



Full wwPDB NMR Structure Validation Report ⓘ

Mar 17, 2026 – 01:35 PM UTC

PDB ID : 6W4F / pdb_00006w4f
BMRB ID : 30735
Title : NMR-driven structure of KRAS4B-GDP homodimer on a lipid bilayer nanodisc
Authors : Lee, K.; Fang, Z.; Enomoto, M.; Gasmi-Seabrook, G.M.; Zheng, L.; Marshall, C.B.; Ikura, M.
Deposited on : 2020-03-10

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.48.1

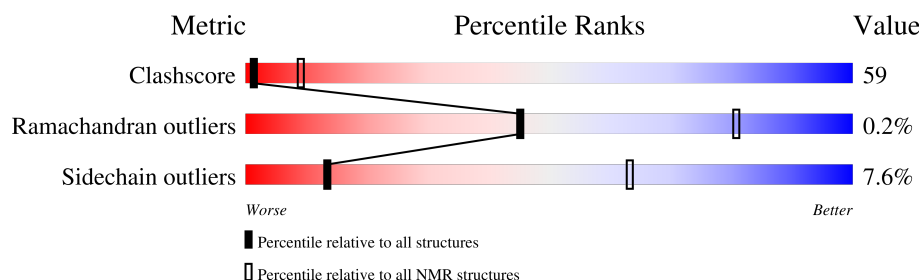
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 2%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	200	80% 12% 6% .
1	D	200	84% 14% .
2	B	184	80% 8% 10% .
2	C	184	82% 8% 8% .

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:214-A:398, D:399-D:595 (382)	0.35	7
2	B:2-B:61, B:65-B:166, C:2-C:61, C:65-C:170 (328)	1.05	15

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 1 single-model cluster was found.

Cluster number	Models
1	3, 5, 6, 11, 13, 14, 17
2	7, 16, 18, 20
3	1, 2, 9, 10
4	4, 12, 15, 19
Single-model clusters	8

3 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12018 atoms, of which 1522 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Apolipoprotein A-I.

Mol	Chain	Residues	Atoms						Trace
1	A	198	Total	C	H	N	O	S	0
			2004	1019	381	287	314	3	
1	D	198	Total	C	H	N	O	S	0
			2002	1019	379	287	314	3	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	GLY	-	expression tag	UNP P02647
A	200	PRO	-	expression tag	UNP P02647
D	397	GLY	-	expression tag	UNP P02647
D	398	PRO	-	expression tag	UNP P02647

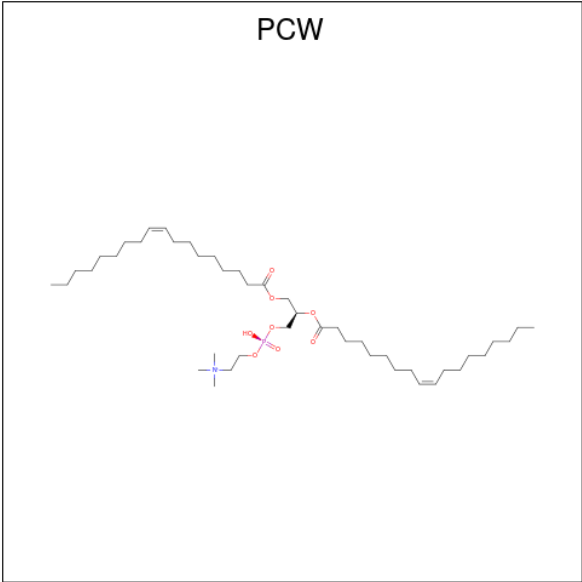
- Molecule 2 is a protein called GTPase KRas.

Mol	Chain	Residues	Atoms						Trace
2	B	180	Total	C	H	N	O	S	0
			1788	898	352	252	279	7	
2	C	180	Total	C	H	N	O	S	0
			1788	898	352	252	279	7	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	12	ASP	GLY	conflict	UNP P01116
C	12	ASP	GLY	conflict	UNP P01116

- Molecule 3 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C₄₄H₈₅NO₈P).



Mol	Chain	Residues	Atoms				
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1

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Mol	Chain	Residues	Atoms				
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1

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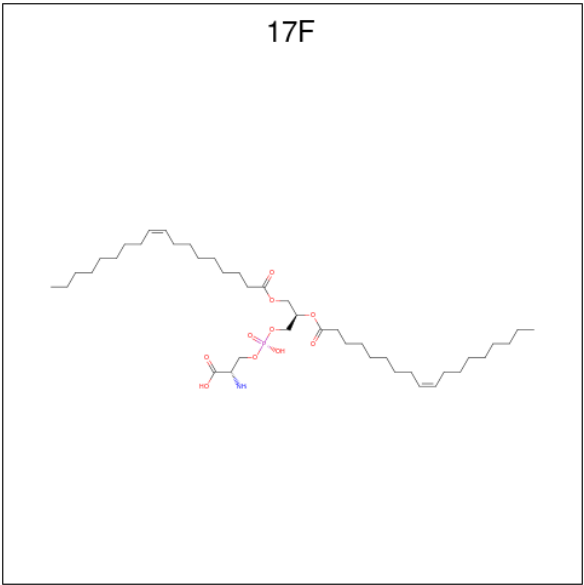
Mol	Chain	Residues	Atoms				
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	D	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1

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Mol	Chain	Residues	Atoms				
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1

- Molecule 4 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propyl}oxy)(hydroxy)phosphoryl]-L-serine (CCD ID: 17F) (formula: C₄₂H₇₈NO₁₀P).



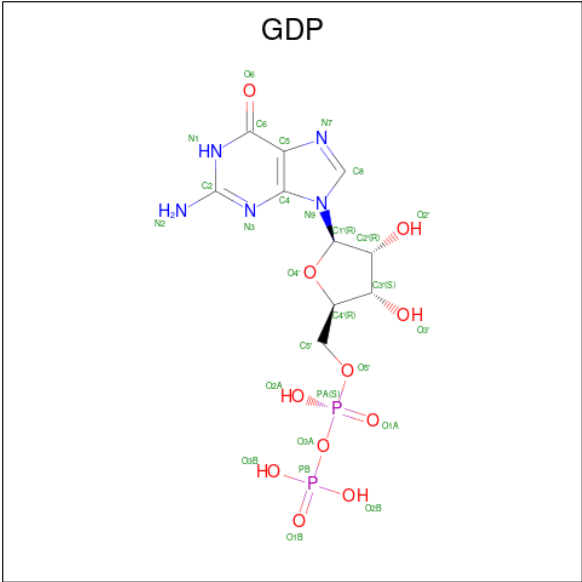
Mol	Chain	Residues	Atoms					
4	A	1	Total	C	H	N	O	P
			57	42	3	1	10	1
4	A	1	Total	C	H	N	O	P
			57	42	3	1	10	1
4	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1

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Mol	Chain	Residues	Atoms					
4	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
4	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
4	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
4	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
4	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
4	D	1	Total	C	H	N	O	P
			57	42	3	1	10	1
4	B	1	Total	C	H	N	O	P
			57	42	3	1	10	1
4	B	1	Total	C	H	N	O	P
			57	42	3	1	10	1
4	B	1	Total	C	H	N	O	P
			57	42	3	1	10	1
4	B	1	Total	C	H	N	O	P
			57	42	3	1	10	1
4	C	1	Total	C	H	N	O	P
			57	42	3	1	10	1
4	C	1	Total	C	H	N	O	P
			57	42	3	1	10	1

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					
5	B	1	Total	C	H	N	O	P
			33	10	5	5	11	2
5	C	1	Total	C	H	N	O	P
			33	10	5	5	11	2

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

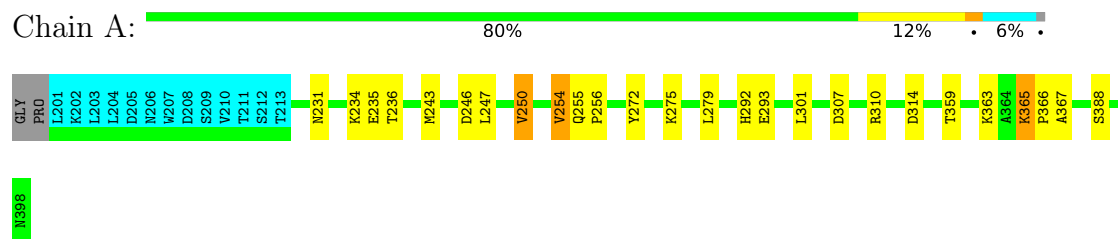
Mol	Chain	Residues	Atoms	
6	B	1	Total	Mg
			1	1
6	C	1	Total	Mg
			1	1

4 Residue-property plots

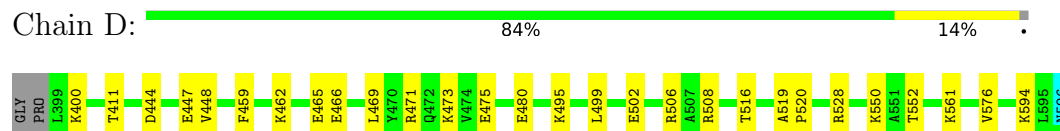
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

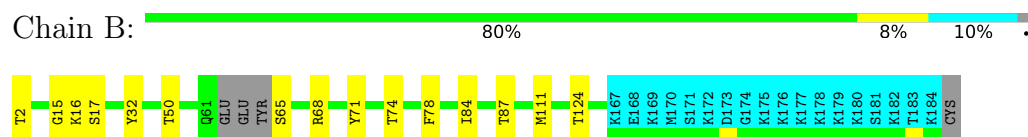
- Molecule 1: Apolipoprotein A-I



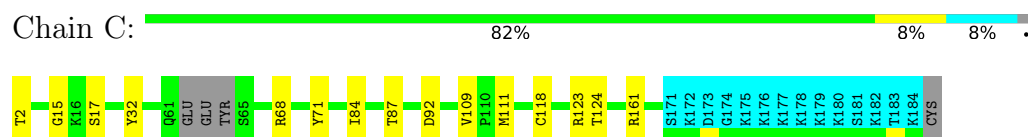
- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas



- Molecule 2: GTPase KRas

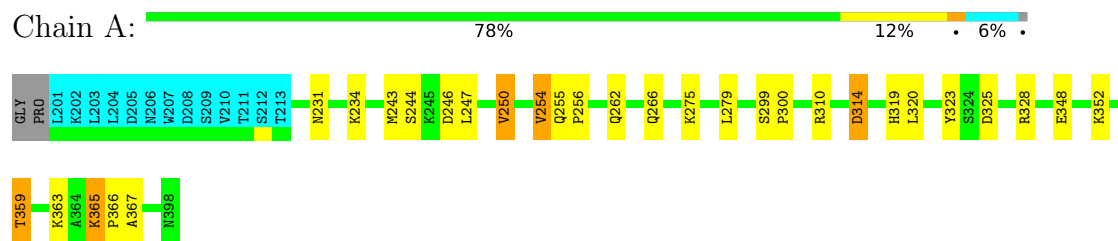


4.2 Scores per residue for each member of the ensemble

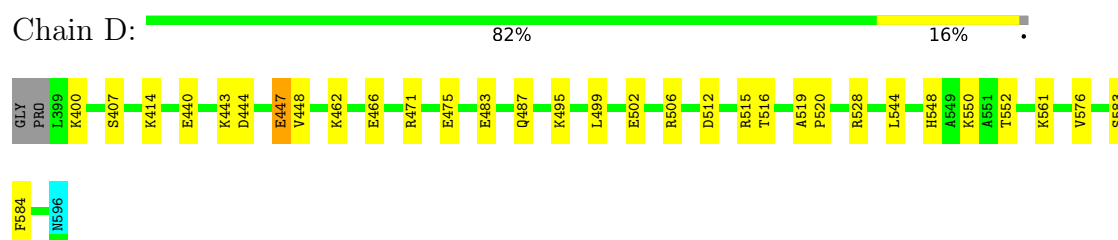
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

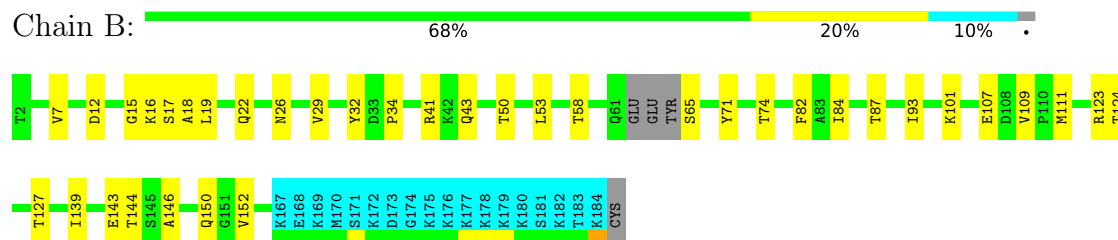
• Molecule 1: Apolipoprotein A-I



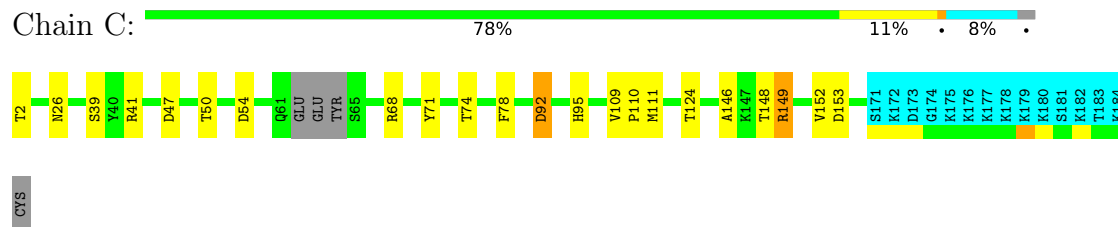
• Molecule 1: Apolipoprotein A-I



• Molecule 2: GTPase KRas

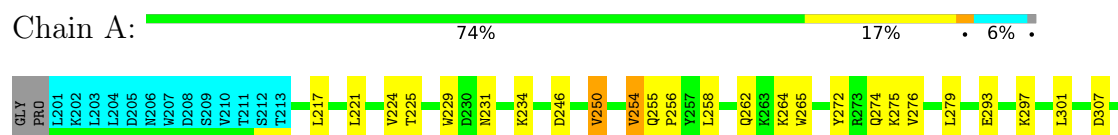


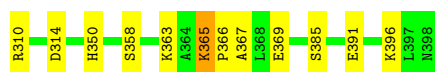
• Molecule 2: GTPase KRas



4.2.2 Score per residue for model 2

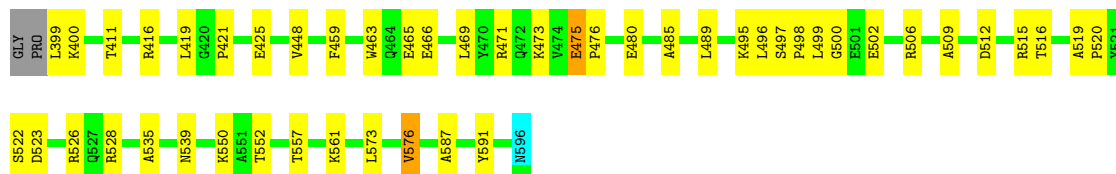
• Molecule 1: Apolipoprotein A-I





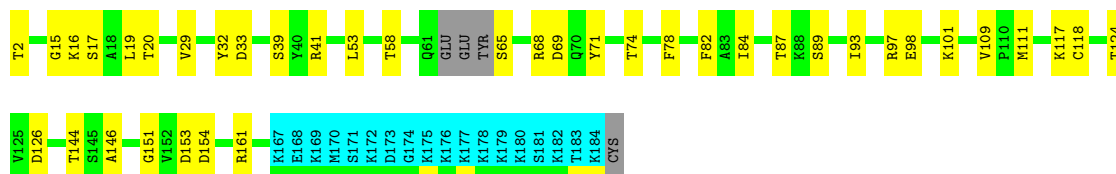
• Molecule 1: Apolipoprotein A-I

Chain D: 74% 23% ..



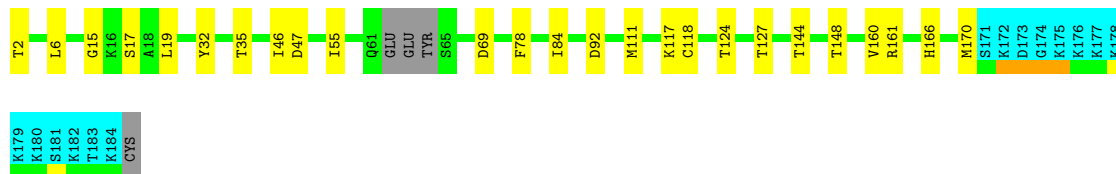
• Molecule 2: GTPase KRas

Chain B: 67% 21% 10% .



• Molecule 2: GTPase KRas

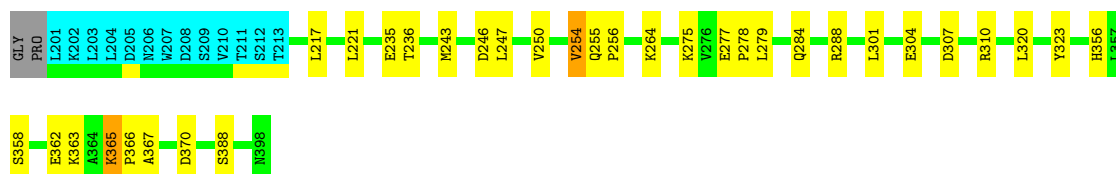
Chain C: 77% 14% 8% .



4.2.3 Score per residue for model 3

• Molecule 1: Apolipoprotein A-I

Chain A: 76% 16% 6% .



• Molecule 1: Apolipoprotein A-I

Chain D: 77% 20% ..





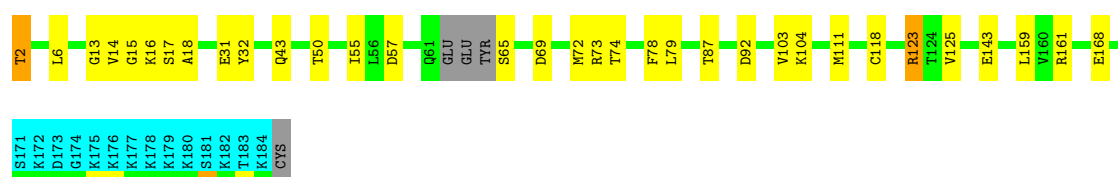
- Molecule 2: GTPase KRas

Chain B: 72% 15% 10%



- Molecule 2: GTPase KRas

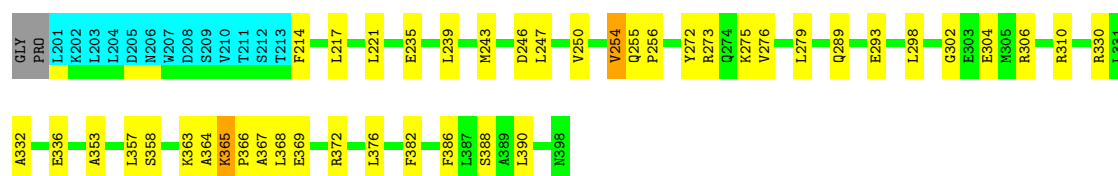
Chain C: 72% 17% 8%



4.2.4 Score per residue for model 4

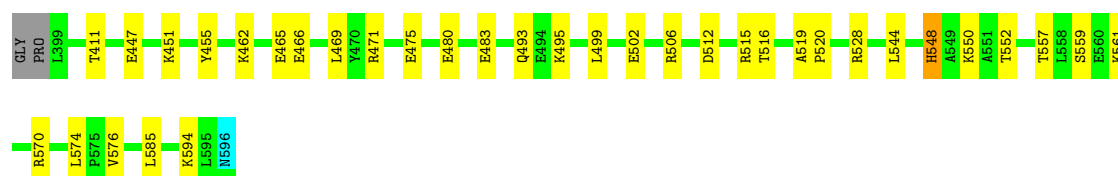
- Molecule 1: Apolipoprotein A-I

Chain A: 71% 20% 6%

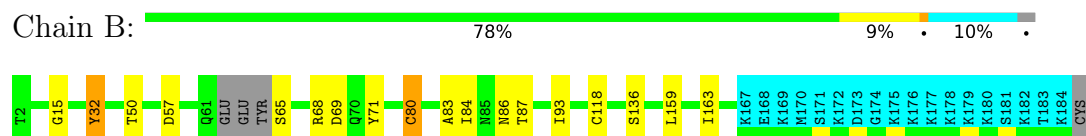


- Molecule 1: Apolipoprotein A-I

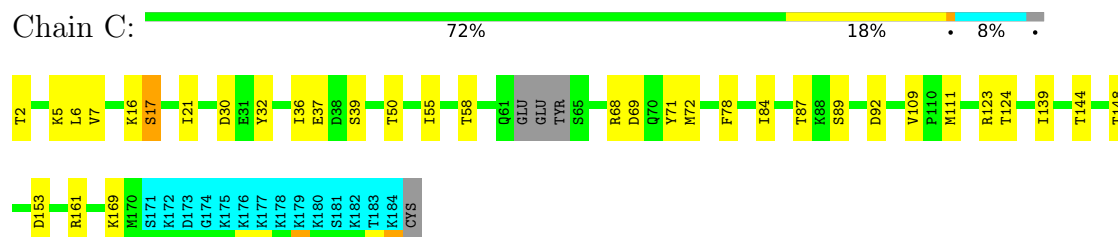
Chain D: 81% 17%



- Molecule 2: GTPase KRas

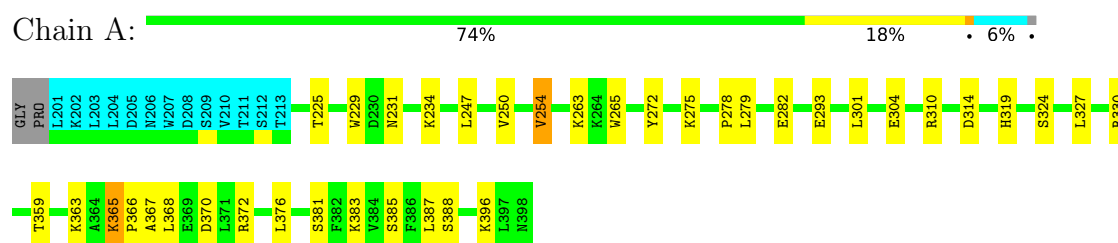


- Molecule 2: GTPase KRas

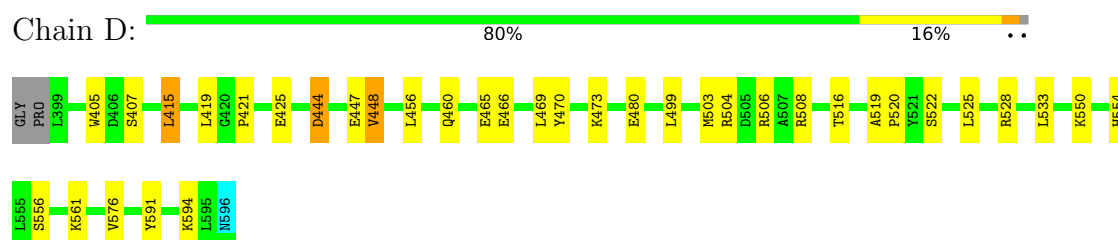


4.2.5 Score per residue for model 5

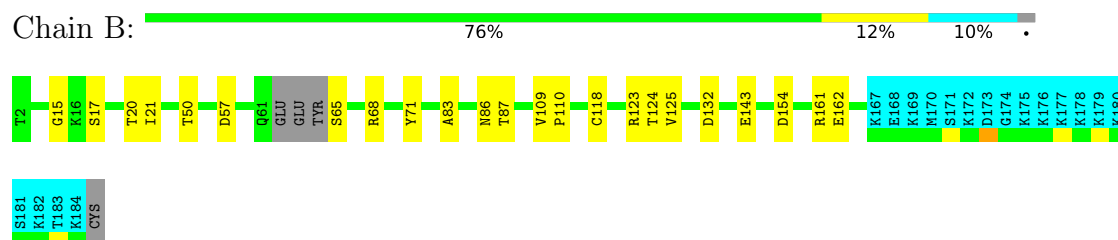
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I

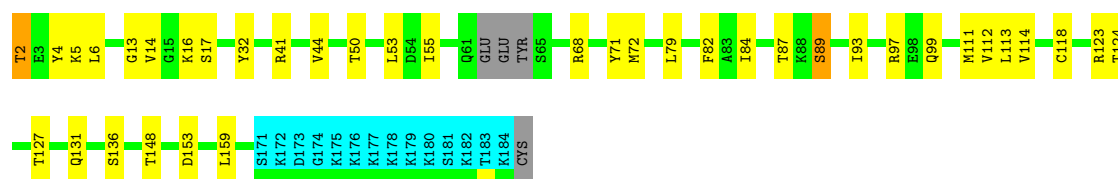


- Molecule 2: GTPase KRas



- Molecule 2: GTPase KRas

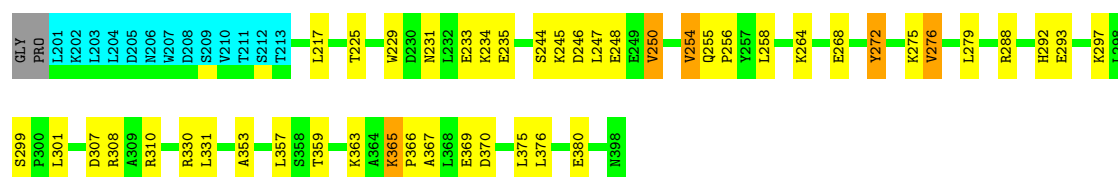




4.2.6 Score per residue for model 6

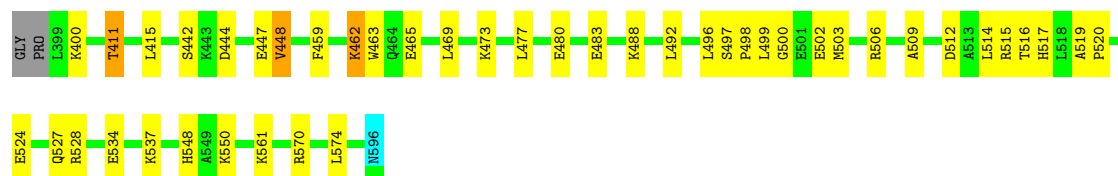
- Molecule 1: Apolipoprotein A-I

Chain A: 70% 20% 6%



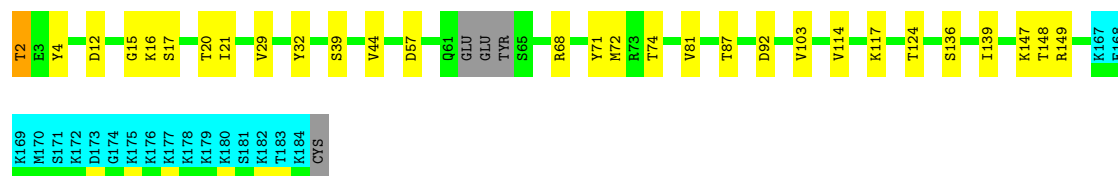
- Molecule 1: Apolipoprotein A-I

Chain D: 76% 20%



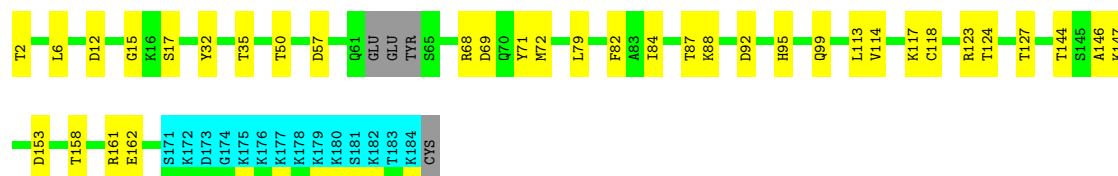
- Molecule 2: GTPase KRas

Chain B: 72% 15% 10%



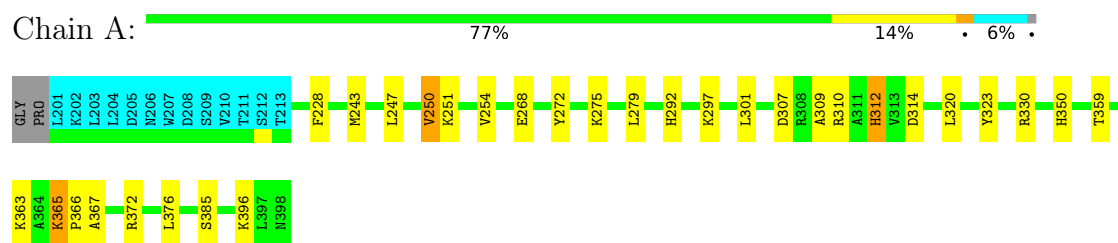
- Molecule 2: GTPase KRas

Chain C: 71% 19% 8%

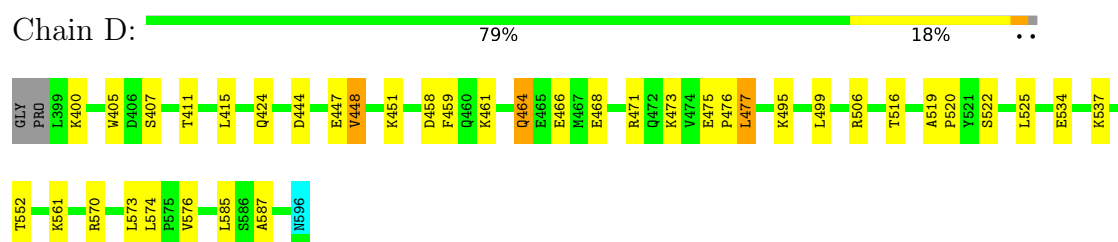


4.2.7 Score per residue for model 7 (medoid)

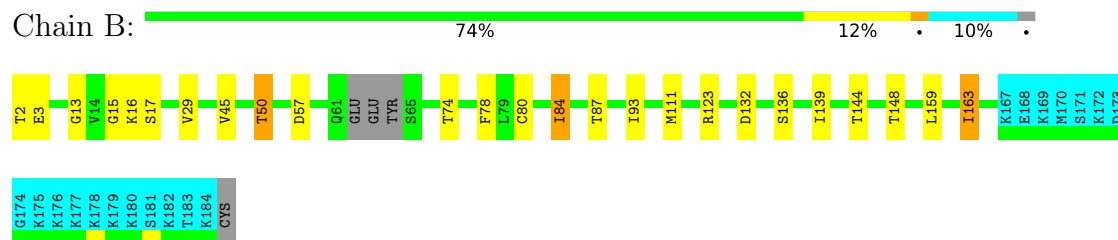
• Molecule 1: Apolipoprotein A-I



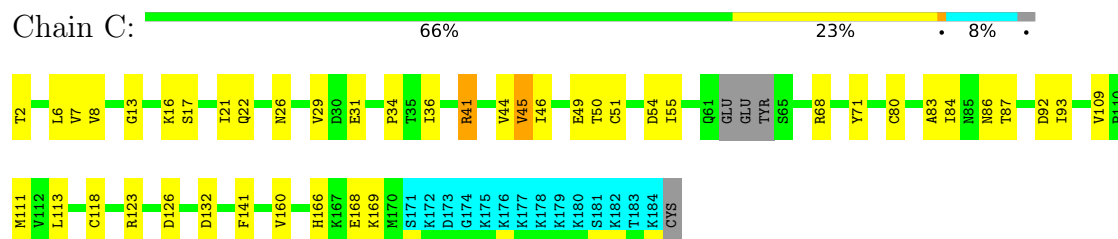
• Molecule 1: Apolipoprotein A-I



• Molecule 2: GTPase KRas

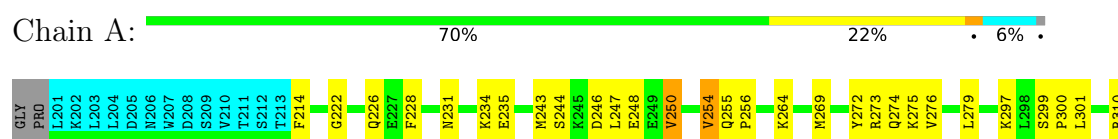


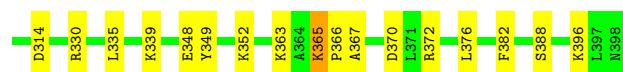
• Molecule 2: GTPase KRas



4.2.8 Score per residue for model 8

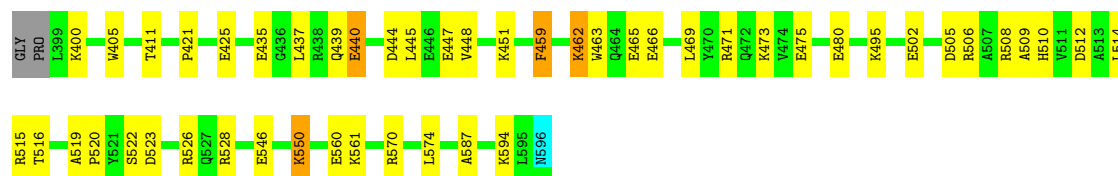
• Molecule 1: Apolipoprotein A-I





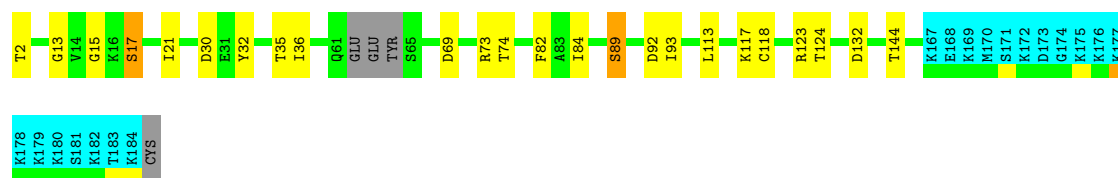
• Molecule 1: Apolipoprotein A-I

Chain D: 74% 22% ..



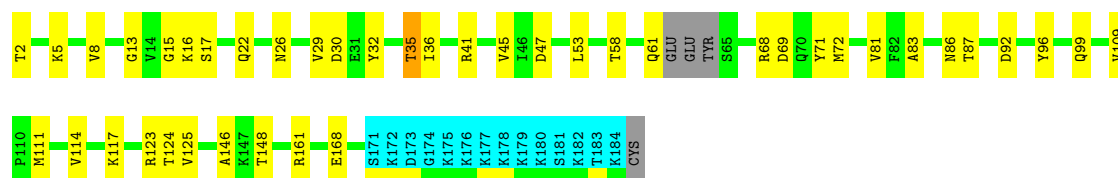
• Molecule 2: GTPase KRas

Chain B: 75% 12% 10% .



• Molecule 2: GTPase KRas

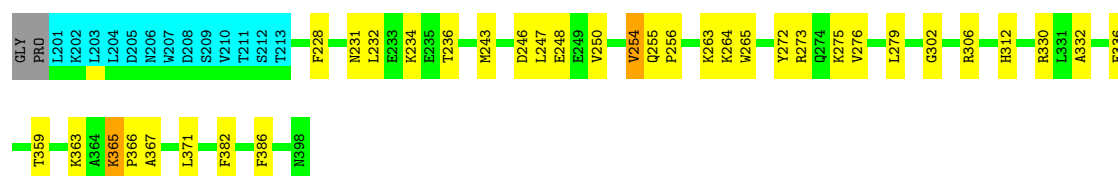
Chain C: 67% 22% 8% .



4.2.9 Score per residue for model 9

• Molecule 1: Apolipoprotein A-I

Chain A: 75% 16% 6% .



• Molecule 1: Apolipoprotein A-I

Chain D: 84% 13% ..



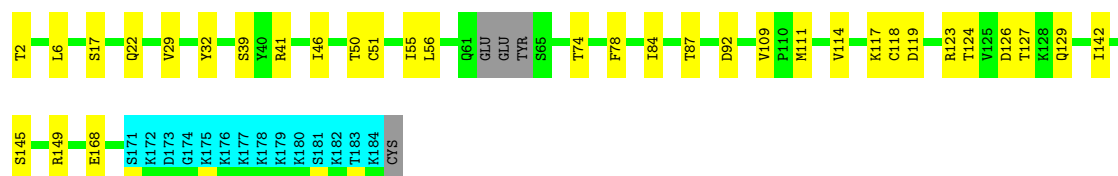
• Molecule 2: GTPase KRas

Chain B: 74% 12% 10%



• Molecule 2: GTPase KRas

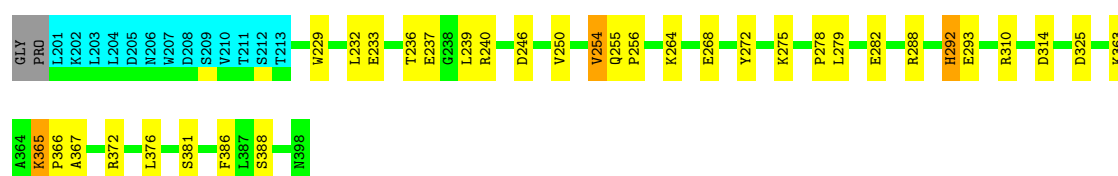
Chain C: 72% 18% 8%



4.2.10 Score per residue for model 10

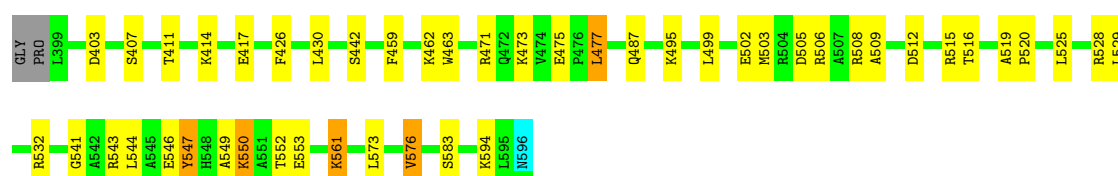
• Molecule 1: Apolipoprotein A-I

Chain A: 76% 16% 6%



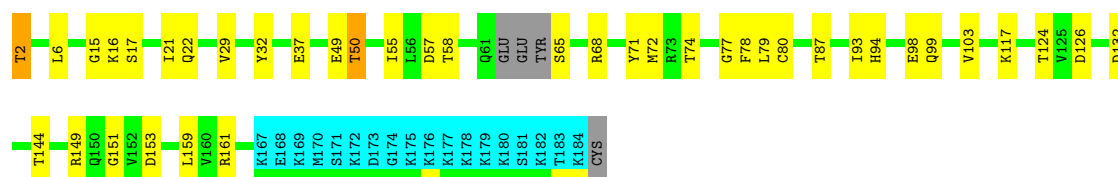
• Molecule 1: Apolipoprotein A-I

Chain D: 75% 21% 2%



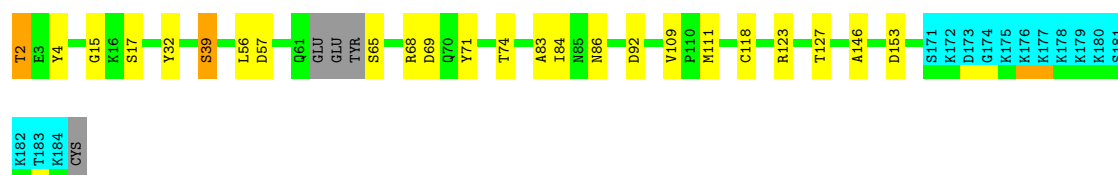
• Molecule 2: GTPase KRas

Chain B: 66% 21% 10%



- Molecule 2: GTPase KRas

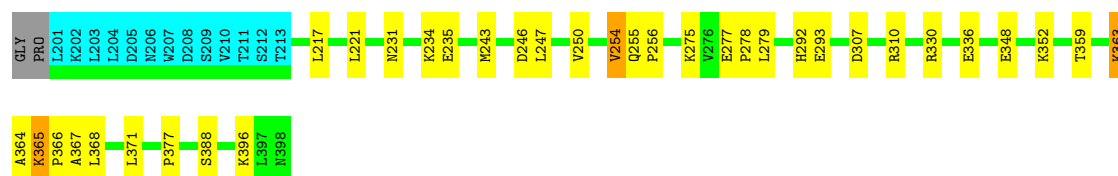
Chain C: 77% 12% 8%



4.2.11 Score per residue for model 11

- Molecule 1: Apolipoprotein A-I

Chain A: 75% 16% 6%



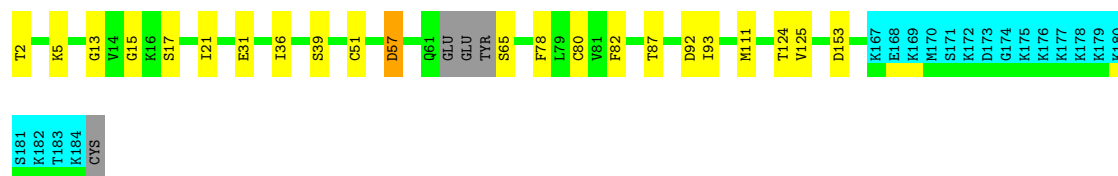
- Molecule 1: Apolipoprotein A-I

Chain D: 77% 20% ..

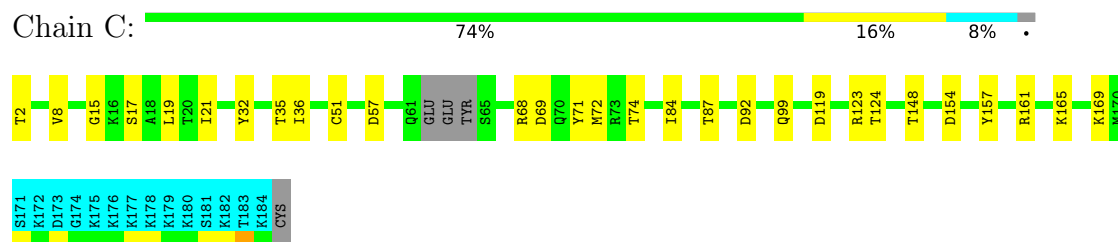


- Molecule 2: GTPase KRas

Chain B: 76% 11% 10%

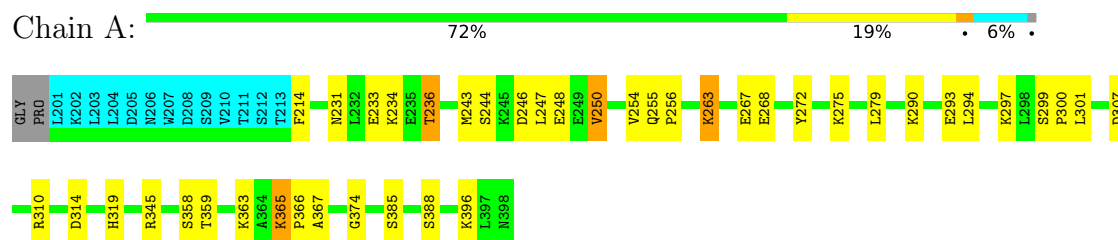


- Molecule 2: GTPase KRas

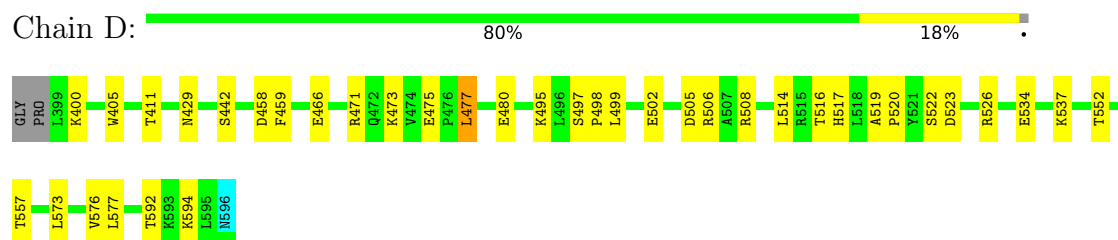


4.2.12 Score per residue for model 12

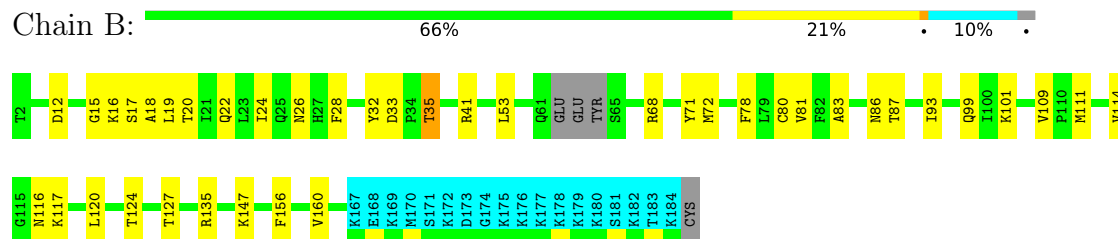
- Molecule 1: Apolipoprotein A-I



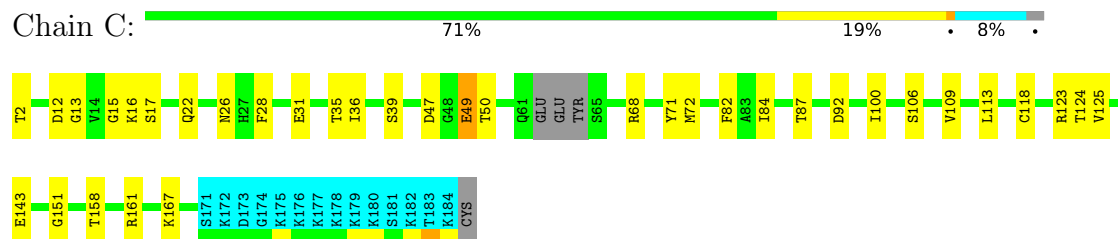
- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas

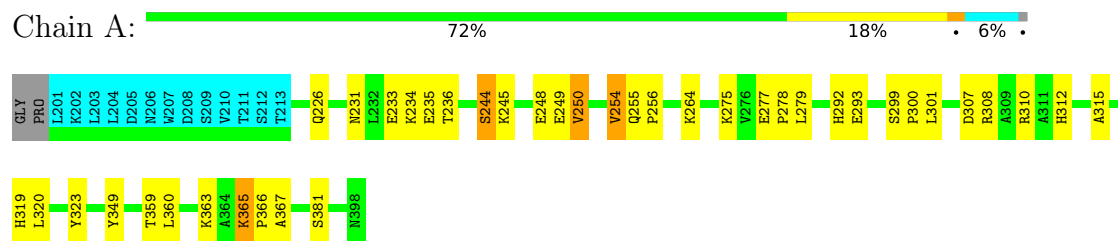


- Molecule 2: GTPase KRas

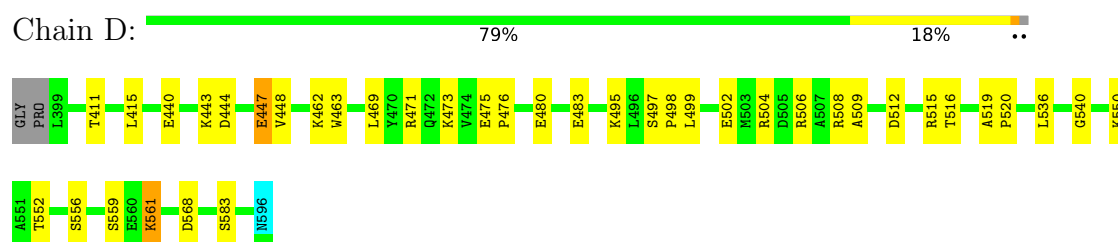


4.2.13 Score per residue for model 13

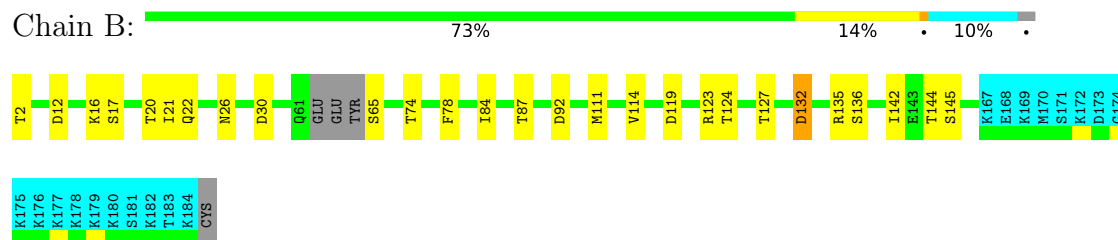
• Molecule 1: Apolipoprotein A-I



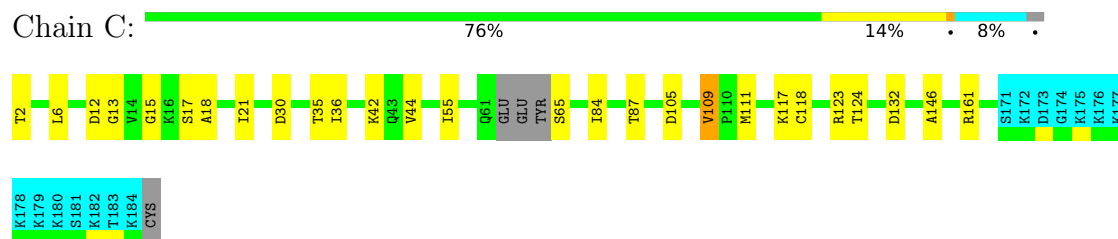
• Molecule 1: Apolipoprotein A-I



• Molecule 2: GTPase KRas

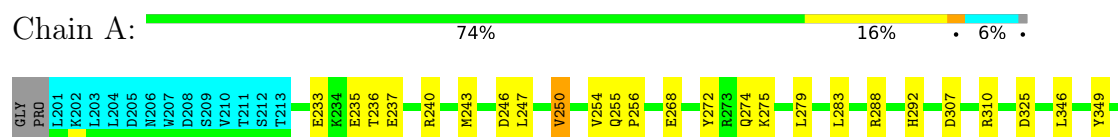


• Molecule 2: GTPase KRas



4.2.14 Score per residue for model 14

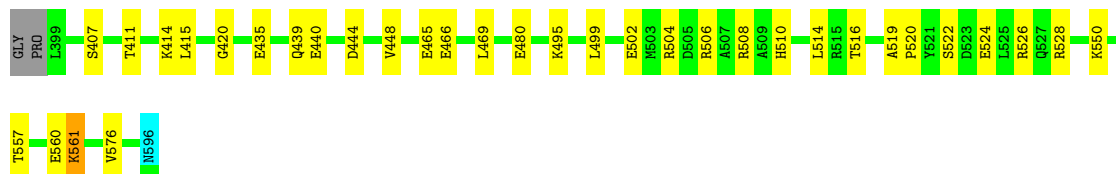
• Molecule 1: Apolipoprotein A-I





• Molecule 1: Apolipoprotein A-I

Chain D: 82% 16% .



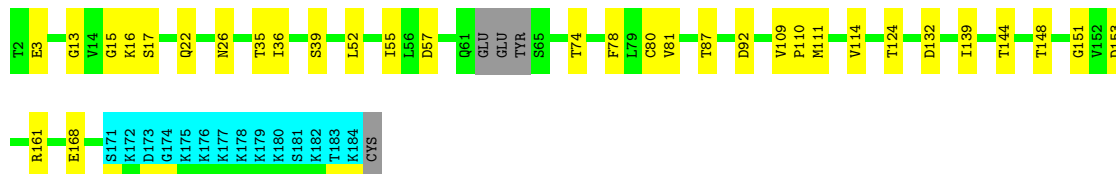
• Molecule 2: GTPase KRas

Chain B: 79% 9% 10% .



• Molecule 2: GTPase KRas

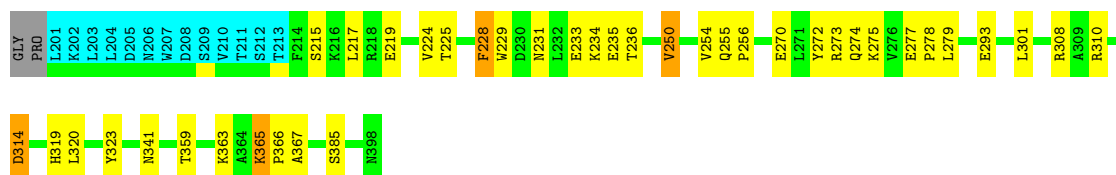
Chain C: 73% 17% 8% .



4.2.15 Score per residue for model 15

• Molecule 1: Apolipoprotein A-I

Chain A: 73% 18% 6% .



• Molecule 1: Apolipoprotein A-I

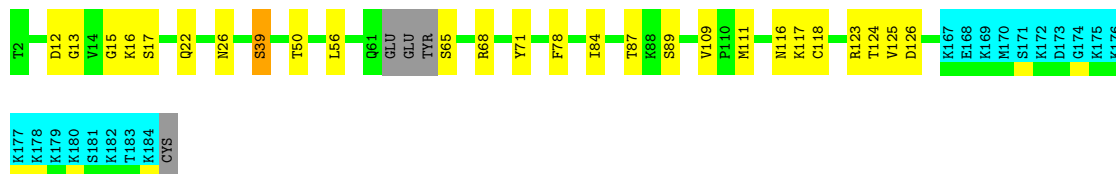
Chain D: 81% 17% .





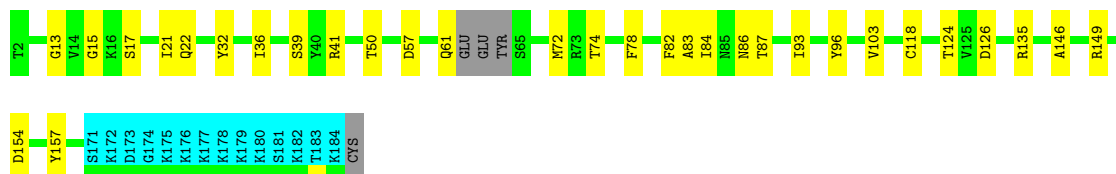
• Molecule 2: GTPase KRas

Chain B: 74% 14% 10%



• Molecule 2: GTPase KRas

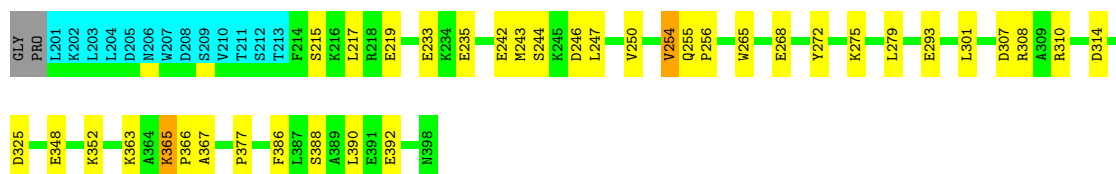
Chain C: 73% 17% 8%



4.2.16 Score per residue for model 16

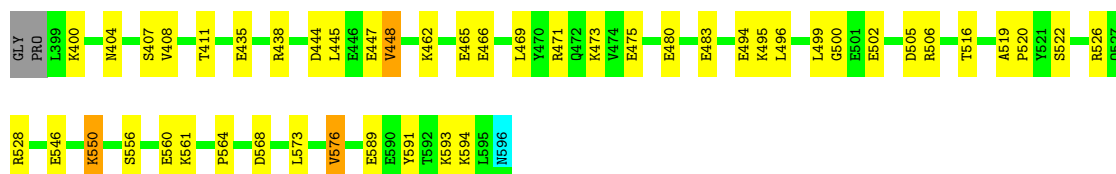
• Molecule 1: Apolipoprotein A-I

Chain A: 74% 18% 6%



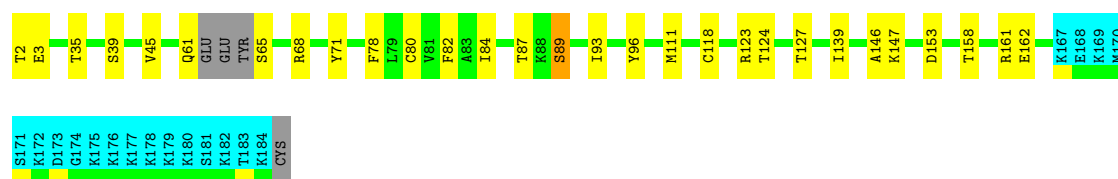
• Molecule 1: Apolipoprotein A-I

Chain D: 75% 22% 3%



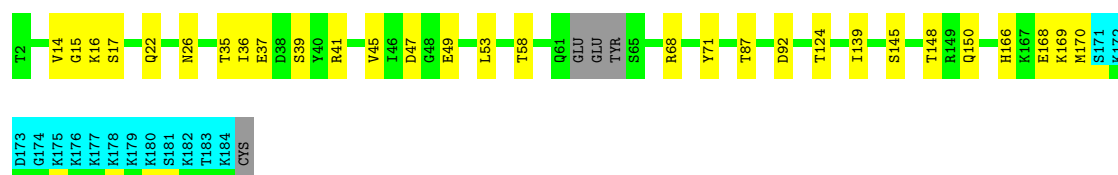
• Molecule 2: GTPase KRas

Chain B: 72% 15% 10%



- Molecule 2: GTPase KRas

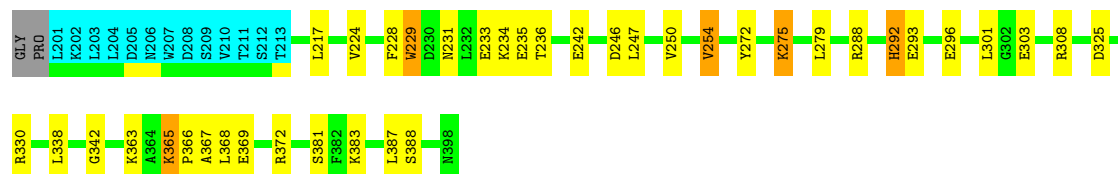
Chain C: 74% 16% 8% .



4.2.17 Score per residue for model 17

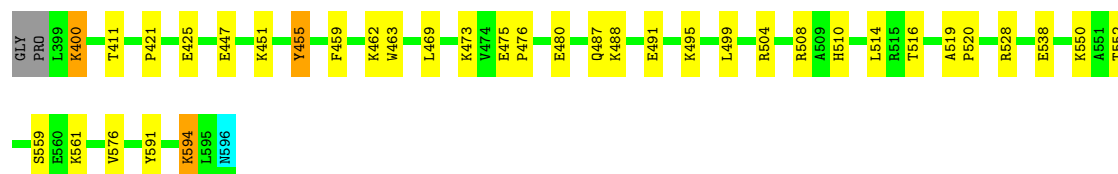
- Molecule 1: Apolipoprotein A-I

Chain A: 73% 17% 6% .



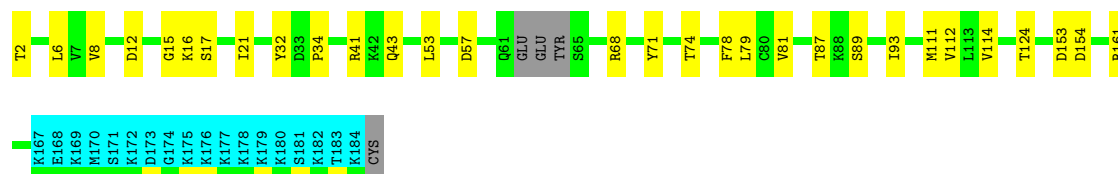
- Molecule 1: Apolipoprotein A-I

Chain D: 80% 16% ..

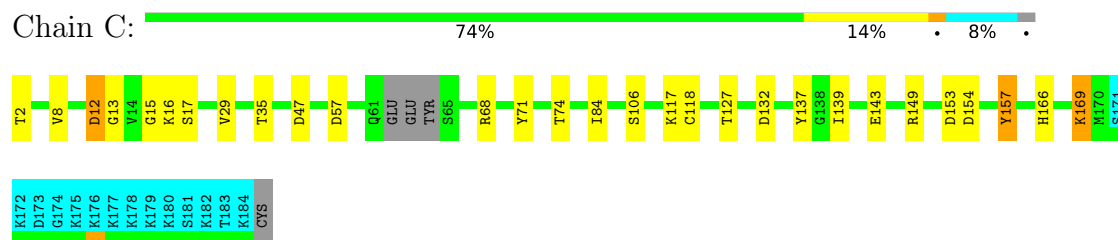


- Molecule 2: GTPase KRas

Chain B: 72% 16% 10% .

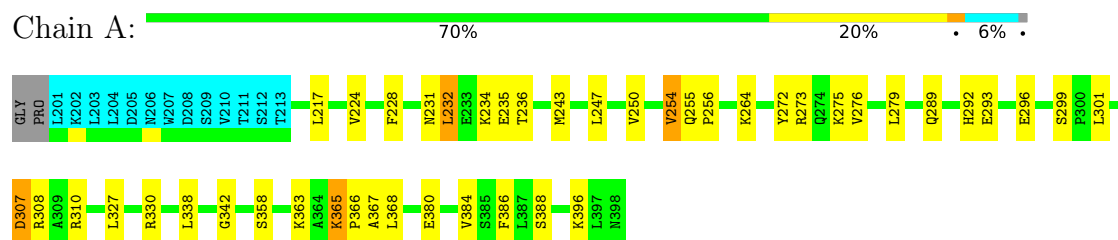


- Molecule 2: GTPase KRas

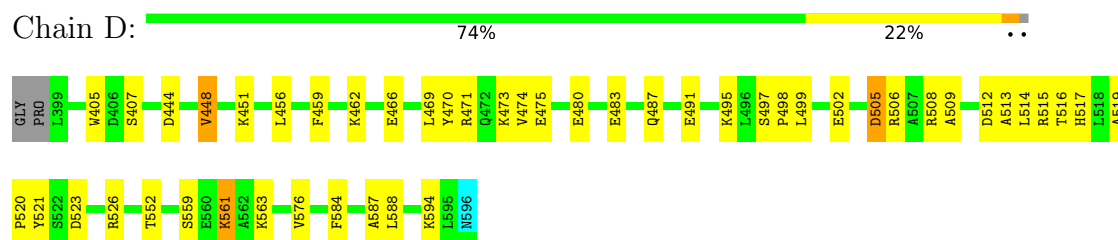


4.2.18 Score per residue for model 18

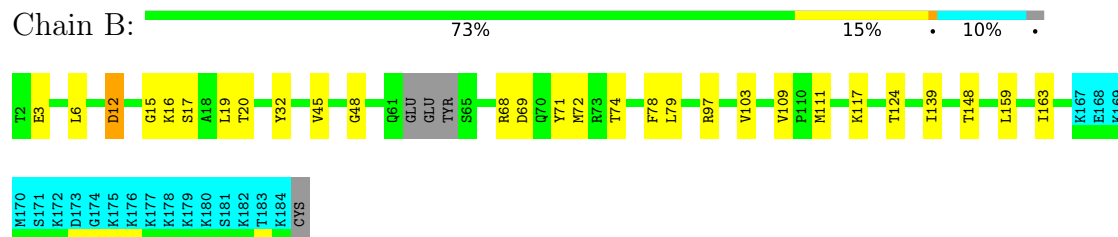
- Molecule 1: Apolipoprotein A-I



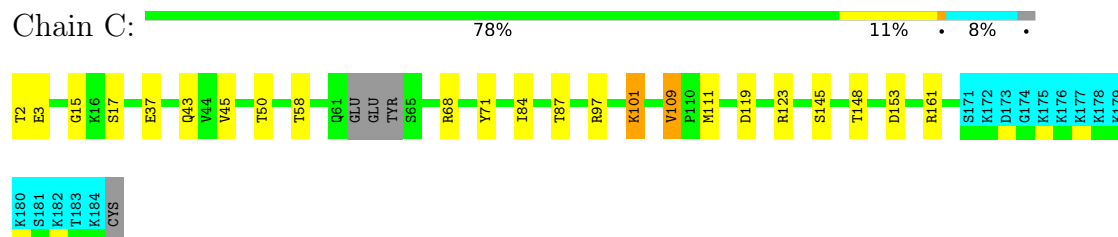
- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas

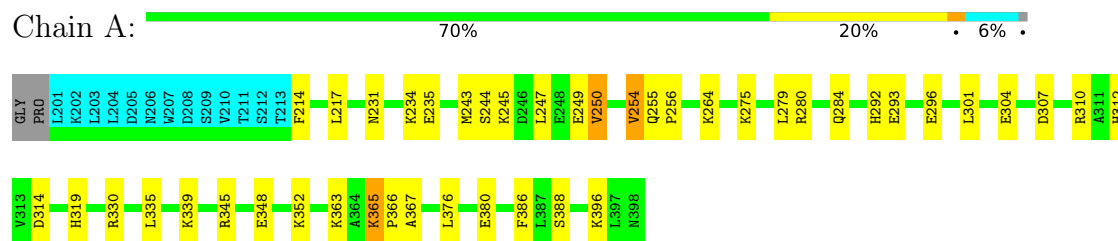


- Molecule 2: GTPase KRas

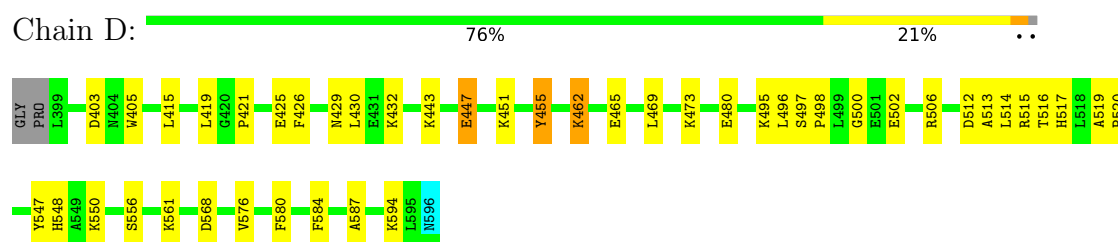


4.2.19 Score per residue for model 19

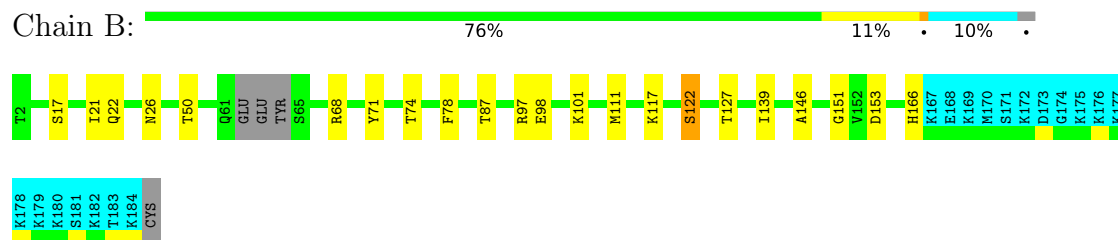
• Molecule 1: Apolipoprotein A-I



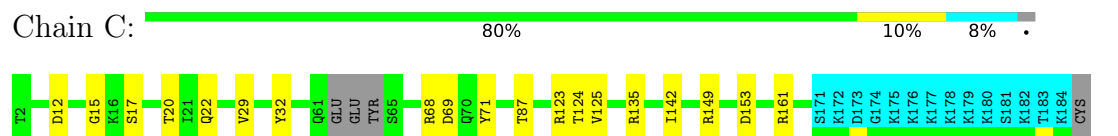
• Molecule 1: Apolipoprotein A-I



• Molecule 2: GTPase KRas

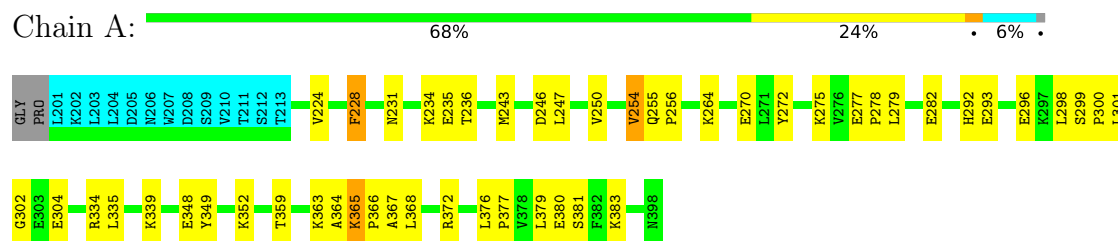


• Molecule 2: GTPase KRas

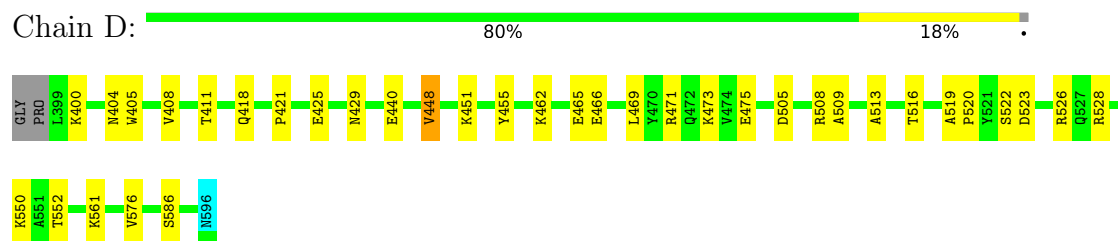


4.2.20 Score per residue for model 20

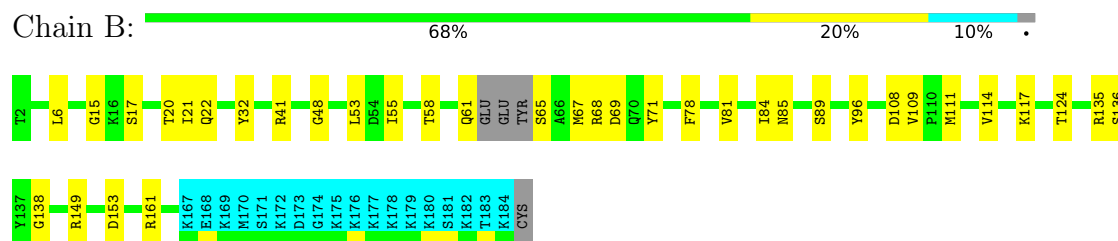
• Molecule 1: Apolipoprotein A-I



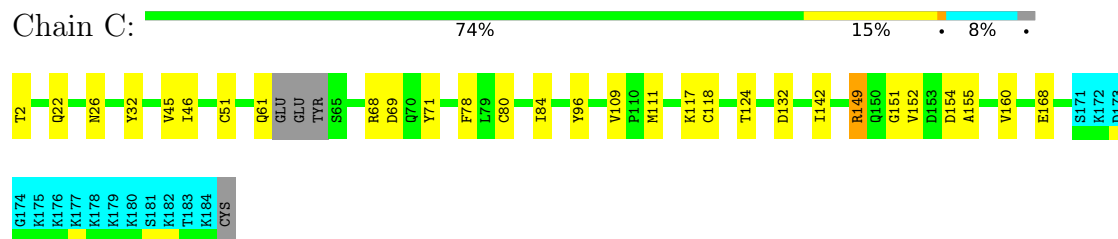
- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas



- Molecule 2: GTPase KRas



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
HADDOCK	refinement	
HADDOCK	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	190
Number of shifts mapped to atoms	70
Number of unparsed shifts	0
Number of shifts with mapping errors	120
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	2%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PCW, GDP, 17F, MG

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1519	358	1524	23±4
1	D	1615	376	1620	20±4
2	B	1289	298	1268	13±4
2	C	1324	308	1309	15±5
3	A	972	0	1440	360±22
3	B	594	0	880	276±18
3	C	432	0	640	202±22
3	D	1458	0	2160	555±25
4	A	108	6	152	33±8
4	B	216	12	304	85±11
4	C	108	6	152	49±8
4	D	432	24	608	164±12
5	B	28	5	12	7±2
5	C	28	5	12	6±3
6	B	1	0	0	1±0
6	C	1	0	0	1±0
All	All	202500	27960	241622	26265

