



Full wwPDB NMR Structure Validation Report ⓘ

Mar 27, 2026 – 10:03 PM UTC

PDB ID : 6PTS / pdb_00006pts
BMRB ID : 30639
Title : NMR data-driven model of KRas-GMPPNP:RBD-CRD complex tethered to a nanodisc (state A)
Authors : Fang, Z.; Lee, K.; Gasmi-Seabrook, G.; Ikura, M.; Marshall, C.B.
Deposited on : 2019-07-16

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 : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

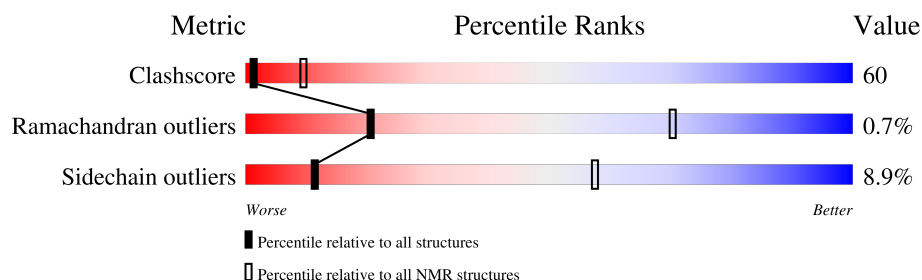
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 6%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	198	89% 10% .
1	C	198	83% 16% .
2	B	185	76% 17% 7% .
3	D	132	80% 19% .

2 Ensemble composition and analysis

This entry contains 10 models. Model 5 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:201-A:398, C:399-C:596 (396)	0.50	5
2	B:1-B:172, D:356-D:487 (304)	1.81	3

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 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	2, 3, 4, 6, 7, 8
2	1, 9, 10
Single-model clusters	5

3 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11566 atoms, of which 1424 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	C	198	Total	C	H	N	O	S	0
			2002	1019	379	287	314	3	

- Molecule 2 is a protein called GTPase KRas.

Mol	Chain	Residues	Atoms						Trace
2	B	185	Total	C	H	N	O	S	0
			1835	923	359	257	287	9	

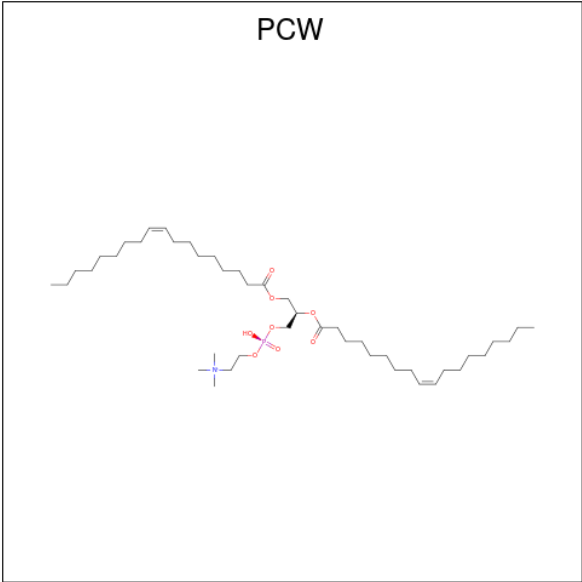
- Molecule 3 is a protein called RAF proto-oncogene serine/threonine-protein kinase.

Mol	Chain	Residues	Atoms						Trace
3	D	132	Total	C	H	N	O	S	0
			1316	677	251	194	182	12	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	403	GLN	HIS	conflict	UNP P04049

- Molecule 4 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C₄₄H₈₅NO₈P).



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

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[illegible]

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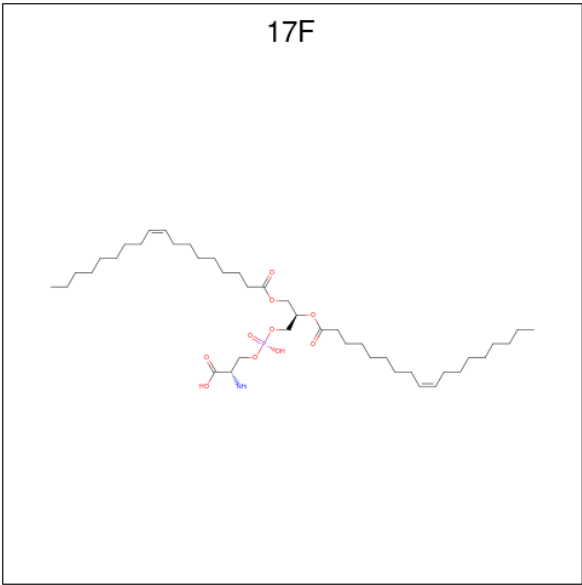
Mol	Chain	Residues	Atoms				
4	C	1	Total	C	N	O	P
			54	44	1	8	1
4	C	1	Total	C	N	O	P
			54	44	1	8	1
4	C	1	Total	C	N	O	P
			54	44	1	8	1
4	C	1	Total	C	N	O	P
			54	44	1	8	1
4	C	1	Total	C	N	O	P
			54	44	1	8	1
4	B	1	Total	C	N	O	P
			54	44	1	8	1
4	B	1	Total	C	N	O	P
			54	44	1	8	1
4	B	1	Total	C	N	O	P
			54	44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

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

- Molecule 5 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propyl}oxy)(hydroxy)phosphoryl]-L-serine (CCD ID: 17F) (formula: C₄₂H₇₈NO₁₀P).



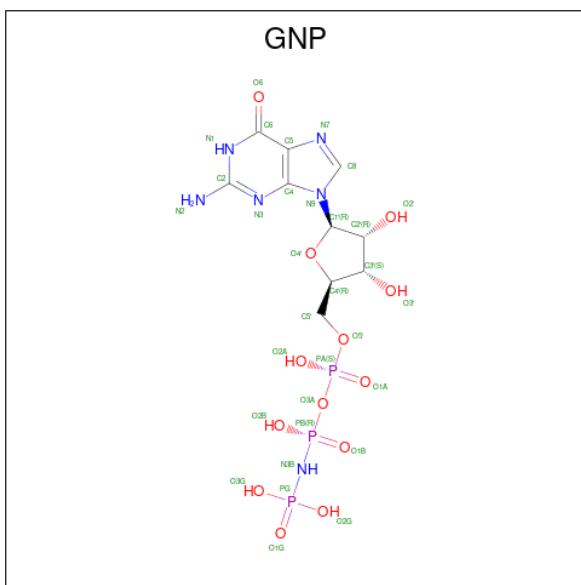
Mol	Chain	Residues	Atoms					
5	A	1	Total	C	H	N	O	P
			57	42	3	1	10	1
5	A	1	Total	C	H	N	O	P
			57	42	3	1	10	1
5	C	1	Total	C	H	N	O	P
			57	42	3	1	10	1

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

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



Mol	Chain	Residues	Atoms					
6	B	1	Total	C	H	N	O	P
			38	10	6	6	13	3

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	
7	B	1	Total	Mg
			1	1

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

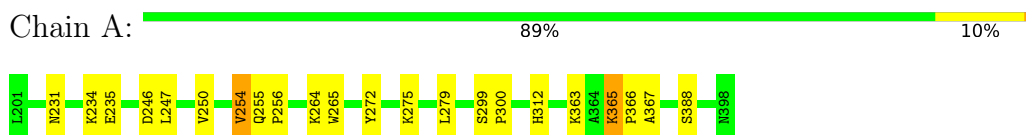
Mol	Chain	Residues	Atoms	
8	D	2	Total	Zn
			2	2

4 Residue-property plots [i](#)

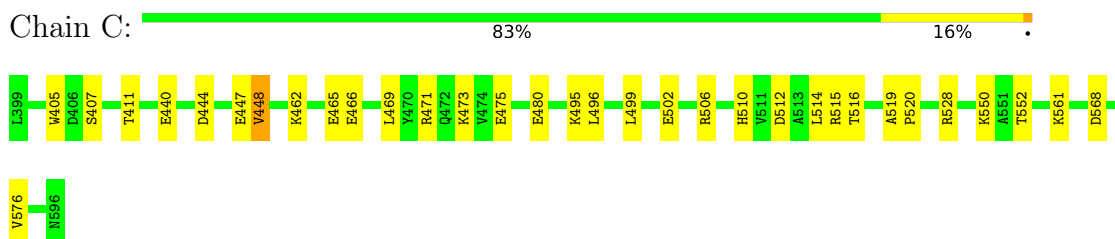
4.1 Average score per residue in the NMR ensemble

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.

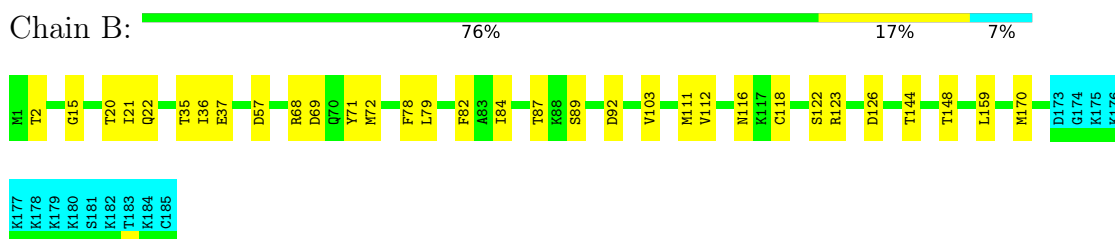
- Molecule 1: Apolipoprotein A-I



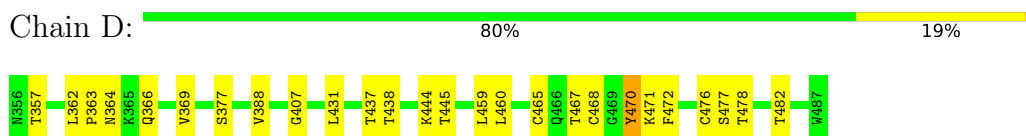
- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas



- Molecule 3: RAF proto-oncogene serine/threonine-protein kinase

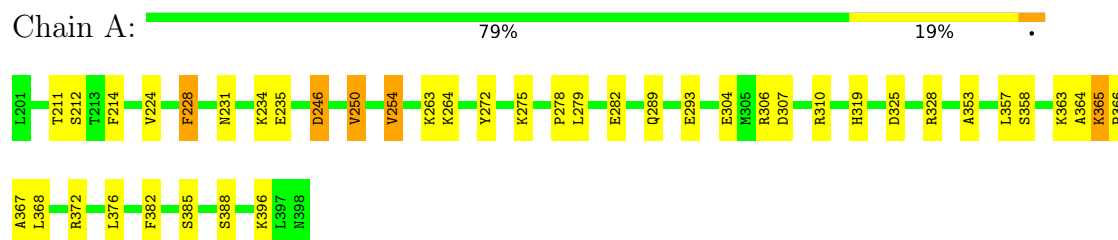


4.2 Scores per residue for each member of the ensemble

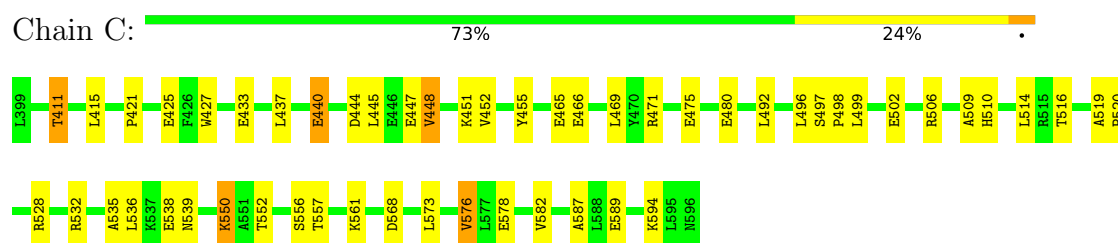
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

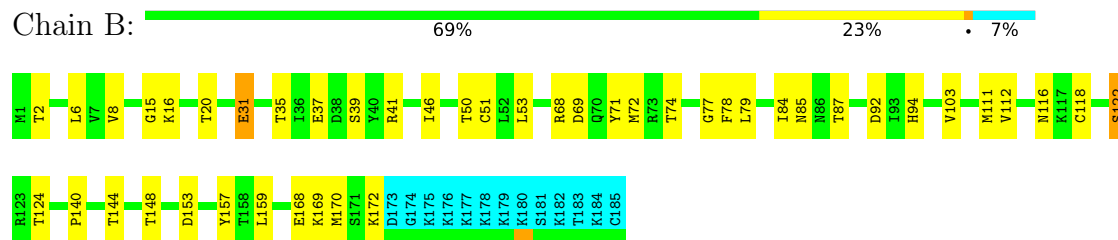
- Molecule 1: Apolipoprotein A-I



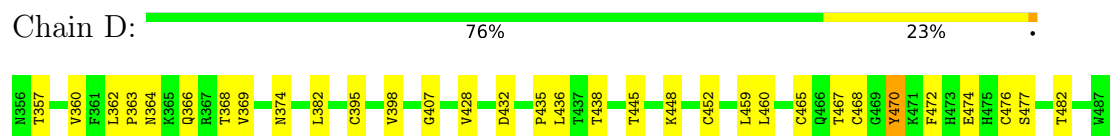
- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas



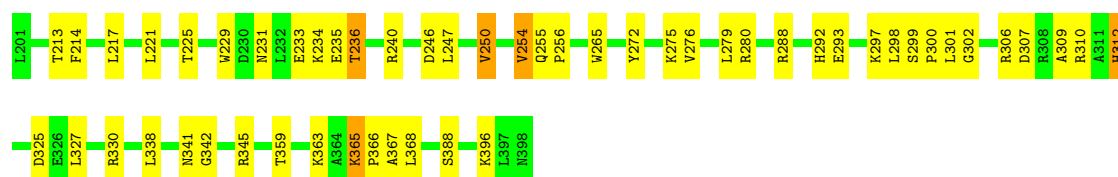
- Molecule 3: RAF proto-oncogene serine/threonine-protein kinase



4.2.2 Score per residue for model 2

- Molecule 1: Apolipoprotein A-I

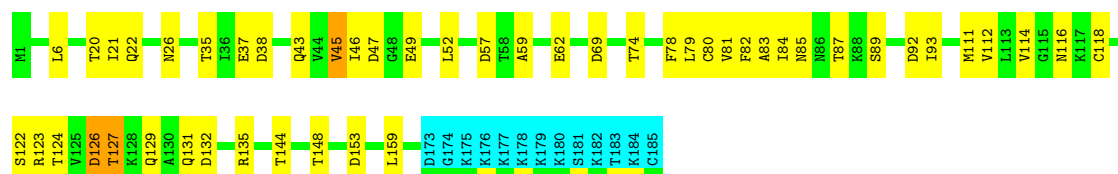




• Molecule 1: Apolipoprotein A-I



• Molecule 2: GTPase KRas

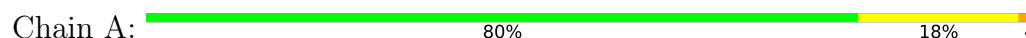


• Molecule 3: RAF proto-oncogene serine/threonine-protein kinase

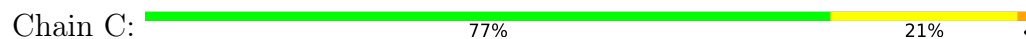


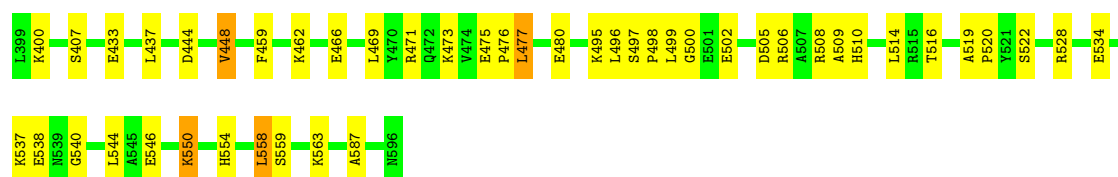
4.2.3 Score per residue for model 3

• Molecule 1: Apolipoprotein A-I



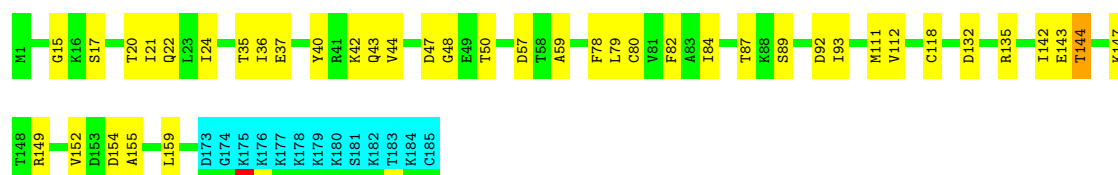
• Molecule 1: Apolipoprotein A-I





- Molecule 2: GTPase KRas

Chain B: 71% 22% 7%



- Molecule 3: RAF proto-oncogene serine/threonine-protein kinase

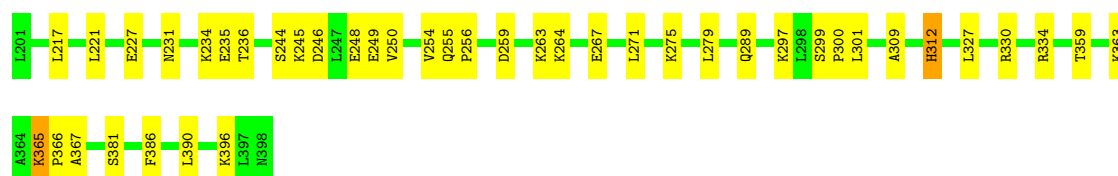
Chain D: 72% 23% 5%



4.2.4 Score per residue for model 4

- Molecule 1: Apolipoprotein A-I

Chain A: 79% 20% 1%

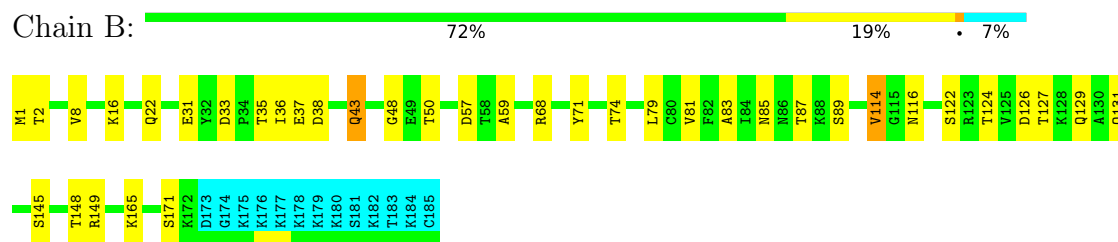


- Molecule 1: Apolipoprotein A-I

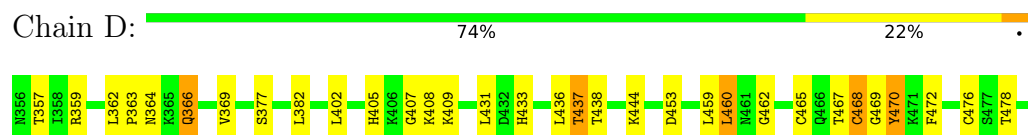
Chain C: 74% 25% 1%



- Molecule 2: GTPase KRas

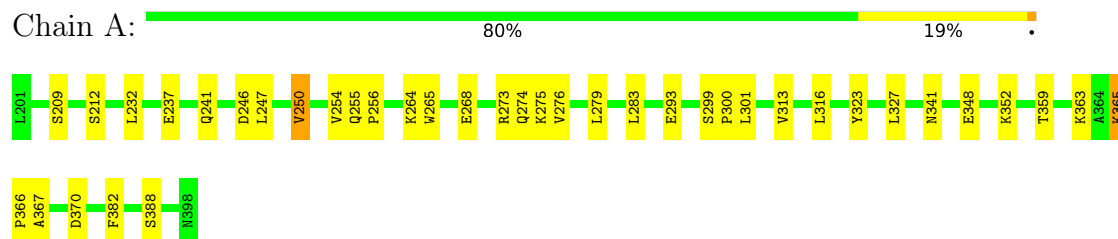


- Molecule 3: RAF proto-oncogene serine/threonine-protein kinase

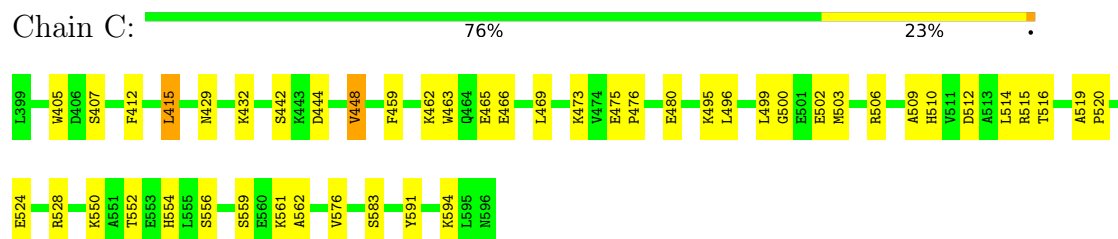


4.2.5 Score per residue for model 5 (medoid)

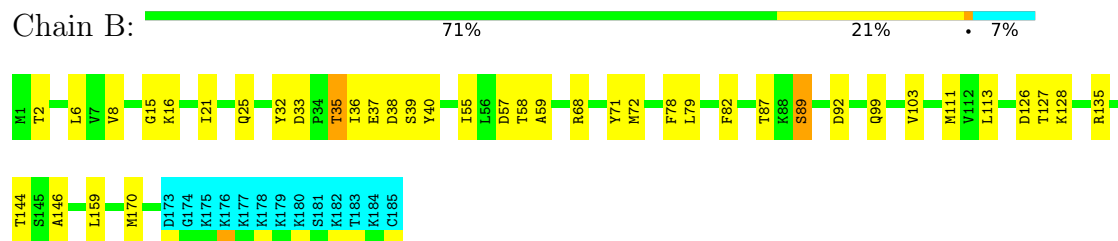
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas



- Molecule 3: RAF proto-oncogene serine/threonine-protein kinase

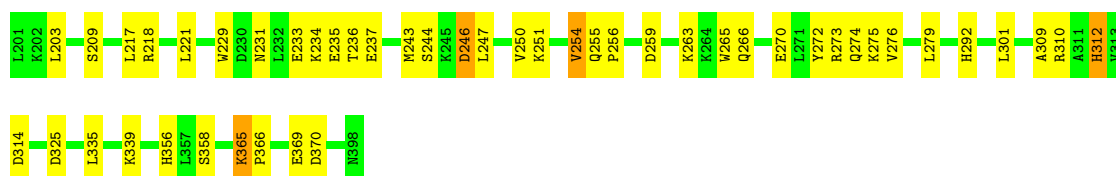
Chain D:  77% 20% ..



4.2.6 Score per residue for model 6

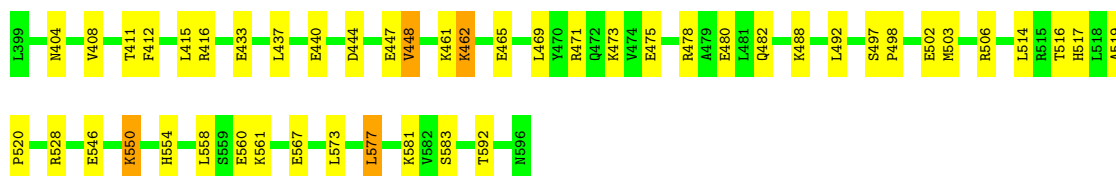
- Molecule 1: Apolipoprotein A-I

Chain A:  76% 22% .



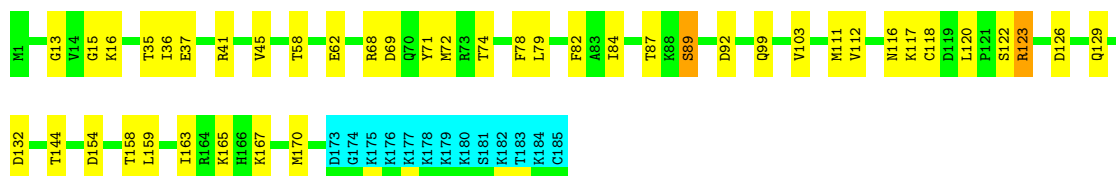
- Molecule 1: Apolipoprotein A-I

Chain C:  76% 22% .



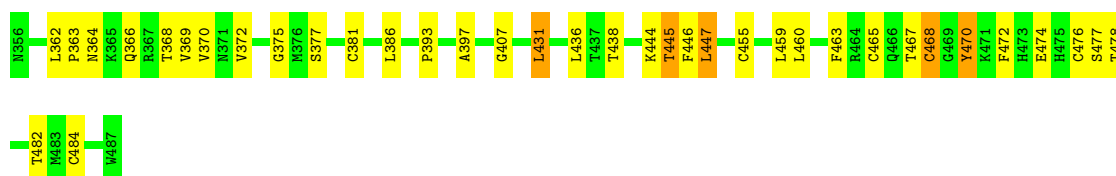
- Molecule 2: GTPase KRas

Chain B:  70% 22% 7% .



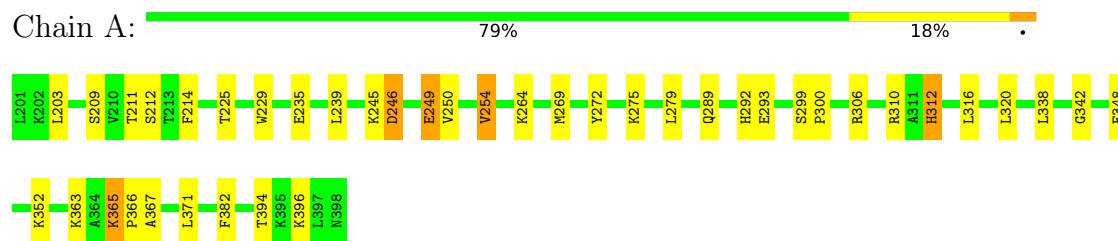
- Molecule 3: RAF proto-oncogene serine/threonine-protein kinase

Chain D:  72% 24% .

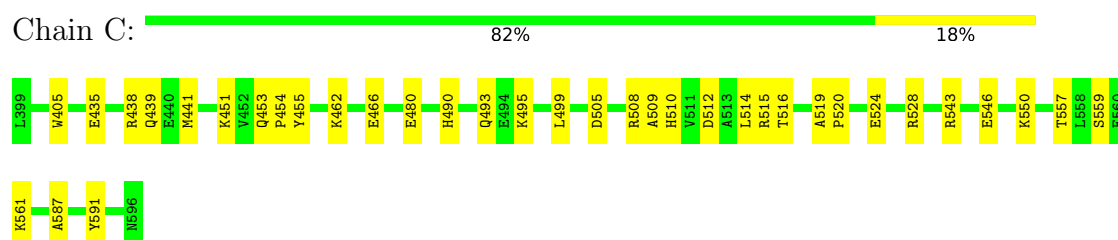


4.2.7 Score per residue for model 7

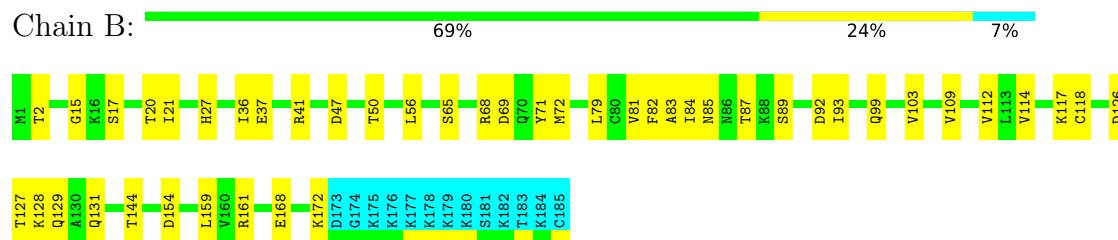
- Molecule 1: Apolipoprotein A-I



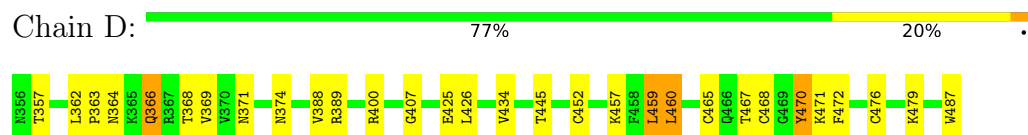
- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas

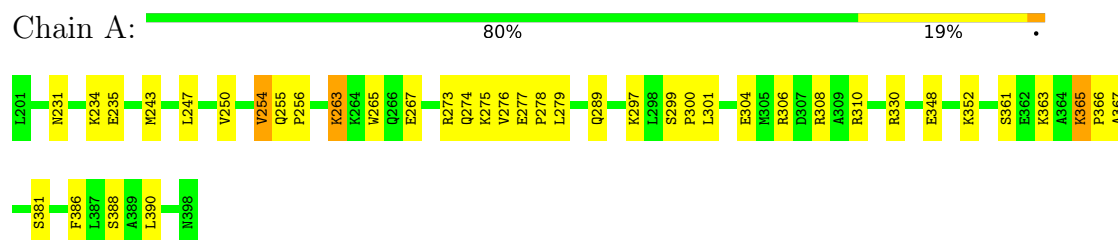


- Molecule 3: RAF proto-oncogene serine/threonine-protein kinase

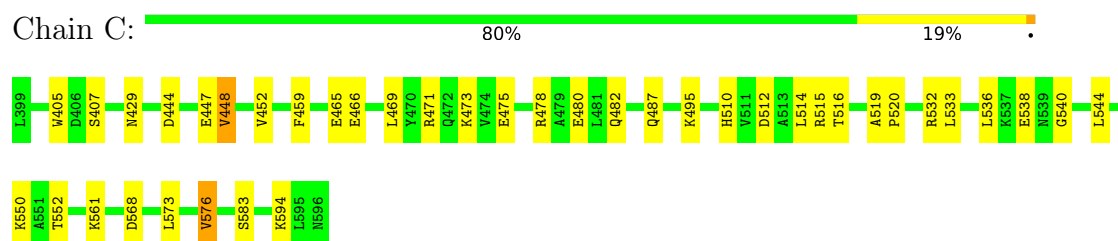


4.2.8 Score per residue for model 8

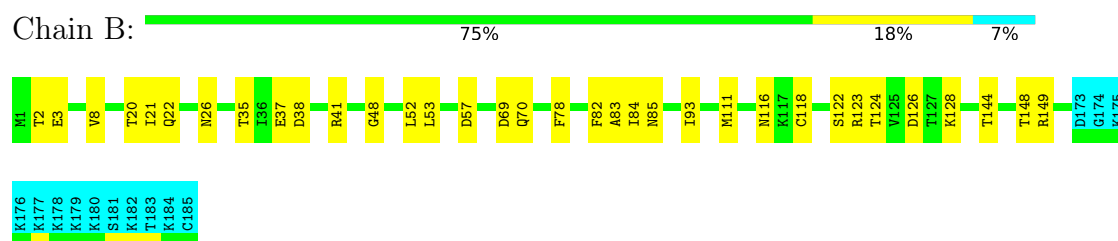
- Molecule 1: Apolipoprotein A-I



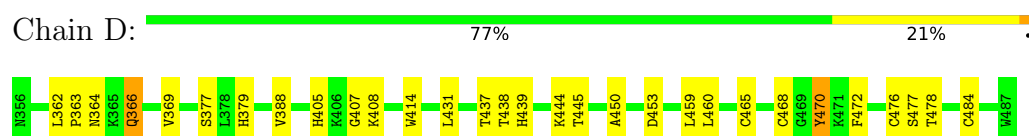
- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas

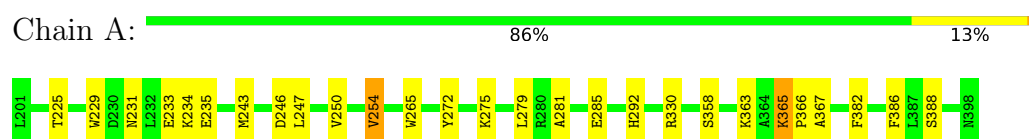


- Molecule 3: RAF proto-oncogene serine/threonine-protein kinase

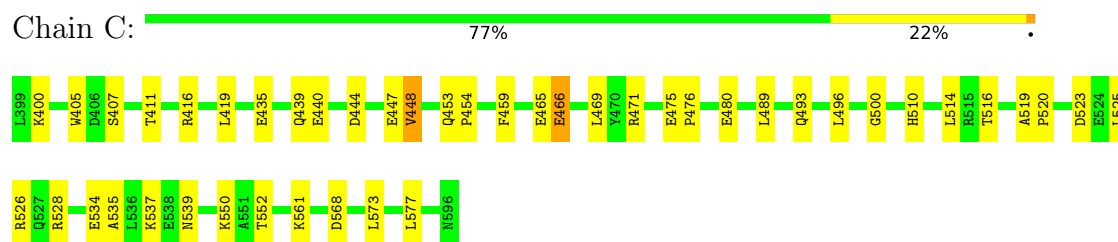


4.2.9 Score per residue for model 9

- Molecule 1: Apolipoprotein A-I

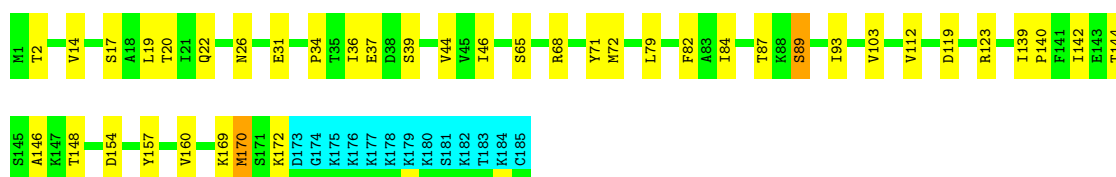


- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas





- Molecule 3: RAF proto-oncogene serine/threonine-protein kinase

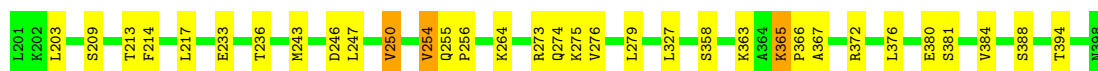
Chain D: 77% 22%



4.2.10 Score per residue for model 10

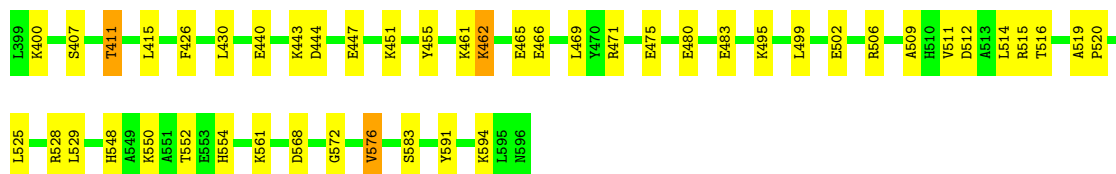
- Molecule 1: Apolipoprotein A-I

Chain A: 83% 15%



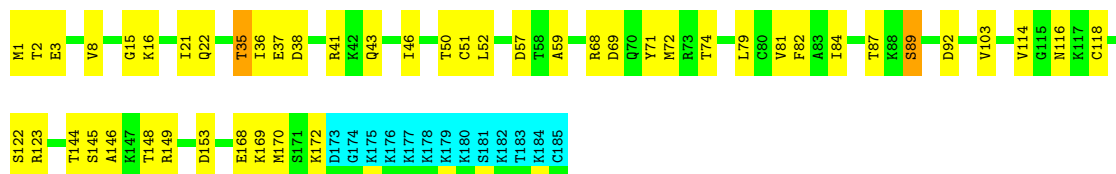
- Molecule 1: Apolipoprotein A-I

Chain C: 76% 22%



- Molecule 2: GTPase KRas

Chain B: 67% 25% 7%



- Molecule 3: RAF proto-oncogene serine/threonine-protein kinase

Chain D: 74% 24%



5 Refinement protocol and experimental data overview

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

Of the 3000 calculated structures, 10 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
CNS	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	557
Number of shifts mapped to atoms	437
Number of unparsed shifts	0
Number of shifts with mapping errors	120
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	6%

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: 17F, ZN, MG, GNP, PCW

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.38±0.00	0±0/1650 (0.0± 0.0%)	0.77±0.01	0±0/2218 (0.0± 0.0%)
1	C	0.39±0.01	0±0/1650 (0.0± 0.0%)	0.81±0.01	0±0/2218 (0.0± 0.0%)
2	B	0.35±0.00	0±0/1395 (0.0± 0.0%)	0.71±0.01	0±0/1880 (0.0± 0.0%)
3	D	0.46±0.01	2±0/1088 (0.2± 0.0%)	2.29±0.01	7±0/1466 (0.5± 0.0%)
All	All	0.39	20/57830 (0.0%)	1.21	70/77820 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
3	D	0.0±0.0	1.0±0.0
All	All	0	10

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
3	D	470	TYR	CB-CG	6.90	1.66	1.51	3	10
3	D	470	TYR	CZ-OH	5.79	1.50	1.38	9	10

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	D	470	TYR	CD1-CG-CD2	-41.66	55.61	118.10	1	10
3	D	470	TYR	CG-CD1-CE1	-36.99	65.71	121.20	9	10
3	D	470	TYR	CG-CD2-CE2	-32.60	72.30	121.20	6	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	D	470	TYR	CE1-CZ-CE2	-31.34	57.61	120.30	10	10
3	D	470	TYR	CZ-CE2-CD2	-30.75	64.24	119.60	3	10
3	D	470	TYR	CD1-CE1-CZ	-27.59	69.93	119.60	9	10
3	D	470	TYR	CB-CG-CD1	9.45	134.97	120.80	3	10

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
3	D	470	TYR	Sidechain	10

6.2 Too-close contacts

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	1623	381	1626	23±6
1	C	1623	379	1626	23±4
2	B	1373	319	1359	24±5
3	D	1065	251	1070	13±2
4	A	810	0	1200	302±24
4	B	648	0	960	281±37
4	C	1350	0	2000	542±22
4	D	648	0	960	282±17
5	A	108	6	152	34±8
5	B	162	9	228	69±11
5	C	378	21	532	149±9
5	D	216	12	304	98±23
6	B	32	6	13	3±2
7	B	1	0	0	0±0
All	All	100390	13840	120300	13345

