



Full wwPDB NMR Structure Validation Report ⓘ

Mar 27, 2026 – 07:10 PM UTC

PDB ID : 7RSE / pdb_00007rse
BMRB ID : 30734
Title : NMR-driven structure of the KRAS4B-G12D "alpha-beta" dimer on a lipid bilayer nanodisc
Authors : Lee, K.; Enomoto, M.; Gebregiworgis, T.; Gasmi-Seabrook, G.M.; Ikura, M.; Marshall, C.B.
Deposited on : 2021-08-11

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

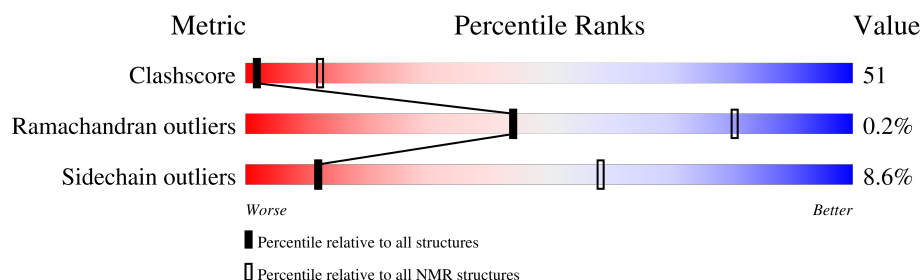
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 1%.

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	185	83% 10% 6% .
1	B	185	78% 10% 11% .
2	D	200	86% 8% 6%
2	E	200	82% 11% 6%

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:2-A:173, B:2-B:28, B:35-B:169 (334)	1.45	20
2	D:255-D:441, E:555-E:741 (374)	0.40	1

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 2 single-model clusters were found.

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

3 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14322 atoms, of which 1540 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called GTPase KRas.

Mol	Chain	Residues	Atoms						Trace
1	A	183	Total	C	H	N	O	S	0
			1822	917	356	255	287	7	
1	B	183	Total	C	H	N	O	S	0
			1822	917	356	255	287	7	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P01116
A	12	ASP	GLY	engineered mutation	UNP P01116
B	1	SER	-	expression tag	UNP P01116
B	12	ASP	GLY	engineered mutation	UNP P01116

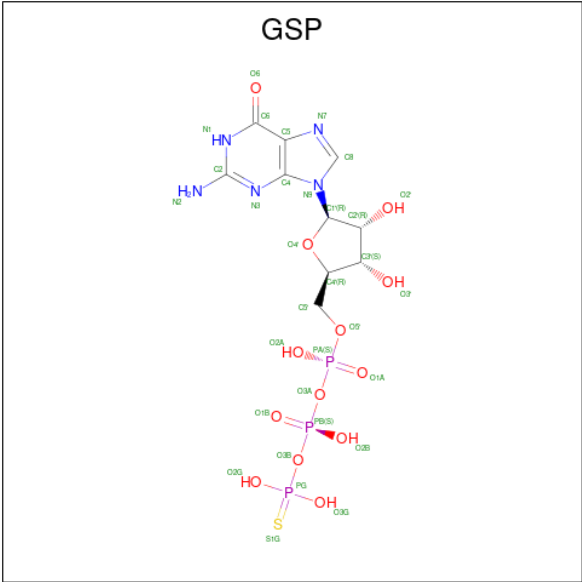
- Molecule 2 is a protein called Apolipoprotein A-I.

Mol	Chain	Residues	Atoms						Trace
2	D	187	Total	C	H	N	O	S	0
			1892	960	360	273	296	3	
2	E	187	Total	C	H	N	O	S	0
			1892	960	360	273	296	3	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	242	GLY	-	expression tag	UNP P02647
D	243	PRO	-	expression tag	UNP P02647
E	542	GLY	-	expression tag	UNP P02647
E	543	PRO	-	expression tag	UNP P02647

- Molecule 3 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S) (labeled as "Ligand of Interest" by depositor).

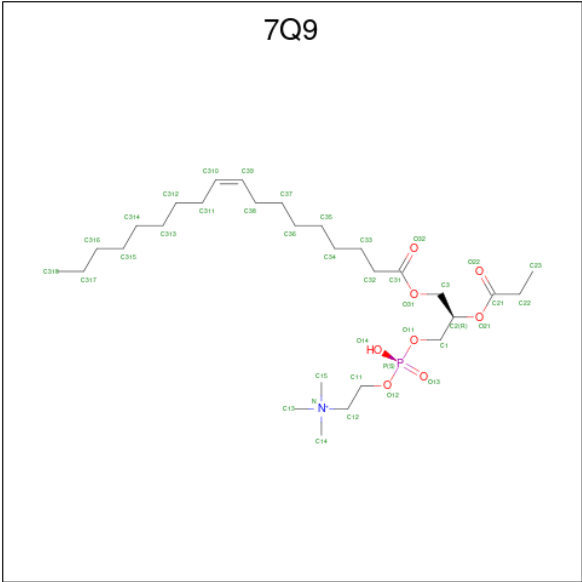


Mol	Chain	Residues	Atoms						
			Total	C	H	N	O	P	S
3	A	1	38	10	6	5	13	3	1
3	B	1	38	10	6	5	13	3	1

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	
			Total	Mg
4	A	1	1	1
4	B	1	1	1

- Molecule 5 is [(2 {R})-3-[oxidanyl-2-(trimethyl- $\text{S}^{\{4\}}$ -azanyl)ethoxy]phosphoryl]oxy-2-propanoyloxy-propyl] ({Z})-octadec-9-enoate (CCD ID: 7Q9) (formula: $\text{C}_{29}\text{H}_{57}\text{NO}_8\text{P}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	A	1	Total	C	N	O	P
			39	29	1	8	1
5	B	1	Total	C	N	O	P
			39	29	1	8	1

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
5	B	1	39	29	1	8	1
5	B	1	39	29	1	8	1
5	B	1	39	29	1	8	1
5	B	1	39	29	1	8	1
5	B	1	39	29	1	8	1
5	B	1	39	29	1	8	1
5	B	1	39	29	1	8	1
5	B	1	39	29	1	8	1
5	B	1	39	29	1	8	1
5	B	1	39	29	1	8	1
5	B	1	39	29	1	8	1
5	B	1	39	29	1	8	1
5	B	1	39	29	1	8	1
5	B	1	39	29	1	8	1
5	D	1	39	29	1	8	1
5	D	1	39	29	1	8	1
5	D	1	39	29	1	8	1
5	D	1	39	29	1	8	1
5	D	1	39	29	1	8	1
5	D	1	39	29	1	8	1
5	D	1	39	29	1	8	1
5	D	1	39	29	1	8	1

Continued on next page...

Continued from previous page...

[illegible]

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
5	D	1	39	29	1	8	1
5	D	1	39	29	1	8	1
5	D	1	39	29	1	8	1
5	D	1	39	29	1	8	1
5	D	1	39	29	1	8	1
5	D	1	39	29	1	8	1
5	D	1	39	29	1	8	1
5	D	1	39	29	1	8	1
5	D	1	39	29	1	8	1
5	D	1	39	29	1	8	1
5	D	1	39	29	1	8	1
5	E	1	39	29	1	8	1
5	E	1	39	29	1	8	1
5	E	1	39	29	1	8	1
5	E	1	39	29	1	8	1
5	E	1	39	29	1	8	1
5	E	1	39	29	1	8	1
5	E	1	39	29	1	8	1
5	E	1	39	29	1	8	1
5	E	1	39	29	1	8	1
5	E	1	39	29	1	8	1
5	E	1	39	29	1	8	1
5	E	1	39	29	1	8	1

Continued on next page...

Continued from previous page...

[illegible]

Continued on next page...

Continued from previous page...

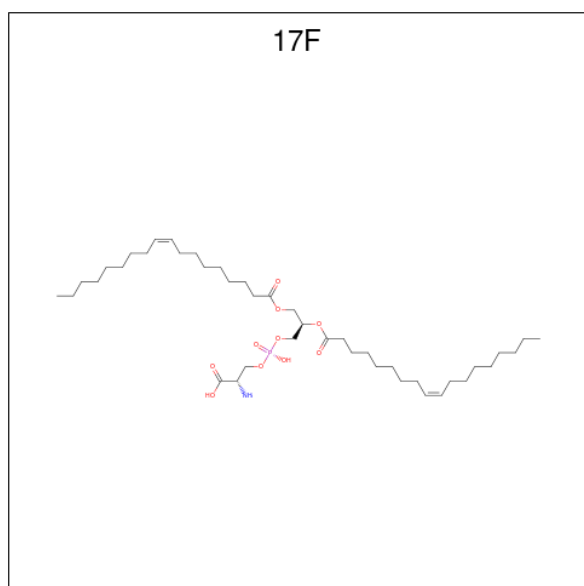
[illegible]

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1
5	E	1	Total	C	N	O	P
			39	29	1	8	1

- Molecule 6 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propyl}oxy)(hydroxy)phosphoryl]-L-serine (CCD ID: 17F) (formula: C₄₂H₇₈NO₁₀P) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

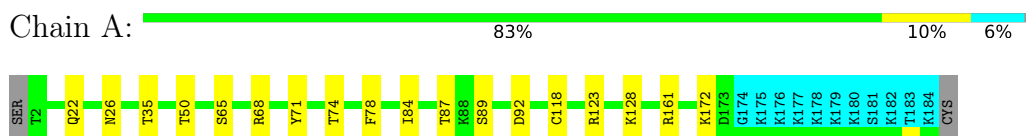
Mol	Chain	Residues	Atoms					
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1
6	E	1	Total	C	H	N	O	P
			57	42	3	1	10	1

4 Residue-property plots [i](#)

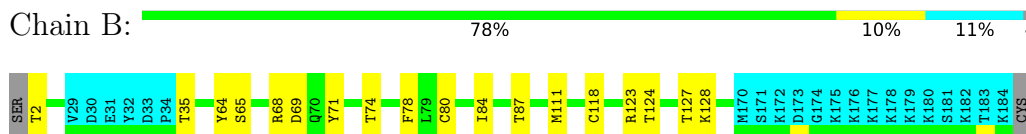
4.1 Average score per residue in the NMR ensemble

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.

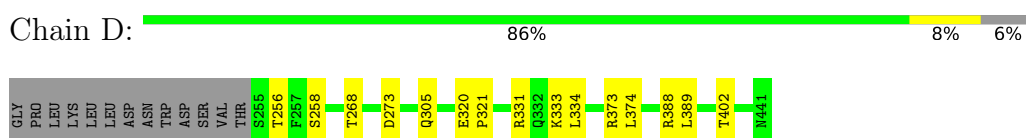
- Molecule 1: GTPase KRas



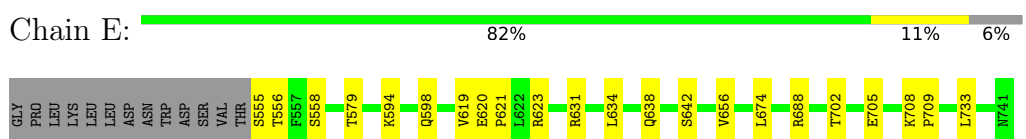
- Molecule 1: GTPase KRas



- Molecule 2: Apolipoprotein A-I



- Molecule 2: Apolipoprotein A-I

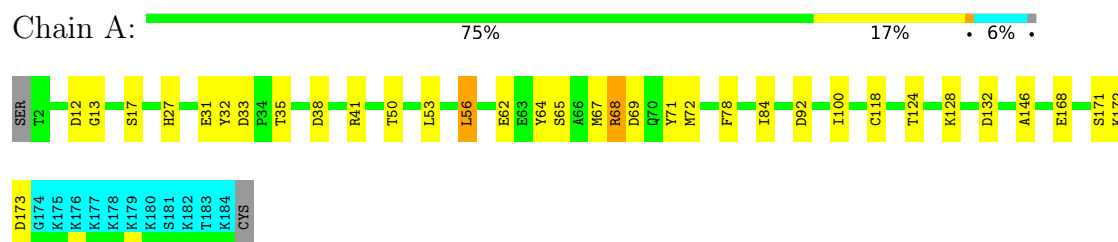


4.2 Scores per residue for each member of the ensemble

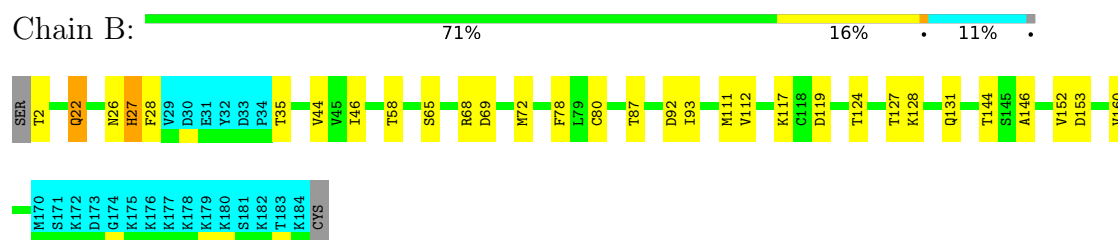
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

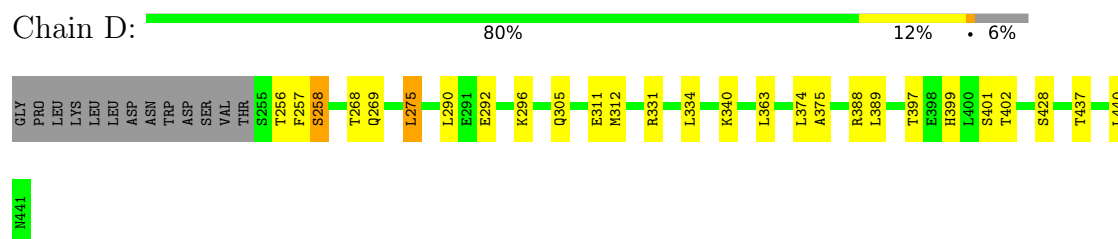
- Molecule 1: GTPase KRas



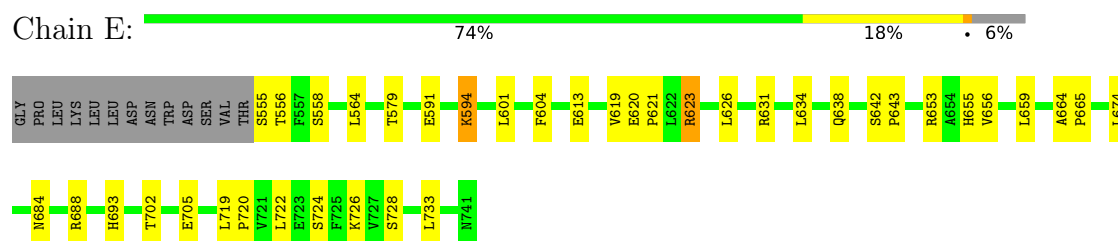
- Molecule 1: GTPase KRas



- Molecule 2: Apolipoprotein A-I

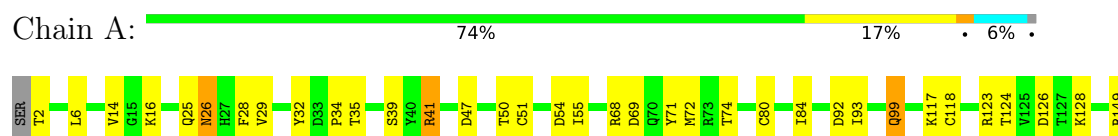


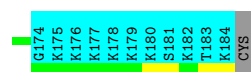
- Molecule 2: Apolipoprotein A-I



4.2.2 Score per residue for model 2

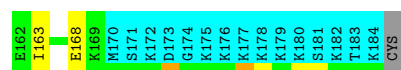
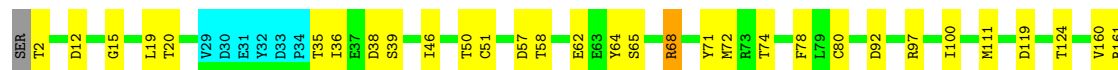
- Molecule 1: GTPase KRas





• Molecule 1: GTPase KRas

Chain B: 70% 17% 11%



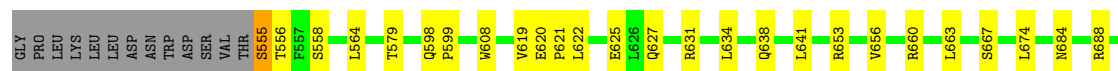
• Molecule 2: Apolipoprotein A-I

Chain D: 80% 14% 6%



• Molecule 2: Apolipoprotein A-I

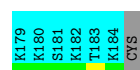
Chain E: 76% 17% 6%



4.2.3 Score per residue for model 3

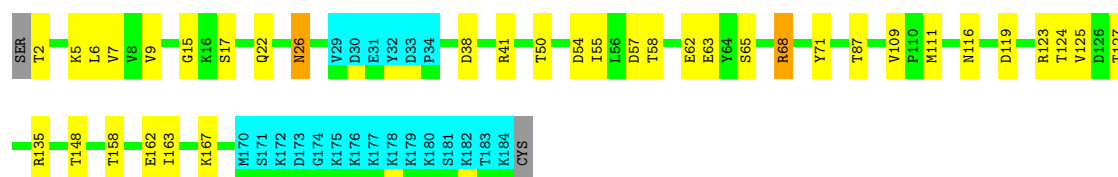
• Molecule 1: GTPase KRas

Chain A: 77% 15% 6%



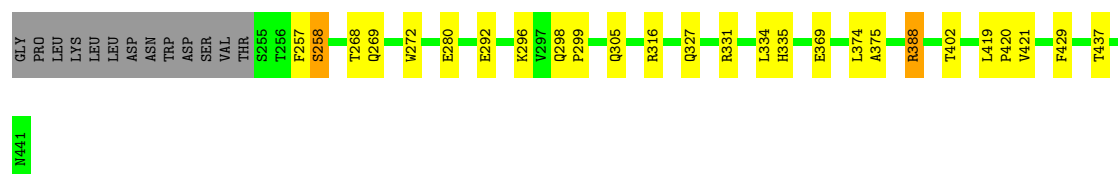
• Molecule 1: GTPase KRas

Chain B: 68% 18% 11%



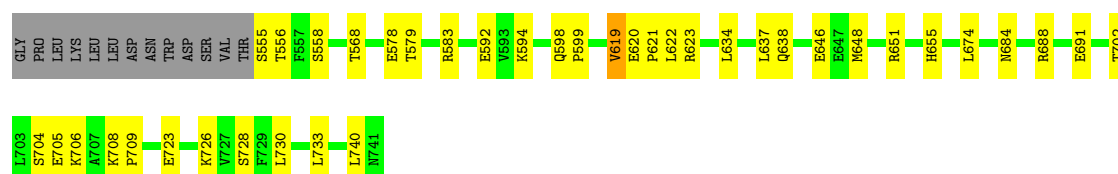
- Molecule 2: Apolipoprotein A-I

Chain D: 80% 12% 6%



- Molecule 2: Apolipoprotein A-I

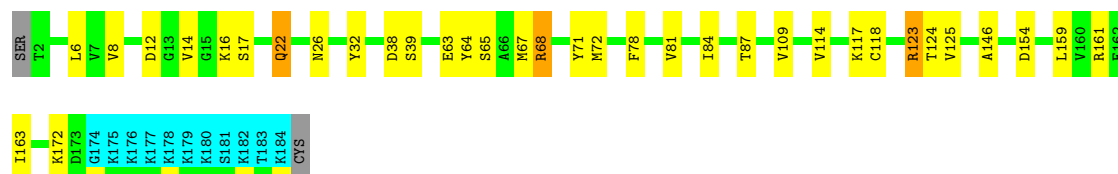
Chain E: 74% 19% 6%



4.2.4 Score per residue for model 4

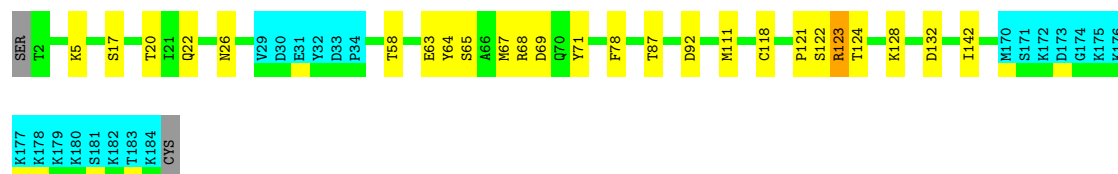
- Molecule 1: GTPase KRas

Chain A: 74% 17% 6%



- Molecule 1: GTPase KRas

Chain B: 74% 13% 11%



- Molecule 2: Apolipoprotein A-I

Chain D:  78% 15% 6%



- Molecule 2: Apolipoprotein A-I

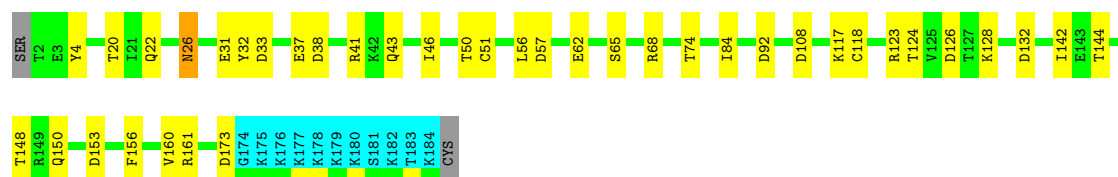
Chain E:  80% 14% 6%



4.2.5 Score per residue for model 5

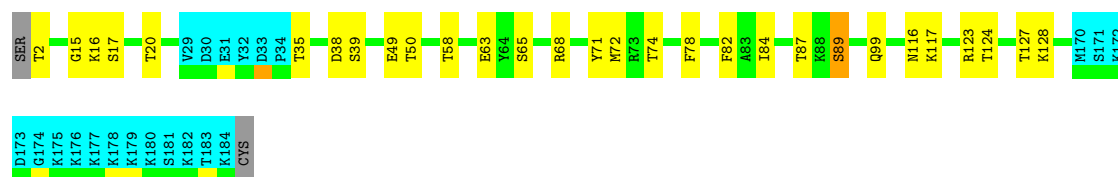
- Molecule 1: GTPase KRas

Chain A:  72% 21% 6%



- Molecule 1: GTPase KRas

Chain B:  72% 15% 11%



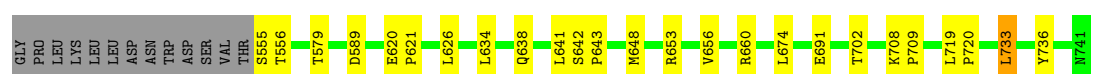
- Molecule 2: Apolipoprotein A-I

Chain D:  80% 14% 6%



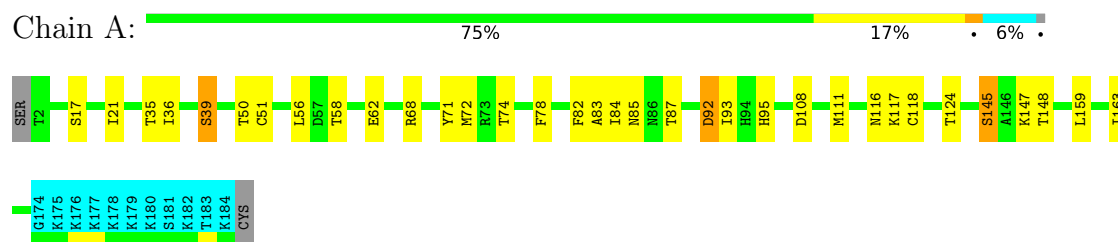
- Molecule 2: Apolipoprotein A-I

Chain E:  81% 12% 6%

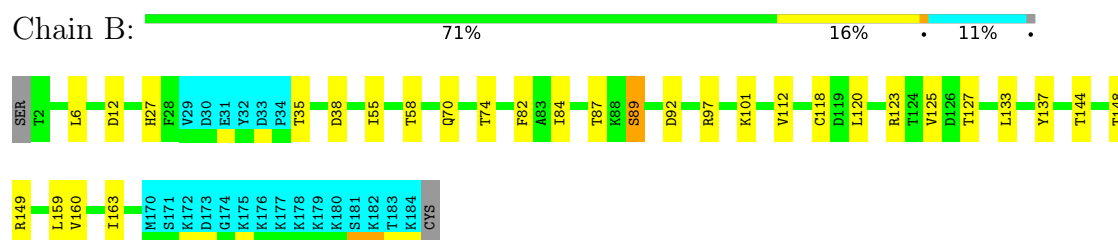


4.2.6 Score per residue for model 6

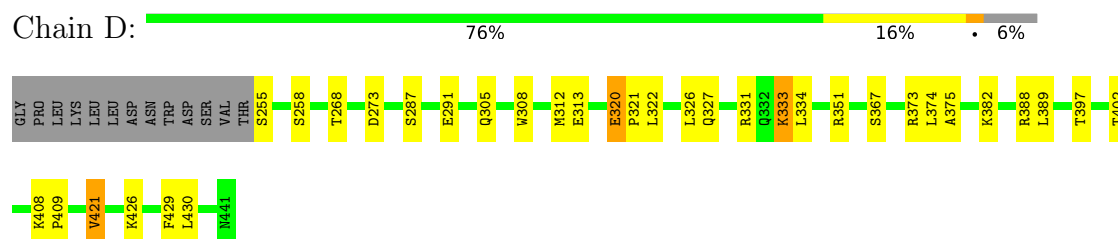
- Molecule 1: GTPase KRas



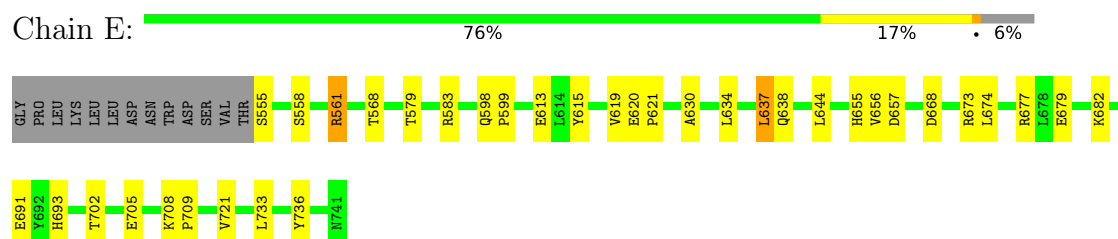
- Molecule 1: GTPase KRas



- Molecule 2: Apolipoprotein A-I

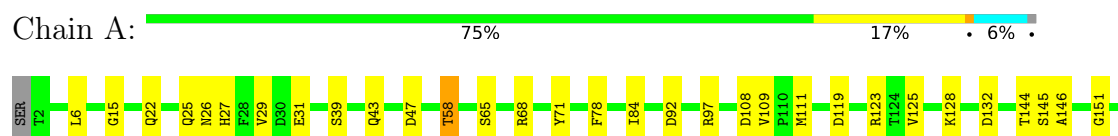


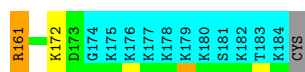
- Molecule 2: Apolipoprotein A-I



4.2.7 Score per residue for model 7

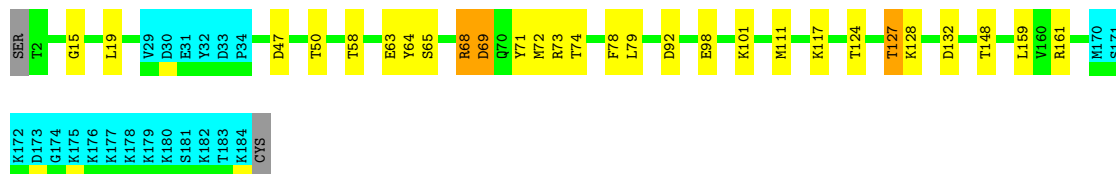
- Molecule 1: GTPase KRas





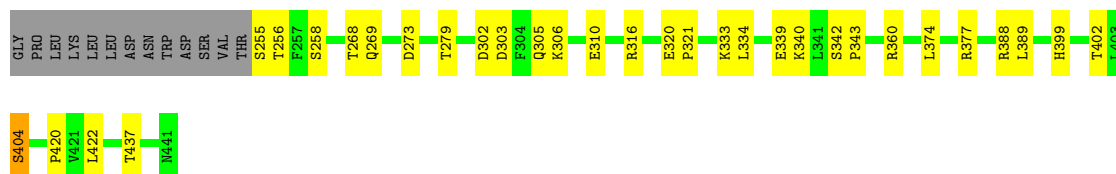
• Molecule 1: GTPase KRas

Chain B: 72% 14% 11%



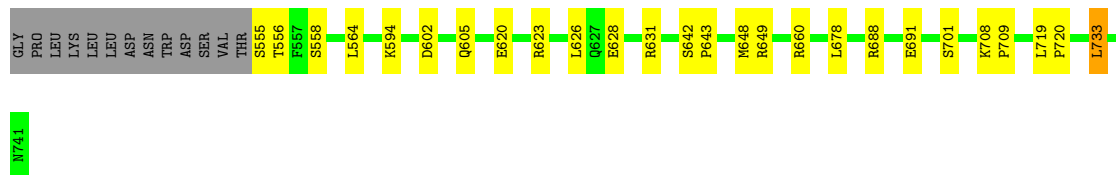
• Molecule 2: Apolipoprotein A-I

Chain D: 78% 16% 6%



• Molecule 2: Apolipoprotein A-I

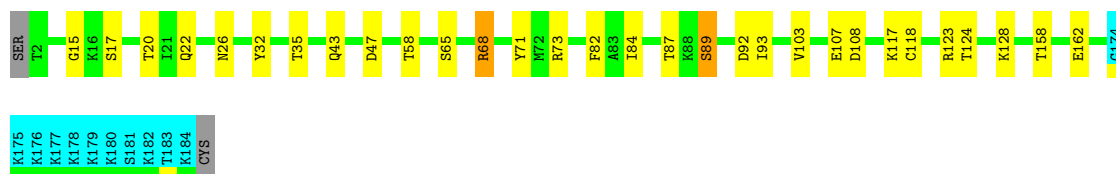
Chain E: 80% 12% 6%



4.2.8 Score per residue for model 8

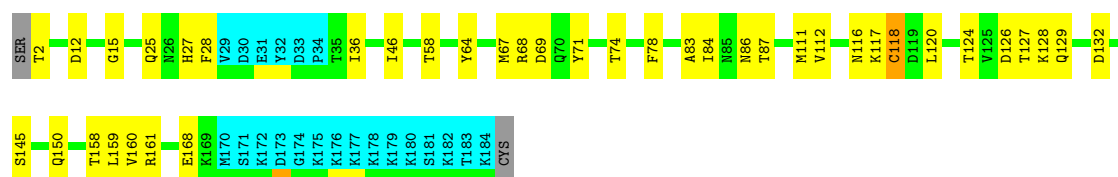
• Molecule 1: GTPase KRas

Chain A: 77% 15% 6%



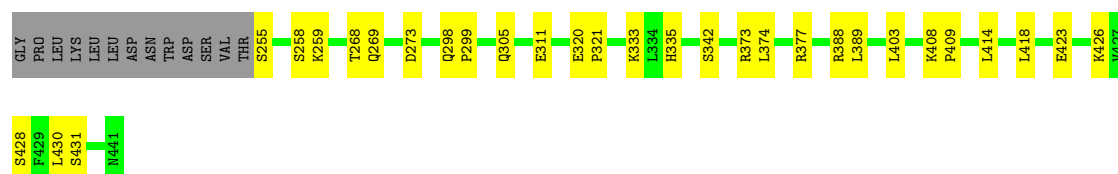
• Molecule 1: GTPase KRas

Chain B: 66% 21% 11%



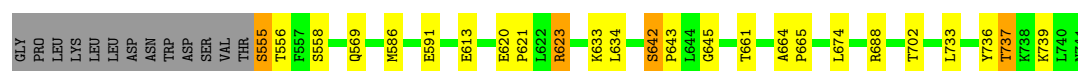
- Molecule 2: Apolipoprotein A-I

Chain D: 78% 15% 6%



- Molecule 2: Apolipoprotein A-I

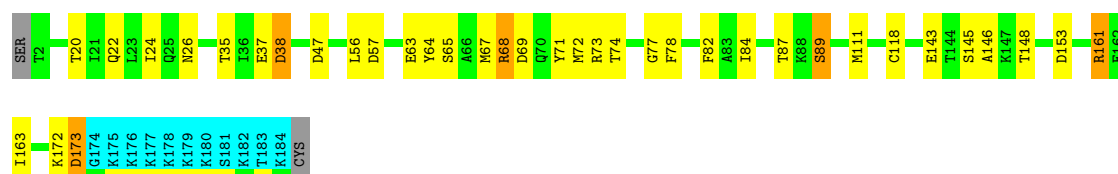
Chain E: 81% 10% 6%



4.2.9 Score per residue for model 9

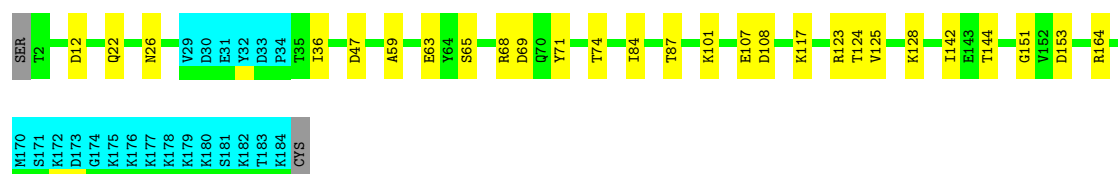
- Molecule 1: GTPase KRas

Chain A: 73% 17% 6%



- Molecule 1: GTPase KRas

Chain B: 73% 15% 11%



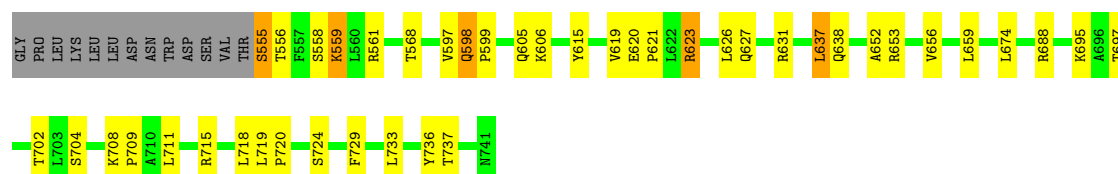
- Molecule 2: Apolipoprotein A-I

Chain D: 76% 16% 6%



• Molecule 2: Apolipoprotein A-I

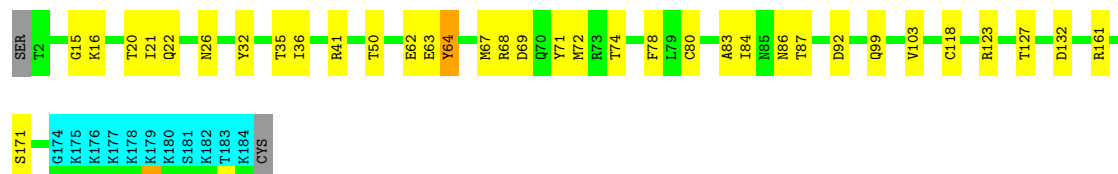
Chain E: 72% 19% 6%



4.2.10 Score per residue for model 10

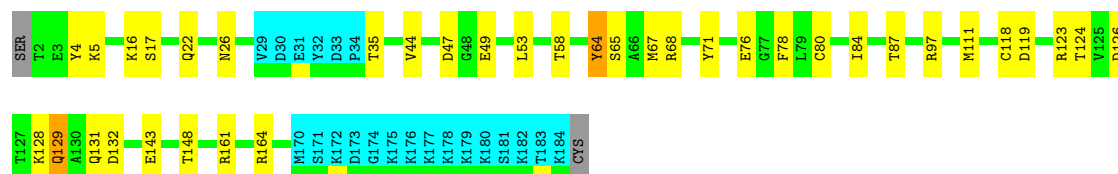
• Molecule 1: GTPase KRas

Chain A: 74% 18% 6%



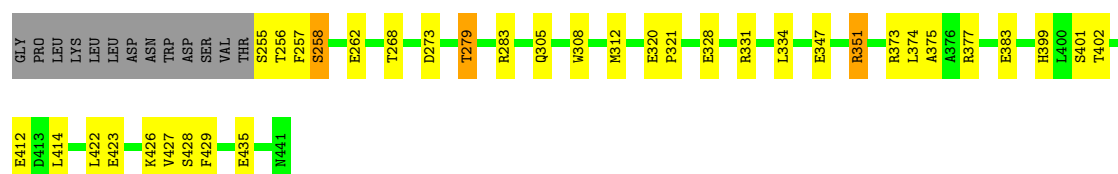
• Molecule 1: GTPase KRas

Chain B: 68% 19% 11%

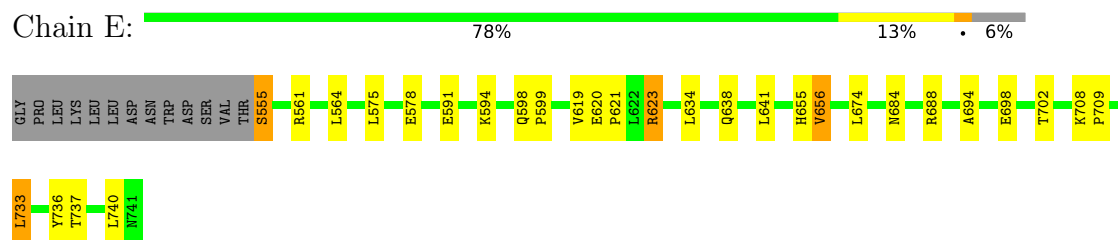


• Molecule 2: Apolipoprotein A-I

Chain D: 76% 16% 6%

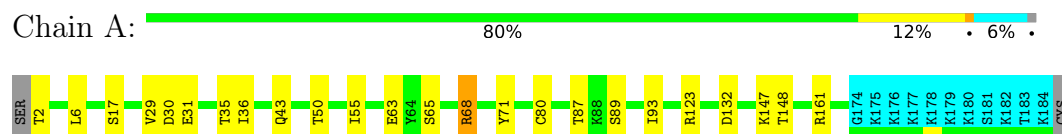


• Molecule 2: Apolipoprotein A-I

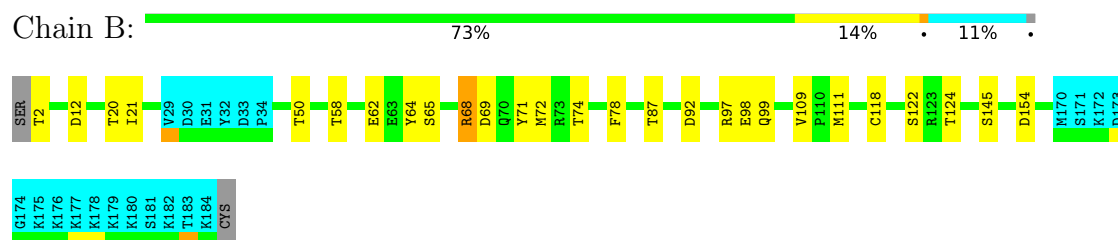


4.2.11 Score per residue for model 11

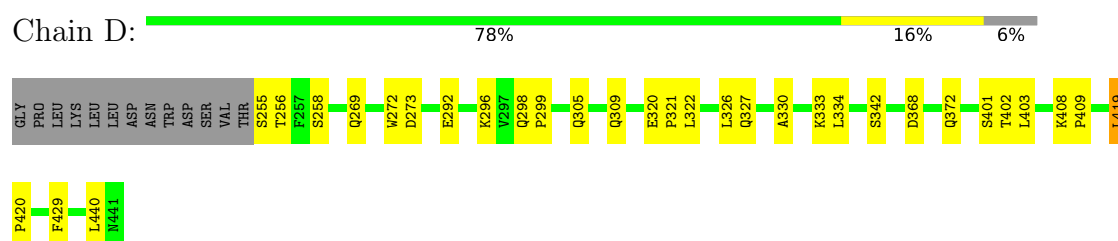
- Molecule 1: GTPase KRas



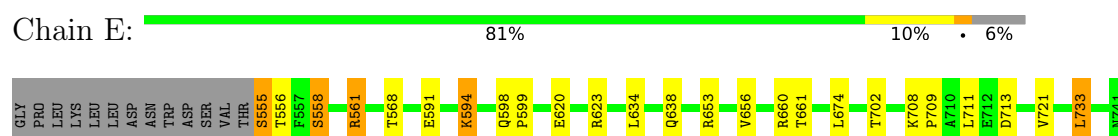
- Molecule 1: GTPase KRas



- Molecule 2: Apolipoprotein A-I

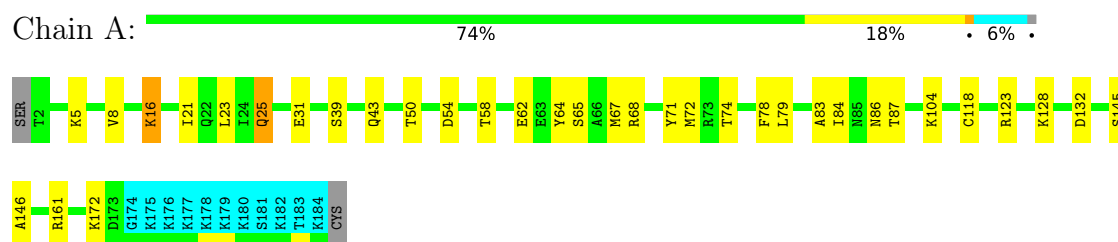


- Molecule 2: Apolipoprotein A-I

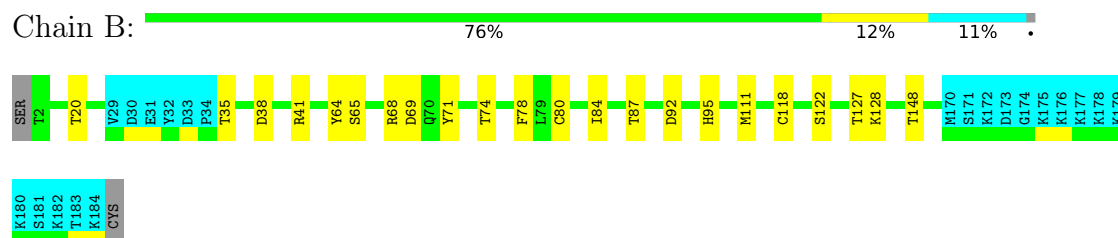


4.2.12 Score per residue for model 12

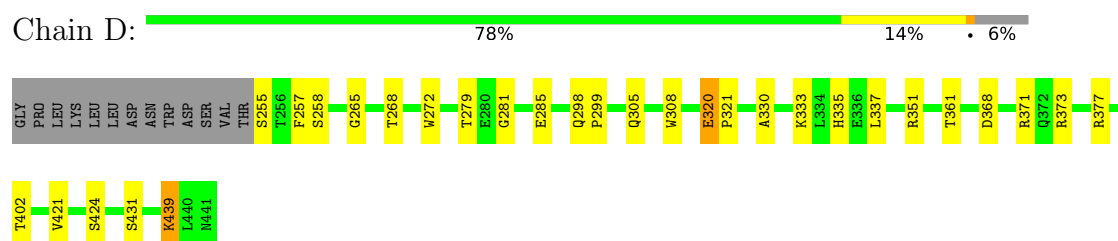
- Molecule 1: GTPase KRas



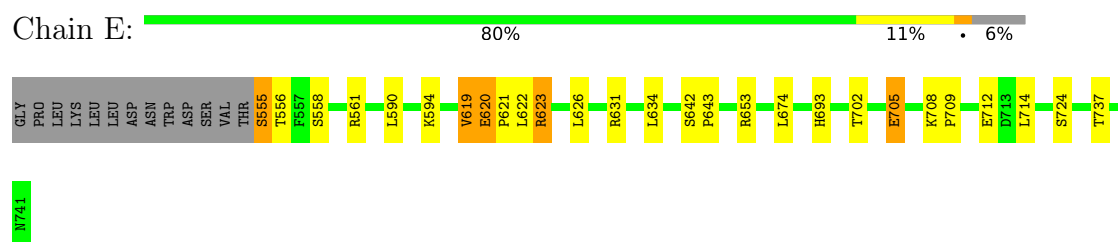
- Molecule 1: GTPase KRas



- Molecule 2: Apolipoprotein A-I

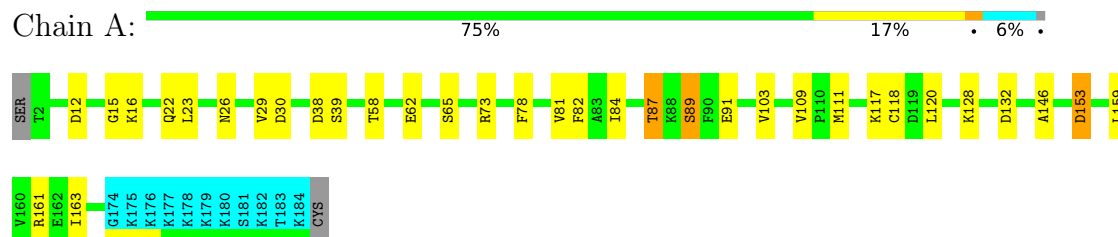


- Molecule 2: Apolipoprotein A-I

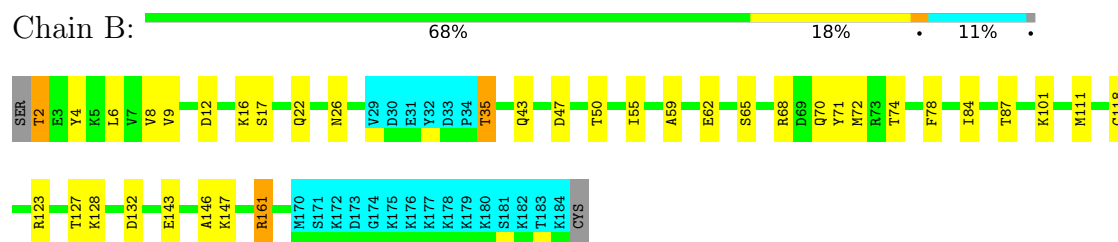


4.2.13 Score per residue for model 13

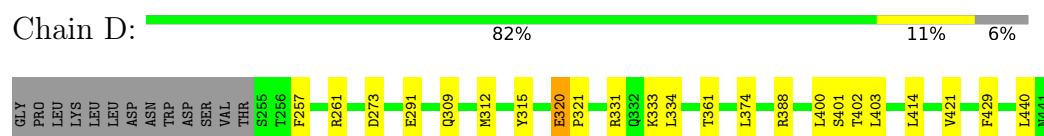
- Molecule 1: GTPase KRas



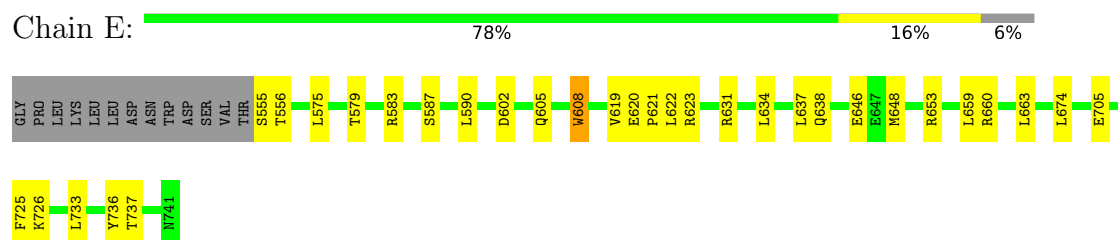
- Molecule 1: GTPase KRas



- Molecule 2: Apolipoprotein A-I

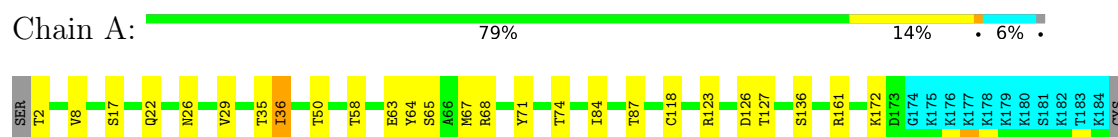


- Molecule 2: Apolipoprotein A-I

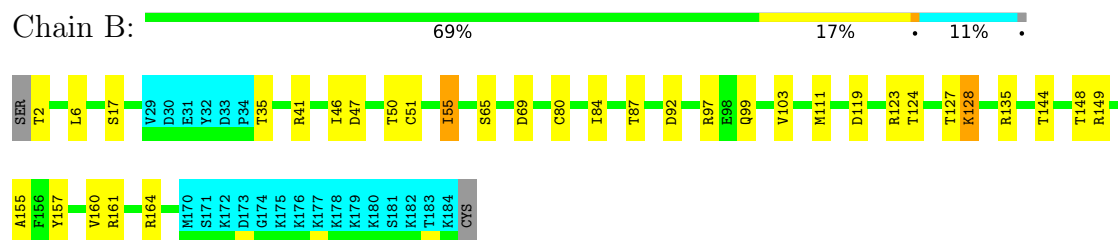


4.2.14 Score per residue for model 14

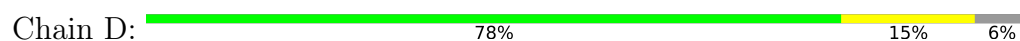
- Molecule 1: GTPase KRas



- Molecule 1: GTPase KRas



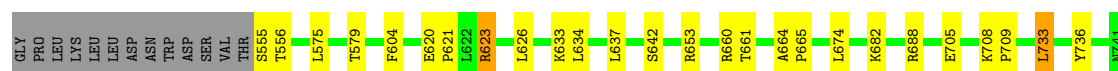
- Molecule 2: Apolipoprotein A-I





- Molecule 2: Apolipoprotein A-I

Chain E: 80% 12% 6%



4.2.15 Score per residue for model 15

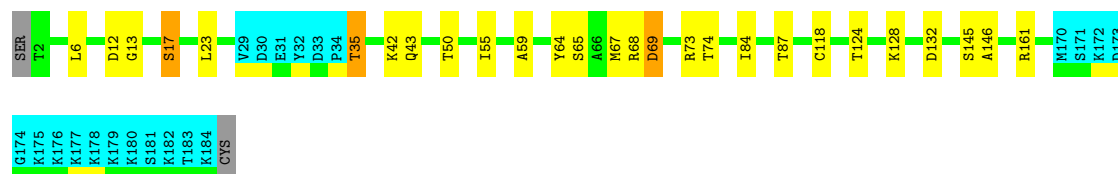
- Molecule 1: GTPase KRas

Chain A: 75% 17% 6%



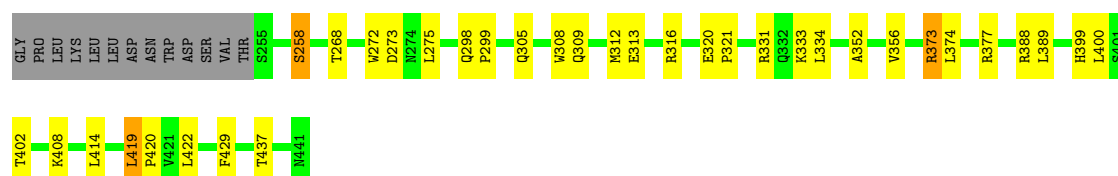
- Molecule 1: GTPase KRas

Chain B: 73% 13% 11%



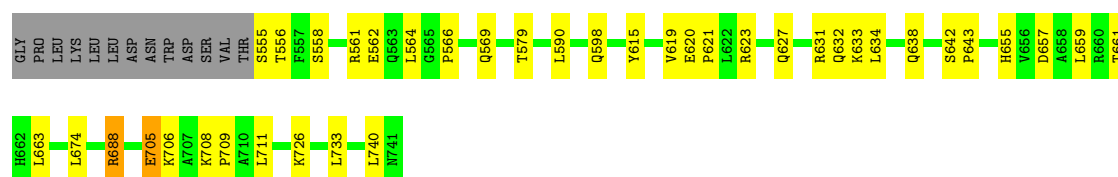
- Molecule 2: Apolipoprotein A-I

Chain D: 76% 16% 6%



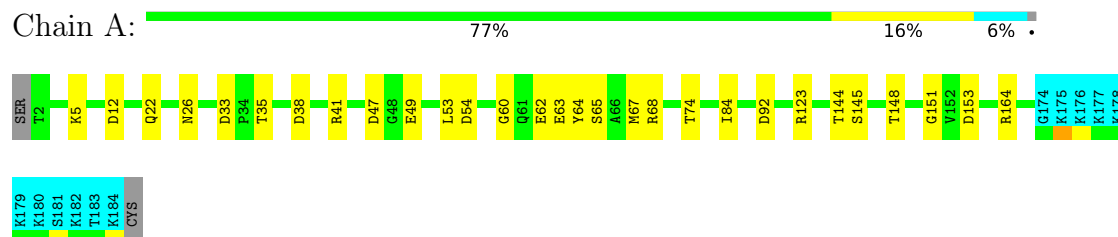
- Molecule 2: Apolipoprotein A-I

Chain E: 74% 18% 6%

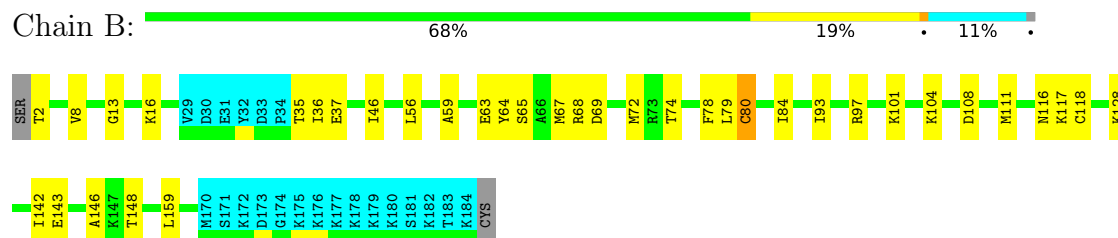


4.2.16 Score per residue for model 16

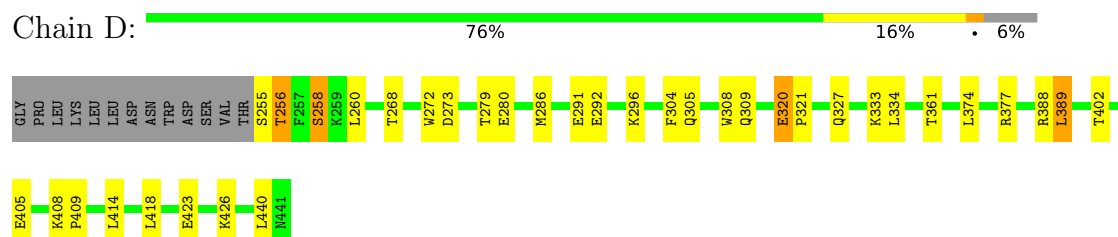
- Molecule 1: GTPase KRas



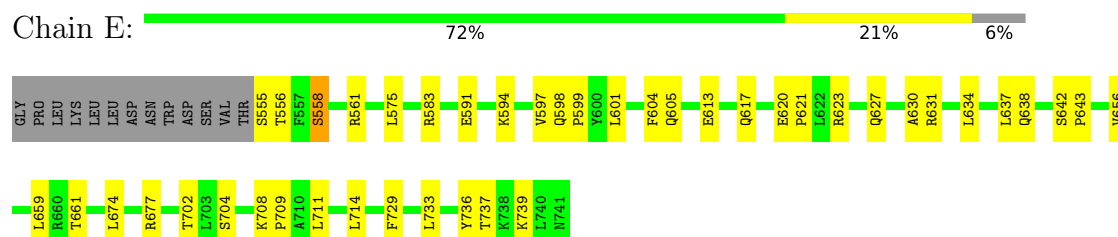
- Molecule 1: GTPase KRas



- Molecule 2: Apolipoprotein A-I

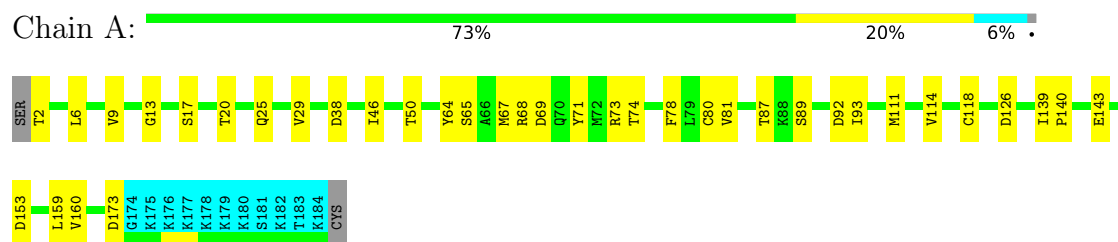


- Molecule 2: Apolipoprotein A-I

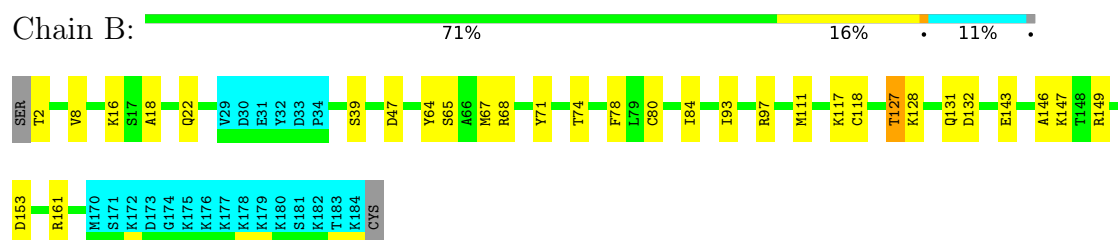


4.2.17 Score per residue for model 17

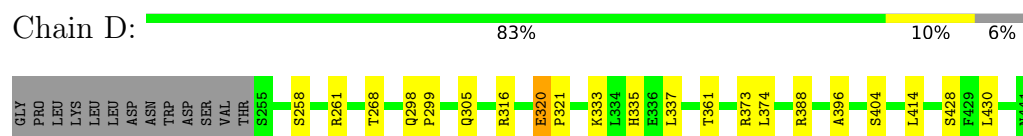
- Molecule 1: GTPase KRas



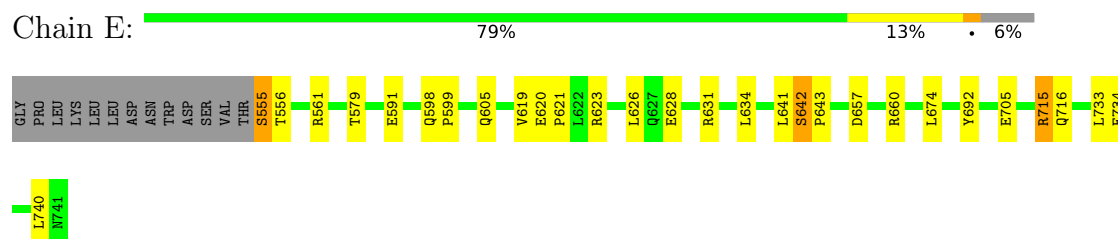
- Molecule 1: GTPase KRas



- Molecule 2: Apolipoprotein A-I

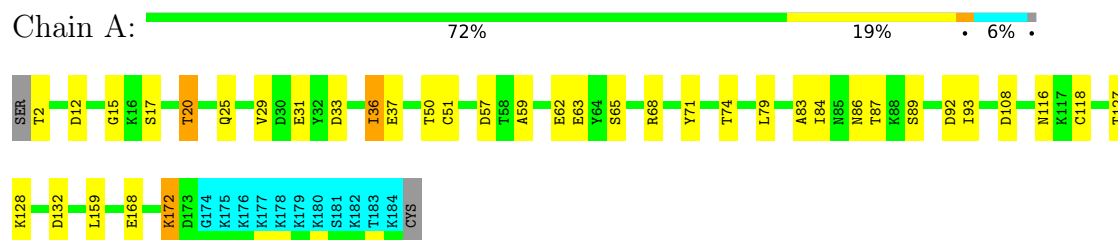


- Molecule 2: Apolipoprotein A-I

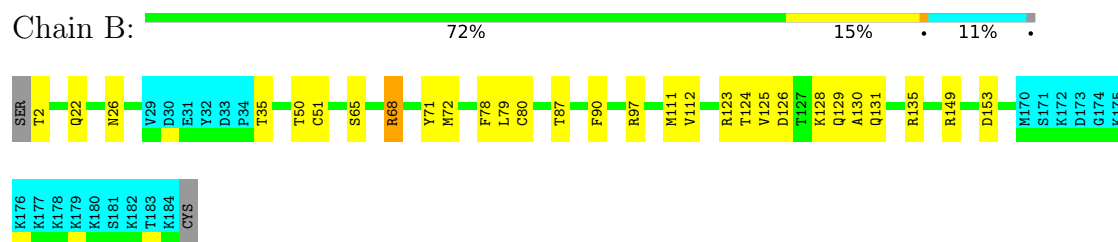


4.2.18 Score per residue for model 18

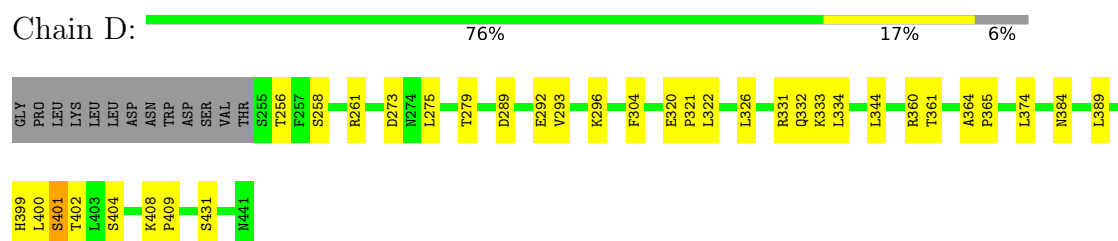
- Molecule 1: GTPase KRas



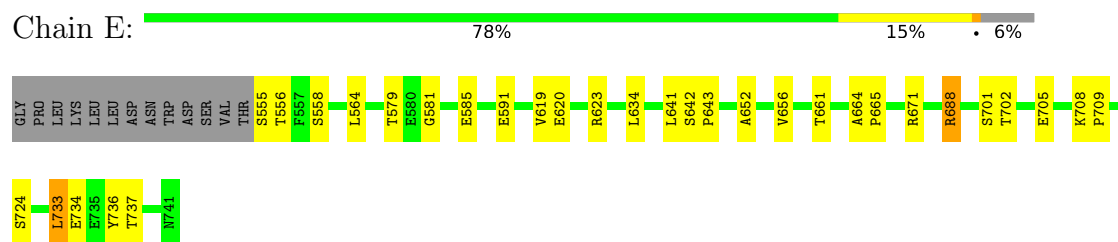
- Molecule 1: GTPase KRas



- Molecule 2: Apolipoprotein A-I

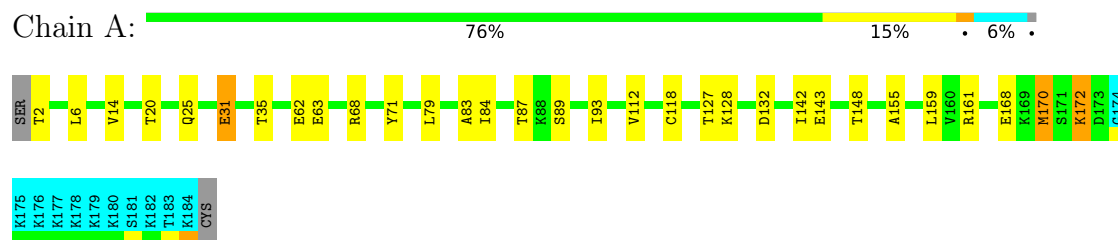


- Molecule 2: Apolipoprotein A-I

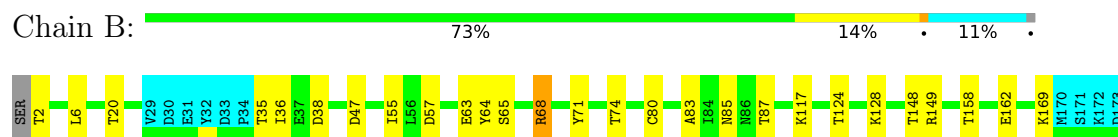


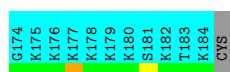
4.2.19 Score per residue for model 19

- Molecule 1: GTPase KRas



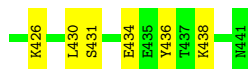
- Molecule 1: GTPase KRas





• Molecule 2: Apolipoprotein A-I

Chain D: 77% 16% 6%



• Molecule 2: Apolipoprotein A-I

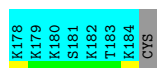
Chain E: 78% 15% 6%



4.2.20 Score per residue for model 20

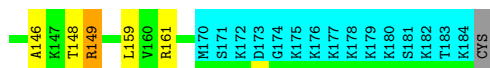
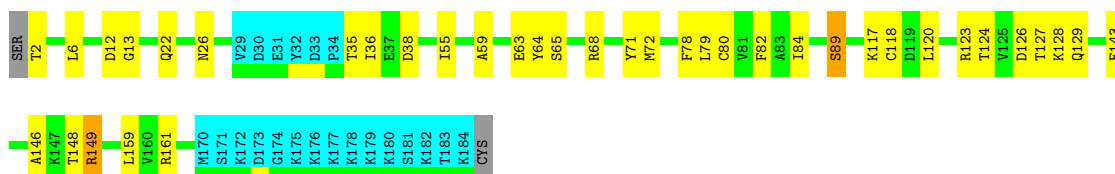
• Molecule 1: GTPase KRas