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 59.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:411:PCW:C19	3:A:411:PCW:H142	1.18	1.69	6	20
3:B:209:PCW:C27	3:B:209:PCW:H222	1.17	1.70	7	3
3:A:401:PCW:H62	3:B:209:PCW:H131	1.16	1.17	19	1
3:B:209:PCW:H272	3:B:209:PCW:C22	1.15	1.72	4	3
3:D:614:PCW:H461	3:D:614:PCW:H421	1.14	1.18	7	20
3:C:208:PCW:H261	3:C:208:PCW:H221	1.14	1.16	11	20
3:A:405:PCW:H461	3:A:405:PCW:H421	1.14	1.17	8	15
3:D:612:PCW:H172	3:D:612:PCW:H212	1.14	1.15	6	18
3:A:411:PCW:H19	3:A:411:PCW:C14	1.14	1.73	17	3
3:B:204:PCW:H251	3:B:204:PCW:H211	1.13	1.20	8	19
3:B:212:PCW:H472	3:B:212:PCW:H432	1.13	1.18	7	20
3:D:617:PCW:H272	3:D:617:PCW:H232	1.13	1.21	20	20
3:D:621:PCW:H141	4:D:634:17F:H6	1.13	1.14	16	17
3:A:403:PCW:H231	3:A:403:PCW:C28	1.13	1.74	10	1
3:B:206:PCW:H461	3:B:206:PCW:H421	1.12	1.21	4	16
4:C:210:17F:H57	4:C:210:17F:H19A	1.12	1.22	1	20
3:B:210:PCW:H472	3:B:210:PCW:H432	1.12	1.19	16	19
3:B:207:PCW:H141	3:B:210:PCW:H321	1.12	1.17	13	5
3:A:413:PCW:H472	3:A:413:PCW:H432	1.12	1.20	14	20
3:A:403:PCW:H282	3:A:403:PCW:C23	1.12	1.74	10	1
3:B:211:PCW:H73	3:B:211:PCW:O1P	1.12	1.42	15	1
3:D:602:PCW:H222	3:D:610:PCW:H351	1.12	1.19	7	15
3:D:612:PCW:H321	3:D:618:PCW:H132	1.12	1.16	17	16
3:A:401:PCW:H252	3:D:614:PCW:H281	1.12	1.14	9	1
3:A:409:PCW:H82	3:C:206:PCW:H371	1.12	1.22	12	3
3:D:605:PCW:H182	3:D:605:PCW:H142	1.11	1.20	3	20
3:C:208:PCW:H121	3:C:208:PCW:H371	1.11	1.19	6	16
3:B:210:PCW:H262	3:B:210:PCW:H222	1.11	1.18	12	19
3:D:626:PCW:H231	3:D:626:PCW:H271	1.11	1.17	12	17
3:B:205:PCW:H212	3:B:205:PCW:H252	1.11	1.12	9	19
3:A:401:PCW:H482	3:D:611:PCW:H232	1.11	1.17	3	4
3:A:419:PCW:H11	3:D:617:PCW:H411	1.11	1.22	18	17
3:D:607:PCW:H431	4:D:628:17F:H34	1.11	1.13	11	17
3:D:611:PCW:H63	3:D:623:PCW:H321	1.11	1.20	17	15
3:A:405:PCW:H472	3:A:405:PCW:H432	1.11	1.15	3	5
3:A:419:PCW:H372	3:D:617:PCW:H431	1.11	1.23	17	17
3:D:601:PCW:H212	3:D:601:PCW:H172	1.11	1.16	17	9
3:C:207:PCW:H281	3:C:208:PCW:H172	1.11	1.20	6	3
3:D:617:PCW:H2	3:D:617:PCW:H41	1.11	1.20	7	4
3:B:209:PCW:H31	3:B:209:PCW:H41	1.11	1.15	20	16
3:D:611:PCW:H162	3:D:619:PCW:H171	1.11	1.18	15	10
3:B:204:PCW:H322	3:B:212:PCW:H141	1.11	1.17	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:404:PCW:H421	3:B:209:PCW:H19	1.11	1.20	3	1
3:A:413:PCW:H181	3:A:413:PCW:H221	1.11	1.20	9	13
3:D:606:PCW:H31	3:D:626:PCW:H372	1.10	1.19	9	14
4:D:629:17F:H18A	4:D:629:17F:O7	1.10	1.44	16	15
3:A:403:PCW:H132	3:C:203:PCW:H12	1.10	1.13	7	3
4:D:628:17F:H57	4:D:628:17F:H19A	1.10	1.23	18	20
3:D:611:PCW:H222	3:D:619:PCW:H442	1.10	1.21	14	3
3:A:419:PCW:H432	3:D:610:PCW:H211	1.10	1.11	3	13
3:D:621:PCW:H132	4:D:634:17F:H4A	1.10	1.22	8	19
3:D:625:PCW:H412	3:D:626:PCW:H412	1.10	1.17	17	15
3:B:206:PCW:H32	3:B:206:PCW:O1P	1.10	1.47	15	4
3:D:602:PCW:H2	3:D:602:PCW:H41	1.10	1.11	14	19
3:D:605:PCW:H172	3:D:605:PCW:H212	1.10	1.14	8	20
3:D:624:PCW:H20	3:D:624:PCW:H241	1.10	1.23	19	20
4:D:629:17F:H68	4:D:634:17F:H29	1.10	1.22	15	11
3:D:620:PCW:H121	4:D:635:17F:H4A	1.10	1.24	20	6
3:D:616:PCW:H39	3:D:618:PCW:H142	1.10	1.21	2	17
3:B:208:PCW:H421	3:B:208:PCW:H372	1.10	1.19	20	10
3:B:205:PCW:H451	3:C:208:PCW:H20	1.10	1.17	16	4
3:B:205:PCW:H283	3:B:212:PCW:H142	1.09	1.22	1	4
3:D:606:PCW:H12	3:D:626:PCW:H372	1.09	1.12	13	16
3:B:205:PCW:H452	3:B:206:PCW:H232	1.09	1.22	1	7
3:B:213:PCW:H20	3:B:213:PCW:H241	1.09	1.22	10	17
3:B:210:PCW:H32	3:B:210:PCW:O4P	1.09	1.47	6	18
3:A:403:PCW:H41	3:A:403:PCW:H31	1.09	1.18	11	12
3:D:622:PCW:H242	3:D:624:PCW:H242	1.09	1.10	18	17
3:A:409:PCW:H51	3:C:206:PCW:H321	1.09	1.10	20	5
3:B:207:PCW:H421	3:B:213:PCW:H252	1.09	1.13	8	5
3:D:611:PCW:H222	3:D:619:PCW:H461	1.09	1.20	9	2
3:D:611:PCW:H321	3:D:623:PCW:H352	1.09	1.25	15	18
3:B:205:PCW:H451	3:C:208:PCW:H19	1.09	1.25	10	7
3:D:617:PCW:H471	3:D:617:PCW:H431	1.09	1.19	11	3
3:B:203:PCW:H332	4:B:215:17F:H35	1.09	1.09	9	4
3:C:203:PCW:H222	3:C:203:PCW:H261	1.09	1.19	11	1
3:B:213:PCW:H421	4:B:217:17F:H12	1.08	1.19	14	6
3:A:408:PCW:H361	3:C:204:PCW:H211	1.08	1.24	10	1
3:A:407:PCW:H251	3:A:407:PCW:H211	1.08	1.21	4	3
4:A:414:17F:H46	3:B:212:PCW:H19	1.08	1.15	4	2
3:A:403:PCW:H31	3:A:403:PCW:O4P	1.08	1.47	18	5
3:A:403:PCW:H141	3:C:203:PCW:H322	1.08	1.21	18	4
4:B:215:17F:H12	4:B:215:17F:H41	1.08	1.17	12	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:621:PCW:H151	4:D:634:17F:H4A	1.08	1.16	2	4
3:A:404:PCW:H231	3:A:404:PCW:H272	1.08	1.20	15	3
3:A:407:PCW:H241	3:A:407:PCW:H282	1.08	1.19	15	3
3:A:413:PCW:H341	4:A:414:17F:H57	1.08	1.19	10	8
3:A:420:PCW:H442	3:D:617:PCW:H211	1.08	1.24	11	4
3:D:627:PCW:H2	3:D:627:PCW:H42	1.08	1.21	19	15
3:A:416:PCW:H451	3:D:617:PCW:H242	1.08	1.25	12	15
3:D:606:PCW:H431	3:D:626:PCW:H472	1.08	1.22	9	8
3:C:209:PCW:H341	3:C:209:PCW:H132	1.08	1.24	15	14
3:C:207:PCW:H51	4:C:211:17F:H1A	1.08	1.16	12	6
3:D:622:PCW:H352	3:D:627:PCW:H20	1.07	1.08	7	9
4:B:214:17F:H1A	3:C:205:PCW:H61	1.07	1.20	6	8
3:A:401:PCW:H362	3:B:209:PCW:H39	1.07	1.08	6	1
3:B:208:PCW:H283	3:B:208:PCW:H231	1.07	1.22	19	1
3:D:621:PCW:H421	4:D:634:17F:H62	1.07	1.09	12	19
4:D:630:17F:H67	4:D:634:17F:H39	1.07	1.26	13	16
3:A:413:PCW:H341	4:A:414:17F:H59	1.07	1.11	12	1
3:A:401:PCW:H181	3:A:401:PCW:H221	1.07	1.21	10	9
3:A:407:PCW:H151	3:C:205:PCW:H151	1.07	1.16	1	10
3:A:419:PCW:H451	3:D:610:PCW:H211	1.07	1.25	18	9
3:A:413:PCW:H371	3:A:413:PCW:H31	1.07	1.09	1	9
3:B:210:PCW:H431	3:B:210:PCW:H472	1.07	1.22	1	1
3:C:204:PCW:H471	4:C:211:17F:H57	1.07	1.26	1	8
3:D:618:PCW:H422	3:D:627:PCW:H231	1.07	1.26	5	11
3:B:208:PCW:H211	4:B:214:17F:H60	1.07	1.25	10	2
3:C:203:PCW:H161	3:C:203:PCW:H421	1.07	1.24	9	3
3:D:609:PCW:H63	4:D:633:17F:H6A	1.07	1.24	2	12
3:A:406:PCW:H341	3:A:411:PCW:C32	1.07	1.79	10	7
3:A:410:PCW:H12	3:C:207:PCW:H381	1.07	1.26	2	3
3:C:205:PCW:H271	3:C:205:PCW:H232	1.07	1.20	7	1
4:A:414:17F:H45	3:C:203:PCW:H411	1.07	1.07	11	1
3:C:203:PCW:H51	3:C:203:PCW:H352	1.07	1.09	11	1
3:C:203:PCW:H262	3:C:203:PCW:H222	1.07	1.22	12	1
3:B:204:PCW:H151	3:B:206:PCW:H321	1.07	1.25	14	1
3:B:208:PCW:H283	3:B:208:PCW:C23	1.07	1.78	19	1
3:A:417:PCW:H351	3:D:612:PCW:H152	1.06	1.27	5	11
3:D:603:PCW:H2	3:D:605:PCW:H82	1.06	1.09	18	13
3:D:603:PCW:H251	4:B:217:17F:H76	1.06	1.21	2	9
3:A:401:PCW:H62	3:B:209:PCW:H2	1.06	1.19	8	2
3:D:609:PCW:H42	4:D:633:17F:O8	1.06	1.48	13	17
3:D:612:PCW:H212	3:D:612:PCW:C17	1.06	1.78	15	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:627:PCW:H2	3:D:627:PCW:C4	1.06	1.80	3	14
3:D:607:PCW:H41	3:D:626:PCW:H222	1.06	1.21	19	17
3:C:203:PCW:H351	3:C:203:PCW:O31	1.06	1.47	6	16
3:A:409:PCW:H171	3:A:409:PCW:H212	1.06	1.09	14	9
3:A:411:PCW:H272	3:A:411:PCW:H472	1.06	1.12	18	4
3:B:211:PCW:H412	3:B:211:PCW:H371	1.06	1.24	2	14
3:A:404:PCW:H211	3:A:404:PCW:C17	1.06	1.80	4	1
3:A:417:PCW:H422	3:D:612:PCW:H231	1.06	1.07	9	13
3:A:406:PCW:H241	3:B:210:PCW:H122	1.06	1.08	2	6
3:D:603:PCW:H381	4:D:629:17F:H36	1.06	1.25	14	12
3:D:615:PCW:H472	3:C:205:PCW:H222	1.06	1.25	2	6
3:B:205:PCW:H471	3:C:208:PCW:H20	1.06	1.26	19	3
3:B:203:PCW:H222	4:C:210:17F:H19	1.06	1.07	20	8
3:B:206:PCW:H422	4:C:211:17F:H47	1.06	1.27	5	4
3:B:212:PCW:H241	4:C:211:17F:H48	1.06	1.22	10	1
3:B:206:PCW:H171	3:C:212:PCW:H281	1.06	1.17	12	1
3:A:403:PCW:H362	3:A:403:PCW:C31	1.06	1.79	15	1
3:A:418:PCW:H40	3:D:625:PCW:H461	1.06	1.24	2	7
3:A:419:PCW:C37	3:D:617:PCW:H431	1.06	1.81	5	16
3:A:403:PCW:H332	3:C:204:PCW:H11	1.06	1.06	4	5
3:B:204:PCW:H362	3:C:204:PCW:H321	1.06	1.25	20	7
3:A:413:PCW:H182	3:A:413:PCW:H142	1.06	1.16	3	1
3:D:615:PCW:H452	3:C:205:PCW:H241	1.06	1.27	13	9
3:D:607:PCW:H63	3:D:626:PCW:H241	1.06	1.27	14	2
3:D:623:PCW:H322	3:D:623:PCW:C36	1.05	1.79	9	19
4:B:215:17F:H41	4:B:215:17F:C12	1.05	1.80	12	11
3:D:623:PCW:H421	3:D:625:PCW:H261	1.05	1.26	5	16
3:C:204:PCW:H451	4:C:211:17F:H60	1.05	1.13	5	1
3:B:207:PCW:H141	3:B:210:PCW:H362	1.05	1.26	18	2
3:D:611:PCW:H351	3:D:611:PCW:H172	1.05	1.15	11	11
3:A:413:PCW:H261	3:C:203:PCW:H432	1.05	1.22	2	1
3:A:406:PCW:H283	4:B:216:17F:H20A	1.05	1.29	3	1
3:B:203:PCW:H451	3:B:211:PCW:H232	1.05	1.19	9	10
3:B:204:PCW:H132	3:B:206:PCW:H11	1.05	1.17	20	5
3:A:413:PCW:H141	4:A:414:17F:H31	1.05	1.25	3	1
3:D:622:PCW:H341	3:C:212:PCW:H442	1.05	1.11	19	11
3:C:204:PCW:H351	4:C:211:17F:H8	1.05	1.16	17	6
3:C:204:PCW:H442	4:C:211:17F:H33	1.05	1.14	15	1
3:B:210:PCW:H441	3:B:213:PCW:H262	1.05	1.23	16	1
3:C:208:PCW:H352	3:C:208:PCW:O31	1.05	1.50	6	18
3:A:409:PCW:H212	3:A:409:PCW:C17	1.05	1.81	5	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:203:PCW:H182	3:C:203:PCW:H221	1.05	1.16	10	7
3:B:205:PCW:H20	3:B:212:PCW:H322	1.05	1.10	11	2
3:A:403:PCW:H182	3:A:403:PCW:H141	1.05	1.23	15	1
3:D:606:PCW:C1	3:D:626:PCW:H372	1.05	1.82	10	16
3:D:623:PCW:H362	3:D:623:PCW:H322	1.05	1.07	3	13
3:C:203:PCW:H182	3:C:203:PCW:C22	1.05	1.82	4	6
3:A:404:PCW:H431	4:B:215:17F:H9A	1.05	1.20	3	3
3:B:211:PCW:H51	3:B:211:PCW:H12	1.05	1.16	18	13
3:D:603:PCW:H482	3:D:626:PCW:H282	1.04	1.18	19	14
3:D:605:PCW:H161	4:D:629:17F:H11A	1.04	1.15	11	15
3:D:618:PCW:H442	3:D:627:PCW:H261	1.04	1.19	15	4
3:D:603:PCW:H461	3:D:626:PCW:H261	1.04	1.23	11	1
3:D:613:PCW:H482	3:D:619:PCW:H211	1.04	1.29	8	18
3:A:405:PCW:H371	3:D:601:PCW:H151	1.04	1.25	2	6
3:D:603:PCW:H461	3:D:626:PCW:H282	1.04	1.05	2	10
3:D:616:PCW:H441	3:D:627:PCW:H232	1.04	1.21	15	8
3:A:410:PCW:H152	3:C:207:PCW:H211	1.04	1.25	5	4
3:D:618:PCW:H412	4:D:633:17F:H41	1.04	1.26	11	3
3:A:407:PCW:H12	4:B:216:17F:H12A	1.04	1.22	15	1
3:A:419:PCW:H39	3:D:616:PCW:H171	1.04	1.27	17	1
3:D:627:PCW:H421	3:D:627:PCW:H381	1.04	1.16	5	5
3:A:402:PCW:H162	3:A:409:PCW:H211	1.04	1.28	19	5
4:A:414:17F:H48	3:C:203:PCW:H421	1.04	1.17	7	1
3:A:413:PCW:H122	4:A:414:17F:H69	1.04	1.27	18	4
3:D:605:PCW:H73	3:D:626:PCW:H19	1.04	1.20	15	12
3:A:412:PCW:H451	3:C:208:PCW:H182	1.04	1.15	14	4
3:A:408:PCW:H342	3:C:204:PCW:H212	1.04	1.21	9	1
3:D:607:PCW:H42	3:D:626:PCW:H242	1.04	1.25	15	2
3:C:204:PCW:H20	4:C:211:17F:H31	1.04	1.23	18	7
3:D:616:PCW:H481	3:B:206:PCW:H40	1.04	1.28	17	1
3:A:401:PCW:H62	3:B:209:PCW:H11	1.04	1.23	20	3
3:B:204:PCW:H152	3:C:204:PCW:H39	1.04	1.22	20	7
3:B:206:PCW:H381	4:C:211:17F:H47	1.04	1.29	4	1
3:A:416:PCW:H282	3:A:419:PCW:H251	1.04	1.23	7	1
3:B:208:PCW:H171	3:C:205:PCW:H322	1.03	1.22	4	2
4:D:630:17F:H9	4:D:630:17F:H18A	1.03	1.13	7	2
3:B:207:PCW:H441	3:B:213:PCW:H252	1.03	1.23	12	2
3:B:208:PCW:H231	3:B:208:PCW:C28	1.03	1.82	19	1
3:A:417:PCW:H431	3:D:612:PCW:H172	1.03	1.26	5	14
3:D:623:PCW:H362	3:D:623:PCW:C32	1.03	1.84	15	20
3:A:417:PCW:H332	3:D:612:PCW:H132	1.03	1.29	14	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:404:PCW:H381	3:B:209:PCW:H352	1.03	1.31	14	2
3:A:420:PCW:H162	4:D:632:17F:H57	1.03	1.27	8	19
3:A:420:PCW:H122	4:D:632:17F:H9	1.03	1.27	5	13
3:D:601:PCW:H261	4:D:631:17F:H76	1.03	1.09	3	3
3:D:602:PCW:H222	3:D:610:PCW:H331	1.03	1.30	16	5
3:B:205:PCW:H461	3:B:206:PCW:H152	1.03	1.10	4	6
3:D:625:PCW:H151	3:D:625:PCW:H19	1.03	1.29	20	19
4:D:635:17F:H52	3:C:205:PCW:H181	1.03	1.27	17	8
3:C:204:PCW:H131	4:C:211:17F:H75	1.03	1.23	2	1
3:A:406:PCW:H242	3:B:210:PCW:H122	1.03	1.30	5	4
3:B:203:PCW:H381	3:B:211:PCW:H441	1.03	1.27	3	5
4:B:215:17F:H18A	4:B:215:17F:H4A	1.03	1.27	9	2
3:B:207:PCW:H412	3:B:213:PCW:H222	1.03	1.31	1	2
3:C:203:PCW:H121	3:C:203:PCW:H382	1.03	1.11	16	4
3:D:618:PCW:H361	3:D:627:PCW:H172	1.03	1.31	10	9
3:B:206:PCW:H482	3:C:212:PCW:H231	1.03	1.22	3	7
3:A:403:PCW:H322	3:C:203:PCW:H11	1.03	1.30	7	2
3:B:205:PCW:H39	4:B:214:17F:H67	1.03	1.30	4	2
3:C:203:PCW:H162	3:C:203:PCW:H421	1.03	1.30	5	1
3:A:401:PCW:H472	3:D:611:PCW:H251	1.03	1.04	19	5
3:B:203:PCW:H411	3:B:211:PCW:H182	1.03	1.31	18	5
3:A:403:PCW:H362	3:A:403:PCW:H322	1.03	1.04	10	1
3:A:406:PCW:H41	3:A:406:PCW:H31	1.03	1.24	11	1
3:D:607:PCW:H181	4:D:631:17F:H11	1.02	1.28	1	14
3:D:608:PCW:H271	4:D:628:17F:H73	1.02	1.30	12	8
3:D:602:PCW:H222	3:D:610:PCW:C33	1.02	1.85	16	9
3:A:411:PCW:H181	3:A:411:PCW:H222	1.02	1.22	8	3
3:A:401:PCW:H482	3:D:611:PCW:H441	1.02	1.28	5	2
3:A:413:PCW:H162	4:A:414:17F:C1Z	1.02	1.84	19	5
3:A:402:PCW:H2	3:A:409:PCW:H272	1.02	1.29	16	1
3:A:409:PCW:H212	3:A:409:PCW:H171	1.02	1.06	13	5
3:A:411:PCW:H142	3:A:411:PCW:H19	1.02	1.23	8	5
3:B:206:PCW:H482	3:C:212:PCW:H232	1.02	1.23	5	2
3:A:413:PCW:H162	4:A:414:17F:H33	1.02	1.08	19	3
3:A:406:PCW:H341	3:A:411:PCW:H322	1.02	1.09	10	5
3:A:402:PCW:H331	3:C:206:PCW:H31	1.02	1.20	10	3
3:B:210:PCW:H42	3:B:210:PCW:H2	1.02	1.29	17	1
3:A:408:PCW:H52	3:C:204:PCW:H121	1.02	1.23	1	6
3:D:607:PCW:H431	4:D:628:17F:C1Z	1.02	1.85	11	11
3:A:416:PCW:H283	3:A:419:PCW:H251	1.02	1.31	20	6
3:A:401:PCW:H322	3:B:209:PCW:H382	1.02	1.23	9	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:601:PCW:H321	4:B:216:17F:H60	1.02	1.29	16	1
3:D:616:PCW:H341	3:C:212:PCW:H341	1.02	1.18	6	16
3:D:616:PCW:H451	3:B:206:PCW:H472	1.02	1.23	7	8
3:A:413:PCW:H141	3:A:413:PCW:H182	1.02	1.26	13	4
3:D:621:PCW:H412	4:D:635:17F:H75	1.02	1.25	19	5
3:A:411:PCW:H371	3:A:411:PCW:H332	1.02	1.24	8	1
3:B:205:PCW:H151	3:B:212:PCW:H362	1.02	1.28	9	1
3:D:616:PCW:H432	3:C:212:PCW:H412	1.02	1.05	11	1
3:D:612:PCW:H212	3:D:612:PCW:H172	1.02	1.05	15	1
3:D:627:PCW:C4	3:D:627:PCW:H2	1.02	1.84	16	3
4:C:211:17F:H12	4:C:211:17F:H65	1.02	1.24	16	3
3:B:211:PCW:H12	4:B:217:17F:H31	1.02	1.32	6	1
3:B:203:PCW:H472	3:B:211:PCW:H251	1.02	1.30	11	9
4:A:414:17F:H8A	4:C:210:17F:H2	1.02	1.24	10	1
4:D:629:17F:H47	4:D:630:17F:H39	1.01	1.29	4	12
3:A:404:PCW:H211	3:A:404:PCW:H172	1.01	1.04	4	1
3:A:409:PCW:H321	3:C:206:PCW:H372	1.01	1.20	5	2
3:A:406:PCW:H231	3:B:207:PCW:H151	1.01	1.28	17	5
3:A:407:PCW:H181	3:C:205:PCW:H362	1.01	1.11	13	4
3:D:610:PCW:H462	3:B:212:PCW:H261	1.01	1.26	17	4
3:B:207:PCW:H231	3:B:210:PCW:H242	1.01	1.27	15	2
3:A:403:PCW:H171	3:C:203:PCW:H122	1.01	1.32	19	8
3:D:621:PCW:H181	3:D:621:PCW:H142	1.01	1.31	9	20
3:B:209:PCW:H231	3:B:209:PCW:H381	1.01	1.29	1	1
3:A:410:PCW:H121	3:C:209:PCW:H352	1.01	1.30	2	1
3:A:416:PCW:H161	3:A:419:PCW:H331	1.01	1.24	12	13
3:D:622:PCW:H352	3:D:627:PCW:C20	1.01	1.84	7	16
3:B:205:PCW:H442	3:B:206:PCW:H161	1.01	1.31	6	5
3:C:203:PCW:C16	3:C:203:PCW:H421	1.01	1.84	10	3
3:C:207:PCW:H272	3:C:209:PCW:H39	1.01	1.22	13	4
3:A:404:PCW:H351	3:B:203:PCW:H171	1.01	1.30	11	2
3:A:401:PCW:H441	3:D:611:PCW:H271	1.01	1.31	14	1
3:B:204:PCW:O11	3:B:206:PCW:H52	1.01	1.54	14	2
3:A:407:PCW:H82	3:B:213:PCW:H322	1.01	1.28	19	1
3:D:613:PCW:H251	4:C:210:17F:H47	1.01	1.33	9	11
3:D:618:PCW:H422	3:D:627:PCW:H261	1.01	1.32	19	10
3:A:407:PCW:H171	3:B:208:PCW:H222	1.01	1.26	2	6
3:A:402:PCW:H321	3:C:206:PCW:H41	1.01	1.23	12	1
4:B:215:17F:H43	4:B:217:17F:H38	1.01	1.30	16	1
3:D:607:PCW:H261	4:D:631:17F:H62	1.01	1.24	20	11
3:D:608:PCW:H483	3:C:205:PCW:H472	1.01	1.27	5	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:612:PCW:H63	3:D:618:PCW:H12	1.01	1.31	7	10
3:B:205:PCW:H171	3:B:205:PCW:H132	1.01	1.24	8	19
3:C:207:PCW:H172	3:C:207:PCW:H212	1.01	1.30	11	2
3:A:413:PCW:H452	4:C:210:17F:H36	1.01	1.33	17	4
3:A:410:PCW:H42	3:C:209:PCW:H32	1.01	1.13	14	4
3:B:205:PCW:H251	3:B:205:PCW:H212	1.01	1.28	19	1
3:D:611:PCW:C32	3:D:623:PCW:H352	1.01	1.86	13	17
3:B:204:PCW:H171	3:B:206:PCW:H321	1.01	1.25	1	1
3:A:420:PCW:H61	4:D:632:17F:H4	1.01	1.07	11	4
4:D:628:17F:H59	4:D:631:17F:H51	1.01	1.32	18	2
3:D:604:PCW:O1P	3:D:613:PCW:H52	1.00	1.53	7	15
3:D:611:PCW:H39	3:D:623:PCW:H462	1.00	1.28	9	16
3:D:604:PCW:H371	3:D:611:PCW:H322	1.00	1.31	4	8
3:B:210:PCW:H451	3:B:213:PCW:H272	1.00	1.30	2	1
4:A:414:17F:H52	3:C:203:PCW:H472	1.00	1.33	3	1
3:B:209:PCW:H222	3:B:209:PCW:H272	1.00	1.03	15	3
3:B:207:PCW:C14	3:B:210:PCW:H321	1.00	1.85	13	3
3:C:204:PCW:H262	3:C:207:PCW:H482	1.00	1.28	12	1
3:D:602:PCW:H2	3:D:602:PCW:C4	1.00	1.86	15	17
3:D:616:PCW:H39	3:D:618:PCW:C14	1.00	1.86	7	11
4:D:630:17F:H59	4:D:630:17F:H12A	1.00	1.31	5	16
3:A:402:PCW:H162	3:A:409:PCW:H231	1.00	1.31	15	4
3:D:602:PCW:H62	3:C:212:PCW:O2P	1.00	1.56	11	5
3:A:403:PCW:H31	3:A:403:PCW:C4	1.00	1.86	13	14
3:A:416:PCW:H452	3:A:420:PCW:H421	1.00	1.30	15	5
3:A:419:PCW:H362	3:D:617:PCW:H412	1.00	1.34	5	19
3:A:420:PCW:O2P	3:D:617:PCW:H42	1.00	1.55	10	5
3:D:604:PCW:H171	3:D:613:PCW:H342	1.00	1.32	13	11
3:A:402:PCW:H411	3:C:205:PCW:H361	1.00	1.34	17	3
3:C:208:PCW:H232	3:C:209:PCW:H431	1.00	1.32	3	6
4:A:415:17F:H18	4:A:415:17F:H9A	1.00	1.25	5	2
3:B:209:PCW:H222	3:B:209:PCW:H432	1.00	1.30	5	1
4:A:415:17F:H76	4:C:210:17F:H73	1.00	1.24	20	3
3:A:406:PCW:H422	3:B:210:PCW:H39	1.00	1.28	10	2
3:D:608:PCW:H182	3:D:615:PCW:H352	1.00	1.30	11	10
3:C:204:PCW:H222	4:C:211:17F:H20	1.00	1.31	9	1
3:B:205:PCW:H172	3:B:212:PCW:H362	1.00	1.03	19	3
3:D:608:PCW:H2	3:D:615:PCW:H61	1.00	1.31	15	12
3:D:621:PCW:H351	4:D:634:17F:H33	1.00	1.31	1	11
3:A:412:PCW:H371	3:C:206:PCW:H40	1.00	1.33	14	3
3:D:611:PCW:H321	3:D:623:PCW:C35	1.00	1.85	13	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:606:PCW:H472	3:B:210:PCW:H483	1.00	1.33	3	4
3:D:620:PCW:H372	3:D:620:PCW:H412	1.00	1.32	10	17
3:A:413:PCW:H471	4:C:210:17F:H12A	1.00	1.32	17	6
3:D:601:PCW:H481	3:D:607:PCW:H231	1.00	1.30	11	3
3:B:206:PCW:H342	3:C:204:PCW:H381	1.00	1.31	20	6
3:A:406:PCW:H39	3:A:406:PCW:C14	1.00	1.86	9	1
3:B:212:PCW:H40	3:C:212:PCW:H283	0.99	1.23	12	4
3:A:407:PCW:H141	3:C:205:PCW:H321	0.99	1.30	4	5
3:D:621:PCW:C14	4:D:634:17F:H6	0.99	1.87	11	18
3:A:407:PCW:H352	3:C:205:PCW:H142	0.99	1.29	7	2
3:D:622:PCW:H262	3:D:624:PCW:H282	0.99	1.27	5	5
3:A:418:PCW:H40	3:D:625:PCW:H441	0.99	1.27	18	15
3:D:607:PCW:H452	4:D:628:17F:H60	0.99	1.26	18	8
4:D:629:17F:C7	4:D:629:17F:H18A	0.99	1.87	19	6
3:D:616:PCW:C39	3:D:618:PCW:H142	0.99	1.87	17	12
3:D:621:PCW:H371	4:D:633:17F:H63	0.99	1.31	19	14
3:A:404:PCW:H351	4:B:215:17F:H42	0.99	1.31	2	1
3:C:208:PCW:H231	3:C:209:PCW:H40	0.99	1.26	3	7
3:D:614:PCW:H52	3:D:625:PCW:O1P	0.99	1.57	20	13
3:A:406:PCW:H252	3:B:207:PCW:H171	0.99	1.33	17	6
3:A:404:PCW:H272	4:A:415:17F:H65	0.99	1.29	12	4
3:D:622:PCW:H362	4:D:629:17F:H76	0.99	1.10	1	2
3:B:207:PCW:H11	4:B:216:17F:H8A	0.99	1.33	19	4
3:D:620:PCW:H152	4:D:635:17F:H18	0.99	1.30	6	9
3:D:622:PCW:H141	4:D:630:17F:H33	0.99	1.29	18	8
3:B:208:PCW:H162	4:B:214:17F:H60	0.99	1.35	8	3
3:D:615:PCW:H282	4:D:635:17F:H46	0.99	1.32	3	3
3:B:206:PCW:H162	3:B:212:PCW:H441	0.99	1.21	4	1
3:B:209:PCW:H332	3:B:209:PCW:H132	0.99	1.30	16	7
3:C:204:PCW:H371	4:C:211:17F:H8A	0.99	1.31	9	4
3:C:207:PCW:H283	3:C:208:PCW:H222	0.99	1.32	17	1
3:A:412:PCW:H332	3:C:206:PCW:H451	0.99	1.28	20	1
3:D:604:PCW:H182	3:D:613:PCW:H362	0.99	1.35	19	17
3:D:622:PCW:H341	3:C:212:PCW:H422	0.99	1.32	1	5
3:C:204:PCW:H351	4:C:211:17F:H9	0.99	1.28	9	4
3:B:204:PCW:H283	3:C:204:PCW:H452	0.99	1.33	17	5
3:D:605:PCW:H252	4:D:629:17F:H38	0.99	1.34	1	7
3:D:611:PCW:H2	3:D:619:PCW:H63	0.99	1.35	5	17
3:D:622:PCW:H141	4:D:630:17F:H32	0.99	1.31	14	15
3:B:206:PCW:H51	3:C:207:PCW:H12	0.99	1.28	16	5
3:B:207:PCW:H441	3:B:213:PCW:H231	0.99	1.32	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:413:PCW:H161	4:A:414:17F:H31	0.99	1.32	12	2
3:B:208:PCW:O1P	3:B:208:PCW:H31	0.99	1.57	5	6
3:A:406:PCW:H131	3:B:210:PCW:H331	0.99	1.33	20	2
3:D:605:PCW:H61	3:D:626:PCW:H281	0.98	1.31	6	16
4:D:629:17F:H69	4:D:634:17F:H11	0.98	1.30	20	7
3:A:410:PCW:H32	3:C:207:PCW:H152	0.98	1.35	16	7
3:D:607:PCW:H141	3:D:608:PCW:H171	0.98	1.25	2	8
3:B:209:PCW:H31	3:B:209:PCW:C4	0.98	1.87	17	17
3:D:622:PCW:C35	3:D:627:PCW:H20	0.98	1.88	7	16
3:D:627:PCW:H42	3:D:627:PCW:C2	0.98	1.87	3	8
3:A:408:PCW:H252	3:A:417:PCW:H262	0.98	1.35	5	1
3:D:602:PCW:H371	3:D:602:PCW:H412	0.98	1.28	5	20
3:D:601:PCW:H142	3:D:601:PCW:H381	0.98	1.32	10	10
3:B:211:PCW:H242	4:B:217:17F:H78	0.98	1.34	15	1
3:D:602:PCW:H222	3:D:610:PCW:C35	0.98	1.87	6	17
3:D:618:PCW:H381	3:D:627:PCW:H161	0.98	1.30	13	15
3:D:623:PCW:C36	3:D:623:PCW:H322	0.98	1.88	5	1
3:A:403:PCW:H231	3:A:403:PCW:H282	0.98	1.06	10	1
3:A:411:PCW:H19	3:A:411:PCW:H142	0.98	0.99	17	1
3:D:623:PCW:H322	3:D:623:PCW:H362	0.98	1.04	5	7
3:B:205:PCW:H39	4:B:214:17F:H63	0.98	1.33	3	1
3:A:406:PCW:H441	3:B:210:PCW:H39	0.98	1.36	16	1
3:A:417:PCW:H431	3:D:612:PCW:C17	0.98	1.88	17	15
3:D:604:PCW:H39	3:D:611:PCW:H341	0.98	1.32	1	15
3:B:203:PCW:H482	4:B:217:17F:H55	0.98	1.26	8	4
3:D:607:PCW:H461	4:D:628:17F:H61	0.98	1.35	15	9
3:D:606:PCW:H12	3:D:626:PCW:C37	0.97	1.88	20	17
3:A:406:PCW:H241	3:B:210:PCW:C12	0.97	1.88	18	6
3:B:208:PCW:H182	3:C:205:PCW:H331	0.97	1.29	13	5
3:B:208:PCW:H161	4:B:214:17F:H56	0.97	1.32	4	5
4:D:635:17F:H53	3:C:205:PCW:H161	0.97	1.36	13	8
3:A:406:PCW:C34	3:A:411:PCW:H322	0.97	1.88	10	3
3:D:611:PCW:H222	3:D:619:PCW:C44	0.97	1.88	18	3
3:A:418:PCW:C40	3:D:625:PCW:H441	0.97	1.89	11	20
3:D:624:PCW:H321	3:D:624:PCW:H73	0.97	1.36	10	7
4:D:629:17F:H19	4:D:629:17F:H5	0.97	1.31	18	11
3:B:207:PCW:H132	3:B:210:PCW:H131	0.97	1.36	7	9
3:A:407:PCW:H161	3:C:205:PCW:H171	0.97	1.32	13	2
3:D:607:PCW:H19	4:D:631:17F:H46	0.97	1.35	12	15
3:C:207:PCW:H241	3:C:209:PCW:H39	0.97	1.29	14	4
3:A:407:PCW:H222	3:C:205:PCW:H451	0.97	1.35	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:615:PCW:H262	4:B:216:17F:H72	0.97	1.35	2	3
3:D:615:PCW:H432	3:C:205:PCW:H262	0.97	1.33	17	6
3:B:206:PCW:C48	3:C:212:PCW:H231	0.97	1.89	6	3
3:C:204:PCW:H351	4:C:211:17F:C8	0.97	1.90	17	6
4:D:629:17F:H76	3:C:212:PCW:H462	0.97	1.32	16	6
3:B:208:PCW:H161	4:B:214:17F:H20A	0.97	1.37	11	4
3:D:624:PCW:H481	4:C:210:17F:H55	0.97	1.34	20	5
3:D:613:PCW:H20	4:C:210:17F:H48	0.97	1.35	1	1
3:B:213:PCW:H422	4:B:217:17F:H67	0.97	1.36	4	3
3:C:207:PCW:H252	3:C:208:PCW:H241	0.97	1.36	6	1
3:B:206:PCW:C34	3:C:204:PCW:H381	0.97	1.90	7	5
3:A:408:PCW:H272	3:D:616:PCW:H211	0.97	1.36	14	1
3:D:601:PCW:H351	4:B:216:17F:H70	0.97	1.32	4	1
3:A:404:PCW:H211	4:A:415:17F:H58	0.97	1.32	5	1
3:A:408:PCW:H281	3:A:417:PCW:H221	0.97	1.35	20	3
3:B:207:PCW:H121	3:B:210:PCW:H341	0.97	1.32	16	1
3:B:204:PCW:O31	3:B:212:PCW:H63	0.97	1.60	17	1
3:C:204:PCW:H122	4:C:211:17F:H8A	0.96	1.35	1	1
3:A:401:PCW:H52	3:A:404:PCW:H32	0.96	1.28	13	1
3:D:626:PCW:H231	3:D:626:PCW:C27	0.96	1.90	20	17
3:C:203:PCW:H221	3:C:203:PCW:C18	0.96	1.90	4	7
3:A:406:PCW:H231	3:B:207:PCW:H171	0.96	1.33	20	4
3:D:601:PCW:H351	4:B:216:17F:H78	0.96	1.36	15	3
3:D:618:PCW:H451	4:D:633:17F:H55	0.96	1.36	9	4
3:D:621:PCW:H19	4:D:633:17F:H5	0.96	1.31	9	16
3:A:406:PCW:H31	3:A:406:PCW:C4	0.96	1.89	11	7
3:A:403:PCW:H461	3:C:203:PCW:H281	0.96	1.31	9	1
3:A:403:PCW:H62	3:A:403:PCW:O11	0.96	1.60	10	1
3:A:407:PCW:H73	4:B:214:17F:O1	0.96	1.60	9	14
3:A:419:PCW:H372	3:D:617:PCW:C43	0.96	1.90	19	19
3:A:409:PCW:H411	3:A:409:PCW:H372	0.96	1.31	8	4
3:B:206:PCW:H482	3:C:212:PCW:C23	0.96	1.90	6	8
3:B:210:PCW:H271	3:B:210:PCW:H421	0.96	1.30	20	3
3:D:604:PCW:H211	3:D:613:PCW:H382	0.96	1.36	1	20
3:B:209:PCW:H182	3:B:209:PCW:H341	0.96	1.36	18	3
3:B:203:PCW:H2	3:B:211:PCW:H372	0.96	1.35	20	4
4:D:629:17F:C38	4:D:634:17F:H11	0.96	1.89	20	6
3:B:205:PCW:H152	4:B:214:17F:H37	0.96	1.37	2	5
3:B:207:PCW:H182	3:B:210:PCW:C20	0.96	1.90	17	3
3:D:621:PCW:H412	4:D:635:17F:H77	0.96	1.37	5	8
3:A:420:PCW:H442	3:D:617:PCW:H20	0.96	1.35	8	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:404:PCW:H332	3:B:203:PCW:H171	0.96	1.34	10	1
3:B:207:PCW:H161	3:B:210:PCW:H211	0.96	1.34	19	2
3:D:616:PCW:H12	3:D:616:PCW:H41	0.96	1.35	1	2
3:D:602:PCW:H261	3:D:610:PCW:H171	0.96	1.35	19	15
4:D:629:17F:H69	4:D:634:17F:H29	0.96	1.36	11	1
3:A:410:PCW:H171	3:C:207:PCW:H232	0.96	1.35	20	4
3:A:409:PCW:H82	3:C:206:PCW:H11	0.96	1.31	1	1
3:D:616:PCW:H19	3:D:617:PCW:H461	0.96	1.35	7	7
3:D:622:PCW:H441	3:B:206:PCW:H272	0.96	1.37	10	10
3:A:407:PCW:H431	4:B:216:17F:H77	0.96	1.34	18	1
3:D:607:PCW:C19	4:D:631:17F:H46	0.96	1.90	20	20
3:A:407:PCW:H141	3:C:205:PCW:H342	0.96	1.32	10	9
3:A:417:PCW:H341	3:D:612:PCW:H132	0.96	1.31	10	2
3:C:204:PCW:H351	4:C:211:17F:O8	0.96	1.58	7	3
3:D:618:PCW:H462	3:C:207:PCW:H231	0.96	1.36	8	1
3:D:623:PCW:H232	3:B:203:PCW:H481	0.96	1.38	3	8
3:B:208:PCW:H441	4:B:214:17F:H33	0.96	1.33	4	4
3:B:204:PCW:H331	3:B:212:PCW:H141	0.96	1.36	17	5
3:D:601:PCW:H261	4:D:631:17F:C42	0.95	1.91	3	7
3:B:206:PCW:H241	3:C:208:PCW:H282	0.95	1.32	5	3
3:A:413:PCW:H121	4:A:414:17F:H33	0.95	1.35	7	1
3:B:212:PCW:H152	3:C:204:PCW:H361	0.95	1.35	13	2
3:D:620:PCW:H2	3:D:620:PCW:H41	0.95	1.35	11	2
3:B:205:PCW:H241	3:B:212:PCW:H362	0.95	1.37	11	1
3:A:407:PCW:H242	3:C:205:PCW:H411	0.95	1.34	7	10
3:A:407:PCW:H222	3:C:205:PCW:H431	0.95	1.37	13	7
3:A:406:PCW:C23	3:B:207:PCW:H171	0.95	1.91	20	3
4:C:211:17F:H12	4:C:211:17F:C36	0.95	1.91	5	3
3:D:608:PCW:H232	3:D:615:PCW:H361	0.95	1.37	3	5
3:D:613:PCW:H121	3:D:619:PCW:H382	0.95	1.36	14	7
3:B:205:PCW:H422	3:B:206:PCW:H161	0.95	1.37	8	5
3:D:603:PCW:H482	3:D:626:PCW:H272	0.95	1.34	11	6
3:C:208:PCW:H121	3:C:208:PCW:C37	0.95	1.91	18	11
3:A:412:PCW:H462	3:C:208:PCW:H19	0.95	1.34	8	1
3:B:204:PCW:H232	3:C:208:PCW:H241	0.95	1.32	8	1
3:D:619:PCW:H451	4:C:210:17F:H74	0.95	1.37	13	1
3:D:601:PCW:H422	4:D:628:17F:H45	0.95	1.38	16	1
3:D:601:PCW:H341	4:B:216:17F:H61	0.95	1.34	2	1
3:A:401:PCW:H362	3:B:209:PCW:C39	0.95	1.91	6	1
3:B:203:PCW:H461	4:B:217:17F:H50	0.95	1.35	8	2
3:A:420:PCW:O31	3:D:617:PCW:H52	0.95	1.60	15	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:606:PCW:H31	3:D:626:PCW:C37	0.95	1.91	9	12
3:D:604:PCW:O31	3:D:613:PCW:H51	0.95	1.62	6	2
3:B:212:PCW:H471	4:B:214:17F:H38	0.95	1.31	13	1
3:A:411:PCW:H2	4:B:215:17F:H33	0.95	1.34	8	4
3:A:420:PCW:H351	3:D:617:PCW:H151	0.95	1.35	1	12
3:D:603:PCW:H41	3:D:603:PCW:H31	0.95	1.37	5	2
3:D:615:PCW:H472	3:C:205:PCW:H20	0.95	1.35	8	1
3:A:417:PCW:H422	3:D:612:PCW:C23	0.95	1.90	5	14
3:D:605:PCW:H212	3:D:605:PCW:C17	0.95	1.90	1	20
3:D:608:PCW:H251	4:D:628:17F:H70	0.95	1.39	16	8
3:B:207:PCW:H39	4:B:215:17F:H6A	0.95	1.36	1	1
3:A:406:PCW:C24	3:B:210:PCW:H122	0.95	1.92	2	8
3:D:627:PCW:H122	3:D:627:PCW:H332	0.95	1.39	5	1
3:D:611:PCW:C22	3:D:619:PCW:H442	0.95	1.91	18	3
3:A:410:PCW:C15	3:C:207:PCW:H211	0.95	1.90	18	2
3:C:206:PCW:H181	3:C:206:PCW:H241	0.95	1.32	16	2
3:D:601:PCW:H462	4:D:628:17F:H66	0.95	1.36	4	1
3:C:204:PCW:H51	3:C:204:PCW:H2	0.95	1.35	5	1
3:A:401:PCW:H73	3:B:209:PCW:H152	0.95	1.35	19	1
3:A:416:PCW:H442	3:D:617:PCW:H212	0.94	1.38	11	5
3:D:621:PCW:C13	4:D:634:17F:H4A	0.94	1.90	12	13
4:D:629:17F:H42	4:D:630:17F:H73	0.94	1.35	6	7
3:B:213:PCW:H442	4:B:217:17F:H40	0.94	1.38	2	3
3:A:413:PCW:H422	4:A:414:17F:H70	0.94	1.37	3	3
3:A:413:PCW:C34	4:A:414:17F:H57	0.94	1.92	20	8
3:D:601:PCW:H212	3:D:601:PCW:C17	0.94	1.91	5	9
3:B:209:PCW:C11	3:B:209:PCW:H73	0.94	1.92	12	13
4:C:211:17F:H69	4:C:211:17F:H12A	0.94	1.39	12	2
3:D:614:PCW:C4	3:D:625:PCW:H42	0.94	1.92	13	1
3:A:401:PCW:H151	3:D:614:PCW:H281	0.94	1.39	1	1
3:D:618:PCW:H382	4:D:633:17F:H41	0.94	1.39	10	12
3:A:410:PCW:H152	3:C:207:PCW:C21	0.94	1.92	18	4
3:A:410:PCW:H52	3:C:209:PCW:H11	0.94	1.38	15	2
3:A:420:PCW:H122	4:D:632:17F:C9	0.94	1.92	16	20
4:B:216:17F:H36	4:B:216:17F:H42	0.94	1.37	2	7
3:B:204:PCW:H152	3:C:204:PCW:C39	0.94	1.91	16	6
3:A:417:PCW:H2	3:A:417:PCW:H42	0.94	1.40	7	3
3:B:205:PCW:H40	4:B:214:17F:H70	0.94	1.36	10	3
3:B:209:PCW:H19	4:B:215:17F:H19A	0.94	1.37	20	2
3:A:404:PCW:H432	3:B:209:PCW:H222	0.94	1.35	14	1
3:A:417:PCW:C33	3:D:612:PCW:H132	0.94	1.92	14	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:602:PCW:H441	3:D:602:PCW:H212	0.94	1.39	11	17
3:C:207:PCW:H322	3:C:207:PCW:H42	0.94	1.38	2	14
3:A:413:PCW:H162	4:A:414:17F:H59	0.94	1.39	17	3
4:D:628:17F:H36	4:D:631:17F:H70	0.94	1.38	10	7
3:D:623:PCW:H371	3:D:623:PCW:H131	0.94	1.34	6	2
3:B:204:PCW:H252	3:C:207:PCW:H262	0.94	1.35	5	2
3:A:413:PCW:H31	3:A:413:PCW:C37	0.94	1.91	3	7
3:B:203:PCW:H51	3:B:211:PCW:H331	0.94	1.40	16	5
3:B:207:PCW:H421	3:B:213:PCW:C25	0.94	1.93	8	3
3:A:417:PCW:H441	3:D:612:PCW:H271	0.94	1.35	10	1
3:A:407:PCW:H62	4:B:214:17F:O1	0.94	1.63	19	2
4:C:211:17F:H54	3:C:212:PCW:H251	0.94	1.40	12	1
3:C:208:PCW:H232	3:C:209:PCW:H451	0.94	1.39	16	3
3:A:417:PCW:H351	3:D:612:PCW:C15	0.94	1.93	11	13
3:D:602:PCW:H421	3:D:610:PCW:H362	0.94	1.37	1	10
3:C:208:PCW:H371	3:C:208:PCW:C12	0.94	1.92	18	10
3:A:412:PCW:H371	3:C:206:PCW:H39	0.94	1.35	5	1
3:A:410:PCW:H41	3:C:209:PCW:H32	0.94	1.36	7	2
3:D:616:PCW:H11	3:C:212:PCW:H342	0.94	1.34	17	3
3:B:206:PCW:H342	3:C:204:PCW:C38	0.94	1.92	7	8
3:A:408:PCW:H212	3:A:417:PCW:C46	0.94	1.91	11	1
3:A:407:PCW:H182	3:C:205:PCW:H151	0.94	1.37	12	3
3:B:207:PCW:H162	3:B:210:PCW:H142	0.94	1.38	12	1
3:A:419:PCW:H482	3:D:616:PCW:H271	0.94	1.39	15	4
2:C:13:GLY:HA2	5:C:201:GDP:H5'	0.94	1.36	12	8
3:B:213:PCW:H421	4:B:217:17F:H10	0.93	1.35	7	2
3:B:213:PCW:H351	4:B:214:17F:H10A	0.93	1.40	16	1
3:A:402:PCW:H441	3:C:205:PCW:H152	0.93	1.38	1	4
3:D:604:PCW:C18	3:D:613:PCW:H362	0.93	1.93	12	20
3:D:621:PCW:C15	4:D:634:17F:H6	0.93	1.92	13	15
3:A:402:PCW:H321	3:C:206:PCW:C4	0.93	1.92	12	1
3:D:620:PCW:O1P	3:D:621:PCW:H52	0.93	1.62	12	9
3:B:211:PCW:H222	3:B:211:PCW:H171	0.93	1.40	4	1
3:A:401:PCW:H452	3:D:611:PCW:H271	0.93	1.41	5	4
3:D:618:PCW:H131	3:D:627:PCW:H151	0.93	1.39	5	15
3:D:625:PCW:C41	3:D:626:PCW:H412	0.93	1.94	17	14
3:D:608:PCW:H452	3:C:205:PCW:H231	0.93	1.38	3	8
3:D:622:PCW:H421	3:B:206:PCW:H272	0.93	1.40	2	4
3:C:206:PCW:H152	3:C:206:PCW:H382	0.93	1.39	4	1
3:B:205:PCW:O1P	3:B:211:PCW:H73	0.93	1.62	10	4
3:B:205:PCW:C17	3:B:212:PCW:H362	0.93	1.94	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:418:PCW:C39	3:D:625:PCW:H441	0.93	1.94	2	9
3:D:611:PCW:H2	3:D:619:PCW:C6	0.93	1.94	5	16
3:B:209:PCW:H41	3:B:209:PCW:C3	0.93	1.94	17	13
3:C:203:PCW:H421	3:C:203:PCW:C16	0.93	1.94	5	4
3:B:213:PCW:H412	4:B:217:17F:H59	0.93	1.34	7	2
3:D:603:PCW:H411	4:D:629:17F:H36	0.93	1.35	10	3
3:B:212:PCW:H40	3:C:212:PCW:H262	0.93	1.35	18	1
3:D:615:PCW:H272	4:D:635:17F:H42	0.93	1.39	3	1
3:B:208:PCW:H182	3:C:205:PCW:H322	0.93	1.35	1	1
3:D:602:PCW:C31	3:D:602:PCW:H42	0.93	1.94	4	4
3:D:615:PCW:H141	4:D:635:17F:H9A	0.93	1.37	12	2
3:A:404:PCW:H272	4:A:415:17F:H69	0.93	1.41	8	3
3:B:211:PCW:H63	3:B:212:PCW:H321	0.93	1.39	14	7
3:B:207:PCW:H421	3:B:213:PCW:H242	0.93	1.38	12	3
3:D:602:PCW:H41	3:D:602:PCW:C2	0.93	1.92	17	18
3:D:604:PCW:H172	3:D:613:PCW:H132	0.93	1.37	18	10
3:B:206:PCW:C40	3:C:212:PCW:H251	0.93	1.93	13	3
3:B:204:PCW:H182	3:B:205:PCW:H482	0.93	1.41	19	4
3:A:407:PCW:H52	4:B:216:17F:H12A	0.93	1.38	19	1
3:A:417:PCW:H371	3:A:417:PCW:H411	0.93	1.41	1	11
3:A:420:PCW:H372	3:D:617:PCW:H141	0.93	1.40	16	8
3:D:605:PCW:H341	3:D:605:PCW:H132	0.93	1.40	16	13
3:A:407:PCW:H241	3:C:205:PCW:H411	0.93	1.41	14	8
3:D:611:PCW:H41	3:D:623:PCW:H342	0.93	1.39	20	7
3:D:617:PCW:H2	3:D:617:PCW:C4	0.93	1.94	18	4
3:A:418:PCW:O1P	3:D:614:PCW:H41	0.93	1.62	15	5
3:A:401:PCW:C6	3:B:209:PCW:H11	0.93	1.94	20	2
3:C:204:PCW:H271	4:C:211:17F:H32	0.93	1.41	2	1
3:D:611:PCW:H221	3:D:619:PCW:H482	0.93	1.39	5	1
3:C:207:PCW:H51	4:C:211:17F:C1	0.93	1.94	10	5
3:C:204:PCW:C44	4:C:211:17F:H33	0.93	1.94	15	1
3:A:410:PCW:H242	3:C:207:PCW:H231	0.92	1.38	16	6
3:A:404:PCW:H40	4:B:215:17F:H10A	0.92	1.37	4	5
3:B:211:PCW:H362	3:B:212:PCW:O2P	0.92	1.64	12	2
4:C:210:17F:H57	4:C:210:17F:C19	0.92	1.94	16	20
3:D:621:PCW:H20	3:D:622:PCW:H82	0.92	1.36	12	9
3:A:403:PCW:H362	3:A:403:PCW:C32	0.92	1.93	10	2
3:B:207:PCW:H422	3:B:213:PCW:H231	0.92	1.36	19	2
3:B:206:PCW:C5	3:C:207:PCW:H12	0.92	1.95	18	4
3:A:417:PCW:C42	3:D:612:PCW:H231	0.92	1.94	9	13
3:D:603:PCW:H31	3:D:603:PCW:O4P	0.92	1.64	15	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:618:PCW:H262	3:C:204:PCW:H281	0.92	1.40	14	3
3:B:206:PCW:H39	3:C:212:PCW:H251	0.92	1.40	18	4
3:A:410:PCW:C4	3:C:209:PCW:H32	0.92	1.95	14	5
3:B:204:PCW:H241	3:C:207:PCW:H252	0.92	1.39	8	1
3:B:204:PCW:C13	3:B:206:PCW:H41	0.92	1.94	19	3
3:A:403:PCW:H322	3:A:403:PCW:C36	0.92	1.94	10	1
3:D:616:PCW:C39	3:D:618:PCW:H162	0.92	1.94	11	14
3:B:205:PCW:H442	3:B:206:PCW:H182	0.92	1.40	9	2
4:D:629:17F:H52	4:D:630:17F:H43	0.92	1.38	2	1
4:D:630:17F:H62	4:D:634:17F:H36	0.92	1.38	3	7
3:A:402:PCW:H421	3:C:205:PCW:H132	0.92	1.40	13	4
3:A:405:PCW:H432	3:A:405:PCW:C47	0.92	1.94	5	5
3:B:204:PCW:H332	3:B:212:PCW:H82	0.92	1.37	11	6
3:C:204:PCW:H352	4:C:211:17F:H4	0.92	1.37	11	2
3:D:622:PCW:C36	4:D:629:17F:H76	0.92	1.95	1	2
3:D:608:PCW:H172	3:D:615:PCW:H331	0.92	1.40	14	8
3:D:602:PCW:H382	3:D:624:PCW:H141	0.92	1.41	8	6
3:B:204:PCW:H182	3:B:205:PCW:H481	0.92	1.38	16	4
3:A:406:PCW:H41	3:A:406:PCW:C3	0.92	1.94	11	1
3:D:616:PCW:H371	3:D:618:PCW:H142	0.92	1.38	18	4
3:D:620:PCW:H141	4:D:635:17F:O9	0.92	1.65	12	17
3:A:402:PCW:C8	3:A:409:PCW:H32	0.92	1.95	5	6
3:C:203:PCW:H421	3:C:203:PCW:H162	0.92	1.40	4	3
3:A:413:PCW:H462	3:D:613:PCW:H231	0.92	1.39	16	5
3:D:615:PCW:H481	3:B:208:PCW:H271	0.92	1.37	7	1
3:A:404:PCW:H451	3:B:209:PCW:H20	0.92	1.37	9	5
3:A:413:PCW:C16	4:A:414:17F:H33	0.92	1.95	19	3
3:B:210:PCW:H451	3:B:213:PCW:H262	0.92	1.39	8	5
3:B:203:PCW:H42	3:B:211:PCW:O31	0.92	1.63	12	1
3:A:406:PCW:H82	4:B:215:17F:O1	0.92	1.65	1	2
3:D:622:PCW:C24	3:D:624:PCW:H242	0.92	1.94	18	14
3:A:402:PCW:H442	3:C:205:PCW:H361	0.92	1.42	7	1
3:A:408:PCW:H241	3:A:417:PCW:H262	0.92	1.37	19	1
3:A:402:PCW:H162	3:A:409:PCW:H251	0.92	1.39	1	1
3:A:413:PCW:H261	3:C:203:PCW:C43	0.92	1.93	2	1
3:A:408:PCW:H262	3:A:417:PCW:H461	0.92	1.42	15	1
3:D:623:PCW:H382	3:D:625:PCW:H171	0.92	1.42	19	12
3:D:608:PCW:H483	3:C:205:PCW:H451	0.92	1.38	9	3
3:A:417:PCW:H39	3:D:612:PCW:H451	0.91	1.40	18	7
3:B:213:PCW:H211	3:B:213:PCW:H162	0.91	1.42	15	3
3:B:210:PCW:O11	3:B:210:PCW:H52	0.91	1.64	10	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:207:PCW:C13	3:B:210:PCW:H131	0.91	1.94	18	4
3:D:625:PCW:H412	3:D:626:PCW:C41	0.91	1.95	11	12
3:B:204:PCW:C17	3:B:206:PCW:H321	0.91	1.95	1	1
4:A:414:17F:H56	4:A:414:17F:H62	0.91	1.40	13	3
3:A:406:PCW:H121	3:A:406:PCW:H39	0.91	1.42	7	1
3:D:616:PCW:C34	3:C:212:PCW:H341	0.91	1.95	14	16
3:A:409:PCW:H82	3:C:206:PCW:H351	0.91	1.40	3	3
3:B:205:PCW:H151	3:B:212:PCW:C36	0.91	1.95	9	1
3:A:402:PCW:H331	3:C:206:PCW:C3	0.91	1.94	10	1
4:D:629:17F:H10	4:D:634:17F:H49	0.91	1.40	1	7
3:A:409:PCW:C16	3:A:409:PCW:H212	0.91	1.94	1	4
3:B:205:PCW:H152	4:B:214:17F:C21	0.91	1.94	2	3
3:B:208:PCW:H161	4:B:214:17F:H60	0.91	1.42	15	2
3:A:404:PCW:H211	3:A:404:PCW:H171	0.91	1.43	18	1
3:D:612:PCW:C32	3:D:618:PCW:H132	0.91	1.95	17	16
3:A:405:PCW:H483	3:A:405:PCW:H152	0.91	1.42	5	3
4:C:211:17F:H12	4:C:211:17F:H66	0.91	1.39	3	3
3:B:203:PCW:C22	4:C:210:17F:H19	0.91	1.96	20	5
3:A:401:PCW:H472	3:D:611:PCW:C25	0.91	1.95	19	2
3:D:618:PCW:H151	3:D:627:PCW:H142	0.91	1.38	13	12
3:D:621:PCW:C15	4:D:634:17F:H4A	0.91	1.95	2	3
3:C:204:PCW:H471	4:C:211:17F:C31	0.91	1.96	18	3
3:D:605:PCW:C6	3:D:626:PCW:H281	0.91	1.95	4	15
3:D:624:PCW:H20	3:D:624:PCW:C24	0.91	1.96	13	20
3:A:402:PCW:H451	4:D:635:17F:H51	0.91	1.42	11	4
3:D:621:PCW:C19	4:D:633:17F:H5	0.91	1.95	7	5
3:A:406:PCW:O4P	3:A:406:PCW:H31	0.91	1.65	15	5
3:A:411:PCW:H142	3:A:411:PCW:C20	0.91	1.94	6	14
3:A:401:PCW:H322	3:B:209:PCW:H251	0.91	1.38	4	1
3:B:204:PCW:H42	3:B:206:PCW:H52	0.91	1.39	13	2
3:B:205:PCW:H61	3:B:213:PCW:H11	0.91	1.38	18	1
3:D:625:PCW:H432	3:D:626:PCW:H432	0.90	1.41	2	4
3:B:210:PCW:H121	4:B:216:17F:H18	0.90	1.42	5	2
3:A:404:PCW:H421	3:B:209:PCW:H432	0.90	1.40	19	1
3:D:604:PCW:H181	3:D:613:PCW:H362	0.90	1.43	5	9
3:D:618:PCW:H351	3:D:627:PCW:H341	0.90	1.40	18	3
3:D:620:PCW:H132	4:D:635:17F:H18	0.90	1.42	1	7
3:D:622:PCW:H141	4:D:630:17F:C1Z	0.90	1.96	20	15
3:B:204:PCW:C33	3:B:212:PCW:H82	0.90	1.96	11	3
3:C:207:PCW:H281	3:C:208:PCW:H152	0.90	1.41	7	4
3:A:409:PCW:H331	3:C:206:PCW:H331	0.90	1.40	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:633:17F:H53	3:C:208:PCW:H242	0.90	1.42	20	1
3:D:612:PCW:H471	3:D:612:PCW:H232	0.90	1.39	1	6
3:A:411:PCW:H432	3:A:418:PCW:H241	0.90	1.42	2	6
3:D:613:PCW:H221	4:C:210:17F:H43	0.90	1.44	10	9
3:A:401:PCW:H411	3:A:404:PCW:H262	0.90	1.41	8	2
3:B:211:PCW:H51	3:B:211:PCW:C1	0.90	1.95	18	4
3:A:408:PCW:H212	3:A:417:PCW:H461	0.90	1.41	11	1
3:D:620:PCW:H11	3:D:620:PCW:H73	0.90	1.40	1	1
3:D:625:PCW:H19	3:D:625:PCW:C15	0.90	1.96	20	19
3:D:603:PCW:H451	3:D:605:PCW:H181	0.90	1.44	1	11
3:D:607:PCW:O1P	3:D:626:PCW:H221	0.90	1.67	20	13
3:B:207:PCW:H182	3:B:210:PCW:H221	0.90	1.38	16	5
1:D:462:LYS:HB3	3:D:601:PCW:H281	0.90	1.41	13	1
3:B:205:PCW:H222	3:B:212:PCW:H351	0.90	1.38	13	2
3:A:404:PCW:H232	3:D:611:PCW:H481	0.90	1.42	1	1
3:B:208:PCW:H162	4:B:214:17F:H56	0.90	1.43	11	7
4:A:414:17F:C30	3:B:212:PCW:H231	0.90	1.97	12	1
3:A:402:PCW:H371	3:A:409:PCW:H261	0.90	1.44	16	1
3:B:213:PCW:H271	4:B:215:17F:H67	0.90	1.44	18	1
3:D:607:PCW:H261	4:D:631:17F:C35	0.90	1.96	15	10
3:B:210:PCW:H432	3:B:210:PCW:C47	0.90	1.97	14	19
3:B:206:PCW:H62	3:C:207:PCW:O1P	0.90	1.67	3	1
4:D:629:17F:H71	4:D:634:17F:H29	0.90	1.41	12	3
3:B:205:PCW:H172	3:B:212:PCW:C36	0.90	1.96	19	2
3:A:403:PCW:H41	3:A:403:PCW:C3	0.90	1.95	12	11
3:A:407:PCW:C15	3:C:205:PCW:H151	0.90	1.97	1	9
3:A:413:PCW:H371	3:A:413:PCW:C3	0.90	1.96	2	7
3:A:416:PCW:H472	3:D:617:PCW:H252	0.90	1.41	10	9
3:D:606:PCW:H431	3:D:626:PCW:C47	0.90	1.96	9	7
3:D:606:PCW:C3	3:D:626:PCW:H372	0.90	1.96	19	15
3:B:209:PCW:H381	3:B:209:PCW:C23	0.90	1.96	1	2
3:D:626:PCW:C20	3:D:626:PCW:H242	0.90	1.97	14	3
3:D:607:PCW:H222	4:D:631:17F:H33	0.90	1.44	16	1
3:B:203:PCW:H39	3:B:211:PCW:H441	0.90	1.41	11	2
3:A:417:PCW:H442	3:D:612:PCW:H162	0.90	1.42	15	1
3:D:605:PCW:H161	4:D:629:17F:C11	0.90	1.97	11	10
3:B:204:PCW:H212	3:C:208:PCW:H262	0.90	1.44	2	2
3:A:402:PCW:H431	3:A:407:PCW:H231	0.90	1.44	4	2
3:B:211:PCW:H12	4:B:217:17F:H19A	0.90	1.41	4	2
3:A:404:PCW:H412	3:B:209:PCW:H361	0.90	1.43	13	2
3:D:614:PCW:H42	3:D:625:PCW:H42	0.90	1.44	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:405:PCW:H421	3:A:405:PCW:C46	0.89	1.97	4	15
3:D:604:PCW:H451	3:D:624:PCW:H441	0.89	1.44	12	10
4:A:415:17F:H71	3:B:203:PCW:H272	0.89	1.44	11	3
3:A:407:PCW:H19	3:B:208:PCW:H241	0.89	1.41	18	1
3:A:409:PCW:H162	3:A:409:PCW:H231	0.89	1.40	12	4
3:D:602:PCW:H162	3:D:624:PCW:H222	0.89	1.42	1	9
3:D:627:PCW:H52	3:D:627:PCW:O31	0.89	1.66	1	2
3:B:208:PCW:H211	4:B:214:17F:H57	0.89	1.41	14	4
3:D:618:PCW:H422	3:D:627:PCW:H282	0.89	1.39	16	2
3:B:204:PCW:C36	3:C:204:PCW:H321	0.89	1.96	20	3
3:B:210:PCW:H73	4:B:216:17F:H18	0.89	1.43	13	1
3:D:601:PCW:H221	3:D:601:PCW:H172	0.89	1.40	8	6
3:B:208:PCW:O11	3:B:208:PCW:H82	0.89	1.67	19	1
3:A:419:PCW:C36	3:D:617:PCW:H412	0.89	1.97	14	17
3:D:621:PCW:H483	4:D:634:17F:H34	0.89	1.40	3	3
3:C:203:PCW:H172	3:C:203:PCW:H462	0.89	1.45	3	1
3:A:417:PCW:H431	3:D:612:PCW:H142	0.89	1.41	15	2
3:D:604:PCW:H2	3:D:613:PCW:H62	0.89	1.43	10	1
3:B:213:PCW:H211	3:B:213:PCW:H421	0.89	1.44	17	1
3:A:403:PCW:H171	3:C:203:PCW:C12	0.89	1.97	11	8
3:C:208:PCW:H261	3:C:208:PCW:C22	0.89	1.97	2	20
3:D:607:PCW:H262	4:D:631:17F:H35	0.89	1.42	9	3
3:D:605:PCW:H51	3:D:605:PCW:O11	0.89	1.67	3	3
3:B:206:PCW:C48	3:C:212:PCW:H232	0.89	1.98	5	1
3:A:412:PCW:H172	3:A:412:PCW:H212	0.89	1.43	1	1
3:D:621:PCW:C42	4:D:634:17F:H62	0.89	1.98	12	19
3:B:213:PCW:H211	3:B:213:PCW:C16	0.89	1.96	15	3
3:B:207:PCW:H32	3:B:210:PCW:H152	0.89	1.42	8	8
3:B:208:PCW:H122	4:B:214:17F:O10	0.89	1.67	2	4
3:B:210:PCW:H73	4:B:216:17F:O2	0.89	1.67	5	2
3:B:207:PCW:C42	3:B:213:PCW:H231	0.89	1.96	19	3
3:C:207:PCW:H172	3:C:207:PCW:C21	0.89	1.96	11	1
3:D:625:PCW:H462	3:D:626:PCW:H482	0.89	1.44	10	5
3:D:616:PCW:H31	3:D:616:PCW:O4P	0.89	1.68	11	12
3:D:614:PCW:H442	3:D:619:PCW:C20	0.89	1.98	4	5
3:B:204:PCW:H321	3:C:204:PCW:H341	0.89	1.41	4	2
3:A:406:PCW:C3	3:A:406:PCW:H42	0.89	1.96	4	2
3:B:207:PCW:C42	3:B:213:PCW:H252	0.89	1.97	8	3
3:C:204:PCW:C37	4:C:211:17F:H8A	0.89	1.98	19	2
3:B:213:PCW:H412	4:B:217:17F:C32	0.89	1.97	20	1
3:D:614:PCW:H461	3:D:614:PCW:C42	0.89	1.98	10	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:615:PCW:H231	3:C:205:PCW:H251	0.89	1.41	12	2
3:B:207:PCW:H221	3:B:210:PCW:H242	0.89	1.42	9	4
3:A:420:PCW:O31	3:D:617:PCW:H51	0.89	1.67	4	1
3:D:607:PCW:H171	4:D:631:17F:H18	0.89	1.42	4	1
3:B:211:PCW:H171	4:B:217:17F:H69	0.89	1.43	6	1
3:B:207:PCW:H411	3:B:213:PCW:H231	0.89	1.42	9	2
3:A:403:PCW:H472	3:C:203:PCW:H281	0.89	1.45	20	2
4:C:210:17F:H19A	4:C:210:17F:C31	0.89	1.98	6	11
3:A:413:PCW:H471	4:C:210:17F:H10A	0.89	1.44	2	1
3:B:209:PCW:O4P	3:B:209:PCW:H31	0.89	1.68	14	2
3:C:208:PCW:H2	3:C:209:PCW:H82	0.89	1.41	4	7
3:D:618:PCW:H412	4:D:633:17F:H45	0.89	1.41	18	6
3:A:404:PCW:H282	4:A:415:17F:H65	0.89	1.45	6	1
4:D:628:17F:H40	4:D:631:17F:H78	0.89	1.42	8	2
3:A:413:PCW:H481	4:C:210:17F:H12A	0.89	1.41	13	1
3:D:603:PCW:H482	3:D:626:PCW:C28	0.89	1.98	19	17
3:D:603:PCW:C2	3:D:605:PCW:H82	0.89	1.98	18	4
3:C:204:PCW:H331	4:C:211:17F:H9	0.89	1.44	3	1
3:A:412:PCW:H482	3:B:205:PCW:H421	0.89	1.45	8	1
3:B:204:PCW:H221	3:C:208:PCW:H283	0.89	1.45	9	1
4:C:211:17F:H65	4:C:211:17F:H35	0.89	1.45	10	2
3:D:616:PCW:H432	3:C:212:PCW:C41	0.89	1.95	11	1
3:B:211:PCW:H82	3:B:212:PCW:O31	0.89	1.68	13	2
3:A:407:PCW:C14	3:C:205:PCW:H321	0.88	1.99	4	4
3:A:416:PCW:H451	3:D:617:PCW:C25	0.88	1.97	9	15
3:A:419:PCW:C1	3:D:617:PCW:H411	0.88	1.98	18	15
3:A:420:PCW:H122	4:D:632:17F:C11	0.88	1.97	2	14
3:D:614:PCW:H421	3:D:614:PCW:C46	0.88	1.97	10	20
3:B:206:PCW:H461	3:B:206:PCW:C42	0.88	1.97	17	16
3:A:406:PCW:C40	3:A:406:PCW:H142	0.88	1.98	8	1
3:D:607:PCW:O1P	3:D:626:PCW:H232	0.88	1.68	8	3
3:B:203:PCW:H252	4:C:210:17F:H78	0.88	1.42	10	1
3:B:208:PCW:H422	4:B:214:17F:H34	0.88	1.45	14	1
3:D:620:PCW:H283	4:D:635:17F:H35	0.88	1.43	15	11
3:A:403:PCW:H321	3:C:204:PCW:H62	0.88	1.44	18	7
3:A:409:PCW:H51	3:C:206:PCW:H351	0.88	1.43	17	5
3:A:406:PCW:H42	3:B:210:PCW:H341	0.88	1.45	8	1
3:B:207:PCW:H12	3:B:213:PCW:H121	0.88	1.43	11	2
3:A:420:PCW:O3	4:D:632:17F:H9	0.88	1.66	8	8
3:B:205:PCW:H212	3:B:205:PCW:C25	0.88	1.97	9	20
3:B:213:PCW:H20	3:B:213:PCW:C24	0.88	1.99	7	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:210:PCW:H51	3:B:210:PCW:O11	0.88	1.69	7	9
3:B:211:PCW:H171	4:B:217:17F:H65	0.88	1.44	12	2
3:A:413:PCW:C14	4:A:414:17F:H31	0.88	1.97	3	1
3:A:417:PCW:H361	3:D:612:PCW:H151	0.88	1.43	4	2
3:A:401:PCW:H371	3:A:401:PCW:H412	0.88	1.42	5	1
3:B:208:PCW:C18	3:C:206:PCW:H122	0.88	1.98	9	1
4:B:216:17F:H4	4:B:216:17F:N1	0.88	1.84	15	6
3:A:420:PCW:C6	4:D:632:17F:H4	0.88	1.98	11	5
3:D:607:PCW:H261	4:D:631:17F:C34	0.88	1.98	7	3
3:D:617:PCW:H283	3:C:203:PCW:H241	0.88	1.41	2	1
3:B:206:PCW:C39	3:C:212:PCW:H251	0.88	1.98	13	4
3:A:410:PCW:O1P	3:A:410:PCW:H31	0.88	1.69	19	4
3:A:407:PCW:H61	3:B:213:PCW:O2P	0.88	1.68	15	3
3:A:402:PCW:H331	3:C:206:PCW:H82	0.88	1.45	18	1
3:A:407:PCW:H62	4:B:214:17F:O8	0.88	1.69	20	1
3:D:616:PCW:H39	3:D:618:PCW:H162	0.88	1.42	11	7
3:D:618:PCW:H431	3:D:627:PCW:H282	0.88	1.43	10	11
3:D:618:PCW:H322	3:D:627:PCW:H152	0.88	1.45	19	2
3:B:207:PCW:C12	3:B:210:PCW:H341	0.88	1.97	16	1
3:D:605:PCW:H422	3:D:608:PCW:H31	0.88	1.45	20	1
3:D:607:PCW:H41	3:D:626:PCW:C22	0.88	1.99	7	12
3:D:608:PCW:O11	3:D:615:PCW:H61	0.88	1.67	5	4
3:A:406:PCW:H441	3:B:207:PCW:H262	0.88	1.46	4	2
3:B:211:PCW:H151	4:B:217:17F:C34	0.88	1.98	11	3
3:D:621:PCW:H222	4:D:633:17F:H31	0.88	1.45	20	9
3:C:204:PCW:H222	4:C:211:17F:H31	0.88	1.45	19	3
3:A:401:PCW:H252	3:D:614:PCW:C28	0.88	1.99	9	1
3:A:403:PCW:H422	3:A:403:PCW:C21	0.88	1.99	13	4
4:D:628:17F:H57	4:D:631:17F:H51	0.88	1.43	15	11
3:A:416:PCW:H19	3:A:419:PCW:H411	0.88	1.45	5	2
3:D:611:PCW:O2P	3:D:613:PCW:H61	0.88	1.67	2	5
3:B:212:PCW:H41	3:B:212:PCW:O31	0.88	1.68	2	10
3:A:407:PCW:H171	3:B:208:PCW:H231	0.88	1.43	10	2
3:A:418:PCW:H82	3:D:626:PCW:H331	0.88	1.42	14	6
3:A:407:PCW:H63	3:B:213:PCW:H321	0.88	1.46	9	5
3:B:205:PCW:H181	3:B:205:PCW:H222	0.88	1.46	11	3
3:B:210:PCW:H42	4:B:216:17F:H4A	0.88	1.46	10	1
4:A:414:17F:H54	3:B:212:PCW:H231	0.88	1.46	12	2
3:A:402:PCW:H141	3:A:409:PCW:H162	0.88	1.46	18	1
3:B:204:PCW:H231	3:C:208:PCW:H251	0.88	1.46	18	1
3:A:407:PCW:H172	3:C:205:PCW:H342	0.88	1.46	4	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:209:PCW:H231	3:B:209:PCW:C38	0.88	1.98	1	1
3:D:616:PCW:H483	3:B:204:PCW:H221	0.88	1.43	2	2
3:D:611:PCW:C6	3:D:623:PCW:H321	0.88	1.98	12	13
3:D:618:PCW:H272	3:B:206:PCW:H442	0.88	1.43	14	2
3:A:401:PCW:C36	3:B:209:PCW:H39	0.88	1.98	6	1
3:A:406:PCW:H39	3:A:406:PCW:H141	0.88	1.45	9	1
3:A:416:PCW:H451	3:D:617:PCW:H252	0.88	1.45	16	2
3:A:404:PCW:H171	3:A:404:PCW:C21	0.88	1.99	18	1
3:B:207:PCW:H39	4:B:215:17F:C6	0.87	1.98	1	1
3:C:208:PCW:H221	3:C:208:PCW:C26	0.87	1.98	2	20
3:B:208:PCW:H412	4:B:214:17F:H10	0.87	1.45	2	5
3:B:209:PCW:H232	3:B:209:PCW:H382	0.87	1.42	16	2
3:A:403:PCW:C11	3:A:403:PCW:H73	0.87	1.99	1	11
3:A:418:PCW:H431	3:D:625:PCW:H462	0.87	1.42	7	9
3:D:604:PCW:H421	3:D:619:PCW:H141	0.87	1.45	14	10
3:A:409:PCW:H171	3:A:409:PCW:C21	0.87	2.00	9	11
3:D:621:PCW:H132	4:D:634:17F:C4	0.87	1.99	7	10
3:B:210:PCW:H121	4:B:216:17F:O9	0.87	1.69	6	7
3:B:208:PCW:H412	4:B:214:17F:H12	0.87	1.46	12	3
3:B:208:PCW:H181	3:C:206:PCW:H19	0.87	1.47	16	1
3:D:622:PCW:H262	3:D:624:PCW:H261	0.87	1.46	18	1
1:A:365:LYS:HB2	1:A:366:PRO:HD3	0.87	1.45	19	20
3:D:602:PCW:H271	3:D:610:PCW:H212	0.87	1.45	19	13
3:D:603:PCW:C46	3:D:626:PCW:H282	0.87	1.98	2	8
3:A:408:PCW:H161	3:A:417:PCW:H282	0.87	1.44	3	1
3:A:401:PCW:H421	3:D:611:PCW:H271	0.87	1.46	9	3
3:D:615:PCW:H221	3:C:205:PCW:H251	0.87	1.46	18	3
3:B:208:PCW:H371	4:B:214:17F:H66	0.87	1.46	9	1
3:D:625:PCW:C15	3:D:625:PCW:H19	0.87	1.99	10	1
3:D:622:PCW:H362	4:D:629:17F:C42	0.87	1.97	1	3
3:D:625:PCW:H39	3:D:626:PCW:H141	0.87	1.45	2	6
3:D:620:PCW:H2	3:D:620:PCW:C4	0.87	1.98	11	5
3:D:622:PCW:H351	3:D:627:PCW:H20	0.87	1.46	20	13
3:D:615:PCW:H221	3:C:205:PCW:H261	0.87	1.47	7	2
3:D:622:PCW:H121	4:D:630:17F:H33	0.87	1.44	19	7
4:D:631:17F:H19A	4:D:631:17F:H9A	0.87	1.45	4	2
3:A:407:PCW:C7	4:B:216:17F:H10A	0.87	2.00	19	1
3:B:209:PCW:H222	4:B:215:17F:O10	0.87	1.68	2	2
3:D:615:PCW:C47	3:C:205:PCW:H222	0.87	1.98	2	5
3:C:207:PCW:H271	3:C:208:PCW:H222	0.87	1.44	6	2
3:A:419:PCW:H362	3:D:617:PCW:H382	0.87	1.45	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:401:PCW:H472	3:D:611:PCW:H283	0.87	1.43	12	1
3:A:416:PCW:H431	3:A:420:PCW:H40	0.87	1.45	2	2
3:D:603:PCW:H461	3:D:626:PCW:C28	0.87	1.97	2	3
3:D:622:PCW:H242	3:D:624:PCW:C24	0.87	1.97	11	14
4:A:414:17F:H53	3:C:203:PCW:H471	0.87	1.43	5	3
3:B:205:PCW:H39	4:B:214:17F:C37	0.87	1.98	4	1
3:A:418:PCW:H431	3:D:625:PCW:C46	0.87	1.99	7	13
3:A:416:PCW:H362	3:A:420:PCW:C37	0.87	2.00	11	3
3:D:607:PCW:H63	3:D:626:PCW:H242	0.87	1.45	18	8
3:B:210:PCW:H162	4:B:216:17F:H8	0.87	1.46	6	1
3:D:611:PCW:O11	3:D:619:PCW:H132	0.87	1.69	9	1
3:A:403:PCW:H122	3:A:403:PCW:H411	0.87	1.46	15	1
3:B:213:PCW:H142	4:B:217:17F:H9A	0.87	1.47	3	6
3:A:410:PCW:H351	3:C:209:PCW:C15	0.87	2.00	16	7
4:B:215:17F:O6	4:B:215:17F:H18A	0.87	1.70	5	7
3:D:601:PCW:H261	4:D:631:17F:H78	0.87	1.47	13	5
3:A:405:PCW:H461	3:A:405:PCW:C42	0.87	2.00	20	14
4:D:628:17F:H36	4:D:631:17F:H74	0.87	1.44	17	4
3:A:413:PCW:H181	3:A:413:PCW:C22	0.87	1.98	9	13
3:A:412:PCW:H483	3:B:206:PCW:H232	0.87	1.46	8	1
3:B:209:PCW:H141	4:B:215:17F:O10	0.87	1.70	18	2
3:D:613:PCW:C20	4:C:210:17F:H48	0.86	2.00	1	5
2:B:32:TYR:HB3	5:B:201:GDP:H3'	0.86	1.46	10	6
3:D:613:PCW:H471	3:D:619:PCW:H431	0.86	1.45	14	6
3:B:205:PCW:H51	3:B:208:PCW:O31	0.86	1.69	17	2
3:B:204:PCW:H362	3:C:204:PCW:H63	0.86	1.46	14	1
3:A:403:PCW:C33	3:C:204:PCW:H11	0.86	1.98	4	2
3:D:606:PCW:H471	3:B:210:PCW:H483	0.86	1.48	14	4
3:A:413:PCW:H372	4:A:414:17F:H69	0.86	1.46	7	5
3:A:407:PCW:H161	3:C:205:PCW:C17	0.86	2.00	13	2
3:B:208:PCW:H182	3:C:206:PCW:H122	0.86	1.47	9	1
3:C:203:PCW:H51	3:C:203:PCW:C35	0.86	1.97	11	1
3:A:401:PCW:H342	3:B:209:PCW:C39	0.86	1.99	16	2
3:D:601:PCW:H462	4:D:628:17F:H65	0.86	1.45	1	6
3:B:204:PCW:H211	3:B:204:PCW:C25	0.86	1.99	13	18
3:A:402:PCW:H82	3:A:409:PCW:H32	0.86	1.45	2	4
3:D:627:PCW:H42	3:D:627:PCW:O31	0.86	1.70	16	3
3:A:411:PCW:H2	4:B:215:17F:C1Y	0.86	2.00	9	4
3:B:213:PCW:H2	4:B:217:17F:O9	0.86	1.69	9	1
3:A:404:PCW:H162	4:A:415:17F:H57	0.86	1.47	11	2
3:A:402:PCW:H40	3:A:409:PCW:H272	0.86	1.45	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:211:PCW:H362	3:B:212:PCW:H11	0.86	1.45	8	8
3:A:406:PCW:O1P	3:A:406:PCW:H31	0.86	1.70	2	5
3:D:627:PCW:H381	3:D:627:PCW:C42	0.86	1.98	5	4
3:B:204:PCW:H372	3:C:204:PCW:O1P	0.86	1.71	16	5
3:A:404:PCW:C21	3:A:404:PCW:H171	0.86	2.00	9	6
3:B:204:PCW:H442	3:C:203:PCW:H351	0.86	1.45	7	1
3:B:211:PCW:C6	3:B:212:PCW:H341	0.86	1.99	20	3
3:A:413:PCW:H321	4:A:414:17F:H32	0.86	1.45	10	3
3:A:401:PCW:H52	3:A:404:PCW:C3	0.86	1.99	13	1
3:C:203:PCW:O2P	3:C:204:PCW:H61	0.86	1.69	15	1
3:A:403:PCW:H52	3:C:203:PCW:O1P	0.86	1.68	20	2
3:D:603:PCW:C48	3:D:626:PCW:H282	0.86	2.01	19	10
3:A:413:PCW:H341	4:A:414:17F:C32	0.86	2.00	12	3
3:A:416:PCW:H362	3:A:420:PCW:H371	0.86	1.46	11	6
3:B:210:PCW:H421	4:B:215:17F:H72	0.86	1.45	9	3
3:A:404:PCW:H381	3:B:209:PCW:H381	0.86	1.47	10	1
3:A:416:PCW:H141	3:A:419:PCW:H341	0.86	1.46	4	12
3:A:403:PCW:H82	3:C:203:PCW:O1P	0.86	1.69	7	2
4:D:634:17F:H74	3:C:206:PCW:H222	0.86	1.48	14	2
3:A:406:PCW:H452	3:B:207:PCW:H251	0.86	1.48	3	1
3:D:606:PCW:O2	3:D:626:PCW:H371	0.86	1.68	5	2
3:A:420:PCW:H61	4:D:632:17F:C4	0.86	1.97	11	4
3:D:611:PCW:H222	3:D:619:PCW:C48	0.86	2.01	6	2
3:A:419:PCW:O2	3:D:617:PCW:H411	0.86	1.70	17	12
3:A:420:PCW:H62	4:D:632:17F:O8	0.86	1.71	1	5
3:B:208:PCW:H372	3:B:208:PCW:C42	0.86	2.00	20	9
3:B:212:PCW:H432	3:B:212:PCW:C47	0.86	2.01	15	20
3:A:405:PCW:H472	3:A:405:PCW:C43	0.86	1.99	11	5
3:A:407:PCW:H52	4:B:216:17F:O8	0.86	1.71	4	1
3:A:410:PCW:C23	3:C:207:PCW:H231	0.86	2.01	20	3
3:B:211:PCW:H12	4:B:217:17F:C1Y	0.86	2.01	6	1
3:D:616:PCW:H451	3:B:206:PCW:C47	0.86	2.01	7	3
3:A:408:PCW:H412	3:C:207:PCW:H422	0.86	1.46	12	1
4:B:217:17F:O6	4:B:217:17F:H18A	0.86	1.71	18	9
3:D:621:PCW:H151	4:D:634:17F:C4	0.86	2.00	2	2
3:A:418:PCW:H63	3:D:626:PCW:H2	0.86	1.47	4	3
3:A:410:PCW:H351	3:C:209:PCW:H162	0.86	1.47	13	5
3:A:406:PCW:H283	4:B:216:17F:H19A	0.86	1.48	6	1
3:B:211:PCW:C1	4:B:217:17F:H19A	0.86	2.00	6	1
3:B:205:PCW:H242	3:B:206:PCW:H372	0.86	1.45	9	1
3:A:401:PCW:H322	3:B:209:PCW:H231	0.86	1.46	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:601:PCW:H362	4:B:216:17F:H67	0.86	1.47	17	3
3:D:625:PCW:H451	3:D:626:PCW:H482	0.86	1.46	12	7
3:A:404:PCW:H231	3:A:404:PCW:C27	0.86	2.01	18	3
3:D:616:PCW:O2P	3:D:616:PCW:H31	0.86	1.67	6	5
3:A:412:PCW:H421	3:C:206:PCW:H39	0.86	1.46	7	1
3:A:402:PCW:H431	3:A:407:PCW:H251	0.85	1.44	1	3
3:D:602:PCW:H52	3:D:602:PCW:O31	0.85	1.69	1	1
3:D:607:PCW:H212	4:D:631:17F:C1X	0.85	2.01	6	11
3:B:208:PCW:H442	4:B:214:17F:H33	0.85	1.48	19	5
3:D:602:PCW:H472	3:D:602:PCW:H231	0.85	1.46	8	7
3:D:604:PCW:C40	3:D:619:PCW:H121	0.85	2.01	6	3
3:B:205:PCW:H231	3:B:212:PCW:H412	0.85	1.46	6	1
3:A:407:PCW:H52	4:B:216:17F:H10A	0.85	1.45	8	4
3:A:411:PCW:H271	3:A:418:PCW:H271	0.85	1.48	14	9
3:B:208:PCW:H421	4:B:214:17F:H32	0.85	1.48	8	1
3:B:206:PCW:C39	4:C:211:17F:H49	0.85	2.01	12	1
3:A:401:PCW:H39	3:A:404:PCW:H231	0.85	1.45	19	2
3:A:403:PCW:H332	3:C:204:PCW:C1	0.85	1.99	4	4
2:C:32:TYR:HB3	5:C:201:GDP:H3'	0.85	1.46	8	8
3:D:614:PCW:H442	3:D:619:PCW:H20	0.85	1.46	4	4
3:A:410:PCW:C35	3:C:209:PCW:H162	0.85	2.00	12	8
3:D:607:PCW:H20	4:D:631:17F:H46	0.85	1.47	18	4
3:B:213:PCW:H432	3:B:213:PCW:H212	0.85	1.47	12	3
3:A:413:PCW:H252	4:A:414:17F:H61	0.85	1.46	12	1
3:B:204:PCW:H272	3:C:207:PCW:H262	0.85	1.46	13	1
3:A:413:PCW:H432	3:A:413:PCW:C47	0.85	2.01	1	20
3:A:413:PCW:C16	4:A:414:17F:H31	0.85	2.01	2	2
3:B:211:PCW:H12	4:B:217:17F:C19	0.85	2.00	4	2
3:A:418:PCW:H52	3:D:626:PCW:O31	0.85	1.71	17	5
4:C:211:17F:H65	4:C:211:17F:C12	0.85	1.98	5	3
3:D:611:PCW:H62	3:D:623:PCW:H321	0.85	1.47	13	2
3:D:615:PCW:H451	4:B:216:17F:H54	0.85	1.47	15	1
3:D:616:PCW:H39	3:D:618:PCW:H141	0.85	1.46	19	1
3:D:622:PCW:H162	3:C:212:PCW:H152	0.85	1.46	1	15
3:B:212:PCW:H472	3:B:212:PCW:C43	0.85	2.01	18	19
3:B:207:PCW:C18	3:B:210:PCW:H221	0.85	2.00	16	5
3:D:612:PCW:H62	3:D:627:PCW:O11	0.85	1.71	20	3
3:B:203:PCW:H431	3:B:211:PCW:H221	0.85	1.44	7	7
3:D:614:PCW:H452	3:D:619:PCW:H222	0.85	1.45	17	2
3:A:412:PCW:H451	3:C:208:PCW:H19	0.85	1.48	11	1
3:A:416:PCW:H162	3:D:617:PCW:H142	0.85	1.44	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:408:PCW:H342	3:C:207:PCW:H442	0.85	1.46	17	1
3:B:208:PCW:H281	4:B:216:17F:H46	0.85	1.46	17	1
3:B:206:PCW:H421	3:B:206:PCW:C46	0.85	2.00	1	16
3:B:207:PCW:H131	3:B:210:PCW:H151	0.85	1.48	3	3
3:A:403:PCW:H472	3:C:203:PCW:C28	0.85	2.01	20	4
4:A:415:17F:H75	3:B:203:PCW:H281	0.85	1.48	11	2
3:D:602:PCW:H261	3:D:610:PCW:H141	0.85	1.45	1	5
3:D:607:PCW:O1P	3:D:626:PCW:H241	0.85	1.72	5	7
3:A:413:PCW:H121	3:A:413:PCW:H352	0.85	1.46	18	7
4:D:635:17F:H52	3:C:205:PCW:H161	0.85	1.45	11	1
3:C:207:PCW:H281	3:C:209:PCW:H39	0.85	1.46	12	1
3:A:410:PCW:C17	3:C:207:PCW:H232	0.85	2.02	20	2
3:D:620:PCW:O1P	3:D:621:PCW:H63	0.85	1.72	16	1
3:A:406:PCW:H341	3:A:411:PCW:H321	0.85	1.46	20	7
3:D:604:PCW:H442	3:D:619:PCW:H483	0.85	1.49	14	3
3:D:617:PCW:H232	3:D:617:PCW:C27	0.85	2.02	18	20
3:B:211:PCW:H342	3:B:212:PCW:H11	0.85	1.48	1	1
3:C:203:PCW:C17	3:C:203:PCW:H462	0.85	2.01	1	1
3:A:416:PCW:H19	3:A:419:PCW:H431	0.85	1.45	9	7
3:A:419:PCW:H31	3:D:617:PCW:H421	0.85	1.47	5	9
3:D:627:PCW:H281	4:D:633:17F:H51	0.85	1.49	4	7
3:A:409:PCW:H162	3:A:409:PCW:C23	0.85	2.02	12	3
3:A:420:PCW:H122	4:D:632:17F:H11	0.85	1.48	2	9
3:D:605:PCW:H142	3:D:605:PCW:C18	0.85	2.02	20	19
3:D:607:PCW:H232	4:D:628:17F:H10A	0.85	1.48	16	4
4:A:414:17F:H46	3:B:212:PCW:C19	0.85	2.00	4	1
3:D:627:PCW:H241	3:C:212:PCW:H451	0.85	1.48	17	8
3:B:203:PCW:H242	4:C:210:17F:H20A	0.85	1.46	6	2
3:D:622:PCW:H341	3:C:212:PCW:C44	0.85	2.01	19	5
3:B:211:PCW:H63	3:B:212:PCW:H341	0.85	1.48	20	2
3:B:208:PCW:O3	4:B:214:17F:H4	0.85	1.72	11	2
4:D:634:17F:H65	4:D:635:17F:H70	0.85	1.49	7	3
3:D:603:PCW:H381	4:D:629:17F:H40	0.85	1.48	20	4
3:B:211:PCW:H472	3:B:211:PCW:C14	0.85	2.02	2	1
3:D:603:PCW:H322	3:D:605:PCW:H122	0.85	1.45	19	6
3:D:621:PCW:H142	3:D:621:PCW:C18	0.85	2.01	11	20
3:D:621:PCW:H262	3:D:622:PCW:H61	0.85	1.48	12	4
3:A:404:PCW:H431	4:B:215:17F:C9	0.85	2.02	9	2
3:A:410:PCW:H20	3:D:627:PCW:H481	0.85	1.47	10	1
3:B:204:PCW:H251	3:B:204:PCW:C21	0.84	2.01	3	19
3:B:207:PCW:H63	4:B:216:17F:H2	0.84	1.46	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:616:PCW:H31	3:D:616:PCW:P	0.84	2.12	9	13
3:D:622:PCW:H283	3:D:624:PCW:H282	0.84	1.48	11	7
3:A:410:PCW:O11	3:C:207:PCW:H152	0.84	1.72	7	1
3:B:204:PCW:H182	3:B:205:PCW:C48	0.84	2.01	16	5
3:B:207:PCW:H141	3:B:210:PCW:C32	0.84	2.00	13	2
3:A:407:PCW:H171	3:B:208:PCW:H20	0.84	1.49	10	1
3:D:617:PCW:H372	3:D:617:PCW:H411	0.84	1.49	11	1
3:A:404:PCW:H62	3:B:203:PCW:C13	0.84	2.02	2	1
3:D:603:PCW:H432	3:D:605:PCW:H181	0.84	1.45	2	2
3:A:411:PCW:H412	3:A:418:PCW:H282	0.84	1.46	4	3
3:A:403:PCW:C31	3:A:403:PCW:H351	0.84	2.03	6	18
3:D:601:PCW:H483	4:D:631:17F:H47	0.84	1.47	1	3
3:A:413:PCW:H221	3:A:413:PCW:C18	0.84	2.00	5	12
3:B:208:PCW:H171	3:C:205:PCW:C32	0.84	2.02	4	1
3:B:208:PCW:C19	3:C:205:PCW:H331	0.84	2.02	6	6
3:B:211:PCW:H152	4:B:217:17F:H58	0.84	1.46	5	2
3:A:401:PCW:H221	3:A:401:PCW:C18	0.84	2.02	10	6
3:D:618:PCW:C35	3:D:627:PCW:H341	0.84	2.01	1	5
3:B:211:PCW:H412	3:B:211:PCW:C37	0.84	2.01	2	5
3:C:204:PCW:H471	4:C:211:17F:H60	0.84	1.48	10	2
3:D:609:PCW:H12	4:D:633:17F:H6	0.84	1.48	6	2
3:C:203:PCW:H171	3:C:203:PCW:H221	0.84	1.45	7	1
3:A:404:PCW:H432	4:B:215:17F:H19A	0.84	1.49	8	1
3:D:611:PCW:H221	3:D:611:PCW:H432	0.84	1.46	11	1
3:B:206:PCW:H171	3:C:212:PCW:C28	0.84	2.02	12	1
3:A:413:PCW:H142	4:A:414:17F:H66	0.84	1.47	18	3
3:A:416:PCW:H451	3:D:617:PCW:C24	0.84	2.02	1	16
3:A:420:PCW:O3P	3:D:617:PCW:H42	0.84	1.71	5	4
3:D:605:PCW:H182	3:D:605:PCW:C14	0.84	2.02	20	20
3:D:611:PCW:H51	3:D:623:PCW:H342	0.84	1.49	1	5
3:A:409:PCW:C22	3:A:409:PCW:H171	0.84	2.02	2	2
3:D:602:PCW:H242	3:D:610:PCW:H352	0.84	1.49	15	12
3:D:623:PCW:H2	3:D:624:PCW:H322	0.84	1.47	10	3
4:B:214:17F:H69	4:B:214:17F:C33	0.84	2.03	4	2
3:B:209:PCW:H181	3:B:209:PCW:H342	0.84	1.47	6	1
3:B:205:PCW:H281	3:B:211:PCW:H431	0.84	1.47	8	1
3:A:403:PCW:H141	3:A:403:PCW:C18	0.84	2.02	15	1
3:A:410:PCW:C8	3:C:209:PCW:H32	0.84	2.02	19	1
3:B:205:PCW:H242	3:B:206:PCW:H352	0.84	1.50	19	1
3:D:609:PCW:H241	3:D:609:PCW:C20	0.84	2.02	7	20
3:D:616:PCW:H342	3:C:212:PCW:H341	0.84	1.48	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:628:17F:H57	4:D:628:17F:C19	0.84	2.03	15	20
3:B:206:PCW:C48	3:C:212:PCW:H211	0.84	2.02	13	2
3:A:401:PCW:H442	3:D:614:PCW:H262	0.84	1.50	8	1
4:C:211:17F:H69	4:C:211:17F:H11	0.84	1.47	8	1
3:C:207:PCW:O4P	4:C:211:17F:H1A	0.84	1.72	14	1
4:B:214:17F:H51	4:B:217:17F:H74	0.84	1.48	19	1
3:D:624:PCW:H472	4:C:210:17F:H55	0.84	1.49	1	3
3:B:208:PCW:H182	3:C:205:PCW:C32	0.84	2.02	1	3
3:D:607:PCW:C4	3:D:626:PCW:H222	0.84	2.01	7	7
3:C:204:PCW:H131	4:C:211:17F:H72	0.84	1.49	3	1
3:A:407:PCW:H211	3:A:407:PCW:C25	0.84	2.03	15	3
3:A:403:PCW:H52	3:A:403:PCW:O11	0.84	1.73	5	3
3:A:409:PCW:H321	3:C:206:PCW:C37	0.84	2.01	5	2
3:A:406:PCW:H282	4:B:216:17F:H19A	0.84	1.46	7	1
3:B:207:PCW:H421	3:B:213:PCW:C24	0.84	2.02	12	4
3:A:404:PCW:H422	4:B:215:17F:H42	0.84	1.50	19	1
3:D:608:PCW:H51	4:D:635:17F:O2	0.84	1.72	1	1
3:B:212:PCW:H421	3:C:212:PCW:H262	0.84	1.48	1	1
3:A:403:PCW:H132	3:C:203:PCW:C1	0.84	2.02	2	1
3:D:618:PCW:H381	3:D:627:PCW:H181	0.84	1.49	9	9
3:A:409:PCW:H82	3:C:206:PCW:H321	0.84	1.48	19	2
3:C:207:PCW:C5	4:C:211:17F:H1A	0.84	2.02	12	4
3:C:204:PCW:H142	4:C:211:17F:H63	0.84	1.47	11	1
3:D:605:PCW:H63	3:D:605:PCW:O11	0.84	1.72	12	15
3:B:210:PCW:H262	3:B:210:PCW:C22	0.84	2.02	8	19
3:B:203:PCW:C5	3:B:211:PCW:H331	0.84	2.03	16	3
3:A:405:PCW:H162	3:A:405:PCW:H462	0.84	1.50	9	3
3:A:401:PCW:H482	3:D:611:PCW:H251	0.84	1.49	6	1
3:B:204:PCW:H122	4:C:211:17F:O1	0.84	1.72	6	2
3:B:208:PCW:C16	4:B:214:17F:H56	0.84	2.03	11	9
3:D:605:PCW:C34	3:D:605:PCW:H132	0.84	2.03	15	7
3:D:606:PCW:C43	3:D:626:PCW:H472	0.84	2.03	9	6
3:B:210:PCW:H462	3:B:213:PCW:H452	0.84	1.48	12	1
3:D:604:PCW:H39	3:D:611:PCW:C34	0.83	2.02	11	13
3:D:610:PCW:H151	3:D:616:PCW:O11	0.83	1.73	1	6
3:D:620:PCW:H461	3:C:205:PCW:H481	0.83	1.50	2	1
3:C:204:PCW:H471	4:C:211:17F:H32	0.83	1.46	12	1
3:D:611:PCW:H39	3:D:623:PCW:C46	0.83	1.98	12	7
3:B:205:PCW:C45	3:B:206:PCW:H232	0.83	2.01	3	3
3:D:613:PCW:H31	3:D:619:PCW:H2	0.83	1.50	9	14
3:D:615:PCW:H483	3:B:208:PCW:H271	0.83	1.46	2	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:204:PCW:H283	4:C:211:17F:H32	0.83	1.49	5	1
3:B:203:PCW:H332	4:B:215:17F:H37	0.83	1.50	20	3
3:A:401:PCW:C32	3:B:209:PCW:H382	0.83	2.03	9	3
4:A:414:17F:H1	4:A:414:17F:H4	0.83	1.47	2	3
3:B:210:PCW:H222	3:B:210:PCW:C26	0.83	2.03	12	18
3:B:213:PCW:C42	4:B:217:17F:H12	0.83	2.02	13	7
3:B:208:PCW:H211	4:B:214:17F:C33	0.83	2.03	10	2
3:D:618:PCW:H342	3:D:627:PCW:H341	0.83	1.49	9	1
3:C:204:PCW:H371	4:C:211:17F:C8	0.83	2.03	19	2
3:A:417:PCW:H422	3:D:612:PCW:H212	0.83	1.48	10	1
3:C:204:PCW:H331	4:C:211:17F:H8	0.83	1.48	11	1
3:A:402:PCW:H482	3:A:409:PCW:H283	0.83	1.50	20	1
3:D:601:PCW:H172	3:D:601:PCW:C21	0.83	2.01	12	11
3:D:615:PCW:H63	4:D:635:17F:H2	0.83	1.49	8	5
3:B:210:PCW:H32	3:B:210:PCW:P	0.83	2.13	5	18
3:C:204:PCW:H51	3:C:204:PCW:C2	0.83	2.03	5	1
3:B:207:PCW:H441	3:B:213:PCW:H272	0.83	1.47	8	1
3:A:404:PCW:H421	3:B:209:PCW:C19	0.83	2.02	3	1
3:D:621:PCW:H19	4:D:633:17F:O10	0.83	1.74	13	5
3:B:205:PCW:H461	3:B:206:PCW:C15	0.83	2.01	4	2
3:B:211:PCW:H222	3:B:211:PCW:C17	0.83	2.02	4	1
3:A:408:PCW:H272	3:A:417:PCW:H241	0.83	1.49	8	5
3:D:625:PCW:H19	3:D:625:PCW:H151	0.83	1.49	10	1
3:B:205:PCW:H12	3:B:211:PCW:H62	0.83	1.48	10	3
3:A:405:PCW:H151	3:A:405:PCW:H483	0.83	1.49	11	1
3:A:407:PCW:C48	4:D:635:17F:H46	0.83	2.02	15	1
3:B:205:PCW:H451	3:C:208:PCW:C19	0.83	2.04	10	8
4:B:214:17F:H69	4:B:214:17F:C34	0.83	2.03	12	2
3:C:204:PCW:H272	4:C:211:17F:H60	0.83	1.50	8	2
3:A:417:PCW:H441	3:D:612:PCW:C27	0.83	2.03	10	2
3:C:204:PCW:H442	4:C:211:17F:C1Z	0.83	2.03	15	1
3:C:206:PCW:H241	3:C:206:PCW:C18	0.83	2.04	16	1
3:D:617:PCW:H272	3:D:617:PCW:C23	0.83	2.03	8	20
3:C:203:PCW:H442	3:C:203:PCW:H161	0.83	1.51	1	4
3:A:406:PCW:H452	3:B:207:PCW:C25	0.83	2.03	3	2
3:D:622:PCW:H372	3:D:627:PCW:H211	0.83	1.46	4	2
3:A:406:PCW:H332	3:A:411:PCW:H341	0.83	1.48	8	1
3:A:406:PCW:H62	3:A:411:PCW:H11	0.83	1.51	9	1
3:A:418:PCW:H12	3:D:614:PCW:H41	0.83	1.51	17	1
3:D:613:PCW:H472	3:D:619:PCW:H231	0.83	1.50	17	4
3:A:401:PCW:H462	3:D:614:PCW:H242	0.83	1.48	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:413:PCW:H141	4:A:414:17F:C37	0.83	2.04	12	2
3:A:407:PCW:H241	3:A:407:PCW:C28	0.83	2.04	15	3
3:D:602:PCW:H162	3:D:624:PCW:C22	0.83	2.02	10	13
3:D:602:PCW:H281	3:D:610:PCW:H232	0.83	1.51	1	4
3:B:210:PCW:H241	3:B:210:PCW:C20	0.83	2.04	1	1
3:A:407:PCW:H19	3:B:208:PCW:H242	0.83	1.47	2	3
3:A:404:PCW:H411	3:B:209:PCW:H171	0.83	1.48	3	1
3:D:618:PCW:P	3:D:627:PCW:H63	0.83	2.14	16	3
3:D:621:PCW:H421	4:D:634:17F:C35	0.83	2.00	12	12
3:B:210:PCW:H422	3:B:210:PCW:H382	0.83	1.48	4	2
3:A:413:PCW:H372	4:A:414:17F:C38	0.83	2.03	7	3
3:B:204:PCW:H132	3:B:206:PCW:C1	0.83	2.04	20	5
3:A:408:PCW:H231	3:A:417:PCW:H262	0.83	1.51	10	4
3:A:405:PCW:H371	3:D:601:PCW:C15	0.83	2.03	3	3
3:B:208:PCW:C16	4:B:214:17F:H60	0.83	2.03	15	2
3:A:401:PCW:C32	3:B:209:PCW:H251	0.83	2.03	4	2
3:A:402:PCW:H181	3:A:409:PCW:H211	0.83	1.49	14	4
3:A:406:PCW:H231	3:B:207:PCW:C15	0.83	2.02	13	4
3:B:213:PCW:H422	4:B:214:17F:H51	0.83	1.49	6	1
3:B:209:PCW:H442	4:B:215:17F:H50	0.83	1.50	9	1
3:A:404:PCW:H82	4:A:415:17F:C3	0.83	2.04	12	2
3:A:407:PCW:H161	3:C:205:PCW:H151	0.83	1.50	13	1
3:A:420:PCW:H19	4:D:632:17F:H57	0.82	1.46	4	8
3:A:417:PCW:C8	3:D:617:PCW:H40	0.82	2.04	5	5
3:D:607:PCW:C17	4:D:631:17F:H18	0.82	2.04	4	1
3:C:204:PCW:H462	4:C:211:17F:H57	0.82	1.48	4	1
3:A:416:PCW:C19	3:A:419:PCW:H411	0.82	2.04	5	2
3:A:404:PCW:C27	4:A:415:17F:H69	0.82	2.03	8	2
3:A:413:PCW:H141	4:A:414:17F:H66	0.82	1.51	12	2
3:D:607:PCW:H42	3:D:626:PCW:C24	0.82	2.03	15	2
3:A:407:PCW:C17	3:C:205:PCW:H341	0.82	2.04	19	1
3:D:611:PCW:H20	3:D:611:PCW:H432	0.82	1.50	6	8
3:A:419:PCW:H422	3:D:616:PCW:H232	0.82	1.48	8	5
3:B:204:PCW:H131	3:C:207:PCW:H11	0.82	1.49	3	3
3:D:604:PCW:O1P	3:D:613:PCW:H62	0.82	1.73	3	1
3:D:614:PCW:H62	3:D:625:PCW:O1P	0.82	1.73	14	2
3:B:208:PCW:H152	3:C:205:PCW:C7	0.82	2.04	12	1
3:A:407:PCW:C16	3:C:205:PCW:H171	0.82	2.04	13	1
3:B:210:PCW:H431	3:B:210:PCW:H271	0.82	1.50	16	1
3:B:205:PCW:H452	3:B:206:PCW:C23	0.82	2.04	3	4
3:D:623:PCW:H421	3:D:625:PCW:C26	0.82	2.04	18	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:211:PCW:C7	3:B:212:PCW:H332	0.82	2.03	4	1
3:A:401:PCW:H40	3:D:611:PCW:H281	0.82	1.52	5	1
3:A:404:PCW:H472	3:B:209:PCW:H442	0.82	1.49	7	2
3:A:407:PCW:H63	3:B:213:PCW:O2	0.82	1.74	12	1
3:A:413:PCW:H182	3:A:413:PCW:C14	0.82	2.02	3	5
3:A:401:PCW:H73	3:B:209:PCW:H12	0.82	1.51	6	1
3:A:404:PCW:H82	4:A:415:17F:H2	0.82	1.51	6	3
3:B:205:PCW:C15	3:B:212:PCW:H362	0.82	2.04	9	1
3:A:408:PCW:H361	3:C:204:PCW:C21	0.82	2.04	10	1
3:A:406:PCW:H242	3:B:210:PCW:H121	0.82	1.50	12	1
3:A:409:PCW:H62	3:A:412:PCW:O1P	0.82	1.74	20	1
3:B:211:PCW:H32	4:B:217:17F:H31	0.82	1.48	8	7
3:A:410:PCW:H82	3:C:209:PCW:O11	0.82	1.74	11	2
3:C:203:PCW:O2P	3:C:204:PCW:H41	0.82	1.75	2	2
3:C:204:PCW:H471	4:C:211:17F:H33	0.82	1.52	2	2
3:A:404:PCW:C43	4:B:215:17F:H9A	0.82	2.04	3	2
3:A:404:PCW:H411	3:B:209:PCW:H352	0.82	1.52	7	2
3:A:410:PCW:H242	3:C:207:PCW:H222	0.82	1.48	14	3
3:B:208:PCW:H19	4:B:214:17F:H57	0.82	1.50	15	4
3:A:406:PCW:H231	3:B:207:PCW:C17	0.82	2.05	20	3
3:D:611:PCW:C22	3:D:619:PCW:H461	0.82	2.03	9	3
3:D:615:PCW:H211	4:D:635:17F:H41	0.82	1.52	15	3
3:B:207:PCW:H132	3:B:210:PCW:H151	0.82	1.51	16	1
3:D:610:PCW:O11	3:D:616:PCW:H62	0.82	1.74	16	3
3:A:413:PCW:H142	3:A:413:PCW:C18	0.82	2.04	3	1
3:D:611:PCW:H222	3:D:619:PCW:H482	0.82	1.50	19	4
3:A:402:PCW:H52	3:A:402:PCW:O11	0.82	1.74	7	2
3:D:621:PCW:O1P	3:D:621:PCW:H31	0.82	1.73	13	1
3:D:606:PCW:H431	3:D:626:PCW:H481	0.82	1.50	2	2
3:B:207:PCW:H181	3:B:210:PCW:H221	0.82	1.49	8	5
3:A:401:PCW:C25	3:D:614:PCW:H281	0.82	2.01	9	2
3:B:208:PCW:H63	3:B:208:PCW:H322	0.82	1.52	5	1
3:A:408:PCW:C34	3:C:207:PCW:H442	0.82	2.03	17	1
3:D:622:PCW:C34	3:C:212:PCW:H422	0.82	2.05	1	4
3:D:626:PCW:H271	3:D:626:PCW:C23	0.82	2.02	17	17
3:A:411:PCW:H39	4:B:215:17F:H65	0.82	1.49	8	2
3:A:402:PCW:H352	3:A:402:PCW:O31	0.82	1.75	12	13
3:B:203:PCW:C38	3:B:211:PCW:H441	0.82	2.05	3	4
3:B:206:PCW:H422	4:C:211:17F:C27	0.82	2.04	18	4
4:B:215:17F:H4A	4:B:215:17F:C18	0.82	2.01	9	2
3:A:401:PCW:C40	3:D:611:PCW:H281	0.82	2.05	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:406:PCW:H142	3:A:406:PCW:H40	0.82	1.49	8	1
3:D:618:PCW:H341	4:D:633:17F:H36	0.82	1.47	8	3
3:D:609:PCW:H62	4:D:633:17F:O6	0.82	1.74	10	1
4:D:628:17F:H58	4:D:631:17F:H51	0.82	1.50	14	6
3:A:410:PCW:H151	3:C:209:PCW:H372	0.82	1.48	2	2
3:B:211:PCW:H231	4:B:217:17F:H73	0.82	1.50	4	2
3:A:413:PCW:H141	4:A:414:17F:H62	0.82	1.51	15	6
3:B:207:PCW:H152	3:B:210:PCW:H371	0.82	1.47	17	2
3:A:406:PCW:C42	3:B:210:PCW:H39	0.82	2.05	10	2
3:B:208:PCW:C28	4:B:214:17F:H31	0.82	2.05	19	1
3:A:402:PCW:H442	3:A:407:PCW:H231	0.82	1.52	1	2
4:D:628:17F:H19A	4:D:628:17F:C31	0.82	2.04	5	20
3:B:204:PCW:H31	3:B:204:PCW:P	0.82	2.15	2	2
3:B:205:PCW:H442	3:B:206:PCW:H181	0.82	1.52	5	5
3:D:601:PCW:C46	4:D:628:17F:H66	0.82	2.04	4	1
4:D:630:17F:H18A	4:D:630:17F:C9	0.82	1.99	16	2
3:A:409:PCW:H122	3:C:206:PCW:H332	0.81	1.52	1	2
3:A:411:PCW:C19	3:A:411:PCW:C14	0.81	2.57	6	19
4:A:414:17F:H2	4:A:414:17F:O1	0.81	1.75	1	16
3:D:603:PCW:C25	4:B:217:17F:H76	0.81	2.05	2	3
3:D:616:PCW:H31	3:D:616:PCW:O2P	0.81	1.74	9	4
3:B:204:PCW:H31	3:B:204:PCW:O1P	0.81	1.73	2	2
3:A:413:PCW:H471	4:C:210:17F:H36	0.81	1.51	3	1
3:D:617:PCW:H431	3:D:617:PCW:C47	0.81	2.04	8	3
3:A:406:PCW:C6	3:A:411:PCW:H11	0.81	2.04	11	2
3:B:205:PCW:H452	3:B:206:PCW:C21	0.81	2.04	9	2
3:B:205:PCW:O2	3:B:208:PCW:H321	0.81	1.75	12	1
3:B:204:PCW:H171	3:B:205:PCW:H481	0.81	1.51	13	1
3:B:208:PCW:H142	4:B:214:17F:H56	0.81	1.52	18	2
3:C:207:PCW:H41	3:C:207:PCW:H322	0.81	1.51	5	2
3:C:203:PCW:H222	3:C:203:PCW:C26	0.81	2.05	11	2
3:A:404:PCW:H52	3:A:404:PCW:O31	0.81	1.75	18	2
3:A:406:PCW:H272	3:B:207:PCW:H19	0.81	1.51	6	5
3:A:413:PCW:H472	3:A:413:PCW:C43	0.81	2.05	1	20
3:A:419:PCW:H362	3:D:617:PCW:C38	0.81	2.05	15	6
3:B:204:PCW:H321	3:C:204:PCW:H361	0.81	1.49	12	3
3:B:211:PCW:H342	3:B:212:PCW:C1	0.81	2.05	1	2
3:A:411:PCW:H272	3:A:411:PCW:C47	0.81	2.02	18	5
3:A:418:PCW:H40	3:D:625:PCW:C46	0.81	2.04	2	2
3:D:608:PCW:H73	3:D:620:PCW:O11	0.81	1.74	4	11
3:C:203:PCW:H421	3:C:203:PCW:H161	0.81	1.50	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:406:PCW:C23	3:B:207:PCW:H151	0.81	2.04	6	3
3:B:211:PCW:H181	3:B:211:PCW:H221	0.81	1.52	18	3
1:A:360:LEU:HD22	3:A:401:PCW:H211	0.81	1.52	13	1
4:B:214:17F:H43	4:B:217:17F:H66	0.81	1.50	13	1
3:B:210:PCW:C44	3:B:213:PCW:H262	0.81	2.03	16	2
3:A:419:PCW:H481	3:D:618:PCW:H283	0.81	1.52	15	1
3:D:605:PCW:C16	4:D:629:17F:H11A	0.81	2.05	16	12
3:D:615:PCW:H211	4:D:635:17F:H38	0.81	1.52	20	9
3:D:616:PCW:O2P	3:C:212:PCW:H51	0.81	1.75	8	4
3:D:621:PCW:H362	4:D:633:17F:H59	0.81	1.51	6	9
3:D:603:PCW:H451	3:D:605:PCW:H141	0.81	1.52	2	2
3:A:413:PCW:H122	4:A:414:17F:H66	0.81	1.52	9	5
3:D:623:PCW:C38	3:D:625:PCW:H182	0.81	2.04	14	8
3:D:607:PCW:H262	4:D:631:17F:H30	0.81	1.51	14	1
3:A:401:PCW:H462	3:D:614:PCW:H262	0.81	1.53	6	1
3:A:410:PCW:H241	4:D:633:17F:H54	0.81	1.50	8	2
3:D:616:PCW:C43	3:C:212:PCW:H412	0.81	1.98	11	1
3:C:207:PCW:C27	3:C:209:PCW:H39	0.81	2.06	13	3
3:D:605:PCW:H172	3:D:605:PCW:C21	0.81	2.05	6	20
3:B:205:PCW:H252	3:B:205:PCW:C21	0.81	2.04	7	19
3:A:403:PCW:H61	4:A:414:17F:O4	0.81	1.76	2	2
3:D:606:PCW:H411	3:D:626:PCW:H472	0.81	1.50	4	5
3:D:610:PCW:C48	3:B:212:PCW:H241	0.81	2.05	3	1
3:B:211:PCW:H162	4:B:217:17F:H65	0.81	1.50	6	1
3:D:601:PCW:H461	3:D:607:PCW:H472	0.81	1.50	10	4
3:A:409:PCW:H32	3:C:206:PCW:H41	0.81	1.49	16	1
3:A:404:PCW:H252	4:A:415:17F:H77	0.81	1.52	1	1
3:A:416:PCW:C45	3:D:617:PCW:H242	0.81	2.05	15	8
3:D:616:PCW:C19	3:D:617:PCW:H461	0.81	2.06	15	6
3:B:207:PCW:H152	3:B:210:PCW:H362	0.81	1.52	20	1
3:D:602:PCW:H261	3:D:610:PCW:C14	0.81	2.06	8	17
3:D:616:PCW:C37	3:D:618:PCW:H142	0.81	2.05	18	5
3:A:419:PCW:H382	3:D:610:PCW:H161	0.81	1.53	8	10
3:D:602:PCW:H462	3:D:610:PCW:H432	0.81	1.51	9	8
3:D:606:PCW:H431	3:D:625:PCW:H471	0.81	1.49	18	6
3:D:625:PCW:H51	3:D:625:PCW:O11	0.81	1.74	14	5
3:D:627:PCW:O31	3:D:627:PCW:H62	0.81	1.76	3	1
3:B:203:PCW:H362	3:B:211:PCW:H162	0.81	1.49	3	2
3:A:402:PCW:H40	3:A:409:PCW:H282	0.81	1.50	13	4
3:A:403:PCW:H342	3:C:203:PCW:H32	0.81	1.51	7	1
3:D:622:PCW:H361	3:C:212:PCW:H462	0.81	1.51	15	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:211:PCW:H151	4:B:217:17F:H61	0.81	1.53	16	4
3:B:206:PCW:H321	3:C:204:PCW:C39	0.81	2.06	18	3
3:D:613:PCW:H221	4:C:210:17F:H51	0.81	1.50	2	1
3:A:411:PCW:H181	3:A:411:PCW:C22	0.81	2.00	8	1
3:A:411:PCW:C2	4:B:215:17F:H33	0.81	2.05	8	1
3:A:402:PCW:H442	3:C:205:PCW:H132	0.81	1.53	19	1
3:D:616:PCW:H271	3:D:618:PCW:H283	0.81	1.51	2	1
4:D:630:17F:H65	4:D:630:17F:H36	0.81	1.51	18	10
3:B:207:PCW:H41	4:B:216:17F:HN1A	0.81	1.34	8	2
3:A:417:PCW:H422	3:D:612:PCW:H251	0.81	1.51	20	5
3:A:401:PCW:H461	3:D:611:PCW:H232	0.81	1.53	11	1
3:B:213:PCW:H352	4:B:214:17F:H9A	0.81	1.53	11	1
3:A:407:PCW:C16	3:C:205:PCW:H151	0.81	2.05	13	1
3:A:401:PCW:H181	3:A:401:PCW:C22	0.80	1.99	10	7
3:B:204:PCW:O31	3:B:212:PCW:H82	0.80	1.76	19	3
3:B:211:PCW:H342	3:B:212:PCW:P	0.80	2.16	10	6
3:C:208:PCW:C23	3:C:209:PCW:H431	0.80	2.06	17	9
3:A:418:PCW:H381	3:D:625:PCW:H262	0.80	1.53	17	3
3:B:203:PCW:C21	4:C:210:17F:H19	0.80	2.06	18	3
3:B:208:PCW:H63	3:B:208:PCW:C32	0.80	2.05	5	1
3:A:406:PCW:H412	3:B:210:PCW:C39	0.80	2.06	9	1
3:C:203:PCW:H261	3:C:203:PCW:C22	0.80	2.05	11	1
3:D:624:PCW:H451	4:C:210:17F:C42	0.80	2.06	13	2
3:A:404:PCW:H222	4:A:415:17F:H58	0.80	1.52	15	2
3:B:213:PCW:H12	4:B:217:17F:O1	0.80	1.74	20	3
3:A:402:PCW:H352	3:A:402:PCW:C31	0.80	2.07	18	20
3:D:608:PCW:H281	4:B:216:17F:H54	0.80	1.51	1	2
3:D:624:PCW:H241	3:D:624:PCW:C20	0.80	2.04	13	20
4:D:628:17F:C32	4:D:631:17F:H51	0.80	2.05	18	7
3:D:625:PCW:H41	3:D:625:PCW:O31	0.80	1.77	20	8
3:D:621:PCW:C22	4:D:633:17F:H31	0.80	2.06	20	15
3:A:402:PCW:C42	3:C:205:PCW:H132	0.80	2.06	13	3
3:D:610:PCW:H462	3:B:212:PCW:C26	0.80	2.07	17	4
3:B:203:PCW:C33	4:B:215:17F:H35	0.80	2.02	9	3
4:B:215:17F:H41	4:B:215:17F:H12	0.80	1.52	19	4
4:A:414:17F:H45	3:C:203:PCW:C41	0.80	2.02	11	1
3:A:420:PCW:C44	3:D:617:PCW:H211	0.80	2.07	11	2
3:B:211:PCW:C24	4:B:217:17F:H73	0.80	2.06	11	3
3:D:615:PCW:H483	3:B:208:PCW:H252	0.80	1.53	12	2
4:B:215:17F:H47	4:B:217:17F:H41	0.80	1.53	16	1
3:D:620:PCW:C13	4:D:635:17F:H18	0.80	2.05	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:207:PCW:H432	4:B:217:17F:H37	0.80	1.50	1	1
3:B:210:PCW:C45	3:B:213:PCW:H272	0.80	2.06	2	1
3:A:404:PCW:H472	4:B:215:17F:H48	0.80	1.53	5	1
3:A:413:PCW:H141	3:A:413:PCW:C18	0.80	2.05	7	4
3:C:203:PCW:C31	3:C:203:PCW:H351	0.80	2.06	17	6
5:C:201:GDP:O2A	5:C:201:GDP:H3'	0.80	1.76	13	1
3:B:205:PCW:H282	3:B:211:PCW:H471	0.80	1.52	16	2
3:D:609:PCW:H63	4:D:633:17F:C6	0.80	2.06	1	8
3:A:410:PCW:C12	3:C:209:PCW:H352	0.80	2.05	2	4
3:D:621:PCW:H231	3:D:622:PCW:H82	0.80	1.52	10	5
3:B:204:PCW:H20	3:B:205:PCW:H481	0.80	1.53	4	1
3:D:611:PCW:H221	3:D:619:PCW:C48	0.80	2.07	5	1
3:A:406:PCW:H322	3:A:411:PCW:H322	0.80	1.53	8	1
3:B:203:PCW:H242	4:C:210:17F:H18	0.80	1.51	13	2
3:D:612:PCW:H172	3:D:612:PCW:C21	0.80	2.06	17	18
3:A:418:PCW:H63	3:D:626:PCW:C31	0.80	2.07	10	11
4:D:629:17F:H10	4:D:634:17F:H48	0.80	1.53	3	5
3:B:212:PCW:C48	3:C:212:PCW:H271	0.80	2.07	4	1
3:B:205:PCW:C40	4:B:214:17F:H70	0.80	2.05	5	3
3:C:208:PCW:H52	3:C:208:PCW:H321	0.80	1.51	16	7
3:A:418:PCW:H482	4:B:217:17F:H54	0.80	1.52	12	1
3:B:208:PCW:H431	4:B:214:17F:H12	0.80	1.51	4	1
3:B:205:PCW:C44	3:B:206:PCW:H161	0.80	2.07	12	4
3:A:412:PCW:H481	3:D:622:PCW:H481	0.80	1.54	8	1
3:A:412:PCW:C45	3:C:208:PCW:H182	0.80	2.03	14	2
3:B:211:PCW:H242	4:B:217:17F:H73	0.80	1.54	11	2
3:A:407:PCW:C18	3:C:205:PCW:H151	0.80	2.07	16	4
3:A:409:PCW:C31	3:C:206:PCW:H331	0.80	2.06	20	1
3:A:403:PCW:H31	3:A:403:PCW:P	0.80	2.16	7	18
3:D:611:PCW:H31	3:D:619:PCW:O11	0.80	1.76	4	13
3:D:621:PCW:H371	4:D:633:17F:C35	0.80	2.06	19	14
3:D:603:PCW:O31	3:D:605:PCW:H82	0.80	1.77	2	10
3:A:404:PCW:H412	3:B:209:PCW:H341	0.80	1.51	6	3
4:D:629:17F:C38	4:D:634:17F:H29	0.80	2.06	13	9
3:D:618:PCW:O1P	3:D:627:PCW:H63	0.80	1.76	3	8
3:B:205:PCW:H40	4:B:214:17F:C38	0.80	2.07	1	1
4:D:632:17F:H5	4:D:632:17F:O8	0.80	1.77	16	8
3:A:401:PCW:H12	3:B:209:PCW:H362	0.80	1.53	12	2
3:B:209:PCW:H412	3:B:209:PCW:H20	0.80	1.50	5	1
3:A:402:PCW:H62	3:A:402:PCW:C33	0.80	2.07	15	1
3:B:204:PCW:H242	3:C:204:PCW:H422	0.80	1.54	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:605:PCW:H132	3:D:605:PCW:C34	0.80	2.07	16	13
3:D:622:PCW:H141	4:D:630:17F:C1Y	0.80	2.06	4	13
4:D:630:17F:H62	4:D:634:17F:C2X	0.80	2.07	3	6
3:A:401:PCW:H62	3:B:209:PCW:O31	0.80	1.76	15	11
3:B:204:PCW:H362	3:C:204:PCW:C32	0.80	2.07	20	4
3:B:208:PCW:H322	3:B:208:PCW:C6	0.80	2.07	5	2
3:A:406:PCW:H131	3:B:210:PCW:C33	0.80	2.06	20	1
3:B:210:PCW:H472	3:B:210:PCW:C43	0.80	2.06	1	20
3:A:404:PCW:H431	4:B:215:17F:H10	0.80	1.54	4	1
3:D:621:PCW:H141	4:D:634:17F:C6	0.80	2.05	11	12
3:C:208:PCW:H182	3:C:208:PCW:H441	0.80	1.54	8	1
3:A:410:PCW:H272	3:D:618:PCW:H452	0.80	1.52	10	1
3:B:204:PCW:H451	3:C:203:PCW:H421	0.80	1.51	12	1
3:A:413:PCW:H351	3:A:413:PCW:O3	0.79	1.76	18	18
3:D:620:PCW:O1P	3:D:621:PCW:H73	0.79	1.76	3	7
4:D:629:17F:H51	4:D:630:17F:H78	0.79	1.52	1	5
3:D:622:PCW:H421	3:B:206:PCW:C27	0.79	2.07	13	4
3:D:622:PCW:H162	3:C:212:PCW:H172	0.79	1.55	15	8
3:A:408:PCW:C16	3:A:417:PCW:H282	0.79	2.07	3	1
3:D:605:PCW:H132	3:D:605:PCW:H341	0.79	1.51	15	7
3:B:205:PCW:C39	4:B:214:17F:H63	0.79	2.07	3	1
3:A:410:PCW:H482	3:C:209:PCW:H232	0.79	1.54	13	3
3:A:407:PCW:H152	3:B:208:PCW:H231	0.79	1.53	7	1
3:A:419:PCW:H461	3:D:616:PCW:H251	0.79	1.54	18	2
3:A:408:PCW:H341	3:C:207:PCW:H422	0.79	1.50	17	1
3:D:607:PCW:C43	4:D:628:17F:H34	0.79	2.01	5	10
4:D:635:17F:C29	3:C:205:PCW:H181	0.79	2.05	1	2
3:A:407:PCW:H251	3:A:407:PCW:C21	0.79	2.06	19	3
3:C:204:PCW:H242	3:C:207:PCW:H482	0.79	1.52	8	1
3:A:406:PCW:H61	3:A:411:PCW:O31	0.79	1.78	11	3
3:D:625:PCW:H351	3:D:625:PCW:O2	0.79	1.78	10	2
3:A:419:PCW:H461	3:D:616:PCW:H272	0.79	1.53	17	1
3:D:604:PCW:O2P	3:D:624:PCW:H82	0.79	1.76	2	10
3:D:607:PCW:C20	4:D:631:17F:H46	0.79	2.08	18	9
3:B:205:PCW:H251	3:B:211:PCW:H471	0.79	1.54	10	3
3:B:207:PCW:H452	4:B:217:17F:H38	0.79	1.54	5	3
3:D:604:PCW:H231	3:D:613:PCW:C39	0.79	2.06	7	14
3:B:207:PCW:H411	4:B:217:17F:H10A	0.79	1.52	14	2
3:B:203:PCW:C39	3:B:211:PCW:H441	0.79	2.07	11	4
3:D:623:PCW:H122	3:D:624:PCW:H331	0.79	1.53	4	4
3:B:213:PCW:C11	4:B:217:17F:H6	0.79	2.08	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:404:PCW:H211	4:A:415:17F:H57	0.79	1.53	7	4
3:D:623:PCW:O31	3:D:624:PCW:H322	0.79	1.77	15	5
3:A:407:PCW:C17	3:B:208:PCW:H20	0.79	2.07	10	1
3:A:403:PCW:H31	3:A:403:PCW:O1P	0.79	1.77	16	11
3:A:419:PCW:C35	3:D:617:PCW:H412	0.79	2.08	9	11
3:D:622:PCW:H121	4:D:630:17F:H32	0.79	1.54	1	1
3:B:213:PCW:H421	3:B:213:PCW:H181	0.79	1.55	1	1
3:D:605:PCW:H252	4:D:629:17F:H41	0.79	1.53	13	10
3:D:604:PCW:C31	3:D:613:PCW:H62	0.79	2.08	15	5
3:B:209:PCW:H232	3:B:209:PCW:H432	0.79	1.54	4	2
3:A:410:PCW:C24	3:C:207:PCW:H231	0.79	2.07	20	5
3:D:627:PCW:H241	3:C:212:PCW:H431	0.79	1.53	6	2
3:A:404:PCW:C41	3:B:209:PCW:H352	0.79	2.07	7	1
3:D:610:PCW:H483	3:B:212:PCW:H242	0.79	1.54	19	3
3:B:210:PCW:H442	3:B:213:PCW:H262	0.79	1.53	14	1
3:A:418:PCW:H381	3:D:625:PCW:H251	0.79	1.52	1	9
2:B:78:PHE:HB2	2:B:111:MET:HG2	0.79	1.55	18	10
3:D:613:PCW:H261	4:C:210:17F:H71	0.79	1.54	17	2
3:A:413:PCW:H181	4:A:414:17F:H34	0.79	1.54	7	1
3:C:203:PCW:H262	3:C:203:PCW:C22	0.79	2.06	12	1
3:B:208:PCW:H281	4:B:214:17F:H31	0.79	1.54	19	1
3:D:605:PCW:H252	4:D:629:17F:C22	0.79	2.07	8	9
3:B:205:PCW:O11	3:B:212:PCW:H361	0.79	1.77	2	2
3:B:208:PCW:C18	3:C:205:PCW:H331	0.79	2.07	13	4
3:A:420:PCW:C16	4:D:632:17F:H57	0.79	2.07	6	6
3:A:406:PCW:H42	3:A:406:PCW:H31	0.79	1.53	4	4
3:A:417:PCW:H361	3:D:612:PCW:H131	0.79	1.55	6	3
3:A:410:PCW:C5	3:C:209:PCW:H11	0.79	2.08	16	1
3:A:404:PCW:C3	3:B:209:PCW:H411	0.79	2.08	1	1
3:D:611:PCW:H63	3:D:623:PCW:C32	0.79	2.08	19	13
3:B:213:PCW:H241	3:B:213:PCW:C20	0.79	2.06	7	20
3:A:413:PCW:H341	4:A:414:17F:H34	0.79	1.53	2	2
3:B:208:PCW:C44	4:B:214:17F:H33	0.79	2.08	5	6
3:B:212:PCW:H51	3:B:212:PCW:O11	0.79	1.76	2	2
3:C:203:PCW:H352	3:C:203:PCW:C5	0.79	2.03	11	1
4:A:414:17F:O8	3:C:203:PCW:H352	0.79	1.78	13	1
3:B:206:PCW:C36	3:C:204:PCW:H40	0.79	2.08	13	1
3:D:605:PCW:H52	3:D:626:PCW:H19	0.79	1.53	20	2
3:A:413:PCW:H321	4:A:414:17F:C1Z	0.79	2.08	1	2
3:B:207:PCW:C41	3:B:213:PCW:H222	0.79	2.07	2	2
3:C:208:PCW:H352	3:C:208:PCW:C31	0.79	2.08	1	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:611:PCW:H41	3:D:623:PCW:C34	0.79	2.07	7	6
3:A:406:PCW:H261	3:B:210:PCW:H122	0.79	1.52	8	1
3:B:208:PCW:C42	4:B:214:17F:H32	0.79	2.08	8	1
3:D:609:PCW:H283	4:D:633:17F:H68	0.79	1.55	9	6
3:A:410:PCW:H242	3:C:207:PCW:C22	0.79	2.06	14	3
3:A:418:PCW:H322	3:D:625:PCW:H342	0.79	1.55	4	5
3:B:204:PCW:H132	3:B:206:PCW:H41	0.79	1.53	19	4
3:A:406:PCW:C32	3:A:411:PCW:H322	0.79	2.08	8	1
3:A:408:PCW:C36	3:C:204:PCW:H211	0.79	2.07	10	1
3:A:410:PCW:H171	3:C:207:PCW:C23	0.79	2.08	20	3
3:A:407:PCW:H12	4:B:216:17F:C12	0.79	2.07	15	1
3:B:205:PCW:O11	3:B:205:PCW:H2	0.79	1.77	9	15
3:D:615:PCW:H272	4:D:635:17F:C24	0.79	2.08	3	1
3:A:408:PCW:H362	3:C:207:PCW:H461	0.79	1.55	5	1
3:D:601:PCW:H481	3:D:607:PCW:C23	0.79	2.08	11	4
3:A:402:PCW:H422	3:A:409:PCW:H132	0.79	1.52	12	1
3:D:627:PCW:H283	3:C:208:PCW:H272	0.79	1.55	13	1
3:B:213:PCW:H222	4:B:217:17F:H12A	0.79	1.52	13	1
3:A:402:PCW:C33	3:C:206:PCW:H82	0.79	2.06	18	1
3:A:407:PCW:H142	3:C:205:PCW:H131	0.78	1.55	1	7
3:D:602:PCW:H412	3:D:602:PCW:C37	0.78	2.08	5	19
4:B:215:17F:H41	4:B:215:17F:H12A	0.78	1.54	9	8
4:A:414:17F:H49	3:B:212:PCW:H222	0.78	1.53	16	2
3:B:211:PCW:H262	4:B:217:17F:H51	0.78	1.54	3	1
3:C:204:PCW:H142	4:C:211:17F:C7	0.78	2.07	4	1
3:D:620:PCW:O2P	3:D:621:PCW:H73	0.78	1.78	5	3
3:A:404:PCW:H431	4:B:215:17F:H10A	0.78	1.55	7	3
3:D:616:PCW:C1	3:C:212:PCW:H342	0.78	2.08	17	2
3:D:620:PCW:P	3:D:621:PCW:H52	0.78	2.17	15	3
3:D:603:PCW:H461	3:D:626:PCW:C26	0.78	2.06	11	1
3:D:622:PCW:C33	3:C:212:PCW:H422	0.78	2.08	20	6
3:D:617:PCW:H471	3:D:617:PCW:C43	0.78	2.06	11	3
3:C:208:PCW:C23	3:C:209:PCW:H40	0.78	2.09	3	3
3:A:410:PCW:H181	3:C:209:PCW:C26	0.78	2.08	16	3
3:B:208:PCW:H483	3:B:208:PCW:H283	0.78	1.53	6	1
3:B:213:PCW:C41	4:B:217:17F:H59	0.78	2.08	7	2
3:C:205:PCW:H232	3:C:205:PCW:C27	0.78	2.05	7	1
3:B:210:PCW:C45	3:B:213:PCW:H262	0.78	2.07	8	3
3:A:413:PCW:H422	4:A:414:17F:H68	0.78	1.55	14	2
3:A:417:PCW:C35	3:D:612:PCW:H132	0.78	2.09	5	7
3:A:417:PCW:C39	3:D:612:PCW:H451	0.78	2.08	18	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:616:PCW:H432	3:D:627:PCW:H232	0.78	1.53	1	3
3:C:204:PCW:O3	4:C:211:17F:H75	0.78	1.79	1	1
3:D:616:PCW:H31	3:D:616:PCW:C4	0.78	2.08	17	3
3:B:213:PCW:H73	4:B:214:17F:H2	0.78	1.56	4	3
3:D:615:PCW:H51	4:D:635:17F:C3	0.78	2.07	7	5
3:B:207:PCW:H152	3:B:210:PCW:H321	0.78	1.53	4	1
3:C:208:PCW:H52	3:C:208:PCW:C32	0.78	2.07	16	3
3:B:211:PCW:H132	4:B:217:17F:H58	0.78	1.54	10	1
3:A:416:PCW:H162	3:D:617:PCW:C14	0.78	2.06	11	1
3:B:212:PCW:H421	3:C:212:PCW:H271	0.78	1.56	11	1
3:A:403:PCW:H422	3:A:403:PCW:H211	0.78	1.53	13	1
4:D:630:17F:H55	3:B:206:PCW:H19	0.78	1.55	13	1
3:A:409:PCW:C5	3:C:206:PCW:H321	0.78	2.01	20	7
3:B:210:PCW:C44	3:B:213:PCW:H283	0.78	2.09	6	3
3:C:208:PCW:O2P	3:C:209:PCW:H51	0.78	1.79	4	10
3:A:403:PCW:H472	3:C:203:PCW:H283	0.78	1.56	4	2
3:B:206:PCW:H361	3:C:204:PCW:H40	0.78	1.56	13	1
3:A:402:PCW:H162	3:A:409:PCW:H182	0.78	1.56	18	1
3:A:401:PCW:C6	3:B:209:PCW:H131	0.78	2.06	19	1
3:A:413:PCW:C16	4:A:414:17F:H56	0.78	2.07	1	2
3:D:615:PCW:H51	4:D:635:17F:O4	0.78	1.77	4	10
4:D:629:17F:H69	4:D:634:17F:H8A	0.78	1.55	5	3
3:A:407:PCW:H82	4:B:216:17F:C10	0.78	2.08	2	1
3:D:604:PCW:C17	3:D:613:PCW:H132	0.78	2.08	18	4
3:A:410:PCW:H261	4:D:633:17F:H55	0.78	1.55	10	2
3:D:618:PCW:H261	3:C:204:PCW:H462	0.78	1.55	11	4
3:A:407:PCW:C17	3:C:205:PCW:H362	0.78	2.08	18	2
3:A:403:PCW:H171	3:C:203:PCW:C11	0.78	2.07	13	5
3:A:411:PCW:H371	3:A:411:PCW:C33	0.78	2.07	8	1
3:D:602:PCW:O11	3:D:603:PCW:H61	0.78	1.79	8	6
3:B:203:PCW:H321	4:B:215:17F:H35	0.78	1.56	13	2
3:A:413:PCW:O2	3:A:413:PCW:H351	0.78	1.78	19	1
1:D:471:ARG:HA	1:D:475:GLU:HG3	0.78	1.55	20	10
3:D:607:PCW:C26	4:D:631:17F:H62	0.78	2.08	20	5
4:B:215:17F:H12A	4:B:215:17F:H41	0.78	1.54	10	3
3:A:405:PCW:H39	4:D:628:17F:H52	0.78	1.52	7	2
3:A:402:PCW:H42	3:C:206:PCW:O2P	0.78	1.79	9	1
3:C:204:PCW:H142	4:C:211:17F:H11A	0.78	1.55	10	1
3:C:204:PCW:H19	4:C:211:17F:H19A	0.78	1.55	18	2
3:C:204:PCW:H122	4:C:211:17F:H6A	0.78	1.52	20	1
4:D:634:17F:H65	4:D:635:17F:C39	0.78	2.09	6	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:407:PCW:H82	4:B:216:17F:H10	0.78	1.53	2	2
3:D:604:PCW:H412	3:D:619:PCW:H121	0.78	1.56	8	4
4:D:629:17F:H29	4:D:630:17F:H8	0.78	1.55	20	2
3:A:407:PCW:H441	3:D:601:PCW:C34	0.78	2.07	12	1
3:D:608:PCW:H241	3:D:615:PCW:H381	0.78	1.55	1	8
3:B:209:PCW:H342	3:B:209:PCW:H182	0.78	1.56	8	6
3:D:618:PCW:C42	3:D:627:PCW:H231	0.78	2.08	5	6
3:B:208:PCW:H171	3:C:206:PCW:H122	0.78	1.52	2	2
3:A:406:PCW:H212	3:B:210:PCW:O31	0.78	1.79	13	4
3:A:419:PCW:H432	3:D:610:PCW:C21	0.78	2.08	17	10
3:A:411:PCW:H412	3:A:418:PCW:C28	0.78	2.08	4	1
3:A:411:PCW:C27	3:A:418:PCW:H271	0.78	2.09	7	6
3:A:417:PCW:C44	3:D:612:PCW:H162	0.78	2.08	15	2
3:A:417:PCW:O31	3:A:417:PCW:H62	0.78	1.78	8	1
3:B:204:PCW:H441	3:B:212:PCW:H19	0.78	1.53	13	1
3:B:205:PCW:C19	3:B:212:PCW:H331	0.78	2.08	13	2
3:B:205:PCW:H132	3:B:205:PCW:C17	0.78	2.09	8	18
3:A:401:PCW:H342	3:B:209:PCW:H472	0.78	1.54	2	1
3:A:407:PCW:H171	3:B:208:PCW:C22	0.78	2.06	2	4
3:A:413:PCW:H483	4:C:210:17F:H65	0.78	1.56	17	2
3:A:419:PCW:H382	3:D:610:PCW:C16	0.78	2.08	13	10
3:D:611:PCW:C16	3:D:619:PCW:H171	0.78	2.03	15	8
3:D:615:PCW:H212	3:C:205:PCW:H282	0.78	1.55	4	1
3:C:207:PCW:H241	3:C:209:PCW:C39	0.78	2.09	14	4
1:A:301:LEU:HD13	1:D:473:LYS:HG3	0.78	1.56	8	2
3:B:211:PCW:H132	4:B:217:17F:C32	0.78	2.09	10	1
3:D:604:PCW:H332	3:D:624:PCW:C8	0.78	2.08	15	8
3:B:203:PCW:C4	3:B:211:PCW:H331	0.78	2.09	7	5
3:A:413:PCW:H122	4:A:414:17F:C37	0.78	2.09	9	6
3:D:611:PCW:H172	3:D:611:PCW:C35	0.78	2.06	11	5
3:C:205:PCW:H372	3:C:206:PCW:H121	0.78	1.54	8	1
3:D:607:PCW:H63	3:D:626:PCW:H222	0.78	1.54	9	3
3:A:406:PCW:H31	3:A:406:PCW:O1P	0.78	1.76	19	6
3:A:404:PCW:C31	3:A:404:PCW:H52	0.77	2.09	1	3
3:A:406:PCW:C34	3:A:411:PCW:H321	0.77	2.09	1	1
3:D:617:PCW:H12	3:D:617:PCW:O31	0.77	1.78	8	16
3:D:620:PCW:H412	3:D:620:PCW:C37	0.77	2.06	10	17
3:D:623:PCW:C38	3:D:625:PCW:H171	0.77	2.08	2	3
3:A:407:PCW:H171	3:C:205:PCW:H362	0.77	1.54	18	2
3:A:406:PCW:H232	3:B:207:PCW:H151	0.77	1.53	5	1
3:D:601:PCW:H332	4:B:216:17F:H61	0.77	1.56	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:624:PCW:C48	4:C:210:17F:H55	0.77	2.08	20	1
3:D:604:PCW:H482	3:D:619:PCW:H471	0.77	1.56	15	4
3:D:622:PCW:H231	3:D:624:PCW:H242	0.77	1.56	1	1
3:D:602:PCW:H261	3:D:610:PCW:H142	0.77	1.52	11	13
3:A:419:PCW:C43	3:D:610:PCW:H211	0.77	2.05	19	7
3:C:204:PCW:C45	4:C:211:17F:H60	0.77	2.05	5	1
3:D:604:PCW:H482	3:D:619:PCW:H441	0.77	1.55	6	1
3:A:401:PCW:H12	3:B:209:PCW:H211	0.77	1.54	7	1
3:A:401:PCW:H411	3:A:404:PCW:C26	0.77	2.09	8	1
3:A:411:PCW:H472	3:A:411:PCW:C27	0.77	2.03	18	2
3:B:213:PCW:H442	4:B:217:17F:H41	0.77	1.56	12	1
3:A:406:PCW:C24	3:B:207:PCW:H151	0.77	2.10	16	1
3:D:622:PCW:H321	3:D:627:PCW:H20	0.77	1.53	11	6
4:A:414:17F:H52	3:C:203:PCW:C47	0.77	2.09	3	1
3:A:404:PCW:H272	3:A:404:PCW:C23	0.77	2.06	15	3
3:C:204:PCW:H241	3:C:207:PCW:H472	0.77	1.55	5	1
3:A:402:PCW:H39	3:A:409:PCW:H261	0.77	1.54	15	2
3:A:413:PCW:H122	4:A:414:17F:C38	0.77	2.08	18	4
3:B:203:PCW:H11	3:B:211:PCW:H352	0.77	1.57	18	1
3:B:210:PCW:H241	3:B:210:PCW:H20	0.77	1.56	1	1
4:B:217:17F:H77	4:B:217:17F:H48	0.77	1.56	10	4
3:D:621:PCW:H141	4:D:634:17F:O8	0.77	1.80	6	6
3:B:209:PCW:H342	3:B:209:PCW:C18	0.77	2.08	6	2
3:A:409:PCW:H372	3:A:409:PCW:C41	0.77	2.10	8	2
3:D:611:PCW:H222	3:D:619:PCW:C46	0.77	2.07	9	2
3:C:208:PCW:H39	3:C:209:PCW:C7	0.77	2.09	19	2
3:D:616:PCW:H421	3:D:627:PCW:H221	0.77	1.56	15	1
3:A:401:PCW:H483	3:D:614:PCW:H471	0.77	1.56	18	1
3:D:602:PCW:C22	3:D:610:PCW:H351	0.77	2.01	10	10
3:C:204:PCW:H122	4:C:211:17F:H10	0.77	1.55	3	1
4:A:414:17F:H41	3:B:204:PCW:H462	0.77	1.54	7	1
3:B:203:PCW:H411	3:B:211:PCW:C18	0.77	2.10	7	3
3:A:406:PCW:H39	3:A:406:PCW:H142	0.77	1.56	9	1
3:C:207:PCW:C21	3:C:207:PCW:C17	0.77	2.62	11	1
3:B:206:PCW:H361	3:C:204:PCW:C40	0.77	2.09	13	1
3:C:204:PCW:C47	4:C:211:17F:H57	0.77	2.02	18	2
3:A:404:PCW:H411	3:B:209:PCW:H19	0.77	1.53	17	1
3:D:624:PCW:H471	4:C:210:17F:H55	0.77	1.54	19	2
3:D:604:PCW:C31	3:D:613:PCW:H82	0.77	2.10	8	7
3:A:413:PCW:H452	4:C:210:17F:H12A	0.77	1.56	2	4
3:A:420:PCW:H322	3:D:617:PCW:H52	0.77	1.53	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:627:PCW:C28	4:D:633:17F:H51	0.77	2.10	7	15
3:C:207:PCW:H322	3:C:207:PCW:C4	0.77	2.10	5	7
3:D:601:PCW:C26	4:D:631:17F:H76	0.77	2.03	3	2
3:C:208:PCW:H321	3:C:208:PCW:C7	0.77	2.09	3	2
3:A:404:PCW:H172	3:A:404:PCW:C21	0.77	1.99	4	1
3:C:205:PCW:H271	3:C:205:PCW:C23	0.77	2.07	7	1
3:B:209:PCW:H19	4:B:215:17F:H19	0.77	1.55	8	1
3:B:203:PCW:C32	4:B:215:17F:H35	0.77	2.10	13	2
3:A:410:PCW:H31	3:A:410:PCW:P	0.77	2.20	11	12
3:C:203:PCW:O31	3:C:203:PCW:C35	0.77	2.33	1	13
4:A:415:17F:H76	4:C:210:17F:H56	0.77	1.54	5	2
3:B:213:PCW:H171	3:B:213:PCW:H381	0.77	1.57	7	4
3:C:207:PCW:C32	3:C:207:PCW:H42	0.77	2.09	14	2
3:A:409:PCW:H41	3:A:409:PCW:O31	0.77	1.80	1	1
3:A:409:PCW:C8	3:C:206:PCW:H11	0.77	2.09	1	1
3:B:203:PCW:H62	3:B:211:PCW:O31	0.77	1.79	6	2
3:C:208:PCW:H142	3:C:208:PCW:H422	0.77	1.57	1	1
3:A:409:PCW:H51	3:A:409:PCW:O31	0.77	1.78	19	5
3:A:420:PCW:H63	3:A:420:PCW:O11	0.77	1.78	5	6
3:A:407:PCW:H282	3:A:407:PCW:C24	0.77	2.06	15	3
3:B:208:PCW:H412	4:B:214:17F:H11A	0.77	1.54	15	4
4:B:216:17F:H4	4:B:216:17F:C2	0.77	2.10	15	2
3:A:417:PCW:H361	3:D:612:PCW:C13	0.77	2.10	6	3
3:A:417:PCW:H381	3:D:612:PCW:H131	0.77	1.55	15	2
3:A:412:PCW:H431	3:C:208:PCW:H381	0.77	1.55	18	1
3:A:404:PCW:H51	4:A:415:17F:C3	0.77	2.10	19	1
3:A:408:PCW:H361	3:C:207:PCW:H462	0.77	1.56	20	1
3:D:609:PCW:C11	4:D:633:17F:H18	0.77	2.09	1	15
3:D:613:PCW:H221	4:C:210:17F:H47	0.77	1.56	7	5
3:C:208:PCW:H232	3:C:209:PCW:H422	0.77	1.55	1	1
3:C:208:PCW:H351	3:C:208:PCW:H121	0.77	1.55	2	3
4:A:415:17F:H72	3:B:203:PCW:H252	0.77	1.54	3	1
3:D:613:PCW:H251	4:C:210:17F:C27	0.77	2.10	9	9
3:D:616:PCW:C34	3:C:212:PCW:H362	0.77	2.10	9	4
1:A:308:ARG:HG3	1:D:469:LEU:HD11	0.77	1.57	18	3
4:D:635:17F:H53	3:C:205:PCW:H141	0.77	1.52	12	2
3:D:601:PCW:H462	4:D:628:17F:C36	0.77	2.10	1	2
3:A:413:PCW:C47	4:C:210:17F:H10A	0.77	2.10	2	1
3:A:416:PCW:H283	3:A:419:PCW:H252	0.77	1.55	5	1
3:C:203:PCW:H121	3:C:203:PCW:C38	0.77	2.04	16	2
3:B:205:PCW:H52	3:B:211:PCW:O2P	0.77	1.79	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:214:17F:C29	4:B:217:17F:H74	0.77	2.10	19	1
3:D:603:PCW:H372	3:D:603:PCW:H422	0.76	1.57	12	17
3:A:412:PCW:H371	3:C:206:PCW:C40	0.76	2.10	14	4
3:D:603:PCW:H381	4:D:629:17F:C2X	0.76	2.10	10	6
4:B:215:17F:H30	4:B:217:17F:H29	0.76	1.57	2	1
3:D:604:PCW:H451	3:D:624:PCW:C44	0.76	2.10	19	7
3:B:205:PCW:H262	4:C:211:17F:H51	0.76	1.55	4	1
4:B:215:17F:H18A	4:B:215:17F:C4	0.76	1.93	9	1
3:A:405:PCW:H371	3:D:601:PCW:H171	0.76	1.55	18	2
3:A:401:PCW:H482	3:D:611:PCW:H162	0.76	1.55	1	1
3:B:204:PCW:H12	3:B:204:PCW:O31	0.76	1.78	9	12
3:B:210:PCW:H431	3:B:210:PCW:C47	0.76	2.09	1	1
3:D:602:PCW:H82	3:D:602:PCW:O31	0.76	1.80	2	5
3:A:401:PCW:H73	3:B:209:PCW:O31	0.76	1.80	17	4
3:D:614:PCW:H63	3:D:625:PCW:O1P	0.76	1.80	16	9
3:B:209:PCW:H212	3:B:209:PCW:H341	0.76	1.57	4	1
3:C:208:PCW:C32	3:C:208:PCW:H52	0.76	2.10	18	6
3:D:612:PCW:C17	3:D:612:PCW:H212	0.76	2.06	17	2
3:A:401:PCW:C48	3:D:611:PCW:H251	0.76	2.10	6	1
3:A:404:PCW:H39	3:B:209:PCW:H62	0.76	1.56	6	1
3:B:212:PCW:C40	3:C:212:PCW:H262	0.76	2.10	18	1
3:D:611:PCW:H41	3:D:623:PCW:H332	0.76	1.56	19	1
3:D:608:PCW:H431	3:C:205:PCW:C24	0.76	2.10	2	6
4:A:414:17F:H45	3:B:204:PCW:H483	0.76	1.57	7	3
3:B:207:PCW:H182	3:B:210:PCW:C22	0.76	2.09	16	2
3:A:406:PCW:H40	3:D:606:PCW:H261	0.76	1.57	11	1
3:A:407:PCW:H42	4:B:214:17F:O1	0.76	1.80	9	9
3:A:420:PCW:C12	4:D:632:17F:H9	0.76	2.11	13	15
3:D:603:PCW:C11	3:D:603:PCW:C31	0.76	2.63	12	5
3:D:608:PCW:H122	3:D:615:PCW:C7	0.76	2.11	5	9
3:A:417:PCW:H442	3:D:612:PCW:H271	0.76	1.57	11	4
3:B:205:PCW:C46	3:B:206:PCW:H152	0.76	2.03	4	2
3:B:207:PCW:H442	3:B:213:PCW:H272	0.76	1.57	4	1
3:B:212:PCW:H482	3:C:212:PCW:H271	0.76	1.58	4	2
3:B:203:PCW:H332	4:B:215:17F:C2X	0.76	2.01	9	2
3:D:616:PCW:P	3:C:212:PCW:H51	0.76	2.21	8	1
3:B:205:PCW:H451	3:B:206:PCW:H232	0.76	1.55	12	1
3:A:417:PCW:H332	3:D:612:PCW:C13	0.76	2.09	14	3
3:B:208:PCW:H31	3:B:208:PCW:C4	0.76	2.11	19	1
3:A:419:PCW:H362	3:D:617:PCW:H381	0.76	1.57	8	3
3:D:603:PCW:H482	3:D:626:PCW:C27	0.76	2.11	6	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:609:PCW:C6	4:D:633:17F:H6A	0.76	2.10	17	8
3:D:605:PCW:H161	4:D:629:17F:H30	0.76	1.56	6	5
3:D:607:PCW:H262	4:D:631:17F:C2X	0.76	2.10	15	12
3:B:205:PCW:H39	4:B:214:17F:C35	0.76	2.10	3	1
3:B:208:PCW:H251	3:B:208:PCW:H483	0.76	1.55	3	2
3:A:404:PCW:H431	4:B:215:17F:C10	0.76	2.11	7	5
3:B:208:PCW:H19	3:C:205:PCW:H331	0.76	1.56	8	4
3:A:405:PCW:H371	3:D:601:PCW:H121	0.76	1.58	19	3
3:D:621:PCW:H212	4:D:633:17F:H31	0.76	1.58	8	6
3:B:205:PCW:H39	4:B:214:17F:H75	0.76	1.57	8	1
3:A:401:PCW:H182	3:A:401:PCW:H221	0.76	1.57	9	1
3:B:207:PCW:C44	3:B:213:PCW:H252	0.76	2.08	12	2
3:A:403:PCW:H362	3:A:403:PCW:H132	0.76	1.58	1	2
3:B:212:PCW:O31	3:B:212:PCW:H41	0.76	1.81	13	4
3:D:604:PCW:O31	3:D:613:PCW:H52	0.76	1.81	16	10
3:D:601:PCW:H482	4:D:628:17F:H56	0.76	1.56	5	1
3:A:413:PCW:H121	4:A:414:17F:C1Z	0.76	2.11	7	1
3:A:408:PCW:C34	3:C:204:PCW:H182	0.76	2.10	10	1
3:A:413:PCW:H321	4:A:414:17F:H18	0.76	1.56	11	1
3:D:613:PCW:H261	4:C:210:17F:H66	0.76	1.56	11	1
3:B:204:PCW:H12	3:B:212:PCW:H61	0.76	1.58	11	1
3:A:410:PCW:H242	3:C:207:PCW:H252	0.76	1.55	12	2
3:A:407:PCW:H211	3:C:205:PCW:H382	0.76	1.56	13	1
3:D:607:PCW:H221	4:D:628:17F:H18	0.76	1.58	18	1
3:C:204:PCW:C19	4:C:211:17F:H19A	0.76	2.11	18	2
3:A:412:PCW:H412	3:A:412:PCW:H372	0.76	1.57	1	1
3:D:605:PCW:C16	4:D:629:17F:H30	0.76	2.11	13	9
3:D:607:PCW:H19	4:D:631:17F:H50	0.76	1.56	16	5
3:D:609:PCW:H62	4:D:633:17F:O1	0.76	1.80	5	4
3:D:604:PCW:H472	3:D:619:PCW:H432	0.76	1.57	17	4
3:D:622:PCW:C7	4:D:633:17F:H11A	0.76	2.10	20	8
3:A:408:PCW:H242	3:A:417:PCW:H262	0.76	1.58	16	3
3:B:205:PCW:H471	3:C:208:PCW:H172	0.76	1.58	8	1
3:A:407:PCW:H161	3:B:208:PCW:H222	0.76	1.57	20	2
3:A:405:PCW:H482	4:D:628:17F:H53	0.76	1.56	4	4
3:A:410:PCW:H152	3:C:207:PCW:H241	0.76	1.58	2	2
3:D:618:PCW:H251	3:B:206:PCW:H442	0.76	1.55	3	1
3:A:402:PCW:H412	3:A:407:PCW:H252	0.76	1.56	4	1
3:D:618:PCW:C35	3:D:627:PCW:H342	0.76	2.11	5	1
3:D:611:PCW:H241	3:D:611:PCW:H452	0.76	1.55	12	2
3:B:210:PCW:H421	3:B:210:PCW:C27	0.76	2.10	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:403:PCW:H41	3:A:403:PCW:O11	0.76	1.80	8	10
3:A:417:PCW:H371	3:A:417:PCW:C41	0.76	2.11	18	11
5:B:201:GDP:O3B	6:B:202:MG:MG	0.76	1.29	3	20
5:C:201:GDP:O3B	6:C:202:MG:MG	0.76	1.29	19	19
3:A:402:PCW:H322	3:C:206:PCW:O4P	0.76	1.81	2	1
3:D:604:PCW:H332	3:D:624:PCW:C7	0.76	2.10	11	11
3:A:401:PCW:H62	3:B:209:PCW:C1	0.76	2.10	20	2
3:A:407:PCW:C20	3:C:205:PCW:H19	0.76	2.11	6	4
3:B:210:PCW:H121	4:B:216:17F:C6	0.76	2.11	3	3
3:A:402:PCW:O2	3:A:402:PCW:H42	0.76	1.80	15	3
3:A:404:PCW:C1	3:A:404:PCW:H73	0.76	2.11	11	3
3:A:403:PCW:C31	3:A:403:PCW:C36	0.76	2.63	15	1
3:A:411:PCW:C17	3:A:411:PCW:H222	0.76	2.10	16	1
3:B:207:PCW:H422	3:B:213:PCW:C23	0.76	2.11	19	2
4:A:414:17F:H6	3:C:203:PCW:H352	0.76	1.56	4	1
3:D:622:PCW:H472	3:B:206:PCW:H252	0.76	1.56	18	7
3:B:210:PCW:H121	4:B:216:17F:C17	0.76	2.10	14	2
3:B:203:PCW:H431	3:B:211:PCW:C22	0.76	2.10	17	6
3:D:608:PCW:C45	3:C:205:PCW:H20	0.76	2.11	9	1
3:A:406:PCW:H283	4:B:216:17F:H32	0.76	1.57	20	2
3:D:603:PCW:H2	3:D:605:PCW:C8	0.75	2.05	8	9
3:A:402:PCW:H162	3:A:409:PCW:C23	0.75	2.11	9	4
3:B:211:PCW:H342	3:B:212:PCW:O2P	0.75	1.81	4	6
4:D:629:17F:H65	4:D:634:17F:H8A	0.75	1.55	4	2
3:B:211:PCW:H171	3:B:211:PCW:C22	0.75	2.09	4	1
3:B:210:PCW:H441	3:B:213:PCW:H283	0.75	1.59	6	3
3:B:205:PCW:H171	3:B:205:PCW:C13	0.75	2.11	8	5
3:C:204:PCW:C27	4:C:211:17F:H60	0.75	2.12	17	3
3:A:409:PCW:C8	3:C:206:PCW:H371	0.75	2.11	11	2
3:D:605:PCW:O31	3:D:605:PCW:H41	0.75	1.82	17	2
3:A:401:PCW:H62	3:B:209:PCW:C13	0.75	2.08	19	1
3:A:417:PCW:H351	3:D:612:PCW:C13	0.75	2.11	1	11
3:B:204:PCW:H451	3:C:203:PCW:H152	0.75	1.58	2	3
1:D:505:ASP:HA	1:D:508:ARG:HD2	0.75	1.56	20	6
3:D:623:PCW:H382	3:D:625:PCW:C17	0.75	2.11	19	7
4:D:631:17F:H19A	4:D:631:17F:C9	0.75	2.12	4	2
3:D:606:PCW:H431	3:D:626:PCW:H482	0.75	1.58	5	1
3:A:404:PCW:H381	3:B:209:PCW:H331	0.75	1.58	6	1
3:A:406:PCW:H422	3:B:210:PCW:C39	0.75	2.10	10	2
3:B:206:PCW:C17	3:C:212:PCW:H281	0.75	2.06	12	1
3:A:401:PCW:H421	3:D:611:PCW:H232	0.75	1.55	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:403:PCW:H141	3:C:203:PCW:C32	0.75	2.07	18	3
3:D:605:PCW:H162	4:D:629:17F:H30	0.75	1.56	8	11
3:A:403:PCW:H321	3:C:204:PCW:H63	0.75	1.58	4	1
3:A:404:PCW:H451	3:B:209:PCW:H431	0.75	1.56	5	1
3:A:413:PCW:H141	4:A:414:17F:H58	0.75	1.59	5	6
3:B:210:PCW:H471	3:B:213:PCW:C19	0.75	2.10	12	4
3:C:208:PCW:H462	3:C:209:PCW:H422	0.75	1.57	7	3
3:D:623:PCW:H281	3:D:624:PCW:H452	0.75	1.57	11	1
3:D:606:PCW:H12	3:D:626:PCW:H362	0.75	1.56	19	2
3:D:622:PCW:H40	3:B:206:PCW:H282	0.75	1.56	13	1
3:B:205:PCW:H431	3:B:206:PCW:H141	0.75	1.57	13	1
3:B:206:PCW:H342	3:C:204:PCW:H382	0.75	1.57	19	2
3:B:208:PCW:H372	3:B:208:PCW:H411	0.75	1.57	11	3
3:D:613:PCW:H431	3:D:619:PCW:C39	0.75	2.11	16	8
3:D:614:PCW:H41	3:D:625:PCW:O1P	0.75	1.80	13	3
3:D:615:PCW:H141	4:D:635:17F:C9	0.75	2.11	12	2
3:D:618:PCW:C15	3:D:627:PCW:H142	0.75	2.11	13	7
3:D:622:PCW:H441	3:B:206:PCW:H252	0.75	1.59	20	5
3:B:204:PCW:H11	3:B:212:PCW:H82	0.75	1.58	4	1
3:A:404:PCW:H73	3:A:404:PCW:O3P	0.75	1.81	11	13
3:A:420:PCW:C37	3:D:617:PCW:H141	0.75	2.12	15	3
3:A:407:PCW:C28	3:A:409:PCW:H172	0.75	2.12	8	1
4:A:414:17F:H8A	4:C:210:17F:C2	0.75	2.09	10	1
3:D:623:PCW:H241	3:D:623:PCW:C20	0.75	2.11	10	1
3:C:207:PCW:C31	3:C:207:PCW:H42	0.75	2.12	11	1
3:B:204:PCW:H63	3:B:212:PCW:H73	0.75	1.58	13	1
3:A:402:PCW:H62	3:A:402:PCW:H332	0.75	1.56	15	1
3:A:403:PCW:H332	3:C:203:PCW:H31	0.75	1.56	15	1
3:A:410:PCW:C23	3:A:410:PCW:H182	0.75	2.11	6	7
3:A:420:PCW:O1P	3:D:617:PCW:H82	0.75	1.82	13	4
4:B:214:17F:O5	3:C:205:PCW:H61	0.75	1.82	4	3
3:A:410:PCW:C8	3:C:209:PCW:H11	0.75	2.12	2	3
3:B:204:PCW:H252	3:C:208:PCW:H241	0.75	1.55	2	1
3:A:404:PCW:C21	3:A:404:PCW:C17	0.75	2.64	18	6
3:C:204:PCW:H351	4:C:211:17F:C9	0.75	2.11	9	3
3:A:406:PCW:H251	3:B:207:PCW:H19	0.75	1.57	11	1
3:B:207:PCW:H131	3:B:210:PCW:H131	0.75	1.58	18	1
3:D:608:PCW:H462	3:C:205:PCW:H472	0.75	1.57	19	1
3:D:625:PCW:H19	3:D:625:PCW:C14	0.75	2.12	10	7
3:D:615:PCW:H262	4:B:216:17F:C40	0.75	2.09	19	3
2:B:68:ARG:HA	2:B:71:TYR:CE1	0.75	2.17	2	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:608:PCW:H442	3:D:615:PCW:H461	0.75	1.57	8	2
3:A:410:PCW:H82	3:C:209:PCW:H11	0.75	1.56	5	1
3:C:204:PCW:H251	4:C:211:17F:H32	0.75	1.57	9	1
3:D:624:PCW:C31	3:D:624:PCW:H41	0.75	2.11	11	1
3:D:605:PCW:H252	4:D:629:17F:H42	0.75	1.55	18	2
3:D:613:PCW:H12	3:D:613:PCW:O31	0.75	1.81	15	13
3:A:410:PCW:C1	3:C:207:PCW:H381	0.75	2.11	2	2
3:D:608:PCW:H422	3:D:615:PCW:H461	0.75	1.58	16	7
3:D:614:PCW:O1P	3:D:625:PCW:H73	0.75	1.80	2	1
3:B:210:PCW:C12	4:B:216:17F:H18	0.75	2.11	5	3
3:A:413:PCW:C18	4:A:414:17F:H34	0.75	2.10	7	1
3:A:401:PCW:C41	3:A:404:PCW:H262	0.75	2.11	8	1
3:A:407:PCW:H352	3:C:205:PCW:H122	0.75	1.59	20	3
3:A:402:PCW:H471	3:C:205:PCW:H361	0.75	1.58	12	1
3:D:619:PCW:C45	4:C:210:17F:H74	0.75	2.10	13	1
3:A:403:PCW:O3	3:A:403:PCW:H382	0.75	1.82	15	1
3:B:205:PCW:H222	3:B:212:PCW:H371	0.75	1.57	19	2
3:B:206:PCW:C32	3:C:204:PCW:H381	0.75	2.12	19	1
3:D:601:PCW:H362	4:B:216:17F:H61	0.75	1.55	1	1
3:D:608:PCW:H2	3:D:615:PCW:C6	0.75	2.12	15	4
3:D:625:PCW:H12	3:D:626:PCW:H12	0.75	1.57	16	6
3:B:204:PCW:H171	3:B:206:PCW:C32	0.75	2.11	1	1
4:D:630:17F:H67	4:D:634:17F:H36	0.75	1.58	7	6
3:A:420:PCW:H321	3:D:617:PCW:H52	0.75	1.57	20	4
3:D:621:PCW:H372	4:D:633:17F:C34	0.75	2.12	13	1
3:B:204:PCW:C27	3:C:207:PCW:H262	0.75	2.12	13	1
3:B:204:PCW:C15	3:B:206:PCW:H321	0.75	2.11	14	1
3:B:210:PCW:H451	4:B:215:17F:H72	0.75	1.56	17	1
3:A:402:PCW:H51	3:A:402:PCW:O11	0.75	1.80	18	6
3:A:406:PCW:H31	3:A:406:PCW:P	0.75	2.22	14	20
3:A:413:PCW:H162	4:A:414:17F:H56	0.75	1.58	12	3
3:D:602:PCW:H271	3:D:610:PCW:H182	0.75	1.59	5	7
3:C:208:PCW:H422	3:C:208:PCW:C14	0.75	2.10	1	1
3:D:617:PCW:C1	3:D:617:PCW:H51	0.75	2.12	2	10
3:A:404:PCW:H441	4:B:215:17F:H44	0.75	1.58	7	3
3:A:417:PCW:C43	3:D:612:PCW:H162	0.75	2.11	6	3
3:B:203:PCW:H12	3:B:211:PCW:H352	0.75	1.56	7	1
3:A:417:PCW:H431	3:D:612:PCW:H171	0.75	1.56	10	1
3:B:207:PCW:C15	3:B:210:PCW:H362	0.75	2.12	20	1
3:B:207:PCW:C14	3:B:210:PCW:H362	0.75	2.12	20	1
3:A:403:PCW:H151	3:A:403:PCW:H382	0.74	1.56	12	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:405:PCW:C39	4:D:628:17F:H52	0.74	2.12	13	9
3:A:403:PCW:C32	3:C:204:PCW:H62	0.74	2.12	7	5
1:D:497:SER:HB2	1:D:498:PRO:HD3	0.74	1.59	2	6
3:C:207:PCW:H42	3:C:207:PCW:C32	0.74	2.12	2	14
3:D:613:PCW:H221	4:C:210:17F:C25	0.74	2.12	19	6
3:C:204:PCW:H462	4:C:211:17F:C31	0.74	2.11	4	1
3:C:204:PCW:H211	4:C:211:17F:H63	0.74	1.59	4	1
3:B:203:PCW:H61	4:B:217:17F:H18	0.74	1.56	6	1
3:B:209:PCW:H132	3:B:209:PCW:C33	0.74	2.11	8	5
3:D:622:PCW:H172	4:D:630:17F:H32	0.74	1.58	13	3
4:D:628:17F:C22	4:D:631:17F:H75	0.74	2.11	15	5
3:B:205:PCW:H51	3:B:208:PCW:C1	0.74	2.12	10	1
3:D:607:PCW:H482	4:D:628:17F:H61	0.74	1.56	14	2
3:D:606:PCW:H432	3:D:626:PCW:C48	0.74	2.12	17	2
3:D:616:PCW:C45	3:B:206:PCW:H472	0.74	2.12	19	8
3:A:419:PCW:H31	3:D:617:PCW:C42	0.74	2.11	8	10
4:D:629:17F:H10	4:D:634:17F:C27	0.74	2.12	14	4
3:C:204:PCW:H142	4:C:211:17F:O7	0.74	1.81	4	1
3:C:209:PCW:H331	3:C:209:PCW:C7	0.74	2.12	4	1
3:A:405:PCW:H483	3:A:405:PCW:C15	0.74	2.12	5	3
3:B:213:PCW:H272	4:B:215:17F:C32	0.74	2.12	6	1
3:A:408:PCW:H342	3:C:204:PCW:C21	0.74	2.10	9	1
3:B:205:PCW:H452	3:B:206:PCW:H212	0.74	1.58	9	4
3:A:410:PCW:H262	3:C:207:PCW:H232	0.74	1.57	10	1
3:A:417:PCW:H442	3:D:612:PCW:H211	0.74	1.58	10	1
3:A:417:PCW:C44	3:D:612:PCW:H271	0.74	2.12	10	1
3:C:204:PCW:H283	3:C:204:PCW:H483	0.74	1.57	10	2
3:A:403:PCW:H19	3:C:203:PCW:H122	0.74	1.59	13	1
3:A:402:PCW:H372	3:A:409:PCW:H282	0.74	1.57	16	1
3:B:206:PCW:H321	3:C:204:PCW:H39	0.74	1.58	18	1
3:B:207:PCW:H451	4:B:215:17F:H10	0.74	1.58	18	1
3:D:607:PCW:C18	4:D:631:17F:H11	0.74	2.10	1	8
3:D:623:PCW:H242	3:B:203:PCW:H481	0.74	1.56	1	1
3:A:404:PCW:H171	3:A:404:PCW:H212	0.74	1.59	2	8
3:A:410:PCW:O1P	3:A:410:PCW:H51	0.74	1.81	2	13
4:D:630:17F:H67	4:D:634:17F:C23	0.74	2.11	12	12
4:D:629:17F:H9A	4:D:629:17F:H20A	0.74	1.56	5	4
3:A:411:PCW:H222	3:A:411:PCW:C18	0.74	2.11	17	4
3:A:417:PCW:H341	3:D:612:PCW:C13	0.74	2.12	4	2
3:D:605:PCW:C7	3:D:626:PCW:H19	0.74	2.08	15	4
3:D:608:PCW:H452	3:C:205:PCW:H20	0.74	1.57	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:204:PCW:H31	4:C:211:17F:H77	0.74	1.58	12	1
3:A:408:PCW:H52	3:C:204:PCW:C12	0.74	2.12	2	4
3:D:602:PCW:H172	3:D:602:PCW:H211	0.74	1.59	15	15
3:D:614:PCW:H51	3:D:625:PCW:O1P	0.74	1.81	5	5
3:B:208:PCW:C16	4:B:214:17F:H20A	0.74	2.13	1	3
3:D:607:PCW:H212	4:D:631:17F:H29	0.74	1.58	6	6
3:C:203:PCW:H442	3:C:203:PCW:H172	0.74	1.56	2	2
4:A:414:17F:C29	3:C:203:PCW:H472	0.74	2.10	3	1
3:A:409:PCW:C12	3:C:206:PCW:H331	0.74	2.12	5	2
3:C:204:PCW:H51	3:C:204:PCW:O11	0.74	1.82	5	1
3:D:616:PCW:H281	3:C:204:PCW:H272	0.74	1.59	14	2
3:A:409:PCW:C5	3:C:206:PCW:H351	0.74	2.13	17	2
3:A:411:PCW:H272	3:A:411:PCW:H482	0.74	1.60	14	6
3:D:604:PCW:H171	3:D:613:PCW:C34	0.74	2.11	13	8
3:D:606:PCW:C41	3:D:626:PCW:H472	0.74	2.12	4	4
3:D:627:PCW:H332	3:D:627:PCW:C12	0.74	2.12	5	1
3:C:204:PCW:H162	4:C:211:17F:H63	0.74	1.59	11	1
3:D:607:PCW:H20	4:D:631:17F:H50	0.74	1.57	14	1
3:D:605:PCW:H62	3:D:626:PCW:H281	0.74	1.57	4	6
3:D:613:PCW:H31	3:D:613:PCW:O31	0.74	1.82	13	10
3:B:206:PCW:C23	3:C:208:PCW:H20	0.74	2.12	5	6
3:D:601:PCW:H73	4:B:216:17F:H1	0.74	1.59	6	1
3:B:206:PCW:H352	3:B:212:PCW:H372	0.74	1.60	6	2
3:B:207:PCW:H462	4:B:215:17F:H60	0.74	1.57	7	2
3:C:204:PCW:H172	4:C:211:17F:O10	0.74	1.83	7	1
3:C:204:PCW:H122	4:C:211:17F:H6	0.74	1.60	8	1
3:B:207:PCW:O1P	4:B:216:17F:H6A	0.74	1.81	9	1
3:A:405:PCW:O1P	3:A:405:PCW:H331	0.74	1.83	11	1
3:A:406:PCW:H61	3:A:411:PCW:H11	0.74	1.59	20	3
3:D:604:PCW:H39	3:D:611:PCW:H322	0.74	1.59	15	1
3:D:601:PCW:H31	3:D:601:PCW:O31	0.74	1.83	2	12
3:D:625:PCW:H151	3:D:625:PCW:C19	0.74	2.12	10	20
3:A:410:PCW:H242	3:C:207:PCW:C23	0.74	2.12	16	5
3:D:603:PCW:H251	4:B:217:17F:C42	0.74	2.09	2	4
3:D:605:PCW:H232	4:D:629:17F:H38	0.74	1.58	18	4
4:B:214:17F:H47	4:B:217:17F:H75	0.74	1.59	3	1
3:D:613:PCW:H212	4:C:210:17F:H51	0.74	1.57	14	5
4:D:628:17F:H18A	4:D:631:17F:H55	0.74	1.59	5	1
3:B:209:PCW:H442	4:B:215:17F:H48	0.74	1.59	8	1
3:A:410:PCW:H232	3:C:207:PCW:H231	0.74	1.58	12	2
3:B:213:PCW:C35	4:B:214:17F:H10A	0.74	2.12	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:207:PCW:H252	3:C:208:PCW:H242	0.74	1.58	18	1
3:A:402:PCW:C44	3:A:407:PCW:H231	0.74	2.12	1	2
3:A:417:PCW:H483	3:D:612:PCW:H281	0.74	1.60	14	5
3:D:612:PCW:H321	3:D:618:PCW:C13	0.74	2.07	17	11
3:D:614:PCW:H452	3:D:619:PCW:C22	0.74	2.13	17	2
3:A:420:PCW:H162	4:D:632:17F:C31	0.74	2.11	10	3
3:B:206:PCW:H222	3:C:208:PCW:H282	0.74	1.59	17	3
3:A:409:PCW:H231	3:A:409:PCW:C16	0.74	2.13	12	1
3:A:407:PCW:H161	3:C:205:PCW:C15	0.74	2.12	13	1
3:A:417:PCW:H471	3:D:612:PCW:H271	0.74	1.60	2	11
3:A:419:PCW:C45	3:D:610:PCW:H211	0.74	2.11	18	7
3:D:602:PCW:H52	3:D:602:PCW:C31	0.74	2.12	1	1
3:D:621:PCW:H283	3:D:622:PCW:H61	0.74	1.59	5	5
3:B:206:PCW:H481	3:C:212:PCW:H40	0.74	1.59	10	4
3:D:622:PCW:H421	3:B:206:PCW:H282	0.74	1.58	14	2
3:C:204:PCW:H142	4:C:211:17F:C35	0.74	2.12	11	1
3:B:204:PCW:H151	3:B:206:PCW:C32	0.74	2.11	14	1
3:A:401:PCW:C47	3:D:611:PCW:H251	0.74	2.00	19	2
3:A:419:PCW:H451	3:D:610:PCW:C21	0.74	2.11	18	4
3:B:208:PCW:H411	4:B:214:17F:H8A	0.74	1.59	2	4
3:B:209:PCW:O11	3:B:209:PCW:H41	0.74	1.82	2	2
3:A:417:PCW:H382	3:D:612:PCW:H231	0.74	1.58	11	3
3:B:211:PCW:H12	4:B:217:17F:C18	0.74	2.12	4	1
3:D:615:PCW:H262	4:B:216:17F:H75	0.74	1.60	5	2
3:A:412:PCW:H362	3:C:206:PCW:H451	0.74	1.57	6	2
3:B:208:PCW:C3	4:B:214:17F:H1	0.74	2.13	17	2
3:A:407:PCW:H372	4:D:635:17F:H55	0.74	1.58	12	1
3:A:407:PCW:H162	3:C:205:PCW:H342	0.74	1.59	18	1
3:A:413:PCW:H321	4:A:414:17F:H34	0.73	1.60	1	1
3:A:413:PCW:H471	4:C:210:17F:H9A	0.73	1.60	1	1
3:D:603:PCW:H31	3:D:603:PCW:P	0.73	2.23	15	18
3:D:622:PCW:H232	3:D:624:PCW:C20	0.73	2.13	3	3
3:C:212:PCW:H11	3:C:212:PCW:O31	0.73	1.83	7	20
3:A:417:PCW:H351	3:D:612:PCW:H151	0.73	1.58	11	3
3:D:623:PCW:H142	3:D:624:PCW:H351	0.73	1.58	3	3
3:A:401:PCW:H421	3:D:611:PCW:C27	0.73	2.12	5	2
4:A:414:17F:H53	3:C:203:PCW:C47	0.73	2.12	5	1
3:C:204:PCW:H122	4:C:211:17F:O8	0.73	1.82	15	4
3:D:609:PCW:H31	4:D:633:17F:O9	0.73	1.83	6	3
3:A:404:PCW:C45	3:B:209:PCW:H20	0.73	2.12	12	2
3:A:402:PCW:H431	3:A:409:PCW:H151	0.73	1.60	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:420:PCW:H351	3:D:617:PCW:H132	0.73	1.59	16	2
3:D:604:PCW:O31	3:D:604:PCW:P	0.73	2.46	6	18
3:D:613:PCW:H483	3:D:619:PCW:H411	0.73	1.57	1	2
4:D:628:17F:H20A	4:D:628:17F:O9	0.73	1.81	11	2
3:A:408:PCW:H63	3:C:204:PCW:O11	0.73	1.82	8	4
4:A:414:17F:H43	4:C:210:17F:H33	0.73	1.58	2	1
3:B:205:PCW:H11	3:B:205:PCW:O31	0.73	1.84	18	15
3:B:204:PCW:H172	3:C:204:PCW:C39	0.73	2.13	14	2
3:A:413:PCW:H422	4:A:414:17F:C39	0.73	2.14	4	2
3:B:211:PCW:C23	4:B:217:17F:H73	0.73	2.12	15	2
3:D:627:PCW:H41	3:D:627:PCW:O31	0.73	1.82	6	2
3:A:406:PCW:C32	3:A:411:PCW:H321	0.73	2.13	11	1
4:A:414:17F:H54	3:B:212:PCW:C23	0.73	2.13	12	1
3:B:208:PCW:H161	4:B:214:17F:C34	0.73	2.13	12	1
3:B:209:PCW:H171	4:B:215:17F:O10	0.73	1.83	20	3
3:D:614:PCW:H31	3:D:614:PCW:C4	0.73	2.13	14	1
3:D:606:PCW:H31	3:D:626:PCW:C39	0.73	2.13	13	7
3:D:616:PCW:H221	3:D:616:PCW:H172	0.73	1.61	4	7
3:A:408:PCW:H361	3:C:207:PCW:C44	0.73	2.13	8	2
3:B:203:PCW:H332	4:B:215:17F:C21	0.73	2.13	8	3
3:D:622:PCW:H162	3:C:212:PCW:C16	0.73	2.12	18	6
3:A:411:PCW:C48	3:A:418:PCW:H212	0.73	2.13	12	1
3:A:407:PCW:H262	3:C:205:PCW:H382	0.73	1.60	15	1
3:D:606:PCW:H31	3:D:626:PCW:H371	0.73	1.57	18	1
3:A:409:PCW:H63	3:A:409:PCW:H321	0.73	1.60	19	1
3:A:407:PCW:C24	3:C:205:PCW:H411	0.73	2.13	6	11
3:A:420:PCW:P	3:D:617:PCW:H42	0.73	2.24	8	10
3:D:609:PCW:H82	4:D:633:17F:O8	0.73	1.82	19	8
4:B:214:17F:H50	4:B:217:17F:H70	0.73	1.59	2	1
3:B:206:PCW:H241	3:C:209:PCW:H481	0.73	1.57	4	1
3:A:412:PCW:H452	3:C:208:PCW:H471	0.73	1.58	10	2
4:D:628:17F:H40	4:D:631:17F:H75	0.73	1.59	10	2
3:D:608:PCW:H251	4:D:628:17F:C39	0.73	2.13	16	3
3:A:401:PCW:H322	3:B:209:PCW:C23	0.73	2.14	19	1
3:A:411:PCW:H412	3:A:418:PCW:H241	0.73	1.60	3	2
3:A:417:PCW:H331	3:D:612:PCW:H132	0.73	1.59	3	9
3:D:617:PCW:H2	3:D:617:PCW:H62	0.73	1.60	1	7
3:D:620:PCW:H73	3:D:620:PCW:C1	0.73	2.12	1	1
3:A:409:PCW:C6	3:C:206:PCW:H371	0.73	2.13	2	2
3:D:607:PCW:H461	4:D:628:17F:C34	0.73	2.13	15	6
3:B:204:PCW:H332	3:B:212:PCW:C8	0.73	2.14	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:411:PCW:H271	3:A:418:PCW:C27	0.73	2.12	19	4
3:A:413:PCW:C47	4:C:210:17F:H12A	0.73	2.13	18	3
3:B:213:PCW:H422	4:B:217:17F:H63	0.73	1.57	8	1
3:D:616:PCW:H451	3:B:206:PCW:H462	0.73	1.58	9	2
3:B:207:PCW:H152	3:B:210:PCW:C36	0.73	2.13	20	2
4:D:629:17F:H76	3:C:212:PCW:C46	0.73	2.13	13	6
1:A:388:SER:HB2	1:D:594:LYS:HE2	0.73	1.60	16	8
3:D:612:PCW:H332	3:D:627:PCW:H131	0.73	1.60	17	6
3:A:405:PCW:H482	4:D:628:17F:H51	0.73	1.58	6	1
3:D:606:PCW:H431	3:D:625:PCW:C47	0.73	2.14	17	3
3:B:204:PCW:H121	3:C:204:PCW:H39	0.73	1.60	20	6
3:C:204:PCW:H271	4:C:211:17F:H60	0.73	1.60	20	3
3:B:210:PCW:H451	3:B:213:PCW:C26	0.73	2.13	8	3
3:D:622:PCW:C32	3:D:627:PCW:H20	0.73	2.14	11	1
3:B:204:PCW:C12	3:C:204:PCW:H372	0.73	2.13	19	2
3:A:407:PCW:H151	3:C:205:PCW:C15	0.73	2.13	14	8
3:A:417:PCW:H422	3:D:612:PCW:C24	0.73	2.13	8	12
3:D:618:PCW:C24	3:B:206:PCW:H442	0.73	2.13	8	3
4:D:629:17F:H46	4:D:630:17F:H73	0.73	1.61	2	8
3:A:413:PCW:H471	4:C:210:17F:C2X	0.73	2.14	3	1
3:A:419:PCW:H362	3:D:617:PCW:C40	0.73	2.14	3	2
3:D:621:PCW:C21	4:D:633:17F:H31	0.73	2.13	11	10
3:B:208:PCW:H412	4:B:214:17F:H30	0.73	1.61	5	2
3:A:410:PCW:H272	3:D:618:PCW:H451	0.73	1.60	6	1
4:C:211:17F:H55	3:C:212:PCW:H162	0.73	1.61	6	1
3:D:615:PCW:H472	3:C:205:PCW:H231	0.73	1.60	7	1
3:A:408:PCW:O1P	3:C:204:PCW:H171	0.73	1.84	9	3
4:D:628:17F:H19A	4:D:631:17F:H51	0.73	1.59	15	3
3:D:620:PCW:H461	3:C:205:PCW:H472	0.73	1.59	12	1
3:A:410:PCW:H152	3:C:207:PCW:H242	0.73	1.59	13	1
3:A:410:PCW:O11	3:A:410:PCW:H2	0.73	1.83	14	1
4:D:629:17F:H68	4:D:634:17F:C1X	0.73	2.10	15	3
3:B:205:PCW:O1P	3:B:211:PCW:H41	0.73	1.83	17	1
1:A:243:MET:HG3	1:A:247:LEU:HD12	0.73	1.61	12	12
3:B:205:PCW:H451	3:C:208:PCW:C20	0.73	2.14	1	6
3:A:409:PCW:H171	3:A:409:PCW:H221	0.73	1.58	2	4
3:D:620:PCW:C15	4:D:635:17F:H18	0.73	2.12	7	7
3:B:204:PCW:H342	3:C:204:PCW:H341	0.73	1.60	20	4
3:A:410:PCW:H242	3:C:207:PCW:H232	0.73	1.61	9	2
3:B:206:PCW:C24	3:C:208:PCW:H20	0.73	2.13	5	3
3:A:418:PCW:H63	3:D:626:PCW:C2	0.73	2.13	4	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:409:PCW:H82	3:C:206:PCW:C36	0.73	2.13	17	2
3:A:419:PCW:H11	3:D:617:PCW:C41	0.73	2.10	12	6
3:B:208:PCW:H162	4:B:214:17F:C33	0.73	2.11	8	4
3:D:618:PCW:H261	3:C:204:PCW:C46	0.73	2.13	11	1
4:D:635:17F:C29	3:C:205:PCW:H161	0.73	2.13	11	1
4:D:628:17F:H76	4:B:216:17F:H53	0.73	1.60	18	1
3:B:208:PCW:H461	4:B:214:17F:H73	0.73	1.58	18	1
3:A:403:PCW:H212	3:A:403:PCW:H422	0.73	1.59	1	4
3:D:627:PCW:O1P	3:D:627:PCW:H51	0.73	1.83	9	10
4:D:629:17F:H42	4:D:630:17F:C40	0.73	2.13	3	6
4:D:630:17F:H60	4:D:630:17F:H10A	0.73	1.59	17	7
3:D:616:PCW:H12	3:D:616:PCW:H42	0.73	1.60	5	1
3:D:618:PCW:H362	4:D:633:17F:H40	0.73	1.60	20	3
3:B:207:PCW:C8	4:B:216:17F:H5	0.73	2.12	9	1
3:B:204:PCW:H31	4:C:211:17F:H4A	0.73	1.60	13	1
3:A:403:PCW:H182	3:A:403:PCW:C14	0.73	2.11	15	1
3:D:603:PCW:H281	3:B:210:PCW:H483	0.73	1.61	16	1
3:A:407:PCW:C17	3:B:208:PCW:H222	0.73	2.10	2	5
3:A:401:PCW:H62	3:B:209:PCW:C2	0.73	2.13	3	2
3:B:208:PCW:H422	4:B:214:17F:H32	0.73	1.59	10	3
3:B:211:PCW:H241	4:B:217:17F:H78	0.73	1.61	3	2
3:C:203:PCW:H382	3:C:203:PCW:C12	0.73	2.05	16	2
3:A:404:PCW:C7	3:A:404:PCW:H132	0.73	2.14	15	3
3:B:208:PCW:H19	4:B:214:17F:C31	0.73	2.13	12	4
3:A:406:PCW:H262	4:B:216:17F:H19A	0.73	1.61	14	3
4:D:635:17F:H4	4:D:635:17F:O10	0.73	1.82	20	3
2:C:72:MET:HE1	2:C:99:GLN:HG2	0.73	1.60	8	4
3:D:601:PCW:O2	4:B:216:17F:H60	0.73	1.83	7	1
3:D:605:PCW:H252	4:D:629:17F:C24	0.73	2.14	18	6
3:A:412:PCW:C45	3:C:208:PCW:H451	0.73	2.14	10	1
3:A:412:PCW:H362	3:C:206:PCW:H452	0.73	1.61	10	1
3:C:204:PCW:H20	4:C:211:17F:C1Y	0.73	2.12	18	4
3:D:616:PCW:H39	3:D:618:PCW:C16	0.72	2.14	1	6
3:B:203:PCW:H73	3:B:211:PCW:O31	0.72	1.83	8	5
3:A:407:PCW:H132	3:C:205:PCW:H321	0.72	1.58	10	5
3:D:603:PCW:C8	4:D:630:17F:H4A	0.72	2.14	15	5
4:D:630:17F:H12A	4:D:630:17F:C32	0.72	2.14	17	11
3:B:208:PCW:H441	4:B:214:17F:C1Z	0.72	2.12	5	3
3:A:404:PCW:H272	4:A:415:17F:C38	0.72	2.13	8	2
3:D:604:PCW:H451	3:D:624:PCW:H442	0.72	1.60	11	1
3:C:204:PCW:C35	4:C:211:17F:H8A	0.72	2.14	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:607:PCW:H212	4:D:631:17F:H30	0.72	1.60	16	8
3:A:406:PCW:H411	3:B:210:PCW:H40	0.72	1.60	6	4
3:A:407:PCW:H63	3:B:213:PCW:C32	0.72	2.14	14	4
3:D:604:PCW:H382	3:D:611:PCW:O2	0.72	1.84	10	13
4:B:214:17F:C1	3:C:205:PCW:H61	0.72	2.14	5	4
3:D:601:PCW:H351	4:B:216:17F:C39	0.72	2.14	4	1
3:B:204:PCW:C4	3:B:206:PCW:H62	0.72	2.13	13	2
3:A:401:PCW:H342	3:B:209:PCW:H371	0.72	1.60	6	1
3:B:209:PCW:H332	3:B:209:PCW:C13	0.72	2.12	8	4
3:B:206:PCW:H472	3:C:212:PCW:C23	0.72	2.14	11	1
4:D:628:17F:H59	4:D:631:17F:C29	0.72	2.14	18	1
4:D:630:17F:H67	4:D:634:17F:H40	0.72	1.59	19	2
3:B:207:PCW:C23	3:B:210:PCW:H242	0.72	2.13	19	1
3:A:408:PCW:O2P	3:C:204:PCW:H171	0.72	1.82	1	1
3:A:410:PCW:H31	3:A:410:PCW:O4P	0.72	1.84	1	3
3:D:608:PCW:C18	3:D:615:PCW:H352	0.72	2.14	14	8
3:D:612:PCW:C17	3:D:612:PCW:C21	0.72	2.64	13	17
3:C:204:PCW:H451	4:C:211:17F:H57	0.72	1.59	3	1
3:D:603:PCW:H31	3:D:603:PCW:C4	0.72	2.14	7	4
3:D:604:PCW:O31	3:D:613:PCW:H62	0.72	1.83	4	5
3:C:208:PCW:H422	3:C:208:PCW:H162	0.72	1.60	18	3
3:A:403:PCW:H242	3:D:617:PCW:H282	0.72	1.60	7	2
3:D:603:PCW:H281	3:D:606:PCW:H483	0.72	1.59	9	1
3:A:402:PCW:H73	3:A:402:PCW:H122	0.72	1.61	15	1
3:A:403:PCW:H52	3:C:203:PCW:P	0.72	2.24	20	1
4:D:635:17F:O8	4:D:635:17F:H5	0.72	1.84	6	18
3:B:208:PCW:O31	3:B:208:PCW:H11	0.72	1.84	5	16
3:C:203:PCW:O2P	3:C:204:PCW:H52	0.72	1.84	9	3
3:D:617:PCW:O31	3:D:617:PCW:H62	0.72	1.83	8	9
3:B:213:PCW:C42	4:B:217:17F:H67	0.72	2.14	4	1
3:A:406:PCW:H362	3:A:411:PCW:H332	0.72	1.61	7	2
3:A:403:PCW:C46	3:C:203:PCW:H281	0.72	2.14	9	1
3:B:205:PCW:C1	3:B:211:PCW:H62	0.72	2.14	10	2
3:D:602:PCW:H41	3:D:602:PCW:O31	0.72	1.84	15	1
3:B:207:PCW:H442	3:B:213:PCW:H282	0.72	1.59	15	1
3:B:206:PCW:H321	3:C:204:PCW:H381	0.72	1.59	19	1
3:C:204:PCW:H271	3:C:204:PCW:H483	0.72	1.62	19	1
3:A:417:PCW:H371	3:D:612:PCW:H151	0.72	1.60	17	4
3:D:611:PCW:C21	3:D:619:PCW:H482	0.72	2.15	2	3
3:D:622:PCW:C14	4:D:630:17F:H33	0.72	2.11	18	7
3:B:204:PCW:C32	3:B:212:PCW:H141	0.72	2.09	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:205:PCW:H12	3:B:211:PCW:C4	0.72	2.14	4	1
3:B:206:PCW:H73	3:C:207:PCW:O1P	0.72	1.85	20	3
3:D:603:PCW:C18	3:B:211:PCW:H283	0.72	2.13	6	1
3:A:416:PCW:H282	3:A:419:PCW:C25	0.72	2.15	10	2
3:A:401:PCW:C27	3:D:614:PCW:H281	0.72	2.14	16	3
3:D:607:PCW:H261	4:D:631:17F:H63	0.72	1.61	15	2
3:B:213:PCW:H241	3:B:213:PCW:H20	0.72	1.59	15	2
3:A:401:PCW:H342	3:B:209:PCW:H39	0.72	1.60	16	1
3:A:406:PCW:H481	3:D:606:PCW:H271	0.72	1.60	17	1
3:B:207:PCW:C15	3:B:210:PCW:H371	0.72	2.14	17	1
3:C:204:PCW:H351	4:C:211:17F:H8A	0.72	1.60	19	1
3:A:405:PCW:H411	3:D:601:PCW:H231	0.72	1.61	20	1
3:D:620:PCW:H283	4:D:635:17F:C21	0.72	2.14	12	9
3:A:408:PCW:H52	3:C:204:PCW:C11	0.72	2.15	2	1
3:A:416:PCW:H61	4:D:632:17F:O5	0.72	1.84	2	2
3:D:603:PCW:C38	4:D:629:17F:H36	0.72	2.11	14	7
3:A:404:PCW:H171	3:A:404:PCW:H211	0.72	1.61	9	6
3:A:402:PCW:H371	3:A:402:PCW:H411	0.72	1.60	12	1
3:D:622:PCW:C34	3:C:212:PCW:H442	0.72	2.05	19	3
3:D:623:PCW:H412	3:D:625:PCW:H212	0.72	1.60	20	1
3:B:205:PCW:H141	4:B:214:17F:H37	0.72	1.59	20	1
3:A:409:PCW:H212	3:A:409:PCW:H162	0.72	1.60	7	2
3:C:209:PCW:H132	3:C:209:PCW:C34	0.72	2.13	20	9
3:D:607:PCW:H282	4:D:631:17F:H67	0.72	1.61	4	1
3:D:621:PCW:H262	3:D:622:PCW:C8	0.72	2.15	19	7
3:B:212:PCW:H40	3:C:212:PCW:C28	0.72	2.13	5	3
3:D:622:PCW:C7	4:D:633:17F:H8	0.72	2.14	9	6
2:C:6:LEU:HB2	2:C:55:ILE:HG22	0.72	1.59	7	1
3:B:205:PCW:H20	3:B:212:PCW:C32	0.72	2.05	11	2
3:A:409:PCW:H61	3:A:412:PCW:H39	0.72	1.60	9	1
3:A:406:PCW:C23	3:B:210:PCW:H122	0.72	2.15	11	2
3:A:404:PCW:H252	4:A:415:17F:H59	0.72	1.62	4	1
3:A:418:PCW:H82	3:D:626:PCW:H362	0.72	1.59	10	2
3:A:420:PCW:O1P	3:D:617:PCW:H63	0.72	1.85	4	1
3:D:607:PCW:H282	4:D:631:17F:C37	0.72	2.15	4	1
3:B:208:PCW:C19	4:B:214:17F:H57	0.72	2.15	4	3
3:B:207:PCW:H182	3:B:210:PCW:C19	0.72	2.14	20	2
3:D:618:PCW:H283	3:C:204:PCW:H281	0.72	1.60	11	1
3:C:207:PCW:H272	3:C:209:PCW:C39	0.72	2.11	13	1
3:A:416:PCW:H31	3:D:610:PCW:C11	0.72	2.15	14	1
3:B:207:PCW:H162	3:B:210:PCW:H181	0.72	1.58	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:616:PCW:H481	3:B:206:PCW:C40	0.72	2.13	17	1
3:D:617:PCW:O3P	3:D:617:PCW:H51	0.72	1.85	1	1
3:B:211:PCW:H152	4:B:217:17F:H61	0.72	1.61	8	2
3:D:603:PCW:C43	3:D:605:PCW:H181	0.72	2.15	2	2
3:D:622:PCW:H172	4:D:630:17F:H34	0.72	1.59	20	5
3:D:606:PCW:H381	3:D:626:PCW:H452	0.72	1.60	6	4
3:A:404:PCW:C28	4:A:415:17F:H65	0.72	2.13	6	1
3:B:204:PCW:C13	3:B:206:PCW:H11	0.72	2.06	20	3
3:D:607:PCW:C19	4:D:631:17F:H39	0.72	2.15	18	4
4:B:214:17F:O4	3:C:205:PCW:H82	0.72	1.85	15	1
1:A:217:LEU:HD13	3:A:408:PCW:H222	0.72	1.62	19	1
3:A:404:PCW:H82	3:A:404:PCW:H132	0.72	1.62	1	1
3:D:618:PCW:C38	3:D:627:PCW:H161	0.72	2.15	5	9
3:B:205:PCW:H471	3:C:208:PCW:C20	0.72	2.13	2	2
3:B:213:PCW:H332	4:B:217:17F:H32	0.72	1.59	2	1
3:D:616:PCW:C36	3:C:212:PCW:H362	0.72	2.13	15	5
4:A:414:17F:H4	4:A:414:17F:O10	0.72	1.85	15	8
3:D:604:PCW:H462	4:C:210:17F:H53	0.72	1.59	10	3
4:D:629:17F:H54	3:B:212:PCW:H452	0.72	1.62	17	3
3:B:205:PCW:C44	3:B:206:PCW:H212	0.72	2.14	20	4
3:B:203:PCW:C33	4:B:215:17F:H37	0.72	2.15	8	2
3:B:204:PCW:H131	3:B:206:PCW:H41	0.72	1.61	19	3
3:C:204:PCW:H472	4:C:211:17F:H32	0.72	1.61	11	1
3:A:411:PCW:C11	4:B:215:17F:H33	0.72	2.15	13	1
3:B:207:PCW:H12	3:B:213:PCW:H132	0.72	1.62	13	1
3:A:407:PCW:H141	3:B:208:PCW:H222	0.72	1.61	15	1
3:B:210:PCW:H441	3:B:213:PCW:C26	0.72	2.10	16	1
3:A:411:PCW:H461	3:A:418:PCW:H241	0.72	1.62	18	1
1:A:231:ASN:HA	1:A:234:LYS:HD2	0.71	1.62	20	14
3:D:605:PCW:C41	4:D:634:17F:H55	0.71	2.14	18	4
3:D:606:PCW:H431	3:D:626:PCW:C48	0.71	2.14	5	7
3:D:611:PCW:H162	3:D:619:PCW:C17	0.71	2.10	15	2
3:D:618:PCW:H131	3:D:627:PCW:C15	0.71	2.15	2	9
3:D:616:PCW:H362	3:C:212:PCW:H362	0.71	1.60	15	2
4:B:214:17F:C34	4:B:214:17F:C38	0.71	2.68	12	2
3:B:207:PCW:H11	4:B:216:17F:O7	0.71	1.85	6	2
3:B:208:PCW:C21	4:B:214:17F:H60	0.71	2.06	6	2
3:B:210:PCW:C28	3:B:210:PCW:H471	0.71	2.15	6	1
3:A:404:PCW:H82	4:A:415:17F:O5	0.71	1.85	7	3
3:A:402:PCW:C33	3:A:409:PCW:H121	0.71	2.15	9	1
3:A:412:PCW:H462	3:C:208:PCW:H472	0.71	1.62	13	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:419:PCW:H31	3:D:617:PCW:H422	0.71	1.62	11	1
3:B:211:PCW:H451	3:B:212:PCW:H31	0.71	1.61	15	1
3:C:203:PCW:H222	3:C:203:PCW:H181	0.71	1.59	15	2
3:D:608:PCW:C24	3:D:615:PCW:H381	0.71	2.14	1	6
3:B:205:PCW:C28	3:B:212:PCW:H142	0.71	2.09	1	1
4:D:628:17F:C2X	4:D:631:17F:H75	0.71	2.15	6	6
3:B:205:PCW:H73	4:B:214:17F:O2	0.71	1.86	13	3
3:B:209:PCW:H62	3:B:209:PCW:H121	0.71	1.61	14	2
3:B:213:PCW:H32	4:B:217:17F:H4A	0.71	1.60	20	2
3:D:616:PCW:H462	3:D:618:PCW:H482	0.71	1.61	5	2
3:C:204:PCW:H141	4:C:211:17F:H8	0.71	1.61	18	3
3:B:204:PCW:H73	3:B:205:PCW:O1P	0.71	1.85	6	1
3:D:613:PCW:C21	4:C:210:17F:H51	0.71	2.16	14	2
3:B:211:PCW:C3	4:B:217:17F:H31	0.71	2.15	13	3
3:C:207:PCW:C28	3:C:208:PCW:H152	0.71	2.13	9	2
3:D:612:PCW:H321	3:D:618:PCW:H152	0.71	1.61	18	2
3:B:207:PCW:H351	3:B:210:PCW:H341	0.71	1.60	11	1
2:C:158:THR:HA	2:C:161:ARG:HD3	0.71	1.60	12	1
3:D:616:PCW:H12	3:D:616:PCW:C4	0.71	2.14	1	3
4:B:214:17F:H1A	3:C:205:PCW:C6	0.71	2.14	5	4
3:A:402:PCW:C43	3:A:407:PCW:H231	0.71	2.14	11	2
3:D:613:PCW:H272	4:C:210:17F:H46	0.71	1.63	16	8
3:B:211:PCW:C1	4:B:217:17F:H31	0.71	2.15	6	1
3:D:618:PCW:H451	4:D:633:17F:C30	0.71	2.13	9	2
3:B:203:PCW:H242	4:C:210:17F:C18	0.71	2.16	13	2
3:B:205:PCW:H231	3:B:212:PCW:H411	0.71	1.61	15	1
3:A:407:PCW:H182	3:C:205:PCW:H171	0.71	1.60	19	1
4:D:628:17F:H69	4:D:631:17F:H48	0.71	1.62	20	1
3:B:207:PCW:H441	3:B:213:PCW:C23	0.71	2.15	20	1
3:B:210:PCW:H20	3:B:210:PCW:C24	0.71	2.14	1	1
3:B:213:PCW:H40	4:B:214:17F:H49	0.71	1.61	4	1
3:A:419:PCW:H40	3:D:616:PCW:C23	0.71	2.15	12	4
3:D:618:PCW:H351	3:D:627:PCW:H342	0.71	1.60	5	1
3:C:204:PCW:C35	4:C:211:17F:H8	0.71	2.15	12	4
3:B:205:PCW:C20	3:B:212:PCW:H322	0.71	2.05	11	2
3:D:607:PCW:C6	3:D:626:PCW:H222	0.71	2.15	9	3
3:D:622:PCW:H441	3:B:206:PCW:C27	0.71	2.16	14	2
3:B:209:PCW:C23	3:B:209:PCW:H341	0.71	2.15	14	1
3:B:207:PCW:C16	3:B:210:PCW:H211	0.71	2.12	19	2
3:B:213:PCW:H32	4:B:217:17F:P1	0.71	2.25	15	1
3:A:411:PCW:C18	3:A:418:PCW:H261	0.71	2.16	15	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:209:PCW:H41	3:B:209:PCW:O11	0.71	1.85	11	10
3:A:404:PCW:H62	3:B:203:PCW:H132	0.71	1.61	2	1
3:A:409:PCW:O31	3:C:206:PCW:H331	0.71	1.85	8	6
3:D:622:PCW:C12	4:D:630:17F:H33	0.71	2.15	16	5
3:A:408:PCW:H252	3:A:417:PCW:C26	0.71	2.14	5	1
3:D:601:PCW:H483	3:D:607:PCW:H231	0.71	1.63	5	1
3:D:615:PCW:H221	3:C:205:PCW:C25	0.71	2.15	18	3
3:A:401:PCW:H381	3:A:404:PCW:H231	0.71	1.62	9	1
4:D:633:17F:H52	3:C:209:PCW:H462	0.71	1.62	19	6
3:A:402:PCW:H361	3:C:205:PCW:H12	0.71	1.62	10	1
3:A:406:PCW:H63	3:A:411:PCW:H11	0.71	1.62	11	1
3:B:210:PCW:H452	3:B:213:PCW:H241	0.71	1.60	12	2
3:B:205:PCW:C28	3:B:212:PCW:H161	0.71	2.16	18	2
3:A:416:PCW:H132	3:D:610:PCW:H121	0.71	1.62	19	1
3:D:622:PCW:H441	3:B:206:PCW:H282	0.71	1.60	1	1
4:D:629:17F:O7	4:D:629:17F:C18	0.71	2.36	8	14
4:D:634:17F:H9	4:D:634:17F:H19A	0.71	1.63	1	13
3:B:205:PCW:H40	4:B:214:17F:H69	0.71	1.61	1	1
3:D:602:PCW:H73	3:C:212:PCW:O3P	0.71	1.85	10	3
3:D:615:PCW:C26	4:B:216:17F:H72	0.71	2.12	2	1
4:A:414:17F:H6	3:C:203:PCW:C35	0.71	2.15	4	1
3:D:601:PCW:H351	4:B:216:17F:C42	0.71	2.14	15	2
3:B:205:PCW:C28	3:B:211:PCW:H451	0.71	2.16	8	2
3:B:209:PCW:H20	3:B:209:PCW:C41	0.71	2.15	5	1
3:A:412:PCW:H421	3:C:206:PCW:C39	0.71	2.15	7	1
3:D:613:PCW:C12	3:D:619:PCW:H382	0.71	2.15	18	3
3:B:204:PCW:H452	3:C:203:PCW:H132	0.71	1.62	20	2
3:B:204:PCW:H42	3:B:206:PCW:C5	0.71	2.16	13	1
3:A:411:PCW:H222	3:A:411:PCW:H171	0.71	1.61	16	1
3:A:407:PCW:H82	3:B:213:PCW:C32	0.71	2.10	19	1
3:A:402:PCW:H342	3:A:409:PCW:H141	0.71	1.62	1	2
3:A:403:PCW:C17	3:C:203:PCW:H122	0.71	2.15	17	7
3:A:413:PCW:C17	4:A:414:17F:H31	0.71	2.16	2	1
4:D:634:17F:H76	3:C:206:PCW:C23	0.71	2.15	2	1
3:B:203:PCW:H362	4:B:215:17F:C22	0.71	2.15	2	1
4:B:217:17F:H72	4:B:217:17F:H44	0.71	1.62	10	2
3:B:204:PCW:C20	3:B:205:PCW:H481	0.71	2.14	4	1
3:A:410:PCW:H241	3:C:208:PCW:H242	0.71	1.62	5	4
4:A:415:17F:H75	4:C:210:17F:H32	0.71	1.62	6	1
3:B:205:PCW:H221	3:B:212:PCW:H351	0.71	1.63	19	2
3:D:602:PCW:H461	3:D:610:PCW:H412	0.71	1.63	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:205:PCW:C42	3:B:206:PCW:H161	0.71	2.15	8	4
3:B:210:PCW:H481	3:B:210:PCW:H281	0.71	1.63	19	1
3:D:604:PCW:O1P	3:D:613:PCW:C5	0.71	2.39	15	8
3:B:208:PCW:H372	3:B:208:PCW:C41	0.71	2.15	11	6
3:A:403:PCW:H452	3:C:203:PCW:H271	0.71	1.63	4	2
3:A:405:PCW:H462	3:A:405:PCW:C16	0.71	2.14	9	2
3:A:409:PCW:H63	3:C:206:PCW:H371	0.71	1.61	5	1
3:B:213:PCW:H272	4:B:215:17F:C33	0.71	2.15	6	1
3:A:419:PCW:H351	3:D:617:PCW:H412	0.71	1.63	8	2
3:B:212:PCW:H52	3:B:212:PCW:H2	0.71	1.61	12	1
3:B:205:PCW:C22	3:B:212:PCW:H371	0.71	2.14	19	1
3:A:404:PCW:H32	3:B:209:PCW:H411	0.71	1.62	1	1
3:A:413:PCW:H351	3:A:413:PCW:C31	0.71	2.16	3	19
3:D:604:PCW:P	3:D:613:PCW:H52	0.71	2.25	9	10