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 60.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:207:PCW:C20	4:B:207:PCW:H251	1.19	1.67	10	1
4:D:508:PCW:C27	4:D:508:PCW:H222	1.17	1.68	9	3
4:A:405:PCW:H142	4:A:405:PCW:C19	1.17	1.70	7	10
4:B:202:PCW:C31	4:B:202:PCW:H362	1.16	1.70	6	2
4:D:508:PCW:H272	4:D:508:PCW:C22	1.16	1.70	1	3
4:D:505:PCW:H212	4:D:505:PCW:H252	1.15	1.16	1	10
4:C:601:PCW:H472	4:C:601:PCW:H432	1.14	1.19	2	3
4:D:504:PCW:H262	4:D:504:PCW:H222	1.14	1.19	2	2
4:B:204:PCW:H441	4:B:212:PCW:H231	1.13	1.15	1	1
4:B:211:PCW:H261	4:B:211:PCW:H221	1.13	1.19	2	10
4:C:616:PCW:H272	4:C:616:PCW:H232	1.13	1.20	10	10
4:C:601:PCW:H461	4:C:601:PCW:H421	1.13	1.14	9	7
4:C:624:PCW:H271	4:C:624:PCW:H231	1.13	1.14	9	9
4:D:503:PCW:H251	4:D:503:PCW:H211	1.13	1.16	3	9
4:A:403:PCW:H51	4:B:209:PCW:H351	1.13	1.18	3	2
4:C:617:PCW:H151	4:C:625:PCW:H142	1.12	1.19	6	8
4:D:510:PCW:H472	4:D:510:PCW:H432	1.12	1.21	1	10
4:D:505:PCW:H221	4:D:510:PCW:H351	1.12	1.14	8	3
4:C:623:PCW:H31	4:C:624:PCW:H32	1.12	1.18	4	2
4:C:614:PCW:H172	4:C:614:PCW:H132	1.12	1.13	9	2
4:B:202:PCW:H41	4:B:202:PCW:H31	1.12	1.14	9	7
4:C:606:PCW:H182	4:C:606:PCW:H142	1.12	1.21	4	10
4:B:207:PCW:H61	5:B:213:17F:H1A	1.12	1.13	9	1
4:A:404:PCW:H31	4:A:404:PCW:O1P	1.12	1.43	5	2
4:C:610:PCW:H321	4:C:622:PCW:H352	1.12	1.22	1	5
4:C:610:PCW:H351	4:C:610:PCW:H172	1.12	1.19	9	5
4:B:205:PCW:H251	4:B:205:PCW:H211	1.12	1.19	5	1
4:C:613:PCW:H421	4:C:613:PCW:H461	1.12	1.19	8	10
4:B:208:PCW:H472	4:B:208:PCW:H432	1.12	1.22	9	10
4:B:211:PCW:H121	4:B:211:PCW:H371	1.11	1.15	4	10
4:D:506:PCW:H461	4:D:506:PCW:H421	1.11	1.22	5	9
5:C:626:17F:H40	5:C:629:17F:H78	1.11	1.22	3	2
4:B:212:PCW:H442	5:D:514:17F:H63	1.11	1.22	10	1
4:B:208:PCW:H262	4:B:208:PCW:H222	1.11	1.20	4	10
4:A:408:PCW:H472	4:A:408:PCW:H432	1.11	1.20	1	10
4:C:610:PCW:H39	4:C:622:PCW:H462	1.11	1.20	9	8
4:B:205:PCW:H241	4:B:205:PCW:H282	1.11	1.20	5	1
4:A:408:PCW:H181	5:A:409:17F:H20A	1.10	1.20	1	1
4:B:206:PCW:C23	4:B:206:PCW:H283	1.10	1.77	5	1
4:A:413:PCW:H431	4:C:611:PCW:H172	1.10	1.19	2	5
4:B:201:PCW:H441	4:B:207:PCW:H141	1.10	1.16	1	1
4:C:620:PCW:H20	4:C:621:PCW:H82	1.10	1.14	5	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:417:PCW:H20	4:A:417:PCW:H241	1.09	1.21	5	10
4:C:620:PCW:H132	5:B:215:17F:H4A	1.09	1.22	1	8
4:A:413:PCW:H271	4:A:413:PCW:H231	1.09	1.21	9	1
4:A:407:PCW:H271	4:A:407:PCW:H232	1.09	1.23	10	1
4:A:413:PCW:H422	4:C:611:PCW:H231	1.09	1.13	2	9
4:C:603:PCW:H2	4:C:603:PCW:H41	1.09	1.15	8	9
5:C:626:17F:H19A	5:C:626:17F:H57	1.09	1.24	6	10
5:D:511:17F:H57	5:D:511:17F:H19A	1.09	1.20	5	8
5:A:409:17F:H6	4:D:504:PCW:H342	1.09	1.22	1	1
4:B:212:PCW:H241	4:B:212:PCW:H20	1.09	1.23	6	10
4:C:605:PCW:H442	4:C:618:PCW:H483	1.08	1.24	2	2
4:C:621:PCW:H341	4:D:516:PCW:H442	1.08	1.23	10	9
4:A:404:PCW:H41	4:A:407:PCW:H32	1.08	1.22	10	1
4:A:407:PCW:H132	4:A:407:PCW:H341	1.08	1.24	9	8
4:A:417:PCW:H242	4:C:621:PCW:H242	1.08	1.19	9	10
5:C:628:17F:H67	5:B:215:17F:H36	1.08	1.19	1	3
4:A:415:PCW:H372	4:C:616:PCW:H431	1.08	1.15	9	7
4:C:610:PCW:H63	4:C:622:PCW:H321	1.08	1.21	2	8
4:C:625:PCW:H2	4:C:625:PCW:H41	1.08	1.13	1	2
4:B:206:PCW:H231	4:B:206:PCW:C28	1.08	1.78	5	1
4:A:405:PCW:C14	4:A:405:PCW:H19	1.08	1.77	7	1
4:C:603:PCW:H222	4:D:515:PCW:H351	1.08	1.20	9	9
4:D:502:PCW:H231	4:D:502:PCW:H272	1.08	1.24	8	1
5:D:512:17F:H52	5:D:514:17F:H46	1.07	1.23	5	1
4:D:502:PCW:H172	4:D:502:PCW:H211	1.07	1.16	8	1
4:C:615:PCW:H39	4:C:617:PCW:H161	1.07	1.26	9	1
4:A:408:PCW:H31	4:A:408:PCW:H371	1.07	1.23	10	8
4:C:620:PCW:H19	5:C:631:17F:H5	1.07	1.20	7	6
4:B:206:PCW:H142	5:B:213:17F:H18	1.07	1.26	9	1
4:C:607:PCW:H431	5:C:626:17F:H34	1.07	1.17	4	7
4:C:619:PCW:H121	5:C:632:17F:H4A	1.07	1.26	9	5
4:C:616:PCW:H471	4:C:616:PCW:H431	1.07	1.22	8	2
4:B:203:PCW:H241	4:B:208:PCW:H122	1.07	1.07	8	2
4:B:206:PCW:H422	5:B:213:17F:H10	1.07	1.25	6	1
4:C:606:PCW:H161	5:C:627:17F:H11A	1.06	1.23	4	9
5:C:628:17F:H67	5:B:215:17F:H39	1.06	1.26	6	5
4:C:622:PCW:H322	4:C:622:PCW:C36	1.06	1.79	3	9
4:B:206:PCW:H283	4:B:206:PCW:H231	1.06	1.14	5	1
4:B:203:PCW:H212	4:B:208:PCW:C32	1.06	1.78	8	1
4:C:620:PCW:H141	5:B:215:17F:H6	1.06	1.14	4	10
5:C:627:17F:O7	5:C:627:17F:H18A	1.06	1.51	6	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:505:PCW:H2	4:D:509:PCW:H62	1.06	1.26	5	2
4:A:401:PCW:H31	4:D:508:PCW:H181	1.06	1.15	7	1
4:A:413:PCW:H372	4:A:413:PCW:H411	1.06	1.19	9	1
4:A:405:PCW:H322	4:B:203:PCW:H341	1.06	1.17	2	4
4:A:405:PCW:H272	4:A:405:PCW:H472	1.06	1.22	10	2
4:A:401:PCW:H472	4:C:610:PCW:H271	1.06	1.25	1	3
4:A:417:PCW:H322	4:C:622:PCW:O31	1.06	1.50	7	4
4:B:211:PCW:H282	4:D:506:PCW:H241	1.06	1.25	9	2
4:C:615:PCW:H39	4:C:617:PCW:H142	1.05	1.07	4	8
4:C:623:PCW:H412	4:C:624:PCW:H412	1.05	1.16	4	8
4:D:505:PCW:H171	4:D:505:PCW:H132	1.05	1.27	10	10
4:C:616:PCW:H2	4:C:616:PCW:H41	1.05	1.25	7	3
4:C:620:PCW:H421	5:B:215:17F:H62	1.05	1.28	6	8
4:B:205:PCW:H141	4:B:206:PCW:H222	1.05	1.26	3	1
5:D:513:17F:H12	5:D:513:17F:H65	1.05	1.18	3	3
4:A:404:PCW:H152	4:B:210:PCW:H211	1.05	1.16	7	3
4:A:405:PCW:H11	4:B:203:PCW:H61	1.05	1.20	5	2
4:C:621:PCW:H141	5:C:628:17F:H32	1.05	1.17	10	4
4:D:507:PCW:H351	5:D:513:17F:H10A	1.05	1.14	9	1
4:D:508:PCW:H19	5:D:512:17F:H19A	1.05	1.22	9	2
4:C:623:PCW:H12	4:C:624:PCW:H12	1.05	1.05	5	6
4:B:211:PCW:H20	4:D:506:PCW:H242	1.05	1.22	7	2
4:A:403:PCW:H132	4:B:201:PCW:H121	1.05	1.25	10	3
4:C:611:PCW:H172	4:C:611:PCW:H212	1.05	1.27	1	8
4:C:621:PCW:H19	5:C:628:17F:H19A	1.05	1.19	1	1
4:B:208:PCW:H52	5:B:214:17F:H4	1.05	1.28	5	3
4:A:403:PCW:H121	4:B:201:PCW:H342	1.05	1.24	7	1
4:D:508:PCW:H412	4:D:508:PCW:H372	1.05	1.22	10	2
4:A:415:PCW:H11	4:C:616:PCW:H411	1.05	1.25	9	7
4:C:609:PCW:H63	5:C:631:17F:H6A	1.05	1.21	1	6
4:B:204:PCW:H151	4:B:208:PCW:H341	1.05	1.24	7	2
4:A:412:PCW:H31	4:C:624:PCW:H371	1.05	1.28	5	1
4:A:412:PCW:H12	4:C:624:PCW:H372	1.04	1.18	9	9
4:C:615:PCW:H451	4:D:506:PCW:H452	1.04	1.11	2	3
4:D:508:PCW:H41	4:D:508:PCW:H31	1.04	1.28	7	7
4:A:404:PCW:H12	4:B:210:PCW:H381	1.04	1.28	9	1
4:B:203:PCW:H271	4:B:204:PCW:H182	1.04	1.13	3	1
4:C:622:PCW:H362	4:C:622:PCW:H322	1.04	1.07	4	5
4:A:407:PCW:H371	4:B:210:PCW:H272	1.04	1.27	1	1
4:A:408:PCW:H121	5:A:409:17F:H33	1.04	1.29	8	2
4:C:604:PCW:H451	4:C:606:PCW:H181	1.04	1.24	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:620:PCW:H32	4:C:620:PCW:O1P	1.04	1.50	8	1
4:A:401:PCW:H411	4:D:502:PCW:H262	1.04	1.28	6	3
4:A:415:PCW:H20	4:A:415:PCW:H242	1.03	1.27	1	1
4:D:505:PCW:H161	4:D:510:PCW:H471	1.03	1.20	1	1
5:B:213:17F:H63	4:D:505:PCW:H39	1.03	1.23	4	3
4:C:623:PCW:H39	4:C:624:PCW:H141	1.03	1.21	3	2
5:C:627:17F:C7	5:C:627:17F:H18A	1.03	1.83	8	2
4:D:506:PCW:H32	4:D:506:PCW:O1P	1.03	1.51	8	3
4:C:604:PCW:H361	5:C:627:17F:H36	1.03	1.29	8	3
4:D:501:PCW:H381	4:D:509:PCW:H422	1.03	1.23	6	2
4:C:611:PCW:H261	4:C:611:PCW:H471	1.03	1.27	5	1
4:A:408:PCW:H162	5:A:409:17F:H59	1.03	1.29	6	1
4:A:415:PCW:H451	4:D:515:PCW:H211	1.03	1.26	9	4
4:A:416:PCW:H122	5:C:630:17F:H9	1.03	1.21	9	9
4:C:617:PCW:H131	4:C:625:PCW:H151	1.03	1.16	9	8
4:C:621:PCW:H362	5:C:627:17F:H76	1.03	1.20	4	2
4:D:501:PCW:H39	4:D:509:PCW:H441	1.03	1.27	7	2
4:A:415:PCW:H422	4:C:615:PCW:H232	1.03	1.09	1	4
4:C:606:PCW:H212	4:C:606:PCW:H172	1.03	1.30	2	10
4:C:622:PCW:H362	4:C:622:PCW:C32	1.03	1.82	3	10
5:A:410:17F:H72	4:D:501:PCW:H252	1.03	1.21	3	1
4:A:413:PCW:H332	4:C:611:PCW:H132	1.03	1.21	3	3
4:C:604:PCW:H381	5:C:627:17F:H36	1.03	1.25	3	5
4:C:605:PCW:H171	4:C:612:PCW:H342	1.03	1.26	6	5
4:D:506:PCW:H342	4:D:507:PCW:H381	1.03	1.25	5	2
4:D:509:PCW:H51	4:D:509:PCW:H12	1.02	1.22	9	8
5:C:630:17F:H65	5:C:630:17F:H58	1.02	1.25	2	1
4:A:405:PCW:H371	5:D:512:17F:H65	1.02	1.31	2	3
4:C:608:PCW:H2	4:C:614:PCW:H61	1.02	1.30	5	6
4:C:621:PCW:H172	5:C:628:17F:H32	1.02	1.06	1	7
5:A:410:17F:H1	4:D:502:PCW:H63	1.02	1.31	7	1
4:D:505:PCW:H422	4:D:506:PCW:H141	1.02	1.21	8	1
4:C:606:PCW:H61	4:C:624:PCW:H281	1.02	1.29	8	6
4:A:403:PCW:H231	4:B:201:PCW:H211	1.02	1.28	6	1
4:D:505:PCW:H361	4:D:506:PCW:H122	1.02	1.10	8	2
4:A:413:PCW:H411	4:A:413:PCW:C37	1.02	1.84	9	6
4:A:403:PCW:H61	4:A:406:PCW:H371	1.02	1.24	6	2
4:C:614:PCW:H452	4:B:207:PCW:H262	1.02	1.26	7	1
4:A:408:PCW:H141	4:A:408:PCW:H182	1.02	1.24	8	2
4:C:607:PCW:H41	4:C:624:PCW:H222	1.02	1.28	2	7
4:C:621:PCW:H141	5:C:628:17F:H33	1.01	1.32	2	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:202:PCW:H332	4:D:507:PCW:H11	1.01	1.28	2	3
4:B:202:PCW:H161	4:D:504:PCW:H322	1.01	1.27	5	4
4:C:603:PCW:H462	4:D:515:PCW:H432	1.01	1.32	4	4
4:A:402:PCW:H281	4:A:413:PCW:H221	1.01	1.25	8	1
4:A:415:PCW:H362	4:C:616:PCW:H412	1.01	1.32	2	8
4:A:401:PCW:H452	4:C:610:PCW:H271	1.01	1.31	4	1
4:A:402:PCW:H221	4:A:413:PCW:H262	1.01	1.25	6	1
4:B:205:PCW:H141	4:B:207:PCW:H321	1.01	1.21	6	1
4:B:206:PCW:H142	5:B:213:17F:H20A	1.01	1.29	8	4
4:A:405:PCW:H142	4:A:405:PCW:H19	1.01	1.25	4	3
4:C:606:PCW:H73	4:C:624:PCW:H19	1.01	1.27	7	6
4:C:621:PCW:H162	4:D:516:PCW:H172	1.01	1.30	2	7
4:A:402:PCW:H231	4:A:413:PCW:H262	1.01	1.20	7	2
4:D:508:PCW:H361	4:D:508:PCW:H221	1.01	1.26	4	2
4:C:614:PCW:H141	5:C:632:17F:H9A	1.01	1.33	5	3
4:B:202:PCW:H181	4:B:202:PCW:C23	1.01	1.84	6	1
4:A:405:PCW:H271	4:A:414:PCW:H281	1.01	1.29	8	1
4:B:203:PCW:H231	4:B:204:PCW:H19	1.01	1.29	8	1
4:A:401:PCW:H12	4:D:508:PCW:H342	1.01	1.23	4	1
5:D:512:17F:H47	5:D:514:17F:H42	1.01	1.30	6	2
5:A:409:17F:H42	5:D:511:17F:C18	1.01	1.85	9	1
4:C:614:PCW:H472	4:B:207:PCW:H231	1.01	1.28	1	1
4:A:401:PCW:H442	4:C:613:PCW:H262	1.00	1.33	2	4
4:A:413:PCW:H431	4:C:611:PCW:C17	1.00	1.85	2	6
5:C:627:17F:H69	5:B:215:17F:C8	1.00	1.85	2	1
4:C:621:PCW:H441	4:D:506:PCW:H272	1.00	1.29	3	3
4:D:501:PCW:H51	4:D:509:PCW:H331	1.00	1.06	9	2
4:C:604:PCW:H461	4:C:624:PCW:H282	1.00	1.28	8	7
4:B:210:PCW:H271	4:B:211:PCW:H222	1.00	1.26	2	2
4:A:412:PCW:H431	4:C:623:PCW:H471	1.00	1.33	5	5
4:C:602:PCW:H362	5:B:214:17F:H67	1.00	1.25	3	2
4:C:613:PCW:H442	4:C:618:PCW:H20	1.00	1.32	7	6
4:A:404:PCW:H242	4:B:210:PCW:H221	1.00	1.06	8	3
4:C:622:PCW:C36	4:C:622:PCW:H322	1.00	1.86	8	1
5:A:409:17F:H42	5:D:511:17F:H18	1.00	1.28	9	1
4:C:608:PCW:H251	5:C:626:17F:H70	1.00	1.23	9	5
4:C:614:PCW:H221	4:B:207:PCW:H251	1.00	1.32	6	3
4:B:212:PCW:H422	5:D:514:17F:H59	1.00	1.32	10	1
4:C:603:PCW:H371	4:C:603:PCW:H412	1.00	1.33	10	10
4:C:603:PCW:H2	4:C:603:PCW:C4	1.00	1.84	5	7
4:B:206:PCW:H361	5:B:213:17F:H5	1.00	1.34	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:602:PCW:H221	4:C:602:PCW:H172	1.00	1.30	8	9
4:D:507:PCW:H471	5:D:513:17F:H32	1.00	1.30	3	1
4:B:206:PCW:O1P	4:B:206:PCW:H31	1.00	1.56	8	4
4:D:509:PCW:H63	4:D:510:PCW:H321	1.00	1.27	7	2
4:A:402:PCW:H62	5:D:513:17F:H18	1.00	1.34	9	1
4:A:413:PCW:H442	4:C:611:PCW:H242	1.00	1.27	10	3
4:D:503:PCW:H152	4:D:507:PCW:H39	1.00	1.33	10	5
4:C:622:PCW:H232	4:D:501:PCW:H481	1.00	1.24	5	1
4:A:416:PCW:H162	5:C:630:17F:H57	1.00	1.27	6	9
4:A:415:PCW:H432	4:D:515:PCW:H211	1.00	1.33	4	5
4:C:601:PCW:H471	4:C:601:PCW:H151	0.99	1.30	4	1
4:C:622:PCW:H421	4:C:623:PCW:H261	0.99	1.29	10	6
5:C:627:17F:H69	5:B:215:17F:H8	0.99	1.06	2	1
4:A:408:PCW:H341	5:A:409:17F:H57	0.99	1.32	6	2
4:C:623:PCW:H412	4:C:624:PCW:H39	0.99	1.34	5	1
4:D:504:PCW:H182	4:D:504:PCW:H221	0.99	1.24	5	3
4:D:507:PCW:H331	5:D:513:17F:C8	0.99	1.87	1	2
4:A:413:PCW:H422	4:C:611:PCW:C23	0.99	1.88	2	8
4:C:607:PCW:H261	5:C:629:17F:H62	0.99	1.32	5	6
4:C:615:PCW:H39	4:C:617:PCW:C14	0.99	1.85	4	7
4:B:206:PCW:H332	4:D:505:PCW:H331	0.99	1.33	10	1
4:D:508:PCW:H222	4:D:508:PCW:H272	0.99	0.99	10	3
4:D:506:PCW:H40	4:D:516:PCW:H251	0.99	1.30	3	2
4:C:606:PCW:H212	4:C:606:PCW:C17	0.99	1.87	6	10
4:D:508:PCW:H362	4:D:508:PCW:H221	0.99	1.34	2	2
4:C:610:PCW:H222	4:C:618:PCW:H442	0.99	1.31	4	1
4:C:625:PCW:H2	4:C:625:PCW:C4	0.99	1.86	7	4
4:C:622:PCW:H232	4:D:501:PCW:H483	0.99	1.32	2	1
4:C:610:PCW:O2P	4:C:618:PCW:H63	0.99	1.57	6	2
4:D:501:PCW:H222	5:D:511:17F:H56	0.99	1.34	9	2
4:C:621:PCW:H162	4:D:516:PCW:H152	0.99	1.29	1	4
4:B:211:PCW:O31	4:B:211:PCW:H352	0.99	1.58	2	10
4:B:204:PCW:H32	4:B:208:PCW:H152	0.99	1.34	2	6
4:A:405:PCW:C32	4:B:203:PCW:H341	0.98	1.85	2	4
4:C:619:PCW:H2	4:C:619:PCW:H41	0.98	1.30	5	1
4:A:403:PCW:H141	4:B:201:PCW:H362	0.98	1.34	7	2
4:B:206:PCW:H171	4:B:207:PCW:H331	0.98	1.32	6	1
4:A:415:PCW:H372	4:C:616:PCW:C43	0.98	1.86	10	7
4:A:415:PCW:C37	4:C:616:PCW:H431	0.98	1.87	2	5
4:A:404:PCW:H242	4:B:210:PCW:H231	0.98	1.33	2	1
4:B:208:PCW:O4P	4:B:208:PCW:H32	0.98	1.59	7	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:504:PCW:H421	4:D:504:PCW:C16	0.98	1.87	5	1
4:B:210:PCW:H482	5:D:513:17F:H32	0.98	1.36	1	1
4:D:504:PCW:H421	4:D:504:PCW:H161	0.98	0.99	5	1
4:C:611:PCW:H212	4:C:611:PCW:C17	0.98	1.86	4	6
4:C:607:PCW:H121	4:C:608:PCW:H171	0.98	1.03	4	1
5:D:513:17F:H11	5:D:513:17F:H65	0.98	1.33	10	1
4:C:610:PCW:C32	4:C:622:PCW:H352	0.98	1.89	1	6
4:C:622:PCW:H322	4:C:622:PCW:H362	0.98	1.04	8	5
4:B:210:PCW:H262	4:D:503:PCW:H252	0.98	1.32	2	2
4:C:619:PCW:O1P	4:C:620:PCW:H52	0.98	1.58	10	7
4:B:203:PCW:H212	4:B:208:PCW:H321	0.98	1.00	8	1
4:C:604:PCW:H212	4:D:509:PCW:H283	0.98	1.36	7	1
4:A:411:PCW:H451	4:C:616:PCW:H242	0.97	1.34	8	9
4:C:605:PCW:H182	4:C:612:PCW:H362	0.97	1.31	6	9
4:A:401:PCW:H62	4:D:508:PCW:H2	0.97	1.35	7	5
4:A:415:PCW:H361	4:D:515:PCW:H161	0.97	1.36	4	1
5:A:409:17F:H60	4:D:504:PCW:H432	0.97	1.32	5	1
4:D:509:PCW:H161	5:D:514:17F:H60	0.97	1.35	10	1
4:B:210:PCW:H261	4:D:503:PCW:H252	0.97	1.32	6	1
4:A:416:PCW:H381	4:C:616:PCW:H151	0.97	1.32	3	3
4:C:620:PCW:H441	5:B:215:17F:H77	0.97	1.30	4	1
4:C:625:PCW:H241	4:D:516:PCW:H451	0.97	1.37	8	4
4:C:604:PCW:H31	4:C:604:PCW:O4P	0.97	1.58	8	10
4:C:620:PCW:H412	5:C:632:17F:H77	0.97	1.36	3	3
4:A:403:PCW:H212	4:A:403:PCW:C16	0.97	1.89	3	6
4:A:416:PCW:H122	5:C:630:17F:H11	0.97	1.36	5	7
4:B:206:PCW:H142	5:B:213:17F:H56	0.97	1.36	6	1
4:D:509:PCW:H82	4:D:510:PCW:H63	0.97	1.36	10	1
4:B:202:PCW:H31	4:B:202:PCW:C4	0.97	1.89	10	7
4:D:507:PCW:C33	5:D:513:17F:H8	0.97	1.89	1	3
4:B:210:PCW:H282	4:D:503:PCW:H212	0.97	1.35	3	1
4:B:212:PCW:H351	5:D:514:17F:H20A	0.97	1.33	9	1
4:B:207:PCW:H251	4:B:207:PCW:H20	0.97	1.03	10	1
4:A:401:PCW:H182	4:A:401:PCW:H221	0.97	1.36	10	4
4:C:607:PCW:H141	4:C:608:PCW:H171	0.97	1.32	2	2
4:B:207:PCW:H351	4:B:209:PCW:H121	0.97	1.34	10	1
4:C:607:PCW:H181	5:C:629:17F:H11	0.97	1.33	4	6
4:A:414:PCW:H431	4:C:623:PCW:H462	0.97	1.35	8	7
4:B:204:PCW:H483	4:D:502:PCW:H442	0.97	1.37	4	1
4:A:411:PCW:H19	4:A:415:PCW:H431	0.97	1.37	7	2
4:B:212:PCW:H372	5:B:213:17F:H29	0.97	1.31	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:620:PCW:H181	4:C:620:PCW:H142	0.97	1.36	7	10
4:D:504:PCW:H351	4:D:504:PCW:O31	0.97	1.58	5	8
4:C:621:PCW:H331	4:C:625:PCW:H20	0.97	1.33	4	1
4:A:416:PCW:H442	4:C:616:PCW:H20	0.97	1.34	3	2
4:A:408:PCW:H141	5:A:409:17F:H63	0.97	1.31	3	2
4:C:602:PCW:H483	5:C:626:17F:H65	0.97	1.36	4	2
4:A:412:PCW:H431	4:C:624:PCW:H472	0.96	1.32	1	2
4:C:614:PCW:H51	5:C:632:17F:O4	0.96	1.60	5	6
4:C:621:PCW:H421	4:D:506:PCW:H282	0.96	1.33	1	2
4:B:204:PCW:H152	4:B:208:PCW:H382	0.96	1.36	1	1
4:A:417:PCW:H321	4:A:417:PCW:H73	0.96	1.35	3	6
4:B:206:PCW:H412	5:B:213:17F:H11A	0.96	1.37	7	2
4:C:624:PCW:H271	4:C:624:PCW:C22	0.96	1.89	7	1
4:D:508:PCW:H31	4:D:508:PCW:C4	0.96	1.90	6	8
4:C:604:PCW:H2	4:C:606:PCW:H82	0.96	1.37	4	8
4:A:408:PCW:H181	4:A:408:PCW:H221	0.96	1.35	3	5
4:B:205:PCW:H52	5:B:214:17F:H10A	0.96	1.35	6	3
5:C:627:17F:H71	5:B:215:17F:H29	0.96	1.34	6	1
4:B:204:PCW:H121	4:B:208:PCW:H342	0.96	1.35	6	1
4:C:607:PCW:H431	5:C:626:17F:C1Z	0.96	1.89	10	4
4:A:401:PCW:H181	4:A:401:PCW:H221	0.96	1.33	4	2
4:C:604:PCW:H283	5:B:213:17F:H51	0.96	1.30	4	3
4:C:615:PCW:H441	4:C:625:PCW:H232	0.96	1.34	7	3
4:A:408:PCW:H121	5:A:409:17F:C1Z	0.96	1.90	1	2
4:B:204:PCW:H11	5:B:214:17F:H8A	0.96	1.34	3	6
5:A:409:17F:H52	4:D:504:PCW:H411	0.96	1.32	4	1
4:C:603:PCW:H222	4:D:515:PCW:C35	0.96	1.90	6	10
4:C:606:PCW:H252	5:C:627:17F:H38	0.96	1.34	6	7
4:D:505:PCW:H181	4:D:505:PCW:H222	0.96	1.37	2	2
4:A:404:PCW:H242	4:B:210:PCW:C22	0.95	1.91	7	3
4:B:206:PCW:H372	5:B:213:17F:H34	0.95	1.32	6	1
4:A:416:PCW:H122	5:C:630:17F:C9	0.95	1.90	1	9
4:B:206:PCW:H41	4:B:206:PCW:H31	0.95	1.36	2	1
4:C:607:PCW:H19	5:C:629:17F:H46	0.95	1.33	4	9
4:D:510:PCW:H42	4:D:510:PCW:H2	0.95	1.34	1	1
4:A:404:PCW:H351	4:A:407:PCW:H152	0.95	1.38	4	2
4:B:206:PCW:H211	5:B:213:17F:H57	0.95	1.37	4	1
4:C:604:PCW:H272	5:D:514:17F:H77	0.95	1.35	6	1
4:C:615:PCW:H341	4:D:516:PCW:H341	0.95	1.35	7	7
4:B:203:PCW:H231	4:B:204:PCW:C19	0.95	1.91	8	1
4:A:401:PCW:H472	4:C:610:PCW:H251	0.95	1.35	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:417:PCW:H141	4:C:603:PCW:H382	0.95	1.35	10	5
4:A:417:PCW:H62	4:A:417:PCW:H2	0.95	1.38	4	1
4:A:407:PCW:H39	4:B:210:PCW:H272	0.95	1.33	7	2
4:D:501:PCW:H62	4:D:509:PCW:H2	0.95	1.39	8	1
4:C:617:PCW:H381	4:C:625:PCW:H161	0.95	1.32	4	8
4:B:211:PCW:H19	4:D:505:PCW:H451	0.95	1.35	4	4
4:C:625:PCW:H42	4:C:625:PCW:C2	0.95	1.92	7	2
4:C:615:PCW:C39	4:C:617:PCW:H142	0.95	1.92	3	7
4:C:603:PCW:H271	4:D:515:PCW:H212	0.94	1.34	10	9
4:C:623:PCW:H19	4:C:623:PCW:H151	0.94	1.36	1	9
4:A:401:PCW:H252	4:C:613:PCW:H281	0.94	1.36	2	2
4:B:212:PCW:H351	5:D:514:17F:C20	0.94	1.92	9	1
4:B:205:PCW:H352	4:B:207:PCW:H132	0.94	1.39	10	1
4:D:502:PCW:H412	4:D:508:PCW:H352	0.94	1.35	1	1
4:C:610:PCW:H283	4:C:618:PCW:H251	0.94	1.32	8	1
4:D:509:PCW:H51	4:D:509:PCW:C1	0.94	1.91	6	7
4:C:619:PCW:H2	4:C:619:PCW:C4	0.94	1.92	5	1
5:C:627:17F:H78	5:B:215:17F:H35	0.94	1.36	8	2
4:C:611:PCW:H321	4:C:617:PCW:H152	0.94	1.40	7	2
4:C:608:PCW:H271	5:C:626:17F:H73	0.94	1.34	2	5
4:C:611:PCW:H471	4:C:611:PCW:H232	0.94	1.35	10	6
4:D:508:PCW:H31	4:D:508:PCW:H42	0.94	1.38	1	1
4:C:610:PCW:H322	4:C:622:PCW:H352	0.94	1.37	7	1
4:A:411:PCW:H452	4:A:416:PCW:H421	0.94	1.36	5	4
4:C:603:PCW:H41	4:C:603:PCW:C2	0.94	1.92	5	9
4:A:411:PCW:H141	4:A:415:PCW:C33	0.94	1.92	9	3
4:A:417:PCW:H451	5:D:511:17F:H75	0.94	1.37	3	4
4:A:414:PCW:H40	4:C:623:PCW:H461	0.94	1.38	7	7
4:D:510:PCW:H51	4:D:510:PCW:O11	0.94	1.61	5	2
4:C:614:PCW:H122	5:C:632:17F:H8	0.94	1.39	7	1
4:C:612:PCW:H121	4:C:618:PCW:H382	0.94	1.38	2	4
4:A:408:PCW:H172	5:A:409:17F:H20	0.94	1.39	9	1
4:D:505:PCW:H262	5:D:513:17F:H50	0.94	1.35	1	1
5:D:511:17F:H57	5:D:511:17F:C19	0.94	1.93	1	8
4:A:414:PCW:H431	4:C:623:PCW:C46	0.94	1.93	4	9
4:C:604:PCW:H482	4:C:624:PCW:H282	0.93	1.33	1	6
4:D:507:PCW:H431	5:D:513:17F:H30	0.93	1.39	1	2
4:D:507:PCW:H351	5:D:513:17F:H9	0.93	1.33	5	1
4:B:208:PCW:H121	5:B:214:17F:C18	0.93	1.93	9	2
4:C:620:PCW:C14	5:B:215:17F:H6	0.93	1.93	9	10
4:B:211:PCW:H121	4:B:211:PCW:C37	0.93	1.93	3	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:504:PCW:H221	4:D:504:PCW:C18	0.93	1.91	5	3
4:C:603:PCW:O11	4:C:604:PCW:H61	0.93	1.62	7	3
4:A:404:PCW:H351	4:A:407:PCW:H162	0.93	1.36	7	2
4:A:413:PCW:H332	4:C:611:PCW:C13	0.93	1.93	3	2
4:A:412:PCW:H472	4:B:208:PCW:H483	0.93	1.37	4	2
4:B:212:PCW:H421	5:D:514:17F:H10	0.93	1.40	9	2
4:C:625:PCW:H2	4:C:625:PCW:H42	0.93	0.96	7	2
4:C:621:PCW:H122	5:C:627:17F:H67	0.93	1.35	10	1
4:C:607:PCW:H261	5:C:629:17F:C35	0.93	1.93	5	6
4:B:202:PCW:H73	4:B:202:PCW:C11	0.93	1.91	7	6
4:B:206:PCW:H461	5:B:213:17F:H68	0.93	1.36	3	1
4:A:403:PCW:H212	4:A:403:PCW:H171	0.93	1.38	1	3
4:A:401:PCW:H39	4:D:502:PCW:H271	0.93	1.37	8	1
4:C:625:PCW:H42	4:C:625:PCW:O31	0.93	1.62	8	1
4:A:408:PCW:H471	5:D:511:17F:H12A	0.93	1.35	10	1
4:B:211:PCW:H261	4:B:211:PCW:C22	0.93	1.93	6	10
4:D:503:PCW:H283	4:D:507:PCW:H451	0.93	1.37	1	1
4:A:404:PCW:C24	4:B:210:PCW:H221	0.93	1.93	8	2
5:C:632:17F:H55	4:B:201:PCW:H442	0.93	1.39	4	1
4:A:411:PCW:H272	4:D:504:PCW:H281	0.93	1.39	6	1
4:C:612:PCW:H251	5:D:511:17F:H47	0.93	1.41	10	4
4:C:615:PCW:H31	4:C:615:PCW:O4P	0.93	1.62	10	7
5:C:627:17F:H47	5:C:628:17F:H39	0.93	1.35	5	3
4:B:204:PCW:H161	4:B:208:PCW:C22	0.93	1.94	3	2
4:B:204:PCW:H172	4:B:204:PCW:H212	0.93	1.38	6	4
4:A:415:PCW:H412	4:D:515:PCW:H231	0.93	1.37	6	1
4:A:417:PCW:H20	4:A:417:PCW:C24	0.93	1.94	4	10
4:C:608:PCW:O31	4:C:614:PCW:H61	0.92	1.62	9	3
4:B:205:PCW:H332	4:B:207:PCW:H121	0.92	1.40	10	1
4:C:607:PCW:H63	4:C:624:PCW:H242	0.92	1.38	3	4
4:B:211:PCW:H221	4:B:211:PCW:C26	0.92	1.95	6	10
5:D:512:17F:H41	5:D:512:17F:C12	0.92	1.94	1	7
4:A:412:PCW:C1	4:C:624:PCW:H372	0.92	1.93	9	9
4:C:602:PCW:H462	5:C:626:17F:H64	0.92	1.40	9	3
4:C:605:PCW:C18	4:C:612:PCW:H362	0.92	1.94	6	9
4:B:202:PCW:H171	4:D:504:PCW:H122	0.92	1.39	7	3
4:D:508:PCW:H182	4:D:508:PCW:H342	0.92	1.39	6	4
5:A:409:17F:O1	4:D:504:PCW:H331	0.92	1.64	9	1
4:B:211:PCW:H371	4:B:211:PCW:C12	0.92	1.94	3	10
4:D:501:PCW:H261	5:D:511:17F:H64	0.92	1.41	1	1
4:C:606:PCW:C7	4:C:624:PCW:H19	0.92	1.94	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:614:PCW:H51	5:C:632:17F:O5	0.92	1.64	3	1
4:A:405:PCW:H142	4:A:405:PCW:C20	0.92	1.94	10	8
4:A:411:PCW:H141	4:A:415:PCW:H341	0.92	1.39	5	9
4:C:613:PCW:H421	4:C:613:PCW:C46	0.92	1.93	2	10
4:A:416:PCW:H321	4:C:616:PCW:H52	0.92	1.41	2	1
4:C:603:PCW:C22	4:D:515:PCW:H351	0.92	1.95	10	6
4:D:502:PCW:H211	4:D:502:PCW:C17	0.92	1.93	8	2
4:A:413:PCW:H39	4:C:611:PCW:H432	0.92	1.37	5	2
4:C:602:PCW:H381	4:C:602:PCW:H142	0.92	1.38	8	8
4:A:413:PCW:H361	4:C:611:PCW:H152	0.92	1.41	3	1
4:D:508:PCW:H451	4:D:508:PCW:H262	0.92	1.42	4	1
4:A:406:PCW:H462	4:D:506:PCW:H251	0.92	1.38	6	1
4:A:413:PCW:H382	4:C:611:PCW:H151	0.92	1.42	6	1
4:D:502:PCW:H412	4:D:508:PCW:H361	0.92	1.42	6	1
4:A:415:PCW:O2P	4:A:415:PCW:H32	0.91	1.65	1	2
4:C:606:PCW:H172	4:C:606:PCW:C21	0.91	1.95	6	10
4:A:408:PCW:C12	5:A:409:17F:H33	0.91	1.95	1	1
4:C:623:PCW:C41	4:C:624:PCW:H412	0.91	1.95	4	6
4:C:609:PCW:H62	5:C:631:17F:O1	0.91	1.66	9	3
4:B:204:PCW:H132	4:B:208:PCW:H131	0.91	1.40	4	1
4:C:603:PCW:H441	4:C:603:PCW:H212	0.91	1.38	5	7
4:D:508:PCW:H382	4:D:508:PCW:H232	0.91	1.39	2	2
4:A:408:PCW:H122	5:A:409:17F:H71	0.91	1.40	10	1
4:A:417:PCW:H222	4:C:603:PCW:H182	0.91	1.39	4	7
5:C:632:17F:H75	5:B:215:17F:H62	0.91	1.41	2	1
4:A:405:PCW:H19	4:A:405:PCW:C14	0.91	1.94	4	1
4:A:403:PCW:H82	4:B:209:PCW:H11	0.91	1.43	7	1
4:A:414:PCW:C40	4:C:623:PCW:H441	0.91	1.95	6	10
4:D:507:PCW:H412	4:D:507:PCW:H371	0.91	1.42	2	4
4:C:614:PCW:H2	4:C:614:PCW:H42	0.91	1.43	8	7
4:B:203:PCW:C21	4:B:208:PCW:H321	0.91	1.94	8	1
4:C:605:PCW:O31	4:C:612:PCW:H51	0.91	1.65	10	4
4:C:620:PCW:H262	4:C:621:PCW:H61	0.91	1.42	5	1
4:C:603:PCW:H421	4:D:515:PCW:H362	0.91	1.39	1	5
2:B:38:ASP:HB3	2:B:57:ASP:HB3	0.91	1.38	10	5
4:A:415:PCW:H422	4:C:615:PCW:C23	0.91	1.96	1	5
4:D:507:PCW:H331	5:D:513:17F:H8	0.91	0.94	1	4
4:A:405:PCW:H461	4:A:414:PCW:H272	0.91	1.39	5	4
4:A:417:PCW:H332	4:C:622:PCW:H122	0.91	1.41	7	2
4:A:413:PCW:H332	4:C:611:PCW:O3	0.91	1.66	2	3
4:A:401:PCW:H483	4:C:613:PCW:H242	0.91	1.39	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:210:PCW:H271	4:B:211:PCW:H231	0.91	1.40	7	1
4:C:606:PCW:H63	4:C:606:PCW:O11	0.90	1.66	10	7
4:A:403:PCW:H372	4:A:403:PCW:H411	0.90	1.38	6	2
4:C:606:PCW:C6	4:C:624:PCW:H281	0.90	1.96	8	9
4:C:607:PCW:H461	5:C:626:17F:H61	0.90	1.43	2	5
4:C:615:PCW:C45	4:D:506:PCW:H452	0.90	1.96	2	2
4:D:508:PCW:H41	4:D:508:PCW:C3	0.90	1.95	6	6
4:D:501:PCW:H381	4:D:509:PCW:C42	0.90	1.97	4	2
4:D:501:PCW:H332	5:D:512:17F:H37	0.90	1.42	6	2
4:B:212:PCW:H272	5:D:512:17F:H61	0.90	1.42	8	1
4:B:208:PCW:H2	4:B:208:PCW:H42	0.90	1.39	1	1
4:B:202:PCW:H382	4:B:202:PCW:O3	0.90	1.67	8	1
4:D:510:PCW:H181	5:D:513:17F:H48	0.90	1.40	2	1
4:D:509:PCW:H412	4:D:509:PCW:H371	0.90	1.43	1	7
4:C:610:PCW:H2	4:C:618:PCW:H63	0.90	1.44	9	4
4:C:602:PCW:H131	5:B:214:17F:H60	0.90	1.42	7	2
4:C:602:PCW:H261	5:C:629:17F:H76	0.90	1.44	8	4
4:A:417:PCW:H451	5:D:511:17F:H77	0.90	1.43	9	1
4:C:610:PCW:C6	4:C:622:PCW:H321	0.90	1.97	5	6
4:B:201:PCW:H352	4:B:201:PCW:O31	0.90	1.66	7	8
4:C:606:PCW:H73	4:C:606:PCW:O11	0.90	1.66	3	1
4:C:621:PCW:C33	4:C:625:PCW:H20	0.90	1.96	4	2
4:C:617:PCW:H422	4:C:625:PCW:H261	0.90	1.43	6	3
4:B:206:PCW:H161	5:B:213:17F:H57	0.90	1.44	10	2
4:C:604:PCW:H381	5:C:627:17F:H40	0.90	1.42	9	4
4:B:211:PCW:H162	4:B:211:PCW:H422	0.90	1.42	1	3
4:A:411:PCW:H161	4:A:415:PCW:H331	0.90	1.41	10	7
4:D:506:PCW:H462	5:D:513:17F:H47	0.90	1.44	3	1
4:C:603:PCW:H442	4:D:515:PCW:H351	0.90	1.44	3	2
4:B:211:PCW:H19	4:D:505:PCW:H432	0.90	1.44	10	2
4:C:620:PCW:H283	4:C:621:PCW:H61	0.90	1.42	8	2
4:D:508:PCW:H73	4:D:508:PCW:C11	0.90	1.97	5	5
5:C:627:17F:H63	5:B:215:17F:H8A	0.90	1.44	4	1
4:C:620:PCW:H132	5:B:215:17F:C4	0.89	1.97	10	6
4:A:412:PCW:H31	4:C:624:PCW:H372	0.89	1.40	7	7
4:A:407:PCW:H82	4:B:211:PCW:H2	0.89	1.44	2	3
4:C:615:PCW:P	4:C:615:PCW:H31	0.89	2.06	7	3
4:B:203:PCW:H283	5:B:214:17F:H20A	0.89	1.41	7	2
4:C:615:PCW:H19	4:C:616:PCW:H461	0.89	1.41	5	2
4:C:614:PCW:H132	4:C:614:PCW:C17	0.89	1.97	9	1
4:D:505:PCW:H422	4:D:506:PCW:C14	0.89	1.96	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:624:PCW:H231	4:C:624:PCW:C27	0.89	1.97	2	8
4:B:202:PCW:H171	4:D:504:PCW:H121	0.89	1.44	3	1
4:D:508:PCW:C19	5:D:512:17F:H19A	0.89	1.97	9	2
4:B:202:PCW:H41	4:B:202:PCW:C3	0.89	1.97	10	7
4:D:507:PCW:H271	4:D:507:PCW:H483	0.89	1.41	3	2
4:B:204:PCW:H131	4:B:208:PCW:H151	0.89	1.41	10	2
4:D:501:PCW:H161	5:D:511:17F:H18	0.89	1.44	10	1
4:A:405:PCW:H271	4:A:414:PCW:H271	0.89	1.44	7	4
4:A:408:PCW:H31	4:A:408:PCW:C37	0.89	1.97	5	4
4:D:506:PCW:H421	4:D:506:PCW:C46	0.89	1.98	2	9
4:A:403:PCW:H231	4:A:403:PCW:H162	0.89	1.43	2	5
4:D:503:PCW:H52	4:D:506:PCW:H62	0.89	1.43	3	1
4:A:401:PCW:H381	4:D:502:PCW:H231	0.89	1.43	4	3
4:C:606:PCW:H62	4:C:624:PCW:H281	0.89	1.41	1	2
4:C:615:PCW:C34	4:D:516:PCW:H341	0.89	1.97	10	6
4:A:411:PCW:H362	4:A:416:PCW:H371	0.89	1.42	7	2
4:D:502:PCW:H381	4:D:508:PCW:H341	0.89	1.43	7	1
4:A:413:PCW:C42	4:C:611:PCW:H231	0.89	1.97	7	8
4:C:617:PCW:H412	5:C:631:17F:H45	0.89	1.38	5	3
4:C:610:PCW:H41	4:C:622:PCW:H342	0.89	1.42	9	3
4:A:408:PCW:H172	4:A:408:PCW:H212	0.89	1.41	5	1
4:D:508:PCW:H372	4:D:508:PCW:C41	0.89	1.98	10	2
5:A:409:17F:H61	5:D:511:17F:H37	0.88	1.43	10	2
4:D:505:PCW:H422	4:D:505:PCW:H381	0.88	1.42	1	1
4:D:506:PCW:H41	4:D:506:PCW:H31	0.88	1.44	8	1
5:C:627:17F:C38	5:B:215:17F:H8	0.88	1.96	2	1
4:D:509:PCW:H12	4:D:509:PCW:C5	0.88	1.97	6	6
4:B:203:PCW:H252	4:B:204:PCW:H151	0.88	1.43	6	1
4:A:403:PCW:H41	4:A:406:PCW:H40	0.88	1.43	8	1
4:C:613:PCW:H461	4:C:613:PCW:C42	0.88	1.97	2	10
4:B:203:PCW:H142	4:B:208:PCW:H371	0.88	1.42	3	1
4:C:607:PCW:C43	5:C:626:17F:H34	0.88	1.97	10	4
4:C:611:PCW:H321	4:C:617:PCW:H132	0.88	1.42	2	5
4:C:614:PCW:H472	4:B:207:PCW:H20	0.88	1.45	3	2
4:C:603:PCW:H242	4:D:515:PCW:C35	0.88	1.99	7	4
4:B:203:PCW:C24	4:B:208:PCW:H122	0.88	1.98	6	3
4:C:624:PCW:H271	4:C:624:PCW:H222	0.88	1.45	7	1
4:C:624:PCW:C27	4:C:624:PCW:H222	0.88	1.99	7	1
4:A:412:PCW:C3	4:C:624:PCW:H372	0.88	1.98	3	8
4:D:506:PCW:H461	4:D:506:PCW:C42	0.88	1.99	2	9
4:A:413:PCW:H362	4:C:611:PCW:C13	0.88	1.97	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:204:PCW:H232	4:B:208:PCW:H283	0.88	1.44	6	1
4:C:605:PCW:H211	4:C:612:PCW:H382	0.88	1.46	9	7
4:B:208:PCW:H432	4:B:208:PCW:C47	0.88	1.99	10	10
4:A:407:PCW:H431	4:B:211:PCW:H232	0.88	1.41	3	4
4:C:611:PCW:H63	4:C:617:PCW:H12	0.88	1.46	3	3
5:A:410:17F:O5	4:D:502:PCW:H51	0.88	1.68	6	2
5:A:409:17F:H39	5:A:409:17F:H29	0.88	1.45	7	1
5:D:514:17F:O6	5:D:514:17F:H18A	0.88	1.67	9	6
4:C:610:PCW:H432	4:C:610:PCW:H221	0.88	1.44	9	3
4:B:204:PCW:H471	5:D:512:17F:H43	0.88	1.43	9	1
4:B:208:PCW:H483	4:B:212:PCW:H262	0.88	1.45	1	1
4:C:621:PCW:C35	4:C:625:PCW:H20	0.88	1.97	9	8
4:C:604:PCW:C19	5:D:514:17F:H53	0.88	1.99	8	1
4:C:620:PCW:C13	5:B:215:17F:H4A	0.88	1.98	10	9
4:A:407:PCW:H382	4:B:211:PCW:H161	0.88	1.43	7	5
4:C:617:PCW:C13	4:C:625:PCW:H151	0.88	1.99	9	3
4:D:502:PCW:H482	4:D:508:PCW:H471	0.88	1.45	6	1
4:D:507:PCW:H351	5:D:513:17F:H8	0.88	1.46	6	2
4:B:204:PCW:H482	5:D:514:17F:H38	0.88	1.44	9	1
4:C:622:PCW:H131	4:C:622:PCW:H371	0.87	1.42	3	3
4:D:508:PCW:H412	4:D:508:PCW:C37	0.87	1.99	10	3
4:C:617:PCW:H422	4:C:625:PCW:H282	0.87	1.45	2	2
4:C:607:PCW:H63	4:C:624:PCW:H241	0.87	1.44	4	1
4:D:510:PCW:H32	4:D:510:PCW:O4P	0.87	1.66	4	1
4:B:201:PCW:H483	4:B:205:PCW:H39	0.87	1.44	9	1
4:C:604:PCW:H482	4:C:624:PCW:H272	0.87	1.46	4	7
4:C:604:PCW:H482	4:C:624:PCW:C28	0.87	2.00	6	8
5:B:213:17F:C35	4:D:505:PCW:H39	0.87	1.98	4	2
4:C:610:PCW:H222	4:C:618:PCW:C44	0.87	1.99	4	1
4:D:507:PCW:H351	5:D:513:17F:C10	0.87	1.99	9	2
4:A:411:PCW:H151	4:A:411:PCW:H39	0.87	1.42	5	3
4:A:408:PCW:H121	5:A:409:17F:H71	0.87	1.46	2	1
4:A:401:PCW:H73	4:D:508:PCW:H131	0.87	1.47	7	2
4:C:615:PCW:H421	4:C:625:PCW:H232	0.87	1.43	6	3
4:C:625:PCW:H222	4:D:516:PCW:H431	0.87	1.45	4	1
4:C:612:PCW:H221	5:D:511:17F:H43	0.87	1.44	6	1
4:A:415:PCW:C42	4:C:615:PCW:H232	0.87	1.97	1	4
4:C:601:PCW:H461	4:C:601:PCW:C42	0.87	2.00	3	7
4:C:608:PCW:H172	4:C:614:PCW:H331	0.87	1.47	1	2
4:D:505:PCW:H283	4:D:510:PCW:H342	0.87	1.44	6	1
4:C:607:PCW:C6	4:C:624:PCW:H283	0.87	1.99	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:204:PCW:C23	4:B:208:PCW:H261	0.87	2.00	9	1
4:B:212:PCW:H20	4:B:212:PCW:C24	0.87	1.99	10	8
4:C:619:PCW:H283	5:C:632:17F:H35	0.87	1.47	3	5
4:B:205:PCW:H241	4:B:207:PCW:H431	0.87	1.45	4	3
4:C:614:PCW:H161	5:C:632:17F:H11A	0.87	1.46	9	2
4:B:206:PCW:H152	4:B:209:PCW:H122	0.87	1.47	6	1
4:A:408:PCW:H162	5:A:409:17F:H56	0.87	1.43	3	1
4:B:205:PCW:H63	4:B:212:PCW:H321	0.87	1.44	3	1
4:D:509:PCW:H61	4:D:510:PCW:H321	0.87	1.43	10	2
4:B:212:PCW:H352	5:B:213:17F:H9A	0.87	1.47	5	2
4:A:403:PCW:H211	4:B:201:PCW:H162	0.87	1.47	8	1
4:B:201:PCW:H352	4:B:201:PCW:C31	0.87	2.00	5	10
4:D:502:PCW:H381	4:D:508:PCW:H352	0.87	1.43	9	2
4:C:620:PCW:H412	5:C:632:17F:H75	0.87	1.43	9	3
4:A:403:PCW:H121	4:B:201:PCW:C34	0.87	1.99	7	1
4:C:607:PCW:C19	5:C:629:17F:H46	0.86	2.00	4	10
4:A:405:PCW:H322	4:B:203:PCW:C34	0.86	1.96	10	5
4:B:207:PCW:H61	5:B:213:17F:O4	0.86	1.68	6	1
5:B:214:17F:H4A	5:B:214:17F:N1	0.86	1.84	10	2
5:D:512:17F:H41	5:D:512:17F:H12	0.86	1.44	6	4
4:D:503:PCW:H352	4:D:510:PCW:H82	0.86	1.43	5	1
4:D:504:PCW:H161	4:D:504:PCW:C42	0.86	1.95	5	1
4:C:610:PCW:H432	4:C:610:PCW:H20	0.86	1.47	1	6
4:C:621:PCW:H172	5:C:628:17F:C1Y	0.86	1.98	1	6
4:C:615:PCW:H482	4:D:503:PCW:H222	0.86	1.47	2	1
5:C:630:17F:H65	5:C:630:17F:C32	0.86	2.00	2	1
4:B:210:PCW:H51	5:D:513:17F:H1A	0.86	1.47	8	4
4:A:416:PCW:O31	4:C:616:PCW:H52	0.86	1.69	8	6
4:B:203:PCW:C27	4:B:204:PCW:H182	0.86	2.00	3	1
4:C:607:PCW:H42	4:C:624:PCW:H242	0.86	1.44	5	2
4:D:509:PCW:H242	5:D:514:17F:H43	0.86	1.45	9	2
4:D:509:PCW:H432	4:D:510:PCW:O2P	0.86	1.69	4	1
4:D:501:PCW:H171	4:D:502:PCW:H332	0.86	1.44	9	2
4:A:403:PCW:H212	4:A:403:PCW:H162	0.86	1.45	3	5
4:B:202:PCW:C32	4:D:507:PCW:H51	0.86	2.01	9	2
4:B:203:PCW:H212	4:B:208:PCW:H2	0.86	1.46	4	1
4:B:206:PCW:H19	5:B:213:17F:H31	0.86	1.48	10	1
4:A:404:PCW:H31	4:A:407:PCW:O3	0.86	1.71	4	5
4:C:610:PCW:H63	4:C:622:PCW:C32	0.86	2.00	3	4
4:B:205:PCW:H161	4:B:206:PCW:H222	0.86	1.48	6	1
5:A:409:17F:H2	5:A:409:17F:O1	0.86	1.70	10	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:602:PCW:H341	5:B:214:17F:H61	0.86	1.47	1	1
4:A:403:PCW:H51	4:B:209:PCW:C35	0.86	2.01	8	2
4:B:203:PCW:C17	4:B:208:PCW:H362	0.86	2.01	3	1
4:B:206:PCW:H19	5:B:213:17F:H57	0.86	1.47	3	1
4:B:208:PCW:H51	4:B:208:PCW:O11	0.86	1.71	9	4
4:C:621:PCW:H162	4:D:516:PCW:H161	0.86	1.46	5	2
4:C:615:PCW:H451	4:D:506:PCW:C45	0.85	2.01	2	3
4:D:504:PCW:H262	4:D:504:PCW:C22	0.85	2.00	8	2
4:A:408:PCW:H341	5:A:409:17F:H59	0.85	1.47	7	2
4:C:617:PCW:H451	5:C:631:17F:H55	0.85	1.44	6	5
4:D:505:PCW:H152	4:D:510:PCW:H471	0.85	1.48	8	1
4:A:417:PCW:H82	4:C:605:PCW:O2P	0.85	1.71	10	4
4:B:208:PCW:H472	4:B:208:PCW:C43	0.85	2.01	6	10
4:D:509:PCW:C1	4:D:509:PCW:H51	0.85	2.02	1	1
4:D:502:PCW:H432	4:D:508:PCW:H20	0.85	1.46	2	1
4:C:605:PCW:H171	4:C:612:PCW:C34	0.85	2.01	6	4
4:D:506:PCW:H171	4:D:510:PCW:H421	0.85	1.49	4	1
4:A:412:PCW:H12	4:C:624:PCW:C37	0.85	2.02	1	9
4:A:415:PCW:C1	4:C:616:PCW:H411	0.85	2.00	4	7
4:C:616:PCW:O31	4:C:616:PCW:H41	0.85	1.72	1	4
4:D:505:PCW:C42	4:D:506:PCW:H141	0.85	2.01	8	1
4:B:207:PCW:C20	4:B:207:PCW:C25	0.85	2.55	10	1
5:D:512:17F:H30	5:D:514:17F:H35	0.85	1.47	3	1
4:B:206:PCW:H52	4:B:206:PCW:O11	0.85	1.71	5	1
4:A:405:PCW:H2	5:D:512:17F:H31	0.85	1.47	10	4
4:B:202:PCW:H351	4:B:202:PCW:C31	0.85	2.01	9	8
4:C:604:PCW:H452	4:C:606:PCW:C18	0.85	2.01	2	5
4:C:605:PCW:C31	4:C:612:PCW:H62	0.85	2.01	6	5
5:C:626:17F:H57	5:C:629:17F:H51	0.85	1.46	5	8
4:B:208:PCW:H121	5:B:214:17F:O9	0.85	1.71	3	3
4:C:602:PCW:H261	5:C:629:17F:C42	0.85	2.02	8	6
4:C:624:PCW:C20	4:C:624:PCW:H242	0.85	2.00	4	1
4:D:504:PCW:H182	4:D:504:PCW:C22	0.85	2.02	5	1
4:C:623:PCW:H451	4:C:624:PCW:H482	0.85	1.47	8	6
4:C:610:PCW:C22	4:C:618:PCW:H442	0.85	2.02	4	1
4:A:401:PCW:H31	4:D:508:PCW:C18	0.85	2.02	7	1
4:D:506:PCW:H431	5:D:513:17F:H38	0.85	1.47	8	2
4:C:614:PCW:H172	4:C:614:PCW:C13	0.85	2.01	9	1
4:A:417:PCW:H242	4:C:621:PCW:C24	0.85	2.01	9	6
4:C:606:PCW:H341	4:C:606:PCW:H132	0.85	1.47	2	6
4:C:617:PCW:H461	4:B:211:PCW:H251	0.85	1.46	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:621:PCW:C7	5:C:631:17F:H8	0.85	2.02	3	4
4:A:403:PCW:C6	4:A:406:PCW:H371	0.85	2.01	6	1
4:D:510:PCW:H432	4:D:510:PCW:C47	0.85	2.02	10	10
4:A:416:PCW:O3	5:C:630:17F:H9	0.85	1.69	4	4
4:D:501:PCW:H372	4:D:509:PCW:H421	0.85	1.47	7	1
4:C:620:PCW:H142	4:C:620:PCW:C18	0.85	2.01	7	10
4:C:621:PCW:C17	5:C:628:17F:H32	0.85	1.99	1	4
4:C:621:PCW:H431	4:D:516:PCW:H481	0.85	1.48	3	1
4:C:620:PCW:H422	5:B:215:17F:H73	0.85	1.46	4	1
4:A:405:PCW:H272	4:A:405:PCW:C47	0.85	2.02	10	2
4:B:204:PCW:H121	4:B:208:PCW:C34	0.85	2.01	6	1
4:B:203:PCW:H232	4:B:208:PCW:H342	0.85	1.49	7	1
4:C:615:PCW:H39	4:C:617:PCW:C16	0.84	2.02	9	4
4:D:505:PCW:H252	4:D:505:PCW:C21	0.84	2.02	1	10
5:C:630:17F:H58	5:C:630:17F:C36	0.84	2.02	2	1
4:A:404:PCW:H351	4:A:407:PCW:C16	0.84	2.02	7	2
4:C:607:PCW:C12	4:C:608:PCW:H171	0.84	1.98	4	1
4:C:608:PCW:H281	5:B:214:17F:H52	0.84	1.49	10	1
4:C:621:PCW:H172	5:C:628:17F:C1Z	0.84	2.03	8	7
4:C:602:PCW:H483	5:C:629:17F:H47	0.84	1.48	1	3
4:C:603:PCW:H52	4:C:603:PCW:O31	0.84	1.72	1	1
4:B:208:PCW:H262	4:B:208:PCW:C22	0.84	2.02	10	10
4:A:403:PCW:H162	4:A:403:PCW:C21	0.84	2.01	3	6
4:B:202:PCW:H171	4:D:504:PCW:C12	0.84	2.03	3	3
4:C:625:PCW:C4	4:C:625:PCW:H2	0.84	2.02	8	1
4:C:621:PCW:H141	5:C:628:17F:C1Z	0.84	2.01	2	7
4:A:413:PCW:H422	4:C:611:PCW:C21	0.84	2.02	6	3
4:A:402:PCW:H272	4:A:413:PCW:H241	0.84	1.48	2	2
4:C:612:PCW:H212	5:D:511:17F:H51	0.84	1.48	7	3
5:C:627:17F:H43	5:C:628:17F:H39	0.84	1.47	3	1
3:D:460:LEU:HD11	4:D:509:PCW:H381	0.84	1.48	4	1
4:C:621:PCW:H472	4:D:506:PCW:H252	0.84	1.48	5	1
4:D:503:PCW:H351	4:D:510:PCW:H141	0.84	1.46	5	1
4:C:610:PCW:H19	4:C:610:PCW:H371	0.84	1.50	7	3
4:B:203:PCW:H252	4:B:204:PCW:H19	0.84	1.48	7	1
4:D:507:PCW:C35	5:D:513:17F:H10A	0.84	2.01	9	1
4:D:503:PCW:H251	4:D:503:PCW:C21	0.84	2.02	3	9
4:A:406:PCW:H431	4:B:211:PCW:H19	0.84	1.48	6	2
4:C:615:PCW:O2P	4:C:615:PCW:H31	0.84	1.71	3	1
4:C:616:PCW:H431	4:C:616:PCW:C47	0.84	2.02	8	2
4:B:206:PCW:H421	4:B:206:PCW:H372	0.84	1.49	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:202:PCW:H422	4:B:202:PCW:H212	0.84	1.47	4	2
4:B:203:PCW:H242	4:B:208:PCW:H122	0.84	1.49	6	3
4:B:204:PCW:H411	5:D:514:17F:H10A	0.84	1.48	5	1
4:C:615:PCW:H31	4:C:615:PCW:C4	0.84	2.02	10	1
4:A:413:PCW:H371	4:A:413:PCW:H411	0.84	1.50	1	5
4:A:417:PCW:H321	4:A:417:PCW:C7	0.84	2.03	7	5
4:B:202:PCW:H141	4:D:504:PCW:H322	0.84	1.47	3	2
4:A:401:PCW:H432	4:C:613:PCW:H262	0.84	1.48	4	1
4:C:604:PCW:C8	5:C:628:17F:H4A	0.84	2.02	10	2
4:B:204:PCW:H141	4:B:208:PCW:H321	0.84	1.49	4	1
4:D:515:PCW:H82	4:D:516:PCW:H73	0.84	1.47	9	2
4:A:405:PCW:C27	4:A:414:PCW:H271	0.84	2.01	3	4
4:C:625:PCW:H182	4:C:625:PCW:H221	0.84	1.47	6	3
4:B:208:PCW:H32	4:B:208:PCW:P	0.84	2.13	6	8
4:D:507:PCW:H271	4:D:507:PCW:H462	0.84	1.46	4	1
4:A:413:PCW:H431	4:C:611:PCW:H151	0.84	1.49	9	1
4:C:621:PCW:H352	4:C:625:PCW:H20	0.84	1.50	9	3
5:A:410:17F:H53	4:C:605:PCW:H281	0.84	1.47	5	1
4:C:610:PCW:H51	4:C:622:PCW:H361	0.84	1.46	6	1
4:D:510:PCW:H421	4:D:516:PCW:H283	0.84	1.50	7	1
4:C:604:PCW:H452	4:C:606:PCW:H181	0.83	1.48	2	3
4:C:605:PCW:O1P	4:C:612:PCW:H52	0.83	1.73	3	4
4:B:205:PCW:H171	4:B:207:PCW:H321	0.83	1.49	3	1
4:A:407:PCW:H39	4:B:210:PCW:H241	0.83	1.49	1	2
4:A:416:PCW:C12	5:C:630:17F:H9	0.83	2.03	3	9
4:C:616:PCW:H232	4:C:616:PCW:C27	0.83	2.03	2	10
4:C:619:PCW:H141	5:C:632:17F:O9	0.83	1.71	8	8
4:B:210:PCW:H322	4:B:210:PCW:H42	0.83	1.49	2	7
4:D:510:PCW:H472	4:D:510:PCW:C43	0.83	2.02	10	10
4:B:205:PCW:H181	4:B:207:PCW:H342	0.83	1.47	3	1
4:B:210:PCW:H262	4:B:211:PCW:H231	0.83	1.49	3	1
5:A:409:17F:H38	4:D:510:PCW:H132	0.83	1.50	6	1
4:A:413:PCW:H451	4:C:611:PCW:H162	0.83	1.47	9	1
4:A:413:PCW:H483	4:C:611:PCW:H281	0.83	1.47	7	3
4:A:405:PCW:H272	4:A:414:PCW:H271	0.83	1.50	3	1
4:C:610:PCW:C16	4:C:618:PCW:H171	0.83	2.03	4	6
4:C:620:PCW:H212	5:C:631:17F:H31	0.83	1.50	1	3
4:D:503:PCW:H211	4:D:503:PCW:C25	0.83	2.02	5	9
4:C:621:PCW:H352	4:C:625:PCW:C20	0.83	2.02	4	7
4:A:408:PCW:H442	5:A:409:17F:H68	0.83	1.47	10	1
4:A:403:PCW:O31	4:A:403:PCW:H51	0.83	1.71	1	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:417:PCW:H222	4:C:603:PCW:C18	0.83	2.02	8	7
4:D:505:PCW:H461	4:D:506:PCW:H161	0.83	1.48	2	2
4:A:404:PCW:C35	4:A:407:PCW:H162	0.83	2.02	3	2
4:C:610:PCW:C4	4:C:622:PCW:H342	0.83	2.03	6	3
4:C:615:PCW:H221	4:C:615:PCW:H172	0.83	1.48	6	5
4:C:603:PCW:H73	4:D:516:PCW:H31	0.83	1.49	2	1
4:C:611:PCW:H332	4:C:625:PCW:H132	0.83	1.51	8	4
4:D:506:PCW:H442	4:D:507:PCW:H442	0.83	1.47	3	1
4:D:504:PCW:H382	4:D:504:PCW:H121	0.83	1.47	4	1
4:C:609:PCW:H63	5:C:631:17F:O1	0.83	1.73	5	1
5:A:410:17F:H77	5:D:511:17F:H73	0.83	1.49	7	1
4:A:408:PCW:H321	5:A:409:17F:H32	0.83	1.48	2	4
5:C:628:17F:H12A	5:C:628:17F:H59	0.83	1.48	9	10
2:B:143:GLU:HB3	4:B:204:PCW:H62	0.83	1.50	3	1
4:B:212:PCW:H422	5:D:514:17F:H64	0.83	1.50	4	1
4:A:405:PCW:H39	5:D:512:17F:H69	0.83	1.50	9	1
4:A:403:PCW:H162	4:A:403:PCW:C23	0.83	2.02	2	6
4:C:601:PCW:H472	4:C:601:PCW:C43	0.83	2.03	2	3
4:C:608:PCW:H2	4:C:614:PCW:C6	0.83	2.04	5	2
5:C:632:17F:H72	5:B:215:17F:H65	0.83	1.49	3	1
4:A:404:PCW:H12	4:B:210:PCW:H361	0.83	1.50	5	1
4:A:407:PCW:H332	4:B:211:PCW:H39	0.83	1.49	5	1
4:C:606:PCW:C34	4:C:606:PCW:H132	0.83	2.02	9	4
4:B:202:PCW:H62	4:B:202:PCW:O11	0.83	1.74	8	1
4:A:413:PCW:H351	4:C:611:PCW:H132	0.83	1.46	10	4
4:B:206:PCW:H2	5:B:213:17F:H4A	0.83	1.51	1	1
4:B:208:PCW:H451	5:D:512:17F:H64	0.83	1.48	1	1
4:C:621:PCW:H361	4:D:516:PCW:H462	0.83	1.51	7	7
4:A:407:PCW:H422	4:B:211:PCW:H461	0.83	1.50	3	1
4:A:413:PCW:H372	4:A:413:PCW:C41	0.83	2.04	9	1
4:C:603:PCW:H261	4:D:515:PCW:H171	0.83	1.47	4	7
4:C:616:PCW:H272	4:C:616:PCW:C23	0.83	2.04	1	10
4:A:403:PCW:H271	4:B:201:PCW:H132	0.83	1.48	2	1
4:C:620:PCW:C42	5:B:215:17F:H62	0.83	2.03	3	5
4:B:211:PCW:H20	4:D:506:PCW:H232	0.83	1.49	9	2
4:B:212:PCW:H171	4:B:212:PCW:H381	0.83	1.49	3	2
5:A:410:17F:H70	4:D:502:PCW:H281	0.83	1.51	4	2
4:C:603:PCW:H222	4:D:515:PCW:C33	0.82	2.04	1	3
4:D:502:PCW:H40	5:D:512:17F:H10A	0.82	1.50	1	2
4:C:613:PCW:C44	4:C:618:PCW:H20	0.82	2.04	7	5
4:C:619:PCW:H372	4:C:619:PCW:H412	0.82	1.48	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:417:PCW:O31	4:A:417:PCW:H62	0.82	1.73	3	1
4:B:203:PCW:H212	4:B:208:PCW:O31	0.82	1.74	7	2
4:D:501:PCW:H171	4:D:502:PCW:C33	0.82	2.03	9	2
4:D:503:PCW:H421	4:D:504:PCW:H40	0.82	1.51	6	1
4:C:604:PCW:H122	4:C:604:PCW:H332	0.82	1.49	2	1
4:C:604:PCW:H412	4:C:606:PCW:H241	0.82	1.49	8	3
5:C:627:17F:H76	4:D:516:PCW:H462	0.82	1.52	3	2
4:B:210:PCW:H362	4:B:210:PCW:H122	0.82	1.50	6	1
4:A:407:PCW:H483	4:D:506:PCW:H261	0.82	1.51	10	1
4:A:408:PCW:H432	4:A:408:PCW:C47	0.82	2.04	10	10
4:C:603:PCW:H52	4:C:603:PCW:C31	0.82	2.04	1	1
4:C:604:PCW:H372	4:C:604:PCW:H422	0.82	1.49	6	6
4:D:505:PCW:H361	4:D:506:PCW:C12	0.82	2.04	6	3
4:D:510:PCW:H242	4:D:515:PCW:H482	0.82	1.48	8	1
4:B:211:PCW:C19	4:D:505:PCW:H432	0.82	2.04	10	1
4:B:205:PCW:H73	5:B:213:17F:O1	0.82	1.74	4	4
1:A:365:LYS:HB2	1:A:366:PRO:HD3	0.82	1.50	1	10
4:A:403:PCW:H82	4:B:209:PCW:H351	0.82	1.50	10	3
4:C:601:PCW:H421	4:C:601:PCW:C46	0.82	2.01	3	7
4:C:605:PCW:C18	4:C:612:PCW:H342	0.82	2.04	5	2
4:C:602:PCW:H351	5:B:214:17F:H77	0.82	1.47	7	1
4:C:603:PCW:H271	4:D:515:PCW:H182	0.82	1.48	7	3
4:A:404:PCW:H241	4:B:211:PCW:H242	0.82	1.51	2	2
4:A:413:PCW:C35	4:C:611:PCW:H132	0.82	2.04	10	4
4:B:210:PCW:H41	5:D:513:17F:H1A	0.82	1.49	2	1
4:D:510:PCW:O31	4:D:510:PCW:H41	0.82	1.75	5	6
4:C:610:PCW:C39	4:C:622:PCW:H462	0.82	2.01	3	3
5:D:513:17F:H12	5:D:513:17F:C36	0.82	2.05	3	2
4:A:413:PCW:H351	4:C:611:PCW:C13	0.82	2.05	2	4
4:C:606:PCW:H182	4:C:606:PCW:C14	0.82	2.05	1	10
4:C:616:PCW:O31	4:C:616:PCW:H62	0.82	1.75	10	4
4:B:206:PCW:H412	5:B:213:17F:H8	0.82	1.49	4	2
4:B:205:PCW:H211	4:B:207:PCW:H431	0.82	1.50	9	2
2:B:84:ILE:HD11	2:B:118:CYS:HA	0.82	1.50	8	7
4:B:208:PCW:H222	4:B:208:PCW:C26	0.82	2.04	2	10
4:A:405:PCW:H2	5:D:512:17F:H33	0.82	1.51	7	3
4:C:623:PCW:H412	4:C:624:PCW:C39	0.82	2.03	5	1
4:B:212:PCW:C44	5:D:514:17F:H12	0.82	2.05	5	1
5:C:628:17F:H53	5:B:213:17F:H73	0.82	1.50	6	1
4:D:505:PCW:H361	4:D:506:PCW:H121	0.82	1.51	9	3
4:B:208:PCW:H121	5:B:214:17F:H18A	0.82	1.50	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:505:PCW:H212	4:D:505:PCW:C25	0.82	2.04	1	10
4:C:603:PCW:H172	4:C:603:PCW:H211	0.82	1.51	6	9
4:B:205:PCW:H142	4:B:207:PCW:H321	0.82	1.50	2	2
4:D:509:PCW:C6	4:D:510:PCW:H321	0.82	2.04	7	3
4:B:210:PCW:H283	4:D:503:PCW:H212	0.82	1.52	4	1
4:D:506:PCW:H381	5:D:513:17F:H46	0.82	1.52	4	1
4:A:402:PCW:H52	5:D:513:17F:H1	0.82	1.49	5	1
4:D:507:PCW:O3	5:D:513:17F:H75	0.82	1.74	8	3
4:C:624:PCW:H271	4:C:624:PCW:C23	0.82	2.05	10	9
4:A:408:PCW:H252	5:A:409:17F:H60	0.82	1.52	3	1
4:C:612:PCW:C20	5:D:511:17F:H47	0.82	2.05	3	2
4:A:404:PCW:H261	4:C:617:PCW:H462	0.82	1.49	4	2
4:A:414:PCW:O1P	4:C:613:PCW:H41	0.82	1.75	5	1
4:C:625:PCW:H281	5:C:631:17F:H51	0.82	1.49	10	2
4:D:505:PCW:H20	4:D:510:PCW:H342	0.82	1.52	10	2
5:C:626:17F:H57	5:C:626:17F:C19	0.81	2.05	8	10
4:C:620:PCW:C15	5:B:215:17F:H6	0.81	2.05	2	8
4:C:623:PCW:C41	4:C:624:PCW:H39	0.81	2.04	5	1
4:A:403:PCW:O3	4:B:209:PCW:H341	0.81	1.74	8	1
4:A:411:PCW:H451	4:C:616:PCW:C24	0.81	2.05	5	8
4:A:415:PCW:H361	4:D:515:PCW:C16	0.81	2.04	4	1
4:A:416:PCW:O1P	4:C:616:PCW:H82	0.81	1.73	8	5
4:B:206:PCW:H82	4:B:209:PCW:O11	0.81	1.75	5	1
4:C:605:PCW:H472	4:C:618:PCW:H432	0.81	1.51	8	3
4:C:611:PCW:C32	4:C:617:PCW:H132	0.81	2.05	3	9
4:D:509:PCW:H61	4:D:510:PCW:H341	0.81	1.51	1	1
4:A:404:PCW:H152	4:B:210:PCW:C21	0.81	2.05	8	3
4:B:212:PCW:H462	5:D:514:17F:H41	0.81	1.53	4	1
4:B:204:PCW:H471	4:D:502:PCW:H442	0.81	1.50	5	1
4:A:411:PCW:O31	4:C:616:PCW:H61	0.81	1.75	6	2
5:C:632:17F:H51	4:B:201:PCW:H442	0.81	1.52	6	1
4:C:609:PCW:H241	4:C:609:PCW:C20	0.81	2.05	3	10
4:C:611:PCW:H172	4:C:611:PCW:C21	0.81	2.00	4	6
5:D:513:17F:H11	5:D:513:17F:C36	0.81	2.06	10	1
5:C:626:17F:H36	5:C:629:17F:H70	0.81	1.50	8	3
2:B:72:MET:HE3	2:B:103:VAL:HG21	0.81	1.50	6	5
4:B:205:PCW:H372	4:B:207:PCW:H122	0.81	1.52	3	1
4:C:606:PCW:H73	4:C:624:PCW:C19	0.81	2.05	7	2
4:C:610:PCW:H452	4:C:618:PCW:H481	0.81	1.53	10	1
4:B:203:PCW:H283	5:B:214:17F:H32	0.81	1.51	10	1
4:A:401:PCW:C47	4:C:610:PCW:H251	0.81	2.06	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:620:PCW:H222	5:C:631:17F:H31	0.81	1.52	6	5
4:A:406:PCW:H431	4:B:211:PCW:C19	0.81	2.05	6	1
4:A:413:PCW:H362	4:C:611:PCW:H131	0.81	1.52	6	1
4:A:411:PCW:C19	4:A:415:PCW:H431	0.81	2.06	7	1
4:B:202:PCW:H131	4:B:202:PCW:H381	0.81	1.49	8	1
4:B:207:PCW:H20	4:B:207:PCW:C25	0.81	1.98	10	1
4:C:607:PCW:H41	4:C:624:PCW:C22	0.81	2.04	2	3
4:D:505:PCW:H242	4:D:506:PCW:H39	0.81	1.51	1	1
5:B:213:17F:H44	4:D:509:PCW:H212	0.81	1.50	3	1
4:A:408:PCW:H472	4:A:408:PCW:C43	0.81	2.05	5	9
4:D:502:PCW:C40	5:D:512:17F:H10A	0.81	2.06	1	3
4:A:405:PCW:H482	4:A:414:PCW:H272	0.81	1.50	3	2
4:C:623:PCW:H412	4:C:624:PCW:C41	0.81	2.04	4	5
5:C:629:17F:H18	5:C:629:17F:C9	0.81	2.05	4	2
5:A:409:17F:H61	5:D:511:17F:C21	0.81	2.04	10	2
4:D:501:PCW:C7	5:D:514:17F:H19A	0.81	2.05	3	1
4:A:407:PCW:H421	4:B:211:PCW:H461	0.81	1.50	4	1
4:C:603:PCW:C46	4:D:515:PCW:H432	0.81	2.05	4	4
4:C:623:PCW:H31	4:C:624:PCW:C3	0.81	2.03	4	1
4:C:623:PCW:C3	4:C:624:PCW:H32	0.81	2.04	4	1
4:C:616:PCW:H2	4:C:616:PCW:C4	0.81	2.03	7	2
4:C:607:PCW:C20	5:C:629:17F:H46	0.81	2.05	5	4
4:D:505:PCW:H221	4:D:510:PCW:C35	0.81	2.05	8	3
4:A:404:PCW:H171	4:B:210:PCW:H222	0.81	1.53	8	2
4:B:204:PCW:H483	4:D:502:PCW:C44	0.81	2.06	4	2
4:B:207:PCW:H241	5:B:214:17F:H55	0.81	1.51	10	1
4:A:401:PCW:H322	4:D:508:PCW:C23	0.80	2.06	2	1
4:C:621:PCW:H421	4:D:506:PCW:H272	0.80	1.51	10	3
4:C:605:PCW:C17	4:C:612:PCW:H342	0.80	2.05	6	4
5:D:511:17F:H19A	5:D:511:17F:C31	0.80	2.04	8	5
4:A:403:PCW:C48	4:B:209:PCW:H262	0.80	2.05	9	1
4:A:411:PCW:H451	4:C:616:PCW:C25	0.80	2.07	10	5
4:B:206:PCW:H332	4:D:505:PCW:C33	0.80	2.07	10	2
4:A:412:PCW:C34	4:C:624:PCW:H381	0.80	2.07	5	1
4:C:619:PCW:H152	5:C:632:17F:H18	0.80	1.51	5	1
4:B:205:PCW:H172	4:B:207:PCW:H342	0.80	1.52	5	2
4:B:211:PCW:H20	4:D:506:PCW:C24	0.80	2.05	5	2
4:A:404:PCW:H32	4:B:210:PCW:H152	0.80	1.51	7	2
4:A:404:PCW:H242	4:B:210:PCW:H232	0.80	1.52	9	2
4:A:412:PCW:H431	4:C:624:PCW:C47	0.80	2.06	7	2
4:A:412:PCW:H431	4:C:624:PCW:H481	0.80	1.51	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:613:PCW:H52	4:C:623:PCW:O1P	0.80	1.76	4	6
4:B:204:PCW:H411	4:B:212:PCW:H231	0.80	1.53	3	1
4:A:406:PCW:H411	4:B:211:PCW:H361	0.80	1.53	5	1
4:A:412:PCW:O3	4:C:624:PCW:H411	0.80	1.77	5	1
4:D:510:PCW:H211	4:D:515:PCW:H483	0.80	1.50	5	1
4:B:212:PCW:H52	5:B:213:17F:C3	0.80	2.06	8	1
4:A:416:PCW:H63	4:A:416:PCW:O11	0.80	1.76	7	2
5:C:627:17F:H29	5:C:628:17F:H8	0.80	1.53	1	2
4:B:205:PCW:H61	4:B:212:PCW:O1P	0.80	1.74	3	1
4:D:505:PCW:C2	4:D:509:PCW:H62	0.80	2.06	5	2
4:D:506:PCW:H352	4:D:510:PCW:H40	0.80	1.53	6	1
4:C:625:PCW:H282	5:C:631:17F:H46	0.80	1.53	7	3
4:D:506:PCW:H462	5:D:513:17F:H50	0.80	1.50	7	1
4:A:405:PCW:C19	4:A:405:PCW:C14	0.80	2.59	1	10
4:C:604:PCW:H262	5:B:213:17F:H53	0.80	1.52	1	1
4:B:204:PCW:H161	4:B:208:PCW:H211	0.80	1.54	7	2
5:A:409:17F:H56	4:D:504:PCW:H331	0.80	1.52	4	1
4:C:621:PCW:H162	4:D:516:PCW:C16	0.80	2.07	8	2
4:C:620:PCW:H141	5:B:215:17F:O8	0.80	1.76	6	1
4:A:401:PCW:H441	4:D:508:PCW:H472	0.80	1.52	8	1
4:B:202:PCW:H162	4:D:504:PCW:H322	0.80	1.52	8	1
4:B:206:PCW:H421	5:B:213:17F:H34	0.80	1.50	9	1
4:A:406:PCW:H371	4:B:209:PCW:H40	0.80	1.52	1	1
4:C:606:PCW:H142	4:C:606:PCW:C18	0.80	2.05	4	10
4:A:416:PCW:H122	5:C:630:17F:C11	0.80	2.05	5	7
4:B:204:PCW:H231	4:B:208:PCW:H261	0.80	1.54	9	3
4:C:607:PCW:H121	4:C:608:PCW:C17	0.80	1.99	4	1
4:D:516:PCW:H372	4:D:516:PCW:H142	0.80	1.52	7	3
4:B:210:PCW:H482	4:D:507:PCW:H242	0.80	1.52	8	1
4:D:501:PCW:H73	5:D:514:17F:H60	0.80	1.50	8	1
4:D:510:PCW:H261	4:D:515:PCW:H462	0.80	1.51	9	1
4:B:204:PCW:H152	4:B:208:PCW:C38	0.80	2.07	1	1
4:B:206:PCW:H382	4:D:505:PCW:O2	0.80	1.76	5	2
4:A:415:PCW:H20	4:A:415:PCW:C24	0.80	2.07	1	1
4:A:413:PCW:H332	4:C:611:PCW:C3	0.80	2.06	2	1
4:B:204:PCW:H432	4:B:212:PCW:H242	0.80	1.50	2	1
4:A:408:PCW:O31	5:A:409:17F:H20	0.80	1.77	3	1
4:B:204:PCW:H151	4:B:208:PCW:C34	0.80	2.05	7	2
4:C:603:PCW:C31	4:C:603:PCW:H42	0.80	2.07	10	2
4:B:204:PCW:H221	4:B:208:PCW:H242	0.80	1.51	4	1
4:C:610:PCW:H172	4:C:610:PCW:C35	0.80	2.04	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:507:PCW:H432	5:D:513:17F:H35	0.80	1.53	9	1
4:A:408:PCW:H181	5:A:409:17F:C20	0.80	2.04	1	1
4:A:416:PCW:C16	5:C:630:17F:H57	0.80	2.07	6	5
4:C:601:PCW:H40	4:C:602:PCW:H231	0.80	1.54	1	3
4:A:415:PCW:O2	4:C:616:PCW:H411	0.80	1.77	2	3
4:D:503:PCW:H332	4:D:510:PCW:H82	0.80	1.52	2	2
4:B:211:PCW:H20	4:D:506:PCW:C23	0.80	2.07	3	4
4:D:505:PCW:C24	4:D:506:PCW:H372	0.80	2.07	9	1
4:C:613:PCW:H452	4:C:618:PCW:H222	0.79	1.53	4	5
4:C:614:PCW:H211	5:C:632:17F:H41	0.79	1.53	7	4
4:B:203:PCW:H31	4:B:203:PCW:O4P	0.79	1.76	4	8
4:D:504:PCW:H351	4:D:504:PCW:C31	0.79	2.06	1	8
4:C:604:PCW:H52	4:C:604:PCW:O11	0.79	1.77	2	2
4:C:604:PCW:H372	4:C:604:PCW:H411	0.79	1.51	2	3
4:C:604:PCW:H451	4:C:606:PCW:C18	0.79	2.07	7	2
4:A:415:PCW:H481	5:D:513:17F:H38	0.79	1.54	7	1
4:A:414:PCW:C39	4:C:623:PCW:H441	0.79	2.06	6	7
4:C:606:PCW:C16	5:C:627:17F:H11A	0.79	2.07	4	9
4:B:211:PCW:H482	4:D:506:PCW:H232	0.79	1.54	8	1
4:D:508:PCW:H19	5:D:512:17F:H31	0.79	1.54	8	1
4:D:506:PCW:H362	4:D:507:PCW:C40	0.79	2.07	9	1
4:C:621:PCW:H141	5:C:628:17F:C1Y	0.79	2.04	10	5
4:B:206:PCW:H161	5:B:213:17F:H60	0.79	1.54	3	1
4:A:403:PCW:H482	4:B:209:PCW:H262	0.79	1.53	8	2
5:C:627:17F:H68	5:B:215:17F:H29	0.79	1.50	9	1
4:A:403:PCW:O11	4:B:201:PCW:H122	0.79	1.77	1	2
4:A:414:PCW:H63	4:C:624:PCW:C31	0.79	2.08	5	7
4:C:617:PCW:C15	4:C:625:PCW:H142	0.79	2.07	5	5
3:D:472:PHE:HB2	3:D:476:CYS:HB2	0.79	1.52	3	10
4:D:501:PCW:H472	4:D:509:PCW:H232	0.79	1.53	1	3
4:A:408:PCW:O3	4:A:408:PCW:H351	0.79	1.75	3	7
4:D:503:PCW:H61	4:D:506:PCW:O3P	0.79	1.77	5	1
4:D:502:PCW:H231	4:D:502:PCW:C27	0.79	2.06	8	1
4:A:417:PCW:C8	4:C:605:PCW:H332	0.79	2.07	7	7
4:B:206:PCW:H31	4:B:206:PCW:C4	0.79	2.06	2	1
4:B:205:PCW:H52	5:B:214:17F:H12A	0.79	1.54	3	1
4:C:622:PCW:C23	4:D:501:PCW:H481	0.79	2.05	5	1
4:D:506:PCW:H342	4:D:507:PCW:C38	0.79	2.07	5	1
4:A:408:PCW:C17	5:A:409:17F:H20	0.79	2.07	9	1
5:A:409:17F:H1	2:B:172:LYS:HB3	0.79	1.55	9	1
4:B:204:PCW:H251	4:B:208:PCW:H283	0.79	1.52	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:408:PCW:H182	4:A:408:PCW:C14	0.79	2.07	8	1
4:B:206:PCW:H142	5:B:213:17F:C18	0.79	2.06	9	1
4:C:623:PCW:H19	4:C:623:PCW:C15	0.79	2.07	7	10
4:B:206:PCW:H372	4:B:206:PCW:H411	0.79	1.53	4	3
4:B:205:PCW:H241	4:B:205:PCW:C28	0.79	2.06	5	1
4:C:614:PCW:H122	5:C:632:17F:C8	0.79	2.08	7	1
4:D:508:PCW:H62	4:D:508:PCW:O11	0.79	1.78	10	1
4:D:509:PCW:H82	4:D:510:PCW:C6	0.79	2.07	10	1
4:A:401:PCW:H62	4:D:508:PCW:H12	0.79	1.52	10	2
4:C:615:PCW:C39	4:C:617:PCW:H162	0.79	2.08	5	7
4:C:621:PCW:H352	4:C:625:PCW:H222	0.79	1.52	1	5
4:B:212:PCW:H241	4:B:212:PCW:C20	0.79	2.08	7	10
4:A:415:PCW:O1P	4:C:616:PCW:H372	0.79	1.78	10	3
4:C:602:PCW:H341	5:B:214:17F:C37	0.79	2.07	2	1
4:C:605:PCW:O31	4:C:612:PCW:H52	0.79	1.77	6	4
4:A:412:PCW:C3	4:C:624:PCW:H371	0.79	2.07	5	1
4:B:211:PCW:H282	4:D:506:PCW:C24	0.79	2.08	9	1
4:C:607:PCW:H19	5:C:629:17F:C26	0.79	2.08	4	4
4:B:205:PCW:H251	4:B:205:PCW:C21	0.79	2.05	5	1
4:C:603:PCW:H261	4:D:515:PCW:C14	0.79	2.07	5	6
4:A:417:PCW:C33	4:C:622:PCW:H122	0.79	2.07	7	3
4:C:601:PCW:H432	4:C:601:PCW:C47	0.79	2.08	4	3
4:C:603:PCW:H261	4:D:515:PCW:H141	0.79	1.54	5	3
4:C:612:PCW:H471	4:C:618:PCW:H431	0.79	1.53	4	3
4:C:621:PCW:H271	4:D:509:PCW:H272	0.79	1.55	6	1
4:C:616:PCW:C1	4:C:616:PCW:H51	0.78	2.09	5	2
4:B:202:PCW:H332	4:D:507:PCW:C1	0.78	2.08	9	2
4:A:401:PCW:C1	4:D:508:PCW:H342	0.78	2.07	4	1
4:C:610:PCW:H39	4:C:622:PCW:C46	0.78	2.02	2	4
4:A:401:PCW:H252	4:C:613:PCW:C28	0.78	2.08	10	2
4:A:415:PCW:H412	4:D:515:PCW:H181	0.78	1.53	2	2
4:C:605:PCW:H172	4:C:612:PCW:H132	0.78	1.54	2	3
4:B:203:PCW:C14	4:B:208:PCW:H371	0.78	2.07	3	1
4:C:614:PCW:H141	5:C:632:17F:C9	0.78	2.08	5	1
4:A:402:PCW:H221	4:A:413:PCW:C26	0.78	2.05	6	1
4:A:407:PCW:H232	4:A:407:PCW:C27	0.78	2.08	10	1
4:C:605:PCW:H472	4:C:618:PCW:C44	0.78	2.08	10	1
4:A:415:PCW:C36	4:C:616:PCW:H412	0.78	2.08	2	8
4:D:509:PCW:H362	4:D:510:PCW:O3P	0.78	1.78	1	1
4:A:417:PCW:C7	4:C:605:PCW:H332	0.78	2.08	4	5
4:C:610:PCW:H2	4:C:618:PCW:C6	0.78	2.09	9	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:403:PCW:H122	4:B:209:PCW:H332	0.78	1.56	7	1
4:D:501:PCW:H171	4:D:502:PCW:H342	0.78	1.55	7	1
4:A:407:PCW:H132	4:A:407:PCW:C34	0.78	2.08	8	5
4:C:619:PCW:H20	5:C:632:17F:H10A	0.78	1.55	8	1
4:C:620:PCW:H141	5:B:215:17F:H4A	0.78	1.54	8	1
4:A:413:PCW:H471	4:C:611:PCW:H271	0.78	1.55	1	4
4:C:603:PCW:H222	4:D:515:PCW:H331	0.78	1.54	1	3
4:D:503:PCW:P	4:D:503:PCW:H31	0.78	2.18	2	2
5:C:629:17F:H18	5:C:629:17F:H9	0.78	1.55	4	2
4:B:209:PCW:H242	4:B:209:PCW:H181	0.78	1.52	6	3
4:B:202:PCW:H161	4:D:504:PCW:C32	0.78	2.08	5	1
4:B:208:PCW:H272	4:B:208:PCW:H471	0.78	1.53	9	1
5:C:628:17F:H67	5:B:215:17F:C2X	0.78	2.05	1	2
4:D:502:PCW:H2	4:D:502:PCW:C7	0.78	2.09	5	5
4:C:617:PCW:H412	5:C:631:17F:H41	0.78	1.55	3	2
4:B:205:PCW:C24	4:B:207:PCW:H431	0.78	2.07	4	2
4:A:406:PCW:H431	4:B:211:PCW:H362	0.78	1.55	5	1
5:A:410:17F:H32	4:D:502:PCW:H211	0.78	1.54	6	1
4:B:204:PCW:H411	5:D:514:17F:H8	0.78	1.55	7	1
4:A:405:PCW:H182	4:A:414:PCW:H261	0.78	1.55	1	1
4:C:608:PCW:C18	4:C:614:PCW:H352	0.78	2.09	1	1
4:D:502:PCW:H441	5:D:512:17F:H44	0.78	1.56	1	2
4:B:204:PCW:C3	4:B:208:PCW:H152	0.78	2.08	4	3
4:D:505:PCW:H442	4:D:506:PCW:H161	0.78	1.56	4	3
4:D:506:PCW:H40	4:D:516:PCW:H242	0.78	1.54	6	1
4:A:403:PCW:H39	4:A:403:PCW:H182	0.78	1.54	10	1
4:C:605:PCW:H421	4:C:618:PCW:H141	0.78	1.53	2	5
4:C:612:PCW:H482	4:C:618:PCW:H211	0.78	1.56	9	9
5:B:213:17F:H38	4:D:505:PCW:H141	0.78	1.54	1	1
4:A:413:PCW:H351	4:C:611:PCW:H152	0.78	1.55	7	3
4:B:203:PCW:H241	4:B:208:PCW:O11	0.78	1.78	2	2
4:B:203:PCW:H232	4:B:208:PCW:H82	0.78	1.55	3	1
4:A:411:PCW:H481	4:D:504:PCW:H181	0.78	1.56	4	1
4:D:510:PCW:H32	4:D:510:PCW:P	0.78	2.18	4	1
4:B:212:PCW:H442	5:D:514:17F:H12	0.78	1.55	5	1
4:D:507:PCW:H19	5:D:513:17F:H19A	0.78	1.56	5	1
4:D:506:PCW:H482	4:D:516:PCW:H231	0.78	1.54	8	2
4:A:402:PCW:H241	4:A:413:PCW:H262	0.78	1.54	5	1
4:A:411:PCW:H283	4:A:415:PCW:H251	0.78	1.52	6	1
4:A:402:PCW:H61	5:D:513:17F:H1	0.78	1.56	7	1
4:B:203:PCW:H252	4:B:204:PCW:C19	0.78	2.08	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:C:627:17F:H19	5:C:627:17F:H5	0.78	1.55	6	3
5:D:513:17F:H69	5:D:513:17F:H12A	0.78	1.54	4	3
4:B:204:PCW:H122	4:B:212:PCW:H172	0.78	1.54	2	2
4:D:508:PCW:H61	5:D:512:17F:O9	0.78	1.79	5	2
5:C:629:17F:H1A	5:C:629:17F:H4	0.78	1.55	5	1
4:B:203:PCW:H51	4:B:204:PCW:H341	0.78	1.55	6	1
4:C:601:PCW:H39	4:C:602:PCW:H171	0.78	1.56	8	2
4:D:502:PCW:H73	4:D:502:PCW:O3P	0.77	1.78	4	9
4:D:505:PCW:H132	4:D:505:PCW:C17	0.77	2.09	4	10
4:D:506:PCW:H441	5:D:513:17F:H38	0.77	1.56	1	1
4:D:507:PCW:H20	5:D:513:17F:H19A	0.77	1.56	2	1
3:D:362:LEU:HB2	3:D:366:GLN:HB3	0.77	1.53	4	5
4:D:507:PCW:H122	5:D:513:17F:O8	0.77	1.79	4	1
5:A:409:17F:H4A	4:D:504:PCW:H352	0.77	1.56	7	1
5:A:410:17F:H71	4:D:501:PCW:H252	0.77	1.56	9	1
4:A:401:PCW:C45	4:C:610:PCW:H251	0.77	2.08	10	1
4:C:609:PCW:H283	5:C:631:17F:H68	0.77	1.54	7	6
4:A:412:PCW:H12	4:C:624:PCW:C36	0.77	2.08	3	7
3:D:445:THR:HG21	4:D:501:PCW:H52	0.77	1.55	3	1
4:B:207:PCW:H40	4:B:209:PCW:H182	0.77	1.55	4	1
4:B:202:PCW:O2P	4:D:507:PCW:H73	0.77	1.79	7	1
4:A:407:PCW:C39	4:B:210:PCW:H241	0.77	2.09	7	2
4:C:615:PCW:H39	4:C:617:PCW:H162	0.77	1.56	5	4
4:B:211:PCW:H422	4:B:211:PCW:C16	0.77	2.09	1	2
5:C:627:17F:H69	5:B:215:17F:H11	0.77	1.53	6	2
4:A:405:PCW:H271	4:A:414:PCW:C28	0.77	2.08	8	1
5:A:409:17F:O1	5:A:409:17F:H2	0.77	1.80	9	1
4:A:414:PCW:H482	4:B:212:PCW:H472	0.77	1.55	9	1
4:B:212:PCW:C38	4:B:212:PCW:H171	0.77	2.08	10	1
4:B:203:PCW:H252	4:B:208:PCW:H122	0.77	1.55	3	1
4:D:508:PCW:H41	4:D:508:PCW:O11	0.77	1.79	5	5
4:C:603:PCW:H442	4:D:515:PCW:H371	0.77	1.54	8	5
4:A:404:PCW:C4	4:A:407:PCW:H32	0.77	2.05	10	1
4:C:615:PCW:H31	4:C:615:PCW:P	0.77	2.20	3	3
4:B:210:PCW:H11	4:D:503:PCW:H131	0.77	1.54	10	3
4:C:608:PCW:H431	4:B:207:PCW:H231	0.77	1.57	4	1
4:C:606:PCW:H422	4:C:608:PCW:H31	0.77	1.54	3	3
4:A:415:PCW:C43	4:D:515:PCW:H211	0.77	2.09	3	4
4:A:415:PCW:H382	4:D:515:PCW:H161	0.77	1.54	10	3
4:C:616:PCW:H12	4:C:616:PCW:O31	0.77	1.80	5	7
4:B:204:PCW:H452	5:D:514:17F:H37	0.77	1.56	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:202:PCW:H181	4:B:202:PCW:H231	0.77	1.55	6	1
4:B:211:PCW:C17	4:D:505:PCW:H432	0.77	2.10	8	1
4:A:408:PCW:H141	4:A:408:PCW:C18	0.77	2.10	8	2
5:A:410:17F:C42	5:D:511:17F:H70	0.77	2.10	6	1
4:B:202:PCW:H181	4:B:202:PCW:H232	0.77	1.55	6	1
4:D:503:PCW:H442	4:D:504:PCW:H121	0.77	1.54	9	1
4:C:620:PCW:C19	5:C:631:17F:H5	0.77	2.09	2	1
2:B:79:LEU:HG	2:B:159:LEU:HD22	0.77	1.55	2	5
4:B:211:PCW:H461	4:B:211:PCW:C18	0.77	2.10	5	2
4:C:621:PCW:H351	4:C:625:PCW:H20	0.77	1.55	7	6
4:A:413:PCW:H361	4:C:611:PCW:C15	0.77	2.09	4	1
4:B:206:PCW:C14	5:B:213:17F:H18	0.77	2.08	9	1
4:A:401:PCW:H62	4:D:508:PCW:C1	0.77	2.10	10	2
4:A:401:PCW:C46	4:C:610:PCW:H251	0.77	2.09	2	2
4:C:621:PCW:H331	4:C:625:PCW:C20	0.77	2.09	4	1
4:C:611:PCW:H352	4:C:625:PCW:O11	0.77	1.80	6	1
4:B:202:PCW:C31	4:B:202:PCW:C36	0.77	2.60	6	2
4:D:505:PCW:H241	4:D:506:PCW:H372	0.77	1.57	9	1
4:B:207:PCW:H51	4:B:207:PCW:O31	0.77	1.79	10	1
4:C:608:PCW:H182	4:C:614:PCW:H352	0.77	1.57	1	3
4:C:609:PCW:C11	5:C:631:17F:H18	0.77	2.10	4	7
4:D:506:PCW:H422	5:D:513:17F:H39	0.77	1.54	1	1
5:D:512:17F:H30	5:D:514:17F:H39	0.77	1.56	4	1
4:C:602:PCW:H461	4:C:607:PCW:H472	0.77	1.57	5	2
5:A:410:17F:H1	4:D:502:PCW:C6	0.77	2.09	7	1
4:D:506:PCW:H462	5:D:513:17F:C28	0.77	2.10	7	1
4:B:203:PCW:C23	4:B:204:PCW:H19	0.77	2.08	8	1
4:B:203:PCW:H161	4:B:208:PCW:H352	0.77	1.55	8	1
4:A:408:PCW:H442	5:A:409:17F:C38	0.77	2.09	10	1
5:D:514:17F:C40	5:D:514:17F:H44	0.77	2.08	10	1
5:C:626:17F:H19A	5:C:626:17F:C31	0.76	2.09	2	10
4:D:502:PCW:H372	4:D:508:PCW:H321	0.76	1.57	1	3
4:A:413:PCW:H61	4:C:616:PCW:H40	0.76	1.54	4	1
4:B:202:PCW:O11	4:B:202:PCW:H52	0.76	1.79	5	1
4:A:406:PCW:H221	4:B:209:PCW:H481	0.76	1.57	9	1
4:A:403:PCW:H211	4:B:201:PCW:H181	0.76	1.56	1	1
4:B:202:PCW:H31	4:B:202:PCW:O1P	0.76	1.81	8	9
4:C:625:PCW:H381	4:C:625:PCW:H421	0.76	1.57	6	4
6:B:216:GNP:O2G	7:B:217:MG:MG	0.76	1.28	7	3
4:A:414:PCW:H63	4:C:624:PCW:C2	0.76	2.09	7	3
4:B:203:PCW:H271	4:B:204:PCW:C18	0.76	2.06	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:205:PCW:H472	5:B:214:17F:H75	0.76	1.57	5	1
5:D:513:17F:H53	4:D:515:PCW:H483	0.76	1.55	2	1
4:A:401:PCW:H181	4:A:401:PCW:C22	0.76	2.10	4	2
5:A:410:17F:H64	4:D:502:PCW:H272	0.76	1.55	6	1
4:A:417:PCW:H241	4:A:417:PCW:C20	0.76	2.09	2	10
4:C:606:PCW:O1P	4:C:624:PCW:H20	0.76	1.80	1	1
4:C:614:PCW:H452	4:B:207:PCW:H241	0.76	1.54	1	1
4:C:613:PCW:H63	4:C:623:PCW:O1P	0.76	1.80	6	7
4:C:603:PCW:H472	4:C:603:PCW:H231	0.76	1.55	3	2
4:A:403:PCW:C12	4:B:209:PCW:H331	0.76	2.09	6	1
4:B:206:PCW:H372	5:B:213:17F:C1Z	0.76	2.09	6	1
4:A:415:PCW:H372	4:C:616:PCW:H422	0.76	1.56	7	1
4:B:211:PCW:H282	4:D:506:PCW:C20	0.76	2.09	8	1
4:D:505:PCW:H422	4:D:506:PCW:H161	0.76	1.56	9	2
4:C:621:PCW:C12	5:C:627:17F:H67	0.76	2.11	10	1
4:A:417:PCW:H221	4:C:621:PCW:H232	0.76	1.57	4	3
4:C:618:PCW:C47	5:D:511:17F:H74	0.76	2.11	7	2
4:B:205:PCW:H82	5:B:214:17F:H10A	0.76	1.55	3	1
5:B:213:17F:H76	5:B:213:17F:H37	0.76	1.57	7	1
4:C:622:PCW:H261	4:D:501:PCW:H422	0.76	1.56	8	1
4:A:403:PCW:H132	4:B:201:PCW:C12	0.76	2.07	10	3
4:C:617:PCW:C35	4:C:625:PCW:H341	0.76	2.09	8	3
4:C:620:PCW:H19	5:C:631:17F:C5	0.76	2.07	7	1
4:D:509:PCW:H241	5:D:514:17F:H69	0.76	1.58	9	1
4:A:404:PCW:O11	4:B:210:PCW:H152	0.76	1.81	1	1
4:C:617:PCW:O2P	4:C:625:PCW:H82	0.76	1.80	1	1
5:C:632:17F:O10	5:C:632:17F:H6	0.76	1.78	1	10
4:C:604:PCW:C46	4:C:624:PCW:H282	0.76	2.11	4	7
4:B:205:PCW:C17	4:B:207:PCW:H321	0.76	2.10	3	1
4:B:210:PCW:H322	4:B:210:PCW:C4	0.76	2.10	7	3
4:A:406:PCW:H462	4:B:211:PCW:H182	0.76	1.57	5	1
4:B:205:PCW:H221	4:B:207:PCW:H152	0.76	1.57	5	1
4:D:505:PCW:H472	4:D:506:PCW:H232	0.76	1.56	5	1
4:C:605:PCW:H462	5:D:511:17F:C30	0.76	2.10	10	3
4:C:610:PCW:H321	4:C:622:PCW:C35	0.76	2.08	1	2
4:B:206:PCW:H462	4:B:206:PCW:H283	0.76	1.56	1	1
4:B:204:PCW:H11	5:B:214:17F:C8	0.76	2.10	3	1
4:D:509:PCW:H242	5:D:514:17F:H78	0.76	1.58	7	2
4:A:408:PCW:H281	4:A:416:PCW:H271	0.76	1.57	6	1
4:A:411:PCW:H431	4:A:416:PCW:H40	0.76	1.57	6	1
4:B:206:PCW:H121	5:B:213:17F:H18	0.76	1.55	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:403:PCW:C14	4:B:201:PCW:H362	0.76	2.10	7	1
4:A:411:PCW:H172	4:A:415:PCW:H411	0.76	1.57	7	1
4:C:604:PCW:H251	5:D:514:17F:H76	0.76	1.56	8	3
4:C:605:PCW:H231	4:C:612:PCW:C38	0.76	2.09	1	5
4:A:412:PCW:H12	4:C:624:PCW:H351	0.76	1.56	2	2
4:C:614:PCW:H472	4:B:207:PCW:C20	0.76	2.09	3	1
4:B:203:PCW:H172	4:B:208:PCW:H362	0.76	1.56	3	1
4:B:205:PCW:C14	4:B:206:PCW:H222	0.76	2.11	3	1
4:B:205:PCW:H211	4:B:205:PCW:C25	0.76	2.06	5	1
4:D:501:PCW:H73	4:D:509:PCW:H2	0.76	1.56	5	1
4:A:412:PCW:H442	4:C:623:PCW:H471	0.76	1.57	1	2
4:A:401:PCW:C48	4:C:613:PCW:H471	0.76	2.10	2	2
4:C:614:PCW:C22	4:B:207:PCW:H272	0.76	2.10	2	1
4:D:503:PCW:C3	5:D:513:17F:H4	0.76	2.10	9	3
4:A:404:PCW:C35	4:A:407:PCW:H152	0.76	2.11	4	2
4:C:625:PCW:H421	4:C:625:PCW:H372	0.76	1.56	10	2
4:A:408:PCW:H212	5:A:409:17F:H34	0.75	1.59	8	2
4:C:620:PCW:H141	5:B:215:17F:C6	0.75	2.04	4	9
4:C:607:PCW:H19	5:C:629:17F:H50	0.75	1.58	9	4
4:C:620:PCW:H451	5:B:215:17F:C42	0.75	2.12	2	1
4:D:504:PCW:H222	4:D:504:PCW:C26	0.75	2.06	2	1
4:C:620:PCW:H262	4:C:621:PCW:C8	0.75	2.10	4	4
4:C:623:PCW:C1	4:C:624:PCW:H12	0.75	2.00	5	3
4:A:403:PCW:H41	4:A:403:PCW:O31	0.75	1.81	7	2
5:C:628:17F:H54	5:B:213:17F:H77	0.75	1.58	1	1
5:A:409:17F:H9A	4:D:504:PCW:H372	0.75	1.57	2	1
4:C:603:PCW:H82	4:C:603:PCW:O31	0.75	1.81	4	3
4:B:202:PCW:H321	4:D:507:PCW:H51	0.75	1.57	2	2
4:B:203:PCW:H42	4:B:204:PCW:H341	0.75	1.58	2	1
4:C:615:PCW:H31	4:C:615:PCW:O2P	0.75	1.81	7	3
4:C:605:PCW:C31	4:C:612:PCW:H51	0.75	2.11	5	1
5:D:513:17F:H65	5:D:513:17F:H10	0.75	1.57	7	1
4:A:413:PCW:H271	4:A:413:PCW:C23	0.75	2.07	9	1
4:D:509:PCW:C26	5:D:514:17F:H73	0.75	2.11	9	1
4:B:203:PCW:H39	4:B:203:PCW:H141	0.75	1.57	10	1
4:C:601:PCW:H372	4:C:602:PCW:H171	0.75	1.54	1	1
4:D:504:PCW:O31	4:D:504:PCW:C35	0.75	2.35	4	7
5:C:630:17F:H5	5:C:630:17F:O8	0.75	1.81	9	3
4:B:203:PCW:C7	5:D:512:17F:H20A	0.75	2.11	5	1
4:D:503:PCW:H352	4:D:510:PCW:C8	0.75	2.11	5	1
5:A:410:17F:H57	4:D:502:PCW:H211	0.75	1.56	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:C:632:17F:H51	4:B:205:PCW:H251	0.75	1.55	4	1
4:A:412:PCW:H131	4:C:624:PCW:H422	0.75	1.58	5	1
4:B:202:PCW:H322	4:D:507:PCW:H51	0.75	1.57	9	2
4:A:403:PCW:H63	4:A:403:PCW:C32	0.75	2.12	4	2
4:B:203:PCW:H231	4:B:208:PCW:H2	0.75	1.58	2	1
4:B:204:PCW:C18	4:B:208:PCW:H221	0.75	2.10	6	3
4:C:610:PCW:H412	4:C:610:PCW:H20	0.75	1.58	8	3
4:A:405:PCW:C8	4:B:203:PCW:H321	0.75	2.11	7	1
4:C:611:PCW:C32	4:C:617:PCW:H152	0.75	2.11	7	1
4:C:615:PCW:H271	4:C:617:PCW:H282	0.75	1.58	7	1
4:C:624:PCW:H271	4:C:624:PCW:C20	0.75	2.12	7	1
4:D:501:PCW:C6	4:D:509:PCW:H2	0.75	2.10	8	1
4:C:620:PCW:H412	5:C:632:17F:C41	0.75	2.11	9	1
4:D:509:PCW:H262	5:D:514:17F:H73	0.75	1.59	9	1
4:B:208:PCW:H52	5:B:214:17F:C4	0.75	2.12	5	2
4:C:621:PCW:H441	4:D:506:PCW:H252	0.75	1.59	8	2
4:B:204:PCW:C14	4:B:208:PCW:H321	0.75	2.11	4	1
4:C:610:PCW:H41	4:C:622:PCW:H332	0.75	1.55	5	1
5:A:410:17F:H74	5:D:511:17F:H68	0.75	1.58	9	1
4:C:615:PCW:H461	4:C:625:PCW:C26	0.75	2.12	8	2
4:C:621:PCW:C14	5:C:628:17F:H33	0.75	2.09	8	7
5:D:513:17F:H53	4:D:516:PCW:H232	0.75	1.59	1	1
4:A:405:PCW:H352	5:D:512:17F:C35	0.75	2.11	2	1
4:A:413:PCW:H332	4:C:611:PCW:C11	0.75	2.11	9	4
4:C:607:PCW:O1P	4:C:624:PCW:H221	0.75	1.81	6	6
4:B:205:PCW:H182	4:B:207:PCW:H151	0.75	1.58	6	3
4:D:502:PCW:H2	4:D:502:PCW:H73	0.75	1.57	5	2
4:B:205:PCW:H282	4:B:205:PCW:C24	0.75	2.06	5	1
5:C:627:17F:C39	5:B:215:17F:H29	0.75	2.11	6	1
4:B:208:PCW:H73	5:B:214:17F:O2	0.75	1.82	10	1
4:C:603:PCW:H412	4:C:603:PCW:C37	0.75	2.11	10	8
4:C:605:PCW:O31	4:C:605:PCW:P	0.75	2.45	8	10
4:B:203:PCW:H31	4:B:203:PCW:P	0.75	2.22	6	10
4:C:622:PCW:H232	4:D:501:PCW:C48	0.75	2.11	2	2
4:D:509:PCW:H342	4:D:510:PCW:P	0.75	2.22	5	3
4:C:602:PCW:H131	5:B:214:17F:C33	0.75	2.12	3	1
4:C:603:PCW:H52	5:C:628:17F:O5	0.75	1.82	3	2
5:C:628:17F:H62	5:B:215:17F:H29	0.75	1.57	4	2
4:B:203:PCW:H231	4:B:204:PCW:C15	0.75	2.11	6	1
4:A:411:PCW:H141	4:A:415:PCW:H331	0.75	1.57	9	1
4:C:609:PCW:H63	5:C:631:17F:C6	0.75	2.12	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:606:PCW:H252	5:C:627:17F:C22	0.75	2.12	10	6
4:C:620:PCW:H151	5:B:215:17F:H4A	0.75	1.56	2	2
4:B:211:PCW:C32	4:B:211:PCW:H52	0.75	2.12	8	4
4:D:506:PCW:H422	5:D:513:17F:C27	0.75	2.12	7	4
4:D:506:PCW:C40	4:D:516:PCW:H251	0.75	2.10	7	3
4:D:508:PCW:H182	4:D:508:PCW:H341	0.75	1.59	4	1
4:C:621:PCW:H19	5:C:628:17F:H20	0.75	1.59	6	5
4:A:411:PCW:H452	4:A:416:PCW:C42	0.74	2.11	7	3
4:B:203:PCW:H231	4:B:204:PCW:H151	0.74	1.57	6	2
4:C:616:PCW:H62	4:C:616:PCW:C31	0.74	2.12	5	1
4:A:403:PCW:H82	4:B:209:PCW:H371	0.74	1.59	6	1
4:C:615:PCW:O2P	4:D:516:PCW:H51	0.74	1.82	6	1
5:B:213:17F:C39	4:D:506:PCW:H162	0.74	2.12	6	1
4:C:607:PCW:H42	4:C:624:PCW:H222	0.74	1.59	5	2
4:C:606:PCW:H132	4:C:606:PCW:H341	0.74	1.57	8	4
4:C:617:PCW:H322	4:C:625:PCW:H121	0.74	1.58	1	3
4:A:416:PCW:P	4:C:616:PCW:H42	0.74	2.23	3	3
4:C:611:PCW:C17	4:C:611:PCW:H212	0.74	2.11	2	2
4:A:403:PCW:C5	4:B:209:PCW:H351	0.74	2.07	3	1
4:A:411:PCW:C3	4:D:515:PCW:H121	0.74	2.12	4	1
4:B:211:PCW:C20	4:D:506:PCW:H242	0.74	2.10	7	2
4:B:204:PCW:O11	4:B:208:PCW:H151	0.74	1.82	6	1
4:A:404:PCW:H242	4:B:210:PCW:H222	0.74	1.57	7	1
4:A:406:PCW:H411	4:B:211:PCW:C38	0.74	2.12	7	1
4:C:611:PCW:H321	4:C:617:PCW:C14	0.74	2.13	1	1
4:C:612:PCW:H431	4:C:618:PCW:H39	0.74	1.59	6	3
4:C:605:PCW:H371	4:C:610:PCW:H322	0.74	1.57	3	2
4:C:610:PCW:H261	4:C:618:PCW:H452	0.74	1.59	3	1
4:B:206:PCW:H462	4:B:206:PCW:H251	0.74	1.58	4	1
4:C:620:PCW:C20	5:C:631:17F:H19A	0.74	2.12	5	1
4:B:205:PCW:C4	5:B:214:17F:H10A	0.74	2.13	5	2
4:D:508:PCW:H141	5:D:512:17F:H19	0.74	1.59	5	1
4:A:413:PCW:H231	4:A:413:PCW:C27	0.74	2.06	9	1
4:A:417:PCW:C22	4:C:603:PCW:H162	0.74	2.13	1	4
4:A:417:PCW:H221	4:C:621:PCW:C23	0.74	2.12	1	5
4:C:612:PCW:H12	4:C:612:PCW:O31	0.74	1.81	1	6
4:A:408:PCW:H352	4:A:408:PCW:H121	0.74	1.58	3	1
4:A:413:PCW:H372	4:C:611:PCW:H182	0.74	1.59	3	1
4:C:603:PCW:H461	4:D:515:PCW:H412	0.74	1.56	6	3
4:C:605:PCW:H462	5:D:511:17F:H53	0.74	1.59	10	1
4:C:621:PCW:H19	5:C:628:17F:C19	0.74	2.06	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:C:626:17F:H58	5:C:629:17F:H51	0.74	1.59	1	1
4:B:211:PCW:O31	4:B:211:PCW:H73	0.74	1.83	1	2
4:C:605:PCW:O31	4:C:612:PCW:H62	0.74	1.82	3	5
4:B:204:PCW:H2	4:B:208:PCW:H132	0.74	1.59	5	2
4:A:403:PCW:H251	4:B:201:PCW:H181	0.74	1.60	3	1
4:A:405:PCW:O2P	4:B:203:PCW:H62	0.74	1.82	6	2
4:B:207:PCW:H441	4:B:209:PCW:H232	0.74	1.58	7	1
4:A:405:PCW:C27	4:A:414:PCW:H281	0.74	2.11	8	1
4:C:617:PCW:H251	4:D:507:PCW:H483	0.74	1.57	9	1
4:C:614:PCW:H472	4:B:207:PCW:C23	0.74	2.12	1	1
4:C:622:PCW:C42	4:C:623:PCW:H261	0.74	2.11	1	3
4:C:623:PCW:H151	4:C:623:PCW:C19	0.74	2.13	9	9
4:C:614:PCW:C21	5:C:632:17F:H38	0.74	2.12	3	2
4:B:208:PCW:H141	5:B:214:17F:O7	0.74	1.83	4	1
4:B:212:PCW:H421	4:B:212:PCW:H222	0.74	1.58	7	1
5:D:514:17F:H44	5:D:514:17F:H72	0.74	1.59	10	1
4:C:610:PCW:H162	4:C:618:PCW:H171	0.74	1.59	4	3
4:D:503:PCW:C33	4:D:510:PCW:H82	0.74	2.12	8	2
4:C:622:PCW:H211	4:D:501:PCW:H481	0.74	1.58	4	1
4:B:210:PCW:H472	4:D:507:PCW:H242	0.74	1.58	7	1
4:A:403:PCW:H151	4:B:201:PCW:H382	0.74	1.57	8	1
4:C:607:PCW:H261	5:C:629:17F:H65	0.74	1.60	9	1
4:D:505:PCW:C20	4:D:510:PCW:H342	0.74	2.10	10	2
4:D:503:PCW:C15	4:D:506:PCW:H321	0.74	2.13	1	2
5:D:513:17F:H10A	5:D:513:17F:H66	0.74	1.59	4	2
4:A:401:PCW:H62	4:D:508:PCW:O31	0.74	1.83	4	5
4:C:613:PCW:H442	4:C:618:PCW:C20	0.74	2.11	7	6
4:C:620:PCW:C22	5:C:631:17F:H31	0.74	2.12	9	6
4:D:507:PCW:H122	5:D:513:17F:C7	0.74	2.13	7	2
4:A:412:PCW:C3	4:C:624:PCW:H411	0.74	2.13	5	1
4:B:201:PCW:H341	4:B:209:PCW:H31	0.74	1.57	8	2
4:B:204:PCW:H42	5:B:214:17F:H2	0.74	1.56	8	1
4:A:405:PCW:C39	5:D:512:17F:H69	0.74	2.13	9	1
4:A:405:PCW:H272	4:A:405:PCW:C48	0.74	2.13	5	3
4:B:203:PCW:H281	4:B:208:PCW:C19	0.74	2.13	3	1
4:C:614:PCW:C22	4:B:207:PCW:H251	0.74	2.13	4	3
4:B:210:PCW:H51	5:D:513:17F:O4	0.74	1.83	4	2
4:B:206:PCW:O4P	4:B:206:PCW:H31	0.74	1.83	5	1
5:C:632:17F:H51	4:B:201:PCW:C44	0.74	2.13	6	1
4:A:408:PCW:O31	5:A:409:17F:H32	0.74	1.83	8	1
4:B:203:PCW:H241	4:B:208:PCW:C12	0.74	2.02	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:417:PCW:H481	5:D:511:17F:H50	0.73	1.59	4	1
4:A:408:PCW:H371	4:A:408:PCW:C3	0.73	2.04	8	9
4:A:415:PCW:C45	4:D:515:PCW:H211	0.73	2.13	7	3
4:A:402:PCW:C22	4:A:413:PCW:H262	0.73	2.12	6	1
5:A:410:17F:C36	4:D:502:PCW:H272	0.73	2.13	6	2
4:C:609:PCW:C28	5:C:631:17F:H68	0.73	2.13	7	2
4:C:625:PCW:H42	4:C:625:PCW:H2	0.73	1.58	8	1
4:B:205:PCW:H52	5:B:214:17F:C9	0.73	2.13	8	1
4:D:506:PCW:C48	4:D:516:PCW:H231	0.73	2.14	8	1
5:C:627:17F:O7	5:C:627:17F:C18	0.73	2.35	7	8
4:B:208:PCW:C48	4:B:212:PCW:H262	0.73	2.14	1	1
4:A:411:PCW:H141	4:A:415:PCW:C34	0.73	2.11	9	4
4:C:621:PCW:H321	4:C:625:PCW:H20	0.73	1.60	7	4
4:A:404:PCW:H31	4:A:407:PCW:C11	0.73	2.13	3	2
4:A:416:PCW:H51	4:A:416:PCW:O11	0.73	1.82	3	1
4:C:614:PCW:H221	5:C:632:17F:H41	0.73	1.59	3	1
4:B:210:PCW:O2P	4:D:506:PCW:H73	0.73	1.83	6	2
4:A:401:PCW:H12	4:D:508:PCW:C34	0.73	2.11	4	1
4:B:201:PCW:H322	4:B:209:PCW:O3	0.73	1.83	4	1
4:B:205:PCW:H142	4:B:206:PCW:C20	0.73	2.13	4	1
4:B:207:PCW:H51	4:B:207:PCW:H322	0.73	1.59	4	2
4:D:507:PCW:H432	5:D:513:17F:H30	0.73	1.58	10	2
4:C:623:PCW:H12	4:C:624:PCW:C1	0.73	2.01	5	2
4:D:509:PCW:H342	4:D:510:PCW:O3P	0.73	1.82	9	2
4:A:403:PCW:H171	4:A:403:PCW:C21	0.73	2.12	9	3
4:A:417:PCW:H472	5:D:511:17F:H55	0.73	1.60	1	1
4:C:608:PCW:H73	4:C:619:PCW:O11	0.73	1.83	4	8
2:B:37:GLU:HB3	3:D:369:VAL:CG2	0.73	2.13	6	9
4:D:505:PCW:H161	4:D:510:PCW:C47	0.73	2.10	1	1
4:C:611:PCW:H332	4:C:625:PCW:C13	0.73	2.13	2	3
4:D:501:PCW:C8	5:D:514:17F:H19A	0.73	2.14	3	1
4:D:501:PCW:H451	4:D:509:PCW:C22	0.73	2.13	4	1
4:B:204:PCW:H441	4:B:212:PCW:C23	0.73	2.07	1	1
4:B:206:PCW:H371	4:D:505:PCW:H321	0.73	1.60	10	2
5:C:626:17F:H19A	5:C:629:17F:H51	0.73	1.59	5	2
4:A:405:PCW:H361	4:B:203:PCW:H372	0.73	1.58	9	1
4:A:417:PCW:C14	4:C:603:PCW:H382	0.73	2.13	2	2
4:D:507:PCW:C35	5:D:513:17F:H8	0.73	2.13	6	2
4:A:405:PCW:H322	4:B:203:PCW:H352	0.73	1.59	9	1
4:C:608:PCW:H332	5:C:632:17F:H20A	0.73	1.59	9	1
4:A:415:PCW:H481	4:C:617:PCW:H283	0.73	1.60	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:606:PCW:H132	4:C:606:PCW:C34	0.73	2.13	2	6
4:B:204:PCW:C41	5:D:514:17F:H8	0.73	2.13	1	2
4:D:502:PCW:H73	4:D:502:PCW:C1	0.73	2.14	5	8
4:A:404:PCW:H52	4:A:407:PCW:H11	0.73	1.58	4	3
4:C:617:PCW:H131	4:C:625:PCW:C15	0.73	2.08	9	7
4:B:205:PCW:H62	5:B:213:17F:O1	0.73	1.84	5	3
4:B:203:PCW:H231	4:B:208:PCW:O31	0.73	1.82	5	1
4:B:210:PCW:O2	4:B:210:PCW:H42	0.73	1.84	5	1
4:B:203:PCW:C25	4:B:204:PCW:H151	0.73	2.13	6	1
4:D:505:PCW:H11	4:D:509:PCW:H73	0.73	1.57	9	2
4:B:212:PCW:H51	5:B:214:17F:H9	0.73	1.60	9	1
5:D:513:17F:H49	4:D:516:PCW:H251	0.73	1.58	10	1
4:A:401:PCW:H322	4:D:508:PCW:C38	0.73	2.13	1	3
4:C:611:PCW:H342	4:C:611:PCW:O2	0.73	1.83	5	9
2:B:135:ARG:NH2	4:B:209:PCW:H2	0.73	1.99	2	1
4:D:502:PCW:H171	4:D:502:PCW:H212	0.73	1.59	6	3
4:B:205:PCW:H52	5:B:214:17F:C10	0.73	2.12	7	3
5:C:628:17F:C37	5:B:215:17F:H39	0.73	2.09	6	2
4:D:503:PCW:H31	5:D:513:17F:O1	0.73	1.84	6	1
4:B:204:PCW:H131	4:B:208:PCW:C15	0.73	2.14	10	1
4:A:413:PCW:H371	4:A:413:PCW:C41	0.73	2.13	1	4
4:A:413:PCW:C35	4:C:611:PCW:C13	0.73	2.67	10	4
4:C:605:PCW:H231	4:C:612:PCW:C39	0.73	2.14	3	4
4:C:601:PCW:H122	4:C:601:PCW:H462	0.73	1.61	2	1
5:C:627:17F:C20	5:C:627:17F:H9A	0.73	2.14	8	2
4:D:507:PCW:H31	5:D:513:17F:H75	0.73	1.59	3	3
4:D:510:PCW:H262	4:D:515:PCW:H462	0.73	1.60	5	1
4:A:405:PCW:H461	4:A:414:PCW:H241	0.73	1.59	6	2
4:D:508:PCW:H342	4:D:508:PCW:C18	0.73	2.13	6	1
5:A:409:17F:H9A	4:D:504:PCW:C40	0.73	2.13	7	1
4:A:403:PCW:H181	4:A:403:PCW:H39	0.73	1.61	8	1
4:A:402:PCW:H342	4:D:507:PCW:H212	0.73	1.60	10	1
4:C:607:PCW:C18	5:C:629:17F:H11	0.73	2.14	5	3
4:A:407:PCW:H382	4:B:211:PCW:H141	0.73	1.61	2	4
4:A:417:PCW:C24	4:C:621:PCW:H242	0.73	2.11	9	5
4:C:622:PCW:C38	4:C:623:PCW:H171	0.73	2.14	4	1
4:B:207:PCW:H441	4:B:209:PCW:H251	0.73	1.60	6	1
4:D:502:PCW:H172	4:D:502:PCW:C21	0.73	2.05	8	1
5:A:410:17F:H78	4:C:618:PCW:H482	0.73	1.59	10	1
4:C:625:PCW:C28	5:C:631:17F:H51	0.72	2.14	10	5
4:D:505:PCW:H282	4:D:509:PCW:H451	0.72	1.60	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:503:PCW:H161	4:D:503:PCW:H271	0.72	1.59	5	1
4:B:206:PCW:O1P	4:B:206:PCW:C3	0.72	2.37	6	2
4:B:202:PCW:H321	4:D:504:PCW:H12	0.72	1.59	8	1
4:D:509:PCW:H82	4:D:510:PCW:H321	0.72	1.60	8	2
4:A:408:PCW:H232	5:A:409:17F:H34	0.72	1.60	9	1
4:B:212:PCW:H371	5:D:514:17F:H33	0.72	1.61	9	1
4:A:407:PCW:H271	4:A:407:PCW:C23	0.72	2.09	10	1
4:A:403:PCW:H32	4:B:201:PCW:C8	0.72	2.13	10	2
4:C:602:PCW:H261	5:C:629:17F:H77	0.72	1.59	3	3
4:B:207:PCW:H61	5:B:213:17F:C1	0.72	2.06	9	1
4:D:501:PCW:H211	5:D:511:17F:H18A	0.72	1.61	10	1
4:A:413:PCW:C33	4:C:611:PCW:H132	0.72	2.14	5	7
5:C:627:17F:H35	5:C:628:17F:H10	0.72	1.60	1	2
4:D:503:PCW:H152	4:D:507:PCW:C39	0.72	2.12	10	3
4:D:503:PCW:O31	4:D:503:PCW:H12	0.72	1.85	9	7
5:A:410:17F:C33	4:D:501:PCW:H241	0.72	2.14	2	1
4:D:507:PCW:H222	5:D:513:17F:H31	0.72	1.61	3	1
4:A:413:PCW:H361	4:C:611:PCW:H151	0.72	1.62	4	1
4:C:607:PCW:C19	5:C:629:17F:H39	0.72	2.14	5	2
2:B:165:LYS:HB3	4:B:209:PCW:H61	0.72	1.58	6	1
4:C:602:PCW:H422	5:C:626:17F:H41	0.72	1.59	7	1
4:B:204:PCW:C23	4:B:208:PCW:H242	0.72	2.13	10	2
4:C:606:PCW:H2	4:C:606:PCW:H41	0.72	1.59	6	8
4:D:505:PCW:H361	4:D:506:PCW:H142	0.72	1.58	1	2
4:B:210:PCW:H262	4:D:503:PCW:C25	0.72	2.15	2	1
4:B:204:PCW:H412	4:B:212:PCW:H231	0.72	1.61	5	1
3:D:447:LEU:HD23	5:D:514:17F:H1A	0.72	1.59	6	1
4:D:501:PCW:H171	4:D:502:PCW:H331	0.72	1.62	6	2
4:B:209:PCW:C39	5:B:213:17F:H64	0.72	2.14	8	1
4:A:408:PCW:H12	4:A:408:PCW:H371	0.72	1.59	1	1
4:C:615:PCW:H451	4:D:506:PCW:H481	0.72	1.62	3	1
4:B:202:PCW:C33	4:D:507:PCW:H11	0.72	2.13	5	2
4:B:202:PCW:O11	4:B:202:PCW:H41	0.72	1.84	6	1
5:D:513:17F:H10	5:D:513:17F:C36	0.72	2.14	7	1
5:C:626:17F:C32	5:C:629:17F:H51	0.72	2.15	1	4
4:B:206:PCW:H2	5:B:213:17F:C4	0.72	2.14	1	1
4:A:411:PCW:C45	4:C:616:PCW:H242	0.72	2.14	4	8
4:B:208:PCW:H162	5:B:214:17F:H8	0.72	1.59	4	2
3:D:437:THR:HG21	3:D:467:THR:HG21	0.72	1.59	4	1
4:D:502:PCW:C41	4:D:508:PCW:H361	0.72	2.13	6	1
4:D:503:PCW:H482	4:D:510:PCW:H19	0.72	1.60	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:504:PCW:H472	4:D:510:PCW:H232	0.72	1.60	1	1
4:A:401:PCW:H481	4:C:613:PCW:H471	0.72	1.60	2	1
4:C:616:PCW:H471	4:C:616:PCW:C43	0.72	2.11	8	2
5:C:627:17F:H42	5:C:628:17F:H73	0.72	1.62	3	3
4:B:204:PCW:H32	4:B:208:PCW:C15	0.72	2.15	6	3
5:D:512:17F:H12	5:D:514:17F:H39	0.72	1.60	3	1
5:B:213:17F:H63	4:D:505:PCW:C39	0.72	2.12	4	1
4:B:212:PCW:H281	5:D:512:17F:H71	0.72	1.61	8	2
4:D:505:PCW:H171	4:D:505:PCW:C13	0.72	2.13	6	9
4:B:206:PCW:H12	5:B:213:17F:H1	0.72	1.59	2	1
4:C:615:PCW:H451	4:D:506:PCW:H472	0.72	1.61	7	2
4:D:503:PCW:H421	4:D:504:PCW:C40	0.72	2.14	6	1
5:B:214:17F:H36	5:B:214:17F:H42	0.72	1.60	9	2
4:A:402:PCW:C26	4:A:413:PCW:H461	0.72	2.14	10	1
4:A:402:PCW:H262	4:A:413:PCW:H461	0.72	1.61	10	1
4:B:201:PCW:H421	4:B:205:PCW:H372	0.72	1.59	10	1
4:A:417:PCW:H211	4:C:603:PCW:C16	0.72	2.14	4	4
4:C:605:PCW:H61	5:C:630:17F:C3	0.72	2.14	2	1
5:A:410:17F:H31	4:D:502:PCW:C17	0.72	2.14	5	1
4:B:201:PCW:H51	4:B:201:PCW:O11	0.72	1.85	10	3
4:A:416:PCW:H141	5:C:630:17F:H11	0.72	1.60	7	1
4:B:202:PCW:O1P	4:B:202:PCW:C3	0.72	2.37	6	3
4:D:507:PCW:H20	5:D:513:17F:H31	0.72	1.61	5	4
4:C:616:PCW:H51	4:C:616:PCW:H2	0.72	1.61	5	3
5:C:632:17F:H5	5:C:632:17F:O8	0.72	1.84	8	7
4:C:612:PCW:H132	4:C:618:PCW:H382	0.72	1.62	3	3
4:B:204:PCW:C15	4:B:208:PCW:H341	0.72	2.10	7	2
4:A:415:PCW:C36	4:D:515:PCW:H161	0.72	2.15	4	1
4:A:416:PCW:H63	4:A:416:PCW:H32	0.72	1.61	6	1
4:C:605:PCW:H441	4:C:618:PCW:H441	0.72	1.62	10	1
4:A:405:PCW:H2	5:D:512:17F:C1Z	0.71	2.14	7	4
4:C:605:PCW:O1P	4:C:612:PCW:H51	0.71	1.84	1	2
5:C:628:17F:H11	5:C:628:17F:H56	0.71	1.60	1	3
4:B:201:PCW:H321	4:B:209:PCW:H31	0.71	1.62	1	1
4:B:210:PCW:C4	4:B:210:PCW:H322	0.71	2.15	5	3
4:C:621:PCW:C19	5:C:628:17F:H29	0.71	2.15	2	1
4:A:404:PCW:H352	4:A:407:PCW:H162	0.71	1.61	3	2
4:A:407:PCW:H431	4:B:211:PCW:C23	0.71	2.14	3	4
4:D:504:PCW:C18	4:D:504:PCW:H221	0.71	2.14	3	1
4:D:507:PCW:H122	5:D:513:17F:O7	0.71	1.84	3	1
4:A:401:PCW:H282	4:D:502:PCW:H241	0.71	1.63	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:510:PCW:C26	4:D:515:PCW:H462	0.71	2.15	5	2
4:B:202:PCW:H231	4:B:202:PCW:C18	0.71	2.15	6	1
5:B:213:17F:H70	4:D:506:PCW:H162	0.71	1.61	6	1
4:C:605:PCW:H442	4:C:618:PCW:C48	0.71	2.12	7	1
4:C:614:PCW:C12	5:C:632:17F:H8	0.71	2.15	7	1
4:D:501:PCW:C39	4:D:509:PCW:H441	0.71	2.13	7	1
4:A:416:PCW:H162	5:C:630:17F:H20	0.71	1.62	7	3
4:B:206:PCW:C16	5:B:213:17F:H56	0.71	2.16	4	3
4:D:506:PCW:H32	4:D:506:PCW:P	0.71	2.24	1	5
5:A:409:17F:H64	5:D:511:17F:H37	0.71	1.62	2	1
4:B:208:PCW:H32	4:B:208:PCW:O4P	0.71	1.85	2	1
4:B:206:PCW:C19	5:B:213:17F:H57	0.71	2.15	3	1
4:C:622:PCW:H211	4:D:501:PCW:C48	0.71	2.14	4	1
4:A:404:PCW:H131	4:B:210:PCW:H161	0.71	1.62	5	1
4:A:408:PCW:H341	5:A:409:17F:C31	0.71	2.15	6	1
4:B:206:PCW:C12	5:B:213:17F:H18	0.71	2.14	10	2
4:A:405:PCW:C7	4:B:203:PCW:H321	0.71	2.15	7	1
4:C:612:PCW:H282	5:D:511:17F:H43	0.71	1.61	9	1
4:A:403:PCW:H132	4:B:201:PCW:H141	0.71	1.61	1	1
4:A:414:PCW:H40	4:C:623:PCW:H441	0.71	1.60	1	5
1:C:497:SER:HB2	1:C:498:PRO:HD3	0.71	1.61	2	5
4:C:605:PCW:H39	4:C:610:PCW:H341	0.71	1.62	8	6
4:D:503:PCW:O11	4:D:506:PCW:H41	0.71	1.86	2	1
4:C:619:PCW:C15	5:C:632:17F:H18	0.71	2.14	5	1
4:A:403:PCW:C21	4:A:403:PCW:H171	0.71	2.15	6	1
4:C:606:PCW:H31	5:C:627:17F:O1	0.71	1.84	6	1
4:B:201:PCW:H382	4:B:207:PCW:H381	0.71	1.63	6	1
4:A:403:PCW:C4	4:A:406:PCW:H40	0.71	2.14	8	1
4:C:608:PCW:C27	5:C:626:17F:H73	0.71	2.14	2	2
5:B:215:17F:H40	5:B:215:17F:H30	0.71	1.60	6	2
4:C:608:PCW:H422	4:C:614:PCW:H452	0.71	1.63	4	1
4:A:403:PCW:H171	4:A:403:PCW:C22	0.71	2.15	6	2
4:C:603:PCW:C27	4:D:515:PCW:H212	0.71	2.14	10	2
4:A:403:PCW:C6	4:A:406:PCW:H422	0.71	2.15	8	1
1:A:388:SER:HB2	1:C:594:LYS:HE2	0.71	1.59	1	2
4:C:608:PCW:O1P	5:C:632:17F:H18A	0.71	1.85	1	2
4:D:503:PCW:H151	4:D:506:PCW:H321	0.71	1.62	8	2
4:D:505:PCW:H442	4:D:506:PCW:H141	0.71	1.61	1	1
1:A:243:MET:HG3	1:A:247:LEU:HD12	0.71	1.62	8	5
4:C:605:PCW:C21	4:C:612:PCW:H382	0.71	2.16	6	4
4:C:619:PCW:H283	5:C:632:17F:C21	0.71	2.15	7	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:604:PCW:H381	5:C:627:17F:C22	0.71	2.16	6	1
4:C:614:PCW:H2	4:C:614:PCW:C4	0.71	2.16	7	4
4:B:205:PCW:H52	5:B:214:17F:H9	0.71	1.61	8	1
4:A:402:PCW:H62	5:D:513:17F:C18	0.71	2.14	9	1
4:B:204:PCW:H442	4:B:212:PCW:H231	0.71	1.60	10	1
4:C:614:PCW:H452	4:B:207:PCW:C24	0.71	2.16	1	1
5:B:215:17F:H19A	5:B:215:17F:H9	0.71	1.62	1	5
4:D:510:PCW:H262	4:D:515:PCW:C46	0.71	2.16	1	3
4:C:625:PCW:O1P	4:C:625:PCW:H51	0.71	1.84	5	2
4:A:411:PCW:H472	4:C:616:PCW:H251	0.71	1.61	3	2
4:C:606:PCW:H411	5:B:215:17F:H55	0.71	1.60	3	1
4:B:202:PCW:H232	4:B:202:PCW:H441	0.71	1.61	4	2
4:D:501:PCW:H451	4:D:509:PCW:H221	0.71	1.63	4	1
4:D:508:PCW:H73	4:D:508:PCW:O11	0.71	1.84	5	2
4:C:620:PCW:H20	4:C:621:PCW:C8	0.71	2.15	8	4
5:C:627:17F:H10	5:B:215:17F:C28	0.71	2.14	9	3
4:C:604:PCW:C38	5:C:627:17F:H40	0.71	2.15	9	2
4:A:405:PCW:H152	5:D:512:17F:H59	0.71	1.63	8	1
4:C:610:PCW:H432	4:C:610:PCW:C22	0.71	2.15	9	2
4:B:202:PCW:C32	4:D:504:PCW:H12	0.71	2.15	8	1
4:C:606:PCW:H161	5:C:627:17F:C11	0.71	2.15	6	7
5:C:631:17F:H53	4:B:211:PCW:H252	0.71	1.63	4	4
4:A:401:PCW:H411	4:D:502:PCW:C26	0.71	2.13	6	1
4:C:625:PCW:H221	4:C:625:PCW:C18	0.71	2.15	6	1
5:D:514:17F:H68	5:D:514:17F:H40	0.71	1.62	10	1
4:C:621:PCW:H172	5:C:628:17F:H34	0.71	1.63	2	6
4:C:617:PCW:H381	4:C:625:PCW:H181	0.71	1.60	3	4
4:D:506:PCW:H362	4:D:507:PCW:C39	0.71	2.15	9	1
4:C:604:PCW:H31	4:C:604:PCW:P	0.71	2.25	5	9
4:C:607:PCW:O1P	4:C:624:PCW:H241	0.71	1.86	1	5
4:A:403:PCW:H52	4:B:209:PCW:O31	0.71	1.85	3	1
4:C:606:PCW:H372	5:C:627:17F:O8	0.71	1.86	9	3
4:D:501:PCW:H73	4:D:509:PCW:O31	0.71	1.86	5	1
4:C:625:PCW:O1P	4:C:625:PCW:H52	0.71	1.85	7	3
4:D:506:PCW:H431	4:D:507:PCW:H422	0.71	1.60	7	1
4:B:202:PCW:H161	4:D:504:PCW:H31	0.71	1.61	10	1
4:B:212:PCW:H422	5:D:514:17F:C32	0.71	2.14	10	1
4:A:407:PCW:C37	4:B:210:PCW:H272	0.71	2.14	1	1
4:C:613:PCW:C5	4:C:623:PCW:O1P	0.71	2.39	6	10
4:B:202:PCW:H63	4:D:504:PCW:O1P	0.71	1.86	3	1
5:A:410:17F:H31	4:D:502:PCW:C16	0.71	2.16	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:206:PCW:C14	5:B:213:17F:H20A	0.71	2.15	6	2
4:D:503:PCW:H31	5:D:513:17F:H4	0.71	1.62	7	2
5:D:514:17F:H4	5:D:514:17F:H2	0.71	1.62	9	1
4:A:401:PCW:H472	4:C:610:PCW:C27	0.70	2.10	1	3
4:A:415:PCW:H242	4:A:415:PCW:C20	0.70	2.13	1	1
4:A:416:PCW:H61	5:C:630:17F:H4	0.70	1.63	5	4
4:C:622:PCW:H421	4:C:623:PCW:C26	0.70	2.14	3	6
4:D:505:PCW:O11	4:D:509:PCW:H62	0.70	1.85	2	2
4:D:505:PCW:H283	4:D:510:PCW:O3	0.70	1.86	3	3
4:C:620:PCW:H141	5:B:215:17F:C4	0.70	2.16	8	1
4:C:623:PCW:C19	4:C:623:PCW:H151	0.70	2.16	8	1
5:C:627:17F:H64	5:C:628:17F:C31	0.70	2.16	10	1
4:B:211:PCW:H282	4:D:506:PCW:H222	0.70	1.61	10	1
4:A:412:PCW:H452	4:C:624:PCW:H481	0.70	1.60	4	2
4:C:617:PCW:H362	5:C:631:17F:C22	0.70	2.16	10	4
4:C:607:PCW:H63	4:C:624:PCW:H222	0.70	1.60	6	1
4:D:507:PCW:H431	5:D:513:17F:H43	0.70	1.63	7	1
4:B:212:PCW:H142	5:D:514:17F:O8	0.70	1.86	8	1
4:C:615:PCW:H461	4:C:625:PCW:H261	0.70	1.62	1	2
4:A:403:PCW:O4P	4:B:209:PCW:H321	0.70	1.86	3	1
4:B:206:PCW:H372	4:B:206:PCW:C42	0.70	2.16	3	1
4:D:501:PCW:H51	4:D:509:PCW:C33	0.70	2.02	9	2
4:A:407:PCW:H451	4:B:211:PCW:H232	0.70	1.63	8	2
5:A:410:17F:H77	5:D:511:17F:H70	0.70	1.63	6	1
5:D:511:17F:C19	5:D:511:17F:C31	0.70	2.68	1	8
4:A:405:PCW:H371	5:D:512:17F:C36	0.70	2.11	2	1
4:A:408:PCW:H141	5:A:409:17F:C37	0.70	2.16	2	1
5:A:409:17F:H46	4:D:510:PCW:H231	0.70	1.60	2	1
4:D:501:PCW:H342	5:D:512:17F:H37	0.70	1.64	2	2
4:C:607:PCW:H42	4:C:624:PCW:C24	0.70	2.17	5	1
4:B:202:PCW:O4P	4:B:202:PCW:H31	0.70	1.85	5	1
4:A:411:PCW:C20	4:A:415:PCW:H431	0.70	2.17	9	1
4:C:607:PCW:C4	4:C:624:PCW:H222	0.70	2.14	1	4
4:A:417:PCW:H211	4:C:603:PCW:H161	0.70	1.61	5	9
4:B:208:PCW:H442	4:B:212:PCW:H283	0.70	1.62	3	1
4:C:621:PCW:H73	5:C:631:17F:H11A	0.70	1.63	4	3
4:C:602:PCW:H39	4:C:602:PCW:C20	0.70	2.16	5	2
4:A:401:PCW:H322	4:D:508:PCW:H381	0.70	1.63	1	2
4:C:602:PCW:H31	4:C:602:PCW:O31	0.70	1.87	6	9
4:C:607:PCW:H452	5:C:626:17F:H60	0.70	1.62	6	5
5:C:628:17F:C37	5:B:215:17F:H36	0.70	2.09	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:622:PCW:H382	4:C:623:PCW:H171	0.70	1.61	3	8
4:C:603:PCW:C44	4:D:515:PCW:H351	0.70	2.16	3	1
4:C:623:PCW:C39	4:C:624:PCW:H141	0.70	2.11	3	1
4:C:617:PCW:C38	4:C:625:PCW:H161	0.70	2.16	4	4
4:D:507:PCW:H31	5:D:513:17F:H77	0.70	1.62	6	1
4:A:401:PCW:H481	4:C:618:PCW:H271	0.70	1.64	7	1
4:C:615:PCW:H471	4:D:506:PCW:H40	0.70	1.61	10	1
4:B:204:PCW:H40	5:D:512:17F:H9	0.70	1.62	9	2
4:D:503:PCW:H321	4:D:507:PCW:H361	0.70	1.63	3	1
5:C:628:17F:H62	5:B:215:17F:C1X	0.70	2.16	5	2
4:C:614:PCW:H452	4:B:207:PCW:C26	0.70	2.13	7	1
4:B:201:PCW:H341	4:B:209:PCW:C3	0.70	2.16	8	2
4:C:610:PCW:H51	4:C:622:PCW:H342	0.70	1.60	10	1
5:C:627:17F:H64	5:C:628:17F:H57	0.70	1.63	10	1
4:B:208:PCW:H462	4:B:212:PCW:H251	0.70	1.63	1	1
4:A:401:PCW:C44	4:C:613:PCW:H262	0.70	2.14	2	2
4:A:413:PCW:H351	4:C:611:PCW:C15	0.70	2.16	7	3
4:D:501:PCW:H41	4:D:509:PCW:H331	0.70	1.64	2	2
4:A:415:PCW:H362	4:C:616:PCW:C38	0.70	2.17	8	2
4:C:621:PCW:C7	5:C:631:17F:H11A	0.70	2.17	4	5
4:D:510:PCW:H63	4:D:510:PCW:H332	0.70	1.61	7	1
4:C:608:PCW:C18	4:C:614:PCW:H341	0.70	2.16	9	1
4:C:603:PCW:H242	4:D:515:PCW:H352	0.70	1.63	7	8
4:C:623:PCW:H41	4:C:623:PCW:O31	0.70	1.87	2	5
4:A:412:PCW:H431	4:C:623:PCW:C47	0.70	2.15	5	3
4:D:501:PCW:H151	4:D:502:PCW:H332	0.70	1.64	4	2
4:D:509:PCW:H452	4:D:510:PCW:C3	0.70	2.17	4	1
4:A:413:PCW:C45	4:C:611:PCW:H162	0.70	2.16	9	1
1:A:250:VAL:O	1:A:254:VAL:HB	0.70	1.86	1	10
4:A:411:PCW:O11	4:D:515:PCW:H121	0.70	1.87	1	1
4:C:612:PCW:H251	5:D:511:17F:C27	0.70	2.17	1	4
4:C:617:PCW:H63	4:C:621:PCW:P	0.70	2.26	8	5
4:C:602:PCW:H362	5:B:214:17F:H61	0.70	1.63	4	3
4:C:621:PCW:C34	4:D:516:PCW:H442	0.70	2.15	7	5
4:C:616:PCW:O11	4:C:616:PCW:H51	0.70	1.86	8	2
4:C:620:PCW:O1P	4:C:620:PCW:C3	0.70	2.38	8	1
5:C:628:17F:H12A	5:C:628:17F:C32	0.69	2.17	9	8
4:B:205:PCW:H42	5:B:213:17F:O1	0.69	1.87	1	1
4:C:603:PCW:H281	4:D:515:PCW:H232	0.69	1.64	10	2
4:D:505:PCW:O11	4:D:505:PCW:H2	0.69	1.87	3	5
4:C:604:PCW:O31	4:C:606:PCW:H82	0.69	1.87	10	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:612:PCW:H411	4:C:618:PCW:H39	0.69	1.60	5	1
4:C:620:PCW:H121	5:B:215:17F:O9	0.69	1.87	8	2
4:B:212:PCW:H52	4:B:212:PCW:O2P	0.69	1.86	9	1
4:D:501:PCW:O11	4:D:509:PCW:H39	0.69	1.87	10	1
1:C:471:ARG:HA	1:C:475:GLU:HG3	0.69	1.64	9	5
4:B:211:PCW:H142	4:B:211:PCW:C39	0.69	2.17	8	6
4:D:508:PCW:C3	4:D:508:PCW:O1P	0.69	2.41	9	9
4:A:403:PCW:H212	4:A:403:PCW:H161	0.69	1.64	2	6
4:A:407:PCW:H421	4:A:407:PCW:H282	0.69	1.63	2	1
4:C:604:PCW:C11	4:C:604:PCW:C31	0.69	2.70	2	2
4:A:411:PCW:H472	4:C:616:PCW:C25	0.69	2.17	8	2
4:C:604:PCW:H472	4:C:606:PCW:H141	0.69	1.63	6	1
4:A:416:PCW:H141	5:C:630:17F:C11	0.69	2.17	7	1
4:C:611:PCW:O11	4:C:611:PCW:H2	0.69	1.87	1	10
4:B:206:PCW:H212	4:B:207:PCW:H452	0.69	1.63	1	1
4:D:502:PCW:C41	4:D:508:PCW:H352	0.69	2.16	1	1
4:A:401:PCW:H381	4:D:502:PCW:H20	0.69	1.63	2	1
4:D:508:PCW:H132	4:D:508:PCW:H332	0.69	1.64	2	2
4:B:202:PCW:H422	4:B:202:PCW:C21	0.69	2.17	4	1
4:D:506:PCW:H422	5:D:513:17F:H47	0.69	1.62	7	2
4:B:203:PCW:C5	4:B:204:PCW:H341	0.69	2.17	6	1
4:A:404:PCW:H31	4:A:404:PCW:P	0.69	2.27	1	4
4:A:412:PCW:H31	4:C:624:PCW:C37	0.69	2.14	7	7
4:D:506:PCW:C3	4:D:506:PCW:O1P	0.69	2.40	1	7
4:A:405:PCW:C31	4:B:203:PCW:H61	0.69	2.17	2	1
4:A:412:PCW:H431	4:C:624:PCW:C48	0.69	2.17	2	2
4:C:616:PCW:H51	4:C:616:PCW:C2	0.69	2.18	5	3
4:C:619:PCW:O2P	4:C:620:PCW:H52	0.69	1.88	2	1
4:C:620:PCW:H181	4:C:620:PCW:C14	0.69	2.14	7	4
4:C:607:PCW:C4	4:C:624:PCW:H242	0.69	2.17	5	1
4:B:205:PCW:C5	5:B:214:17F:H10A	0.69	2.14	7	3
4:B:205:PCW:C14	4:B:207:PCW:H321	0.69	2.10	6	2
4:A:411:PCW:H411	4:A:411:PCW:H371	0.69	1.65	8	1
4:C:620:PCW:C20	4:C:621:PCW:H82	0.69	2.06	5	5
4:D:505:PCW:H11	4:D:505:PCW:O31	0.69	1.88	7	8
4:C:603:PCW:H62	4:D:516:PCW:P	0.69	2.27	2	5
4:A:406:PCW:H411	4:B:211:PCW:H381	0.69	1.62	7	1
4:A:415:PCW:H372	4:C:616:PCW:C42	0.69	2.17	7	1
4:B:205:PCW:H62	4:B:212:PCW:O2P	0.69	1.88	8	1
4:A:402:PCW:H283	4:A:413:PCW:H452	0.69	1.63	10	1
5:A:409:17F:C34	5:D:511:17F:H37	0.69	2.16	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:A:409:17F:H6	4:D:504:PCW:C34	0.69	2.09	1	1
4:A:411:PCW:H283	4:B:202:PCW:H483	0.69	1.65	1	1
4:C:605:PCW:H152	4:C:612:PCW:O2	0.69	1.87	6	5
4:B:202:PCW:H41	4:B:202:PCW:O11	0.69	1.86	1	5
4:D:502:PCW:H73	4:D:502:PCW:C2	0.69	2.17	5	5
5:D:514:17F:H61	5:D:514:17F:H30	0.69	1.63	5	2
4:A:408:PCW:H162	5:A:409:17F:C31	0.69	2.15	3	1
4:B:202:PCW:H141	4:D:504:PCW:C32	0.69	2.17	3	2
4:C:607:PCW:H241	5:C:629:17F:H30	0.69	1.61	4	1
4:A:408:PCW:H162	5:A:409:17F:C32	0.69	2.13	6	1
4:C:620:PCW:C14	5:B:215:17F:H4A	0.69	2.18	8	2
4:D:504:PCW:O31	4:D:504:PCW:H41	0.69	1.87	9	1
4:C:619:PCW:H121	5:C:632:17F:C17	0.69	2.18	10	1
4:C:623:PCW:H282	5:D:514:17F:H54	0.69	1.63	10	1
4:B:212:PCW:H412	5:D:514:17F:H33	0.69	1.63	10	1
4:D:505:PCW:H262	5:D:513:17F:C28	0.69	2.16	1	1
4:C:609:PCW:H132	4:C:609:PCW:H342	0.69	1.63	5	3
4:B:210:PCW:C27	4:B:211:PCW:H222	0.69	2.14	2	1
4:A:407:PCW:C43	4:B:211:PCW:H232	0.69	2.18	3	2
4:A:408:PCW:H181	4:A:408:PCW:C22	0.69	2.08	3	5
4:C:614:PCW:H211	5:C:632:17F:H38	0.69	1.65	5	3
4:B:204:PCW:C15	4:B:208:PCW:H361	0.69	2.18	7	2
4:C:607:PCW:H20	5:C:629:17F:H46	0.69	1.64	5	2
4:A:403:PCW:H483	4:B:209:PCW:H461	0.69	1.65	6	1
4:A:415:PCW:H451	4:D:515:PCW:H231	0.69	1.64	7	1
4:D:505:PCW:H281	4:D:509:PCW:H451	0.69	1.65	10	2
4:C:605:PCW:H40	4:C:618:PCW:H141	0.69	1.63	10	1
4:A:403:PCW:H212	4:A:403:PCW:C17	0.69	2.11	1	4
4:C:612:PCW:H141	4:C:618:PCW:C39	0.69	2.18	3	2
4:C:623:PCW:C46	4:C:624:PCW:H482	0.69	2.18	7	5
5:C:626:17F:C21	5:C:629:17F:H75	0.69	2.17	2	4
4:A:415:PCW:H432	4:D:515:PCW:C21	0.69	2.18	3	3
4:A:416:PCW:H19	5:C:630:17F:H57	0.69	1.64	2	2
4:C:604:PCW:C45	4:C:606:PCW:H181	0.69	2.15	7	7
4:D:505:PCW:H211	4:D:509:PCW:H472	0.69	1.63	3	2
4:D:509:PCW:H342	4:D:510:PCW:O2P	0.69	1.88	2	2
4:D:509:PCW:H82	4:D:510:PCW:O31	0.69	1.87	7	3
4:A:403:PCW:H321	4:B:209:PCW:H372	0.69	1.63	3	1
4:C:618:PCW:H481	5:D:511:17F:H74	0.69	1.63	3	1
5:C:626:17F:H36	5:C:629:17F:H74	0.69	1.64	4	3
4:B:206:PCW:H442	5:B:213:17F:H33	0.69	1.64	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:407:PCW:H462	5:C:631:17F:H52	0.69	1.64	4	1
5:C:627:17F:H10	5:B:215:17F:H49	0.69	1.63	9	3
4:B:206:PCW:H341	4:B:206:PCW:C6	0.69	2.17	6	1
4:A:415:PCW:H381	4:C:616:PCW:H481	0.69	1.64	8	1
4:B:202:PCW:H131	4:B:202:PCW:C38	0.69	2.18	8	1
4:D:503:PCW:C3	4:D:503:PCW:O1P	0.69	2.40	8	1
4:B:205:PCW:H182	4:B:207:PCW:C17	0.69	2.17	9	1
4:B:205:PCW:H352	4:B:207:PCW:C13	0.69	2.15	10	1
4:A:408:PCW:C31	4:A:408:PCW:H351	0.69	2.18	10	3
4:A:415:PCW:H52	4:A:415:PCW:O1P	0.69	1.88	9	3
4:C:602:PCW:C48	5:C:629:17F:H47	0.69	2.16	1	3
5:C:626:17F:H18A	5:C:629:17F:H55	0.69	1.65	2	4
5:C:626:17F:H40	5:C:629:17F:C42	0.69	2.18	9	2
4:D:507:PCW:H31	5:D:513:17F:C42	0.69	2.18	4	2
4:A:403:PCW:H332	4:B:209:PCW:H411	0.69	1.63	8	1
4:D:505:PCW:C22	4:D:510:PCW:H351	0.69	2.07	8	1
4:A:403:PCW:C8	4:B:209:PCW:H371	0.69	2.18	10	1
4:C:604:PCW:H411	5:C:627:17F:H36	0.69	1.65	10	1
4:A:408:PCW:H371	4:A:408:PCW:H31	0.69	1.65	1	1
4:C:619:PCW:H271	5:C:632:17F:H37	0.69	1.62	1	1
4:B:201:PCW:H331	4:B:209:PCW:O2	0.69	1.88	1	1
4:B:208:PCW:C22	4:B:208:PCW:C26	0.69	2.69	9	9
5:D:513:17F:H2	5:D:513:17F:O2	0.69	1.88	2	9
4:A:408:PCW:C12	5:A:409:17F:H71	0.69	2.17	2	1
4:C:623:PCW:H471	4:C:624:PCW:H482	0.69	1.64	2	4
4:B:206:PCW:H122	5:B:213:17F:O10	0.69	1.87	10	3
4:D:503:PCW:C5	4:D:506:PCW:H62	0.69	2.17	3	1
4:B:204:PCW:H411	5:D:514:17F:C10	0.69	2.18	5	1
4:C:612:PCW:H472	4:C:618:PCW:H231	0.69	1.62	6	3
4:A:412:PCW:H451	4:C:624:PCW:H481	0.69	1.64	7	1
4:B:206:PCW:H142	5:B:213:17F:C20	0.69	2.15	8	1
4:C:623:PCW:C28	5:D:514:17F:H54	0.69	2.18	10	1
4:A:412:PCW:H381	4:C:624:PCW:H431	0.68	1.65	1	1
4:D:508:PCW:H42	4:D:508:PCW:O11	0.68	1.88	1	1
4:D:516:PCW:O31	4:D:516:PCW:H11	0.68	1.89	4	10
4:A:408:PCW:H232	5:A:409:17F:C33	0.68	2.18	2	1
4:C:612:PCW:H31	4:C:612:PCW:O31	0.68	1.88	6	4
4:C:619:PCW:H121	5:C:632:17F:C4	0.68	2.18	3	2
4:A:404:PCW:H131	4:B:210:PCW:C16	0.68	2.18	5	1
4:C:610:PCW:H241	4:C:610:PCW:H452	0.68	1.62	8	1
4:A:407:PCW:H51	4:B:211:PCW:O2P	0.68	1.88	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:502:PCW:H441	5:D:512:17F:C25	0.68	2.18	9	1
4:C:604:PCW:H372	4:C:604:PCW:C41	0.68	2.18	2	7
4:B:201:PCW:C31	4:B:201:PCW:C35	0.68	2.70	5	10
4:D:503:PCW:H151	4:D:506:PCW:H342	0.68	1.64	1	1
4:D:507:PCW:C43	5:D:513:17F:H30	0.68	2.17	10	2
4:A:404:PCW:O1P	4:A:404:PCW:H51	0.68	1.89	9	7
4:D:502:PCW:H381	4:D:508:PCW:H361	0.68	1.65	2	1
4:A:414:PCW:H82	4:C:624:PCW:H331	0.68	1.64	8	5
2:B:37:GLU:HB3	3:D:369:VAL:HG23	0.68	1.63	3	5
4:C:610:PCW:H241	4:C:610:PCW:C45	0.68	2.17	8	1
4:B:212:PCW:H122	5:D:514:17F:O9	0.68	1.87	8	1
4:D:505:PCW:C15	4:D:510:PCW:H471	0.68	2.17	8	1
5:C:627:17F:H43	5:C:628:17F:H35	0.68	1.65	10	1
4:D:509:PCW:C8	4:D:510:PCW:H63	0.68	2.16	10	1
4:A:417:PCW:H452	4:C:622:PCW:C28	0.68	2.18	2	2
4:C:605:PCW:C26	4:C:612:PCW:H181	0.68	2.18	5	2
5:A:409:17F:H53	4:D:504:PCW:H471	0.68	1.64	5	1
4:A:411:PCW:H442	4:C:616:PCW:H242	0.68	1.65	6	1
4:A:411:PCW:H172	4:A:415:PCW:C41	0.68	2.18	7	1
4:C:610:PCW:H161	4:C:618:PCW:H151	0.68	1.65	10	1
4:B:211:PCW:H19	4:D:505:PCW:C43	0.68	2.17	10	1
4:A:417:PCW:H221	4:C:621:PCW:H231	0.68	1.65	1	4
5:C:628:17F:C39	5:B:215:17F:H39	0.68	2.18	1	1
4:A:408:PCW:H351	4:A:408:PCW:C31	0.68	2.18	7	7
4:C:608:PCW:C2	4:C:614:PCW:H61	0.68	2.14	5	2
4:B:204:PCW:C12	4:B:212:PCW:H172	0.68	2.18	8	2
4:C:613:PCW:C45	4:C:618:PCW:H222	0.68	2.19	4	2
4:A:406:PCW:H411	4:B:211:PCW:H171	0.68	1.63	6	1
4:A:417:PCW:H211	4:C:603:PCW:H162	0.68	1.63	4	2
4:C:612:PCW:H431	4:C:618:PCW:C39	0.68	2.19	6	4
4:C:617:PCW:O1P	4:C:625:PCW:H63	0.68	1.87	3	3
4:B:209:PCW:O11	4:B:209:PCW:H2	0.68	1.88	6	9
4:C:605:PCW:H39	4:C:610:PCW:C34	0.68	2.18	7	4
4:B:206:PCW:H452	5:B:213:17F:H76	0.68	1.64	2	1
4:C:616:PCW:O3P	4:C:616:PCW:H51	0.68	1.89	3	1
4:A:405:PCW:H171	4:D:508:PCW:H281	0.68	1.64	5	1
5:C:628:17F:H67	5:B:215:17F:C23	0.68	2.18	7	5
4:A:408:PCW:C34	5:A:409:17F:H57	0.68	2.13	6	1
4:A:415:PCW:H372	4:C:616:PCW:C41	0.68	2.18	7	1
4:C:602:PCW:H481	4:C:607:PCW:H231	0.68	1.64	7	1
4:B:211:PCW:H282	4:D:506:PCW:H261	0.68	1.65	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:B:213:17F:H37	5:B:213:17F:C42	0.68	2.19	7	1
5:A:409:17F:O5	4:B:202:PCW:H61	0.68	1.87	9	1
4:B:210:PCW:H19	4:B:210:PCW:H452	0.68	1.63	10	1
4:D:507:PCW:C20	5:D:513:17F:H31	0.68	2.18	9	2
4:C:612:PCW:O11	4:C:612:PCW:H2	0.68	1.89	5	9
4:D:501:PCW:C4	4:D:509:PCW:H331	0.68	2.18	5	2
4:D:510:PCW:O31	4:D:510:PCW:C4	0.68	2.42	7	7
4:D:509:PCW:H82	4:D:510:PCW:H41	0.68	1.64	3	1
4:A:414:PCW:C43	4:C:623:PCW:H462	0.68	2.18	4	2
4:B:203:PCW:H82	4:B:204:PCW:H351	0.68	1.66	6	1
4:A:408:PCW:H172	5:A:409:17F:H31	0.68	1.64	7	1
4:D:505:PCW:H82	4:D:509:PCW:H11	0.68	1.66	8	1
5:A:410:17F:H72	4:D:501:PCW:H272	0.68	1.66	9	1
5:C:628:17F:O6	5:C:628:17F:H2	0.68	1.88	9	1
4:B:212:PCW:H451	5:D:514:17F:H71	0.68	1.65	9	1
4:A:415:PCW:H451	4:D:515:PCW:C21	0.68	2.17	7	3
4:C:602:PCW:H462	5:C:626:17F:C36	0.68	2.18	9	4
4:C:621:PCW:H372	4:C:625:PCW:H211	0.68	1.65	3	3
4:B:202:PCW:C31	4:B:202:PCW:C35	0.68	2.71	9	8
4:C:602:PCW:H341	5:B:214:17F:H67	0.68	1.65	2	2
4:D:504:PCW:C22	4:D:504:PCW:C26	0.68	2.72	8	2
4:D:507:PCW:H19	5:D:513:17F:O10	0.68	1.89	2	1
4:C:616:PCW:H51	4:C:616:PCW:O31	0.68	1.89	3	1
4:A:401:PCW:H442	4:C:613:PCW:H242	0.68	1.64	4	2
4:C:602:PCW:H432	5:B:214:17F:H68	0.68	1.65	4	1
4:A:402:PCW:H251	4:A:413:PCW:H482	0.68	1.64	6	1
5:A:409:17F:H29	4:D:504:PCW:H461	0.68	1.64	6	1
4:A:407:PCW:C38	4:B:211:PCW:H161	0.68	2.19	7	2
5:B:213:17F:H63	4:D:505:PCW:H371	0.68	1.63	10	1
4:C:605:PCW:H482	4:C:618:PCW:H441	0.68	1.64	6	2
4:B:205:PCW:H2	4:B:205:PCW:O1P	0.68	1.89	10	10
4:A:403:PCW:H271	4:B:201:PCW:H172	0.68	1.65	3	1
4:A:401:PCW:C45	4:C:610:PCW:H271	0.68	2.16	4	1
4:A:405:PCW:O31	5:D:512:17F:H33	0.68	1.89	4	3
4:B:204:PCW:H481	5:D:512:17F:H48	0.68	1.65	5	1
4:D:507:PCW:H131	5:D:513:17F:H75	0.68	1.65	5	1
4:C:620:PCW:H171	5:C:631:17F:H5	0.68	1.65	8	1
4:B:204:PCW:H232	4:B:208:PCW:H242	0.68	1.63	10	1
4:C:606:PCW:H442	4:C:608:PCW:H12	0.68	1.63	1	2
4:C:607:PCW:C46	5:C:626:17F:H61	0.68	2.19	2	3
4:D:501:PCW:H211	5:D:511:17F:H19	0.68	1.65	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:508:PCW:C41	4:D:508:PCW:C37	0.68	2.69	10	3
4:A:415:PCW:C2	4:C:616:PCW:H411	0.68	2.19	2	3
4:C:607:PCW:H262	5:C:629:17F:H30	0.68	1.65	10	4
4:A:404:PCW:C11	4:A:407:PCW:H121	0.68	2.17	3	2
4:B:207:PCW:H82	5:B:213:17F:H1A	0.68	1.65	4	1
4:A:403:PCW:H73	4:A:406:PCW:H371	0.68	1.66	5	1
5:A:410:17F:H19A	4:D:502:PCW:H162	0.68	1.64	5	1
5:A:410:17F:C40	4:D:501:PCW:H272	0.68	2.19	9	1
4:B:202:PCW:H31	4:B:202:PCW:P	0.68	2.29	5	9
4:B:202:PCW:O31	4:B:202:PCW:H11	0.68	1.89	2	10
4:C:619:PCW:H372	4:C:619:PCW:C41	0.68	2.18	5	2
4:B:204:PCW:H421	5:D:512:17F:H60	0.68	1.64	2	1
4:B:210:PCW:H42	4:B:210:PCW:C32	0.68	2.19	2	5
4:C:620:PCW:H283	4:C:621:PCW:C6	0.68	2.18	3	2
4:A:415:PCW:H382	4:D:515:PCW:H181	0.68	1.64	4	1
4:A:416:PCW:H62	5:C:630:17F:O8	0.68	1.89	6	3
4:A:405:PCW:C17	4:D:508:PCW:H281	0.68	2.19	5	1
4:B:206:PCW:H412	5:B:213:17F:C11	0.68	2.16	5	1
4:D:502:PCW:C48	4:D:508:PCW:H471	0.68	2.16	6	1
4:C:614:PCW:H51	5:C:632:17F:H2	0.68	1.65	7	1
4:C:607:PCW:C26	5:C:629:17F:H65	0.68	2.19	9	1
4:A:401:PCW:H221	4:A:401:PCW:C18	0.67	2.18	9	8
4:A:407:PCW:C7	4:B:211:PCW:H372	0.67	2.19	5	3
4:B:205:PCW:C17	4:B:207:PCW:H342	0.67	2.17	5	2
4:B:208:PCW:O11	4:B:208:PCW:H51	0.67	1.88	2	3
4:D:505:PCW:H211	4:D:509:PCW:C47	0.67	2.19	3	2
4:A:407:PCW:H40	4:B:211:PCW:H231	0.67	1.64	6	2
4:C:612:PCW:H282	5:D:511:17F:H12	0.67	1.63	3	1
4:C:608:PCW:H241	4:C:614:PCW:H381	0.67	1.64	5	4
4:C:620:PCW:C42	5:B:215:17F:H73	0.67	2.20	4	1
4:B:204:PCW:C14	4:B:208:PCW:H362	0.67	2.19	6	1
4:D:504:PCW:H51	4:D:504:PCW:H341	0.67	1.64	6	1
4:C:603:PCW:H242	4:D:515:PCW:H351	0.67	1.65	7	1
4:A:405:PCW:C39	5:D:512:17F:H68	0.67	2.17	8	1
4:D:503:PCW:H142	4:D:505:PCW:H482	0.67	1.65	8	1
4:C:612:PCW:H352	4:C:618:PCW:H351	0.67	1.63	9	1
4:B:204:PCW:H452	4:D:502:PCW:H461	0.67	1.66	10	1
4:A:412:PCW:H412	4:C:624:PCW:H472	0.67	1.66	8	2
4:B:212:PCW:H411	4:B:212:PCW:H181	0.67	1.65	5	2
4:C:603:PCW:H73	4:D:516:PCW:O3P	0.67	1.88	4	2
1:C:512:ASP:HA	1:C:515:ARG:HD2	0.67	1.65	7	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:502:PCW:C36	4:D:508:PCW:H352	0.67	2.20	2	1
4:A:405:PCW:H361	4:B:203:PCW:C36	0.67	2.20	3	2
5:D:512:17F:C12	5:D:514:17F:H29	0.67	2.18	5	1
4:A:408:PCW:C16	5:A:409:17F:H34	0.67	2.19	6	1
4:C:615:PCW:C45	4:D:506:PCW:H472	0.67	2.19	6	3
4:B:206:PCW:H63	4:B:206:PCW:H322	0.67	1.64	6	1
4:B:206:PCW:C20	5:B:213:17F:H31	0.67	2.19	9	1
4:C:611:PCW:C33	4:C:617:PCW:H132	0.67	2.18	4	2
4:A:404:PCW:H32	4:B:210:PCW:C15	0.67	2.19	8	2
4:C:610:PCW:H222	4:C:618:PCW:C43	0.67	2.19	4	1
4:A:401:PCW:H332	4:D:502:PCW:C19	0.67	2.19	5	1
4:B:208:PCW:H162	5:B:214:17F:H11A	0.67	1.67	5	2
4:B:210:PCW:H42	4:B:210:PCW:H322	0.67	1.66	5	1
4:B:206:PCW:C17	4:B:207:PCW:H331	0.67	2.13	6	1
4:D:508:PCW:H221	4:D:508:PCW:H382	0.67	1.65	6	1
4:B:212:PCW:H361	5:B:213:17F:H11	0.67	1.66	9	1
5:C:628:17F:H36	5:C:628:17F:H65	0.67	1.66	6	5
3:D:382:LEU:HD21	3:D:428:VAL:HG21	0.67	1.65	1	3
5:D:513:17F:H6A	5:D:513:17F:O10	0.67	1.90	6	5
4:C:617:PCW:H412	5:C:631:17F:H50	0.67	1.66	2	1
4:C:622:PCW:C23	4:D:501:PCW:H483	0.67	2.18	2	1
5:C:632:17F:H4	5:C:632:17F:O10	0.67	1.87	9	4
4:A:402:PCW:C36	4:B:210:PCW:H441	0.67	2.19	3	2
4:B:206:PCW:O2P	4:B:206:PCW:C3	0.67	2.42	3	2
4:D:506:PCW:H40	4:D:516:PCW:C25	0.67	2.17	3	2
4:C:610:PCW:H221	4:C:610:PCW:C43	0.67	2.20	9	2
5:A:409:17F:C1	2:B:172:LYS:HB3	0.67	2.19	9	1
4:D:501:PCW:C22	5:D:511:17F:H56	0.67	2.16	9	1
4:D:508:PCW:H171	5:D:512:17F:O10	0.67	1.90	10	2
4:C:625:PCW:H41	4:C:625:PCW:C2	0.67	2.17	9	2
4:B:206:PCW:P	4:B:206:PCW:H31	0.67	2.30	9	3
4:D:501:PCW:H211	5:D:511:17F:C19	0.67	2.20	1	1
4:C:605:PCW:C32	4:C:612:PCW:H62	0.67	2.19	3	5
4:C:619:PCW:O1P	4:C:620:PCW:H63	0.67	1.90	3	1
4:C:623:PCW:H151	4:C:623:PCW:H19	0.67	1.64	8	1
4:A:404:PCW:O2P	4:B:210:PCW:H361	0.67	1.88	9	1
4:D:508:PCW:O1P	4:D:508:PCW:H31	0.67	1.90	9	2
5:D:514:17F:H4	5:D:514:17F:C2	0.67	2.20	9	1
4:A:417:PCW:H281	4:D:509:PCW:H282	0.67	1.67	10	1
4:A:402:PCW:O11	4:A:402:PCW:H2	0.67	1.90	10	9
4:C:607:PCW:H63	4:C:624:PCW:C24	0.67	2.19	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:615:PCW:H39	4:C:617:PCW:C15	0.67	2.20	1	2
4:A:412:PCW:H12	4:C:624:PCW:C35	0.67	2.18	2	2
4:D:506:PCW:O1P	4:D:506:PCW:C3	0.67	2.42	3	3
4:A:402:PCW:H382	4:B:210:PCW:H461	0.67	1.67	4	1
4:D:505:PCW:C20	4:D:510:PCW:H351	0.67	2.19	5	1
4:A:403:PCW:H82	4:B:209:PCW:O31	0.67	1.89	7	1
4:A:407:PCW:H411	4:A:407:PCW:H283	0.67	1.65	7	1
2:B:37:GLU:HB2	3:D:369:VAL:CG2	0.67	2.20	8	1
4:C:621:PCW:H362	5:C:627:17F:C42	0.67	2.12	4	4
4:B:204:PCW:H411	5:D:514:17F:C8	0.67	2.20	1	1
4:B:205:PCW:C18	4:B:207:PCW:H151	0.67	2.20	5	3
4:A:413:PCW:H411	4:C:611:PCW:C18	0.67	2.20	3	1
4:C:618:PCW:H481	5:D:511:17F:C41	0.67	2.19	3	1
4:B:207:PCW:H371	4:B:209:PCW:H161	0.67	1.67	6	1
4:B:210:PCW:H282	4:D:503:PCW:H181	0.67	1.67	6	1
4:C:606:PCW:C16	5:C:627:17F:H30	0.67	2.20	7	3
5:D:512:17F:H30	5:D:514:17F:H29	0.67	1.66	7	1
4:C:625:PCW:O31	4:C:625:PCW:H63	0.67	1.90	8	1
4:A:405:PCW:H272	4:A:405:PCW:H482	0.67	1.64	5	5
4:B:211:PCW:C20	4:D:505:PCW:H451	0.67	2.19	1	2
1:C:561:LYS:HA	1:C:561:LYS:HE3	0.67	1.66	2	2
5:D:513:17F:H65	5:D:513:17F:C12	0.67	2.20	7	2
4:A:401:PCW:H483	4:C:613:PCW:H471	0.67	1.67	10	2
4:C:605:PCW:H212	4:C:612:PCW:H382	0.67	1.67	6	1
4:B:204:PCW:H331	4:B:208:PCW:H332	0.67	1.65	6	1
4:D:502:PCW:H451	4:D:508:PCW:H281	0.67	1.67	10	1
4:C:609:PCW:H172	5:C:631:17F:H61	0.67	1.65	1	1
4:A:412:PCW:C41	4:C:624:PCW:H472	0.67	2.20	2	3
4:C:605:PCW:P	4:C:612:PCW:H52	0.67	2.30	6	2
4:C:619:PCW:H283	5:C:632:17F:C2X	0.67	2.19	3	5
4:C:621:PCW:H341	4:D:516:PCW:C44	0.67	2.20	3	5
4:C:622:PCW:H382	4:C:623:PCW:C17	0.67	2.20	5	3
4:A:411:PCW:H61	5:C:630:17F:C3	0.67	2.21	5	1
4:C:602:PCW:H481	5:C:629:17F:H44	0.67	1.66	9	1
4:B:212:PCW:C5	5:B:214:17F:H9	0.67	2.20	9	1
4:B:203:PCW:O2P	4:B:203:PCW:H51	0.66	1.91	9	5
4:D:503:PCW:H271	4:D:507:PCW:H40	0.66	1.64	1	1
4:D:509:PCW:C6	4:D:510:PCW:H341	0.66	2.20	1	1
4:C:612:PCW:C48	4:C:618:PCW:H431	0.66	2.20	2	2
5:D:512:17F:H2	5:D:512:17F:O2	0.66	1.89	7	9
4:A:408:PCW:H221	4:A:408:PCW:C18	0.66	2.16	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:601:PCW:C42	4:C:601:PCW:C46	0.66	2.71	3	4
4:C:606:PCW:H62	4:C:624:PCW:H19	0.66	1.68	5	1
4:A:403:PCW:H51	4:B:209:PCW:H352	0.66	1.67	8	1
4:B:202:PCW:C23	4:B:202:PCW:H182	0.66	2.21	8	1
4:D:510:PCW:O3P	4:D:510:PCW:O31	0.66	2.13	3	5
4:C:605:PCW:H61	5:C:630:17F:O4	0.66	1.90	2	1
4:B:204:PCW:H332	4:B:208:PCW:H322	0.66	1.66	3	2
4:B:204:PCW:C39	5:D:514:17F:H10A	0.66	2.20	3	1
4:B:203:PCW:H31	4:B:203:PCW:O1P	0.66	1.90	7	6
4:B:212:PCW:C44	4:B:212:PCW:H222	0.66	2.20	4	1
4:A:416:PCW:H381	4:C:616:PCW:C15	0.66	2.19	5	2
4:C:620:PCW:C19	5:C:631:17F:H19A	0.66	2.20	5	1
4:B:210:PCW:H322	4:B:210:PCW:C7	0.66	2.21	5	1
4:D:508:PCW:H231	4:D:508:PCW:H382	0.66	1.67	5	1
4:C:612:PCW:H282	5:D:511:17F:H36	0.66	1.66	6	1
4:B:205:PCW:C16	4:B:206:PCW:H222	0.66	2.20	6	1
4:B:207:PCW:H322	4:B:207:PCW:H63	0.66	1.65	10	1
4:A:415:PCW:C48	4:C:617:PCW:H281	0.66	2.20	5	2
4:B:201:PCW:H411	4:B:207:PCW:H381	0.66	1.67	1	1
2:B:22:GLN:HG3	2:B:149:ARG:HG3	0.66	1.66	3	3
4:B:208:PCW:O11	4:B:208:PCW:H2	0.66	1.91	9	5
4:C:625:PCW:O31	4:C:625:PCW:H52	0.66	1.89	5	1
5:D:513:17F:H11A	5:D:513:17F:H69	0.66	1.66	5	1
4:B:203:PCW:H272	4:B:204:PCW:H171	0.66	1.66	6	1
4:A:407:PCW:H371	4:B:211:PCW:H141	0.66	1.67	8	1
4:A:407:PCW:C39	4:B:211:PCW:H161	0.66	2.21	10	2
4:D:508:PCW:O31	4:D:508:PCW:H11	0.66	1.88	9	3
4:A:411:PCW:O1P	4:A:411:PCW:H52	0.66	1.89	9	7
4:C:604:PCW:C3	4:C:606:PCW:H82	0.66	2.20	1	1
4:C:603:PCW:H62	4:D:516:PCW:O3P	0.66	1.90	5	3
4:C:604:PCW:H482	4:C:624:PCW:C27	0.66	2.20	5	6
4:B:204:PCW:H161	4:B:208:PCW:H222	0.66	1.66	3	1
4:B:206:PCW:H372	4:B:206:PCW:C41	0.66	2.20	4	3
4:B:212:PCW:C20	4:B:212:PCW:C24	0.66	2.74	9	4
4:A:404:PCW:O4P	4:A:407:PCW:H32	0.66	1.90	5	1
5:A:409:17F:C33	4:D:504:PCW:H432	0.66	2.14	5	1
5:B:213:17F:H66	4:D:505:PCW:H40	0.66	1.65	5	1
4:C:623:PCW:H432	4:C:624:PCW:H441	0.66	1.67	6	1
4:C:602:PCW:H172	4:C:602:PCW:C22	0.66	2.20	1	5
4:B:210:PCW:C26	4:D:503:PCW:H252	0.66	2.14	2	1
4:C:622:PCW:H131	4:C:622:PCW:C37	0.66	2.19	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:510:PCW:H41	4:D:510:PCW:O31	0.66	1.91	3	1
4:A:411:PCW:H442	4:C:616:PCW:H212	0.66	1.65	5	3
4:C:606:PCW:H432	5:B:215:17F:H55	0.66	1.64	4	1
4:D:507:PCW:H451	5:D:513:17F:C31	0.66	2.20	8	2
4:C:622:PCW:H382	4:C:623:PCW:C18	0.66	2.20	5	1
4:B:208:PCW:H282	5:D:512:17F:H78	0.66	1.65	6	1
4:C:604:PCW:C2	4:C:606:PCW:H82	0.66	2.19	1	2
4:D:508:PCW:O11	4:D:508:PCW:H62	0.66	1.89	1	1
5:D:512:17F:H41	5:D:512:17F:H12A	0.66	1.66	1	5
5:A:409:17F:C3	4:B:202:PCW:H61	0.66	2.20	2	1
4:B:208:PCW:O31	4:B:208:PCW:H12	0.66	1.89	5	7
4:D:506:PCW:O1P	4:D:506:PCW:H32	0.66	1.89	6	5
4:A:412:PCW:H451	4:C:623:PCW:C48	0.66	2.20	4	2
4:B:206:PCW:H39	4:D:505:PCW:H122	0.66	1.66	3	1
4:A:401:PCW:H472	4:C:610:PCW:H232	0.66	1.66	5	1
4:A:401:PCW:H452	4:C:610:PCW:H251	0.66	1.67	10	1
4:A:407:PCW:H371	4:B:210:PCW:C27	0.66	2.16	1	1
4:B:206:PCW:O31	4:B:206:PCW:H11	0.66	1.91	3	10
4:B:211:PCW:H352	4:B:211:PCW:C31	0.66	2.20	2	10
5:B:214:17F:O8	5:B:214:17F:H5	0.66	1.91	10	5
4:D:502:PCW:H152	4:D:508:PCW:H39	0.66	1.67	1	3
4:D:504:PCW:C31	4:D:504:PCW:C35	0.66	2.73	1	6
4:A:407:PCW:H82	4:B:211:PCW:C2	0.66	2.20	2	2
4:A:417:PCW:H431	4:C:622:PCW:H281	0.66	1.65	2	1
4:A:413:PCW:H321	4:C:611:PCW:H121	0.66	1.67	3	1
4:C:608:PCW:C39	4:C:614:PCW:H421	0.66	2.21	3	2
4:D:503:PCW:C26	4:D:507:PCW:H472	0.66	2.21	3	1
5:A:410:17F:H71	4:D:501:PCW:H242	0.66	1.66	5	1
4:C:621:PCW:H372	4:C:625:PCW:H242	0.66	1.67	7	3
5:C:627:17F:H51	5:C:628:17F:H78	0.66	1.66	5	1
4:B:202:PCW:H162	4:D:504:PCW:C32	0.66	2.21	8	1
4:C:603:PCW:H261	4:D:515:PCW:H142	0.66	1.65	3	6
4:D:501:PCW:C26	5:D:511:17F:H64	0.66	2.18	1	1
4:D:509:PCW:H2	5:D:514:17F:H58	0.66	1.68	1	1
5:D:514:17F:O2	5:D:514:17F:N1	0.66	2.26	10	10
4:A:415:PCW:H31	4:C:616:PCW:C42	0.66	2.21	9	6
1:C:462:LYS:HB3	4:C:602:PCW:H281	0.66	1.67	6	1
4:A:403:PCW:O11	4:B:201:PCW:H142	0.66	1.90	8	1
4:A:403:PCW:H212	4:B:201:PCW:H162	0.66	1.66	10	1
4:C:609:PCW:C20	4:C:609:PCW:C24	0.66	2.73	3	10
4:D:503:PCW:H362	4:D:507:PCW:H321	0.66	1.68	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:403:PCW:C16	4:A:403:PCW:H231	0.66	2.21	3	4
4:A:405:PCW:O2P	4:B:203:PCW:H63	0.66	1.91	2	1
4:D:516:PCW:C32	4:D:516:PCW:H52	0.66	2.21	4	2
4:A:404:PCW:H331	4:A:407:PCW:H151	0.66	1.66	3	1
4:B:203:PCW:C23	4:B:204:PCW:H151	0.66	2.21	6	2
4:C:607:PCW:H63	4:C:624:PCW:H283	0.66	1.68	7	1
4:B:207:PCW:H63	5:B:213:17F:O4	0.66	1.91	9	1
4:B:212:PCW:C42	5:D:514:17F:H10	0.66	2.18	9	1
4:D:508:PCW:H19	5:D:512:17F:C19	0.66	2.11	9	2
4:C:613:PCW:H51	4:C:623:PCW:O1P	0.66	1.91	1	3
4:B:204:PCW:H451	4:D:502:PCW:H442	0.66	1.68	1	1
4:A:402:PCW:C27	4:A:413:PCW:H241	0.66	2.21	2	2
4:C:620:PCW:H283	4:C:621:PCW:C8	0.66	2.21	2	1
4:B:205:PCW:H161	4:B:207:PCW:H171	0.66	1.66	4	1
5:A:410:17F:H56	4:D:502:PCW:H151	0.66	1.68	5	1
4:C:607:PCW:H42	4:C:624:PCW:C22	0.66	2.21	5	1
4:A:417:PCW:H141	4:C:603:PCW:H411	0.66	1.66	6	1
4:C:604:PCW:H172	4:C:604:PCW:H211	0.66	1.64	6	1
4:B:205:PCW:H19	4:B:206:PCW:C24	0.66	2.21	6	1
5:C:626:17F:H36	5:C:629:17F:H73	0.66	1.68	7	1
4:A:403:PCW:C21	4:B:201:PCW:H162	0.66	2.19	8	2
4:B:205:PCW:H161	4:B:206:PCW:H182	0.66	1.66	8	1
4:C:614:PCW:H63	4:C:614:PCW:O31	0.66	1.91	9	1
4:D:509:PCW:H231	5:D:514:17F:H65	0.66	1.66	10	1
4:C:611:PCW:H321	4:C:617:PCW:C13	0.65	2.18	2	4
4:C:612:PCW:H272	5:D:511:17F:H46	0.65	1.68	1	2
5:C:632:17F:C30	4:B:207:PCW:H161	0.65	2.20	6	2
4:B:203:PCW:H242	4:B:208:PCW:C12	0.65	2.21	7	1
4:D:506:PCW:H321	4:D:507:PCW:C38	0.65	2.21	10	1
4:C:620:PCW:C21	5:C:631:17F:H31	0.65	2.20	1	6
4:D:510:PCW:H421	4:D:516:PCW:H262	0.65	1.66	8	2
4:C:607:PCW:H262	5:C:629:17F:C2X	0.65	2.20	2	6
5:C:627:17F:C7	5:C:627:17F:C18	0.65	2.69	8	2
4:A:416:PCW:P	4:C:616:PCW:H82	0.65	2.31	4	3
4:A:405:PCW:H332	4:B:203:PCW:H361	0.65	1.68	5	1
4:A:408:PCW:H212	4:A:408:PCW:C17	0.65	2.19	5	1
5:B:213:17F:H70	4:D:505:PCW:H422	0.65	1.67	5	1
4:A:407:PCW:H412	4:B:211:PCW:C44	0.65	2.21	7	1
5:D:514:17F:H48	5:D:514:17F:C42	0.65	2.21	7	1
4:B:208:PCW:H41	4:B:208:PCW:O31	0.65	1.90	8	1
5:A:410:17F:H75	5:D:511:17F:H64	0.65	1.67	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:212:PCW:H442	5:D:514:17F:C35	0.65	2.13	10	1
4:A:401:PCW:C47	4:C:610:PCW:H271	0.65	2.22	9	2
2:B:16:LYS:HB3	6:B:216:GNP:O1G	0.65	1.92	6	3
2:B:84:ILE:HD12	2:B:123:ARG:HG3	0.65	1.67	2	4
4:D:502:PCW:H361	4:D:508:PCW:H352	0.65	1.67	2	1
4:A:407:PCW:H422	4:B:211:PCW:C46	0.65	2.21	3	2
4:A:401:PCW:H73	4:D:508:PCW:O31	0.65	1.91	8	2
4:A:415:PCW:H11	4:C:616:PCW:C39	0.65	2.20	7	1
4:D:501:PCW:C47	4:D:509:PCW:H232	0.65	2.21	7	1
4:C:612:PCW:C25	5:D:511:17F:H47	0.65	2.21	9	2
4:C:604:PCW:C48	4:C:624:PCW:H282	0.65	2.20	10	4
5:C:627:17F:H47	5:C:628:17F:C22	0.65	2.21	10	4
1:A:279:LEU:HD22	1:C:495:LYS:HE3	0.65	1.68	10	7
4:A:405:PCW:H352	5:D:512:17F:H63	0.65	1.67	2	1
4:C:605:PCW:H231	4:C:612:PCW:H381	0.65	1.66	2	1
4:A:402:PCW:H281	1:C:558:LEU:HD21	0.65	1.68	6	1
4:C:617:PCW:H352	4:C:625:PCW:H341	0.65	1.68	8	1
4:C:617:PCW:P	4:C:625:PCW:H52	0.65	2.32	9	1
1:A:275:LYS:O	1:A:279:LEU:HG	0.65	1.91	4	10
4:A:405:PCW:H2	5:D:512:17F:C1Y	0.65	2.21	1	5
4:C:611:PCW:C21	4:C:611:PCW:C17	0.65	2.73	6	2
4:C:613:PCW:C46	4:C:613:PCW:C42	0.65	2.69	2	8
4:D:505:PCW:H211	4:D:510:PCW:H412	0.65	1.67	1	1
4:C:612:PCW:O31	4:C:612:PCW:H12	0.65	1.92	6	4
4:C:614:PCW:H222	4:B:207:PCW:H272	0.65	1.68	2	1
5:C:626:17F:C19	5:C:626:17F:C31	0.65	2.74	4	8
4:A:402:PCW:C23	4:A:413:PCW:H262	0.65	2.11	7	2
4:A:414:PCW:H63	4:C:624:PCW:H2	0.65	1.67	7	4
4:B:207:PCW:C8	5:B:213:17F:H1A	0.65	2.22	4	1
4:B:203:PCW:H231	4:B:204:PCW:C14	0.65	2.21	6	1
4:A:403:PCW:H231	4:A:403:PCW:C16	0.65	2.21	7	1
4:D:505:PCW:H381	4:D:506:PCW:H142	0.65	1.68	9	1
4:A:402:PCW:H241	4:A:413:PCW:H461	0.65	1.69	1	1
4:A:408:PCW:C18	5:A:409:17F:H20A	0.65	2.12	1	1
4:A:408:PCW:H321	5:A:409:17F:H19A	0.65	1.67	1	3
4:A:412:PCW:C43	4:C:624:PCW:H472	0.65	2.20	10	4
3:D:362:LEU:HB3	3:D:363:PRO:HD2	0.65	1.67	4	7
4:D:503:PCW:H372	4:D:507:PCW:O2P	0.65	1.91	1	1
4:B:206:PCW:H63	4:B:206:PCW:C13	0.65	2.22	2	1
4:B:208:PCW:C8	5:B:214:17F:H19A	0.65	2.22	2	2
4:C:620:PCW:H441	5:B:215:17F:H73	0.65	1.68	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:204:PCW:H481	5:D:512:17F:H44	0.65	1.69	6	1
4:A:408:PCW:C17	5:A:409:17F:H31	0.65	2.22	7	1
4:B:203:PCW:H31	4:B:203:PCW:H42	0.65	1.68	7	1
4:D:507:PCW:H451	5:D:513:17F:C1Z	0.65	2.22	8	1
4:C:614:PCW:H181	5:C:632:17F:H12	0.65	1.69	9	1
4:B:204:PCW:H412	5:D:514:17F:H8	0.65	1.68	1	1
4:D:503:PCW:H172	4:D:507:PCW:H40	0.65	1.68	3	2
4:A:406:PCW:H451	4:B:211:PCW:H182	0.65	1.69	3	1
4:D:501:PCW:H39	4:D:509:PCW:C44	0.65	2.15	7	2
4:D:502:PCW:H462	5:D:512:17F:C8	0.65	2.22	3	1
4:B:203:PCW:H252	4:B:204:PCW:H171	0.65	1.68	4	2
4:D:505:PCW:H361	4:D:506:PCW:C14	0.65	2.22	1	1
4:A:403:PCW:O2	4:A:403:PCW:H342	0.65	1.91	5	3
4:C:619:PCW:H412	4:C:619:PCW:C37	0.65	2.14	5	4
4:C:622:PCW:H39	4:C:622:PCW:H131	0.65	1.69	2	2
4:B:206:PCW:H40	5:B:213:17F:H75	0.65	1.69	2	2
4:A:403:PCW:C31	4:B:209:PCW:H352	0.65	2.22	3	1
4:A:415:PCW:H362	4:C:616:PCW:C39	0.65	2.22	3	1
4:A:408:PCW:H351	4:A:408:PCW:O3	0.65	1.91	10	2
4:C:620:PCW:C26	4:C:621:PCW:H61	0.65	2.21	5	1
4:C:610:PCW:O2P	4:C:618:PCW:H41	0.65	1.92	6	2
4:D:505:PCW:H341	4:D:506:PCW:C11	0.65	2.22	7	2
4:B:205:PCW:C18	4:B:207:PCW:H172	0.65	2.22	9	1
4:A:416:PCW:H372	4:C:616:PCW:C15	0.65	2.22	10	1
1:C:462:LYS:HD2	4:C:602:PCW:H281	0.65	1.68	10	1
4:C:610:PCW:H242	4:C:618:PCW:C48	0.65	2.21	10	1
5:C:626:17F:H78	5:B:214:17F:H51	0.65	1.69	10	1
4:C:619:PCW:C12	5:C:632:17F:H4A	0.65	2.16	9	3
4:C:621:PCW:H341	4:D:516:PCW:H422	0.65	1.69	3	2
4:B:206:PCW:H351	4:D:505:PCW:H332	0.65	1.67	4	2
4:A:402:PCW:H271	4:A:413:PCW:H241	0.65	1.69	8	1
4:D:501:PCW:H73	5:D:514:17F:C33	0.65	2.21	8	1
1:A:363:LYS:HA	1:A:367:ALA:HB3	0.65	1.68	8	9
4:A:408:PCW:H321	5:A:409:17F:C1Y	0.65	2.22	2	2
4:C:605:PCW:C48	4:C:618:PCW:H441	0.65	2.21	6	2
4:C:612:PCW:O31	4:C:612:PCW:H31	0.65	1.91	8	6
4:C:611:PCW:C17	4:C:611:PCW:C21	0.65	2.59	4	5
4:C:614:PCW:C20	5:C:632:17F:H38	0.65	2.22	6	4
4:A:413:PCW:H422	4:C:611:PCW:H212	0.65	1.68	6	2
4:A:413:PCW:C40	4:C:611:PCW:H231	0.65	2.22	4	2
5:A:410:17F:H53	4:C:605:PCW:C28	0.65	2.20	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:606:PCW:H331	4:C:607:PCW:C7	0.65	2.22	5	1
4:A:413:PCW:H431	4:C:611:PCW:C15	0.65	2.22	9	1
4:A:402:PCW:P	4:D:507:PCW:H171	0.65	2.32	10	1
4:C:605:PCW:H472	4:C:618:PCW:H442	0.65	1.69	10	1
4:C:617:PCW:H241	4:D:506:PCW:H432	0.65	1.69	10	1
4:A:401:PCW:H2	4:A:401:PCW:O2P	0.64	1.92	8	5
5:A:409:17F:O1	5:A:409:17F:C2	0.64	2.44	3	9
4:A:416:PCW:C6	5:C:630:17F:H4	0.64	2.22	3	3
5:C:626:17F:C2X	5:C:629:17F:H75	0.64	2.22	5	5
4:D:506:PCW:C42	4:D:506:PCW:C46	0.64	2.73	1	5
4:D:505:PCW:H251	4:D:509:PCW:H471	0.64	1.67	2	1
4:D:510:PCW:O31	4:D:510:PCW:O3P	0.64	2.15	7	4
4:A:413:PCW:C37	4:C:611:PCW:H182	0.64	2.22	3	1
4:B:208:PCW:H412	4:B:208:PCW:H281	0.64	1.67	3	1
4:A:403:PCW:H63	4:A:403:PCW:C31	0.64	2.23	4	1
4:D:504:PCW:O1P	4:D:507:PCW:H52	0.64	1.91	6	1
4:C:620:PCW:C28	4:C:621:PCW:H61	0.64	2.22	8	1
4:D:506:PCW:H421	4:D:516:PCW:H251	0.64	1.68	9	1
1:A:231:ASN:HA	1:A:234:LYS:HD2	0.64	1.69	3	6
4:A:416:PCW:H61	5:C:630:17F:C4	0.64	2.22	3	4
4:B:201:PCW:O2P	4:B:209:PCW:H41	0.64	1.92	1	1
4:D:503:PCW:H132	4:D:506:PCW:H332	0.64	1.67	1	1
4:D:503:PCW:O11	4:D:503:PCW:H2	0.64	1.89	10	9
4:C:623:PCW:H471	4:C:624:PCW:C48	0.64	2.22	2	4
4:B:205:PCW:C7	5:B:213:17F:H6	0.64	2.21	2	1
4:B:208:PCW:C43	4:B:208:PCW:C47	0.64	2.70	6	4
5:A:410:17F:H72	4:D:501:PCW:C25	0.64	2.13	3	1
4:C:606:PCW:H2	4:C:606:PCW:H42	0.64	1.68	3	1
4:C:612:PCW:C28	5:D:511:17F:H12	0.64	2.21	3	1
4:C:615:PCW:H341	4:D:516:PCW:C34	0.64	2.18	7	4
4:C:617:PCW:H412	5:C:631:17F:C26	0.64	2.19	5	2
4:A:403:PCW:H171	4:A:403:PCW:H221	0.64	1.69	6	1
4:A:407:PCW:C42	4:B:211:PCW:H462	0.64	2.22	6	1
4:C:604:PCW:C36	5:C:627:17F:H36	0.64	2.22	6	1
4:B:207:PCW:C35	4:B:209:PCW:H141	0.64	2.21	6	1
4:B:208:PCW:C28	5:D:512:17F:H78	0.64	2.23	6	1
4:B:210:PCW:H11	4:D:503:PCW:H122	0.64	1.69	6	1
4:A:414:PCW:H39	4:C:623:PCW:H422	0.64	1.69	7	1
4:D:515:PCW:H51	4:D:516:PCW:H73	0.64	1.69	7	1
4:B:208:PCW:H121	5:B:214:17F:H18	0.64	1.68	9	1
4:A:404:PCW:C8	4:A:407:PCW:H11	0.64	2.20	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:414:PCW:H381	4:C:623:PCW:H262	0.64	1.69	4	3
4:C:606:PCW:H211	5:B:215:17F:H52	0.64	1.68	1	1
5:C:627:17F:H70	5:C:628:17F:H62	0.64	1.67	2	2
2:B:78:PHE:HB2	2:B:111:MET:HG2	0.64	1.67	6	5
4:D:504:PCW:O31	4:D:504:PCW:O3	0.64	2.14	6	9
4:D:508:PCW:H221	4:D:508:PCW:C36	0.64	2.16	2	2
4:A:403:PCW:O3	4:B:209:PCW:H331	0.64	1.91	3	1
4:C:607:PCW:H461	5:C:626:17F:H60	0.64	1.69	8	2
4:D:506:PCW:H422	5:D:513:17F:H48	0.64	1.70	3	1
4:C:606:PCW:H51	4:C:606:PCW:O11	0.64	1.91	6	1
4:C:624:PCW:H222	4:C:624:PCW:C26	0.64	2.21	7	1
4:B:211:PCW:H251	4:D:503:PCW:H231	0.64	1.70	8	1
4:C:605:PCW:H482	4:C:618:PCW:H471	0.64	1.68	9	1
5:B:213:17F:H37	4:D:505:PCW:H142	0.64	1.67	9	1
4:D:502:PCW:H421	4:D:508:PCW:H221	0.64	1.68	9	1
4:D:515:PCW:H82	4:D:516:PCW:C7	0.64	2.22	9	2
4:A:417:PCW:C6	4:A:417:PCW:O4P	0.64	2.46	2	8
4:D:506:PCW:O1P	4:D:506:PCW:H31	0.64	1.93	1	3
4:C:616:PCW:C27	4:C:616:PCW:C23	0.64	2.75	10	9