Chain A: 77% 15% 6%



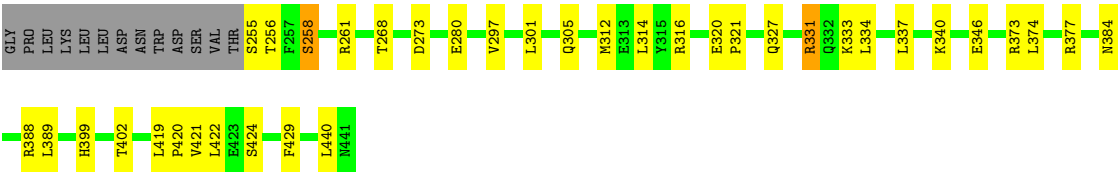
• Molecule 1: GTPase KRas

Chain B: 67% 19% 11%



• Molecule 2: Apolipoprotein A-I

Chain D: 75% 18% 6%



• Molecule 2: Apolipoprotein A-I



5 Refinement protocol and experimental data overview

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

Of the 1000 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
HADDOCK	refinement	
HADDOCK	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	154
Number of shifts mapped to atoms	61
Number of unparsed shifts	0
Number of shifts with mapping errors	93
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	1%

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: 7Q9, MG, 17F, GSP

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	0.35±0.01	0±0/1399 (0.0± 0.0%)	0.72±0.01	0±0/1887 (0.0± 0.0%)
1	B	0.35±0.01	0±0/1315 (0.0± 0.0%)	0.71±0.01	0±0/1773 (0.0± 0.0%)
2	D	0.37±0.00	0±0/1557 (0.0± 0.0%)	0.74±0.01	0±0/2090 (0.0± 0.0%)
2	E	0.37±0.01	0±0/1557 (0.0± 0.0%)	0.74±0.01	0±0/2090 (0.0± 0.0%)
All	All	0.36	0/116560 (0.0%)	0.73	1/156800 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	36	ILE	N-CA-C	-5.16	107.54	111.62	19	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1377	319	1353	14±4
1	B	1295	305	1282	12±4
2	D	1532	360	1535	19±5
2	E	1532	360	1535	23±5
3	A	32	6	12	6±2

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes
3	B	32	6	12	4±3
4	A	1	0	0	1±0
4	B	1	0	0	0±1
5	A	507	0	0	53±8
5	B	546	0	0	74±8
5	D	1521	0	0	172±16
5	E	2418	0	0	294±30
6	A	108	6	152	39±6
6	B	216	12	304	65±9
6	D	540	30	760	213±19
6	E	864	48	1216	253±58
All	All	250440	29040	163227	20932

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 51.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:510:17F:C9	6:D:516:17F:H9	1.24	1.62	17	14
6:D:510:17F:H9A	6:D:516:17F:C9	1.21	1.66	19	15
6:D:510:17F:C9	6:D:516:17F:H8A	1.19	1.67	12	5
6:D:516:17F:H47	6:D:516:17F:C22	1.17	1.68	5	1
6:D:510:17F:H19	6:D:527:17F:C19	1.16	1.70	1	6
6:D:510:17F:H9A	6:D:516:17F:C8	1.16	1.69	8	20
6:A:208:17F:H31	6:B:208:17F:H30	1.15	1.18	16	9
6:D:516:17F:H47	6:D:516:17F:H39	1.15	1.17	14	15
6:D:510:17F:C12	6:D:516:17F:H8A	1.15	1.71	4	18
6:A:208:17F:H55	6:A:208:17F:H46	1.15	1.19	17	17
6:D:510:17F:C9	6:D:516:17F:H11	1.14	1.72	12	4
6:D:528:17F:H50	6:D:528:17F:H42	1.13	1.19	13	20
6:D:517:17F:H48	6:D:517:17F:H67	1.13	1.20	9	12
6:E:805:17F:H54	6:E:805:17F:H45	1.12	1.21	10	20
6:E:809:17F:H29	6:E:809:17F:H40	1.12	1.21	20	19
6:E:819:17F:H32	6:E:819:17F:H36	1.12	1.18	10	3
6:A:214:17F:H56	6:A:214:17F:H64	1.12	1.12	4	11
6:D:533:17F:H19A	6:D:533:17F:H57	1.12	1.19	9	19
6:E:856:17F:H68	6:E:874:17F:H65	1.12	1.21	13	12
6:D:510:17F:O9	6:D:516:17F:H9A	1.11	1.44	1	16
6:D:516:17F:H38	6:D:516:17F:C27	1.11	1.73	5	1
6:D:516:17F:C23	6:D:516:17F:H49	1.11	1.74	18	3
6:D:533:17F:H57	6:D:533:17F:C18	1.11	1.75	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:510:17F:H50	6:D:516:17F:H38	1.11	1.18	12	15
6:D:510:17F:C17	6:D:527:17F:H19A	1.11	1.75	11	8
6:B:219:17F:H29	6:B:219:17F:H18A	1.11	1.16	17	1
6:D:510:17F:H31	6:D:516:17F:H10	1.10	1.14	5	7
6:D:527:17F:O9	6:D:527:17F:H32	1.10	1.46	16	14
6:D:501:17F:H12A	6:D:501:17F:H8A	1.10	1.21	6	11
6:D:527:17F:H40	6:D:527:17F:H72	1.10	1.23	2	3
6:E:838:17F:H11	6:E:838:17F:H65	1.10	1.23	19	15
6:D:510:17F:H9	6:D:516:17F:C11	1.10	1.76	6	1
6:D:501:17F:H31	6:D:501:17F:H8	1.09	1.14	6	7
6:E:874:17F:H49	6:E:874:17F:H78	1.09	1.25	3	19
6:D:527:17F:H49	6:E:856:17F:H74	1.09	1.13	13	6
6:D:510:17F:H12	6:D:516:17F:H8A	1.09	1.17	4	17
6:D:510:17F:O7	6:D:516:17F:H9	1.09	1.43	11	8
6:D:510:17F:H8A	6:D:516:17F:H19A	1.08	1.15	17	19
6:E:801:17F:H57	6:E:801:17F:H62	1.08	1.18	9	20
6:D:546:17F:H65	6:D:546:17F:H73	1.08	1.24	2	2
6:D:501:17F:H8	6:D:501:17F:H12A	1.08	1.21	9	7
6:B:208:17F:H49	6:B:208:17F:H68	1.08	1.25	14	16
6:B:208:17F:H43	6:B:208:17F:H57	1.08	1.10	9	15
6:E:838:17F:H73	6:E:856:17F:H41	1.08	1.21	1	4
6:B:214:17F:H5	6:B:219:17F:H9	1.08	1.21	15	6
6:E:856:17F:H65	6:E:874:17F:H61	1.07	1.18	9	12
6:D:510:17F:C8	6:D:516:17F:H19A	1.07	1.78	20	20
6:D:527:17F:H55	6:E:856:17F:H47	1.07	1.08	20	3
6:D:501:17F:H12	6:D:501:17F:H31	1.07	1.23	16	1
6:E:807:17F:H18A	6:E:809:17F:H20	1.07	1.25	4	4
6:B:214:17F:H61	6:B:214:17F:H68	1.07	1.22	11	16
6:E:801:17F:H33	6:E:801:17F:H36	1.07	1.22	7	14
6:D:516:17F:H49	6:D:516:17F:H39	1.07	1.22	18	3
6:D:510:17F:H9A	6:D:516:17F:H9	1.06	1.13	13	15
6:D:527:17F:H77	6:D:527:17F:H50	1.06	1.21	5	11
6:D:533:17F:C31	6:D:533:17F:H18	1.06	1.80	14	1
6:D:534:17F:H58	6:D:534:17F:H30	1.06	1.23	16	11
6:D:510:17F:H12	6:D:516:17F:H10A	1.06	1.28	18	8
6:D:510:17F:H46	6:D:516:17F:H68	1.06	1.23	5	9
6:A:208:17F:H31	6:B:208:17F:H37	1.06	1.23	3	3
6:E:807:17F:H42	6:E:809:17F:H62	1.06	1.10	4	5
6:E:856:17F:H67	6:E:874:17F:C33	1.06	1.80	12	1
6:D:510:17F:H18A	6:D:516:17F:H10	1.05	1.23	12	7
6:D:510:17F:H18A	6:D:527:17F:H19A	1.05	1.20	9	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:B:214:17F:H39	6:B:214:17F:H11	1.05	1.28	4	16
6:E:809:17F:H61	6:E:809:17F:H52	1.05	1.23	16	16
6:D:510:17F:O3	6:D:516:17F:H4	1.05	1.51	5	20
5:E:803:7Q9:C3	6:E:807:17F:H8A	1.05	1.81	10	8
6:E:838:17F:H68	6:E:856:17F:H41	1.05	1.27	2	8
6:D:517:17F:H68	6:D:517:17F:H51	1.05	1.14	17	1
6:D:510:17F:H12	6:D:516:17F:C8	1.05	1.80	3	19
6:D:511:17F:H2	6:D:511:17F:H18A	1.05	1.29	12	2
6:E:807:17F:H33	6:E:818:17F:H9A	1.05	1.26	19	5
6:E:818:17F:H30	6:E:818:17F:H39	1.04	1.26	13	16
6:D:510:17F:H9A	6:D:516:17F:O7	1.04	1.51	6	4
6:D:546:17F:H41	6:D:546:17F:H66	1.04	1.27	11	2
6:D:510:17F:H9A	6:D:516:17F:H11	1.04	1.18	12	4
6:D:510:17F:H12A	6:D:516:17F:H8	1.04	1.27	12	3
6:D:510:17F:H6A	6:D:527:17F:H20A	1.04	1.20	14	1
6:D:510:17F:H46	6:D:516:17F:H66	1.04	1.05	16	1
6:A:208:17F:H57	6:A:208:17F:H63	1.04	1.20	5	17
6:D:510:17F:H12A	6:D:516:17F:H8A	1.04	1.23	5	7
6:D:510:17F:H18	6:D:516:17F:H10	1.04	1.17	20	5
6:D:533:17F:H57	6:D:533:17F:H18	1.04	1.20	14	1
6:D:534:17F:H59	6:D:534:17F:H65	1.03	1.16	15	15
6:D:510:17F:H50	6:D:516:17F:C22	1.03	1.82	10	13
6:B:215:17F:H67	6:B:215:17F:H54	1.03	1.31	5	10
6:D:510:17F:H5	6:D:527:17F:H19A	1.03	1.25	8	5
6:D:510:17F:H9A	6:D:516:17F:H8A	1.03	1.04	9	5
6:D:533:17F:H76	6:E:870:17F:H68	1.03	1.23	13	4
6:D:510:17F:H56	6:D:516:17F:H10A	1.03	1.30	6	1
6:E:818:17F:H41	6:E:818:17F:H67	1.03	1.15	15	2
6:B:208:17F:H33	6:B:214:17F:H12	1.03	1.29	14	1
6:E:807:17F:H20A	6:E:818:17F:H11	1.02	1.26	16	6
6:D:510:17F:H9	6:D:516:17F:H9	1.02	1.31	14	5
6:D:501:17F:H74	6:E:809:17F:H55	1.02	1.09	20	3
6:E:819:17F:H36	6:E:819:17F:C1Y	1.02	1.85	15	3
6:D:501:17F:H41	6:D:501:17F:H60	1.02	1.02	13	3
6:A:214:17F:H35	6:A:214:17F:H42	1.02	1.30	13	15
6:E:819:17F:H52	6:E:819:17F:H73	1.02	1.10	6	8
6:D:516:17F:H76	6:E:838:17F:H74	1.02	1.23	5	6
6:D:501:17F:H44	6:D:501:17F:H61	1.02	1.27	14	4
6:E:819:17F:H18	5:E:852:7Q9:C33	1.02	1.85	3	5
6:E:805:17F:H73	5:E:816:7Q9:C318	1.02	1.83	11	10
6:E:818:17F:H45	6:E:818:17F:H74	1.02	1.21	20	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:510:17F:H8A	6:D:516:17F:H34	1.01	1.19	3	14
6:E:838:17F:H56	6:E:838:17F:H19	1.01	1.32	18	20
6:B:219:17F:H20	6:B:219:17F:H36	1.01	1.31	9	11
6:E:807:17F:H33	6:E:818:17F:C9	1.01	1.86	19	10
6:D:501:17F:H20A	6:D:501:17F:O1	1.01	1.53	18	7
6:E:818:17F:H12A	6:E:819:17F:H30	1.01	1.31	3	6
6:E:856:17F:H68	6:E:874:17F:H61	1.01	1.25	5	4
6:D:510:17F:C28	6:D:516:17F:H38	1.01	1.84	10	12
6:D:533:17F:H50	6:D:533:17F:H75	1.01	1.29	17	12
6:E:807:17F:H56	6:E:819:17F:H29	1.01	1.29	16	9
6:B:208:17F:H31	6:B:214:17F:H10A	1.01	1.33	11	2
6:E:856:17F:H67	6:E:874:17F:H61	1.01	1.29	7	2
6:D:510:17F:H46	6:D:516:17F:H67	1.01	1.32	18	3
6:B:214:17F:H31	5:B:220:7Q9:C34	1.00	1.86	13	9
2:D:273:ASP:HB2	6:D:534:17F:H34	1.00	1.30	18	12
6:E:809:17F:HN1A	6:E:818:17F:H4A	1.00	1.08	2	1
6:B:214:17F:H74	6:B:214:17F:H48	1.00	1.33	18	4
6:E:856:17F:H67	6:E:874:17F:H60	1.00	1.01	12	5
6:E:838:17F:H12	6:E:856:17F:H12	1.00	1.15	6	11
6:D:510:17F:H1	6:D:516:17F:H6	1.00	1.33	16	10
6:D:516:17F:H39	6:D:516:17F:C28	1.00	1.86	18	3
6:D:510:17F:H39	6:D:510:17F:H29	1.00	1.29	14	1
6:E:809:17F:H40	6:E:809:17F:C1X	1.00	1.86	10	19
6:D:516:17F:H44	6:D:527:17F:H38	1.00	1.28	7	4
6:D:510:17F:H18A	6:D:527:17F:H20A	1.00	1.34	15	2
6:D:510:17F:H9A	6:D:516:17F:C10	0.99	1.87	11	8
6:B:214:17F:O10	6:B:219:17F:H11A	0.99	1.57	13	6
6:E:809:17F:N1	6:E:818:17F:H4A	0.99	1.70	2	1
6:D:516:17F:H41	6:D:527:17F:H38	0.99	1.32	2	7
6:D:511:17F:H66	6:D:511:17F:H39	0.99	1.28	15	6
6:D:510:17F:H18A	6:D:527:17F:C20	0.99	1.86	15	3
6:E:801:17F:H62	6:E:801:17F:C31	0.99	1.86	18	16
6:D:510:17F:H47	6:D:516:17F:H62	0.99	1.32	2	3
6:D:501:17F:H44	6:D:501:17F:C34	0.99	1.87	16	3
6:D:501:17F:H61	6:D:501:17F:C25	0.99	1.88	16	2
5:A:204:7Q9:C313	6:A:208:17F:H78	0.98	1.89	3	10
5:D:512:7Q9:C13	6:D:528:17F:H4	0.98	1.87	17	6
6:B:208:17F:H33	6:B:214:17F:H10	0.98	1.30	3	2
6:B:219:17F:H20	6:B:219:17F:C2X	0.98	1.89	13	12
6:E:807:17F:H20A	6:E:818:17F:H9A	0.98	1.30	2	7
6:D:501:17F:H31	6:D:501:17F:H10A	0.98	1.29	19	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:B:208:17F:H64	6:B:208:17F:H45	0.98	1.31	1	11
6:E:838:17F:H65	6:E:838:17F:C11	0.98	1.89	5	8
6:D:517:17F:H30	6:D:517:17F:H39	0.97	1.33	9	19
6:E:818:17F:H78	6:E:818:17F:H47	0.97	1.35	7	8
6:E:819:17F:H32	6:E:819:17F:C2X	0.97	1.89	15	3
6:D:510:17F:H42	6:D:516:17F:H68	0.97	1.30	18	1
6:B:208:17F:C1Z	6:B:214:17F:H12	0.97	1.89	14	1
6:D:510:17F:H12	6:D:516:17F:C10	0.97	1.89	5	8
6:D:511:17F:H53	6:E:828:17F:H66	0.97	1.28	19	2
5:B:211:7Q9:C23	6:D:501:17F:H57	0.97	1.88	15	5
6:D:510:17F:H19A	6:D:516:17F:C9	0.97	1.88	9	2
6:E:819:17F:C20	6:E:819:17F:H12	0.97	1.89	10	2
6:D:510:17F:H46	6:D:516:17F:H64	0.97	1.33	8	10
6:E:855:17F:H38	6:E:855:17F:H68	0.97	1.37	16	17
6:D:501:17F:H46	6:D:501:17F:C34	0.97	1.89	20	2
6:D:501:17F:H40	6:D:501:17F:H34	0.97	1.37	19	2
6:D:510:17F:H9A	6:D:516:17F:C7	0.96	1.88	6	9
6:D:510:17F:H19	6:D:527:17F:H19A	0.96	1.37	1	7
6:E:807:17F:H33	6:E:818:17F:H10A	0.96	1.35	6	9
6:D:528:17F:H60	6:D:528:17F:H10A	0.96	1.37	8	14
5:E:802:7Q9:O13	6:E:807:17F:H2	0.96	1.58	7	7
6:E:838:17F:H57	6:E:838:17F:H65	0.96	1.36	20	3
6:D:517:17F:H42	6:D:517:17F:H66	0.96	1.32	19	1
6:D:501:17F:H8A	6:D:501:17F:C12	0.96	1.90	1	8
6:A:214:17F:H55	6:A:214:17F:H72	0.96	1.35	3	5
6:B:219:17F:H20	6:B:219:17F:H29	0.96	1.33	4	2
6:A:214:17F:H32	6:A:214:17F:H11	0.96	1.37	17	8
6:D:533:17F:H63	6:D:533:17F:H38	0.96	1.36	12	7
6:E:807:17F:H76	6:E:807:17F:H51	0.96	1.35	4	4
6:E:807:17F:H75	6:E:818:17F:H54	0.96	1.34	17	2
6:D:533:17F:H59	6:D:533:17F:H65	0.96	1.34	14	1
2:E:674:LEU:HD21	6:E:855:17F:H12	0.95	1.34	11	9
6:D:501:17F:H41	6:D:501:17F:C33	0.95	1.90	13	4
6:E:809:17F:H10A	5:E:810:7Q9:C33	0.95	1.90	19	9
6:A:208:17F:H61	6:B:208:17F:H69	0.95	1.36	11	2
6:E:856:17F:H65	6:E:874:17F:C34	0.95	1.91	20	12
6:E:856:17F:C37	6:E:874:17F:H60	0.95	1.91	12	3
6:D:501:17F:H56	6:D:501:17F:H63	0.95	1.38	9	7
6:D:501:17F:C26	6:D:501:17F:H61	0.95	1.91	11	1
6:E:838:17F:H11A	6:E:856:17F:H35	0.95	1.36	3	8
5:E:869:7Q9:O12	6:E:872:17F:H9	0.95	1.61	12	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:510:17F:O10	6:D:527:17F:H19A	0.95	1.61	6	8
6:D:501:17F:H49	6:D:501:17F:C37	0.95	1.92	15	3
6:E:807:17F:H33	6:E:818:17F:C10	0.94	1.92	6	10
6:A:208:17F:H19	6:B:208:17F:H30	0.94	1.37	8	5
6:D:501:17F:H35	5:D:506:7Q9:C22	0.94	1.93	7	1
5:E:824:7Q9:C33	6:E:841:17F:H20A	0.94	1.91	2	9
6:B:215:17F:H36	5:B:216:7Q9:C311	0.94	1.92	11	5
6:D:510:17F:H9	6:D:516:17F:H11A	0.94	1.35	6	1
6:D:510:17F:H20A	6:D:516:17F:H9A	0.94	1.35	8	2
6:E:817:17F:H8A	5:E:820:7Q9:C23	0.94	1.91	13	5
6:A:214:17F:H54	5:E:840:7Q9:C318	0.94	1.93	15	13
6:B:214:17F:H74	6:B:214:17F:H46	0.94	1.40	5	1
6:D:516:17F:H39	6:D:516:17F:C27	0.93	1.94	10	18
6:D:501:17F:H31	6:D:501:17F:C8	0.93	1.91	7	5
6:D:516:17F:C17	6:D:516:17F:H1A	0.93	1.92	14	4
6:D:511:17F:H76	6:E:828:17F:H54	0.93	1.41	5	7
6:E:818:17F:H10A	6:E:819:17F:H30	0.93	1.40	19	4
6:A:208:17F:C1Y	6:B:208:17F:H30	0.93	1.92	20	9
6:D:533:17F:H19A	6:D:533:17F:C31	0.93	1.92	8	19
6:E:838:17F:H33	6:E:838:17F:H35	0.93	1.39	3	11
6:A:208:17F:H19A	6:B:208:17F:H30	0.93	1.40	10	2
6:E:819:17F:H12	6:E:819:17F:H20	0.93	1.36	10	2
6:D:510:17F:H18	6:D:516:17F:H8	0.93	1.39	2	3
6:D:510:17F:C18	6:D:516:17F:H10	0.93	1.94	12	8
6:E:809:17F:H61	6:E:809:17F:C29	0.93	1.94	20	7
6:D:501:17F:H41	6:D:501:17F:H61	0.93	1.40	5	4
6:D:510:17F:H19A	6:D:516:17F:C10	0.93	1.93	9	2
6:D:516:17F:H48	6:D:516:17F:H60	0.93	1.41	2	1
6:D:501:17F:H41	6:D:501:17F:C34	0.93	1.93	15	5
6:E:807:17F:H20A	6:E:818:17F:C11	0.93	1.94	15	6
6:D:510:17F:H8A	6:D:516:17F:C19	0.92	1.92	20	10
6:E:874:17F:H78	6:E:874:17F:C28	0.92	1.94	7	19
6:E:807:17F:H30	6:E:807:17F:H58	0.92	1.41	5	5
5:E:824:7Q9:C32	6:E:841:17F:H18	0.92	1.94	20	6
6:E:805:17F:H47	5:E:812:7Q9:C314	0.92	1.94	13	4
2:E:659:LEU:HD21	6:E:856:17F:H77	0.92	1.41	13	2
6:E:874:17F:H49	6:E:874:17F:C42	0.92	1.95	7	10
6:D:510:17F:C1Y	6:D:516:17F:H10	0.92	1.95	5	3
6:E:838:17F:H65	6:E:838:17F:H11	0.92	1.39	20	4
6:D:510:17F:C1	6:D:516:17F:H6	0.92	1.95	9	6
5:B:211:7Q9:C22	6:D:501:17F:H57	0.92	1.93	3	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:510:17F:H8	6:D:516:17F:H19A	0.92	1.42	6	3
6:B:214:17F:H18	6:B:219:17F:C8	0.92	1.94	4	1
6:E:807:17F:H63	6:E:807:17F:H12A	0.92	1.38	15	1
6:D:534:17F:H10	5:D:539:7Q9:C36	0.92	1.95	5	5
6:B:214:17F:H46	5:B:217:7Q9:C37	0.92	1.95	18	5
6:D:510:17F:H31	6:D:516:17F:C10	0.92	1.95	5	2
6:D:510:17F:C26	6:D:516:17F:H66	0.92	1.95	16	1
6:E:838:17F:H50	6:E:874:17F:H55	0.91	1.39	20	3
6:D:510:17F:H19	6:D:527:17F:H19	0.91	1.39	1	5
6:E:809:17F:H52	6:E:809:17F:C34	0.91	1.94	20	8
6:E:819:17F:H6	5:E:836:7Q9:C21	0.91	1.94	15	2
6:D:501:17F:H39	6:D:501:17F:H60	0.91	1.38	2	1
6:B:208:17F:H33	6:B:214:17F:C10	0.91	1.95	3	2
6:D:510:17F:H9A	6:D:516:17F:H10A	0.91	1.38	11	3
6:E:801:17F:H60	5:E:803:7Q9:C23	0.91	1.96	2	10
6:B:208:17F:H43	6:B:208:17F:C31	0.91	1.96	20	15
6:D:534:17F:H30	6:D:534:17F:C32	0.91	1.96	15	9
6:D:516:17F:H61	6:D:516:17F:H69	0.91	1.40	16	1
6:E:856:17F:H57	6:E:856:17F:H36	0.91	1.43	11	6
6:D:501:17F:H60	6:D:501:17F:C24	0.91	1.95	13	2
6:E:809:17F:H60	6:E:818:17F:H70	0.90	1.40	6	1
5:B:211:7Q9:C313	6:B:215:17F:H19A	0.90	1.95	14	1
6:E:805:17F:H37	6:E:805:17F:H19	0.90	1.42	1	5
6:E:805:17F:H73	5:E:816:7Q9:C317	0.90	1.95	13	8
6:E:856:17F:H70	6:E:874:17F:H61	0.90	1.40	4	2
6:B:214:17F:H62	6:B:214:17F:H57	0.90	1.42	17	1
6:B:219:17F:H76	6:B:219:17F:H53	0.90	1.43	20	7
6:D:510:17F:H12	6:D:516:17F:C7	0.90	1.96	7	7
6:D:510:17F:O7	6:D:516:17F:H4A	0.90	1.66	10	9
6:E:818:17F:H45	6:E:818:17F:H75	0.90	1.43	12	1
6:D:501:17F:H51	5:D:508:7Q9:C316	0.90	1.97	20	3
6:E:807:17F:C31	6:E:819:17F:H29	0.90	1.97	1	8
6:E:807:17F:H66	5:E:813:7Q9:C310	0.90	1.94	15	5
6:D:510:17F:H20A	6:D:516:17F:C10	0.90	1.97	11	2
6:D:534:17F:H10	5:D:539:7Q9:C33	0.90	1.96	3	12
6:E:818:17F:H48	6:E:818:17F:H78	0.90	1.43	16	4
6:D:501:17F:H10	6:D:501:17F:C34	0.90	1.96	13	2
6:E:819:17F:H6	5:E:836:7Q9:O22	0.90	1.67	13	5
6:D:510:17F:H56	6:D:516:17F:H12A	0.90	1.41	18	3
6:D:510:17F:H12A	6:D:516:17F:C8	0.90	1.97	12	4
6:D:516:17F:C42	6:E:838:17F:H74	0.90	1.96	5	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:807:17F:H60	6:E:819:17F:H12A	0.90	1.43	14	3
6:D:516:17F:H47	6:D:516:17F:C23	0.90	1.96	6	16
6:E:819:17F:H57	6:E:819:17F:H40	0.90	1.44	16	3
6:D:510:17F:C27	6:D:516:17F:H37	0.90	1.97	11	2
6:E:818:17F:H1	5:E:837:7Q9:C11	0.90	1.97	18	1
5:D:537:7Q9:C3	6:D:546:17F:H11A	0.89	1.95	15	12
6:E:819:17F:H45	6:E:819:17F:H38	0.89	1.44	1	15
6:E:838:17F:H48	6:E:838:17F:H77	0.89	1.42	18	2
6:D:527:17F:C42	6:D:527:17F:H50	0.89	1.96	2	2
6:D:501:17F:H40	6:D:501:17F:C11	0.89	1.96	18	4
6:A:214:17F:H56	6:A:214:17F:C36	0.89	1.96	12	6
6:D:510:17F:H53	6:D:510:17F:H78	0.89	1.42	20	4
6:E:805:17F:H74	5:E:810:7Q9:C315	0.89	1.97	20	4
6:B:219:17F:H18A	6:B:219:17F:C1X	0.89	1.97	17	1
6:D:501:17F:H60	6:D:501:17F:H36	0.89	1.42	2	1
6:E:838:17F:H33	6:E:838:17F:H40	0.89	1.44	6	9
6:E:817:17F:H18	5:E:833:7Q9:O32	0.89	1.67	13	5
6:B:219:17F:H2	6:B:219:17F:H4A	0.89	1.42	11	3
5:D:515:7Q9:O31	6:D:517:17F:H19	0.89	1.67	4	1
5:E:803:7Q9:O32	6:E:807:17F:H9	0.89	1.67	19	2
5:A:204:7Q9:C315	6:A:208:17F:H78	0.89	1.98	7	2
6:D:516:17F:C24	6:D:527:17F:H38	0.89	1.98	2	8
6:B:214:17F:H61	6:B:214:17F:C38	0.89	1.96	11	17
5:B:211:7Q9:C311	6:D:501:17F:H65	0.89	1.97	15	5
5:E:824:7Q9:C33	6:E:841:17F:H18	0.89	1.97	15	1
6:D:511:17F:H77	6:D:511:17F:H49	0.89	1.42	15	14
6:D:533:17F:H37	6:D:533:17F:H62	0.89	1.43	7	5
6:D:510:17F:H19A	6:D:516:17F:H9A	0.89	1.42	9	3
6:E:874:17F:H36	6:E:874:17F:H41	0.89	1.44	20	19
6:D:501:17F:H39	5:D:508:7Q9:C35	0.88	1.98	9	2
6:D:534:17F:H11A	6:D:534:17F:H31	0.88	1.43	16	1
6:D:510:17F:C9	6:D:516:17F:C9	0.88	2.52	7	14
6:D:510:17F:H46	6:D:516:17F:C38	0.88	1.96	5	10
6:E:807:17F:H55	6:E:818:17F:C42	0.88	1.98	1	9
6:E:805:17F:H54	6:E:805:17F:H72	0.88	1.45	1	5
6:E:818:17F:H10	6:E:819:17F:H10	0.88	1.44	1	5
2:E:634:LEU:HB2	5:E:878:7Q9:C316	0.88	1.98	19	9
6:B:208:17F:H57	6:B:208:17F:C25	0.88	1.99	4	13
6:D:510:17F:H38	6:D:511:17F:H72	0.88	1.45	4	1
5:D:507:7Q9:C314	6:D:516:17F:H53	0.88	1.98	6	1
6:D:534:17F:H61	6:D:534:17F:H47	0.88	1.45	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:527:17F:H55	6:E:856:17F:C27	0.88	1.99	20	2
6:A:214:17F:H64	6:A:214:17F:C31	0.88	1.98	12	7
6:D:501:17F:H40	6:D:501:17F:H11A	0.88	1.41	18	2
6:D:510:17F:H6A	6:D:527:17F:H19A	0.88	1.44	17	1
5:E:837:7Q9:C12	6:E:841:17F:H18	0.88	1.98	1	1
6:D:517:17F:H67	6:D:517:17F:C27	0.88	1.98	20	9
6:E:818:17F:H73	6:E:818:17F:H45	0.88	1.44	15	2
6:E:828:17F:H11	5:E:832:7Q9:C38	0.88	1.99	3	5
6:E:807:17F:H54	6:E:809:17F:H53	0.88	1.40	20	4
6:D:510:17F:H49	6:D:516:17F:H64	0.88	1.46	17	1
6:D:510:17F:C7	6:D:516:17F:H9	0.88	1.97	18	15
6:E:856:17F:C36	6:E:874:17F:H61	0.88	1.99	10	12
6:B:208:17F:H71	6:B:208:17F:H54	0.88	1.42	4	9
6:D:533:17F:H57	6:D:533:17F:C19	0.88	1.99	2	20
6:D:517:17F:H48	6:D:517:17F:C37	0.88	1.98	15	8
6:A:214:17F:H29	6:A:214:17F:H59	0.88	1.43	8	2
6:D:510:17F:H20A	6:D:516:17F:C9	0.88	1.98	8	2
6:B:214:17F:C1Z	6:B:219:17F:H12	0.88	1.97	17	1
6:E:818:17F:H59	6:E:818:17F:H65	0.88	1.45	2	5
6:B:208:17F:H43	6:B:208:17F:C1Z	0.88	1.99	15	10
6:D:510:17F:H18A	6:D:516:17F:H8	0.88	1.45	10	3
6:E:807:17F:H19A	6:E:818:17F:H9A	0.88	1.44	9	6
6:E:856:17F:H67	6:E:874:17F:C34	0.88	1.99	7	1
6:E:838:17F:H77	6:E:838:17F:H49	0.87	1.43	13	7
6:A:208:17F:H12	5:A:209:7Q9:C39	0.87	1.98	11	8
6:E:807:17F:H42	6:E:809:17F:C35	0.87	2.00	8	4
6:E:807:17F:C20	6:E:818:17F:H11	0.87	1.98	15	4
6:D:510:17F:H29	6:D:510:17F:C23	0.87	1.99	14	1
6:D:510:17F:H46	6:D:516:17F:C37	0.87	1.97	16	9
6:D:546:17F:H71	6:D:546:17F:H45	0.87	1.46	1	6
6:D:510:17F:H9	6:D:516:17F:H11	0.87	1.45	8	5
6:B:214:17F:C17	6:B:219:17F:H11A	0.87	1.98	15	6
6:D:516:17F:H76	6:E:838:17F:C41	0.87	1.98	5	3
6:E:818:17F:C10	6:E:819:17F:H10A	0.87	2.00	13	6
6:E:801:17F:H57	6:E:801:17F:C35	0.87	1.99	12	18
6:E:805:17F:H6A	5:E:816:7Q9:O31	0.87	1.70	15	2
5:D:508:7Q9:C314	6:E:818:17F:H52	0.87	1.99	16	1
5:D:512:7Q9:C33	6:D:528:17F:H6A	0.87	1.99	2	4
6:D:528:17F:H50	6:D:528:17F:C24	0.87	1.99	20	20
6:D:510:17F:O8	6:D:516:17F:H19A	0.87	1.68	4	5
6:E:801:17F:H39	5:E:804:7Q9:C38	0.87	2.00	13	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:B:219:17F:H20	6:B:219:17F:C1X	0.87	1.98	4	5
6:E:856:17F:C38	6:E:874:17F:H61	0.87	1.99	5	4
5:A:204:7Q9:C313	6:A:208:17F:H65	0.87	1.99	19	13
6:D:516:17F:H44	6:D:527:17F:H41	0.87	1.46	19	3
6:E:838:17F:H11	6:E:838:17F:C36	0.86	1.99	20	10
6:E:874:17F:O3	6:E:874:17F:H6	0.86	1.70	9	4
6:E:807:17F:H55	6:E:818:17F:H75	0.86	1.47	5	6
6:A:208:17F:H46	6:A:208:17F:C30	0.86	2.00	16	17
6:D:501:17F:H12	6:D:501:17F:C23	0.86	2.00	15	5
6:E:801:17F:H9A	5:E:802:7Q9:O14	0.86	1.69	6	1
6:D:511:17F:H49	6:D:511:17F:C42	0.86	1.99	9	4
6:D:501:17F:H46	6:D:501:17F:H61	0.86	1.45	20	2
6:E:807:17F:C41	6:E:807:17F:H51	0.86	1.99	6	10
6:E:818:17F:C12	6:E:819:17F:H30	0.86	2.00	3	5
6:E:818:17F:H10	6:E:819:17F:H10A	0.86	1.43	2	6
6:D:501:17F:H38	5:D:508:7Q9:C33	0.86	2.01	3	1
6:E:841:17F:H9A	5:E:876:7Q9:O14	0.86	1.71	10	2
6:D:510:17F:H10A	6:D:516:17F:H58	0.86	1.46	20	1
6:D:516:17F:C25	6:D:527:17F:H38	0.86	2.01	17	6
6:E:856:17F:H69	6:E:856:17F:H58	0.86	1.46	7	8
6:B:214:17F:H6	5:B:217:7Q9:O32	0.86	1.69	16	5
6:E:872:17F:H20A	6:E:872:17F:H36	0.86	1.47	9	8
6:B:208:17F:H39	6:B:208:17F:H64	0.86	1.44	9	10
6:D:510:17F:H76	6:D:516:17F:H75	0.86	1.45	5	1
6:E:818:17F:H78	6:E:818:17F:C27	0.86	2.01	16	6
5:B:211:7Q9:C312	6:D:501:17F:H65	0.86	2.00	20	5
6:D:510:17F:H20A	6:D:516:17F:H10	0.85	1.45	11	2
5:D:537:7Q9:C31	6:D:546:17F:H29	0.85	2.01	19	5
6:D:534:17F:H61	6:D:534:17F:H44	0.85	1.47	5	6
6:D:501:17F:H8	6:D:501:17F:C1Y	0.85	2.00	6	6
6:D:501:17F:H45	5:D:508:7Q9:C36	0.85	2.00	16	2
6:D:527:17F:C28	6:E:856:17F:H74	0.85	1.99	15	5
6:E:817:17F:H61	5:E:826:7Q9:C36	0.85	2.02	9	6
6:D:501:17F:H10A	6:D:501:17F:C1Y	0.85	2.01	19	1
5:E:824:7Q9:C34	6:E:841:17F:H18	0.85	2.01	15	1
6:E:856:17F:H29	6:E:874:17F:C33	0.85	2.00	11	5
6:D:510:17F:H9A	6:D:516:17F:C11	0.85	2.00	12	4
6:D:534:17F:H65	6:D:534:17F:C32	0.85	2.02	15	12
5:D:515:7Q9:C3	6:D:517:17F:H6A	0.85	2.00	8	1
6:D:510:17F:C26	6:D:516:17F:H64	0.85	2.01	9	9
6:E:817:17F:H11	5:E:833:7Q9:C33	0.85	2.01	13	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:533:17F:H67	6:D:533:17F:H43	0.85	1.47	14	6
6:D:501:17F:H12A	6:D:501:17F:C8	0.85	2.01	6	18
6:E:819:17F:H31	5:E:829:7Q9:C22	0.85	2.02	10	2
6:A:208:17F:H63	6:A:208:17F:C31	0.85	1.99	5	12
6:E:856:17F:C38	6:E:874:17F:H65	0.85	2.01	10	6
6:B:215:17F:H10A	6:B:215:17F:H63	0.84	1.49	12	5
6:D:501:17F:H49	6:D:501:17F:H66	0.84	1.47	20	3
5:B:220:7Q9:C22	6:D:533:17F:H6	0.84	2.02	19	4
6:D:510:17F:H5	6:D:527:17F:C19	0.84	2.02	8	4
3:B:201:GSP:H5'1	3:B:201:GSP:O1B	0.84	1.71	12	4
6:D:501:17F:H49	6:D:501:17F:H67	0.84	1.48	15	1
6:D:501:17F:H12	6:D:501:17F:C1Y	0.84	2.02	16	1
5:E:857:7Q9:O32	6:E:874:17F:H10A	0.84	1.72	13	8
6:D:527:17F:H50	6:D:527:17F:H78	0.84	1.48	2	1
6:E:856:17F:H11	6:E:874:17F:H59	0.84	1.47	19	6
6:A:208:17F:H30	5:A:209:7Q9:C39	0.84	2.02	12	3
6:E:819:17F:H45	6:E:819:17F:C22	0.84	2.02	11	20
6:E:838:17F:C11	6:E:838:17F:H65	0.84	2.02	9	2
6:D:501:17F:C11	6:D:501:17F:H39	0.84	2.02	3	2
6:D:527:17F:H30	6:D:527:17F:H67	0.84	1.46	8	5
6:E:807:17F:H46	6:E:809:17F:H62	0.84	1.49	20	5
6:D:533:17F:H66	6:D:533:17F:H38	0.84	1.46	14	1
6:A:214:17F:H10	6:A:214:17F:H19A	0.84	1.49	8	13
6:E:817:17F:H11	5:E:833:7Q9:C32	0.84	2.03	20	10
6:B:219:17F:H29	6:B:219:17F:C20	0.84	2.02	4	3
6:E:838:17F:C12	6:E:856:17F:H12	0.84	2.02	6	6
6:E:856:17F:C11	6:E:874:17F:H59	0.84	2.01	19	6
6:E:818:17F:H61	6:E:841:17F:H67	0.84	1.45	4	4
6:D:510:17F:H50	6:D:516:17F:H37	0.84	1.49	5	3
6:E:828:17F:H9	5:E:832:7Q9:C33	0.84	2.03	12	2
6:D:510:17F:C4	6:D:516:17F:H4A	0.83	2.03	11	18
6:E:838:17F:H33	6:E:838:17F:C23	0.83	2.02	4	11
6:D:510:17F:C26	6:D:516:17F:H68	0.83	2.03	5	7
6:D:516:17F:H47	6:D:516:17F:H38	0.83	0.86	5	1
6:D:510:17F:C30	6:D:527:17F:H55	0.83	2.03	10	4
6:B:215:17F:H18	6:D:501:17F:H9A	0.83	1.49	10	1
6:D:501:17F:H76	6:E:818:17F:H51	0.83	1.49	14	1
6:E:819:17F:H61	5:E:836:7Q9:C36	0.83	2.03	15	13
6:E:801:17F:H20	6:E:801:17F:H12	0.83	1.49	18	12
6:D:510:17F:H8	6:D:516:17F:C17	0.83	2.02	13	13
6:E:807:17F:C20	6:E:818:17F:H9A	0.83	2.03	10	9