4:C:210:17F:C19	4:C:210:17F:C31	0.71	2.68	16	19
3:B:210:PCW:H12	3:B:210:PCW:O31	0.71	1.84	15	13
3:A:406:PCW:H283	4:B:216:17F:C20	0.71	2.13	3	1
3:D:613:PCW:H471	3:D:619:PCW:C43	0.71	2.15	14	7
3:B:205:PCW:C39	4:B:214:17F:H67	0.71	2.14	4	2
3:B:208:PCW:H162	4:B:214:17F:C31	0.71	2.16	13	4
3:A:411:PCW:H332	3:A:411:PCW:C37	0.71	2.11	8	1
3:B:204:PCW:O3	3:C:204:PCW:H372	0.71	1.86	17	3
3:D:616:PCW:C45	3:B:206:PCW:H462	0.71	2.15	9	1
3:A:403:PCW:H19	3:C:203:PCW:C14	0.71	2.16	14	1
4:A:414:17F:H9A	3:C:203:PCW:H372	0.71	1.60	15	1
3:B:206:PCW:H441	4:C:211:17F:C22	0.71	2.15	15	1
3:A:413:PCW:O31	4:A:414:17F:H20	0.71	1.85	1	3
3:D:624:PCW:H321	3:D:624:PCW:C7	0.71	2.14	10	12
3:A:416:PCW:H283	3:A:419:PCW:C25	0.71	2.16	5	5
3:D:620:PCW:H372	3:D:620:PCW:C41	0.71	2.16	10	8
3:B:206:PCW:H362	3:C:204:PCW:H411	0.71	1.62	2	1
3:B:206:PCW:H431	3:C:204:PCW:H442	0.71	1.60	2	1
3:D:608:PCW:C48	3:C:205:PCW:H472	0.71	2.15	14	3
3:B:210:PCW:H272	3:B:210:PCW:H471	0.71	1.63	14	6
3:C:204:PCW:C35	4:C:211:17F:H9	0.71	2.13	9	2
3:A:401:PCW:O2	3:B:209:PCW:H231	0.71	1.86	16	2
3:A:413:PCW:H322	3:A:413:PCW:H63	0.71	1.60	11	1
4:A:414:17F:C26	3:C:203:PCW:H411	0.71	2.02	11	1
3:B:211:PCW:H82	3:B:212:PCW:O1P	0.71	1.86	11	2
3:B:204:PCW:C28	4:C:211:17F:H20A	0.71	2.16	14	1
3:B:211:PCW:O3P	3:B:211:PCW:H62	0.71	1.85	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:407:PCW:H82	4:B:216:17F:H9	0.70	1.63	8	6
3:D:620:PCW:H121	4:D:635:17F:C17	0.70	2.16	1	2
3:A:410:PCW:H31	3:A:410:PCW:O2P	0.70	1.86	2	2
3:D:601:PCW:H39	3:D:601:PCW:C20	0.70	2.15	13	2
3:D:601:PCW:H462	4:D:628:17F:C37	0.70	2.15	4	1
3:D:624:PCW:H451	4:C:210:17F:H75	0.70	1.63	8	7
3:A:410:PCW:H272	3:D:618:PCW:C45	0.70	2.16	6	1
3:A:403:PCW:H342	3:C:203:PCW:C3	0.70	2.16	7	1
3:B:212:PCW:C24	4:C:211:17F:H48	0.70	2.11	10	1
3:A:404:PCW:H162	4:A:415:17F:C31	0.70	2.16	20	2
3:B:204:PCW:H42	3:B:206:PCW:H62	0.70	1.62	13	1
3:B:207:PCW:H121	3:B:210:PCW:C34	0.70	2.15	16	1
3:A:419:PCW:C2	3:D:617:PCW:H411	0.70	2.16	1	14
4:D:635:17F:O10	4:D:635:17F:H6	0.70	1.86	17	20
4:D:629:17F:H12	4:D:634:17F:H47	0.70	1.61	3	3
3:C:208:PCW:H321	3:C:208:PCW:H73	0.70	1.64	3	1
3:C:208:PCW:C31	3:C:208:PCW:H52	0.70	2.15	6	1
3:A:401:PCW:H63	3:A:404:PCW:O2P	0.70	1.85	20	2
3:A:409:PCW:H52	3:C:206:PCW:O2P	0.70	1.86	7	1
3:B:210:PCW:H451	3:B:213:PCW:H472	0.70	1.62	7	2
3:A:411:PCW:O2	3:A:411:PCW:H342	0.70	1.85	8	1
3:A:403:PCW:H19	3:C:203:PCW:H141	0.70	1.62	14	1
3:A:403:PCW:O3P	3:C:204:PCW:H61	0.70	1.86	16	2
3:D:603:PCW:H242	4:B:217:17F:H76	0.70	1.61	16	2
3:A:410:PCW:H182	3:A:410:PCW:H231	0.70	1.62	1	6
3:B:205:PCW:C47	3:C:208:PCW:H20	0.70	2.14	19	3
3:A:416:PCW:C41	3:A:416:PCW:H371	0.70	2.15	5	7
3:D:615:PCW:H181	4:D:635:17F:H12	0.70	1.64	3	1
3:B:204:PCW:C23	3:C:208:PCW:H262	0.70	2.16	12	4
3:B:205:PCW:H432	3:C:208:PCW:H19	0.70	1.63	7	1
3:A:404:PCW:H351	3:B:203:PCW:C17	0.70	2.15	11	1
3:B:205:PCW:H40	4:B:214:17F:H67	0.70	1.62	12	1
3:A:407:PCW:H482	4:D:635:17F:H50	0.70	1.61	15	1
4:D:628:17F:H66	4:D:631:17F:H52	0.70	1.63	20	1
3:D:618:PCW:H362	4:D:633:17F:C22	0.70	2.16	13	12
3:D:604:PCW:C37	3:D:611:PCW:H322	0.70	2.13	4	4
4:D:629:17F:H46	4:D:630:17F:H78	0.70	1.63	10	7
3:D:614:PCW:C44	3:D:619:PCW:H20	0.70	2.17	4	4
3:D:616:PCW:H361	3:C:212:PCW:H362	0.70	1.63	11	3
3:D:618:PCW:C44	3:D:627:PCW:H261	0.70	2.13	5	1
3:D:604:PCW:H462	4:C:210:17F:C30	0.70	2.16	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:403:PCW:H483	3:A:416:PCW:H271	0.70	1.61	10	1
3:A:418:PCW:H483	3:B:213:PCW:H471	0.70	1.61	15	3
3:D:624:PCW:H232	4:C:211:17F:C30	0.70	2.16	11	1
3:B:207:PCW:H382	4:B:215:17F:H60	0.70	1.62	16	1
3:A:409:PCW:H82	3:C:206:PCW:O31	0.70	1.86	1	1
3:A:405:PCW:H382	4:D:628:17F:H54	0.70	1.62	2	1
3:D:623:PCW:H441	3:D:625:PCW:H262	0.70	1.63	2	2
4:D:628:17F:C21	4:D:631:17F:H75	0.70	2.16	20	7
3:D:623:PCW:H122	3:D:624:PCW:H332	0.70	1.61	3	10
3:A:402:PCW:H451	3:A:407:PCW:H39	0.70	1.61	4	1
3:A:407:PCW:H182	3:C:205:PCW:H172	0.70	1.61	4	2
3:A:419:PCW:C39	3:D:617:PCW:H451	0.70	2.16	6	2
3:C:207:PCW:H322	3:C:207:PCW:C8	0.70	2.17	10	2
3:A:401:PCW:H272	3:D:614:PCW:H281	0.70	1.63	7	6
3:A:404:PCW:H272	4:A:415:17F:C36	0.70	2.16	16	2
3:A:405:PCW:O1P	3:A:405:PCW:H52	0.70	1.86	7	1
3:D:615:PCW:H63	4:D:635:17F:C2	0.70	2.15	14	3
3:C:207:PCW:H62	4:C:211:17F:O5	0.70	1.86	10	1
3:C:204:PCW:H251	4:C:211:17F:H60	0.70	1.63	1	2
3:C:206:PCW:H52	3:C:206:PCW:O1P	0.70	1.84	14	17
3:A:403:PCW:H482	3:C:203:PCW:H281	0.70	1.63	2	1
3:D:611:PCW:C39	3:D:623:PCW:H462	0.70	2.14	2	4
4:D:635:17F:H48	3:C:205:PCW:H211	0.70	1.61	9	4
3:D:606:PCW:H12	3:D:626:PCW:C36	0.70	2.17	17	11
4:A:415:17F:H9A	4:A:415:17F:C18	0.70	2.14	5	1
3:C:204:PCW:H222	4:C:211:17F:C1Y	0.70	2.17	19	2
3:A:409:PCW:H411	3:A:409:PCW:C37	0.70	2.14	8	1
3:B:213:PCW:H422	4:B:217:17F:H36	0.70	1.63	17	2
1:A:279:LEU:HD22	1:D:495:LYS:HE3	0.70	1.64	3	15
3:A:402:PCW:C44	3:C:205:PCW:H152	0.70	2.16	9	3
3:B:211:PCW:C34	3:B:212:PCW:H11	0.70	2.16	1	1
3:D:603:PCW:H451	3:D:605:PCW:C14	0.70	2.16	2	2
3:C:204:PCW:C45	4:C:211:17F:H57	0.70	2.17	3	1
3:D:602:PCW:H162	3:D:624:PCW:H211	0.70	1.64	9	5
3:C:208:PCW:H141	3:C:209:PCW:H382	0.70	1.62	18	5
3:D:603:PCW:H452	3:D:605:PCW:H181	0.70	1.62	15	2
3:A:408:PCW:C36	3:C:207:PCW:H442	0.70	2.16	7	2
4:C:211:17F:H69	4:C:211:17F:C11	0.70	2.16	8	1
3:A:409:PCW:O3	3:C:206:PCW:H331	0.70	1.86	11	4
3:B:213:PCW:H2	4:B:217:17F:C17	0.70	2.16	9	1
3:A:406:PCW:H483	3:D:606:PCW:C28	0.70	2.17	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:413:PCW:H411	4:C:210:17F:C9	0.70	2.16	13	1
3:A:402:PCW:H482	3:A:409:PCW:C28	0.70	2.16	20	1
4:A:414:17F:H54	3:C:203:PCW:H452	0.70	1.63	20	1
4:D:629:17F:H68	4:D:634:17F:H11	0.70	1.62	1	3
3:B:204:PCW:H2	3:B:204:PCW:O11	0.70	1.87	18	14
3:A:410:PCW:H121	3:C:209:PCW:C35	0.70	2.13	2	1
3:D:601:PCW:H172	3:D:601:PCW:C22	0.70	2.17	2	7
3:A:404:PCW:C3	3:B:209:PCW:H322	0.70	2.16	12	2
4:B:214:17F:H46	4:B:217:17F:H66	0.70	1.63	20	3
4:D:629:17F:C39	4:D:634:17F:H29	0.70	2.17	12	3
3:D:622:PCW:H122	4:D:629:17F:H68	0.70	1.63	6	1
3:D:624:PCW:H451	4:C:210:17F:H77	0.70	1.64	13	1
3:B:206:PCW:H182	4:B:214:17F:H72	0.70	1.64	13	1
3:D:602:PCW:H82	3:D:602:PCW:C31	0.70	2.16	15	1
3:A:407:PCW:C18	3:C:205:PCW:H171	0.70	2.16	19	2
3:A:416:PCW:O1P	3:A:416:PCW:H52	0.70	1.87	16	17
3:D:622:PCW:H162	3:C:212:PCW:C15	0.70	2.17	18	9
3:B:205:PCW:H281	3:B:212:PCW:H161	0.70	1.63	18	2
3:B:207:PCW:H372	4:B:217:17F:H8	0.70	1.64	1	1
3:B:208:PCW:C18	3:C:205:PCW:H322	0.70	2.17	1	1
3:A:411:PCW:H462	3:A:418:PCW:H221	0.70	1.64	2	2
3:D:620:PCW:H132	4:D:635:17F:C18	0.70	2.16	13	5
3:B:206:PCW:C3	3:B:206:PCW:O1P	0.70	2.40	5	13
3:B:205:PCW:O2	3:B:208:PCW:H382	0.70	1.86	14	4
3:B:207:PCW:H61	3:B:213:PCW:O2P	0.70	1.87	4	1
3:B:208:PCW:C41	4:B:214:17F:H11A	0.70	2.16	15	5
3:A:412:PCW:C37	3:C:206:PCW:H39	0.70	2.17	5	1
3:A:413:PCW:H162	4:A:414:17F:H34	0.70	1.64	18	4
3:C:212:PCW:H142	3:C:212:PCW:H372	0.70	1.61	20	4
3:A:401:PCW:H322	3:B:209:PCW:C38	0.70	2.17	12	3
3:C:204:PCW:C20	4:C:211:17F:H18	0.70	2.17	9	1
3:A:407:PCW:H161	3:B:208:PCW:C22	0.70	2.16	18	2
3:B:208:PCW:H31	3:B:208:PCW:H42	0.70	1.62	19	1
3:A:403:PCW:C3	3:A:403:PCW:O1P	0.70	2.40	10	15
3:A:406:PCW:H51	3:A:406:PCW:O2P	0.70	1.87	7	8
3:B:208:PCW:H452	4:B:214:17F:H78	0.70	1.63	1	2
3:A:419:PCW:C48	3:D:618:PCW:H281	0.70	2.16	2	3
3:D:615:PCW:H172	3:D:615:PCW:H132	0.70	1.61	12	3
3:B:207:PCW:H142	3:B:210:PCW:H382	0.70	1.63	18	2
3:A:404:PCW:H40	4:B:215:17F:H8	0.70	1.63	9	1
3:A:404:PCW:H412	3:B:209:PCW:H381	0.70	1.62	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:417:PCW:H82	3:D:617:PCW:H40	0.70	1.63	14	1
3:D:609:PCW:H12	4:D:633:17F:H4	0.70	1.63	20	3
3:A:403:PCW:C11	3:A:403:PCW:H52	0.70	2.17	18	1
3:A:407:PCW:H162	3:B:208:PCW:H222	0.69	1.62	1	1
3:A:411:PCW:H182	3:A:418:PCW:H261	0.69	1.64	11	3
3:D:602:PCW:H212	3:D:602:PCW:C44	0.69	2.17	10	3
3:D:621:PCW:H422	4:D:634:17F:H66	0.69	1.63	5	4
3:D:608:PCW:H431	3:C:205:PCW:H241	0.69	1.64	2	2
3:A:404:PCW:H31	3:B:209:PCW:H322	0.69	1.64	12	2
3:A:406:PCW:H212	3:B:210:PCW:C32	0.69	2.16	6	3
3:D:616:PCW:H483	3:D:618:PCW:H482	0.69	1.64	9	3
3:A:409:PCW:O31	3:C:206:PCW:H352	0.69	1.87	17	2
3:A:413:PCW:C25	4:A:414:17F:H61	0.69	2.17	12	1
3:B:213:PCW:H281	4:B:215:17F:H77	0.69	1.64	13	1
3:B:207:PCW:H231	3:B:210:PCW:C24	0.69	2.13	15	2
4:D:629:17F:H29	4:D:630:17F:H10	0.69	1.64	18	1
3:A:401:PCW:C42	3:D:611:PCW:H232	0.69	2.16	1	1
3:A:417:PCW:H382	3:D:612:PCW:C23	0.69	2.17	11	4
3:B:204:PCW:C15	3:C:204:PCW:H39	0.69	2.16	19	3
3:B:211:PCW:H362	3:B:212:PCW:C1	0.69	2.17	8	4
3:C:204:PCW:H131	4:C:211:17F:C40	0.69	2.16	3	1
3:A:417:PCW:H361	3:D:612:PCW:C15	0.69	2.17	16	3
3:D:601:PCW:H12	3:D:601:PCW:O31	0.69	1.86	12	8
3:D:602:PCW:H222	3:D:610:PCW:H332	0.69	1.62	4	4
3:C:203:PCW:H161	3:C:203:PCW:C42	0.69	2.11	9	5
3:D:623:PCW:H331	3:D:624:PCW:C32	0.69	2.17	9	1
3:A:407:PCW:H181	3:C:205:PCW:H151	0.69	1.64	16	2
3:D:623:PCW:H421	3:D:625:PCW:H262	0.69	1.62	18	2
3:A:420:PCW:H351	3:D:617:PCW:C14	0.69	2.17	3	3
3:C:208:PCW:H132	3:C:209:PCW:C32	0.69	2.17	5	4
3:A:410:PCW:H31	3:C:209:PCW:O3	0.69	1.87	12	4
3:A:418:PCW:H40	3:D:625:PCW:C44	0.69	2.12	18	2
3:D:607:PCW:H19	4:D:631:17F:C26	0.69	2.16	20	6
3:D:615:PCW:H251	4:B:216:17F:H75	0.69	1.63	6	1
4:D:630:17F:H9	4:D:630:17F:C18	0.69	2.00	16	2
3:A:403:PCW:H472	3:C:203:PCW:H271	0.69	1.64	18	1
3:A:404:PCW:H381	3:A:404:PCW:H422	0.69	1.63	18	1
3:D:602:PCW:H222	3:D:610:PCW:H352	0.69	1.62	1	2
3:D:620:PCW:H283	4:D:635:17F:C2X	0.69	2.17	18	8
3:C:206:PCW:O11	3:C:206:PCW:H2	0.69	1.86	4	19
3:A:409:PCW:O31	3:C:206:PCW:H321	0.69	1.87	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:605:PCW:H161	4:D:629:17F:C12	0.69	2.18	4	7
3:D:612:PCW:H332	3:D:627:PCW:C13	0.69	2.16	17	10
3:D:622:PCW:H172	4:D:630:17F:C1Z	0.69	2.17	18	5
3:A:410:PCW:H272	3:C:204:PCW:H481	0.69	1.63	4	1
3:A:411:PCW:H161	3:B:209:PCW:H281	0.69	1.62	8	1
3:A:412:PCW:H461	3:B:205:PCW:H432	0.69	1.63	8	1
3:B:204:PCW:H372	3:C:204:PCW:H63	0.69	1.62	10	1
3:C:207:PCW:H52	3:C:207:PCW:H322	0.69	1.63	17	1
3:B:208:PCW:H282	4:B:214:17F:H19	0.69	1.63	19	1
3:A:407:PCW:H141	3:C:205:PCW:C32	0.69	2.13	4	4
3:A:409:PCW:H162	3:A:409:PCW:C21	0.69	2.17	1	4
3:D:623:PCW:H381	3:D:625:PCW:H171	0.69	1.64	1	2
3:D:625:PCW:C15	3:D:625:PCW:C19	0.69	2.70	10	9
3:D:618:PCW:H361	3:D:627:PCW:C17	0.69	2.16	3	4
2:B:15:GLY:HA2	5:B:201:GDP:C8	0.69	2.22	8	4
3:A:403:PCW:C14	3:C:203:PCW:H322	0.69	2.10	18	2
3:A:413:PCW:H431	4:C:210:17F:H29	0.69	1.62	17	2
3:B:209:PCW:C41	3:B:209:PCW:H372	0.69	2.17	15	2
3:D:626:PCW:C20	3:D:626:PCW:C24	0.69	2.70	14	3
3:B:210:PCW:H141	4:B:216:17F:O7	0.69	1.88	16	2
4:B:216:17F:H55	3:C:205:PCW:H221	0.69	1.64	20	1
3:D:603:PCW:C45	3:D:605:PCW:H181	0.69	2.17	1	13
3:D:608:PCW:H271	4:D:628:17F:C40	0.69	2.14	2	2
3:D:621:PCW:H222	4:D:633:17F:H19A	0.69	1.64	12	6
3:D:623:PCW:H122	3:D:624:PCW:C33	0.69	2.17	3	13
3:D:607:PCW:H82	3:D:608:PCW:H20	0.69	1.62	4	1
3:B:203:PCW:H271	4:B:215:17F:C30	0.69	2.18	5	1
3:D:618:PCW:O2P	3:D:627:PCW:H52	0.69	1.87	6	1
3:D:616:PCW:H371	3:D:618:PCW:H122	0.69	1.63	20	2
3:D:621:PCW:O1P	3:D:621:PCW:C3	0.69	2.40	13	1
3:D:602:PCW:H271	3:D:610:PCW:C21	0.69	2.17	19	3
3:C:207:PCW:P	4:C:211:17F:H1A	0.69	2.28	14	1
3:A:408:PCW:H63	4:C:211:17F:O6	0.69	1.88	15	1
3:B:205:PCW:C17	3:B:205:PCW:H132	0.69	2.16	19	1
1:A:250:VAL:O	1:A:254:VAL:HB	0.69	1.88	7	19
3:D:602:PCW:H141	3:D:624:PCW:H182	0.69	1.63	2	7
3:A:403:PCW:H421	3:A:403:PCW:H381	0.69	1.65	2	2
3:A:409:PCW:H122	3:C:206:PCW:H331	0.69	1.62	5	2
3:B:204:PCW:H322	3:B:206:PCW:H341	0.69	1.63	3	1
3:D:622:PCW:H352	3:D:627:PCW:H222	0.69	1.63	4	5
3:A:408:PCW:H361	3:C:207:PCW:H441	0.69	1.65	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:613:PCW:C28	4:C:210:17F:H35	0.69	2.18	18	5
3:A:401:PCW:C6	3:B:209:PCW:H2	0.69	2.11	8	3
3:A:408:PCW:P	3:C:204:PCW:H171	0.69	2.28	8	2
3:B:207:PCW:H141	3:B:210:PCW:C36	0.69	2.13	18	2
3:A:402:PCW:C35	3:C:205:PCW:H12	0.69	2.18	10	1
3:A:404:PCW:H172	3:B:209:PCW:H251	0.69	1.63	10	1
3:A:419:PCW:H432	3:D:610:PCW:H231	0.69	1.63	11	1
3:D:625:PCW:H12	3:D:626:PCW:H32	0.69	1.63	12	1
3:D:607:PCW:H171	4:D:631:17F:H18A	0.69	1.63	17	1
3:A:418:PCW:H441	4:B:215:17F:H76	0.69	1.63	19	1
3:A:417:PCW:H431	3:D:612:PCW:C16	0.69	2.18	17	6
3:D:602:PCW:C16	3:D:624:PCW:H222	0.69	2.17	16	7
3:D:615:PCW:H261	4:D:635:17F:H45	0.69	1.64	1	2
3:B:211:PCW:H472	3:B:211:PCW:H142	0.69	1.65	2	1
3:B:213:PCW:C24	3:B:213:PCW:H20	0.69	2.18	16	2
3:C:204:PCW:C27	4:C:211:17F:H32	0.69	2.17	2	1
3:A:411:PCW:H352	4:B:215:17F:H65	0.69	1.63	14	2
3:D:613:PCW:H142	3:D:619:PCW:H382	0.69	1.65	3	1
3:D:621:PCW:H371	4:D:633:17F:C34	0.69	2.18	20	12
3:A:419:PCW:C11	3:D:617:PCW:H421	0.69	2.17	10	2
3:B:208:PCW:H2	4:B:214:17F:H4A	0.69	1.63	11	5
3:A:404:PCW:H483	3:B:207:PCW:H471	0.69	1.64	6	1
3:A:420:PCW:H162	4:D:632:17F:H20	0.69	1.63	7	3
3:B:205:PCW:H221	3:B:212:PCW:H371	0.69	1.64	6	1
3:A:404:PCW:C40	4:B:215:17F:H10A	0.69	2.18	17	4
4:B:216:17F:O1	4:B:216:17F:H2	0.69	1.87	9	4
3:B:210:PCW:H421	4:B:215:17F:C40	0.69	2.17	9	1
3:A:411:PCW:H352	4:B:215:17F:H62	0.69	1.63	10	2
3:A:413:PCW:H341	4:A:414:17F:C31	0.69	2.07	20	4
3:A:417:PCW:H372	3:D:612:PCW:H182	0.69	1.65	10	1
3:C:204:PCW:H151	4:C:211:17F:H72	0.69	1.63	14	2
3:C:207:PCW:H62	4:C:211:17F:C3	0.69	2.17	10	1
3:A:407:PCW:O4P	4:B:216:17F:H10A	0.69	1.88	11	1
3:B:203:PCW:H261	4:C:210:17F:H19	0.69	1.61	11	1
3:D:604:PCW:O2P	3:D:613:PCW:H62	0.69	1.88	14	1
3:B:206:PCW:H322	3:B:212:PCW:H39	0.69	1.61	15	1
3:B:206:PCW:C33	3:C:204:PCW:H381	0.69	2.17	19	3
3:A:416:PCW:H231	3:D:617:PCW:H481	0.69	1.64	18	1
3:A:410:PCW:H152	3:C:207:PCW:H232	0.69	1.65	20	1
4:D:628:17F:C38	4:D:631:17F:H48	0.69	2.18	20	1
3:A:409:PCW:O3	3:C:206:PCW:H322	0.69	1.87	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:612:PCW:O11	3:D:612:PCW:H2	0.69	1.87	9	17
3:D:618:PCW:C34	3:D:627:PCW:H341	0.69	2.18	9	2
3:D:606:PCW:H361	3:D:626:PCW:H431	0.69	1.65	2	5
3:B:209:PCW:H162	3:B:209:PCW:H332	0.69	1.63	2	2
3:B:206:PCW:H381	4:C:211:17F:C27	0.69	2.13	4	1
3:B:205:PCW:H283	3:B:212:PCW:H161	0.69	1.64	14	2
3:B:213:PCW:H341	4:B:214:17F:H9A	0.69	1.64	5	2
3:B:205:PCW:C20	3:B:212:PCW:H342	0.69	2.18	7	2
3:B:209:PCW:H372	3:B:209:PCW:H411	0.69	1.65	15	2
3:A:402:PCW:C36	3:C:205:PCW:H12	0.69	2.18	10	1
3:D:618:PCW:H272	3:B:206:PCW:H462	0.69	1.63	11	1
3:A:410:PCW:H351	3:C:209:PCW:C16	0.69	2.17	16	5
3:B:205:PCW:H251	3:B:205:PCW:C21	0.69	2.13	19	1
3:D:623:PCW:C23	3:B:203:PCW:H481	0.69	2.15	3	3
3:C:203:PCW:H462	3:C:203:PCW:H171	0.69	1.64	1	1
3:D:623:PCW:H441	3:D:625:PCW:C26	0.69	2.18	2	3
3:D:615:PCW:C21	4:D:635:17F:H38	0.69	2.17	18	5
3:B:206:PCW:H232	3:C:208:PCW:H20	0.69	1.63	5	3
3:A:404:PCW:C41	3:B:209:PCW:H341	0.69	2.17	16	2
3:B:206:PCW:H351	3:B:212:PCW:H39	0.69	1.64	6	1
3:A:413:PCW:H283	3:C:203:PCW:C45	0.69	2.18	7	1
3:D:623:PCW:H211	3:B:203:PCW:H481	0.69	1.65	20	2
3:A:401:PCW:C5	3:A:404:PCW:H32	0.69	2.14	13	1
3:B:210:PCW:C8	4:B:216:17F:H18	0.69	2.18	15	1
3:D:623:PCW:H232	3:B:203:PCW:H483	0.69	1.65	20	2
3:B:204:PCW:H31	4:C:211:17F:H4	0.69	1.64	16	2
3:B:208:PCW:C41	4:B:214:17F:H10	0.68	2.18	18	4
3:C:208:PCW:H422	3:C:208:PCW:H382	0.68	1.65	2	1
3:B:204:PCW:C34	3:B:212:PCW:H82	0.68	2.18	11	2
3:D:606:PCW:C38	3:D:626:PCW:H452	0.68	2.18	6	5
4:D:630:17F:H53	3:B:212:PCW:H451	0.68	1.65	4	1
3:A:410:PCW:C16	3:C:207:PCW:H232	0.68	2.17	20	3
3:D:620:PCW:H271	4:D:635:17F:H35	0.68	1.65	6	1
4:C:211:17F:H9A	4:C:211:17F:H65	0.68	1.65	7	1
3:B:205:PCW:H12	3:B:211:PCW:O1P	0.68	1.87	15	1
3:A:407:PCW:H52	4:B:216:17F:C12	0.68	2.16	19	1
3:A:413:PCW:H121	4:A:414:17F:H66	0.68	1.63	12	3
3:B:213:PCW:H39	4:B:217:17F:C36	0.68	2.17	1	1
4:B:215:17F:O2	4:B:215:17F:H2	0.68	1.87	7	14
4:D:629:17F:H42	4:D:630:17F:H74	0.68	1.64	10	7
3:A:402:PCW:H162	3:A:409:PCW:C21	0.68	2.18	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:403:PCW:H20	3:C:203:PCW:H251	0.68	1.65	5	3
3:B:209:PCW:H362	3:B:209:PCW:H221	0.68	1.65	8	1
3:D:601:PCW:C37	4:B:216:17F:H77	0.68	2.17	9	1
3:A:402:PCW:C43	3:A:409:PCW:H151	0.68	2.18	12	1
3:A:413:PCW:H411	4:C:210:17F:H9A	0.68	1.65	13	1
3:D:617:PCW:H51	3:D:617:PCW:C1	0.68	2.19	1	1
3:D:622:PCW:H341	3:C:212:PCW:C42	0.68	2.16	1	2
3:D:625:PCW:H471	3:D:626:PCW:H482	0.68	1.65	16	7
3:D:602:PCW:C26	3:D:610:PCW:H171	0.68	2.18	9	9
3:B:206:PCW:H262	3:C:208:PCW:C48	0.68	2.18	7	2
3:A:404:PCW:H2	3:A:404:PCW:C7	0.68	2.18	9	7
3:D:614:PCW:H452	3:D:619:PCW:C20	0.68	2.19	5	7
3:A:404:PCW:C39	3:B:209:PCW:H62	0.68	2.18	6	1
3:D:613:PCW:H411	3:D:619:PCW:H39	0.68	1.65	16	3
2:B:81:VAL:HG22	2:B:114:VAL:HB	0.68	1.64	17	2
3:B:205:PCW:H361	3:B:206:PCW:H122	0.68	1.65	13	2
3:D:611:PCW:H31	3:D:619:PCW:C11	0.68	2.18	13	4
2:B:13:GLY:HA2	5:B:201:GDP:H5'	0.68	1.63	7	4
3:B:206:PCW:H231	3:C:208:PCW:H20	0.68	1.64	8	3
1:D:561:LYS:HE3	1:D:561:LYS:HA	0.68	1.65	14	5
3:B:205:PCW:H272	3:B:211:PCW:H471	0.68	1.65	11	1
3:A:401:PCW:C39	3:A:404:PCW:H231	0.68	2.18	16	3
3:B:207:PCW:H141	3:B:210:PCW:H351	0.68	1.64	17	1
1:A:363:LYS:HA	1:A:367:ALA:HB3	0.68	1.65	5	20
4:B:217:17F:O2	4:B:217:17F:N1	0.68	2.23	2	19
3:A:407:PCW:H352	3:C:205:PCW:C12	0.68	2.19	2	4
3:B:204:PCW:O1P	3:B:204:PCW:C3	0.68	2.40	2	2
3:A:407:PCW:H482	3:D:615:PCW:C28	0.68	2.17	17	4
3:A:407:PCW:H182	3:C:205:PCW:H152	0.68	1.65	4	1
3:A:418:PCW:H483	3:B:213:PCW:H481	0.68	1.63	5	1
3:D:602:PCW:H442	3:D:610:PCW:H371	0.68	1.65	13	4
3:A:407:PCW:H222	3:C:205:PCW:C43	0.68	2.16	13	2
3:A:411:PCW:H371	4:B:215:17F:H65	0.68	1.65	10	1
4:A:415:17F:H20	4:A:415:17F:O8	0.68	1.88	15	3
3:B:206:PCW:C40	4:C:211:17F:H47	0.68	2.18	20	1
3:A:403:PCW:H11	3:A:403:PCW:O31	0.68	1.88	11	19
3:A:408:PCW:C23	3:A:417:PCW:H262	0.68	2.19	10	3
3:D:601:PCW:H351	4:B:216:17F:H77	0.68	1.64	10	5
3:D:627:PCW:H421	3:D:627:PCW:C38	0.68	2.18	15	5
3:A:419:PCW:H412	3:D:610:PCW:H181	0.68	1.64	12	3
3:A:404:PCW:H151	4:A:415:17F:H31	0.68	1.66	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:213:PCW:O31	3:B:213:PCW:O3	0.68	2.11	17	9
3:C:204:PCW:H2	3:C:204:PCW:C5	0.68	2.18	5	1
3:B:211:PCW:C23	4:B:217:17F:H47	0.68	2.18	6	1
3:A:401:PCW:H381	3:A:404:PCW:C23	0.68	2.19	9	1
3:D:602:PCW:H73	3:C:212:PCW:H31	0.68	1.65	14	3
3:B:208:PCW:C44	4:B:214:17F:H58	0.68	2.18	9	1
3:A:408:PCW:H342	3:C:204:PCW:H182	0.68	1.65	10	1
3:C:203:PCW:C18	3:C:203:PCW:H222	0.68	2.18	18	1
3:B:213:PCW:C20	3:B:213:PCW:C24	0.68	2.72	8	3
3:C:207:PCW:H161	3:C:207:PCW:H261	0.68	1.64	2	1
3:A:402:PCW:H421	3:C:205:PCW:C13	0.68	2.18	13	2
3:A:417:PCW:C41	3:D:612:PCW:H231	0.68	2.17	18	7
4:A:415:17F:H18	4:A:415:17F:C9	0.68	2.13	5	1
3:B:203:PCW:H222	4:C:210:17F:H18	0.68	1.66	14	1
3:D:606:PCW:C3	3:D:626:PCW:H371	0.68	2.18	18	1
3:C:207:PCW:H252	3:C:208:PCW:C24	0.68	2.19	18	1
3:B:207:PCW:H451	4:B:215:17F:C33	0.68	2.19	19	1
3:D:605:PCW:H442	3:D:608:PCW:O2	0.68	1.88	5	5
3:B:210:PCW:O11	3:B:210:PCW:H2	0.68	1.88	10	11
3:C:203:PCW:H351	3:C:203:PCW:C31	0.68	2.19	14	3
3:D:623:PCW:H232	3:B:203:PCW:C48	0.68	2.19	16	8
4:D:635:17F:C30	3:C:205:PCW:H161	0.68	2.15	13	8
3:B:211:PCW:H132	4:B:217:17F:H57	0.68	1.63	5	1
4:B:215:17F:O7	4:B:215:17F:H18A	0.68	1.89	6	2
3:A:401:PCW:C44	3:D:614:PCW:H262	0.68	2.19	8	1
3:D:616:PCW:C43	3:B:206:PCW:H483	0.68	2.18	12	2
3:A:406:PCW:H321	3:A:411:PCW:H321	0.68	1.65	11	1
3:A:413:PCW:H261	4:C:210:17F:H38	0.68	1.64	11	1
3:C:204:PCW:C14	4:C:211:17F:H63	0.68	2.19	11	1
3:B:205:PCW:C22	3:B:212:PCW:H351	0.68	2.17	13	4
3:B:211:PCW:O3	4:B:217:17F:H31	0.68	1.88	13	1
3:D:616:PCW:O2	3:D:616:PCW:O4P	0.68	2.11	12	4
3:A:409:PCW:H321	3:C:206:PCW:H352	0.68	1.65	2	3
3:D:617:PCW:H51	3:D:617:PCW:O3P	0.68	1.89	16	10
3:B:210:PCW:C22	3:B:210:PCW:C26	0.68	2.71	6	16
4:B:216:17F:O8	4:B:216:17F:H5	0.68	1.88	11	7
3:A:410:PCW:H51	3:A:410:PCW:O2P	0.68	1.87	6	4
3:D:623:PCW:H381	3:D:625:PCW:H182	0.68	1.66	14	6
3:D:615:PCW:H82	4:D:635:17F:O4	0.68	1.87	7	5
3:A:404:PCW:H421	3:B:209:PCW:H221	0.68	1.65	9	1
3:D:605:PCW:H41	3:D:605:PCW:H2	0.68	1.63	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:204:PCW:H141	4:C:211:17F:H9	0.68	1.66	11	1
3:B:206:PCW:H483	3:C:212:PCW:H211	0.68	1.64	13	1
3:B:207:PCW:H472	4:B:215:17F:H42	0.68	1.65	16	1
3:D:614:PCW:C5	3:D:625:PCW:O1P	0.68	2.42	4	16
3:C:205:PCW:H441	3:C:206:PCW:H231	0.68	1.64	1	1
3:B:204:PCW:H51	3:B:204:PCW:H12	0.68	1.64	2	1
3:A:412:PCW:C45	3:C:208:PCW:H472	0.68	2.19	3	2
3:A:420:PCW:C36	3:D:617:PCW:H141	0.68	2.19	15	2
4:C:211:17F:H66	4:C:211:17F:C12	0.68	2.19	3	2
3:A:405:PCW:H40	3:D:601:PCW:H251	0.68	1.64	14	2
3:A:411:PCW:H2	4:B:215:17F:H31	0.68	1.64	15	5
3:C:208:PCW:H231	3:C:209:PCW:H431	0.68	1.64	9	3
4:D:634:17F:H75	3:C:206:PCW:H283	0.68	1.65	7	1
3:A:412:PCW:C45	3:C:208:PCW:H19	0.68	2.19	11	1
3:C:207:PCW:H62	4:C:211:17F:H1A	0.68	1.66	15	1
3:A:408:PCW:H342	3:C:207:PCW:C44	0.68	2.19	17	1
3:A:416:PCW:C19	3:A:419:PCW:H431	0.68	2.19	18	5
3:D:611:PCW:O2P	3:D:619:PCW:H41	0.68	1.89	17	3
4:D:628:17F:C19	4:D:628:17F:C31	0.68	2.72	15	12
3:B:208:PCW:H62	3:C:208:PCW:O1P	0.68	1.89	1	1
3:A:410:PCW:H181	3:C:209:PCW:H262	0.68	1.66	16	3
3:A:417:PCW:H442	3:D:612:PCW:H242	0.68	1.64	19	6
3:B:203:PCW:H472	4:B:217:17F:H50	0.68	1.65	2	1
3:B:204:PCW:H442	3:C:203:PCW:H132	0.68	1.66	2	1
3:A:406:PCW:H121	3:A:406:PCW:C39	0.68	2.17	7	1
3:A:416:PCW:C47	3:D:617:PCW:H252	0.68	2.18	10	3
3:A:419:PCW:H121	3:D:617:PCW:H442	0.68	1.66	8	1
4:D:628:17F:H8	4:D:631:17F:H33	0.68	1.64	10	2
2:C:6:LEU:HB2	2:C:55:ILE:HG12	0.68	1.65	9	1
4:C:211:17F:H65	4:C:211:17F:C2X	0.68	2.19	9	2
3:A:407:PCW:H271	3:A:409:PCW:H20	0.68	1.66	11	1
3:A:410:PCW:H42	3:C:209:PCW:C3	0.68	2.08	14	2
3:A:406:PCW:H232	3:B:210:PCW:O3	0.68	1.88	18	2
3:C:203:PCW:H252	4:C:211:17F:H73	0.68	1.65	14	1
3:D:601:PCW:H141	4:D:628:17F:H54	0.68	1.66	16	1
3:B:210:PCW:C40	4:B:215:17F:H77	0.68	2.18	16	1
3:B:204:PCW:C48	3:B:212:PCW:H19	0.68	2.19	20	1
3:A:419:PCW:O1P	3:D:617:PCW:H372	0.67	1.87	20	10
3:D:602:PCW:C28	3:D:610:PCW:H232	0.67	2.18	1	1
3:D:615:PCW:H2	3:D:615:PCW:H42	0.67	1.64	6	11
3:D:627:PCW:O31	3:D:627:PCW:C5	0.67	2.41	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:204:PCW:O11	3:C:204:PCW:H2	0.67	1.88	11	15
3:A:403:PCW:H332	3:C:204:PCW:H12	0.67	1.67	20	2
3:B:211:PCW:H242	4:B:217:17F:H47	0.67	1.64	3	3
3:D:616:PCW:H482	3:C:208:PCW:H271	0.67	1.66	7	1
3:D:608:PCW:H63	3:D:620:PCW:O11	0.67	1.88	8	1
3:A:408:PCW:C21	3:A:417:PCW:H461	0.67	2.18	11	1
3:A:416:PCW:C16	3:D:617:PCW:H142	0.67	2.19	11	1
3:B:209:PCW:H262	3:B:209:PCW:H471	0.67	1.66	16	2
3:D:604:PCW:C39	3:D:611:PCW:H322	0.67	2.19	15	1
3:A:409:PCW:C3	3:C:206:PCW:H41	0.67	2.20	16	1
3:D:616:PCW:C43	3:B:206:PCW:H472	0.67	2.19	1	1
4:C:211:17F:H2	4:C:211:17F:O2	0.67	1.89	10	17
3:B:208:PCW:H161	4:B:214:17F:C31	0.67	2.16	4	3
3:A:406:PCW:H212	3:B:210:PCW:C31	0.67	2.18	18	6
3:D:614:PCW:H452	3:D:619:PCW:H20	0.67	1.65	15	7
3:B:206:PCW:H362	3:C:204:PCW:C39	0.67	2.19	5	1
3:D:604:PCW:C31	3:D:613:PCW:H51	0.67	2.19	14	2
3:D:610:PCW:H31	3:D:616:PCW:H41	0.67	1.65	15	1
3:B:207:PCW:H452	4:B:215:17F:C24	0.67	2.20	16	1
3:A:403:PCW:H281	3:A:413:PCW:H222	0.67	1.67	1	1
3:A:411:PCW:H142	3:A:411:PCW:C18	0.67	2.18	4	17
3:A:417:PCW:H39	3:D:612:PCW:C45	0.67	2.17	18	6
3:D:602:PCW:H421	3:D:610:PCW:C36	0.67	2.17	1	1
3:D:605:PCW:O11	3:D:605:PCW:H2	0.67	1.88	20	18
4:D:633:17F:O10	4:D:633:17F:O7	0.67	2.12	6	19
3:C:208:PCW:H441	3:C:208:PCW:H161	0.67	1.65	18	3
3:A:413:PCW:H471	4:C:210:17F:C10	0.67	2.19	2	1
3:A:420:PCW:H321	3:D:617:PCW:C5	0.67	2.19	20	2
3:D:604:PCW:O31	3:D:613:PCW:H61	0.67	1.89	19	3
4:A:414:17F:H6	3:C:203:PCW:C34	0.67	2.19	4	1
3:D:616:PCW:H431	3:B:206:PCW:H481	0.67	1.63	4	1
3:C:203:PCW:C39	3:C:203:PCW:H141	0.67	2.19	4	2
4:D:634:17F:H65	4:D:635:17F:H72	0.67	1.63	15	3
3:A:413:PCW:H431	4:C:210:17F:H12A	0.67	1.65	7	3
3:D:604:PCW:P	3:D:604:PCW:O31	0.67	2.52	11	2
3:D:608:PCW:H483	3:C:205:PCW:C45	0.67	2.16	9	2
3:D:616:PCW:C45	3:B:206:PCW:H471	0.67	2.19	12	1
3:A:407:PCW:H352	3:C:205:PCW:H121	0.67	1.65	2	1
3:D:618:PCW:H282	4:C:211:17F:H60	0.67	1.66	2	1
3:A:401:PCW:C6	3:B:209:PCW:O31	0.67	2.42	9	6
3:B:211:PCW:H231	4:B:217:17F:H47	0.67	1.65	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:204:PCW:C20	4:C:211:17F:H31	0.67	2.17	10	5
3:A:404:PCW:H73	3:A:404:PCW:C1	0.67	2.20	17	5
3:D:601:PCW:H481	4:D:631:17F:H47	0.67	1.64	8	1
3:A:412:PCW:H452	3:C:208:PCW:H451	0.67	1.66	10	1
3:C:204:PCW:C14	4:C:211:17F:H11A	0.67	2.20	10	1
3:D:603:PCW:C46	3:D:626:PCW:H261	0.67	2.13	11	1
3:B:207:PCW:H472	4:B:215:17F:H44	0.67	1.64	12	1
3:D:618:PCW:C26	3:C:204:PCW:H281	0.67	2.17	14	1
3:B:210:PCW:H162	4:B:216:17F:H8A	0.67	1.64	16	1
3:B:208:PCW:C27	4:B:214:17F:H31	0.67	2.19	19	1
3:D:609:PCW:C20	3:D:609:PCW:C24	0.67	2.71	7	20
3:D:613:PCW:C48	3:D:619:PCW:H431	0.67	2.19	11	3
3:B:203:PCW:H51	3:B:211:PCW:C33	0.67	2.18	16	4
3:A:402:PCW:H331	3:C:206:PCW:O3P	0.67	1.88	2	1
3:A:405:PCW:C37	3:D:601:PCW:H151	0.67	2.16	10	3
4:D:630:17F:H12A	4:D:630:17F:C33	0.67	2.19	17	8
3:A:417:PCW:H431	3:D:612:PCW:H162	0.67	1.66	6	3
3:D:619:PCW:H481	4:C:210:17F:H74	0.67	1.65	7	2
3:B:205:PCW:H283	3:B:212:PCW:O3	0.67	1.89	8	1
3:C:204:PCW:C19	4:C:211:17F:H18	0.67	2.18	9	1
3:A:420:PCW:H442	3:D:617:PCW:C21	0.67	2.12	11	2
3:B:208:PCW:H283	3:B:208:PCW:C24	0.67	2.19	19	1
3:B:208:PCW:C3	3:B:208:PCW:O1P	0.67	2.42	19	1
3:A:407:PCW:H39	4:D:635:17F:H55	0.67	1.65	5	4
3:B:209:PCW:H182	3:B:209:PCW:C34	0.67	2.17	18	6
3:D:608:PCW:H252	3:D:615:PCW:H381	0.67	1.63	3	4
3:B:207:PCW:C13	3:B:210:PCW:H151	0.67	2.20	15	3
3:B:208:PCW:H151	4:B:214:17F:H56	0.67	1.65	3	2
1:A:364:ALA:HA	1:A:368:LEU:HD12	0.67	1.67	11	3
3:A:401:PCW:C7	3:B:209:PCW:H131	0.67	2.20	4	1
3:D:610:PCW:H51	3:C:212:PCW:H73	0.67	1.67	6	2
3:D:616:PCW:H462	3:D:618:PCW:C48	0.67	2.20	15	2
3:B:207:PCW:C44	3:B:213:PCW:H272	0.67	2.19	8	1
3:B:211:PCW:H321	3:B:212:PCW:C1	0.67	2.19	13	2
3:A:401:PCW:H441	3:D:611:PCW:C27	0.67	2.15	14	1
3:D:603:PCW:H452	3:D:605:PCW:C18	0.67	2.20	17	2
3:A:417:PCW:H381	3:D:612:PCW:H432	0.67	1.66	19	1
3:D:618:PCW:H442	3:D:627:PCW:C26	0.67	2.10	15	6
3:C:208:PCW:O31	3:C:208:PCW:H73	0.67	1.90	18	7
3:B:203:PCW:H11	3:B:203:PCW:O31	0.67	1.89	3	2
4:B:214:17F:H46	4:B:217:17F:C37	0.67	2.19	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:407:PCW:H11	3:A:407:PCW:H41	0.67	1.66	15	2
3:B:209:PCW:H73	3:B:209:PCW:O11	0.67	1.90	11	7
3:D:603:PCW:C39	4:D:629:17F:H40	0.67	2.19	6	1
3:A:416:PCW:C28	3:A:419:PCW:H251	0.67	2.11	7	4
4:D:630:17F:O10	4:D:630:17F:H20A	0.67	1.89	7	1
3:B:204:PCW:C36	3:C:204:PCW:H63	0.67	2.19	14	1
3:A:407:PCW:H221	3:C:205:PCW:H152	0.67	1.67	16	1
3:C:208:PCW:H142	3:C:208:PCW:H412	0.67	1.67	17	1
3:D:611:PCW:H261	3:D:619:PCW:H452	0.67	1.66	1	2
3:B:212:PCW:O31	3:B:212:PCW:C4	0.67	2.42	10	14
3:C:207:PCW:H281	3:C:208:PCW:H242	0.67	1.67	1	1
3:A:413:PCW:H341	4:A:414:17F:C1Z	0.67	2.18	11	5
3:D:605:PCW:C25	4:D:629:17F:H41	0.67	2.20	2	5
3:D:618:PCW:H241	3:B:206:PCW:H442	0.67	1.67	8	3
3:D:602:PCW:H62	3:C:212:PCW:P	0.67	2.30	17	9
3:B:211:PCW:H132	4:B:217:17F:H56	0.67	1.65	3	2
3:A:401:PCW:H322	3:B:209:PCW:C25	0.67	2.18	4	1
4:A:414:17F:P1	4:A:414:17F:C17	0.67	2.83	4	1
3:A:420:PCW:H63	4:D:632:17F:O8	0.67	1.89	6	2
3:B:204:PCW:C18	3:B:205:PCW:H482	0.67	2.20	7	2
3:A:411:PCW:C28	3:A:411:PCW:H472	0.67	2.20	9	2
4:D:630:17F:H67	4:D:634:17F:H43	0.67	1.66	11	1
3:D:604:PCW:H461	3:D:619:PCW:H471	0.67	1.65	14	1
3:B:213:PCW:H342	4:B:216:17F:H37	0.67	1.67	16	1
3:B:208:PCW:H281	4:B:216:17F:C26	0.67	2.19	17	1
3:D:605:PCW:C5	3:D:626:PCW:H19	0.67	2.20	20	1
3:D:613:PCW:C48	3:D:619:PCW:H211	0.67	2.19	20	8
3:D:622:PCW:C23	3:D:624:PCW:H221	0.67	2.19	8	10
2:B:144:THR:HG22	2:B:151:GLY:HA3	0.67	1.67	10	2
4:C:211:17F:H12	4:C:211:17F:C37	0.67	2.20	3	3
3:B:207:PCW:H31	3:B:207:PCW:O31	0.67	1.89	4	1
3:A:408:PCW:C25	3:A:417:PCW:H262	0.67	2.17	5	1
3:B:213:PCW:H341	4:B:214:17F:C9	0.67	2.19	5	1
3:A:406:PCW:C25	3:B:207:PCW:H171	0.67	2.16	17	4
3:D:606:PCW:H471	3:B:210:PCW:C48	0.67	2.20	14	1
3:B:210:PCW:O11	4:B:216:17F:H6	0.67	1.89	14	1
3:A:404:PCW:H362	3:B:203:PCW:H19	0.67	1.67	18	2
3:B:207:PCW:C38	4:B:215:17F:H60	0.67	2.19	16	1
3:C:208:PCW:H451	3:C:209:PCW:H412	0.67	1.65	17	1
3:A:408:PCW:H82	4:C:211:17F:O2	0.67	1.89	19	1
3:A:404:PCW:H252	4:A:415:17F:C42	0.67	2.19	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:624:PCW:O4P	3:D:624:PCW:C6	0.67	2.43	5	20
3:A:412:PCW:H452	3:C:208:PCW:H452	0.67	1.67	2	3
3:A:419:PCW:H481	3:D:618:PCW:H281	0.67	1.67	3	4
3:D:605:PCW:H352	4:D:629:17F:O7	0.67	1.90	5	1
3:D:609:PCW:H241	3:D:609:PCW:C19	0.67	2.20	14	3
3:A:406:PCW:H232	3:B:210:PCW:O31	0.67	1.89	8	1
3:A:408:PCW:H282	3:A:417:PCW:H162	0.67	1.66	11	1
3:B:207:PCW:H442	3:B:213:PCW:C23	0.67	2.20	11	1
3:A:404:PCW:H381	3:B:209:PCW:C35	0.67	2.19	13	2
3:B:207:PCW:H452	4:B:215:17F:H41	0.67	1.66	16	1
3:A:407:PCW:H39	4:D:635:17F:C30	0.67	2.20	17	1
3:D:620:PCW:O2P	3:D:621:PCW:H52	0.67	1.88	19	1
3:D:624:PCW:H481	4:C:210:17F:H50	0.67	1.67	19	1
3:D:603:PCW:H231	4:B:217:17F:H76	0.67	1.66	20	1
3:D:625:PCW:H471	3:D:626:PCW:C48	0.66	2.21	16	5
3:B:212:PCW:O11	3:B:212:PCW:H2	0.66	1.89	6	14
3:A:409:PCW:O31	3:A:409:PCW:H51	0.66	1.90	2	2
1:D:523:ASP:HA	1:D:526:ARG:HD2	0.66	1.66	15	7
3:D:627:PCW:O1P	3:D:627:PCW:H52	0.66	1.91	3	7
4:A:415:17F:H77	3:B:203:PCW:H261	0.66	1.67	3	1
3:A:419:PCW:C3	3:D:617:PCW:H422	0.66	2.20	8	3
3:B:207:PCW:H212	3:B:207:PCW:H172	0.66	1.66	11	3
3:A:409:PCW:O3P	3:A:409:PCW:O31	0.66	2.13	7	5
3:A:410:PCW:O1P	3:A:410:PCW:C3	0.66	2.41	19	7
3:B:213:PCW:H281	4:B:215:17F:H67	0.66	1.66	6	1
3:B:210:PCW:H51	3:B:210:PCW:C11	0.66	2.20	15	2
3:A:417:PCW:C34	3:D:612:PCW:H132	0.66	2.15	10	1
3:A:403:PCW:C18	3:A:403:PCW:C14	0.66	2.74	15	1
4:A:414:17F:C28	3:B:212:PCW:H20	0.66	2.20	18	1
3:D:612:PCW:H332	3:D:627:PCW:H132	0.66	1.65	2	6
3:A:407:PCW:H241	3:C:205:PCW:C41	0.66	2.19	2	5
3:D:604:PCW:H322	3:D:613:PCW:C8	0.66	2.21	8	2
3:A:411:PCW:C14	3:A:411:PCW:H19	0.66	2.20	5	3
3:A:418:PCW:H472	3:D:625:PCW:H483	0.66	1.67	5	8
3:B:206:PCW:C42	3:B:206:PCW:C46	0.66	2.69	17	10
3:A:403:PCW:H322	3:C:203:PCW:C1	0.66	2.20	18	2
1:D:470:TYR:HE2	4:D:631:17F:H68	0.66	1.50	5	1
3:D:621:PCW:C42	4:D:634:17F:H66	0.66	2.21	5	1
3:A:404:PCW:C48	3:B:207:PCW:H471	0.66	2.20	6	1
3:A:404:PCW:C41	3:B:209:PCW:H361	0.66	2.20	13	2
3:B:206:PCW:H481	3:C:212:PCW:C40	0.66	2.20	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:418:PCW:H431	3:D:625:PCW:C44	0.66	2.20	11	3
3:B:204:PCW:H272	3:C:207:PCW:C20	0.66	2.21	11	1
3:A:413:PCW:H362	4:C:210:17F:O8	0.66	1.90	19	3
3:D:612:PCW:H62	3:D:618:PCW:H31	0.66	1.67	19	1
3:A:403:PCW:C31	3:A:403:PCW:C35	0.66	2.73	13	18
1:D:512:ASP:HA	1:D:515:ARG:HD2	0.66	1.65	10	10
3:D:622:PCW:C35	3:D:627:PCW:C20	0.66	2.73	20	13
3:A:401:PCW:C7	3:B:209:PCW:O31	0.66	2.42	17	2
3:A:404:PCW:C42	3:B:209:PCW:H19	0.66	2.11	3	1
3:A:407:PCW:H20	3:C:205:PCW:H19	0.66	1.67	6	3
3:A:417:PCW:C40	3:D:612:PCW:H231	0.66	2.21	16	7
4:D:628:17F:C31	4:D:628:17F:C19	0.66	2.73	5	8
3:A:407:PCW:H182	3:C:205:PCW:C17	0.66	2.19	4	1
3:A:407:PCW:C18	3:C:205:PCW:H152	0.66	2.20	4	1
3:A:413:PCW:H251	3:C:203:PCW:C43	0.66	2.20	4	2
3:B:211:PCW:H231	4:B:217:17F:C40	0.66	2.20	4	1
3:B:213:PCW:H432	3:B:213:PCW:H181	0.66	1.66	19	3
3:D:627:PCW:O31	3:D:627:PCW:H63	0.66	1.90	5	1
3:B:210:PCW:H2	3:B:210:PCW:O11	0.66	1.89	5	2
3:A:409:PCW:O2	3:A:409:PCW:H342	0.66	1.90	9	5
3:D:623:PCW:H331	3:D:624:PCW:H322	0.66	1.65	9	1
3:B:211:PCW:H32	4:B:217:17F:C1Y	0.66	2.19	9	2
3:D:625:PCW:O31	3:D:625:PCW:C4	0.66	2.43	20	2
3:A:413:PCW:H352	4:A:414:17F:H34	0.66	1.67	11	1
3:D:615:PCW:H231	3:C:205:PCW:C25	0.66	2.17	12	1
3:A:409:PCW:H63	3:A:409:PCW:C32	0.66	2.19	19	2
3:A:404:PCW:H63	4:A:415:17F:C3	0.66	2.21	16	1
3:B:203:PCW:C41	3:B:211:PCW:H182	0.66	2.17	18	1
3:A:410:PCW:O3P	3:A:410:PCW:H63	0.66	1.90	8	3
3:D:626:PCW:C27	3:D:626:PCW:C23	0.66	2.68	20	17
3:B:207:PCW:H412	3:B:213:PCW:C22	0.66	2.19	2	2
3:B:212:PCW:O31	3:B:212:PCW:O3P	0.66	2.13	1	16
4:C:211:17F:O10	4:C:211:17F:H6A	0.66	1.89	14	6
3:A:409:PCW:C21	3:A:409:PCW:C17	0.66	2.70	9	5
3:C:208:PCW:O2P	3:C:209:PCW:H82	0.66	1.90	7	8
3:A:408:PCW:H362	3:C:207:PCW:H462	0.66	1.66	7	2
3:D:610:PCW:H482	3:B:212:PCW:H241	0.66	1.66	3	1
3:B:204:PCW:H283	4:C:211:17F:H20	0.66	1.67	3	1
3:C:204:PCW:H122	4:C:211:17F:C10	0.66	2.19	3	1
3:A:412:PCW:H411	3:C:208:PCW:H361	0.66	1.68	4	1
3:B:213:PCW:H431	4:B:214:17F:H55	0.66	1.66	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:419:PCW:H39	3:D:617:PCW:H451	0.66	1.68	6	2
3:C:203:PCW:H342	3:C:203:PCW:C7	0.66	2.21	7	1
3:A:404:PCW:H411	3:B:209:PCW:H341	0.66	1.65	16	2
3:A:406:PCW:C25	3:B:207:PCW:H19	0.66	2.20	11	1
3:B:206:PCW:H482	3:C:212:PCW:H211	0.66	1.67	13	1
3:D:625:PCW:H451	3:D:626:PCW:C47	0.66	2.20	19	1
3:D:625:PCW:C46	3:D:626:PCW:H482	0.66	2.20	11	7
4:D:634:17F:H40	4:D:634:17F:H30	0.66	1.67	6	7
3:B:205:PCW:H432	3:C:208:PCW:H171	0.66	1.66	1	1
3:A:413:PCW:H321	4:A:414:17F:H20	0.66	1.68	2	1
3:D:602:PCW:H242	3:D:610:PCW:C35	0.66	2.20	15	6
3:C:207:PCW:H451	3:C:207:PCW:H19	0.66	1.67	2	1
3:C:203:PCW:H172	3:C:203:PCW:C46	0.66	2.21	3	1
3:A:405:PCW:H382	4:D:628:17F:H52	0.66	1.67	5	2
3:B:211:PCW:H342	3:B:212:PCW:O3P	0.66	1.90	16	6
3:B:204:PCW:H232	3:C:208:PCW:C24	0.66	2.18	8	1
4:B:214:17F:H2	4:B:214:17F:O2	0.66	1.90	12	1
3:B:212:PCW:C15	3:C:204:PCW:H361	0.66	2.19	13	1
4:B:217:17F:H63	4:B:217:17F:H30	0.66	1.68	14	1
3:A:406:PCW:H481	3:D:606:PCW:C26	0.66	2.20	5	2
3:A:406:PCW:C3	3:A:406:PCW:O1P	0.66	2.44	11	7
3:A:408:PCW:O11	3:A:408:PCW:H2	0.66	1.90	1	17
3:B:207:PCW:C14	3:B:210:PCW:H382	0.66	2.20	7	3
3:D:621:PCW:C37	4:D:633:17F:H63	0.66	2.17	19	4
3:B:205:PCW:C39	4:B:214:17F:H66	0.66	2.21	6	2
3:B:208:PCW:H421	3:B:208:PCW:C37	0.66	2.11	20	2
3:A:413:PCW:H252	4:A:414:17F:C33	0.66	2.21	16	2
3:D:604:PCW:C42	3:D:619:PCW:H141	0.66	2.19	11	3
3:D:613:PCW:C21	4:C:210:17F:H47	0.66	2.20	6	10
3:D:613:PCW:H212	4:C:210:17F:H47	0.66	1.66	20	8
3:B:212:PCW:C43	3:B:212:PCW:C47	0.66	2.71	18	3
3:B:213:PCW:H462	4:B:217:17F:H40	0.66	1.68	8	1
3:D:614:PCW:C45	3:D:619:PCW:H222	0.66	2.18	17	2
3:A:404:PCW:H82	4:A:415:17F:O2	0.66	1.89	11	1
3:B:205:PCW:C41	3:B:206:PCW:H162	0.66	2.20	11	1
3:C:204:PCW:C35	4:C:211:17F:H4	0.66	2.17	11	1
3:D:604:PCW:H482	4:C:210:17F:H75	0.66	1.68	13	1
3:B:205:PCW:C20	3:B:212:PCW:H331	0.66	2.21	13	2
3:A:413:PCW:C16	4:A:414:17F:H34	0.66	2.20	14	2
4:D:628:17F:H76	4:B:216:17F:C30	0.66	2.21	18	1
3:B:213:PCW:H122	4:B:217:17F:O10	0.66	1.90	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:610:PCW:H262	3:D:610:PCW:C42	0.66	2.20	16	3
3:B:205:PCW:H362	3:C:208:PCW:H332	0.66	1.66	1	1
3:B:206:PCW:O1P	3:B:206:PCW:C3	0.66	2.44	8	5
3:D:613:PCW:H251	4:C:210:17F:H43	0.66	1.65	19	3
3:B:210:PCW:C47	3:B:210:PCW:H281	0.66	2.20	3	2
3:A:409:PCW:H182	3:A:409:PCW:H39	0.66	1.66	19	3
3:A:403:PCW:H342	3:C:203:PCW:H12	0.66	1.68	11	3
3:B:203:PCW:H271	4:B:215:17F:H55	0.66	1.67	5	1
3:A:403:PCW:C13	3:C:203:PCW:H12	0.66	2.08	7	2
3:D:615:PCW:H452	3:C:205:PCW:H242	0.66	1.66	7	1
3:C:204:PCW:H19	4:C:211:17F:C18	0.66	2.21	7	1
3:D:616:PCW:H452	3:B:206:PCW:H471	0.66	1.67	12	2
3:B:208:PCW:C41	4:B:214:17F:H12	0.66	2.19	12	2
3:B:204:PCW:H451	3:C:203:PCW:H132	0.66	1.68	15	2
4:D:630:17F:H53	4:B:214:17F:H73	0.66	1.68	16	1
3:D:622:PCW:C47	3:B:206:PCW:H272	0.66	2.20	18	1
3:A:406:PCW:H11	3:A:411:PCW:H82	0.66	1.67	1	1
3:D:604:PCW:C39	3:D:611:PCW:H341	0.66	2.17	14	8
3:D:621:PCW:H421	4:D:634:17F:H59	0.66	1.67	11	5
3:D:625:PCW:H39	3:D:626:PCW:C14	0.66	2.19	2	3
3:A:404:PCW:C3	3:B:209:PCW:H382	0.66	2.20	4	1
3:A:420:PCW:H19	4:D:632:17F:C31	0.66	2.19	4	6
3:A:420:PCW:H442	3:D:617:PCW:C22	0.66	2.21	5	1
3:A:407:PCW:C6	3:B:213:PCW:H322	0.66	2.21	8	1
4:C:211:17F:H11	4:C:211:17F:C38	0.66	2.21	8	1
3:A:404:PCW:H262	4:A:415:17F:H68	0.66	1.67	18	1
3:B:207:PCW:C1	4:B:216:17F:H8A	0.66	2.18	19	1
3:A:404:PCW:H132	3:A:404:PCW:C8	0.66	2.21	1	1
3:D:614:PCW:C46	3:D:614:PCW:C42	0.66	2.72	17	18
3:B:210:PCW:C20	3:B:210:PCW:C24	0.66	2.72	1	1
2:C:46:ILE:HD13	2:C:160:VAL:HG21	0.66	1.65	2	3
3:C:208:PCW:H372	3:C:209:PCW:C7	0.66	2.21	10	2
3:B:210:PCW:H121	4:B:216:17F:O7	0.66	1.89	3	1
3:A:419:PCW:H40	3:D:616:PCW:H232	0.66	1.68	12	3
3:A:402:PCW:H82	3:A:409:PCW:O11	0.66	1.91	6	1
3:A:408:PCW:H361	3:C:207:PCW:H442	0.66	1.65	7	2
3:D:612:PCW:H471	3:D:612:PCW:H252	0.66	1.67	20	3
3:D:616:PCW:H221	3:D:616:PCW:C18	0.66	2.20	12	2
3:A:409:PCW:H82	3:C:206:PCW:C37	0.66	2.20	17	3
3:B:207:PCW:H442	3:B:213:PCW:H231	0.66	1.67	11	1
3:A:403:PCW:H411	3:A:403:PCW:C12	0.66	2.20	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:207:PCW:H152	3:B:210:PCW:C37	0.66	2.21	17	1
3:A:409:PCW:C12	3:C:206:PCW:H332	0.66	2.20	1	3
4:D:629:17F:H5	4:D:629:17F:C19	0.66	2.04	18	10
3:A:401:PCW:H452	3:D:611:PCW:H251	0.66	1.68	4	2
3:A:407:PCW:C18	3:C:205:PCW:H172	0.66	2.20	7	2
4:A:414:17F:C26	3:B:212:PCW:H19	0.66	2.09	4	2
3:D:602:PCW:H162	3:D:624:PCW:C21	0.66	2.20	9	4
3:A:404:PCW:C21	4:A:415:17F:H58	0.66	2.18	5	1
3:A:403:PCW:H122	3:A:403:PCW:C41	0.66	2.21	15	1
3:B:211:PCW:H242	4:B:217:17F:C42	0.66	2.18	15	1
3:B:210:PCW:H281	3:B:210:PCW:H482	0.66	1.65	17	1
3:B:211:PCW:H19	3:B:211:PCW:H482	0.66	1.68	19	1
3:D:614:PCW:H11	3:D:614:PCW:O31	0.65	1.90	7	15
3:C:208:PCW:C26	3:C:208:PCW:C22	0.65	2.72	18	8
3:A:405:PCW:C39	4:D:628:17F:H54	0.65	2.21	2	1
3:D:622:PCW:H352	3:D:627:PCW:C21	0.65	2.21	2	13
3:A:416:PCW:H371	3:A:416:PCW:H411	0.65	1.67	5	4
3:D:605:PCW:C6	3:D:605:PCW:O4P	0.65	2.44	10	4
3:B:213:PCW:H421	4:B:217:17F:C12	0.65	2.04	13	5
3:D:613:PCW:O31	3:D:619:PCW:H2	0.65	1.91	7	6
3:B:205:PCW:C19	3:B:212:PCW:H342	0.65	2.21	7	4
3:B:210:PCW:H121	4:B:216:17F:C18	0.65	2.19	5	1
3:B:211:PCW:H451	3:B:212:PCW:H131	0.65	1.68	6	1
3:A:410:PCW:H121	3:C:209:PCW:H161	0.65	1.68	8	1
3:C:206:PCW:H152	3:C:206:PCW:H361	0.65	1.67	13	2
3:D:615:PCW:H161	4:D:635:17F:C11	0.65	2.21	12	1
3:C:207:PCW:C28	3:C:209:PCW:H39	0.65	2.19	12	1
3:A:404:PCW:C44	4:B:215:17F:H37	0.65	2.21	16	1
3:A:404:PCW:H441	4:B:215:17F:H37	0.65	1.67	16	1
3:B:207:PCW:H442	3:B:213:PCW:H261	0.65	1.67	19	1
3:A:416:PCW:H161	3:A:419:PCW:H352	0.65	1.67	1	1
3:B:204:PCW:H322	3:B:206:PCW:C34	0.65	2.22	3	1
3:A:420:PCW:C31	3:D:617:PCW:H51	0.65	2.20	4	1
3:D:609:PCW:H172	4:D:633:17F:H61	0.65	1.66	4	8
4:D:635:17F:H65	3:C:205:PCW:H482	0.65	1.68	5	3
3:A:406:PCW:H31	3:A:406:PCW:O4P	0.65	1.91	14	7
3:A:413:PCW:C12	4:A:414:17F:H33	0.65	2.17	7	1
3:B:204:PCW:H442	3:C:203:PCW:C35	0.65	2.20	7	1
3:B:211:PCW:H221	3:B:211:PCW:H181	0.65	1.69	17	2
4:C:211:17F:H20A	4:C:211:17F:O9	0.65	1.90	7	1
3:A:407:PCW:C37	4:D:635:17F:H55	0.65	2.22	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:413:PCW:H381	4:C:210:17F:H9A	0.65	1.67	15	2
3:A:408:PCW:H272	3:D:616:PCW:C21	0.65	2.19	14	1
3:C:207:PCW:H252	3:C:208:PCW:H231	0.65	1.68	14	1
3:A:403:PCW:C32	3:C:204:PCW:H51	0.65	2.20	1	2
3:D:607:PCW:O11	3:D:607:PCW:H2	0.65	1.91	6	19
3:D:618:PCW:H63	3:D:622:PCW:P	0.65	2.31	14	9
3:A:410:PCW:O2P	3:A:410:PCW:C3	0.65	2.45	2	1
3:A:410:PCW:H122	3:C:207:PCW:H272	0.65	1.67	2	1
3:D:623:PCW:C2	3:D:624:PCW:H322	0.65	2.21	10	3
3:A:410:PCW:C24	3:C:208:PCW:H242	0.65	2.21	12	4
3:D:601:PCW:H483	3:D:607:PCW:C23	0.65	2.22	5	1
3:C:208:PCW:H132	3:C:209:PCW:H321	0.65	1.68	5	1
3:A:403:PCW:O1P	3:A:403:PCW:C3	0.65	2.44	16	2
3:D:621:PCW:H483	4:D:634:17F:H56	0.65	1.67	12	1
3:C:204:PCW:C43	4:C:211:17F:H30	0.65	2.21	12	1
3:A:419:PCW:H39	3:D:616:PCW:C17	0.65	2.13	17	1
3:C:208:PCW:C14	3:C:209:PCW:H382	0.65	2.20	18	1
3:D:616:PCW:H342	3:C:212:PCW:C34	0.65	2.20	1	1
3:D:602:PCW:C31	3:D:602:PCW:C4	0.65	2.73	4	4
3:D:611:PCW:H161	3:D:619:PCW:H151	0.65	1.68	10	6
4:D:628:17F:O10	4:D:628:17F:C7	0.65	2.45	2	18
3:B:211:PCW:H472	3:B:211:PCW:H141	0.65	1.65	2	1
3:A:416:PCW:O11	3:D:617:PCW:H332	0.65	1.90	10	2
3:B:203:PCW:H222	4:C:210:17F:C19	0.65	2.20	7	3
3:B:211:PCW:H152	4:B:217:17F:H35	0.65	1.69	7	1
3:A:410:PCW:O1P	3:C:207:PCW:H152	0.65	1.91	8	1
3:B:206:PCW:H231	3:C:208:PCW:C20	0.65	2.22	10	1
3:B:208:PCW:H161	4:B:214:17F:C33	0.65	2.19	15	2
3:D:620:PCW:H272	4:D:635:17F:H37	0.65	1.68	13	1
3:A:411:PCW:H152	3:B:209:PCW:C28	0.65	2.21	16	1
3:C:207:PCW:H281	3:C:208:PCW:C24	0.65	2.20	1	1
3:A:411:PCW:H482	3:A:411:PCW:H262	0.65	1.67	3	1
4:D:630:17F:C37	4:D:634:17F:H39	0.65	2.21	3	5
3:B:210:PCW:H121	4:B:216:17F:H6	0.65	1.67	9	5
3:A:404:PCW:H452	4:B:215:17F:H44	0.65	1.68	5	1
3:A:413:PCW:H141	4:A:414:17F:C32	0.65	2.22	14	3
3:B:209:PCW:O31	3:B:209:PCW:H11	0.65	1.91	5	2
3:B:204:PCW:O2	3:C:204:PCW:H352	0.65	1.90	20	2
3:B:204:PCW:H151	3:B:206:PCW:O2	0.65	1.91	20	4
4:A:414:17F:H29	3:C:203:PCW:C40	0.65	2.22	19	2
3:A:413:PCW:H121	4:A:414:17F:H59	0.65	1.68	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:68:ARG:HA	2:B:71:TYR:CD1	0.65	2.27	9	1
3:A:401:PCW:H471	3:D:614:PCW:H222	0.65	1.67	10	1
3:A:404:PCW:H461	3:B:209:PCW:H471	0.65	1.68	10	1
3:D:624:PCW:H232	4:C:211:17F:H54	0.65	1.69	11	1
3:B:208:PCW:H32	4:B:214:17F:H1	0.65	1.68	17	2
3:B:210:PCW:H141	4:B:216:17F:C6	0.65	2.22	15	2
3:B:210:PCW:H162	4:B:216:17F:H29	0.65	1.69	18	1
1:A:275:LYS:O	1:A:279:LEU:HG	0.65	1.92	8	20
3:B:204:PCW:C25	3:B:204:PCW:C21	0.65	2.73	7	10
4:D:630:17F:H62	4:D:634:17F:H29	0.65	1.68	19	6
4:A:415:17F:O9	4:A:415:17F:H20	0.65	1.91	10	9
3:B:203:PCW:O1P	3:B:211:PCW:H331	0.65	1.90	5	1
3:A:408:PCW:O4P	3:C:204:PCW:H171	0.65	1.91	7	1
4:A:415:17F:H78	3:D:611:PCW:H472	0.65	1.68	8	1
3:D:604:PCW:H232	3:D:613:PCW:H161	0.65	1.67	8	1
4:D:633:17F:H78	3:C:206:PCW:H281	0.65	1.67	20	2
3:B:205:PCW:C44	3:B:206:PCW:H182	0.65	2.17	9	1
3:B:204:PCW:C8	3:B:212:PCW:H62	0.65	2.22	11	1
3:D:608:PCW:C27	4:D:628:17F:H73	0.65	2.22	13	3
4:D:635:17F:H65	3:C:205:PCW:H483	0.65	1.67	12	1
3:D:621:PCW:H151	4:D:634:17F:H6	0.65	1.65	13	1
3:D:616:PCW:C33	3:C:212:PCW:H341	0.65	2.22	14	2
3:B:213:PCW:H32	4:B:217:17F:O1	0.65	1.91	18	4
3:A:401:PCW:H321	3:B:209:PCW:H381	0.65	1.67	15	1
3:B:207:PCW:H422	3:B:213:PCW:H261	0.65	1.68	15	1
3:B:210:PCW:H82	4:B:216:17F:H18	0.65	1.67	15	1
3:A:411:PCW:C14	3:A:411:PCW:C19	0.65	2.56	17	1
4:C:211:17F:H62	4:C:211:17F:H11	0.65	1.68	17	1
3:B:210:PCW:H482	4:B:214:17F:H54	0.65	1.69	18	1
3:C:209:PCW:H321	3:C:209:PCW:C7	0.65	2.21	18	1
3:A:410:PCW:H52	3:C:209:PCW:O11	0.65	1.92	19	1
3:A:407:PCW:H63	3:B:213:PCW:C31	0.65	2.22	20	1
3:A:407:PCW:H52	3:B:213:PCW:H321	0.65	1.69	20	1
1:A:299:SER:HB2	1:A:300:PRO:HD3	0.65	1.66	20	5
3:A:417:PCW:C35	3:D:612:PCW:C13	0.65	2.75	5	9
3:D:615:PCW:O1P	3:D:615:PCW:H52	0.65	1.90	7	12
3:D:625:PCW:O11	3:D:625:PCW:H2	0.65	1.91	19	15
3:D:623:PCW:H39	3:D:623:PCW:H131	0.65	1.66	9	3
3:B:207:PCW:H41	4:B:216:17F:N1	0.65	2.05	8	2
3:B:213:PCW:C24	3:B:213:PCW:C20	0.65	2.75	16	14
3:A:418:PCW:H452	3:D:625:PCW:H462	0.65	1.67	12	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:624:PCW:H271	3:B:212:PCW:H281	0.65	1.68	4	1
4:D:630:17F:C7	4:D:630:17F:C17	0.65	2.75	16	2
3:B:204:PCW:C44	3:C:203:PCW:H351	0.65	2.21	7	1
3:C:208:PCW:H181	3:C:208:PCW:H461	0.65	1.69	18	2
3:A:401:PCW:H452	3:D:611:PCW:C27	0.65	2.22	18	3
3:B:206:PCW:H172	3:C:212:PCW:H281	0.65	1.66	10	1
3:D:606:PCW:H451	3:D:625:PCW:H471	0.65	1.68	19	1
3:A:402:PCW:O11	3:A:402:PCW:C5	0.65	2.45	1	8
3:D:618:PCW:H63	3:D:622:PCW:O2P	0.65	1.92	14	6
3:B:207:PCW:O3	3:B:207:PCW:O31	0.65	2.15	1	15
3:A:402:PCW:H451	4:D:635:17F:C29	0.65	2.21	11	2
3:A:407:PCW:C28	3:A:407:PCW:C24	0.65	2.74	15	3
3:D:603:PCW:H361	4:D:629:17F:H36	0.65	1.68	4	4
3:D:603:PCW:H412	3:D:605:PCW:H241	0.65	1.67	13	8
3:A:404:PCW:H151	4:A:415:17F:H56	0.65	1.69	7	2
3:A:401:PCW:H442	3:D:614:PCW:H242	0.65	1.68	9	1
3:D:605:PCW:H372	4:D:629:17F:O8	0.65	1.91	11	2
4:A:415:17F:H71	3:B:203:PCW:C27	0.65	2.21	11	1
3:D:616:PCW:H461	3:C:212:PCW:H451	0.65	1.68	11	1
3:A:406:PCW:H82	3:B:207:PCW:H371	0.65	1.68	13	1
3:C:208:PCW:H52	3:C:208:PCW:C31	0.65	2.22	19	2
3:C:207:PCW:H63	4:C:211:17F:O4	0.65	1.92	17	1
3:D:601:PCW:H483	4:D:628:17F:H65	0.65	1.69	18	1
4:D:628:17F:C31	4:D:631:17F:H51	0.65	2.20	15	9
3:B:205:PCW:H40	4:B:214:17F:C39	0.65	2.19	10	3
3:D:601:PCW:H422	4:D:628:17F:H42	0.65	1.69	2	1
4:D:629:17F:C26	4:D:630:17F:H73	0.65	2.22	5	4
3:B:207:PCW:H421	3:B:213:PCW:C23	0.65	2.22	14	3
3:D:607:PCW:H211	4:D:631:17F:H20	0.65	1.68	4	2
3:A:412:PCW:H451	3:C:208:PCW:C18	0.65	2.21	5	2
3:B:212:PCW:C40	3:C:212:PCW:H283	0.65	2.21	5	2
3:D:618:PCW:H362	4:D:633:17F:C23	0.65	2.21	20	3
3:A:419:PCW:H452	3:D:616:PCW:H232	0.65	1.69	10	1
4:A:415:17F:H77	3:D:611:PCW:C47	0.65	2.21	18	2
3:B:205:PCW:H272	3:B:211:PCW:C47	0.65	2.21	11	1
3:A:404:PCW:H411	3:B:209:PCW:C19	0.65	2.21	17	2
3:D:622:PCW:H162	3:C:212:PCW:C17	0.65	2.21	19	3
3:A:406:PCW:H221	3:B:210:PCW:O11	0.65	1.91	16	1
3:D:616:PCW:C48	3:B:206:PCW:H40	0.65	2.14	17	1
3:B:205:PCW:H282	3:B:211:PCW:H451	0.65	1.69	1	3
3:A:409:PCW:H221	3:A:409:PCW:C17	0.65	2.21	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:410:PCW:C6	3:A:410:PCW:O4P	0.65	2.45	12	19
3:D:609:PCW:C24	3:D:609:PCW:H20	0.65	2.22	18	14
3:D:613:PCW:C47	3:D:619:PCW:H431	0.65	2.22	14	3
3:B:211:PCW:H321	3:B:212:PCW:O3P	0.65	1.91	5	3
3:B:205:PCW:H52	3:B:208:PCW:C1	0.65	2.22	7	1
4:B:216:17F:H55	3:C:205:PCW:H251	0.65	1.67	7	1
3:A:413:PCW:C12	4:A:414:17F:H69	0.65	2.22	19	4
4:A:414:17F:H11	3:C:203:PCW:H381	0.65	1.68	8	2
3:A:404:PCW:H63	4:A:415:17F:H2	0.65	1.68	9	1
3:A:404:PCW:H162	4:A:415:17F:H56	0.65	1.66	20	2
3:A:407:PCW:H482	3:D:615:PCW:H281	0.65	1.66	17	4
3:D:611:PCW:P	3:D:613:PCW:H61	0.65	2.31	17	3
3:D:616:PCW:H482	3:C:208:PCW:H283	0.65	1.67	10	4
3:A:407:PCW:H441	3:D:601:PCW:H341	0.65	1.67	12	1
4:B:214:17F:H41	4:B:217:17F:H66	0.65	1.68	20	2
3:A:402:PCW:H442	3:C:205:PCW:H381	0.65	1.69	18	1
3:B:208:PCW:H231	3:B:208:PCW:C27	0.65	2.22	19	1
3:B:208:PCW:O2P	3:B:208:PCW:C3	0.64	2.44	13	6
4:B:214:17F:H20	4:B:214:17F:O10	0.64	1.92	1	6
3:C:208:PCW:C31	3:C:208:PCW:C35	0.64	2.75	15	17
3:A:411:PCW:C39	4:B:215:17F:H65	0.64	2.22	2	2
3:A:407:PCW:H182	3:C:205:PCW:C15	0.64	2.22	4	1
4:D:629:17F:H54	3:B:212:PCW:C45	0.64	2.22	6	2
3:A:413:PCW:C46	3:D:613:PCW:H231	0.64	2.22	18	3
3:C:204:PCW:H351	4:C:211:17F:C7	0.64	2.22	20	3
3:D:623:PCW:H131	3:D:623:PCW:C39	0.64	2.21	9	1
3:A:404:PCW:H412	3:B:209:PCW:C38	0.64	2.22	10	1
3:A:416:PCW:H282	3:A:419:PCW:H252	0.64	1.67	10	2
3:D:616:PCW:C45	3:C:212:PCW:H431	0.64	2.20	11	1
3:B:212:PCW:O4P	3:B:212:PCW:H32	0.64	1.92	12	1
3:A:410:PCW:H351	3:C:209:PCW:H151	0.64	1.68	20	2
3:A:410:PCW:H32	3:C:207:PCW:H141	0.64	1.69	17	1
3:D:618:PCW:H483	3:B:204:PCW:H242	0.64	1.69	17	1
3:C:207:PCW:C23	3:C:208:PCW:H241	0.64	2.22	19	1
3:A:410:PCW:C15	3:C:207:PCW:H232	0.64	2.21	20	1
3:D:624:PCW:C24	3:D:624:PCW:C20	0.64	2.73	20	20
3:B:209:PCW:H31	3:B:209:PCW:P	0.64	2.30	2	7
4:D:630:17F:H62	4:D:634:17F:C1X	0.64	2.21	14	6
3:B:210:PCW:H32	3:B:210:PCW:O2P	0.64	1.91	11	6
3:D:614:PCW:H442	3:D:619:PCW:H19	0.64	1.67	18	8
3:B:206:PCW:H40	3:C:212:PCW:H251	0.64	1.70	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:213:PCW:H281	4:B:215:17F:C37	0.64	2.23	6	1
3:A:407:PCW:H19	3:B:208:PCW:H261	0.64	1.69	9	2
4:D:630:17F:H54	4:B:214:17F:C42	0.64	2.23	10	1
3:A:403:PCW:H19	3:C:203:PCW:C12	0.64	2.22	13	1
3:A:403:PCW:H232	3:A:403:PCW:H461	0.64	1.69	17	1
3:B:208:PCW:H142	4:B:214:17F:C31	0.64	2.22	18	1
3:D:618:PCW:H342	3:D:627:PCW:C34	0.64	2.22	9	2
3:D:601:PCW:C48	4:D:628:17F:H56	0.64	2.20	5	4
3:C:203:PCW:H442	3:C:203:PCW:C17	0.64	2.22	2	2
3:A:409:PCW:P	3:A:412:PCW:O1P	0.64	2.55	13	3
3:A:413:PCW:C14	3:A:413:PCW:C18	0.64	2.73	3	3
3:D:615:PCW:C27	4:D:635:17F:H42	0.64	2.20	3	1
3:A:407:PCW:C1	4:B:216:17F:H29	0.64	2.23	7	1
3:A:420:PCW:H122	4:D:632:17F:H9A	0.64	1.69	16	7
3:B:204:PCW:H121	3:C:204:PCW:C39	0.64	2.22	12	4
3:D:622:PCW:H421	3:B:206:PCW:C28	0.64	2.21	9	1
3:D:624:PCW:H62	3:D:624:PCW:H2	0.64	1.69	14	3
3:A:407:PCW:C16	3:B:208:PCW:H222	0.64	2.23	1	3
3:D:621:PCW:C28	4:D:633:17F:H30	0.64	2.22	17	7
3:C:203:PCW:O31	3:C:203:PCW:O3	0.64	2.16	13	15
3:C:208:PCW:H252	3:C:209:PCW:H442	0.64	1.69	1	1
3:A:403:PCW:H482	3:D:617:PCW:H281	0.64	1.69	6	1
3:A:406:PCW:H242	3:B:210:PCW:C12	0.64	2.22	16	2
3:D:622:PCW:H232	3:D:624:PCW:H221	0.64	1.69	10	3
3:D:624:PCW:H481	4:C:210:17F:C30	0.64	2.22	7	2
3:D:614:PCW:C42	3:D:614:PCW:C46	0.64	2.69	10	2
3:B:207:PCW:H73	3:B:213:PCW:H41	0.64	1.69	12	1
3:D:601:PCW:H371	4:B:216:17F:H70	0.64	1.69	17	1
3:C:212:PCW:O31	3:C:212:PCW:C1	0.64	2.44	18	17
3:A:406:PCW:O1P	3:A:406:PCW:C3	0.64	2.46	16	7
3:B:211:PCW:C7	3:B:212:PCW:H62	0.64	2.22	2	1
3:D:604:PCW:C48	3:D:619:PCW:H432	0.64	2.23	3	2
5:C:201:GDP:O3B	5:C:201:GDP:O2A	0.64	2.15	3	1
3:B:205:PCW:C45	3:C:208:PCW:H19	0.64	2.13	10	2
3:A:404:PCW:H51	4:A:415:17F:O5	0.64	1.92	6	3
3:D:604:PCW:C48	3:D:619:PCW:H421	0.64	2.21	6	2
3:D:622:PCW:H73	4:D:633:17F:H11A	0.64	1.69	6	3
3:D:622:PCW:H271	3:D:624:PCW:H261	0.64	1.69	7	1
3:C:208:PCW:C46	3:C:209:PCW:H422	0.64	2.22	7	3
3:A:413:PCW:H481	4:A:414:17F:H68	0.64	1.68	11	1
3:B:205:PCW:H452	3:C:208:PCW:H282	0.64	1.68	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:208:PCW:H181	3:C:206:PCW:C19	0.64	2.22	16	1
3:B:213:PCW:C34	4:B:216:17F:H37	0.64	2.23	16	1
3:A:410:PCW:H162	3:C:207:PCW:H211	0.64	1.68	19	1
3:A:409:PCW:H212	3:A:409:PCW:H161	0.64	1.68	1	4
3:A:409:PCW:C39	3:A:409:PCW:H182	0.64	2.22	2	2
3:C:208:PCW:H2	3:C:209:PCW:C8	0.64	2.19	4	3
3:A:404:PCW:O11	3:A:404:PCW:H2	0.64	1.91	19	2
3:B:212:PCW:H421	3:C:212:PCW:H283	0.64	1.69	20	2
2:C:68:ARG:HA	2:C:71:TYR:CE1	0.64	2.28	6	9
3:D:615:PCW:C45	3:C:205:PCW:H241	0.64	2.20	14	3
3:B:205:PCW:C45	3:B:206:PCW:H212	0.64	2.23	9	3
4:A:415:17F:H74	4:C:210:17F:H68	0.64	1.68	16	4
3:B:208:PCW:H352	4:B:214:17F:H59	0.64	1.70	9	1
3:C:204:PCW:H431	4:C:211:17F:H30	0.64	1.68	12	1
3:A:407:PCW:H482	4:D:635:17F:H46	0.64	1.68	15	1
3:A:411:PCW:H152	3:B:209:PCW:H281	0.64	1.70	16	1
3:D:611:PCW:C8	3:D:625:PCW:H141	0.64	2.23	1	1
3:B:204:PCW:O1P	3:C:207:PCW:H63	0.64	1.93	1	1
3:B:206:PCW:H12	3:B:206:PCW:O31	0.64	1.90	3	10
3:A:403:PCW:C28	3:A:413:PCW:H271	0.64	2.23	2	1
3:B:204:PCW:O31	3:B:204:PCW:H11	0.64	1.93	2	3
3:B:209:PCW:H251	3:B:209:PCW:H432	0.64	1.69	2	1
3:A:401:PCW:H451	3:D:614:PCW:H262	0.64	1.68	3	1
3:B:206:PCW:C24	3:C:208:PCW:H282	0.64	2.22	14	3
3:B:213:PCW:H122	4:B:217:17F:O8	0.64	1.92	4	4
3:B:206:PCW:C38	4:C:211:17F:H47	0.64	2.15	4	1
3:A:408:PCW:H261	3:A:417:PCW:H241	0.64	1.68	5	1
3:B:208:PCW:H2	4:B:214:17F:C4	0.64	2.22	5	4
3:B:211:PCW:C6	3:B:212:PCW:H321	0.64	2.21	5	5
3:B:213:PCW:H441	3:B:213:PCW:H222	0.64	1.68	8	3
3:C:204:PCW:C22	4:C:211:17F:H20	0.64	2.18	9	1
3:A:405:PCW:C46	3:A:405:PCW:C42	0.64	2.72	4	11
3:A:411:PCW:H272	3:A:411:PCW:C48	0.64	2.22	1	4
3:A:407:PCW:C18	3:C:205:PCW:H362	0.64	2.23	11	6
3:A:418:PCW:H39	3:D:625:PCW:H441	0.64	1.69	2	2
4:D:629:17F:C10	4:D:634:17F:H48	0.64	2.21	3	5
4:D:634:17F:C41	3:C:206:PCW:H283	0.64	2.22	7	3
3:B:207:PCW:O1P	4:B:216:17F:N1	0.64	2.31	4	2
3:B:205:PCW:H19	3:B:212:PCW:H342	0.64	1.70	5	2
3:B:206:PCW:C43	3:C:204:PCW:H441	0.64	2.22	5	2
3:A:417:PCW:H471	3:D:612:PCW:C27	0.64	2.23	12	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:417:PCW:O31	3:A:417:PCW:O3P	0.64	2.16	8	3
3:D:608:PCW:H131	3:D:615:PCW:C7	0.64	2.23	8	1
3:B:206:PCW:H341	3:C:204:PCW:H381	0.64	1.69	10	1
3:A:419:PCW:H371	3:D:610:PCW:H162	0.64	1.70	11	1
3:D:611:PCW:H412	3:D:611:PCW:H20	0.64	1.70	11	2
3:D:622:PCW:H381	3:C:212:PCW:H483	0.64	1.70	12	1
3:A:403:PCW:H422	3:A:403:PCW:H212	0.64	1.70	13	1
3:A:403:PCW:C16	3:C:203:PCW:H122	0.64	2.23	1	2
3:A:413:PCW:H321	4:A:414:17F:C20	0.64	2.23	2	2
3:D:620:PCW:P	3:D:621:PCW:H42	0.64	2.33	3	2
3:B:212:PCW:H421	3:C:212:PCW:C26	0.64	2.23	1	1
3:B:213:PCW:H411	3:B:213:PCW:C18	0.64	2.21	2	1
3:B:210:PCW:H52	3:B:210:PCW:H2	0.64	1.70	3	2
3:A:402:PCW:C16	3:A:409:PCW:H211	0.64	2.20	5	1
3:D:608:PCW:H122	3:D:615:PCW:H73	0.64	1.69	13	3
3:D:621:PCW:C41	4:D:635:17F:H77	0.64	2.18	13	7
4:D:633:17F:H53	3:C:208:PCW:H252	0.64	1.69	7	2
3:B:211:PCW:H451	3:B:212:PCW:C13	0.64	2.23	6	1
3:B:203:PCW:H461	4:B:217:17F:H52	0.64	1.70	10	1
3:B:203:PCW:H19	4:B:215:17F:H42	0.64	1.69	11	1
3:D:605:PCW:H52	3:D:626:PCW:C19	0.64	2.21	14	1
3:A:416:PCW:C45	3:D:617:PCW:H252	0.64	2.23	16	1
3:D:604:PCW:C26	3:D:613:PCW:H181	0.64	2.23	19	2
3:A:407:PCW:H171	3:C:205:PCW:H341	0.64	1.67	19	1
3:A:407:PCW:H73	4:B:214:17F:H6	0.64	1.70	20	1
3:A:412:PCW:H332	3:C:206:PCW:C45	0.64	2.14	20	1
3:A:409:PCW:O31	3:A:409:PCW:O3P	0.64	2.16	1	2
3:A:420:PCW:H341	3:D:617:PCW:H132	0.64	1.67	1	2
3:D:601:PCW:H252	4:D:631:17F:H76	0.64	1.67	1	1
3:A:404:PCW:H62	3:B:203:PCW:H131	0.64	1.68	2	1
3:B:210:PCW:H141	4:B:216:17F:H18A	0.64	1.69	7	2
3:A:405:PCW:C48	4:D:628:17F:H51	0.64	2.23	6	1
3:A:405:PCW:C42	3:A:405:PCW:C46	0.64	2.75	7	4
3:A:413:PCW:H181	4:A:414:17F:C1Z	0.64	2.22	7	1
3:B:207:PCW:H432	4:B:215:17F:H60	0.64	1.70	11	1
3:B:206:PCW:H40	3:C:212:PCW:C25	0.64	2.22	12	1
3:D:603:PCW:H232	4:B:217:17F:H53	0.64	1.70	14	1
3:C:204:PCW:H141	4:C:211:17F:O8	0.64	1.92	14	1
3:A:402:PCW:H412	3:C:205:PCW:C38	0.64	2.23	15	1
3:B:210:PCW:C47	3:B:213:PCW:H283	0.64	2.22	17	1
3:D:605:PCW:H152	4:D:629:17F:H8	0.64	1.70	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:213:PCW:C3	4:B:217:17F:H4A	0.64	2.23	20	1
3:A:409:PCW:H82	3:C:206:PCW:C1	0.63	2.17	1	1
3:D:613:PCW:O31	3:D:613:PCW:H31	0.63	1.93	18	10
3:D:616:PCW:H482	3:B:204:PCW:H262	0.63	1.69	1	1
3:A:420:PCW:H381	3:D:617:PCW:C15	0.63	2.22	2	2
3:B:207:PCW:H421	3:B:213:PCW:H231	0.63	1.68	14	2
3:B:213:PCW:H421	4:B:217:17F:H36	0.63	1.70	3	1
3:A:416:PCW:C16	3:A:419:PCW:H331	0.63	2.23	4	3
3:C:204:PCW:H442	4:C:211:17F:H58	0.63	1.70	4	1
3:A:401:PCW:C4	3:B:209:PCW:H2	0.63	2.22	6	1
3:D:617:PCW:O31	3:D:617:PCW:H73	0.63	1.92	12	3
3:A:413:PCW:C32	4:A:414:17F:H32	0.63	2.21	10	2
3:C:208:PCW:O4P	3:C:208:PCW:O31	0.63	2.15	15	3
3:A:416:PCW:H412	3:D:610:PCW:H261	0.63	1.69	11	1
3:D:613:PCW:H241	4:C:210:17F:H66	0.63	1.70	13	1
4:D:629:17F:H35	4:D:630:17F:H10	0.63	1.71	20	1
3:D:616:PCW:H221	3:D:616:PCW:C17	0.63	2.23	12	4
3:D:618:PCW:H322	3:D:627:PCW:H121	0.63	1.69	1	7
3:D:621:PCW:C27	3:D:622:PCW:H61	0.63	2.23	1	2
3:B:206:PCW:C46	3:B:206:PCW:C42	0.63	2.72	1	6
4:B:215:17F:H30	4:B:217:17F:H35	0.63	1.70	1	1
3:D:602:PCW:O1P	3:D:602:PCW:O2	0.63	2.16	10	4
3:A:405:PCW:C47	3:A:405:PCW:C43	0.63	2.71	5	4
1:D:444:ASP:O	1:D:448:VAL:HB	0.63	1.94	7	8
3:B:208:PCW:C17	3:C:205:PCW:H322	0.63	2.13	4	1
3:C:204:PCW:H462	4:C:211:17F:C32	0.63	2.22	4	1
3:A:418:PCW:H31	3:D:614:PCW:C11	0.63	2.23	18	2
3:D:608:PCW:H52	4:D:635:17F:HN1	0.63	1.52	5	3
3:A:404:PCW:H422	4:B:215:17F:C24	0.63	2.22	19	2
3:D:612:PCW:C6	3:D:618:PCW:H12	0.63	2.19	7	2
3:B:207:PCW:H462	4:B:215:17F:C33	0.63	2.23	7	1
3:B:205:PCW:H73	3:B:208:PCW:H12	0.63	1.68	8	1
3:A:413:PCW:H442	4:A:414:17F:H68	0.63	1.70	9	1
3:A:406:PCW:H232	3:B:210:PCW:H122	0.63	1.71	20	2
3:A:402:PCW:H422	3:A:409:PCW:C13	0.63	2.23	12	1
4:A:414:17F:H56	4:A:414:17F:C35	0.63	2.18	13	2
4:B:215:17F:H1	4:B:215:17F:H4A	0.63	1.69	19	1
3:A:413:PCW:C47	3:A:413:PCW:C43	0.63	2.76	18	17
4:A:415:17F:H2	4:A:415:17F:O1	0.63	1.94	1	5
3:D:605:PCW:C25	4:D:629:17F:H38	0.63	2.18	8	5
3:A:406:PCW:C33	3:A:411:PCW:H322	0.63	2.22	8	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:409:PCW:H61	3:C:206:PCW:H371	0.63	1.70	2	1
3:D:611:PCW:H211	3:D:619:PCW:H482	0.63	1.68	16	2
3:D:607:PCW:H121	3:D:608:PCW:H171	0.63	1.68	16	3
3:A:410:PCW:H162	3:C:207:PCW:H232	0.63	1.68	5	1
4:A:414:17F:C30	3:C:203:PCW:H471	0.63	2.21	5	1
3:D:624:PCW:C47	4:C:210:17F:H55	0.63	2.24	16	8
3:B:204:PCW:H172	3:C:204:PCW:C40	0.63	2.23	16	3
3:D:603:PCW:H482	3:D:605:PCW:H61	0.63	1.71	12	2
3:A:401:PCW:C48	3:D:614:PCW:H222	0.63	2.23	10	1
3:D:616:PCW:C44	3:C:212:PCW:H431	0.63	2.23	11	1
3:D:610:PCW:H483	3:B:212:PCW:C26	0.63	2.22	13	1
3:B:204:PCW:H42	3:B:206:PCW:C6	0.63	2.23	14	2
3:B:211:PCW:C45	3:B:212:PCW:H31	0.63	2.23	15	1
3:A:406:PCW:H481	3:D:606:PCW:C27	0.63	2.23	17	1
3:A:420:PCW:O2P	3:D:617:PCW:H82	0.63	1.94	18	1
3:A:404:PCW:H472	3:B:209:PCW:H451	0.63	1.70	19	1
3:D:606:PCW:C11	3:D:606:PCW:O31	0.63	2.47	19	19
3:D:622:PCW:H231	3:D:624:PCW:H221	0.63	1.70	11	9
3:B:212:PCW:C47	3:B:212:PCW:C43	0.63	2.75	20	17
3:C:203:PCW:O4P	3:C:204:PCW:H62	0.63	1.93	1	1
3:A:411:PCW:H172	3:A:418:PCW:H261	0.63	1.70	2	2
3:B:210:PCW:P	3:B:210:PCW:C3	0.63	2.86	5	18
3:C:207:PCW:H382	3:C:207:PCW:H151	0.63	1.69	2	2
3:C:208:PCW:C22	3:C:208:PCW:C26	0.63	2.75	5	12
3:A:402:PCW:H431	3:A:407:PCW:C23	0.63	2.22	4	1
3:B:203:PCW:H62	3:B:211:PCW:O2P	0.63	1.94	7	1
3:A:408:PCW:H322	3:C:204:PCW:H181	0.63	1.69	9	1
3:A:410:PCW:C27	3:D:618:PCW:H452	0.63	2.24	10	1
3:D:622:PCW:H472	3:B:206:PCW:C25	0.63	2.23	16	5
3:D:625:PCW:O2	3:D:625:PCW:C35	0.63	2.46	10	2
3:A:413:PCW:H371	3:A:413:PCW:H12	0.63	1.70	11	2
3:D:620:PCW:C28	4:D:635:17F:H35	0.63	2.23	11	2
3:C:204:PCW:H331	4:C:211:17F:C8	0.63	2.24	11	1
3:C:204:PCW:H232	3:C:207:PCW:H472	0.63	1.70	17	2
3:A:413:PCW:H341	4:A:414:17F:H32	0.63	1.71	17	3
3:A:416:PCW:H481	3:C:203:PCW:H19	0.63	1.70	16	1
3:A:417:PCW:H381	3:D:612:PCW:H151	0.63	1.69	16	1
3:A:408:PCW:C5	3:C:204:PCW:H121	0.63	2.14	1	1
3:A:418:PCW:H381	3:D:625:PCW:C25	0.63	2.23	15	6
3:D:603:PCW:H451	3:D:605:PCW:C18	0.63	2.21	9	9
3:D:616:PCW:H431	3:B:206:PCW:C47	0.63	2.23	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:210:PCW:C43	3:B:210:PCW:C47	0.63	2.75	1	4
3:B:211:PCW:H321	3:B:212:PCW:H12	0.63	1.70	1	2
3:D:603:PCW:O31	3:D:603:PCW:O3	0.63	2.17	13	3
3:D:616:PCW:C48	3:B:204:PCW:H221	0.63	2.23	10	2
3:C:204:PCW:H131	4:C:211:17F:C41	0.63	2.12	2	1
3:A:401:PCW:H461	3:D:611:PCW:H251	0.63	1.69	3	1
3:A:404:PCW:H12	3:B:209:PCW:H11	0.63	1.68	13	3
4:A:414:17F:H39	4:A:414:17F:H29	0.63	1.70	13	3
3:A:416:PCW:O11	3:A:416:PCW:H2	0.63	1.93	17	5
3:D:616:PCW:C43	3:B:206:PCW:H481	0.63	2.23	4	1
3:B:205:PCW:C25	3:B:205:PCW:C21	0.63	2.74	7	10
3:B:205:PCW:C20	3:B:212:PCW:H351	0.63	2.24	6	2
3:B:206:PCW:H231	3:C:208:PCW:H282	0.63	1.70	7	5
3:A:406:PCW:H39	3:A:406:PCW:C12	0.63	2.20	7	1
3:D:622:PCW:C44	3:B:206:PCW:H272	0.63	2.18	10	2
3:C:203:PCW:C31	3:C:203:PCW:C35	0.63	2.77	8	7
3:D:622:PCW:H121	4:D:630:17F:C1Z	0.63	2.22	19	3
3:B:204:PCW:H232	3:C:208:PCW:H262	0.63	1.70	12	3
1:A:308:ARG:HG3	1:D:469:LEU:HD21	0.63	1.69	16	3
2:C:13:GLY:CA	5:C:201:GDP:H5'	0.63	2.23	13	1
3:A:403:PCW:C33	3:C:203:PCW:H31	0.63	2.21	15	1
3:D:616:PCW:H421	3:D:627:PCW:C22	0.63	2.22	15	2
3:B:207:PCW:H11	4:B:216:17F:C8	0.63	2.20	19	1
3:A:402:PCW:C31	3:A:402:PCW:C35	0.63	2.76	18	20
3:A:417:PCW:O3P	3:A:417:PCW:O31	0.63	2.15	18	14
3:D:611:PCW:C5	3:D:623:PCW:H342	0.63	2.22	17	5
3:D:618:PCW:H131	3:D:627:PCW:C14	0.63	2.23	19	8
4:D:630:17F:H59	4:D:630:17F:C12	0.63	2.16	5	8
3:A:413:PCW:C42	4:A:414:17F:H70	0.63	2.18	3	1
3:D:620:PCW:H20	4:D:635:17F:H10A	0.63	1.70	3	2
3:C:204:PCW:C33	4:C:211:17F:H9	0.63	2.23	3	1
4:B:214:17F:H46	4:B:217:17F:H70	0.63	1.70	4	2
3:C:204:PCW:C46	4:C:211:17F:H57	0.63	2.23	4	1
3:D:604:PCW:C21	3:D:613:PCW:H382	0.63	2.24	13	3
3:D:605:PCW:H42	3:D:626:PCW:C19	0.63	2.23	16	2
3:D:616:PCW:C38	3:D:618:PCW:H142	0.63	2.23	9	1
3:A:412:PCW:H432	3:C:208:PCW:H432	0.63	1.70	10	1
3:A:411:PCW:H483	3:A:418:PCW:H212	0.63	1.68	12	2
3:A:406:PCW:H241	3:B:207:PCW:H151	0.63	1.69	16	1
3:D:607:PCW:H62	3:D:626:PCW:H222	0.63	1.70	17	1
3:D:613:PCW:O31	3:D:613:PCW:C1	0.63	2.46	15	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:211:PCW:H152	4:B:217:17F:C34	0.63	2.23	8	2
3:C:203:PCW:H462	3:C:203:PCW:H172	0.63	1.70	1	1
3:A:409:PCW:H82	3:C:206:PCW:C35	0.63	2.22	3	4
3:D:616:PCW:C27	3:D:618:PCW:H283	0.63	2.23	2	1
3:D:616:PCW:H331	3:C:212:PCW:H321	0.63	1.69	6	3
3:B:205:PCW:H322	3:B:206:PCW:H122	0.63	1.69	3	2
3:A:405:PCW:C37	3:D:601:PCW:H171	0.63	2.22	18	2
3:B:207:PCW:H171	3:B:210:PCW:H131	0.63	1.71	4	1
3:A:416:PCW:H161	3:A:419:PCW:C33	0.63	2.14	12	4
3:A:404:PCW:H372	3:B:209:PCW:O11	0.63	1.94	6	1
3:B:204:PCW:C14	3:C:207:PCW:H11	0.63	2.23	6	1
3:A:417:PCW:O31	3:A:417:PCW:P	0.63	2.56	18	3
3:A:410:PCW:H222	4:D:633:17F:H49	0.63	1.70	8	1
3:A:407:PCW:H161	3:C:205:PCW:C16	0.63	2.23	13	1
3:A:411:PCW:H122	4:B:215:17F:C1Z	0.63	2.24	13	1
4:D:628:17F:H19A	4:D:631:17F:H55	0.63	1.70	13	1
3:A:403:PCW:H472	3:C:203:PCW:C25	0.63	2.24	15	1
3:A:407:PCW:H232	4:D:635:17F:H51	0.63	1.71	19	1
3:A:404:PCW:H371	4:B:215:17F:C10	0.63	2.23	1	1
3:A:411:PCW:H242	3:A:418:PCW:H271	0.63	1.71	11	2
3:A:416:PCW:O3P	3:A:416:PCW:O31	0.63	2.17	13	5
3:B:213:PCW:H39	4:B:217:17F:H64	0.63	1.69	1	1
3:D:603:PCW:C38	4:D:629:17F:H40	0.63	2.23	2	4
3:B:208:PCW:H171	3:C:206:PCW:C12	0.63	2.24	2	2
3:A:420:PCW:H351	3:D:617:PCW:H141	0.63	1.68	3	2
3:D:618:PCW:H131	3:D:627:PCW:H142	0.63	1.70	10	5
3:D:622:PCW:H372	3:D:627:PCW:C21	0.63	2.21	4	1
3:B:209:PCW:O1P	3:B:209:PCW:C3	0.63	2.47	5	4
3:D:603:PCW:H31	3:D:603:PCW:H41	0.63	1.69	7	1
3:C:204:PCW:C47	4:C:211:17F:H56	0.63	2.24	7	1
3:C:205:PCW:H371	3:C:205:PCW:H411	0.63	1.69	15	2
3:C:204:PCW:H51	3:C:204:PCW:O31	0.63	1.94	10	1
3:A:413:PCW:C35	4:A:414:17F:H34	0.63	2.24	11	1
3:A:420:PCW:H161	4:D:632:17F:H60	0.63	1.71	17	2
3:D:615:PCW:H222	3:C:205:PCW:H272	0.63	1.71	15	3
3:D:609:PCW:H241	3:D:609:PCW:H20	0.63	1.70	18	9
3:D:625:PCW:C45	3:D:626:PCW:H482	0.63	2.22	12	6
3:B:209:PCW:O11	3:B:209:PCW:H73	0.63	1.94	2	2
3:D:603:PCW:O3	3:D:603:PCW:O31	0.63	2.17	6	12
3:C:208:PCW:O2P	3:C:209:PCW:C5	0.63	2.47	3	7
3:D:608:PCW:C39	3:D:615:PCW:H421	0.63	2.24	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:213:PCW:H42	4:B:214:17F:O2	0.63	1.93	4	1
3:A:402:PCW:H39	3:A:409:PCW:H272	0.63	1.69	17	4
3:A:416:PCW:H121	3:D:617:PCW:H331	0.63	1.70	10	4
3:A:401:PCW:H61	3:B:209:PCW:H2	0.63	1.70	15	2
3:D:615:PCW:H483	3:B:208:PCW:C25	0.63	2.22	12	1
3:D:604:PCW:H39	3:D:611:PCW:C32	0.63	2.24	15	1
3:A:407:PCW:H162	3:B:208:PCW:C20	0.63	2.23	16	1
3:B:206:PCW:H422	4:C:211:17F:C28	0.63	2.24	16	2
4:B:215:17F:H36	4:B:215:17F:H41	0.63	1.70	18	1
3:A:406:PCW:H241	3:B:210:PCW:H121	0.62	1.71	1	1
3:D:609:PCW:H52	3:D:609:PCW:O1P	0.62	1.94	3	12
3:D:617:PCW:C27	3:D:617:PCW:C23	0.62	2.76	15	16
2:B:84:ILE:HD12	2:B:123:ARG:HB3	0.62	1.71	9	5
3:B:209:PCW:C11	3:B:209:PCW:C31	0.62	2.77	11	7
3:A:403:PCW:H342	3:C:203:PCW:C1	0.62	2.24	11	2
3:A:417:PCW:C6	3:A:417:PCW:O4P	0.62	2.47	18	10
3:A:419:PCW:H362	3:D:617:PCW:C39	0.62	2.24	3	1
3:D:613:PCW:H251	4:C:210:17F:C26	0.62	2.24	4	10
3:D:616:PCW:H19	3:D:617:PCW:C46	0.62	2.18	7	3
4:D:635:17F:C36	3:C:205:PCW:H461	0.62	2.23	11	2
3:A:402:PCW:H73	3:A:402:PCW:H332	0.62	1.69	7	1
3:A:409:PCW:C21	3:A:409:PCW:H171	0.62	2.23	15	2
3:D:611:PCW:H19	3:D:611:PCW:H371	0.62	1.69	19	3
3:A:412:PCW:H20	3:C:206:PCW:H481	0.62	1.72	12	3
3:D:608:PCW:O1P	4:D:635:17F:H20A	0.62	1.94	10	3
3:D:616:PCW:H452	3:C:212:PCW:C43	0.62	2.24	11	1
3:D:618:PCW:C39	3:D:627:PCW:H161	0.62	2.23	11	2
3:C:204:PCW:C47	4:C:211:17F:H32	0.62	2.24	11	1
3:D:607:PCW:H262	4:D:631:17F:C1X	0.62	2.24	14	1
3:B:211:PCW:H241	4:B:217:17F:H73	0.62	1.71	17	1
3:A:406:PCW:C24	3:B:210:PCW:H121	0.62	2.23	12	2
3:D:615:PCW:H171	3:D:615:PCW:H212	0.62	1.70	5	3
3:B:203:PCW:H211	4:C:210:17F:H56	0.62	1.70	1	1
3:D:616:PCW:H421	3:D:627:PCW:H232	0.62	1.69	20	8
3:D:622:PCW:H172	4:D:630:17F:C1Y	0.62	2.23	13	5
3:B:210:PCW:O11	3:B:210:PCW:C5	0.62	2.47	3	10
4:A:414:17F:H62	4:A:414:17F:C31	0.62	2.13	13	3
3:B:204:PCW:H131	3:C:207:PCW:C1	0.62	2.24	3	2
3:C:206:PCW:H152	3:C:206:PCW:C38	0.62	2.22	4	1
3:A:404:PCW:H31	3:B:209:PCW:H321	0.62	1.69	5	1
1:D:462:LYS:HB3	3:D:601:PCW:H283	0.62	1.71	19	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:203:PCW:H332	4:B:215:17F:C22	0.62	2.24	8	1
3:A:413:PCW:C37	3:A:413:PCW:H12	0.62	2.24	11	1
3:B:206:PCW:H472	3:C:212:PCW:H231	0.62	1.71	11	1
3:A:406:PCW:H232	3:B:207:PCW:H171	0.62	1.69	12	1
3:A:407:PCW:H372	4:D:635:17F:C30	0.62	2.24	12	1
3:D:601:PCW:H362	4:B:216:17F:C39	0.62	2.24	13	1
3:D:607:PCW:C6	3:D:626:PCW:H241	0.62	2.17	14	2
3:D:602:PCW:H241	3:D:610:PCW:H142	0.62	1.70	1	2
3:D:602:PCW:H141	3:D:624:PCW:C18	0.62	2.24	3	7
3:D:604:PCW:O31	3:D:604:PCW:O3P	0.62	2.18	14	18
3:D:616:PCW:H39	3:D:618:PCW:C15	0.62	2.23	1	3
3:D:611:PCW:C2	3:D:619:PCW:H63	0.62	2.24	4	8
3:D:616:PCW:H452	3:B:206:PCW:H472	0.62	1.70	2	3
3:B:204:PCW:O31	3:B:204:PCW:C1	0.62	2.44	9	8
3:A:411:PCW:H11	3:A:411:PCW:O31	0.62	1.93	3	2
3:B:211:PCW:H132	4:B:217:17F:C31	0.62	2.25	3	3
3:C:203:PCW:H351	3:C:203:PCW:C8	0.62	2.23	3	1
3:D:627:PCW:H182	3:D:627:PCW:H221	0.62	1.68	9	5
3:A:407:PCW:H82	4:B:216:17F:C9	0.62	2.23	7	2
3:C:203:PCW:H252	4:C:211:17F:H78	0.62	1.70	8	1
3:D:608:PCW:C48	3:C:205:PCW:H451	0.62	2.22	9	1
3:D:612:PCW:H322	3:D:618:PCW:H132	0.62	1.71	18	3
3:A:401:PCW:H472	3:D:611:PCW:C24	0.62	2.23	13	1
3:D:607:PCW:C20	4:D:631:17F:H50	0.62	2.23	14	1
3:A:417:PCW:C41	3:A:417:PCW:C37	0.62	2.75	9	8
4:B:217:17F:H20A	4:B:217:17F:O10	0.62	1.93	13	14
3:A:416:PCW:C8	4:D:632:17F:H1	0.62	2.24	20	4
3:A:419:PCW:C42	3:D:616:PCW:H232	0.62	2.25	19	5
1:D:573:LEU:HA	1:D:576:VAL:HG12	0.62	1.70	16	7
3:B:204:PCW:C21	3:B:204:PCW:C25	0.62	2.77	4	9
3:B:210:PCW:C47	3:B:210:PCW:C43	0.62	2.76	18	16
4:C:211:17F:O10	4:C:211:17F:H4A	0.62	1.93	2	1
3:A:417:PCW:H332	3:D:612:PCW:O3	0.62	1.95	19	4
3:A:419:PCW:C39	3:D:617:PCW:H472	0.62	2.24	3	2
3:A:420:PCW:H351	3:D:617:PCW:C15	0.62	2.25	4	5
3:D:622:PCW:C14	4:D:630:17F:H32	0.62	2.18	14	2
3:A:408:PCW:C26	3:A:417:PCW:H241	0.62	2.25	5	1
3:A:412:PCW:H362	3:C:206:PCW:C45	0.62	2.24	6	2
3:A:409:PCW:H152	3:C:205:PCW:H39	0.62	1.69	11	1
3:A:401:PCW:H322	3:B:209:PCW:C39	0.62	2.25	12	1
3:A:405:PCW:C43	3:A:405:PCW:C47	0.62	2.76	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:635:17F:H54	3:C:205:PCW:H161	0.62	1.69	12	2
4:A:414:17F:O1	4:A:414:17F:C2	0.62	2.47	15	14
3:A:408:PCW:C36	3:C:204:PCW:H232	0.62	2.25	2	2
3:B:206:PCW:H51	3:C:207:PCW:P	0.62	2.34	2	1
3:C:206:PCW:H471	3:C:208:PCW:H411	0.62	1.70	2	1
3:A:406:PCW:C8	3:B:207:PCW:H362	0.62	2.24	3	1
3:A:407:PCW:H171	3:B:208:PCW:C23	0.62	2.24	10	3
3:D:615:PCW:C4	3:D:615:PCW:H2	0.62	2.24	19	4
3:A:402:PCW:H422	3:C:205:PCW:H152	0.62	1.70	6	2
3:D:608:PCW:C40	3:D:615:PCW:H441	0.62	2.25	20	2
3:C:208:PCW:H441	3:C:208:PCW:C18	0.62	2.23	8	1
3:A:416:PCW:H40	3:D:610:PCW:H242	0.62	1.69	11	1
3:B:205:PCW:H241	3:B:212:PCW:C36	0.62	2.22	11	1
3:D:609:PCW:H63	4:D:633:17F:O1	0.62	1.95	18	3
3:B:210:PCW:H73	4:B:216:17F:C18	0.62	2.21	13	1
3:D:613:PCW:C20	4:C:210:17F:H51	0.62	2.24	14	1
3:D:626:PCW:C8	3:D:626:PCW:H182	0.62	2.24	19	1
3:B:203:PCW:H283	4:B:215:17F:H55	0.62	1.71	20	1
3:B:208:PCW:O2P	3:B:208:PCW:H31	0.62	1.95	13	2
3:D:603:PCW:H372	3:D:603:PCW:C42	0.62	2.25	20	7
4:D:628:17F:H36	4:D:631:17F:H75	0.62	1.71	9	6
3:B:206:PCW:O1P	3:B:206:PCW:H32	0.62	1.94	6	9
3:A:407:PCW:H2	3:A:407:PCW:O1P	0.62	1.94	12	8
3:A:412:PCW:H452	3:C:208:PCW:H472	0.62	1.69	5	3
3:D:618:PCW:C13	3:D:627:PCW:H142	0.62	2.24	3	6
3:D:607:PCW:C8	3:D:608:PCW:H20	0.62	2.25	4	1
3:B:204:PCW:H11	3:B:204:PCW:O31	0.62	1.93	4	1
3:A:406:PCW:H362	3:A:411:PCW:C33	0.62	2.25	7	1
3:B:211:PCW:C8	3:B:212:PCW:H321	0.62	2.24	16	3
3:B:206:PCW:H371	3:B:212:PCW:H39	0.62	1.71	11	1
3:A:410:PCW:C37	3:C:209:PCW:H162	0.62	2.25	20	3
3:A:406:PCW:H441	3:B:207:PCW:H251	0.62	1.70	13	1
3:D:610:PCW:C46	3:B:212:PCW:H261	0.62	2.25	14	2
3:A:416:PCW:H19	3:A:419:PCW:C43	0.62	2.22	18	2
3:B:207:PCW:C42	3:B:213:PCW:H242	0.62	2.23	16	1
3:A:407:PCW:C13	3:C:205:PCW:H321	0.62	2.24	1	3
3:D:621:PCW:H481	4:D:634:17F:H12	0.62	1.72	1	1
4:D:631:17F:O7	4:D:631:17F:C17	0.62	2.48	7	20
3:B:205:PCW:H283	3:B:212:PCW:C14	0.62	2.14	1	2
3:A:404:PCW:C4	3:B:203:PCW:H31	0.62	2.25	2	1
4:D:629:17F:C7	4:D:629:17F:C18	0.62	2.74	19	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:207:PCW:H442	4:B:215:17F:H57	0.62	1.71	6	1
3:D:607:PCW:H222	4:D:628:17F:H10A	0.62	1.72	19	2
4:D:629:17F:H54	3:B:212:PCW:H451	0.62	1.72	7	1
3:D:601:PCW:H371	4:B:216:17F:H77	0.62	1.72	9	3
3:C:204:PCW:H412	4:C:211:17F:H8A	0.62	1.71	9	1
3:B:204:PCW:C37	3:C:204:PCW:H63	0.62	2.24	10	1
3:A:413:PCW:H341	4:A:414:17F:H33	0.62	1.71	11	1
3:B:205:PCW:C42	3:B:206:PCW:H162	0.62	2.23	11	1
3:B:208:PCW:H40	4:B:214:17F:H30	0.62	1.70	11	1
3:D:616:PCW:H483	3:B:204:PCW:H232	0.62	1.71	14	1
3:A:403:PCW:H152	3:C:203:PCW:H282	0.62	1.69	15	1
3:A:404:PCW:C27	3:A:404:PCW:C23	0.62	2.76	15	2
3:B:208:PCW:H412	4:B:214:17F:C11	0.62	2.24	15	1
3:D:606:PCW:H451	3:D:625:PCW:C48	0.62	2.24	17	1
3:D:606:PCW:H11	3:D:626:PCW:H372	0.62	1.71	17	1
3:B:204:PCW:H442	3:C:203:PCW:H40	0.62	1.72	19	1
3:A:412:PCW:H171	3:C:206:PCW:H481	0.62	1.70	20	1
3:A:402:PCW:H162	3:A:409:PCW:H222	0.62	1.70	1	2
3:A:407:PCW:C8	4:B:216:17F:H9	0.62	2.25	9	3
4:A:414:17F:H42	4:C:210:17F:H31	0.62	1.70	1	1
3:A:419:PCW:O2	3:D:617:PCW:C41	0.62	2.46	17	9
3:B:209:PCW:H20	4:B:215:17F:H19	0.62	1.71	1	1
3:D:607:PCW:H251	4:D:631:17F:H63	0.62	1.71	2	1
3:A:408:PCW:H262	3:A:417:PCW:H482	0.62	1.70	4	2
3:D:621:PCW:H222	4:D:633:17F:C1Y	0.62	2.24	20	4
3:D:615:PCW:H242	4:D:635:17F:H41	0.62	1.72	5	2
3:B:207:PCW:C45	4:B:217:17F:H38	0.62	2.24	5	1
3:D:621:PCW:H182	4:D:633:17F:O10	0.62	1.94	7	1
3:C:203:PCW:H341	3:C:203:PCW:O31	0.62	1.95	7	1
3:D:614:PCW:H82	3:D:625:PCW:O1P	0.62	1.94	15	5
3:D:604:PCW:H471	3:D:613:PCW:H162	0.62	1.71	14	4
3:A:413:PCW:O31	4:A:414:17F:H34	0.62	1.94	12	1
3:D:624:PCW:H73	3:D:624:PCW:C32	0.62	2.20	12	1
3:A:408:PCW:H231	3:A:417:PCW:H252	0.62	1.71	13	1
3:D:614:PCW:O2P	3:D:614:PCW:H51	0.62	1.95	13	1
3:A:401:PCW:C32	3:B:209:PCW:H381	0.62	2.24	15	1
3:A:402:PCW:H451	4:D:635:17F:H53	0.62	1.71	15	1
3:D:616:PCW:H451	3:B:206:PCW:H452	0.62	1.72	15	1
3:A:412:PCW:C33	3:C:206:PCW:H451	0.62	2.15	20	1
3:A:412:PCW:H372	3:A:412:PCW:C41	0.62	2.24	1	1
3:A:420:PCW:O31	3:A:420:PCW:O3P	0.62	2.18	2	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:307:ASP:HA	1:A:310:ARG:HD2	0.62	1.72	3	9
4:D:631:17F:O7	4:D:631:17F:O10	0.62	2.18	7	19
4:B:214:17F:O10	4:B:214:17F:H4	0.62	1.94	2	3
3:A:418:PCW:H431	3:D:625:PCW:H461	0.62	1.71	3	6
3:B:210:PCW:H62	4:B:216:17F:O2	0.62	1.94	3	2
3:D:615:PCW:C20	4:D:635:17F:H38	0.62	2.25	15	9
3:B:211:PCW:H431	3:B:212:PCW:C3	0.62	2.24	4	1
3:B:212:PCW:H481	3:C:212:PCW:H252	0.62	1.72	4	1
3:B:203:PCW:H451	3:B:211:PCW:C22	0.62	2.25	5	2
3:A:404:PCW:H82	4:A:415:17F:C2	0.62	2.24	6	2
3:A:406:PCW:H212	3:B:210:PCW:H322	0.62	1.71	6	1
3:A:417:PCW:C36	3:D:612:PCW:H131	0.62	2.24	6	1
4:C:210:17F:C31	4:C:210:17F:C19	0.62	2.71	6	1
3:D:602:PCW:H441	3:D:602:PCW:C21	0.62	2.24	7	5
3:B:205:PCW:O4P	3:B:208:PCW:H11	0.62	1.93	12	2
2:C:168:GLU:CD	3:C:206:PCW:H61	0.62	2.20	8	1
3:B:204:PCW:H40	3:C:203:PCW:H73	0.62	1.71	10	1
3:D:605:PCW:C25	4:D:629:17F:H42	0.62	2.24	18	2
3:B:213:PCW:H283	3:B:213:PCW:H482	0.62	1.71	12	2
3:A:404:PCW:H381	3:B:209:PCW:C36	0.62	2.24	13	1
2:B:132:ASP:HA	2:B:135:ARG:NH1	0.62	2.10	13	1
3:B:206:PCW:H421	3:C:212:PCW:H232	0.62	1.71	13	1
3:A:406:PCW:H321	3:A:411:PCW:H42	0.62	1.72	17	1
3:A:404:PCW:C11	3:A:404:PCW:O31	0.62	2.48	15	13
3:C:209:PCW:C11	3:C:209:PCW:O31	0.62	2.47	5	13
3:A:401:PCW:H341	3:A:404:PCW:C19	0.62	2.25	3	1
3:D:606:PCW:H432	3:D:626:PCW:C47	0.62	2.25	3	3
4:D:630:17F:H10A	4:D:630:17F:H56	0.62	1.72	12	2
3:B:204:PCW:H241	3:C:204:PCW:H472	0.62	1.72	4	1
3:A:413:PCW:H262	4:A:414:17F:C34	0.62	2.25	5	1
3:D:603:PCW:H482	3:D:626:PCW:H281	0.62	1.72	5	5
3:D:613:PCW:H241	4:C:210:17F:H71	0.62	1.71	5	1
3:D:618:PCW:H381	3:D:627:PCW:C16	0.62	2.18	13	7
3:B:208:PCW:H412	4:B:214:17F:C1X	0.62	2.25	5	2
1:A:396:LYS:HE2	1:D:587:ALA:HA	0.62	1.71	7	3
4:A:414:17F:H8	3:C:203:PCW:C7	0.62	2.25	7	1
3:A:420:PCW:H442	3:D:617:PCW:C20	0.62	2.24	9	5
3:D:623:PCW:H39	3:D:623:PCW:C13	0.62	2.25	9	2
3:B:209:PCW:H251	3:B:209:PCW:H451	0.62	1.72	11	3
3:B:209:PCW:H471	3:B:209:PCW:H261	0.62	1.72	18	2
3:D:606:PCW:C47	3:B:210:PCW:H483	0.62	2.23	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:402:PCW:H61	3:A:409:PCW:O11	0.62	1.95	15	1
3:A:411:PCW:O3	4:B:215:17F:H34	0.61	1.95	4	2
3:D:605:PCW:H411	4:D:634:17F:H55	0.61	1.71	2	7
3:D:607:PCW:C14	3:D:608:PCW:H171	0.61	2.15	2	6
3:D:618:PCW:O2P	3:D:627:PCW:H42	0.61	1.94	1	2
3:A:411:PCW:C17	3:A:418:PCW:H261	0.61	2.24	20	3
3:D:607:PCW:C25	4:D:631:17F:H63	0.61	2.25	2	2
3:B:208:PCW:P	3:B:208:PCW:H31	0.61	2.35	11	9
3:B:210:PCW:H281	3:B:210:PCW:C48	0.61	2.25	17	3
3:B:212:PCW:H421	3:C:212:PCW:C28	0.61	2.25	3	4
3:B:213:PCW:C42	4:B:217:17F:H36	0.61	2.25	3	2
4:B:214:17F:H4	4:B:214:17F:O10	0.61	1.93	7	6
3:A:407:PCW:H262	3:C:205:PCW:C40	0.61	2.25	4	1
3:D:602:PCW:H271	3:D:610:PCW:C18	0.61	2.25	7	2
3:A:411:PCW:C33	3:A:411:PCW:C37	0.61	2.76	8	1
4:C:211:17F:H69	4:C:211:17F:H37	0.61	1.71	10	1
3:A:409:PCW:H52	3:C:206:PCW:H321	0.61	1.71	12	2
3:D:625:PCW:C1	3:D:626:PCW:H12	0.61	2.25	12	2
3:A:413:PCW:H482	4:C:210:17F:H63	0.61	1.71	13	1
3:A:407:PCW:C26	3:C:205:PCW:H382	0.61	2.25	15	1
3:A:402:PCW:H411	3:C:205:PCW:H381	0.61	1.72	1	1
3:A:402:PCW:C41	3:C:205:PCW:H381	0.61	2.25	11	5
3:A:404:PCW:H82	3:A:404:PCW:O31	0.61	1.95	1	1
3:C:204:PCW:H351	4:C:211:17F:H10	0.61	1.70	1	2
3:A:408:PCW:C37	3:C:204:PCW:H232	0.61	2.25	2	1
3:C:208:PCW:O2P	3:C:209:PCW:H63	0.61	1.94	14	4
3:A:419:PCW:H381	3:D:617:PCW:H481	0.61	1.71	11	2
3:D:622:PCW:H262	3:D:624:PCW:C28	0.61	2.15	5	1
3:A:402:PCW:H332	3:A:409:PCW:H121	0.61	1.71	9	1
1:A:374:GLY:CA	1:D:400:LYS:HE3	0.61	2.26	12	1
4:A:414:17F:H53	3:C:203:PCW:H452	0.61	1.72	14	1
4:B:215:17F:C19	4:B:215:17F:H5	0.61	2.26	14	1
3:D:616:PCW:H451	3:B:206:PCW:C45	0.61	2.25	15	1
4:D:629:17F:C1X	4:D:630:17F:H10	0.61	2.24	18	1
3:A:408:PCW:H361	3:C:207:PCW:C46	0.61	2.25	20	1
3:A:420:PCW:H372	3:D:617:PCW:C15	0.61	2.25	13	5
3:D:618:PCW:H422	3:D:627:PCW:C26	0.61	2.21	3	3
1:D:475:GLU:HB2	1:D:476:PRO:HD3	0.61	1.72	13	4
3:D:616:PCW:C40	3:D:618:PCW:H162	0.61	2.23	2	6
4:D:634:17F:H65	4:D:635:17F:H71	0.61	1.72	11	4
3:D:604:PCW:H212	3:D:613:PCW:H152	0.61	1.72	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:210:PCW:C26	3:B:210:PCW:C22	0.61	2.76	18	3
2:C:84:ILE:HD12	2:C:123:ARG:HB3	0.61	1.72	7	10
3:C:204:PCW:H232	3:C:207:PCW:H452	0.61	1.71	5	1
3:D:613:PCW:O31	3:D:613:PCW:H12	0.61	1.94	6	6
3:A:409:PCW:H171	3:A:409:PCW:C22	0.61	2.25	9	3
3:A:410:PCW:C20	3:D:627:PCW:H482	0.61	2.25	8	1
3:D:602:PCW:H32	3:D:603:PCW:C7	0.61	2.25	10	2
3:D:616:PCW:H432	3:B:206:PCW:H483	0.61	1.72	9	3
3:B:205:PCW:H51	3:B:208:PCW:H12	0.61	1.72	9	2
3:B:203:PCW:H2	3:B:211:PCW:H39	0.61	1.70	10	1
3:B:206:PCW:C40	3:C:212:PCW:H261	0.61	2.25	12	2
3:A:404:PCW:H222	4:A:415:17F:C32	0.61	2.25	15	1
3:A:402:PCW:C37	3:A:409:PCW:H261	0.61	2.23	16	1
3:A:416:PCW:H141	3:A:419:PCW:C34	0.61	2.24	15	3
3:D:619:PCW:O31	3:D:619:PCW:H11	0.61	1.95	18	16
3:D:615:PCW:H472	3:C:205:PCW:C22	0.61	2.16	2	3
3:A:407:PCW:H121	3:C:205:PCW:H151	0.61	1.72	4	1
3:A:411:PCW:H412	3:A:418:PCW:H251	0.61	1.72	10	2
3:A:420:PCW:C44	3:D:617:PCW:H222	0.61	2.26	5	1
3:D:610:PCW:H82	3:C:212:PCW:H73	0.61	1.71	20	3
3:C:208:PCW:H281	3:C:212:PCW:H471	0.61	1.72	8	1
3:A:417:PCW:H422	3:D:612:PCW:C21	0.61	2.22	10	1
3:D:603:PCW:H251	4:B:217:17F:H75	0.61	1.72	11	1
3:B:208:PCW:C27	4:B:216:17F:H50	0.61	2.25	11	1
3:B:205:PCW:C28	3:B:211:PCW:H471	0.61	2.25	16	2
3:D:616:PCW:C45	3:B:206:PCW:H452	0.61	2.25	15	2
3:D:601:PCW:H422	4:D:628:17F:C26	0.61	2.22	16	1
3:D:606:PCW:H432	3:D:626:PCW:H481	0.61	1.70	17	2
3:D:621:PCW:H181	3:D:621:PCW:C14	0.61	2.19	2	11
3:A:401:PCW:O11	3:A:401:PCW:H2	0.61	1.95	10	3
3:D:605:PCW:O11	3:D:605:PCW:H51	0.61	1.96	13	7
3:B:208:PCW:H412	4:B:214:17F:C10	0.61	2.25	2	1
3:D:604:PCW:H152	3:D:613:PCW:O2	0.61	1.95	5	6
3:D:611:PCW:H11	3:D:619:PCW:H63	0.61	1.71	7	2
3:B:207:PCW:H422	3:B:213:PCW:H252	0.61	1.73	19	2
4:A:415:17F:H76	4:C:210:17F:C31	0.61	2.24	5	1
3:B:203:PCW:H451	3:B:211:PCW:C23	0.61	2.16	11	4
3:D:603:PCW:H182	3:B:211:PCW:H283	0.61	1.72	6	1
3:B:203:PCW:O11	3:B:203:PCW:H2	0.61	1.95	13	4
3:D:615:PCW:H272	4:D:635:17F:H45	0.61	1.70	7	2
3:D:604:PCW:C32	3:D:613:PCW:H82	0.61	2.26	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:205:PCW:H332	3:B:208:PCW:H321	0.61	1.70	8	1
3:B:205:PCW:H451	3:C:208:PCW:C17	0.61	2.24	8	1
3:A:410:PCW:C24	3:C:207:PCW:H232	0.61	2.24	9	1
4:D:633:17F:H53	3:C:208:PCW:H251	0.61	1.71	9	1
3:B:203:PCW:H222	4:C:210:17F:H56	0.61	1.73	9	3
3:C:204:PCW:H222	4:C:211:17F:C20	0.61	2.19	9	1
3:A:413:PCW:H12	3:A:413:PCW:C38	0.61	2.26	11	1
3:D:604:PCW:C48	3:D:619:PCW:H471	0.61	2.26	15	1
3:B:207:PCW:H63	4:B:216:17F:C2	0.61	2.24	17	1
3:B:207:PCW:C14	3:B:210:PCW:H351	0.61	2.26	17	1
3:D:615:PCW:H432	3:C:205:PCW:H283	0.61	1.69	19	1
3:A:406:PCW:C33	3:A:411:PCW:H321	0.61	2.25	1	1
4:B:216:17F:O10	4:B:216:17F:C7	0.61	2.49	8	8
3:A:407:PCW:C19	3:B:208:PCW:H242	0.61	2.26	9	3
3:D:603:PCW:H412	3:D:605:PCW:H232	0.61	1.71	6	3
3:D:605:PCW:O11	3:D:605:PCW:C5	0.61	2.49	10	10
3:D:611:PCW:H61	3:D:625:PCW:H141	0.61	1.71	15	3
3:B:208:PCW:C17	3:C:206:PCW:H122	0.61	2.25	2	2
3:D:623:PCW:H332	3:D:624:PCW:H73	0.61	1.72	3	2
3:D:625:PCW:O31	3:D:625:PCW:O3P	0.61	2.18	14	13
3:B:210:PCW:O31	3:B:210:PCW:H12	0.61	1.94	13	4
1:A:247:LEU:HD23	3:A:412:PCW:H283	0.61	1.73	4	2
4:D:629:17F:H47	4:D:630:17F:C23	0.61	2.17	4	5
3:C:203:PCW:C16	3:C:203:PCW:C42	0.61	2.75	5	2
3:A:420:PCW:H442	3:D:617:PCW:H222	0.61	1.70	5	1
3:D:605:PCW:H411	4:D:634:17F:H50	0.61	1.72	6	1
3:B:204:PCW:C6	3:B:204:PCW:O4P	0.61	2.49	20	4
3:B:206:PCW:H39	4:C:211:17F:H49	0.61	1.69	12	1
3:C:208:PCW:H172	3:C:208:PCW:H211	0.61	1.72	18	2
3:B:211:PCW:H82	3:B:212:PCW:H41	0.61	1.71	13	2
3:B:204:PCW:H281	4:C:211:17F:H20A	0.61	1.72	14	1
3:B:206:PCW:C39	3:C:212:PCW:H261	0.61	2.25	14	1
3:D:605:PCW:H73	3:D:626:PCW:H281	0.61	1.73	20	1
3:A:405:PCW:H482	4:D:628:17F:C30	0.61	2.25	2	2
3:A:406:PCW:C6	3:A:406:PCW:O4P	0.61	2.49	11	12
3:A:413:PCW:H172	4:A:414:17F:H31	0.61	1.71	2	1
4:D:635:17F:H52	3:C:205:PCW:C18	0.61	2.22	3	4
3:A:404:PCW:C23	3:A:404:PCW:C27	0.61	2.78	4	1
3:B:211:PCW:H222	3:B:211:PCW:C18	0.61	2.26	4	1
3:D:608:PCW:H442	3:D:615:PCW:H472	0.61	1.73	14	3
3:B:204:PCW:C48	3:B:212:PCW:H20	0.61	2.26	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:206:PCW:C42	4:C:211:17F:H47	0.61	2.17	18	2
3:B:210:PCW:O11	3:B:210:PCW:H51	0.61	1.96	5	1
3:D:623:PCW:H382	3:D:625:PCW:H182	0.61	1.71	14	2
3:A:406:PCW:H412	3:B:210:PCW:H39	0.61	1.70	9	1
3:A:403:PCW:H231	3:A:403:PCW:C27	0.61	2.26	10	1
3:A:403:PCW:H282	3:A:403:PCW:C24	0.61	2.25	10	1
3:D:623:PCW:C20	3:D:623:PCW:C24	0.61	2.79	10	1
3:B:203:PCW:H2	3:B:211:PCW:C39	0.61	2.25	10	1
3:A:403:PCW:H211	3:A:403:PCW:H422	0.61	1.71	11	1
2:B:72:MET:HE1	2:B:99:GLN:HG2	0.61	1.72	12	1
3:A:407:PCW:H12	4:B:216:17F:H11	0.61	1.70	14	1
3:C:208:PCW:H242	3:C:209:PCW:H451	0.61	1.71	19	1
3:A:406:PCW:C27	3:B:207:PCW:H19	0.61	2.24	10	3
3:A:417:PCW:H351	3:D:612:PCW:H132	0.61	1.72	1	5
3:D:618:PCW:C45	3:C:207:PCW:H231	0.61	2.26	1	1
4:D:632:17F:O8	4:D:632:17F:H5	0.61	1.95	8	4
3:D:621:PCW:C14	4:D:634:17F:H4A	0.61	2.25	8	6
2:B:98:GLU:HA	2:B:101:LYS:HE2	0.61	1.73	19	2
3:B:210:PCW:H382	3:B:210:PCW:C42	0.61	2.19	8	2
2:C:79:LEU:HG	2:C:114:VAL:HG21	0.61	1.72	5	2
3:A:412:PCW:C20	3:C:206:PCW:H481	0.61	2.25	12	2
3:D:601:PCW:H461	3:D:607:PCW:C47	0.61	2.23	10	1
4:D:628:17F:H8	4:D:631:17F:C1Z	0.61	2.25	10	1
4:D:630:17F:H54	4:B:214:17F:H77	0.61	1.73	10	1
3:B:210:PCW:H52	4:B:216:17F:H4	0.61	1.73	19	2
3:C:203:PCW:C26	3:C:203:PCW:C22	0.61	2.74	11	1
3:A:404:PCW:H483	3:B:207:PCW:C48	0.61	2.26	13	1
3:A:407:PCW:C35	3:C:205:PCW:H122	0.61	2.26	20	2
3:B:212:PCW:C47	4:B:214:17F:H38	0.61	2.18	13	1
3:A:416:PCW:H20	3:A:419:PCW:H431	0.61	1.72	16	1
4:A:414:17F:H50	3:B:212:PCW:H20	0.61	1.72	18	1
3:A:403:PCW:H121	3:C:203:PCW:H322	0.61	1.73	1	1
3:A:420:PCW:H73	4:D:632:17F:H4	0.61	1.72	1	1
3:D:621:PCW:H231	3:D:622:PCW:C8	0.61	2.25	10	5
1:A:301:LEU:HD13	1:D:473:LYS:HG2	0.61	1.71	2	6
3:A:403:PCW:H342	3:C:203:PCW:H11	0.61	1.73	2	1
3:D:611:PCW:C22	3:D:619:PCW:H482	0.61	2.24	19	5
3:C:207:PCW:H322	3:C:207:PCW:C7	0.61	2.26	2	3
3:B:209:PCW:H222	3:B:209:PCW:C26	0.61	2.25	7	3
3:B:209:PCW:H372	3:B:209:PCW:H412	0.61	1.70	4	1
3:D:609:PCW:H281	4:D:633:17F:H72	0.61	1.73	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:406:PCW:C32	3:A:411:PCW:H41	0.61	2.26	7	1
3:A:413:PCW:H282	3:C:203:PCW:H432	0.61	1.73	9	1
3:A:417:PCW:H411	3:D:612:PCW:H181	0.61	1.72	10	1
3:D:616:PCW:C28	3:C:204:PCW:H272	0.61	2.25	10	1
4:D:628:17F:C8	4:D:631:17F:H33	0.61	2.26	10	1
3:B:207:PCW:C44	3:B:213:PCW:H231	0.61	2.25	11	2
1:A:301:LEU:HD22	1:D:473:LYS:HG2	0.61	1.72	18	4
4:A:414:17F:H69	4:C:210:17F:H29	0.61	1.73	16	1
3:B:213:PCW:H421	3:B:213:PCW:C21	0.61	2.23	17	2
3:D:621:PCW:H19	4:D:633:17F:C5	0.61	2.20	19	1
3:D:605:PCW:C18	3:D:605:PCW:C14	0.61	2.77	4	9
3:D:605:PCW:H2	3:D:605:PCW:H41	0.61	1.73	8	12
3:D:609:PCW:H342	3:D:609:PCW:H132	0.61	1.72	20	3
2:C:149:ARG:HG2	2:C:152:VAL:HG21	0.61	1.73	20	2
1:D:465:GLU:O	1:D:469:LEU:HG	0.61	1.96	5	12
3:D:604:PCW:H172	3:D:613:PCW:C13	0.61	2.26	14	3
3:D:617:PCW:C23	3:D:617:PCW:C27	0.61	2.78	11	4
3:D:622:PCW:O4P	3:D:622:PCW:C6	0.61	2.49	8	2
2:B:15:GLY:HA3	5:B:201:GDP:C8	0.61	2.31	2	7
3:A:416:PCW:H442	3:D:617:PCW:C21	0.61	2.26	3	6
3:D:615:PCW:H451	4:B:216:17F:C30	0.61	2.22	15	3
3:A:404:PCW:C28	4:A:415:17F:H69	0.61	2.26	8	2
3:D:607:PCW:H41	3:D:626:PCW:H241	0.61	1.72	8	1
3:B:203:PCW:C45	3:B:211:PCW:H232	0.61	2.12	9	2
3:A:413:PCW:C43	3:A:413:PCW:C47	0.61	2.77	15	3
3:A:420:PCW:O31	3:D:617:PCW:H63	0.61	1.96	11	1
3:A:413:PCW:H252	4:A:414:17F:H63	0.61	1.73	13	1
3:B:209:PCW:H341	3:B:209:PCW:H232	0.61	1.72	14	1
3:A:404:PCW:C45	4:B:215:17F:H12A	0.61	2.26	18	1
3:D:611:PCW:C11	3:D:611:PCW:O31	0.60	2.48	18	7
3:D:622:PCW:C16	3:C:212:PCW:H152	0.60	2.25	1	5
3:D:601:PCW:H441	4:D:628:17F:H38	0.60	1.72	2	1
3:D:616:PCW:O2P	3:D:616:PCW:C3	0.60	2.49	9	9
3:D:624:PCW:H62	3:D:624:PCW:O4P	0.60	1.96	14	4
3:B:213:PCW:C40	4:B:217:17F:H66	0.60	2.26	14	2
3:D:610:PCW:H483	3:B:212:PCW:H241	0.60	1.73	3	2
3:A:417:PCW:C36	3:D:612:PCW:H151	0.60	2.24	4	1
3:D:607:PCW:C28	4:D:631:17F:H67	0.60	2.26	4	1
4:D:628:17F:H78	4:B:216:17F:H48	0.60	1.73	4	1
3:B:204:PCW:C1	3:B:212:PCW:H82	0.60	2.24	4	1
3:B:206:PCW:H162	3:B:212:PCW:C44	0.60	2.12	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:215:17F:O6	4:B:215:17F:C18	0.60	2.47	17	4
3:A:404:PCW:C40	3:B:209:PCW:H121	0.60	2.25	6	1
3:D:622:PCW:H51	3:D:622:PCW:O3P	0.60	1.96	7	1
3:B:211:PCW:H61	3:B:212:PCW:H341	0.60	1.72	7	2
3:A:402:PCW:H412	3:A:407:PCW:H262	0.60	1.72	9	1
3:B:213:PCW:H281	4:B:215:17F:H71	0.60	1.73	9	1
4:A:415:17F:H77	3:D:611:PCW:H472	0.60	1.73	18	2
3:B:207:PCW:H483	3:B:213:PCW:C48	0.60	2.25	11	1
3:D:603:PCW:H52	3:D:603:PCW:O11	0.60	1.96	12	2
3:C:204:PCW:H132	4:C:211:17F:H75	0.60	1.72	14	1
3:A:408:PCW:H271	3:A:417:PCW:H241	0.60	1.73	20	2
3:D:601:PCW:C42	4:D:628:17F:H45	0.60	2.23	16	1
3:B:213:PCW:H271	4:B:215:17F:H75	0.60	1.73	16	1
3:D:622:PCW:C11	4:D:629:17F:H62	0.60	2.25	17	1
3:A:407:PCW:C21	3:A:407:PCW:C25	0.60	2.76	19	1
3:A:410:PCW:H181	3:C:209:PCW:H282	0.60	1.72	19	1
3:C:208:PCW:H32	3:C:209:PCW:H12	0.60	1.73	19	1
3:D:601:PCW:O4P	3:D:601:PCW:C6	0.60	2.48	4	20
3:A:401:PCW:H221	3:A:401:PCW:H182	0.60	1.71	3	1
3:D:611:PCW:C4	3:D:623:PCW:H342	0.60	2.26	8	5
4:D:629:17F:C20	4:D:629:17F:H9A	0.60	2.26	3	2
3:B:204:PCW:H341	3:B:212:PCW:C8	0.60	2.26	4	2
3:A:406:PCW:H481	3:D:606:PCW:H261	0.60	1.72	5	1
3:A:416:PCW:H472	3:D:617:PCW:C25	0.60	2.23	10	2
4:D:634:17F:H74	3:C:206:PCW:H251	0.60	1.71	7	1
3:B:206:PCW:C48	3:C:212:PCW:H40	0.60	2.27	12	2
3:A:404:PCW:H63	4:A:415:17F:C2	0.60	2.26	9	1
3:D:603:PCW:H251	4:B:217:17F:C41	0.60	2.26	11	1
3:B:208:PCW:C40	4:B:214:17F:H30	0.60	2.27	11	1
3:A:410:PCW:H122	3:C:209:PCW:H352	0.60	1.71	20	3
4:B:214:17F:H32	4:B:214:17F:H10	0.60	1.70	12	1
3:A:403:PCW:H331	4:C:211:17F:H76	0.60	1.71	14	1
3:A:407:PCW:H221	3:C:205:PCW:C15	0.60	2.27	16	1
3:B:203:PCW:H222	4:C:210:17F:C31	0.60	2.26	16	1
3:A:408:PCW:C28	3:A:417:PCW:H221	0.60	2.19	20	2
3:A:412:PCW:H451	3:C:208:PCW:C38	0.60	2.26	18	1
3:B:213:PCW:H272	4:B:215:17F:H61	0.60	1.73	20	1
3:A:420:PCW:H372	3:D:617:PCW:C14	0.60	2.22	16	5
3:D:601:PCW:O31	3:D:601:PCW:H12	0.60	1.96	9	12
3:D:622:PCW:H121	4:D:630:17F:C1Y	0.60	2.24	1	4
3:D:624:PCW:O4P	3:D:624:PCW:H62	0.60	1.96	5	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:616:PCW:H421	3:D:627:PCW:C23	0.60	2.27	20	7
3:B:210:PCW:O2P	3:B:210:PCW:C3	0.60	2.49	11	3
3:D:602:PCW:C18	3:D:624:PCW:H222	0.60	2.26	3	2
3:D:604:PCW:H82	4:D:632:17F:O4	0.60	1.95	3	1
3:A:416:PCW:H482	3:C:203:PCW:H462	0.60	1.73	4	1
3:A:419:PCW:C36	3:D:617:PCW:H431	0.60	2.26	12	5
3:D:607:PCW:H63	3:D:626:PCW:C24	0.60	2.24	5	3
3:A:420:PCW:H51	3:A:420:PCW:O11	0.60	1.96	6	1
3:A:404:PCW:C21	4:A:415:17F:H57	0.60	2.25	7	1
3:A:408:PCW:H471	3:A:410:PCW:C32	0.60	2.25	8	1
3:C:204:PCW:C16	4:C:211:17F:H63	0.60	2.26	11	1
3:C:204:PCW:H351	4:C:211:17F:C10	0.60	2.26	12	1
1:A:392:GLU:HB3	1:D:591:TYR:HE1	0.60	1.54	16	1
3:B:210:PCW:H73	3:B:210:PCW:O11	0.60	1.95	17	1
3:A:410:PCW:H472	3:C:209:PCW:H221	0.60	1.73	19	1
3:A:406:PCW:C23	3:B:210:PCW:H121	0.60	2.26	1	1
3:A:409:PCW:C6	3:A:412:PCW:H371	0.60	2.26	1	1
3:D:605:PCW:H331	3:D:607:PCW:H61	0.60	1.74	1	2
3:D:623:PCW:C24	3:B:203:PCW:H481	0.60	2.27	1	1
3:D:613:PCW:H431	3:D:619:PCW:H39	0.60	1.73	5	7
4:D:633:17F:H52	3:C:209:PCW:H452	0.60	1.73	3	1
4:D:634:17F:H75	3:C:206:PCW:H252	0.60	1.72	3	1
1:A:330:ARG:HH21	1:D:447:GLU:HB3	0.60	1.55	5	7
3:A:413:PCW:C11	3:A:413:PCW:H371	0.60	2.25	4	5
3:B:205:PCW:O31	3:B:205:PCW:C1	0.60	2.48	18	5
3:B:209:PCW:H272	3:B:209:PCW:C23	0.60	2.25	7	3
3:A:401:PCW:H41	3:B:209:PCW:H2	0.60	1.72	6	1
3:A:419:PCW:C38	3:D:610:PCW:H161	0.60	2.25	8	1
3:A:409:PCW:H181	3:A:409:PCW:C40	0.60	2.25	14	2
3:C:204:PCW:H432	4:C:211:17F:H11A	0.60	1.72	12	1
3:D:620:PCW:C27	4:D:635:17F:H37	0.60	2.26	13	1
3:D:624:PCW:C31	3:D:624:PCW:H62	0.60	2.26	15	1
3:B:203:PCW:H482	4:B:217:17F:C29	0.60	2.26	16	1
3:B:204:PCW:O31	3:B:204:PCW:H12	0.60	1.96	17	2
3:B:207:PCW:H182	3:B:210:PCW:H20	0.60	1.72	17	1
3:A:403:PCW:C13	3:A:403:PCW:H362	0.60	2.27	2	1
3:A:405:PCW:C38	4:D:628:17F:H54	0.60	2.25	2	1
3:B:207:PCW:C3	3:B:210:PCW:H152	0.60	2.25	13	3
3:B:208:PCW:H352	4:B:214:17F:H34	0.60	1.71	3	2
3:A:413:PCW:C34	4:A:414:17F:H59	0.60	2.07	12	2
3:A:417:PCW:H441	3:D:612:PCW:H272	0.60	1.74	16	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:419:PCW:C3	3:D:617:PCW:H421	0.60	2.26	5	2
3:D:602:PCW:C46	3:D:610:PCW:H432	0.60	2.26	5	3
3:B:204:PCW:C11	3:C:207:PCW:H11	0.60	2.26	7	3
3:A:411:PCW:H461	3:A:418:PCW:H272	0.60	1.73	10	3
3:D:601:PCW:H483	4:D:628:17F:H58	0.60	1.72	13	3
3:D:613:PCW:C20	4:C:210:17F:H47	0.60	2.25	6	2
3:A:406:PCW:H282	4:B:216:17F:C19	0.60	2.22	7	1
3:B:213:PCW:H432	3:B:213:PCW:C21	0.60	2.27	7	3
3:C:204:PCW:H42	3:C:204:PCW:H11	0.60	1.72	19	4
3:D:603:PCW:C28	3:D:606:PCW:H483	0.60	2.26	9	1
3:D:623:PCW:H131	3:D:623:PCW:H371	0.60	1.73	9	2
2:B:22:GLN:HB3	2:B:149:ARG:HG3	0.60	1.72	10	2
3:B:205:PCW:H283	3:B:212:PCW:H331	0.60	1.72	11	1
3:A:411:PCW:H432	3:A:418:PCW:H272	0.60	1.74	13	2
3:A:402:PCW:H451	4:D:635:17F:C30	0.60	2.25	15	1
3:B:204:PCW:H331	3:B:212:PCW:C14	0.60	2.20	17	2
3:A:406:PCW:O4P	3:A:406:PCW:C6	0.60	2.50	14	8
3:A:407:PCW:C7	4:B:214:17F:O1	0.60	2.47	10	14
3:D:611:PCW:O11	3:D:619:PCW:C8	0.60	2.49	15	7
3:D:625:PCW:C47	3:D:626:PCW:H482	0.60	2.27	11	5
3:A:411:PCW:H182	3:A:418:PCW:H283	0.60	1.73	19	5
3:B:204:PCW:C45	3:C:203:PCW:H152	0.60	2.26	9	3
3:B:209:PCW:H271	4:B:215:17F:H32	0.60	1.72	2	1
3:B:211:PCW:O4P	3:B:211:PCW:C6	0.60	2.50	12	4
3:A:401:PCW:H12	3:B:209:PCW:H181	0.60	1.72	15	2
3:D:601:PCW:O31	3:D:601:PCW:H31	0.60	1.96	4	8
3:D:601:PCW:H483	4:D:628:17F:C37	0.60	2.26	4	1
3:B:206:PCW:H151	3:B:212:PCW:H421	0.60	1.73	4	1
3:B:212:PCW:O4P	3:B:212:PCW:O31	0.60	2.20	6	3
3:B:213:PCW:H421	4:B:217:17F:H67	0.60	1.72	6	1
3:A:417:PCW:O31	3:A:417:PCW:O4P	0.60	2.19	18	2
3:C:207:PCW:H272	3:C:209:PCW:C37	0.60	2.27	7	1
3:D:621:PCW:C20	4:D:633:17F:H19A	0.60	2.27	8	1
3:B:209:PCW:H19	4:B:215:17F:C19	0.60	2.26	8	2
3:B:209:PCW:H61	4:B:215:17F:O9	0.60	1.96	8	1
3:C:207:PCW:H261	3:C:207:PCW:H131	0.60	1.73	11	1
3:D:608:PCW:C36	3:C:205:PCW:H281	0.60	2.25	13	1
3:D:614:PCW:C3	3:D:614:PCW:H42	0.60	2.27	14	1
3:A:402:PCW:H342	3:A:409:PCW:H121	0.60	1.71	15	1
3:D:618:PCW:O2P	3:D:627:PCW:H63	0.60	1.96	16	1
3:B:203:PCW:H211	4:C:210:17F:H19	0.60	1.73	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:207:PCW:O11	3:B:213:PCW:H172	0.60	1.97	16	1
4:A:414:17F:O10	4:A:414:17F:O6	0.60	2.19	1	8
3:D:612:PCW:H342	3:D:612:PCW:O2	0.60	1.97	14	19
3:B:205:PCW:H382	3:C:208:PCW:H342	0.60	1.74	1	1
3:D:613:PCW:C41	3:D:619:PCW:H39	0.60	2.25	6	3
3:A:409:PCW:H52	3:C:206:PCW:P	0.60	2.36	7	1
4:A:414:17F:H48	3:C:203:PCW:C42	0.60	2.10	7	1
3:C:204:PCW:H471	4:C:211:17F:H56	0.60	1.72	7	1
3:B:208:PCW:H441	4:B:214:17F:H62	0.60	1.73	9	1
3:D:609:PCW:C12	4:D:633:17F:H18	0.60	2.26	11	1
3:B:205:PCW:H261	3:B:212:PCW:H351	0.60	1.74	11	1
3:B:205:PCW:H422	3:B:206:PCW:H162	0.60	1.73	11	1
3:D:601:PCW:H483	4:D:628:17F:C36	0.60	2.26	18	2
3:B:204:PCW:O2	3:C:204:PCW:H372	0.60	1.96	12	1
3:C:204:PCW:H451	4:C:211:17F:H33	0.60	1.73	12	1
3:C:207:PCW:C19	3:C:207:PCW:H452	0.60	2.27	12	1
3:D:618:PCW:H151	3:D:627:PCW:H162	0.60	1.72	14	1
3:A:416:PCW:C20	3:A:419:PCW:H431	0.60	2.26	16	2
3:D:610:PCW:H483	3:B:212:PCW:C24	0.60	2.27	16	2
3:A:404:PCW:H451	4:B:215:17F:C22	0.60	2.26	18	1
3:A:407:PCW:C16	3:C:205:PCW:H342	0.60	2.26	18	1
3:D:602:PCW:H252	3:D:610:PCW:H171	0.60	1.74	1	3
3:D:603:PCW:H82	4:D:630:17F:H4A	0.60	1.73	1	1
3:D:609:PCW:H63	4:D:633:17F:O8	0.60	1.95	1	7
3:D:614:PCW:C6	3:D:625:PCW:O1P	0.60	2.49	18	11
3:D:623:PCW:C36	3:D:623:PCW:C32	0.60	2.63	9	16
3:B:208:PCW:H162	4:B:214:17F:H20A	0.60	1.73	1	1
3:B:208:PCW:H31	3:B:208:PCW:P	0.60	2.36	13	7
3:B:210:PCW:O4P	3:B:210:PCW:O31	0.60	2.20	17	2
3:A:402:PCW:H73	3:C:206:PCW:O2P	0.60	1.96	9	2
3:D:602:PCW:H331	3:D:624:PCW:H121	0.60	1.72	2	3
3:D:622:PCW:H352	3:D:627:PCW:H211	0.60	1.71	6	3
3:D:608:PCW:H431	3:C:205:PCW:H242	0.60	1.73	5	3
3:D:603:PCW:H41	3:D:603:PCW:O11	0.60	1.96	5	1
3:C:203:PCW:C12	3:C:203:PCW:H382	0.60	2.27	6	1
3:A:410:PCW:H62	3:C:209:PCW:O11	0.60	1.97	7	1
3:B:208:PCW:H51	3:B:208:PCW:O3P	0.60	1.97	20	5
3:B:208:PCW:H381	4:B:214:17F:H11A	0.60	1.73	8	1
3:B:205:PCW:H142	3:B:211:PCW:H131	0.60	1.74	10	1
3:A:406:PCW:C8	3:B:207:PCW:H371	0.60	2.26	13	1
3:D:618:PCW:H261	3:C:204:PCW:H461	0.60	1.73	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:604:PCW:H261	3:D:613:PCW:H181	0.60	1.72	17	1
3:A:404:PCW:C42	3:B:209:PCW:H432	0.60	2.23	19	1
3:B:204:PCW:H352	3:B:212:PCW:C7	0.60	2.26	19	1
3:A:402:PCW:H362	3:A:409:PCW:H151	0.60	1.74	20	1
3:D:604:PCW:C32	3:D:611:PCW:H12	0.60	2.27	14	6
4:D:635:17F:O10	4:D:635:17F:H4	0.60	1.97	15	14
3:C:206:PCW:H11	3:C:206:PCW:O31	0.60	1.97	10	5
3:D:604:PCW:H231	3:D:613:PCW:C38	0.60	2.26	8	9
3:C:207:PCW:H181	3:C:207:PCW:H251	0.60	1.74	2	2
3:A:401:PCW:H51	3:B:209:PCW:H11	0.60	1.74	3	1
3:A:409:PCW:C17	3:A:409:PCW:C21	0.60	2.59	6	6
3:A:404:PCW:C17	3:A:404:PCW:C21	0.60	2.62	4	1
3:D:601:PCW:H483	4:D:628:17F:H67	0.60	1.73	4	1
3:D:608:PCW:C45	3:C:205:PCW:H231	0.60	2.25	6	4
3:B:211:PCW:C1	4:B:217:17F:H18	0.60	2.26	4	1
3:C:204:PCW:H19	4:C:211:17F:H18	0.60	1.73	7	1
3:B:213:PCW:H432	3:B:213:PCW:H211	0.60	1.72	14	2
3:C:203:PCW:C18	3:C:203:PCW:C22	0.60	2.72	9	3
3:D:601:PCW:C46	4:D:628:17F:H65	0.60	2.25	11	1
3:B:208:PCW:C21	4:B:214:17F:H57	0.60	2.22	14	3
3:A:403:PCW:O3P	3:A:403:PCW:O31	0.60	2.18	15	1
3:A:407:PCW:H141	3:C:205:PCW:C34	0.60	2.27	18	1
3:B:209:PCW:H172	4:B:215:17F:O10	0.60	1.97	19	1
3:B:211:PCW:H482	3:B:211:PCW:C19	0.60	2.27	19	1
3:D:601:PCW:C48	4:D:631:17F:H47	0.60	2.26	1	2
3:D:604:PCW:O1P	3:D:604:PCW:H52	0.60	1.97	18	10
3:D:617:PCW:H2	3:D:617:PCW:O11	0.60	1.97	11	10
4:D:629:17F:H54	3:B:212:PCW:H462	0.60	1.74	1	2
2:B:109:VAL:HB	2:B:111:MET:HE2	0.60	1.73	15	6
3:B:205:PCW:C21	3:B:205:PCW:C25	0.60	2.80	20	10
3:A:403:PCW:H362	3:A:403:PCW:H131	0.60	1.71	2	2
4:D:633:17F:H52	3:C:209:PCW:H471	0.60	1.74	2	1
3:B:205:PCW:C40	4:B:214:17F:H66	0.60	2.25	2	2
3:A:407:PCW:C14	3:C:205:PCW:H342	0.60	2.25	6	4
3:B:208:PCW:C41	4:B:214:17F:H8A	0.60	2.27	13	2
3:A:419:PCW:H351	3:D:617:PCW:H422	0.60	1.73	16	3
3:B:206:PCW:H431	3:C:204:PCW:H441	0.60	1.74	13	2
3:B:213:PCW:H371	4:B:217:17F:H57	0.60	1.72	7	1
3:D:623:PCW:O2	3:D:625:PCW:H162	0.60	1.97	9	1
3:B:206:PCW:H211	3:C:208:PCW:H282	0.60	1.73	9	1
3:A:417:PCW:C42	3:D:612:PCW:H212	0.60	2.26	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:409:PCW:H51	3:C:206:PCW:C35	0.60	2.27	12	3
3:A:404:PCW:H152	3:B:209:PCW:C40	0.60	2.27	12	1
3:B:203:PCW:C22	4:C:210:17F:H18	0.60	2.27	14	1
3:D:607:PCW:C46	4:D:628:17F:H61	0.60	2.22	15	2
3:B:204:PCW:H172	3:C:204:PCW:H40	0.60	1.72	18	3
3:B:208:PCW:O3	4:B:214:17F:H1	0.60	1.97	17	1
3:D:604:PCW:H262	3:D:613:PCW:H181	0.60	1.73	19	2
3:D:622:PCW:H171	3:C:212:PCW:H121	0.59	1.73	8	4
3:D:615:PCW:C48	3:B:208:PCW:H271	0.59	2.23	7	2
3:D:622:PCW:O4P	3:D:622:PCW:H62	0.59	1.96	8	2
3:D:620:PCW:O1P	3:D:621:PCW:H42	0.59	1.97	3	3
3:D:601:PCW:C35	4:B:216:17F:H70	0.59	2.20	4	1
3:D:613:PCW:O31	3:D:613:PCW:C3	0.59	2.48	13	8
3:A:403:PCW:H481	3:C:203:PCW:H283	0.59	1.72	7	1
3:A:403:PCW:H461	3:C:203:PCW:C28	0.59	2.19	9	1
3:A:413:PCW:C34	4:A:414:17F:H58	0.59	2.27	9	1
3:C:203:PCW:C22	3:C:203:PCW:C26	0.59	2.77	12	1
3:C:206:PCW:H152	3:C:206:PCW:C36	0.59	2.26	13	1
3:A:410:PCW:H52	3:C:209:PCW:O2P	0.59	1.96	16	1
3:D:622:PCW:H162	3:C:212:PCW:H161	0.59	1.74	18	3
3:A:413:PCW:O31	3:A:413:PCW:H351	0.59	1.97	17	1
3:B:208:PCW:H322	3:B:208:PCW:H62	0.59	1.72	17	1
3:D:607:PCW:H181	4:D:631:17F:H29	0.59	1.74	20	2
3:D:618:PCW:C32	3:D:627:PCW:H152	0.59	2.24	19	1
3:C:207:PCW:H121	3:C:207:PCW:H362	0.59	1.74	19	1
3:A:410:PCW:H152	3:C:207:PCW:C23	0.59	2.26	20	1
3:A:403:PCW:C28	3:A:413:PCW:H222	0.59	2.26	1	1
3:D:604:PCW:O31	3:D:613:PCW:H82	0.59	1.97	1	6
3:B:212:PCW:H451	4:B:214:17F:H77	0.59	1.72	2	1
2:C:15:GLY:HA3	5:C:201:GDP:C8	0.59	2.33	18	9
3:D:604:PCW:C31	3:D:613:PCW:H61	0.59	2.27	3	1
3:D:613:PCW:C14	3:D:619:PCW:H382	0.59	2.27	3	1
3:B:211:PCW:C13	4:B:217:17F:H58	0.59	2.26	10	3
3:A:404:PCW:H341	3:A:404:PCW:H132	0.59	1.73	6	3
3:B:204:PCW:H252	3:C:207:PCW:H182	0.59	1.73	6	1
3:A:408:PCW:C27	3:A:417:PCW:H241	0.59	2.27	16	7
3:A:406:PCW:C25	3:B:207:PCW:H151	0.59	2.27	16	2
3:D:607:PCW:H63	3:D:626:PCW:C22	0.59	2.25	9	1
3:D:623:PCW:C31	3:D:624:PCW:H322	0.59	2.27	14	2
3:C:207:PCW:H62	4:C:211:17F:O4	0.59	1.97	12	2
3:C:203:PCW:H19	3:C:203:PCW:C48	0.59	2.26	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:607:PCW:H172	4:D:631:17F:O10	0.59	1.98	1	4
3:A:406:PCW:H31	3:A:406:PCW:H42	0.59	1.73	2	2
3:D:618:PCW:H352	3:D:627:PCW:H341	0.59	1.74	16	2
3:D:613:PCW:H251	4:C:210:17F:H46	0.59	1.74	6	4
3:B:206:PCW:C15	3:B:212:PCW:H421	0.59	2.27	4	1
4:B:214:17F:C26	4:B:217:17F:H70	0.59	2.27	4	2
3:A:406:PCW:H283	4:B:216:17F:C19	0.59	2.26	6	1
3:A:410:PCW:H371	3:C:209:PCW:H162	0.59	1.75	6	3
3:C:207:PCW:H452	3:C:207:PCW:H19	0.59	1.73	12	2
3:A:407:PCW:H12	4:B:216:17F:H29	0.59	1.74	7	2
3:D:602:PCW:H231	3:D:602:PCW:C47	0.59	2.26	8	1
3:D:627:PCW:O4P	3:D:627:PCW:H2	0.59	1.98	10	2
4:C:211:17F:H29	4:C:211:17F:H65	0.59	1.74	17	1
4:C:211:17F:H54	3:C:212:PCW:H232	0.59	1.72	17	1
3:A:407:PCW:C15	3:B:208:PCW:H222	0.59	2.27	19	1
3:A:404:PCW:C39	3:B:209:PCW:H63	0.59	2.27	20	1
3:D:616:PCW:H372	3:D:618:PCW:H142	0.59	1.72	20	1
3:D:621:PCW:O31	3:D:621:PCW:O3P	0.59	2.20	3	17
3:A:417:PCW:H422	3:D:612:PCW:H242	0.59	1.75	8	5
3:A:403:PCW:O11	3:A:403:PCW:C4	0.59	2.50	9	4
3:D:615:PCW:H122	4:D:635:17F:C6	0.59	2.27	4	1
3:A:410:PCW:C23	3:A:410:PCW:C18	0.59	2.80	8	3
3:D:612:PCW:C21	3:D:612:PCW:C17	0.59	2.79	18	2
3:C:208:PCW:H442	3:C:209:PCW:H422	0.59	1.74	7	1
3:D:611:PCW:O2P	3:D:619:PCW:H63	0.59	1.96	8	1
4:B:215:17F:C18	4:B:215:17F:C4	0.59	2.69	9	1
4:A:415:17F:N1	4:A:415:17F:O10	0.59	2.35	10	2
3:D:625:PCW:H19	3:D:625:PCW:C12	0.59	2.27	10	2
3:A:410:PCW:O1P	3:C:207:PCW:C14	0.59	2.51	13	1
3:B:209:PCW:C46	4:B:215:17F:H50	0.59	2.28	13	1
3:A:406:PCW:H422	3:B:210:PCW:C40	0.59	2.28	15	1
3:D:614:PCW:O1P	3:D:625:PCW:H51	0.59	1.96	17	1
3:B:213:PCW:H271	4:B:215:17F:H61	0.59	1.74	18	1
3:A:407:PCW:H171	3:C:205:PCW:H361	0.59	1.73	19	1
3:B:208:PCW:O11	3:B:208:PCW:C8	0.59	2.49	19	1
3:C:208:PCW:H441	3:C:209:PCW:H382	0.59	1.74	19	1
4:C:211:17F:H55	3:C:212:PCW:H212	0.59	1.72	19	1
3:D:616:PCW:H483	3:B:204:PCW:H222	0.59	1.73	20	1
3:D:616:PCW:H483	3:B:204:PCW:C22	0.59	2.27	20	1
3:A:410:PCW:P	3:A:410:PCW:C3	0.59	2.90	11	9
3:D:602:PCW:H42	3:D:602:PCW:H2	0.59	1.73	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:604:PCW:H211	3:D:613:PCW:C38	0.59	2.18	12	4
3:A:419:PCW:C3	3:D:617:PCW:C42	0.59	2.80	8	5
3:D:616:PCW:H261	3:C:204:PCW:H272	0.59	1.75	3	1
3:D:617:PCW:C47	3:D:617:PCW:C43	0.59	2.78	8	2
3:A:407:PCW:H251	3:C:205:PCW:H411	0.59	1.75	4	1
3:D:614:PCW:O1P	3:D:614:PCW:H51	0.59	1.97	7	7
3:B:211:PCW:C1	4:B:217:17F:C18	0.59	2.80	4	1
3:A:416:PCW:C44	3:D:617:PCW:H231	0.59	2.28	5	1
3:B:204:PCW:H182	3:C:207:PCW:H283	0.59	1.75	5	1
3:B:206:PCW:H242	3:C:208:PCW:H221	0.59	1.73	5	1
3:D:603:PCW:H412	3:D:605:PCW:C24	0.59	2.27	11	4
3:A:413:PCW:C14	4:A:414:17F:H33	0.59	2.28	8	1
4:D:628:17F:C23	4:D:631:17F:H75	0.59	2.26	10	2
3:A:416:PCW:H142	3:D:617:PCW:H141	0.59	1.75	11	1
3:D:616:PCW:H452	3:C:212:PCW:H431	0.59	1.71	11	1
3:C:207:PCW:H261	3:C:207:PCW:C13	0.59	2.28	11	1
3:A:408:PCW:H412	3:C:207:PCW:C42	0.59	2.26	12	1
3:D:616:PCW:H431	3:B:206:PCW:H483	0.59	1.74	12	1
4:B:214:17F:H50	4:B:217:17F:H71	0.59	1.74	17	2
4:A:414:17F:H52	3:C:203:PCW:H462	0.59	1.73	15	1
3:A:420:PCW:C35	3:D:617:PCW:H132	0.59	2.25	16	2
3:D:627:PCW:H282	4:D:633:17F:H46	0.59	1.74	18	1
3:D:626:PCW:H182	3:D:626:PCW:H82	0.59	1.72	19	2
4:B:216:17F:H4A	4:B:216:17F:N1	0.59	2.12	20	1
3:D:608:PCW:H271	4:D:628:17F:H71	0.59	1.73	1	2
3:B:209:PCW:C22	4:B:215:17F:O10	0.59	2.50	1	1
3:B:211:PCW:H362	3:B:212:PCW:H32	0.59	1.74	1	1
3:D:607:PCW:H462	3:B:207:PCW:H271	0.59	1.74	2	1
3:A:407:PCW:H211	3:C:205:PCW:H411	0.59	1.73	5	3
3:D:627:PCW:H2	3:D:627:PCW:H41	0.59	1.75	5	1
3:D:623:PCW:H262	3:B:212:PCW:H282	0.59	1.74	6	1
3:C:203:PCW:H382	3:C:203:PCW:C14	0.59	2.27	6	1
3:D:622:PCW:H51	3:D:622:PCW:O31	0.59	1.98	7	1
3:B:207:PCW:O11	3:B:210:PCW:H152	0.59	1.97	10	1
3:D:604:PCW:O3P	3:D:624:PCW:H82	0.59	1.97	14	4
3:D:623:PCW:C32	3:D:623:PCW:C36	0.59	2.79	19	2
3:C:207:PCW:H51	4:C:211:17F:O4	0.59	1.97	14	1
3:B:208:PCW:H432	4:B:214:17F:C42	0.59	2.28	19	1
3:A:406:PCW:O11	3:B:210:PCW:H332	0.59	1.97	20	1
3:A:410:PCW:H222	4:D:633:17F:H54	0.59	1.74	20	1
3:D:622:PCW:H431	3:C:212:PCW:H481	0.59	1.74	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:216:17F:C30	3:C:205:PCW:H221	0.59	2.26	20	1
4:C:211:17F:H50	3:C:212:PCW:H212	0.59	1.73	20	1
4:B:217:17F:O6	4:B:217:17F:C18	0.59	2.51	14	4
3:A:412:PCW:H432	3:C:208:PCW:H451	0.59	1.74	2	1
3:D:601:PCW:O31	3:D:601:PCW:C3	0.59	2.47	2	15
3:D:623:PCW:C42	3:D:625:PCW:H261	0.59	2.25	13	5
3:B:205:PCW:O11	3:B:205:PCW:C2	0.59	2.44	9	6
3:A:409:PCW:C32	3:C:206:PCW:H372	0.59	2.13	5	1
4:D:629:17F:H65	4:D:634:17F:O7	0.59	1.98	20	2
4:A:415:17F:C42	4:C:210:17F:H73	0.59	2.27	16	3
3:A:416:PCW:H411	3:A:416:PCW:H371	0.59	1.75	7	1
3:D:622:PCW:H421	3:B:206:PCW:H261	0.59	1.73	7	3
3:A:403:PCW:H321	3:C:204:PCW:H73	0.59	1.73	9	1
3:A:408:PCW:O2P	3:A:408:PCW:C31	0.59	2.51	13	1
3:A:409:PCW:C16	3:A:409:PCW:C21	0.59	2.81	12	4
3:D:608:PCW:H271	4:D:628:17F:C39	0.59	2.28	1	2
3:D:621:PCW:C19	4:D:633:17F:O10	0.59	2.48	13	10
3:A:403:PCW:O11	3:A:403:PCW:C5	0.59	2.51	19	14
3:D:605:PCW:C14	3:D:605:PCW:C18	0.59	2.80	5	11
3:D:616:PCW:H441	3:D:627:PCW:H251	0.59	1.72	8	3
3:C:208:PCW:H351	3:C:208:PCW:C12	0.59	2.26	10	3
3:A:404:PCW:H451	4:B:215:17F:O10	0.59	1.98	3	1
3:B:204:PCW:C4	3:B:206:PCW:H52	0.59	2.22	13	2
3:D:608:PCW:H422	3:D:615:PCW:H441	0.59	1.74	14	2
3:D:620:PCW:H141	4:D:635:17F:C17	0.59	2.28	11	3
3:D:601:PCW:H51	3:D:601:PCW:O1P	0.59	1.98	18	2
3:B:207:PCW:O2P	3:B:207:PCW:O2	0.59	2.21	12	5
3:B:206:PCW:H422	4:C:211:17F:H39	0.59	1.72	8	2
3:D:610:PCW:C48	3:B:212:PCW:H261	0.59	2.28	13	1
3:B:204:PCW:H171	3:B:205:PCW:C48	0.59	2.28	13	1
4:B:215:17F:H5	4:B:215:17F:H19	0.59	1.73	14	1
3:D:618:PCW:H481	3:C:204:PCW:H472	0.59	1.74	15	1
3:D:618:PCW:C48	3:B:204:PCW:H242	0.59	2.28	17	1
3:B:204:PCW:C33	3:B:212:PCW:H121	0.59	2.28	19	2
3:D:612:PCW:C6	3:D:618:PCW:H31	0.59	2.27	19	2
3:C:207:PCW:H281	3:C:208:PCW:C17	0.59	2.27	20	1
3:A:403:PCW:H362	3:A:403:PCW:C13	0.59	2.26	1	2
3:D:603:PCW:H51	3:D:603:PCW:O11	0.59	1.98	1	1
3:D:609:PCW:C17	4:D:633:17F:H61	0.59	2.27	19	8
3:B:204:PCW:H241	3:C:207:PCW:H271	0.59	1.74	1	1
3:B:211:PCW:O11	3:B:211:PCW:O2	0.59	2.21	13	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:203:PCW:O4P	3:C:203:PCW:H2	0.59	1.97	2	2
3:D:605:PCW:O4P	3:D:605:PCW:H62	0.59	1.97	3	4
3:A:403:PCW:P	3:A:403:PCW:C3	0.59	2.91	7	6
3:D:604:PCW:C32	3:D:613:PCW:H62	0.59	2.28	12	4
3:D:601:PCW:C46	3:D:607:PCW:H472	0.59	2.28	10	3
3:A:404:PCW:C43	4:B:215:17F:H19A	0.59	2.26	8	1
3:B:205:PCW:H283	3:B:212:PCW:H181	0.59	1.74	9	1
3:A:402:PCW:H63	3:A:402:PCW:O11	0.59	1.97	10	2
3:A:413:PCW:C14	4:A:414:17F:H66	0.59	2.26	12	5
3:B:206:PCW:H421	3:C:212:PCW:H251	0.59	1.75	11	1
3:A:411:PCW:H122	4:B:215:17F:H33	0.59	1.73	13	1
3:A:413:PCW:H162	4:A:414:17F:C32	0.59	2.22	17	3
3:B:207:PCW:C6	3:B:207:PCW:O4P	0.59	2.51	15	1
3:B:206:PCW:C36	3:C:204:PCW:H411	0.59	2.26	2	1
3:D:616:PCW:O1P	3:D:616:PCW:H52	0.59	1.98	5	1
3:A:407:PCW:C1	4:B:216:17F:H11	0.59	2.28	8	2
3:A:413:PCW:H132	4:A:414:17F:H33	0.59	1.73	20	2
3:B:204:PCW:H231	3:C:207:PCW:H271	0.59	1.74	8	1
3:A:417:PCW:O4P	3:A:417:PCW:O31	0.59	2.21	19	2
3:B:212:PCW:H232	4:C:211:17F:H44	0.59	1.75	10	1
3:D:611:PCW:H241	3:D:611:PCW:C45	0.59	2.27	11	2
3:D:613:PCW:H483	3:D:619:PCW:H431	0.59	1.73	11	1
3:B:205:PCW:H271	3:B:212:PCW:H161	0.59	1.73	12	1
3:C:208:PCW:H121	3:C:208:PCW:H351	0.59	1.74	19	3
3:D:610:PCW:H483	3:B:212:PCW:H261	0.59	1.72	13	1
3:B:204:PCW:C26	3:C:207:PCW:H262	0.59	2.28	13	1
3:A:402:PCW:H321	2:C:170:MET:HB3	0.59	1.74	16	1
3:B:204:PCW:H42	3:B:206:PCW:H51	0.59	1.74	17	1
3:A:401:PCW:C42	3:D:611:PCW:H271	0.59	2.28	18	1
3:B:206:PCW:H321	3:C:204:PCW:C38	0.59	2.28	19	1
3:A:413:PCW:C31	4:A:414:17F:H20	0.58	2.28	1	1
3:A:417:PCW:H411	3:A:417:PCW:C37	0.58	2.13	1	10
3:C:204:PCW:O3P	3:C:204:PCW:O31	0.58	2.20	12	11
3:D:604:PCW:O2P	3:D:613:PCW:H63	0.58	1.98	2	3
3:D:620:PCW:H2	3:D:620:PCW:O4P	0.58	1.97	20	8
3:D:621:PCW:H362	4:D:633:17F:C33	0.58	2.28	18	6
3:A:401:PCW:H341	3:A:404:PCW:H19	0.58	1.73	3	1
3:D:608:PCW:H452	3:C:205:PCW:C23	0.58	2.25	6	4
3:A:404:PCW:H222	4:A:415:17F:H57	0.58	1.75	4	1
3:D:615:PCW:H212	3:C:205:PCW:C28	0.58	2.28	4	1
4:D:629:17F:H9A	4:D:629:17F:C20	0.58	2.27	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:204:PCW:H131	4:C:211:17F:H62	0.58	1.74	6	1
3:A:420:PCW:H122	4:D:632:17F:H11A	0.58	1.74	7	5
3:C:207:PCW:H272	3:C:209:PCW:H371	0.58	1.74	7	1
3:D:620:PCW:H11	3:D:620:PCW:C7	0.58	2.27	8	2
3:C:206:PCW:C17	3:C:206:PCW:H381	0.58	2.28	8	1
3:A:401:PCW:H471	3:D:614:PCW:H242	0.58	1.75	10	2
3:B:205:PCW:H12	3:B:211:PCW:H73	0.58	1.75	11	4
3:A:411:PCW:C12	4:B:215:17F:H33	0.58	2.28	13	1
3:A:413:PCW:H252	4:A:414:17F:C35	0.58	2.29	13	1
3:B:213:PCW:C28	4:B:215:17F:H77	0.58	2.28	13	1
3:C:203:PCW:H222	3:C:203:PCW:C18	0.58	2.27	15	1
3:A:412:PCW:H12	3:A:412:PCW:H41	0.58	1.74	20	2
3:D:609:PCW:C8	4:D:633:17F:O8	0.58	2.50	6	2
3:D:611:PCW:H51	3:D:623:PCW:C34	0.58	2.26	1	1
3:D:620:PCW:O3P	3:D:620:PCW:O31	0.58	2.21	1	5
2:B:22:GLN:O	2:B:26:ASN:HA	0.58	1.98	3	6
3:A:402:PCW:H82	3:A:409:PCW:C3	0.58	2.27	2	1
3:D:607:PCW:H121	3:D:608:PCW:H161	0.58	1.75	2	3
3:B:205:PCW:H40	4:B:214:17F:H66	0.58	1.75	15	2
1:A:250:VAL:HG21	3:A:412:PCW:H271	0.58	1.73	3	1
3:B:206:PCW:H242	3:C:208:PCW:H20	0.58	1.75	8	3
3:B:204:PCW:H141	3:C:204:PCW:H39	0.58	1.74	4	1
3:B:207:PCW:H171	3:B:210:PCW:C13	0.58	2.27	4	1
3:D:608:PCW:C11	3:D:608:PCW:O31	0.58	2.51	15	6
3:A:411:PCW:C43	3:A:418:PCW:H282	0.58	2.28	10	4
3:B:213:PCW:C40	4:B:217:17F:H59	0.58	2.28	7	1
4:B:215:17F:H5	4:B:215:17F:O8	0.58	1.98	18	6
3:A:410:PCW:C22	4:D:633:17F:H49	0.58	2.28	8	1
3:A:419:PCW:H372	3:D:617:PCW:C40	0.58	2.28	8	1
3:D:603:PCW:C48	3:D:605:PCW:H61	0.58	2.27	12	2
3:B:203:PCW:H482	4:B:217:17F:H51	0.58	1.75	16	2
3:D:601:PCW:H481	3:D:607:PCW:H232	0.58	1.75	10	1
3:D:604:PCW:H471	3:D:613:PCW:C16	0.58	2.27	14	2
3:C:209:PCW:O11	3:C:209:PCW:H2	0.58	1.97	10	1
3:A:401:PCW:H351	3:B:209:PCW:H472	0.58	1.75	11	2
3:B:210:PCW:C46	3:B:213:PCW:H452	0.58	2.25	12	1
3:B:212:PCW:H32	3:B:212:PCW:P	0.58	2.38	12	1
3:D:610:PCW:H262	3:D:610:PCW:H421	0.58	1.74	16	1
3:D:601:PCW:H371	4:B:216:17F:H78	0.58	1.74	17	1
3:A:403:PCW:H342	3:C:203:PCW:H31	0.58	1.74	1	1
4:A:415:17F:C7	4:A:415:17F:C17	0.58	2.81	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:603:PCW:C41	3:D:603:PCW:H372	0.58	2.29	17	4
3:D:605:PCW:H2	3:D:605:PCW:C4	0.58	2.28	17	7
3:A:406:PCW:H62	3:A:411:PCW:O2P	0.58	1.97	3	1
3:D:620:PCW:C12	4:D:635:17F:H4A	0.58	2.15	20	2
3:B:205:PCW:H241	3:B:206:PCW:H372	0.58	1.73	10	2
3:A:401:PCW:H371	3:A:401:PCW:C41	0.58	2.22	5	1
3:A:404:PCW:H472	4:B:215:17F:C27	0.58	2.28	5	1
3:A:420:PCW:H141	4:D:632:17F:C11	0.58	2.28	13	2
3:C:203:PCW:H382	3:C:203:PCW:H141	0.58	1.74	6	1
3:B:212:PCW:O3P	3:B:212:PCW:O31	0.58	2.22	16	3
3:D:616:PCW:H451	3:B:206:PCW:H481	0.58	1.75	11	1
3:C:207:PCW:H152	3:C:209:PCW:H31	0.58	1.74	11	1
3:A:402:PCW:C47	3:C:205:PCW:H361	0.58	2.28	12	1
3:D:622:PCW:C16	3:C:212:PCW:H172	0.58	2.29	19	3
3:B:205:PCW:C40	4:B:214:17F:H67	0.58	2.28	17	2
3:A:401:PCW:H472	3:D:611:PCW:H241	0.58	1.75	13	2
3:B:207:PCW:H141	3:B:210:PCW:H342	0.58	1.74	16	1
3:D:615:PCW:C43	3:C:205:PCW:H262	0.58	2.20	17	3
3:A:410:PCW:H181	3:C:209:PCW:C28	0.58	2.28	19	1
1:A:246:ASP:HA	1:D:528:ARG:NH1	0.58	2.13	17	10
3:A:406:PCW:H411	3:B:210:PCW:C40	0.58	2.29	3	3
3:D:607:PCW:C19	4:D:631:17F:H50	0.58	2.25	19	4
3:B:204:PCW:H322	3:B:206:PCW:C33	0.58	2.28	3	2
3:C:208:PCW:O31	3:C:208:PCW:C35	0.58	2.42	6	6
3:A:401:PCW:H251	3:D:614:PCW:H281	0.58	1.76	5	1
3:A:404:PCW:H412	3:B:209:PCW:C34	0.58	2.26	6	1
3:A:407:PCW:H171	3:B:208:PCW:H242	0.58	1.74	6	1
3:C:206:PCW:C18	3:C:206:PCW:H241	0.58	2.28	7	1
3:D:616:PCW:H341	3:C:212:PCW:H362	0.58	1.75	9	2
3:A:401:PCW:C47	3:D:614:PCW:H222	0.58	2.26	10	1
3:A:413:PCW:C5	4:A:415:17F:O4	0.58	2.51	10	1
3:A:406:PCW:C44	3:B:207:PCW:H251	0.58	2.27	13	1
3:D:608:PCW:H281	4:B:216:17F:H53	0.58	1.73	13	1
3:B:209:PCW:H151	4:B:215:17F:H1	0.58	1.76	14	1
3:D:625:PCW:H451	3:D:626:PCW:H472	0.58	1.75	19	1
3:A:401:PCW:H281	3:D:614:PCW:H271	0.58	1.73	2	1
3:B:209:PCW:H361	3:B:209:PCW:C23	0.58	2.27	2	1
3:C:208:PCW:O31	3:C:208:PCW:O4P	0.58	2.21	2	1
3:D:616:PCW:H282	3:C:204:PCW:H252	0.58	1.74	3	1
3:A:401:PCW:H52	3:A:404:PCW:O2P	0.58	1.99	4	1
3:D:614:PCW:N	3:D:625:PCW:O1P	0.58	2.36	9	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:206:PCW:C16	3:B:212:PCW:H441	0.58	2.13	4	1
3:A:409:PCW:H52	3:C:206:PCW:O31	0.58	1.98	9	2
3:A:403:PCW:H252	3:D:617:PCW:H282	0.58	1.73	8	1
3:A:406:PCW:H332	3:A:411:PCW:C34	0.58	2.27	8	1
3:A:407:PCW:C17	3:C:205:PCW:H342	0.58	2.28	16	4
3:B:213:PCW:H131	3:B:213:PCW:O31	0.58	1.98	13	1
3:A:417:PCW:H431	3:D:612:PCW:C14	0.58	2.24	15	1
3:C:205:PCW:H371	3:C:205:PCW:C41	0.58	2.28	15	1
3:B:209:PCW:H61	4:B:215:17F:O7	0.58	1.98	16	2
3:B:203:PCW:H19	4:B:215:17F:H38	0.58	1.75	17	1
3:A:407:PCW:H431	4:B:216:17F:C42	0.58	2.21	18	1
3:A:405:PCW:C39	3:D:601:PCW:H151	0.58	2.29	19	1
3:A:404:PCW:H362	4:B:215:17F:H42	0.58	1.75	1	1
3:D:601:PCW:H62	3:D:601:PCW:O4P	0.58	1.97	16	3
3:D:618:PCW:O1P	3:D:627:PCW:C6	0.58	2.52	7	6
3:A:412:PCW:H432	3:C:208:PCW:C45	0.58	2.28	2	1
3:D:611:PCW:H32	3:D:619:PCW:H31	0.58	1.75	2	2
4:D:634:17F:H76	3:C:206:PCW:H231	0.58	1.74	2	1
3:B:207:PCW:O11	3:B:210:PCW:C15	0.58	2.52	14	3
3:A:404:PCW:H322	3:B:209:PCW:O4P	0.58	1.99	3	1
3:D:614:PCW:H442	3:D:619:PCW:C19	0.58	2.29	3	8
4:D:632:17F:O10	4:D:632:17F:C7	0.58	2.52	10	2
3:B:210:PCW:H471	3:B:210:PCW:C27	0.58	2.29	3	4
3:C:203:PCW:C35	3:C:203:PCW:C8	0.58	2.82	3	1
3:A:409:PCW:O31	3:C:206:PCW:C35	0.58	2.51	17	2
3:B:204:PCW:H252	3:C:207:PCW:C26	0.58	2.22	5	1
3:C:204:PCW:C22	4:C:211:17F:H31	0.58	2.24	19	3
3:A:417:PCW:C44	3:D:612:PCW:H242	0.58	2.28	10	1
3:A:407:PCW:C22	3:C:205:PCW:H411	0.58	2.28	13	1
3:D:617:PCW:O1P	3:D:617:PCW:O2	0.58	2.21	13	1
3:D:604:PCW:H481	3:D:619:PCW:H432	0.58	1.75	16	1
3:A:410:PCW:H242	3:C:207:PCW:H221	0.58	1.75	17	2
3:D:605:PCW:H131	3:D:605:PCW:C6	0.58	2.28	17	1
3:C:204:PCW:H232	3:C:207:PCW:C47	0.58	2.29	17	1
3:C:204:PCW:H122	4:C:211:17F:C7	0.58	2.29	18	1
3:B:205:PCW:H222	3:B:212:PCW:C37	0.58	2.26	19	1
3:A:413:PCW:H162	4:A:414:17F:H62	0.58	1.74	1	2
3:D:609:PCW:C4	4:D:633:17F:O8	0.58	2.51	14	7
3:D:618:PCW:H341	4:D:633:17F:C21	0.58	2.29	1	3
3:D:622:PCW:H152	3:C:212:PCW:H122	0.58	1.74	1	1
3:B:213:PCW:O31	4:B:217:17F:C20	0.58	2.52	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:414:17F:H52	3:C:203:PCW:C46	0.58	2.29	15	2
3:B:208:PCW:C19	4:B:214:17F:C31	0.58	2.81	4	1
3:D:601:PCW:H482	4:D:628:17F:C31	0.58	2.28	5	1
2:B:118:CYS:SG	2:B:143:GLU:HB3	0.58	2.38	5	1
3:C:205:PCW:H441	3:C:206:PCW:H251	0.58	1.73	8	1
3:D:613:PCW:H31	3:D:619:PCW:C2	0.58	2.28	9	2
3:D:616:PCW:H381	3:D:618:PCW:H142	0.58	1.74	9	1
3:D:603:PCW:H281	3:B:213:PCW:C47	0.58	2.28	11	1
3:D:603:PCW:H281	3:B:213:PCW:H471	0.58	1.76	11	1
4:D:635:17F:H65	3:C:205:PCW:H461	0.58	1.76	11	1
3:B:208:PCW:H142	4:B:214:17F:H60	0.58	1.74	18	1
3:C:209:PCW:H341	3:C:209:PCW:O31	0.58	1.99	15	8
4:A:415:17F:H2	4:A:415:17F:O2	0.58	1.99	3	1
3:A:417:PCW:H422	3:D:612:PCW:C25	0.58	2.26	20	7
4:D:630:17F:C35	4:D:634:17F:H36	0.58	2.27	14	2
3:A:417:PCW:C43	3:D:612:PCW:H172	0.58	2.16	5	2
3:C:208:PCW:H232	3:C:209:PCW:C43	0.58	2.26	17	2
3:A:401:PCW:H2	3:A:401:PCW:O2P	0.58	1.97	15	6
3:B:204:PCW:O4P	3:B:204:PCW:H62	0.58	1.97	12	4
3:B:211:PCW:O31	3:B:211:PCW:O3P	0.58	2.22	8	3
3:A:408:PCW:H282	3:A:417:PCW:C16	0.58	2.29	11	1
3:D:618:PCW:C27	3:B:206:PCW:H462	0.58	2.28	11	1
3:B:207:PCW:C43	4:B:215:17F:H60	0.58	2.29	11	1
3:C:204:PCW:H222	4:C:211:17F:H60	0.58	1.75	11	1
3:B:208:PCW:C20	4:B:214:17F:H60	0.58	2.29	12	1
3:A:402:PCW:H141	3:A:409:PCW:H232	0.58	1.75	15	1
3:A:413:PCW:H232	4:A:414:17F:H59	0.58	1.75	16	1
3:D:605:PCW:H283	4:B:214:17F:H52	0.58	1.74	16	1
3:D:603:PCW:C23	4:B:217:17F:H76	0.58	2.29	20	1
3:A:403:PCW:C4	3:A:403:PCW:O11	0.58	2.52	19	6
3:D:620:PCW:C14	4:D:635:17F:H18	0.58	2.29	4	4
3:C:203:PCW:O2P	3:C:204:PCW:H73	0.58	1.98	6	2
3:A:413:PCW:H141	4:A:414:17F:C1Y	0.58	2.16	3	1
3:D:616:PCW:H341	3:C:212:PCW:C34	0.58	2.17	3	7
3:A:407:PCW:C19	3:C:205:PCW:H172	0.58	2.29	7	2
3:D:621:PCW:C14	3:D:621:PCW:H181	0.58	2.23	4	7
3:D:621:PCW:H451	4:D:634:17F:C37	0.58	2.29	5	1
3:D:613:PCW:H282	4:C:210:17F:H35	0.58	1.74	6	3
3:A:413:PCW:H283	3:C:203:PCW:H452	0.58	1.73	7	1
3:B:205:PCW:H441	3:B:206:PCW:H212	0.58	1.76	19	3
3:B:210:PCW:C8	4:B:216:17F:H19	0.58	2.29	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:211:PCW:C15	4:B:217:17F:H61	0.58	2.29	11	3
3:D:616:PCW:H362	3:C:212:PCW:H382	0.58	1.73	9	1
4:B:216:17F:H5	4:B:216:17F:O8	0.58	1.97	9	1
3:A:420:PCW:H362	3:D:617:PCW:H132	0.58	1.74	10	1
2:B:50:THR:H	3:C:207:PCW:H61	0.58	1.59	10	1
3:D:616:PCW:O3P	3:C:212:PCW:H51	0.58	1.99	11	1
3:B:205:PCW:C1	3:B:211:PCW:H73	0.58	2.28	11	2
3:B:204:PCW:O2	4:C:211:17F:N1	0.58	2.35	15	1
2:C:82:PHE:HB3	2:C:93:ILE:HD11	0.58	1.75	15	1
3:B:207:PCW:H332	3:B:210:PCW:H332	0.58	1.74	16	1
4:D:628:17F:H8A	4:D:631:17F:H33	0.58	1.75	17	1
3:B:204:PCW:O11	3:B:206:PCW:H82	0.58	1.98	17	1
3:B:207:PCW:C45	4:B:215:17F:H60	0.58	2.28	19	1
3:A:406:PCW:H332	3:A:411:PCW:H321	0.58	1.75	3	2
3:D:614:PCW:H73	3:D:614:PCW:O4P	0.58	1.99	5	14
3:D:621:PCW:H20	3:D:622:PCW:C8	0.58	2.29	10	4
3:C:204:PCW:H222	4:C:211:17F:H56	0.58	1.75	16	5
3:A:406:PCW:C41	3:B:210:PCW:H39	0.58	2.29	9	2
4:A:414:17F:H52	3:C:203:PCW:H452	0.58	1.75	3	3
3:A:407:PCW:C25	3:A:407:PCW:C21	0.58	2.73	15	2
3:B:210:PCW:H461	4:B:215:17F:H78	0.58	1.74	4	2
3:C:206:PCW:H231	3:C:206:PCW:H182	0.58	1.76	4	1
3:A:420:PCW:H61	4:D:632:17F:H5	0.58	1.76	6	1
3:A:401:PCW:O2	3:B:209:PCW:H241	0.58	1.98	7	1
3:A:403:PCW:H321	3:C:204:PCW:C4	0.58	2.29	7	2
3:A:413:PCW:C18	3:A:413:PCW:C14	0.58	2.82	11	2
3:A:402:PCW:H412	3:C:205:PCW:H381	0.58	1.76	15	3
3:A:404:PCW:C15	4:A:415:17F:H57	0.58	2.29	8	1
3:B:208:PCW:H182	3:C:205:PCW:H321	0.58	1.75	11	1
3:B:213:PCW:H212	3:B:213:PCW:C43	0.58	2.27	12	2
3:A:408:PCW:C26	3:A:417:PCW:H461	0.58	2.26	15	1
3:C:204:PCW:H282	4:C:211:17F:H60	0.58	1.75	15	1
3:D:601:PCW:C32	4:B:216:17F:H60	0.58	2.20	16	1
3:D:605:PCW:H442	3:D:608:PCW:C31	0.58	2.28	16	1
3:B:206:PCW:H39	3:C:212:PCW:C26	0.58	2.29	19	2
4:A:414:17F:H53	3:C:203:PCW:H472	0.58	1.74	17	1
3:D:603:PCW:C26	4:B:217:17F:H76	0.58	2.28	18	1
3:A:407:PCW:H152	3:B:208:PCW:H182	0.58	1.74	19	1
3:D:618:PCW:C42	3:D:627:PCW:H261	0.57	2.22	3	4
3:B:209:PCW:C3	3:B:209:PCW:O1P	0.57	2.52	20	10
3:D:610:PCW:H341	3:D:610:PCW:O31	0.57	1.99	7	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:622:PCW:H19	4:D:630:17F:H20	0.57	1.75	10	5
3:A:402:PCW:H121	3:A:409:PCW:H132	0.57	1.75	6	2
3:D:624:PCW:O3	3:D:624:PCW:O31	0.57	2.21	3	9
3:A:404:PCW:H412	3:B:209:PCW:H372	0.57	1.76	4	1
4:D:635:17F:O10	4:D:635:17F:C6	0.57	2.51	13	10
3:C:203:PCW:H121	3:C:203:PCW:C37	0.57	2.28	6	1
3:C:204:PCW:H161	4:C:211:17F:H18	0.57	1.75	9	1
3:D:607:PCW:C45	4:D:628:17F:H60	0.57	2.17	18	5
3:B:206:PCW:H20	3:C:208:PCW:C28	0.57	2.29	10	1
3:C:204:PCW:H241	3:C:207:PCW:H482	0.57	1.75	10	1
3:A:406:PCW:O31	3:A:406:PCW:H11	0.57	1.98	11	1
3:A:406:PCW:H241	3:B:210:PCW:H131	0.57	1.75	16	1
3:A:407:PCW:H422	3:D:601:PCW:H342	0.57	1.76	18	1
3:D:627:PCW:C28	4:D:633:17F:H46	0.57	2.29	18	2
3:B:210:PCW:C48	4:B:214:17F:H54	0.57	2.28	18	1
3:D:615:PCW:C28	4:D:635:17F:H46	0.57	2.29	18	6
3:A:417:PCW:C42	3:D:612:PCW:H251	0.57	2.29	4	1
3:C:203:PCW:H121	3:C:203:PCW:H371	0.57	1.75	4	3
3:A:405:PCW:H482	4:D:628:17F:C29	0.57	2.29	6	2
3:A:413:PCW:H351	3:A:413:PCW:C3	0.57	2.30	6	2
1:D:462:LYS:HB3	3:D:601:PCW:C28	0.57	2.28	6	2
3:B:204:PCW:O2P	3:B:212:PCW:C7	0.57	2.52	11	2
3:D:613:PCW:H32	3:D:619:PCW:C11	0.57	2.29	11	5
3:A:412:PCW:H461	3:B:205:PCW:C43	0.57	2.29	8	1
3:A:417:PCW:H411	3:D:612:PCW:C18	0.57	2.30	10	1
3:D:620:PCW:C3	3:D:620:PCW:H73	0.57	2.30	10	1
3:A:407:PCW:H51	4:B:214:17F:O6	0.57	1.99	11	1
3:C:204:PCW:H471	4:C:211:17F:C1Y	0.57	2.25	12	1
3:B:209:PCW:H462	4:B:215:17F:H50	0.57	1.76	13	1
2:C:109:VAL:HG23	2:C:111:MET:HE2	0.57	1.74	13	2
3:A:404:PCW:C43	3:B:209:PCW:H222	0.57	2.21	14	1
3:D:616:PCW:H441	3:D:627:PCW:H261	0.57	1.76	16	1
3:D:615:PCW:H181	4:D:635:17F:H37	0.57	1.74	18	1
3:A:411:PCW:O3	3:A:411:PCW:O31	0.57	2.22	12	4
3:A:412:PCW:H412	3:A:412:PCW:C37	0.57	2.24	1	1
3:A:420:PCW:C7	4:D:632:17F:O2	0.57	2.53	10	8
3:D:603:PCW:P	3:D:603:PCW:C3	0.57	2.93	15	17
3:B:208:PCW:H161	4:B:214:17F:H18	0.57	1.76	1	1
3:A:409:PCW:C32	3:C:206:PCW:H352	0.57	2.29	13	4
3:A:416:PCW:C44	3:D:617:PCW:H242	0.57	2.29	2	2
3:C:205:PCW:O31	3:C:205:PCW:O3	0.57	2.22	6	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:602:PCW:H161	3:D:624:PCW:H211	0.57	1.74	3	5
3:A:404:PCW:H132	3:A:404:PCW:H73	0.57	1.73	4	2
3:A:420:PCW:C6	4:D:632:17F:O8	0.57	2.51	6	2
3:D:605:PCW:H411	4:D:634:17F:C28	0.57	2.29	6	1
3:D:615:PCW:H221	3:C:205:PCW:C26	0.57	2.29	18	2
3:A:410:PCW:C19	3:D:627:PCW:H482	0.57	2.29	8	1
3:D:618:PCW:H341	4:D:633:17F:C2X	0.57	2.25	8	2
3:D:624:PCW:C45	4:C:210:17F:H75	0.57	2.29	18	3
3:C:208:PCW:C18	3:C:208:PCW:H461	0.57	2.28	8	1
3:A:403:PCW:C32	3:A:403:PCW:C36	0.57	2.71	10	1
3:A:417:PCW:H372	3:D:612:PCW:C18	0.57	2.28	10	1
3:D:614:PCW:H31	3:D:614:PCW:H42	0.57	1.75	14	1
3:A:419:PCW:C36	3:D:617:PCW:H382	0.57	2.27	15	1
3:A:408:PCW:H61	4:C:211:17F:H1	0.57	1.75	18	1
3:B:207:PCW:C45	4:B:215:17F:H10	0.57	2.29	18	1
4:C:211:17F:O2	4:C:211:17F:H2	0.57	1.98	19	1
3:D:627:PCW:H52	3:D:627:PCW:H2	0.57	1.75	1	1
3:D:627:PCW:H2	3:D:627:PCW:O4P	0.57	1.99	6	4
3:B:211:PCW:C35	3:B:212:PCW:H11	0.57	2.30	1	1
3:D:607:PCW:O1P	3:D:626:PCW:C22	0.57	2.52	14	6
3:A:410:PCW:C3	3:A:410:PCW:O2P	0.57	2.51	3	5
4:D:634:17F:C41	3:C:206:PCW:H252	0.57	2.29	3	2
3:B:205:PCW:H341	3:B:206:PCW:H122	0.57	1.76	3	2
3:A:402:PCW:H362	3:A:409:PCW:H141	0.57	1.76	4	1
4:D:630:17F:C33	4:D:630:17F:H10A	0.57	2.29	5	2
3:B:204:PCW:H483	3:B:212:PCW:H20	0.57	1.76	17	2
3:C:207:PCW:H281	3:C:208:PCW:C15	0.57	2.25	7	3
3:A:411:PCW:H2	4:B:215:17F:C1Z	0.57	2.20	8	5
3:A:413:PCW:C39	4:A:414:17F:H68	0.57	2.28	8	1
3:D:611:PCW:O2P	3:D:619:PCW:C6	0.57	2.51	8	1
3:C:208:PCW:H182	3:C:208:PCW:C44	0.57	2.29	8	1
3:B:205:PCW:H281	3:B:212:PCW:H212	0.57	1.75	9	1
3:A:407:PCW:C20	3:C:205:PCW:H172	0.57	2.30	11	1
3:A:410:PCW:O1P	3:C:209:PCW:H32	0.57	1.99	12	1
3:D:602:PCW:C22	3:D:610:PCW:H331	0.57	2.19	16	3
3:D:618:PCW:H461	3:C:208:PCW:H271	0.57	1.75	12	1
3:A:403:PCW:H63	3:C:203:PCW:O2P	0.57	1.99	14	1
3:A:402:PCW:H73	3:A:402:PCW:O11	0.57	2.00	15	1
4:A:415:17F:H20	4:A:415:17F:O9	0.57	1.99	15	1
3:A:403:PCW:H321	3:C:204:PCW:H41	0.57	1.75	20	2
3:D:608:PCW:C25	4:D:628:17F:H70	0.57	2.30	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:608:PCW:C25	3:D:615:PCW:H381	0.57	2.30	3	4
3:A:410:PCW:H152	3:C:207:PCW:C24	0.57	2.30	13	4
3:C:207:PCW:H42	3:C:207:PCW:C31	0.57	2.30	10	5
3:A:402:PCW:O4P	3:A:402:PCW:O2	0.57	2.22	12	8
3:A:413:PCW:C13	4:A:414:17F:H31	0.57	2.30	3	1
3:C:208:PCW:H461	3:C:209:PCW:H422	0.57	1.75	18	4
3:A:407:PCW:H152	3:B:208:PCW:H222	0.57	1.75	19	2
3:C:206:PCW:H182	3:C:206:PCW:C23	0.57	2.30	15	5
4:D:630:17F:H56	4:D:630:17F:C10	0.57	2.30	12	2
1:A:363:LYS:HE2	1:D:411:THR:HG22	0.57	1.75	9	2
3:B:205:PCW:H441	3:B:206:PCW:H232	0.57	1.76	7	2
3:A:404:PCW:H421	3:B:209:PCW:C22	0.57	2.29	9	1
3:A:402:PCW:C33	3:C:206:PCW:H31	0.57	2.14	10	1
4:B:216:17F:C2	4:B:216:17F:H4	0.57	2.30	13	1
3:A:410:PCW:H63	3:A:410:PCW:O2P	0.57	2.00	14	1
3:B:211:PCW:H251	4:B:217:17F:H51	0.57	1.75	15	1
3:A:411:PCW:C18	3:A:411:PCW:C22	0.57	2.78	17	2
2:B:3:GLU:HB3	3:B:213:PCW:H61	0.57	1.76	16	1
3:B:210:PCW:H271	3:B:210:PCW:C43	0.57	2.26	16	1
3:D:610:PCW:H462	3:B:212:PCW:H241	0.57	1.77	19	1
3:D:623:PCW:H371	3:D:623:PCW:O3	0.57	1.99	19	1
1:A:365:LYS:HB2	1:A:366:PRO:CD	0.57	2.24	19	14
3:A:404:PCW:H371	4:B:215:17F:H10	0.57	1.75	1	1
3:A:420:PCW:C11	4:D:632:17F:H9	0.57	2.30	10	9
3:D:616:PCW:C48	3:B:204:PCW:H262	0.57	2.30	1	1
3:D:627:PCW:O31	3:D:627:PCW:H12	0.57	1.99	1	3
3:D:606:PCW:C1	3:D:626:PCW:C37	0.57	2.74	17	6
3:D:607:PCW:H461	4:D:628:17F:C33	0.57	2.29	3	3
3:B:204:PCW:H271	3:B:204:PCW:H161	0.57	1.75	3	2
3:A:403:PCW:O31	3:A:403:PCW:C1	0.57	2.51	11	11
3:B:210:PCW:C3	3:B:210:PCW:O2P	0.57	2.53	5	6
3:A:404:PCW:H121	3:B:209:PCW:H362	0.57	1.77	5	1
3:A:420:PCW:O11	3:A:420:PCW:C6	0.57	2.52	5	1
3:B:205:PCW:H442	3:B:206:PCW:C16	0.57	2.21	6	3
4:A:414:17F:H48	3:B:204:PCW:H471	0.57	1.75	10	1
3:A:407:PCW:C8	4:B:216:17F:H10	0.57	2.29	11	1
3:A:418:PCW:H441	4:B:215:17F:H74	0.57	1.76	11	1
3:B:208:PCW:C41	3:B:208:PCW:C37	0.57	2.82	11	2
3:A:403:PCW:C32	3:C:203:PCW:H31	0.57	2.29	15	1
3:A:407:PCW:C5	4:B:216:17F:H12A	0.57	2.22	19	1
3:A:409:PCW:H321	3:A:412:PCW:H39	0.57	1.77	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:413:PCW:O31	3:A:413:PCW:O3	0.57	2.23	17	2
3:A:413:PCW:C12	4:A:414:17F:H66	0.57	2.29	12	2
3:A:418:PCW:O1P	3:D:625:PCW:H321	0.57	2.00	2	1
3:D:604:PCW:O31	3:D:613:PCW:C5	0.57	2.52	16	5
3:D:607:PCW:O1P	3:D:626:PCW:C24	0.57	2.53	2	4
3:B:209:PCW:H381	3:B:209:PCW:H232	0.57	1.76	2	5
3:A:412:PCW:H481	3:C:206:PCW:H39	0.57	1.77	4	1
3:D:618:PCW:H271	3:B:206:PCW:H452	0.57	1.74	4	1
3:D:613:PCW:C22	4:C:210:17F:H47	0.57	2.27	7	5
4:B:215:17F:C12	4:B:215:17F:C24	0.57	2.70	12	4
3:A:417:PCW:H361	3:D:612:PCW:H152	0.57	1.77	10	2
3:B:213:PCW:H381	3:B:213:PCW:C17	0.57	2.29	10	1
3:B:204:PCW:H272	3:C:207:PCW:C19	0.57	2.29	11	1
3:B:205:PCW:C28	3:B:212:PCW:H331	0.57	2.30	11	1
3:C:207:PCW:H42	3:C:207:PCW:H322	0.57	1.76	14	2
3:D:616:PCW:H441	3:D:627:PCW:C23	0.57	2.30	17	4
3:A:404:PCW:H483	3:B:207:PCW:H481	0.57	1.77	13	1
3:D:618:PCW:H261	3:C:204:PCW:H281	0.57	1.77	17	2
2:B:147:LYS:HE3	5:B:201:GDP:N2	0.57	2.15	16	1
3:C:208:PCW:H232	3:C:209:PCW:C45	0.57	2.23	16	2
3:B:209:PCW:H341	3:B:209:PCW:C18	0.57	2.22	18	1
3:D:622:PCW:C23	3:D:624:PCW:H242	0.57	2.27	1	4
3:B:212:PCW:O31	3:B:212:PCW:P	0.57	2.63	4	13
3:B:213:PCW:H371	4:B:217:17F:H63	0.57	1.77	1	1
3:B:213:PCW:H11	3:B:213:PCW:O31	0.57	1.99	15	4
3:D:601:PCW:O4P	3:D:601:PCW:H62	0.57	2.00	5	14
3:D:604:PCW:H421	3:D:619:PCW:C14	0.57	2.28	11	4
3:A:402:PCW:H42	3:A:402:PCW:C32	0.57	2.29	7	2
3:D:602:PCW:C2	3:D:602:PCW:C4	0.57	2.83	4	2
3:B:209:PCW:H242	3:B:209:PCW:H381	0.57	1.75	4	1
3:D:606:PCW:H442	3:D:625:PCW:H481	0.57	1.77	5	1
3:D:611:PCW:H39	3:D:623:PCW:H442	0.57	1.77	6	1
3:D:612:PCW:H252	3:D:612:PCW:C47	0.57	2.30	20	2
3:D:622:PCW:C25	3:D:624:PCW:H242	0.57	2.29	7	1
3:D:615:PCW:H63	4:D:635:17F:O4	0.57	1.99	14	3
3:B:205:PCW:H442	3:B:206:PCW:C18	0.57	2.25	9	2
3:A:403:PCW:C28	3:A:403:PCW:C23	0.57	2.59	10	1
1:D:463:TRP:HE1	4:D:631:17F:H75	0.57	1.60	11	1
3:B:209:PCW:C23	3:B:209:PCW:H432	0.57	2.29	15	1
3:C:208:PCW:H141	3:C:208:PCW:C42	0.57	2.30	15	1
3:A:404:PCW:C39	3:B:207:PCW:H451	0.57	2.30	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:406:PCW:O4P	3:A:406:PCW:H62	0.57	1.98	1	13
3:A:420:PCW:C12	4:D:632:17F:C9	0.57	2.81	10	8
3:D:612:PCW:O3P	3:D:612:PCW:O31	0.57	2.21	2	17
3:D:613:PCW:C20	4:C:210:17F:C27	0.57	2.82	20	4
3:D:621:PCW:C26	3:D:622:PCW:H61	0.57	2.30	1	2
3:D:621:PCW:H412	4:D:635:17F:C41	0.57	2.29	6	5
3:B:206:PCW:H352	3:B:212:PCW:H39	0.57	1.77	1	1
3:D:625:PCW:C19	3:D:625:PCW:C15	0.57	2.82	17	6
3:B:211:PCW:C17	4:B:217:17F:H65	0.57	2.25	12	2