5:C:630:17F:C32	5:C:630:17F:C36	0.64	2.69	2	1
4:B:208:PCW:P	4:B:208:PCW:C3	0.64	2.86	9	8
4:A:402:PCW:H272	4:A:413:PCW:C24	0.64	2.23	3	1
4:C:612:PCW:C19	5:D:511:17F:H47	0.64	2.23	3	1
4:C:613:PCW:H82	4:C:623:PCW:O1P	0.64	1.93	8	2
4:B:203:PCW:H232	4:B:208:PCW:C8	0.64	2.23	3	1
4:C:604:PCW:H251	5:D:514:17F:H75	0.64	1.68	5	1
2:B:36:ILE:HD11	3:D:371:ASN:HB2	0.64	1.68	5	3
4:C:604:PCW:C21	4:D:509:PCW:H283	0.64	2.18	7	1
4:C:617:PCW:H341	5:C:631:17F:H36	0.64	1.70	8	3
4:A:408:PCW:C14	4:A:408:PCW:C18	0.64	2.75	8	1
4:A:411:PCW:H371	4:A:411:PCW:C41	0.64	2.23	8	1
4:C:614:PCW:H121	5:C:632:17F:O7	0.64	1.92	8	2
4:B:204:PCW:C20	4:B:208:PCW:H371	0.64	2.23	8	1
4:B:205:PCW:H171	4:B:205:PCW:H212	0.64	1.67	8	1
4:B:211:PCW:H171	4:D:505:PCW:H432	0.64	1.70	8	1
4:C:613:PCW:H51	4:C:623:PCW:O31	0.64	1.91	1	1
4:A:414:PCW:H431	4:C:623:PCW:H461	0.64	1.68	7	5
4:A:415:PCW:H372	4:C:616:PCW:H432	0.64	1.69	3	1
4:B:202:PCW:H472	4:D:504:PCW:H271	0.64	1.69	3	1
4:C:601:PCW:C47	4:C:601:PCW:C43	0.64	2.75	4	1
4:C:605:PCW:H272	4:C:612:PCW:H412	0.64	1.69	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:606:PCW:O11	4:C:606:PCW:H63	0.64	1.91	6	1
4:C:615:PCW:H451	4:D:506:PCW:C47	0.64	2.23	7	2
4:C:605:PCW:H181	4:C:612:PCW:H362	0.64	1.67	10	2
4:D:505:PCW:H422	4:D:506:PCW:C16	0.64	2.22	9	2
4:B:206:PCW:H251	4:B:206:PCW:C48	0.64	2.22	9	1
5:C:626:17F:C31	5:C:626:17F:C19	0.64	2.75	5	2
4:C:623:PCW:H432	4:C:624:PCW:H432	0.64	1.70	3	2
4:B:201:PCW:H331	4:B:209:PCW:C3	0.64	2.23	3	1
4:A:401:PCW:H381	4:D:502:PCW:C23	0.64	2.21	4	3
4:C:615:PCW:C33	4:D:516:PCW:H341	0.64	2.22	4	2
4:A:411:PCW:H472	4:C:616:PCW:H252	0.64	1.69	8	3
4:A:403:PCW:H121	4:B:209:PCW:H331	0.64	1.68	6	1
4:C:605:PCW:H442	4:C:618:PCW:H451	0.64	1.69	6	1
4:B:212:PCW:C37	5:B:213:17F:H29	0.64	2.17	9	1
4:C:605:PCW:H231	4:C:612:PCW:H382	0.64	1.70	5	3
4:D:501:PCW:H222	5:D:511:17F:H57	0.64	1.69	1	1
4:D:502:PCW:H381	4:D:508:PCW:C35	0.64	2.23	1	1
4:A:404:PCW:H242	4:B:210:PCW:C23	0.64	2.16	2	2
4:A:417:PCW:H282	4:C:621:PCW:H262	0.64	1.70	6	2
5:C:626:17F:C18	5:C:629:17F:H55	0.64	2.22	2	3
4:B:205:PCW:H11	5:B:214:17F:H29	0.64	1.67	3	1
4:D:502:PCW:H472	4:D:508:PCW:H271	0.64	1.68	4	1
4:D:507:PCW:H271	4:D:507:PCW:C46	0.64	2.21	4	1
4:C:604:PCW:H251	5:D:514:17F:C41	0.64	2.22	5	1
4:B:202:PCW:H151	4:B:202:PCW:H361	0.64	1.68	6	1
4:A:416:PCW:H322	4:C:616:PCW:C5	0.64	2.22	1	1
4:C:611:PCW:H322	4:C:617:PCW:H132	0.64	1.70	10	5
4:B:212:PCW:C27	5:D:512:17F:H61	0.64	2.21	8	2
4:C:612:PCW:H20	5:D:511:17F:H43	0.64	1.68	3	1
4:B:205:PCW:C8	5:B:214:17F:H10A	0.64	2.23	3	1
4:C:624:PCW:C20	4:C:624:PCW:C24	0.64	2.72	4	1
4:D:501:PCW:C26	5:D:511:17F:H73	0.64	2.22	4	1
4:C:608:PCW:H452	4:B:207:PCW:H231	0.64	1.67	9	3
4:B:202:PCW:H182	4:B:202:PCW:H232	0.64	1.70	8	1
4:A:416:PCW:C31	4:C:616:PCW:H52	0.64	2.23	1	4
4:C:621:PCW:C19	5:C:628:17F:H19A	0.64	2.11	1	1
5:C:630:17F:O8	5:C:630:17F:H5	0.64	1.92	6	3
4:A:407:PCW:C38	4:B:211:PCW:H141	0.64	2.23	8	4
5:A:409:17F:C26	4:D:510:PCW:H231	0.64	2.22	2	1
4:C:607:PCW:H432	5:C:626:17F:C33	0.64	2.23	8	2
4:C:621:PCW:H441	4:D:506:PCW:C27	0.64	2.18	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:508:PCW:H361	4:D:508:PCW:C22	0.64	2.14	4	2
4:B:206:PCW:H231	4:B:206:PCW:C27	0.64	2.22	5	1
4:A:405:PCW:H321	4:B:203:PCW:H341	0.64	1.67	6	4
4:A:416:PCW:H161	5:C:630:17F:H60	0.64	1.70	6	2
4:D:502:PCW:H272	4:D:502:PCW:C23	0.64	2.11	8	1
4:A:416:PCW:H322	4:C:616:PCW:H52	0.64	1.68	1	1
1:C:444:ASP:O	1:C:448:VAL:HB	0.64	1.93	8	7
4:C:621:PCW:H422	4:D:516:PCW:H483	0.64	1.69	1	1
4:D:506:PCW:H12	4:D:510:PCW:C8	0.64	2.23	3	1
5:D:513:17F:C7	5:D:513:17F:C17	0.64	2.75	3	1
4:A:411:PCW:H32	4:D:515:PCW:H121	0.64	1.69	4	1
4:B:203:PCW:H212	4:B:208:PCW:C2	0.64	2.20	4	1
4:C:606:PCW:C7	4:C:624:PCW:H171	0.64	2.23	5	1
4:C:610:PCW:C4	4:C:622:PCW:H332	0.64	2.23	5	1
4:A:406:PCW:C46	4:D:506:PCW:H251	0.64	2.17	6	1
4:A:407:PCW:H82	4:B:211:PCW:O2P	0.64	1.92	6	1
4:B:203:PCW:H241	4:B:204:PCW:H132	0.64	1.69	6	1
4:A:406:PCW:H462	4:D:506:PCW:H271	0.64	1.70	9	1
4:C:610:PCW:C5	4:C:622:PCW:H342	0.64	2.22	10	1
4:D:507:PCW:C3	5:D:513:17F:H75	0.64	2.23	10	1
4:B:206:PCW:H411	5:B:213:17F:H8A	0.63	1.68	1	1
4:A:415:PCW:H31	4:C:616:PCW:H421	0.63	1.69	9	4
4:C:601:PCW:H122	4:C:601:PCW:C46	0.63	2.23	2	1
4:C:609:PCW:O1P	4:C:609:PCW:H52	0.63	1.93	6	6
4:A:413:PCW:C36	4:C:611:PCW:H151	0.63	2.23	4	1
5:D:512:17F:H35	5:D:514:17F:H43	0.63	1.70	4	1
4:A:404:PCW:H152	4:B:210:PCW:C22	0.63	2.23	8	1
4:D:508:PCW:H251	4:D:508:PCW:H412	0.63	1.68	8	1
4:A:401:PCW:C39	4:D:502:PCW:H231	0.63	2.23	9	1
4:A:408:PCW:C47	4:A:408:PCW:C43	0.63	2.76	3	9
4:C:625:PCW:C24	4:D:516:PCW:H451	0.63	2.20	8	3
4:A:414:PCW:H82	4:C:624:PCW:O31	0.63	1.93	7	3
4:B:211:PCW:H461	4:B:211:PCW:H181	0.63	1.69	5	2
4:D:510:PCW:C43	4:D:510:PCW:C47	0.63	2.73	9	3
5:A:409:17F:H4	5:A:409:17F:O10	0.63	1.93	10	3
4:D:504:PCW:H382	4:D:504:PCW:H122	0.63	1.70	9	1
4:B:208:PCW:H442	4:B:212:PCW:H271	0.63	1.70	10	1
4:C:604:PCW:H381	5:C:627:17F:C24	0.63	2.22	1	2
4:C:606:PCW:H252	5:C:627:17F:H42	0.63	1.69	2	1
4:C:617:PCW:H131	4:C:625:PCW:C14	0.63	2.23	3	3
4:B:206:PCW:H432	5:B:213:17F:H76	0.63	1.69	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:413:PCW:C38	4:C:611:PCW:H151	0.63	2.19	6	2
4:C:608:PCW:H361	4:B:207:PCW:H281	0.63	1.69	4	1
4:C:621:PCW:H352	4:C:625:PCW:C21	0.63	2.23	9	6
4:B:206:PCW:H161	5:B:213:17F:H20A	0.63	1.70	4	2
4:D:503:PCW:C25	4:D:503:PCW:C21	0.63	2.74	4	5
4:C:621:PCW:C47	4:D:506:PCW:H252	0.63	2.23	5	1
4:B:208:PCW:H412	4:B:208:PCW:H272	0.63	1.70	6	2
4:B:203:PCW:H422	4:B:208:PCW:H39	0.63	1.68	7	1
4:C:614:PCW:H483	4:B:206:PCW:H252	0.63	1.69	10	1
4:A:417:PCW:H441	4:C:605:PCW:H451	0.63	1.69	5	3
4:C:605:PCW:O31	4:C:612:PCW:C5	0.63	2.46	8	4
4:C:614:PCW:H82	5:C:632:17F:O4	0.63	1.93	2	3
4:A:405:PCW:H461	4:A:414:PCW:C27	0.63	2.22	5	2
4:C:621:PCW:C33	4:D:516:PCW:H422	0.63	2.23	8	6
4:A:408:PCW:H141	5:A:409:17F:H62	0.63	1.70	4	1
4:A:412:PCW:H471	4:A:414:PCW:C47	0.63	2.23	5	1
4:D:501:PCW:O11	4:D:501:PCW:H2	0.63	1.91	8	3
4:D:505:PCW:H2	4:D:505:PCW:O11	0.63	1.93	5	2
4:A:405:PCW:C46	4:A:414:PCW:H241	0.63	2.23	10	2
4:C:610:PCW:H41	4:C:622:PCW:H321	0.63	1.68	8	1
4:C:609:PCW:C28	5:C:631:17F:H72	0.63	2.23	9	1
4:B:208:PCW:C12	5:B:214:17F:H18A	0.63	2.22	10	1
4:A:401:PCW:H461	4:C:610:PCW:H251	0.63	1.69	10	3
4:A:412:PCW:C11	4:A:412:PCW:O31	0.63	2.46	8	9
4:C:609:PCW:H42	5:C:631:17F:O8	0.63	1.93	4	6
4:D:505:PCW:C21	4:D:505:PCW:C25	0.63	2.75	6	7
4:B:207:PCW:O1P	4:B:209:PCW:H32	0.63	1.93	3	1
4:C:603:PCW:O1P	4:C:603:PCW:O2	0.63	2.17	4	2
4:C:622:PCW:H20	5:D:514:17F:H53	0.63	1.68	5	1
4:C:603:PCW:H472	4:C:603:PCW:H212	0.63	1.71	6	1
1:C:523:ASP:HA	1:C:526:ARG:HD2	0.63	1.70	9	1
4:C:614:PCW:C17	4:C:614:PCW:C13	0.63	2.70	9	1
4:D:504:PCW:O31	4:D:504:PCW:C4	0.63	2.47	9	1
4:D:506:PCW:H321	4:D:507:PCW:H381	0.63	1.70	10	1
4:A:408:PCW:C21	5:A:409:17F:H34	0.63	2.22	8	2
4:C:605:PCW:H382	4:C:610:PCW:O2	0.63	1.94	5	5
4:B:208:PCW:H483	4:B:212:PCW:C26	0.63	2.22	1	1
4:B:208:PCW:H482	4:B:208:PCW:H281	0.63	1.69	1	1
4:B:212:PCW:C24	4:B:212:PCW:C20	0.63	2.74	2	5
4:D:510:PCW:C47	4:D:510:PCW:C43	0.63	2.73	6	7
4:A:407:PCW:H341	4:A:407:PCW:C13	0.63	2.23	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:504:PCW:H272	5:D:513:17F:C38	0.63	2.23	2	1
4:A:412:PCW:H432	4:C:624:PCW:H472	0.63	1.70	4	3
4:C:612:PCW:C48	4:C:618:PCW:H211	0.63	2.24	7	3
4:B:204:PCW:C16	4:B:208:PCW:H211	0.63	2.24	7	2
4:C:609:PCW:C4	5:C:631:17F:H6A	0.63	2.24	5	1
4:A:412:PCW:H483	4:C:604:PCW:H283	0.63	1.70	6	1
5:C:632:17F:C29	4:B:201:PCW:H442	0.63	2.24	6	1
4:C:612:PCW:H20	5:D:511:17F:H47	0.63	1.71	7	1
4:A:413:PCW:H352	4:C:611:PCW:C13	0.63	2.24	9	2
4:D:501:PCW:H381	4:D:509:PCW:H442	0.63	1.71	10	1
4:C:607:PCW:H212	5:C:629:17F:C1X	0.63	2.24	1	5
4:C:614:PCW:C46	4:B:206:PCW:H261	0.63	2.24	1	1
4:C:620:PCW:H19	5:C:631:17F:O10	0.63	1.94	1	2
4:C:624:PCW:C27	4:C:624:PCW:C23	0.63	2.75	2	9
4:A:414:PCW:H381	4:C:623:PCW:C26	0.63	2.23	4	3
4:D:505:PCW:H452	4:D:506:PCW:H232	0.63	1.71	3	2
4:A:408:PCW:H141	5:A:409:17F:C35	0.63	2.24	4	1
4:C:620:PCW:C44	5:B:215:17F:H77	0.63	2.17	4	1
4:B:208:PCW:H421	5:D:512:17F:H72	0.63	1.69	4	2
4:C:615:PCW:H271	4:C:617:PCW:C28	0.63	2.23	7	2
4:C:601:PCW:H39	4:C:602:PCW:C17	0.63	2.24	10	2
4:D:502:PCW:C42	4:D:508:PCW:H221	0.63	2.23	9	1
4:B:204:PCW:H452	4:D:502:PCW:C46	0.63	2.23	10	1
4:B:204:PCW:C47	4:D:502:PCW:H482	0.63	2.23	10	1
4:C:606:PCW:H442	4:C:608:PCW:H31	0.63	1.70	1	1
4:B:212:PCW:H40	5:D:514:17F:H71	0.63	1.69	1	1
5:A:410:17F:O5	4:D:502:PCW:H82	0.63	1.93	2	2
4:A:411:PCW:H11	4:D:515:PCW:H32	0.63	1.71	2	1
4:A:417:PCW:C45	5:D:511:17F:H75	0.63	2.21	3	2
4:D:503:PCW:H262	4:D:507:PCW:H472	0.63	1.71	3	1
4:B:201:PCW:H452	4:B:205:PCW:C25	0.63	2.24	6	1
4:B:201:PCW:C44	4:B:207:PCW:H141	0.63	2.10	1	1
4:B:211:PCW:C26	4:B:211:PCW:C22	0.63	2.74	2	7
4:A:401:PCW:C25	4:C:613:PCW:H281	0.63	2.21	2	2
5:A:409:17F:O2	5:A:409:17F:C17	0.63	2.47	4	3
5:C:627:17F:H47	5:C:628:17F:C23	0.63	2.23	8	2
4:D:507:PCW:H222	5:D:513:17F:H56	0.63	1.71	2	2
5:C:628:17F:H10A	5:C:628:17F:H60	0.63	1.70	3	3
4:D:505:PCW:C28	4:D:509:PCW:H451	0.63	2.24	3	1
4:A:404:PCW:C15	4:B:210:PCW:H211	0.63	2.07	4	2
4:A:404:PCW:C11	4:B:210:PCW:H142	0.63	2.24	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:505:PCW:H19	4:D:509:PCW:H63	0.63	1.71	6	1
4:A:411:PCW:C14	4:A:415:PCW:H331	0.63	2.24	9	1
4:A:407:PCW:H82	4:B:211:PCW:O31	0.62	1.94	5	3
4:C:611:PCW:O1P	4:C:611:PCW:H52	0.62	1.94	5	1
4:D:508:PCW:H182	4:D:508:PCW:H362	0.62	1.70	5	1
4:A:402:PCW:H251	4:A:413:PCW:H241	0.62	1.70	7	1
4:C:615:PCW:H461	4:C:625:PCW:H251	0.62	1.69	7	2
4:B:205:PCW:C21	4:B:207:PCW:H411	0.62	2.24	9	1
4:C:614:PCW:H52	4:C:614:PCW:O1P	0.62	1.93	8	8
1:A:299:SER:HB2	1:A:300:PRO:HD3	0.62	1.72	3	6
4:D:503:PCW:H342	4:D:507:PCW:H341	0.62	1.71	3	4
4:D:501:PCW:C5	4:D:509:PCW:H331	0.62	2.23	3	1
4:B:206:PCW:C19	5:B:213:17F:H20A	0.62	2.24	5	1
4:B:206:PCW:H161	5:B:213:17F:C31	0.62	2.22	10	2
5:A:409:17F:H6	4:D:504:PCW:H372	0.62	1.71	7	1
4:A:402:PCW:C28	4:A:413:PCW:H221	0.62	2.16	8	1
4:C:604:PCW:H252	5:D:514:17F:H75	0.62	1.70	9	1
4:B:205:PCW:C21	4:B:207:PCW:H431	0.62	2.24	9	1
4:A:413:PCW:O3P	4:A:413:PCW:O31	0.62	2.17	5	6
4:C:620:PCW:C41	5:C:632:17F:H77	0.62	2.22	10	2
4:A:408:PCW:H141	5:A:409:17F:H66	0.62	1.71	2	1
5:C:632:17F:H52	4:B:207:PCW:H181	0.62	1.69	2	1
4:B:206:PCW:H31	4:B:206:PCW:P	0.62	2.33	5	4
4:A:411:PCW:H271	4:B:202:PCW:H483	0.62	1.72	3	1
4:C:621:PCW:H341	4:D:516:PCW:C43	0.62	2.24	3	1
4:B:212:PCW:H171	4:B:212:PCW:C38	0.62	2.21	3	1
4:D:506:PCW:H442	4:D:507:PCW:C44	0.62	2.23	3	1
4:B:211:PCW:H52	4:B:211:PCW:H321	0.62	1.70	10	5
4:A:408:PCW:H161	5:A:409:17F:H34	0.62	1.70	6	1
4:C:608:PCW:H261	4:C:614:PCW:H411	0.62	1.71	10	2
4:D:505:PCW:H271	4:D:510:PCW:H161	0.62	1.70	7	1
4:C:620:PCW:O11	4:C:620:PCW:H2	0.62	1.93	8	1
4:B:210:PCW:C28	4:D:505:PCW:H451	0.62	2.24	8	1
4:B:206:PCW:C37	4:D:505:PCW:H321	0.62	2.24	10	1
4:A:401:PCW:H341	4:D:502:PCW:H172	0.62	1.70	4	2
4:C:606:PCW:C44	4:C:608:PCW:H12	0.62	2.23	1	1
4:C:623:PCW:O11	4:C:623:PCW:H2	0.62	1.92	7	9
4:C:607:PCW:H19	5:C:629:17F:C28	0.62	2.24	3	4
4:C:622:PCW:H12	4:C:623:PCW:H161	0.62	1.71	3	2
5:D:513:17F:O10	5:D:513:17F:H6A	0.62	1.92	2	2
4:C:623:PCW:H371	4:C:624:PCW:H121	0.62	1.68	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:202:PCW:C14	4:D:504:PCW:H322	0.62	2.24	3	1
4:D:501:PCW:H461	5:D:514:17F:H52	0.62	1.71	3	1
4:B:203:PCW:C21	4:B:208:PCW:O31	0.62	2.47	4	1
4:D:503:PCW:H282	5:D:513:17F:H20A	0.62	1.71	4	1
4:B:205:PCW:C21	4:B:205:PCW:C25	0.62	2.75	5	1
4:B:208:PCW:H121	5:B:214:17F:C17	0.62	2.24	5	2
4:A:415:PCW:C39	4:C:616:PCW:H472	0.62	2.24	8	1
4:C:620:PCW:H231	4:C:621:PCW:C8	0.62	2.24	9	3
4:B:201:PCW:H483	4:B:205:PCW:C39	0.62	2.21	9	1
4:D:505:PCW:H341	4:D:506:PCW:H121	0.62	1.69	9	1
4:C:619:PCW:H271	5:C:632:17F:C21	0.62	2.23	1	1
4:D:506:PCW:P	4:D:506:PCW:C3	0.62	2.88	1	1
4:A:415:PCW:H11	4:C:616:PCW:C41	0.62	2.18	4	3
4:C:602:PCW:H483	5:C:626:17F:H58	0.62	1.70	2	1
4:A:411:PCW:C44	4:C:616:PCW:H242	0.62	2.24	3	3
4:B:203:PCW:H261	4:B:208:PCW:H122	0.62	1.71	5	1
4:D:503:PCW:C45	4:D:504:PCW:H152	0.62	2.25	5	1
5:D:513:17F:H65	5:D:513:17F:C10	0.62	2.25	7	1
4:B:205:PCW:H73	4:B:212:PCW:H41	0.62	1.72	8	1
4:A:405:PCW:C32	4:B:203:PCW:H352	0.62	2.23	9	1
4:C:617:PCW:C42	4:C:625:PCW:H231	0.62	2.24	9	1
4:C:619:PCW:H11	4:C:619:PCW:C7	0.62	2.24	10	1
4:D:501:PCW:H472	4:D:509:PCW:H252	0.62	1.70	10	1
4:A:411:PCW:C45	4:A:416:PCW:H421	0.62	2.21	1	3
4:B:208:PCW:H63	5:B:214:17F:O9	0.62	1.95	1	1
4:B:208:PCW:C27	4:B:208:PCW:H412	0.62	2.25	2	1
4:A:403:PCW:H152	4:B:207:PCW:H39	0.62	1.71	7	2
4:A:405:PCW:C48	4:A:414:PCW:H272	0.62	2.23	3	1
4:C:612:PCW:H471	4:C:618:PCW:C43	0.62	2.25	3	2
4:D:501:PCW:H12	4:D:501:PCW:H41	0.62	1.71	3	1
4:D:506:PCW:C46	5:D:513:17F:H47	0.62	2.22	3	1
4:A:408:PCW:H282	4:A:416:PCW:C28	0.62	2.25	4	1
4:C:601:PCW:H371	4:C:602:PCW:H171	0.62	1.70	7	4
4:D:505:PCW:H452	4:D:506:PCW:H251	0.62	1.71	5	1
4:C:612:PCW:H212	5:D:511:17F:H47	0.62	1.70	6	1
4:C:615:PCW:C42	4:C:625:PCW:H232	0.62	2.23	6	1
4:C:617:PCW:H341	5:C:631:17F:C2X	0.62	2.24	8	2
2:B:21:ILE:HD13	3:D:388:VAL:HG13	0.62	1.69	7	1
4:D:505:PCW:H452	4:D:506:PCW:H211	0.62	1.71	7	1
4:A:401:PCW:H40	4:D:502:PCW:C28	0.62	2.24	8	1
4:D:510:PCW:H242	4:D:515:PCW:C48	0.62	2.24	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:507:PCW:C19	5:D:513:17F:H31	0.62	2.25	9	1
4:C:612:PCW:O31	4:C:612:PCW:C1	0.62	2.46	1	5
4:B:203:PCW:O4P	4:B:203:PCW:C6	0.62	2.47	5	10
4:B:205:PCW:C17	4:B:207:PCW:H362	0.62	2.24	1	2
4:B:212:PCW:H222	5:D:514:17F:H12A	0.62	1.70	1	1
4:A:401:PCW:H322	4:D:508:PCW:H231	0.62	1.71	2	1
4:A:414:PCW:H381	4:C:623:PCW:H251	0.62	1.72	10	3
4:C:612:PCW:C12	4:C:618:PCW:H382	0.62	2.21	2	1
4:B:202:PCW:H19	4:D:504:PCW:H142	0.62	1.71	3	2
4:C:603:PCW:C31	4:C:603:PCW:C4	0.62	2.77	4	2
5:A:410:17F:H31	4:D:502:PCW:H162	0.62	1.69	5	1
4:A:408:PCW:H121	5:A:409:17F:H63	0.62	1.71	6	1
4:B:210:PCW:H472	4:D:507:PCW:H232	0.62	1.72	6	1
4:A:408:PCW:H172	5:A:409:17F:C1Y	0.62	2.25	7	1
4:A:417:PCW:H351	4:C:622:PCW:H142	0.62	1.72	7	2
4:C:608:PCW:H122	4:C:614:PCW:C7	0.62	2.24	1	3
4:B:205:PCW:H182	4:B:207:PCW:H172	0.62	1.69	9	2
4:A:404:PCW:C24	4:B:211:PCW:H242	0.62	2.25	2	1
4:A:412:PCW:H361	4:C:624:PCW:H431	0.62	1.71	7	3
5:C:632:17F:H75	5:B:215:17F:C35	0.62	2.22	2	1
4:D:506:PCW:C46	4:D:506:PCW:C42	0.62	2.74	4	4
4:B:203:PCW:H212	4:B:208:PCW:H63	0.62	1.70	3	1
4:D:507:PCW:H471	5:D:513:17F:H57	0.62	1.70	4	4
4:B:211:PCW:C22	4:B:211:PCW:C26	0.62	2.65	6	3
4:B:206:PCW:H42	4:B:209:PCW:H82	0.62	1.71	6	1
4:B:212:PCW:H211	5:D:514:17F:H10	0.62	1.70	8	1
4:B:206:PCW:H161	5:B:213:17F:C20	0.62	2.24	9	1
4:D:503:PCW:H362	4:D:507:PCW:C32	0.62	2.24	9	1
4:A:406:PCW:H452	4:B:211:PCW:H471	0.62	1.70	10	1
5:A:410:17F:H78	4:C:618:PCW:C48	0.62	2.24	10	1
4:C:603:PCW:H212	4:C:603:PCW:C44	0.62	2.22	5	2
4:C:605:PCW:O31	4:C:605:PCW:O3P	0.62	2.18	1	8
4:C:606:PCW:H152	5:C:627:17F:H8	0.62	1.71	2	1
5:C:626:17F:C31	5:C:629:17F:H51	0.62	2.24	6	6
4:A:404:PCW:C23	4:B:210:PCW:H222	0.62	2.25	4	3
4:D:501:PCW:H61	5:D:514:17F:O7	0.62	1.95	4	1
4:C:619:PCW:C14	5:C:632:17F:H18	0.62	2.24	5	3
4:C:602:PCW:C2	5:B:214:17F:H57	0.62	2.23	8	1
4:C:604:PCW:H252	5:D:514:17F:C41	0.62	2.25	9	1
4:D:509:PCW:O3	5:D:514:17F:H31	0.62	1.95	9	1
5:D:513:17F:H5	5:D:513:17F:O2	0.62	1.95	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:502:PCW:H40	5:D:512:17F:C10	0.62	2.23	1	2
4:A:417:PCW:H261	4:C:621:PCW:H242	0.62	1.71	2	1
1:C:588:LEU:HD22	5:C:630:17F:H48	0.62	1.69	2	1
4:C:613:PCW:H452	4:C:618:PCW:H20	0.62	1.72	2	1
4:C:625:PCW:H421	4:C:625:PCW:C38	0.62	2.25	6	3
4:C:622:PCW:H412	4:C:623:PCW:H212	0.62	1.70	3	1
4:D:503:PCW:H52	4:D:506:PCW:C6	0.62	2.23	3	1
4:D:504:PCW:H382	4:D:504:PCW:C12	0.62	2.23	4	1
4:A:413:PCW:H372	4:C:611:PCW:H231	0.62	1.71	5	1
4:C:610:PCW:H31	4:C:618:PCW:C11	0.62	2.25	6	1
4:B:203:PCW:C28	5:B:214:17F:H20A	0.62	2.21	7	1
4:D:515:PCW:H122	4:D:515:PCW:H332	0.62	1.72	7	1
4:C:612:PCW:H262	5:D:511:17F:H74	0.62	1.70	9	1
4:A:402:PCW:O2P	4:D:507:PCW:H151	0.62	1.94	10	1
4:A:417:PCW:C28	4:D:509:PCW:H282	0.62	2.25	10	1
4:C:615:PCW:H452	4:D:506:PCW:H482	0.62	1.71	10	1
4:C:604:PCW:O3	4:C:604:PCW:O31	0.61	2.18	8	6
4:B:209:PCW:H52	4:B:209:PCW:O1P	0.61	1.93	6	9
4:C:621:PCW:C35	4:C:625:PCW:C20	0.61	2.78	10	5
4:B:206:PCW:H283	4:B:206:PCW:C24	0.61	2.25	5	1
4:C:608:PCW:H462	4:B:207:PCW:H472	0.61	1.70	6	1
4:B:204:PCW:H182	4:B:208:PCW:H221	0.61	1.72	6	1
4:C:615:PCW:C36	4:D:516:PCW:H362	0.61	2.25	7	2
4:D:508:PCW:H472	4:D:508:PCW:C26	0.61	2.25	7	1
4:A:407:PCW:C37	4:B:211:PCW:H141	0.61	2.24	8	2
4:C:608:PCW:H131	4:C:614:PCW:C7	0.61	2.25	8	1
4:C:615:PCW:H11	4:D:516:PCW:H342	0.61	1.71	3	3
4:A:403:PCW:H251	4:B:201:PCW:H141	0.61	1.72	2	2
4:C:612:PCW:C21	5:D:511:17F:H51	0.61	2.25	2	2
4:C:620:PCW:H222	5:C:631:17F:C19	0.61	2.25	2	1
4:D:507:PCW:C20	5:D:513:17F:H19A	0.61	2.25	2	1
4:B:206:PCW:O2P	4:B:206:PCW:H31	0.61	1.94	3	1
5:A:409:17F:H60	4:D:504:PCW:H331	0.61	1.71	4	1
4:C:617:PCW:H252	4:D:507:PCW:H281	0.61	1.73	4	2
4:C:620:PCW:H483	5:B:215:17F:H34	0.61	1.70	7	1
4:D:505:PCW:C42	4:D:506:PCW:H161	0.61	2.25	8	2
4:A:406:PCW:H431	4:B:211:PCW:H182	0.61	1.71	9	1
4:B:212:PCW:H222	5:D:514:17F:H10A	0.61	1.72	10	1
4:A:413:PCW:C41	4:A:413:PCW:C37	0.61	2.77	1	4
4:B:208:PCW:C47	4:B:208:PCW:C43	0.61	2.75	4	6
5:A:409:17F:H29	4:D:503:PCW:H462	0.61	1.70	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:C:630:17F:O10	5:C:630:17F:P1	0.61	2.58	2	1
4:A:414:PCW:H321	4:C:623:PCW:H362	0.61	1.72	4	1
4:A:401:PCW:C41	4:D:502:PCW:H262	0.61	2.17	6	1
4:B:210:PCW:H283	4:D:505:PCW:H481	0.61	1.70	6	1
4:A:402:PCW:H322	4:D:507:PCW:H181	0.61	1.73	10	1
4:C:606:PCW:C45	4:C:608:PCW:H12	0.61	2.25	1	1
4:B:207:PCW:H442	4:B:209:PCW:H251	0.61	1.72	7	2
4:C:616:PCW:H51	4:C:616:PCW:O3P	0.61	1.95	2	2
5:C:627:17F:H72	5:B:215:17F:H10A	0.61	1.72	2	1
4:D:507:PCW:H451	5:D:513:17F:H33	0.61	1.71	8	2
4:C:606:PCW:H132	4:C:606:PCW:H342	0.61	1.70	9	4
5:C:627:17F:C38	5:B:215:17F:H29	0.61	2.26	9	2
4:C:606:PCW:H162	5:C:627:17F:H30	0.61	1.71	7	4
5:B:213:17F:H67	4:D:505:PCW:H372	0.61	1.73	7	1
4:D:505:PCW:H11	4:D:509:PCW:C7	0.61	2.25	9	2
4:C:613:PCW:H31	4:C:613:PCW:O4P	0.61	1.94	9	1
4:C:617:PCW:H422	4:C:625:PCW:C26	0.61	2.23	9	1
4:D:501:PCW:H61	5:D:514:17F:H1	0.61	1.73	9	1
4:D:508:PCW:H121	5:D:512:17F:O9	0.61	1.95	9	1
4:A:405:PCW:H432	4:A:414:PCW:H282	0.61	1.71	10	4
5:C:626:17F:O10	5:C:626:17F:C7	0.61	2.49	2	9
4:C:602:PCW:H152	5:C:626:17F:H49	0.61	1.73	8	2
5:C:627:17F:H10	5:B:215:17F:C27	0.61	2.25	9	2
1:A:327:LEU:HD11	4:C:601:PCW:H241	0.61	1.70	10	2
4:C:604:PCW:O31	4:C:604:PCW:O3	0.61	2.18	10	2
4:A:404:PCW:H2	4:B:210:PCW:H381	0.61	1.71	5	1
5:D:512:17F:C29	5:D:514:17F:H46	0.61	2.13	5	1
5:D:513:17F:H69	5:D:513:17F:C11	0.61	2.24	5	1
4:B:206:PCW:H142	5:B:213:17F:C31	0.61	2.21	6	1
4:A:408:PCW:H172	5:A:409:17F:C20	0.61	2.25	7	1
5:D:513:17F:H65	5:D:513:17F:C11	0.61	2.19	10	2
4:B:203:PCW:H261	4:B:204:PCW:H19	0.61	1.70	10	1
4:B:204:PCW:H121	4:B:204:PCW:H362	0.61	1.70	10	1
4:C:610:PCW:H161	4:C:618:PCW:H171	0.61	1.72	4	4
5:D:514:17F:O10	5:D:514:17F:H20A	0.61	1.95	8	9
5:A:409:17F:H50	4:D:510:PCW:H231	0.61	1.71	2	1
4:C:601:PCW:C43	4:C:601:PCW:C47	0.61	2.74	2	2
4:C:602:PCW:H341	5:B:214:17F:H66	0.61	1.72	2	1
4:A:417:PCW:H73	4:A:417:PCW:C32	0.61	2.21	3	2
4:C:621:PCW:C34	4:D:516:PCW:H422	0.61	2.25	3	2
4:B:204:PCW:H152	4:B:208:PCW:H361	0.61	1.71	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:412:PCW:H471	4:A:414:PCW:H472	0.61	1.72	5	2
4:C:614:PCW:C4	4:C:614:PCW:H2	0.61	2.25	4	3
4:D:508:PCW:H232	4:D:508:PCW:H381	0.61	1.72	4	1
4:B:208:PCW:H431	4:B:212:PCW:H262	0.61	1.72	5	1
4:B:210:PCW:O2P	4:D:503:PCW:H32	0.61	1.95	5	1
4:B:202:PCW:C23	4:B:202:PCW:C18	0.61	2.70	6	1
4:A:416:PCW:H372	4:C:616:PCW:H141	0.61	1.71	10	1
4:B:212:PCW:H462	5:D:514:17F:H67	0.61	1.73	10	1
4:C:602:PCW:O31	4:C:602:PCW:H12	0.61	1.93	3	10
4:C:602:PCW:O4P	4:C:602:PCW:C6	0.61	2.49	6	10
4:C:625:PCW:C25	4:D:516:PCW:H451	0.61	2.25	1	1
4:D:503:PCW:C21	4:D:503:PCW:C25	0.61	2.75	10	4
5:A:409:17F:H19	4:D:504:PCW:H342	0.61	1.72	2	2
4:A:414:PCW:H63	4:C:624:PCW:O31	0.61	1.96	2	3
4:A:416:PCW:C38	4:C:616:PCW:H151	0.61	2.19	3	1
4:C:619:PCW:H41	4:C:619:PCW:O31	0.61	1.94	8	3
2:B:24:ILE:HG23	2:B:42:LYS:HD3	0.61	1.72	3	1
5:D:513:17F:H19	5:D:513:17F:H8A	0.61	1.71	3	1
4:A:415:PCW:H481	4:C:617:PCW:H281	0.61	1.73	5	1
4:C:614:PCW:C14	5:C:632:17F:H9A	0.61	2.18	5	1
4:D:507:PCW:H131	5:D:513:17F:C41	0.61	2.26	5	2
4:C:604:PCW:H361	5:C:627:17F:C2X	0.61	2.26	6	2
4:B:203:PCW:H252	4:B:204:PCW:C15	0.61	2.23	6	1
4:C:617:PCW:H341	5:C:631:17F:C21	0.61	2.26	8	2
4:B:204:PCW:H462	4:D:502:PCW:H461	0.61	1.73	7	1
4:B:206:PCW:H442	5:B:213:17F:H58	0.61	1.70	7	1
4:A:411:PCW:H451	4:C:616:PCW:H252	0.61	1.72	10	1
5:C:631:17F:O10	5:C:631:17F:O7	0.61	2.19	6	9
4:B:208:PCW:O31	4:B:208:PCW:O3P	0.61	2.18	8	2
4:D:515:PCW:H341	4:D:515:PCW:O31	0.61	1.96	8	8
4:A:411:PCW:O31	4:A:411:PCW:P	0.61	2.58	9	2
4:A:413:PCW:C40	4:C:611:PCW:H251	0.61	2.26	5	1
4:B:204:PCW:C40	5:D:514:17F:H8	0.61	2.25	5	2
4:B:206:PCW:H19	5:B:213:17F:H20A	0.61	1.73	5	1
4:B:207:PCW:H62	5:B:213:17F:O4	0.61	1.95	5	1
4:C:613:PCW:C42	4:C:613:PCW:C46	0.61	2.74	6	2
4:B:204:PCW:C11	4:B:208:PCW:H131	0.61	2.25	6	1
4:C:610:PCW:H242	4:C:618:PCW:H483	0.61	1.73	10	1
4:C:620:PCW:H412	5:C:632:17F:C42	0.61	2.20	3	2
4:D:509:PCW:H412	4:D:509:PCW:C37	0.61	2.22	8	4
4:D:509:PCW:H362	4:D:510:PCW:C1	0.61	2.26	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:510:PCW:H2	4:D:510:PCW:O11	0.61	1.96	6	4
4:B:205:PCW:H73	5:B:213:17F:H6	0.61	1.73	2	1
4:D:503:PCW:P	4:D:503:PCW:C3	0.61	2.89	2	1
4:A:417:PCW:H62	4:A:417:PCW:O4P	0.61	1.94	10	3
4:C:603:PCW:H441	4:C:603:PCW:C21	0.61	2.26	9	3
4:C:606:PCW:H52	4:C:624:PCW:H281	0.61	1.72	3	1
4:C:608:PCW:C24	4:C:614:PCW:H381	0.61	2.26	5	4
4:C:610:PCW:H63	4:C:622:PCW:H361	0.61	1.72	4	1
5:A:409:17F:C22	4:D:510:PCW:H132	0.61	2.25	6	1
4:B:210:PCW:H283	4:D:505:PCW:C48	0.61	2.26	6	1
4:A:403:PCW:C6	4:A:406:PCW:H39	0.61	2.26	7	1
2:B:168:GLU:HG2	2:B:172:LYS:HE2	0.61	1.72	7	2
4:B:203:PCW:C16	4:B:208:PCW:H352	0.61	2.25	8	1
4:C:610:PCW:H481	4:D:501:PCW:H281	0.61	1.71	9	1
4:A:413:PCW:C44	4:C:611:PCW:H242	0.61	2.17	10	1
4:C:616:PCW:O1P	4:C:616:PCW:O2	0.61	2.18	10	1
4:B:206:PCW:H41	4:B:206:PCW:C3	0.61	2.23	2	1
4:C:618:PCW:O31	4:C:618:PCW:H11	0.61	1.96	8	7
4:C:620:PCW:H222	5:C:631:17F:H19A	0.61	1.72	3	4
4:D:509:PCW:O3P	4:D:509:PCW:O31	0.61	2.18	7	4
5:A:409:17F:H56	4:D:504:PCW:C33	0.61	2.26	4	1
4:C:609:PCW:H63	5:C:631:17F:O8	0.61	1.95	4	1
4:C:611:PCW:H51	4:C:611:PCW:H341	0.61	1.70	4	1
5:C:626:17F:H36	5:C:629:17F:H75	0.61	1.73	5	2
4:B:208:PCW:H82	5:B:214:17F:H19A	0.61	1.72	7	2
4:D:502:PCW:C12	4:D:508:PCW:H372	0.61	2.26	5	1
4:A:405:PCW:H271	4:A:414:PCW:C27	0.61	2.26	6	2
5:A:409:17F:H38	4:D:510:PCW:C13	0.61	2.25	6	1
4:D:503:PCW:O4P	4:D:503:PCW:C6	0.61	2.48	7	1
4:C:617:PCW:H251	4:D:506:PCW:H442	0.61	1.73	8	1
4:D:501:PCW:H63	4:D:509:PCW:O31	0.61	1.96	8	1
4:D:509:PCW:H242	5:D:514:17F:C25	0.61	2.25	8	1
4:B:210:PCW:H11	4:D:503:PCW:C11	0.61	2.26	9	1
4:B:201:PCW:H73	4:B:209:PCW:O2P	0.61	1.96	10	1
4:C:608:PCW:H422	4:C:614:PCW:H461	0.60	1.72	1	3
4:C:615:PCW:H361	4:D:516:PCW:H362	0.60	1.71	1	4
4:D:503:PCW:C28	4:D:507:PCW:H451	0.60	2.21	1	1
4:D:505:PCW:H242	4:D:506:PCW:C39	0.60	2.25	1	1
4:C:605:PCW:H322	4:C:612:PCW:H62	0.60	1.72	3	2
4:C:621:PCW:H162	4:D:516:PCW:C17	0.60	2.26	8	2
4:A:413:PCW:C37	4:C:611:PCW:H151	0.60	2.26	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:204:PCW:H162	4:B:208:PCW:H211	0.60	1.71	6	1
4:D:507:PCW:H351	5:D:513:17F:C8	0.60	2.25	10	2
4:C:615:PCW:H62	4:D:515:PCW:O11	0.60	1.95	8	1
4:B:203:PCW:H231	4:B:204:PCW:C18	0.60	2.26	8	1
4:A:402:PCW:H262	4:A:413:PCW:C46	0.60	2.26	10	1
4:A:404:PCW:H261	5:C:631:17F:H55	0.60	1.73	9	2
4:A:411:PCW:C41	4:A:411:PCW:H371	0.60	2.26	10	5
4:C:606:PCW:C14	4:C:606:PCW:C18	0.60	2.77	5	5
4:C:607:PCW:H461	5:C:626:17F:C34	0.60	2.22	2	5
4:C:611:PCW:H321	4:C:617:PCW:C15	0.60	2.27	1	2
4:D:503:PCW:H11	4:D:503:PCW:O31	0.60	1.95	2	2
4:D:508:PCW:H382	4:D:508:PCW:C23	0.60	2.20	2	3
4:C:614:PCW:H181	5:C:632:17F:H30	0.60	1.71	4	1
4:B:212:PCW:O1P	4:B:212:PCW:C31	0.60	2.50	4	2
5:B:215:17F:O10	5:B:215:17F:P1	0.60	2.59	4	1
4:A:416:PCW:H41	4:A:416:PCW:C2	0.60	2.26	6	2
4:C:608:PCW:C25	5:C:626:17F:H70	0.60	2.16	9	1
4:C:612:PCW:C26	5:D:511:17F:H74	0.60	2.26	9	1
5:C:627:17F:H54	4:D:510:PCW:H462	0.60	1.71	10	2
4:C:612:PCW:O31	4:C:618:PCW:H2	0.60	1.96	9	3
4:C:612:PCW:H221	5:D:511:17F:H47	0.60	1.72	8	5
5:C:629:17F:C17	5:C:629:17F:O7	0.60	2.49	1	5
4:D:501:PCW:H472	4:D:509:PCW:C23	0.60	2.26	1	2
4:D:505:PCW:H272	4:D:510:PCW:H481	0.60	1.72	1	1
4:D:506:PCW:H172	4:D:516:PCW:H281	0.60	1.73	4	2
4:A:403:PCW:O3P	4:A:403:PCW:O31	0.60	2.19	3	2
4:B:211:PCW:H241	4:D:503:PCW:C23	0.60	2.26	3	1
4:B:205:PCW:C28	4:B:205:PCW:C24	0.60	2.75	5	1
4:B:211:PCW:H282	4:D:506:PCW:H231	0.60	1.72	6	1
4:C:602:PCW:H221	4:C:602:PCW:C17	0.60	2.18	8	1
4:B:208:PCW:H52	5:B:214:17F:H6	0.60	1.73	8	1
4:B:204:PCW:H442	4:B:212:PCW:C23	0.60	2.26	10	1
4:D:502:PCW:H31	4:D:508:PCW:O31	0.60	1.96	10	1
4:C:602:PCW:C34	5:B:214:17F:H61	0.60	2.25	1	1
4:B:211:PCW:H461	4:B:211:PCW:H212	0.60	1.74	1	1
4:D:501:PCW:O11	4:D:509:PCW:H381	0.60	1.96	1	1
4:A:401:PCW:C6	4:D:508:PCW:O31	0.60	2.49	2	4
4:C:625:PCW:H381	4:C:625:PCW:C42	0.60	2.22	6	4
4:C:617:PCW:H361	4:C:625:PCW:H172	0.60	1.71	3	5
4:D:505:PCW:H461	4:D:506:PCW:C16	0.60	2.26	3	1
4:D:506:PCW:H171	4:D:510:PCW:C42	0.60	2.25	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:510:PCW:P	4:D:510:PCW:C3	0.60	2.89	4	1
4:A:416:PCW:O1P	4:C:616:PCW:H42	0.60	1.96	10	2
4:C:616:PCW:C1	4:C:616:PCW:O31	0.60	2.46	5	1
4:C:620:PCW:H231	4:C:621:PCW:H82	0.60	1.72	6	3
4:A:403:PCW:C15	4:B:201:PCW:H382	0.60	2.26	8	1
4:A:403:PCW:H171	4:B:205:PCW:C27	0.60	2.26	8	1
4:A:408:PCW:H212	5:A:409:17F:C1Z	0.60	2.26	8	1
4:B:211:PCW:H172	4:D:505:PCW:H432	0.60	1.71	8	1
4:D:503:PCW:H11	4:D:510:PCW:C8	0.60	2.26	8	1
4:B:207:PCW:O1P	4:B:209:PCW:H42	0.60	1.95	9	1
4:A:401:PCW:H442	4:C:613:PCW:C26	0.60	2.20	2	2
4:A:414:PCW:H483	4:B:212:PCW:H471	0.60	1.72	2	1
4:A:417:PCW:H141	4:C:603:PCW:H351	0.60	1.72	2	1
4:C:602:PCW:C36	5:B:214:17F:H61	0.60	2.26	3	2
4:C:620:PCW:H151	5:B:215:17F:C4	0.60	2.27	2	2
4:C:616:PCW:O3P	4:C:616:PCW:O31	0.60	2.19	3	1
4:D:503:PCW:O1P	5:D:513:17F:N1	0.60	2.34	6	1
4:A:403:PCW:C15	4:B:207:PCW:H39	0.60	2.27	7	1
4:A:408:PCW:H321	5:A:409:17F:C1Z	0.60	2.26	7	1
4:A:416:PCW:C14	5:C:630:17F:H11	0.60	2.26	7	1
4:B:204:PCW:O31	4:B:208:PCW:H32	0.60	1.97	8	1
4:C:615:PCW:H452	4:D:506:PCW:C48	0.60	2.26	10	1
4:A:416:PCW:C11	5:C:630:17F:H9	0.60	2.26	4	5
4:C:613:PCW:C6	4:C:623:PCW:O1P	0.60	2.49	9	8
4:C:606:PCW:C18	4:C:606:PCW:C14	0.60	2.77	4	5
4:C:612:PCW:C20	5:D:511:17F:H51	0.60	2.26	2	1
4:A:405:PCW:H361	4:B:203:PCW:H362	0.60	1.72	3	1
4:D:506:PCW:H331	4:D:510:PCW:H351	0.60	1.72	3	1
4:D:510:PCW:O11	4:D:510:PCW:H2	0.60	1.97	4	4
4:D:501:PCW:C25	5:D:511:17F:H73	0.60	2.27	4	1
4:D:501:PCW:C7	4:D:509:PCW:H2	0.60	2.26	5	1
4:C:606:PCW:O11	4:C:606:PCW:C5	0.60	2.50	6	3
4:B:205:PCW:H121	4:B:207:PCW:H142	0.60	1.71	10	2
4:A:404:PCW:H482	4:A:407:PCW:C22	0.60	2.26	9	1
4:C:620:PCW:O3P	4:C:620:PCW:O31	0.60	2.20	2	9
4:C:613:PCW:H11	4:C:613:PCW:O31	0.60	1.97	8	8
4:D:504:PCW:H121	4:D:504:PCW:C38	0.60	2.25	4	1
5:C:628:17F:H62	5:B:215:17F:H36	0.60	1.71	8	3
4:B:204:PCW:C41	4:B:212:PCW:H231	0.60	2.26	5	1
4:B:209:PCW:H152	4:B:209:PCW:H382	0.60	1.72	8	1
4:A:404:PCW:H482	4:A:407:PCW:H221	0.60	1.71	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:403:PCW:H372	4:A:403:PCW:C41	0.60	2.21	6	6
5:A:409:17F:H55	5:D:511:17F:H63	0.60	1.74	1	1
4:D:508:PCW:H272	4:D:508:PCW:C23	0.60	2.26	1	3
4:B:205:PCW:C1	5:B:214:17F:H11	0.60	2.27	3	3
3:D:468:CYS:HB3	3:D:484:CYS:HB3	0.60	1.72	2	2
4:A:413:PCW:C42	4:C:611:PCW:H181	0.60	2.27	3	1
4:C:622:PCW:O2	4:C:623:PCW:H162	0.60	1.97	3	1
4:B:204:PCW:H161	4:B:208:PCW:C21	0.60	2.25	7	2
4:B:210:PCW:H42	4:B:210:PCW:C31	0.60	2.27	5	1
4:A:411:PCW:H283	4:A:415:PCW:C25	0.60	2.27	6	1
4:B:206:PCW:C15	4:B:209:PCW:H122	0.60	2.24	6	1
4:C:601:PCW:H39	5:C:626:17F:H52	0.60	1.70	7	2
4:C:607:PCW:O1P	4:C:624:PCW:H242	0.60	1.97	7	1
4:B:205:PCW:H62	5:B:213:17F:O8	0.60	1.97	9	1
4:B:210:PCW:O2P	5:D:513:17F:H4A	0.60	1.97	10	2
4:D:503:PCW:H372	4:D:507:PCW:O1P	0.60	1.96	9	1
4:A:408:PCW:C32	5:A:409:17F:H32	0.60	2.23	2	2
4:C:608:PCW:O1P	5:C:632:17F:H20A	0.60	1.97	10	2
4:B:208:PCW:O2P	5:B:214:17F:N1	0.60	2.35	1	2
4:C:620:PCW:H283	4:C:621:PCW:C7	0.60	2.27	2	2
4:C:606:PCW:O11	4:C:606:PCW:C7	0.60	2.49	3	1
4:B:204:PCW:C14	4:B:208:PCW:H341	0.60	2.27	3	1
4:D:501:PCW:H151	4:D:502:PCW:H382	0.60	1.72	3	1
4:C:608:PCW:H452	4:B:207:PCW:H20	0.60	1.74	4	2
4:D:505:PCW:H19	4:D:510:PCW:H322	0.60	1.74	7	1
4:D:505:PCW:C36	4:D:506:PCW:H121	0.60	2.25	9	1
4:D:506:PCW:H422	5:D:513:17F:H49	0.60	1.71	9	1
4:C:612:PCW:C43	4:C:618:PCW:H39	0.60	2.26	1	1
4:D:506:PCW:C39	5:D:513:17F:H49	0.60	2.27	1	1
4:D:508:PCW:H222	4:D:508:PCW:C26	0.60	2.26	9	3
4:C:610:PCW:O4P	4:C:618:PCW:H62	0.60	1.95	9	4
4:C:622:PCW:C13	4:C:622:PCW:H39	0.60	2.27	3	2
4:C:625:PCW:H262	4:B:211:PCW:C27	0.60	2.27	4	1
4:C:614:PCW:H161	5:C:632:17F:C11	0.60	2.26	5	1
4:D:502:PCW:H152	4:D:508:PCW:C39	0.60	2.27	5	2
4:B:202:PCW:C17	4:D:504:PCW:H122	0.60	2.23	7	1
4:A:401:PCW:C39	4:D:502:PCW:H271	0.60	2.22	8	1
4:D:502:PCW:C27	4:D:502:PCW:C23	0.60	2.77	8	1
4:B:203:PCW:H452	4:B:204:PCW:C26	0.60	2.26	9	1
4:B:212:PCW:H181	4:B:212:PCW:H432	0.60	1.74	10	1
5:B:214:17F:H4A	5:B:214:17F:C2	0.60	2.27	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:601:PCW:C37	4:C:602:PCW:H171	0.59	2.27	1	2
5:C:626:17F:C8	5:C:629:17F:H33	0.59	2.26	2	3
2:B:46:ILE:HB	2:B:51:CYS:SG	0.59	2.37	10	2
4:A:401:PCW:H52	4:D:502:PCW:O2P	0.59	1.96	2	2
4:D:506:PCW:H321	4:D:507:PCW:C39	0.59	2.26	2	2
4:A:402:PCW:H52	4:D:507:PCW:H121	0.59	1.71	3	1
4:C:602:PCW:O31	4:C:602:PCW:H31	0.59	1.95	3	1
4:B:203:PCW:H142	4:B:208:PCW:C37	0.59	2.25	3	1
4:D:509:PCW:C8	4:D:510:PCW:H41	0.59	2.27	3	1
4:A:417:PCW:H40	4:C:622:PCW:H272	0.59	1.74	4	1
4:B:206:PCW:H422	5:B:213:17F:H32	0.59	1.72	10	2
4:D:510:PCW:H242	4:D:515:PCW:H483	0.59	1.74	9	2
4:A:401:PCW:C5	4:D:508:PCW:O31	0.59	2.50	7	1
5:A:409:17F:H36	5:A:409:17F:H42	0.59	1.74	7	1
4:A:403:PCW:C33	4:B:209:PCW:H411	0.59	2.27	8	1
4:A:417:PCW:H451	5:D:511:17F:C42	0.59	2.22	9	1
4:C:601:PCW:H371	4:C:602:PCW:H151	0.59	1.74	9	1
4:D:502:PCW:H122	4:D:508:PCW:C39	0.59	2.27	10	2
4:D:509:PCW:H161	5:D:514:17F:C33	0.59	2.22	10	1
4:A:417:PCW:H452	4:C:622:PCW:H281	0.59	1.71	2	2
4:A:417:PCW:C47	5:D:511:17F:H55	0.59	2.27	10	3
4:C:608:PCW:C11	4:C:608:PCW:O31	0.59	2.50	8	5
4:C:609:PCW:H241	4:C:609:PCW:H20	0.59	1.73	4	6
4:C:615:PCW:H483	4:D:503:PCW:H221	0.59	1.74	1	2
5:C:628:17F:H70	5:B:215:17F:H39	0.59	1.74	1	1
5:C:632:17F:O10	5:C:632:17F:H4	0.59	1.96	4	6
5:C:632:17F:H52	4:B:207:PCW:H161	0.59	1.72	3	1
4:A:401:PCW:H472	4:C:610:PCW:H262	0.59	1.73	4	1
4:A:408:PCW:H282	4:A:416:PCW:H283	0.59	1.72	4	1
4:C:607:PCW:H181	5:C:629:17F:C11	0.59	2.19	4	2
4:A:412:PCW:H341	4:C:624:PCW:C38	0.59	2.27	5	1
4:A:411:PCW:C27	4:D:504:PCW:H281	0.59	2.24	6	1
4:C:614:PCW:H481	4:B:207:PCW:H19	0.59	1.74	6	1
4:C:625:PCW:C28	5:C:631:17F:H46	0.59	2.27	6	3
4:B:204:PCW:C12	4:B:208:PCW:C34	0.59	2.80	6	1
4:B:206:PCW:H232	4:B:206:PCW:H482	0.59	1.73	6	1
4:B:206:PCW:C37	5:B:213:17F:H34	0.59	2.20	6	2
4:A:407:PCW:H412	4:B:211:PCW:H442	0.59	1.74	7	1
1:A:277:GLU:HB2	1:A:278:PRO:HD3	0.59	1.71	8	1
4:D:503:PCW:H482	4:D:510:PCW:C19	0.59	2.26	8	1
4:A:417:PCW:C24	4:A:417:PCW:C20	0.59	2.74	10	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:417:PCW:C18	4:C:603:PCW:H141	0.59	2.27	10	4
4:C:604:PCW:P	4:C:604:PCW:C3	0.59	2.90	1	9
5:C:631:17F:H53	4:B:211:PCW:C25	0.59	2.26	4	2
4:C:619:PCW:H141	5:C:632:17F:C17	0.59	2.26	8	2
4:C:615:PCW:H441	4:C:625:PCW:C23	0.59	2.22	7	2
4:B:212:PCW:H321	4:D:505:PCW:C7	0.59	2.28	7	2
4:A:416:PCW:H2	4:A:416:PCW:H41	0.59	1.72	8	1
4:D:510:PCW:H40	4:D:516:PCW:H262	0.59	1.74	8	1
4:B:208:PCW:H282	4:B:208:PCW:H481	0.59	1.73	9	1
4:A:402:PCW:C5	5:D:513:17F:O5	0.59	2.50	10	1
4:A:408:PCW:H262	5:A:409:17F:H59	0.59	1.72	10	1
4:C:609:PCW:C24	4:C:609:PCW:H20	0.59	2.27	4	8
4:B:206:PCW:H162	5:B:213:17F:H60	0.59	1.73	4	2
4:A:401:PCW:N	4:D:508:PCW:O31	0.59	2.36	7	3
4:A:404:PCW:H351	4:A:407:PCW:H151	0.59	1.74	2	1
4:A:403:PCW:H461	4:B:209:PCW:H272	0.59	1.75	8	2
4:C:620:PCW:H222	5:C:631:17F:C1Y	0.59	2.23	6	4
4:B:210:PCW:H62	5:D:513:17F:O4	0.59	1.96	4	1
5:A:410:17F:O5	4:D:502:PCW:C5	0.59	2.48	6	1
4:A:415:PCW:C41	4:D:515:PCW:H231	0.59	2.21	6	1
4:B:209:PCW:H182	4:B:209:PCW:C23	0.59	2.28	7	1
5:A:409:17F:H43	5:D:511:17F:H34	0.59	1.74	8	1
4:C:615:PCW:C44	4:C:625:PCW:H232	0.59	2.26	9	1
4:A:404:PCW:C23	4:A:404:PCW:H182	0.59	2.27	2	1
4:A:414:PCW:C8	4:C:624:PCW:O31	0.59	2.51	2	1
4:A:408:PCW:C25	5:A:409:17F:H60	0.59	2.27	3	1
4:B:204:PCW:H39	5:D:514:17F:H8	0.59	1.73	3	1
4:C:621:PCW:H421	4:D:506:PCW:H261	0.59	1.73	8	2
4:A:412:PCW:O3	4:C:624:PCW:C41	0.59	2.51	5	1
4:D:508:PCW:H382	4:D:508:PCW:C22	0.59	2.27	6	1
4:D:501:PCW:C40	4:D:509:PCW:H162	0.59	2.28	7	1
4:B:202:PCW:H172	4:D:504:PCW:H122	0.59	1.74	8	1
4:B:212:PCW:H421	5:D:514:17F:C10	0.59	2.23	9	1
4:B:212:PCW:C36	5:B:213:17F:H11	0.59	2.27	9	1
4:A:405:PCW:H352	5:D:512:17F:H62	0.59	1.74	1	2
4:A:413:PCW:H471	4:C:611:PCW:C27	0.59	2.28	8	3
4:C:607:PCW:H212	5:C:629:17F:H30	0.59	1.75	1	2
5:C:629:17F:O7	5:C:629:17F:O10	0.59	2.21	7	8
4:D:509:PCW:H242	5:D:514:17F:H51	0.59	1.74	1	1
4:D:510:PCW:H461	4:D:516:PCW:H221	0.59	1.73	1	1
5:D:514:17F:O6	5:D:514:17F:C18	0.59	2.50	1	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:414:PCW:H63	4:C:624:PCW:H11	0.59	1.72	2	1
4:A:416:PCW:H442	4:C:616:PCW:C20	0.59	2.27	2	2
4:A:416:PCW:O3P	4:A:416:PCW:O31	0.59	2.20	5	4
4:C:615:PCW:C20	4:C:616:PCW:H461	0.59	2.27	2	1
4:B:202:PCW:C3	4:B:202:PCW:O1P	0.59	2.50	3	7
4:C:615:PCW:O2P	4:C:615:PCW:C3	0.59	2.51	7	4
4:B:212:PCW:H352	5:B:214:17F:C21	0.59	2.27	3	1
4:D:505:PCW:C25	4:D:505:PCW:C21	0.59	2.78	4	3
5:C:627:17F:C10	5:B:215:17F:H48	0.59	2.27	9	2
4:C:605:PCW:H282	4:C:612:PCW:H412	0.59	1.73	6	1
4:B:205:PCW:H19	4:B:206:PCW:H241	0.59	1.74	6	1
4:D:505:PCW:H452	4:D:506:PCW:C23	0.59	2.28	6	1
1:A:348:GLU:HB3	1:A:352:LYS:HE2	0.59	1.73	8	1
4:B:203:PCW:H241	4:B:204:PCW:H171	0.59	1.75	10	1
4:B:206:PCW:C36	4:D:505:PCW:H321	0.59	2.26	10	1
1:A:246:ASP:HA	1:C:528:ARG:NH1	0.59	2.12	10	9
4:C:606:PCW:H2	4:C:606:PCW:C4	0.59	2.28	6	6
4:B:205:PCW:H121	4:B:207:PCW:H171	0.59	1.73	1	1
4:B:206:PCW:C7	4:B:209:PCW:H12	0.59	2.28	1	1
4:B:210:PCW:H461	5:D:513:17F:C20	0.59	2.27	1	1
4:D:508:PCW:O1P	4:D:508:PCW:H32	0.59	1.97	1	5
4:C:623:PCW:C47	4:C:624:PCW:H482	0.59	2.27	7	4
4:D:502:PCW:H432	4:D:508:PCW:C20	0.59	2.25	2	1
4:D:506:PCW:H171	4:D:516:PCW:H281	0.59	1.74	10	2
5:A:409:17F:H52	5:D:511:17F:H39	0.59	1.74	3	1
4:B:204:PCW:H332	4:B:208:PCW:H321	0.59	1.73	5	1
4:A:403:PCW:C21	4:A:403:PCW:C17	0.59	2.80	10	3
4:C:617:PCW:H131	4:C:625:PCW:H132	0.59	1.75	6	1
4:B:206:PCW:H341	4:B:206:PCW:H62	0.59	1.74	6	1
4:A:401:PCW:C7	4:D:508:PCW:O31	0.59	2.50	8	2
4:A:404:PCW:H371	4:A:407:PCW:H182	0.59	1.73	7	1
4:A:415:PCW:C48	5:D:513:17F:H38	0.59	2.27	7	1
5:C:627:17F:N1	5:C:627:17F:O10	0.59	2.36	7	2
4:D:506:PCW:H41	4:D:506:PCW:C3	0.59	2.22	8	1
4:A:406:PCW:O2P	4:B:211:PCW:H63	0.59	1.97	9	1
4:C:621:PCW:O4P	4:C:621:PCW:C6	0.59	2.50	10	1
4:A:416:PCW:O31	4:C:616:PCW:H82	0.59	1.98	1	1
4:C:607:PCW:O11	4:C:607:PCW:H2	0.59	1.98	6	10
4:C:612:PCW:H482	4:C:618:PCW:H181	0.59	1.74	7	3
4:A:413:PCW:O4P	4:A:413:PCW:C6	0.59	2.50	5	3
4:B:208:PCW:C26	4:B:208:PCW:C22	0.59	2.74	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:505:PCW:C1	4:D:509:PCW:H73	0.59	2.27	8	3
4:C:612:PCW:H482	4:C:618:PCW:C21	0.59	2.28	8	2
4:B:206:PCW:C16	5:B:213:17F:H60	0.59	2.26	3	2
3:D:452:CYS:HA	3:D:459:LEU:HD23	0.59	1.74	7	4
4:A:412:PCW:O31	4:A:412:PCW:O3	0.59	2.21	8	3
4:C:606:PCW:H482	5:C:632:17F:H59	0.59	1.74	4	1
4:B:206:PCW:H442	5:B:213:17F:H32	0.59	1.72	4	1
4:B:210:PCW:C5	5:D:513:17F:H1A	0.59	2.28	4	3
4:D:507:PCW:C27	4:D:507:PCW:H483	0.59	2.28	4	1
5:A:410:17F:H78	4:C:610:PCW:H471	0.59	1.74	7	1
5:C:627:17F:H78	5:B:215:17F:C2X	0.59	2.24	7	2
4:D:501:PCW:C16	5:D:511:17F:H18	0.59	2.24	10	1
4:A:403:PCW:H63	4:A:403:PCW:H321	0.59	1.75	1	2
4:A:417:PCW:C21	4:C:603:PCW:H162	0.59	2.28	4	2
1:C:465:GLU:O	1:C:469:LEU:HG	0.59	1.98	8	8
4:C:609:PCW:C4	5:C:631:17F:O8	0.59	2.51	4	3
4:B:205:PCW:H152	4:B:206:PCW:H172	0.59	1.74	1	1
4:C:622:PCW:H131	4:C:622:PCW:C39	0.59	2.27	3	2
5:C:632:17F:C29	4:B:207:PCW:H161	0.59	2.28	3	1
4:C:617:PCW:H381	4:C:625:PCW:C16	0.59	2.19	4	2
4:D:501:PCW:H261	5:D:511:17F:H73	0.59	1.74	4	1
4:D:508:PCW:H451	4:D:508:PCW:C26	0.59	2.25	4	1
4:A:404:PCW:H171	4:B:210:PCW:C21	0.59	2.28	5	1
4:A:403:PCW:H171	4:A:403:PCW:H212	0.59	1.74	6	1
4:A:403:PCW:O31	4:A:403:PCW:C4	0.59	2.51	7	1
5:D:514:17F:H48	5:D:514:17F:H77	0.59	1.75	7	1
4:A:403:PCW:C11	4:B:201:PCW:H82	0.59	2.28	9	1
4:C:605:PCW:H472	4:C:618:PCW:H441	0.59	1.75	10	1
4:A:401:PCW:O3	4:A:401:PCW:O31	0.59	2.21	5	7
4:C:602:PCW:H261	5:C:629:17F:H78	0.59	1.75	6	3
4:D:507:PCW:H412	4:D:507:PCW:C37	0.59	2.26	2	1
4:C:605:PCW:C40	4:C:618:PCW:H141	0.59	2.28	10	2
4:C:622:PCW:H131	4:C:622:PCW:H39	0.59	1.73	3	1
4:B:212:PCW:H381	4:B:212:PCW:C17	0.59	2.28	10	2
4:D:501:PCW:H151	4:D:502:PCW:C33	0.59	2.28	4	1
4:D:501:PCW:C38	4:D:509:PCW:H422	0.59	2.20	4	2
4:C:620:PCW:H422	5:B:215:17F:H66	0.59	1.75	6	1
4:C:612:PCW:C26	5:D:511:17F:H50	0.59	2.28	7	2
4:C:605:PCW:P	4:C:612:PCW:H61	0.59	2.38	9	1
4:B:207:PCW:C24	5:B:214:17F:H55	0.59	2.26	10	1
4:A:403:PCW:C21	4:B:201:PCW:H181	0.58	2.26	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:204:PCW:C42	5:D:512:17F:H60	0.58	2.28	2	1
4:C:602:PCW:H362	5:B:214:17F:C34	0.58	2.28	4	1
4:C:607:PCW:H241	5:C:629:17F:C1X	0.58	2.28	4	1
4:A:406:PCW:H462	4:B:211:PCW:C18	0.58	2.27	5	1
4:C:619:PCW:H132	5:C:632:17F:C18	0.58	2.28	5	2
4:B:202:PCW:H2	4:B:202:PCW:H382	0.58	1.74	6	1
4:C:604:PCW:C3	4:C:604:PCW:O1P	0.58	2.50	1	5
4:C:605:PCW:O1P	4:C:612:PCW:C5	0.58	2.51	2	4
4:C:619:PCW:C27	5:C:632:17F:H37	0.58	2.27	1	1
4:A:417:PCW:H82	4:C:605:PCW:O3P	0.58	1.98	7	3
4:C:611:PCW:H352	4:C:625:PCW:H131	0.58	1.74	2	1
4:C:621:PCW:H321	4:C:625:PCW:C20	0.58	2.28	2	3
4:B:210:PCW:O1P	4:B:210:PCW:O2	0.58	2.21	6	2
4:D:516:PCW:O31	4:D:516:PCW:C1	0.58	2.49	5	9
4:A:404:PCW:C35	4:A:407:PCW:C15	0.58	2.80	4	1
5:A:409:17F:C31	4:D:504:PCW:H331	0.58	2.26	4	1
4:A:406:PCW:H431	4:B:211:PCW:C36	0.58	2.28	5	1
4:A:402:PCW:H322	4:D:507:PCW:H171	0.58	1.74	6	1
4:B:204:PCW:H221	4:B:208:PCW:H261	0.58	1.75	6	1
1:C:453:GLN:HB2	1:C:454:PRO:HD3	0.58	1.74	7	1
4:C:623:PCW:H462	4:C:624:PCW:H482	0.58	1.75	7	2
4:C:617:PCW:O1P	4:C:625:PCW:H82	0.58	1.98	9	1
2:B:142:ILE:HD12	4:B:210:PCW:H62	0.58	1.75	9	1
4:C:604:PCW:H381	5:C:627:17F:C2X	0.58	2.27	10	1
4:B:203:PCW:H261	4:B:204:PCW:C19	0.58	2.28	10	1
4:A:404:PCW:C6	4:A:404:PCW:O4P	0.58	2.51	3	9
4:A:412:PCW:H262	4:B:203:PCW:H481	0.58	1.72	6	2
4:C:620:PCW:H351	5:B:215:17F:H33	0.58	1.76	1	3
4:B:210:PCW:C48	5:D:513:17F:H32	0.58	2.22	1	1
2:B:21:ILE:HD13	3:D:388:VAL:CG1	0.58	2.28	5	5
4:A:408:PCW:H341	5:A:409:17F:H34	0.58	1.74	3	1
4:A:404:PCW:H171	4:B:210:PCW:C20	0.58	2.28	5	1
4:D:503:PCW:C17	4:D:507:PCW:H40	0.58	2.28	6	1
4:A:408:PCW:H321	5:A:409:17F:H33	0.58	1.73	7	1
4:C:606:PCW:O11	4:C:606:PCW:H51	0.58	1.98	9	2
4:B:208:PCW:H462	4:B:212:PCW:H212	0.58	1.73	8	1
4:C:617:PCW:H422	4:C:625:PCW:H231	0.58	1.75	9	2
5:B:214:17F:H36	5:B:214:17F:C24	0.58	2.24	9	1
4:B:204:PCW:H371	4:B:208:PCW:H342	0.58	1.74	10	1
4:A:407:PCW:H422	4:B:211:PCW:H462	0.58	1.75	1	2
4:A:415:PCW:H482	4:C:617:PCW:H281	0.58	1.75	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:601:PCW:H452	4:C:601:PCW:H322	0.58	1.75	1	1
4:C:620:PCW:C14	4:C:620:PCW:H181	0.58	2.26	10	6
4:D:505:PCW:C24	4:D:506:PCW:H39	0.58	2.26	1	1
4:A:405:PCW:O31	4:B:203:PCW:C7	0.58	2.52	2	1
4:A:414:PCW:N	4:C:624:PCW:O31	0.58	2.36	2	1
4:A:415:PCW:O2P	4:A:415:PCW:H52	0.58	1.99	8	3
4:C:624:PCW:O11	4:C:624:PCW:O2	0.58	2.21	2	1
4:A:407:PCW:C43	4:B:211:PCW:H212	0.58	2.28	7	2
4:B:205:PCW:C1	5:B:214:17F:H29	0.58	2.28	3	1
4:D:501:PCW:H351	5:D:512:17F:H37	0.58	1.76	3	1
4:C:615:PCW:H331	4:D:516:PCW:H341	0.58	1.75	4	1
4:B:205:PCW:H11	5:B:214:17F:H12A	0.58	1.75	4	1
5:A:410:17F:O1	4:D:502:PCW:H82	0.58	1.99	5	1
4:C:621:PCW:C11	5:C:627:17F:H65	0.58	2.29	5	2
4:B:206:PCW:O11	4:B:206:PCW:C5	0.58	2.51	5	2
4:B:210:PCW:O1P	4:B:210:PCW:H52	0.58	1.98	5	1
4:B:203:PCW:H221	4:B:208:PCW:O11	0.58	1.97	7	1
4:B:204:PCW:O11	4:B:212:PCW:H161	0.58	1.98	7	1
4:B:206:PCW:H19	5:B:213:17F:H19	0.58	1.75	8	1
4:A:404:PCW:C1	4:B:210:PCW:H381	0.58	2.18	9	1
4:B:201:PCW:H361	4:B:207:PCW:H31	0.58	1.75	9	1
4:B:212:PCW:H471	5:D:514:17F:C41	0.58	2.29	9	1
4:C:604:PCW:C28	5:B:213:17F:H51	0.58	2.28	10	1
4:C:608:PCW:C28	5:B:214:17F:H52	0.58	2.26	10	1
1:A:396:LYS:HG2	1:C:587:ALA:HB2	0.58	1.74	1	3
4:A:408:PCW:H231	5:A:409:17F:H56	0.58	1.73	1	1
1:A:330:ARG:HH21	1:C:447:GLU:HB3	0.58	1.59	2	3
4:A:403:PCW:C25	4:B:201:PCW:H162	0.58	2.28	5	2
4:A:405:PCW:H142	4:A:405:PCW:C18	0.58	2.27	5	6
4:B:201:PCW:H321	4:B:207:PCW:O2P	0.58	1.98	3	1
4:B:208:PCW:H442	4:B:212:PCW:C28	0.58	2.29	3	1
4:D:516:PCW:H372	4:D:516:PCW:H141	0.58	1.74	4	2
4:C:610:PCW:H471	4:D:501:PCW:H271	0.58	1.75	4	1
5:C:632:17F:H69	5:C:632:17F:H58	0.58	1.76	4	1
4:B:207:PCW:C40	4:B:209:PCW:H182	0.58	2.26	4	1
4:C:617:PCW:H63	4:C:621:PCW:O2P	0.58	1.99	5	2
4:A:413:PCW:H381	4:C:611:PCW:H432	0.58	1.76	10	1
4:C:606:PCW:C26	5:C:627:17F:H42	0.58	2.29	1	2
4:C:614:PCW:H51	5:C:632:17F:C3	0.58	2.29	7	4
2:B:15:GLY:HA3	6:B:216:GNP:H8	0.58	1.74	1	3
4:B:204:PCW:O4P	4:B:204:PCW:H82	0.58	1.98	6	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:508:PCW:C41	4:D:508:PCW:H372	0.58	2.28	1	1
4:C:609:PCW:H82	5:C:631:17F:O8	0.58	1.99	4	2
4:D:508:PCW:H232	4:D:508:PCW:C38	0.58	2.29	4	2
4:B:207:PCW:H462	4:B:209:PCW:H20	0.58	1.76	7	1
4:B:208:PCW:H52	5:B:214:17F:O9	0.58	1.98	9	1
4:B:203:PCW:H283	5:B:214:17F:C1Y	0.58	2.28	10	1
4:D:502:PCW:H471	4:D:508:PCW:H281	0.58	1.76	10	1
4:A:405:PCW:C2	5:D:512:17F:H31	0.58	2.26	1	2
4:A:417:PCW:O4P	4:A:417:PCW:H62	0.58	1.97	7	7
5:D:513:17F:H10A	5:D:513:17F:C37	0.58	2.28	1	1
4:C:620:PCW:H451	5:B:215:17F:H77	0.58	1.73	2	1
2:B:126:ASP:HB3	2:B:129:GLN:HG3	0.58	1.75	4	4
4:B:208:PCW:H442	4:B:212:PCW:H262	0.58	1.74	2	3
4:B:206:PCW:C46	5:B:213:17F:H68	0.58	2.22	3	1
4:A:407:PCW:H421	4:B:211:PCW:C46	0.58	2.27	4	2
4:C:604:PCW:H283	5:B:213:17F:C29	0.58	2.28	10	3
2:B:116:ASN:OD1	2:B:145:SER:HA	0.58	1.98	4	2
4:D:509:PCW:H452	4:D:510:PCW:H31	0.58	1.75	4	1
4:A:413:PCW:H441	4:C:611:PCW:C27	0.58	2.29	6	1
4:B:210:PCW:H282	4:D:503:PCW:C18	0.58	2.28	6	1
4:A:404:PCW:C24	4:B:210:PCW:H222	0.58	2.28	7	1
5:C:627:17F:C42	5:B:215:17F:H35	0.58	2.25	7	2
4:B:203:PCW:H242	4:B:208:PCW:C13	0.58	2.28	7	1
4:C:615:PCW:H61	4:C:616:PCW:H371	0.58	1.74	8	1
4:B:203:PCW:H63	4:B:203:PCW:O3P	0.58	1.98	9	1
4:C:606:PCW:O3P	4:C:606:PCW:O31	0.58	2.21	3	7
5:C:632:17F:H75	5:B:215:17F:C33	0.58	2.28	1	1
4:C:604:PCW:H411	4:C:604:PCW:C37	0.58	2.19	2	4
4:C:615:PCW:H482	4:D:503:PCW:C22	0.58	2.26	2	1
4:B:204:PCW:H42	5:B:214:17F:O4	0.58	1.99	10	2
4:C:620:PCW:H362	5:C:631:17F:C33	0.58	2.29	7	2
4:C:621:PCW:H341	4:D:516:PCW:C42	0.58	2.29	3	1
4:C:603:PCW:H462	4:D:515:PCW:C43	0.58	2.21	4	1
4:C:612:PCW:C47	4:C:618:PCW:H411	0.58	2.27	4	1
4:C:615:PCW:C40	4:C:617:PCW:H162	0.58	2.29	4	2
4:C:614:PCW:H231	4:B:207:PCW:H272	0.58	1.75	5	1
1:C:577:LEU:HD22	1:C:581:LYS:HE3	0.58	1.74	6	1
5:C:627:17F:H55	5:B:213:17F:H42	0.58	1.75	8	1
4:B:203:PCW:H382	4:B:203:PCW:H141	0.58	1.74	8	1
4:B:203:PCW:H82	4:B:204:PCW:H362	0.58	1.75	8	1
4:A:401:PCW:H182	4:A:401:PCW:C22	0.58	2.17	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:605:PCW:O31	4:C:612:PCW:H61	0.58	1.99	9	1
4:D:502:PCW:H431	5:D:512:17F:H10	0.58	1.75	9	1
4:A:408:PCW:H341	5:A:409:17F:H32	0.58	1.74	1	1
5:A:410:17F:O9	5:A:410:17F:H20	0.58	1.99	5	3
4:C:625:PCW:H251	4:D:516:PCW:H451	0.58	1.76	1	1
2:B:68:ARG:HA	2:B:71:TYR:CZ	0.58	2.34	5	6
4:C:622:PCW:H371	4:C:622:PCW:C13	0.58	2.26	3	1
4:B:203:PCW:H172	4:B:208:PCW:C36	0.58	2.28	3	1
4:A:404:PCW:H32	4:B:210:PCW:C14	0.58	2.29	4	2
4:C:608:PCW:H483	4:B:207:PCW:H481	0.58	1.76	5	1
4:B:206:PCW:H62	4:B:206:PCW:O11	0.58	1.98	6	1
4:A:407:PCW:H422	4:B:211:PCW:H442	0.58	1.74	8	1
4:C:616:PCW:C4	4:C:616:PCW:H2	0.58	2.29	8	1
4:B:203:PCW:C8	4:B:204:PCW:H362	0.58	2.29	8	1
4:A:415:PCW:H32	4:A:415:PCW:O4P	0.58	1.98	9	1
4:A:416:PCW:C32	4:C:616:PCW:H52	0.58	2.28	1	4
4:C:614:PCW:H462	4:B:206:PCW:H261	0.58	1.74	1	1
4:C:623:PCW:C45	4:C:624:PCW:H482	0.58	2.27	4	4
4:B:208:PCW:C48	4:B:208:PCW:H281	0.58	2.29	1	1
4:D:510:PCW:C12	4:D:510:PCW:H73	0.58	2.29	1	1
4:C:620:PCW:H151	5:B:215:17F:H6	0.58	1.75	2	1
4:C:620:PCW:H222	5:C:631:17F:H19	0.58	1.75	2	1
4:C:621:PCW:H482	4:D:506:PCW:H212	0.58	1.75	10	2
4:C:607:PCW:H432	5:C:626:17F:C34	0.58	2.29	8	2
4:A:404:PCW:H281	4:D:507:PCW:C48	0.58	2.28	4	1
4:C:604:PCW:O31	4:C:606:PCW:C8	0.58	2.52	7	5
5:C:629:17F:H4	5:C:629:17F:C1	0.58	2.26	5	1
4:C:617:PCW:H261	4:D:507:PCW:H483	0.58	1.76	6	1
4:A:407:PCW:H422	4:B:211:PCW:H181	0.58	1.75	7	1
4:C:614:PCW:H51	5:C:632:17F:C2	0.58	2.28	7	1
4:C:617:PCW:H351	4:C:625:PCW:H341	0.58	1.75	9	3
4:D:506:PCW:H482	4:D:516:PCW:C23	0.58	2.28	8	2
4:B:203:PCW:H39	4:B:203:PCW:C14	0.58	2.28	10	1
4:A:411:PCW:H39	4:A:411:PCW:C15	0.57	2.24	5	2
4:C:613:PCW:H432	4:C:618:PCW:H20	0.57	1.75	1	2
4:A:408:PCW:C43	4:A:408:PCW:C47	0.57	2.76	2	1
4:A:408:PCW:H212	5:A:409:17F:H59	0.57	1.76	2	1
4:A:412:PCW:C43	4:C:624:PCW:H481	0.57	2.29	8	3
4:C:612:PCW:H251	5:D:511:17F:H50	0.57	1.76	7	2
5:C:627:17F:H65	5:B:215:17F:C7	0.57	2.29	2	1
4:B:206:PCW:C41	5:B:213:17F:H8	0.57	2.28	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:210:PCW:H472	4:D:507:PCW:H221	0.57	1.76	4	1
5:B:213:17F:O7	5:B:213:17F:O10	0.57	2.21	5	4
4:C:603:PCW:H441	4:C:603:PCW:H231	0.57	1.76	8	2
4:D:508:PCW:H472	4:D:508:PCW:H262	0.57	1.74	7	1
4:A:403:PCW:C4	4:A:403:PCW:O31	0.57	2.51	8	1
4:B:212:PCW:H471	5:D:514:17F:H72	0.57	1.76	9	1
4:B:204:PCW:C41	5:D:514:17F:C8	0.57	2.80	1	1
4:A:417:PCW:H242	4:C:621:PCW:C23	0.57	2.29	2	1
5:B:213:17F:O10	5:B:213:17F:H20	0.57	1.98	2	3
3:D:459:LEU:HG	3:D:471:LYS:HB2	0.57	1.76	7	4
4:B:212:PCW:H352	5:B:214:17F:H37	0.57	1.77	3	1
4:A:406:PCW:H421	4:B:209:PCW:H40	0.57	1.74	4	1
4:B:205:PCW:H241	4:B:207:PCW:C43	0.57	2.27	4	1
4:B:206:PCW:H411	4:B:206:PCW:C37	0.57	2.20	4	3
1:C:478:ARG:O	1:C:482:GLN:HB2	0.57	1.99	8	2
4:C:603:PCW:O4P	5:C:628:17F:H1A	0.57	1.98	6	1
4:C:610:PCW:P	4:C:618:PCW:H63	0.57	2.39	6	1
4:B:206:PCW:H152	4:B:209:PCW:C12	0.57	2.27	6	1
4:A:415:PCW:H11	4:C:616:PCW:C38	0.57	2.29	7	1
4:D:508:PCW:O31	4:D:508:PCW:C1	0.57	2.50	9	2
4:C:615:PCW:C47	4:D:506:PCW:H40	0.57	2.29	10	1
4:D:509:PCW:C6	4:D:509:PCW:O4P	0.57	2.52	10	1
4:A:415:PCW:O2P	4:A:415:PCW:C3	0.57	2.50	1	1
4:C:606:PCW:O11	4:C:606:PCW:H2	0.57	1.99	5	9
5:C:632:17F:C42	5:B:215:17F:H58	0.57	2.29	1	1
4:B:204:PCW:C15	4:B:208:PCW:H382	0.57	2.24	1	1
4:D:510:PCW:H262	4:D:515:PCW:H461	0.57	1.75	1	2
4:A:407:PCW:H341	4:A:407:PCW:O31	0.57	2.00	5	4
4:D:504:PCW:O31	4:D:504:PCW:C36	0.57	2.52	6	5
4:C:617:PCW:O1P	4:C:625:PCW:H52	0.57	1.98	4	1
4:B:203:PCW:P	4:B:203:PCW:H63	0.57	2.39	5	1
4:A:406:PCW:C39	4:B:211:PCW:H362	0.57	2.30	6	1
4:B:202:PCW:O11	4:B:202:PCW:H63	0.57	1.99	6	1
4:B:206:PCW:H151	5:B:213:17F:H60	0.57	1.76	6	1
4:A:402:PCW:H231	4:A:413:PCW:C26	0.57	2.13	7	1
4:C:614:PCW:H211	5:C:632:17F:C22	0.57	2.28	8	1
4:C:615:PCW:H441	4:C:625:PCW:H231	0.57	1.77	8	1
4:A:404:PCW:C48	4:A:407:PCW:H221	0.57	2.30	9	1
4:C:608:PCW:H281	5:B:214:17F:C29	0.57	2.26	10	1
4:C:613:PCW:H62	4:C:623:PCW:O1P	0.57	1.99	1	1
4:B:208:PCW:O31	4:B:208:PCW:C4	0.57	2.52	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:509:PCW:H61	4:D:510:PCW:C34	0.57	2.26	1	1
4:B:212:PCW:H442	5:D:514:17F:H71	0.57	1.76	2	1
4:D:506:PCW:H171	4:D:510:PCW:H422	0.57	1.74	3	1
4:A:404:PCW:H32	4:B:210:PCW:H142	0.57	1.76	4	2
4:C:610:PCW:O2P	4:C:618:PCW:H52	0.57	1.99	9	2
4:B:201:PCW:H452	4:B:205:PCW:H282	0.57	1.76	5	1
4:C:610:PCW:O4P	4:C:622:PCW:H342	0.57	2.00	10	2
4:B:204:PCW:H142	4:B:208:PCW:H362	0.57	1.76	6	1
4:B:201:PCW:H321	4:B:207:PCW:P	0.57	2.40	9	1
4:D:507:PCW:H432	5:D:513:17F:H40	0.57	1.76	9	1
5:C:632:17F:C30	4:B:207:PCW:H172	0.57	2.29	10	1
4:A:403:PCW:C16	4:A:403:PCW:C21	0.57	2.81	7	6
4:A:414:PCW:C6	4:C:624:PCW:O31	0.57	2.51	2	1
2:B:82:PHE:HB3	2:B:93:ILE:HD11	0.57	1.74	8	5
5:A:410:17F:H61	5:D:511:17F:H19	0.57	1.76	3	1
4:A:412:PCW:H432	4:C:624:PCW:C47	0.57	2.29	10	3
4:C:607:PCW:O1P	4:C:624:PCW:C22	0.57	2.52	4	3
4:A:414:PCW:C32	4:C:623:PCW:H342	0.57	2.29	4	1
4:A:412:PCW:H342	4:C:624:PCW:H381	0.57	1.75	5	1
2:B:170:MET:HE2	2:B:170:MET:HA	0.57	1.77	10	4
4:B:203:PCW:H51	4:B:204:PCW:C34	0.57	2.26	6	1
4:C:604:PCW:H212	4:D:509:PCW:C28	0.57	2.23	7	1
4:C:614:PCW:H42	4:C:614:PCW:C2	0.57	2.28	9	1
3:D:402:LEU:HD11	3:D:409:LYS:HA	0.57	1.76	9	1
4:A:401:PCW:C6	4:D:508:PCW:H12	0.57	2.28	10	2
4:A:403:PCW:H132	4:B:201:PCW:C14	0.57	2.29	1	1
4:B:201:PCW:H282	4:B:205:PCW:H283	0.57	1.75	1	1
4:D:502:PCW:C11	4:D:502:PCW:O31	0.57	2.52	3	10
4:D:505:PCW:H181	4:D:505:PCW:C22	0.57	2.12	2	1
4:D:508:PCW:H132	4:D:508:PCW:C33	0.57	2.29	6	3
5:D:512:17F:O6	5:D:512:17F:H18A	0.57	1.99	4	4
4:A:407:PCW:H442	4:B:211:PCW:H482	0.57	1.75	3	1
4:B:202:PCW:C16	4:D:504:PCW:H322	0.57	2.29	8	2
4:A:404:PCW:C24	4:B:210:PCW:C22	0.57	2.81	4	2
5:A:410:17F:H73	4:D:501:PCW:H251	0.57	1.75	4	1
4:A:415:PCW:H40	4:C:615:PCW:C23	0.57	2.29	4	1
4:C:601:PCW:O1P	4:C:601:PCW:H331	0.57	2.00	4	1
4:B:207:PCW:H241	5:B:214:17F:H53	0.57	1.75	5	1
5:D:512:17F:C27	5:D:514:17F:H42	0.57	2.20	6	2
4:C:610:PCW:H31	4:C:618:PCW:O11	0.57	1.99	9	4
4:A:403:PCW:O31	4:A:403:PCW:O3P	0.57	2.23	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:615:PCW:C39	4:C:617:PCW:C16	0.57	2.81	9	2
4:A:415:PCW:H362	4:C:616:PCW:H382	0.57	1.76	8	1
5:A:409:17F:C24	5:D:511:17F:H18	0.57	2.17	9	1
4:A:403:PCW:C13	4:B:201:PCW:H141	0.57	2.30	1	1
4:A:408:PCW:H12	4:A:408:PCW:C37	0.57	2.29	1	1
4:C:605:PCW:O1P	4:C:605:PCW:H52	0.57	1.98	10	7
5:A:409:17F:P1	4:D:504:PCW:H341	0.57	2.40	2	1
4:C:607:PCW:C26	5:C:629:17F:H62	0.57	2.28	6	4
5:D:511:17F:O7	5:D:511:17F:O10	0.57	2.23	9	6
4:A:411:PCW:O3P	4:A:411:PCW:O31	0.57	2.23	3	2
4:C:616:PCW:O31	4:C:616:PCW:C5	0.57	2.52	3	1
4:B:210:PCW:O2P	4:B:210:PCW:H51	0.57	2.00	3	1
4:C:606:PCW:C6	4:C:624:PCW:H19	0.57	2.30	5	1
4:D:502:PCW:H121	4:D:508:PCW:H372	0.57	1.76	5	1
1:A:301:LEU:HD13	1:C:473:LYS:HG2	0.57	1.77	8	2
5:B:215:17F:O10	5:B:215:17F:O6	0.57	2.23	6	1
5:D:512:17F:H1	5:D:512:17F:H4	0.57	1.76	6	3
4:A:403:PCW:H162	4:A:403:PCW:H231	0.57	1.77	8	1
4:A:405:PCW:H321	4:B:203:PCW:C34	0.57	2.30	8	1
4:C:605:PCW:C48	4:C:618:PCW:H471	0.57	2.29	9	1
4:B:212:PCW:C35	5:B:213:17F:H11	0.57	2.30	9	1
1:A:341:ASN:HD21	1:C:432:LYS:HB3	0.57	1.60	2	2
4:C:612:PCW:H261	5:D:511:17F:H66	0.57	1.75	7	2
4:C:621:PCW:C16	4:D:516:PCW:H172	0.57	2.18	2	4
4:B:210:PCW:H252	4:B:211:PCW:H241	0.57	1.76	2	2
4:A:404:PCW:H351	4:A:407:PCW:C15	0.57	2.24	4	3
4:A:408:PCW:H341	5:A:409:17F:C32	0.57	2.26	7	2
4:C:604:PCW:C16	4:C:604:PCW:H211	0.57	2.29	3	1
4:C:608:PCW:C7	4:C:619:PCW:O11	0.57	2.52	4	3
4:C:618:PCW:H481	5:D:511:17F:C40	0.57	2.30	3	1
4:B:204:PCW:H412	4:B:212:PCW:H252	0.57	1.75	3	1
4:A:403:PCW:H82	4:B:209:PCW:C35	0.57	2.26	10	2
4:C:613:PCW:H452	4:C:618:PCW:C22	0.57	2.29	4	2
4:C:605:PCW:H262	4:C:612:PCW:H181	0.57	1.75	5	1
2:B:37:GLU:O	3:D:368:THR:HA	0.57	1.99	5	3
4:B:208:PCW:H121	5:B:214:17F:O7	0.57	1.99	7	2
4:D:508:PCW:C11	4:D:508:PCW:C31	0.57	2.82	7	2
3:D:447:LEU:HA	5:D:514:17F:C1	0.57	2.30	6	1
4:A:416:PCW:H442	4:C:616:PCW:H211	0.57	1.75	7	1
4:A:411:PCW:O31	4:A:411:PCW:O3P	0.57	2.23	9	1
4:B:204:PCW:H482	5:D:514:17F:C22	0.57	2.25	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:416:PCW:H372	4:C:616:PCW:C14	0.57	2.29	10	1
4:C:605:PCW:H481	4:C:618:PCW:H421	0.57	1.75	1	2
4:C:623:PCW:C15	4:C:623:PCW:C19	0.57	2.79	3	6
5:C:630:17F:H20A	5:C:630:17F:O10	0.57	1.99	9	5
4:D:507:PCW:H351	5:D:513:17F:H10	0.57	1.75	10	3
4:D:507:PCW:O11	4:D:507:PCW:H2	0.57	1.99	5	7
4:A:408:PCW:C34	5:A:409:17F:H59	0.57	2.29	3	1
4:A:412:PCW:H432	4:C:624:PCW:C48	0.57	2.30	3	1
4:A:415:PCW:H362	4:C:616:PCW:H381	0.57	1.75	3	2
2:B:36:ILE:HA	2:B:59:ALA:HB2	0.57	1.75	3	3
2:B:135:ARG:CZ	4:B:209:PCW:H82	0.57	2.30	3	1
4:A:405:PCW:H19	4:A:405:PCW:C15	0.57	2.29	4	1
5:A:410:17F:O2	4:D:502:PCW:H82	0.57	1.99	4	1
4:A:411:PCW:H442	4:C:616:PCW:C21	0.57	2.29	8	4
4:C:607:PCW:C6	4:C:624:PCW:H241	0.57	2.24	4	1
4:B:203:PCW:H283	5:B:214:17F:C20	0.57	2.30	4	2
4:B:204:PCW:H212	4:B:204:PCW:C17	0.57	2.25	9	3
4:B:205:PCW:O4P	5:B:214:17F:H10A	0.57	2.00	4	1
4:B:206:PCW:H162	5:B:213:17F:H56	0.57	1.77	4	1
4:A:401:PCW:C6	4:D:508:PCW:H2	0.57	2.28	5	2
4:B:205:PCW:H162	4:B:206:PCW:H182	0.57	1.77	6	1
4:A:413:PCW:C41	4:A:413:PCW:H371	0.57	2.30	8	1
4:C:608:PCW:H182	4:C:614:PCW:H341	0.57	1.76	9	1
4:B:212:PCW:H471	5:D:514:17F:C40	0.57	2.29	9	1
4:D:502:PCW:C21	4:D:502:PCW:H171	0.57	2.29	9	1
4:D:503:PCW:H32	5:D:513:17F:H4	0.57	1.76	9	1
4:A:408:PCW:H161	5:A:409:17F:H31	0.57	1.76	3	1
4:C:603:PCW:H472	4:C:603:PCW:C23	0.57	2.29	3	1
4:C:616:PCW:C47	4:C:616:PCW:C43	0.57	2.78	8	2
4:B:202:PCW:H332	4:D:507:PCW:O2P	0.57	2.00	3	1
4:B:205:PCW:H242	4:B:207:PCW:H411	0.57	1.75	3	2
4:A:401:PCW:C3	4:D:508:PCW:H231	0.57	2.29	4	2
5:A:410:17F:C42	4:C:618:PCW:H452	0.57	2.30	4	1
5:C:629:17F:H9	5:C:629:17F:C18	0.57	2.30	4	2
4:A:404:PCW:O4P	4:A:404:PCW:C6	0.57	2.53	5	1
4:A:408:PCW:C16	5:A:409:17F:H59	0.57	2.18	6	1
5:A:410:17F:H2	5:A:410:17F:O1	0.57	1.99	9	3
4:A:403:PCW:H32	4:B:201:PCW:H82	0.57	1.75	10	1
4:D:508:PCW:H19	5:D:512:17F:H32	0.57	1.74	10	1
4:A:408:PCW:H351	4:A:408:PCW:O2	0.56	2.00	1	1
4:C:615:PCW:P	4:C:615:PCW:C3	0.56	2.93	8	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:618:PCW:O4P	4:C:618:PCW:H82	0.56	2.00	2	10
5:C:627:17F:H70	5:C:628:17F:C35	0.56	2.30	2	2
4:B:206:PCW:P	4:B:206:PCW:C3	0.56	2.93	9	6
5:B:215:17F:O7	5:B:215:17F:O10	0.56	2.22	7	7
4:D:509:PCW:C8	4:D:510:PCW:H341	0.56	2.29	1	1
4:D:510:PCW:O4P	4:D:510:PCW:O31	0.56	2.22	1	1
4:A:408:PCW:H442	5:A:409:17F:H70	0.56	1.74	2	1
4:D:507:PCW:H371	4:D:507:PCW:C41	0.56	2.23	2	1
4:C:603:PCW:H52	5:C:628:17F:C3	0.56	2.30	3	2
5:C:627:17F:H68	5:B:215:17F:H11	0.56	1.76	3	1
4:B:210:PCW:O4P	5:D:513:17F:H4	0.56	2.00	5	1
4:D:503:PCW:C35	4:D:510:PCW:C8	0.56	2.83	5	1
4:D:506:PCW:H342	4:D:507:PCW:C40	0.56	2.29	6	1
4:A:404:PCW:C17	4:B:210:PCW:H222	0.56	2.28	8	1
4:A:405:PCW:C28	4:A:405:PCW:H472	0.56	2.30	8	1
4:C:602:PCW:C8	5:B:214:17F:O2	0.56	2.53	9	1
4:B:206:PCW:H251	4:B:206:PCW:H483	0.56	1.75	9	1
4:D:501:PCW:H261	5:D:511:17F:C34	0.56	2.30	9	1
4:A:416:PCW:C37	4:C:616:PCW:H141	0.56	2.30	10	1
4:B:204:PCW:O31	4:B:204:PCW:O3	0.56	2.21	5	8
4:A:407:PCW:H421	4:A:407:PCW:C28	0.56	2.30	2	1
4:A:417:PCW:C3	4:C:603:PCW:H31	0.56	2.30	3	1
4:A:412:PCW:O3	4:A:412:PCW:O31	0.56	2.22	5	1
4:C:612:PCW:H431	4:C:618:PCW:C40	0.56	2.29	5	1
4:D:503:PCW:H52	4:D:510:PCW:H62	0.56	1.75	5	1
4:D:505:PCW:C13	4:D:505:PCW:C17	0.56	2.81	6	3
4:C:605:PCW:O3P	4:C:605:PCW:O31	0.56	2.23	7	1
5:D:514:17F:O8	5:D:514:17F:O9	0.56	2.22	8	1
2:B:169:LYS:HG3	4:B:202:PCW:H82	0.56	1.77	10	2
4:B:205:PCW:H212	4:B:207:PCW:H411	0.56	1.76	9	1
4:A:404:PCW:H63	4:A:404:PCW:O2	0.56	2.00	10	1
4:B:205:PCW:H152	4:B:206:PCW:H182	0.56	1.76	10	1
4:B:212:PCW:C28	5:D:512:17F:H71	0.56	2.28	10	1
4:B:212:PCW:C41	5:D:514:17F:H33	0.56	2.30	10	1
1:A:396:LYS:HE2	1:C:587:ALA:HA	0.56	1.76	1	5
4:A:412:PCW:H31	4:C:624:PCW:C39	0.56	2.30	1	5
4:C:607:PCW:H63	4:C:624:PCW:H262	0.56	1.76	7	2
4:C:622:PCW:H52	4:C:622:PCW:O1P	0.56	2.00	10	6
4:B:208:PCW:H483	4:B:212:PCW:H241	0.56	1.77	1	1
4:D:505:PCW:O31	4:D:505:PCW:C1	0.56	2.50	7	4
4:A:407:PCW:C11	4:A:407:PCW:O31	0.56	2.53	3	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:413:PCW:C43	4:C:611:PCW:H172	0.56	2.12	2	3
4:B:209:PCW:H2	4:B:209:PCW:O11	0.56	2.00	2	1
4:D:506:PCW:H342	4:D:507:PCW:H411	0.56	1.76	2	1
4:A:405:PCW:C39	5:D:512:17F:H64	0.56	2.30	3	1
1:C:534:GLU:HA	1:C:537:LYS:HE3	0.56	1.78	9	2
4:D:504:PCW:H221	4:D:504:PCW:H182	0.56	1.77	3	1
4:D:507:PCW:H351	5:D:513:17F:O8	0.56	2.00	3	1
4:A:404:PCW:H42	4:A:407:PCW:H32	0.56	1.77	4	1
4:B:205:PCW:H142	4:B:206:PCW:C19	0.56	2.29	4	1
5:C:627:17F:H46	5:C:628:17F:H78	0.56	1.75	5	1
4:D:503:PCW:C4	4:D:510:PCW:C7	0.56	2.83	5	1
4:A:403:PCW:H152	4:B:207:PCW:C39	0.56	2.29	7	1
5:A:410:17F:H65	4:D:501:PCW:H241	0.56	1.76	7	1
4:B:203:PCW:C25	4:B:204:PCW:H19	0.56	2.27	7	1
4:C:613:PCW:H442	4:C:618:PCW:H19	0.56	1.77	9	1
4:B:210:PCW:H241	4:B:211:PCW:H242	0.56	1.77	9	1
4:A:413:PCW:C47	4:C:611:PCW:H271	0.56	2.30	10	1
4:C:610:PCW:O4P	4:C:622:PCW:C34	0.56	2.53	10	1
4:C:620:PCW:H381	5:C:632:17F:C42	0.56	2.30	1	1
4:B:212:PCW:H422	5:D:514:17F:H68	0.56	1.77	1	1
4:C:612:PCW:H272	5:D:511:17F:H50	0.56	1.77	2	2
4:C:615:PCW:H271	4:C:617:PCW:H283	0.56	1.77	5	2
4:C:614:PCW:H272	5:C:632:17F:H45	0.56	1.77	4	2
4:C:617:PCW:H151	4:C:625:PCW:C14	0.56	2.15	7	2
4:C:614:PCW:H211	5:C:632:17F:C24	0.56	2.30	6	1
4:A:417:PCW:H472	5:D:511:17F:H54	0.56	1.76	7	1
4:B:201:PCW:O11	4:B:201:PCW:H63	0.56	2.01	7	1
4:A:402:PCW:H361	4:B:210:PCW:H442	0.56	1.76	8	1
4:B:212:PCW:C40	5:D:514:17F:H30	0.56	2.30	8	1
4:C:601:PCW:H61	4:C:602:PCW:H32	0.56	1.76	9	1
4:D:502:PCW:H152	4:D:508:PCW:C40	0.56	2.31	10	1
4:C:608:PCW:O31	4:C:608:PCW:O3	0.56	2.23	5	3
5:C:628:17F:C30	5:B:213:17F:H77	0.56	2.30	1	1
4:D:505:PCW:C16	4:D:510:PCW:H471	0.56	2.13	1	1
5:A:409:17F:C28	4:D:510:PCW:H231	0.56	2.30	2	1
4:D:508:PCW:C31	4:D:508:PCW:C11	0.56	2.84	6	2
5:C:629:17F:O7	5:C:629:17F:C17	0.56	2.54	7	3
5:C:632:17F:H53	4:B:207:PCW:H161	0.56	1.75	6	2
4:A:414:PCW:H322	4:C:623:PCW:H342	0.56	1.78	4	1
4:C:615:PCW:H432	4:C:625:PCW:H232	0.56	1.76	4	1
4:D:505:PCW:C28	4:D:509:PCW:H481	0.56	2.31	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:32:TYR:HD1	6:B:216:GNP:H5'1	0.56	1.61	5	1
4:D:504:PCW:H52	4:D:504:PCW:H352	0.56	1.76	6	1
4:A:415:PCW:H451	4:D:515:PCW:C23	0.56	2.29	7	1
4:D:504:PCW:H171	4:D:504:PCW:H483	0.56	1.75	7	1
4:A:403:PCW:H481	4:B:209:PCW:H262	0.56	1.73	9	1
4:B:206:PCW:H421	5:B:213:17F:C1Z	0.56	2.28	9	1
4:C:619:PCW:O1P	4:C:620:PCW:C5	0.56	2.50	1	1
5:C:630:17F:O10	5:C:630:17F:O6	0.56	2.24	6	7
4:B:211:PCW:H461	4:B:211:PCW:C21	0.56	2.31	1	1
4:C:607:PCW:C19	5:C:629:17F:H50	0.56	2.31	6	4
4:A:404:PCW:H232	4:B:210:PCW:H222	0.56	1.76	4	1
4:A:407:PCW:H362	4:B:211:PCW:H141	0.56	1.77	6	1
4:A:417:PCW:H242	4:C:621:PCW:H241	0.56	1.77	6	1
1:C:573:LEU:HA	1:C:576:VAL:HG12	0.56	1.77	8	3
4:C:607:PCW:C6	4:C:624:PCW:H242	0.56	2.25	2	2
4:B:205:PCW:O3	4:B:205:PCW:O31	0.56	2.24	2	8
4:B:208:PCW:P	5:B:214:17F:HN1	0.56	2.23	1	1
4:D:505:PCW:H381	4:D:505:PCW:C42	0.56	2.22	1	1
4:D:507:PCW:H121	5:D:513:17F:O8	0.56	2.00	1	1
4:A:403:PCW:H162	4:A:403:PCW:C22	0.56	2.29	3	2
4:D:504:PCW:O2P	4:D:507:PCW:H52	0.56	2.00	2	1
4:A:413:PCW:H431	4:C:611:PCW:H171	0.56	1.75	3	2
4:C:602:PCW:O31	4:C:602:PCW:C3	0.56	2.53	8	4
4:C:606:PCW:C43	5:B:215:17F:H55	0.56	2.30	4	1
4:C:608:PCW:H431	4:B:207:PCW:C23	0.56	2.30	4	1
4:C:620:PCW:C21	5:C:631:17F:H19A	0.56	2.31	5	1
5:D:512:17F:H52	5:D:514:17F:C26	0.56	2.16	5	1
4:D:505:PCW:H442	4:D:506:PCW:C16	0.56	2.30	7	2
4:B:210:PCW:H262	4:D:503:PCW:H262	0.56	1.77	8	1
4:A:413:PCW:H352	4:C:611:PCW:H131	0.56	1.76	9	1
5:B:215:17F:H5	5:B:215:17F:O1	0.56	2.00	4	5
4:A:407:PCW:H321	4:A:407:PCW:C7	0.56	2.31	10	3
4:A:411:PCW:C28	4:A:415:PCW:H251	0.56	2.31	3	1
5:C:626:17F:C23	5:C:629:17F:H78	0.56	2.16	3	2
4:B:203:PCW:C23	4:B:208:PCW:H82	0.56	2.31	3	1
4:B:205:PCW:H372	4:B:207:PCW:C12	0.56	2.28	3	1
4:A:407:PCW:H332	4:B:211:PCW:C39	0.56	2.27	5	1
4:A:407:PCW:C33	4:B:211:PCW:H39	0.56	2.29	5	1
4:A:412:PCW:C34	4:C:624:PCW:C38	0.56	2.82	5	1
4:A:413:PCW:H422	4:C:611:PCW:C27	0.56	2.30	5	1
4:C:611:PCW:H261	4:C:611:PCW:C47	0.56	2.18	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:204:PCW:H181	4:B:208:PCW:H221	0.56	1.77	5	3
4:A:403:PCW:H151	4:B:201:PCW:C38	0.56	2.31	8	1
4:A:403:PCW:H161	4:B:201:PCW:H141	0.56	1.78	8	1
5:D:512:17F:H36	5:D:514:17F:H37	0.56	1.76	8	1
4:A:404:PCW:H241	5:C:631:17F:H54	0.56	1.75	9	1
4:A:408:PCW:H162	5:A:409:17F:H33	0.56	1.75	9	1
4:C:609:PCW:H62	5:C:631:17F:P1	0.56	2.39	9	2
4:A:407:PCW:C27	4:A:407:PCW:C23	0.56	2.78	10	1
4:C:604:PCW:H381	5:C:627:17F:H41	0.56	1.77	2	2
4:C:605:PCW:H472	4:C:618:PCW:C43	0.56	2.29	1	1
4:A:405:PCW:O31	4:B:203:PCW:H61	0.56	2.00	2	1
4:A:416:PCW:H61	5:C:630:17F:O2	0.56	2.01	2	1
4:D:505:PCW:O11	4:D:505:PCW:C2	0.56	2.51	3	2
5:A:409:17F:O10	5:A:409:17F:O6	0.56	2.24	7	2
4:C:613:PCW:C8	4:C:623:PCW:O1P	0.56	2.54	8	2
4:D:516:PCW:H372	4:D:516:PCW:C14	0.56	2.31	4	4
4:A:402:PCW:O4P	4:A:402:PCW:H82	0.56	2.01	5	3
5:B:214:17F:O10	5:B:214:17F:C7	0.56	2.53	8	4
4:D:503:PCW:H262	4:D:507:PCW:C42	0.56	2.31	4	1
4:A:413:PCW:H422	4:C:611:PCW:H272	0.56	1.76	5	1
4:B:210:PCW:H262	4:D:503:PCW:H272	0.56	1.77	5	2
4:B:203:PCW:C24	4:B:204:PCW:H151	0.56	2.31	6	1
4:C:620:PCW:H483	5:B:215:17F:C1Z	0.56	2.31	7	1
4:A:401:PCW:H252	4:C:613:PCW:C27	0.56	2.31	10	1
4:A:413:PCW:H422	4:C:611:PCW:C24	0.56	2.31	4	3
4:C:601:PCW:C46	4:C:601:PCW:C42	0.56	2.74	1	3
4:B:205:PCW:H121	4:B:207:PCW:C17	0.56	2.31	1	1
4:D:503:PCW:H172	4:D:507:PCW:C40	0.56	2.31	1	1
4:D:503:PCW:H82	4:D:503:PCW:O4P	0.56	2.01	10	8
4:A:407:PCW:C31	4:A:407:PCW:H52	0.56	2.31	8	4
4:A:404:PCW:H331	4:A:407:PCW:C15	0.56	2.31	3	1
4:D:505:PCW:C46	4:D:506:PCW:H161	0.56	2.28	3	1
4:A:407:PCW:O31	4:A:407:PCW:C11	0.56	2.54	5	2
4:A:417:PCW:H481	5:D:511:17F:C28	0.56	2.30	4	1
4:B:207:PCW:H63	3:D:447:LEU:O	0.56	2.01	5	1
4:B:211:PCW:C19	4:D:505:PCW:H471	0.56	2.31	5	1
5:B:213:17F:C21	4:D:505:PCW:H152	0.56	2.31	5	1
4:D:509:PCW:H63	4:D:510:PCW:H341	0.56	1.77	5	1
4:B:208:PCW:H272	4:B:208:PCW:C41	0.56	2.32	6	1
4:D:502:PCW:H39	5:D:512:17F:H8	0.56	1.76	6	1
4:B:211:PCW:H171	4:D:505:PCW:H412	0.56	1.77	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:502:PCW:C31	4:D:502:PCW:H52	0.56	2.31	8	1
4:B:204:PCW:H221	4:B:208:PCW:H221	0.56	1.76	9	1
5:A:409:17F:O4	4:B:202:PCW:C8	0.56	2.53	10	1
4:C:603:PCW:C22	4:D:515:PCW:H331	0.55	2.29	1	1
4:C:615:PCW:O3	4:C:615:PCW:O31	0.55	2.24	10	9
4:D:506:PCW:H12	4:D:506:PCW:O31	0.55	2.01	2	6
4:C:623:PCW:C19	4:C:623:PCW:C15	0.55	2.84	8	4
4:A:417:PCW:O4P	4:A:417:PCW:C6	0.55	2.54	10	2
4:B:201:PCW:H331	4:B:209:PCW:H31	0.55	1.77	3	1
4:B:202:PCW:H342	4:D:504:PCW:H31	0.55	1.78	3	2
4:D:502:PCW:H483	5:D:512:17F:H9A	0.55	1.78	3	1
4:D:506:PCW:H331	4:D:510:PCW:C35	0.55	2.32	3	1
4:A:417:PCW:H2	4:A:417:PCW:C6	0.55	2.24	4	1
4:D:502:PCW:H421	4:D:508:PCW:C20	0.55	2.29	4	1
4:C:605:PCW:H212	4:C:612:PCW:H141	0.55	1.78	5	1
4:D:503:PCW:C35	4:D:510:PCW:H141	0.55	2.27	5	1
4:D:508:PCW:H121	5:D:512:17F:O10	0.55	2.01	8	2
4:C:621:PCW:H19	5:C:628:17F:C20	0.55	2.30	6	2
4:B:204:PCW:O31	4:B:204:PCW:O3P	0.55	2.24	6	1
4:D:508:PCW:C11	4:D:508:PCW:H73	0.55	2.31	6	1
4:A:405:PCW:H421	4:A:414:PCW:C24	0.55	2.31	7	1
4:C:614:PCW:H283	5:B:214:17F:H74	0.55	1.78	8	1
4:A:406:PCW:C46	4:D:506:PCW:H271	0.55	2.31	9	1
4:D:502:PCW:H471	4:D:508:PCW:H271	0.55	1.78	9	1
4:A:406:PCW:H483	4:D:506:PCW:H262	0.55	1.77	10	1
5:A:409:17F:H56	4:D:504:PCW:C43	0.55	2.31	10	1
4:A:411:PCW:H61	5:C:630:17F:H2	0.55	1.77	10	1
4:B:212:PCW:C40	5:B:213:17F:H50	0.55	2.29	10	1
4:A:416:PCW:O31	4:A:416:PCW:O3P	0.55	2.24	4	6
1:C:448:VAL:HG22	1:C:452:VAL:HG23	0.55	1.77	8	2
5:C:626:17F:H8	5:C:629:17F:H33	0.55	1.76	2	3
4:B:212:PCW:H421	5:D:514:17F:H12	0.55	1.77	1	2
4:D:507:PCW:O3P	4:D:507:PCW:O31	0.55	2.25	1	4
5:C:632:17F:H52	4:B:207:PCW:C18	0.55	2.31	2	1
2:B:21:ILE:HD13	3:D:388:VAL:HG11	0.55	1.77	5	3
4:A:401:PCW:O3P	4:A:401:PCW:O31	0.55	2.24	3	1
4:A:411:PCW:O11	4:A:411:PCW:H2	0.55	2.00	3	2
4:A:412:PCW:H31	4:C:624:PCW:C38	0.55	2.31	4	6
4:C:615:PCW:H421	4:C:625:PCW:C23	0.55	2.27	6	2
1:A:334:ARG:HD3	1:C:440:GLU:OE1	0.55	2.02	4	1
4:A:417:PCW:H282	4:C:621:PCW:H283	0.55	1.76	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:212:PCW:H442	5:D:514:17F:H68	0.55	1.78	4	1
4:D:505:PCW:H2	4:D:509:PCW:C6	0.55	2.17	5	1
5:D:512:17F:H12	5:D:514:17F:H29	0.55	1.77	5	1
4:C:615:PCW:C38	4:C:617:PCW:H142	0.55	2.31	10	2
4:C:601:PCW:H40	4:C:602:PCW:C23	0.55	2.31	10	3
4:C:601:PCW:C39	5:C:626:17F:H52	0.55	2.32	6	4
4:C:611:PCW:H332	4:C:625:PCW:H131	0.55	1.77	1	1
4:C:613:PCW:H19	4:C:622:PCW:H481	0.55	1.78	1	1
4:C:620:PCW:H371	5:C:631:17F:C34	0.55	2.32	1	5
4:B:202:PCW:O31	4:B:202:PCW:C1	0.55	2.52	6	6
4:D:505:PCW:H151	4:D:510:PCW:H431	0.55	1.78	1	1
4:B:206:PCW:H452	5:B:213:17F:C42	0.55	2.31	2	1
4:A:403:PCW:O4P	4:A:403:PCW:O31	0.55	2.25	3	1
4:A:413:PCW:H372	4:C:611:PCW:C18	0.55	2.31	3	1
2:B:47:ASP:HA	3:D:448:LYS:HD3	0.55	1.78	3	1
4:A:413:PCW:H352	4:C:611:PCW:H181	0.55	1.76	4	1
4:B:206:PCW:C44	5:B:213:17F:H32	0.55	2.31	4	2
4:D:502:PCW:C45	4:D:508:PCW:H20	0.55	2.30	4	1
4:A:413:PCW:C42	4:C:611:PCW:H272	0.55	2.31	5	1
5:C:632:17F:H71	5:B:215:17F:H65	0.55	1.78	5	2
4:B:204:PCW:C2	4:B:208:PCW:H132	0.55	2.30	5	1
4:B:206:PCW:C41	5:B:213:17F:H11A	0.55	2.20	5	2
4:A:405:PCW:H322	4:B:203:PCW:C35	0.55	2.29	9	1
4:B:208:PCW:O31	4:B:208:PCW:O4P	0.55	2.24	1	1
4:B:212:PCW:O2P	5:B:214:17F:H10	0.55	2.01	1	1
4:B:212:PCW:C40	5:D:514:17F:H71	0.55	2.30	1	1
4:D:505:PCW:C15	4:D:510:PCW:H452	0.55	2.31	1	1
5:D:514:17F:O9	5:D:514:17F:O8	0.55	2.23	6	6
4:A:406:PCW:C43	4:B:211:PCW:H19	0.55	2.30	2	1
1:C:463:TRP:CD1	5:C:629:17F:H71	0.55	2.36	5	2
4:C:613:PCW:C45	4:C:618:PCW:H20	0.55	2.32	7	2
4:C:616:PCW:O11	4:C:616:PCW:H2	0.55	2.01	2	3
4:B:202:PCW:C19	4:D:504:PCW:H122	0.55	2.32	2	2
4:D:509:PCW:O31	4:D:509:PCW:O3P	0.55	2.24	5	4
5:D:514:17F:H30	5:D:514:17F:C34	0.55	2.30	2	1
4:D:510:PCW:H40	4:D:516:PCW:H283	0.55	1.78	4	1
4:B:209:PCW:H281	5:B:215:17F:H74	0.55	1.78	5	1
4:C:607:PCW:C6	4:C:624:PCW:H222	0.55	2.31	6	1
4:B:202:PCW:H362	4:B:202:PCW:C32	0.55	2.31	6	2
4:B:203:PCW:H272	4:B:204:PCW:H19	0.55	1.78	7	1
4:C:602:PCW:H151	5:C:626:17F:H54	0.55	1.77	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:503:PCW:O1P	4:D:503:PCW:H32	0.55	2.00	8	1
4:B:208:PCW:H441	5:D:512:17F:H72	0.55	1.77	10	1
4:B:210:PCW:H252	4:D:503:PCW:H252	0.55	1.78	10	1
4:C:610:PCW:C3	4:C:618:PCW:H63	0.55	2.32	1	2
4:C:621:PCW:H171	4:D:516:PCW:H121	0.55	1.78	1	1
4:B:211:PCW:H31	4:D:506:PCW:C8	0.55	2.31	1	1
4:D:505:PCW:H461	4:D:506:PCW:H121	0.55	1.77	1	1
4:D:509:PCW:O11	4:D:509:PCW:O2	0.55	2.23	6	9
4:A:401:PCW:H361	4:D:502:PCW:C19	0.55	2.31	2	1
4:A:413:PCW:C32	4:C:611:PCW:H32	0.55	2.31	2	1
4:C:606:PCW:H442	4:C:608:PCW:O2	0.55	2.02	10	2
5:C:627:17F:C24	5:C:628:17F:H73	0.55	2.32	3	1
5:C:628:17F:H10A	5:C:628:17F:C33	0.55	2.30	3	2
4:D:503:PCW:P	5:D:513:17F:O1	0.55	2.65	3	3
4:B:201:PCW:O4P	4:B:201:PCW:O2	0.55	2.23	4	4
5:A:410:17F:H31	4:D:502:PCW:H171	0.55	1.77	5	1
4:C:602:PCW:H461	4:C:607:PCW:C47	0.55	2.30	5	1
5:D:513:17F:H69	5:D:513:17F:C12	0.55	2.32	5	1
4:A:408:PCW:H121	5:A:409:17F:C35	0.55	2.31	6	1
4:B:207:PCW:H332	4:B:209:PCW:H121	0.55	1.78	6	1
4:D:504:PCW:O31	4:D:504:PCW:H362	0.55	2.02	6	2
4:C:603:PCW:O11	4:C:604:PCW:C6	0.55	2.48	7	1
4:A:406:PCW:H483	4:B:211:PCW:H182	0.55	1.77	8	1
5:A:409:17F:H43	5:D:511:17F:C1Z	0.55	2.32	8	1
4:A:406:PCW:O31	4:A:406:PCW:O3	0.55	2.25	1	7
4:C:613:PCW:C7	4:C:613:PCW:O4P	0.55	2.55	1	2
4:C:606:PCW:C25	5:C:627:17F:H38	0.55	2.32	9	4
2:B:35:THR:O	2:B:59:ALA:HA	0.55	2.02	2	3
4:B:210:PCW:H19	4:B:210:PCW:H431	0.55	1.79	2	1
4:D:510:PCW:O31	4:D:510:PCW:O4P	0.55	2.25	9	6
4:A:411:PCW:H282	4:A:415:PCW:H251	0.55	1.77	3	2
2:B:48:GLY:HA2	3:D:450:ALA:HA	0.55	1.76	3	1
5:D:512:17F:H11A	5:D:514:17F:H29	0.55	1.78	6	2
4:B:207:PCW:H241	5:B:214:17F:C30	0.55	2.32	5	1
4:C:606:PCW:H352	5:C:627:17F:O8	0.55	2.02	6	1
4:B:201:PCW:O11	4:B:201:PCW:C5	0.55	2.54	7	2
4:A:412:PCW:H483	4:A:414:PCW:H481	0.55	1.79	7	1
4:A:414:PCW:H40	4:C:623:PCW:C46	0.55	2.24	7	2
4:C:603:PCW:C24	4:D:515:PCW:H351	0.55	2.31	7	1
5:C:626:17F:H40	5:C:629:17F:H75	0.55	1.79	8	1
4:D:503:PCW:H131	4:D:506:PCW:C5	0.55	2.31	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:417:PCW:H472	5:D:511:17F:H76	0.55	1.77	9	1
4:B:208:PCW:C8	5:B:214:17F:H19	0.55	2.31	10	2
4:C:617:PCW:H431	4:C:625:PCW:H282	0.55	1.78	10	1
4:A:405:PCW:O2P	4:B:203:PCW:H61	0.55	2.01	9	2
4:A:405:PCW:H361	4:B:203:PCW:H361	0.55	1.77	5	2
4:A:412:PCW:H432	4:C:624:PCW:H481	0.55	1.77	5	2
4:A:406:PCW:H421	4:B:209:PCW:C40	0.55	2.31	4	1
4:A:411:PCW:H152	4:D:515:PCW:H162	0.55	1.79	4	1
4:C:606:PCW:H41	4:C:606:PCW:O31	0.55	2.02	6	3
5:A:410:17F:H65	4:D:502:PCW:H272	0.55	1.78	10	1
4:A:416:PCW:C12	5:C:630:17F:H11	0.55	2.32	7	5
4:A:417:PCW:H451	5:D:511:17F:C41	0.55	2.22	3	1
4:A:417:PCW:O31	4:A:417:PCW:C6	0.55	2.50	3	1
4:A:401:PCW:C43	4:C:613:PCW:H262	0.55	2.29	4	2
4:C:609:PCW:C6	5:C:631:17F:O8	0.55	2.55	4	1
5:C:629:17F:C9	5:C:629:17F:C18	0.55	2.83	4	2
4:A:408:PCW:H51	4:A:408:PCW:O2P	0.55	2.01	5	1
4:A:404:PCW:H482	4:A:407:PCW:H231	0.55	1.77	6	1
4:D:505:PCW:C36	4:D:506:PCW:H122	0.55	2.32	6	2
4:A:408:PCW:H272	4:D:504:PCW:H162	0.55	1.79	7	1
4:B:210:PCW:C4	5:D:513:17F:H1A	0.55	2.32	7	1
4:C:602:PCW:H2	5:B:214:17F:H57	0.55	1.78	8	1
4:A:415:PCW:O31	4:A:415:PCW:O3	0.55	2.24	9	1
4:A:402:PCW:H73	5:D:513:17F:O5	0.55	2.02	10	1
4:C:601:PCW:H421	5:C:626:17F:H52	0.55	1.77	10	1
4:D:501:PCW:C21	5:D:511:17F:H18A	0.55	2.31	10	1
4:A:415:PCW:C24	4:A:415:PCW:C20	0.55	2.78	1	1
5:C:627:17F:H29	5:C:628:17F:C8	0.55	2.30	1	1
4:B:208:PCW:H462	4:B:212:PCW:C25	0.55	2.31	1	1
4:D:502:PCW:C38	4:D:508:PCW:H352	0.55	2.28	1	2
4:C:614:PCW:H221	4:B:207:PCW:H272	0.55	1.76	2	1
5:C:627:17F:H9A	5:C:627:17F:H20A	0.55	1.77	3	2
4:B:201:PCW:H331	4:B:209:PCW:O3	0.55	2.02	3	1
2:B:82:PHE:HB2	2:B:89:SER:HB2	0.55	1.77	5	4
4:B:205:PCW:H442	5:B:214:17F:H73	0.55	1.77	5	1
4:B:212:PCW:H441	5:D:514:17F:H12	0.55	1.79	5	1
4:B:202:PCW:H361	4:B:202:PCW:C15	0.55	2.32	6	1
5:D:513:17F:H10	5:D:513:17F:C37	0.55	2.32	7	1
4:A:402:PCW:C36	4:B:210:PCW:H442	0.55	2.32	8	1
4:A:411:PCW:C15	4:A:411:PCW:H39	0.55	2.32	8	1
4:D:501:PCW:H181	5:D:511:17F:H19	0.55	1.77	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:205:PCW:H352	4:B:207:PCW:C14	0.55	2.32	9	1
4:D:506:PCW:C42	4:D:516:PCW:H251	0.55	2.32	9	1
4:A:408:PCW:H261	4:D:504:PCW:H441	0.55	1.79	10	1
4:C:625:PCW:H421	4:C:625:PCW:C37	0.55	2.31	10	1
4:B:208:PCW:H461	5:D:512:17F:H78	0.55	1.78	10	1
4:C:620:PCW:C19	5:C:631:17F:O10	0.55	2.55	10	6
4:C:623:PCW:O11	4:C:623:PCW:C2	0.55	2.54	7	6
4:D:505:PCW:C36	4:D:506:PCW:H142	0.55	2.32	1	1
4:A:401:PCW:H381	4:D:502:PCW:C20	0.55	2.32	2	1
4:D:501:PCW:O31	4:D:501:PCW:H11	0.55	2.02	9	3
4:A:417:PCW:O31	4:A:417:PCW:O3	0.55	2.25	7	3
4:A:403:PCW:H411	4:A:403:PCW:C37	0.55	2.22	6	1
5:A:410:17F:C41	4:C:612:PCW:H241	0.55	2.31	6	1
4:B:212:PCW:H222	4:B:212:PCW:H432	0.55	1.78	6	1
4:C:604:PCW:C25	5:D:514:17F:H76	0.55	2.32	8	1
4:D:502:PCW:H12	4:D:508:PCW:H11	0.55	1.77	9	2
4:C:614:PCW:H483	4:B:206:PCW:C25	0.55	2.31	10	1
4:C:601:PCW:H341	4:C:601:PCW:O31	0.54	2.02	9	9
4:C:622:PCW:H382	4:C:623:PCW:H182	0.54	1.78	5	2
4:B:203:PCW:O4P	4:B:203:PCW:H62	0.54	2.02	10	7
4:A:401:PCW:O2	4:D:508:PCW:H231	0.54	2.02	4	3
4:A:406:PCW:C40	4:D:505:PCW:H471	0.54	2.31	2	1
5:A:409:17F:O4	4:B:202:PCW:H61	0.54	2.01	2	1
4:D:505:PCW:H482	4:D:506:PCW:H152	0.54	1.80	2	2
4:A:404:PCW:C23	4:B:210:PCW:C22	0.54	2.85	4	2
4:C:620:PCW:H421	5:B:215:17F:H66	0.54	1.77	4	1
4:C:625:PCW:O31	4:C:625:PCW:C5	0.54	2.55	9	2
2:B:126:ASP:OD2	4:B:210:PCW:H62	0.54	2.02	5	1
4:D:504:PCW:H19	4:D:515:PCW:H282	0.54	1.78	5	1
4:A:413:PCW:H441	4:C:611:PCW:H271	0.54	1.79	6	1
4:D:506:PCW:C19	4:D:516:PCW:H281	0.54	2.31	7	1
4:B:203:PCW:H241	4:B:204:PCW:C17	0.54	2.31	10	1
4:D:505:PCW:C17	4:D:505:PCW:C13	0.54	2.80	4	6
4:C:601:PCW:H422	5:C:626:17F:H52	0.54	1.79	2	1
4:C:602:PCW:H462	5:C:626:17F:H65	0.54	1.79	2	1
4:C:606:PCW:C5	4:C:624:PCW:H281	0.54	2.31	3	1
4:C:617:PCW:C41	5:C:631:17F:H41	0.54	2.28	3	2
4:B:202:PCW:H382	4:B:202:PCW:H151	0.54	1.80	4	2
4:C:608:PCW:H211	4:C:614:PCW:H372	0.54	1.79	4	3
4:B:207:PCW:H51	4:B:207:PCW:C32	0.54	2.32	4	1
4:B:210:PCW:H63	4:D:506:PCW:H73	0.54	1.80	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:512:17F:H30	5:D:514:17F:C1X	0.54	2.32	7	2
5:C:627:17F:H5	5:C:627:17F:C19	0.54	2.22	6	2
4:B:206:PCW:O2	4:B:206:PCW:H51	0.54	2.02	6	1
4:C:608:PCW:O11	4:C:614:PCW:C8	0.54	2.55	7	2
4:C:622:PCW:H242	4:D:501:PCW:C43	0.54	2.32	8	1
4:A:413:PCW:C23	4:A:413:PCW:C27	0.54	2.76	9	1
4:D:502:PCW:C12	4:D:508:PCW:H371	0.54	2.33	10	1
4:C:603:PCW:O31	4:C:603:PCW:O3	0.54	2.25	1	3
4:C:603:PCW:H371	4:C:603:PCW:C41	0.54	2.33	6	4
2:B:8:VAL:HG12	2:B:79:LEU:HB2	0.54	1.78	4	4
2:B:15:GLY:CA	6:B:216:GNP:H8	0.54	2.32	5	4
4:C:619:PCW:H11	4:C:619:PCW:H62	0.54	1.80	2	1
4:D:501:PCW:H451	4:D:509:PCW:H232	0.54	1.80	2	1
4:D:503:PCW:H451	4:D:504:PCW:H39	0.54	1.79	2	1
4:B:212:PCW:H452	4:B:212:PCW:C21	0.54	2.33	3	1
4:B:206:PCW:H211	5:B:213:17F:C31	0.54	2.25	4	1
4:B:212:PCW:H222	4:B:212:PCW:H441	0.54	1.80	4	1
4:D:502:PCW:H452	4:D:508:PCW:H20	0.54	1.80	4	1
4:D:507:PCW:H31	5:D:513:17F:C41	0.54	2.33	10	2
4:A:415:PCW:H382	4:D:515:PCW:C16	0.54	2.33	9	4
4:C:606:PCW:C33	4:C:607:PCW:C7	0.54	2.86	5	1
4:B:205:PCW:C47	5:B:214:17F:H75	0.54	2.31	5	1
4:B:205:PCW:H161	4:B:206:PCW:C22	0.54	2.28	6	1
4:A:401:PCW:H381	4:D:502:PCW:H232	0.54	1.78	7	1
4:A:415:PCW:H11	4:C:616:PCW:H381	0.54	1.78	7	2
4:A:415:PCW:H471	4:D:515:PCW:H222	0.54	1.79	7	1
4:B:205:PCW:C20	4:B:206:PCW:H222	0.54	2.32	7	1
5:B:213:17F:H29	4:D:505:PCW:H141	0.54	1.78	7	1
4:D:503:PCW:H42	4:D:506:PCW:H52	0.54	1.78	7	1
4:D:504:PCW:H122	4:D:504:PCW:C38	0.54	2.32	9	1
5:D:514:17F:N1	5:D:514:17F:C4	0.54	2.70	9	1
5:A:410:17F:O10	5:A:410:17F:O6	0.54	2.25	7	6
4:C:611:PCW:H321	4:C:617:PCW:H141	0.54	1.79	1	1
4:B:202:PCW:O11	4:B:202:PCW:C5	0.54	2.55	5	7
4:B:208:PCW:C45	5:D:512:17F:H64	0.54	2.29	1	1
4:B:212:PCW:H271	5:D:512:17F:H61	0.54	1.78	1	1
4:D:510:PCW:H421	4:D:516:PCW:C26	0.54	2.32	8	2
4:D:503:PCW:H39	4:D:504:PCW:H73	0.54	1.79	2	1
4:C:606:PCW:H161	5:C:627:17F:H8	0.54	1.78	3	1
4:C:618:PCW:C48	5:D:511:17F:H74	0.54	2.33	3	1
4:D:502:PCW:H462	5:D:512:17F:H8	0.54	1.79	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:211:PCW:H52	4:B:211:PCW:C32	0.54	2.32	10	2
4:B:202:PCW:H381	4:B:202:PCW:H141	0.54	1.79	6	1
4:B:205:PCW:C16	4:B:206:PCW:H182	0.54	2.31	8	2
4:B:210:PCW:H161	4:D:503:PCW:H282	0.54	1.79	6	1
4:A:416:PCW:C13	5:C:630:17F:H11	0.54	2.32	7	1
4:C:610:PCW:C3	4:C:618:PCW:O11	0.54	2.56	7	2
4:C:625:PCW:C31	4:C:625:PCW:O3	0.54	2.54	7	2
4:D:503:PCW:O1P	4:D:503:PCW:H31	0.54	2.00	8	1
4:A:415:PCW:O3	4:A:415:PCW:C31	0.54	2.55	9	1
4:D:508:PCW:O2	4:D:508:PCW:O11	0.54	2.25	9	1
5:D:513:17F:O2	5:D:513:17F:H2	0.54	2.02	9	1
4:A:415:PCW:H481	4:C:617:PCW:C28	0.54	2.31	10	1
4:D:509:PCW:C23	5:D:514:17F:H65	0.54	2.31	10	1
1:A:325:ASP:HA	1:A:328:ARG:HD2	0.54	1.78	1	2
4:A:401:PCW:C31	4:A:401:PCW:O3	0.54	2.54	10	4
4:C:617:PCW:O3P	4:C:617:PCW:O31	0.54	2.25	5	5
1:A:276:VAL:O	1:A:280:ARG:HB2	0.54	2.02	2	1
4:C:607:PCW:H262	5:C:629:17F:C1X	0.54	2.33	2	3
4:C:621:PCW:H421	4:D:506:PCW:C27	0.54	2.32	6	3
4:B:205:PCW:H142	4:B:207:PCW:C32	0.54	2.28	2	1
4:D:505:PCW:H20	4:D:510:PCW:H331	0.54	1.78	2	3
2:B:40:TYR:HE1	2:B:57:ASP:HB2	0.54	1.62	3	1
4:B:205:PCW:H171	4:B:207:PCW:C32	0.54	2.29	3	1
1:C:503:MET:HA	1:C:506:ARG:HD2	0.54	1.79	5	3
4:D:503:PCW:H262	4:D:507:PCW:H421	0.54	1.79	4	1
4:C:619:PCW:P	4:C:620:PCW:H52	0.54	2.43	5	4
4:B:205:PCW:H262	4:B:207:PCW:H422	0.54	1.79	6	1
4:B:203:PCW:H362	4:B:203:PCW:H121	0.54	1.78	8	1
4:D:501:PCW:H62	4:D:509:PCW:C2	0.54	2.25	8	1
4:D:506:PCW:H411	5:D:513:17F:H39	0.54	1.78	8	1
4:C:617:PCW:C42	4:C:625:PCW:H261	0.54	2.26	9	1
4:B:203:PCW:H452	4:B:204:PCW:H262	0.54	1.78	9	1
4:B:204:PCW:H472	5:D:514:17F:H37	0.54	1.79	9	1
4:B:212:PCW:H40	5:B:213:17F:H50	0.54	1.79	10	1
5:C:628:17F:H59	5:C:628:17F:C12	0.54	2.31	5	2
4:D:501:PCW:C11	4:D:501:PCW:O31	0.54	2.55	6	4
4:B:206:PCW:O31	4:B:206:PCW:C1	0.54	2.54	10	4
3:D:444:LYS:HB2	3:D:464:ARG:HD3	0.54	1.80	2	1
5:B:213:17F:H43	4:D:509:PCW:C17	0.54	2.31	3	1
4:B:204:PCW:H40	5:D:514:17F:H8	0.54	1.79	5	1
4:A:414:PCW:C8	4:C:624:PCW:H331	0.54	2.32	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:613:PCW:N	4:C:623:PCW:O1P	0.54	2.41	7	2
4:B:209:PCW:H182	4:B:209:PCW:H231	0.54	1.79	7	1
3:D:460:LEU:HD13	4:D:501:PCW:H121	0.54	1.79	7	1
4:A:404:PCW:C27	4:C:617:PCW:H462	0.54	2.31	8	1
4:D:505:PCW:C8	4:D:509:PCW:H11	0.54	2.32	8	1
5:C:628:17F:H10A	5:C:628:17F:H56	0.54	1.80	9	1
1:A:224:VAL:HG22	1:C:550:LYS:HD3	0.54	1.80	1	1
4:A:408:PCW:H232	5:A:409:17F:H59	0.54	1.79	8	2
5:A:409:17F:H6A	2:B:172:LYS:HD2	0.54	1.80	1	1
4:C:621:PCW:H421	4:D:506:PCW:C28	0.54	2.23	1	1
4:D:508:PCW:C20	5:D:512:17F:H19A	0.54	2.32	1	1
4:A:417:PCW:H331	4:C:622:PCW:H122	0.54	1.78	2	3
4:C:610:PCW:C11	4:C:610:PCW:O31	0.54	2.56	2	5
4:A:401:PCW:H442	4:C:613:PCW:H261	0.54	1.79	3	1
4:C:603:PCW:C6	4:D:516:PCW:P	0.54	2.95	8	3
4:A:414:PCW:O31	4:A:414:PCW:O3P	0.54	2.26	4	1
3:D:359:ARG:HG2	3:D:369:VAL:HG22	0.54	1.78	4	1
4:A:406:PCW:H452	4:B:211:PCW:H472	0.54	1.80	6	2
4:A:408:PCW:H481	5:A:410:17F:H70	0.54	1.78	6	1
4:C:601:PCW:O31	4:C:601:PCW:O3	0.54	2.26	6	1
4:C:625:PCW:H282	5:C:631:17F:C26	0.54	2.32	6	1
4:B:208:PCW:H272	4:B:208:PCW:C40	0.54	2.32	6	1
4:C:624:PCW:C22	4:C:624:PCW:C27	0.54	2.68	7	1
4:B:205:PCW:H181	4:B:207:PCW:H151	0.54	1.79	8	1
4:C:614:PCW:H212	5:C:632:17F:H38	0.54	1.80	9	1
4:A:405:PCW:H472	4:A:405:PCW:C27	0.54	2.15	10	1
4:C:605:PCW:H322	4:C:610:PCW:O3P	0.54	2.03	10	1
4:D:509:PCW:H132	5:D:514:17F:H19A	0.54	1.79	10	1
1:C:519:ALA:HB3	1:C:520:PRO:HD3	0.54	1.78	10	10
4:C:616:PCW:O31	4:C:616:PCW:H12	0.54	2.01	1	1
4:D:509:PCW:H242	5:D:514:17F:C29	0.54	2.32	1	1
4:C:617:PCW:H131	4:C:625:PCW:H142	0.54	1.79	3	2
4:C:620:PCW:C28	5:C:631:17F:H12	0.54	2.32	2	1
2:B:15:GLY:HA2	6:B:216:GNP:H8	0.54	1.80	6	2
4:D:503:PCW:H322	4:D:510:PCW:C8	0.54	2.33	3	1
4:C:608:PCW:H381	4:B:207:PCW:C28	0.54	2.33	4	1
4:C:619:PCW:H283	5:C:632:17F:H37	0.54	1.80	4	1
4:D:501:PCW:O3	4:D:501:PCW:O31	0.54	2.25	4	1
5:A:410:17F:C19	4:D:502:PCW:H162	0.54	2.33	5	1
4:B:202:PCW:H82	4:D:504:PCW:O2P	0.54	2.03	5	1
4:B:208:PCW:H281	4:B:208:PCW:H40	0.54	1.78	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:503:PCW:C35	4:D:510:PCW:H82	0.54	2.29	5	1
2:B:36:ILE:HD12	3:D:370:VAL:HA	0.54	1.80	6	1
4:B:204:PCW:H483	4:D:502:PCW:H441	0.54	1.80	6	1
5:B:215:17F:O8	5:B:215:17F:O9	0.54	2.24	6	1
5:A:410:17F:H78	4:C:610:PCW:C47	0.54	2.32	7	1
4:D:501:PCW:H222	5:D:511:17F:H20A	0.54	1.78	7	1
5:A:410:17F:H72	4:C:610:PCW:C47	0.54	2.33	8	1
4:B:205:PCW:H442	5:B:214:17F:H77	0.54	1.78	8	1
4:B:210:PCW:C1	4:D:503:PCW:C11	0.54	2.86	9	1
4:B:212:PCW:H342	5:B:213:17F:H9A	0.54	1.80	9	1
4:D:502:PCW:H431	5:D:512:17F:C10	0.54	2.32	9	1
4:D:501:PCW:H481	4:D:509:PCW:C27	0.54	2.32	10	1
1:C:471:ARG:HA	1:C:475:GLU:CG	0.54	2.33	1	1
4:C:604:PCW:H211	4:C:604:PCW:H162	0.54	1.80	3	3
4:B:205:PCW:C7	4:B:212:PCW:H73	0.54	2.33	1	1
4:B:206:PCW:O11	4:B:206:PCW:O2	0.54	2.26	9	7
4:C:605:PCW:C44	4:C:618:PCW:H483	0.54	2.21	7	2
5:C:627:17F:H10	5:B:215:17F:H48	0.54	1.79	3	2
4:B:203:PCW:O11	4:B:203:PCW:H42	0.54	2.02	3	1
4:B:204:PCW:H42	5:B:214:17F:HN1A	0.54	1.63	3	1
5:B:213:17F:H66	4:D:505:PCW:C40	0.54	2.32	5	2
4:A:412:PCW:C45	4:C:624:PCW:H481	0.54	2.33	4	1
4:A:417:PCW:C6	4:A:417:PCW:O31	0.54	2.56	4	2
4:D:504:PCW:H381	4:D:504:PCW:H421	0.54	1.80	4	1
5:A:410:17F:C37	4:D:501:PCW:H252	0.54	2.33	5	1
5:A:410:17F:H57	4:D:502:PCW:C21	0.54	2.31	7	2
1:C:461:LYS:O	1:C:465:GLU:HG3	0.54	2.02	10	2
4:C:615:PCW:H441	4:C:625:PCW:H251	0.54	1.80	6	1
4:B:207:PCW:H352	4:B:209:PCW:H141	0.54	1.80	6	1
4:B:210:PCW:H181	4:D:503:PCW:H282	0.54	1.79	6	1
4:D:502:PCW:H52	4:D:502:PCW:C32	0.54	2.33	8	1
4:A:411:PCW:C16	4:A:415:PCW:H331	0.54	2.32	9	2
4:A:403:PCW:H2	4:A:403:PCW:O4P	0.54	2.03	1	4
4:A:413:PCW:H39	4:C:611:PCW:C43	0.54	2.32	1	1
4:A:404:PCW:O3P	4:A:404:PCW:O31	0.54	2.26	4	6
4:A:413:PCW:O4P	4:A:413:PCW:H62	0.54	2.03	5	2
4:C:607:PCW:O3P	4:C:607:PCW:O31	0.54	2.25	8	2
4:A:401:PCW:H472	4:C:610:PCW:C23	0.54	2.32	5	1
4:B:208:PCW:C43	4:B:212:PCW:H283	0.54	2.33	5	1
5:B:213:17F:H76	5:B:213:17F:C21	0.54	2.30	7	1
4:B:206:PCW:C38	4:D:505:PCW:H31	0.54	2.33	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:509:PCW:H371	4:D:509:PCW:C41	0.54	2.31	8	1
4:A:404:PCW:H231	4:A:404:PCW:H182	0.54	1.80	9	1
4:C:610:PCW:C2	4:C:618:PCW:H63	0.54	2.29	9	1
4:B:205:PCW:H352	4:B:207:PCW:H142	0.54	1.79	9	1
4:B:212:PCW:C35	5:D:514:17F:H20A	0.54	2.21	9	1
4:B:207:PCW:O31	4:B:207:PCW:O3	0.54	2.26	10	1
5:A:410:17F:O9	5:A:410:17F:O8	0.53	2.26	4	5
4:D:502:PCW:H461	5:D:512:17F:H48	0.53	1.80	1	2
4:B:208:PCW:C3	4:B:208:PCW:O2P	0.53	2.56	9	4
4:B:203:PCW:H261	5:B:214:17F:H18	0.53	1.79	3	1
4:C:609:PCW:H82	5:C:631:17F:H4A	0.53	1.80	5	1
4:D:510:PCW:C24	4:D:515:PCW:H462	0.53	2.34	5	1
4:A:416:PCW:H162	5:C:630:17F:C31	0.53	2.18	6	1
4:A:415:PCW:H451	4:D:515:PCW:C22	0.53	2.34	7	1
4:C:612:PCW:C25	5:D:511:17F:H50	0.53	2.33	7	1
4:D:502:PCW:H52	4:D:502:PCW:H321	0.53	1.79	8	1
2:B:19:LEU:HD23	2:B:146:ALA:HB2	0.53	1.81	9	1
4:B:207:PCW:C35	4:B:209:PCW:H121	0.53	2.23	10	1
3:D:448:LYS:HD3	4:D:503:PCW:H51	0.53	1.80	1	1
4:A:408:PCW:H281	4:A:411:PCW:H461	0.53	1.80	2	1
4:D:501:PCW:H19	4:D:502:PCW:H342	0.53	1.80	2	1
2:B:143:GLU:O	4:B:204:PCW:H73	0.53	2.03	3	1
4:B:205:PCW:C18	4:B:207:PCW:H342	0.53	2.27	3	1
4:C:625:PCW:O31	4:C:625:PCW:H12	0.53	2.03	5	1
4:B:207:PCW:C6	5:B:213:17F:O4	0.53	2.56	9	2
4:D:507:PCW:H19	5:D:513:17F:H31	0.53	1.80	9	1
4:C:605:PCW:C44	4:C:618:PCW:H441	0.53	2.32	10	1
4:B:208:PCW:C12	5:B:214:17F:C18	0.53	2.86	10	1
4:D:501:PCW:H73	5:D:514:17F:O5	0.53	2.04	10	1
4:C:609:PCW:H172	5:C:631:17F:C34	0.53	2.31	1	1
4:C:613:PCW:O4P	4:C:613:PCW:H73	0.53	2.03	1	5
5:C:626:17F:C22	5:C:629:17F:H75	0.53	2.33	8	3
4:D:505:PCW:H361	4:D:506:PCW:C15	0.53	2.33	1	1
1:A:225:THR:O	1:A:229:TRP:HB2	0.53	2.03	3	4
4:A:406:PCW:C37	4:B:211:PCW:H362	0.53	2.33	2	1
4:B:203:PCW:H261	5:B:214:17F:C18	0.53	2.33	3	1
4:A:411:PCW:H132	4:D:515:PCW:H141	0.53	1.80	4	1
4:D:504:PCW:H141	4:D:504:PCW:H382	0.53	1.79	5	1
5:C:632:17F:H52	4:B:205:PCW:C23	0.53	2.33	6	1
4:B:206:PCW:C14	5:B:213:17F:H56	0.53	2.23	6	1
4:B:207:PCW:H412	4:B:209:PCW:H182	0.53	1.80	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:405:PCW:H472	4:A:405:PCW:H282	0.53	1.80	8	1
5:A:409:17F:H20A	4:D:504:PCW:H361	0.53	1.80	8	1
4:C:608:PCW:H351	5:C:632:17F:H31	0.53	1.80	9	1
4:B:202:PCW:C5	4:B:202:PCW:O11	0.53	2.56	9	1
4:A:414:PCW:O31	4:A:414:PCW:O3	0.53	2.27	1	6
4:D:508:PCW:H372	4:D:508:PCW:H412	0.53	1.81	1	1
4:B:204:PCW:O2	4:B:204:PCW:O2P	0.53	2.26	7	3
5:B:213:17F:H43	4:D:509:PCW:C16	0.53	2.34	3	1
4:D:503:PCW:C34	4:D:507:PCW:H341	0.53	2.33	3	1
4:D:507:PCW:H451	5:D:513:17F:H57	0.53	1.81	8	3
5:A:410:17F:O1	4:D:502:PCW:C8	0.53	2.56	5	1
5:D:512:17F:H47	5:D:514:17F:C24	0.53	2.26	5	1
4:B:205:PCW:C18	4:B:207:PCW:H171	0.53	2.33	6	1
4:A:413:PCW:H39	4:C:611:PCW:H451	0.53	1.79	8	2
4:C:621:PCW:H122	5:C:627:17F:C37	0.53	2.24	10	1
4:B:202:PCW:C4	4:B:202:PCW:O11	0.53	2.56	1	7
4:C:602:PCW:H282	5:C:629:17F:H78	0.53	1.81	2	1
4:C:606:PCW:C25	5:C:627:17F:H42	0.53	2.34	2	1
4:B:205:PCW:H19	4:B:206:PCW:H221	0.53	1.81	3	1
4:D:502:PCW:H462	5:D:512:17F:C9	0.53	2.34	3	1
4:C:625:PCW:H182	4:C:625:PCW:C22	0.53	2.29	6	1
4:C:621:PCW:H331	4:D:516:PCW:H422	0.53	1.79	7	1
4:B:205:PCW:H221	4:B:207:PCW:H151	0.53	1.79	7	1
4:D:509:PCW:H82	4:D:510:PCW:C32	0.53	2.31	8	1
4:B:205:PCW:H211	4:B:207:PCW:C43	0.53	2.30	9	1
4:A:402:PCW:H283	4:C:611:PCW:H182	0.53	1.81	1	1
4:C:616:PCW:C23	4:C:616:PCW:C27	0.53	2.74	1	1
4:C:619:PCW:O3P	4:C:619:PCW:O31	0.53	2.26	6	2
4:C:622:PCW:C36	4:C:622:PCW:C32	0.53	2.67	6	7
4:B:203:PCW:H20	4:B:208:PCW:H321	0.53	1.80	1	1
4:D:508:PCW:C4	4:D:508:PCW:O11	0.53	2.56	1	3
4:A:406:PCW:H461	4:C:621:PCW:C47	0.53	2.34	2	1
4:C:615:PCW:H431	4:D:506:PCW:C45	0.53	2.33	2	1
4:B:202:PCW:O11	4:B:202:PCW:H51	0.53	2.04	4	4
4:B:206:PCW:H63	4:B:206:PCW:H131	0.53	1.79	2	1
4:A:412:PCW:H451	4:C:623:PCW:H481	0.53	1.80	4	2
2:B:142:ILE:HG21	2:B:155:ALA:HB2	0.53	1.79	3	1
4:C:608:PCW:C25	4:C:614:PCW:H381	0.53	2.34	4	3
4:C:613:PCW:H73	4:C:613:PCW:O4P	0.53	2.04	7	5
4:C:617:PCW:C42	4:C:625:PCW:H282	0.53	2.32	4	1
5:D:513:17F:C17	5:D:513:17F:O7	0.53	2.56	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:403:PCW:C48	4:B:209:PCW:H461	0.53	2.33	6	1
4:A:404:PCW:H482	4:A:407:PCW:C23	0.53	2.34	6	1
4:B:206:PCW:H73	4:B:209:PCW:H63	0.53	1.81	7	1
4:B:210:PCW:O2P	5:D:513:17F:O3	0.53	2.27	8	2
4:A:405:PCW:H321	4:B:203:PCW:C33	0.53	2.33	8	1
4:A:405:PCW:H39	5:D:512:17F:H68	0.53	1.79	8	1
4:C:610:PCW:H20	4:C:610:PCW:C41	0.53	2.32	8	1
5:C:632:17F:O8	5:C:632:17F:C5	0.53	2.51	8	1
4:B:203:PCW:C14	4:B:203:PCW:C39	0.53	2.86	10	1
4:B:206:PCW:H351	4:D:505:PCW:C33	0.53	2.34	10	1
4:A:404:PCW:P	4:A:404:PCW:C3	0.53	2.96	1	3
4:A:416:PCW:H122	5:C:630:17F:H9A	0.53	1.76	1	2
4:C:606:PCW:H62	4:C:624:PCW:C28	0.53	2.27	1	1
4:B:202:PCW:H41	4:B:202:PCW:C11	0.53	2.34	10	4
4:B:210:PCW:H322	4:B:210:PCW:H41	0.53	1.80	1	2
4:D:503:PCW:O1P	4:D:503:PCW:H51	0.53	2.03	2	1
4:D:503:PCW:O31	4:D:503:PCW:C1	0.53	2.54	7	4
4:C:610:PCW:H471	4:D:501:PCW:C27	0.53	2.34	4	1
4:C:612:PCW:H31	4:C:618:PCW:H2	0.53	1.80	4	3
2:B:1:MET:HA	2:B:50:THR:O	0.53	2.04	4	1
4:B:203:PCW:H241	4:B:208:PCW:H2	0.53	1.81	5	1
4:A:413:PCW:H82	4:A:413:PCW:O4P	0.53	2.04	6	1
4:B:204:PCW:H122	4:B:208:PCW:C36	0.53	2.33	6	1
4:C:620:PCW:H221	5:C:631:17F:H31	0.53	1.79	8	1
4:C:622:PCW:H12	4:C:623:PCW:H162	0.53	1.81	8	1
4:B:204:PCW:C35	4:B:208:PCW:H332	0.53	2.34	10	1
4:A:402:PCW:H283	4:C:611:PCW:C18	0.53	2.33	1	1
4:A:417:PCW:H62	4:A:417:PCW:C31	0.53	2.33	9	4
4:C:623:PCW:O31	4:C:623:PCW:O3P	0.53	2.26	5	6
4:A:406:PCW:H372	4:B:211:PCW:H362	0.53	1.79	2	1
4:C:615:PCW:H342	4:D:516:PCW:H362	0.53	1.80	2	3
4:C:619:PCW:C28	5:C:632:17F:H35	0.53	2.32	2	1
4:B:206:PCW:C1	5:B:213:17F:H4	0.53	2.33	2	1
4:C:608:PCW:H251	5:C:626:17F:H73	0.53	1.81	3	2
5:C:627:17F:C42	4:D:516:PCW:H462	0.53	2.31	3	1
4:B:203:PCW:O4P	4:B:203:PCW:H31	0.53	2.04	3	1
4:C:614:PCW:H142	5:C:632:17F:C8	0.53	2.34	4	1
4:A:403:PCW:H272	4:B:201:PCW:H371	0.53	1.80	5	1
5:A:410:17F:H71	4:D:501:PCW:C24	0.53	2.33	5	1
4:A:413:PCW:H422	4:C:611:PCW:C25	0.53	2.33	5	1
4:A:402:PCW:O2	4:A:402:PCW:O1P	0.53	2.26	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:604:PCW:H2	4:C:606:PCW:C8	0.53	2.34	6	3
4:C:606:PCW:O31	4:C:606:PCW:O3P	0.53	2.27	6	1
4:C:614:PCW:C21	5:C:632:17F:H41	0.53	2.34	6	1
4:B:203:PCW:H242	4:B:208:PCW:H131	0.53	1.80	7	1
4:A:404:PCW:H182	4:A:404:PCW:C23	0.53	2.34	9	1
5:D:513:17F:H11A	5:D:513:17F:H62	0.53	1.80	9	1
4:C:610:PCW:H222	4:C:618:PCW:C48	0.53	2.33	10	1
5:A:409:17F:H50	5:D:511:17F:H33	0.53	1.79	1	1
4:C:613:PCW:C5	4:C:623:PCW:O31	0.53	2.57	1	1
4:C:613:PCW:C43	4:C:618:PCW:H20	0.53	2.34	3	2
4:A:401:PCW:H51	4:D:502:PCW:H12	0.53	1.78	2	1
4:D:505:PCW:C20	4:D:510:PCW:H322	0.53	2.34	3	2
4:A:407:PCW:C32	4:B:211:PCW:H132	0.53	2.33	6	2
4:A:412:PCW:C47	4:B:208:PCW:H483	0.53	2.34	10	3
4:C:609:PCW:C8	5:C:631:17F:O8	0.53	2.57	4	1
4:D:504:PCW:O4P	4:D:504:PCW:H2	0.53	2.04	5	1
1:A:233:GLU:HA	1:A:236:THR:OG1	0.53	2.04	10	2
1:C:443:LYS:O	1:C:447:GLU:HB2	0.53	2.04	10	1
4:D:502:PCW:H372	4:D:508:PCW:C32	0.53	2.34	10	1
1:A:365:LYS:HB2	1:A:366:PRO:CD	0.53	2.31	6	5
4:A:417:PCW:H181	4:C:603:PCW:C14	0.53	2.34	1	2
1:C:411:THR:O	1:C:415:LEU:HG	0.53	2.04	1	2
4:C:603:PCW:C31	4:C:603:PCW:C5	0.53	2.84	1	1
5:C:628:17F:H12A	5:C:628:17F:C33	0.53	2.34	3	7
4:B:203:PCW:H241	4:B:204:PCW:H19	0.53	1.79	1	1
4:D:506:PCW:H39	5:D:513:17F:H49	0.53	1.79	1	1
4:D:506:PCW:C17	4:D:516:PCW:H281	0.53	2.33	1	2
4:A:413:PCW:H431	4:C:611:PCW:C16	0.53	2.34	7	2
4:C:605:PCW:C39	4:C:610:PCW:H341	0.53	2.33	7	2
4:B:205:PCW:H221	4:B:207:PCW:C17	0.53	2.34	2	1
4:A:413:PCW:C41	4:C:611:PCW:H181	0.53	2.34	3	1
4:B:208:PCW:H121	5:B:214:17F:H6	0.53	1.81	4	1
4:A:412:PCW:O31	4:A:412:PCW:C11	0.53	2.56	5	1
4:A:413:PCW:H422	4:C:611:PCW:H251	0.53	1.80	8	2
4:C:614:PCW:H161	5:C:632:17F:C10	0.53	2.34	5	1
4:B:212:PCW:C21	4:B:212:PCW:H432	0.53	2.33	5	1
4:D:505:PCW:H20	4:D:510:PCW:H351	0.53	1.81	5	1
4:A:401:PCW:C3	4:D:508:PCW:H181	0.53	2.10	7	1
4:C:602:PCW:H362	5:B:214:17F:C37	0.53	2.29	7	1
4:A:404:PCW:O2P	4:A:404:PCW:C3	0.53	2.57	9	1
4:C:606:PCW:H61	4:C:624:PCW:C28	0.53	2.24	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:408:PCW:H371	4:A:408:PCW:C1	0.52	2.33	1	1
4:D:502:PCW:H361	4:D:508:PCW:H371	0.52	1.80	1	1
4:C:606:PCW:H252	5:C:627:17F:C24	0.52	2.34	8	2
4:C:612:PCW:H32	4:C:618:PCW:C11	0.52	2.34	9	3
5:A:409:17F:C33	4:D:504:PCW:H331	0.52	2.33	4	1
1:C:435:GLU:O	1:C:439:GLN:HG3	0.52	2.04	9	3
4:B:210:PCW:H51	5:D:513:17F:C1	0.52	2.28	8	2
4:A:407:PCW:H442	4:B:211:PCW:H212	0.52	1.80	5	1
4:A:415:PCW:C11	4:C:616:PCW:H421	0.52	2.35	6	1
4:B:205:PCW:C19	4:B:207:PCW:H171	0.52	2.34	6	1
4:B:208:PCW:C16	5:B:214:17F:H11A	0.52	2.34	6	1
5:C:627:17F:H18A	5:C:627:17F:C6	0.52	2.29	7	1
4:D:505:PCW:H182	4:D:509:PCW:C47	0.52	2.33	8	1
4:D:506:PCW:H382	4:D:507:PCW:H411	0.52	1.79	9	1
4:D:507:PCW:O3	5:D:513:17F:H77	0.52	2.04	9	1
5:A:409:17F:H46	5:D:511:17F:H33	0.52	1.82	1	1
4:A:404:PCW:O4P	4:A:404:PCW:H62	0.52	2.04	6	5
4:C:608:PCW:H251	5:C:626:17F:C39	0.52	2.34	3	5
4:D:502:PCW:C43	4:D:508:PCW:H20	0.52	2.27	2	1
5:D:513:17F:O2	5:D:513:17F:C2	0.52	2.57	2	2
4:C:609:PCW:H241	4:C:609:PCW:C19	0.52	2.35	6	2
4:C:621:PCW:H281	4:D:509:PCW:H282	0.52	1.81	4	1
5:C:629:17F:C17	5:C:629:17F:C7	0.52	2.87	4	2
4:D:501:PCW:H12	4:D:509:PCW:H352	0.52	1.80	5	1
4:D:507:PCW:C19	5:D:513:17F:H19A	0.52	2.32	5	1
4:C:615:PCW:H452	4:D:506:PCW:H472	0.52	1.81	6	1
3:D:446:PHE:O	5:D:514:17F:H1	0.52	2.04	6	1
4:D:502:PCW:H411	4:D:508:PCW:H19	0.52	1.81	7	1
5:D:514:17F:H20A	5:D:514:17F:O10	0.52	2.04	9	1
4:C:621:PCW:O4P	4:C:621:PCW:H62	0.52	2.03	10	1
4:C:624:PCW:C8	4:C:624:PCW:H182	0.52	2.33	10	1
4:B:208:PCW:H73	5:B:214:17F:P1	0.52	2.44	10	1
4:A:413:PCW:H451	4:C:611:PCW:H171	0.52	1.82	1	1
4:B:211:PCW:C31	4:B:211:PCW:C35	0.52	2.87	10	10
4:D:516:PCW:O11	4:D:516:PCW:O2	0.52	2.28	6	8
4:A:401:PCW:C5	4:D:502:PCW:H12	0.52	2.34	2	1
4:A:407:PCW:H132	4:A:407:PCW:O31	0.52	2.04	8	2
4:A:408:PCW:C44	5:A:409:17F:H70	0.52	2.34	2	1
4:A:413:PCW:H371	4:C:611:PCW:H151	0.52	1.80	10	3
4:C:608:PCW:H251	5:C:626:17F:C40	0.52	2.35	3	3
4:A:415:PCW:H31	4:C:616:PCW:H422	0.52	1.82	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:608:PCW:H51	5:C:632:17F:O2	0.52	2.04	3	2
5:C:626:17F:O10	5:C:626:17F:O7	0.52	2.27	8	5
4:D:509:PCW:H221	4:D:509:PCW:H181	0.52	1.80	3	1
5:A:410:17F:H76	4:C:618:PCW:H452	0.52	1.81	4	2
4:D:501:PCW:C15	4:D:502:PCW:H332	0.52	2.32	4	1
4:C:625:PCW:H282	5:C:631:17F:H51	0.52	1.81	5	2
4:B:212:PCW:H222	5:D:514:17F:H10	0.52	1.80	7	2
4:A:401:PCW:C5	4:D:502:PCW:O2P	0.52	2.57	6	1
4:A:413:PCW:H341	4:C:611:PCW:C11	0.52	2.34	6	1
4:A:407:PCW:H421	4:B:211:PCW:H462	0.52	1.79	7	1
4:A:417:PCW:O31	4:A:417:PCW:C11	0.52	2.57	7	2
4:B:206:PCW:C44	5:B:213:17F:H58	0.52	2.35	7	1
5:B:213:17F:H29	4:D:505:PCW:H122	0.52	1.80	7	1
4:D:507:PCW:C43	5:D:513:17F:H35	0.52	2.32	9	1
4:A:402:PCW:H62	5:D:513:17F:O1	0.52	2.04	1	1
4:B:204:PCW:H471	5:D:512:17F:C27	0.52	2.34	1	1
4:B:203:PCW:H241	4:B:208:PCW:H51	0.52	1.80	2	1
5:D:512:17F:H52	5:D:514:17F:C25	0.52	2.35	2	1
4:A:415:PCW:H12	4:C:616:PCW:H351	0.52	1.80	3	2
4:B:206:PCW:H442	5:B:213:17F:C1Z	0.52	2.33	3	1
5:C:630:17F:O10	5:C:630:17F:H20A	0.52	2.04	8	2
5:C:632:17F:H55	4:B:201:PCW:C44	0.52	2.25	4	1
4:A:405:PCW:H432	4:A:414:PCW:C28	0.52	2.34	5	1
4:C:616:PCW:H2	4:C:616:PCW:O11	0.52	2.04	5	1
4:D:506:PCW:H171	4:D:516:PCW:C28	0.52	2.34	7	2
4:D:510:PCW:H412	4:D:516:PCW:H262	0.52	1.80	7	1
5:C:627:17F:H9A	5:C:627:17F:H20	0.52	1.81	8	1
4:D:503:PCW:C3	4:D:503:PCW:P	0.52	2.98	8	1
5:A:409:17F:H42	5:D:511:17F:H18A	0.52	1.74	9	1
4:C:615:PCW:C43	4:D:506:PCW:H472	0.52	2.34	10	1
4:B:208:PCW:C7	5:B:214:17F:H19	0.52	2.34	10	1
4:A:408:PCW:H321	5:A:409:17F:C19	0.52	2.35	1	1
4:A:408:PCW:C32	5:A:409:17F:H19A	0.52	2.34	1	3
4:A:408:PCW:O31	4:A:408:PCW:O3	0.52	2.28	1	3
4:C:611:PCW:O31	4:C:611:PCW:O3P	0.52	2.27	2	9
4:D:509:PCW:O31	5:D:514:17F:H56	0.52	2.04	7	2
4:A:415:PCW:O2	4:A:415:PCW:H342	0.52	2.04	9	4
4:D:510:PCW:H181	5:D:513:17F:C27	0.52	2.26	2	1
4:A:405:PCW:H482	4:A:414:PCW:C27	0.52	2.31	3	1
1:C:475:GLU:HB2	1:C:476:PRO:HD3	0.52	1.81	3	3
4:B:204:PCW:H122	4:B:212:PCW:H19	0.52	1.81	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:202:PCW:P	4:B:202:PCW:C3	0.52	2.98	5	1
4:C:619:PCW:H141	5:C:632:17F:H18	0.52	1.81	6	2
4:D:501:PCW:C33	5:D:512:17F:H37	0.52	2.25	6	1
4:D:506:PCW:C40	4:D:516:PCW:H242	0.52	2.30	6	1
4:A:417:PCW:H442	5:D:511:17F:H76	0.52	1.80	7	1
4:D:501:PCW:H342	5:D:512:17F:C21	0.52	2.35	7	1
4:B:206:PCW:C42	5:B:213:17F:H19A	0.52	2.35	8	1
4:A:405:PCW:C32	4:B:203:PCW:C35	0.52	2.87	9	1
4:C:608:PCW:H232	4:C:614:PCW:H361	0.52	1.81	1	3
4:B:203:PCW:P	4:B:203:PCW:C3	0.52	2.97	2	7
4:A:408:PCW:O3	4:A:408:PCW:O31	0.52	2.27	2	5
4:A:417:PCW:C7	4:A:417:PCW:H321	0.52	2.35	2	1
4:C:610:PCW:O11	4:C:618:PCW:C6	0.52	2.57	4	3
4:B:206:PCW:C3	4:B:206:PCW:O1P	0.52	2.58	2	2
4:A:407:PCW:H431	4:B:211:PCW:H212	0.52	1.80	3	1
4:C:612:PCW:O4P	4:C:612:PCW:H63	0.52	2.04	6	2
4:C:617:PCW:C43	4:C:625:PCW:H282	0.52	2.35	4	2
4:B:203:PCW:H31	4:B:203:PCW:C4	0.52	2.33	7	2
4:B:208:PCW:O2P	5:B:214:17F:H1A	0.52	2.04	3	1
4:B:203:PCW:H52	4:B:204:PCW:H362	0.52	1.82	4	2
4:A:402:PCW:C24	4:A:413:PCW:H262	0.52	2.32	5	1
4:A:407:PCW:C42	4:B:211:PCW:H442	0.52	2.35	5	2
4:A:415:PCW:H32	4:A:415:PCW:P	0.52	2.45	9	2
4:D:501:PCW:C7	4:D:509:PCW:O31	0.52	2.57	5	1
2:B:154:ASP:OD2	4:B:212:PCW:H52	0.52	2.04	6	1
4:B:204:PCW:H421	4:B:212:PCW:H242	0.52	1.82	8	1
4:A:415:PCW:P	4:A:415:PCW:C3	0.52	2.98	9	1
4:A:415:PCW:C31	4:A:415:PCW:O3	0.52	2.58	2	9
1:C:510:HIS:O	1:C:514:LEU:HG	0.52	2.05	7	7
4:B:204:PCW:H411	5:D:514:17F:H8A	0.52	1.79	1	1
4:B:207:PCW:O3	4:B:207:PCW:O31	0.52	2.28	5	7
4:D:502:PCW:H73	4:D:502:PCW:H2	0.52	1.82	10	3
4:A:404:PCW:H182	4:A:404:PCW:H231	0.52	1.81	2	1
4:A:417:PCW:H32	4:C:603:PCW:H31	0.52	1.79	3	1
4:C:602:PCW:O31	4:C:602:PCW:C1	0.52	2.56	9	3
5:B:213:17F:H66	4:D:505:PCW:H39	0.52	1.81	3	1
4:C:616:PCW:O31	4:C:616:PCW:C1	0.52	2.53	4	2
4:D:507:PCW:H131	5:D:513:17F:C40	0.52	2.34	5	1
4:A:417:PCW:H282	4:C:621:PCW:C26	0.52	2.35	6	1
4:C:604:PCW:H31	4:C:604:PCW:C4	0.52	2.35	6	1
4:A:402:PCW:O1P	4:A:402:PCW:C31	0.52	2.57	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:A:409:17F:H51	5:D:511:17F:C34	0.52	2.35	8	1
5:A:410:17F:H32	4:D:502:PCW:C15	0.52	2.33	8	1
4:C:614:PCW:H151	4:B:207:PCW:H281	0.52	1.82	8	1
4:B:211:PCW:C25	4:D:503:PCW:H231	0.52	2.34	8	1
4:D:503:PCW:C14	4:D:505:PCW:H482	0.52	2.32	8	1
4:A:404:PCW:H181	4:A:407:PCW:C26	0.52	2.35	9	1
4:D:504:PCW:O31	4:D:504:PCW:O3P	0.52	2.28	9	1
4:A:403:PCW:H261	4:B:201:PCW:H39	0.52	1.81	10	1
4:C:619:PCW:H141	5:C:632:17F:C5	0.52	2.35	1	1
2:B:81:VAL:HG12	2:B:114:VAL:HB	0.52	1.80	2	4
5:B:213:17F:H43	4:D:509:PCW:H161	0.52	1.81	3	1
4:A:408:PCW:H211	4:B:202:PCW:H281	0.52	1.81	4	1
4:C:621:PCW:C34	4:C:625:PCW:H20	0.52	2.34	4	1
5:C:626:17F:C2X	5:C:629:17F:H74	0.52	2.33	4	2
4:C:604:PCW:H432	4:C:606:PCW:H181	0.52	1.80	5	1
4:D:503:PCW:H42	4:D:510:PCW:H73	0.52	1.81	5	1
4:A:408:PCW:H281	4:A:416:PCW:C27	0.52	2.33	6	1
4:B:201:PCW:H452	4:B:205:PCW:H251	0.52	1.81	6	1
4:B:202:PCW:H382	4:B:202:PCW:C11	0.52	2.34	8	1
5:D:512:17F:H30	5:D:514:17F:H11	0.52	1.81	8	1
3:D:456:GLN:HB3	4:D:508:PCW:C7	0.52	2.34	9	1
4:D:507:PCW:H20	5:D:513:17F:H56	0.52	1.79	9	1
4:B:204:PCW:C37	4:B:208:PCW:H342	0.52	2.35	10	1
4:C:619:PCW:O4P	4:C:619:PCW:H2	0.52	2.05	2	2
4:B:205:PCW:H141	4:B:207:PCW:C33	0.52	2.35	1	1
4:B:210:PCW:H482	5:D:513:17F:C1Y	0.52	2.24	1	1
4:C:621:PCW:H19	5:C:628:17F:H29	0.52	1.82	2	1
4:D:510:PCW:O31	4:D:510:PCW:P	0.52	2.68	7	7
4:A:401:PCW:O11	4:A:401:PCW:H2	0.52	2.05	3	2
4:B:205:PCW:C7	5:B:213:17F:O1	0.52	2.57	3	3
4:A:403:PCW:H222	4:B:201:PCW:H162	0.52	1.80	4	1
4:A:417:PCW:H261	4:C:621:PCW:H262	0.52	1.81	4	2
4:C:610:PCW:H471	4:D:501:PCW:C28	0.52	2.34	4	1
4:B:202:PCW:H362	4:B:202:PCW:C13	0.52	2.35	4	2
4:D:503:PCW:H361	4:D:507:PCW:H321	0.52	1.80	4	1
5:C:629:17F:H1A	5:C:629:17F:C4	0.52	2.33	5	1
4:A:403:PCW:H483	4:B:209:PCW:C46	0.52	2.32	6	1
4:B:206:PCW:H171	4:B:207:PCW:C33	0.52	2.22	6	1
4:A:401:PCW:H62	4:D:508:PCW:C2	0.52	2.24	7	3
4:A:405:PCW:H431	4:A:414:PCW:C28	0.52	2.34	7	1
4:B:203:PCW:H231	4:B:204:PCW:H171	0.52	1.81	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:404:PCW:O4P	4:A:404:PCW:H31	0.52	2.05	10	1
4:D:503:PCW:H121	4:D:507:PCW:H39	0.52	1.81	10	1
4:D:505:PCW:H20	4:D:510:PCW:C34	0.52	2.33	10	1
4:A:411:PCW:C1	4:D:515:PCW:H32	0.52	2.35	2	1
4:C:602:PCW:O4P	4:C:602:PCW:H62	0.52	2.05	3	9
4:D:502:PCW:H31	4:D:508:PCW:H322	0.52	1.81	4	2
4:D:509:PCW:H63	4:D:510:PCW:H322	0.52	1.82	2	1
4:C:623:PCW:O31	4:C:623:PCW:O4P	0.52	2.28	3	1
4:A:401:PCW:H452	4:C:610:PCW:C27	0.52	2.21	4	1
4:D:508:PCW:H441	5:D:512:17F:H48	0.52	1.80	4	1
4:A:401:PCW:O3	4:A:401:PCW:C31	0.52	2.57	5	3
4:D:507:PCW:H331	5:D:513:17F:O8	0.52	2.05	7	1
4:A:401:PCW:H40	4:D:502:PCW:H281	0.52	1.82	8	1
4:C:610:PCW:H241	4:C:610:PCW:C46	0.52	2.34	8	1
4:C:610:PCW:H41	4:C:622:PCW:C34	0.52	2.28	9	1
4:B:210:PCW:P	5:D:513:17F:H4A	0.52	2.44	10	2
4:A:413:PCW:C35	4:C:611:PCW:H131	0.51	2.35	2	3
4:C:604:PCW:H381	5:C:627:17F:C23	0.51	2.34	1	2
5:C:627:17F:C2X	5:C:628:17F:H10	0.51	2.35	1	1
5:A:409:17F:H46	4:D:510:PCW:C23	0.51	2.31	2	1
4:C:604:PCW:C41	4:C:604:PCW:C37	0.51	2.85	2	1
1:C:473:LYS:O	1:C:477:LEU:HB2	0.51	2.05	3	1
4:C:614:PCW:C31	4:C:614:PCW:O3	0.51	2.58	10	2
4:B:212:PCW:O1P	4:B:212:PCW:O2	0.51	2.28	6	3
4:D:505:PCW:H20	4:D:510:PCW:O2	0.51	2.06	3	1
1:A:245:LYS:O	1:A:249:GLU:HB2	0.51	2.05	7	2
4:C:619:PCW:O1P	4:C:620:PCW:H62	0.51	2.05	4	2
4:A:417:PCW:H472	5:D:511:17F:C42	0.51	2.35	6	2
4:B:207:PCW:C8	5:B:213:17F:O4	0.51	2.58	6	1
5:A:410:17F:H65	4:D:501:PCW:C24	0.51	2.34	7	1
4:A:401:PCW:H452	4:C:610:PCW:C25	0.51	2.35	10	1
4:C:607:PCW:C20	5:C:629:17F:H50	0.51	2.34	10	1
1:C:451:LYS:O	1:C:455:TYR:HB2	0.51	2.05	10	5
4:B:202:PCW:H381	4:B:202:PCW:H421	0.51	1.81	1	1
4:C:603:PCW:O2P	5:C:628:17F:H1	0.51	2.05	2	1
5:C:632:17F:C41	5:B:215:17F:H62	0.51	2.26	2	1
4:A:407:PCW:C39	4:B:210:PCW:H252	0.51	2.35	3	1
4:C:607:PCW:H121	4:C:608:PCW:H19	0.51	1.80	3	1
4:C:619:PCW:O31	4:C:619:PCW:O3P	0.51	2.28	8	2
4:D:506:PCW:H131	4:D:510:PCW:H381	0.51	1.81	3	1
4:C:610:PCW:H63	4:C:622:PCW:C36	0.51	2.35	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:619:PCW:H132	5:C:632:17F:H18	0.51	1.81	10	2
4:A:405:PCW:O31	4:B:203:PCW:C6	0.51	2.57	5	1
4:D:510:PCW:H412	4:D:516:PCW:C28	0.51	2.35	5	1
4:C:611:PCW:C6	4:C:617:PCW:H31	0.51	2.35	6	2
4:C:619:PCW:H73	4:C:619:PCW:O4P	0.51	2.04	6	2
4:D:501:PCW:H42	4:D:509:PCW:H331	0.51	1.82	6	1
4:D:503:PCW:C3	5:D:513:17F:O1	0.51	2.58	6	1
4:D:504:PCW:H341	4:D:504:PCW:C5	0.51	2.34	6	1
4:C:623:PCW:H411	4:C:624:PCW:H412	0.51	1.81	8	1
4:B:203:PCW:O1P	4:B:203:PCW:C3	0.51	2.59	9	2
4:A:408:PCW:C14	5:A:409:17F:H66	0.51	2.35	9	1
1:A:214:PHE:HD2	4:A:413:PCW:H282	0.51	1.65	10	1
1:A:275:LYS:HG2	1:C:499:LEU:HD21	0.51	1.82	1	4
4:A:405:PCW:H11	4:A:405:PCW:O31	0.51	2.05	10	3
5:C:628:17F:H11	5:C:628:17F:C31	0.51	2.34	1	1
5:C:628:17F:H56	5:C:628:17F:C11	0.51	2.35	1	1
5:C:632:17F:H77	5:B:215:17F:H58	0.51	1.82	1	1
4:B:205:PCW:C15	4:B:206:PCW:H172	0.51	2.34	1	1
4:D:508:PCW:C27	4:D:508:PCW:C22	0.51	2.56	9	3
4:A:405:PCW:C17	4:D:502:PCW:H483	0.51	2.35	2	1
4:A:412:PCW:H411	4:C:624:PCW:H472	0.51	1.83	9	2
2:B:79:LEU:HD23	2:B:112:VAL:HB	0.51	1.81	7	5
4:A:404:PCW:H32	4:B:210:PCW:H141	0.51	1.82	3	1
4:C:614:PCW:O3	4:C:614:PCW:O31	0.51	2.28	10	2
1:A:386:PHE:O	1:A:390:LEU:HG	0.51	2.06	8	2
4:C:615:PCW:C31	4:C:615:PCW:O3	0.51	2.59	6	2
4:B:212:PCW:H52	5:B:213:17F:C2	0.51	2.34	8	1
4:D:504:PCW:H121	4:D:504:PCW:C39	0.51	2.35	9	1
4:C:602:PCW:C7	5:B:214:17F:O10	0.51	2.58	10	1
4:C:607:PCW:O1P	4:C:624:PCW:C24	0.51	2.58	10	4
4:C:610:PCW:O3	4:C:610:PCW:O31	0.51	2.27	8	3
3:D:395:CYS:HA	3:D:432:ASP:HB3	0.51	1.82	1	1
4:A:415:PCW:C35	4:C:616:PCW:H412	0.51	2.35	5	3
4:A:416:PCW:O3P	4:C:616:PCW:H42	0.51	2.06	2	1
4:C:614:PCW:H63	5:C:632:17F:H2	0.51	1.80	2	2
4:A:411:PCW:H442	4:C:616:PCW:H211	0.51	1.83	3	2
4:B:205:PCW:C6	5:B:213:17F:O1	0.51	2.57	6	3
4:B:204:PCW:H2	4:B:208:PCW:C13	0.51	2.35	5	1
4:A:417:PCW:C14	4:C:603:PCW:H411	0.51	2.33	6	1
4:C:605:PCW:H372	4:C:605:PCW:H411	0.51	1.82	6	2
4:B:203:PCW:H62	4:B:203:PCW:O4P	0.51	2.06	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:269:MET:HE1	4:B:201:PCW:H252	0.51	1.81	7	1
4:A:403:PCW:O3	4:B:209:PCW:H322	0.51	2.05	7	1
4:C:625:PCW:O2	4:C:625:PCW:C11	0.51	2.59	8	1
4:A:408:PCW:C16	5:A:409:17F:H20	0.51	2.35	9	1
4:C:605:PCW:O1P	4:C:612:PCW:C6	0.51	2.58	9	1
4:A:403:PCW:H39	4:A:403:PCW:C18	0.51	2.32	10	1
4:D:502:PCW:H432	4:D:508:PCW:H221	0.51	1.80	10	1
4:C:606:PCW:O11	4:C:606:PCW:C6	0.51	2.57	1	2
4:B:212:PCW:C22	5:D:514:17F:H12A	0.51	2.35	1	1
5:B:213:17F:O10	5:B:213:17F:O7	0.51	2.28	2	1
4:C:612:PCW:H482	4:C:618:PCW:H231	0.51	1.81	3	1
4:B:211:PCW:H241	4:D:503:PCW:H231	0.51	1.80	3	1
5:B:213:17F:C25	4:D:509:PCW:H212	0.51	2.29	3	1
4:D:505:PCW:H20	4:D:510:PCW:C32	0.51	2.36	4	1
5:C:628:17F:H62	5:B:215:17F:C2X	0.51	2.35	8	2
4:D:504:PCW:C19	4:D:515:PCW:H282	0.51	2.35	5	1
4:A:417:PCW:C6	4:A:417:PCW:C31	0.51	2.88	7	2
4:A:417:PCW:C28	4:C:621:PCW:H262	0.51	2.34	6	1
4:C:610:PCW:C28	4:C:618:PCW:H272	0.51	2.34	6	1
4:C:612:PCW:C22	5:D:511:17F:H43	0.51	2.27	6	1
4:B:204:PCW:H122	4:B:208:PCW:H361	0.51	1.81	6	1
4:B:205:PCW:H182	4:B:207:PCW:H171	0.51	1.83	6	2
4:B:208:PCW:H421	5:D:512:17F:H77	0.51	1.82	6	1
4:A:403:PCW:H421	4:B:201:PCW:H221	0.51	1.81	8	1
5:C:632:17F:H67	5:B:215:17F:H65	0.51	1.82	8	1
4:C:621:PCW:H352	4:C:625:PCW:H211	0.51	1.82	9	1
4:B:203:PCW:C39	4:B:208:PCW:H39	0.51	2.34	9	1
5:D:514:17F:H4	5:D:514:17F:N1	0.51	2.21	9	1
4:C:616:PCW:O31	4:C:616:PCW:O3	0.51	2.28	10	1
4:B:202:PCW:H342	4:D:507:PCW:H11	0.51	1.83	10	1
4:B:206:PCW:H351	4:D:505:PCW:C32	0.51	2.35	10	1
4:B:208:PCW:H42	5:B:214:17F:O3	0.51	2.06	10	1
4:D:508:PCW:H31	4:D:508:PCW:O1P	0.51	2.04	5	5
1:C:546:GLU:O	1:C:550:LYS:HD2	0.51	2.06	6	2
4:B:204:PCW:C41	4:B:212:PCW:H252	0.51	2.34	3	1
4:D:508:PCW:H31	4:D:508:PCW:P	0.51	2.46	3	5
4:C:606:PCW:C21	4:C:606:PCW:C17	0.51	2.77	9	3
4:B:205:PCW:H221	4:B:207:PCW:H19	0.51	1.82	4	1
4:C:607:PCW:H181	5:C:629:17F:H29	0.51	1.82	5	1
4:D:507:PCW:H122	5:D:513:17F:H8A	0.51	1.82	8	1
4:A:411:PCW:C3	4:D:515:PCW:O3	0.51	2.58	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:619:PCW:H121	5:C:632:17F:O9	0.51	2.06	10	1
4:B:204:PCW:H351	4:B:208:PCW:C33	0.51	2.36	10	1
4:B:204:PCW:H182	4:B:208:PCW:C19	0.51	2.35	10	1
4:D:501:PCW:C6	4:D:509:PCW:O2P	0.51	2.58	2	1
4:D:509:PCW:C6	4:D:510:PCW:H322	0.51	2.36	2	1
4:A:412:PCW:C43	4:C:623:PCW:H471	0.51	2.28	3	2
4:A:415:PCW:H362	4:C:616:PCW:C40	0.51	2.36	3	1
4:C:602:PCW:H481	5:C:629:17F:H47	0.51	1.82	3	1
4:C:620:PCW:H421	5:B:215:17F:C35	0.51	2.32	10	4
4:B:205:PCW:C6	4:B:212:PCW:H321	0.51	2.29	3	1
4:B:206:PCW:H461	5:B:213:17F:C38	0.51	2.25	3	1
4:D:516:PCW:H52	4:D:516:PCW:H322	0.51	1.80	4	1
4:B:202:PCW:C34	4:D:507:PCW:H11	0.51	2.35	5	2
4:B:204:PCW:C41	5:D:514:17F:H10A	0.51	2.30	5	1
4:A:412:PCW:C2	4:C:624:PCW:H372	0.51	2.35	7	3
4:D:501:PCW:O31	4:D:501:PCW:O3	0.51	2.29	6	2
5:C:628:17F:H67	5:B:215:17F:H40	0.51	1.81	7	1
4:D:503:PCW:H281	5:D:513:17F:C20	0.51	2.36	7	1
4:C:614:PCW:C24	5:C:632:17F:H41	0.51	2.36	8	1
4:B:202:PCW:C33	4:D:507:PCW:H32	0.51	2.36	9	1
4:B:203:PCW:H142	4:B:203:PCW:C40	0.51	2.36	10	1
4:B:204:PCW:H63	5:B:214:17F:O4	0.51	2.06	10	1
4:B:212:PCW:H462	5:D:514:17F:C37	0.51	2.36	10	1
4:C:603:PCW:C46	4:D:515:PCW:H412	0.51	2.35	1	1
4:C:614:PCW:C45	4:B:207:PCW:H241	0.51	2.30	1	1
4:C:603:PCW:O4P	5:C:628:17F:O1	0.51	2.28	2	3
4:C:609:PCW:H19	4:C:620:PCW:H39	0.51	1.82	2	1
4:D:502:PCW:H171	4:D:502:PCW:C21	0.51	2.34	6	4
4:A:402:PCW:C8	5:D:513:17F:O5	0.51	2.59	3	1
4:C:607:PCW:H212	5:C:629:17F:H29	0.51	1.83	5	2
4:A:414:PCW:O31	4:A:414:PCW:O2P	0.51	2.28	4	1
1:A:313:VAL:HA	1:A:316:LEU:HD12	0.51	1.83	5	1
4:C:622:PCW:C32	4:C:622:PCW:C36	0.51	2.83	5	2
4:B:211:PCW:H461	4:B:211:PCW:H182	0.51	1.82	5	1
4:D:502:PCW:C7	4:D:502:PCW:O11	0.51	2.59	5	1
4:D:505:PCW:O11	4:D:509:PCW:C6	0.51	2.58	5	1
4:A:413:PCW:C42	4:C:611:PCW:C23	0.51	2.86	6	1
4:A:416:PCW:H41	4:A:416:PCW:H2	0.51	1.82	6	1
4:C:614:PCW:C19	5:C:632:17F:H38	0.51	2.35	7	2
4:B:201:PCW:H472	4:B:205:PCW:C28	0.51	2.36	6	1
4:C:615:PCW:C45	4:D:506:PCW:C47	0.51	2.89	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:205:PCW:H211	4:B:207:PCW:H411	0.51	1.82	8	1
4:A:404:PCW:O31	4:A:404:PCW:H11	0.51	2.05	10	2
4:D:507:PCW:C43	5:D:513:17F:H40	0.51	2.36	9	1
4:B:202:PCW:H31	4:B:202:PCW:O4P	0.51	2.06	10	1
4:A:415:PCW:H351	4:C:616:PCW:H431	0.51	1.82	1	1
4:A:417:PCW:H222	4:C:603:PCW:H162	0.51	1.83	1	1
4:A:417:PCW:H472	5:D:511:17F:C30	0.51	2.35	1	2
4:C:607:PCW:O11	4:C:607:PCW:C2	0.51	2.58	3	6
4:C:620:PCW:O11	4:C:620:PCW:O2	0.51	2.28	3	5
5:D:512:17F:H52	5:D:514:17F:H43	0.51	1.82	2	1
4:A:404:PCW:H42	4:A:404:PCW:H12	0.51	1.81	8	2
5:D:514:17F:C2X	5:D:514:17F:H67	0.51	2.36	3	1
4:C:602:PCW:H51	2:B:131:GLN:OE1	0.51	2.06	7	2
4:C:617:PCW:C25	4:D:507:PCW:H281	0.51	2.36	9	2
2:B:43:GLN:O	3:D:469:GLY:HA3	0.51	2.05	4	1
4:B:208:PCW:H162	5:B:214:17F:C8	0.51	2.35	4	1
4:A:407:PCW:H321	4:B:211:PCW:H132	0.51	1.82	6	1
4:A:411:PCW:H451	4:C:616:PCW:H251	0.51	1.81	6	1
5:C:628:17F:H53	5:B:213:17F:C40	0.51	2.30	6	1
4:B:206:PCW:C40	4:D:505:PCW:H122	0.51	2.35	6	1
4:B:212:PCW:H2	5:D:514:17F:O1	0.51	2.05	7	1
3:D:476:CYS:HA	3:D:479:LYS:HB3	0.51	1.83	7	1
4:C:622:PCW:H242	4:D:501:PCW:C44	0.51	2.36	8	1
2:B:3:GLU:HG3	2:B:52:LEU:HD22	0.51	1.83	8	1
4:D:502:PCW:C17	4:D:502:PCW:C21	0.51	2.68	8	1
4:B:210:PCW:H2	5:D:513:17F:H18A	0.51	1.83	9	1
4:B:208:PCW:C7	5:B:214:17F:O2	0.51	2.57	10	1
6:B:216:GNP:O2B	6:B:216:GNP:H5'2	0.51	2.06	10	1
4:D:506:PCW:H39	4:D:516:PCW:H261	0.51	1.81	10	1
4:D:509:PCW:H62	4:D:509:PCW:H12	0.51	1.81	10	1
1:A:364:ALA:HA	1:A:368:LEU:HD12	0.51	1.82	1	1
4:C:604:PCW:O1P	4:C:604:PCW:H32	0.51	2.06	1	1
4:C:614:PCW:H181	5:C:632:17F:C21	0.51	2.36	1	1
4:B:205:PCW:H141	4:B:207:PCW:C34	0.51	2.36	1	1
4:D:505:PCW:C21	4:D:510:PCW:H412	0.51	2.36	1	1
4:A:408:PCW:H212	5:A:409:17F:C32	0.51	2.36	2	1
4:A:408:PCW:H481	5:D:511:17F:H12A	0.51	1.82	2	1
4:A:405:PCW:C19	4:A:405:PCW:C15	0.51	2.89	5	5
4:C:612:PCW:H141	4:C:618:PCW:H39	0.51	1.80	3	2
4:C:614:PCW:H242	5:C:632:17F:H41	0.51	1.80	3	2
4:C:623:PCW:H39	4:C:624:PCW:C14	0.51	2.36	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:203:PCW:H171	4:B:208:PCW:H362	0.51	1.77	3	1
4:A:404:PCW:C26	4:C:617:PCW:H462	0.51	2.34	8	2
4:D:507:PCW:C12	5:D:513:17F:O8	0.51	2.55	4	1
4:A:416:PCW:H422	4:C:616:PCW:H211	0.51	1.83	5	1
4:D:503:PCW:C7	4:D:503:PCW:O4P	0.51	2.58	5	1
4:A:407:PCW:C40	4:B:210:PCW:H241	0.51	2.36	7	1
4:C:609:PCW:C12	5:C:631:17F:H18	0.51	2.37	7	1
4:B:210:PCW:O4P	5:D:513:17F:H1A	0.51	2.06	7	1
4:D:509:PCW:C8	4:D:510:PCW:H321	0.51	2.35	8	1
4:B:210:PCW:H452	4:B:210:PCW:C19	0.51	2.36	10	1
5:B:215:17F:C17	5:B:215:17F:O7	0.50	2.59	1	2
4:A:408:PCW:C43	5:A:409:17F:H70	0.50	2.36	2	1
4:A:408:PCW:H141	5:A:409:17F:H67	0.50	1.82	2	1
5:D:513:17F:O10	5:D:513:17F:C6	0.50	2.52	6	3
4:A:402:PCW:H283	4:A:413:PCW:H482	0.50	1.82	4	2
4:C:611:PCW:H471	4:C:611:PCW:C26	0.50	2.19	5	1
1:A:203:LEU:HD21	4:A:415:PCW:H282	0.50	1.81	10	3
4:B:206:PCW:H121	5:B:213:17F:C18	0.50	2.32	6	1
4:B:206:PCW:C6	4:B:206:PCW:O11	0.50	2.59	6	1
4:D:505:PCW:H442	4:D:506:PCW:H181	0.50	1.82	6	1
4:D:506:PCW:C39	4:D:516:PCW:H261	0.50	2.36	6	2
4:D:501:PCW:H222	5:D:511:17F:C20	0.50	2.36	7	1
5:B:214:17F:H2	5:B:214:17F:O1	0.50	2.05	8	1
4:A:408:PCW:H122	5:A:409:17F:C39	0.50	2.25	10	1
4:B:204:PCW:H472	4:D:502:PCW:H482	0.50	1.82	10	1
4:B:206:PCW:H412	5:B:213:17F:H8A	0.50	1.82	10	1
4:A:405:PCW:C46	4:A:414:PCW:H222	0.50	2.35	1	1
5:A:409:17F:H55	5:D:511:17F:C35	0.50	2.36	1	1
4:A:416:PCW:H63	5:C:630:17F:O8	0.50	2.06	3	3
4:C:606:PCW:H262	5:C:627:17F:H42	0.50	1.83	1	1
4:C:610:PCW:H39	4:C:622:PCW:C45	0.50	2.37	1	1
4:C:622:PCW:C38	4:C:623:PCW:H182	0.50	2.37	5	3
5:D:511:17F:H20	5:D:511:17F:O10	0.50	2.05	5	4
4:A:404:PCW:H272	4:C:617:PCW:H483	0.50	1.82	8	2
4:A:405:PCW:H342	5:D:512:17F:H34	0.50	1.82	4	1
4:C:606:PCW:H73	4:C:624:PCW:H171	0.50	1.82	4	2
4:D:505:PCW:H32	4:D:510:PCW:H341	0.50	1.84	4	1
4:C:605:PCW:H181	4:C:612:PCW:H342	0.50	1.81	5	1
4:B:201:PCW:H431	4:B:205:PCW:H251	0.50	1.83	6	1
4:B:204:PCW:C23	4:B:208:PCW:H283	0.50	2.30	6	1
4:C:615:PCW:C47	4:D:506:PCW:H472	0.50	2.36	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:621:PCW:H122	5:C:627:17F:H69	0.50	1.83	8	1
4:B:212:PCW:H422	5:D:514:17F:C11	0.50	2.36	8	1
4:D:504:PCW:H272	5:D:513:17F:H74	0.50	1.83	9	1
4:D:505:PCW:C44	4:D:506:PCW:H161	0.50	2.34	9	1
4:C:608:PCW:H452	4:B:207:PCW:H281	0.50	1.82	10	1
4:B:204:PCW:H471	5:D:512:17F:H48	0.50	1.84	1	1
4:D:503:PCW:O11	4:D:503:PCW:C2	0.50	2.56	4	2
4:C:617:PCW:O3	4:C:625:PCW:H151	0.50	2.06	2	1
4:C:621:PCW:H121	5:C:628:17F:H33	0.50	1.83	3	2
4:C:622:PCW:H39	4:C:622:PCW:C13	0.50	2.36	2	1
4:B:203:PCW:H52	4:B:204:PCW:C35	0.50	2.35	2	1
4:A:413:PCW:H332	4:C:611:PCW:C14	0.50	2.36	3	1
4:A:417:PCW:O31	4:A:417:PCW:O4P	0.50	2.30	3	1
4:D:505:PCW:H12	4:D:509:PCW:H73	0.50	1.83	3	2
4:A:402:PCW:H241	4:A:413:PCW:H241	0.50	1.83	6	1
4:B:202:PCW:H171	4:D:504:PCW:H31	0.50	1.82	6	1
4:A:403:PCW:H322	4:A:406:PCW:H351	0.50	1.83	7	1
4:A:413:PCW:C48	4:C:611:PCW:H281	0.50	2.36	8	2
4:A:402:PCW:C36	4:B:210:PCW:C44	0.50	2.89	8	1
4:A:405:PCW:H181	4:A:405:PCW:H222	0.50	1.84	8	1
4:B:211:PCW:H212	4:D:506:PCW:H231	0.50	1.82	8	1
4:D:506:PCW:H431	5:D:513:17F:C22	0.50	2.30	8	1
4:A:415:PCW:H31	4:A:415:PCW:O2P	0.50	2.07	9	1
4:C:608:PCW:H381	4:C:614:PCW:H421	0.50	1.83	9	1
4:A:402:PCW:N	5:D:513:17F:O5	0.50	2.44	10	1
4:C:617:PCW:O2P	4:C:625:PCW:C4	0.50	2.59	10	1
4:B:206:PCW:H351	4:D:505:PCW:H321	0.50	1.84	10	1
5:A:410:17F:H2	5:A:410:17F:O2	0.50	2.05	1	1
4:C:615:PCW:C2	4:D:516:PCW:H342	0.50	2.36	1	1
4:A:403:PCW:O31	4:A:403:PCW:O4P	0.50	2.30	2	2
4:C:618:PCW:H481	5:D:511:17F:C42	0.50	2.36	2	2
4:B:206:PCW:C42	5:B:213:17F:H32	0.50	2.36	4	1
4:C:619:PCW:C41	4:C:619:PCW:C37	0.50	2.86	5	1
4:D:510:PCW:H242	4:D:515:PCW:H462	0.50	1.84	5	1
4:C:606:PCW:C6	4:C:606:PCW:O11	0.50	2.59	6	3
4:D:502:PCW:C39	5:D:512:17F:H8	0.50	2.36	6	1
4:D:508:PCW:H182	4:D:508:PCW:C34	0.50	2.26	6	1
4:A:403:PCW:H62	4:A:406:PCW:H39	0.50	1.83	7	1
4:A:415:PCW:H482	5:D:513:17F:H37	0.50	1.83	7	1
4:C:617:PCW:H451	5:C:631:17F:C30	0.50	2.32	7	1
4:B:202:PCW:H73	4:B:202:PCW:O11	0.50	2.05	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:C:628:17F:H54	5:B:213:17F:H72	0.50	1.82	9	1
4:D:503:PCW:O11	4:D:506:PCW:C8	0.50	2.59	10	1
4:C:608:PCW:O31	4:C:608:PCW:H131	0.50	2.07	7	4
4:A:405:PCW:O2P	4:B:203:PCW:O3P	0.50	2.30	5	2
4:A:408:PCW:C48	5:D:511:17F:H12A	0.50	2.36	2	1
4:C:608:PCW:H271	5:C:626:17F:C40	0.50	2.32	6	2
4:A:415:PCW:C44	4:D:515:PCW:H211	0.50	2.36	3	1
4:A:411:PCW:C8	5:C:630:17F:H1	0.50	2.37	5	1
4:B:203:PCW:O2P	4:B:203:PCW:C5	0.50	2.59	5	3
4:C:612:PCW:H262	5:D:511:17F:H75	0.50	1.83	6	1
4:C:617:PCW:H131	4:C:625:PCW:C13	0.50	2.36	6	1
4:B:205:PCW:H262	4:B:207:PCW:C42	0.50	2.36	6	1
4:B:202:PCW:C17	4:D:504:PCW:H131	0.50	2.36	9	1
4:B:206:PCW:H441	5:B:213:17F:H33	0.50	1.83	9	1
4:A:407:PCW:H382	4:B:211:PCW:H422	0.50	1.83	10	1
5:C:632:17F:H52	4:B:207:PCW:C17	0.50	2.36	10	1
4:B:203:PCW:C41	4:B:208:PCW:H372	0.50	2.36	10	1
5:D:512:17F:H5	5:D:512:17F:O8	0.50	2.06	10	1
4:C:608:PCW:H281	5:B:214:17F:H54	0.50	1.84	1	1
4:D:505:PCW:H20	4:D:510:PCW:C36	0.50	2.36	1	1
4:D:508:PCW:O11	4:D:508:PCW:C6	0.50	2.58	1	2
5:A:409:17F:H50	4:D:510:PCW:H252	0.50	1.83	2	1
4:A:414:PCW:H52	4:C:624:PCW:O31	0.50	2.06	3	3
4:B:210:PCW:C31	4:B:210:PCW:O3	0.50	2.59	8	6
4:C:615:PCW:H451	4:D:506:PCW:C48	0.50	2.37	3	1
4:C:615:PCW:C48	4:D:503:PCW:H221	0.50	2.37	6	2
4:C:621:PCW:H421	4:D:506:PCW:C26	0.50	2.36	6	3
4:D:501:PCW:H252	5:D:511:17F:H73	0.50	1.84	4	1
4:C:620:PCW:C19	5:C:631:17F:C17	0.50	2.90	5	1
4:B:203:PCW:H261	4:B:208:PCW:C12	0.50	2.34	5	1
4:D:501:PCW:C27	4:D:508:PCW:H431	0.50	2.36	5	1
4:A:407:PCW:H482	4:D:506:PCW:C26	0.50	2.36	6	1
4:C:615:PCW:H381	4:C:617:PCW:H142	0.50	1.83	8	2
4:C:621:PCW:H472	4:D:506:PCW:H221	0.50	1.82	8	1
4:D:501:PCW:C7	5:D:514:17F:H60	0.50	2.32	8	1
4:D:503:PCW:H342	4:D:507:PCW:C34	0.50	2.36	9	1
4:C:607:PCW:H20	5:C:629:17F:H50	0.50	1.83	10	1
4:D:508:PCW:H19	5:D:512:17F:C1Y	0.50	2.36	10	1
4:A:412:PCW:H442	4:C:623:PCW:C47	0.50	2.34	1	2
4:C:606:PCW:H442	4:C:608:PCW:C1	0.50	2.33	1	1
4:D:502:PCW:C47	4:D:508:PCW:H271	0.50	2.37	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:503:PCW:H121	4:D:507:PCW:C39	0.50	2.37	10	2
4:A:404:PCW:H122	4:A:407:PCW:H352	0.50	1.83	3	1
4:C:615:PCW:H461	4:C:625:PCW:H262	0.50	1.81	8	2
4:B:205:PCW:C5	5:B:214:17F:H12A	0.50	2.33	3	1
4:A:413:PCW:H422	4:C:611:PCW:H242	0.50	1.83	4	1
5:C:626:17F:C42	4:B:207:PCW:H262	0.50	2.37	5	1
5:C:628:17F:O7	5:C:628:17F:O10	0.50	2.30	8	3
5:C:630:17F:O7	5:C:630:17F:O10	0.50	2.30	5	1
4:D:509:PCW:H12	4:D:509:PCW:H51	0.50	1.83	5	1
4:D:510:PCW:H412	4:D:516:PCW:H283	0.50	1.84	5	1
4:A:405:PCW:C11	5:D:512:17F:H31	0.50	2.36	6	1
4:C:612:PCW:H20	5:D:511:17F:C25	0.50	2.36	6	1
4:B:205:PCW:H161	4:B:206:PCW:H242	0.50	1.82	6	1
4:A:403:PCW:O31	4:A:403:PCW:P	0.50	2.70	7	1
4:B:204:PCW:H12	4:B:205:PCW:H63	0.50	1.84	8	1
4:B:202:PCW:H121	4:B:202:PCW:H62	0.50	1.84	9	1
4:B:206:PCW:C16	5:B:213:17F:H20A	0.50	2.37	9	1
4:A:401:PCW:H31	4:D:508:PCW:H241	0.50	1.82	1	1