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:501:17F:H45	6:D:501:17F:H35	0.83	1.45	10	3
6:D:510:17F:H8	6:D:516:17F:C19	0.83	2.02	6	4
6:E:807:17F:H12A	6:E:807:17F:C35	0.83	2.02	15	3
6:E:856:17F:H56	6:E:856:17F:H63	0.83	1.48	18	14
5:E:837:7Q9:O13	6:E:841:17F:H5	0.83	1.73	3	4
6:B:208:17F:H40	6:B:208:17F:H34	0.83	1.48	4	4
6:D:510:17F:H37	6:D:511:17F:H56	0.83	1.47	18	2
6:D:510:17F:H47	6:D:516:17F:H37	0.83	1.49	18	2
6:D:533:17F:H38	6:D:533:17F:C37	0.83	2.03	14	2
6:B:208:17F:H43	6:B:208:17F:H58	0.83	1.48	2	1
5:B:203:7Q9:C310	6:B:208:17F:H73	0.83	2.03	9	5
5:E:804:7Q9:C13	6:E:805:17F:H8A	0.83	2.03	14	1
5:E:837:7Q9:O32	6:E:841:17F:H12A	0.83	1.72	2	6
6:E:838:17F:H12	6:E:856:17F:C12	0.83	2.03	6	8
6:B:215:17F:H36	5:B:216:7Q9:C312	0.83	2.02	5	2
6:D:501:17F:H74	6:E:809:17F:H53	0.83	1.47	5	1
5:E:848:7Q9:C312	5:E:851:7Q9:C34	0.83	2.57	15	5
6:D:516:17F:H69	6:D:516:17F:C34	0.83	2.04	16	1
6:D:501:17F:H8	6:D:501:17F:C12	0.83	2.03	16	7
6:D:517:17F:H68	6:D:517:17F:C29	0.83	2.01	17	2
6:B:219:17F:O10	6:B:219:17F:H6A	0.83	1.73	15	15
6:D:501:17F:H31	6:D:501:17F:C12	0.83	2.04	16	1
5:E:869:7Q9:C22	6:E:872:17F:H10	0.82	2.04	4	13
6:D:510:17F:H50	6:D:516:17F:C21	0.82	2.04	5	5
6:E:819:17F:H18A	5:E:829:7Q9:C23	0.82	2.03	15	3
5:A:215:7Q9:C37	6:D:534:17F:H50	0.82	2.04	6	1
6:E:807:17F:H55	6:E:818:17F:H76	0.82	1.46	1	8
6:D:501:17F:H61	6:D:501:17F:H45	0.82	1.48	11	1
6:D:516:17F:H74	6:E:838:17F:H74	0.82	1.52	13	1
6:E:828:17F:H30	5:E:832:7Q9:C35	0.82	2.03	14	3
6:B:219:17F:H29	6:B:219:17F:H19	0.82	1.48	15	11
2:D:312:MET:HE1	6:D:527:17F:H64	0.82	1.48	10	4
6:E:872:17F:H36	6:E:872:17F:C20	0.82	2.04	13	19
6:E:838:17F:C1Z	6:E:838:17F:H40	0.82	2.03	13	5
6:E:819:17F:H52	6:E:819:17F:C40	0.82	2.00	6	3
6:B:215:17F:H12	6:B:215:17F:H64	0.82	1.49	2	5
6:E:856:17F:H70	6:E:874:17F:H68	0.82	1.49	9	5
6:D:546:17F:H67	6:D:546:17F:H56	0.82	1.50	11	4
5:D:513:7Q9:C38	6:D:528:17F:H65	0.82	2.04	8	4
6:D:516:17F:H61	6:D:516:17F:C38	0.82	2.05	16	1
1:A:33:ASP:HB2	1:B:128:LYS:HD2	0.82	1.50	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:B:211:7Q9:C312	6:D:501:17F:H64	0.82	2.04	13	3
5:E:824:7Q9:O32	6:E:841:17F:H61	0.82	1.75	14	2
6:B:214:17F:O10	6:B:219:17F:H9	0.82	1.75	5	3
6:E:819:17F:H19A	5:E:852:7Q9:C35	0.82	2.04	19	4
6:D:528:17F:H42	6:D:528:17F:C28	0.81	2.03	16	20
6:D:527:17F:H39	6:D:527:17F:H68	0.81	1.50	16	5
6:E:807:17F:H56	6:E:819:17F:C1X	0.81	2.05	9	7
6:B:214:17F:H34	6:B:219:17F:H37	0.81	1.50	15	4
5:B:206:7Q9:C314	6:E:805:17F:H75	0.81	2.04	16	10
6:D:501:17F:H29	5:D:509:7Q9:C23	0.81	2.06	10	2
6:D:534:17F:H59	6:D:534:17F:C36	0.81	1.95	15	14
6:E:807:17F:H38	6:E:809:17F:H20	0.81	1.47	11	3
6:D:501:17F:H45	6:D:501:17F:H36	0.81	1.50	20	5
5:E:802:7Q9:C315	6:E:809:17F:H66	0.81	2.04	15	7
6:B:219:17F:H18A	5:D:545:7Q9:C35	0.81	2.05	10	2
6:D:510:17F:H64	6:D:527:17F:H75	0.81	1.52	11	2
3:A:201:GSP:O3B	3:A:201:GSP:H5'1	0.81	1.75	14	1
6:D:516:17F:H50	6:D:516:17F:C33	0.81	2.05	14	1
6:B:219:17F:H69	5:D:522:7Q9:C311	0.81	2.04	13	6
6:E:805:17F:H54	6:E:805:17F:C26	0.81	2.06	19	20
6:E:856:17F:H36	6:E:856:17F:C31	0.81	2.05	11	11
6:D:546:17F:H65	6:D:546:17F:C40	0.81	2.06	11	2
6:D:501:17F:H39	6:D:501:17F:H11A	0.81	1.51	13	7
2:E:733:LEU:HG	5:E:875:7Q9:C37	0.81	2.05	11	16
6:E:841:17F:H64	6:E:841:17F:H59	0.81	1.51	17	7
6:B:215:17F:H71	5:E:824:7Q9:C318	0.81	2.05	20	1
6:E:805:17F:H45	6:E:805:17F:C30	0.81	2.05	8	20
6:E:856:17F:H11	6:E:874:17F:C33	0.81	2.05	13	7
6:E:807:17F:H58	6:E:807:17F:C1X	0.81	2.06	5	8
6:A:208:17F:H55	6:A:208:17F:C26	0.81	2.05	10	17
6:D:501:17F:H29	5:D:509:7Q9:O22	0.81	1.76	6	3
6:B:208:17F:H40	6:B:208:17F:H58	0.81	1.53	19	7
6:D:516:17F:C27	6:D:516:17F:H60	0.81	2.06	3	1
6:E:818:17F:H42	5:E:835:7Q9:C37	0.81	2.06	7	4
6:D:501:17F:H74	6:E:809:17F:C30	0.81	2.02	20	6
6:E:817:17F:H8A	5:E:820:7Q9:C22	0.81	2.05	20	1
6:E:819:17F:H38	6:E:819:17F:C26	0.81	2.06	1	9
6:D:527:17F:H49	6:E:856:17F:C41	0.81	2.05	16	6
6:B:208:17F:H49	6:B:208:17F:C38	0.81	2.05	11	13
5:A:204:7Q9:C311	6:A:208:17F:H72	0.81	2.05	19	6
6:E:818:17F:H10A	6:E:819:17F:H12A	0.81	1.51	16	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:B:211:7Q9:C312	6:D:501:17F:H70	0.81	2.06	16	4
6:D:510:17F:H18A	6:D:527:17F:C19	0.81	2.06	9	2
6:E:819:17F:H18A	5:E:829:7Q9:C22	0.81	2.06	13	5
6:D:510:17F:C29	6:D:516:17F:H67	0.81	2.05	14	1
6:D:510:17F:C19	6:D:527:17F:H19A	0.81	2.06	1	4
6:D:510:17F:C6	6:D:516:17F:H4A	0.81	2.06	6	14
6:E:838:17F:H77	6:E:838:17F:C27	0.81	2.06	1	10
6:B:219:17F:O6	6:B:219:17F:H2	0.81	1.76	20	6
6:D:510:17F:H57	6:D:527:17F:H61	0.81	1.51	2	3
6:E:807:17F:H74	6:E:807:17F:H47	0.81	1.51	20	7
6:D:501:17F:H34	6:D:501:17F:H37	0.81	1.53	16	2
6:E:809:17F:H10A	5:E:810:7Q9:O32	0.80	1.76	18	1
6:B:214:17F:H4A	5:B:217:7Q9:O32	0.80	1.76	1	1
6:E:807:17F:C1Z	6:E:818:17F:H9A	0.80	2.05	19	5
6:E:801:17F:H36	6:E:801:17F:C1Z	0.80	2.05	8	7
6:B:214:17F:H52	5:E:827:7Q9:C318	0.80	2.06	18	2
6:E:807:17F:C18	6:E:809:17F:H20	0.80	2.07	14	1
5:E:804:7Q9:O32	6:E:811:17F:H31	0.80	1.74	18	11
6:B:214:17F:H20	6:B:219:17F:O2	0.80	1.77	4	1
6:E:838:17F:H10A	6:E:856:17F:H12	0.80	1.54	16	7
6:D:517:17F:H43	6:D:517:17F:H67	0.80	1.51	7	2
6:E:818:17F:H10A	6:E:819:17F:C12	0.80	2.07	16	1
6:D:510:17F:H8	6:D:516:17F:O9	0.80	1.76	10	7
6:B:214:17F:O10	6:B:214:17F:H6A	0.80	1.77	14	11
5:A:204:7Q9:C311	6:A:208:17F:H78	0.80	2.06	18	6
5:D:512:7Q9:O13	6:D:528:17F:H4A	0.80	1.77	8	3
6:E:809:17F:H31	6:E:818:17F:H63	0.80	1.51	13	3
6:D:510:17F:H39	6:D:510:17F:C1X	0.80	2.06	14	1
6:A:208:17F:C19	6:B:208:17F:H30	0.80	2.07	10	6
2:E:634:LEU:HG	5:E:862:7Q9:C310	0.80	2.07	6	8
6:E:819:17F:H58	6:E:819:17F:H44	0.80	1.51	20	8
6:D:501:17F:H39	6:D:501:17F:C11	0.80	2.07	13	3
6:D:510:17F:O9	6:D:516:17F:C9	0.80	2.30	6	19
6:E:817:17F:H59	5:E:833:7Q9:C35	0.80	2.07	15	5
6:B:214:17F:H39	6:B:214:17F:C11	0.80	2.07	16	11
6:B:215:17F:H54	6:B:215:17F:H61	0.80	1.51	8	4
6:E:819:17F:H73	6:E:819:17F:C29	0.80	2.03	6	3
6:E:817:17F:H49	5:E:820:7Q9:C318	0.80	2.07	9	2
6:D:546:17F:H68	6:D:546:17F:H30	0.80	1.52	11	1
6:D:510:17F:C18	6:D:527:17F:H19A	0.79	2.06	9	5
6:D:511:17F:H39	6:D:511:17F:C37	0.79	2.06	15	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:872:17F:C33	6:E:872:17F:H55	0.79	2.07	13	7
6:E:807:17F:C24	6:E:809:17F:H62	0.79	2.03	4	3
5:D:504:7Q9:C32	6:D:516:17F:H31	0.79	2.06	6	1
6:D:510:17F:C12	6:D:516:17F:C8	0.79	2.61	15	13
6:E:818:17F:C27	6:E:818:17F:H78	0.79	2.06	3	7
6:D:510:17F:C42	6:D:510:17F:H53	0.79	2.06	18	4
6:D:527:17F:H42	5:D:535:7Q9:C310	0.79	2.07	6	6
5:E:869:7Q9:C14	6:E:872:17F:H8A	0.79	2.07	7	5
6:E:807:17F:C32	6:E:807:17F:H30	0.79	2.08	16	8
5:E:824:7Q9:C32	6:E:841:17F:H20A	0.79	2.08	2	5
6:D:533:17F:H65	6:D:533:17F:C32	0.79	2.07	14	2
6:B:219:17F:H41	5:D:545:7Q9:C39	0.79	2.07	11	6
6:E:838:17F:H40	6:E:838:17F:C1Z	0.79	2.08	6	7
6:D:510:17F:H19A	6:D:516:17F:H10	0.79	1.53	9	2
6:B:219:17F:H18	5:D:522:7Q9:C3	0.79	2.06	19	4
6:E:841:17F:H4A	6:E:841:17F:H2	0.79	1.53	3	1
6:D:501:17F:H61	6:D:501:17F:H46	0.79	1.52	19	3
6:B:214:17F:H6A	6:B:219:17F:H9	0.79	1.55	17	2
6:B:214:17F:C34	6:B:214:17F:H68	0.79	2.06	5	3
6:E:856:17F:H68	6:E:874:17F:C36	0.79	2.08	2	10
6:E:874:17F:H6	6:E:874:17F:P1	0.79	2.18	2	20
6:E:870:17F:H12	6:E:870:17F:H32	0.79	1.55	2	7
6:D:510:17F:H9	6:D:516:17F:C9	0.79	2.07	14	4
5:A:217:7Q9:C34	6:D:546:17F:H36	0.79	2.08	7	2
5:E:824:7Q9:C316	6:E:841:17F:H71	0.79	2.08	12	1
6:D:517:17F:H69	6:D:517:17F:H52	0.79	1.52	20	8
6:D:501:17F:C8	6:D:501:17F:H31	0.79	2.07	4	2
6:D:527:17F:H72	6:D:527:17F:H46	0.79	1.55	10	7
6:D:510:17F:H55	6:D:516:17F:H38	0.79	1.51	6	1
6:D:510:17F:C7	6:D:516:17F:H11A	0.79	2.06	8	4
6:D:510:17F:H19	5:D:524:7Q9:O32	0.79	1.76	9	2
6:D:501:17F:H37	5:D:509:7Q9:C22	0.79	2.07	18	2
2:E:555:SER:HA	6:E:872:17F:H65	0.79	1.53	15	10
6:D:510:17F:C19	6:D:516:17F:H10	0.79	2.08	9	2
6:E:807:17F:H20	6:E:809:17F:H20	0.79	1.55	6	1
6:A:208:17F:H37	5:A:211:7Q9:C36	0.79	2.08	16	2
6:E:807:17F:H20A	6:E:818:17F:C10	0.79	2.08	3	1
5:A:204:7Q9:C314	6:A:208:17F:H44	0.79	2.07	13	5
6:E:805:17F:H47	5:E:812:7Q9:C313	0.79	2.08	9	1
5:E:824:7Q9:C38	6:E:841:17F:H58	0.79	2.08	19	1
6:D:510:17F:C7	6:D:516:17F:H19A	0.78	2.08	2	16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:B:219:17F:H19	6:B:219:17F:H10A	0.78	1.52	11	4
6:D:510:17F:C5	6:D:527:17F:H19A	0.78	2.06	4	5
6:D:527:17F:C30	6:E:856:17F:H43	0.78	2.08	9	4
5:E:850:7Q9:C39	6:E:870:17F:H20A	0.78	2.08	10	2
5:E:850:7Q9:C35	6:E:870:17F:H20	0.78	2.09	12	5
6:E:805:17F:H72	6:E:805:17F:C30	0.78	2.09	20	3
6:E:818:17F:H31	6:E:818:17F:H8	0.78	1.52	2	1
6:D:510:17F:O2	6:D:516:17F:H6	0.78	1.79	10	4
6:E:818:17F:H45	6:E:818:17F:C41	0.78	2.04	20	2
6:E:856:17F:H78	6:E:874:17F:H61	0.78	1.55	14	1
6:D:510:17F:H49	6:D:516:17F:H67	0.78	1.55	8	10
6:E:801:17F:H49	6:E:801:17F:C42	0.78	2.08	20	9
6:E:819:17F:H18A	5:E:829:7Q9:O11	0.78	1.77	19	2
6:E:807:17F:H74	6:E:807:17F:H51	0.78	1.56	5	4
5:D:524:7Q9:O22	6:D:527:17F:H18	0.78	1.78	20	5
6:D:501:17F:H35	6:D:501:17F:C26	0.78	2.09	10	1
6:E:817:17F:H9	5:E:820:7Q9:C23	0.78	2.09	8	4
6:D:516:17F:H43	6:D:527:17F:H38	0.78	1.56	17	3
6:E:809:17F:H8A	5:E:810:7Q9:C34	0.78	2.08	16	3
6:E:838:17F:H19A	6:E:874:17F:H8	0.78	1.55	10	2
6:D:510:17F:O10	6:D:510:17F:H4	0.78	1.79	11	20
6:D:510:17F:H63	5:D:524:7Q9:C313	0.78	2.09	3	2
5:E:837:7Q9:O32	6:E:841:17F:H19	0.78	1.78	3	2
5:E:837:7Q9:C32	6:E:841:17F:H31	0.78	2.07	3	3
6:E:809:17F:H32	6:E:818:17F:H68	0.78	1.55	19	2
6:A:214:17F:H59	6:A:214:17F:H64	0.78	1.54	19	1
6:D:517:17F:H55	5:E:842:7Q9:C318	0.78	2.09	20	5
6:E:818:17F:H1A	5:E:835:7Q9:O14	0.78	1.79	6	4
6:D:510:17F:H18	6:D:516:17F:C10	0.78	2.04	20	5
6:E:807:17F:C31	6:E:819:17F:H12A	0.78	2.09	7	3
6:B:219:17F:H36	6:B:219:17F:C20	0.77	2.08	15	4
6:E:807:17F:H51	6:E:807:17F:H74	0.77	1.56	6	3
6:E:807:17F:H58	6:E:807:17F:H12	0.77	1.56	11	12
6:E:838:17F:H77	6:E:838:17F:H47	0.77	1.56	8	2
6:E:807:17F:H19	6:E:809:17F:H18	0.77	1.53	14	1
6:E:819:17F:H20	5:E:829:7Q9:O14	0.77	1.80	3	4
6:E:819:17F:H65	5:E:836:7Q9:C37	0.77	2.07	4	1
6:E:809:17F:C33	6:E:818:17F:H70	0.77	2.09	6	1
2:D:334:LEU:HB2	5:D:532:7Q9:C312	0.77	2.10	19	14
5:E:833:7Q9:O12	6:E:838:17F:H2	0.77	1.79	1	1
6:D:510:17F:C31	6:D:516:17F:H29	0.77	2.09	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:872:17F:H36	6:E:872:17F:H20A	0.77	1.55	13	11
6:B:208:17F:C1Z	6:B:214:17F:H10	0.77	2.08	3	3
6:D:517:17F:H57	6:D:517:17F:H40	0.77	1.54	3	5
6:B:214:17F:H75	5:B:217:7Q9:C37	0.77	2.08	6	4
6:E:801:17F:O10	6:E:807:17F:N1	0.77	2.18	18	4
6:E:809:17F:N1	6:E:818:17F:O10	0.77	2.17	20	1
6:E:809:17F:H60	6:E:818:17F:H71	0.77	1.55	1	3
5:E:834:7Q9:C34	6:E:855:17F:H19A	0.77	2.10	8	1
6:D:510:17F:H51	6:D:516:17F:H67	0.77	1.53	14	1
6:B:214:17F:H68	6:B:214:17F:C34	0.77	2.10	19	17
6:B:219:17F:H31	5:D:522:7Q9:C3	0.77	2.10	3	1
6:B:214:17F:H18	6:B:219:17F:H11A	0.77	1.56	7	1
6:D:510:17F:C20	6:D:516:17F:H9A	0.77	2.09	8	1
6:D:517:17F:H35	6:D:517:17F:H57	0.77	1.56	15	2
6:D:510:17F:O2	6:D:510:17F:N1	0.77	2.17	17	17
6:E:818:17F:C34	6:E:841:17F:H67	0.77	2.09	4	2
5:A:204:7Q9:C31	6:A:208:17F:H6	0.77	2.09	12	3
2:D:305:GLN:HE22	6:D:527:17F:H10A	0.77	1.38	10	4
5:D:525:7Q9:C311	5:D:525:7Q9:C37	0.77	2.59	16	15
6:E:872:17F:H57	6:E:872:17F:H62	0.77	1.56	4	11
6:D:510:17F:H57	6:D:527:17F:C34	0.77	2.09	2	2
6:D:511:17F:H76	6:E:828:17F:H50	0.77	1.55	2	2
5:E:824:7Q9:C35	6:E:841:17F:H56	0.77	2.09	9	3
6:D:501:17F:H2	5:D:508:7Q9:O13	0.77	1.79	12	1
6:E:838:17F:H50	6:E:874:17F:H51	0.77	1.56	14	1
6:E:856:17F:H70	6:E:874:17F:C34	0.77	2.10	14	3
6:E:807:17F:C1Y	6:E:818:17F:H9A	0.77	2.10	10	1
5:E:813:7Q9:C38	6:E:819:17F:H77	0.76	2.10	17	7
6:E:838:17F:H35	6:E:838:17F:C1Z	0.76	2.08	3	9
6:D:528:17F:H10A	6:D:528:17F:C33	0.76	2.10	8	7
6:E:855:17F:H68	6:E:855:17F:C22	0.76	2.09	10	7
6:B:214:17F:H18	6:B:219:17F:H8	0.76	1.56	4	1
5:D:537:7Q9:C1	6:D:546:17F:H29	0.76	2.09	12	2
5:E:808:7Q9:C32	6:E:811:17F:H12A	0.76	2.10	5	6
2:E:634:LEU:HB2	5:E:878:7Q9:C317	0.76	2.11	17	2
5:D:506:7Q9:C36	6:D:517:17F:H56	0.76	2.10	2	2
6:D:510:17F:C9	6:D:516:17F:H10A	0.76	2.09	11	3
6:E:818:17F:H40	6:E:819:17F:H41	0.76	1.56	8	1
5:E:802:7Q9:C310	6:E:807:17F:H45	0.76	2.09	15	4
6:D:533:17F:H63	6:D:533:17F:C22	0.76	2.10	10	5
6:B:208:17F:H43	6:B:208:17F:C33	0.76	2.10	5	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:B:215:17F:H40	5:E:821:7Q9:C315	0.76	2.08	17	3
6:E:818:17F:H46	5:E:835:7Q9:C311	0.76	2.10	17	5
6:D:528:17F:H49	5:E:852:7Q9:C317	0.76	2.10	10	1
6:D:510:17F:C6	6:D:527:17F:H20A	0.76	2.06	14	1
6:E:870:17F:C21	6:E:870:17F:H58	0.76	2.10	11	10
6:D:510:17F:C20	6:D:516:17F:H10	0.76	2.09	11	2
3:B:201:GSP:H5'1	3:B:201:GSP:S1G	0.76	2.21	6	1
5:D:507:7Q9:C39	6:D:516:17F:H60	0.76	2.10	15	7
6:E:838:17F:H40	6:E:838:17F:H33	0.76	1.55	13	1
6:E:818:17F:H41	6:E:818:17F:C37	0.76	2.07	15	1
5:B:212:7Q9:C34	5:B:212:7Q9:C39	0.76	2.63	19	1
6:B:208:17F:H41	6:B:214:17F:H12A	0.76	1.55	1	2
6:B:214:17F:H69	6:B:219:17F:H12	0.76	1.55	4	1
6:E:801:17F:H77	6:E:801:17F:H49	0.76	1.55	14	4
6:E:818:17F:H1A	5:E:835:7Q9:O13	0.76	1.80	11	3
5:D:515:7Q9:C12	6:D:517:17F:H4A	0.76	2.10	7	1
6:E:841:17F:H42	6:E:841:17F:H56	0.76	1.58	7	1
6:E:807:17F:H63	6:E:807:17F:C12	0.76	2.10	15	1
6:D:510:17F:C19	6:D:527:17F:C19	0.76	2.62	1	4
5:E:848:7Q9:C34	5:E:851:7Q9:C32	0.76	2.64	17	14
6:D:527:17F:H77	6:D:527:17F:C28	0.76	2.08	5	4
6:D:528:17F:H35	5:D:532:7Q9:C315	0.76	2.10	19	3
5:D:524:7Q9:C2	6:D:527:17F:H18	0.76	2.11	9	2
6:D:501:17F:H4	6:D:501:17F:O10	0.76	1.79	5	13
6:D:510:17F:C1	6:D:516:17F:H4	0.76	2.11	7	10
6:E:807:17F:H51	6:E:807:17F:C42	0.76	2.10	4	7
5:A:215:7Q9:O14	6:D:534:17F:H43	0.76	1.80	4	1
6:B:208:17F:H57	6:B:214:17F:H10	0.76	1.57	5	1
6:D:533:17F:H48	5:D:543:7Q9:C23	0.76	2.10	7	2
2:E:674:LEU:HD21	6:E:855:17F:H35	0.76	1.58	9	9
6:D:501:17F:H76	6:E:807:17F:H53	0.76	1.57	19	1
6:E:838:17F:C33	6:E:838:17F:H9A	0.75	2.11	2	11
6:D:516:17F:H48	6:D:516:17F:C33	0.75	2.11	2	1
2:E:663:LEU:HD21	6:E:874:17F:H42	0.75	1.57	19	4
6:E:870:17F:H6A	6:E:870:17F:O10	0.75	1.78	3	5
1:A:31:GLU:HB2	1:B:128:LYS:HD3	0.75	1.58	18	1
6:D:534:17F:H58	6:D:534:17F:C1X	0.75	2.08	16	6
6:E:801:17F:H33	6:E:801:17F:C2X	0.75	2.11	15	10
6:D:510:17F:C28	6:D:516:17F:H37	0.75	2.11	5	2
6:D:510:17F:C9	6:D:516:17F:H11A	0.75	2.12	6	1
6:E:819:17F:H69	6:E:819:17F:H52	0.75	1.58	11	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:870:17F:H58	6:E:870:17F:H35	0.75	1.58	20	10
6:E:838:17F:C28	6:E:874:17F:H55	0.75	2.11	20	3
6:B:219:17F:H52	5:E:846:7Q9:C317	0.75	2.11	10	6
2:E:620:GLU:HA	5:E:858:7Q9:C311	0.75	2.12	18	14
5:E:850:7Q9:C315	6:E:870:17F:H20	0.75	2.12	3	3
6:D:510:17F:H12	6:D:516:17F:H8	0.75	1.57	8	2
6:D:501:17F:H20A	6:D:501:17F:O9	0.75	1.81	12	3
6:E:807:17F:H49	6:E:809:17F:H62	0.75	1.56	5	6
6:B:208:17F:H64	6:B:208:17F:H39	0.75	1.58	17	4
6:D:510:17F:O6	6:D:516:17F:H4A	0.75	1.80	13	17
6:D:511:17F:H66	6:D:511:17F:C23	0.75	2.11	15	10
6:B:208:17F:H4	6:B:208:17F:O10	0.75	1.80	4	13
5:A:204:7Q9:C312	6:A:208:17F:H65	0.75	2.11	4	4
6:B:214:17F:C1Z	6:B:219:17F:H37	0.75	2.11	15	5
6:E:818:17F:H10A	6:E:819:17F:H10A	0.75	1.58	13	4
5:E:814:7Q9:C318	6:E:828:17F:H67	0.75	2.11	3	7
5:E:802:7Q9:C314	6:E:809:17F:H66	0.75	2.11	2	4
6:E:856:17F:C39	6:E:874:17F:H68	0.75	2.11	9	4
6:E:872:17F:C23	6:E:872:17F:H20	0.75	2.10	3	7
5:A:204:7Q9:C315	6:E:811:17F:H70	0.75	2.12	4	1
6:D:546:17F:C7	6:D:546:17F:H57	0.75	2.12	14	15
5:E:806:7Q9:C13	6:E:817:17F:H4A	0.75	2.12	3	2
6:E:818:17F:H10	6:E:819:17F:C10	0.75	2.12	16	11
6:E:838:17F:H38	5:E:857:7Q9:C39	0.75	2.12	11	5
6:E:872:17F:H20	6:E:872:17F:H39	0.75	1.57	13	14
6:E:801:17F:H31	5:E:803:7Q9:C23	0.75	2.12	18	7
6:A:214:17F:H37	6:A:214:17F:H20	0.75	1.58	12	3
6:D:501:17F:C41	6:E:809:17F:H55	0.75	2.03	20	3
6:D:546:17F:H41	6:D:546:17F:C37	0.75	2.09	11	3
6:D:516:17F:O10	6:D:516:17F:H6A	0.75	1.81	12	9
6:E:872:17F:H48	6:E:872:17F:H60	0.75	1.56	13	8
6:E:856:17F:H11	6:E:874:17F:C32	0.75	2.11	19	6
5:E:802:7Q9:C313	6:E:805:17F:H64	0.75	2.11	8	2
6:B:214:17F:C5	6:B:219:17F:H9	0.75	2.10	20	3
6:D:527:17F:H36	6:D:527:17F:H42	0.74	1.57	13	5
5:D:507:7Q9:C32	6:D:516:17F:H32	0.74	2.12	15	4
6:E:818:17F:H10A	6:E:819:17F:C1X	0.74	2.11	19	4
6:E:818:17F:C41	6:E:818:17F:H45	0.74	2.12	9	1
5:D:504:7Q9:C3	6:D:516:17F:H18A	0.74	2.11	10	3
6:D:501:17F:C42	6:E:818:17F:H51	0.74	2.12	14	1
6:D:501:17F:C12	6:D:501:17F:C8	0.74	2.65	8	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:B:207:7Q9:C13	6:D:501:17F:H18A	0.74	2.12	2	1
6:A:208:17F:H31	6:B:208:17F:C21	0.74	2.11	4	1
5:E:824:7Q9:C35	6:E:841:17F:H30	0.74	2.12	20	5
6:B:215:17F:H48	6:B:215:17F:H67	0.74	1.57	13	2
6:D:516:17F:H35	6:D:527:17F:H38	0.74	1.56	10	1
5:E:832:7Q9:C23	6:E:838:17F:H4	0.74	2.13	13	2
6:D:510:17F:H4A	6:D:516:17F:H4A	0.74	1.59	8	5
6:D:510:17F:C18	6:D:516:17F:H8	0.74	2.11	2	6
5:E:802:7Q9:C315	6:E:809:17F:H70	0.74	2.12	19	2
6:E:809:17F:C1Y	6:E:818:17F:H68	0.74	2.13	19	1
6:D:511:17F:C42	6:E:828:17F:H54	0.74	2.12	5	7
5:E:813:7Q9:C314	6:E:818:17F:H54	0.74	2.12	11	7
6:B:208:17F:H33	6:B:214:17F:H41	0.74	1.57	2	3
6:B:208:17F:H57	6:B:214:17F:H45	0.74	1.59	2	1
6:E:807:17F:H51	6:E:807:17F:H75	0.74	1.56	20	9
6:B:215:17F:H12A	5:B:216:7Q9:C38	0.74	2.13	5	3
6:D:510:17F:C26	6:D:516:17F:H67	0.74	2.11	20	3
6:A:214:17F:H35	6:A:214:17F:C24	0.74	2.10	5	8
5:E:848:7Q9:C315	5:E:851:7Q9:C38	0.74	2.65	18	6
6:D:510:17F:H8A	6:D:516:17F:C1Z	0.74	2.07	3	2
6:D:510:17F:C9	6:D:516:17F:C8	0.74	2.65	6	3
6:E:801:17F:C31	6:E:801:17F:C35	0.74	2.61	7	4
6:A:208:17F:C19	6:B:208:17F:H37	0.74	2.13	8	3
5:E:802:7Q9:C312	6:E:805:17F:H64	0.74	2.13	4	2
6:E:819:17F:H61	5:E:836:7Q9:C34	0.74	2.12	6	2
6:D:527:17F:C37	6:D:527:17F:H58	0.74	2.13	14	1
6:E:811:17F:H75	5:E:822:7Q9:C315	0.74	2.11	20	2
5:D:508:7Q9:C313	6:E:818:17F:H52	0.74	2.12	13	6
6:B:219:17F:C20	6:B:219:17F:H36	0.74	2.12	16	2
6:B:214:17F:H46	6:B:214:17F:H75	0.74	1.58	14	1
6:E:809:17F:H53	6:E:818:17F:C42	0.74	2.13	15	2
6:D:546:17F:H56	6:D:546:17F:H62	0.74	1.58	17	18
6:E:818:17F:H42	5:E:835:7Q9:C311	0.74	2.13	13	5
6:E:838:17F:H57	6:E:838:17F:H35	0.74	1.60	1	1
6:B:219:17F:H71	5:D:522:7Q9:C311	0.74	2.13	19	1
6:E:818:17F:H42	5:E:835:7Q9:C310	0.73	2.13	5	7
6:E:818:17F:H61	6:E:841:17F:H68	0.73	1.59	7	3
6:D:546:17F:H66	6:D:546:17F:C24	0.73	2.10	11	1
6:E:818:17F:H67	6:E:818:17F:C24	0.73	2.05	15	1
6:D:510:17F:H46	6:D:516:17F:C36	0.73	2.13	9	10
6:E:838:17F:H71	6:E:838:17F:H48	0.73	1.61	8	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:B:219:17F:H33	5:D:522:7Q9:C37	0.73	2.12	5	9
5:D:505:7Q9:C316	6:E:819:17F:H74	0.73	2.14	11	2
2:D:305:GLN:NE2	6:D:527:17F:H10A	0.73	1.97	10	6
5:D:504:7Q9:C318	6:D:511:17F:H74	0.73	2.12	11	2
2:E:638:GLN:HB2	5:E:862:7Q9:C312	0.73	2.13	2	8
1:A:68:ARG:HG2	1:A:72:MET:HE3	0.73	1.60	10	5
2:E:660:ARG:HD2	6:E:874:17F:H20A	0.73	1.60	4	3
6:B:214:17F:H46	6:B:214:17F:H76	0.73	1.58	11	2
6:B:208:17F:H31	6:B:214:17F:H12	0.73	1.58	12	1
5:E:857:7Q9:C36	6:E:874:17F:H37	0.73	2.13	10	7
5:B:217:7Q9:C37	5:B:217:7Q9:C311	0.73	2.64	6	5
5:D:505:7Q9:C310	6:D:511:17F:H52	0.73	2.14	9	6
5:E:857:7Q9:C31	6:E:874:17F:H10A	0.73	2.12	16	5
6:D:511:17F:H4	6:D:511:17F:O10	0.73	1.83	6	20
6:B:214:17F:C33	6:B:214:17F:H68	0.73	2.14	4	1
5:B:217:7Q9:C311	5:B:217:7Q9:C37	0.73	2.65	12	11
5:D:537:7Q9:C32	6:D:546:17F:H11A	0.73	2.12	11	1
5:D:507:7Q9:C32	6:D:516:17F:H31	0.73	2.13	14	3
5:D:537:7Q9:O14	5:D:537:7Q9:C3	0.73	2.37	1	3
6:E:801:17F:C35	6:E:801:17F:C31	0.73	2.64	12	13
6:D:510:17F:C12	6:D:516:17F:H8	0.73	2.13	15	4
6:D:501:17F:H42	5:D:508:7Q9:C36	0.73	2.13	11	1
6:E:809:17F:C30	6:E:818:17F:H77	0.73	2.14	16	2
6:D:510:17F:C8	6:D:516:17F:C19	0.73	2.64	14	12
6:B:219:17F:H29	6:B:219:17F:C18	0.73	2.07	17	2
6:E:807:17F:H18A	6:E:809:17F:C20	0.73	2.09	14	2
6:E:856:17F:H65	6:E:874:17F:H60	0.73	1.59	8	2
6:D:528:17F:H29	5:D:532:7Q9:C315	0.73	2.13	13	4
6:E:856:17F:C37	6:E:874:17F:H61	0.73	2.13	8	3
6:B:208:17F:H54	6:B:208:17F:C39	0.73	2.13	4	10
5:D:506:7Q9:C36	6:D:517:17F:H57	0.73	2.14	6	1
5:D:513:7Q9:O22	6:D:528:17F:H10	0.73	1.84	8	1
6:D:528:17F:C22	6:D:528:17F:H69	0.73	2.13	15	2
6:D:516:17F:H11A	6:D:527:17F:H31	0.73	1.60	14	1
2:E:726:LYS:HD3	6:E:870:17F:H11	0.73	1.59	15	2
6:E:818:17F:H74	6:E:818:17F:C26	0.73	2.10	20	1
2:E:659:LEU:HD23	6:E:856:17F:H67	0.73	1.61	20	4
6:E:838:17F:N1	6:E:874:17F:O8	0.73	2.21	9	13
1:A:32:TYR:HB2	3:A:201:GSP:H3'	0.73	1.60	10	1
6:B:214:17F:C17	6:B:219:17F:H9	0.73	2.14	5	2
6:E:838:17F:H37	5:E:857:7Q9:C310	0.73	2.13	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:510:17F:H4A	6:D:516:17F:C4	0.73	2.14	8	5
6:E:809:17F:H53	6:E:818:17F:H77	0.73	1.61	16	3
6:E:818:17F:H1A	5:E:837:7Q9:C11	0.73	2.14	14	1
6:B:215:17F:H67	6:B:215:17F:H50	0.72	1.61	1	1
6:D:510:17F:O7	6:D:516:17F:O7	0.72	2.07	2	20
6:E:809:17F:C33	6:E:818:17F:H71	0.72	2.14	1	3
5:E:869:7Q9:C21	6:E:872:17F:H10	0.72	2.14	12	1
1:B:68:ARG:HG2	1:B:72:MET:HE3	0.72	1.61	11	5
6:E:807:17F:H58	6:E:807:17F:C12	0.72	2.14	11	11
6:E:870:17F:H58	6:E:870:17F:C2X	0.72	2.14	2	18
5:E:834:7Q9:C318	6:E:855:17F:H70	0.72	2.14	6	6
6:E:807:17F:H75	6:E:818:17F:C30	0.72	2.14	4	3
5:E:832:7Q9:C23	6:E:838:17F:H6A	0.72	2.14	20	1
6:A:214:17F:H50	5:E:840:7Q9:C317	0.72	2.14	16	5
6:D:516:17F:H41	6:D:527:17F:C22	0.72	2.15	19	5
5:E:802:7Q9:O32	6:E:807:17F:H5	0.72	1.84	10	14
6:A:214:17F:H41	5:E:840:7Q9:C318	0.72	2.13	5	3
6:E:838:17F:H56	6:E:838:17F:C19	0.72	2.13	20	20
6:A:214:17F:H71	5:E:840:7Q9:C318	0.72	2.15	5	4
6:E:807:17F:H47	6:E:807:17F:C42	0.72	2.14	8	7
5:A:204:7Q9:C310	6:A:208:17F:H72	0.72	2.15	8	3
6:B:214:17F:H74	6:B:214:17F:C26	0.72	2.13	5	1
6:E:855:17F:O10	6:E:855:17F:H6A	0.72	1.84	5	17
5:A:204:7Q9:C317	6:E:811:17F:H46	0.72	2.14	6	4
6:D:528:17F:H37	6:D:528:17F:H69	0.72	1.61	19	2
6:B:219:17F:H58	5:D:522:7Q9:C38	0.72	2.14	20	9
5:E:861:7Q9:C314	5:E:861:7Q9:C310	0.72	2.68	8	20
6:D:501:17F:H36	6:D:501:17F:C33	0.72	2.13	2	1
6:E:874:17F:H6	6:E:874:17F:O3	0.72	1.85	20	12
6:E:811:17F:H5	5:E:823:7Q9:C11	0.72	2.15	5	9
6:E:809:17F:H29	6:E:809:17F:C23	0.72	2.14	6	6
6:D:527:17F:H57	6:D:527:17F:H6A	0.72	1.59	16	4
5:E:850:7Q9:C38	6:E:870:17F:H20A	0.72	2.13	10	1
6:D:534:17F:H12A	5:D:539:7Q9:C36	0.72	2.13	17	1
6:E:838:17F:N1	6:E:874:17F:H6A	0.72	2.00	10	5
5:E:850:7Q9:C313	6:E:870:17F:H20	0.72	2.14	19	2
5:A:204:7Q9:C310	6:A:208:17F:H57	0.72	2.14	20	6
6:E:819:17F:C31	6:E:819:17F:H44	0.72	2.14	9	1
5:D:544:7Q9:C22	6:D:546:17F:H19	0.72	2.15	18	1
6:E:805:17F:H4A	5:E:810:7Q9:C14	0.72	2.15	5	1
6:E:809:17F:H60	6:E:818:17F:C39	0.72	2.14	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:527:17F:H48	6:E:874:17F:H75	0.72	1.59	7	1
6:D:517:17F:H40	6:D:517:17F:H59	0.72	1.61	11	5
6:D:534:17F:H8	5:D:539:7Q9:C33	0.72	2.15	5	5
1:A:37:GLU:HG2	1:A:56:LEU:HD11	0.72	1.61	20	3
6:D:510:17F:C31	6:D:516:17F:H10A	0.72	2.11	6	1
6:B:208:17F:H75	5:B:212:7Q9:C316	0.72	2.14	17	1
5:A:217:7Q9:O13	6:D:546:17F:N1	0.72	2.23	1	4
6:E:856:17F:H5	6:E:856:17F:O1	0.72	1.85	3	8
6:B:208:17F:H44	6:B:214:17F:H41	0.72	1.61	3	1
6:D:501:17F:H39	6:D:501:17F:C12	0.72	2.14	15	3
6:D:516:17F:H60	6:D:516:17F:H48	0.72	1.61	3	1
6:E:856:17F:H57	6:E:856:17F:H40	0.72	1.60	16	6
6:B:214:17F:H46	5:B:217:7Q9:C38	0.72	2.15	7	1
6:D:501:17F:C33	6:D:501:17F:H41	0.72	2.15	20	1
2:E:638:GLN:HB2	5:E:862:7Q9:C311	0.71	2.15	16	12
6:A:208:17F:C1Y	6:B:208:17F:H37	0.71	2.10	3	3
6:B:214:17F:O9	6:B:219:17F:H11A	0.71	1.84	16	4
6:E:807:17F:H1	5:E:813:7Q9:C14	0.71	2.14	18	4
6:B:214:17F:H74	6:B:214:17F:C27	0.71	2.13	18	3
6:D:511:17F:C41	6:E:828:17F:H54	0.71	2.14	20	1
6:E:818:17F:H2	6:E:818:17F:O2	0.71	1.84	13	15
6:E:805:17F:H44	5:E:816:7Q9:C317	0.71	2.14	20	7
6:E:841:17F:H37	5:E:876:7Q9:O31	0.71	1.85	3	3
6:A:208:17F:C27	6:E:811:17F:H70	0.71	2.14	3	1
6:D:527:17F:H78	6:D:527:17F:H50	0.71	1.62	14	1
6:D:533:17F:H6	5:D:543:7Q9:C15	0.71	2.14	17	1
5:E:848:7Q9:C313	5:E:851:7Q9:C311	0.71	2.68	15	11
5:B:211:7Q9:C316	6:B:215:17F:H34	0.71	2.15	8	2
2:D:429:PHE:HZ	6:D:533:17F:H41	0.71	1.43	11	1
3:A:201:GSP:H5'1	3:A:201:GSP:PG	0.71	2.25	14	1
6:E:838:17F:H12	6:E:856:17F:H9A	0.71	1.62	1	2
6:E:838:17F:C10	6:E:856:17F:H35	0.71	2.15	20	3
6:E:856:17F:H36	6:E:856:17F:H57	0.71	1.61	6	5
6:B:208:17F:H43	6:B:208:17F:H34	0.71	1.63	15	2
5:D:513:7Q9:C2	6:D:528:17F:H8A	0.71	2.15	8	1
2:E:633:LYS:HB3	5:E:878:7Q9:C318	0.71	2.16	19	3
6:D:501:17F:O1	6:D:501:17F:H19A	0.71	1.84	10	1
5:E:857:7Q9:C3	6:E:874:17F:H2	0.71	2.15	10	1
6:D:546:17F:H42	6:D:546:17F:H33	0.71	1.60	11	1
6:E:801:17F:N1	5:E:808:7Q9:O22	0.71	2.22	12	1
6:D:510:17F:H53	6:D:510:17F:H76	0.71	1.61	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:809:17F:H51	6:E:818:17F:C41	0.71	2.15	20	1
6:D:510:17F:O7	6:D:516:17F:H9A	0.71	1.86	13	10
6:D:517:17F:H52	6:D:517:17F:C38	0.71	2.15	20	6
6:D:546:17F:H73	6:D:546:17F:C36	0.71	2.13	2	2
5:E:869:7Q9:C23	6:E:872:17F:H12A	0.71	2.16	5	1
2:E:674:LEU:HD11	6:E:855:17F:H35	0.71	1.61	11	3
2:E:555:SER:HA	6:E:872:17F:H67	0.71	1.60	13	1
5:D:505:7Q9:C2	6:D:511:17F:H6	0.71	2.16	18	1
6:D:510:17F:O7	6:D:516:17F:H11A	0.71	1.86	8	4
6:E:818:17F:H30	5:E:835:7Q9:C37	0.71	2.15	9	4
6:D:533:17F:C42	6:E:870:17F:H68	0.71	2.11	13	2
6:A:214:17F:H55	6:A:214:17F:C40	0.71	2.15	7	4
6:E:838:17F:HN1A	6:E:874:17F:H6A	0.71	1.45	13	3
6:A:208:17F:H31	6:B:208:17F:C1X	0.71	2.15	20	5
2:D:333:LYS:HD2	5:E:878:7Q9:C318	0.71	2.16	17	2
6:B:215:17F:H43	5:E:810:7Q9:C318	0.71	2.16	7	1
6:D:510:17F:H54	6:D:516:17F:H71	0.71	1.61	8	4
6:D:510:17F:C29	6:D:510:17F:H67	0.71	2.15	16	1
5:E:806:7Q9:C31	5:E:806:7Q9:C21	0.71	2.68	9	5
6:E:805:17F:H45	6:E:805:17F:H72	0.71	1.62	5	2
6:E:819:17F:C22	6:E:819:17F:C26	0.71	2.69	11	17
6:B:215:17F:H67	6:B:215:17F:C30	0.71	2.15	5	3
6:B:215:17F:H19A	6:D:517:17F:H60	0.71	1.62	6	1
6:D:546:17F:O8	6:D:546:17F:H57	0.71	1.86	7	2
6:E:809:17F:H9A	6:E:809:17F:H18A	0.71	1.62	9	1
6:E:809:17F:H34	6:E:818:17F:H64	0.71	1.63	11	1
2:D:312:MET:HE1	6:D:527:17F:H70	0.71	1.60	13	3
6:B:214:17F:H47	5:B:217:7Q9:C312	0.71	2.16	19	1
6:E:828:17F:O10	6:E:828:17F:H6A	0.71	1.85	17	20
6:A:214:17F:H54	5:E:840:7Q9:C317	0.71	2.16	19	6
6:E:818:17F:H1A	5:E:835:7Q9:P	0.71	2.26	11	3
6:B:214:17F:H19A	6:B:219:17F:H11A	0.71	1.62	5	3
5:D:544:7Q9:O31	6:D:546:17F:H18	0.71	1.86	20	3
5:D:544:7Q9:O21	6:D:546:17F:H18	0.70	1.86	1	1
6:D:501:17F:H45	6:D:501:17F:C2X	0.70	2.15	10	4
6:D:501:17F:C8	6:D:501:17F:C12	0.70	2.67	6	8
6:D:516:17F:C28	6:D:516:17F:H60	0.70	2.16	4	1
5:B:206:7Q9:O32	5:B:206:7Q9:C1	0.70	2.38	8	7
6:D:501:17F:H44	5:D:508:7Q9:C35	0.70	2.17	15	2
6:E:874:17F:H10	6:E:874:17F:O7	0.70	1.85	9	1
5:E:850:7Q9:C39	6:E:870:17F:H60	0.70	2.15	14	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:829:7Q9:P	5:E:829:7Q9:O22	0.70	2.49	13	6
6:E:807:17F:H38	6:E:809:17F:H58	0.70	1.61	14	3
3:A:201:GSP:O1B	3:A:201:GSP:S1G	0.70	2.50	9	3
6:D:527:17F:H58	6:D:527:17F:H67	0.70	1.63	14	1
6:D:510:17F:C28	6:D:516:17F:H64	0.70	2.16	17	1
6:D:501:17F:H37	5:D:509:7Q9:C23	0.70	2.15	20	3
6:E:818:17F:H12A	6:E:819:17F:C1X	0.70	2.14	3	4
5:B:212:7Q9:C38	5:B:212:7Q9:C313	0.70	2.69	2	3
6:B:214:17F:H68	6:B:214:17F:H61	0.70	1.62	2	2
6:E:856:17F:O8	6:E:856:17F:C4	0.70	2.40	4	10
6:A:208:17F:H19A	6:B:208:17F:H37	0.70	1.64	8	2
5:B:209:7Q9:C317	5:B:209:7Q9:C313	0.70	2.70	20	16
6:E:872:17F:H20	6:E:872:17F:C23	0.70	2.17	13	5
1:A:82:PHE:HB2	1:A:89:SER:HB2	0.70	1.62	13	4
6:D:517:17F:H76	5:D:541:7Q9:C317	0.70	2.17	4	1
6:E:807:17F:C33	6:E:819:17F:H12A	0.70	2.15	14	3
6:E:807:17F:C19	6:E:818:17F:H9A	0.70	2.15	9	5
2:E:634:LEU:HD22	5:E:878:7Q9:C316	0.70	2.17	11	1
5:E:820:7Q9:C3	6:E:838:17F:H4A	0.70	2.17	14	2
5:B:206:7Q9:C313	5:B:206:7Q9:C317	0.70	2.70	7	20
5:B:212:7Q9:O11	5:B:212:7Q9:C31	0.70	2.39	2	3
5:A:204:7Q9:C312	6:A:208:17F:H35	0.70	2.15	3	3
6:E:805:17F:H69	5:E:816:7Q9:C317	0.70	2.17	16	5
6:D:510:17F:H47	6:D:516:17F:C21	0.70	2.17	18	1
6:D:501:17F:H58	6:D:501:17F:H65	0.70	1.61	1	2
5:E:808:7Q9:C33	5:E:808:7Q9:C37	0.70	2.70	12	20
6:D:510:17F:H65	6:D:527:17F:H74	0.70	1.62	2	2
5:E:824:7Q9:O32	5:E:824:7Q9:C1	0.70	2.40	15	11
5:D:506:7Q9:C311	6:D:517:17F:H44	0.70	2.16	5	1
6:E:801:17F:H49	6:E:801:17F:H78	0.70	1.64	6	2
2:D:331:ARG:HA	5:D:532:7Q9:C310	0.70	2.16	10	6
6:D:501:17F:H46	5:D:508:7Q9:C316	0.70	2.17	9	2
5:E:832:7Q9:C23	6:E:856:17F:H6A	0.70	2.16	1	2
5:E:815:7Q9:C31	5:E:815:7Q9:O11	0.70	2.40	20	15
5:E:824:7Q9:C318	6:E:841:17F:H68	0.70	2.16	11	3
6:D:510:17F:H19A	5:D:524:7Q9:C3	0.70	2.17	14	2
6:E:818:17F:C10	6:E:819:17F:H30	0.70	2.16	19	2
5:B:212:7Q9:C318	6:E:805:17F:H77	0.70	2.17	16	6
2:E:733:LEU:HA	5:E:875:7Q9:C311	0.70	2.16	16	9
6:D:510:17F:C9	6:D:516:17F:O7	0.70	2.38	6	1
6:E:872:17F:C20	6:E:872:17F:H39	0.69	2.17	13	11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:501:17F:H40	6:D:501:17F:C12	0.69	2.16	7	2
6:E:805:17F:H6A	5:E:816:7Q9:C32	0.69	2.16	13	1
6:E:870:17F:H64	6:E:870:17F:H43	0.69	1.63	20	2
6:A:214:17F:H8A	5:D:539:7Q9:C3	0.69	2.17	1	1
6:A:214:17F:H42	6:A:214:17F:C2X	0.69	2.17	17	6
6:E:807:17F:H46	6:E:809:17F:C35	0.69	2.18	20	3
6:D:533:17F:O10	6:D:533:17F:H6A	0.69	1.86	7	15
6:E:809:17F:C2X	6:E:809:17F:H57	0.69	2.16	1	1
5:E:845:7Q9:C314	5:E:845:7Q9:C310	0.69	2.69	11	20
6:D:501:17F:H46	6:D:501:17F:C35	0.69	2.17	20	1
6:E:819:17F:H44	6:E:819:17F:C32	0.69	2.16	14	15
6:E:805:17F:H54	6:E:805:17F:H68	0.69	1.64	12	4
6:E:841:17F:H38	5:E:876:7Q9:C34	0.69	2.17	6	3
5:D:507:7Q9:C32	6:D:516:17F:H20	0.69	2.17	4	2
6:E:874:17F:O1	6:E:874:17F:H6	0.69	1.87	6	3
6:E:818:17F:H10	6:E:819:17F:H9A	0.69	1.64	15	1
6:A:208:17F:O8	6:A:208:17F:C4	0.69	2.40	4	19
5:D:513:7Q9:C314	5:D:513:7Q9:C310	0.69	2.71	12	20
5:D:506:7Q9:C34	6:D:517:17F:H37	0.69	2.18	4	1
6:A:208:17F:H69	6:B:208:17F:H78	0.69	1.61	11	1
6:E:805:17F:H45	6:E:805:17F:H68	0.69	1.64	12	3
6:E:801:17F:O8	6:E:801:17F:C17	0.69	2.40	17	19
6:E:856:17F:H68	6:E:874:17F:C34	0.69	2.12	5	5
6:E:870:17F:H38	6:E:870:17F:H64	0.69	1.63	9	5
6:B:215:17F:H41	6:B:215:17F:H66	0.69	1.64	4	2
6:D:501:17F:H12	5:D:509:7Q9:C22	0.69	2.18	11	1
6:E:817:17F:H61	5:E:826:7Q9:C34	0.69	2.18	15	1
6:D:533:17F:C31	6:D:533:17F:C19	0.69	2.69	7	16
6:E:807:17F:H71	6:E:818:17F:H47	0.69	1.62	3	5
6:B:214:17F:H57	5:B:220:7Q9:C34	0.69	2.18	19	5
6:D:501:17F:C10	6:D:501:17F:H56	0.69	2.18	3	3
6:D:533:17F:H62	6:D:533:17F:C21	0.69	2.16	7	6
6:A:214:17F:H29	6:A:214:17F:C32	0.69	2.17	8	2
6:E:807:17F:H30	6:E:807:17F:H59	0.69	1.63	16	4
6:E:855:17F:H37	5:E:857:7Q9:C317	0.69	2.17	12	1
2:E:631:ARG:HG2	5:E:878:7Q9:C37	0.69	2.17	9	3
2:E:656:VAL:HG13	6:E:856:17F:H64	0.69	1.61	6	8
6:E:838:17F:C40	6:E:856:17F:H41	0.69	2.13	1	3
6:B:219:17F:H33	5:D:522:7Q9:C38	0.69	2.17	5	1
6:B:214:17F:H48	6:B:214:17F:C41	0.69	2.16	16	3
5:E:816:7Q9:O12	5:E:816:7Q9:O32	0.69	2.10	9	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:807:17F:H49	6:E:809:17F:H65	0.69	1.65	15	2
6:D:516:17F:H37	6:D:516:17F:H62	0.69	1.63	18	1
5:A:209:7Q9:C313	6:A:214:17F:H62	0.69	2.18	1	1
5:B:206:7Q9:C316	6:E:805:17F:H53	0.69	2.18	20	8
6:B:214:17F:C35	6:B:214:17F:H56	0.69	2.17	1	2
5:D:514:7Q9:C33	5:D:514:7Q9:C37	0.69	2.70	17	13
6:D:534:17F:H44	6:D:534:17F:C34	0.69	2.17	5	6
5:D:537:7Q9:O32	6:D:546:17F:H10A	0.69	1.87	2	1
6:D:516:17F:H49	6:D:516:17F:C24	0.69	2.18	4	3
5:A:203:7Q9:C316	6:E:801:17F:H53	0.69	2.18	17	4
6:D:546:17F:H56	6:D:546:17F:C37	0.69	2.17	11	2
6:D:510:17F:H67	6:D:510:17F:H51	0.69	1.65	20	5
6:E:809:17F:C29	6:E:818:17F:H77	0.69	2.17	13	3
6:D:501:17F:C34	6:D:501:17F:C10	0.69	2.70	13	2
6:E:801:17F:H77	6:E:801:17F:C28	0.69	2.18	14	2
6:D:511:17F:H74	6:E:828:17F:H54	0.69	1.65	20	1
5:A:204:7Q9:C312	6:A:208:17F:H57	0.69	2.17	1	1
6:B:219:17F:H29	6:B:219:17F:C19	0.69	2.18	13	11
6:E:819:17F:C18	5:E:852:7Q9:C33	0.69	2.70	3	4
5:E:864:7Q9:C35	5:E:864:7Q9:C39	0.69	2.71	6	20
5:E:864:7Q9:C315	5:E:864:7Q9:C311	0.69	2.70	14	20
6:A:214:17F:H70	6:A:214:17F:H55	0.69	1.64	2	4
5:A:217:7Q9:C32	6:D:546:17F:H36	0.69	2.17	6	5
5:E:867:7Q9:C21	5:E:867:7Q9:O32	0.69	2.41	14	6
6:D:501:17F:C23	6:D:501:17F:C12	0.69	2.71	15	3
5:E:857:7Q9:C39	6:E:874:17F:H44	0.69	2.18	7	2
6:B:208:17F:H39	6:B:208:17F:C36	0.69	2.18	17	5
6:D:501:17F:H31	6:D:501:17F:C10	0.69	2.13	19	1
6:D:510:17F:C27	6:D:516:17F:H67	0.69	2.18	19	1
6:D:510:17F:C8	6:D:516:17F:H9	0.68	2.17	20	10
6:A:208:17F:H6A	6:B:208:17F:H37	0.68	1.62	2	1
6:E:856:17F:H46	6:E:856:17F:H59	0.68	1.64	14	9
6:D:533:17F:H6	5:D:543:7Q9:C12	0.68	2.18	4	1
5:D:544:7Q9:C313	6:D:546:17F:H50	0.68	2.18	5	4
6:A:208:17F:H69	6:B:208:17F:C40	0.68	2.18	6	1
2:D:305:GLN:OE1	6:D:527:17F:H10A	0.68	1.89	8	7
6:D:510:17F:O9	6:D:516:17F:H9	0.68	1.88	15	5
6:B:214:17F:O8	6:B:219:17F:H11A	0.68	1.88	10	1
6:B:215:17F:C18	6:D:501:17F:H9A	0.68	2.17	10	1
6:B:219:17F:H4A	6:B:219:17F:C2	0.68	2.17	11	1
5:E:802:7Q9:O32	6:E:807:17F:H6A	0.68	1.88	13	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:819:17F:H65	5:E:836:7Q9:C38	0.68	2.18	5	8
6:D:534:17F:C32	6:D:534:17F:H30	0.68	2.18	9	3
6:E:805:17F:C30	6:E:805:17F:H72	0.68	2.18	15	3
6:D:510:17F:C10	6:D:516:17F:H58	0.68	2.17	20	1
5:E:840:7Q9:O32	5:E:840:7Q9:C1	0.68	2.41	19	17
6:D:510:17F:C33	6:D:510:17F:H48	0.68	2.18	6	1
6:D:527:17F:C30	6:E:856:17F:H47	0.68	2.03	20	2
6:D:533:17F:H2	6:D:533:17F:H19	0.68	1.65	18	1
5:B:213:7Q9:C35	5:B:213:7Q9:C39	0.68	2.71	6	20
6:E:807:17F:H75	6:E:818:17F:H55	0.68	1.65	1	3
6:E:838:17F:H35	6:E:838:17F:C31	0.68	2.18	1	8
6:E:819:17F:H20A	6:E:819:17F:O9	0.68	1.89	10	2
5:E:824:7Q9:C34	6:E:841:17F:H20A	0.68	2.17	11	4
5:A:204:7Q9:C39	6:A:208:17F:H9A	0.68	2.17	9	9
1:A:32:TYR:CD1	3:A:201:GSP:H5'2	0.68	2.24	15	2
5:B:206:7Q9:C315	6:E:805:17F:H75	0.68	2.17	16	6
6:E:855:17F:H53	5:E:867:7Q9:C315	0.68	2.18	1	5
6:D:501:17F:H31	6:D:501:17F:C9	0.68	2.18	3	2
6:B:219:17F:H41	5:D:545:7Q9:C310	0.68	2.19	12	3
6:E:809:17F:H51	6:E:818:17F:H77	0.68	1.63	13	4
6:A:214:17F:H58	6:A:214:17F:H11	0.68	1.63	6	2
6:E:811:17F:H18A	5:E:815:7Q9:O13	0.68	1.87	11	1
6:E:818:17F:H62	5:E:824:7Q9:C318	0.68	2.19	12	1
6:D:546:17F:H70	6:D:546:17F:H45	0.68	1.65	2	1
6:E:807:17F:H20A	6:E:818:17F:C9	0.68	2.17	10	3
5:A:210:7Q9:C315	6:E:817:17F:H70	0.68	2.19	4	1
5:B:211:7Q9:C38	5:B:211:7Q9:C313	0.68	2.71	12	7
6:E:818:17F:H60	6:E:841:17F:H65	0.68	1.64	8	1
6:B:214:17F:H71	5:B:217:7Q9:C37	0.68	2.19	18	4
6:A:208:17F:H70	6:E:811:17F:H47	0.68	1.64	14	1
6:D:510:17F:O7	6:D:516:17F:C9	0.68	2.33	11	15
5:E:844:7Q9:C318	5:E:844:7Q9:C314	0.68	2.71	19	20
6:D:501:17F:H61	6:D:501:17F:C24	0.68	2.17	5	3
6:B:214:17F:H75	5:B:217:7Q9:C311	0.68	2.19	16	5
6:D:511:17F:H43	5:D:513:7Q9:C316	0.68	2.17	9	5
6:D:534:17F:H10	5:D:539:7Q9:C35	0.68	2.19	13	4
6:E:818:17F:H45	6:E:818:17F:C40	0.68	2.19	15	2
5:E:832:7Q9:C315	6:E:856:17F:H51	0.68	2.19	10	1
6:D:510:17F:O10	6:D:510:17F:C4	0.68	2.42	2	12
5:E:843:7Q9:C37	5:E:843:7Q9:C33	0.68	2.72	3	20
5:E:845:7Q9:C37	5:E:845:7Q9:C33	0.68	2.71	16	20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:855:17F:H2	5:E:857:7Q9:C13	0.68	2.17	2	3
6:E:838:17F:H77	6:E:838:17F:H48	0.68	1.64	19	5
3:B:201:GSP:O1A	3:B:201:GSP:O3G	0.68	2.12	10	1
6:D:501:17F:O1	6:D:501:17F:C20	0.68	2.38	18	6
6:A:208:17F:H5	6:A:208:17F:O1	0.68	1.88	1	8
5:D:506:7Q9:C317	6:E:841:17F:H74	0.68	2.19	20	4
6:D:527:17F:O9	6:D:527:17F:C1Y	0.68	2.36	10	14
6:D:528:17F:H69	6:D:528:17F:C21	0.68	2.19	1	5
6:D:546:17F:H31	6:D:546:17F:C17	0.68	2.19	17	20
6:E:807:17F:H20A	6:E:818:17F:H10A	0.68	1.65	3	1
6:D:510:17F:C6	6:D:516:17F:H11A	0.68	2.19	8	4
6:E:817:17F:H39	5:E:833:7Q9:C311	0.68	2.19	15	2
5:E:843:7Q9:C314	5:E:843:7Q9:C310	0.68	2.72	5	20
6:E:838:17F:H10A	6:E:856:17F:H35	0.68	1.63	2	3
5:E:852:7Q9:O21	5:E:852:7Q9:O14	0.68	2.12	2	13
6:A:208:17F:H32	6:B:208:17F:H30	0.68	1.63	13	4
6:E:809:17F:H51	6:E:818:17F:H72	0.68	1.64	9	3
6:E:817:17F:C11	5:E:833:7Q9:C33	0.68	2.72	20	6
5:E:848:7Q9:C313	5:E:851:7Q9:C314	0.68	2.72	16	3
6:B:208:17F:H1	6:B:208:17F:H4	0.67	1.64	6	3
5:D:505:7Q9:C11	6:D:511:17F:H4A	0.67	2.19	1	1
5:E:840:7Q9:C36	5:E:840:7Q9:C32	0.67	2.72	18	20
6:D:528:17F:H72	5:E:862:7Q9:C317	0.67	2.18	2	2
6:E:807:17F:H55	6:E:818:17F:C41	0.67	2.19	10	5
6:D:510:17F:H76	6:D:516:17F:C41	0.67	2.19	5	1
5:E:857:7Q9:C3	6:E:874:17F:H10	0.67	2.18	20	3
6:B:215:17F:H4	6:B:215:17F:O10	0.67	1.89	19	3
2:D:374:LEU:HD23	5:D:529:7Q9:C39	0.67	2.19	20	12
6:E:828:17F:N1	5:E:848:7Q9:O14	0.67	2.27	3	6
6:B:215:17F:H12	6:B:215:17F:C36	0.67	2.19	2	2
6:E:805:17F:H44	5:E:816:7Q9:C316	0.67	2.19	9	4
6:E:819:17F:H4A	6:E:819:17F:C7	0.67	2.20	7	10
6:E:841:17F:H2	6:E:841:17F:C4	0.67	2.18	3	1
6:B:214:17F:H57	5:B:220:7Q9:C36	0.67	2.19	5	1
6:E:841:17F:H56	6:E:841:17F:C24	0.67	2.19	7	1
5:E:857:7Q9:C310	6:E:874:17F:H48	0.67	2.19	7	2
5:E:824:7Q9:C37	6:E:841:17F:H58	0.67	2.19	11	3
6:D:546:17F:C24	6:D:546:17F:H33	0.67	2.19	11	1
6:A:208:17F:H38	5:E:823:7Q9:C318	0.67	2.19	12	1
5:D:505:7Q9:O13	5:D:505:7Q9:O21	0.67	2.13	18	1
6:D:510:17F:C27	6:D:516:17F:H38	0.67	2.19	19	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:B:208:17F:H41	6:B:214:17F:C12	0.67	2.19	1	3
6:B:219:17F:H57	6:B:219:17F:H62	0.67	1.65	10	10
2:D:269:GLN:O	6:D:534:17F:H34	0.67	1.88	1	2
6:E:817:17F:H5	6:E:817:17F:O8	0.67	1.90	5	11
6:E:819:17F:O10	6:E:819:17F:H6A	0.67	1.89	17	12
5:E:844:7Q9:C37	5:E:844:7Q9:C311	0.67	2.70	14	7
6:A:208:17F:H69	5:E:804:7Q9:C318	0.67	2.19	7	1
5:D:513:7Q9:C312	6:D:528:17F:H72	0.67	2.19	7	1
5:B:211:7Q9:C317	6:D:501:17F:H73	0.67	2.19	8	1
5:D:506:7Q9:C310	6:D:517:17F:H58	0.67	2.19	10	1
5:D:519:7Q9:C21	5:D:519:7Q9:O32	0.67	2.42	2	11
5:D:539:7Q9:C318	5:D:539:7Q9:C314	0.67	2.73	5	20
6:E:807:17F:H74	6:E:807:17F:C29	0.67	2.19	5	3
1:B:117:LYS:HE2	3:B:201:GSP:C4	0.67	2.24	17	1
3:A:201:GSP:O3G	3:A:201:GSP:O2B	0.67	2.12	7	4
6:B:219:17F:H44	6:B:219:17F:H59	0.67	1.65	12	10
6:B:219:17F:O10	6:B:219:17F:C6	0.67	2.41	13	8
6:E:807:17F:H30	6:E:807:17F:C32	0.67	2.19	5	4
6:E:841:17F:O5	6:E:841:17F:H4A	0.67	1.90	14	1
6:E:828:17F:C34	6:E:828:17F:H43	0.67	2.20	15	1
5:B:220:7Q9:C313	6:D:533:17F:H47	0.67	2.20	19	1
5:B:212:7Q9:C39	5:B:212:7Q9:C35	0.67	2.73	18	18
2:D:292:GLU:HG2	2:D:296:LYS:HE3	0.67	1.67	11	7
5:D:545:7Q9:C33	5:D:545:7Q9:C37	0.67	2.72	6	15
5:E:836:7Q9:C313	5:E:836:7Q9:C317	0.67	2.72	1	20
5:E:848:7Q9:C313	5:E:851:7Q9:C38	0.67	2.73	14	10
6:A:214:17F:H4	6:A:214:17F:O10	0.67	1.89	5	3
6:B:214:17F:H42	5:B:217:7Q9:C37	0.67	2.20	17	2
6:E:819:17F:H44	6:E:819:17F:H57	0.67	1.67	17	5
5:E:824:7Q9:C318	6:E:841:17F:H69	0.67	2.20	9	2
6:A:208:17F:H61	6:B:208:17F:C38	0.67	2.19	11	1
6:D:510:17F:H12	6:D:516:17F:C9	0.67	2.20	19	6
5:A:204:7Q9:O32	6:A:208:17F:N1	0.67	2.26	2	1
5:D:544:7Q9:C35	6:D:546:17F:H59	0.67	2.20	4	1
6:E:809:17F:HN1A	6:E:818:17F:H6	0.67	1.48	8	1
6:B:214:17F:O1	6:B:214:17F:H2	0.67	1.88	9	1
6:D:510:17F:H76	6:E:856:17F:H48	0.67	1.67	20	1
5:E:825:7Q9:C35	5:E:825:7Q9:C31	0.67	2.73	5	20
5:E:834:7Q9:C311	5:E:834:7Q9:C37	0.67	2.71	4	16
6:E:818:17F:H39	6:E:818:17F:C1X	0.67	2.09	2	15
5:D:507:7Q9:C310	6:D:516:17F:H69	0.67	2.19	3	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:201:GSP:O2A	3:A:201:GSP:S1G	0.67	2.52	13	4
6:E:801:17F:H46	5:E:806:7Q9:C316	0.67	2.20	8	2
6:E:807:17F:H66	6:E:819:17F:H29	0.67	1.67	14	2
2:D:429:PHE:CE1	6:D:533:17F:H66	0.67	2.24	10	3
6:B:214:17F:H75	5:B:217:7Q9:C312	0.67	2.20	9	5
5:A:204:7Q9:C31	5:A:204:7Q9:O11	0.67	2.43	10	1
6:D:501:17F:H29	5:D:509:7Q9:C22	0.67	2.20	19	3
5:D:503:7Q9:C318	5:D:503:7Q9:C314	0.67	2.73	14	3
6:D:528:17F:C24	6:D:528:17F:C28	0.67	2.73	15	19
6:E:801:17F:O8	6:E:801:17F:H10	0.67	1.89	16	12
5:E:848:7Q9:C310	5:E:851:7Q9:C311	0.67	2.73	15	13
6:E:874:17F:H6	6:E:874:17F:O1	0.67	1.90	13	14
6:E:809:17F:H61	6:E:818:17F:H71	0.67	1.65	10	3
1:A:118:CYS:SG	1:A:143:GLU:HB3	0.67	2.30	9	2
6:D:510:17F:H18A	6:D:527:17F:H20	0.67	1.67	20	3
2:D:333:LYS:HE2	2:E:630:ALA:HB1	0.67	1.66	19	1
6:B:219:17F:N1	5:B:220:7Q9:O13	0.66	2.29	1	1
6:E:838:17F:H12	6:E:856:17F:C1X	0.66	2.20	2	2
6:E:870:17F:H58	6:E:870:17F:C21	0.66	2.20	2	8
6:E:838:17F:H29	6:E:856:17F:H30	0.66	1.67	3	1
1:B:36:ILE:HA	1:B:59:ALA:HB2	0.66	1.67	16	3
5:B:206:7Q9:C35	5:B:212:7Q9:O32	0.66	2.43	13	5
6:B:208:17F:H76	5:E:812:7Q9:C318	0.66	2.20	13	4
6:D:517:17F:H1A	6:D:517:17F:H8	0.66	1.68	11	1
6:D:510:17F:H49	6:D:516:17F:H72	0.66	1.66	19	1
6:D:516:17F:O2	6:D:516:17F:H5	0.66	1.90	12	10
5:D:544:7Q9:C316	5:D:544:7Q9:C312	0.66	2.74	4	19
6:E:838:17F:H42	6:E:838:17F:H71	0.66	1.68	1	2
6:E:819:17F:C26	6:E:819:17F:H38	0.66	2.20	4	9
6:B:215:17F:H44	5:E:810:7Q9:C318	0.66	2.19	8	1
2:E:726:LYS:HE2	6:E:870:17F:H29	0.66	1.66	13	1
6:D:510:17F:H67	6:D:510:17F:C29	0.66	2.21	20	1
3:B:201:GSP:O3G	4:B:202:MG:MG	0.66	1.38	1	9
6:E:801:17F:H1	5:E:806:7Q9:C12	0.66	2.21	14	3
6:D:546:17F:H31	6:D:546:17F:O10	0.66	1.90	10	5
6:B:208:17F:H1	6:B:208:17F:C4	0.66	2.20	6	4
6:D:516:17F:H35	6:D:516:17F:H41	0.66	1.68	7	1
5:A:204:7Q9:C314	6:A:208:17F:H65	0.66	2.20	16	1
1:B:78:PHE:HB2	1:B:111:MET:HG2	0.66	1.67	11	11
5:E:815:7Q9:C1	5:E:815:7Q9:O22	0.66	2.43	13	15
5:E:848:7Q9:C312	5:E:851:7Q9:C35	0.66	2.73	6	13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:510:17F:C8	6:D:516:17F:H34	0.66	2.10	3	3
1:B:13:GLY:HA2	3:B:201:GSP:H5'1	0.66	1.66	20	1
6:A:208:17F:O8	6:A:208:17F:H4A	0.66	1.90	7	17
3:B:201:GSP:O2A	3:B:201:GSP:S1G	0.66	2.54	8	4
6:B:215:17F:H5	6:B:215:17F:O8	0.66	1.89	2	17
6:D:510:17F:O6	6:D:516:17F:C4	0.66	2.44	6	15
6:E:828:17F:N1	5:E:851:7Q9:O14	0.66	2.28	3	6
6:A:208:17F:H48	5:A:209:7Q9:C317	0.66	2.20	6	1
6:D:510:17F:C7	6:D:516:17F:C11	0.66	2.74	8	4
6:E:818:17F:C10	6:E:819:17F:H10	0.66	2.18	16	3
5:E:824:7Q9:O22	5:E:824:7Q9:C3	0.66	2.39	20	16
6:E:838:17F:H73	6:E:856:17F:C24	0.66	2.13	1	2
5:D:547:7Q9:C318	5:D:547:7Q9:C314	0.66	2.74	14	7
6:E:818:17F:C33	6:E:841:17F:H53	0.66	2.21	4	1
6:D:501:17F:N1	5:D:508:7Q9:O22	0.66	2.27	17	4
6:D:527:17F:H53	6:E:856:17F:H43	0.66	1.67	9	4
6:E:838:17F:H68	6:E:856:17F:C24	0.66	2.20	5	3
6:D:528:17F:C37	6:D:528:17F:H37	0.66	2.20	7	1
6:E:818:17F:H40	6:E:819:17F:H46	0.66	1.66	10	2
5:A:217:7Q9:C32	6:D:546:17F:H40	0.66	2.21	17	2
6:E:807:17F:H68	6:E:818:17F:H38	0.66	1.68	14	2
6:D:510:17F:C6	6:D:527:17F:H19A	0.66	2.20	17	1
6:E:872:17F:H39	6:E:872:17F:C20	0.66	2.20	17	1
5:B:205:7Q9:C14	5:B:205:7Q9:O12	0.66	2.44	3	20
6:E:807:17F:H49	6:E:809:17F:C36	0.66	2.21	11	8
6:E:807:17F:C28	6:E:809:17F:H62	0.66	2.20	5	5
6:E:856:17F:H11A	6:E:874:17F:H59	0.66	1.68	1	2
5:E:813:7Q9:C37	6:E:819:17F:H36	0.66	2.21	2	3
6:D:501:17F:H61	6:D:501:17F:C26	0.66	2.20	20	3
6:D:511:17F:H61	6:D:511:17F:H12	0.66	1.66	15	3
6:D:546:17F:H49	6:D:546:17F:H78	0.66	1.67	11	1
6:B:208:17F:H68	6:B:208:17F:C28	0.66	2.08	3	12
6:E:870:17F:O8	6:E:870:17F:C17	0.66	2.44	6	15
6:D:517:17F:H10	5:D:529:7Q9:C23	0.66	2.20	5	2
5:E:824:7Q9:C33	6:E:841:17F:H31	0.66	2.21	9	1
6:B:214:17F:C6	6:B:219:17F:H9	0.66	2.20	10	1
6:B:219:17F:H45	5:D:543:7Q9:C311	0.66	2.20	10	1
6:B:219:17F:H68	5:D:522:7Q9:C312	0.66	2.21	17	1
3:A:201:GSP:O3G	4:A:202:MG:MG	0.66	1.39	10	12
5:A:215:7Q9:C313	5:A:215:7Q9:C317	0.66	2.74	8	20
5:B:217:7Q9:C31	5:B:217:7Q9:C21	0.66	2.74	7	10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:B:214:17F:C34	6:B:214:17F:C38	0.66	2.72	5	9
6:E:805:17F:O7	6:E:805:17F:O3	0.66	2.14	15	4
5:E:813:7Q9:C313	6:E:819:17F:H54	0.66	2.21	3	5
6:E:817:17F:H35	6:E:817:17F:H41	0.66	1.66	4	8
6:E:819:17F:H19A	5:E:852:7Q9:C33	0.66	2.21	2	1
6:E:828:17F:H51	5:E:832:7Q9:C317	0.66	2.21	6	2
6:E:809:17F:C1Y	6:E:818:17F:H63	0.66	2.21	16	2
6:E:870:17F:H51	6:E:870:17F:C41	0.66	2.20	13	1
5:B:211:7Q9:C314	6:B:215:17F:H33	0.66	2.21	17	1
5:D:506:7Q9:C33	6:D:517:17F:H11	0.66	2.21	19	1
6:A:208:17F:C7	6:A:208:17F:H4A	0.65	2.21	2	11
5:B:213:7Q9:O32	5:B:213:7Q9:C1	0.65	2.43	3	13
6:D:517:17F:H39	6:D:517:17F:C1X	0.65	2.19	3	17
5:D:525:7Q9:C318	5:D:525:7Q9:C314	0.65	2.75	7	20
5:B:211:7Q9:C311	6:D:501:17F:H70	0.65	2.20	9	3
6:E:818:17F:H20A	6:E:818:17F:O8	0.65	1.91	2	1
3:B:201:GSP:O2B	3:B:201:GSP:O3G	0.65	2.11	3	1
6:B:215:17F:H67	6:B:215:17F:H48	0.65	1.66	4	2
6:D:501:17F:H11A	6:D:501:17F:C23	0.65	2.21	7	4
5:D:504:7Q9:C34	6:D:516:17F:H31	0.65	2.21	12	1
6:D:501:17F:H12	6:D:501:17F:H40	0.65	1.67	15	2
5:D:505:7Q9:C311	6:D:511:17F:H52	0.65	2.21	13	1
1:B:22:GLN:HG2	1:B:28:PHE:HA	0.65	1.68	1	1
6:E:818:17F:H19A	5:E:837:7Q9:C14	0.65	2.20	6	2
2:D:273:ASP:HB2	6:D:534:17F:C1Z	0.65	2.18	5	6
6:B:214:17F:H75	5:B:217:7Q9:C38	0.65	2.22	8	3
5:E:813:7Q9:O22	5:E:829:7Q9:C15	0.65	2.44	10	1
6:E:872:17F:O6	6:E:872:17F:H2	0.65	1.91	16	2
6:E:807:17F:H43	6:E:809:17F:H62	0.65	1.67	18	1
6:E:807:17F:H1A	6:E:807:17F:H4A	0.65	1.68	20	1
5:D:535:7Q9:O21	5:D:535:7Q9:O14	0.65	2.13	15	19
6:B:208:17F:H40	6:B:208:17F:C1Z	0.65	2.21	4	1
6:E:838:17F:C23	6:E:838:17F:C1Z	0.65	2.72	4	4
6:D:501:17F:H66	6:D:501:17F:H43	0.65	1.67	6	1
6:D:501:17F:H41	5:D:508:7Q9:C318	0.65	2.22	9	1
5:B:203:7Q9:C1	5:B:206:7Q9:C22	0.65	2.73	18	3
6:A:214:17F:H47	6:A:214:17F:H71	0.65	1.65	12	1
5:B:213:7Q9:O22	5:B:213:7Q9:C3	0.65	2.42	2	17
6:D:510:17F:P1	6:D:516:17F:H4	0.65	2.31	7	10
6:E:807:17F:O10	6:E:807:17F:H4	0.65	1.90	18	16
5:E:839:7Q9:C311	5:E:839:7Q9:C36	0.65	2.75	5	9