3:D:613:PCW:H482	3:D:619:PCW:H181	0.57	1.76	3	3
3:D:623:PCW:O1P	3:D:623:PCW:H52	0.57	1.99	9	13
4:A:414:17F:H65	4:C:210:17F:H29	0.57	1.76	4	1
3:D:613:PCW:C48	3:D:619:PCW:H181	0.57	2.30	4	2
3:D:615:PCW:C24	4:D:635:17F:H41	0.57	2.30	5	1
4:D:635:17F:O10	4:D:635:17F:C4	0.57	2.48	20	3
3:D:618:PCW:O1P	3:D:627:PCW:C8	0.57	2.53	11	4
3:D:608:PCW:H442	3:D:615:PCW:C46	0.57	2.30	8	1
2:B:82:PHE:HE2	2:B:113:LEU:HG	0.57	1.60	8	1
3:C:204:PCW:H122	4:C:211:17F:C6	0.57	2.27	20	2
4:D:633:17F:H53	3:C:208:PCW:C25	0.57	2.30	9	1
3:B:205:PCW:C28	3:B:212:PCW:H181	0.57	2.30	9	1
4:B:216:17F:O8	4:B:216:17F:C5	0.57	2.51	17	4
4:C:211:17F:O2	4:C:211:17F:H5	0.57	2.00	12	1
3:B:207:PCW:H382	3:B:213:PCW:H231	0.57	1.77	15	1
3:C:203:PCW:H19	3:C:203:PCW:H483	0.57	1.75	17	1
3:D:622:PCW:H332	3:C:212:PCW:H422	0.57	1.75	19	2
3:B:204:PCW:H212	3:C:208:PCW:H283	0.57	1.76	19	1
3:C:204:PCW:H141	4:C:211:17F:O10	0.57	2.00	19	1
3:D:613:PCW:H471	3:D:619:PCW:C42	0.57	2.30	20	1
3:D:606:PCW:H451	3:D:626:PCW:H481	0.57	1.76	9	2
3:D:607:PCW:H431	4:D:628:17F:H33	0.57	1.74	1	1
3:D:616:PCW:C34	3:C:212:PCW:C34	0.57	2.83	1	2
3:A:403:PCW:H161	3:C:203:PCW:H322	0.57	1.76	14	3
3:D:603:PCW:H181	3:B:211:PCW:H283	0.57	1.76	6	2
3:B:204:PCW:H322	3:B:212:PCW:C14	0.57	2.11	2	1
3:B:211:PCW:C8	3:B:212:PCW:H42	0.57	2.30	2	1
3:D:611:PCW:C1	3:D:619:PCW:H63	0.57	2.30	4	2
3:D:620:PCW:H12	3:D:621:PCW:O2P	0.57	2.00	4	4
4:D:629:17F:H69	4:D:634:17F:C11	0.57	2.28	4	1
3:A:420:PCW:O1P	3:D:617:PCW:H42	0.57	2.00	7	2
3:D:615:PCW:H272	4:D:635:17F:C26	0.57	2.30	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:203:PCW:C2	3:B:211:PCW:H372	0.57	2.30	7	1
3:A:419:PCW:O3	3:D:617:PCW:H422	0.57	2.00	8	1
3:B:207:PCW:C41	3:B:213:PCW:H231	0.57	2.23	9	1
3:B:213:PCW:H422	4:B:217:17F:H64	0.57	1.77	20	2
3:B:207:PCW:O3	3:B:210:PCW:H152	0.57	2.00	16	1
3:A:418:PCW:H483	3:B:213:PCW:C47	0.57	2.30	17	1
3:B:203:PCW:C1	3:B:211:PCW:H352	0.57	2.28	18	1
3:D:615:PCW:C4	4:D:635:17F:HN1A	0.57	2.13	19	1
3:B:213:PCW:C27	4:B:215:17F:H67	0.57	2.29	20	1
3:A:406:PCW:H272	3:B:207:PCW:H171	0.56	1.75	8	2
3:D:624:PCW:H472	4:C:210:17F:C30	0.56	2.26	1	1
4:A:414:17F:H4	4:A:414:17F:C1	0.56	2.27	2	1
3:D:605:PCW:H352	4:D:629:17F:C7	0.56	2.30	2	2
3:D:612:PCW:H51	3:D:618:PCW:O11	0.56	2.00	19	4
3:A:406:PCW:C45	3:B:207:PCW:H251	0.56	2.27	3	2
3:D:618:PCW:C38	3:D:627:PCW:H181	0.56	2.30	3	4
4:D:629:17F:H12	4:D:634:17F:C27	0.56	2.29	3	3
3:C:204:PCW:H412	3:C:204:PCW:H371	0.56	1.77	3	4
3:C:204:PCW:H131	4:C:211:17F:C35	0.56	2.30	6	1
3:D:601:PCW:H131	4:B:216:17F:H60	0.56	1.77	8	1
3:A:408:PCW:O4P	3:C:204:PCW:H151	0.56	2.00	9	1
3:D:618:PCW:C45	4:D:633:17F:H55	0.56	2.23	9	1
3:C:207:PCW:H51	4:C:211:17F:H1	0.56	1.74	10	1
4:D:629:17F:H71	4:D:634:17F:H36	0.56	1.77	11	1
3:B:205:PCW:C36	3:B:206:PCW:H122	0.56	2.29	13	1
3:B:208:PCW:H19	3:C:205:PCW:C32	0.56	2.30	13	2
4:B:215:17F:H30	4:B:217:17F:H30	0.56	1.77	14	1
3:C:208:PCW:H11	3:C:209:PCW:O1P	0.56	1.99	14	1
3:A:402:PCW:H431	3:A:407:PCW:H272	0.56	1.77	15	1
3:B:208:PCW:C3	4:B:214:17F:H4	0.56	2.30	15	1
2:B:79:LEU:HD13	2:B:159:LEU:HD22	0.56	1.77	18	1
3:B:203:PCW:C45	4:B:217:17F:H46	0.56	2.30	20	1
1:A:275:LYS:HG2	1:D:499:LEU:HD21	0.56	1.76	14	4
3:A:403:PCW:C12	3:C:203:PCW:H322	0.56	2.30	1	1
3:A:407:PCW:H142	3:C:205:PCW:C13	0.56	2.30	1	5
4:D:631:17F:O10	4:D:631:17F:O7	0.56	2.23	1	1
3:B:204:PCW:O31	3:B:212:PCW:C8	0.56	2.52	13	5
3:C:204:PCW:H131	4:C:211:17F:H77	0.56	1.76	3	1
3:A:404:PCW:H121	3:B:209:PCW:C36	0.56	2.30	5	1
3:A:420:PCW:O31	3:D:617:PCW:H82	0.56	2.00	5	1
3:C:207:PCW:P	4:C:211:17F:H4A	0.56	2.40	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:203:PCW:H141	3:C:203:PCW:C39	0.56	2.30	6	2
3:B:205:PCW:H52	3:B:208:PCW:H11	0.56	1.76	7	1
3:A:406:PCW:H142	3:A:406:PCW:C39	0.56	2.29	9	1
3:B:205:PCW:H181	3:B:205:PCW:C22	0.56	2.16	11	1
3:A:408:PCW:H61	2:C:49:GLU:OE1	0.56	1.99	12	1
3:A:411:PCW:C43	3:A:418:PCW:H272	0.56	2.29	12	2
3:B:209:PCW:C17	4:B:215:17F:O10	0.56	2.53	19	3
2:C:12:ASP:HA	2:C:16:LYS:NZ	0.56	2.15	17	2
3:B:204:PCW:C39	3:B:212:PCW:H132	0.56	2.30	13	1
3:B:210:PCW:H141	4:B:216:17F:H6	0.56	1.77	15	2
3:A:413:PCW:H241	4:A:414:17F:C33	0.56	2.30	17	1
3:D:612:PCW:C11	3:D:612:PCW:O31	0.56	2.52	18	1
3:A:404:PCW:H472	3:B:209:PCW:C45	0.56	2.30	19	1
3:D:605:PCW:C4	3:D:626:PCW:H19	0.56	2.30	20	1
3:A:401:PCW:P	3:A:401:PCW:O31	0.56	2.64	1	2
3:A:411:PCW:H412	3:A:418:PCW:C24	0.56	2.30	3	3
3:A:413:PCW:H232	4:A:414:17F:C34	0.56	2.30	12	2
3:A:420:PCW:C12	4:D:632:17F:H11	0.56	2.30	14	6
3:D:603:PCW:C47	3:D:626:PCW:H282	0.56	2.30	6	4
3:D:608:PCW:O3	3:D:608:PCW:O31	0.56	2.24	14	8
3:D:611:PCW:O4P	3:D:619:PCW:H62	0.56	2.00	14	9
3:B:205:PCW:C43	3:B:206:PCW:H161	0.56	2.30	18	3
4:B:214:17F:O10	4:B:214:17F:O7	0.56	2.22	1	5
3:D:604:PCW:O2P	3:D:624:PCW:C8	0.56	2.54	4	3
3:D:620:PCW:P	3:D:621:PCW:H41	0.56	2.41	2	1
4:D:629:17F:H42	4:D:630:17F:C41	0.56	2.30	16	6
3:A:401:PCW:C18	3:A:401:PCW:C22	0.56	2.72	10	3
3:A:406:PCW:H141	3:A:406:PCW:H382	0.56	1.76	4	1
4:D:634:17F:C34	4:D:635:17F:H74	0.56	2.30	6	2
3:B:213:PCW:H422	4:B:217:17F:C37	0.56	2.22	4	2
3:D:603:PCW:O1P	3:D:603:PCW:C3	0.56	2.54	14	3
3:D:614:PCW:O1P	3:D:625:PCW:H62	0.56	2.00	14	4
3:D:618:PCW:C13	3:D:627:PCW:H151	0.56	2.23	5	2
3:A:417:PCW:C38	3:D:612:PCW:H131	0.56	2.28	15	2
3:A:404:PCW:H171	4:A:415:17F:H57	0.56	1.76	7	2
3:D:615:PCW:C5	4:D:635:17F:O4	0.56	2.53	9	4
3:B:206:PCW:H262	3:C:208:PCW:H481	0.56	1.76	7	2
3:A:407:PCW:H283	3:A:409:PCW:H172	0.56	1.77	8	1
3:A:410:PCW:H31	3:A:410:PCW:O1P	0.56	2.00	8	2
3:A:418:PCW:H441	4:B:215:17F:C42	0.56	2.30	11	1
3:A:401:PCW:C1	3:B:209:PCW:H362	0.56	2.29	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:615:PCW:C23	3:C:205:PCW:H251	0.56	2.25	12	1
3:D:615:PCW:H182	4:D:635:17F:H37	0.56	1.77	12	1
3:A:404:PCW:H381	3:B:209:PCW:H361	0.56	1.77	13	1
3:C:203:PCW:O1P	3:C:203:PCW:H2	0.56	1.99	13	1
3:C:208:PCW:O31	3:C:208:PCW:P	0.56	2.63	13	2
3:A:409:PCW:H331	3:C:206:PCW:H352	0.56	1.77	14	1
3:A:407:PCW:H242	3:C:205:PCW:H382	0.56	1.74	16	2
3:D:608:PCW:H442	3:D:615:PCW:H482	0.56	1.75	16	1
3:B:204:PCW:H482	3:B:212:PCW:H20	0.56	1.76	16	1
3:C:203:PCW:H11	3:C:204:PCW:O2P	0.56	2.00	18	1
3:A:401:PCW:C7	3:B:209:PCW:H152	0.56	2.23	19	1
3:B:208:PCW:H281	4:B:214:17F:C1Y	0.56	2.29	19	1
3:D:620:PCW:H141	4:D:635:17F:H5	0.56	1.76	20	1
3:A:407:PCW:C31	3:A:407:PCW:O3	0.56	2.53	2	10
3:D:622:PCW:H472	3:B:206:PCW:C28	0.56	2.31	1	1
3:A:403:PCW:C8	4:A:414:17F:O4	0.56	2.52	2	1
3:A:410:PCW:H12	3:C:207:PCW:C38	0.56	2.17	2	1
3:A:416:PCW:O31	3:D:617:PCW:H61	0.56	2.00	18	2
3:D:606:PCW:H432	3:D:626:PCW:H472	0.56	1.77	11	5
3:B:204:PCW:H321	3:C:204:PCW:C34	0.56	2.30	3	1
3:D:607:PCW:H272	4:D:628:17F:H37	0.56	1.77	4	1
4:D:628:17F:H40	4:D:631:17F:C42	0.56	2.30	4	1
3:B:207:PCW:H171	3:B:210:PCW:C12	0.56	2.30	4	1
3:D:622:PCW:H321	3:D:627:PCW:C20	0.56	2.30	6	3
3:A:418:PCW:C43	3:D:625:PCW:H462	0.56	2.25	7	1
3:A:403:PCW:C48	3:A:416:PCW:H271	0.56	2.30	10	1
2:B:17:SER:HB2	5:B:201:GDP:O2A	0.56	2.00	10	2
3:C:209:PCW:O31	3:C:209:PCW:O4P	0.56	2.23	10	1
3:B:207:PCW:H351	3:B:210:PCW:C34	0.56	2.29	11	1
3:A:404:PCW:H441	3:B:207:PCW:H462	0.56	1.77	12	1
3:A:410:PCW:H52	3:C:209:PCW:C1	0.56	2.24	15	1
4:C:211:17F:H11	4:C:211:17F:C35	0.56	2.30	17	1
3:A:406:PCW:H52	3:B:207:PCW:C34	0.56	2.30	18	1
3:D:605:PCW:H411	4:D:634:17F:C30	0.56	2.30	20	1
3:A:401:PCW:O31	3:A:401:PCW:O3P	0.56	2.23	1	2
3:A:410:PCW:O4P	3:A:410:PCW:C6	0.56	2.53	1	1
3:D:618:PCW:H451	3:C:207:PCW:H231	0.56	1.76	1	1
3:A:409:PCW:O3P	3:A:412:PCW:O1P	0.56	2.22	14	2
3:D:605:PCW:H61	3:D:626:PCW:C28	0.56	2.30	17	2
3:A:403:PCW:H321	3:C:204:PCW:C6	0.56	2.28	4	1
3:B:211:PCW:C43	3:B:212:PCW:H31	0.56	2.30	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:407:PCW:H151	3:C:205:PCW:H171	0.56	1.76	5	1
3:A:410:PCW:H231	3:C:207:PCW:H231	0.56	1.78	5	1
3:D:622:PCW:H122	4:D:629:17F:C38	0.56	2.30	6	1
3:A:409:PCW:O31	3:A:409:PCW:O4P	0.56	2.23	9	4
3:B:211:PCW:C16	4:B:217:17F:H35	0.56	2.30	7	1
3:A:404:PCW:H39	3:B:209:PCW:H63	0.56	1.78	20	2
3:B:206:PCW:H20	3:C:208:PCW:H282	0.56	1.78	10	1
3:A:401:PCW:C44	3:D:611:PCW:H271	0.56	2.20	14	1
3:D:601:PCW:H321	4:B:216:17F:C33	0.56	2.19	16	1
3:A:413:PCW:C16	4:A:414:17F:C1Z	0.56	2.84	20	2
3:B:209:PCW:H451	3:B:209:PCW:C26	0.56	2.30	18	1
3:D:606:PCW:H442	3:D:625:PCW:H471	0.56	1.76	12	3
3:B:207:PCW:H422	3:B:213:PCW:H232	0.56	1.76	15	2
3:A:403:PCW:H152	3:C:203:PCW:H31	0.56	1.76	7	4
3:D:603:PCW:H412	3:D:605:PCW:C23	0.56	2.31	11	4
3:A:404:PCW:H63	4:A:415:17F:O5	0.56	2.01	3	2
3:D:621:PCW:C20	3:D:622:PCW:H82	0.56	2.24	12	5
3:D:611:PCW:H222	3:D:619:PCW:H483	0.56	1.75	6	1
3:B:205:PCW:H122	3:B:208:PCW:C40	0.56	2.30	6	1
3:D:622:PCW:H251	3:D:624:PCW:H242	0.56	1.77	7	1
3:C:208:PCW:H462	3:C:209:PCW:C42	0.56	2.30	14	3
3:D:601:PCW:H461	3:D:607:PCW:C48	0.56	2.31	19	2
3:A:411:PCW:H472	3:A:411:PCW:H272	0.56	1.78	9	2
3:A:401:PCW:H39	3:D:614:PCW:H271	0.56	1.75	11	1
3:B:203:PCW:H63	3:B:211:PCW:O3P	0.56	2.01	12	1
3:B:204:PCW:O11	3:B:206:PCW:C8	0.56	2.54	12	1
4:D:629:17F:H76	3:C:212:PCW:H461	0.56	1.76	13	2
3:D:601:PCW:C36	4:B:216:17F:H70	0.56	2.30	15	1
3:B:211:PCW:H73	3:B:211:PCW:P	0.56	2.40	15	1
3:A:404:PCW:H382	4:B:215:17F:H42	0.56	1.76	17	1
3:C:204:PCW:H20	4:C:211:17F:H20	0.56	1.78	19	1
3:D:603:PCW:H231	4:B:217:17F:C42	0.56	2.31	20	1
3:A:404:PCW:H31	3:B:209:PCW:H411	0.56	1.77	1	1
3:A:417:PCW:H332	3:D:612:PCW:C11	0.56	2.30	6	4
3:D:611:PCW:O11	3:D:619:PCW:C6	0.56	2.53	11	7
4:D:634:17F:O10	4:D:634:17F:O7	0.56	2.22	14	10
3:B:204:PCW:O4P	3:B:204:PCW:H82	0.56	2.01	18	15
3:C:203:PCW:O31	3:C:203:PCW:C36	0.56	2.54	13	5
3:C:203:PCW:H272	4:C:211:17F:H78	0.56	1.76	1	1
3:A:413:PCW:O3	3:A:413:PCW:O31	0.56	2.24	16	10
3:B:209:PCW:O31	3:B:209:PCW:O3	0.56	2.23	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:602:PCW:C16	3:D:624:PCW:C22	0.56	2.83	16	6
3:B:208:PCW:O11	3:B:208:PCW:O2	0.56	2.24	8	14
3:A:404:PCW:H252	4:A:415:17F:C32	0.56	2.30	4	1
3:B:204:PCW:H212	3:C:208:PCW:H241	0.56	1.77	4	1
3:A:416:PCW:H451	3:D:617:PCW:C23	0.56	2.31	5	1
3:B:204:PCW:H482	3:B:212:PCW:H19	0.56	1.77	5	2
1:A:244:SER:HA	1:A:248:GLU:HG3	0.56	1.77	6	1
3:D:602:PCW:H261	3:D:610:PCW:C17	0.56	2.31	20	4
3:B:211:PCW:H32	4:B:217:17F:H56	0.56	1.76	6	2
3:D:611:PCW:O11	3:D:611:PCW:H2	0.56	2.00	7	2
3:A:413:PCW:H352	4:A:414:17F:H57	0.56	1.76	8	1
3:D:602:PCW:H142	3:D:622:PCW:H221	0.56	1.75	8	1
1:A:239:LEU:HD13	3:A:410:PCW:H421	0.56	1.78	10	1
3:A:405:PCW:C40	4:D:628:17F:H52	0.56	2.31	10	2
4:A:414:17F:C8	4:C:210:17F:H2	0.56	2.16	10	1
3:B:205:PCW:H251	3:B:211:PCW:C47	0.56	2.30	10	1
3:A:402:PCW:H451	3:C:205:PCW:H361	0.56	1.77	12	1
3:A:407:PCW:H141	3:B:208:PCW:H231	0.56	1.77	13	1
4:B:216:17F:H4	4:B:216:17F:H2	0.56	1.78	15	2
3:B:205:PCW:H461	3:B:206:PCW:H161	0.56	1.76	15	2
3:A:407:PCW:H472	3:D:615:PCW:H281	0.56	1.77	15	1
3:B:205:PCW:H231	3:B:212:PCW:C41	0.56	2.30	15	1
4:B:216:17F:H53	3:C:205:PCW:H262	0.56	1.78	15	1
3:A:401:PCW:H62	3:B:209:PCW:C31	0.56	2.31	16	2
3:D:616:PCW:P	3:D:616:PCW:C3	0.56	2.89	9	9
4:B:217:17F:O9	4:B:217:17F:O8	0.56	2.23	5	6
3:A:404:PCW:H31	3:B:209:PCW:C31	0.56	2.31	3	1
3:D:605:PCW:C21	3:D:605:PCW:C17	0.56	2.78	9	8
3:B:206:PCW:H32	3:B:206:PCW:P	0.56	2.40	11	5
3:B:210:PCW:H421	4:B:215:17F:C38	0.56	2.31	4	1
3:C:204:PCW:O31	3:C:204:PCW:O4P	0.56	2.24	5	1
1:D:473:LYS:O	1:D:477:LEU:HB2	0.56	2.00	12	4
3:A:403:PCW:H73	3:A:403:PCW:O11	0.56	2.01	8	2
3:A:403:PCW:H20	3:C:203:PCW:C25	0.56	2.31	9	1
3:D:620:PCW:H73	3:D:620:PCW:H32	0.56	1.76	10	1
3:A:416:PCW:P	3:A:416:PCW:O31	0.56	2.64	14	4
3:D:607:PCW:H482	4:D:628:17F:C34	0.56	2.29	14	1
3:A:401:PCW:H322	3:B:209:PCW:C24	0.56	2.31	15	2
3:D:615:PCW:H483	3:B:208:PCW:H251	0.56	1.77	15	1
3:D:623:PCW:H40	3:D:625:PCW:H261	0.56	1.78	16	1
3:A:410:PCW:H231	3:C:207:PCW:H222	0.56	1.78	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:204:PCW:H122	3:C:204:PCW:H372	0.56	1.78	19	1
3:A:402:PCW:H432	3:A:409:PCW:H261	0.56	1.78	20	1
3:A:403:PCW:O1P	3:A:403:PCW:H32	0.56	2.00	10	2
3:A:406:PCW:H481	3:D:606:PCW:H262	0.56	1.77	1	1
3:D:618:PCW:C43	3:D:627:PCW:H282	0.56	2.31	9	6
3:A:408:PCW:H362	3:C:204:PCW:H232	0.56	1.75	2	2
3:D:617:PCW:H51	3:D:617:PCW:H2	0.56	1.76	13	9
3:B:204:PCW:H322	3:B:206:PCW:H332	0.56	1.77	5	2
3:A:405:PCW:C48	4:D:628:17F:H53	0.56	2.31	4	1
3:B:212:PCW:H73	3:B:212:PCW:O11	0.56	2.01	4	4
3:B:203:PCW:C24	4:C:210:17F:H20A	0.56	2.25	6	1
2:C:22:GLN:O	2:C:26:ASN:HA	0.56	2.01	14	6
3:C:203:PCW:H252	4:C:211:17F:C42	0.56	2.31	8	1
3:C:204:PCW:C20	4:C:211:17F:H19A	0.56	2.31	20	2
3:A:417:PCW:C48	3:D:612:PCW:H281	0.56	2.31	12	3
3:D:605:PCW:O11	3:D:605:PCW:H63	0.56	2.01	11	2
3:B:211:PCW:C15	4:B:217:17F:H58	0.56	2.30	10	1
3:A:403:PCW:H422	3:A:403:PCW:H181	0.56	1.77	14	2
3:B:208:PCW:H281	4:B:216:17F:H50	0.56	1.77	11	1
3:D:616:PCW:H221	3:D:616:PCW:H181	0.56	1.77	12	1
3:A:407:PCW:H181	3:C:205:PCW:C36	0.56	2.07	13	1
3:A:403:PCW:C1	3:C:204:PCW:H61	0.56	2.31	16	1
3:A:402:PCW:C41	3:C:205:PCW:H361	0.56	2.22	17	1
3:A:403:PCW:H332	3:C:204:PCW:O4P	0.56	2.01	17	1
3:A:401:PCW:C7	3:B:209:PCW:H382	0.56	2.31	1	1
3:A:420:PCW:O1P	3:D:617:PCW:C8	0.56	2.54	8	2
3:D:622:PCW:H19	4:D:630:17F:H18A	0.56	1.78	1	1
4:D:629:17F:H10	4:D:634:17F:C28	0.56	2.31	20	6
3:B:211:PCW:C34	3:B:212:PCW:C1	0.56	2.81	1	1
3:D:607:PCW:O11	3:D:607:PCW:C2	0.56	2.52	6	13
3:B:203:PCW:H211	4:C:210:17F:H32	0.56	1.78	9	2
3:B:213:PCW:H462	4:B:217:17F:H44	0.56	1.77	2	1
3:D:620:PCW:H283	4:D:635:17F:H37	0.56	1.77	12	2
3:A:407:PCW:C5	4:B:216:17F:O8	0.56	2.51	4	1
3:C:212:PCW:H372	3:C:212:PCW:H141	0.56	1.78	6	4
3:A:418:PCW:H39	3:D:625:PCW:H422	0.56	1.78	5	1
4:D:629:17F:C27	4:D:630:17F:H39	0.56	2.30	5	1
3:B:207:PCW:C46	4:B:215:17F:H60	0.56	2.28	20	2
4:D:630:17F:C38	4:D:630:17F:H40	0.56	2.31	7	1
3:D:622:PCW:H141	4:D:630:17F:H34	0.56	1.76	9	3
3:D:618:PCW:P	3:D:627:PCW:H51	0.56	2.41	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:212:PCW:H422	3:C:212:PCW:H271	0.56	1.78	18	1
3:A:406:PCW:H422	3:B:210:PCW:H40	0.56	1.76	19	1
3:D:626:PCW:O11	3:D:626:PCW:O2	0.56	2.23	19	1
3:B:208:PCW:H19	4:B:214:17F:H56	0.56	1.76	19	1
3:A:401:PCW:H411	3:D:611:PCW:H251	0.55	1.77	1	1
3:A:419:PCW:H351	3:D:617:PCW:C42	0.55	2.32	17	5
1:D:443:LYS:O	1:D:447:GLU:HB2	0.55	2.01	1	3
3:B:205:PCW:H422	4:B:214:17F:H75	0.55	1.76	1	1
3:D:602:PCW:H351	3:D:624:PCW:H141	0.55	1.77	13	2
3:D:617:PCW:H62	3:D:617:PCW:C31	0.55	2.31	6	4
2:B:28:PHE:HZ	5:B:201:GDP:C2	0.55	2.18	3	1
3:D:602:PCW:C46	3:D:610:PCW:H412	0.55	2.31	8	3
3:B:207:PCW:H381	3:B:213:PCW:H231	0.55	1.76	10	1
3:D:604:PCW:C17	3:D:613:PCW:H362	0.55	2.30	13	1
3:B:204:PCW:H421	3:B:212:PCW:H171	0.55	1.78	13	1
3:B:205:PCW:H12	3:B:211:PCW:C7	0.55	2.31	15	3
3:B:208:PCW:H142	4:B:214:17F:H20A	0.55	1.78	15	1
4:C:211:17F:C30	3:C:212:PCW:H212	0.55	2.31	17	1
3:A:420:PCW:H63	3:A:420:PCW:H32	0.55	1.77	9	3
1:D:519:ALA:HB3	1:D:520:PRO:HD3	0.55	1.78	11	20
3:D:602:PCW:O31	3:D:602:PCW:O3	0.55	2.23	1	5
4:D:632:17F:O10	4:D:632:17F:H20A	0.55	2.00	4	13
3:A:407:PCW:C6	3:B:213:PCW:O2	0.55	2.55	2	3
3:A:416:PCW:H141	3:A:419:PCW:C33	0.55	2.31	10	4
3:D:620:PCW:O2P	3:D:621:PCW:H42	0.55	2.00	18	3
3:B:208:PCW:C35	4:B:214:17F:H34	0.55	2.31	3	2
4:A:414:17F:C6	3:C:203:PCW:H341	0.55	2.31	4	1
3:B:203:PCW:H42	3:B:211:PCW:H331	0.55	1.78	4	3
4:B:217:17F:H47	4:B:217:17F:H77	0.55	1.78	5	1
3:A:407:PCW:H171	3:B:208:PCW:C24	0.55	2.32	6	1
3:D:608:PCW:H251	4:D:628:17F:C40	0.55	2.31	7	1
2:B:15:GLY:HA2	5:B:201:GDP:H8	0.55	1.61	10	5
3:C:204:PCW:H19	4:C:211:17F:C17	0.55	2.31	7	1
3:B:205:PCW:H422	3:B:206:PCW:C16	0.55	2.27	13	4
3:B:213:PCW:C46	4:B:217:17F:H40	0.55	2.31	8	1
3:B:203:PCW:H472	3:B:211:PCW:C25	0.55	2.18	11	2
3:B:209:PCW:H341	3:B:209:PCW:H231	0.55	1.79	14	1
3:B:209:PCW:H262	3:B:209:PCW:C47	0.55	2.31	16	1
3:A:405:PCW:H372	3:D:601:PCW:H152	0.55	1.76	20	1
3:D:626:PCW:O31	3:D:626:PCW:O3	0.55	2.25	1	11
3:B:207:PCW:O4P	3:B:207:PCW:H82	0.55	2.01	4	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:403:PCW:H131	3:A:403:PCW:C36	0.55	2.31	2	1
3:A:404:PCW:C35	4:B:215:17F:H42	0.55	2.19	2	1
3:D:624:PCW:O11	3:D:624:PCW:H2	0.55	2.01	17	2
4:D:634:17F:H76	3:C:206:PCW:H232	0.55	1.78	2	1
3:C:203:PCW:C31	3:C:203:PCW:O3	0.55	2.54	2	7
3:C:212:PCW:O11	3:C:212:PCW:O2	0.55	2.25	14	14
3:C:212:PCW:C32	3:C:212:PCW:H52	0.55	2.31	14	2
3:A:407:PCW:H352	3:C:205:PCW:C14	0.55	2.29	4	4
3:A:401:PCW:H381	3:A:404:PCW:H281	0.55	1.77	4	1
3:B:207:PCW:C31	3:B:207:PCW:O2P	0.55	2.55	4	1
3:A:407:PCW:H19	3:B:208:PCW:H222	0.55	1.78	8	1
3:A:409:PCW:H39	3:A:409:PCW:H181	0.55	1.76	8	2
4:A:414:17F:H40	3:C:203:PCW:H411	0.55	1.78	8	1
3:B:203:PCW:C47	3:B:211:PCW:H251	0.55	2.21	11	2
3:D:624:PCW:H41	3:D:624:PCW:O2	0.55	2.01	11	1
3:B:213:PCW:H222	4:B:217:17F:H10	0.55	1.76	11	1
3:A:407:PCW:C14	3:B:208:PCW:H20	0.55	2.31	13	1
3:D:614:PCW:C45	3:D:619:PCW:H20	0.55	2.31	14	1
3:B:213:PCW:H462	4:B:217:17F:H41	0.55	1.77	17	2
3:B:206:PCW:H51	3:C:207:PCW:C1	0.55	2.18	16	2
3:C:208:PCW:H161	3:C:209:PCW:C39	0.55	2.31	20	2
3:B:210:PCW:H471	3:B:213:PCW:H283	0.55	1.78	17	1
3:B:203:PCW:H451	4:B:217:17F:H43	0.55	1.78	19	1
3:A:401:PCW:O2P	3:A:401:PCW:H51	0.55	2.02	1	1
3:B:203:PCW:C11	3:B:203:PCW:O31	0.55	2.54	19	7
3:D:617:PCW:O31	3:D:617:PCW:C1	0.55	2.49	6	3
3:A:406:PCW:H381	3:B:210:PCW:H352	0.55	1.79	4	1
3:B:207:PCW:H152	3:B:210:PCW:C32	0.55	2.28	4	1
4:D:629:17F:H43	4:D:630:17F:H73	0.55	1.79	13	2
3:A:401:PCW:H361	3:A:404:PCW:H172	0.55	1.79	19	2
3:B:204:PCW:C1	3:B:212:PCW:C8	0.55	2.84	6	1
3:C:204:PCW:O2	4:C:211:17F:H75	0.55	2.01	12	2
3:A:403:PCW:O4P	3:A:403:PCW:O11	0.55	2.24	16	2
3:D:615:PCW:C22	3:C:205:PCW:H261	0.55	2.27	7	1
3:B:205:PCW:O3	3:B:208:PCW:H382	0.55	2.01	7	1
3:B:211:PCW:C15	4:B:217:17F:H35	0.55	2.30	7	1
2:C:80:CYS:HB3	2:C:93:ILE:HD12	0.55	1.77	7	1
3:C:207:PCW:O31	3:C:207:PCW:H342	0.55	2.00	7	2
3:A:406:PCW:H362	3:A:411:PCW:H361	0.55	1.77	9	1
3:A:420:PCW:H63	3:A:420:PCW:C11	0.55	2.30	9	1
3:A:407:PCW:H19	3:B:208:PCW:C24	0.55	2.28	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:613:PCW:H182	4:C:210:17F:H52	0.55	1.79	10	1
3:B:208:PCW:H11	3:B:208:PCW:O31	0.55	2.01	12	2
3:D:617:PCW:C43	3:D:617:PCW:C47	0.55	2.75	11	1
3:A:420:PCW:H11	3:A:420:PCW:H41	0.55	1.77	15	2
3:D:608:PCW:H381	3:C:205:PCW:H283	0.55	1.77	20	2
3:D:614:PCW:H19	3:D:623:PCW:C48	0.55	2.32	16	1
3:A:406:PCW:H162	3:B:210:PCW:H322	0.55	1.78	20	1
3:B:212:PCW:C42	3:C:212:PCW:H283	0.55	2.31	20	1
3:A:410:PCW:O31	3:A:410:PCW:H11	0.55	2.01	6	11
3:A:409:PCW:C8	3:C:206:PCW:H351	0.55	2.26	3	2
3:A:410:PCW:H252	4:D:633:17F:H54	0.55	1.77	5	2
3:D:611:PCW:C3	3:D:619:PCW:H63	0.55	2.32	20	2
3:A:417:PCW:H352	3:D:612:PCW:H181	0.55	1.78	4	1
3:D:615:PCW:H272	4:D:635:17F:H41	0.55	1.77	4	2
3:B:212:PCW:O4P	3:B:212:PCW:H2	0.55	2.01	11	4
4:C:211:17F:H12	4:C:211:17F:H62	0.55	1.77	4	2
3:B:211:PCW:H63	3:B:212:PCW:C32	0.55	2.31	13	4
3:A:404:PCW:H411	3:B:209:PCW:H121	0.55	1.77	6	1
3:D:612:PCW:H352	3:D:627:PCW:O11	0.55	2.02	6	2
3:D:613:PCW:C43	3:D:619:PCW:C39	0.55	2.85	6	1
3:D:614:PCW:H19	3:D:623:PCW:H481	0.55	1.78	16	2
3:A:403:PCW:C32	3:C:203:PCW:H11	0.55	2.21	7	1
3:B:210:PCW:H471	3:B:213:PCW:H19	0.55	1.79	20	2
3:B:211:PCW:H181	3:B:211:PCW:C22	0.55	2.25	8	3
1:D:463:TRP:CD1	4:D:631:17F:H71	0.55	2.37	13	3
3:D:601:PCW:H371	4:B:216:17F:C42	0.55	2.32	17	4
3:A:413:PCW:H73	4:A:415:17F:O4	0.55	2.01	10	1
3:D:616:PCW:H441	3:D:627:PCW:C26	0.55	2.30	10	2
3:B:205:PCW:H351	3:B:208:PCW:H332	0.55	1.77	10	2
3:D:603:PCW:H432	3:D:605:PCW:H221	0.55	1.77	11	3
3:D:605:PCW:H152	4:D:629:17F:H11A	0.55	1.77	12	3
4:D:634:17F:H74	3:C:206:PCW:C22	0.55	2.30	14	1
3:B:204:PCW:C1	3:B:212:PCW:C7	0.55	2.84	15	1
3:A:401:PCW:H461	3:D:611:PCW:H262	0.55	1.77	18	1
3:B:205:PCW:H73	4:B:214:17F:H6A	0.55	1.78	18	1
3:A:404:PCW:O31	3:A:404:PCW:C11	0.55	2.54	1	2
3:A:420:PCW:C11	3:A:420:PCW:H63	0.55	2.31	1	1
3:D:615:PCW:C31	3:D:615:PCW:O3	0.55	2.55	5	10
3:D:616:PCW:H431	3:B:206:PCW:H472	0.55	1.77	1	1
3:D:617:PCW:H62	3:D:617:PCW:O31	0.55	2.02	19	2
5:B:201:GDP:H2'	5:B:201:GDP:O5'	0.55	2.01	8	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:401:PCW:H281	3:D:614:PCW:C27	0.55	2.31	2	1
3:D:605:PCW:H161	4:D:629:17F:H12	0.55	1.78	4	3
3:D:613:PCW:H251	4:C:210:17F:H55	0.55	1.78	2	1
3:D:621:PCW:H362	4:D:633:17F:C32	0.55	2.31	3	5
4:D:630:17F:H56	4:D:630:17F:H11	0.55	1.79	2	3
3:B:209:PCW:C19	3:B:209:PCW:H342	0.55	2.32	3	1
3:A:420:PCW:H141	4:D:632:17F:H11A	0.55	1.78	20	3
3:B:208:PCW:H212	4:B:214:17F:H60	0.55	1.77	5	1
3:A:416:PCW:H142	3:A:416:PCW:H39	0.55	1.77	6	1
3:A:417:PCW:H361	3:D:612:PCW:O3	0.55	2.01	6	2
3:C:208:PCW:H441	3:C:209:PCW:C36	0.55	2.31	6	1
3:A:416:PCW:H371	3:A:416:PCW:C41	0.55	2.31	7	1
3:A:417:PCW:H141	3:D:617:PCW:H462	0.55	1.79	14	2
3:D:616:PCW:H342	3:C:212:PCW:H362	0.55	1.79	9	1
3:A:413:PCW:H122	4:A:414:17F:C20	0.55	2.31	11	1
3:D:609:PCW:H121	4:D:633:17F:H18	0.55	1.79	11	1
3:D:613:PCW:H471	3:D:619:PCW:C44	0.55	2.31	11	1
3:A:403:PCW:H322	3:C:204:PCW:H51	0.55	1.77	13	1
2:B:158:THR:O	2:B:162:GLU:HG2	0.55	2.01	16	1
3:B:207:PCW:C39	4:B:215:17F:H60	0.55	2.31	16	1
3:A:407:PCW:C1	4:B:216:17F:H10	0.55	2.31	18	1
3:A:409:PCW:O31	3:A:409:PCW:C4	0.55	2.55	1	6
3:D:619:PCW:O4P	3:D:619:PCW:H82	0.55	2.02	8	20
4:D:628:17F:H5	4:D:628:17F:O8	0.55	2.01	1	1
2:C:109:VAL:HB	2:C:111:MET:HE2	0.55	1.78	8	8
3:A:401:PCW:C48	3:D:611:PCW:H232	0.55	2.12	3	2
3:A:401:PCW:O3	3:A:401:PCW:O31	0.55	2.24	7	12
3:A:410:PCW:O4P	3:A:410:PCW:H62	0.55	2.01	15	12
3:A:419:PCW:O31	3:A:419:PCW:O3	0.55	2.25	16	2
3:B:204:PCW:C47	3:C:203:PCW:H171	0.55	2.31	5	1
4:B:216:17F:H57	4:B:216:17F:H62	0.55	1.78	13	2
3:C:208:PCW:H442	3:C:209:PCW:C42	0.55	2.32	7	2
3:A:405:PCW:C37	3:D:601:PCW:H121	0.55	2.31	11	1
3:D:620:PCW:H41	3:D:620:PCW:O31	0.55	2.02	11	1
4:D:635:17F:H62	3:C:205:PCW:H461	0.55	1.77	13	1
3:A:410:PCW:H261	3:C:208:PCW:C24	0.55	2.32	17	1
3:D:607:PCW:C17	4:D:631:17F:C18	0.55	2.85	17	1
3:B:205:PCW:H52	3:B:208:PCW:O31	0.55	2.02	18	1
4:C:211:17F:H66	4:C:211:17F:H10	0.55	1.78	18	1
3:A:401:PCW:C11	3:A:401:PCW:O31	0.55	2.55	19	1
3:A:402:PCW:H442	3:C:205:PCW:C13	0.55	2.30	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:407:PCW:H372	3:C:205:PCW:H121	0.55	1.76	20	1
3:D:616:PCW:H482	3:B:204:PCW:H242	0.55	1.79	1	1
3:D:603:PCW:O3	3:D:603:PCW:C31	0.55	2.54	7	15
3:B:208:PCW:H182	3:C:205:PCW:C33	0.55	2.29	2	2
3:B:207:PCW:C11	3:B:210:PCW:H152	0.55	2.31	10	3
3:B:210:PCW:C12	4:B:216:17F:H6	0.55	2.32	9	3
3:D:607:PCW:C27	4:D:631:17F:H67	0.55	2.31	4	1
3:D:613:PCW:H141	3:D:619:PCW:C39	0.55	2.31	6	4
3:A:411:PCW:C26	3:A:411:PCW:H472	0.55	2.32	7	1
3:D:616:PCW:C44	3:D:627:PCW:H232	0.55	2.27	20	5
3:B:204:PCW:H271	3:C:204:PCW:H422	0.55	1.78	8	2
3:A:406:PCW:H252	3:B:207:PCW:H151	0.55	1.79	9	3
4:A:414:17F:H49	3:B:212:PCW:H241	0.55	1.77	8	1
3:A:403:PCW:C33	3:C:204:PCW:H51	0.55	2.32	13	1
3:A:410:PCW:H272	3:D:618:PCW:H462	0.55	1.79	18	2
3:A:412:PCW:C39	3:C:206:PCW:H40	0.55	2.32	13	1
3:D:616:PCW:H31	3:D:616:PCW:O1P	0.55	2.02	13	1
3:A:406:PCW:H261	3:B:207:PCW:H19	0.55	1.77	15	1
3:B:208:PCW:O11	3:B:208:PCW:H41	0.55	2.02	19	1
3:B:211:PCW:C36	3:B:212:PCW:H11	0.55	2.32	1	2
3:C:208:PCW:H161	3:C:208:PCW:C44	0.55	2.32	1	1
3:A:407:PCW:H62	3:B:213:PCW:O2	0.55	2.02	2	1
3:B:204:PCW:P	3:B:204:PCW:C3	0.55	2.93	2	2
4:D:628:17F:O7	4:D:628:17F:O10	0.55	2.25	15	2
3:B:203:PCW:O31	3:B:203:PCW:C1	0.55	2.54	3	1
3:C:204:PCW:H451	4:C:211:17F:C31	0.55	2.30	3	1
3:B:208:PCW:H172	4:B:214:17F:H20A	0.55	1.78	4	1
3:B:211:PCW:H483	3:B:212:PCW:H212	0.55	1.79	4	1
3:B:213:PCW:C7	4:B:214:17F:H2	0.55	2.30	9	3
3:D:622:PCW:C26	3:D:624:PCW:H282	0.55	2.19	5	1
3:B:205:PCW:H73	3:B:213:PCW:O2P	0.55	2.02	5	1
3:D:604:PCW:C41	3:D:619:PCW:H121	0.55	2.31	9	2
2:C:22:GLN:HB3	2:C:149:ARG:HG3	0.55	1.78	9	2
3:A:410:PCW:H261	4:D:633:17F:C30	0.55	2.30	10	1
1:D:573:LEU:O	1:D:577:LEU:HG	0.55	2.02	12	1
3:B:206:PCW:H40	3:C:212:PCW:H232	0.55	1.78	13	1
3:B:204:PCW:H332	3:B:212:PCW:C7	0.55	2.32	14	1
1:D:487:GLN:O	1:D:491:GLU:HG3	0.55	2.01	15	2
3:D:607:PCW:H452	4:D:628:17F:C33	0.55	2.17	18	1
3:A:407:PCW:C18	3:C:205:PCW:C17	0.55	2.85	19	1
3:A:418:PCW:H82	3:D:626:PCW:O31	0.55	2.01	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:417:PCW:H411	3:D:612:PCW:H231	0.55	1.78	20	1
3:D:604:PCW:O31	3:D:613:PCW:C6	0.55	2.55	10	4
4:D:628:17F:C18	4:D:631:17F:H55	0.55	2.32	13	3
3:A:420:PCW:C32	3:D:617:PCW:H52	0.55	2.29	20	3
3:D:601:PCW:C42	4:D:628:17F:H42	0.55	2.32	2	1
3:D:602:PCW:H371	3:D:602:PCW:C41	0.55	2.30	19	8
3:D:607:PCW:H19	4:D:631:17F:C28	0.55	2.32	16	3
3:B:205:PCW:H341	3:B:206:PCW:C12	0.55	2.32	3	1
3:B:205:PCW:H452	3:B:206:PCW:H211	0.55	1.78	9	2
3:B:213:PCW:O2	3:B:213:PCW:O1P	0.55	2.25	4	2
4:D:635:17F:H65	3:C:205:PCW:C48	0.55	2.31	6	2
3:A:410:PCW:P	3:A:410:PCW:H63	0.55	2.41	6	3
3:D:603:PCW:C40	4:D:629:17F:H40	0.55	2.31	6	1
3:D:604:PCW:H481	3:D:619:PCW:H421	0.55	1.78	14	4
3:D:623:PCW:H382	3:D:625:PCW:C18	0.55	2.31	14	3
3:B:211:PCW:H12	4:B:217:17F:C20	0.55	2.31	6	1
3:A:402:PCW:H442	3:C:205:PCW:C36	0.55	2.25	7	1
3:D:607:PCW:H431	4:D:628:17F:C33	0.55	2.32	13	4
3:B:207:PCW:H441	3:B:213:PCW:C27	0.55	2.29	8	1
4:B:214:17F:O7	4:B:214:17F:O10	0.55	2.25	10	2
3:A:403:PCW:H332	3:C:204:PCW:H51	0.55	1.78	9	2
3:C:203:PCW:H182	3:C:203:PCW:C23	0.55	2.32	11	1
3:B:211:PCW:C15	4:B:217:17F:H65	0.55	2.32	14	1
3:B:209:PCW:H232	3:B:209:PCW:C38	0.55	2.23	16	2
4:A:415:17F:H75	3:B:203:PCW:C28	0.55	2.32	19	1
3:A:417:PCW:H39	3:D:612:PCW:C42	0.55	2.32	19	1
3:D:623:PCW:H362	3:D:623:PCW:C31	0.55	2.32	19	1
4:D:633:17F:C29	3:C:209:PCW:H462	0.55	2.31	19	1
3:A:418:PCW:O3	3:A:418:PCW:O31	0.54	2.25	11	12
3:D:601:PCW:O31	3:D:601:PCW:C1	0.54	2.53	6	7
3:D:611:PCW:C3	3:D:619:PCW:H31	0.54	2.31	13	2
3:B:206:PCW:H51	3:C:207:PCW:O2P	0.54	2.02	2	1
3:A:420:PCW:C35	3:D:617:PCW:H141	0.54	2.32	3	1
3:B:206:PCW:H131	3:B:212:PCW:H40	0.54	1.77	4	1
4:D:630:17F:H71	4:D:634:17F:H39	0.54	1.77	19	2
3:B:205:PCW:C25	3:B:211:PCW:H471	0.54	2.28	10	2
3:A:404:PCW:H39	3:B:209:PCW:C6	0.54	2.29	6	1
3:D:627:PCW:O31	3:D:627:PCW:C4	0.54	2.55	6	1
4:C:211:17F:O10	4:C:211:17F:C6	0.54	2.51	6	2
3:B:203:PCW:C7	3:B:211:PCW:O31	0.54	2.54	8	2
3:A:410:PCW:H352	3:C:209:PCW:H162	0.54	1.78	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:411:PCW:H272	3:A:411:PCW:C46	0.54	2.32	9	1
3:A:412:PCW:H452	3:C:208:PCW:C47	0.54	2.31	19	2
3:D:611:PCW:H483	3:B:209:PCW:H461	0.54	1.77	10	1
3:A:406:PCW:C24	4:B:216:17F:H18	0.54	2.31	11	2
3:A:407:PCW:C27	3:A:409:PCW:H232	0.54	2.31	11	1
3:A:413:PCW:H371	3:A:413:PCW:C1	0.54	2.31	11	1
3:A:416:PCW:H322	3:D:610:PCW:C39	0.54	2.33	11	1
3:A:418:PCW:H441	4:B:215:17F:C41	0.54	2.32	11	1
3:A:403:PCW:H182	3:A:403:PCW:H411	0.54	1.77	12	1
3:B:204:PCW:H441	3:B:212:PCW:C19	0.54	2.30	13	1
3:A:402:PCW:C18	3:A:409:PCW:H211	0.54	2.28	17	2
3:A:402:PCW:C39	3:A:409:PCW:H261	0.54	2.32	15	1
3:B:207:PCW:H142	3:B:210:PCW:C36	0.54	2.31	16	1
4:C:211:17F:H11	4:C:211:17F:C36	0.54	2.31	17	1
3:A:409:PCW:H331	3:C:206:PCW:C33	0.54	2.23	18	1
4:B:215:17F:H36	4:B:215:17F:C24	0.54	2.31	18	1
4:D:632:17F:O10	4:D:632:17F:O6	0.54	2.25	2	12
3:A:403:PCW:O11	3:A:403:PCW:H51	0.54	2.03	16	3
3:B:208:PCW:C17	3:C:205:PCW:H331	0.54	2.31	2	1
3:A:401:PCW:C46	3:D:611:PCW:H251	0.54	2.31	3	2
3:A:408:PCW:H272	3:A:417:PCW:H221	0.54	1.78	3	2
4:B:215:17F:H40	4:B:215:17F:H12	0.54	1.77	13	2
3:A:412:PCW:C41	3:C:208:PCW:H361	0.54	2.32	20	2
1:D:471:ARG:HA	1:D:475:GLU:CG	0.54	2.32	7	3
3:D:601:PCW:H142	3:D:601:PCW:C38	0.54	2.32	4	2
3:D:613:PCW:H282	4:C:210:17F:H39	0.54	1.78	6	4
3:B:207:PCW:C16	3:B:210:PCW:H131	0.54	2.32	4	1
4:D:635:17F:H64	3:C:205:PCW:H461	0.54	1.78	6	2
3:B:208:PCW:P	3:B:208:PCW:C3	0.54	2.96	11	8
3:B:211:PCW:H451	3:B:212:PCW:C11	0.54	2.32	6	1
3:C:207:PCW:H271	3:C:208:PCW:C22	0.54	2.32	16	2
3:D:608:PCW:H272	3:D:615:PCW:H411	0.54	1.79	7	2
3:C:204:PCW:C17	4:C:211:17F:O10	0.54	2.53	7	1
3:A:403:PCW:H483	3:A:416:PCW:C27	0.54	2.31	10	1
1:D:543:ARG:O	1:D:547:TYR:HB2	0.54	2.01	10	1
3:B:213:PCW:C16	3:B:213:PCW:C21	0.54	2.80	15	2
3:A:402:PCW:C42	3:A:409:PCW:H132	0.54	2.29	12	1
3:D:604:PCW:H322	3:D:613:PCW:H62	0.54	1.78	12	1
3:B:204:PCW:H32	4:C:211:17F:H4	0.54	1.78	12	1
3:B:204:PCW:H271	3:C:204:PCW:H40	0.54	1.78	14	1
3:D:621:PCW:C41	4:D:634:17F:H62	0.54	2.32	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:209:PCW:C36	3:B:209:PCW:H221	0.54	2.32	16	1
3:B:210:PCW:H412	3:B:210:PCW:H261	0.54	1.80	17	1
3:A:410:PCW:H472	3:C:209:PCW:C22	0.54	2.32	19	1
4:D:634:17F:H9	4:D:634:17F:C19	0.54	2.32	20	4
3:A:402:PCW:H442	3:C:205:PCW:H152	0.54	1.79	2	2
3:D:622:PCW:H481	3:B:205:PCW:H441	0.54	1.79	3	1
4:D:629:17F:C24	4:D:630:17F:H73	0.54	2.28	3	4
3:D:602:PCW:O4P	4:D:630:17F:O1	0.54	2.25	17	9
3:B:207:PCW:H432	3:B:213:PCW:H231	0.54	1.80	5	2
3:B:208:PCW:O1P	3:B:208:PCW:C3	0.54	2.46	5	2
3:D:620:PCW:H252	4:D:635:17F:H12A	0.54	1.78	6	2
3:C:208:PCW:O31	3:C:208:PCW:C7	0.54	2.55	6	2
3:B:205:PCW:C17	3:B:205:PCW:C13	0.54	2.84	7	3
3:B:205:PCW:O4P	3:B:208:PCW:O31	0.54	2.26	7	1
3:B:206:PCW:P	3:B:206:PCW:C3	0.54	2.95	11	2
3:A:401:PCW:H342	3:B:209:PCW:H282	0.54	1.78	10	1
3:B:207:PCW:H483	3:B:213:PCW:H482	0.54	1.79	11	1
3:A:403:PCW:H483	3:A:416:PCW:H281	0.54	1.79	12	1
3:A:417:PCW:H141	3:D:617:PCW:H483	0.54	1.79	15	2
3:A:401:PCW:H431	3:B:209:PCW:H481	0.54	1.79	15	1
3:D:601:PCW:H362	4:B:216:17F:H70	0.54	1.78	15	1
3:D:622:PCW:H361	3:C:212:PCW:C46	0.54	2.30	15	2
3:A:406:PCW:C24	3:B:210:PCW:H131	0.54	2.32	16	1
3:A:410:PCW:C23	3:C:207:PCW:H222	0.54	2.32	18	1
3:B:208:PCW:H171	3:C:205:PCW:H331	0.54	1.79	18	1
3:B:206:PCW:H283	3:C:208:PCW:H481	0.54	1.77	20	1
3:B:213:PCW:H283	4:B:215:17F:H78	0.54	1.78	20	1
4:D:630:17F:H54	4:B:214:17F:H72	0.54	1.77	1	1
3:B:207:PCW:H411	4:B:217:17F:H12A	0.54	1.79	2	2
3:A:408:PCW:H342	3:C:204:PCW:H181	0.54	1.78	2	1
3:D:608:PCW:H483	3:C:205:PCW:C47	0.54	2.28	14	2
3:D:604:PCW:H372	3:D:604:PCW:H411	0.54	1.77	3	4
3:D:622:PCW:H182	3:C:212:PCW:H152	0.54	1.79	7	1
3:C:205:PCW:C27	3:C:205:PCW:C23	0.54	2.75	7	1
3:A:408:PCW:H471	3:A:410:PCW:H321	0.54	1.77	8	1
3:D:605:PCW:H482	4:D:635:17F:H56	0.54	1.77	10	1
3:D:621:PCW:H121	4:D:634:17F:O9	0.54	2.03	16	3
3:B:210:PCW:H442	3:B:213:PCW:H251	0.54	1.77	11	1
3:C:207:PCW:H282	3:C:207:PCW:O11	0.54	2.03	11	1
3:B:203:PCW:C4	3:B:211:PCW:O31	0.54	2.49	12	1
3:B:210:PCW:O1P	4:B:216:17F:N1	0.54	2.37	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:15:GLY:HA2	5:C:201:GDP:H8	0.54	1.61	12	1
3:A:411:PCW:H482	3:A:411:PCW:H281	0.54	1.79	13	1
3:B:211:PCW:H63	3:B:212:PCW:H322	0.54	1.80	13	1
3:D:605:PCW:C7	3:D:626:PCW:H281	0.54	2.33	17	1
3:D:622:PCW:H472	3:B:206:PCW:H272	0.54	1.79	18	1
3:B:203:PCW:H172	3:B:203:PCW:H211	0.54	1.79	19	1
3:A:406:PCW:C48	3:D:606:PCW:H262	0.54	2.32	1	1
3:A:407:PCW:C15	3:C:205:PCW:C15	0.54	2.81	3	6
3:D:612:PCW:H232	3:D:612:PCW:C47	0.54	2.26	1	1
3:A:403:PCW:H131	3:A:403:PCW:C37	0.54	2.33	2	2
3:C:204:PCW:H141	4:C:211:17F:H67	0.54	1.80	3	1
3:D:602:PCW:C22	3:D:610:PCW:H332	0.54	2.32	4	1
3:D:627:PCW:O4P	3:D:627:PCW:H82	0.54	2.02	8	8
4:D:630:17F:H10A	4:D:630:17F:H60	0.54	1.79	5	2
3:A:420:PCW:C6	4:D:632:17F:H5	0.54	2.32	6	1
3:B:208:PCW:H342	4:B:214:17F:H5	0.54	1.78	11	3
4:A:414:17F:H49	3:C:203:PCW:H472	0.54	1.78	8	1
3:D:606:PCW:C43	3:D:626:PCW:C47	0.54	2.85	13	4
3:D:616:PCW:C36	3:C:212:PCW:H382	0.54	2.32	9	1
3:B:210:PCW:C42	4:B:215:17F:H72	0.54	2.27	9	1
3:A:407:PCW:C8	4:B:216:17F:C10	0.54	2.86	11	1
3:A:408:PCW:C14	3:A:417:PCW:H261	0.54	2.32	11	1
3:C:203:PCW:H372	3:C:203:PCW:H52	0.54	1.78	11	1
3:A:420:PCW:H11	3:A:420:PCW:C4	0.54	2.32	12	2
3:D:614:PCW:C7	3:D:614:PCW:O4P	0.54	2.54	13	4
4:D:628:17F:H40	4:D:631:17F:H74	0.54	1.78	14	1
3:A:406:PCW:H20	3:B:210:PCW:O3P	0.54	2.02	15	1
3:B:207:PCW:H161	3:B:210:PCW:C21	0.54	2.23	19	2
3:B:204:PCW:H482	3:B:212:PCW:C20	0.54	2.32	16	1
3:A:404:PCW:C39	4:B:215:17F:H10A	0.54	2.33	17	1
3:A:403:PCW:C33	3:C:204:PCW:C3	0.54	2.86	20	1
3:A:412:PCW:C38	3:C:208:PCW:H361	0.54	2.33	20	1
3:A:410:PCW:C3	3:A:410:PCW:O1P	0.54	2.55	1	1
2:B:12:ASP:HA	2:B:16:LYS:NZ	0.54	2.18	17	7
3:B:204:PCW:P	4:C:211:17F:O1	0.54	2.65	1	1
3:B:211:PCW:H242	4:B:217:17F:H51	0.54	1.80	6	3
3:C:203:PCW:O2P	3:C:204:PCW:C5	0.54	2.56	1	2
3:A:406:PCW:H332	3:A:411:PCW:H322	0.54	1.77	2	2
3:A:419:PCW:H482	3:D:618:PCW:H281	0.54	1.79	2	2
1:D:495:LYS:O	1:D:499:LEU:HB2	0.54	2.02	17	10
3:C:204:PCW:H251	4:C:211:17F:H20	0.54	1.79	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:206:PCW:O11	3:C:206:PCW:C2	0.54	2.53	17	10
3:D:616:PCW:C27	3:C:204:PCW:H272	0.54	2.33	3	1
3:D:601:PCW:H381	3:D:601:PCW:C14	0.54	2.31	4	1
3:D:622:PCW:H442	3:C:212:PCW:H481	0.54	1.78	18	4
3:A:413:PCW:C18	3:A:413:PCW:C22	0.54	2.72	5	2
3:A:401:PCW:H41	3:B:209:PCW:C2	0.54	2.33	6	1
3:A:416:PCW:H382	3:D:617:PCW:H141	0.54	1.80	10	2
3:A:404:PCW:H40	4:B:215:17F:C8	0.54	2.33	9	1
3:D:622:PCW:H431	3:C:212:PCW:C48	0.54	2.32	20	2
3:C:207:PCW:C6	4:C:211:17F:O5	0.54	2.55	10	1
3:D:617:PCW:H411	3:D:617:PCW:C37	0.54	2.27	11	1
3:D:618:PCW:H241	3:B:206:PCW:H483	0.54	1.79	11	1
3:C:204:PCW:H352	4:C:211:17F:O7	0.54	2.02	11	1
4:C:211:17F:H53	3:C:212:PCW:H232	0.54	1.78	12	1
4:B:216:17F:H53	3:C:205:PCW:C26	0.54	2.32	15	1
3:A:406:PCW:C44	3:B:210:PCW:H39	0.54	2.22	16	1
3:D:601:PCW:H82	4:B:216:17F:O5	0.54	2.02	16	1
2:B:79:LEU:HD12	2:B:112:VAL:HB	0.54	1.80	17	1
3:A:406:PCW:H332	3:A:411:PCW:C32	0.54	2.33	3	3
3:A:419:PCW:C31	3:A:419:PCW:O3	0.54	2.55	18	17
3:D:609:PCW:H152	4:D:633:17F:C33	0.54	2.32	10	3
3:D:614:PCW:O4P	3:D:614:PCW:C7	0.54	2.54	5	13
3:B:207:PCW:C42	3:B:213:PCW:H232	0.54	2.32	1	2
3:D:607:PCW:H462	3:B:207:PCW:C27	0.54	2.32	2	1
3:A:411:PCW:H352	4:B:215:17F:C36	0.54	2.32	3	1
4:C:211:17F:O7	4:C:211:17F:O10	0.54	2.25	9	3
3:A:402:PCW:H42	3:A:402:PCW:C31	0.54	2.33	4	1
3:A:404:PCW:H31	3:B:209:PCW:C37	0.54	2.32	4	1
3:A:411:PCW:C2	4:B:215:17F:H31	0.54	2.32	7	3
3:A:404:PCW:C41	3:B:209:PCW:H121	0.54	2.33	6	1
3:A:418:PCW:H481	3:D:603:PCW:H281	0.54	1.78	7	1
3:D:607:PCW:H171	4:D:631:17F:C18	0.54	2.32	17	2
3:B:207:PCW:H422	3:B:213:PCW:H283	0.54	1.79	10	1
3:A:417:PCW:H141	3:D:617:PCW:C48	0.54	2.33	12	1
3:A:410:PCW:O11	3:C:207:PCW:H161	0.54	2.03	13	1
3:A:416:PCW:C28	3:A:419:PCW:H252	0.54	2.33	13	1
3:D:603:PCW:H232	4:B:217:17F:C30	0.54	2.32	14	1
2:B:12:ASP:HA	2:B:16:LYS:HZ1	0.54	1.62	15	2
4:B:216:17F:H2	4:B:216:17F:C4	0.54	2.33	15	1
3:C:205:PCW:H411	3:C:205:PCW:C37	0.54	2.31	15	1
3:A:402:PCW:H321	2:C:170:MET:CB	0.54	2.32	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:C:201:GDP:O2B	5:C:201:GDP:H5'	0.54	2.02	19	1
3:D:613:PCW:H141	3:D:619:PCW:H39	0.54	1.79	20	1
3:D:622:PCW:H361	3:C:212:PCW:H442	0.54	1.80	1	2
4:D:630:17F:O7	4:D:630:17F:O10	0.54	2.26	10	9
3:B:213:PCW:H181	3:B:213:PCW:C42	0.54	2.32	1	1
3:A:402:PCW:C45	4:D:635:17F:H51	0.54	2.25	2	1
3:A:419:PCW:O3	3:A:419:PCW:O31	0.54	2.25	18	14
3:D:601:PCW:H221	3:D:601:PCW:C17	0.54	2.31	2	2
3:A:401:PCW:C31	3:A:401:PCW:O3	0.54	2.56	9	8
3:D:615:PCW:C21	3:C:205:PCW:H282	0.54	2.32	4	1
3:B:204:PCW:H11	3:B:212:PCW:C8	0.54	2.31	4	2
3:D:612:PCW:H63	3:D:618:PCW:H31	0.54	1.78	5	1
3:A:404:PCW:C5	4:A:415:17F:O5	0.54	2.56	6	2
3:D:606:PCW:H452	3:D:626:PCW:H481	0.54	1.80	7	2
3:B:204:PCW:H452	3:C:203:PCW:C14	0.54	2.32	7	1
3:A:407:PCW:H141	3:B:208:PCW:H262	0.54	1.78	8	1
3:D:614:PCW:C8	3:D:625:PCW:O1P	0.54	2.56	15	4
3:A:404:PCW:H211	4:A:415:17F:C31	0.54	2.33	9	1
3:D:616:PCW:H461	3:D:627:PCW:H262	0.54	1.78	9	1
3:A:406:PCW:H61	3:A:411:PCW:C31	0.54	2.33	10	1
3:D:622:PCW:H182	3:C:212:PCW:H172	0.54	1.80	16	2
2:B:49:GLU:HA	3:C:207:PCW:C6	0.54	2.33	10	1
3:B:213:PCW:H181	3:B:213:PCW:H411	0.54	1.80	10	3
3:B:209:PCW:H451	3:B:209:PCW:C25	0.54	2.33	18	2
3:A:420:PCW:H19	4:D:632:17F:H56	0.54	1.79	13	1
3:D:615:PCW:C48	3:B:208:PCW:H252	0.54	2.33	13	3
3:A:402:PCW:H73	3:A:402:PCW:C12	0.54	2.32	15	1
1:D:453:GLN:HB2	1:D:454:PRO:HD3	0.54	1.79	15	1
3:B:211:PCW:C6	3:B:211:PCW:O11	0.54	2.56	15	1
3:D:605:PCW:H73	3:D:626:PCW:H171	0.54	1.78	16	1
3:B:207:PCW:H141	3:B:210:PCW:C34	0.54	2.32	16	1
3:B:208:PCW:C18	3:C:206:PCW:H19	0.54	2.30	16	1
3:D:605:PCW:H412	4:D:634:17F:H55	0.54	1.79	18	1
3:D:615:PCW:H181	4:D:635:17F:C21	0.54	2.33	18	1
3:A:409:PCW:O1P	3:A:412:PCW:H42	0.54	2.03	20	1
3:A:408:PCW:H73	3:C:204:PCW:O11	0.54	2.03	1	1
3:A:412:PCW:O31	3:A:412:PCW:O3	0.54	2.26	19	12
3:D:615:PCW:H2	3:D:615:PCW:C4	0.54	2.33	6	6
3:C:203:PCW:C27	4:C:211:17F:H78	0.54	2.33	1	1
3:A:408:PCW:H372	3:C:204:PCW:H232	0.54	1.79	2	1
3:C:203:PCW:O2P	3:C:204:PCW:H63	0.54	2.03	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:406:PCW:H452	3:B:207:PCW:C26	0.54	2.33	3	1
3:B:213:PCW:H351	4:B:214:17F:H9A	0.54	1.79	7	3
4:B:214:17F:H47	4:B:217:17F:C41	0.54	2.31	3	1
3:C:204:PCW:H331	4:C:211:17F:C9	0.54	2.29	3	1
3:A:404:PCW:C43	4:B:215:17F:H10	0.54	2.32	4	1
3:A:411:PCW:H32	4:B:215:17F:H31	0.54	1.80	4	1
3:B:206:PCW:H172	3:B:206:PCW:H211	0.54	1.79	4	1
3:C:207:PCW:H19	3:C:207:PCW:H431	0.54	1.79	4	1
3:B:209:PCW:H242	3:B:209:PCW:H412	0.54	1.79	15	2
3:A:412:PCW:H481	3:D:622:PCW:C48	0.54	2.31	8	1
3:D:625:PCW:H39	3:D:626:PCW:H142	0.54	1.79	8	1
3:C:206:PCW:C36	3:C:206:PCW:H152	0.54	2.33	8	1
3:D:608:PCW:O11	3:D:615:PCW:C7	0.54	2.56	17	5
3:B:205:PCW:H411	3:B:206:PCW:H162	0.54	1.80	11	1
3:A:411:PCW:H382	4:B:215:17F:H65	0.54	1.79	17	1
1:A:217:LEU:HD11	3:A:408:PCW:H232	0.54	1.80	18	1
3:A:407:PCW:H73	4:B:214:17F:O6	0.54	2.03	20	1
3:D:605:PCW:H261	4:D:630:17F:H74	0.54	1.79	20	1
3:D:607:PCW:H181	4:D:631:17F:C11	0.54	2.19	1	5
3:D:620:PCW:O1P	3:D:621:PCW:C5	0.54	2.55	1	6
4:D:628:17F:H4A	4:D:628:17F:O10	0.54	2.03	11	2
3:A:410:PCW:H232	3:A:410:PCW:H171	0.54	1.80	8	3
3:D:607:PCW:H141	3:D:608:PCW:C17	0.54	2.18	2	1
3:B:205:PCW:H39	4:B:214:17F:H66	0.54	1.80	18	3
3:B:207:PCW:C6	4:B:216:17F:H2	0.54	2.33	2	1
3:A:411:PCW:H19	3:A:411:PCW:C15	0.54	2.33	8	4
3:A:413:PCW:H452	4:C:210:17F:C21	0.54	2.33	3	1
3:A:403:PCW:H161	3:C:203:PCW:H332	0.54	1.80	4	1
3:B:207:PCW:C17	3:B:210:PCW:H131	0.54	2.32	4	1
3:A:420:PCW:O3P	3:A:420:PCW:O31	0.54	2.26	5	2
3:D:621:PCW:C28	3:D:622:PCW:H61	0.54	2.33	5	4
3:B:210:PCW:H141	4:B:216:17F:C18	0.54	2.33	5	1
3:A:404:PCW:C37	3:B:209:PCW:H51	0.54	2.32	6	1
3:D:604:PCW:H462	4:C:210:17F:H55	0.54	1.79	6	1
3:D:609:PCW:C28	4:D:633:17F:H72	0.54	2.33	13	5
3:B:204:PCW:H452	4:C:211:17F:H78	0.54	1.80	6	1
3:D:621:PCW:C14	3:D:621:PCW:C18	0.54	2.79	11	6
3:D:611:PCW:H20	3:D:611:PCW:H412	0.54	1.79	10	1
3:D:608:PCW:C17	3:D:615:PCW:H331	0.54	2.27	11	1
3:A:418:PCW:O3P	3:A:418:PCW:O31	0.54	2.26	16	2
3:D:621:PCW:H462	4:D:634:17F:H59	0.54	1.80	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:208:PCW:H151	4:B:214:17F:H63	0.54	1.78	12	1
3:D:606:PCW:H382	3:D:626:PCW:H452	0.54	1.80	14	2
3:D:606:PCW:C43	3:D:626:PCW:H481	0.54	2.33	20	2
3:A:402:PCW:H141	3:A:409:PCW:H212	0.54	1.80	16	1
3:B:207:PCW:H142	3:B:210:PCW:H361	0.54	1.80	16	1
3:B:207:PCW:O2P	3:B:213:PCW:H121	0.54	2.03	17	1
3:C:209:PCW:C31	3:C:209:PCW:H52	0.54	2.32	18	1
3:B:204:PCW:O3	3:C:204:PCW:H352	0.54	2.01	19	1
3:D:613:PCW:H132	3:D:619:PCW:H382	0.53	1.80	20	3
3:B:207:PCW:H40	4:B:215:17F:H9	0.53	1.79	1	1
2:C:68:ARG:HA	2:C:71:TYR:CZ	0.53	2.38	10	6
3:C:207:PCW:H161	3:C:207:PCW:C26	0.53	2.32	2	1
3:D:605:PCW:H132	3:D:605:PCW:H342	0.53	1.78	5	5
4:B:217:17F:N1	4:B:217:17F:H4	0.53	2.17	11	2
3:A:404:PCW:C22	4:A:415:17F:H57	0.53	2.33	4	1
3:D:605:PCW:H42	3:D:626:PCW:H19	0.53	1.80	16	3
3:D:620:PCW:O2P	3:D:621:PCW:C7	0.53	2.54	5	1
2:B:80:CYS:HB3	2:B:93:ILE:HD12	0.53	1.78	10	5
2:C:168:GLU:OE2	3:C:206:PCW:H61	0.53	2.03	8	1
3:A:413:PCW:H422	4:A:414:17F:C38	0.53	2.33	9	1
3:D:604:PCW:H321	3:D:611:PCW:H12	0.53	1.80	14	4
3:D:605:PCW:C48	4:D:635:17F:H56	0.53	2.33	11	1
3:A:408:PCW:H121	3:A:417:PCW:C27	0.53	2.33	14	1
3:A:401:PCW:H381	3:A:404:PCW:H20	0.53	1.79	15	1
3:D:611:PCW:O2P	3:D:613:PCW:C7	0.53	2.57	15	1
3:C:208:PCW:C14	3:C:208:PCW:H412	0.53	2.33	15	1
3:A:404:PCW:H421	3:B:209:PCW:C43	0.53	2.25	19	1
3:B:208:PCW:O1P	3:B:208:PCW:H32	0.53	2.02	19	1
3:C:208:PCW:H441	3:C:209:PCW:C38	0.53	2.32	19	1
2:C:84:ILE:HD13	2:C:118:CYS:HA	0.53	1.81	5	11
3:A:401:PCW:O3	3:A:401:PCW:C31	0.53	2.56	7	6
3:D:605:PCW:O11	3:D:605:PCW:C2	0.53	2.51	20	6
3:C:204:PCW:H131	4:C:211:17F:C42	0.53	2.33	3	1
3:A:404:PCW:H441	4:B:215:17F:C10	0.53	2.33	5	1
3:A:406:PCW:C24	3:B:207:PCW:H171	0.53	2.33	5	1
3:A:413:PCW:H431	4:C:210:17F:C1X	0.53	2.33	17	2
3:D:614:PCW:H432	3:D:619:PCW:H20	0.53	1.80	7	3
3:D:620:PCW:C7	3:D:620:PCW:O4P	0.53	2.55	8	1
3:B:209:PCW:H442	4:B:215:17F:C27	0.53	2.32	8	1
3:A:419:PCW:H382	3:D:610:PCW:H162	0.53	1.79	13	4
3:B:205:PCW:H51	3:B:208:PCW:H11	0.53	1.81	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:211:17F:O2	4:C:211:17F:C2	0.53	2.55	15	4
3:B:205:PCW:C27	3:B:211:PCW:H471	0.53	2.34	11	1
3:B:207:PCW:C35	3:B:210:PCW:H341	0.53	2.31	11	1
3:B:208:PCW:H411	3:B:208:PCW:C37	0.53	2.25	11	2
3:C:203:PCW:C35	3:C:203:PCW:C31	0.53	2.85	11	1
3:A:419:PCW:H481	3:D:618:PCW:C28	0.53	2.33	13	3
3:B:203:PCW:H63	3:B:211:PCW:O31	0.53	2.03	12	1
4:D:628:17F:C19	4:D:631:17F:H55	0.53	2.32	13	1
3:A:404:PCW:O3	3:B:209:PCW:H371	0.53	2.03	19	2
3:A:413:PCW:H141	4:A:414:17F:C35	0.53	2.33	17	1
4:B:214:17F:O4	3:C:205:PCW:C6	0.53	2.56	17	1
4:D:635:17F:H62	3:C:205:PCW:H482	0.53	1.80	19	1
3:A:403:PCW:H332	3:C:204:PCW:C3	0.53	2.32	20	1
1:A:246:ASP:HA	1:D:528:ARG:CZ	0.53	2.33	3	6
3:A:407:PCW:H61	3:B:213:PCW:O3P	0.53	2.03	14	3
4:A:415:17F:H76	3:D:613:PCW:H261	0.53	1.79	1	1
3:D:604:PCW:H182	3:D:613:PCW:C36	0.53	2.30	1	6
4:D:629:17F:C25	4:D:630:17F:H73	0.53	2.33	2	7
2:C:15:GLY:O	2:C:19:LEU:HG	0.53	2.03	2	2
3:A:404:PCW:H451	4:B:215:17F:C17	0.53	2.33	3	1
3:A:408:PCW:H82	4:C:211:17F:C7	0.53	2.34	3	1
3:D:620:PCW:O4P	3:D:620:PCW:C7	0.53	2.56	3	3
3:B:203:PCW:C36	3:B:211:PCW:H162	0.53	2.29	3	1
3:D:609:PCW:H31	4:D:633:17F:H18	0.53	1.80	4	1
4:D:629:17F:H65	4:D:634:17F:C8	0.53	2.32	4	1
4:C:210:17F:O10	4:C:210:17F:H20	0.53	2.03	13	13
3:B:206:PCW:C44	3:C:204:PCW:H441	0.53	2.33	5	1
3:A:401:PCW:C42	3:A:404:PCW:H262	0.53	2.33	8	1
3:B:211:PCW:H82	3:B:212:PCW:H62	0.53	1.80	10	1
3:B:205:PCW:H222	3:B:205:PCW:C18	0.53	2.27	11	1
3:B:205:PCW:C13	3:B:205:PCW:C17	0.53	2.84	11	2
3:D:603:PCW:H252	4:B:217:17F:C29	0.53	2.33	14	1
3:B:210:PCW:H40	4:B:215:17F:H77	0.53	1.79	16	1
3:A:404:PCW:H52	3:A:404:PCW:C31	0.53	2.33	18	1
3:B:208:PCW:H272	4:B:214:17F:H31	0.53	1.80	19	1
3:D:611:PCW:H321	3:D:623:PCW:H372	0.53	1.81	20	1
3:D:623:PCW:H122	3:D:624:PCW:H352	0.53	1.79	1	1
3:B:207:PCW:H231	3:B:210:PCW:H272	0.53	1.80	1	1
1:A:264:LYS:HE2	1:D:509:ALA:HB1	0.53	1.80	13	9
3:A:404:PCW:H372	4:B:215:17F:C10	0.53	2.32	2	1
3:D:605:PCW:O3P	3:D:605:PCW:O31	0.53	2.27	10	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:611:PCW:C16	3:D:619:PCW:H151	0.53	2.33	2	1
3:C:208:PCW:H372	3:C:209:PCW:C8	0.53	2.33	2	1
3:D:625:PCW:H31	3:D:626:PCW:H32	0.53	1.81	15	3
3:B:208:PCW:H151	4:B:214:17F:H60	0.53	1.79	3	1
3:A:417:PCW:O4P	3:A:417:PCW:H2	0.53	2.03	4	1
3:B:208:PCW:O31	3:B:208:PCW:C1	0.53	2.45	5	8
3:A:410:PCW:O2P	3:A:410:PCW:C5	0.53	2.56	6	2
3:A:420:PCW:H62	4:D:632:17F:H6A	0.53	1.79	7	1
3:D:611:PCW:H321	3:D:623:PCW:C36	0.53	2.34	9	1
3:C:204:PCW:H161	4:C:211:17F:C18	0.53	2.33	9	1
3:D:623:PCW:H282	4:C:210:17F:H77	0.53	1.79	11	1
3:B:207:PCW:C16	3:B:210:PCW:H142	0.53	2.25	12	1
3:D:621:PCW:C37	4:D:633:17F:C34	0.53	2.86	13	1
3:C:203:PCW:O4P	3:C:204:PCW:H63	0.53	2.03	13	1
3:A:413:PCW:H341	4:A:414:17F:C1Y	0.53	2.33	17	2
3:A:403:PCW:H62	4:A:414:17F:C3	0.53	2.33	18	1
3:A:410:PCW:C16	3:C:207:PCW:H211	0.53	2.33	19	1
3:A:410:PCW:H63	3:A:410:PCW:O2	0.53	2.04	7	2
3:A:407:PCW:H241	3:C:205:PCW:C42	0.53	2.33	3	3
3:A:401:PCW:N	3:B:209:PCW:O31	0.53	2.41	3	4
3:A:406:PCW:H381	3:B:210:PCW:H372	0.53	1.81	4	1
3:D:608:PCW:H381	3:D:615:PCW:H421	0.53	1.80	4	1
3:B:212:PCW:O11	3:B:212:PCW:C7	0.53	2.56	4	1
3:D:604:PCW:C45	3:D:624:PCW:H441	0.53	2.33	19	4
3:D:627:PCW:O31	3:D:627:PCW:H73	0.53	2.04	6	1
3:D:602:PCW:H62	3:C:212:PCW:O3P	0.53	2.03	16	3
3:C:204:PCW:H483	3:C:204:PCW:H262	0.53	1.80	7	1
3:B:205:PCW:C33	3:B:208:PCW:H321	0.53	2.33	8	1
1:A:315:ALA:O	1:A:319:HIS:HB2	0.53	2.04	13	1
3:D:612:PCW:H51	3:D:618:PCW:H31	0.53	1.78	13	1
3:B:207:PCW:O11	3:B:210:PCW:H151	0.53	2.03	14	1
3:A:417:PCW:C14	3:D:617:PCW:H483	0.53	2.34	15	1
3:D:601:PCW:C8	4:B:216:17F:H2	0.53	2.33	16	1
3:C:207:PCW:H271	3:C:208:PCW:C23	0.53	2.33	16	1
3:A:407:PCW:H162	3:C:205:PCW:C34	0.53	2.33	18	1
3:A:412:PCW:H451	3:C:208:PCW:H382	0.53	1.79	18	1
3:A:405:PCW:O31	3:A:405:PCW:H341	0.53	2.04	19	9
3:D:611:PCW:H452	3:D:611:PCW:H221	0.53	1.81	1	1
4:D:634:17F:C36	4:D:635:17F:H70	0.53	2.32	6	2
3:B:207:PCW:H461	3:B:213:PCW:H461	0.53	1.80	1	1
3:D:621:PCW:H262	3:D:622:PCW:C7	0.53	2.32	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:214:17F:H1A	3:C:205:PCW:H63	0.53	1.78	2	1
3:B:213:PCW:H421	4:B:217:17F:C2X	0.53	2.34	3	1
3:A:413:PCW:H252	4:A:414:17F:H60	0.53	1.81	17	3
4:A:414:17F:O1	4:A:414:17F:C17	0.53	2.57	4	1
3:C:204:PCW:C2	3:C:204:PCW:C5	0.53	2.84	5	1
3:A:404:PCW:H281	4:A:415:17F:H69	0.53	1.79	11	2
3:A:411:PCW:H39	4:B:215:17F:C36	0.53	2.30	8	1
3:A:404:PCW:H2	3:A:404:PCW:H73	0.53	1.81	16	2
3:B:212:PCW:H152	3:C:204:PCW:C36	0.53	2.33	10	1
4:D:629:17F:H67	4:D:630:17F:H58	0.53	1.80	11	2
3:B:204:PCW:H181	3:C:204:PCW:H39	0.53	1.80	11	1
3:D:602:PCW:H12	3:D:602:PCW:O31	0.53	2.02	19	3
4:B:214:17F:H50	4:B:217:17F:C39	0.53	2.34	12	2
3:A:409:PCW:C33	3:C:206:PCW:H352	0.53	2.33	14	1
3:A:402:PCW:O2P	2:C:170:MET:HE2	0.53	2.04	16	1
3:A:410:PCW:H171	3:C:207:PCW:H222	0.53	1.78	16	1
3:A:412:PCW:H452	3:C:208:PCW:H422	0.53	1.80	16	1
3:C:208:PCW:H422	3:C:209:PCW:H382	0.53	1.79	17	1
3:A:402:PCW:H331	3:C:206:PCW:C8	0.53	2.27	18	1
3:A:409:PCW:C31	3:A:409:PCW:H51	0.53	2.33	18	1
3:A:410:PCW:H241	4:D:633:17F:H55	0.53	1.80	19	1
3:D:609:PCW:O2P	3:D:609:PCW:H52	0.53	2.04	20	1
3:A:413:PCW:H162	4:A:414:17F:C35	0.53	2.34	1	2
3:D:602:PCW:H63	4:D:630:17F:O1	0.53	2.04	1	1
3:B:210:PCW:O31	3:B:210:PCW:O3P	0.53	2.26	1	2
3:A:404:PCW:H332	3:B:203:PCW:H342	0.53	1.80	2	1
3:A:407:PCW:H62	3:B:213:PCW:O2P	0.53	2.02	3	2
3:A:417:PCW:O4P	3:A:417:PCW:H62	0.53	2.02	9	7
4:D:634:17F:H76	3:C:206:PCW:H222	0.53	1.81	4	1
3:A:402:PCW:H421	3:C:205:PCW:H152	0.53	1.79	5	1
3:A:413:PCW:H121	3:A:413:PCW:C35	0.53	2.28	18	3
3:C:204:PCW:O31	3:C:204:PCW:O3P	0.53	2.26	5	2
3:C:203:PCW:C7	3:C:203:PCW:H352	0.53	2.33	6	1
3:B:207:PCW:H432	3:B:213:PCW:C23	0.53	2.33	9	1
3:A:401:PCW:H342	3:B:209:PCW:H421	0.53	1.81	11	1
3:A:420:PCW:P	3:D:617:PCW:H52	0.53	2.44	11	1
3:C:204:PCW:H471	4:C:211:17F:C1Z	0.53	2.33	11	2
3:A:407:PCW:H162	3:B:208:PCW:C19	0.53	2.34	16	1
3:D:607:PCW:C17	4:D:631:17F:H18A	0.53	2.34	17	1
3:A:412:PCW:H452	3:C:208:PCW:C48	0.53	2.34	19	1
3:C:205:PCW:O1P	3:C:206:PCW:C8	0.53	2.57	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:402:PCW:C45	3:A:407:PCW:H231	0.53	2.34	1	1
3:D:606:PCW:H462	3:D:625:PCW:H481	0.53	1.80	1	1
3:D:608:PCW:C12	3:D:615:PCW:C7	0.53	2.86	7	3
3:C:209:PCW:O31	3:C:209:PCW:C11	0.53	2.57	19	2
3:A:408:PCW:H61	2:C:170:MET:O	0.53	2.04	2	1
3:A:410:PCW:C15	3:C:207:PCW:H241	0.53	2.31	2	1
3:D:601:PCW:H483	4:D:628:17F:H56	0.53	1.79	2	2
3:D:603:PCW:O31	3:D:605:PCW:C8	0.53	2.56	13	10
3:D:604:PCW:O1P	3:D:604:PCW:H2	0.53	2.04	15	9
3:B:203:PCW:C48	4:B:217:17F:H55	0.53	2.18	8	2
3:D:603:PCW:C3	3:D:603:PCW:O1P	0.53	2.56	10	4
3:D:607:PCW:H461	4:D:628:17F:H60	0.53	1.79	3	1
3:D:621:PCW:H441	4:D:634:17F:H73	0.53	1.79	5	2
1:A:288:ARG:O	1:A:292:HIS:HB2	0.53	2.03	17	4
3:A:413:PCW:H161	4:A:414:17F:C1Y	0.53	2.20	12	1
3:D:606:PCW:C47	3:B:210:PCW:H272	0.53	2.34	12	1
3:B:208:PCW:C47	3:B:208:PCW:H282	0.53	2.33	12	1
3:A:403:PCW:C19	3:C:203:PCW:H122	0.53	2.32	13	1
3:A:416:PCW:H452	3:A:420:PCW:C42	0.53	2.33	19	2
3:B:209:PCW:H61	4:B:215:17F:C8	0.53	2.34	17	1
2:C:13:GLY:HA2	5:C:201:GDP:C5'	0.53	2.31	17	1
3:D:618:PCW:H252	3:C:204:PCW:H281	0.53	1.80	19	1
3:C:212:PCW:C14	3:C:212:PCW:H372	0.53	2.34	19	1
3:D:616:PCW:O3	3:D:616:PCW:O31	0.53	2.27	11	15
3:A:410:PCW:H181	3:C:209:PCW:H261	0.53	1.81	18	5
3:A:419:PCW:H342	3:D:617:PCW:H412	0.53	1.80	3	2
3:D:613:PCW:C47	3:D:619:PCW:H231	0.53	2.33	5	2
4:D:632:17F:O7	4:D:632:17F:O10	0.53	2.27	5	5
2:B:32:TYR:HA	5:B:201:GDP:H5''	0.53	1.80	3	1
2:C:15:GLY:HA2	5:C:201:GDP:C8	0.53	2.38	12	4
4:C:211:17F:O7	4:C:211:17F:C17	0.53	2.57	9	9
4:A:414:17F:H29	4:A:414:17F:H40	0.53	1.81	4	1
3:D:622:PCW:C14	4:D:630:17F:C1Z	0.53	2.85	16	4
1:D:534:GLU:HA	1:D:537:LYS:HE3	0.53	1.78	7	3
3:D:622:PCW:H171	3:C:212:PCW:C12	0.53	2.34	8	1
3:A:408:PCW:O2	3:A:408:PCW:O2P	0.53	2.27	15	3
3:D:615:PCW:O31	3:D:615:PCW:O3	0.53	2.27	17	4
3:A:407:PCW:H41	4:B:216:17F:H12A	0.53	1.81	12	1
3:B:204:PCW:H172	3:C:204:PCW:C38	0.53	2.34	14	1
3:D:602:PCW:C6	3:C:212:PCW:O2P	0.53	2.56	17	2
3:B:207:PCW:H181	3:B:210:PCW:C19	0.53	2.34	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:408:PCW:H262	3:A:417:PCW:H241	0.53	1.80	19	1
3:D:625:PCW:H412	3:D:626:PCW:H421	0.53	1.81	19	1
3:A:404:PCW:H382	4:B:215:17F:H44	0.53	1.81	1	1
3:D:605:PCW:C15	4:D:629:17F:H11A	0.53	2.34	14	4
3:D:608:PCW:H261	3:D:615:PCW:H411	0.53	1.81	1	3
3:D:624:PCW:H62	3:D:624:PCW:C31	0.53	2.34	7	6
3:C:208:PCW:H161	3:C:208:PCW:C45	0.53	2.34	1	1
3:D:604:PCW:C47	3:D:619:PCW:H432	0.53	2.34	2	2
3:D:606:PCW:H31	3:D:626:PCW:C38	0.53	2.33	11	5
3:D:621:PCW:H283	4:D:633:17F:H30	0.53	1.80	17	6
3:D:602:PCW:H472	3:D:602:PCW:C23	0.53	2.28	3	2
1:A:273:ARG:HA	1:A:276:VAL:HG12	0.53	1.79	18	4
1:D:502:GLU:HG2	1:D:506:ARG:HE	0.53	1.63	4	4
3:D:602:PCW:C22	3:D:610:PCW:C33	0.53	2.86	4	1
3:A:409:PCW:H51	3:C:206:PCW:C32	0.53	2.07	20	2
3:A:418:PCW:H82	3:D:626:PCW:C33	0.53	2.32	7	3
3:B:205:PCW:C5	3:B:208:PCW:H12	0.53	2.33	9	1
3:D:616:PCW:H372	3:D:618:PCW:C14	0.53	2.34	20	2
1:A:250:VAL:HG11	3:A:412:PCW:H271	0.53	1.80	13	3
3:D:604:PCW:H341	3:D:624:PCW:H342	0.53	1.80	15	1
3:A:413:PCW:H241	4:A:414:17F:C34	0.53	2.34	17	1
3:D:611:PCW:O2P	3:D:619:PCW:C4	0.53	2.57	17	1
3:D:618:PCW:H483	3:B:204:PCW:H232	0.53	1.81	19	1
3:C:207:PCW:H232	3:C:208:PCW:H241	0.53	1.79	19	1
3:A:406:PCW:H252	3:B:207:PCW:H19	0.53	1.81	20	1
3:A:403:PCW:H171	3:C:203:PCW:H142	0.52	1.81	1	1
3:D:604:PCW:O31	3:D:613:PCW:H63	0.52	2.03	1	4
4:D:634:17F:H71	3:C:206:PCW:H211	0.52	1.80	1	1
3:A:403:PCW:C6	4:A:414:17F:O4	0.52	2.55	2	1
3:A:404:PCW:H121	3:B:209:PCW:H352	0.52	1.79	3	1
4:A:414:17F:H45	3:B:204:PCW:H462	0.52	1.81	4	1
3:D:615:PCW:H122	4:D:635:17F:O7	0.52	2.04	4	1
3:B:207:PCW:H422	3:B:213:PCW:C25	0.52	2.33	4	2
3:D:611:PCW:H221	3:D:619:PCW:H461	0.52	1.79	5	1
3:A:404:PCW:H442	4:B:215:17F:H10A	0.52	1.80	6	1
1:D:503:MET:HA	1:D:506:ARG:HD2	0.52	1.81	6	2
3:D:601:PCW:C21	3:D:601:PCW:H172	0.52	2.35	6	1
3:A:410:PCW:H152	3:C:207:PCW:H212	0.52	1.79	7	1
3:A:419:PCW:C46	3:C:203:PCW:H281	0.52	2.34	11	1
3:D:604:PCW:H482	3:D:619:PCW:H451	0.52	1.81	14	1
3:B:205:PCW:H172	3:B:212:PCW:H342	0.52	1.82	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:208:PCW:H422	4:B:214:17F:C1Z	0.52	2.29	14	1
3:B:211:PCW:H132	4:B:217:17F:C33	0.52	2.33	14	1
1:A:341:ASN:HD21	1:D:432:LYS:HB3	0.52	1.64	15	1
3:B:210:PCW:H271	3:B:210:PCW:C41	0.52	2.34	15	1
3:D:622:PCW:H341	3:C:212:PCW:C43	0.52	2.34	18	1
4:C:211:17F:C11	4:C:211:17F:H69	0.52	2.34	18	1
3:A:401:PCW:O31	3:A:401:PCW:O3	0.52	2.27	19	1
3:B:207:PCW:C39	4:B:215:17F:H6A	0.52	2.23	1	1
3:B:207:PCW:H132	3:B:210:PCW:C13	0.52	2.25	13	3
3:A:413:PCW:H172	4:A:414:17F:C1Y	0.52	2.34	2	1
4:B:214:17F:O10	4:B:214:17F:C4	0.52	2.56	7	2
3:A:407:PCW:H482	3:D:615:PCW:H283	0.52	1.81	9	2
4:B:217:17F:H30	4:B:217:17F:H61	0.52	1.80	5	2
2:C:118:CYS:SG	2:C:143:GLU:HB3	0.52	2.44	3	3
3:A:413:PCW:H351	3:A:413:PCW:O31	0.52	2.03	15	4
4:A:414:17F:C21	3:B:211:PCW:H422	0.52	2.34	4	1
3:D:602:PCW:H121	3:D:624:PCW:H161	0.52	1.80	4	3
3:D:618:PCW:O3P	3:D:618:PCW:O31	0.52	2.27	16	7
3:B:208:PCW:H412	4:B:214:17F:C12	0.52	2.34	5	2
3:B:210:PCW:O11	3:B:210:PCW:C2	0.52	2.54	7	5
3:B:211:PCW:H471	3:B:212:PCW:H131	0.52	1.81	6	1
3:A:413:PCW:H352	4:A:414:17F:H65	0.52	1.82	7	1
4:D:634:17F:H69	4:D:635:17F:H67	0.52	1.79	7	1
3:B:207:PCW:H12	3:B:207:PCW:O31	0.52	2.05	9	1
4:C:211:17F:H65	4:C:211:17F:C1X	0.52	2.35	9	1
3:A:402:PCW:C40	3:A:409:PCW:H282	0.52	2.34	10	2
4:D:634:17F:H75	3:C:206:PCW:H271	0.52	1.81	10	1
3:B:203:PCW:C25	4:C:210:17F:H78	0.52	2.24	10	1
3:A:407:PCW:H272	3:A:409:PCW:H232	0.52	1.79	11	1
3:A:419:PCW:H432	3:D:610:PCW:C23	0.52	2.33	11	1
3:A:419:PCW:H412	3:D:610:PCW:H211	0.52	1.80	11	1
3:D:605:PCW:H31	4:D:629:17F:O1	0.52	2.04	16	1
3:B:210:PCW:H73	3:B:210:PCW:H122	0.52	1.80	17	1
3:A:407:PCW:H12	4:B:216:17F:H10	0.52	1.80	18	1
3:D:622:PCW:C47	3:B:206:PCW:H252	0.52	2.32	18	1
3:A:402:PCW:H412	3:C:205:PCW:H352	0.52	1.81	19	1
4:D:628:17F:C37	4:D:631:17F:H48	0.52	2.35	20	1
3:A:403:PCW:O11	3:A:403:PCW:O2	0.52	2.26	18	13
3:A:404:PCW:H52	3:A:404:PCW:C32	0.52	2.34	15	3
3:D:611:PCW:C3	3:D:619:PCW:O11	0.52	2.57	11	3
3:D:613:PCW:C14	3:D:619:PCW:C39	0.52	2.88	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:627:PCW:O2	3:D:627:PCW:C11	0.52	2.58	14	3
2:B:41:ARG:HA	2:B:53:LEU:O	0.52	2.05	9	5
3:B:209:PCW:O11	3:B:209:PCW:C5	0.52	2.57	14	7
3:D:605:PCW:H161	4:D:629:17F:C1X	0.52	2.34	2	3
3:A:401:PCW:C45	3:D:614:PCW:H262	0.52	2.34	3	1
3:A:406:PCW:H82	3:B:207:PCW:H362	0.52	1.81	3	1
1:D:433:GLU:O	1:D:437:LEU:HB2	0.52	2.04	3	1
4:B:215:17F:O2	4:B:215:17F:C2	0.52	2.58	7	5
3:A:404:PCW:C3	3:B:209:PCW:H321	0.52	2.34	5	1
3:B:206:PCW:H442	3:C:204:PCW:H441	0.52	1.81	5	1
3:A:401:PCW:H41	3:B:209:PCW:C1	0.52	2.35	6	1
3:A:412:PCW:C48	3:B:206:PCW:H271	0.52	2.35	6	1
3:D:609:PCW:H61	4:D:633:17F:H6A	0.52	1.79	6	1
3:B:206:PCW:H462	4:C:211:17F:H49	0.52	1.81	6	1
3:A:407:PCW:H242	3:C:205:PCW:C41	0.52	2.33	18	2
4:B:214:17F:O10	4:B:214:17F:H20	0.52	2.03	10	2
3:D:623:PCW:O2	3:D:625:PCW:C16	0.52	2.57	9	1
3:D:606:PCW:H361	3:D:626:PCW:H442	0.52	1.81	10	1
3:B:208:PCW:H422	4:B:214:17F:C1Y	0.52	2.33	10	1
3:A:410:PCW:O1P	3:C:207:PCW:H142	0.52	2.04	13	1
3:A:408:PCW:H142	3:A:417:PCW:H251	0.52	1.80	14	1
3:B:203:PCW:H483	3:B:209:PCW:H481	0.52	1.79	14	1
3:B:206:PCW:H39	3:C:212:PCW:H261	0.52	1.81	19	2
3:B:206:PCW:H39	3:C:212:PCW:C25	0.52	2.34	19	2
3:B:204:PCW:C24	3:C:204:PCW:H422	0.52	2.33	19	1
3:B:208:PCW:C23	3:B:208:PCW:C28	0.52	2.60	19	1
3:A:403:PCW:C8	4:A:414:17F:H1	0.52	2.34	20	1
3:D:616:PCW:H461	3:D:627:PCW:H251	0.52	1.82	20	1
3:A:407:PCW:H262	3:C:205:PCW:C39	0.52	2.35	4	4
3:D:617:PCW:H51	3:D:617:PCW:C2	0.52	2.34	19	10
3:C:204:PCW:C3	4:C:211:17F:H75	0.52	2.33	1	1
3:C:207:PCW:O2P	4:C:211:17F:H4A	0.52	2.03	1	2
1:A:396:LYS:HG2	1:D:587:ALA:HB2	0.52	1.80	18	2
3:D:606:PCW:O31	3:D:606:PCW:O3	0.52	2.28	9	13
3:A:408:PCW:H262	3:A:417:PCW:C48	0.52	2.34	4	2
3:D:613:PCW:C3	3:D:619:PCW:H2	0.52	2.33	3	3
3:D:618:PCW:H331	3:D:627:PCW:H172	0.52	1.79	19	2
3:D:627:PCW:C31	3:D:627:PCW:O3	0.52	2.57	3	2
4:D:634:17F:C19	4:D:634:17F:H9	0.52	2.34	6	2
4:B:214:17F:H46	4:B:217:17F:C39	0.52	2.34	16	2
3:A:403:PCW:H441	3:A:403:PCW:H232	0.52	1.81	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:606:PCW:H442	3:D:625:PCW:C48	0.52	2.34	5	1
3:B:212:PCW:H421	3:C:212:PCW:H281	0.52	1.80	19	2
3:A:404:PCW:H372	3:B:209:PCW:H51	0.52	1.81	6	1
3:A:404:PCW:C40	4:B:215:17F:H8	0.52	2.33	9	1
3:D:607:PCW:H221	4:D:628:17F:H8A	0.52	1.82	9	1
3:D:613:PCW:H182	4:C:210:17F:C29	0.52	2.34	10	1
4:D:629:17F:HN1	4:D:629:17F:C17	0.52	2.17	11	1
3:C:204:PCW:H352	4:C:211:17F:C4	0.52	2.24	11	1
1:A:374:GLY:HA2	1:D:400:LYS:HE3	0.52	1.81	12	1
3:A:408:PCW:O2P	3:A:408:PCW:O2	0.52	2.26	13	2
3:A:418:PCW:C48	3:D:603:PCW:H272	0.52	2.34	13	1
3:A:411:PCW:O31	4:B:215:17F:H33	0.52	2.05	15	1
3:B:210:PCW:H381	3:B:210:PCW:H422	0.52	1.81	16	1
3:A:410:PCW:H152	3:C:207:PCW:H222	0.52	1.82	17	1
4:A:414:17F:H55	3:B:212:PCW:C24	0.52	2.34	18	1
3:B:213:PCW:C48	4:B:217:17F:H44	0.52	2.35	20	1
3:A:402:PCW:H442	3:A:407:PCW:C23	0.52	2.32	1	1
3:B:209:PCW:C32	3:B:209:PCW:H132	0.52	2.34	1	1
3:A:410:PCW:H162	3:C:209:PCW:C41	0.52	2.34	2	1
3:A:419:PCW:H422	3:D:616:PCW:C23	0.52	2.34	2	4
3:D:611:PCW:H141	3:D:619:PCW:H171	0.52	1.79	2	1
3:C:208:PCW:H212	3:C:209:PCW:H441	0.52	1.81	4	1
3:A:417:PCW:H352	3:D:612:PCW:C13	0.52	2.34	5	2
3:D:622:PCW:H331	3:D:627:PCW:H20	0.52	1.82	7	2
3:C:203:PCW:C38	3:C:203:PCW:H141	0.52	2.34	6	1
3:A:409:PCW:H331	3:C:206:PCW:H322	0.52	1.81	7	1
3:A:408:PCW:H82	3:C:204:PCW:H121	0.52	1.81	8	1
3:C:204:PCW:H351	4:C:211:17F:O7	0.52	2.05	15	2
1:A:233:GLU:HA	1:A:236:THR:OG1	0.52	2.04	14	4
3:D:615:PCW:H221	3:C:205:PCW:H252	0.52	1.80	11	1
3:A:402:PCW:O2P	3:C:206:PCW:H73	0.52	2.04	12	1
3:A:411:PCW:C35	4:B:215:17F:H62	0.52	2.35	13	1
3:B:206:PCW:H431	3:C:204:PCW:C44	0.52	2.34	13	2
3:A:417:PCW:C8	3:D:617:PCW:C40	0.52	2.87	14	1
3:D:602:PCW:H52	4:D:630:17F:O5	0.52	2.05	14	1
4:D:634:17F:H61	4:D:635:17F:H70	0.52	1.81	14	1
3:A:411:PCW:H171	3:A:411:PCW:C22	0.52	2.34	16	1
3:B:212:PCW:O11	3:B:212:PCW:H82	0.52	2.05	17	1
3:D:622:PCW:H471	3:B:206:PCW:H272	0.52	1.82	18	1
3:B:208:PCW:H40	4:B:214:17F:H76	0.52	1.80	19	1
3:B:209:PCW:H442	4:B:215:17F:H45	0.52	1.82	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:404:PCW:H471	3:B:209:PCW:H271	0.52	1.82	20	1
3:A:406:PCW:H61	3:A:411:PCW:O2P	0.52	2.03	20	1
3:D:617:PCW:H2	3:D:617:PCW:C6	0.52	2.33	1	4
3:B:204:PCW:C13	3:C:207:PCW:H11	0.52	2.28	3	2
3:A:406:PCW:H382	3:A:406:PCW:C14	0.52	2.35	4	1
3:D:604:PCW:H39	3:D:611:PCW:O3	0.52	2.05	5	1
3:C:204:PCW:H451	4:C:211:17F:C33	0.52	2.09	5	1
3:A:405:PCW:H39	3:D:601:PCW:H151	0.52	1.81	19	2
3:A:409:PCW:O31	3:A:409:PCW:H41	0.52	2.04	6	3
3:B:211:PCW:C16	4:B:217:17F:H65	0.52	2.31	6	1
3:C:206:PCW:H182	3:C:206:PCW:H231	0.52	1.81	15	3
3:C:207:PCW:C25	3:C:208:PCW:H241	0.52	2.24	6	1
3:A:403:PCW:C48	3:C:203:PCW:H283	0.52	2.34	7	1
3:A:417:PCW:H442	3:D:612:PCW:C27	0.52	2.34	8	4
3:A:419:PCW:H451	3:D:610:PCW:C20	0.52	2.34	8	1
1:D:463:TRP:NE1	4:D:631:17F:H75	0.52	2.20	17	3
3:B:209:PCW:H221	3:B:209:PCW:C36	0.52	2.34	8	1
3:B:211:PCW:H32	4:B:217:17F:H32	0.52	1.80	9	1
3:A:403:PCW:O1P	3:A:403:PCW:H31	0.52	2.05	10	1
3:A:413:PCW:H371	3:A:413:PCW:C2	0.52	2.34	11	1
3:A:406:PCW:H241	3:B:207:PCW:H19	0.52	1.81	12	1
3:A:408:PCW:H262	3:A:417:PCW:C46	0.52	2.28	15	1
3:D:603:PCW:H211	3:D:603:PCW:H162	0.52	1.81	15	1
3:A:416:PCW:H211	3:D:617:PCW:H472	0.52	1.80	18	1
3:C:209:PCW:H52	3:C:209:PCW:O2	0.52	2.05	18	1
3:A:408:PCW:H82	4:C:211:17F:H2	0.52	1.82	19	1
3:A:413:PCW:H241	4:A:414:17F:H59	0.52	1.80	19	1
4:D:633:17F:C42	3:C:206:PCW:H281	0.52	2.33	20	1
3:B:207:PCW:H332	3:B:210:PCW:O2P	0.52	2.04	20	1
3:D:611:PCW:H63	3:D:623:PCW:C33	0.52	2.35	1	1
4:D:634:17F:H5	4:D:634:17F:O1	0.52	2.04	4	4
3:A:416:PCW:O3	3:A:416:PCW:O31	0.52	2.27	6	7
3:D:626:PCW:O2	3:D:626:PCW:P	0.52	2.68	18	9
3:A:410:PCW:C11	3:C:209:PCW:H121	0.52	2.35	18	2
3:A:419:PCW:H362	3:D:617:PCW:C41	0.52	2.34	11	4
3:B:206:PCW:O31	3:B:206:PCW:C1	0.52	2.55	3	2
3:C:208:PCW:O2P	3:C:209:PCW:N	0.52	2.43	13	5
3:C:209:PCW:H341	3:C:209:PCW:C13	0.52	2.30	13	2
3:A:406:PCW:H141	3:A:406:PCW:H362	0.52	1.80	4	1
3:D:602:PCW:H211	3:D:610:PCW:H331	0.52	1.82	4	1
3:B:204:PCW:H332	3:B:212:PCW:H121	0.52	1.81	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:414:17F:H50	3:B:212:PCW:H231	0.52	1.80	5	1
3:B:204:PCW:H471	3:C:203:PCW:H171	0.52	1.81	5	1
3:D:604:PCW:H481	3:D:613:PCW:H162	0.52	1.79	6	1
3:C:203:PCW:O31	3:C:203:PCW:H51	0.52	2.05	6	1
3:A:407:PCW:H61	3:B:213:PCW:O1P	0.52	2.05	11	2
3:A:411:PCW:H272	3:A:418:PCW:H271	0.52	1.80	7	1
3:A:411:PCW:H431	3:A:418:PCW:H282	0.52	1.80	7	1
3:D:602:PCW:H212	3:D:602:PCW:H472	0.52	1.79	7	2
3:B:211:PCW:C22	3:B:211:PCW:H181	0.52	2.34	17	3
3:A:406:PCW:C4	3:B:210:PCW:H341	0.52	2.28	8	1
3:A:413:PCW:H121	4:A:414:17F:H65	0.52	1.82	20	2
3:B:208:PCW:H441	4:B:214:17F:H58	0.52	1.82	9	1
3:C:204:PCW:C25	4:C:211:17F:H32	0.52	2.32	9	1
3:D:616:PCW:C37	3:D:618:PCW:C14	0.52	2.88	10	1
3:A:413:PCW:H482	4:C:210:17F:C35	0.52	2.34	13	1
3:A:411:PCW:H222	3:A:411:PCW:C17	0.52	2.34	17	1
3:C:208:PCW:C45	3:C:209:PCW:H412	0.52	2.35	17	1
3:D:604:PCW:O31	3:D:613:PCW:C8	0.52	2.58	1	5
3:A:409:PCW:O31	3:C:206:PCW:C32	0.52	2.57	3	2
3:A:410:PCW:H32	3:C:207:PCW:C15	0.52	2.35	13	2
4:A:414:17F:H64	4:C:210:17F:H37	0.52	1.81	2	1
2:B:16:LYS:HB2	5:B:201:GDP:O3B	0.52	2.03	6	4
3:B:213:PCW:H40	4:B:217:17F:C37	0.52	2.34	2	2
3:A:401:PCW:C5	3:B:209:PCW:O31	0.52	2.58	3	2
3:A:419:PCW:H412	3:D:610:PCW:C18	0.52	2.35	19	3
3:A:402:PCW:O31	3:A:402:PCW:H11	0.52	2.03	19	5
3:A:419:PCW:O3	3:A:419:PCW:C31	0.52	2.58	5	3
3:D:607:PCW:C6	3:D:626:PCW:H242	0.52	2.30	16	2
3:B:203:PCW:H321	4:B:215:17F:H37	0.52	1.80	5	1
4:A:415:17F:O8	4:A:415:17F:O9	0.52	2.28	6	6
3:B:211:PCW:H11	4:B:217:17F:H19A	0.52	1.81	6	1
4:B:215:17F:H19	4:B:215:17F:H5	0.52	1.81	6	1
3:A:407:PCW:C35	3:C:205:PCW:H142	0.52	2.20	7	1
3:A:417:PCW:C37	3:D:612:PCW:H182	0.52	2.35	10	1
3:D:620:PCW:H141	4:D:635:17F:C5	0.52	2.34	20	3
3:D:623:PCW:H281	3:D:624:PCW:H462	0.52	1.80	12	4
3:B:212:PCW:O31	3:B:212:PCW:H12	0.52	2.04	12	1
3:D:622:PCW:H283	3:D:624:PCW:C28	0.52	2.35	14	1
3:B:210:PCW:H42	4:B:216:17F:O3	0.52	2.05	14	1
3:A:407:PCW:C14	3:B:208:PCW:H182	0.52	2.35	15	1
3:A:419:PCW:H412	3:D:610:PCW:H182	0.52	1.82	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:204:PCW:H331	4:C:211:17F:O8	0.52	2.05	16	2
3:D:603:PCW:H271	4:B:217:17F:C42	0.52	2.35	18	1
3:A:404:PCW:H212	3:B:203:PCW:H281	0.52	1.82	1	1
3:A:409:PCW:O4P	3:A:409:PCW:H2	0.52	2.05	3	9
4:A:415:17F:O10	4:A:415:17F:O6	0.52	2.27	16	10
3:A:416:PCW:O31	3:A:416:PCW:P	0.52	2.67	5	4
3:D:608:PCW:C8	3:D:608:PCW:O4P	0.52	2.58	6	14
3:D:611:PCW:O31	3:D:619:PCW:H61	0.52	2.05	5	3
2:C:78:PHE:HB2	2:C:111:MET:HG2	0.52	1.81	9	7
2:C:117:LYS:HE2	5:C:201:GDP:C4	0.52	2.40	17	5
3:A:407:PCW:H63	3:B:213:PCW:H322	0.52	1.82	8	2
3:D:602:PCW:H442	3:D:610:PCW:H351	0.52	1.81	9	4
4:D:628:17F:C2X	4:D:631:17F:H74	0.52	2.34	3	1
4:D:634:17F:O8	4:D:634:17F:O9	0.52	2.28	10	4
3:B:204:PCW:H172	3:C:204:PCW:H39	0.52	1.81	15	2
3:B:213:PCW:H162	4:B:217:17F:C10	0.52	2.35	17	2
5:C:201:GDP:H2'	5:C:201:GDP:O5'	0.52	2.05	3	5
3:A:409:PCW:O31	3:A:409:PCW:O3	0.52	2.27	18	7
4:A:415:17F:C41	4:C:210:17F:H68	0.52	2.34	11	4
3:C:207:PCW:H19	3:C:207:PCW:H451	0.52	1.81	4	1
3:A:404:PCW:H441	4:B:215:17F:H10	0.52	1.82	5	1
3:A:413:PCW:C14	4:A:414:17F:H62	0.52	2.31	15	4
3:C:207:PCW:C28	3:C:208:PCW:H172	0.52	2.34	20	2
3:D:607:PCW:H172	4:D:631:17F:C18	0.52	2.35	7	2
3:A:413:PCW:C34	4:A:414:17F:C1Z	0.52	2.88	11	1
3:A:406:PCW:H241	3:B:207:PCW:C19	0.52	2.35	12	2
3:D:608:PCW:H362	3:C:205:PCW:H281	0.52	1.81	13	1
3:D:616:PCW:O1P	3:D:616:PCW:C3	0.52	2.58	13	1
3:A:402:PCW:H451	3:A:407:PCW:H251	0.52	1.82	14	1
3:A:404:PCW:H63	4:A:415:17F:O4	0.52	2.05	16	1
3:A:412:PCW:H461	3:C:208:PCW:H182	0.52	1.81	16	1
3:B:210:PCW:C46	3:B:213:PCW:H283	0.52	2.34	17	1
1:A:292:HIS:O	1:A:296:GLU:HG2	0.52	2.05	19	3
3:D:603:PCW:H262	4:B:217:17F:H76	0.52	1.80	18	1
3:D:605:PCW:C23	4:D:629:17F:H38	0.52	2.32	18	1
3:B:210:PCW:H482	4:B:214:17F:C30	0.52	2.34	18	1
3:B:211:PCW:H19	3:B:211:PCW:C48	0.52	2.34	19	1
3:A:419:PCW:O2P	3:A:419:PCW:H52	0.52	2.04	1	6
3:B:208:PCW:H161	4:B:214:17F:C18	0.52	2.35	1	1
3:A:404:PCW:H51	3:B:203:PCW:C3	0.52	2.34	2	1
3:D:615:PCW:H161	4:D:635:17F:H11A	0.52	1.80	13	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:203:PCW:O3	3:C:203:PCW:O31	0.52	2.27	2	1
3:C:203:PCW:O31	3:C:203:PCW:H341	0.52	2.05	2	1
3:A:406:PCW:H42	3:A:406:PCW:O3	0.52	2.05	4	1
1:D:570:ARG:O	1:D:574:LEU:HG	0.52	2.05	4	4
3:D:624:PCW:H271	3:B:212:PCW:C28	0.52	2.34	4	1
3:A:407:PCW:H151	3:C:205:PCW:C16	0.52	2.35	5	1
3:D:617:PCW:O31	3:D:617:PCW:H12	0.52	2.04	5	1
3:D:622:PCW:H482	3:B:206:PCW:H221	0.52	1.82	5	1
3:B:204:PCW:H452	4:C:211:17F:C42	0.52	2.35	6	1
3:A:405:PCW:H271	1:D:451:LYS:HD3	0.52	1.82	7	1
3:D:602:PCW:C6	3:C:212:PCW:P	0.52	2.98	18	3
3:C:208:PCW:C44	3:C:209:PCW:H422	0.52	2.34	7	1
3:C:208:PCW:H483	3:C:209:PCW:H442	0.52	1.81	7	1
3:A:404:PCW:H272	4:A:415:17F:C37	0.52	2.35	8	1
4:D:634:17F:C34	4:D:635:17F:H75	0.52	2.35	8	1
3:A:410:PCW:H471	1:D:532:ARG:NH1	0.52	2.20	10	1
3:D:614:PCW:H52	3:D:625:PCW:H41	0.52	1.80	10	1
3:B:207:PCW:H12	3:B:213:PCW:C12	0.52	2.27	11	1
3:A:402:PCW:C32	3:C:206:PCW:H41	0.52	2.16	12	1
4:D:630:17F:H10A	4:D:630:17F:C33	0.52	2.32	17	2
3:A:411:PCW:H162	3:A:418:PCW:C28	0.52	2.35	13	1
3:C:203:PCW:H171	3:C:203:PCW:H483	0.52	1.82	13	1
3:A:405:PCW:C38	4:D:628:17F:H52	0.52	2.34	17	2
3:B:205:PCW:H39	4:B:214:17F:H64	0.52	1.80	17	2
3:A:420:PCW:P	3:D:617:PCW:H82	0.52	2.44	15	1
4:B:215:17F:H18	4:B:215:17F:C7	0.52	2.35	16	1
3:B:207:PCW:C15	3:B:210:PCW:H351	0.52	2.35	17	1
3:A:406:PCW:H52	3:B:207:PCW:H341	0.52	1.81	18	1
3:A:417:PCW:C41	3:A:417:PCW:H371	0.52	2.34	20	1
3:B:206:PCW:H40	4:C:211:17F:H47	0.52	1.81	20	1
3:D:609:PCW:C6	4:D:633:17F:O8	0.51	2.57	1	2
3:D:617:PCW:C1	3:D:617:PCW:O31	0.51	2.57	16	3
3:A:404:PCW:H351	4:B:215:17F:C24	0.51	2.22	2	1
1:D:421:PRO:O	1:D:425:GLU:HG2	0.51	2.05	5	7
3:D:621:PCW:O11	3:D:621:PCW:O2	0.51	2.28	20	14
3:A:420:PCW:O1P	3:D:617:PCW:C6	0.51	2.57	4	1
3:D:618:PCW:H381	3:D:627:PCW:C18	0.51	2.33	10	4
3:D:623:PCW:O31	3:D:623:PCW:O3P	0.51	2.27	4	6
3:A:404:PCW:H432	3:B:209:PCW:C20	0.51	2.34	5	1
3:B:208:PCW:H63	3:B:208:PCW:H321	0.51	1.81	5	1
3:A:404:PCW:H31	3:B:209:PCW:H11	0.51	1.82	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:413:PCW:H462	3:D:613:PCW:C23	0.51	2.33	18	2
3:A:408:PCW:H471	3:A:410:PCW:C33	0.51	2.35	8	1
3:D:602:PCW:C7	3:C:212:PCW:H31	0.51	2.35	9	2
3:D:623:PCW:H2	3:D:624:PCW:C32	0.51	2.28	10	1
3:A:403:PCW:H51	3:A:403:PCW:O11	0.51	2.04	14	2
3:A:417:PCW:O4P	3:A:417:PCW:H82	0.51	2.05	20	2
3:D:602:PCW:H141	3:D:624:PCW:H211	0.51	1.80	11	1
3:B:208:PCW:H281	4:B:216:17F:C28	0.51	2.34	11	1
3:D:603:PCW:H271	4:B:217:17F:H75	0.51	1.80	13	1
3:A:407:PCW:H11	3:A:407:PCW:C4	0.51	2.35	15	1
3:A:406:PCW:H161	3:B:210:PCW:H371	0.51	1.81	19	1
3:B:204:PCW:H451	3:C:203:PCW:H141	0.51	1.82	20	1
3:A:406:PCW:P	3:A:406:PCW:C3	0.51	2.99	7	13
3:A:406:PCW:H283	4:B:216:17F:H33	0.51	1.81	1	1
3:D:622:PCW:H472	3:B:206:PCW:H282	0.51	1.82	1	1
3:B:209:PCW:C4	3:B:209:PCW:O11	0.51	2.58	14	10
3:B:206:PCW:O1P	3:B:206:PCW:H31	0.51	2.05	18	10
3:D:606:PCW:O3	3:D:606:PCW:O31	0.51	2.28	3	1
3:C:204:PCW:C13	4:C:211:17F:H77	0.51	2.35	3	1
3:B:209:PCW:H412	3:B:209:PCW:C37	0.51	2.32	4	1
3:D:611:PCW:H221	3:D:619:PCW:C46	0.51	2.35	5	1
3:B:213:PCW:O2P	4:B:214:17F:O2	0.51	2.28	5	1
3:C:208:PCW:C13	3:C:209:PCW:C32	0.51	2.88	5	1
3:A:403:PCW:C47	3:C:203:PCW:H283	0.51	2.36	8	1
3:B:209:PCW:C44	4:B:215:17F:H48	0.51	2.32	8	1
3:B:213:PCW:H422	4:B:217:17F:C35	0.51	2.34	8	1
3:A:405:PCW:H483	3:A:405:PCW:H121	0.51	1.83	9	1
4:A:415:17F:H9A	4:A:415:17F:H20A	0.51	1.81	10	1
3:A:408:PCW:H212	3:A:417:PCW:H462	0.51	1.80	11	1
4:C:210:17F:H10	4:C:210:17F:H59	0.51	1.81	14	2
3:D:605:PCW:H131	3:D:626:PCW:H281	0.51	1.81	13	1
3:D:610:PCW:H41	3:D:616:PCW:O2P	0.51	2.06	13	1
3:D:618:PCW:O1P	3:D:627:PCW:H51	0.51	2.05	13	1
3:B:212:PCW:H39	3:C:212:PCW:H262	0.51	1.81	13	1
3:D:606:PCW:H12	3:D:626:PCW:C35	0.51	2.35	17	2
3:B:206:PCW:H73	3:C:207:PCW:H12	0.51	1.82	14	1
3:A:407:PCW:O3P	3:A:407:PCW:O31	0.51	2.28	15	1
1:D:469:LEU:HD22	1:D:473:LYS:HE3	0.51	1.81	15	1
3:A:407:PCW:C1	4:B:216:17F:H12A	0.51	2.36	17	1
3:C:207:PCW:P	3:C:207:PCW:O2	0.51	2.68	17	1
3:A:408:PCW:H63	4:C:211:17F:O1	0.51	2.06	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:359:THR:HG22	1:D:414:LYS:HD2	0.51	1.82	14	2
3:A:403:PCW:H221	3:C:203:PCW:H252	0.51	1.81	2	1
3:A:420:PCW:H381	3:D:617:PCW:H151	0.51	1.82	2	3
3:D:603:PCW:H372	3:D:603:PCW:H411	0.51	1.82	17	2
3:B:207:PCW:C8	4:B:216:17F:O8	0.51	2.58	2	1
3:A:409:PCW:H122	3:C:206:PCW:C33	0.51	2.35	3	1
3:A:417:PCW:H351	3:D:612:PCW:H131	0.51	1.80	3	2
3:B:208:PCW:H182	3:C:205:PCW:H351	0.51	1.82	5	2
3:A:406:PCW:H362	3:A:406:PCW:H121	0.51	1.83	4	1
3:A:416:PCW:O11	3:A:416:PCW:C2	0.51	2.54	17	4
3:A:417:PCW:H341	3:D:612:PCW:H152	0.51	1.81	4	1
3:A:420:PCW:C44	3:D:617:PCW:C22	0.51	2.88	5	1
3:B:211:PCW:O3P	3:B:211:PCW:O31	0.51	2.29	13	6
3:A:409:PCW:H40	3:A:409:PCW:C18	0.51	2.35	6	2
3:C:212:PCW:H372	3:C:212:PCW:C14	0.51	2.34	6	3
3:A:413:PCW:C37	4:A:414:17F:H69	0.51	2.28	7	1
3:D:618:PCW:O2	3:D:627:PCW:H121	0.51	2.05	7	2
3:B:204:PCW:H283	3:C:204:PCW:C45	0.51	2.25	7	2
3:A:404:PCW:H151	4:A:415:17F:H57	0.51	1.82	8	1
3:A:419:PCW:C11	3:D:617:PCW:H422	0.51	2.35	8	1
3:A:406:PCW:H251	3:B:207:PCW:H171	0.51	1.82	9	1
3:A:411:PCW:O31	4:B:215:17F:H34	0.51	2.05	12	2
3:A:401:PCW:O11	3:A:401:PCW:C2	0.51	2.55	10	2
3:A:403:PCW:C28	3:A:413:PCW:H20	0.51	2.36	10	1
3:C:208:PCW:O31	3:C:208:PCW:H63	0.51	2.05	10	1
3:A:413:PCW:C34	4:A:414:17F:H34	0.51	2.35	11	1
3:A:402:PCW:H471	3:C:205:PCW:C36	0.51	2.35	12	1
3:B:207:PCW:C6	3:B:213:PCW:O2P	0.51	2.59	12	1
3:D:614:PCW:C4	3:D:625:PCW:O1P	0.51	2.58	19	2
3:B:203:PCW:H171	3:B:209:PCW:O2P	0.51	2.05	14	1
3:B:203:PCW:H342	4:B:215:17F:H38	0.51	1.82	14	1
3:A:403:PCW:H332	3:C:203:PCW:C3	0.51	2.32	15	1
3:A:410:PCW:C17	3:C:207:PCW:H211	0.51	2.35	15	1
3:A:402:PCW:H442	3:C:205:PCW:H172	0.51	1.82	17	1
3:A:403:PCW:C5	3:C:203:PCW:O1P	0.51	2.56	19	1
3:A:404:PCW:H472	3:B:209:PCW:C46	0.51	2.35	19	1
3:A:418:PCW:C40	3:D:625:PCW:C44	0.51	2.86	4	5
3:B:203:PCW:O31	3:B:203:PCW:H341	0.51	2.05	3	1
4:A:415:17F:H75	4:C:210:17F:H68	0.51	1.82	4	1
3:D:601:PCW:H462	4:D:628:17F:H70	0.51	1.82	4	1
3:D:613:PCW:H282	4:C:210:17F:C23	0.51	2.34	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:408:PCW:C36	3:C:207:PCW:H441	0.51	2.36	5	1
3:D:612:PCW:O11	3:D:612:PCW:C2	0.51	2.51	9	4
3:D:601:PCW:H52	4:B:216:17F:O1	0.51	2.05	6	1
3:D:604:PCW:H231	3:D:613:PCW:H382	0.51	1.81	8	2
3:C:208:PCW:H132	3:C:209:PCW:H322	0.51	1.81	11	2
4:D:634:17F:C9	4:D:634:17F:H19A	0.51	2.36	7	1
3:A:406:PCW:H241	3:B:210:PCW:O11	0.51	2.06	8	1
3:B:204:PCW:H32	3:C:207:PCW:O2P	0.51	2.06	8	1
3:A:405:PCW:H39	3:D:601:PCW:H152	0.51	1.81	10	1
2:C:15:GLY:HA3	5:C:201:GDP:H8	0.51	1.64	18	3
3:D:615:PCW:H271	4:B:216:17F:H75	0.51	1.80	11	1
3:C:203:PCW:H172	3:C:203:PCW:H471	0.51	1.80	11	1
3:A:407:PCW:C17	3:C:205:PCW:H151	0.51	2.34	13	1
3:A:413:PCW:H442	4:A:414:17F:H74	0.51	1.81	1	1
3:D:621:PCW:C18	3:D:621:PCW:C14	0.51	2.88	8	8
3:B:207:PCW:H162	3:B:210:PCW:H172	0.51	1.81	1	1
3:B:212:PCW:O31	3:B:212:PCW:O4P	0.51	2.28	16	5
1:A:365:LYS:CB	1:A:366:PRO:HD3	0.51	2.34	7	9
3:A:410:PCW:C3	3:C:207:PCW:H152	0.51	2.27	3	2
3:B:210:PCW:H451	3:B:213:PCW:C27	0.51	2.36	19	3
3:D:606:PCW:O31	3:D:606:PCW:C11	0.51	2.58	3	1
2:B:83:ALA:HB3	2:B:86:ASN:HB3	0.51	1.82	12	3
3:B:207:PCW:C15	3:B:210:PCW:H321	0.51	2.35	13	2
3:C:208:PCW:C39	3:C:208:PCW:H142	0.51	2.35	4	2
3:D:622:PCW:C33	3:D:627:PCW:H20	0.51	2.36	7	2
3:C:204:PCW:O11	3:C:204:PCW:C5	0.51	2.57	5	1
3:A:407:PCW:C20	3:C:205:PCW:H431	0.51	2.35	8	1
3:B:210:PCW:H481	3:B:210:PCW:H272	0.51	1.82	8	1
3:A:404:PCW:H381	3:B:209:PCW:C38	0.51	2.30	10	1
3:D:616:PCW:H482	3:C:208:PCW:C28	0.51	2.35	20	3
4:D:629:17F:H71	4:D:634:17F:C2X	0.51	2.35	11	1
3:D:603:PCW:H252	4:B:217:17F:H52	0.51	1.82	14	1
3:A:404:PCW:H262	4:A:415:17F:H64	0.51	1.81	15	1
3:D:615:PCW:O3	3:D:615:PCW:C31	0.51	2.58	17	3
3:B:204:PCW:H12	3:B:212:PCW:C7	0.51	2.34	15	1
3:A:401:PCW:H272	3:D:614:PCW:C28	0.51	2.36	17	1
3:A:408:PCW:C27	3:A:417:PCW:H221	0.51	2.35	18	1
3:A:413:PCW:H232	4:A:414:17F:H61	0.51	1.83	1	1
3:D:616:PCW:C4	3:D:616:PCW:C1	0.51	2.88	1	1
3:A:416:PCW:H472	3:D:617:PCW:H251	0.51	1.82	15	2
3:C:208:PCW:H73	3:C:208:PCW:C32	0.51	2.34	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:204:PCW:C14	3:C:204:PCW:H39	0.51	2.35	4	1
3:C:206:PCW:H382	3:C:206:PCW:C15	0.51	2.26	4	1
2:C:117:LYS:HG2	5:C:201:GDP:C6	0.51	2.41	20	3
4:D:630:17F:O10	4:D:630:17F:C20	0.51	2.59	7	1
3:D:602:PCW:C38	3:D:624:PCW:H141	0.51	2.24	8	1
3:A:413:PCW:H352	4:A:414:17F:H58	0.51	1.81	9	1
3:D:614:PCW:H52	3:D:625:PCW:C4	0.51	2.36	15	2
3:A:418:PCW:H63	3:D:626:PCW:O2	0.51	2.06	11	2
3:A:407:PCW:C7	4:B:214:17F:O3	0.51	2.59	12	1
3:C:203:PCW:H272	4:C:211:17F:H74	0.51	1.83	13	1
4:B:214:17F:H47	4:B:217:17F:H74	0.51	1.81	16	1
3:B:213:PCW:H162	4:B:217:17F:H10	0.51	1.80	17	1
3:A:406:PCW:C23	3:B:207:PCW:H19	0.51	2.36	19	1
3:A:403:PCW:C48	3:C:203:PCW:H281	0.51	2.33	2	1
3:A:404:PCW:C6	3:B:203:PCW:H132	0.51	2.35	2	1
3:D:607:PCW:C26	4:D:631:17F:C35	0.51	2.88	2	1
3:A:404:PCW:C41	3:B:209:PCW:H171	0.51	2.29	3	1
3:A:406:PCW:H472	3:B:207:PCW:H262	0.51	1.83	3	1
3:D:617:PCW:H51	3:D:617:PCW:O11	0.51	2.06	3	1
3:B:206:PCW:H40	3:C:212:PCW:H242	0.51	1.83	3	3
3:B:208:PCW:C3	3:B:208:PCW:O2P	0.51	2.59	15	5
3:D:627:PCW:H332	3:D:627:PCW:C11	0.51	2.35	5	1
3:B:207:PCW:H11	4:B:216:17F:C7	0.51	2.35	5	1
3:A:407:PCW:H61	3:B:213:PCW:P	0.51	2.45	7	3
3:B:205:PCW:H441	3:B:206:PCW:C21	0.51	2.36	7	2
3:B:209:PCW:O11	3:B:209:PCW:O2	0.51	2.28	19	7
3:D:605:PCW:O11	3:D:605:PCW:C6	0.51	2.58	13	4
3:B:213:PCW:C42	4:B:217:17F:H63	0.51	2.35	8	1
3:C:206:PCW:H381	3:C:206:PCW:H171	0.51	1.82	8	1
2:B:68:ARG:HA	2:B:71:TYR:HD1	0.51	1.65	9	1
3:B:213:PCW:C41	4:B:217:17F:H12	0.51	2.35	15	2
3:C:207:PCW:O2P	4:C:211:17F:H4	0.51	2.05	10	1
3:B:213:PCW:C35	4:B:214:17F:H9A	0.51	2.33	11	1
3:B:204:PCW:H452	3:C:203:PCW:C8	0.51	2.35	13	1
3:A:402:PCW:O2P	3:C:206:PCW:C7	0.51	2.59	14	1
3:D:612:PCW:C32	3:D:618:PCW:H152	0.51	2.33	18	1
3:C:208:PCW:H422	3:C:208:PCW:C16	0.51	2.36	18	1
3:A:406:PCW:C13	3:B:210:PCW:H331	0.51	2.21	20	1
3:B:205:PCW:H442	3:B:206:PCW:C17	0.51	2.36	20	1
3:C:206:PCW:H242	3:C:206:PCW:C18	0.51	2.36	1	1
3:A:403:PCW:C25	3:D:617:PCW:H282	0.51	2.36	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:410:PCW:O1P	3:A:410:PCW:C5	0.51	2.58	2	5
3:D:611:PCW:H39	3:D:623:PCW:C45	0.51	2.35	2	2
3:D:618:PCW:C48	3:B:204:PCW:H232	0.51	2.36	19	2
3:A:403:PCW:H19	3:C:203:PCW:H142	0.51	1.82	3	1
3:D:602:PCW:H11	3:D:624:PCW:H32	0.51	1.82	17	2
3:A:406:PCW:H82	3:B:210:PCW:O2P	0.51	2.06	4	1
3:D:608:PCW:O11	3:D:615:PCW:C8	0.51	2.59	4	2
4:D:630:17F:C30	3:B:212:PCW:H451	0.51	2.32	4	1
3:C:208:PCW:H161	3:C:209:PCW:C41	0.51	2.36	4	1
3:A:401:PCW:H73	3:B:209:PCW:C1	0.51	2.30	6	1
3:A:410:PCW:C15	3:C:207:PCW:H242	0.51	2.36	7	2
3:D:616:PCW:H31	3:D:616:PCW:H42	0.51	1.82	7	2
3:B:208:PCW:H381	4:B:214:17F:H8A	0.51	1.83	18	2
3:C:208:PCW:H461	3:C:208:PCW:C19	0.51	2.35	8	1
3:D:602:PCW:H441	3:D:602:PCW:H181	0.51	1.83	10	1
1:A:377:PRO:HG2	1:D:400:LYS:HE3	0.51	1.83	11	2
3:A:406:PCW:H483	3:D:606:PCW:H283	0.51	1.81	11	1
1:A:250:VAL:HG11	3:A:412:PCW:H282	0.51	1.82	12	1
3:A:407:PCW:H61	3:B:213:PCW:H11	0.51	1.83	12	1
3:D:603:PCW:H122	3:D:603:PCW:H332	0.51	1.83	12	1
3:B:206:PCW:H421	3:C:212:PCW:H242	0.51	1.82	12	1
3:B:204:PCW:H272	3:C:207:PCW:C26	0.51	2.28	13	1
3:B:204:PCW:O11	3:B:206:PCW:H51	0.51	2.06	13	1
4:B:215:17F:H30	4:B:217:17F:C1X	0.51	2.36	14	1
3:A:401:PCW:H431	3:B:209:PCW:C48	0.51	2.36	15	1
3:A:404:PCW:H451	3:B:209:PCW:H221	0.51	1.81	15	1
3:A:403:PCW:C31	3:C:204:PCW:H62	0.51	2.36	16	1
3:A:419:PCW:H11	3:D:617:PCW:C40	0.51	2.35	16	1
3:D:627:PCW:H42	3:D:627:PCW:C31	0.51	2.36	16	1
4:D:629:17F:O9	4:D:629:17F:O3	0.51	2.28	20	2
3:A:405:PCW:H40	4:D:628:17F:H52	0.51	1.81	19	1
1:A:325:ASP:HA	1:A:328:ARG:HD2	0.51	1.81	1	1
3:A:403:PCW:H322	3:C:203:PCW:H12	0.51	1.82	18	2
3:D:608:PCW:H241	3:D:615:PCW:C38	0.51	2.33	1	1
4:D:629:17F:H69	4:D:634:17F:C8	0.51	2.35	20	2
3:B:207:PCW:C42	3:B:213:PCW:C23	0.51	2.89	1	1
3:D:617:PCW:C28	3:C:203:PCW:H241	0.51	2.27	2	2
3:D:621:PCW:H152	4:D:634:17F:H6	0.51	1.83	5	2
4:B:215:17F:C1X	4:B:217:17F:H29	0.51	2.35	2	1
3:B:210:PCW:H32	3:B:210:PCW:C4	0.51	2.36	3	2
3:A:401:PCW:H73	3:B:209:PCW:C13	0.51	2.36	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:213:PCW:H431	4:B:214:17F:C30	0.51	2.35	4	1
3:D:615:PCW:H262	4:B:216:17F:C41	0.51	2.34	5	2
3:B:213:PCW:O4P	3:B:213:PCW:H82	0.51	2.05	5	1
3:B:213:PCW:C34	4:B:214:17F:H9A	0.51	2.35	5	1
3:C:204:PCW:C35	4:C:211:17F:C8	0.51	2.85	6	1
3:D:624:PCW:H481	4:C:210:17F:H54	0.51	1.80	7	1
3:C:208:PCW:H371	3:C:208:PCW:C13	0.51	2.36	12	2
3:A:420:PCW:H372	3:D:617:PCW:H151	0.51	1.82	8	1
4:D:628:17F:H40	4:D:631:17F:C41	0.51	2.32	10	2
3:A:405:PCW:O1P	3:A:405:PCW:C33	0.51	2.57	11	1
1:D:418:GLN:O	1:D:422:VAL:HB	0.51	2.06	11	1
3:B:208:PCW:C14	4:B:214:17F:H56	0.51	2.36	12	1
3:D:627:PCW:H283	3:C:208:PCW:C27	0.51	2.35	13	1
3:B:211:PCW:C6	3:B:212:PCW:C32	0.51	2.89	13	2
4:B:215:17F:H40	4:B:215:17F:C12	0.51	2.36	13	1
3:A:413:PCW:H141	4:A:414:17F:H59	0.51	1.83	14	1
3:B:203:PCW:H342	4:B:215:17F:C22	0.51	2.36	14	1
1:D:462:LYS:HD2	3:D:601:PCW:H283	0.51	1.81	15	1
3:A:402:PCW:C44	3:C:205:PCW:H172	0.51	2.36	17	1
3:A:420:PCW:O2P	3:D:617:PCW:C8	0.51	2.59	18	1
3:B:210:PCW:H481	3:B:213:PCW:H182	0.51	1.82	18	1
3:B:210:PCW:H52	4:B:216:17F:H18	0.51	1.82	18	1
3:A:407:PCW:O3	3:A:407:PCW:O31	0.51	2.29	16	11
1:D:463:TRP:HE1	4:D:631:17F:H77	0.51	1.65	9	2
3:D:604:PCW:O2P	3:D:613:PCW:C6	0.51	2.59	2	1
3:D:606:PCW:H12	3:D:626:PCW:H371	0.51	1.80	20	2
3:B:207:PCW:C41	4:B:217:17F:H10A	0.51	2.35	2	1
3:B:211:PCW:H371	3:B:211:PCW:C41	0.51	2.36	20	2
3:B:213:PCW:O31	4:B:217:17F:H20	0.51	2.05	2	1
4:B:216:17F:H36	4:B:216:17F:C24	0.51	2.22	19	5
3:A:401:PCW:O11	3:B:209:PCW:H232	0.51	2.06	3	1
3:A:404:PCW:C7	3:A:404:PCW:O31	0.51	2.59	3	2
3:A:406:PCW:H231	3:B:207:PCW:H152	0.51	1.83	16	3
4:A:414:17F:H6	3:C:203:PCW:H341	0.51	1.80	4	2
3:D:614:PCW:O31	3:D:614:PCW:C1	0.51	2.50	7	5
3:D:616:PCW:C26	3:C:204:PCW:H272	0.51	2.35	3	1
3:A:409:PCW:O31	3:C:206:PCW:C33	0.51	2.58	17	2
3:A:405:PCW:H39	3:D:601:PCW:C15	0.51	2.36	6	2
3:B:204:PCW:H12	3:B:212:PCW:C8	0.51	2.36	6	1
3:C:203:PCW:O2P	3:C:204:PCW:C7	0.51	2.59	6	1
3:A:403:PCW:H221	3:D:617:PCW:C28	0.51	2.36	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:630:17F:H43	4:D:630:17F:H72	0.51	1.82	7	1
4:D:630:17F:H44	4:D:630:17F:H68	0.51	1.82	16	2
2:C:168:GLU:OE1	3:C:206:PCW:H61	0.51	2.06	8	1
1:A:386:PHE:CZ	4:A:414:17F:H76	0.51	2.41	9	2
3:D:608:PCW:H272	4:B:216:17F:H54	0.51	1.81	9	1
3:B:213:PCW:H73	4:B:214:17F:O2	0.51	2.06	9	1
3:C:203:PCW:P	3:C:204:PCW:H52	0.51	2.46	9	1
3:A:417:PCW:H431	3:D:612:PCW:C21	0.51	2.35	11	1
3:A:403:PCW:H412	3:A:403:PCW:H212	0.51	1.82	12	1
3:C:207:PCW:H73	4:C:211:17F:O4	0.51	2.05	19	2
3:D:615:PCW:C28	4:D:635:17F:H45	0.51	2.36	13	1
3:D:620:PCW:H73	3:D:620:PCW:O4P	0.51	2.05	13	2
3:C:203:PCW:H351	3:C:203:PCW:O1P	0.51	2.05	13	1
4:A:415:17F:H53	3:D:619:PCW:H261	0.51	1.81	17	1
3:B:209:PCW:C44	4:B:215:17F:H45	0.51	2.35	19	1
3:A:411:PCW:C19	3:A:411:PCW:C15	0.50	2.89	16	15
3:A:413:PCW:C31	3:A:413:PCW:C35	0.50	2.89	11	9
3:D:604:PCW:C31	3:D:613:PCW:C8	0.50	2.88	1	1
3:D:623:PCW:H381	3:D:625:PCW:C17	0.50	2.36	1	2
3:D:627:PCW:H52	3:D:627:PCW:C31	0.50	2.35	1	1
3:B:208:PCW:C41	3:B:208:PCW:H372	0.50	2.36	1	2
3:A:410:PCW:H162	3:C:209:PCW:H411	0.50	1.83	2	1
3:D:606:PCW:C2	3:D:626:PCW:H372	0.50	2.36	2	6
3:A:402:PCW:C42	3:C:205:PCW:H152	0.50	2.36	5	2
1:D:532:ARG:O	1:D:536:LEU:HG	0.50	2.06	3	1
3:D:602:PCW:H182	3:D:624:PCW:H222	0.50	1.83	12	4
3:D:613:PCW:O4P	3:D:613:PCW:H63	0.50	2.06	3	4
3:B:204:PCW:H452	3:C:203:PCW:H39	0.50	1.82	3	1
3:B:208:PCW:C15	4:B:214:17F:H60	0.50	2.35	3	1
1:A:239:LEU:CD1	3:A:410:PCW:H442	0.50	2.36	4	1
3:D:618:PCW:H151	3:D:627:PCW:C15	0.50	2.36	5	1
2:C:84:ILE:CD1	2:C:118:CYS:HA	0.50	2.36	9	7
3:A:413:PCW:H351	3:A:413:PCW:O2	0.50	2.06	11	3
3:A:418:PCW:C5	3:D:626:PCW:O31	0.50	2.56	6	2
3:C:209:PCW:O31	3:C:209:PCW:H341	0.50	2.05	8	3
1:A:228:PHE:HE1	3:A:408:PCW:H462	0.50	1.66	7	1
3:A:413:PCW:H122	4:A:414:17F:C36	0.50	2.36	7	2
3:A:402:PCW:O11	3:A:402:PCW:O2	0.50	2.29	9	4
3:B:205:PCW:H73	3:B:208:PCW:C1	0.50	2.35	8	1
3:A:418:PCW:H452	3:D:625:PCW:H483	0.50	1.83	9	2
2:B:31:GLU:O	5:B:201:GDP:H3'	0.50	2.05	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:404:PCW:H61	4:A:415:17F:C33	0.50	2.36	10	1
3:C:204:PCW:H341	4:C:211:17F:O1	0.50	2.06	11	1
3:A:408:PCW:H371	3:C:207:PCW:H422	0.50	1.83	12	1
3:B:212:PCW:C4	3:B:212:PCW:O11	0.50	2.59	12	1
3:B:204:PCW:H382	3:B:212:PCW:H132	0.50	1.82	13	1
3:D:616:PCW:H331	3:C:212:PCW:H341	0.50	1.83	14	1
2:B:68:ARG:HA	2:B:71:TYR:CZ	0.50	2.41	14	2
3:D:606:PCW:C3	3:D:626:PCW:H411	0.50	2.36	19	1
3:D:621:PCW:H283	3:D:622:PCW:C7	0.50	2.36	20	1
3:D:613:PCW:O11	3:D:613:PCW:H2	0.50	2.06	14	9
3:B:211:PCW:H61	3:B:212:PCW:O31	0.50	2.06	2	1
3:C:207:PCW:O3	3:C:207:PCW:O31	0.50	2.29	6	14
4:A:414:17F:C29	3:C:203:PCW:H452	0.50	2.37	3	2
4:D:634:17F:O10	4:D:634:17F:O6	0.50	2.28	5	4
4:B:215:17F:C12	4:B:215:17F:H40	0.50	2.36	3	1
3:A:412:PCW:H481	3:C:206:PCW:C39	0.50	2.36	4	1
3:D:611:PCW:H62	3:D:623:PCW:H342	0.50	1.83	4	1
3:B:209:PCW:H372	3:B:209:PCW:C41	0.50	2.37	4	1
3:D:610:PCW:H483	3:B:212:PCW:H262	0.50	1.83	5	1
2:B:17:SER:O	2:B:21:ILE:HG12	0.50	2.07	8	8
3:A:403:PCW:H62	3:C:203:PCW:O3P	0.50	2.05	6	1
3:A:405:PCW:H382	4:D:628:17F:C30	0.50	2.36	6	2
3:C:208:PCW:H441	3:C:209:PCW:H362	0.50	1.83	6	1
4:C:210:17F:H58	4:C:210:17F:H10	0.50	1.82	6	1
3:A:413:PCW:O31	4:A:414:17F:H32	0.50	2.05	7	2
3:B:205:PCW:H441	3:B:206:PCW:C23	0.50	2.36	7	1
2:C:113:LEU:HB3	2:C:141:PHE:HD1	0.50	1.66	7	1
3:A:401:PCW:H31	3:B:209:PCW:H231	0.50	1.82	8	1
3:D:601:PCW:H461	3:D:607:PCW:H482	0.50	1.84	8	1
3:A:404:PCW:H452	3:B:209:PCW:H222	0.50	1.82	9	1
3:A:405:PCW:H162	3:A:405:PCW:C46	0.50	2.32	9	1
3:A:403:PCW:H283	3:A:413:PCW:H20	0.50	1.83	10	1
3:A:412:PCW:C43	3:C:208:PCW:H432	0.50	2.36	10	1
3:B:204:PCW:H19	3:B:205:PCW:H472	0.50	1.82	13	1
5:C:201:GDP:O2A	5:C:201:GDP:C3'	0.50	2.56	13	1
3:A:402:PCW:C31	3:A:402:PCW:O2P	0.50	2.59	15	2
3:A:401:PCW:H39	3:A:404:PCW:C23	0.50	2.29	19	2
3:B:213:PCW:H52	4:B:214:17F:H2	0.50	1.82	18	1
3:B:208:PCW:O11	3:B:208:PCW:C4	0.50	2.59	19	1
3:A:405:PCW:H73	3:D:601:PCW:C6	0.50	2.36	20	1
3:B:213:PCW:C1	4:B:217:17F:O1	0.50	2.55	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:607:PCW:O3P	3:D:607:PCW:O31	0.50	2.29	1	6
3:B:211:PCW:C3	4:B:217:17F:H56	0.50	2.36	1	1
3:A:412:PCW:H362	3:C:206:PCW:H431	0.50	1.84	2	1
3:D:604:PCW:H442	3:D:624:PCW:C44	0.50	2.36	2	1
3:B:206:PCW:C5	3:C:207:PCW:O2P	0.50	2.60	2	1
3:B:211:PCW:H11	3:B:211:PCW:O31	0.50	2.04	2	1
3:A:402:PCW:H381	3:C:205:PCW:H31	0.50	1.82	3	2
3:A:418:PCW:C32	3:D:625:PCW:H342	0.50	2.34	4	2
3:D:604:PCW:C41	3:D:604:PCW:H372	0.50	2.36	5	2
3:D:621:PCW:H451	4:D:634:17F:H67	0.50	1.81	5	3
3:D:627:PCW:H63	3:D:627:PCW:C31	0.50	2.36	5	1
3:A:401:PCW:H462	3:D:614:PCW:C26	0.50	2.34	6	1
3:A:420:PCW:H61	4:D:632:17F:C5	0.50	2.36	6	1
3:A:411:PCW:H472	3:A:411:PCW:H262	0.50	1.82	7	1
3:D:602:PCW:H142	3:D:622:PCW:C22	0.50	2.36	8	1
3:A:407:PCW:C17	3:B:208:PCW:C20	0.50	2.87	10	1
3:D:616:PCW:H441	3:D:627:PCW:C25	0.50	2.37	10	1
3:B:207:PCW:C48	4:B:217:17F:H41	0.50	2.36	11	1
3:B:207:PCW:H482	4:B:217:17F:H41	0.50	1.81	11	1
4:D:628:17F:C23	4:D:631:17F:H78	0.50	2.35	12	1
3:D:605:PCW:H63	3:D:605:PCW:H131	0.50	1.83	17	2
3:B:206:PCW:C40	3:C:212:PCW:H232	0.50	2.36	13	1
3:D:606:PCW:H12	3:D:626:PCW:H351	0.50	1.83	17	2
3:B:204:PCW:H232	3:C:204:PCW:H451	0.50	1.83	15	1
3:A:410:PCW:H212	3:C:209:PCW:H262	0.50	1.81	17	1
3:C:204:PCW:H251	4:C:211:17F:C31	0.50	2.35	17	1
3:B:210:PCW:C26	3:B:210:PCW:H40	0.50	2.37	18	1
3:D:602:PCW:C7	3:C:212:PCW:P	0.50	3.00	1	1
3:A:408:PCW:H362	3:C:204:PCW:H212	0.50	1.83	2	1
4:D:628:17F:O10	4:D:628:17F:O7	0.50	2.29	13	9
3:D:601:PCW:H232	4:D:628:17F:H48	0.50	1.83	3	2
3:D:613:PCW:H32	3:D:619:PCW:H32	0.50	1.81	3	1
3:C:204:PCW:C13	4:C:211:17F:H72	0.50	2.32	3	1
3:A:412:PCW:C40	3:C:208:PCW:H362	0.50	2.37	5	2
3:A:413:PCW:O2P	3:A:413:PCW:H51	0.50	2.06	5	2
3:B:211:PCW:H342	3:B:212:PCW:O1P	0.50	2.06	6	1
3:D:619:PCW:C48	4:C:210:17F:H74	0.50	2.36	8	1
3:B:204:PCW:H271	3:C:204:PCW:C42	0.50	2.37	8	1
3:B:205:PCW:H341	3:B:205:PCW:O31	0.50	2.06	8	1
3:B:204:PCW:H441	3:C:203:PCW:H40	0.50	1.82	9	1
3:D:620:PCW:H121	4:D:635:17F:C4	0.50	2.28	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:208:PCW:C28	4:B:216:17F:H50	0.50	2.36	11	1
3:D:614:PCW:O4P	3:D:614:PCW:H73	0.50	2.06	12	5
3:D:622:PCW:H352	3:D:627:PCW:C22	0.50	2.36	16	2
3:B:206:PCW:C35	3:B:212:PCW:H372	0.50	2.37	13	1
3:A:401:PCW:H371	3:B:209:PCW:H282	0.50	1.84	14	1
3:A:412:PCW:O31	3:A:412:PCW:H11	0.50	2.06	15	1
3:D:602:PCW:C27	3:D:610:PCW:H212	0.50	2.29	19	2
1:A:330:ARG:HH21	1:D:447:GLU:HB2	0.50	1.67	17	1
3:A:407:PCW:H172	3:C:205:PCW:H341	0.50	1.81	19	1
3:C:207:PCW:H51	4:C:211:17F:HN1	0.50	1.64	20	1
3:A:403:PCW:C17	3:C:203:PCW:H142	0.50	2.36	1	1
3:D:622:PCW:C12	4:D:630:17F:H32	0.50	2.34	1	1
4:D:634:17F:O7	4:D:634:17F:C17	0.50	2.59	7	10
5:B:201:GDP:H5'	5:B:201:GDP:O1B	0.50	2.07	18	2
3:D:611:PCW:O1P	3:D:623:PCW:H341	0.50	2.06	7	3
2:B:117:LYS:HE2	5:B:201:GDP:C4	0.50	2.41	18	4
3:C:207:PCW:H171	3:C:207:PCW:H431	0.50	1.82	2	1
3:A:419:PCW:C38	3:D:617:PCW:H472	0.50	2.36	3	1
3:D:602:PCW:C31	3:D:602:PCW:O3	0.50	2.60	4	3
3:B:208:PCW:C20	4:B:214:17F:H57	0.50	2.35	4	1
1:A:375:LEU:HD11	4:A:415:17F:H40	0.50	1.84	6	1
3:D:603:PCW:O1P	3:D:623:PCW:C8	0.50	2.59	15	5
4:D:633:17F:O10	4:D:633:17F:H4A	0.50	2.05	7	1
3:A:410:PCW:H241	4:D:633:17F:C30	0.50	2.33	8	2
3:B:203:PCW:H332	4:B:215:17F:H38	0.50	1.83	8	1
3:B:212:PCW:H482	3:C:212:PCW:H252	0.50	1.83	8	2
3:A:420:PCW:H73	4:D:632:17F:O2	0.50	2.05	10	2
3:A:413:PCW:H321	4:A:414:17F:C18	0.50	2.33	11	1
3:D:602:PCW:C28	3:D:610:PCW:H212	0.50	2.37	11	1
3:A:407:PCW:H211	3:C:205:PCW:C38	0.50	2.34	13	1
3:D:621:PCW:C41	4:D:634:17F:H58	0.50	2.37	14	1
3:D:621:PCW:H462	4:D:634:17F:H34	0.50	1.84	14	1
3:D:615:PCW:C48	3:B:208:PCW:H251	0.50	2.37	15	1
3:D:603:PCW:H242	4:B:217:17F:C42	0.50	2.35	16	1
4:D:630:17F:H53	4:B:214:17F:C40	0.50	2.36	16	1
3:A:407:PCW:H372	3:C:205:PCW:H141	0.50	1.83	17	1
4:D:630:17F:H36	4:D:630:17F:C36	0.50	2.33	18	1
2:C:168:GLU:HG3	3:C:205:PCW:H52	0.50	1.83	20	1
3:A:412:PCW:H39	3:C:206:PCW:H351	0.50	1.83	1	1
3:D:610:PCW:O2	3:D:610:PCW:O11	0.50	2.29	1	2
3:D:611:PCW:H472	3:D:611:PCW:H241	0.50	1.83	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:621:PCW:H281	4:D:633:17F:H30	0.50	1.83	18	2
3:D:623:PCW:H441	3:D:625:PCW:H261	0.50	1.83	13	2
3:B:203:PCW:C6	3:B:211:PCW:O31	0.50	2.60	1	2
3:D:620:PCW:P	3:D:621:PCW:C4	0.50	3.00	2	1
1:A:386:PHE:O	1:A:390:LEU:HG	0.50	2.07	4	3
3:A:410:PCW:H351	3:C:209:PCW:H152	0.50	1.82	18	3
3:A:407:PCW:H142	3:C:205:PCW:C14	0.50	2.37	5	1
2:B:147:LYS:HB2	5:B:201:GDP:N1	0.50	2.21	6	1
3:B:205:PCW:H361	3:B:206:PCW:C12	0.50	2.37	11	3
3:C:203:PCW:O2P	3:C:204:PCW:H62	0.50	2.06	6	2
3:B:210:PCW:H73	4:B:216:17F:P1	0.50	2.47	7	1
3:B:213:PCW:C40	4:B:217:17F:C32	0.50	2.90	7	1
3:D:604:PCW:C17	3:D:613:PCW:H342	0.50	2.36	8	4
3:B:204:PCW:C3	3:C:204:PCW:H352	0.50	2.37	8	2
3:B:213:PCW:C31	3:B:213:PCW:O1P	0.50	2.60	8	1
3:A:402:PCW:H162	3:A:409:PCW:H232	0.50	1.84	9	1
3:A:409:PCW:H39	3:A:409:PCW:C18	0.50	2.37	9	1
3:A:406:PCW:O3P	3:A:406:PCW:H63	0.50	2.06	10	1
3:A:410:PCW:C20	3:D:627:PCW:H481	0.50	2.30	10	1
3:A:419:PCW:C44	3:C:203:PCW:H281	0.50	2.37	11	1
3:D:602:PCW:O11	3:D:603:PCW:C7	0.50	2.59	11	1
3:C:204:PCW:C14	4:C:211:17F:H9	0.50	2.34	11	1
3:A:407:PCW:H441	3:D:601:PCW:H342	0.50	1.82	12	1
2:B:33:ASP:OD2	2:B:35:THR:HG22	0.50	2.07	12	1
3:B:209:PCW:C19	4:B:215:17F:O10	0.50	2.59	12	2
2:C:13:GLY:C	5:C:201:GDP:H5'	0.50	2.32	13	1
3:B:213:PCW:H171	3:B:213:PCW:H411	0.50	1.83	15	1
3:A:402:PCW:C19	3:A:409:PCW:H40	0.50	2.36	16	1
3:B:203:PCW:H222	4:C:210:17F:H57	0.50	1.82	16	1
2:C:32:TYR:HB3	5:C:201:GDP:H5''	0.50	1.84	19	2
3:A:404:PCW:H39	3:B:207:PCW:H451	0.50	1.82	1	1
3:B:206:PCW:C35	3:B:212:PCW:H39	0.50	2.37	1	1
3:D:611:PCW:C39	3:D:623:PCW:H442	0.50	2.36	2	2
3:B:203:PCW:H362	4:B:215:17F:H38	0.50	1.82	2	2
3:A:419:PCW:H40	3:D:616:PCW:H231	0.50	1.84	3	3
3:D:613:PCW:C25	4:C:210:17F:H43	0.50	2.37	3	1
3:D:622:PCW:H371	3:D:627:PCW:H20	0.50	1.84	4	1
3:C:204:PCW:O11	3:C:204:PCW:C2	0.50	2.52	11	6
3:A:407:PCW:H61	3:B:213:PCW:O2	0.50	2.07	17	3
3:B:204:PCW:H472	4:C:211:17F:H73	0.50	1.81	6	1
3:B:205:PCW:H461	3:B:206:PCW:C16	0.50	2.37	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:611:PCW:H20	3:D:611:PCW:C43	0.50	2.36	8	1
3:A:408:PCW:C34	3:C:204:PCW:H212	0.50	2.15	9	1
3:A:413:PCW:C35	4:A:414:17F:H58	0.50	2.36	9	1
3:B:208:PCW:H441	4:B:214:17F:C35	0.50	2.36	9	1
3:D:613:PCW:H251	4:C:210:17F:C25	0.50	2.37	19	2
3:C:208:PCW:H351	3:C:208:PCW:C11	0.50	2.36	10	2
3:A:409:PCW:C48	3:C:206:PCW:H272	0.50	2.36	12	1
2:B:135:ARG:HD3	2:C:151:GLY:HA3	0.50	1.82	12	1
3:C:207:PCW:C6	4:C:211:17F:O4	0.50	2.59	12	2
3:B:205:PCW:H261	3:C:204:PCW:C38	0.50	2.36	13	1
3:D:621:PCW:H483	4:D:634:17F:C1Z	0.50	2.36	14	1
3:B:211:PCW:H151	4:B:217:17F:H65	0.50	1.82	14	1
3:A:409:PCW:C11	3:C:206:PCW:H42	0.50	2.36	16	1
3:A:420:PCW:H341	3:D:617:PCW:O11	0.50	2.06	16	1
4:C:211:17F:H69	4:C:211:17F:H11A	0.50	1.84	18	1
3:A:406:PCW:H231	3:B:207:PCW:H19	0.50	1.84	19	1
1:A:320:LEU:HA	1:A:323:TYR:HB2	0.50	1.83	13	5
3:A:417:PCW:C35	3:D:612:PCW:H131	0.50	2.37	19	4
3:D:608:PCW:C27	3:D:615:PCW:H411	0.50	2.36	16	2
3:C:204:PCW:H251	4:C:211:17F:C33	0.50	2.35	1	1
3:D:603:PCW:O2P	3:D:623:PCW:C8	0.50	2.60	2	1
3:B:209:PCW:P	3:B:209:PCW:C3	0.50	2.99	2	2
4:C:211:17F:O10	4:C:211:17F:C4	0.50	2.57	2	1
4:A:414:17F:H39	4:A:414:17F:C1X	0.50	2.36	3	2
4:A:414:17F:H29	4:A:414:17F:C23	0.50	2.37	3	1
1:D:463:TRP:HD1	4:D:631:17F:H70	0.50	1.66	3	1
3:D:604:PCW:C40	3:D:619:PCW:H141	0.50	2.37	3	3
3:B:210:PCW:H281	3:B:210:PCW:H471	0.50	1.82	3	1
3:B:210:PCW:H471	3:B:210:PCW:C28	0.50	2.37	3	1
3:D:608:PCW:O31	3:D:608:PCW:O3	0.50	2.29	18	6
4:B:214:17F:C3	3:C:205:PCW:H61	0.50	2.37	4	2
3:C:207:PCW:H382	3:C:207:PCW:C15	0.50	2.37	4	1
3:C:203:PCW:O31	3:C:203:PCW:H362	0.50	2.06	13	3
3:A:417:PCW:H161	3:D:617:PCW:C48	0.50	2.36	9	2
3:A:402:PCW:H181	3:A:409:PCW:H39	0.50	1.83	12	1
3:B:205:PCW:O2	3:B:208:PCW:C32	0.50	2.54	12	1
3:A:407:PCW:C21	3:C:205:PCW:H411	0.50	2.37	13	1
4:B:216:17F:N1	4:B:216:17F:C4	0.50	2.75	13	1
4:D:629:17F:H76	3:C:212:PCW:C44	0.50	2.37	14	1
3:D:616:PCW:C28	3:C:204:PCW:H262	0.50	2.36	15	1
3:A:410:PCW:H242	3:C:207:PCW:H251	0.50	1.83	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:210:PCW:H73	3:B:210:PCW:C11	0.50	2.37	17	1
3:B:210:PCW:C45	4:B:215:17F:H72	0.50	2.34	17	1
3:D:622:PCW:C17	4:D:630:17F:H32	0.50	2.36	18	1
3:C:208:PCW:H181	3:C:208:PCW:C46	0.50	2.37	18	1
3:A:403:PCW:O11	3:A:403:PCW:H41	0.50	2.06	20	1
3:A:401:PCW:H481	3:D:619:PCW:C17	0.50	2.37	1	1
3:A:406:PCW:H272	3:B:207:PCW:C19	0.50	2.37	1	1
3:D:601:PCW:C46	4:D:628:17F:C36	0.50	2.89	1	1
3:D:610:PCW:H421	3:D:610:PCW:H262	0.50	1.83	1	3
2:B:84:ILE:CD1	2:B:118:CYS:HA	0.50	2.37	2	6
3:B:206:PCW:H342	3:C:204:PCW:C39	0.50	2.37	2	1
3:C:208:PCW:O31	3:C:209:PCW:H82	0.50	2.07	10	4
4:A:415:17F:H72	3:B:203:PCW:C25	0.50	2.31	3	1
3:C:208:PCW:O2P	3:C:209:PCW:C6	0.50	2.60	14	3
1:A:217:LEU:HD13	3:A:408:PCW:H231	0.50	1.83	4	1
3:A:401:PCW:H51	3:A:404:PCW:C1	0.50	2.37	4	1
3:A:410:PCW:H481	3:C:209:PCW:H241	0.50	1.83	4	1
3:A:416:PCW:H451	3:D:617:PCW:H231	0.50	1.84	5	1
3:A:416:PCW:H121	3:D:617:PCW:C33	0.50	2.36	10	3
3:B:213:PCW:O2P	4:B:214:17F:P1	0.50	2.70	5	1
4:D:629:17F:H18A	4:D:629:17F:O8	0.50	2.05	19	2
3:B:209:PCW:H332	3:B:209:PCW:C12	0.50	2.37	6	1
3:A:406:PCW:C39	3:A:406:PCW:C12	0.50	2.87	7	1
3:D:615:PCW:C8	4:D:635:17F:O4	0.50	2.58	9	2
3:A:405:PCW:H283	1:D:451:LYS:HB3	0.50	1.83	8	1
3:B:212:PCW:P	3:B:212:PCW:O31	0.50	2.70	16	2
3:C:204:PCW:C15	4:C:211:17F:H63	0.50	2.37	11	1
3:B:207:PCW:H182	3:B:210:PCW:C14	0.50	2.37	12	1
3:A:403:PCW:H161	3:C:203:PCW:C32	0.50	2.37	13	1
3:D:613:PCW:H251	4:C:210:17F:H50	0.50	1.83	14	1
3:B:207:PCW:C39	4:B:217:17F:H8	0.50	2.36	14	1
3:B:205:PCW:C44	3:B:206:PCW:H211	0.50	2.37	16	1
3:B:205:PCW:C5	3:B:208:PCW:O31	0.50	2.60	18	2
3:B:210:PCW:H452	3:B:213:PCW:H262	0.50	1.84	18	1
3:B:208:PCW:H31	3:B:208:PCW:O1P	0.50	2.07	19	1
3:D:624:PCW:O1P	3:D:624:PCW:H51	0.50	2.07	20	1
3:A:403:PCW:H321	3:C:204:PCW:H51	0.49	1.83	1	1
3:D:606:PCW:H462	3:D:625:PCW:C48	0.49	2.37	1	1
3:D:613:PCW:H142	3:D:619:PCW:C39	0.49	2.37	1	2
3:D:625:PCW:O11	3:D:625:PCW:C2	0.49	2.52	1	8
4:A:414:17F:O9	4:A:414:17F:O8	0.49	2.29	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:618:PCW:H63	3:D:622:PCW:O1P	0.49	2.07	2	1
3:B:203:PCW:H261	4:C:210:17F:H73	0.49	1.81	2	1
3:D:615:PCW:H142	4:D:635:17F:H8	0.49	1.84	18	2
3:A:404:PCW:H52	3:A:404:PCW:H321	0.49	1.83	4	1
3:B:208:PCW:H121	4:B:214:17F:O10	0.49	2.07	12	2
4:B:216:17F:H55	3:C:205:PCW:H262	0.49	1.84	4	1
3:A:404:PCW:H73	3:A:404:PCW:C2	0.49	2.36	16	4
3:D:611:PCW:O31	3:D:611:PCW:O3	0.49	2.30	9	6
3:B:204:PCW:C37	3:C:204:PCW:O1P	0.49	2.60	8	2
3:A:411:PCW:C16	3:B:209:PCW:H281	0.49	2.35	8	1
3:D:615:PCW:C47	3:C:205:PCW:H20	0.49	2.24	8	1
3:B:208:PCW:C37	4:B:214:17F:H63	0.49	2.36	9	1
2:C:114:VAL:HG12	2:C:142:ILE:HB	0.49	1.84	9	1
1:A:239:LEU:HD22	3:A:410:PCW:H441	0.49	1.84	10	1
3:A:403:PCW:H212	3:A:403:PCW:C41	0.49	2.37	12	1
3:D:607:PCW:H222	4:D:631:17F:C1Z	0.49	2.30	16	1
3:A:410:PCW:H261	3:C:208:PCW:H242	0.49	1.83	17	1
3:D:625:PCW:O4P	3:D:625:PCW:O31	0.49	2.30	17	1
4:D:629:17F:C42	3:C:212:PCW:H462	0.49	2.33	18	1
3:B:206:PCW:H52	3:C:207:PCW:H12	0.49	1.78	18	1
3:D:605:PCW:C42	3:D:608:PCW:H31	0.49	2.28	20	1
3:B:203:PCW:C28	4:B:215:17F:H55	0.49	2.36	20	1
3:A:402:PCW:C16	3:A:409:PCW:H251	0.49	2.26	1	1
3:A:406:PCW:C1	3:A:411:PCW:H82	0.49	2.36	1	1
3:A:419:PCW:C3	3:D:617:PCW:H411	0.49	2.37	9	4
1:D:483:GLU:O	1:D:487:GLN:HG2	0.49	2.07	1	1
3:B:209:PCW:H231	3:B:209:PCW:C36	0.49	2.37	1	1
3:C:204:PCW:C25	4:C:211:17F:H60	0.49	2.35	1	2
3:A:418:PCW:H31	3:D:614:PCW:H122	0.49	1.82	2	1
3:D:605:PCW:C6	3:D:605:PCW:O11	0.49	2.60	6	4
3:D:614:PCW:O11	3:D:614:PCW:O2	0.49	2.30	2	5
4:D:629:17F:H46	4:D:630:17F:C40	0.49	2.35	2	1
4:D:628:17F:H36	4:D:631:17F:C41	0.49	2.37	8	3
1:A:372:ARG:O	1:A:376:LEU:HG	0.49	2.07	4	6
3:A:402:PCW:H321	3:C:206:PCW:H31	0.49	1.84	4	2
3:D:609:PCW:H152	4:D:633:17F:C34	0.49	2.38	4	1
3:D:627:PCW:C20	4:D:633:17F:H38	0.49	2.37	4	2
3:B:211:PCW:C22	3:B:211:PCW:C18	0.49	2.89	4	1
3:C:204:PCW:H142	4:C:211:17F:C6	0.49	2.36	4	1
1:A:247:LEU:HA	1:A:250:VAL:HG12	0.49	1.84	5	1
3:B:208:PCW:C39	4:B:214:17F:H76	0.49	2.37	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:212:PCW:O11	3:B:212:PCW:C2	0.49	2.52	6	2
3:C:204:PCW:H19	4:C:211:17F:O10	0.49	2.07	7	1
3:D:609:PCW:O11	3:D:609:PCW:H2	0.49	2.06	8	1
3:A:406:PCW:H271	3:B:207:PCW:H171	0.49	1.83	9	1
3:A:413:PCW:H282	3:C:203:PCW:C43	0.49	2.37	9	1
1:A:367:ALA:O	1:A:371:LEU:HG	0.49	2.07	11	1
3:D:611:PCW:H221	3:D:611:PCW:C43	0.49	2.30	11	1
3:B:206:PCW:H472	3:C:212:PCW:H232	0.49	1.82	11	1
3:C:203:PCW:O1P	3:C:204:PCW:H52	0.49	2.07	11	1
3:A:409:PCW:H2	3:C:206:PCW:H331	0.49	1.83	12	1
3:D:611:PCW:C23	3:D:619:PCW:H442	0.49	2.38	12	1
3:C:207:PCW:H252	3:C:208:PCW:C23	0.49	2.37	14	1
3:B:209:PCW:C6	4:B:215:17F:H8	0.49	2.36	17	1
3:A:403:PCW:C47	3:C:203:PCW:H271	0.49	2.37	18	1
2:B:97:ARG:HG3	2:B:111:MET:HE1	0.49	1.82	18	1
4:A:415:17F:H64	4:A:415:17F:H59	0.49	1.82	19	1
3:D:603:PCW:H372	3:D:603:PCW:C41	0.49	2.36	20	1
4:D:629:17F:H43	4:D:630:17F:H35	0.49	1.83	20	1
3:A:407:PCW:C7	3:B:213:PCW:O2P	0.49	2.60	1	2
3:A:407:PCW:C7	3:A:407:PCW:O4P	0.49	2.59	17	5
5:B:201:GDP:O5'	5:B:201:GDP:C2'	0.49	2.60	8	6
3:B:203:PCW:C5	3:B:211:PCW:O31	0.49	2.60	1	1
3:A:410:PCW:O2P	3:A:410:PCW:H31	0.49	2.06	3	1
2:B:117:LYS:HE2	5:B:201:GDP:C5	0.49	2.43	3	1
4:D:634:17F:C33	4:D:635:17F:H74	0.49	2.38	19	3
3:C:208:PCW:H161	3:C:209:PCW:H382	0.49	1.84	5	3
3:A:406:PCW:O31	3:A:406:PCW:O3	0.49	2.30	9	6
3:A:417:PCW:C37	3:D:612:PCW:H131	0.49	2.37	6	1
3:A:407:PCW:C5	4:B:216:17F:H10A	0.49	2.37	12	3
4:A:414:17F:H44	3:C:203:PCW:H452	0.49	1.84	8	1
3:D:616:PCW:P	3:D:616:PCW:O2	0.49	2.71	8	1
3:B:205:PCW:H451	3:C:208:PCW:H172	0.49	1.84	8	1
3:A:416:PCW:O11	3:D:617:PCW:H341	0.49	2.07	16	2
3:B:207:PCW:H82	4:B:216:17F:O6	0.49	2.06	9	1
4:B:215:17F:H12	4:B:215:17F:C24	0.49	2.36	15	2
4:D:629:17F:H49	3:B:212:PCW:C47	0.49	2.37	11	1
3:A:406:PCW:C8	4:B:215:17F:O1	0.49	2.61	13	1
3:A:411:PCW:H281	3:A:411:PCW:C48	0.49	2.38	13	1
3:D:620:PCW:H141	4:D:635:17F:H18	0.49	1.83	14	1
3:A:405:PCW:C15	3:A:405:PCW:H471	0.49	2.37	20	2
3:D:611:PCW:O11	3:D:619:PCW:H82	0.49	2.06	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:402:PCW:C20	3:A:409:PCW:H40	0.49	2.37	16	1
3:A:411:PCW:H431	3:A:418:PCW:C28	0.49	2.37	16	1
3:A:416:PCW:C20	3:A:419:PCW:H411	0.49	2.36	16	1
3:B:204:PCW:O31	3:B:212:PCW:C6	0.49	2.49	17	1
3:D:609:PCW:O4P	4:D:633:17F:O1	0.49	2.29	18	1
3:A:417:PCW:C38	3:D:612:PCW:H432	0.49	2.37	19	1
3:A:402:PCW:H331	3:C:206:PCW:O2P	0.49	2.06	20	1
3:A:403:PCW:H61	4:A:414:17F:O1	0.49	2.06	20	1
3:C:204:PCW:C35	4:C:211:17F:O8	0.49	2.57	20	1
3:A:407:PCW:C14	3:C:205:PCW:H131	0.49	2.33	1	1
3:D:605:PCW:C17	3:D:605:PCW:C21	0.49	2.78	7	5
4:D:628:17F:H78	3:C:205:PCW:H261	0.49	1.82	1	1
2:B:19:LEU:HD23	2:B:146:ALA:HB2	0.49	1.83	1	2
3:C:208:PCW:O2P	3:C:209:PCW:C8	0.49	2.60	10	5
3:A:401:PCW:C45	3:D:611:PCW:H271	0.49	2.36	18	3
3:D:607:PCW:H282	4:D:631:17F:H65	0.49	1.83	5	1
3:C:208:PCW:H141	3:C:209:PCW:H362	0.49	1.84	11	2
3:A:401:PCW:O1P	3:A:401:PCW:H52	0.49	2.07	6	1
3:B:211:PCW:H32	4:B:217:17F:C31	0.49	2.37	6	1
3:A:404:PCW:H162	4:A:415:17F:H31	0.49	1.83	7	1
3:A:406:PCW:H241	3:B:210:PCW:C11	0.49	2.37	8	1
3:A:405:PCW:H462	3:A:405:PCW:C15	0.49	2.37	9	1
3:D:616:PCW:H462	3:D:618:PCW:H472	0.49	1.84	9	1
3:A:401:PCW:H342	3:B:209:PCW:H452	0.49	1.83	11	1
3:A:417:PCW:C38	3:D:612:PCW:H231	0.49	2.35	11	1
3:D:602:PCW:C14	3:D:624:PCW:H211	0.49	2.37	11	1
4:C:210:17F:H59	4:C:210:17F:C10	0.49	2.37	11	2
3:A:412:PCW:H462	3:C:208:PCW:C47	0.49	2.37	12	1
4:D:630:17F:H53	3:B:206:PCW:H19	0.49	1.82	15	1
3:C:208:PCW:H412	3:C:208:PCW:H142	0.49	1.83	15	1
3:A:406:PCW:H182	3:B:210:PCW:H352	0.49	1.83	17	1
3:A:407:PCW:H412	4:B:216:17F:H73	0.49	1.84	18	1
3:B:209:PCW:H221	3:B:209:PCW:H361	0.49	1.85	18	1
3:B:213:PCW:H483	4:B:217:17F:H48	0.49	1.83	20	1
4:B:214:17F:O7	4:B:214:17F:C17	0.49	2.60	12	7
3:A:406:PCW:H62	3:A:406:PCW:O4P	0.49	2.07	3	2
3:B:208:PCW:H352	4:B:214:17F:H20	0.49	1.82	8	3
2:C:72:MET:HB2	2:C:103:VAL:HG11	0.49	1.82	15	2
3:A:403:PCW:H161	3:C:203:PCW:C33	0.49	2.36	4	1
3:A:409:PCW:H82	3:C:206:PCW:H362	0.49	1.82	17	2
3:A:416:PCW:H411	3:A:416:PCW:C37	0.49	2.31	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:420:PCW:O3P	3:D:617:PCW:C4	0.49	2.53	5	1
1:D:525:LEU:HD23	1:D:528:ARG:HD2	0.49	1.85	5	1
3:D:618:PCW:H352	3:D:627:PCW:H342	0.49	1.85	5	1
2:C:14:VAL:HG23	2:C:16:LYS:HG3	0.49	1.84	5	2
3:B:213:PCW:H40	4:B:217:17F:H67	0.49	1.84	6	2
1:A:335:LEU:O	1:A:339:LYS:HB2	0.49	2.06	20	3
3:A:419:PCW:C12	3:D:617:PCW:H442	0.49	2.36	8	1
3:D:602:PCW:H142	3:D:622:PCW:C23	0.49	2.36	8	1
3:B:204:PCW:H372	3:C:204:PCW:P	0.49	2.47	8	1
3:B:208:PCW:H31	3:B:208:PCW:O2P	0.49	2.08	10	2
3:C:207:PCW:H41	3:C:207:PCW:C32	0.49	2.33	9	1
3:A:406:PCW:H11	3:A:411:PCW:C8	0.49	2.37	18	2
3:D:604:PCW:C31	3:D:613:PCW:C6	0.49	2.90	10	1
3:A:404:PCW:H332	3:B:203:PCW:H172	0.49	1.85	17	2
3:A:413:PCW:C24	4:A:414:17F:H61	0.49	2.37	12	1
3:D:625:PCW:H12	3:D:626:PCW:C3	0.49	2.35	12	1
1:D:536:LEU:O	1:D:540:GLY:HA3	0.49	2.06	13	1
3:D:601:PCW:H39	3:D:601:PCW:C19	0.49	2.37	13	1
3:B:203:PCW:C7	4:B:217:17F:O5	0.49	2.60	19	1
3:B:208:PCW:C28	3:B:208:PCW:C24	0.49	2.91	19	1
3:B:203:PCW:O11	3:B:211:PCW:H372	0.49	2.06	1	1
3:A:411:PCW:C46	3:A:418:PCW:H221	0.49	2.34	2	1
1:D:463:TRP:CD1	4:D:631:17F:H70	0.49	2.42	3	1
1:D:533:LEU:HD23	1:D:536:LEU:HD12	0.49	1.83	3	1
3:D:608:PCW:O31	3:D:608:PCW:C11	0.49	2.61	10	4
3:B:211:PCW:C43	3:B:212:PCW:C3	0.49	2.91	4	1
2:C:97:ARG:HG3	2:C:111:MET:HE1	0.49	1.85	5	1
3:A:407:PCW:H242	3:C:205:PCW:C38	0.49	2.38	13	2
4:A:415:17F:C41	4:C:210:17F:H56	0.49	2.38	6	1
3:D:603:PCW:C31	3:D:605:PCW:H82	0.49	2.37	13	3
3:D:604:PCW:C39	3:D:619:PCW:H121	0.49	2.37	6	2
3:D:607:PCW:C21	4:D:631:17F:H29	0.49	2.36	6	2
3:A:404:PCW:H281	4:A:415:17F:C38	0.49	2.38	11	2
3:A:411:PCW:H261	3:A:418:PCW:H281	0.49	1.84	7	1
3:D:601:PCW:H422	4:D:628:17F:H41	0.49	1.83	7	2
3:D:618:PCW:C46	3:C:207:PCW:H231	0.49	2.25	8	1
1:D:414:LYS:HA	1:D:417:GLU:HG3	0.49	1.83	10	1
3:D:615:PCW:H161	4:D:635:17F:C12	0.49	2.36	12	1
3:B:206:PCW:H331	3:B:212:PCW:H352	0.49	1.84	13	1
2:C:18:ALA:HB3	5:C:201:GDP:C8	0.49	2.43	13	1
4:C:210:17F:H41	4:C:210:17F:H36	0.49	1.84	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:402:PCW:C40	3:A:409:PCW:H272	0.49	2.31	14	1
4:A:414:17F:C30	3:C:203:PCW:H452	0.49	2.37	14	1
3:A:407:PCW:H82	3:B:213:PCW:O2	0.49	2.07	15	1
3:A:409:PCW:C11	3:C:206:PCW:C4	0.49	2.90	16	1
3:D:607:PCW:H252	4:D:631:17F:H33	0.49	1.85	16	1
3:B:208:PCW:C6	3:B:208:PCW:C32	0.49	2.91	17	1
3:A:403:PCW:H452	3:C:203:PCW:H272	0.49	1.85	18	1
3:B:209:PCW:H31	3:B:209:PCW:O4P	0.49	2.07	18	1
3:D:608:PCW:C46	3:C:205:PCW:H472	0.49	2.34	19	1
3:D:602:PCW:H241	3:D:610:PCW:C14	0.49	2.36	1	1
3:B:213:PCW:O11	3:B:213:PCW:O2	0.49	2.30	1	3
4:C:210:17F:O10	4:C:210:17F:O7	0.49	2.31	2	10
3:A:412:PCW:O3	3:A:412:PCW:C31	0.49	2.61	13	12
1:D:496:LEU:O	1:D:500:GLY:HA3	0.49	2.08	2	4
3:A:406:PCW:H122	3:B:210:PCW:H352	0.49	1.85	3	1
3:A:411:PCW:C14	3:A:411:PCW:C18	0.49	2.90	4	6
3:A:413:PCW:H251	3:C:203:PCW:H432	0.49	1.84	4	1
3:D:611:PCW:H483	4:B:215:17F:H54	0.49	1.83	4	1
3:B:208:PCW:H121	4:B:214:17F:C17	0.49	2.38	4	1
3:B:211:PCW:C17	3:B:211:PCW:C22	0.49	2.83	4	1
3:C:206:PCW:C38	3:C:206:PCW:H172	0.49	2.38	10	2
3:C:208:PCW:H272	3:C:209:PCW:H482	0.49	1.85	4	1
3:A:420:PCW:O11	3:A:420:PCW:C5	0.49	2.61	5	1
3:B:211:PCW:O31	3:B:211:PCW:H11	0.49	2.07	6	1
3:A:402:PCW:C31	3:A:402:PCW:H42	0.49	2.37	7	1
4:B:216:17F:C30	3:C:205:PCW:H251	0.49	2.37	7	1
3:A:402:PCW:H431	3:A:407:PCW:C25	0.49	2.37	8	1
3:A:411:PCW:H161	3:B:209:PCW:C28	0.49	2.35	8	1
3:D:613:PCW:H272	4:C:210:17F:H50	0.49	1.85	9	2
4:D:630:17F:C12	4:D:630:17F:H59	0.49	2.37	20	2
3:A:412:PCW:H451	3:C:208:PCW:C19	0.49	2.30	11	1
3:A:420:PCW:H19	4:D:632:17F:H20	0.49	1.83	11	1
3:B:203:PCW:H182	4:B:215:17F:H38	0.49	1.83	13	2
3:C:204:PCW:C35	4:C:211:17F:O7	0.49	2.59	15	2
3:A:407:PCW:C6	3:B:213:PCW:O2P	0.49	2.61	14	1
3:A:407:PCW:O3P	4:B:216:17F:H9A	0.49	2.07	14	1
3:D:603:PCW:O1P	3:D:603:PCW:H31	0.49	2.08	14	1
3:D:613:PCW:H121	3:D:619:PCW:C38	0.49	2.26	14	2
3:D:618:PCW:H481	3:C:204:PCW:C47	0.49	2.37	15	1
3:A:410:PCW:C18	3:C:209:PCW:H262	0.49	2.36	16	1
4:D:630:17F:C30	4:B:214:17F:H73	0.49	2.36	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:627:PCW:H282	4:D:633:17F:H51	0.49	1.84	18	2
3:B:210:PCW:H271	3:B:210:PCW:C42	0.49	2.34	18	2
4:B:215:17F:H41	4:B:215:17F:C2X	0.49	2.38	18	1
3:C:204:PCW:H161	4:C:211:17F:H19A	0.49	1.84	19	1
3:A:407:PCW:H372	3:C:205:PCW:C12	0.49	2.38	20	1
3:A:410:PCW:C6	3:A:410:PCW:O2	0.49	2.61	1	2
3:D:616:PCW:H431	3:B:206:PCW:C45	0.49	2.37	1	1
3:D:621:PCW:C20	4:D:633:17F:O10	0.49	2.60	9	5
3:D:623:PCW:C28	3:D:624:PCW:H462	0.49	2.37	1	4
3:A:412:PCW:C37	3:C:206:PCW:H40	0.49	2.37	2	2
3:B:213:PCW:C8	3:B:213:PCW:O4P	0.49	2.61	10	11
3:D:626:PCW:C31	3:D:626:PCW:O3	0.49	2.61	17	11
3:B:210:PCW:O11	3:B:210:PCW:C7	0.49	2.60	17	2
2:C:79:LEU:HD13	2:C:159:LEU:HD22	0.49	1.85	3	1
3:C:209:PCW:H132	3:C:209:PCW:O31	0.49	2.08	3	6
3:A:410:PCW:C5	3:C:209:PCW:H32	0.49	2.38	4	2
1:D:451:LYS:O	1:D:455:TYR:HB2	0.49	2.07	17	4
3:D:608:PCW:C38	3:D:615:PCW:H421	0.49	2.38	4	1
3:D:622:PCW:C42	3:B:206:PCW:H272	0.49	2.37	4	1
4:D:629:17F:H10	4:D:634:17F:H47	0.49	1.84	6	1
4:D:630:17F:H65	4:D:630:17F:C2X	0.49	2.36	6	1
3:A:401:PCW:C7	3:B:209:PCW:H2	0.49	2.38	7	1
3:D:601:PCW:H462	4:D:628:17F:H64	0.49	1.84	8	1
3:B:204:PCW:C45	3:C:203:PCW:H132	0.49	2.38	8	2
3:C:206:PCW:H132	3:C:206:PCW:H342	0.49	1.85	9	2
3:D:621:PCW:C23	3:D:622:PCW:H82	0.49	2.31	10	1
3:A:409:PCW:C16	3:A:409:PCW:H231	0.49	2.38	11	1
3:D:604:PCW:H322	3:D:611:PCW:O3P	0.49	2.08	12	2
3:D:616:PCW:H181	3:D:616:PCW:C22	0.49	2.37	12	1
3:B:206:PCW:C48	3:C:212:PCW:C40	0.49	2.91	12	1
3:B:213:PCW:H73	3:B:213:PCW:O4P	0.49	2.08	12	1
3:A:403:PCW:H171	3:C:203:PCW:O3	0.49	2.08	13	1
4:D:631:17F:H11A	4:D:631:17F:H32	0.49	1.83	16	1
3:B:206:PCW:H422	4:C:211:17F:H49	0.49	1.83	16	1
3:D:621:PCW:C13	4:D:634:17F:H6	0.49	2.37	17	1
2:C:166:HIS:HA	2:C:169:LYS:HD2	0.49	1.85	17	1
3:B:208:PCW:H411	4:B:214:17F:H10	0.49	1.84	18	1
3:D:624:PCW:H481	4:C:210:17F:C28	0.49	2.36	19	1
3:C:208:PCW:C12	3:C:208:PCW:H351	0.49	2.38	19	1
4:C:211:17F:O10	4:C:211:17F:O7	0.49	2.31	19	1
4:B:215:17F:O8	4:B:215:17F:C5	0.49	2.59	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:412:PCW:H212	3:A:412:PCW:C17	0.49	2.19	1	1
3:D:604:PCW:P	3:D:613:PCW:C5	0.49	3.01	4	3
3:D:613:PCW:H63	3:D:624:PCW:C8	0.49	2.38	2	2
3:A:407:PCW:O31	3:A:407:PCW:P	0.49	2.71	4	1
2:B:32:TYR:CD1	5:B:201:GDP:H3'	0.49	2.42	4	2
3:A:406:PCW:C41	3:B:210:PCW:H40	0.49	2.35	6	2
3:D:618:PCW:O1P	3:D:627:PCW:H61	0.49	2.07	11	2
3:A:405:PCW:O3	3:A:405:PCW:O31	0.49	2.31	16	2
3:D:615:PCW:H63	4:D:635:17F:C3	0.49	2.38	8	2
2:C:61:GLN:HA	2:C:96:TYR:OH	0.49	2.06	20	3
3:C:205:PCW:C37	3:C:206:PCW:H121	0.49	2.33	8	1
3:D:602:PCW:H32	3:D:603:PCW:C8	0.49	2.38	9	1
3:D:609:PCW:O4P	4:D:633:17F:H6	0.49	2.07	9	1
1:D:525:LEU:O	1:D:529:LEU:HG	0.49	2.08	10	1
2:C:39:SER:HB3	2:C:56:LEU:HD12	0.49	1.82	10	1
3:D:605:PCW:H372	4:D:629:17F:H8A	0.49	1.85	18	2
3:A:405:PCW:H40	3:D:601:PCW:C25	0.49	2.35	14	1
3:A:413:PCW:H462	3:D:613:PCW:H252	0.49	1.85	14	1
3:B:209:PCW:C11	3:B:209:PCW:H51	0.49	2.38	14	1
3:A:406:PCW:H212	3:B:210:PCW:H321	0.49	1.84	20	2
3:A:402:PCW:H412	3:C:205:PCW:C35	0.49	2.38	19	1
3:D:616:PCW:H40	3:D:618:PCW:H162	0.49	1.84	19	1
3:A:403:PCW:H121	3:A:403:PCW:H62	0.49	1.83	20	1
3:A:404:PCW:H182	4:A:415:17F:H57	0.49	1.85	20	1
4:D:630:17F:H59	4:D:630:17F:H29	0.49	1.85	20	1
3:B:205:PCW:C2	3:B:211:PCW:H62	0.49	2.38	20	1
3:A:403:PCW:H73	3:A:403:PCW:C12	0.49	2.38	1	1
3:D:612:PCW:H321	3:D:618:PCW:C12	0.49	2.38	1	1
3:D:623:PCW:O3	3:D:624:PCW:H332	0.49	2.08	1	1
4:A:414:17F:H52	3:C:203:PCW:C45	0.49	2.38	3	1
3:D:602:PCW:H172	3:D:602:PCW:C21	0.49	2.38	3	3
3:A:416:PCW:H451	3:D:617:PCW:H251	0.49	1.83	4	1
3:D:602:PCW:C16	3:D:624:PCW:H211	0.49	2.38	10	4
3:B:204:PCW:H20	3:B:205:PCW:C48	0.49	2.30	4	1
3:A:407:PCW:C14	3:C:205:PCW:H151	0.49	2.37	5	1
3:B:213:PCW:C40	4:B:217:17F:H67	0.49	2.38	6	1
3:B:211:PCW:H152	4:B:217:17F:C2X	0.49	2.38	7	1
4:D:633:17F:H53	3:C:209:PCW:C43	0.49	2.38	8	1
3:A:406:PCW:H271	3:B:207:PCW:H19	0.49	1.83	10	1
3:D:623:PCW:H282	3:D:624:PCW:H431	0.49	1.85	10	1
3:A:404:PCW:H31	3:B:209:PCW:C32	0.49	2.36	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:601:PCW:C48	4:D:628:17F:C36	0.49	2.91	12	1
3:A:406:PCW:H242	3:B:210:PCW:C11	0.49	2.38	16	1
3:D:607:PCW:C22	4:D:631:17F:H20	0.49	2.38	16	1
3:A:410:PCW:O3	3:C:209:PCW:H121	0.49	2.07	18	1
3:D:603:PCW:C32	3:D:605:PCW:H122	0.49	2.36	18	1
3:C:208:PCW:C24	3:C:209:PCW:H451	0.49	2.37	19	1
3:A:406:PCW:C21	3:B:210:PCW:H321	0.49	2.38	20	1
3:A:411:PCW:C8	3:A:411:PCW:O4P	0.48	2.60	19	6
3:D:615:PCW:C26	4:D:635:17F:H45	0.48	2.35	1	1
3:A:410:PCW:H171	3:A:410:PCW:C23	0.48	2.37	2	1
3:B:203:PCW:H362	4:B:215:17F:C21	0.48	2.37	2	1
3:B:206:PCW:C23	3:C:208:PCW:H282	0.48	2.37	3	3
3:C:208:PCW:C13	3:C:209:PCW:H322	0.48	2.38	11	2
3:B:207:PCW:C23	3:B:210:PCW:H261	0.48	2.38	4	1
3:B:211:PCW:O4P	3:B:211:PCW:H62	0.48	2.08	6	3
3:A:412:PCW:C31	3:A:412:PCW:O3	0.48	2.61	17	2
3:A:418:PCW:H63	3:D:626:PCW:O31	0.48	2.08	19	2
3:B:206:PCW:C40	3:C:212:PCW:C25	0.48	2.90	6	1
3:B:210:PCW:C16	4:B:216:17F:H11A	0.48	2.38	6	1
3:C:212:PCW:O31	3:C:212:PCW:H52	0.48	2.08	13	2
3:B:204:PCW:H122	3:C:207:PCW:H12	0.48	1.84	8	1
3:C:204:PCW:H251	4:C:211:17F:C1Y	0.48	2.33	9	1
3:B:204:PCW:C31	3:B:206:PCW:H331	0.48	2.37	11	1
3:A:403:PCW:H382	3:A:403:PCW:C11	0.48	2.38	15	1
3:D:606:PCW:C43	3:D:625:PCW:H471	0.48	2.30	18	2
2:B:12:ASP:OD2	5:B:201:GDP:O3B	0.48	2.31	18	1
3:A:405:PCW:H421	3:A:405:PCW:H381	0.48	1.84	19	1
3:B:211:PCW:H232	4:B:217:17F:H47	0.48	1.83	20	1
4:C:211:17F:H4	4:C:211:17F:O10	0.48	2.07	20	1
3:D:613:PCW:H471	3:D:619:PCW:H422	0.48	1.84	2	2
3:D:627:PCW:O1P	3:D:627:PCW:C5	0.48	2.59	9	4
1:D:485:ALA:O	1:D:489:LEU:HG	0.48	2.08	15	2
4:D:630:17F:O10	4:D:630:17F:O6	0.48	2.31	2	1
3:B:207:PCW:H82	4:B:216:17F:O8	0.48	2.08	2	1
3:B:213:PCW:H411	3:B:213:PCW:H182	0.48	1.84	2	1
3:B:213:PCW:C40	4:B:217:17F:C37	0.48	2.90	2	1
3:B:204:PCW:H122	4:C:211:17F:H18A	0.48	1.83	3	1
3:A:417:PCW:H341	3:D:612:PCW:C15	0.48	2.38	4	1
3:A:418:PCW:H322	3:D:625:PCW:C34	0.48	2.33	4	2
2:C:7:VAL:HG11	2:C:71:TYR:CD2	0.48	2.43	4	1
3:A:401:PCW:C48	3:D:611:PCW:H441	0.48	2.19	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:614:PCW:H51	3:D:625:PCW:P	0.48	2.48	5	1
3:C:206:PCW:C23	3:C:206:PCW:C18	0.48	2.91	5	3
3:A:417:PCW:H332	3:D:612:PCW:C3	0.48	2.38	6	1
3:C:208:PCW:O31	3:C:208:PCW:H52	0.48	2.07	6	1
3:A:406:PCW:C27	3:B:207:PCW:H171	0.48	2.39	9	2
3:A:416:PCW:H211	3:D:617:PCW:C48	0.48	2.38	8	1
3:D:621:PCW:H412	4:D:634:17F:H62	0.48	1.84	8	1
4:D:629:17F:O6	4:D:629:17F:N1	0.48	2.46	8	1
3:D:610:PCW:O11	3:D:616:PCW:C6	0.48	2.61	9	2
3:A:417:PCW:C41	3:D:612:PCW:H181	0.48	2.37	10	1
3:A:413:PCW:O31	3:A:413:PCW:H51	0.48	2.08	11	1
3:C:207:PCW:H472	4:C:211:17F:H18	0.48	1.84	11	1
3:C:203:PCW:O1P	3:C:203:PCW:C2	0.48	2.60	13	1
3:A:413:PCW:C36	4:C:210:17F:O8	0.48	2.60	15	1
3:B:208:PCW:H461	4:B:214:17F:C40	0.48	2.34	18	1
4:C:211:17F:H10	4:C:211:17F:C37	0.48	2.38	18	1
3:D:606:PCW:H451	3:D:625:PCW:C47	0.48	2.36	19	1
3:B:208:PCW:H442	4:B:214:17F:C1Z	0.48	2.31	19	1
3:A:420:PCW:H41	3:A:420:PCW:C2	0.48	2.37	9	2
3:D:615:PCW:H211	4:D:635:17F:C22	0.48	2.39	3	2
3:C:204:PCW:H20	4:C:211:17F:H18	0.48	1.84	2	1
3:D:620:PCW:O4P	3:D:620:PCW:H73	0.48	2.08	3	2
3:B:211:PCW:C31	3:B:211:PCW:O3	0.48	2.60	9	2
3:A:402:PCW:C40	3:A:407:PCW:H272	0.48	2.39	4	1
3:A:413:PCW:C34	4:A:414:17F:C32	0.48	2.91	4	1
3:B:213:PCW:H73	4:B:214:17F:C2	0.48	2.35	4	1
4:A:414:17F:O10	4:A:414:17F:C4	0.48	2.54	18	2
2:C:41:ARG:HD2	2:C:54:ASP:OD2	0.48	2.08	7	1
3:C:207:PCW:C32	3:C:207:PCW:C4	0.48	2.90	20	4
3:D:616:PCW:H482	3:C:208:PCW:H262	0.48	1.85	8	1
4:D:629:17F:H47	4:D:630:17F:C22	0.48	2.38	8	2
3:B:205:PCW:C28	3:B:212:PCW:H212	0.48	2.38	9	1
3:B:211:PCW:O3	3:B:211:PCW:O31	0.48	2.31	9	1
1:A:237:GLU:HA	1:A:240:ARG:HD2	0.48	1.84	14	2
3:A:404:PCW:H61	4:A:415:17F:H60	0.48	1.86	10	1
3:A:404:PCW:C8	4:A:415:17F:H61	0.48	2.38	10	1
3:D:625:PCW:H19	3:D:625:PCW:H142	0.48	1.84	10	1
3:A:405:PCW:P	3:A:405:PCW:C31	0.48	3.02	11	1
3:D:618:PCW:H411	3:D:627:PCW:H181	0.48	1.84	11	2
3:D:627:PCW:H421	3:D:627:PCW:H372	0.48	1.83	11	1
4:D:629:17F:C10	4:D:634:17F:H49	0.48	2.35	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:633:17F:H52	3:C:209:PCW:C46	0.48	2.38	14	2
3:B:204:PCW:C34	3:B:212:PCW:C8	0.48	2.91	11	1
3:B:208:PCW:H142	4:B:214:17F:H18	0.48	1.85	11	2
3:D:604:PCW:O1P	3:D:613:PCW:H73	0.48	2.08	13	2
3:B:207:PCW:H52	4:B:216:17F:O4	0.48	2.08	13	1
3:C:203:PCW:H483	3:C:203:PCW:C17	0.48	2.38	13	2
3:A:407:PCW:H222	3:C:205:PCW:C45	0.48	2.23	15	1
3:B:210:PCW:H271	3:B:210:PCW:H411	0.48	1.85	15	1
3:D:606:PCW:H451	3:D:625:PCW:H481	0.48	1.84	17	1
3:A:407:PCW:H181	3:C:205:PCW:C17	0.48	2.38	19	1
3:B:206:PCW:C39	4:C:211:17F:H47	0.48	2.37	19	1
3:A:402:PCW:H412	3:A:409:PCW:H241	0.48	1.85	20	1
3:D:625:PCW:H432	3:D:626:PCW:H412	0.48	1.84	20	1
4:D:633:17F:C30	3:C:208:PCW:H242	0.48	2.28	20	1
3:D:601:PCW:C21	3:D:601:PCW:C17	0.48	2.88	3	3
3:D:606:PCW:H442	3:D:625:PCW:C47	0.48	2.38	1	1
3:B:209:PCW:H132	3:B:209:PCW:H321	0.48	1.84	1	1
3:D:613:PCW:H221	4:C:210:17F:H44	0.48	1.84	3	1
3:C:212:PCW:C8	3:C:212:PCW:O4P	0.48	2.61	3	14
3:A:401:PCW:H73	3:B:209:PCW:H131	0.48	1.83	4	1
1:D:504:ARG:O	1:D:508:ARG:HG3	0.48	2.08	17	5
3:D:608:PCW:H462	3:C:205:PCW:C46	0.48	2.39	5	1
3:A:419:PCW:H371	3:D:610:PCW:H152	0.48	1.84	6	1
3:D:608:PCW:O31	3:D:608:PCW:H131	0.48	2.07	6	7
2:C:147:LYS:HB2	5:C:201:GDP:N1	0.48	2.24	6	1
3:A:402:PCW:H211	3:A:409:PCW:C20	0.48	2.38	8	1
3:C:204:PCW:H242	3:C:207:PCW:C48	0.48	2.32	8	1
3:A:404:PCW:H152	3:B:209:PCW:H39	0.48	1.84	10	1
2:B:117:LYS:HG2	5:B:201:GDP:C6	0.48	2.43	20	3
3:B:205:PCW:O31	3:B:212:PCW:H361	0.48	2.08	10	1
3:A:406:PCW:H251	3:B:207:PCW:C19	0.48	2.36	11	1
3:A:413:PCW:C12	4:A:414:17F:C20	0.48	2.91	11	1
3:A:419:PCW:H381	3:D:617:PCW:C48	0.48	2.39	11	1
3:D:615:PCW:H161	4:D:635:17F:H12	0.48	1.84	12	1
3:D:621:PCW:C19	4:D:633:17F:H20	0.48	2.38	13	2
3:D:622:PCW:H351	3:D:627:PCW:C20	0.48	2.37	13	1
3:B:213:PCW:C41	4:B:217:17F:H63	0.48	2.38	13	1
2:B:151:GLY:HA2	2:C:135:ARG:HD3	0.48	1.83	19	1
3:B:213:PCW:H432	3:B:213:PCW:C18	0.48	2.38	19	1
3:A:407:PCW:H181	3:C:205:PCW:C15	0.48	2.39	20	1
3:A:403:PCW:H41	3:A:403:PCW:C11	0.48	2.38	6	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:404:PCW:H232	3:D:611:PCW:C48	0.48	2.26	1	1
3:A:416:PCW:C15	3:D:602:PCW:H272	0.48	2.38	1	1
3:B:209:PCW:H222	4:B:215:17F:C19	0.48	2.37	1	1
3:C:206:PCW:H242	3:C:206:PCW:H181	0.48	1.86	1	1
3:A:410:PCW:H39	3:C:209:PCW:C18	0.48	2.39	2	1
3:D:619:PCW:O31	3:D:619:PCW:C1	0.48	2.58	7	6
4:A:414:17F:H42	3:B:212:PCW:H171	0.48	1.85	4	1
3:B:206:PCW:C24	3:C:209:PCW:H481	0.48	2.34	4	1
3:B:207:PCW:O31	3:B:207:PCW:H12	0.48	2.08	4	1
3:C:206:PCW:O1P	3:C:206:PCW:C5	0.48	2.61	11	4
3:D:618:PCW:C37	3:D:627:PCW:H161	0.48	2.39	5	3
3:B:213:PCW:H272	4:B:215:17F:H58	0.48	1.84	6	2
3:A:405:PCW:O31	3:A:405:PCW:O3P	0.48	2.31	7	2
3:A:402:PCW:H162	3:A:409:PCW:H212	0.48	1.85	8	1
3:A:408:PCW:H322	3:C:204:PCW:H182	0.48	1.86	8	1
3:D:610:PCW:C8	3:C:212:PCW:H73	0.48	2.39	8	1
4:D:632:17F:O8	4:D:632:17F:C5	0.48	2.56	8	3
1:A:371:LEU:HD23	4:A:415:17F:H40	0.48	1.84	9	1
3:A:411:PCW:C2	4:B:215:17F:C1Y	0.48	2.84	9	1
3:D:603:PCW:H281	3:D:606:PCW:C48	0.48	2.35	9	1
3:C:207:PCW:C4	3:C:207:PCW:C32	0.48	2.88	9	2
3:A:406:PCW:C7	3:A:411:PCW:O31	0.48	2.61	17	2
3:C:204:PCW:C20	4:C:211:17F:H56	0.48	2.38	10	1
3:A:417:PCW:H431	3:D:612:PCW:H211	0.48	1.86	11	1
3:A:419:PCW:H12	3:D:617:PCW:H351	0.48	1.84	13	2
3:B:203:PCW:H39	3:B:211:PCW:C44	0.48	2.27	11	1
3:A:401:PCW:H322	3:B:209:PCW:H39	0.48	1.86	12	1
3:A:410:PCW:H241	3:C:208:PCW:C24	0.48	2.39	12	1
3:D:621:PCW:O31	3:D:621:PCW:C1	0.48	2.55	13	1
4:D:630:17F:C30	3:B:206:PCW:H19	0.48	2.35	13	1
3:D:605:PCW:H42	3:D:626:PCW:C20	0.48	2.39	16	1
3:B:204:PCW:O11	3:B:204:PCW:C2	0.48	2.53	18	1
1:A:217:LEU:CD1	3:A:408:PCW:H222	0.48	2.37	19	1
3:A:412:PCW:H381	3:C:208:PCW:H361	0.48	1.85	20	1
3:A:408:PCW:O11	3:A:408:PCW:C2	0.48	2.53	1	5
3:A:417:PCW:O3P	3:A:417:PCW:C31	0.48	2.62	3	5
3:D:615:PCW:O3	3:D:615:PCW:O31	0.48	2.31	9	8
3:B:210:PCW:H342	3:B:210:PCW:O2	0.48	2.08	1	1
1:A:217:LEU:O	1:A:221:LEU:HG	0.48	2.09	2	3
3:A:413:PCW:H141	4:A:414:17F:H67	0.48	1.84	2	2
3:D:616:PCW:O3	3:D:616:PCW:C31	0.48	2.62	12	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:213:PCW:H181	3:B:213:PCW:C41	0.48	2.38	2	1
3:C:203:PCW:H182	3:C:203:PCW:H222	0.48	1.85	2	1
3:B:210:PCW:H52	3:B:210:PCW:C2	0.48	2.39	3	1
3:A:419:PCW:H31	3:D:617:PCW:C41	0.48	2.39	4	2
1:A:383:LYS:O	1:A:387:LEU:HG	0.48	2.08	5	2
3:D:613:PCW:H482	3:D:619:PCW:C21	0.48	2.38	17	2
3:D:620:PCW:H62	3:D:620:PCW:H11	0.48	1.86	5	1
3:D:627:PCW:C11	3:D:627:PCW:C31	0.48	2.92	5	1
3:A:404:PCW:H381	3:B:209:PCW:C33	0.48	2.34	6	1
3:B:204:PCW:C31	3:B:212:PCW:H82	0.48	2.39	6	1
3:D:602:PCW:H161	3:D:624:PCW:C21	0.48	2.39	7	1
3:D:607:PCW:H172	4:D:631:17F:H18	0.48	1.86	7	1
3:A:410:PCW:H20	3:D:627:PCW:H482	0.48	1.85	8	1
3:D:627:PCW:O4P	3:D:627:PCW:C8	0.48	2.62	8	2
4:D:632:17F:H1	4:D:632:17F:H4A	0.48	1.83	8	1
3:A:404:PCW:C38	3:B:209:PCW:H381	0.48	2.33	10	1
3:A:411:PCW:H432	3:A:418:PCW:H282	0.48	1.83	10	1
3:A:418:PCW:O31	3:A:418:PCW:C11	0.48	2.62	11	1
3:A:420:PCW:O3P	3:D:617:PCW:H52	0.48	2.08	11	1
3:D:612:PCW:H52	3:D:618:PCW:H31	0.48	1.86	11	1
3:D:616:PCW:H441	3:C:212:PCW:H431	0.48	1.85	11	1
3:A:404:PCW:H40	4:B:215:17F:C9	0.48	2.39	12	1
1:D:411:THR:O	1:D:415:LEU:HG	0.48	2.07	13	2
3:C:207:PCW:O2P	4:C:211:17F:H1A	0.48	2.07	14	1
3:A:410:PCW:H172	3:C:207:PCW:H211	0.48	1.83	15	1
3:C:205:PCW:O4P	3:C:206:PCW:H82	0.48	2.08	15	1
3:A:420:PCW:H351	3:D:617:PCW:C13	0.48	2.36	16	1
3:B:211:PCW:H131	4:B:217:17F:H60	0.48	1.85	16	1
3:D:617:PCW:H41	3:D:617:PCW:C2	0.48	2.15	18	1
3:B:206:PCW:C5	3:C:207:PCW:O1P	0.48	2.61	19	1
3:A:406:PCW:C6	3:A:411:PCW:O2P	0.48	2.62	20	1
3:A:404:PCW:H421	3:B:209:PCW:H471	0.48	1.85	1	1
3:D:622:PCW:H231	3:D:624:PCW:C24	0.48	2.35	1	1
2:B:15:GLY:O	2:B:19:LEU:HG	0.48	2.08	12	3
3:D:611:PCW:C20	3:D:619:PCW:H482	0.48	2.38	2	1
3:D:625:PCW:H371	3:D:626:PCW:H121	0.48	1.84	2	1
3:A:401:PCW:C31	3:B:209:PCW:H251	0.48	2.37	4	1
3:D:620:PCW:O3	3:D:620:PCW:O31	0.48	2.32	20	4
3:D:627:PCW:O31	3:D:627:PCW:H51	0.48	2.09	5	1
3:A:406:PCW:C28	4:B:216:17F:H19A	0.48	2.29	7	2
4:A:414:17F:H29	3:C:203:PCW:C41	0.48	2.39	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:546:GLU:O	1:D:550:LYS:HD2	0.48	2.08	8	3
3:D:626:PCW:H242	3:D:626:PCW:C19	0.48	2.36	14	2
3:B:208:PCW:H381	4:B:214:17F:H8	0.48	1.85	8	1
3:A:413:PCW:H341	4:A:414:17F:H58	0.48	1.84	9	1
3:D:605:PCW:H211	4:D:634:17F:C30	0.48	2.39	10	1
3:D:613:PCW:H471	3:D:619:PCW:H441	0.48	1.84	11	1
3:A:410:PCW:H31	3:C:209:PCW:C11	0.48	2.39	12	1
3:D:615:PCW:C22	3:C:205:PCW:H272	0.48	2.39	18	2
3:B:208:PCW:H282	3:B:208:PCW:H471	0.48	1.86	12	1
2:C:28:PHE:HZ	5:C:201:GDP:C2	0.48	2.27	12	1
4:A:414:17F:C35	4:A:414:17F:C31	0.48	2.85	13	1
4:A:415:17F:O9	4:A:415:17F:C20	0.48	2.61	18	2
3:B:205:PCW:C46	3:B:206:PCW:H161	0.48	2.39	14	1
3:A:403:PCW:H411	3:A:403:PCW:O3	0.48	2.08	15	1
3:D:611:PCW:O3P	3:D:623:PCW:H341	0.48	2.08	15	1
3:B:213:PCW:H211	3:B:213:PCW:H161	0.48	1.83	15	1
3:D:601:PCW:O2	4:B:216:17F:H56	0.48	2.09	16	1
3:B:205:PCW:C45	3:C:208:PCW:H20	0.48	2.12	16	1
3:A:420:PCW:C16	4:D:632:17F:H60	0.48	2.39	17	1
2:B:8:VAL:HB	2:B:57:ASP:HA	0.48	1.84	17	1
3:A:404:PCW:H481	3:B:209:PCW:H271	0.48	1.85	18	1
3:A:406:PCW:H11	3:A:406:PCW:O31	0.48	2.08	1	2
3:A:409:PCW:O31	3:A:409:PCW:P	0.48	2.71	9	4
2:B:146:ALA:N	5:B:201:GDP:O6	0.48	2.46	1	4
3:B:213:PCW:H40	4:B:217:17F:H66	0.48	1.86	2	1
3:D:618:PCW:C24	3:B:206:PCW:H472	0.48	2.39	4	1
3:A:401:PCW:H412	3:A:401:PCW:C37	0.48	2.27	5	1
3:A:419:PCW:O2	3:D:617:PCW:H422	0.48	2.08	7	2
2:C:166:HIS:HA	2:C:169:LYS:HG2	0.48	1.85	7	1
4:A:414:17F:C28	3:C:203:PCW:H472	0.48	2.39	8	1
3:C:204:PCW:H251	4:C:211:17F:H56	0.48	1.86	8	2
3:B:205:PCW:H12	3:B:211:PCW:C6	0.48	2.39	19	2
3:A:407:PCW:H52	4:B:216:17F:C10	0.48	2.36	12	2
3:B:205:PCW:C14	4:B:214:17F:H37	0.48	2.38	12	1
3:A:407:PCW:H242	3:C:205:PCW:H381	0.48	1.85	13	1
3:A:409:PCW:H152	3:C:205:PCW:C39	0.48	2.38	15	1
3:A:404:PCW:C8	4:A:415:17F:O5	0.48	2.60	16	1
3:D:604:PCW:H382	3:D:611:PCW:H31	0.48	1.84	17	2
1:A:348:GLU:HB3	1:A:352:LYS:HE2	0.48	1.84	8	5
3:A:402:PCW:C43	3:A:407:PCW:H251	0.48	2.30	1	1
3:A:403:PCW:H212	3:A:403:PCW:C42	0.48	2.35	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:418:PCW:O11	3:A:418:PCW:H2	0.48	2.08	2	1
4:D:630:17F:C7	4:D:630:17F:O9	0.48	2.62	7	2
3:A:401:PCW:H63	2:C:2:THR:HG23	0.48	1.85	3	1
3:A:407:PCW:H52	4:B:216:17F:H9	0.48	1.85	4	1
3:A:407:PCW:C1	4:B:216:17F:H10A	0.48	2.39	4	1
3:A:410:PCW:O3P	3:A:410:PCW:O31	0.48	2.31	20	3
2:C:17:SER:O	2:C:21:ILE:HG12	0.48	2.08	11	5
3:A:407:PCW:H151	3:C:205:PCW:C17	0.48	2.39	5	1
1:A:297:LYS:O	1:A:301:LEU:HB2	0.48	2.09	6	2
3:D:601:PCW:H172	3:D:601:PCW:H221	0.48	1.84	6	1
3:B:203:PCW:H242	4:C:210:17F:C20	0.48	2.39	14	2
2:C:92:ASP:HA	2:C:95:HIS:HD2	0.48	1.67	6	1
4:D:634:17F:C42	3:C:206:PCW:H222	0.48	2.39	7	1
3:C:204:PCW:H20	4:C:211:17F:H19	0.48	1.84	7	1
4:C:211:17F:O10	4:C:211:17F:H4	0.48	2.07	7	1
3:A:412:PCW:C46	3:C:208:PCW:H472	0.48	2.39	9	2
3:B:203:PCW:C8	3:B:203:PCW:O4P	0.48	2.61	13	4
4:D:635:17F:H52	3:C:205:PCW:C16	0.48	2.31	11	1
3:D:604:PCW:O2P	3:D:613:PCW:C7	0.48	2.62	13	1
3:A:413:PCW:C25	4:A:414:17F:H60	0.48	2.38	17	2
3:A:401:PCW:H331	3:B:209:PCW:H251	0.48	1.84	15	1
3:A:412:PCW:O11	3:A:412:PCW:O2	0.48	2.31	15	1
3:D:616:PCW:C45	3:B:206:PCW:C45	0.48	2.92	15	1
3:B:205:PCW:H422	4:B:214:17F:H70	0.48	1.85	15	1
3:B:205:PCW:H442	3:B:206:PCW:H211	0.48	1.85	16	1
3:B:210:PCW:H451	4:B:215:17F:H68	0.48	1.85	17	1
3:A:411:PCW:H131	3:A:411:PCW:H342	0.48	1.85	14	3
3:D:616:PCW:C43	3:B:206:PCW:C47	0.48	2.90	1	1
3:D:616:PCW:O1P	3:C:212:PCW:H42	0.48	2.08	1	1
3:D:626:PCW:O3	3:D:626:PCW:C31	0.48	2.61	2	6
4:D:634:17F:H19A	4:D:634:17F:C9	0.48	2.37	12	2
3:D:620:PCW:H461	3:C:205:PCW:C48	0.48	2.34	2	1
3:A:402:PCW:C4	3:A:402:PCW:H322	0.48	2.39	4	1
3:D:608:PCW:H381	3:D:615:PCW:C40	0.48	2.39	4	1
3:A:405:PCW:H382	4:D:628:17F:H53	0.48	1.86	7	1
3:A:409:PCW:C5	3:C:206:PCW:O2P	0.48	2.60	7	1
3:D:622:PCW:O3P	3:D:622:PCW:C5	0.48	2.62	7	1
3:A:407:PCW:C22	3:C:205:PCW:H431	0.48	2.38	8	1
3:A:413:PCW:C35	4:A:414:17F:H57	0.48	2.37	8	1
3:D:622:PCW:H422	3:C:212:PCW:H483	0.48	1.85	8	1
2:C:35:THR:HG23	2:C:36:ILE:HG23	0.48	1.85	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:406:PCW:P	3:A:411:PCW:O2P	0.48	2.72	9	1
3:B:211:PCW:H151	4:B:217:17F:H62	0.48	1.85	9	1
3:A:412:PCW:H452	3:C:208:PCW:C45	0.48	2.37	10	1
3:A:420:PCW:H362	3:D:617:PCW:C13	0.48	2.39	10	1
3:D:625:PCW:O31	3:D:625:PCW:O4P	0.48	2.32	10	1
3:B:203:PCW:H41	3:B:211:PCW:H352	0.48	1.84	10	2
4:D:629:17F:H49	3:B:212:PCW:H462	0.48	1.86	11	1
3:C:204:PCW:H132	4:C:211:17F:H67	0.48	1.84	11	1
1:A:268:GLU:HG2	1:D:506:ARG:HD3	0.48	1.85	12	1
3:A:410:PCW:O3	3:C:209:PCW:C12	0.48	2.61	14	1
3:A:416:PCW:C3	3:D:610:PCW:C11	0.48	2.92	14	1
2:B:25:GLN:HB3	2:B:27:HIS:CD2	0.48	2.44	14	1
3:A:416:PCW:H442	3:D:617:PCW:H211	0.48	1.84	15	1
3:A:417:PCW:C8	3:A:419:PCW:H31	0.48	2.39	15	1
3:A:419:PCW:H412	3:D:610:PCW:H161	0.48	1.84	20	2
3:A:404:PCW:C36	3:B:203:PCW:H19	0.48	2.38	18	1
3:A:412:PCW:H451	3:C:208:PCW:H412	0.48	1.85	18	1
3:A:402:PCW:H322	3:C:206:PCW:C4	0.48	2.39	19	1
3:A:401:PCW:O1P	3:A:401:PCW:H2	0.47	2.08	5	2
4:D:633:17F:O7	4:D:633:17F:C17	0.47	2.62	13	13
3:D:605:PCW:H352	4:D:629:17F:C8	0.47	2.39	2	1