4:A:405:PCW:O11	4:A:405:PCW:O2	0.50	2.30	1	1
4:C:604:PCW:O3	4:C:604:PCW:C31	0.50	2.60	8	8
4:C:613:PCW:O1P	4:C:623:PCW:H62	0.50	2.07	2	3
4:C:622:PCW:O3P	4:C:622:PCW:O31	0.50	2.30	1	2
5:C:627:17F:O9	5:C:627:17F:O1	0.50	2.29	1	1
2:B:77:GLY:HA3	2:B:159:LEU:HD21	0.50	1.83	1	1
4:B:206:PCW:H42	3:D:474:GLU:CD	0.50	2.32	1	1
4:C:605:PCW:H261	4:C:612:PCW:H181	0.50	1.83	5	2
3:D:465:CYS:HB3	3:D:468:CYS:SG	0.50	2.46	2	2
4:A:407:PCW:H40	4:B:211:PCW:C23	0.50	2.37	3	1
4:A:416:PCW:H351	4:C:616:PCW:H151	0.50	1.83	10	2
4:A:401:PCW:C33	4:D:502:PCW:H172	0.50	2.36	5	1
4:B:208:PCW:H431	4:B:212:PCW:H283	0.50	1.84	5	1
4:A:403:PCW:O3	4:A:403:PCW:O31	0.50	2.30	6	1
4:B:207:PCW:C41	4:B:209:PCW:H182	0.50	2.36	6	1
4:C:602:PCW:C15	5:C:626:17F:H49	0.50	2.36	8	1
4:A:415:PCW:C39	4:D:515:PCW:H161	0.50	2.37	1	2
4:B:203:PCW:H241	4:B:204:PCW:C19	0.50	2.37	1	1
4:B:207:PCW:H421	4:B:209:PCW:H182	0.50	1.83	1	1
4:B:209:PCW:O31	4:B:209:PCW:H11	0.50	2.07	9	7
4:D:503:PCW:H151	4:D:506:PCW:C34	0.50	2.36	1	1
4:D:505:PCW:H20	4:D:510:PCW:C37	0.50	2.37	1	1
4:C:601:PCW:H462	4:C:601:PCW:C12	0.50	2.36	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:604:PCW:H412	4:C:606:PCW:C24	0.50	2.35	2	4
2:B:132:ASP:HA	4:B:209:PCW:H63	0.50	1.84	2	1
4:B:208:PCW:H451	4:B:212:PCW:H452	0.50	1.84	2	1
4:C:608:PCW:H62	4:C:619:PCW:O11	0.50	2.06	3	2
4:A:402:PCW:C28	4:A:413:PCW:H482	0.50	2.37	4	1
4:C:608:PCW:O31	4:C:608:PCW:C11	0.50	2.59	7	2
4:B:202:PCW:C3	4:B:202:PCW:P	0.50	3.00	10	2
4:D:503:PCW:C28	5:D:513:17F:H20A	0.50	2.36	4	1
1:A:279:LEU:O	1:A:283:LEU:HG	0.50	2.07	5	1
4:A:403:PCW:C23	4:B:201:PCW:H211	0.50	2.20	6	1
4:C:605:PCW:O2P	4:C:612:PCW:C5	0.50	2.60	6	1
4:C:614:PCW:O2	4:C:614:PCW:C11	0.50	2.59	6	1
4:D:504:PCW:C35	4:D:504:PCW:C5	0.50	2.90	6	1
4:B:202:PCW:H171	4:D:504:PCW:H131	0.50	1.84	9	1
4:A:405:PCW:H332	4:B:203:PCW:H362	0.50	1.82	10	1
4:A:417:PCW:H181	4:C:603:PCW:H141	0.50	1.84	10	1
4:D:509:PCW:O4P	4:D:509:PCW:H62	0.50	2.06	10	1
4:C:623:PCW:O11	4:C:623:PCW:H51	0.49	2.07	9	2
4:B:211:PCW:H20	4:D:505:PCW:H451	0.49	1.84	1	1
5:A:410:17F:H65	4:D:502:PCW:C28	0.49	2.37	2	1
4:A:417:PCW:O11	4:A:417:PCW:H2	0.49	2.06	3	1
4:C:614:PCW:H242	5:C:632:17F:C24	0.49	2.37	3	1
4:C:609:PCW:H42	5:C:631:17F:H6A	0.49	1.82	5	1
4:D:505:PCW:H283	4:D:510:PCW:H142	0.49	1.84	5	1
4:A:401:PCW:C48	4:C:613:PCW:H242	0.49	2.26	6	1
1:C:495:LYS:O	1:C:499:LEU:HB2	0.49	2.07	7	1
4:C:606:PCW:H62	4:C:624:PCW:H20	0.49	1.82	7	1
4:D:509:PCW:H2	5:D:514:17F:H57	0.49	1.82	7	1
4:A:413:PCW:H481	4:C:611:PCW:H281	0.49	1.84	8	1
4:C:604:PCW:C19	4:D:509:PCW:H281	0.49	2.36	9	1
4:C:604:PCW:C25	5:D:514:17F:H70	0.49	2.37	10	1
4:B:212:PCW:H171	4:B:212:PCW:H382	0.49	1.83	10	1
5:C:632:17F:H52	4:B:207:PCW:H182	0.49	1.82	1	1
4:A:404:PCW:C23	4:A:404:PCW:C18	0.49	2.89	2	1
4:C:617:PCW:C32	4:C:625:PCW:H121	0.49	2.36	2	1
4:B:205:PCW:H171	4:B:207:PCW:H342	0.49	1.83	2	1
4:A:403:PCW:O11	4:B:201:PCW:H82	0.49	2.07	3	1
4:A:404:PCW:C35	4:A:407:PCW:C16	0.49	2.81	3	1
4:B:204:PCW:H411	4:B:212:PCW:C23	0.49	2.32	3	1
4:C:625:PCW:H262	4:B:211:PCW:H271	0.49	1.83	4	1
4:D:507:PCW:H252	5:D:513:17F:H60	0.49	1.82	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:A:409:17F:H48	4:D:510:PCW:H19	0.49	1.84	5	1
4:D:503:PCW:H42	4:D:510:PCW:C7	0.49	2.37	5	1
4:C:619:PCW:O4P	4:C:619:PCW:C7	0.49	2.60	6	1
4:B:203:PCW:C24	4:B:208:PCW:H131	0.49	2.38	7	1
4:B:205:PCW:H82	5:B:214:17F:H9	0.49	1.84	7	1
4:A:413:PCW:H351	4:C:611:PCW:H131	0.49	1.84	8	1
4:C:610:PCW:H63	4:C:622:PCW:C31	0.49	2.37	8	1
4:B:212:PCW:H40	5:D:514:17F:H30	0.49	1.84	8	1
4:A:406:PCW:C41	4:D:505:PCW:H412	0.49	2.36	9	1
4:B:203:PCW:C40	4:B:208:PCW:H39	0.49	2.38	9	1
4:C:607:PCW:H171	5:C:629:17F:H18A	0.49	1.84	1	2
4:C:614:PCW:C5	5:C:632:17F:O4	0.49	2.59	10	3
4:A:415:PCW:O2	4:C:616:PCW:C41	0.49	2.57	2	3
1:C:418:GLN:O	1:C:422:VAL:HB	0.49	2.06	2	1
4:A:413:PCW:H422	4:C:611:PCW:H181	0.49	1.84	3	1
5:B:213:17F:H51	5:D:514:17F:H74	0.49	1.82	3	1
5:B:215:17F:O7	5:B:215:17F:C17	0.49	2.59	7	5
4:D:503:PCW:H262	4:D:507:PCW:C47	0.49	2.37	3	1
4:D:506:PCW:C31	4:D:510:PCW:H352	0.49	2.37	3	1
4:B:207:PCW:C39	4:B:209:PCW:H161	0.49	2.38	4	1
4:D:508:PCW:H232	4:D:508:PCW:H421	0.49	1.84	5	1
4:A:405:PCW:H421	4:A:414:PCW:H241	0.49	1.83	7	1
5:A:409:17F:C26	4:D:510:PCW:H19	0.49	2.37	7	1
4:C:620:PCW:C15	5:B:215:17F:H4A	0.49	2.37	7	1
4:A:412:PCW:H271	4:B:203:PCW:H481	0.49	1.84	8	1
4:C:604:PCW:H19	5:D:514:17F:H53	0.49	1.79	8	1
4:B:205:PCW:C6	4:B:212:PCW:O2P	0.49	2.59	8	1
4:D:501:PCW:O11	4:D:501:PCW:C2	0.49	2.56	8	2
4:D:507:PCW:H211	4:D:507:PCW:H162	0.49	1.83	9	1
1:A:246:ASP:O	1:A:250:VAL:HB	0.49	2.06	1	1
4:B:206:PCW:H31	4:B:206:PCW:O1P	0.49	2.08	9	2
4:A:414:PCW:C5	4:C:624:PCW:O31	0.49	2.60	2	1
4:A:415:PCW:H351	4:C:616:PCW:H422	0.49	1.84	2	1
4:B:202:PCW:O11	4:B:202:PCW:O2	0.49	2.29	10	9
4:C:612:PCW:C47	4:C:618:PCW:H431	0.49	2.37	3	2
4:D:503:PCW:H322	4:D:510:PCW:H82	0.49	1.84	3	1
5:D:513:17F:H19	5:D:513:17F:C8	0.49	2.37	3	1
4:A:414:PCW:H322	4:C:623:PCW:C34	0.49	2.37	4	1
4:B:206:PCW:H162	5:B:213:17F:C31	0.49	2.37	4	1
5:A:409:17F:H37	4:D:509:PCW:H431	0.49	1.84	5	1
4:B:206:PCW:C4	4:B:209:PCW:H82	0.49	2.36	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:403:PCW:C12	4:B:209:PCW:H332	0.49	2.35	7	1
5:A:410:17F:C1	4:D:502:PCW:H63	0.49	2.21	7	1
4:B:203:PCW:H422	4:B:208:PCW:C39	0.49	2.37	7	1
2:B:48:GLY:HA2	3:D:450:ALA:CB	0.49	2.37	8	1
4:B:204:PCW:H411	5:D:514:17F:H9A	0.49	1.84	8	1
4:B:212:PCW:C12	5:D:514:17F:H4A	0.49	2.37	8	1
4:D:510:PCW:C40	4:D:516:PCW:H262	0.49	2.37	8	1
4:D:509:PCW:H151	5:D:514:17F:H60	0.49	1.83	9	1
4:C:619:PCW:C7	4:C:619:PCW:O4P	0.49	2.60	10	1
4:A:403:PCW:O31	4:A:403:PCW:O3	0.49	2.31	4	4
4:D:503:PCW:C14	4:D:506:PCW:H321	0.49	2.36	1	1
5:A:409:17F:H52	5:D:511:17F:C22	0.49	2.38	3	1
5:A:409:17F:H60	4:D:504:PCW:C33	0.49	2.36	4	1
4:C:611:PCW:C31	4:C:611:PCW:O4P	0.49	2.60	4	1
4:C:615:PCW:H431	4:D:506:PCW:H481	0.49	1.83	5	1
5:A:410:17F:H32	4:D:502:PCW:H182	0.49	1.84	6	1
4:B:204:PCW:H32	4:B:208:PCW:C13	0.49	2.38	6	1
4:A:405:PCW:H161	4:D:508:PCW:H281	0.49	1.84	7	1
4:C:610:PCW:H11	4:C:612:PCW:H61	0.49	1.84	7	1
4:B:202:PCW:H322	4:D:504:PCW:H12	0.49	1.85	7	1
4:A:403:PCW:H171	4:B:205:PCW:H272	0.49	1.83	8	1
5:C:632:17F:H64	4:B:207:PCW:H482	0.49	1.83	9	1
4:D:504:PCW:H32	4:D:507:PCW:O2P	0.49	2.07	9	1
4:C:603:PCW:H442	4:D:515:PCW:C35	0.49	2.37	1	2
4:C:607:PCW:H172	5:C:629:17F:C18	0.49	2.38	9	2
4:C:608:PCW:C12	4:C:614:PCW:C7	0.49	2.91	1	2
5:C:631:17F:O7	5:C:631:17F:C17	0.49	2.60	6	7
1:A:246:ASP:HA	1:C:528:ARG:CZ	0.49	2.38	5	2
4:A:415:PCW:O3	4:A:415:PCW:O31	0.49	2.30	2	4
1:C:533:LEU:HD23	1:C:536:LEU:HD12	0.49	1.85	2	2
4:D:507:PCW:H471	5:D:513:17F:C31	0.49	2.38	2	1
5:A:409:17F:C29	5:D:511:17F:H39	0.49	2.38	3	1
4:B:210:PCW:C1	4:D:503:PCW:H131	0.49	2.37	3	2
4:A:404:PCW:H11	4:B:210:PCW:H141	0.49	1.83	8	2
4:C:606:PCW:H161	5:C:627:17F:C12	0.49	2.37	5	2
4:B:212:PCW:H352	5:B:213:17F:C9	0.49	2.32	5	1
4:C:603:PCW:H52	5:C:628:17F:C1	0.49	2.38	6	1
4:C:610:PCW:H412	4:C:610:PCW:C20	0.49	2.35	8	2
4:C:623:PCW:O3P	4:C:623:PCW:O31	0.49	2.30	6	1
4:D:501:PCW:H222	5:D:511:17F:C19	0.49	2.37	7	1
4:D:508:PCW:H232	4:D:508:PCW:C36	0.49	2.38	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:605:PCW:O1P	4:C:612:PCW:H61	0.49	2.07	9	1
4:C:625:PCW:O31	4:C:625:PCW:H73	0.49	2.08	9	1
5:C:628:17F:H56	5:C:628:17F:C10	0.49	2.37	9	1
4:D:504:PCW:C39	4:D:504:PCW:C12	0.49	2.90	9	1
4:D:515:PCW:H82	4:D:516:PCW:H42	0.49	1.84	9	1
4:A:413:PCW:H442	4:C:611:PCW:H211	0.49	1.83	10	1
4:C:608:PCW:H471	4:B:205:PCW:C22	0.49	2.38	10	1
4:B:204:PCW:H352	4:B:208:PCW:H332	0.49	1.84	10	1
4:A:408:PCW:C31	4:A:408:PCW:C35	0.49	2.91	7	7
4:C:612:PCW:O31	4:C:612:PCW:C3	0.49	2.59	3	5
4:B:205:PCW:C8	4:B:212:PCW:O1P	0.49	2.61	1	1
4:B:212:PCW:O31	4:B:212:PCW:O3	0.49	2.30	10	3
4:D:504:PCW:H272	5:D:513:17F:H68	0.49	1.83	2	1
4:A:401:PCW:H472	4:C:610:PCW:C26	0.49	2.37	4	1
4:D:505:PCW:C45	4:D:506:PCW:H251	0.49	2.38	5	1
2:B:62:GLU:HB3	2:B:68:ARG:NH2	0.49	2.21	6	1
4:A:401:PCW:H322	4:D:508:PCW:C39	0.49	2.37	7	1
4:A:413:PCW:H382	4:C:611:PCW:H221	0.49	1.83	8	2
4:C:608:PCW:C13	4:C:614:PCW:C7	0.49	2.90	8	1
4:C:611:PCW:H352	4:C:625:PCW:C11	0.49	2.38	8	1
4:C:608:PCW:C38	4:C:614:PCW:H421	0.49	2.37	9	1
5:C:632:17F:H51	4:B:201:PCW:H451	0.49	1.84	9	1
4:D:505:PCW:H341	4:D:506:PCW:C12	0.49	2.38	9	1
3:D:399:PHE:HE2	3:D:429:ASP:HB3	0.49	1.67	10	1
5:A:409:17F:H55	5:D:511:17F:C34	0.49	2.37	1	1
4:B:212:PCW:H40	5:D:514:17F:C39	0.49	2.38	1	1
4:A:415:PCW:H412	4:D:515:PCW:C18	0.49	2.37	10	2
4:A:417:PCW:C42	4:C:605:PCW:H451	0.49	2.38	2	1
4:B:201:PCW:O31	4:B:201:PCW:H11	0.49	2.07	10	4
4:A:404:PCW:O3	4:A:407:PCW:H121	0.49	2.08	3	1
5:A:410:17F:H75	5:D:511:17F:H61	0.49	1.84	3	1
4:A:413:PCW:H411	4:C:611:PCW:H181	0.49	1.85	3	1
4:B:204:PCW:C11	4:B:208:PCW:H151	0.49	2.37	3	1
4:B:204:PCW:H231	4:B:208:PCW:H242	0.49	1.85	7	3
4:C:605:PCW:C47	4:C:618:PCW:H421	0.49	2.38	4	1
4:B:212:PCW:C44	5:D:514:17F:H68	0.49	2.38	4	1
5:D:512:17F:C1X	5:D:514:17F:H39	0.49	2.33	4	1
4:C:606:PCW:C15	5:C:627:17F:H11A	0.49	2.37	5	2
4:C:617:PCW:H322	4:C:625:PCW:H152	0.49	1.83	6	1
4:B:204:PCW:O3P	4:B:204:PCW:C31	0.49	2.61	6	1
1:A:312:HIS:CD2	4:C:602:PCW:H283	0.49	2.43	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:602:PCW:H481	4:C:607:PCW:C23	0.49	2.37	7	1
4:C:609:PCW:H152	5:C:631:17F:C33	0.49	2.38	7	1
4:B:208:PCW:H122	5:B:214:17F:H18	0.49	1.84	7	1
4:C:614:PCW:H171	4:C:614:PCW:H212	0.49	1.84	8	1
4:C:625:PCW:H2	4:C:625:PCW:O4P	0.49	2.07	8	2
4:B:205:PCW:H212	4:B:205:PCW:C17	0.49	2.34	8	1
4:B:205:PCW:C7	4:B:212:PCW:H41	0.49	2.37	8	1
4:B:208:PCW:O31	4:B:208:PCW:P	0.49	2.70	8	1
4:B:212:PCW:H272	5:D:512:17F:H67	0.49	1.84	8	1
5:D:513:17F:H69	5:D:513:17F:H10A	0.49	1.84	8	1
4:A:415:PCW:H461	4:C:615:PCW:H251	0.49	1.85	9	1
4:D:515:PCW:C8	4:D:516:PCW:H42	0.49	2.38	9	1
4:B:204:PCW:C35	4:B:208:PCW:C33	0.49	2.91	10	1
4:B:206:PCW:H122	5:B:213:17F:H18	0.49	1.84	10	1
4:B:211:PCW:H19	4:D:505:PCW:C42	0.49	2.37	10	1
4:C:604:PCW:H372	4:C:604:PCW:C42	0.49	2.37	1	4
4:C:607:PCW:C17	5:C:629:17F:C18	0.49	2.90	1	1
4:C:611:PCW:O11	4:C:611:PCW:C2	0.49	2.57	6	6
2:B:15:GLY:HA3	6:B:216:GNP:C8	0.49	2.38	1	2
4:D:504:PCW:H481	4:D:510:PCW:H20	0.49	1.84	1	1
5:A:409:17F:H52	5:D:511:17F:C23	0.49	2.37	3	1
4:C:621:PCW:C36	5:C:627:17F:H76	0.49	2.38	3	1
5:C:628:17F:H65	5:C:628:17F:C2X	0.49	2.38	3	1
4:B:211:PCW:H52	4:B:211:PCW:H322	0.49	1.83	4	1
4:C:613:PCW:O1P	4:C:613:PCW:H51	0.49	2.07	7	4
4:B:206:PCW:H122	5:B:213:17F:H4	0.49	1.85	5	1
4:C:603:PCW:H442	4:D:515:PCW:H362	0.49	1.85	6	1
4:B:203:PCW:C8	5:D:512:17F:H1A	0.49	2.38	6	1
4:A:407:PCW:C39	4:B:210:PCW:H272	0.49	2.22	7	2
4:D:509:PCW:H2	5:D:514:17F:C31	0.49	2.38	7	1
4:B:209:PCW:H39	5:B:213:17F:H64	0.49	1.84	8	1
4:A:401:PCW:C39	4:D:502:PCW:C23	0.49	2.91	9	1
4:B:208:PCW:O11	4:B:208:PCW:C2	0.49	2.53	9	1
1:A:307:ASP:HA	1:A:310:ARG:HD2	0.49	1.83	2	2
4:A:417:PCW:C44	4:C:605:PCW:H451	0.49	2.38	2	2
4:C:624:PCW:C31	4:C:624:PCW:O3	0.49	2.61	7	6
5:B:214:17F:O8	5:B:214:17F:C5	0.49	2.53	1	2
4:D:501:PCW:H222	5:D:511:17F:C31	0.49	2.36	1	3
4:D:510:PCW:C7	4:D:510:PCW:H121	0.49	2.37	1	1
4:A:401:PCW:H322	4:D:508:PCW:H232	0.49	1.83	2	1
4:D:505:PCW:H222	4:D:505:PCW:C18	0.49	2.24	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:447:GLU:O	1:C:451:LYS:HG2	0.49	2.08	4	1
4:C:605:PCW:C48	4:C:618:PCW:H421	0.49	2.38	4	1
4:B:205:PCW:C1	5:B:214:17F:H12A	0.49	2.37	4	2
4:C:604:PCW:H231	5:D:514:17F:H76	0.49	1.85	5	1
4:D:509:PCW:C1	4:D:509:PCW:C5	0.49	2.77	6	1
4:D:508:PCW:H442	5:D:512:17F:C27	0.49	2.38	7	2
4:A:403:PCW:C40	4:B:201:PCW:H221	0.49	2.38	8	1
4:A:403:PCW:H62	4:A:406:PCW:H422	0.49	1.84	8	1
4:C:602:PCW:H232	5:C:626:17F:H48	0.49	1.83	8	1
5:C:627:17F:H55	5:B:213:17F:C24	0.49	2.38	8	1
4:D:505:PCW:H421	4:D:506:PCW:H161	0.49	1.83	8	1
4:D:501:PCW:H62	4:D:509:PCW:O31	0.49	2.08	9	1
4:B:203:PCW:C3	4:B:203:PCW:O1P	0.49	2.61	10	1
4:C:602:PCW:H172	4:C:602:PCW:C21	0.48	2.37	1	2
4:C:604:PCW:H171	4:D:509:PCW:H283	0.48	1.84	1	1
4:C:606:PCW:H442	4:C:608:PCW:C3	0.48	2.38	1	1
4:C:615:PCW:H2	4:D:516:PCW:H342	0.48	1.85	1	1
4:B:210:PCW:C4	4:B:210:PCW:C32	0.48	2.91	1	1
4:D:503:PCW:C36	4:D:507:PCW:H321	0.48	2.38	3	3
5:D:513:17F:O2	5:D:513:17F:H5	0.48	2.08	1	1
5:C:630:17F:O1	5:C:630:17F:N1	0.48	2.39	2	1
4:D:504:PCW:C23	4:D:504:PCW:H182	0.48	2.38	2	1
4:A:414:PCW:H63	4:C:624:PCW:O2	0.48	2.08	7	3
4:C:613:PCW:O4P	4:C:613:PCW:C7	0.48	2.61	4	6
5:B:213:17F:H66	4:D:505:PCW:C39	0.48	2.38	3	1
4:D:509:PCW:H181	4:D:509:PCW:C22	0.48	2.38	3	1
4:B:205:PCW:C6	4:B:212:PCW:H322	0.48	2.38	4	1
4:B:212:PCW:C42	5:D:514:17F:H12	0.48	2.37	4	1
4:B:204:PCW:H411	5:D:514:17F:C9	0.48	2.38	5	1
4:B:212:PCW:H411	4:B:212:PCW:H211	0.48	1.85	5	1
4:A:417:PCW:O11	4:C:603:PCW:H331	0.48	2.08	6	1
4:D:502:PCW:H482	4:D:508:PCW:C47	0.48	2.29	6	1
4:D:508:PCW:H332	4:D:508:PCW:C13	0.48	2.36	6	1
5:A:409:17F:H60	4:D:504:PCW:H441	0.48	1.85	7	1
4:A:415:PCW:H362	4:C:616:PCW:H411	0.48	1.85	7	1
4:C:614:PCW:O31	4:C:614:PCW:O3	0.48	2.31	7	2
2:B:117:LYS:HG2	6:B:216:GNP:C6	0.48	2.37	7	1
4:B:212:PCW:H421	4:B:212:PCW:C22	0.48	2.35	7	1
4:A:411:PCW:H411	4:A:411:PCW:C37	0.48	2.29	8	1
4:B:205:PCW:H172	4:B:207:PCW:H362	0.48	1.85	8	1
4:C:610:PCW:H20	4:C:610:PCW:C43	0.48	2.30	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:210:PCW:H41	4:B:210:PCW:C32	0.48	2.37	1	1
4:D:501:PCW:C21	5:D:511:17F:H19	0.48	2.35	1	1
4:D:501:PCW:H11	4:D:509:PCW:H352	0.48	1.85	1	1
4:D:504:PCW:C31	4:D:504:PCW:O3	0.48	2.61	6	4
4:D:508:PCW:O11	4:D:508:PCW:O2	0.48	2.30	3	4
4:A:414:PCW:H381	4:C:623:PCW:C25	0.48	2.38	2	2
4:B:203:PCW:H52	4:B:204:PCW:H351	0.48	1.84	2	1
1:C:540:GLY:O	1:C:544:LEU:HG	0.48	2.07	3	2
4:C:615:PCW:H341	4:D:516:PCW:C35	0.48	2.38	4	3
4:C:620:PCW:H421	5:B:215:17F:H59	0.48	1.84	3	1
4:B:203:PCW:H241	5:B:214:17F:H18	0.48	1.84	3	1
4:B:203:PCW:H272	4:B:208:PCW:H142	0.48	1.85	3	1
4:C:606:PCW:H131	4:C:624:PCW:H281	0.48	1.83	4	1
4:B:201:PCW:C32	4:B:209:PCW:O3	0.48	2.59	4	1
4:B:206:PCW:C28	4:B:206:PCW:H451	0.48	2.38	4	1
5:A:410:17F:H67	4:D:501:PCW:H252	0.48	1.83	5	1
4:C:623:PCW:H462	4:C:624:PCW:C48	0.48	2.38	5	1
4:A:411:PCW:C43	4:A:416:PCW:H40	0.48	2.35	6	1
4:A:417:PCW:H472	5:D:511:17F:H77	0.48	1.83	6	1
4:B:204:PCW:C12	4:B:208:PCW:C36	0.48	2.90	6	1
4:C:614:PCW:O3	4:C:614:PCW:C31	0.48	2.61	7	2
4:D:505:PCW:C43	4:D:506:PCW:H161	0.48	2.39	9	1
1:A:264:LYS:HE2	1:C:509:ALA:HB1	0.48	1.84	5	4
1:A:372:ARG:O	1:A:376:LEU:HG	0.48	2.08	1	2
4:A:405:PCW:H321	4:B:203:PCW:H332	0.48	1.86	8	2
4:C:614:PCW:H181	5:C:632:17F:C22	0.48	2.37	1	1
1:C:544:LEU:O	1:C:548:HIS:HB2	0.48	2.09	2	1
4:C:605:PCW:O1P	4:C:605:PCW:H2	0.48	2.09	4	7
4:C:612:PCW:C14	4:C:618:PCW:C39	0.48	2.91	7	2
4:B:210:PCW:H342	4:B:210:PCW:H122	0.48	1.83	3	1
5:A:409:17F:O5	4:B:202:PCW:C8	0.48	2.60	4	1
4:C:624:PCW:O31	4:C:624:PCW:O3	0.48	2.31	7	6
4:B:204:PCW:C11	4:B:208:PCW:C15	0.48	2.90	4	2
4:A:401:PCW:H452	4:C:610:PCW:H241	0.48	1.83	5	1
4:C:615:PCW:H52	4:C:615:PCW:O2P	0.48	2.09	5	1
4:C:610:PCW:O2P	4:C:618:PCW:C6	0.48	2.48	6	2
4:C:619:PCW:H141	5:C:632:17F:C18	0.48	2.39	6	2
4:B:204:PCW:C33	4:B:208:PCW:H332	0.48	2.36	6	1
5:D:513:17F:H10A	5:D:513:17F:H59	0.48	1.85	7	1
4:C:602:PCW:O3	5:B:214:17F:H57	0.48	2.09	8	1
4:C:615:PCW:H452	4:D:506:PCW:C47	0.48	2.38	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:502:PCW:O31	4:D:502:PCW:O3	0.48	2.30	8	1
4:B:204:PCW:C40	5:D:512:17F:H9	0.48	2.35	9	1
4:B:207:PCW:O4P	4:B:207:PCW:H2	0.48	2.08	10	1
4:A:411:PCW:O3	4:A:411:PCW:O31	0.48	2.31	5	4
4:C:606:PCW:C16	5:C:627:17F:C11	0.48	2.90	1	1
4:C:618:PCW:O4P	4:C:618:PCW:C8	0.48	2.62	2	9
4:A:408:PCW:H471	5:D:511:17F:C1X	0.48	2.38	2	1
5:A:410:17F:H65	4:D:502:PCW:H282	0.48	1.84	2	1
4:B:204:PCW:H12	4:B:212:PCW:H322	0.48	1.85	2	1
4:B:210:PCW:H19	4:B:210:PCW:C43	0.48	2.38	2	1
4:A:413:PCW:C33	4:C:611:PCW:C13	0.48	2.82	3	1
4:B:204:PCW:H332	4:B:208:PCW:C32	0.48	2.37	5	2
4:D:505:PCW:H221	4:D:510:PCW:H331	0.48	1.85	3	1
4:A:405:PCW:O2P	4:B:203:PCW:C6	0.48	2.62	4	1
4:A:413:PCW:C36	4:C:611:PCW:C15	0.48	2.87	4	1
4:C:603:PCW:H62	4:D:516:PCW:O2P	0.48	2.08	9	2
5:A:409:17F:H40	4:D:503:PCW:C40	0.48	2.38	5	1
4:A:405:PCW:C43	4:A:414:PCW:H282	0.48	2.39	6	1
4:A:411:PCW:O31	4:A:411:PCW:O3	0.48	2.31	6	2
4:A:413:PCW:H362	4:C:611:PCW:H132	0.48	1.78	6	1
4:B:202:PCW:H31	4:B:202:PCW:H41	0.48	1.84	6	1
4:B:204:PCW:H221	4:B:204:PCW:H181	0.48	1.85	6	1
4:B:206:PCW:H32	5:B:213:17F:H4	0.48	1.85	6	1
5:A:409:17F:H9A	4:D:504:PCW:C39	0.48	2.38	7	1
4:C:602:PCW:H63	2:B:128:LYS:HB2	0.48	1.84	7	1
4:C:615:PCW:H41	4:D:515:PCW:H131	0.48	1.85	7	1
4:B:208:PCW:H462	4:B:212:PCW:H441	0.48	1.85	8	1
4:A:402:PCW:C7	5:D:513:17F:O5	0.48	2.61	10	1
4:B:201:PCW:O31	4:B:207:PCW:H12	0.48	2.07	10	1
4:B:206:PCW:C41	4:B:206:PCW:C37	0.48	2.87	10	1
4:A:408:PCW:O2	4:A:408:PCW:C35	0.48	2.61	1	1
4:C:610:PCW:O3	4:C:618:PCW:H63	0.48	2.08	1	1
5:C:626:17F:H78	5:B:214:17F:H53	0.48	1.85	1	1
4:B:208:PCW:H2	4:B:208:PCW:O11	0.48	2.09	1	2
1:A:231:ASN:HA	1:A:234:LYS:HE3	0.48	1.86	2	1
1:A:365:LYS:CB	1:A:366:PRO:HD3	0.48	2.39	7	5
4:A:403:PCW:H222	4:B:201:PCW:H141	0.48	1.85	2	1
4:A:406:PCW:H372	4:B:211:PCW:C36	0.48	2.37	2	2
1:A:323:TYR:O	1:A:327:LEU:HG	0.48	2.08	5	2
4:D:504:PCW:C18	4:D:504:PCW:C22	0.48	2.62	5	2
4:A:404:PCW:H281	4:D:507:PCW:H482	0.48	1.83	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:620:PCW:H441	5:B:215:17F:C42	0.48	2.22	4	1
4:C:607:PCW:H20	5:C:629:17F:C26	0.48	2.35	5	2
4:C:623:PCW:H462	4:C:624:PCW:H483	0.48	1.83	5	1
5:C:632:17F:C39	5:B:215:17F:H65	0.48	2.39	5	1
2:B:128:LYS:HG3	4:D:503:PCW:O1P	0.48	2.08	5	1
4:B:202:PCW:H342	4:D:504:PCW:C1	0.48	2.39	5	1
4:B:204:PCW:H63	5:B:214:17F:O8	0.48	2.09	5	1
4:A:403:PCW:C41	4:A:403:PCW:C37	0.48	2.87	6	1
5:A:410:17F:O7	5:A:410:17F:O10	0.48	2.32	6	1
4:A:417:PCW:H282	4:C:621:PCW:C28	0.48	2.38	6	1
4:B:207:PCW:H351	4:B:209:PCW:H141	0.48	1.85	6	1
4:B:208:PCW:H40	5:D:512:17F:H71	0.48	1.86	6	1
4:C:608:PCW:H452	4:B:207:PCW:C24	0.48	2.38	7	1
4:C:608:PCW:H232	4:C:614:PCW:H381	0.48	1.84	7	1
4:C:613:PCW:O31	4:C:613:PCW:C1	0.48	2.58	7	1
4:D:508:PCW:H442	5:D:512:17F:H48	0.48	1.84	7	1
4:A:404:PCW:H82	4:A:407:PCW:H11	0.48	1.85	9	1
4:A:416:PCW:H11	4:A:416:PCW:C4	0.48	2.38	10	1
4:A:414:PCW:H452	4:C:623:PCW:H462	0.48	1.84	4	4
4:A:416:PCW:O1P	4:C:616:PCW:C8	0.48	2.57	8	2
4:B:204:PCW:C47	5:D:512:17F:H47	0.48	2.38	1	1
4:B:206:PCW:H381	5:B:213:17F:H8	0.48	1.83	1	1
4:D:516:PCW:O4P	4:D:516:PCW:C8	0.48	2.62	3	10
4:A:414:PCW:H483	4:B:212:PCW:C47	0.48	2.38	2	1
4:C:604:PCW:H332	4:C:604:PCW:C12	0.48	2.30	2	1
4:B:208:PCW:O11	4:B:208:PCW:C5	0.48	2.59	4	2
4:D:505:PCW:H221	4:D:510:PCW:C36	0.48	2.39	2	1
4:A:405:PCW:H19	4:D:508:PCW:H283	0.48	1.84	3	1
4:C:612:PCW:H32	4:C:618:PCW:O3	0.48	2.09	3	1
4:A:407:PCW:C8	4:B:211:PCW:O31	0.48	2.61	9	3
4:C:608:PCW:H252	4:C:614:PCW:H381	0.48	1.85	4	1
4:B:204:PCW:C11	4:B:208:PCW:H152	0.48	2.38	7	2
4:B:205:PCW:H61	4:B:212:PCW:P	0.48	2.49	4	1
4:A:413:PCW:H341	4:C:611:PCW:O3	0.48	2.09	6	1
4:B:206:PCW:C15	5:B:213:17F:H60	0.48	2.38	6	1
4:A:413:PCW:H471	4:C:611:PCW:H272	0.48	1.84	8	1
4:B:210:PCW:H461	4:D:507:PCW:H221	0.48	1.83	8	1
4:B:201:PCW:C36	4:B:207:PCW:H31	0.48	2.38	9	1
4:B:206:PCW:H441	5:B:213:17F:C1Z	0.48	2.38	9	1
4:D:507:PCW:H432	5:D:513:17F:C2X	0.48	2.34	9	1
4:D:509:PCW:H11	5:D:514:17F:O1	0.48	2.09	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:604:PCW:C38	5:C:627:17F:H36	0.48	2.35	10	1
4:C:608:PCW:H41	5:C:632:17F:O10	0.48	2.09	10	1
4:C:603:PCW:C8	4:D:516:PCW:P	0.48	3.02	1	1
4:C:612:PCW:H462	4:C:618:PCW:C39	0.48	2.38	1	2
4:C:612:PCW:C21	5:D:511:17F:H47	0.48	2.38	7	2
4:B:203:PCW:C6	4:B:203:PCW:O2	0.48	2.62	1	1
4:B:209:PCW:O11	4:B:209:PCW:C2	0.48	2.52	6	5
4:B:210:PCW:H481	4:D:507:PCW:H462	0.48	1.85	1	1
4:D:506:PCW:H441	5:D:513:17F:C22	0.48	2.36	1	1
4:C:613:PCW:H452	4:C:618:PCW:C20	0.48	2.38	2	1
4:B:202:PCW:H19	4:D:504:PCW:H122	0.48	1.85	2	1
4:C:606:PCW:H351	5:C:627:17F:H6	0.48	1.86	3	1
4:C:621:PCW:H332	4:D:516:PCW:H422	0.48	1.85	8	2
4:C:621:PCW:C44	4:D:506:PCW:H252	0.48	2.38	4	1
4:C:616:PCW:H62	4:C:616:PCW:H2	0.48	1.86	5	1
4:C:614:PCW:O2	4:C:614:PCW:O11	0.48	2.31	6	1
4:A:403:PCW:C8	4:B:209:PCW:O31	0.48	2.62	7	1
4:C:610:PCW:H41	4:C:622:PCW:C32	0.48	2.39	8	1
5:A:409:17F:H35	5:D:511:17F:C5	0.48	2.39	9	1
4:C:602:PCW:H351	5:B:214:17F:H78	0.48	1.83	9	1
4:D:501:PCW:H482	5:D:514:17F:H50	0.48	1.86	9	1
5:A:409:17F:H56	4:D:504:PCW:H431	0.48	1.85	10	1
4:C:617:PCW:H322	4:C:625:PCW:C12	0.48	2.38	2	2
2:B:85:ASN:HB2	2:B:122:SER:HB2	0.48	1.85	1	1
4:B:206:PCW:H73	4:B:209:PCW:H12	0.48	1.84	1	1
1:C:474:VAL:O	1:C:478:ARG:HB2	0.48	2.09	2	1
1:C:505:ASP:HA	1:C:508:ARG:HD2	0.48	1.85	7	3
4:C:601:PCW:C42	5:C:626:17F:H52	0.48	2.38	2	1
4:C:620:PCW:C20	5:C:631:17F:O10	0.48	2.62	2	2
4:B:205:PCW:H221	4:B:207:PCW:H172	0.48	1.86	2	1
4:B:206:PCW:H2	5:B:213:17F:C5	0.48	2.39	2	1
4:A:402:PCW:H362	4:B:210:PCW:H441	0.48	1.85	7	2
4:A:411:PCW:H31	4:D:515:PCW:C11	0.48	2.39	3	1
4:C:602:PCW:H412	5:B:214:17F:H68	0.48	1.83	3	1
4:C:605:PCW:H322	4:C:612:PCW:C6	0.48	2.37	3	1
4:C:609:PCW:H12	5:C:631:17F:H6	0.48	1.86	3	1
4:C:625:PCW:H12	4:C:625:PCW:O31	0.48	2.08	3	1
4:B:212:PCW:H352	5:B:214:17F:C22	0.48	2.38	3	1
4:D:501:PCW:H342	5:D:512:17F:H29	0.48	1.86	3	1
4:B:202:PCW:H131	4:B:202:PCW:C37	0.48	2.38	4	1
4:C:601:PCW:H382	5:C:626:17F:H54	0.48	1.85	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:205:PCW:H221	4:B:207:PCW:C15	0.48	2.39	7	1
5:B:213:17F:C1X	4:D:505:PCW:H141	0.48	2.39	7	1
4:A:408:PCW:H332	5:D:511:17F:C7	0.48	2.38	8	1
4:B:203:PCW:H131	4:B:208:PCW:H331	0.48	1.84	8	1
4:B:202:PCW:H332	4:D:507:PCW:H32	0.48	1.85	9	1
5:B:214:17F:H42	5:B:214:17F:C2X	0.48	2.36	9	1
4:D:505:PCW:H20	4:D:510:PCW:H322	0.48	1.85	9	1
4:A:404:PCW:H171	4:B:210:PCW:H232	0.48	1.84	1	1
4:C:608:PCW:O4P	4:C:608:PCW:C8	0.48	2.62	2	8
4:D:503:PCW:H483	4:D:510:PCW:H19	0.48	1.85	1	1
1:A:327:LEU:HD23	1:A:330:ARG:HD2	0.48	1.85	2	2
4:A:406:PCW:H40	4:D:505:PCW:H471	0.48	1.85	2	1
4:A:413:PCW:C33	4:C:611:PCW:C3	0.48	2.89	2	1
4:D:505:PCW:C21	4:D:509:PCW:H472	0.48	2.39	3	1
4:C:605:PCW:H211	4:C:612:PCW:C38	0.48	2.32	4	1
4:D:510:PCW:H12	4:D:510:PCW:O31	0.48	2.09	4	1
2:B:6:LEU:HB2	2:B:55:ILE:HG22	0.48	1.85	5	1
4:B:205:PCW:C26	4:B:207:PCW:H422	0.48	2.39	6	1
4:D:502:PCW:H411	4:D:508:PCW:C19	0.48	2.39	7	2
4:C:601:PCW:H471	4:C:601:PCW:H121	0.48	1.84	7	1
4:B:203:PCW:H382	4:B:203:PCW:C14	0.48	2.39	8	1
4:D:503:PCW:O11	4:D:506:PCW:H11	0.48	2.09	8	1
4:B:206:PCW:C15	5:B:213:17F:H20A	0.48	2.39	9	1
4:D:507:PCW:H451	5:D:513:17F:H35	0.48	1.85	9	1
4:B:211:PCW:H19	4:D:505:PCW:H412	0.48	1.85	10	1
4:D:506:PCW:H241	4:D:516:PCW:H471	0.48	1.84	1	1
1:A:213:THR:O	1:A:217:LEU:HG	0.48	2.09	10	2
4:C:614:PCW:C8	5:C:632:17F:O4	0.48	2.62	2	1
4:C:617:PCW:C13	4:C:625:PCW:H142	0.48	2.39	2	2
2:B:79:LEU:CD2	2:B:112:VAL:HB	0.48	2.39	2	4
4:C:606:PCW:H73	4:C:606:PCW:C11	0.48	2.35	3	1
4:B:205:PCW:C14	4:B:206:PCW:C20	0.48	2.90	4	1
4:D:508:PCW:H132	4:D:508:PCW:C32	0.48	2.39	5	2
4:D:509:PCW:H142	4:D:509:PCW:H482	0.48	1.86	6	1
4:A:408:PCW:C16	5:A:409:17F:H31	0.48	2.39	7	1
1:A:229:TRP:O	1:A:233:GLU:HG2	0.48	2.09	9	1
4:D:506:PCW:H422	5:D:513:17F:C28	0.48	2.38	9	1
4:A:417:PCW:H321	4:C:622:PCW:H331	0.48	1.85	10	1
4:C:621:PCW:H372	4:C:625:PCW:C21	0.47	2.39	1	1
4:D:503:PCW:O4P	4:D:503:PCW:C8	0.47	2.63	1	7
4:C:620:PCW:H281	5:C:631:17F:H37	0.47	1.87	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:506:PCW:C32	4:D:510:PCW:H372	0.47	2.39	2	1
4:D:506:PCW:C20	4:D:516:PCW:H281	0.47	2.38	3	2
4:A:411:PCW:H32	4:D:515:PCW:C12	0.47	2.39	4	1
4:C:608:PCW:O31	4:C:614:PCW:C6	0.47	2.62	5	2
4:C:610:PCW:H242	4:C:618:PCW:H442	0.47	1.85	4	1
4:A:412:PCW:H31	4:C:624:PCW:H411	0.47	1.86	5	1
4:D:501:PCW:H73	4:D:509:PCW:C31	0.47	2.38	5	1
4:D:501:PCW:H42	4:D:509:PCW:C31	0.47	2.39	5	1
5:D:512:17F:H30	5:D:514:17F:H30	0.47	1.85	5	1
4:C:609:PCW:H171	5:C:631:17F:H61	0.47	1.86	7	1
4:A:405:PCW:C32	4:B:203:PCW:H332	0.47	2.39	8	1
4:C:611:PCW:H372	4:C:625:PCW:O11	0.47	2.09	8	1
4:C:621:PCW:H442	4:D:516:PCW:H481	0.47	1.85	9	1
5:C:627:17F:C36	5:C:628:17F:H57	0.47	2.37	10	1
4:B:202:PCW:H341	4:D:507:PCW:H32	0.47	1.84	10	1
4:D:503:PCW:H42	4:D:506:PCW:C7	0.47	2.38	10	1
4:C:624:PCW:O3	4:C:624:PCW:O31	0.47	2.32	1	1
2:B:112:VAL:HG13	2:B:140:PRO:HG2	0.47	1.85	1	1
4:B:201:PCW:O11	4:B:201:PCW:O2	0.47	2.32	2	3
4:A:405:PCW:O3	5:D:512:17F:H31	0.47	2.09	4	2
4:B:212:PCW:H422	5:D:514:17F:H67	0.47	1.86	2	1
4:D:502:PCW:H361	4:D:508:PCW:H372	0.47	1.86	2	2
4:A:401:PCW:H462	4:C:613:PCW:H261	0.47	1.85	3	1
4:C:617:PCW:H412	5:C:631:17F:C24	0.47	2.33	3	1
4:B:204:PCW:O4P	4:B:204:PCW:C8	0.47	2.62	6	3
4:D:502:PCW:H462	5:D:512:17F:H9A	0.47	1.86	3	1
1:A:267:GLU:O	1:A:271:LEU:HG	0.47	2.08	4	1
5:A:410:17F:H73	4:D:501:PCW:C25	0.47	2.38	4	1
4:C:620:PCW:H471	5:B:215:17F:H67	0.47	1.85	4	1
4:C:625:PCW:O1P	4:C:625:PCW:C5	0.47	2.60	5	1
4:D:503:PCW:H362	4:D:507:PCW:H341	0.47	1.86	6	1
4:A:415:PCW:C45	4:D:515:PCW:H231	0.47	2.39	7	1
4:A:401:PCW:H372	4:D:502:PCW:H212	0.47	1.85	8	1
4:C:614:PCW:H261	5:C:632:17F:H45	0.47	1.86	8	1
4:D:502:PCW:H442	5:D:512:17F:H48	0.47	1.84	8	1
4:D:508:PCW:C19	5:D:512:17F:H31	0.47	2.35	8	1
4:A:415:PCW:C3	4:A:415:PCW:O2P	0.47	2.62	9	1
4:A:415:PCW:C39	4:C:616:PCW:H451	0.47	2.38	10	1
4:D:501:PCW:H73	5:D:514:17F:C3	0.47	2.39	10	1
4:A:403:PCW:H41	4:A:406:PCW:O1P	0.47	2.09	1	1
4:C:603:PCW:C26	4:D:515:PCW:H171	0.47	2.38	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:288:ARG:O	1:A:292:HIS:HB2	0.47	2.09	2	1
4:D:509:PCW:H321	4:D:510:PCW:O3P	0.47	2.09	5	2
4:C:604:PCW:C16	4:C:604:PCW:C21	0.47	2.92	3	1
4:C:619:PCW:O31	4:C:619:PCW:C4	0.47	2.62	3	2
4:B:210:PCW:P	4:B:210:PCW:O2	0.47	2.72	3	1
4:A:405:PCW:C31	5:D:512:17F:H33	0.47	2.40	4	1
4:A:417:PCW:C48	5:D:511:17F:H55	0.47	2.39	4	1
4:C:608:PCW:H381	4:B:207:PCW:H283	0.47	1.85	4	1
4:C:614:PCW:H142	5:C:632:17F:H8	0.47	1.86	4	1
4:D:502:PCW:H461	4:D:508:PCW:H442	0.47	1.87	4	1
4:C:617:PCW:H382	5:C:631:17F:H41	0.47	1.85	7	4
4:A:417:PCW:H20	4:C:621:PCW:H242	0.47	1.84	6	1
4:A:403:PCW:C32	4:A:406:PCW:H351	0.47	2.39	7	1
4:A:403:PCW:H332	4:B:209:PCW:C41	0.47	2.38	8	1
4:B:208:PCW:C46	4:B:212:PCW:H212	0.47	2.38	8	1
4:C:620:PCW:C41	5:B:215:17F:H62	0.47	2.39	10	1
4:B:210:PCW:O31	4:B:210:PCW:O3	0.47	2.33	9	5
4:D:502:PCW:C40	4:D:508:PCW:H331	0.47	2.39	1	1
5:D:513:17F:C30	4:D:516:PCW:H232	0.47	2.34	1	1
4:C:614:PCW:H63	5:C:632:17F:C2	0.47	2.39	2	1
4:A:403:PCW:C5	4:B:209:PCW:H321	0.47	2.40	3	1
4:A:404:PCW:H482	4:A:407:PCW:H241	0.47	1.85	3	1
4:C:603:PCW:H73	4:D:516:PCW:P	0.47	2.49	4	1
1:A:273:ARG:HA	1:A:276:VAL:HG12	0.47	1.86	6	4
4:A:403:PCW:C26	4:B:201:PCW:H162	0.47	2.40	5	1
5:C:627:17F:H12	5:B:215:17F:C27	0.47	2.39	5	1
4:D:503:PCW:C48	4:D:515:PCW:H281	0.47	2.39	5	1
5:C:632:17F:H54	4:B:207:PCW:H181	0.47	1.84	6	1
4:B:206:PCW:C35	5:B:213:17F:H59	0.47	2.39	6	1
4:B:211:PCW:O31	4:B:211:PCW:C35	0.47	2.50	10	3
4:D:501:PCW:H171	4:D:502:PCW:C34	0.47	2.34	7	1
4:D:507:PCW:H451	5:D:513:17F:H58	0.47	1.84	7	1
4:C:609:PCW:C11	5:C:631:17F:C18	0.47	2.93	8	1
4:B:203:PCW:H211	4:B:204:PCW:H19	0.47	1.86	8	1
4:D:510:PCW:P	4:D:510:PCW:O31	0.47	2.72	9	1
4:B:202:PCW:H51	4:D:507:PCW:H62	0.47	1.87	10	1
4:B:206:PCW:O31	4:D:505:PCW:C5	0.47	2.62	10	1
1:A:224:VAL:O	1:A:228:PHE:HB2	0.47	2.09	1	1
4:C:608:PCW:H442	4:C:614:PCW:H482	0.47	1.87	1	1
4:C:625:PCW:H252	4:D:516:PCW:H471	0.47	1.85	1	1
4:B:202:PCW:H73	4:B:202:PCW:C12	0.47	2.39	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:408:PCW:H322	5:A:409:17F:H19A	0.47	1.85	2	1
5:A:409:17F:C19	4:D:504:PCW:H342	0.47	2.39	2	2
4:C:606:PCW:C15	5:C:627:17F:H8	0.47	2.39	2	1
4:C:620:PCW:H151	5:B:215:17F:C6	0.47	2.39	2	1
4:A:416:PCW:C44	4:C:616:PCW:H20	0.47	2.24	3	1
4:B:205:PCW:H162	4:B:206:PCW:C22	0.47	2.39	3	1
4:D:503:PCW:O2	4:D:507:PCW:H361	0.47	2.10	3	2
4:B:205:PCW:H61	4:B:212:PCW:O2P	0.47	2.09	4	1
4:D:505:PCW:H283	4:D:509:PCW:H481	0.47	1.86	4	1
1:A:268:GLU:OE1	1:C:506:ARG:HD3	0.47	2.09	5	1
4:A:403:PCW:C7	4:A:406:PCW:H371	0.47	2.37	5	1
5:A:410:17F:H32	4:D:502:PCW:C21	0.47	2.40	5	1
4:C:617:PCW:C41	5:C:631:17F:H45	0.47	2.25	5	1
4:B:206:PCW:H431	5:B:213:17F:H12	0.47	1.85	6	1
5:C:626:17F:H36	5:C:629:17F:C40	0.47	2.39	7	1
4:A:405:PCW:H39	5:D:512:17F:H72	0.47	1.84	8	1
4:B:204:PCW:C19	4:B:208:PCW:H371	0.47	2.39	8	1
4:B:212:PCW:C27	5:D:512:17F:H67	0.47	2.40	8	1
4:D:505:PCW:H182	4:D:509:PCW:H481	0.47	1.84	8	1
4:A:402:PCW:H52	5:D:513:17F:O5	0.47	2.08	10	1
4:D:505:PCW:H442	4:D:506:PCW:H132	0.47	1.86	10	1
4:D:505:PCW:H272	4:D:509:PCW:H471	0.47	1.86	10	1
4:A:416:PCW:O11	4:A:416:PCW:H51	0.47	2.10	1	1
4:B:205:PCW:H141	4:B:207:PCW:H331	0.47	1.85	1	1
5:A:409:17F:H64	5:D:511:17F:C21	0.47	2.37	2	1
4:A:411:PCW:C1	4:D:515:PCW:C3	0.47	2.92	2	1
4:D:501:PCW:H472	4:D:509:PCW:H251	0.47	1.86	2	2
4:A:405:PCW:H461	4:A:414:PCW:C28	0.47	2.39	3	1
4:C:605:PCW:C23	4:C:612:PCW:H382	0.47	2.40	3	1
4:C:607:PCW:H461	5:C:626:17F:C33	0.47	2.37	8	2
4:B:210:PCW:H283	4:B:211:PCW:H222	0.47	1.85	3	1
4:B:212:PCW:C8	4:B:212:PCW:O4P	0.47	2.62	3	5
2:B:165:LYS:HD3	4:B:206:PCW:O2P	0.47	2.08	4	1
4:B:210:PCW:H283	4:D:503:PCW:H181	0.47	1.86	4	1
5:D:514:17F:N1	5:D:514:17F:H4A	0.47	2.24	4	1
4:A:402:PCW:C25	4:A:413:PCW:H482	0.47	2.39	6	1
4:A:404:PCW:H371	4:A:407:PCW:H171	0.47	1.86	6	1
4:A:413:PCW:H341	4:C:611:PCW:H132	0.47	1.86	6	1
4:C:612:PCW:H20	5:D:511:17F:H44	0.47	1.86	6	1
4:C:623:PCW:H19	4:C:623:PCW:C14	0.47	2.39	7	2
4:B:202:PCW:H362	4:B:202:PCW:H131	0.47	1.87	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:A:410:17F:H75	4:D:501:PCW:C27	0.47	2.38	8	1
4:C:608:PCW:H271	5:C:626:17F:C39	0.47	2.38	8	1
4:D:505:PCW:C43	4:D:506:PCW:H141	0.47	2.39	8	1
5:A:409:17F:H35	5:D:511:17F:H5	0.47	1.86	9	1
4:A:417:PCW:H82	4:C:605:PCW:P	0.47	2.49	10	1
4:D:503:PCW:C15	4:D:507:PCW:H39	0.47	2.23	10	1
1:A:306:ARG:O	1:A:310:ARG:HG3	0.47	2.09	7	4
4:B:205:PCW:H162	4:B:207:PCW:H351	0.47	1.86	1	1
4:D:505:PCW:H20	4:D:510:PCW:H371	0.47	1.85	1	1
4:C:604:PCW:H452	4:C:606:PCW:C19	0.47	2.40	2	1
4:C:611:PCW:C23	4:C:611:PCW:H471	0.47	2.29	2	1
4:C:612:PCW:H121	4:C:618:PCW:C38	0.47	2.27	2	1
4:C:615:PCW:O3	4:C:615:PCW:C31	0.47	2.62	2	3
4:B:206:PCW:H12	5:B:213:17F:H4	0.47	1.86	2	1
4:A:407:PCW:H39	4:B:210:PCW:H271	0.47	1.86	3	1
4:B:207:PCW:O1P	4:B:209:PCW:C3	0.47	2.62	3	1
4:A:416:PCW:C12	5:C:630:17F:C9	0.47	2.90	4	1
1:C:463:TRP:CD1	5:C:629:17F:H75	0.47	2.45	4	1
4:C:611:PCW:H63	4:C:625:PCW:O11	0.47	2.09	4	1
4:C:615:PCW:H482	4:B:211:PCW:H283	0.47	1.86	4	1
4:B:202:PCW:H472	4:D:504:PCW:H281	0.47	1.87	5	2
4:B:208:PCW:H381	5:D:512:17F:H64	0.47	1.86	4	1
4:B:210:PCW:H283	4:D:503:PCW:C18	0.47	2.40	4	1
4:A:402:PCW:H241	4:A:413:PCW:C26	0.47	2.33	5	1
4:A:402:PCW:O4P	4:A:402:PCW:C8	0.47	2.63	5	1
4:C:616:PCW:O31	4:C:616:PCW:H73	0.47	2.09	5	1
4:D:503:PCW:H452	4:D:504:PCW:H152	0.47	1.87	5	1
4:A:412:PCW:H483	4:C:604:PCW:C28	0.47	2.39	6	1
4:C:604:PCW:O1P	4:C:622:PCW:C7	0.47	2.62	9	3
5:C:626:17F:H40	5:C:629:17F:C41	0.47	2.40	6	1
5:C:627:17F:P1	5:C:627:17F:O9	0.47	2.72	6	1
4:B:202:PCW:O11	4:B:202:PCW:C6	0.47	2.63	6	1
4:B:210:PCW:C47	4:D:507:PCW:H232	0.47	2.40	6	1
4:D:505:PCW:H241	4:D:510:PCW:H382	0.47	1.85	6	1
4:D:515:PCW:H472	4:D:515:PCW:C28	0.47	2.40	6	1
4:C:618:PCW:H472	5:D:511:17F:H74	0.47	1.86	7	1
4:A:404:PCW:C3	4:B:210:PCW:H152	0.47	2.39	8	1
4:C:608:PCW:O31	4:C:608:PCW:C13	0.47	2.62	8	2
4:C:622:PCW:H242	4:D:501:PCW:H431	0.47	1.86	8	1
4:C:608:PCW:H181	4:C:614:PCW:H341	0.47	1.87	9	1
4:C:610:PCW:O2P	4:C:618:PCW:C5	0.47	2.63	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:212:PCW:O2P	4:B:212:PCW:C5	0.47	2.61	9	1
4:D:505:PCW:H381	4:D:506:PCW:C14	0.47	2.40	9	1
4:D:505:PCW:C34	4:D:506:PCW:H121	0.47	2.38	9	1
4:A:413:PCW:H442	4:C:611:PCW:C24	0.47	2.19	10	1
4:B:204:PCW:H351	4:B:208:PCW:H321	0.47	1.87	10	1
4:A:416:PCW:C6	5:C:630:17F:O8	0.47	2.62	4	4
4:C:605:PCW:H412	4:C:618:PCW:H121	0.47	1.86	1	1
4:B:210:PCW:C28	4:B:211:PCW:H152	0.47	2.40	1	1
4:C:604:PCW:H2	4:C:606:PCW:C7	0.47	2.40	3	1
1:A:396:LYS:HE2	1:C:587:ALA:CA	0.47	2.40	4	1
4:A:402:PCW:H19	4:A:402:PCW:H39	0.47	1.86	4	1
4:A:403:PCW:H61	4:A:406:PCW:C37	0.47	2.32	4	2
4:C:610:PCW:H63	4:C:622:PCW:H342	0.47	1.86	4	1
4:C:610:PCW:C6	4:C:622:PCW:H342	0.47	2.40	4	1
1:A:301:LEU:HD22	1:C:473:LYS:HG2	0.47	1.85	5	1
4:D:506:PCW:H39	4:D:516:PCW:H251	0.47	1.86	5	1
4:A:413:PCW:H422	4:C:611:PCW:H211	0.47	1.84	6	1
4:C:601:PCW:H39	4:C:602:PCW:H172	0.47	1.85	10	2
4:C:606:PCW:H2	4:C:606:PCW:O11	0.47	2.10	6	1
4:C:621:PCW:H162	4:D:516:PCW:C15	0.47	2.40	7	2
5:D:513:17F:H10A	5:D:513:17F:C32	0.47	2.40	7	1
3:D:378:LEU:HD21	3:D:421:LEU:HD12	0.47	1.85	9	1
4:B:204:PCW:H471	4:D:502:PCW:H482	0.47	1.86	10	1
4:B:210:PCW:H252	4:D:503:PCW:C25	0.47	2.40	10	1
4:A:412:PCW:H11	4:C:624:PCW:H372	0.47	1.85	2	1
4:A:415:PCW:H351	4:C:616:PCW:C42	0.47	2.40	5	2
4:C:606:PCW:C15	5:C:627:17F:C8	0.47	2.93	2	1
4:B:204:PCW:H51	4:B:212:PCW:O2P	0.47	2.09	2	1
1:A:244:SER:HA	1:A:248:GLU:HG3	0.47	1.87	3	2
4:C:606:PCW:H411	5:B:215:17F:C30	0.47	2.35	3	1
4:B:212:PCW:H432	4:B:212:PCW:H211	0.47	1.86	3	1
4:D:501:PCW:H411	4:D:509:PCW:H182	0.47	1.86	3	1
4:C:615:PCW:C44	4:D:506:PCW:H472	0.47	2.40	5	1
4:B:206:PCW:C23	4:B:206:PCW:C28	0.47	2.60	5	1
4:D:503:PCW:O4P	4:D:503:PCW:H73	0.47	2.09	5	1
4:A:417:PCW:H451	4:C:622:PCW:C28	0.47	2.40	6	1
4:B:202:PCW:H362	4:B:202:PCW:O31	0.47	2.04	6	1
3:D:397:ALA:HB2	3:D:431:LEU:HD23	0.47	1.86	6	1
4:B:204:PCW:H151	4:B:208:PCW:H361	0.47	1.87	7	1
4:B:205:PCW:C19	4:B:206:PCW:H222	0.47	2.40	7	1
4:C:614:PCW:H151	4:B:207:PCW:C28	0.47	2.40	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:154:ASP:HA	2:B:157:TYR:HD2	0.47	1.69	9	1
4:A:407:PCW:H321	4:A:407:PCW:H73	0.47	1.85	10	1
1:C:426:PHE:O	1:C:430:LEU:HG	0.47	2.10	10	1
3:D:384:LYS:O	3:D:387:LYS:HG2	0.47	2.10	10	1
4:A:405:PCW:H461	4:A:414:PCW:H242	0.47	1.87	1	1
4:A:416:PCW:H141	5:C:630:17F:H11A	0.47	1.86	1	3
4:D:510:PCW:H73	4:D:510:PCW:C11	0.47	2.40	1	1
1:A:309:ALA:HA	1:A:312:HIS:HB2	0.47	1.87	6	3
4:A:408:PCW:C28	4:A:411:PCW:H461	0.47	2.40	2	1
4:A:412:PCW:C1	4:C:624:PCW:C37	0.47	2.94	3	5
1:C:514:LEU:HA	1:C:517:HIS:HB2	0.47	1.86	2	2
4:C:610:PCW:O11	4:C:618:PCW:C8	0.47	2.62	6	2
4:A:414:PCW:C6	4:C:624:PCW:C31	0.47	2.93	7	3
4:B:206:PCW:C46	4:B:206:PCW:H283	0.47	2.40	4	1
4:D:508:PCW:O11	4:D:508:PCW:C5	0.47	2.63	4	2
4:D:509:PCW:O2	4:D:509:PCW:C11	0.47	2.63	4	2
4:D:503:PCW:H451	4:D:504:PCW:H152	0.47	1.85	5	1
4:B:203:PCW:C8	4:B:204:PCW:H351	0.47	2.38	6	1
4:B:210:PCW:O2P	4:D:506:PCW:C7	0.47	2.61	6	1
4:C:618:PCW:H481	5:D:511:17F:H76	0.47	1.87	7	1
4:B:209:PCW:H11	4:B:209:PCW:O31	0.47	2.10	7	1
4:A:404:PCW:C15	4:B:210:PCW:H232	0.47	2.39	8	1
4:D:509:PCW:H262	5:D:514:17F:H47	0.47	1.85	8	1
4:A:407:PCW:H322	4:B:211:PCW:H132	0.47	1.86	10	1
4:C:605:PCW:C40	4:C:618:PCW:H121	0.47	2.40	10	1
4:C:601:PCW:O31	4:C:601:PCW:O3P	0.46	2.33	7	2
4:C:608:PCW:H452	4:B:207:PCW:C23	0.46	2.40	1	3
4:C:621:PCW:H422	4:D:506:PCW:H261	0.46	1.86	1	1
4:B:208:PCW:H32	4:B:208:PCW:O2P	0.46	2.10	2	2
4:A:408:PCW:H471	4:C:612:PCW:C23	0.46	2.41	3	1
4:B:212:PCW:H452	4:B:212:PCW:H222	0.46	1.86	3	1
4:A:401:PCW:H321	4:D:502:PCW:H172	0.46	1.87	5	1
1:C:591:TYR:HB3	5:C:630:17F:H48	0.46	1.87	7	3
4:C:601:PCW:H482	5:C:626:17F:H51	0.46	1.86	5	2
4:B:208:PCW:H141	5:B:214:17F:H8	0.46	1.87	5	1
4:D:509:PCW:H231	5:D:514:17F:H73	0.46	1.86	5	1
4:B:204:PCW:H172	4:B:204:PCW:C21	0.46	2.23	6	1
5:D:512:17F:O2	5:D:512:17F:C2	0.46	2.62	7	2
5:C:626:17F:H36	5:C:629:17F:C41	0.46	2.40	9	1
4:B:205:PCW:H332	4:B:207:PCW:H142	0.46	1.85	9	1
4:A:417:PCW:O3P	4:A:417:PCW:C31	0.46	2.62	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:204:PCW:H431	4:B:212:PCW:H252	0.46	1.86	10	1
1:A:278:PRO:O	1:A:282:GLU:HG3	0.46	2.10	1	1
4:A:411:PCW:O2P	4:A:411:PCW:H2	0.46	2.10	8	3
4:C:609:PCW:H42	5:C:631:17F:H6	0.46	1.86	1	2
4:B:211:PCW:H172	4:D:505:PCW:H471	0.46	1.87	1	1
1:A:247:LEU:O	1:A:250:VAL:HG12	0.46	2.10	5	2
4:C:622:PCW:O4P	4:C:622:PCW:C7	0.46	2.63	2	1
4:C:622:PCW:O4P	4:C:622:PCW:H73	0.46	2.09	2	1
4:C:625:PCW:H283	4:B:211:PCW:H272	0.46	1.87	2	2
4:B:204:PCW:C47	5:D:512:17F:H44	0.46	2.40	3	1
4:D:501:PCW:H252	5:D:511:17F:H68	0.46	1.88	4	1
4:C:601:PCW:C48	5:C:626:17F:H51	0.46	2.41	5	1
2:B:128:LYS:HE2	4:D:503:PCW:P	0.46	2.50	5	1
4:C:614:PCW:H12	4:C:614:PCW:O31	0.46	2.09	6	1
4:C:610:PCW:H20	4:C:610:PCW:H412	0.46	1.86	7	1
5:C:632:17F:C30	4:B:207:PCW:H181	0.46	2.40	7	1
4:D:506:PCW:C42	5:D:513:17F:H47	0.46	2.38	7	1
1:A:214:PHE:CD2	4:A:413:PCW:H282	0.46	2.44	10	1
4:B:204:PCW:C4	5:B:214:17F:O4	0.46	2.62	10	1
4:B:206:PCW:C35	4:D:505:PCW:H321	0.46	2.40	10	1
4:B:207:PCW:H251	4:B:207:PCW:C21	0.46	2.34	10	1
4:D:509:PCW:C16	5:D:514:17F:H60	0.46	2.24	10	1
4:B:201:PCW:H51	4:B:201:PCW:H332	0.46	1.86	1	1
4:A:404:PCW:C24	4:B:210:PCW:H231	0.46	2.24	2	1
4:C:617:PCW:O2	4:C:625:PCW:H121	0.46	2.10	2	1
4:D:501:PCW:C34	5:D:512:17F:H37	0.46	2.39	2	2
4:D:507:PCW:H471	5:D:513:17F:H33	0.46	1.86	2	1
4:A:401:PCW:C35	4:D:502:PCW:H19	0.46	2.41	3	1
4:B:206:PCW:H19	5:B:213:17F:C31	0.46	2.32	3	1
5:D:512:17F:H11A	5:D:514:17F:C2X	0.46	2.40	3	1
5:C:627:17F:C38	5:C:628:17F:H63	0.46	2.40	4	1
3:D:485:VAL:HG12	3:D:487:TRP:HZ3	0.46	1.69	4	1
4:C:602:PCW:H282	5:C:629:17F:C42	0.46	2.40	5	1
4:C:622:PCW:H421	4:C:623:PCW:H241	0.46	1.85	5	1
4:A:417:PCW:C20	4:C:621:PCW:H242	0.46	2.41	6	1
4:C:603:PCW:H41	4:C:603:PCW:O31	0.46	2.10	6	1
4:C:610:PCW:H283	4:C:618:PCW:H272	0.46	1.87	6	1
4:D:501:PCW:H342	5:D:512:17F:H35	0.46	1.86	6	1
4:A:403:PCW:O31	4:A:406:PCW:H351	0.46	2.10	7	1
4:C:614:PCW:H122	5:C:632:17F:C7	0.46	2.39	7	1
5:C:628:17F:O9	5:C:628:17F:O1	0.46	2.34	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:140:PRO:HB3	5:D:513:17F:N1	0.46	2.23	9	1
4:B:208:PCW:C12	5:B:214:17F:H18	0.46	2.39	9	1
4:A:404:PCW:H62	4:A:407:PCW:O11	0.46	2.09	10	1
4:B:204:PCW:H422	4:B:212:PCW:H231	0.46	1.85	10	1
4:D:502:PCW:H451	4:D:508:PCW:C28	0.46	2.39	10	1
4:D:507:PCW:H451	5:D:513:17F:C32	0.46	2.40	10	1
4:C:620:PCW:H371	5:C:631:17F:H63	0.46	1.86	9	3
5:D:513:17F:H10A	5:D:513:17F:C38	0.46	2.40	1	2
2:B:154:ASP:OD1	4:B:212:PCW:H52	0.46	2.10	3	2
4:B:202:PCW:C19	4:D:504:PCW:H142	0.46	2.41	3	2
4:B:210:PCW:O2	4:B:210:PCW:O4P	0.46	2.33	3	1
1:A:259:ASP:O	1:A:263:LYS:HB2	0.46	2.11	4	2
4:B:203:PCW:H282	4:B:208:PCW:H142	0.46	1.88	5	1
4:B:205:PCW:H431	5:B:214:17F:H66	0.46	1.86	5	1
4:B:206:PCW:O11	4:B:206:PCW:H73	0.46	2.10	6	1
4:C:615:PCW:C4	4:D:515:PCW:O11	0.46	2.64	7	1
4:B:207:PCW:H462	4:B:209:PCW:C20	0.46	2.39	7	1
3:D:400:ARG:HA	3:D:426:LEU:HG	0.46	1.88	7	1
1:C:471:ARG:HA	1:C:475:GLU:HG2	0.46	1.88	8	1
4:C:603:PCW:H451	4:D:515:PCW:H412	0.46	1.88	10	1
4:C:608:PCW:H471	4:B:205:PCW:H221	0.46	1.85	10	1
4:C:616:PCW:O31	4:C:616:PCW:C11	0.46	2.64	10	1
4:B:210:PCW:H12	4:D:506:PCW:C8	0.46	2.41	10	1
4:C:613:PCW:H442	4:C:618:PCW:C19	0.46	2.40	9	2
5:C:628:17F:H71	5:B:215:17F:H39	0.46	1.84	1	1
4:C:607:PCW:H171	5:C:629:17F:C18	0.46	2.41	2	1
4:C:606:PCW:H42	4:C:606:PCW:C2	0.46	2.38	3	1
4:C:610:PCW:O11	4:C:618:PCW:H63	0.46	2.11	4	1
4:A:401:PCW:H462	4:C:613:PCW:H222	0.46	1.87	5	1
4:B:205:PCW:C18	4:B:207:PCW:C15	0.46	2.93	5	1
4:A:416:PCW:H362	5:C:630:17F:C10	0.46	2.41	6	1
4:D:504:PCW:H51	4:D:504:PCW:C34	0.46	2.39	6	1
4:A:401:PCW:C7	4:D:508:PCW:H131	0.46	2.33	7	1
4:A:403:PCW:C14	4:B:207:PCW:H39	0.46	2.41	7	1
4:C:610:PCW:H39	4:C:622:PCW:H442	0.46	1.87	7	1
4:A:412:PCW:C27	4:B:203:PCW:H481	0.46	2.41	8	1
4:A:417:PCW:H73	4:C:622:PCW:C33	0.46	2.41	9	1
4:C:605:PCW:O2P	4:C:612:PCW:H61	0.46	2.11	9	1
4:D:506:PCW:H342	4:D:507:PCW:H39	0.46	1.87	9	1
4:B:201:PCW:H411	4:B:207:PCW:O11	0.46	2.10	10	1
4:A:404:PCW:H61	4:B:210:PCW:H331	0.46	1.88	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:406:PCW:H12	4:A:406:PCW:H41	0.46	1.87	1	2
1:C:532:ARG:O	1:C:536:LEU:HG	0.46	2.10	1	3
2:B:153:ASP:HB2	4:B:210:PCW:H63	0.46	1.87	1	1
4:B:204:PCW:C44	4:B:212:PCW:H231	0.46	2.10	1	2
4:C:610:PCW:C8	4:C:623:PCW:C14	0.46	2.94	2	1
4:A:403:PCW:H271	4:B:201:PCW:C17	0.46	2.38	3	1
4:B:206:PCW:H452	5:B:213:17F:H73	0.46	1.88	3	1
4:C:615:PCW:H40	4:C:617:PCW:H162	0.46	1.87	4	1
4:B:206:PCW:C35	4:D:505:PCW:H332	0.46	2.39	4	1
4:D:502:PCW:C40	5:D:512:17F:H9A	0.46	2.40	4	1
4:C:609:PCW:H132	4:C:609:PCW:C34	0.46	2.38	5	1
4:D:507:PCW:H351	5:D:513:17F:C9	0.46	2.24	5	1
4:D:508:PCW:O11	4:D:508:PCW:C4	0.46	2.60	5	1
4:A:404:PCW:H222	5:C:631:17F:H54	0.46	1.87	6	1
4:A:415:PCW:H31	4:C:616:PCW:C41	0.46	2.40	6	1
2:B:99:GLN:O	2:B:103:VAL:HG23	0.46	2.11	6	2
4:A:411:PCW:H61	5:C:630:17F:O4	0.46	2.10	7	1
4:C:615:PCW:C6	4:C:616:PCW:H371	0.46	2.40	8	1
5:A:409:17F:O8	4:D:504:PCW:C8	0.46	2.64	9	1
4:A:411:PCW:C15	4:C:603:PCW:H272	0.46	2.40	9	1
3:D:451:PHE:CE1	4:D:501:PCW:H63	0.46	2.46	10	1
4:C:601:PCW:H421	4:C:601:PCW:H381	0.46	1.87	1	1
4:A:401:PCW:H483	4:C:613:PCW:C48	0.46	2.41	2	1
5:A:409:17F:H50	4:D:510:PCW:C23	0.46	2.41	2	1
3:D:465:CYS:HB2	3:D:469:GLY:N	0.46	2.25	2	1
4:A:403:PCW:C2	4:B:209:PCW:H331	0.46	2.41	3	1
4:C:616:PCW:H372	4:C:616:PCW:H411	0.46	1.87	3	1
4:C:619:PCW:H472	4:B:207:PCW:H481	0.46	1.87	3	1
4:D:502:PCW:C7	4:D:502:PCW:C2	0.46	2.89	3	1
5:D:512:17F:H40	5:D:514:17F:H43	0.46	1.87	3	1
1:C:404:ASN:O	1:C:408:VAL:HG23	0.46	2.11	4	2
5:C:629:17F:H18	5:C:629:17F:H9A	0.46	1.80	4	1
5:A:410:17F:C1Y	4:D:502:PCW:H162	0.46	2.41	5	1
4:C:606:PCW:C17	4:C:606:PCW:C21	0.46	2.80	7	2
4:C:622:PCW:H232	4:D:501:PCW:H472	0.46	1.87	6	1
5:C:628:17F:O7	5:C:628:17F:C17	0.46	2.64	8	2
2:B:16:LYS:NZ	6:B:216:GNP:O3G	0.46	2.48	10	2
4:A:408:PCW:H172	5:A:409:17F:H20A	0.46	1.86	7	1
4:C:622:PCW:H242	4:D:501:PCW:H442	0.46	1.88	8	1
4:D:503:PCW:O11	4:D:506:PCW:H52	0.46	2.11	8	1
4:A:415:PCW:H422	4:C:615:PCW:H231	0.46	1.82	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:509:PCW:C24	5:D:514:17F:H43	0.46	2.31	9	1
4:A:412:PCW:C43	4:C:624:PCW:C47	0.46	2.90	10	1
5:C:632:17F:H52	4:B:207:PCW:C21	0.46	2.41	1	1
4:B:206:PCW:H42	3:D:474:GLU:OE2	0.46	2.10	1	1
1:A:341:ASN:ND2	1:C:432:LYS:HB3	0.46	2.25	5	2
4:C:606:PCW:H331	4:C:607:PCW:H61	0.46	1.87	2	2
4:B:204:PCW:C43	4:B:212:PCW:H242	0.46	2.32	2	1
4:D:503:PCW:O31	4:D:510:PCW:C8	0.46	2.64	8	2
5:B:213:17F:O10	5:B:213:17F:H4	0.46	2.11	7	2
4:D:503:PCW:C32	4:D:507:PCW:H361	0.46	2.38	3	1
4:A:411:PCW:H481	4:D:504:PCW:C18	0.46	2.35	4	1
4:C:619:PCW:C28	5:C:632:17F:H37	0.46	2.41	4	1
4:D:505:PCW:H272	4:D:510:PCW:H142	0.46	1.87	4	1
5:B:213:17F:O7	5:B:213:17F:C17	0.46	2.64	6	3
4:D:507:PCW:C35	5:D:513:17F:H9	0.46	2.23	5	1
4:A:402:PCW:H412	4:B:210:PCW:H461	0.46	1.87	6	1
4:A:411:PCW:H382	4:A:416:PCW:H39	0.46	1.86	6	1
4:C:620:PCW:H283	5:C:631:17F:H30	0.46	1.88	9	2
4:A:403:PCW:H232	4:B:205:PCW:C27	0.46	2.40	7	1
4:C:624:PCW:H222	4:C:624:PCW:H262	0.46	1.87	7	1
4:B:205:PCW:C25	4:B:207:PCW:H382	0.46	2.41	7	1
4:D:515:PCW:H332	4:D:515:PCW:C12	0.46	2.40	7	1
5:A:410:17F:H32	4:D:502:PCW:H152	0.46	1.87	8	1
4:C:607:PCW:H261	5:C:629:17F:H63	0.46	1.82	8	1
4:C:620:PCW:O31	4:C:620:PCW:C1	0.46	2.62	8	1
4:C:607:PCW:H272	5:C:629:17F:H69	0.46	1.88	9	1
2:B:142:ILE:HD12	4:B:210:PCW:C6	0.46	2.41	9	1
4:D:504:PCW:O2P	4:D:507:PCW:C4	0.46	2.64	9	1
4:D:501:PCW:C7	5:D:514:17F:O5	0.46	2.63	10	1
4:A:408:PCW:H341	5:A:409:17F:C1Y	0.46	2.40	1	1
4:A:417:PCW:C18	4:C:603:PCW:C14	0.46	2.94	1	1
1:C:492:LEU:O	1:C:496:LEU:HG	0.46	2.10	1	1
4:A:401:PCW:C48	4:C:613:PCW:C47	0.46	2.89	2	1
4:C:621:PCW:H181	5:C:628:17F:H37	0.46	1.87	2	1
4:D:503:PCW:C31	4:D:510:PCW:H82	0.46	2.41	2	2
5:A:409:17F:O6	5:A:409:17F:C17	0.46	2.63	7	2
4:B:205:PCW:H82	5:B:214:17F:C10	0.46	2.35	3	1
4:B:206:PCW:H422	5:B:213:17F:H34	0.46	1.88	3	1
4:D:506:PCW:H211	4:D:516:PCW:H281	0.46	1.88	3	1
4:C:601:PCW:P	4:C:601:PCW:C31	0.46	3.04	4	1
4:D:507:PCW:H483	4:D:507:PCW:C26	0.46	2.40	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:559:SER:HA	1:C:562:ALA:HB3	0.46	1.87	5	1
4:D:501:PCW:H482	5:D:514:17F:H51	0.46	1.88	5	1
4:D:510:PCW:C21	4:D:515:PCW:H483	0.46	2.32	5	1
5:A:410:17F:H57	4:D:502:PCW:H212	0.46	1.87	6	1
4:A:417:PCW:H451	4:C:622:PCW:H283	0.46	1.86	6	1
4:B:206:PCW:C12	5:B:213:17F:C17	0.46	2.94	6	1
4:B:206:PCW:H421	5:B:213:17F:H32	0.46	1.87	6	2
4:B:204:PCW:H162	4:B:208:PCW:H181	0.46	1.87	7	2
1:A:308:ARG:HG3	1:C:469:LEU:HD21	0.46	1.88	8	1
4:A:413:PCW:C41	4:C:611:PCW:H231	0.46	2.41	8	1
4:A:408:PCW:H252	5:A:409:17F:H59	0.46	1.88	9	1
4:C:615:PCW:C46	4:C:625:PCW:H251	0.46	2.40	9	1
4:A:403:PCW:O31	4:B:209:PCW:C32	0.46	2.64	10	1
4:A:417:PCW:H141	4:C:603:PCW:C38	0.46	2.25	10	1
4:A:417:PCW:O31	4:A:417:PCW:O3P	0.46	2.34	10	1
4:C:614:PCW:H221	4:B:207:PCW:C26	0.46	2.41	10	1
4:C:621:PCW:H352	4:C:625:PCW:C22	0.46	2.33	1	3
4:B:205:PCW:H171	4:B:207:PCW:H362	0.46	1.88	8	2
4:B:206:PCW:H42	3:D:474:GLU:OE1	0.46	2.10	1	1
4:A:417:PCW:C43	4:C:622:PCW:H281	0.46	2.39	2	1
4:C:603:PCW:P	5:C:628:17F:O1	0.46	2.74	2	1
4:A:402:PCW:H361	4:B:210:PCW:H441	0.46	1.86	3	1
4:A:411:PCW:H282	4:A:415:PCW:C25	0.46	2.41	3	1
1:C:559:SER:HB3	1:C:563:LYS:HE3	0.46	1.88	3	1
4:C:623:PCW:C37	4:C:624:PCW:H121	0.46	2.40	8	2
4:B:203:PCW:C28	4:B:208:PCW:H172	0.46	2.41	3	1
5:B:213:17F:C24	4:D:509:PCW:H172	0.46	2.41	3	1
4:A:414:PCW:C31	4:C:623:PCW:H342	0.46	2.41	4	1
4:C:615:PCW:O4P	4:C:615:PCW:C3	0.46	2.63	4	3
4:A:403:PCW:H262	4:B:201:PCW:H162	0.46	1.87	5	1
4:C:611:PCW:O2	4:C:611:PCW:C34	0.46	2.59	5	1
4:C:608:PCW:C46	4:B:207:PCW:H472	0.46	2.40	6	1
3:D:463:PHE:CE2	3:D:474:GLU:HG2	0.46	2.46	6	1
4:B:203:PCW:C23	4:B:208:PCW:H342	0.46	2.34	7	1
4:A:414:PCW:C48	4:B:212:PCW:H472	0.46	2.36	9	1
5:C:627:17F:H54	4:D:510:PCW:C46	0.46	2.41	9	1
2:B:46:ILE:HG21	2:B:160:VAL:HG21	0.46	1.87	9	1
4:C:605:PCW:H82	5:C:630:17F:O4	0.46	2.10	10	1
4:B:210:PCW:H281	4:B:211:PCW:H152	0.45	1.88	1	1
1:A:217:LEU:O	1:A:221:LEU:HG	0.45	2.11	4	3
4:D:501:PCW:H472	4:D:509:PCW:C25	0.45	2.41	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:203:PCW:H11	4:B:203:PCW:O31	0.45	2.10	3	2
4:B:205:PCW:H182	4:B:207:PCW:H152	0.45	1.87	3	1
4:D:505:PCW:C19	4:D:510:PCW:H322	0.45	2.40	7	2
4:C:615:PCW:C48	4:D:503:PCW:C22	0.45	2.94	4	1
4:B:210:PCW:H12	4:D:506:PCW:H51	0.45	1.88	4	1
4:D:507:PCW:C13	5:D:513:17F:H75	0.45	2.39	5	1
1:A:335:LEU:O	1:A:339:LYS:HB2	0.45	2.11	6	1
5:C:632:17F:H49	4:B:207:PCW:H211	0.45	1.87	6	1
4:C:609:PCW:H121	5:C:631:17F:H18	0.45	1.87	7	1
4:A:411:PCW:C41	4:A:411:PCW:C37	0.45	2.88	8	1
4:A:404:PCW:O1P	4:A:404:PCW:C5	0.45	2.63	9	1
4:C:620:PCW:H371	5:C:631:17F:C35	0.45	2.41	9	1
5:A:410:17F:H4	5:A:410:17F:H1A	0.45	1.88	10	1
4:B:208:PCW:C42	5:D:512:17F:H68	0.45	2.41	10	1
4:B:204:PCW:H351	5:D:512:17F:O1	0.45	2.11	1	1
4:B:206:PCW:H381	5:B:213:17F:C8	0.45	2.41	1	1
5:B:213:17F:O8	4:D:505:PCW:H73	0.45	2.11	1	1
4:A:408:PCW:H162	5:A:409:17F:H62	0.45	1.87	2	1
4:A:413:PCW:O3P	4:A:413:PCW:C31	0.45	2.63	10	3
4:C:605:PCW:H461	4:C:618:PCW:H471	0.45	1.87	2	1
4:C:606:PCW:H161	5:C:627:17F:H10	0.45	1.88	2	1
2:B:22:GLN:O	2:B:26:ASN:HA	0.45	2.12	8	3
4:B:203:PCW:C24	4:B:208:PCW:O11	0.45	2.59	2	1
3:D:473:HIS:HB2	3:D:476:CYS:SG	0.45	2.51	2	2
4:D:506:PCW:C42	5:D:513:17F:H48	0.45	2.40	3	1
4:A:417:PCW:C7	4:A:417:PCW:O31	0.45	2.64	10	2
4:B:205:PCW:H142	4:B:206:PCW:H20	0.45	1.88	4	1
4:C:601:PCW:C40	5:C:626:17F:H52	0.45	2.42	5	1
4:B:205:PCW:H62	5:B:213:17F:P1	0.45	2.51	5	1
4:A:402:PCW:C11	4:A:402:PCW:O31	0.45	2.64	6	1
3:D:386:LEU:HD21	3:D:393:PRO:HD3	0.45	1.88	6	1
1:A:361:SER:HB3	1:A:365:LYS:HE3	0.45	1.87	8	1
5:A:409:17F:H39	5:D:511:17F:H31	0.45	1.86	8	1
5:C:626:17F:C23	5:C:629:17F:H75	0.45	2.41	8	1
4:B:212:PCW:H52	5:B:213:17F:H2	0.45	1.88	8	1
4:D:503:PCW:H41	4:D:506:PCW:C7	0.45	2.41	9	1
4:A:405:PCW:O4P	4:A:405:PCW:C8	0.45	2.65	2	6
4:A:406:PCW:H461	4:C:621:PCW:H472	0.45	1.87	2	1
4:C:620:PCW:C15	5:B:215:17F:C6	0.45	2.89	2	1
3:D:465:CYS:HB2	3:D:470:TYR:H	0.45	1.69	2	1
4:A:401:PCW:C18	4:A:401:PCW:C22	0.45	2.85	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:411:PCW:O11	4:A:411:PCW:C2	0.45	2.60	9	2
4:C:608:PCW:C6	4:C:619:PCW:O11	0.45	2.64	3	1
4:D:507:PCW:H483	4:D:507:PCW:C27	0.45	2.29	3	1
4:A:401:PCW:H73	4:D:508:PCW:C31	0.45	2.42	4	1
4:B:212:PCW:H222	4:B:212:PCW:C43	0.45	2.41	4	1
4:A:407:PCW:C8	4:B:211:PCW:H372	0.45	2.41	5	1
4:D:505:PCW:C2	4:D:505:PCW:O11	0.45	2.59	5	1
4:D:505:PCW:H19	4:D:510:PCW:H342	0.45	1.88	5	1
4:C:603:PCW:C17	4:C:603:PCW:C21	0.45	2.94	6	1
5:C:632:17F:H52	4:B:205:PCW:H231	0.45	1.88	6	1
2:B:165:LYS:HB3	4:B:209:PCW:C6	0.45	2.36	6	1
2:B:165:LYS:NZ	5:B:213:17F:O4	0.45	2.50	6	1
4:B:206:PCW:O11	4:B:206:PCW:N	0.45	2.50	6	1
4:B:207:PCW:H421	4:B:209:PCW:H251	0.45	1.88	6	1
4:C:605:PCW:H482	5:D:511:17F:H70	0.45	1.87	7	1
4:C:612:PCW:H20	5:D:511:17F:C27	0.45	2.41	7	1
5:C:627:17F:HN1	5:C:627:17F:C17	0.45	2.23	7	1
4:A:401:PCW:H322	4:D:508:PCW:H362	0.45	1.86	8	1
4:B:212:PCW:H52	5:B:213:17F:O5	0.45	2.11	8	1
4:C:620:PCW:H381	5:C:632:17F:H76	0.45	1.89	9	1
4:C:612:PCW:H251	5:D:511:17F:C26	0.45	2.41	1	1
4:C:613:PCW:O11	4:C:613:PCW:O2	0.45	2.34	9	2
1:A:255:GLN:HB2	1:A:256:PRO:CD	0.45	2.42	4	6
4:C:604:PCW:C38	5:C:627:17F:H41	0.45	2.41	2	1
4:C:617:PCW:C38	4:C:625:PCW:H181	0.45	2.39	3	1
4:A:401:PCW:H282	4:C:613:PCW:H283	0.45	1.88	4	1
4:C:602:PCW:C32	5:B:214:17F:H61	0.45	2.42	5	1
3:D:468:CYS:CB	3:D:484:CYS:HB3	0.45	2.42	6	1
4:D:504:PCW:C35	4:D:504:PCW:H52	0.45	2.41	6	1
4:A:402:PCW:C6	5:D:513:17F:H1	0.45	2.36	7	1
4:C:603:PCW:C8	4:C:603:PCW:H131	0.45	2.41	7	1
4:C:617:PCW:C35	4:C:625:PCW:C34	0.45	2.94	7	1
1:A:388:SER:HB2	1:C:594:LYS:HE3	0.45	1.88	8	1
4:A:404:PCW:H372	4:A:407:PCW:H162	0.45	1.88	9	1
4:A:416:PCW:H342	4:C:616:PCW:H132	0.45	1.88	9	1
4:C:610:PCW:H351	4:C:610:PCW:C17	0.45	2.14	9	1
4:B:204:PCW:H481	5:D:512:17F:H52	0.45	1.87	9	1
4:B:207:PCW:H42	4:B:209:PCW:O1P	0.45	2.11	9	1
4:C:625:PCW:H281	5:C:631:17F:H46	0.45	1.87	10	1
4:D:508:PCW:C1	4:D:508:PCW:O31	0.45	2.55	10	1
5:D:514:17F:H44	5:D:514:17F:H73	0.45	1.85	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:413:PCW:H431	4:C:611:PCW:H212	0.45	1.89	10	2
2:B:6:LEU:HD22	2:B:159:LEU:HD23	0.45	1.89	2	2
4:B:206:PCW:H151	5:B:213:17F:H56	0.45	1.87	1	2
4:D:503:PCW:H262	4:D:507:PCW:C45	0.45	2.42	1	1
4:A:406:PCW:C41	4:B:211:PCW:H171	0.45	2.41	2	1
4:A:406:PCW:H422	4:D:505:PCW:C47	0.45	2.41	2	1
4:C:608:PCW:C11	4:C:614:PCW:C7	0.45	2.94	2	1
4:C:612:PCW:H241	5:D:511:17F:H69	0.45	1.88	2	1
2:B:83:ALA:HB1	2:B:85:ASN:OD1	0.45	2.11	2	4
4:D:501:PCW:H42	4:D:509:PCW:O31	0.45	2.12	2	1
4:D:502:PCW:H211	4:D:502:PCW:H171	0.45	1.88	2	1
4:D:506:PCW:C3	4:D:506:PCW:P	0.45	3.04	2	1
2:B:144:THR:HB	2:B:152:VAL:HG22	0.45	1.88	3	1
1:A:255:GLN:HB2	1:A:256:PRO:HD3	0.45	1.89	4	4
4:B:205:PCW:C14	4:B:206:PCW:H20	0.45	2.40	4	1
4:B:206:PCW:H283	4:B:206:PCW:H471	0.45	1.89	4	1
4:D:501:PCW:O31	4:D:501:PCW:C11	0.45	2.65	4	1
4:B:207:PCW:C44	4:B:209:PCW:H251	0.45	2.37	6	1
5:A:409:17F:H45	4:D:510:PCW:H19	0.45	1.88	7	1
4:A:415:PCW:C37	4:C:616:PCW:C41	0.45	2.92	7	1
4:A:417:PCW:H332	4:C:622:PCW:C12	0.45	2.29	7	1
4:C:602:PCW:H82	2:B:127:THR:HB	0.45	1.87	7	1
4:D:515:PCW:C11	4:D:515:PCW:C31	0.45	2.94	7	1
4:C:608:PCW:H131	4:C:608:PCW:O31	0.45	2.12	8	1
4:C:624:PCW:O3	4:C:624:PCW:C31	0.45	2.64	8	2
4:B:211:PCW:C24	4:D:503:PCW:H231	0.45	2.41	8	1
5:D:514:17F:C38	5:D:514:17F:H35	0.45	2.41	8	1
4:B:202:PCW:H332	4:D:507:PCW:C3	0.45	2.41	9	1
4:D:504:PCW:H121	4:D:504:PCW:H39	0.45	1.87	9	1
1:C:445:LEU:O	1:C:448:VAL:HG12	0.45	2.12	1	1
4:C:603:PCW:O4P	4:C:603:PCW:O2	0.45	2.34	1	1
1:C:496:LEU:O	1:C:500:GLY:HA3	0.45	2.11	2	5
4:C:620:PCW:H282	5:C:631:17F:H10	0.45	1.89	2	1
4:C:624:PCW:O2	4:C:624:PCW:C11	0.45	2.64	2	1
5:A:410:17F:H77	4:D:501:PCW:H272	0.45	1.87	3	1
4:A:411:PCW:H271	4:B:202:PCW:C48	0.45	2.40	3	1
4:D:503:PCW:H262	4:D:507:PCW:C46	0.45	2.42	3	1
4:D:504:PCW:O3	4:D:504:PCW:C31	0.45	2.65	4	3
4:A:406:PCW:H372	4:B:211:PCW:H361	0.45	1.86	6	1
2:B:13:GLY:N	6:B:216:GNP:O2B	0.45	2.50	6	1
4:B:201:PCW:C38	4:B:207:PCW:H381	0.45	2.39	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:202:PCW:H381	4:B:202:PCW:C14	0.45	2.41	6	1
4:B:206:PCW:C28	4:B:206:PCW:H483	0.45	2.41	6	1
4:B:210:PCW:H161	4:D:503:PCW:C28	0.45	2.41	6	1
4:A:414:PCW:H482	4:C:604:PCW:H272	0.45	1.87	8	1
4:B:212:PCW:H422	5:D:514:17F:H11A	0.45	1.88	8	1
4:D:508:PCW:H361	4:D:508:PCW:C23	0.45	2.41	8	1
4:D:510:PCW:C42	4:D:516:PCW:H262	0.45	2.40	8	1
4:D:508:PCW:O11	4:D:508:PCW:H41	0.45	2.12	9	1
4:B:203:PCW:H412	4:B:208:PCW:H372	0.45	1.87	10	1
4:D:516:PCW:C11	4:D:516:PCW:O2	0.45	2.65	10	1
4:C:617:PCW:C13	4:C:625:PCW:H132	0.45	2.41	1	1
4:D:503:PCW:H451	4:D:504:PCW:H132	0.45	1.88	1	1
5:A:409:17F:C36	5:D:511:17F:H37	0.45	2.38	2	1
4:A:401:PCW:O3	4:D:508:PCW:H231	0.45	2.11	4	1
4:B:204:PCW:H132	4:B:208:PCW:C13	0.45	2.28	4	1
4:C:610:PCW:H461	4:C:610:PCW:H242	0.45	1.87	7	2
4:C:614:PCW:C16	5:C:632:17F:H11A	0.45	2.42	5	1
4:C:616:PCW:H2	4:C:616:PCW:C5	0.45	2.39	5	1
4:C:606:PCW:H63	4:C:606:PCW:C11	0.45	2.42	6	1
4:B:203:PCW:H231	4:B:204:PCW:H141	0.45	1.89	6	1
4:A:401:PCW:H342	4:D:508:PCW:H39	0.45	1.88	7	1
2:B:161:ARG:NH1	4:B:212:PCW:H51	0.45	2.26	7	1
4:B:201:PCW:H331	4:B:209:PCW:O3P	0.45	2.11	7	1
4:D:501:PCW:H61	5:D:514:17F:H31	0.45	1.88	8	1
4:D:510:PCW:H421	4:D:516:PCW:C27	0.45	2.42	8	1
4:A:404:PCW:C6	4:A:404:PCW:O2	0.45	2.63	10	1
5:C:627:17F:C1X	5:C:628:17F:H8	0.45	2.33	1	1
4:B:206:PCW:H162	5:B:213:17F:C33	0.45	2.41	1	1
4:D:501:PCW:H2	4:D:509:PCW:H372	0.45	1.87	1	1
4:D:503:PCW:H151	4:D:506:PCW:C32	0.45	2.40	8	2
4:D:516:PCW:O2	4:D:516:PCW:C11	0.45	2.64	4	6
1:A:236:THR:O	1:A:240:ARG:HG3	0.45	2.11	2	1
4:A:411:PCW:O11	4:C:616:PCW:H341	0.45	2.12	8	2
4:C:615:PCW:C48	4:D:503:PCW:C20	0.45	2.95	2	1
4:D:507:PCW:H20	5:D:513:17F:C19	0.45	2.36	2	1
4:A:407:PCW:H452	5:C:631:17F:H53	0.45	1.88	3	1
4:C:622:PCW:O2	4:C:623:PCW:C16	0.45	2.65	3	1
4:C:605:PCW:H472	4:C:618:PCW:H421	0.45	1.87	4	1
4:B:212:PCW:H411	4:B:212:PCW:C18	0.45	2.40	5	1
4:C:605:PCW:C47	4:C:618:PCW:H441	0.45	2.42	6	1
3:D:444:LYS:HG3	3:D:445:THR:N	0.45	2.26	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:401:PCW:H322	4:D:508:PCW:H39	0.45	1.89	7	1
4:C:612:PCW:H142	4:C:618:PCW:C39	0.45	2.42	7	1
4:B:211:PCW:C19	4:D:505:PCW:H421	0.45	2.42	8	1
1:C:573:LEU:O	1:C:577:LEU:HG	0.45	2.11	9	1
4:D:504:PCW:H171	4:D:504:PCW:H221	0.45	1.87	9	1
4:C:610:PCW:C24	4:C:618:PCW:H483	0.45	2.42	10	1
4:A:403:PCW:H122	4:B:209:PCW:H331	0.45	1.89	1	1
4:B:204:PCW:C47	5:D:512:17F:C27	0.45	2.95	1	1
4:A:407:PCW:H82	4:B:211:PCW:C3	0.45	2.42	2	1
4:B:203:PCW:H52	4:B:204:PCW:C36	0.45	2.41	2	1
4:B:211:PCW:C16	4:B:211:PCW:H441	0.45	2.42	5	2
4:B:204:PCW:H452	5:D:514:17F:H38	0.45	1.88	3	1
4:C:614:PCW:C27	5:C:632:17F:H45	0.45	2.42	4	1
4:C:615:PCW:H431	4:D:506:PCW:C47	0.45	2.42	4	1
4:C:621:PCW:H482	4:D:506:PCW:H181	0.45	1.87	4	1
4:B:210:PCW:H283	4:D:503:PCW:C21	0.45	2.32	4	1
4:C:611:PCW:H63	4:C:617:PCW:H31	0.45	1.87	6	1
4:B:203:PCW:C24	4:B:204:PCW:H132	0.45	2.41	6	1
4:B:205:PCW:C8	4:B:205:PCW:O4P	0.45	2.65	8	3
5:A:410:17F:H66	4:D:502:PCW:C28	0.45	2.42	7	1
4:B:212:PCW:C39	5:D:514:17F:H63	0.45	2.42	7	1
4:D:501:PCW:H362	5:D:512:17F:H37	0.45	1.87	7	1
4:C:601:PCW:C39	4:C:602:PCW:H171	0.45	2.36	8	1
4:A:408:PCW:C11	4:A:408:PCW:C37	0.45	2.94	9	1
4:B:210:PCW:C48	4:D:507:PCW:H242	0.45	2.42	9	1
4:A:411:PCW:H371	4:A:411:PCW:H411	0.45	1.89	10	1
4:B:204:PCW:H351	4:B:208:PCW:C32	0.45	2.42	10	1
5:B:213:17F:C35	4:D:505:PCW:H371	0.45	2.39	10	1
1:C:502:GLU:O	1:C:506:ARG:HG3	0.45	2.12	5	7
4:A:405:PCW:H412	4:A:414:PCW:H282	0.45	1.89	8	2
4:A:407:PCW:H181	4:A:407:PCW:H222	0.45	1.89	10	2
4:C:603:PCW:H172	4:C:603:PCW:C21	0.45	2.40	3	3
4:B:204:PCW:H182	4:B:208:PCW:H211	0.45	1.88	2	1
4:A:416:PCW:C6	5:C:630:17F:C4	0.45	2.92	3	1
4:C:604:PCW:C47	4:C:624:PCW:H282	0.45	2.42	3	2
4:C:612:PCW:C13	4:C:618:PCW:H382	0.45	2.39	3	1
4:C:621:PCW:H481	4:D:505:PCW:H441	0.45	1.87	4	1
4:B:204:PCW:H221	4:B:208:PCW:C24	0.45	2.32	4	1
4:A:408:PCW:H351	4:A:408:PCW:C3	0.45	2.42	5	1
2:B:32:TYR:CD1	6:B:216:GNP:H5'1	0.45	2.45	5	1
4:A:413:PCW:O4P	4:A:413:PCW:C8	0.45	2.65	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:605:PCW:H282	4:C:612:PCW:H432	0.45	1.88	6	1
4:C:601:PCW:H483	4:C:601:PCW:H151	0.45	1.87	7	1
4:C:611:PCW:C33	4:C:617:PCW:H152	0.45	2.42	7	1
5:C:627:17F:H42	5:C:628:17F:C40	0.45	2.41	7	1
4:B:206:PCW:C7	4:B:209:PCW:H63	0.45	2.41	7	1
4:A:405:PCW:H152	5:D:512:17F:C32	0.45	2.40	8	1
4:C:603:PCW:H442	4:D:515:PCW:C37	0.45	2.36	8	1
5:D:514:17F:H35	5:D:514:17F:C37	0.45	2.42	8	1
4:A:406:PCW:H362	4:B:209:PCW:H40	0.45	1.89	9	1
4:A:402:PCW:C36	4:B:210:PCW:H422	0.45	2.42	10	1
2:B:168:GLU:OE1	4:D:504:PCW:H61	0.44	2.13	1	1
4:D:502:PCW:H122	4:D:508:PCW:H39	0.44	1.88	9	2
4:D:510:PCW:C40	4:D:516:PCW:H283	0.44	2.42	2	1
4:A:405:PCW:C47	4:A:414:PCW:H272	0.44	2.41	3	1
4:A:407:PCW:H431	4:B:211:PCW:C21	0.44	2.42	3	1
5:D:512:17F:C12	5:D:514:17F:H39	0.44	2.38	3	1
4:C:605:PCW:H182	4:C:612:PCW:C36	0.44	2.41	4	1
4:C:622:PCW:H381	4:C:623:PCW:C17	0.44	2.43	4	1
5:C:632:17F:H65	4:B:207:PCW:H482	0.44	1.87	4	1
4:A:404:PCW:O1P	4:A:407:PCW:C11	0.44	2.65	5	1
4:C:605:PCW:H232	4:C:612:PCW:H172	0.44	1.88	5	1
4:C:616:PCW:O31	4:C:616:PCW:C6	0.44	2.64	5	1
4:C:620:PCW:C14	4:C:620:PCW:C18	0.44	2.91	5	2
4:B:212:PCW:C34	5:B:213:17F:O8	0.44	2.65	5	1
4:D:504:PCW:H442	4:D:504:PCW:H172	0.44	1.88	5	1
4:D:516:PCW:H142	4:D:516:PCW:C37	0.44	2.39	5	1
1:A:316:LEU:O	1:A:320:LEU:HG	0.44	2.11	7	1
5:A:409:17F:H45	4:D:510:PCW:C19	0.44	2.42	7	1
4:A:411:PCW:C7	5:C:630:17F:O4	0.44	2.65	7	1
4:A:413:PCW:H331	4:C:611:PCW:H132	0.44	1.88	7	1
5:B:213:17F:H55	5:D:514:17F:H71	0.44	1.89	7	1
4:C:610:PCW:H283	4:C:618:PCW:C25	0.44	2.24	8	1
4:D:503:PCW:O31	4:D:510:PCW:C6	0.44	2.65	8	1
4:A:403:PCW:H42	4:A:406:PCW:H11	0.44	1.89	9	1
4:A:405:PCW:C33	4:B:203:PCW:H362	0.44	2.41	10	1
4:A:405:PCW:H483	4:A:414:PCW:H221	0.44	1.89	10	1
4:B:204:PCW:H162	4:B:208:PCW:H151	0.44	1.89	10	1
5:A:409:17F:H1A	2:B:169:LYS:HD3	0.44	1.87	1	1
4:B:206:PCW:C41	4:B:206:PCW:H372	0.44	2.42	1	1
4:A:411:PCW:H31	4:D:515:PCW:O3	0.44	2.11	2	2
4:C:615:PCW:H231	4:C:616:PCW:H461	0.44	1.88	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:210:PCW:O3	4:B:210:PCW:O31	0.44	2.36	3	3
4:A:411:PCW:H61	5:C:630:17F:O5	0.44	2.11	5	1
4:C:614:PCW:H451	5:B:214:17F:H55	0.44	1.89	5	1
4:B:201:PCW:H452	4:B:205:PCW:C28	0.44	2.42	5	1
1:C:488:LYS:O	1:C:492:LEU:HG	0.44	2.12	6	1
4:A:416:PCW:O11	4:A:416:PCW:C6	0.44	2.60	7	1
5:C:632:17F:H74	5:B:215:17F:C33	0.44	2.42	7	1
4:D:505:PCW:H372	4:D:506:PCW:H142	0.44	1.88	8	1
4:A:405:PCW:C32	4:B:203:PCW:C34	0.44	2.95	9	1
4:B:204:PCW:H39	5:D:512:17F:O8	0.44	2.12	9	1
4:B:206:PCW:H162	5:B:213:17F:H57	0.44	1.87	9	1
4:A:411:PCW:C6	5:C:630:17F:H2	0.44	2.40	10	1
4:C:605:PCW:H462	5:D:511:17F:H55	0.44	1.88	10	1
1:A:301:LEU:HB3	1:C:473:LYS:HE3	0.44	1.90	8	2
4:D:503:PCW:H482	4:D:510:PCW:H171	0.44	1.88	2	1
4:D:507:PCW:H442	5:D:513:17F:H30	0.44	1.88	2	1
1:A:264:LYS:HE3	1:C:509:ALA:HB1	0.44	1.89	3	1
4:B:203:PCW:C25	4:B:208:PCW:H122	0.44	2.36	3	1
5:B:213:17F:C37	4:D:505:PCW:H39	0.44	2.42	3	1
5:D:512:17F:C1X	5:D:514:17F:H35	0.44	2.34	3	1
1:C:592:THR:O	1:C:596:ASN:HB2	0.44	2.11	4	1
4:C:615:PCW:C34	4:D:516:PCW:C34	0.44	2.89	4	1
4:A:407:PCW:H52	4:A:407:PCW:O2	0.44	2.13	5	1
4:A:405:PCW:H412	4:A:414:PCW:H251	0.44	1.88	6	1
1:C:412:PHE:O	1:C:416:ARG:HG3	0.44	2.12	6	1
4:B:206:PCW:C4	4:B:209:PCW:C8	0.44	2.95	6	1
1:C:591:TYR:CB	5:C:630:17F:H48	0.44	2.42	7	1
4:B:207:PCW:C46	4:B:209:PCW:H20	0.44	2.42	7	1
5:D:512:17F:C23	5:D:512:17F:C12	0.44	2.95	7	1
4:B:208:PCW:C45	4:B:212:PCW:H212	0.44	2.42	8	1
4:C:614:PCW:H212	5:C:632:17F:C22	0.44	2.42	9	1
4:A:402:PCW:H322	4:D:507:PCW:C18	0.44	2.40	10	1
4:A:403:PCW:H331	4:B:209:PCW:H331	0.44	1.87	10	1
5:C:628:17F:H53	5:B:213:17F:H72	0.44	1.89	10	1
5:D:513:17F:H11	5:D:513:17F:C37	0.44	2.42	10	1
4:A:406:PCW:H371	4:B:209:PCW:H431	0.44	1.89	1	1
4:D:505:PCW:C37	4:D:506:PCW:H162	0.44	2.42	1	1
4:A:401:PCW:H472	4:C:610:PCW:C25	0.44	2.37	2	1
4:B:203:PCW:C23	4:B:208:PCW:H2	0.44	2.39	2	1
5:B:213:17F:H2	5:B:213:17F:O2	0.44	2.12	2	1
1:A:279:LEU:HD11	1:C:499:LEU:HD11	0.44	1.89	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:401:PCW:H221	4:A:401:PCW:H182	0.44	1.89	3	1
4:A:411:PCW:O31	4:A:411:PCW:O4P	0.44	2.35	3	1
2:B:47:ASP:HA	3:D:448:LYS:CD	0.44	2.42	3	1
4:D:507:PCW:O11	4:D:507:PCW:C2	0.44	2.62	3	1
4:C:611:PCW:H321	4:C:617:PCW:C12	0.44	2.42	4	1
4:C:612:PCW:H471	4:C:618:PCW:H411	0.44	1.88	4	1
4:C:608:PCW:H462	4:B:207:PCW:H482	0.44	1.88	5	1
4:B:208:PCW:O31	4:B:208:PCW:C1	0.44	2.57	6	2
4:D:501:PCW:O2P	5:D:514:17F:H19A	0.44	2.13	5	1
1:A:310:ARG:O	1:A:314:ASP:HB2	0.44	2.13	6	1
4:A:415:PCW:C3	4:C:616:PCW:C42	0.44	2.96	6	1
4:A:403:PCW:H322	4:A:406:PCW:C35	0.44	2.41	7	1
4:D:503:PCW:O4P	4:D:503:PCW:H62	0.44	2.12	7	1
4:A:407:PCW:H451	4:B:211:PCW:C23	0.44	2.40	8	1
4:D:509:PCW:H261	5:D:514:17F:H73	0.44	1.85	9	1
4:C:606:PCW:H261	5:C:628:17F:H78	0.44	1.89	10	1
4:B:204:PCW:H342	4:B:208:PCW:O2	0.44	2.13	10	1
4:A:403:PCW:O11	4:B:201:PCW:C12	0.44	2.60	1	1
4:A:417:PCW:H161	4:C:603:PCW:H121	0.44	1.90	1	1
4:C:611:PCW:C32	4:C:617:PCW:C13	0.44	2.96	1	1
4:C:621:PCW:C42	4:D:516:PCW:H483	0.44	2.42	1	1
1:A:338:LEU:O	1:A:342:GLY:HA3	0.44	2.12	3	3
4:A:402:PCW:O11	4:A:402:PCW:C2	0.44	2.64	2	4
4:B:204:PCW:H462	4:D:502:PCW:H441	0.44	1.89	2	1
4:B:205:PCW:H172	4:B:207:PCW:H131	0.44	1.88	2	1
1:A:308:ARG:HG3	1:C:469:LEU:HD11	0.44	1.89	3	1
4:B:206:PCW:C18	4:B:207:PCW:H331	0.44	2.42	3	1
4:D:510:PCW:O2P	4:D:510:PCW:C3	0.44	2.66	4	1
4:A:408:PCW:H252	5:A:409:17F:H67	0.44	1.90	5	1
4:B:208:PCW:H431	4:B:212:PCW:C26	0.44	2.42	5	1
4:D:503:PCW:H61	4:D:506:PCW:P	0.44	2.52	5	1
4:A:404:PCW:C37	4:A:407:PCW:H171	0.44	2.42	6	1
4:A:405:PCW:C27	4:A:414:PCW:C27	0.44	2.95	6	1
5:C:627:17F:O9	5:C:627:17F:O3	0.44	2.35	6	1
2:B:172:LYS:HB3	4:B:201:PCW:H73	0.44	1.90	7	1
4:D:506:PCW:C46	5:D:513:17F:H50	0.44	2.33	7	1
5:C:628:17F:H20	5:C:628:17F:H11	0.44	1.90	8	1
4:B:203:PCW:C21	4:B:204:PCW:H19	0.44	2.43	8	1
4:B:205:PCW:H242	4:B:207:PCW:C41	0.44	2.42	8	1
4:D:505:PCW:C37	4:D:506:PCW:H142	0.44	2.43	8	1
4:C:617:PCW:O2P	4:C:625:PCW:H52	0.44	2.13	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:201:PCW:C48	4:B:205:PCW:H39	0.44	2.30	9	1
4:B:206:PCW:H483	4:B:206:PCW:C28	0.44	2.43	9	1
4:B:208:PCW:H212	4:B:212:PCW:H172	0.44	1.89	9	1
4:B:212:PCW:H222	5:D:514:17F:C10	0.44	2.42	10	1
3:D:450:ALA:HB1	3:D:471:LYS:HE2	0.44	1.90	10	1
4:A:408:PCW:C34	5:A:409:17F:H32	0.44	2.42	1	1
4:B:204:PCW:H481	5:D:512:17F:H47	0.44	1.88	1	2
4:D:509:PCW:H382	4:D:510:PCW:C1	0.44	2.42	1	1
1:A:388:SER:HB3	1:C:594:LYS:HE2	0.44	1.87	2	1
4:A:415:PCW:C3	4:C:616:PCW:H421	0.44	2.41	2	2
4:D:505:PCW:H20	4:D:510:PCW:C33	0.44	2.41	2	2
4:C:608:PCW:N	4:C:619:PCW:O11	0.44	2.51	3	1
4:D:501:PCW:H351	5:D:512:17F:C21	0.44	2.43	3	1
4:B:208:PCW:C28	4:B:208:PCW:H471	0.44	2.43	4	1
3:D:402:LEU:HD21	3:D:409:LYS:HA	0.44	1.90	4	1
4:D:516:PCW:H141	4:D:516:PCW:C37	0.44	2.40	4	1
4:C:607:PCW:C18	5:C:629:17F:H29	0.44	2.42	5	1
4:C:612:PCW:O11	4:C:612:PCW:C2	0.44	2.53	5	1
4:C:612:PCW:C28	5:D:511:17F:H43	0.44	2.43	5	1
4:A:405:PCW:H432	4:A:414:PCW:C24	0.44	2.43	6	1
4:C:607:PCW:C47	5:C:626:17F:H61	0.44	2.43	6	1
4:B:202:PCW:C36	4:B:202:PCW:O31	0.44	2.66	6	1
1:C:438:ARG:HA	1:C:441:MET:HB2	0.44	1.90	7	1
4:C:625:PCW:O3	4:C:625:PCW:O31	0.44	2.36	7	1
4:D:507:PCW:O3	5:D:513:17F:H71	0.44	2.12	7	1
5:D:513:17F:C10	5:D:513:17F:H59	0.44	2.42	7	1
4:C:612:PCW:C27	5:D:511:17F:H50	0.44	2.42	8	1
4:A:412:PCW:C38	4:C:624:PCW:H452	0.44	2.41	9	1
4:C:625:PCW:H73	4:C:625:PCW:C31	0.44	2.43	9	1
4:D:506:PCW:H431	4:D:507:PCW:H431	0.44	1.90	9	1
4:A:408:PCW:C26	4:D:504:PCW:H441	0.44	2.42	10	1
4:C:602:PCW:H422	5:C:626:17F:H42	0.44	1.88	10	1
4:C:604:PCW:H411	4:C:604:PCW:H372	0.44	1.88	10	1
4:C:605:PCW:C39	4:C:618:PCW:H121	0.44	2.43	10	1
4:C:610:PCW:H222	4:C:618:PCW:H471	0.44	1.89	10	1
4:A:405:PCW:C18	4:A:414:PCW:H261	0.44	2.37	1	1
4:A:406:PCW:O3	4:A:406:PCW:C31	0.44	2.66	9	3
1:C:433:GLU:O	1:C:437:LEU:HG	0.44	2.13	1	3
4:A:404:PCW:H331	4:A:407:PCW:H122	0.44	1.87	4	2
4:A:417:PCW:C45	4:C:622:PCW:H281	0.44	2.42	2	1
3:D:446:PHE:O	4:D:501:PCW:H63	0.44	2.13	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:417:PCW:C21	4:C:603:PCW:C16	0.44	2.93	4	1
4:C:615:PCW:C34	4:D:516:PCW:H362	0.44	2.43	4	1
4:C:621:PCW:C48	4:D:505:PCW:H441	0.44	2.43	4	1
5:C:630:17F:O6	5:C:630:17F:C17	0.44	2.65	4	3
2:B:68:ARG:HA	2:B:71:TYR:CE1	0.44	2.47	10	3
4:B:203:PCW:H271	4:B:204:PCW:H171	0.44	1.89	5	1
4:B:206:PCW:C28	4:B:206:PCW:C24	0.44	2.96	5	1
5:D:512:17F:C1X	5:D:514:17F:H29	0.44	2.43	5	1
2:B:117:LYS:HB3	2:B:120:LEU:HD12	0.44	1.90	6	1
4:B:201:PCW:H452	4:B:205:PCW:H252	0.44	1.88	6	1
4:B:205:PCW:H182	4:B:207:PCW:C15	0.44	2.36	6	1
4:B:207:PCW:C7	5:B:213:17F:H1A	0.44	2.43	6	1
4:C:618:PCW:H471	5:D:511:17F:H74	0.44	1.86	7	1
5:C:627:17F:O3	5:C:627:17F:O9	0.44	2.36	7	1
4:B:208:PCW:H441	5:D:512:17F:C38	0.44	2.43	7	1
4:D:501:PCW:O2	4:D:501:PCW:H341	0.44	2.13	7	1
4:A:406:PCW:H441	4:B:209:PCW:H451	0.44	1.89	8	1
4:A:404:PCW:H181	4:A:407:PCW:H261	0.44	1.88	9	1
4:A:406:PCW:C40	4:D:505:PCW:H412	0.44	2.43	9	1
4:B:208:PCW:C8	5:B:214:17F:C19	0.44	2.95	9	1
4:C:604:PCW:H251	5:D:514:17F:H70	0.44	1.89	10	1
4:C:612:PCW:H281	5:D:511:17F:H35	0.44	1.89	10	1
4:B:206:PCW:H32	5:B:213:17F:H1	0.44	1.88	10	1
4:B:202:PCW:H421	4:B:202:PCW:C38	0.44	2.43	1	1
4:D:503:PCW:C3	4:D:507:PCW:H352	0.44	2.43	1	1
4:A:413:PCW:H332	4:C:611:PCW:H32	0.44	1.85	2	1
4:A:413:PCW:H381	4:C:611:PCW:H151	0.44	1.89	4	1
4:D:507:PCW:H462	4:D:507:PCW:C27	0.44	2.31	4	1
2:B:39:SER:O	3:D:366:GLN:HG3	0.44	2.12	5	1
4:A:408:PCW:C48	5:A:410:17F:H70	0.44	2.43	6	1
4:A:401:PCW:H322	4:D:508:PCW:H371	0.44	1.88	7	1
4:A:403:PCW:H152	4:B:207:PCW:H381	0.44	1.89	7	1
4:A:407:PCW:H412	4:B:211:PCW:H441	0.44	1.89	7	1
4:C:614:PCW:H472	4:B:207:PCW:H222	0.44	1.89	7	1
4:B:210:PCW:H271	4:B:211:PCW:C23	0.44	2.29	7	1
4:D:503:PCW:H321	4:D:507:PCW:H341	0.44	1.89	7	1
5:D:513:17F:O7	5:D:513:17F:O10	0.44	2.36	7	1
4:A:416:PCW:H422	4:C:616:PCW:C20	0.44	2.42	8	1
4:B:205:PCW:H162	4:B:206:PCW:C17	0.44	2.42	8	1
4:C:621:PCW:C32	4:C:625:PCW:H20	0.44	2.42	9	1
5:C:628:17F:H53	5:B:213:17F:H77	0.44	1.88	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:502:PCW:H421	4:D:508:PCW:C22	0.44	2.42	9	1
4:D:504:PCW:O31	4:D:504:PCW:P	0.44	2.76	9	1
4:A:402:PCW:H73	5:D:513:17F:C3	0.44	2.43	10	1
4:A:411:PCW:H61	5:C:630:17F:C2	0.44	2.43	10	1
4:D:503:PCW:H162	4:D:505:PCW:H472	0.44	1.88	10	1
4:B:209:PCW:H212	4:B:209:PCW:H181	0.44	1.55	1	1
4:C:608:PCW:H442	4:C:614:PCW:H461	0.44	1.89	2	1
2:B:135:ARG:HG2	4:B:209:PCW:H82	0.44	1.89	2	1
5:B:213:17F:H64	4:D:505:PCW:C40	0.44	2.43	2	1
3:D:399:PHE:HB3	3:D:409:LYS:HB2	0.44	1.90	2	1
4:A:405:PCW:C40	5:D:512:17F:H64	0.44	2.43	3	1
4:A:408:PCW:H422	5:A:409:17F:C39	0.44	2.42	3	1
4:B:203:PCW:H73	4:B:204:PCW:H342	0.44	1.90	3	1
4:B:212:PCW:H452	4:B:212:PCW:C22	0.44	2.43	3	1
4:D:508:PCW:H471	4:D:508:PCW:H251	0.44	1.90	3	1
4:B:203:PCW:O4P	4:B:203:PCW:C3	0.44	2.60	4	1
4:B:203:PCW:H51	4:B:204:PCW:H351	0.44	1.90	4	1
4:A:417:PCW:H182	4:C:603:PCW:H141	0.44	1.90	10	2
4:C:621:PCW:H182	4:D:516:PCW:H172	0.44	1.89	8	2
4:B:206:PCW:C38	4:D:505:PCW:O3	0.44	2.66	5	1
4:A:407:PCW:C32	4:B:211:PCW:C13	0.44	2.96	6	1
4:B:205:PCW:O3	4:B:205:PCW:C31	0.44	2.66	7	1
4:A:402:PCW:H361	4:B:210:PCW:C44	0.44	2.43	8	1
5:A:410:17F:C40	4:C:610:PCW:C47	0.44	2.96	8	1
4:D:508:PCW:H442	5:D:512:17F:C26	0.44	2.42	9	1
2:B:3:GLU:HA	2:B:52:LEU:HB3	0.44	1.88	10	1
4:A:408:PCW:H412	5:D:511:17F:H9A	0.43	1.89	1	1
4:A:413:PCW:H451	4:C:611:PCW:C17	0.43	2.43	1	1
4:C:612:PCW:C22	5:D:511:17F:H47	0.43	2.43	7	2
4:C:621:PCW:C18	5:C:628:17F:H29	0.43	2.43	2	1
4:B:205:PCW:H73	5:B:213:17F:C7	0.43	2.43	2	1
4:D:507:PCW:H152	5:D:513:17F:O8	0.43	2.13	2	1
4:D:508:PCW:H61	5:D:512:17F:H6	0.43	1.89	2	1
4:C:624:PCW:H181	4:C:624:PCW:H211	0.43	1.50	3	2
5:C:630:17F:O8	5:C:630:17F:C5	0.43	2.55	6	3
3:D:377:SER:HA	3:D:417:ASP:HA	0.43	1.89	3	1
4:D:509:PCW:C8	4:D:510:PCW:O31	0.43	2.66	3	1
4:A:406:PCW:C31	4:A:406:PCW:O3	0.43	2.65	4	1
4:A:401:PCW:H472	4:C:610:PCW:C24	0.43	2.42	5	1
4:C:601:PCW:H482	5:C:626:17F:C29	0.43	2.43	5	1
4:C:606:PCW:H62	4:C:624:PCW:C19	0.43	2.42	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:146:ALA:N	6:B:216:GNP:O6	0.43	2.51	10	2
3:D:463:PHE:HB2	3:D:472:PHE:CE1	0.43	2.48	6	1
4:A:405:PCW:C14	4:A:405:PCW:C18	0.43	2.92	8	2
4:A:406:PCW:O2P	4:B:211:PCW:C6	0.43	2.66	9	1
4:A:408:PCW:H371	4:A:408:PCW:C11	0.43	2.42	9	1
5:A:409:17F:C2X	5:D:511:17F:C17	0.43	2.96	9	1
5:A:410:17F:C41	5:D:511:17F:H68	0.43	2.37	9	1
2:B:84:ILE:HD13	2:B:123:ARG:HG3	0.43	1.89	9	1
4:D:504:PCW:C35	4:D:504:PCW:O31	0.43	2.65	10	1
4:C:613:PCW:O31	4:C:613:PCW:H11	0.43	2.13	1	1
4:C:621:PCW:H142	5:C:628:17F:H33	0.43	1.87	1	1
4:C:622:PCW:H12	4:C:623:PCW:C16	0.43	2.43	2	2
4:A:404:PCW:C48	4:A:407:PCW:H241	0.43	2.42	3	1
4:A:412:PCW:H12	4:C:624:PCW:H362	0.43	1.85	3	3
1:C:554:HIS:O	1:C:558:LEU:HB2	0.43	2.13	3	1
5:C:627:17F:H68	5:B:215:17F:C11	0.43	2.43	3	1
1:C:440:GLU:O	1:C:444:ASP:HB2	0.43	2.13	6	4
4:C:608:PCW:H422	4:C:614:PCW:C45	0.43	2.41	4	1
4:C:605:PCW:H261	4:C:612:PCW:H412	0.43	1.89	6	1
4:D:509:PCW:O3P	4:D:509:PCW:C31	0.43	2.66	7	2
4:A:406:PCW:H462	4:B:211:PCW:H19	0.43	1.90	7	1
5:A:409:17F:C9	4:D:504:PCW:C40	0.43	2.93	7	1
4:C:607:PCW:H172	5:C:629:17F:O10	0.43	2.13	7	1
4:B:207:PCW:H441	4:B:209:PCW:C23	0.43	2.37	7	1
4:B:210:PCW:H212	4:B:210:PCW:H181	0.43	1.55	7	1
4:C:608:PCW:H471	4:B:205:PCW:C23	0.43	2.44	10	1
4:D:510:PCW:H461	4:D:516:PCW:H20	0.43	1.89	1	1
4:A:402:PCW:H242	4:A:413:PCW:H262	0.43	1.91	2	1
4:C:620:PCW:C18	4:C:620:PCW:C14	0.43	2.88	2	2
4:A:403:PCW:C46	4:B:209:PCW:H272	0.43	2.43	3	1
4:C:605:PCW:O1P	4:C:605:PCW:O31	0.43	2.36	3	1
4:C:605:PCW:C32	4:C:610:PCW:H12	0.43	2.43	3	1
4:D:506:PCW:O31	4:D:510:PCW:H82	0.43	2.13	3	1
4:C:609:PCW:C6	5:C:631:17F:H6A	0.43	2.29	4	1
4:A:417:PCW:H322	4:C:622:PCW:H2	0.43	1.91	5	2
4:B:206:PCW:H161	5:B:213:17F:H56	0.43	1.89	5	1
4:B:209:PCW:C28	5:B:215:17F:H74	0.43	2.42	5	1
5:D:512:17F:H11A	5:D:514:17F:H11	0.43	1.90	5	1
4:A:416:PCW:H161	5:C:630:17F:C33	0.43	2.40	6	1
4:C:605:PCW:H372	4:C:605:PCW:C41	0.43	2.43	6	1
4:C:613:PCW:C13	4:C:622:PCW:H481	0.43	2.44	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:208:PCW:H272	4:B:208:PCW:C39	0.43	2.44	6	1
4:C:612:PCW:H261	5:D:511:17F:C37	0.43	2.43	7	1
4:C:617:PCW:C37	4:C:625:PCW:H161	0.43	2.43	7	1
2:B:37:GLU:HB2	3:D:369:VAL:HG23	0.43	1.89	8	1
4:D:505:PCW:H182	4:D:509:PCW:C48	0.43	2.43	8	1
1:C:489:LEU:O	1:C:493:GLN:HG3	0.43	2.13	9	1
4:C:615:PCW:H451	4:D:506:PCW:H483	0.43	1.89	9	1
4:D:506:PCW:C42	5:D:513:17F:H49	0.43	2.42	9	1
4:A:408:PCW:C26	5:A:409:17F:H59	0.43	2.42	10	1
5:B:213:17F:H41	5:D:514:17F:C31	0.43	2.43	10	1
5:D:514:17F:H48	5:D:514:17F:H78	0.43	1.89	10	1
4:A:408:PCW:H211	5:A:409:17F:C1Y	0.43	2.44	1	1
4:C:612:PCW:C28	5:D:511:17F:H35	0.43	2.43	1	1
4:C:622:PCW:H212	4:C:622:PCW:H182	0.43	1.58	1	2
4:B:203:PCW:H232	4:B:204:PCW:H171	0.43	1.89	1	1
4:B:204:PCW:H132	4:B:208:PCW:O3	0.43	2.13	1	1
4:D:501:PCW:C21	5:D:511:17F:C19	0.43	2.94	1	1
4:A:405:PCW:C2	5:D:512:17F:H33	0.43	2.37	2	1
4:C:606:PCW:H161	5:C:627:17F:C10	0.43	2.43	2	1
4:C:604:PCW:C45	4:C:606:PCW:C18	0.43	2.97	3	2
4:A:412:PCW:C3	4:C:624:PCW:C39	0.43	2.95	4	1
4:A:413:PCW:H361	4:C:611:PCW:C13	0.43	2.44	4	1
4:B:208:PCW:H121	5:B:214:17F:C6	0.43	2.43	4	1
4:D:504:PCW:H2	4:D:504:PCW:H41	0.43	1.90	4	1
4:D:508:PCW:H182	4:D:508:PCW:C36	0.43	2.40	5	1
4:C:625:PCW:C18	4:C:625:PCW:C22	0.43	2.82	6	1
5:C:632:17F:H65	4:B:207:PCW:H483	0.43	1.88	6	1
4:B:206:PCW:H39	5:B:213:17F:H76	0.43	1.90	6	1
4:C:609:PCW:C17	5:C:631:17F:H61	0.43	2.43	7	1
4:B:201:PCW:H52	4:B:209:PCW:O2P	0.43	2.14	7	1
4:D:502:PCW:H32	4:D:508:PCW:H371	0.43	1.90	8	1
5:D:512:17F:H35	5:D:514:17F:H29	0.43	1.89	8	1
4:B:208:PCW:H471	4:B:208:PCW:C27	0.43	2.35	9	1
4:A:402:PCW:C34	4:D:507:PCW:H212	0.43	2.38	10	1
4:A:415:PCW:C41	4:D:515:PCW:H181	0.43	2.39	10	1
4:D:501:PCW:H481	4:D:509:PCW:H271	0.43	1.91	10	1
1:A:299:SER:HB2	1:A:300:PRO:CD	0.43	2.44	2	2
4:A:407:PCW:H63	4:B:211:PCW:O2P	0.43	2.14	2	1
4:B:201:PCW:C31	4:B:201:PCW:O4P	0.43	2.66	2	2
4:A:405:PCW:C46	4:A:414:PCW:H272	0.43	2.43	3	1
4:A:408:PCW:C16	5:A:409:17F:H56	0.43	2.31	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:43:GLN:NE2	3:D:468:CYS:HA	0.43	2.29	3	1
4:B:212:PCW:H422	5:D:514:17F:H70	0.43	1.89	3	1
5:B:213:17F:H29	4:D:505:PCW:H142	0.43	1.91	3	1
4:A:411:PCW:H121	4:C:616:PCW:C33	0.43	2.44	4	1
4:D:501:PCW:O2P	5:D:514:17F:H30	0.43	2.13	4	1
4:A:404:PCW:H131	4:B:210:PCW:C15	0.43	2.44	5	1
4:A:406:PCW:H422	4:B:209:PCW:H39	0.43	1.90	5	1
4:D:503:PCW:H41	4:D:510:PCW:C7	0.43	2.42	5	1
4:D:508:PCW:H132	4:D:508:PCW:H321	0.43	1.90	5	1
5:D:512:17F:H59	5:D:512:17F:H62	0.43	1.53	5	1
4:A:413:PCW:C34	4:C:611:PCW:O3	0.43	2.67	6	1
4:A:416:PCW:H32	4:A:416:PCW:C6	0.43	2.39	6	1
5:B:215:17F:O9	5:B:215:17F:C7	0.43	2.66	6	1
5:A:410:17F:O5	4:D:502:PCW:H63	0.43	2.14	7	1
4:A:417:PCW:C47	5:D:511:17F:H54	0.43	2.42	7	1
4:C:612:PCW:C20	5:D:511:17F:C27	0.43	2.95	7	1
3:D:366:GLN:HG2	3:D:389:ARG:NH2	0.43	2.27	7	1
4:D:505:PCW:O11	4:D:509:PCW:H31	0.43	2.12	7	1
1:A:281:ALA:O	1:A:285:GLU:HG3	0.43	2.13	9	1
4:B:212:PCW:C37	5:D:514:17F:H33	0.43	2.41	9	1
4:B:212:PCW:H342	5:B:213:17F:C9	0.43	2.43	9	1
4:D:503:PCW:H20	4:D:516:PCW:H282	0.43	1.88	9	1
2:B:21:ILE:HG21	3:D:388:VAL:HB	0.43	1.88	10	1
4:B:208:PCW:H421	5:D:512:17F:C40	0.43	2.43	10	1
5:B:214:17F:C4	5:B:214:17F:H2	0.43	2.43	10	1
1:C:421:PRO:O	1:C:425:GLU:HG2	0.43	2.13	1	1
4:C:608:PCW:H452	4:B:207:PCW:H232	0.43	1.91	1	1
5:B:213:17F:H4	5:B:213:17F:O10	0.43	2.14	1	1
4:A:404:PCW:C18	4:A:404:PCW:H232	0.43	2.43	2	1
4:A:404:PCW:H162	4:A:407:PCW:H411	0.43	1.90	2	1
4:C:608:PCW:H442	4:C:614:PCW:H472	0.43	1.91	4	1
4:D:505:PCW:C27	4:D:510:PCW:H142	0.43	2.43	4	1
4:D:506:PCW:C41	4:D:516:PCW:H251	0.43	2.43	9	2
4:B:206:PCW:C23	4:B:206:PCW:C27	0.43	2.95	5	1
4:D:510:PCW:O11	4:D:510:PCW:C2	0.43	2.65	5	1
4:C:604:PCW:H482	4:C:624:PCW:H281	0.43	1.84	6	1
4:A:401:PCW:H481	4:C:618:PCW:C27	0.43	2.41	7	1
4:B:201:PCW:H322	4:B:209:PCW:O4P	0.43	2.14	7	1
4:B:205:PCW:H151	4:B:207:PCW:H151	0.43	1.91	7	1
4:A:415:PCW:H382	4:D:515:PCW:H162	0.43	1.91	8	1
4:C:617:PCW:C48	4:D:507:PCW:H461	0.43	2.44	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:C:627:17F:H9A	5:C:627:17F:C18	0.43	2.44	8	1
4:B:204:PCW:H172	4:B:208:PCW:C37	0.43	2.43	8	1
4:B:206:PCW:H462	4:B:206:PCW:H262	0.43	1.91	8	1
4:D:503:PCW:C34	4:D:510:PCW:H82	0.43	2.43	8	1
4:B:203:PCW:O2	4:B:203:PCW:H342	0.43	2.13	9	1
4:B:204:PCW:H471	5:D:512:17F:C25	0.43	2.32	9	1
4:B:206:PCW:H161	5:B:213:17F:C1Y	0.43	2.43	9	1
4:D:502:PCW:H441	5:D:512:17F:H43	0.43	1.88	9	1
4:D:507:PCW:H271	4:D:507:PCW:H481	0.43	1.90	9	1
4:C:615:PCW:O11	4:C:615:PCW:H42	0.43	2.13	10	1
4:C:604:PCW:H262	5:B:213:17F:C30	0.43	2.35	1	1
2:B:31:GLU:H	2:B:31:GLU:CD	0.43	2.22	1	1
4:B:202:PCW:O1P	4:B:202:PCW:H32	0.43	2.13	1	1
4:B:209:PCW:C22	5:B:215:17F:H74	0.43	2.43	1	1
4:D:505:PCW:H152	4:D:510:PCW:H452	0.43	1.89	1	1
4:D:507:PCW:C22	5:D:513:17F:H31	0.43	2.39	3	1
5:D:514:17F:H18	5:D:514:17F:H5	0.43	1.39	10	3
4:C:601:PCW:H471	4:C:601:PCW:C15	0.43	2.22	4	1
4:B:201:PCW:H331	4:B:209:PCW:H132	0.43	1.89	4	1
4:D:504:PCW:H381	4:D:504:PCW:C42	0.43	2.43	4	1
4:A:412:PCW:C36	4:C:624:PCW:H381	0.43	2.43	5	1
4:D:508:PCW:O11	4:D:508:PCW:H332	0.43	2.13	5	1
4:C:605:PCW:P	4:C:612:PCW:C5	0.43	3.06	6	1
4:A:407:PCW:H382	4:B:211:PCW:C16	0.43	2.28	7	1
4:A:415:PCW:C1	4:C:616:PCW:H381	0.43	2.44	7	1
4:B:204:PCW:O11	4:B:212:PCW:C16	0.43	2.66	7	1
4:D:502:PCW:H412	4:D:508:PCW:H341	0.43	1.90	7	1
4:D:505:PCW:H461	4:D:506:PCW:H152	0.43	1.91	7	1
4:C:615:PCW:H61	4:C:616:PCW:C37	0.43	2.42	8	1
3:D:472:PHE:HB2	3:D:476:CYS:CB	0.43	2.37	8	1
5:D:512:17F:C2X	5:D:514:17F:H29	0.43	2.44	8	1
5:D:514:17F:H35	5:D:514:17F:H67	0.43	1.90	8	1
5:D:512:17F:O8	5:D:512:17F:H5	0.43	2.13	9	1
4:B:207:PCW:C20	4:B:207:PCW:C24	0.43	2.96	10	1
5:D:514:17F:H36	5:D:514:17F:H64	0.43	1.90	10	1
1:A:353:ALA:O	1:A:357:LEU:HG	0.43	2.14	1	1
4:A:404:PCW:H261	5:C:631:17F:C30	0.43	2.43	1	1
1:C:535:ALA:O	1:C:539:ASN:HB2	0.43	2.13	9	2
4:B:205:PCW:H162	4:B:207:PCW:C35	0.43	2.43	1	1
4:A:411:PCW:H12	4:D:515:PCW:C3	0.43	2.44	2	1
4:A:408:PCW:O3	4:A:408:PCW:C35	0.43	2.60	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:37:GLU:OE1	3:D:367:ARG:HD2	0.43	2.13	3	1
4:C:616:PCW:H2	4:C:616:PCW:C6	0.43	2.43	5	1
4:B:203:PCW:O2P	4:B:203:PCW:H63	0.43	2.14	5	2
4:C:617:PCW:H482	4:D:503:PCW:H222	0.43	1.91	6	1
4:C:607:PCW:H431	5:C:626:17F:C33	0.43	2.43	7	1
4:C:607:PCW:H63	4:C:624:PCW:C28	0.43	2.41	7	1
2:B:37:GLU:HG3	2:B:56:LEU:HD11	0.43	1.89	7	1
4:B:206:PCW:C42	5:B:213:17F:H59	0.43	2.44	7	1
5:C:627:17F:H18A	5:C:627:17F:O8	0.43	2.06	8	1
4:A:411:PCW:H151	4:C:603:PCW:H272	0.43	1.90	9	1
4:C:614:PCW:H42	4:C:614:PCW:C3	0.43	2.44	9	1
5:C:632:17F:H70	5:B:215:17F:H65	0.43	1.91	9	1
4:D:501:PCW:H61	5:D:514:17F:C1	0.43	2.42	9	1
4:D:516:PCW:O2	4:D:516:PCW:O11	0.43	2.35	10	1
5:B:213:17F:H64	4:D:505:PCW:C39	0.43	2.44	2	1
4:D:504:PCW:H182	4:D:504:PCW:H231	0.43	1.91	2	1
4:C:606:PCW:O11	4:C:606:PCW:C2	0.43	2.61	3	2
4:A:417:PCW:C40	4:C:622:PCW:H272	0.43	2.43	4	1
4:B:210:PCW:H281	4:D:505:PCW:C47	0.43	2.44	4	1
4:D:501:PCW:H451	4:D:509:PCW:H222	0.43	1.87	4	1
4:A:402:PCW:O2	4:A:402:PCW:P	0.43	2.76	5	1
4:B:212:PCW:H432	4:B:212:PCW:H212	0.43	1.89	5	1
5:B:213:17F:H29	4:D:505:PCW:C14	0.43	2.44	7	1
4:A:407:PCW:H212	4:A:407:PCW:H181	0.43	1.61	8	1
4:B:212:PCW:O31	4:D:505:PCW:C7	0.43	2.66	8	1
5:A:409:17F:H35	5:D:511:17F:C17	0.43	2.43	9	1
4:A:415:PCW:O1P	4:A:415:PCW:C5	0.43	2.65	9	1
4:D:506:PCW:H342	4:D:507:PCW:C39	0.43	2.44	9	1
4:A:403:PCW:H51	4:A:403:PCW:C31	0.43	2.44	10	1
4:B:206:PCW:H122	5:B:213:17F:C17	0.43	2.44	10	1
4:D:501:PCW:C7	5:D:514:17F:C3	0.43	2.97	10	1
4:B:201:PCW:C44	4:B:205:PCW:H231	0.43	2.44	1	1
4:B:205:PCW:H20	4:B:207:PCW:H431	0.43	1.91	1	1
4:B:207:PCW:O3	4:B:207:PCW:C31	0.43	2.66	4	3
4:B:208:PCW:H462	4:B:212:PCW:C26	0.43	2.43	1	1
4:C:617:PCW:H412	5:C:631:17F:C28	0.43	2.41	2	1
4:B:205:PCW:H161	4:B:207:PCW:H151	0.43	1.90	3	1
5:D:512:17F:H18	5:D:512:17F:H5	0.43	1.61	3	3
4:A:414:PCW:O31	4:A:414:PCW:P	0.43	2.76	4	1
4:C:602:PCW:H342	5:B:214:17F:H77	0.43	1.91	5	1
5:C:627:17F:C26	5:C:628:17F:H73	0.43	2.43	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:211:PCW:H441	4:B:211:PCW:H161	0.43	1.91	5	1
4:D:508:PCW:H362	4:D:508:PCW:C18	0.43	2.43	5	1
4:C:608:PCW:O11	4:C:614:PCW:C7	0.43	2.67	6	1
4:B:205:PCW:H221	4:B:207:PCW:C19	0.43	2.44	6	1
4:A:405:PCW:C18	4:A:405:PCW:H222	0.43	2.44	7	1
5:A:409:17F:H60	4:D:504:PCW:C44	0.43	2.42	7	1
4:C:610:PCW:H242	4:C:610:PCW:C46	0.43	2.44	7	1
4:B:203:PCW:C28	5:B:214:17F:C20	0.43	2.95	7	1
4:A:403:PCW:H131	4:B:201:PCW:C14	0.43	2.44	8	1
4:A:407:PCW:C39	4:B:211:PCW:H141	0.43	2.44	8	1
4:A:413:PCW:H442	4:C:611:PCW:H272	0.43	1.91	8	1
4:D:502:PCW:C43	4:D:508:PCW:H221	0.43	2.44	9	1
4:B:202:PCW:O11	4:D:507:PCW:C5	0.43	2.67	10	1
4:A:414:PCW:H481	4:C:604:PCW:H272	0.42	1.89	1	1
4:C:617:PCW:H462	4:D:503:PCW:H242	0.42	1.90	1	1
5:A:410:17F:O5	4:D:502:PCW:C8	0.42	2.65	2	1
2:B:127:THR:O	2:B:131:GLN:HG3	0.42	2.14	2	1
4:B:206:PCW:H2	5:B:213:17F:H5	0.42	1.90	2	1
4:A:404:PCW:O3P	4:A:404:PCW:C31	0.42	2.66	3	1
4:A:416:PCW:C7	5:C:630:17F:O2	0.42	2.67	3	2
4:C:612:PCW:H282	5:D:511:17F:C12	0.42	2.38	3	1
4:D:508:PCW:H162	4:D:508:PCW:H342	0.42	1.90	3	1
4:A:413:PCW:H441	4:C:611:PCW:H272	0.42	1.91	4	1
4:B:207:PCW:H371	4:B:209:PCW:H141	0.42	1.91	4	2
4:B:210:PCW:O4P	5:D:513:17F:C1	0.42	2.67	4	1
5:A:410:17F:O9	5:A:410:17F:C20	0.42	2.68	5	1
4:A:413:PCW:O2	4:A:413:PCW:H342	0.42	2.14	8	2
1:A:229:TRP:CH2	4:A:402:PCW:H462	0.42	2.48	6	1
4:A:416:PCW:H63	4:A:416:PCW:C3	0.42	2.38	6	1
4:B:211:PCW:C19	4:D:505:PCW:H451	0.42	2.44	6	1
5:A:410:17F:C39	4:D:502:PCW:H281	0.42	2.38	7	1
4:A:416:PCW:H62	5:C:630:17F:H6A	0.42	1.90	7	1
4:C:624:PCW:O2	4:C:624:PCW:P	0.42	2.76	9	3
2:B:17:SER:OG	6:B:216:GNP:O2G	0.42	2.36	7	1
4:B:201:PCW:C34	4:B:209:PCW:H31	0.42	2.43	7	1
4:B:207:PCW:H412	4:B:209:PCW:C14	0.42	2.44	7	1
4:A:402:PCW:H52	5:D:513:17F:O10	0.42	2.14	9	1
4:B:205:PCW:C20	4:B:207:PCW:H431	0.42	2.42	9	1
4:C:615:PCW:H31	4:C:615:PCW:H42	0.42	1.89	10	1
4:B:211:PCW:H412	4:B:211:PCW:H382	0.42	1.63	10	1
3:D:359:ARG:HA	3:D:369:VAL:HG22	0.42	1.91	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:612:PCW:H141	4:C:618:PCW:H382	0.42	1.89	1	1
2:B:116:ASN:HA	2:B:144:THR:O	0.42	2.14	8	3
4:C:616:PCW:O3P	4:C:616:PCW:C5	0.42	2.67	2	1
4:C:615:PCW:C1	4:D:516:PCW:H342	0.42	2.43	3	1
3:D:405:HIS:CE1	3:D:408:LYS:HB3	0.42	2.49	4	3
5:C:632:17F:H53	4:B:207:PCW:H152	0.42	1.90	4	1
5:A:409:17F:O10	5:A:409:17F:C4	0.42	2.60	5	1
4:C:614:PCW:H141	5:C:632:17F:C8	0.42	2.44	5	1
4:C:601:PCW:O3	4:C:601:PCW:C31	0.42	2.67	6	1
4:A:407:PCW:C28	4:B:211:PCW:H442	0.42	2.44	7	1
4:C:611:PCW:C7	4:C:617:PCW:H31	0.42	2.43	7	1
4:B:204:PCW:C13	4:B:208:PCW:H151	0.42	2.43	7	1
4:B:207:PCW:C41	4:B:207:PCW:H371	0.42	2.44	7	1
4:B:212:PCW:H231	5:D:514:17F:H10A	0.42	1.91	7	1
4:D:501:PCW:C22	5:D:511:17F:H20A	0.42	2.44	7	1
4:A:403:PCW:H461	4:B:209:PCW:C27	0.42	2.42	8	1
4:C:614:PCW:H212	4:C:614:PCW:C17	0.42	2.44	8	1
4:C:603:PCW:O4P	5:C:628:17F:H1	0.42	2.14	9	1
4:C:616:PCW:H41	4:C:616:PCW:H2	0.42	1.91	9	1
4:C:624:PCW:C11	4:C:624:PCW:H51	0.42	2.44	10	1
4:B:205:PCW:H121	4:B:207:PCW:C14	0.42	2.43	10	1
4:D:508:PCW:C19	5:D:512:17F:H32	0.42	2.44	10	1
5:C:627:17F:H52	5:C:628:17F:H39	0.42	1.90	1	1
2:B:6:LEU:HD11	2:B:53:LEU:HD22	0.42	1.91	1	1
4:A:413:PCW:C33	4:C:611:PCW:H32	0.42	2.44	2	1
4:D:503:PCW:H332	4:D:510:PCW:C8	0.42	2.36	2	1
5:D:513:17F:H62	5:D:513:17F:H59	0.42	1.60	2	1
4:C:614:PCW:C22	5:C:632:17F:H41	0.42	2.36	3	1
4:C:617:PCW:C46	4:B:211:PCW:H251	0.42	2.34	3	1
4:D:508:PCW:H41	4:D:508:PCW:C11	0.42	2.44	3	1
4:D:508:PCW:C11	4:D:508:PCW:O2	0.42	2.67	3	1
4:C:614:PCW:C28	5:C:632:17F:H49	0.42	2.44	4	1
4:D:507:PCW:H122	5:D:513:17F:C8	0.42	2.44	4	1
1:A:316:LEU:HD13	4:C:601:PCW:H442	0.42	1.91	5	1
4:A:417:PCW:H141	4:C:603:PCW:C41	0.42	2.42	6	1
4:C:610:PCW:C5	4:C:622:PCW:H361	0.42	2.33	6	1
4:A:411:PCW:H39	4:A:411:PCW:H151	0.42	1.91	8	1
4:A:407:PCW:C5	4:B:211:PCW:O2P	0.42	2.64	9	1
5:B:213:17F:H41	5:D:514:17F:H57	0.42	1.90	10	1
4:A:405:PCW:O31	4:A:405:PCW:C1	0.42	2.65	1	1
1:C:437:LEU:O	1:C:440:GLU:HG3	0.42	2.14	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:B:215:17F:H19A	5:B:215:17F:C9	0.42	2.40	1	1
4:C:613:PCW:H381	4:C:613:PCW:H411	0.42	1.59	4	3
4:B:203:PCW:C4	4:B:204:PCW:H341	0.42	2.40	2	1
4:B:206:PCW:O1P	4:B:206:PCW:H32	0.42	2.14	2	1
4:D:503:PCW:C39	4:D:504:PCW:H73	0.42	2.44	2	1
4:A:401:PCW:H283	4:C:613:PCW:H281	0.42	1.90	3	1
4:A:417:PCW:O31	4:A:417:PCW:C4	0.42	2.68	3	1
4:C:617:PCW:H442	4:C:625:PCW:H282	0.42	1.89	3	1
4:D:506:PCW:H151	4:D:510:PCW:C39	0.42	2.44	3	1
4:A:402:PCW:H342	4:D:507:PCW:H182	0.42	1.90	4	1
4:A:408:PCW:H451	5:A:409:17F:H69	0.42	1.92	4	1
4:C:621:PCW:H73	5:C:631:17F:C11	0.42	2.40	4	1
4:B:204:PCW:H181	4:B:208:PCW:H242	0.42	1.90	4	1
5:A:410:17F:C31	4:D:502:PCW:H151	0.42	2.43	5	1
4:C:619:PCW:H132	5:C:632:17F:H18A	0.42	1.90	5	1
4:C:625:PCW:O4P	4:C:625:PCW:H2	0.42	2.14	5	1
5:C:627:17F:H42	5:C:628:17F:H74	0.42	1.90	5	1
4:C:605:PCW:H462	5:D:511:17F:H51	0.42	1.90	6	1
4:C:608:PCW:H462	4:B:207:PCW:H451	0.42	1.90	6	1
5:A:409:17F:H60	4:D:504:PCW:C43	0.42	2.45	7	1
4:A:415:PCW:C3	4:C:616:PCW:H422	0.42	2.43	8	1
4:C:608:PCW:H271	5:C:626:17F:H71	0.42	1.89	8	1
4:C:620:PCW:H171	5:C:631:17F:C5	0.42	2.40	8	1
2:B:41:ARG:HA	2:B:53:LEU:O	0.42	2.13	8	1
4:B:204:PCW:C47	5:D:514:17F:H37	0.42	2.44	9	1
4:D:504:PCW:H221	4:D:504:PCW:C17	0.42	2.45	9	1
5:D:512:17F:H36	5:D:512:17F:H40	0.42	1.63	9	1
5:A:409:17F:O9	4:D:504:PCW:H361	0.42	2.14	10	1
4:A:412:PCW:H382	4:C:624:PCW:H452	0.42	1.89	10	1
4:C:620:PCW:H181	4:C:620:PCW:H212	0.42	1.65	10	1
4:B:206:PCW:H371	4:D:505:PCW:C32	0.42	2.38	10	1
4:C:605:PCW:P	4:C:612:PCW:H51	0.42	2.54	1	1
4:B:204:PCW:H221	4:B:208:PCW:H20	0.42	1.90	1	1
4:D:502:PCW:C48	4:D:508:PCW:H462	0.42	2.44	1	1
4:D:504:PCW:H351	4:D:504:PCW:O2	0.42	2.14	1	1
4:D:507:PCW:C35	5:D:513:17F:H10	0.42	2.45	1	1
4:A:404:PCW:H31	4:A:407:PCW:C3	0.42	2.44	2	1
1:C:584:PHE:O	1:C:588:LEU:HG	0.42	2.15	2	1
4:D:504:PCW:H272	5:D:513:17F:H69	0.42	1.91	2	1
4:B:211:PCW:H20	4:D:506:PCW:H231	0.42	1.85	3	1
4:A:411:PCW:C11	4:A:411:PCW:O31	0.42	2.67	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:513:17F:H59	5:D:513:17F:H62	0.42	1.64	10	2
1:A:348:GLU:O	1:A:352:LYS:HG3	0.42	2.15	7	2
5:A:410:17F:N1	5:A:410:17F:O10	0.42	2.52	5	1
4:A:417:PCW:C8	4:C:605:PCW:O2P	0.42	2.68	5	1
4:B:205:PCW:H172	4:B:207:PCW:C34	0.42	2.37	5	1
5:B:213:17F:H76	4:D:510:PCW:H441	0.42	1.89	5	1
1:C:462:LYS:HB3	4:C:602:PCW:C28	0.42	2.42	6	1
2:B:158:THR:OG1	4:B:212:PCW:H63	0.42	2.15	6	1
4:C:625:PCW:O31	4:C:625:PCW:H62	0.42	2.15	7	1
1:C:487:GLN:OE1	1:C:487:GLN:HA	0.42	2.14	8	1
4:C:610:PCW:H371	4:C:610:PCW:C19	0.42	2.33	8	1
4:B:202:PCW:H332	4:D:504:PCW:H31	0.42	1.92	8	1
1:C:466:GLU:OE2	4:C:602:PCW:H262	0.42	2.14	9	1
4:C:613:PCW:O4P	4:C:613:PCW:C3	0.42	2.66	9	1
4:B:201:PCW:H63	4:B:201:PCW:O11	0.42	2.13	9	1
4:A:417:PCW:H62	4:A:417:PCW:O31	0.42	2.14	10	1
4:B:201:PCW:C7	4:B:209:PCW:O2P	0.42	2.67	10	1
4:B:208:PCW:H52	5:B:214:17F:H18	0.42	1.91	10	1
4:A:403:PCW:C11	4:B:201:PCW:H122	0.42	2.43	1	1
4:A:405:PCW:C27	4:A:414:PCW:H241	0.42	2.45	1	1
4:B:205:PCW:O2P	5:B:214:17F:H12A	0.42	2.14	1	1
4:B:208:PCW:P	5:B:214:17F:N1	0.42	2.92	1	1
4:C:620:PCW:H20	5:C:631:17F:O10	0.42	2.14	2	1
4:B:201:PCW:O2	4:B:201:PCW:O4P	0.42	2.37	2	1
4:B:206:PCW:H63	4:B:206:PCW:C11	0.42	2.44	2	1
4:B:204:PCW:C12	4:B:212:PCW:H19	0.42	2.43	3	1
4:B:205:PCW:H11	5:B:214:17F:C1X	0.42	2.44	3	1
4:D:508:PCW:C3	4:D:508:PCW:P	0.42	3.08	3	1
4:B:203:PCW:H232	4:B:208:PCW:C11	0.42	2.44	4	1
4:B:204:PCW:H161	4:B:208:PCW:H262	0.42	1.91	6	2
4:A:403:PCW:H221	4:A:403:PCW:C17	0.42	2.41	6	1
4:B:206:PCW:H42	4:B:209:PCW:C8	0.42	2.44	6	1
4:B:206:PCW:O11	4:B:206:PCW:C7	0.42	2.68	6	1
4:C:606:PCW:H161	5:C:627:17F:H30	0.42	1.89	7	2
4:D:506:PCW:H441	5:D:513:17F:H47	0.42	1.90	7	1
4:B:203:PCW:C22	4:B:204:PCW:H19	0.42	2.44	8	1
4:D:510:PCW:C24	4:D:515:PCW:H482	0.42	2.33	8	1
4:A:401:PCW:C38	4:D:502:PCW:H231	0.42	2.44	9	1
4:D:504:PCW:C7	4:D:504:PCW:H352	0.42	2.45	9	1
4:C:603:PCW:C31	4:C:603:PCW:O3	0.42	2.67	10	1
4:C:606:PCW:H251	5:C:628:17F:H74	0.42	1.92	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:502:PCW:H471	4:D:508:PCW:C28	0.42	2.44	10	1
1:C:578:GLU:O	1:C:582:VAL:HG23	0.42	2.15	2	2
4:C:621:PCW:C16	4:D:516:PCW:H152	0.42	2.22	1	1
4:B:206:PCW:C12	5:B:213:17F:O10	0.42	2.68	1	1
3:D:452:CYS:HB2	3:D:459:LEU:HB2	0.42	1.90	1	1
4:D:508:PCW:H42	4:D:508:PCW:C3	0.42	2.28	1	1
4:C:605:PCW:C17	4:C:612:PCW:H132	0.42	2.35	2	1
4:B:204:PCW:H161	4:B:208:PCW:H221	0.42	1.84	3	1
4:B:210:PCW:H382	4:B:210:PCW:H411	0.42	1.67	5	2
4:D:506:PCW:O3P	4:D:510:PCW:H61	0.42	2.14	3	1
4:A:403:PCW:O31	4:A:403:PCW:C5	0.42	2.66	4	1
4:C:617:PCW:O1P	4:C:625:PCW:C7	0.42	2.68	4	1
4:D:506:PCW:H382	4:D:506:PCW:H411	0.42	1.57	4	2
4:D:507:PCW:H271	4:D:507:PCW:C47	0.42	2.45	4	1
4:A:414:PCW:H452	4:C:623:PCW:H483	0.42	1.92	5	1
4:C:612:PCW:H32	4:C:618:PCW:H2	0.42	1.91	5	1
4:B:204:PCW:H41	5:B:214:17F:H6A	0.42	1.90	5	1
4:C:605:PCW:H462	5:D:511:17F:C29	0.42	2.45	6	1
5:C:626:17F:H57	5:C:629:17F:C29	0.42	2.38	6	1
2:B:154:ASP:OD1	4:B:212:PCW:H82	0.42	2.15	6	1
4:B:210:PCW:O2P	4:D:506:PCW:C5	0.42	2.68	6	1
4:D:501:PCW:H382	4:D:501:PCW:H412	0.42	1.58	6	1
5:C:632:17F:H53	4:B:207:PCW:H181	0.42	1.91	7	1
4:B:202:PCW:H211	4:B:202:PCW:H181	0.42	1.64	7	1
5:A:410:17F:C40	4:C:610:PCW:H472	0.42	2.44	8	1
4:D:510:PCW:C42	4:D:516:PCW:H283	0.42	2.44	8	1
4:C:601:PCW:C47	4:C:601:PCW:H151	0.42	2.44	9	1
4:C:604:PCW:C25	5:D:514:17F:C41	0.42	2.97	9	1
4:C:607:PCW:C25	5:C:629:17F:H65	0.42	2.45	9	1
5:C:627:17F:C38	5:B:215:17F:H11	0.42	2.42	9	1
4:B:203:PCW:C28	5:B:214:17F:H57	0.42	2.45	10	1
4:A:408:PCW:O2	4:A:408:PCW:C36	0.42	2.68	1	1
4:C:606:PCW:H262	5:C:627:17F:C24	0.42	2.44	1	1
4:D:509:PCW:H51	4:D:509:PCW:O3P	0.42	2.14	1	1
5:C:627:17F:H47	5:C:628:17F:H35	0.42	1.90	2	1
4:B:202:PCW:O4P	4:D:507:PCW:C8	0.42	2.68	2	1
4:D:505:PCW:H82	4:D:509:PCW:O1P	0.42	2.13	3	1
1:A:297:LYS:O	1:A:301:LEU:HB2	0.42	2.14	4	2
4:D:501:PCW:H61	5:D:514:17F:C6	0.42	2.45	4	1
4:B:211:PCW:H241	4:D:503:PCW:H212	0.42	1.91	5	1
4:D:502:PCW:H472	4:D:508:PCW:H252	0.42	1.91	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:610:PCW:O1P	4:C:612:PCW:C7	0.42	2.67	6	1
4:B:206:PCW:H483	4:B:206:PCW:H282	0.42	1.91	6	1
4:D:508:PCW:H181	4:D:508:PCW:H212	0.42	1.60	6	1
4:A:401:PCW:H51	4:D:508:PCW:O31	0.42	2.14	7	1
4:C:606:PCW:H12	5:C:627:17F:O1	0.42	2.15	7	1
4:B:201:PCW:H11	4:B:201:PCW:O31	0.42	2.15	8	1
4:B:212:PCW:H462	5:D:514:17F:H40	0.42	1.92	9	1
4:A:403:PCW:C18	4:A:403:PCW:C39	0.42	2.97	10	1
4:A:411:PCW:H211	4:C:616:PCW:H472	0.42	1.92	10	1
4:B:204:PCW:H181	4:B:208:PCW:C20	0.42	2.45	10	1
4:A:408:PCW:H361	5:D:511:17F:O8	0.42	2.15	1	1
4:A:411:PCW:H481	4:D:504:PCW:H172	0.42	1.92	1	1
4:A:417:PCW:C11	4:A:417:PCW:O31	0.42	2.68	1	1
4:C:614:PCW:H212	4:C:614:PCW:H182	0.42	1.59	1	1
5:C:627:17F:O9	5:C:627:17F:P1	0.42	2.77	1	1
4:B:205:PCW:H162	4:B:207:PCW:C36	0.42	2.44	1	1
4:B:210:PCW:H281	4:B:211:PCW:C15	0.42	2.45	1	1
4:D:501:PCW:O4P	4:D:501:PCW:C8	0.42	2.67	1	3
1:A:341:ASN:O	1:A:345:ARG:HG3	0.42	2.15	2	1
5:C:630:17F:P1	5:C:630:17F:HN1	0.42	2.38	2	1
1:A:244:SER:HA	1:A:248:GLU:CG	0.42	2.44	3	1
4:C:606:PCW:C8	4:C:624:PCW:H281	0.42	2.44	3	1
4:B:206:PCW:H182	4:B:207:PCW:H322	0.42	1.91	3	1
4:C:615:PCW:H181	4:C:615:PCW:H211	0.42	1.65	4	1
4:D:507:PCW:H483	4:D:507:PCW:H262	0.42	1.92	4	1
1:A:388:SER:HB2	1:C:594:LYS:CE	0.42	2.45	5	1
4:C:605:PCW:C42	4:C:618:PCW:H141	0.42	2.40	5	1
4:C:609:PCW:C6	5:C:631:17F:O1	0.42	2.60	5	1
4:B:206:PCW:H63	4:B:209:PCW:H12	0.42	1.90	5	1
5:B:213:17F:C3	3:D:448:LYS:HG3	0.42	2.45	5	1
3:D:378:LEU:O	3:D:382:LEU:HG	0.42	2.15	5	1
4:D:501:PCW:C5	4:D:509:PCW:O31	0.42	2.68	5	1
4:A:403:PCW:H231	4:B:201:PCW:H181	0.42	1.91	6	1
4:A:411:PCW:O3	4:A:411:PCW:C31	0.42	2.68	6	1
4:D:502:PCW:C21	4:D:502:PCW:C17	0.42	2.97	6	1
4:B:201:PCW:C32	4:B:209:PCW:O4P	0.42	2.67	7	1
4:A:413:PCW:H382	4:C:611:PCW:C22	0.42	2.44	8	1
4:B:204:PCW:H231	4:B:208:PCW:H211	0.42	1.90	8	1
4:B:209:PCW:H172	4:B:209:PCW:C38	0.42	2.43	8	1
3:D:439:HIS:HB2	3:D:484:CYS:HB2	0.42	1.90	8	1
4:A:402:PCW:O31	4:A:402:PCW:H11	0.42	2.14	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:CE2	0.42	2.49	9	1
4:C:602:PCW:H422	5:C:626:17F:C24	0.42	2.45	10	1
4:A:408:PCW:C18	4:A:408:PCW:C14	0.42	2.90	1	1
5:A:409:17F:H1A	2:B:169:LYS:CD	0.42	2.45	1	1
4:B:208:PCW:H342	4:B:208:PCW:O2	0.42	2.15	1	1
3:D:360:VAL:HB	3:D:368:THR:O	0.42	2.14	1	1
4:D:503:PCW:O3	4:D:507:PCW:H372	0.42	2.14	1	1
4:D:508:PCW:C22	4:D:508:PCW:C26	0.42	2.95	9	2
4:D:501:PCW:H62	4:D:509:PCW:O2P	0.42	2.15	2	1
4:C:621:PCW:O3P	4:C:621:PCW:O31	0.42	2.38	3	1
5:C:632:17F:C37	5:C:632:17F:C32	0.42	2.97	3	1
5:B:214:17F:H30	5:B:214:17F:H39	0.42	1.92	3	1
4:C:608:PCW:C36	4:B:207:PCW:H281	0.42	2.42	4	1
4:B:208:PCW:H382	4:B:208:PCW:H422	0.42	1.91	4	1
4:D:508:PCW:C44	5:D:512:17F:H48	0.42	2.45	4	1
4:A:403:PCW:H251	4:B:201:PCW:H162	0.42	1.90	5	1
4:C:609:PCW:O3	4:C:609:PCW:C31	0.42	2.68	5	1
4:B:205:PCW:H212	4:B:205:PCW:H181	0.42	1.58	6	2
1:C:573:LEU:O	1:C:577:LEU:HB2	0.42	2.15	6	1
4:D:505:PCW:H211	4:D:505:PCW:H181	0.42	1.69	6	1
5:A:410:17F:C42	5:D:511:17F:H73	0.42	2.33	7	1
4:B:212:PCW:H341	4:D:505:PCW:C8	0.42	2.45	7	1
3:D:379:HIS:HB2	3:D:414:TRP:HB3	0.42	1.91	8	1
4:A:414:PCW:H31	4:C:613:PCW:H121	0.42	1.92	9	1
4:C:625:PCW:O31	4:C:625:PCW:H51	0.42	2.15	9	1
4:A:405:PCW:C41	4:A:414:PCW:H282	0.41	2.45	1	1
4:A:405:PCW:H411	4:A:405:PCW:H381	0.41	1.70	1	1
4:A:412:PCW:H182	4:A:412:PCW:H211	0.41	1.66	1	1
4:A:414:PCW:H412	4:A:414:PCW:H382	0.41	1.58	1	2
4:C:611:PCW:O3P	4:C:611:PCW:C31	0.41	2.68	8	2
4:D:516:PCW:H382	4:D:516:PCW:H411	0.41	1.52	2	2
4:A:404:PCW:H232	4:A:404:PCW:H171	0.41	1.90	3	1
4:A:417:PCW:H211	4:A:417:PCW:H182	0.41	1.67	3	1
4:C:610:PCW:C26	4:C:618:PCW:H452	0.41	2.40	3	1
1:A:244:SER:C	1:A:248:GLU:HB2	0.41	2.40	4	1
4:B:205:PCW:C16	4:B:207:PCW:H171	0.41	2.39	4	1
4:A:407:PCW:C7	4:A:407:PCW:H321	0.41	2.44	5	1
4:A:412:PCW:C31	4:C:624:PCW:H372	0.41	2.45	5	1
4:C:617:PCW:H431	5:C:631:17F:H50	0.41	1.92	5	1
4:B:203:PCW:P	4:B:203:PCW:C6	0.41	3.07	5	1
4:A:415:PCW:C39	4:D:515:PCW:H211	0.41	2.44	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:372:VAL:HG11	3:D:381:CYS:SG	0.41	2.55	6	1
4:C:608:PCW:C23	4:C:614:PCW:H381	0.41	2.45	7	1
4:B:212:PCW:H483	5:D:514:17F:H41	0.41	1.92	7	1
4:A:415:PCW:O2P	4:A:415:PCW:C5	0.41	2.68	8	1
4:C:610:PCW:H221	4:C:610:PCW:C44	0.41	2.44	8	1
4:C:603:PCW:C6	4:D:516:PCW:O2P	0.41	2.68	9	1
4:C:606:PCW:H442	4:C:608:PCW:C2	0.41	2.44	1	1
4:B:210:PCW:O3	4:B:210:PCW:C31	0.41	2.68	1	2
4:D:503:PCW:H31	4:D:507:PCW:H352	0.41	1.93	1	1
4:A:417:PCW:C26	4:C:621:PCW:H242	0.41	2.45	2	1
4:A:411:PCW:C27	4:B:202:PCW:H483	0.41	2.42	3	1
4:B:204:PCW:C3	4:B:208:PCW:C15	0.41	2.96	3	1
4:A:416:PCW:O2P	4:C:616:PCW:C8	0.41	2.68	4	1
4:C:609:PCW:O3P	4:C:609:PCW:O31	0.41	2.38	10	2
5:A:409:17F:H31	4:D:504:PCW:H361	0.41	1.92	5	1
4:B:205:PCW:H11	5:B:214:17F:H11	0.41	1.92	5	1
4:B:205:PCW:C22	4:B:207:PCW:H152	0.41	2.38	5	1
4:C:616:PCW:H282	4:B:202:PCW:H281	0.41	1.92	6	1
4:C:621:PCW:H271	4:D:509:PCW:C27	0.41	2.39	6	1
4:C:623:PCW:H412	4:C:624:PCW:C42	0.41	2.44	6	1
4:A:415:PCW:C36	4:C:616:PCW:H411	0.41	2.45	7	1
1:C:520:PRO:O	1:C:524:GLU:HG3	0.41	2.15	7	1
4:A:401:PCW:H31	4:D:508:PCW:H231	0.41	1.92	8	1
5:A:410:17F:H72	4:C:610:PCW:H471	0.41	1.91	8	1
4:A:413:PCW:H121	4:C:611:PCW:H171	0.41	1.90	8	1
5:C:628:17F:C10	5:C:628:17F:H56	0.41	2.46	8	1
4:D:506:PCW:H351	4:D:510:PCW:H39	0.41	1.90	8	1
4:A:415:PCW:H40	4:C:615:PCW:H172	0.41	1.92	9	1
4:C:621:PCW:H472	4:D:506:PCW:H272	0.41	1.91	9	1
4:B:206:PCW:C16	5:B:213:17F:H57	0.41	2.45	9	1
4:A:408:PCW:H261	4:D:504:PCW:H472	0.41	1.91	10	1
2:B:1:MET:HA	2:B:50:THR:HB	0.41	1.92	10	1
4:A:416:PCW:H211	4:A:416:PCW:H181	0.41	1.65	6	2
4:C:608:PCW:C27	5:B:214:17F:H54	0.41	2.45	1	1
5:C:627:17F:C39	5:C:628:17F:H62	0.41	2.43	2	1
2:B:78:PHE:O	2:B:111:MET:HA	0.41	2.15	2	1
4:B:206:PCW:C3	4:B:206:PCW:P	0.41	3.08	2	1
4:A:413:PCW:C42	4:C:611:PCW:H212	0.41	2.43	3	1
4:D:503:PCW:H411	4:D:503:PCW:H381	0.41	1.70	3	1
4:D:507:PCW:C35	5:D:513:17F:O8	0.41	2.68	3	1
5:D:514:17F:H30	5:D:514:17F:H63	0.41	1.91	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:202:PCW:C48	4:D:504:PCW:H281	0.41	2.44	5	1
4:A:405:PCW:O2P	4:B:203:PCW:H322	0.41	2.15	9	2
4:A:415:PCW:C48	5:D:513:17F:C22	0.41	2.98	7	1
2:B:68:ARG:O	2:B:72:MET:HB2	0.41	2.16	7	1
4:B:203:PCW:H271	5:B:214:17F:H20	0.41	1.90	7	1
4:B:210:PCW:C27	4:B:211:PCW:H231	0.41	2.28	7	1
4:A:405:PCW:C39	5:D:512:17F:C38	0.41	2.95	8	1
4:C:603:PCW:H252	4:D:515:PCW:C19	0.41	2.45	9	1
2:B:14:VAL:N	6:B:216:GNP:O2B	0.41	2.51	9	1
4:A:414:PCW:C6	4:C:624:PCW:H2	0.41	2.44	10	1
4:B:206:PCW:H32	5:B:213:17F:C1	0.41	2.45	10	1
4:A:404:PCW:H61	4:B:210:PCW:C33	0.41	2.45	1	1
5:C:632:17F:O10	5:C:632:17F:C6	0.41	2.56	6	2
5:C:632:17F:O8	5:C:632:17F:H5	0.41	2.13	1	1
4:D:503:PCW:H372	4:D:507:PCW:P	0.41	2.55	1	1
1:A:298:LEU:O	1:A:302:GLY:HA3	0.41	2.16	2	1
5:A:410:17F:C31	4:D:502:PCW:H162	0.41	2.45	2	1
4:C:621:PCW:C19	5:C:628:17F:C1X	0.41	2.95	2	1
4:B:206:PCW:H432	5:B:213:17F:C42	0.41	2.42	2	1
4:C:608:PCW:C40	4:C:614:PCW:H441	0.41	2.45	3	1
4:B:208:PCW:C44	4:B:212:PCW:H283	0.41	2.42	3	2
4:D:501:PCW:H39	4:D:509:PCW:H442	0.41	1.90	3	1
5:D:514:17F:H67	5:D:514:17F:H36	0.41	1.91	3	1
4:C:604:PCW:H461	4:C:624:PCW:C28	0.41	2.23	4	1
4:A:402:PCW:H412	4:A:402:PCW:H382	0.41	1.63	5	1
4:D:503:PCW:H481	4:D:515:PCW:H281	0.41	1.92	5	1
4:A:401:PCW:H51	4:D:508:PCW:C31	0.41	2.46	6	1
1:C:469:LEU:HB3	1:C:473:LYS:NZ	0.41	2.31	6	1
2:B:116:ASN:ND2	6:B:216:GNP:N7	0.41	2.68	6	1
1:A:273:ARG:O	1:A:277:GLU:HG3	0.41	2.15	8	1
4:A:401:PCW:H51	4:D:508:PCW:H321	0.41	1.91	8	1
5:C:627:17F:H55	5:B:213:17F:C23	0.41	2.45	8	1
4:B:202:PCW:H172	4:D:504:PCW:C12	0.41	2.45	8	1
4:D:508:PCW:H121	5:D:512:17F:C17	0.41	2.45	8	1
4:D:510:PCW:H411	4:D:510:PCW:H382	0.41	1.57	8	1
4:B:205:PCW:H141	4:B:206:PCW:H182	0.41	1.92	9	1
4:B:209:PCW:H412	4:B:209:PCW:H381	0.41	1.68	9	1
4:C:623:PCW:O31	4:C:623:PCW:C4	0.41	2.66	10	1
4:A:403:PCW:H211	4:B:201:PCW:C18	0.41	2.36	1	1
4:A:405:PCW:H462	4:A:414:PCW:H222	0.41	1.91	1	1
5:A:410:17F:H73	4:C:610:PCW:C47	0.41	2.45	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:604:PCW:C17	4:D:509:PCW:H283	0.41	2.44	1	1
4:D:507:PCW:H181	4:D:507:PCW:H212	0.41	1.57	1	1
4:A:401:PCW:H462	4:C:613:PCW:H241	0.41	1.91	3	1
5:A:410:17F:C41	5:D:511:17F:H61	0.41	2.45	3	1
4:C:619:PCW:O31	4:C:619:PCW:P	0.41	2.78	3	1
4:C:622:PCW:H412	4:C:623:PCW:H241	0.41	1.93	3	1
4:B:205:PCW:C17	4:B:207:PCW:H151	0.41	2.46	3	1
4:D:507:PCW:H211	4:D:507:PCW:C16	0.41	2.45	9	2
4:A:417:PCW:H421	4:C:605:PCW:H451	0.41	1.93	4	1
4:C:604:PCW:H452	4:C:606:PCW:H182	0.41	1.93	5	1
4:D:502:PCW:O31	4:D:502:PCW:H341	0.41	2.16	5	1
4:C:610:PCW:H20	4:C:610:PCW:H432	0.41	1.92	6	1
4:A:401:PCW:H361	4:D:502:PCW:C20	0.41	2.45	7	1
4:C:603:PCW:H271	4:D:515:PCW:C18	0.41	2.33	7	1
4:C:609:PCW:H151	5:C:631:17F:C34	0.41	2.46	7	1
4:C:617:PCW:O1P	4:C:625:PCW:C8	0.41	2.69	8	1
4:C:617:PCW:C25	4:D:506:PCW:H442	0.41	2.44	8	1
4:C:625:PCW:H411	4:C:625:PCW:H381	0.41	1.65	8	1
1:C:572:GLY:O	1:C:576:VAL:HB	0.41	2.15	10	1
5:D:512:17F:H62	5:D:512:17F:H59	0.41	1.57	10	1
4:A:404:PCW:H152	4:B:210:PCW:H242	0.41	1.93	1	1
4:C:606:PCW:O31	4:C:606:PCW:P	0.41	2.78	3	2
4:C:619:PCW:C14	5:C:632:17F:O9	0.41	2.67	1	1
4:D:508:PCW:H222	4:D:508:PCW:C28	0.41	2.41	1	1
4:C:604:PCW:C39	5:C:627:17F:H41	0.41	2.45	2	1
4:B:207:PCW:H11	4:B:209:PCW:C7	0.41	2.45	2	1
4:B:208:PCW:C45	4:B:212:PCW:H452	0.41	2.45	2	1
4:C:602:PCW:C26	5:C:629:17F:H77	0.41	2.39	3	1
4:B:210:PCW:C31	4:B:210:PCW:O4P	0.41	2.68	3	1
4:D:507:PCW:H161	5:D:513:17F:H19A	0.41	1.91	3	1
5:D:514:17F:O9	5:D:514:17F:C7	0.41	2.68	3	2
4:A:405:PCW:H461	4:A:414:PCW:H281	0.41	1.91	4	1
4:A:408:PCW:H211	4:B:202:PCW:C28	0.41	2.46	4	1
1:A:348:GLU:OE1	1:C:429:ASN:HB2	0.41	2.16	5	1
4:B:201:PCW:H411	4:B:201:PCW:H382	0.41	1.67	5	1
1:A:251:LYS:O	1:A:254:VAL:HG12	0.41	2.15	6	1
4:D:503:PCW:H171	4:D:507:PCW:H40	0.41	1.91	6	1
4:D:508:PCW:C5	4:D:508:PCW:O11	0.41	2.69	6	1
4:C:607:PCW:H63	4:C:624:PCW:C26	0.41	2.45	7	1
4:A:403:PCW:H252	4:B:201:PCW:H39	0.41	1.92	8	1
4:A:413:PCW:C7	4:C:616:PCW:H421	0.41	2.46	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:212:PCW:C21	5:D:514:17F:H10	0.41	2.42	8	1
4:D:507:PCW:O31	4:D:507:PCW:O3P	0.41	2.39	10	1
5:A:409:17F:C6	2:B:172:LYS:HD2	0.41	2.45	1	1
4:C:608:PCW:H181	4:C:614:PCW:H352	0.41	1.89	1	1
4:C:611:PCW:C47	4:C:611:PCW:H252	0.41	2.45	1	1
4:C:617:PCW:H132	4:C:625:PCW:H132	0.41	1.92	1	1
4:B:208:PCW:H483	4:B:212:PCW:C24	0.41	2.44	1	1
4:B:210:PCW:H461	5:D:513:17F:H20	0.41	1.90	1	1
4:D:505:PCW:C20	4:D:510:PCW:H362	0.41	2.46	1	1
4:D:515:PCW:H212	4:D:515:PCW:H182	0.41	1.71	1	1
4:C:621:PCW:H212	4:C:621:PCW:H182	0.41	1.67	2	2
4:C:604:PCW:C28	5:B:213:17F:H52	0.41	2.45	3	1
4:C:609:PCW:H31	5:C:631:17F:O9	0.41	2.15	3	1
4:B:206:PCW:O2P	4:B:206:PCW:H32	0.41	2.15	3	1
4:B:212:PCW:H442	5:D:514:17F:H75	0.41	1.92	3	1
4:B:212:PCW:C35	5:B:214:17F:H37	0.41	2.44	3	1
4:C:610:PCW:C24	4:C:618:PCW:H442	0.41	2.45	4	1
4:B:205:PCW:O4P	4:B:205:PCW:C8	0.41	2.69	4	1
4:A:401:PCW:H332	4:D:502:PCW:H19	0.41	1.92	5	1
4:A:401:PCW:C32	4:D:502:PCW:H172	0.41	2.45	5	1
5:A:410:17F:O10	5:A:410:17F:H2	0.41	2.16	5	1
4:C:606:PCW:H152	5:C:627:17F:H11A	0.41	1.93	5	1
4:C:614:PCW:C14	5:C:632:17F:O7	0.41	2.69	5	1
4:C:617:PCW:H342	4:C:625:PCW:H341	0.41	1.93	5	1
2:B:25:GLN:HG2	2:B:40:TYR:HE2	0.41	1.75	5	1
4:C:603:PCW:H211	4:C:603:PCW:C17	0.41	2.32	6	1
4:B:201:PCW:H412	4:B:207:PCW:H381	0.41	1.92	6	1
4:A:401:PCW:H322	4:D:508:PCW:C37	0.41	2.46	7	1
4:A:403:PCW:H131	4:B:201:PCW:H141	0.41	1.93	8	1
4:C:604:PCW:H251	5:D:514:17F:C42	0.41	2.36	8	1
4:C:620:PCW:C28	5:C:631:17F:H30	0.41	2.46	9	2
4:A:404:PCW:C24	4:B:210:PCW:H232	0.41	2.35	9	1
4:C:602:PCW:H481	5:C:629:17F:C25	0.41	2.42	9	1
4:B:202:PCW:H482	4:D:504:PCW:H281	0.41	1.93	10	1
4:B:203:PCW:C24	4:B:204:PCW:H171	0.41	2.43	10	1
4:A:403:PCW:H82	4:B:209:PCW:H321	0.41	1.92	1	1
4:A:405:PCW:C24	4:A:414:PCW:H262	0.41	2.46	1	1
4:A:408:PCW:C41	5:D:511:17F:H9A	0.41	2.46	1	1
4:C:623:PCW:O31	4:C:623:PCW:H41	0.41	2.16	1	1
2:B:157:TYR:CD2	4:D:503:PCW:H61	0.41	2.50	1	1
4:B:201:PCW:H51	4:B:201:PCW:C33	0.41	2.45	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:501:PCW:H211	5:D:511:17F:C18	0.41	2.46	1	1
1:A:312:HIS:HE1	1:C:465:GLU:HB2	0.41	1.76	4	1
4:A:405:PCW:C3	5:D:512:17F:H31	0.41	2.46	4	1
5:C:627:17F:H75	4:D:516:PCW:H462	0.41	1.93	4	1
4:A:406:PCW:C43	4:B:211:PCW:H382	0.41	2.45	5	1
4:A:407:PCW:C34	4:A:407:PCW:O31	0.41	2.68	5	1
5:A:409:17F:C23	4:D:503:PCW:C40	0.41	2.98	5	1
4:A:411:PCW:H281	4:B:202:PCW:H481	0.41	1.91	5	1
4:C:605:PCW:H211	4:C:605:PCW:H182	0.41	1.66	5	1
4:C:620:PCW:H262	4:C:621:PCW:C6	0.41	2.31	5	1
5:C:627:17F:H46	5:C:628:17F:H73	0.41	1.91	5	1
4:B:202:PCW:H342	4:D:504:PCW:H12	0.41	1.93	5	1
4:B:206:PCW:H222	4:B:206:PCW:H182	0.41	1.92	6	1
4:A:403:PCW:C31	4:A:406:PCW:H351	0.41	2.45	7	1
4:A:405:PCW:H222	4:A:405:PCW:C17	0.41	2.46	7	1
4:C:603:PCW:C23	4:D:515:PCW:H351	0.41	2.45	7	1
4:C:624:PCW:C22	4:C:624:PCW:C26	0.41	2.95	7	1
4:B:204:PCW:H231	4:B:208:PCW:C26	0.41	2.45	7	1
4:D:506:PCW:O31	4:D:506:PCW:H12	0.41	2.16	7	1
4:D:508:PCW:H442	5:D:512:17F:C28	0.41	2.45	7	1
4:C:602:PCW:H332	5:B:214:17F:H60	0.41	1.91	8	1
4:B:212:PCW:H341	5:B:213:17F:O8	0.41	2.16	8	1
4:D:510:PCW:H422	4:D:516:PCW:H283	0.41	1.91	8	1
4:B:206:PCW:C16	5:B:213:17F:C31	0.41	2.99	9	1
4:B:212:PCW:H471	5:D:514:17F:H75	0.41	1.91	9	1
4:D:507:PCW:C35	5:D:513:17F:H8A	0.41	2.45	9	1
4:B:205:PCW:O1P	4:B:205:PCW:C2	0.41	2.65	10	1
4:B:212:PCW:C39	5:B:213:17F:H50	0.41	2.45	10	1
4:A:415:PCW:H371	4:D:515:PCW:H152	0.41	1.93	1	1
1:C:451:LYS:HB3	4:C:601:PCW:H283	0.41	1.92	1	1
4:B:205:PCW:H141	4:B:207:PCW:H342	0.41	1.92	1	1
4:B:211:PCW:H371	4:B:211:PCW:H142	0.41	1.92	1	1
5:D:512:17F:H40	5:D:512:17F:H36	0.41	1.69	1	1
1:A:297:LYS:HG3	1:C:477:LEU:HD21	0.41	1.92	2	1
4:A:403:PCW:H261	4:B:201:PCW:H371	0.41	1.93	2	1
4:A:408:PCW:H321	5:A:409:17F:C20	0.41	2.46	2	1
4:A:408:PCW:H471	5:D:511:17F:H29	0.41	1.93	2	1
5:A:409:17F:O10	5:A:409:17F:H4	0.41	2.15	9	2
4:C:615:PCW:C19	4:C:616:PCW:H461	0.41	2.45	2	1
4:B:212:PCW:H222	5:D:514:17F:H36	0.41	1.93	2	1
4:A:403:PCW:C32	4:B:209:PCW:H352	0.41	2.46	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:404:PCW:H272	4:D:507:PCW:H482	0.41	1.93	3	1
4:A:404:PCW:C41	4:A:404:PCW:H372	0.41	2.46	3	1
4:A:408:PCW:C22	4:A:408:PCW:C18	0.41	2.84	3	1
5:B:213:17F:H43	4:D:509:PCW:H172	0.41	1.92	3	1
4:D:501:PCW:C8	4:D:501:PCW:O4P	0.41	2.69	10	2
4:A:403:PCW:C31	4:A:403:PCW:O3	0.41	2.69	4	1
4:A:411:PCW:H161	4:A:415:PCW:C33	0.41	2.44	4	1
1:C:564:PRO:O	1:C:568:ASP:HB2	0.41	2.16	4	1
4:C:607:PCW:H51	4:C:607:PCW:O3P	0.41	2.15	4	1
5:C:626:17F:H35	5:C:626:17F:H39	0.41	1.64	4	1
5:B:215:17F:H36	5:B:215:17F:H40	0.41	1.65	4	1
4:A:403:PCW:C27	4:B:201:PCW:H371	0.41	2.46	5	1
4:A:404:PCW:O11	4:B:210:PCW:H142	0.41	2.15	5	1
1:C:412:PHE:O	1:C:415:LEU:HB3	0.41	2.16	5	1
4:C:601:PCW:H412	4:C:601:PCW:H381	0.41	1.66	5	1
2:B:128:LYS:HE2	4:D:503:PCW:O1P	0.41	2.16	5	1
4:B:202:PCW:H19	4:D:504:PCW:O11	0.41	2.16	6	1
4:B:204:PCW:C12	4:B:208:PCW:H362	0.41	2.46	6	1
4:B:206:PCW:C12	5:B:213:17F:C18	0.41	2.99	6	1
4:B:212:PCW:C40	5:D:514:17F:H59	0.41	2.46	6	1
4:D:501:PCW:C45	5:D:514:17F:H47	0.41	2.46	6	1
1:C:543:ARG:HA	1:C:546:GLU:HB2	0.41	1.93	7	1
4:B:204:PCW:H251	4:B:208:PCW:C28	0.41	2.37	7	1
4:B:212:PCW:H32	5:D:514:17F:O2	0.41	2.16	7	1
4:B:212:PCW:H39	5:D:514:17F:H63	0.41	1.93	7	1
4:D:507:PCW:C33	5:D:513:17F:O8	0.41	2.68	7	1
4:A:402:PCW:H362	4:B:210:PCW:C44	0.41	2.46	8	1
4:A:407:PCW:H371	4:B:211:PCW:C14	0.41	2.44	8	1
4:A:407:PCW:C13	4:A:407:PCW:O31	0.41	2.68	8	1
4:C:613:PCW:H411	4:C:613:PCW:H381	0.41	1.64	8	1
4:B:211:PCW:C12	4:B:211:PCW:H351	0.41	2.46	8	1
4:D:501:PCW:H61	5:D:514:17F:C1Y	0.41	2.46	8	1
4:A:404:PCW:C11	4:B:210:PCW:H152	0.41	2.45	9	1
4:C:605:PCW:H482	5:D:511:17F:H78	0.41	1.93	9	1
4:C:615:PCW:H371	4:C:615:PCW:H412	0.41	1.93	9	1
4:B:206:PCW:H131	4:B:206:PCW:H341	0.41	1.92	9	1
4:A:407:PCW:H381	4:A:407:PCW:H412	0.41	1.59	10	1
5:C:628:17F:O10	5:C:628:17F:O7	0.41	2.39	10	1
4:B:211:PCW:H19	4:D:505:PCW:C41	0.41	2.46	10	1
4:B:212:PCW:O2	4:B:212:PCW:P	0.41	2.79	10	1
3:D:358:ILE:O	3:D:369:VAL:HG13	0.41	2.15	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:608:PCW:C28	5:B:214:17F:H54	0.41	2.45	1	1
5:C:630:17F:H39	5:C:630:17F:H36	0.41	1.63	1	1
4:C:604:PCW:H41	5:C:628:17F:O2	0.41	2.16	2	1
4:C:605:PCW:H182	4:C:605:PCW:H211	0.41	1.68	2	1
5:C:627:17F:C27	5:C:628:17F:H39	0.41	2.39	2	1
2:B:49:GLU:HA	3:D:471:LYS:HE3	0.41	1.93	2	1
4:D:503:PCW:O31	4:D:510:PCW:H82	0.41	2.16	2	1
4:D:507:PCW:H471	5:D:513:17F:C1Z	0.41	2.46	2	1
4:D:508:PCW:C6	5:D:512:17F:H6	0.41	2.46	9	2
4:A:404:PCW:H152	4:B:210:PCW:H221	0.41	1.93	3	1
4:C:602:PCW:C36	5:B:214:17F:H67	0.41	2.19	3	1
4:C:603:PCW:H231	4:C:603:PCW:C47	0.41	2.38	3	1
4:B:204:PCW:H412	4:B:204:PCW:H382	0.41	1.74	3	1
5:B:214:17F:O10	5:B:214:17F:H4A	0.41	2.16	3	1
1:A:264:LYS:NZ	1:C:513:ALA:HB2	0.41	2.30	4	1
4:A:405:PCW:H381	4:A:405:PCW:H411	0.41	1.70	4	1
4:A:405:PCW:H352	5:D:512:17F:H59	0.41	1.92	4	1
4:B:202:PCW:C11	4:B:202:PCW:H73	0.41	2.46	4	1
4:C:616:PCW:O31	4:C:616:PCW:N	0.41	2.54	5	1
4:C:619:PCW:O1P	4:C:620:PCW:C7	0.41	2.68	6	1
4:C:620:PCW:H451	5:B:215:17F:C37	0.41	2.46	6	1
4:A:407:PCW:C42	4:B:211:PCW:H212	0.41	2.45	7	1
4:C:614:PCW:C48	4:B:206:PCW:H271	0.41	2.45	7	1
1:A:263:LYS:O	1:A:267:GLU:HG3	0.41	2.15	8	1
4:A:403:PCW:H2	4:B:209:PCW:H331	0.41	1.92	8	1
4:B:212:PCW:H63	5:B:213:17F:O5	0.41	2.16	8	1
4:A:413:PCW:C44	4:C:611:PCW:H162	0.41	2.45	9	1
4:A:407:PCW:H472	5:C:631:17F:H53	0.41	1.91	10	1
4:C:608:PCW:H471	4:B:205:PCW:H232	0.41	1.91	10	1
5:C:632:17F:H52	4:B:207:PCW:H172	0.41	1.91	10	1
4:B:203:PCW:C39	4:B:203:PCW:H142	0.41	2.46	10	1
4:B:204:PCW:C13	4:B:208:PCW:C15	0.41	2.95	10	1
4:B:208:PCW:H442	4:B:212:PCW:C27	0.41	2.42	10	1
4:B:212:PCW:H40	5:B:213:17F:H46	0.41	1.92	10	1
4:C:612:PCW:C43	4:C:618:PCW:C39	0.40	2.95	1	1
4:A:401:PCW:H481	4:C:613:PCW:C47	0.40	2.38	2	1
4:C:607:PCW:O31	4:C:607:PCW:O3P	0.40	2.39	2	1
4:A:404:PCW:H31	4:A:407:PCW:C12	0.40	2.47	3	1
4:C:620:PCW:C41	5:B:215:17F:H58	0.40	2.45	3	1
4:D:508:PCW:C6	5:D:512:17F:H4A	0.40	2.46	3	1
1:C:413:SER:O	1:C:417:GLU:HG3	0.40	2.16	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:611:PCW:O4P	4:C:611:PCW:H322	0.40	2.16	4	1
4:C:620:PCW:H451	5:B:215:17F:H67	0.40	1.91	4	1
4:B:201:PCW:H411	4:B:201:PCW:H381	0.40	1.68	4	1
4:A:417:PCW:C21	4:C:603:PCW:H161	0.40	2.39	5	1
1:A:266:GLN:O	1:A:270:GLU:HG2	0.40	2.16	6	1
4:A:404:PCW:H242	4:B:210:PCW:C20	0.40	2.46	6	1
5:A:410:17F:H75	4:C:612:PCW:H241	0.40	1.92	6	1
4:C:611:PCW:H51	4:C:617:PCW:O11	0.40	2.16	6	1
4:B:203:PCW:O3	4:B:203:PCW:O31	0.40	2.39	6	1
4:B:205:PCW:H19	4:B:206:PCW:H242	0.40	1.92	6	1
4:C:607:PCW:C22	5:C:626:17F:H10A	0.40	2.46	7	1
4:A:408:PCW:C3	4:A:408:PCW:H351	0.40	2.45	8	1
4:A:405:PCW:H372	4:B:203:PCW:H39	0.40	1.92	9	1
4:A:406:PCW:H40	4:D:505:PCW:C40	0.40	2.46	9	1
4:B:212:PCW:O31	5:D:514:17F:H4A	0.40	2.16	9	1
1:C:525:LEU:O	1:C:529:LEU:HG	0.40	2.16	10	1
4:C:612:PCW:C20	5:D:511:17F:H48	0.40	2.46	10	1
4:B:204:PCW:C43	4:B:212:PCW:H252	0.40	2.46	10	1
4:B:206:PCW:O31	4:D:505:PCW:H52	0.40	2.17	10	1
4:B:210:PCW:C25	4:D:503:PCW:H252	0.40	2.44	10	1
5:B:214:17F:C2	5:B:214:17F:C4	0.40	2.99	10	1
4:A:415:PCW:O2	4:C:616:PCW:H422	0.40	2.16	1	1
4:C:604:PCW:H432	4:C:606:PCW:H221	0.40	1.92	2	1
4:C:606:PCW:H42	4:C:624:PCW:H20	0.40	1.93	2	1
4:C:608:PCW:H412	5:C:632:17F:H60	0.40	1.94	2	1
4:C:617:PCW:P	4:C:625:PCW:H42	0.40	2.55	2	1
4:A:402:PCW:H52	4:D:507:PCW:C12	0.40	2.45	3	1
4:C:617:PCW:H442	4:C:625:PCW:C28	0.40	2.46	3	1
4:C:617:PCW:C44	4:C:625:PCW:H282	0.40	2.46	3	1
4:C:606:PCW:H232	5:C:627:17F:H37	0.40	1.94	4	1
4:D:504:PCW:H41	4:D:504:PCW:C2	0.40	2.47	4	1
4:A:403:PCW:H73	4:A:406:PCW:C37	0.40	2.42	5	1
4:A:403:PCW:C7	4:A:406:PCW:C37	0.40	2.99	5	1
4:C:617:PCW:H242	4:D:506:PCW:H451	0.40	1.92	5	1
5:C:629:17F:C1	5:C:629:17F:C4	0.40	2.97	5	1
2:B:82:PHE:HE2	2:B:113:LEU:HG	0.40	1.75	5	1
2:B:135:ARG:NH2	4:D:509:PCW:H341	0.40	2.31	5	1
4:A:403:PCW:H211	4:B:201:PCW:C21	0.40	2.46	6	1
4:A:407:PCW:H411	4:A:407:PCW:C28	0.40	2.44	7	1
4:A:416:PCW:P	4:C:616:PCW:H52	0.40	2.56	7	1
4:B:202:PCW:H362	4:B:202:PCW:O2	0.40	2.10	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:416:ARG:HA	1:C:419:LEU:HD12	0.40	1.93	9	1
1:C:453:GLN:HB2	1:C:454:PRO:CD	0.40	2.47	9	1
1:A:380:GLU:O	1:A:384:VAL:HG23	0.40	2.16	10	1
4:A:402:PCW:H351	4:D:507:PCW:H232	0.40	1.92	10	1
4:A:402:PCW:H261	4:A:413:PCW:H461	0.40	1.91	10	1
4:A:403:PCW:O3	4:A:403:PCW:C31	0.40	2.68	1	1
4:B:208:PCW:C6	5:B:214:17F:O9	0.40	2.66	1	1
4:C:606:PCW:H232	5:C:627:17F:H38	0.40	1.93	2	1
5:C:632:17F:H36	5:C:632:17F:H39	0.40	1.58	2	2
4:A:415:PCW:C37	4:C:616:PCW:C40	0.40	2.99	3	1
5:C:627:17F:H43	5:C:628:17F:C23	0.40	2.32	3	1
4:A:414:PCW:H382	4:A:414:PCW:H412	0.40	1.59	4	1
4:B:202:PCW:C20	4:D:504:PCW:H271	0.40	2.46	4	1
1:A:237:GLU:O	1:A:241:GLN:HG3	0.40	2.16	5	1
4:C:615:PCW:O11	4:D:515:PCW:H151	0.40	2.17	5	1
4:C:616:PCW:O31	4:C:616:PCW:C7	0.40	2.68	5	1
4:C:620:PCW:C18	5:C:631:17F:H19A	0.40	2.46	5	1
5:B:213:17F:C22	4:D:510:PCW:H471	0.40	2.46	5	1
4:C:619:PCW:O3P	4:C:619:PCW:C31	0.40	2.69	6	1
2:B:163:ILE:HG22	2:B:167:LYS:HE2	0.40	1.92	6	1
4:B:209:PCW:O1P	4:B:209:PCW:C5	0.40	2.68	6	1
4:A:416:PCW:H122	5:C:630:17F:C10	0.40	2.46	7	1
5:A:410:17F:H75	4:D:501:PCW:H281	0.40	1.93	8	1
4:A:404:PCW:C3	4:A:404:PCW:P	0.40	3.10	9	1
4:A:411:PCW:C14	4:A:415:PCW:C33	0.40	2.80	9	1
4:A:415:PCW:H361	4:D:515:PCW:H152	0.40	1.93	9	1
1:A:247:LEU:HA	1:A:250:VAL:HG12	0.40	1.93	10	1
4:A:417:PCW:H281	4:D:509:PCW:C28	0.40	2.41	10	1
1:C:511:VAL:HA	1:C:514:LEU:HD12	0.40	1.93	10	1
4:B:202:PCW:H482	4:D:504:PCW:C28	0.40	2.46	10	1
4:B:202:PCW:H181	4:B:202:PCW:H211	0.40	1.67	10	1
4:B:204:PCW:H381	4:B:204:PCW:H412	0.40	1.65	10	1
3:D:399:PHE:CE2	3:D:429:ASP:HB3	0.40	2.51	10	1
4:D:501:PCW:H481	4:D:509:PCW:H272	0.40	1.92	10	1
4:A:405:PCW:C35	5:D:512:17F:H62	0.40	2.43	1	1
5:A:409:17F:C28	5:D:511:17F:H33	0.40	2.46	1	1
4:B:207:PCW:C40	4:B:209:PCW:H161	0.40	2.47	1	1
4:A:404:PCW:H12	4:A:407:PCW:H31	0.40	1.93	2	1
4:A:415:PCW:H11	4:C:616:PCW:C40	0.40	2.46	2	1
4:A:403:PCW:H231	4:A:403:PCW:C15	0.40	2.45	3	1
4:A:407:PCW:C42	4:B:211:PCW:C46	0.40	2.98	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:621:PCW:H472	4:D:506:PCW:C27	0.40	2.47	3	1
4:A:414:PCW:H182	4:A:414:PCW:H211	0.40	1.66	4	1
4:A:414:PCW:C44	4:C:623:PCW:H462	0.40	2.46	4	1
4:C:608:PCW:C45	4:B:207:PCW:H20	0.40	2.46	4	1
2:B:16:LYS:N	6:B:216:GNP:O1B	0.40	2.54	4	2
4:D:509:PCW:H432	4:D:510:PCW:P	0.40	2.55	4	1
4:C:605:PCW:H63	5:C:630:17F:N1	0.40	2.31	5	1
4:C:607:PCW:H63	4:C:624:PCW:H271	0.40	1.93	5	1
4:B:206:PCW:H51	4:B:207:PCW:C8	0.40	2.46	5	1
3:D:464:ARG:HA	3:D:470:TYR:O	0.40	2.17	5	1
5:D:514:17F:O10	5:D:514:17F:C20	0.40	2.68	5	1
4:C:603:PCW:H62	5:C:628:17F:O5	0.40	2.16	6	1
4:C:605:PCW:O31	4:C:612:PCW:C6	0.40	2.68	6	1
4:B:204:PCW:C3	4:B:208:PCW:C13	0.40	2.99	6	1
4:B:210:PCW:H11	4:D:503:PCW:C12	0.40	2.45	6	1
4:D:505:PCW:H281	4:D:509:PCW:H452	0.40	1.94	6	1
4:B:212:PCW:H231	5:D:514:17F:C10	0.40	2.47	7	1
4:A:412:PCW:C26	4:B:203:PCW:H481	0.40	2.47	8	1
4:C:618:PCW:O31	4:C:618:PCW:C1	0.40	2.58	8	1
4:D:506:PCW:H322	4:D:510:PCW:H372	0.40	1.94	8	1
5:D:512:17F:H11A	5:D:514:17F:H8	0.40	1.93	8	1
4:C:612:PCW:H31	4:C:618:PCW:C3	0.40	2.46	9	1
2:B:112:VAL:HG22	2:B:140:PRO:HG2	0.40	1.92	9	1
4:A:402:PCW:H62	5:D:513:17F:O5	0.40	2.15	10	1
4:A:415:PCW:C48	4:C:617:PCW:H283	0.40	2.40	10	1
4:C:606:PCW:H381	4:C:606:PCW:H412	0.40	1.55	10	1
4:C:614:PCW:H272	5:C:632:17F:C26	0.40	2.46	10	1
4:B:206:PCW:H31	4:B:206:PCW:O2P	0.40	2.16	10	1
4:C:614:PCW:C18	5:C:632:17F:C22	0.40	3.00	1	1
4:B:204:PCW:H182	4:B:208:PCW:H181	0.40	1.94	1	1
4:B:206:PCW:O3	5:B:213:17F:H4	0.40	2.16	1	1
4:B:208:PCW:O11	4:B:208:PCW:H62	0.40	2.16	1	1
5:D:512:17F:H12	5:D:512:17F:C24	0.40	2.33	1	1
4:C:610:PCW:C8	4:C:623:PCW:H142	0.40	2.47	2	1
4:C:622:PCW:O3	4:C:622:PCW:C31	0.40	2.69	2	1
4:D:502:PCW:O3P	4:D:502:PCW:C7	0.40	2.68	2	1
4:C:606:PCW:H51	4:C:624:PCW:H19	0.40	1.94	3	1
4:B:203:PCW:H251	4:B:204:PCW:C18	0.40	2.46	3	1
4:C:610:PCW:H162	4:C:618:PCW:C17	0.40	2.38	4	1
5:C:630:17F:H36	5:C:630:17F:H39	0.40	1.57	4	1
4:D:501:PCW:H332	5:D:512:17F:C21	0.40	2.46	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:507:PCW:H31	5:D:513:17F:H76	0.40	1.93	4	1
1:A:316:LEU:HD13	4:C:601:PCW:C44	0.40	2.46	5	1
4:D:505:PCW:H452	4:D:506:PCW:C25	0.40	2.46	5	1
5:A:410:17F:C1Y	4:D:502:PCW:H211	0.40	2.36	6	1
4:A:415:PCW:C40	4:D:515:PCW:H211	0.40	2.47	6	1
4:C:609:PCW:O1P	4:C:609:PCW:C5	0.40	2.68	6	1
4:C:624:PCW:P	4:C:624:PCW:O2	0.40	2.80	6	1
4:B:206:PCW:C6	4:B:206:PCW:H322	0.40	2.43	6	1
4:D:505:PCW:H381	4:D:505:PCW:H411	0.40	1.67	6	1
4:A:401:PCW:H361	4:D:502:PCW:H20	0.40	1.94	7	1
4:B:212:PCW:O2	4:B:212:PCW:O1P	0.40	2.39	7	1
5:D:512:17F:H5	5:D:512:17F:H18	0.40	1.56	7	1
4:C:620:PCW:O11	4:C:620:PCW:C2	0.40	2.58	8	1
5:C:632:17F:H39	5:C:632:17F:H36	0.40	1.71	8	1
4:B:205:PCW:H411	4:B:205:PCW:H382	0.40	1.59	8	1
4:D:504:PCW:O31	4:D:504:PCW:O4P	0.40	2.39	9	1
5:C:627:17F:H64	5:C:628:17F:C1Z	0.40	2.46	10	1
4:B:212:PCW:C42	5:D:514:17F:H33	0.40	2.47	10	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	196/198 (99%)	190±1 (97±1%)	5±1 (2±1%)	1±0 (1±0%)	23	72
1	C	196/198 (99%)	190±1 (97±1%)	6±1 (3±1%)	0±0 (0±0%)	100	100
2	B	171/185 (92%)	162±2 (95±1%)	8±2 (5±1%)	0±0 (0±0%)	44	80
3	D	130/132 (98%)	112±2 (86±2%)	15±3 (12±2%)	3±1 (2±1%)	7	44
All	All	6930/7130 (97%)	6543 (94%)	341 (5%)	46 (1%)	20	70