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:B:211:7Q9:O14	6:D:501:17F:H5	0.65	1.91	6	5
6:E:856:17F:H8	6:E:874:17F:O10	0.65	1.90	3	2
6:D:510:17F:C8	6:D:516:17F:H8A	0.65	2.21	9	2
6:E:838:17F:H57	6:E:838:17F:C36	0.65	2.18	20	1
2:D:331:ARG:HA	5:D:532:7Q9:C311	0.65	2.21	9	7
5:D:543:7Q9:O22	5:D:543:7Q9:C3	0.65	2.43	6	18
6:E:805:17F:H60	5:E:810:7Q9:C35	0.65	2.21	1	2
6:D:501:17F:O10	6:D:501:17F:C4	0.65	2.44	5	9
6:E:805:17F:H74	5:E:816:7Q9:C318	0.65	2.21	5	1
6:D:511:17F:H69	6:D:511:17F:C32	0.65	2.22	19	6
5:A:216:7Q9:C318	6:E:855:17F:H77	0.65	2.21	13	2
5:E:802:7Q9:C32	6:E:809:17F:H18A	0.65	2.21	18	1
6:B:215:17F:H50	6:B:215:17F:C37	0.65	2.22	1	1
6:E:872:17F:H19	6:E:872:17F:C1X	0.65	2.21	7	16
5:A:204:7Q9:C310	6:A:208:17F:H66	0.65	2.20	3	2
6:A:208:17F:H35	6:A:208:17F:H42	0.65	1.68	5	3
6:D:517:17F:H9A	5:D:538:7Q9:C32	0.65	2.22	6	3
2:E:555:SER:HA	6:E:872:17F:C36	0.65	2.21	20	5
6:D:511:17F:H69	6:D:511:17F:H58	0.65	1.69	19	2
1:B:126:ASP:HB2	1:B:129:GLN:HB2	0.65	1.69	18	1
5:A:212:7Q9:O32	5:A:212:7Q9:C1	0.65	2.45	19	12
6:E:818:17F:H45	6:E:818:17F:H78	0.65	1.68	1	1
6:D:517:17F:O10	6:D:517:17F:H6A	0.65	1.92	4	7
6:E:807:17F:H74	6:E:807:17F:C27	0.65	2.22	5	6
6:D:516:17F:H39	6:D:516:17F:H60	0.65	1.68	4	2
6:E:856:17F:H63	6:E:856:17F:C31	0.65	2.18	18	9
6:D:501:17F:H40	6:D:501:17F:H12	0.65	1.67	17	3
6:E:811:17F:H4A	5:E:822:7Q9:C13	0.65	2.21	11	3
5:E:821:7Q9:C31	5:E:821:7Q9:C21	0.65	2.74	14	2
5:D:544:7Q9:C32	6:D:546:17F:H19	0.65	2.22	9	5
6:E:811:17F:H75	5:E:822:7Q9:C316	0.65	2.21	15	4
5:D:544:7Q9:C312	6:D:546:17F:H50	0.65	2.22	10	1
6:E:807:17F:H69	5:E:813:7Q9:C310	0.65	2.22	17	3
6:D:510:17F:H49	6:D:516:17F:H68	0.65	1.69	13	1
6:E:818:17F:H30	6:E:818:17F:C23	0.65	2.14	13	1
6:A:214:17F:H73	5:A:215:7Q9:C318	0.65	2.22	14	1
6:E:819:17F:H36	6:E:819:17F:C20	0.65	2.22	15	1
6:D:510:17F:H66	5:D:524:7Q9:C317	0.65	2.22	1	2
5:D:520:7Q9:O21	5:D:520:7Q9:O14	0.65	2.14	2	16
6:D:516:17F:C2X	6:D:527:17F:H38	0.65	2.20	10	2
5:E:850:7Q9:C315	6:E:870:17F:H34	0.65	2.22	19	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:828:17F:H40	6:E:828:17F:C32	0.65	2.22	15	1
6:E:874:17F:N1	6:E:874:17F:H10	0.65	2.07	17	2
5:D:543:7Q9:C36	5:D:543:7Q9:C32	0.65	2.75	4	8
6:E:838:17F:O7	6:E:838:17F:O10	0.65	2.15	11	16
6:B:208:17F:H43	6:B:208:17F:C32	0.65	2.22	2	2
1:A:15:GLY:HA2	3:A:201:GSP:O2B	0.65	1.92	10	3
5:D:514:7Q9:O13	5:D:514:7Q9:O21	0.65	2.15	12	12
6:D:533:17F:C19	6:D:533:17F:C31	0.65	2.70	3	4
6:E:838:17F:H19	6:E:838:17F:C31	0.65	2.17	15	12
6:E:838:17F:H47	6:E:838:17F:C42	0.65	2.22	8	1
6:D:501:17F:H62	6:D:501:17F:H46	0.65	1.66	15	1
5:B:211:7Q9:C318	6:E:809:17F:H74	0.65	2.21	1	2
5:B:220:7Q9:C314	6:D:533:17F:H52	0.65	2.22	19	2
6:D:546:17F:H45	6:D:546:17F:C39	0.65	2.22	1	1
5:E:802:7Q9:C316	5:E:802:7Q9:C312	0.65	2.75	2	19
5:E:802:7Q9:C32	6:E:809:17F:H18	0.65	2.21	9	3
5:D:507:7Q9:C311	6:D:516:17F:H55	0.65	2.22	13	4
6:E:872:17F:O2	6:E:872:17F:H8	0.65	1.92	14	3
6:B:219:17F:C2X	6:B:219:17F:C20	0.65	2.75	9	5
6:D:510:17F:H6A	6:D:527:17F:C20	0.65	2.11	14	1
6:D:510:17F:H54	6:D:516:17F:H38	0.65	1.69	14	1
6:D:533:17F:H6	5:D:543:7Q9:C2	0.65	2.22	15	1
6:D:528:17F:O10	6:D:528:17F:C7	0.64	2.46	15	17
5:E:834:7Q9:C314	5:E:834:7Q9:C310	0.64	2.74	14	20
6:D:510:17F:C17	6:D:527:17F:C19	0.64	2.75	10	4
5:E:816:7Q9:O12	5:E:816:7Q9:C3	0.64	2.45	13	7
6:E:819:17F:H44	6:E:819:17F:H58	0.64	1.68	3	5
6:D:510:17F:H33	5:D:524:7Q9:C310	0.64	2.22	13	1
6:D:510:17F:H51	6:D:516:17F:C40	0.64	2.22	14	1
6:A:208:17F:H18A	5:A:211:7Q9:O32	0.64	1.92	19	2
5:E:842:7Q9:O22	5:E:842:7Q9:C31	0.64	2.45	9	18
5:B:218:7Q9:C31	5:B:218:7Q9:O11	0.64	2.45	4	12
6:E:819:17F:H44	6:E:819:17F:C31	0.64	2.22	17	6
6:E:838:17F:C11	6:E:856:17F:H35	0.64	2.22	10	5
6:D:501:17F:O10	6:D:501:17F:N1	0.64	2.30	20	3
5:E:848:7Q9:C311	5:E:851:7Q9:C34	0.64	2.75	13	3
6:A:208:17F:C34	6:B:208:17F:H69	0.64	2.19	11	1
1:B:8:VAL:HG12	1:B:16:LYS:HD2	0.64	1.69	13	2
5:A:204:7Q9:C312	6:A:208:17F:H63	0.64	2.22	1	1
6:B:214:17F:H51	5:E:827:7Q9:C317	0.64	2.22	1	3
6:D:510:17F:H39	6:D:511:17F:H73	0.64	1.68	1	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:511:17F:H43	5:D:513:7Q9:C317	0.64	2.22	1	4
6:D:527:17F:O9	6:D:527:17F:O1	0.64	2.15	1	20
6:E:819:17F:O8	6:E:819:17F:C4	0.64	2.45	18	9
1:A:109:VAL:HB	1:A:111:MET:HE2	0.64	1.70	13	3
5:D:543:7Q9:C34	5:D:543:7Q9:O31	0.64	2.46	6	10
6:E:809:17F:H10A	5:E:810:7Q9:C34	0.64	2.22	15	2
5:A:212:7Q9:C14	6:A:214:17F:H2	0.64	2.22	17	1
6:D:528:17F:H69	6:D:528:17F:H37	0.64	1.69	1	2
6:E:818:17F:H78	6:E:818:17F:C26	0.64	2.23	6	3
6:E:841:17F:O10	6:E:841:17F:H6A	0.64	1.92	14	19
6:E:841:17F:H8	5:E:876:7Q9:C12	0.64	2.21	3	2
2:D:327:GLN:HG3	6:D:528:17F:H56	0.64	1.69	9	6
6:E:807:17F:H51	6:E:807:17F:C41	0.64	2.22	5	5
5:D:507:7Q9:C310	6:D:516:17F:H60	0.64	2.22	10	4
1:A:68:ARG:HA	1:A:71:TYR:CE1	0.64	2.26	8	3
6:E:856:17F:H78	6:E:874:17F:H65	0.64	1.68	18	4
6:D:501:17F:H42	6:D:501:17F:C2X	0.64	2.23	16	4
6:D:511:17F:H47	5:D:513:7Q9:C317	0.64	2.23	13	3
6:D:528:17F:H46	5:E:852:7Q9:C317	0.64	2.22	13	1
6:D:510:17F:H63	5:D:524:7Q9:C314	0.64	2.22	9	4
5:E:827:7Q9:C1	5:E:827:7Q9:O22	0.64	2.43	16	7
6:D:534:17F:H30	6:D:534:17F:H58	0.64	1.67	9	2
6:E:807:17F:H57	6:E:819:17F:H12A	0.64	1.68	20	4
6:E:870:17F:H31	6:E:870:17F:H35	0.64	1.69	2	2
6:D:527:17F:C17	6:D:527:17F:H32	0.64	2.22	5	5
5:D:535:7Q9:C318	6:E:874:17F:H55	0.64	2.23	5	1
1:B:92:ASP:HA	1:B:95:HIS:HD2	0.64	1.52	12	1
5:D:536:7Q9:C21	5:D:536:7Q9:C31	0.64	2.75	12	1
6:B:214:17F:H33	6:B:219:17F:H12	0.64	1.68	17	1
5:D:518:7Q9:C313	6:D:533:17F:H46	0.64	2.23	2	3
6:E:856:17F:H56	6:E:856:17F:C35	0.64	2.23	9	10
6:D:517:17F:C37	6:D:517:17F:H52	0.64	2.23	13	5
6:D:516:17F:H18A	6:D:516:17F:N1	0.64	2.07	14	1
6:D:510:17F:H56	6:D:516:17F:H29	0.64	1.70	10	5
6:D:534:17F:H12A	5:D:539:7Q9:C35	0.64	2.23	1	1
6:D:510:17F:H66	5:D:524:7Q9:C318	0.64	2.23	5	1
1:A:29:VAL:HG21	1:B:128:LYS:HB2	0.64	1.68	7	1
5:E:850:7Q9:C314	6:E:870:17F:H61	0.64	2.23	8	2
6:E:805:17F:C26	6:E:805:17F:C30	0.64	2.75	19	3
6:B:214:17F:C38	6:B:214:17F:C34	0.64	2.73	14	7
5:D:547:7Q9:O22	5:D:547:7Q9:O11	0.64	2.16	20	13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:72:MET:SD	1:B:100:ILE:HA	0.64	2.33	2	1
6:E:809:17F:C34	6:E:818:17F:H71	0.64	2.22	2	5
6:E:817:17F:H4	6:E:817:17F:O10	0.64	1.93	11	11
6:D:527:17F:O10	6:D:527:17F:H6A	0.64	1.92	3	3
5:B:207:7Q9:C316	6:E:801:17F:H68	0.64	2.23	7	4
6:D:516:17F:H49	6:D:516:17F:C22	0.64	2.22	18	3
5:E:863:7Q9:C35	5:E:863:7Q9:O31	0.64	2.46	14	7
6:B:214:17F:H46	5:B:217:7Q9:C311	0.64	2.23	17	3
6:E:805:17F:H70	5:E:810:7Q9:C315	0.64	2.22	10	1
5:E:823:7Q9:O22	5:E:845:7Q9:C12	0.64	2.46	14	1
6:A:214:17F:H76	5:E:822:7Q9:C310	0.64	2.23	20	2
6:E:818:17F:C19	6:E:841:17F:H57	0.64	2.23	18	1
6:E:838:17F:H9A	6:E:838:17F:C34	0.64	2.23	19	8
6:D:511:17F:H1A	5:D:526:7Q9:C12	0.64	2.23	3	1
6:E:818:17F:H78	6:E:818:17F:H45	0.64	1.70	6	3
6:B:219:17F:H36	6:B:219:17F:H20A	0.64	1.69	16	2
6:D:501:17F:C34	6:D:501:17F:H41	0.64	2.23	20	2
5:B:216:7Q9:C14	5:B:216:7Q9:C1	0.64	2.76	12	1
2:E:602:ASP:HA	5:E:866:7Q9:C38	0.64	2.23	13	1
6:E:807:17F:C30	6:E:818:17F:H76	0.64	2.22	16	3
5:D:539:7Q9:O32	5:D:539:7Q9:C1	0.64	2.46	14	14
2:E:591:GLU:HG2	5:E:861:7Q9:C37	0.64	2.23	4	8
5:E:852:7Q9:O22	5:E:852:7Q9:C3	0.64	2.44	5	14
6:D:527:17F:H68	6:D:527:17F:C23	0.64	2.23	16	3
6:D:534:17F:H35	6:D:534:17F:C34	0.64	2.23	18	3
6:E:805:17F:C30	6:E:805:17F:H68	0.64	2.22	9	7
6:B:215:17F:H48	6:B:215:17F:C37	0.64	2.23	13	4
5:B:220:7Q9:C22	6:D:533:17F:H11A	0.64	2.22	4	2
6:E:838:17F:H50	6:E:874:17F:C30	0.64	2.21	20	4
6:A:214:17F:H47	6:A:214:17F:C39	0.64	2.23	12	1
6:E:874:17F:H36	6:E:874:17F:C24	0.63	2.17	9	16
6:A:208:17F:C30	6:A:208:17F:C26	0.63	2.75	6	12
6:E:807:17F:H69	5:E:813:7Q9:C312	0.63	2.23	13	5
6:E:838:17F:C38	6:E:856:17F:H41	0.63	2.17	2	2
5:E:850:7Q9:C315	6:E:870:17F:H60	0.63	2.23	10	2
6:E:805:17F:H73	5:E:816:7Q9:C316	0.63	2.24	9	4
1:A:117:LYS:HE2	3:A:201:GSP:C4	0.63	2.29	13	3
1:A:146:ALA:HB3	3:A:201:GSP:N7	0.63	2.07	12	6
6:D:516:17F:C23	6:D:516:17F:C27	0.63	2.70	6	3
6:A:208:17F:H44	5:E:822:7Q9:C315	0.63	2.23	6	2
6:E:807:17F:H49	6:E:809:17F:H51	0.63	1.68	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:528:17F:H35	5:D:532:7Q9:C317	0.63	2.23	11	1
5:E:824:7Q9:C34	6:E:841:17F:H31	0.63	2.23	13	3
6:D:533:17F:H18	6:D:533:17F:C1Z	0.63	2.22	14	1
6:D:501:17F:H40	6:D:501:17F:C1Z	0.63	2.23	20	1
5:A:216:7Q9:O14	5:A:216:7Q9:O21	0.63	2.16	2	17
6:D:510:17F:H33	5:D:524:7Q9:C39	0.63	2.23	2	1
5:E:837:7Q9:C12	6:E:841:17F:O10	0.63	2.47	5	5
6:D:527:17F:H50	6:D:527:17F:C42	0.63	2.22	3	5
6:D:510:17F:C42	6:D:516:17F:H75	0.63	2.22	5	1
6:B:214:17F:H4	6:B:214:17F:O10	0.63	1.92	20	5
5:A:209:7Q9:C318	5:E:823:7Q9:C310	0.63	2.76	13	3
2:D:330:ALA:HB2	6:D:528:17F:H78	0.63	1.70	11	1
6:E:838:17F:H38	5:E:857:7Q9:C310	0.63	2.23	15	5
3:A:201:GSP:O2G	4:A:202:MG:MG	0.63	1.41	17	1
1:A:32:TYR:CE2	3:A:201:GSP:H5'2	0.63	2.28	1	1
5:E:863:7Q9:C37	5:E:863:7Q9:C22	0.63	2.77	12	15
6:A:208:17F:H2	6:A:208:17F:O1	0.63	1.92	2	1
6:A:208:17F:H38	5:E:823:7Q9:C316	0.63	2.23	2	1
6:E:818:17F:C10	6:E:819:17F:C10	0.63	2.76	13	8
5:E:820:7Q9:C31	5:E:820:7Q9:C21	0.63	2.77	12	3
6:D:527:17F:H10	5:D:535:7Q9:C34	0.63	2.24	9	3
6:D:510:17F:H56	6:D:516:17F:C10	0.63	2.19	6	1
6:E:809:17F:C23	6:E:809:17F:C1X	0.63	2.74	6	1
6:E:856:17F:H70	6:E:874:17F:H65	0.63	1.69	7	2
6:E:819:17F:C11	6:E:819:17F:O7	0.63	2.45	15	3
5:B:205:7Q9:C31	5:B:205:7Q9:C21	0.63	2.76	16	1
6:E:856:17F:H30	6:E:874:17F:H64	0.63	1.68	16	1
6:D:501:17F:H55	5:D:508:7Q9:C314	0.63	2.24	19	1
5:D:537:7Q9:O31	6:D:546:17F:H11A	0.63	1.93	15	5
6:D:546:17F:H68	6:D:546:17F:H41	0.63	1.68	14	2
5:E:802:7Q9:C317	6:E:809:17F:H69	0.63	2.24	9	5
6:E:805:17F:C17	6:E:805:17F:O8	0.63	2.46	1	2
6:D:510:17F:C36	6:D:527:17F:H74	0.63	2.24	2	3
6:E:818:17F:H59	6:E:818:17F:C36	0.63	2.21	18	5
1:B:68:ARG:HA	1:B:71:TYR:CE1	0.63	2.29	20	5
6:D:527:17F:H1A	5:D:535:7Q9:C13	0.63	2.23	8	2
6:B:219:17F:H63	5:D:522:7Q9:C311	0.63	2.24	20	6
6:E:807:17F:H49	6:E:809:17F:H64	0.63	1.69	9	3
6:D:517:17F:C29	6:D:517:17F:H66	0.63	2.22	10	1
5:E:825:7Q9:O32	5:E:825:7Q9:C35	0.63	2.46	18	1
6:E:819:17F:H6A	5:E:836:7Q9:C2	0.63	2.24	1	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:534:17F:H76	5:E:863:7Q9:C316	0.63	2.23	5	3
5:B:203:7Q9:O13	5:B:205:7Q9:C13	0.63	2.47	3	6
6:A:208:17F:H19	6:B:208:17F:C1X	0.63	2.21	8	4
2:E:645:GLY:HA2	5:E:851:7Q9:C318	0.63	2.23	8	1
6:D:546:17F:H41	6:D:546:17F:C38	0.63	2.23	14	1
6:D:510:17F:H32	6:D:527:17F:H34	0.63	1.70	1	2
5:D:520:7Q9:O22	5:D:520:7Q9:C3	0.63	2.44	15	15
6:E:818:17F:H2	6:E:818:17F:O1	0.63	1.93	2	1
6:A:214:17F:H50	5:E:840:7Q9:C318	0.63	2.23	4	3
6:E:872:17F:H20	6:E:872:17F:H40	0.63	1.69	16	4
5:D:507:7Q9:O32	6:D:516:17F:N1	0.63	2.32	6	2
5:B:211:7Q9:C33	6:B:215:17F:H57	0.63	2.24	12	1
6:B:214:17F:H11	6:B:214:17F:C23	0.63	2.16	4	3
6:E:818:17F:O6	6:E:818:17F:C7	0.63	2.47	16	7
5:E:848:7Q9:C37	5:E:851:7Q9:C32	0.63	2.76	1	3
5:A:215:7Q9:O11	5:A:215:7Q9:C31	0.63	2.46	3	8
6:A:208:17F:H43	5:A:209:7Q9:C315	0.63	2.23	6	1
6:D:501:17F:H6	5:D:506:7Q9:C14	0.63	2.24	13	3
5:E:821:7Q9:C1	5:E:821:7Q9:C15	0.63	2.76	13	6
6:D:527:17F:H72	6:D:527:17F:C23	0.63	2.15	2	1
5:B:204:7Q9:C13	5:B:207:7Q9:O22	0.63	2.47	9	8
6:D:528:17F:H69	6:D:528:17F:H38	0.63	1.71	15	6
5:D:507:7Q9:C318	6:E:838:17F:H47	0.63	2.23	16	1
6:E:809:17F:H47	6:E:818:17F:H72	0.63	1.70	20	1
2:E:620:GLU:HB3	2:E:621:PRO:HD3	0.63	1.69	1	17
6:E:805:17F:C30	6:E:805:17F:C26	0.63	2.75	2	17
6:E:805:17F:H60	5:E:810:7Q9:C36	0.63	2.24	1	5
1:A:117:LYS:NZ	3:A:201:GSP:N7	0.63	2.47	2	2
6:A:214:17F:H76	5:E:822:7Q9:C39	0.63	2.24	2	2
6:D:516:17F:H60	6:D:516:17F:H50	0.63	1.70	4	1
6:B:214:17F:C18	6:B:219:17F:H11A	0.63	2.23	7	1
6:B:219:17F:H19	6:B:219:17F:C1X	0.63	2.23	16	3
6:E:807:17F:C1X	6:E:807:17F:H58	0.63	2.24	9	2
3:B:201:GSP:O1A	4:B:202:MG:MG	0.63	1.40	10	1
6:B:208:17F:H33	6:B:214:17F:C12	0.63	2.16	14	1
5:E:853:7Q9:C311	5:E:853:7Q9:C37	0.62	2.76	3	17
6:E:801:17F:H64	5:E:803:7Q9:C39	0.62	2.24	2	1
6:B:219:17F:H53	6:B:219:17F:H71	0.62	1.70	3	1
5:E:802:7Q9:O32	6:E:807:17F:C6	0.62	2.47	15	7
6:E:874:17F:H78	6:E:874:17F:H49	0.62	1.71	6	1
5:E:848:7Q9:C34	5:E:851:7Q9:C33	0.62	2.76	13	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:A:208:17F:H47	5:E:823:7Q9:C317	0.62	2.23	19	4
6:A:214:17F:H72	5:E:840:7Q9:C318	0.62	2.23	15	3
6:B:219:17F:C1X	6:B:219:17F:H18A	0.62	2.24	18	1
6:D:501:17F:H44	5:D:508:7Q9:C36	0.62	2.23	20	1
6:E:818:17F:H49	5:E:835:7Q9:C311	0.62	2.25	7	2
6:B:214:17F:H9	5:B:217:7Q9:C37	0.62	2.24	5	1
6:A:214:17F:H11	6:A:214:17F:H32	0.62	1.70	6	1
6:D:510:17F:H55	6:D:516:17F:C22	0.62	2.23	6	1
5:E:832:7Q9:C13	6:E:838:17F:H4	0.62	2.24	10	3
5:B:220:7Q9:C22	6:D:533:17F:H36	0.62	2.24	7	2
5:E:824:7Q9:C35	6:E:841:17F:H34	0.62	2.24	11	2
2:D:400:LEU:HG	5:D:542:7Q9:C312	0.62	2.25	19	2
5:D:504:7Q9:O21	5:D:504:7Q9:O32	0.62	2.16	20	17
5:D:503:7Q9:O32	5:D:503:7Q9:C21	0.62	2.47	13	14
6:A:208:17F:H19	6:B:208:17F:H37	0.62	1.69	4	2
6:D:533:17F:H50	6:D:533:17F:C41	0.62	2.17	17	4
6:D:534:17F:C1X	6:D:534:17F:H64	0.62	2.24	5	4
6:D:510:17F:H1	6:D:516:17F:C6	0.62	2.22	20	4
6:E:818:17F:C34	6:E:841:17F:H68	0.62	2.25	12	1
6:D:501:17F:H76	6:E:807:17F:C30	0.62	2.24	19	1
1:A:72:MET:HA	1:A:78:PHE:HZ	0.62	1.54	1	5
5:B:211:7Q9:C311	6:D:501:17F:H64	0.62	2.24	1	1
6:E:872:17F:H6A	6:E:872:17F:O10	0.62	1.94	7	12
6:D:516:17F:C23	6:D:516:17F:C28	0.62	2.64	4	3
6:E:801:17F:O8	6:E:801:17F:O9	0.62	2.18	1	11
5:E:829:7Q9:O22	5:E:829:7Q9:O11	0.62	2.18	15	12
6:B:208:17F:N1	6:B:214:17F:O1	0.62	2.32	11	2
5:D:507:7Q9:C11	5:D:507:7Q9:O21	0.62	2.48	5	2
5:E:850:7Q9:C35	6:E:870:17F:C20	0.62	2.77	18	5
5:D:505:7Q9:C318	6:E:828:17F:H71	0.62	2.25	13	5
6:D:501:17F:H40	6:D:501:17F:C33	0.62	2.25	10	1
5:B:203:7Q9:C36	5:B:203:7Q9:C311	0.62	2.77	4	6
6:B:208:17F:O9	6:B:208:17F:O8	0.62	2.18	3	20
6:D:534:17F:H35	6:D:534:17F:C33	0.62	2.25	8	9
6:D:534:17F:H4	6:D:534:17F:O10	0.62	1.95	17	14
5:E:802:7Q9:O13	6:E:807:17F:N1	0.62	2.32	8	5
6:B:219:17F:H2	6:B:219:17F:O2	0.62	1.94	18	3
5:D:504:7Q9:C34	6:D:516:17F:H32	0.62	2.25	6	1
6:E:818:17F:H2	6:E:818:17F:H4A	0.62	1.72	7	1
6:D:510:17F:C4	6:D:510:17F:O10	0.62	2.41	11	7
6:D:501:17F:C26	5:D:508:7Q9:C36	0.62	2.75	16	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:A:208:17F:C26	6:A:208:17F:C30	0.62	2.74	10	5
6:E:841:17F:H29	6:E:841:17F:H41	0.62	1.71	10	2
5:E:848:7Q9:C22	5:E:852:7Q9:C11	0.62	2.77	3	2
6:E:838:17F:H77	6:E:838:17F:C28	0.62	2.24	20	3
6:E:818:17F:H61	6:E:841:17F:C38	0.62	2.24	7	1
6:A:214:17F:H32	6:A:214:17F:C11	0.62	2.18	8	1
6:D:528:17F:H76	5:D:532:7Q9:C313	0.62	2.25	14	1
6:A:214:17F:H6	5:D:539:7Q9:C15	0.62	2.25	17	1
5:E:802:7Q9:C39	6:E:807:17F:H41	0.62	2.25	9	6
6:E:856:17F:O2	6:E:856:17F:N1	0.62	2.31	4	5
6:D:546:17F:H2	6:D:546:17F:O1	0.62	1.95	2	14
5:E:858:7Q9:O22	5:E:858:7Q9:C1	0.62	2.46	11	13
5:D:519:7Q9:C3	5:D:519:7Q9:O22	0.62	2.45	9	6
2:E:733:LEU:HA	5:E:875:7Q9:C310	0.62	2.24	9	5
6:E:805:17F:H69	5:E:816:7Q9:C318	0.62	2.25	15	4
6:A:208:17F:H10	5:A:209:7Q9:C33	0.62	2.24	12	1
6:D:534:17F:C32	6:D:534:17F:H65	0.62	2.22	13	1
5:E:843:7Q9:C21	5:E:843:7Q9:O13	0.62	2.48	16	18
5:E:866:7Q9:O31	5:E:866:7Q9:O22	0.62	2.18	9	20
2:D:333:LYS:HD3	5:E:878:7Q9:C318	0.62	2.24	4	3
6:A:208:17F:H47	5:E:823:7Q9:C318	0.62	2.25	16	3
6:B:214:17F:O10	6:B:214:17F:N1	0.62	2.32	20	3
1:A:23:LEU:HD21	1:A:153:ASP:HA	0.62	1.72	13	1
1:A:32:TYR:CE1	3:A:201:GSP:H5'2	0.62	2.30	15	1
6:E:818:17F:H20	5:E:837:7Q9:C14	0.62	2.25	18	1
2:D:340:LYS:HD3	2:E:626:LEU:HD21	0.62	1.70	1	5
5:D:540:7Q9:C15	5:D:540:7Q9:O12	0.62	2.48	13	20
2:E:733:LEU:HG	5:E:875:7Q9:C38	0.62	2.24	15	5
5:D:515:7Q9:C313	6:D:517:17F:H78	0.62	2.24	6	1
6:E:811:17F:H41	6:E:811:17F:H36	0.62	1.71	6	1
6:E:874:17F:H41	6:E:874:17F:C2X	0.62	2.21	20	3
6:E:874:17F:O10	6:E:874:17F:C7	0.62	2.47	9	1
6:E:819:17F:H18	5:E:852:7Q9:C34	0.62	2.25	11	2
6:E:856:17F:O1	6:E:856:17F:N1	0.62	2.33	14	1
6:E:841:17F:H4A	6:E:841:17F:C7	0.62	2.25	19	1
5:B:209:7Q9:O12	5:B:209:7Q9:C13	0.61	2.47	3	18
6:E:819:17F:C7	6:E:819:17F:C4	0.61	2.78	7	6
6:A:214:17F:H55	6:A:214:17F:C39	0.61	2.25	5	2
5:A:204:7Q9:C313	6:A:208:17F:C42	0.61	2.78	19	10
6:B:208:17F:H40	6:B:208:17F:H64	0.61	1.70	7	2
6:D:546:17F:H57	6:D:546:17F:O8	0.61	1.94	19	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:E:711:LEU:HB2	5:E:865:7Q9:C311	0.61	2.25	15	3
6:D:533:17F:C18	6:D:533:17F:C31	0.61	2.58	14	1
5:E:802:7Q9:C37	6:E:807:17F:H36	0.61	2.25	16	1
6:B:208:17F:H64	6:B:208:17F:C26	0.61	2.18	1	1
5:B:216:7Q9:O14	5:B:216:7Q9:O21	0.61	2.18	12	10
5:E:803:7Q9:C31	5:E:803:7Q9:O22	0.61	2.48	10	9
5:A:207:7Q9:O22	5:A:207:7Q9:C3	0.61	2.45	16	10
5:E:848:7Q9:C34	5:E:851:7Q9:O31	0.61	2.47	14	12
6:D:533:17F:H37	6:D:533:17F:C35	0.61	2.25	3	3
6:E:870:17F:O10	6:E:870:17F:C6	0.61	2.43	3	3
6:D:510:17F:H38	6:D:511:17F:H73	0.61	1.70	8	3
6:D:510:17F:H50	6:D:510:17F:C42	0.61	2.26	14	1
6:E:870:17F:C22	6:E:870:17F:H64	0.61	2.26	16	2
6:B:214:17F:C31	6:B:219:17F:H12	0.61	2.26	17	1
5:E:837:7Q9:C32	6:E:841:17F:H32	0.61	2.25	1	2
5:E:847:7Q9:O31	6:E:872:17F:N1	0.61	2.34	7	8
6:E:856:17F:H46	6:E:856:17F:C32	0.61	2.25	3	3
5:D:535:7Q9:C1	5:D:535:7Q9:C14	0.61	2.78	20	5
6:D:534:17F:H54	6:D:534:17F:H63	0.61	1.72	12	3
6:E:819:17F:H75	5:E:852:7Q9:C310	0.61	2.25	8	1
5:B:211:7Q9:C314	6:B:215:17F:H34	0.61	2.26	12	2
6:D:501:17F:O10	6:D:501:17F:H4	0.61	1.94	19	3
2:E:555:SER:HA	6:E:872:17F:C37	0.61	2.24	13	1
5:A:204:7Q9:C38	6:A:208:17F:H10A	0.61	2.25	16	1
6:E:819:17F:H74	5:E:852:7Q9:C311	0.61	2.24	18	1
6:E:872:17F:H36	6:E:872:17F:H20	0.61	1.73	7	4
6:E:801:17F:H10	6:E:801:17F:H18	0.61	1.70	3	7
5:E:837:7Q9:C14	6:E:841:17F:H19A	0.61	2.25	3	2
5:E:850:7Q9:C315	6:E:870:17F:C20	0.61	2.78	3	1
1:A:46:ILE:HD13	1:A:160:VAL:HG21	0.61	1.70	17	2
5:D:544:7Q9:C312	5:D:544:7Q9:C316	0.61	2.79	10	1
6:E:801:17F:H39	5:E:804:7Q9:C312	0.61	2.25	12	2
6:B:208:17F:H33	6:B:214:17F:H10A	0.61	1.69	18	1
6:B:214:17F:C37	6:B:219:17F:H47	0.61	2.25	18	1
6:E:841:17F:H10	6:E:841:17F:O7	0.61	1.93	19	1
5:D:507:7Q9:C2	5:D:507:7Q9:O32	0.61	2.46	8	7
5:E:850:7Q9:C313	6:E:870:17F:H20A	0.61	2.25	3	2
2:D:333:LYS:HE2	5:E:878:7Q9:C318	0.61	2.25	2	2
5:D:513:7Q9:C36	5:D:526:7Q9:C39	0.61	2.77	3	5
6:B:215:17F:C19	6:D:517:17F:H60	0.61	2.24	6	1
5:E:857:7Q9:C2	6:E:874:17F:H2	0.61	2.26	10	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:A:208:17F:H69	6:B:208:17F:C42	0.61	2.25	11	1
6:E:870:17F:H64	6:E:870:17F:H38	0.61	1.72	16	3
6:D:527:17F:H30	6:D:527:17F:C37	0.61	2.25	19	1
5:D:515:7Q9:O12	5:D:515:7Q9:C13	0.61	2.49	1	20
6:D:528:17F:O2	6:D:528:17F:O9	0.61	2.19	10	16
5:D:503:7Q9:C318	6:D:516:17F:H77	0.61	2.25	7	1
6:D:533:17F:H59	6:D:533:17F:C36	0.61	2.06	14	2
5:E:859:7Q9:C21	5:E:859:7Q9:O32	0.61	2.48	5	12
5:A:211:7Q9:C22	6:B:214:17F:H30	0.61	2.25	4	1
6:D:511:17F:H10A	5:D:513:7Q9:C23	0.61	2.26	8	3
6:B:214:17F:H48	6:B:214:17F:H74	0.61	1.71	9	1
6:D:511:17F:H52	6:E:828:17F:H78	0.61	1.71	10	1
6:E:811:17F:H77	6:E:811:17F:H45	0.61	1.72	13	1
6:E:856:17F:C42	6:E:874:17F:H61	0.61	2.26	14	1
2:D:401:SER:HB3	5:D:542:7Q9:C37	0.61	2.26	18	1
5:E:832:7Q9:C2	6:E:856:17F:H6A	0.61	2.26	18	1
5:D:524:7Q9:O22	5:D:524:7Q9:C1	0.61	2.47	13	7
6:E:807:17F:C26	6:E:809:17F:H62	0.61	2.25	20	4
5:D:509:7Q9:O22	5:D:509:7Q9:C3	0.61	2.47	12	17
5:E:815:7Q9:O32	5:E:815:7Q9:C11	0.61	2.49	9	7
6:E:818:17F:H20A	6:E:818:17F:O9	0.61	1.96	2	1
6:E:856:17F:C35	6:E:856:17F:H56	0.61	2.26	13	5
6:B:219:17F:C18	5:D:545:7Q9:C35	0.61	2.79	10	2
6:B:219:17F:O10	5:D:522:7Q9:C2	0.61	2.48	13	6
5:E:852:7Q9:C11	5:E:852:7Q9:C3	0.61	2.79	9	3
1:B:16:LYS:HB2	3:B:201:GSP:O2G	0.61	1.95	13	1
5:E:824:7Q9:C36	6:E:841:17F:H39	0.61	2.26	16	1
5:B:204:7Q9:C15	5:B:204:7Q9:O12	0.61	2.48	16	20
6:D:517:17F:H40	6:D:517:17F:C31	0.61	2.26	20	4
6:D:510:17F:H64	6:D:527:17F:C41	0.61	2.24	11	3
6:E:801:17F:H58	5:E:803:7Q9:C22	0.61	2.26	4	1
6:B:219:17F:H58	5:D:522:7Q9:C39	0.61	2.26	20	4
5:B:220:7Q9:C316	6:D:533:17F:H52	0.61	2.26	5	1
6:D:533:17F:C32	6:D:533:17F:H65	0.61	2.26	8	2
6:E:807:17F:H56	6:E:819:17F:H12A	0.61	1.70	7	1
6:D:533:17F:H38	6:D:533:17F:C35	0.61	2.22	12	1
6:B:214:17F:H62	6:B:214:17F:C31	0.61	2.17	17	1
1:A:68:ARG:HA	1:A:71:TYR:CZ	0.61	2.30	2	12
5:B:212:7Q9:O22	5:B:212:7Q9:C3	0.61	2.47	9	14
5:D:536:7Q9:O21	5:D:536:7Q9:O12	0.61	2.19	6	3
2:D:327:GLN:CD	6:D:528:17F:H32	0.61	2.20	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:516:17F:O10	6:D:516:17F:C6	0.61	2.45	12	3
5:D:543:7Q9:O21	5:D:543:7Q9:O14	0.61	2.19	9	2
6:E:818:17F:H10	6:E:819:17F:C9	0.61	2.25	10	3
5:D:504:7Q9:O31	6:D:516:17F:H31	0.61	1.94	13	1
2:D:333:LYS:HZ2	6:D:528:17F:C22	0.61	2.09	16	1
6:D:533:17F:H46	5:D:543:7Q9:C22	0.61	2.26	17	1
6:B:214:17F:H46	6:B:214:17F:C41	0.60	2.23	5	4
6:A:214:17F:H52	5:E:840:7Q9:C312	0.60	2.26	2	2
3:B:201:GSP:H2'	3:B:201:GSP:O5'	0.60	1.97	11	8
5:A:204:7Q9:C316	6:A:208:17F:H71	0.60	2.25	3	2
6:D:516:17F:H41	6:D:527:17F:H40	0.60	1.71	3	1
1:A:6:LEU:HD21	1:A:163:ILE:HD11	0.60	1.73	4	1
6:E:805:17F:H20	5:E:810:7Q9:C22	0.60	2.25	5	1
6:E:838:17F:H65	6:E:838:17F:H57	0.60	1.71	10	7
6:D:534:17F:H37	5:D:539:7Q9:C35	0.60	2.26	7	1
5:E:816:7Q9:C36	5:E:816:7Q9:C311	0.60	2.78	20	5
5:D:521:7Q9:O32	5:D:525:7Q9:C32	0.60	2.49	2	2
5:E:814:7Q9:O12	5:E:814:7Q9:C15	0.60	2.49	5	20
6:E:838:17F:H12	6:E:856:17F:C9	0.60	2.26	1	3
5:E:869:7Q9:C23	6:E:872:17F:H10	0.60	2.26	3	4
5:B:203:7Q9:C315	6:B:208:17F:H74	0.60	2.26	14	3
5:D:505:7Q9:C37	6:D:511:17F:H30	0.60	2.27	4	1
6:E:809:17F:H52	6:E:818:17F:H71	0.60	1.73	6	1
6:D:510:17F:H1A	6:D:516:17F:O2	0.60	1.97	7	1
6:D:510:17F:H49	6:D:516:17F:C37	0.60	2.26	20	5
2:D:400:LEU:HG	5:D:542:7Q9:C313	0.60	2.27	13	1
6:E:838:17F:C36	6:E:838:17F:C11	0.60	2.76	20	2
5:E:804:7Q9:O13	5:E:804:7Q9:O21	0.60	2.18	2	20
6:D:510:17F:C8	6:D:516:17F:C17	0.60	2.79	2	3
5:D:536:7Q9:C1	5:D:547:7Q9:O22	0.60	2.50	4	2
6:D:534:17F:H35	6:D:534:17F:H44	0.60	1.72	20	4
6:D:527:17F:H42	5:D:535:7Q9:C313	0.60	2.25	8	1
2:E:605:GLN:HB2	5:E:866:7Q9:C313	0.60	2.27	9	1
6:E:818:17F:H67	5:E:824:7Q9:C318	0.60	2.27	12	1
6:E:870:17F:H58	6:E:870:17F:H30	0.60	1.72	16	2
6:D:501:17F:H40	6:D:501:17F:C1Y	0.60	2.26	20	1
5:D:505:7Q9:C31	5:D:505:7Q9:O22	0.60	2.49	6	6
6:D:527:17F:H36	6:D:527:17F:C24	0.60	2.24	9	6
5:E:849:7Q9:C311	5:E:849:7Q9:C37	0.60	2.76	10	16
5:E:804:7Q9:C31	6:E:811:17F:H31	0.60	2.26	2	1
6:D:501:17F:C11	6:D:501:17F:C23	0.60	2.79	4	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:A:208:17F:H57	6:A:208:17F:C35	0.60	2.13	5	2
6:D:510:17F:C12	6:D:516:17F:H10A	0.60	2.18	18	3
6:D:511:17F:H76	6:E:828:17F:C30	0.60	2.27	6	2
6:D:510:17F:P1	6:D:516:17F:H6	0.60	2.36	6	2
5:D:506:7Q9:C36	6:D:517:17F:H60	0.60	2.27	7	1
5:A:204:7Q9:C318	6:E:811:17F:H46	0.60	2.26	10	1
2:E:631:ARG:HG3	5:E:878:7Q9:C34	0.60	2.26	12	1
5:D:518:7Q9:O12	5:D:518:7Q9:C15	0.60	2.50	3	20
5:D:539:7Q9:C1	5:D:539:7Q9:C31	0.60	2.80	5	20
6:D:510:17F:C9	6:D:516:17F:C10	0.60	2.72	11	3
6:D:510:17F:C21	6:D:511:17F:H56	0.60	2.24	18	3
5:E:803:7Q9:C3	6:E:807:17F:C8	0.60	2.77	6	2
6:E:809:17F:C29	6:E:818:17F:H75	0.60	2.26	6	1
5:E:837:7Q9:O32	6:E:841:17F:H31	0.60	1.97	6	2
6:E:855:17F:H18	5:E:867:7Q9:C12	0.60	2.26	11	1
5:D:505:7Q9:O14	6:D:511:17F:H4A	0.60	1.95	17	1
5:D:506:7Q9:C33	6:D:517:17F:H57	0.60	2.26	17	1
5:B:212:7Q9:C15	5:B:212:7Q9:O12	0.60	2.49	17	20
6:B:214:17F:O10	6:B:214:17F:C6	0.60	2.44	13	7
5:D:548:7Q9:O32	5:D:548:7Q9:O21	0.60	2.19	10	19
6:E:805:17F:H37	6:E:805:17F:C19	0.60	2.23	12	3
5:E:868:7Q9:C14	5:E:868:7Q9:O12	0.60	2.49	14	20
2:D:320:GLU:HB3	2:D:321:PRO:HD3	0.60	1.73	14	18
6:E:838:17F:H9A	6:E:838:17F:H60	0.60	1.72	2	1
6:D:546:17F:C1Y	6:D:546:17F:O10	0.60	2.49	4	3
5:E:836:7Q9:O22	5:E:836:7Q9:C1	0.60	2.48	15	8
5:D:507:7Q9:C318	6:E:838:17F:H54	0.60	2.27	10	2
5:E:824:7Q9:C35	6:E:841:17F:C1X	0.60	2.79	15	5
6:D:501:17F:H34	6:D:501:17F:C23	0.60	2.27	20	1
5:A:217:7Q9:O32	5:A:217:7Q9:C21	0.60	2.50	5	19
5:B:206:7Q9:O22	5:B:206:7Q9:C3	0.60	2.48	20	16
5:B:206:7Q9:O14	5:B:206:7Q9:C2	0.60	2.49	2	6
5:B:210:7Q9:C3	5:B:210:7Q9:O22	0.60	2.48	9	15
5:E:831:7Q9:O22	5:E:831:7Q9:C3	0.60	2.47	15	14
6:D:516:17F:C27	6:D:516:17F:C33	0.60	2.80	3	1
6:E:818:17F:H78	6:E:818:17F:H48	0.60	1.74	3	2
6:B:214:17F:H69	6:B:219:17F:C12	0.60	2.27	4	1
5:A:216:7Q9:C33	5:D:507:7Q9:C23	0.60	2.80	9	2
6:D:533:17F:H43	6:D:533:17F:C37	0.60	2.24	14	1
5:E:830:7Q9:C311	6:E:870:17F:H50	0.60	2.27	14	1
6:D:511:17F:H61	6:D:511:17F:C12	0.60	2.27	15	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:817:17F:H56	5:E:833:7Q9:O32	0.60	1.96	15	1
6:E:838:17F:H10A	6:E:856:17F:C12	0.60	2.27	20	3
6:A:208:17F:C4	6:A:208:17F:C7	0.60	2.80	2	19
5:E:827:7Q9:C15	5:E:827:7Q9:O12	0.60	2.50	9	20
5:E:850:7Q9:O22	5:E:850:7Q9:C3	0.60	2.47	2	14
1:A:84:ILE:HD11	1:A:118:CYS:HA	0.60	1.73	19	7
6:D:510:17F:H47	6:D:516:17F:C35	0.60	2.24	3	1
6:E:856:17F:C39	6:E:874:17F:H65	0.60	2.26	10	2
5:D:509:7Q9:C31	5:D:509:7Q9:C1	0.60	2.80	9	1
6:D:510:17F:H58	6:D:516:17F:H37	0.60	1.74	10	2
5:B:212:7Q9:O13	5:B:212:7Q9:O21	0.60	2.20	1	16
5:D:543:7Q9:C14	5:D:543:7Q9:O12	0.60	2.50	12	20
5:E:816:7Q9:P	5:E:816:7Q9:C3	0.60	2.90	2	11
5:E:837:7Q9:C11	6:E:841:17F:O10	0.60	2.50	1	3
5:E:845:7Q9:C2	5:E:845:7Q9:O32	0.60	2.47	10	14
5:E:868:7Q9:C3	5:E:868:7Q9:O22	0.60	2.47	20	7
1:A:72:MET:HE1	1:A:99:GLN:HG2	0.60	1.74	2	1
6:E:805:17F:O8	6:E:805:17F:O9	0.60	2.19	3	19
6:A:208:17F:H2	6:A:208:17F:O2	0.60	1.96	7	9
6:B:208:17F:C31	6:B:214:17F:H10	0.60	2.25	5	2
5:D:504:7Q9:C32	6:D:516:17F:C1Y	0.60	2.80	6	1
5:E:802:7Q9:C315	6:E:809:17F:H72	0.60	2.26	8	2
6:E:838:17F:C10	6:E:856:17F:H12	0.60	2.26	16	4
6:D:517:17F:H48	6:D:517:17F:H62	0.60	1.73	10	1
1:A:6:LEU:HD12	1:A:55:ILE:HG12	0.60	1.72	11	1
6:E:809:17F:C1Z	6:E:818:17F:H64	0.60	2.26	11	1
5:A:211:7Q9:C38	5:A:213:7Q9:C314	0.60	2.80	13	1
6:E:811:17F:H6A	5:E:823:7Q9:C11	0.60	2.27	13	1
5:D:544:7Q9:O12	5:D:544:7Q9:C13	0.60	2.50	14	20
5:D:549:7Q9:C2	5:D:549:7Q9:O32	0.60	2.47	10	13
6:E:809:17F:C1X	6:E:809:17F:C23	0.60	2.67	10	9
5:E:824:7Q9:C1	5:E:824:7Q9:C31	0.60	2.79	3	11
5:E:824:7Q9:C315	6:E:841:17F:H69	0.60	2.26	3	1
5:E:812:7Q9:C13	5:E:816:7Q9:C22	0.60	2.80	17	7
6:B:214:17F:H77	5:B:217:7Q9:C316	0.60	2.27	9	3
6:E:809:17F:C7	6:E:809:17F:C17	0.60	2.80	9	1
6:D:533:17F:H66	6:D:533:17F:C22	0.60	2.24	14	1
6:B:214:17F:C6	5:B:217:7Q9:O32	0.60	2.49	15	1
6:A:208:17F:H6A	6:A:208:17F:O10	0.59	1.97	18	17
5:D:518:7Q9:C12	5:D:518:7Q9:O22	0.59	2.50	1	9
5:D:549:7Q9:C15	6:E:856:17F:O1	0.59	2.50	6	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:534:17F:H36	6:D:534:17F:H58	0.59	1.72	4	1
5:B:209:7Q9:C311	5:B:209:7Q9:C37	0.59	2.80	6	1
6:D:527:17F:H55	6:E:856:17F:H43	0.59	1.73	13	3
6:E:807:17F:H55	6:E:818:17F:H78	0.59	1.73	11	1
6:B:214:17F:H76	6:B:214:17F:H48	0.59	1.74	12	1
5:B:212:7Q9:C312	5:B:212:7Q9:C38	0.59	2.78	1	1
5:B:220:7Q9:O22	5:B:220:7Q9:O11	0.59	2.19	2	20
5:D:508:7Q9:O32	5:D:508:7Q9:O21	0.59	2.20	15	15
6:B:219:17F:H35	6:B:219:17F:H20	0.59	1.72	3	1
5:E:803:7Q9:O22	5:E:803:7Q9:O31	0.59	2.20	3	17
5:A:212:7Q9:C317	6:A:214:17F:H76	0.59	2.27	18	2
2:D:389:LEU:HD22	5:D:540:7Q9:C312	0.59	2.27	20	4
6:E:828:17F:H11A	6:E:828:17F:H39	0.59	1.72	8	2
5:D:518:7Q9:O32	5:D:518:7Q9:C21	0.59	2.51	20	19
5:E:812:7Q9:C14	5:E:812:7Q9:O12	0.59	2.50	18	20
5:E:813:7Q9:C35	6:E:819:17F:H12	0.59	2.27	14	2
1:A:64:TYR:HB3	1:A:67:MET:HB3	0.59	1.73	9	4
6:D:510:17F:C17	6:D:516:17F:H9A	0.59	2.27	18	4
6:E:841:17F:H29	6:E:841:17F:H39	0.59	1.75	14	4
6:E:856:17F:O10	6:E:856:17F:H6A	0.59	1.95	7	14
6:B:208:17F:H64	6:B:208:17F:C23	0.59	2.27	7	3
1:B:4:TYR:HB2	1:B:53:LEU:HD23	0.59	1.73	10	1
6:D:510:17F:H78	6:D:510:17F:C30	0.59	2.28	11	3
5:A:209:7Q9:O22	5:A:209:7Q9:O11	0.59	2.20	11	20
5:D:508:7Q9:C21	5:D:508:7Q9:O32	0.59	2.51	8	9
6:D:516:17F:C27	6:D:516:17F:C23	0.59	2.73	7	14
5:E:804:7Q9:C312	5:E:804:7Q9:C38	0.59	2.77	19	11
5:E:821:7Q9:C15	5:E:821:7Q9:O12	0.59	2.49	10	19
5:D:539:7Q9:C1	5:D:539:7Q9:O32	0.59	2.50	5	5
5:E:804:7Q9:C3	6:E:811:17F:H19	0.59	2.26	10	4
5:D:512:7Q9:C318	6:D:528:17F:H36	0.59	2.28	6	2
5:B:218:7Q9:C311	6:B:219:17F:H67	0.59	2.27	7	1
6:B:214:17F:H5	6:B:219:17F:C9	0.59	2.13	15	2
6:E:870:17F:H58	6:E:870:17F:C1X	0.59	2.28	16	2
5:D:520:7Q9:C15	5:D:520:7Q9:O12	0.59	2.50	19	20
5:D:526:7Q9:C35	5:D:526:7Q9:O31	0.59	2.50	19	9
5:E:833:7Q9:C11	6:E:838:17F:H2	0.59	2.27	1	1
5:E:849:7Q9:C21	5:E:849:7Q9:O32	0.59	2.49	19	15
6:D:517:17F:H52	6:D:517:17F:C37	0.59	2.27	20	2
5:E:840:7Q9:C3	5:E:840:7Q9:O22	0.59	2.48	18	10
5:B:218:7Q9:C1	5:B:218:7Q9:O22	0.59	2.48	9	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:818:17F:H40	6:E:819:17F:H38	0.59	1.73	11	2
5:E:824:7Q9:C36	5:E:842:7Q9:C33	0.59	2.80	3	1
6:E:838:17F:H51	6:E:874:17F:H51	0.59	1.75	3	2
6:E:838:17F:O10	6:E:838:17F:C7	0.59	2.50	16	5
6:B:208:17F:H68	6:B:208:17F:H45	0.59	1.74	7	2
5:B:217:7Q9:C13	5:D:522:7Q9:O22	0.59	2.51	14	2
2:D:333:LYS:HG3	5:E:878:7Q9:C318	0.59	2.26	16	2
6:E:811:17F:H8	6:E:811:17F:H34	0.59	1.75	12	1
5:E:866:7Q9:C1	5:E:876:7Q9:O13	0.59	2.50	18	3
6:B:214:17F:H62	6:B:219:17F:H37	0.59	1.73	1	2
5:D:537:7Q9:O32	5:D:537:7Q9:C2	0.59	2.48	2	5
5:E:852:7Q9:C312	5:E:852:7Q9:C38	0.59	2.79	1	9
5:E:816:7Q9:C3	5:E:816:7Q9:P	0.59	2.90	13	9
6:E:819:17F:O8	6:E:819:17F:H4A	0.59	1.96	18	3
6:B:214:17F:H18	6:B:219:17F:H8A	0.59	1.70	4	1
6:D:534:17F:H61	6:D:534:17F:H54	0.59	1.73	6	1
6:E:817:17F:H61	5:E:826:7Q9:C35	0.59	2.26	15	4
6:D:501:17F:H37	6:D:501:17F:C1Z	0.59	2.27	16	1
6:B:214:17F:H18	6:B:219:17F:C2	0.59	2.27	17	1
2:D:436:TYR:HB3	5:D:537:7Q9:C314	0.59	2.27	19	1
6:D:528:17F:H76	5:E:878:7Q9:C318	0.59	2.27	20	1
5:B:203:7Q9:C32	6:B:208:17F:H6	0.59	2.27	1	1
5:D:531:7Q9:C1	5:D:531:7Q9:O32	0.59	2.51	20	6
5:E:839:7Q9:O32	5:E:839:7Q9:C21	0.59	2.50	3	10
5:E:846:7Q9:O22	5:E:846:7Q9:C3	0.59	2.46	12	10
5:E:867:7Q9:O22	5:E:867:7Q9:C3	0.59	2.49	13	14
5:E:871:7Q9:O32	5:E:871:7Q9:O21	0.59	2.21	4	16
6:E:807:17F:H69	5:E:813:7Q9:C313	0.59	2.28	2	1
6:D:534:17F:H65	6:D:534:17F:C1X	0.59	2.27	19	2
1:A:17:SER:HB2	3:A:201:GSP:O1A	0.59	1.97	1	2
6:D:510:17F:H76	6:D:510:17F:H53	0.59	1.74	1	2
5:D:519:7Q9:C14	5:D:519:7Q9:O12	0.59	2.51	20	20
5:E:816:7Q9:C3	5:E:816:7Q9:O12	0.59	2.50	2	10
5:E:829:7Q9:O22	5:E:829:7Q9:P	0.59	2.61	6	6
5:E:839:7Q9:O12	5:E:839:7Q9:C13	0.59	2.51	16	20
5:E:854:7Q9:O32	5:E:854:7Q9:C21	0.59	2.51	9	19
5:E:878:7Q9:C15	5:E:878:7Q9:O12	0.59	2.51	2	20
2:E:708:LYS:HB2	2:E:709:PRO:HD3	0.59	1.75	20	15
5:A:205:7Q9:O22	5:B:204:7Q9:C12	0.59	2.51	4	3
6:B:208:17F:H34	6:B:208:17F:C23	0.59	2.26	4	1
2:D:330:ALA:HA	2:D:333:LYS:HE2	0.59	1.74	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:A:213:7Q9:O12	5:A:213:7Q9:C14	0.59	2.51	17	19
5:A:215:7Q9:O12	5:A:215:7Q9:C14	0.59	2.50	16	20
6:B:219:17F:C20	6:B:219:17F:C2X	0.59	2.79	15	4
6:D:510:17F:H73	5:E:832:7Q9:C315	0.59	2.28	1	2
5:D:522:7Q9:C13	5:D:522:7Q9:O12	0.59	2.51	4	20
6:D:527:17F:C23	6:D:527:17F:H68	0.59	2.28	3	3
6:E:807:17F:C31	6:E:819:17F:C1X	0.59	2.80	9	7
5:E:833:7Q9:O31	5:E:833:7Q9:O22	0.59	2.20	19	19
5:A:207:7Q9:O32	5:A:207:7Q9:C1	0.59	2.50	8	2
5:E:802:7Q9:C312	5:E:802:7Q9:C316	0.59	2.80	4	1
6:B:208:17F:H44	5:B:212:7Q9:C37	0.59	2.28	7	1
6:E:818:17F:H47	6:E:818:17F:C42	0.59	2.27	10	2
6:D:510:17F:O10	6:D:527:17F:N1	0.59	2.34	9	1
5:E:802:7Q9:C314	6:E:809:17F:H70	0.59	2.28	18	3
6:D:510:17F:H50	6:D:510:17F:H78	0.59	1.75	14	1
6:D:510:17F:C28	6:D:516:17F:H67	0.59	2.27	19	2
5:D:525:7Q9:C14	5:D:525:7Q9:O12	0.59	2.51	2	20
5:D:538:7Q9:C14	5:D:538:7Q9:O12	0.59	2.51	1	20
6:E:811:17F:O10	6:E:811:17F:H6A	0.59	1.98	16	16
6:E:811:17F:O8	6:E:811:17F:O6	0.59	2.21	11	13
5:E:815:7Q9:O12	5:E:815:7Q9:C13	0.59	2.50	15	20
5:E:826:7Q9:O12	5:E:826:7Q9:C13	0.59	2.50	5	20
5:D:512:7Q9:C33	6:D:528:17F:C6	0.59	2.78	2	2
6:E:818:17F:N1	5:E:835:7Q9:O13	0.59	2.36	2	1
6:E:874:17F:O1	6:E:874:17F:C6	0.59	2.50	6	14
6:B:219:17F:H19	6:B:219:17F:H29	0.59	1.75	3	1
5:A:204:7Q9:C311	6:A:208:17F:H65	0.59	2.28	14	3
1:B:64:TYR:HB3	1:B:67:MET:HB3	0.59	1.75	16	5
5:D:504:7Q9:C318	6:D:516:17F:H68	0.59	2.27	20	3
6:B:214:17F:H6	5:B:217:7Q9:C32	0.59	2.28	6	1
6:A:214:17F:H4A	5:D:539:7Q9:C13	0.59	2.28	17	3
6:B:208:17F:H41	6:B:214:17F:C22	0.59	2.27	11	1
5:E:835:7Q9:O13	5:E:837:7Q9:C13	0.59	2.51	18	2
5:B:207:7Q9:C11	5:B:211:7Q9:C22	0.59	2.81	14	1
6:A:214:17F:O8	6:A:214:17F:C17	0.58	2.51	18	14
5:B:207:7Q9:C13	6:D:501:17F:H19A	0.58	2.28	1	1
5:B:217:7Q9:O12	5:B:217:7Q9:C14	0.58	2.51	14	20
6:D:510:17F:H53	6:D:510:17F:C42	0.58	2.27	12	2
5:D:531:7Q9:O12	5:D:531:7Q9:C13	0.58	2.51	10	20
6:E:801:17F:H39	5:E:804:7Q9:C37	0.58	2.28	1	3
5:E:835:7Q9:O12	5:E:835:7Q9:C15	0.58	2.51	19	20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:531:7Q9:C38	5:D:540:7Q9:C37	0.58	2.81	15	5