2:B:97:ARG:O	2:B:101:LYS:HG3	0.47	2.09	2	2
3:D:604:PCW:H372	3:D:604:PCW:C41	0.47	2.38	3	1
3:B:203:PCW:O3	3:B:203:PCW:O31	0.47	2.31	15	3
3:A:404:PCW:H73	3:A:404:PCW:H2	0.47	1.86	8	3
3:A:418:PCW:O11	3:D:614:PCW:H121	0.47	2.09	5	1
3:B:204:PCW:C8	3:B:212:PCW:H73	0.47	2.38	5	1
1:A:376:LEU:O	1:A:380:GLU:HG3	0.47	2.09	19	3
3:D:609:PCW:H12	4:D:633:17F:C6	0.47	2.31	6	1
3:C:204:PCW:H162	4:C:211:17F:C35	0.47	2.39	10	2
3:A:407:PCW:H271	3:A:409:PCW:C20	0.47	2.38	11	1
3:D:613:PCW:H361	3:D:619:PCW:H371	0.47	1.86	11	1
3:A:410:PCW:H251	3:C:207:PCW:H231	0.47	1.86	12	1
3:A:407:PCW:H222	3:C:205:PCW:H411	0.47	1.85	13	1
3:A:411:PCW:O3	4:B:215:17F:H33	0.47	2.08	13	1
4:A:415:17F:H33	4:A:415:17F:H62	0.47	1.85	14	1
3:A:402:PCW:H122	3:A:402:PCW:C7	0.47	2.37	15	1
4:A:414:17F:H30	3:B:204:PCW:H40	0.47	1.86	15	1
1:A:386:PHE:HZ	4:A:414:17F:H76	0.47	1.69	18	1
2:B:72:MET:HE3	2:B:103:VAL:HG21	0.47	1.84	18	1
4:B:214:17F:H40	4:B:217:17F:H70	0.47	1.85	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:409:PCW:C8	3:C:206:PCW:O31	0.47	2.62	1	1
3:A:418:PCW:C38	3:D:625:PCW:H271	0.47	2.39	1	1
3:B:203:PCW:H41	3:B:203:PCW:H12	0.47	1.85	1	3
3:B:205:PCW:H322	3:B:206:PCW:H121	0.47	1.85	1	1
3:D:608:PCW:C38	3:C:205:PCW:H283	0.47	2.39	2	2
3:D:623:PCW:H142	3:D:624:PCW:C35	0.47	2.35	3	2
3:A:407:PCW:H172	3:C:205:PCW:C34	0.47	2.31	4	2
3:A:408:PCW:C26	3:A:417:PCW:H482	0.47	2.38	15	2
3:D:604:PCW:H141	3:D:613:PCW:H132	0.47	1.84	4	2
1:D:514:LEU:HA	1:D:517:HIS:HB2	0.47	1.85	19	4
3:D:616:PCW:C43	3:D:627:PCW:H232	0.47	2.37	7	1
2:B:78:PHE:O	2:B:111:MET:HA	0.47	2.09	17	2
3:C:206:PCW:H241	3:C:206:PCW:H182	0.47	1.85	7	1
3:D:607:PCW:O1P	3:D:626:PCW:C23	0.47	2.62	13	2
3:B:208:PCW:H372	4:B:214:17F:H63	0.47	1.86	9	1
4:B:215:17F:H12A	4:B:215:17F:C24	0.47	2.34	10	2
3:A:407:PCW:H152	3:C:205:PCW:H151	0.47	1.79	11	1
3:A:417:PCW:C35	3:D:612:PCW:H151	0.47	2.33	11	1
3:B:205:PCW:H142	4:B:214:17F:H37	0.47	1.86	12	1
3:B:209:PCW:H19	4:B:215:17F:O10	0.47	2.09	12	2
3:A:401:PCW:H322	3:B:209:PCW:H232	0.47	1.87	13	2
3:B:204:PCW:C42	3:B:212:PCW:H171	0.47	2.38	13	1
3:D:607:PCW:C48	4:D:628:17F:H61	0.47	2.36	14	1
3:B:207:PCW:C43	3:B:213:PCW:H231	0.47	2.39	14	1
3:C:207:PCW:H452	4:C:211:17F:H20	0.47	1.86	14	1
3:A:407:PCW:H482	4:D:635:17F:C28	0.47	2.38	15	1
3:D:621:PCW:H381	4:D:635:17F:C42	0.47	2.39	18	2
3:B:208:PCW:C32	3:B:208:PCW:H63	0.47	2.39	17	1
3:A:401:PCW:H372	3:A:404:PCW:C20	0.47	2.39	19	1
3:A:416:PCW:O31	3:A:416:PCW:O3P	0.47	2.32	19	1
3:B:203:PCW:H472	4:B:217:17F:H47	0.47	1.85	19	1
3:B:207:PCW:H422	3:B:213:PCW:C24	0.47	2.39	19	1
3:D:626:PCW:H182	3:D:626:PCW:C8	0.47	2.39	20	1
3:D:619:PCW:O4P	3:D:619:PCW:C8	0.47	2.63	11	10
3:D:620:PCW:O1P	3:D:621:PCW:C7	0.47	2.55	3	5
3:B:207:PCW:H162	3:B:210:PCW:C19	0.47	2.40	1	1
3:B:207:PCW:H141	3:B:210:PCW:H382	0.47	1.86	1	1
3:B:213:PCW:H142	4:B:217:17F:C9	0.47	2.39	1	1
3:C:207:PCW:H19	3:C:207:PCW:C45	0.47	2.39	2	1
3:A:406:PCW:C23	3:B:207:PCW:H152	0.47	2.39	3	1
3:A:406:PCW:O1P	3:A:406:PCW:H51	0.47	2.10	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:417:PCW:H2	3:A:417:PCW:C4	0.47	2.39	5	4
3:D:624:PCW:H451	4:C:210:17F:H76	0.47	1.86	5	1
3:D:611:PCW:H322	3:D:623:PCW:H352	0.47	1.84	9	2
3:B:211:PCW:C17	4:B:217:17F:H69	0.47	2.29	6	1
3:D:602:PCW:O4P	4:D:630:17F:H1A	0.47	2.09	7	1
3:C:203:PCW:H221	3:C:203:PCW:C17	0.47	2.29	7	1
3:A:407:PCW:H62	3:B:213:PCW:H322	0.47	1.86	8	1
3:C:206:PCW:H171	3:C:206:PCW:C38	0.47	2.40	8	1
3:A:408:PCW:H362	3:C:204:PCW:C20	0.47	2.39	11	1
3:C:203:PCW:H182	3:C:203:PCW:H231	0.47	1.85	11	1
3:B:205:PCW:H452	3:B:206:PCW:H172	0.47	1.86	12	1
3:A:402:PCW:H331	3:C:206:PCW:H322	0.47	1.86	14	1
1:A:388:SER:HB2	1:D:594:LYS:HD3	0.47	1.85	17	1
3:A:419:PCW:C39	3:D:616:PCW:H171	0.47	2.19	17	1
3:B:210:PCW:H2	3:B:210:PCW:C4	0.47	2.20	17	1
3:D:618:PCW:H251	3:B:206:PCW:H451	0.47	1.87	18	1
3:B:204:PCW:H331	3:B:212:PCW:H121	0.47	1.86	19	1
3:A:404:PCW:C16	4:A:415:17F:C31	0.47	2.92	20	1
3:D:617:PCW:O3P	3:D:617:PCW:C5	0.47	2.62	1	5
2:B:17:SER:OG	5:B:201:GDP:O3B	0.47	2.32	8	12
2:B:18:ALA:HB2	5:B:201:GDP:O2A	0.47	2.09	1	1
3:A:406:PCW:H42	3:A:406:PCW:C3	0.47	2.39	2	1
3:A:416:PCW:C6	4:D:632:17F:O5	0.47	2.62	18	2
3:B:204:PCW:H73	3:B:212:PCW:C7	0.47	2.38	2	1
3:C:207:PCW:C31	3:C:207:PCW:O3	0.47	2.63	5	4
3:A:419:PCW:C34	3:D:617:PCW:H412	0.47	2.39	3	2
4:D:628:17F:C21	4:D:631:17F:H70	0.47	2.39	4	1
3:B:209:PCW:H341	3:B:209:PCW:H182	0.47	1.85	4	1
4:B:215:17F:H1	4:B:215:17F:H4	0.47	1.86	4	2
3:A:401:PCW:H272	3:D:614:PCW:H271	0.47	1.87	5	1
3:D:603:PCW:O1P	3:D:623:PCW:C7	0.47	2.62	8	3
3:D:616:PCW:C39	3:D:618:PCW:C16	0.47	2.93	5	1
3:B:207:PCW:C18	3:B:210:PCW:C19	0.47	2.92	7	2
3:A:413:PCW:C11	4:A:414:17F:H69	0.47	2.39	8	1
3:D:605:PCW:H331	3:D:607:PCW:C7	0.47	2.39	10	1
3:D:616:PCW:H281	3:C:204:PCW:C27	0.47	2.38	10	1
3:D:621:PCW:C20	3:D:622:PCW:C8	0.47	2.92	11	1
2:B:17:SER:HA	2:B:57:ASP:OD1	0.47	2.09	11	1
3:A:402:PCW:C46	3:C:205:PCW:H361	0.47	2.40	12	1
3:D:625:PCW:H12	3:D:626:PCW:C1	0.47	2.38	12	1
3:B:208:PCW:H411	4:B:214:17F:H33	0.47	1.87	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:615:PCW:C6	4:D:635:17F:O4	0.47	2.63	14	1
3:B:208:PCW:C27	4:B:216:17F:H46	0.47	2.38	14	1
3:A:401:PCW:H322	3:B:209:PCW:H242	0.47	1.86	15	1
3:A:409:PCW:H162	3:A:409:PCW:H371	0.47	1.85	15	1
3:B:207:PCW:H41	4:B:216:17F:C3	0.47	2.39	15	1
3:C:208:PCW:H141	3:C:208:PCW:H422	0.47	1.87	15	1
3:B:207:PCW:C11	3:B:210:PCW:C15	0.47	2.93	16	1
3:D:607:PCW:H462	3:B:207:PCW:H281	0.47	1.85	18	1
3:C:208:PCW:H211	3:C:208:PCW:C17	0.47	2.36	18	1
3:A:402:PCW:H39	3:A:409:PCW:C24	0.47	2.40	19	1
4:B:215:17F:H4A	4:B:215:17F:C1	0.47	2.39	19	1
3:B:203:PCW:H461	4:B:217:17F:C28	0.47	2.32	20	1
3:C:208:PCW:H161	3:C:209:PCW:H39	0.47	1.85	20	1
3:B:203:PCW:N	3:B:211:PCW:O31	0.47	2.48	1	1
4:A:414:17F:C36	4:C:210:17F:H37	0.47	2.39	2	1
3:A:407:PCW:H241	3:C:205:PCW:H422	0.47	1.86	3	1
3:D:618:PCW:C35	3:D:627:PCW:C34	0.47	2.89	18	2
4:B:215:17F:C12	4:B:215:17F:C23	0.47	2.93	3	4
3:A:402:PCW:H42	3:A:402:PCW:H322	0.47	1.87	4	2
3:D:602:PCW:H142	3:D:624:PCW:C18	0.47	2.39	9	2
3:A:410:PCW:H222	3:C:209:PCW:H432	0.47	1.87	9	2
3:C:203:PCW:O4P	3:C:204:PCW:H52	0.47	2.10	6	1
3:A:413:PCW:H121	4:A:414:17F:C31	0.47	2.40	7	1
3:C:207:PCW:C28	3:C:208:PCW:H131	0.47	2.39	7	1
3:B:204:PCW:H131	3:B:206:PCW:C4	0.47	2.38	8	3
3:B:205:PCW:C39	4:B:214:17F:H75	0.47	2.35	8	1
3:A:410:PCW:H372	3:C:209:PCW:C17	0.47	2.39	9	1
3:D:625:PCW:O31	3:D:625:PCW:H41	0.47	2.09	10	2
3:C:208:PCW:H121	3:C:208:PCW:C35	0.47	2.40	19	2
4:D:629:17F:C38	4:D:634:17F:C1X	0.47	2.90	11	2
3:D:603:PCW:H251	4:B:217:17F:H52	0.47	1.84	12	1
4:D:635:17F:C30	3:C:205:PCW:H141	0.47	2.33	12	1
3:A:408:PCW:H121	3:A:417:PCW:C26	0.47	2.39	14	1
2:C:144:THR:HG22	2:C:151:GLY:HA3	0.47	1.85	14	1
4:C:211:17F:H49	3:C:212:PCW:H251	0.47	1.87	14	1
3:A:419:PCW:H351	3:D:617:PCW:C43	0.47	2.39	17	1
4:D:629:17F:H29	4:D:630:17F:C8	0.47	2.35	20	1
3:B:213:PCW:C28	4:B:215:17F:H78	0.47	2.39	20	1
1:A:297:LYS:HB3	1:A:301:LEU:HD12	0.47	1.87	2	3
3:A:418:PCW:C48	3:B:213:PCW:H472	0.47	2.39	2	1
3:D:624:PCW:O3P	3:D:624:PCW:C31	0.47	2.62	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:406:PCW:C28	4:B:216:17F:H20A	0.47	2.22	3	1
3:D:602:PCW:H73	3:C:212:PCW:P	0.47	2.49	4	2
3:A:403:PCW:C32	3:C:203:PCW:O2P	0.47	2.62	5	1
3:A:420:PCW:H51	3:A:420:PCW:O2P	0.47	2.10	7	1
4:B:217:17F:O7	4:B:217:17F:O10	0.47	2.32	7	1
3:D:604:PCW:C32	3:D:613:PCW:C8	0.47	2.90	8	1
3:B:204:PCW:H441	3:C:203:PCW:C40	0.47	2.40	9	1
3:B:206:PCW:C21	3:C:208:PCW:H282	0.47	2.39	9	1
3:B:203:PCW:H351	4:B:215:17F:H37	0.47	1.85	11	1
4:D:629:17F:H54	3:B:212:PCW:C46	0.47	2.40	12	1
3:A:410:PCW:C27	3:D:618:PCW:H462	0.47	2.39	18	3
3:A:408:PCW:H121	3:A:417:PCW:H261	0.47	1.87	14	1
3:D:615:PCW:H412	3:C:205:PCW:H283	0.47	1.86	14	3
3:A:401:PCW:H63	3:A:404:PCW:H12	0.47	1.86	15	1
3:A:401:PCW:O3P	3:B:209:PCW:H161	0.47	2.09	15	1
3:A:402:PCW:C7	3:A:409:PCW:O11	0.47	2.62	15	1
3:D:605:PCW:H321	3:D:607:PCW:C8	0.47	2.39	15	1
3:B:205:PCW:H40	4:B:214:17F:C37	0.47	2.39	15	1
3:B:207:PCW:O4P	3:B:207:PCW:H62	0.47	2.09	15	1
3:A:407:PCW:H52	4:B:216:17F:H11	0.47	1.84	16	1
4:B:214:17F:H29	4:B:217:17F:H58	0.47	1.86	16	1
3:A:401:PCW:H452	3:D:611:PCW:C28	0.47	2.38	18	1
3:D:607:PCW:C20	4:D:631:17F:H39	0.47	2.38	18	1
3:D:623:PCW:H362	3:D:623:PCW:O2	0.47	2.09	19	1
3:A:418:PCW:H422	3:D:625:PCW:H442	0.47	1.85	20	1
3:D:611:PCW:H461	3:D:611:PCW:H241	0.47	1.85	20	1
3:D:613:PCW:H73	3:D:624:PCW:C8	0.47	2.40	20	1
3:A:402:PCW:H52	3:C:206:PCW:C7	0.47	2.40	1	1
3:A:406:PCW:O31	3:A:411:PCW:H52	0.47	2.10	1	1
3:A:406:PCW:H261	3:B:210:PCW:H141	0.47	1.86	1	1
4:A:415:17F:H75	3:B:203:PCW:H272	0.47	1.86	1	1
1:D:440:GLU:O	1:D:444:ASP:HB2	0.47	2.09	13	3
3:B:204:PCW:H51	3:B:212:PCW:H73	0.47	1.87	1	1
3:B:208:PCW:H161	4:B:214:17F:C20	0.47	2.40	1	1
3:B:211:PCW:H82	3:B:211:PCW:O4P	0.47	2.10	1	1
3:A:416:PCW:O3	3:A:416:PCW:C31	0.47	2.63	6	3
3:D:605:PCW:H63	3:D:605:PCW:C11	0.47	2.40	17	2
3:D:608:PCW:H62	3:D:620:PCW:O11	0.47	2.09	2	1
3:D:615:PCW:H121	4:D:635:17F:H8	0.47	1.85	2	1
3:B:204:PCW:H12	3:B:204:PCW:C7	0.47	2.40	2	1
3:C:204:PCW:H141	4:C:211:17F:H6A	0.47	1.87	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:618:PCW:C46	3:B:204:PCW:H232	0.47	2.40	3	1
2:B:72:MET:HB2	2:B:103:VAL:HG11	0.47	1.86	3	2
3:B:203:PCW:H19	4:B:215:17F:C26	0.47	2.40	3	1
3:C:203:PCW:O3	3:C:203:PCW:C31	0.47	2.62	3	3
3:A:401:PCW:H381	3:A:404:PCW:C28	0.47	2.40	4	1
3:A:407:PCW:C12	3:C:205:PCW:H151	0.47	2.39	4	1
4:D:628:17F:C42	4:B:216:17F:H48	0.47	2.40	4	1
1:A:388:SER:HB3	1:D:594:LYS:HE2	0.47	1.86	10	2
3:A:404:PCW:H432	3:B:209:PCW:C19	0.47	2.39	5	1
3:D:624:PCW:O31	3:D:624:PCW:C11	0.47	2.63	16	4
3:B:204:PCW:H362	3:C:204:PCW:C33	0.47	2.40	5	1
3:B:207:PCW:H182	3:B:210:PCW:H19	0.47	1.85	7	1
3:C:208:PCW:H281	3:C:212:PCW:C47	0.47	2.38	8	1
3:A:409:PCW:C6	3:A:412:PCW:H39	0.47	2.37	9	1
3:B:209:PCW:H361	3:B:209:PCW:H231	0.47	1.87	9	1
3:D:604:PCW:O31	3:D:613:PCW:C7	0.47	2.62	10	1
3:B:204:PCW:H321	3:B:212:PCW:H141	0.47	1.85	10	1
3:D:611:PCW:H452	3:D:611:PCW:C24	0.47	2.38	11	1
3:B:205:PCW:H151	3:B:208:PCW:C39	0.47	2.40	11	1
3:B:210:PCW:C44	3:B:213:PCW:H251	0.47	2.40	11	1
3:D:615:PCW:H161	4:D:635:17F:C10	0.47	2.39	12	1
3:D:616:PCW:H432	3:B:206:PCW:C48	0.47	2.39	12	1
3:D:627:PCW:H241	3:C:212:PCW:C45	0.47	2.39	12	1
3:A:413:PCW:C31	3:A:413:PCW:H51	0.47	2.39	13	1
3:D:601:PCW:H362	4:B:216:17F:H68	0.47	1.84	13	1
3:B:210:PCW:O4P	3:B:210:PCW:C3	0.47	2.43	13	1
3:D:622:PCW:H121	4:D:630:17F:H31	0.47	1.85	14	1
3:A:402:PCW:H382	3:C:205:PCW:H381	0.47	1.86	15	1
3:A:417:PCW:H361	3:D:612:PCW:H132	0.47	1.86	15	1
4:B:216:17F:C2	4:B:216:17F:C4	0.47	2.89	15	1
3:B:206:PCW:H182	4:B:214:17F:H71	0.47	1.86	16	1
3:B:207:PCW:H442	4:B:215:17F:H61	0.47	1.85	16	1
2:B:8:VAL:CG1	2:B:16:LYS:HB3	0.47	2.40	17	1
3:B:213:PCW:H422	4:B:217:17F:H12	0.47	1.85	17	1
3:A:405:PCW:H371	3:D:601:PCW:C12	0.47	2.36	19	1
3:D:624:PCW:O31	3:D:624:PCW:H61	0.47	2.09	19	1
3:A:403:PCW:C20	3:C:203:PCW:H251	0.47	2.40	20	1
3:D:605:PCW:H422	3:D:608:PCW:C3	0.47	2.30	20	1
3:D:616:PCW:C42	3:D:627:PCW:H232	0.47	2.39	20	1
3:D:601:PCW:C34	4:B:216:17F:H61	0.47	2.25	2	1
4:B:217:17F:O9	4:B:217:17F:C7	0.47	2.62	6	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:416:PCW:C41	3:A:416:PCW:C37	0.47	2.85	10	5
3:D:613:PCW:C43	3:D:619:PCW:H39	0.47	2.39	3	2
3:A:410:PCW:H51	3:C:209:PCW:H32	0.47	1.86	4	1
3:B:208:PCW:H411	4:B:214:17F:H11A	0.47	1.87	5	2
3:B:209:PCW:O1P	3:B:209:PCW:H32	0.47	2.09	5	4
3:B:204:PCW:H212	3:C:207:PCW:C26	0.47	2.40	6	1
3:B:210:PCW:C16	4:B:216:17F:H8	0.47	2.32	6	1
3:A:416:PCW:H61	4:D:632:17F:C3	0.47	2.40	7	1
3:B:210:PCW:H422	3:B:210:PCW:C38	0.47	2.33	8	1
3:D:607:PCW:H63	3:D:626:PCW:C23	0.47	2.39	9	1
3:A:401:PCW:C34	3:B:209:PCW:H282	0.47	2.40	10	1
3:A:406:PCW:C44	3:B:207:PCW:H262	0.47	2.39	11	1
3:A:419:PCW:C37	3:D:610:PCW:H162	0.47	2.38	11	1
3:A:419:PCW:C43	3:D:610:PCW:H231	0.47	2.39	11	1
3:A:409:PCW:H483	3:C:206:PCW:H272	0.47	1.86	12	1
3:B:210:PCW:C12	4:B:216:17F:C18	0.47	2.93	13	1
3:A:401:PCW:C33	3:B:209:PCW:H251	0.47	2.40	15	1
3:A:403:PCW:H472	3:C:203:PCW:H251	0.47	1.87	15	1
3:D:607:PCW:C25	4:D:631:17F:H58	0.47	2.40	16	1
3:A:412:PCW:C43	3:C:208:PCW:H381	0.47	2.37	18	1
1:D:517:HIS:O	1:D:521:TYR:HB2	0.47	2.10	18	1
3:D:609:PCW:H332	4:D:633:17F:H18A	0.47	1.86	20	1
2:B:138:GLY:HA2	2:C:154:ASP:OD1	0.47	2.09	20	1
3:D:627:PCW:O2	3:D:627:PCW:O11	0.47	2.33	1	1
3:B:210:PCW:C47	3:B:210:PCW:C28	0.47	2.93	6	2
2:C:15:GLY:CA	5:C:201:GDP:C8	0.47	2.97	12	4
4:D:633:17F:C29	3:C:209:PCW:H452	0.47	2.38	3	1
2:B:81:VAL:HA	2:B:114:VAL:O	0.47	2.10	17	4
3:B:205:PCW:C24	3:B:206:PCW:H372	0.47	2.40	3	1
3:B:209:PCW:C27	3:B:209:PCW:C22	0.47	2.59	15	3
3:B:204:PCW:H482	3:B:212:PCW:C19	0.47	2.39	5	1
3:C:204:PCW:O31	3:C:204:PCW:P	0.47	2.73	5	1
3:D:618:PCW:P	3:D:627:PCW:H52	0.47	2.50	6	1
3:D:611:PCW:H63	3:D:623:PCW:H342	0.47	1.85	7	1
3:B:203:PCW:H431	3:B:211:PCW:H222	0.47	1.87	8	1
3:D:620:PCW:H141	4:D:635:17F:C18	0.47	2.40	11	2
3:A:410:PCW:O31	3:A:410:PCW:C1	0.47	2.61	19	2
3:A:410:PCW:H331	3:C:209:PCW:H151	0.47	1.85	16	2
3:B:207:PCW:H382	4:B:215:17F:C33	0.47	2.36	16	1
3:A:410:PCW:C7	3:C:209:PCW:O11	0.47	2.62	19	1
2:C:168:GLU:OE2	3:C:205:PCW:H63	0.47	2.10	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:203:PCW:C43	3:B:211:PCW:H222	0.47	2.40	1	1
3:A:404:PCW:C6	3:B:203:PCW:H162	0.47	2.40	2	1
3:A:404:PCW:C42	3:B:209:PCW:H442	0.47	2.40	2	1
3:D:602:PCW:C24	3:D:610:PCW:H352	0.47	2.31	2	1
3:B:204:PCW:C7	3:B:204:PCW:C1	0.47	2.93	2	1
1:A:255:GLN:HB2	1:A:256:PRO:HD3	0.47	1.86	3	5
3:D:613:PCW:H32	3:D:619:PCW:C3	0.47	2.40	3	1
3:A:403:PCW:H331	3:C:204:PCW:H32	0.47	1.85	20	2
3:A:410:PCW:O2P	3:C:207:PCW:H361	0.47	2.09	5	2
3:C:207:PCW:O31	3:C:207:PCW:O3	0.47	2.33	7	2
3:A:410:PCW:H121	3:C:209:PCW:C16	0.47	2.37	8	1
3:D:607:PCW:H411	4:D:628:17F:H33	0.47	1.86	8	1
3:A:408:PCW:H322	3:C:204:PCW:C18	0.47	2.40	9	1
3:B:207:PCW:C42	3:B:213:PCW:H283	0.47	2.40	10	1
3:A:418:PCW:H431	3:D:625:PCW:H442	0.47	1.87	19	2
3:B:206:PCW:H262	3:C:208:PCW:C28	0.47	2.40	11	1
3:D:601:PCW:H362	4:B:216:17F:C38	0.47	2.40	13	1
3:B:205:PCW:H283	3:B:212:PCW:C16	0.47	2.38	14	1
1:A:265:TRP:HH2	3:A:409:PCW:H451	0.47	1.70	16	1
3:A:418:PCW:C43	3:D:625:PCW:H442	0.47	2.40	19	1
3:D:607:PCW:C22	4:D:628:17F:H10A	0.47	2.38	19	1
3:B:207:PCW:H122	3:B:213:PCW:H172	0.47	1.86	19	1
3:B:211:PCW:H63	3:B:212:PCW:C34	0.47	2.32	20	1
3:D:615:PCW:H212	3:D:615:PCW:C17	0.46	2.36	5	3
3:D:622:PCW:O3P	3:D:622:PCW:O31	0.46	2.32	1	6
3:B:204:PCW:H272	3:C:207:PCW:H252	0.46	1.86	3	1
3:D:614:PCW:C43	3:D:619:PCW:H20	0.46	2.40	4	1
3:B:206:PCW:H51	3:C:207:PCW:O11	0.46	2.09	4	1
3:B:213:PCW:H483	4:B:217:17F:H45	0.46	1.87	5	1
2:C:41:ARG:HA	2:C:53:LEU:O	0.46	2.10	8	3
3:A:410:PCW:C18	3:A:410:PCW:H232	0.46	2.40	8	2
3:D:611:PCW:C22	3:D:619:PCW:H483	0.46	2.40	6	1
3:B:213:PCW:O4P	3:B:213:PCW:C7	0.46	2.62	6	1
3:D:608:PCW:H283	4:D:628:17F:H73	0.46	1.86	8	1
3:B:205:PCW:C32	3:B:208:PCW:H321	0.46	2.39	8	1
3:D:601:PCW:H372	4:B:216:17F:H77	0.46	1.88	9	1
2:B:116:ASN:ND2	5:B:201:GDP:N7	0.46	2.62	12	1
3:B:204:PCW:C3	4:C:211:17F:H4	0.46	2.38	16	3
3:C:207:PCW:H452	3:C:207:PCW:C20	0.46	2.40	12	1
3:D:621:PCW:H151	4:D:634:17F:C6	0.46	2.38	13	1
3:B:211:PCW:H451	3:B:212:PCW:C3	0.46	2.39	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:412:PCW:C46	3:C:208:PCW:H182	0.46	2.41	16	1
3:B:203:PCW:H412	3:B:203:PCW:H371	0.46	1.86	17	1
3:B:209:PCW:C14	4:B:215:17F:O10	0.46	2.63	17	1
3:B:210:PCW:H462	3:B:213:PCW:H283	0.46	1.86	17	1
3:A:407:PCW:H121	3:C:205:PCW:H142	0.46	1.86	18	1
3:B:203:PCW:H212	4:C:210:17F:H19	0.46	1.81	18	1
2:B:32:TYR:HB2	5:B:201:GDP:H5"	0.46	1.86	1	1
1:A:225:THR:O	1:A:229:TRP:HB2	0.46	2.10	15	4
3:A:404:PCW:C37	4:B:215:17F:H10	0.46	2.40	2	1
3:A:409:PCW:C22	3:A:409:PCW:C17	0.46	2.84	2	1
3:A:413:PCW:H483	4:C:210:17F:C36	0.46	2.40	2	1
3:B:209:PCW:H361	3:B:209:PCW:H232	0.46	1.87	2	1
3:B:210:PCW:O31	3:B:210:PCW:C1	0.46	2.50	15	4
3:A:418:PCW:C11	3:D:614:PCW:H121	0.46	2.41	5	1
3:B:204:PCW:C18	3:C:207:PCW:H283	0.46	2.39	5	1
3:B:209:PCW:H31	3:B:209:PCW:O1P	0.46	2.10	8	5
3:D:617:PCW:O31	3:D:617:PCW:C6	0.46	2.63	19	2
2:C:17:SER:N	5:C:201:GDP:O1A	0.46	2.48	8	5
3:A:411:PCW:C3	4:B:215:17F:H31	0.46	2.39	7	1
3:B:206:PCW:H422	4:C:211:17F:C23	0.46	2.40	15	2
3:A:402:PCW:H181	3:A:409:PCW:H231	0.46	1.87	9	1
2:B:17:SER:N	5:B:201:GDP:O2A	0.46	2.48	11	2
3:A:404:PCW:C17	3:B:209:PCW:H251	0.46	2.38	10	1
3:A:407:PCW:H171	3:B:208:PCW:C20	0.46	2.32	10	1
3:A:413:PCW:H252	4:A:414:17F:C34	0.46	2.41	10	1
3:D:604:PCW:C2	3:D:613:PCW:H62	0.46	2.28	10	1
3:D:608:PCW:H41	4:D:635:17F:O10	0.46	2.10	10	1
2:B:6:LEU:O	2:B:55:ILE:HA	0.46	2.11	20	2
4:D:634:17F:C17	4:D:634:17F:O7	0.46	2.63	13	3
3:B:211:PCW:H151	4:B:217:17F:C33	0.46	2.39	11	1
4:C:211:17F:C30	3:C:212:PCW:H232	0.46	2.40	12	1
3:D:606:PCW:H361	3:D:626:PCW:C43	0.46	2.40	13	1
3:D:614:PCW:H31	3:D:614:PCW:O4P	0.46	2.09	14	1
3:B:211:PCW:C15	4:B:217:17F:C36	0.46	2.93	14	1
1:A:215:SER:O	1:A:219:GLU:HG3	0.46	2.11	16	2
3:B:207:PCW:H342	3:B:210:PCW:C33	0.46	2.40	15	1
3:B:213:PCW:H422	4:B:217:17F:C2X	0.46	2.40	17	1
4:A:415:17F:H59	4:A:415:17F:C36	0.46	2.40	19	1
4:D:628:17F:H18	4:D:631:17F:H55	0.46	1.87	1	1
2:B:101:LYS:HD2	2:B:107:GLU:HA	0.46	1.87	1	1
3:D:604:PCW:H322	3:D:613:PCW:H82	0.46	1.87	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:15:GLY:CA	5:B:201:GDP:H8	0.46	2.24	14	6
4:B:216:17F:H39	4:B:216:17F:H30	0.46	1.86	20	2
3:A:401:PCW:H51	3:A:404:PCW:H12	0.46	1.87	3	1
3:B:208:PCW:C15	4:B:214:17F:H56	0.46	2.39	7	2
3:B:209:PCW:C11	3:B:209:PCW:O2	0.46	2.63	3	3
5:C:201:GDP:O5'	5:C:201:GDP:C2'	0.46	2.63	3	3
3:A:406:PCW:O2P	3:A:406:PCW:C5	0.46	2.62	7	2
2:C:29:VAL:HB	2:C:31:GLU:HG2	0.46	1.86	7	1
4:B:216:17F:H4A	4:B:216:17F:O10	0.46	2.10	9	1
3:A:403:PCW:H483	3:A:416:PCW:C28	0.46	2.40	10	2
4:C:211:17F:H30	4:C:211:17F:H66	0.46	1.87	10	1
3:A:406:PCW:O31	3:A:406:PCW:C1	0.46	2.58	11	1
3:A:418:PCW:C45	3:D:625:PCW:H462	0.46	2.41	19	2
3:D:604:PCW:C41	3:D:619:PCW:H141	0.46	2.40	11	1
3:B:211:PCW:H321	3:B:212:PCW:P	0.46	2.50	11	2
3:A:406:PCW:H63	3:A:406:PCW:O2	0.46	2.10	12	1
2:C:72:MET:SD	2:C:100:ILE:HG12	0.46	2.50	12	1
3:D:602:PCW:C8	3:D:602:PCW:H131	0.46	2.40	13	1
3:A:409:PCW:H181	3:A:409:PCW:H40	0.46	1.86	14	1
3:A:403:PCW:C21	3:A:403:PCW:H171	0.46	2.41	15	1
3:A:412:PCW:O3	3:A:412:PCW:O31	0.46	2.34	17	1
3:D:605:PCW:C25	4:D:629:17F:C24	0.46	2.91	17	1
3:A:403:PCW:C8	3:C:203:PCW:P	0.46	3.03	18	1
3:D:620:PCW:C8	3:D:620:PCW:O4P	0.46	2.63	18	1
4:B:214:17F:H51	4:B:217:17F:C41	0.46	2.32	19	1
2:C:92:ASP:HA	2:C:95:HIS:CD2	0.46	2.45	1	1
3:B:213:PCW:H462	4:B:217:17F:C25	0.46	2.40	2	1
3:C:203:PCW:O2P	3:C:204:PCW:C6	0.46	2.64	6	4
3:A:413:PCW:C11	3:A:413:PCW:C37	0.46	2.93	5	4
3:C:204:PCW:H20	4:C:211:17F:H59	0.46	1.87	4	1
3:D:611:PCW:O1P	3:D:613:PCW:C7	0.46	2.64	5	1
3:D:627:PCW:H281	4:D:633:17F:H46	0.46	1.86	16	3
3:C:203:PCW:O2P	3:C:204:PCW:N	0.46	2.49	6	1
3:A:401:PCW:O2	3:B:209:PCW:C24	0.46	2.64	7	1
3:D:615:PCW:H211	4:D:635:17F:C24	0.46	2.39	7	1
3:D:624:PCW:C6	3:D:624:PCW:C31	0.46	2.93	19	3
3:A:407:PCW:H181	3:C:205:PCW:H342	0.46	1.88	8	1
3:A:409:PCW:O2P	3:A:409:PCW:H52	0.46	2.11	8	1
3:A:413:PCW:H372	4:A:414:17F:H68	0.46	1.86	8	1
3:A:413:PCW:H141	4:A:414:17F:H33	0.46	1.87	8	1
3:D:611:PCW:O1P	3:D:613:PCW:H61	0.46	2.11	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:410:PCW:C16	3:C:209:PCW:H372	0.46	2.40	9	1
3:A:403:PCW:H31	3:A:403:PCW:H42	0.46	1.87	10	1
3:D:625:PCW:H11	3:D:626:PCW:H32	0.46	1.88	10	1
3:A:408:PCW:H261	3:A:417:PCW:H162	0.46	1.87	11	1
3:B:207:PCW:H182	3:B:210:PCW:H141	0.46	1.85	12	1
3:A:402:PCW:H431	3:A:409:PCW:C28	0.46	2.40	14	1
3:D:618:PCW:C27	3:B:206:PCW:H442	0.46	2.28	14	1
3:D:611:PCW:H181	3:D:619:PCW:H151	0.46	1.85	15	1
3:B:204:PCW:O2	3:C:204:PCW:H361	0.46	2.10	17	1
2:B:3:GLU:OE1	3:B:207:PCW:H73	0.46	2.10	18	1
3:B:213:PCW:C27	4:B:215:17F:H61	0.46	2.40	18	1
4:A:415:17F:H72	3:D:611:PCW:H481	0.46	1.85	20	1
3:B:207:PCW:C16	3:B:210:PCW:H172	0.46	2.40	1	2
3:B:209:PCW:H231	3:B:209:PCW:H361	0.46	1.88	1	1
3:C:205:PCW:O3	3:C:205:PCW:C31	0.46	2.63	6	2
3:D:622:PCW:C37	3:D:627:PCW:H20	0.46	2.40	4	1
3:B:204:PCW:H471	3:C:203:PCW:C16	0.46	2.41	5	1
3:A:410:PCW:C27	3:D:618:PCW:H451	0.46	2.37	6	1
3:B:204:PCW:H212	3:B:205:PCW:H472	0.46	1.86	7	1
2:C:45:VAL:HA	2:C:49:GLU:O	0.46	2.10	7	1
3:D:617:PCW:H182	3:D:617:PCW:H221	0.46	1.88	11	1
3:D:625:PCW:H451	3:D:626:PCW:H461	0.46	1.88	11	1
3:D:609:PCW:C6	4:D:633:17F:O1	0.46	2.64	13	1
3:A:407:PCW:H142	3:B:208:PCW:H182	0.46	1.88	15	1
3:B:211:PCW:H431	3:B:212:PCW:H32	0.46	1.87	15	1
3:A:401:PCW:C47	3:D:611:PCW:H241	0.46	2.40	16	1
3:B:206:PCW:H332	3:C:204:PCW:H381	0.46	1.87	16	2
3:A:411:PCW:H39	4:B:215:17F:H69	0.46	1.87	17	1
3:D:618:PCW:H483	3:B:204:PCW:C24	0.46	2.39	17	1
3:D:624:PCW:H62	3:D:624:PCW:O31	0.46	2.10	17	1
3:B:208:PCW:C28	4:B:214:17F:H19	0.46	2.39	19	1
4:A:415:17F:C41	3:B:203:PCW:H272	0.46	2.41	1	1
3:D:613:PCW:C8	3:D:613:PCW:O4P	0.46	2.63	17	5
1:D:416:ARG:HA	1:D:419:LEU:HD12	0.46	1.86	2	1
3:D:604:PCW:H40	3:D:619:PCW:H141	0.46	1.88	3	1
2:B:28:PHE:CZ	5:B:201:GDP:C2	0.46	3.03	3	1
2:C:16:LYS:HE2	2:C:57:ASP:OD2	0.46	2.11	3	1
3:D:617:PCW:C4	3:D:617:PCW:H2	0.46	2.40	4	1
3:B:205:PCW:O3	3:B:208:PCW:C38	0.46	2.63	6	2
3:A:410:PCW:C6	3:C:207:PCW:H341	0.46	2.41	5	1
3:D:617:PCW:H62	3:D:617:PCW:H2	0.46	1.86	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:203:PCW:H381	3:B:211:PCW:H421	0.46	1.87	5	1
3:B:207:PCW:H442	4:B:215:17F:C31	0.46	2.40	6	1
3:C:204:PCW:C13	4:C:211:17F:H62	0.46	2.40	6	1
3:D:616:PCW:O1P	3:C:212:PCW:H51	0.46	2.11	8	1
3:B:208:PCW:C42	4:B:214:17F:H58	0.46	2.41	9	1
3:A:410:PCW:C26	3:D:618:PCW:H452	0.46	2.41	10	1
3:D:610:PCW:O31	3:D:610:PCW:H11	0.46	2.10	10	2
3:D:622:PCW:H362	4:D:629:17F:H77	0.46	1.87	10	1
3:A:408:PCW:C28	3:A:417:PCW:H162	0.46	2.39	11	1
3:A:420:PCW:C13	4:D:632:17F:H11	0.46	2.40	13	1
2:B:114:VAL:HG12	2:B:142:ILE:HB	0.46	1.86	13	1
3:A:403:PCW:H342	3:C:203:PCW:O11	0.46	2.11	14	1
3:B:207:PCW:C40	4:B:217:17F:H8	0.46	2.40	14	1
1:A:224:VAL:O	1:A:228:PHE:HB2	0.46	2.10	15	4
3:A:419:PCW:H351	3:D:617:PCW:H431	0.46	1.86	17	2
1:A:310:ARG:O	1:A:314:ASP:HB2	0.46	2.11	16	9
3:B:203:PCW:H73	3:B:211:PCW:H2	0.46	1.88	1	1
3:A:419:PCW:H372	3:D:617:PCW:H472	0.46	1.87	3	1
3:A:401:PCW:H51	3:A:404:PCW:H11	0.46	1.87	4	1
3:D:603:PCW:C36	4:D:629:17F:H36	0.46	2.40	4	1
3:D:622:PCW:C37	3:D:627:PCW:H211	0.46	2.32	4	1
3:C:206:PCW:H181	3:C:206:PCW:H231	0.46	1.86	5	1
3:A:413:PCW:C12	4:A:414:17F:H58	0.46	2.41	7	1
4:D:634:17F:H19A	4:D:634:17F:H9	0.46	1.87	7	1
3:A:410:PCW:H232	3:A:410:PCW:C17	0.46	2.41	8	1
3:D:611:PCW:C8	3:D:625:PCW:H142	0.46	2.41	17	3
3:B:208:PCW:H19	3:C:205:PCW:C33	0.46	2.36	8	1
3:B:209:PCW:H141	4:B:215:17F:H6	0.46	1.87	9	1
3:B:207:PCW:H212	3:B:207:PCW:C17	0.46	2.34	11	1
2:C:32:TYR:CD1	5:C:201:GDP:H3'	0.46	2.46	11	1
3:C:207:PCW:C48	4:C:211:17F:H19A	0.46	2.41	11	1
3:B:205:PCW:H451	3:B:206:PCW:C23	0.46	2.33	12	1
3:D:621:PCW:O31	3:D:621:PCW:H11	0.46	2.10	13	1
3:B:208:PCW:H131	4:B:214:17F:O10	0.46	2.10	13	2
4:B:215:17F:H11A	4:B:217:17F:H29	0.46	1.85	14	1
3:A:403:PCW:H151	3:C:203:PCW:H261	0.46	1.87	15	1
3:B:213:PCW:O2	3:B:213:PCW:O11	0.46	2.33	15	1
3:A:411:PCW:H431	3:A:418:PCW:H272	0.46	1.88	16	1
3:B:208:PCW:C28	4:B:216:17F:H46	0.46	2.31	17	1
1:A:228:PHE:O	1:A:232:LEU:HB2	0.46	2.11	18	1
4:A:414:17F:H50	3:B:212:PCW:C20	0.46	2.41	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:608:PCW:H332	4:D:635:17F:H20A	0.46	1.85	20	1
3:D:610:PCW:H82	3:C:212:PCW:C7	0.46	2.40	20	1
3:C:207:PCW:H51	4:C:211:17F:N1	0.46	2.26	20	1
3:D:604:PCW:H63	4:D:632:17F:O4	0.46	2.11	5	3
3:D:608:PCW:C27	4:D:628:17F:C39	0.46	2.94	1	1
3:D:622:PCW:H232	3:D:624:PCW:C19	0.46	2.41	1	1
4:D:630:17F:H72	4:D:630:17F:C25	0.46	2.41	1	1
2:B:82:PHE:HB3	2:B:93:ILE:HD11	0.46	1.87	16	3
3:B:211:PCW:C32	3:B:212:PCW:H12	0.46	2.39	1	1
1:A:246:ASP:O	1:A:250:VAL:HB	0.46	2.11	2	2
3:D:606:PCW:H471	3:B:210:PCW:H462	0.46	1.87	2	1
3:B:209:PCW:H271	4:B:215:17F:C1Y	0.46	2.41	2	1
3:B:213:PCW:H371	4:B:217:17F:H59	0.46	1.88	2	1
3:A:420:PCW:C31	3:D:617:PCW:H52	0.46	2.41	3	1
3:B:210:PCW:H451	3:B:213:PCW:H283	0.46	1.87	3	2
3:C:207:PCW:O3	3:C:207:PCW:C31	0.46	2.64	3	5
3:A:420:PCW:O11	3:A:420:PCW:H51	0.46	2.10	5	1
3:D:608:PCW:H442	3:D:615:PCW:C47	0.46	2.41	14	2
3:B:204:PCW:H471	3:C:203:PCW:C17	0.46	2.40	5	1
3:B:208:PCW:H211	4:B:214:17F:C31	0.46	2.37	5	1
2:C:89:SER:O	2:C:93:ILE:HG12	0.46	2.11	5	1
3:C:204:PCW:C24	3:C:207:PCW:H472	0.46	2.33	5	1
1:A:254:VAL:HG22	1:A:258:LEU:HG	0.46	1.87	6	1
3:A:404:PCW:H132	3:A:404:PCW:C34	0.46	2.40	6	1
3:B:210:PCW:H162	4:B:216:17F:H11A	0.46	1.87	6	2
3:A:413:PCW:C19	4:A:414:17F:H34	0.46	2.41	7	1
3:B:204:PCW:H31	3:C:204:PCW:H352	0.46	1.87	8	1
3:D:623:PCW:H281	3:D:624:PCW:C45	0.46	2.37	11	1
3:B:208:PCW:C15	4:B:214:17F:H63	0.46	2.40	12	1
3:A:410:PCW:C3	3:A:410:PCW:P	0.46	3.04	14	1
3:D:611:PCW:H242	3:D:619:PCW:H442	0.46	1.87	14	1
3:A:406:PCW:C23	3:B:207:PCW:C15	0.46	2.94	16	1
3:D:616:PCW:C2	3:C:212:PCW:H342	0.46	2.41	17	1
3:D:608:PCW:H462	3:C:205:PCW:C47	0.46	2.37	19	1
3:A:405:PCW:H411	3:D:601:PCW:C23	0.46	2.39	20	1
3:A:405:PCW:H471	3:A:405:PCW:H162	0.46	1.88	20	1
3:C:208:PCW:C23	3:C:209:PCW:H422	0.46	2.36	1	1
2:B:15:GLY:CA	5:B:201:GDP:C8	0.46	2.99	2	6
3:B:208:PCW:H151	4:B:214:17F:C31	0.46	2.40	3	1
3:B:209:PCW:O2	3:B:209:PCW:O11	0.46	2.33	3	1
3:B:213:PCW:H452	3:B:213:PCW:H212	0.46	1.86	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:618:PCW:O2P	3:D:627:PCW:H82	0.46	2.11	17	2
3:A:412:PCW:H482	3:B:206:PCW:H271	0.46	1.88	6	1
3:D:608:PCW:O31	3:D:608:PCW:C13	0.46	2.64	18	5
3:D:615:PCW:H251	4:B:216:17F:C41	0.46	2.39	6	1
3:D:622:PCW:H331	3:D:627:PCW:H222	0.46	1.88	6	3
3:C:204:PCW:H12	4:C:211:17F:H77	0.46	1.87	6	1
3:C:207:PCW:C27	3:C:209:PCW:H371	0.46	2.40	7	1
3:D:617:PCW:O31	3:D:617:PCW:C7	0.46	2.64	19	3
1:D:426:PHE:O	1:D:430:LEU:HG	0.46	2.11	19	2
3:B:209:PCW:H51	3:B:209:PCW:O11	0.46	2.11	10	1
3:A:402:PCW:H441	3:C:205:PCW:C14	0.46	2.40	11	1
3:A:406:PCW:H262	4:B:216:17F:C20	0.46	2.41	11	1
3:A:419:PCW:H371	3:D:610:PCW:C16	0.46	2.41	11	1
3:D:613:PCW:H281	4:C:210:17F:H35	0.46	1.87	13	1
3:B:205:PCW:H261	3:C:204:PCW:H381	0.46	1.88	13	1
3:A:409:PCW:C37	3:A:409:PCW:H182	0.46	2.41	15	1
3:D:624:PCW:C31	3:D:624:PCW:C6	0.46	2.93	15	1
3:A:416:PCW:O1P	3:A:416:PCW:C5	0.46	2.63	16	1
2:B:6:LEU:HD21	2:B:163:ILE:HD11	0.46	1.88	18	1
3:A:418:PCW:C8	3:D:626:PCW:O31	0.46	2.63	19	1
3:A:406:PCW:H352	3:A:411:PCW:H332	0.46	1.88	1	1
4:B:214:17F:O10	4:B:214:17F:C20	0.46	2.63	1	1
1:D:522:SER:O	1:D:526:ARG:HG3	0.46	2.11	20	5
2:C:6:LEU:O	2:C:55:ILE:HA	0.46	2.11	3	5
3:A:410:PCW:C27	3:C:204:PCW:H481	0.46	2.40	4	1
1:A:278:PRO:O	1:A:282:GLU:HG3	0.46	2.12	20	3
3:A:413:PCW:C48	4:C:210:17F:H65	0.46	2.41	5	2
4:A:414:17F:H49	3:B:212:PCW:H232	0.46	1.87	5	1
3:D:613:PCW:C24	4:C:210:17F:H71	0.46	2.40	5	1
3:B:205:PCW:O1P	3:B:211:PCW:H52	0.46	2.11	6	1
3:A:401:PCW:C1	3:B:209:PCW:H211	0.46	2.33	7	1
3:B:203:PCW:H41	3:B:211:PCW:H331	0.46	1.87	20	2
3:A:402:PCW:H422	3:C:205:PCW:H132	0.46	1.87	10	1
3:A:403:PCW:C42	3:C:203:PCW:H271	0.46	2.41	10	1
3:B:203:PCW:H461	4:B:217:17F:C29	0.46	2.41	10	1
3:C:204:PCW:H142	4:C:211:17F:H66	0.46	1.87	10	1
3:A:413:PCW:C35	3:A:413:PCW:O2	0.46	2.64	11	1
3:B:209:PCW:H471	3:B:209:PCW:C26	0.46	2.41	11	1
3:A:406:PCW:C6	3:A:406:PCW:O2	0.46	2.64	12	1
3:B:204:PCW:O1P	4:C:211:17F:O3	0.46	2.33	12	1
3:B:211:PCW:H42	3:B:212:PCW:O1P	0.46	2.10	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:213:PCW:H222	3:B:213:PCW:C44	0.46	2.38	14	1
3:A:404:PCW:C26	4:A:415:17F:H64	0.46	2.40	15	1
2:C:37:GLU:HG2	2:C:58:THR:HA	0.46	1.86	16	2
2:C:166:HIS:O	2:C:169:LYS:HG2	0.46	2.11	16	1
3:A:404:PCW:H451	4:B:215:17F:H42	0.46	1.88	18	1
3:D:606:PCW:C2	3:D:626:PCW:H371	0.46	2.41	18	1
4:D:634:17F:C34	4:D:635:17F:H70	0.46	2.41	19	1
3:B:211:PCW:H242	4:B:217:17F:H44	0.46	1.88	19	1
3:B:204:PCW:H483	3:B:212:PCW:H19	0.46	1.87	20	1
3:B:211:PCW:C36	3:B:212:PCW:H32	0.45	2.41	1	1
3:C:207:PCW:O1P	3:C:207:PCW:H52	0.45	2.11	1	2
3:A:403:PCW:C6	3:C:203:PCW:O1P	0.45	2.64	2	1
3:D:612:PCW:O3P	3:D:612:PCW:C31	0.45	2.64	2	7
3:D:618:PCW:H251	3:C:204:PCW:H462	0.45	1.88	2	1
4:C:211:17F:H8A	4:C:211:17F:C39	0.45	2.41	2	1
4:A:414:17F:O6	4:A:414:17F:C17	0.45	2.64	6	5
3:D:605:PCW:O4P	3:D:605:PCW:H2	0.45	2.11	3	2
3:D:605:PCW:O31	3:D:605:PCW:P	0.45	2.74	3	1
3:B:205:PCW:H40	4:B:214:17F:H71	0.45	1.88	4	1
3:A:410:PCW:C37	3:C:209:PCW:H182	0.45	2.41	5	1
3:A:416:PCW:C45	3:D:617:PCW:H231	0.45	2.41	5	1
3:B:207:PCW:H82	3:B:207:PCW:O4P	0.45	2.11	9	3
3:B:211:PCW:H171	4:B:217:17F:C38	0.45	2.31	6	1
3:A:403:PCW:C34	3:C:203:PCW:H32	0.45	2.32	7	1
3:B:205:PCW:C47	3:C:208:PCW:H172	0.45	2.38	8	1
3:A:411:PCW:H2	4:B:215:17F:H34	0.45	1.87	9	2
4:B:214:17F:H46	4:B:217:17F:H71	0.45	1.87	9	1
4:A:414:17F:H51	3:C:203:PCW:H422	0.45	1.87	10	1
3:D:608:PCW:H211	3:D:615:PCW:H361	0.45	1.88	10	1
3:D:625:PCW:H19	3:D:625:PCW:H121	0.45	1.88	10	1
1:A:290:LYS:O	1:A:294:LEU:HG	0.45	2.11	12	1
1:A:307:ASP:O	1:A:310:ARG:HB2	0.45	2.10	13	3
3:D:604:PCW:C18	3:D:613:PCW:C36	0.45	2.83	12	1
3:A:402:PCW:C16	3:A:409:PCW:H231	0.45	2.23	15	1
3:A:409:PCW:H172	3:C:205:PCW:H40	0.45	1.87	15	1
3:B:211:PCW:H271	4:B:217:17F:H51	0.45	1.87	15	1
3:A:418:PCW:C38	3:D:625:PCW:H251	0.45	2.41	16	1
3:D:601:PCW:H51	4:B:216:17F:O5	0.45	2.11	16	1
3:D:602:PCW:C44	3:D:610:PCW:H351	0.45	2.40	16	1
3:D:604:PCW:H232	3:D:613:PCW:H181	0.45	1.88	17	1
1:A:386:PHE:CZ	4:A:414:17F:H77	0.45	2.46	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:615:PCW:C43	3:C:205:PCW:H283	0.45	2.41	19	1
3:B:205:PCW:H472	3:C:208:PCW:H282	0.45	1.87	19	1
3:A:412:PCW:C41	3:A:412:PCW:C37	0.45	2.89	1	1
3:B:205:PCW:C40	4:B:214:17F:H69	0.45	2.39	1	1
3:B:207:PCW:C17	3:B:210:PCW:H172	0.45	2.41	1	1
1:A:272:TYR:O	1:A:276:VAL:HB	0.45	2.11	6	2
3:D:615:PCW:H431	4:B:216:17F:H49	0.45	1.87	4	1
3:B:206:PCW:C14	3:B:212:PCW:H421	0.45	2.40	4	1
3:D:623:PCW:H281	3:D:624:PCW:C46	0.45	2.41	5	1
3:A:403:PCW:H51	3:C:203:PCW:O2P	0.45	2.10	8	2
3:D:603:PCW:H411	4:D:629:17F:C2X	0.45	2.25	10	1
3:D:610:PCW:O11	3:D:616:PCW:H41	0.45	2.11	10	1
3:D:622:PCW:H282	3:B:211:PCW:H281	0.45	1.87	10	1
3:D:625:PCW:H32	3:D:626:PCW:H32	0.45	1.88	10	2
4:D:629:17F:P1	4:D:629:17F:O9	0.45	2.74	16	2
3:A:410:PCW:H221	4:D:633:17F:H54	0.45	1.88	11	1
3:B:212:PCW:C42	3:C:212:PCW:H271	0.45	2.37	11	1
3:C:203:PCW:C23	3:C:203:PCW:C18	0.45	2.94	11	1
3:A:402:PCW:H411	3:A:402:PCW:C37	0.45	2.34	12	1
3:A:402:PCW:C45	3:C:205:PCW:H361	0.45	2.41	12	1
1:D:453:GLN:CB	1:D:454:PRO:HD3	0.45	2.42	15	1
3:A:408:PCW:H61	4:C:211:17F:O6	0.45	2.11	16	1
3:A:411:PCW:H431	3:A:418:PCW:C27	0.45	2.41	16	1
3:A:404:PCW:H382	4:B:215:17F:C24	0.45	2.40	17	1
3:A:408:PCW:C34	3:C:207:PCW:C44	0.45	2.86	17	1
3:B:213:PCW:H482	3:B:213:PCW:C28	0.45	2.41	19	1
3:D:623:PCW:H211	3:B:211:PCW:H281	0.45	1.87	1	1
3:B:205:PCW:H461	3:B:206:PCW:H182	0.45	1.87	1	1
3:B:205:PCW:H421	4:B:214:17F:H70	0.45	1.88	1	1
3:C:207:PCW:H42	3:C:207:PCW:O2	0.45	2.10	10	2
1:A:356:HIS:HB3	3:A:401:PCW:H211	0.45	1.88	3	1
4:A:414:17F:C30	3:C:203:PCW:H472	0.45	2.41	3	1
3:C:209:PCW:O31	3:C:209:PCW:O3	0.45	2.35	11	4
3:A:417:PCW:O31	3:A:417:PCW:O3	0.45	2.34	4	1
2:C:16:LYS:HB2	5:C:201:GDP:O3B	0.45	2.11	4	3
2:C:17:SER:HB2	5:C:201:GDP:O1A	0.45	2.11	4	3
3:D:603:PCW:C4	3:D:603:PCW:O11	0.45	2.64	5	1
3:A:413:PCW:C13	4:A:414:17F:C20	0.45	2.94	6	1
2:B:117:LYS:HG2	5:B:201:GDP:C2	0.45	2.47	8	2
3:A:403:PCW:H19	3:C:203:PCW:H131	0.45	1.88	7	1
4:A:414:17F:H48	3:C:203:PCW:H452	0.45	1.86	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:204:PCW:H122	3:C:207:PCW:C1	0.45	2.42	8	1
3:D:616:PCW:C48	3:C:208:PCW:H283	0.45	2.41	20	3
1:D:448:VAL:HA	1:D:451:LYS:HB2	0.45	1.88	11	2
3:D:616:PCW:C45	3:B:206:PCW:H481	0.45	2.41	11	1
4:B:214:17F:O2	4:B:214:17F:C2	0.45	2.64	12	1
3:A:403:PCW:H322	3:C:204:PCW:C5	0.45	2.40	13	1
3:D:603:PCW:H461	3:D:626:PCW:C27	0.45	2.41	13	1
3:B:213:PCW:C40	4:B:217:17F:H63	0.45	2.42	13	1
3:A:402:PCW:H42	3:A:402:PCW:O11	0.45	2.10	15	1
3:B:209:PCW:O31	3:B:209:PCW:O3P	0.45	2.34	15	1
4:D:629:17F:H70	4:D:630:17F:H63	0.45	1.88	16	1
1:D:463:TRP:CD1	4:D:631:17F:H75	0.45	2.46	17	1
3:C:207:PCW:H262	3:C:208:PCW:H241	0.45	1.87	17	1
3:C:208:PCW:H32	3:C:209:PCW:C1	0.45	2.41	19	1
3:D:616:PCW:O2	3:D:616:PCW:P	0.45	2.74	1	2
3:A:407:PCW:O4P	3:A:407:PCW:C8	0.45	2.64	2	5
3:B:209:PCW:H442	4:B:215:17F:C28	0.45	2.42	3	1
3:B:205:PCW:H12	3:B:211:PCW:H42	0.45	1.85	4	1
3:B:205:PCW:H20	3:B:212:PCW:H351	0.45	1.88	6	1
2:C:83:ALA:HB3	2:C:86:ASN:HB3	0.45	1.86	10	4
3:A:413:PCW:C13	4:A:414:17F:H33	0.45	2.42	8	1
3:A:407:PCW:H212	3:C:205:PCW:C17	0.45	2.41	9	1
3:A:408:PCW:C35	3:C:204:PCW:H232	0.45	2.42	9	1
3:A:419:PCW:H351	3:D:617:PCW:C41	0.45	2.41	9	1
3:D:607:PCW:C22	4:D:628:17F:H8A	0.45	2.41	9	1
3:A:416:PCW:C28	3:A:419:PCW:C25	0.45	2.94	10	1
4:D:634:17F:O7	4:D:634:17F:O10	0.45	2.34	13	2
3:A:411:PCW:H482	3:A:418:PCW:H212	0.45	1.85	12	1
3:D:612:PCW:C6	3:D:627:PCW:H32	0.45	2.40	12	1
3:B:205:PCW:O2P	3:B:208:PCW:C8	0.45	2.64	12	1
3:A:401:PCW:H461	3:D:611:PCW:H283	0.45	1.87	14	1
3:A:407:PCW:H262	3:C:205:PCW:H381	0.45	1.86	14	1
3:A:412:PCW:H342	3:C:206:PCW:H451	0.45	1.87	14	1
3:C:208:PCW:P	3:C:209:PCW:H63	0.45	2.52	14	1
3:A:409:PCW:H51	3:A:409:PCW:C31	0.45	2.42	15	1
3:A:420:PCW:H362	3:D:617:PCW:H141	0.45	1.88	15	1
3:B:208:PCW:H222	3:B:208:PCW:H182	0.45	1.87	15	2
3:A:402:PCW:C2	3:A:409:PCW:H272	0.45	2.20	16	1
3:A:403:PCW:H212	3:A:403:PCW:H452	0.45	1.87	17	1
1:D:400:LYS:HB2	1:D:400:LYS:NZ	0.45	2.27	17	1
4:B:214:17F:C22	4:B:217:17F:H70	0.45	2.41	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:255:GLN:HB2	1:A:256:PRO:CD	0.45	2.41	3	17
1:A:348:GLU:O	1:A:352:LYS:HG3	0.45	2.11	20	4
3:D:620:PCW:C1	3:D:620:PCW:C7	0.45	2.90	1	1
4:D:628:17F:O9	4:D:628:17F:C20	0.45	2.59	11	2
3:C:207:PCW:O4P	4:C:211:17F:N1	0.45	2.50	2	1
3:A:409:PCW:O3	3:A:409:PCW:C31	0.45	2.63	14	3
3:A:417:PCW:H421	3:D:612:PCW:H251	0.45	1.88	4	1
3:B:204:PCW:H122	3:C:204:PCW:H39	0.45	1.87	4	1
2:C:158:THR:O	2:C:162:GLU:HG2	0.45	2.11	6	1
3:A:410:PCW:H42	3:C:209:PCW:O11	0.45	2.12	8	2
3:D:620:PCW:O31	3:D:620:PCW:H342	0.45	2.11	9	1
3:A:406:PCW:H40	3:D:606:PCW:C26	0.45	2.37	11	1
3:A:408:PCW:H141	3:A:417:PCW:H261	0.45	1.89	11	1
3:D:604:PCW:C47	3:D:619:PCW:H421	0.45	2.41	11	1
3:D:616:PCW:H272	3:C:204:PCW:H272	0.45	1.87	11	1
3:A:407:PCW:C20	3:C:205:PCW:H171	0.45	2.41	14	1
2:C:3:GLU:HA	2:C:52:LEU:O	0.45	2.12	14	1
3:B:205:PCW:H152	4:B:214:17F:C22	0.45	2.42	15	1
3:B:207:PCW:H152	3:B:210:PCW:H361	0.45	1.89	15	1
3:A:407:PCW:C5	4:B:216:17F:H11	0.45	2.42	16	1
3:D:603:PCW:C28	3:B:210:PCW:H483	0.45	2.38	16	1
3:B:207:PCW:C33	3:B:210:PCW:H332	0.45	2.42	16	1
3:A:404:PCW:C41	3:B:209:PCW:C19	0.45	2.94	17	1
4:D:628:17F:H8A	4:D:631:17F:C1Z	0.45	2.40	17	1
3:A:404:PCW:H381	3:A:404:PCW:C42	0.45	2.33	18	1
3:A:405:PCW:H261	1:D:451:LYS:HD2	0.45	1.86	18	1
3:D:604:PCW:H2	3:D:613:PCW:C6	0.45	2.41	3	1
4:D:633:17F:C30	3:C:209:PCW:H452	0.45	2.41	3	1
3:A:401:PCW:H462	3:D:614:PCW:C22	0.45	2.42	4	1
4:D:630:17F:C29	3:B:212:PCW:H451	0.45	2.42	4	1
3:B:210:PCW:H421	4:B:215:17F:H68	0.45	1.89	4	1
3:C:203:PCW:C42	3:C:203:PCW:H161	0.45	2.40	5	1
4:A:415:17F:H75	4:C:210:17F:H56	0.45	1.88	6	1
3:D:610:PCW:H41	3:D:616:PCW:O1P	0.45	2.12	6	1
3:D:623:PCW:H131	3:D:623:PCW:C37	0.45	2.40	9	2
3:A:406:PCW:H122	3:B:210:PCW:H331	0.45	1.89	7	1
2:C:44:VAL:HG23	2:C:51:CYS:HB2	0.45	1.89	7	1
3:C:204:PCW:H11	3:C:204:PCW:H42	0.45	1.88	7	1
3:C:208:PCW:H462	3:C:209:PCW:H442	0.45	1.88	7	1
3:D:622:PCW:H421	3:B:206:PCW:C26	0.45	2.42	8	1
3:B:205:PCW:O31	3:B:205:PCW:H11	0.45	2.10	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:213:PCW:H171	3:B:213:PCW:H361	0.45	1.87	10	1
3:A:416:PCW:O2	3:D:610:PCW:H381	0.45	2.11	11	1
3:D:602:PCW:H121	3:D:624:PCW:H181	0.45	1.87	11	1
3:C:204:PCW:C33	4:C:211:17F:H8	0.45	2.32	11	1
3:A:404:PCW:H441	3:B:207:PCW:C46	0.45	2.41	12	1
3:A:409:PCW:C41	3:A:409:PCW:H372	0.45	2.42	12	1
4:A:414:17F:H55	3:B:212:PCW:H231	0.45	1.85	12	1
3:A:418:PCW:H481	3:D:603:PCW:H272	0.45	1.87	13	1
3:D:603:PCW:H182	3:B:211:PCW:C28	0.45	2.42	13	1
3:B:205:PCW:H222	3:B:212:PCW:C35	0.45	2.27	13	1
3:A:412:PCW:C43	3:C:206:PCW:H40	0.45	2.41	15	1
3:A:417:PCW:H82	3:D:617:PCW:H421	0.45	1.87	15	1
3:D:602:PCW:C4	3:D:602:PCW:O31	0.45	2.60	15	1
3:C:205:PCW:H452	3:C:206:PCW:H20	0.45	1.87	15	1
3:A:412:PCW:C45	3:C:208:PCW:H471	0.45	2.39	19	1
3:B:205:PCW:C44	3:B:206:PCW:C21	0.45	2.94	19	1
3:D:602:PCW:H451	3:D:610:PCW:H412	0.45	1.89	20	1
3:D:605:PCW:H262	4:D:629:17F:H41	0.45	1.87	20	1
1:A:262:GLN:O	1:A:266:GLN:HG3	0.45	2.11	1	1
3:A:402:PCW:H321	3:C:205:PCW:O2P	0.45	2.12	1	1
3:A:408:PCW:H282	3:A:417:PCW:H482	0.45	1.89	2	1
3:C:204:PCW:H20	4:C:211:17F:C18	0.45	2.41	2	1
3:D:602:PCW:O31	3:D:602:PCW:C8	0.45	2.62	9	2
3:D:614:PCW:O31	3:D:614:PCW:H11	0.45	2.12	5	2
3:A:406:PCW:H252	3:B:207:PCW:C19	0.45	2.41	20	2
3:D:623:PCW:O2	3:D:623:PCW:C11	0.45	2.65	6	2
3:B:204:PCW:H382	3:B:212:PCW:H141	0.45	1.88	6	1
3:A:403:PCW:C8	3:C:203:PCW:O1P	0.45	2.54	7	2
3:D:608:PCW:H251	4:D:628:17F:H73	0.45	1.87	7	1
2:C:81:VAL:HA	2:C:114:VAL:O	0.45	2.11	8	2
3:B:207:PCW:C8	4:B:216:17F:C5	0.45	2.90	9	1
3:B:204:PCW:H12	3:B:212:PCW:C6	0.45	2.38	11	1
3:B:204:PCW:C38	3:B:212:PCW:H132	0.45	2.41	13	1
3:C:204:PCW:H31	4:C:211:17F:H75	0.45	1.87	13	1
3:C:207:PCW:C14	3:C:209:PCW:H31	0.45	2.42	14	1
3:A:403:PCW:C15	3:C:203:PCW:H261	0.45	2.42	15	1
3:A:404:PCW:O31	3:A:404:PCW:H73	0.45	2.12	15	1
3:A:403:PCW:H322	3:C:203:PCW:O2P	0.45	2.12	17	1
3:B:212:PCW:O4P	3:B:212:PCW:C7	0.45	2.64	17	1
3:D:603:PCW:H271	4:B:217:17F:H77	0.45	1.87	18	1
3:A:413:PCW:C12	4:A:414:17F:C38	0.45	2.91	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:207:PCW:H231	3:C:208:PCW:H241	0.45	1.85	19	1
3:D:606:PCW:H412	3:D:626:PCW:H472	0.45	1.89	20	1
2:B:135:ARG:HD3	2:C:151:GLY:HA2	0.45	1.87	20	1
3:A:404:PCW:C8	3:A:404:PCW:O4P	0.45	2.64	1	1
3:D:613:PCW:H221	4:C:210:17F:C27	0.45	2.40	1	1
3:B:210:PCW:O2P	4:B:216:17F:O3	0.45	2.35	1	1
3:B:213:PCW:H39	4:B:217:17F:C37	0.45	2.42	1	1
3:C:212:PCW:O2	3:C:212:PCW:C11	0.45	2.64	4	8
4:A:414:17F:C25	4:C:210:17F:H33	0.45	2.38	2	1
3:A:416:PCW:H442	3:D:617:PCW:H242	0.45	1.88	2	1
3:A:411:PCW:O31	3:A:411:PCW:C1	0.45	2.56	3	1
3:D:602:PCW:H141	3:D:624:PCW:H181	0.45	1.87	3	1
3:D:625:PCW:C39	3:D:626:PCW:H141	0.45	2.42	10	2
3:A:404:PCW:O31	3:A:404:PCW:O3	0.45	2.34	15	2
3:A:416:PCW:C8	4:D:632:17F:O5	0.45	2.65	4	2
3:A:417:PCW:C36	3:D:612:PCW:O3	0.45	2.64	6	1
3:A:403:PCW:H321	3:C:204:PCW:H42	0.45	1.89	7	1
3:A:405:PCW:O1P	3:A:405:PCW:C5	0.45	2.64	7	1
3:D:621:PCW:H221	4:D:633:17F:H31	0.45	1.89	7	1
4:D:629:17F:H68	4:D:630:17F:H62	0.45	1.89	8	1
3:B:209:PCW:C19	4:B:215:17F:H19	0.45	2.34	8	1
3:A:404:PCW:H472	3:B:209:PCW:H252	0.45	1.89	9	1
3:B:206:PCW:C22	3:C:208:PCW:H282	0.45	2.41	9	3
3:A:402:PCW:H441	3:C:205:PCW:H141	0.45	1.89	11	1
3:D:618:PCW:C46	3:C:208:PCW:H271	0.45	2.42	12	1
3:D:620:PCW:C14	4:D:635:17F:O9	0.45	2.61	13	2
3:B:206:PCW:C42	3:C:212:PCW:H232	0.45	2.41	13	1
3:D:604:PCW:H322	3:D:611:PCW:C1	0.45	2.42	14	1
3:A:409:PCW:H182	3:A:409:PCW:C39	0.45	2.38	19	2
3:B:211:PCW:C37	3:B:211:PCW:C41	0.45	2.92	15	1
3:A:402:PCW:H321	3:C:206:PCW:O1P	0.45	2.12	18	1
3:D:621:PCW:H421	4:D:634:17F:H63	0.45	1.89	20	1
3:D:611:PCW:H82	3:D:625:PCW:H141	0.45	1.87	1	1
3:B:205:PCW:H431	3:B:206:PCW:H161	0.45	1.88	18	2
4:D:630:17F:O6	4:D:630:17F:C17	0.45	2.64	2	2
3:D:618:PCW:C25	3:B:206:PCW:H442	0.45	2.34	3	1
3:D:623:PCW:H12	3:D:625:PCW:H161	0.45	1.89	3	2
3:B:210:PCW:H281	3:B:210:PCW:H481	0.45	1.89	3	1
3:B:210:PCW:C45	3:B:213:PCW:H283	0.45	2.41	3	1
2:C:123:ARG:HD3	2:C:125:VAL:O	0.45	2.12	12	4
2:C:17:SER:OG	5:C:201:GDP:O3B	0.45	2.35	19	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:413:PCW:C45	4:C:210:17F:H40	0.45	2.42	5	1
2:C:127:THR:HG22	2:C:131:GLN:HE21	0.45	1.71	5	1
2:B:21:ILE:HG21	2:B:29:VAL:HG13	0.45	1.89	6	1
4:D:630:17F:O9	4:D:630:17F:O8	0.45	2.35	7	1
3:D:604:PCW:H212	3:D:613:PCW:C15	0.45	2.41	8	1
3:A:411:PCW:C1	4:B:215:17F:H31	0.45	2.42	9	1
2:B:14:VAL:HG23	2:B:16:LYS:HG3	0.45	1.89	14	2
3:D:604:PCW:H132	3:D:613:PCW:H2	0.45	1.89	11	1
3:B:212:PCW:H2	3:B:212:PCW:O11	0.45	2.11	11	2
3:B:213:PCW:C22	4:B:217:17F:H10	0.45	2.41	11	1
3:B:212:PCW:O31	3:B:212:PCW:C1	0.45	2.63	12	1
3:A:419:PCW:H421	3:D:616:PCW:H232	0.45	1.88	13	2
2:C:6:LEU:HD12	2:C:55:ILE:HD11	0.45	1.88	13	1
3:D:616:PCW:H281	3:C:204:PCW:H262	0.45	1.88	15	1
3:D:622:PCW:H181	4:D:630:17F:H29	0.45	1.89	15	1
3:B:210:PCW:C13	4:B:216:17F:H6	0.45	2.42	15	1
3:B:211:PCW:H62	3:B:211:PCW:O2	0.45	2.11	15	1
3:A:411:PCW:H431	3:A:418:PCW:H281	0.45	1.89	16	1
3:B:209:PCW:H221	3:B:209:PCW:H362	0.45	1.89	16	1
3:A:403:PCW:H212	3:A:403:PCW:C46	0.45	2.42	17	1
3:D:606:PCW:H431	3:D:625:PCW:H472	0.45	1.85	17	1
3:B:213:PCW:H39	4:B:217:17F:H67	0.45	1.88	18	1
3:C:207:PCW:H342	3:C:207:PCW:H121	0.45	1.89	18	1
3:A:407:PCW:H272	3:A:409:PCW:H242	0.45	1.89	20	1
3:A:404:PCW:H222	4:A:415:17F:H77	0.45	1.88	1	1
3:B:212:PCW:C42	3:C:212:PCW:H262	0.45	2.31	1	1
3:D:604:PCW:O2P	3:D:613:PCW:C5	0.45	2.64	2	2
3:C:204:PCW:O3	4:C:211:17F:C41	0.45	2.65	2	1
3:A:401:PCW:H482	3:D:611:PCW:C23	0.45	2.12	3	1
3:D:618:PCW:H462	3:B:204:PCW:H232	0.45	1.88	3	1
3:B:210:PCW:H471	3:B:210:PCW:H272	0.45	1.88	3	1
3:A:401:PCW:H281	3:D:614:PCW:H281	0.45	1.88	4	1
4:A:414:17F:O8	4:A:414:17F:H5	0.45	2.10	4	1
3:B:207:PCW:O4P	3:B:207:PCW:C8	0.45	2.65	4	2
3:B:210:PCW:C14	4:B:216:17F:H18A	0.45	2.42	4	1
3:A:402:PCW:H181	3:A:409:PCW:C20	0.45	2.42	5	1
3:A:413:PCW:H452	4:C:210:17F:H40	0.45	1.89	5	1
4:B:216:17F:H4	4:B:216:17F:HN1	0.45	1.70	6	1
3:A:406:PCW:H362	3:A:411:PCW:C32	0.45	2.42	7	1
3:A:413:PCW:H372	4:A:414:17F:C36	0.45	2.42	8	1
3:C:204:PCW:H20	4:C:211:17F:H19A	0.45	1.89	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:406:PCW:H63	3:A:406:PCW:O2P	0.45	2.12	9	1
3:A:409:PCW:O3	3:C:206:PCW:C33	0.45	2.65	9	1
3:D:621:PCW:H20	4:D:633:17F:O10	0.45	2.12	9	1
3:A:413:PCW:C12	4:A:414:17F:H20	0.45	2.42	11	1
4:D:631:17F:H1	4:D:631:17F:H4	0.45	1.89	20	2
3:B:206:PCW:H482	3:C:212:PCW:C21	0.45	2.39	13	1
3:A:402:PCW:C38	3:C:205:PCW:H381	0.45	2.42	15	1
3:A:407:PCW:C14	3:B:208:PCW:H242	0.45	2.41	15	1
3:D:607:PCW:C26	4:D:631:17F:H63	0.45	2.39	15	2
3:D:607:PCW:C21	4:D:631:17F:H20	0.45	2.41	16	1
3:D:621:PCW:H381	4:D:635:17F:H77	0.45	1.89	18	1
3:A:418:PCW:H82	3:D:626:PCW:C31	0.45	2.42	19	1
3:B:204:PCW:O4P	3:B:204:PCW:C8	0.44	2.66	6	9
3:A:403:PCW:H152	3:C:203:PCW:C3	0.44	2.42	2	1
3:D:616:PCW:H61	3:D:617:PCW:C36	0.44	2.41	18	2
4:B:216:17F:C24	4:B:216:17F:C2X	0.44	2.91	2	1
2:C:13:GLY:N	5:C:201:GDP:O2B	0.44	2.48	3	1
3:D:601:PCW:H282	4:D:631:17F:H72	0.44	1.89	4	1
3:D:602:PCW:C25	3:D:610:PCW:H171	0.44	2.43	4	1
2:B:84:ILE:HD13	2:B:118:CYS:HA	0.44	1.87	4	2
3:D:623:PCW:C38	3:D:625:PCW:C18	0.44	2.96	6	1
3:B:211:PCW:C45	3:B:212:PCW:H131	0.44	2.41	6	1
4:A:414:17F:H40	3:C:203:PCW:H372	0.44	1.89	7	1
3:D:607:PCW:H261	4:D:631:17F:C33	0.44	2.42	7	1
3:D:608:PCW:C7	3:D:620:PCW:O11	0.44	2.64	12	2
4:D:629:17F:O10	4:D:629:17F:N1	0.44	2.50	7	1
4:A:415:17F:H76	3:D:619:PCW:C47	0.44	2.42	8	1
3:D:612:PCW:C7	3:D:618:PCW:H31	0.44	2.42	8	1
1:A:332:ALA:O	1:A:336:GLU:HB2	0.44	2.12	9	1
4:A:415:17F:O9	4:A:415:17F:O8	0.44	2.35	19	2
3:A:406:PCW:C45	3:B:207:PCW:H282	0.44	2.41	12	1
4:D:630:17F:O7	4:D:630:17F:C17	0.44	2.65	12	2
3:D:603:PCW:H182	3:B:211:PCW:H281	0.44	1.89	13	1
3:C:204:PCW:H181	4:C:211:17F:H63	0.44	1.89	14	1
3:B:205:PCW:C1	3:B:205:PCW:O31	0.44	2.62	17	1
3:A:404:PCW:C45	4:B:215:17F:H42	0.44	2.42	18	1
3:B:210:PCW:H281	4:B:215:17F:H74	0.44	1.87	18	1
3:D:626:PCW:C31	3:D:626:PCW:O2P	0.44	2.66	19	1
3:D:622:PCW:H481	3:B:205:PCW:H421	0.44	1.90	20	1
4:B:214:17F:C24	4:B:217:17F:H66	0.44	2.41	20	1
3:C:208:PCW:H141	3:C:209:PCW:H371	0.44	1.89	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:615:PCW:H241	4:D:635:17F:H41	0.44	1.89	1	1
4:D:632:17F:O6	4:D:632:17F:C17	0.44	2.65	1	7
3:B:210:PCW:C45	3:B:213:PCW:H271	0.44	2.43	1	1
3:A:403:PCW:H281	3:A:413:PCW:H271	0.44	1.87	2	1
3:A:404:PCW:H252	4:A:415:17F:H69	0.44	1.88	2	1
3:A:413:PCW:C3	3:A:413:PCW:H351	0.44	2.42	11	2
3:B:203:PCW:H382	3:B:211:PCW:H182	0.44	1.89	3	2
3:A:408:PCW:H42	3:C:204:PCW:H171	0.44	1.89	5	1
3:D:606:PCW:O2	3:D:626:PCW:C37	0.44	2.53	5	1
3:B:203:PCW:C7	4:B:217:17F:H18	0.44	2.43	7	1
3:D:611:PCW:H20	3:D:611:PCW:C42	0.44	2.43	8	1
3:B:213:PCW:H483	4:B:217:17F:H44	0.44	1.89	8	1
3:A:401:PCW:H182	3:A:401:PCW:C22	0.44	2.37	9	1
3:A:401:PCW:H73	3:B:209:PCW:C31	0.44	2.42	9	1
3:B:203:PCW:C21	4:C:210:17F:H32	0.44	2.41	9	1
3:A:411:PCW:C37	4:B:215:17F:H65	0.44	2.40	10	1
3:C:207:PCW:H212	3:C:207:PCW:C17	0.44	2.08	11	1
3:D:618:PCW:O2P	3:D:627:PCW:O4P	0.44	2.35	12	1
3:D:614:PCW:H41	3:D:625:PCW:H42	0.44	1.81	13	1
3:B:210:PCW:C12	4:B:216:17F:H18A	0.44	2.42	13	1
3:D:607:PCW:C26	4:D:631:17F:H30	0.44	2.32	14	1
3:A:407:PCW:C24	3:C:205:PCW:H382	0.44	2.41	16	1
1:D:435:GLU:OE1	1:D:438:ARG:HD2	0.44	2.13	16	1
3:D:603:PCW:C7	4:D:630:17F:P1	0.44	3.05	16	1
2:B:82:PHE:HB2	2:B:89:SER:HB2	0.44	1.88	16	1
1:A:338:LEU:O	1:A:342:GLY:HA3	0.44	2.12	17	2
4:D:628:17F:C8	4:D:631:17F:C1Z	0.44	2.96	17	1
3:A:409:PCW:C31	3:A:409:PCW:O3	0.44	2.65	18	1
3:B:208:PCW:C14	4:B:214:17F:H60	0.44	2.41	18	1
3:D:615:PCW:H41	4:D:635:17F:HN1A	0.44	1.71	19	1
3:D:610:PCW:O2	3:D:610:PCW:C11	0.44	2.65	1	1
3:D:627:PCW:C5	3:D:627:PCW:H2	0.44	2.41	1	1
3:B:203:PCW:H172	4:C:210:17F:H19	0.44	1.88	1	1
3:A:410:PCW:H39	3:C:209:PCW:H182	0.44	1.88	2	1
3:D:604:PCW:H461	3:D:624:PCW:H441	0.44	1.90	2	1
4:D:629:17F:H18A	4:D:629:17F:C6	0.44	2.36	2	1
4:D:628:17F:C23	4:D:631:17F:H74	0.44	2.42	3	2
2:B:46:ILE:HG21	2:B:160:VAL:HG21	0.44	1.88	3	1
2:C:78:PHE:HE2	2:C:104:LYS:HD2	0.44	1.72	3	1
1:A:306:ARG:O	1:A:310:ARG:HG3	0.44	2.12	4	1
3:D:626:PCW:O3	3:D:626:PCW:O31	0.44	2.35	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:204:PCW:C47	3:C:203:PCW:H152	0.44	2.42	5	1
3:B:204:PCW:H132	3:B:206:PCW:C4	0.44	2.41	6	1
3:B:204:PCW:C40	3:B:212:PCW:H151	0.44	2.42	6	1
3:C:203:PCW:C35	3:C:203:PCW:C7	0.44	2.95	6	1
3:A:410:PCW:H62	3:C:209:PCW:C11	0.44	2.42	7	1
3:D:609:PCW:O31	3:D:609:PCW:H11	0.44	2.10	8	1
3:B:211:PCW:H221	3:B:211:PCW:C18	0.44	2.37	8	1
3:C:206:PCW:C15	3:C:206:PCW:H362	0.44	2.43	8	1
2:C:126:ASP:O	2:C:129:GLN:HG2	0.44	2.11	9	1
3:D:603:PCW:C28	3:B:213:PCW:H471	0.44	2.40	11	1
3:D:622:PCW:H352	3:D:627:PCW:C24	0.44	2.42	11	1
3:A:406:PCW:H63	3:A:406:PCW:O3P	0.44	2.12	12	1
3:B:213:PCW:H412	4:B:217:17F:H12	0.44	1.89	12	1
3:C:204:PCW:H211	3:C:204:PCW:H162	0.44	1.89	13	2
3:A:407:PCW:H141	3:B:208:PCW:H20	0.44	1.89	13	1
3:D:621:PCW:C20	4:D:633:17F:H31	0.44	2.42	13	1
3:B:205:PCW:C43	3:B:206:PCW:H141	0.44	2.35	13	1
3:D:603:PCW:H11	3:D:605:PCW:H61	0.44	1.89	14	1
3:B:210:PCW:H122	4:B:216:17F:H18	0.44	1.89	14	1
3:A:401:PCW:H381	3:A:404:PCW:C20	0.44	2.42	15	1
3:B:206:PCW:H41	3:B:206:PCW:H31	0.44	1.88	15	1
3:B:210:PCW:C14	4:B:216:17F:H6	0.44	2.42	15	1
4:D:629:17F:C26	4:D:630:17F:H78	0.44	2.41	16	1
3:D:614:PCW:O4P	3:D:614:PCW:H31	0.44	2.12	17	1
3:B:210:PCW:H73	3:B:210:PCW:C12	0.44	2.42	17	1
3:A:404:PCW:O4P	3:A:404:PCW:H2	0.44	2.13	18	1
4:D:629:17F:O9	4:D:629:17F:O1	0.44	2.36	18	1
3:A:413:PCW:H382	4:C:210:17F:H9A	0.44	1.90	19	1
3:D:608:PCW:H381	3:C:205:PCW:C28	0.44	2.42	20	1
3:A:412:PCW:C39	3:C:206:PCW:H351	0.44	2.41	1	1
3:D:602:PCW:C42	3:D:610:PCW:H362	0.44	2.26	1	1
3:A:407:PCW:H82	4:B:216:17F:H10A	0.44	1.86	2	2
3:A:420:PCW:H381	3:D:617:PCW:C14	0.44	2.43	2	1
3:D:608:PCW:H382	3:C:205:PCW:H283	0.44	1.89	2	1
3:B:213:PCW:C44	4:B:217:17F:H40	0.44	2.27	2	1
3:A:406:PCW:H472	3:B:207:PCW:C26	0.44	2.43	3	1
3:A:413:PCW:H251	3:C:203:PCW:H431	0.44	1.89	4	1
3:B:206:PCW:C36	3:C:204:PCW:H381	0.44	2.42	5	1
4:B:217:17F:H77	4:B:217:17F:C27	0.44	2.42	5	1
3:D:611:PCW:O1P	3:D:613:PCW:H73	0.44	2.13	6	1
3:B:204:PCW:O2P	3:B:212:PCW:H61	0.44	2.12	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:407:PCW:H141	3:B:208:PCW:C26	0.44	2.42	8	1
3:D:613:PCW:C48	3:D:619:PCW:H161	0.44	2.42	9	2
1:D:541:GLY:HA2	1:D:544:LEU:HD12	0.44	1.88	10	1
3:D:616:PCW:H431	3:D:618:PCW:H232	0.44	1.88	11	1
3:A:408:PCW:O2	3:A:408:PCW:P	0.44	2.75	12	1
4:D:635:17F:C36	3:C:205:PCW:H483	0.44	2.40	12	1
3:B:210:PCW:O1P	4:B:216:17F:C1	0.44	2.65	12	1
2:C:28:PHE:CZ	5:C:201:GDP:C2	0.44	3.05	12	1
3:B:208:PCW:C44	4:B:214:17F:H32	0.44	2.41	13	1
3:D:618:PCW:H482	3:B:204:PCW:H242	0.44	1.90	14	1
3:A:406:PCW:H52	3:B:207:PCW:C35	0.44	2.42	18	1
3:B:204:PCW:H283	3:C:204:PCW:H422	0.44	1.90	1	1
3:B:207:PCW:H142	3:B:210:PCW:H411	0.44	1.88	1	1
1:A:250:VAL:HG21	3:A:412:PCW:C27	0.44	2.42	3	1
3:C:203:PCW:H382	3:C:203:PCW:C13	0.44	2.42	3	1
3:C:206:PCW:O31	3:C:206:PCW:H11	0.44	2.11	19	3
2:C:58:THR:HG21	2:C:71:TYR:CE1	0.44	2.47	4	1
3:B:213:PCW:H40	4:B:214:17F:H55	0.44	1.90	5	1
3:D:626:PCW:H181	3:D:626:PCW:H211	0.44	1.51	6	4
2:B:16:LYS:NZ	5:B:201:GDP:O1B	0.44	2.50	7	1
1:A:244:SER:O	1:A:248:GLU:HB2	0.44	2.12	8	1
3:A:408:PCW:H471	3:A:410:PCW:H332	0.44	1.90	8	1
3:A:419:PCW:H482	3:D:618:PCW:C28	0.44	2.43	8	1
1:D:435:GLU:O	1:D:439:GLN:HG3	0.44	2.12	8	2
3:D:615:PCW:H472	3:C:205:PCW:C20	0.44	2.25	8	1
4:B:217:17F:N1	4:B:217:17F:H4A	0.44	2.27	8	2
2:B:49:GLU:HG3	3:C:207:PCW:H61	0.44	1.90	9	1
3:A:411:PCW:H411	3:A:418:PCW:C28	0.44	2.43	12	1
3:A:418:PCW:H2	3:A:418:PCW:O2P	0.44	2.13	16	2
3:B:207:PCW:C34	3:B:210:PCW:H341	0.44	2.42	12	1
3:A:419:PCW:H432	3:D:610:PCW:H212	0.44	1.89	13	1
3:D:601:PCW:C8	4:B:216:17F:P1	0.44	3.06	13	1
3:B:207:PCW:C3	3:B:210:PCW:H132	0.44	2.43	14	1
3:A:402:PCW:H73	3:A:402:PCW:C11	0.44	2.43	15	1
3:A:407:PCW:H142	3:C:205:PCW:H321	0.44	1.88	16	2
3:D:615:PCW:H221	3:C:205:PCW:H272	0.44	1.89	16	1
3:D:622:PCW:H331	3:C:212:PCW:H422	0.44	1.89	17	1
3:B:207:PCW:H152	3:B:210:PCW:H351	0.44	1.89	17	1
3:A:401:PCW:C46	3:D:611:PCW:H262	0.44	2.43	18	1
3:D:605:PCW:H232	4:D:629:17F:C22	0.44	2.39	18	1
3:B:208:PCW:H432	4:B:214:17F:H76	0.44	1.88	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:208:PCW:C23	3:C:209:PCW:H451	0.44	2.41	20	1
4:A:414:17F:H36	4:C:210:17F:H20	0.44	1.90	1	1
3:D:603:PCW:O11	3:D:603:PCW:C5	0.44	2.65	4	2
3:C:205:PCW:C35	3:C:206:PCW:H122	0.44	2.43	1	1
1:A:279:LEU:HD11	1:D:499:LEU:HD11	0.44	1.88	2	3
3:A:406:PCW:C34	3:A:411:PCW:C32	0.44	2.95	2	1
3:D:604:PCW:H471	3:D:619:PCW:H432	0.44	1.88	2	1
3:D:608:PCW:C5	4:D:635:17F:N1	0.44	2.80	4	1
3:B:211:PCW:C7	3:B:212:PCW:C33	0.44	2.90	4	1
3:C:209:PCW:H331	3:C:209:PCW:H52	0.44	1.90	4	1
3:D:605:PCW:H41	3:D:605:PCW:O31	0.44	2.11	5	2
3:B:203:PCW:H451	3:B:211:PCW:H221	0.44	1.88	5	1
2:C:82:PHE:HE2	2:C:113:LEU:HG	0.44	1.73	5	3
3:B:204:PCW:H142	3:C:207:PCW:H11	0.44	1.89	6	1
3:A:402:PCW:C44	3:C:205:PCW:H361	0.44	2.29	7	1
4:A:414:17F:C24	3:B:204:PCW:H462	0.44	2.35	7	1
3:B:203:PCW:O11	3:B:203:PCW:C2	0.44	2.57	13	2
3:B:203:PCW:H331	4:B:215:17F:H37	0.44	1.89	10	1
3:A:411:PCW:H261	3:A:418:PCW:H271	0.44	1.89	11	1
3:C:207:PCW:H242	3:C:207:PCW:H142	0.44	1.89	11	1
3:D:615:PCW:H161	4:D:635:17F:H10	0.44	1.89	12	1
3:A:411:PCW:H162	3:A:418:PCW:H283	0.44	1.90	13	1
3:A:401:PCW:O2P	3:A:404:PCW:H32	0.44	2.13	14	1
3:A:402:PCW:H61	3:A:409:PCW:H32	0.44	1.88	15	1
3:A:407:PCW:H242	3:C:205:PCW:H442	0.44	1.88	15	1
3:B:207:PCW:H141	3:B:210:PCW:H341	0.44	1.90	15	1
3:A:402:PCW:H322	3:C:206:PCW:H41	0.44	1.90	19	1
3:A:403:PCW:H19	3:C:203:PCW:C13	0.44	2.43	19	1
3:B:204:PCW:C34	3:C:204:PCW:H341	0.44	2.37	20	1
3:D:608:PCW:H261	3:D:615:PCW:C40	0.44	2.42	1	1
3:A:402:PCW:H432	3:C:205:PCW:H152	0.44	1.88	3	1
3:A:404:PCW:H452	3:B:209:PCW:C20	0.44	2.42	3	1
3:A:409:PCW:C12	3:C:206:PCW:C33	0.44	2.95	3	1
3:C:208:PCW:H231	3:C:209:PCW:C40	0.44	2.19	3	1
1:A:353:ALA:O	1:A:357:LEU:HG	0.44	2.13	4	2
3:A:401:PCW:H442	3:D:614:PCW:H241	0.44	1.89	4	1
3:D:607:PCW:H152	4:D:631:17F:O10	0.44	2.12	4	1
3:B:211:PCW:C32	3:B:212:PCW:O3P	0.44	2.66	4	1
3:C:206:PCW:H362	3:C:206:PCW:H132	0.44	1.89	4	1
2:C:82:PHE:CE2	2:C:113:LEU:HG	0.44	2.48	5	1
1:A:247:LEU:O	1:A:250:VAL:HG12	0.44	2.12	8	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:203:PCW:H341	3:C:203:PCW:C8	0.44	2.43	6	1
3:C:204:PCW:C21	4:C:211:17F:H31	0.44	2.42	6	1
4:A:414:17F:H45	3:B:204:PCW:C48	0.44	2.37	7	1
4:C:211:17F:C30	3:C:212:PCW:H182	0.44	2.43	8	1
3:A:401:PCW:C4	3:B:209:PCW:H321	0.44	2.43	9	1
3:B:208:PCW:H352	4:B:214:17F:O10	0.44	2.13	11	1
2:B:20:THR:O	2:B:24:ILE:HG12	0.44	2.13	12	1
3:B:206:PCW:H40	3:C:212:PCW:C24	0.44	2.43	19	2
3:D:604:PCW:H322	3:D:613:PCW:H61	0.44	1.88	13	1
3:D:617:PCW:O31	3:D:617:PCW:O3	0.44	2.36	13	1
3:B:204:PCW:H19	3:B:205:PCW:C47	0.44	2.43	13	1
3:A:404:PCW:H361	3:B:209:PCW:H351	0.44	1.90	14	1
3:B:211:PCW:H152	4:B:217:17F:C36	0.44	2.42	14	1
3:C:207:PCW:O4P	4:C:211:17F:C1	0.44	2.56	14	1
1:A:273:ARG:O	1:A:277:GLU:HG3	0.44	2.13	15	1
3:A:402:PCW:H332	3:A:402:PCW:C6	0.44	2.38	15	1
3:A:410:PCW:H171	3:C:207:PCW:C24	0.44	2.43	15	1
3:D:618:PCW:C26	3:C:204:PCW:H461	0.44	2.43	15	1
3:A:419:PCW:O2	3:D:617:PCW:C42	0.44	2.66	16	1
3:D:627:PCW:O3	3:D:627:PCW:O31	0.44	2.35	17	1
4:D:634:17F:H74	3:C:206:PCW:H283	0.44	1.88	17	1
3:B:205:PCW:C19	3:B:212:PCW:C34	0.44	2.96	17	1
4:B:214:17F:C23	4:B:217:17F:H70	0.44	2.43	18	1
3:A:417:PCW:H39	3:D:612:PCW:H421	0.44	1.89	19	1
3:D:621:PCW:H451	4:D:634:17F:H63	0.44	1.90	19	1
3:B:203:PCW:H461	4:B:217:17F:H46	0.44	1.89	19	1
3:C:204:PCW:H20	4:C:211:17F:C20	0.44	2.42	19	1
3:A:408:PCW:C36	3:C:207:PCW:H462	0.44	2.36	20	1
2:B:32:TYR:HB3	5:B:201:GDP:H5''	0.44	1.89	20	1
3:A:418:PCW:H381	3:D:625:PCW:C26	0.44	2.42	1	2
3:D:622:PCW:O3P	3:D:622:PCW:C31	0.44	2.66	1	2
2:B:32:TYR:CB	5:B:201:GDP:H3'	0.44	2.39	1	1
2:C:146:ALA:N	5:C:201:GDP:O6	0.44	2.51	8	4
3:D:624:PCW:O3P	3:D:624:PCW:O31	0.44	2.35	2	2
3:D:607:PCW:C46	4:D:628:17F:H60	0.44	2.42	3	2
3:B:208:PCW:H483	3:B:208:PCW:C25	0.44	2.36	3	1
3:B:210:PCW:O3P	3:B:210:PCW:H51	0.44	2.13	13	2
3:D:603:PCW:C45	3:D:605:PCW:C18	0.44	2.94	17	4
3:B:205:PCW:H161	3:B:212:PCW:H431	0.44	1.89	7	1
3:A:404:PCW:C14	4:A:415:17F:H57	0.44	2.43	8	1
4:A:414:17F:O10	4:A:414:17F:H4	0.44	2.13	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:601:PCW:H152	4:D:628:17F:H49	0.44	1.89	8	1
2:B:147:LYS:HD3	5:B:201:GDP:N2	0.44	2.28	9	1
3:B:210:PCW:C47	3:B:210:PCW:H272	0.44	2.41	9	1
4:C:211:17F:H30	4:C:211:17F:C37	0.44	2.43	10	1
3:A:411:PCW:C31	4:B:215:17F:H34	0.44	2.42	12	1
3:D:609:PCW:O31	3:D:609:PCW:O3P	0.44	2.36	12	2
3:D:615:PCW:C23	3:C:205:PCW:H272	0.44	2.42	12	1
4:D:634:17F:H65	4:D:635:17F:H68	0.44	1.90	13	1
3:B:203:PCW:H321	4:B:215:17F:C2X	0.44	2.37	13	1
3:B:204:PCW:H251	3:B:204:PCW:H181	0.44	1.89	13	1
3:B:206:PCW:H362	3:C:204:PCW:C38	0.44	2.42	15	1
4:B:215:17F:H41	4:B:215:17F:H36	0.44	1.88	16	1
3:B:211:PCW:C11	4:B:217:17F:H56	0.44	2.42	17	1
3:A:417:PCW:C39	3:D:612:PCW:H432	0.44	2.42	19	1
4:D:630:17F:H54	4:B:214:17F:H73	0.44	1.89	20	1
3:B:208:PCW:C20	4:B:214:17F:H19	0.44	2.43	1	1
3:A:404:PCW:C37	4:B:215:17F:C10	0.44	2.96	2	1
3:A:404:PCW:H422	3:B:209:PCW:H442	0.44	1.90	2	1
3:A:410:PCW:H371	3:C:209:PCW:C16	0.44	2.43	2	2
3:C:203:PCW:H442	3:C:203:PCW:C18	0.44	2.42	2	1
3:A:408:PCW:O1P	3:A:408:PCW:C31	0.44	2.66	3	2
3:A:411:PCW:H271	3:A:418:PCW:H281	0.44	1.89	4	1
4:B:216:17F:O10	4:B:216:17F:O7	0.44	2.35	4	1
4:A:414:17F:H50	3:B:212:PCW:C23	0.44	2.43	5	1
4:D:634:17F:O5	4:D:634:17F:H4	0.44	2.12	5	1
3:D:611:PCW:H39	3:D:623:PCW:C44	0.44	2.43	6	1
3:A:413:PCW:H211	4:A:414:17F:H59	0.44	1.90	7	1
1:D:400:LYS:HZ3	1:D:400:LYS:HB3	0.44	1.73	7	1
3:C:204:PCW:C19	4:C:211:17F:O10	0.44	2.66	7	1
1:D:510:HIS:O	1:D:514:LEU:HG	0.44	2.13	8	3
2:B:13:GLY:HA2	5:B:201:GDP:C5'	0.44	2.39	8	1
3:A:413:PCW:H321	4:A:414:17F:H19A	0.44	1.89	9	1
3:D:623:PCW:H131	3:D:623:PCW:C38	0.44	2.43	9	1
3:D:618:PCW:C26	3:C:204:PCW:H462	0.44	2.37	11	2
3:A:406:PCW:H241	4:B:216:17F:H18	0.44	1.90	11	1
3:A:413:PCW:O4P	3:A:413:PCW:H2	0.44	2.13	11	1
4:D:629:17F:H69	4:D:634:17F:C1X	0.44	2.25	11	1
3:A:410:PCW:C25	3:C:207:PCW:H231	0.44	2.42	12	1
3:D:601:PCW:H483	4:D:628:17F:H64	0.44	1.90	12	1
3:D:615:PCW:H182	3:D:615:PCW:H212	0.44	1.55	17	2
3:A:404:PCW:C35	3:B:203:PCW:H19	0.44	2.43	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:410:PCW:H372	3:A:410:PCW:H411	0.44	1.89	14	1
3:A:407:PCW:H141	3:B:208:PCW:H242	0.44	1.89	15	1
3:D:622:PCW:H19	4:D:630:17F:H11	0.44	1.89	15	1
2:C:154:ASP:HA	2:C:157:TYR:HB2	0.44	1.88	15	2
3:D:608:PCW:H211	3:D:615:PCW:H372	0.44	1.89	17	1
3:A:409:PCW:O31	3:A:409:PCW:C5	0.44	2.61	19	1
3:A:417:PCW:H39	3:D:612:PCW:C43	0.44	2.42	19	1
3:D:627:PCW:H42	3:D:627:PCW:C3	0.44	2.42	19	1
3:B:207:PCW:H231	3:B:210:PCW:H261	0.44	1.89	19	1
3:A:403:PCW:C35	3:A:403:PCW:O31	0.44	2.66	20	1
3:D:611:PCW:H63	3:D:623:PCW:H332	0.43	1.90	1	1
2:B:7:VAL:HG11	2:B:71:TYR:CD2	0.43	2.47	1	1
3:B:213:PCW:O4P	3:B:213:PCW:C8	0.43	2.66	5	3
3:C:203:PCW:P	3:C:204:PCW:H62	0.43	2.53	6	2
3:D:603:PCW:C41	3:D:603:PCW:C37	0.43	2.94	2	3
4:D:630:17F:H11	4:D:630:17F:C31	0.43	2.41	2	1
3:A:419:PCW:O2	3:A:419:PCW:H342	0.43	2.13	4	4
4:D:630:17F:H55	3:B:206:PCW:C18	0.43	2.42	4	1
3:B:209:PCW:H212	3:B:209:PCW:C34	0.43	2.37	4	1
3:D:603:PCW:C11	3:D:603:PCW:O31	0.43	2.66	5	1
2:B:123:ARG:HD3	2:B:125:VAL:O	0.43	2.13	5	2
3:D:602:PCW:H382	3:D:624:PCW:C14	0.43	2.43	13	2
3:D:622:PCW:H342	4:D:629:17F:H78	0.43	1.90	7	1
3:B:204:PCW:H261	3:C:207:PCW:H221	0.43	1.90	9	1
3:D:605:PCW:H331	3:D:607:PCW:C8	0.43	2.43	10	1
3:B:208:PCW:C1	3:B:208:PCW:O31	0.43	2.64	10	1
4:D:630:17F:C37	4:D:634:17F:H43	0.43	2.42	11	1
3:B:205:PCW:H422	3:B:206:PCW:H182	0.43	1.88	11	1
3:C:203:PCW:C35	3:C:203:PCW:O31	0.43	2.63	11	2
3:D:603:PCW:H271	4:B:217:17F:H52	0.43	1.89	12	1
3:D:611:PCW:H242	3:D:619:PCW:H452	0.43	1.89	12	1
3:D:616:PCW:C18	3:D:616:PCW:C22	0.43	2.86	12	1
3:D:626:PCW:O2	3:D:626:PCW:O2P	0.43	2.36	14	3
3:B:208:PCW:H121	4:B:214:17F:H20	0.43	1.90	12	1
3:D:622:PCW:C42	3:B:206:PCW:H282	0.43	2.37	14	1
2:B:39:SER:HB3	2:B:56:LEU:HD12	0.43	1.90	15	1
3:A:409:PCW:C31	3:C:206:PCW:H352	0.43	2.43	17	1
3:D:616:PCW:H472	3:B:206:PCW:H482	0.43	1.89	17	1
3:B:210:PCW:H122	3:B:210:PCW:C7	0.43	2.43	17	1
3:C:207:PCW:O2	3:C:207:PCW:O4P	0.43	2.36	17	1
3:A:417:PCW:H352	3:D:612:PCW:H131	0.43	1.90	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:211:PCW:C24	4:B:217:17F:H51	0.43	2.43	18	1
4:C:211:17F:C12	4:C:211:17F:H69	0.43	2.43	18	1
3:A:407:PCW:C23	4:D:635:17F:H51	0.43	2.41	19	1
4:D:634:17F:H75	3:C:206:PCW:H282	0.43	1.90	19	1
3:A:403:PCW:H332	3:C:204:PCW:H31	0.43	1.90	20	1
3:B:205:PCW:H442	3:B:206:PCW:H212	0.43	1.89	20	1
3:A:411:PCW:C12	3:B:209:PCW:H281	0.43	2.43	1	1
3:D:601:PCW:H252	4:D:631:17F:C42	0.43	2.39	1	2
2:C:41:ARG:HD2	2:C:54:ASP:CG	0.43	2.39	1	1
3:D:612:PCW:C33	3:D:618:PCW:H132	0.43	2.43	2	1
4:D:632:17F:H36	4:D:632:17F:H39	0.43	1.58	18	3
3:B:209:PCW:O3	3:B:209:PCW:C31	0.43	2.66	4	2
3:D:605:PCW:O31	3:D:605:PCW:O3P	0.43	2.35	5	3
3:B:211:PCW:H152	4:B:217:17F:C33	0.43	2.43	3	1
3:D:601:PCW:C28	4:D:631:17F:H78	0.43	2.43	4	1
1:A:324:SER:HA	1:A:327:LEU:HD12	0.43	1.90	5	1
3:A:418:PCW:H483	3:B:213:PCW:C48	0.43	2.40	5	1
1:A:217:LEU:HD13	3:A:408:PCW:H251	0.43	1.90	6	1
4:A:415:17F:H75	4:C:210:17F:C1Y	0.43	2.41	6	1
4:A:415:17F:O9	4:A:415:17F:C7	0.43	2.66	6	2
1:A:309:ALA:HA	1:A:312:HIS:HB2	0.43	1.89	7	1
3:D:611:PCW:O11	3:D:611:PCW:C2	0.43	2.60	7	1
3:B:213:PCW:H351	4:B:214:17F:C9	0.43	2.43	7	1
3:C:204:PCW:C24	3:C:207:PCW:H461	0.43	2.43	7	1
3:C:206:PCW:C36	3:C:206:PCW:C15	0.43	2.96	8	1
3:D:615:PCW:N	4:D:635:17F:O4	0.43	2.51	9	2
4:D:634:17F:C41	3:C:206:PCW:H221	0.43	2.44	9	1
3:A:404:PCW:C40	4:B:215:17F:H42	0.43	2.42	10	1
3:D:625:PCW:H39	3:D:626:PCW:H121	0.43	1.88	10	1
3:D:624:PCW:O2	3:D:624:PCW:C4	0.43	2.66	11	1
3:A:402:PCW:H52	3:C:206:PCW:O2P	0.43	2.13	13	1
3:A:402:PCW:H431	3:A:409:PCW:H272	0.43	1.89	14	1
3:D:611:PCW:H483	3:B:209:PCW:C47	0.43	2.42	14	1
4:D:629:17F:H76	3:C:212:PCW:H441	0.43	1.90	14	1
3:B:211:PCW:H131	4:B:217:17F:H58	0.43	1.90	14	1
3:B:211:PCW:H61	3:B:212:PCW:C32	0.43	2.44	15	1
1:A:264:LYS:NZ	1:D:513:ALA:HB2	0.43	2.29	18	3
3:A:408:PCW:H61	4:C:211:17F:O4	0.43	2.12	18	1
4:D:634:17F:H4A	4:D:634:17F:H1A	0.43	1.90	18	1
3:C:206:PCW:H181	3:C:206:PCW:H212	0.43	1.54	1	2
3:D:626:PCW:H211	3:D:626:PCW:H181	0.43	1.54	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:204:PCW:H432	4:C:211:17F:H30	0.43	1.89	2	1
4:C:211:17F:H71	4:C:211:17F:O8	0.43	2.13	2	1
3:A:416:PCW:H39	3:A:416:PCW:C15	0.43	2.43	3	1
3:D:615:PCW:O31	3:D:615:PCW:H12	0.43	2.13	3	1
3:B:211:PCW:H432	3:B:212:PCW:H31	0.43	1.90	16	2
3:C:204:PCW:H20	4:C:211:17F:C32	0.43	2.43	4	1
3:A:408:PCW:H281	1:D:554:HIS:CE1	0.43	2.49	5	1
1:D:470:TYR:CE2	4:D:631:17F:H68	0.43	2.39	5	1
2:C:112:VAL:HG23	2:C:159:LEU:HD13	0.43	1.89	5	1
3:A:408:PCW:H362	3:C:207:PCW:C46	0.43	2.42	7	1
3:D:622:PCW:H331	3:D:627:PCW:C20	0.43	2.43	7	1
4:D:630:17F:H40	4:D:630:17F:H69	0.43	1.89	7	1
3:B:204:PCW:C44	3:C:203:PCW:C35	0.43	2.92	7	1
3:B:213:PCW:H421	4:B:217:17F:C10	0.43	2.25	7	1
3:A:407:PCW:C8	3:B:207:PCW:C8	0.43	2.96	8	1
3:A:407:PCW:H20	3:C:205:PCW:H431	0.43	1.89	8	1
3:A:408:PCW:C36	3:C:207:PCW:C44	0.43	2.94	8	1
3:D:626:PCW:O2P	3:D:626:PCW:O2	0.43	2.37	15	2
4:C:211:17F:H11	4:C:211:17F:C37	0.43	2.43	8	1
4:C:211:17F:C28	3:C:212:PCW:H212	0.43	2.43	8	1
3:D:621:PCW:H32	4:D:634:17F:O2	0.43	2.12	10	1
3:A:413:PCW:O2	3:A:413:PCW:C36	0.43	2.66	11	1
3:D:613:PCW:H2	3:D:613:PCW:O11	0.43	2.13	11	1
3:D:616:PCW:H431	3:D:618:PCW:C24	0.43	2.43	11	1
3:B:203:PCW:C22	4:C:210:17F:H20A	0.43	2.44	11	1
3:B:204:PCW:H352	3:B:212:PCW:C8	0.43	2.43	11	1
4:B:215:17F:H40	4:B:215:17F:H36	0.43	1.57	11	1
3:B:206:PCW:H411	4:C:211:17F:H39	0.43	1.91	12	1
3:C:204:PCW:C26	3:C:207:PCW:H482	0.43	2.21	12	1
3:A:413:PCW:H481	4:C:210:17F:C12	0.43	2.28	13	1
3:D:623:PCW:C31	3:D:623:PCW:O3	0.43	2.66	13	1
4:D:628:17F:C22	4:D:631:17F:H74	0.43	2.43	14	1
3:C:207:PCW:H472	4:C:211:17F:H32	0.43	1.90	14	1
3:A:413:PCW:C22	3:A:413:PCW:C18	0.43	2.78	15	1
3:A:402:PCW:H382	3:A:402:PCW:H411	0.43	1.51	16	2
3:A:407:PCW:O3	3:A:407:PCW:C31	0.43	2.66	16	1
3:A:418:PCW:O31	3:A:418:PCW:P	0.43	2.76	16	1
3:D:614:PCW:C19	3:D:623:PCW:H481	0.43	2.43	16	1
3:D:622:PCW:C19	4:D:630:17F:H29	0.43	2.43	16	1
2:B:6:LEU:HD13	2:B:159:LEU:HD23	0.43	1.90	18	1
3:A:401:PCW:H63	3:B:209:PCW:O31	0.43	2.13	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:404:PCW:H51	4:A:415:17F:O4	0.43	2.12	19	1
3:A:404:PCW:H452	3:B:209:PCW:H432	0.43	1.89	19	1
1:D:502:GLU:O	1:D:506:ARG:HG3	0.43	2.14	14	8
3:D:608:PCW:C26	3:D:615:PCW:H411	0.43	2.43	1	1
3:D:613:PCW:H20	4:C:210:17F:C27	0.43	2.25	1	2
1:A:224:VAL:HG22	1:D:550:LYS:HE2	0.43	1.90	2	1
3:A:410:PCW:C25	4:D:633:17F:H54	0.43	2.42	2	1
4:A:415:17F:H18A	4:A:415:17F:H9A	0.43	1.90	2	1
3:D:604:PCW:C38	3:D:611:PCW:H322	0.43	2.44	2	2
3:A:417:PCW:C39	3:D:612:PCW:H231	0.43	2.43	3	2
3:C:207:PCW:O1P	3:C:207:PCW:O2	0.43	2.37	18	2
1:A:221:LEU:HD11	3:A:408:PCW:H182	0.43	1.89	4	1
3:A:402:PCW:C45	3:A:407:PCW:H39	0.43	2.39	4	1
4:D:635:17F:H44	3:C:205:PCW:H251	0.43	1.89	4	1
3:D:618:PCW:H261	3:C:204:PCW:C48	0.43	2.43	5	1
1:D:473:LYS:O	1:D:477:LEU:HG	0.43	2.13	6	1
4:D:629:17F:H9A	4:D:629:17F:H18	0.43	1.90	6	1
3:B:209:PCW:H221	3:B:209:PCW:H172	0.43	1.89	6	1
2:C:146:ALA:HB3	5:C:201:GDP:N7	0.43	2.29	13	3
2:C:16:LYS:NZ	5:C:201:GDP:O2B	0.43	2.51	14	3
2:C:93:ILE:HG21	2:C:113:LEU:HD11	0.43	1.89	7	1
3:C:205:PCW:C41	3:C:205:PCW:H371	0.43	2.44	8	1
3:D:616:PCW:H461	3:D:627:PCW:C26	0.43	2.43	9	1
3:A:402:PCW:C4	3:A:402:PCW:H31	0.43	2.43	10	1
3:B:206:PCW:C20	3:C:208:PCW:H282	0.43	2.41	10	1
3:A:407:PCW:O4P	3:A:407:PCW:C7	0.43	2.66	11	1
3:D:618:PCW:H262	3:C:204:PCW:H283	0.43	1.89	11	1
3:B:204:PCW:H172	3:C:204:PCW:H381	0.43	1.91	11	1
3:B:208:PCW:C11	4:B:214:17F:H4	0.43	2.42	11	1
3:B:211:PCW:H61	3:B:212:PCW:H321	0.43	1.91	11	1
3:D:601:PCW:C17	3:D:601:PCW:C21	0.43	2.71	12	1
3:D:605:PCW:C16	4:D:629:17F:C11	0.43	2.96	12	1
3:D:616:PCW:C43	3:B:206:PCW:C48	0.43	2.94	12	1
2:B:117:LYS:HB3	2:B:120:LEU:HD12	0.43	1.90	12	1
3:A:410:PCW:H42	3:C:209:PCW:H11	0.43	1.90	13	1
3:D:621:PCW:H421	4:D:634:17F:C32	0.43	2.42	14	1
3:D:627:PCW:C25	3:C:212:PCW:H451	0.43	2.43	14	1
3:B:209:PCW:C41	3:B:209:PCW:C37	0.43	2.85	15	1
3:C:205:PCW:H452	3:C:206:PCW:C20	0.43	2.43	15	1
3:A:408:PCW:H341	3:C:207:PCW:C42	0.43	2.34	17	1
3:A:408:PCW:H61	4:C:211:17F:C1	0.43	2.43	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:217:17F:O10	4:B:217:17F:H20A	0.43	2.13	18	1
3:A:408:PCW:C8	4:C:211:17F:O2	0.43	2.65	19	1
3:D:601:PCW:H483	4:D:628:17F:C33	0.43	2.42	19	1
3:A:406:PCW:C31	3:A:411:PCW:H82	0.43	2.43	20	1
3:A:406:PCW:C20	3:B:210:PCW:C32	0.43	2.96	20	1
3:D:618:PCW:C13	3:D:627:PCW:C14	0.43	2.94	3	2
3:D:627:PCW:C4	3:D:627:PCW:C2	0.43	2.73	3	2
4:B:217:17F:C2X	4:B:217:17F:H64	0.43	2.44	3	1
2:C:18:ALA:N	5:C:201:GDP:O1A	0.43	2.51	3	1
3:D:603:PCW:O11	3:D:603:PCW:H51	0.43	2.14	4	1
3:D:606:PCW:H182	3:D:606:PCW:H211	0.43	1.63	13	4
3:D:613:PCW:H352	3:D:619:PCW:H351	0.43	1.89	4	2
3:B:206:PCW:H222	3:C:208:PCW:H281	0.43	1.89	4	1
3:A:404:PCW:H2	3:A:404:PCW:O11	0.43	2.13	5	1
1:D:415:LEU:O	1:D:419:LEU:HG	0.43	2.14	5	2
4:B:214:17F:O4	3:C:205:PCW:C8	0.43	2.67	5	1
1:D:524:GLU:HA	1:D:527:GLN:NE2	0.43	2.29	6	1
2:C:15:GLY:CA	5:C:201:GDP:H8	0.43	2.26	6	3
3:C:204:PCW:C14	4:C:211:17F:H62	0.43	2.44	6	1
3:A:406:PCW:O1P	3:A:406:PCW:H32	0.43	2.13	7	1
3:A:410:PCW:H121	3:C:209:PCW:H121	0.43	1.90	7	1
3:A:410:PCW:H371	3:C:209:PCW:H171	0.43	1.88	7	1
3:B:206:PCW:C39	4:C:211:17F:H43	0.43	2.44	7	1
3:B:204:PCW:C12	3:C:204:PCW:H39	0.43	2.44	8	1
3:B:205:PCW:H381	3:B:205:PCW:H411	0.43	1.51	17	3
3:A:417:PCW:C36	3:D:612:PCW:H152	0.43	2.42	10	1
3:A:402:PCW:C7	3:C:206:PCW:H322	0.43	2.43	11	1
3:A:413:PCW:H281	3:C:203:PCW:H483	0.43	1.90	11	1
3:D:603:PCW:C25	4:B:217:17F:H52	0.43	2.44	12	1
3:C:205:PCW:O2	3:C:205:PCW:H341	0.43	2.13	12	1
3:D:606:PCW:C3	3:D:626:PCW:C39	0.43	2.94	13	1
3:A:411:PCW:P	3:A:411:PCW:O2	0.43	2.76	14	2
3:A:403:PCW:O31	3:A:403:PCW:H351	0.43	2.13	15	1
3:A:406:PCW:H261	3:B:207:PCW:C19	0.43	2.42	15	1
3:A:407:PCW:H472	3:D:615:PCW:C28	0.43	2.44	15	1
3:D:603:PCW:H411	3:D:603:PCW:H372	0.43	1.90	15	1
3:B:203:PCW:H461	4:B:217:17F:H47	0.43	1.91	16	1
3:D:601:PCW:H362	4:B:216:17F:C37	0.43	2.31	17	1
3:D:618:PCW:P	3:D:627:PCW:H82	0.43	2.54	17	1
1:A:327:LEU:HD23	1:A:330:ARG:HD2	0.43	1.91	18	1
3:A:404:PCW:H451	4:B:215:17F:H12A	0.43	1.90	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:402:PCW:H39	3:A:409:PCW:H241	0.43	1.90	19	1
3:D:626:PCW:O2	3:D:626:PCW:C11	0.43	2.67	19	1
3:B:207:PCW:C45	4:B:215:17F:C33	0.43	2.90	19	1
3:C:206:PCW:H462	3:C:208:PCW:H482	0.43	1.90	19	1
3:A:401:PCW:H471	3:D:614:PCW:H451	0.43	1.89	1	1
3:A:419:PCW:H31	3:D:617:PCW:H411	0.43	1.89	4	4
3:D:605:PCW:H412	3:D:605:PCW:H381	0.43	1.55	12	3
3:D:614:PCW:H381	3:D:614:PCW:H411	0.43	1.54	1	5
1:D:535:ALA:O	1:D:539:ASN:HB2	0.43	2.14	2	1
3:D:607:PCW:C12	3:D:608:PCW:H19	0.43	2.43	2	1
3:D:616:PCW:H271	3:D:618:PCW:C28	0.43	2.33	2	1
3:D:604:PCW:C32	3:D:624:PCW:C8	0.43	2.96	3	1
1:D:522:SER:HA	1:D:525:LEU:HB2	0.43	1.89	5	2
3:D:618:PCW:H151	3:D:627:PCW:C14	0.43	2.44	5	1
1:A:229:TRP:O	1:A:233:GLU:HG2	0.43	2.14	6	1
1:A:268:GLU:OE1	1:D:506:ARG:HD3	0.43	2.13	16	5
3:C:207:PCW:H412	3:C:207:PCW:H382	0.43	1.60	6	1
3:A:412:PCW:C42	3:C:206:PCW:H39	0.43	2.32	7	1
3:A:413:PCW:H381	4:C:210:17F:H11	0.43	1.90	7	1
3:D:611:PCW:H231	3:D:619:PCW:H442	0.43	1.90	7	1
3:D:616:PCW:O2P	3:C:212:PCW:C5	0.43	2.59	8	1
3:B:204:PCW:C34	3:C:204:PCW:H321	0.43	2.42	8	1
3:D:601:PCW:H351	4:B:216:17F:H73	0.43	1.91	9	1
3:A:412:PCW:H412	3:C:208:PCW:H412	0.43	1.90	10	1
3:D:601:PCW:C35	4:B:216:17F:H77	0.43	2.39	10	2
3:D:603:PCW:H2	3:D:605:PCW:H52	0.43	1.89	10	1
2:B:17:SER:HB2	5:B:201:GDP:PA	0.43	2.53	10	2
3:A:405:PCW:H331	3:A:405:PCW:P	0.43	2.54	11	1
3:D:618:PCW:C28	4:C:211:17F:H37	0.43	2.43	11	1
3:B:204:PCW:C8	3:B:204:PCW:O4P	0.43	2.67	11	1
3:B:204:PCW:H283	4:C:211:17F:O9	0.43	2.13	11	1
3:B:208:PCW:O2P	3:B:208:PCW:H32	0.43	2.13	11	2
3:A:403:PCW:H171	3:C:203:PCW:H31	0.43	1.91	12	1
1:D:523:ASP:O	1:D:526:ARG:HB2	0.43	2.13	12	1
3:A:403:PCW:H181	3:A:403:PCW:C42	0.43	2.42	14	1
3:B:208:PCW:H32	4:B:214:17F:H4	0.43	1.90	15	1
3:C:203:PCW:H442	3:C:203:PCW:C16	0.43	2.37	16	1
3:D:605:PCW:H63	3:D:605:PCW:C13	0.43	2.44	17	1
4:D:631:17F:H63	4:D:631:17F:H58	0.43	1.60	18	1
4:D:630:17F:C37	4:D:634:17F:H36	0.43	2.39	19	1
3:B:205:PCW:H222	3:B:212:PCW:C36	0.43	2.44	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:334:ARG:HD3	1:D:440:GLU:OE1	0.43	2.13	20	1
3:B:209:PCW:H11	3:B:209:PCW:O31	0.43	2.13	20	1
3:A:412:PCW:H482	4:D:634:17F:H76	0.43	1.90	1	1
1:A:277:GLU:HB2	1:A:278:PRO:CD	0.43	2.44	13	5
4:D:634:17F:O9	4:D:634:17F:C7	0.43	2.67	3	3
3:C:207:PCW:H282	3:C:209:PCW:H371	0.43	1.90	3	1
3:C:208:PCW:H73	3:C:208:PCW:C31	0.43	2.44	3	1
4:C:211:17F:H66	4:C:211:17F:H35	0.43	1.91	3	1
3:D:609:PCW:H62	4:D:633:17F:P1	0.43	2.54	10	3
3:D:624:PCW:O4P	3:D:624:PCW:C31	0.43	2.67	4	1
3:B:206:PCW:H242	3:C:208:PCW:H482	0.43	1.90	4	1
3:A:407:PCW:H142	3:C:205:PCW:H142	0.43	1.90	5	1
3:B:210:PCW:H471	3:B:210:PCW:H282	0.43	1.86	6	1
3:B:213:PCW:O3	3:B:213:PCW:C31	0.43	2.66	12	2
3:B:208:PCW:H182	3:C:206:PCW:C12	0.43	2.34	9	1
3:D:605:PCW:H62	3:D:626:PCW:H20	0.43	1.89	10	1
3:C:204:PCW:H51	3:C:204:PCW:O3P	0.43	2.14	10	1
3:D:603:PCW:C27	3:B:213:PCW:H471	0.43	2.43	11	1
3:B:209:PCW:H412	3:B:209:PCW:H381	0.43	1.54	11	1
3:A:417:PCW:C8	3:D:617:PCW:H421	0.43	2.43	12	1
3:A:420:PCW:H41	3:A:420:PCW:C1	0.43	2.44	15	2
3:B:204:PCW:C40	3:C:203:PCW:H73	0.43	2.44	12	1
3:B:213:PCW:H222	3:B:213:PCW:H421	0.43	1.89	12	1
3:B:212:PCW:C39	3:C:212:PCW:H262	0.43	2.44	13	1
3:B:203:PCW:H452	4:B:215:17F:H55	0.43	1.91	14	1
3:C:212:PCW:H52	3:C:212:PCW:H322	0.43	1.90	14	1
3:A:420:PCW:H211	3:A:420:PCW:H181	0.43	1.54	15	1
3:B:203:PCW:H411	3:B:211:PCW:C19	0.43	2.43	15	1
3:B:207:PCW:H371	4:B:215:17F:H58	0.43	1.91	16	1
1:D:488:LYS:HA	1:D:491:GLU:OE1	0.43	2.14	17	1
3:B:207:PCW:H52	4:B:216:17F:O5	0.43	2.14	17	1
3:A:410:PCW:C24	3:C:207:PCW:H222	0.43	2.43	18	1
3:A:411:PCW:H432	3:A:418:PCW:C24	0.43	2.42	18	2
3:B:208:PCW:O3	4:B:214:17F:O10	0.43	2.36	18	1
3:B:211:PCW:H12	3:B:211:PCW:C5	0.43	2.37	19	1
4:D:630:17F:H36	4:D:630:17F:H69	0.43	1.91	20	1
3:B:206:PCW:O31	3:B:206:PCW:H12	0.43	2.14	20	4
1:A:284:GLN:O	1:A:288:ARG:HG3	0.43	2.14	3	1
3:A:404:PCW:H151	3:B:209:PCW:H411	0.43	1.90	3	1
3:A:416:PCW:H281	3:C:203:PCW:C28	0.43	2.44	3	1
4:B:217:17F:O8	4:B:217:17F:O9	0.43	2.36	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:298:LEU:O	1:A:302:GLY:HA3	0.43	2.13	20	2
3:A:412:PCW:C48	3:C:206:PCW:H39	0.43	2.42	4	1
3:D:613:PCW:C28	4:C:210:17F:H39	0.43	2.43	6	5
3:B:205:PCW:H12	3:B:211:PCW:C5	0.43	2.43	4	1
3:A:404:PCW:H121	3:B:209:PCW:C37	0.43	2.44	5	1
4:C:211:17F:H59	4:C:211:17F:H62	0.43	1.54	20	3
1:A:251:LYS:O	1:A:254:VAL:HG12	0.43	2.13	7	1
3:A:401:PCW:H411	3:A:404:PCW:C28	0.43	2.43	7	1
3:A:401:PCW:C11	3:B:209:PCW:H231	0.43	2.44	8	1
3:A:401:PCW:C3	3:B:209:PCW:H231	0.43	2.43	8	1
3:A:420:PCW:H63	3:A:420:PCW:C3	0.43	2.43	9	1
3:D:614:PCW:C44	3:D:619:PCW:C20	0.43	2.96	9	1
3:D:620:PCW:O31	3:D:620:PCW:O3	0.43	2.37	9	1
3:B:203:PCW:H482	4:B:217:17F:C30	0.43	2.43	9	2
3:D:605:PCW:O11	3:D:605:PCW:N	0.43	2.51	10	1
3:D:622:PCW:C18	3:C:212:PCW:H172	0.43	2.43	10	1
3:C:208:PCW:H39	3:C:209:PCW:H73	0.43	1.90	10	1
3:B:204:PCW:O11	3:B:204:PCW:H2	0.43	2.14	14	1
3:D:614:PCW:H52	3:D:625:PCW:H42	0.43	1.90	15	1
3:A:419:PCW:H342	3:D:617:PCW:C41	0.43	2.44	17	1
2:B:32:TYR:CG	5:B:201:GDP:H3'	0.43	2.48	18	1
3:A:411:PCW:O31	3:A:411:PCW:H342	0.43	2.12	19	1
3:D:608:PCW:O31	3:D:615:PCW:H61	0.43	2.14	19	1
3:A:401:PCW:C6	3:A:404:PCW:O2P	0.43	2.62	20	1
3:D:604:PCW:C6	4:D:632:17F:O4	0.43	2.67	1	1
3:B:207:PCW:H432	4:B:217:17F:C21	0.43	2.34	1	1
3:B:208:PCW:C3	3:B:208:PCW:P	0.43	3.06	13	3
3:A:404:PCW:H372	4:B:215:17F:H10A	0.43	1.89	2	1
3:B:208:PCW:H352	4:B:214:17F:C1Z	0.43	2.43	3	1
3:D:615:PCW:H212	3:D:615:PCW:H182	0.43	1.57	14	4
3:D:617:PCW:O4P	3:D:617:PCW:O11	0.43	2.37	4	1
4:D:635:17F:C37	4:D:635:17F:C32	0.43	2.97	5	2
3:B:204:PCW:C48	3:B:212:PCW:C20	0.43	2.96	5	1
4:C:211:17F:H36	4:C:211:17F:H40	0.43	1.59	10	2
3:A:406:PCW:H252	3:B:207:PCW:C17	0.43	2.32	6	1
3:C:207:PCW:C28	3:C:209:PCW:H371	0.43	2.43	7	1
3:D:623:PCW:C33	3:D:624:PCW:H73	0.43	2.43	9	1
3:B:204:PCW:H283	4:C:211:17F:C17	0.43	2.43	11	1
3:A:402:PCW:H451	3:C:205:PCW:C36	0.43	2.42	12	1
3:A:407:PCW:H61	4:B:214:17F:O1	0.43	2.14	12	1
3:B:208:PCW:H141	4:B:214:17F:H20A	0.43	1.91	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:212:PCW:P	3:B:212:PCW:C3	0.43	3.05	12	1
3:B:212:PCW:H51	3:B:212:PCW:O3P	0.43	2.13	12	1
3:A:401:PCW:C5	3:A:404:PCW:C3	0.43	2.86	13	1
3:D:615:PCW:H282	4:D:635:17F:H45	0.43	1.91	13	1
3:B:204:PCW:C38	3:B:212:PCW:H151	0.43	2.43	13	1
3:A:406:PCW:H242	3:B:210:PCW:O11	0.43	2.14	16	1
3:D:613:PCW:C25	4:C:210:17F:H47	0.43	2.40	16	1
4:D:631:17F:H9A	4:D:631:17F:C19	0.43	2.42	16	1
3:A:411:PCW:C38	4:B:215:17F:H65	0.43	2.43	17	1
3:A:401:PCW:H372	3:A:404:PCW:C19	0.43	2.43	19	1
3:D:606:PCW:H31	3:D:626:PCW:H411	0.43	1.90	19	1
3:D:610:PCW:H283	3:D:610:PCW:C44	0.43	2.44	19	1
3:C:207:PCW:H73	4:C:211:17F:C3	0.43	2.44	19	1
3:A:403:PCW:C33	3:C:204:PCW:H32	0.43	2.43	20	1
3:A:403:PCW:C3	3:A:403:PCW:P	0.43	3.07	1	1
3:A:404:PCW:H472	3:B:209:PCW:H481	0.43	1.91	1	1
3:A:404:PCW:H281	4:C:210:17F:H70	0.43	1.89	1	1
3:A:411:PCW:H122	3:B:209:PCW:C28	0.43	2.43	1	1
3:D:602:PCW:C7	3:C:212:PCW:O2P	0.43	2.67	1	1
3:B:208:PCW:H372	3:B:208:PCW:H421	0.43	1.89	1	1
3:A:410:PCW:H151	3:C:209:PCW:C37	0.43	2.35	2	1
3:D:608:PCW:O3	3:D:608:PCW:C31	0.43	2.67	3	2
3:D:609:PCW:H171	4:D:633:17F:H61	0.43	1.89	18	3
3:B:206:PCW:H142	3:B:212:PCW:C42	0.43	2.44	4	1
3:C:207:PCW:H212	3:C:207:PCW:H181	0.43	1.56	4	1
3:A:402:PCW:H211	3:A:409:PCW:H20	0.43	1.91	5	1
3:A:410:PCW:H32	3:A:410:PCW:O2P	0.43	2.14	5	1
3:B:210:PCW:C44	3:B:213:PCW:C28	0.43	2.93	5	1
3:D:602:PCW:H161	3:D:624:PCW:C22	0.43	2.43	14	2
3:D:623:PCW:H212	3:D:623:PCW:H182	0.43	1.64	7	3
4:D:628:17F:H36	4:D:631:17F:C40	0.43	2.44	8	1
3:A:403:PCW:O31	3:A:403:PCW:C35	0.43	2.67	9	2
3:A:404:PCW:C38	3:B:209:PCW:H412	0.43	2.44	10	1
2:B:77:GLY:HA3	2:B:159:LEU:HD11	0.43	1.90	10	1
3:C:208:PCW:O3	3:C:209:PCW:H321	0.43	2.14	10	1
1:A:330:ARG:NH2	1:D:447:GLU:HB3	0.43	2.28	11	1
3:A:419:PCW:H432	3:D:610:PCW:C22	0.43	2.44	11	1
1:D:540:GLY:O	1:D:544:LEU:HG	0.43	2.14	11	1
4:D:629:17F:H49	3:B:212:PCW:C46	0.43	2.44	11	1
4:D:629:17F:H71	4:D:634:17F:C1X	0.43	2.27	12	1
3:B:212:PCW:H2	3:B:212:PCW:C5	0.43	2.38	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:214:17F:C25	4:B:217:17F:H66	0.43	2.35	13	1
4:B:217:17F:O10	4:B:217:17F:C20	0.43	2.66	13	1
3:C:206:PCW:H381	3:C:206:PCW:H172	0.43	1.90	13	1
3:A:406:PCW:C26	4:B:216:17F:H19A	0.43	2.40	14	1
2:B:84:ILE:HD11	2:B:118:CYS:HA	0.43	1.90	14	1
1:A:217:LEU:HD21	3:A:408:PCW:H252	0.43	1.90	16	1
3:A:418:PCW:C6	3:D:626:PCW:H2	0.43	2.44	16	1
3:B:204:PCW:H231	3:C:208:PCW:H241	0.43	1.89	16	1
3:D:603:PCW:H231	3:B:211:PCW:C28	0.43	2.44	19	1
3:B:204:PCW:H242	3:C:204:PCW:H441	0.43	1.91	19	1
3:A:405:PCW:C7	3:D:601:PCW:C6	0.43	2.96	20	1
3:A:409:PCW:H63	3:A:412:PCW:C39	0.42	2.43	1	1
3:D:620:PCW:O1P	3:D:621:PCW:C4	0.42	2.67	1	2
3:C:206:PCW:H12	3:C:208:PCW:C8	0.42	2.44	1	1
1:D:463:TRP:NE1	4:D:631:17F:H77	0.42	2.28	2	1
3:B:207:PCW:H171	3:B:210:PCW:H122	0.42	1.89	4	1
3:A:404:PCW:H152	3:B:209:PCW:H382	0.42	1.91	5	1
3:C:204:PCW:H11	3:C:204:PCW:H52	0.42	1.91	5	1
3:A:401:PCW:H361	3:A:404:PCW:C17	0.42	2.44	6	1
3:A:416:PCW:H431	3:A:420:PCW:C40	0.42	2.44	6	1
3:A:417:PCW:H411	3:D:612:PCW:H142	0.42	1.91	6	1
3:D:612:PCW:O2	3:D:612:PCW:C34	0.42	2.67	13	3
4:A:414:17F:H45	3:B:212:PCW:H232	0.42	1.91	8	1
3:A:405:PCW:H421	4:D:628:17F:C29	0.42	2.44	9	1
3:A:404:PCW:H382	3:B:209:PCW:H412	0.42	1.91	10	1
1:D:549:ALA:O	1:D:553:GLU:HG3	0.42	2.14	10	1
2:B:37:GLU:HA	2:B:57:ASP:O	0.42	2.14	10	1
3:A:413:PCW:H12	3:A:413:PCW:H382	0.42	1.91	11	1
3:B:211:PCW:C32	3:B:212:PCW:C1	0.42	2.96	11	1
1:A:345:ARG:HG2	1:D:429:ASN:OD1	0.42	2.14	12	2
3:D:615:PCW:H231	3:C:205:PCW:C26	0.42	2.44	12	1
3:B:208:PCW:O3	4:B:214:17F:H5	0.42	2.13	12	1
3:D:605:PCW:C37	4:D:629:17F:O8	0.42	2.67	13	1
3:D:611:PCW:H242	3:D:619:PCW:C44	0.42	2.44	14	1
3:B:206:PCW:H483	3:C:212:PCW:H231	0.42	1.85	14	1
3:D:627:PCW:C42	3:D:627:PCW:C38	0.42	2.85	15	1
3:D:609:PCW:H42	4:D:633:17F:H6A	0.42	1.91	20	1
2:C:142:ILE:HG21	2:C:155:ALA:HB2	0.42	1.91	20	1
3:A:401:PCW:C41	3:D:611:PCW:H251	0.42	2.44	1	1
3:C:205:PCW:H352	3:C:206:PCW:H122	0.42	1.90	1	1
3:A:408:PCW:H39	3:A:408:PCW:H19	0.42	1.89	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:212:PCW:H451	4:B:214:17F:C42	0.42	2.43	2	1
4:D:628:17F:H58	4:D:631:17F:C29	0.42	2.42	3	1
3:B:206:PCW:O4P	3:B:206:PCW:C8	0.42	2.67	3	1
3:C:208:PCW:H382	3:C:208:PCW:H412	0.42	1.55	3	1
3:B:211:PCW:H351	3:B:212:PCW:C1	0.42	2.44	4	1
1:D:503:MET:SD	1:D:506:ARG:HD2	0.42	2.53	5	2
3:B:208:PCW:C44	4:B:214:17F:C1Z	0.42	2.88	5	2
3:A:413:PCW:H182	3:A:413:PCW:H211	0.42	1.62	7	1
4:A:414:17F:O8	3:C:203:PCW:C8	0.42	2.67	7	1
1:D:437:LEU:O	1:D:440:GLU:HG3	0.42	2.14	8	1
3:D:604:PCW:C17	3:D:613:PCW:H131	0.42	2.44	16	2
2:C:17:SER:N	5:C:201:GDP:O3B	0.42	2.52	12	3
3:A:402:PCW:H331	3:C:206:PCW:O2	0.42	2.13	11	1
3:A:416:PCW:H212	3:A:416:PCW:H181	0.42	1.58	11	1
4:B:214:17F:H1A	3:C:205:PCW:C8	0.42	2.44	11	1
3:A:403:PCW:H271	3:A:413:PCW:H211	0.42	1.90	12	1
3:D:618:PCW:O2P	3:D:627:PCW:H51	0.42	2.14	13	1
3:B:206:PCW:H441	4:C:211:17F:H47	0.42	1.91	13	1
3:B:213:PCW:H211	3:B:213:PCW:H181	0.42	1.68	17	3
2:C:78:PHE:O	2:C:111:MET:HA	0.42	2.14	14	1
1:A:377:PRO:HG2	1:D:400:LYS:HE2	0.42	1.91	16	1
3:A:406:PCW:C24	3:B:207:PCW:C15	0.42	2.93	16	1
2:B:6:LEU:HD11	2:B:53:LEU:HD22	0.42	1.91	17	1
3:A:418:PCW:C8	3:D:626:PCW:H331	0.42	2.42	19	1
3:D:625:PCW:H451	3:D:626:PCW:H471	0.42	1.90	19	1
3:A:411:PCW:H412	3:A:418:PCW:H242	0.42	1.91	20	1
3:C:207:PCW:H281	3:C:208:PCW:C16	0.42	2.43	20	1
3:A:409:PCW:H321	3:A:412:PCW:C39	0.42	2.43	1	1
3:A:416:PCW:O31	3:A:416:PCW:O4P	0.42	2.37	1	1
3:B:209:PCW:C23	3:B:209:PCW:H361	0.42	2.45	1	1
3:B:209:PCW:C20	4:B:215:17F:H19	0.42	2.41	1	1
3:C:212:PCW:O2	3:C:212:PCW:O11	0.42	2.37	1	2
3:A:413:PCW:H321	4:A:414:17F:C19	0.42	2.45	2	1
4:B:217:17F:H18	4:B:217:17F:H5	0.42	1.60	2	4
3:B:210:PCW:H442	3:B:213:PCW:C27	0.42	2.44	3	1
3:A:403:PCW:C47	3:C:203:PCW:C28	0.42	2.94	4	1
3:A:407:PCW:C25	3:C:205:PCW:H411	0.42	2.42	4	1
1:D:544:LEU:O	1:D:548:HIS:HB2	0.42	2.14	4	1
3:B:207:PCW:O2	3:B:207:PCW:P	0.42	2.77	4	2
3:C:204:PCW:H462	4:C:211:17F:C33	0.42	2.44	4	1
3:C:204:PCW:C14	4:C:211:17F:H6A	0.42	2.43	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:417:PCW:H352	3:D:612:PCW:H132	0.42	1.87	5	1
3:D:611:PCW:O31	3:D:611:PCW:C11	0.42	2.68	5	2
3:B:204:PCW:H342	3:C:204:PCW:C34	0.42	2.45	5	1
3:B:206:PCW:H242	3:C:208:PCW:C20	0.42	2.43	5	1
3:C:204:PCW:H52	3:C:204:PCW:O2P	0.42	2.13	5	1
3:D:619:PCW:C44	4:C:210:17F:H74	0.42	2.45	6	1
3:C:208:PCW:H181	3:C:208:PCW:H211	0.42	1.56	6	1
1:D:458:ASP:HA	1:D:461:LYS:HD2	0.42	1.92	7	1
3:D:602:PCW:H271	3:D:610:PCW:C17	0.42	2.45	7	1
2:B:89:SER:O	2:B:93:ILE:HG12	0.42	2.14	17	2
3:A:402:PCW:H352	3:C:205:PCW:H12	0.42	1.91	10	1
3:C:208:PCW:H63	3:C:209:PCW:C8	0.42	2.44	10	1
4:A:414:17F:H48	3:C:203:PCW:H431	0.42	1.90	11	1
3:D:605:PCW:C33	3:D:607:PCW:H61	0.42	2.45	11	1
3:B:204:PCW:H272	3:C:207:PCW:H20	0.42	1.91	11	1
3:B:207:PCW:C15	3:B:210:PCW:H382	0.42	2.44	12	1
3:A:406:PCW:H322	3:A:411:PCW:H321	0.42	1.90	13	1
3:A:408:PCW:H121	3:A:417:PCW:H272	0.42	1.90	14	1
3:A:401:PCW:C38	3:A:404:PCW:H20	0.42	2.45	15	1
3:A:407:PCW:H41	3:A:407:PCW:C1	0.42	2.40	15	1
3:B:205:PCW:H422	4:B:214:17F:C39	0.42	2.44	15	1
3:B:206:PCW:H231	3:C:208:PCW:C28	0.42	2.44	15	1
3:A:411:PCW:H222	3:A:411:PCW:H181	0.42	1.91	16	1
3:D:601:PCW:C8	4:B:216:17F:O5	0.42	2.67	16	1
2:B:61:GLN:HA	2:B:96:TYR:OH	0.42	2.14	16	2
3:A:405:PCW:H382	4:D:628:17F:C29	0.42	2.42	17	1
3:B:209:PCW:H73	3:B:209:PCW:C11	0.42	2.44	18	1
3:B:210:PCW:H471	3:B:213:PCW:C20	0.42	2.44	18	1
3:A:407:PCW:H152	3:B:208:PCW:C20	0.42	2.44	20	1
3:B:203:PCW:H452	4:B:217:17F:H46	0.42	1.90	20	1
3:B:203:PCW:H161	4:C:210:17F:H20A	0.42	1.91	2	1
3:D:614:PCW:H51	3:D:614:PCW:O1P	0.42	2.14	3	1
3:B:204:PCW:H352	3:B:212:PCW:H82	0.42	1.92	3	1
3:C:203:PCW:H121	3:C:203:PCW:H362	0.42	1.90	3	1
3:D:602:PCW:C21	3:D:610:PCW:H331	0.42	2.44	4	1
2:B:80:CYS:HB2	2:B:93:ILE:HD12	0.42	1.91	4	1
2:C:2:THR:HB	2:C:4:TYR:CE2	0.42	2.50	5	2
3:D:603:PCW:H322	3:D:605:PCW:C12	0.42	2.43	6	1
3:D:622:PCW:C11	4:D:629:17F:H64	0.42	2.44	6	1
3:B:207:PCW:C1	4:B:216:17F:O7	0.42	2.65	6	1
3:B:213:PCW:H422	4:B:214:17F:C29	0.42	2.35	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:228:PHE:CE1	3:A:408:PCW:H462	0.42	2.49	7	1
3:A:408:PCW:C24	3:A:417:PCW:H262	0.42	2.45	7	1
3:B:205:PCW:H432	3:C:208:PCW:C19	0.42	2.39	7	1
3:A:402:PCW:C34	3:A:409:PCW:H121	0.42	2.43	9	1
3:A:413:PCW:C28	3:C:203:PCW:H432	0.42	2.43	9	1
3:D:602:PCW:C14	3:D:624:PCW:C18	0.42	2.97	9	1
3:B:212:PCW:H2	3:B:212:PCW:O4P	0.42	2.13	10	3
3:D:618:PCW:H381	3:D:627:PCW:C17	0.42	2.45	11	1
4:B:215:17F:H5	4:B:215:17F:H18	0.42	1.49	11	1
3:A:411:PCW:O4P	3:A:411:PCW:C8	0.42	2.67	12	1
3:A:413:PCW:H381	3:A:413:PCW:H411	0.42	1.58	12	1
3:C:207:PCW:H281	3:C:209:PCW:C39	0.42	2.32	12	1
3:B:204:PCW:O3P	3:B:206:PCW:H62	0.42	2.14	14	1
4:A:415:17F:H35	4:A:415:17F:H39	0.42	1.57	15	1
3:A:420:PCW:C34	3:D:617:PCW:H132	0.42	2.44	16	1
3:B:212:PCW:H451	4:B:214:17F:H72	0.42	1.91	16	1
3:D:607:PCW:H41	3:D:626:PCW:H221	0.42	1.87	17	1
3:D:622:PCW:C44	3:C:212:PCW:H481	0.42	2.44	18	1
4:D:629:17F:H29	4:D:630:17F:C10	0.42	2.41	18	1
3:D:623:PCW:H351	3:D:624:PCW:H322	0.42	1.91	19	1
2:C:32:TYR:CB	5:C:201:GDP:H5"	0.42	2.44	19	1
3:D:606:PCW:H362	3:D:626:PCW:H431	0.42	1.92	20	1
4:D:629:17F:C2X	4:D:630:17F:H10	0.42	2.43	20	1
4:B:214:17F:C26	4:B:217:17F:H66	0.42	2.39	20	1
3:A:413:PCW:C32	4:A:414:17F:H20	0.42	2.43	1	2
4:A:415:17F:C42	3:D:613:PCW:H261	0.42	2.44	1	1
3:D:613:PCW:H251	4:C:210:17F:C30	0.42	2.44	2	1
3:D:607:PCW:C27	4:D:628:17F:H37	0.42	2.45	4	1
3:B:213:PCW:H181	3:B:213:PCW:H211	0.42	1.63	5	2
3:D:601:PCW:H471	4:D:631:17F:H44	0.42	1.92	6	1
3:A:407:PCW:H11	4:B:216:17F:H11	0.42	1.91	8	1
3:D:608:PCW:H63	3:D:620:PCW:C3	0.42	2.43	8	1
3:B:204:PCW:C24	3:C:207:PCW:H252	0.42	2.27	8	1
3:A:405:PCW:H421	4:D:628:17F:H52	0.42	1.92	9	1
3:D:605:PCW:H442	3:D:608:PCW:H12	0.42	1.91	9	1
3:A:402:PCW:H361	3:C:205:PCW:C1	0.42	2.41	10	1
3:A:419:PCW:C11	3:D:617:PCW:C42	0.42	2.96	10	1
3:A:420:PCW:C19	4:D:632:17F:H20	0.42	2.45	11	1
3:D:602:PCW:C26	3:D:610:PCW:H142	0.42	2.35	11	1
3:A:402:PCW:C44	3:A:409:PCW:H151	0.42	2.45	12	1
2:B:18:ALA:N	5:B:201:GDP:O2A	0.42	2.51	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:624:PCW:C11	3:D:624:PCW:O31	0.42	2.68	13	1
3:B:204:PCW:C19	3:B:205:PCW:H472	0.42	2.44	13	1
1:A:279:LEU:O	1:A:283:LEU:HG	0.42	2.14	14	1
3:A:408:PCW:H181	3:A:408:PCW:H211	0.42	1.59	15	1
3:A:411:PCW:O31	4:B:215:17F:C1Z	0.42	2.67	15	1
3:A:402:PCW:H451	3:A:407:PCW:C39	0.42	2.45	16	1
3:A:404:PCW:C7	3:A:404:PCW:C2	0.42	2.94	16	1
3:D:607:PCW:H262	4:D:631:17F:H36	0.42	1.91	16	1
2:C:145:SER:HB3	2:C:150:GLN:HB3	0.42	1.91	16	1
3:A:409:PCW:O31	3:C:206:PCW:H322	0.42	2.14	19	1
3:A:417:PCW:H442	3:D:612:PCW:H272	0.42	1.92	20	1
3:D:609:PCW:C4	4:D:633:17F:H6	0.42	2.45	20	1
4:D:630:17F:H59	4:D:630:17F:C1X	0.42	2.43	20	1
4:B:214:17F:H39	4:B:214:17F:H36	0.42	1.59	2	1
3:A:402:PCW:O2	3:A:402:PCW:C4	0.42	2.64	4	1
3:D:607:PCW:H63	3:D:626:PCW:H262	0.42	1.90	4	1
1:A:363:LYS:HA	1:A:367:ALA:CB	0.42	2.41	5	2
4:A:414:17F:C28	3:B:212:PCW:C23	0.42	2.98	5	1
4:B:215:17F:H59	4:B:215:17F:H62	0.42	1.61	5	3
1:D:524:GLU:O	1:D:528:ARG:HG3	0.42	2.15	6	1
3:D:609:PCW:H181	3:D:609:PCW:H212	0.42	1.62	6	2
3:B:210:PCW:H451	3:B:213:PCW:H471	0.42	1.90	6	1
3:A:403:PCW:H61	4:A:414:17F:C3	0.42	2.44	7	1
3:B:205:PCW:H281	3:B:211:PCW:H451	0.42	1.92	7	1
2:C:7:VAL:HG21	2:C:71:TYR:HB2	0.42	1.91	7	1
3:A:406:PCW:C26	3:B:210:PCW:H122	0.42	2.35	8	1
1:D:445:LEU:O	1:D:448:VAL:HG12	0.42	2.14	16	2
3:D:601:PCW:O3	4:B:216:17F:H60	0.42	2.13	8	1
3:A:404:PCW:C6	4:A:415:17F:H2	0.42	2.40	9	1
3:D:611:PCW:H381	3:D:623:PCW:H442	0.42	1.91	9	1
3:B:207:PCW:H411	3:B:213:PCW:C23	0.42	2.30	9	1
3:A:406:PCW:H411	3:A:411:PCW:H372	0.42	1.91	10	1
3:A:406:PCW:C3	3:A:406:PCW:P	0.42	3.07	11	1
3:A:419:PCW:H442	3:C:203:PCW:C28	0.42	2.45	11	1
3:D:613:PCW:H283	4:C:210:17F:H63	0.42	1.90	11	1
3:D:623:PCW:O2	3:D:623:PCW:O11	0.42	2.36	11	1
3:B:210:PCW:H451	3:B:213:PCW:C25	0.42	2.44	11	1
1:A:250:VAL:HG11	3:A:412:PCW:C28	0.42	2.44	12	1
1:D:497:SER:HB2	1:D:498:PRO:CD	0.42	2.44	18	4
3:B:205:PCW:H332	3:B:208:PCW:H322	0.42	1.92	12	1
3:A:420:PCW:C24	4:C:210:17F:H54	0.42	2.45	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:601:PCW:C8	4:B:216:17F:O2	0.42	2.68	13	1
4:D:631:17F:H1A	4:D:631:17F:H4	0.42	1.91	13	1
1:A:392:GLU:HB3	1:D:591:TYR:CE1	0.42	2.44	16	1
3:B:212:PCW:O11	3:B:212:PCW:C8	0.42	2.66	17	1
1:D:580:PHE:O	1:D:584:PHE:HB2	0.42	2.15	19	1
3:A:402:PCW:H40	3:A:409:PCW:H261	0.42	1.91	20	1
3:D:622:PCW:C44	3:B:206:PCW:H252	0.42	2.40	20	1
3:A:407:PCW:C5	4:B:214:17F:O1	0.42	2.68	1	2
3:D:602:PCW:H371	3:D:610:PCW:H342	0.42	1.91	1	1
3:D:609:PCW:H342	3:D:609:PCW:O31	0.42	2.14	1	1
3:B:212:PCW:H212	3:B:212:PCW:H181	0.42	1.58	1	1
4:B:217:17F:H5	4:B:217:17F:H18	0.42	1.48	1	2
3:A:403:PCW:H211	3:A:403:PCW:H181	0.42	1.63	11	2
3:A:405:PCW:O3P	3:A:405:PCW:C31	0.42	2.68	3	2
3:A:407:PCW:C6	4:B:214:17F:O1	0.42	2.68	4	1
3:D:608:PCW:H131	3:D:608:PCW:O31	0.42	2.14	4	1
2:C:72:MET:HA	2:C:78:PHE:HZ	0.42	1.73	15	2
3:A:413:PCW:O3	3:A:413:PCW:C35	0.42	2.61	5	1
3:B:211:PCW:H152	4:B:217:17F:C32	0.42	2.41	10	2
3:D:605:PCW:C35	4:D:629:17F:O7	0.42	2.68	6	1
3:D:618:PCW:H281	4:C:211:17F:H37	0.42	1.91	6	1
3:D:613:PCW:O4P	3:D:613:PCW:C8	0.42	2.67	11	4
4:B:217:17F:H78	4:B:217:17F:H51	0.42	1.91	7	1
1:A:222:GLY:O	1:A:226:GLN:HG3	0.42	2.14	8	1
3:A:411:PCW:C3	4:B:215:17F:H33	0.42	2.42	8	1
3:D:616:PCW:H281	3:D:618:PCW:C28	0.42	2.45	8	1
3:D:608:PCW:H73	3:D:620:PCW:H31	0.42	1.90	9	2
3:B:208:PCW:O2	3:B:208:PCW:C11	0.42	2.67	9	1
3:B:211:PCW:C3	4:B:217:17F:C1Y	0.42	2.93	9	1
3:B:213:PCW:H73	4:B:214:17F:P1	0.42	2.55	9	1
3:A:403:PCW:C23	3:A:403:PCW:C27	0.42	2.96	10	1
3:A:408:PCW:H341	3:C:204:PCW:H182	0.42	1.87	10	1
3:A:416:PCW:H142	3:D:617:PCW:C14	0.42	2.45	11	1
3:D:621:PCW:H483	4:D:634:17F:C31	0.42	2.42	12	1
3:D:621:PCW:H471	4:D:634:17F:H63	0.42	1.92	12	1
3:D:609:PCW:H151	4:D:633:17F:C34	0.42	2.44	13	1
3:D:618:PCW:O1P	3:D:627:PCW:C5	0.42	2.68	13	1
3:B:211:PCW:H242	4:B:217:17F:C40	0.42	2.44	13	1
3:A:404:PCW:H452	3:B:209:PCW:C44	0.42	2.45	14	1
3:C:207:PCW:H141	3:C:209:PCW:H31	0.42	1.90	14	1
3:A:417:PCW:C44	3:D:612:PCW:H272	0.42	2.43	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:217:LEU:CD1	3:A:408:PCW:H232	0.42	2.45	17	1
1:D:470:TYR:O	1:D:474:VAL:HB	0.42	2.14	18	1
3:B:208:PCW:C23	3:B:208:PCW:C27	0.42	2.95	19	1
3:A:412:PCW:C41	3:C:208:PCW:C36	0.42	2.97	20	1
3:A:417:PCW:H411	3:A:417:PCW:H371	0.42	1.90	20	1
3:B:206:PCW:C48	4:C:211:17F:H49	0.42	2.44	20	1
3:D:602:PCW:C8	3:C:212:PCW:P	0.42	3.08	1	1
3:D:623:PCW:H281	3:D:624:PCW:C43	0.42	2.45	4	2
3:A:418:PCW:O11	3:A:418:PCW:C2	0.42	2.65	2	1
3:D:616:PCW:H481	3:B:204:PCW:H20	0.42	1.91	2	1
3:B:204:PCW:C45	3:C:203:PCW:H39	0.42	2.43	3	1
3:A:406:PCW:O3	3:A:406:PCW:C31	0.42	2.67	4	1
1:D:591:TYR:HB3	4:D:632:17F:H48	0.42	1.91	15	2
3:C:206:PCW:C23	3:C:206:PCW:H181	0.42	2.44	5	1
3:A:410:PCW:C6	3:A:410:PCW:P	0.42	3.08	6	1
3:A:417:PCW:H411	3:D:612:PCW:C14	0.42	2.44	6	1
3:B:203:PCW:H61	4:B:217:17F:C18	0.42	2.36	6	1
3:B:203:PCW:O4P	3:B:203:PCW:C8	0.42	2.68	7	3
3:B:211:PCW:H2	4:B:217:17F:H19A	0.42	1.92	7	1
3:A:408:PCW:C32	3:C:204:PCW:H182	0.42	2.43	8	1
3:B:206:PCW:C8	3:C:207:PCW:O1P	0.42	2.68	9	1
3:A:404:PCW:C33	3:B:203:PCW:H171	0.42	2.25	10	1
3:A:408:PCW:C37	3:C:204:PCW:H231	0.42	2.43	10	1
3:A:413:PCW:C32	4:A:414:17F:H18	0.42	2.39	11	1
3:B:205:PCW:C27	3:B:212:PCW:H161	0.42	2.41	12	1
2:C:167:LYS:HD3	3:C:207:PCW:H61	0.42	1.92	12	1
3:C:204:PCW:H211	3:C:204:PCW:C16	0.42	2.44	12	2
3:C:205:PCW:H412	3:C:205:PCW:H382	0.42	1.65	12	1
3:A:404:PCW:H361	3:B:209:PCW:H352	0.42	1.92	13	1
3:D:614:PCW:C4	3:D:625:PCW:C4	0.42	2.83	13	1
3:B:208:PCW:C11	3:B:208:PCW:O2	0.42	2.68	13	1
3:A:404:PCW:O3	3:B:209:PCW:H321	0.42	2.14	14	1
3:D:619:PCW:C8	3:D:619:PCW:O4P	0.42	2.68	15	1
3:A:409:PCW:C3	3:C:206:PCW:C4	0.42	2.96	16	1
4:A:415:17F:H39	4:A:415:17F:H35	0.42	1.60	19	1
3:D:608:PCW:H39	3:D:615:PCW:H421	0.42	1.91	20	1
3:A:412:PCW:C40	3:C:206:PCW:H371	0.42	2.45	1	1
2:B:72:MET:HA	2:B:78:PHE:HZ	0.42	1.75	10	2
3:B:205:PCW:H411	3:B:205:PCW:H381	0.42	1.61	16	2
3:B:211:PCW:H231	4:B:217:17F:H69	0.42	1.90	4	1
3:A:403:PCW:C12	3:C:203:PCW:H12	0.42	2.44	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:611:PCW:H452	3:D:619:PCW:H481	0.42	1.90	6	1
3:D:612:PCW:C35	3:D:627:PCW:O11	0.42	2.68	6	2
3:B:208:PCW:C40	4:B:214:17F:H76	0.42	2.44	6	1
3:C:209:PCW:O1P	3:C:209:PCW:H51	0.42	2.15	6	2
2:B:45:VAL:HG22	2:B:50:THR:HG23	0.42	1.92	7	1
3:B:209:PCW:C22	3:B:209:PCW:C26	0.42	2.97	15	2
3:A:407:PCW:H372	3:C:205:PCW:H122	0.42	1.91	8	1
3:A:419:PCW:C37	3:D:617:PCW:C40	0.42	2.97	8	2
3:D:613:PCW:C47	3:D:619:PCW:H422	0.42	2.45	8	1
3:D:616:PCW:C39	3:D:618:PCW:C14	0.42	2.83	9	1
3:A:401:PCW:H471	3:D:614:PCW:C22	0.42	2.42	10	1
3:A:416:PCW:H39	3:A:416:PCW:H151	0.42	1.91	11	1
3:A:420:PCW:C6	4:D:632:17F:H6A	0.42	2.45	11	1
3:B:203:PCW:C26	4:C:210:17F:H19	0.42	2.39	11	1
3:A:410:PCW:H261	3:D:618:PCW:H462	0.42	1.92	13	1
3:D:620:PCW:C27	4:D:635:17F:C21	0.42	2.98	13	1
3:B:203:PCW:H251	3:B:209:PCW:H441	0.42	1.91	13	1
3:B:208:PCW:O2	3:B:208:PCW:O11	0.42	2.38	13	1
3:A:408:PCW:H283	3:A:417:PCW:C45	0.42	2.45	15	1
3:D:618:PCW:H252	3:C:204:PCW:C47	0.42	2.45	15	1
3:D:623:PCW:O31	3:D:624:PCW:C32	0.42	2.59	15	1
3:A:403:PCW:O3P	3:C:204:PCW:C6	0.42	2.64	16	1
3:C:204:PCW:C23	3:C:207:PCW:H472	0.42	2.41	17	1
3:A:405:PCW:H372	3:D:601:PCW:C15	0.42	2.45	20	1
3:B:206:PCW:H382	3:B:206:PCW:H411	0.42	1.59	20	1
3:B:208:PCW:O3P	3:B:208:PCW:C5	0.42	2.66	20	1
1:D:444:ASP:O	1:D:448:VAL:HG23	0.42	2.15	1	1
3:A:401:PCW:H12	3:B:209:PCW:H242	0.42	1.90	2	1
3:B:210:PCW:C27	3:B:210:PCW:H431	0.42	2.44	2	1
3:B:213:PCW:H462	4:B:217:17F:C24	0.42	2.45	2	1
1:A:362:GLU:HA	1:A:366:PRO:HD2	0.42	1.92	3	1
3:A:401:PCW:C11	3:B:209:PCW:H251	0.42	2.45	3	1
3:A:404:PCW:C6	4:A:415:17F:O5	0.42	2.66	3	1
1:D:413:SER:O	1:D:417:GLU:HG3	0.42	2.15	3	1
3:B:210:PCW:O11	3:B:210:PCW:H73	0.42	2.15	3	1
2:C:69:ASP:O	2:C:73:ARG:HG3	0.42	2.15	3	1
3:D:608:PCW:H52	4:D:635:17F:N1	0.42	2.30	4	1
3:D:627:PCW:H221	3:D:627:PCW:C18	0.42	2.44	4	1
2:B:159:LEU:O	2:B:163:ILE:HG13	0.42	2.15	7	2
3:B:213:PCW:H122	4:B:217:17F:C7	0.42	2.45	4	1
3:A:404:PCW:C12	3:B:209:PCW:H362	0.42	2.43	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:415:17F:H62	4:A:415:17F:H59	0.42	1.60	5	2
3:A:420:PCW:H382	3:A:420:PCW:H411	0.42	1.56	5	1
3:B:205:PCW:H51	4:B:214:17F:H6A	0.42	1.92	7	1
4:A:415:17F:C42	3:D:611:PCW:H472	0.42	2.44	8	1
3:B:205:PCW:H131	3:B:211:PCW:O11	0.42	2.14	9	1
3:B:205:PCW:H221	3:B:212:PCW:H342	0.42	1.91	11	1
4:C:210:17F:H62	4:C:210:17F:H58	0.42	1.52	11	1
3:A:420:PCW:H141	4:D:632:17F:H11	0.42	1.91	13	1
3:D:623:PCW:O31	3:D:623:PCW:O3	0.42	2.37	13	1
4:B:216:17F:O10	4:B:216:17F:H20A	0.42	2.15	13	1
3:B:205:PCW:C17	3:B:212:PCW:H342	0.42	2.44	14	1
3:A:407:PCW:H141	3:B:208:PCW:C22	0.42	2.40	15	1
3:B:210:PCW:H281	3:B:210:PCW:H412	0.42	1.91	15	1
3:B:213:PCW:H332	4:B:214:17F:H9A	0.42	1.92	16	1
3:A:410:PCW:C21	3:C:209:PCW:H262	0.42	2.45	17	1
3:A:413:PCW:C24	4:A:414:17F:C33	0.42	2.98	17	1
3:B:208:PCW:C13	4:B:214:17F:O10	0.42	2.68	17	1
3:A:407:PCW:H382	3:A:407:PCW:H411	0.42	1.62	19	1
3:A:407:PCW:H412	3:D:601:PCW:H322	0.42	1.91	19	1
3:D:606:PCW:C43	3:D:626:PCW:C48	0.42	2.98	20	1
4:D:634:17F:H40	4:D:634:17F:H36	0.42	1.67	20	1
3:B:213:PCW:H272	4:B:215:17F:C34	0.42	2.44	20	1
3:D:623:PCW:H122	3:D:624:PCW:C35	0.41	2.44	1	1
3:B:208:PCW:C6	3:C:208:PCW:O1P	0.41	2.64	1	1
4:D:634:17F:O10	4:D:634:17F:P1	0.41	2.78	8	4
3:A:418:PCW:H382	3:A:418:PCW:H412	0.41	1.52	5	4
4:D:630:17F:P1	4:D:630:17F:O9	0.41	2.78	3	1
2:C:32:TYR:CB	5:C:201:GDP:H3'	0.41	2.45	11	2
3:D:624:PCW:C27	3:B:212:PCW:H281	0.41	2.42	4	1
3:C:204:PCW:H412	3:C:204:PCW:H382	0.41	1.63	4	1
3:A:401:PCW:H122	3:B:209:PCW:H471	0.41	1.92	5	1
3:A:407:PCW:H212	3:C:205:PCW:H172	0.41	1.91	5	1
3:D:623:PCW:C28	3:D:624:PCW:H452	0.41	2.45	5	1
1:D:488:LYS:O	1:D:492:LEU:HG	0.41	2.15	6	1
3:B:206:PCW:H482	3:C:212:PCW:C22	0.41	2.43	6	1
3:A:401:PCW:O1P	3:B:209:PCW:H161	0.41	2.14	7	1
3:A:403:PCW:C7	4:A:414:17F:O4	0.41	2.68	7	1
3:A:410:PCW:O1P	3:A:410:PCW:H32	0.41	2.15	7	1
3:D:602:PCW:O11	3:D:603:PCW:C8	0.41	2.68	7	1
3:D:623:PCW:H211	3:B:211:PCW:H271	0.41	1.91	7	1
4:D:634:17F:H74	3:C:206:PCW:C25	0.41	2.45	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:203:PCW:H2	3:B:211:PCW:C37	0.41	2.42	7	1
3:A:401:PCW:C43	3:D:614:PCW:H262	0.41	2.45	9	1
3:A:403:PCW:H452	3:C:203:PCW:C28	0.41	2.44	10	1
3:B:203:PCW:C18	4:B:215:17F:H38	0.41	2.45	11	1
3:B:203:PCW:H222	4:C:210:17F:H20A	0.41	1.91	11	1
3:A:402:PCW:H31	3:A:402:PCW:H41	0.41	1.91	12	1
3:A:404:PCW:H462	4:B:215:17F:H56	0.41	1.92	12	1
3:B:210:PCW:H221	3:B:210:PCW:C18	0.41	2.45	12	1
1:D:469:LEU:O	1:D:473:LYS:HB2	0.41	2.15	13	1
3:A:404:PCW:O31	3:A:404:PCW:H341	0.41	2.14	14	1
3:A:413:PCW:H431	4:C:210:17F:C12	0.41	2.41	15	1
3:D:608:PCW:H461	4:D:635:17F:H62	0.41	1.91	15	1
4:D:635:17F:H52	3:C:205:PCW:C19	0.41	2.45	15	1
4:D:629:17F:O9	4:D:629:17F:P1	0.41	2.78	18	1
3:B:210:PCW:H471	3:B:213:PCW:C18	0.41	2.45	18	1
3:A:404:PCW:H122	3:B:209:PCW:H39	0.41	1.92	19	1
4:D:633:17F:C30	3:C:209:PCW:H462	0.41	2.45	19	1
3:D:623:PCW:H182	3:D:623:PCW:H222	0.41	1.91	1	1
3:B:205:PCW:C15	4:B:214:17F:H37	0.41	2.26	2	1
3:A:411:PCW:H411	3:A:411:PCW:H381	0.41	1.63	3	1
1:D:567:GLU:O	1:D:571:GLN:HG3	0.41	2.15	3	1
3:A:417:PCW:C8	3:A:419:PCW:O11	0.41	2.68	4	1
3:D:607:PCW:H41	3:D:626:PCW:H242	0.41	1.92	4	1
3:B:204:PCW:H122	3:C:204:PCW:C39	0.41	2.46	4	1
3:B:211:PCW:H431	3:B:212:PCW:O3	0.41	2.15	4	1
3:A:403:PCW:H181	3:A:403:PCW:H211	0.41	1.63	5	1
3:C:207:PCW:H181	3:C:207:PCW:H212	0.41	1.56	16	2
3:A:416:PCW:C45	3:A:420:PCW:H421	0.41	2.26	6	1
3:D:604:PCW:C46	4:C:210:17F:H53	0.41	2.44	6	1
3:D:613:PCW:H432	3:D:619:PCW:C40	0.41	2.45	6	1
3:D:622:PCW:H472	3:B:206:PCW:H221	0.41	1.91	6	1
3:C:209:PCW:O31	3:C:209:PCW:H132	0.41	2.15	6	1
3:B:211:PCW:H171	3:B:211:PCW:H482	0.41	1.92	7	1
3:A:407:PCW:H181	3:B:208:PCW:H222	0.41	1.92	9	1
4:D:630:17F:H12A	4:D:630:17F:H59	0.41	1.92	9	1
3:B:204:PCW:H40	3:C:203:PCW:C7	0.41	2.43	10	1
4:A:414:17F:H46	3:B:204:PCW:C44	0.41	2.45	11	1
3:A:419:PCW:C42	3:D:610:PCW:H211	0.41	2.46	11	1
1:D:475:GLU:O	1:D:478:ARG:HB2	0.41	2.14	11	1
4:D:635:17F:H39	4:D:635:17F:H36	0.41	1.65	11	2
3:A:407:PCW:H221	3:D:608:PCW:H451	0.41	1.91	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:611:PCW:H242	3:D:619:PCW:C45	0.41	2.45	12	1
3:B:206:PCW:H362	3:C:204:PCW:H40	0.41	1.85	13	1
3:A:407:PCW:C6	3:B:213:PCW:C31	0.41	2.98	14	1
3:A:411:PCW:H39	4:B:215:17F:H73	0.41	1.93	14	1
4:C:211:17F:H54	3:C:212:PCW:H221	0.41	1.92	14	1
1:D:455:TYR:O	1:D:459:PHE:HB2	0.41	2.14	15	1
3:B:209:PCW:H432	3:B:209:PCW:H232	0.41	1.92	15	1
3:A:411:PCW:H19	3:A:411:PCW:C13	0.41	2.40	16	1
3:B:212:PCW:H40	3:C:212:PCW:H281	0.41	1.91	17	1
1:A:359:THR:HG21	1:D:418:GLN:NE2	0.41	2.30	20	1
3:A:402:PCW:H212	3:A:409:PCW:H39	0.41	1.92	20	1
3:D:616:PCW:H181	3:D:616:PCW:H211	0.41	1.67	20	1
4:D:628:17F:H69	4:D:631:17F:C27	0.41	2.42	20	1
3:B:210:PCW:C7	4:B:216:17F:HN1	0.41	2.27	20	1
3:D:618:PCW:H322	3:D:627:PCW:C12	0.41	2.44	1	1
3:D:618:PCW:C32	3:D:627:PCW:H121	0.41	2.42	1	1
3:B:203:PCW:C21	4:C:210:17F:H56	0.41	2.44	1	1
3:B:210:PCW:H451	3:B:213:PCW:H271	0.41	1.91	1	1
4:A:414:17F:H36	4:C:210:17F:H5	0.41	1.92	2	1
3:C:204:PCW:H20	4:C:211:17F:C17	0.41	2.46	2	1
3:D:615:PCW:H142	4:D:635:17F:C8	0.41	2.46	3	1
4:B:216:17F:H39	4:B:216:17F:H36	0.41	1.57	3	1
3:A:404:PCW:H151	4:A:415:17F:C1Y	0.41	2.42	4	1
3:D:602:PCW:C37	3:D:602:PCW:C41	0.41	2.95	14	2
3:D:609:PCW:C3	4:D:633:17F:H18	0.41	2.43	4	1
3:B:207:PCW:H42	4:B:216:17F:O1	0.41	2.15	4	1
3:A:409:PCW:O2	3:A:409:PCW:C34	0.41	2.67	6	1
3:A:410:PCW:H63	3:A:410:PCW:O3P	0.41	2.15	7	1
3:D:601:PCW:H321	4:B:216:17F:H61	0.41	1.92	7	1
3:D:622:PCW:C27	3:D:624:PCW:H261	0.41	2.42	7	1
3:B:203:PCW:C7	4:B:217:17F:C18	0.41	2.98	7	1
3:C:207:PCW:H321	3:C:207:PCW:H41	0.41	1.92	7	1
3:A:408:PCW:H82	3:C:204:PCW:C12	0.41	2.45	8	1
1:D:459:PHE:CD2	3:D:601:PCW:H281	0.41	2.50	8	1
3:D:621:PCW:H412	4:D:635:17F:C42	0.41	2.33	8	1
3:D:621:PCW:H222	4:D:633:17F:C19	0.41	2.46	8	1
3:B:204:PCW:H231	3:C:208:PCW:H262	0.41	1.92	9	1
3:A:413:PCW:H52	4:A:415:17F:O4	0.41	2.14	10	1
3:A:417:PCW:C42	3:D:612:PCW:H181	0.41	2.45	10	1
3:D:602:PCW:H271	3:D:610:PCW:H171	0.41	1.92	11	1
3:D:614:PCW:H411	3:D:614:PCW:H381	0.41	1.56	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:207:PCW:H131	3:C:207:PCW:C26	0.41	2.45	11	1
3:A:410:PCW:H242	3:C:207:PCW:C25	0.41	2.35	12	1
1:A:245:LYS:O	1:A:249:GLU:HB2	0.41	2.15	13	2
3:A:417:PCW:C43	3:D:612:PCW:H142	0.41	2.30	15	1
3:D:617:PCW:O31	3:D:617:PCW:H41	0.41	2.15	15	1
3:A:407:PCW:H52	4:B:216:17F:H9A	0.41	1.91	16	1
3:D:603:PCW:H411	3:D:603:PCW:H381	0.41	1.70	16	1
3:A:410:PCW:C18	3:A:410:PCW:C23	0.41	2.98	17	1
3:A:419:PCW:H321	3:D:617:PCW:H422	0.41	1.92	17	1
3:B:204:PCW:C22	3:C:208:PCW:H262	0.41	2.46	17	1
2:C:12:ASP:HA	2:C:16:LYS:HZ2	0.41	1.73	17	1
3:C:208:PCW:H412	3:C:208:PCW:C14	0.41	2.43	17	1
1:D:584:PHE:O	1:D:588:LEU:HG	0.41	2.15	18	1
3:A:418:PCW:C6	3:D:626:PCW:O31	0.41	2.67	19	1
1:A:379:LEU:O	1:A:383:LYS:HG3	0.41	2.15	20	1
3:B:213:PCW:H412	4:B:217:17F:H58	0.41	1.85	20	1
3:D:601:PCW:C25	4:D:631:17F:H76	0.41	2.41	1	1
3:D:601:PCW:C14	3:D:601:PCW:H381	0.41	2.45	11	2
3:D:623:PCW:H281	3:D:624:PCW:H432	0.41	1.92	1	1
3:B:203:PCW:H172	4:C:210:17F:C19	0.41	2.45	1	1
3:D:603:PCW:H411	3:D:603:PCW:C37	0.41	2.46	15	2
3:B:208:PCW:H181	3:B:208:PCW:H212	0.41	1.59	3	1
1:A:332:ALA:O	1:A:336:GLU:HG3	0.41	2.16	4	1
3:D:608:PCW:O4P	3:D:608:PCW:C8	0.41	2.68	5	1
3:B:211:PCW:O2	3:B:211:PCW:C11	0.41	2.68	5	2
4:B:215:17F:O7	4:B:215:17F:C18	0.41	2.67	6	1
2:B:17:SER:N	5:B:201:GDP:O3B	0.41	2.53	7	1
3:A:401:PCW:H51	3:B:209:PCW:C31	0.41	2.45	8	1
3:A:416:PCW:H181	3:A:416:PCW:H212	0.41	1.58	8	2
3:A:418:PCW:H412	3:A:418:PCW:H382	0.41	1.63	8	5
3:D:618:PCW:H241	3:B:206:PCW:C44	0.41	2.42	8	1
3:D:621:PCW:C22	4:D:633:17F:H19A	0.41	2.46	8	1
2:B:82:PHE:CE2	2:B:113:LEU:HG	0.41	2.46	8	1
1:D:463:TRP:NE1	4:D:631:17F:H71	0.41	2.30	9	1
3:B:207:PCW:H381	3:B:213:PCW:H221	0.41	1.91	9	1
3:A:416:PCW:H362	3:A:420:PCW:H372	0.41	1.85	11	1
4:C:210:17F:C10	4:C:210:17F:C32	0.41	2.98	11	1
4:C:210:17F:H40	4:C:210:17F:H36	0.41	1.65	11	1
3:D:615:PCW:C14	4:D:635:17F:H9A	0.41	2.26	12	1
3:C:204:PCW:H331	4:C:211:17F:H8A	0.41	1.92	12	1
2:C:42:LYS:HE3	2:C:44:VAL:HG11	0.41	1.93	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:621:PCW:O3	4:D:634:17F:O9	0.41	2.38	14	1
3:A:419:PCW:C46	3:D:616:PCW:H251	0.41	2.41	15	1
2:B:15:GLY:HA3	2:B:116:ASN:ND2	0.41	2.31	15	1
3:D:613:PCW:H283	4:C:210:17F:H66	0.41	1.92	17	1
3:B:209:PCW:C6	4:B:215:17F:C8	0.41	2.98	17	1
3:C:207:PCW:H262	3:C:208:PCW:C24	0.41	2.45	17	1
3:A:404:PCW:H451	4:B:215:17F:C24	0.41	2.45	18	1
3:A:404:PCW:C46	4:B:215:17F:H42	0.41	2.45	18	1
3:A:412:PCW:H52	2:C:3:GLU:OE1	0.41	2.16	18	1
3:D:607:PCW:H221	4:D:628:17F:C18	0.41	2.38	18	1
3:B:211:PCW:C3	4:B:217:17F:H60	0.41	2.46	18	1
3:C:207:PCW:O2	3:C:207:PCW:P	0.41	2.79	18	1
3:D:605:PCW:C4	3:D:626:PCW:C19	0.41	2.98	20	1
3:D:622:PCW:H73	4:D:633:17F:C11	0.41	2.45	20	1
3:A:402:PCW:C16	3:A:409:PCW:H222	0.41	2.44	1	1
3:A:405:PCW:H381	3:A:405:PCW:H412	0.41	1.58	10	2
3:A:413:PCW:H331	4:A:414:17F:H9	0.41	1.93	1	1
3:A:418:PCW:O1P	3:D:614:PCW:C4	0.41	2.68	8	2
3:D:604:PCW:H442	3:D:624:PCW:H442	0.41	1.91	2	1
2:C:14:VAL:HG23	5:C:201:GDP:O1B	0.41	2.15	3	1
3:A:411:PCW:H482	3:A:411:PCW:C28	0.41	2.46	4	1
3:D:623:PCW:O3P	3:D:623:PCW:C31	0.41	2.69	4	1
3:C:203:PCW:C22	3:C:203:PCW:C18	0.41	2.59	4	1
3:C:208:PCW:H451	3:C:209:PCW:H382	0.41	1.90	6	1
3:A:407:PCW:H11	4:B:216:17F:H29	0.41	1.91	7	1
1:D:464:GLN:O	1:D:468:GLU:HG3	0.41	2.14	7	1
3:B:205:PCW:C5	3:B:208:PCW:H11	0.41	2.43	7	1
3:A:408:PCW:O1P	3:C:204:PCW:C17	0.41	2.69	8	1
3:D:607:PCW:C43	4:D:628:17F:C33	0.41	2.98	8	1
3:D:613:PCW:C48	3:D:619:PCW:H441	0.41	2.46	8	1
3:B:208:PCW:C40	4:B:214:17F:H12	0.41	2.45	8	1
3:D:611:PCW:O3	3:D:611:PCW:C31	0.41	2.68	9	1
3:D:623:PCW:C13	3:D:623:PCW:H371	0.41	2.44	9	1
3:A:413:PCW:C7	4:A:415:17F:O4	0.41	2.68	10	1
3:D:611:PCW:H371	3:D:611:PCW:H19	0.41	1.93	10	1
3:A:409:PCW:O1P	3:A:412:PCW:H11	0.41	2.16	11	1
3:A:410:PCW:H381	3:A:410:PCW:H411	0.41	1.65	11	1
1:D:521:TYR:O	1:D:525:LEU:HG	0.41	2.16	11	1
3:D:608:PCW:H362	3:C:205:PCW:C28	0.41	2.45	11	1
3:D:621:PCW:H372	4:D:633:17F:C33	0.41	2.44	13	1
3:B:205:PCW:C22	3:B:212:PCW:C35	0.41	2.96	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:216:17F:H62	4:B:216:17F:C31	0.41	2.41	13	1
2:C:15:GLY:HA2	5:C:201:GDP:O5'	0.41	2.15	13	1
4:D:630:17F:C36	4:D:634:17F:H36	0.41	2.45	14	1
4:C:211:17F:H54	3:C:212:PCW:C22	0.41	2.45	14	1
3:D:607:PCW:H20	4:D:631:17F:C26	0.41	2.44	15	1
3:B:207:PCW:C35	3:B:210:PCW:H331	0.41	2.45	15	1
3:D:606:PCW:H472	3:B:210:PCW:H282	0.41	1.92	16	1
3:D:622:PCW:H182	3:D:622:PCW:H212	0.41	1.64	16	1
3:B:207:PCW:C14	3:B:210:PCW:C36	0.41	2.99	16	1
3:A:417:PCW:H39	3:D:612:PCW:H432	0.41	1.92	18	2
3:A:413:PCW:C24	4:A:414:17F:H59	0.41	2.44	19	1
4:D:635:17F:H36	4:D:635:17F:H39	0.41	1.64	19	1
3:A:403:PCW:C31	3:C:204:PCW:C6	0.41	2.98	20	1
3:A:412:PCW:H382	3:A:412:PCW:H412	0.41	1.62	20	1
3:B:205:PCW:O11	3:B:211:PCW:H62	0.41	2.15	20	1
3:B:205:PCW:H2	3:B:211:PCW:H62	0.41	1.91	20	1
4:B:216:17F:H55	3:C:205:PCW:C22	0.41	2.41	20	1
3:C:204:PCW:H11	3:C:204:PCW:C4	0.41	2.44	20	1
3:A:417:PCW:O2	3:A:417:PCW:H342	0.41	2.15	8	2
3:D:611:PCW:H32	3:D:619:PCW:H63	0.41	1.93	3	2
4:D:634:17F:C34	4:D:635:17F:H72	0.41	2.46	3	1
3:B:210:PCW:C5	3:B:210:PCW:O3P	0.41	2.69	3	1
3:D:615:PCW:C20	4:D:635:17F:C22	0.41	2.99	4	1
3:A:409:PCW:H121	3:C:206:PCW:C33	0.41	2.46	5	1
2:B:110:PRO:HB3	2:B:162:GLU:HB3	0.41	1.93	5	1
3:B:206:PCW:H361	3:C:204:PCW:H381	0.41	1.91	5	1
3:B:211:PCW:C1	3:B:211:PCW:O31	0.41	2.67	6	1
3:A:411:PCW:O31	3:A:411:PCW:H11	0.41	2.16	8	1
3:C:204:PCW:H271	4:C:211:17F:H57	0.41	1.93	9	1
3:A:404:PCW:H19	3:B:209:PCW:H242	0.41	1.92	10	1
3:B:203:PCW:C4	3:B:211:PCW:H352	0.41	2.46	10	1
3:C:207:PCW:H51	4:C:211:17F:O5	0.41	2.15	10	1
3:A:401:PCW:H482	3:D:611:PCW:H212	0.41	1.91	11	1
3:A:419:PCW:H462	3:C:203:PCW:H281	0.41	1.91	11	1
3:D:603:PCW:C27	4:B:217:17F:H52	0.41	2.45	12	1
3:B:208:PCW:C18	3:B:208:PCW:H222	0.41	2.46	12	1
3:D:610:PCW:H462	3:B:212:PCW:H283	0.41	1.92	13	1
3:D:623:PCW:C12	3:D:624:PCW:H332	0.41	2.42	14	1
3:B:203:PCW:H212	3:B:203:PCW:H181	0.41	1.57	14	1
3:B:209:PCW:H151	4:B:215:17F:C1	0.41	2.44	14	1
3:A:404:PCW:H122	3:B:209:PCW:C39	0.41	2.44	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:418:PCW:H63	3:D:626:PCW:C32	0.41	2.46	15	1
3:A:419:PCW:H382	3:D:610:PCW:C15	0.41	2.46	15	1
3:D:603:PCW:H331	4:D:630:17F:O8	0.41	2.15	15	1
3:D:622:PCW:H181	4:D:630:17F:C1X	0.41	2.45	15	1
3:A:407:PCW:C16	3:B:208:PCW:C20	0.41	2.97	16	1
3:B:212:PCW:C44	4:B:214:17F:H72	0.41	2.44	16	1
3:C:204:PCW:H221	3:C:207:PCW:C47	0.41	2.46	16	1
3:A:403:PCW:C17	3:C:203:PCW:C12	0.41	2.83	17	1
3:D:605:PCW:H381	3:D:605:PCW:H412	0.41	1.56	17	2
3:D:613:PCW:H282	4:C:210:17F:C2X	0.41	2.45	18	1
3:D:603:PCW:C24	4:B:217:17F:H76	0.41	2.45	19	1
4:B:214:17F:O4	3:C:205:PCW:H62	0.41	2.16	19	1
3:A:404:PCW:H211	4:A:415:17F:C32	0.41	2.46	20	1
3:D:605:PCW:C15	4:D:629:17F:H8	0.41	2.44	20	1
3:A:416:PCW:H152	3:D:602:PCW:H272	0.41	1.93	1	1
3:A:404:PCW:O4P	3:A:404:PCW:C8	0.41	2.68	9	2
3:A:408:PCW:H371	3:A:408:PCW:H412	0.41	1.93	2	1
3:D:621:PCW:H132	4:D:634:17F:O6	0.41	2.16	2	1
3:B:204:PCW:H442	3:C:203:PCW:C13	0.41	2.43	2	1
3:B:210:PCW:O11	3:B:210:PCW:O4P	0.41	2.38	2	1
3:A:418:PCW:H31	3:D:614:PCW:H121	0.41	1.93	3	1
3:B:203:PCW:H432	3:B:211:PCW:H212	0.41	1.91	3	1
3:A:406:PCW:H182	3:A:406:PCW:H211	0.41	1.57	5	2
3:D:601:PCW:H482	4:D:628:17F:C32	0.41	2.45	5	1
3:B:206:PCW:C7	3:C:207:PCW:O1P	0.41	2.68	5	1
3:A:401:PCW:H442	3:D:614:PCW:H271	0.41	1.92	6	1
3:A:408:PCW:C4	3:C:204:PCW:H171	0.41	2.45	7	1
3:A:410:PCW:H231	3:C:207:PCW:H232	0.41	1.93	7	1
3:A:412:PCW:C46	3:C:208:PCW:H19	0.41	2.25	8	1
4:A:414:17F:H9A	3:C:203:PCW:H361	0.41	1.93	8	1
4:D:628:17F:H39	4:D:628:17F:H35	0.41	1.64	11	2
3:D:603:PCW:H332	3:D:603:PCW:C12	0.41	2.45	12	1
3:B:208:PCW:C19	4:B:214:17F:C33	0.41	2.98	12	1
3:D:608:PCW:H462	3:C:205:PCW:C45	0.41	2.45	13	1
3:A:410:PCW:H331	3:C:209:PCW:C15	0.41	2.45	14	1
4:D:635:17F:H54	3:C:205:PCW:H181	0.41	1.92	15	1
3:D:601:PCW:H82	4:B:216:17F:C2	0.41	2.46	16	1
3:C:207:PCW:H382	3:C:207:PCW:H411	0.41	1.66	16	1
1:A:229:TRP:CE3	1:A:229:TRP:HA	0.41	2.51	17	1
4:A:414:17F:H48	3:C:203:PCW:H40	0.41	1.91	18	1
1:D:559:SER:O	1:D:563:LYS:HG3	0.41	2.15	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:210:PCW:H52	4:B:216:17F:C18	0.41	2.46	18	1
3:B:213:PCW:C39	4:B:217:17F:H67	0.41	2.45	18	1
4:D:629:17F:O8	4:D:629:17F:H5	0.41	2.16	19	1
3:B:205:PCW:C24	3:B:206:PCW:H352	0.41	2.33	19	1
2:C:22:GLN:CD	2:C:149:ARG:HG3	0.41	2.40	19	1
3:C:208:PCW:H452	3:C:209:PCW:H412	0.41	1.91	19	1
3:C:212:PCW:H372	3:C:212:PCW:H142	0.41	1.92	19	1
3:A:416:PCW:H2	3:A:416:PCW:O2P	0.41	2.15	20	1
3:D:604:PCW:H332	3:D:624:PCW:H73	0.41	1.93	20	1
3:B:207:PCW:C18	3:B:210:PCW:C20	0.41	2.98	20	1
3:A:402:PCW:H411	3:A:402:PCW:H382	0.41	1.56	3	2
3:A:406:PCW:H321	3:A:411:PCW:H52	0.41	1.93	1	1
3:D:621:PCW:H271	3:D:622:PCW:H61	0.41	1.90	1	1
3:A:404:PCW:H221	4:A:415:17F:C36	0.41	2.45	2	1
3:D:618:PCW:H181	3:D:618:PCW:H212	0.41	1.73	10	2
3:A:403:PCW:C28	3:A:413:PCW:H211	0.41	2.46	3	1
3:A:416:PCW:C8	4:D:632:17F:C3	0.41	2.98	4	1
3:A:417:PCW:O3	3:A:417:PCW:C31	0.41	2.69	4	1
4:D:628:17F:H36	4:D:631:17F:C39	0.41	2.46	4	1
1:D:456:LEU:O	1:D:460:GLN:HB2	0.41	2.15	5	1
3:D:602:PCW:C45	3:D:610:PCW:H432	0.41	2.46	5	1
3:D:613:PCW:H141	3:D:619:PCW:H382	0.41	1.92	6	1
3:A:403:PCW:H481	3:C:203:PCW:C28	0.41	2.44	7	1
3:D:613:PCW:C13	3:D:619:PCW:H382	0.41	2.46	8	1
3:A:404:PCW:H40	4:B:215:17F:O7	0.41	2.16	9	1
3:B:213:PCW:C41	4:B:217:17F:H64	0.41	2.45	9	1
3:A:406:PCW:C25	3:B:207:PCW:C19	0.41	2.97	11	1
3:C:208:PCW:C35	3:C:208:PCW:C31	0.41	2.98	11	1
3:A:406:PCW:C47	3:B:207:PCW:H282	0.41	2.46	12	1
3:B:206:PCW:C40	3:C:212:PCW:C26	0.41	2.98	12	1
3:A:408:PCW:H182	3:A:408:PCW:H211	0.41	1.68	13	1
3:C:208:PCW:O11	3:C:208:PCW:O2	0.41	2.38	13	1
4:A:415:17F:H62	4:A:415:17F:C1Z	0.41	2.46	14	1
3:D:602:PCW:C5	4:D:630:17F:O5	0.41	2.68	14	1
3:D:608:PCW:H422	3:D:615:PCW:C44	0.41	2.43	14	1
3:A:404:PCW:H262	4:A:415:17F:C36	0.41	2.46	15	1
3:A:416:PCW:C8	4:D:632:17F:O4	0.41	2.69	15	1
3:D:601:PCW:C8	4:B:216:17F:C2	0.41	2.98	16	1
3:B:203:PCW:H461	4:B:217:17F:C27	0.41	2.46	16	1
3:B:206:PCW:C34	3:C:204:PCW:C38	0.41	2.97	16	2
3:A:418:PCW:C11	3:A:418:PCW:O31	0.41	2.68	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:401:PCW:H471	3:D:611:PCW:H271	0.41	1.93	19	1
3:A:402:PCW:O11	3:A:402:PCW:C4	0.41	2.68	1	2
4:D:632:17F:H39	4:D:632:17F:H36	0.41	1.66	1	2
2:B:32:TYR:CB	5:B:201:GDP:H5''	0.41	2.46	1	1
1:A:258:LEU:O	1:A:262:GLN:HB2	0.41	2.16	2	1
3:A:404:PCW:C11	3:B:209:PCW:C40	0.41	2.99	2	1
3:D:601:PCW:H411	3:D:601:PCW:H382	0.41	1.73	2	1
3:D:615:PCW:C25	4:B:216:17F:H72	0.41	2.45	2	1
3:D:625:PCW:H411	3:D:626:PCW:H412	0.41	1.92	2	1
3:C:207:PCW:H431	3:C:207:PCW:C19	0.41	2.46	2	1
4:A:415:17F:H4	4:A:415:17F:H1	0.41	1.92	3	1
2:B:16:LYS:HE3	2:B:58:THR:O	0.41	2.16	3	1
3:B:213:PCW:H40	4:B:214:17F:H50	0.41	1.93	3	1
3:C:204:PCW:H451	4:C:211:17F:C32	0.41	2.46	3	1
3:C:212:PCW:H411	3:C:212:PCW:H382	0.41	1.59	5	2
3:A:402:PCW:O2P	3:A:402:PCW:C31	0.41	2.69	4	1
3:B:205:PCW:C40	4:B:214:17F:H71	0.41	2.45	4	1
3:B:212:PCW:H382	3:B:212:PCW:H411	0.41	1.65	4	1
4:B:215:17F:H1	4:B:215:17F:C4	0.41	2.46	4	1
3:A:416:PCW:C11	3:D:617:PCW:H332	0.41	2.45	5	1
3:D:608:PCW:H462	3:C:205:PCW:H461	0.41	1.93	5	1
3:D:614:PCW:C45	3:D:619:PCW:C20	0.41	2.95	5	1
3:B:204:PCW:C25	3:C:207:PCW:H262	0.41	2.27	5	1
3:C:203:PCW:H161	3:C:203:PCW:C40	0.41	2.45	5	1
1:D:463:TRP:HD1	3:D:601:PCW:H282	0.41	1.74	6	1
3:D:620:PCW:C27	4:D:635:17F:H35	0.41	2.43	6	2
4:B:215:17F:H36	4:B:215:17F:H40	0.41	1.63	6	1
4:C:210:17F:H10	4:C:210:17F:C32	0.41	2.46	6	1
3:A:402:PCW:C8	3:A:409:PCW:O2P	0.41	2.69	7	1
3:D:603:PCW:H52	4:D:630:17F:H4A	0.41	1.92	7	1
2:B:84:ILE:HB	2:B:123:ARG:HB2	0.41	1.93	7	1
3:B:207:PCW:C41	3:B:213:PCW:H252	0.41	2.45	8	1
3:A:403:PCW:H482	3:C:203:PCW:C28	0.41	2.45	9	1
3:D:610:PCW:H212	3:D:610:PCW:H182	0.41	1.69	9	2
3:D:611:PCW:C31	3:D:623:PCW:H352	0.41	2.46	9	1
3:D:622:PCW:H212	3:D:622:PCW:H182	0.41	1.69	9	1
3:A:401:PCW:O2P	3:A:401:PCW:O31	0.41	2.39	10	1
3:A:408:PCW:H361	3:C:204:PCW:H231	0.41	1.93	10	1
3:A:416:PCW:C14	3:A:419:PCW:H341	0.41	2.46	10	1
3:D:604:PCW:H2	3:D:604:PCW:O1P	0.41	2.16	10	1
4:C:211:17F:H69	4:C:211:17F:C21	0.41	2.44	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:615:PCW:H262	4:B:216:17F:H73	0.41	1.93	11	1
4:D:635:17F:H65	3:C:205:PCW:C46	0.41	2.45	11	1
2:B:82:PHE:CE1	2:B:125:VAL:HG11	0.41	2.51	11	1
3:C:204:PCW:C47	4:C:211:17F:C1Y	0.41	2.99	11	1
1:A:263:LYS:O	1:A:267:GLU:HG3	0.41	2.14	12	1
3:A:406:PCW:H381	3:A:406:PCW:H412	0.41	1.63	12	1
2:B:28:PHE:CD1	2:B:147:LYS:HA	0.41	2.51	12	1
3:A:403:PCW:H19	3:C:203:PCW:C11	0.41	2.46	13	1
3:D:608:PCW:C36	3:C:205:PCW:C28	0.41	2.98	13	1
1:A:375:LEU:O	1:A:379:LEU:HG	0.41	2.16	14	1
3:A:412:PCW:H212	3:A:412:PCW:H182	0.41	1.73	14	1
3:D:618:PCW:H252	3:C:204:PCW:H482	0.41	1.91	15	1
4:D:635:17F:C30	3:C:205:PCW:H181	0.41	2.46	15	1
3:B:210:PCW:H381	3:B:210:PCW:C42	0.41	2.40	16	1
2:C:8:VAL:HB	2:C:57:ASP:HA	0.41	1.92	17	1
2:C:137:TYR:HB2	2:C:139:ILE:HG12	0.41	1.91	17	1
3:C:206:PCW:H412	3:C:206:PCW:H381	0.41	1.66	18	1
3:D:606:PCW:O3	3:D:626:PCW:H411	0.41	2.16	19	1
3:D:621:PCW:H451	4:D:634:17F:C35	0.41	2.45	19	1
3:B:207:PCW:H442	3:B:213:PCW:C26	0.41	2.44	19	1
3:C:206:PCW:O31	3:C:206:PCW:C1	0.41	2.64	20	1
3:A:407:PCW:N	4:B:214:17F:O1	0.41	2.53	1	1
4:A:414:17F:H1	4:A:414:17F:C4	0.41	2.46	1	1
3:B:212:PCW:H381	3:B:212:PCW:H411	0.41	1.59	1	1
3:A:404:PCW:H212	3:A:404:PCW:C17	0.41	2.33	2	1
3:A:410:PCW:H212	3:A:410:PCW:H182	0.41	1.63	2	1
4:C:211:17F:H8A	4:C:211:17F:H71	0.41	1.92	2	1
3:A:401:PCW:C6	3:B:209:PCW:C1	0.41	2.94	3	1
3:A:405:PCW:O3P	3:A:405:PCW:O31	0.41	2.39	3	1
3:D:606:PCW:H211	3:D:606:PCW:H182	0.41	1.66	17	2
3:A:406:PCW:H31	3:A:406:PCW:C5	0.41	2.46	4	1
3:A:406:PCW:C38	3:B:210:PCW:H372	0.41	2.45	4	1
3:A:420:PCW:O31	3:D:617:PCW:H62	0.41	2.16	4	1
3:D:604:PCW:C48	3:D:613:PCW:H162	0.41	2.45	6	1
3:D:626:PCW:H411	3:D:626:PCW:H381	0.41	1.75	6	1
3:B:205:PCW:O3	3:B:208:PCW:H381	0.41	2.16	6	1
3:A:404:PCW:H382	4:B:215:17F:H38	0.41	1.92	7	1
3:C:209:PCW:H181	3:C:209:PCW:H212	0.41	1.65	8	1
1:A:228:PHE:O	1:A:232:LEU:HG	0.41	2.16	9	1
3:A:406:PCW:H271	3:B:207:PCW:C19	0.41	2.46	9	1
3:A:412:PCW:C39	3:C:206:PCW:H39	0.41	2.46	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:213:PCW:H2	4:B:217:17F:O10	0.41	2.16	9	1
3:A:417:PCW:C35	3:D:612:PCW:H152	0.41	2.46	10	1
3:D:616:PCW:C3	3:D:616:PCW:O4P	0.41	2.68	10	1
2:B:94:HIS:O	2:B:98:GLU:HG2	0.41	2.16	10	1
3:A:411:PCW:C41	3:A:418:PCW:H282	0.41	2.46	12	1
3:D:615:PCW:H172	3:D:615:PCW:C13	0.41	2.41	12	1
3:C:203:PCW:H412	3:C:203:PCW:H382	0.41	1.73	12	1
3:B:204:PCW:C19	3:B:205:PCW:C47	0.41	2.98	13	1
3:A:417:PCW:H141	3:D:617:PCW:C46	0.41	2.44	14	1
3:D:602:PCW:H161	3:D:624:PCW:H222	0.41	1.93	14	1
3:B:206:PCW:H431	4:C:211:17F:C22	0.41	2.45	14	1
4:A:414:17F:H65	4:C:210:17F:C1X	0.41	2.46	16	1
1:D:589:GLU:O	1:D:593:LYS:HG3	0.41	2.16	16	1
3:D:604:PCW:H481	3:D:619:PCW:C43	0.41	2.45	16	1
3:A:402:PCW:C39	3:A:409:PCW:H272	0.41	2.43	17	1
3:A:408:PCW:H272	3:A:417:PCW:C24	0.41	2.36	17	1
3:A:410:PCW:C24	3:C:207:PCW:H251	0.41	2.45	17	1
4:C:210:17F:H58	4:C:210:17F:H62	0.41	1.67	17	1
3:A:412:PCW:H432	3:C:206:PCW:H442	0.41	1.93	18	1
3:A:413:PCW:H462	3:D:613:PCW:C24	0.41	2.46	18	1
3:C:212:PCW:O4P	3:C:212:PCW:C8	0.41	2.69	18	1
3:A:420:PCW:H181	3:A:420:PCW:H212	0.41	1.58	19	1
3:D:620:PCW:H342	3:D:620:PCW:O31	0.41	2.16	19	1
3:C:204:PCW:C36	4:C:211:17F:H8A	0.41	2.43	19	1
1:A:376:LEU:HB2	1:A:377:PRO:HD3	0.41	1.92	20	1
3:A:405:PCW:C8	3:D:601:PCW:H11	0.41	2.45	20	1
3:B:206:PCW:H483	4:C:211:17F:H49	0.41	1.93	20	1
3:A:403:PCW:H63	3:C:203:PCW:O1P	0.40	2.16	2	1
1:D:555:LEU:HA	1:D:558:LEU:HD12	0.40	1.91	3	1
4:D:629:17F:H18A	4:D:629:17F:H5	0.40	1.61	3	2
3:D:604:PCW:O2P	3:D:613:PCW:H51	0.40	2.15	5	1
3:B:205:PCW:C7	3:B:213:PCW:O1P	0.40	2.69	5	1
2:B:2:THR:HB	2:B:4:TYR:CE2	0.40	2.51	6	1
3:B:210:PCW:C8	4:B:216:17F:H19A	0.40	2.46	8	1
3:B:211:PCW:C36	3:B:212:PCW:C1	0.40	2.97	8	1
1:A:302:GLY:O	1:A:306:ARG:HG3	0.40	2.16	9	1
4:D:634:17F:O1	4:D:634:17F:H5	0.40	2.16	9	1
3:A:406:PCW:H242	4:B:216:17F:H18	0.40	1.93	11	1
3:B:207:PCW:C34	3:B:210:PCW:C34	0.40	2.99	11	1
3:C:207:PCW:H482	4:C:211:17F:H19A	0.40	1.92	11	1
1:A:247:LEU:CD2	3:A:412:PCW:H272	0.40	2.47	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:403:PCW:H212	3:A:403:PCW:H441	0.40	1.93	13	1
1:D:471:ARG:HA	1:D:475:GLU:HG2	0.40	1.92	13	1
3:A:404:PCW:C36	3:B:209:PCW:H322	0.40	2.45	14	1
3:A:407:PCW:C48	4:D:635:17F:H50	0.40	2.42	15	1
3:A:417:PCW:C6	3:D:617:PCW:H40	0.40	2.46	15	1
3:D:603:PCW:C34	4:D:630:17F:O8	0.40	2.69	15	1
3:D:608:PCW:C46	4:D:635:17F:H62	0.40	2.46	15	1
3:C:209:PCW:C34	3:C:209:PCW:O31	0.40	2.69	15	1
3:A:417:PCW:C44	3:D:612:PCW:C27	0.40	2.99	16	1
3:A:418:PCW:C39	3:D:625:PCW:H251	0.40	2.45	16	1
1:A:380:GLU:O	1:A:384:VAL:HG23	0.40	2.16	18	1
3:D:611:PCW:O11	3:D:619:PCW:H63	0.40	2.17	18	1
4:B:214:17F:H38	4:B:217:17F:H70	0.40	1.93	18	1
2:C:97:ARG:NH1	2:C:101:LYS:HE2	0.40	2.31	18	1
3:D:612:PCW:C6	3:D:618:PCW:C3	0.40	2.99	19	1
3:B:207:PCW:O31	3:B:207:PCW:H341	0.40	2.16	19	1
2:B:117:LYS:HG2	5:B:201:GDP:C5	0.40	2.51	20	1
3:A:407:PCW:C35	3:C:205:PCW:H121	0.40	2.41	2	1
3:D:615:PCW:H182	3:C:205:PCW:H282	0.40	1.93	4	1
3:D:618:PCW:H241	3:B:206:PCW:H472	0.40	1.92	4	1
3:A:409:PCW:H121	3:C:206:PCW:H331	0.40	1.91	5	1
3:D:613:PCW:H241	4:C:210:17F:C39	0.40	2.44	5	1
3:B:206:PCW:H352	3:B:212:PCW:C37	0.40	2.41	6	1
3:D:611:PCW:C6	3:D:623:PCW:H342	0.40	2.46	7	1
3:D:613:PCW:H31	3:D:619:PCW:C3	0.40	2.47	7	1
4:D:635:17F:H63	4:D:635:17F:H58	0.40	1.70	8	2
3:D:602:PCW:O31	3:D:602:PCW:C4	0.40	2.69	9	1
3:B:207:PCW:H221	3:B:210:PCW:C24	0.40	2.32	9	1
3:A:418:PCW:H471	3:B:210:PCW:H462	0.40	1.93	10	1
3:D:625:PCW:O31	3:D:625:PCW:P	0.40	2.80	10	1
3:C:207:PCW:C5	4:C:211:17F:O5	0.40	2.70	10	1
3:A:419:PCW:C41	3:D:610:PCW:H211	0.40	2.46	11	1
3:B:204:PCW:H351	3:B:212:PCW:H141	0.40	1.92	11	1
3:D:601:PCW:C48	4:D:628:17F:H64	0.40	2.45	12	1
3:D:608:PCW:H411	3:D:608:PCW:H382	0.40	1.57	12	2
3:C:212:PCW:H382	3:C:212:PCW:H411	0.40	1.53	12	1
3:A:407:PCW:C15	3:B:208:PCW:H242	0.40	2.47	15	1
3:C:209:PCW:H262	3:C:209:PCW:H432	0.40	1.91	15	1
1:D:404:ASN:O	1:D:408:VAL:HG23	0.40	2.16	20	2
3:D:622:PCW:H73	4:D:633:17F:H8	0.40	1.92	16	1
3:D:623:PCW:O3	3:D:624:PCW:C33	0.40	2.70	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:414:17F:H49	3:B:212:PCW:H20	0.40	1.90	18	1
3:B:204:PCW:H40	3:C:203:PCW:C5	0.40	2.47	18	1
1:D:429:ASN:HA	1:D:432:LYS:HD2	0.40	1.92	19	1
3:A:402:PCW:H162	3:A:409:PCW:H181	0.40	1.94	20	1
3:A:417:PCW:O4P	3:A:417:PCW:C8	0.40	2.67	20	1
3:D:610:PCW:H262	3:D:610:PCW:H422	0.40	1.93	20	1
3:D:625:PCW:C37	3:D:626:PCW:H121	0.40	2.46	2	1
3:D:604:PCW:H322	3:D:624:PCW:C8	0.40	2.46	3	1
3:B:204:PCW:H412	3:B:204:PCW:H381	0.40	1.54	3	1
3:D:608:PCW:H381	3:D:615:PCW:C41	0.40	2.47	4	1
3:A:409:PCW:O31	3:C:206:PCW:H351	0.40	2.17	5	1
3:B:207:PCW:H63	4:B:216:17F:HN1A	0.40	1.76	5	1
3:A:409:PCW:C5	3:C:206:PCW:O31	0.40	2.69	6	1
3:D:622:PCW:H182	3:C:212:PCW:C15	0.40	2.45	7	1
3:D:623:PCW:H161	3:D:624:PCW:H371	0.40	1.92	8	1
3:C:204:PCW:C25	4:C:211:17F:H56	0.40	2.46	8	1
3:A:406:PCW:O4P	3:A:411:PCW:O2P	0.40	2.39	9	1
2:C:84:ILE:HD12	2:C:123:ARG:CB	0.40	2.46	9	1
4:C:211:17F:H40	4:C:211:17F:H36	0.40	1.73	9	2
3:A:420:PCW:H411	3:A:420:PCW:H381	0.40	1.73	10	1
2:B:2:THR:HG23	3:B:206:PCW:H62	0.40	1.92	10	1
3:C:204:PCW:O31	3:C:204:PCW:C5	0.40	2.66	10	1
3:A:416:PCW:C8	4:D:632:17F:H2	0.40	2.47	11	1
3:A:420:PCW:C12	4:D:632:17F:H9A	0.40	2.44	11	1
1:A:319:HIS:CE1	1:D:458:ASP:HB2	0.40	2.52	12	1
4:D:635:17F:H52	3:C:205:PCW:H152	0.40	1.92	12	1
4:B:216:17F:H59	4:B:216:17F:H62	0.40	1.66	12	1
3:A:410:PCW:C26	3:D:618:PCW:H462	0.40	2.46	13	1
3:A:403:PCW:H371	3:A:403:PCW:H131	0.40	1.93	14	1
4:B:215:17F:C12	4:B:217:17F:H29	0.40	2.46	14	1
3:C:212:PCW:H141	3:C:212:PCW:C37	0.40	2.47	14	1
3:D:622:PCW:C36	3:C:212:PCW:H462	0.40	2.34	15	1
3:A:408:PCW:H231	3:A:417:PCW:H283	0.40	1.94	16	1
3:A:402:PCW:H442	3:A:407:PCW:H212	0.40	1.93	17	1
3:A:410:PCW:H32	3:A:410:PCW:O1P	0.40	2.16	17	1
3:C:208:PCW:O4P	3:C:208:PCW:H63	0.40	2.17	17	1
3:A:401:PCW:C48	3:D:614:PCW:H471	0.40	2.39	18	1
3:A:406:PCW:H52	3:B:207:PCW:H351	0.40	1.93	18	1
1:A:280:ARG:O	1:A:284:GLN:HB2	0.40	2.17	19	1
3:A:404:PCW:C42	3:B:209:PCW:C43	0.40	2.94	19	1
3:A:409:PCW:C39	3:A:409:PCW:C18	0.40	3.00	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:204:PCW:H242	3:C:204:PCW:C42	0.40	2.35	19	1
3:B:207:PCW:H452	4:B:215:17F:H60	0.40	1.93	19	1
4:D:634:17F:C7	4:D:634:17F:O9	0.40	2.69	20	1
3:A:403:PCW:H161	3:C:203:PCW:H122	0.40	1.93	1	1
3:A:408:PCW:H62	4:C:211:17F:C7	0.40	2.46	1	1
3:D:607:PCW:C17	4:D:631:17F:O10	0.40	2.69	1	1
4:D:629:17F:H58	4:D:629:17F:H63	0.40	1.75	1	1
3:B:208:PCW:C19	4:B:214:17F:H18	0.40	2.47	1	1
3:B:206:PCW:H342	3:C:204:PCW:C36	0.40	2.46	3	1
3:D:611:PCW:C26	3:D:619:PCW:H452	0.40	2.46	4	1
3:B:207:PCW:C7	3:B:213:PCW:O2P	0.40	2.70	4	1
3:B:213:PCW:C12	4:B:217:17F:H6	0.40	2.46	4	1
4:A:414:17F:C28	3:B:212:PCW:H232	0.40	2.47	5	1
3:A:417:PCW:C35	3:D:612:PCW:C15	0.40	2.88	5	1
3:D:618:PCW:H411	3:D:627:PCW:H212	0.40	1.93	5	1
3:B:204:PCW:H212	3:C:207:PCW:H261	0.40	1.94	6	1
3:B:211:PCW:H462	3:B:212:PCW:H162	0.40	1.92	6	1
3:D:603:PCW:O11	3:D:603:PCW:H73	0.40	2.16	7	1
3:B:206:PCW:C3	3:B:206:PCW:P	0.40	3.09	7	1
3:B:204:PCW:C23	3:C:207:PCW:H271	0.40	2.45	8	1
3:A:409:PCW:C41	3:A:409:PCW:C37	0.40	3.00	10	1
3:A:418:PCW:H182	3:A:418:PCW:H211	0.40	1.69	10	1
4:D:632:17F:O10	4:D:632:17F:O7	0.40	2.40	10	1
3:B:203:PCW:O31	3:B:203:PCW:O3	0.40	2.40	10	1
4:A:414:17F:H36	4:A:414:17F:H40	0.40	1.54	11	1
3:D:611:PCW:C3	3:D:619:PCW:C11	0.40	3.00	11	1
3:D:620:PCW:C14	4:D:635:17F:C18	0.40	3.00	11	1
1:A:214:PHE:CE1	3:A:417:PCW:H282	0.40	2.50	12	1
1:A:244:SER:HA	1:A:248:GLU:CG	0.40	2.46	13	1
1:A:299:SER:HB2	1:A:300:PRO:CD	0.40	2.46	13	1
3:B:213:PCW:H412	4:B:217:17F:H63	0.40	1.94	13	1
4:C:211:17F:H35	4:C:211:17F:H40	0.40	1.71	14	1
3:A:403:PCW:C31	3:A:403:PCW:O3P	0.40	2.69	15	1
3:A:403:PCW:H411	3:A:403:PCW:C11	0.40	2.47	15	1
3:D:622:PCW:H19	4:D:630:17F:C11	0.40	2.46	15	1
4:D:630:17F:H53	3:B:206:PCW:C19	0.40	2.47	15	1
3:B:207:PCW:C33	3:B:210:PCW:C33	0.40	2.99	16	1
3:B:213:PCW:O3	3:B:213:PCW:O31	0.40	2.39	18	1
1:A:277:GLU:HB2	1:A:278:PRO:HD3	0.40	1.94	20	1
3:A:406:PCW:H162	3:B:210:PCW:C32	0.40	2.45	20	1
3:A:407:PCW:C8	3:A:407:PCW:O4P	0.40	2.69	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:412:PCW:H411	3:C:208:PCW:C36	0.40	2.47	20	1
3:A:404:PCW:H452	3:B:209:PCW:H471	0.40	1.94	1	1
3:D:623:PCW:H182	3:D:623:PCW:C22	0.40	2.45	1	1
3:B:204:PCW:H441	3:C:203:PCW:H141	0.40	1.92	2	1
3:D:604:PCW:C8	4:D:632:17F:O4	0.40	2.67	3	1
3:B:210:PCW:H442	3:B:213:PCW:H271	0.40	1.93	3	1
3:A:402:PCW:C39	3:A:407:PCW:H272	0.40	2.47	4	1
4:B:216:17F:H62	4:B:216:17F:H58	0.40	1.56	5	1
4:D:631:17F:H29	4:D:631:17F:C23	0.40	2.46	6	1
3:D:611:PCW:H141	3:D:619:PCW:H19	0.40	1.92	7	1
3:B:204:PCW:H452	3:C:203:PCW:H142	0.40	1.92	7	1
3:B:211:PCW:C15	4:B:217:17F:C34	0.40	2.99	8	1
3:C:209:PCW:H421	3:C:209:PCW:H283	0.40	1.94	8	1
3:D:608:PCW:O31	3:D:615:PCW:C6	0.40	2.70	9	1
3:B:207:PCW:C8	4:B:216:17F:O6	0.40	2.69	9	1
2:C:46:ILE:HB	2:C:51:CYS:SG	0.40	2.56	9	1
3:D:612:PCW:H212	3:D:612:PCW:H181	0.40	1.52	10	1
2:B:99:GLN:O	2:B:103:VAL:HG23	0.40	2.16	10	1
2:B:156:PHE:O	2:B:160:VAL:HG23	0.40	2.17	12	1
3:B:213:PCW:H121	4:B:217:17F:O8	0.40	2.17	12	1
3:C:207:PCW:C7	4:C:211:17F:O4	0.40	2.70	12	1
3:A:411:PCW:H131	3:A:411:PCW:C34	0.40	2.46	13	1
3:A:413:PCW:C31	3:A:413:PCW:O3	0.40	2.69	13	1
4:B:216:17F:H42	4:B:216:17F:C2X	0.40	2.45	13	1
3:A:406:PCW:C41	3:B:210:PCW:C40	0.40	2.99	14	1
3:D:613:PCW:H142	3:D:619:PCW:H39	0.40	1.92	14	1
4:B:215:17F:C11	4:B:217:17F:H29	0.40	2.47	14	1
3:C:208:PCW:C1	3:C:209:PCW:O1P	0.40	2.68	14	1
3:A:407:PCW:H482	4:D:635:17F:C26	0.40	2.42	15	1
4:A:414:17F:C38	4:C:210:17F:H29	0.40	2.46	16	1
1:D:564:PRO:O	1:D:568:ASP:HB2	0.40	2.16	16	1
3:B:207:PCW:H182	3:B:210:PCW:C23	0.40	2.47	16	1
1:A:369:GLU:OE2	1:A:372:ARG:HD2	0.40	2.17	17	1
3:D:620:PCW:C28	4:D:635:17F:C21	0.40	2.99	17	1
3:A:410:PCW:H82	3:C:209:PCW:H32	0.40	1.87	19	1
3:B:204:PCW:C13	3:B:206:PCW:C4	0.40	2.85	19	1
3:B:210:PCW:H171	4:B:216:17F:H39	0.40	1.94	19	1
3:D:612:PCW:C6	3:D:627:PCW:O11	0.40	2.58	20	1