All 15 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	10
3	D	364	ASN	10
3	D	407	GLY	10
3	D	374	ASN	5
3	D	435	PRO	1
2	B	45	VAL	1
1	A	300	PRO	1
2	B	48	GLY	1
3	D	433	HIS	1
3	D	462	GLY	1
2	B	123	ARG	1
3	D	375	GLY	1
3	D	447	LEU	1
3	D	434	VAL	1
2	B	34	PRO	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	174/174 (100%)	162±4 (93±2%)	12±4 (7±2%)	17	65
1	C	174/174 (100%)	159±2 (91±1%)	15±2 (9±1%)	12	58
2	B	152/164 (93%)	138±2 (91±2%)	14±2 (9±2%)	11	57
3	D	119/119 (100%)	104±3 (87±2%)	15±3 (13±2%)	6	48
All	All	6190/6310 (98%)	5639 (91%)	551 (9%)	11	57

All 178 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	C	516	THR	10
1	C	550	LYS	10
3	D	460	LEU	10
3	D	468	CYS	10
1	C	480	GLU	9
1	C	561	LYS	9
2	B	87	THR	9

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Mol	Chain	Res	Type	Models (Total)
3	D	438	THR	9
1	A	235	GLU	8
1	C	448	VAL	8
1	C	466	GLU	8
3	D	465	CYS	8
2	B	89	SER	8
3	D	459	LEU	8
3	D	478	THR	8
1	A	254	VAL	7
2	B	2	THR	7
2	B	35	THR	7
2	B	92	ASP	7
3	D	477	SER	7
1	C	462	LYS	7
1	A	272	TYR	6
1	C	552	THR	6
1	C	568	ASP	6
2	B	20	THR	6
2	B	69	ASP	6
2	B	122	SER	6
2	B	148	THR	6
3	D	357	THR	6
3	D	366	GLN	6
3	D	445	THR	6
3	D	467	THR	6
3	D	482	THR	6
1	A	265	TRP	6
1	C	405	TRP	6
1	C	407	SER	6
3	D	431	LEU	6
2	B	144	THR	6
3	D	377	SER	6
1	A	289	GLN	5
1	C	576	VAL	5
2	B	74	THR	5
1	C	459	PHE	5
3	D	437	THR	5
1	A	209	SER	5
3	D	453	ASP	5
1	A	250	VAL	4
1	A	293	GLU	4
1	A	358	SER	4

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Mol	Chain	Res	Type	Models (Total)
1	A	382	PHE	4
1	C	411	THR	4
2	B	41	ARG	4
2	B	124	THR	4
1	A	312	HIS	4
1	C	400	LYS	4
3	D	444	LYS	4
1	A	274	GLN	4
1	C	583	SER	4
1	A	212	SER	3
1	A	214	PHE	3
1	A	246	ASP	3
1	C	538	GLU	3
1	C	556	SER	3
1	C	557	THR	3
2	B	31	GLU	3
2	B	50	THR	3
3	D	398	VAL	3
3	D	436	LEU	3
1	A	359	THR	3
2	B	43	GLN	3
2	B	127	THR	3
3	D	381	CYS	3
1	A	381	SER	3
1	C	554	HIS	3
1	A	292	HIS	3
1	A	211	THR	2
1	A	263	LYS	2
1	A	304	GLU	2
1	C	447	GLU	2
2	B	39	SER	2
2	B	170	MET	2
1	A	236	THR	2
1	A	325	ASP	2
1	A	368	LEU	2
1	C	523	ASP	2
1	C	548	HIS	2
1	C	560	GLU	2
2	B	45	VAL	2
2	B	47	ASP	2
2	B	80	CYS	2
2	B	126	ASP	2

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Mol	Chain	Res	Type	Models (Total)
2	B	153	ASP	2
2	B	17	SER	2
2	B	44	VAL	2
2	B	132	ASP	2
3	D	420	SER	2
3	D	476	CYS	2
1	C	483	GLU	2
1	C	490	HIS	2
2	B	33	ASP	2
1	A	370	ASP	2
1	C	415	LEU	2
2	B	58	THR	2
3	D	455	CYS	2
1	A	394	THR	2
2	B	65	SER	2
3	D	433	HIS	2
1	A	228	PHE	1
1	A	319	HIS	1
1	A	385	SER	1
1	C	427	TRP	1
1	C	440	GLU	1
1	C	589	GLU	1
2	B	94	HIS	1
1	A	233	GLU	1
2	B	46	ILE	1
2	B	52	LEU	1
2	B	62	GLU	1
3	D	361	PHE	1
3	D	403	GLN	1
3	D	485	VAL	1
1	A	225	THR	1
1	A	269	MET	1
1	A	277	GLU	1
1	A	299	SER	1
1	A	314	ASP	1
1	A	349	TYR	1
1	C	477	LEU	1
1	C	522	SER	1
1	C	558	LEU	1
2	B	147	LYS	1
3	D	365	LYS	1
3	D	367	ARG	1

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Mol	Chain	Res	Type	Models (Total)
3	D	434	VAL	1
3	D	486	ASP	1
1	A	227	GLU	1
1	C	473	LYS	1
2	B	114	VAL	1
2	B	171	SER	1
3	D	382	LEU	1
1	A	232	LEU	1
1	C	442	SER	1
1	C	524	GLU	1
2	B	99	GLN	1
3	D	432	ASP	1
1	A	218	ARG	1
1	A	237	GLU	1
1	A	244	SER	1
1	A	356	HIS	1
1	A	369	GLU	1
1	C	567	GLU	1
1	C	577	LEU	1
1	C	592	THR	1
3	D	368	THR	1
1	A	239	LEU	1
1	A	249	GLU	1
1	A	371	LEU	1
1	C	493	GLN	1
1	C	559	SER	1
2	B	27	HIS	1
2	B	109	VAL	1
3	D	425	GLU	1
3	D	457	LYS	1
3	D	487	TRP	1
1	C	429	ASN	1
2	B	8	VAL	1
2	B	70	GLN	1
2	B	128	LYS	1
2	B	149	ARG	1
1	A	386	PHE	1
1	A	388	SER	1
1	C	525	LEU	1
2	B	119	ASP	1
2	B	139	ILE	1
3	D	412	LEU	1

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Mol	Chain	Res	Type	Models (Total)
3	D	470	TYR	1
3	D	484	CYS	1
3	D	471	LYS	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, 3 are monoatomic - leaving 81 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
5	17F	C	628	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	17F	B	213	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	17F	D	511	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	C	612	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	C	630	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	D	508	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	C	631	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	B	210	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	403	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	607	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	413	-	53,53,53	0.82±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PCW	C	617	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	613	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	B	205	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	B	206	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	406	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	510	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	603	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	414	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	615	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	405	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	417	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	608	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	604	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	605	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	412	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	611	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	C	626	-	52,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	601	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	620	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	516	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	506	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	415	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	614	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	B	207	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	C	627	-	52,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	407	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	B	208	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	408	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	606	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	D	512	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	17F	A	410	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	B	209	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	B	204	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	503	-	53,53,53	0.82±0.00	0±0 (0±0%)
6	GNP	B	216	-	34,34,34	1.22±0.02	2±1 (7±1%)
4	PCW	A	401	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	502	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	624	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	509	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	515	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	616	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	411	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	C	629	-	52,53,53	0.83±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PCW	C	625	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	C	632	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	A	402	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	A	409	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	D	504	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	D	514	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	C	618	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	609	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	B	201	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	404	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	623	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	B	202	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	B	211	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	610	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	505	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	621	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	416	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	501	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	B	215	-	52,53,53	0.82±0.00	0±0 (0±0%)
5	17F	D	513	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	C	619	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	B	212	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	507	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	622	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	B	214	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	B	203	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	602	-	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
5	17F	C	628	-	54,60,60	1.09±0.04	5±0 (8±0%)
5	17F	B	213	-	54,60,60	1.12±0.03	4±0 (7±0%)
5	17F	D	511	-	54,60,60	1.11±0.03	5±0 (9±0%)
4	PCW	C	612	-	59,61,61	2.60±0.01	6±1 (10±1%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
5	17F	C	630	-	54,60,60	1.34±0.04	9±0 (16±0%)
4	PCW	D	508	-	59,61,61	2.59±0.01	6±0 (10±0%)
5	17F	C	631	-	54,60,60	1.12±0.05	4±0 (7±0%)
4	PCW	B	210	-	59,61,61	2.62±0.01	7±0 (11±0%)
4	PCW	A	403	-	59,61,61	2.58±0.01	6±0 (10±0%)
4	PCW	C	607	-	59,61,61	2.60±0.01	6±1 (10±1%)
4	PCW	A	413	-	59,61,61	2.61±0.02	7±1 (11±1%)
4	PCW	C	617	-	59,61,61	2.61±0.01	7±0 (11±0%)
4	PCW	C	613	-	59,61,61	2.61±0.01	7±0 (11±0%)
4	PCW	B	205	-	59,61,61	2.60±0.01	6±0 (11±0%)
4	PCW	B	206	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	A	406	-	59,61,61	2.60±0.01	6±0 (10±0%)
4	PCW	D	510	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	C	603	-	59,61,61	2.61±0.01	7±1 (11±1%)
4	PCW	A	414	-	59,61,61	2.60±0.01	7±1 (12±1%)
4	PCW	C	615	-	59,61,61	2.58±0.00	6±0 (10±0%)
4	PCW	A	405	-	59,61,61	2.58±0.01	6±0 (10±0%)
4	PCW	A	417	-	59,61,61	2.58±0.02	6±1 (10±1%)
4	PCW	C	608	-	59,61,61	2.59±0.01	7±1 (11±1%)
4	PCW	C	604	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	C	605	-	59,61,61	2.63±0.01	7±0 (12±0%)
4	PCW	A	412	-	59,61,61	2.59±0.01	6±0 (11±0%)
4	PCW	C	611	-	59,61,61	2.61±0.01	6±0 (10±0%)
5	17F	C	626	-	54,60,60	1.10±0.02	4±0 (7±0%)
4	PCW	C	601	-	59,61,61	2.61±0.01	7±1 (11±1%)
4	PCW	C	620	-	59,61,61	2.58±0.01	6±0 (11±0%)
4	PCW	D	516	-	59,61,61	2.67±0.01	10±0 (17±0%)
4	PCW	D	506	-	59,61,61	2.60±0.01	7±1 (11±1%)
4	PCW	A	415	-	59,61,61	2.61±0.01	6±0 (10±0%)
4	PCW	C	614	-	59,61,61	2.61±0.01	6±0 (10±0%)
4	PCW	B	207	-	59,61,61	2.60±0.01	6±0 (10±0%)
5	17F	C	627	-	54,60,60	1.12±0.02	5±1 (9±0%)
4	PCW	A	407	-	59,61,61	2.59±0.00	6±0 (10±0%)
4	PCW	B	208	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	A	408	-	59,61,61	2.62±0.01	7±1 (12±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PCW	C	606	-	59,61,61	2.59±0.01	6±0 (10±0%)
5	17F	D	512	-	54,60,60	1.14±0.03	5±1 (8±1%)
5	17F	A	410	-	54,60,60	1.14±0.01	4±0 (8±0%)
4	PCW	B	209	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	B	204	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	D	503	-	59,61,61	2.69±0.01	10±0 (17±0%)
6	GNP	B	216	-	47,54,54	1.81±0.02	11±1 (24±1%)
4	PCW	A	401	-	59,61,61	2.60±0.01	6±0 (10±0%)
4	PCW	D	502	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	C	624	-	59,61,61	2.62±0.01	6±0 (10±0%)
4	PCW	D	509	-	59,61,61	2.60±0.01	6±0 (10±0%)
4	PCW	D	515	-	59,61,61	2.61±0.01	7±0 (11±0%)
4	PCW	C	616	-	59,61,61	2.61±0.01	6±0 (11±0%)
4	PCW	A	411	-	59,61,61	2.60±0.01	7±0 (11±0%)
5	17F	C	629	-	54,60,60	1.13±0.02	4±0 (7±0%)
4	PCW	C	625	-	59,61,61	2.59±0.02	7±1 (11±1%)
5	17F	C	632	-	54,60,60	1.10±0.05	4±0 (8±0%)
4	PCW	A	402	-	59,61,61	2.61±0.01	6±0 (10±0%)
5	17F	A	409	-	54,60,60	1.35±0.03	8±0 (15±0%)
4	PCW	D	504	-	59,61,61	2.59±0.01	6±0 (10±0%)
5	17F	D	514	-	54,60,60	1.24±0.03	4±0 (7±0%)
4	PCW	C	618	-	59,61,61	2.58±0.01	6±0 (10±0%)
4	PCW	C	609	-	59,61,61	2.59±0.01	6±1 (11±1%)
4	PCW	B	201	-	59,61,61	2.60±0.01	6±0 (10±0%)
4	PCW	A	404	-	59,61,61	2.59±0.01	7±0 (11±0%)
4	PCW	C	623	-	59,61,61	2.57±0.01	6±0 (9±0%)
4	PCW	B	202	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	B	211	-	59,61,61	2.59±0.01	7±0 (11±0%)
4	PCW	C	610	-	59,61,61	2.59±0.01	7±0 (11±0%)
4	PCW	D	505	-	59,61,61	2.60±0.01	6±0 (10±0%)
4	PCW	C	621	-	59,61,61	2.61±0.01	7±0 (12±0%)
4	PCW	A	416	-	59,61,61	2.58±0.01	7±0 (11±0%)
4	PCW	D	501	-	59,61,61	2.60±0.01	7±0 (11±0%)
5	17F	B	215	-	54,60,60	1.13±0.04	4±0 (8±0%)
5	17F	D	513	-	54,60,60	1.15±0.02	4±0 (7±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PCW	C	619	-	59,61,61	2.59±0.01	7±0 (11±0%)
4	PCW	B	212	-	59,61,61	2.60±0.01	7±0 (11±0%)
4	PCW	D	507	-	59,61,61	2.60±0.01	6±0 (10±0%)
4	PCW	C	622	-	59,61,61	2.59±0.02	6±0 (10±0%)
5	17F	B	214	-	54,60,60	1.13±0.03	4±0 (7±0%)
4	PCW	B	203	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	C	602	-	59,61,61	2.59±0.00	6±0 (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
5	17F	B	213	-	-	0±0,59,59,59	-
4	PCW	B	210	-	-	0±0,57,57,57	-
4	PCW	C	607	-	-	0±0,57,57,57	-
4	PCW	B	206	-	-	0±0,57,57,57	-
4	PCW	D	508	-	-	0±0,57,57,57	-
4	PCW	A	403	-	-	0±0,57,57,57	-
4	PCW	B	207	-	-	0±0,57,57,57	-
4	PCW	C	613	-	-	0±0,57,57,57	-
4	PCW	B	209	-	-	0±0,57,57,57	-
4	PCW	D	503	-	-	0±0,57,57,57	-
4	PCW	D	504	-	-	0±0,57,57,57	-
4	PCW	C	615	-	-	0±0,57,57,57	-
4	PCW	A	407	-	-	0±0,57,57,57	-
5	17F	C	628	-	-	0±0,59,59,59	-
5	17F	D	511	-	-	0±0,59,59,59	-
4	PCW	A	405	-	-	0±0,57,57,57	-
4	PCW	C	605	-	-	0±0,57,57,57	-
4	PCW	D	509	-	-	0±0,57,57,57	-
5	17F	C	626	-	-	0±0,59,59,59	-
4	PCW	B	201	-	-	0±0,57,57,57	-
4	PCW	D	510	-	-	0±0,57,57,57	-
4	PCW	C	625	-	-	0±0,57,57,57	-
4	PCW	A	402	-	-	0±0,57,57,57	-
5	17F	A	410	-	-	0±0,59,59,59	-
4	PCW	C	603	-	-	0±0,57,57,57	-
4	PCW	B	203	-	-	0±0,57,57,57	-
4	PCW	D	515	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	A	413	-	-	0±0,57,57,57	-
4	PCW	D	505	-	-	0±0,57,57,57	-
4	PCW	C	621	-	-	0±0,57,57,57	-
4	PCW	A	414	-	-	0±0,57,57,57	-
5	17F	A	409	-	-	0±0,59,59,59	-
4	PCW	C	601	-	-	0±0,57,57,57	-
4	PCW	A	417	-	-	0±0,57,57,57	-
4	PCW	B	204	-	-	0±0,57,57,57	-
4	PCW	B	212	-	-	0±0,57,57,57	-
5	17F	D	512	-	-	1±0,59,59,59	-
4	PCW	C	604	-	-	0±0,57,57,57	-
4	PCW	C	612	-	-	0±0,57,57,57	-
4	PCW	B	208	-	-	0±0,57,57,57	-
5	17F	B	214	-	-	0±0,59,59,59	-
4	PCW	C	606	-	-	0±0,57,57,57	-
4	PCW	C	622	-	-	0±0,57,57,57	-
4	PCW	C	619	-	-	0±0,57,57,57	-
5	17F	C	629	-	-	0±0,59,59,59	-
4	PCW	A	408	-	-	0±0,57,57,57	-
4	PCW	A	415	-	-	0±0,57,57,57	-
5	17F	C	630	-	-	0±0,59,59,59	-
4	PCW	C	608	-	-	0±0,57,57,57	-
5	17F	D	514	-	-	1±0,59,59,59	-
4	PCW	C	609	-	-	0±0,57,57,57	-
4	PCW	D	502	-	-	0±0,57,57,57	-
4	PCW	C	611	-	-	0±0,57,57,57	-
4	PCW	A	416	-	-	0±0,57,57,57	-
4	PCW	C	614	-	-	0±0,57,57,57	-
4	PCW	A	401	-	-	0±0,57,57,57	-
4	PCW	D	506	-	-	0±0,57,57,57	-
5	17F	D	513	-	-	0±0,59,59,59	-
4	PCW	D	501	-	-	0±0,57,57,57	-
4	PCW	B	202	-	-	0±0,57,57,57	-
4	PCW	A	411	-	-	0±0,57,57,57	-
4	PCW	C	620	-	-	0±0,57,57,57	-
4	PCW	C	624	-	-	0±0,57,57,57	-
4	PCW	A	412	-	-	0±0,57,57,57	-
4	PCW	D	516	-	-	0±0,57,57,57	-
4	PCW	C	618	-	-	0±0,57,57,57	-
5	17F	C	632	-	-	0±0,59,59,59	-
4	PCW	D	507	-	-	0±0,57,57,57	-
4	PCW	A	404	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	C	617	-	-	0±0,57,57,57	-
4	PCW	A	406	-	-	0±0,57,57,57	-
5	17F	C	627	-	-	1±0,59,59,59	-
5	17F	B	215	-	-	0±0,59,59,59	-
4	PCW	C	623	-	-	0±0,57,57,57	-
5	17F	C	631	-	-	0±0,59,59,59	-
4	PCW	C	616	-	-	0±0,57,57,57	-
4	PCW	B	205	-	-	0±0,57,57,57	-
6	GNP	B	216	-	-	0±0,18,38,38	0±0,3,3,3
4	PCW	C	602	-	-	0±0,57,57,57	-
4	PCW	B	211	-	-	0±0,57,57,57	-
4	PCW	C	610	-	-	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
6	B	216	GNP	PB-O2B	3.16	1.48	1.56	10	10
6	B	216	GNP	C5-N7	2.90	1.33	1.39	9	10
6	B	216	GNP	PA-O3A	2.17	1.61	1.59	6	1
6	B	216	GNP	PB-O3A	2.16	1.61	1.59	6	3

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
4	D	516	PCW	C8-N-C7	17.71	62.47	108.98	9	10
4	C	607	PCW	C8-N-C7	17.69	62.52	108.98	8	10
4	A	405	PCW	C8-N-C7	17.68	62.52	108.98	5	10
4	A	413	PCW	C8-N-C7	17.68	62.52	108.98	3	10
4	C	609	PCW	C8-N-C7	17.68	62.53	108.98	6	10
4	C	601	PCW	C8-N-C7	17.68	62.53	108.98	8	10
4	C	613	PCW	C8-N-C7	17.68	62.53	108.98	3	10
4	C	619	PCW	C8-N-C7	17.68	62.53	108.98	6	10
4	C	606	PCW	C8-N-C7	17.68	62.54	108.98	8	10
4	B	201	PCW	C8-N-C7	17.68	62.54	108.98	10	10
4	A	406	PCW	C8-N-C7	17.68	62.55	108.98	2	10
4	A	412	PCW	C8-N-C7	17.68	62.55	108.98	4	10
4	A	414	PCW	C8-N-C7	17.68	62.54	108.98	7	10
4	B	208	PCW	C8-N-C7	17.68	62.54	108.98	3	10
4	A	408	PCW	C8-N-C7	17.67	62.55	108.98	2	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	C	610	PCW	C8-N-C7	17.67	62.55	108.98	2	10
4	A	416	PCW	C8-N-C7	17.67	62.55	108.98	7	10
4	A	417	PCW	C8-N-C7	17.67	62.55	108.98	1	10
4	C	616	PCW	C8-N-C7	17.67	62.55	108.98	9	10
4	C	618	PCW	C8-N-C7	17.67	62.55	108.98	7	10
4	C	625	PCW	C8-N-C7	17.67	62.55	108.98	7	10
4	C	605	PCW	C8-N-C7	17.67	62.55	108.98	5	10
4	B	206	PCW	C8-N-C7	17.67	62.56	108.98	5	10
4	D	502	PCW	C8-N-C7	17.67	62.56	108.98	10	10
4	B	212	PCW	C8-N-C7	17.67	62.56	108.98	2	10
4	D	501	PCW	C8-N-C7	17.67	62.56	108.98	9	10
4	A	402	PCW	C8-N-C7	17.67	62.56	108.98	1	10
4	D	506	PCW	C8-N-C7	17.67	62.56	108.98	3	10
4	D	508	PCW	C8-N-C7	17.67	62.56	108.98	7	10
4	A	415	PCW	C8-N-C7	17.67	62.56	108.98	6	10
4	D	509	PCW	C8-N-C7	17.67	62.56	108.98	9	10
4	C	611	PCW	C8-N-C7	17.67	62.57	108.98	4	10
4	C	612	PCW	C8-N-C7	17.67	62.57	108.98	9	10
4	C	620	PCW	C8-N-C7	17.67	62.57	108.98	3	10
4	C	622	PCW	C8-N-C7	17.67	62.57	108.98	8	10
4	B	210	PCW	C8-N-C7	17.67	62.57	108.98	5	10
4	D	504	PCW	C8-N-C7	17.67	62.57	108.98	2	10
4	A	403	PCW	C8-N-C7	17.67	62.57	108.98	5	10
4	A	411	PCW	C8-N-C7	17.67	62.57	108.98	5	10
4	B	203	PCW	C8-N-C7	17.67	62.57	108.98	8	10
4	B	204	PCW	C8-N-C7	17.67	62.57	108.98	2	10
4	A	401	PCW	C8-N-C7	17.66	62.58	108.98	3	10
4	A	404	PCW	C8-N-C7	17.66	62.57	108.98	9	10
4	C	602	PCW	C8-N-C7	17.67	62.57	108.98	4	10
4	B	205	PCW	C8-N-C7	17.66	62.58	108.98	5	10
4	D	507	PCW	C8-N-C7	17.66	62.58	108.98	5	10
4	C	603	PCW	C8-N-C7	17.66	62.58	108.98	10	10
4	C	604	PCW	C8-N-C7	17.66	62.58	108.98	7	10
4	C	614	PCW	C8-N-C7	17.66	62.58	108.98	6	10
4	B	207	PCW	C8-N-C7	17.66	62.58	108.98	4	10
4	B	209	PCW	C8-N-C7	17.66	62.58	108.98	10	10
4	D	505	PCW	C8-N-C7	17.66	62.58	108.98	8	10
4	D	510	PCW	C8-N-C7	17.66	62.58	108.98	8	10
4	A	407	PCW	C8-N-C7	17.66	62.59	108.98	10	10
4	C	608	PCW	C8-N-C7	17.66	62.59	108.98	8	10
4	C	617	PCW	C8-N-C7	17.66	62.59	108.98	4	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	B	202	PCW	C8-N-C7	17.66	62.59	108.98	7	10
4	C	621	PCW	C8-N-C7	17.66	62.59	108.98	6	10
4	C	623	PCW	C8-N-C7	17.66	62.59	108.98	5	10
4	D	503	PCW	C8-N-C7	17.66	62.59	108.98	3	10
4	C	624	PCW	C8-N-C7	17.66	62.59	108.98	1	10
4	B	211	PCW	C8-N-C7	17.66	62.59	108.98	10	10
4	D	515	PCW	C8-N-C7	17.66	62.59	108.98	7	10
4	C	615	PCW	C8-N-C7	17.65	62.61	108.98	1	10
5	D	514	17F	O3-C1-C2	5.66	113.00	108.06	6	10
6	B	216	GNP	C2-N3-C4	5.42	121.64	112.30	2	10
6	B	216	GNP	C5-C4-N3	4.95	120.51	128.39	2	10
5	C	630	17F	O3-C1-C2	4.89	112.32	108.06	2	10
5	C	627	17F	O9-C17-C18	4.43	121.06	111.48	1	10
5	D	512	17F	O9-C17-C18	4.39	120.97	111.48	5	10
4	A	413	PCW	O2-C31-C32	4.31	120.80	111.48	7	10
4	C	624	PCW	O2-C31-C32	4.30	120.78	111.48	3	10
5	C	628	17F	O3-C1-C2	4.25	111.76	108.06	2	10
4	C	625	PCW	C2-O2-C31	4.24	107.64	117.80	9	10
5	B	214	17F	O3-C1-C2	4.24	111.75	108.06	3	10
5	C	632	17F	O9-C17-C18	4.24	120.65	111.48	9	10
5	D	514	17F	O9-C17-C18	4.22	120.62	111.48	9	10
5	D	512	17F	O3-C1-C2	4.21	111.72	108.06	10	10
5	A	409	17F	O9-C17-C18	4.18	120.53	111.48	3	10
4	A	415	PCW	O2-C31-C32	4.17	120.51	111.48	3	10
5	A	409	17F	O3-C1-C2	4.16	111.69	108.06	1	10
5	D	511	17F	O3-C1-C2	4.15	111.67	108.06	3	10
4	A	413	PCW	C2-O2-C31	4.12	107.92	117.80	8	10
4	C	624	PCW	C2-O2-C31	4.12	107.94	117.80	3	10
4	A	415	PCW	C2-O2-C31	4.10	107.97	117.80	3	10
4	C	603	PCW	O2-C31-C32	4.10	120.36	111.48	7	10
4	C	605	PCW	O2-C31-C32	4.10	120.36	111.48	1	10
4	C	625	PCW	O2-C31-C32	4.09	120.34	111.48	9	10
4	C	611	PCW	O2-C31-C32	4.09	120.33	111.48	1	10
4	C	614	PCW	O2-C31-C32	4.08	120.31	111.48	3	10
4	B	208	PCW	O2-C31-C32	4.07	120.28	111.48	8	10
5	C	627	17F	O3-C1-C2	4.06	111.60	108.06	7	10
4	C	622	PCW	O2-C31-C32	4.05	120.25	111.48	5	10
5	C	632	17F	O3-C1-C2	4.05	111.59	108.06	6	10
4	A	408	PCW	O2-C31-C32	4.04	120.21	111.48	6	10
5	C	631	17F	O9-C17-C18	4.03	120.21	111.48	1	10
5	A	410	17F	O9-C17-C18	4.03	120.20	111.48	6	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	B	213	17F	O3-C1-C2	4.02	111.56	108.06	2	10
5	A	410	17F	O3-C1-C2	4.01	111.55	108.06	9	10
5	C	629	17F	O9-C17-C18	3.99	120.12	111.48	9	10
4	C	604	PCW	O2-C31-C32	3.99	120.11	111.48	10	10
4	C	613	PCW	O2-C31-C32	3.99	120.11	111.48	10	10
4	C	616	PCW	O2-C31-C32	3.99	120.11	111.48	9	10
5	B	215	17F	O9-C17-C18	3.99	120.11	111.48	9	10
4	B	210	PCW	O2-C31-C32	3.98	120.10	111.48	5	10
4	C	612	PCW	O2-C31-C32	3.97	120.06	111.48	2	10
5	D	513	17F	O3-C1-C2	3.97	111.52	108.06	7	10
4	D	505	PCW	O2-C31-C32	3.96	120.05	111.48	8	10
4	A	401	PCW	O2-C31-C32	3.95	120.03	111.48	5	10
5	D	513	17F	C5-O9-C17	3.95	108.34	117.80	7	10
5	D	513	17F	O9-C17-C18	3.95	120.02	111.48	7	10
4	B	207	PCW	O2-C31-C32	3.94	120.01	111.48	7	10
5	B	214	17F	O9-C17-C18	3.93	119.99	111.48	5	10
4	A	417	PCW	O2-C31-C32	3.93	119.98	111.48	3	10
4	B	210	PCW	C2-O2-C31	3.92	108.41	117.80	8	10
4	A	406	PCW	O2-C31-C32	3.91	119.94	111.48	7	10
4	A	412	PCW	O2-C31-C32	3.91	119.93	111.48	3	10
4	B	203	PCW	O2-C31-C32	3.91	119.93	111.48	6	10
4	C	601	PCW	O2-C31-C32	3.90	119.93	111.48	5	10
5	C	629	17F	O3-C1-C2	3.89	111.45	108.06	5	10
4	B	202	PCW	O2-C31-C32	3.89	119.90	111.48	10	10
5	C	629	17F	C5-O9-C17	3.88	108.51	117.80	10	10
4	D	515	PCW	O2-C31-C32	3.88	119.88	111.48	8	10
4	A	403	PCW	O2-C31-C32	3.88	119.86	111.48	10	10
4	A	402	PCW	O2-C31-C32	3.87	119.86	111.48	10	10
5	B	215	17F	O3-C1-C2	3.86	111.42	108.06	7	10
5	C	626	17F	O3-C1-C2	3.86	111.42	108.06	6	10
4	D	503	PCW	O2-C31-C32	3.86	119.83	111.48	8	10
4	A	411	PCW	O2-C31-C32	3.85	119.81	111.48	6	10
4	D	501	PCW	O2-C31-C32	3.85	119.81	111.48	9	10
4	C	607	PCW	O2-C31-C32	3.85	119.81	111.48	4	10
4	A	404	PCW	O2-C31-C32	3.84	119.78	111.48	3	10
4	D	505	PCW	C2-O2-C31	3.83	108.63	117.80	5	10
6	B	216	GNP	O2B-PB-O1B	3.83	118.08	109.87	2	10
4	C	609	PCW	O2-C31-C32	3.82	119.75	111.48	2	10
4	D	504	PCW	O2-C31-C32	3.82	119.74	111.48	6	10
5	B	213	17F	O9-C17-C18	3.82	119.75	111.48	10	10
4	C	620	PCW	O2-C31-C32	3.81	119.73	111.48	8	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	414	PCW	O2-C31-C32	3.81	119.72	111.48	2	10
4	C	606	PCW	O2-C31-C32	3.81	119.72	111.48	2	10
4	A	405	PCW	O2-C31-C32	3.81	119.71	111.48	3	10
4	D	508	PCW	O2-C31-C32	3.80	119.71	111.48	8	10
4	D	506	PCW	O2-C31-C32	3.80	119.70	111.48	4	10
4	B	201	PCW	O2-C31-C32	3.79	119.68	111.48	5	10
4	B	205	PCW	O2-C31-C32	3.79	119.68	111.48	2	10
4	C	614	PCW	C2-O2-C31	3.78	108.74	117.80	9	10
4	B	209	PCW	O2-C31-C32	3.78	119.66	111.48	9	10
4	B	212	PCW	O2-C31-C32	3.78	119.65	111.48	3	10
4	B	204	PCW	O2-C31-C32	3.78	119.65	111.48	1	10
5	C	626	17F	O9-C17-C18	3.77	119.64	111.48	6	10
4	D	510	PCW	O2-C31-C32	3.77	119.63	111.48	4	10
4	C	617	PCW	O2-C31-C32	3.77	119.63	111.48	10	10
5	C	630	17F	O9-C17-C18	3.76	119.61	111.48	6	10
4	C	610	PCW	O2-C31-C32	3.75	119.60	111.48	4	10
4	B	206	PCW	O2-C31-C32	3.75	119.58	111.48	6	10
4	A	407	PCW	O2-C31-C32	3.74	119.58	111.48	6	10
4	C	621	PCW	O2-C31-C32	3.73	119.56	111.48	2	10
4	C	602	PCW	O2-C31-C32	3.73	119.55	111.48	6	10
4	D	509	PCW	O2-C31-C32	3.73	119.54	111.48	6	10
4	D	502	PCW	O2-C31-C32	3.72	119.54	111.48	3	10
4	C	601	PCW	C2-O2-C31	3.71	108.91	117.80	9	10
5	D	511	17F	O9-C17-C18	3.71	119.51	111.48	7	10
5	C	631	17F	C5-O9-C17	3.70	108.95	117.80	1	9
4	C	618	PCW	O2-C31-C32	3.69	119.47	111.48	3	10
4	D	507	PCW	O2-C31-C32	3.69	119.47	111.48	8	10
4	C	622	PCW	C2-O2-C31	3.68	108.99	117.80	7	10
4	B	207	PCW	C2-O2-C31	3.67	109.00	117.80	7	10
4	C	608	PCW	O2-C31-C32	3.67	119.42	111.48	8	10
5	A	409	17F	C5-O9-C17	3.67	109.01	117.80	3	10
4	C	611	PCW	C2-O2-C31	3.66	109.03	117.80	2	10
4	A	416	PCW	O2-C31-C32	3.66	119.40	111.48	4	10
5	C	628	17F	O9-C17-C18	3.65	119.38	111.48	8	10
4	C	613	PCW	C2-O2-C31	3.64	109.09	117.80	5	10
4	C	619	PCW	O2-C31-C32	3.64	119.35	111.48	8	10
4	C	616	PCW	C2-O2-C31	3.61	109.15	117.80	9	10
4	C	603	PCW	C2-O2-C31	3.61	109.16	117.80	7	10
5	C	631	17F	O3-C1-C2	3.60	111.19	108.06	8	10
4	B	211	PCW	O2-C31-C32	3.56	119.19	111.48	2	10
4	D	515	PCW	C2-O2-C31	3.56	109.28	117.80	8	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	402	PCW	C2-O2-C31	3.55	109.30	117.80	1	10
4	C	604	PCW	C2-O2-C31	3.54	109.33	117.80	10	10
4	B	202	PCW	C2-O2-C31	3.54	109.33	117.80	10	10
5	C	630	17F	C5-O9-C17	3.53	109.34	117.80	9	10
4	C	615	PCW	O2-C31-C32	3.53	119.12	111.48	1	10
4	D	516	PCW	O2-C31-C32	3.53	119.11	111.48	2	10
4	C	601	PCW	C7-N-C6	3.51	118.19	108.98	5	10
5	A	410	17F	C5-O9-C17	3.50	109.41	117.80	2	10
5	B	213	17F	C5-O9-C17	3.50	109.41	117.80	10	10
4	A	405	PCW	C2-O2-C31	3.49	109.44	117.80	3	10
4	A	401	PCW	C2-O2-C31	3.49	109.44	117.80	10	10
4	C	607	PCW	C2-O2-C31	3.49	109.44	117.80	2	10
4	A	406	PCW	C2-O2-C31	3.48	109.46	117.80	4	10
4	C	612	PCW	C7-N-C6	3.48	118.11	108.98	3	10
4	A	417	PCW	C7-N-C6	3.46	118.06	108.98	3	10
4	C	609	PCW	C7-N-C6	3.46	118.06	108.98	9	10
4	C	607	PCW	C7-N-C6	3.46	118.06	108.98	3	10
4	D	505	PCW	C8-N-C6	3.45	118.04	108.98	5	10
5	C	632	17F	C5-O9-C17	3.45	109.55	117.80	9	10
4	B	209	PCW	C2-O2-C31	3.44	109.56	117.80	9	10
4	A	403	PCW	C2-O2-C31	3.44	109.57	117.80	10	10
4	D	504	PCW	C2-O2-C31	3.43	109.58	117.80	4	10
4	A	408	PCW	C2-O2-C31	3.43	109.59	117.80	8	10
4	C	621	PCW	C2-O2-C31	3.43	109.58	117.80	8	10
4	C	609	PCW	C2-O2-C31	3.43	109.59	117.80	8	10
4	C	612	PCW	C8-N-C6	3.41	117.95	108.98	1	10
5	D	514	17F	C5-O9-C17	3.41	109.62	117.80	5	10
4	D	503	PCW	C2-O2-C31	3.41	109.63	117.80	6	10
4	C	612	PCW	C2-O2-C31	3.41	109.64	117.80	8	10
4	C	617	PCW	C2-O2-C31	3.41	109.64	117.80	9	10
4	C	625	PCW	C7-N-C6	3.41	117.92	108.98	5	10
4	A	413	PCW	C8-N-C6	3.40	117.92	108.98	10	10
4	B	207	PCW	C8-N-C6	3.40	117.92	108.98	9	10
4	D	506	PCW	C8-N-C6	3.40	117.92	108.98	9	10
4	B	201	PCW	C2-O2-C31	3.39	109.68	117.80	5	10
4	C	609	PCW	C8-N-C6	3.39	117.88	108.98	3	10
4	A	413	PCW	C7-N-C6	3.38	117.86	108.98	2	10
4	C	605	PCW	C2-O2-C31	3.38	109.70	117.80	3	10
4	D	509	PCW	C2-O2-C31	3.38	109.71	117.80	10	10
4	D	508	PCW	C2-O2-C31	3.38	109.71	117.80	5	10
4	C	618	PCW	C8-N-C6	3.37	117.83	108.98	9	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	B	215	17F	C5-O9-C17	3.37	109.73	117.80	1	10
4	A	414	PCW	C8-N-C6	3.37	117.82	108.98	7	10
5	B	214	17F	C5-O9-C17	3.37	109.74	117.80	5	10
4	A	401	PCW	C7-N-C6	3.36	117.81	108.98	2	10
4	A	411	PCW	C2-O2-C31	3.36	109.75	117.80	6	10
4	B	205	PCW	C2-O2-C31	3.36	109.75	117.80	7	10
4	D	508	PCW	C7-N-C6	3.36	117.80	108.98	1	10
4	A	411	PCW	C8-N-C6	3.35	117.78	108.98	6	10
4	B	212	PCW	C2-O2-C31	3.35	109.77	117.80	3	10
4	B	203	PCW	C7-N-C6	3.35	117.78	108.98	9	10
4	B	210	PCW	C7-N-C6	3.35	117.78	108.98	5	10
4	D	501	PCW	C2-O2-C31	3.35	109.78	117.80	9	10
4	D	506	PCW	C2-O2-C31	3.35	109.78	117.80	3	10
4	D	507	PCW	C2-O2-C31	3.35	109.79	117.80	10	10
4	C	614	PCW	C7-N-C6	3.34	117.76	108.98	7	10
4	C	619	PCW	C8-N-C6	3.34	117.76	108.98	1	10
4	B	204	PCW	C2-O2-C31	3.34	109.79	117.80	4	10
4	B	206	PCW	C7-N-C6	3.34	117.76	108.98	8	10
4	B	203	PCW	C2-O2-C31	3.34	109.80	117.80	3	10
4	C	620	PCW	C7-N-C6	3.34	117.74	108.98	9	10
4	B	206	PCW	C2-O2-C31	3.34	109.81	117.80	3	10
4	C	616	PCW	C7-N-C6	3.33	117.73	108.98	5	10
6	B	216	GNP	N9-C4-N3	3.33	132.62	125.95	3	10
4	C	619	PCW	C2-O2-C31	3.33	109.82	117.80	10	10
4	C	616	PCW	C8-N-C6	3.33	117.72	108.98	7	10
4	C	613	PCW	C8-N-C6	3.33	117.72	108.98	6	10
4	D	503	PCW	C7-N-C6	3.32	117.71	108.98	10	10
4	C	605	PCW	C8-N-C6	3.32	117.70	108.98	9	10
4	C	606	PCW	C8-N-C6	3.32	117.70	108.98	10	10
4	C	620	PCW	C2-O2-C31	3.32	109.85	117.80	8	10
4	A	406	PCW	C7-N-C6	3.32	117.69	108.98	2	10
4	C	620	PCW	C8-N-C6	3.32	117.69	108.98	1	10
4	D	515	PCW	C7-N-C6	3.32	117.69	108.98	5	10
4	C	623	PCW	C7-N-C6	3.32	117.69	108.98	3	10
4	D	507	PCW	C8-N-C6	3.31	117.68	108.98	7	10
4	C	608	PCW	C7-N-C6	3.31	117.67	108.98	2	10
4	D	510	PCW	C2-O2-C31	3.31	109.88	117.80	4	10
4	C	603	PCW	C7-N-C6	3.30	117.65	108.98	8	10
4	C	604	PCW	C7-N-C6	3.30	117.65	108.98	1	10
4	C	602	PCW	C8-N-C6	3.30	117.64	108.98	1	10
4	B	208	PCW	C8-N-C6	3.30	117.64	108.98	10	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	D	508	PCW	C8-N-C6	3.30	117.64	108.98	6	10
4	B	211	PCW	C7-N-C6	3.30	117.63	108.98	8	10
4	D	510	PCW	C7-N-C6	3.30	117.63	108.98	5	10
4	C	625	PCW	C8-N-C6	3.29	117.63	108.98	4	10
4	D	503	PCW	C8-N-C6	3.29	117.63	108.98	9	10
4	D	516	PCW	C7-N-C6	3.29	117.62	108.98	8	10
4	C	603	PCW	C8-N-C6	3.29	117.62	108.98	10	10
4	B	204	PCW	C8-N-C6	3.29	117.62	108.98	4	10
4	C	614	PCW	C8-N-C6	3.29	117.61	108.98	9	10
4	C	622	PCW	C7-N-C6	3.29	117.61	108.98	8	10
4	A	407	PCW	C7-N-C6	3.29	117.61	108.98	5	10
4	A	407	PCW	C8-N-C6	3.29	117.61	108.98	7	10
4	A	415	PCW	C7-N-C6	3.29	117.61	108.98	2	10
4	D	502	PCW	C8-N-C6	3.29	117.61	108.98	7	10
4	A	412	PCW	C7-N-C6	3.29	117.61	108.98	3	10
4	B	202	PCW	C8-N-C6	3.29	117.61	108.98	3	10
4	A	403	PCW	C7-N-C6	3.28	117.60	108.98	8	10
4	A	414	PCW	C2-O2-C31	3.28	109.94	117.80	5	10
4	C	623	PCW	O2-C31-C32	3.28	118.59	111.48	9	10
4	A	402	PCW	C7-N-C6	3.28	117.60	108.98	10	10
4	C	607	PCW	C8-N-C6	3.28	117.60	108.98	8	10
4	B	208	PCW	C7-N-C6	3.28	117.60	108.98	8	10
4	D	506	PCW	C7-N-C6	3.28	117.60	108.98	7	10
4	C	610	PCW	C2-O2-C31	3.28	109.94	117.80	10	10
4	C	611	PCW	C7-N-C6	3.28	117.60	108.98	4	10
4	C	602	PCW	C7-N-C6	3.28	117.59	108.98	7	10
4	C	604	PCW	C8-N-C6	3.28	117.59	108.98	3	10
4	B	204	PCW	C7-N-C6	3.28	117.59	108.98	9	10
6	B	216	GNP	C2-N1-C6	3.28	119.16	125.11	8	10
4	B	210	PCW	C8-N-C6	3.28	117.59	108.98	2	10
4	D	507	PCW	C7-N-C6	3.28	117.59	108.98	1	10
4	B	205	PCW	C7-N-C6	3.28	117.59	108.98	7	10
4	D	504	PCW	C8-N-C6	3.28	117.59	108.98	2	10
4	A	406	PCW	C8-N-C6	3.28	117.58	108.98	3	10
4	A	408	PCW	C7-N-C6	3.28	117.58	108.98	10	10
4	A	408	PCW	C8-N-C6	3.28	117.58	108.98	1	10
4	C	615	PCW	C7-N-C6	3.28	117.58	108.98	4	10
4	B	207	PCW	C7-N-C6	3.28	117.58	108.98	3	10
4	D	505	PCW	C7-N-C6	3.28	117.58	108.98	6	10
4	C	624	PCW	C8-N-C6	3.27	117.58	108.98	4	10
4	B	212	PCW	C7-N-C6	3.27	117.58	108.98	9	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	402	PCW	C8-N-C6	3.27	117.57	108.98	6	10
4	A	404	PCW	C7-N-C6	3.27	117.57	108.98	2	10
4	C	618	PCW	C7-N-C6	3.27	117.57	108.98	8	10
4	C	601	PCW	C8-N-C6	3.27	117.57	108.98	4	10
4	A	405	PCW	C8-N-C6	3.27	117.57	108.98	8	10
4	A	416	PCW	C8-N-C6	3.27	117.56	108.98	3	10
4	B	209	PCW	C8-N-C6	3.27	117.56	108.98	1	10
4	D	504	PCW	C7-N-C6	3.27	117.57	108.98	5	10
4	A	404	PCW	C2-O2-C31	3.27	109.98	117.80	10	10
4	A	415	PCW	C8-N-C6	3.27	117.56	108.98	3	10
4	C	618	PCW	C2-O2-C31	3.27	109.98	117.80	5	10
4	D	501	PCW	C7-N-C6	3.27	117.56	108.98	2	10
4	D	502	PCW	C7-N-C6	3.27	117.56	108.98	2	10
4	A	412	PCW	C8-N-C6	3.26	117.55	108.98	10	10
4	B	209	PCW	C7-N-C6	3.26	117.55	108.98	6	10
4	D	501	PCW	C8-N-C6	3.26	117.55	108.98	8	10
4	C	610	PCW	C8-N-C6	3.26	117.54	108.98	2	10
4	C	610	PCW	C7-N-C6	3.26	117.54	108.98	6	10
4	C	617	PCW	C7-N-C6	3.26	117.54	108.98	9	10
4	B	202	PCW	C7-N-C6	3.26	117.54	108.98	8	10
4	B	205	PCW	C8-N-C6	3.26	117.54	108.98	1	10
4	A	416	PCW	C7-N-C6	3.26	117.53	108.98	2	10
4	C	611	PCW	C8-N-C6	3.26	117.53	108.98	8	10
4	A	405	PCW	C7-N-C6	3.26	117.53	108.98	9	10
4	C	605	PCW	C7-N-C6	3.26	117.53	108.98	2	10
4	C	623	PCW	C8-N-C6	3.26	117.53	108.98	7	10
4	D	509	PCW	C8-N-C6	3.26	117.53	108.98	3	10
4	A	414	PCW	C7-N-C6	3.25	117.52	108.98	8	10
4	C	621	PCW	C7-N-C6	3.25	117.52	108.98	5	10
4	B	211	PCW	C8-N-C6	3.25	117.52	108.98	1	10
4	D	509	PCW	C7-N-C6	3.25	117.51	108.98	5	10
4	C	622	PCW	C8-N-C6	3.25	117.50	108.98	3	10
4	B	206	PCW	C8-N-C6	3.25	117.50	108.98	7	10
4	A	411	PCW	C7-N-C6	3.24	117.50	108.98	5	10
4	A	417	PCW	C2-O2-C31	3.24	110.03	117.80	10	5
4	C	624	PCW	C7-N-C6	3.24	117.50	108.98	5	10
4	A	403	PCW	C8-N-C6	3.24	117.49	108.98	2	10
4	C	619	PCW	C7-N-C6	3.24	117.49	108.98	5	10
4	D	515	PCW	C8-N-C6	3.24	117.49	108.98	5	10
4	C	606	PCW	C2-O2-C31	3.24	110.04	117.80	4	10
4	C	621	PCW	C8-N-C6	3.24	117.47	108.98	3	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	B	201	PCW	C7-N-C6	3.23	117.46	108.98	8	10
4	B	201	PCW	C8-N-C6	3.23	117.46	108.98	10	10
4	D	510	PCW	C8-N-C6	3.23	117.46	108.98	8	10
4	B	208	PCW	C2-O2-C31	3.23	110.07	117.80	4	10
4	B	212	PCW	C8-N-C6	3.23	117.45	108.98	5	10
4	C	617	PCW	C8-N-C6	3.23	117.45	108.98	1	10
5	C	628	17F	C5-O9-C17	3.23	110.08	117.80	8	10
5	D	511	17F	C5-O9-C17	3.22	110.08	117.80	7	10
4	A	404	PCW	C8-N-C6	3.22	117.44	108.98	8	10
4	C	606	PCW	C7-N-C6	3.22	117.44	108.98	2	10
4	D	516	PCW	C8-N-C6	3.22	117.44	108.98	8	10
4	C	615	PCW	C8-N-C6	3.22	117.43	108.98	10	10
4	B	203	PCW	C8-N-C6	3.21	117.42	108.98	4	10
4	A	401	PCW	C8-N-C6	3.20	117.39	108.98	6	10
5	C	630	17F	O3-P1-O1	3.20	96.25	108.94	3	10
4	C	613	PCW	C7-N-C6	3.20	117.37	108.98	3	10
4	C	608	PCW	C8-N-C6	3.19	117.35	108.98	6	10
5	C	626	17F	C5-O9-C17	3.18	110.18	117.80	1	10
4	A	412	PCW	C2-O2-C31	3.15	110.26	117.80	3	9
4	D	503	PCW	O4P-P-O2P	3.14	96.51	108.94	10	10
4	D	502	PCW	C2-O2-C31	3.12	110.34	117.80	3	10
4	A	407	PCW	C2-O2-C31	3.11	110.35	117.80	10	10
4	A	417	PCW	C8-N-C6	3.11	117.15	108.98	5	10
4	C	602	PCW	C2-O2-C31	3.10	110.38	117.80	6	10
4	B	211	PCW	C2-O2-C31	3.07	110.44	117.80	10	10
5	A	409	17F	O3-P1-O1	3.07	96.76	108.94	6	10
4	C	608	PCW	C2-O2-C31	3.07	110.46	117.80	5	10
4	D	516	PCW	O4P-P-O2P	3.05	96.84	108.94	7	10
4	C	615	PCW	C2-O2-C31	3.03	110.55	117.80	8	10
5	D	512	17F	C5-O9-C17	3.01	110.60	117.80	8	10
4	D	516	PCW	C2-O2-C31	2.95	110.74	117.80	7	10
4	C	614	PCW	O3-C11-C12	2.90	120.69	111.83	6	10
4	A	416	PCW	C2-O2-C31	2.89	110.87	117.80	10	10
4	A	408	PCW	O3-C11-C12	2.89	120.64	111.83	6	10
4	A	414	PCW	O3-C11-C12	2.89	120.63	111.83	6	10
4	C	605	PCW	O3-C11-C12	2.87	120.59	111.83	10	10
4	C	603	PCW	O3-C11-C12	2.87	120.59	111.83	4	10
5	D	511	17F	O7-C7-C8	2.81	120.40	111.83	1	10
4	A	416	PCW	O3-C11-C12	2.77	120.29	111.83	2	10
6	B	216	GNP	C3'-C2'-C1'	2.77	96.23	101.46	5	10
4	C	616	PCW	O3-C11-C12	2.77	120.27	111.83	2	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	417	PCW	O3-C11-C12	2.76	120.25	111.83	1	10
4	D	506	PCW	O3-C11-C12	2.76	120.24	111.83	8	10
5	C	630	17F	O7-C7-C8	2.76	120.25	111.83	1	10
4	B	211	PCW	O3-C11-C12	2.75	120.23	111.83	7	10
4	C	620	PCW	O3-C11-C12	2.75	120.22	111.83	8	10
4	B	208	PCW	O3-C11-C12	2.73	120.16	111.83	6	10
5	A	409	17F	O2-P1-O1	2.73	125.15	112.44	5	10
4	D	515	PCW	O3-C11-C12	2.73	120.15	111.83	3	10
4	B	205	PCW	O3-C11-C12	2.73	120.15	111.83	4	10
4	C	621	PCW	O3-C11-C12	2.72	120.14	111.83	1	10
4	A	411	PCW	O3-C11-C12	2.72	120.13	111.83	7	10
5	C	630	17F	O2-P1-O1	2.72	125.09	112.44	4	10
4	D	503	PCW	O1P-P-O2P	2.72	125.08	112.44	1	10
4	D	516	PCW	O3-C11-C12	2.70	120.08	111.83	10	10
4	B	210	PCW	O3-C11-C12	2.70	120.07	111.83	6	10
5	C	627	17F	C5-O9-C17	2.69	111.35	117.80	7	10
4	A	408	PCW	C3-O3-C11	2.69	107.28	117.12	6	9
4	D	516	PCW	O1P-P-O2P	2.69	124.96	112.44	7	10
4	A	413	PCW	O3-C11-C12	2.67	119.98	111.83	10	10
4	A	404	PCW	O3-C11-C12	2.67	119.97	111.83	7	10
4	C	625	PCW	O3-C11-C12	2.67	119.97	111.83	8	10
4	C	608	PCW	O3-C11-C12	2.67	119.97	111.83	5	10
4	C	617	PCW	O3-C11-C12	2.67	119.96	111.83	10	10
4	D	501	PCW	O3-C11-C12	2.66	119.95	111.83	6	10
4	B	207	PCW	O3-C11-C12	2.66	119.94	111.83	8	10
5	A	410	17F	O7-C7-C8	2.65	119.92	111.83	2	10
4	C	624	PCW	O3-C11-C12	2.65	119.92	111.83	3	10
5	A	409	17F	O7-C7-C8	2.65	119.90	111.83	7	10
4	C	610	PCW	O3-C11-C12	2.64	119.90	111.83	10	10
4	C	619	PCW	O3-C11-C12	2.64	119.89	111.83	5	10
5	C	631	17F	O7-C7-C8	2.64	119.89	111.83	5	10
4	D	509	PCW	O3-C11-C12	2.64	119.87	111.83	7	10
4	A	412	PCW	O3-C11-C12	2.62	119.82	111.83	7	10
4	D	510	PCW	O3-C11-C12	2.61	119.80	111.83	10	10
5	D	513	17F	O7-C7-C8	2.61	119.81	111.83	3	10
4	C	622	PCW	O3-C11-C12	2.60	119.78	111.83	3	10
4	C	601	PCW	O3-C11-C12	2.60	119.77	111.83	7	10
4	D	502	PCW	O3-C11-C12	2.60	119.76	111.83	5	10
4	B	209	PCW	O3-C11-C12	2.60	119.75	111.83	3	10
5	D	512	17F	O7-C7-C8	2.60	119.76	111.83	7	10
4	D	503	PCW	O3-C11-C12	2.59	119.74	111.83	9	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	B	204	PCW	O3-C11-C12	2.59	119.73	111.83	8	10
4	C	611	PCW	O3-C11-C12	2.59	119.72	111.83	4	10
4	C	613	PCW	O3-C11-C12	2.58	119.72	111.83	10	10
4	B	212	PCW	O3-C11-C12	2.58	119.71	111.83	7	10
5	C	632	17F	O7-C7-C8	2.58	119.71	111.83	9	10
5	C	626	17F	O7-C7-C8	2.58	119.70	111.83	4	10
5	B	215	17F	O7-C7-C8	2.58	119.69	111.83	6	10
4	D	505	PCW	O3-C11-C12	2.57	119.69	111.83	4	10
4	B	202	PCW	O3-C11-C12	2.57	119.68	111.83	1	10
4	A	402	PCW	O3-C11-C12	2.57	119.67	111.83	10	10
4	A	407	PCW	O3-C11-C12	2.57	119.67	111.83	9	10
4	C	615	PCW	O3-C11-C12	2.57	119.66	111.83	3	10
4	B	203	PCW	O3-C11-C12	2.56	119.65	111.83	4	10
5	B	214	17F	O7-C7-C8	2.56	119.65	111.83	9	10
4	C	605	PCW	C3-O3-C11	2.56	107.77	117.12	9	10
4	B	201	PCW	O3-C11-C12	2.55	119.60	111.83	7	10
5	A	409	17F	O2-P1-O3	2.55	96.02	107.57	2	10
4	C	602	PCW	O3-C11-C12	2.55	119.60	111.83	9	10
4	C	623	PCW	O3-C11-C12	2.54	119.59	111.83	5	10
5	D	514	17F	O7-C7-C8	2.54	119.58	111.83	3	10
4	A	403	PCW	O3-C11-C12	2.54	119.57	111.83	9	10
4	A	406	PCW	O3-C11-C12	2.54	119.57	111.83	2	10
4	C	607	PCW	O3-C11-C12	2.53	119.55	111.83	5	10
5	B	213	17F	O7-C7-C8	2.53	119.54	111.83	2	10
4	D	503	PCW	O1P-P-O4P	2.53	96.12	107.57	8	10
4	C	623	PCW	C2-O2-C31	2.52	111.75	117.80	10	7
4	D	508	PCW	O3-C11-C12	2.52	119.52	111.83	3	10
4	C	612	PCW	O3-C11-C12	2.51	119.49	111.83	4	10
5	C	628	17F	O7-C7-C8	2.51	119.50	111.83	2	10
5	C	629	17F	O7-C7-C8	2.51	119.50	111.83	6	10
4	C	609	PCW	O3-C11-C12	2.51	119.48	111.83	6	10
4	C	611	PCW	C3-C2-C1	2.51	105.94	111.78	7	1
5	C	627	17F	O7-C7-C8	2.50	119.45	111.83	8	10
4	D	507	PCW	O3-C11-C12	2.49	119.43	111.83	5	10
4	D	504	PCW	O3-C11-C12	2.49	119.42	111.83	6	10
4	C	625	PCW	C3-O3-C11	2.48	108.06	117.12	4	3
4	D	516	PCW	O1P-P-O4P	2.48	96.34	107.57	2	10
4	C	606	PCW	O3-C11-C12	2.47	119.37	111.83	3	10
5	D	511	17F	C6-O7-C7	2.46	108.12	117.12	1	9
4	A	416	PCW	C3-O3-C11	2.46	108.13	117.12	2	5
4	A	405	PCW	O3-C11-C12	2.45	119.30	111.83	7	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	B	206	PCW	O3-C11-C12	2.45	119.30	111.83	1	10
6	B	216	GNP	C4-C5-N7	2.43	106.81	110.67	2	9
4	A	417	PCW	C3-O3-C11	2.43	108.23	117.12	4	8
4	A	414	PCW	C3-O3-C11	2.42	108.28	117.12	6	8
4	C	617	PCW	C3-O3-C11	2.40	108.33	117.12	10	9
4	A	401	PCW	O3-C11-C12	2.40	119.16	111.83	5	10
6	B	216	GNP	C8-N7-C5	2.39	108.51	104.26	2	10
4	C	616	PCW	C3-O3-C11	2.38	108.42	117.12	3	5
4	C	621	PCW	C3-O3-C11	2.38	108.42	117.12	6	10
4	A	415	PCW	O3-C11-C12	2.38	119.08	111.83	4	10
4	C	604	PCW	O3-C11-C12	2.37	119.06	111.83	7	10
4	C	603	PCW	C3-O3-C11	2.37	108.46	117.12	2	5
4	C	614	PCW	C3-O3-C11	2.36	108.49	117.12	6	4
4	B	211	PCW	C3-O3-C11	2.36	108.50	117.12	7	9
4	B	205	PCW	C3-O3-C11	2.35	108.52	117.12	3	5
5	C	630	17F	O2-P1-O3	2.35	96.91	107.57	2	10
4	A	411	PCW	C3-O3-C11	2.33	108.60	117.12	6	6
4	D	502	PCW	C3-O3-C11	2.33	108.61	117.12	5	4
4	D	516	PCW	O1P-P-O3P	2.33	118.12	107.57	6	10
4	D	503	PCW	O1P-P-O3P	2.33	118.12	107.57	3	10
5	C	628	17F	C6-O7-C7	2.31	108.67	117.12	2	8
5	C	630	17F	O6-P1-O1	2.31	118.09	108.94	3	10
5	C	630	17F	C6-O7-C7	2.31	108.68	117.12	2	9
5	A	409	17F	O6-P1-O1	2.31	118.08	108.94	3	10
4	B	207	PCW	C3-O3-C11	2.30	108.72	117.12	8	4
4	B	210	PCW	C3-O3-C11	2.30	108.72	117.12	9	7
4	D	501	PCW	C3-O3-C11	2.30	108.72	117.12	6	6
4	C	610	PCW	C3-O3-C11	2.28	108.78	117.12	10	5
4	D	515	PCW	C3-O3-C11	2.28	108.78	117.12	9	7
5	B	215	17F	C6-O7-C7	2.28	108.80	117.12	2	4
6	B	216	GNP	O4'-C1'-C2'	2.28	101.74	106.62	4	2
4	D	506	PCW	C3-O3-C11	2.27	108.81	117.12	6	6
5	C	631	17F	C6-O7-C7	2.27	108.81	117.12	10	4
6	B	216	GNP	N9-C8-N7	2.27	109.20	113.40	6	10
4	C	618	PCW	O3-C11-C12	2.26	118.74	111.83	9	10
4	A	413	PCW	C3-O3-C11	2.25	108.89	117.12	1	4
6	B	216	GNP	O6-C6-C5	2.25	120.60	126.53	9	10
5	D	512	17F	C6-O7-C7	2.20	109.06	117.12	7	2
4	C	609	PCW	C4-C5-N	2.20	108.77	115.82	1	4
4	C	619	PCW	C3-O3-C11	2.20	109.08	117.12	9	5
4	A	404	PCW	C3-O3-C11	2.19	109.10	117.12	4	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	C	627	17F	O9-C17-O10	2.19	118.59	123.70	9	9
4	C	613	PCW	C3-O3-C11	2.18	109.15	117.12	8	6
4	B	208	PCW	C3-O3-C11	2.17	109.18	117.12	6	1
4	C	608	PCW	C3-O3-C11	2.17	109.20	117.12	1	7
6	B	216	GNP	C5-C6-N1	2.17	118.77	113.25	8	10
5	A	409	17F	C6-O7-C7	2.16	109.21	117.12	7	3
4	B	204	PCW	C3-O3-C11	2.16	109.22	117.12	7	4
4	C	621	PCW	C4-C5-N	2.15	108.91	115.82	3	3
5	B	214	17F	C6-O7-C7	2.15	109.25	117.12	9	2
4	A	412	PCW	C3-O3-C11	2.15	109.26	117.12	7	5
5	C	632	17F	C6-O7-C7	2.15	109.27	117.12	1	4
4	C	601	PCW	C3-O3-C11	2.14	109.29	117.12	7	3
4	B	212	PCW	C3-O3-C11	2.14	109.29	117.12	7	7
4	C	624	PCW	C3-O3-C11	2.14	109.29	117.12	8	3
5	A	410	17F	C6-O7-C7	2.13	109.32	117.12	2	4
5	C	626	17F	C6-O7-C7	2.13	109.32	117.12	8	2
4	D	503	PCW	C3-O3-C11	2.12	109.38	117.12	9	2
4	C	620	PCW	C3-O3-C11	2.11	109.39	117.12	8	2
5	D	513	17F	C6-O7-C7	2.10	109.43	117.12	2	2
4	A	414	PCW	C4-C5-N	2.10	109.09	115.82	6	2
4	C	622	PCW	C3-O3-C11	2.10	109.45	117.12	3	3
4	C	621	PCW	C3-C2-C1	2.09	106.90	111.78	6	1
6	B	216	GNP	O1B-PB-N3B	2.09	108.69	111.77	9	2
4	A	406	PCW	C3-O3-C11	2.09	109.47	117.12	10	1
4	C	610	PCW	C4-C5-N	2.08	109.16	115.82	2	1
4	C	603	PCW	C4-C5-N	2.07	109.17	115.82	8	3
4	C	607	PCW	C4-C5-N	2.07	109.17	115.82	3	2
4	A	408	PCW	C4-C5-N	2.07	109.18	115.82	10	2
4	C	625	PCW	C8-N-C5	2.07	118.14	109.91	1	1
4	C	601	PCW	C4-C5-N	2.07	109.18	115.82	8	4
4	C	619	PCW	C4-C5-N	2.06	109.20	115.82	1	3
4	D	504	PCW	C3-O3-C11	2.06	109.58	117.12	2	1
4	C	607	PCW	C3-O3-C11	2.06	109.58	117.12	5	1
4	A	416	PCW	C4-C5-N	2.06	109.21	115.82	6	1
4	C	612	PCW	C4-C5-N	2.06	109.21	115.82	4	2
4	C	625	PCW	C7-N-C5	2.06	118.09	109.91	9	2
5	C	627	17F	C6-O7-C7	2.05	109.61	117.12	10	2
4	D	505	PCW	C3-O3-C11	2.05	109.62	117.12	6	1
4	D	503	PCW	C4-C5-N	2.05	109.25	115.82	10	1
4	A	411	PCW	C3-C2-C1	2.04	107.02	111.78	3	1
5	D	514	17F	C6-O7-C7	2.04	109.64	117.12	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	407	PCW	C4-C5-N	2.04	109.27	115.82	10	3
4	A	413	PCW	C4-C5-N	2.04	109.27	115.82	4	1
4	B	209	PCW	C3-O3-C11	2.04	109.66	117.12	3	1
4	C	615	PCW	C3-O3-C11	2.04	109.67	117.12	3	3
4	D	504	PCW	C4-C5-N	2.03	109.29	115.82	9	2
5	D	514	17F	O9-C17-O10	2.04	118.95	123.70	9	1
4	A	413	PCW	O2-C31-O31	2.03	118.96	123.70	7	1
4	C	620	PCW	C4-C5-N	2.03	109.30	115.82	9	2
4	D	506	PCW	C4-C5-N	2.03	109.30	115.82	3	2
4	C	612	PCW	C3-O3-C11	2.03	109.70	117.12	6	1
4	D	516	PCW	C3-O3-C11	2.03	109.70	117.12	2	1
4	C	609	PCW	C7-N-C5	2.03	117.97	109.91	7	1
5	D	512	17F	O9-C17-O10	2.03	118.97	123.70	9	4
4	A	407	PCW	C3-O3-C11	2.03	109.72	117.12	9	1
4	D	510	PCW	C4-C5-N	2.03	109.32	115.82	9	1
4	C	620	PCW	C7-N-C5	2.02	117.95	109.91	3	1
4	D	507	PCW	C4-C5-N	2.02	109.33	115.82	1	1
4	C	604	PCW	C4-C5-N	2.02	109.33	115.82	4	1
4	C	607	PCW	C7-N-C5	2.02	117.93	109.91	3	1
4	C	625	PCW	C4-C5-N	2.02	109.35	115.82	2	1
4	D	510	PCW	C3-O3-C11	2.02	109.74	117.12	10	1
4	B	201	PCW	C3-O3-C11	2.01	109.76	117.12	3	2
4	B	201	PCW	C4-C5-N	2.01	109.37	115.82	6	2
4	B	202	PCW	C4-C5-N	2.01	109.36	115.82	10	1
4	C	605	PCW	C3-C2-C1	2.01	107.10	111.78	7	1
4	C	619	PCW	C7-N-C5	2.01	117.90	109.91	10	1
4	A	412	PCW	C4-C5-N	2.01	109.38	115.82	1	1
4	C	612	PCW	C7-N-C5	2.01	117.89	109.91	6	1
5	B	213	17F	C6-O7-C7	2.01	109.77	117.12	2	1
4	A	414	PCW	C8-N-C5	2.01	117.89	109.91	7	1
4	C	605	PCW	C4-C5-N	2.01	109.38	115.82	5	1
4	C	608	PCW	C7-N-C5	2.01	117.89	109.91	4	1
4	C	619	PCW	C8-N-C5	2.01	117.89	109.91	6	1
4	B	208	PCW	C4-C5-N	2.01	109.38	115.82	9	1
4	C	606	PCW	C4-C5-N	2.00	109.39	115.82	10	1
4	B	203	PCW	C3-O3-C11	2.00	109.80	117.12	4	1