6:E:838:17F:H59	6:E:838:17F:H18A	0.58	1.75	4	10
6:D:510:17F:O6	6:D:516:17F:H4	0.58	1.96	6	2
6:E:801:17F:H33	6:E:801:17F:C21	0.58	2.28	17	5
6:E:817:17F:C32	5:E:833:7Q9:C35	0.58	2.81	15	4
6:D:534:17F:H51	5:D:536:7Q9:C318	0.58	2.28	10	1
6:E:819:17F:C7	6:E:819:17F:H11	0.58	2.28	15	3
1:A:12:ASP:HB2	3:A:201:GSP:S1G	0.58	2.37	18	1
6:E:811:17F:H61	5:E:823:7Q9:C32	0.58	2.28	19	2
5:B:207:7Q9:C15	6:D:501:17F:H18A	0.58	2.28	1	2
5:D:503:7Q9:O22	5:D:503:7Q9:C3	0.58	2.48	7	6
5:E:803:7Q9:O12	5:E:803:7Q9:C13	0.58	2.50	7	20
5:E:810:7Q9:C15	5:E:810:7Q9:O12	0.58	2.51	6	20
5:E:830:7Q9:C14	5:E:830:7Q9:O12	0.58	2.51	9	20
6:E:838:17F:H52	5:E:857:7Q9:C312	0.58	2.28	6	7
5:E:857:7Q9:O32	5:E:857:7Q9:O21	0.58	2.21	16	5
5:A:204:7Q9:C12	6:B:208:17F:H9	0.58	2.27	2	1
5:D:538:7Q9:C12	5:D:538:7Q9:O32	0.58	2.51	3	5
5:B:203:7Q9:C314	6:B:208:17F:H74	0.58	2.28	3	2
5:E:802:7Q9:C3	6:E:809:17F:O1	0.58	2.50	5	3
6:E:818:17F:H43	5:E:835:7Q9:C311	0.58	2.28	16	3
6:D:510:17F:H77	6:D:516:17F:H74	0.58	1.75	20	1
2:D:258:SER:HB3	5:D:544:7Q9:C38	0.58	2.28	20	8
5:D:507:7Q9:C32	6:D:516:17F:C1Y	0.58	2.80	11	6
6:D:528:17F:O7	6:D:528:17F:O10	0.58	2.21	6	4
5:E:834:7Q9:C15	5:E:834:7Q9:O12	0.58	2.51	7	20
5:B:203:7Q9:O22	5:B:203:7Q9:C3	0.58	2.49	16	16
6:B:208:17F:C1Z	6:B:214:17F:H41	0.58	2.27	2	1
6:D:527:17F:H40	6:D:527:17F:C40	0.58	2.16	2	1
6:E:807:17F:H47	6:E:807:17F:C41	0.58	2.25	2	6
5:E:864:7Q9:O13	5:E:864:7Q9:C21	0.58	2.51	4	12
5:D:544:7Q9:C34	6:D:546:17F:H59	0.58	2.27	4	1
6:E:856:17F:O8	6:E:856:17F:H4A	0.58	1.98	16	4
5:E:813:7Q9:C313	6:E:819:17F:H55	0.58	2.29	10	2
6:E:819:17F:C19	5:E:852:7Q9:C35	0.58	2.81	19	2
6:E:855:17F:H29	6:E:855:17F:C33	0.58	2.28	15	2
6:D:511:17F:H53	6:E:828:17F:C37	0.58	2.16	19	1
5:A:210:7Q9:C14	5:A:210:7Q9:O12	0.58	2.50	15	20
5:D:503:7Q9:C13	5:D:503:7Q9:O12	0.58	2.52	20	20
5:E:802:7Q9:C13	5:E:802:7Q9:O12	0.58	2.50	19	20
5:E:804:7Q9:O22	5:E:804:7Q9:C3	0.58	2.49	18	17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:841:17F:H37	5:E:876:7Q9:C31	0.58	2.28	3	3
6:D:501:17F:H9	5:D:509:7Q9:O22	0.58	1.97	2	1
6:D:501:17F:H46	6:D:501:17F:C37	0.58	2.28	5	1
6:D:501:17F:H51	6:D:501:17F:H71	0.58	1.74	12	1
5:D:509:7Q9:O12	5:D:509:7Q9:C13	0.58	2.52	2	20
5:D:513:7Q9:C15	5:D:513:7Q9:O12	0.58	2.51	12	20
6:D:510:17F:H70	5:D:524:7Q9:C318	0.58	2.29	2	1
6:E:805:17F:O2	6:E:805:17F:N1	0.58	2.30	9	3
6:E:819:17F:O10	6:E:819:17F:O6	0.58	2.21	2	2
5:E:844:7Q9:C3	5:E:844:7Q9:O22	0.58	2.48	14	8
5:E:851:7Q9:O32	5:E:851:7Q9:C21	0.58	2.51	9	14
5:E:859:7Q9:O32	5:E:859:7Q9:O21	0.58	2.21	10	8
5:E:878:7Q9:O11	5:E:878:7Q9:O22	0.58	2.22	2	11
6:D:510:17F:C22	6:D:511:17F:H56	0.58	2.28	6	1
5:D:514:7Q9:C1	5:D:514:7Q9:O22	0.58	2.50	11	2
6:E:809:17F:C29	6:E:818:17F:H72	0.58	2.28	16	3
6:D:517:17F:H46	5:D:520:7Q9:C312	0.58	2.28	12	1
6:D:534:17F:H1A	5:D:539:7Q9:C32	0.58	2.28	12	1
5:E:832:7Q9:C23	6:E:856:17F:H39	0.58	2.29	14	1
1:B:59:ALA:HA	3:B:201:GSP:O2G	0.58	1.98	15	1
5:A:205:7Q9:O12	5:A:205:7Q9:C13	0.58	2.51	5	20
5:B:216:7Q9:C34	5:D:519:7Q9:C22	0.58	2.81	9	7
6:D:546:17F:O10	6:D:546:17F:H6A	0.58	1.98	11	10
5:E:824:7Q9:C14	5:E:824:7Q9:O12	0.58	2.51	4	20
5:E:832:7Q9:C1	5:E:832:7Q9:O22	0.58	2.49	17	13
1:A:78:PHE:HB2	1:A:111:MET:HG2	0.58	1.73	17	8
5:A:207:7Q9:C1	5:A:207:7Q9:C31	0.58	2.82	8	2
6:B:208:17F:H57	6:B:208:17F:C26	0.58	2.29	12	6
6:D:533:17F:H9A	6:D:533:17F:H60	0.58	1.76	4	1
6:E:818:17F:H12	6:E:819:17F:H9A	0.58	1.75	4	1
6:D:534:17F:H35	6:D:534:17F:C25	0.58	2.29	20	4
6:E:838:17F:O2	6:E:838:17F:H5	0.58	1.99	6	7
6:B:208:17F:H41	6:B:214:17F:C21	0.58	2.29	11	1
5:D:537:7Q9:C31	6:D:546:17F:H11A	0.58	2.28	11	2
6:D:511:17F:H2	6:D:511:17F:C18	0.58	2.19	12	1
5:B:220:7Q9:C22	5:D:543:7Q9:O14	0.58	2.52	1	2
6:D:511:17F:C28	6:D:511:17F:H77	0.58	2.29	1	2
5:D:537:7Q9:O32	6:D:546:17F:H29	0.58	1.98	1	2
5:E:844:7Q9:C15	5:E:844:7Q9:O12	0.58	2.52	9	20
5:E:857:7Q9:C3	6:E:874:17F:C10	0.58	2.82	1	8
1:B:38:ASP:HB2	1:B:57:ASP:HB3	0.58	1.75	3	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:510:17F:H8	6:D:516:17F:C18	0.58	2.27	14	4
6:E:817:17F:C31	5:E:833:7Q9:C35	0.58	2.81	13	5
2:E:736:TYR:HD1	5:E:875:7Q9:C310	0.58	2.12	13	5
6:B:208:17F:H41	6:B:214:17F:H38	0.58	1.76	11	1
6:B:215:17F:H72	5:D:515:7Q9:C317	0.58	2.29	14	1
1:B:146:ALA:HB3	3:B:201:GSP:N7	0.58	2.13	15	2
6:D:517:17F:H66	6:E:841:17F:C42	0.58	2.28	16	1
6:E:828:17F:O10	6:E:828:17F:C6	0.58	2.50	17	8
5:E:836:7Q9:C1	5:E:836:7Q9:O22	0.58	2.50	16	5
5:B:206:7Q9:C316	6:E:805:17F:H71	0.58	2.29	3	1
5:B:205:7Q9:O13	5:B:211:7Q9:C15	0.58	2.52	4	1
6:D:510:17F:C4	6:D:516:17F:C4	0.58	2.82	6	6
6:E:818:17F:H65	6:E:818:17F:C32	0.58	2.27	18	3
6:B:215:17F:H54	6:B:215:17F:H67	0.58	1.75	8	1
5:A:212:7Q9:O32	6:A:214:17F:N1	0.58	2.36	10	1
6:D:510:17F:H32	6:D:527:17F:H60	0.58	1.76	12	2
5:D:537:7Q9:C35	6:D:546:17F:H73	0.58	2.29	14	2
6:E:818:17F:H19A	5:E:824:7Q9:C13	0.58	2.28	20	1
6:B:208:17F:C31	6:B:214:17F:H45	0.58	2.28	2	1
5:D:506:7Q9:C311	6:D:517:17F:H58	0.58	2.29	2	1
6:D:510:17F:H57	6:D:527:17F:C33	0.58	2.27	2	1
6:D:546:17F:C40	6:D:546:17F:C36	0.58	2.78	11	2
6:D:510:17F:H36	6:D:510:17F:C25	0.58	2.29	3	4
5:E:802:7Q9:C2	5:E:802:7Q9:O32	0.58	2.50	20	7
6:D:510:17F:C9	6:D:516:17F:C11	0.58	2.75	8	3
6:D:510:17F:H20	6:D:527:17F:H60	0.58	1.75	6	1
5:D:519:7Q9:C312	5:D:540:7Q9:C39	0.58	2.82	6	1
6:E:841:17F:O4	5:E:876:7Q9:C15	0.58	2.51	11	1
6:A:208:17F:H12	5:A:209:7Q9:C310	0.58	2.28	1	3
5:A:212:7Q9:C1	5:A:212:7Q9:C31	0.58	2.82	13	16
6:D:527:17F:O10	6:D:527:17F:H4	0.58	1.99	19	8
5:E:802:7Q9:O22	5:E:802:7Q9:O11	0.58	2.21	9	16
5:E:813:7Q9:C1	5:E:813:7Q9:O22	0.58	2.50	5	5
5:E:825:7Q9:C1	5:E:825:7Q9:O22	0.58	2.48	2	9
5:E:833:7Q9:C35	5:E:833:7Q9:C31	0.58	2.82	8	20
5:E:849:7Q9:C14	5:E:849:7Q9:O12	0.58	2.52	12	20
5:B:207:7Q9:O12	5:B:207:7Q9:C13	0.58	2.52	7	18
5:D:506:7Q9:O22	5:D:506:7Q9:O12	0.58	2.21	3	1
6:D:511:17F:H43	5:D:513:7Q9:C315	0.58	2.29	6	4
6:E:807:17F:H20A	6:E:818:17F:C7	0.58	2.29	10	1
2:D:309:GLN:HG3	6:D:527:17F:H58	0.58	1.75	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:E:605:GLN:HB2	5:E:866:7Q9:C311	0.58	2.28	13	2
5:D:547:7Q9:C14	5:D:547:7Q9:O12	0.57	2.51	17	20
5:D:548:7Q9:O11	5:D:548:7Q9:O22	0.57	2.22	6	13
5:E:829:7Q9:C14	5:E:829:7Q9:O12	0.57	2.51	10	20
5:E:873:7Q9:C21	5:E:873:7Q9:O32	0.57	2.52	18	12
6:E:874:17F:O7	6:E:874:17F:O10	0.57	2.22	15	16
5:E:877:7Q9:C31	5:E:877:7Q9:O22	0.57	2.52	5	15
5:E:853:7Q9:O32	5:E:853:7Q9:O21	0.57	2.22	10	13
5:E:857:7Q9:O21	5:E:857:7Q9:O32	0.57	2.22	8	13
6:E:805:17F:O1	6:E:805:17F:N1	0.57	2.31	6	8
6:D:546:17F:O10	6:D:546:17F:C1Y	0.57	2.52	10	3
5:E:876:7Q9:C3	5:E:876:7Q9:O22	0.57	2.50	16	4
2:D:269:GLN:HG2	6:D:534:17F:H32	0.57	1.75	11	2
6:E:874:17F:H4	6:E:874:17F:O10	0.57	1.98	10	1
5:A:203:7Q9:C317	6:E:801:17F:H53	0.57	2.29	14	4
5:D:502:7Q9:C21	5:D:502:7Q9:O32	0.57	2.52	7	16
5:D:507:7Q9:O12	5:D:507:7Q9:C13	0.57	2.51	1	20
6:E:807:17F:H49	6:E:809:17F:C35	0.57	2.29	1	3
5:E:822:7Q9:C14	5:E:822:7Q9:O12	0.57	2.52	4	20
5:E:860:7Q9:O12	5:E:860:7Q9:C15	0.57	2.52	2	20
6:A:208:17F:H4A	6:A:208:17F:C7	0.57	2.30	7	8
5:B:211:7Q9:C22	6:D:501:17F:C31	0.57	2.82	13	5
6:D:510:17F:H48	6:D:510:17F:H60	0.57	1.76	6	1
5:B:217:7Q9:C15	6:B:219:17F:O10	0.57	2.53	8	3
5:E:824:7Q9:C37	6:E:841:17F:H34	0.57	2.29	11	1
5:B:213:7Q9:C36	5:D:514:7Q9:C36	0.57	2.82	13	1
6:E:818:17F:H61	6:E:841:17F:C37	0.57	2.28	18	2
5:D:513:7Q9:C21	5:D:513:7Q9:C31	0.57	2.81	15	1
6:D:510:17F:H54	6:D:516:17F:C42	0.57	2.28	16	1
2:E:642:SER:H	2:E:643:PRO:HD2	0.57	1.58	17	1
6:E:819:17F:H66	5:E:852:7Q9:C310	0.57	2.29	17	1
6:D:516:17F:C21	6:D:516:17F:H62	0.57	2.29	18	1
1:A:35:THR:HG23	3:A:201:GSP:H5'2	0.57	1.74	19	1
6:D:501:17F:H61	6:D:501:17F:H41	0.57	1.75	19	1
1:B:22:GLN:O	1:B:26:ASN:HA	0.57	1.99	13	8
5:B:203:7Q9:O12	5:B:203:7Q9:C13	0.57	2.51	17	20
5:B:213:7Q9:C1	5:B:213:7Q9:C31	0.57	2.82	4	19
5:D:505:7Q9:C14	5:D:505:7Q9:O12	0.57	2.52	19	20
5:D:530:7Q9:C14	5:D:530:7Q9:O12	0.57	2.52	15	20
5:D:537:7Q9:C15	5:D:537:7Q9:O12	0.57	2.52	8	20
5:E:835:7Q9:O32	5:E:835:7Q9:O21	0.57	2.23	10	12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:818:17F:O9	6:E:818:17F:H32	0.57	1.99	12	6
6:E:819:17F:H58	6:E:819:17F:C25	0.57	2.27	4	3
5:E:853:7Q9:O14	5:E:853:7Q9:C21	0.57	2.51	4	1
5:B:207:7Q9:C318	6:E:801:17F:H68	0.57	2.29	5	3
6:A:214:17F:C30	6:A:214:17F:H70	0.57	2.29	6	1
6:D:510:17F:H9	6:D:516:17F:H8A	0.57	1.74	6	1
5:D:515:7Q9:C318	6:D:517:17F:H52	0.57	2.29	6	1
5:E:806:7Q9:C23	6:E:817:17F:H5	0.57	2.29	8	1
5:A:212:7Q9:C31	6:A:214:17F:H18A	0.57	2.30	16	1
6:D:517:17F:H51	6:D:517:17F:C38	0.57	2.08	17	1
6:B:208:17F:H56	5:B:212:7Q9:C36	0.57	2.28	18	1
5:A:216:7Q9:C15	5:A:216:7Q9:O12	0.57	2.52	4	20
6:D:510:17F:H56	6:D:516:17F:C1X	0.57	2.30	1	4
5:D:539:7Q9:C14	5:D:539:7Q9:O12	0.57	2.52	11	20
5:D:549:7Q9:O12	5:D:549:7Q9:C13	0.57	2.53	11	20
5:E:804:7Q9:O12	5:E:804:7Q9:C14	0.57	2.52	4	19
5:E:812:7Q9:O31	5:E:812:7Q9:O22	0.57	2.22	16	16
5:E:875:7Q9:C14	5:E:875:7Q9:O12	0.57	2.52	14	20
5:B:205:7Q9:O22	5:B:205:7Q9:O11	0.57	2.22	9	14
6:B:215:17F:H47	6:B:215:17F:H65	0.57	1.77	2	1
6:B:219:17F:C17	6:B:219:17F:O8	0.57	2.52	17	6
5:D:525:7Q9:O14	5:D:525:7Q9:C21	0.57	2.52	20	12
5:D:541:7Q9:C2	5:D:541:7Q9:O32	0.57	2.49	12	8
5:D:543:7Q9:C312	5:D:543:7Q9:C38	0.57	2.81	9	7
6:B:208:17F:H20A	6:B:214:17F:O1	0.57	2.00	5	1
6:A:208:17F:H51	5:E:823:7Q9:C317	0.57	2.29	6	1
6:E:838:17F:H12	6:E:856:17F:C11	0.57	2.29	9	3
6:D:533:17F:C30	6:E:870:17F:H68	0.57	2.28	11	1
2:D:403:LEU:HD11	6:E:872:17F:H71	0.57	1.76	13	1
6:E:817:17F:H11A	5:E:833:7Q9:C33	0.57	2.29	16	2
5:A:212:7Q9:C31	5:A:212:7Q9:C1	0.57	2.83	16	1
5:A:209:7Q9:C13	5:A:209:7Q9:O12	0.57	2.52	1	20
5:A:210:7Q9:O22	5:A:210:7Q9:C3	0.57	2.47	16	14
5:D:508:7Q9:O12	5:D:508:7Q9:C14	0.57	2.53	9	20
5:D:512:7Q9:O32	5:D:512:7Q9:O21	0.57	2.23	16	17
5:D:514:7Q9:C21	5:D:514:7Q9:O12	0.57	2.53	10	6
5:E:857:7Q9:O12	5:E:857:7Q9:C14	0.57	2.53	2	20
1:A:32:TYR:HB3	3:A:201:GSP:O2'	0.57	1.99	2	1
5:E:852:7Q9:C3	5:E:852:7Q9:C12	0.57	2.82	2	3
6:E:856:17F:C4	6:E:856:17F:C7	0.57	2.83	15	16
6:D:510:17F:H36	6:D:510:17F:H43	0.57	1.75	3	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:539:7Q9:O32	5:D:539:7Q9:C15	0.57	2.53	10	8
5:B:216:7Q9:C31	5:D:519:7Q9:C23	0.57	2.82	4	1
6:A:214:17F:O4	5:D:539:7Q9:C13	0.57	2.52	5	1
6:D:501:17F:C1X	5:D:509:7Q9:O22	0.57	2.50	6	2
6:D:510:17F:C10	6:D:516:17F:H8A	0.57	2.26	12	2
6:E:805:17F:C26	6:E:805:17F:H68	0.57	2.30	19	3
1:B:37:GLU:HG2	1:B:56:LEU:HD11	0.57	1.76	16	1
6:B:215:17F:O7	6:B:215:17F:O10	0.57	2.23	16	1
5:A:203:7Q9:C14	5:A:203:7Q9:O12	0.57	2.53	9	20
5:A:212:7Q9:C14	5:A:212:7Q9:O12	0.57	2.52	20	20
5:D:504:7Q9:C1	5:D:504:7Q9:O22	0.57	2.50	17	7
6:E:819:17F:O10	6:E:819:17F:C6	0.57	2.50	17	8
5:E:848:7Q9:C14	5:E:848:7Q9:O12	0.57	2.52	11	20
5:E:859:7Q9:O12	5:E:859:7Q9:C14	0.57	2.52	10	20
5:E:871:7Q9:C13	5:E:871:7Q9:O12	0.57	2.53	16	20
5:D:535:7Q9:O22	5:D:535:7Q9:C3	0.57	2.51	13	10
5:E:810:7Q9:C2	5:E:810:7Q9:O32	0.57	2.50	3	5
1:B:117:LYS:NZ	3:B:201:GSP:N7	0.57	2.52	7	2
5:E:857:7Q9:C33	6:E:874:17F:H37	0.57	2.29	8	2
5:B:209:7Q9:C32	5:B:209:7Q9:C13	0.57	2.82	9	2
6:E:817:17F:H9	5:E:833:7Q9:C32	0.57	2.30	9	1
6:D:517:17F:O8	6:D:517:17F:C17	0.57	2.53	12	9
6:D:534:17F:C32	6:D:534:17F:C36	0.57	2.79	5	9
5:E:843:7Q9:C15	5:E:843:7Q9:O12	0.57	2.53	10	20
5:E:867:7Q9:O12	5:E:867:7Q9:C14	0.57	2.53	5	20
6:E:870:17F:H2	6:E:870:17F:O2	0.57	2.00	10	11
6:D:534:17F:C2X	6:D:534:17F:C33	0.57	2.83	2	4
5:E:868:7Q9:O32	5:E:873:7Q9:C15	0.57	2.53	4	3
5:E:849:7Q9:O21	5:E:849:7Q9:O32	0.57	2.23	15	5
5:A:204:7Q9:C318	6:E:811:17F:H42	0.57	2.30	4	1
5:D:507:7Q9:O14	5:D:507:7Q9:C21	0.57	2.51	10	4
5:D:522:7Q9:O22	5:D:522:7Q9:O11	0.57	2.22	12	6
5:D:513:7Q9:C14	5:D:526:7Q9:C11	0.57	2.83	5	1
5:B:204:7Q9:C318	6:E:801:17F:H75	0.57	2.29	9	3
5:E:810:7Q9:O13	5:E:821:7Q9:C11	0.57	2.53	10	1
5:D:503:7Q9:C23	6:D:510:17F:H37	0.57	2.29	14	1
6:A:214:17F:H47	6:A:214:17F:H70	0.57	1.76	16	2
6:A:214:17F:H37	6:A:214:17F:H33	0.57	1.77	18	1
2:D:334:LEU:HB3	5:D:532:7Q9:C310	0.57	2.30	3	7
5:D:529:7Q9:C13	5:D:529:7Q9:O12	0.57	2.53	4	20
5:D:532:7Q9:O32	5:D:532:7Q9:C21	0.57	2.52	2	16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:B:207:7Q9:C2	5:B:207:7Q9:O32	0.57	2.49	14	7
6:B:214:17F:C1Y	5:B:220:7Q9:C34	0.57	2.80	9	4
6:E:818:17F:H42	5:E:835:7Q9:C39	0.57	2.30	6	4
5:E:802:7Q9:C310	6:E:807:17F:H46	0.57	2.29	5	3
5:E:861:7Q9:C3	5:E:876:7Q9:C11	0.57	2.81	10	2
6:E:817:17F:H56	5:E:833:7Q9:C35	0.57	2.30	13	4
5:A:204:7Q9:C314	6:A:208:17F:C42	0.57	2.82	16	1
6:A:214:17F:H6A	6:A:214:17F:O10	0.57	1.98	16	1
6:E:805:17F:H19A	5:E:810:7Q9:C22	0.57	2.29	20	1
6:E:809:17F:H51	6:E:818:17F:H75	0.57	1.76	20	1
6:D:510:17F:H78	6:D:510:17F:H52	0.57	1.77	11	3
6:D:511:17F:O4	5:D:524:7Q9:C15	0.57	2.53	8	5
5:E:803:7Q9:O22	5:E:803:7Q9:C35	0.57	2.53	17	8
5:E:847:7Q9:C14	5:E:847:7Q9:O12	0.57	2.53	3	20
5:E:803:7Q9:O22	5:E:803:7Q9:C31	0.57	2.53	9	6
6:D:528:17F:H37	6:D:528:17F:H66	0.57	1.77	12	8
6:D:501:17F:H47	5:D:508:7Q9:C318	0.57	2.29	5	1
6:D:534:17F:H54	6:D:534:17F:C34	0.57	2.30	6	1
6:E:817:17F:H19	6:E:817:17F:H1	0.57	1.76	9	1
5:A:205:7Q9:O13	5:B:209:7Q9:C15	0.57	2.53	11	1
5:D:515:7Q9:C2	5:D:515:7Q9:O32	0.57	2.50	10	10
5:E:866:7Q9:C15	5:E:866:7Q9:O12	0.57	2.53	6	20
5:E:876:7Q9:C14	5:E:876:7Q9:O12	0.57	2.53	14	20
5:D:530:7Q9:O32	5:D:530:7Q9:C21	0.57	2.53	16	11
6:D:534:17F:C33	6:D:534:17F:H35	0.57	2.29	2	1
5:E:815:7Q9:C3	5:E:827:7Q9:O32	0.57	2.52	2	3
1:A:22:GLN:O	1:A:26:ASN:HA	0.57	1.99	13	10
6:D:501:17F:H55	5:D:508:7Q9:C316	0.57	2.30	4	1
6:B:219:17F:H20	6:B:219:17F:H35	0.57	1.76	5	2
6:A:208:17F:H69	6:B:208:17F:H72	0.57	1.76	6	1
5:D:505:7Q9:C39	6:D:528:17F:H41	0.57	2.29	8	2
6:E:856:17F:HN1	6:E:856:17F:P1	0.57	2.23	18	3
6:D:510:17F:C24	6:D:516:17F:H68	0.57	2.19	18	1
5:A:204:7Q9:C13	5:A:204:7Q9:O12	0.56	2.53	10	20
5:A:211:7Q9:O12	5:A:211:7Q9:C13	0.56	2.53	6	20
6:D:501:17F:H74	6:E:807:17F:H53	0.56	1.75	1	2
5:D:521:7Q9:C15	5:D:521:7Q9:O12	0.56	2.53	19	20
5:A:203:7Q9:C3	5:A:203:7Q9:O22	0.56	2.51	18	10
5:D:549:7Q9:C15	6:E:856:17F:H5	0.56	2.30	11	6
6:E:801:17F:H70	5:E:803:7Q9:C316	0.56	2.30	3	1
6:D:510:17F:C18	6:D:516:17F:C10	0.56	2.80	12	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:515:7Q9:C3	6:D:517:17F:C6	0.56	2.79	8	1
6:D:534:17F:H44	6:D:534:17F:H61	0.56	1.77	8	1
2:D:429:PHE:CE1	6:D:533:17F:H68	0.56	2.35	13	3
5:B:212:7Q9:P	5:B:217:7Q9:O31	0.56	2.62	15	1
5:D:504:7Q9:C318	6:D:516:17F:H70	0.56	2.30	18	1
5:B:211:7Q9:C311	6:D:501:17F:H58	0.56	2.30	20	1
5:B:206:7Q9:O12	5:B:206:7Q9:C14	0.56	2.53	7	19
6:B:219:17F:H34	5:D:545:7Q9:C39	0.56	2.30	1	4
6:D:528:17F:H38	6:D:528:17F:H74	0.56	1.75	1	3
5:D:542:7Q9:O22	5:D:542:7Q9:C3	0.56	2.51	16	14
5:E:820:7Q9:O31	5:E:820:7Q9:O22	0.56	2.23	9	11
5:E:836:7Q9:O12	5:E:836:7Q9:C13	0.56	2.53	3	20
6:E:801:17F:H34	6:E:801:17F:H36	0.56	1.75	2	1
6:E:817:17F:H51	5:E:820:7Q9:C318	0.56	2.30	6	1
6:E:838:17F:H8A	6:E:856:17F:C21	0.56	2.30	17	2
5:B:209:7Q9:C13	5:B:209:7Q9:O12	0.56	2.54	9	2
6:A:208:17F:H43	5:E:822:7Q9:C315	0.56	2.30	10	2
6:D:528:17F:H4A	5:D:532:7Q9:C13	0.56	2.30	11	1
5:B:205:7Q9:C310	6:E:809:17F:H77	0.56	2.30	15	2
6:E:805:17F:H19A	5:E:810:7Q9:C23	0.56	2.30	13	1
6:A:208:17F:H32	6:B:208:17F:H37	0.56	1.77	15	1
6:E:809:17F:C1Z	6:E:818:17F:H63	0.56	2.30	20	1
5:A:215:7Q9:O22	5:A:215:7Q9:C3	0.56	2.51	19	14
5:B:211:7Q9:C15	5:B:211:7Q9:O12	0.56	2.53	19	20
2:D:363:LEU:HD13	2:E:601:LEU:HD11	0.56	1.75	1	1
6:D:501:17F:H55	6:D:501:17F:H68	0.56	1.77	16	5
6:E:809:17F:C31	6:E:809:17F:H29	0.56	2.31	1	1
5:E:845:7Q9:C15	5:E:845:7Q9:O12	0.56	2.53	19	20
5:E:850:7Q9:C15	5:E:850:7Q9:O12	0.56	2.54	6	20
5:E:863:7Q9:C15	5:E:863:7Q9:O12	0.56	2.53	19	20
6:E:874:17F:P1	6:E:874:17F:C6	0.56	2.94	2	19
1:A:117:LYS:HG2	3:A:201:GSP:O6	0.56	2.00	8	2
6:D:501:17F:O1	6:D:501:17F:O9	0.56	2.23	2	4
6:D:534:17F:H65	6:D:534:17F:H30	0.56	1.76	18	7
5:E:848:7Q9:C310	5:E:851:7Q9:C38	0.56	2.84	3	5
6:E:856:17F:H36	6:E:856:17F:H56	0.56	1.77	2	2
1:A:35:THR:HG22	1:B:135:ARG:HH22	0.56	1.60	3	1
1:A:68:ARG:HA	1:A:71:TYR:CE2	0.56	2.35	15	3
5:A:217:7Q9:C317	6:D:546:17F:H51	0.56	2.30	4	1
5:B:220:7Q9:C12	6:D:533:17F:H8A	0.56	2.30	4	2
5:A:204:7Q9:C310	6:A:208:17F:H63	0.56	2.30	16	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:B:210:7Q9:O13	6:B:215:17F:N1	0.56	2.37	17	2
1:A:35:THR:HG21	1:A:38:ASP:HB2	0.56	1.75	9	1
6:B:208:17F:H35	6:B:208:17F:H62	0.56	1.75	10	2
6:D:510:17F:H54	6:D:527:17F:H55	0.56	1.75	10	1
6:D:510:17F:H34	6:D:516:17F:H10	0.56	1.76	11	1
6:D:501:17F:H56	6:D:501:17F:H10A	0.56	1.77	15	1
6:E:818:17F:H40	5:E:835:7Q9:C311	0.56	2.30	20	2
6:B:214:17F:C5	6:B:219:17F:H11A	0.56	2.30	16	1
6:B:214:17F:H33	6:B:219:17F:H37	0.56	1.76	16	1
5:D:513:7Q9:C23	6:D:528:17F:H53	0.56	2.30	18	1
6:A:214:17F:H59	6:A:214:17F:C36	0.56	2.24	19	1
6:D:510:17F:C28	6:D:516:17F:H72	0.56	2.30	19	1
6:D:516:17F:H77	6:E:838:17F:H78	0.56	1.76	20	1
5:D:520:7Q9:C318	2:E:601:LEU:HD21	0.56	2.31	20	1
6:B:214:17F:C35	6:B:214:17F:C31	0.56	2.83	1	2
2:D:269:GLN:HG3	6:D:534:17F:H32	0.56	1.76	1	1
6:D:501:17F:H68	6:D:501:17F:C30	0.56	2.31	16	2
5:E:831:7Q9:O12	5:E:831:7Q9:C14	0.56	2.54	15	20
5:E:851:7Q9:O12	5:E:851:7Q9:C13	0.56	2.53	14	20
6:E:872:17F:H19	6:E:872:17F:H29	0.56	1.77	7	8
5:B:206:7Q9:C1	5:B:206:7Q9:C31	0.56	2.83	14	7
5:D:514:7Q9:C2	5:D:514:7Q9:O32	0.56	2.52	7	5
5:E:876:7Q9:C21	5:E:876:7Q9:O32	0.56	2.52	13	12
5:A:211:7Q9:C38	5:A:213:7Q9:C313	0.56	2.83	16	2
5:E:836:7Q9:O32	5:E:836:7Q9:O21	0.56	2.24	18	7
1:B:47:ASP:HB2	1:B:164:ARG:HH12	0.56	1.61	10	3
5:E:850:7Q9:C38	6:E:870:17F:C20	0.56	2.82	10	1
6:D:501:17F:H4	6:D:501:17F:N1	0.56	2.16	11	1
6:B:214:17F:C34	6:B:214:17F:H40	0.56	2.31	16	1
6:A:208:17F:H38	5:A:213:7Q9:C316	0.56	2.29	20	1
5:B:210:7Q9:O12	5:B:210:7Q9:C13	0.56	2.53	10	20
5:D:525:7Q9:O21	5:D:525:7Q9:O32	0.56	2.24	6	18
5:E:832:7Q9:O32	5:E:832:7Q9:O21	0.56	2.23	2	18
5:E:863:7Q9:C35	5:E:863:7Q9:O32	0.56	2.54	15	8
6:D:527:17F:H50	6:D:527:17F:H77	0.56	1.76	2	2
6:E:856:17F:O4	6:E:874:17F:H4	0.56	2.01	3	2
5:B:213:7Q9:C1	5:B:213:7Q9:O32	0.56	2.53	4	6
6:D:510:17F:H64	6:D:527:17F:H74	0.56	1.75	4	1
1:B:84:ILE:HD12	1:B:123:ARG:HB3	0.56	1.78	20	6
5:B:205:7Q9:C15	5:B:210:7Q9:O22	0.56	2.53	6	1
5:E:840:7Q9:C1	5:E:849:7Q9:C22	0.56	2.84	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:863:7Q9:C13	5:E:873:7Q9:O13	0.56	2.53	8	2
6:E:855:17F:H54	5:E:867:7Q9:C315	0.56	2.30	9	2
6:E:818:17F:H41	6:E:818:17F:H71	0.56	1.78	12	2
5:E:834:7Q9:C317	6:E:855:17F:H66	0.56	2.31	11	1
2:D:388:ARG:HD2	2:E:575:LEU:HG	0.56	1.76	14	1
5:B:218:7Q9:C1	5:D:542:7Q9:C15	0.56	2.83	2	4
5:D:506:7Q9:C13	5:D:506:7Q9:O12	0.56	2.53	11	19
5:D:535:7Q9:O12	5:D:535:7Q9:C14	0.56	2.54	18	15
6:E:811:17F:O10	6:E:811:17F:C6	0.56	2.51	16	13
6:E:872:17F:O9	6:E:872:17F:O1	0.56	2.23	1	13
5:D:503:7Q9:C311	5:D:503:7Q9:C37	0.56	2.82	11	4
5:D:548:7Q9:P	5:D:548:7Q9:O22	0.56	2.63	2	3
5:E:837:7Q9:C31	6:E:841:17F:H12A	0.56	2.31	5	5
1:B:109:VAL:HB	1:B:111:MET:HE3	0.56	1.78	3	1
6:D:517:17F:H30	6:D:517:17F:C23	0.56	2.27	14	4
5:E:812:7Q9:C13	5:E:816:7Q9:O22	0.56	2.54	6	2
5:D:513:7Q9:C34	6:D:528:17F:H62	0.56	2.31	7	2
6:E:817:17F:H18	5:E:820:7Q9:C22	0.56	2.31	8	1
5:E:847:7Q9:O14	6:E:872:17F:H1A	0.56	2.00	8	1
6:E:817:17F:H40	6:E:817:17F:H30	0.56	1.78	20	4
6:D:510:17F:H54	6:D:516:17F:H78	0.56	1.77	16	1
5:E:802:7Q9:C310	6:E:807:17F:H41	0.56	2.30	16	1
6:B:214:17F:H66	6:B:219:17F:H47	0.56	1.76	18	1
5:D:506:7Q9:C2	5:D:506:7Q9:O32	0.56	2.51	1	3
5:D:524:7Q9:C33	5:D:524:7Q9:C37	0.56	2.84	6	15
5:D:524:7Q9:O32	5:D:524:7Q9:O21	0.56	2.24	16	16
5:D:545:7Q9:O12	5:D:545:7Q9:C15	0.56	2.53	17	20
5:E:806:7Q9:O12	5:E:806:7Q9:C15	0.56	2.54	17	20
5:E:808:7Q9:C14	5:E:808:7Q9:O12	0.56	2.54	8	20
6:D:510:17F:H18	6:D:516:17F:C8	0.56	2.24	2	1
6:A:208:17F:H47	6:E:811:17F:H70	0.56	1.78	3	1
6:D:510:17F:C21	6:D:511:17F:H57	0.56	2.31	5	1
6:B:214:17F:H6	5:B:217:7Q9:C31	0.56	2.30	8	2
5:A:203:7Q9:C13	5:B:204:7Q9:O22	0.56	2.54	11	1
6:A:208:17F:H67	6:B:208:17F:H72	0.56	1.78	11	1
6:E:805:17F:H72	6:E:805:17F:H53	0.56	1.77	15	2
5:E:848:7Q9:C37	5:E:851:7Q9:C33	0.56	2.83	15	1
5:A:204:7Q9:C316	6:A:208:17F:H45	0.56	2.31	16	1
6:B:208:17F:H55	6:B:214:17F:H54	0.56	1.78	17	1
6:B:215:17F:H47	6:B:215:17F:C34	0.56	2.31	17	1
5:B:220:7Q9:C23	6:D:533:17F:H11A	0.56	2.31	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:A:208:17F:H48	5:A:211:7Q9:C318	0.56	2.31	18	1
6:E:841:17F:O8	6:E:841:17F:C4	0.56	2.53	19	1
6:D:510:17F:H43	6:D:510:17F:H36	0.56	1.77	9	5
5:D:536:7Q9:O12	5:D:536:7Q9:C13	0.56	2.53	11	20
5:E:813:7Q9:C15	5:E:813:7Q9:O12	0.56	2.53	13	20
5:E:823:7Q9:O12	5:E:823:7Q9:C14	0.56	2.54	17	20
5:E:837:7Q9:C15	5:E:837:7Q9:O12	0.56	2.54	11	19
5:E:833:7Q9:C14	5:E:833:7Q9:O12	0.56	2.53	2	19
6:B:219:17F:H19	6:B:219:17F:C10	0.56	2.30	3	2
6:D:516:17F:H47	6:D:516:17F:H60	0.56	1.76	3	1
6:D:527:17F:O10	6:D:527:17F:C6	0.56	2.53	3	2
5:E:824:7Q9:C32	6:E:841:17F:C18	0.56	2.83	3	4
5:E:839:7Q9:O32	5:E:839:7Q9:O21	0.56	2.24	9	7
5:D:531:7Q9:O13	5:D:540:7Q9:C12	0.56	2.53	4	1
6:B:208:17F:H64	6:B:208:17F:H40	0.56	1.78	5	1
5:E:875:7Q9:O22	5:E:875:7Q9:C3	0.56	2.52	10	8
2:E:555:SER:OG	6:E:872:17F:H65	0.56	2.00	7	2
6:E:807:17F:H42	6:E:809:17F:C34	0.56	2.30	8	1
5:E:824:7Q9:C35	6:E:841:17F:H20A	0.56	2.30	11	1
5:A:207:7Q9:O12	5:A:207:7Q9:C14	0.56	2.54	20	20
5:D:512:7Q9:C13	5:D:512:7Q9:O12	0.56	2.54	19	20
5:D:520:7Q9:C313	5:D:538:7Q9:C313	0.56	2.84	2	2
5:E:832:7Q9:C14	5:E:832:7Q9:O12	0.56	2.54	3	20
5:E:845:7Q9:O22	5:E:845:7Q9:O11	0.56	2.24	17	15
5:E:844:7Q9:C14	5:E:864:7Q9:O22	0.56	2.54	5	6
6:E:828:17F:H4	5:E:851:7Q9:O13	0.56	2.01	3	1
5:D:504:7Q9:C318	6:D:516:17F:H73	0.56	2.31	4	1
6:E:838:17F:O10	6:E:838:17F:O7	0.56	2.24	16	2
5:B:203:7Q9:O32	6:B:208:17F:H6	0.56	2.01	5	1
6:D:517:17F:H48	6:D:517:17F:H69	0.56	1.77	6	2
5:D:521:7Q9:C314	5:D:525:7Q9:C315	0.56	2.84	11	3
6:D:501:17F:H46	6:D:501:17F:H62	0.56	1.78	20	1
5:A:213:7Q9:C14	5:A:213:7Q9:C1	0.56	2.84	4	4
6:B:214:17F:H56	6:B:214:17F:H63	0.56	1.77	1	2
5:D:512:7Q9:C14	5:D:513:7Q9:C1	0.56	2.84	1	2
5:D:541:7Q9:C13	5:D:541:7Q9:O12	0.56	2.53	11	20
5:E:848:7Q9:O32	5:E:848:7Q9:O21	0.56	2.23	2	16
5:A:204:7Q9:C312	6:A:208:17F:H39	0.56	2.31	2	2
6:E:801:17F:H18A	6:E:801:17F:H10	0.56	1.77	2	1
6:E:811:17F:H66	6:E:811:17F:H36	0.56	1.78	2	1
5:A:213:7Q9:C22	5:A:213:7Q9:C12	0.56	2.84	13	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:B:206:7Q9:C13	5:B:210:7Q9:O32	0.56	2.54	17	7
6:D:510:17F:O3	6:D:516:17F:C4	0.56	2.47	15	6
6:A:214:17F:H63	6:A:214:17F:H29	0.56	1.75	19	2
1:A:31:GLU:OE2	3:A:201:GSP:S1G	0.56	2.64	7	1
5:D:521:7Q9:O32	5:D:521:7Q9:O21	0.56	2.24	8	4
5:A:216:7Q9:O22	5:A:216:7Q9:O11	0.56	2.24	15	3
6:D:533:17F:H6	5:D:543:7Q9:C1	0.56	2.31	9	2
5:E:815:7Q9:O11	5:E:815:7Q9:O32	0.56	2.23	9	5
5:E:869:7Q9:C11	6:E:872:17F:H9	0.56	2.31	14	2
6:D:510:17F:C30	6:D:516:17F:H38	0.56	2.31	14	1
6:D:510:17F:H60	6:D:510:17F:H42	0.56	1.77	14	1
5:E:804:7Q9:C13	6:E:805:17F:C8	0.56	2.83	14	1
1:A:84:ILE:CD1	1:A:118:CYS:HA	0.55	2.31	8	11
5:D:509:7Q9:O32	5:D:509:7Q9:C1	0.55	2.54	1	2
5:D:522:7Q9:O22	5:D:522:7Q9:C3	0.55	2.52	18	11
5:D:523:7Q9:C14	5:D:523:7Q9:O12	0.55	2.54	3	20
5:D:549:7Q9:O22	5:D:549:7Q9:C1	0.55	2.51	7	7
5:E:877:7Q9:O12	5:E:877:7Q9:C15	0.55	2.54	9	20
6:E:841:17F:H4A	6:E:841:17F:C2	0.55	2.30	3	1
5:E:821:7Q9:C12	5:E:825:7Q9:O13	0.55	2.54	18	2
6:B:215:17F:H72	5:E:821:7Q9:C317	0.55	2.31	15	3
2:E:555:SER:HA	6:E:872:17F:H64	0.55	1.78	9	1
5:A:206:7Q9:O22	5:A:206:7Q9:C3	0.55	2.53	18	4
5:E:824:7Q9:C315	6:E:841:17F:H72	0.55	2.31	13	1
6:E:838:17F:C1Z	6:E:838:17F:H35	0.55	2.28	13	1
6:E:841:17F:C4	6:E:841:17F:H2	0.55	2.31	14	1
2:D:375:ALA:HB2	5:D:529:7Q9:C35	0.55	2.31	3	6
6:D:510:17F:C25	6:D:516:17F:H64	0.55	2.31	1	4
5:D:524:7Q9:C14	5:D:524:7Q9:O12	0.55	2.54	12	20
5:D:526:7Q9:O12	5:D:526:7Q9:C15	0.55	2.53	5	20
6:E:838:17F:H57	6:E:838:17F:C2X	0.55	2.30	1	1
6:E:856:17F:O8	6:E:856:17F:H4	0.55	2.02	10	8
5:A:212:7Q9:C31	6:A:214:17F:H20A	0.55	2.32	6	1
6:D:546:17F:H51	5:E:865:7Q9:C315	0.55	2.31	6	1
6:D:534:17F:H12A	5:D:539:7Q9:C33	0.55	2.31	7	1
6:B:208:17F:HN1	6:B:214:17F:H1	0.55	1.60	12	1
2:D:419:LEU:H	2:D:420:PRO:HD2	0.55	1.61	15	1
6:D:534:17F:H29	6:D:534:17F:H64	0.55	1.77	15	1
6:E:819:17F:C6	5:E:836:7Q9:C2	0.55	2.84	16	1
6:E:855:17F:H40	6:E:855:17F:H56	0.55	1.75	18	1
6:D:510:17F:H10A	6:D:516:17F:C32	0.55	2.28	20	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:B:213:7Q9:O12	5:B:213:7Q9:C13	0.55	2.55	9	20
5:D:536:7Q9:P	5:D:536:7Q9:O21	0.55	2.63	20	16
5:E:825:7Q9:O12	5:E:825:7Q9:C14	0.55	2.54	9	20
5:E:842:7Q9:O12	5:E:842:7Q9:C14	0.55	2.53	6	20
5:B:209:7Q9:C15	5:D:505:7Q9:O13	0.55	2.54	2	3
5:E:808:7Q9:C312	6:E:811:17F:H55	0.55	2.30	4	1
5:A:204:7Q9:C22	5:A:206:7Q9:C33	0.55	2.84	6	1
6:D:510:17F:H37	6:D:511:17F:C31	0.55	2.28	18	2
2:E:555:SER:N	6:E:872:17F:H68	0.55	2.17	8	2
5:D:525:7Q9:C11	5:D:525:7Q9:O21	0.55	2.54	9	6
6:E:838:17F:H39	6:E:838:17F:H34	0.55	1.78	17	2
5:E:843:7Q9:O22	5:E:844:7Q9:C34	0.55	2.55	9	2
5:E:832:7Q9:C23	6:E:838:17F:H8A	0.55	2.31	11	1
5:B:217:7Q9:C12	5:D:522:7Q9:O22	0.55	2.54	12	1
6:E:805:17F:H19	6:E:805:17F:C21	0.55	2.27	12	1
5:E:824:7Q9:C37	5:E:824:7Q9:C33	0.55	2.84	12	2
6:B:208:17F:H4	6:B:208:17F:H1	0.55	1.77	18	2
5:E:832:7Q9:C22	6:E:856:17F:H6	0.55	2.32	16	1
6:E:809:17F:H34	6:E:818:17F:H63	0.55	1.78	20	1
6:D:517:17F:H11A	5:D:538:7Q9:C34	0.55	2.32	1	1
5:D:526:7Q9:C39	5:D:526:7Q9:C22	0.55	2.85	8	17
5:D:538:7Q9:O32	5:D:538:7Q9:O21	0.55	2.24	17	12
6:E:818:17F:H39	5:E:835:7Q9:C37	0.55	2.32	12	4
5:E:861:7Q9:C14	5:E:861:7Q9:O12	0.55	2.55	11	20
5:E:867:7Q9:C34	5:E:867:7Q9:O31	0.55	2.55	3	13
5:E:834:7Q9:C1	5:E:834:7Q9:O22	0.55	2.52	11	2
5:D:520:7Q9:C313	5:D:538:7Q9:C314	0.55	2.85	3	2
6:E:807:17F:H33	6:E:819:17F:H12A	0.55	1.77	3	2
6:E:838:17F:C1Z	6:E:838:17F:C23	0.55	2.81	16	7
5:B:203:7Q9:C310	6:B:208:17F:H66	0.55	2.31	9	3
6:D:510:17F:O9	6:D:516:17F:C10	0.55	2.54	15	3
6:E:807:17F:C32	6:E:807:17F:C1X	0.55	2.81	16	3
2:D:429:PHE:CZ	6:D:533:17F:H68	0.55	2.37	20	2
1:B:6:LEU:HB2	1:B:55:ILE:HG22	0.55	1.77	14	1
5:B:216:7Q9:C14	5:B:216:7Q9:O12	0.55	2.55	10	20
5:B:218:7Q9:C14	5:B:218:7Q9:O12	0.55	2.55	5	20
5:E:851:7Q9:C310	5:E:862:7Q9:C38	0.55	2.84	19	6
5:E:858:7Q9:C15	5:E:858:7Q9:O12	0.55	2.54	15	20
6:D:511:17F:O9	6:D:511:17F:O8	0.55	2.23	2	13
2:D:408:LYS:HB2	2:D:409:PRO:HD3	0.55	1.77	8	9
6:D:510:17F:H9	6:D:516:17F:C8	0.55	2.29	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:801:17F:H78	6:E:801:17F:C28	0.55	2.30	6	1
6:E:809:17F:H48	6:E:818:17F:H71	0.55	1.77	6	1
6:E:874:17F:H46	6:E:874:17F:H66	0.55	1.77	6	1
6:E:809:17F:H60	6:E:818:17F:H69	0.55	1.77	9	2
6:E:809:17F:H52	6:E:818:17F:H72	0.55	1.77	16	1
5:D:548:7Q9:O12	5:D:548:7Q9:C13	0.55	2.55	13	20
5:E:802:7Q9:O32	6:E:807:17F:C5	0.55	2.55	15	9
5:E:803:7Q9:C311	5:E:814:7Q9:C38	0.55	2.84	6	4
5:E:878:7Q9:C2	5:E:878:7Q9:O32	0.55	2.52	3	8
5:B:211:7Q9:C22	6:D:501:17F:H56	0.55	2.31	2	2
5:D:529:7Q9:C3	5:D:529:7Q9:O22	0.55	2.53	12	11
6:E:807:17F:H32	6:E:818:17F:H37	0.55	1.79	20	2
6:B:208:17F:H31	6:B:214:17F:H10	0.55	1.77	18	3
6:E:801:17F:N1	5:E:808:7Q9:O13	0.55	2.40	7	1
6:D:534:17F:H64	6:D:534:17F:H46	0.55	1.79	12	1
5:E:816:7Q9:C11	5:E:831:7Q9:O13	0.55	2.55	14	1
6:E:801:17F:H49	6:E:801:17F:H77	0.55	1.77	15	1
2:E:594:LYS:HD3	5:E:861:7Q9:C316	0.55	2.32	16	1
3:A:201:GSP:H5'1	3:A:201:GSP:O2B	0.55	2.01	17	1
5:D:504:7Q9:O12	5:D:504:7Q9:C14	0.55	2.55	7	20
6:D:510:17F:N1	6:D:510:17F:P1	0.55	2.80	6	15
6:D:511:17F:O10	6:D:511:17F:C4	0.55	2.51	1	11
5:E:813:7Q9:C15	5:E:813:7Q9:O13	0.55	2.55	17	14
5:E:822:7Q9:O31	5:E:822:7Q9:O22	0.55	2.25	8	17
5:E:853:7Q9:O12	5:E:853:7Q9:C13	0.55	2.55	1	20
5:E:864:7Q9:C14	5:E:864:7Q9:O12	0.55	2.55	10	20
5:B:209:7Q9:C38	5:D:502:7Q9:C35	0.55	2.85	2	1
5:A:204:7Q9:C317	6:E:811:17F:H70	0.55	2.32	5	1
5:A:212:7Q9:C32	6:A:214:17F:H34	0.55	2.31	6	1
5:E:840:7Q9:C1	5:E:840:7Q9:O32	0.55	2.55	6	1
6:D:517:17F:C38	6:D:517:17F:H48	0.55	2.32	18	2
5:D:502:7Q9:C23	5:D:502:7Q9:C13	0.55	2.85	8	2
5:B:218:7Q9:C37	5:D:514:7Q9:C33	0.55	2.85	20	2
5:E:815:7Q9:O32	5:E:815:7Q9:C14	0.55	2.54	9	2
2:D:322:LEU:O	2:D:326:LEU:HG	0.55	2.02	18	2
6:E:819:17F:H40	6:E:819:17F:C31	0.55	2.30	13	1
6:E:838:17F:H8A	6:E:856:17F:H39	0.55	1.78	14	1
5:A:206:7Q9:O32	5:A:206:7Q9:C21	0.55	2.55	1	13
6:D:501:17F:H46	5:D:508:7Q9:C318	0.55	2.32	1	1
5:E:814:7Q9:O32	5:E:814:7Q9:O21	0.55	2.25	16	18
5:E:863:7Q9:C32	5:E:873:7Q9:C32	0.55	2.85	5	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:B:212:7Q9:P	5:B:212:7Q9:O21	0.55	2.65	2	1
6:D:510:17F:C31	6:D:527:17F:H61	0.55	2.27	2	2
5:D:544:7Q9:C2	5:D:544:7Q9:O32	0.55	2.49	11	2
5:E:865:7Q9:C3	5:E:865:7Q9:O22	0.55	2.50	10	5
5:D:513:7Q9:O31	5:D:513:7Q9:O22	0.55	2.25	11	11
5:D:514:7Q9:C15	5:D:514:7Q9:O12	0.55	2.55	3	14
5:E:837:7Q9:C32	6:E:841:17F:C1Y	0.55	2.85	11	3
6:D:511:17F:O5	5:D:526:7Q9:C15	0.55	2.54	5	1
5:B:220:7Q9:O22	6:D:533:17F:H11A	0.55	2.02	7	1
2:D:400:LEU:HB3	5:D:542:7Q9:C313	0.55	2.32	9	2
6:D:501:17F:H45	5:D:508:7Q9:C35	0.55	2.32	9	1
6:E:838:17F:H68	6:E:856:17F:C22	0.55	2.32	9	1
6:E:838:17F:H39	6:E:838:17F:C1Z	0.55	2.32	17	2
6:B:214:17F:H46	6:B:214:17F:C42	0.55	2.30	11	1
6:B:215:17F:O2	5:D:506:7Q9:C15	0.55	2.55	14	1
6:B:215:17F:H38	5:B:216:7Q9:C317	0.55	2.32	14	1
5:E:813:7Q9:C33	5:E:829:7Q9:C23	0.55	2.85	15	2
6:B:214:17F:C6	5:B:217:7Q9:C31	0.55	2.85	18	1
6:D:501:17F:C25	5:D:508:7Q9:C36	0.55	2.85	20	1
5:B:204:7Q9:O32	5:B:204:7Q9:O21	0.55	2.25	13	17
5:B:213:7Q9:C37	5:D:514:7Q9:C310	0.55	2.84	20	3
6:B:214:17F:H34	5:B:220:7Q9:C32	0.55	2.31	12	4
6:D:510:17F:P1	6:D:510:17F:HN1	0.55	2.24	6	8
6:D:511:17F:H11	5:D:526:7Q9:O14	0.55	2.01	5	3
5:D:530:7Q9:O22	5:D:530:7Q9:C3	0.55	2.52	5	5
5:D:542:7Q9:O12	5:D:542:7Q9:C13	0.55	2.55	16	20
6:E:801:17F:O9	6:E:801:17F:C7	0.55	2.55	1	5
5:B:216:7Q9:O31	5:B:216:7Q9:O22	0.55	2.25	6	13
5:D:548:7Q9:O14	5:E:847:7Q9:C13	0.55	2.55	10	6
6:D:517:17F:H76	5:D:541:7Q9:C318	0.55	2.32	4	1
5:E:821:7Q9:O12	5:E:821:7Q9:O21	0.55	2.24	18	2
6:D:501:17F:H46	6:D:501:17F:H66	0.55	1.78	5	2
6:E:828:17F:H11A	5:E:832:7Q9:C38	0.55	2.32	15	3
5:D:502:7Q9:C23	5:D:508:7Q9:C22	0.55	2.85	8	2
6:E:828:17F:H72	5:E:829:7Q9:C318	0.55	2.32	12	1
5:E:837:7Q9:C14	6:E:841:17F:O10	0.55	2.55	16	2
5:A:206:7Q9:C318	6:E:811:17F:H76	0.55	2.32	1	4
5:E:824:7Q9:O13	5:E:824:7Q9:C2	0.55	2.55	2	18
5:E:862:7Q9:C13	5:E:862:7Q9:O12	0.55	2.55	14	20
6:E:801:17F:H59	5:E:803:7Q9:C39	0.55	2.32	2	1
5:D:537:7Q9:C3	6:D:546:17F:C11	0.55	2.81	15	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:ILE:HD13	1:A:118:CYS:HA	0.55	1.79	10	7
5:A:215:7Q9:P	6:D:534:17F:H43	0.55	2.42	4	1
6:D:528:17F:C28	6:D:528:17F:C24	0.55	2.77	4	1
6:B:208:17F:H45	6:B:208:17F:C38	0.55	2.32	7	2
5:D:521:7Q9:O31	5:D:525:7Q9:O31	0.55	2.25	5	6
2:E:682:LYS:NZ	5:E:867:7Q9:O32	0.55	2.39	6	1
5:E:835:7Q9:C13	5:E:835:7Q9:O22	0.55	2.56	12	1
6:D:510:17F:C28	6:D:516:17F:H68	0.55	2.32	13	1
6:D:533:17F:O5	6:D:533:17F:H10	0.55	2.01	19	1
1:B:13:GLY:HA2	3:B:201:GSP:C5'	0.55	2.32	20	1
5:D:518:7Q9:O32	5:D:518:7Q9:O21	0.54	2.24	12	12
5:E:830:7Q9:O32	5:E:830:7Q9:O21	0.54	2.25	3	16
6:B:208:17F:O10	6:B:208:17F:C4	0.54	2.48	4	4
6:D:528:17F:O10	6:D:528:17F:H9	0.54	2.02	10	11
6:D:510:17F:O9	6:D:516:17F:H11A	0.54	2.02	4	3
5:B:207:7Q9:C1	5:B:207:7Q9:O22	0.54	2.53	15	6
5:B:220:7Q9:O14	6:D:533:17F:H4A	0.54	2.02	11	1
2:D:429:PHE:CZ	6:D:533:17F:H41	0.54	2.32	11	1
2:E:555:SER:N	6:E:872:17F:H65	0.54	2.17	12	3
5:E:820:7Q9:C21	5:E:820:7Q9:O14	0.54	2.55	13	1
5:A:204:7Q9:C313	6:A:208:17F:H77	0.54	2.32	14	1
6:E:819:17F:O7	6:E:819:17F:H11	0.54	2.03	15	1
6:D:517:17F:H57	6:D:517:17F:C22	0.54	2.32	18	1
5:A:206:7Q9:C15	5:A:206:7Q9:O12	0.54	2.55	20	20
6:D:501:17F:C7	6:D:501:17F:O9	0.54	2.55	18	5
5:E:804:7Q9:C1	5:E:815:7Q9:O13	0.54	2.56	1	1
5:E:837:7Q9:O32	6:E:841:17F:H19A	0.54	2.01	1	1
5:E:873:7Q9:O12	5:E:873:7Q9:C14	0.54	2.55	13	20
5:D:508:7Q9:O32	5:D:508:7Q9:C21	0.54	2.55	2	8
6:E:856:17F:C4	6:E:856:17F:O8	0.54	2.55	11	5
6:D:527:17F:O2	5:D:535:7Q9:C15	0.54	2.56	11	2
6:E:805:17F:H39	6:E:805:17F:H29	0.54	1.78	3	3
5:E:816:7Q9:C311	5:E:825:7Q9:C313	0.54	2.85	10	2
5:A:212:7Q9:C311	5:E:822:7Q9:C317	0.54	2.85	5	7
6:E:811:17F:H10	5:E:822:7Q9:O22	0.54	2.02	8	2
6:D:511:17F:O1	5:D:513:7Q9:C14	0.54	2.56	8	1
2:D:309:GLN:OE1	6:D:527:17F:H63	0.54	2.02	11	1
5:E:862:7Q9:O32	5:E:878:7Q9:C14	0.54	2.55	11	2
5:A:206:7Q9:O22	5:A:210:7Q9:C12	0.54	2.55	12	2
5:B:211:7Q9:C317	6:B:215:17F:H51	0.54	2.32	1	1
5:E:837:7Q9:C31	6:E:841:17F:H32	0.54	2.32	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:869:7Q9:C12	6:E:872:17F:O4	0.54	2.55	1	1
5:B:216:7Q9:O22	5:D:514:7Q9:C13	0.54	2.55	19	3