6.3 Torsion angles

6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	184/200 (92%)	179±1 (97±1%)	4±1 (2±1%)	1±0 (1±0%)	27	74
1	D	196/200 (98%)	190±2 (97±1%)	6±2 (3±1%)	0±0 (0±0%)	100	100
2	B	159/184 (86%)	154±2 (97±1%)	5±2 (3±1%)	0±0 (0±0%)	45	81
2	C	163/184 (89%)	157±2 (96±1%)	6±2 (3±1%)	0±0 (0±0%)	50	84
All	All	14040/15360 (91%)	13600 (97%)	411 (3%)	29 (0%)	45	81

All 8 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	365	LYS	20
2	B	34	PRO	2
2	C	110	PRO	2
2	B	163	ILE	1
2	C	34	PRO	1
1	D	420	GLY	1
2	B	122	SER	1
2	B	48	GLY	1

6.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	161/175 (92%)	151±2 (94±1%)	10±2 (6±1%)	17	69
1	D	173/175 (99%)	159±2 (92±1%)	14±2 (8±1%)	12	62
2	B	143/164 (87%)	132±3 (92±2%)	11±3 (8±2%)	13	63
2	C	147/164 (90%)	135±3 (92±2%)	12±3 (8±2%)	11	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	12480/13560 (92%)	11530 (92%)	950 (8%)	13 63

All 230 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	D	516	THR	19
1	D	561	LYS	18
1	A	254	VAL	17
2	B	87	THR	17
1	D	550	LYS	16
1	D	576	VAL	16
2	B	124	THR	16
2	C	2	THR	16
1	D	480	GLU	16
2	C	124	THR	15
2	C	87	THR	15
1	D	466	GLU	14
1	A	293	GLU	14
1	A	272	TYR	14
1	D	552	THR	13
1	D	448	VAL	13
1	A	235	GLU	13
2	C	92	ASP	12
1	D	411	THR	12
2	B	2	THR	12
1	D	462	LYS	11
2	B	65	SER	11
2	B	74	THR	11
1	D	459	PHE	11
1	A	250	VAL	10
1	A	359	THR	10
1	D	407	SER	10
2	C	50	THR	10
2	C	161	ARG	10
1	D	405	TRP	10
2	B	50	THR	9
2	C	148	THR	9
2	C	153	ASP	9
2	C	39	SER	8
2	C	74	THR	8
2	C	35	THR	8

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Mol	Chain	Res	Type	Models (Total)
2	C	69	ASP	8
2	B	20	THR	7
2	B	153	ASP	7
1	A	236	THR	7
2	C	36	ILE	7
1	D	400	LYS	6
2	B	29	VAL	6
2	B	139	ILE	6
2	C	47	ASP	6
1	D	557	THR	6
2	B	69	ASP	6
2	B	161	ARG	6
2	B	92	ASP	6
1	D	483	GLU	6
1	A	381	SER	6
1	A	244	SER	5
2	B	58	THR	5
2	B	127	THR	5
1	A	358	SER	5
1	A	385	SER	5
2	B	39	SER	5
2	B	89	SER	5
2	C	127	THR	5
1	A	304	GLU	5
1	A	370	ASP	5
2	C	168	GLU	5
2	B	57	ASP	5
2	B	136	SER	5
1	D	556	SER	5
2	B	132	ASP	5
2	C	57	ASP	5
1	A	292	HIS	5
2	C	132	ASP	5
1	A	319	HIS	4
1	D	447	GLU	4
1	D	548	HIS	4
1	D	583	SER	4
2	B	144	THR	4
1	A	274	GLN	4
2	B	126	ASP	4
2	B	148	THR	4
1	D	559	SER	4

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Mol	Chain	Res	Type	Models (Total)
2	B	32	TYR	4
2	C	12	ASP	4
1	A	312	HIS	4
2	C	45	VAL	4
1	A	349	TYR	4
2	C	29	VAL	4
1	D	568	ASP	4
1	A	325	ASP	4
1	A	314	ASP	3
2	C	149	ARG	3
1	A	265	TRP	3
1	A	369	GLU	3
2	B	154	ASP	3
2	C	17	SER	3
2	C	144	THR	3
2	C	65	SER	3
1	A	214	PHE	3
1	A	382	PHE	3
2	C	5	LYS	3
2	C	30	ASP	3
2	C	139	ILE	3
2	C	169	LYS	3
1	A	263	LYS	3
1	A	368	LEU	3
1	A	396	LYS	3
1	D	415	LEU	3
1	D	442	SER	3
1	D	477	LEU	3
2	C	8	VAL	3
2	C	41	ARG	3
1	A	228	PHE	3
1	D	522	SER	3
1	D	560	GLU	3
2	B	35	THR	3
1	D	547	TYR	3
2	B	45	VAL	3
2	C	119	ASP	3
1	D	538	GLU	3
2	C	109	VAL	3
1	A	233	GLU	3
2	B	43	GLN	2
1	A	350	HIS	2

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Mol	Chain	Res	Type	Models (Total)
1	D	591	TYR	2
2	C	31	GLU	2
2	C	43	GLN	2
1	A	289	GLN	2
1	D	585	LEU	2
2	C	89	SER	2
2	B	109	VAL	2
1	A	299	SER	2
2	B	84	ILE	2
2	C	126	ASP	2
1	D	440	GLU	2
2	B	17	SER	2
2	B	30	ASP	2
2	B	36	ILE	2
1	A	248	GLU	2
2	B	31	GLU	2
2	C	32	TYR	2
2	C	145	SER	2
1	A	229	TRP	2
1	A	232	LEU	2
1	D	403	ASP	2
1	D	487	GLN	2
2	C	51	CYS	2
2	C	157	TYR	2
2	C	49	GLU	2
2	C	106	SER	2
2	B	12	ASP	2
2	B	166	HIS	2
2	C	80	CYS	2
1	A	270	GLU	2
1	A	242	GLU	2
1	D	505	ASP	2
1	D	455	TYR	2
1	D	544	LEU	1
1	D	584	PHE	1
2	B	143	GLU	1
2	B	150	GLN	1
2	B	152	VAL	1
2	C	26	ASN	1
1	A	391	GLU	1
1	D	399	LEU	1
1	D	475	GLU	1

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Mol	Chain	Res	Type	Models (Total)
2	B	33	ASP	1
2	C	166	HIS	1
1	D	412	PHE	1
1	D	437	LEU	1
2	B	47	ASP	1
2	B	159	LEU	1
2	C	123	ARG	1
1	D	493	GLN	1
2	B	80	CYS	1
2	C	37	GLU	1
1	D	444	ASP	1
1	D	533	LEU	1
2	C	44	VAL	1
2	C	136	SER	1
1	A	245	LYS	1
1	A	276	VAL	1
1	A	331	LEU	1
2	B	44	VAL	1
2	B	149	ARG	1
2	C	6	LEU	1
2	C	88	LYS	1
1	D	424	GLN	1
1	D	464	GLN	1
1	D	499	LEU	1
2	B	3	GLU	1
1	A	243	MET	1
1	A	269	MET	1
2	B	73	ARG	1
2	C	58	THR	1
1	D	434	THR	1
2	B	147	LYS	1
2	C	56	LEU	1
1	A	386	PHE	1
2	B	79	LEU	1
1	A	336	GLU	1
1	A	363	LYS	1
2	B	5	LYS	1
2	B	51	CYS	1
2	C	154	ASP	1
2	C	165	LYS	1
1	D	592	THR	1
2	B	101	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	226	GLN	1
2	B	119	ASP	1
2	B	145	SER	1
2	C	105	ASP	1
1	A	346	LEU	1
1	D	524	GLU	1
2	C	55	ILE	1
1	D	502	GLU	1
2	C	135	ARG	1
1	D	494	GLU	1
1	A	275	LYS	1
1	A	296	GLU	1
1	A	303	GLU	1
1	D	594	LYS	1
2	B	41	ARG	1
1	A	307	ASP	1
1	D	456	LEU	1
2	C	101	LYS	1
2	B	122	SER	1
2	C	20	THR	1
2	C	142	ILE	1
1	D	429	ASN	1
1	D	586	SER	1
2	B	67	MET	1
2	B	85	ASN	1
2	B	108	ASP	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry

Of 84 ligands modelled in this entry, 2 are monoatomic - leaving 82 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PCW	B	211	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	C	205	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	413	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	403	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	B	206	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	D	633	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	D	602	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	610	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	627	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	626	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	C	212	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	410	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	B	213	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	619	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	609	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	606	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	608	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	624	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	418	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	A	414	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	D	604	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	C	210	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	A	419	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	B	216	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	D	617	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	420	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	401	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	D	630	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	B	205	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	607	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	614	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	605	-	53,53,53	0.82±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
5	GDP	C	201	-	25,30,30	1.53±0.02	3±0 (13±1%)
3	PCW	A	406	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	404	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	C	211	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	D	625	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	620	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	B	208	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	C	209	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	B	210	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	412	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	402	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	A	415	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	17F	B	215	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	A	408	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	601	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	613	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	B	212	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	612	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	C	203	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	618	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	622	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	417	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	615	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	C	206	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	GDP	B	201	-	25,30,30	1.37±0.02	2±0 (9±1%)
3	PCW	C	207	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	D	635	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	B	207	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	D	631	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	D	623	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	407	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	616	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	D	634	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	A	411	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	416	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	B	209	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	B	204	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	D	628	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	C	208	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	603	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	C	204	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	A	409	-	53,53,53	0.82±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	17F	D	632	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	17F	D	629	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	B	203	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	621	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	17F	B	214	-	52,53,53	0.82±0.00	0±0 (0±0%)
4	17F	B	217	-	52,53,53	0.83±0.00	0±0 (0±0%)
3	PCW	A	405	-	53,53,53	0.82±0.00	0±0 (0±0%)
3	PCW	D	611	-	53,53,53	0.82±0.00	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PCW	B	211	-	59,61,61	2.59±0.02	6±1 (10±0%)
3	PCW	C	205	-	59,61,61	2.61±0.01	7±0 (11±0%)
3	PCW	A	413	-	59,61,61	2.62±0.02	7±1 (12±1%)
3	PCW	A	403	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	B	206	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	17F	D	633	-	54,60,60	1.15±0.03	4±0 (7±0%)
3	PCW	D	602	-	59,61,61	2.61±0.01	7±1 (11±0%)
3	PCW	D	610	-	59,61,61	2.61±0.01	7±0 (11±0%)
3	PCW	D	627	-	59,61,61	2.59±0.02	7±1 (11±1%)
3	PCW	D	626	-	59,61,61	2.62±0.01	6±1 (10±0%)
3	PCW	C	212	-	59,61,61	2.67±0.01	10±0 (17±0%)
3	PCW	A	410	-	59,61,61	2.58±0.01	6±0 (10±0%)
3	PCW	B	213	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	D	619	-	59,61,61	2.58±0.01	6±0 (10±0%)
3	PCW	D	609	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	D	606	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	D	608	-	59,61,61	2.59±0.01	7±0 (11±0%)
3	PCW	D	624	-	59,61,61	2.57±0.01	6±1 (10±1%)
3	PCW	A	418	-	59,61,61	2.60±0.02	7±0 (11±0%)
4	17F	A	414	-	54,60,60	1.34±0.03	8±0 (15±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PCW	D	604	-	59,61,61	2.64±0.01	7±0 (12±0%)
4	17F	C	210	-	54,60,60	1.11±0.03	5±0 (9±0%)
3	PCW	A	419	-	59,61,61	2.61±0.01	6±0 (10±0%)
4	17F	B	216	-	54,60,60	1.11±0.03	4±0 (7±0%)
3	PCW	D	617	-	59,61,61	2.61±0.01	7±0 (11±0%)
3	PCW	A	420	-	59,61,61	2.59±0.01	7±1 (11±1%)
3	PCW	A	401	-	59,61,61	2.60±0.01	6±0 (10±0%)
4	17F	D	630	-	54,60,60	1.12±0.04	5±0 (8±0%)
3	PCW	B	205	-	59,61,61	2.61±0.01	6±1 (11±1%)
3	PCW	D	607	-	59,61,61	2.60±0.01	7±1 (11±0%)
3	PCW	D	614	-	59,61,61	2.61±0.01	6±0 (10±0%)
3	PCW	D	605	-	59,61,61	2.59±0.00	6±0 (10±0%)
5	GDP	C	201	-	30,47,47	1.58±0.03	6±0 (20±0%)
3	PCW	A	406	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	A	404	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	17F	C	211	-	54,60,60	1.16±0.04	4±0 (7±0%)
3	PCW	D	625	-	59,61,61	2.57±0.01	6±0 (10±0%)
3	PCW	D	620	-	59,61,61	2.59±0.01	7±1 (11±1%)
3	PCW	B	208	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	C	209	-	59,61,61	2.59±0.01	6±1 (10±0%)
3	PCW	B	210	-	59,61,61	2.59±0.02	6±0 (10±0%)
3	PCW	A	412	-	59,61,61	2.60±0.01	6±0 (10±0%)
3	PCW	A	402	-	59,61,61	2.60±0.01	6±0 (10±0%)
4	17F	A	415	-	54,60,60	1.13±0.04	4±0 (7±0%)
4	17F	B	215	-	54,60,60	1.14±0.03	5±1 (8±1%)
3	PCW	A	408	-	59,61,61	2.60±0.01	6±0 (10±0%)
3	PCW	D	601	-	59,61,61	2.58±0.01	6±0 (10±0%)
3	PCW	D	613	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	B	212	-	59,61,61	2.58±0.01	6±0 (10±0%)
3	PCW	D	612	-	59,61,61	2.61±0.01	6±0 (10±0%)
3	PCW	C	203	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	D	618	-	59,61,61	2.61±0.01	7±0 (11±0%)
3	PCW	D	622	-	59,61,61	2.61±0.01	7±1 (12±0%)
3	PCW	A	417	-	59,61,61	2.61±0.02	7±1 (11±1%)
3	PCW	D	615	-	59,61,61	2.61±0.02	6±0 (10±0%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
3	PCW	C	206	-	59,61,61	2.59±0.01	6±0 (10±0%)
5	GDP	B	201	-	30,47,47	1.43±0.03	5±0 (16±0%)
3	PCW	C	207	-	59,61,61	2.61±0.01	7±0 (11±0%)
4	17F	D	635	-	54,60,60	1.09±0.05	4±0 (8±0%)
3	PCW	B	207	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	17F	D	631	-	54,60,60	1.12±0.03	4±0 (7±0%)
3	PCW	D	623	-	59,61,61	2.58±0.02	6±0 (10±0%)
3	PCW	A	407	-	59,61,61	2.61±0.01	7±1 (11±1%)
3	PCW	D	616	-	59,61,61	2.58±0.01	6±0 (10±0%)
4	17F	D	634	-	54,60,60	1.12±0.03	4±0 (8±0%)
3	PCW	A	411	-	59,61,61	2.58±0.01	6±1 (10±0%)
3	PCW	A	416	-	59,61,61	2.60±0.02	7±0 (11±0%)
3	PCW	B	209	-	59,61,61	2.60±0.01	6±0 (10±0%)
3	PCW	B	204	-	59,61,61	2.68±0.01	10±0 (17±0%)
4	17F	D	628	-	54,60,60	1.09±0.02	4±0 (7±0%)
3	PCW	C	208	-	59,61,61	2.59±0.01	7±0 (11±0%)
3	PCW	D	603	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	C	204	-	59,61,61	2.60±0.01	6±0 (10±0%)
3	PCW	A	409	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	17F	D	632	-	54,60,60	1.33±0.03	9±0 (16±0%)
4	17F	D	629	-	54,60,60	1.13±0.03	5±1 (10±1%)
3	PCW	B	203	-	59,61,61	2.59±0.01	6±0 (10±0%)
3	PCW	D	621	-	59,61,61	2.57±0.01	6±1 (10±0%)
4	17F	B	214	-	54,60,60	1.09±0.03	4±0 (7±0%)
4	17F	B	217	-	54,60,60	1.24±0.02	4±0 (8±0%)
3	PCW	A	405	-	59,61,61	2.60±0.01	7±1 (11±1%)
3	PCW	D	611	-	59,61,61	2.59±0.01	6±1 (10±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	D	602	-	-	0±0,57,57,57	-
3	PCW	D	609	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	B	208	-	-	0±0,57,57,57	-
4	17F	A	415	-	-	0±0,59,59,59	-
3	PCW	B	207	-	-	0±0,57,57,57	-
3	PCW	B	212	-	-	0±0,57,57,57	-
3	PCW	B	213	-	-	0±0,57,57,57	-
3	PCW	D	613	-	-	0±0,57,57,57	-
3	PCW	A	413	-	-	0±0,57,57,57	-
3	PCW	B	211	-	-	0±0,57,57,57	-
4	17F	B	214	-	-	0±0,59,59,59	-
3	PCW	A	410	-	-	0±0,57,57,57	-
3	PCW	D	603	-	-	0±0,57,57,57	-
3	PCW	D	621	-	-	0±0,57,57,57	-
3	PCW	A	405	-	-	0±0,57,57,57	-
3	PCW	D	607	-	-	0±0,57,57,57	-
3	PCW	D	626	-	-	0±0,57,57,57	-
3	PCW	D	606	-	-	0±0,57,57,57	-
4	17F	D	632	-	-	0±0,59,59,59	-
3	PCW	A	407	-	-	0±0,57,57,57	-
3	PCW	D	608	-	-	0±0,57,57,57	-
3	PCW	D	624	-	-	0±0,57,57,57	-
3	PCW	D	618	-	-	0±0,57,57,57	-
3	PCW	D	615	-	-	0±0,57,57,57	-
3	PCW	D	614	-	-	0±0,57,57,57	-
4	17F	D	629	-	-	2±0,59,59,59	-
3	PCW	A	404	-	-	0±0,57,57,57	-
3	PCW	C	207	-	-	0±0,57,57,57	-
3	PCW	B	204	-	-	0±0,57,57,57	-
3	PCW	C	209	-	-	0±0,57,57,57	-
3	PCW	B	210	-	-	0±0,57,57,57	-
3	PCW	D	617	-	-	0±0,57,57,57	-
3	PCW	D	623	-	-	0±0,57,57,57	-
3	PCW	D	625	-	-	0±0,57,57,57	-
3	PCW	D	604	-	-	0±0,57,57,57	-
3	PCW	A	411	-	-	0±0,57,57,57	-
4	17F	D	630	-	-	0±0,59,59,59	-
3	PCW	C	205	-	-	0±0,57,57,57	-
3	PCW	C	212	-	-	0±0,57,57,57	-
3	PCW	A	416	-	-	0±0,57,57,57	-
3	PCW	D	610	-	-	0±0,57,57,57	-
3	PCW	A	412	-	-	0±0,57,57,57	-
3	PCW	D	611	-	-	0±0,57,57,57	-
3	PCW	A	417	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	D	605	-	-	0±0,57,57,57	-
4	17F	B	217	-	-	1±0,59,59,59	-
4	17F	D	634	-	-	0±0,59,59,59	-
3	PCW	B	203	-	-	0±0,57,57,57	-
4	17F	D	635	-	-	0±0,59,59,59	-
3	PCW	D	622	-	-	0±0,57,57,57	-
3	PCW	B	206	-	-	0±0,57,57,57	-
4	17F	C	211	-	-	0±0,59,59,59	-
4	17F	D	628	-	-	0±0,59,59,59	-
3	PCW	C	203	-	-	0±0,57,57,57	-
3	PCW	D	612	-	-	0±0,57,57,57	-
3	PCW	A	401	-	-	0±0,57,57,57	-
4	17F	B	216	-	-	0±0,59,59,59	-
4	17F	D	631	-	-	0±0,59,59,59	-
3	PCW	A	420	-	-	0±0,57,57,57	-
3	PCW	A	406	-	-	0±0,57,57,57	-
3	PCW	B	209	-	-	0±0,57,57,57	-
4	17F	A	414	-	-	0±0,59,59,59	-
3	PCW	D	620	-	-	0±0,57,57,57	-
3	PCW	B	205	-	-	0±0,57,57,57	-
3	PCW	C	206	-	-	0±0,57,57,57	-
4	17F	C	210	-	-	0±0,59,59,59	-
5	GDP	B	201	-	-	0±0,12,32,32	0±0,3,3,3
3	PCW	A	402	-	-	0±0,57,57,57	-
3	PCW	A	418	-	-	0±0,57,57,57	-
4	17F	B	215	-	-	1±0,59,59,59	-
3	PCW	A	408	-	-	0±0,57,57,57	-
4	17F	D	633	-	-	0±0,59,59,59	-
3	PCW	D	619	-	-	0±0,57,57,57	-
5	GDP	C	201	-	-	0±0,12,32,32	0±0,3,3,3
3	PCW	A	403	-	-	0±0,57,57,57	-
3	PCW	D	616	-	-	0±0,57,57,57	-
3	PCW	A	419	-	-	0±0,57,57,57	-
3	PCW	D	627	-	-	0±0,57,57,57	-
3	PCW	D	601	-	-	0±0,57,57,57	-
3	PCW	A	409	-	-	0±0,57,57,57	-
3	PCW	C	208	-	-	0±0,57,57,57	-
3	PCW	C	204	-	-	0±0,57,57,57	-

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
5	B	201	GDP	C5-C6	4.30	1.38	1.47	14	20
5	C	201	GDP	C5-C6	4.30	1.38	1.47	1	20
5	C	201	GDP	PB-O1B	3.59	1.61	1.50	4	20
5	C	201	GDP	O4'-C1'	2.74	1.44	1.40	20	20
5	B	201	GDP	O4'-C1'	2.64	1.44	1.40	3	20
5	B	201	GDP	PA-O3A	2.35	1.62	1.59	12	7
5	C	201	GDP	PA-O3A	2.11	1.61	1.59	17	6

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	B	213	PCW	C8-N-C7	17.69	62.50	108.98	6	20
3	A	413	PCW	C8-N-C7	17.69	62.52	108.98	16	20
3	A	417	PCW	C8-N-C7	17.69	62.52	108.98	7	20
3	D	616	PCW	C8-N-C7	17.69	62.52	108.98	19	20
3	D	613	PCW	C8-N-C7	17.68	62.53	108.98	10	20
3	C	212	PCW	C8-N-C7	17.68	62.53	108.98	20	20
3	A	402	PCW	C8-N-C7	17.68	62.53	108.98	10	20
3	A	410	PCW	C8-N-C7	17.68	62.53	108.98	18	20
3	A	407	PCW	C8-N-C7	17.68	62.54	108.98	10	20
3	A	411	PCW	C8-N-C7	17.68	62.54	108.98	10	20
3	D	623	PCW	C8-N-C7	17.68	62.53	108.98	19	20
3	B	209	PCW	C8-N-C7	17.68	62.53	108.98	19	20
3	B	212	PCW	C8-N-C7	17.68	62.54	108.98	11	20
3	D	614	PCW	C8-N-C7	17.68	62.54	108.98	18	20
3	A	416	PCW	C8-N-C7	17.68	62.55	108.98	17	20
3	D	617	PCW	C8-N-C7	17.68	62.55	108.98	11	20
3	D	619	PCW	C8-N-C7	17.68	62.54	108.98	18	20
3	B	210	PCW	C8-N-C7	17.68	62.54	108.98	3	20
3	B	204	PCW	C8-N-C7	17.68	62.55	108.98	16	20
3	B	206	PCW	C8-N-C7	17.68	62.54	108.98	20	20
3	C	203	PCW	C8-N-C7	17.68	62.54	108.98	10	20
3	C	206	PCW	C8-N-C7	17.68	62.55	108.98	20	20
3	B	203	PCW	C8-N-C7	17.67	62.55	108.98	3	20
3	B	207	PCW	C8-N-C7	17.68	62.55	108.98	14	20
3	A	409	PCW	C8-N-C7	17.67	62.55	108.98	16	20
3	A	401	PCW	C8-N-C7	17.67	62.56	108.98	3	20
3	A	408	PCW	C8-N-C7	17.67	62.55	108.98	3	20
3	A	419	PCW	C8-N-C7	17.67	62.55	108.98	19	20
3	A	420	PCW	C8-N-C7	17.67	62.55	108.98	10	20
3	D	604	PCW	C8-N-C7	17.67	62.55	108.98	17	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	D	620	PCW	C8-N-C7	17.67	62.55	108.98	2	20
3	D	605	PCW	C8-N-C7	17.67	62.55	108.98	10	20
3	D	609	PCW	C8-N-C7	17.67	62.56	108.98	18	20
3	D	601	PCW	C8-N-C7	17.67	62.56	108.98	5	20
3	D	607	PCW	C8-N-C7	17.67	62.56	108.98	18	20
3	D	615	PCW	C8-N-C7	17.67	62.56	108.98	7	20
3	B	208	PCW	C8-N-C7	17.67	62.56	108.98	4	20
3	B	211	PCW	C8-N-C7	17.67	62.56	108.98	15	20
3	D	622	PCW	C8-N-C7	17.67	62.56	108.98	14	20
3	D	626	PCW	C8-N-C7	17.67	62.56	108.98	2	20
3	D	627	PCW	C8-N-C7	17.67	62.56	108.98	4	20
3	A	405	PCW	C8-N-C7	17.67	62.56	108.98	5	20
3	A	403	PCW	C8-N-C7	17.67	62.57	108.98	2	20
3	D	610	PCW	C8-N-C7	17.67	62.56	108.98	11	20
3	D	621	PCW	C8-N-C7	17.67	62.56	108.98	15	20
3	A	412	PCW	C8-N-C7	17.67	62.57	108.98	3	20
3	D	602	PCW	C8-N-C7	17.67	62.56	108.98	13	20
3	D	611	PCW	C8-N-C7	17.67	62.57	108.98	9	20
3	D	612	PCW	C8-N-C7	17.67	62.57	108.98	7	20
3	D	624	PCW	C8-N-C7	17.67	62.56	108.98	6	20
3	D	625	PCW	C8-N-C7	17.67	62.56	108.98	18	20
3	C	205	PCW	C8-N-C7	17.67	62.56	108.98	2	20
3	C	207	PCW	C8-N-C7	17.67	62.57	108.98	18	20
3	C	209	PCW	C8-N-C7	17.67	62.56	108.98	4	20
3	D	603	PCW	C8-N-C7	17.67	62.57	108.98	10	20
3	D	606	PCW	C8-N-C7	17.67	62.57	108.98	2	20
3	B	205	PCW	C8-N-C7	17.67	62.57	108.98	5	20
3	A	404	PCW	C8-N-C7	17.66	62.58	108.98	10	20
3	A	406	PCW	C8-N-C7	17.66	62.58	108.98	10	20
3	A	418	PCW	C8-N-C7	17.66	62.58	108.98	16	20
3	D	618	PCW	C8-N-C7	17.66	62.58	108.98	13	20
3	C	204	PCW	C8-N-C7	17.66	62.58	108.98	1	20
3	D	608	PCW	C8-N-C7	17.66	62.59	108.98	19	20
3	C	208	PCW	C8-N-C7	17.66	62.59	108.98	2	20
4	B	217	17F	O3-C1-C2	5.44	112.80	108.06	1	20
5	C	201	GDP	C4'-O4'-C1'	4.79	105.54	109.92	14	20
4	D	629	17F	O3-C1-C2	4.57	112.04	108.06	8	20
4	B	216	17F	O3-C1-C2	4.55	112.03	108.06	7	20
4	D	629	17F	O9-C17-C18	4.55	121.31	111.48	8	20
4	D	630	17F	O3-C1-C2	4.53	112.01	108.06	15	20
3	A	417	PCW	O2-C31-C32	4.50	121.21	111.48	17	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	D	633	17F	O3-C1-C2	4.43	111.92	108.06	7	20
3	D	627	PCW	O2-C31-C32	4.35	120.88	111.48	3	20
4	C	210	17F	O3-C1-C2	4.33	111.84	108.06	17	20
3	A	413	PCW	O2-C31-C32	4.32	120.83	111.48	19	20
4	D	632	17F	O3-C1-C2	4.32	111.82	108.06	5	20
4	B	215	17F	O9-C17-C18	4.29	120.77	111.48	2	20
3	D	626	PCW	O2-C31-C32	4.29	120.76	111.48	17	20
3	A	419	PCW	O2-C31-C32	4.28	120.73	111.48	7	20
3	D	615	PCW	O2-C31-C32	4.25	120.67	111.48	4	20
4	C	211	17F	C5-O9-C17	4.24	107.66	117.80	4	20
4	A	415	17F	O3-C1-C2	4.23	111.75	108.06	13	20
4	D	635	17F	O9-C17-C18	4.22	120.61	111.48	10	20
3	B	210	PCW	O2-C31-C32	4.22	120.60	111.48	18	20
4	D	634	17F	O3-C1-C2	4.22	111.73	108.06	9	20
3	D	602	PCW	O2-C31-C32	4.21	120.59	111.48	19	20
3	D	627	PCW	C2-O2-C31	4.21	107.72	117.80	3	20
4	A	414	17F	O9-C17-C18	4.20	120.57	111.48	13	20
4	B	217	17F	O9-C17-C18	4.20	120.57	111.48	2	20
3	D	626	PCW	C2-O2-C31	4.18	107.79	117.80	17	20
3	D	623	PCW	O2-C31-C32	4.17	120.51	111.48	19	20
4	D	633	17F	O9-C17-C18	4.17	120.51	111.48	11	20
4	B	214	17F	O9-C17-C18	4.16	120.48	111.48	12	20
3	C	205	PCW	O2-C31-C32	4.16	120.47	111.48	11	20
4	B	214	17F	C5-O9-C17	4.14	107.89	117.80	12	20
4	C	211	17F	O3-C1-C2	4.14	111.67	108.06	11	20
3	D	625	PCW	O2-C31-C32	4.13	120.43	111.48	20	20
3	A	409	PCW	O2-C31-C32	4.12	120.39	111.48	17	20
4	A	415	17F	O9-C17-C18	4.11	120.38	111.48	13	20
3	A	417	PCW	C2-O2-C31	4.11	107.97	117.80	11	20
3	B	205	PCW	O2-C31-C32	4.10	120.34	111.48	17	20
3	D	604	PCW	O2-C31-C32	4.09	120.33	111.48	8	20
4	D	635	17F	O3-C1-C2	4.09	111.62	108.06	5	20
3	A	407	PCW	O2-C31-C32	4.08	120.31	111.48	5	20
4	C	211	17F	O9-C17-C18	4.08	120.30	111.48	4	20
4	D	631	17F	O9-C17-C18	4.07	120.30	111.48	6	20
4	D	634	17F	O9-C17-C18	4.07	120.29	111.48	4	20
4	D	630	17F	O9-C17-C18	4.07	120.28	111.48	16	20
4	D	630	17F	C5-O9-C17	4.06	108.08	117.80	16	20
3	D	614	PCW	O2-C31-C32	4.05	120.23	111.48	7	20
4	D	628	17F	O3-C1-C2	4.02	111.56	108.06	6	20
3	B	210	PCW	C2-O2-C31	4.02	108.17	117.80	18	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	D	617	PCW	O2-C31-C32	4.02	120.18	111.48	2	20
3	D	612	PCW	O2-C31-C32	4.01	120.15	111.48	4	20
4	D	631	17F	O3-C1-C2	4.01	111.55	108.06	14	20
3	D	610	PCW	O2-C31-C32	4.00	120.13	111.48	7	20
3	A	401	PCW	O2-C31-C32	3.99	120.12	111.48	13	20
3	B	211	PCW	O2-C31-C32	3.98	120.10	111.48	3	20
3	B	207	PCW	O2-C31-C32	3.98	120.08	111.48	14	20
3	B	209	PCW	O2-C31-C32	3.97	120.06	111.48	6	20
4	D	632	17F	O9-C17-C18	3.97	120.07	111.48	4	20
3	D	613	PCW	O2-C31-C32	3.96	120.05	111.48	10	20
3	D	603	PCW	O2-C31-C32	3.96	120.04	111.48	2	20
4	A	414	17F	O3-C1-C2	3.96	111.51	108.06	3	20
3	A	411	PCW	O2-C31-C32	3.95	120.03	111.48	18	20
3	C	203	PCW	O2-C31-C32	3.95	120.03	111.48	2	20
4	B	215	17F	O3-C1-C2	3.95	111.50	108.06	11	20
3	A	412	PCW	O2-C31-C32	3.93	119.99	111.48	13	20
3	D	607	PCW	O2-C31-C32	3.93	119.99	111.48	12	20
3	C	208	PCW	O2-C31-C32	3.93	119.99	111.48	13	20
3	A	418	PCW	O2-C31-C32	3.92	119.97	111.48	20	20
3	B	213	PCW	O2-C31-C32	3.91	119.94	111.48	9	20
3	A	401	PCW	C2-O2-C31	3.90	108.46	117.80	13	19
3	A	408	PCW	O2-C31-C32	3.90	119.92	111.48	16	20
3	A	416	PCW	O2-C31-C32	3.90	119.91	111.48	6	20
5	B	201	GDP	C4'-O4'-C1'	3.89	106.36	109.92	9	20
3	C	205	PCW	C2-O2-C31	3.89	108.48	117.80	11	20
3	D	624	PCW	O2-C31-C32	3.89	119.89	111.48	17	20
3	D	609	PCW	O2-C31-C32	3.89	119.89	111.48	1	20
3	A	419	PCW	C2-O2-C31	3.88	108.50	117.80	7	20
3	A	403	PCW	O2-C31-C32	3.88	119.88	111.48	7	20
3	D	618	PCW	O2-C31-C32	3.88	119.88	111.48	13	20
3	C	207	PCW	O2-C31-C32	3.87	119.86	111.48	2	20
3	D	605	PCW	O2-C31-C32	3.87	119.85	111.48	5	20
3	D	620	PCW	O2-C31-C32	3.86	119.83	111.48	13	20
4	B	216	17F	O9-C17-C18	3.86	119.83	111.48	1	20
3	C	206	PCW	O2-C31-C32	3.85	119.82	111.48	15	20
3	A	406	PCW	O2-C31-C32	3.85	119.82	111.48	3	20
3	B	203	PCW	O2-C31-C32	3.85	119.80	111.48	2	20
3	B	208	PCW	O2-C31-C32	3.84	119.79	111.48	14	20
3	B	211	PCW	C2-O2-C31	3.84	108.61	117.80	3	20
3	D	611	PCW	O2-C31-C32	3.84	119.78	111.48	18	20
3	A	410	PCW	O2-C31-C32	3.83	119.77	111.48	14	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	B	206	PCW	O2-C31-C32	3.82	119.75	111.48	15	20
3	D	606	PCW	O2-C31-C32	3.82	119.75	111.48	16	20
3	B	204	PCW	O2-C31-C32	3.81	119.72	111.48	12	20
3	B	205	PCW	C2-O2-C31	3.81	108.67	117.80	17	20
3	C	204	PCW	O2-C31-C32	3.81	119.72	111.48	2	20
3	D	614	PCW	C2-O2-C31	3.81	108.69	117.80	8	20
3	C	209	PCW	O2-C31-C32	3.80	119.69	111.48	6	20
3	A	404	PCW	O2-C31-C32	3.79	119.69	111.48	12	20
3	D	619	PCW	O2-C31-C32	3.79	119.68	111.48	17	20
3	A	402	PCW	O2-C31-C32	3.78	119.66	111.48	19	20
3	A	405	PCW	O2-C31-C32	3.78	119.65	111.48	8	20
4	A	414	17F	C5-O9-C17	3.77	108.77	117.80	13	20
3	A	420	PCW	O2-C31-C32	3.77	119.64	111.48	15	20
3	A	407	PCW	C2-O2-C31	3.77	108.78	117.80	5	20
3	D	623	PCW	C2-O2-C31	3.77	108.78	117.80	19	20
4	D	628	17F	O9-C17-C18	3.76	119.62	111.48	14	20
4	C	210	17F	O9-C17-C18	3.75	119.59	111.48	6	20
3	B	212	PCW	O2-C31-C32	3.73	119.56	111.48	8	20
4	D	631	17F	C5-O9-C17	3.74	108.86	117.80	9	20
3	A	412	PCW	C2-O2-C31	3.73	108.86	117.80	17	20
4	B	214	17F	O3-C1-C2	3.73	111.31	108.06	10	20
3	D	612	PCW	C2-O2-C31	3.73	108.88	117.80	5	20
3	D	615	PCW	C2-O2-C31	3.72	108.90	117.80	4	20
3	D	610	PCW	C2-O2-C31	3.71	108.93	117.80	6	20
3	A	409	PCW	C2-O2-C31	3.70	108.95	117.80	14	20
3	D	601	PCW	O2-C31-C32	3.69	119.47	111.48	1	20
3	D	622	PCW	O2-C31-C32	3.69	119.47	111.48	4	20
3	D	602	PCW	C2-O2-C31	3.68	109.00	117.80	19	20
3	D	620	PCW	C2-O2-C31	3.67	109.02	117.80	13	20
4	A	415	17F	C5-O9-C17	3.66	109.05	117.80	14	20
3	A	413	PCW	C2-O2-C31	3.64	109.08	117.80	6	20
3	D	616	PCW	O2-C31-C32	3.64	119.36	111.48	1	20
3	D	607	PCW	C2-O2-C31	3.64	109.09	117.80	9	20
3	D	621	PCW	O2-C31-C32	3.64	119.35	111.48	17	20
3	C	207	PCW	C2-O2-C31	3.64	109.09	117.80	2	20
3	D	608	PCW	O2-C31-C32	3.63	119.34	111.48	8	20
4	D	635	17F	C5-O9-C17	3.63	109.11	117.80	10	20
3	D	604	PCW	C2-O2-C31	3.62	109.13	117.80	18	20
3	C	212	PCW	O2-C31-C32	3.62	119.31	111.48	16	20
3	D	622	PCW	C2-O2-C31	3.60	109.17	117.80	5	20
3	D	617	PCW	C2-O2-C31	3.60	109.18	117.80	11	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	C	206	PCW	C2-O2-C31	3.57	109.24	117.80	15	20
4	D	632	17F	C5-O9-C17	3.57	109.24	117.80	4	20
3	B	205	PCW	C7-N-C6	3.57	118.34	108.98	10	20
3	C	208	PCW	C2-O2-C31	3.57	109.26	117.80	13	20
4	D	633	17F	C5-O9-C17	3.56	109.28	117.80	4	19
3	C	203	PCW	C2-O2-C31	3.55	109.29	117.80	2	20
3	D	627	PCW	C8-N-C6	3.54	118.27	108.98	17	20
3	D	613	PCW	C7-N-C6	3.52	118.23	108.98	10	20
3	D	609	PCW	C2-O2-C31	3.51	109.39	117.80	6	20
3	B	209	PCW	C2-O2-C31	3.51	109.41	117.80	6	20
3	A	408	PCW	C2-O2-C31	3.50	109.41	117.80	16	20
3	C	204	PCW	C2-O2-C31	3.50	109.42	117.80	11	20
3	B	206	PCW	C2-O2-C31	3.50	109.43	117.80	18	20
3	D	624	PCW	C2-O2-C31	3.49	109.44	117.80	17	10
3	B	206	PCW	C8-N-C6	3.49	118.14	108.98	6	20
3	D	618	PCW	C2-O2-C31	3.49	109.45	117.80	13	20
4	D	634	17F	C5-O9-C17	3.48	109.46	117.80	11	20
3	A	403	PCW	C2-O2-C31	3.48	109.47	117.80	13	20
3	D	603	PCW	C2-O2-C31	3.48	109.47	117.80	19	20
3	B	207	PCW	C7-N-C6	3.48	118.11	108.98	14	20
3	D	613	PCW	C8-N-C6	3.47	118.08	108.98	19	20
3	B	208	PCW	C2-O2-C31	3.46	109.50	117.80	2	20
3	B	213	PCW	C2-O2-C31	3.45	109.54	117.80	18	19
4	B	216	17F	C5-O9-C17	3.45	109.55	117.80	9	20
3	A	411	PCW	C2-O2-C31	3.45	109.55	117.80	18	20
3	D	627	PCW	C7-N-C6	3.45	118.03	108.98	8	20
3	C	203	PCW	C7-N-C6	3.44	118.01	108.98	4	20
3	A	402	PCW	C2-O2-C31	3.44	109.56	117.80	4	20
4	C	210	17F	C5-O9-C17	3.44	109.57	117.80	12	20
3	B	204	PCW	C2-O2-C31	3.43	109.59	117.80	18	20
3	D	619	PCW	C8-N-C6	3.42	117.95	108.98	4	20
3	A	401	PCW	C7-N-C6	3.41	117.94	108.98	9	20
3	A	405	PCW	C7-N-C6	3.41	117.94	108.98	17	20
3	D	602	PCW	C7-N-C6	3.39	117.89	108.98	18	20
3	A	413	PCW	C7-N-C6	3.39	117.87	108.98	19	20
3	A	405	PCW	C8-N-C6	3.38	117.86	108.98	9	20
3	D	609	PCW	C7-N-C6	3.38	117.86	108.98	16	20
3	A	416	PCW	C2-O2-C31	3.38	109.71	117.80	6	19
3	D	609	PCW	C8-N-C6	3.38	117.85	108.98	2	20
3	A	407	PCW	C7-N-C6	3.37	117.84	108.98	19	20
3	D	621	PCW	C7-N-C6	3.37	117.82	108.98	15	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	403	PCW	C8-N-C6	3.36	117.81	108.98	1	20
3	A	417	PCW	C7-N-C6	3.36	117.81	108.98	18	20
3	A	416	PCW	C8-N-C6	3.36	117.81	108.98	6	20
3	D	602	PCW	C8-N-C6	3.36	117.81	108.98	10	20
3	D	614	PCW	C8-N-C6	3.36	117.81	108.98	6	20
3	A	406	PCW	C2-O2-C31	3.36	109.76	117.80	2	20
3	A	410	PCW	C2-O2-C31	3.36	109.76	117.80	14	20
3	A	413	PCW	C8-N-C6	3.36	117.80	108.98	17	20
3	D	615	PCW	C7-N-C6	3.36	117.80	108.98	20	20
3	D	604	PCW	C8-N-C6	3.36	117.79	108.98	15	20
3	B	207	PCW	C2-O2-C31	3.35	109.77	117.80	16	19
3	A	408	PCW	C7-N-C6	3.35	117.78	108.98	16	20
3	D	621	PCW	C8-N-C6	3.35	117.78	108.98	11	20
3	D	608	PCW	C7-N-C6	3.35	117.78	108.98	6	20
3	C	207	PCW	C7-N-C6	3.35	117.77	108.98	12	20
3	D	624	PCW	C7-N-C6	3.35	117.77	108.98	15	20
3	B	207	PCW	C8-N-C6	3.35	117.77	108.98	9	20
3	D	620	PCW	C7-N-C6	3.34	117.76	108.98	6	20
3	D	610	PCW	C7-N-C6	3.34	117.75	108.98	9	20
5	C	201	GDP	C8-N7-C5	3.34	108.24	102.55	15	20
3	C	205	PCW	C8-N-C6	3.34	117.75	108.98	17	20
3	C	206	PCW	C8-N-C6	3.34	117.75	108.98	20	20
3	D	607	PCW	C7-N-C6	3.34	117.74	108.98	3	20
3	D	605	PCW	C8-N-C6	3.34	117.74	108.98	8	20
3	A	408	PCW	C8-N-C6	3.33	117.73	108.98	5	20
4	D	628	17F	C5-O9-C17	3.34	109.81	117.80	14	20
3	B	212	PCW	C8-N-C6	3.33	117.73	108.98	17	20
3	C	208	PCW	C8-N-C6	3.33	117.73	108.98	7	20
3	A	402	PCW	C7-N-C6	3.33	117.72	108.98	15	20
3	C	203	PCW	C8-N-C6	3.33	117.72	108.98	20	20
3	D	606	PCW	C7-N-C6	3.33	117.72	108.98	7	20
3	D	612	PCW	C8-N-C6	3.33	117.72	108.98	1	20
3	A	418	PCW	C2-O2-C31	3.33	109.83	117.80	9	20
3	D	601	PCW	C7-N-C6	3.33	117.72	108.98	5	20
3	D	616	PCW	C8-N-C6	3.33	117.72	108.98	19	20
3	C	204	PCW	C7-N-C6	3.33	117.72	108.98	1	20
5	B	201	GDP	C8-N7-C5	3.33	108.21	102.55	16	20
3	A	412	PCW	C7-N-C6	3.32	117.71	108.98	9	20
3	D	617	PCW	C8-N-C6	3.32	117.70	108.98	4	20
3	C	208	PCW	C7-N-C6	3.32	117.70	108.98	17	20
3	D	601	PCW	C8-N-C6	3.32	117.69	108.98	17	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	406	PCW	C7-N-C6	3.32	117.69	108.98	7	20
5	C	201	GDP	C2-N1-C6	3.32	119.04	125.11	15	20
3	A	417	PCW	C8-N-C6	3.31	117.68	108.98	20	20
3	D	603	PCW	C8-N-C6	3.31	117.68	108.98	8	20
3	B	205	PCW	C8-N-C6	3.31	117.68	108.98	12	20
3	B	213	PCW	C7-N-C6	3.31	117.68	108.98	13	20
3	B	213	PCW	C8-N-C6	3.31	117.68	108.98	6	20
3	A	420	PCW	C8-N-C6	3.31	117.67	108.98	14	20
3	D	623	PCW	C7-N-C6	3.31	117.67	108.98	3	20
3	D	623	PCW	C8-N-C6	3.31	117.67	108.98	12	20
3	A	403	PCW	C7-N-C6	3.31	117.67	108.98	10	20
3	D	626	PCW	C8-N-C6	3.31	117.67	108.98	19	20
3	A	407	PCW	C8-N-C6	3.31	117.66	108.98	17	20
3	D	616	PCW	C7-N-C6	3.30	117.66	108.98	1	20
3	A	406	PCW	C8-N-C6	3.30	117.65	108.98	20	20
3	D	617	PCW	C7-N-C6	3.30	117.65	108.98	5	20
3	D	622	PCW	C7-N-C6	3.30	117.65	108.98	8	20
3	D	622	PCW	C8-N-C6	3.30	117.65	108.98	7	20
3	B	204	PCW	C8-N-C6	3.30	117.64	108.98	18	20
3	B	210	PCW	C7-N-C6	3.30	117.64	108.98	1	20
3	D	620	PCW	C8-N-C6	3.30	117.64	108.98	20	20
3	C	209	PCW	C2-O2-C31	3.30	109.90	117.80	14	20
3	B	204	PCW	C7-N-C6	3.30	117.64	108.98	9	20
3	C	205	PCW	C7-N-C6	3.29	117.63	108.98	19	20
3	A	405	PCW	C2-O2-C31	3.29	109.92	117.80	12	20
3	A	418	PCW	C8-N-C6	3.29	117.62	108.98	4	20
3	D	603	PCW	C7-N-C6	3.29	117.63	108.98	1	20
3	A	416	PCW	C7-N-C6	3.29	117.62	108.98	14	20
3	D	606	PCW	C8-N-C6	3.29	117.62	108.98	14	20
3	D	626	PCW	C7-N-C6	3.29	117.61	108.98	9	20
3	C	209	PCW	C7-N-C6	3.29	117.61	108.98	7	20
3	D	612	PCW	C7-N-C6	3.29	117.61	108.98	13	20
3	B	203	PCW	C2-O2-C31	3.29	109.93	117.80	13	20
3	B	212	PCW	C7-N-C6	3.29	117.61	108.98	13	20
3	D	625	PCW	C7-N-C6	3.29	117.61	108.98	20	20
3	B	208	PCW	C7-N-C6	3.28	117.60	108.98	1	20
3	A	402	PCW	C8-N-C6	3.28	117.60	108.98	5	20
3	B	209	PCW	C8-N-C6	3.28	117.60	108.98	3	20
3	A	410	PCW	C7-N-C6	3.28	117.59	108.98	15	20
5	B	201	GDP	C2-N1-C6	3.28	119.10	125.11	12	20
3	A	411	PCW	C7-N-C6	3.28	117.59	108.98	4	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	419	PCW	C7-N-C6	3.28	117.59	108.98	3	20
3	B	210	PCW	C8-N-C6	3.28	117.59	108.98	5	20
3	C	212	PCW	C8-N-C6	3.28	117.59	108.98	5	20
3	A	409	PCW	C7-N-C6	3.27	117.58	108.98	14	20
3	A	412	PCW	C8-N-C6	3.28	117.58	108.98	7	20
3	A	409	PCW	C8-N-C6	3.27	117.58	108.98	7	20
3	D	614	PCW	C7-N-C6	3.27	117.58	108.98	13	20
3	B	203	PCW	C8-N-C6	3.27	117.58	108.98	17	20
3	A	404	PCW	C8-N-C6	3.27	117.57	108.98	3	20
3	B	211	PCW	C7-N-C6	3.27	117.57	108.98	15	20
3	D	604	PCW	C7-N-C6	3.27	117.56	108.98	12	20
3	D	613	PCW	C2-O2-C31	3.27	109.97	117.80	10	20
3	A	419	PCW	C8-N-C6	3.27	117.56	108.98	8	20
3	D	610	PCW	C8-N-C6	3.27	117.56	108.98	16	20
3	D	618	PCW	C8-N-C6	3.27	117.56	108.98	8	20
3	D	615	PCW	C8-N-C6	3.27	117.56	108.98	5	20
3	D	625	PCW	C8-N-C6	3.27	117.56	108.98	18	20
3	C	212	PCW	C7-N-C6	3.26	117.55	108.98	15	20
3	C	209	PCW	C8-N-C6	3.26	117.55	108.98	14	20
3	A	404	PCW	C7-N-C6	3.26	117.54	108.98	20	20
3	A	418	PCW	C7-N-C6	3.26	117.54	108.98	17	20
3	B	211	PCW	C8-N-C6	3.26	117.54	108.98	13	20
3	C	204	PCW	C8-N-C6	3.26	117.54	108.98	5	20
3	C	207	PCW	C8-N-C6	3.26	117.54	108.98	19	20
3	D	605	PCW	C7-N-C6	3.26	117.53	108.98	20	20
3	B	208	PCW	C8-N-C6	3.26	117.53	108.98	13	20
3	B	209	PCW	C7-N-C6	3.26	117.53	108.98	7	20
3	D	608	PCW	C8-N-C6	3.25	117.51	108.98	8	20
3	D	611	PCW	C7-N-C6	3.25	117.51	108.98	6	20
3	C	206	PCW	C7-N-C6	3.25	117.51	108.98	11	20
3	B	206	PCW	C7-N-C6	3.25	117.51	108.98	19	20
3	D	607	PCW	C8-N-C6	3.25	117.50	108.98	7	20
3	D	611	PCW	C8-N-C6	3.25	117.50	108.98	7	20
3	D	619	PCW	C7-N-C6	3.24	117.50	108.98	13	20
3	A	420	PCW	C7-N-C6	3.24	117.49	108.98	17	20
3	B	203	PCW	C7-N-C6	3.24	117.49	108.98	10	20
3	A	411	PCW	C8-N-C6	3.24	117.49	108.98	5	20
3	D	618	PCW	C7-N-C6	3.24	117.49	108.98	19	20
3	D	611	PCW	C2-O2-C31	3.23	110.07	117.80	14	20
3	A	401	PCW	C8-N-C6	3.22	117.44	108.98	1	20
3	A	410	PCW	C8-N-C6	3.22	117.44	108.98	3	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	D	619	PCW	C2-O2-C31	3.22	110.09	117.80	6	20
3	D	624	PCW	C8-N-C6	3.22	117.43	108.98	11	20
4	B	217	17F	C5-O9-C17	3.20	110.13	117.80	4	20
4	D	632	17F	O3-P1-O1	3.19	96.29	108.94	13	20
3	B	212	PCW	C2-O2-C31	3.18	110.19	117.80	12	20
3	A	404	PCW	C2-O2-C31	3.16	110.23	117.80	6	20
3	D	616	PCW	C2-O2-C31	3.16	110.23	117.80	5	20
4	A	414	17F	O3-P1-O1	3.16	96.42	108.94	20	20
4	B	215	17F	C5-O9-C17	3.16	110.23	117.80	6	20
3	B	204	PCW	O4P-P-O2P	3.15	96.45	108.94	18	20
3	D	605	PCW	C2-O2-C31	3.13	110.32	117.80	12	20
3	C	212	PCW	O4P-P-O2P	3.12	96.58	108.94	13	20
3	D	608	PCW	C2-O2-C31	3.10	110.39	117.80	2	20
3	D	606	PCW	C2-O2-C31	3.09	110.41	117.80	16	20
3	D	602	PCW	O3-C11-C12	3.06	121.17	111.83	19	20
3	C	212	PCW	C2-O2-C31	3.02	110.57	117.80	16	20
5	C	201	GDP	O2B-PB-O3A	3.02	114.76	104.64	11	20
3	D	625	PCW	C2-O2-C31	3.02	110.58	117.80	20	18
3	D	601	PCW	C2-O2-C31	3.01	110.59	117.80	4	20
3	D	621	PCW	C2-O2-C31	2.98	110.66	117.80	15	20
3	D	604	PCW	O3-C11-C12	2.96	120.85	111.83	20	20
3	A	413	PCW	O3-C11-C12	2.90	120.68	111.83	14	20
3	D	620	PCW	O3-C11-C12	2.84	120.48	111.83	7	20
3	D	622	PCW	O3-C11-C12	2.82	120.43	111.83	12	20
3	A	417	PCW	O3-C11-C12	2.82	120.42	111.83	8	20
3	A	416	PCW	O3-C11-C12	2.81	120.42	111.83	7	20
4	D	632	17F	O7-C7-C8	2.81	120.40	111.83	4	20
3	D	617	PCW	O3-C11-C12	2.80	120.38	111.83	13	20
5	B	201	GDP	O4'-C1'-N9	2.80	112.46	108.75	9	20
3	A	418	PCW	O3-C11-C12	2.80	120.36	111.83	20	20
3	B	205	PCW	O3-C11-C12	2.79	120.35	111.83	9	20
3	D	618	PCW	O3-C11-C12	2.79	120.34	111.83	4	20
3	D	627	PCW	O3-C11-C12	2.79	120.33	111.83	14	20
3	B	210	PCW	O3-C11-C12	2.79	120.33	111.83	14	20
3	B	206	PCW	O3-C11-C12	2.78	120.33	111.83	3	20
4	A	415	17F	O7-C7-C8	2.78	120.32	111.83	8	20
3	D	611	PCW	O3-C11-C12	2.76	120.25	111.83	13	20
3	C	208	PCW	O3-C11-C12	2.75	120.23	111.83	3	20
5	C	201	GDP	O4'-C1'-N9	2.75	112.40	108.75	5	20
4	A	414	17F	O7-C7-C8	2.75	120.23	111.83	4	20
3	A	407	PCW	O3-C11-C12	2.75	120.22	111.83	13	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	420	PCW	C2-O2-C31	2.75	111.22	117.80	15	20
3	A	420	PCW	O3-C11-C12	2.75	120.21	111.83	7	20
3	D	610	PCW	O3-C11-C12	2.75	120.21	111.83	16	20
4	C	210	17F	O7-C7-C8	2.75	120.21	111.83	18	20
3	D	624	PCW	O3-C11-C12	2.74	120.20	111.83	2	20
4	B	217	17F	O7-C7-C8	2.74	120.19	111.83	4	20
3	B	204	PCW	O1P-P-O2P	2.74	125.19	112.44	14	20
4	D	632	17F	O2-P1-O1	2.74	125.17	112.44	20	20
4	D	630	17F	O7-C7-C8	2.73	120.17	111.83	16	20
3	C	212	PCW	O1P-P-O2P	2.72	125.12	112.44	16	20
3	B	213	PCW	O3-C11-C12	2.72	120.13	111.83	4	20
4	A	414	17F	O2-P1-O1	2.72	125.08	112.44	18	20
3	A	403	PCW	O3-C11-C12	2.70	120.07	111.83	7	20
3	D	615	PCW	O3-C11-C12	2.70	120.07	111.83	13	20
3	B	211	PCW	O3-C11-C12	2.70	120.06	111.83	3	20
3	A	406	PCW	O3-C11-C12	2.69	120.02	111.83	12	20
4	D	629	17F	O7-C7-C8	2.68	120.02	111.83	10	20
3	C	212	PCW	O3-C11-C12	2.68	120.01	111.83	3	20
3	B	203	PCW	O3-C11-C12	2.68	120.00	111.83	10	20
4	D	633	17F	O7-C7-C8	2.67	119.98	111.83	18	20
3	A	410	PCW	O3-C11-C12	2.66	119.96	111.83	20	20
3	D	608	PCW	O3-C11-C12	2.67	119.96	111.83	18	20
3	D	626	PCW	O3-C11-C12	2.66	119.95	111.83	13	20
3	D	616	PCW	O3-C11-C12	2.66	119.94	111.83	1	20
3	B	209	PCW	O3-C11-C12	2.66	119.94	111.83	14	20
3	C	205	PCW	O3-C11-C12	2.66	119.93	111.83	4	20
3	A	408	PCW	O3-C11-C12	2.65	119.92	111.83	10	20
4	D	635	17F	O7-C7-C8	2.65	119.92	111.83	16	20
3	B	207	PCW	O3-C11-C12	2.65	119.91	111.83	13	20
3	B	212	PCW	O3-C11-C12	2.64	119.89	111.83	12	20
3	A	405	PCW	O3-C11-C12	2.63	119.84	111.83	7	20
3	A	412	PCW	O3-C11-C12	2.63	119.84	111.83	7	20
4	D	634	17F	O7-C7-C8	2.63	119.84	111.83	2	20
3	A	402	PCW	O3-C11-C12	2.62	119.83	111.83	10	20
3	C	207	PCW	O3-C11-C12	2.62	119.83	111.83	2	20
3	A	404	PCW	O3-C11-C12	2.62	119.83	111.83	14	20
3	A	411	PCW	O3-C11-C12	2.62	119.83	111.83	5	20
4	B	216	17F	O7-C7-C8	2.62	119.83	111.83	11	20
3	D	607	PCW	O3-C11-C12	2.62	119.82	111.83	1	20
4	B	215	17F	O7-C7-C8	2.62	119.82	111.83	19	20
3	A	413	PCW	C3-O3-C11	2.62	107.55	117.12	8	17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	D	609	PCW	O3-C11-C12	2.61	119.80	111.83	7	20
4	D	628	17F	O7-C7-C8	2.61	119.79	111.83	11	20
3	D	623	PCW	O3-C11-C12	2.60	119.76	111.83	9	20
3	D	604	PCW	C3-O3-C11	2.60	107.63	117.12	1	20
3	C	204	PCW	O3-C11-C12	2.60	119.75	111.83	4	20
3	D	612	PCW	O3-C11-C12	2.59	119.75	111.83	13	20
3	A	409	PCW	O3-C11-C12	2.59	119.74	111.83	8	20
3	D	625	PCW	O3-C11-C12	2.59	119.74	111.83	1	20
3	D	606	PCW	O3-C11-C12	2.59	119.73	111.83	3	20
3	B	204	PCW	O3-C11-C12	2.58	119.70	111.83	17	20
3	C	206	PCW	O3-C11-C12	2.58	119.69	111.83	15	20
3	D	618	PCW	C3-O3-C11	2.57	107.73	117.12	4	16
3	C	209	PCW	O3-C11-C12	2.57	119.66	111.83	2	20
3	A	401	PCW	O3-C11-C12	2.55	119.62	111.83	16	20
3	B	208	PCW	O3-C11-C12	2.55	119.62	111.83	16	20
3	D	613	PCW	O3-C11-C12	2.55	119.62	111.83	3	20
4	C	211	17F	O7-C7-C8	2.55	119.62	111.83	12	20
4	B	214	17F	O7-C7-C8	2.54	119.59	111.83	11	20
3	D	620	PCW	C3-O3-C11	2.53	107.86	117.12	7	14
3	D	601	PCW	O3-C11-C12	2.53	119.54	111.83	7	20
3	D	614	PCW	O3-C11-C12	2.53	119.53	111.83	3	20
3	D	602	PCW	C3-O3-C11	2.52	107.92	117.12	19	5
3	D	605	PCW	O3-C11-C12	2.52	119.50	111.83	14	20
5	B	201	GDP	C5-C6-N1	2.51	118.86	114.07	14	20
3	C	212	PCW	O1P-P-O4P	2.50	96.22	107.57	5	20
3	A	420	PCW	C3-O3-C11	2.49	108.03	117.12	4	11
3	D	610	PCW	C3-O3-C11	2.49	108.03	117.12	16	12
4	D	629	17F	C5-O9-C17	2.48	111.86	117.80	19	16
4	C	210	17F	C6-O7-C7	2.48	108.06	117.12	4	20
3	B	204	PCW	O1P-P-O4P	2.48	96.34	107.57	4	20
3	C	203	PCW	O3-C11-C12	2.47	119.38	111.83	17	20
3	D	621	PCW	O3-C11-C12	2.45	119.29	111.83	17	20
4	D	632	17F	O2-P1-O3	2.44	96.49	107.57	15	20
5	C	201	GDP	C5-C6-N1	2.44	118.73	114.07	15	20
3	A	416	PCW	C3-O3-C11	2.43	108.22	117.12	7	11
3	D	603	PCW	O3-C11-C12	2.43	119.25	111.83	16	17
3	A	419	PCW	O3-C11-C12	2.42	119.22	111.83	8	20
3	A	417	PCW	C3-O3-C11	2.41	108.30	117.12	5	11
3	D	627	PCW	C3-O3-C11	2.41	108.32	117.12	10	11
3	D	622	PCW	C3-O3-C11	2.40	108.33	117.12	11	18
4	A	414	17F	C6-O7-C7	2.39	108.37	117.12	4	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	D	630	17F	C6-O7-C7	2.39	108.37	117.12	17	14
3	B	204	PCW	O1P-P-O3P	2.39	118.39	107.57	2	20
3	C	208	PCW	C3-O3-C11	2.39	108.39	117.12	3	14
4	A	414	17F	O2-P1-O3	2.39	96.75	107.57	9	20
4	B	217	17F	C6-O7-C7	2.39	108.39	117.12	20	6
4	D	632	17F	C6-O7-C7	2.38	108.42	117.12	4	14
3	A	418	PCW	C3-O3-C11	2.37	108.44	117.12	20	13
4	A	414	17F	O6-P1-O1	2.37	118.34	108.94	4	20
3	D	616	PCW	C3-O3-C11	2.35	108.51	117.12	1	8
3	D	617	PCW	C3-O3-C11	2.35	108.54	117.12	13	16
3	A	407	PCW	C3-O3-C11	2.34	108.56	117.12	13	15
3	C	212	PCW	O1P-P-O3P	2.34	118.17	107.57	2	20
3	B	205	PCW	C3-O3-C11	2.33	108.60	117.12	9	1
3	A	405	PCW	C3-O3-C11	2.32	108.62	117.12	9	9
3	D	624	PCW	C3-O3-C11	2.32	108.63	117.12	2	17
4	D	632	17F	O6-P1-O1	2.31	118.09	108.94	5	20
3	D	615	PCW	C3-O3-C11	2.30	108.71	117.12	13	4
4	D	635	17F	C6-O7-C7	2.29	108.75	117.12	17	7
4	D	633	17F	C6-O7-C7	2.28	108.77	117.12	18	5
4	D	631	17F	O7-C7-C8	2.28	118.79	111.83	16	16
3	A	404	PCW	C3-O3-C11	2.28	108.79	117.12	4	8
4	D	629	17F	C6-O7-C7	2.28	108.80	117.12	10	13
3	D	611	PCW	C3-O3-C11	2.26	108.85	117.12	3	8
3	D	609	PCW	C3-O3-C11	2.24	108.92	117.12	7	1
3	B	210	PCW	C3-O3-C11	2.24	108.92	117.12	12	4
3	D	619	PCW	O3-C11-C12	2.24	118.67	111.83	5	19
3	D	621	PCW	C4-C5-N	2.23	108.67	115.82	2	2
3	B	213	PCW	C3-O3-C11	2.22	109.00	117.12	4	5
3	C	207	PCW	C3-O3-C11	2.20	109.07	117.12	13	13
4	D	629	17F	O9-C17-O10	2.20	118.56	123.70	8	20
3	D	614	PCW	C3-O3-C11	2.19	109.10	117.12	8	7
3	D	606	PCW	C3-O3-C11	2.19	109.13	117.12	3	6
3	D	608	PCW	C3-O3-C11	2.19	109.13	117.12	11	13
4	A	415	17F	C6-O7-C7	2.18	109.14	117.12	8	5
3	A	402	PCW	C3-O3-C11	2.18	109.16	117.12	10	3
3	D	620	PCW	C4-C5-N	2.18	108.83	115.82	7	1
3	C	205	PCW	C3-O3-C11	2.17	109.17	117.12	4	17
3	A	411	PCW	C3-O3-C11	2.17	109.18	117.12	5	2
3	B	207	PCW	C3-O3-C11	2.17	109.20	117.12	19	9
3	D	607	PCW	C4-C5-N	2.16	108.88	115.82	20	7
3	B	203	PCW	C3-O3-C11	2.16	109.22	117.12	1	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	D	634	17F	C6-O7-C7	2.16	109.22	117.12	2	7
3	A	409	PCW	C3-O3-C11	2.15	109.24	117.12	8	2
4	B	215	17F	C6-O7-C7	2.15	109.26	117.12	19	6
3	D	602	PCW	C4-C5-N	2.15	108.93	115.82	4	6
3	D	626	PCW	C3-O3-C11	2.15	109.27	117.12	13	6
4	C	211	17F	C6-O7-C7	2.15	109.26	117.12	6	3
3	B	212	PCW	C3-O3-C11	2.15	109.27	117.12	17	5
3	A	416	PCW	C3-C2-C1	2.15	106.78	111.78	4	1
3	C	204	PCW	C3-C2-C1	2.14	106.79	111.78	20	1
3	D	618	PCW	C3-C2-C1	2.14	106.80	111.78	4	2
3	A	405	PCW	C4-C5-N	2.13	108.99	115.82	9	6
3	A	413	PCW	C7-N-C5	2.13	118.36	109.91	13	3
3	D	609	PCW	C4-C5-N	2.12	109.00	115.82	19	5
3	D	609	PCW	C8-N-C5	2.12	118.33	109.91	1	1
3	B	211	PCW	C3-O3-C11	2.12	109.38	117.12	18	6
3	D	627	PCW	C8-N-C5	2.11	118.31	109.91	12	5
4	B	216	17F	C6-O7-C7	2.11	109.41	117.12	11	4
3	D	604	PCW	C3-C2-C1	2.11	106.88	111.78	15	5
3	D	622	PCW	C3-C2-C1	2.10	106.88	111.78	7	1
3	B	213	PCW	C8-N-C5	2.10	118.25	109.91	5	2
3	D	627	PCW	C4-C5-N	2.10	109.10	115.82	12	4
3	B	205	PCW	C4-C5-N	2.10	109.09	115.82	5	5
3	B	205	PCW	C8-N-C5	2.09	118.20	109.91	1	3
3	A	406	PCW	C3-O3-C11	2.08	109.50	117.12	6	4
3	A	408	PCW	C3-O3-C11	2.09	109.50	117.12	11	5
3	D	623	PCW	C3-O3-C11	2.08	109.51	117.12	6	2
3	A	402	PCW	C4-C5-N	2.08	109.15	115.82	5	2
3	D	615	PCW	C4-C5-N	2.08	109.15	115.82	5	1
3	B	206	PCW	C3-O3-C11	2.08	109.53	117.12	15	4
3	A	409	PCW	C4-C5-N	2.07	109.18	115.82	2	4
3	A	410	PCW	C3-O3-C11	2.07	109.55	117.12	20	3
3	D	607	PCW	C8-N-C5	2.07	118.14	109.91	9	2
3	B	211	PCW	C4-C5-N	2.07	109.17	115.82	13	2
3	C	203	PCW	C4-C5-N	2.07	109.19	115.82	13	5
3	D	622	PCW	C4-C5-N	2.06	109.19	115.82	19	6
3	D	627	PCW	O2-C31-O31	2.06	118.88	123.70	3	1
3	B	205	PCW	C7-N-C5	2.06	118.12	109.91	6	1
3	D	613	PCW	C4-C5-N	2.06	109.20	115.82	10	2
3	A	411	PCW	C4-C5-N	2.06	109.21	115.82	8	2
3	B	213	PCW	C7-N-C5	2.06	118.10	109.91	17	1
3	D	605	PCW	C3-O3-C11	2.06	109.59	117.12	19	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	C	203	PCW	C3-O3-C11	2.06	109.59	117.12	14	2
3	B	208	PCW	C3-O3-C11	2.06	109.60	117.12	13	2
3	D	619	PCW	C8-N-C5	2.05	118.07	109.91	18	3
4	D	628	17F	C6-O7-C7	2.05	109.62	117.12	2	2
3	A	401	PCW	C3-O3-C11	2.05	109.63	117.12	16	4
4	B	215	17F	C6-C5-C4	2.05	107.01	111.78	5	1
3	C	209	PCW	C4-C5-N	2.05	109.25	115.82	17	3
3	A	408	PCW	C4-C5-N	2.05	109.25	115.82	10	1
3	A	412	PCW	C3-O3-C11	2.04	109.65	117.12	7	2
3	D	613	PCW	C7-N-C5	2.04	118.04	109.91	9	1
3	A	417	PCW	O2-C31-O31	2.04	118.93	123.70	17	2
3	B	209	PCW	C4-C5-N	2.04	109.27	115.82	3	1
3	A	413	PCW	C4-C5-N	2.04	109.28	115.82	15	3
3	A	416	PCW	C4-C5-N	2.04	109.28	115.82	14	1
3	A	420	PCW	C4-C5-N	2.04	109.28	115.82	7	2
3	C	204	PCW	C3-O3-C11	2.04	109.67	117.12	4	1
3	C	209	PCW	C3-O3-C11	2.04	109.67	117.12	2	2
4	B	214	17F	C6-O7-C7	2.04	109.68	117.12	16	1
4	B	215	17F	O9-C17-O10	2.04	118.94	123.70	16	4
3	A	405	PCW	C3-C2-C1	2.03	107.04	111.78	9	1
3	B	212	PCW	C4-C5-N	2.03	109.30	115.82	3	2
3	A	413	PCW	C8-N-C5	2.03	117.99	109.91	20	4
3	C	204	PCW	C4-C5-N	2.03	109.30	115.82	16	2
3	D	625	PCW	C4-C5-N	2.03	109.31	115.82	18	1
3	D	626	PCW	C4-C5-N	2.03	109.31	115.82	6	2
3	A	417	PCW	C4-C5-N	2.03	109.32	115.82	14	3
3	D	603	PCW	C4-C5-N	2.03	109.32	115.82	11	1
3	D	611	PCW	C4-C5-N	2.03	109.32	115.82	13	1
3	D	613	PCW	C8-N-C5	2.03	117.97	109.91	8	4
3	B	206	PCW	C4-C5-N	2.03	109.32	115.82	7	1
3	A	411	PCW	C8-N-C5	2.02	117.96	109.91	6	1
3	C	206	PCW	C3-O3-C11	2.03	109.72	117.12	16	1
3	A	417	PCW	C8-N-C5	2.02	117.95	109.91	11	1
3	D	607	PCW	C7-N-C5	2.02	117.95	109.91	17	2
3	C	205	PCW	C4-C5-N	2.02	109.33	115.82	17	2
4	B	217	17F	O9-C17-O10	2.02	118.97	123.70	2	1
3	D	614	PCW	C7-N-C5	2.02	117.94	109.91	13	1
3	D	601	PCW	C3-O3-C11	2.02	109.74	117.12	14	1
3	B	207	PCW	C8-N-C5	2.02	117.94	109.91	14	1
3	B	210	PCW	C4-C5-N	2.02	109.34	115.82	4	1
3	D	620	PCW	C7-N-C5	2.02	117.93	109.91	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	D	625	PCW	C3-O3-C11	2.01	109.75	117.12	10	1
3	C	212	PCW	C3-O3-C11	2.02	109.75	117.12	7	1
3	D	621	PCW	C7-N-C5	2.01	117.90	109.91	12	2
3	A	420	PCW	C8-N-C5	2.01	117.89	109.91	2	1
3	D	618	PCW	C4-C5-N	2.01	109.37	115.82	17	1
3	D	610	PCW	C4-C5-N	2.01	109.38	115.82	1	1
3	B	209	PCW	C3-O3-C11	2.01	109.79	117.12	3	1
3	A	407	PCW	C7-N-C5	2.00	117.88	109.91	8	3
3	D	620	PCW	C8-N-C5	2.00	117.88	109.91	7	1
3	A	417	PCW	C7-N-C5	2.00	117.87	109.91	6	1
3	A	419	PCW	C4-C5-N	2.00	109.40	115.82	16	1
3	C	208	PCW	C4-C5-N	2.00	109.39	115.82	10	1
3	B	204	PCW	C4-C5-N	2.00	109.40	115.82	7	1

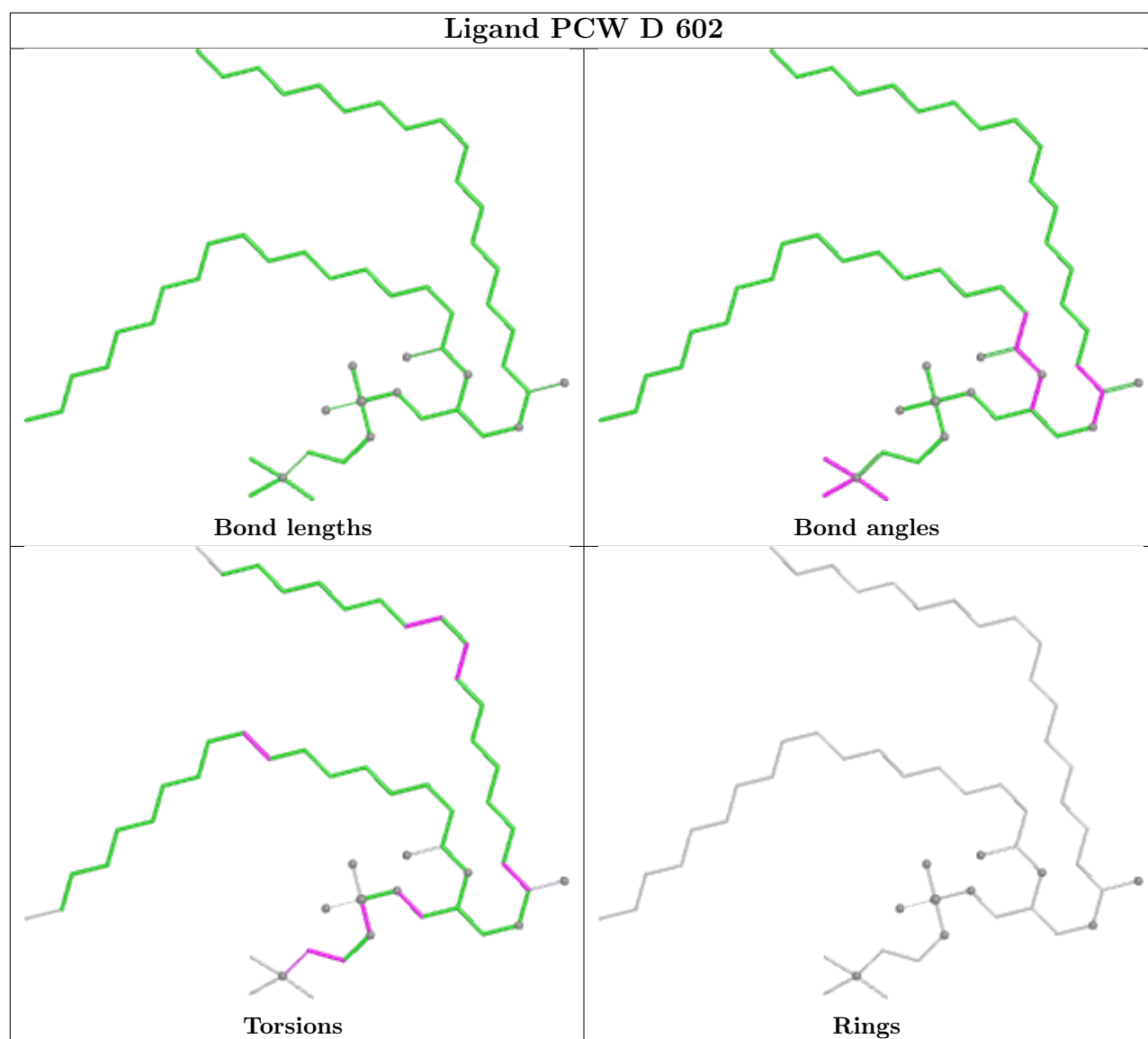
There are no chirality outliers.

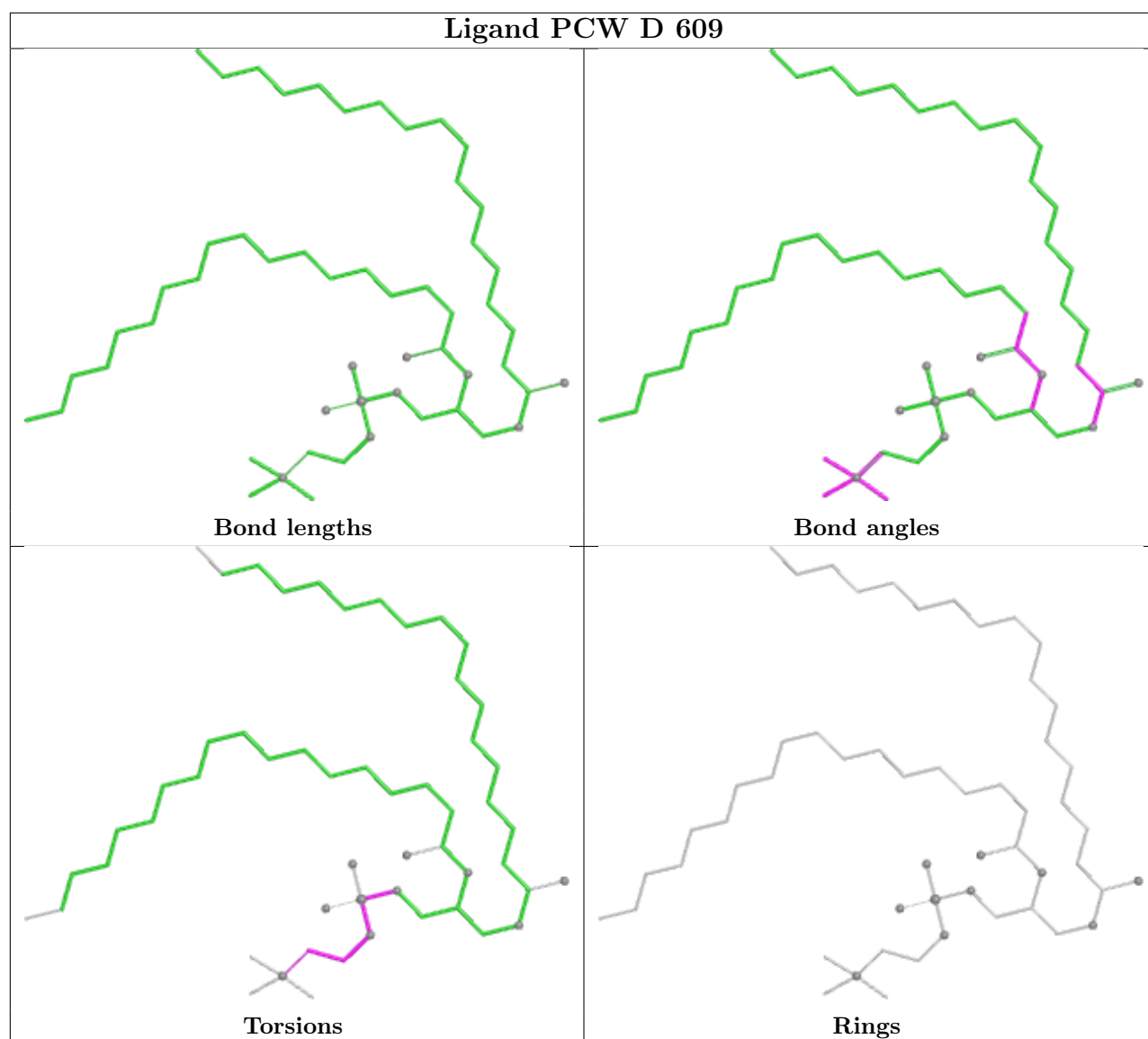
All unique torsion outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

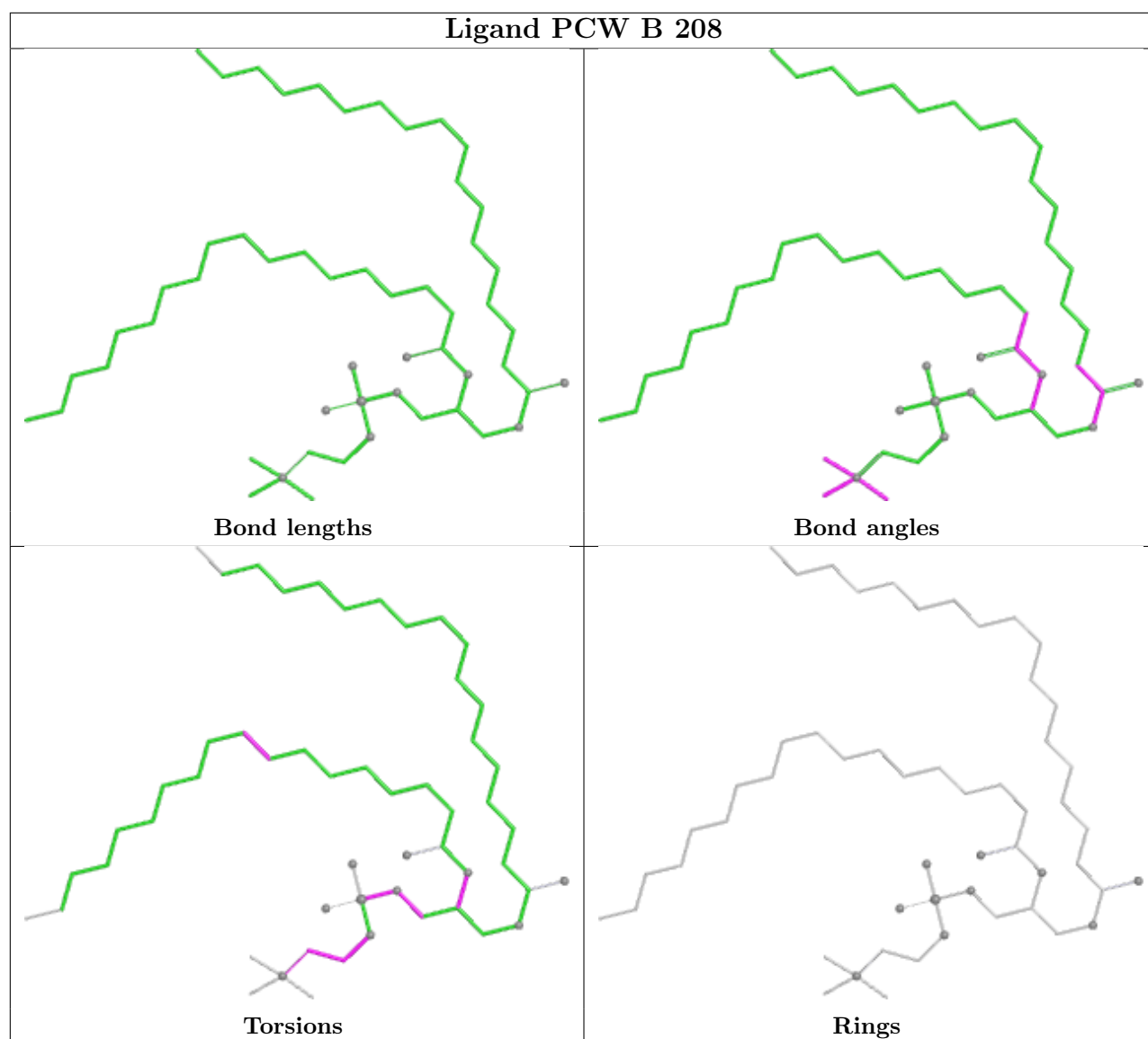
Mol	Chain	Res	Type	Atoms	Models (Total)
4	D	629	17F	O10-C17-O9-C5	20
4	B	215	17F	O10-C17-O9-C5	20
4	B	217	17F	O10-C17-O9-C5	16
4	B	217	17F	C18-C17-O9-C5	7
4	D	629	17F	C18-C17-O9-C5	6
4	B	215	17F	C18-C17-O9-C5	2

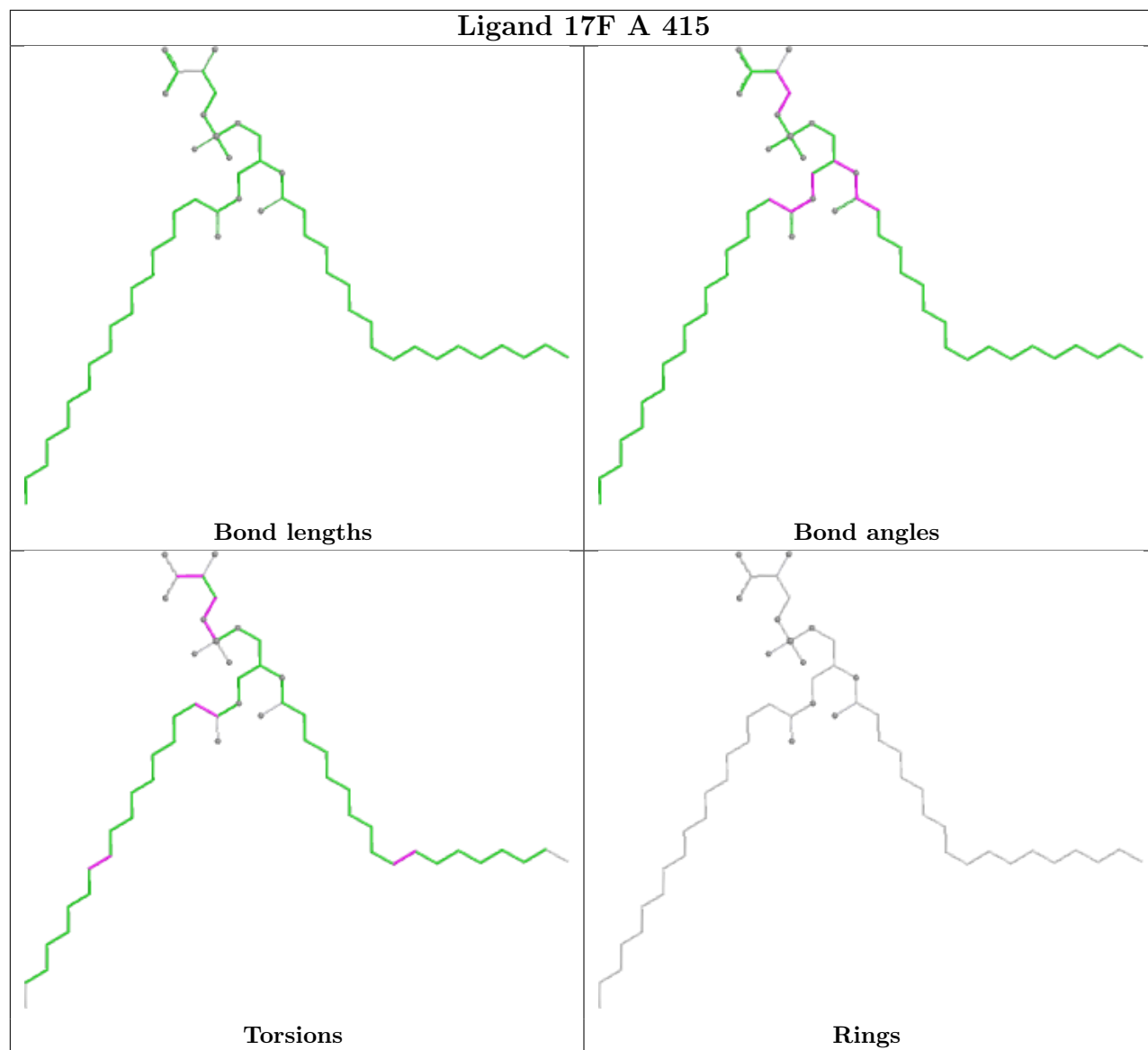
There are no ring outliers.