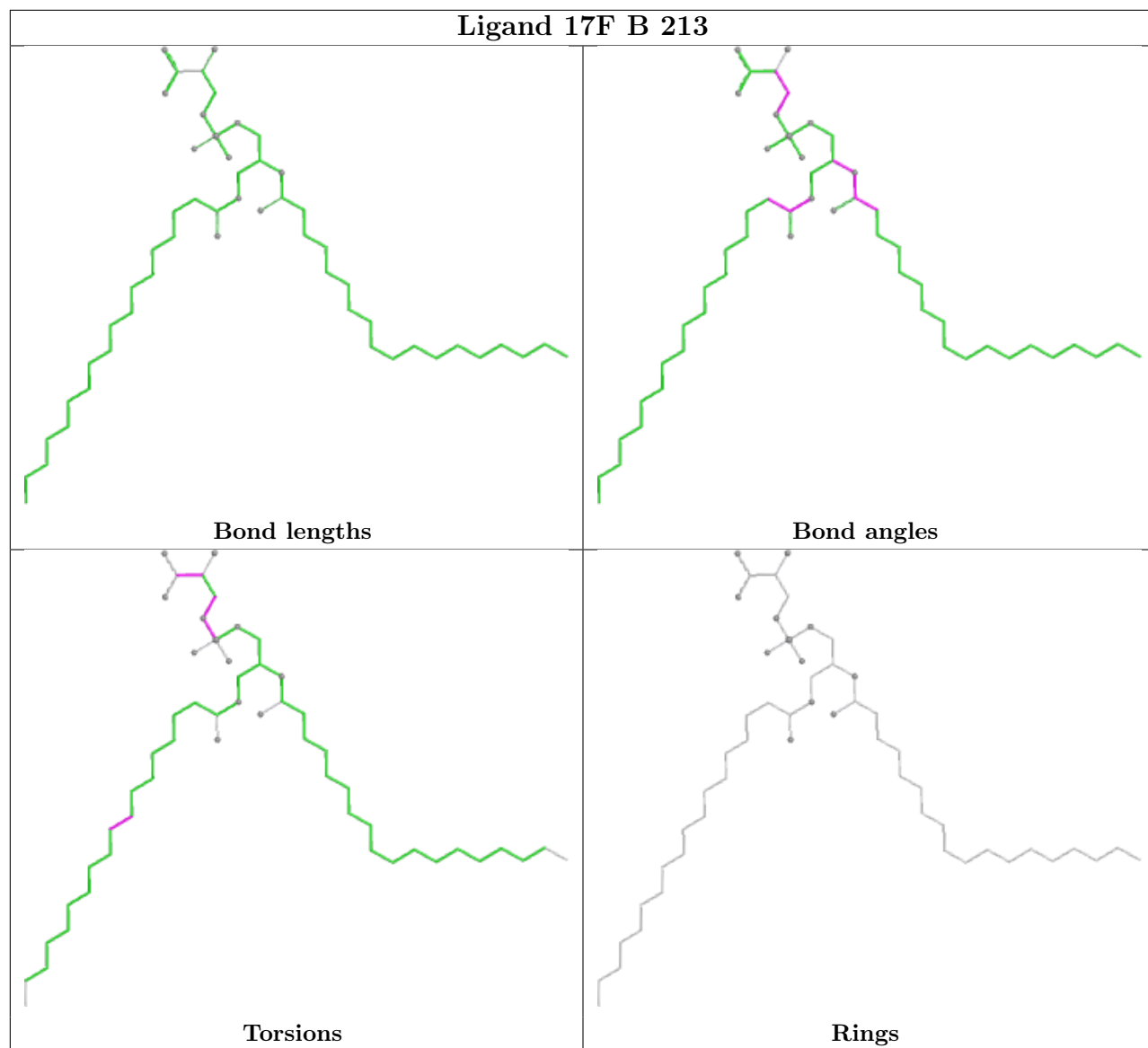
There are no chirality outliers.

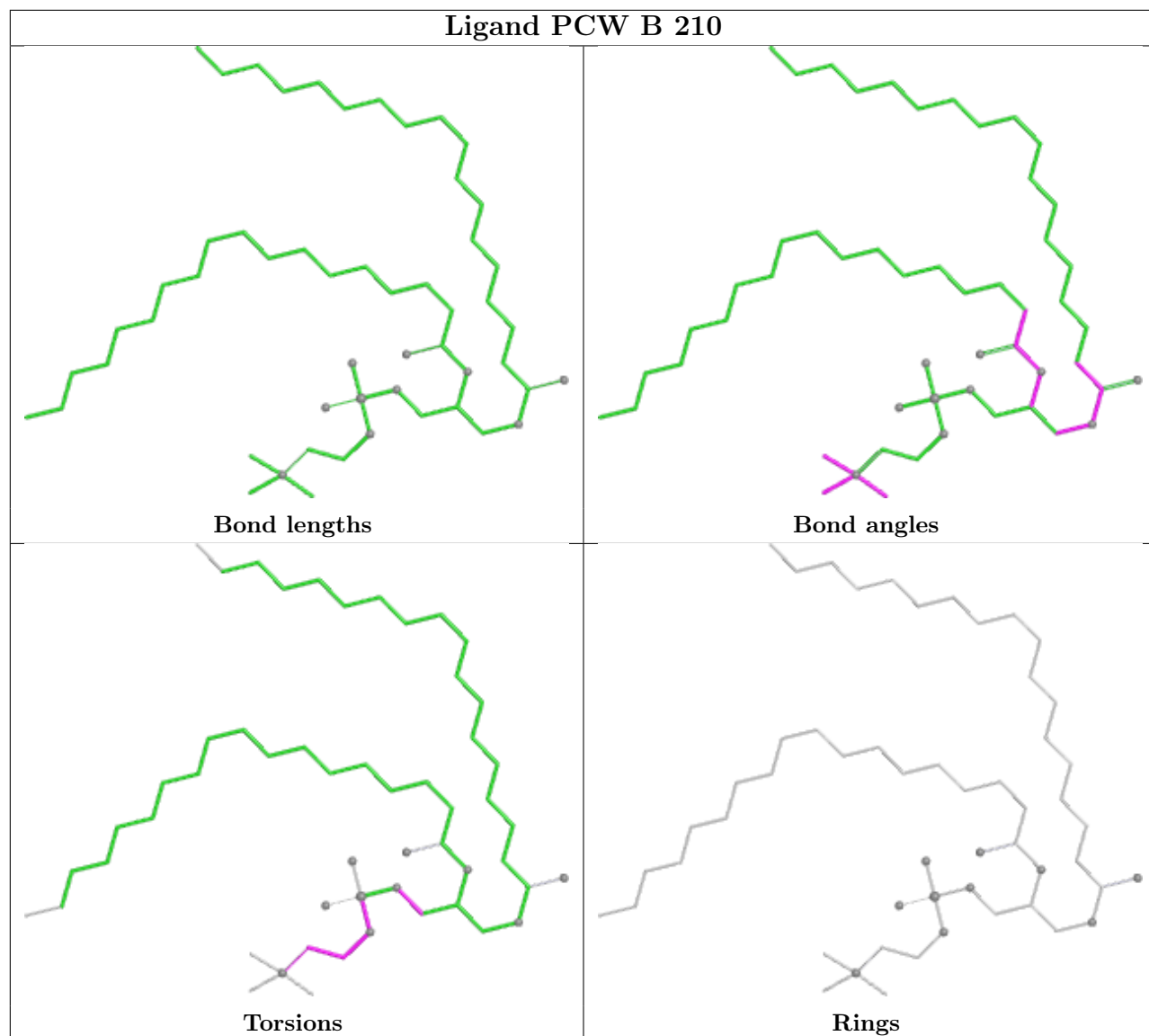
All unique torsion outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

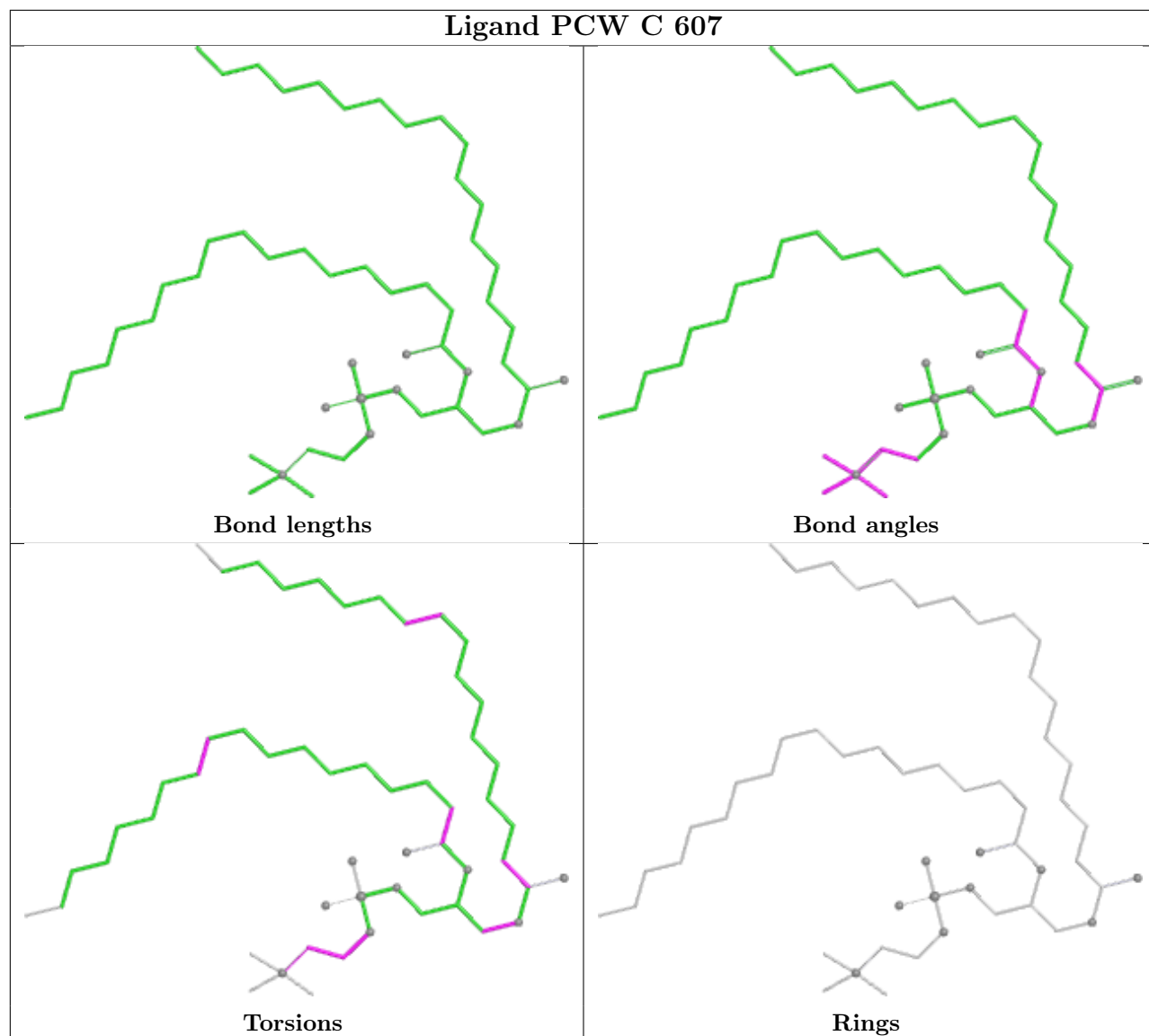
Mol	Chain	Res	Type	Atoms	Models (Total)
5	C	627	17F	O10-C17-O9-C5	10
5	D	512	17F	O10-C17-O9-C5	10
5	D	514	17F	O10-C17-O9-C5	10
5	D	512	17F	C18-C17-O9-C5	3
5	D	514	17F	C18-C17-O9-C5	2
5	C	627	17F	C18-C17-O9-C5	1

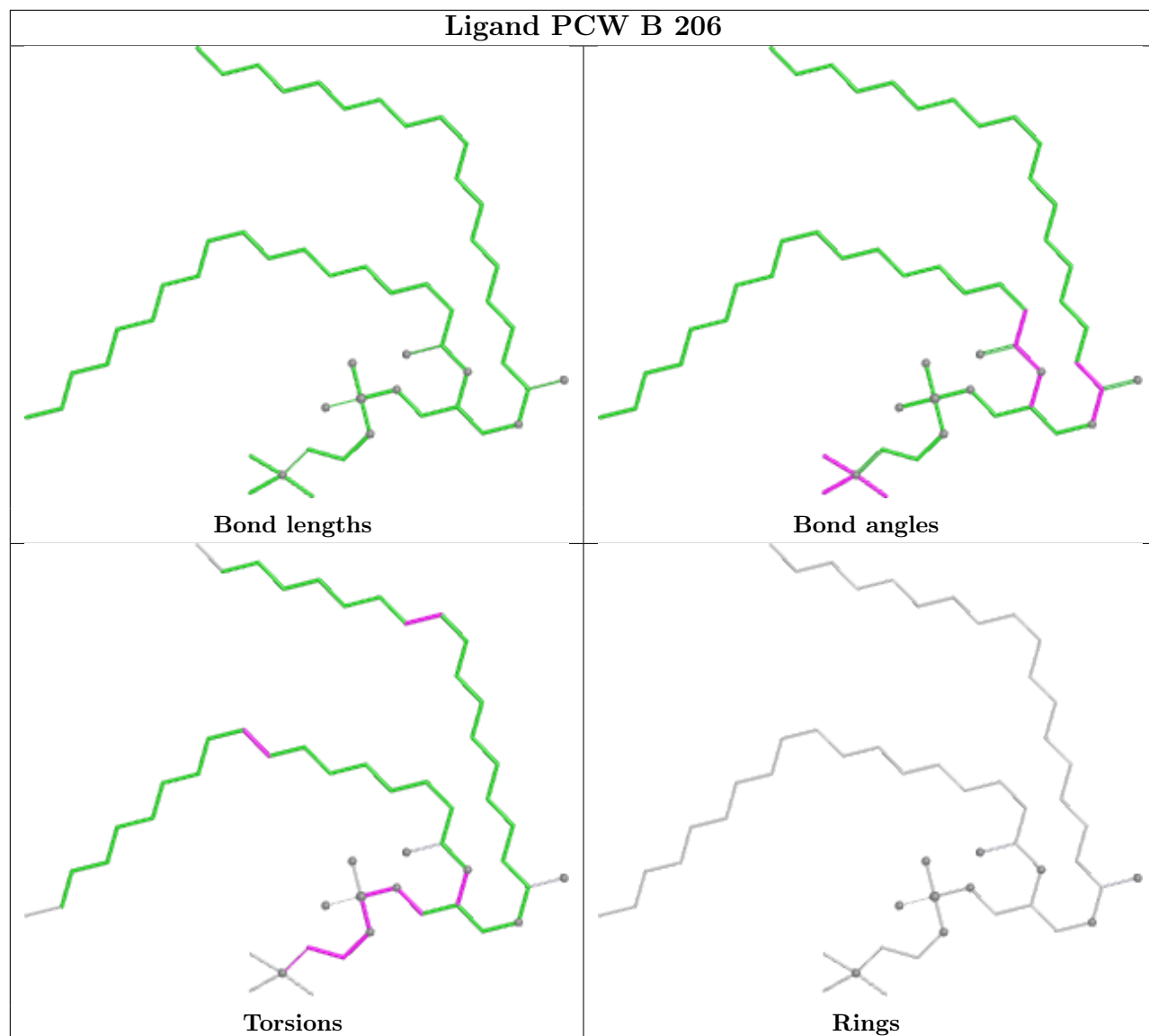
There are no ring outliers.

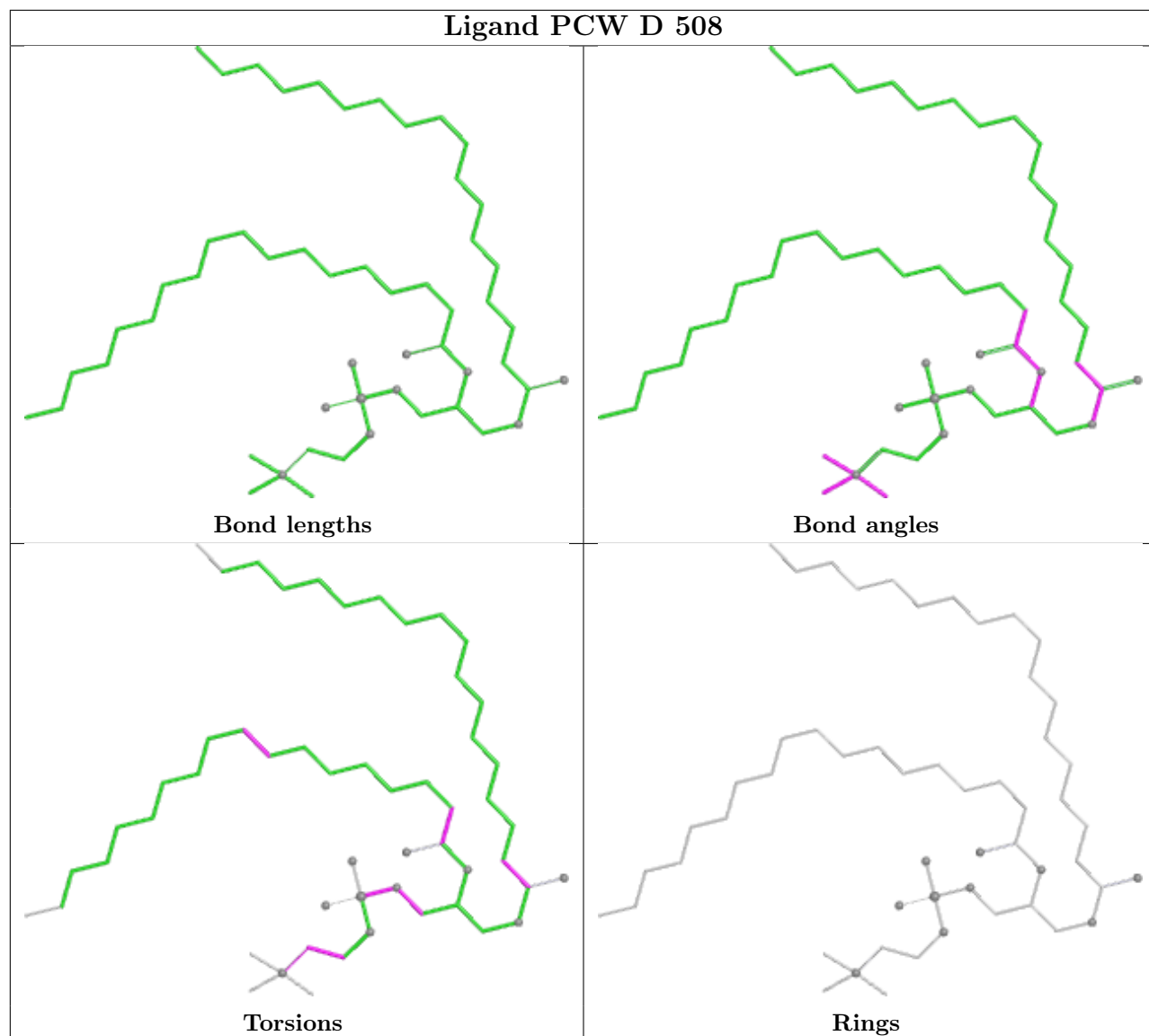
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