5:E:816:7Q9:C37	5:E:825:7Q9:C2	0.54	2.86	4	1
5:A:207:7Q9:C33	5:D:504:7Q9:O32	0.54	2.55	5	2
5:D:515:7Q9:O22	5:D:519:7Q9:C15	0.54	2.55	8	2
5:A:204:7Q9:C39	6:A:208:17F:H72	0.54	2.32	16	2
2:E:659:LEU:HD21	6:E:856:17F:C42	0.54	2.26	13	1
5:E:877:7Q9:O22	5:E:877:7Q9:O31	0.54	2.25	15	1
6:A:208:17F:H40	5:E:823:7Q9:C316	0.54	2.31	1	1
5:B:206:7Q9:C32	5:B:212:7Q9:C37	0.54	2.84	1	1
5:E:840:7Q9:O12	5:E:840:7Q9:C13	0.54	2.56	14	20
5:E:861:7Q9:C1	5:E:861:7Q9:O22	0.54	2.53	11	9
5:D:507:7Q9:O22	5:D:507:7Q9:C1	0.54	2.52	11	6
5:E:829:7Q9:O22	5:E:829:7Q9:C3	0.54	2.54	5	5
6:D:516:17F:H39	6:D:516:17F:C33	0.54	2.33	3	2
5:D:537:7Q9:C1	5:D:537:7Q9:O22	0.54	2.50	5	3
1:B:72:MET:HA	1:B:78:PHE:HZ	0.54	1.61	5	2
6:B:215:17F:H31	6:D:517:17F:H61	0.54	1.77	6	1
5:B:217:7Q9:O21	5:B:217:7Q9:O32	0.54	2.26	18	5
2:D:291:GLU:HG2	5:D:547:7Q9:C310	0.54	2.33	6	1
5:A:203:7Q9:C14	5:B:204:7Q9:O22	0.54	2.55	11	1
5:B:211:7Q9:C312	6:D:501:17F:C36	0.54	2.81	20	4
6:D:501:17F:H29	5:D:509:7Q9:C21	0.54	2.32	15	2
6:B:214:17F:H10A	6:B:214:17F:H41	0.54	1.79	5	3
6:D:528:17F:H69	6:D:528:17F:C22	0.54	2.33	1	4
5:D:536:7Q9:O21	5:D:536:7Q9:P	0.54	2.66	6	4
6:E:856:17F:C31	6:E:856:17F:H63	0.54	2.32	2	3
3:A:201:GSP:O5'	3:A:201:GSP:H2'	0.54	2.02	17	4
5:B:207:7Q9:O22	5:B:207:7Q9:C1	0.54	2.53	9	2
6:E:819:17F:C4	6:E:819:17F:C7	0.54	2.86	14	4
6:A:208:17F:H50	6:E:811:17F:H68	0.54	1.78	4	1
2:D:348:MET:HE3	2:D:348:MET:HA	0.54	1.77	4	1
6:D:501:17F:C12	6:D:501:17F:H40	0.54	2.32	4	2
6:D:517:17F:H66	6:D:517:17F:C27	0.54	2.33	10	2
6:B:215:17F:H30	6:B:215:17F:H46	0.54	1.78	6	1
5:B:217:7Q9:O22	5:B:217:7Q9:O11	0.54	2.26	16	7
5:E:816:7Q9:O32	5:E:816:7Q9:O21	0.54	2.24	20	2
6:E:819:17F:H32	6:E:819:17F:C21	0.54	2.30	15	1
5:E:837:7Q9:C34	6:E:841:17F:H55	0.54	2.32	18	1
6:E:818:17F:H4	6:E:818:17F:O10	0.54	2.02	2	13
6:E:856:17F:C7	6:E:856:17F:H4A	0.54	2.33	18	13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:522:7Q9:C3	5:D:522:7Q9:O22	0.54	2.52	19	3
5:E:825:7Q9:C33	5:E:844:7Q9:C38	0.54	2.86	12	2
5:E:820:7Q9:O32	5:E:820:7Q9:O21	0.54	2.25	7	5
3:B:201:GSP:O5'	3:B:201:GSP:C2'	0.54	2.56	11	6
6:E:807:17F:H42	6:E:809:17F:H63	0.54	1.79	6	2
6:B:214:17F:O10	6:B:214:17F:C4	0.54	2.54	20	5
6:A:208:17F:H60	6:B:208:17F:H65	0.54	1.78	10	1
2:D:333:LYS:HE3	5:D:532:7Q9:C313	0.54	2.33	12	1
5:B:218:7Q9:O14	5:D:522:7Q9:C22	0.54	2.56	17	1
5:E:833:7Q9:C12	5:E:857:7Q9:O14	0.54	2.56	11	4
5:D:548:7Q9:O22	5:D:548:7Q9:O12	0.54	2.25	3	6
5:E:863:7Q9:C12	5:E:873:7Q9:O13	0.54	2.56	2	3
5:D:549:7Q9:C33	6:E:856:17F:H54	0.54	2.32	4	1
6:E:828:17F:H9A	5:E:832:7Q9:C37	0.54	2.32	5	1
6:B:208:17F:C4	6:B:208:17F:C1	0.54	2.86	6	3
6:E:818:17F:C12	6:E:819:17F:H10A	0.54	2.31	12	1
6:E:817:17F:H18	5:E:833:7Q9:C3	0.54	2.33	16	3
5:E:824:7Q9:C33	6:E:841:17F:H34	0.54	2.33	20	2
6:D:510:17F:C7	6:D:516:17F:C9	0.54	2.83	20	9
5:D:518:7Q9:C313	6:D:533:17F:H40	0.54	2.32	3	2
5:D:526:7Q9:O22	5:D:526:7Q9:C3	0.54	2.53	14	16
6:E:809:17F:H61	6:E:818:17F:H75	0.54	1.78	1	1
5:E:826:7Q9:C2	5:E:826:7Q9:O32	0.54	2.54	4	13
5:E:869:7Q9:C15	5:E:869:7Q9:O12	0.54	2.56	3	17
5:D:536:7Q9:O22	5:D:536:7Q9:O31	0.54	2.26	7	14
5:D:539:7Q9:O22	5:D:539:7Q9:C3	0.54	2.53	2	10
6:E:818:17F:C23	6:E:819:17F:H38	0.54	2.33	2	3
6:E:817:17F:H29	5:E:820:7Q9:C23	0.54	2.33	5	1
5:A:204:7Q9:C316	6:A:208:17F:H54	0.54	2.32	6	3
6:D:517:17F:O8	6:D:517:17F:O9	0.54	2.26	8	3
6:B:214:17F:O9	6:B:214:17F:O8	0.54	2.25	17	6
5:D:520:7Q9:C1	5:D:538:7Q9:C1	0.54	2.85	9	2
1:A:16:LYS:HB2	3:A:201:GSP:O2G	0.54	2.02	10	1
5:E:834:7Q9:C39	6:E:855:17F:H63	0.54	2.32	19	2
5:A:217:7Q9:C313	6:D:546:17F:H51	0.54	2.33	14	1
6:B:219:17F:H39	6:B:219:17F:H20	0.54	1.77	16	1
6:A:208:17F:C1Z	6:B:208:17F:H37	0.54	2.33	17	1
6:B:214:17F:H66	6:B:219:17F:C27	0.54	2.33	18	1
5:A:215:7Q9:C39	6:D:534:17F:H45	0.54	2.32	1	1
5:B:220:7Q9:C13	5:B:220:7Q9:O12	0.54	2.56	6	20
6:D:501:17F:O9	6:D:501:17F:O8	0.54	2.25	7	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:852:7Q9:C15	5:E:852:7Q9:O12	0.54	2.55	9	20
5:E:865:7Q9:C15	5:E:865:7Q9:O12	0.54	2.56	6	20
6:E:870:17F:H75	6:E:870:17F:H48	0.54	1.78	1	1
5:B:218:7Q9:C39	5:D:514:7Q9:C35	0.54	2.86	10	5
5:B:205:7Q9:C32	5:B:211:7Q9:C37	0.54	2.86	12	2
5:A:204:7Q9:C12	5:B:203:7Q9:O32	0.54	2.56	5	1
6:D:534:17F:C34	6:D:534:17F:H35	0.54	2.33	5	1
6:D:501:17F:H66	6:D:501:17F:C25	0.54	2.33	6	1
5:E:813:7Q9:C314	6:E:818:17F:H52	0.54	2.33	17	2
6:D:534:17F:H70	5:D:539:7Q9:C314	0.54	2.33	7	1
5:B:206:7Q9:C13	5:B:210:7Q9:C32	0.54	2.86	20	5
6:E:807:17F:C31	6:E:819:17F:C12	0.54	2.86	16	2
5:E:852:7Q9:C3	5:E:852:7Q9:O22	0.54	2.53	16	3
2:D:273:ASP:OD1	6:D:534:17F:H20	0.54	2.02	16	1
5:D:525:7Q9:O14	5:D:525:7Q9:O21	0.54	2.25	18	1
6:E:841:17F:C7	6:E:841:17F:C4	0.54	2.86	19	1
5:D:502:7Q9:C15	5:D:502:7Q9:O12	0.54	2.56	4	20
5:D:532:7Q9:O32	5:D:532:7Q9:O21	0.54	2.26	16	9
2:E:623:ARG:HB2	5:E:858:7Q9:C313	0.54	2.33	8	11
6:E:838:17F:H65	6:E:838:17F:H36	0.54	1.80	1	1
5:D:540:7Q9:O31	5:D:540:7Q9:O22	0.54	2.25	4	16
5:A:209:7Q9:C2	5:A:209:7Q9:O32	0.54	2.52	12	8
6:B:219:17F:O9	6:B:219:17F:O1	0.54	2.26	17	4
6:E:874:17F:H49	6:E:874:17F:H72	0.54	1.78	6	3
5:D:506:7Q9:C36	6:D:517:17F:C31	0.54	2.85	6	1
6:D:510:17F:H76	6:D:516:17F:C40	0.54	2.33	6	2
6:D:511:17F:O4	5:D:524:7Q9:C12	0.54	2.56	8	2
6:E:874:17F:H18A	6:E:874:17F:N1	0.54	2.17	20	2
5:A:211:7Q9:C311	5:A:213:7Q9:C313	0.54	2.86	9	3
1:A:8:VAL:HG12	1:A:16:LYS:HD2	0.54	1.80	12	2
2:D:352:ALA:HB1	5:D:521:7Q9:C317	0.54	2.33	14	1
6:E:818:17F:C10	6:E:819:17F:H9A	0.54	2.33	15	2
5:A:212:7Q9:C1	5:A:212:7Q9:O32	0.54	2.55	16	4
6:B:214:17F:H19A	6:B:219:17F:H12	0.54	1.79	16	2
6:E:819:17F:C26	6:E:819:17F:C22	0.54	2.76	15	1
6:D:510:17F:H65	5:D:524:7Q9:C317	0.54	2.33	16	1
6:D:501:17F:C41	6:E:807:17F:H53	0.54	2.33	18	1
1:B:6:LEU:HB2	1:B:55:ILE:HG12	0.54	1.78	19	1
2:E:725:PHE:HE1	6:E:870:17F:H65	0.54	1.62	19	1
5:D:532:7Q9:O12	5:D:532:7Q9:C15	0.53	2.56	8	19
6:E:807:17F:H57	6:E:819:17F:H29	0.53	1.79	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:825:7Q9:O32	5:E:825:7Q9:O21	0.53	2.27	9	14
6:E:801:17F:H1A	6:E:801:17F:H4	0.53	1.79	2	2
5:E:824:7Q9:C32	6:E:841:17F:H18A	0.53	2.33	2	5
6:D:511:17F:H77	6:D:511:17F:C28	0.53	2.33	4	2
5:D:537:7Q9:C2	5:D:537:7Q9:O32	0.53	2.52	7	7
5:D:544:7Q9:O32	5:D:544:7Q9:C2	0.53	2.55	15	10
5:E:837:7Q9:C12	6:E:841:17F:H19A	0.53	2.33	6	1
5:D:524:7Q9:C2	6:D:527:17F:C18	0.53	2.87	9	1
5:A:215:7Q9:C3	5:D:536:7Q9:C39	0.53	2.86	10	1
5:E:852:7Q9:C3	5:E:852:7Q9:C11	0.53	2.85	13	2
5:B:206:7Q9:C33	5:B:212:7Q9:C37	0.53	2.86	1	1
6:D:546:17F:H56	6:D:546:17F:H9	0.53	1.78	12	3
6:D:546:17F:H62	6:D:546:17F:C31	0.53	2.26	17	12
6:E:809:17F:O7	6:E:809:17F:O10	0.53	2.26	10	14
5:E:824:7Q9:C33	6:E:841:17F:C20	0.53	2.81	10	5
5:B:213:7Q9:C2	5:B:213:7Q9:O14	0.53	2.56	5	3
2:D:404:SER:HB2	5:D:542:7Q9:C312	0.53	2.33	5	2
5:E:802:7Q9:O32	6:E:807:17F:H6	0.53	2.03	6	1
5:E:844:7Q9:O22	5:E:844:7Q9:C3	0.53	2.54	7	1
6:D:533:17F:H55	6:E:870:17F:H68	0.53	1.80	11	2
5:E:820:7Q9:C315	6:E:828:17F:H52	0.53	2.33	12	1
6:D:510:17F:C29	6:D:516:17F:H38	0.53	2.34	14	1
6:E:838:17F:C11	6:E:838:17F:H64	0.53	2.34	20	1
6:A:208:17F:O10	6:A:208:17F:C6	0.53	2.54	20	7
5:A:216:7Q9:C3	5:A:216:7Q9:O22	0.53	2.52	4	8
5:A:217:7Q9:C14	5:A:217:7Q9:O12	0.53	2.55	18	20
5:B:206:7Q9:C14	5:B:206:7Q9:C22	0.53	2.87	3	3
6:D:527:17F:H53	6:E:838:17F:H75	0.53	1.80	1	1
5:E:846:7Q9:O12	5:E:846:7Q9:C14	0.53	2.57	18	16
6:E:855:17F:H31	5:E:867:7Q9:C35	0.53	2.33	1	1
5:E:860:7Q9:O32	5:E:860:7Q9:O21	0.53	2.27	4	17
6:E:817:17F:H11	5:E:820:7Q9:C23	0.53	2.33	5	1
6:E:870:17F:C21	6:E:870:17F:C32	0.53	2.85	10	9
6:E:818:17F:C27	6:E:818:17F:C42	0.53	2.86	6	3
5:E:842:7Q9:O21	5:E:842:7Q9:O13	0.53	2.27	15	2
6:D:528:17F:H78	2:E:637:LEU:HD22	0.53	1.79	13	3
6:D:501:17F:O9	6:D:501:17F:C20	0.53	2.55	12	2
6:D:510:17F:C1Z	6:D:516:17F:H10	0.53	2.34	11	1
6:E:855:17F:H29	6:E:855:17F:C34	0.53	2.34	15	2
5:E:863:7Q9:C23	5:E:863:7Q9:C37	0.53	2.87	19	1
6:B:219:17F:H76	6:B:219:17F:C30	0.53	2.33	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:837:7Q9:O31	5:E:837:7Q9:O22	0.53	2.25	1	8
5:E:842:7Q9:O22	5:E:842:7Q9:O31	0.53	2.26	7	3
6:B:208:17F:H45	6:B:208:17F:C36	0.53	2.30	17	2
5:B:209:7Q9:C15	5:D:503:7Q9:O14	0.53	2.57	2	2
2:E:598:GLN:HB2	2:E:599:PRO:HD3	0.53	1.80	11	10
6:E:805:17F:O10	6:E:805:17F:H4	0.53	2.03	9	7
5:A:207:7Q9:C34	5:D:504:7Q9:O32	0.53	2.56	16	4
5:D:524:7Q9:C1	5:D:524:7Q9:O22	0.53	2.53	9	7
5:E:832:7Q9:C13	5:E:832:7Q9:C22	0.53	2.86	4	3
5:E:839:7Q9:O22	5:E:839:7Q9:C3	0.53	2.54	17	7
6:D:510:17F:H49	6:D:516:17F:H71	0.53	1.80	6	1
6:D:534:17F:C10	5:D:539:7Q9:C33	0.53	2.87	9	5
5:E:804:7Q9:C14	6:E:805:17F:H8A	0.53	2.33	12	2
5:E:826:7Q9:O22	5:E:840:7Q9:C12	0.53	2.56	8	1
5:D:537:7Q9:P	5:D:537:7Q9:C15	0.53	2.97	11	1
6:E:856:17F:C42	6:E:874:17F:H65	0.53	2.33	18	2
6:E:856:17F:H29	6:E:874:17F:C34	0.53	2.33	15	2
6:B:214:17F:O10	6:B:214:17F:H4	0.53	2.04	15	1
6:B:208:17F:C24	6:B:214:17F:H12A	0.53	2.30	1	1
5:D:506:7Q9:O22	5:D:506:7Q9:O31	0.53	2.27	5	8
6:E:874:17F:O10	6:E:874:17F:O7	0.53	2.26	3	1
3:A:201:GSP:O2G	3:A:201:GSP:H5'2	0.53	2.04	6	1
5:B:218:7Q9:C1	5:B:218:7Q9:C14	0.53	2.87	17	2
6:D:501:17F:H63	6:D:501:17F:C31	0.53	2.17	9	3
6:E:817:17F:C18	5:E:833:7Q9:O32	0.53	2.56	16	4
6:E:818:17F:H45	6:E:818:17F:H73	0.53	1.80	9	1
5:A:209:7Q9:C315	5:E:822:7Q9:C312	0.53	2.87	11	3
5:D:513:7Q9:C23	6:D:528:17F:H64	0.53	2.33	12	2
6:E:807:17F:H74	6:E:807:17F:C28	0.53	2.33	12	1
6:D:501:17F:C34	6:D:501:17F:H46	0.53	2.33	13	1
6:D:534:17F:H63	6:D:534:17F:C30	0.53	2.34	14	1
5:D:538:7Q9:C22	5:D:538:7Q9:C14	0.53	2.87	15	1
6:D:517:17F:H66	6:E:841:17F:H76	0.53	1.80	16	1
6:A:208:17F:H70	5:E:804:7Q9:C318	0.53	2.33	1	1
6:E:819:17F:H6A	6:E:819:17F:O10	0.53	2.04	1	3
5:D:521:7Q9:C1	5:D:521:7Q9:O22	0.53	2.54	5	9
6:E:805:17F:HN1	6:E:805:17F:P1	0.53	2.27	4	7
5:E:814:7Q9:O22	5:E:814:7Q9:O11	0.53	2.27	20	17
5:E:840:7Q9:O13	5:E:840:7Q9:C2	0.53	2.57	16	12
5:A:211:7Q9:C36	5:A:213:7Q9:C313	0.53	2.87	3	1
5:E:843:7Q9:C22	5:E:844:7Q9:C14	0.53	2.87	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:E:660:ARG:HG3	6:E:874:17F:H31	0.53	1.80	5	1
6:B:208:17F:O10	5:B:212:7Q9:C13	0.53	2.56	17	3
6:D:501:17F:C34	6:D:501:17F:C24	0.53	2.81	15	4
5:D:530:7Q9:C22	5:D:530:7Q9:C311	0.53	2.87	10	4
6:D:510:17F:H49	6:D:516:17F:C38	0.53	2.34	12	3
5:E:824:7Q9:C34	6:E:841:17F:H30	0.53	2.34	9	2
1:A:83:ALA:HB3	1:A:86:ASN:HB3	0.53	1.79	12	4
6:A:214:17F:H77	5:E:840:7Q9:C310	0.53	2.34	10	1
5:B:220:7Q9:C11	6:D:533:17F:H10A	0.53	2.33	17	2
6:D:510:17F:C1	6:D:516:17F:C6	0.53	2.83	16	2
5:E:820:7Q9:C23	6:E:838:17F:H32	0.53	2.34	17	1
5:B:205:7Q9:O32	5:B:205:7Q9:O21	0.53	2.27	6	14
5:D:535:7Q9:C317	6:E:874:17F:H50	0.53	2.34	1	4
6:E:809:17F:H57	6:E:809:17F:H36	0.53	1.78	1	1
5:E:816:7Q9:O12	5:E:816:7Q9:C15	0.53	2.57	20	18
6:B:219:17F:O6	6:B:219:17F:C2	0.53	2.55	20	2
6:D:501:17F:C12	6:D:501:17F:C23	0.53	2.86	17	2
5:E:837:7Q9:C32	6:E:841:17F:H50	0.53	2.34	14	2
1:A:92:ASP:HA	1:A:95:HIS:HD2	0.53	1.63	6	1
1:A:147:LYS:HB2	3:A:201:GSP:N1	0.53	2.19	6	1
6:B:215:17F:H74	5:E:842:7Q9:C318	0.53	2.34	8	1
5:A:217:7Q9:C312	5:A:217:7Q9:C38	0.53	2.86	9	2
6:D:510:17F:C18	6:D:527:17F:C19	0.53	2.80	9	1
6:D:510:17F:C28	6:D:516:17F:C22	0.53	2.77	20	6
5:E:802:7Q9:C33	6:E:809:17F:H18	0.53	2.33	9	1
6:B:208:17F:H54	6:B:208:17F:H71	0.53	1.81	11	2
6:D:510:17F:C30	6:D:510:17F:H78	0.53	2.32	10	1
6:D:528:17F:H72	5:E:862:7Q9:C315	0.53	2.34	13	1
6:B:215:17F:O10	6:B:215:17F:C4	0.53	2.53	19	1
6:E:805:17F:H78	5:E:816:7Q9:C318	0.53	2.33	19	1
1:A:64:TYR:HB3	1:A:67:MET:HB2	0.53	1.79	12	3
3:B:201:GSP:S1G	3:B:201:GSP:H5'2	0.53	2.43	8	2
6:B:215:17F:H53	6:E:809:17F:H42	0.53	1.79	1	1
5:D:535:7Q9:C318	6:E:838:17F:H51	0.53	2.33	20	5
6:D:546:17F:C17	6:D:546:17F:C1Y	0.53	2.87	8	18
6:A:208:17F:O8	6:A:208:17F:H4	0.53	2.04	17	7
5:E:852:7Q9:C11	5:E:852:7Q9:O31	0.53	2.56	4	1
1:B:84:ILE:HD12	1:B:123:ARG:HG2	0.53	1.81	5	1
5:E:846:7Q9:P	5:E:846:7Q9:C14	0.53	2.97	10	3
5:A:209:7Q9:C318	5:E:839:7Q9:C314	0.53	2.87	15	3
5:E:849:7Q9:P	5:E:849:7Q9:O22	0.53	2.67	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LEU:HD22	1:A:159:LEU:HD23	0.53	1.80	19	2
6:A:214:17F:H72	6:A:214:17F:C30	0.53	2.33	20	5
6:E:805:17F:H70	5:E:816:7Q9:C318	0.53	2.34	1	2
5:E:857:7Q9:C3	6:E:874:17F:H9	0.53	2.34	1	1
6:B:219:17F:H2	6:B:219:17F:C4	0.53	2.24	11	2
6:D:501:17F:H19A	6:D:501:17F:HN1	0.53	1.64	2	1
5:D:548:7Q9:O22	5:D:548:7Q9:O11	0.53	2.26	3	5
6:E:838:17F:H12	6:E:856:17F:H30	0.53	1.80	15	2
6:D:510:17F:HN1	6:D:510:17F:P1	0.53	2.25	16	7
6:A:208:17F:H12	5:A:209:7Q9:C37	0.53	2.33	4	2
5:D:548:7Q9:O12	5:D:548:7Q9:O22	0.53	2.27	8	6
5:B:216:7Q9:C32	5:D:519:7Q9:C22	0.53	2.87	14	4
5:A:215:7Q9:C37	5:A:215:7Q9:C311	0.53	2.85	6	2
6:E:838:17F:O2	6:E:838:17F:N1	0.53	2.37	7	3
2:D:269:GLN:HG2	6:D:534:17F:C1Y	0.53	2.34	11	2
5:A:206:7Q9:C11	5:A:206:7Q9:O21	0.53	2.57	13	1
6:D:510:17F:H76	6:D:516:17F:H72	0.53	1.81	13	1
5:E:808:7Q9:C13	6:E:817:17F:O1	0.53	2.56	18	2
5:D:523:7Q9:C1	5:D:523:7Q9:O22	0.53	2.52	19	5
6:E:807:17F:H51	6:E:807:17F:H76	0.53	1.81	1	3
5:D:523:7Q9:O21	5:D:523:7Q9:O32	0.53	2.27	19	9
5:E:810:7Q9:C1	5:E:810:7Q9:O22	0.53	2.55	13	3
2:E:631:ARG:HG2	5:E:878:7Q9:C34	0.53	2.34	13	3
6:D:510:17F:H6A	6:D:516:17F:H11A	0.53	1.81	8	1
5:D:520:7Q9:C1	5:D:538:7Q9:O22	0.53	2.57	13	2
6:E:809:17F:H51	6:E:818:17F:C40	0.53	2.33	20	2
6:E:818:17F:H42	5:E:835:7Q9:C38	0.53	2.34	10	1
5:E:868:7Q9:C36	5:E:873:7Q9:C38	0.53	2.87	12	2
5:E:862:7Q9:C13	5:E:862:7Q9:P	0.53	2.97	19	3
6:E:818:17F:H19	6:E:841:17F:H57	0.53	1.78	18	1
5:D:513:7Q9:C11	5:D:513:7Q9:O21	0.52	2.57	16	12
6:B:219:17F:H18	5:D:545:7Q9:C35	0.52	2.34	4	1
5:E:850:7Q9:C310	6:E:870:17F:H44	0.52	2.34	4	3
6:E:828:17F:H40	6:E:828:17F:C33	0.52	2.35	15	3
5:E:868:7Q9:O32	5:E:873:7Q9:C22	0.52	2.56	20	4
1:A:39:SER:HB3	1:A:56:LEU:HD12	0.52	1.82	6	1
5:A:217:7Q9:O13	6:D:546:17F:H1	0.52	2.03	6	1
6:D:510:17F:H50	6:D:516:17F:C23	0.52	2.35	6	1
6:E:809:17F:H52	6:E:818:17F:H75	0.52	1.79	6	1
6:E:841:17F:H64	6:E:841:17F:C32	0.52	2.34	18	2
2:D:333:LYS:HD2	5:D:532:7Q9:C314	0.52	2.34	7	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:B:217:7Q9:C15	6:B:219:17F:H6	0.52	2.34	10	2
6:D:501:17F:N1	6:D:501:17F:O10	0.52	2.42	11	1
2:D:374:LEU:HD13	2:E:590:LEU:HD21	0.52	1.80	13	1
5:D:506:7Q9:C317	6:E:841:17F:H52	0.52	2.33	20	2
6:B:219:17F:H20A	6:B:219:17F:C2X	0.52	2.33	16	1
2:E:558:SER:OG	6:E:872:17F:H65	0.52	2.04	16	2
5:A:212:7Q9:O22	5:A:212:7Q9:C3	0.52	2.52	1	12
5:A:215:7Q9:C15	5:A:216:7Q9:O14	0.52	2.57	1	4
5:E:833:7Q9:O12	5:E:833:7Q9:C14	0.52	2.57	1	1
5:E:848:7Q9:C312	5:E:851:7Q9:C38	0.52	2.88	3	1
5:E:810:7Q9:C12	5:E:816:7Q9:C32	0.52	2.87	14	4
5:A:216:7Q9:O22	5:A:216:7Q9:C3	0.52	2.54	12	7
6:E:874:17F:H78	6:E:874:17F:C27	0.52	2.34	5	4
5:D:502:7Q9:C1	5:D:502:7Q9:C15	0.52	2.87	6	1
6:E:805:17F:H71	5:E:810:7Q9:C317	0.52	2.35	6	1
5:D:544:7Q9:O31	6:D:546:17F:H4	0.52	2.04	7	1
6:D:546:17F:H57	6:D:546:17F:C7	0.52	2.34	7	1
5:E:853:7Q9:C1	5:E:853:7Q9:O22	0.52	2.53	11	3
2:E:559:LYS:HE3	2:E:559:LYS:HA	0.52	1.79	9	1
6:D:534:17F:H30	6:D:534:17F:C33	0.52	2.33	16	1
6:E:870:17F:H69	6:E:870:17F:H43	0.52	1.79	18	1
6:B:208:17F:H40	6:B:208:17F:C32	0.52	2.32	19	2
2:D:348:MET:HE2	2:E:612:MET:SD	0.52	2.44	19	1
5:A:215:7Q9:C38	6:D:534:17F:H45	0.52	2.34	1	2
2:D:440:LEU:HD11	5:D:537:7Q9:C313	0.52	2.35	11	2
5:E:820:7Q9:C14	5:E:820:7Q9:O12	0.52	2.57	2	20
1:B:68:ARG:HA	1:B:71:TYR:CZ	0.52	2.39	19	8
6:D:510:17F:C27	6:D:516:17F:H62	0.52	2.21	2	1
5:E:821:7Q9:O22	5:E:821:7Q9:O31	0.52	2.28	5	4
1:B:6:LEU:O	1:B:55:ILE:HA	0.52	2.04	6	7
5:E:816:7Q9:O22	5:E:816:7Q9:C1	0.52	2.56	15	11
5:E:820:7Q9:C1	6:E:838:17F:H18	0.52	2.34	4	2
5:E:853:7Q9:O14	5:E:853:7Q9:O21	0.52	2.27	20	6
6:D:516:17F:H42	6:D:527:17F:H38	0.52	1.82	5	1
5:D:515:7Q9:O13	5:D:519:7Q9:C12	0.52	2.57	11	1
5:E:804:7Q9:C14	5:E:804:7Q9:O12	0.52	2.57	12	1
6:A:208:17F:C19	6:B:208:17F:C1X	0.52	2.87	13	1
2:D:333:LYS:HZ2	6:D:528:17F:H38	0.52	1.63	16	1
6:D:516:17F:C25	6:D:527:17F:C22	0.52	2.85	17	1
6:B:219:17F:H32	5:D:545:7Q9:C37	0.52	2.34	1	1
5:A:213:7Q9:C3	5:A:213:7Q9:O22	0.52	2.52	2	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:838:17F:H47	6:E:838:17F:H77	0.52	1.80	2	1
5:D:512:7Q9:O11	5:D:512:7Q9:O22	0.52	2.27	9	13
2:E:641:LEU:HG	5:E:851:7Q9:C313	0.52	2.33	4	2
5:A:211:7Q9:C3	5:A:211:7Q9:O22	0.52	2.53	7	4
5:A:215:7Q9:C36	5:D:536:7Q9:C310	0.52	2.88	9	1
6:B:214:17F:H52	5:E:815:7Q9:C318	0.52	2.34	9	3
6:E:819:17F:H12	6:E:819:17F:C1Y	0.52	2.34	13	2
6:E:819:17F:H12A	5:E:829:7Q9:O14	0.52	2.05	10	1
5:D:530:7Q9:C13	5:D:530:7Q9:C32	0.52	2.88	20	2
6:E:809:17F:H53	6:E:818:17F:H78	0.52	1.81	15	1
5:B:220:7Q9:C312	6:D:533:17F:H47	0.52	2.35	19	1
5:A:204:7Q9:C1	5:A:204:7Q9:O22	0.52	2.53	12	8
6:D:528:17F:H38	6:D:528:17F:C41	0.52	2.34	1	2
5:A:217:7Q9:O32	5:A:217:7Q9:O21	0.52	2.28	5	4
5:B:209:7Q9:C3	5:D:505:7Q9:C22	0.52	2.88	4	1
5:D:548:7Q9:O22	5:D:548:7Q9:P	0.52	2.68	5	8
2:D:309:GLN:HB2	6:D:527:17F:H63	0.52	1.81	9	1
1:A:64:TYR:HB2	1:A:67:MET:HB2	0.52	1.81	10	1
5:E:834:7Q9:C38	6:E:855:17F:H63	0.52	2.34	11	1
5:B:205:7Q9:O14	5:B:206:7Q9:C15	0.52	2.57	12	2
6:D:533:17F:C32	6:D:533:17F:C36	0.52	2.77	14	1
5:D:536:7Q9:C3	5:D:547:7Q9:C21	0.52	2.88	15	1
6:B:214:17F:C17	6:B:219:17F:C11	0.52	2.87	16	1
5:D:519:7Q9:C32	5:D:541:7Q9:C22	0.52	2.88	19	2
6:D:527:17F:O9	6:D:527:17F:H1	0.52	2.05	17	1
5:D:545:7Q9:C22	5:D:545:7Q9:C13	0.52	2.87	1	5
5:E:847:7Q9:O32	5:E:847:7Q9:O21	0.52	2.28	7	17
5:E:854:7Q9:C14	5:E:854:7Q9:O12	0.52	2.58	12	19
5:A:213:7Q9:C31	5:D:518:7Q9:C34	0.52	2.88	2	1
5:B:218:7Q9:O22	5:D:542:7Q9:C15	0.52	2.58	5	6
5:B:220:7Q9:C22	5:D:543:7Q9:P	0.52	2.98	3	1
5:E:806:7Q9:O32	5:E:806:7Q9:O21	0.52	2.28	3	7
5:A:213:7Q9:C14	5:A:213:7Q9:O12	0.52	2.57	4	1
5:B:203:7Q9:C39	6:B:208:17F:H73	0.52	2.33	7	3
2:D:418:LEU:HD22	2:E:736:TYR:HA	0.52	1.81	8	1
6:E:818:17F:H10A	6:E:819:17F:C10	0.52	2.35	20	2
5:D:506:7Q9:O22	5:D:506:7Q9:C31	0.52	2.58	10	1
6:D:534:17F:C33	6:D:534:17F:H36	0.52	2.34	18	2
6:D:501:17F:O8	5:D:506:7Q9:C14	0.52	2.58	11	1
6:D:534:17F:H64	6:D:534:17F:H30	0.52	1.81	11	1
5:A:211:7Q9:C316	5:A:213:7Q9:C315	0.52	2.87	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:520:7Q9:C3	5:D:538:7Q9:O22	0.52	2.57	13	1
5:D:521:7Q9:C311	5:D:521:7Q9:C37	0.52	2.87	20	2
6:D:501:17F:O1	6:D:501:17F:C7	0.52	2.58	18	1
5:D:515:7Q9:C35	6:D:517:17F:H70	0.52	2.35	19	1
6:D:501:17F:C7	5:D:506:7Q9:C15	0.52	2.87	20	1
1:B:46:ILE:HD13	1:B:160:VAL:HG21	0.52	1.80	14	4
5:B:209:7Q9:O32	5:B:209:7Q9:O21	0.52	2.28	6	10
2:E:664:ALA:HB3	2:E:665:PRO:HD3	0.52	1.81	18	3
6:E:818:17F:O6	6:E:818:17F:O8	0.52	2.27	9	4
2:E:555:SER:CA	6:E:872:17F:H65	0.52	2.35	11	5
5:B:203:7Q9:O13	5:B:205:7Q9:C15	0.52	2.57	4	3
6:B:214:17F:H69	6:B:219:17F:H37	0.52	1.82	4	1
5:A:209:7Q9:C316	5:E:822:7Q9:C312	0.52	2.87	7	4
2:D:305:GLN:OE1	6:D:527:17F:H29	0.52	2.05	7	2
5:D:515:7Q9:C318	6:D:517:17F:H73	0.52	2.35	8	2
6:E:801:17F:O5	5:E:808:7Q9:C14	0.52	2.58	8	1
6:B:208:17F:H76	5:E:804:7Q9:C318	0.52	2.35	11	2
6:E:838:17F:H12	6:E:856:17F:H11A	0.52	1.82	15	2
5:E:813:7Q9:C21	5:E:829:7Q9:O13	0.52	2.57	10	1
6:B:214:17F:H78	6:B:219:17F:C42	0.52	2.35	14	1
6:D:510:17F:H51	6:D:516:17F:C37	0.52	2.30	14	1
5:D:548:7Q9:C23	5:E:816:7Q9:C22	0.52	2.88	20	1
5:B:205:7Q9:C311	5:B:205:7Q9:C37	0.52	2.87	12	3
5:B:209:7Q9:C1	5:B:209:7Q9:O22	0.52	2.53	1	7
5:E:863:7Q9:C35	5:E:863:7Q9:C31	0.52	2.88	10	7
5:B:211:7Q9:C22	6:D:501:17F:H31	0.52	2.34	2	1
5:D:548:7Q9:C13	5:D:548:7Q9:O14	0.52	2.57	7	6
6:B:219:17F:H19	6:B:219:17F:O8	0.52	2.05	4	2
6:E:856:17F:H4A	6:E:856:17F:C7	0.52	2.35	4	3
5:A:209:7Q9:C313	6:A:214:17F:H61	0.52	2.35	5	2
6:B:214:17F:O10	6:B:219:17F:C9	0.52	2.56	5	1
5:E:848:7Q9:C317	5:E:851:7Q9:C316	0.52	2.88	6	3
6:E:817:17F:H59	5:E:833:7Q9:C34	0.52	2.34	13	4
6:E:870:17F:H51	6:E:870:17F:H75	0.52	1.80	13	1
6:D:546:17F:H4	6:D:546:17F:H1A	0.52	1.80	14	1
2:D:399:HIS:CE1	2:E:564:LEU:HB2	0.52	2.39	7	7
6:D:510:17F:H43	6:D:516:17F:H64	0.52	1.80	1	3
5:B:210:7Q9:C38	5:B:210:7Q9:C22	0.52	2.87	15	6
6:D:534:17F:O8	6:D:534:17F:O9	0.52	2.27	14	11
6:D:528:17F:H4A	5:D:532:7Q9:C14	0.52	2.34	3	1
5:A:217:7Q9:C3	6:D:546:17F:H18A	0.52	2.35	6	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:326:LEU:HD22	2:E:637:LEU:HG	0.52	1.81	6	1
6:E:819:17F:H75	5:E:829:7Q9:C23	0.52	2.35	6	1
6:B:219:17F:H36	6:B:219:17F:H20	0.52	1.82	16	2
5:E:859:7Q9:O22	5:E:859:7Q9:C3	0.52	2.55	13	2
5:B:203:7Q9:C22	5:B:204:7Q9:C3	0.52	2.88	8	1
5:E:848:7Q9:C39	5:E:862:7Q9:C37	0.52	2.87	16	2
2:D:330:ALA:HA	2:D:333:LYS:CE	0.52	2.34	11	1
6:E:809:17F:H34	6:E:818:17F:C36	0.52	2.35	11	1
6:E:818:17F:H12A	6:E:819:17F:H10A	0.52	1.81	12	1
5:A:215:7Q9:C39	5:D:536:7Q9:C310	0.52	2.88	15	2
5:D:522:7Q9:C36	5:D:545:7Q9:C314	0.52	2.87	20	3
5:B:212:7Q9:C35	5:B:212:7Q9:C31	0.52	2.87	17	1
6:B:215:17F:O2	5:D:506:7Q9:C14	0.52	2.58	17	1
6:E:819:17F:O2	5:E:829:7Q9:C14	0.52	2.58	17	1
6:D:510:17F:H46	6:D:516:17F:C40	0.52	2.35	18	1
2:E:663:LEU:HD21	6:E:874:17F:C24	0.52	2.33	19	1
5:E:823:7Q9:O32	5:E:823:7Q9:O21	0.52	2.28	10	15
5:E:840:7Q9:C1	5:E:840:7Q9:C31	0.52	2.88	2	18
5:E:864:7Q9:C14	5:E:864:7Q9:O11	0.52	2.58	7	15
5:E:878:7Q9:C37	5:E:878:7Q9:C311	0.52	2.87	17	5
1:A:80:CYS:HB3	1:A:93:ILE:HD12	0.52	1.82	17	3
6:E:819:17F:H41	5:E:835:7Q9:C37	0.52	2.35	2	4
5:E:850:7Q9:C38	6:E:870:17F:H20	0.52	2.34	2	1
5:A:204:7Q9:C312	6:A:208:17F:H12A	0.52	2.35	3	1
6:B:214:17F:H39	6:B:214:17F:C12	0.52	2.35	16	3
5:E:873:7Q9:O32	5:E:873:7Q9:O21	0.52	2.28	3	12
1:B:17:SER:HB2	3:B:201:GSP:O1A	0.52	2.04	13	2
5:A:205:7Q9:O14	5:B:204:7Q9:C12	0.52	2.58	6	1
5:E:871:7Q9:C1	5:E:871:7Q9:O22	0.52	2.55	14	6
5:D:525:7Q9:C11	5:D:525:7Q9:O32	0.52	2.58	9	4
2:E:729:PHE:CD2	6:E:870:17F:H63	0.52	2.40	16	2
6:D:516:17F:H44	5:D:535:7Q9:C314	0.52	2.35	10	1
1:A:117:LYS:HG2	3:A:201:GSP:C6	0.52	2.40	13	1
6:D:510:17F:C27	6:D:516:17F:H64	0.52	2.35	13	2
6:D:533:17F:H76	6:E:870:17F:C38	0.52	2.17	13	1
5:E:843:7Q9:O13	5:E:843:7Q9:O21	0.52	2.27	19	4
5:D:525:7Q9:C1	5:D:525:7Q9:O22	0.51	2.57	1	1
2:E:558:SER:OG	6:E:872:17F:H63	0.51	2.05	9	5
5:E:846:7Q9:C1	5:E:850:7Q9:C3	0.51	2.88	16	2
5:D:535:7Q9:C14	5:D:535:7Q9:C1	0.51	2.88	7	8
5:D:544:7Q9:C34	6:D:546:17F:C19	0.51	2.88	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:514:7Q9:C1	5:D:514:7Q9:C15	0.51	2.88	13	4
6:A:208:17F:H35	6:A:208:17F:C24	0.51	2.31	5	2
5:D:535:7Q9:C14	5:D:535:7Q9:O12	0.51	2.59	15	5
5:B:211:7Q9:C318	6:E:809:17F:H55	0.51	2.35	6	1
6:E:801:17F:H50	6:E:801:17F:H77	0.51	1.82	7	1
6:B:214:17F:O9	6:B:214:17F:C7	0.51	2.58	15	6
6:D:533:17F:C35	6:D:533:17F:H38	0.51	2.34	9	2
6:D:517:17F:C31	6:D:517:17F:H40	0.51	2.36	10	1
6:A:208:17F:H69	6:B:208:17F:C41	0.51	2.35	11	1
2:E:634:LEU:HD21	5:E:862:7Q9:C310	0.51	2.34	12	1
5:D:508:7Q9:O31	5:D:509:7Q9:C23	0.51	2.57	13	2
5:E:802:7Q9:C314	6:E:809:17F:H59	0.51	2.35	13	1
6:D:527:17F:C37	6:D:527:17F:C32	0.51	2.87	14	1
5:E:833:7Q9:C13	6:E:838:17F:O5	0.51	2.58	19	1
6:D:528:17F:H37	6:D:528:17F:C38	0.51	2.32	19	3
6:E:856:17F:H6A	6:E:856:17F:O10	0.51	2.04	1	2
6:A:214:17F:O8	6:A:214:17F:O9	0.51	2.29	2	3
5:D:537:7Q9:C3	6:D:546:17F:H10	0.51	2.35	2	2
5:E:815:7Q9:C32	5:E:830:7Q9:C3	0.51	2.88	2	4
2:E:623:ARG:HB3	5:E:858:7Q9:C310	0.51	2.35	20	4
6:E:807:17F:H54	6:E:809:17F:H64	0.51	1.82	3	1
1:B:15:GLY:HA3	3:B:201:GSP:C8	0.51	2.40	5	1
5:B:211:7Q9:O22	5:B:211:7Q9:C1	0.51	2.53	6	5
5:E:842:7Q9:O31	5:E:861:7Q9:C22	0.51	2.58	13	5
5:E:864:7Q9:C2	5:E:864:7Q9:O32	0.51	2.54	12	6
6:E:841:17F:H42	6:E:841:17F:C31	0.51	2.34	7	1
5:D:549:7Q9:C14	5:E:851:7Q9:O13	0.51	2.58	8	1
6:D:510:17F:C19	6:D:516:17F:H9A	0.51	2.29	9	2
6:D:510:17F:C33	6:D:516:17F:H37	0.51	2.36	9	1
6:D:527:17F:C10	5:D:535:7Q9:C34	0.51	2.89	9	1
6:E:818:17F:H40	5:E:835:7Q9:C310	0.51	2.35	9	2
6:E:838:17F:H40	6:E:838:17F:H34	0.51	1.80	13	2
2:D:315:TYR:CE2	2:E:648:MET:HB2	0.51	2.40	13	1
5:E:802:7Q9:C23	6:E:805:17F:H34	0.51	2.35	14	1
5:D:506:7Q9:C33	6:D:517:17F:H56	0.51	2.36	18	1
6:E:809:17F:C33	6:E:809:17F:H48	0.51	2.36	20	1
6:B:208:17F:O1	6:B:208:17F:H10A	0.51	2.04	1	1
5:B:216:7Q9:C34	5:D:519:7Q9:C23	0.51	2.87	1	3
5:E:835:7Q9:C14	5:E:836:7Q9:O13	0.51	2.57	1	2
5:A:209:7Q9:C318	5:E:823:7Q9:C312	0.51	2.88	16	4
5:B:211:7Q9:C15	5:B:211:7Q9:C3	0.51	2.88	2	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:E:641:LEU:HD21	5:E:851:7Q9:C318	0.51	2.36	10	2
6:E:817:17F:H29	5:E:833:7Q9:C32	0.51	2.35	10	2
5:A:204:7Q9:C312	6:A:208:17F:C2X	0.51	2.88	8	2
5:E:851:7Q9:O32	5:E:851:7Q9:O21	0.51	2.28	3	8
6:D:516:17F:C28	6:D:516:17F:C24	0.51	2.88	4	3
6:E:841:17F:H29	6:E:841:17F:C23	0.51	2.35	7	4
2:D:311:GLU:HG2	2:E:648:MET:HE1	0.51	1.81	5	1
6:D:516:17F:H44	6:D:527:17F:C22	0.51	2.19	7	1
6:B:208:17F:N1	6:B:214:17F:O4	0.51	2.43	8	1
5:D:505:7Q9:C12	6:D:511:17F:O2	0.51	2.58	8	1
5:E:802:7Q9:C316	6:E:809:17F:H72	0.51	2.36	8	1
5:B:218:7Q9:C32	5:D:514:7Q9:C32	0.51	2.89	9	3
6:B:208:17F:H31	6:B:214:17F:C10	0.51	2.35	10	1
6:D:517:17F:H10	5:D:529:7Q9:C22	0.51	2.36	11	1
6:E:817:17F:H47	6:E:817:17F:H76	0.51	1.82	12	1
6:E:828:17F:H41	5:E:832:7Q9:C311	0.51	2.36	15	2
6:D:501:17F:H8A	5:D:506:7Q9:C15	0.51	2.35	19	2
5:D:539:7Q9:C15	5:D:539:7Q9:O32	0.51	2.58	17	1
5:D:505:7Q9:C1	6:D:511:17F:H6	0.51	2.36	18	1
6:D:517:17F:O8	6:D:517:17F:H10A	0.51	2.04	12	6
5:D:518:7Q9:O12	5:D:518:7Q9:C2	0.51	2.59	6	2
5:E:848:7Q9:C34	5:E:851:7Q9:C31	0.51	2.88	1	3
6:D:517:17F:H10	5:D:529:7Q9:O22	0.51	2.06	2	1
5:D:544:7Q9:C34	6:D:546:17F:H19	0.51	2.36	6	3
6:E:838:17F:C11	6:E:838:17F:C36	0.51	2.88	16	4
1:B:5:LYS:HA	1:B:54:ASP:HB3	0.51	1.81	3	1
6:E:807:17F:C1Z	6:E:819:17F:H29	0.51	2.34	3	1
6:E:817:17F:O8	6:E:817:17F:C5	0.51	2.53	4	4
6:B:214:17F:C38	6:B:214:17F:H61	0.51	2.35	5	1
5:E:833:7Q9:O13	6:E:838:17F:H20A	0.51	2.05	11	4
5:B:213:7Q9:O21	5:B:213:7Q9:C12	0.51	2.57	6	3
6:D:510:17F:C11	6:D:516:17F:H8A	0.51	2.35	6	1
5:B:216:7Q9:O32	5:D:519:7Q9:C15	0.51	2.58	17	2
5:D:512:7Q9:O13	6:D:528:17F:C4	0.51	2.59	7	2
6:D:517:17F:H40	6:D:517:17F:C32	0.51	2.36	15	4
6:E:805:17F:C25	5:E:816:7Q9:C316	0.51	2.88	9	1
5:B:217:7Q9:C318	5:D:548:7Q9:C318	0.51	2.88	13	5
6:E:807:17F:O5	5:E:813:7Q9:C14	0.51	2.58	10	2
1:B:68:ARG:HB3	1:B:99:GLN:HE22	0.51	1.64	11	1
5:E:804:7Q9:C2	5:E:815:7Q9:C22	0.51	2.88	20	2
6:D:510:17F:H51	6:D:516:17F:H72	0.51	1.82	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:516:17F:H57	5:D:535:7Q9:C314	0.51	2.35	14	1
2:D:334:LEU:HB2	5:D:532:7Q9:C315	0.51	2.35	16	2
5:A:211:7Q9:C33	5:A:213:7Q9:C36	0.51	2.88	16	1
1:A:36:ILE:HA	1:A:59:ALA:HB2	0.51	1.83	18	1
3:B:201:GSP:O3G	3:B:201:GSP:O2B	0.51	2.29	1	1
5:B:203:7Q9:O13	5:B:205:7Q9:C12	0.51	2.59	1	2
2:E:558:SER:OG	6:E:872:17F:H69	0.51	2.06	1	3
5:E:824:7Q9:C33	5:E:824:7Q9:C37	0.51	2.89	3	4
5:E:862:7Q9:O32	5:E:862:7Q9:O21	0.51	2.28	16	16
6:E:874:17F:C6	6:E:874:17F:O1	0.51	2.58	7	4
6:D:534:17F:H65	6:D:534:17F:H59	0.51	1.81	2	1
6:E:801:17F:H20A	6:E:801:17F:H12	0.51	1.82	2	1
5:D:506:7Q9:O12	5:D:506:7Q9:C13	0.51	2.58	3	1
5:E:816:7Q9:C39	5:E:831:7Q9:C23	0.51	2.88	3	1
5:E:834:7Q9:C318	6:E:855:17F:H66	0.51	2.35	3	1
1:A:84:ILE:HD12	1:A:123:ARG:HB3	0.51	1.83	5	9
5:B:207:7Q9:C13	5:B:207:7Q9:P	0.51	2.99	9	14
5:B:217:7Q9:O22	5:B:217:7Q9:O31	0.51	2.29	9	2
6:E:817:17F:C34	5:E:826:7Q9:C36	0.51	2.84	9	3
6:D:510:17F:H78	6:D:510:17F:C29	0.51	2.35	11	2
6:A:208:17F:H63	6:A:208:17F:H57	0.51	1.81	16	1
5:B:203:7Q9:C315	6:B:208:17F:H78	0.51	2.34	17	1
6:B:208:17F:H20	5:B:212:7Q9:C32	0.51	2.36	17	1
5:B:218:7Q9:C34	5:B:218:7Q9:O31	0.51	2.59	18	2
6:D:517:17F:H48	6:D:517:17F:H70	0.51	1.82	18	1
1:A:32:TYR:CD2	3:A:201:GSP:H5'2	0.51	2.41	1	1
5:B:213:7Q9:C22	5:B:213:7Q9:C14	0.51	2.89	1	1
5:B:220:7Q9:O32	5:B:220:7Q9:O21	0.51	2.29	18	12
2:E:659:LEU:CD2	6:E:856:17F:H67	0.51	2.36	1	2
5:E:810:7Q9:O32	5:E:810:7Q9:C2	0.51	2.56	11	8
5:E:813:7Q9:O21	5:E:813:7Q9:O32	0.51	2.29	12	10
5:D:548:7Q9:C33	5:E:831:7Q9:C23	0.51	2.89	3	2
5:D:514:7Q9:O13	5:D:531:7Q9:C15	0.51	2.59	4	1
5:E:849:7Q9:C314	5:E:867:7Q9:C314	0.51	2.88	4	5
6:E:856:17F:O7	6:E:856:17F:H10	0.51	2.05	12	3
6:D:527:17F:H68	6:D:527:17F:H40	0.51	1.82	8	1
6:E:811:17F:O8	5:E:822:7Q9:C11	0.51	2.59	11	1
6:E:818:17F:H75	6:E:818:17F:C26	0.51	2.28	12	1
2:E:660:ARG:HH12	6:E:874:17F:C3	0.51	2.18	14	1
5:E:813:7Q9:C314	6:E:819:17F:H54	0.51	2.36	16	1
6:D:501:17F:C34	6:D:501:17F:C26	0.51	2.78	20	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:835:7Q9:C31	5:E:837:7Q9:C23	0.51	2.88	20	1
6:B:219:17F:H18	5:D:545:7Q9:C33	0.51	2.36	1	1
2:E:693:HIS:HB2	5:E:863:7Q9:C39	0.51	2.35	2	4
6:E:801:17F:H4	6:E:801:17F:O10	0.51	2.06	1	1
6:E:807:17F:H58	6:E:807:17F:H30	0.51	1.83	1	2
5:E:821:7Q9:C15	5:E:821:7Q9:C1	0.51	2.89	15	5
5:D:540:7Q9:C12	5:D:540:7Q9:O22	0.51	2.58	10	4
6:E:807:17F:H68	6:E:818:17F:H44	0.51	1.82	6	1
2:D:423:GLU:HA	2:D:426:LYS:HE2	0.51	1.83	8	2
5:D:535:7Q9:C318	6:E:874:17F:H76	0.51	2.35	8	1
5:E:842:7Q9:O11	5:E:842:7Q9:O22	0.51	2.28	13	2
5:D:520:7Q9:C34	5:D:520:7Q9:O32	0.51	2.59	9	1
5:E:813:7Q9:C311	6:E:819:17F:H77	0.51	2.36	16	3
1:B:126:ASP:HB3	1:B:129:GLN:HB3	0.51	1.82	10	1
2:D:422:LEU:HG	2:D:426:LYS:HE2	0.51	1.82	10	1
5:E:839:7Q9:O32	5:E:840:7Q9:C22	0.51	2.59	11	1
1:A:58:THR:HG21	1:A:71:TYR:CZ	0.51	2.41	12	1
5:A:204:7Q9:O32	6:A:208:17F:H6	0.51	2.06	12	1
6:E:838:17F:H62	6:E:838:17F:H57	0.51	1.81	12	1
5:D:502:7Q9:C315	5:E:813:7Q9:C317	0.51	2.88	13	2
5:E:848:7Q9:C315	5:E:851:7Q9:C311	0.51	2.89	13	1
6:B:214:17F:H10A	6:B:214:17F:C24	0.51	2.36	14	1
6:E:805:17F:H55	6:E:805:17F:H68	0.51	1.83	15	1
5:A:204:7Q9:C314	6:A:208:17F:H77	0.51	2.35	16	1
6:B:215:17F:O10	6:B:215:17F:C7	0.51	2.59	16	1
6:E:872:17F:O10	6:E:872:17F:H6A	0.51	2.05	16	2
5:E:857:7Q9:C310	6:E:874:17F:H51	0.51	2.36	18	1
6:B:208:17F:O9	6:B:208:17F:C7	0.51	2.59	14	16
5:D:540:7Q9:O22	5:D:540:7Q9:O31	0.51	2.28	10	3
5:E:834:7Q9:O21	5:E:834:7Q9:O32	0.51	2.29	14	16
5:D:518:7Q9:C13	6:D:533:17F:H8A	0.51	2.35	2	1
5:D:538:7Q9:C14	5:D:538:7Q9:C22	0.51	2.88	13	5
5:E:842:7Q9:C314	5:E:842:7Q9:C37	0.51	2.89	16	5
5:E:863:7Q9:C31	5:E:863:7Q9:C35	0.51	2.89	16	5
5:E:837:7Q9:C31	6:E:841:17F:H31	0.51	2.35	3	2
6:D:501:17F:H74	6:E:818:17F:C42	0.51	2.36	4	1
5:D:524:7Q9:C312	5:D:524:7Q9:C38	0.51	2.86	9	2
5:E:813:7Q9:C33	5:E:829:7Q9:C22	0.51	2.89	5	2
5:E:863:7Q9:C3	5:E:863:7Q9:O22	0.51	2.55	9	1
1:B:118:CYS:SG	1:B:143:GLU:HB3	0.51	2.46	10	2
6:B:214:17F:H31	5:B:220:7Q9:C32	0.51	2.36	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:503:7Q9:C23	6:D:510:17F:C2X	0.51	2.89	12	1
2:D:291:GLU:HG3	5:D:547:7Q9:C310	0.51	2.36	13	1
6:D:534:17F:H64	6:D:534:17F:C1X	0.51	2.36	15	1
5:E:824:7Q9:C34	6:E:841:17F:C18	0.51	2.85	15	1
6:D:528:17F:O2	5:D:532:7Q9:C14	0.51	2.59	17	1
5:A:203:7Q9:O22	5:A:203:7Q9:C3	0.51	2.55	3	4
5:E:802:7Q9:O32	5:E:802:7Q9:C2	0.51	2.53	1	10
5:E:847:7Q9:C1	5:E:847:7Q9:O22	0.51	2.53	14	11
5:E:854:7Q9:O32	5:E:854:7Q9:O21	0.51	2.29	15	7
5:B:216:7Q9:O21	5:B:216:7Q9:P	0.51	2.68	2	14
6:E:817:17F:H35	6:E:817:17F:C24	0.51	2.33	4	6
6:D:501:17F:H62	6:D:501:17F:H10	0.51	1.81	3	1
5:E:816:7Q9:C15	5:E:816:7Q9:O12	0.51	2.58	11	2
5:A:209:7Q9:C318	5:E:839:7Q9:C312	0.51	2.89	7	3
6:D:511:17F:H8A	5:D:513:7Q9:C14	0.51	2.36	7	3
5:E:810:7Q9:C39	5:E:825:7Q9:C312	0.51	2.88	5	2
6:E:841:17F:H59	6:E:841:17F:C36	0.51	2.24	17	3
1:A:73:ARG:HG3	1:A:103:VAL:HG12	0.51	1.82	13	2
6:A:208:17F:H41	5:E:823:7Q9:C318	0.51	2.35	19	3
6:D:510:17F:H6	6:D:516:17F:H4A	0.51	1.82	9	1
6:E:855:17F:H38	6:E:855:17F:C38	0.51	2.26	16	3
6:B:219:17F:H52	5:E:846:7Q9:C318	0.51	2.35	10	2
6:D:501:17F:H38	6:D:501:17F:H20A	0.51	1.82	10	1
6:B:208:17F:H41	6:B:214:17F:H37	0.51	1.80	11	1
2:D:403:LEU:HD11	2:E:561:ARG:HG3	0.51	1.83	11	1
6:D:501:17F:O1	6:D:501:17F:O7	0.51	2.29	11	1
5:E:808:7Q9:C32	6:E:811:17F:C12	0.51	2.87	13	1
6:D:516:17F:H50	6:D:516:17F:C34	0.51	2.36	14	1
6:D:501:17F:H56	6:D:501:17F:C10	0.51	2.36	15	1
6:E:819:17F:C18	5:E:829:7Q9:C23	0.51	2.85	15	2
5:A:215:7Q9:C34	5:A:215:7Q9:O31	0.51	2.58	16	1
5:D:536:7Q9:C21	5:D:536:7Q9:O31	0.51	2.58	14	4
6:B:215:17F:O8	6:B:215:17F:C5	0.51	2.57	9	4
5:D:502:7Q9:O32	5:D:502:7Q9:O21	0.51	2.30	7	6
5:D:509:7Q9:C312	5:D:525:7Q9:C316	0.51	2.89	2	1
1:A:72:MET:HA	1:A:78:PHE:CZ	0.51	2.39	3	3
5:B:218:7Q9:C312	5:D:522:7Q9:C22	0.51	2.89	3	1
6:D:510:17F:O9	6:D:527:17F:H19A	0.51	2.05	10	2
6:D:510:17F:P1	6:D:510:17F:N1	0.51	2.84	18	5
5:E:821:7Q9:O21	5:E:821:7Q9:P	0.51	2.69	18	2
5:E:843:7Q9:O14	5:E:859:7Q9:C32	0.51	2.59	8	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:872:17F:H59	6:E:872:17F:H44	0.51	1.83	12	2
6:B:208:17F:C7	6:B:208:17F:O9	0.51	2.59	10	2
5:D:506:7Q9:C22	5:D:520:7Q9:C22	0.51	2.89	9	3
5:D:509:7Q9:C314	5:E:835:7Q9:C316	0.51	2.88	16	4
6:A:208:17F:H10A	5:A:209:7Q9:C37	0.51	2.36	10	1
6:D:510:17F:C30	6:D:510:17F:C42	0.51	2.89	11	1
6:B:214:17F:O10	6:B:219:17F:C11	0.51	2.59	19	2