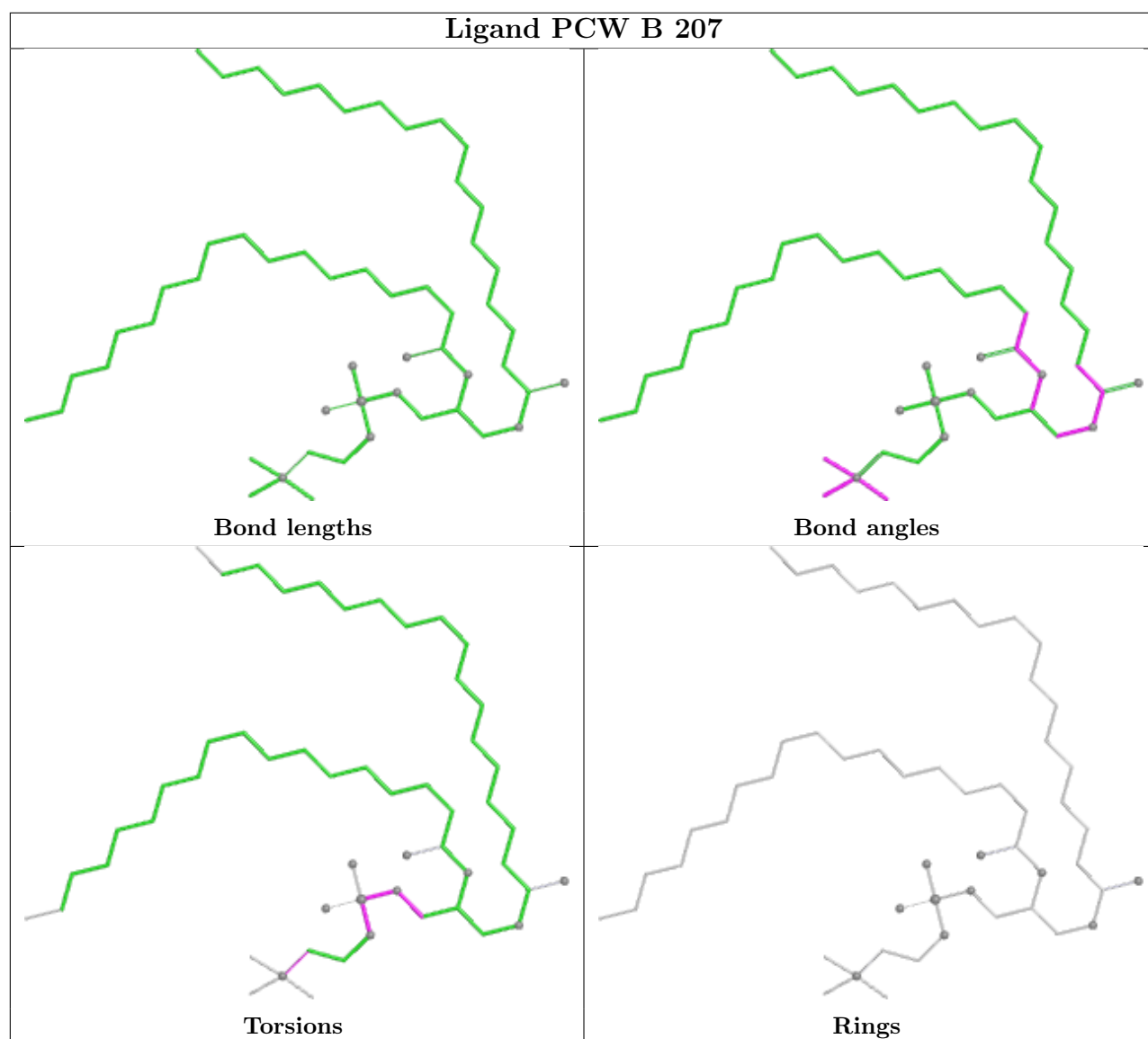
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

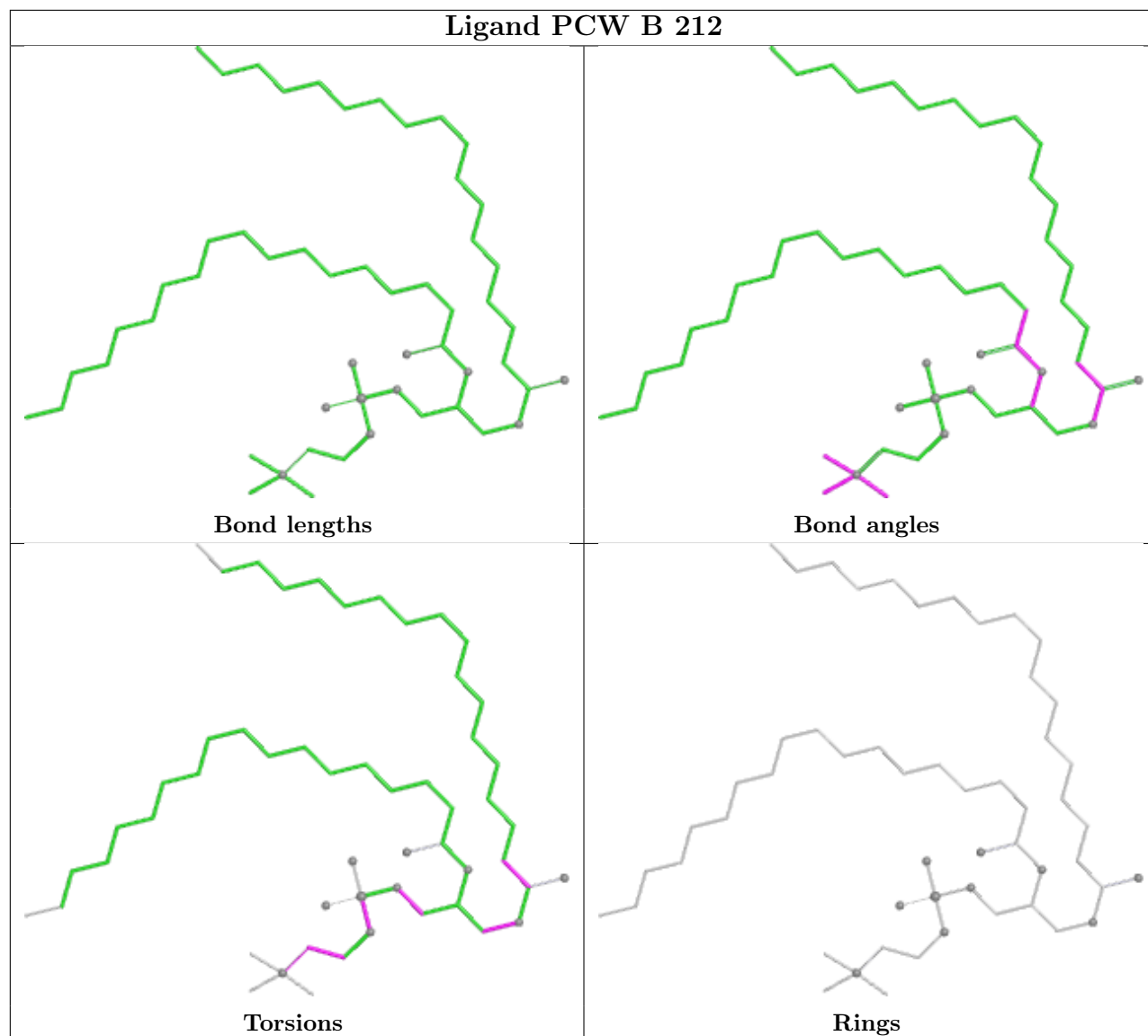


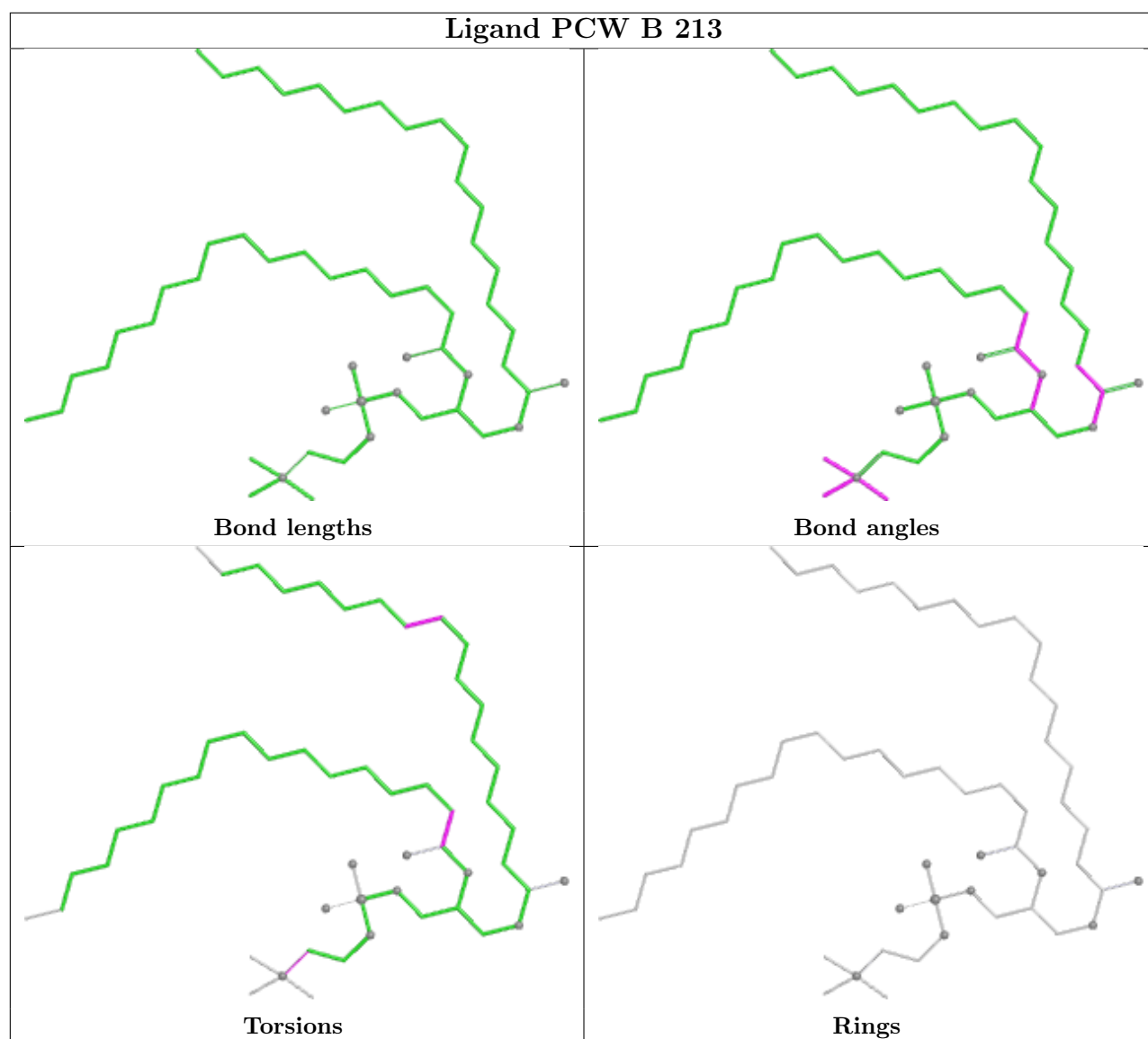


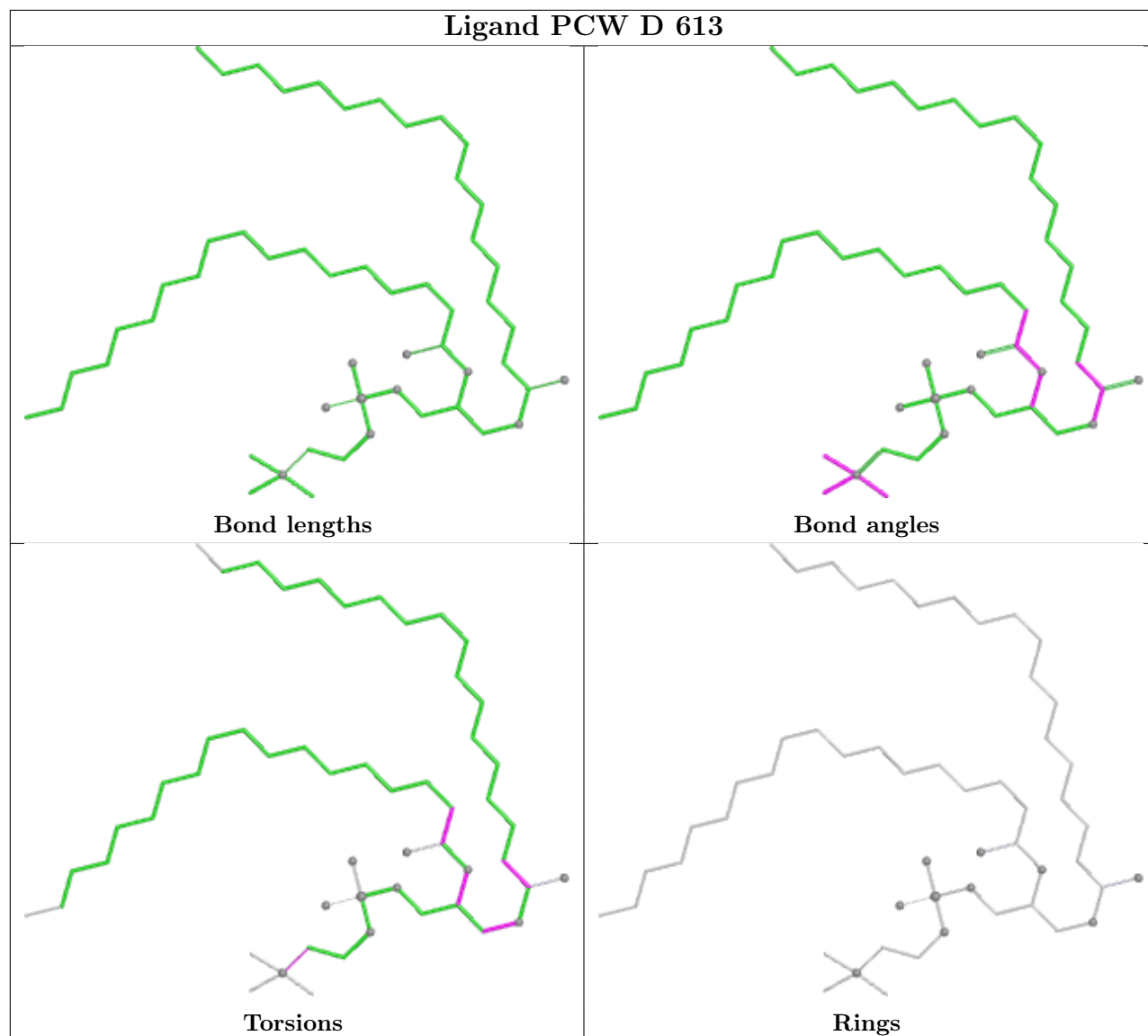


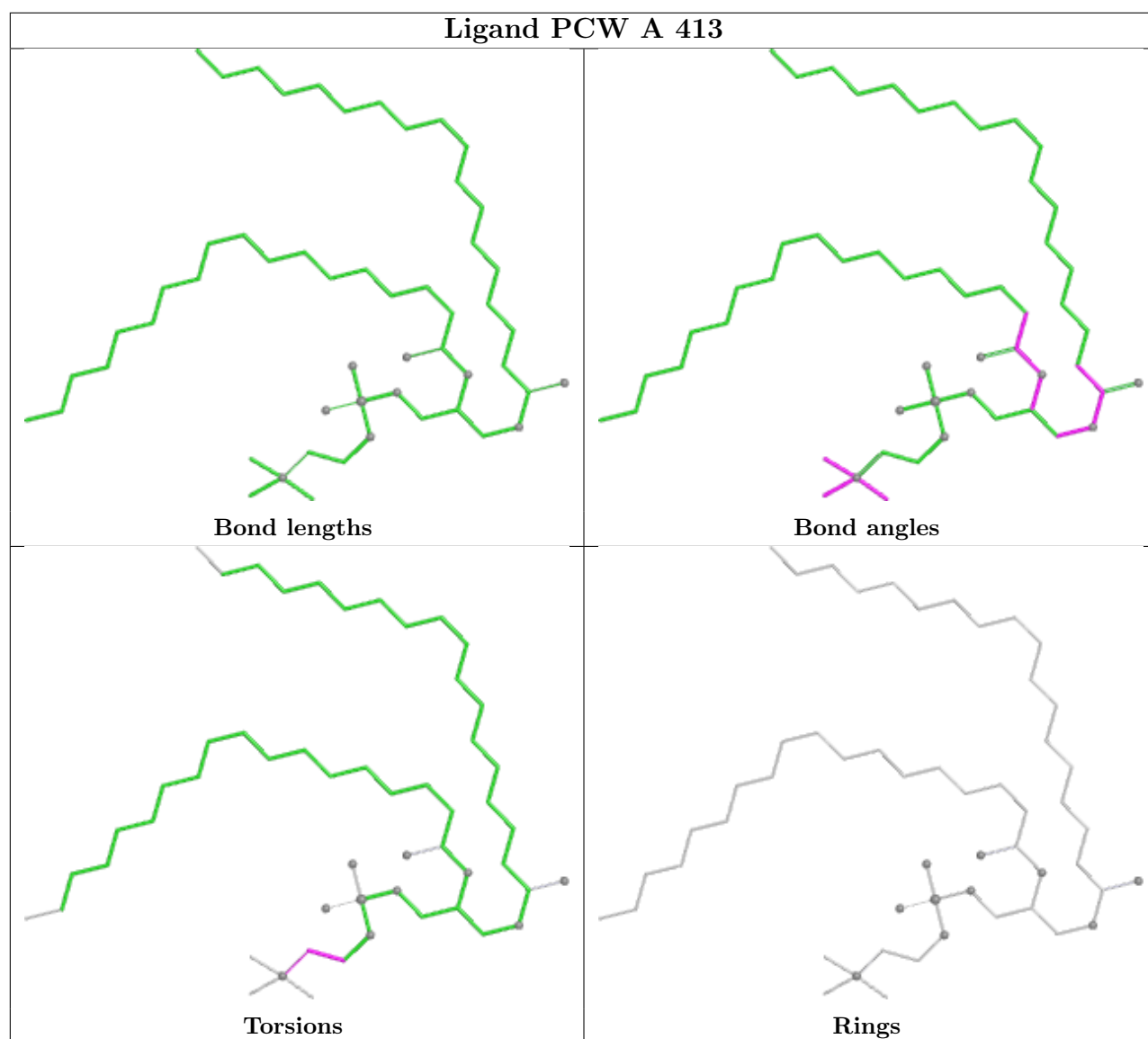


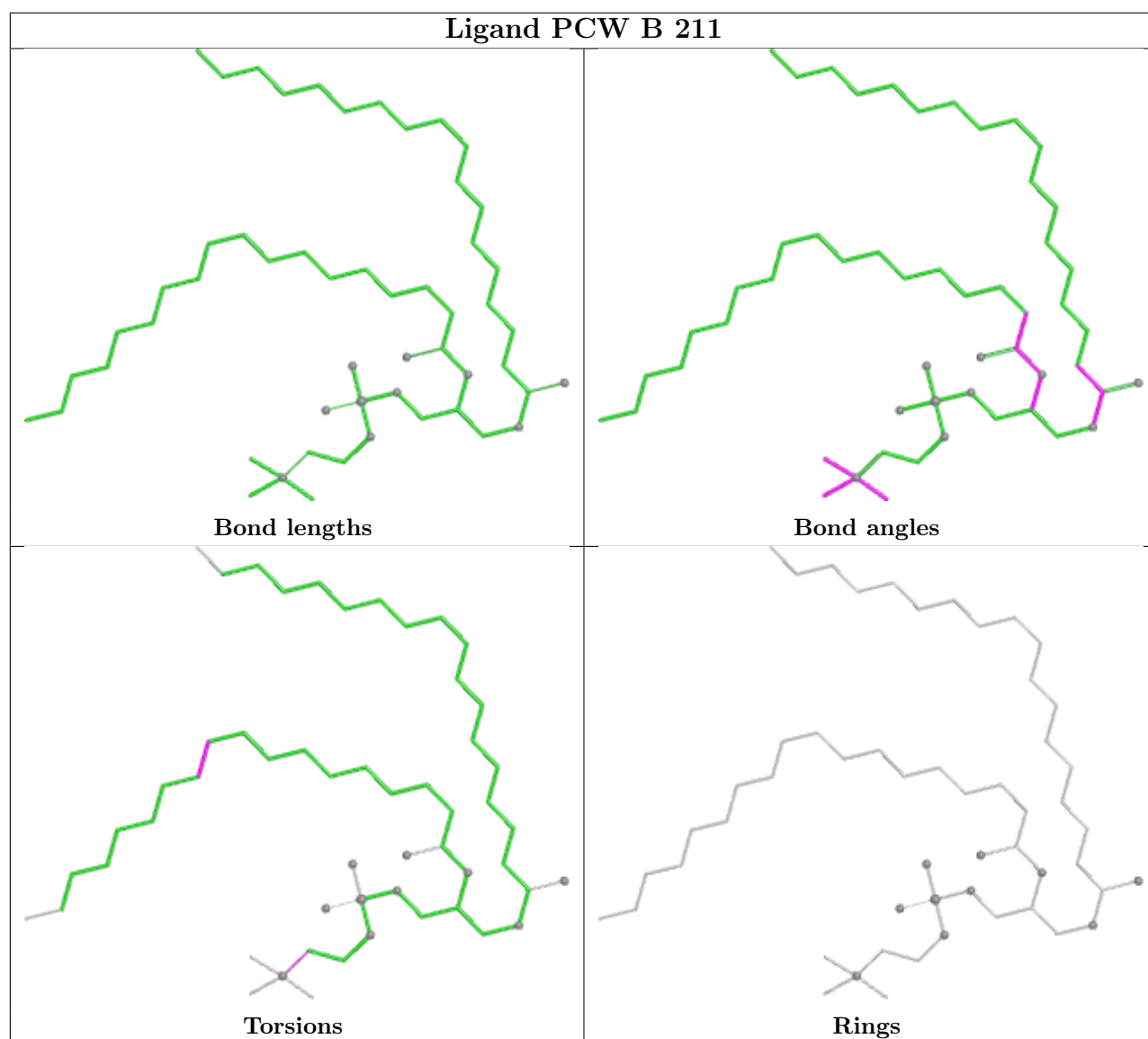


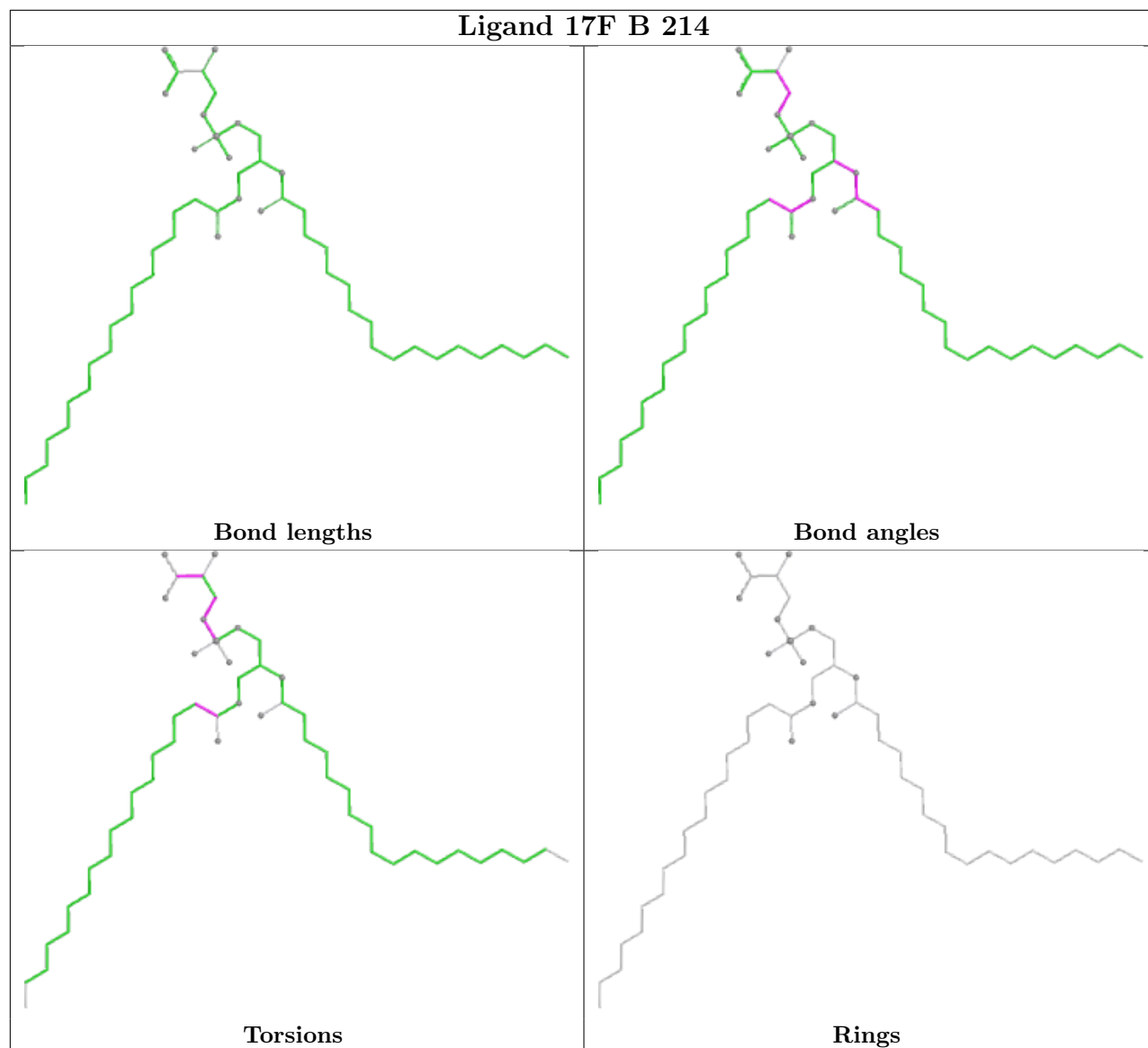


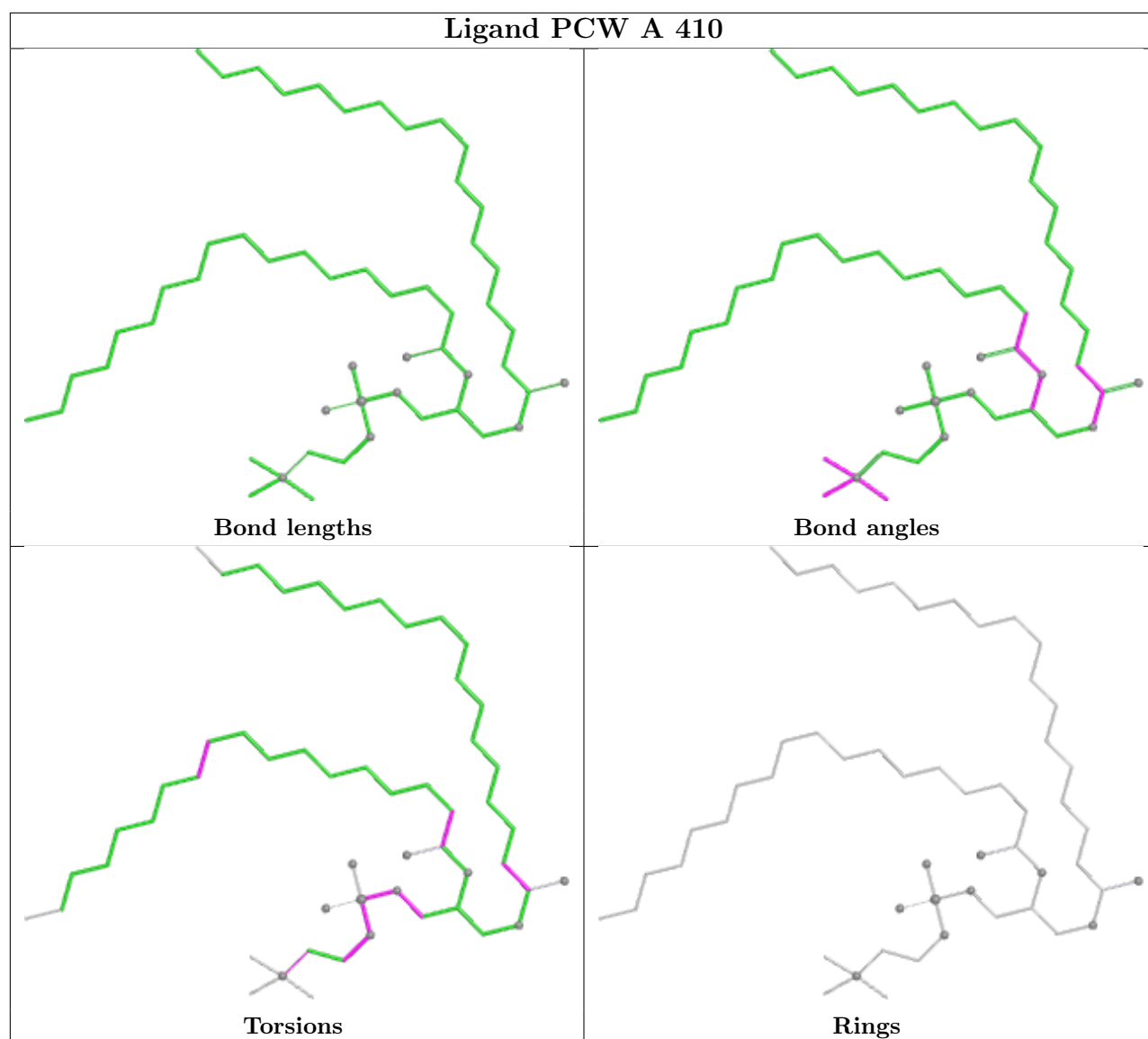


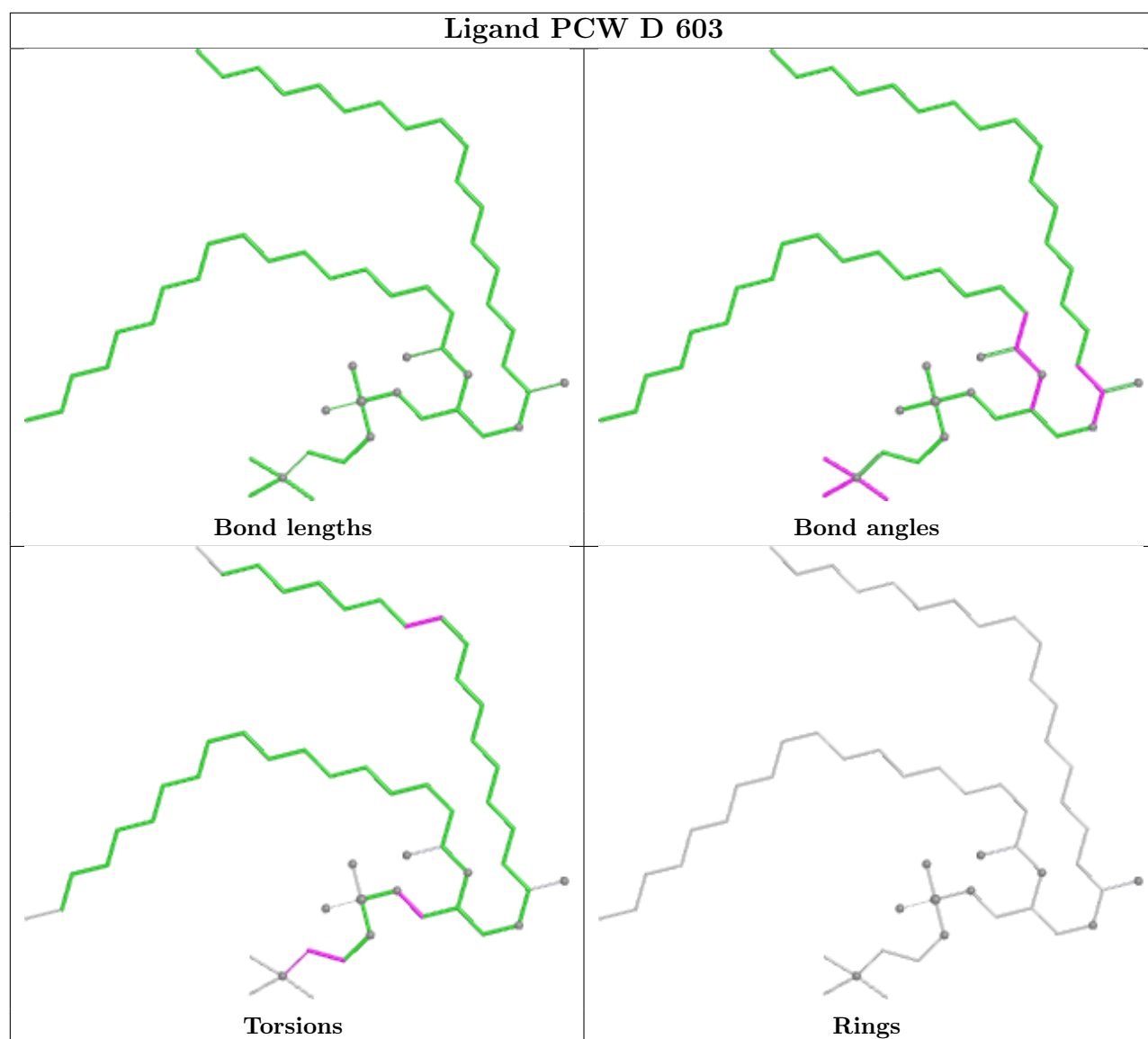


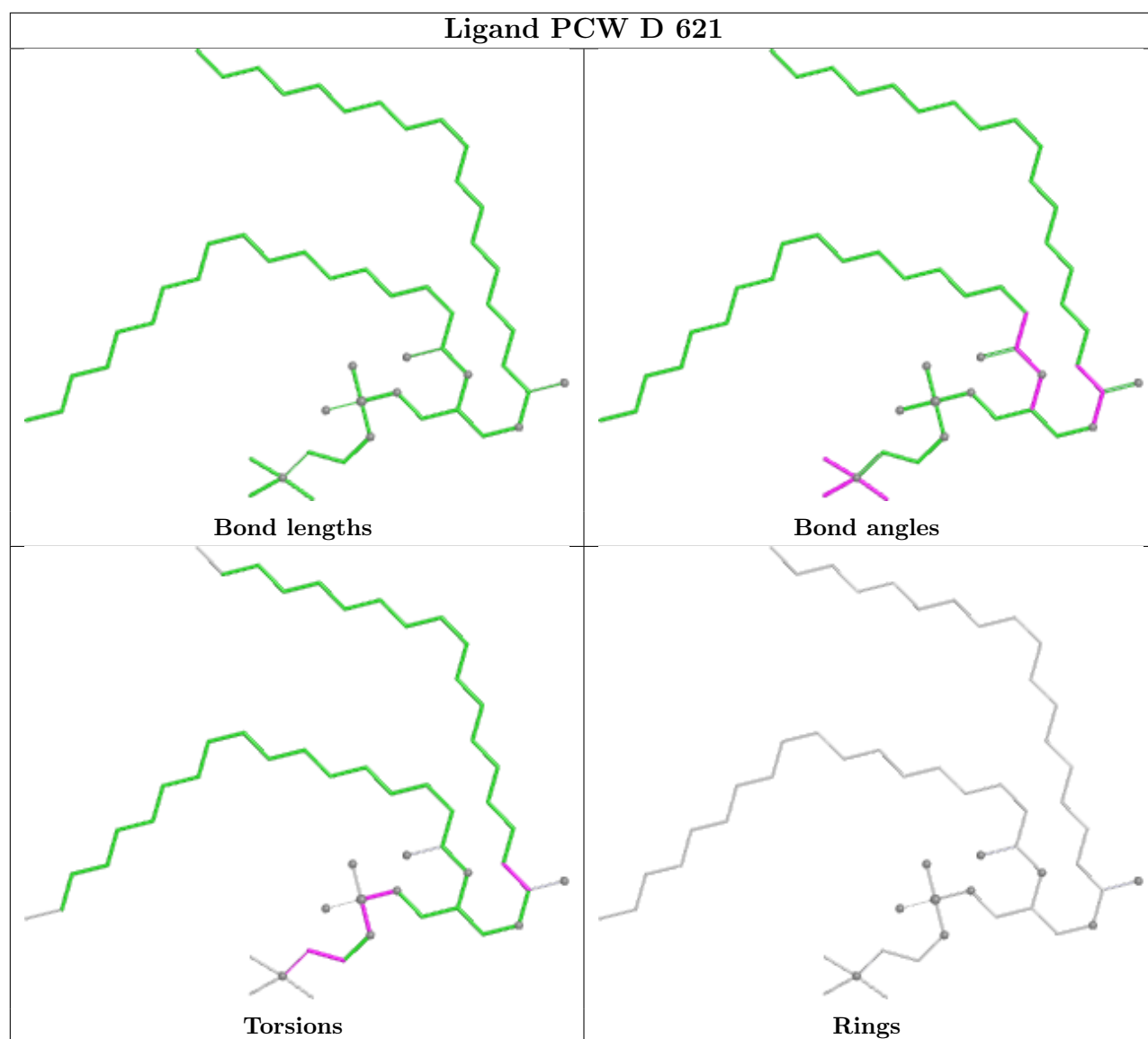


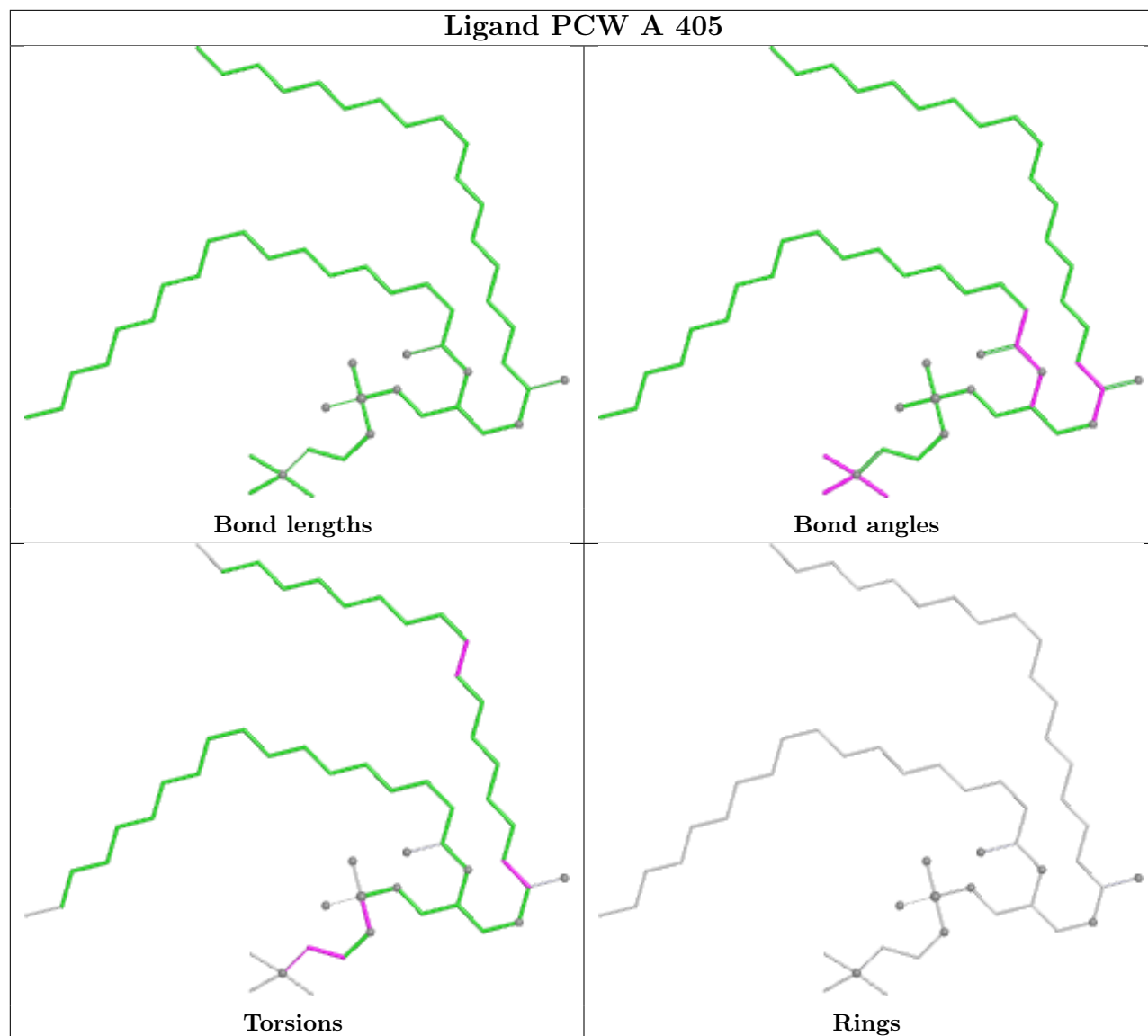


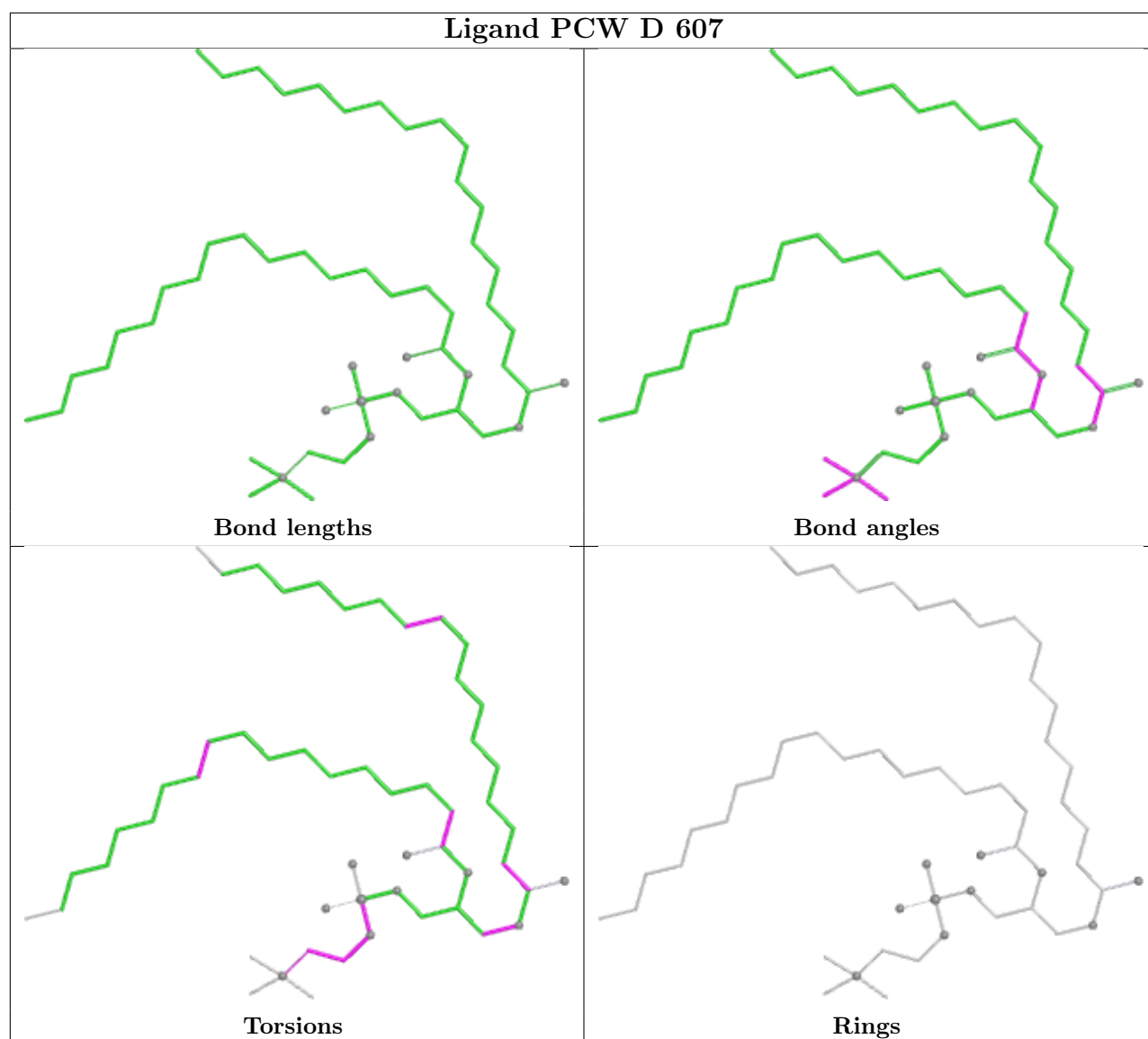


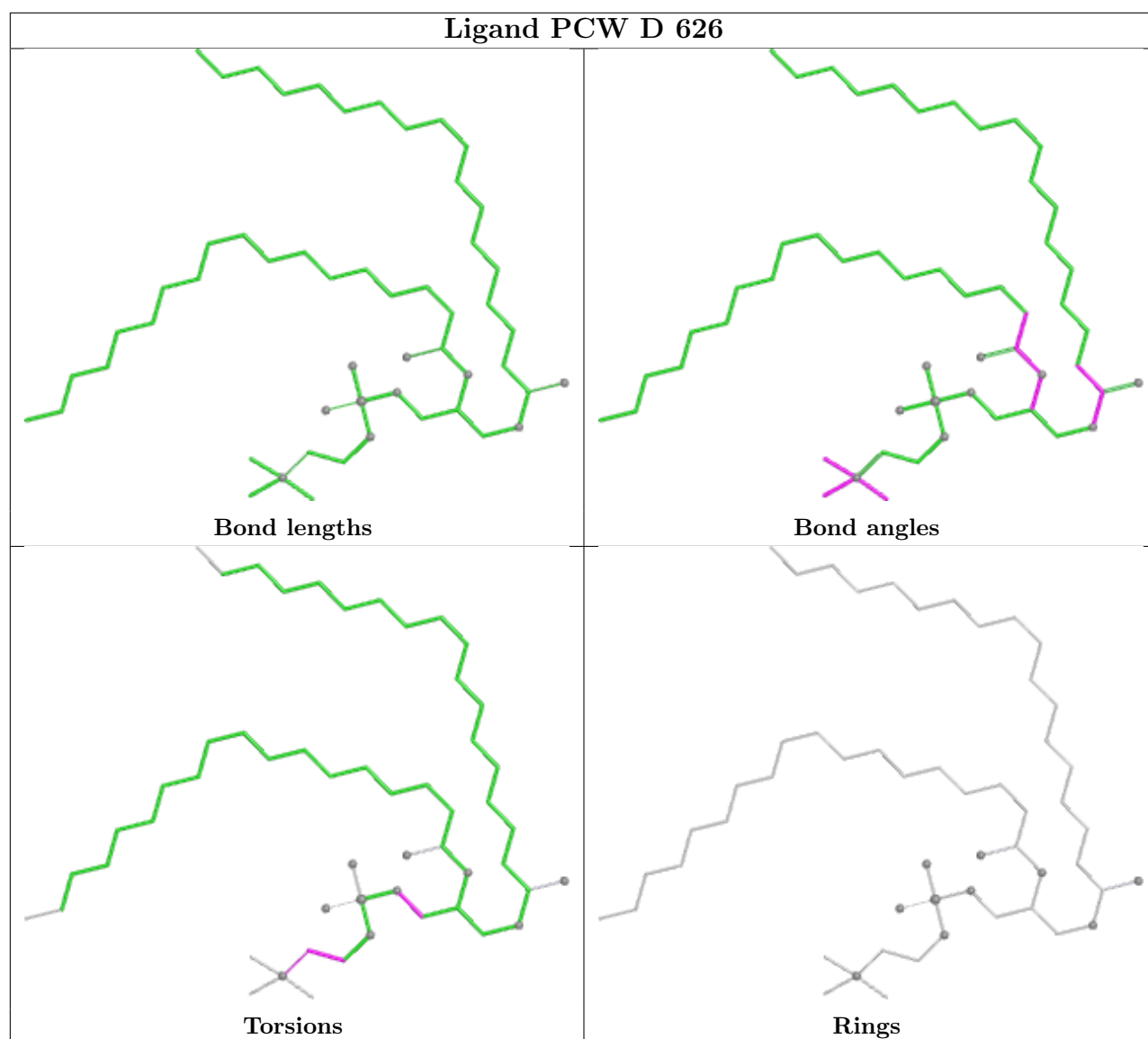


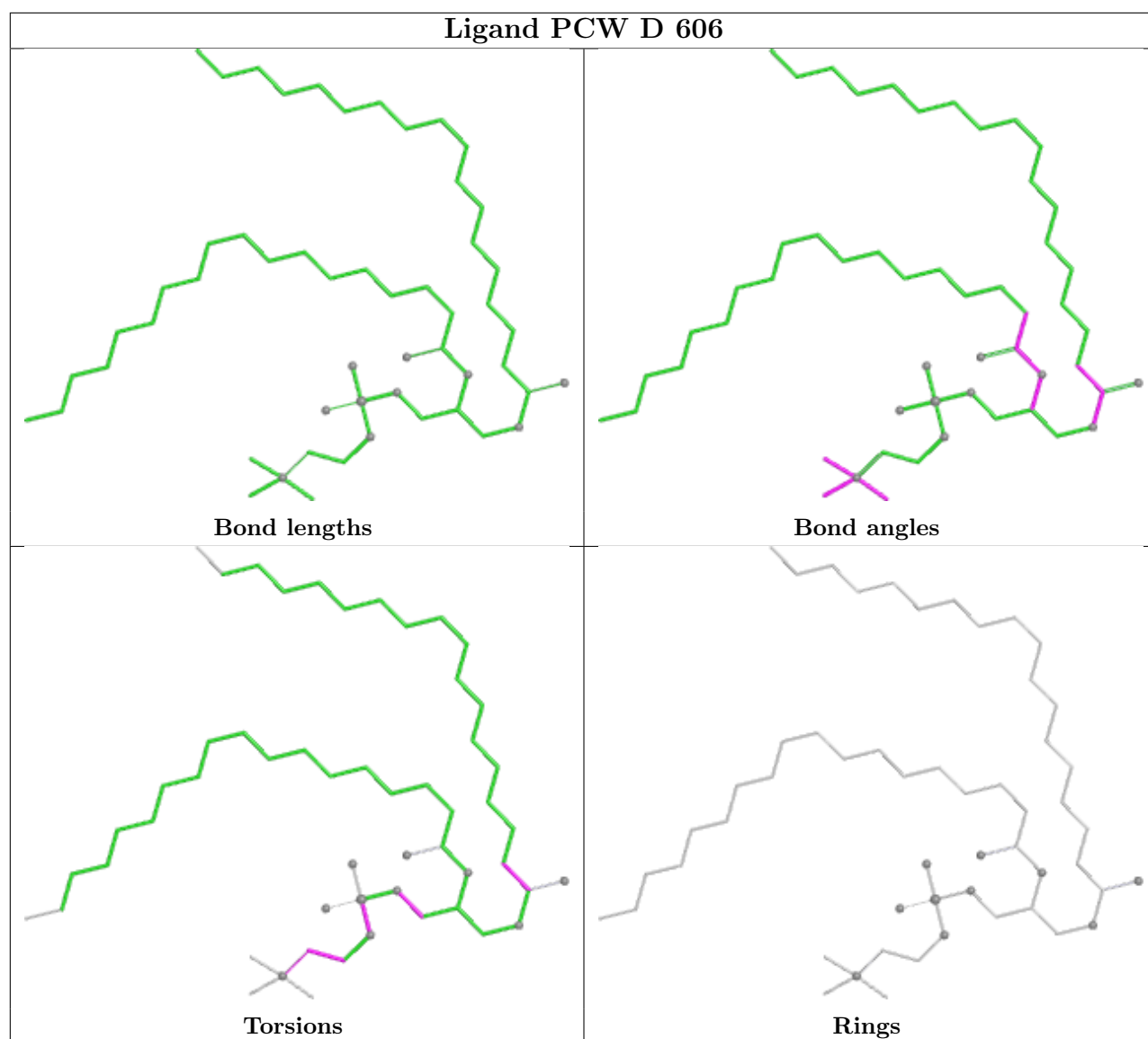


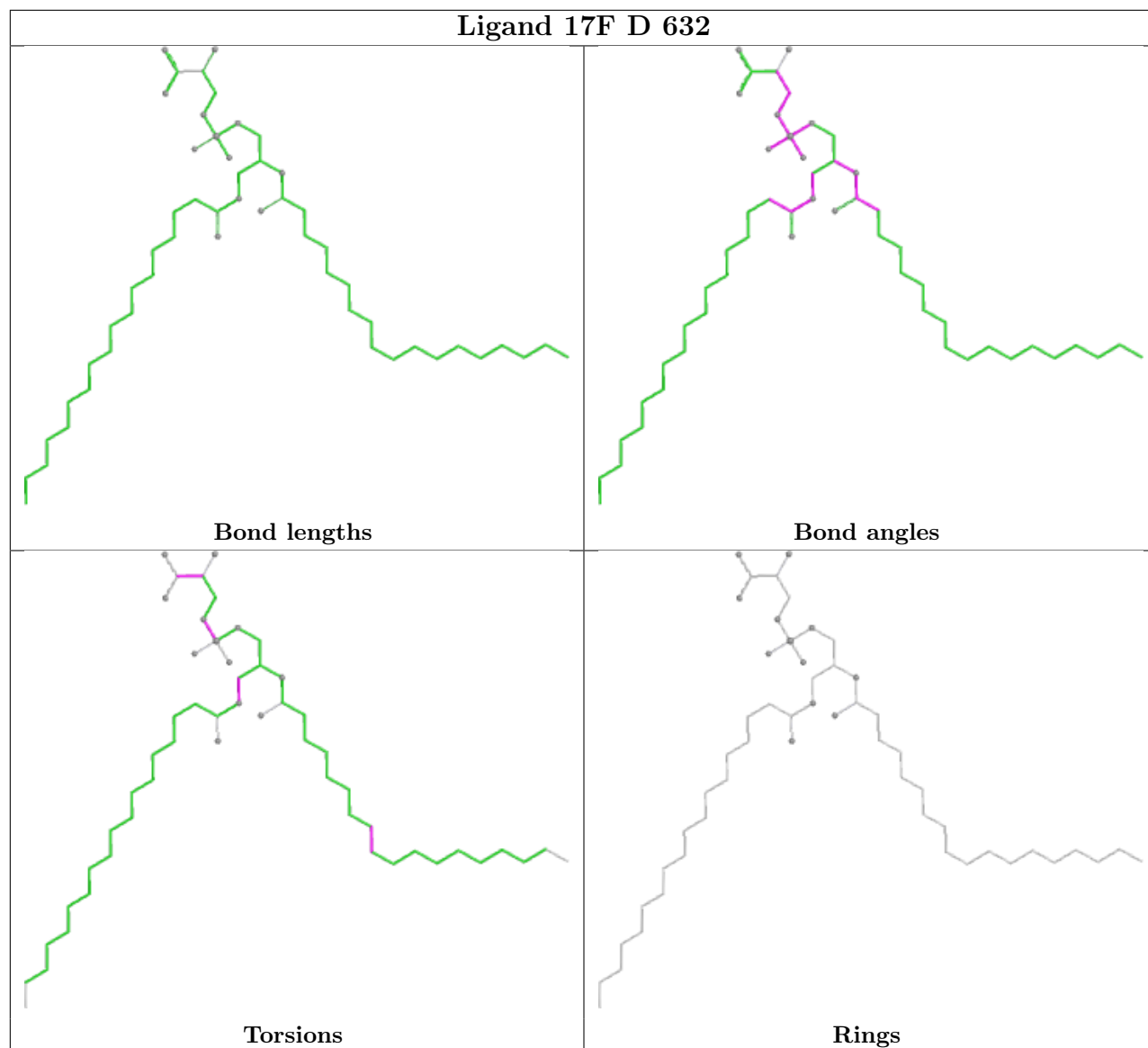


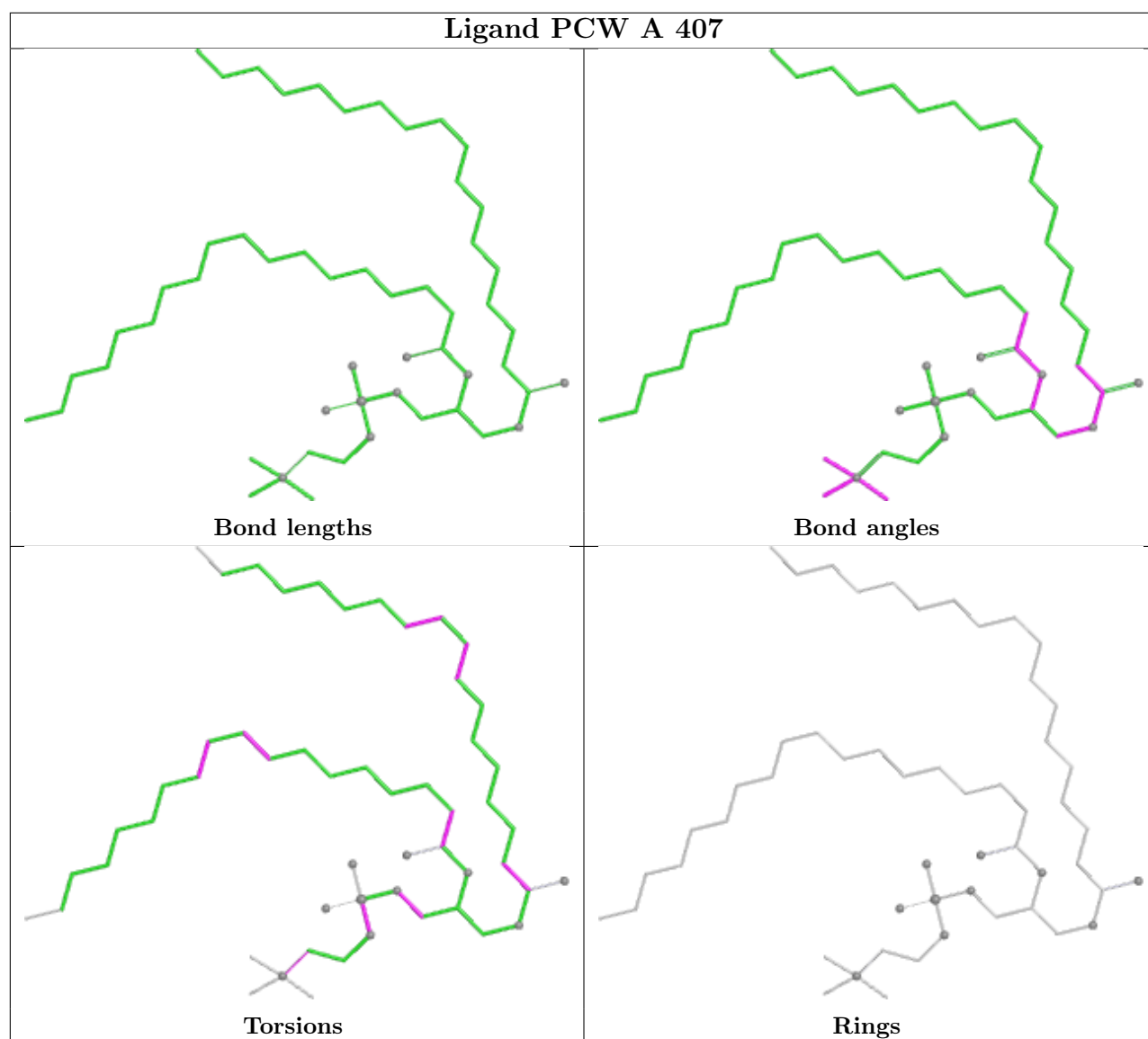


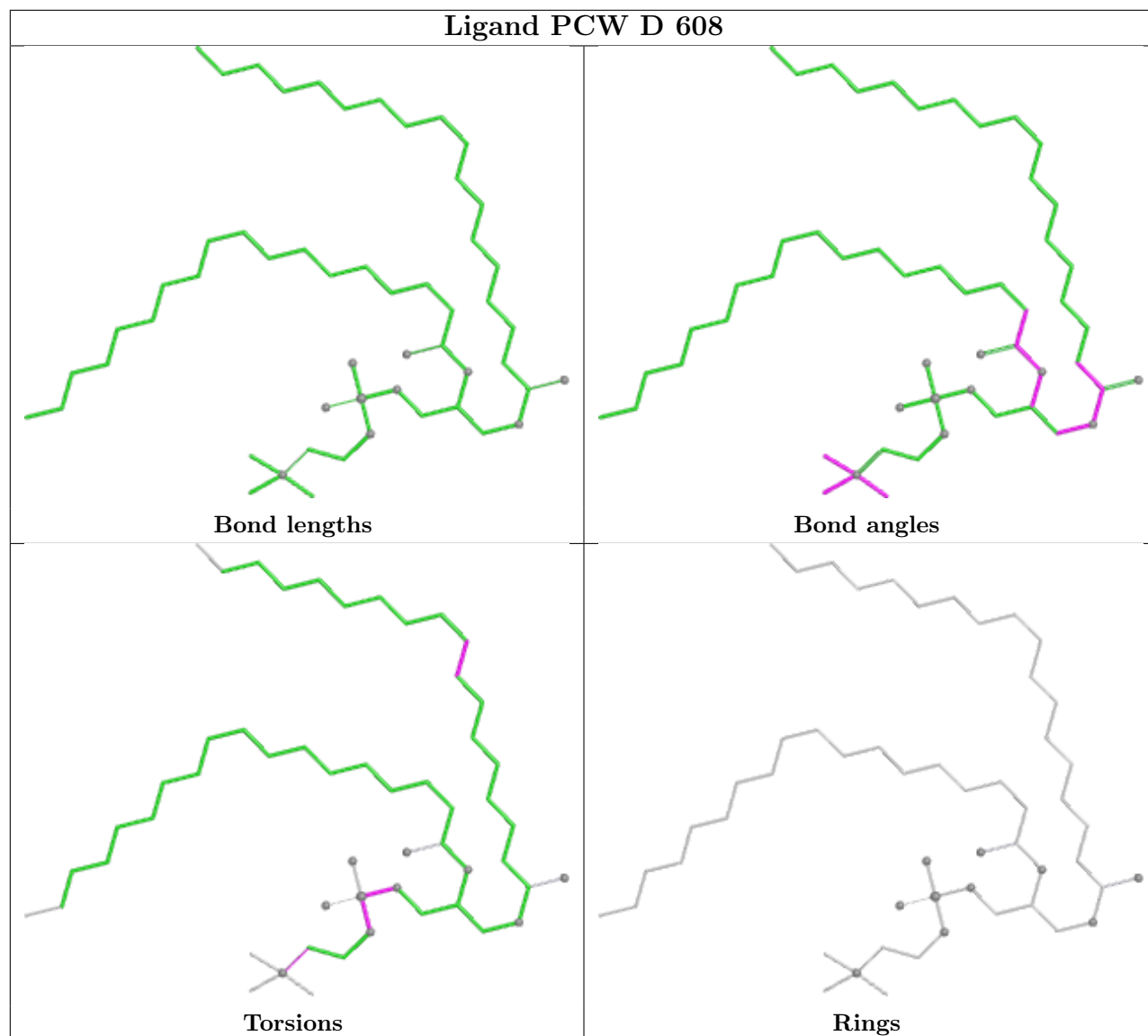


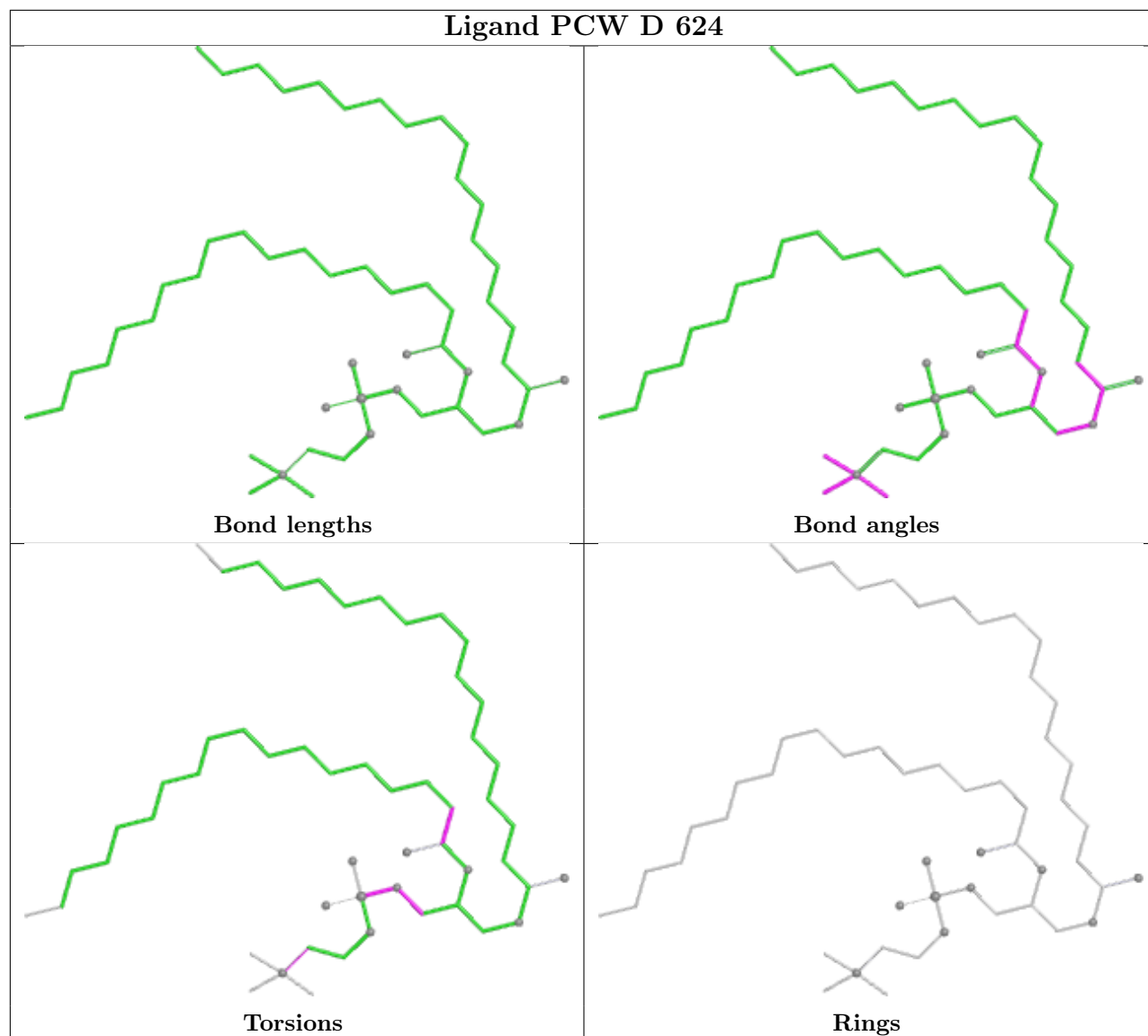


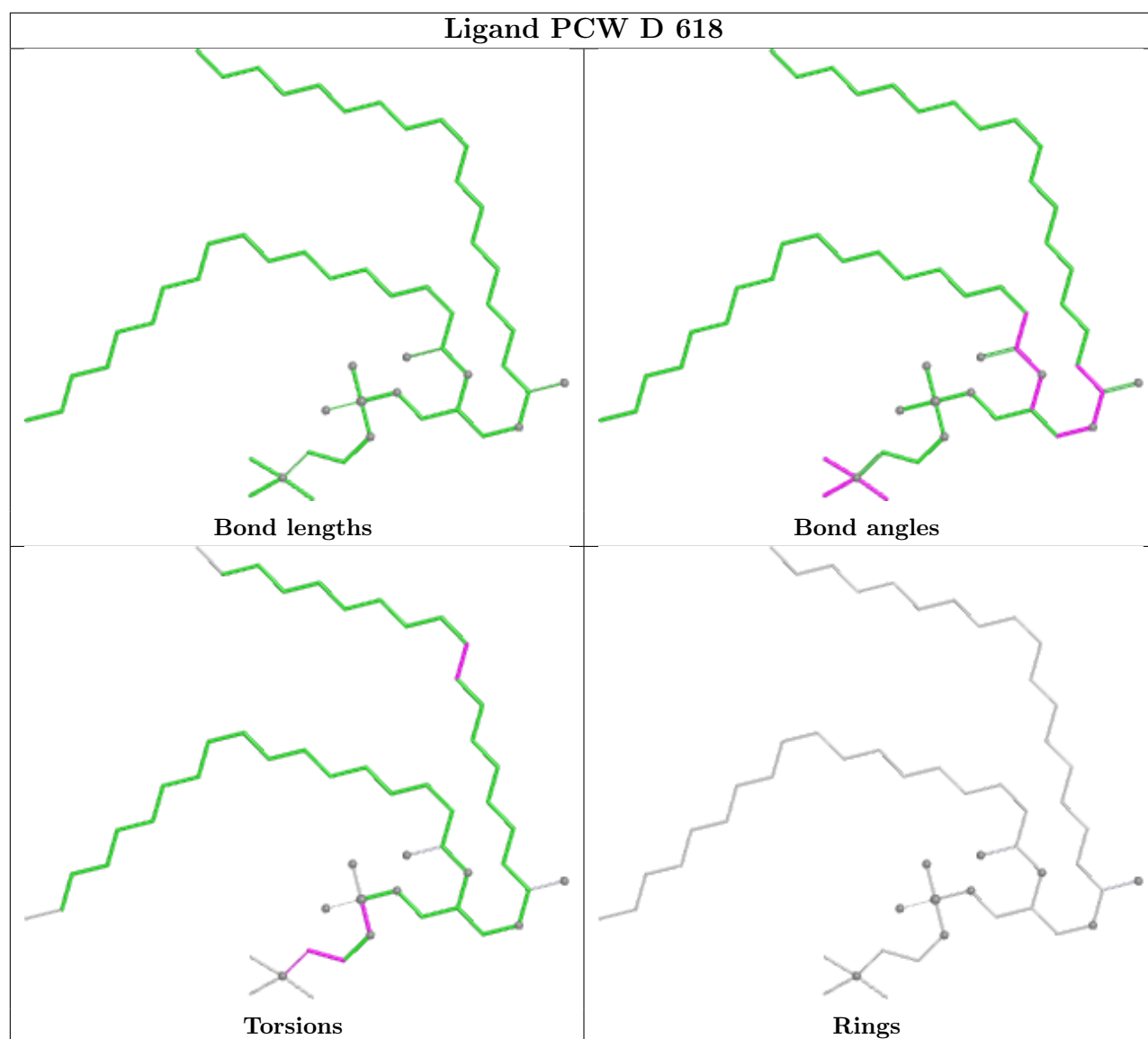


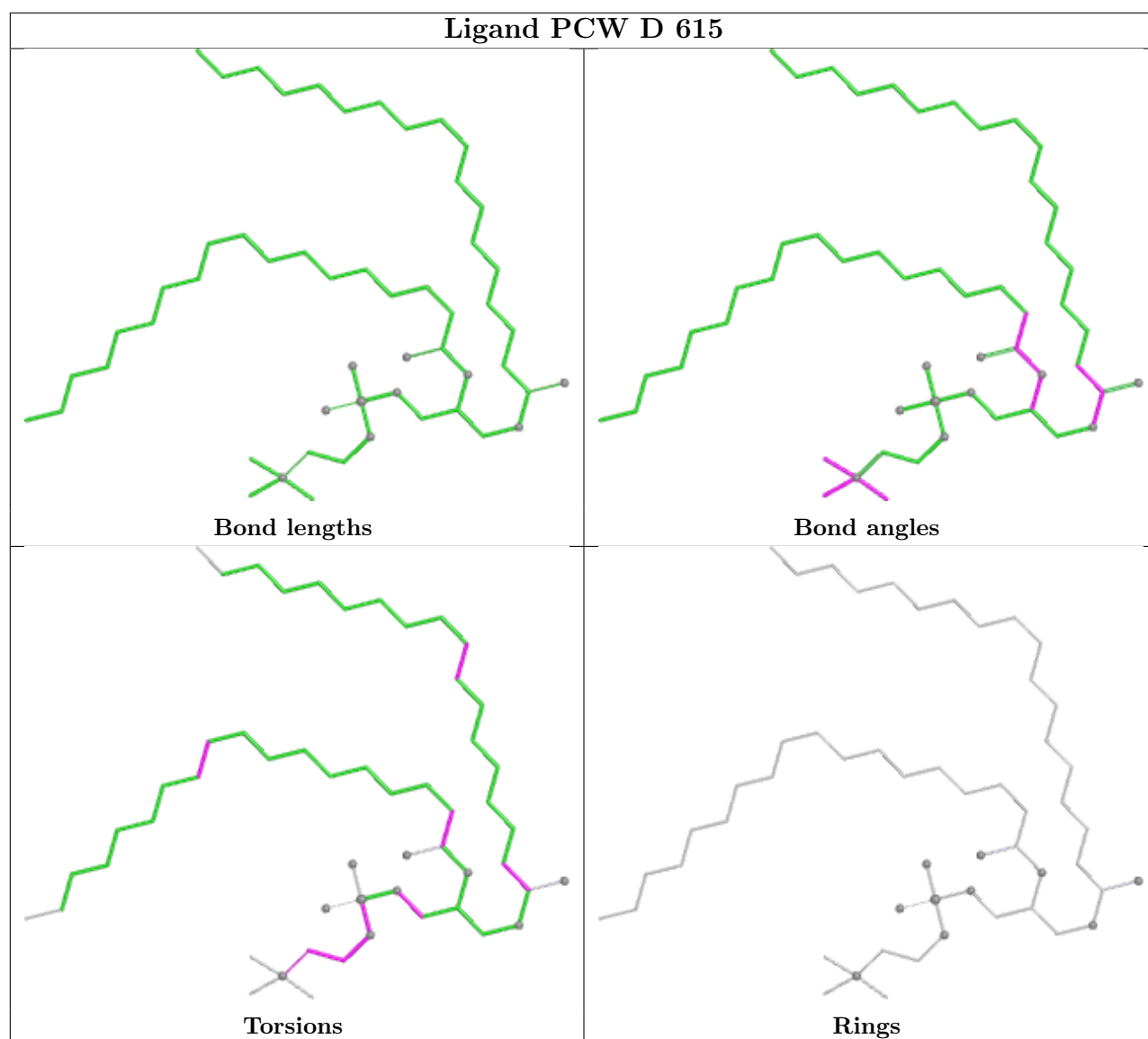


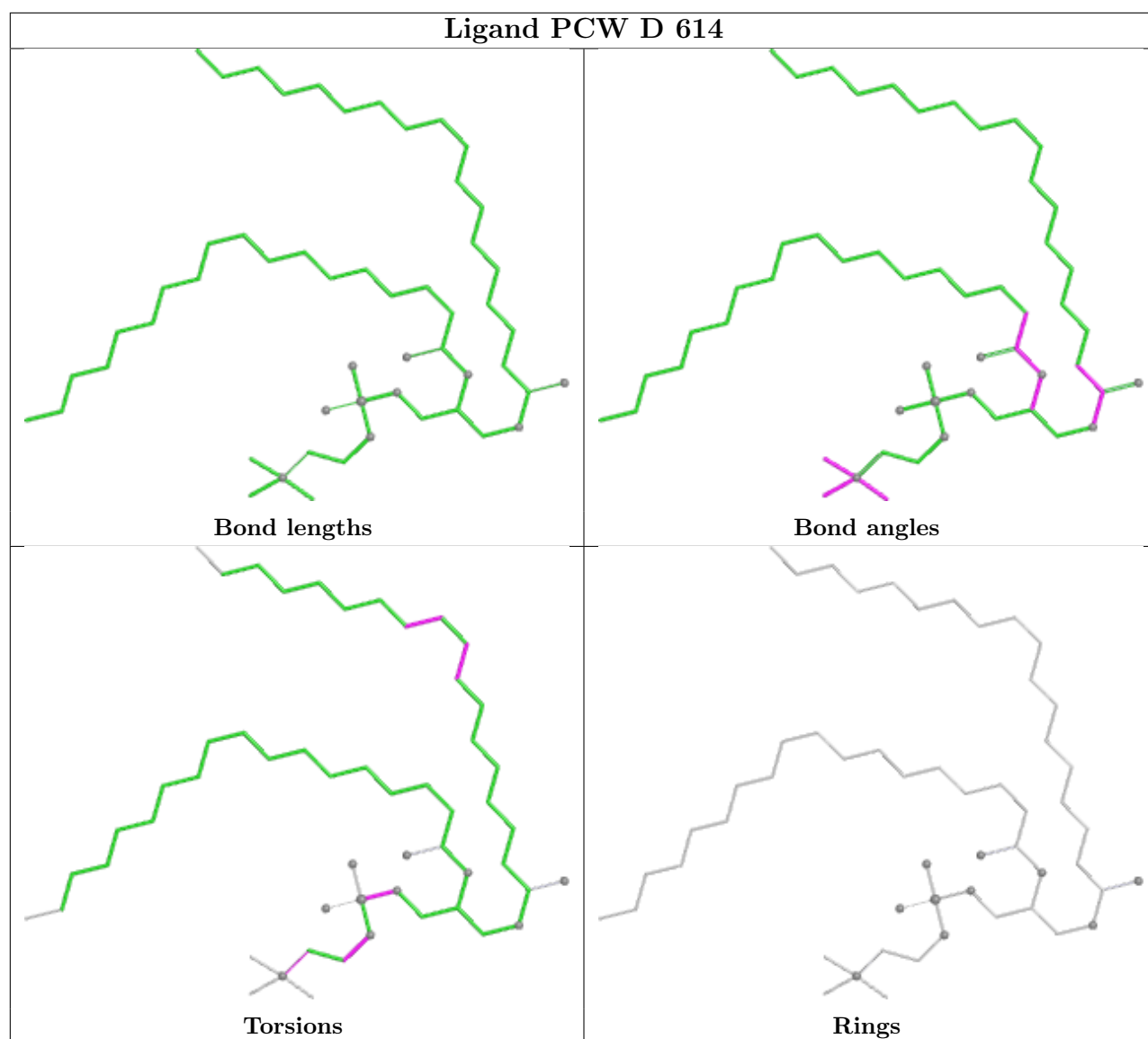


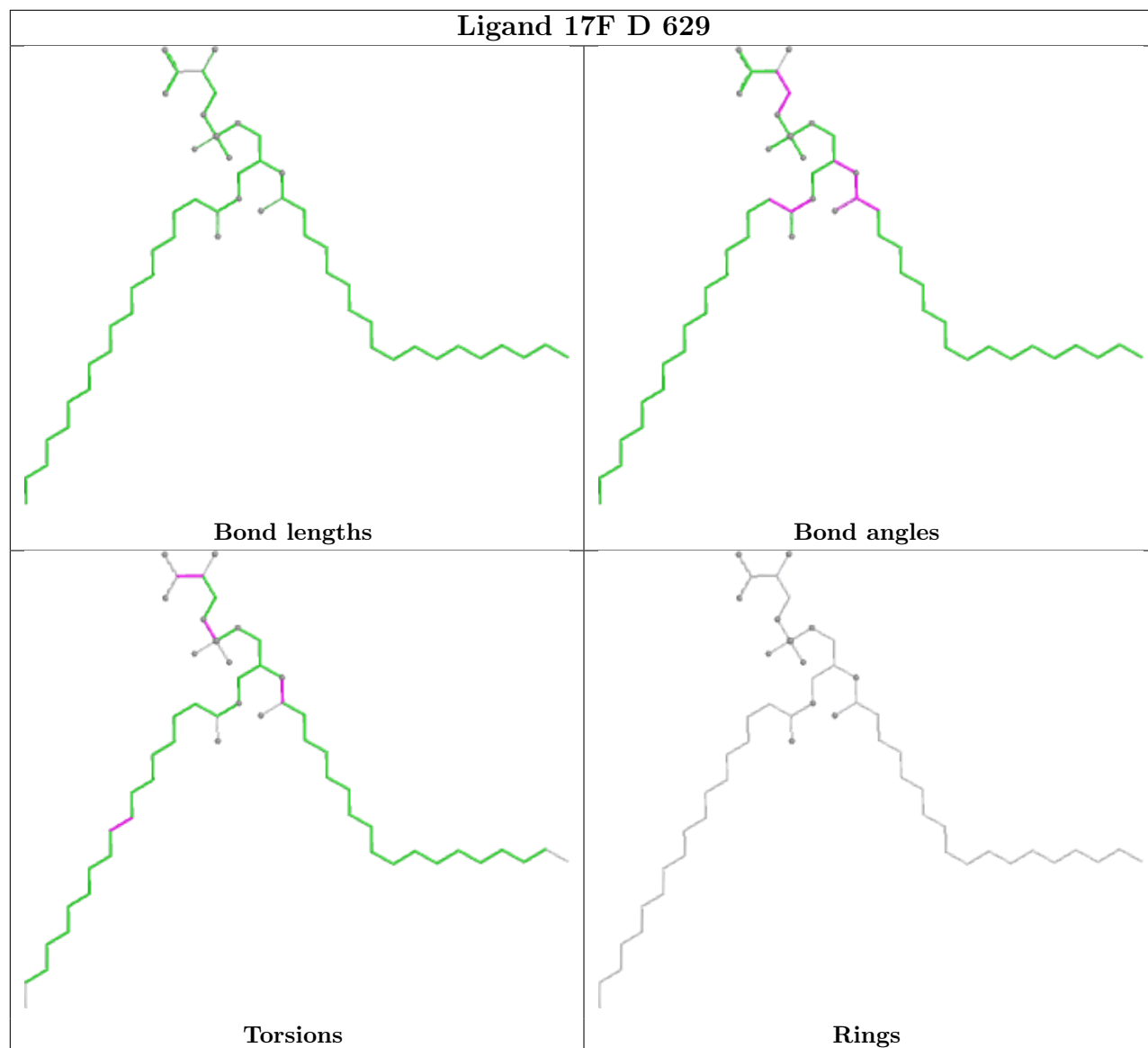


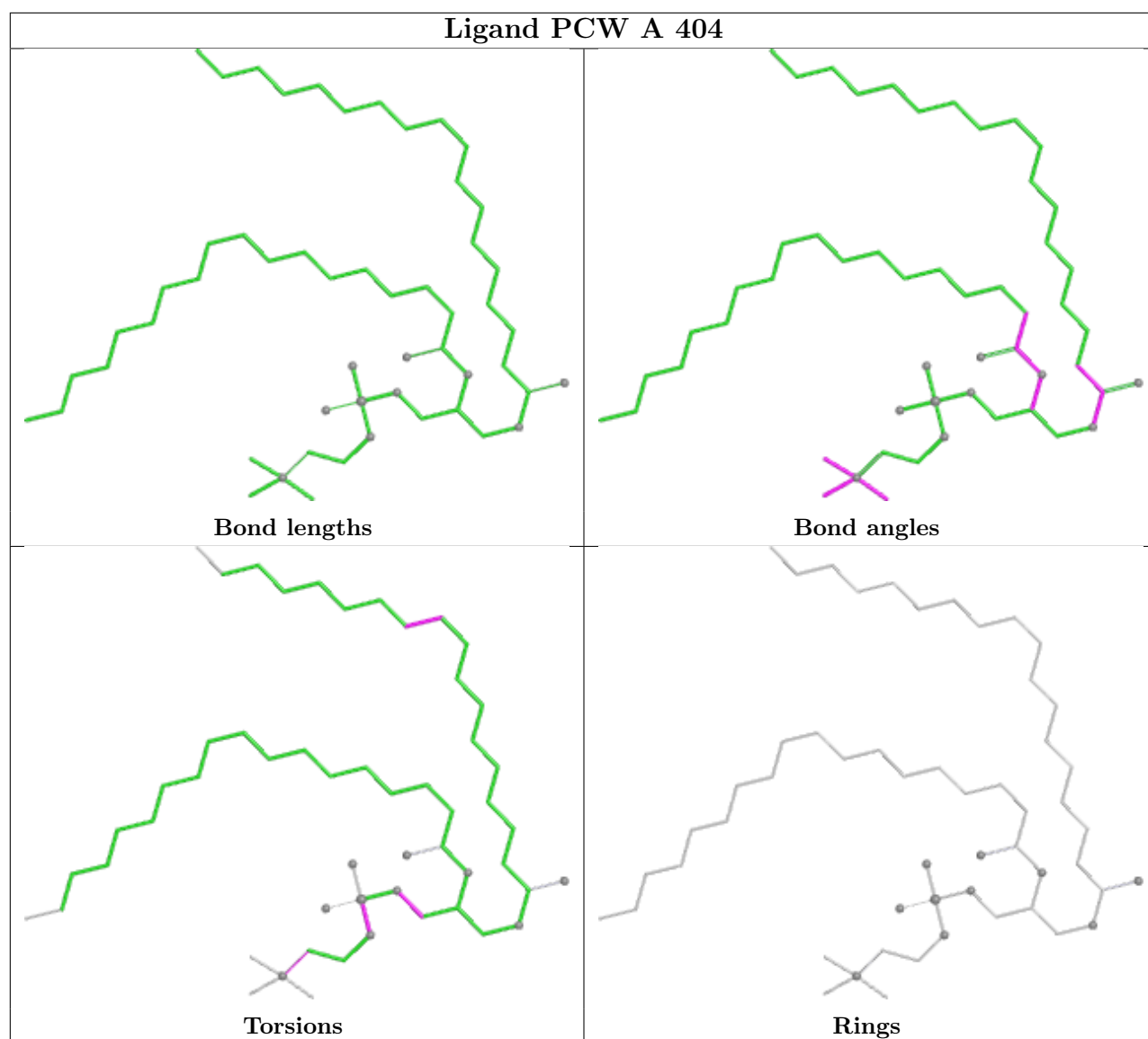


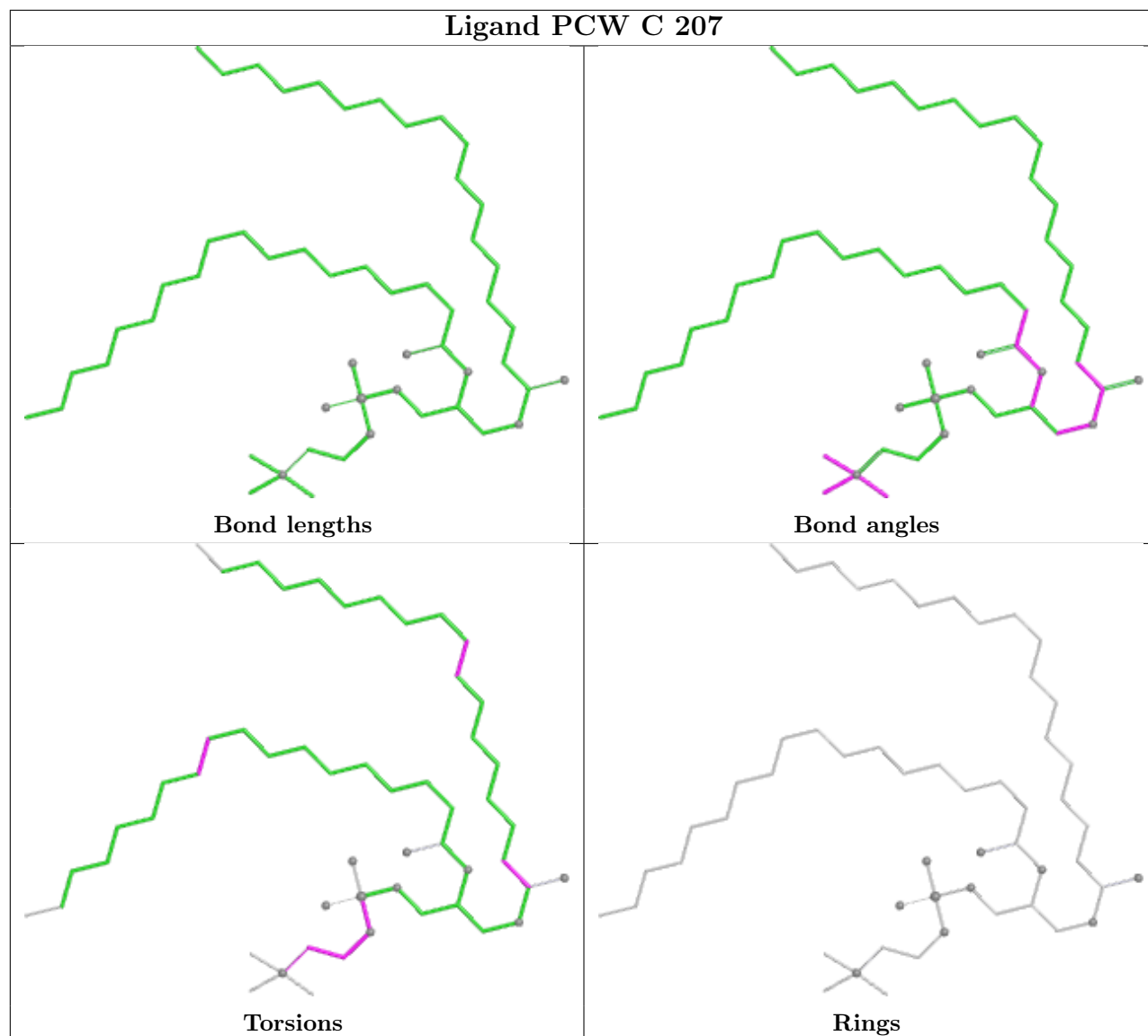


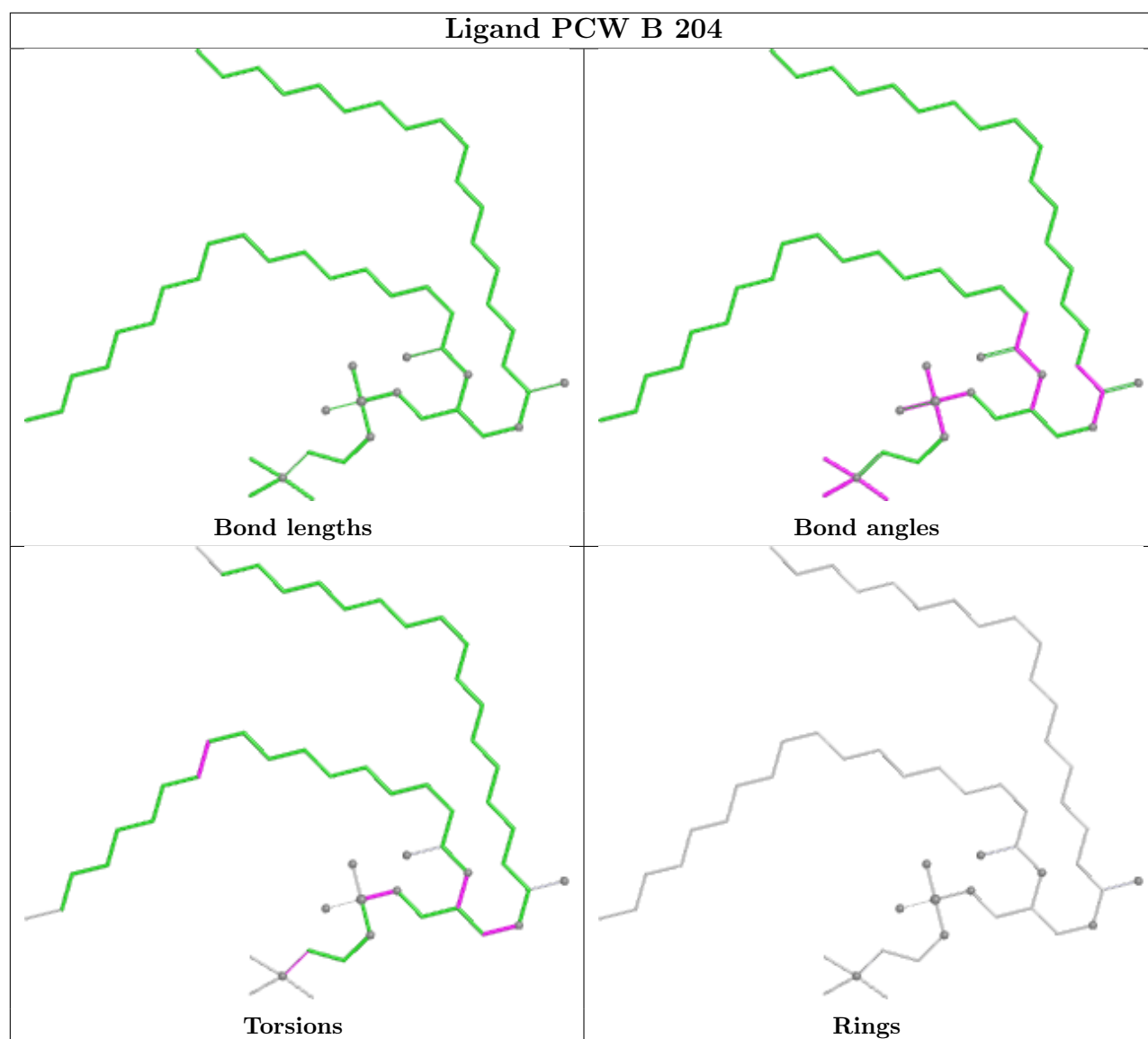


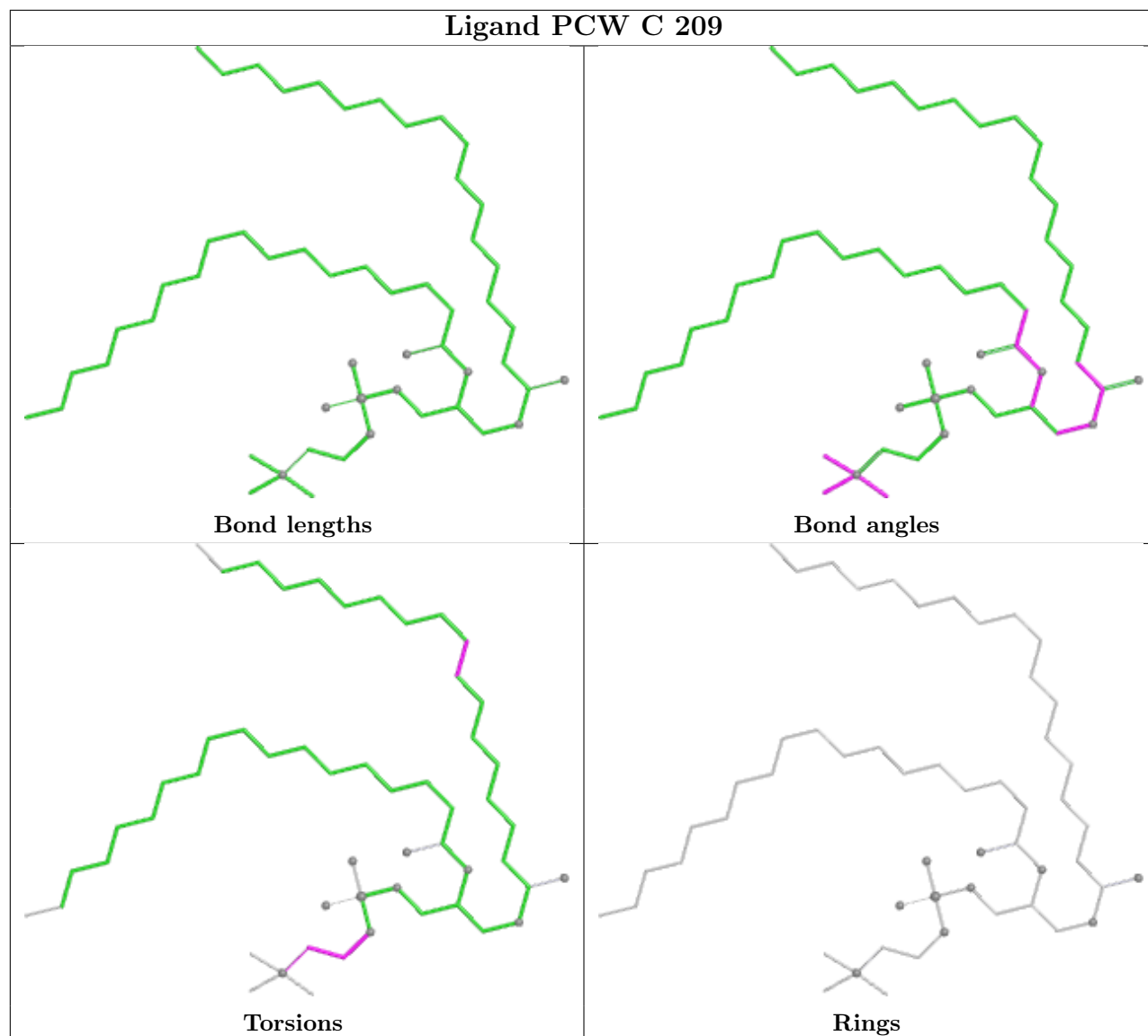


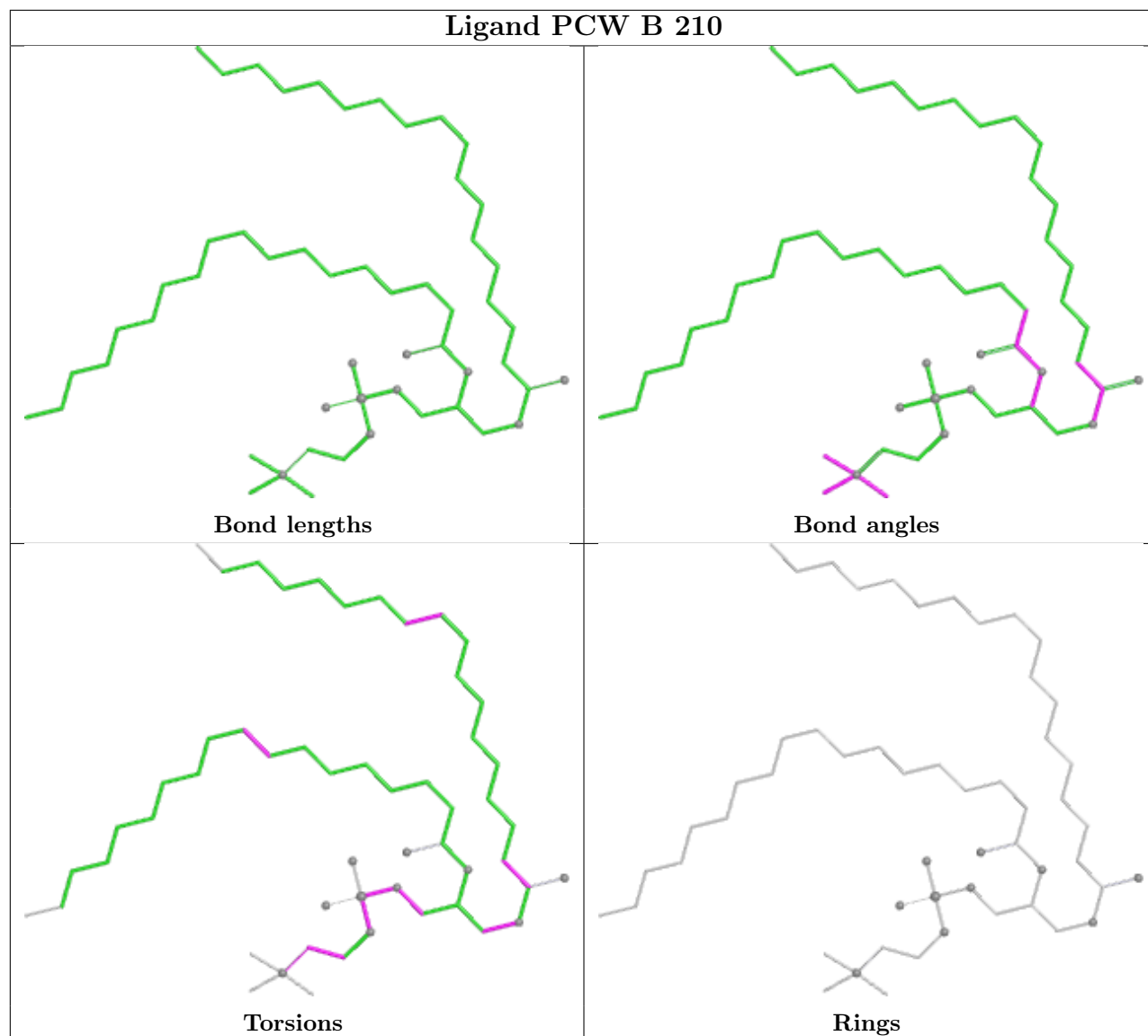


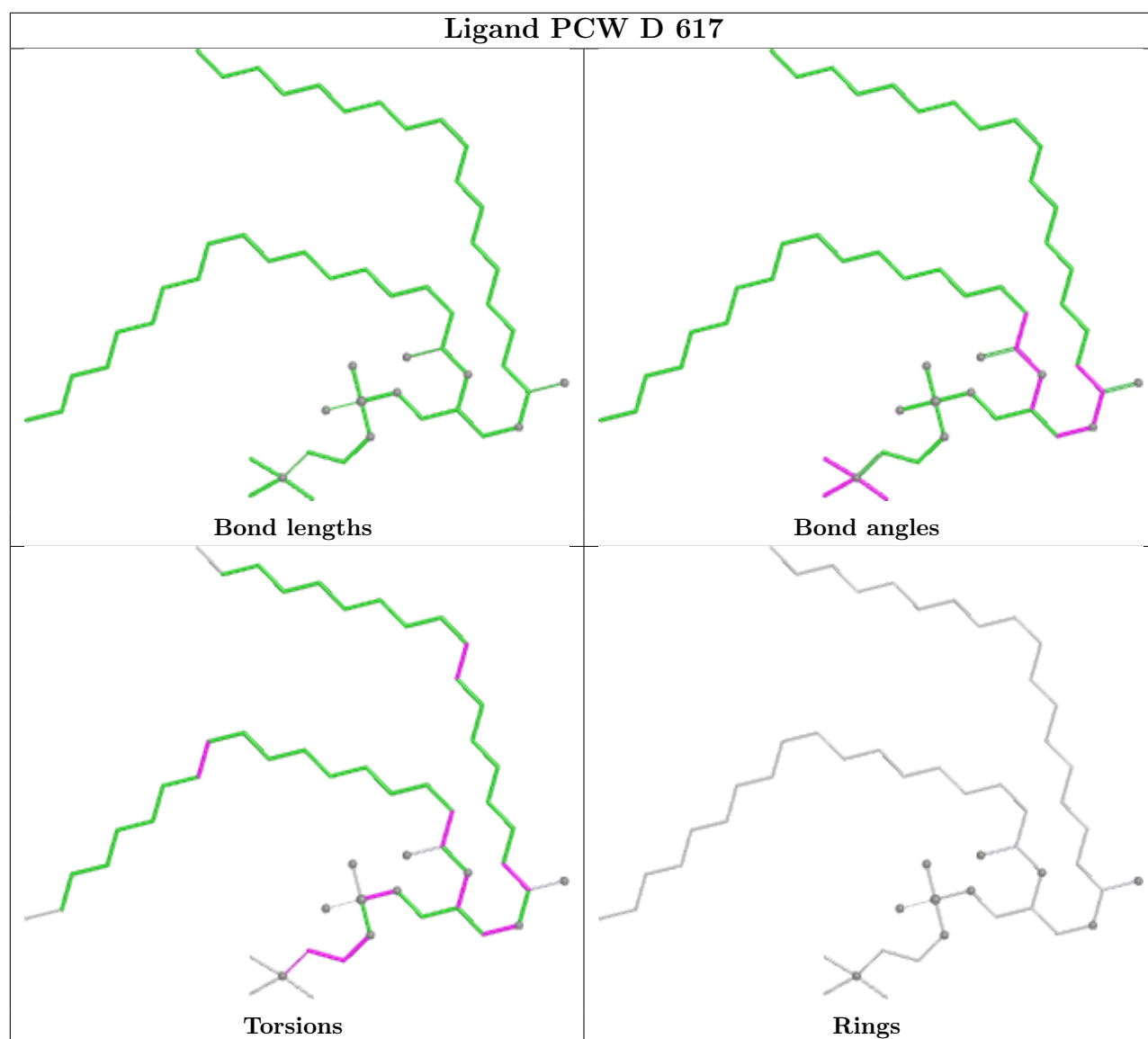


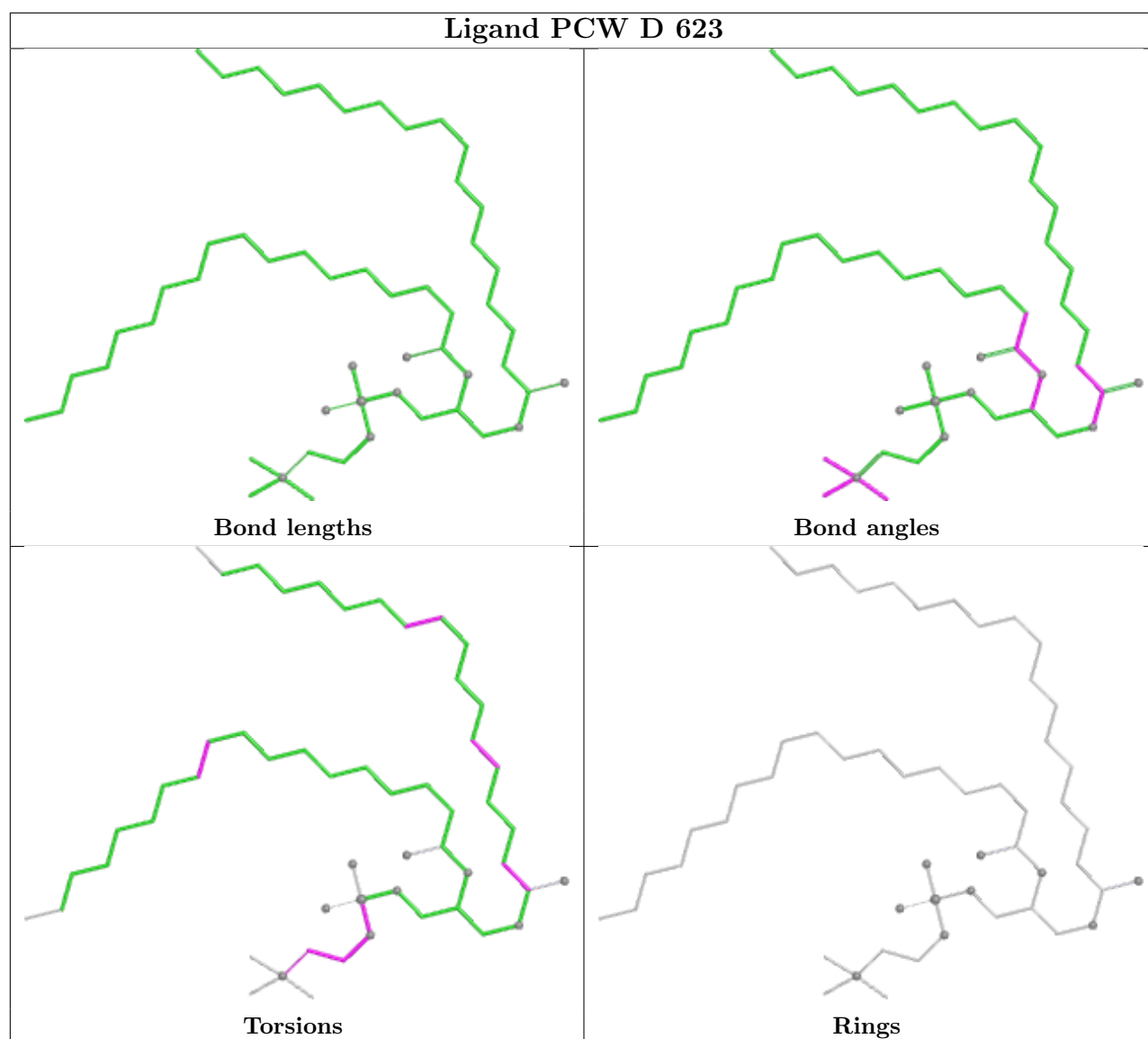


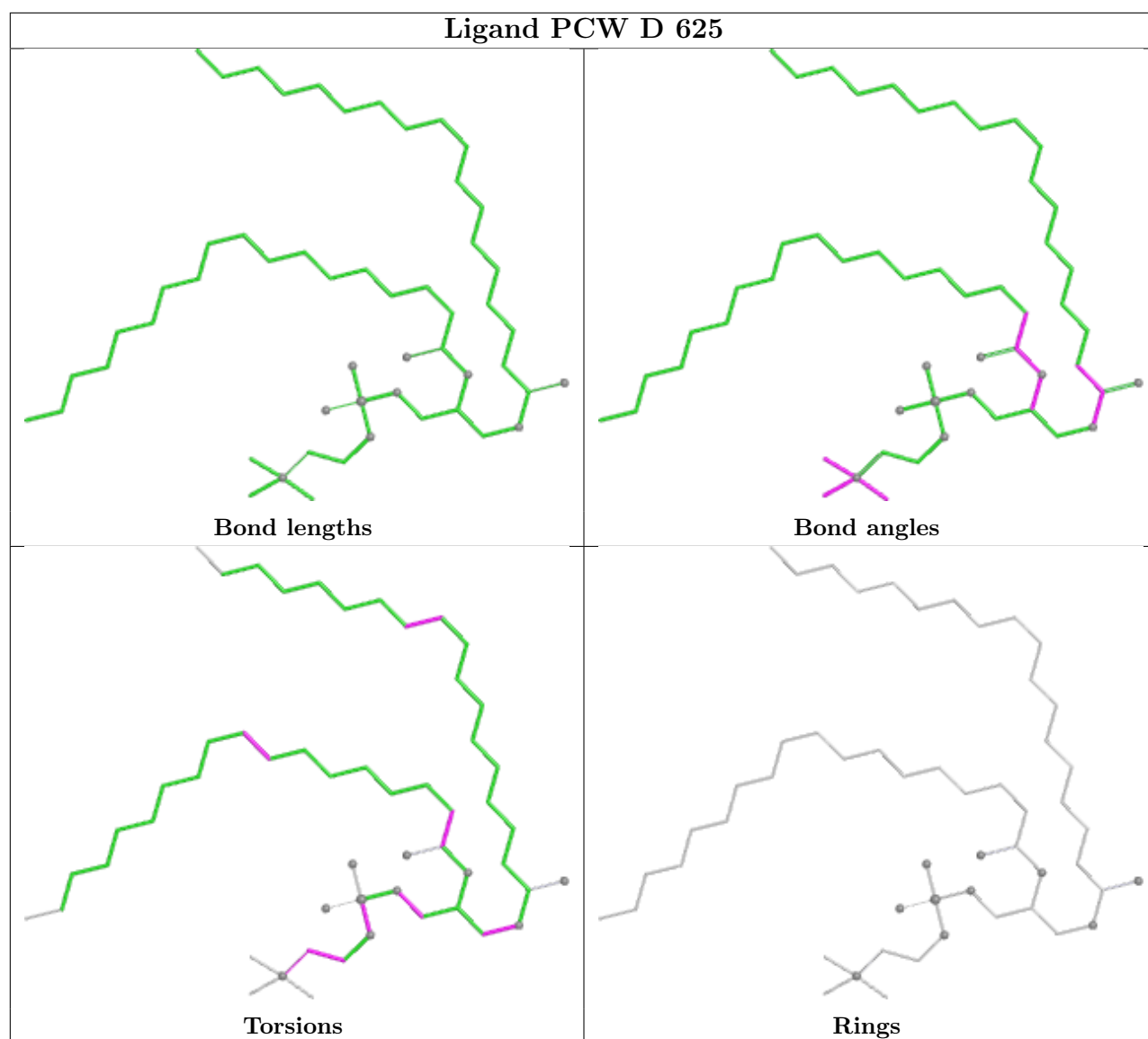


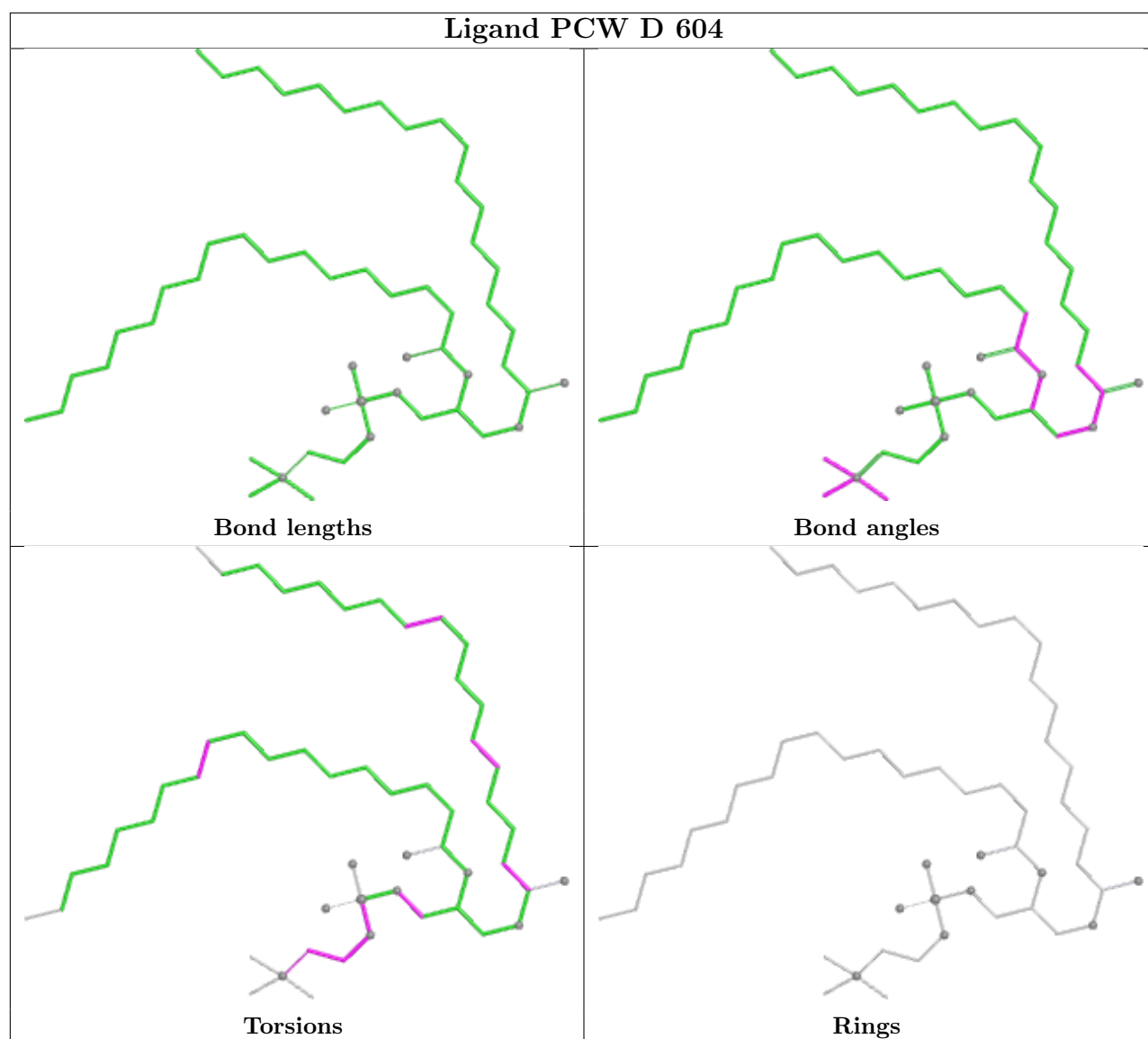


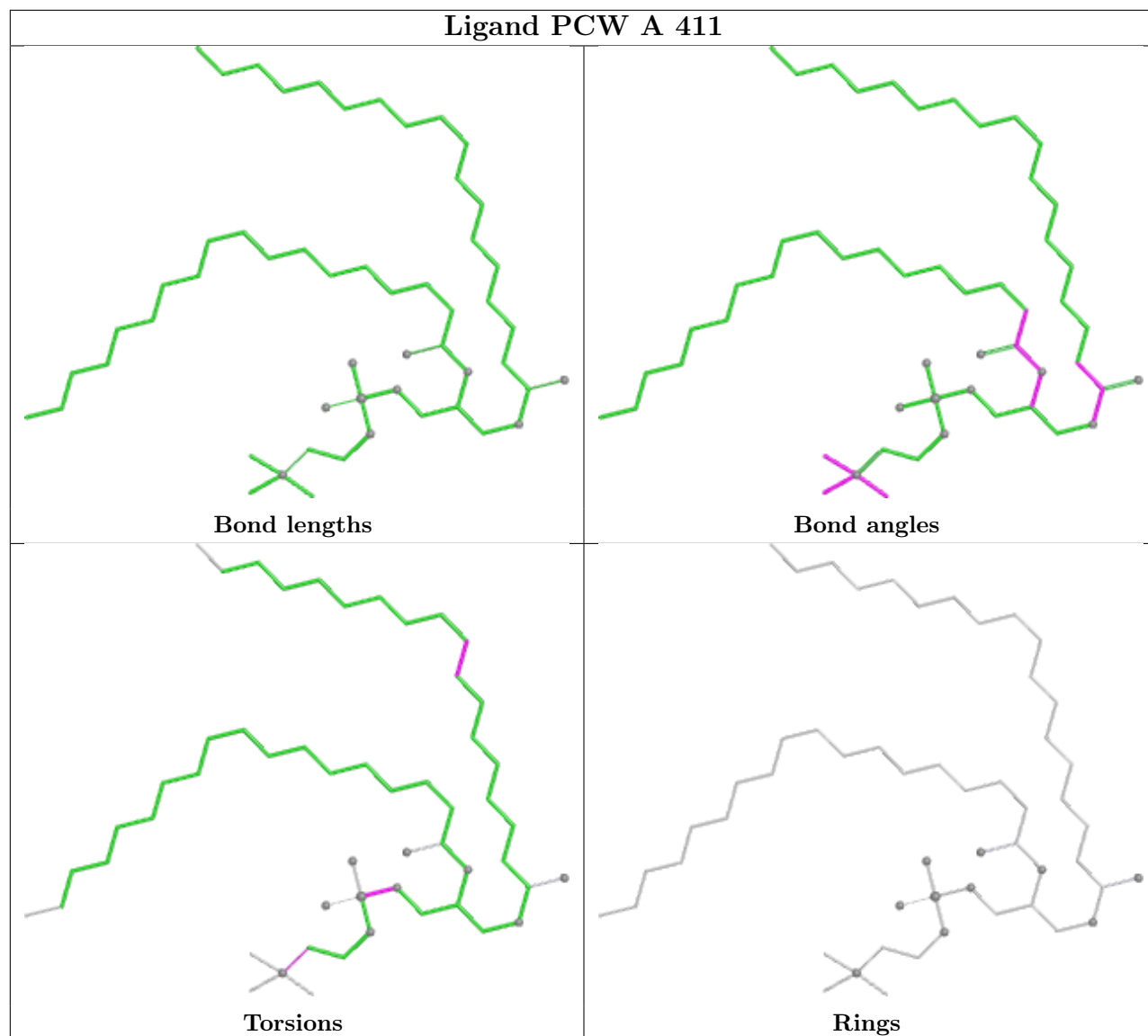


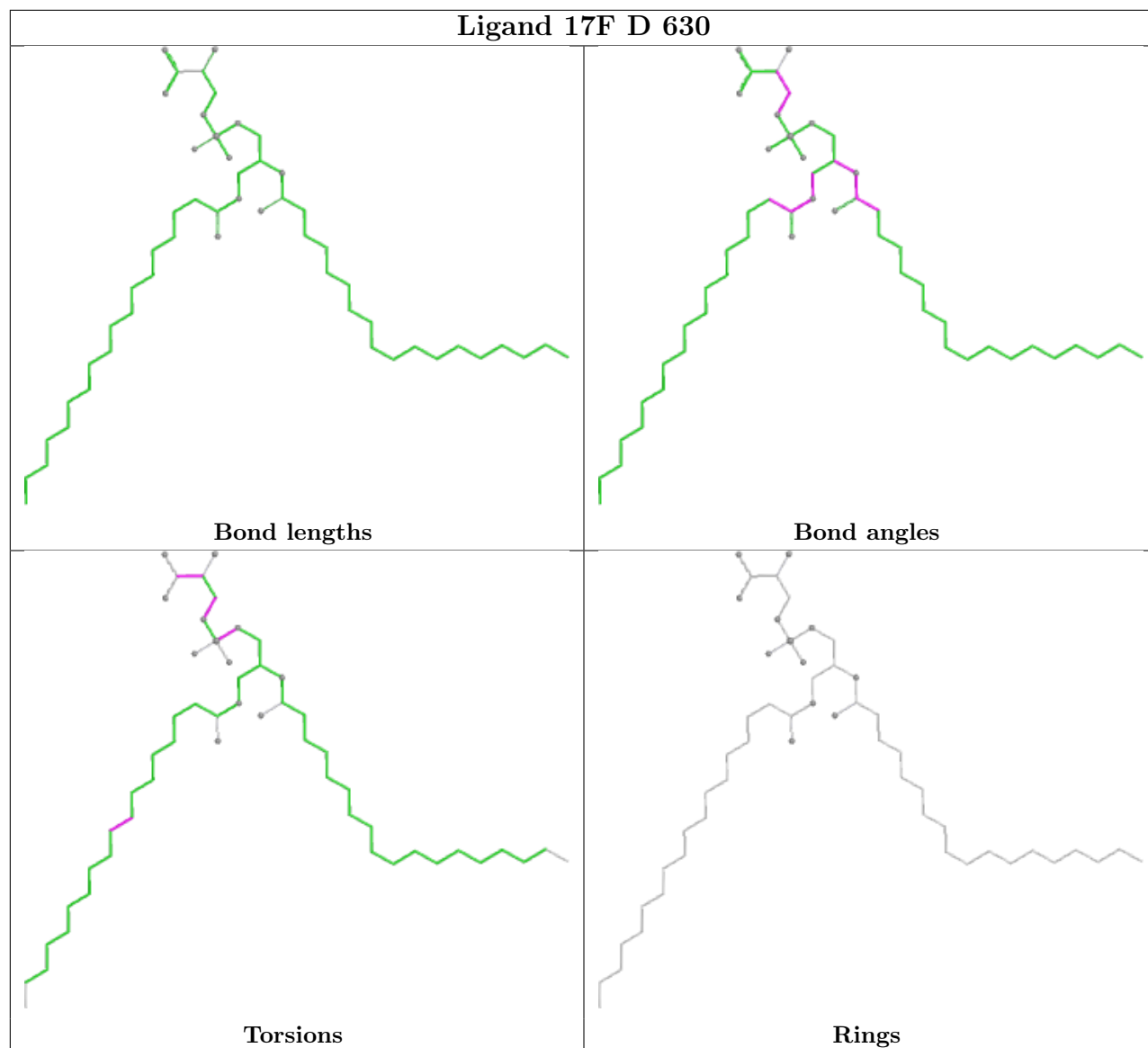


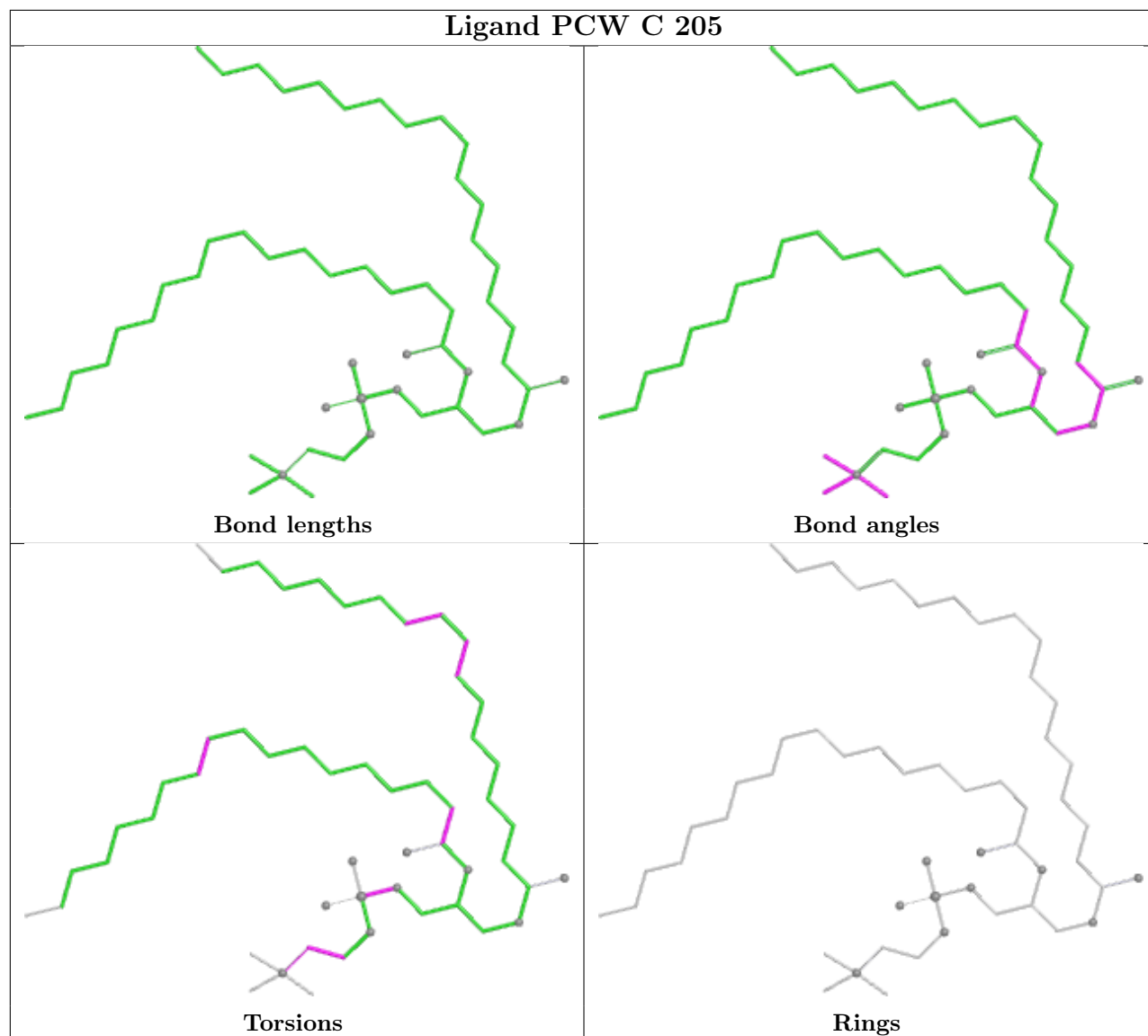


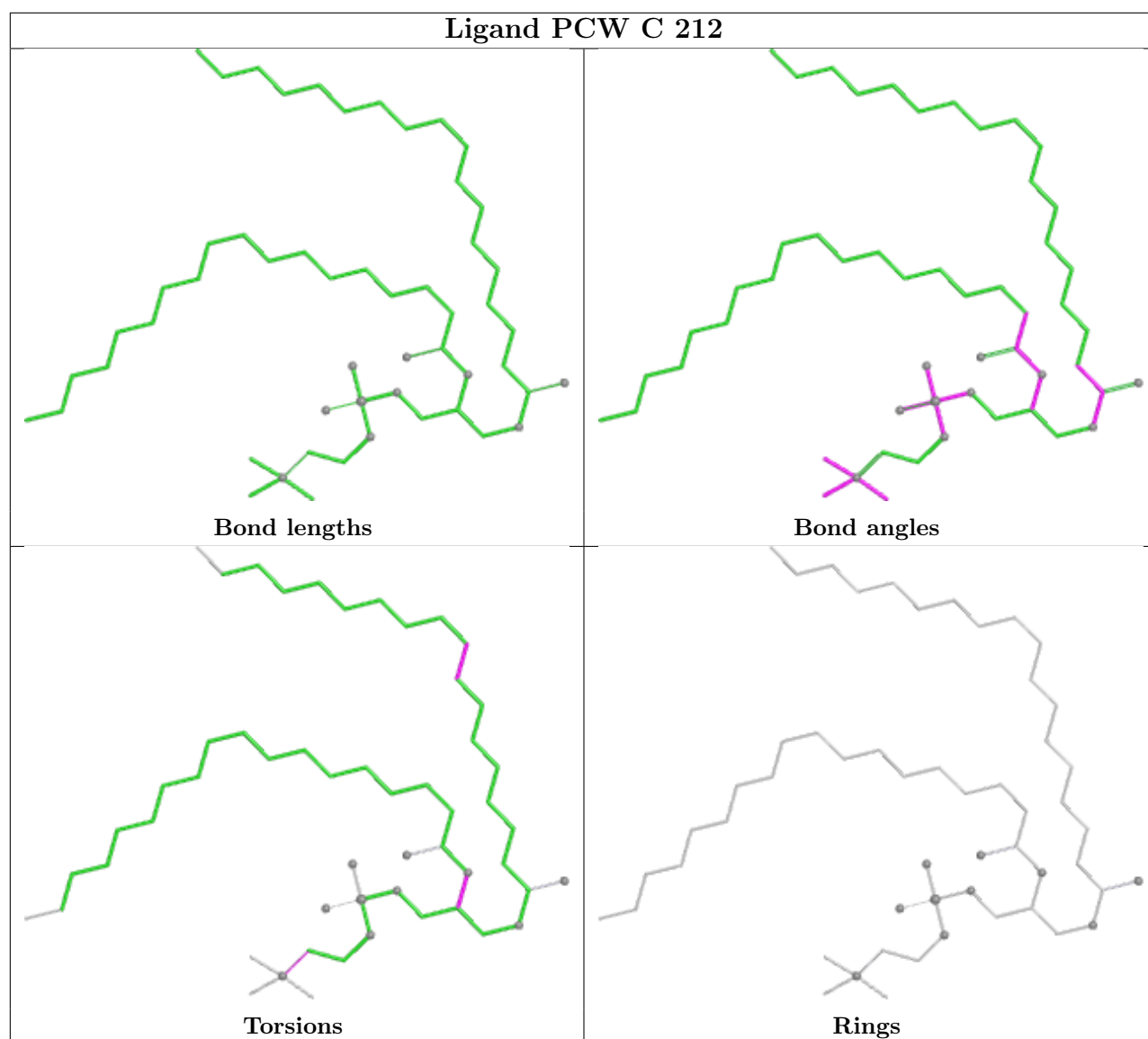


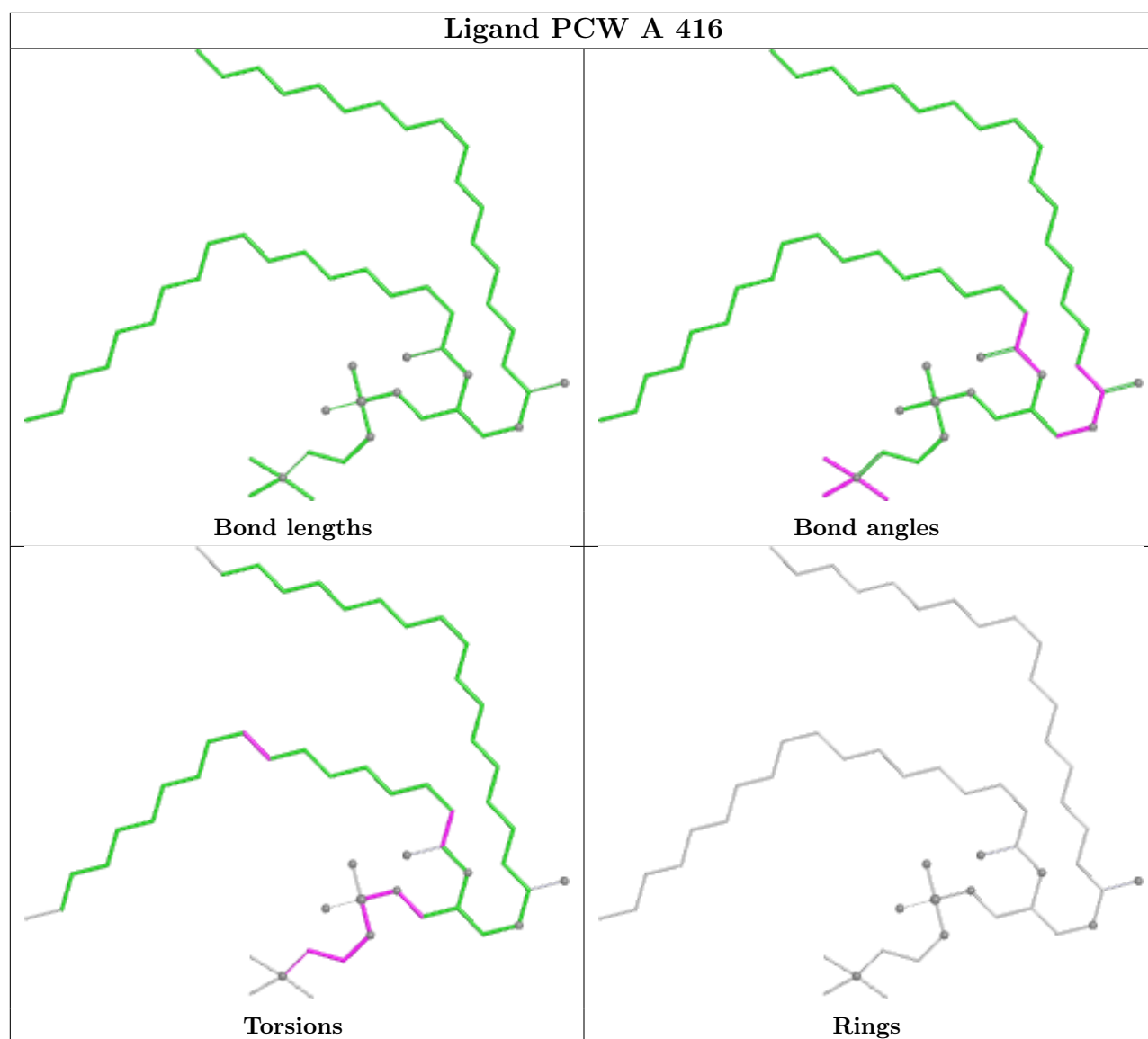


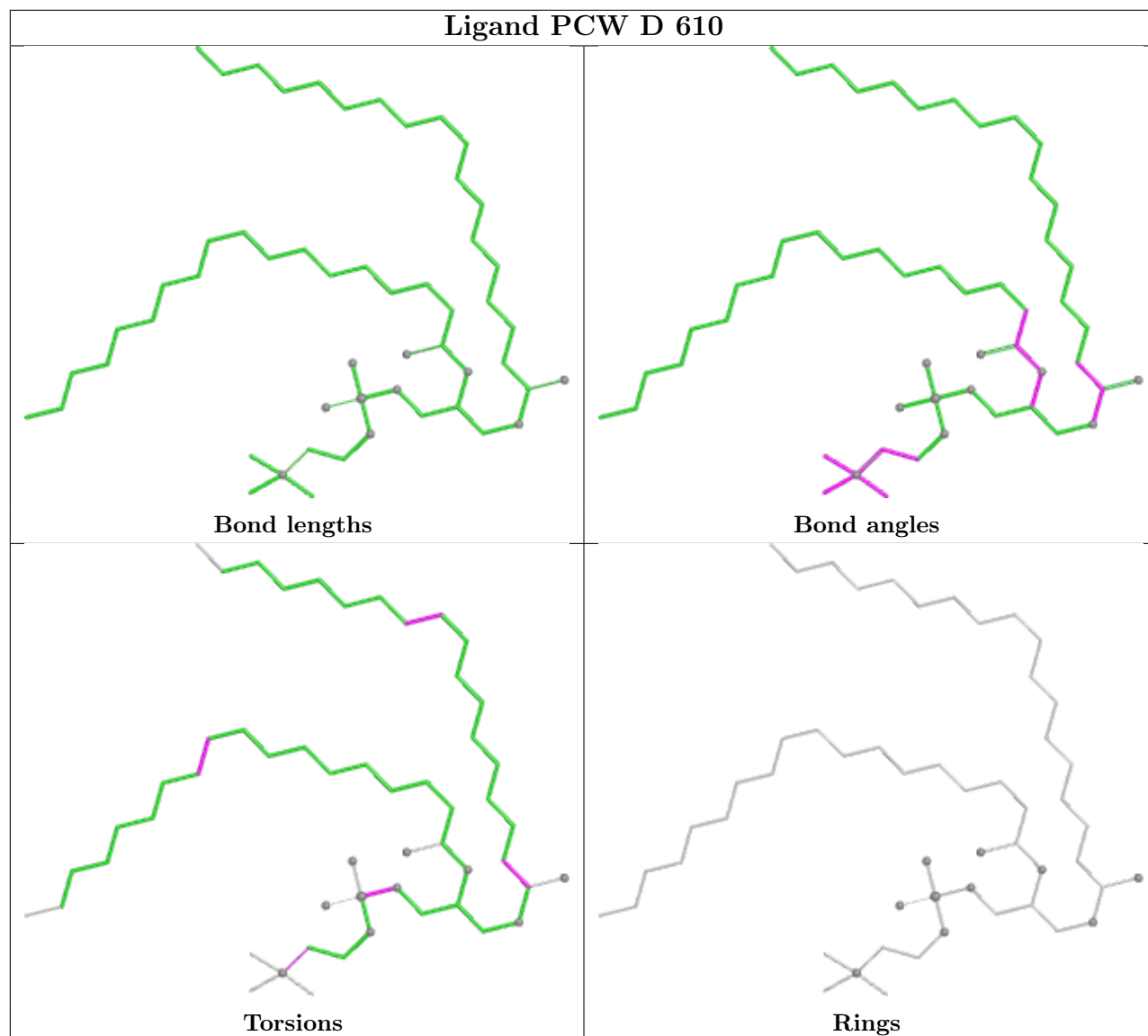


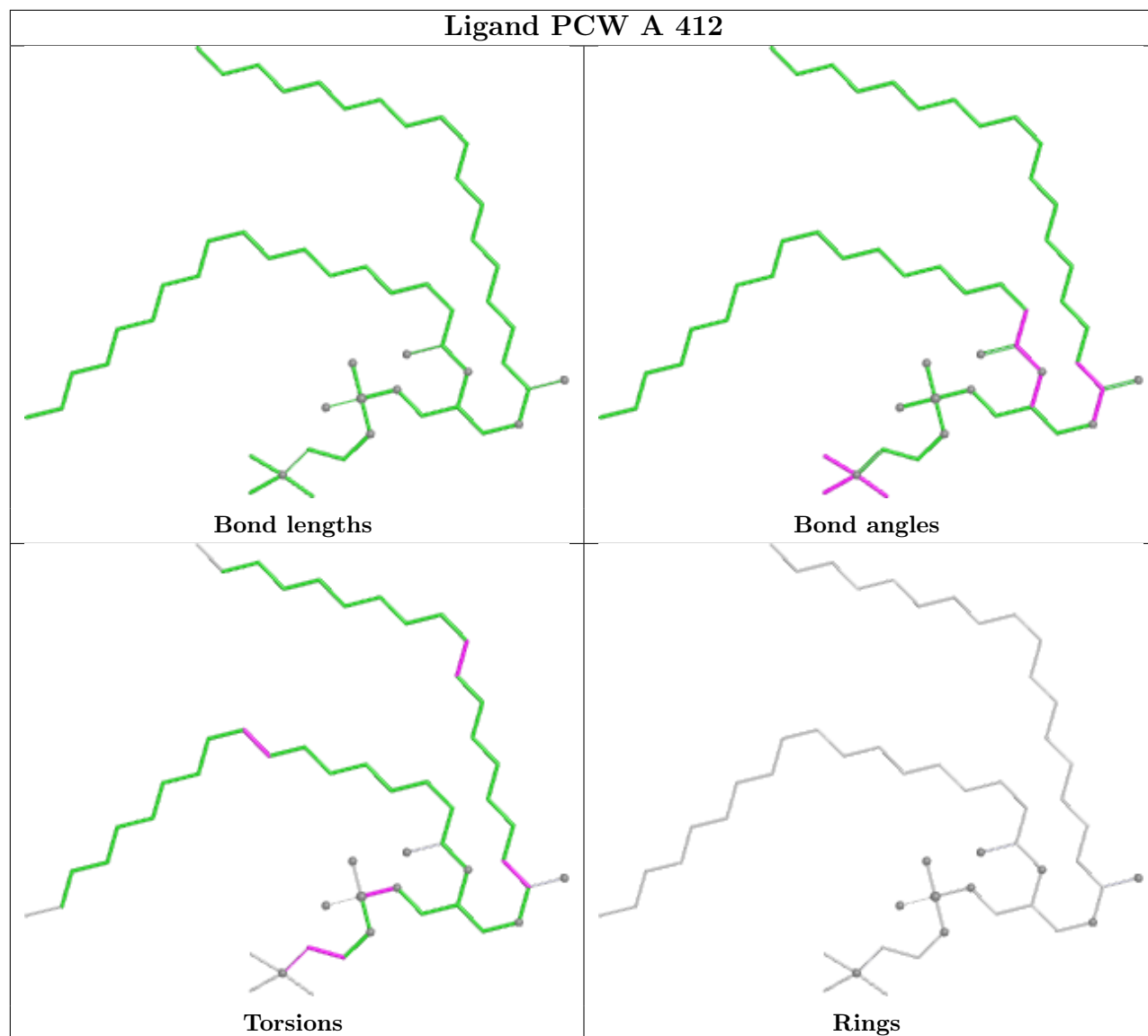


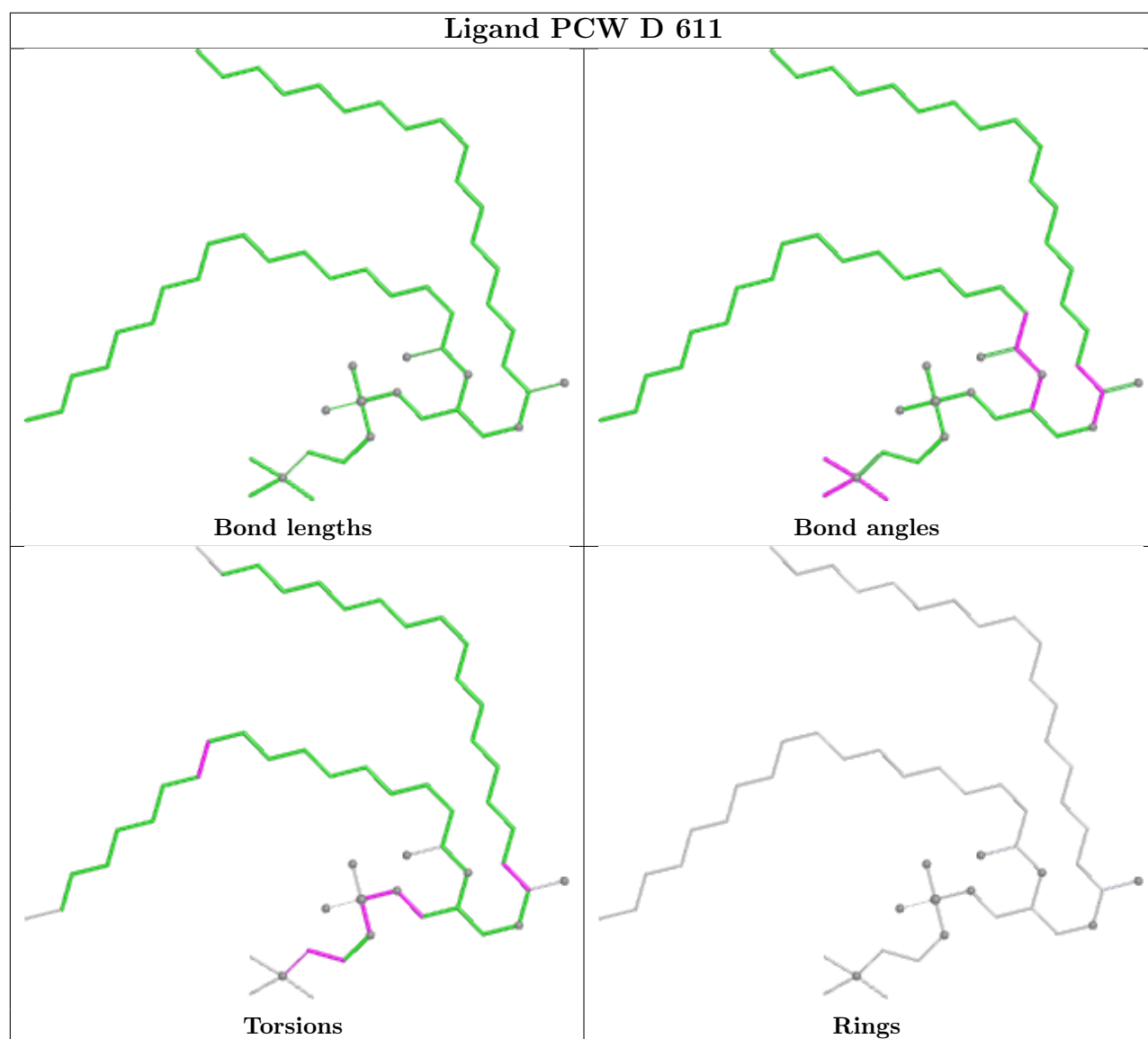


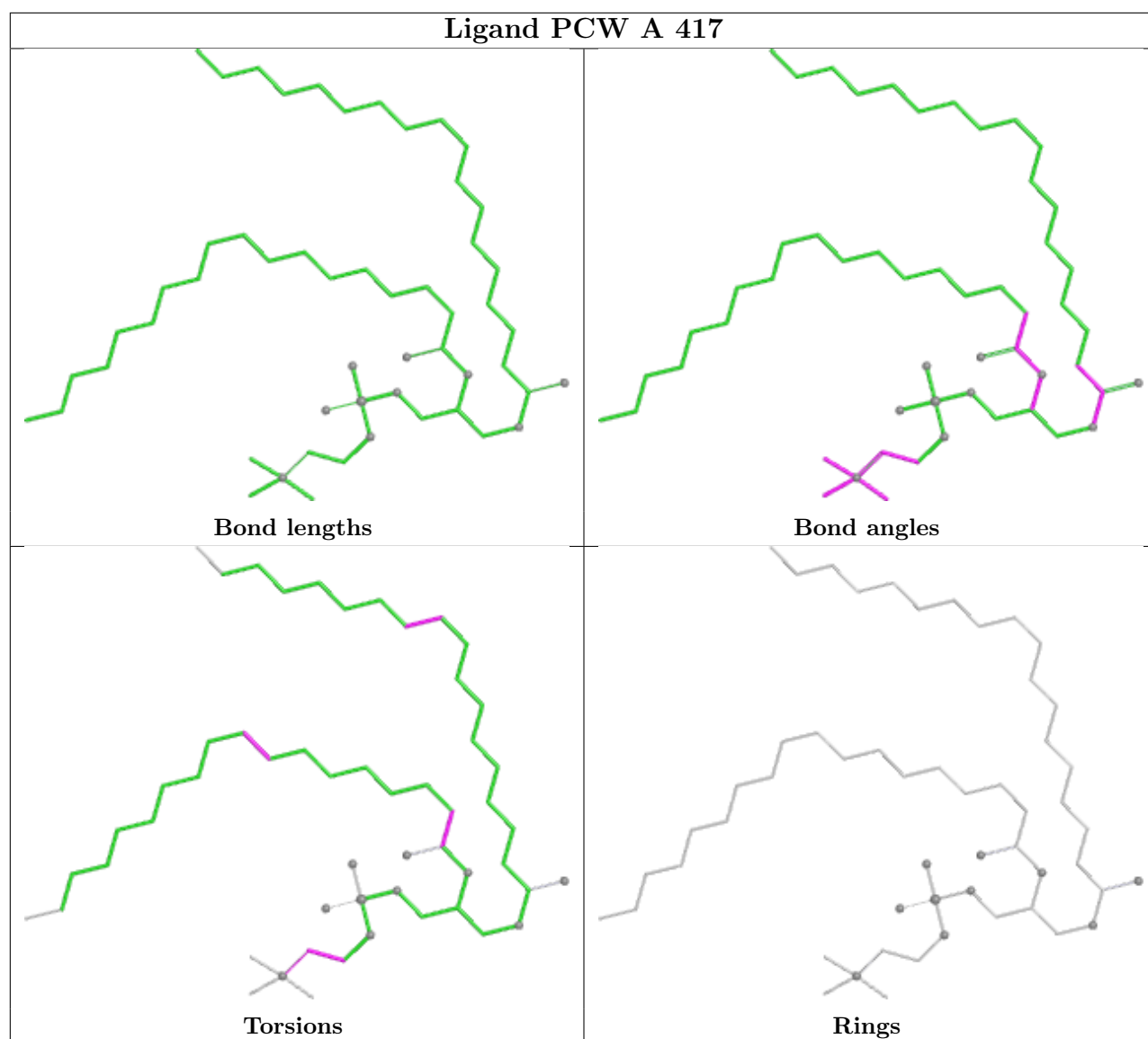


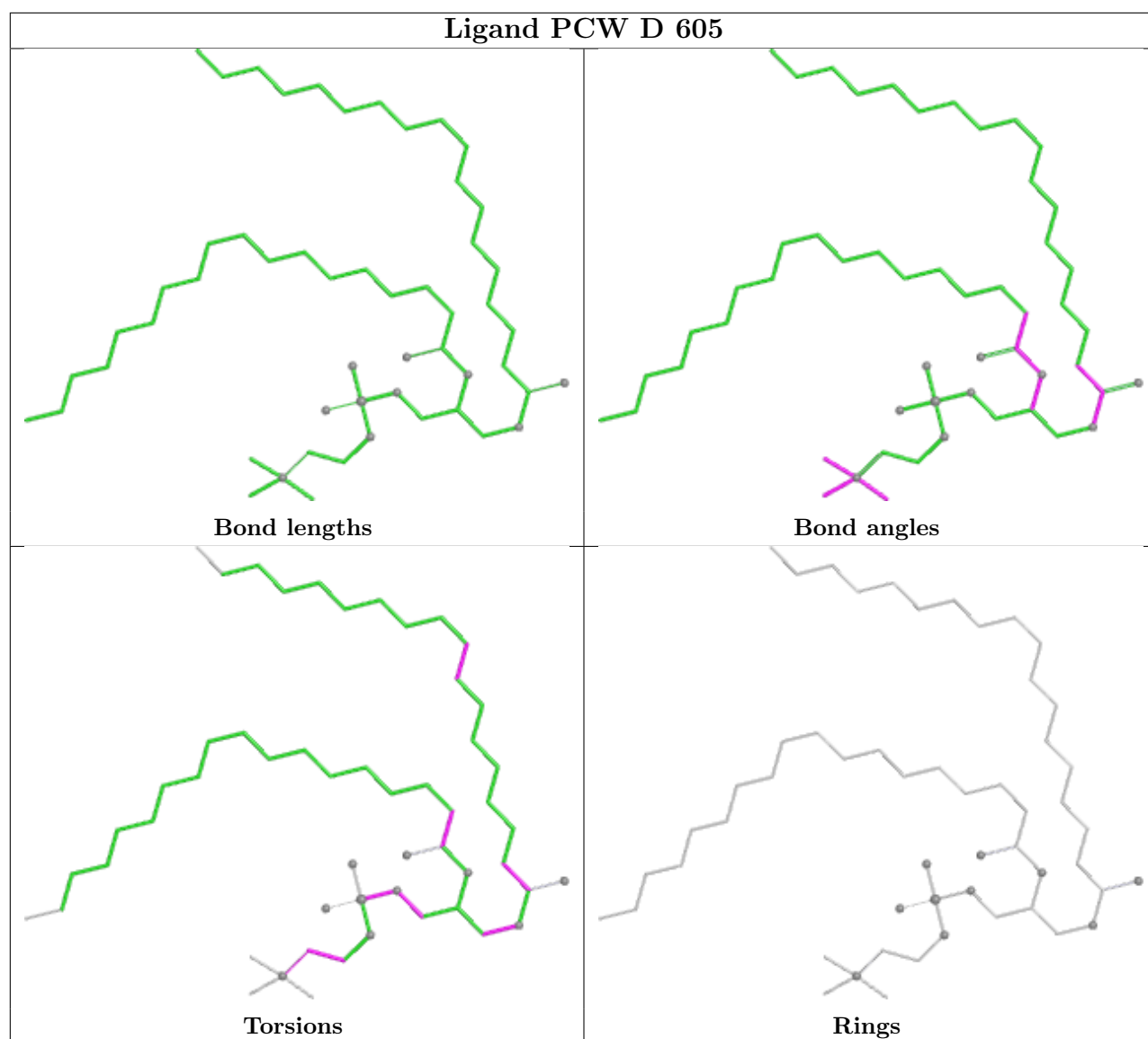




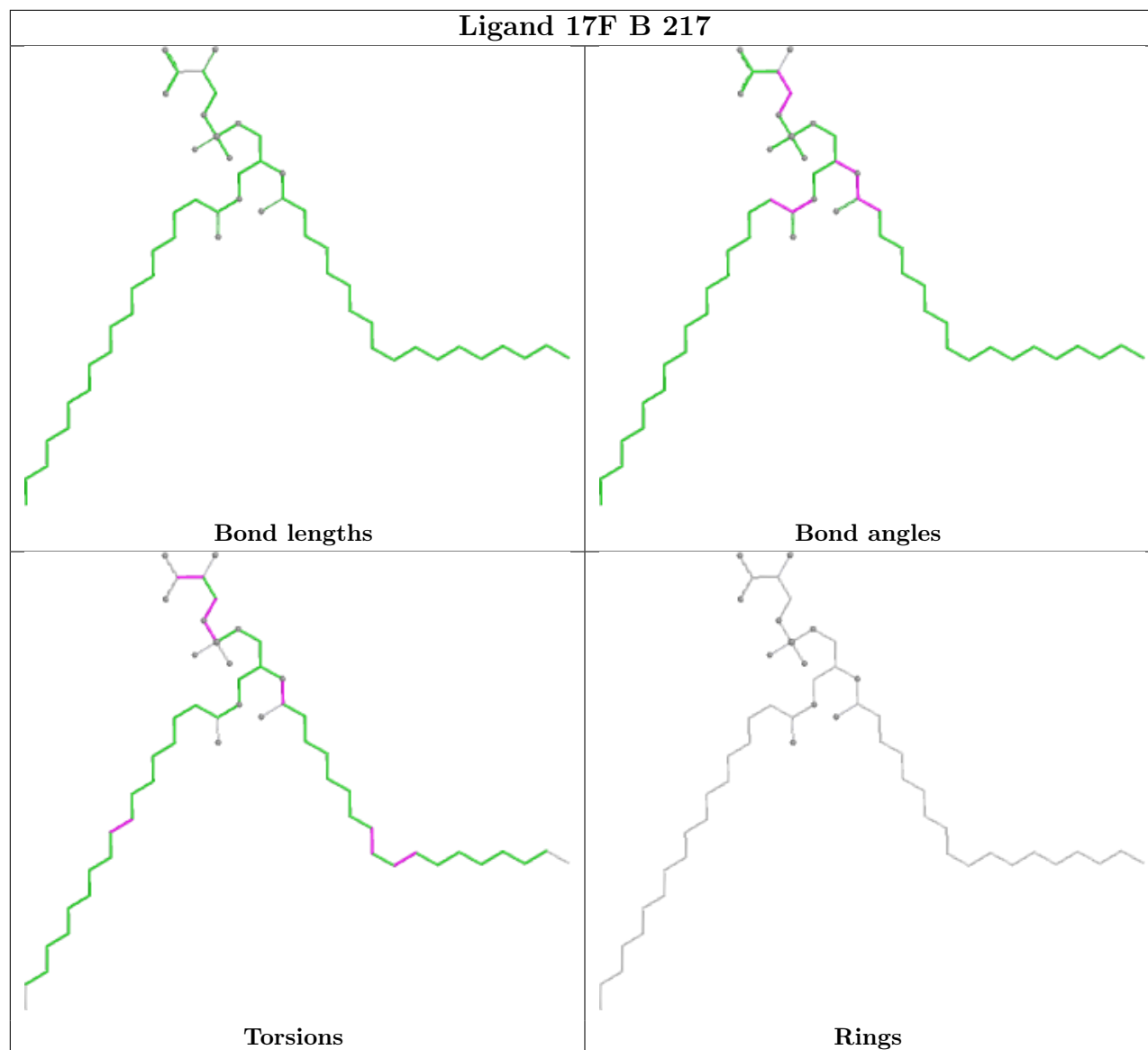


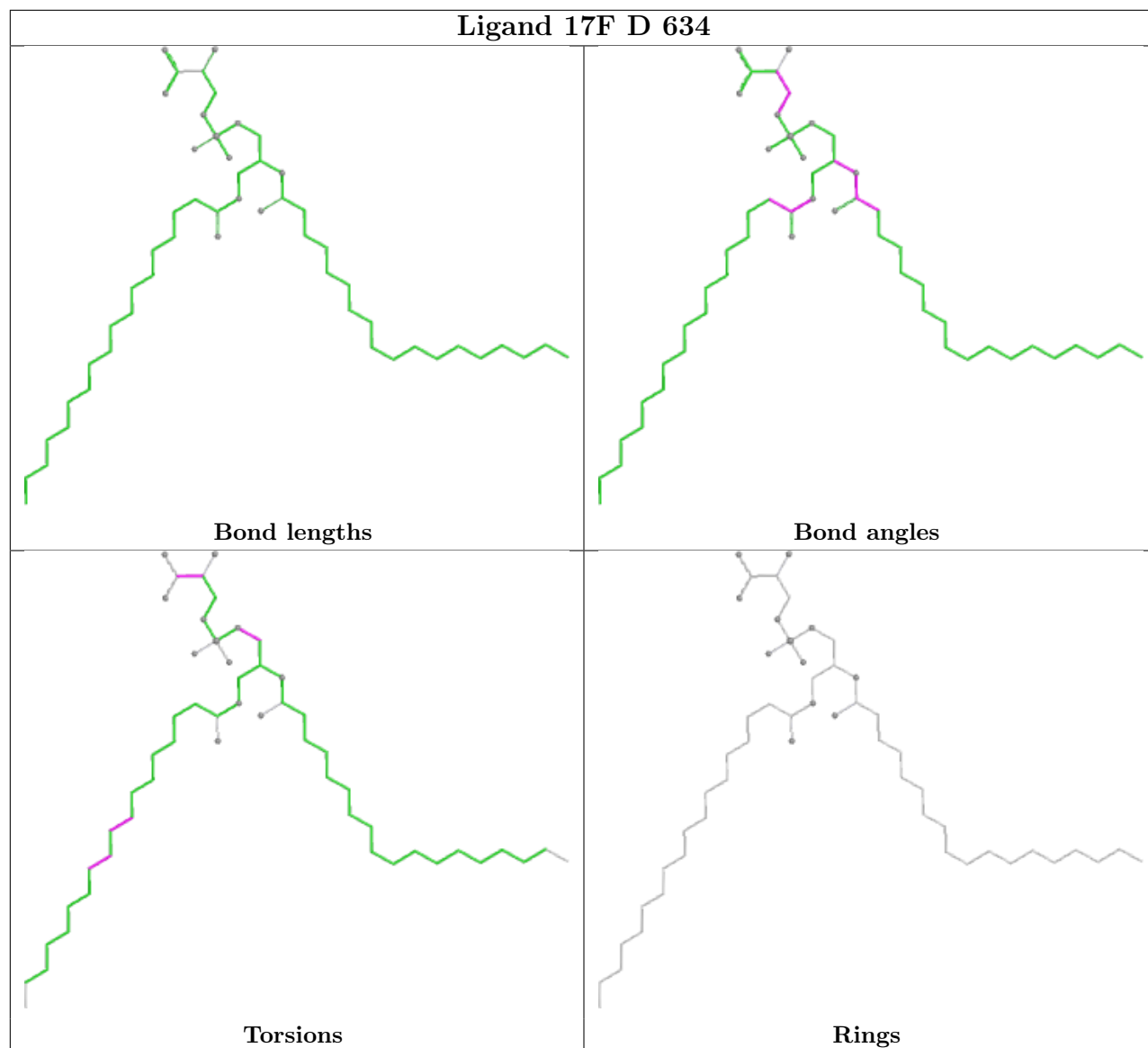


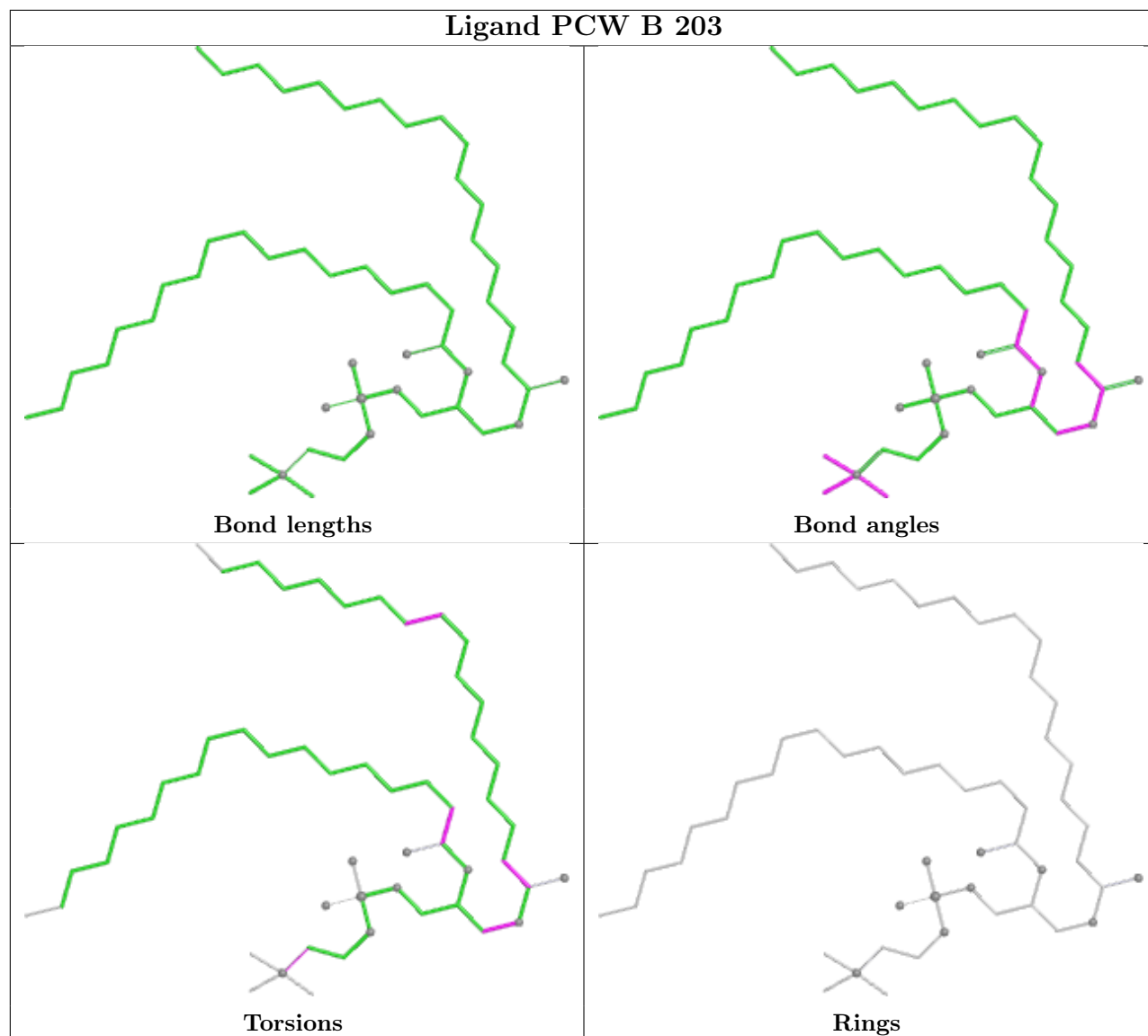


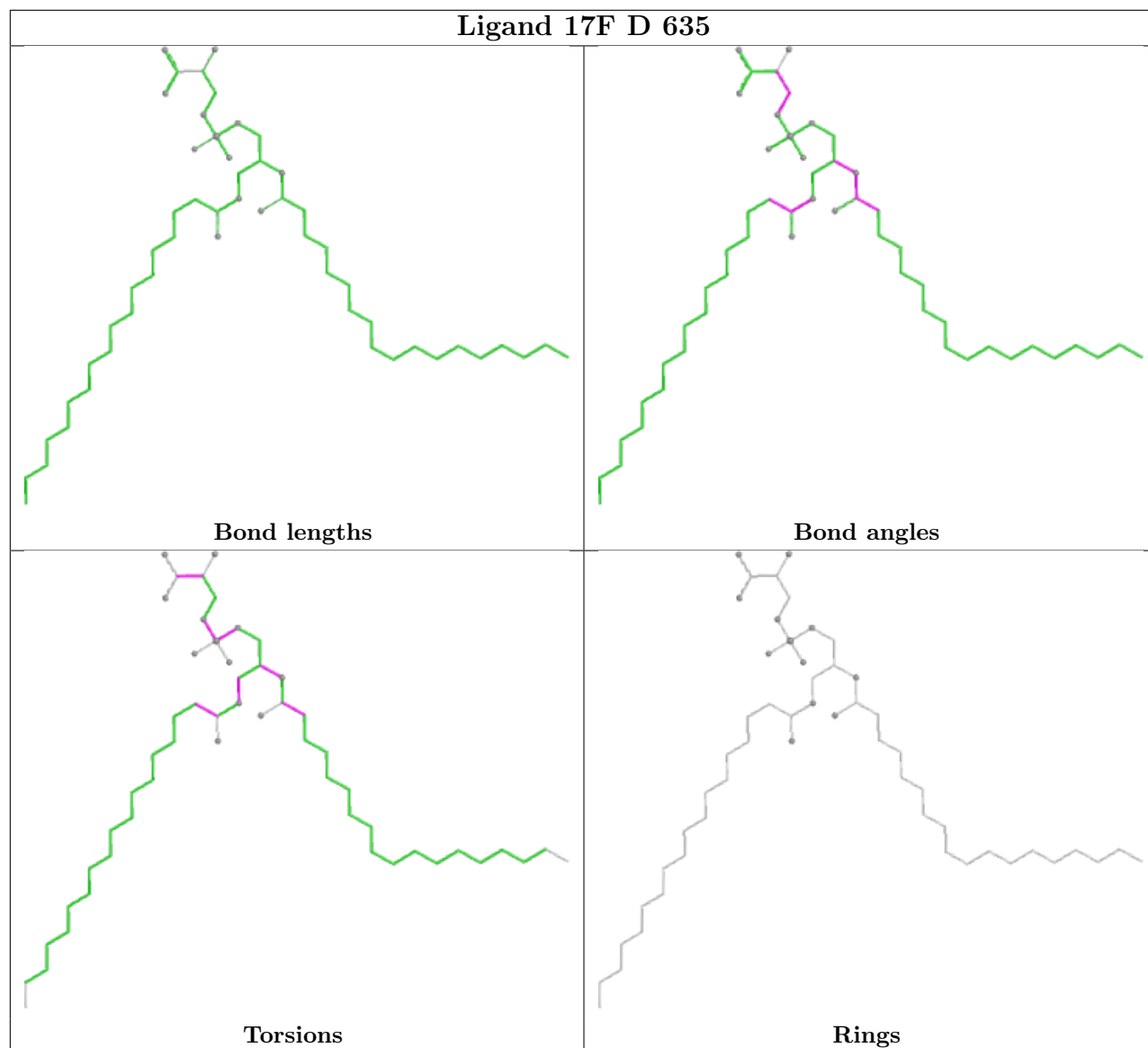


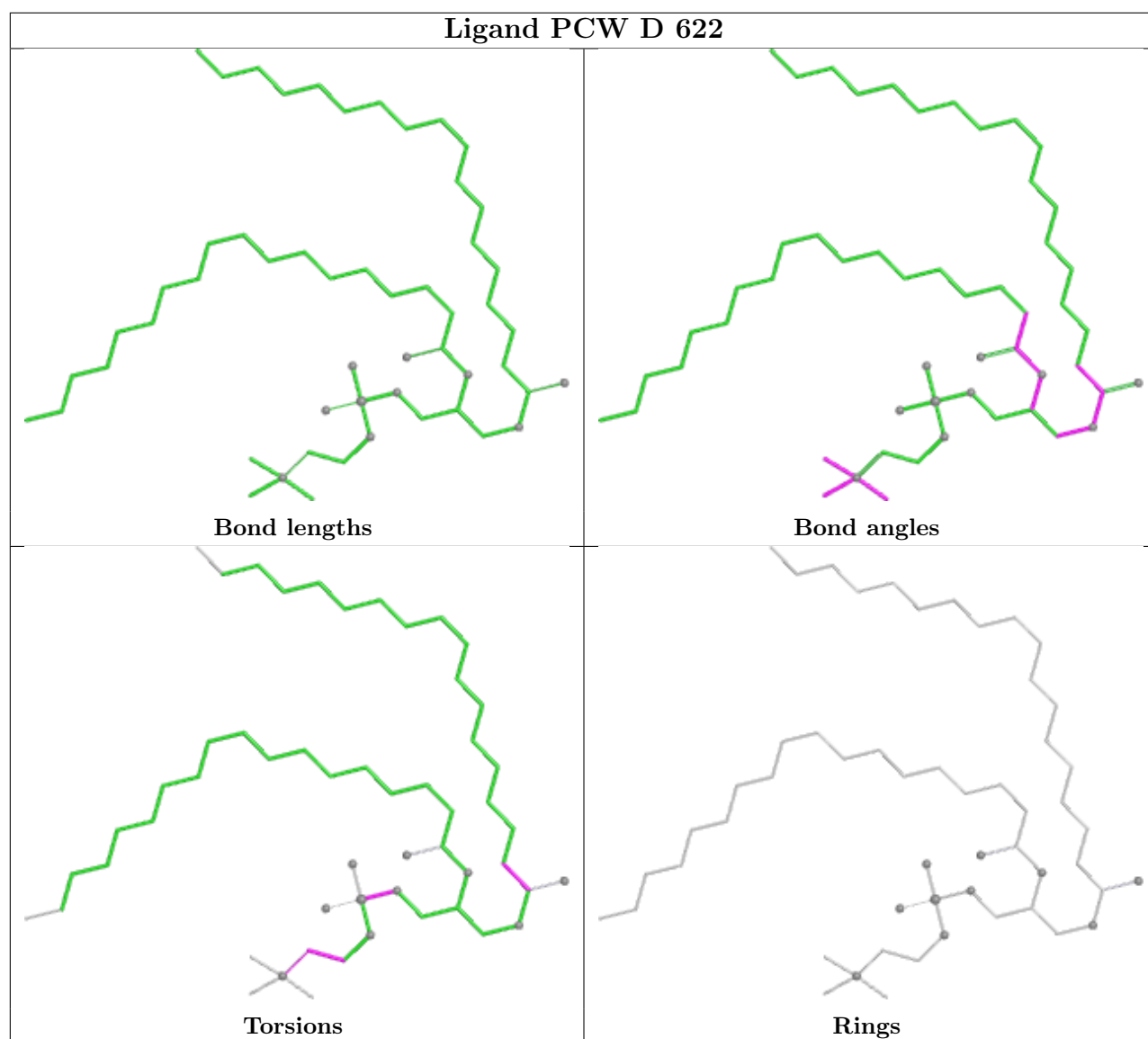
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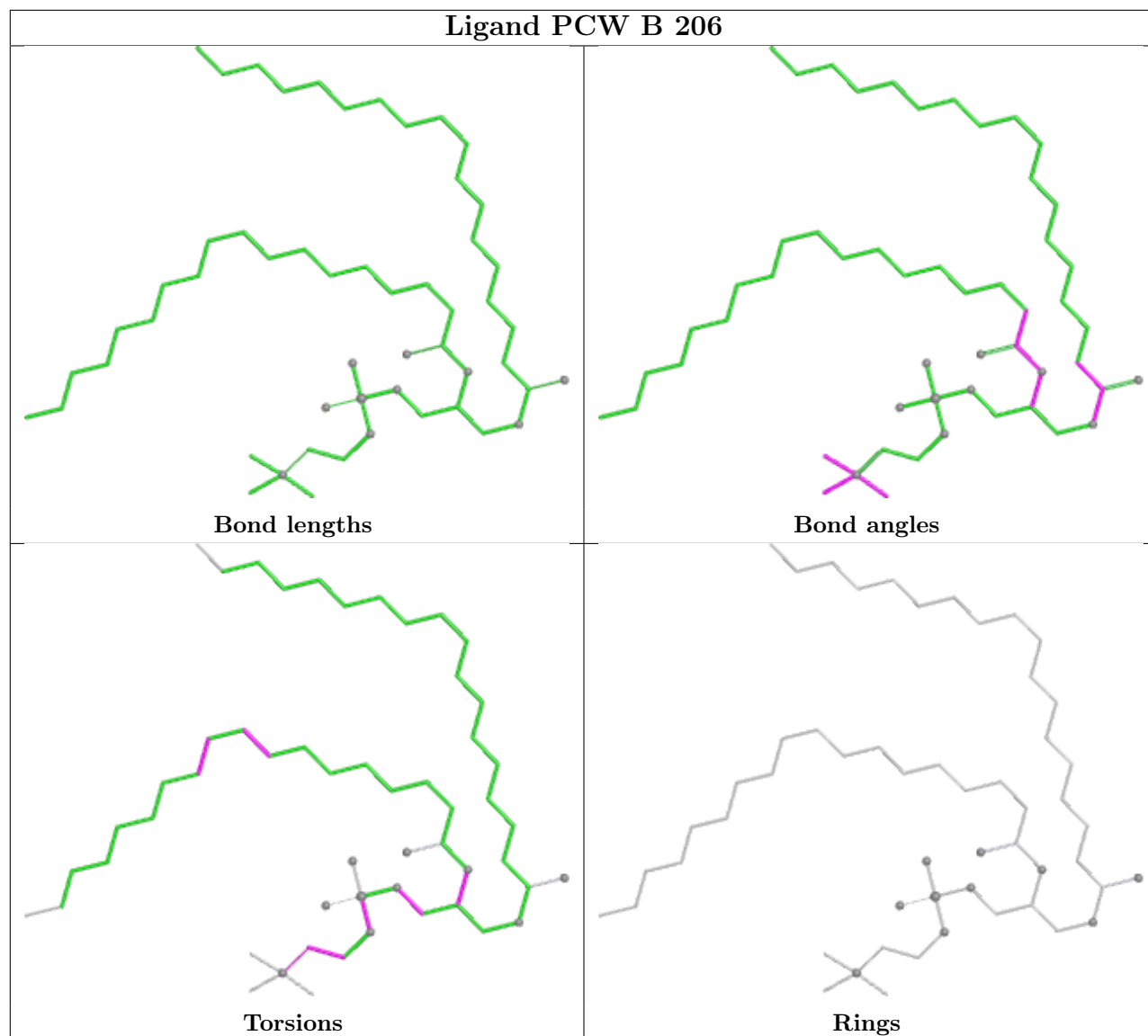