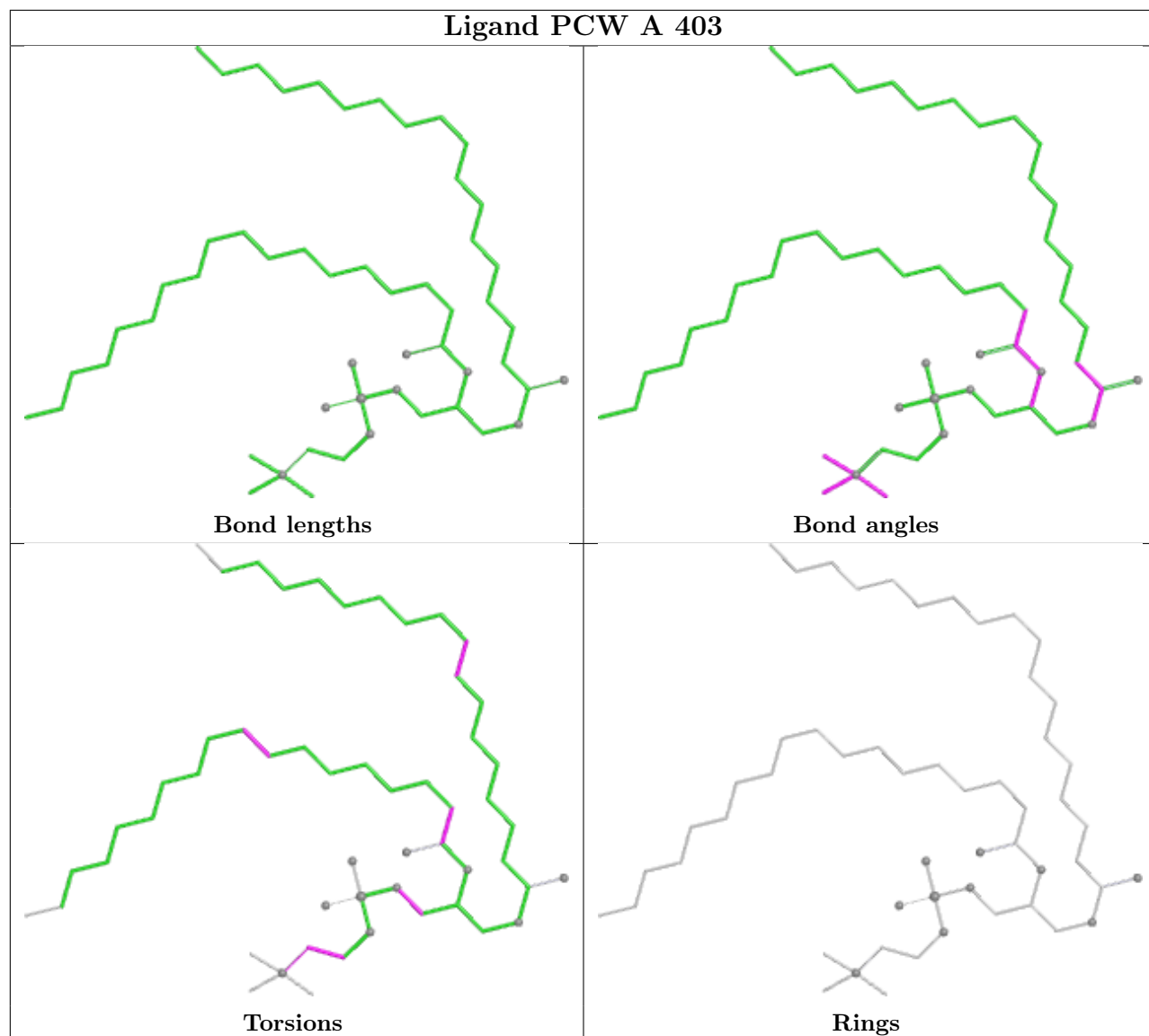


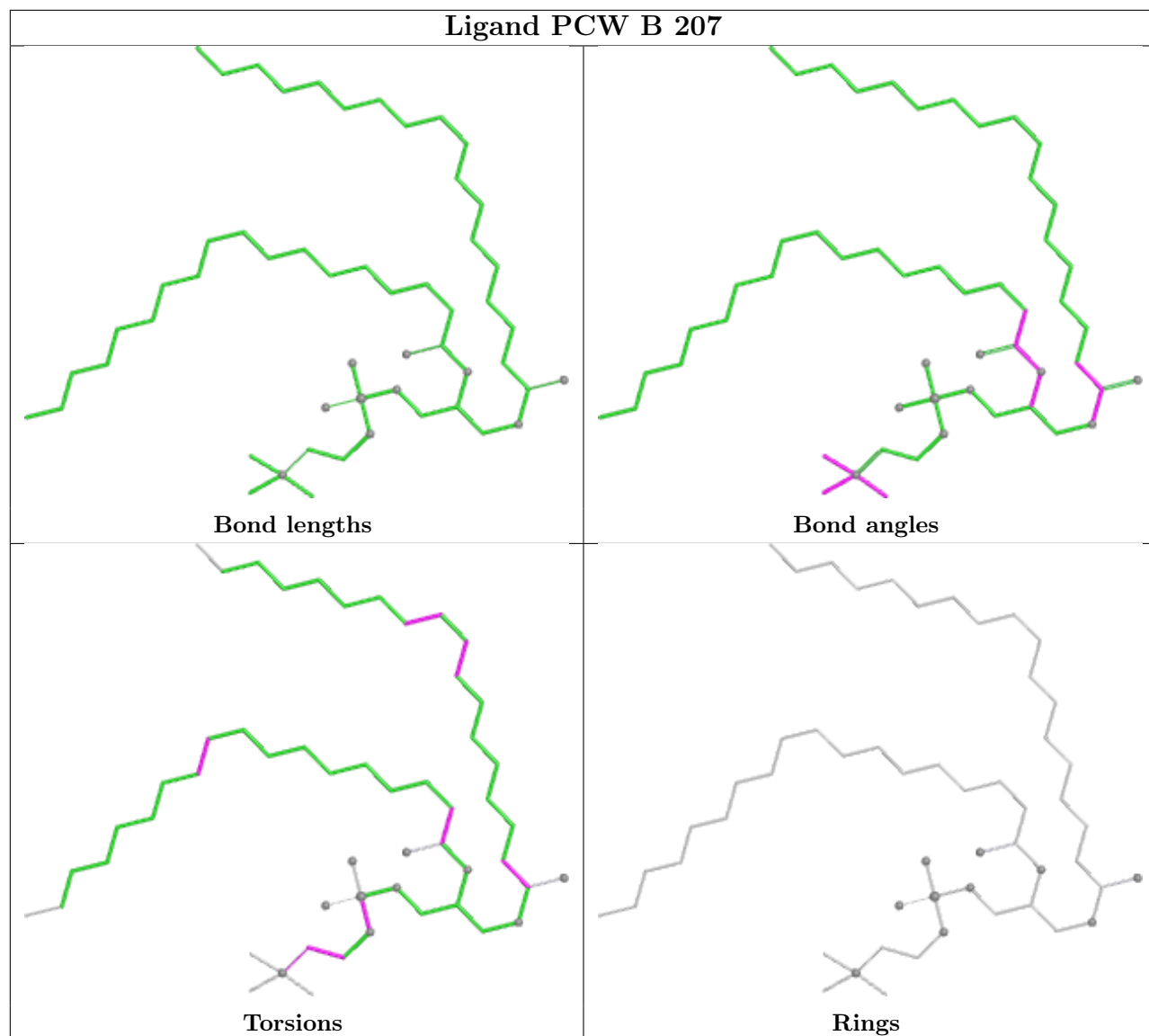


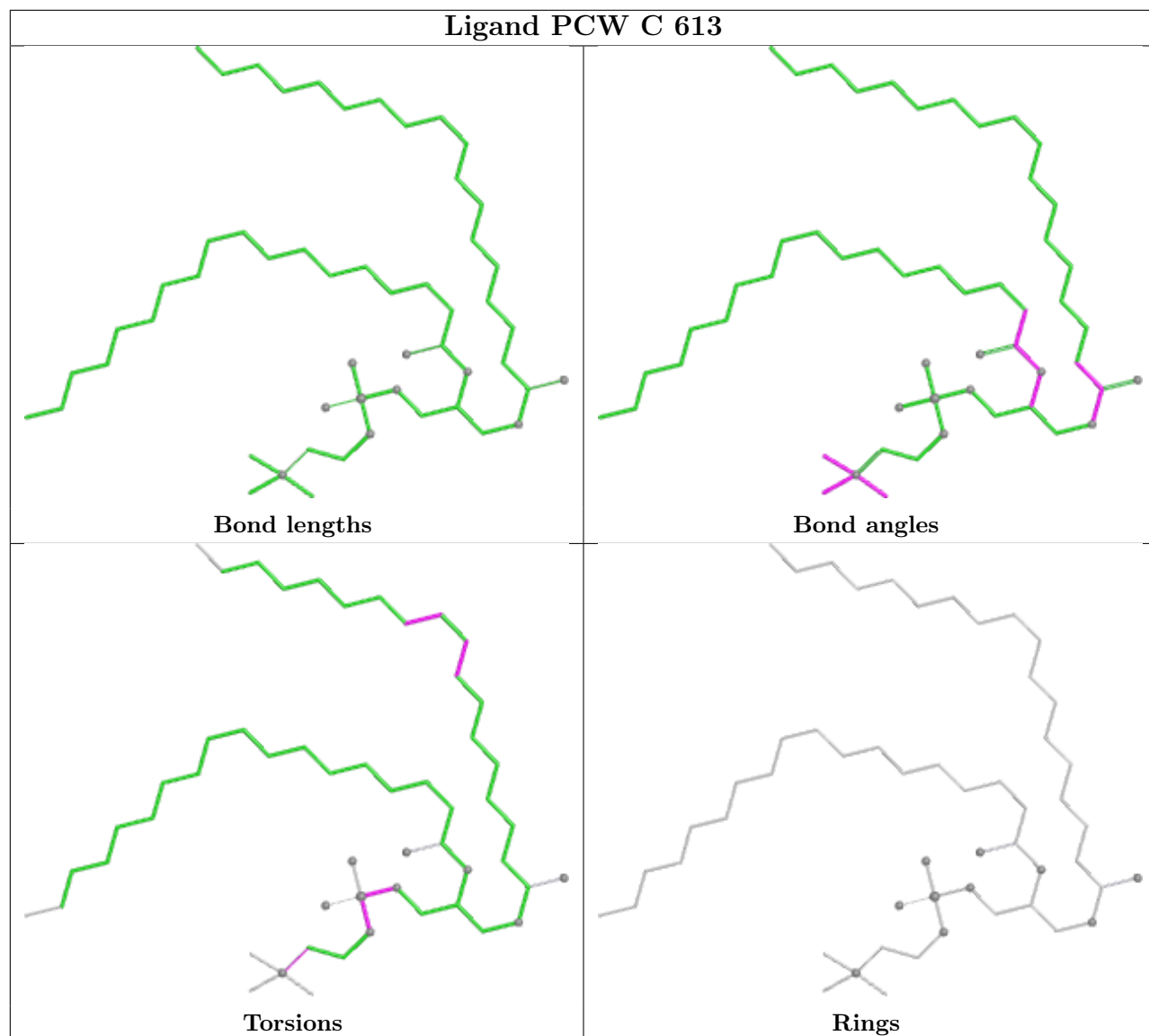


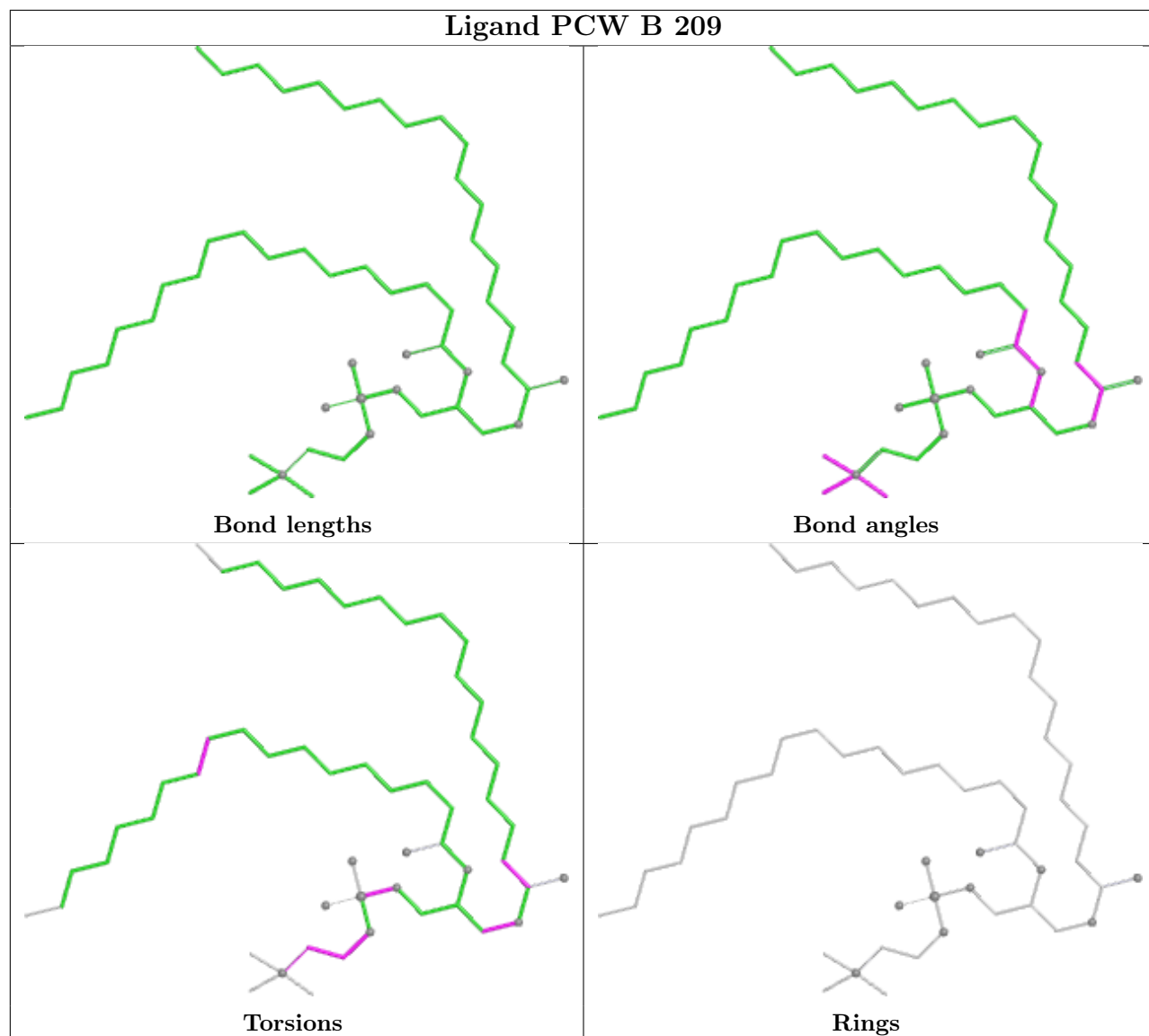


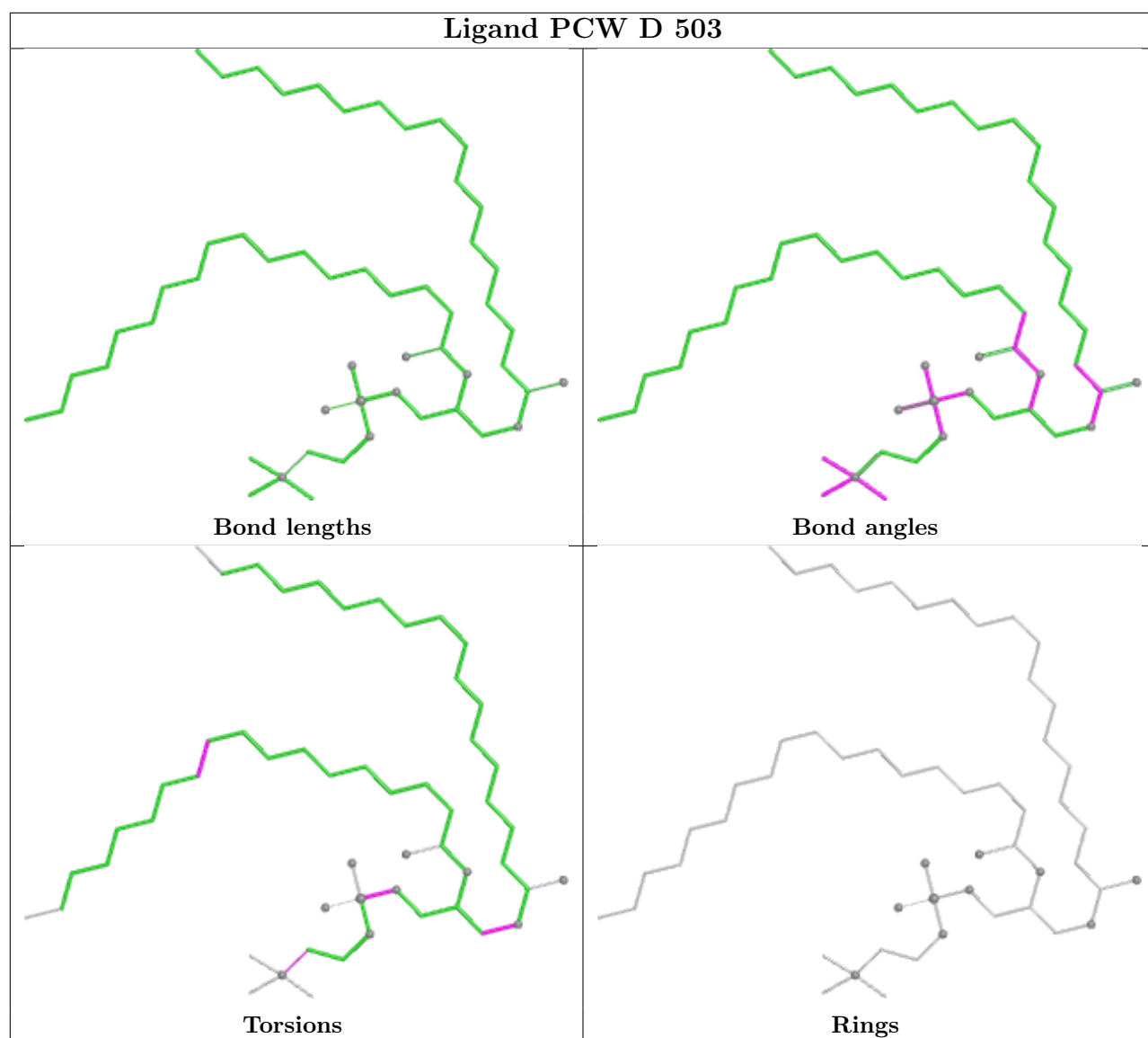


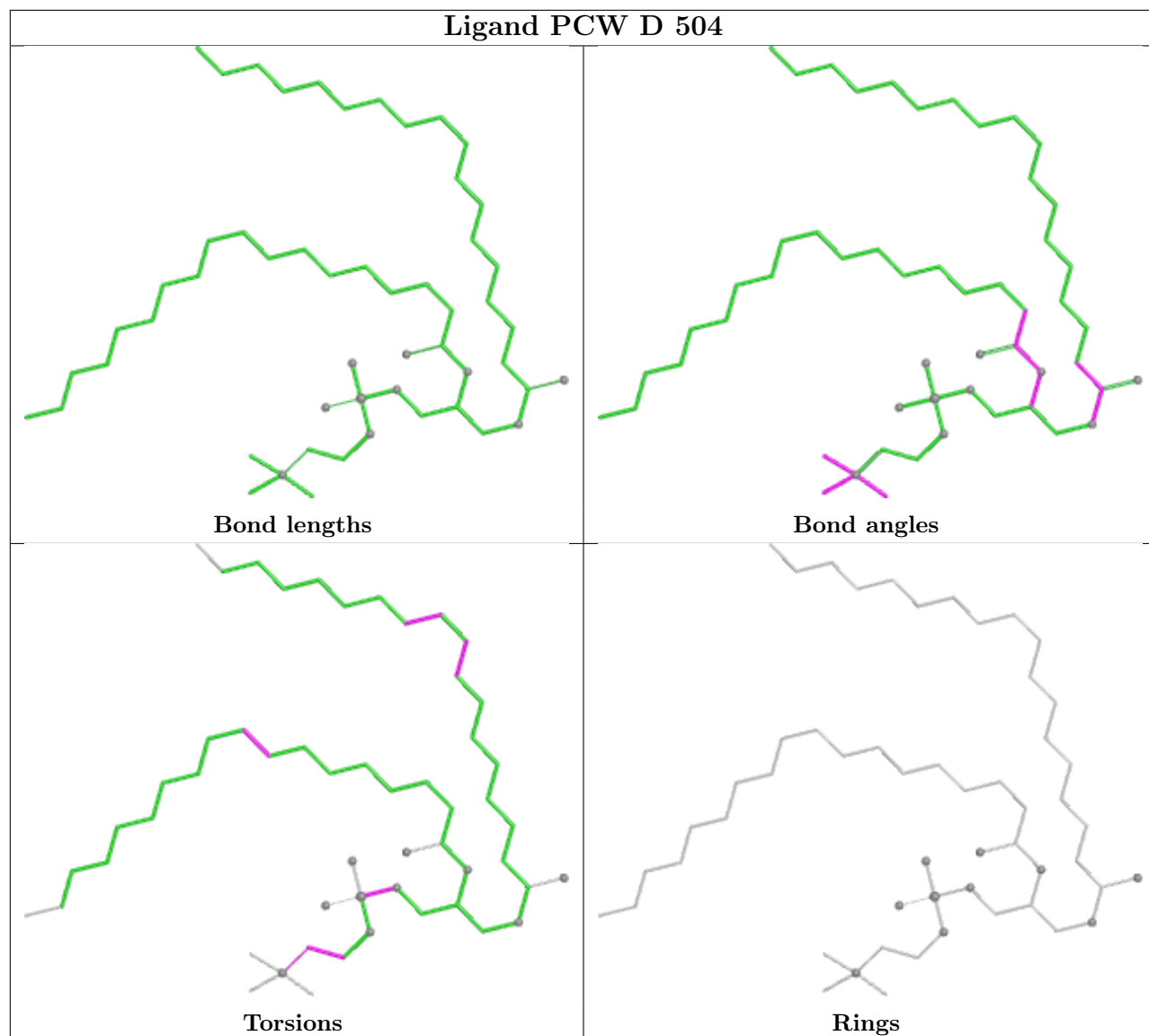


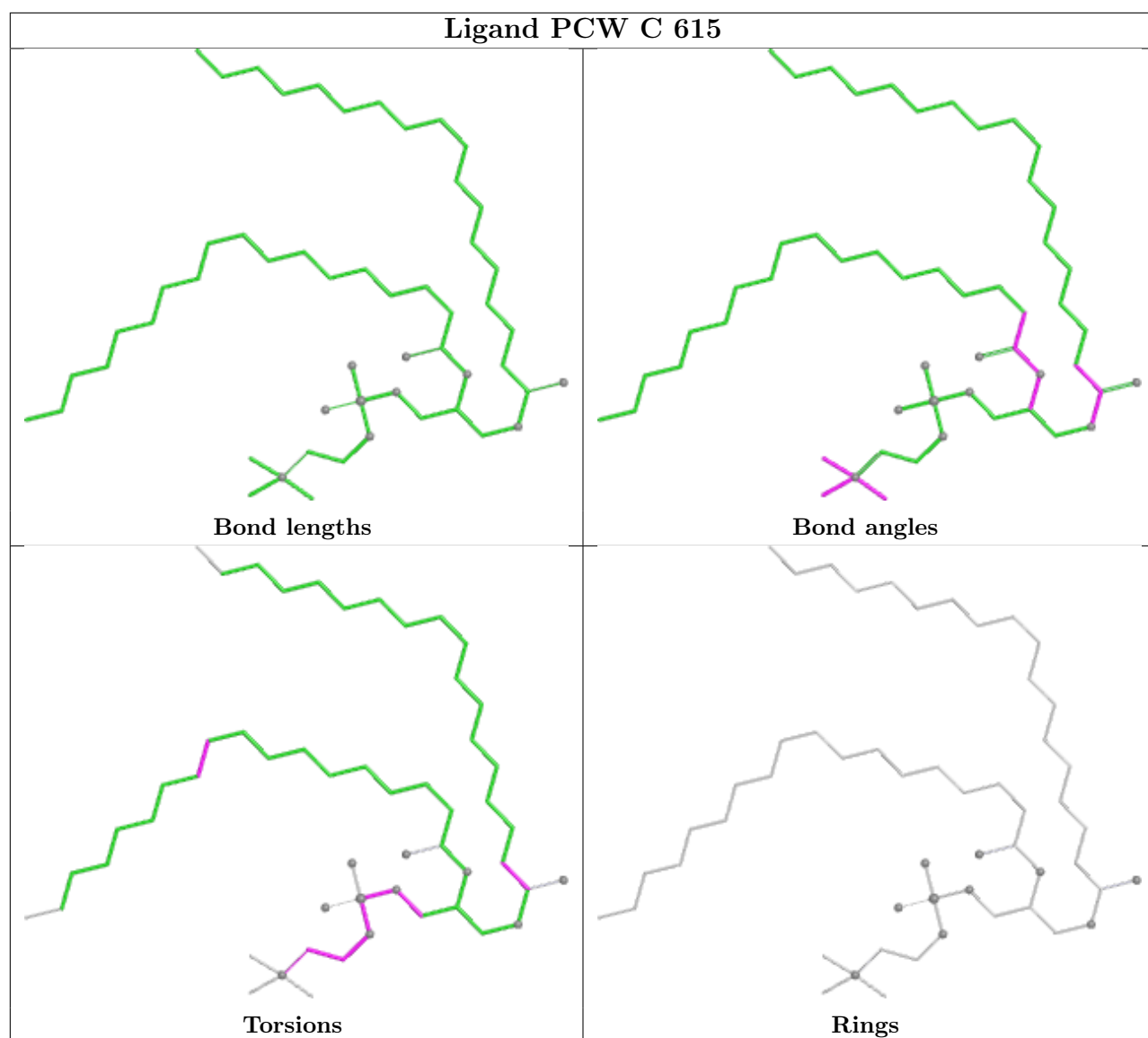


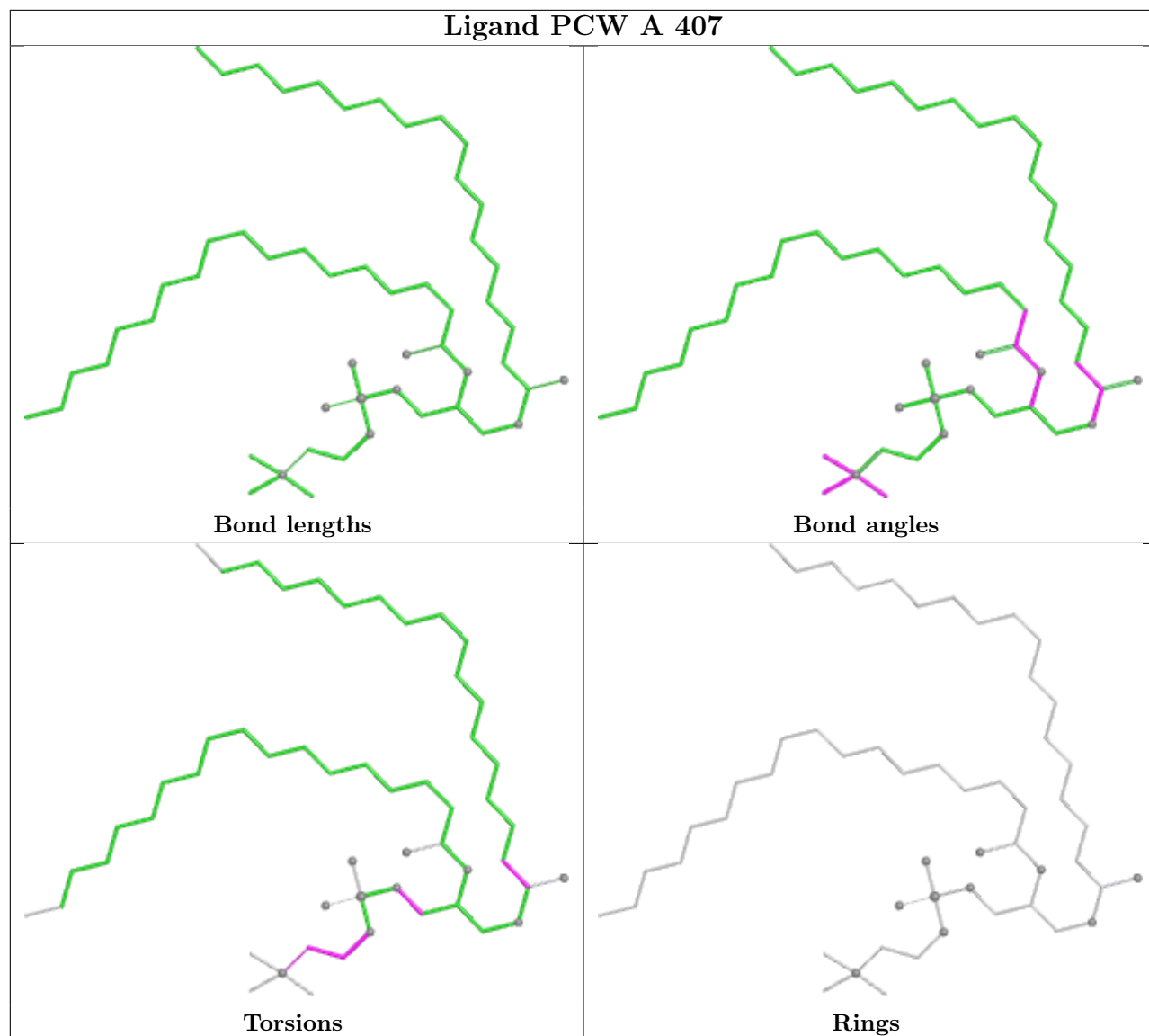


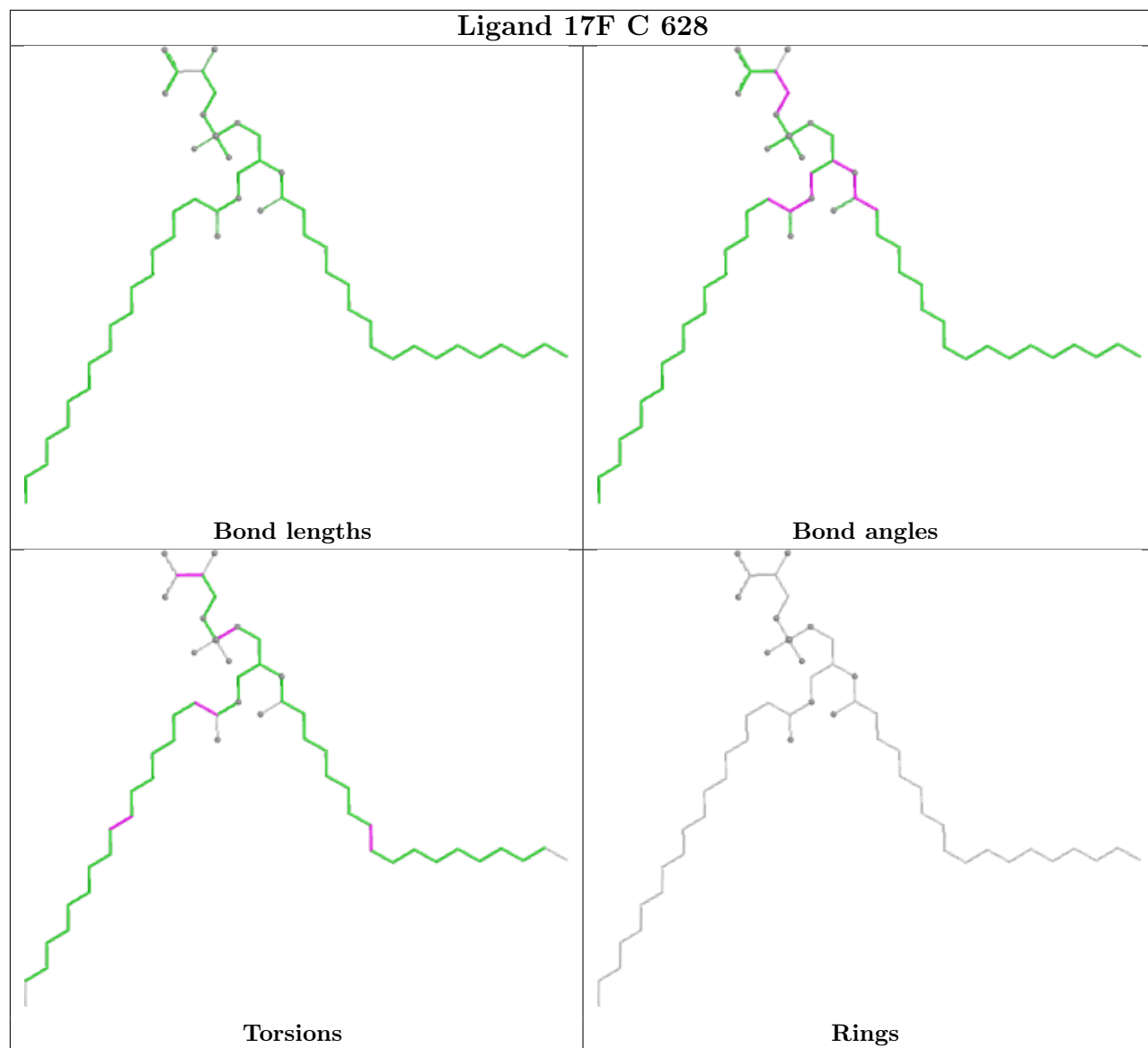


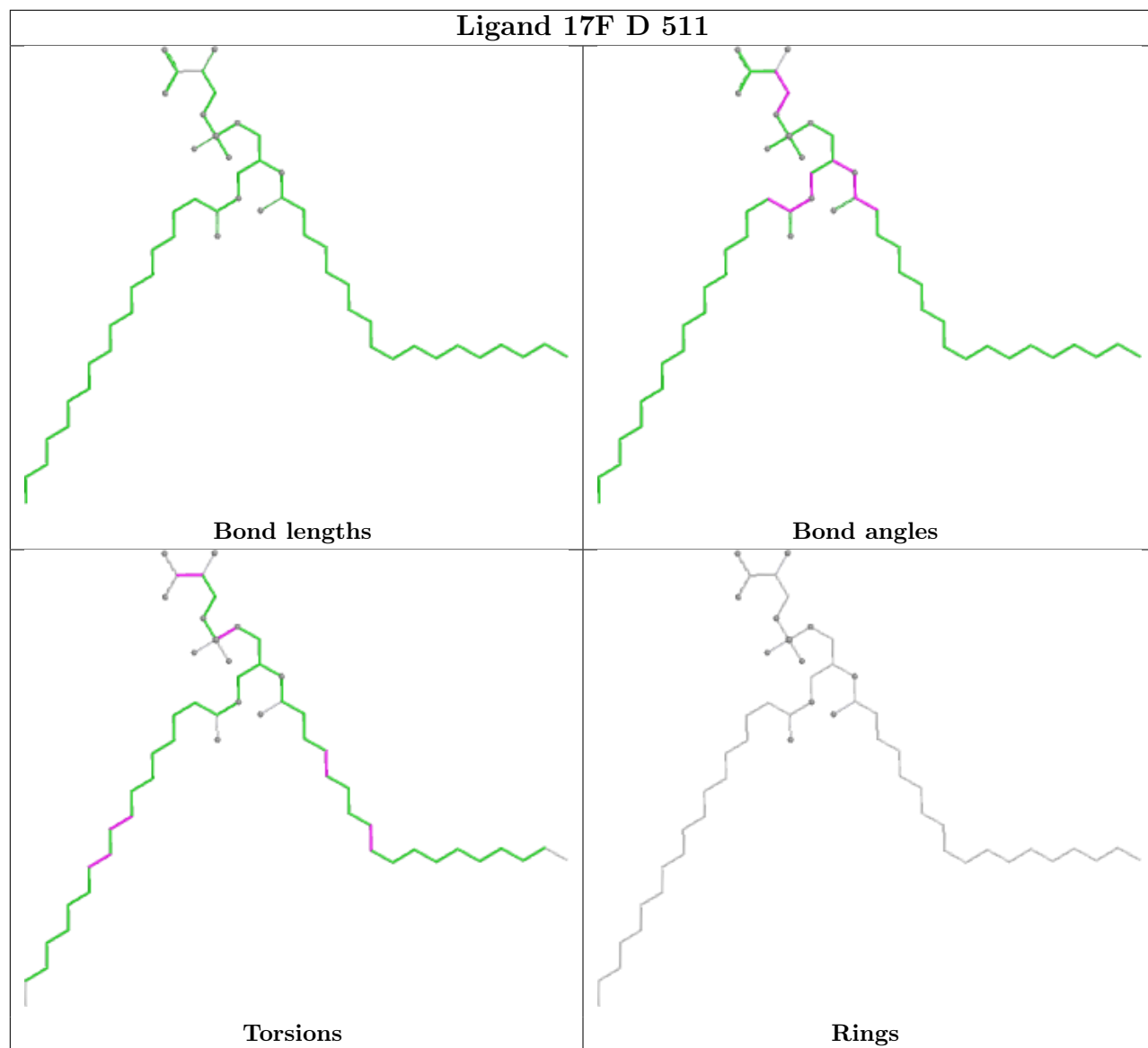


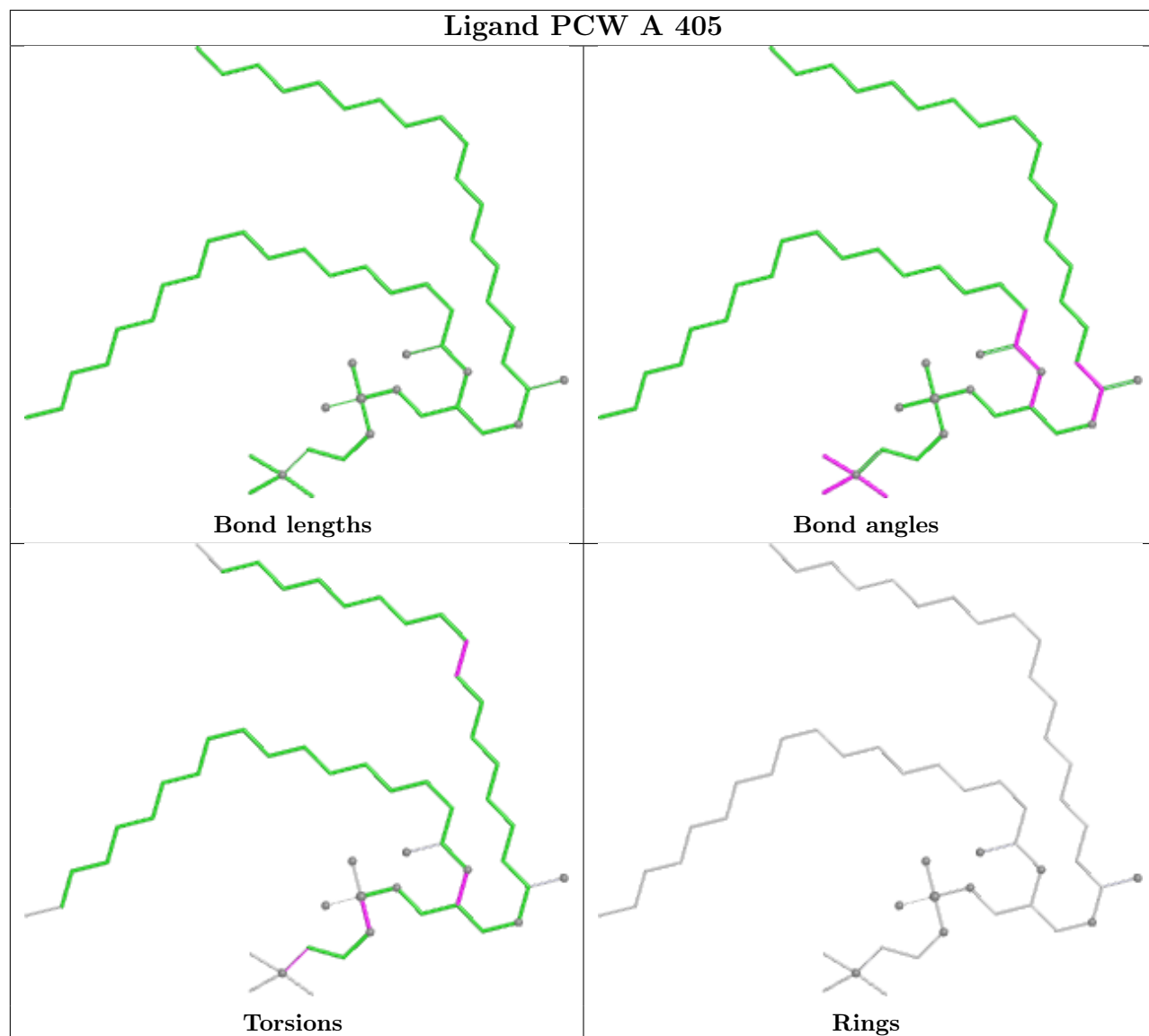


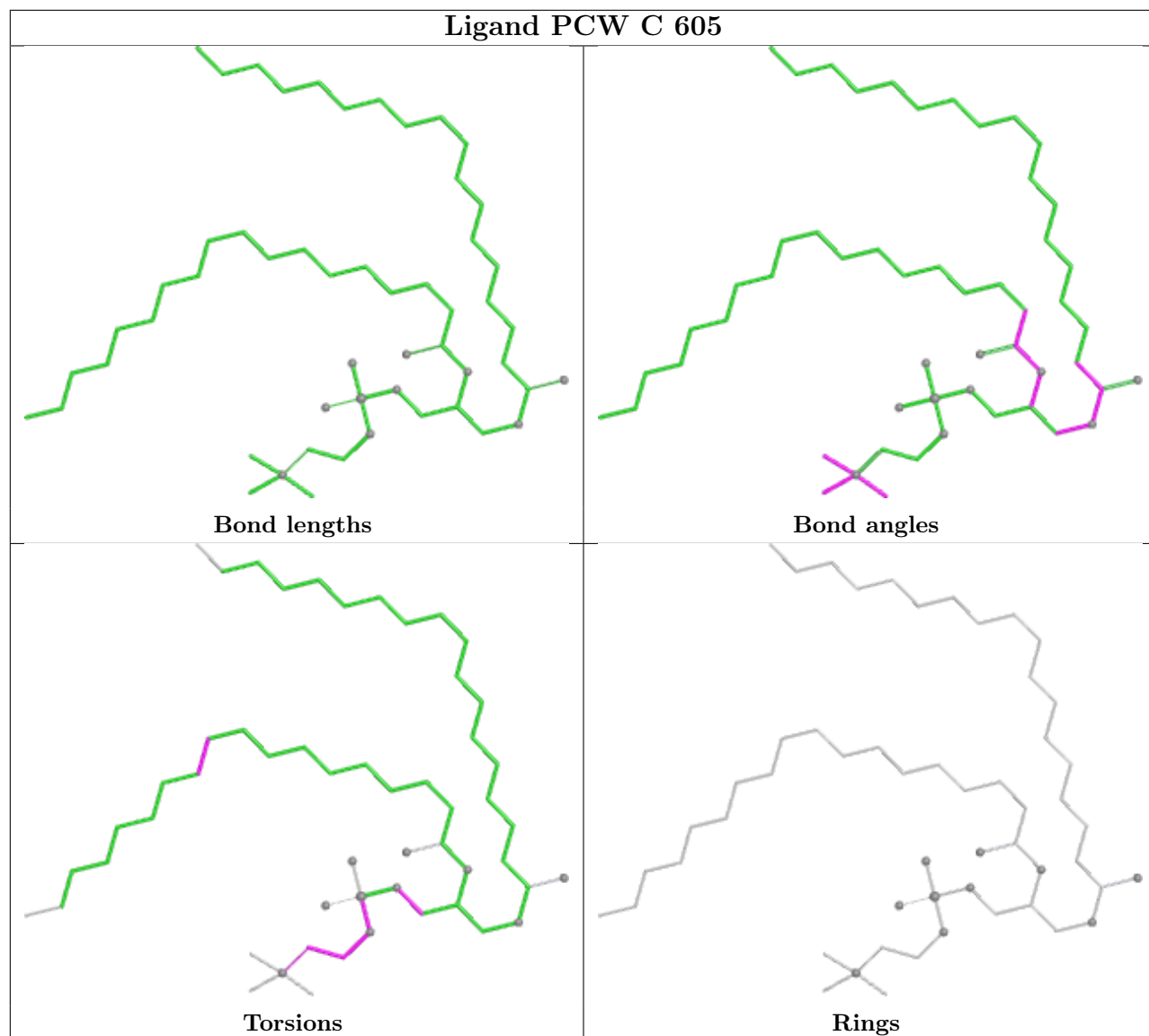


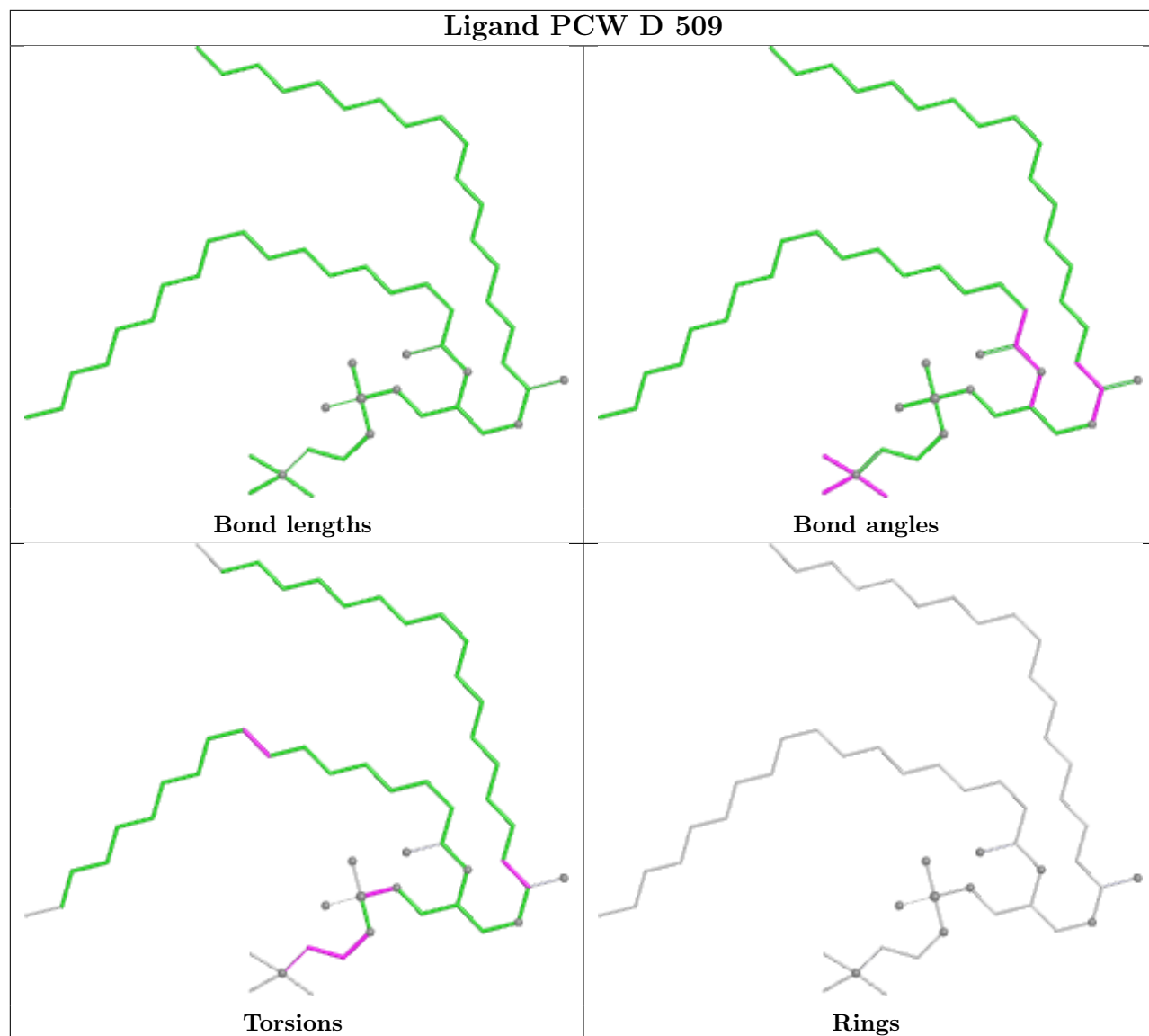


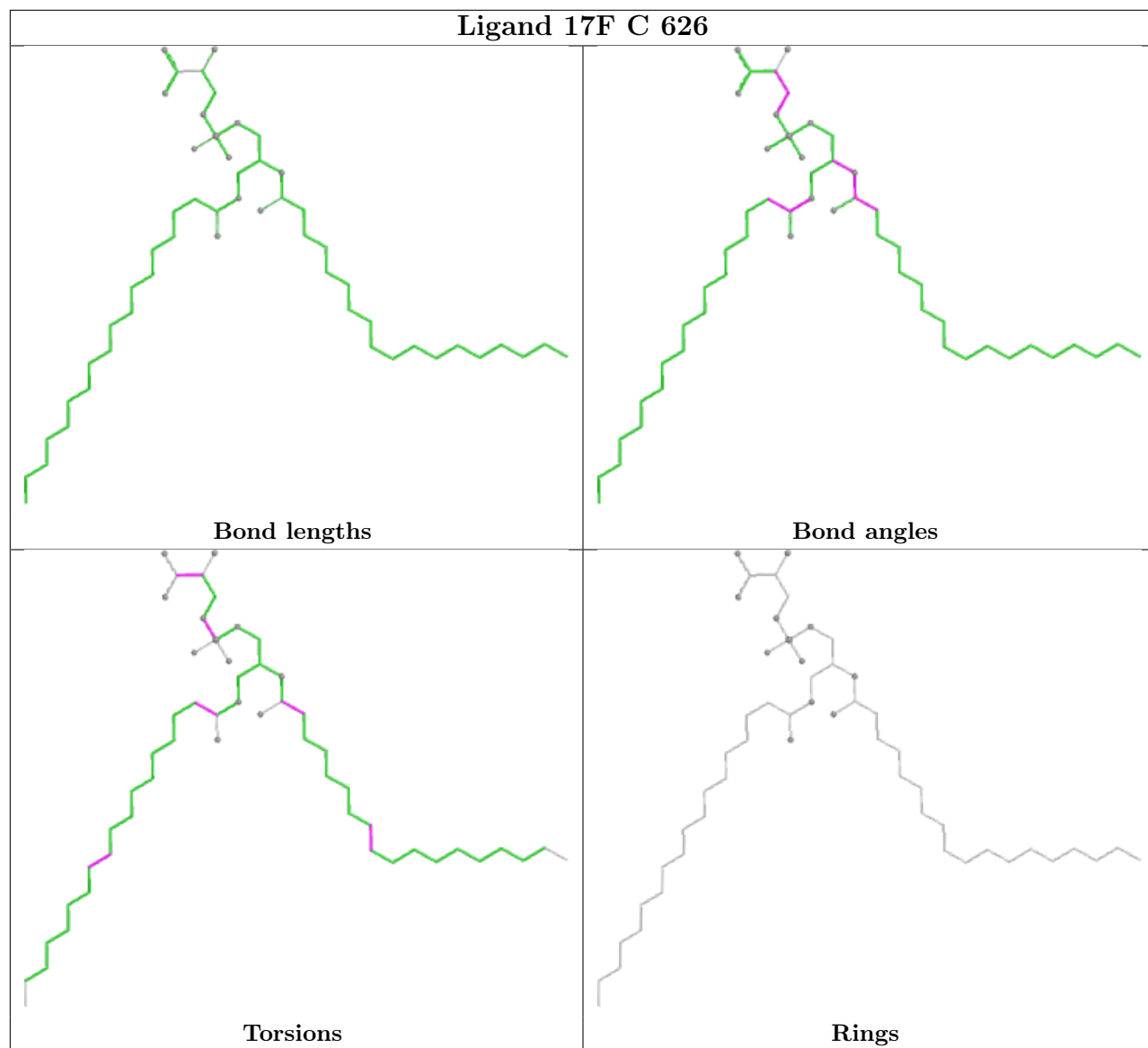


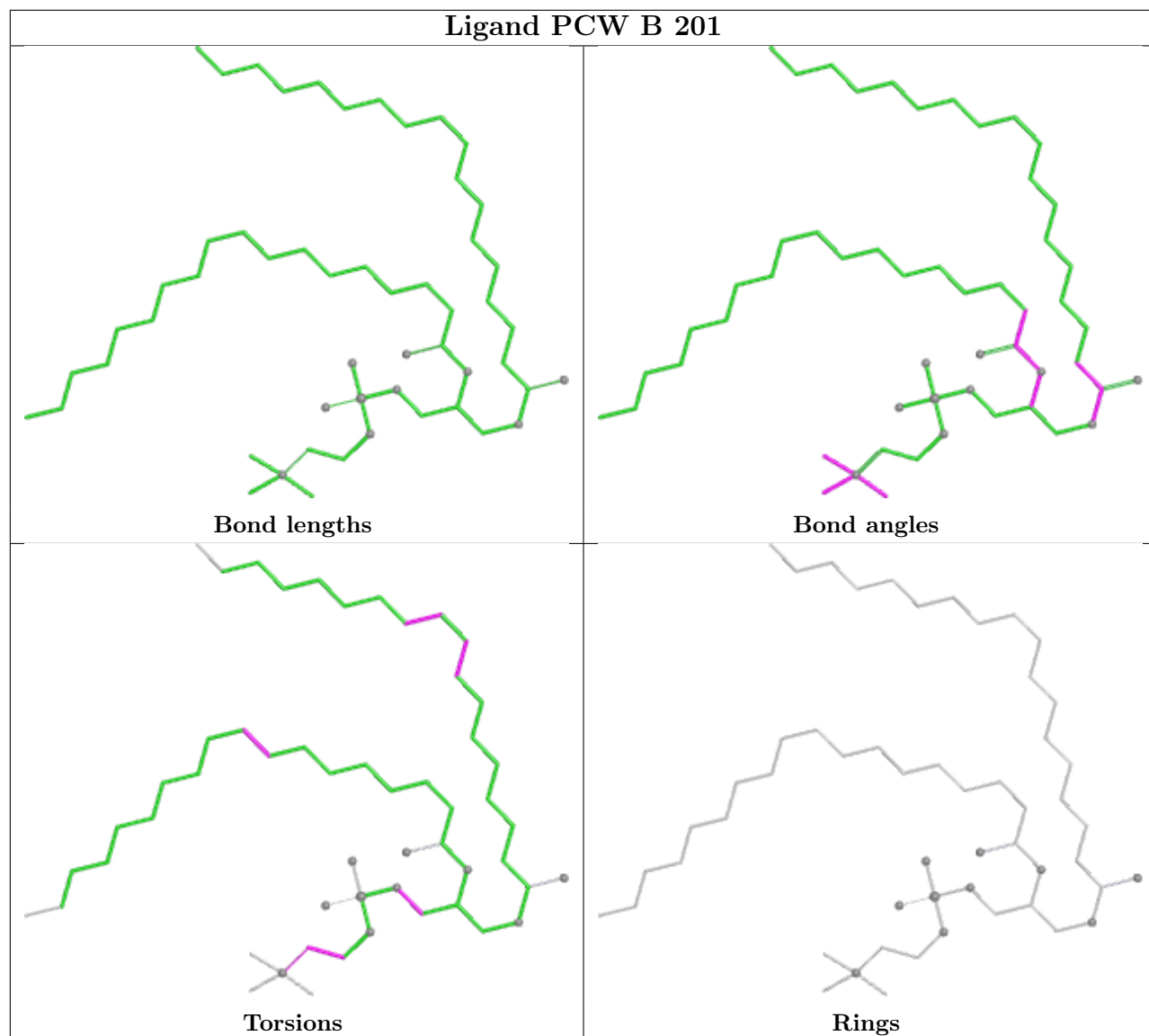


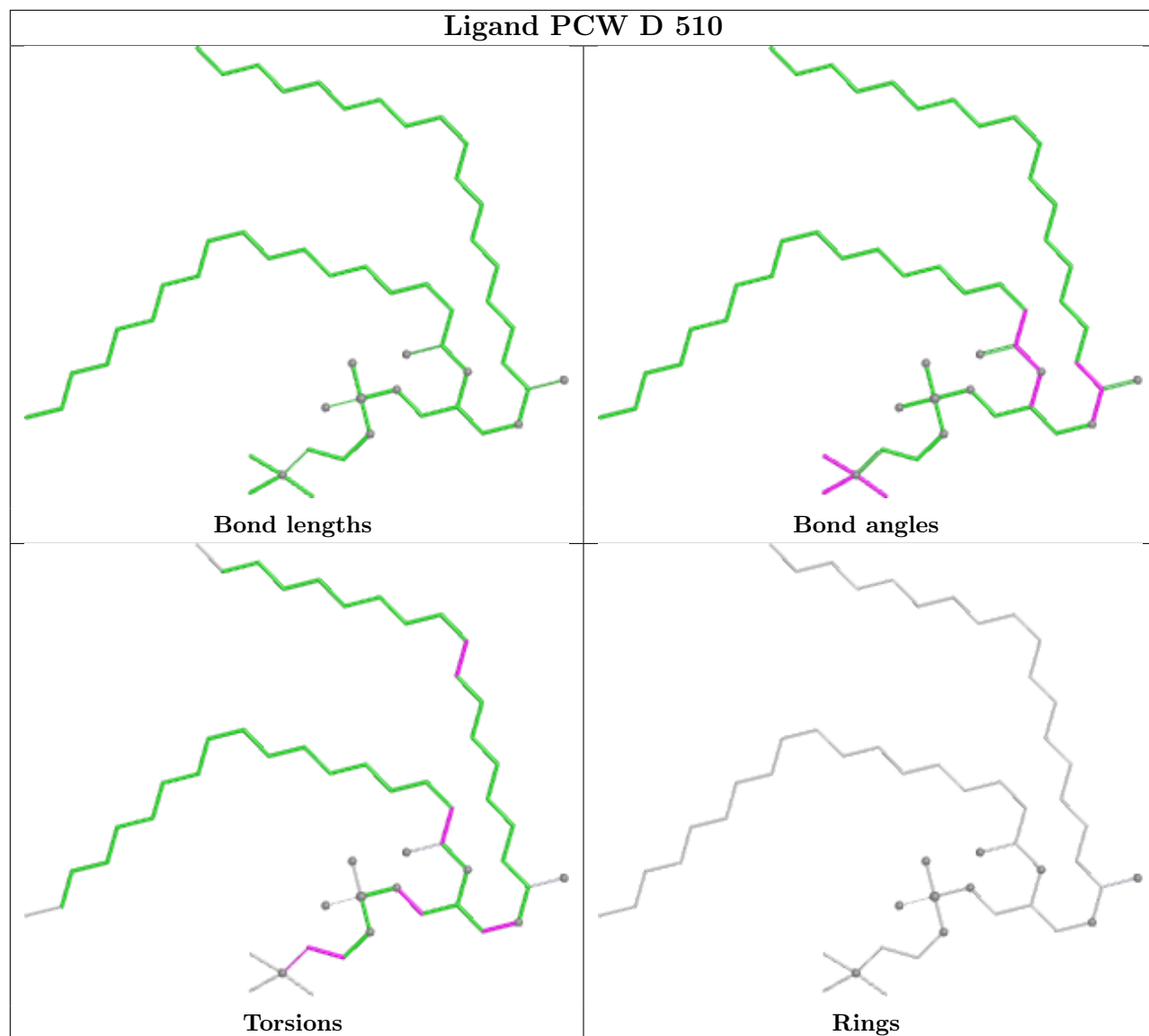


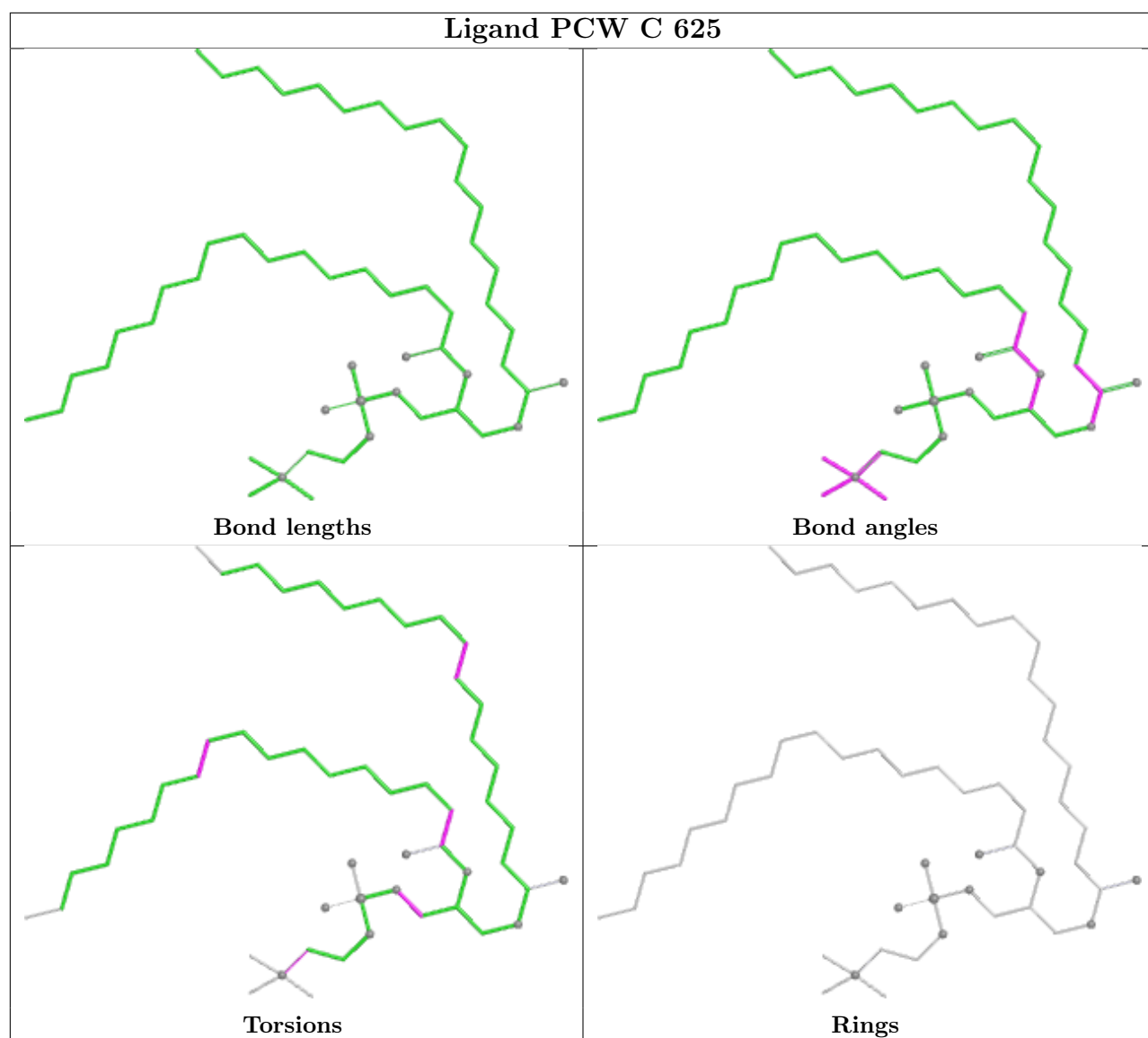


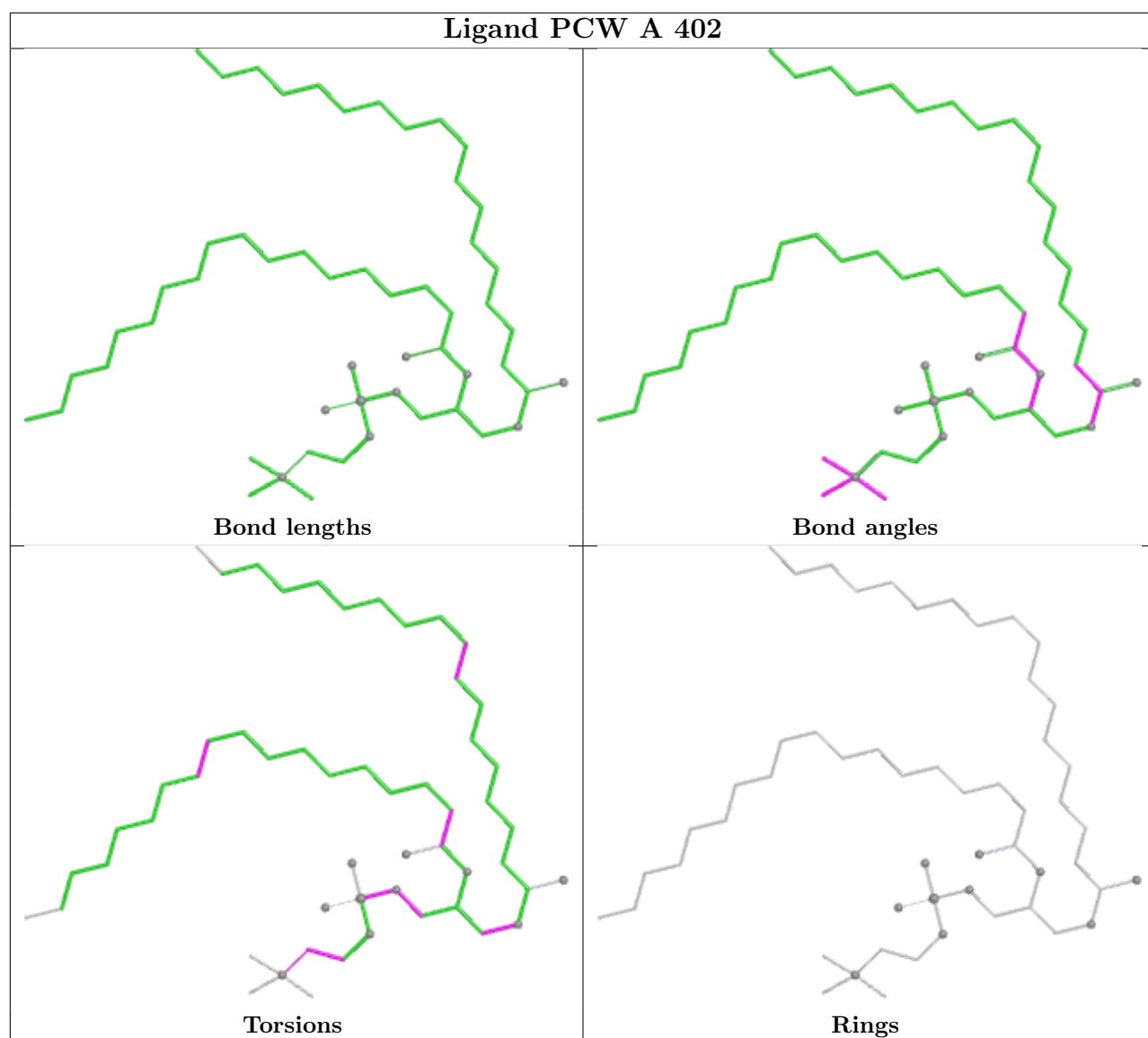


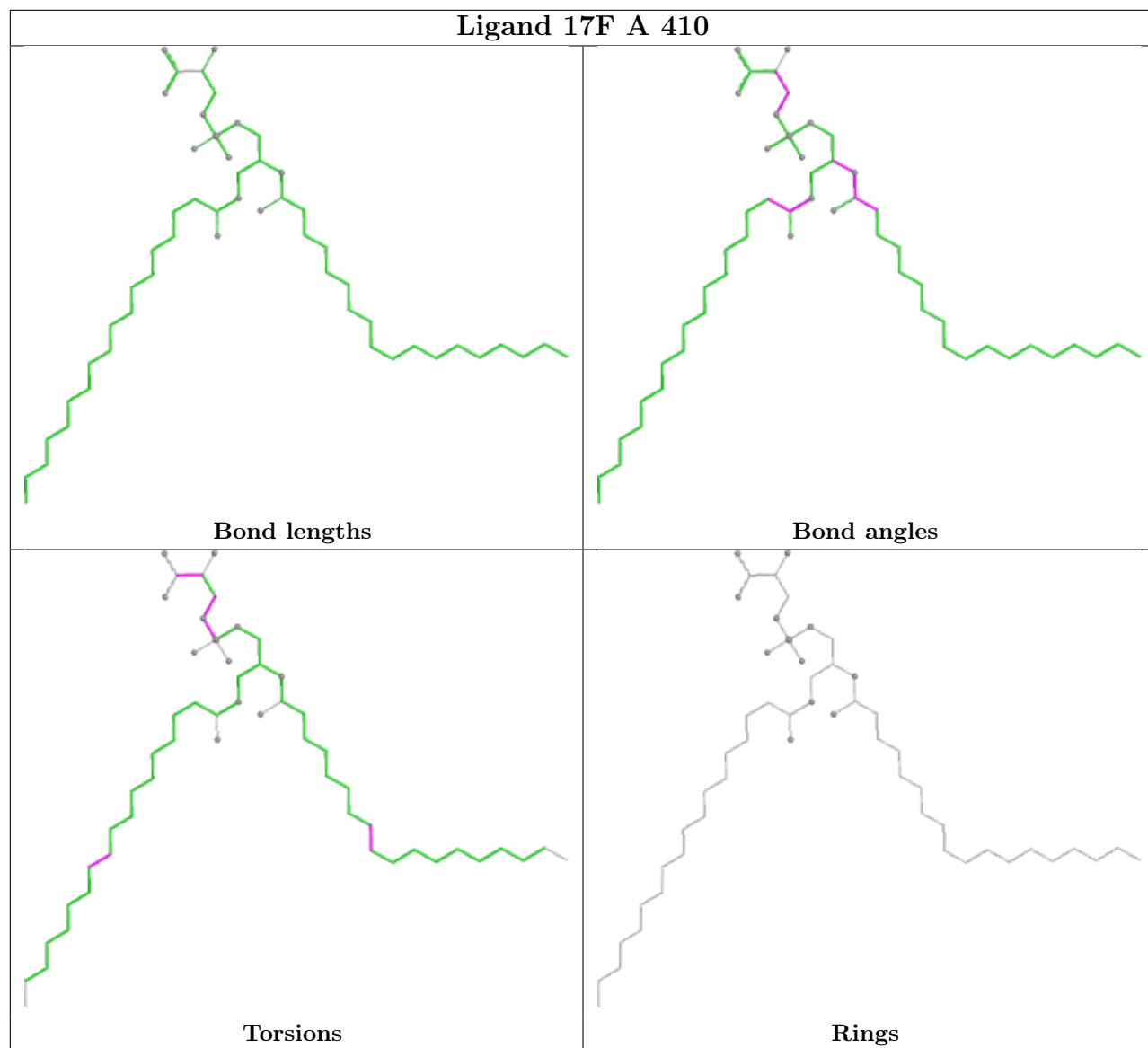


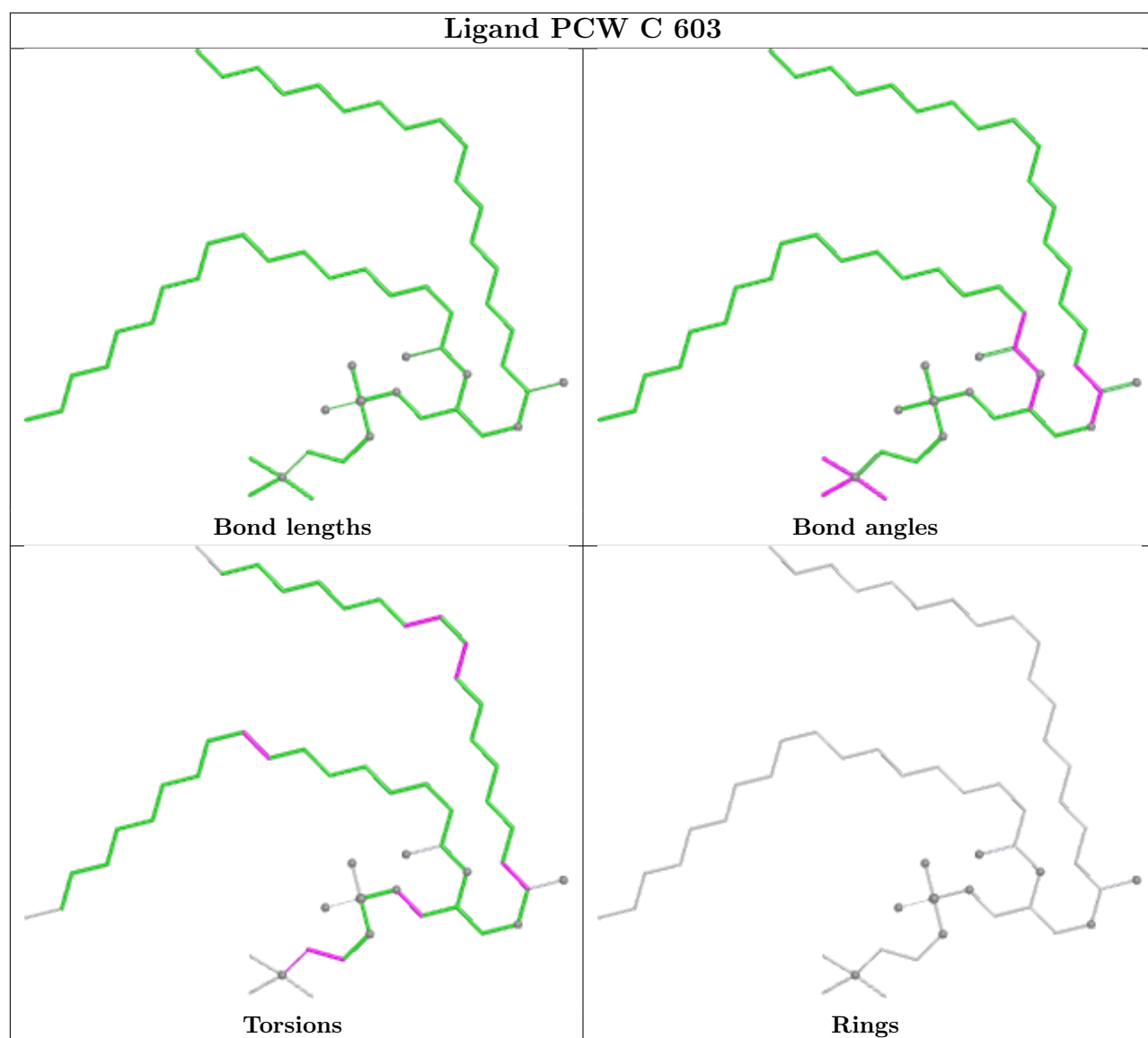


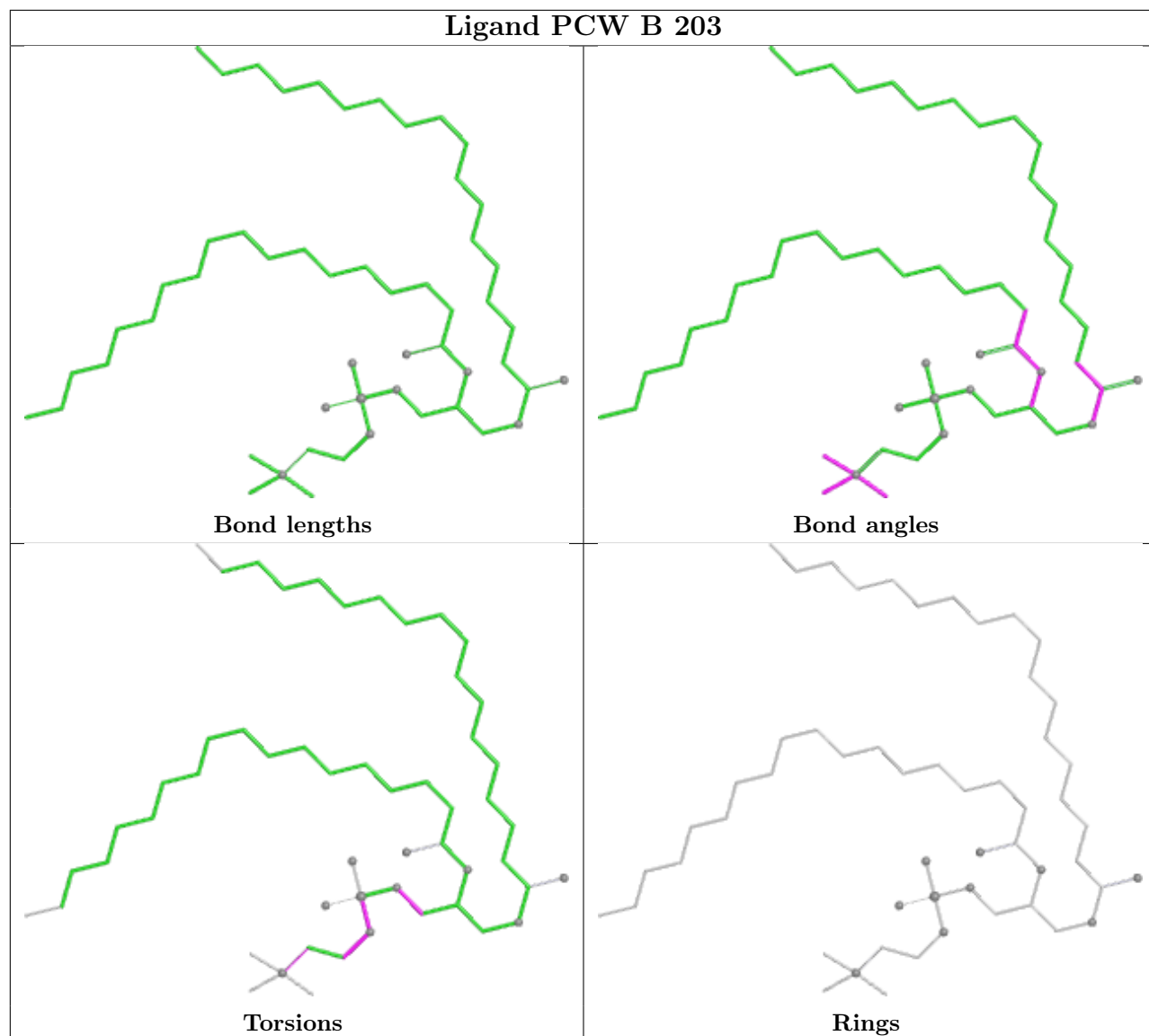


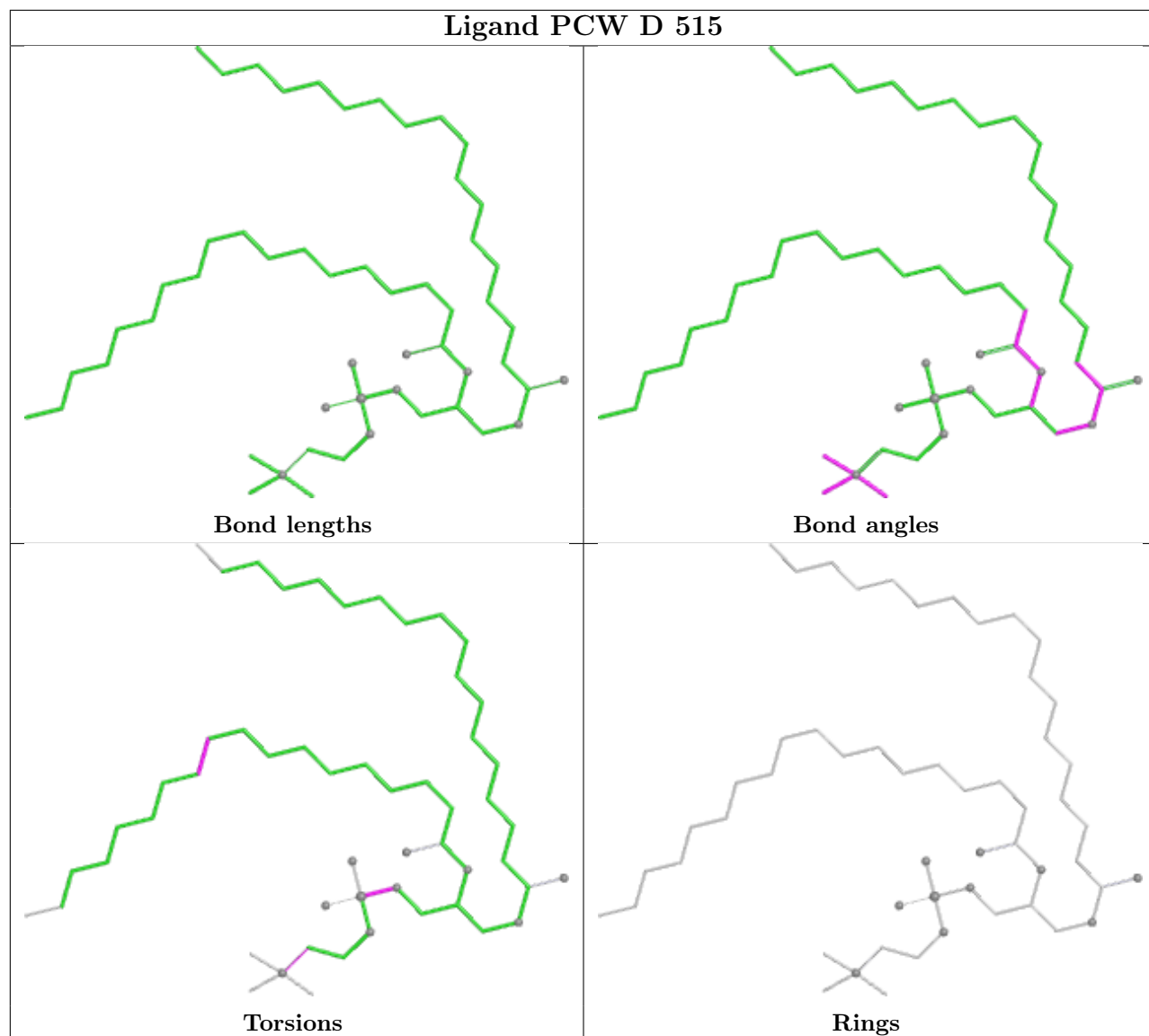


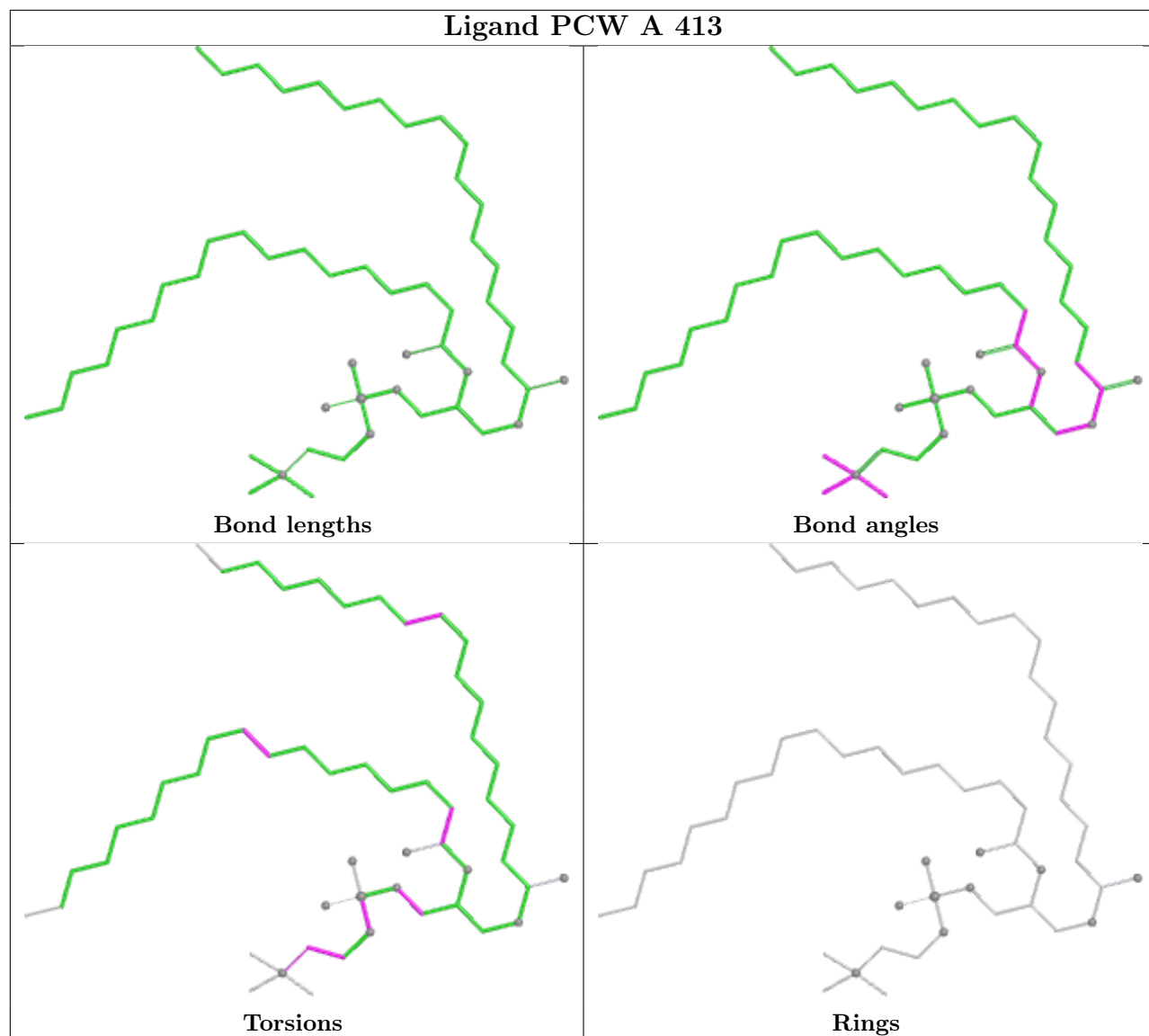


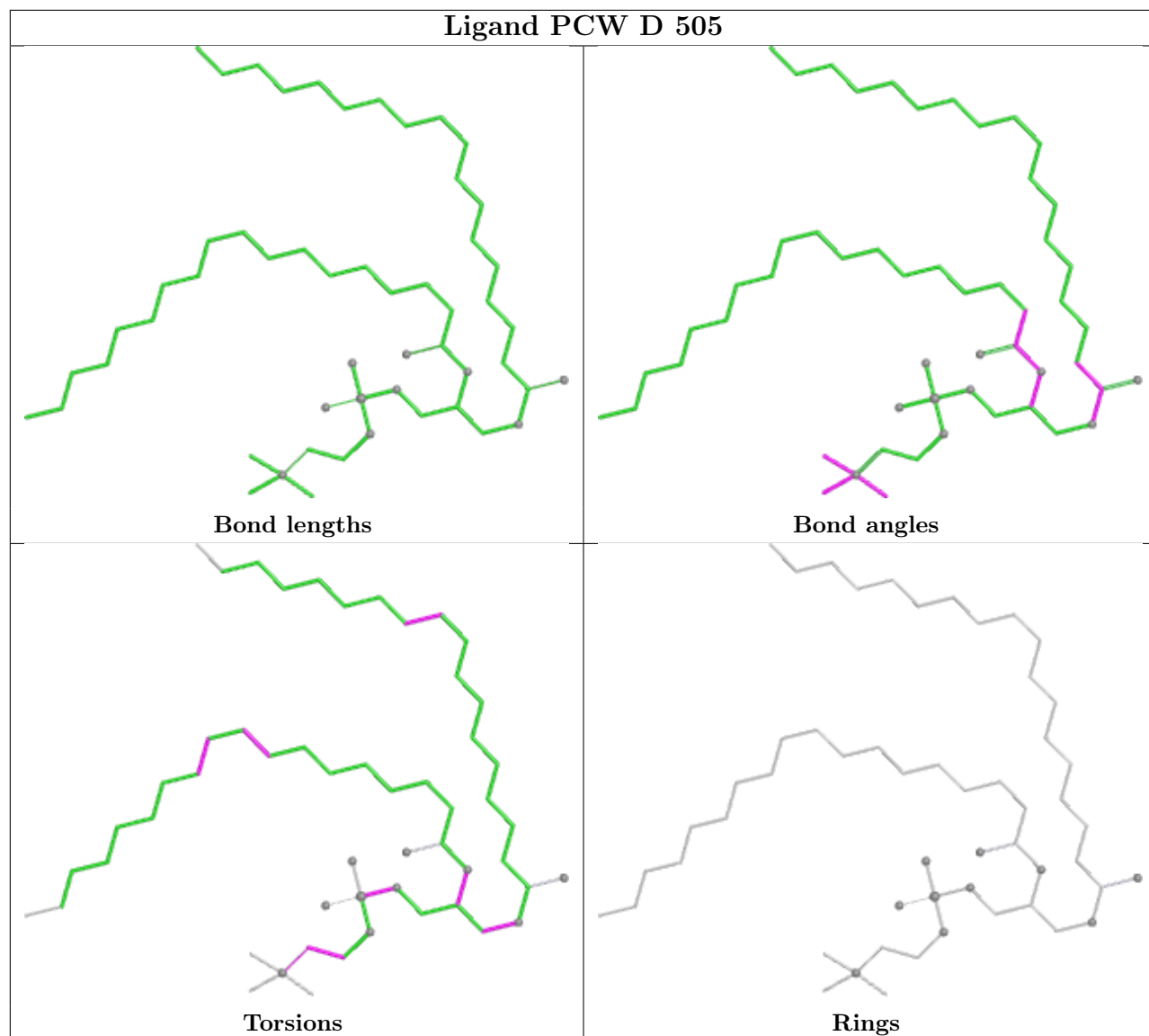


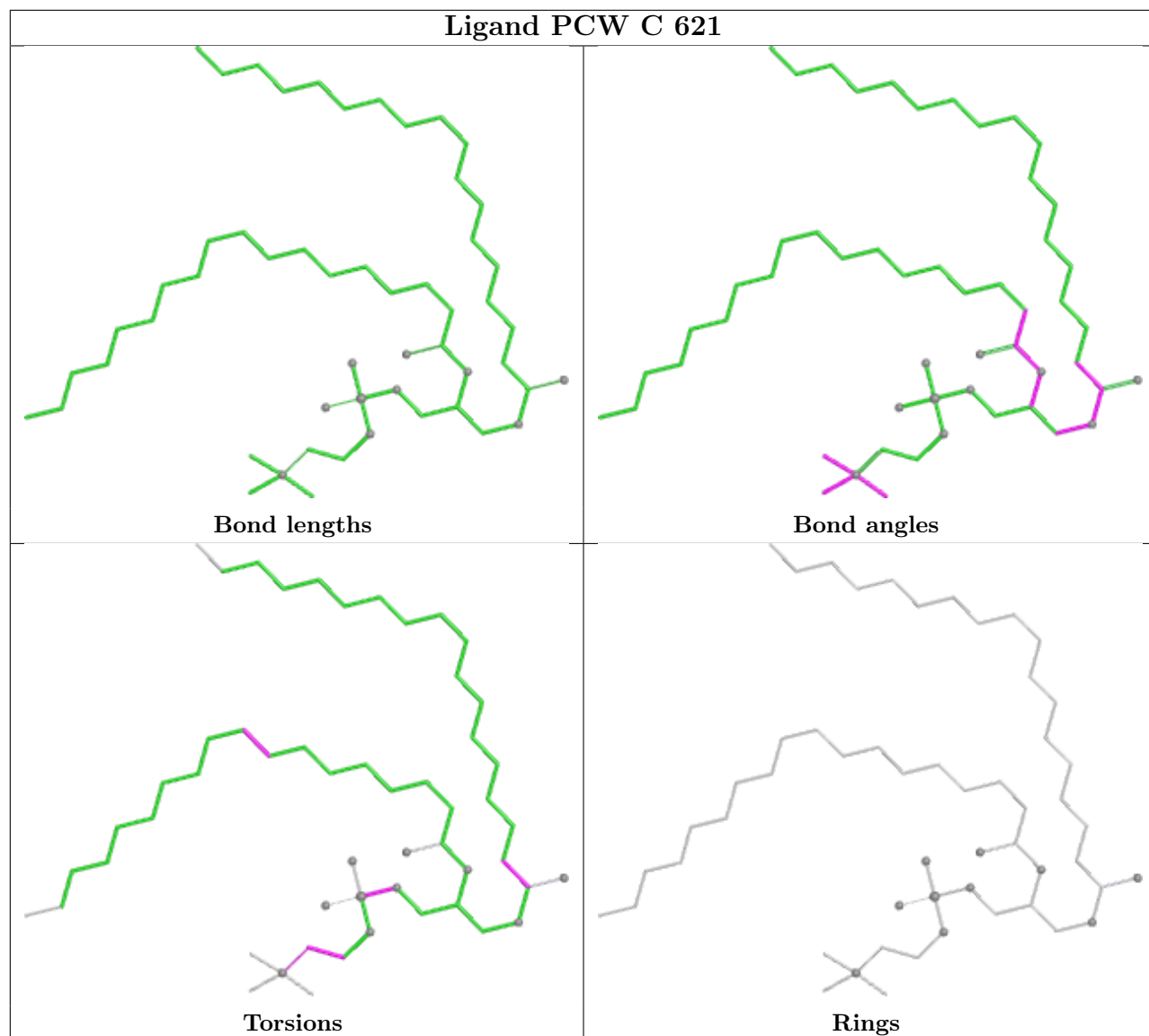


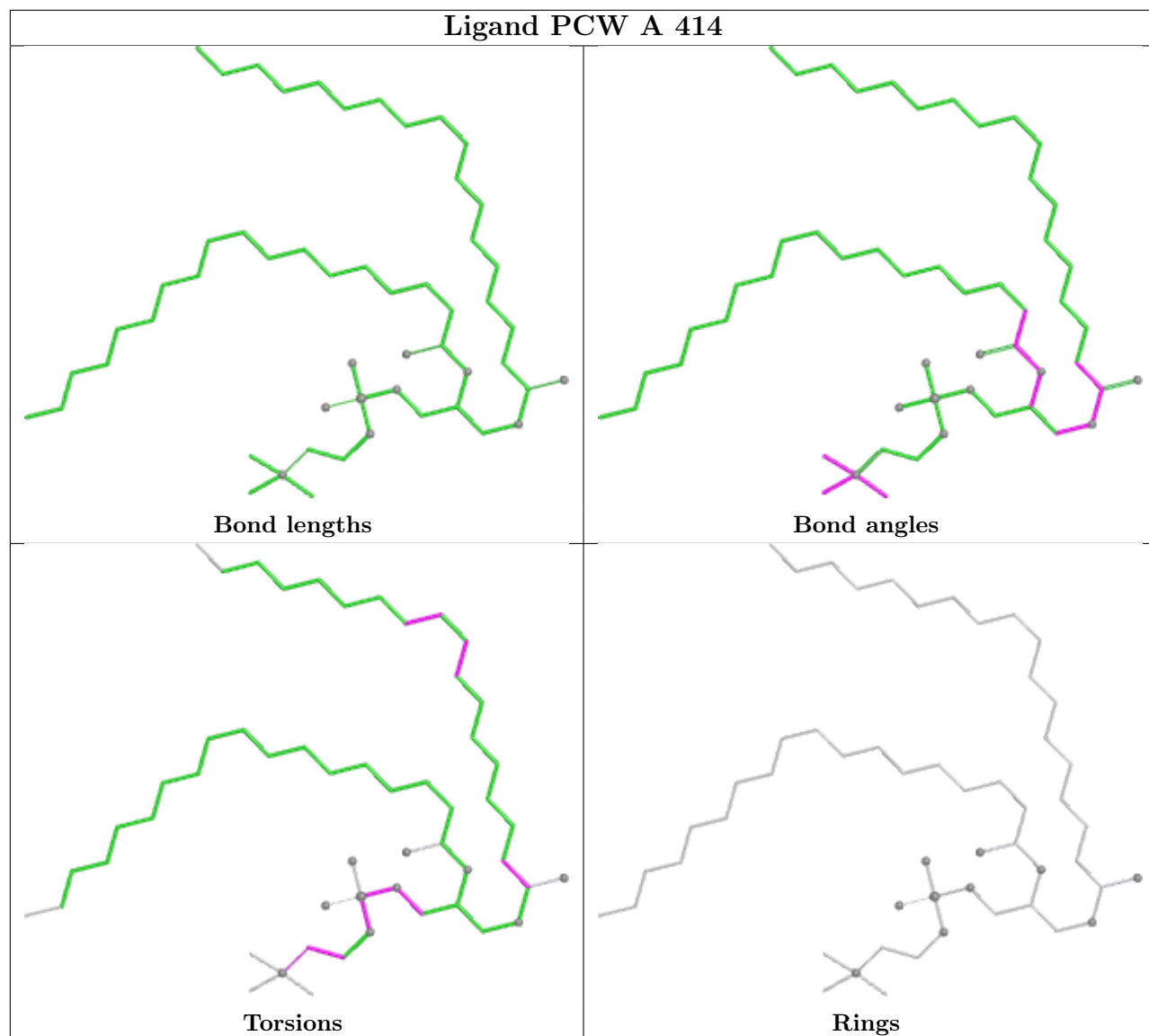


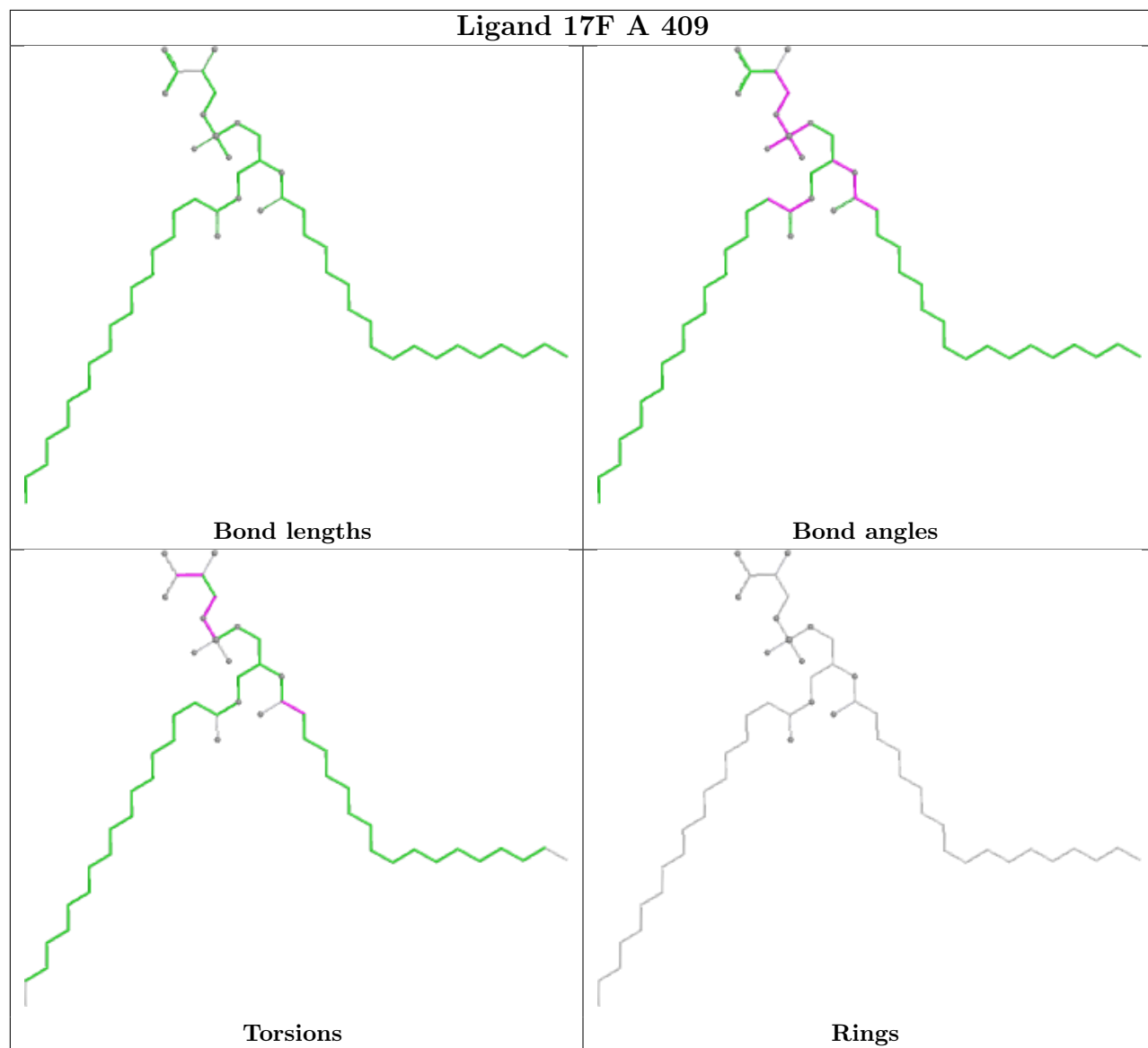


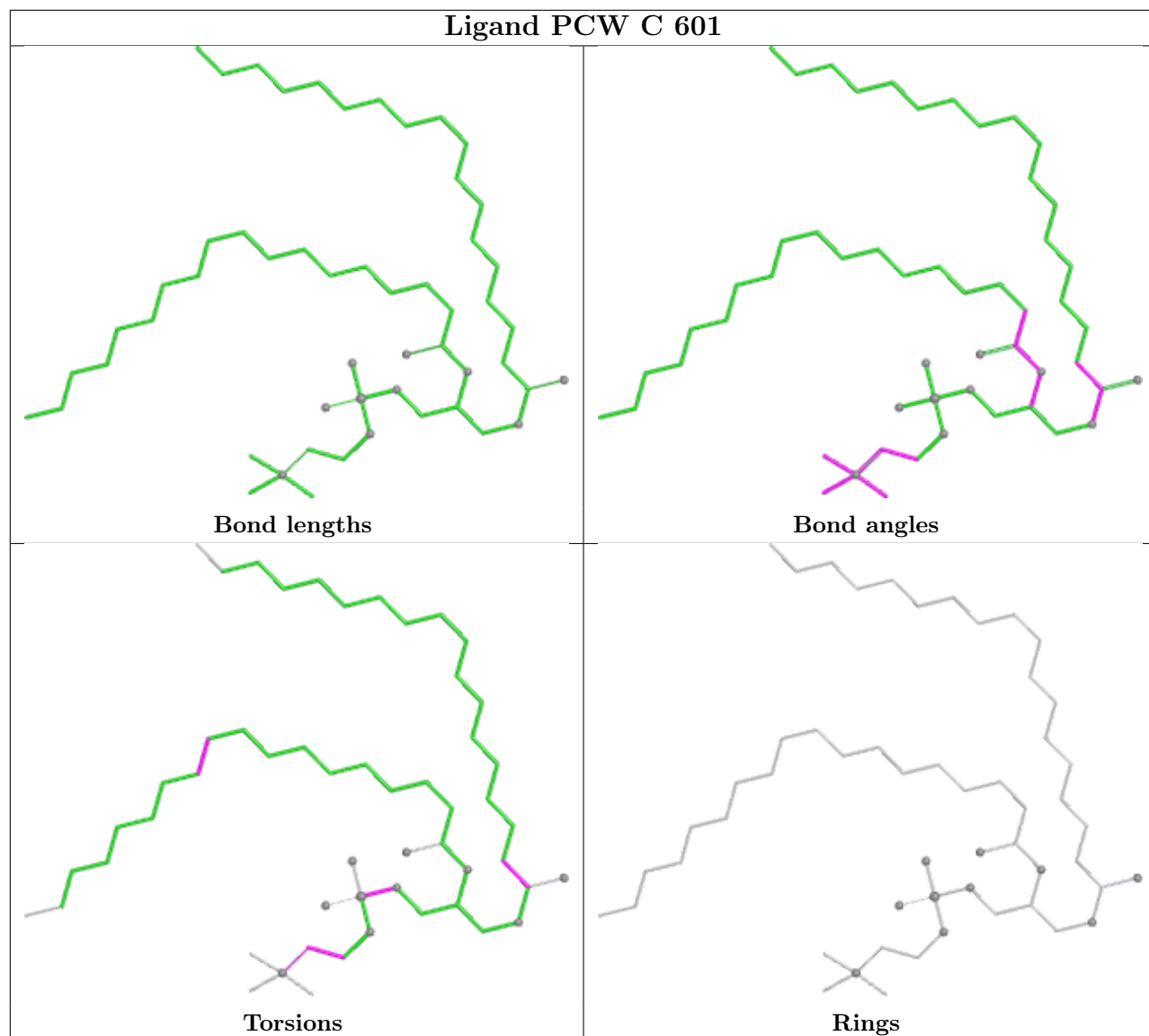


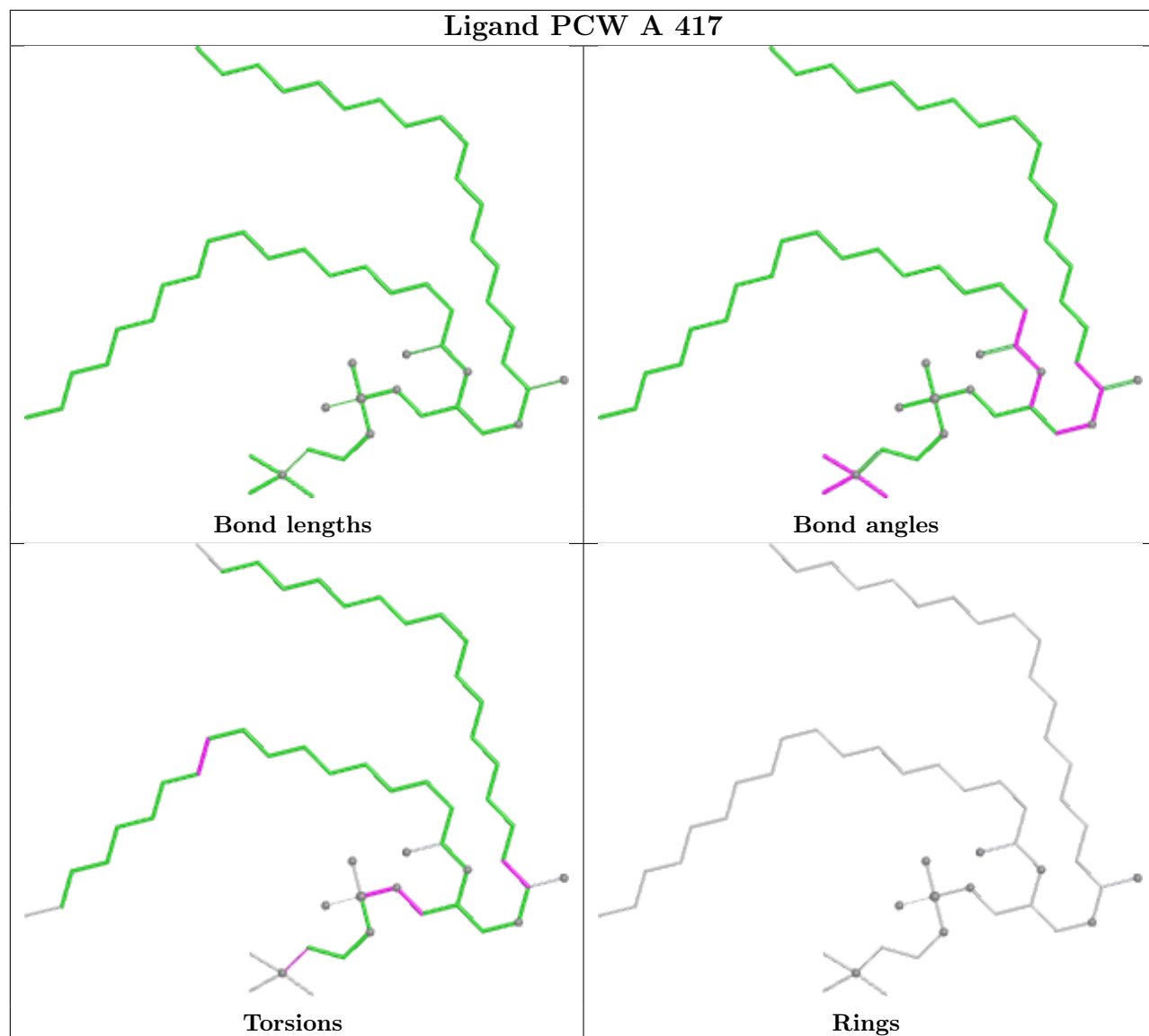


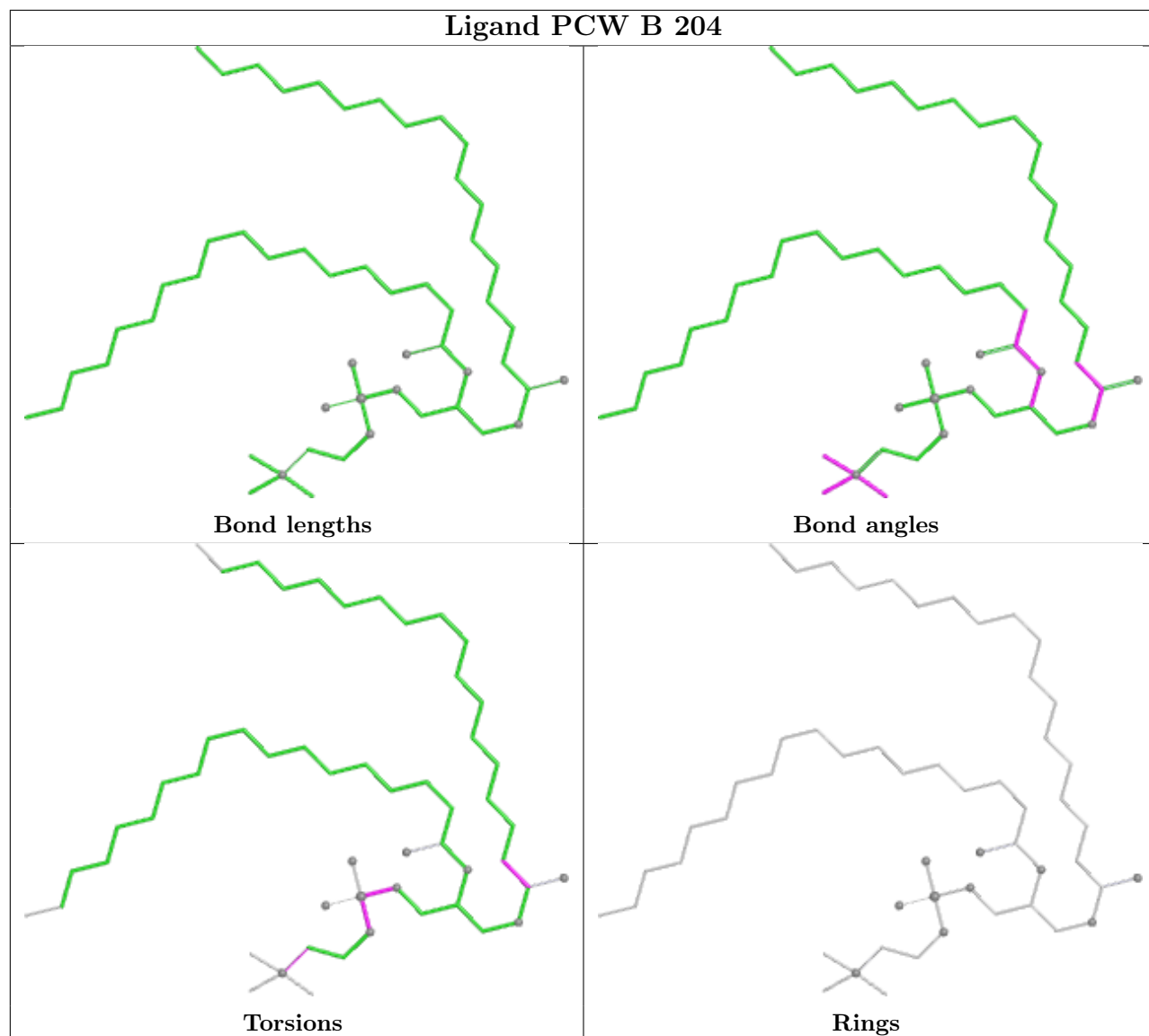


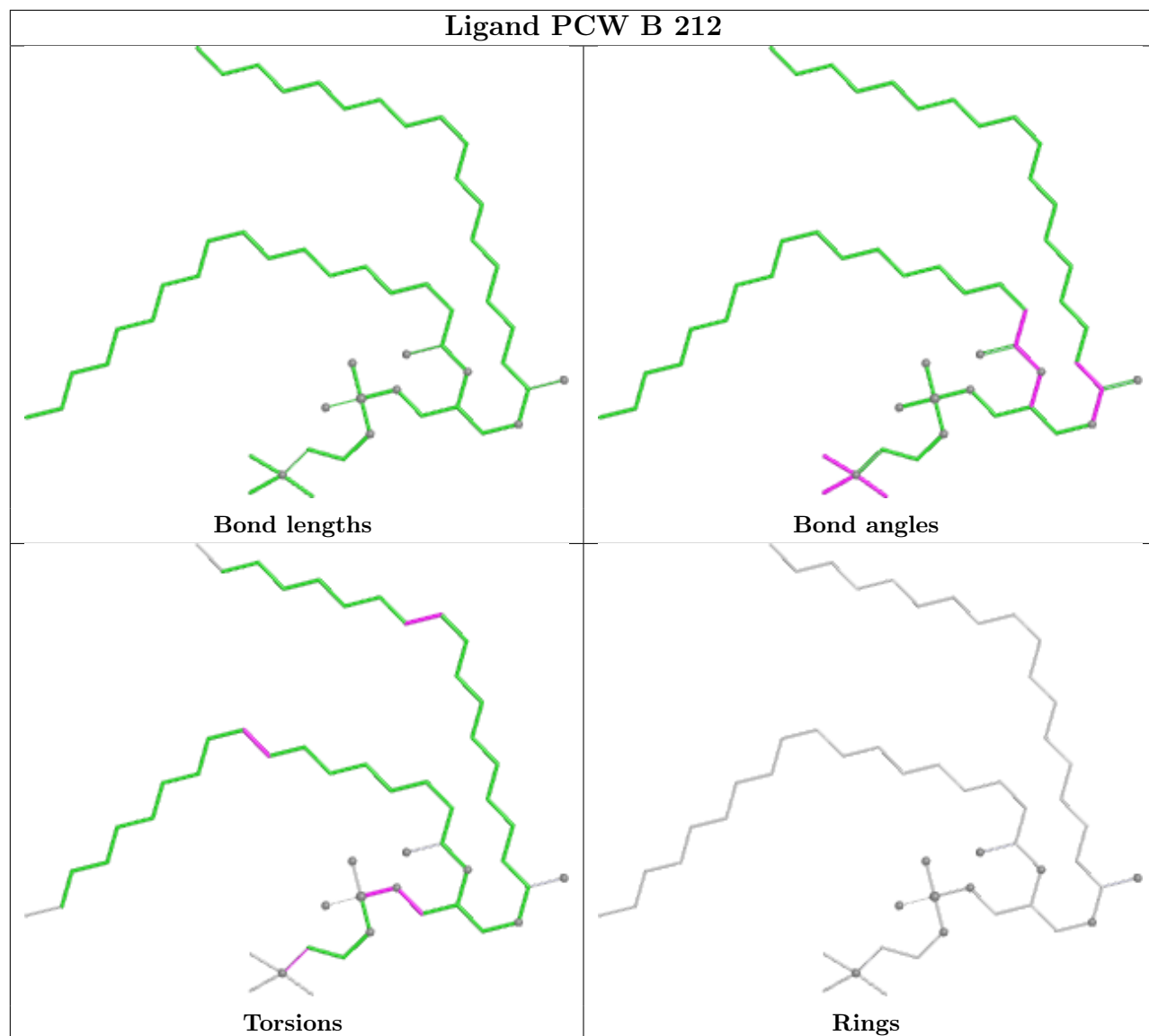




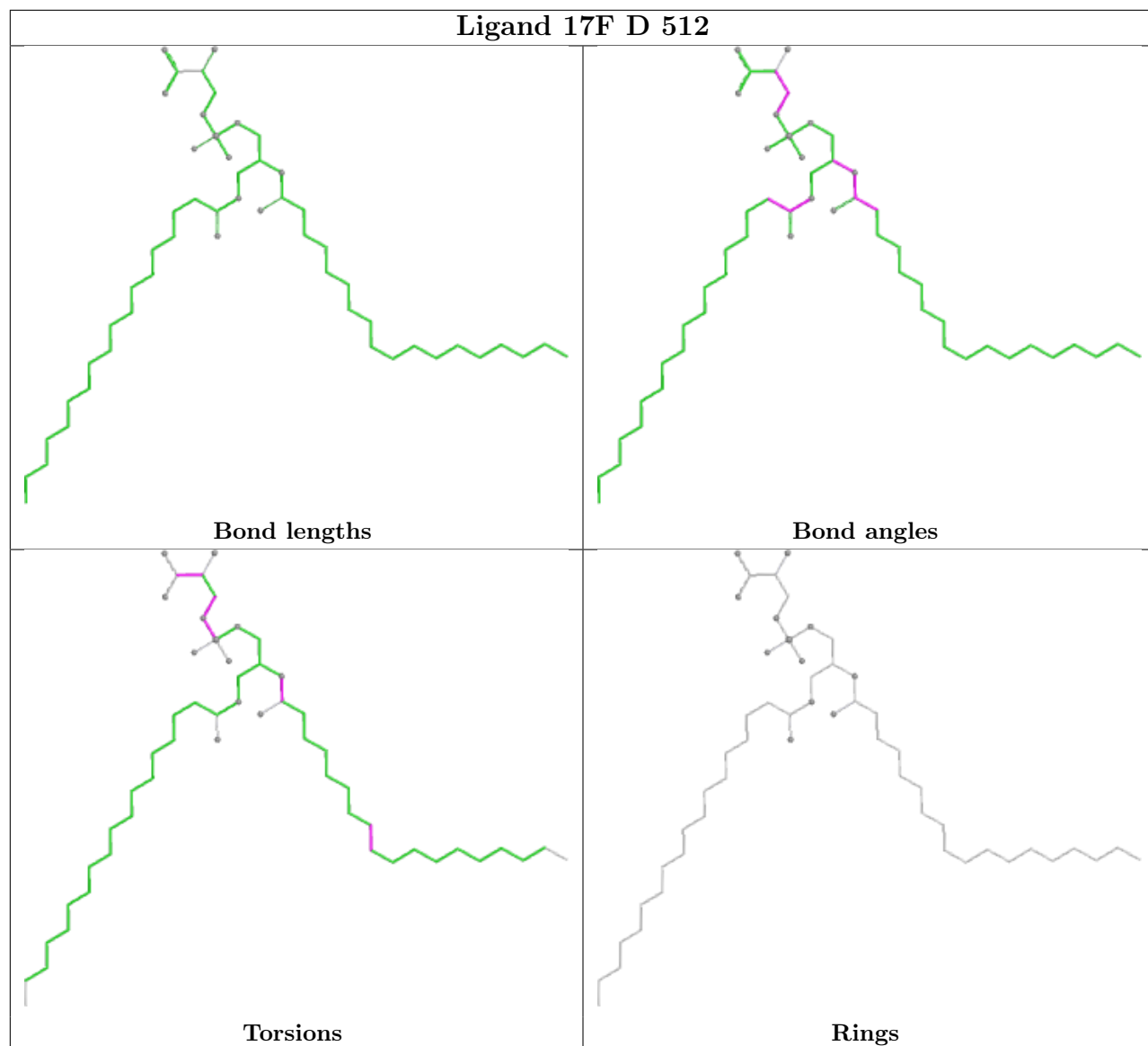


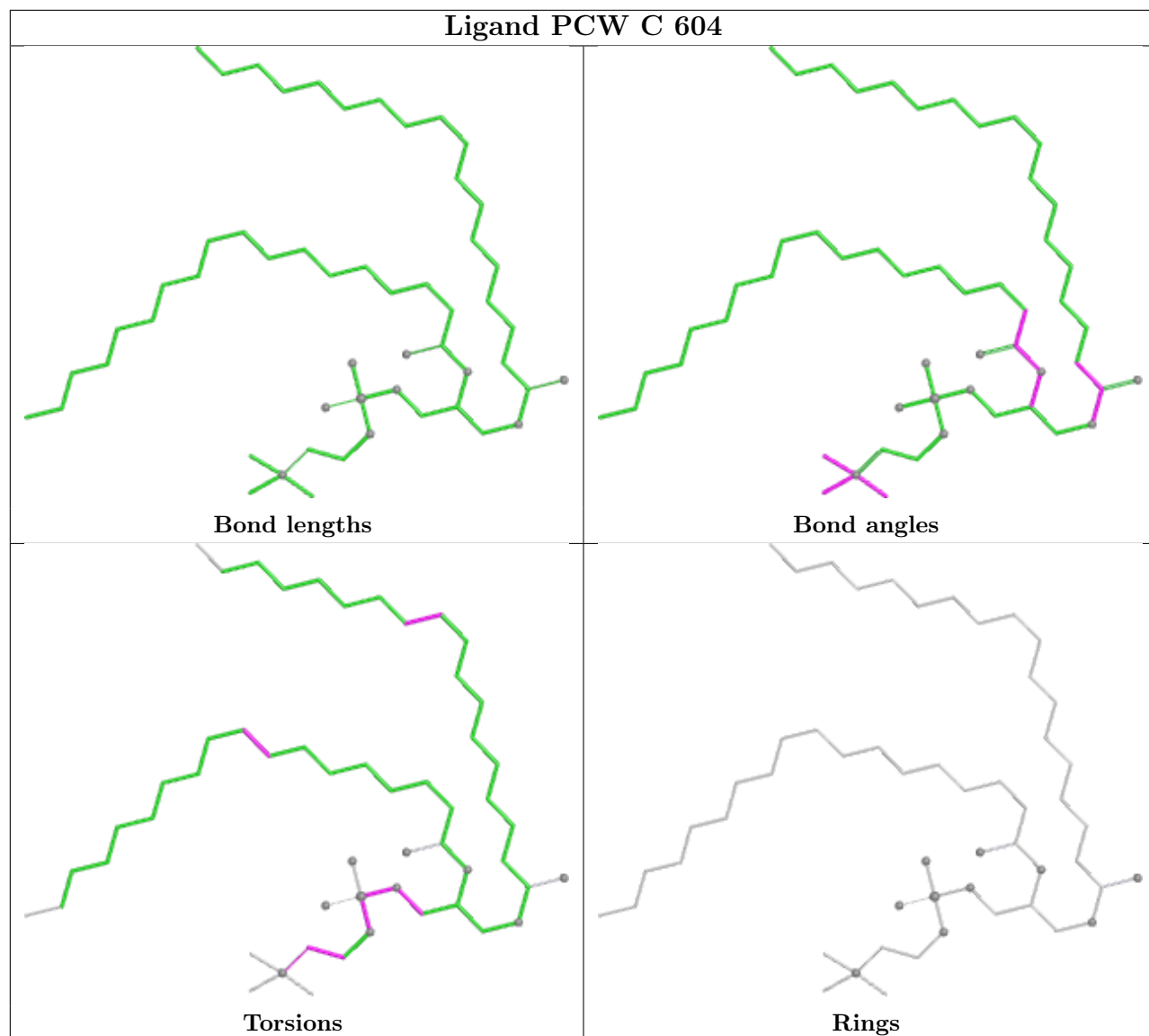


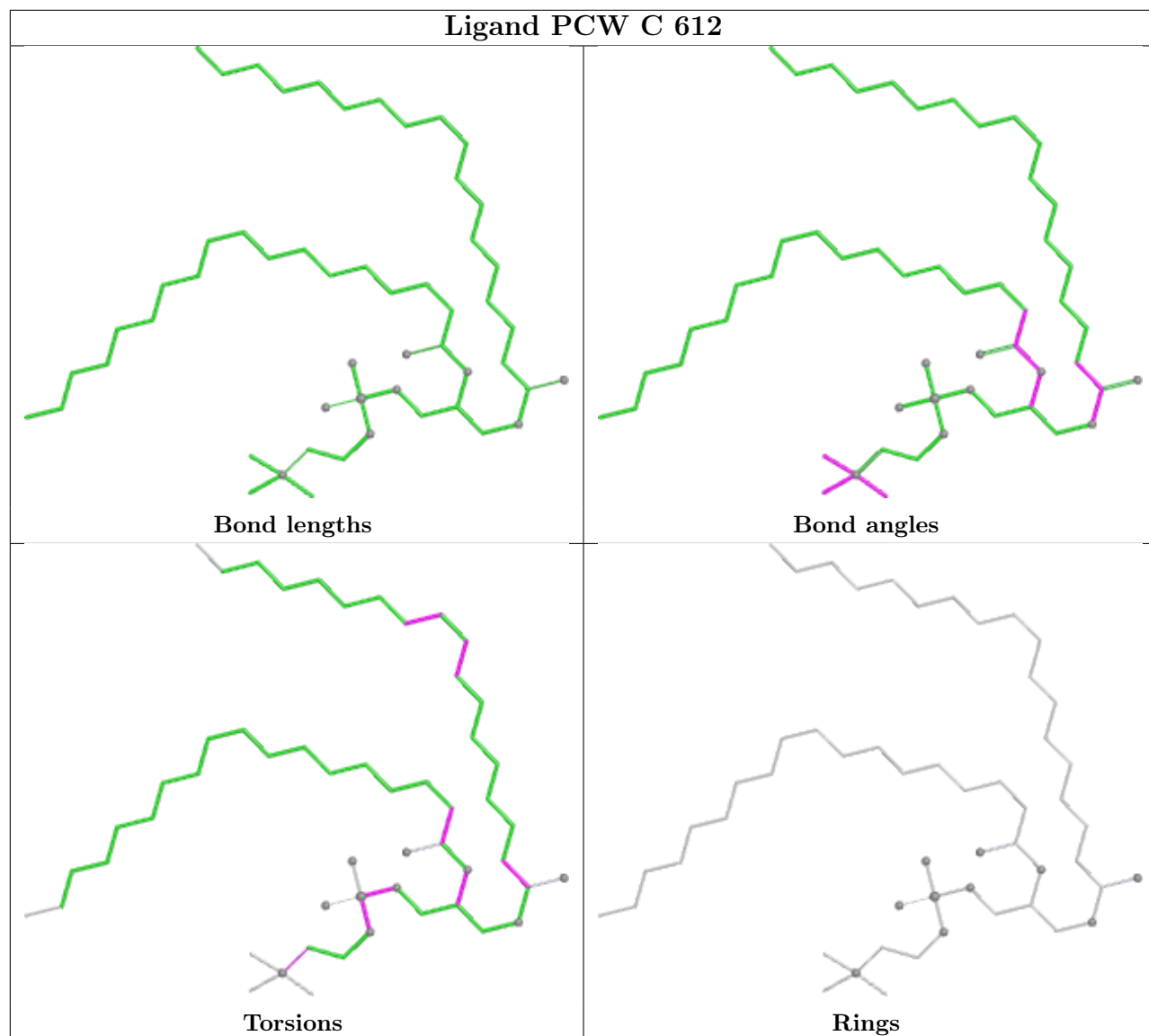


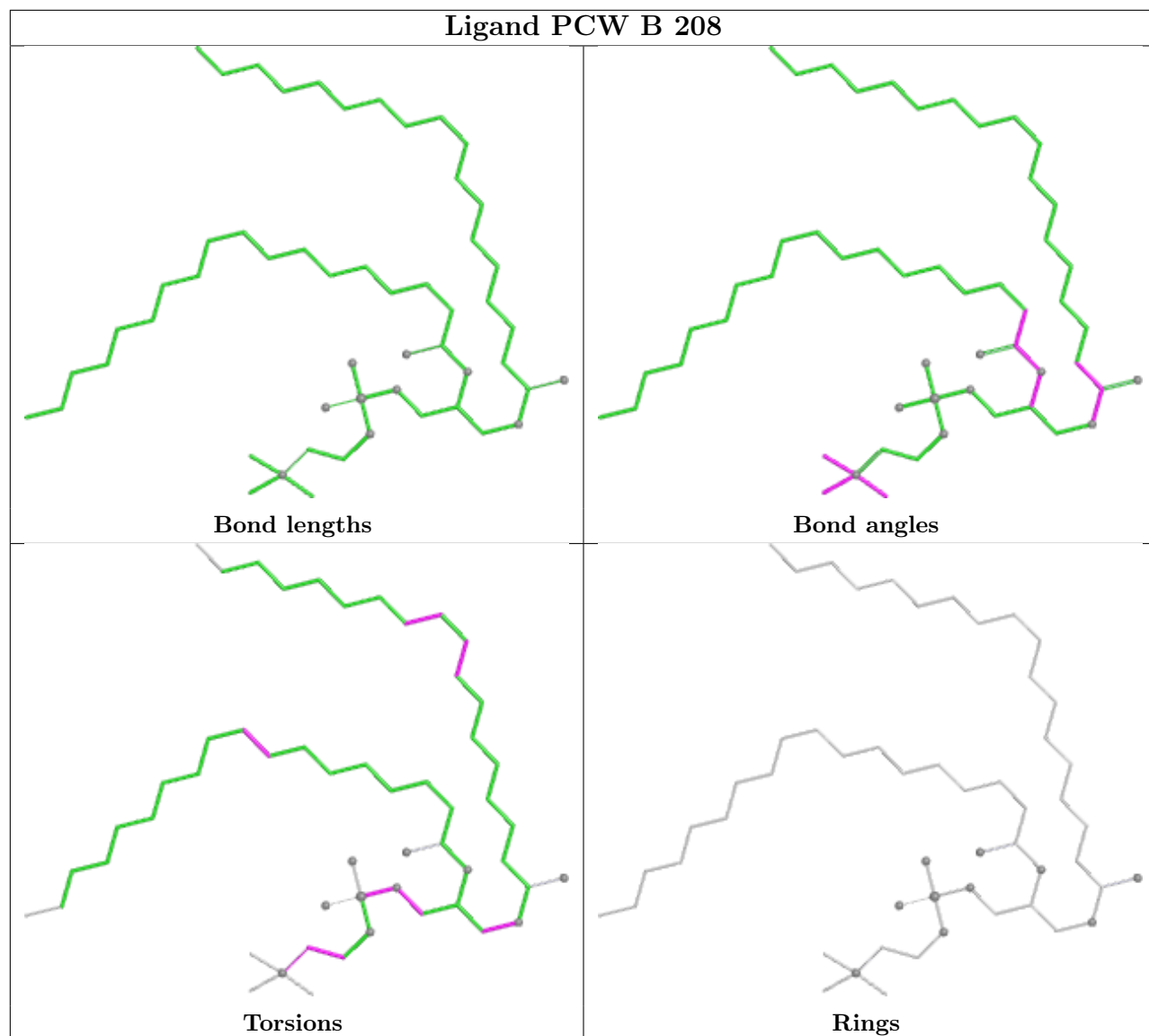


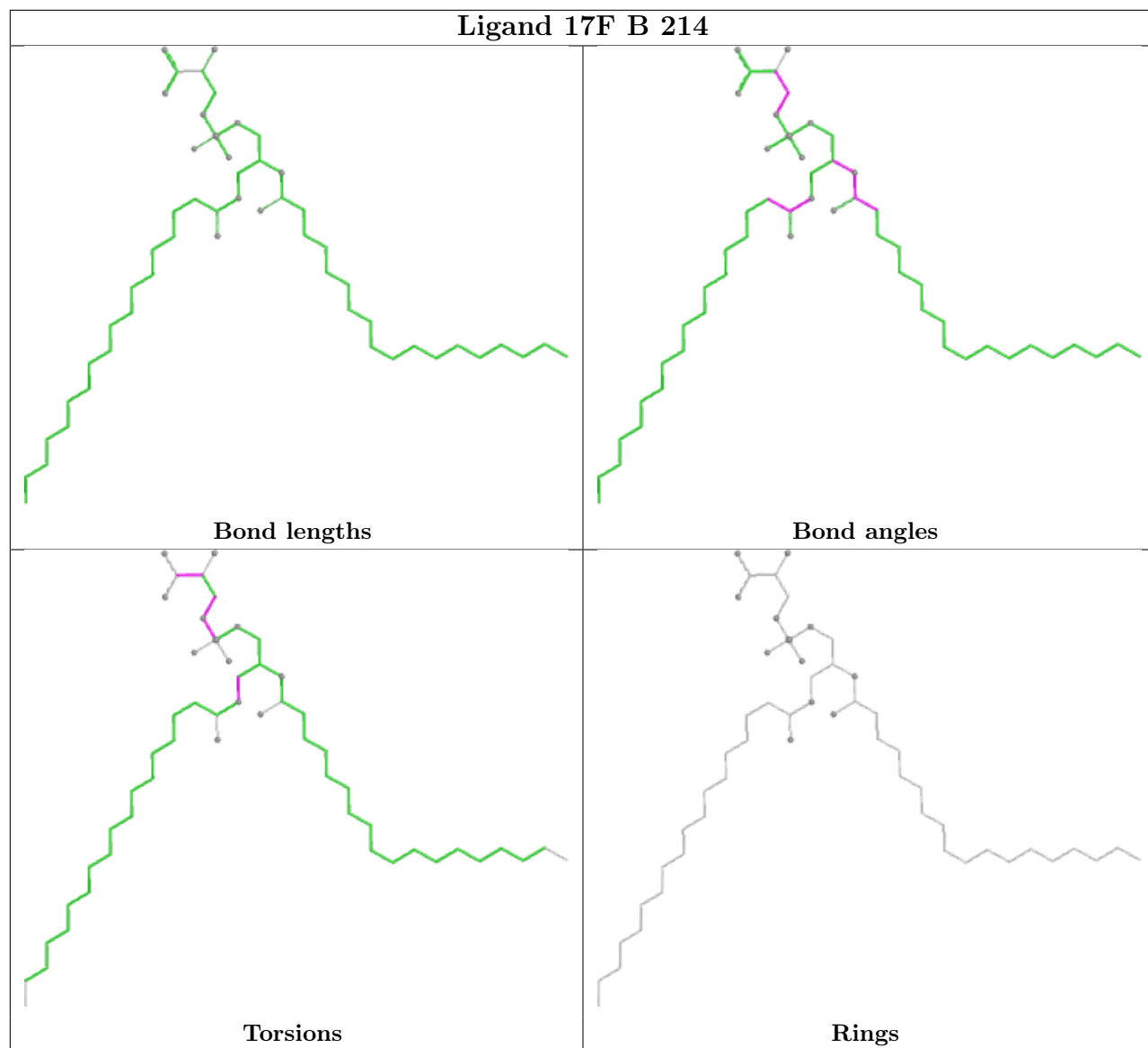
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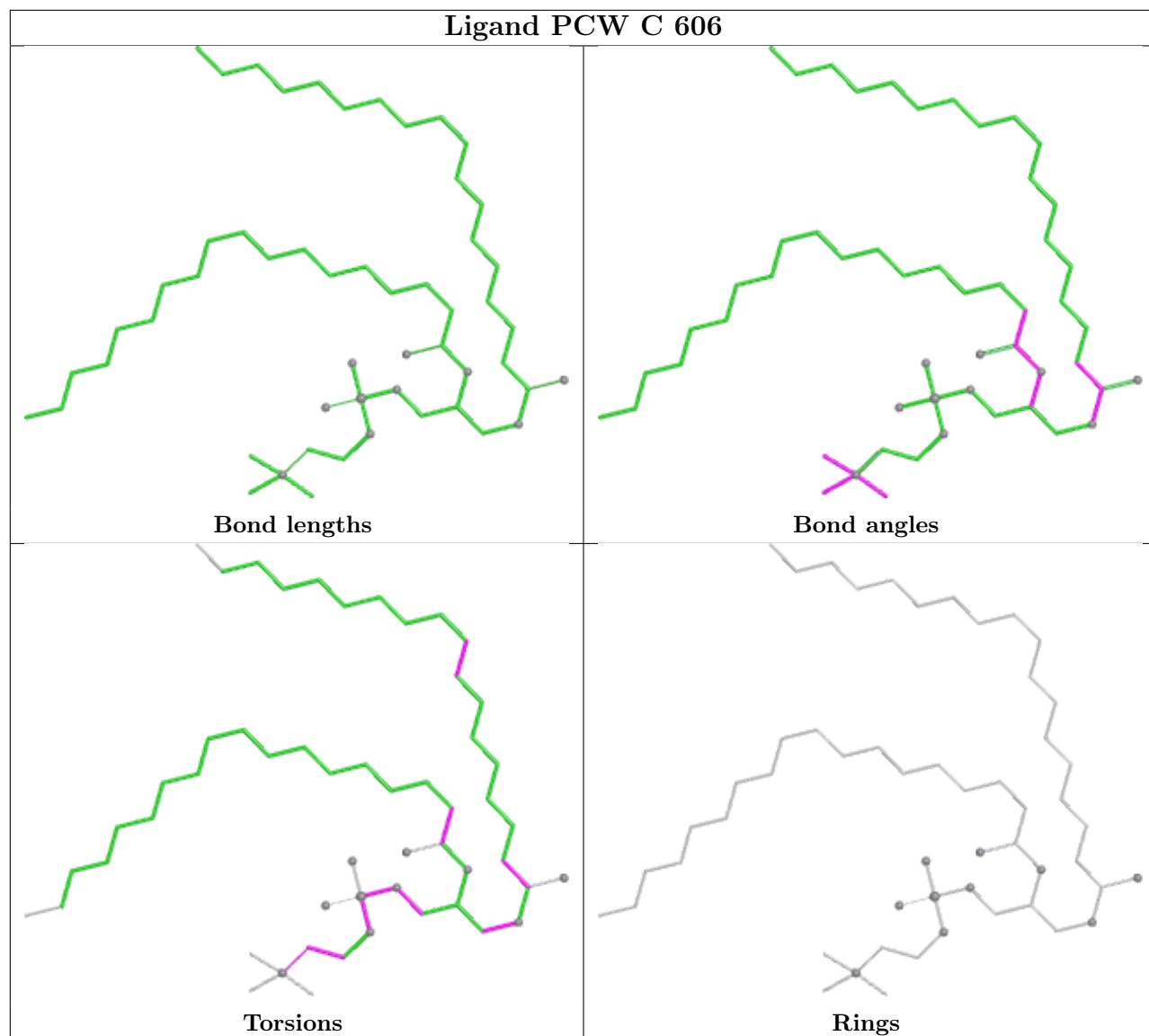


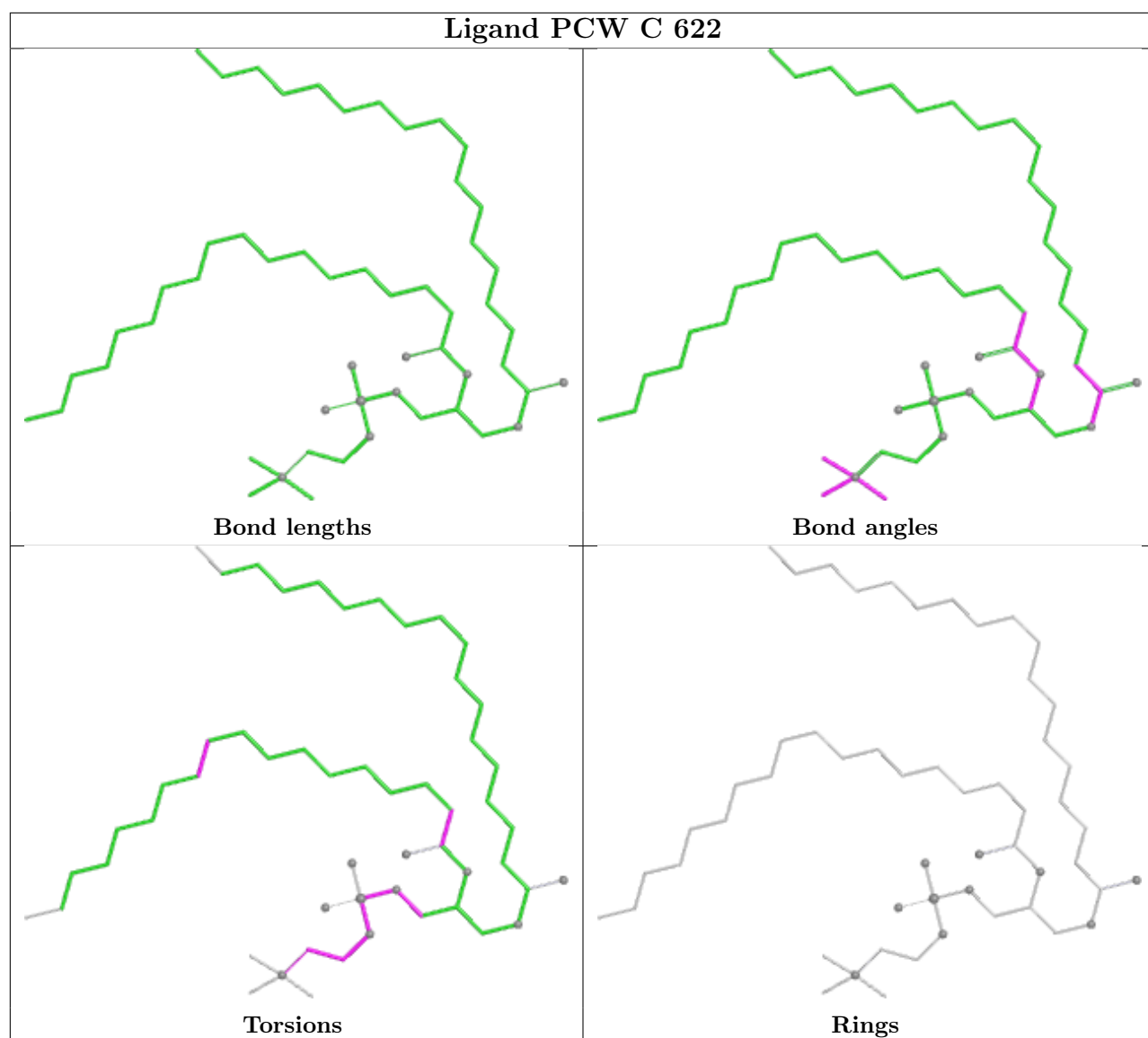


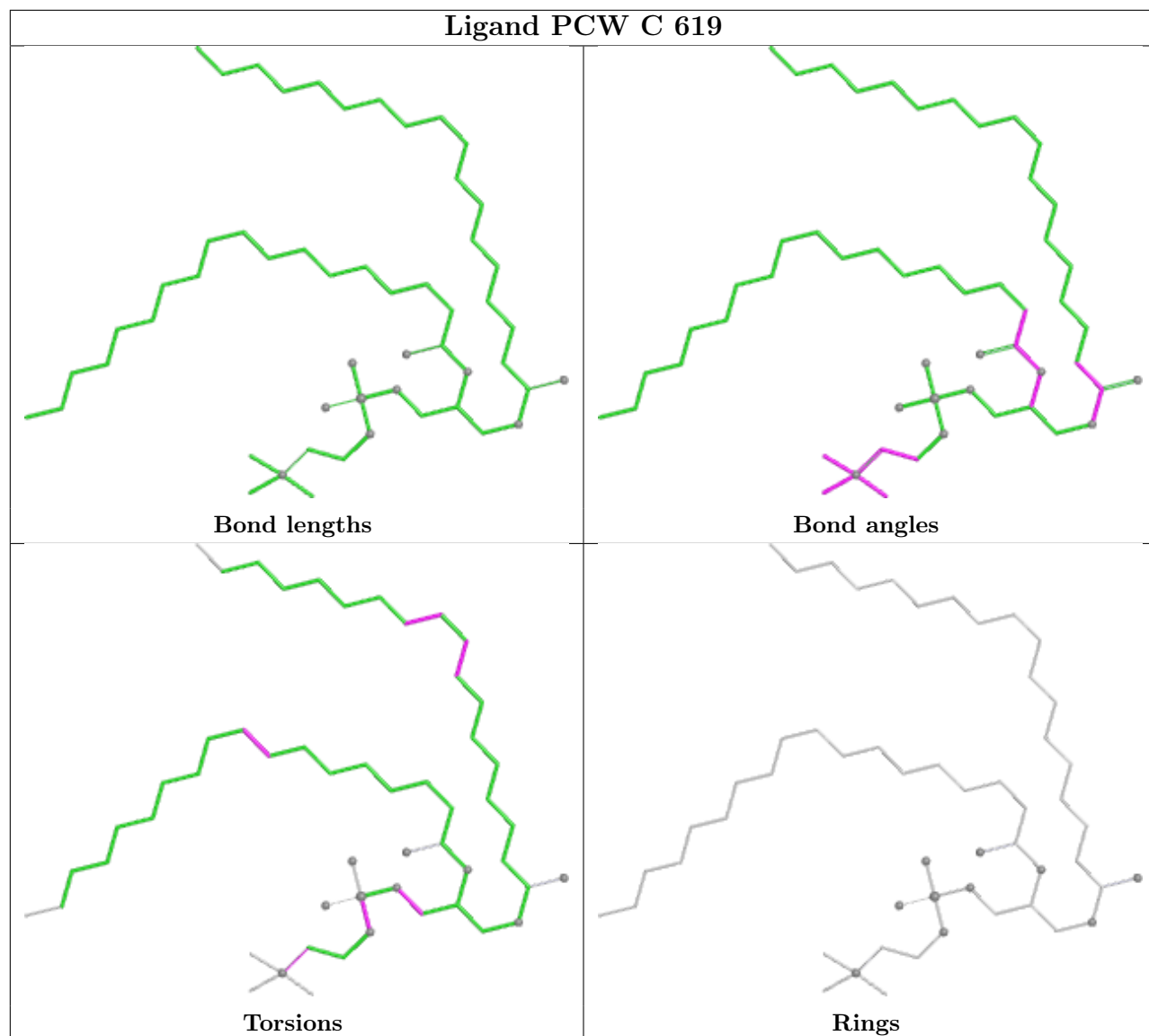


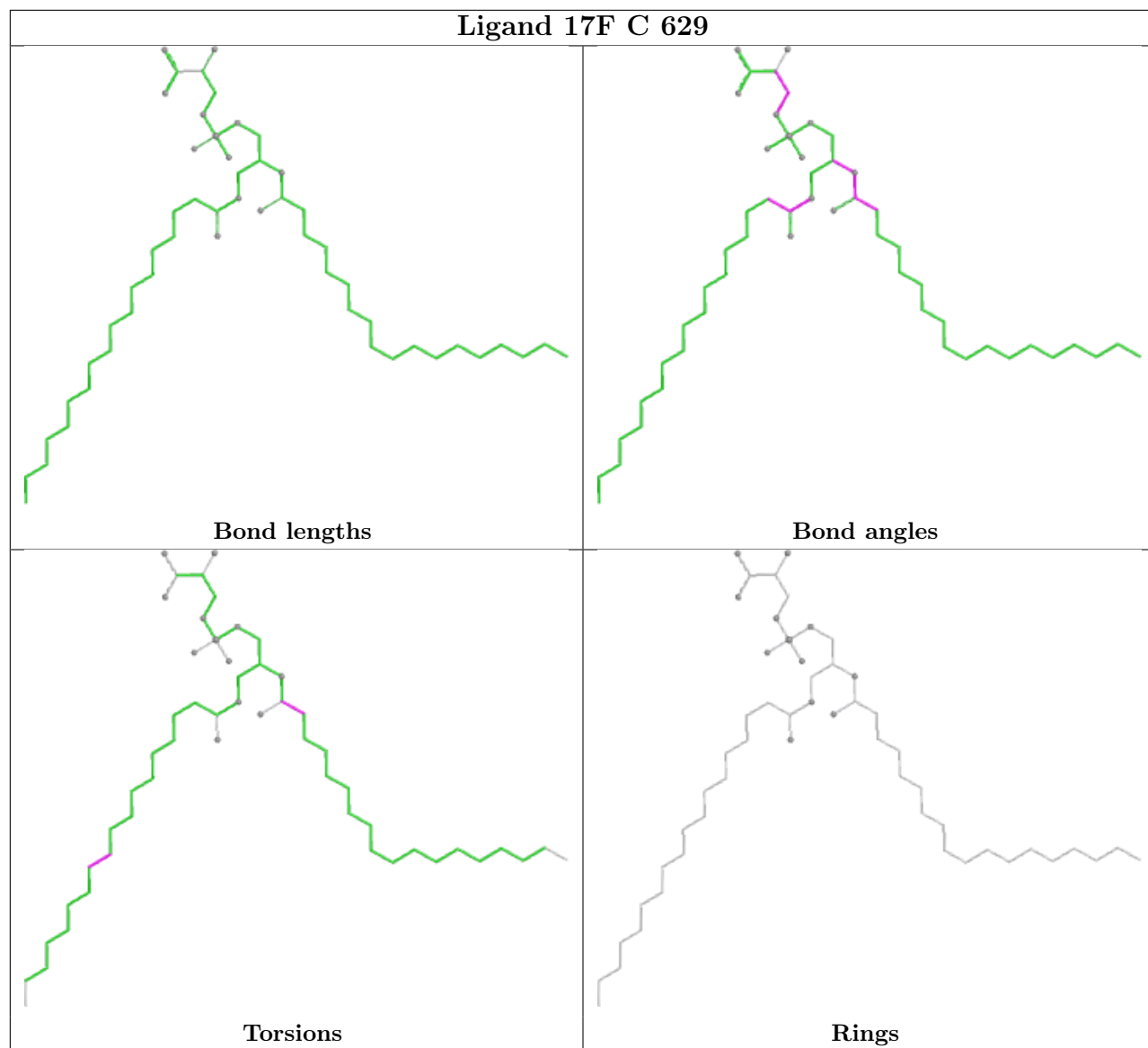


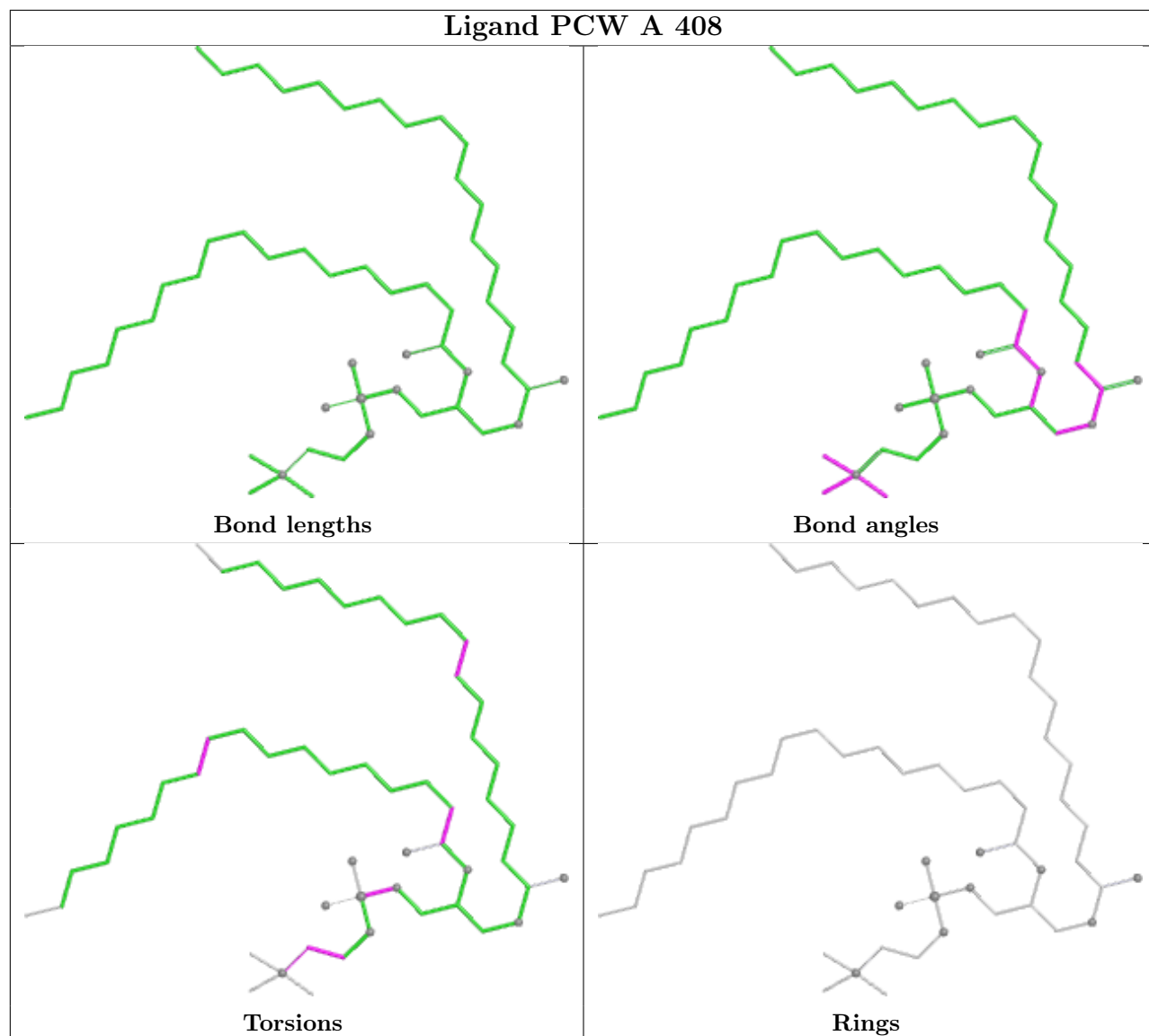


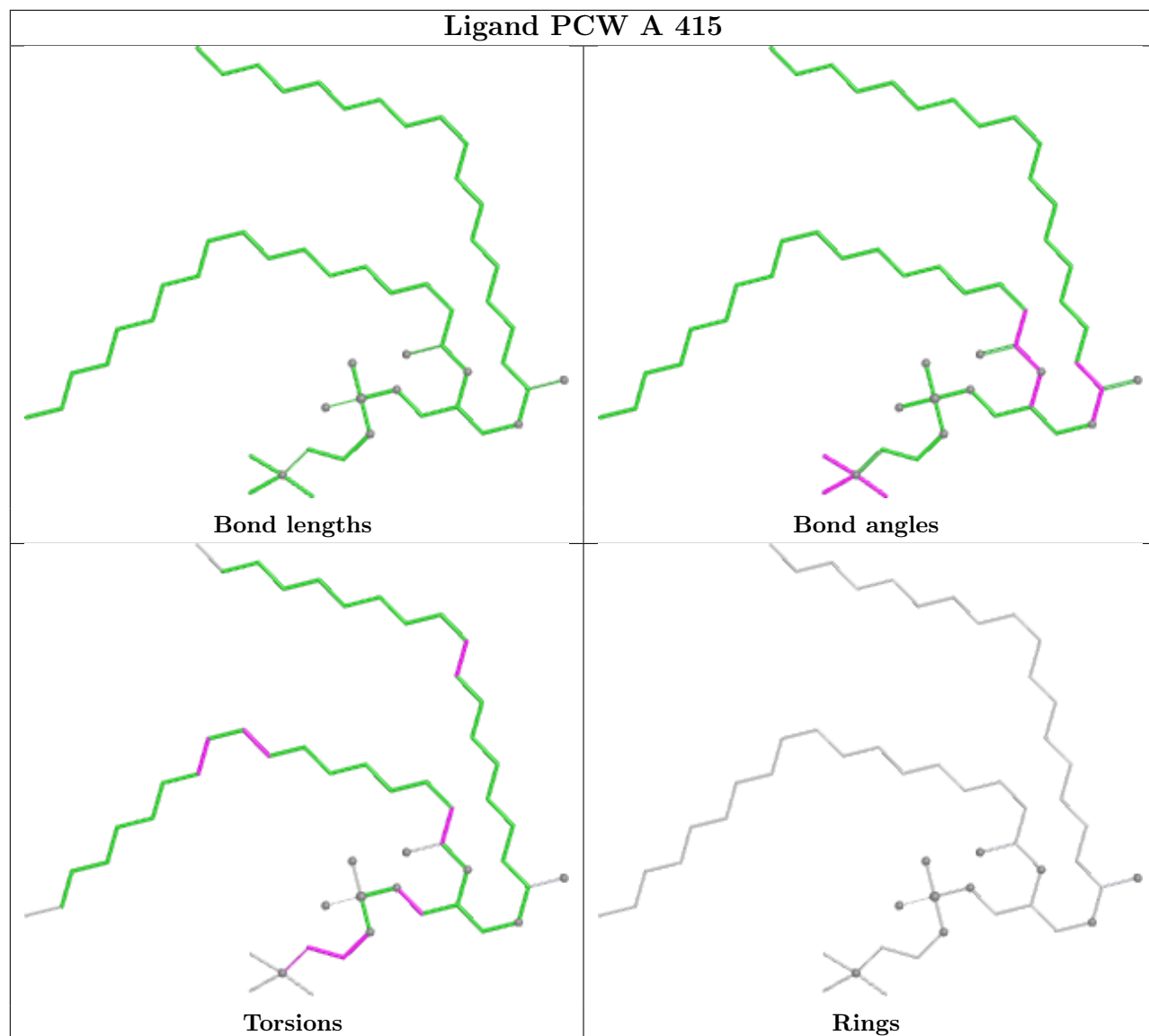


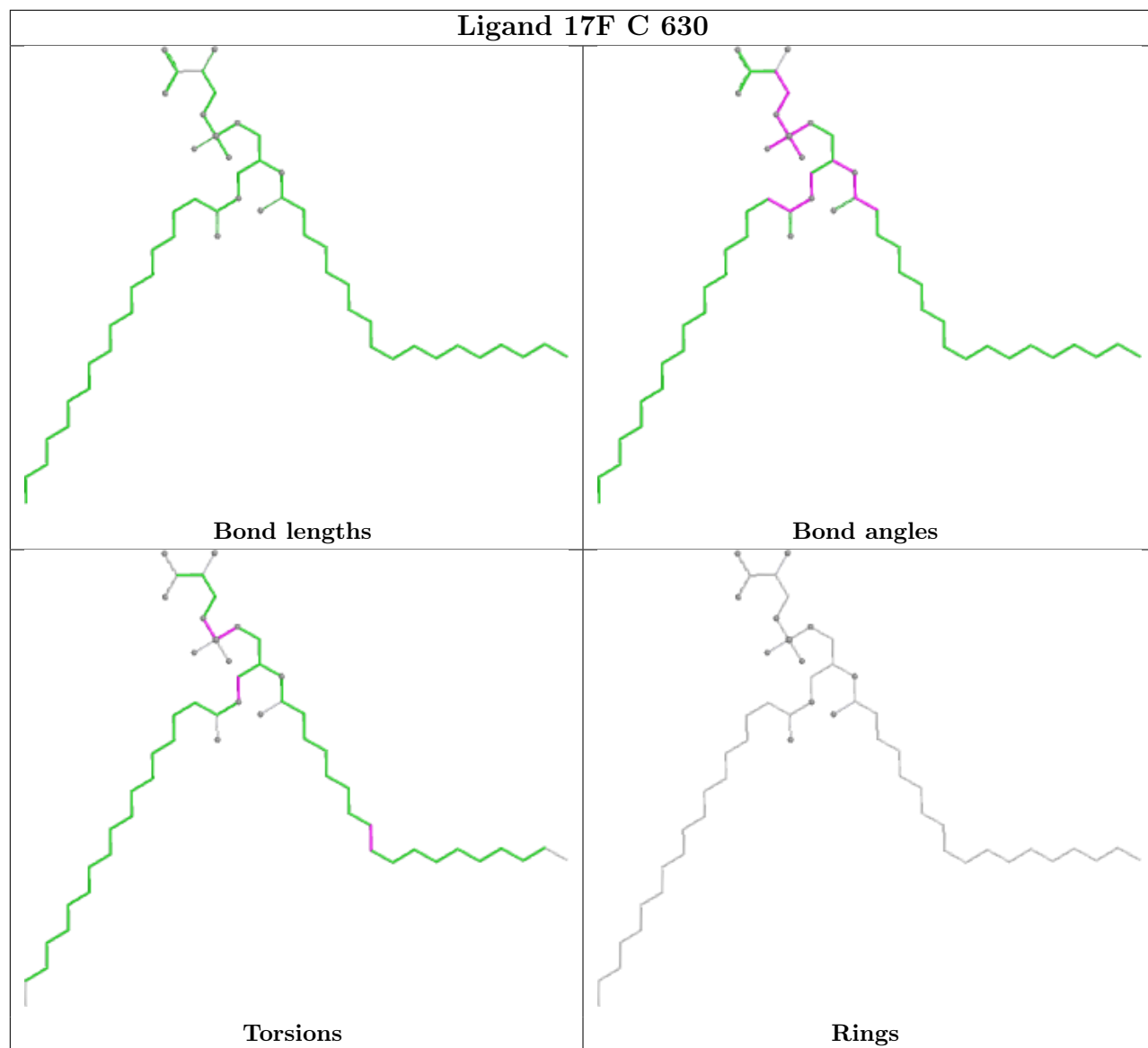


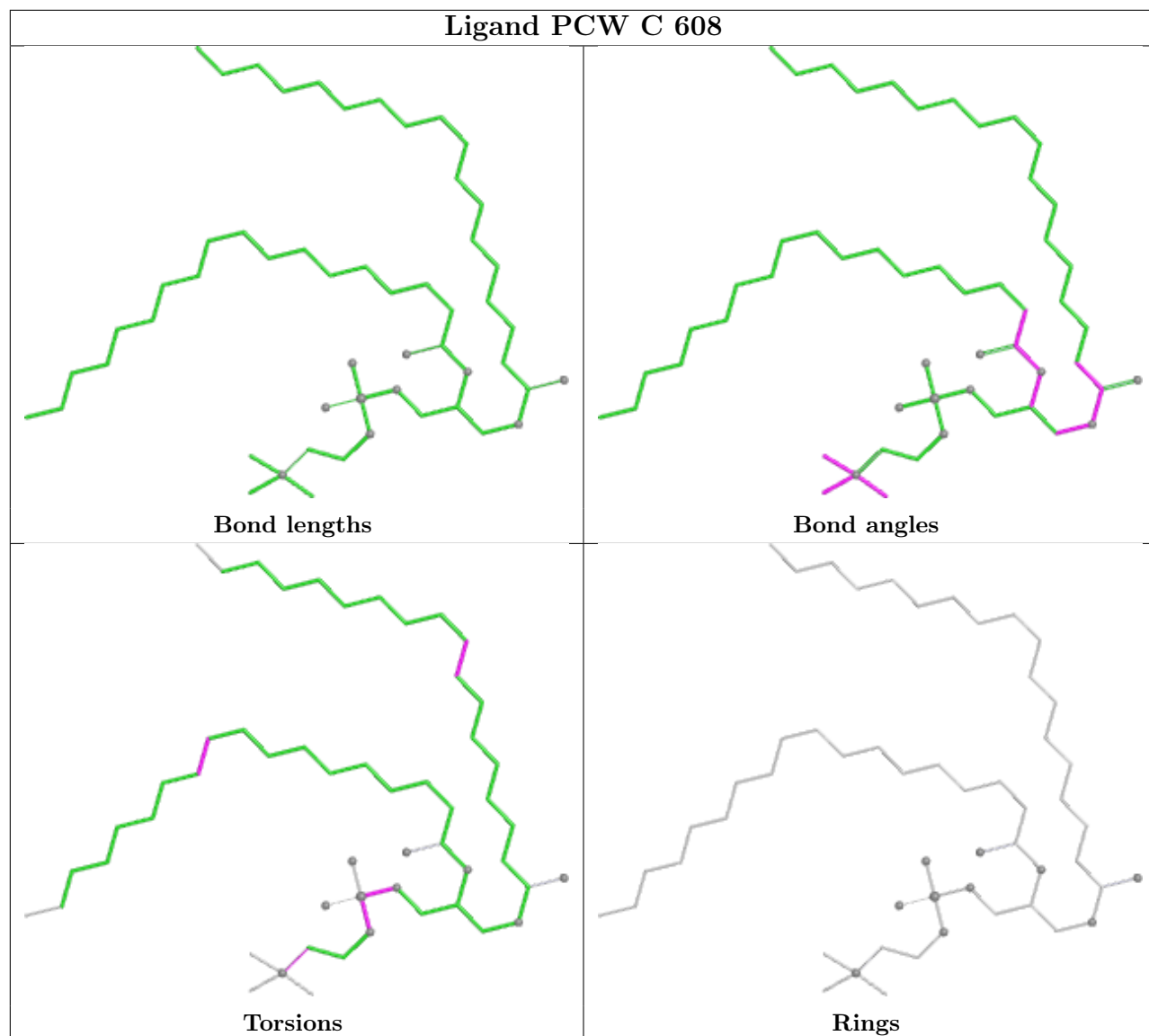




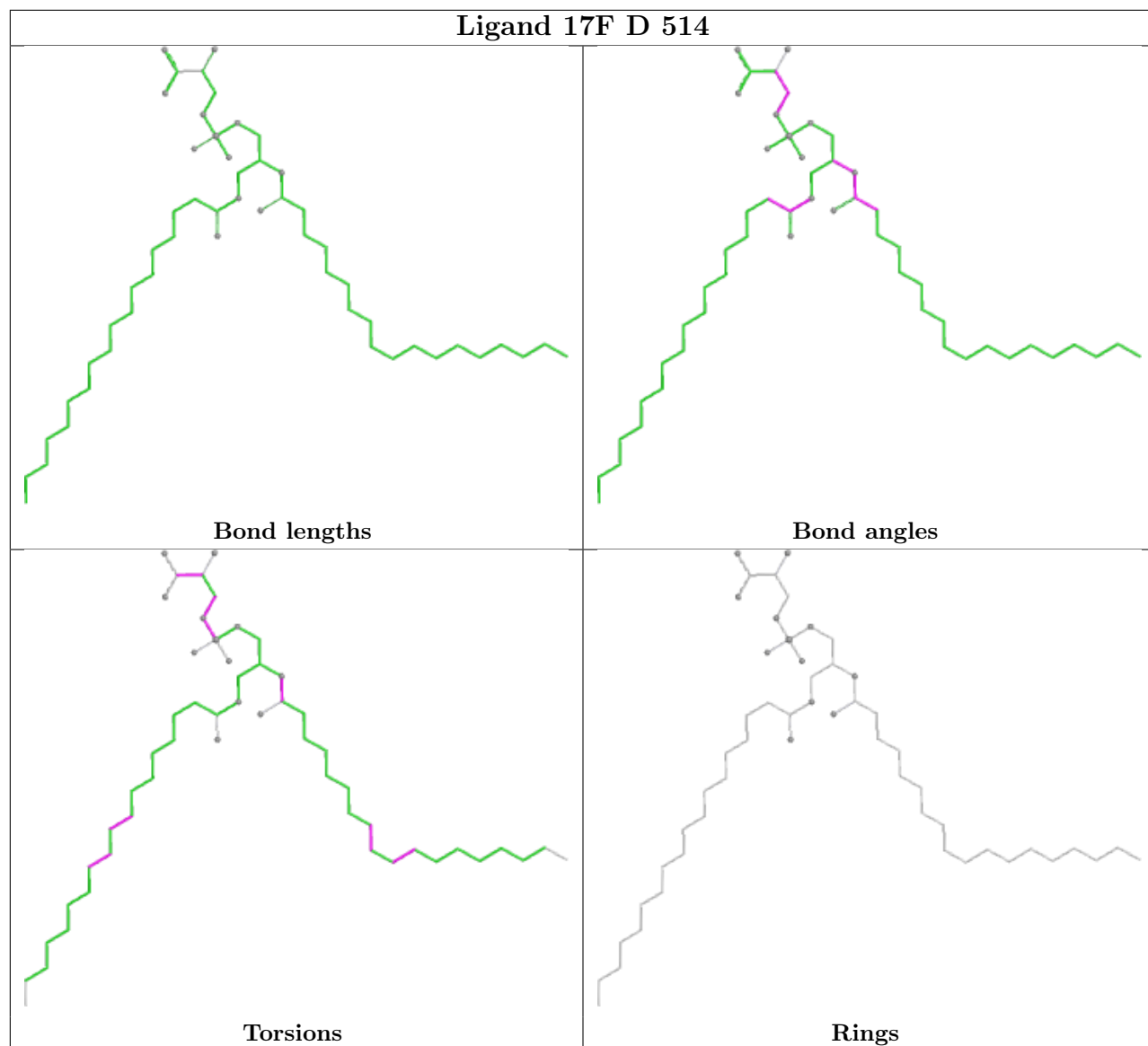


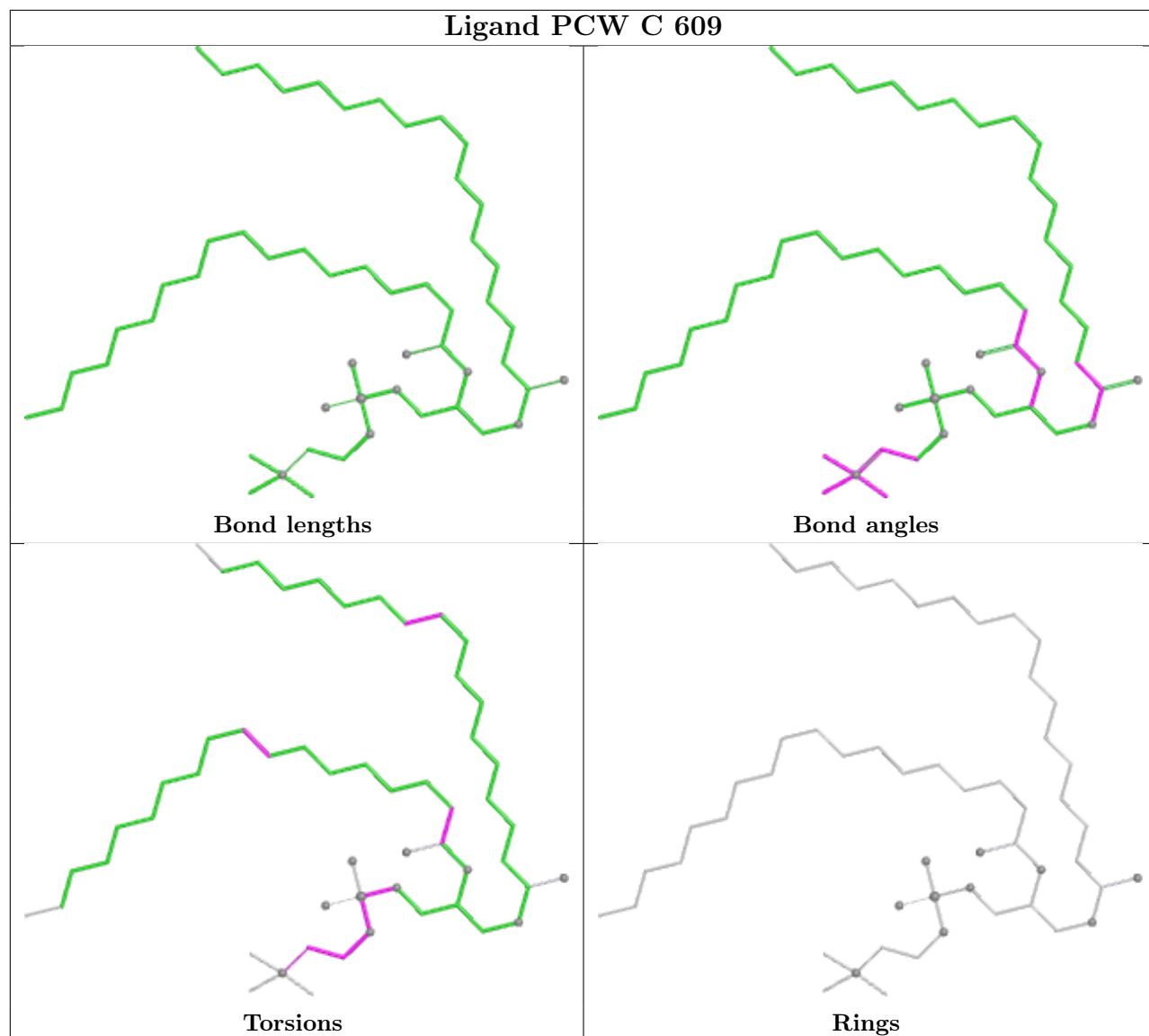


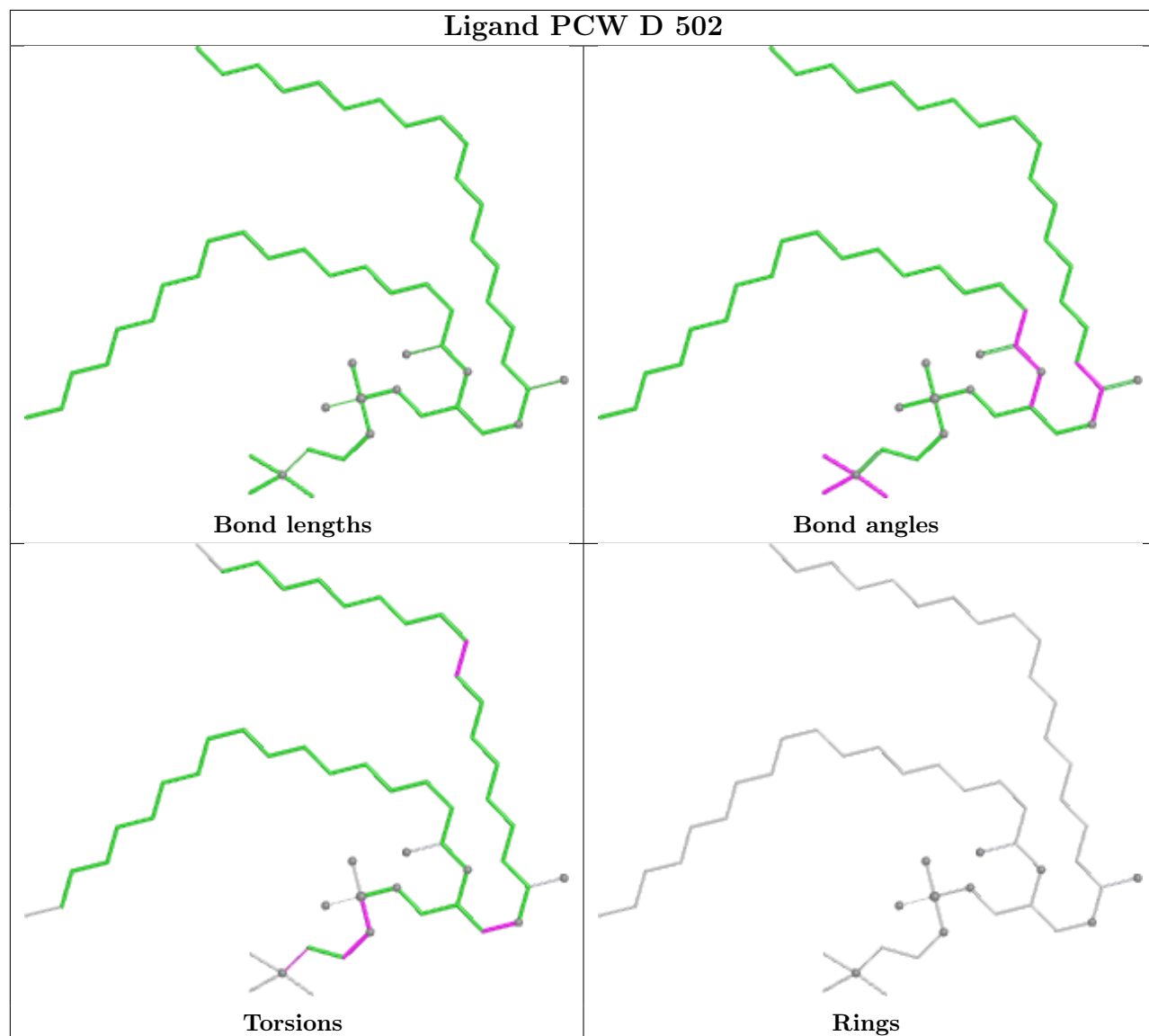


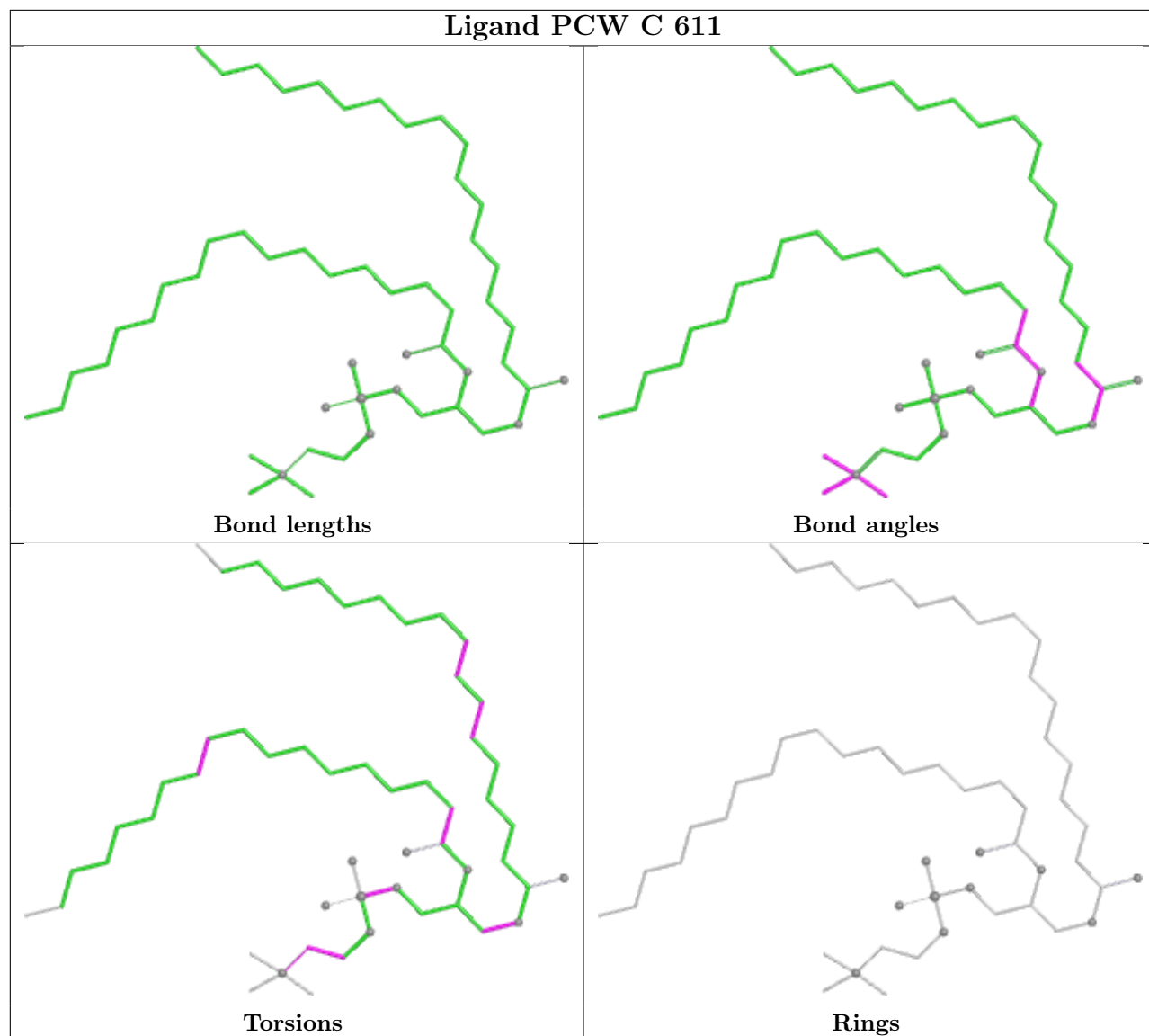


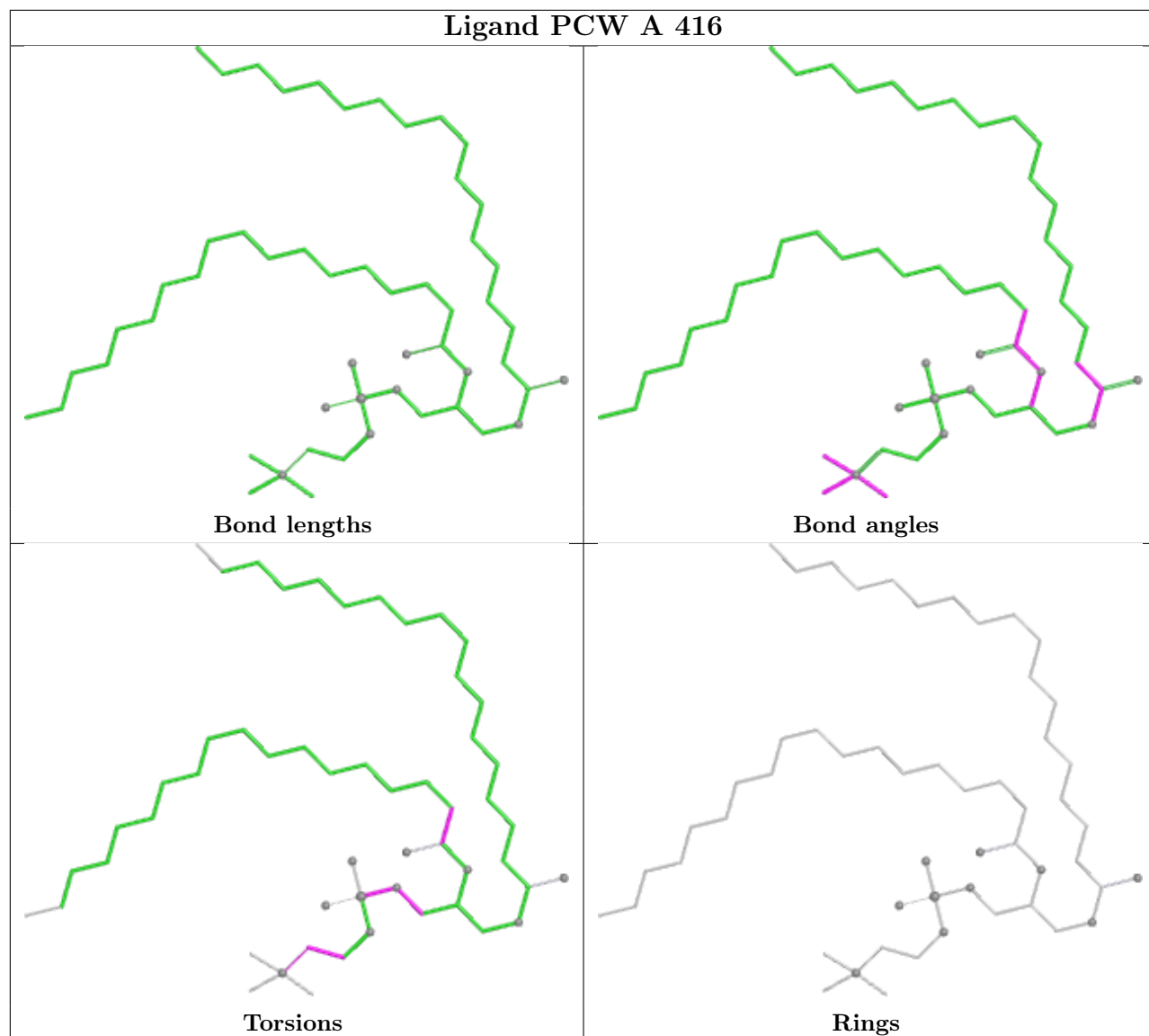
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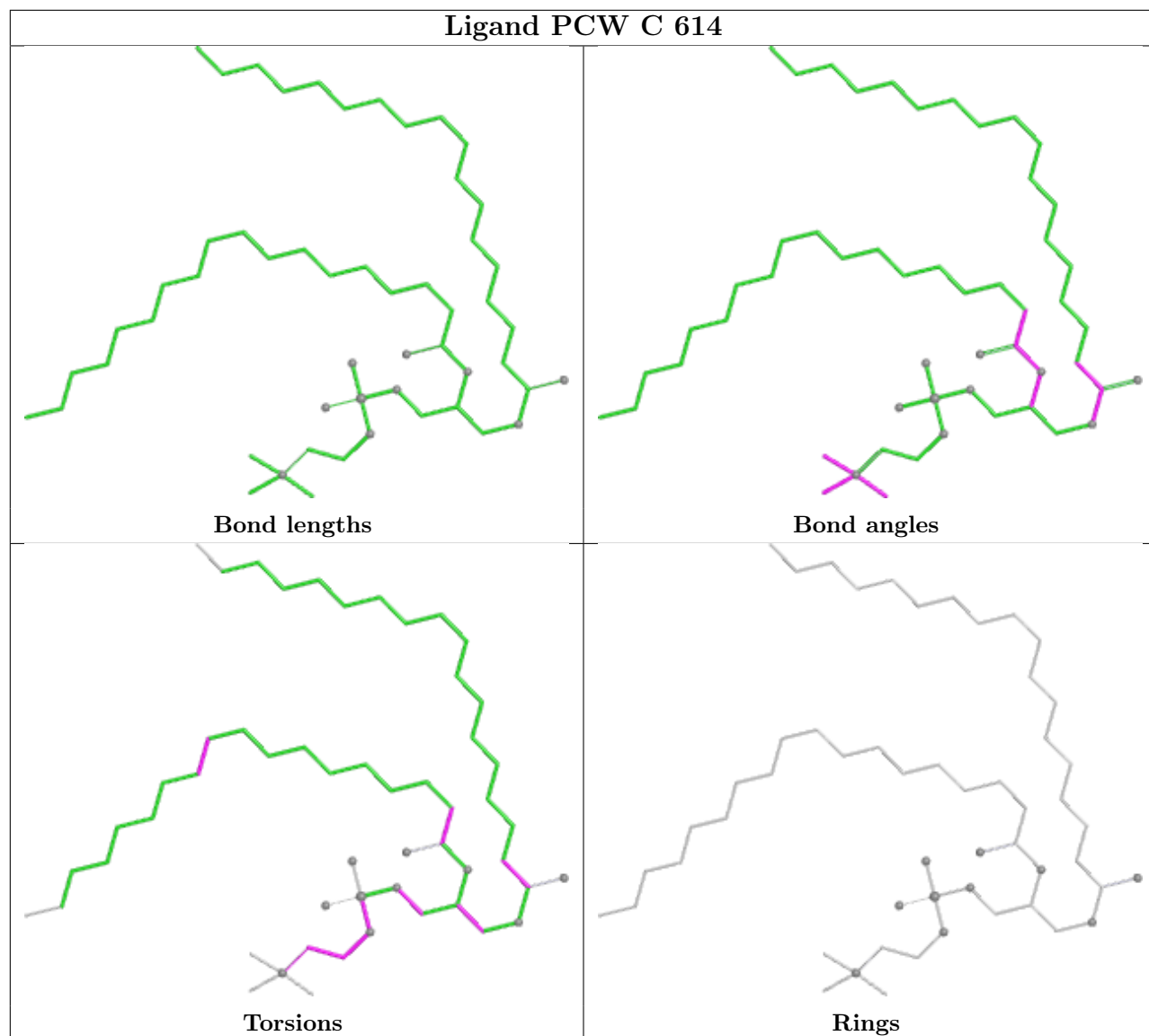