5:E:813:7Q9:O22	5:E:813:7Q9:C1	0.51	2.54	12	2
6:B:215:17F:H55	5:E:810:7Q9:C318	0.51	2.36	14	1
1:A:32:TYR:HE1	3:A:201:GSP:O3A	0.51	1.88	15	1
2:D:334:LEU:HB3	5:D:532:7Q9:C312	0.51	2.36	16	1
6:B:214:17F:H56	6:B:219:17F:H12	0.51	1.82	17	1
6:B:219:17F:H4	5:D:545:7Q9:C33	0.51	2.36	17	1
5:B:205:7Q9:C3	5:B:207:7Q9:C11	0.51	2.89	18	1
5:E:832:7Q9:C23	6:E:856:17F:H36	0.51	2.35	18	1
5:E:834:7Q9:C35	6:E:855:17F:H59	0.51	2.36	19	1
2:D:334:LEU:H	5:D:532:7Q9:C312	0.51	2.19	20	1
6:D:510:17F:H77	6:D:516:17F:C41	0.51	2.35	20	1
2:D:275:LEU:HG	2:E:688:ARG:HG2	0.50	1.81	1	1
5:E:816:7Q9:C3	5:E:816:7Q9:O13	0.50	2.58	15	10
6:E:819:17F:H4A	6:E:819:17F:O8	0.50	2.05	6	3
5:E:846:7Q9:C14	5:E:846:7Q9:P	0.50	2.99	17	15
6:E:805:17F:C40	5:E:816:7Q9:C318	0.50	2.87	6	5
6:E:855:17F:O10	6:E:855:17F:C6	0.50	2.51	14	2
5:E:849:7Q9:O32	5:E:849:7Q9:C21	0.50	2.59	13	3
5:D:505:7Q9:O22	5:D:505:7Q9:O11	0.50	2.29	4	1
6:E:870:17F:H5	6:E:870:17F:O1	0.50	2.05	18	13
6:A:208:17F:H68	5:B:203:7Q9:C318	0.50	2.36	7	1
2:D:404:SER:HB3	5:D:542:7Q9:C315	0.50	2.36	7	1
5:A:212:7Q9:C14	6:A:214:17F:O4	0.50	2.60	10	1
6:B:219:17F:H63	5:D:522:7Q9:C38	0.50	2.36	10	1
5:B:209:7Q9:C13	5:B:209:7Q9:O14	0.50	2.60	11	1
6:E:819:17F:C7	6:E:819:17F:C11	0.50	2.90	13	1
5:E:840:7Q9:C11	5:E:849:7Q9:O22	0.50	2.59	14	1
5:D:504:7Q9:C318	6:D:516:17F:H69	0.50	2.35	15	1
6:D:516:17F:C34	6:D:516:17F:C38	0.50	2.73	16	1
6:B:219:17F:C18	5:D:545:7Q9:C33	0.50	2.89	8	3
6:D:511:17F:O4	5:D:526:7Q9:C15	0.50	2.59	1	2
5:E:862:7Q9:O22	5:E:862:7Q9:C1	0.50	2.56	12	13
5:E:866:7Q9:O31	5:E:866:7Q9:C21	0.50	2.58	13	20
6:B:214:17F:H61	6:B:214:17F:C39	0.50	2.36	19	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:510:17F:C36	6:D:527:17F:C41	0.50	2.89	5	2
5:E:826:7Q9:O32	5:E:826:7Q9:C2	0.50	2.53	5	6
5:E:853:7Q9:C39	5:E:877:7Q9:C35	0.50	2.90	15	2
2:E:660:ARG:HD2	6:E:874:17F:C20	0.50	2.32	4	2
6:E:838:17F:H8A	6:E:856:17F:H35	0.50	1.83	4	2
5:D:538:7Q9:C1	5:D:538:7Q9:O22	0.50	2.56	5	2
5:E:878:7Q9:O32	5:E:878:7Q9:C2	0.50	2.55	19	7
1:B:79:LEU:HD13	1:B:159:LEU:HD22	0.50	1.83	16	3
6:E:856:17F:H37	6:E:856:17F:H68	0.50	1.83	8	2
6:D:501:17F:H44	6:D:501:17F:C35	0.50	2.36	9	1
5:B:211:7Q9:C312	6:D:501:17F:H62	0.50	2.36	17	1
5:E:827:7Q9:O13	5:E:850:7Q9:C1	0.50	2.59	18	1
6:E:818:17F:H12A	6:E:819:17F:C21	0.50	2.36	20	1
6:D:528:17F:H72	5:E:862:7Q9:C316	0.50	2.36	11	3
6:E:807:17F:H57	6:E:819:17F:C12	0.50	2.36	1	3
5:E:868:7Q9:C34	5:E:873:7Q9:C37	0.50	2.89	1	2
6:E:801:17F:H1A	6:E:801:17F:C4	0.50	2.35	2	1
5:E:827:7Q9:O32	5:E:827:7Q9:O21	0.50	2.30	15	8
6:D:516:17F:H44	6:D:527:17F:H47	0.50	1.84	3	1
5:A:206:7Q9:C39	5:E:822:7Q9:C318	0.50	2.90	4	1
6:E:807:17F:O10	6:E:807:17F:C4	0.50	2.57	17	5
5:E:860:7Q9:C1	5:E:860:7Q9:O22	0.50	2.57	11	5
6:D:533:17F:H38	6:D:533:17F:H63	0.50	1.81	9	1
5:A:207:7Q9:C35	5:D:504:7Q9:C36	0.50	2.90	16	2
2:D:308:TRP:CH2	6:E:856:17F:H75	0.50	2.41	15	1
6:A:208:17F:H34	6:B:208:17F:H37	0.50	1.83	17	1
5:E:868:7Q9:C21	5:E:868:7Q9:O32	0.50	2.60	18	1
5:A:207:7Q9:C35	5:D:504:7Q9:C33	0.50	2.89	19	1
6:D:510:17F:H76	6:E:856:17F:H44	0.50	1.83	20	1
6:E:807:17F:H1A	6:E:807:17F:C4	0.50	2.36	20	1
5:B:203:7Q9:C32	6:B:208:17F:C6	0.50	2.90	1	1
6:D:501:17F:H68	6:D:501:17F:C29	0.50	2.37	1	1
6:E:811:17F:C6	5:E:823:7Q9:C3	0.50	2.89	1	2
6:E:855:17F:C21	6:E:855:17F:H65	0.50	2.37	6	4
1:A:41:ARG:HD2	1:A:54:ASP:OD1	0.50	2.07	2	1
6:D:527:17F:C17	6:D:527:17F:C1Y	0.50	2.89	17	5
6:D:510:17F:H38	6:D:511:17F:C40	0.50	2.29	4	1
6:B:208:17F:H45	6:B:208:17F:C37	0.50	2.36	5	2
5:D:531:7Q9:C3	5:D:531:7Q9:O22	0.50	2.55	19	3
6:E:838:17F:HN1	6:E:874:17F:H6A	0.50	1.64	10	1
6:A:208:17F:H1	5:A:209:7Q9:C15	0.50	2.36	19	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:504:7Q9:O31	6:D:516:17F:O10	0.50	2.29	12	1
5:A:212:7Q9:O13	5:A:212:7Q9:C2	0.50	2.60	10	10
6:E:807:17F:C1Z	6:E:818:17F:H10A	0.50	2.36	2	2
6:D:501:17F:O9	6:D:501:17F:C7	0.50	2.59	8	4
5:E:837:7Q9:C36	6:E:841:17F:H50	0.50	2.37	3	1
6:A:208:17F:C12	5:A:209:7Q9:C39	0.50	2.89	5	3
5:E:834:7Q9:C35	6:E:855:17F:H32	0.50	2.36	8	2
5:B:216:7Q9:C32	5:D:519:7Q9:C15	0.50	2.89	9	1
2:E:605:GLN:HG3	2:E:606:LYS:N	0.50	2.20	9	1
6:A:208:17F:H45	6:E:811:17F:H70	0.50	1.84	12	1
6:D:511:17F:H30	6:D:528:17F:C30	0.50	2.37	17	2
5:E:857:7Q9:C31	6:E:874:17F:C10	0.50	2.90	16	1
6:B:214:17F:H18	6:B:219:17F:H2	0.50	1.81	17	1
6:A:208:17F:H10	5:A:209:7Q9:C310	0.50	2.36	1	1
5:E:843:7Q9:C2	5:E:843:7Q9:O32	0.50	2.56	15	13
6:E:872:17F:H20A	6:E:872:17F:C2X	0.50	2.32	2	2
5:A:211:7Q9:O14	5:A:213:7Q9:C14	0.50	2.60	3	1
6:D:501:17F:H51	5:D:508:7Q9:C318	0.50	2.36	3	1
5:D:512:7Q9:C34	6:D:528:17F:H6A	0.50	2.37	3	2
5:D:521:7Q9:C15	5:D:521:7Q9:P	0.50	3.00	14	3
5:E:868:7Q9:C31	5:E:873:7Q9:C13	0.50	2.90	19	7
5:D:536:7Q9:O31	5:D:536:7Q9:C21	0.50	2.60	6	10
5:B:216:7Q9:C316	5:E:843:7Q9:C318	0.50	2.89	5	2
2:E:623:ARG:HD2	5:E:858:7Q9:C316	0.50	2.37	7	1
6:D:510:17F:H8	6:D:516:17F:O7	0.50	2.07	8	2
6:D:510:17F:C19	5:D:524:7Q9:O32	0.50	2.57	11	2
5:E:866:7Q9:C33	5:E:876:7Q9:C35	0.50	2.90	9	2
5:A:210:7Q9:C2	5:A:216:7Q9:O22	0.50	2.60	13	1
6:B:214:17F:O10	6:B:219:17F:H10	0.50	2.07	14	1
5:A:206:7Q9:C1	5:A:210:7Q9:C15	0.50	2.89	15	1
5:B:209:7Q9:C318	5:D:503:7Q9:C311	0.50	2.89	20	2
6:B:214:17F:C7	6:B:214:17F:O9	0.50	2.60	18	1
6:D:510:17F:N1	6:D:510:17F:O2	0.50	2.36	18	1
5:E:833:7Q9:O22	6:E:838:17F:H31	0.50	2.07	18	1
5:A:210:7Q9:O13	5:A:215:7Q9:C13	0.50	2.60	3	3
6:D:501:17F:O8	5:D:506:7Q9:C15	0.50	2.60	2	1
5:E:823:7Q9:O22	5:E:823:7Q9:C1	0.50	2.57	14	4
5:A:213:7Q9:O22	5:A:213:7Q9:C3	0.50	2.58	3	5
5:D:536:7Q9:C3	5:D:547:7Q9:C2	0.50	2.89	9	2
1:B:116:ASN:ND2	3:B:201:GSP:N7	0.50	2.58	5	2
5:B:206:7Q9:O13	5:B:212:7Q9:C13	0.50	2.60	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:837:7Q9:C32	6:E:841:17F:H56	0.50	2.36	6	1
5:D:521:7Q9:P	5:D:521:7Q9:C15	0.50	2.99	10	1
6:E:818:17F:C1X	6:E:818:17F:C23	0.50	2.87	10	1
6:B:214:17F:H56	6:B:219:17F:H37	0.50	1.82	17	2
2:D:275:LEU:HG	2:E:688:ARG:HD2	0.50	1.84	15	2
6:D:501:17F:H67	6:D:501:17F:C28	0.50	2.30	15	1
5:E:821:7Q9:O12	5:E:821:7Q9:C15	0.50	2.59	18	1
5:D:520:7Q9:C318	5:E:837:7Q9:C313	0.50	2.90	2	1
5:E:820:7Q9:C2	6:E:838:17F:H18	0.50	2.35	6	2
5:E:835:7Q9:C1	5:E:835:7Q9:O22	0.50	2.56	9	5
6:B:215:17F:C30	6:B:215:17F:H61	0.50	2.37	4	1
6:D:534:17F:H36	6:D:534:17F:C32	0.50	2.37	4	1
5:E:863:7Q9:C1	5:E:863:7Q9:O22	0.50	2.55	4	3
5:E:869:7Q9:O12	5:E:869:7Q9:C15	0.50	2.60	17	3
1:B:72:MET:HA	1:B:78:PHE:CZ	0.50	2.41	5	4
6:B:214:17F:H6	5:B:217:7Q9:C33	0.50	2.37	5	1
5:E:804:7Q9:C3	5:E:804:7Q9:O22	0.50	2.54	5	3
6:D:511:17F:H35	6:D:511:17F:H42	0.50	1.83	6	1
6:E:809:17F:C29	6:E:818:17F:H71	0.50	2.37	6	1
5:E:833:7Q9:C11	6:E:874:17F:O8	0.50	2.60	6	2
5:E:865:7Q9:O22	5:E:871:7Q9:C3	0.50	2.60	19	2
5:B:203:7Q9:C39	6:B:208:17F:H66	0.50	2.37	7	1
6:D:517:17F:N1	5:D:529:7Q9:O13	0.50	2.44	8	1
1:A:35:THR:OG1	3:A:201:GSP:O3G	0.50	2.30	15	4
2:D:309:GLN:HB2	6:D:527:17F:C35	0.50	2.37	9	1
6:D:510:17F:C19	6:D:516:17F:C10	0.50	2.74	9	1
6:D:510:17F:O10	6:D:527:17F:C19	0.50	2.57	10	2
1:B:46:ILE:HG23	1:B:157:TYR:HD1	0.50	1.67	14	1
2:E:682:LYS:HD2	5:E:867:7Q9:C31	0.50	2.37	14	1
6:E:811:17F:C18	5:E:815:7Q9:O14	0.50	2.60	16	1
5:D:545:7Q9:C15	5:D:545:7Q9:O31	0.50	2.60	17	1
5:D:514:7Q9:C14	5:D:519:7Q9:O22	0.50	2.60	19	1
6:D:510:17F:H62	5:D:524:7Q9:C314	0.50	2.37	20	1
5:E:806:7Q9:O21	5:E:806:7Q9:C31	0.50	2.60	10	11
5:E:825:7Q9:C11	5:E:844:7Q9:O32	0.50	2.60	1	1
5:E:843:7Q9:O32	5:E:843:7Q9:C2	0.50	2.57	5	7
6:E:838:17F:C19	6:E:838:17F:C31	0.50	2.87	15	12
5:E:844:7Q9:C318	5:E:864:7Q9:C312	0.50	2.90	2	2
5:D:549:7Q9:C13	5:D:549:7Q9:O14	0.50	2.60	14	10
5:E:846:7Q9:C14	5:E:846:7Q9:O12	0.50	2.59	10	4
5:B:206:7Q9:C33	5:B:212:7Q9:C32	0.50	2.89	6	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:B:210:7Q9:C313	6:B:215:17F:H10	0.50	2.37	7	1
5:D:503:7Q9:O13	5:D:505:7Q9:C1	0.50	2.59	18	2
5:E:863:7Q9:C22	5:E:867:7Q9:C23	0.50	2.90	7	2
5:D:512:7Q9:C13	6:D:528:17F:C4	0.50	2.90	12	2
5:D:547:7Q9:C21	5:D:547:7Q9:C12	0.50	2.90	13	2
6:E:817:17F:H50	5:E:820:7Q9:C318	0.50	2.35	8	1
6:E:807:17F:H18	6:E:807:17F:C1X	0.50	2.37	13	1
6:E:819:17F:H32	6:E:819:17F:C1X	0.50	2.37	13	1
5:E:869:7Q9:C1	5:E:869:7Q9:O22	0.50	2.57	20	3
6:E:838:17F:H9	6:E:856:17F:H9A	0.50	1.82	20	1
5:B:207:7Q9:C13	5:B:207:7Q9:O12	0.49	2.60	2	2
5:D:507:7Q9:C34	6:D:516:17F:H57	0.49	2.37	1	1
5:E:848:7Q9:C317	5:E:851:7Q9:C318	0.49	2.90	1	1
5:E:850:7Q9:C311	5:E:850:7Q9:C37	0.49	2.89	3	4
5:B:212:7Q9:C22	5:B:213:7Q9:O22	0.49	2.59	2	2
2:E:693:HIS:HB2	5:E:863:7Q9:C310	0.49	2.37	2	1
5:E:849:7Q9:O32	5:E:849:7Q9:O21	0.49	2.30	16	6
6:D:533:17F:C30	5:E:850:7Q9:C318	0.49	2.89	3	1
6:D:510:17F:H53	6:D:527:17F:H55	0.49	1.83	5	2
6:E:805:17F:H70	5:E:816:7Q9:C317	0.49	2.37	8	2
6:E:807:17F:C34	6:E:819:17F:H29	0.49	2.36	7	2
6:E:838:17F:H8A	6:E:856:17F:C2X	0.49	2.37	7	2
5:D:540:7Q9:C318	5:E:877:7Q9:C317	0.49	2.90	8	1
6:E:801:17F:H40	5:E:804:7Q9:C37	0.49	2.37	8	1
5:D:512:7Q9:C317	6:D:528:17F:H36	0.49	2.36	10	1
6:A:208:17F:C25	5:E:822:7Q9:C315	0.49	2.90	17	2
6:E:855:17F:H36	6:E:855:17F:H56	0.49	1.84	13	2
5:E:824:7Q9:C316	6:E:841:17F:H75	0.49	2.36	17	1
5:B:205:7Q9:C34	5:B:211:7Q9:C37	0.49	2.90	20	1
6:A:208:17F:H1A	5:A:209:7Q9:C12	0.49	2.38	1	1
5:B:217:7Q9:C13	5:D:522:7Q9:O14	0.49	2.60	1	3
6:D:510:17F:H18A	6:D:516:17F:C10	0.49	2.37	18	3
5:E:848:7Q9:O21	5:E:848:7Q9:C31	0.49	2.60	6	14
5:A:205:7Q9:C36	5:D:504:7Q9:C23	0.49	2.90	3	4
5:A:206:7Q9:O32	5:A:206:7Q9:O21	0.49	2.30	3	5
5:D:531:7Q9:O22	5:D:531:7Q9:C3	0.49	2.55	9	3
6:D:546:17F:O10	6:D:546:17F:H31	0.49	2.06	4	1
2:E:634:LEU:HG	5:E:862:7Q9:C312	0.49	2.37	5	2
6:D:510:17F:C5	6:D:516:17F:H9	0.49	2.37	8	1
1:B:126:ASP:CB	1:B:129:GLN:HB3	0.49	2.37	10	1
5:E:823:7Q9:O22	5:E:845:7Q9:C14	0.49	2.60	12	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:B:219:17F:C1X	6:B:219:17F:C20	0.49	2.90	13	1
5:E:837:7Q9:O32	6:E:841:17F:H44	0.49	2.08	14	1
6:E:809:17F:C30	6:E:809:17F:H64	0.49	2.37	16	1
5:D:538:7Q9:O32	5:D:538:7Q9:C12	0.49	2.60	1	2
6:A:214:17F:H52	5:E:840:7Q9:C311	0.49	2.38	5	2
5:B:212:7Q9:C22	5:B:213:7Q9:C2	0.49	2.90	2	1
5:E:815:7Q9:C34	5:E:815:7Q9:O31	0.49	2.60	19	9
1:B:158:THR:O	1:B:162:GLU:HG2	0.49	2.06	19	2
5:B:216:7Q9:C312	5:B:216:7Q9:C38	0.49	2.88	16	3
5:E:843:7Q9:C1	5:E:844:7Q9:C34	0.49	2.90	6	2
5:B:204:7Q9:C13	5:B:207:7Q9:C22	0.49	2.90	7	1
1:B:117:LYS:HB3	1:B:120:LEU:HD12	0.49	1.84	8	2
6:B:214:17F:C26	5:B:217:7Q9:C311	0.49	2.90	8	1
5:B:207:7Q9:C12	5:B:211:7Q9:O22	0.49	2.60	10	1
6:D:528:17F:O7	5:D:532:7Q9:C35	0.49	2.60	10	1
1:B:109:VAL:HB	1:B:111:MET:HE2	0.49	1.83	11	1
6:D:546:17F:H73	6:D:546:17F:H45	0.49	1.83	11	1
6:D:534:17F:H64	6:D:534:17F:C26	0.49	2.37	12	1
5:D:548:7Q9:C15	5:E:812:7Q9:C15	0.49	2.90	12	1
5:E:852:7Q9:C15	5:E:852:7Q9:O11	0.49	2.60	12	1
6:D:527:17F:H54	6:E:856:17F:H71	0.49	1.83	13	1
6:E:805:17F:O9	6:E:805:17F:C7	0.49	2.59	9	5
1:A:144:THR:HB	1:A:150:GLN:O	0.49	2.07	5	1
5:B:216:7Q9:O14	5:B:216:7Q9:C21	0.49	2.60	5	3
6:E:819:17F:O9	5:E:829:7Q9:C11	0.49	2.61	5	1
6:E:838:17F:H11A	6:E:856:17F:C2X	0.49	2.32	10	2
6:D:517:17F:H67	6:D:517:17F:H43	0.49	1.83	11	1
5:D:504:7Q9:C318	6:D:510:17F:H42	0.49	2.37	12	1
5:A:213:7Q9:O22	5:A:217:7Q9:C35	0.49	2.60	16	2
2:D:309:GLN:OE1	6:D:527:17F:H58	0.49	2.08	16	1
5:B:206:7Q9:C14	5:B:206:7Q9:O12	0.49	2.60	3	1
6:E:807:17F:H33	6:E:819:17F:C12	0.49	2.38	3	1
6:E:817:17F:H47	6:E:817:17F:C42	0.49	2.38	12	3
6:B:215:17F:H54	6:B:215:17F:C34	0.49	2.32	8	3
2:D:374:LEU:HD11	5:D:529:7Q9:C318	0.49	2.37	4	2
6:D:510:17F:C21	6:D:511:17F:C31	0.49	2.90	10	2
2:E:634:LEU:HD13	5:E:878:7Q9:C316	0.49	2.37	16	2
6:E:809:17F:C27	6:E:818:17F:H71	0.49	2.38	6	1
6:D:501:17F:O1	6:D:501:17F:C19	0.49	2.58	10	1
5:D:519:7Q9:C314	5:D:540:7Q9:C316	0.49	2.91	10	2
6:E:819:17F:H61	5:E:852:7Q9:C311	0.49	2.38	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:SER:HB2	3:A:201:GSP:O2'	0.49	2.07	14	1
6:D:533:17F:H57	6:D:533:17F:C17	0.49	2.35	14	1
5:D:537:7Q9:C34	6:D:546:17F:H73	0.49	2.37	14	1
6:D:510:17F:C35	5:D:524:7Q9:C313	0.49	2.90	15	2
6:D:534:17F:H76	2:E:692:TYR:HE2	0.49	1.67	17	1
6:E:838:17F:H52	5:E:857:7Q9:C313	0.49	2.37	18	1
6:D:501:17F:H34	6:D:501:17F:C24	0.49	2.37	20	1
5:E:837:7Q9:C314	5:E:866:7Q9:C318	0.49	2.91	1	5
6:D:510:17F:C8	6:D:516:17F:C18	0.49	2.91	2	2
5:D:503:7Q9:O13	6:D:511:17F:H5	0.49	2.07	3	1
6:D:511:17F:C7	6:D:511:17F:O9	0.49	2.60	4	3
5:D:537:7Q9:C31	6:D:546:17F:H10A	0.49	2.38	5	1
6:E:874:17F:H49	6:E:874:17F:C41	0.49	2.38	5	1
5:E:802:7Q9:C316	6:E:809:17F:H64	0.49	2.36	6	1
2:D:377:ARG:HD2	2:E:586:MET:HB3	0.49	1.83	8	1
6:E:807:17F:H60	6:E:819:17F:H29	0.49	1.83	8	1
6:E:838:17F:C31	6:E:838:17F:H35	0.49	2.38	8	1
5:D:513:7Q9:O32	5:D:513:7Q9:O21	0.49	2.31	9	1
6:D:516:17F:C2X	6:D:527:17F:C22	0.49	2.90	10	1
5:E:857:7Q9:C33	6:E:874:17F:H30	0.49	2.38	10	1
1:B:2:THR:HB	1:B:4:TYR:CE2	0.49	2.42	13	1
5:E:853:7Q9:C13	5:E:853:7Q9:P	0.49	3.01	13	2
6:D:517:17F:H48	6:D:517:17F:C39	0.49	2.38	18	1
2:E:620:GLU:HA	5:E:858:7Q9:C310	0.49	2.37	20	1
5:D:509:7Q9:C1	5:D:509:7Q9:C31	0.49	2.90	16	2
5:D:504:7Q9:C3	6:D:516:17F:O10	0.49	2.60	2	1
6:E:801:17F:H4	6:E:801:17F:C1	0.49	2.38	2	1
5:A:203:7Q9:C14	5:A:203:7Q9:O13	0.49	2.60	6	7
6:D:528:17F:O10	6:D:528:17F:O7	0.49	2.30	3	6
5:E:837:7Q9:C34	6:E:841:17F:H44	0.49	2.37	10	2
5:E:854:7Q9:C14	5:E:854:7Q9:P	0.49	3.01	20	4
5:D:506:7Q9:O11	5:D:506:7Q9:O22	0.49	2.30	6	3
5:E:833:7Q9:C2	5:E:833:7Q9:O13	0.49	2.60	12	5
5:D:506:7Q9:C318	5:D:520:7Q9:C318	0.49	2.91	8	1
5:D:508:7Q9:O22	5:D:508:7Q9:C3	0.49	2.58	18	3
5:E:837:7Q9:C15	5:E:837:7Q9:O11	0.49	2.60	10	1
2:D:334:LEU:CB	5:D:532:7Q9:C312	0.49	2.91	13	2
5:E:833:7Q9:O22	5:E:833:7Q9:O31	0.49	2.31	18	1
5:E:843:7Q9:C312	5:E:859:7Q9:C313	0.49	2.91	19	1
6:D:534:17F:C36	6:D:534:17F:C32	0.49	2.79	20	1
6:E:870:17F:H35	6:E:870:17F:C32	0.49	2.36	20	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:807:17F:C12	6:E:807:17F:C32	0.49	2.90	15	4
5:E:854:7Q9:C32	5:E:858:7Q9:C35	0.49	2.91	1	4
5:B:203:7Q9:O14	5:B:206:7Q9:C22	0.49	2.61	2	1
6:E:801:17F:H10	6:E:801:17F:C18	0.49	2.38	2	1
5:E:824:7Q9:C34	6:E:841:17F:H18A	0.49	2.37	3	2
5:E:846:7Q9:C310	5:E:847:7Q9:C313	0.49	2.91	3	1
6:D:516:17F:C22	6:D:516:17F:C27	0.49	2.57	5	1
6:E:819:17F:C4	6:E:819:17F:O8	0.49	2.61	5	1
2:E:634:LEU:HD22	5:E:878:7Q9:C35	0.49	2.37	20	2
5:E:862:7Q9:C11	5:E:878:7Q9:C14	0.49	2.91	19	2
6:E:809:17F:C33	6:E:818:17F:H69	0.49	2.37	13	3
2:D:388:ARG:HH11	2:E:575:LEU:HG	0.49	1.67	16	1
5:D:506:7Q9:C34	6:D:517:17F:H34	0.49	2.37	18	1
5:A:210:7Q9:P	5:A:215:7Q9:C13	0.49	3.01	19	1
5:B:212:7Q9:C31	5:B:212:7Q9:C1	0.49	2.91	2	1
5:D:514:7Q9:O12	5:D:514:7Q9:C15	0.49	2.61	10	5
6:D:533:17F:H63	6:D:533:17F:C21	0.49	2.38	4	3
5:E:861:7Q9:C2	5:E:876:7Q9:C11	0.49	2.91	2	2
6:A:208:17F:H41	5:E:823:7Q9:C316	0.49	2.37	3	1
5:D:503:7Q9:C14	6:D:511:17F:H6	0.49	2.38	4	1
5:B:204:7Q9:C1	5:B:204:7Q9:O22	0.49	2.58	16	4
5:E:802:7Q9:C38	6:E:807:17F:H42	0.49	2.38	5	1
6:E:809:17F:H51	6:E:818:17F:C42	0.49	2.36	13	3
5:E:843:7Q9:O22	5:E:844:7Q9:C35	0.49	2.61	5	1
5:D:530:7Q9:O32	5:D:530:7Q9:O21	0.49	2.30	20	4
5:A:209:7Q9:O32	5:A:209:7Q9:C2	0.49	2.59	16	5
6:E:801:17F:C34	5:E:803:7Q9:C39	0.49	2.91	7	1
5:A:211:7Q9:C14	6:B:214:17F:O5	0.49	2.60	8	2
6:B:214:17F:O8	6:B:214:17F:O9	0.49	2.31	10	1
5:A:210:7Q9:C318	5:E:826:7Q9:C312	0.49	2.91	11	1
6:A:214:17F:H75	5:E:839:7Q9:C315	0.49	2.38	11	1
2:D:272:TRP:HZ3	6:D:534:17F:H71	0.49	1.68	11	1
6:E:818:17F:C39	6:E:818:17F:H45	0.49	2.38	11	1
6:D:510:17F:C37	6:D:511:17F:H74	0.49	2.38	14	1
1:B:117:LYS:HE2	3:B:201:GSP:N3	0.49	2.23	17	2
6:B:214:17F:H56	6:B:214:17F:H62	0.49	1.84	19	1
5:E:812:7Q9:C1	5:E:815:7Q9:C2	0.49	2.90	19	1
6:E:838:17F:H33	6:E:838:17F:C2X	0.49	2.30	19	1
5:A:205:7Q9:C13	5:A:205:7Q9:C21	0.49	2.90	5	2
6:D:511:17F:C11	5:D:526:7Q9:O14	0.49	2.61	1	3
5:D:538:7Q9:O14	5:D:538:7Q9:C21	0.49	2.61	6	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:540:7Q9:O22	5:D:540:7Q9:C12	0.49	2.61	11	5
5:E:814:7Q9:O21	5:E:814:7Q9:C31	0.49	2.61	4	17
1:A:14:VAL:HG23	1:A:16:LYS:HG3	0.49	1.83	2	2
5:D:523:7Q9:C3	5:D:535:7Q9:O22	0.49	2.61	2	4
5:A:213:7Q9:C14	5:A:213:7Q9:C22	0.49	2.91	5	1
6:E:809:17F:C33	6:E:818:17F:C39	0.49	2.84	6	1
5:A:205:7Q9:C1	5:B:204:7Q9:C14	0.49	2.91	7	1
6:A:214:17F:H11	6:A:214:17F:H58	0.49	1.84	10	2
1:B:83:ALA:HB3	1:B:86:ASN:HB3	0.49	1.84	8	1
5:D:537:7Q9:C12	5:D:537:7Q9:O13	0.49	2.60	11	3
5:A:215:7Q9:C13	5:A:216:7Q9:O14	0.49	2.60	11	1
6:E:855:17F:H53	5:E:867:7Q9:C317	0.49	2.37	11	1
6:D:501:17F:H34	6:D:501:17F:C21	0.49	2.35	16	2
5:E:837:7Q9:C14	6:E:841:17F:H5	0.49	2.38	13	1
6:E:838:17F:H9A	6:E:838:17F:C33	0.49	2.37	19	1
2:D:389:LEU:HD11	5:D:540:7Q9:C313	0.48	2.38	1	2
2:E:594:LYS:HE2	5:E:861:7Q9:C318	0.48	2.38	1	1
6:E:817:17F:H61	5:E:826:7Q9:C37	0.48	2.38	1	1
6:E:828:17F:C11	5:E:832:7Q9:C38	0.48	2.91	19	4
5:D:504:7Q9:C33	5:D:507:7Q9:O32	0.48	2.61	2	2
6:E:807:17F:H56	6:E:819:17F:H30	0.48	1.85	2	1
6:D:533:17F:C21	6:D:533:17F:C35	0.48	2.90	3	1
6:A:208:17F:H42	5:A:209:7Q9:C39	0.48	2.37	4	1
5:D:513:7Q9:O21	5:D:513:7Q9:C31	0.48	2.60	7	4
6:E:805:17F:H56	5:E:810:7Q9:O22	0.48	2.08	5	1
1:B:35:THR:HA	1:B:38:ASP:OD2	0.48	2.08	6	1
2:D:414:LEU:HD11	2:E:739:LYS:HB3	0.48	1.85	8	1
2:D:389:LEU:HD22	5:D:540:7Q9:C314	0.48	2.37	9	1
6:E:818:17F:O8	6:E:818:17F:P1	0.48	2.71	9	1
6:D:510:17F:H10A	6:D:516:17F:H34	0.48	1.82	10	1
6:E:818:17F:C42	6:E:818:17F:C27	0.48	2.91	10	1
5:B:218:7Q9:C33	5:B:218:7Q9:O14	0.48	2.61	13	3
5:A:209:7Q9:C316	5:E:822:7Q9:C313	0.48	2.91	13	1
6:D:501:17F:H6	5:D:506:7Q9:C13	0.48	2.38	13	2
6:D:501:17F:H76	6:E:818:17F:C29	0.48	2.33	14	1
5:E:806:7Q9:O22	5:E:806:7Q9:C1	0.48	2.59	17	2
5:E:851:7Q9:C12	5:E:851:7Q9:O22	0.48	2.61	15	1
6:B:214:17F:H33	6:B:219:17F:C12	0.48	2.37	17	1
6:A:214:17F:O4	5:D:539:7Q9:C14	0.48	2.61	18	1
1:A:68:ARG:HG3	1:A:71:TYR:OH	0.48	2.07	19	1
5:B:217:7Q9:C15	6:B:219:17F:H6A	0.48	2.37	19	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:517:17F:C1Z	6:D:517:17F:H63	0.48	2.37	19	1
5:E:858:7Q9:O32	5:E:858:7Q9:O21	0.48	2.32	20	11
5:D:521:7Q9:O13	5:D:521:7Q9:C12	0.48	2.61	10	4
1:B:15:GLY:HA3	1:B:116:ASN:ND2	0.48	2.23	3	2
5:E:830:7Q9:C39	5:E:830:7Q9:C22	0.48	2.91	16	8
6:B:208:17F:H43	6:B:208:17F:C34	0.48	2.39	5	1
6:D:516:17F:H42	6:D:527:17F:H47	0.48	1.84	6	1
5:D:549:7Q9:O32	5:D:549:7Q9:C2	0.48	2.59	19	2
5:E:864:7Q9:O32	5:E:864:7Q9:C2	0.48	2.56	15	6
1:A:27:HIS:HE1	1:B:127:THR:HG21	0.48	1.67	7	1
5:E:848:7Q9:C36	5:E:851:7Q9:C33	0.48	2.90	16	4
6:A:208:17F:H64	6:B:208:17F:H72	0.48	1.83	10	1
5:E:852:7Q9:O11	5:E:852:7Q9:C12	0.48	2.61	10	2
6:D:527:17F:H11A	5:D:535:7Q9:C37	0.48	2.38	12	1
5:E:851:7Q9:C36	5:E:851:7Q9:C311	0.48	2.91	12	1
5:E:869:7Q9:C22	6:E:872:17F:C10	0.48	2.86	12	1
6:D:511:17F:H61	6:D:511:17F:H36	0.48	1.84	14	1
6:E:856:17F:H70	6:E:874:17F:C33	0.48	2.37	14	1
6:E:805:17F:H42	5:E:812:7Q9:C313	0.48	2.38	16	1
6:E:818:17F:C10	6:E:819:17F:H12A	0.48	2.34	16	1
5:D:505:7Q9:C310	6:D:528:17F:H41	0.48	2.39	17	1
5:D:514:7Q9:O12	5:D:514:7Q9:C21	0.48	2.61	18	1
1:A:38:ASP:O	1:A:56:LEU:HA	0.48	2.09	1	1
5:B:204:7Q9:O11	5:B:204:7Q9:O31	0.48	2.31	10	7
6:B:219:17F:O10	5:D:522:7Q9:C1	0.48	2.62	8	2
6:B:214:17F:C1Z	5:B:220:7Q9:C32	0.48	2.90	2	1
5:D:544:7Q9:O22	5:D:544:7Q9:O11	0.48	2.31	15	10
5:E:804:7Q9:C316	6:E:811:17F:H52	0.48	2.38	2	1
5:E:854:7Q9:C14	5:E:854:7Q9:O11	0.48	2.61	9	7
6:D:533:17F:O7	6:D:533:17F:O6	0.48	2.32	20	6
5:E:820:7Q9:C14	5:E:820:7Q9:P	0.48	3.02	7	8
5:D:507:7Q9:O32	6:D:516:17F:H20	0.48	2.08	6	1
5:E:850:7Q9:C39	6:E:870:17F:H20	0.48	2.38	6	1
5:A:205:7Q9:C318	6:E:817:17F:H55	0.48	2.38	7	1
2:D:389:LEU:HD11	5:D:540:7Q9:C314	0.48	2.38	7	1
5:E:823:7Q9:O22	5:E:845:7Q9:C13	0.48	2.61	7	3
5:A:209:7Q9:C318	5:E:822:7Q9:C312	0.48	2.90	15	3
6:E:841:17F:H9A	5:E:876:7Q9:P	0.48	2.47	10	1
6:A:208:17F:C37	6:B:208:17F:H72	0.48	2.38	11	1
6:B:215:17F:O2	5:D:506:7Q9:C13	0.48	2.60	11	1
2:D:272:TRP:CZ3	6:D:534:17F:H71	0.48	2.42	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:823:7Q9:C315	5:E:845:7Q9:C315	0.48	2.92	11	1
5:E:824:7Q9:C36	6:E:841:17F:H34	0.48	2.38	11	1
6:B:208:17F:H43	6:B:208:17F:H33	0.48	1.85	13	1
6:D:501:17F:O7	5:D:506:7Q9:C15	0.48	2.61	13	1
5:E:848:7Q9:C315	5:E:851:7Q9:C314	0.48	2.91	14	2
2:D:286:MET:HB3	2:E:677:ARG:HD3	0.48	1.83	16	1
5:E:804:7Q9:C38	5:E:804:7Q9:C312	0.48	2.90	16	1
6:D:510:17F:H48	6:D:510:17F:H61	0.48	1.84	20	1
1:A:33:ASP:O	3:A:201:GSP:S1G	0.48	2.70	1	2
5:A:215:7Q9:C36	6:D:534:17F:H38	0.48	2.38	1	1
6:D:511:17F:O4	5:D:526:7Q9:C13	0.48	2.62	1	3
5:B:220:7Q9:C314	6:D:533:17F:H47	0.48	2.38	2	1
6:E:809:17F:O7	6:E:809:17F:C17	0.48	2.62	2	8
6:E:856:17F:H57	6:E:856:17F:C2X	0.48	2.38	2	1
5:A:204:7Q9:O32	6:B:208:17F:H12	0.48	2.08	3	1
5:E:820:7Q9:C3	6:E:838:17F:O9	0.48	2.62	3	1
6:E:838:17F:H43	5:E:857:7Q9:C310	0.48	2.39	3	3
6:D:533:17F:H9A	6:D:533:17F:C33	0.48	2.38	4	1
5:E:810:7Q9:O22	5:E:810:7Q9:C1	0.48	2.60	9	4
5:E:826:7Q9:C318	5:E:840:7Q9:C310	0.48	2.92	4	1
6:E:841:17F:H39	6:E:841:17F:C1X	0.48	2.36	18	4
6:D:510:17F:H72	6:E:856:17F:H51	0.48	1.84	5	1
6:D:510:17F:O10	5:D:524:7Q9:C3	0.48	2.60	6	1
5:D:526:7Q9:C38	5:D:526:7Q9:C22	0.48	2.91	18	2
2:E:674:LEU:CD2	6:E:855:17F:H12	0.48	2.24	11	3
5:D:513:7Q9:C2	6:D:528:17F:H10	0.48	2.39	7	1
6:D:534:17F:H64	6:D:534:17F:H29	0.48	1.84	7	1
1:B:117:LYS:HE2	3:B:201:GSP:C6	0.48	2.43	8	1
6:D:510:17F:O7	6:D:516:17F:C11	0.48	2.60	8	2
6:E:801:17F:H51	5:E:806:7Q9:C316	0.48	2.38	8	1
5:E:865:7Q9:O22	5:E:865:7Q9:C3	0.48	2.56	19	3
1:A:77:GLY:HA3	1:A:163:ILE:HD11	0.48	1.85	9	1
6:E:817:17F:H9	5:E:833:7Q9:C33	0.48	2.38	9	2
5:E:848:7Q9:C310	5:E:851:7Q9:C37	0.48	2.91	20	3
6:D:511:17F:C3	5:D:526:7Q9:C12	0.48	2.92	10	2
5:D:504:7Q9:C3	6:D:516:17F:C18	0.48	2.92	13	1
5:E:844:7Q9:C14	5:E:864:7Q9:C22	0.48	2.91	13	2
6:D:510:17F:H60	6:D:510:17F:C24	0.48	2.38	14	1
6:E:856:17F:H78	6:E:874:17F:C34	0.48	2.34	14	1
6:D:501:17F:H74	6:E:809:17F:H54	0.48	1.84	15	1
5:D:512:7Q9:C318	6:D:528:17F:H40	0.48	2.39	20	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:533:17F:H75	6:D:533:17F:C28	0.48	2.20	17	1
6:E:874:17F:H1A	6:E:874:17F:O9	0.48	2.08	18	1
2:D:421:VAL:HG21	2:E:735:GLU:HG2	0.48	1.84	20	1
5:B:203:7Q9:C31	6:B:208:17F:H6	0.48	2.38	1	2
5:B:211:7Q9:C311	6:D:501:17F:C36	0.48	2.91	9	3
5:E:814:7Q9:C318	6:E:828:17F:H61	0.48	2.39	1	1
5:E:830:7Q9:C1	5:E:830:7Q9:O22	0.48	2.56	5	4
5:A:205:7Q9:C1	5:A:205:7Q9:O22	0.48	2.56	11	2
6:D:511:17F:C42	6:D:511:17F:H54	0.48	2.38	2	2
6:E:818:17F:O9	6:E:818:17F:C20	0.48	2.61	2	1
6:D:511:17F:H20A	5:D:524:7Q9:C34	0.48	2.38	10	2
5:D:543:7Q9:C37	5:D:545:7Q9:C38	0.48	2.92	4	1
5:D:503:7Q9:C14	5:D:505:7Q9:O14	0.48	2.62	7	3
6:E:801:17F:H50	6:E:801:17F:H65	0.48	1.84	5	1
5:B:205:7Q9:C12	5:B:210:7Q9:O32	0.48	2.62	6	1
5:E:827:7Q9:C22	5:E:830:7Q9:C31	0.48	2.92	6	1
1:B:84:ILE:HD13	1:B:118:CYS:HA	0.48	1.85	17	4
6:E:818:17F:C42	6:E:818:17F:H48	0.48	2.39	9	1
6:E:818:17F:C1	5:E:837:7Q9:C11	0.48	2.84	18	2
2:E:719:LEU:HB2	2:E:720:PRO:HD3	0.48	1.84	4	5
6:E:838:17F:H35	6:E:838:17F:H33	0.48	1.83	8	2
5:E:846:7Q9:O13	5:E:846:7Q9:C12	0.48	2.61	17	14
6:D:510:17F:C1X	6:D:516:17F:H8A	0.48	2.38	3	3
5:B:220:7Q9:C317	6:D:533:17F:H52	0.48	2.38	5	1
5:E:848:7Q9:C22	5:E:852:7Q9:C14	0.48	2.92	11	3
5:A:211:7Q9:O22	5:A:211:7Q9:C3	0.48	2.57	12	5
1:B:84:ILE:CD1	1:B:118:CYS:HA	0.48	2.38	16	6
6:D:510:17F:H29	6:D:516:17F:C8	0.48	2.38	6	1
6:D:534:17F:C34	6:D:534:17F:H44	0.48	2.39	6	1
6:E:807:17F:C30	6:E:809:17F:H53	0.48	2.38	6	1
5:D:515:7Q9:O22	5:D:519:7Q9:C13	0.48	2.61	8	1
6:D:501:17F:C28	6:D:501:17F:H66	0.48	2.39	9	1
6:E:817:17F:C9	5:E:833:7Q9:C33	0.48	2.91	9	1
6:E:856:17F:O5	6:E:874:17F:H4	0.48	2.08	11	1
5:B:216:7Q9:C15	5:D:515:7Q9:O14	0.48	2.61	12	1
6:D:534:17F:H64	6:D:534:17F:C25	0.48	2.38	12	1
6:D:546:17F:C37	6:D:546:17F:H41	0.48	2.39	12	1
3:A:201:GSP:O5'	3:A:201:GSP:C2'	0.48	2.61	17	3
2:D:337:LEU:HD22	2:E:626:LEU:HB3	0.48	1.84	17	1
1:B:131:GLN:HB3	1:B:135:ARG:NH2	0.48	2.23	18	1
5:D:507:7Q9:C316	6:E:817:17F:H46	0.48	2.38	19	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:337:LEU:HG	2:E:626:LEU:HD22	0.48	1.83	20	1
5:D:549:7Q9:C15	6:E:856:17F:O6	0.48	2.62	1	1
6:E:819:17F:O9	6:E:819:17F:C20	0.48	2.60	2	1
5:E:822:7Q9:O31	5:E:822:7Q9:C21	0.48	2.61	15	10
6:E:819:17F:C6	5:E:836:7Q9:O22	0.48	2.62	3	1
5:B:210:7Q9:C35	5:B:210:7Q9:O14	0.48	2.62	5	2
6:E:856:17F:H29	6:E:874:17F:H60	0.48	1.84	5	1
6:E:872:17F:H56	6:E:872:17F:H39	0.48	1.85	5	2
6:D:517:17F:H67	6:D:517:17F:C25	0.48	2.36	6	2
6:A:208:17F:C38	5:E:804:7Q9:C318	0.48	2.92	7	1
5:D:541:7Q9:O32	5:D:541:7Q9:C2	0.48	2.58	9	4
5:E:833:7Q9:O32	5:E:834:7Q9:C14	0.48	2.61	7	1
5:B:209:7Q9:C3	5:D:505:7Q9:C1	0.48	2.92	9	1
5:E:821:7Q9:P	5:E:821:7Q9:O21	0.48	2.71	9	2
6:B:214:17F:H66	6:B:219:17F:H43	0.48	1.84	10	1
6:D:510:17F:H9	6:D:516:17F:H30	0.48	1.85	11	1
5:E:820:7Q9:C315	6:E:828:17F:C29	0.48	2.92	12	1
6:E:838:17F:H51	6:E:874:17F:H55	0.48	1.86	13	1
6:B:208:17F:H60	5:B:212:7Q9:C34	0.48	2.39	19	1
5:A:211:7Q9:C32	5:A:213:7Q9:C36	0.48	2.92	20	1
1:B:13:GLY:CA	3:B:201:GSP:H5'1	0.48	2.38	20	1
2:D:333:LYS:HD3	5:D:532:7Q9:C314	0.48	2.39	20	1
6:B:215:17F:H10A	6:B:215:17F:C35	0.48	2.32	12	2
5:D:507:7Q9:O32	5:D:507:7Q9:C2	0.48	2.61	2	6
5:D:536:7Q9:O14	5:D:536:7Q9:O21	0.48	2.32	2	2
5:E:852:7Q9:C22	5:E:878:7Q9:C22	0.48	2.92	2	3
1:B:123:ARG:HD3	1:B:125:VAL:O	0.48	2.09	3	4
5:D:512:7Q9:O13	5:D:532:7Q9:C14	0.48	2.62	3	1
6:D:516:17F:H47	6:D:516:17F:C33	0.48	2.38	3	1
5:E:840:7Q9:O22	5:E:873:7Q9:C37	0.48	2.61	19	3
5:E:832:7Q9:C23	6:E:838:17F:O2	0.48	2.62	4	1
6:A:214:17F:O8	6:A:214:17F:H10	0.48	2.09	6	2
6:B:214:17F:C26	5:B:217:7Q9:C37	0.48	2.92	7	1
5:D:531:7Q9:C39	5:D:540:7Q9:C318	0.48	2.91	7	1
2:D:255:SER:O	2:D:259:LYS:HG2	0.48	2.09	8	1
5:E:832:7Q9:O22	5:E:832:7Q9:C1	0.48	2.57	12	4
5:E:837:7Q9:C314	6:E:841:17F:H49	0.48	2.39	9	1
6:D:511:17F:C29	6:E:828:17F:H78	0.48	2.39	10	1
6:E:818:17F:H45	6:E:818:17F:H70	0.48	1.83	11	1
5:E:877:7Q9:O32	5:E:877:7Q9:C2	0.48	2.52	12	2
6:D:517:17F:H52	6:D:517:17F:H69	0.48	1.86	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:528:17F:O7	5:D:532:7Q9:C37	0.48	2.62	13	1
6:E:805:17F:C27	5:E:812:7Q9:C314	0.48	2.84	13	2
6:E:818:17F:H20	5:E:837:7Q9:C12	0.48	2.39	14	1
6:E:819:17F:H8A	6:E:819:17F:H32	0.48	1.85	16	1
6:A:214:17F:C30	5:E:840:7Q9:C317	0.48	2.91	19	1
6:E:809:17F:H32	6:E:818:17F:C38	0.48	2.33	19	1
6:A:214:17F:H52	5:E:840:7Q9:C313	0.48	2.39	7	2
6:D:527:17F:O1	6:D:527:17F:H20A	0.48	2.08	11	2
5:A:204:7Q9:O22	5:A:204:7Q9:C1	0.48	2.59	4	3
5:E:848:7Q9:C1	5:E:848:7Q9:O22	0.48	2.57	19	6
5:E:863:7Q9:C15	5:E:863:7Q9:P	0.48	3.02	16	7
6:B:214:17F:O10	6:B:219:17F:C8	0.48	2.62	3	1
5:E:829:7Q9:C2	5:E:829:7Q9:O13	0.48	2.62	3	3
6:E:838:17F:H56	6:E:838:17F:H12A	0.48	1.83	3	1
6:D:510:17F:C4	6:D:516:17F:H4	0.48	2.39	6	1
5:E:845:7Q9:C37	6:E:870:17F:H54	0.48	2.38	7	1
5:D:515:7Q9:O22	5:D:515:7Q9:C1	0.48	2.55	17	2
5:E:857:7Q9:C1	5:E:857:7Q9:O22	0.48	2.57	12	3
6:D:534:17F:H11	5:D:539:7Q9:C36	0.48	2.39	10	1
6:D:501:17F:H51	6:D:501:17F:C39	0.48	2.39	12	1
6:E:838:17F:H33	6:E:838:17F:H39	0.48	1.85	12	2
5:E:853:7Q9:O14	5:E:853:7Q9:C12	0.48	2.62	13	3
5:D:544:7Q9:C22	6:D:546:17F:C19	0.48	2.90	18	1
2:D:327:GLN:O	2:D:331:ARG:HB2	0.48	2.08	20	1
6:D:516:17F:H77	6:E:838:17F:C42	0.48	2.39	20	1
5:E:816:7Q9:O21	5:E:816:7Q9:C31	0.48	2.62	20	1
5:B:207:7Q9:C15	5:B:211:7Q9:O13	0.48	2.61	1	1
5:B:207:7Q9:O13	5:B:207:7Q9:C12	0.48	2.61	13	13
2:E:619:VAL:HA	2:E:622:LEU:HD12	0.48	1.86	12	4
5:E:808:7Q9:C38	6:E:811:17F:H37	0.48	2.39	2	1
5:E:850:7Q9:C316	6:E:870:17F:H61	0.48	2.39	10	2
6:D:516:17F:H41	6:D:527:17F:C23	0.48	2.38	19	2
6:A:208:17F:H42	5:A:209:7Q9:C310	0.48	2.39	4	2
5:B:220:7Q9:O14	5:B:220:7Q9:C13	0.48	2.62	5	1
6:D:534:17F:C36	6:D:534:17F:H30	0.48	2.39	5	2
5:E:820:7Q9:O22	5:E:820:7Q9:C1	0.48	2.57	5	3
6:E:838:17F:H65	6:E:838:17F:C10	0.48	2.39	5	1
5:B:210:7Q9:C22	5:B:210:7Q9:C38	0.48	2.91	6	1
6:D:534:17F:H54	6:D:534:17F:C35	0.48	2.39	6	2
2:E:558:SER:O	2:E:561:ARG:HD3	0.48	2.08	6	1
6:D:533:17F:C41	6:D:533:17F:H44	0.48	2.39	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:815:7Q9:C317	5:E:830:7Q9:C318	0.48	2.91	8	1
6:E:870:17F:C10	5:E:871:7Q9:O14	0.48	2.62	8	1
6:D:501:17F:C2X	6:D:501:17F:C24	0.48	2.91	12	2
6:D:510:17F:C41	6:E:856:17F:H44	0.48	2.39	9	1
2:D:422:LEU:HD13	5:E:875:7Q9:C317	0.48	2.39	15	3
1:B:59:ALA:HA	3:B:201:GSP:S1G	0.48	2.49	13	1
5:D:506:7Q9:C21	5:D:506:7Q9:C11	0.48	2.91	13	1
5:D:509:7Q9:O22	5:D:509:7Q9:O11	0.48	2.32	16	1
6:D:510:17F:H78	6:D:510:17F:H53	0.48	1.85	16	1
1:B:97:ARG:HG3	1:B:111:MET:HE1	0.48	1.86	18	1
6:B:214:17F:C37	6:B:219:17F:C27	0.48	2.91	18	1
5:D:502:7Q9:C23	5:D:508:7Q9:C23	0.48	2.92	19	1
1:B:6:LEU:HD22	1:B:159:LEU:HG	0.48	1.86	20	1
1:A:34:PRO:HG3	3:A:201:GSP:H5'2	0.47	1.86	2	1
5:A:213:7Q9:C23	5:A:213:7Q9:C15	0.47	2.92	2	1
5:E:820:7Q9:C3	6:E:838:17F:H18	0.47	2.38	2	1
6:E:801:17F:H45	6:E:801:17F:H63	0.47	1.86	4	1
6:D:501:17F:H10	6:D:501:17F:C35	0.47	2.38	5	1
6:E:872:17F:H44	6:E:872:17F:H60	0.47	1.86	5	1
6:A:208:17F:H69	6:B:208:17F:H73	0.47	1.86	6	1
6:D:517:17F:H48	6:D:517:17F:C38	0.47	2.38	6	1
5:D:541:7Q9:C1	5:D:541:7Q9:O22	0.47	2.56	7	2
5:E:868:7Q9:O13	5:E:873:7Q9:C13	0.47	2.62	8	1
6:D:510:17F:H10A	6:D:516:17F:H59	0.47	1.84	9	1
5:E:802:7Q9:C38	6:E:807:17F:H41	0.47	2.39	13	4
6:B:208:17F:H62	6:B:208:17F:C2X	0.47	2.38	10	1
6:E:819:17F:C12	5:E:829:7Q9:O14	0.47	2.62	10	1
6:D:516:17F:H1A	6:D:516:17F:C5	0.47	2.38	11	1
6:E:819:17F:C18	5:E:852:7Q9:C34	0.47	2.92	11	1
1:B:84:ILE:HD11	1:B:118:CYS:HA	0.47	1.86	12	2
6:D:501:17F:H11	5:D:506:7Q9:C23	0.47	2.39	12	1
5:D:503:7Q9:C23	6:D:510:17F:H35	0.47	2.38	12	1
6:E:838:17F:P1	6:E:838:17F:HN1	0.47	2.32	14	2
5:E:863:7Q9:O12	5:E:873:7Q9:C32	0.47	2.61	14	1
6:D:534:17F:C7	6:D:534:17F:O9	0.47	2.62	16	1
6:D:517:17F:H78	5:E:842:7Q9:C318	0.47	2.39	17	1
6:E:855:17F:H58	6:E:855:17F:H40	0.47	1.84	17	1
5:A:204:7Q9:C311	6:A:208:17F:H63	0.47	2.39	20	1
5:D:514:7Q9:P	5:D:514:7Q9:C15	0.47	3.02	20	1
5:A:217:7Q9:C32	6:D:546:17F:C2X	0.47	2.91	1	1
5:D:531:7Q9:C1	5:D:531:7Q9:C31	0.47	2.92	19	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:532:7Q9:C15	5:D:532:7Q9:O13	0.47	2.62	1	4
5:E:837:7Q9:O32	6:E:841:17F:H32	0.47	2.09	1	1
5:E:869:7Q9:C14	6:E:872:17F:O4	0.47	2.62	1	3
6:D:511:17F:C23	6:D:511:17F:C37	0.47	2.92	12	2
2:D:414:LEU:HD21	2:E:740:LEU:HD23	0.47	1.85	10	4
1:B:72:MET:SD	1:B:99:GLN:HG2	0.47	2.49	5	1
5:E:816:7Q9:C12	5:E:831:7Q9:O13	0.47	2.62	7	3
5:E:845:7Q9:O32	5:E:845:7Q9:C2	0.47	2.57	11	3
5:E:850:7Q9:C15	5:E:850:7Q9:P	0.47	3.02	16	4
5:D:503:7Q9:C37	5:D:505:7Q9:C37	0.47	2.92	6	1
5:E:876:7Q9:O32	5:E:876:7Q9:O21	0.47	2.31	15	4
6:B:214:17F:C17	6:B:214:17F:O8	0.47	2.62	8	1
1:A:57:ASP:OD2	3:A:201:GSP:O3G	0.47	2.32	15	2
5:D:507:7Q9:C311	6:D:516:17F:H50	0.47	2.40	9	1
1:A:117:LYS:HB3	1:A:120:LEU:HD12	0.47	1.85	13	1
6:E:838:17F:H71	6:E:874:17F:H53	0.47	1.86	14	1
5:E:846:7Q9:C13	6:E:872:17F:O4	0.47	2.62	14	1
1:A:14:VAL:HA	1:A:83:ALA:HB2	0.47	1.86	19	1
2:E:733:LEU:HD12	5:E:875:7Q9:C311	0.47	2.38	19	1
5:B:212:7Q9:C12	5:B:217:7Q9:O22	0.47	2.62	2	1
5:D:504:7Q9:O22	5:D:504:7Q9:C1	0.47	2.58	7	4
6:D:528:17F:H40	5:D:532:7Q9:C316	0.47	2.38	9	2
5:D:536:7Q9:O32	5:D:547:7Q9:C3	0.47	2.62	2	2
1:B:7:VAL:HG11	1:B:71:TYR:CD2	0.47	2.44	3	1
5:B:207:7Q9:O32	5:B:207:7Q9:C2	0.47	2.59	13	6
5:A:211:7Q9:C13	6:B:214:17F:O5	0.47	2.62	8	1
6:E:828:17F:H8A	5:E:832:7Q9:C11	0.47	2.39	8	1
5:B:220:7Q9:O21	5:B:220:7Q9:C31	0.47	2.63	9	4
5:D:509:7Q9:C1	5:D:509:7Q9:O32	0.47	2.61	9	1
5:D:522:7Q9:C313	5:D:545:7Q9:C316	0.47	2.92	9	2
5:D:524:7Q9:O21	5:D:524:7Q9:C31	0.47	2.62	12	5
6:B:215:17F:C19	6:D:501:17F:H9A	0.47	2.39	10	1
6:E:811:17F:H9A	5:E:822:7Q9:C1	0.47	2.39	10	1
5:E:813:7Q9:C37	6:E:819:17F:H37	0.47	2.39	10	1
5:B:216:7Q9:C310	5:D:515:7Q9:C39	0.47	2.91	11	1
6:D:501:17F:C17	6:D:501:17F:O3	0.47	2.63	11	1
6:D:511:17F:O5	5:D:526:7Q9:C12	0.47	2.62	11	1
5:E:840:7Q9:C13	5:E:840:7Q9:P	0.47	3.03	11	2
1:A:9:VAL:HB	1:A:80:CYS:HA	0.47	1.86	17	1
3:A:201:GSP:PB	3:A:201:GSP:C5'	0.47	3.02	17	1
6:A:208:17F:H12A	5:E:822:7Q9:C318	0.47	2.39	19	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:B:219:17F:H75	6:B:219:17F:C32	0.47	2.39	19	1
5:E:806:7Q9:O22	5:E:814:7Q9:C13	0.47	2.61	19	1
5:D:509:7Q9:C312	5:D:525:7Q9:C318	0.47	2.93	20	1
5:B:209:7Q9:C13	5:B:209:7Q9:C32	0.47	2.93	1	5
5:B:213:7Q9:C37	5:D:514:7Q9:C39	0.47	2.92	1	2
5:D:543:7Q9:O14	5:D:543:7Q9:O21	0.47	2.32	1	1
6:A:214:17F:H19A	6:A:214:17F:C10	0.47	2.32	9	5
6:E:801:17F:H35	6:E:801:17F:H42	0.47	1.85	2	2
6:D:534:17F:C32	6:D:534:17F:C2X	0.47	2.92	4	1
5:E:825:7Q9:O22	5:E:825:7Q9:C1	0.47	2.59	13	7
5:E:848:7Q9:C33	5:E:851:7Q9:C32	0.47	2.92	7	1
5:D:509:7Q9:O32	5:D:525:7Q9:C36	0.47	2.62	10	1