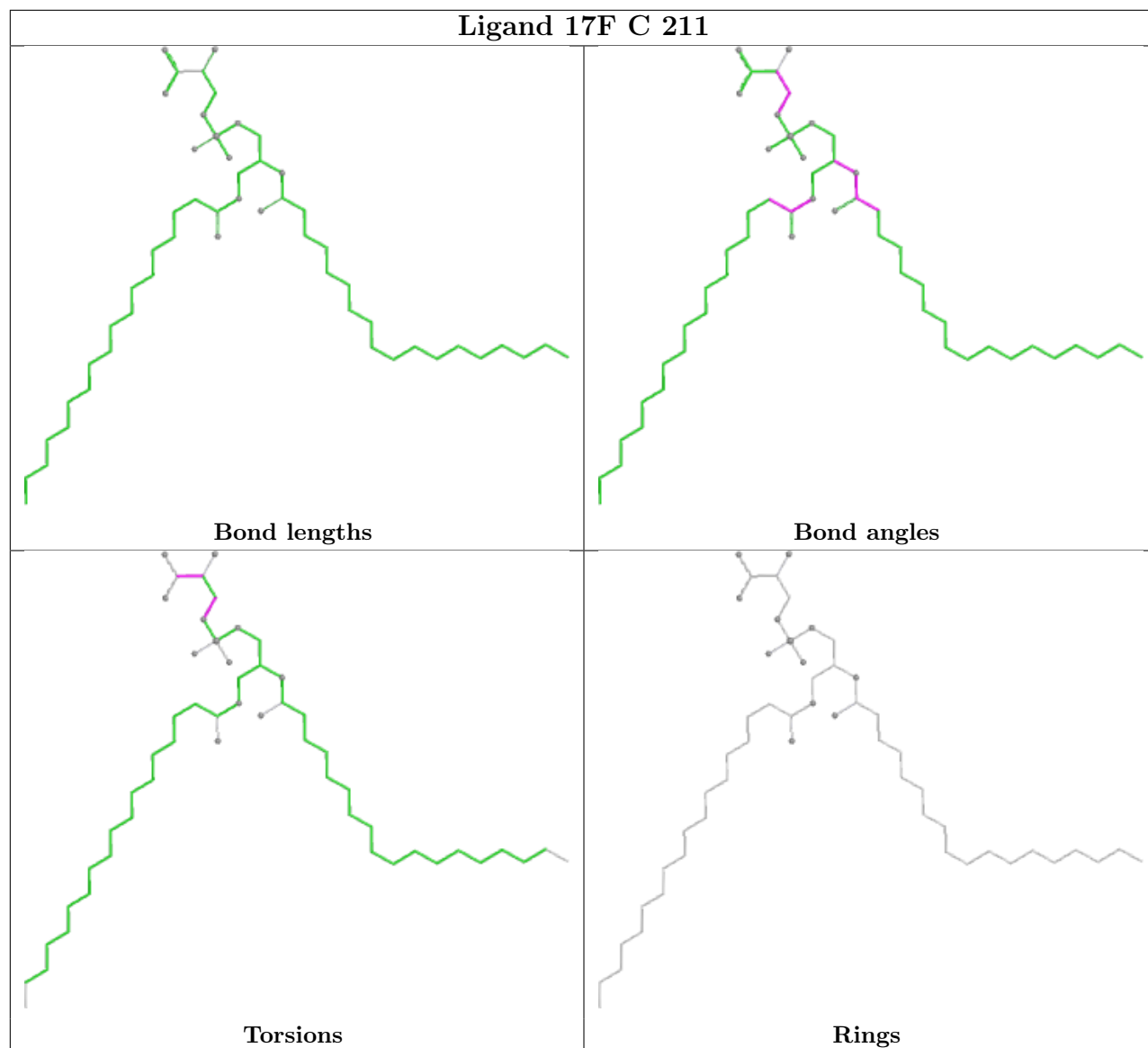


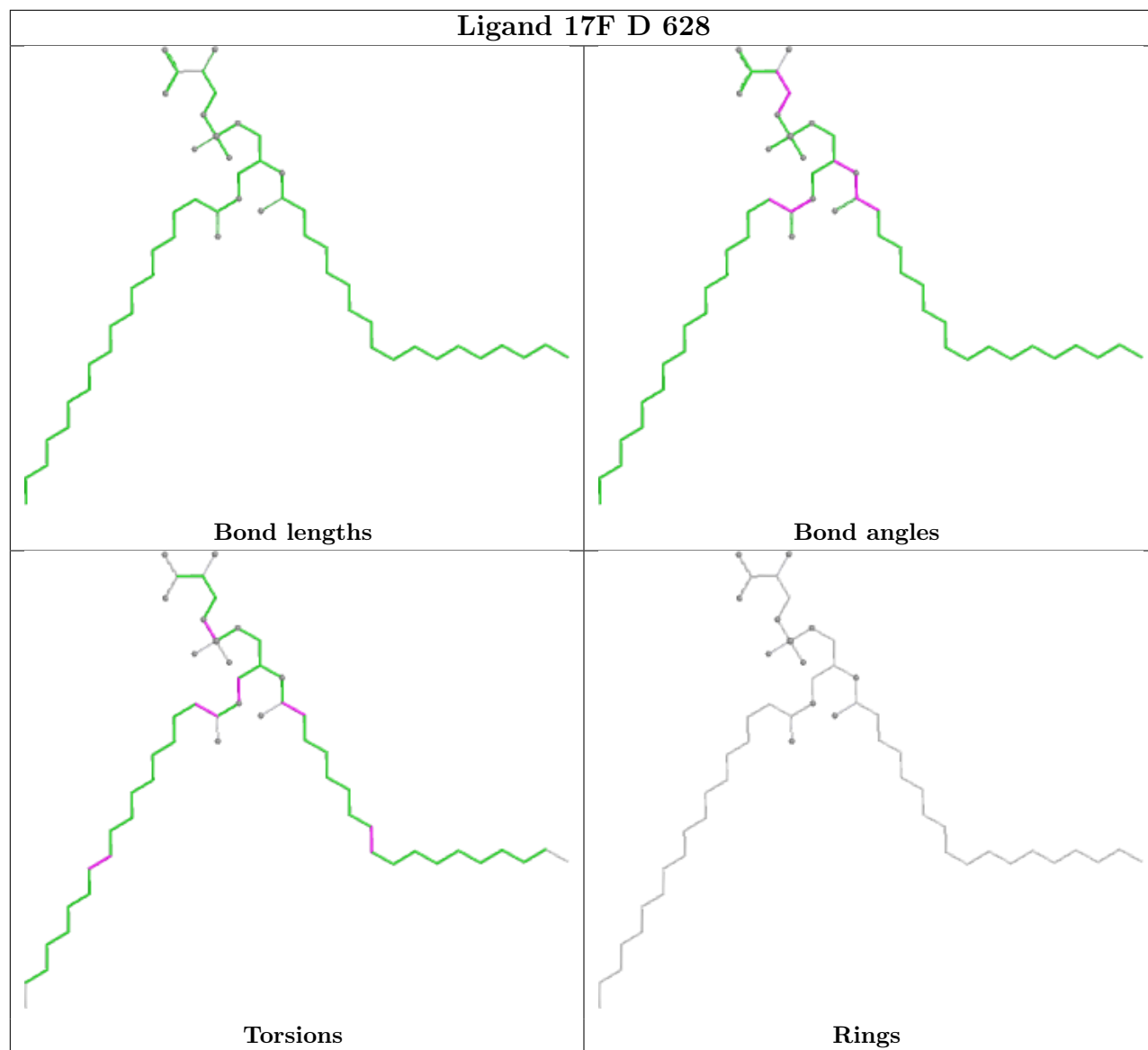


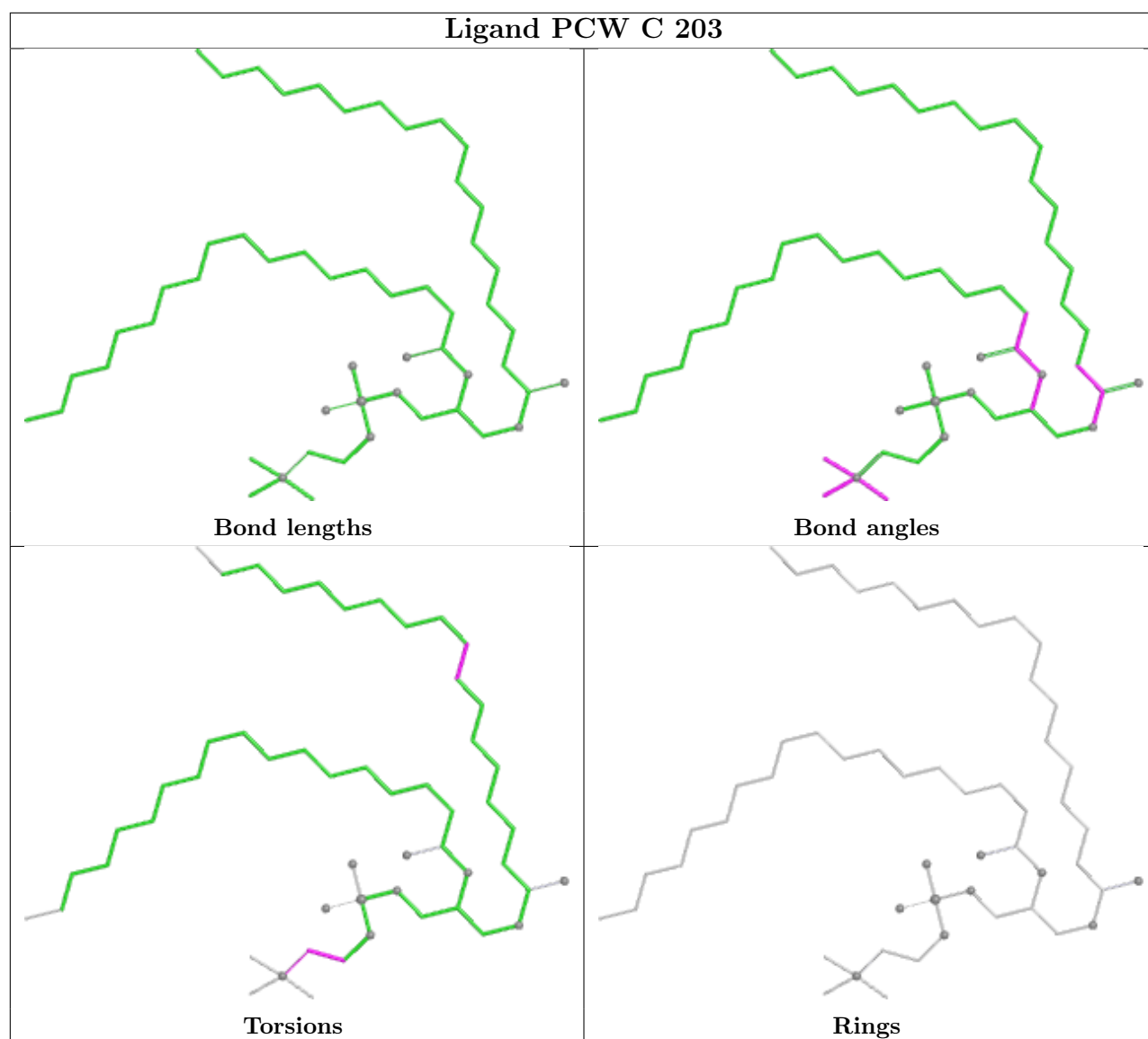


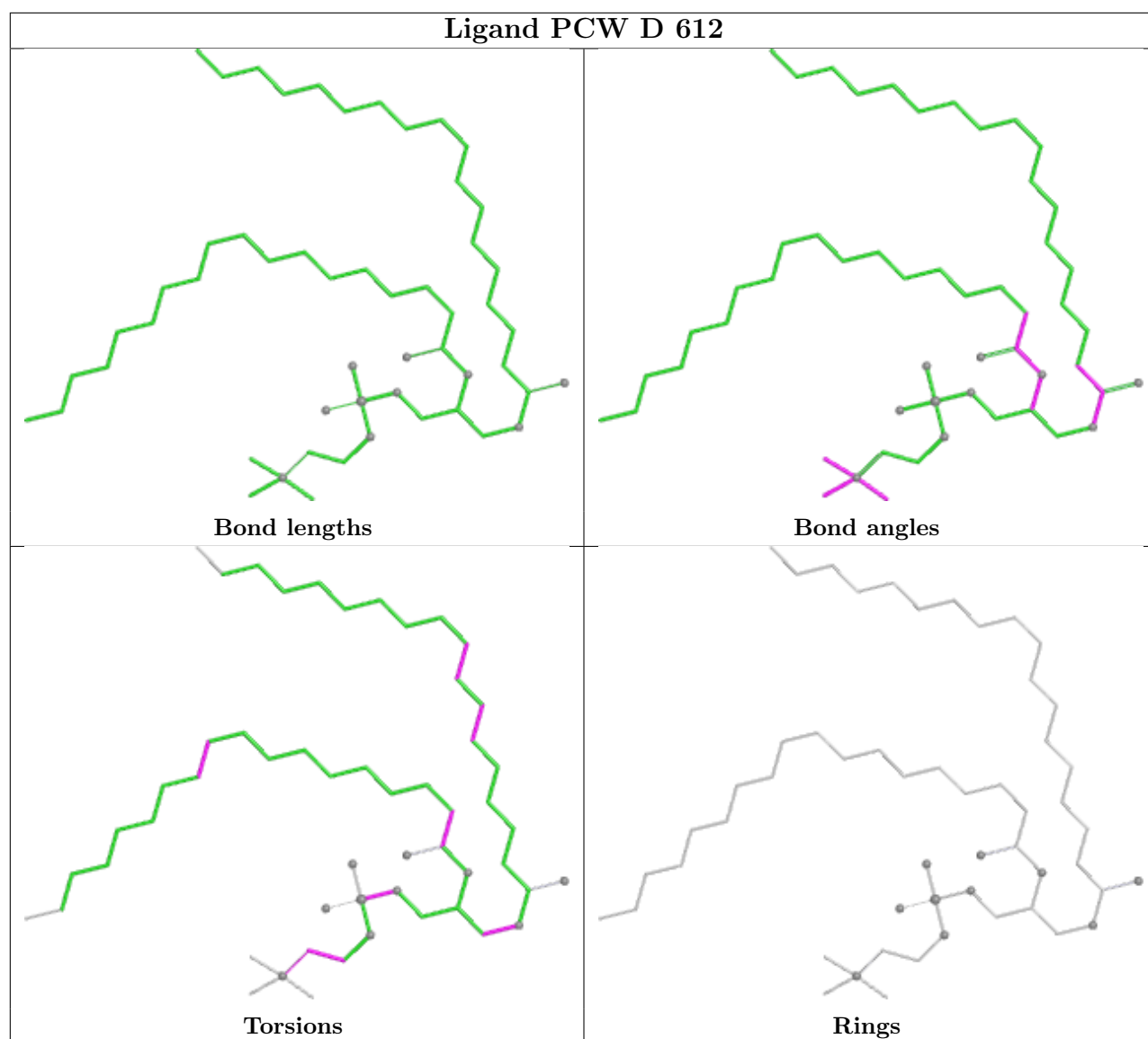


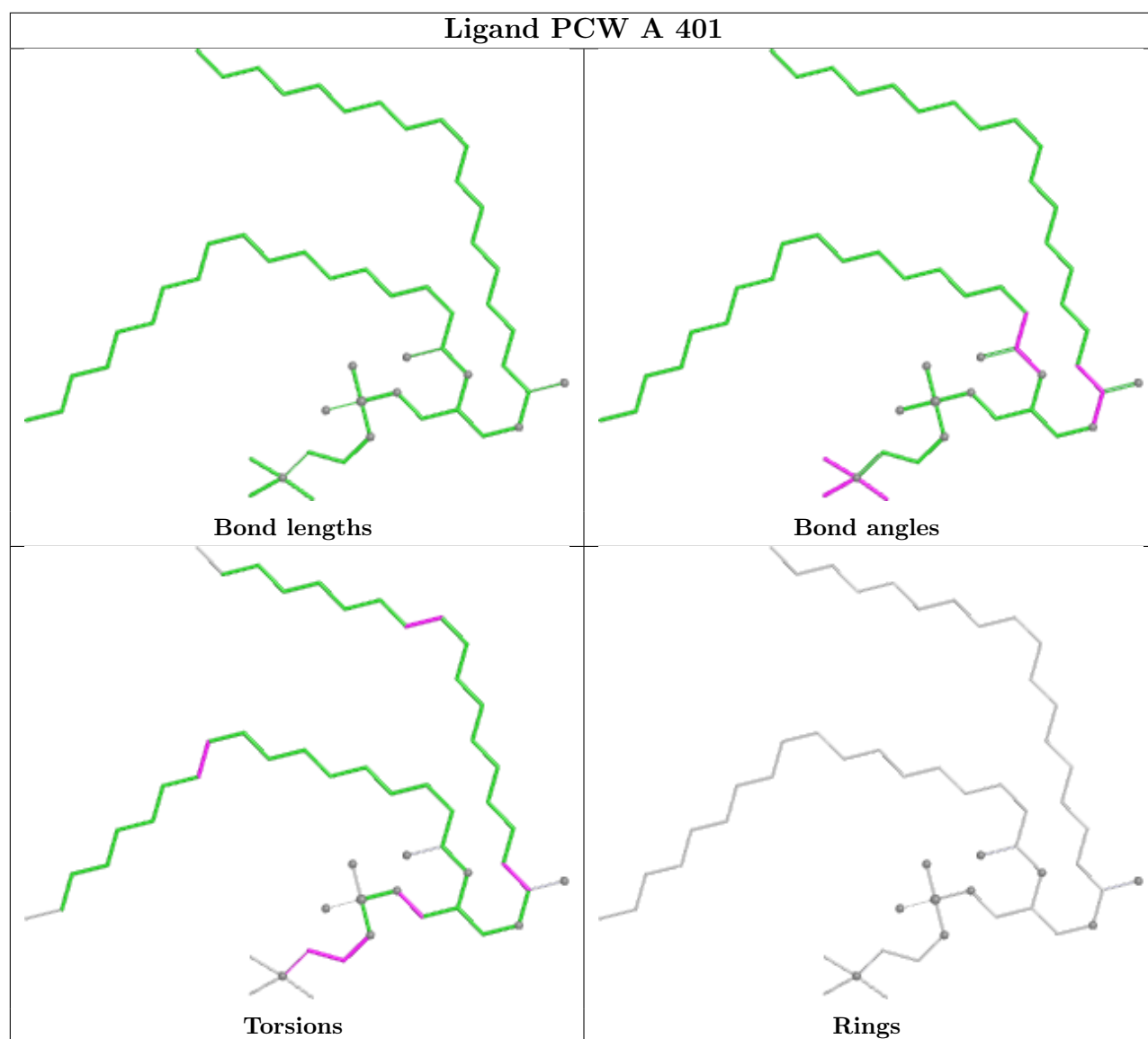


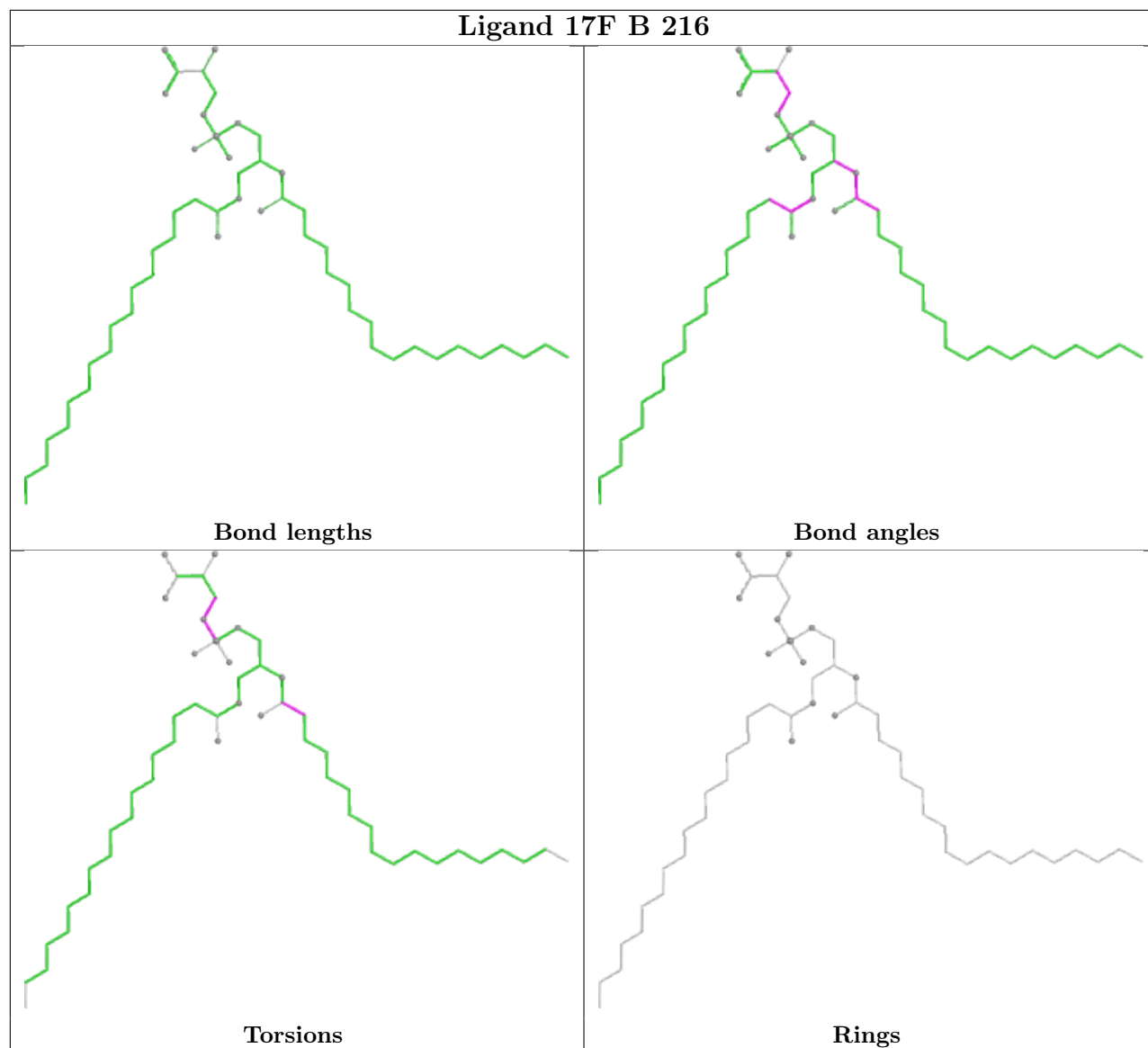


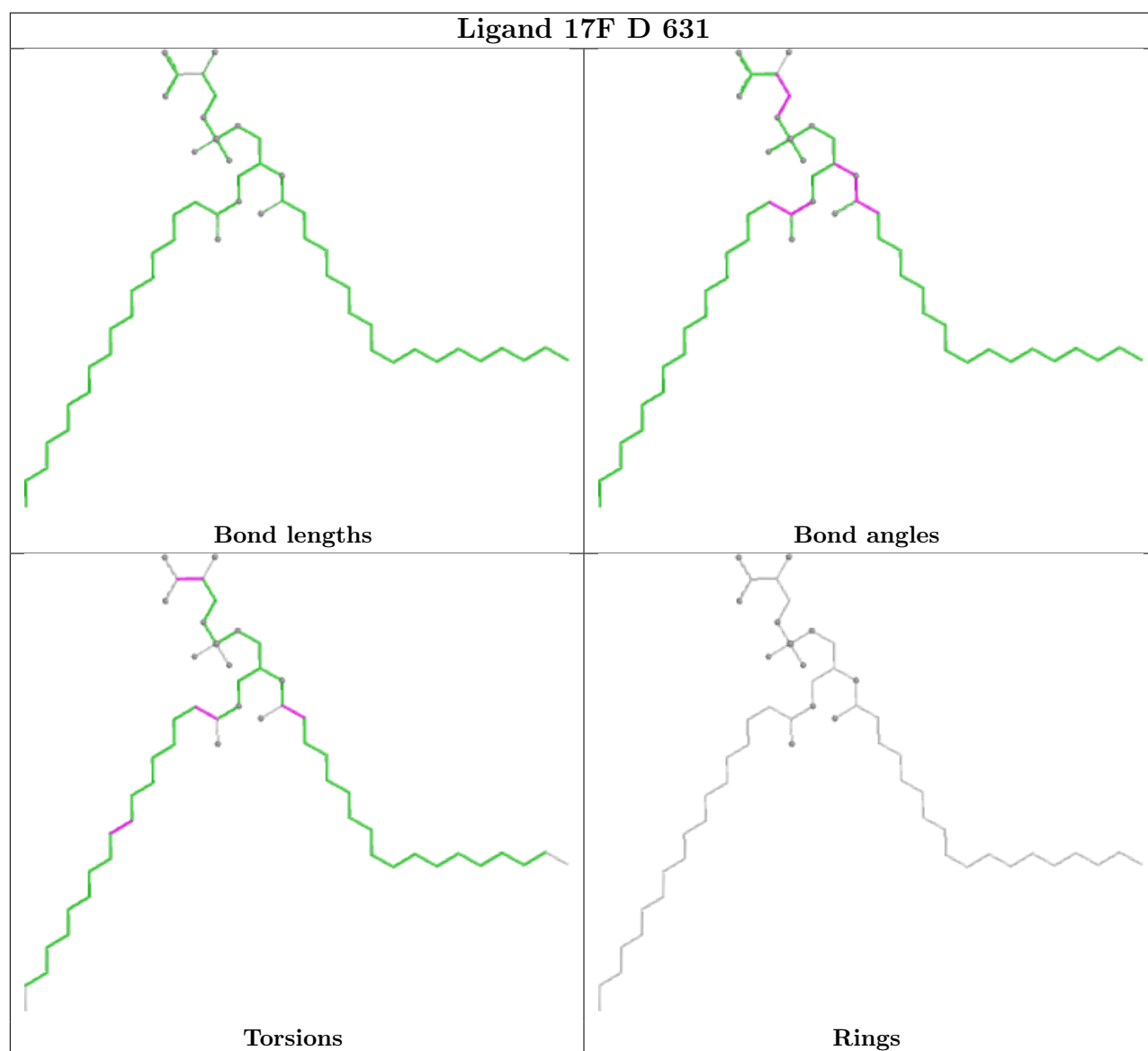


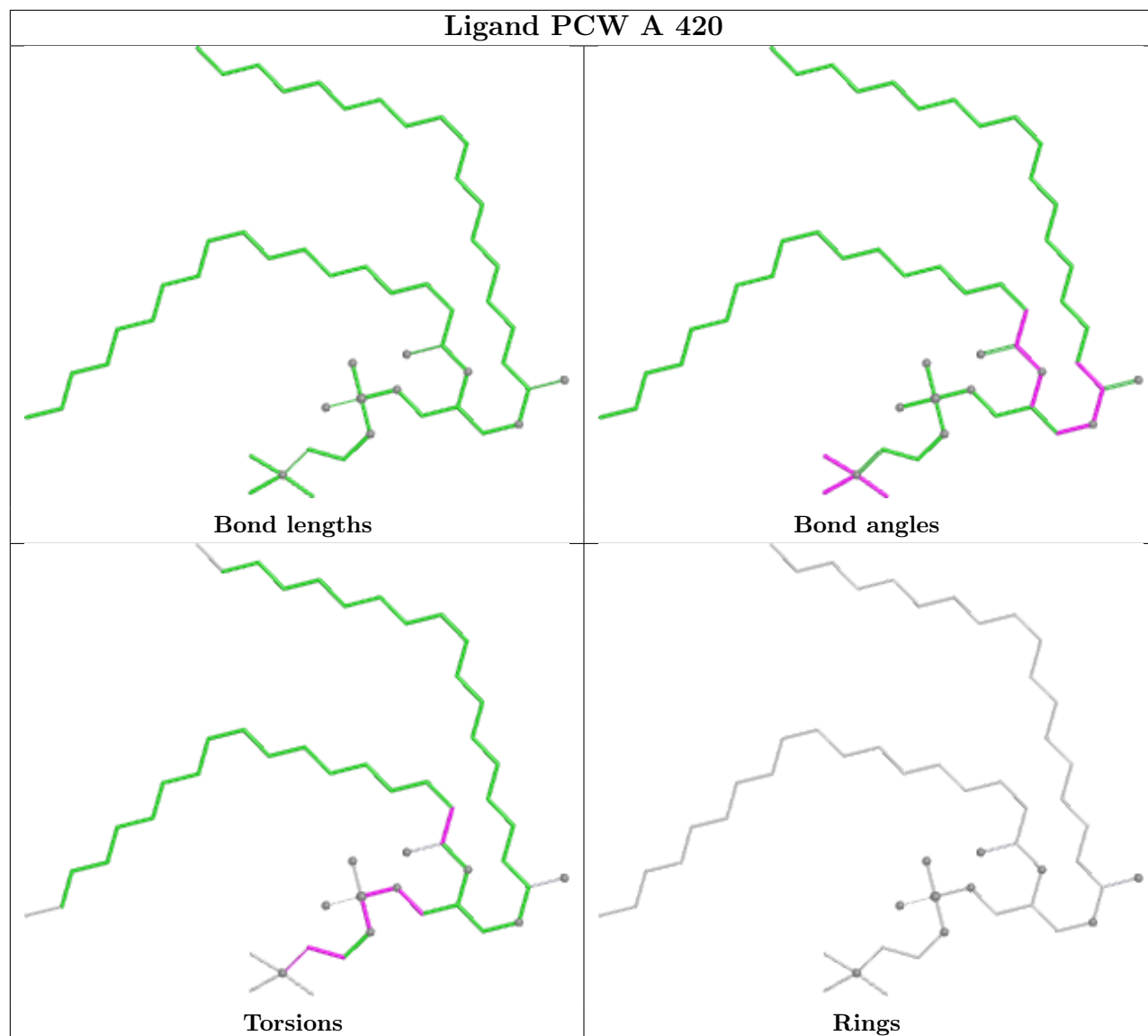


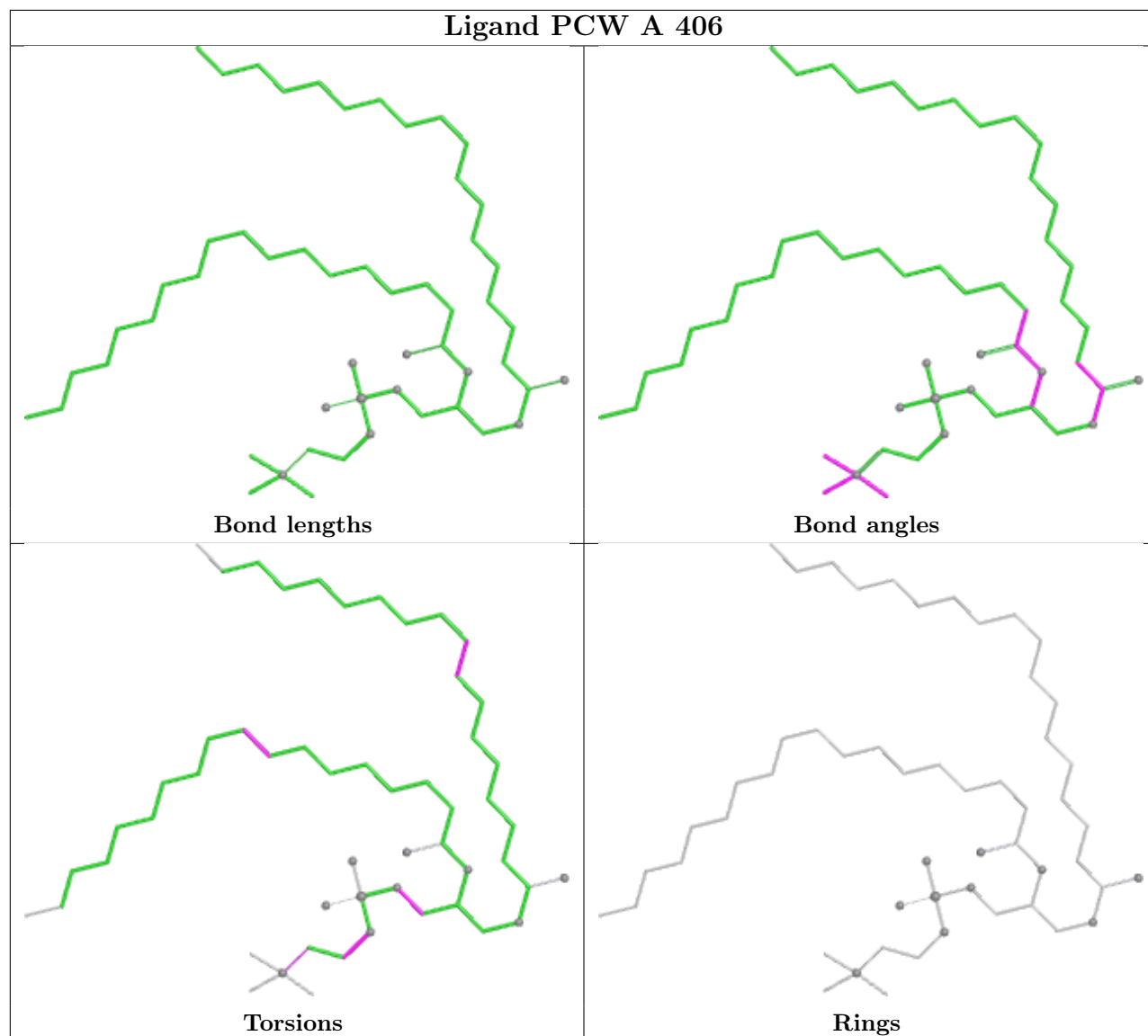


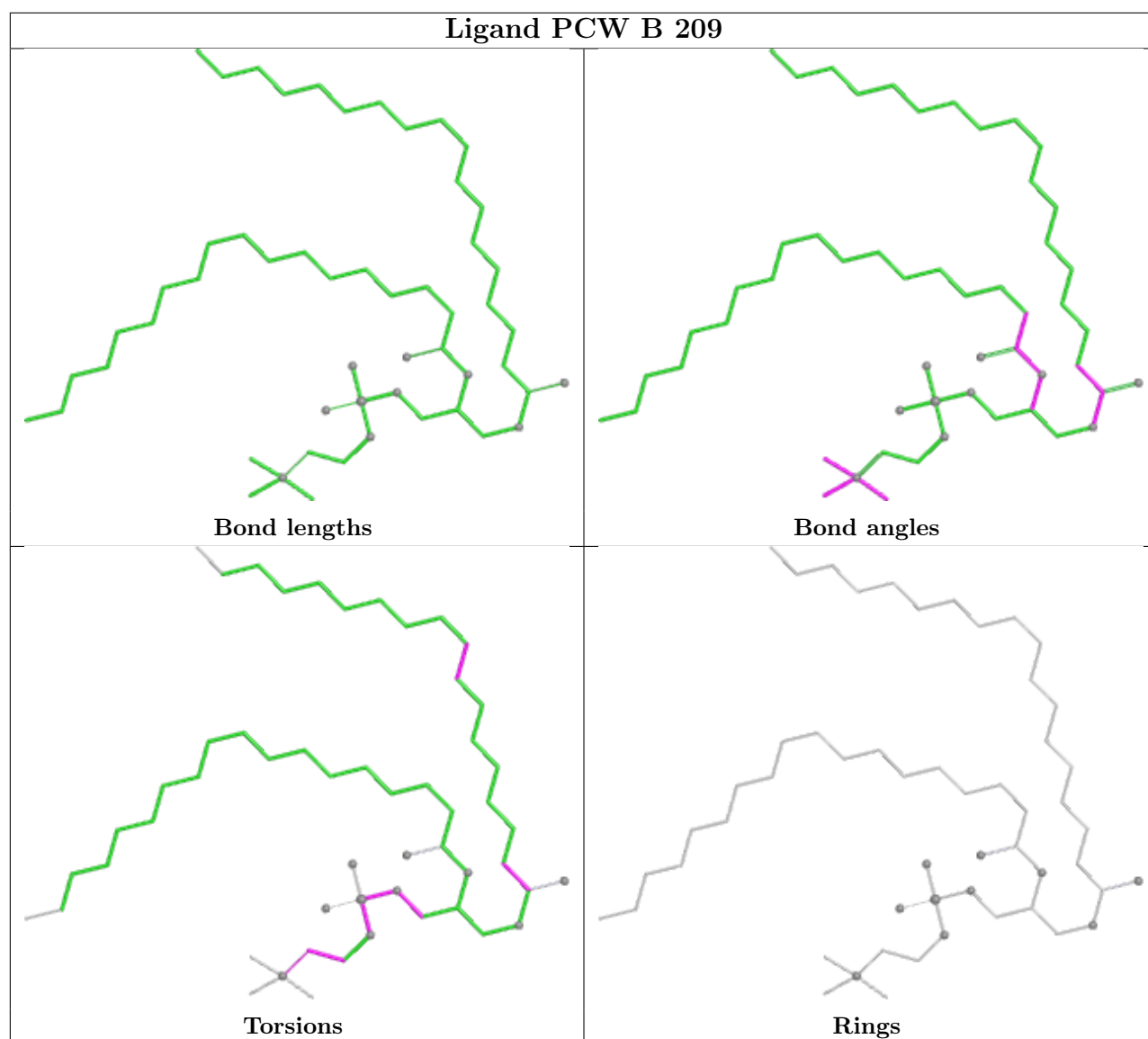


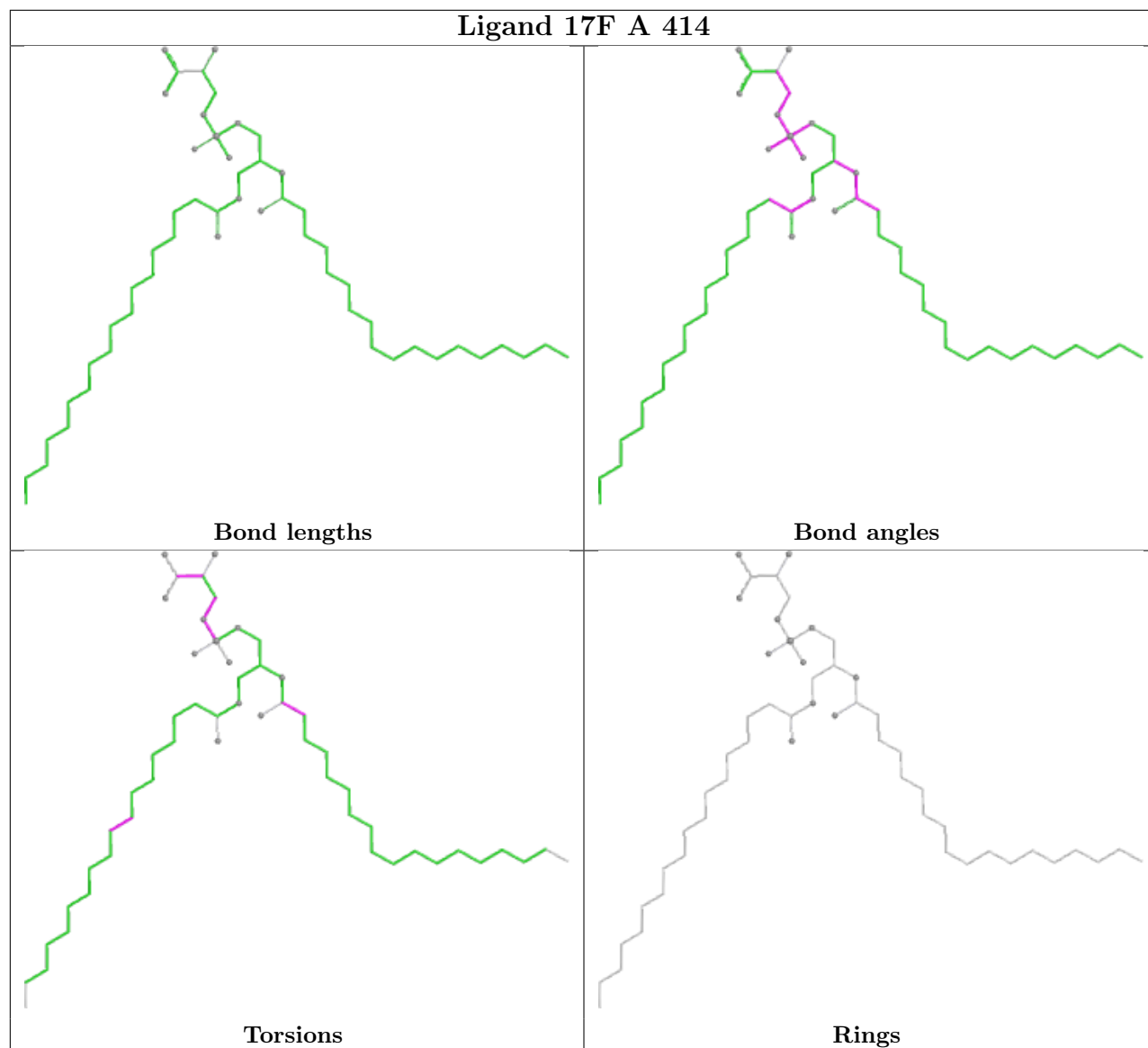


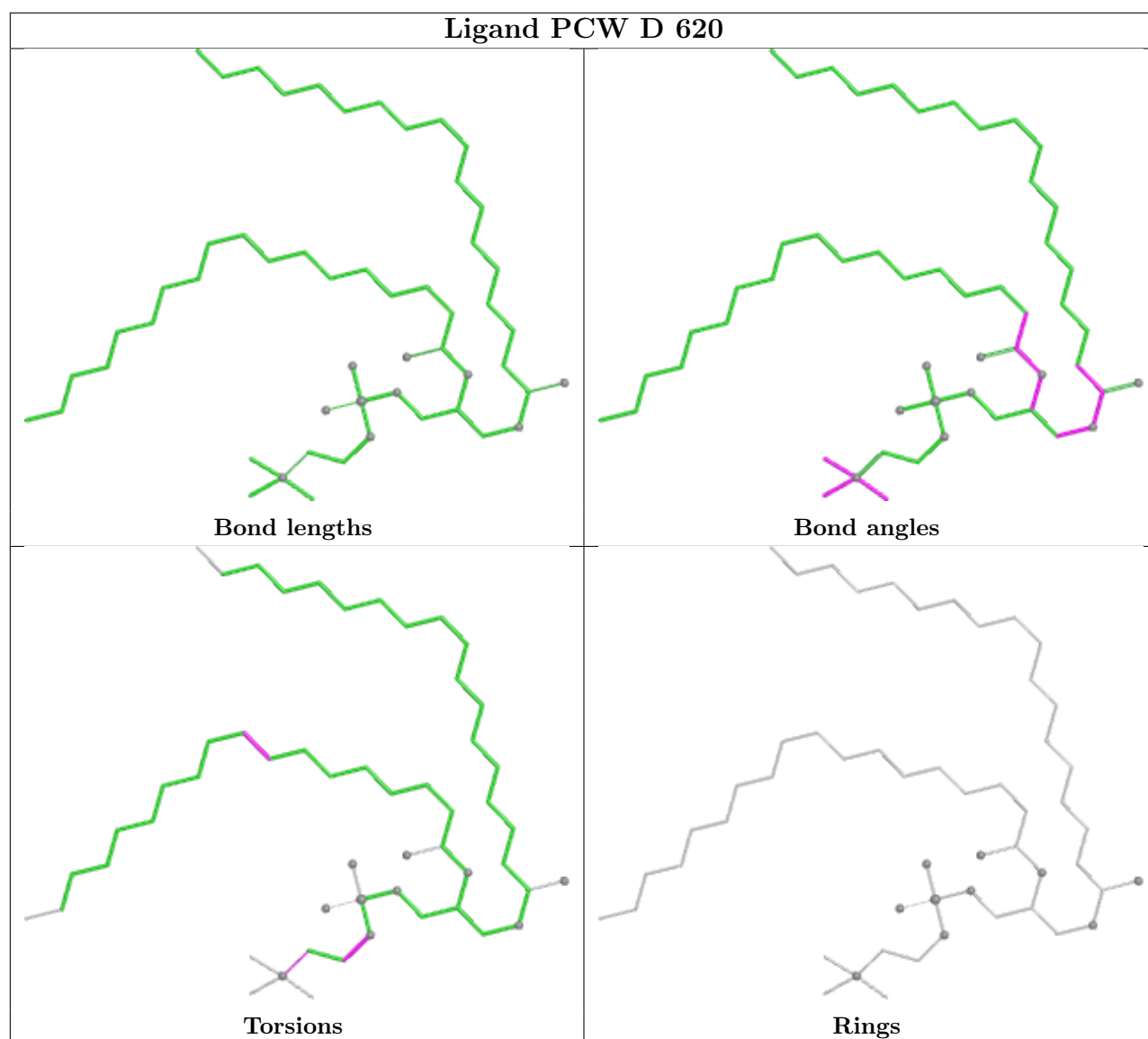


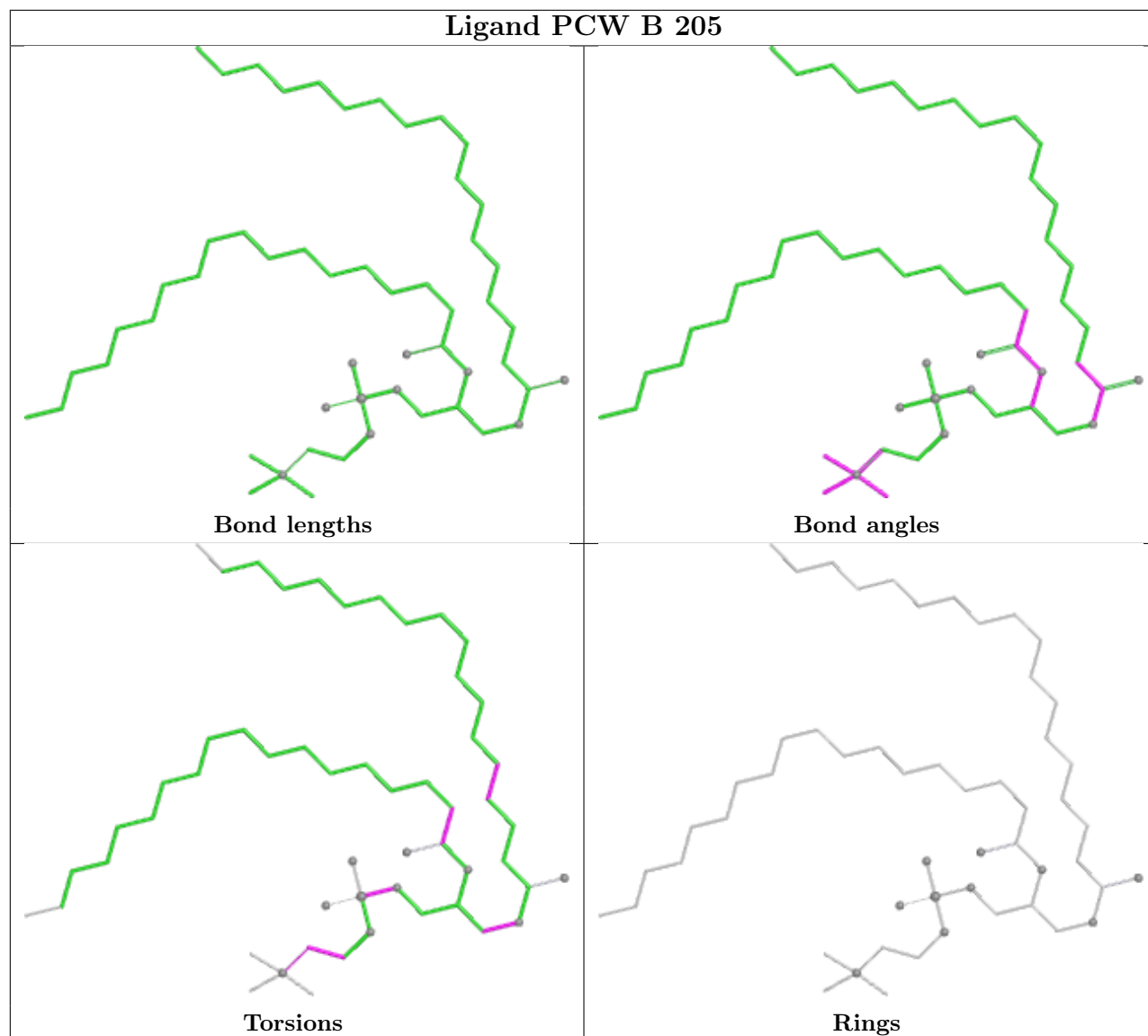


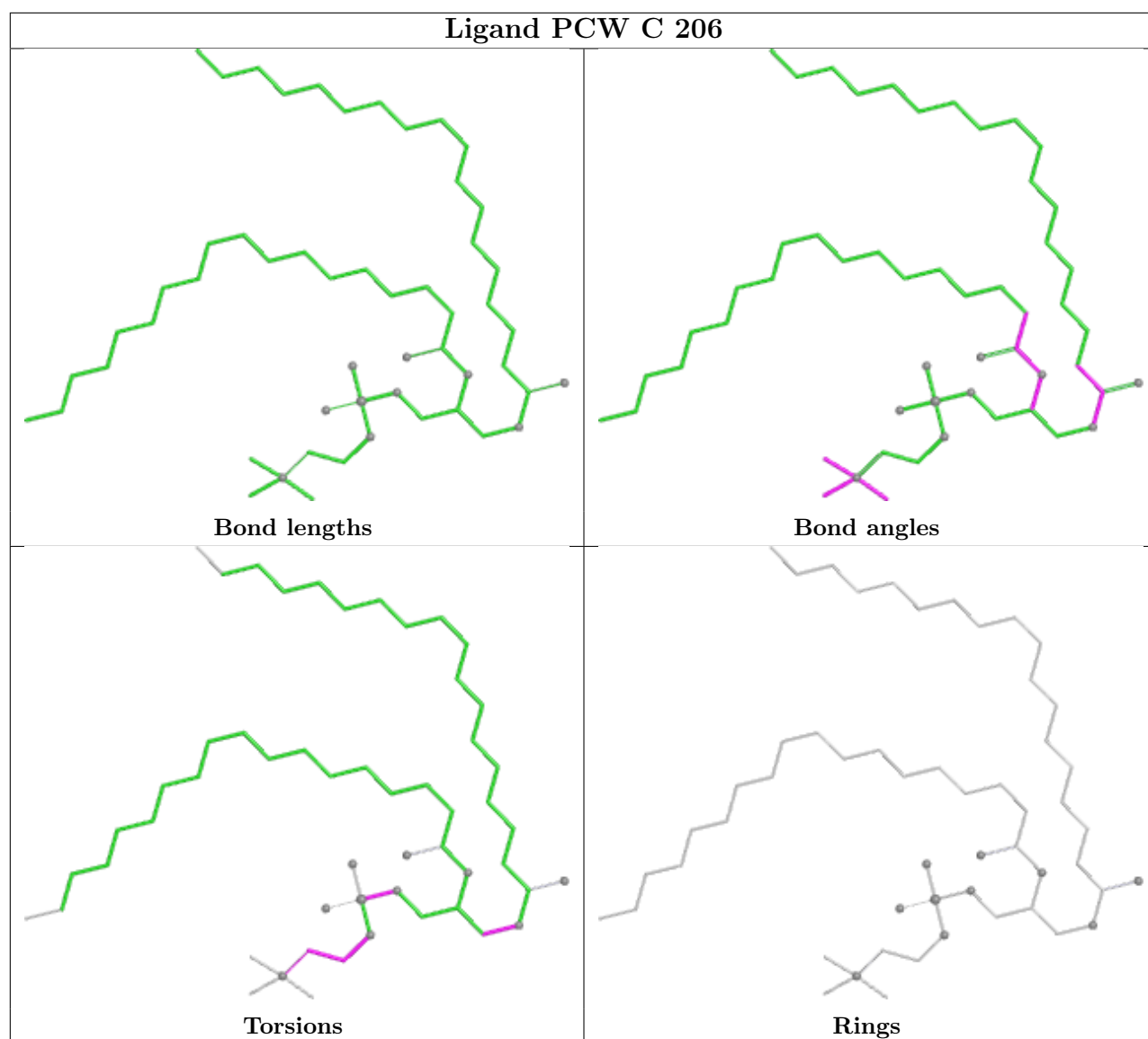


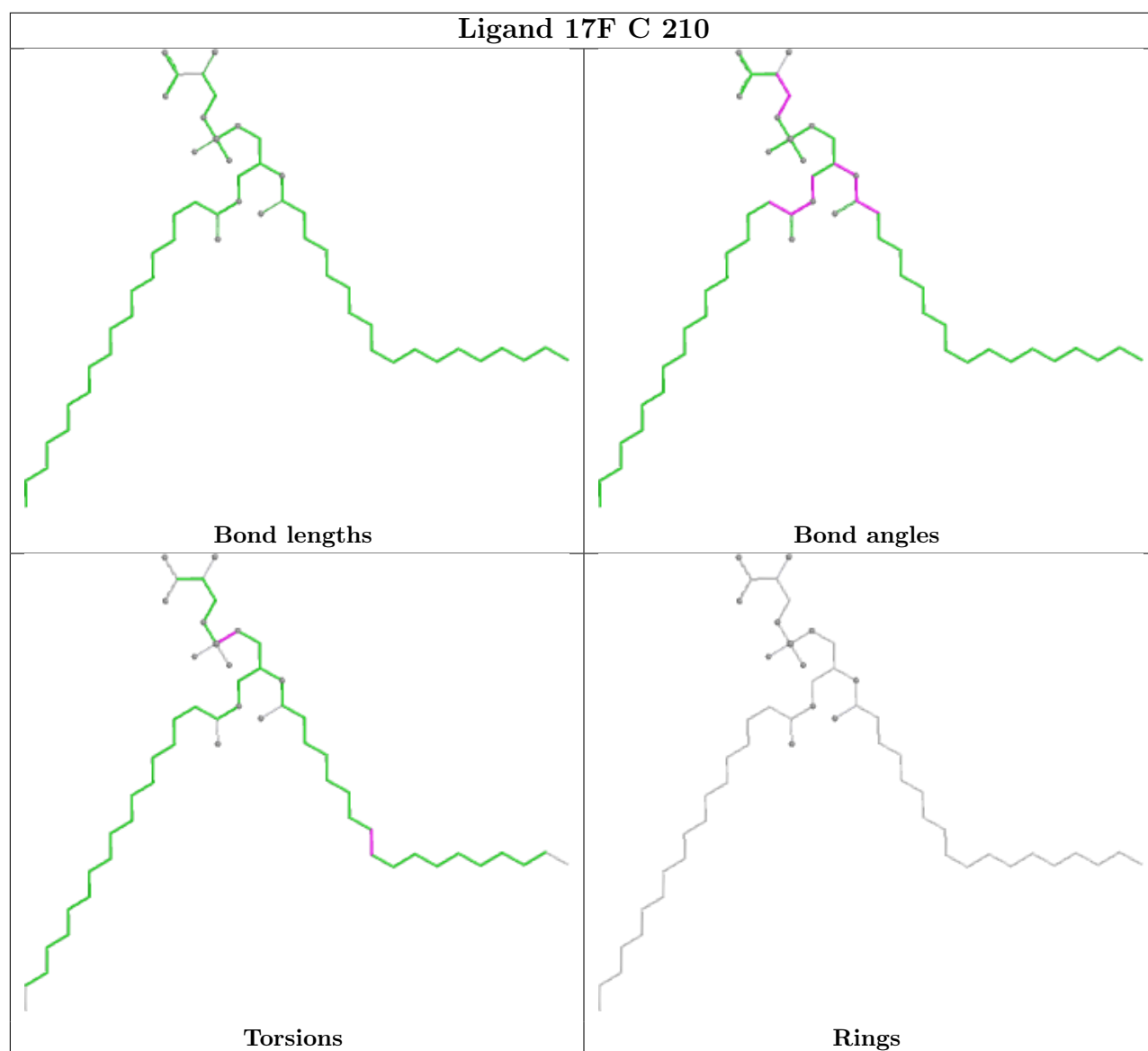


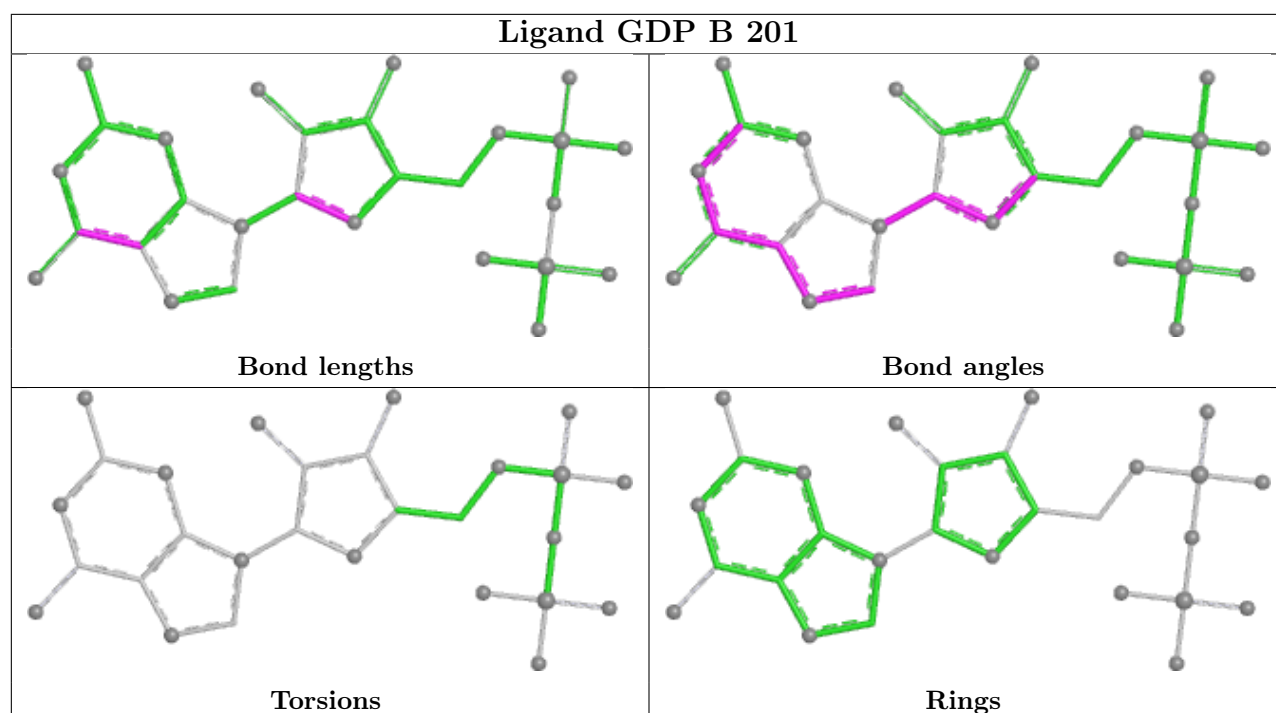


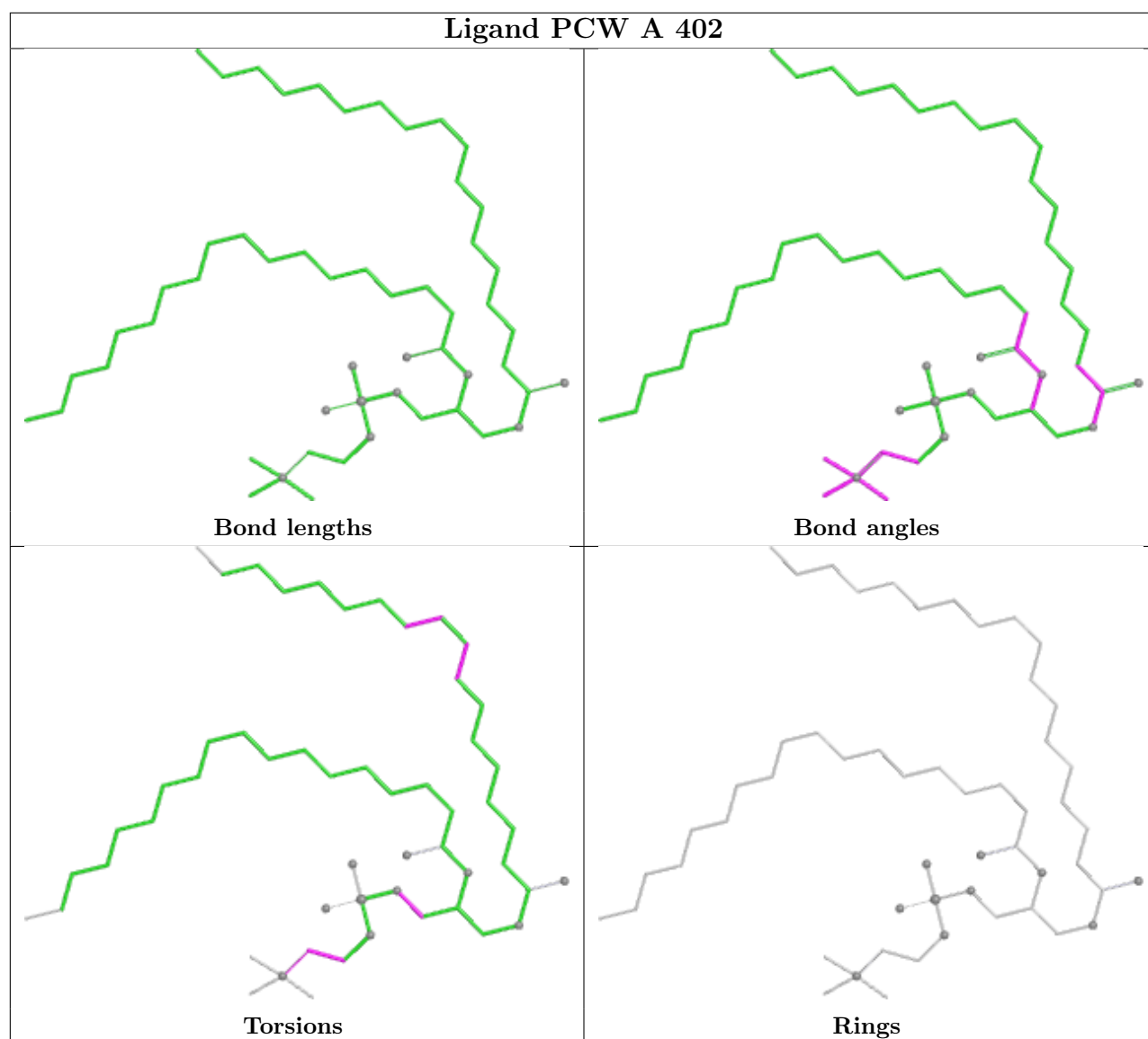


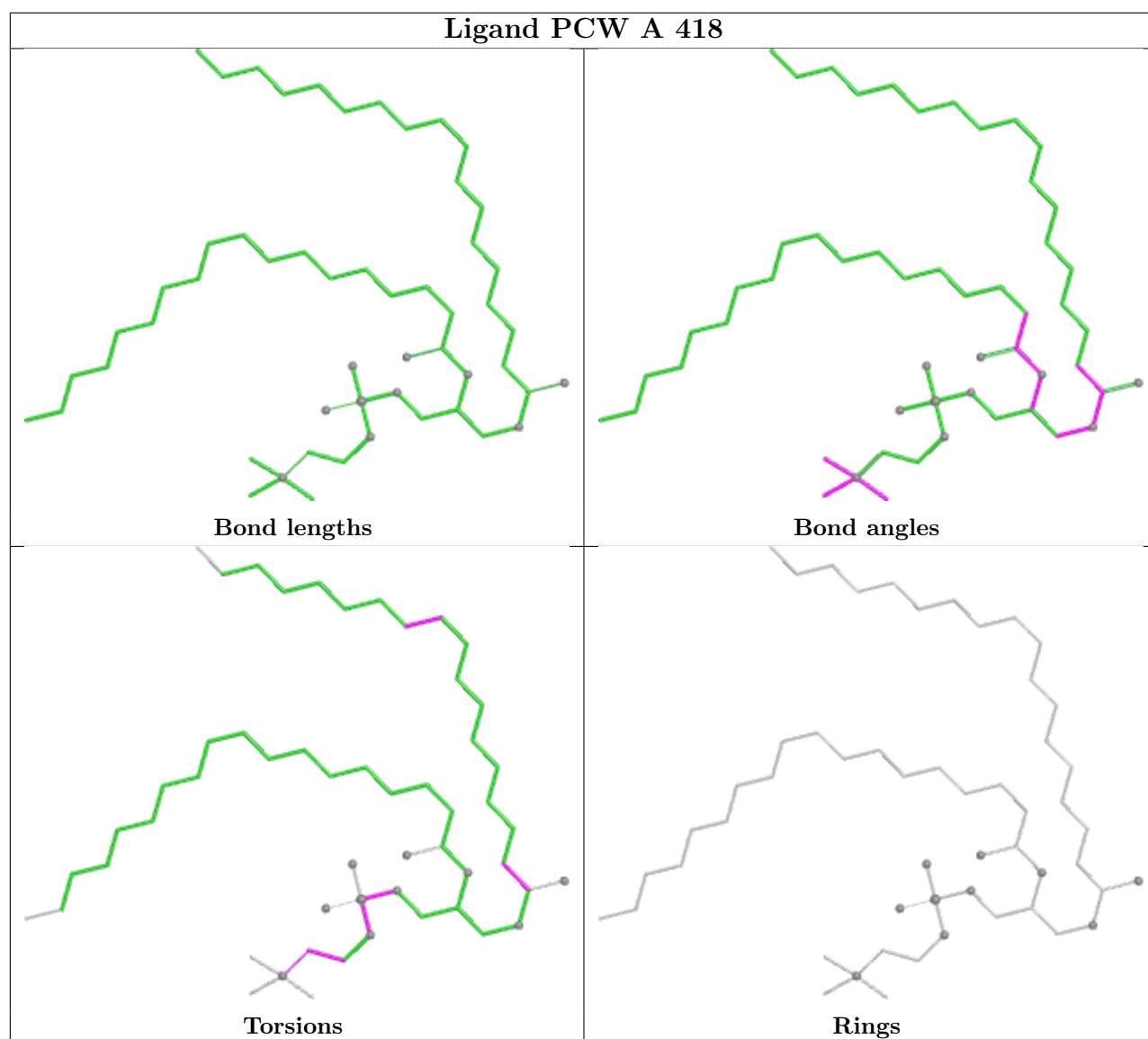


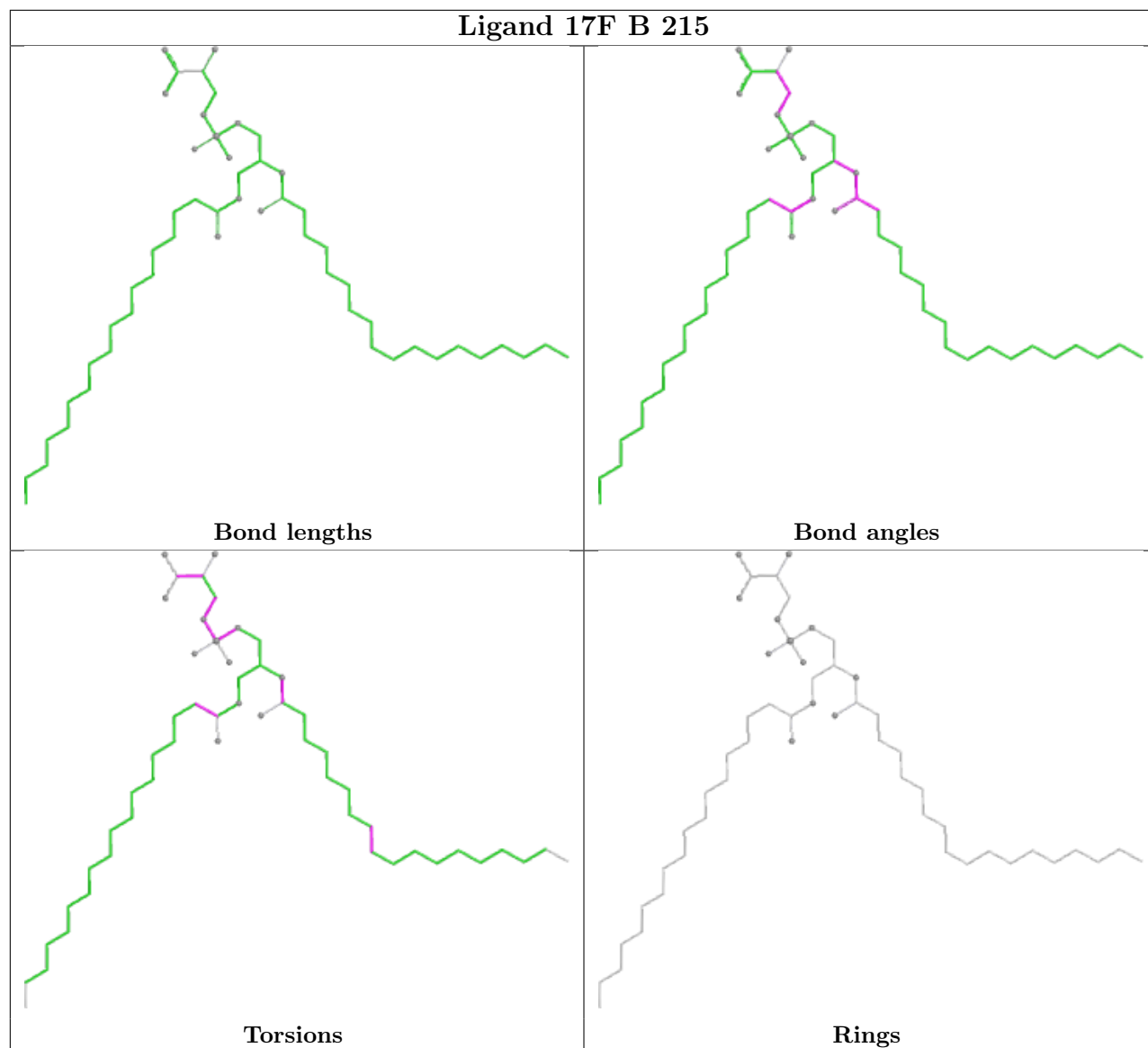


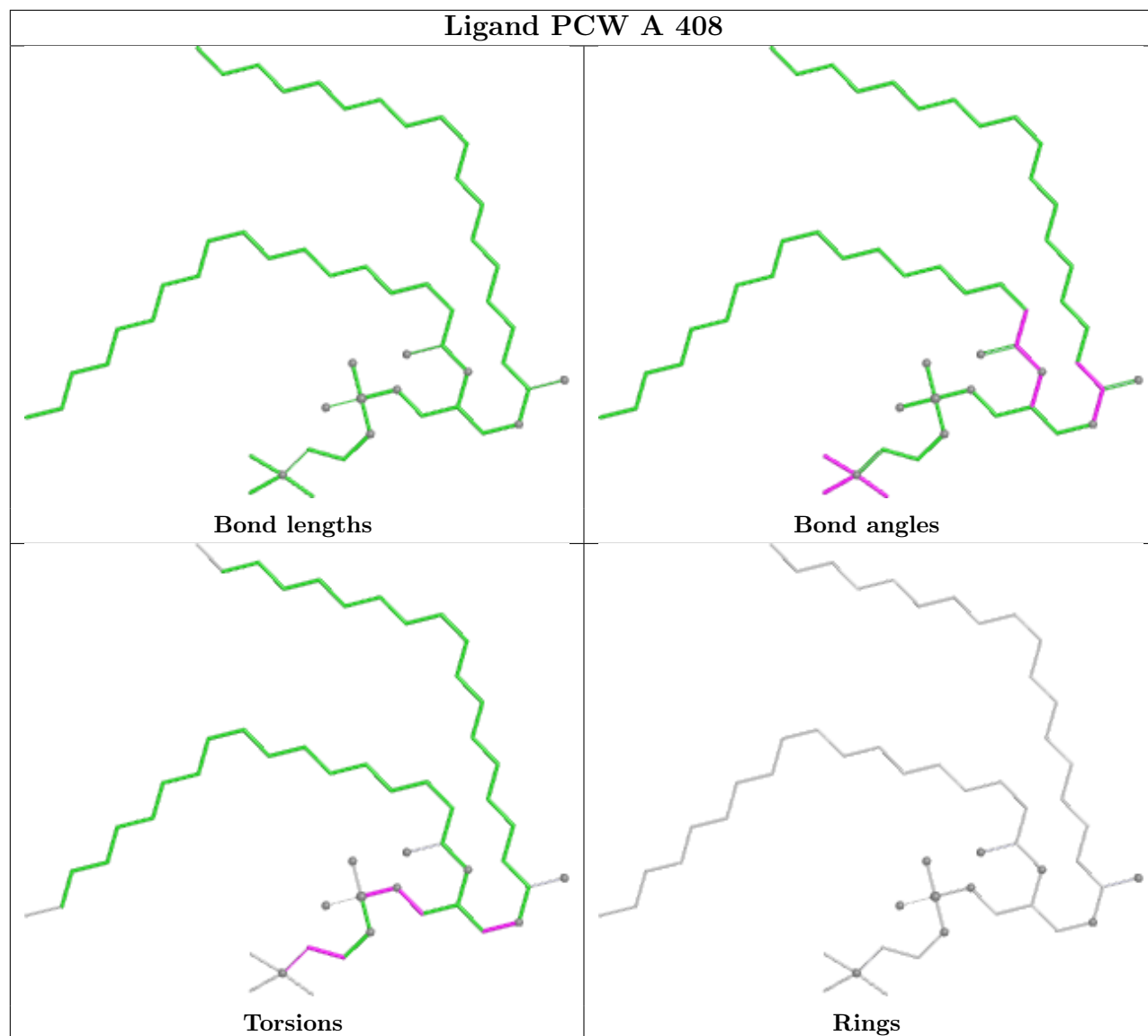




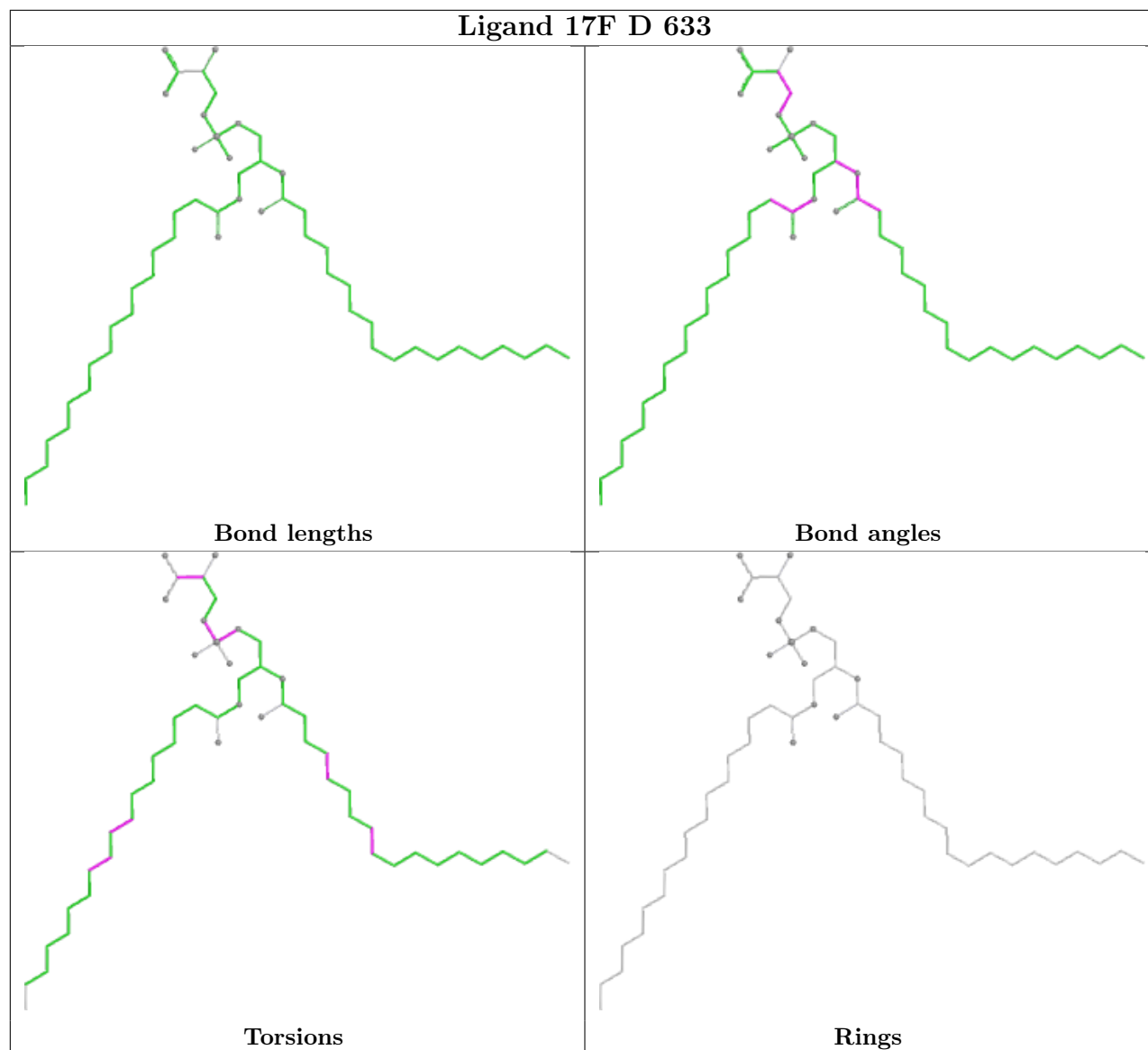


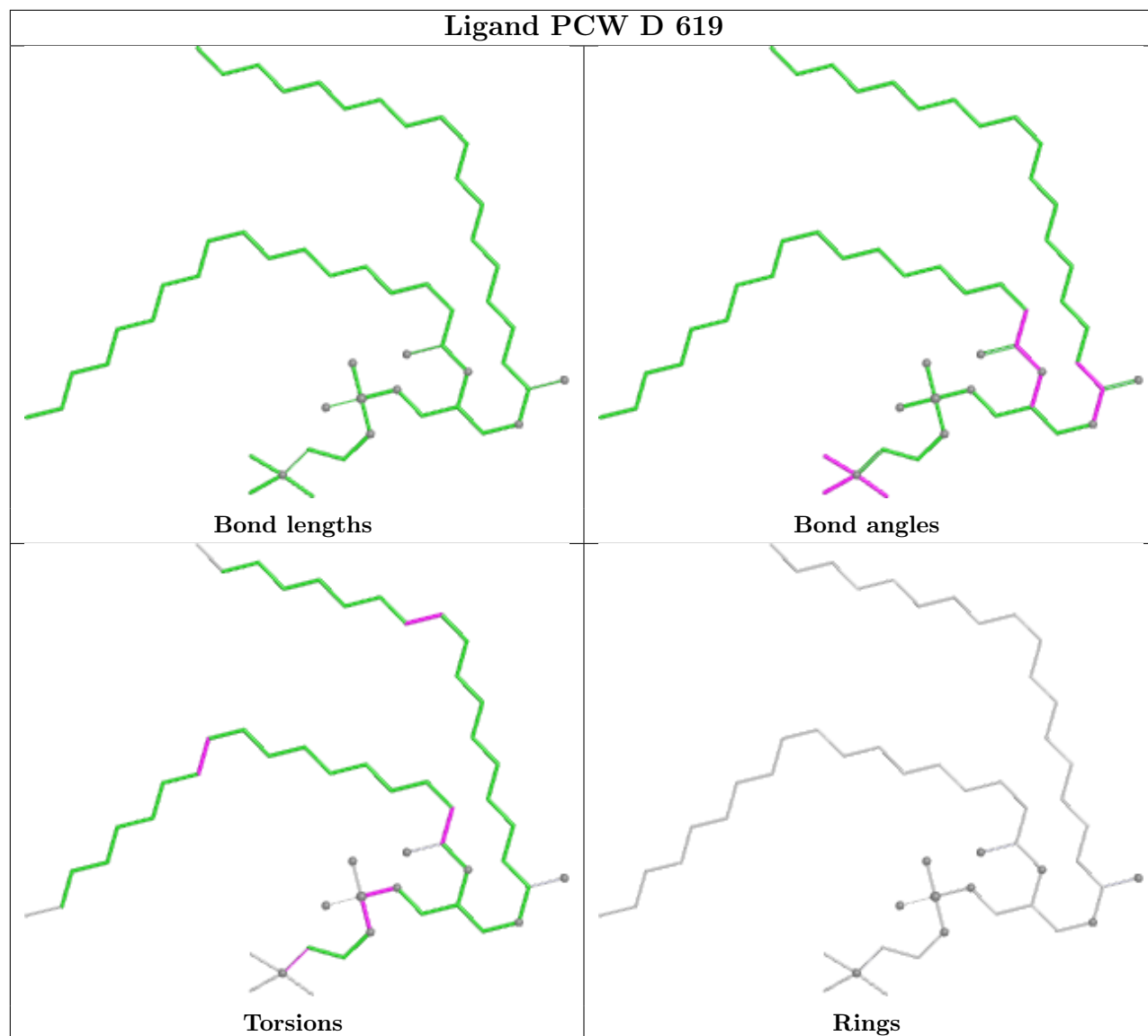


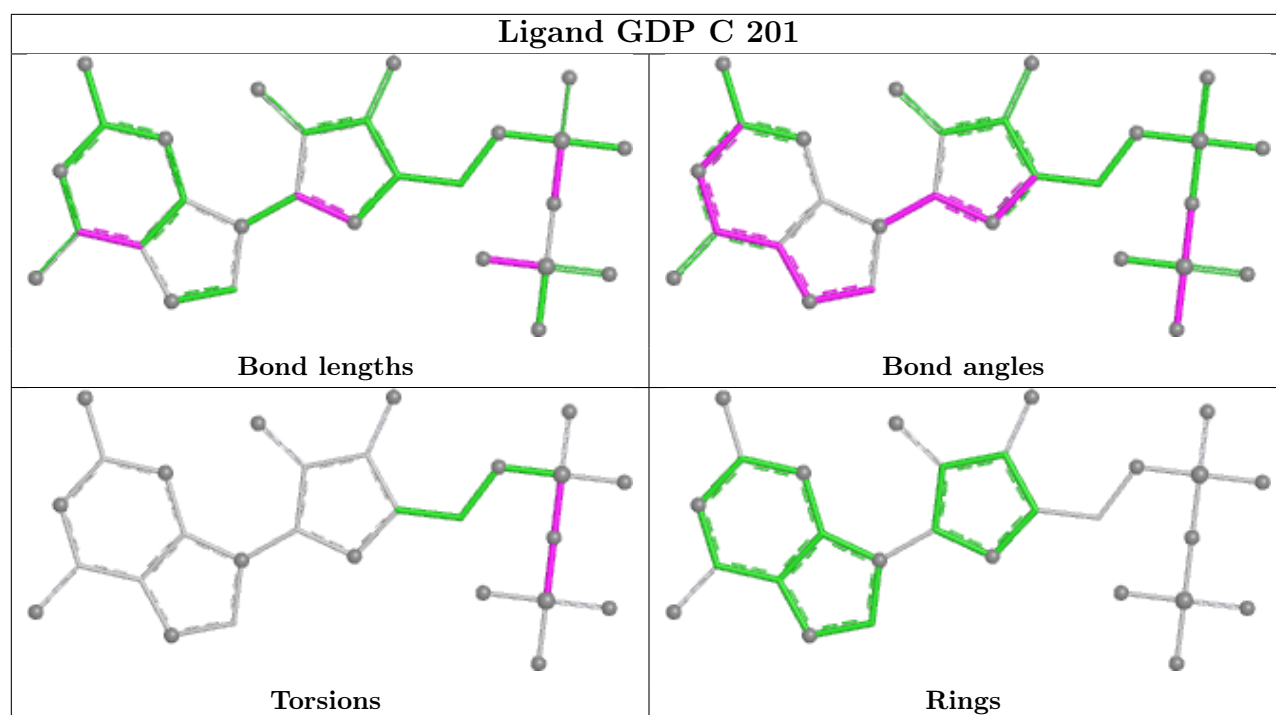


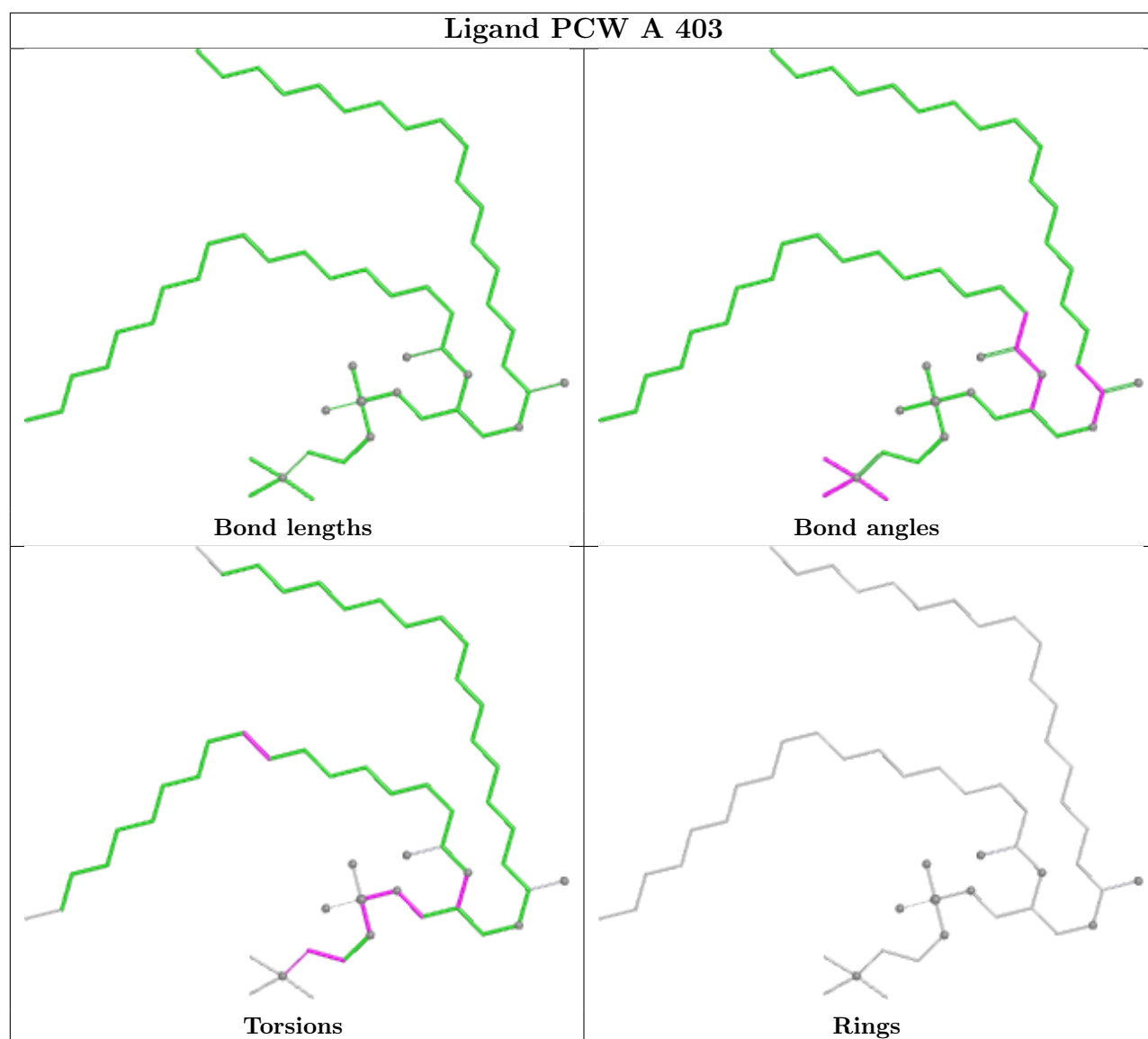


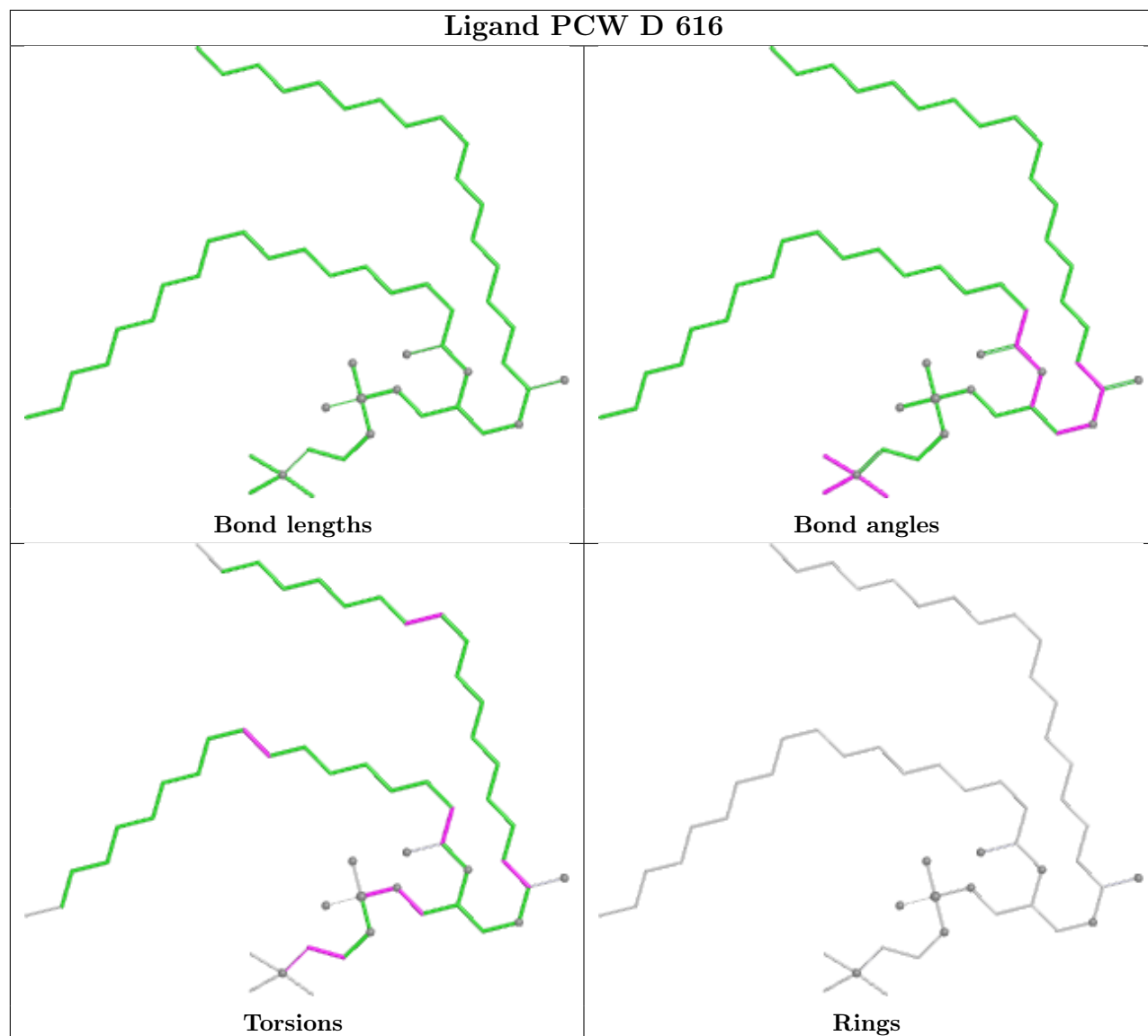
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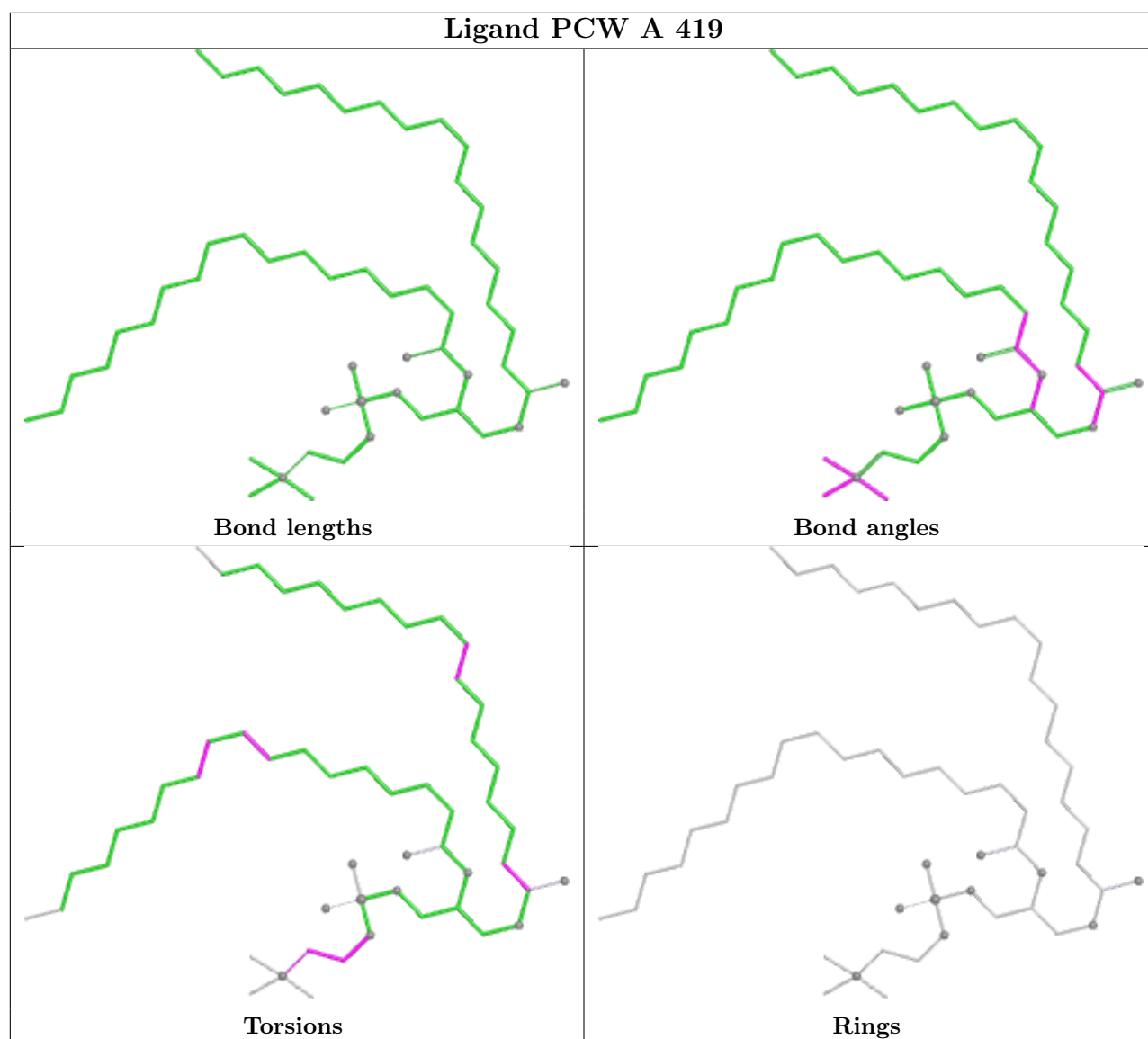


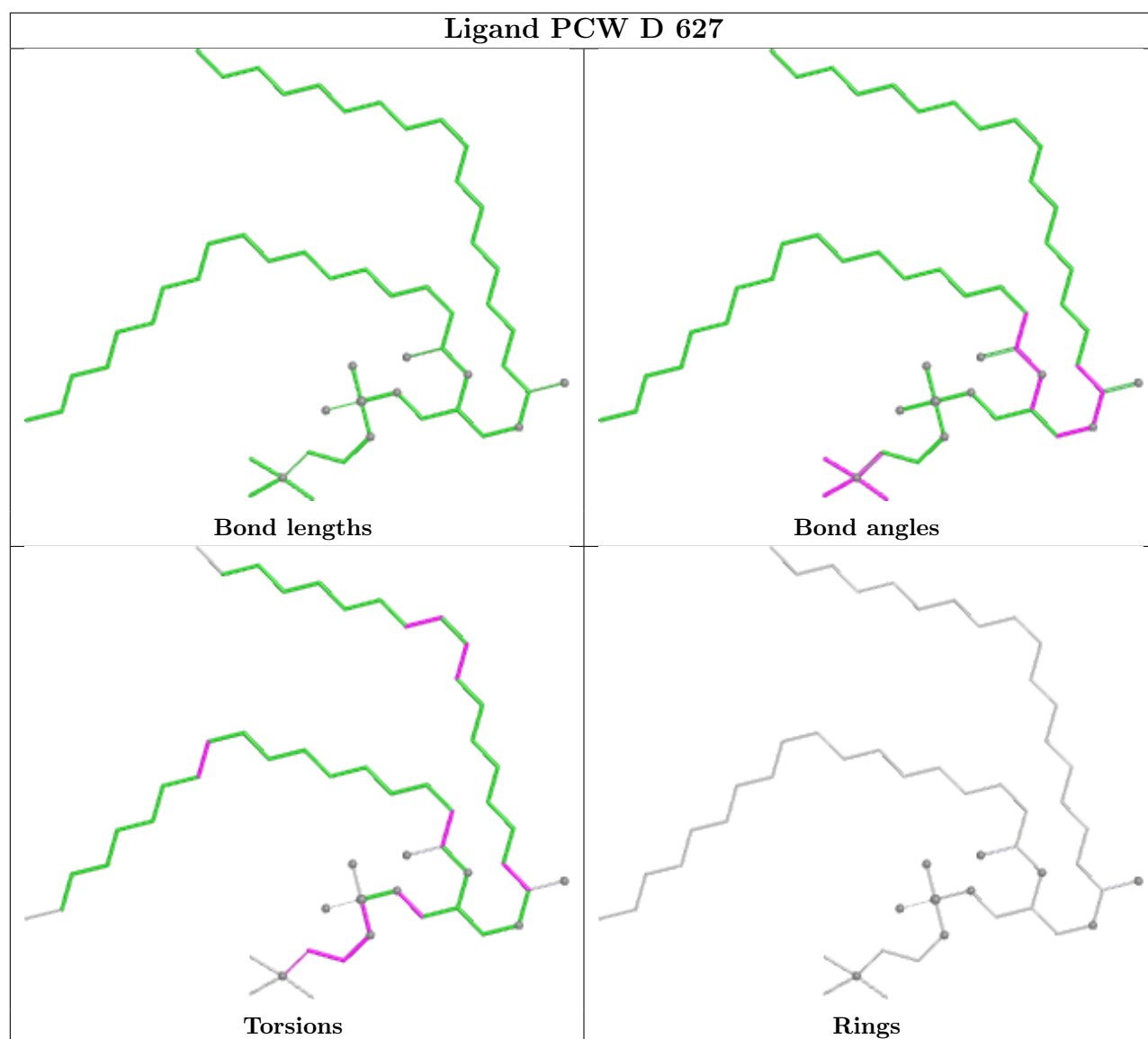


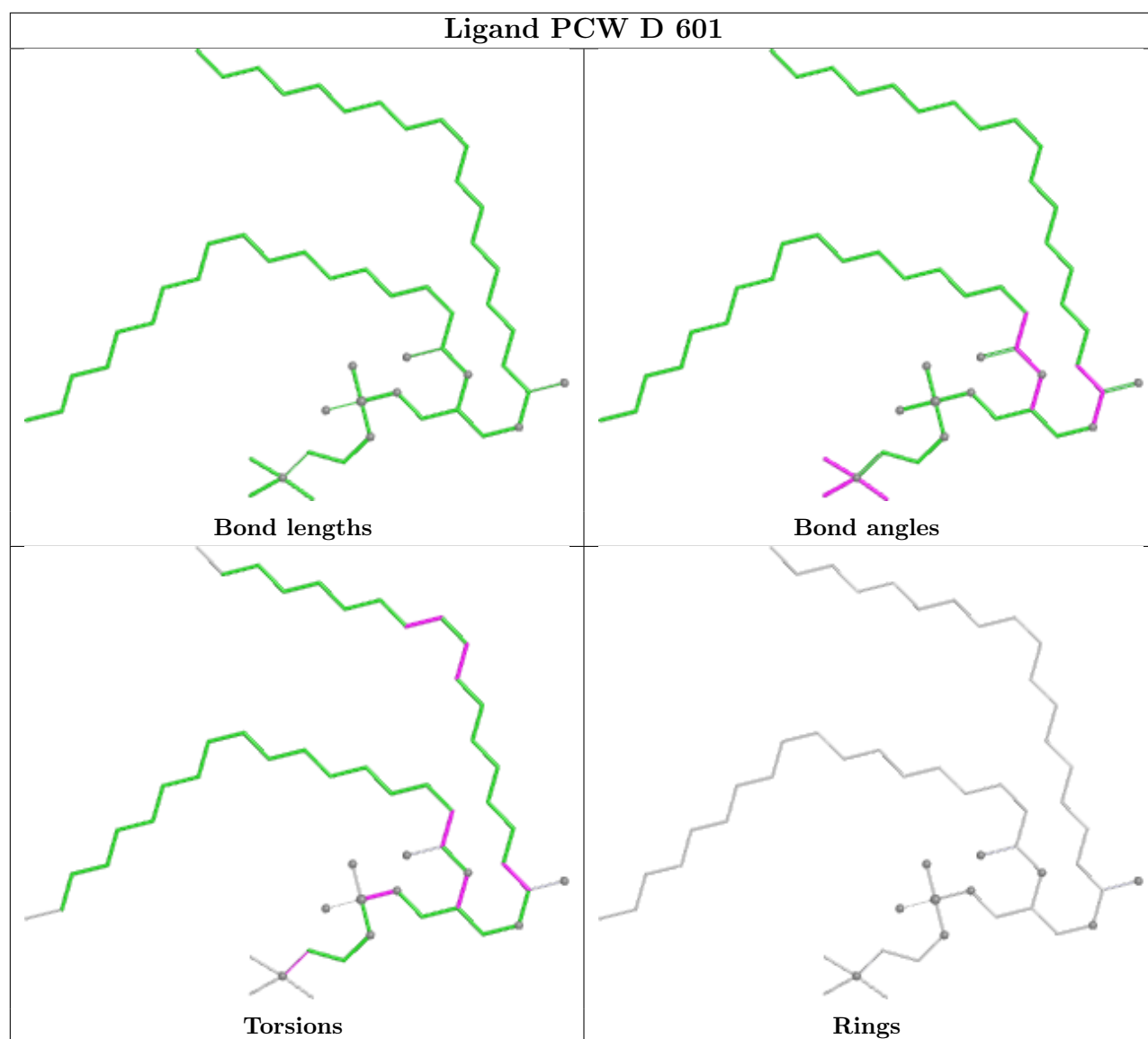


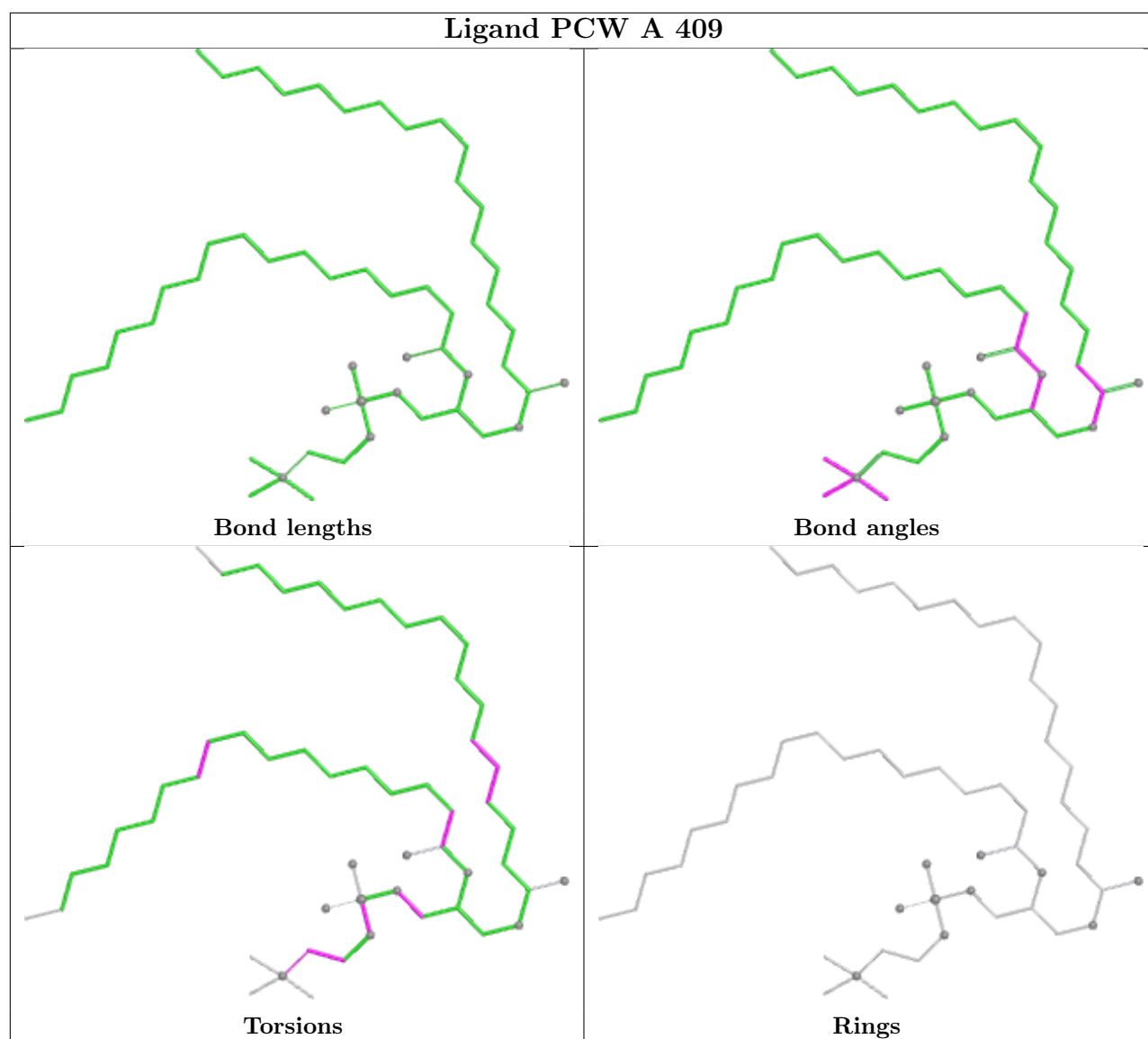


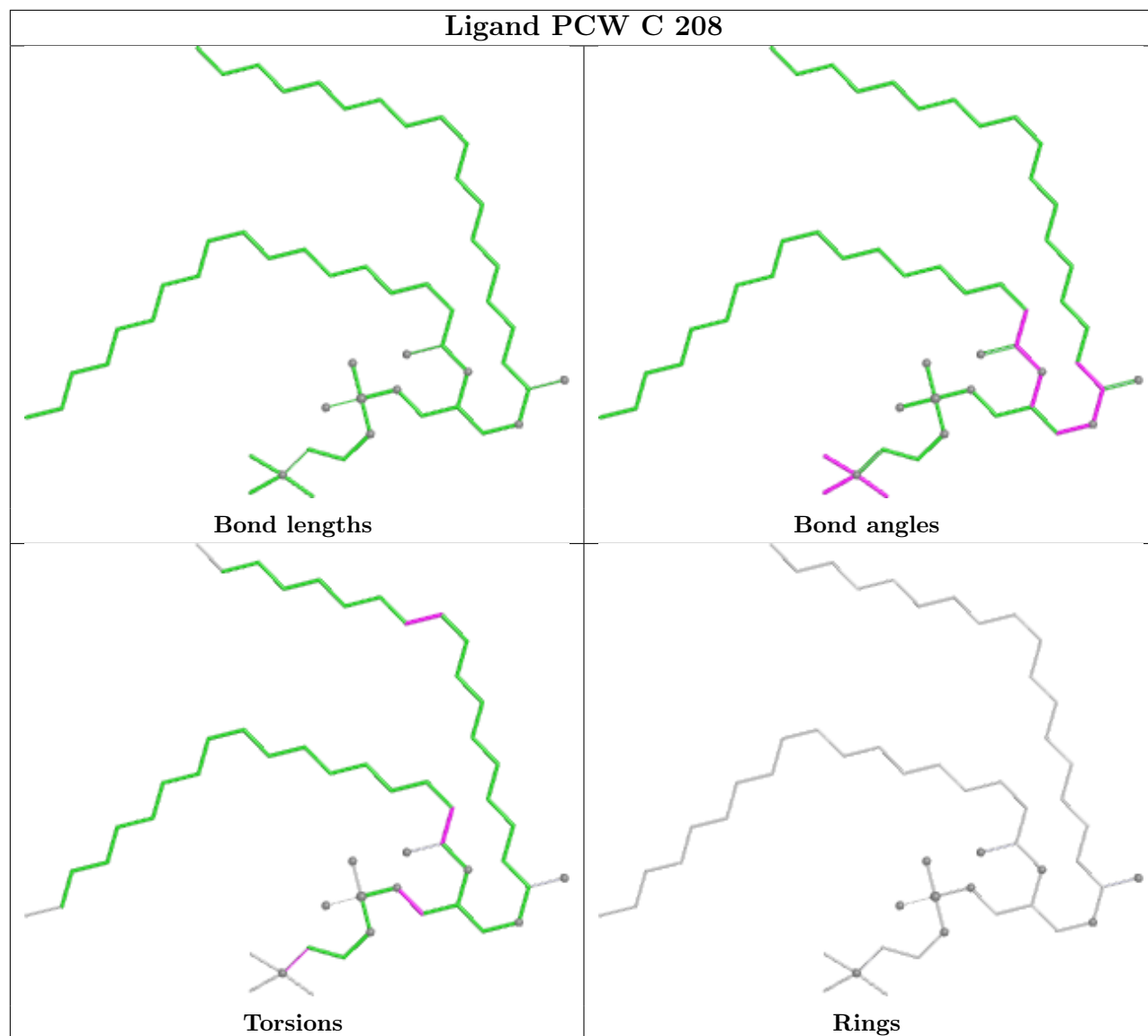


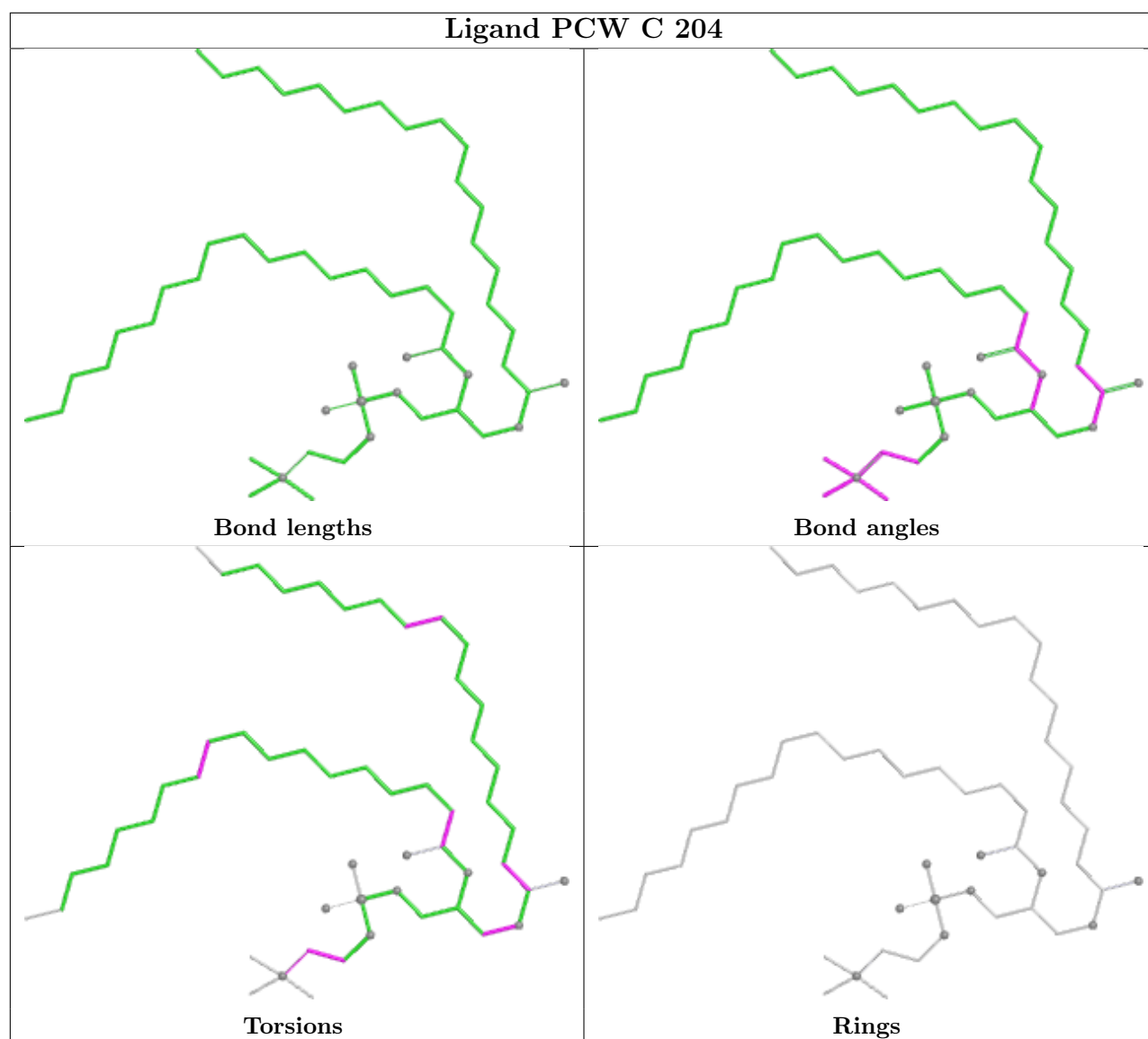












6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 2% for the well-defined parts and 2% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	190
Number of shifts mapped to atoms	70
Number of unparsed shifts	0
Number of shifts with mapping errors	120
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 120 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	6	LEU	HD11	0.7649	.	2
1	B	6	LEU	HD12	0.7649	.	2
1	B	6	LEU	HD13	0.7649	.	2
1	B	6	LEU	HD21	0.4933	.	2
1	B	6	LEU	HD22	0.4933	.	2
1	B	6	LEU	HD23	0.4933	.	2
1	B	8	VAL	HG11	0.7753	.	2
1	B	8	VAL	HG12	0.7753	.	2
1	B	8	VAL	HG13	0.7753	.	2
1	B	14	VAL	HG11	0.9972	.	2
1	B	14	VAL	HG12	0.9972	.	2
1	B	14	VAL	HG13	0.9972	.	2
1	B	19	LEU	HD11	0.4324	.	2
1	B	19	LEU	HD12	0.4324	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	19	LEU	HD13	0.4324	.	2
1	B	19	LEU	HD21	0.5838	.	2
1	B	19	LEU	HD22	0.5838	.	2
1	B	19	LEU	HD23	0.5838	.	2
1	B	21	ILE	HD11	-0.1199	.	1
1	B	21	ILE	HD12	-0.1199	.	1
1	B	21	ILE	HD13	-0.1199	.	1
1	B	23	LEU	HD11	-0.4194	.	2
1	B	23	LEU	HD12	-0.4194	.	2
1	B	23	LEU	HD13	-0.4194	.	2
1	B	24	ILE	HD11	0.2711	.	1
1	B	24	ILE	HD12	0.2711	.	1
1	B	24	ILE	HD13	0.2711	.	1
1	B	29	VAL	HG11	0.4389	.	2
1	B	29	VAL	HG12	0.4389	.	2
1	B	29	VAL	HG13	0.4389	.	2
1	B	29	VAL	HG21	0.5738	.	2
1	B	29	VAL	HG22	0.5738	.	2
1	B	29	VAL	HG23	0.5738	.	2
1	B	36	ILE	HD11	0.5128	.	1
1	B	36	ILE	HD12	0.5128	.	1
1	B	36	ILE	HD13	0.5128	.	1
1	B	44	VAL	HG11	0.5439	.	2
1	B	44	VAL	HG12	0.5439	.	2
1	B	44	VAL	HG13	0.5439	.	2
1	B	45	VAL	HG11	0.4386	.	2
1	B	45	VAL	HG12	0.4386	.	2
1	B	45	VAL	HG13	0.4386	.	2
1	B	46	ILE	HD11	0.2688	.	1
1	B	46	ILE	HD12	0.2688	.	1
1	B	46	ILE	HD13	0.2688	.	1
1	B	55	ILE	HD11	0.3484	.	1
1	B	55	ILE	HD12	0.3484	.	1
1	B	55	ILE	HD13	0.3484	.	1
1	B	56	LEU	HD11	0.3279	.	2
1	B	56	LEU	HD12	0.3279	.	2
1	B	56	LEU	HD13	0.3279	.	2
1	B	79	LEU	HD11	-0.0802	.	2
1	B	79	LEU	HD12	-0.0802	.	2
1	B	79	LEU	HD13	-0.0802	.	2
1	B	79	LEU	HD21	-0.0067	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	79	LEU	HD22	-0.0067	.	2
1	B	79	LEU	HD23	-0.0067	.	2
1	B	81	VAL	HG11	0.3718	.	2
1	B	81	VAL	HG12	0.3718	.	2
1	B	81	VAL	HG13	0.3718	.	2
1	B	81	VAL	HG21	0.4788	.	2
1	B	81	VAL	HG22	0.4788	.	2
1	B	81	VAL	HG23	0.4788	.	2
1	B	84	ILE	HD11	0.5835	.	1
1	B	84	ILE	HD12	0.5835	.	1
1	B	84	ILE	HD13	0.5835	.	1
1	B	93	ILE	HD11	0.6278	.	1
1	B	93	ILE	HD12	0.6278	.	1
1	B	93	ILE	HD13	0.6278	.	1
1	B	100	ILE	HD11	0.2013	.	1
1	B	100	ILE	HD12	0.2013	.	1
1	B	100	ILE	HD13	0.2013	.	1
1	B	103	VAL	HG11	0.8609	.	2
1	B	103	VAL	HG12	0.8609	.	2
1	B	103	VAL	HG13	0.8609	.	2
1	B	103	VAL	HG21	0.7641	.	2
1	B	103	VAL	HG22	0.7641	.	2
1	B	103	VAL	HG23	0.7641	.	2
1	B	109	VAL	HG11	0.5231	.	2
1	B	109	VAL	HG12	0.5231	.	2
1	B	109	VAL	HG13	0.5231	.	2
1	B	112	VAL	HG11	0.5984	.	2
1	B	112	VAL	HG12	0.5984	.	2
1	B	112	VAL	HG13	0.5984	.	2
1	B	113	LEU	HD11	0.8924	.	2
1	B	113	LEU	HD12	0.8924	.	2
1	B	113	LEU	HD13	0.8924	.	2
1	B	114	VAL	HG11	0.511	.	2
1	B	114	VAL	HG12	0.511	.	2
1	B	114	VAL	HG13	0.511	.	2
1	B	120	LEU	HD11	0.7114	.	2
1	B	120	LEU	HD12	0.7114	.	2
1	B	120	LEU	HD13	0.7114	.	2
1	B	125	VAL	HG11	-0.35	.	2
1	B	125	VAL	HG12	-0.35	.	2
1	B	125	VAL	HG13	-0.35	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	125	VAL	HG21	0.4923	.	2
1	B	125	VAL	HG22	0.4923	.	2
1	B	125	VAL	HG23	0.4923	.	2
1	B	133	LEU	HD11	0.2492	.	2
1	B	133	LEU	HD12	0.2492	.	2
1	B	133	LEU	HD13	0.2492	.	2
1	B	139	ILE	HD11	0.7014	.	1
1	B	139	ILE	HD12	0.7014	.	1
1	B	139	ILE	HD13	0.7014	.	1
1	B	142	ILE	HD11	0.5153	.	1
1	B	142	ILE	HD12	0.5153	.	1
1	B	142	ILE	HD13	0.5153	.	1
1	B	159	LEU	HD11	0.5167	.	2
1	B	159	LEU	HD12	0.5167	.	2
1	B	159	LEU	HD13	0.5167	.	2
1	B	160	VAL	HG11	-0.146	.	2
1	B	160	VAL	HG12	-0.146	.	2
1	B	160	VAL	HG13	-0.146	.	2
1	B	160	VAL	HG21	0.4847	.	2
1	B	160	VAL	HG22	0.4847	.	2
1	B	160	VAL	HG23	0.4847	.	2
1	B	163	ILE	HD11	0.4805	.	1
1	B	163	ILE	HD12	0.4805	.	1
1	B	163	ILE	HD13	0.4805	.	1

7.1.2 Chemical shift referencing ⓘ

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 2%, i.e. 174 atoms were assigned a chemical shift out of a possible 9964. 0 out of 130 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	14/3540 (0%)	7/1432 (0%)	0/1420 (0%)	7/688 (1%)
Sidechain	160/5800 (3%)	120/3731 (3%)	40/1812 (2%)	0/257 (0%)
Aromatic	0/624 (0%)	0/308 (0%)	0/291 (0%)	0/25 (0%)
Overall	174/9964 (2%)	127/5471 (2%)	40/3523 (1%)	7/970 (1%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 2%, i.e. 190 atoms were assigned a chemical shift out of a possible 10622. 0 out of 134 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	30/3772 (1%)	15/1526 (1%)	0/1512 (0%)	15/734 (2%)
Sidechain	160/6214 (3%)	120/3990 (3%)	40/1944 (2%)	0/280 (0%)
Aromatic	0/636 (0%)	0/314 (0%)	0/296 (0%)	0/26 (0%)
Overall	190/10622 (2%)	135/5830 (2%)	40/3752 (1%)	15/1040 (1%)

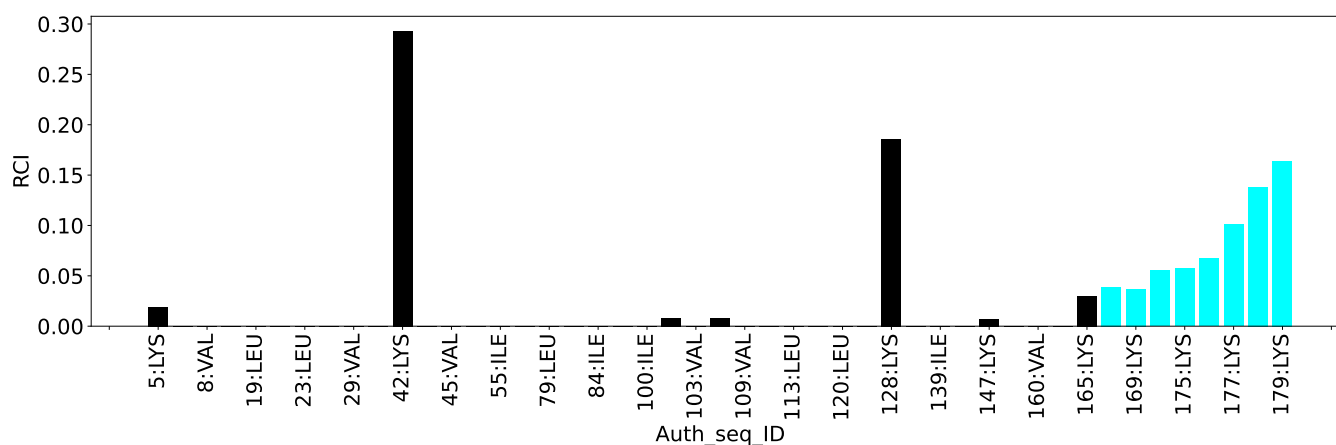
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain B:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	226
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	0
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	0
Inter-chain	226
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.3
Number of long range restraints per residue ¹	0.0

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.7	0.19
0.2-0.5 (Medium)	1.5	0.5
>0.5 (Large)	16.9	14.25

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

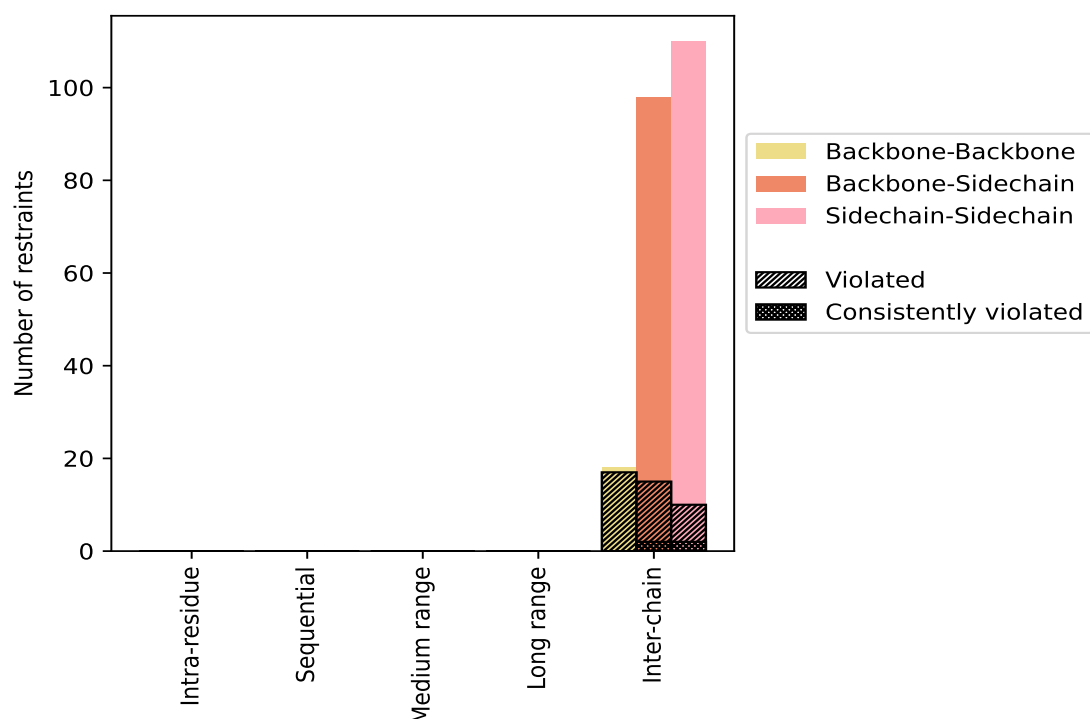
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	226	100.0	42	18.6	18.6	4	1.8	1.8
Backbone-Backbone	18	8.0	17	94.4	7.5	0	0.0	0.0
Backbone-Sidechain	98	43.4	15	15.3	6.6	2	2.0	0.9
Sidechain-Sidechain	110	48.7	10	9.1	4.4	2	1.8	0.9
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	226	100.0	42	18.6	18.6	4	1.8	1.8
Backbone-Backbone	18	8.0	17	94.4	7.5	0	0.0	0.0
Backbone-Sidechain	98	43.4	15	15.3	6.6	2	2.0	0.9
Sidechain-Sidechain	110	48.7	10	9.1	4.4	2	1.8	0.9

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	0	0	0	15	15	2.62	7.76	2.53	1.67
2	0	0	0	0	17	17	2.7	9.36	2.61	2.23
3	0	0	0	0	17	17	4.33	11.65	3.61	2.22
4	0	0	0	0	15	15	3.7	9.48	3.32	2.48
5	0	0	0	0	30	30	3.79	13.68	3.97	2.4
6	0	0	0	0	23	23	3.95	13.41	3.83	2.16
7	0	0	0	0	16	16	2.98	7.87	2.19	2.06
8	0	0	0	0	12	12	4.16	10.06	2.85	3.4
9	0	0	0	0	16	16	2.9	8.04	2.36	2.42
10	0	0	0	0	21	21	2.03	5.53	1.16	1.89

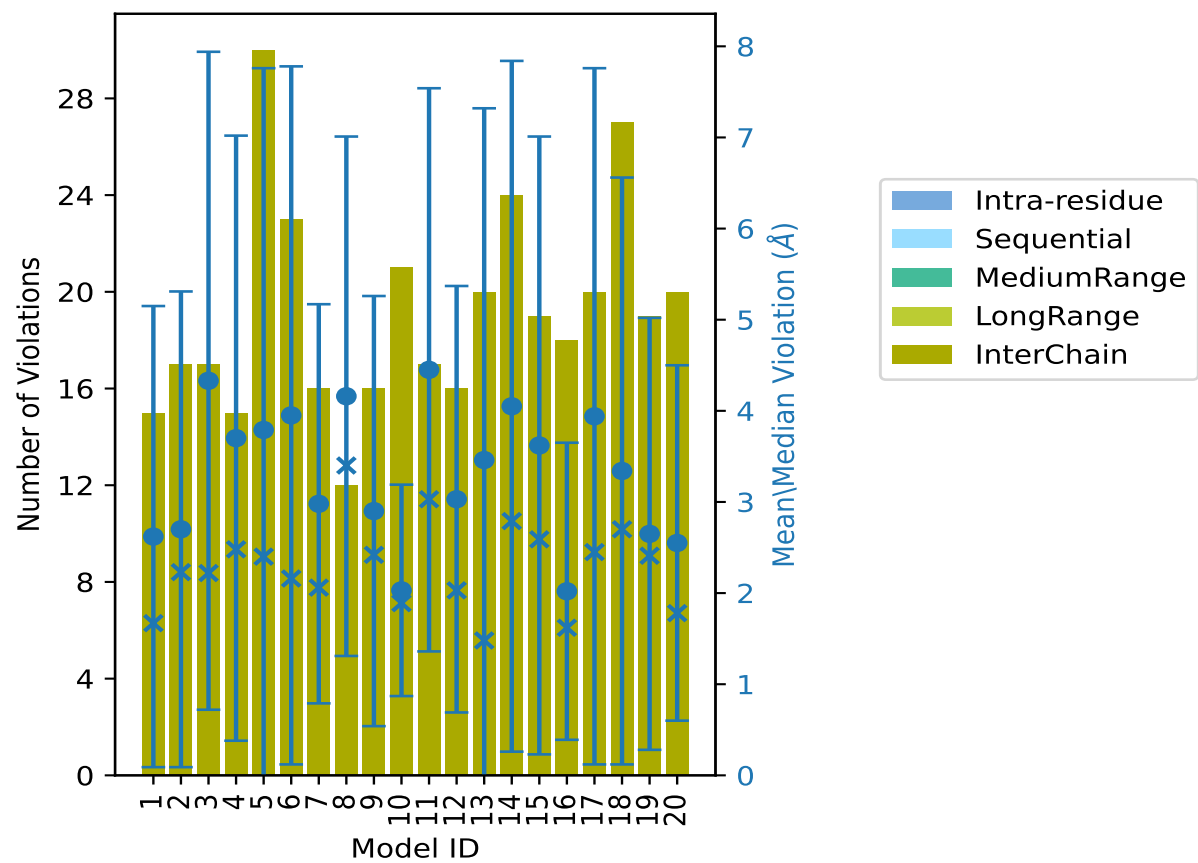
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	0	0	17	17	4.45	11.29	3.09	3.03
12	0	0	0	0	16	16	3.03	8.66	2.34	2.03
13	0	0	0	0	20	20	3.46	12.01	3.86	1.48
14	0	0	0	0	24	24	4.05	13.51	3.79	2.79
15	0	0	0	0	19	19	3.62	13.58	3.39	2.59
16	0	0	0	0	18	18	2.02	6.2	1.63	1.62
17	0	0	0	0	20	20	3.94	12.84	3.82	2.45
18	0	0	0	0	27	27	3.34	14.25	3.22	2.7
19	0	0	0	0	19	19	2.65	9.71	2.37	2.41
20	0	0	0	0	20	20	2.55	7.77	1.95	1.78

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble

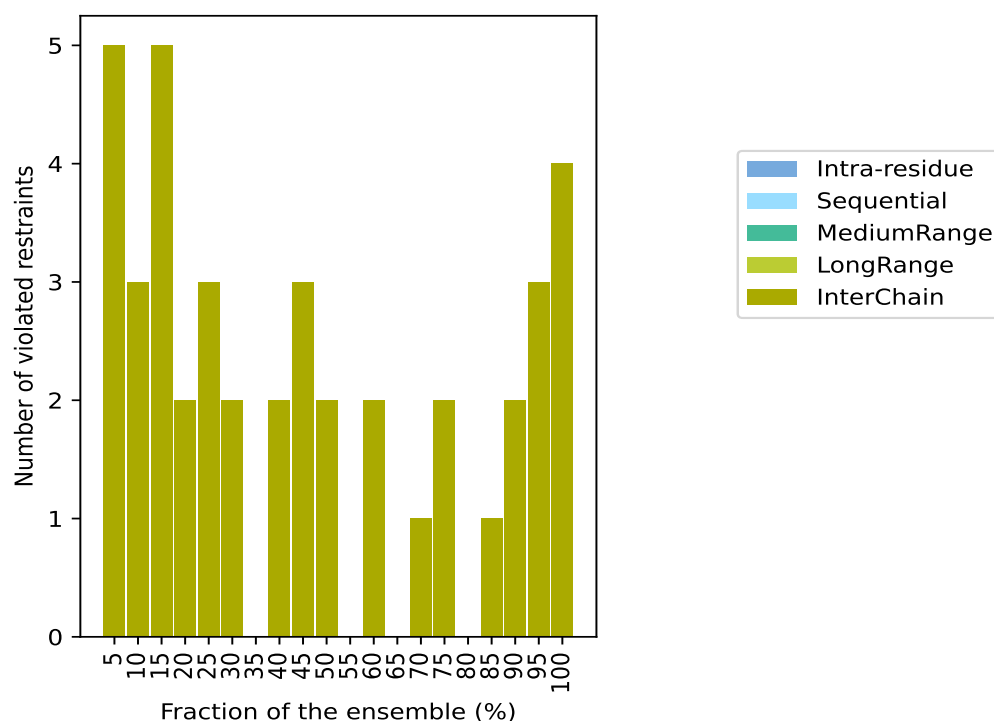
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 184(IR:0, SQ:0, MR:0, LR:0, IC:184) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	5	5	1	5.0
0	0	0	0	3	3	2	10.0
0	0	0	0	5	5	3	15.0
0	0	0	0	2	2	4	20.0
0	0	0	0	3	3	5	25.0
0	0	0	0	2	2	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	2	2	8	40.0
0	0	0	0	3	3	9	45.0
0	0	0	0	2	2	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	2	2	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	1	1	14	70.0
0	0	0	0	2	2	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	1	1	17	85.0
0	0	0	0	2	2	18	90.0
0	0	0	0	3	3	19	95.0
0	0	0	0	4	4	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

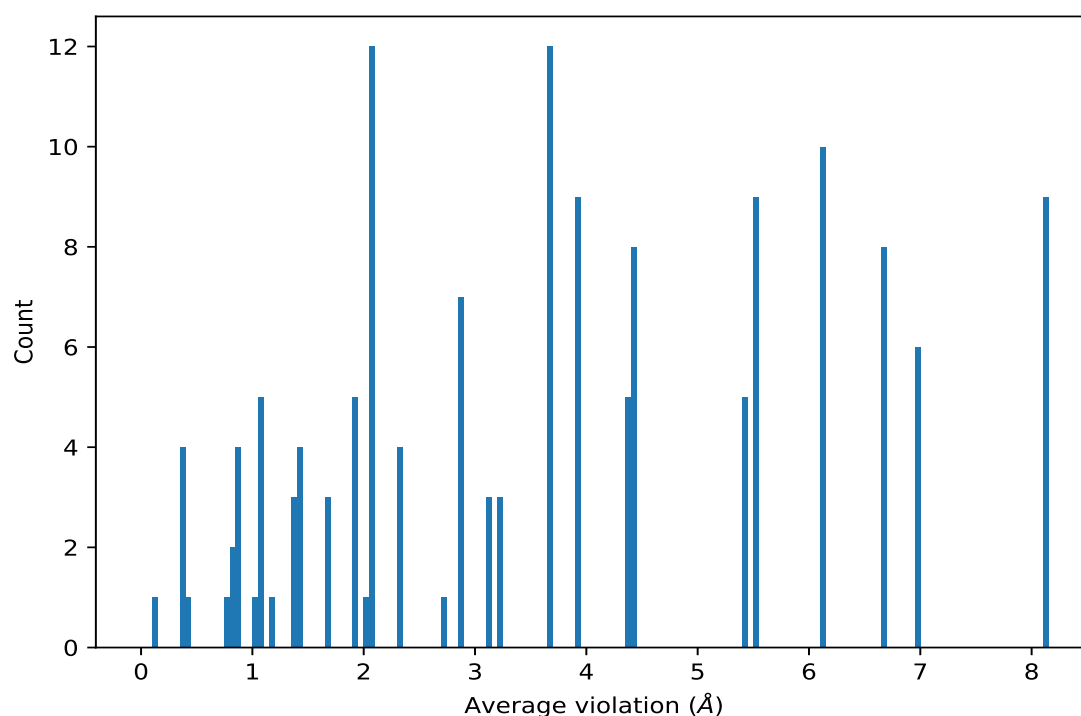
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,45)	2:36:B:ILE:CD1	3:412:A:PCW:C6	20	8.1	3.89	7.58
(1,45)	2:36:B:ILE:CD1	3:412:A:PCW:C5	20	8.1	3.89	7.58
(1,45)	2:36:B:ILE:CD1	3:402:A:PCW:C4	20	8.1	3.89	7.58
(1,45)	2:36:B:ILE:CD1	3:405:A:PCW:C6	20	8.1	3.89	7.58
(1,45)	2:36:B:ILE:CD1	3:402:A:PCW:C6	20	8.1	3.89	7.58
(1,45)	2:36:B:ILE:CD1	3:404:A:PCW:C4	20	8.1	3.89	7.58
(1,45)	2:36:B:ILE:CD1	3:407:A:PCW:C7	20	8.1	3.89	7.58
(1,45)	2:36:B:ILE:CD1	3:406:A:PCW:C6	20	8.1	3.89	7.58
(1,45)	2:36:B:ILE:CD1	3:411:A:PCW:C7	20	8.1	3.89	7.58
(1,32)	2:36:C:ILE:CD1	4:414:A:17F:N1	20	3.93	2.45	3.5
(1,32)	2:36:C:ILE:CD1	4:415:A:17F:O4	20	3.93	2.45	3.5
(1,32)	2:36:C:ILE:CD1	3:410:A:PCW:C7	20	3.93	2.45	3.5
(1,32)	2:36:C:ILE:CD1	4:415:A:17F:O5	20	3.93	2.45	3.5
(1,32)	2:36:C:ILE:CD1	3:412:A:PCW:C8	20	3.93	2.45	3.5
(1,32)	2:36:C:ILE:CD1	3:411:A:PCW:C7	20	3.93	2.45	3.5
(1,32)	2:36:C:ILE:CD1	4:415:A:17F:C1	20	3.93	2.45	3.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,32)	2:36:C:ILE:CD1	3:412:A:PCW:C5	20	3.93	2.45	3.5
(1,32)	2:36:C:ILE:CD1	3:402:A:PCW:C7	20	3.93	2.45	3.5
(1,24)	2:170:B:MET:CG	2:163:C:ILE:CD1	20	2.86	1.02	2.79
(1,9)	2:170:C:MET:CG	2:163:B:ILE:CD1	20	2.73	1.28	2.84
(1,48)	2:6:B:LEU:N	3:410:A:PCW:C5	19	6.95	2.5	7.52
(1,48)	2:6:B:LEU:N	3:410:A:PCW:C7	19	6.95	2.5	7.52
(1,48)	2:6:B:LEU:N	3:407:A:PCW:C7	19	6.95	2.5	7.52
(1,48)	2:6:B:LEU:N	3:407:A:PCW:C6	19	6.95	2.5	7.52
(1,48)	2:6:B:LEU:N	4:415:A:17F:O4	19	6.95	2.5	7.52
(1,48)	2:6:B:LEU:N	3:407:A:PCW:C8	19	6.95	2.5	7.52
(1,50)	2:105:B:ASP:N	3:407:A:PCW:C7	19	5.54	2.16	5.34
(1,50)	2:105:B:ASP:N	3:405:A:PCW:C6	19	5.54	2.16	5.34
(1,50)	2:105:B:ASP:N	3:407:A:PCW:C6	19	5.54	2.16	5.34
(1,50)	2:105:B:ASP:N	3:411:A:PCW:C6	19	5.54	2.16	5.34
(1,50)	2:105:B:ASP:N	3:408:A:PCW:C6	19	5.54	2.16	5.34
(1,50)	2:105:B:ASP:N	3:402:A:PCW:C4	19	5.54	2.16	5.34
(1,50)	2:105:B:ASP:N	3:403:A:PCW:C8	19	5.54	2.16	5.34
(1,50)	2:105:B:ASP:N	3:408:A:PCW:C7	19	5.54	2.16	5.34
(1,50)	2:105:B:ASP:N	4:414:A:17F:O5	19	5.54	2.16	5.34
(1,12)	2:170:C:MET:CG	2:170:B:MET:N	19	1.66	0.89	1.83
(1,44)	2:24:B:ILE:CD1	3:410:A:PCW:C5	18	6.65	3.81	6.44
(1,44)	2:24:B:ILE:CD1	3:410:A:PCW:C7	18	6.65	3.81	6.44
(1,44)	2:24:B:ILE:CD1	3:407:A:PCW:C7	18	6.65	3.81	6.44
(1,44)	2:24:B:ILE:CD1	3:405:A:PCW:C6	18	6.65	3.81	6.44
(1,44)	2:24:B:ILE:CD1	3:411:A:PCW:C8	18	6.65	3.81	6.44
(1,44)	2:24:B:ILE:CD1	3:407:A:PCW:C8	18	6.65	3.81	6.44
(1,44)	2:24:B:ILE:CD1	3:410:A:PCW:C8	18	6.65	3.81	6.44
(1,44)	2:24:B:ILE:CD1	3:411:A:PCW:C7	18	6.65	3.81	6.44
(1,27)	2:170:B:MET:CG	2:170:C:MET:N	18	1.68	0.71	1.85
(1,49)	2:43:B:GLN:N	3:410:A:PCW:C5	17	6.14	4.07	7.2
(1,49)	2:43:B:GLN:N	3:410:A:PCW:C7	17	6.14	4.07	7.2
(1,49)	2:43:B:GLN:N	3:402:A:PCW:C4	17	6.14	4.07	7.2
(1,49)	2:43:B:GLN:N	3:407:A:PCW:C6	17	6.14	4.07	7.2
(1,49)	2:43:B:GLN:N	3:405:A:PCW:C5	17	6.14	4.07	7.2
(1,49)	2:43:B:GLN:N	3:407:A:PCW:C8	17	6.14	4.07	7.2
(1,49)	2:43:B:GLN:N	3:410:A:PCW:C8	17	6.14	4.07	7.2
(1,49)	2:43:B:GLN:N	3:407:A:PCW:C7	17	6.14	4.07	7.2
(1,49)	2:43:B:GLN:N	3:405:A:PCW:C6	17	6.14	4.07	7.2
(1,49)	2:43:B:GLN:N	3:405:A:PCW:C7	17	6.14	4.07	7.2
(1,13)	2:170:C:MET:CG	2:173:B:ASP:N	15	2.03	0.98	1.97
(1,28)	2:170:B:MET:CG	2:173:C:ASP:N	15	1.69	0.71	1.66
(1,47)	2:46:B:ILE:CG2	3:408:A:PCW:C8	14	3.69	2.64	2.76

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,47)	2:46:B:ILE:CG1	3:410:A:PCW:C7	14	3.69	2.64	2.76
(1,47)	2:46:B:ILE:CG2	3:413:A:PCW:C6	14	3.69	2.64	2.76
(1,47)	2:46:B:ILE:CG2	3:403:A:PCW:C7	14	3.69	2.64	2.76
(1,47)	2:46:B:ILE:CG2	3:413:A:PCW:C7	14	3.69	2.64	2.76
(1,47)	2:46:B:ILE:CG1	3:407:A:PCW:C7	14	3.69	2.64	2.76
(1,47)	2:46:B:ILE:CG2	4:414:A:17F:O4	14	3.69	2.64	2.76
(1,47)	2:46:B:ILE:CG1	3:407:A:PCW:C6	14	3.69	2.64	2.76
(1,47)	2:46:B:ILE:CG2	3:413:A:PCW:C8	14	3.69	2.64	2.76
(1,47)	2:46:B:ILE:CG2	3:404:A:PCW:C5	14	3.69	2.64	2.76
(1,47)	2:46:B:ILE:CG2	3:409:A:PCW:C4	14	3.69	2.64	2.76
(1,47)	2:46:B:ILE:CG1	3:405:A:PCW:C7	14	3.69	2.64	2.76
(1,7)	2:170:C:MET:CG	2:46:B:ILE:CD1	12	1.2	0.86	0.92
(1,8)	2:170:C:MET:CG	2:160:B:VAL:CG1	12	1.06	0.86	0.71
(1,43)	2:180:C:LYS:N	3:403:A:PCW:C7	10	4.4	4.85	2.24
(1,43)	2:180:C:LYS:N	3:403:A:PCW:C5	10	4.4	4.85	2.24
(1,43)	2:180:C:LYS:N	3:409:A:PCW:C6	10	4.4	4.85	2.24
(1,43)	2:180:C:LYS:N	3:410:A:PCW:C4	10	4.4	4.85	2.24
(1,43)	2:180:C:LYS:N	3:402:A:PCW:C4	10	4.4	4.85	2.24
(1,43)	2:180:C:LYS:N	3:403:A:PCW:C4	10	4.4	4.85	2.24
(1,43)	2:180:C:LYS:N	3:410:A:PCW:C5	10	4.4	4.85	2.24
(1,43)	2:180:C:LYS:N	3:405:A:PCW:C6	10	4.4	4.85	2.24
(1,22)	2:170:B:MET:CG	2:46:C:ILE:CD1	10	1.42	1.01	1.11
(1,31)	2:24:C:ILE:CD1	3:404:A:PCW:C4	9	2.06	2.34	0.64
(1,31)	2:24:C:ILE:CD1	4:415:A:17F:O5	9	2.06	2.34	0.64
(1,31)	2:24:C:ILE:CD1	3:412:A:PCW:C4	9	2.06	2.34	0.64
(1,31)	2:24:C:ILE:CD1	3:405:A:PCW:C4	9	2.06	2.34	0.64
(1,31)	2:24:C:ILE:CD1	4:415:A:17F:C1	9	2.06	2.34	0.64
(1,31)	2:24:C:ILE:CD1	3:410:A:PCW:C6	9	2.06	2.34	0.64
(1,31)	2:24:C:ILE:CD1	3:402:A:PCW:C7	9	2.06	2.34	0.64
(1,36)	2:43:C:GLN:N	3:404:A:PCW:C4	9	2.06	1.29	1.56
(1,36)	2:43:C:GLN:N	3:412:A:PCW:C4	9	2.06	1.29	1.56
(1,36)	2:43:C:GLN:N	3:405:A:PCW:C4	9	2.06	1.29	1.56
(1,36)	2:43:C:GLN:N	4:415:A:17F:C1	9	2.06	1.29	1.56
(1,36)	2:43:C:GLN:N	3:410:A:PCW:C6	9	2.06	1.29	1.56
(1,23)	2:170:B:MET:CG	2:160:C:VAL:CG1	9	1.02	0.85	0.77
(1,56)	2:180:B:LYS:N	3:404:A:PCW:C6	8	2.88	1.52	3.08
(1,56)	2:180:B:LYS:N	3:405:A:PCW:C4	8	2.88	1.52	3.08
(1,56)	2:180:B:LYS:N	3:410:A:PCW:C7	8	2.88	1.52	3.08
(1,56)	2:180:B:LYS:N	3:411:A:PCW:C5	8	2.88	1.52	3.08
(1,56)	2:180:B:LYS:N	3:412:A:PCW:C4	8	2.88	1.52	3.08
(1,56)	2:180:B:LYS:N	3:412:A:PCW:C5	8	2.88	1.52	3.08
(1,37)	2:105:C:ASP:N	3:403:A:PCW:C4	8	2.34	2.36	1.66

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,37)	2:105:C:ASP:N	3:402:A:PCW:C4	8	2.34	2.36	1.66
(1,37)	2:105:C:ASP:N	3:407:A:PCW:C6	8	2.34	2.36	1.66
(1,37)	2:105:C:ASP:N	3:410:A:PCW:C7	8	2.34	2.36	1.66
(1,42)	2:179:C:LYS:N	3:403:A:PCW:C7	6	5.43	3.81	2.94
(1,42)	2:179:C:LYS:N	3:403:A:PCW:C5	6	5.43	3.81	2.94
(1,42)	2:179:C:LYS:N	3:403:A:PCW:C4	6	5.43	3.81	2.94
(1,42)	2:179:C:LYS:N	3:410:A:PCW:C5	6	5.43	3.81	2.94
(1,42)	2:179:C:LYS:N	3:405:A:PCW:C6	6	5.43	3.81	2.94
(1,41)	2:178:C:LYS:N	3:403:A:PCW:C7	6	4.36	2.9	3.29
(1,41)	2:178:C:LYS:N	3:403:A:PCW:C6	6	4.36	2.9	3.29
(1,41)	2:178:C:LYS:N	3:403:A:PCW:C4	6	4.36	2.9	3.29
(1,41)	2:178:C:LYS:N	3:408:A:PCW:C7	6	4.36	2.9	3.29
(1,41)	2:178:C:LYS:N	3:402:A:PCW:C4	6	4.36	2.9	3.29
(1,39)	2:176:C:LYS:N	4:414:A:17F:O4	5	1.94	0.92	1.65
(1,39)	2:176:C:LYS:N	3:413:A:PCW:C7	5	1.94	0.92	1.65
(1,39)	2:176:C:LYS:N	3:403:A:PCW:C5	5	1.94	0.92	1.65
(1,39)	2:176:C:LYS:N	3:405:A:PCW:C6	5	1.94	0.92	1.65
(1,39)	2:176:C:LYS:N	3:402:A:PCW:C4	5	1.94	0.92	1.65
(1,10)	2:170:C:MET:CG	2:166:B:HIS:N	5	0.79	0.34	0.88
(1,54)	2:178:B:LYS:N	3:404:A:PCW:C4	5	0.38	0.36	0.17
(1,54)	2:178:B:LYS:N	3:404:A:PCW:C6	5	0.38	0.36	0.17
(1,54)	2:178:B:LYS:N	3:410:A:PCW:C7	5	0.38	0.36	0.17
(1,55)	2:179:B:LYS:N	3:404:A:PCW:C4	4	1.09	1.0	0.66
(1,55)	2:179:B:LYS:N	3:412:A:PCW:C4	4	1.09	1.0	0.66
(1,55)	2:179:B:LYS:N	3:412:A:PCW:C5	4	1.09	1.0	0.66
(1,55)	2:179:B:LYS:N	3:404:A:PCW:C7	4	1.09	1.0	0.66
(1,34)	2:46:C:ILE:CG2	3:405:A:PCW:C6	4	0.87	0.76	0.6
(1,34)	2:46:C:ILE:CG1	4:415:A:17F:O5	4	0.87	0.76	0.6
(1,34)	2:46:C:ILE:CG1	3:410:A:PCW:C6	4	0.87	0.76	0.6
(1,34)	2:46:C:ILE:CG1	3:404:A:PCW:C4	4	0.87	0.76	0.6
(1,35)	2:6:C:LEU:N	3:407:A:PCW:C7	3	3.21	1.81	2.91
(1,35)	2:6:C:LEU:N	3:412:A:PCW:C5	3	3.21	1.81	2.91
(1,35)	2:6:C:LEU:N	3:410:A:PCW:C7	3	3.21	1.81	2.91
(1,40)	2:177:C:LYS:N	3:402:A:PCW:C4	3	3.12	0.93	2.81
(1,40)	2:177:C:LYS:N	3:403:A:PCW:C7	3	3.12	0.93	2.81
(1,40)	2:177:C:LYS:N	3:403:A:PCW:C6	3	3.12	0.93	2.81
(1,46)	2:45:B:VAL:CG1	4:414:A:17F:O5	3	1.41	0.45	1.6
(1,46)	2:45:B:VAL:CG1	4:414:A:17F:O4	3	1.41	0.45	1.6
(1,46)	2:45:B:VAL:CG1	3:403:A:PCW:C5	3	1.41	0.45	1.6
(1,51)	2:173:B:ASP:N	3:413:A:PCW:C8	3	1.37	0.53	1.05
(1,51)	2:173:B:ASP:N	3:407:A:PCW:C6	3	1.37	0.53	1.05
(1,51)	2:173:B:ASP:N	3:411:A:PCW:C6	3	1.37	0.53	1.05

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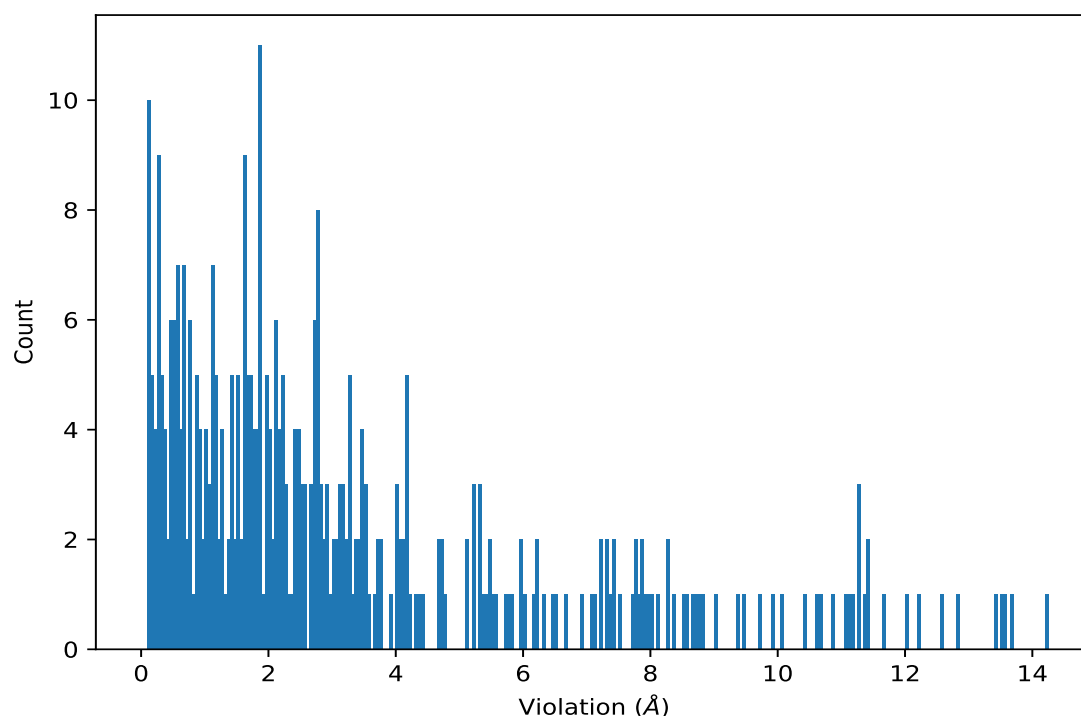
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,25)	2:170:B:MET:CG	2:166:C:HIS:N	3	0.39	0.29	0.28
(1,38)	2:173:C:ASP:N	3:402:A:PCW:C4	2	0.84	0.18	0.84
(1,38)	2:173:C:ASP:N	3:413:A:PCW:C6	2	0.84	0.18	0.84
(2,85)	2:39:C:SER:OG	2:180:B:LYS:N	2	0.41	0.3	0.41
(1,3)	2:118:C:CYS:SG	2:139:B:ILE:CD1	2	0.14	0.03	0.14

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	2:180:C:LYS:N	3:405:A:PCW:C6	18	14.25
(1,43)	2:180:C:LYS:N	3:403:A:PCW:C7	5	13.68
(1,45)	2:36:B:ILE:CD1	3:407:A:PCW:C7	15	13.58
(1,45)	2:36:B:ILE:CD1	3:402:A:PCW:C4	14	13.51
(1,45)	2:36:B:ILE:CD1	3:402:A:PCW:C4	6	13.41
(1,45)	2:36:B:ILE:CD1	3:402:A:PCW:C6	17	12.84
(1,44)	2:24:B:ILE:CD1	3:407:A:PCW:C7	14	12.55
(1,49)	2:43:B:GLN:N	3:407:A:PCW:C6	6	12.23
(1,49)	2:43:B:GLN:N	3:410:A:PCW:C8	13	12.01
(1,45)	2:36:B:ILE:CD1	3:402:A:PCW:C4	3	11.65
(1,44)	2:24:B:ILE:CD1	3:407:A:PCW:C7	6	11.41
(1,49)	2:43:B:GLN:N	3:410:A:PCW:C8	14	11.4
(1,44)	2:24:B:ILE:CD1	3:410:A:PCW:C7	5	11.37
(1,45)	2:36:B:ILE:CD1	3:412:A:PCW:C5	11	11.29
(1,48)	2:6:B:LEU:N	3:407:A:PCW:C7	17	11.26
(1,45)	2:36:B:ILE:CD1	3:402:A:PCW:C4	13	11.26
(1,42)	2:179:C:LYS:N	3:405:A:PCW:C6	18	11.19
(1,49)	2:43:B:GLN:N	3:410:A:PCW:C7	3	11.13
(1,44)	2:24:B:ILE:CD1	3:407:A:PCW:C7	13	11.07
(1,45)	2:36:B:ILE:CD1	3:402:A:PCW:C6	5	10.87
(1,48)	2:6:B:LEU:N	3:407:A:PCW:C6	11	10.69
(1,44)	2:24:B:ILE:CD1	3:410:A:PCW:C8	17	10.61
(1,42)	2:179:C:LYS:N	3:403:A:PCW:C7	5	10.42
(1,32)	2:36:C:ILE:CD1	3:411:A:PCW:C7	8	10.06
(1,44)	2:24:B:ILE:CD1	3:407:A:PCW:C7	3	9.94
(1,32)	2:36:C:ILE:CD1	3:412:A:PCW:C5	19	9.71
(1,50)	2:105:B:ASP:N	3:407:A:PCW:C6	4	9.48
(1,48)	2:6:B:LEU:N	3:410:A:PCW:C7	2	9.36
(1,45)	2:36:B:ILE:CD1	3:405:A:PCW:C6	4	9.01
(1,49)	2:43:B:GLN:N	3:410:A:PCW:C5	17	8.83
(1,49)	2:43:B:GLN:N	3:410:A:PCW:C7	5	8.75
(1,41)	2:178:C:LYS:N	3:402:A:PCW:C4	18	8.72
(1,48)	2:6:B:LEU:N	4:415:A:17F:O4	12	8.66
(1,48)	2:6:B:LEU:N	3:407:A:PCW:C7	14	8.57
(1,48)	2:6:B:LEU:N	3:407:A:PCW:C7	6	8.51
(1,48)	2:6:B:LEU:N	3:407:A:PCW:C7	5	8.36
(1,44)	2:24:B:ILE:CD1	3:410:A:PCW:C7	11	8.29
(1,37)	2:105:C:ASP:N	3:407:A:PCW:C6	8	8.26
(1,44)	2:24:B:ILE:CD1	3:407:A:PCW:C7	15	8.12
(1,50)	2:105:B:ASP:N	3:407:A:PCW:C7	9	8.04
(1,47)	2:46:B:ILE:CG2	3:404:A:PCW:C5	14	7.98
(1,48)	2:6:B:LEU:N	3:407:A:PCW:C7	15	7.91
(1,50)	2:105:B:ASP:N	3:408:A:PCW:C6	7	7.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	2:178:C:LYS:N	3:403:A:PCW:C7	5	7.86
(1,45)	2:36:B:ILE:CD1	3:412:A:PCW:C5	2	7.82
(1,50)	2:105:B:ASP:N	3:407:A:PCW:C6	20	7.77
(1,50)	2:105:B:ASP:N	3:407:A:PCW:C7	1	7.76
(1,48)	2:6:B:LEU:N	3:410:A:PCW:C5	1	7.74
(1,48)	2:6:B:LEU:N	3:407:A:PCW:C7	13	7.52
(1,47)	2:46:B:ILE:CG2	3:413:A:PCW:C6	3	7.43
(1,44)	2:24:B:ILE:CD1	3:405:A:PCW:C6	4	7.43
(1,49)	2:43:B:GLN:N	3:407:A:PCW:C7	15	7.39
(1,49)	2:43:B:GLN:N	3:410:A:PCW:C7	11	7.34
(1,45)	2:36:B:ILE:CD1	3:412:A:PCW:C5	9	7.34
(1,45)	2:36:B:ILE:CD1	3:404:A:PCW:C4	12	7.24
(1,49)	2:43:B:GLN:N	3:402:A:PCW:C4	4	7.2
(1,50)	2:105:B:ASP:N	3:407:A:PCW:C7	17	7.14
(1,48)	2:6:B:LEU:N	3:407:A:PCW:C7	3	7.09
(1,31)	2:24:C:ILE:CD1	3:405:A:PCW:C4	8	6.92
(1,47)	2:46:B:ILE:CG2	3:413:A:PCW:C8	13	6.67
(1,47)	2:46:B:ILE:CG2	3:413:A:PCW:C7	6	6.52
(1,48)	2:6:B:LEU:N	3:407:A:PCW:C8	19	6.46
(1,48)	2:6:B:LEU:N	3:410:A:PCW:C7	9	6.34
(1,50)	2:105:B:ASP:N	3:408:A:PCW:C7	16	6.2
(1,48)	2:6:B:LEU:N	3:407:A:PCW:C6	4	6.2
(1,45)	2:36:B:ILE:CD1	3:412:A:PCW:C6	1	6.17
(1,45)	2:36:B:ILE:CD1	3:404:A:PCW:C4	7	6.03
(1,32)	2:36:C:ILE:CD1	3:410:A:PCW:C7	4	5.97
(1,50)	2:105:B:ASP:N	3:407:A:PCW:C7	2	5.96
(1,50)	2:105:B:ASP:N	3:403:A:PCW:C8	15	5.85
(1,47)	2:46:B:ILE:CG2	3:403:A:PCW:C7	5	5.76
(1,48)	2:6:B:LEU:N	3:407:A:PCW:C7	7	5.74
(1,35)	2:6:C:LEU:N	3:407:A:PCW:C7	8	5.56
(1,56)	2:180:B:LYS:N	3:404:A:PCW:C6	10	5.53
(1,24)	2:170:B:MET:CG	2:163:C:ILE:CD1	5	5.49
(1,44)	2:24:B:ILE:CD1	3:407:A:PCW:C8	12	5.45
(1,32)	2:36:C:ILE:CD1	3:402:A:PCW:C7	20	5.4
(1,32)	2:36:C:ILE:CD1	4:415:A:17F:O4	3	5.37
(1,50)	2:105:B:ASP:N	3:411:A:PCW:C6	6	5.34
(1,32)	2:36:C:ILE:CD1	3:410:A:PCW:C7	12	5.34
(1,9)	2:170:C:MET:CG	2:163:B:ILE:CD1	11	5.32
(1,50)	2:105:B:ASP:N	3:405:A:PCW:C6	5	5.21
(1,50)	2:105:B:ASP:N	3:408:A:PCW:C6	18	5.2
(1,31)	2:24:C:ILE:CD1	3:410:A:PCW:C6	19	5.2
(1,50)	2:105:B:ASP:N	3:407:A:PCW:C7	11	5.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	2:24:B:ILE:CD1	3:411:A:PCW:C8	7	5.13
(1,47)	2:46:B:ILE:CG2	4:414:A:17F:O4	11	4.75
(1,50)	2:105:B:ASP:N	3:411:A:PCW:C6	14	4.74
(1,49)	2:43:B:GLN:N	3:405:A:PCW:C5	7	4.71
(1,44)	2:24:B:ILE:CD1	3:411:A:PCW:C7	20	4.67
(1,45)	2:36:B:ILE:CD1	3:406:A:PCW:C6	16	4.66
(1,9)	2:170:C:MET:CG	2:163:B:ILE:CD1	6	4.41
(1,40)	2:177:C:LYS:N	3:402:A:PCW:C4	18	4.38
(1,49)	2:43:B:GLN:N	3:405:A:PCW:C7	20	4.34
(1,24)	2:170:B:MET:CG	2:163:C:ILE:CD1	18	4.21
(1,36)	2:43:C:GLN:N	3:405:A:PCW:C4	8	4.18
(1,9)	2:170:C:MET:CG	2:163:B:ILE:CD1	14	4.17
(1,32)	2:36:C:ILE:CD1	4:414:A:17F:N1	1	4.16
(1,9)	2:170:C:MET:CG	2:163:B:ILE:CD1	18	4.16
(1,32)	2:36:C:ILE:CD1	4:415:A:17F:C1	10	4.15
(1,44)	2:24:B:ILE:CD1	3:407:A:PCW:C7	19	4.12
(1,56)	2:180:B:LYS:N	3:412:A:PCW:C5	20	4.11
(1,45)	2:36:B:ILE:CD1	3:404:A:PCW:C4	20	4.09
(1,36)	2:43:C:GLN:N	3:404:A:PCW:C4	14	4.08
(1,22)	2:170:B:MET:CG	2:46:C:ILE:CD1	5	4.04
(1,9)	2:170:C:MET:CG	2:163:B:ILE:CD1	15	4.03
(1,50)	2:105:B:ASP:N	3:405:A:PCW:C6	3	4.01
(1,32)	2:36:C:ILE:CD1	4:415:A:17F:O4	6	3.94
(1,24)	2:170:B:MET:CG	2:163:C:ILE:CD1	6	3.79
(1,43)	2:180:C:LYS:N	3:410:A:PCW:C5	17	3.78
(1,24)	2:170:B:MET:CG	2:163:C:ILE:CD1	15	3.72
(1,9)	2:170:C:MET:CG	2:163:B:ILE:CD1	9	3.72
(1,13)	2:170:C:MET:CG	2:173:B:ASP:N	18	3.66
(1,45)	2:36:B:ILE:CD1	3:404:A:PCW:C4	19	3.58
(1,32)	2:36:C:ILE:CD1	4:415:A:17F:C1	14	3.55
(1,13)	2:170:C:MET:CG	2:173:B:ASP:N	9	3.54
(1,24)	2:170:B:MET:CG	2:163:C:ILE:CD1	13	3.52
(1,56)	2:180:B:LYS:N	3:405:A:PCW:C4	8	3.46
(1,48)	2:6:B:LEU:N	3:407:A:PCW:C8	20	3.46
(1,9)	2:170:C:MET:CG	2:163:B:ILE:CD1	17	3.46
(1,56)	2:180:B:LYS:N	3:410:A:PCW:C7	16	3.45
(1,32)	2:36:C:ILE:CD1	3:412:A:PCW:C8	7	3.44
(1,39)	2:176:C:LYS:N	3:402:A:PCW:C4	18	3.43
(1,48)	2:6:B:LEU:N	3:407:A:PCW:C7	16	3.39
(1,41)	2:178:C:LYS:N	3:402:A:PCW:C4	19	3.39
(1,50)	2:105:B:ASP:N	3:402:A:PCW:C4	8	3.33
(1,31)	2:24:C:ILE:CD1	3:404:A:PCW:C4	14	3.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	2:170:B:MET:CG	2:170:C:MET:N	18	3.3
(1,24)	2:170:B:MET:CG	2:163:C:ILE:CD1	14	3.29
(1,49)	2:43:B:GLN:N	3:407:A:PCW:C8	12	3.27
(1,24)	2:170:B:MET:CG	2:163:C:ILE:CD1	12	3.25
(1,45)	2:36:B:ILE:CD1	3:411:A:PCW:C7	18	3.23
(1,23)	2:170:B:MET:CG	2:160:C:VAL:CG1	5	3.22
(1,41)	2:178:C:LYS:N	3:403:A:PCW:C6	6	3.19
(1,8)	2:170:C:MET:CG	2:160:B:VAL:CG1	11	3.18
(1,13)	2:170:C:MET:CG	2:173:B:ASP:N	2	3.16
(1,50)	2:105:B:ASP:N	3:411:A:PCW:C6	13	3.13
(1,44)	2:24:B:ILE:CD1	3:410:A:PCW:C7	2	3.13
(1,42)	2:179:C:LYS:N	3:403:A:PCW:C4	14	3.12
(1,24)	2:170:B:MET:CG	2:163:C:ILE:CD1	1	3.08
(1,9)	2:170:C:MET:CG	2:163:B:ILE:CD1	16	3.07
(1,12)	2:170:C:MET:CG	2:170:B:MET:N	18	3.05
(1,7)	2:170:C:MET:CG	2:46:B:ILE:CD1	11	3.03
(1,24)	2:170:B:MET:CG	2:163:C:ILE:CD1	10	2.98
(1,47)	2:46:B:ILE:CG2	3:409:A:PCW:C4	15	2.93
(1,9)	2:170:C:MET:CG	2:163:B:ILE:CD1	20	2.93
(1,35)	2:6:C:LEU:N	3:412:A:PCW:C5	19	2.91
(1,12)	2:170:C:MET:CG	2:170:B:MET:N	9	2.85
(1,9)	2:170:C:MET:CG	2:163:B:ILE:CD1	2	2.85
(1,9)	2:170:C:MET:CG	2:163:B:ILE:CD1	5	2.83
(1,40)	2:177:C:LYS:N	3:403:A:PCW:C7	5	2.81
(1,13)	2:170:C:MET:CG	2:173:B:ASP:N	11	2.81
(1,55)	2:179:B:LYS:N	3:404:A:PCW:C4	10	2.8
(1,28)	2:170:B:MET:CG	2:173:C:ASP:N	18	2.8
(1,24)	2:170:B:MET:CG	2:163:C:ILE:CD1	11	2.8
(1,24)	2:170:B:MET:CG	2:163:C:ILE:CD1	4	2.78
(1,24)	2:170:B:MET:CG	2:163:C:ILE:CD1	9	2.78
(1,24)	2:170:B:MET:CG	2:163:C:ILE:CD1	17	2.78
(1,42)	2:179:C:LYS:N	3:403:A:PCW:C5	6	2.76
(1,28)	2:170:B:MET:CG	2:173:C:ASP:N	17	2.75
(1,50)	2:105:B:ASP:N	3:407:A:PCW:C7	10	2.74
(1,37)	2:105:C:ASP:N	3:402:A:PCW:C4	7	2.74
(1,32)	2:36:C:ILE:CD1	4:415:A:17F:O5	13	2.72
(1,24)	2:170:B:MET:CG	2:163:C:ILE:CD1	2	2.72
(1,13)	2:170:C:MET:CG	2:173:B:ASP:N	15	2.71
(1,56)	2:180:B:LYS:N	3:412:A:PCW:C4	18	2.7
(1,36)	2:43:C:GLN:N	3:404:A:PCW:C4	5	2.67
(1,42)	2:179:C:LYS:N	3:410:A:PCW:C5	17	2.66
(1,32)	2:36:C:ILE:CD1	4:414:A:17F:N1	9	2.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	2:170:C:MET:CG	2:170:B:MET:N	15	2.59
(1,47)	2:46:B:ILE:CG1	3:407:A:PCW:C6	12	2.58
(1,27)	2:170:B:MET:CG	2:170:C:MET:N	11	2.56
(1,48)	2:6:B:LEU:N	3:410:A:PCW:C7	10	2.52
(1,12)	2:170:C:MET:CG	2:170:B:MET:N	11	2.52
(1,12)	2:170:C:MET:CG	2:170:B:MET:N	2	2.51
(1,9)	2:170:C:MET:CG	2:163:B:ILE:CD1	4	2.48
(1,43)	2:180:C:LYS:N	3:403:A:PCW:C4	14	2.46
(1,39)	2:176:C:LYS:N	3:405:A:PCW:C6	16	2.45
(1,28)	2:170:B:MET:CG	2:173:C:ASP:N	16	2.45
(1,45)	2:36:B:ILE:CD1	3:412:A:PCW:C6	8	2.43
(1,42)	2:179:C:LYS:N	3:405:A:PCW:C6	19	2.43
(1,49)	2:43:B:GLN:N	3:407:A:PCW:C7	19	2.42
(1,36)	2:43:C:GLN:N	3:410:A:PCW:C6	19	2.41
(1,43)	2:180:C:LYS:N	3:409:A:PCW:C6	8	2.38
(1,48)	2:6:B:LEU:N	3:407:A:PCW:C7	18	2.33
(1,44)	2:24:B:ILE:CD1	3:405:A:PCW:C6	16	2.3
(1,44)	2:24:B:ILE:CD1	3:407:A:PCW:C7	18	2.27
(1,28)	2:170:B:MET:CG	2:173:C:ASP:N	11	2.26
(1,32)	2:36:C:ILE:CD1	4:414:A:17F:N1	2	2.23
(1,32)	2:36:C:ILE:CD1	4:415:A:17F:O4	17	2.23
(1,13)	2:170:C:MET:CG	2:173:B:ASP:N	3	2.23
(1,7)	2:170:C:MET:CG	2:46:B:ILE:CD1	3	2.22
(1,28)	2:170:B:MET:CG	2:173:C:ASP:N	3	2.2
(1,27)	2:170:B:MET:CG	2:170:C:MET:N	9	2.17
(1,40)	2:177:C:LYS:N	3:403:A:PCW:C6	6	2.16
(1,41)	2:178:C:LYS:N	3:403:A:PCW:C4	14	2.15
(1,34)	2:46:C:ILE:CG1	4:415:A:17F:O5	10	2.15
(1,12)	2:170:C:MET:CG	2:170:B:MET:N	10	2.13
(1,56)	2:180:B:LYS:N	3:404:A:PCW:C6	5	2.12
(1,51)	2:173:B:ASP:N	3:413:A:PCW:C8	9	2.12
(1,37)	2:105:C:ASP:N	3:402:A:PCW:C4	20	2.12
(1,7)	2:170:C:MET:CG	2:46:B:ILE:CD1	6	2.12
(1,43)	2:180:C:LYS:N	3:403:A:PCW:C5	6	2.1
(1,28)	2:170:B:MET:CG	2:173:C:ASP:N	7	2.09
(1,12)	2:170:C:MET:CG	2:170:B:MET:N	12	2.09
(1,27)	2:170:B:MET:CG	2:170:C:MET:N	2	2.04
(1,13)	2:170:C:MET:CG	2:173:B:ASP:N	7	2.03
(1,22)	2:170:B:MET:CG	2:46:C:ILE:CD1	2	2.02
(1,12)	2:170:C:MET:CG	2:170:B:MET:N	3	2.0
(1,24)	2:170:B:MET:CG	2:163:C:ILE:CD1	8	1.99
(1,27)	2:170:B:MET:CG	2:170:C:MET:N	10	1.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	2:170:C:MET:CG	2:173:B:ASP:N	12	1.97
(1,24)	2:170:B:MET:CG	2:163:C:ILE:CD1	3	1.96
(1,8)	2:170:C:MET:CG	2:160:B:VAL:CG1	14	1.96
(1,47)	2:46:B:ILE:CG2	3:403:A:PCW:C7	17	1.93
(1,28)	2:170:B:MET:CG	2:173:C:ASP:N	10	1.9
(1,27)	2:170:B:MET:CG	2:170:C:MET:N	17	1.9
(1,45)	2:36:B:ILE:CD1	3:412:A:PCW:C5	10	1.89
(1,27)	2:170:B:MET:CG	2:170:C:MET:N	12	1.89
(1,24)	2:170:B:MET:CG	2:163:C:ILE:CD1	19	1.88
(1,9)	2:170:C:MET:CG	2:163:B:ILE:CD1	3	1.88
(1,27)	2:170:B:MET:CG	2:170:C:MET:N	15	1.87
(1,13)	2:170:C:MET:CG	2:173:B:ASP:N	10	1.87
(1,32)	2:36:C:ILE:CD1	3:410:A:PCW:C7	15	1.85
(1,27)	2:170:B:MET:CG	2:170:C:MET:N	20	1.85
(1,12)	2:170:C:MET:CG	2:170:B:MET:N	14	1.85
(1,27)	2:170:B:MET:CG	2:170:C:MET:N	7	1.84
(1,46)	2:45:B:VAL:CG1	4:414:A:17F:O4	6	1.83
(1,22)	2:170:B:MET:CG	2:46:C:ILE:CD1	6	1.83
(1,12)	2:170:C:MET:CG	2:170:B:MET:N	17	1.83
(1,37)	2:105:C:ASP:N	3:403:A:PCW:C4	9	1.77
(1,27)	2:170:B:MET:CG	2:170:C:MET:N	14	1.76
(1,13)	2:170:C:MET:CG	2:173:B:ASP:N	17	1.76
(1,13)	2:170:C:MET:CG	2:173:B:ASP:N	1	1.75
(1,27)	2:170:B:MET:CG	2:170:C:MET:N	3	1.74
(1,9)	2:170:C:MET:CG	2:163:B:ILE:CD1	1	1.74
(1,43)	2:180:C:LYS:N	3:410:A:PCW:C4	10	1.73
(1,47)	2:46:B:ILE:CG1	3:407:A:PCW:C7	7	1.71
(1,24)	2:170:B:MET:CG	2:163:C:ILE:CD1	16	1.71
(1,47)	2:46:B:ILE:CG1	3:405:A:PCW:C7	20	1.7
(1,32)	2:36:C:ILE:CD1	4:415:A:17F:O4	11	1.67
(1,12)	2:170:C:MET:CG	2:170:B:MET:N	1	1.67
(1,9)	2:170:C:MET:CG	2:163:B:ILE:CD1	13	1.67
(1,28)	2:170:B:MET:CG	2:173:C:ASP:N	9	1.66
(1,39)	2:176:C:LYS:N	4:414:A:17F:O4	5	1.65
(1,8)	2:170:C:MET:CG	2:160:B:VAL:CG1	18	1.65
(1,44)	2:24:B:ILE:CD1	3:410:A:PCW:C5	1	1.64
(1,28)	2:170:B:MET:CG	2:173:C:ASP:N	20	1.64
(1,12)	2:170:C:MET:CG	2:170:B:MET:N	7	1.63
(1,43)	2:180:C:LYS:N	3:405:A:PCW:C6	19	1.62
(1,7)	2:170:C:MET:CG	2:46:B:ILE:CD1	14	1.62
(1,9)	2:170:C:MET:CG	2:163:B:ILE:CD1	10	1.61
(1,46)	2:45:B:VAL:CG1	3:403:A:PCW:C5	14	1.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	2:170:C:MET:CG	2:170:B:MET:N	20	1.57
(1,36)	2:43:C:GLN:N	3:404:A:PCW:C4	3	1.56
(1,37)	2:105:C:ASP:N	3:402:A:PCW:C4	16	1.54
(1,9)	2:170:C:MET:CG	2:163:B:ILE:CD1	12	1.53
(1,8)	2:170:C:MET:CG	2:160:B:VAL:CG1	6	1.53
(1,12)	2:170:C:MET:CG	2:170:B:MET:N	13	1.52
(1,24)	2:170:B:MET:CG	2:163:C:ILE:CD1	20	1.5
(1,43)	2:180:C:LYS:N	3:402:A:PCW:C4	12	1.49
(1,32)	2:36:C:ILE:CD1	3:412:A:PCW:C8	18	1.47
(1,37)	2:105:C:ASP:N	3:402:A:PCW:C4	18	1.45
(1,27)	2:170:B:MET:CG	2:170:C:MET:N	16	1.45
(1,27)	2:170:B:MET:CG	2:170:C:MET:N	13	1.44
(1,39)	2:176:C:LYS:N	3:413:A:PCW:C7	6	1.41
(1,32)	2:36:C:ILE:CD1	3:412:A:PCW:C8	16	1.41
(1,49)	2:43:B:GLN:N	3:407:A:PCW:C7	18	1.38
(1,7)	2:170:C:MET:CG	2:46:B:ILE:CD1	18	1.36
(1,52)	2:176:B:LYS:N	3:404:A:PCW:C4	10	1.31
(1,36)	2:43:C:GLN:N	3:404:A:PCW:C4	13	1.28
(1,23)	2:170:B:MET:CG	2:160:C:VAL:CG1	18	1.25
(1,22)	2:170:B:MET:CG	2:46:C:ILE:CD1	15	1.25
(1,8)	2:170:C:MET:CG	2:160:B:VAL:CG1	15	1.25
(1,47)	2:46:B:ILE:CG1	3:407:A:PCW:C6	19	1.21
(1,28)	2:170:B:MET:CG	2:173:C:ASP:N	12	1.21
(1,36)	2:43:C:GLN:N	4:415:A:17F:C1	10	1.2
(1,32)	2:36:C:ILE:CD1	4:415:A:17F:O5	5	1.18
(1,7)	2:170:C:MET:CG	2:46:B:ILE:CD1	10	1.18
(1,56)	2:180:B:LYS:N	3:411:A:PCW:C5	17	1.17
(1,28)	2:170:B:MET:CG	2:173:C:ASP:N	15	1.16
(1,35)	2:6:C:LEU:N	3:410:A:PCW:C7	4	1.15
(1,27)	2:170:B:MET:CG	2:170:C:MET:N	1	1.14
(1,10)	2:170:C:MET:CG	2:166:B:HIS:N	11	1.13
(1,49)	2:43:B:GLN:N	3:405:A:PCW:C6	16	1.12
(1,23)	2:170:B:MET:CG	2:160:C:VAL:CG1	6	1.11
(1,22)	2:170:B:MET:CG	2:46:C:ILE:CD1	4	1.11
(1,22)	2:170:B:MET:CG	2:46:C:ILE:CD1	12	1.11
(1,23)	2:170:B:MET:CG	2:160:C:VAL:CG1	12	1.09
(1,54)	2:178:B:LYS:N	3:404:A:PCW:C4	10	1.08
(1,51)	2:173:B:ASP:N	3:407:A:PCW:C6	10	1.05
(1,10)	2:170:C:MET:CG	2:166:B:HIS:N	18	1.04
(1,22)	2:170:B:MET:CG	2:46:C:ILE:CD1	14	1.03
(1,38)	2:173:C:ASP:N	3:402:A:PCW:C4	20	1.02
(1,22)	2:170:B:MET:CG	2:46:C:ILE:CD1	13	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	2:170:C:MET:CG	2:163:B:ILE:CD1	19	0.98
(1,13)	2:170:C:MET:CG	2:173:B:ASP:N	13	0.97
(1,51)	2:173:B:ASP:N	3:411:A:PCW:C6	11	0.95
(1,9)	2:170:C:MET:CG	2:163:B:ILE:CD1	7	0.95
(1,28)	2:170:B:MET:CG	2:173:C:ASP:N	14	0.93
(1,28)	2:170:B:MET:CG	2:173:C:ASP:N	1	0.9
(1,24)	2:170:B:MET:CG	2:163:C:ILE:CD1	7	0.88
(1,13)	2:170:C:MET:CG	2:173:B:ASP:N	20	0.88
(1,10)	2:170:C:MET:CG	2:166:B:HIS:N	15	0.88
(1,41)	2:178:C:LYS:N	3:408:A:PCW:C7	17	0.87
(1,28)	2:170:B:MET:CG	2:173:C:ASP:N	13	0.87
(1,8)	2:170:C:MET:CG	2:160:B:VAL:CG1	17	0.81
(1,46)	2:45:B:VAL:CG1	4:414:A:17F:O5	13	0.79
(1,25)	2:170:B:MET:CG	2:166:C:HIS:N	18	0.79
(1,9)	2:170:C:MET:CG	2:163:B:ILE:CD1	8	0.79
(1,39)	2:176:C:LYS:N	3:403:A:PCW:C5	14	0.78
(1,31)	2:24:C:ILE:CD1	3:404:A:PCW:C4	3	0.78
(1,23)	2:170:B:MET:CG	2:160:C:VAL:CG1	4	0.77
(1,10)	2:170:C:MET:CG	2:166:B:HIS:N	9	0.73
(2,85)	2:39:C:SER:OG	2:180:B:LYS:N	13	0.71
(1,55)	2:179:B:LYS:N	3:404:A:PCW:C7	5	0.68
(1,38)	2:173:C:ASP:N	3:413:A:PCW:C6	5	0.66
(1,7)	2:170:C:MET:CG	2:46:B:ILE:CD1	4	0.66
(1,55)	2:179:B:LYS:N	3:412:A:PCW:C4	18	0.65
(1,13)	2:170:C:MET:CG	2:173:B:ASP:N	19	0.65
(1,7)	2:170:C:MET:CG	2:46:B:ILE:CD1	5	0.65
(1,7)	2:170:C:MET:CG	2:46:B:ILE:CD1	15	0.65
(1,34)	2:46:C:ILE:CG1	3:404:A:PCW:C4	5	0.64
(1,31)	2:24:C:ILE:CD1	3:404:A:PCW:C4	13	0.64
(1,37)	2:105:C:ASP:N	3:403:A:PCW:C4	2	0.61
(1,8)	2:170:C:MET:CG	2:160:B:VAL:CG1	20	0.61
(1,7)	2:170:C:MET:CG	2:46:B:ILE:CD1	20	0.6
(1,12)	2:170:C:MET:CG	2:170:B:MET:N	4	0.59
(1,36)	2:43:C:GLN:N	3:412:A:PCW:C4	7	0.58
(1,36)	2:43:C:GLN:N	3:404:A:PCW:C4	6	0.57
(1,34)	2:46:C:ILE:CG2	3:405:A:PCW:C6	8	0.57
(1,23)	2:170:B:MET:CG	2:160:C:VAL:CG1	14	0.57
(1,23)	2:170:B:MET:CG	2:160:C:VAL:CG1	15	0.56
(1,22)	2:170:B:MET:CG	2:46:C:ILE:CD1	1	0.54
(1,8)	2:170:C:MET:CG	2:160:B:VAL:CG1	4	0.52
(1,31)	2:24:C:ILE:CD1	4:415:A:17F:C1	10	0.51
(1,27)	2:170:B:MET:CG	2:170:C:MET:N	5	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	2:180:B:LYS:N	3:404:A:PCW:C6	3	0.5
(1,28)	2:170:B:MET:CG	2:173:C:ASP:N	2	0.5
(1,49)	2:43:B:GLN:N	3:410:A:PCW:C5	1	0.49
(1,43)	2:180:C:LYS:N	3:402:A:PCW:C4	15	0.49
(1,13)	2:170:C:MET:CG	2:173:B:ASP:N	16	0.47
(1,31)	2:24:C:ILE:CD1	4:415:A:17F:O5	5	0.46
(1,49)	2:43:B:GLN:N	3:410:A:PCW:C7	2	0.45
(1,27)	2:170:B:MET:CG	2:170:C:MET:N	19	0.45
(1,31)	2:24:C:ILE:CD1	3:402:A:PCW:C7	20	0.44
(1,50)	2:105:B:ASP:N	4:414:A:17F:O5	19	0.42
(1,54)	2:178:B:LYS:N	3:404:A:PCW:C6	13	0.39
(1,12)	2:170:C:MET:CG	2:170:B:MET:N	19	0.39
(1,12)	2:170:C:MET:CG	2:170:B:MET:N	5	0.38
(1,27)	2:170:B:MET:CG	2:170:C:MET:N	6	0.36
(1,23)	2:170:B:MET:CG	2:160:C:VAL:CG1	10	0.35
(1,31)	2:24:C:ILE:CD1	3:412:A:PCW:C4	7	0.33
(1,47)	2:46:B:ILE:CG2	3:408:A:PCW:C8	1	0.32
(1,8)	2:170:C:MET:CG	2:160:B:VAL:CG1	5	0.32
(1,8)	2:170:C:MET:CG	2:160:B:VAL:CG1	9	0.31
(1,1)	2:118:C:CYS:SG	2:112:B:VAL:CG1	5	0.3
(1,1)	2:118:C:CYS:SG	2:112:B:VAL:CG2	5	0.3
(1,25)	2:170:B:MET:CG	2:166:C:HIS:N	5	0.28
(1,21)	2:170:B:MET:CG	2:46:C:ILE:CG1	5	0.27
(1,21)	2:170:B:MET:CG	2:46:C:ILE:CG2	5	0.27
(1,8)	2:170:C:MET:CG	2:160:B:VAL:CG1	2	0.26
(1,8)	2:170:C:MET:CG	2:160:B:VAL:CG1	16	0.26
(1,44)	2:24:B:ILE:CD1	3:410:A:PCW:C7	9	0.25
(1,37)	2:105:C:ASP:N	3:410:A:PCW:C7	12	0.25
(1,12)	2:170:C:MET:CG	2:170:B:MET:N	6	0.24
(1,55)	2:179:B:LYS:N	3:412:A:PCW:C5	20	0.23
(1,23)	2:170:B:MET:CG	2:160:C:VAL:CG1	1	0.23
(1,22)	2:170:B:MET:CG	2:46:C:ILE:CD1	18	0.21
(1,7)	2:170:C:MET:CG	2:46:B:ILE:CD1	2	0.19
(1,12)	2:170:C:MET:CG	2:170:B:MET:N	16	0.18
(1,3)	2:118:C:CYS:SG	2:139:B:ILE:CD1	5	0.18
(1,54)	2:178:B:LYS:N	3:410:A:PCW:C7	18	0.17
(1,10)	2:170:C:MET:CG	2:166:B:HIS:N	17	0.16
(2,154)	2:170:B:MET:CG	2:179:C:LYS:N	4	0.15
(1,54)	2:178:B:LYS:N	3:410:A:PCW:C7	16	0.14
(1,34)	2:46:C:ILE:CG1	3:410:A:PCW:C6	19	0.13
(1,54)	2:178:B:LYS:N	3:404:A:PCW:C4	14	0.12
(2,85)	2:39:C:SER:OG	2:180:B:LYS:N	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	2:46:B:ILE:CG1	3:410:A:PCW:C7	2	0.11
(1,25)	2:170:B:MET:CG	2:166:C:HIS:N	17	0.11
(1,18)	2:118:B:CYS:SG	2:139:C:ILE:CD1	6	0.11
(1,3)	2:118:C:CYS:SG	2:139:B:ILE:CD1	13	0.11
(1,7)	2:170:C:MET:CG	2:46:B:ILE:CD1	16	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found