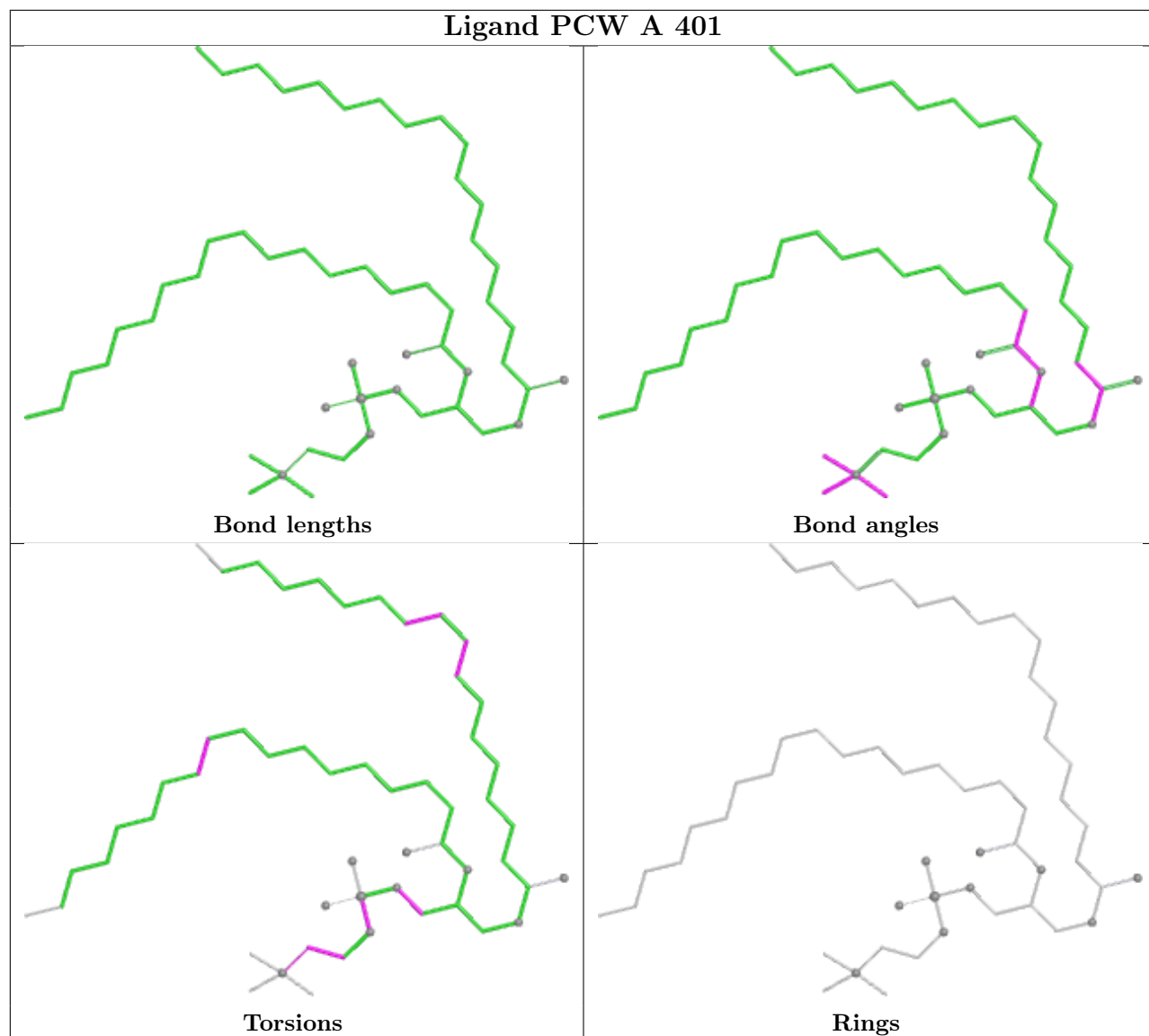


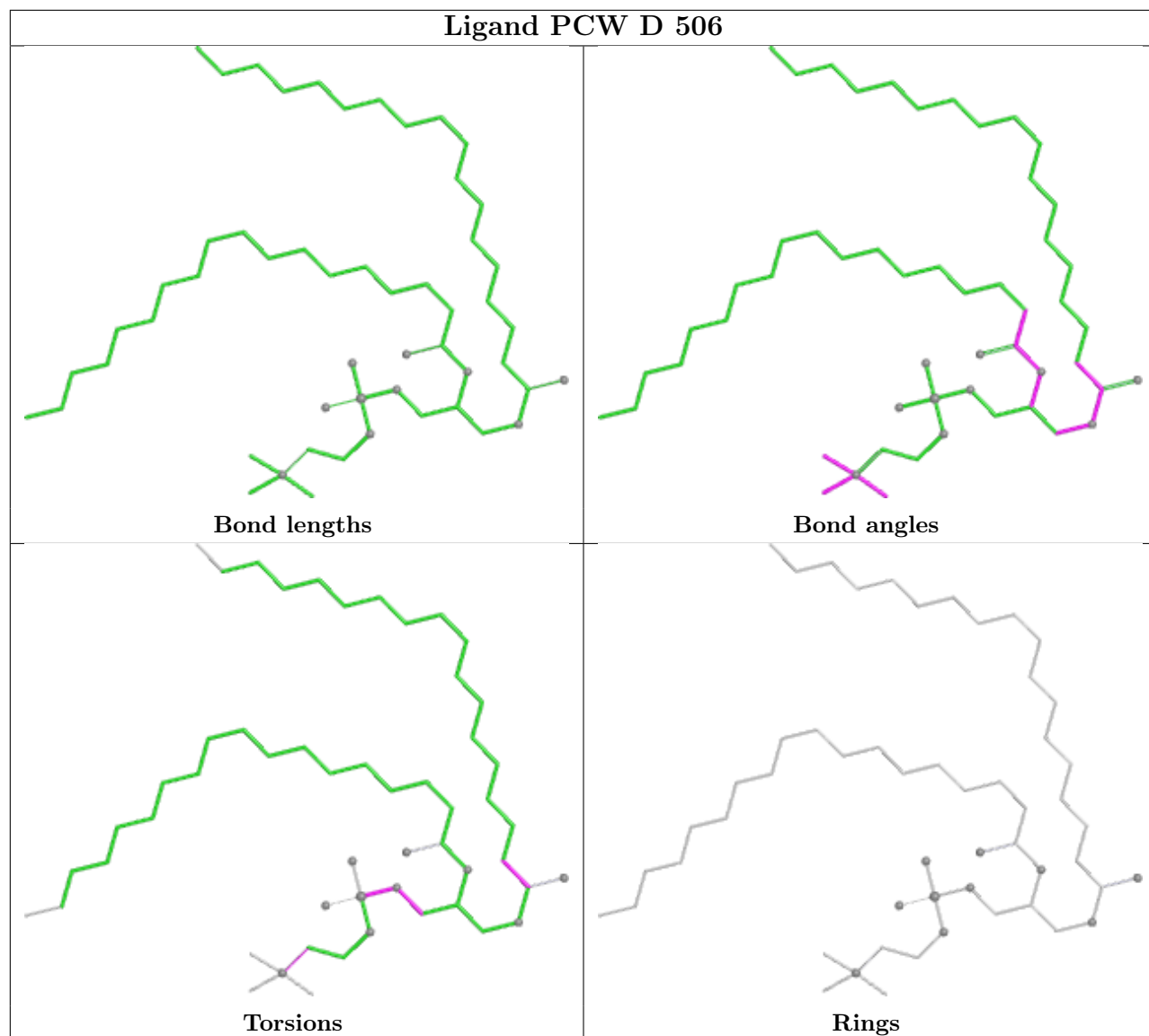


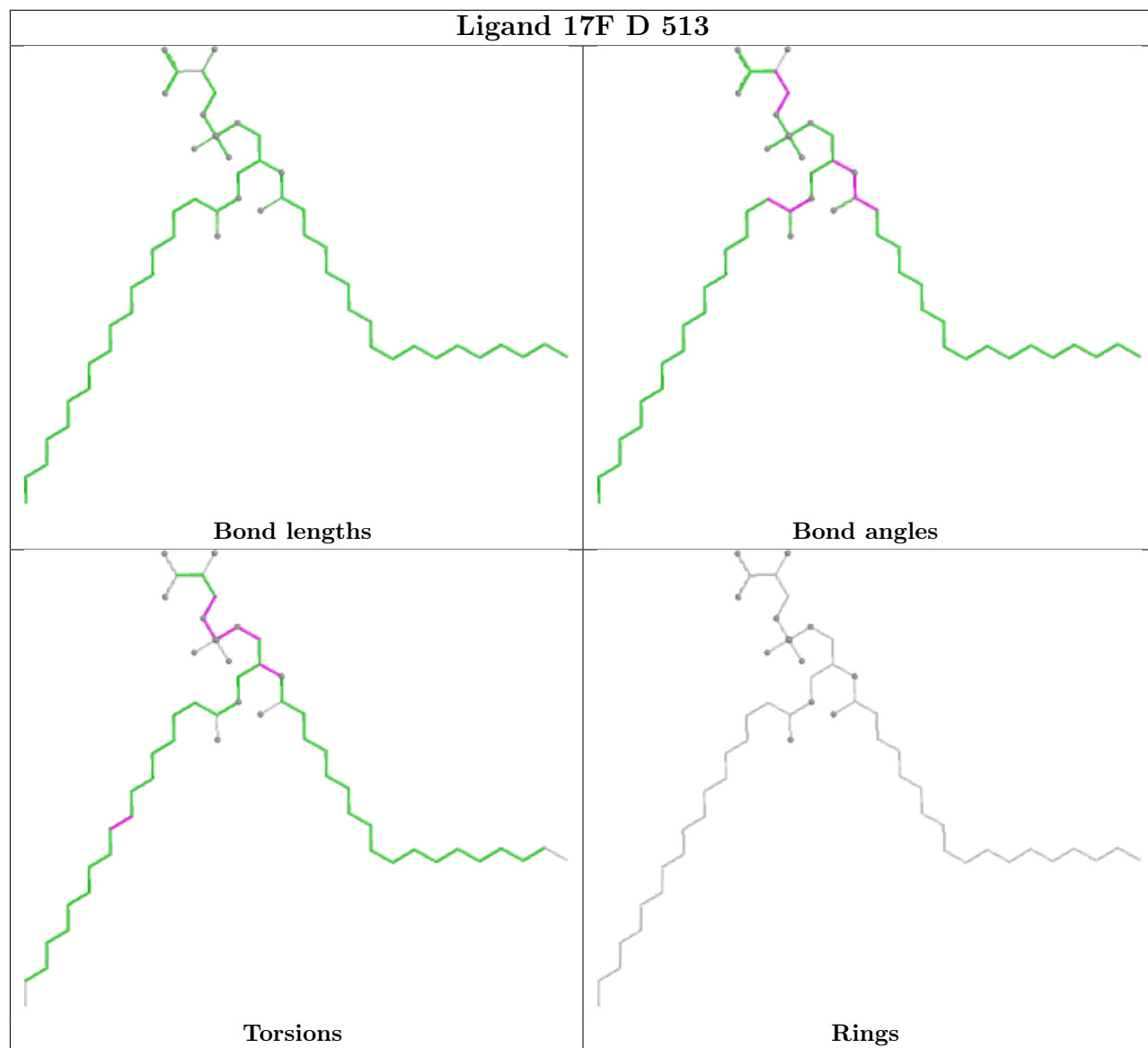


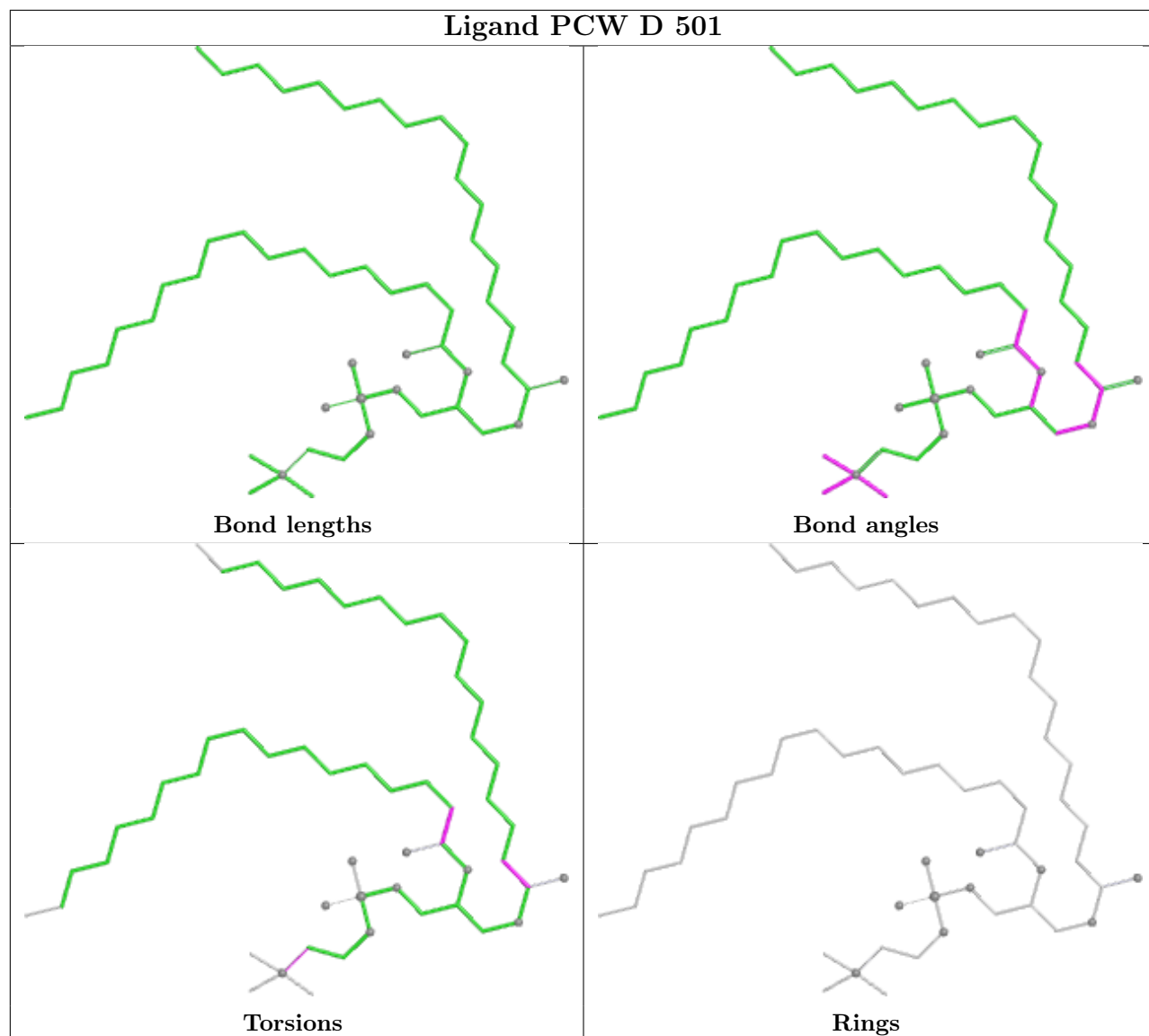


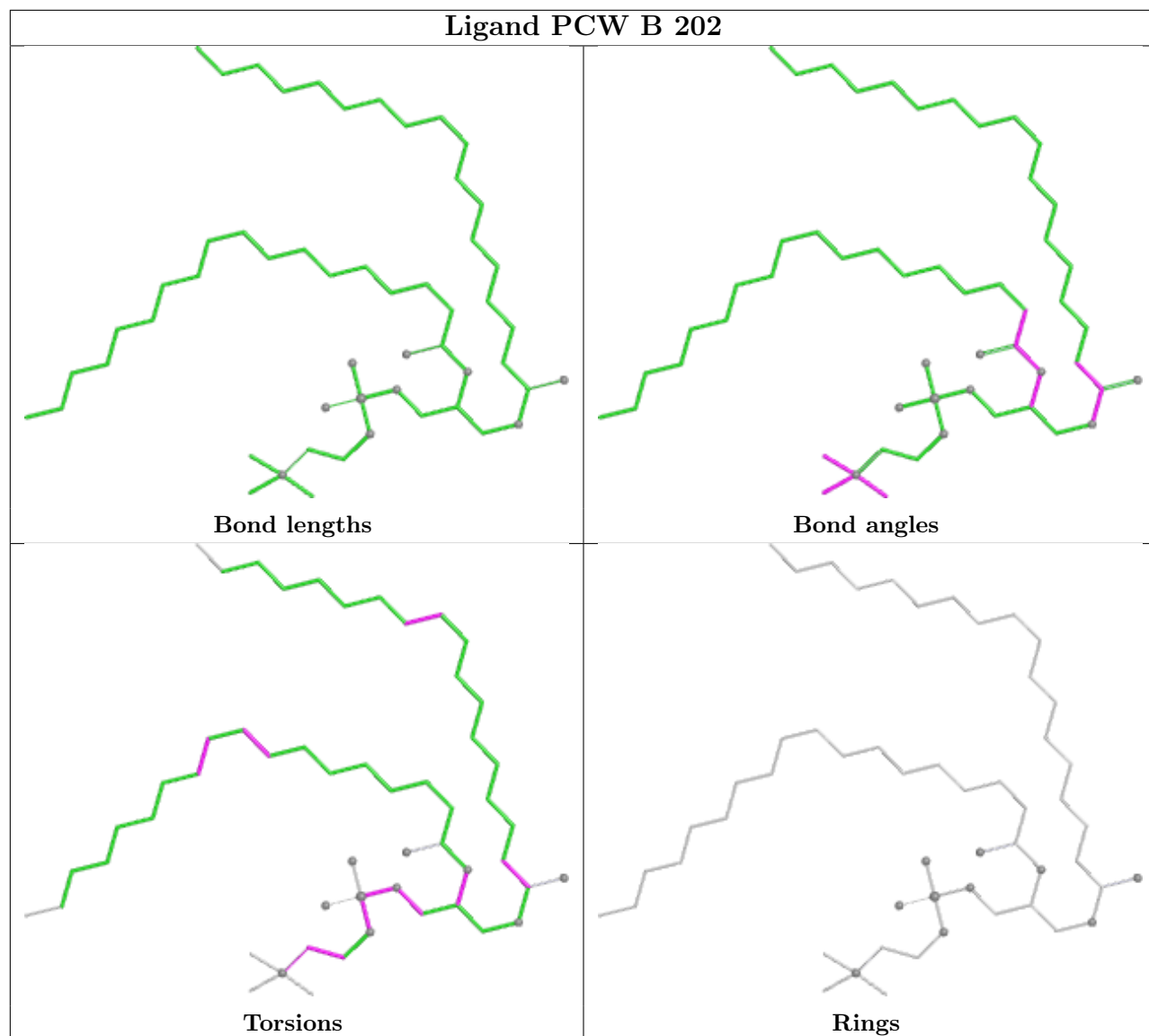


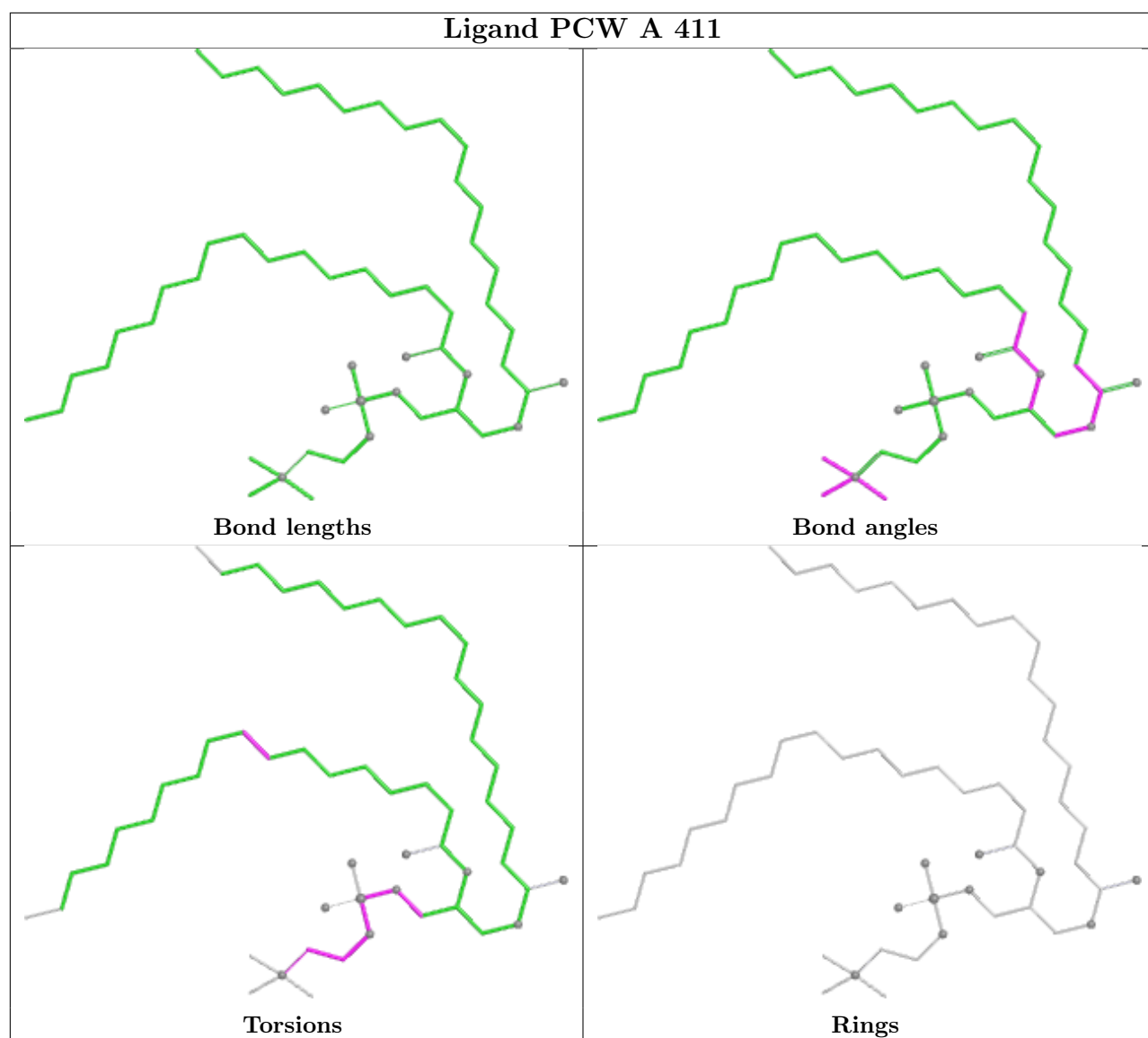


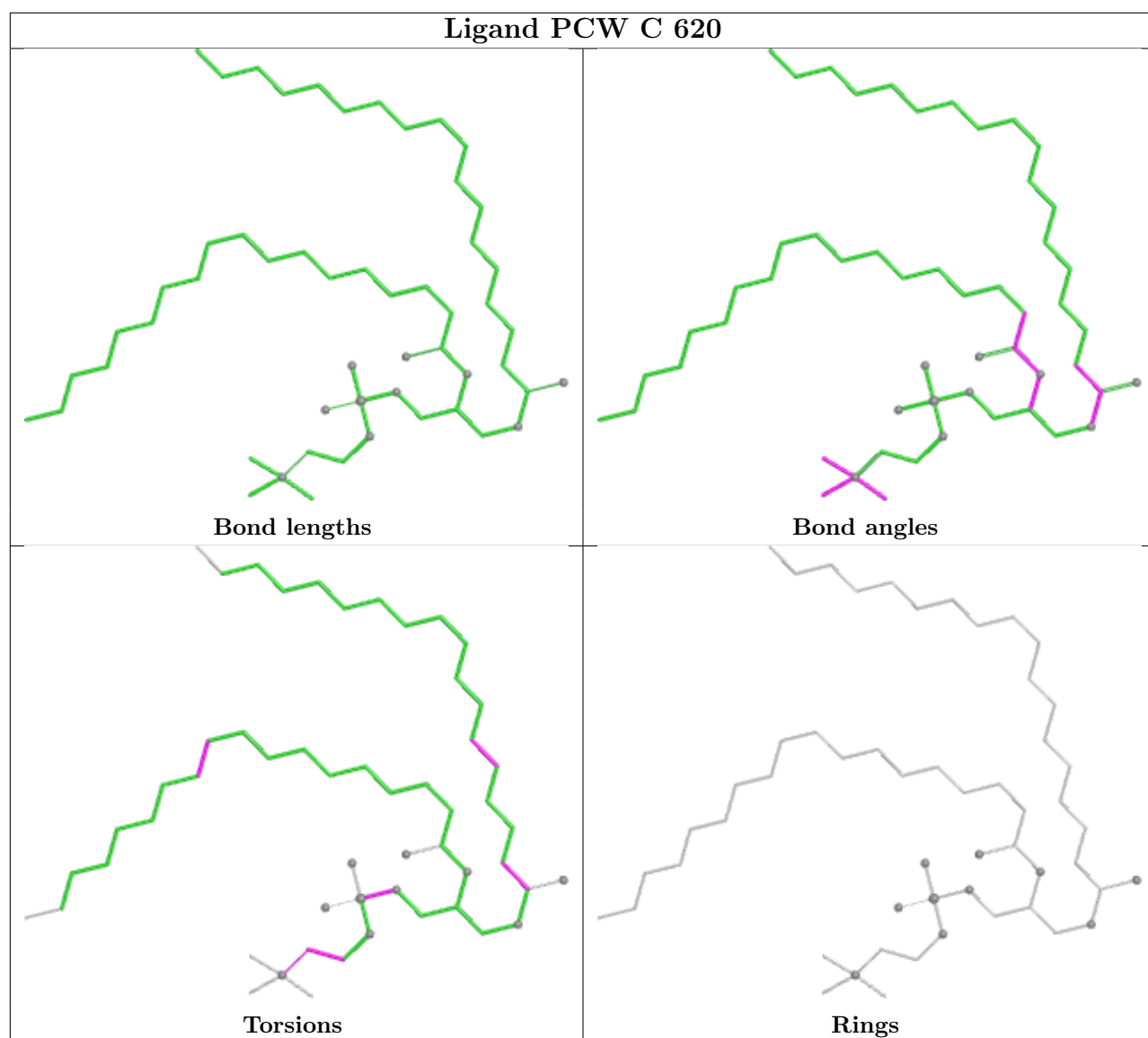


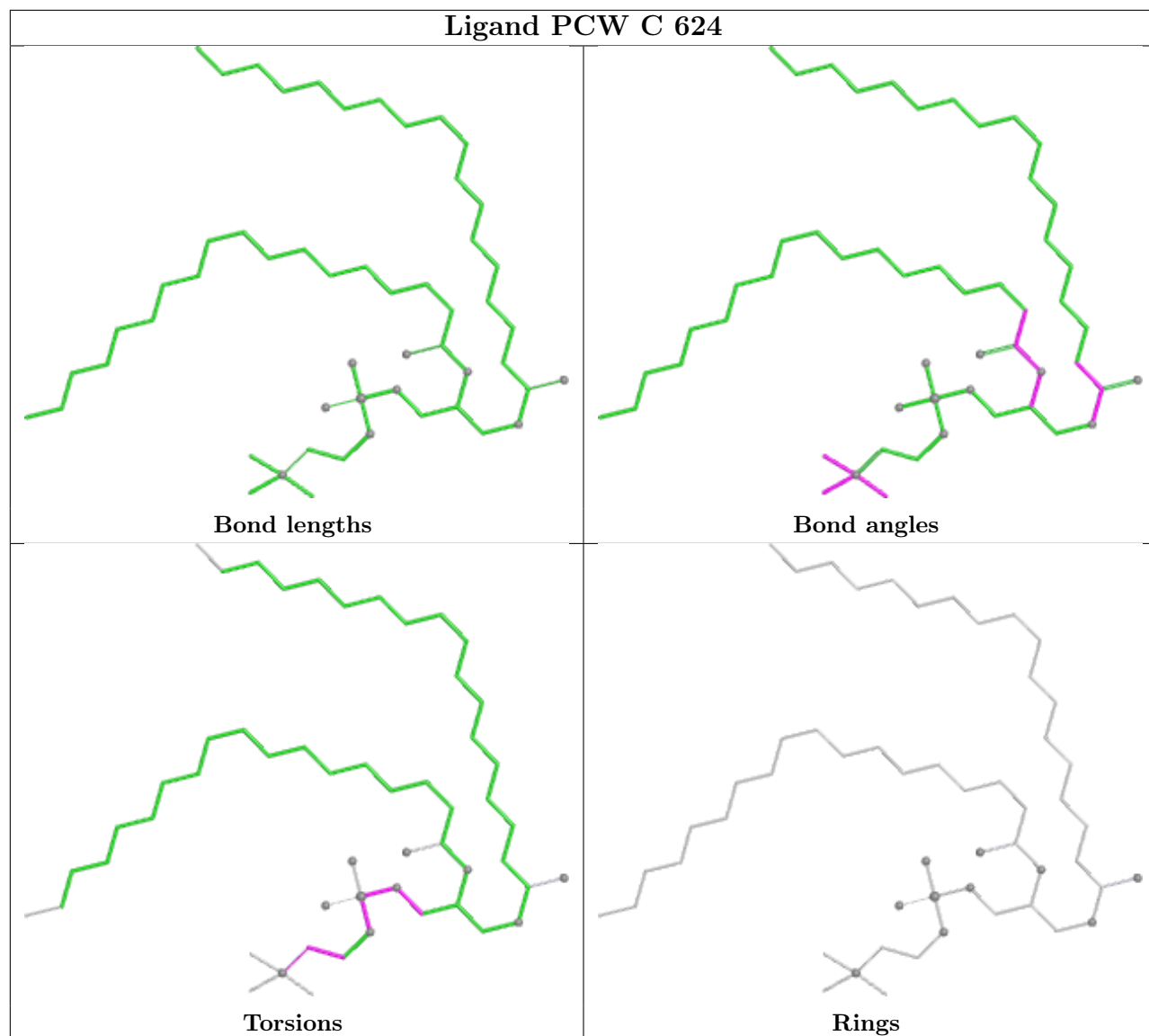


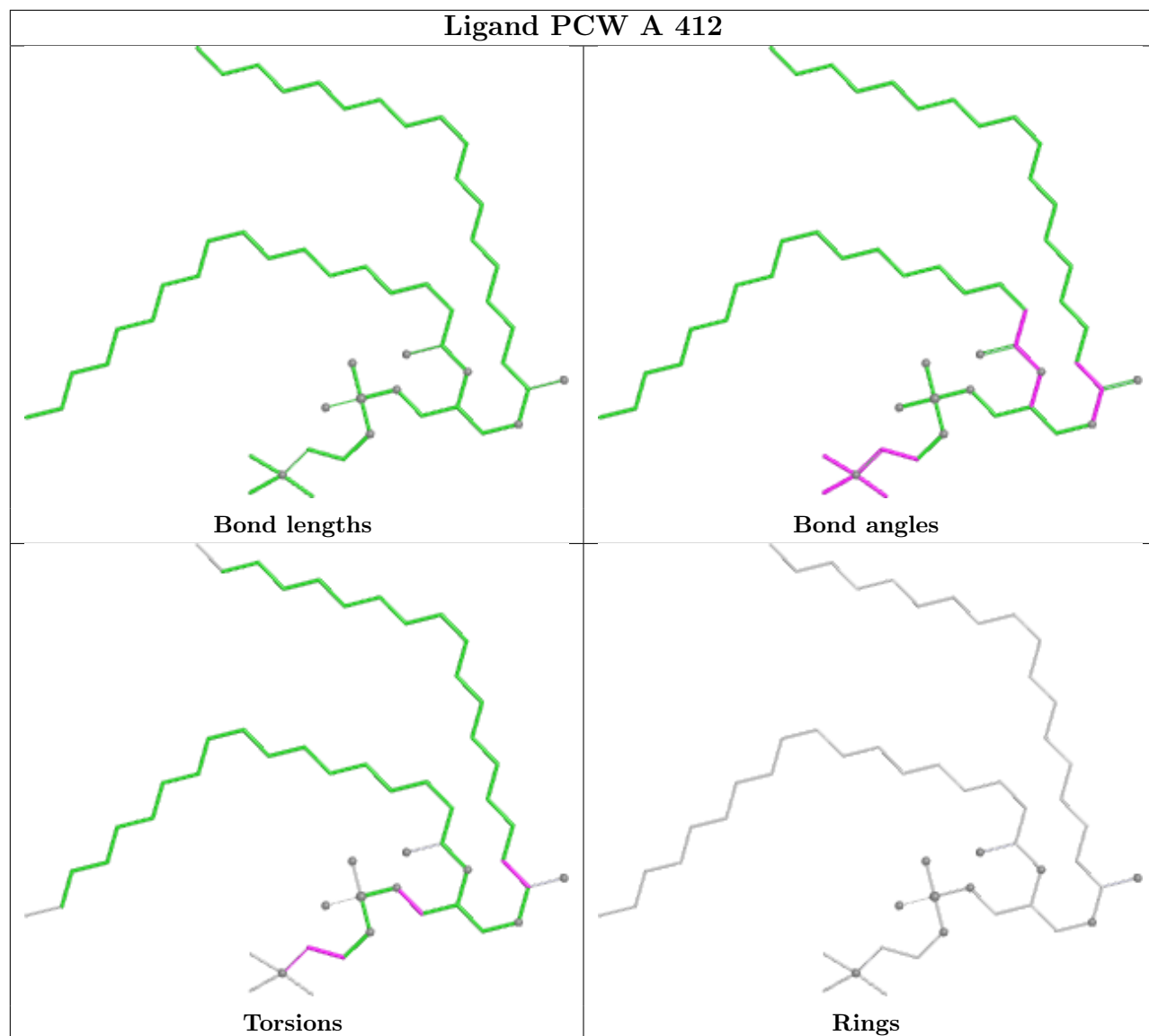


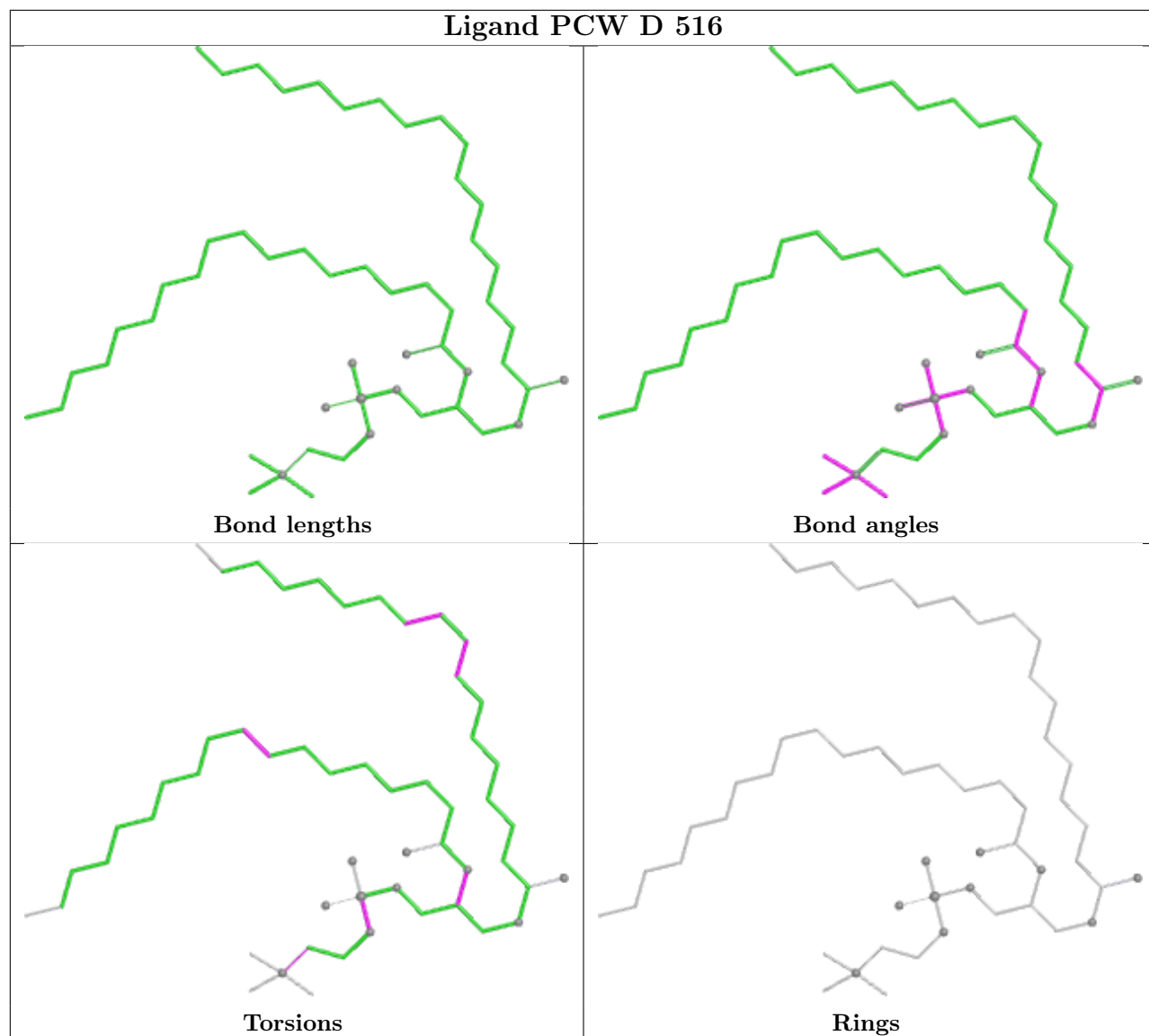


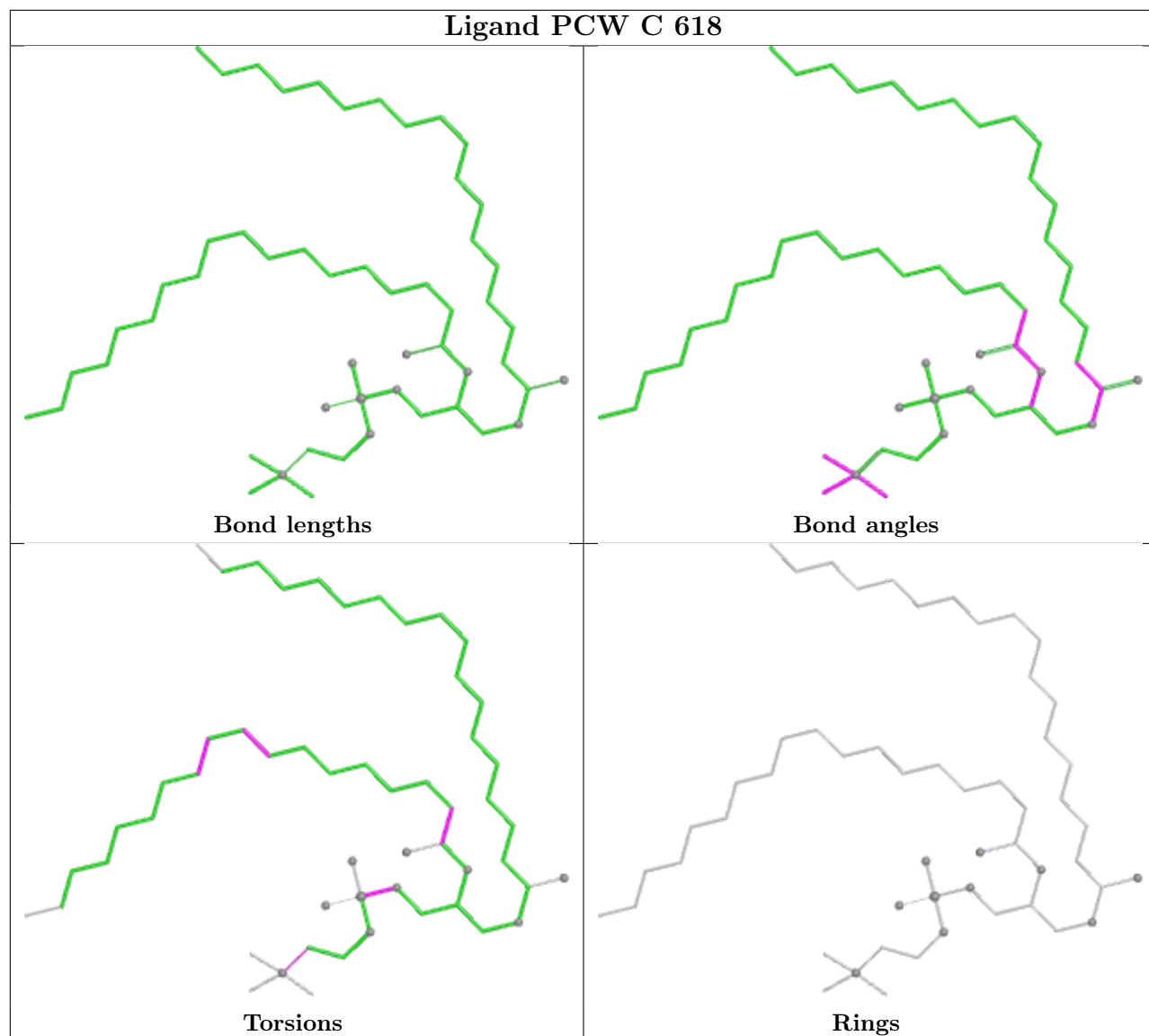


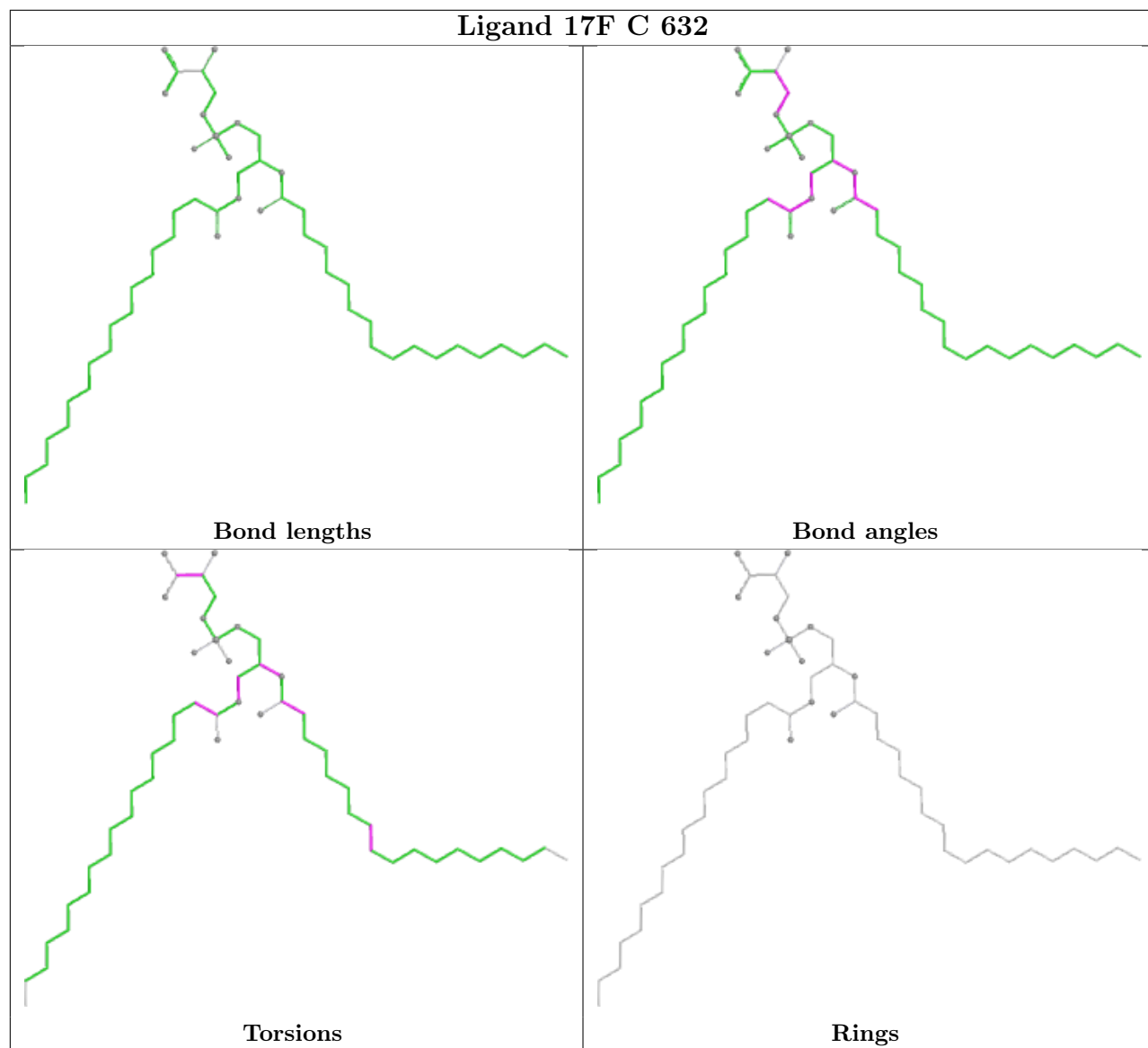


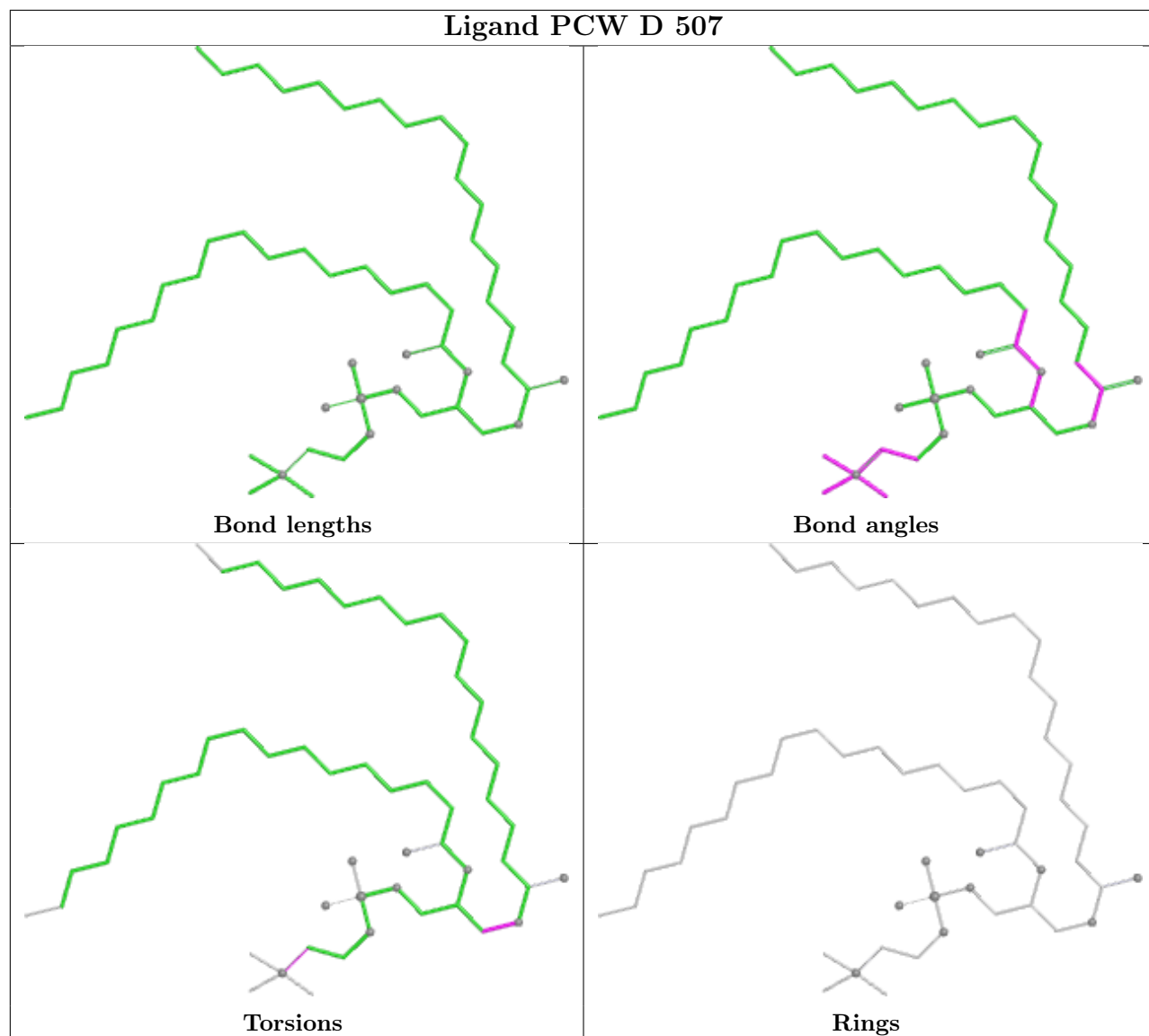


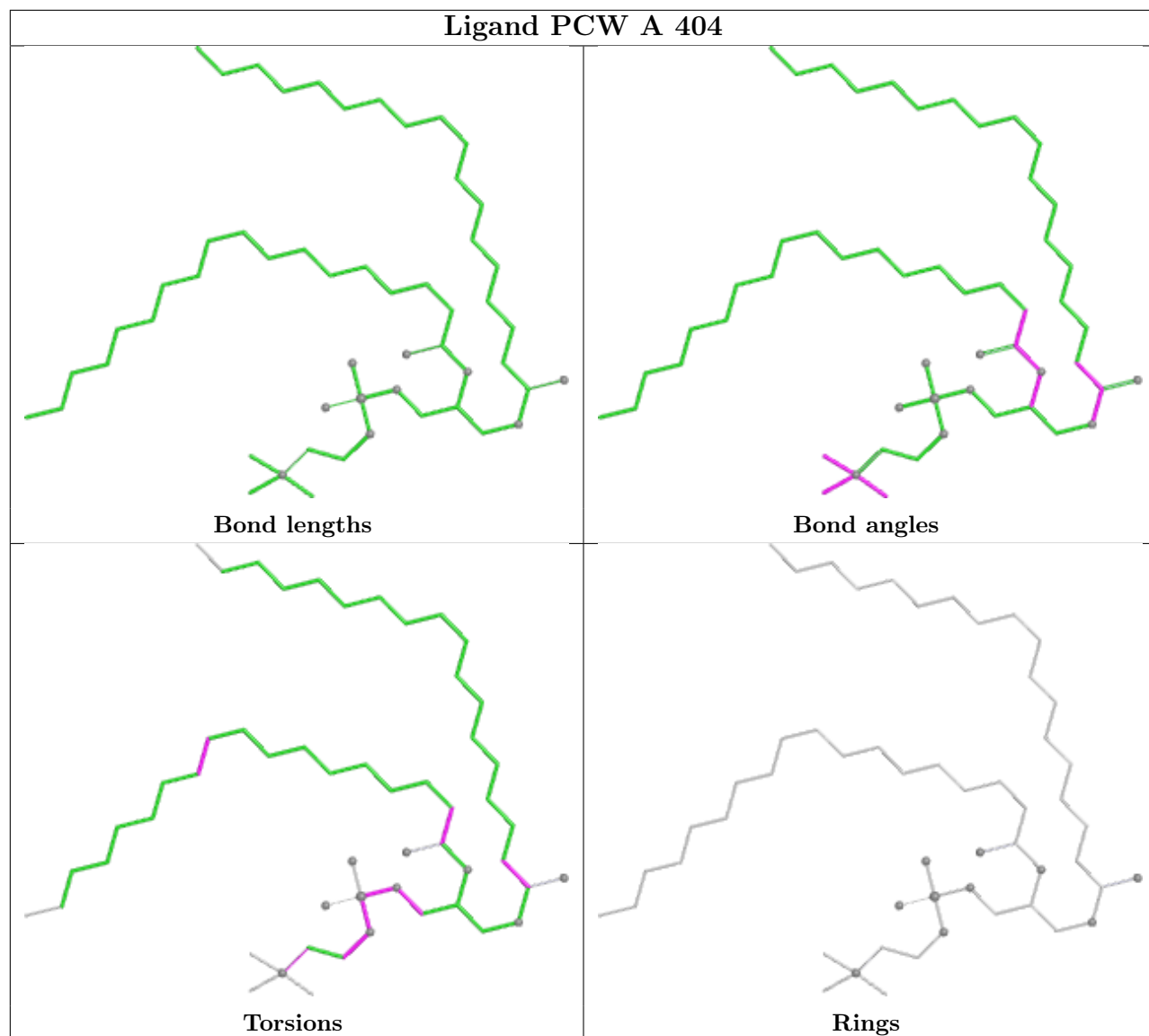


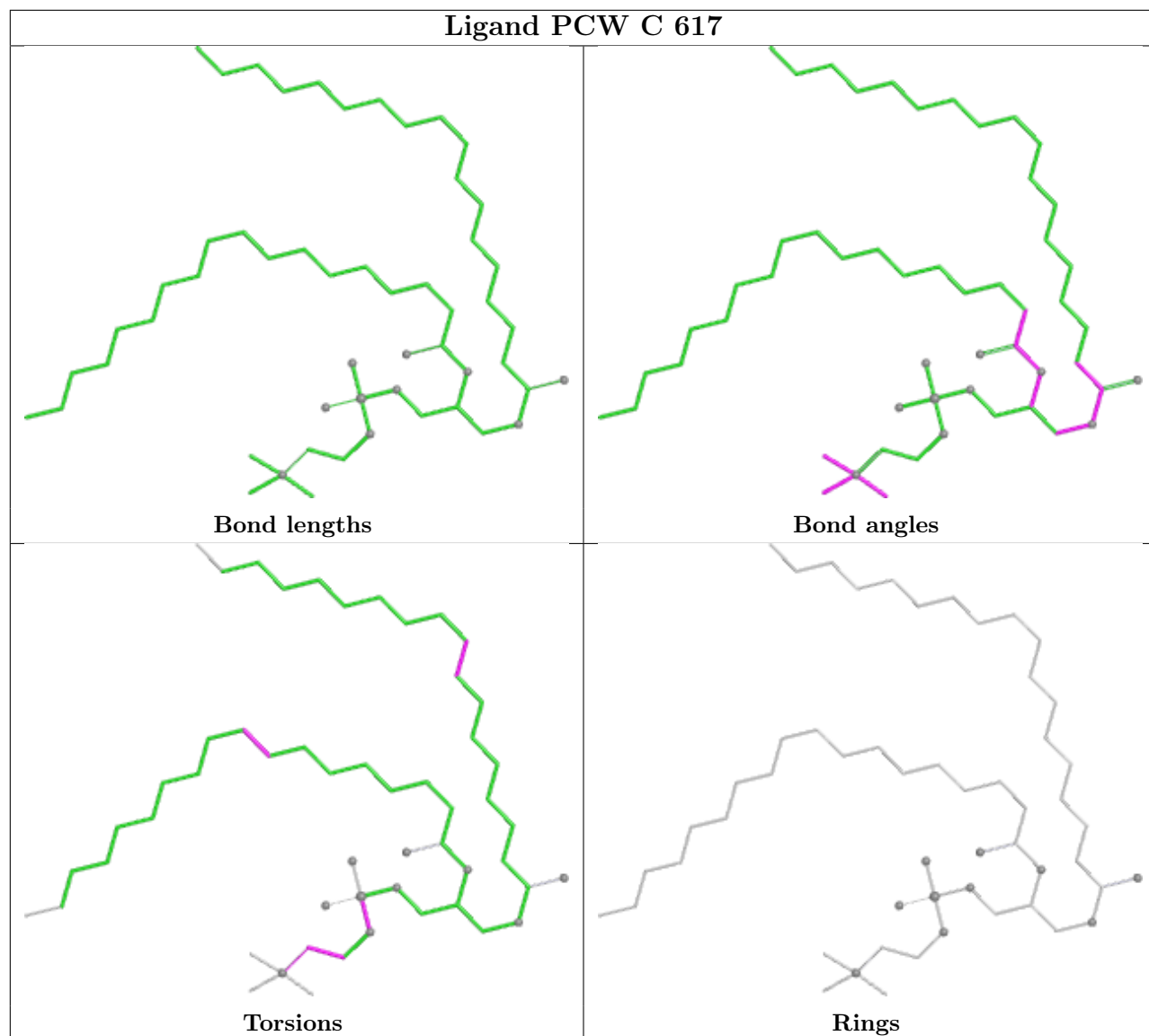


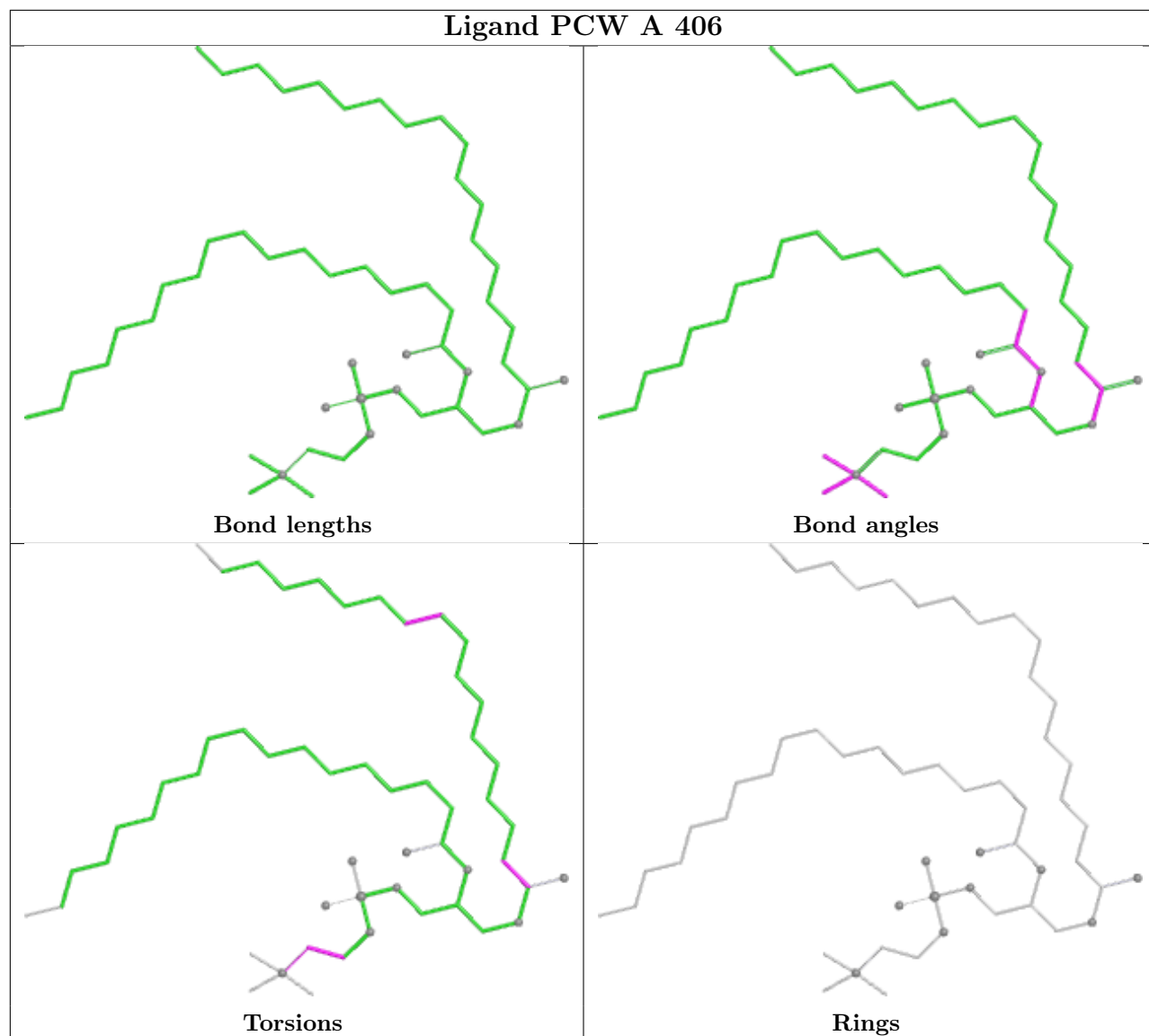


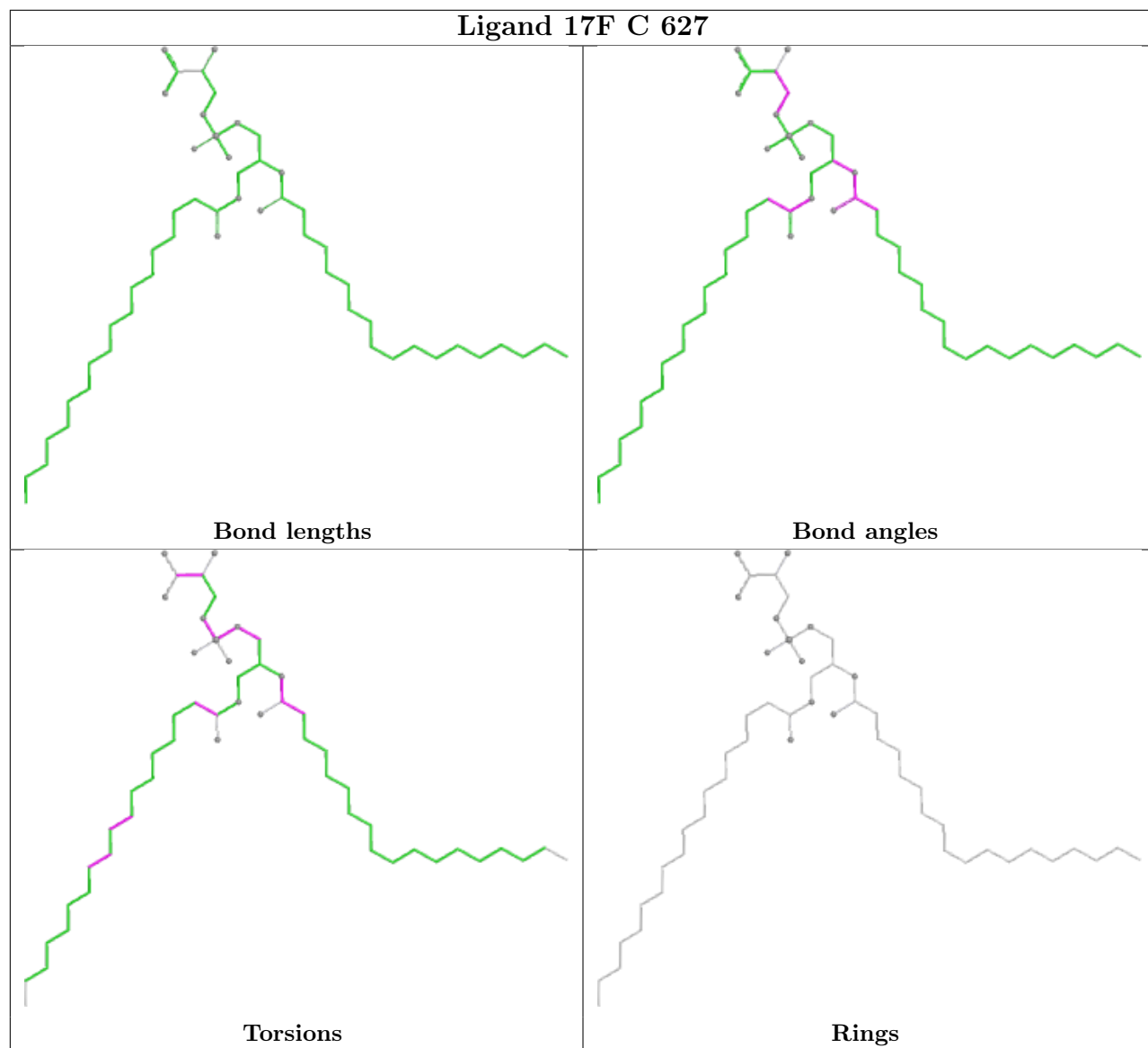


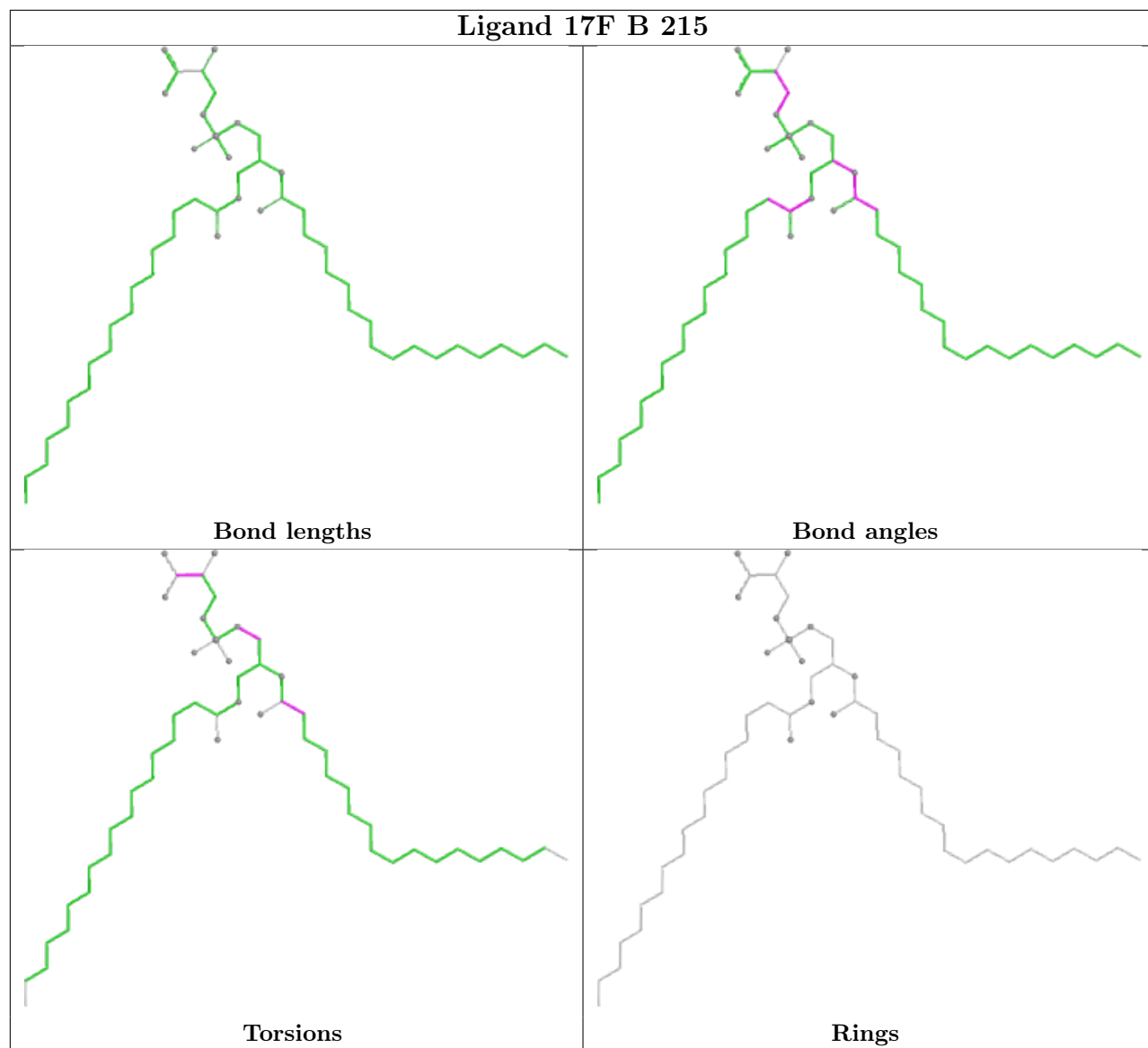


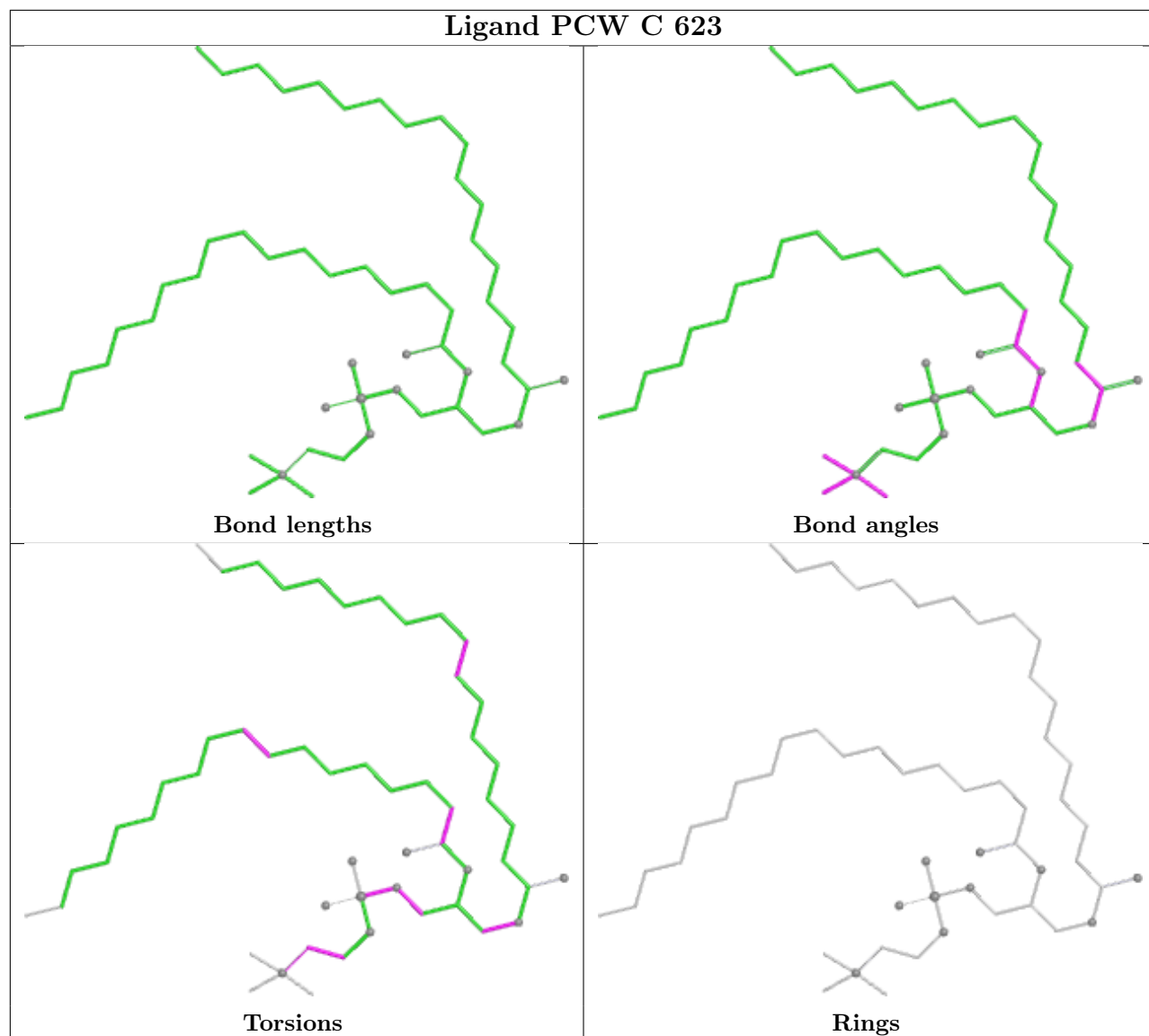




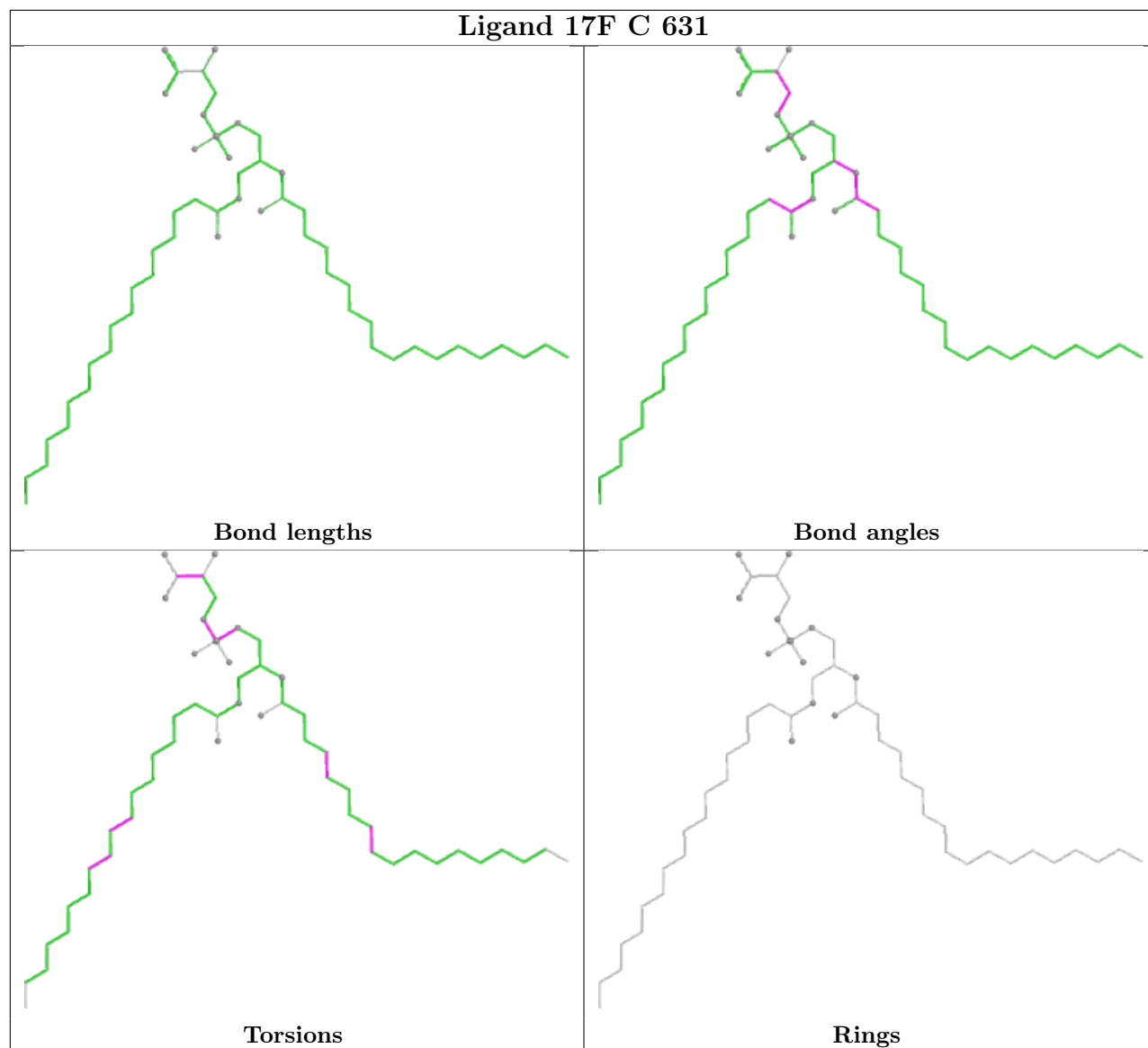


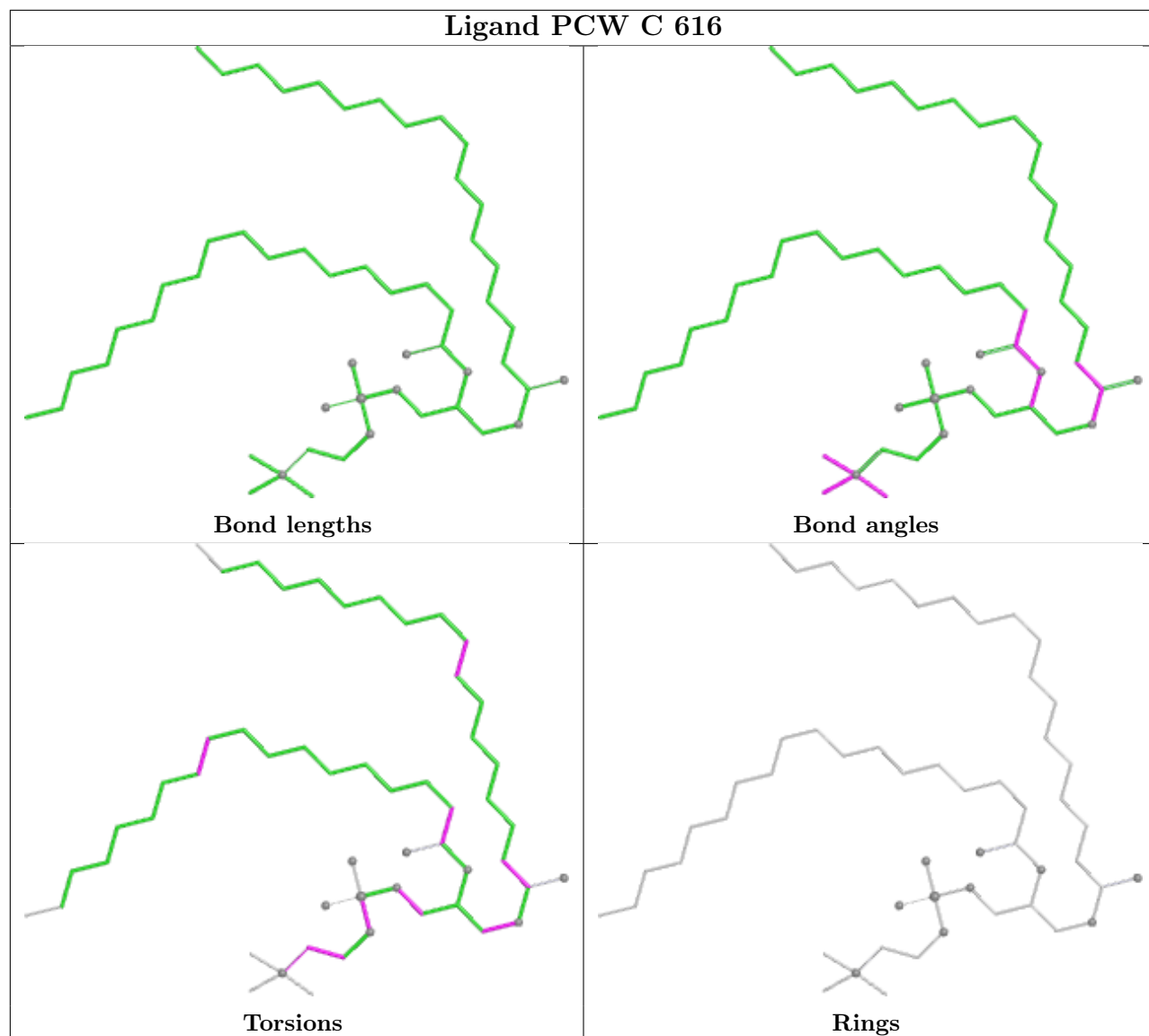


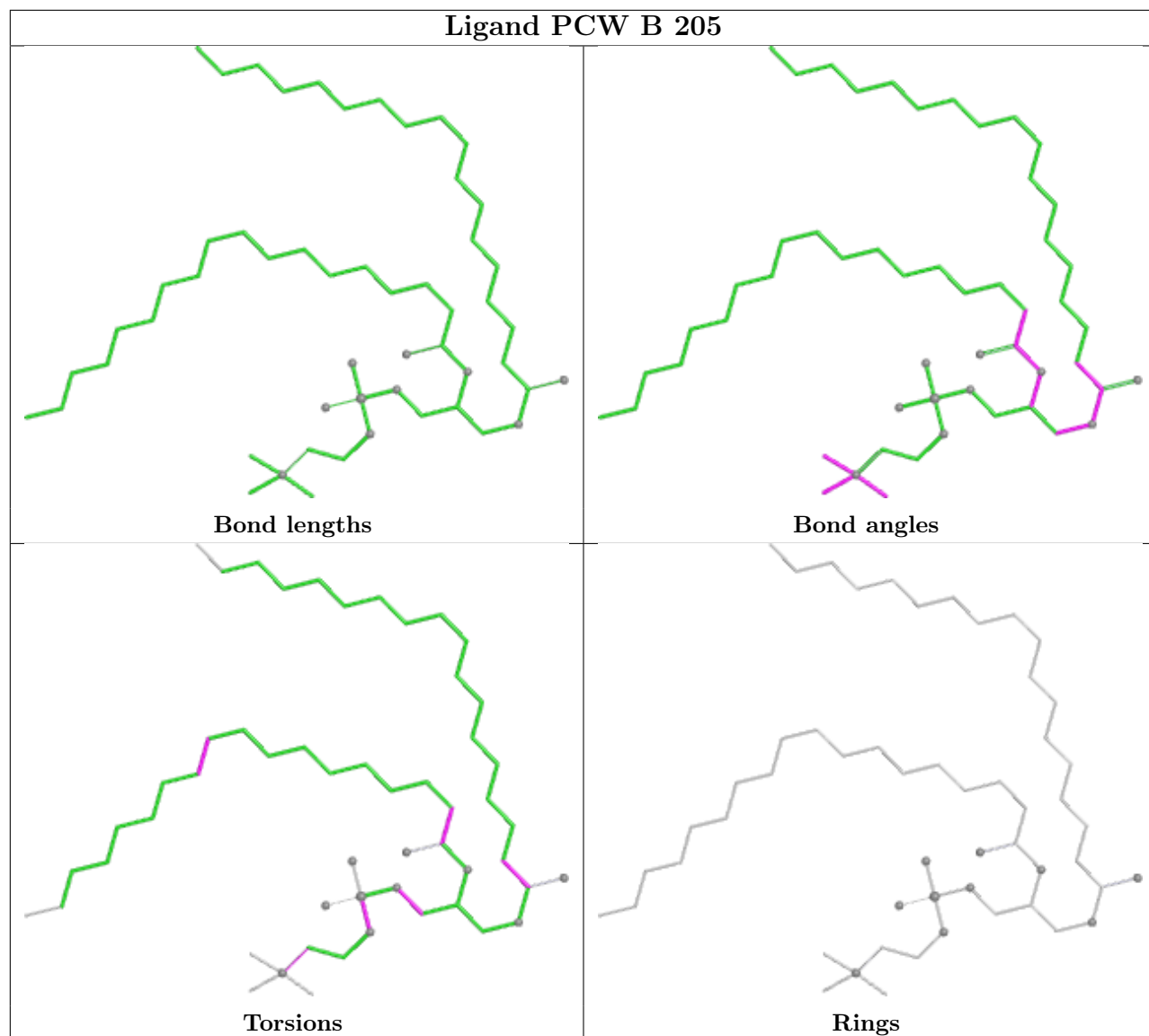


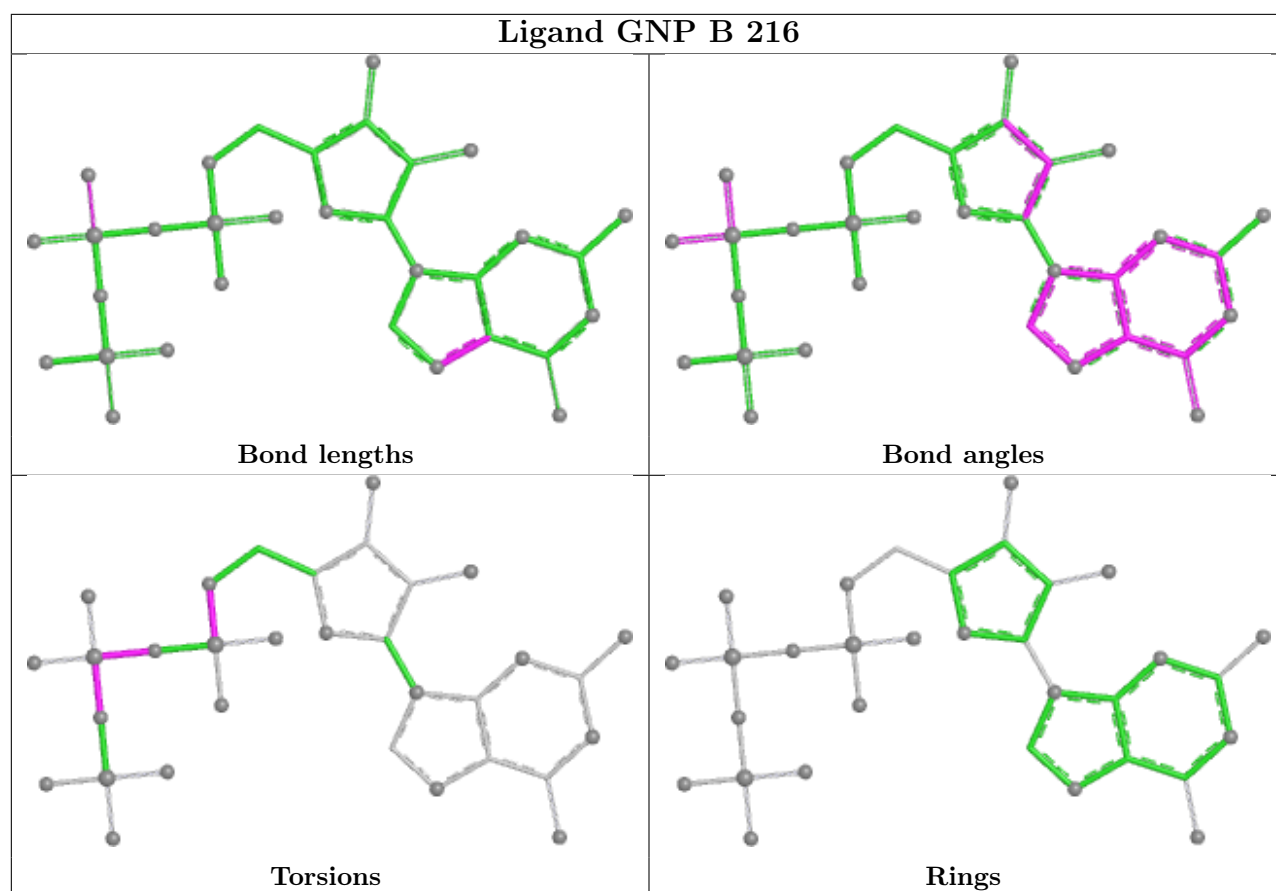


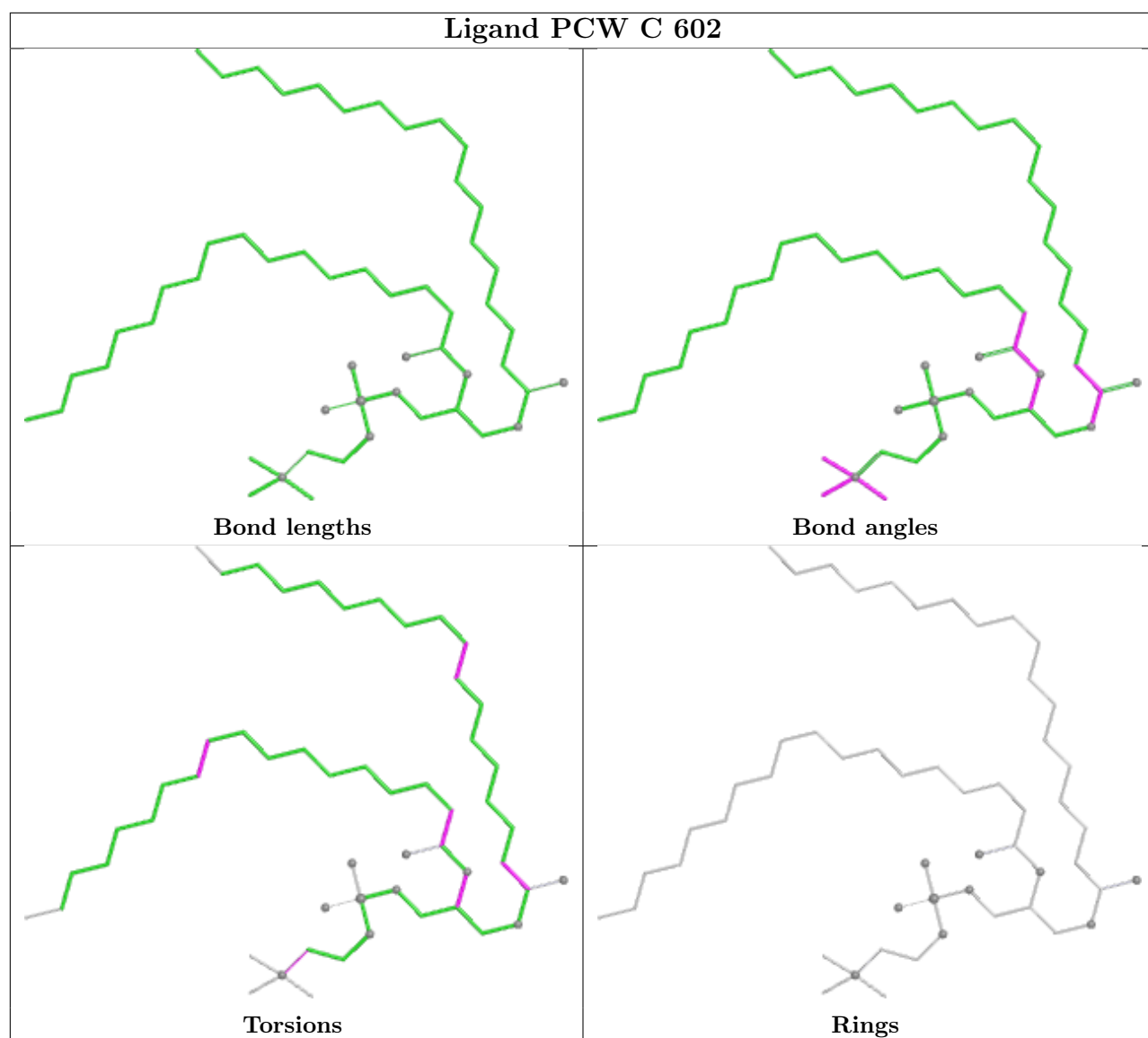
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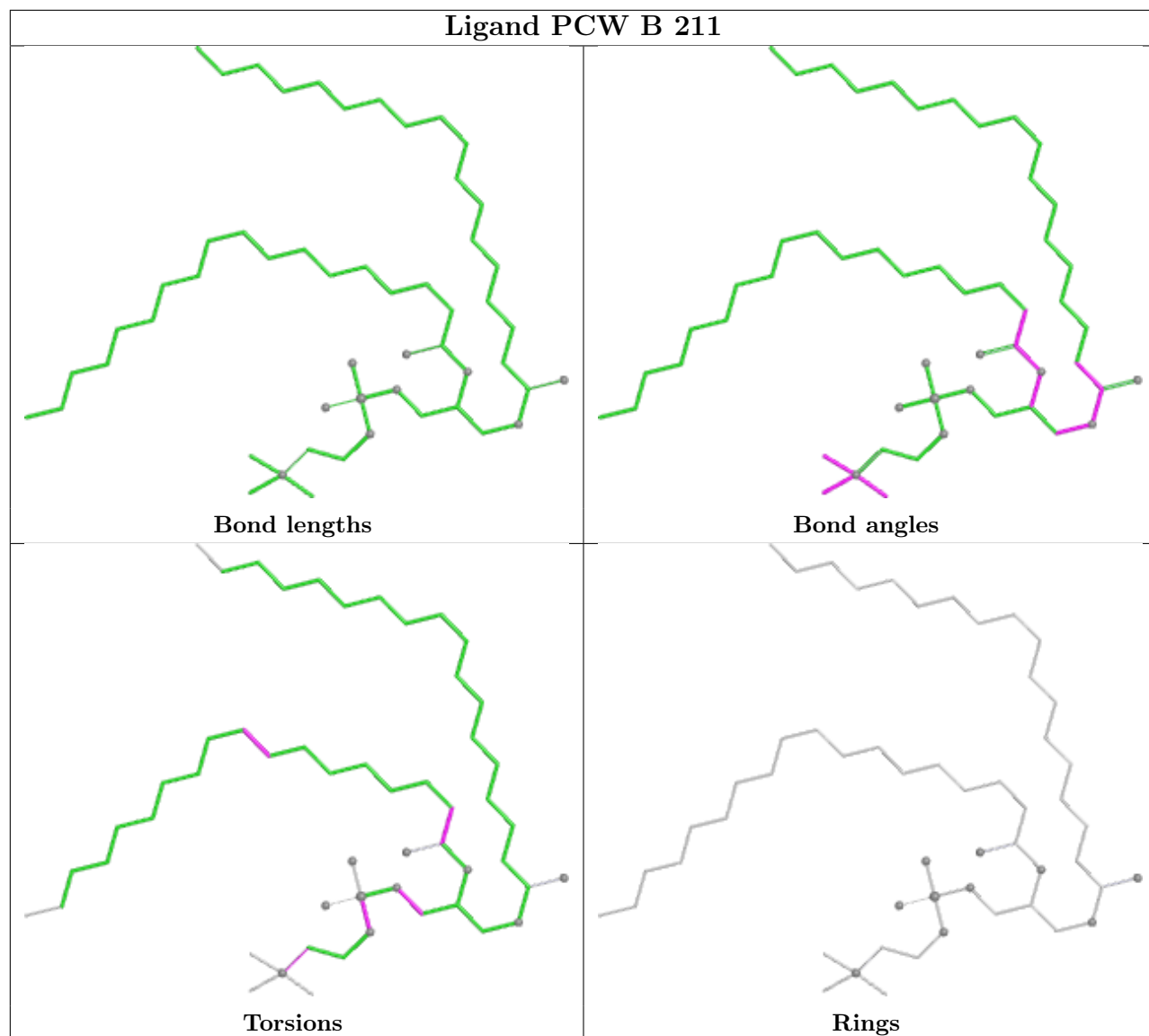


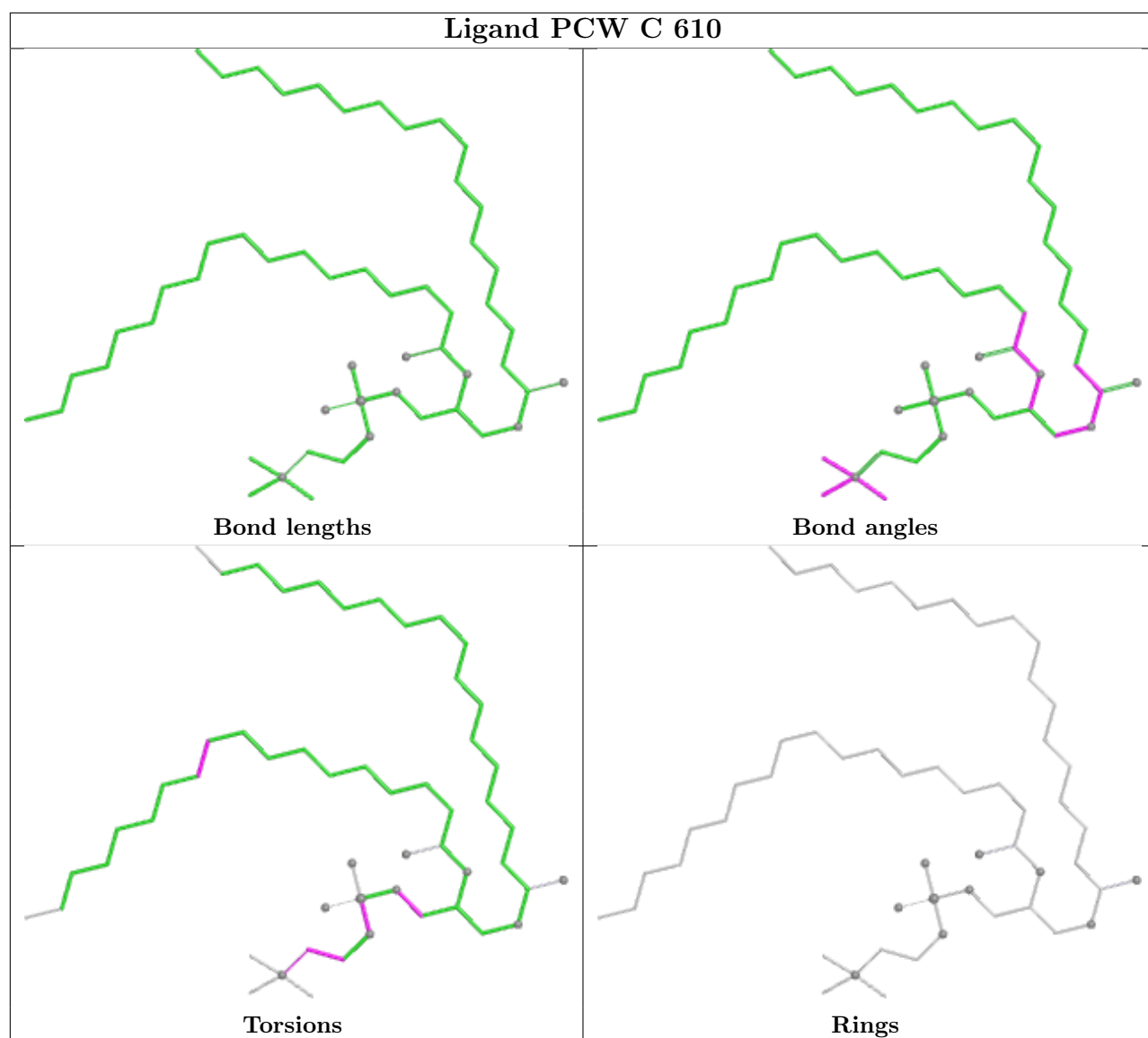












6.7 Other polymers [i](#)

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 6% for the well-defined parts and 6% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

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	557
Number of shifts mapped to atoms	437
Number of unparsed shifts	0
Number of shifts with mapping errors	120
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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	C	401	LEU	HD21	0.714	.	.
1	C	401	LEU	HD22	0.714	.	.
1	C	401	LEU	HD23	0.714	.	.
1	B	6	LEU	HD21	0.982	.	.
1	B	6	LEU	HD22	0.982	.	.
1	B	6	LEU	HD23	0.982	.	.
1	B	19	LEU	HD11	0.65	.	.
1	B	19	LEU	HD12	0.65	.	.
1	B	19	LEU	HD13	0.65	.	.
1	B	21	ILE	HD11	0.649	.	1
1	B	21	ILE	HD12	0.649	.	1
1	B	21	ILE	HD13	0.649	.	1
1	B	23	LEU	HD11	-0.175	.	.
1	B	23	LEU	HD12	-0.175	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	23	LEU	HD13	-0.175	.	.
1	B	24	ILE	HD11	0.486	.	1
1	B	24	ILE	HD12	0.486	.	1
1	B	24	ILE	HD13	0.486	.	1
1	B	36	ILE	HD11	0.691	.	1
1	B	36	ILE	HD12	0.691	.	1
1	B	36	ILE	HD13	0.691	.	1
1	B	46	ILE	HD11	0.466	.	1
1	B	46	ILE	HD12	0.466	.	1
1	B	46	ILE	HD13	0.466	.	1
1	B	55	ILE	HD11	0.567	.	1
1	B	55	ILE	HD12	0.567	.	1
1	B	55	ILE	HD13	0.567	.	1
1	B	79	LEU	HD11	0.154	.	.
1	B	79	LEU	HD12	0.154	.	.
1	B	79	LEU	HD13	0.154	.	.
1	B	79	LEU	HD21	0.208	.	.
1	B	79	LEU	HD22	0.208	.	.
1	B	79	LEU	HD23	0.208	.	.
1	B	84	ILE	HD11	0.802	.	1
1	B	84	ILE	HD12	0.802	.	1
1	B	84	ILE	HD13	0.802	.	1
1	B	93	ILE	HD11	0.833	.	1
1	B	93	ILE	HD12	0.833	.	1
1	B	93	ILE	HD13	0.833	.	1
1	B	100	ILE	HD11	0.34	.	1
1	B	100	ILE	HD12	0.34	.	1
1	B	100	ILE	HD13	0.34	.	1
1	B	113	LEU	HD11	1.088	.	.
1	B	113	LEU	HD12	1.088	.	.
1	B	113	LEU	HD13	1.088	.	.
1	B	113	LEU	HD21	1.352	.	.
1	B	113	LEU	HD22	1.352	.	.
1	B	113	LEU	HD23	1.352	.	.
1	B	120	LEU	HD21	0.91	.	.
1	B	120	LEU	HD22	0.91	.	.
1	B	120	LEU	HD23	0.91	.	.
1	B	125	VAL	HG11	-0.082	.	.
1	B	125	VAL	HG12	-0.082	.	.
1	B	125	VAL	HG13	-0.082	.	.
1	B	133	LEU	HD11	0.413	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	133	LEU	HD12	0.413	.	.
1	B	133	LEU	HD13	0.413	.	.
1	B	133	LEU	HD21	0.476	.	.
1	B	133	LEU	HD22	0.476	.	.
1	B	133	LEU	HD23	0.476	.	.
1	B	139	ILE	HD11	0.922	.	1
1	B	139	ILE	HD12	0.922	.	1
1	B	139	ILE	HD13	0.922	.	1
1	B	142	ILE	HD11	0.715	.	1
1	B	142	ILE	HD12	0.715	.	1
1	B	142	ILE	HD13	0.715	.	1
1	B	159	LEU	HD11	0.729	.	.
1	B	159	LEU	HD12	0.729	.	.
1	B	159	LEU	HD13	0.729	.	.
1	B	160	VAL	HG11	0.038	.	.
1	B	160	VAL	HG12	0.038	.	.
1	B	160	VAL	HG13	0.038	.	.
1	B	163	ILE	HD11	0.737	.	1
1	B	163	ILE	HD12	0.737	.	1
1	B	163	ILE	HD13	0.737	.	1
1	D	358	ILE	HD11	0.625	.	1
1	D	358	ILE	HD12	0.625	.	1
1	D	358	ILE	HD13	0.625	.	1
1	D	370	VAL	HG11	0.794	.	.
1	D	370	VAL	HG12	0.794	.	.
1	D	370	VAL	HG13	0.794	.	.
1	D	378	LEU	HD11	0.581	.	.
1	D	378	LEU	HD12	0.581	.	.
1	D	378	LEU	HD13	0.581	.	.
1	D	386	LEU	HD21	0.698	.	.
1	D	386	LEU	HD22	0.698	.	.
1	D	386	LEU	HD23	0.698	.	.
1	D	388	VAL	HG11	1.126	.	.
1	D	388	VAL	HG12	1.126	.	.
1	D	388	VAL	HG13	1.126	.	.
1	D	388	VAL	HG21	1.087	.	.
1	D	388	VAL	HG22	1.087	.	.
1	D	388	VAL	HG23	1.087	.	.
1	D	398	VAL	HG21	0.273	.	.
1	D	398	VAL	HG22	0.273	.	.
1	D	398	VAL	HG23	0.273	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	D	412	LEU	HD11	0.652	.	.
1	D	412	LEU	HD12	0.652	.	.
1	D	412	LEU	HD13	0.652	.	.
1	D	421	LEU	HD11	0.839	.	.
1	D	421	LEU	HD12	0.839	.	.
1	D	421	LEU	HD13	0.839	.	.
1	D	422	ILE	HD11	0.954	.	1
1	D	422	ILE	HD12	0.954	.	1
1	D	422	ILE	HD13	0.954	.	1
1	D	436	LEU	HD21	0.712	.	.
1	D	436	LEU	HD22	0.712	.	.
1	D	436	LEU	HD23	0.712	.	.
1	D	454	ILE	HD11	0.674	.	1
1	D	454	ILE	HD12	0.674	.	1
1	D	454	ILE	HD13	0.674	.	1
1	D	459	LEU	HD11	-0.052	.	.
1	D	459	LEU	HD12	-0.052	.	.
1	D	459	LEU	HD13	-0.052	.	.
1	D	480	VAL	HG11	0.57	.	.
1	D	480	VAL	HG12	0.57	.	.
1	D	480	VAL	HG13	0.57	.	.
1	D	485	VAL	HG11	0.712	.	.
1	D	485	VAL	HG12	0.712	.	.
1	D	485	VAL	HG13	0.712	.	.

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	198	-0.53 ± 0.24	Should be applied

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 6%, i.e. 555 atoms were assigned a chemical shift out of a possible 9878. 0 out of 134 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	394/3487 (11%)	197/1409 (14%)	0/1400 (0%)	197/678 (29%)
Sidechain	161/5732 (3%)	120/3690 (3%)	41/1786 (2%)	0/256 (0%)
Aromatic	0/659 (0%)	0/329 (0%)	0/300 (0%)	0/30 (0%)
Overall	555/9878 (6%)	317/5428 (6%)	41/3486 (1%)	197/964 (20%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 6%, i.e. 557 atoms were assigned a chemical shift out of a possible 10064. 0 out of 134 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	396/3553 (11%)	198/1436 (14%)	0/1426 (0%)	198/691 (29%)
Sidechain	161/5852 (3%)	120/3764 (3%)	41/1824 (2%)	0/264 (0%)
Aromatic	0/659 (0%)	0/329 (0%)	0/300 (0%)	0/30 (0%)
Overall	557/10064 (6%)	318/5529 (6%)	41/3550 (1%)	198/985 (20%)

7.1.4 Statistically unusual chemical shifts [i](#)

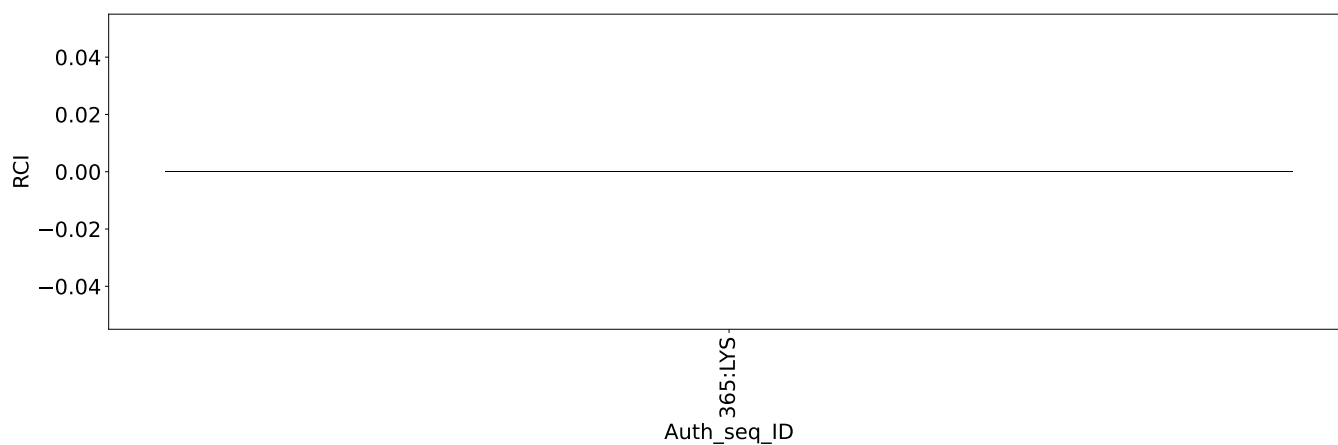
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	48	GLY	N	140.27	91.59 – 127.52	8.6

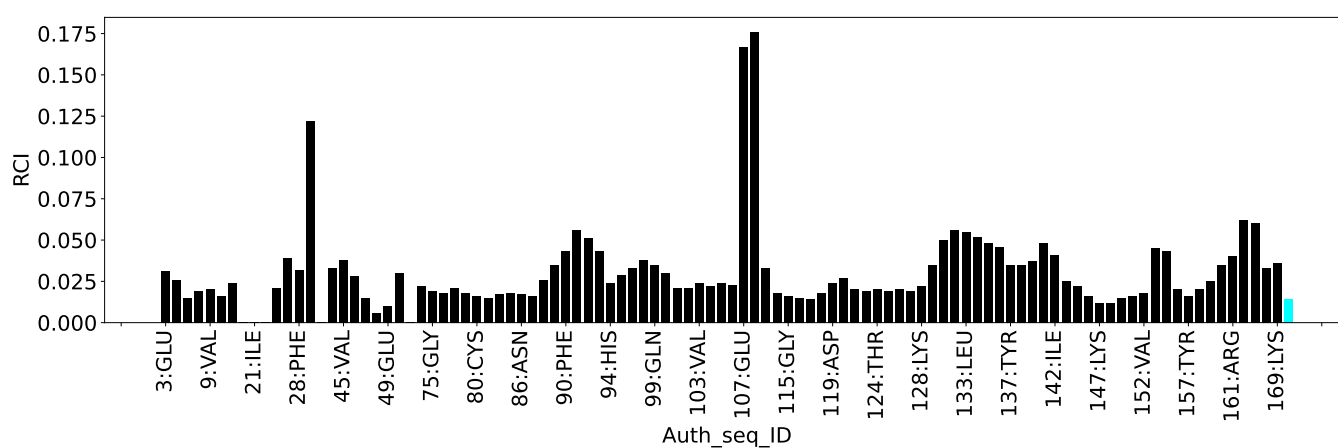
7.1.5 Random Coil Index (RCI) plots [i](#)

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.

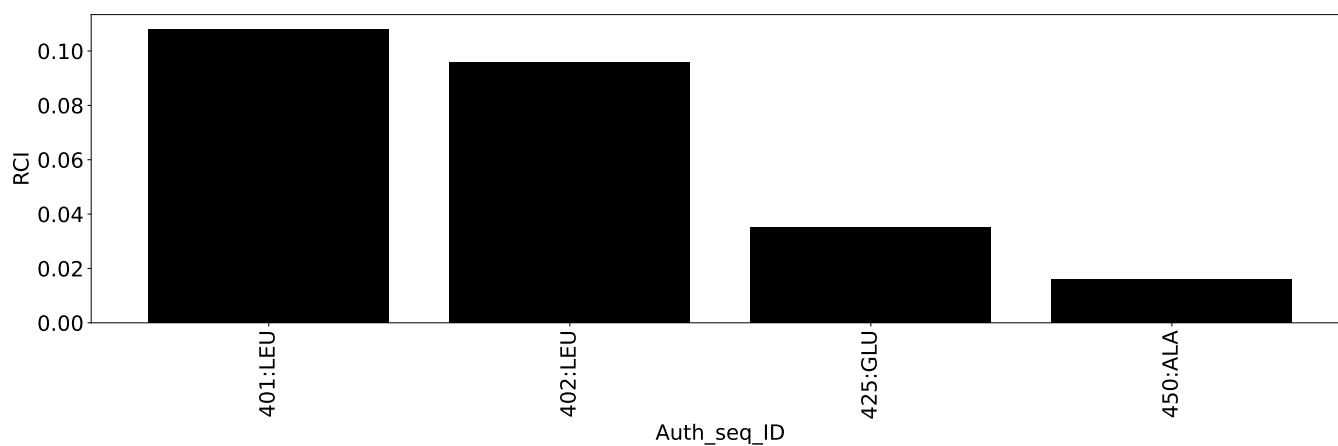
Random coil index (RCI) for chain A:



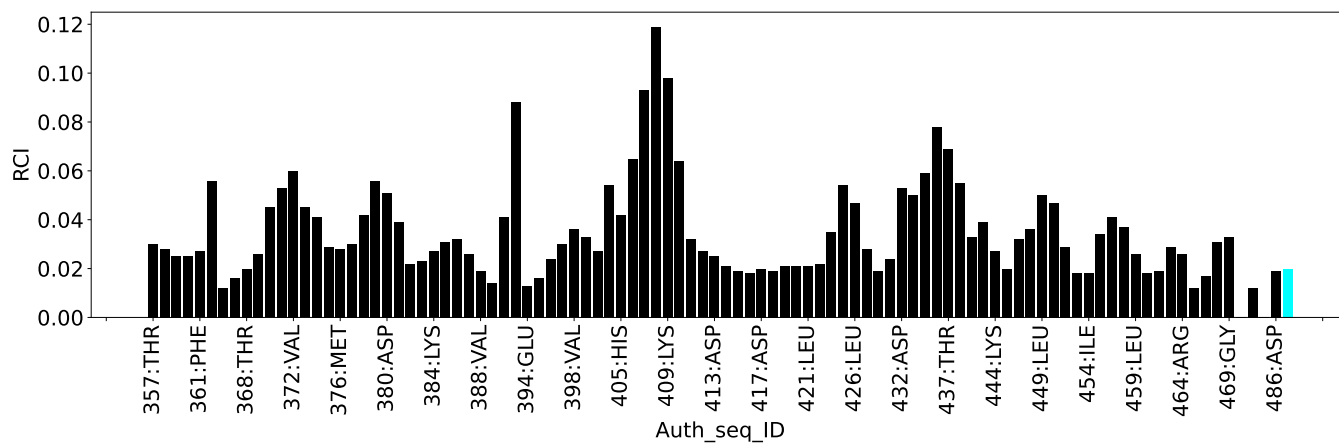
Random coil index (RCI) for chain B:



Random coil index (RCI) for chain C:



Random coil index (RCI) for chain D:



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	51
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	2
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	0
Inter-chain	49
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.1
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)	None	None
0.2-0.5 (Medium)	0.4	0.5
>0.5 (Large)	46.3	33.32

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 ⓘ

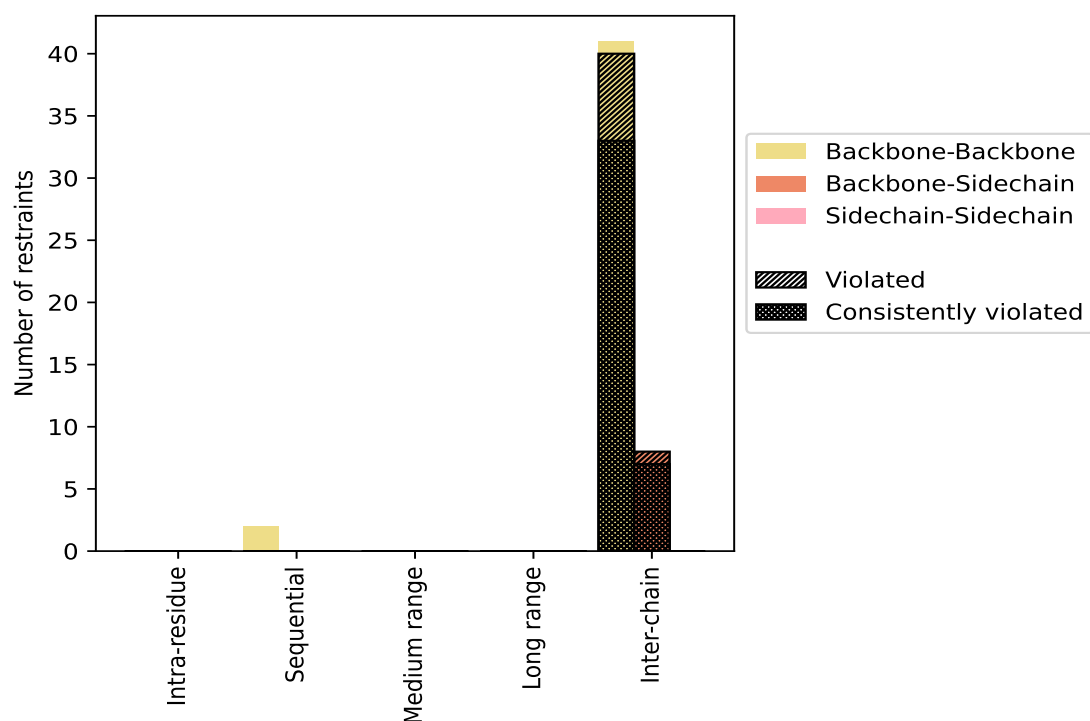
9.1 Summary of distance violations ⓘ

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)	2	3.9	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	2	3.9	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	49	96.1	48	98.0	94.1	40	81.6	78.4
Backbone-Backbone	41	80.4	40	97.6	78.4	33	80.5	64.7
Backbone-Sidechain	8	15.7	8	100.0	15.7	7	87.5	13.7
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
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	51	100.0	48	94.1	94.1	40	78.4	78.4
Backbone-Backbone	43	84.3	40	93.0	78.4	33	76.7	64.7
Backbone-Sidechain	8	15.7	8	100.0	15.7	7	87.5	13.7
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0

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

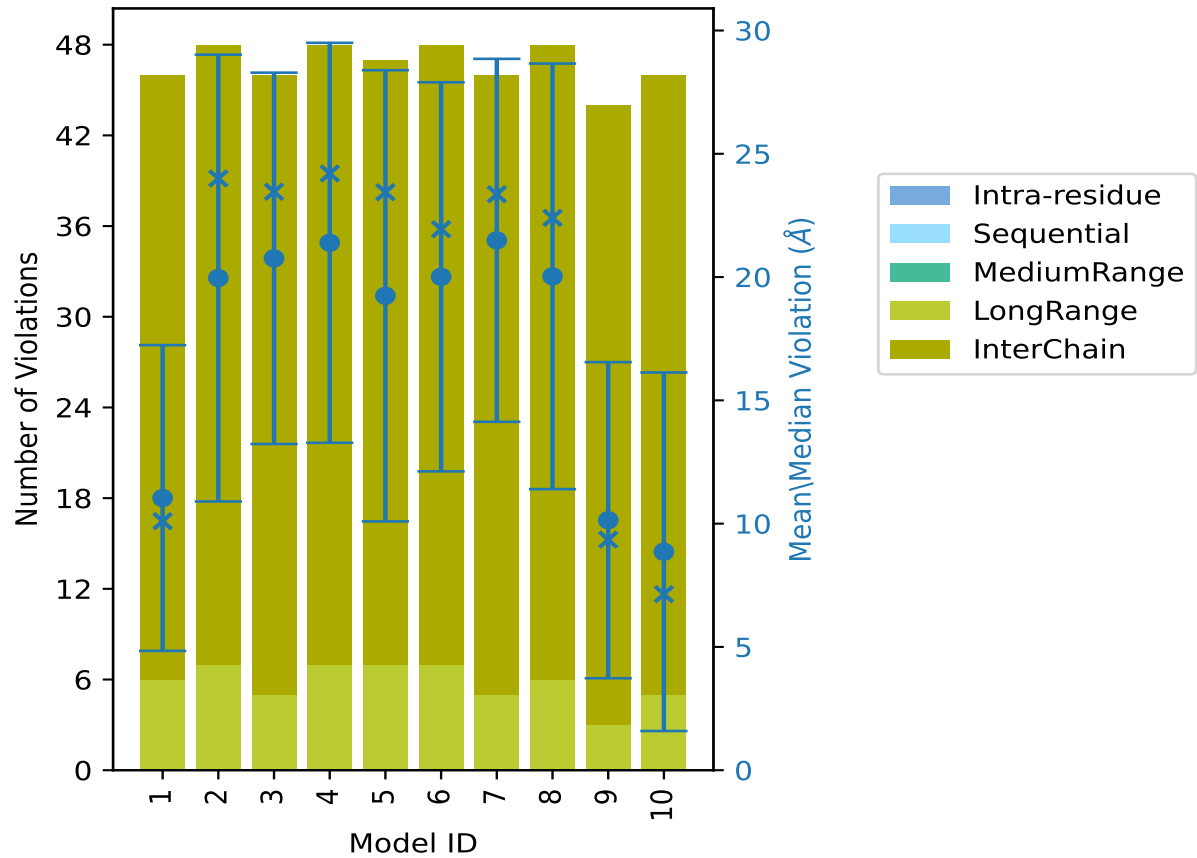
9.2 Distance violation statistics for each model [i](#)

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	6	40	46	11.04	24.8	6.2	10.1
2	0	0	0	7	41	48	19.96	33.32	9.06	24.0
3	0	0	0	5	41	46	20.76	30.61	7.53	23.46
4	0	0	0	7	41	48	21.39	32.62	8.11	24.2
5	0	0	0	7	40	47	19.24	30.78	9.15	23.44
6	0	0	0	7	41	48	20.01	32.19	7.89	21.94
7	0	0	0	5	41	46	21.49	32.6	7.36	23.36
8	0	0	0	6	42	48	20.03	32.59	8.63	22.4
9	0	0	0	3	41	44	10.14	24.44	6.41	9.35
10	0	0	0	5	41	46	8.86	23.14	7.27	7.14

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, 3(IR:0, SQ:2, MR:0, LR:0, IC:1) 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	0	0	1	10.0
0	0	0	0	0	0	2	20.0
0	0	0	0	0	0	3	30.0

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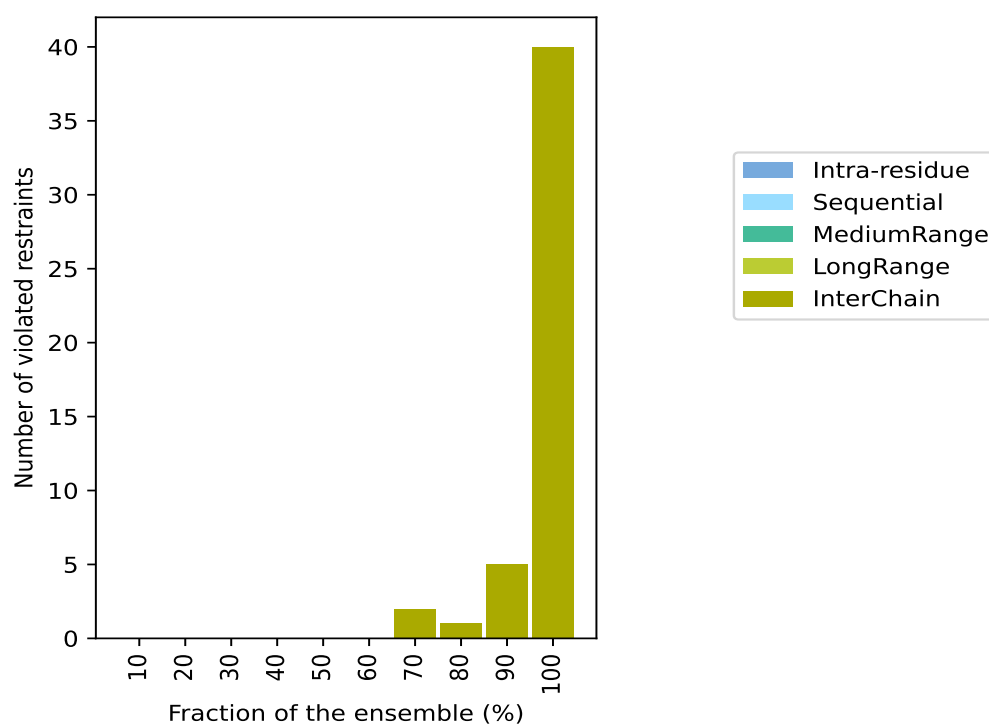
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	4	40.0
0	0	0	0	0	0	5	50.0
0	0	0	0	0	0	6	60.0
0	0	0	0	2	2	7	70.0
0	0	0	0	1	1	8	80.0
0	0	0	0	5	5	9	90.0
0	0	0	0	40	40	10	100.0

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](#)

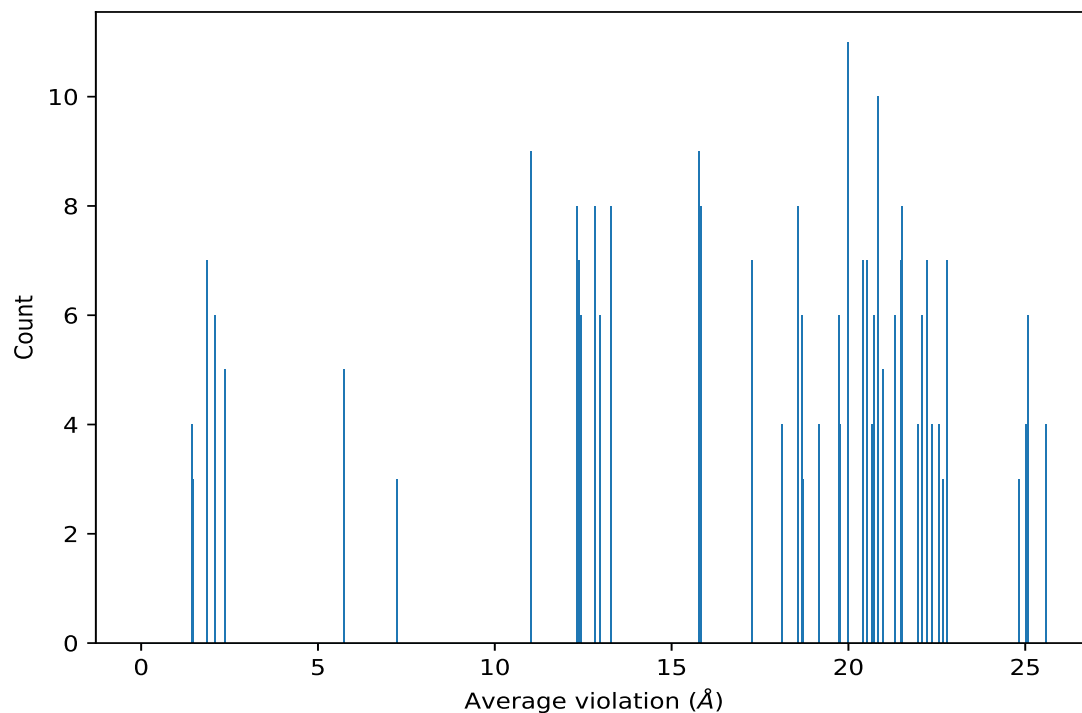


9.4 Most violated distance restraints in the ensemble [i](#)

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)
(1,37)	1:237:A:GLU:O	4:210:B:PCW:O3	10	25.56	1.41	25.2
(1,37)	1:237:A:GLU:O	4:211:B:PCW:O3	10	25.56	1.41	25.2
(1,37)	1:237:A:GLU:O	2:143:B:GLU:OE1	10	25.56	1.41	25.2
(1,37)	1:237:A:GLU:O	2:143:B:GLU:OE2	10	25.56	1.41	25.2
(1,1)	1:201:A:LEU:N	2:132:B:ASP:OD1	10	25.07	10.86	31.48
(1,1)	1:201:A:LEU:N	4:210:B:PCW:C4	10	25.07	10.86	31.48
(1,1)	1:201:A:LEU:N	4:210:B:PCW:C7	10	25.07	10.86	31.48
(1,1)	1:201:A:LEU:N	4:210:B:PCW:C6	10	25.07	10.86	31.48
(1,1)	1:201:A:LEU:N	2:185:B:CYS:O	10	25.07	10.86	31.48
(1,1)	1:201:A:LEU:N	2:185:B:CYS:HG	10	25.07	10.86	31.48
(1,34)	1:234:A:LYS:O	2:143:B:GLU:OE2	10	25.01	1.25	25.2
(1,34)	1:234:A:LYS:O	4:211:B:PCW:O3	10	25.01	1.25	25.2
(1,34)	1:234:A:LYS:O	4:210:B:PCW:O3	10	25.01	1.25	25.2
(1,34)	1:234:A:LYS:O	2:132:B:ASP:OD1	10	25.01	1.25	25.2
(1,40)	1:240:A:ARG:O	4:211:B:PCW:O3	10	24.84	1.36	24.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,40)	1:240:A:ARG:O	4:210:B:PCW:O3	10	24.84	1.36	24.38
(1,40)	1:240:A:ARG:O	2:143:B:GLU:OE2	10	24.84	1.36	24.38
(1,5)	1:205:A:ASP:N	2:132:B:ASP:OD1	10	22.78	11.03	29.65
(1,5)	1:205:A:ASP:N	4:210:B:PCW:C4	10	22.78	11.03	29.65
(1,5)	1:205:A:ASP:N	4:210:B:PCW:C7	10	22.78	11.03	29.65
(1,5)	1:205:A:ASP:N	4:210:B:PCW:C2	10	22.78	11.03	29.65
(1,5)	1:205:A:ASP:N	4:210:B:PCW:C6	10	22.78	11.03	29.65
(1,5)	1:205:A:ASP:N	2:185:B:CYS:O	10	22.78	11.03	29.65
(1,5)	1:205:A:ASP:N	2:185:B:CYS:HG	10	22.78	11.03	29.65
(1,39)	1:239:A:LEU:O	4:211:B:PCW:O3	10	22.65	1.17	22.34
(1,39)	1:239:A:LEU:O	4:210:B:PCW:O3	10	22.65	1.17	22.34
(1,39)	1:239:A:LEU:O	2:143:B:GLU:OE2	10	22.65	1.17	22.34
(1,35)	1:235:A:GLU:O	4:210:B:PCW:O3	10	22.56	0.97	22.33
(1,35)	1:235:A:GLU:O	4:211:B:PCW:O3	10	22.56	0.97	22.33
(1,35)	1:235:A:GLU:O	2:143:B:GLU:OE1	10	22.56	0.97	22.33
(1,35)	1:235:A:GLU:O	2:143:B:GLU:OE2	10	22.56	0.97	22.33
(1,36)	1:236:A:THR:O	4:210:B:PCW:O3	10	22.36	1.44	22.04
(1,36)	1:236:A:THR:O	4:211:B:PCW:O3	10	22.36	1.44	22.04
(1,36)	1:236:A:THR:O	2:143:B:GLU:OE1	10	22.36	1.44	22.04
(1,36)	1:236:A:THR:O	2:143:B:GLU:OE2	10	22.36	1.44	22.04
(1,6)	1:206:A:ASN:N	2:132:B:ASP:OD1	10	22.21	10.82	29.01
(1,6)	1:206:A:ASN:N	4:210:B:PCW:C4	10	22.21	10.82	29.01
(1,6)	1:206:A:ASN:N	4:210:B:PCW:C7	10	22.21	10.82	29.01
(1,6)	1:206:A:ASN:N	4:210:B:PCW:C2	10	22.21	10.82	29.01
(1,6)	1:206:A:ASN:N	4:210:B:PCW:C6	10	22.21	10.82	29.01
(1,6)	1:206:A:ASN:N	2:185:B:CYS:O	10	22.21	10.82	29.01
(1,6)	1:206:A:ASN:N	2:185:B:CYS:HG	10	22.21	10.82	29.01
(1,3)	1:203:A:LEU:N	2:132:B:ASP:OD1	10	22.07	10.58	28.44
(1,3)	1:203:A:LEU:N	4:210:B:PCW:C4	10	22.07	10.58	28.44
(1,3)	1:203:A:LEU:N	4:210:B:PCW:C7	10	22.07	10.58	28.44
(1,3)	1:203:A:LEU:N	4:210:B:PCW:C6	10	22.07	10.58	28.44
(1,3)	1:203:A:LEU:N	2:185:B:CYS:O	10	22.07	10.58	28.44
(1,3)	1:203:A:LEU:N	2:185:B:CYS:HG	10	22.07	10.58	28.44
(1,27)	1:227:A:GLU:N	2:143:B:GLU:OE2	10	21.96	4.11	24.26
(1,27)	1:227:A:GLU:N	4:211:B:PCW:C3	10	21.96	4.11	24.26
(1,27)	1:227:A:GLU:N	4:210:B:PCW:O3	10	21.96	4.11	24.26
(1,27)	1:227:A:GLU:N	2:132:B:ASP:OD1	10	21.96	4.11	24.26
(1,23)	1:223:A:PRO:N	2:143:B:GLU:OE1	10	21.54	5.72	24.72
(1,23)	1:223:A:PRO:N	4:210:B:PCW:O3	10	21.54	5.72	24.72
(1,23)	1:223:A:PRO:N	2:132:B:ASP:OD1	10	21.54	5.72	24.72
(1,23)	1:223:A:PRO:N	2:185:B:CYS:O	10	21.54	5.72	24.72
(1,30)	1:230:A:ASP:N	2:143:B:GLU:OE2	10	21.54	3.15	23.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,30)	1:230:A:ASP:N	4:211:B:PCW:O3	10	21.54	3.15	23.4
(1,30)	1:230:A:ASP:N	4:210:B:PCW:O3	10	21.54	3.15	23.4
(1,30)	1:230:A:ASP:N	2:132:B:ASP:OD1	10	21.54	3.15	23.4
(1,9)	1:209:A:SER:N	2:132:B:ASP:OD1	10	21.46	10.38	27.72
(1,9)	1:209:A:SER:N	4:210:B:PCW:C4	10	21.46	10.38	27.72
(1,9)	1:209:A:SER:N	4:210:B:PCW:O3	10	21.46	10.38	27.72
(1,9)	1:209:A:SER:N	4:210:B:PCW:C2	10	21.46	10.38	27.72
(1,9)	1:209:A:SER:N	4:210:B:PCW:C7	10	21.46	10.38	27.72
(1,9)	1:209:A:SER:N	2:185:B:CYS:C	10	21.46	10.38	27.72
(1,9)	1:209:A:SER:N	2:185:B:CYS:HG	10	21.46	10.38	27.72
(1,4)	1:204:A:LEU:N	2:132:B:ASP:OD1	10	21.34	10.61	27.88
(1,4)	1:204:A:LEU:N	4:210:B:PCW:C4	10	21.34	10.61	27.88
(1,4)	1:204:A:LEU:N	4:210:B:PCW:C7	10	21.34	10.61	27.88
(1,4)	1:204:A:LEU:N	4:210:B:PCW:C6	10	21.34	10.61	27.88
(1,4)	1:204:A:LEU:N	2:185:B:CYS:O	10	21.34	10.61	27.88
(1,4)	1:204:A:LEU:N	2:185:B:CYS:HG	10	21.34	10.61	27.88
(1,16)	1:216:A:LYS:N	2:132:B:ASP:H	10	20.97	8.0	25.54
(1,16)	1:216:A:LYS:N	4:210:B:PCW:O3	10	20.97	8.0	25.54
(1,16)	1:216:A:LYS:N	4:210:B:PCW:C7	10	20.97	8.0	25.54
(1,16)	1:216:A:LYS:N	2:132:B:ASP:OD1	10	20.97	8.0	25.54
(1,16)	1:216:A:LYS:N	2:185:B:CYS:CB	10	20.97	8.0	25.54
(1,24)	1:224:A:VAL:N	2:143:B:GLU:OE1	10	20.81	5.0	23.58
(1,24)	1:224:A:VAL:N	4:210:B:PCW:O3	10	20.81	5.0	23.58
(1,24)	1:224:A:VAL:N	2:132:B:ASP:OD1	10	20.81	5.0	23.58
(1,24)	1:224:A:VAL:N	2:185:B:CYS:O	10	20.81	5.0	23.58
(1,13)	1:213:A:THR:N	2:132:B:ASP:CB	10	20.7	8.69	25.77
(1,13)	1:213:A:THR:N	4:210:B:PCW:O3	10	20.7	8.69	25.77
(1,13)	1:213:A:THR:N	4:210:B:PCW:C2	10	20.7	8.69	25.77
(1,13)	1:213:A:THR:N	4:210:B:PCW:C4	10	20.7	8.69	25.77
(1,13)	1:213:A:THR:N	2:185:B:CYS:H	10	20.7	8.69	25.77
(1,13)	1:213:A:THR:N	2:185:B:CYS:HG	10	20.7	8.69	25.77
(1,28)	1:228:A:PHE:N	2:143:B:GLU:OE2	10	20.66	3.37	22.42
(1,28)	1:228:A:PHE:N	4:211:B:PCW:O3	10	20.66	3.37	22.42
(1,28)	1:228:A:PHE:N	4:210:B:PCW:O3	10	20.66	3.37	22.42
(1,28)	1:228:A:PHE:N	2:132:B:ASP:OD1	10	20.66	3.37	22.42
(1,12)	1:212:A:SER:N	2:132:B:ASP:OD1	10	20.51	9.53	26.32
(1,12)	1:212:A:SER:N	4:210:B:PCW:C7	10	20.51	9.53	26.32
(1,12)	1:212:A:SER:N	4:210:B:PCW:O3	10	20.51	9.53	26.32
(1,12)	1:212:A:SER:N	4:210:B:PCW:C4	10	20.51	9.53	26.32
(1,12)	1:212:A:SER:N	4:210:B:PCW:C2	10	20.51	9.53	26.32
(1,12)	1:212:A:SER:N	2:185:B:CYS:H	10	20.51	9.53	26.32
(1,12)	1:212:A:SER:N	2:185:B:CYS:HG	10	20.51	9.53	26.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,8)	1:208:A:ASP:N	2:132:B:ASP:OD1	10	20.41	10.63	26.95
(1,8)	1:208:A:ASP:N	4:210:B:PCW:C7	10	20.41	10.63	26.95
(1,8)	1:208:A:ASP:N	4:210:B:PCW:C4	10	20.41	10.63	26.95
(1,8)	1:208:A:ASP:N	4:210:B:PCW:C2	10	20.41	10.63	26.95
(1,8)	1:208:A:ASP:N	4:210:B:PCW:C6	10	20.41	10.63	26.95
(1,8)	1:208:A:ASP:N	2:185:B:CYS:C	10	20.41	10.63	26.95
(1,8)	1:208:A:ASP:N	2:185:B:CYS:HG	10	20.41	10.63	26.95
(1,7)	1:207:A:TRP:N	2:132:B:ASP:OD1	10	19.99	10.4	26.41
(1,7)	1:207:A:TRP:N	4:210:B:PCW:C4	10	19.99	10.4	26.41
(1,7)	1:207:A:TRP:N	4:210:B:PCW:C7	10	19.99	10.4	26.41
(1,7)	1:207:A:TRP:N	4:210:B:PCW:C2	10	19.99	10.4	26.41
(1,7)	1:207:A:TRP:N	4:210:B:PCW:C6	10	19.99	10.4	26.41
(1,7)	1:207:A:TRP:N	2:185:B:CYS:C	10	19.99	10.4	26.41
(1,7)	1:207:A:TRP:N	2:185:B:CYS:HG	10	19.99	10.4	26.41
(1,26)	1:226:A:GLN:N	2:143:B:GLU:OE2	10	19.97	4.57	22.53
(1,26)	1:226:A:GLN:N	4:211:B:PCW:C3	10	19.97	4.57	22.53
(1,26)	1:226:A:GLN:N	4:210:B:PCW:O3	10	19.97	4.57	22.53
(1,26)	1:226:A:GLN:N	2:132:B:ASP:OD1	10	19.97	4.57	22.53
(1,17)	1:217:A:LEU:N	2:132:B:ASP:H	10	19.75	7.1	23.72
(1,17)	1:217:A:LEU:N	4:210:B:PCW:O3	10	19.75	7.1	23.72
(1,17)	1:217:A:LEU:N	2:132:B:ASP:OD1	10	19.75	7.1	23.72
(1,17)	1:217:A:LEU:N	2:185:B:CYS:C	10	19.75	7.1	23.72
(1,10)	1:210:A:VAL:N	2:132:B:ASP:OD1	10	19.7	9.54	25.38
(1,10)	1:210:A:VAL:N	4:210:B:PCW:C4	10	19.7	9.54	25.38
(1,10)	1:210:A:VAL:N	4:210:B:PCW:O3	10	19.7	9.54	25.38
(1,10)	1:210:A:VAL:N	4:210:B:PCW:C2	10	19.7	9.54	25.38
(1,10)	1:210:A:VAL:N	2:185:B:CYS:H	10	19.7	9.54	25.38
(1,10)	1:210:A:VAL:N	2:185:B:CYS:HG	10	19.7	9.54	25.38
(1,22)	1:222:A:GLY:N	2:143:B:GLU:OE1	10	19.18	6.04	22.52
(1,22)	1:222:A:GLY:N	4:210:B:PCW:O3	10	19.18	6.04	22.52
(1,22)	1:222:A:GLY:N	2:132:B:ASP:OD1	10	19.18	6.04	22.52
(1,22)	1:222:A:GLY:N	2:185:B:CYS:O	10	19.18	6.04	22.52
(1,25)	1:225:A:THR:N	2:143:B:GLU:OE1	10	18.71	4.49	21.2
(1,25)	1:225:A:THR:N	4:210:B:PCW:O3	10	18.71	4.49	21.2
(1,25)	1:225:A:THR:N	2:132:B:ASP:OD1	10	18.71	4.49	21.2
(1,14)	1:214:A:PHE:N	2:132:B:ASP:H	10	18.65	7.99	23.16
(1,14)	1:214:A:PHE:N	4:210:B:PCW:O3	10	18.65	7.99	23.16
(1,14)	1:214:A:PHE:N	4:210:B:PCW:C2	10	18.65	7.99	23.16
(1,14)	1:214:A:PHE:N	4:210:B:PCW:C4	10	18.65	7.99	23.16
(1,14)	1:214:A:PHE:N	2:132:B:ASP:OD1	10	18.65	7.99	23.16
(1,14)	1:214:A:PHE:N	2:185:B:CYS:CB	10	18.65	7.99	23.16
(1,18)	1:218:A:ARG:N	2:143:B:GLU:OE1	10	18.14	7.07	22.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,18)	1:218:A:ARG:N	4:210:B:PCW:O3	10	18.14	7.07	22.2
(1,18)	1:218:A:ARG:N	2:132:B:ASP:OD1	10	18.14	7.07	22.2
(1,18)	1:218:A:ARG:N	2:185:B:CYS:C	10	18.14	7.07	22.2
(1,32)	4:408:A:PCW:C7	2:161:B:ARG:O	10	17.25	4.29	19.26
(1,32)	4:408:A:PCW:C7	2:45:B:VAL:CG1	10	17.25	4.29	19.26
(1,32)	4:408:A:PCW:C7	2:45:B:VAL:CG2	10	17.25	4.29	19.26
(1,32)	4:408:A:PCW:C4	2:185:B:CYS:CB	10	17.25	4.29	19.26
(1,32)	1:232:A:LEU:N	4:210:B:PCW:O3	10	17.25	4.29	19.26
(1,32)	4:408:A:PCW:C7	2:47:B:ASP:OD1	10	17.25	4.29	19.26
(1,32)	4:408:A:PCW:C6	2:161:B:ARG:O	10	17.25	4.29	19.26
(1,44)	2:79:B:LEU:CD2	4:402:A:PCW:C7	10	15.82	5.68	18.43
(1,44)	2:79:B:LEU:CD2	4:406:A:PCW:C8	10	15.82	5.68	18.43
(1,44)	2:79:B:LEU:CD2	4:403:A:PCW:C7	10	15.82	5.68	18.43
(1,44)	2:79:B:LEU:CD1	4:405:A:PCW:C4	10	15.82	5.68	18.43
(1,44)	2:79:B:LEU:CD2	4:404:A:PCW:C7	10	15.82	5.68	18.43
(1,44)	5:215:B:17F:C9	4:403:A:PCW:C8	10	15.82	5.68	18.43
(1,44)	2:79:B:LEU:CD2	4:403:A:PCW:C8	10	15.82	5.68	18.43
(1,44)	2:79:B:LEU:CD2	4:402:A:PCW:C8	10	15.82	5.68	18.43
(1,43)	2:46:B:ILE:CG2	4:402:A:PCW:C6	10	15.77	3.4	16.42
(1,43)	2:46:B:ILE:CG2	4:406:A:PCW:C8	10	15.77	3.4	16.42
(1,43)	2:46:B:ILE:CG2	4:403:A:PCW:C7	10	15.77	3.4	16.42
(1,43)	2:46:B:ILE:O	4:404:A:PCW:C8	10	15.77	3.4	16.42
(1,43)	2:46:B:ILE:O	4:405:A:PCW:C7	10	15.77	3.4	16.42
(1,43)	2:46:B:ILE:O	4:403:A:PCW:C7	10	15.77	3.4	16.42
(1,43)	2:46:B:ILE:O	4:407:A:PCW:C6	10	15.77	3.4	16.42
(1,43)	2:46:B:ILE:O	4:408:A:PCW:C7	10	15.77	3.4	16.42
(1,43)	2:46:B:ILE:CG2	4:402:A:PCW:C7	10	15.77	3.4	16.42
(1,45)	2:113:B:LEU:O	4:402:A:PCW:C8	10	13.25	7.39	13.95
(1,45)	2:113:B:LEU:H	4:406:A:PCW:C8	10	13.25	7.39	13.95
(1,45)	2:113:B:LEU:H	4:403:A:PCW:C7	10	13.25	7.39	13.95
(1,45)	2:113:B:LEU:O	4:405:A:PCW:C4	10	13.25	7.39	13.95
(1,45)	2:113:B:LEU:CD2	5:409:A:17F:O5	10	13.25	7.39	13.95
(1,45)	2:113:B:LEU:H	4:403:A:PCW:C8	10	13.25	7.39	13.95
(1,45)	2:113:B:LEU:H	4:403:A:PCW:C5	10	13.25	7.39	13.95
(1,45)	2:113:B:LEU:H	4:402:A:PCW:C7	10	13.25	7.39	13.95
(1,46)	2:133:B:LEU:C	4:402:A:PCW:C8	10	12.98	7.79	11.49
(1,46)	2:133:B:LEU:O	4:403:A:PCW:C8	10	12.98	7.79	11.49
(1,46)	2:133:B:LEU:O	4:406:A:PCW:C8	10	12.98	7.79	11.49
(1,46)	2:133:B:LEU:O	4:403:A:PCW:C5	10	12.98	7.79	11.49
(1,46)	2:133:B:LEU:CD1	5:409:A:17F:O4	10	12.98	7.79	11.49
(1,46)	2:133:B:LEU:N	4:402:A:PCW:C4	10	12.98	7.79	11.49
(1,48)	2:160:B:VAL:H	4:402:A:PCW:C7	10	12.83	4.06	13.77

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,48)	2:160:B:VAL:O	4:406:A:PCW:C8	10	12.83	4.06	13.77
(1,48)	2:160:B:VAL:O	4:403:A:PCW:C7	10	12.83	4.06	13.77
(1,48)	2:160:B:VAL:O	4:407:A:PCW:C8	10	12.83	4.06	13.77
(1,48)	2:160:B:VAL:O	4:405:A:PCW:C7	10	12.83	4.06	13.77
(1,48)	2:160:B:VAL:O	4:403:A:PCW:C4	10	12.83	4.06	13.77
(1,48)	2:160:B:VAL:O	4:403:A:PCW:C8	10	12.83	4.06	13.77
(1,48)	2:160:B:VAL:N	4:402:A:PCW:C7	10	12.83	4.06	13.77
(1,33)	5:409:A:17F:O5	2:161:B:ARG:O	10	12.42	5.99	13.59
(1,33)	5:409:A:17F:O5	4:210:B:PCW:C6	10	12.42	5.99	13.59
(1,33)	5:409:A:17F:O4	4:210:B:PCW:C7	10	12.42	5.99	13.59
(1,33)	5:409:A:17F:O5	4:210:B:PCW:C5	10	12.42	5.99	13.59
(1,33)	5:409:A:17F:O5	2:132:B:ASP:OD2	10	12.42	5.99	13.59
(1,33)	5:409:A:17F:O4	4:210:B:PCW:C5	10	12.42	5.99	13.59
(1,2)	1:202:A:LYS:N	2:132:B:ASP:OD1	10	12.39	3.84	13.42
(1,2)	4:401:A:PCW:C6	2:45:B:VAL:CG2	10	12.39	3.84	13.42
(1,2)	4:401:A:PCW:C6	2:22:B:GLN:HE22	10	12.39	3.84	13.42
(1,2)	4:401:A:PCW:C4	2:185:B:CYS:HG	10	12.39	3.84	13.42
(1,2)	4:401:A:PCW:C7	2:45:B:VAL:CG1	10	12.39	3.84	13.42
(1,2)	1:202:A:LYS:N	2:185:B:CYS:O	10	12.39	3.84	13.42
(1,2)	1:202:A:LYS:N	2:185:B:CYS:HG	10	12.39	3.84	13.42
(1,49)	2:185:B:CYS:N	1:201:A:LEU:N	10	11.0	6.6	11.7
(1,49)	2:185:B:CYS:HG	4:403:A:PCW:C8	10	11.0	6.6	11.7
(1,49)	2:185:B:CYS:HG	4:406:A:PCW:C8	10	11.0	6.6	11.7
(1,49)	2:185:B:CYS:HG	5:410:A:17F:O6	10	11.0	6.6	11.7
(1,49)	2:185:B:CYS:N	4:403:A:PCW:C5	10	11.0	6.6	11.7
(1,49)	2:185:B:CYS:O	4:403:A:PCW:C6	10	11.0	6.6	11.7
(1,49)	2:185:B:CYS:C	4:406:A:PCW:C4	10	11.0	6.6	11.7
(1,49)	2:185:B:CYS:O	1:203:A:LEU:N	10	11.0	6.6	11.7
(1,49)	2:185:B:CYS:HG	1:211:A:THR:N	10	11.0	6.6	11.7
(1,21)	4:405:A:PCW:C7	4:208:B:PCW:C1	10	7.22	1.13	7.54
(1,21)	4:405:A:PCW:C8	4:208:B:PCW:C1	10	7.22	1.13	7.54
(1,21)	4:405:A:PCW:C4	4:208:B:PCW:C1	10	7.22	1.13	7.54
(1,29)	4:406:A:PCW:C4	4:211:B:PCW:C8	10	5.74	3.8	6.3
(1,29)	4:406:A:PCW:C4	4:209:B:PCW:C4	10	5.74	3.8	6.3
(1,29)	4:406:A:PCW:C4	4:209:B:PCW:O2	10	5.74	3.8	6.3
(1,29)	4:406:A:PCW:C4	4:211:B:PCW:C6	10	5.74	3.8	6.3
(1,29)	4:406:A:PCW:C4	2:185:B:CYS:C	10	5.74	3.8	6.3
(1,11)	1:211:A:THR:N	2:132:B:ASP:OD1	9	20.8	7.18	24.55
(1,11)	1:211:A:THR:N	4:210:B:PCW:C7	9	20.8	7.18	24.55
(1,11)	1:211:A:THR:N	4:210:B:PCW:O3	9	20.8	7.18	24.55
(1,11)	1:211:A:THR:N	4:210:B:PCW:C4	9	20.8	7.18	24.55
(1,11)	1:211:A:THR:N	4:210:B:PCW:C2	9	20.8	7.18	24.55

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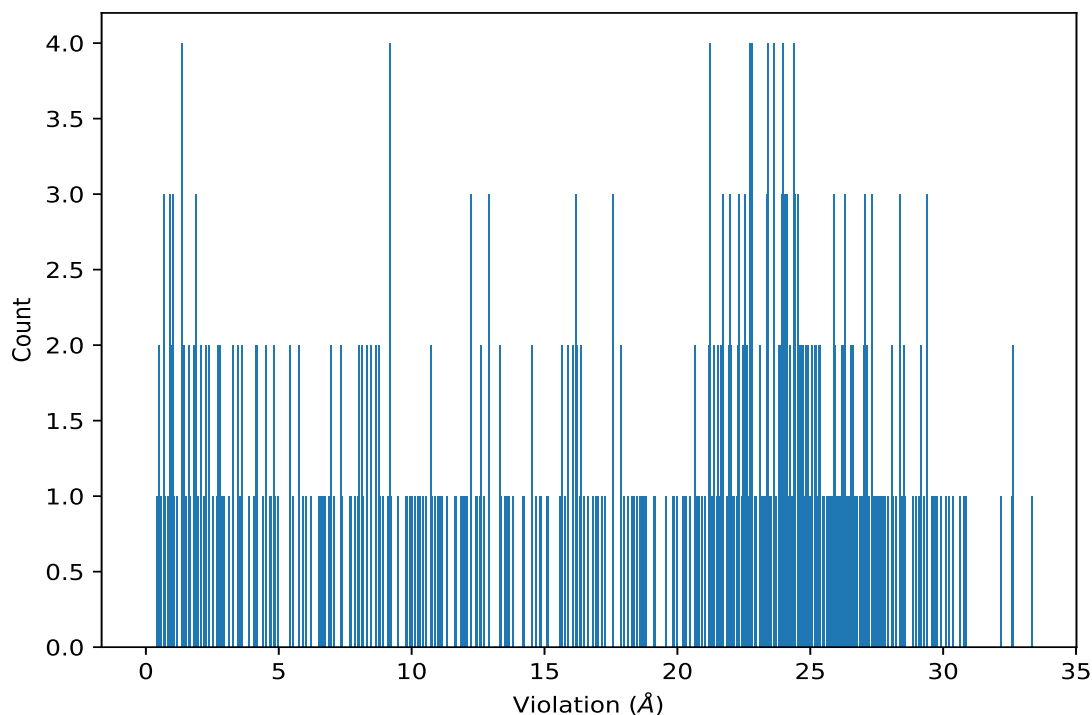
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,11)	1:211:A:THR:N	2:185:B:CYS:H	9	20.8	7.18	24.55
(1,38)	5:410:A:17F:N1	2:47:B:ASP:O	9	18.56	2.6	18.15
(1,38)	5:410:A:17F:O5	2:45:B:VAL:CG2	9	18.56	2.6	18.15
(1,38)	5:410:A:17F:O4	2:45:B:VAL:CG2	9	18.56	2.6	18.15
(1,38)	5:410:A:17F:N1	2:45:B:VAL:CG2	9	18.56	2.6	18.15
(1,38)	5:410:A:17F:O5	2:25:B:GLN:O	9	18.56	2.6	18.15
(1,38)	5:410:A:17F:O5	2:45:B:VAL:CG1	9	18.56	2.6	18.15
(1,38)	5:410:A:17F:O4	2:47:B:ASP:OD1	9	18.56	2.6	18.15
(1,38)	5:410:A:17F:C2	2:47:B:ASP:O	9	18.56	2.6	18.15
(1,47)	2:142:B:ILE:CD1	4:406:A:PCW:C8	9	12.3	5.93	14.51
(1,47)	2:142:B:ILE:CD1	4:403:A:PCW:C7	9	12.3	5.93	14.51
(1,47)	2:142:B:ILE:CG2	4:405:A:PCW:C4	9	12.3	5.93	14.51
(1,47)	2:142:B:ILE:C	4:404:A:PCW:C7	9	12.3	5.93	14.51
(1,47)	2:142:B:ILE:CG2	4:405:A:PCW:C7	9	12.3	5.93	14.51
(1,47)	2:142:B:ILE:CG2	4:405:A:PCW:C8	9	12.3	5.93	14.51
(1,47)	2:142:B:ILE:CD1	4:402:A:PCW:C7	9	12.3	5.93	14.51
(1,47)	2:142:B:ILE:CD1	4:402:A:PCW:C6	9	12.3	5.93	14.51
(1,20)	4:404:A:PCW:C6	4:210:B:PCW:C7	9	2.06	0.9	1.87
(1,20)	4:404:A:PCW:C8	4:211:B:PCW:C1	9	2.06	0.9	1.87
(1,20)	4:404:A:PCW:C5	4:210:B:PCW:O2	9	2.06	0.9	1.87
(1,20)	4:404:A:PCW:C5	4:210:B:PCW:C8	9	2.06	0.9	1.87
(1,20)	4:404:A:PCW:C8	4:210:B:PCW:C8	9	2.06	0.9	1.87
(1,20)	4:404:A:PCW:C8	2:143:B:GLU:OE2	9	2.06	0.9	1.87
(1,42)	4:210:B:PCW:C7	4:404:A:PCW:C6	9	1.88	0.93	1.85
(1,42)	4:210:B:PCW:C4	4:402:A:PCW:C8	9	1.88	0.93	1.85
(1,42)	4:210:B:PCW:C7	4:402:A:PCW:C6	9	1.88	0.93	1.85
(1,42)	4:210:B:PCW:C8	4:404:A:PCW:C8	9	1.88	0.93	1.85
(1,42)	4:210:B:PCW:C8	4:404:A:PCW:C5	9	1.88	0.93	1.85
(1,42)	4:210:B:PCW:C6	4:402:A:PCW:C6	9	1.88	0.93	1.85
(1,42)	4:210:B:PCW:C4	4:402:A:PCW:C6	9	1.88	0.93	1.85
(1,41)	4:209:B:PCW:O2	4:403:A:PCW:C8	8	1.46	1.05	1.19
(1,41)	4:209:B:PCW:O2	4:403:A:PCW:C6	8	1.46	1.05	1.19
(1,41)	4:209:B:PCW:O2	4:403:A:PCW:C5	8	1.46	1.05	1.19
(1,15)	4:402:A:PCW:C8	4:210:B:PCW:C4	7	2.36	0.86	2.38
(1,15)	4:402:A:PCW:C6	4:210:B:PCW:C7	7	2.36	0.86	2.38
(1,15)	4:402:A:PCW:C6	4:210:B:PCW:C4	7	2.36	0.86	2.38
(1,15)	4:402:A:PCW:C5	4:210:B:PCW:C4	7	2.36	0.86	2.38
(1,15)	4:402:A:PCW:C6	4:210:B:PCW:C6	7	2.36	0.86	2.38
(1,19)	4:403:A:PCW:C8	4:209:B:PCW:O2	7	1.4	1.17	1.01
(1,19)	4:403:A:PCW:C6	4:209:B:PCW:O2	7	1.4	1.17	1.01
(1,19)	4:403:A:PCW:C4	4:211:B:PCW:C8	7	1.4	1.17	1.01
(1,19)	4:403:A:PCW:C5	4:209:B:PCW:O2	7	1.4	1.17	1.01

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)
(1,1)	1:201:A:LEU:N	4:210:B:PCW:C4	2	33.32
(1,1)	1:201:A:LEU:N	4:210:B:PCW:C4	4	32.62
(1,1)	1:201:A:LEU:N	4:210:B:PCW:C4	7	32.6
(1,1)	1:201:A:LEU:N	4:210:B:PCW:C4	8	32.59
(1,1)	1:201:A:LEU:N	4:210:B:PCW:C6	6	32.19
(1,5)	1:205:A:ASP:N	4:210:B:PCW:C4	2	30.88
(1,1)	1:201:A:LEU:N	2:132:B:ASP:OD1	5	30.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:201:A:LEU:N	4:210:B:PCW:C7	3	30.61
(1,5)	1:205:A:ASP:N	4:210:B:PCW:C4	4	30.36
(1,6)	1:206:A:ASN:N	4:210:B:PCW:C4	2	30.22
(1,5)	1:205:A:ASP:N	4:210:B:PCW:C4	8	30.14
(1,5)	1:205:A:ASP:N	4:210:B:PCW:C4	7	29.93
(1,3)	1:203:A:LEU:N	4:210:B:PCW:C4	2	29.78
(1,5)	1:205:A:ASP:N	4:210:B:PCW:C2	5	29.67
(1,5)	1:205:A:ASP:N	4:210:B:PCW:C7	3	29.62
(1,6)	1:206:A:ASN:N	4:210:B:PCW:C4	4	29.55
(1,3)	1:203:A:LEU:N	4:210:B:PCW:C4	7	29.4
(1,6)	1:206:A:ASN:N	4:210:B:PCW:C7	3	29.39
(1,9)	1:209:A:SER:N	4:210:B:PCW:C4	2	29.35
(1,6)	1:206:A:ASN:N	4:210:B:PCW:C4	8	29.28
(1,5)	1:205:A:ASP:N	4:210:B:PCW:C6	6	29.17
(1,6)	1:206:A:ASN:N	4:210:B:PCW:C4	7	29.16
(1,3)	1:203:A:LEU:N	4:210:B:PCW:C4	4	29.12
(1,4)	1:204:A:LEU:N	4:210:B:PCW:C4	2	29.07
(1,3)	1:203:A:LEU:N	4:210:B:PCW:C4	8	28.96
(1,6)	1:206:A:ASN:N	4:210:B:PCW:C6	6	28.86
(1,9)	1:209:A:SER:N	4:210:B:PCW:C4	4	28.58
(1,4)	1:204:A:LEU:N	4:210:B:PCW:C4	4	28.54
(1,3)	1:203:A:LEU:N	4:210:B:PCW:C7	3	28.5
(1,4)	1:204:A:LEU:N	4:210:B:PCW:C4	7	28.48
(1,9)	1:209:A:SER:N	4:210:B:PCW:O3	3	28.43
(1,8)	1:208:A:ASP:N	4:210:B:PCW:C7	2	28.37
(1,3)	1:203:A:LEU:N	4:210:B:PCW:C6	6	28.37
(1,4)	1:204:A:LEU:N	4:210:B:PCW:C4	8	28.36
(1,9)	1:209:A:SER:N	4:210:B:PCW:C4	8	28.23
(1,4)	1:204:A:LEU:N	2:132:B:ASP:OD1	5	28.14
(1,6)	1:206:A:ASN:N	4:210:B:PCW:C2	5	28.08
(1,9)	1:209:A:SER:N	4:210:B:PCW:C4	7	28.05
(1,3)	1:203:A:LEU:N	2:132:B:ASP:OD1	5	27.94
(1,12)	1:212:A:SER:N	4:210:B:PCW:C7	2	27.81
(1,7)	1:207:A:TRP:N	4:210:B:PCW:C4	2	27.74
(1,8)	1:208:A:ASP:N	4:210:B:PCW:C4	4	27.69
(1,4)	1:204:A:LEU:N	4:210:B:PCW:C7	3	27.62
(1,4)	1:204:A:LEU:N	4:210:B:PCW:C6	6	27.55
(1,13)	1:213:A:THR:N	4:210:B:PCW:O3	2	27.5
(1,37)	1:237:A:GLU:O	4:211:B:PCW:O3	4	27.49
(1,8)	1:208:A:ASP:N	4:210:B:PCW:C7	3	27.42
(1,9)	1:209:A:SER:N	4:210:B:PCW:C2	5	27.4
(1,8)	1:208:A:ASP:N	4:210:B:PCW:C4	8	27.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:216:A:LYS:N	4:210:B:PCW:O3	2	27.33
(1,37)	1:237:A:GLU:O	4:210:B:PCW:O3	5	27.3
(1,34)	1:234:A:LYS:O	4:211:B:PCW:O3	4	27.22
(1,12)	1:212:A:SER:N	4:210:B:PCW:C4	4	27.14
(1,10)	1:210:A:VAL:N	4:210:B:PCW:C4	2	27.13
(1,16)	1:216:A:LYS:N	4:210:B:PCW:O3	4	27.09
(1,37)	1:237:A:GLU:O	4:211:B:PCW:O3	3	27.08
(1,9)	1:209:A:SER:N	4:210:B:PCW:C7	6	27.05
(1,8)	1:208:A:ASP:N	4:210:B:PCW:C4	7	27.04
(1,7)	1:207:A:TRP:N	4:210:B:PCW:C4	4	27.04
(1,13)	1:213:A:THR:N	4:210:B:PCW:C2	4	26.97
(1,7)	1:207:A:TRP:N	4:210:B:PCW:C7	3	26.94
(1,8)	1:208:A:ASP:N	4:210:B:PCW:C2	5	26.86
(1,7)	1:207:A:TRP:N	4:210:B:PCW:C4	8	26.77
(1,23)	1:223:A:PRO:N	4:210:B:PCW:O3	2	26.68
(1,40)	1:240:A:ARG:O	4:211:B:PCW:O3	5	26.64
(1,40)	1:240:A:ARG:O	4:210:B:PCW:O3	7	26.6
(1,7)	1:207:A:TRP:N	4:210:B:PCW:C4	7	26.55
(1,12)	1:212:A:SER:N	4:210:B:PCW:C4	7	26.53
(1,12)	1:212:A:SER:N	4:210:B:PCW:O3	3	26.52
(1,13)	1:213:A:THR:N	4:210:B:PCW:C4	7	26.47
(1,12)	1:212:A:SER:N	4:210:B:PCW:C4	8	26.45
(1,23)	1:223:A:PRO:N	4:210:B:PCW:O3	4	26.35
(1,37)	1:237:A:GLU:O	4:210:B:PCW:O3	7	26.31
(1,16)	1:216:A:LYS:N	4:210:B:PCW:C7	7	26.31
(1,10)	1:210:A:VAL:N	4:210:B:PCW:C4	4	26.3
(1,8)	1:208:A:ASP:N	4:210:B:PCW:C6	6	26.28
(1,7)	1:207:A:TRP:N	4:210:B:PCW:C6	6	26.27
(1,40)	1:240:A:ARG:O	4:211:B:PCW:O3	4	26.23
(1,12)	1:212:A:SER:N	4:210:B:PCW:C2	5	26.2
(1,13)	1:213:A:THR:N	4:210:B:PCW:C4	8	26.18
(1,34)	1:234:A:LYS:O	4:210:B:PCW:O3	5	26.14
(1,13)	1:213:A:THR:N	4:210:B:PCW:O3	3	26.06
(1,34)	1:234:A:LYS:O	4:210:B:PCW:O3	3	26.03
(1,40)	1:240:A:ARG:O	4:211:B:PCW:O3	3	25.99
(1,10)	1:210:A:VAL:N	4:210:B:PCW:C4	8	25.95
(1,10)	1:210:A:VAL:N	4:210:B:PCW:O3	3	25.92
(1,11)	1:211:A:THR:N	4:210:B:PCW:C7	2	25.9
(1,16)	1:216:A:LYS:N	4:210:B:PCW:O3	8	25.89
(1,10)	1:210:A:VAL:N	4:210:B:PCW:C4	7	25.89
(1,27)	1:227:A:GLU:N	4:211:B:PCW:C3	2	25.8
(1,7)	1:207:A:TRP:N	4:210:B:PCW:C2	5	25.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:227:A:GLU:N	4:210:B:PCW:O3	4	25.71
(1,16)	1:216:A:LYS:N	4:210:B:PCW:O3	3	25.69
(1,24)	1:224:A:VAL:N	4:210:B:PCW:O3	2	25.63
(1,17)	1:217:A:LEU:N	4:210:B:PCW:O3	2	25.5
(1,13)	1:213:A:THR:N	4:210:B:PCW:O3	5	25.48
(1,34)	1:234:A:LYS:O	4:211:B:PCW:O3	8	25.38
(1,16)	1:216:A:LYS:N	4:210:B:PCW:O3	5	25.38
(1,17)	1:217:A:LEU:N	4:210:B:PCW:O3	4	25.34
(1,23)	1:223:A:PRO:N	4:210:B:PCW:O3	7	25.31
(1,12)	1:212:A:SER:N	4:210:B:PCW:C7	6	25.26
(1,37)	1:237:A:GLU:O	4:211:B:PCW:O3	8	25.23
(1,34)	1:234:A:LYS:O	4:210:B:PCW:O3	6	25.21
(1,34)	1:234:A:LYS:O	4:210:B:PCW:O3	7	25.19
(1,37)	1:237:A:GLU:O	4:211:B:PCW:O3	2	25.18
(1,24)	1:224:A:VAL:N	4:210:B:PCW:O3	4	25.09
(1,11)	1:211:A:THR:N	4:210:B:PCW:C4	4	25.09
(1,37)	1:237:A:GLU:O	4:211:B:PCW:O3	6	25.02
(1,30)	1:230:A:ASP:N	4:210:B:PCW:O3	4	24.97
(1,23)	1:223:A:PRO:N	4:210:B:PCW:O3	5	24.95
(1,14)	1:214:A:PHE:N	4:210:B:PCW:O3	2	24.95
(1,10)	1:210:A:VAL:N	4:210:B:PCW:C2	5	24.87
(1,34)	1:234:A:LYS:O	4:211:B:PCW:O3	2	24.82
(1,37)	1:237:A:GLU:O	4:210:B:PCW:O3	1	24.8
(1,13)	1:213:A:THR:N	4:210:B:PCW:O3	6	24.78
(1,23)	1:223:A:PRO:N	4:210:B:PCW:O3	8	24.74
(1,11)	1:211:A:THR:N	4:210:B:PCW:O3	3	24.71
(1,23)	1:223:A:PRO:N	4:210:B:PCW:O3	3	24.69
(1,10)	1:210:A:VAL:N	4:210:B:PCW:O3	6	24.66
(1,16)	1:216:A:LYS:N	4:210:B:PCW:O3	6	24.65
(1,17)	1:217:A:LEU:N	4:210:B:PCW:O3	7	24.6
(1,11)	1:211:A:THR:N	4:210:B:PCW:C4	8	24.58
(1,11)	1:211:A:THR:N	4:210:B:PCW:C4	7	24.55
(1,36)	1:236:A:THR:O	4:211:B:PCW:O3	4	24.53
(1,14)	1:214:A:PHE:N	4:210:B:PCW:C2	4	24.53
(1,27)	1:227:A:GLU:N	4:210:B:PCW:O3	7	24.5
(1,22)	1:222:A:GLY:N	4:210:B:PCW:O3	2	24.45
(1,37)	1:237:A:GLU:O	2:143:B:GLU:OE1	9	24.44
(1,27)	1:227:A:GLU:N	4:210:B:PCW:O3	3	24.42
(1,40)	1:240:A:ARG:O	2:143:B:GLU:OE2	9	24.4
(1,27)	1:227:A:GLU:N	4:210:B:PCW:O3	5	24.38
(1,40)	1:240:A:ARG:O	4:211:B:PCW:O3	2	24.35
(1,39)	1:239:A:LEU:O	4:211:B:PCW:O3	5	24.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:239:A:LEU:O	4:210:B:PCW:O3	7	24.34
(1,35)	1:235:A:GLU:O	4:211:B:PCW:O3	4	24.23
(1,26)	1:226:A:GLN:N	4:211:B:PCW:C3	2	24.23
(1,22)	1:222:A:GLY:N	4:210:B:PCW:O3	4	24.18
(1,11)	1:211:A:THR:N	4:210:B:PCW:C2	5	24.15
(1,27)	1:227:A:GLU:N	4:210:B:PCW:O3	8	24.14
(1,40)	1:240:A:ARG:O	4:211:B:PCW:O3	8	24.13
(1,24)	1:224:A:VAL:N	4:210:B:PCW:O3	7	24.08
(1,30)	1:230:A:ASP:N	4:211:B:PCW:O3	2	24.06
(1,17)	1:217:A:LEU:N	4:210:B:PCW:O3	3	24.06
(1,26)	1:226:A:GLN:N	4:210:B:PCW:O3	4	24.01
(1,23)	1:223:A:PRO:N	4:210:B:PCW:O3	6	24.01
(1,17)	1:217:A:LEU:N	4:210:B:PCW:O3	8	24.0
(1,28)	1:228:A:PHE:N	4:210:B:PCW:O3	4	23.98
(1,36)	1:236:A:THR:O	4:210:B:PCW:O3	5	23.97
(1,36)	1:236:A:THR:O	4:210:B:PCW:O3	3	23.96
(1,14)	1:214:A:PHE:N	4:210:B:PCW:C4	7	23.96
(1,18)	1:218:A:ARG:N	4:210:B:PCW:O3	2	23.94
(1,40)	1:240:A:ARG:O	4:211:B:PCW:O3	1	23.92
(1,28)	1:228:A:PHE:N	4:211:B:PCW:O3	2	23.92
(1,18)	1:218:A:ARG:N	4:210:B:PCW:O3	4	23.89
(1,35)	1:235:A:GLU:O	4:210:B:PCW:O3	5	23.85
(1,46)	2:133:B:LEU:O	4:403:A:PCW:C5	4	23.84
(1,34)	1:234:A:LYS:O	2:143:B:GLU:OE2	1	23.82
(1,39)	1:239:A:LEU:O	4:211:B:PCW:O3	4	23.71
(1,24)	1:224:A:VAL:N	4:210:B:PCW:O3	8	23.67
(1,14)	1:214:A:PHE:N	4:210:B:PCW:O3	8	23.65
(1,35)	1:235:A:GLU:O	4:210:B:PCW:O3	3	23.64
(1,24)	1:224:A:VAL:N	4:210:B:PCW:O3	5	23.64
(1,40)	1:240:A:ARG:O	4:211:B:PCW:O3	6	23.63
(1,24)	1:224:A:VAL:N	4:210:B:PCW:O3	3	23.53
(1,39)	1:239:A:LEU:O	4:211:B:PCW:O3	3	23.48
(1,30)	1:230:A:ASP:N	4:210:B:PCW:O3	3	23.45
(1,30)	1:230:A:ASP:N	4:210:B:PCW:O3	5	23.45
(1,17)	1:217:A:LEU:N	4:210:B:PCW:O3	5	23.44
(1,30)	1:230:A:ASP:N	4:210:B:PCW:O3	7	23.43
(1,14)	1:214:A:PHE:N	4:210:B:PCW:O3	3	23.4
(1,30)	1:230:A:ASP:N	4:210:B:PCW:O3	8	23.38
(1,11)	1:211:A:THR:N	4:210:B:PCW:C7	6	23.37
(1,22)	1:222:A:GLY:N	4:210:B:PCW:O3	7	23.3
(1,27)	1:227:A:GLU:N	4:210:B:PCW:O3	6	23.27
(1,34)	1:234:A:LYS:O	2:132:B:ASP:OD1	9	23.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:234:A:LYS:O	2:143:B:GLU:OE2	10	23.14
(1,25)	1:225:A:THR:N	4:210:B:PCW:O3	2	23.12
(1,36)	1:236:A:THR:O	4:210:B:PCW:O3	7	22.96
(1,14)	1:214:A:PHE:N	4:210:B:PCW:O3	5	22.93
(1,28)	1:228:A:PHE:N	4:210:B:PCW:O3	7	22.83
(1,18)	1:218:A:ARG:N	4:210:B:PCW:O3	7	22.82
(1,38)	5:410:A:17F:C2	2:47:B:ASP:O	10	22.8
(1,22)	1:222:A:GLY:N	4:210:B:PCW:O3	5	22.8
(1,37)	1:237:A:GLU:O	2:143:B:GLU:OE2	10	22.76
(1,26)	1:226:A:GLN:N	4:210:B:PCW:O3	7	22.74
(1,17)	1:217:A:LEU:N	4:210:B:PCW:O3	6	22.74
(1,39)	1:239:A:LEU:O	2:143:B:GLU:OE2	9	22.73
(1,26)	1:226:A:GLN:N	4:210:B:PCW:O3	3	22.73
(1,25)	1:225:A:THR:N	4:210:B:PCW:O3	4	22.68
(1,28)	1:228:A:PHE:N	4:210:B:PCW:O3	5	22.63
(1,24)	1:224:A:VAL:N	4:210:B:PCW:O3	6	22.6
(1,26)	1:226:A:GLN:N	4:210:B:PCW:O3	5	22.57
(1,28)	1:228:A:PHE:N	4:210:B:PCW:O3	3	22.56
(1,22)	1:222:A:GLY:N	4:210:B:PCW:O3	3	22.52
(1,22)	1:222:A:GLY:N	4:210:B:PCW:O3	8	22.52
(1,35)	1:235:A:GLU:O	4:210:B:PCW:O3	7	22.51
(1,26)	1:226:A:GLN:N	4:210:B:PCW:O3	8	22.49
(1,40)	1:240:A:ARG:O	2:143:B:GLU:OE2	10	22.46
(1,35)	1:235:A:GLU:O	4:211:B:PCW:O3	6	22.45
(1,18)	1:218:A:ARG:N	4:210:B:PCW:O3	3	22.32
(1,44)	2:79:B:LEU:CD1	4:405:A:PCW:C4	4	22.31
(1,18)	1:218:A:ARG:N	4:210:B:PCW:O3	8	22.3
(1,28)	1:228:A:PHE:N	4:210:B:PCW:O3	8	22.29
(1,14)	1:214:A:PHE:N	4:210:B:PCW:O3	6	22.26
(1,35)	1:235:A:GLU:O	4:211:B:PCW:O3	8	22.21
(1,18)	1:218:A:ARG:N	4:210:B:PCW:O3	5	22.11
(1,36)	1:236:A:THR:O	4:211:B:PCW:O3	8	22.09
(1,30)	1:230:A:ASP:N	4:210:B:PCW:O3	6	22.04
(1,32)	1:232:A:LEU:N	4:210:B:PCW:O3	8	22.03
(1,36)	1:236:A:THR:O	4:211:B:PCW:O3	6	21.99
(1,36)	1:236:A:THR:O	4:211:B:PCW:O3	2	21.98
(1,35)	1:235:A:GLU:O	4:211:B:PCW:O3	2	21.97
(1,39)	1:239:A:LEU:O	4:211:B:PCW:O3	2	21.94
(1,35)	1:235:A:GLU:O	2:143:B:GLU:OE1	9	21.93
(1,22)	1:222:A:GLY:N	4:210:B:PCW:O3	6	21.89
(1,39)	1:239:A:LEU:O	4:211:B:PCW:O3	8	21.74
(1,39)	1:239:A:LEU:O	4:211:B:PCW:O3	1	21.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,38)	5:410:A:17F:O5	2:25:B:GLN:O	7	21.71
(1,46)	2:133:B:LEU:O	4:403:A:PCW:C8	7	21.7
(1,26)	1:226:A:GLN:N	4:210:B:PCW:O3	6	21.7
(1,44)	2:79:B:LEU:CD2	4:403:A:PCW:C7	8	21.64
(1,45)	2:113:B:LEU:H	4:406:A:PCW:C8	6	21.62
(1,35)	1:235:A:GLU:O	4:210:B:PCW:O3	1	21.59
(1,25)	1:225:A:THR:N	4:210:B:PCW:O3	7	21.54
(1,36)	1:236:A:THR:O	4:210:B:PCW:O3	1	21.52
(1,44)	2:79:B:LEU:CD2	4:403:A:PCW:C8	7	21.47
(1,45)	2:113:B:LEU:O	4:405:A:PCW:C4	4	21.38
(1,28)	1:228:A:PHE:N	4:210:B:PCW:O3	6	21.38
(1,39)	1:239:A:LEU:O	4:211:B:PCW:O3	6	21.3
(1,49)	2:185:B:CYS:N	4:403:A:PCW:C5	6	21.27
(1,39)	1:239:A:LEU:O	2:143:B:GLU:OE2	10	21.22
(1,25)	1:225:A:THR:N	4:210:B:PCW:O3	3	21.22
(1,25)	1:225:A:THR:N	4:210:B:PCW:O3	5	21.21
(1,18)	1:218:A:ARG:N	4:210:B:PCW:O3	6	21.21
(1,25)	1:225:A:THR:N	4:210:B:PCW:O3	8	21.2
(1,35)	1:235:A:GLU:O	2:143:B:GLU:OE2	10	21.17
(1,36)	1:236:A:THR:O	2:143:B:GLU:OE1	9	21.03
(1,32)	1:232:A:LEU:N	4:210:B:PCW:O3	6	20.93
(1,46)	2:133:B:LEU:O	4:406:A:PCW:C8	6	20.82
(1,43)	2:46:B:ILE:O	4:405:A:PCW:C7	5	20.72
(1,46)	2:133:B:LEU:O	4:403:A:PCW:C5	8	20.69
(1,38)	5:410:A:17F:O5	2:45:B:VAL:CG1	8	20.66
(1,45)	2:113:B:LEU:H	4:403:A:PCW:C5	8	20.46
(1,45)	2:113:B:LEU:H	4:403:A:PCW:C8	7	20.3
(1,33)	5:409:A:17F:O5	4:210:B:PCW:C6	6	20.26
(1,25)	1:225:A:THR:N	4:210:B:PCW:O3	6	20.23
(1,32)	4:408:A:PCW:C7	2:45:B:VAL:CG2	4	19.97
(1,32)	4:408:A:PCW:C7	2:45:B:VAL:CG2	7	19.85
(1,32)	4:408:A:PCW:C7	2:45:B:VAL:CG2	3	19.8
(1,36)	1:236:A:THR:O	2:143:B:GLU:OE2	10	19.59
(1,38)	5:410:A:17F:O5	2:45:B:VAL:CG2	6	19.17
(1,48)	2:160:B:VAL:O	4:405:A:PCW:C7	5	19.15
(1,43)	2:46:B:ILE:O	4:403:A:PCW:C7	6	18.81
(1,47)	2:142:B:ILE:CG2	4:405:A:PCW:C7	7	18.77
(1,32)	4:408:A:PCW:C4	2:185:B:CYS:CB	5	18.73
(1,44)	5:215:B:17F:C9	4:403:A:PCW:C8	6	18.67
(1,44)	2:79:B:LEU:CD2	4:404:A:PCW:C7	5	18.58
(1,43)	2:46:B:ILE:O	4:404:A:PCW:C8	4	18.46
(1,33)	5:409:A:17F:O4	4:210:B:PCW:C7	3	18.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	2:79:B:LEU:CD2	4:403:A:PCW:C7	3	18.28
(1,38)	5:410:A:17F:N1	2:45:B:VAL:CG2	4	18.15
(1,48)	2:160:B:VAL:O	4:407:A:PCW:C8	4	17.98
(1,47)	2:142:B:ILE:CG2	4:405:A:PCW:C8	8	17.87
(1,33)	5:409:A:17F:O5	4:210:B:PCW:C6	2	17.86
(1,30)	1:230:A:ASP:N	2:132:B:ASP:OD1	10	17.59
(1,43)	2:46:B:ILE:CG2	4:403:A:PCW:C7	8	17.57
(1,38)	5:410:A:17F:O5	2:45:B:VAL:CG2	2	17.57
(1,49)	2:185:B:CYS:N	1:201:A:LEU:N	1	17.28
(1,47)	2:142:B:ILE:CG2	4:405:A:PCW:C7	6	17.19
(1,33)	5:409:A:17F:O5	4:210:B:PCW:C5	4	17.01
(1,49)	2:185:B:CYS:HG	4:403:A:PCW:C8	4	16.93
(1,30)	1:230:A:ASP:N	2:143:B:GLU:OE2	1	16.83
(1,43)	2:46:B:ILE:O	4:407:A:PCW:C6	7	16.64
(1,2)	4:401:A:PCW:C6	2:45:B:VAL:CG2	2	16.47
(1,2)	4:401:A:PCW:C7	2:45:B:VAL:CG1	8	16.4
(1,49)	2:185:B:CYS:O	4:403:A:PCW:C6	7	16.36
(1,38)	5:410:A:17F:O4	2:45:B:VAL:CG2	3	16.32
(1,28)	1:228:A:PHE:N	2:132:B:ASP:OD1	10	16.22
(1,43)	2:46:B:ILE:CG2	4:403:A:PCW:C7	3	16.21
(1,30)	1:230:A:ASP:N	2:132:B:ASP:OD1	9	16.18
(1,38)	5:410:A:17F:N1	2:47:B:ASP:O	1	16.17
(1,27)	1:227:A:GLU:N	2:132:B:ASP:OD1	10	16.17
(1,28)	1:228:A:PHE:N	2:143:B:GLU:OE2	1	16.08
(1,27)	1:227:A:GLU:N	2:143:B:GLU:OE2	1	16.08
(1,48)	2:160:B:VAL:O	4:403:A:PCW:C4	6	15.89
(1,43)	2:46:B:ILE:CG2	4:406:A:PCW:C8	2	15.88
(1,2)	4:401:A:PCW:C6	2:45:B:VAL:CG2	6	15.75
(1,45)	2:113:B:LEU:H	4:403:A:PCW:C7	3	15.69
(1,32)	4:408:A:PCW:C7	2:45:B:VAL:CG1	2	15.65
(1,47)	2:142:B:ILE:CG2	4:405:A:PCW:C4	4	15.64
(1,32)	4:408:A:PCW:C6	2:161:B:ARG:O	10	15.6
(1,27)	1:227:A:GLU:N	2:132:B:ASP:OD1	9	15.11
(1,33)	5:409:A:17F:O4	4:210:B:PCW:C5	7	15.08
(1,46)	2:133:B:LEU:O	4:406:A:PCW:C8	3	14.88
(1,2)	4:401:A:PCW:C6	2:22:B:GLN:HE22	4	14.82
(1,28)	1:228:A:PHE:N	2:132:B:ASP:OD1	9	14.69
(1,38)	5:410:A:17F:O4	2:47:B:ASP:OD1	9	14.52
(1,47)	2:142:B:ILE:CD1	4:403:A:PCW:C7	3	14.51
(1,48)	2:160:B:VAL:O	4:403:A:PCW:C8	7	14.23
(1,24)	1:224:A:VAL:N	2:143:B:GLU:OE1	1	14.2
(1,48)	2:160:B:VAL:O	4:403:A:PCW:C7	3	13.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	2:160:B:VAL:O	4:403:A:PCW:C7	8	13.7
(1,23)	1:223:A:PRO:N	2:143:B:GLU:OE1	1	13.55
(1,2)	4:401:A:PCW:C6	2:22:B:GLN:HE22	3	13.53
(1,26)	1:226:A:GLN:N	2:132:B:ASP:OD1	10	13.39
(1,26)	1:226:A:GLN:N	2:143:B:GLU:OE2	1	13.35
(1,2)	4:401:A:PCW:C6	2:22:B:GLN:HE22	7	13.32
(1,24)	1:224:A:VAL:N	2:132:B:ASP:OD1	9	12.95
(1,23)	1:223:A:PRO:N	2:132:B:ASP:OD1	9	12.91
(1,44)	2:79:B:LEU:CD2	4:406:A:PCW:C8	2	12.9
(1,24)	1:224:A:VAL:N	2:185:B:CYS:O	10	12.73
(1,32)	4:408:A:PCW:C7	2:161:B:ARG:O	1	12.63
(1,43)	2:46:B:ILE:CG2	4:402:A:PCW:C7	10	12.61
(1,25)	1:225:A:THR:N	2:143:B:GLU:OE1	1	12.56
(1,26)	1:226:A:GLN:N	2:132:B:ASP:OD1	9	12.47
(1,49)	2:185:B:CYS:HG	4:406:A:PCW:C8	3	12.44
(1,25)	1:225:A:THR:N	2:132:B:ASP:OD1	10	12.22
(1,45)	2:113:B:LEU:CD2	5:409:A:17F:O5	5	12.21
(1,23)	1:223:A:PRO:N	2:185:B:CYS:O	10	12.21
(1,33)	5:409:A:17F:O5	4:210:B:PCW:C6	8	12.1
(1,47)	2:142:B:ILE:CD1	4:406:A:PCW:C8	2	12.04
(1,16)	1:216:A:LYS:N	2:132:B:ASP:OD1	9	11.93
(1,17)	1:217:A:LEU:N	2:132:B:ASP:H	1	11.86
(1,2)	1:202:A:LYS:N	2:132:B:ASP:OD1	1	11.65
(1,43)	2:46:B:ILE:O	4:408:A:PCW:C7	9	11.63
(1,1)	1:201:A:LEU:N	2:132:B:ASP:OD1	1	11.3
(1,25)	1:225:A:THR:N	2:132:B:ASP:OD1	9	11.11
(1,29)	4:406:A:PCW:C4	4:211:B:PCW:C8	5	11.08
(1,17)	1:217:A:LEU:N	2:132:B:ASP:OD1	9	11.03
(1,49)	2:185:B:CYS:HG	4:403:A:PCW:C8	2	10.96
(1,16)	1:216:A:LYS:N	2:132:B:ASP:H	1	10.89
(1,22)	1:222:A:GLY:N	2:143:B:GLU:OE1	1	10.79
(1,45)	2:113:B:LEU:H	4:406:A:PCW:C8	2	10.72
(1,13)	1:213:A:THR:N	2:185:B:CYS:H	9	10.72
(1,12)	1:212:A:SER:N	2:185:B:CYS:H	9	10.51
(1,29)	4:406:A:PCW:C4	4:209:B:PCW:O2	4	10.4
(1,14)	1:214:A:PHE:N	2:132:B:ASP:OD1	9	10.32
(1,13)	1:213:A:THR:N	2:132:B:ASP:CB	1	10.29
(1,3)	1:203:A:LEU:N	2:132:B:ASP:OD1	1	10.21
(1,22)	1:222:A:GLY:N	2:132:B:ASP:OD1	9	10.14
(1,48)	2:160:B:VAL:H	4:402:A:PCW:C7	9	10.01
(1,18)	1:218:A:ARG:N	2:143:B:GLU:OE1	1	9.98
(1,47)	2:142:B:ILE:C	4:404:A:PCW:C7	5	9.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:206:A:ASN:N	2:132:B:ASP:OD1	1	9.8
(1,29)	4:406:A:PCW:C4	4:209:B:PCW:O2	7	9.76
(1,44)	2:79:B:LEU:CD2	4:402:A:PCW:C7	10	9.46
(1,1)	1:201:A:LEU:N	2:185:B:CYS:HG	10	9.24
(1,43)	2:46:B:ILE:CG2	4:402:A:PCW:C6	1	9.2
(1,33)	5:409:A:17F:O5	2:161:B:ARG:O	10	9.2
(1,2)	4:401:A:PCW:C4	2:185:B:CYS:HG	5	9.2
(1,22)	1:222:A:GLY:N	2:185:B:CYS:O	10	9.19
(1,14)	1:214:A:PHE:N	2:132:B:ASP:H	1	9.11
(1,10)	1:210:A:VAL:N	2:132:B:ASP:OD1	1	8.92
(1,2)	1:202:A:LYS:N	2:185:B:CYS:HG	10	8.81
(1,9)	1:209:A:SER:N	2:132:B:ASP:OD1	1	8.79
(1,21)	4:405:A:PCW:C7	4:208:B:PCW:C1	5	8.77
(1,18)	1:218:A:ARG:N	2:132:B:ASP:OD1	9	8.69
(1,44)	2:79:B:LEU:CD2	4:402:A:PCW:C8	9	8.67
(1,5)	1:205:A:ASP:N	2:132:B:ASP:OD1	1	8.47
(1,48)	2:160:B:VAL:N	4:402:A:PCW:C7	10	8.46
(1,21)	4:405:A:PCW:C8	4:208:B:PCW:C1	2	8.33
(1,48)	2:160:B:VAL:O	4:406:A:PCW:C8	2	8.31
(1,33)	5:409:A:17F:O5	2:161:B:ARG:O	9	8.16
(1,46)	2:133:B:LEU:O	4:403:A:PCW:C8	2	8.1
(1,21)	4:405:A:PCW:C7	4:208:B:PCW:C1	7	8.1
(1,12)	1:212:A:SER:N	2:132:B:ASP:OD1	1	8.04
(1,21)	4:405:A:PCW:C8	4:208:B:PCW:C1	9	8.02
(1,11)	1:211:A:THR:N	2:185:B:CYS:H	9	7.95
(1,7)	1:207:A:TRP:N	2:132:B:ASP:OD1	1	7.89
(1,21)	4:405:A:PCW:C4	4:208:B:PCW:C1	4	7.73
(1,4)	1:204:A:LEU:N	2:132:B:ASP:OD1	1	7.69
(1,29)	4:406:A:PCW:C4	4:211:B:PCW:C6	10	7.39
(1,21)	4:405:A:PCW:C7	4:208:B:PCW:C1	1	7.34
(1,32)	4:408:A:PCW:C7	2:47:B:ASP:OD1	9	7.33
(1,29)	4:406:A:PCW:C4	4:211:B:PCW:C8	1	7.06
(1,21)	4:405:A:PCW:C8	4:208:B:PCW:C1	6	6.98
(1,9)	1:209:A:SER:N	2:185:B:CYS:C	9	6.98
(1,3)	1:203:A:LEU:N	2:185:B:CYS:HG	10	6.9
(1,11)	1:211:A:THR:N	2:132:B:ASP:OD1	1	6.89
(1,48)	2:160:B:VAL:H	4:402:A:PCW:C7	1	6.71
(1,46)	2:133:B:LEU:C	4:402:A:PCW:C8	1	6.67
(1,8)	1:208:A:ASP:N	2:132:B:ASP:OD1	1	6.6
(1,10)	1:210:A:VAL:N	2:185:B:CYS:H	9	6.55
(1,44)	2:79:B:LEU:CD2	4:402:A:PCW:C7	1	6.21
(1,8)	1:208:A:ASP:N	2:185:B:CYS:C	9	6.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,49)	2:185:B:CYS:C	4:406:A:PCW:C4	8	5.92
(1,21)	4:405:A:PCW:C7	4:208:B:PCW:C1	3	5.8
(1,21)	4:405:A:PCW:C8	4:208:B:PCW:C1	8	5.75
(1,29)	4:406:A:PCW:C4	4:209:B:PCW:C4	3	5.54
(1,1)	1:201:A:LEU:N	2:185:B:CYS:O	9	5.41
(1,21)	4:405:A:PCW:C8	4:208:B:PCW:C1	10	5.4
(1,17)	1:217:A:LEU:N	2:185:B:CYS:C	10	4.95
(1,46)	2:133:B:LEU:CD1	5:409:A:17F:O4	5	4.88
(1,5)	1:205:A:ASP:N	2:185:B:CYS:O	9	4.85
(1,4)	1:204:A:LEU:N	2:185:B:CYS:HG	10	4.83
(1,46)	2:133:B:LEU:N	4:402:A:PCW:C4	9	4.73
(1,5)	1:205:A:ASP:N	2:185:B:CYS:HG	10	4.69
(1,49)	2:185:B:CYS:O	1:203:A:LEU:N	9	4.52
(1,16)	1:216:A:LYS:N	2:185:B:CYS:CB	10	4.52
(1,45)	2:113:B:LEU:O	4:402:A:PCW:C8	9	4.41
(1,6)	1:206:A:ASN:N	2:185:B:CYS:HG	10	4.19
(1,18)	1:218:A:ARG:N	2:185:B:CYS:C	10	4.17
(1,41)	4:209:B:PCW:O2	4:403:A:PCW:C8	2	4.13
(1,19)	4:403:A:PCW:C8	4:209:B:PCW:O2	2	4.13
(1,33)	5:409:A:17F:O5	2:161:B:ARG:O	1	4.08
(1,2)	1:202:A:LYS:N	2:185:B:CYS:O	9	3.9
(1,15)	4:402:A:PCW:C6	4:210:B:PCW:C4	4	3.64
(1,6)	1:206:A:ASN:N	2:185:B:CYS:O	9	3.62
(1,20)	4:404:A:PCW:C5	4:210:B:PCW:O2	3	3.57
(1,45)	2:113:B:LEU:H	4:402:A:PCW:C7	10	3.51
(1,42)	4:210:B:PCW:C8	4:404:A:PCW:C8	4	3.49
(1,46)	2:133:B:LEU:C	4:402:A:PCW:C8	10	3.46
(1,20)	4:404:A:PCW:C8	4:210:B:PCW:C8	6	3.3
(1,7)	1:207:A:TRP:N	2:185:B:CYS:C	9	3.28
(1,4)	1:204:A:LEU:N	2:185:B:CYS:O	9	3.13
(1,29)	4:406:A:PCW:C4	2:185:B:CYS:C	8	2.92
(1,15)	4:402:A:PCW:C5	4:210:B:PCW:C4	5	2.88
(1,42)	4:210:B:PCW:C6	4:402:A:PCW:C6	6	2.8
(1,15)	4:402:A:PCW:C6	4:210:B:PCW:C6	6	2.8
(1,47)	2:142:B:ILE:CD1	4:402:A:PCW:C6	10	2.73
(1,20)	4:404:A:PCW:C8	4:211:B:PCW:C1	2	2.72
(1,49)	2:185:B:CYS:HG	5:410:A:17F:O6	5	2.68
(1,13)	1:213:A:THR:N	2:185:B:CYS:HG	10	2.52
(1,42)	4:210:B:PCW:C4	4:402:A:PCW:C8	2	2.38
(1,15)	4:402:A:PCW:C8	4:210:B:PCW:C4	2	2.38
(1,42)	4:210:B:PCW:C4	4:402:A:PCW:C8	8	2.3
(1,15)	4:402:A:PCW:C8	4:210:B:PCW:C4	8	2.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	2:113:B:LEU:O	4:402:A:PCW:C8	1	2.18
(1,33)	5:409:A:17F:O5	2:132:B:ASP:OD2	5	2.09
(1,20)	4:404:A:PCW:C8	4:211:B:PCW:C1	4	2.06
(1,47)	2:142:B:ILE:CD1	4:402:A:PCW:C7	9	1.97
(1,20)	4:404:A:PCW:C8	4:210:B:PCW:C8	7	1.87
(1,42)	4:210:B:PCW:C7	4:402:A:PCW:C6	3	1.85
(1,15)	4:402:A:PCW:C6	4:210:B:PCW:C7	3	1.85
(1,42)	4:210:B:PCW:C8	4:404:A:PCW:C5	5	1.81
(1,20)	4:404:A:PCW:C5	4:210:B:PCW:C8	5	1.81
(1,9)	1:209:A:SER:N	2:185:B:CYS:HG	10	1.7
(1,49)	2:185:B:CYS:HG	1:211:A:THR:N	10	1.65
(1,7)	1:207:A:TRP:N	2:185:B:CYS:HG	10	1.64
(1,3)	1:203:A:LEU:N	2:185:B:CYS:O	9	1.52
(1,29)	4:406:A:PCW:C4	4:211:B:PCW:C6	6	1.48
(1,41)	4:209:B:PCW:O2	4:403:A:PCW:C8	9	1.44
(1,14)	1:214:A:PHE:N	2:185:B:CYS:CB	10	1.42
(1,41)	4:209:B:PCW:O2	4:403:A:PCW:C6	5	1.39
(1,19)	4:403:A:PCW:C6	4:209:B:PCW:O2	5	1.39
(1,41)	4:209:B:PCW:O2	4:403:A:PCW:C8	4	1.37
(1,19)	4:403:A:PCW:C8	4:209:B:PCW:O2	4	1.37
(1,20)	4:404:A:PCW:C8	4:211:B:PCW:C1	8	1.19
(1,20)	4:404:A:PCW:C8	2:143:B:GLU:OE2	10	1.05
(1,29)	4:406:A:PCW:C4	4:211:B:PCW:C6	9	1.02
(1,41)	4:209:B:PCW:O2	4:403:A:PCW:C5	10	1.01
(1,19)	4:403:A:PCW:C5	4:209:B:PCW:O2	10	1.01
(1,42)	4:210:B:PCW:C7	4:404:A:PCW:C6	1	0.99
(1,20)	4:404:A:PCW:C6	4:210:B:PCW:C7	1	0.99
(1,41)	4:209:B:PCW:O2	4:403:A:PCW:C5	8	0.95
(1,19)	4:403:A:PCW:C5	4:209:B:PCW:O2	8	0.95
(1,41)	4:209:B:PCW:O2	4:403:A:PCW:C5	6	0.92
(1,10)	1:210:A:VAL:N	2:185:B:CYS:HG	10	0.84
(1,29)	4:406:A:PCW:C4	4:211:B:PCW:C8	2	0.73
(1,42)	4:210:B:PCW:C4	4:402:A:PCW:C6	7	0.67
(1,15)	4:402:A:PCW:C6	4:210:B:PCW:C4	7	0.67
(1,12)	1:212:A:SER:N	2:185:B:CYS:HG	10	0.67
(1,42)	4:210:B:PCW:C6	4:402:A:PCW:C6	10	0.6
(1,19)	4:403:A:PCW:C4	4:211:B:PCW:C8	6	0.5
(1,41)	4:209:B:PCW:O2	4:403:A:PCW:C8	1	0.46
(1,19)	4:403:A:PCW:C8	4:209:B:PCW:O2	1	0.46
(1,8)	1:208:A:ASP:N	2:185:B:CYS:HG	10	0.44

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found