5:D:545:7Q9:C15	5:D:545:7Q9:C21	0.47	2.92	11	1
6:D:501:17F:C33	6:D:501:17F:C10	0.47	2.92	13	1
6:D:501:17F:H29	5:D:509:7Q9:C3	0.47	2.40	13	1
6:D:501:17F:H39	5:D:508:7Q9:C36	0.47	2.40	16	1
6:E:870:17F:H64	6:E:870:17F:C21	0.47	2.40	16	1
6:B:219:17F:H31	5:D:522:7Q9:O22	0.47	2.09	19	1
1:A:13:GLY:HA2	3:A:201:GSP:H5'1	0.47	1.86	1	1
5:D:536:7Q9:O31	5:D:536:7Q9:O22	0.47	2.32	15	4
5:E:840:7Q9:O14	5:E:840:7Q9:C12	0.47	2.63	11	7
1:B:68:ARG:HA	1:B:71:TYR:CE2	0.47	2.44	18	2
5:E:821:7Q9:C14	5:E:825:7Q9:O13	0.47	2.62	12	3
6:D:528:17F:H77	2:E:634:LEU:HD13	0.47	1.84	3	1
5:D:507:7Q9:C32	6:D:516:17F:C20	0.47	2.92	20	2
6:A:214:17F:C24	6:A:214:17F:C2X	0.47	2.84	5	2
5:E:848:7Q9:O22	5:E:848:7Q9:C13	0.47	2.63	5	1
6:D:510:17F:C6	6:D:516:17F:H9	0.47	2.39	6	2
6:E:856:17F:O10	6:E:856:17F:C6	0.47	2.57	7	3
6:E:870:17F:H9A	5:E:871:7Q9:O13	0.47	2.08	7	1
5:E:852:7Q9:C22	5:E:878:7Q9:C23	0.47	2.92	11	1
2:D:281:GLY:O	2:D:285:GLU:HG2	0.47	2.10	12	1
5:D:532:7Q9:C15	5:D:532:7Q9:O12	0.47	2.61	12	1
5:E:836:7Q9:O14	5:E:854:7Q9:C14	0.47	2.62	12	2
6:E:838:17F:C31	6:E:838:17F:H62	0.47	2.38	12	1
5:B:216:7Q9:C38	5:D:515:7Q9:C22	0.47	2.93	18	1
5:D:520:7Q9:C313	5:D:538:7Q9:C315	0.47	2.93	20	1
6:E:807:17F:H54	6:E:809:17F:C30	0.47	2.28	20	1
6:E:838:17F:H10A	6:E:856:17F:C2X	0.47	2.38	20	1
6:D:501:17F:C39	6:D:501:17F:H51	0.47	2.39	1	1
5:D:509:7Q9:O14	5:D:520:7Q9:C14	0.47	2.62	3	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:514:7Q9:O32	5:D:514:7Q9:C2	0.47	2.60	11	9
2:E:642:SER:N	2:E:643:PRO:HD2	0.47	2.25	5	10
5:A:206:7Q9:C316	5:E:808:7Q9:C310	0.47	2.93	2	1
5:B:218:7Q9:O13	5:D:542:7Q9:C15	0.47	2.63	2	2
6:D:510:17F:C6	6:D:516:17F:H9A	0.47	2.39	13	2
2:E:621:PRO:O	2:E:625:GLU:HG3	0.47	2.09	4	2
5:E:826:7Q9:C13	5:E:849:7Q9:O14	0.47	2.62	2	1
5:D:506:7Q9:O13	5:D:506:7Q9:C12	0.47	2.62	17	4
5:D:540:7Q9:O31	5:D:540:7Q9:C21	0.47	2.63	13	10
6:E:838:17F:C42	6:E:838:17F:C27	0.47	2.92	5	1
5:B:205:7Q9:O31	5:B:205:7Q9:O22	0.47	2.33	7	1
5:D:549:7Q9:O22	2:E:649:ARG:HD3	0.47	2.08	7	1
6:E:801:17F:O7	6:E:801:17F:O6	0.47	2.33	13	6
6:E:807:17F:H47	6:E:807:17F:H74	0.47	1.86	8	1
2:D:331:ARG:HA	5:D:532:7Q9:C39	0.47	2.40	10	2
5:A:204:7Q9:C3	6:A:208:17F:H6	0.47	2.40	11	1
5:E:834:7Q9:C318	6:E:855:17F:H67	0.47	2.40	11	1
6:D:501:17F:C1X	5:D:509:7Q9:C22	0.47	2.93	12	1
5:D:537:7Q9:C32	6:D:546:17F:H29	0.47	2.39	13	1
5:A:210:7Q9:C317	5:E:808:7Q9:C39	0.47	2.92	17	2
1:A:47:ASP:HB2	1:A:164:ARG:HH12	0.47	1.69	16	1
5:E:808:7Q9:C1	5:E:808:7Q9:O22	0.47	2.60	16	1
6:E:872:17F:C23	6:E:872:17F:C20	0.47	2.91	16	1
6:E:819:17F:H65	5:E:836:7Q9:C36	0.47	2.39	17	1
6:D:533:17F:H8	6:D:533:17F:C2	0.47	2.40	19	1
6:D:510:17F:C11	6:D:516:17F:H58	0.47	2.38	20	1
1:B:80:CYS:HB3	1:B:93:ILE:HD12	0.47	1.86	1	2
5:B:207:7Q9:C318	6:E:801:17F:H73	0.47	2.40	3	2
6:D:510:17F:H56	6:D:516:17F:C12	0.47	2.40	19	2
5:E:869:7Q9:C15	5:E:869:7Q9:O14	0.47	2.62	1	9
6:D:528:17F:H60	6:D:528:17F:C10	0.47	2.31	15	2
6:E:819:17F:H18	5:E:852:7Q9:C32	0.47	2.40	6	2
5:E:832:7Q9:O21	5:E:832:7Q9:C31	0.47	2.63	19	4
5:E:840:7Q9:C314	5:E:849:7Q9:C318	0.47	2.92	13	7
1:A:147:LYS:HD3	3:A:201:GSP:O6	0.47	2.09	3	1
5:A:205:7Q9:C23	5:A:207:7Q9:C3	0.47	2.92	3	3
5:B:203:7Q9:C12	5:B:204:7Q9:O31	0.47	2.62	10	5
5:D:532:7Q9:O22	5:D:532:7Q9:C3	0.47	2.57	3	2
5:E:847:7Q9:O22	5:E:847:7Q9:C1	0.47	2.61	13	6
5:A:204:7Q9:C317	6:E:811:17F:H42	0.47	2.38	4	1
6:B:215:17F:H41	6:B:215:17F:C37	0.47	2.38	4	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:421:VAL:HG11	2:E:735:GLU:HG2	0.47	1.86	4	1
5:E:834:7Q9:C35	6:E:855:17F:C33	0.47	2.93	4	1
5:A:205:7Q9:C15	5:A:207:7Q9:O32	0.47	2.62	5	1
2:D:337:LEU:HG	2:E:626:LEU:HB3	0.47	1.85	5	1
5:A:205:7Q9:C35	5:D:504:7Q9:C23	0.47	2.93	7	1
5:E:806:7Q9:C312	5:E:814:7Q9:C38	0.47	2.92	8	1
6:E:807:17F:H60	6:E:819:17F:C1X	0.47	2.39	8	1
6:E:870:17F:H10A	5:E:871:7Q9:O14	0.47	2.10	8	1
5:E:863:7Q9:C32	5:E:873:7Q9:C31	0.47	2.92	10	5
6:D:510:17F:C1Y	6:D:527:17F:H60	0.47	2.40	10	1
6:A:214:17F:H75	5:E:839:7Q9:C316	0.47	2.40	11	1
6:D:528:17F:H71	5:E:862:7Q9:C318	0.47	2.40	11	1
1:B:47:ASP:OD2	1:B:161:ARG:HD2	0.47	2.10	13	1
6:B:208:17F:H41	6:B:214:17F:H30	0.47	1.87	14	1
6:D:510:17F:H66	6:D:511:17F:H74	0.47	1.86	14	1
5:E:824:7Q9:C313	6:E:841:17F:H71	0.47	2.40	14	1
6:E:807:17F:C37	5:E:813:7Q9:C310	0.47	2.84	15	1
6:D:533:17F:H9A	6:D:533:17F:H56	0.47	1.87	16	1
5:E:831:7Q9:O32	5:E:831:7Q9:C21	0.47	2.62	16	1
6:E:856:17F:P1	6:E:856:17F:N1	0.47	2.88	18	2
5:A:207:7Q9:C33	5:D:504:7Q9:C15	0.47	2.92	17	1
6:B:214:17F:H18	6:B:219:17F:N1	0.47	2.25	17	1
2:D:289:ASP:O	2:D:293:VAL:HG23	0.47	2.10	18	1
5:E:803:7Q9:C1	5:E:813:7Q9:C11	0.47	2.93	18	1
5:E:802:7Q9:C32	6:E:809:17F:C18	0.47	2.93	20	1
6:A:208:17F:H30	6:A:208:17F:H42	0.47	1.86	1	1
5:E:836:7Q9:O21	5:E:836:7Q9:C31	0.47	2.62	17	11
6:D:534:17F:O10	6:D:534:17F:H4	0.47	2.09	2	2
6:E:809:17F:H72	5:E:810:7Q9:C318	0.47	2.38	2	1
6:E:855:17F:C2	5:E:857:7Q9:C13	0.47	2.91	2	1
5:E:810:7Q9:C13	5:E:816:7Q9:O32	0.47	2.63	4	1
1:B:117:LYS:HA	3:B:201:GSP:C6	0.47	2.44	5	1
6:E:841:17F:O10	6:E:841:17F:C6	0.47	2.56	17	4
6:A:214:17F:H67	6:A:214:17F:H42	0.47	1.86	12	1
5:D:519:7Q9:C14	5:D:519:7Q9:C1	0.47	2.93	12	1
6:E:807:17F:H30	6:E:807:17F:H31	0.47	1.86	13	1
5:A:212:7Q9:O31	6:A:214:17F:H18A	0.47	2.10	16	1
6:E:809:17F:H64	6:E:809:17F:H54	0.47	1.86	16	1
5:E:837:7Q9:C38	5:E:860:7Q9:C39	0.47	2.93	16	1
5:A:210:7Q9:O22	5:A:210:7Q9:O11	0.47	2.33	17	1
5:A:212:7Q9:C32	6:A:214:17F:H57	0.47	2.39	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:B:214:17F:C34	6:B:214:17F:H35	0.47	2.40	17	1
6:E:807:17F:C25	6:E:809:17F:H62	0.47	2.37	18	1
5:A:209:7Q9:C23	6:A:214:17F:H31	0.47	2.39	19	1
6:D:510:17F:H19A	5:D:524:7Q9:O32	0.47	2.09	2	1
6:D:517:17F:H62	6:D:517:17F:H43	0.47	1.85	4	1
6:B:208:17F:H11A	6:B:208:17F:H32	0.47	1.87	5	1
5:E:834:7Q9:O22	5:E:834:7Q9:C1	0.47	2.60	10	5
6:D:510:17F:C8	6:D:516:17F:H11A	0.47	2.40	6	1
6:E:801:17F:C42	6:E:801:17F:C28	0.47	2.93	6	4
5:E:813:7Q9:C316	6:E:819:17F:C30	0.47	2.93	6	1
5:A:204:7Q9:C311	6:A:208:17F:H11	0.47	2.40	8	1
5:D:548:7Q9:C3	5:E:831:7Q9:O14	0.47	2.63	8	1
6:D:517:17F:H9A	5:D:538:7Q9:O31	0.47	2.10	9	1
5:A:203:7Q9:C15	5:A:205:7Q9:O22	0.47	2.63	10	1
1:B:17:SER:OG	3:B:201:GSP:O3G	0.47	2.33	15	3
5:E:802:7Q9:C31	6:E:807:17F:H5	0.47	2.40	10	1
6:D:528:17F:H66	6:D:528:17F:C21	0.47	2.39	12	2
5:E:848:7Q9:C316	5:E:851:7Q9:C318	0.47	2.93	11	1
6:B:215:17F:H66	6:B:215:17F:H48	0.47	1.87	12	1
5:D:512:7Q9:O13	6:D:528:17F:H4	0.47	2.10	12	1
5:B:205:7Q9:C32	5:B:211:7Q9:O22	0.47	2.63	13	1
2:E:583:ARG:HD2	5:E:859:7Q9:C318	0.47	2.40	16	2
5:E:844:7Q9:C12	5:E:877:7Q9:O13	0.47	2.63	14	1
6:D:534:17F:C8	5:D:539:7Q9:C33	0.47	2.92	15	1
6:D:501:17F:H10	6:D:501:17F:H61	0.47	1.87	17	1
6:E:801:17F:H59	5:E:806:7Q9:C315	0.47	2.40	17	1
5:B:206:7Q9:C316	6:E:805:17F:H52	0.47	2.40	19	1
5:B:212:7Q9:C34	5:B:212:7Q9:C38	0.47	2.93	19	1
5:B:207:7Q9:O12	6:D:501:17F:H19	0.47	2.10	1	1
5:B:217:7Q9:C14	5:B:217:7Q9:P	0.47	3.03	1	1
5:D:535:7Q9:C318	6:E:874:17F:H50	0.47	2.40	2	3
5:E:840:7Q9:O22	5:E:840:7Q9:C3	0.47	2.61	10	4
1:A:6:LEU:HB2	1:A:55:ILE:HG12	0.47	1.87	2	1
6:B:208:17F:C2	6:B:214:17F:O1	0.47	2.63	2	1
6:E:801:17F:H12	6:E:801:17F:C20	0.47	2.39	2	1
6:E:807:17F:H12	6:E:807:17F:C32	0.47	2.36	2	4
6:E:811:17F:O8	5:E:823:7Q9:C3	0.47	2.63	3	1
6:B:208:17F:H60	5:B:212:7Q9:C37	0.47	2.39	5	2
5:E:859:7Q9:O32	5:E:864:7Q9:C12	0.47	2.63	7	1
6:E:807:17F:H47	6:E:807:17F:H76	0.47	1.86	8	1
1:A:21:ILE:HG12	1:B:131:GLN:HE22	0.47	1.69	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:544:7Q9:C23	6:D:546:17F:H19A	0.47	2.40	10	1
6:E:819:17F:C11	6:E:819:17F:C7	0.47	2.93	15	2
6:D:516:17F:H1A	6:D:516:17F:H5	0.47	1.87	11	1
2:E:594:LYS:HE2	5:E:861:7Q9:C316	0.47	2.40	11	1
6:E:838:17F:P1	6:E:838:17F:N1	0.47	2.88	12	2
5:B:218:7Q9:C14	5:B:218:7Q9:O13	0.47	2.63	13	3
6:D:510:17F:H29	6:D:510:17F:C24	0.47	2.40	14	1
6:B:214:17F:C32	6:B:214:17F:H35	0.47	2.40	16	1
5:D:512:7Q9:O22	5:D:530:7Q9:C15	0.47	2.63	17	1
6:D:527:17F:O10	6:D:527:17F:H33	0.47	2.10	17	1
6:D:534:17F:HN1	5:D:539:7Q9:C11	0.47	2.23	17	1
5:B:205:7Q9:O14	5:B:210:7Q9:C14	0.47	2.62	19	1
5:D:538:7Q9:O22	5:D:538:7Q9:C1	0.46	2.61	13	4
5:E:834:7Q9:O14	5:E:849:7Q9:C12	0.46	2.64	1	1
6:E:838:17F:C11	6:E:856:17F:H12	0.46	2.40	1	1
5:B:206:7Q9:C315	6:E:805:17F:H71	0.46	2.40	9	3
6:D:501:17F:C8	6:D:501:17F:C1Y	0.46	2.78	7	4
6:D:516:17F:O2	6:D:516:17F:C5	0.46	2.63	5	5
5:E:806:7Q9:C15	5:E:806:7Q9:C21	0.46	2.93	12	4
5:D:506:7Q9:C13	5:D:506:7Q9:O13	0.46	2.63	12	2
6:D:510:17F:C8	6:D:516:17F:O7	0.46	2.63	8	2
5:E:814:7Q9:C37	6:E:817:17F:H8	0.46	2.40	8	1
5:E:865:7Q9:C15	5:E:865:7Q9:O13	0.46	2.63	18	3
1:A:20:THR:O	1:A:24:ILE:HG12	0.46	2.09	9	2
6:B:208:17F:H58	6:B:208:17F:H36	0.46	1.87	19	2
6:D:511:17F:C3	5:D:524:7Q9:C12	0.46	2.92	10	1
6:B:208:17F:H49	6:B:208:17F:C39	0.46	2.40	11	1
6:D:501:17F:H48	6:D:501:17F:H66	0.46	1.86	11	1
2:E:674:LEU:HD21	6:E:855:17F:C12	0.46	2.40	12	1
5:E:803:7Q9:C13	5:E:814:7Q9:O22	0.46	2.63	12	1
6:D:510:17F:H51	6:D:510:17F:C37	0.46	2.40	13	1
2:D:364:ALA:HB3	2:D:365:PRO:HD3	0.46	1.86	18	2
5:E:802:7Q9:C313	6:E:805:17F:H61	0.46	2.40	14	1
1:A:25:GLN:HG3	1:B:131:GLN:HE21	0.46	1.70	17	1
5:B:205:7Q9:C3	5:B:211:7Q9:O22	0.46	2.64	17	1
6:B:219:17F:O2	6:B:219:17F:C2	0.46	2.64	17	1
6:E:807:17F:H32	6:E:818:17F:H10A	0.46	1.86	17	1
5:E:833:7Q9:C12	6:E:855:17F:O5	0.46	2.62	17	1
5:E:833:7Q9:C15	5:E:857:7Q9:O14	0.46	2.63	19	1
6:E:838:17F:H42	6:E:838:17F:C39	0.46	2.40	1	1
5:A:206:7Q9:C316	5:E:808:7Q9:C312	0.46	2.93	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:837:7Q9:C21	5:E:837:7Q9:O31	0.46	2.64	14	7
5:D:518:7Q9:C2	5:D:518:7Q9:C11	0.46	2.93	6	1
6:D:527:17F:H35	5:D:535:7Q9:C310	0.46	2.40	7	1
6:E:817:17F:O10	5:E:820:7Q9:C13	0.46	2.63	8	1
6:E:856:17F:C31	6:E:856:17F:C35	0.46	2.87	9	2
5:E:824:7Q9:C33	6:E:841:17F:C1Y	0.46	2.94	9	1
6:E:838:17F:N1	6:E:874:17F:C7	0.46	2.77	13	1
6:D:510:17F:H32	5:D:524:7Q9:C23	0.46	2.40	15	1
6:E:807:17F:O10	6:E:818:17F:H6A	0.46	2.11	15	1
6:E:870:17F:H30	6:E:870:17F:C32	0.46	2.40	16	2
2:D:308:TRP:CZ3	6:D:527:17F:H74	0.46	2.46	16	1
6:E:811:17F:H18A	5:E:815:7Q9:O14	0.46	2.10	16	1
5:D:545:7Q9:C15	5:D:545:7Q9:O11	0.46	2.64	17	1
5:A:204:7Q9:C310	6:A:208:17F:H9A	0.46	2.41	1	2
6:E:838:17F:H48	6:E:838:17F:H71	0.46	1.86	1	2
5:A:217:7Q9:O22	5:D:544:7Q9:C23	0.46	2.63	2	1
5:B:212:7Q9:C1	5:B:212:7Q9:O32	0.46	2.63	2	1
6:B:215:17F:H65	6:B:215:17F:C27	0.46	2.39	2	1
6:E:818:17F:O2	5:E:824:7Q9:C12	0.46	2.63	2	1
5:E:860:7Q9:O22	5:E:860:7Q9:C1	0.46	2.60	16	4
5:D:521:7Q9:C3	5:D:525:7Q9:O31	0.46	2.63	3	1
6:E:856:17F:H10A	6:E:874:17F:O10	0.46	2.10	8	2
6:B:208:17F:H78	5:E:804:7Q9:C318	0.46	2.40	4	1
6:D:517:17F:H53	5:E:842:7Q9:C318	0.46	2.39	4	1
6:B:214:17F:H41	6:B:214:17F:C10	0.46	2.41	5	1
6:E:811:17F:H6	5:E:823:7Q9:C3	0.46	2.41	5	1
6:E:807:17F:C33	6:E:819:17F:H29	0.46	2.40	8	1
5:D:536:7Q9:C13	5:D:536:7Q9:C1	0.46	2.93	9	1
6:E:838:17F:H49	6:E:838:17F:C42	0.46	2.30	13	2
6:D:516:17F:H44	5:D:535:7Q9:C315	0.46	2.41	10	1
6:D:527:17F:O1	6:D:527:17F:C17	0.46	2.64	14	2
5:E:806:7Q9:C23	5:E:820:7Q9:C13	0.46	2.93	12	1
5:E:840:7Q9:C3	5:E:873:7Q9:C39	0.46	2.93	17	3
5:E:846:7Q9:C13	5:E:869:7Q9:C12	0.46	2.93	12	1
5:E:863:7Q9:O31	5:E:873:7Q9:C32	0.46	2.64	12	2
6:B:208:17F:H34	6:B:214:17F:H12	0.46	1.78	14	1
2:E:562:GLU:O	2:E:566:PRO:HD2	0.46	2.10	15	1
6:E:838:17F:C12	6:E:856:17F:H30	0.46	2.40	15	1
5:A:211:7Q9:C311	5:A:213:7Q9:C310	0.46	2.94	16	1
6:D:546:17F:H57	6:D:546:17F:C9	0.46	2.40	16	1
6:B:214:17F:H20	6:B:219:17F:HN1A	0.46	1.71	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:819:17F:H34	5:E:852:7Q9:C32	0.46	2.40	17	1
1:B:79:LEU:HD12	1:B:112:VAL:HB	0.46	1.87	18	1
6:D:510:17F:C27	6:D:516:17F:C21	0.46	2.91	18	1
2:D:290:LEU:HG	5:D:547:7Q9:C314	0.46	2.40	1	1
1:B:20:THR:HG21	1:B:57:ASP:HB2	0.46	1.87	2	1
5:B:212:7Q9:O22	5:B:213:7Q9:C12	0.46	2.63	2	1
5:B:220:7Q9:C13	5:B:220:7Q9:P	0.46	3.04	2	6
5:D:515:7Q9:O32	5:D:515:7Q9:C2	0.46	2.60	16	6
5:E:802:7Q9:C311	6:E:807:17F:H42	0.46	2.41	2	1
6:D:510:17F:H19	6:D:527:17F:C18	0.46	2.41	3	1
5:E:868:7Q9:C312	5:E:873:7Q9:C313	0.46	2.93	4	1
6:D:534:17F:C33	6:D:534:17F:C2X	0.46	2.94	7	4
6:E:828:17F:H6	5:E:851:7Q9:O13	0.46	2.10	6	1
5:D:513:7Q9:O21	5:D:513:7Q9:O32	0.46	2.33	7	2
6:E:819:17F:C36	5:E:836:7Q9:C38	0.46	2.93	8	1
2:E:627:GLN:O	2:E:631:ARG:HG3	0.46	2.11	15	3
6:E:817:17F:O10	6:E:817:17F:C4	0.46	2.59	16	3
5:B:217:7Q9:O32	5:B:217:7Q9:O21	0.46	2.32	15	1
5:B:205:7Q9:O31	5:B:211:7Q9:C1	0.46	2.63	16	1
6:B:208:17F:C42	5:E:812:7Q9:C318	0.46	2.93	16	2
2:E:714:LEU:HD22	5:E:865:7Q9:C317	0.46	2.40	16	1
2:D:396:ALA:HA	5:D:531:7Q9:C316	0.46	2.40	17	1
5:E:823:7Q9:C1	5:E:823:7Q9:O22	0.46	2.62	17	1
6:D:517:17F:H58	6:D:517:17F:H43	0.46	1.88	20	1
5:B:217:7Q9:O14	5:B:217:7Q9:C12	0.46	2.63	1	2
6:D:534:17F:C32	6:D:534:17F:C1X	0.46	2.84	16	2
2:D:327:GLN:OE1	6:D:528:17F:H32	0.46	2.11	11	2
6:D:534:17F:H11	5:D:539:7Q9:C311	0.46	2.41	2	2
2:E:719:LEU:N	2:E:720:PRO:HD2	0.46	2.25	2	1
1:A:32:TYR:HE2	3:A:201:GSP:H4'	0.46	1.71	4	1
5:D:515:7Q9:O32	5:D:519:7Q9:C15	0.46	2.64	4	1
5:E:812:7Q9:C2	5:E:812:7Q9:O13	0.46	2.64	4	4
2:D:297:VAL:HA	2:D:300:TYR:HD2	0.46	1.70	5	1
2:D:421:VAL:HB	2:E:736:TYR:HE2	0.46	1.71	6	3
5:B:205:7Q9:C15	5:B:205:7Q9:C23	0.46	2.94	6	1
5:E:813:7Q9:C22	6:E:828:17F:H33	0.46	2.41	7	1
6:E:809:17F:HN1A	6:E:818:17F:C6	0.46	2.22	8	1
6:E:811:17F:H9A	5:E:822:7Q9:C2	0.46	2.40	8	1
6:D:501:17F:H42	6:D:501:17F:H35	0.46	1.87	16	3
2:E:715:ARG:O	2:E:719:LEU:HG	0.46	2.11	20	2
6:E:801:17F:C23	5:E:804:7Q9:C38	0.46	2.94	16	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:49:GLU:HB3	1:B:164:ARG:NH2	0.46	2.25	10	1
6:D:517:17F:H40	6:D:517:17F:H57	0.46	1.87	10	1
6:E:828:17F:C1X	5:E:832:7Q9:C35	0.46	2.87	14	2
5:B:206:7Q9:C33	5:B:212:7Q9:O32	0.46	2.64	20	2
6:E:870:17F:H64	6:E:870:17F:C22	0.46	2.38	15	1
5:A:215:7Q9:O32	5:A:215:7Q9:C1	0.46	2.63	16	1
1:A:13:GLY:HA2	3:A:201:GSP:C4'	0.46	2.40	17	1
5:E:832:7Q9:C23	6:E:856:17F:C2X	0.46	2.93	18	1
6:E:807:17F:O4	5:E:813:7Q9:C14	0.46	2.63	1	3
6:E:819:17F:C19	5:E:852:7Q9:C33	0.46	2.94	2	1
5:E:859:7Q9:O32	5:E:859:7Q9:C21	0.46	2.64	2	2
5:E:862:7Q9:O21	5:E:862:7Q9:C31	0.46	2.64	16	8
5:D:506:7Q9:C13	5:D:506:7Q9:P	0.46	3.04	3	5
5:B:218:7Q9:C1	5:B:218:7Q9:O32	0.46	2.64	15	3
5:A:211:7Q9:C1	5:A:213:7Q9:C22	0.46	2.94	5	1
1:B:97:ARG:HD3	1:B:101:LYS:HE2	0.46	1.85	6	1
3:B:201:GSP:S1G	3:B:201:GSP:C5'	0.46	3.00	6	1
5:D:545:7Q9:C1	5:D:545:7Q9:O22	0.46	2.57	6	1
5:E:848:7Q9:O21	5:E:848:7Q9:O32	0.46	2.33	19	2
1:A:17:SER:OG	3:A:201:GSP:O3G	0.46	2.33	15	2
5:E:804:7Q9:C318	5:E:812:7Q9:C318	0.46	2.94	9	1
5:A:215:7Q9:O14	5:D:536:7Q9:C22	0.46	2.64	10	1
2:D:279:THR:O	2:D:283:ARG:HG3	0.46	2.11	10	1
2:E:702:THR:HA	2:E:705:GLU:HG2	0.46	1.87	12	1
5:E:867:7Q9:C312	5:E:867:7Q9:C38	0.46	2.93	17	4
5:D:526:7Q9:C317	5:D:549:7Q9:C318	0.46	2.94	16	1
6:D:516:17F:H50	6:D:516:17F:H62	0.46	1.87	17	1
1:A:41:ARG:HA	1:A:53:LEU:O	0.46	2.11	1	2
5:E:835:7Q9:O22	5:E:835:7Q9:C1	0.46	2.60	8	4
5:A:217:7Q9:C14	5:A:217:7Q9:P	0.46	3.03	5	4
5:B:212:7Q9:C12	5:B:217:7Q9:O31	0.46	2.64	2	1
6:D:511:17F:O9	6:D:511:17F:C7	0.46	2.64	8	6
6:D:546:17F:H56	6:D:546:17F:C35	0.46	2.37	2	1
5:A:205:7Q9:O13	5:B:209:7Q9:C13	0.46	2.64	3	1
5:A:211:7Q9:O13	5:D:518:7Q9:C13	0.46	2.64	3	1
2:E:579:THR:O	2:E:583:ARG:HG3	0.46	2.11	3	2
5:E:820:7Q9:C1	6:E:838:17F:C18	0.46	2.94	4	1
1:B:112:VAL:HG23	1:B:159:LEU:HD13	0.46	1.88	6	2
6:E:856:17F:O1	6:E:856:17F:H5	0.46	2.11	11	3
6:B:215:17F:H61	6:B:215:17F:C30	0.46	2.40	7	2
6:E:801:17F:H50	6:E:801:17F:C42	0.46	2.40	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:842:7Q9:C2	5:E:842:7Q9:O32	0.46	2.61	13	2
5:D:520:7Q9:P	5:D:520:7Q9:O21	0.46	2.74	13	3
6:E:838:17F:H48	6:E:838:17F:C42	0.46	2.40	10	1
5:E:849:7Q9:O22	5:E:849:7Q9:O11	0.46	2.32	10	1
5:D:529:7Q9:O22	5:D:529:7Q9:C3	0.46	2.60	17	4
2:E:660:ARG:CG	6:E:874:17F:H31	0.46	2.41	11	1
6:B:208:17F:H20A	6:B:214:17F:H10	0.46	1.87	12	1
5:E:853:7Q9:O32	5:E:853:7Q9:C15	0.46	2.63	12	1
6:D:510:17F:H68	6:D:510:17F:H53	0.46	1.88	13	1
5:E:820:7Q9:O21	5:E:820:7Q9:C31	0.46	2.64	18	2
5:D:536:7Q9:C3	5:D:547:7Q9:O22	0.46	2.64	20	2
2:D:418:LEU:HD23	2:E:739:LYS:HD2	0.46	1.87	16	1
6:D:501:17F:H1	5:D:508:7Q9:C3	0.46	2.40	17	1
5:E:813:7Q9:C39	6:E:819:17F:C21	0.46	2.94	17	1
6:E:819:17F:H70	5:E:852:7Q9:C310	0.46	2.40	17	1
5:B:220:7Q9:O14	5:B:220:7Q9:C12	0.46	2.64	2	4
5:D:537:7Q9:O22	5:D:537:7Q9:C1	0.46	2.60	19	5
2:E:648:MET:SD	2:E:651:ARG:HD2	0.46	2.51	3	1
2:E:730:LEU:HD12	2:E:733:LEU:HD22	0.46	1.87	3	1
1:B:17:SER:HB2	3:B:201:GSP:O2G	0.46	2.11	4	1
5:E:876:7Q9:O32	5:E:876:7Q9:C34	0.46	2.64	8	4
5:D:515:7Q9:O13	5:D:519:7Q9:C13	0.46	2.64	5	2
1:A:82:PHE:HB3	1:A:93:ILE:HD11	0.46	1.87	6	1
6:E:807:17F:C24	6:E:809:17F:H63	0.46	2.40	6	1
5:E:808:7Q9:C13	6:E:817:17F:O2	0.46	2.64	7	1
5:E:832:7Q9:C39	6:E:856:17F:H53	0.46	2.40	8	1
5:E:816:7Q9:P	5:E:816:7Q9:C15	0.46	3.04	12	3
6:D:546:17F:C31	6:D:546:17F:C9	0.46	2.94	12	2
5:B:211:7Q9:C23	6:D:501:17F:H56	0.46	2.41	13	1
6:D:510:17F:C5	6:D:516:17F:H9A	0.46	2.36	16	4
2:D:429:PHE:CZ	6:D:533:17F:H66	0.46	2.46	15	1
1:A:35:THR:OG1	3:A:201:GSP:O1A	0.46	2.34	19	1
6:A:208:17F:H10	5:A:209:7Q9:C39	0.46	2.41	1	1
5:D:545:7Q9:O22	5:D:545:7Q9:C1	0.46	2.59	18	4
5:E:820:7Q9:O13	5:E:820:7Q9:C12	0.46	2.63	7	12
6:B:208:17F:H2	6:B:214:17F:O1	0.46	2.11	2	1
5:D:505:7Q9:O22	5:D:505:7Q9:O31	0.46	2.33	6	3
5:D:509:7Q9:O14	5:D:520:7Q9:C13	0.46	2.64	2	1
5:B:207:7Q9:C14	5:B:211:7Q9:O13	0.46	2.64	8	2
6:E:819:17F:C36	5:E:836:7Q9:C37	0.46	2.88	4	1
6:B:208:17F:H4	6:B:208:17F:C1	0.46	2.39	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:B:205:7Q9:C316	5:B:206:7Q9:C318	0.46	2.93	7	1
6:D:533:17F:H62	6:D:533:17F:H37	0.46	1.88	8	1
5:B:211:7Q9:C310	6:D:501:17F:H70	0.46	2.41	9	1
6:E:838:17F:H9	6:E:856:17F:C9	0.46	2.41	9	1
1:B:5:LYS:HB2	1:B:76:GLU:HG3	0.46	1.88	10	1
2:D:347:GLU:HG2	2:D:351:ARG:HH12	0.46	1.70	10	1
1:B:64:TYR:O	1:B:68:ARG:HB2	0.46	2.11	19	2
6:D:546:17F:H34	6:D:546:17F:H9A	0.46	1.86	11	1
6:E:801:17F:C31	6:E:801:17F:H62	0.46	2.39	11	1
6:E:809:17F:H48	6:E:809:17F:H60	0.46	1.87	20	3
5:D:514:7Q9:O14	5:D:514:7Q9:C12	0.46	2.64	20	4
5:E:863:7Q9:O22	5:E:863:7Q9:C3	0.46	2.59	16	2
6:B:214:17F:H62	6:B:219:17F:C21	0.46	2.41	14	1
5:E:803:7Q9:C1	5:E:813:7Q9:C14	0.46	2.94	17	1
5:A:204:7Q9:C311	6:A:208:17F:H66	0.46	2.40	19	1
6:E:805:17F:C6	5:E:816:7Q9:O31	0.46	2.64	20	1
5:D:540:7Q9:C15	5:D:540:7Q9:O22	0.46	2.64	1	1
5:E:810:7Q9:C3	5:E:825:7Q9:C35	0.46	2.94	9	4
5:E:834:7Q9:C13	5:E:834:7Q9:C22	0.46	2.94	2	2
1:A:32:TYR:CE1	3:A:201:GSP:H3'	0.46	2.45	3	1
6:D:527:17F:O9	6:D:527:17F:P1	0.46	2.74	18	4
5:E:848:7Q9:C314	5:E:851:7Q9:C314	0.46	2.94	3	1
1:A:37:GLU:HA	1:A:57:ASP:O	0.46	2.11	5	1
6:D:510:17F:C18	6:D:527:17F:H20	0.46	2.41	5	1
6:E:817:17F:H74	6:E:817:17F:H43	0.46	1.88	6	1
5:B:218:7Q9:O22	5:D:542:7Q9:C14	0.46	2.64	15	2
6:D:528:17F:H9A	5:D:532:7Q9:C38	0.46	2.41	9	1
6:D:501:17F:H40	6:D:501:17F:C34	0.46	2.40	10	1
5:D:539:7Q9:O13	5:D:544:7Q9:C11	0.46	2.64	10	1
6:D:533:17F:H61	5:D:543:7Q9:C22	0.46	2.41	12	1
6:D:501:17F:C33	6:D:501:17F:H10A	0.46	2.41	17	2
5:E:815:7Q9:C14	5:E:815:7Q9:O32	0.46	2.64	13	1
2:D:256:THR:O	2:D:260:LEU:HG	0.46	2.10	16	1
5:E:834:7Q9:O14	5:E:849:7Q9:C15	0.46	2.64	16	1
6:D:516:17F:H62	6:D:516:17F:C28	0.46	2.40	17	1
5:B:216:7Q9:O32	5:D:519:7Q9:C12	0.46	2.64	19	2
5:E:825:7Q9:C36	5:E:844:7Q9:C39	0.46	2.94	18	1
5:D:505:7Q9:C15	6:D:511:17F:H6	0.46	2.41	20	1
6:D:501:17F:H58	6:D:501:17F:C36	0.45	2.32	1	2
5:D:520:7Q9:C314	5:E:837:7Q9:C315	0.45	2.93	1	1
5:A:204:7Q9:C22	5:A:209:7Q9:C32	0.45	2.94	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:A:209:7Q9:C36	6:A:214:17F:H57	0.45	2.41	3	1
5:A:204:7Q9:C314	6:A:208:17F:H46	0.45	2.41	14	2
5:E:837:7Q9:C37	5:E:860:7Q9:C39	0.45	2.95	6	2
5:D:508:7Q9:O13	5:D:508:7Q9:C2	0.45	2.64	17	4
5:E:803:7Q9:C23	5:E:806:7Q9:C33	0.45	2.94	6	1
5:E:808:7Q9:C14	5:E:808:7Q9:P	0.45	3.04	6	1
6:E:818:17F:O1	5:E:835:7Q9:C3	0.45	2.64	6	1
5:E:834:7Q9:C15	6:E:855:17F:O4	0.45	2.64	18	2
6:D:510:17F:C7	6:D:516:17F:H11	0.45	2.41	9	1
6:E:874:17F:H11A	6:E:874:17F:HN1A	0.45	1.70	11	1
5:D:513:7Q9:C23	6:D:528:17F:H54	0.45	2.41	12	1
6:D:546:17F:C9	6:D:546:17F:C31	0.45	2.94	14	2
5:D:547:7Q9:O22	5:D:547:7Q9:C3	0.45	2.59	19	4
6:E:841:17F:H2	6:E:841:17F:O6	0.45	2.10	14	1
5:D:549:7Q9:C312	5:E:848:7Q9:C318	0.45	2.94	18	1
5:A:205:7Q9:C22	5:A:207:7Q9:O22	0.45	2.64	20	1
5:B:216:7Q9:C22	5:D:514:7Q9:C13	0.45	2.95	13	2
5:D:521:7Q9:O22	5:D:521:7Q9:C1	0.45	2.62	19	7
5:D:532:7Q9:C15	5:D:532:7Q9:P	0.45	3.04	19	4
5:A:217:7Q9:O14	5:A:217:7Q9:C12	0.45	2.63	2	2
5:D:549:7Q9:C11	5:E:832:7Q9:C2	0.45	2.94	2	1
5:B:220:7Q9:C22	5:D:543:7Q9:O13	0.45	2.64	3	1
6:D:534:17F:C36	6:D:534:17F:C1X	0.45	2.95	13	6
5:E:827:7Q9:O22	5:E:827:7Q9:C1	0.45	2.61	10	6
5:E:876:7Q9:C34	5:E:876:7Q9:O32	0.45	2.64	5	1
5:A:215:7Q9:C31	5:A:215:7Q9:C1	0.45	2.94	14	5
5:D:507:7Q9:C3	6:D:516:17F:N1	0.45	2.79	7	1
5:B:204:7Q9:O22	5:B:204:7Q9:C1	0.45	2.61	9	2
6:E:819:17F:H41	5:E:835:7Q9:C38	0.45	2.41	9	1
6:B:219:17F:H45	5:D:543:7Q9:C310	0.45	2.42	10	1
6:E:807:17F:H60	5:E:813:7Q9:C35	0.45	2.41	10	1
6:D:510:17F:H9	6:D:516:17F:C1X	0.45	2.41	11	1
6:E:828:17F:H46	5:E:832:7Q9:C318	0.45	2.41	11	1
5:E:853:7Q9:O21	5:E:853:7Q9:C31	0.45	2.64	12	2
6:B:215:17F:H64	6:B:215:17F:C12	0.45	2.42	12	1
1:B:46:ILE:HB	1:B:51:CYS:SG	0.45	2.51	14	1
6:E:807:17F:C19	6:E:809:17F:H18	0.45	2.34	14	1
6:B:214:17F:H71	5:B:217:7Q9:C38	0.45	2.41	15	2
5:E:824:7Q9:C35	6:E:841:17F:H29	0.45	2.40	16	1
5:B:209:7Q9:C32	5:B:209:7Q9:C15	0.45	2.94	18	1
5:E:837:7Q9:C34	6:E:841:17F:H50	0.45	2.41	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:B:218:7Q9:O11	5:B:218:7Q9:O32	0.45	2.34	4	5
2:D:272:TRP:CZ3	6:D:534:17F:H78	0.45	2.47	3	2
6:B:215:17F:H66	6:B:215:17F:C24	0.45	2.40	4	1
5:E:850:7Q9:C39	6:E:870:17F:C20	0.45	2.95	6	1
3:B:201:GSP:O1B	3:B:201:GSP:C5'	0.45	2.61	17	2
6:D:511:17F:H57	5:D:524:7Q9:C36	0.45	2.41	9	1
2:E:652:ALA:O	2:E:656:VAL:HG23	0.45	2.11	9	2
6:E:807:17F:H20A	6:E:818:17F:O8	0.45	2.11	10	1
5:A:215:7Q9:C14	5:D:536:7Q9:C22	0.45	2.95	11	1
2:E:725:PHE:HE1	6:E:870:17F:H71	0.45	1.71	13	1
6:E:801:17F:C28	6:E:801:17F:C42	0.45	2.91	14	1
5:A:210:7Q9:C2	5:A:216:7Q9:C21	0.45	2.94	15	1
5:E:804:7Q9:C23	5:E:812:7Q9:C23	0.45	2.95	16	1
5:B:210:7Q9:C34	5:B:210:7Q9:O14	0.45	2.64	18	1
5:E:858:7Q9:O21	5:E:858:7Q9:C31	0.45	2.64	20	1
1:A:168:GLU:HG2	1:A:172:LYS:HE3	0.45	1.88	1	1
5:A:211:7Q9:C1	5:A:213:7Q9:C34	0.45	2.95	1	2
5:E:824:7Q9:C35	6:E:841:17F:H31	0.45	2.41	1	1
6:E:838:17F:H11	6:E:838:17F:H64	0.45	1.87	1	1
6:D:501:17F:H39	6:D:501:17F:C33	0.45	2.27	2	1
5:D:518:7Q9:C318	6:E:870:17F:H52	0.45	2.41	3	1
5:D:525:7Q9:O21	5:D:525:7Q9:C11	0.45	2.65	4	1
6:D:517:17F:H54	5:E:842:7Q9:C318	0.45	2.42	6	1
5:D:526:7Q9:C22	5:D:526:7Q9:C39	0.45	2.93	6	1
6:E:838:17F:C12	6:E:856:17F:C9	0.45	2.93	6	1
1:B:69:ASP:O	1:B:73:ARG:HG3	0.45	2.11	15	2
5:A:213:7Q9:C1	5:A:217:7Q9:C36	0.45	2.94	8	1
2:E:656:VAL:HG22	6:E:856:17F:H61	0.45	1.87	9	1
5:A:205:7Q9:C22	5:A:207:7Q9:C3	0.45	2.94	10	1
2:E:656:VAL:CG2	6:E:856:17F:H64	0.45	2.41	10	1
6:E:809:17F:C34	6:E:818:17F:C39	0.45	2.94	10	1
6:E:819:17F:O7	6:E:819:17F:H11A	0.45	2.11	10	2
6:E:838:17F:H19A	6:E:874:17F:C8	0.45	2.37	10	1
6:A:214:17F:H64	6:A:214:17F:C32	0.45	2.41	11	1
6:E:817:17F:H40	6:E:817:17F:C1X	0.45	2.41	13	2
5:B:207:7Q9:C15	5:B:211:7Q9:C22	0.45	2.94	14	2
6:B:214:17F:H57	5:B:220:7Q9:C313	0.45	2.41	14	1
6:E:856:17F:H65	6:E:874:17F:C35	0.45	2.40	15	1
6:B:208:17F:C1Y	6:B:214:17F:H10	0.45	2.40	18	1
6:B:214:17F:C29	5:E:827:7Q9:C318	0.45	2.90	18	1
5:E:820:7Q9:C2	6:E:838:17F:H6	0.45	2.42	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:828:17F:N1	5:E:832:7Q9:O13	0.45	2.49	18	1
6:E:801:17F:H20	6:E:801:17F:C12	0.45	2.36	20	1
6:D:511:17F:H40	6:D:511:17F:H66	0.45	1.87	1	2
1:B:15:GLY:O	1:B:19:LEU:HG	0.45	2.11	2	2
2:D:388:ARG:HH22	2:E:578:GLU:HB2	0.45	1.70	3	1
5:E:821:7Q9:C2	5:E:824:7Q9:C22	0.45	2.95	3	1
5:B:206:7Q9:C33	5:B:212:7Q9:C3	0.45	2.95	4	1
5:B:211:7Q9:O32	5:B:211:7Q9:O21	0.45	2.34	4	1
5:E:840:7Q9:C38	5:E:849:7Q9:C317	0.45	2.95	4	1
5:E:852:7Q9:C11	5:E:852:7Q9:C34	0.45	2.94	4	1
5:D:506:7Q9:O32	5:D:506:7Q9:C2	0.45	2.58	6	2
5:D:514:7Q9:O22	5:D:514:7Q9:C1	0.45	2.58	6	2
5:D:543:7Q9:C318	5:E:875:7Q9:C313	0.45	2.95	6	2
5:E:808:7Q9:O14	5:E:808:7Q9:C12	0.45	2.64	6	1
5:B:207:7Q9:C15	5:B:211:7Q9:C1	0.45	2.95	8	1
6:E:801:17F:O4	5:E:806:7Q9:C13	0.45	2.64	8	1
5:B:211:7Q9:C13	5:B:211:7Q9:O32	0.45	2.65	10	1
2:E:656:VAL:HG23	6:E:856:17F:H64	0.45	1.88	10	1
6:E:807:17F:H20A	6:E:818:17F:C8	0.45	2.41	10	1
5:D:505:7Q9:O32	5:D:505:7Q9:C2	0.45	2.59	11	2
5:E:816:7Q9:O14	5:E:816:7Q9:C12	0.45	2.63	12	3
1:A:87:THR:O	1:A:91:GLU:HG3	0.45	2.11	13	1
5:D:521:7Q9:O31	5:D:525:7Q9:C3	0.45	2.65	17	2
6:D:527:17F:H76	6:E:856:17F:H50	0.45	1.89	20	2
5:E:848:7Q9:C312	5:E:851:7Q9:C37	0.45	2.95	16	1
6:B:214:17F:H47	5:B:217:7Q9:C311	0.45	2.41	18	1
6:D:516:17F:HN1	6:D:516:17F:H18A	0.45	1.72	1	1
5:E:831:7Q9:C34	5:E:831:7Q9:O32	0.45	2.65	19	2
5:E:833:7Q9:C13	6:E:838:17F:O4	0.45	2.65	2	1
5:A:207:7Q9:C3	5:A:207:7Q9:O22	0.45	2.59	3	1
6:B:215:17F:H12A	5:B:216:7Q9:C311	0.45	2.42	3	1
5:D:503:7Q9:O13	6:D:511:17F:C6	0.45	2.64	3	1
6:E:856:17F:O1	6:E:856:17F:C5	0.45	2.62	3	3
6:E:872:17F:H59	6:E:872:17F:C25	0.45	2.41	12	2
6:B:215:17F:H19A	6:D:517:17F:C33	0.45	2.39	6	1
5:D:505:7Q9:C21	5:D:505:7Q9:O31	0.45	2.64	7	3
5:E:802:7Q9:O13	6:E:807:17F:C2	0.45	2.65	8	2
5:E:833:7Q9:O13	5:E:833:7Q9:C2	0.45	2.65	11	4
6:E:838:17F:C27	6:E:838:17F:C42	0.45	2.88	8	3
6:D:501:17F:H55	5:D:509:7Q9:C311	0.45	2.42	10	1
5:A:211:7Q9:C34	5:A:213:7Q9:O32	0.45	2.65	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:549:7Q9:C12	6:E:856:17F:O10	0.45	2.65	11	1
5:E:852:7Q9:C34	5:E:852:7Q9:O32	0.45	2.64	11	1
2:D:344:LEU:HD13	2:E:619:VAL:HG12	0.45	1.87	18	1
1:A:170:MET:HE2	1:A:170:MET:HA	0.45	1.88	19	1
5:B:220:7Q9:C22	6:D:533:17F:C6	0.45	2.88	19	1
5:D:514:7Q9:C15	5:D:519:7Q9:O22	0.45	2.65	19	1
5:D:525:7Q9:O14	5:D:525:7Q9:C23	0.45	2.65	19	1
1:A:146:ALA:N	3:A:201:GSP:O6	0.45	2.50	7	3
5:A:209:7Q9:C311	6:A:214:17F:H61	0.45	2.42	1	1
6:B:219:17F:C17	5:D:545:7Q9:C33	0.45	2.95	1	1
5:D:513:7Q9:C1	5:D:513:7Q9:O22	0.45	2.54	1	1
6:D:510:17F:C17	6:D:516:17F:H8	0.45	2.41	2	1
6:D:510:17F:C17	6:D:527:17F:C18	0.45	2.95	3	1
6:E:838:17F:H11	6:E:838:17F:H57	0.45	1.89	6	3
5:A:212:7Q9:C317	5:E:822:7Q9:C38	0.45	2.95	14	2
1:B:126:ASP:O	1:B:129:GLN:HG2	0.45	2.12	20	2
5:E:867:7Q9:O13	5:E:867:7Q9:C2	0.45	2.64	12	2
5:E:803:7Q9:C3	6:E:807:17F:H9	0.45	2.41	9	1
1:A:99:GLN:O	1:A:103:VAL:HG23	0.45	2.12	10	1
5:E:864:7Q9:C23	5:E:877:7Q9:C1	0.45	2.95	10	1
6:D:517:17F:H69	6:D:517:17F:C29	0.45	2.41	13	2
6:B:219:17F:O8	6:B:219:17F:H10A	0.45	2.11	17	2
5:D:524:7Q9:C21	6:D:527:17F:H19A	0.45	2.42	15	1
6:D:510:17F:H51	6:D:510:17F:H61	0.45	1.88	16	1
6:D:527:17F:H46	6:D:527:17F:C40	0.45	2.41	16	1
5:D:531:7Q9:C36	5:D:540:7Q9:C37	0.45	2.95	16	1
6:E:838:17F:O10	6:E:838:17F:C9	0.45	2.65	16	2
5:A:206:7Q9:C15	5:A:206:7Q9:C1	0.45	2.95	17	1
5:A:203:7Q9:C22	5:A:207:7Q9:C311	0.45	2.95	18	1
3:B:201:GSP:S1G	3:B:201:GSP:O1B	0.45	2.74	19	1
5:B:212:7Q9:C38	5:B:212:7Q9:C312	0.45	2.92	19	1
6:D:510:17F:O1	5:D:524:7Q9:C3	0.45	2.65	20	1
6:B:214:17F:C31	6:B:214:17F:H63	0.45	2.41	1	1
6:D:527:17F:H10	5:D:535:7Q9:C32	0.45	2.41	1	1
6:E:856:17F:O10	6:E:856:17F:H20A	0.45	2.10	1	1
6:A:208:17F:O1	6:A:208:17F:C2	0.45	2.62	2	1
5:B:209:7Q9:O22	5:B:209:7Q9:C1	0.45	2.62	20	6
1:A:35:THR:HG22	1:B:135:ARG:NH2	0.45	2.27	3	1
5:A:210:7Q9:O13	5:A:215:7Q9:C15	0.45	2.64	3	2
6:D:501:17F:H56	6:D:501:17F:H10	0.45	1.88	3	2
5:D:524:7Q9:C15	5:D:526:7Q9:C15	0.45	2.94	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:841:17F:O4	5:E:876:7Q9:C12	0.45	2.65	3	2
5:B:211:7Q9:C1	5:B:211:7Q9:O22	0.45	2.61	16	2
6:D:533:17F:C34	6:D:533:17F:H37	0.45	2.42	4	1
5:B:207:7Q9:C23	5:B:209:7Q9:C311	0.45	2.95	5	1
5:B:209:7Q9:O14	5:B:209:7Q9:C12	0.45	2.65	6	1
5:A:204:7Q9:C315	6:A:208:17F:C42	0.45	2.86	7	1
6:A:214:17F:H72	6:A:214:17F:H47	0.45	1.87	7	1
5:D:514:7Q9:O21	5:D:514:7Q9:P	0.45	2.75	8	3
5:D:549:7Q9:C310	5:E:848:7Q9:C318	0.45	2.95	8	2
1:A:69:ASP:O	1:A:73:ARG:HG3	0.45	2.12	9	2
6:A:208:17F:C27	5:E:823:7Q9:C317	0.45	2.95	9	1
5:D:540:7Q9:O12	5:D:540:7Q9:C2	0.45	2.64	11	2
5:E:857:7Q9:C3	6:E:874:17F:C2	0.45	2.94	10	1
6:D:510:17F:C7	6:D:516:17F:C19	0.45	2.93	11	1
1:B:46:ILE:HG23	1:B:157:TYR:CD1	0.45	2.47	14	1
5:B:213:7Q9:C35	5:B:218:7Q9:C37	0.45	2.95	14	1
1:A:49:GLU:HB3	1:A:164:ARG:NH2	0.45	2.27	16	1
3:A:201:GSP:S1G	3:A:201:GSP:PA	0.45	3.14	16	1
6:E:805:17F:H42	5:E:812:7Q9:C314	0.45	2.42	16	1
5:A:205:7Q9:O14	5:B:204:7Q9:C14	0.45	2.64	17	1
5:A:217:7Q9:O32	5:A:217:7Q9:C23	0.45	2.65	17	1
6:D:534:17F:H76	2:E:692:TYR:CE2	0.45	2.46	17	1
5:B:207:7Q9:C13	6:D:501:17F:C19	0.45	2.94	1	1
5:D:512:7Q9:C317	6:D:528:17F:H35	0.45	2.41	3	1
2:D:426:LYS:O	2:D:430:LEU:HG	0.45	2.12	19	4
5:E:813:7Q9:C3	5:E:829:7Q9:O13	0.45	2.65	4	1
6:E:838:17F:C27	6:E:838:17F:H78	0.45	2.42	5	1
1:A:17:SER:OG	3:A:201:GSP:O2B	0.45	2.35	6	1
6:E:819:17F:C34	5:E:836:7Q9:C34	0.45	2.92	6	1
2:D:269:GLN:HG2	6:D:534:17F:H33	0.45	1.89	7	1
6:E:818:17F:O5	6:E:818:17F:C4	0.45	2.65	8	1
5:B:213:7Q9:C314	5:D:548:7Q9:C316	0.45	2.95	9	1
5:E:803:7Q9:C3	6:E:807:17F:C9	0.45	2.94	9	1
6:B:215:17F:H40	5:E:821:7Q9:C316	0.45	2.42	10	1
5:E:806:7Q9:C1	5:E:806:7Q9:O22	0.45	2.59	12	2
2:D:272:TRP:HB3	6:D:534:17F:H76	0.45	1.89	12	1
6:D:527:17F:H53	6:E:856:17F:H38	0.45	1.89	16	1
5:B:213:7Q9:C318	5:E:825:7Q9:C316	0.45	2.95	17	1
5:B:217:7Q9:C31	5:B:217:7Q9:O21	0.45	2.64	18	1
5:E:806:7Q9:C23	6:E:817:17F:O8	0.45	2.65	18	1
6:A:214:17F:O8	6:A:214:17F:H19A	0.45	2.12	19	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:852:7Q9:C12	5:E:852:7Q9:O11	0.45	2.64	19	1
1:A:14:VAL:CG2	1:A:16:LYS:HG3	0.45	2.41	4	2
6:D:510:17F:O10	6:D:527:17F:H18	0.45	2.12	3	1
6:D:501:17F:H8	6:D:501:17F:C20	0.45	2.42	18	2
6:D:517:17F:H48	6:D:517:17F:H66	0.45	1.87	4	1
6:E:819:17F:H55	5:E:835:7Q9:C317	0.45	2.43	4	2
1:A:89:SER:O	1:A:93:ILE:HG12	0.45	2.11	8	3
5:E:857:7Q9:C33	6:E:874:17F:C21	0.45	2.95	8	1
6:E:811:17F:H75	5:E:822:7Q9:C313	0.45	2.42	11	1
2:D:439:LYS:HE3	2:E:714:LEU:HD12	0.45	1.87	12	1
5:E:865:7Q9:C310	5:E:868:7Q9:C39	0.45	2.95	12	1
2:D:312:MET:CE	6:D:527:17F:H65	0.45	2.42	13	1
6:D:534:17F:O9	6:D:534:17F:C7	0.45	2.65	13	3
5:A:207:7Q9:C37	5:D:504:7Q9:C22	0.45	2.95	14	1
6:D:510:17F:C5	6:D:527:17F:C20	0.45	2.95	14	1
5:A:204:7Q9:C317	6:A:208:17F:H54	0.45	2.42	16	1
5:D:518:7Q9:O32	5:D:518:7Q9:C23	0.45	2.66	16	1
5:E:834:7Q9:C38	5:E:849:7Q9:C310	0.45	2.95	17	1
5:D:519:7Q9:O22	5:D:519:7Q9:C3	0.45	2.60	19	1
5:D:531:7Q9:C311	5:D:531:7Q9:C37	0.45	2.95	20	1
5:D:536:7Q9:O21	5:D:536:7Q9:O14	0.45	2.35	20	1
5:E:842:7Q9:C31	5:E:861:7Q9:C22	0.45	2.95	20	1
6:E:807:17F:H57	6:E:819:17F:C1X	0.44	2.41	1	1
5:E:810:7Q9:O13	5:E:821:7Q9:C12	0.44	2.65	1	1
6:E:811:17F:O6	6:E:811:17F:C7	0.44	2.65	11	5
6:B:215:17F:C36	6:B:215:17F:H47	0.44	2.40	2	1
6:B:215:17F:O10	6:B:215:17F:H4	0.44	2.11	2	2
2:D:419:LEU:HB3	2:D:420:PRO:HD3	0.44	1.90	3	5
5:E:806:7Q9:O21	5:E:806:7Q9:O32	0.44	2.34	2	4
3:A:201:GSP:H5'1	3:A:201:GSP:O1B	0.44	2.13	3	1
2:D:298:GLN:N	2:D:299:PRO:HD2	0.44	2.27	4	8
6:D:534:17F:H58	6:D:534:17F:C2X	0.44	2.42	4	2
6:E:805:17F:P1	6:E:805:17F:N1	0.44	2.89	4	2
1:B:35:THR:OG1	3:B:201:GSP:O3G	0.44	2.35	15	3
6:D:533:17F:H60	5:D:543:7Q9:O22	0.44	2.12	5	1
6:E:838:17F:C12	6:E:856:17F:H9A	0.44	2.42	6	1
6:E:819:17F:O8	6:E:819:17F:H4	0.44	2.12	7	1
6:E:801:17F:H60	5:E:803:7Q9:C22	0.44	2.43	9	1
6:A:214:17F:H44	5:E:840:7Q9:C318	0.44	2.41	11	1
5:E:810:7Q9:C310	5:E:825:7Q9:C312	0.44	2.94	15	4
5:A:209:7Q9:C313	5:E:822:7Q9:C312	0.44	2.95	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:822:7Q9:O13	5:E:822:7Q9:C12	0.44	2.65	17	3
1:A:16:LYS:HG2	3:A:201:GSP:PB	0.44	2.52	13	1
6:E:805:17F:C40	5:E:816:7Q9:C317	0.44	2.84	13	1
5:E:802:7Q9:C310	6:E:807:17F:C26	0.44	2.89	15	1
5:B:211:7Q9:C3	5:B:211:7Q9:C13	0.44	2.95	17	1
3:A:201:GSP:O2A	3:A:201:GSP:PG	0.44	2.75	18	1
6:D:510:17F:H58	6:D:527:17F:H71	0.44	1.88	19	1
5:E:852:7Q9:C15	5:E:852:7Q9:O13	0.44	2.65	20	1
6:A:208:17F:O1	6:A:208:17F:C5	0.44	2.65	7	3
5:D:506:7Q9:C31	5:D:520:7Q9:C22	0.44	2.95	2	1
6:E:841:17F:H9A	5:E:876:7Q9:C11	0.44	2.42	3	1
6:E:838:17F:H38	5:E:857:7Q9:C312	0.44	2.41	4	1
6:E:807:17F:C1Y	6:E:818:17F:H11	0.44	2.42	6	1
2:E:602:ASP:O	2:E:605:GLN:HG2	0.44	2.12	7	1
5:A:205:7Q9:C13	5:A:205:7Q9:O14	0.44	2.65	8	1
5:B:207:7Q9:C15	5:B:211:7Q9:O22	0.44	2.65	10	2
6:D:528:17F:H37	6:D:528:17F:C37	0.44	2.42	8	2
6:D:501:17F:C37	6:D:501:17F:H50	0.44	2.42	9	1
5:E:820:7Q9:C14	5:E:820:7Q9:O13	0.44	2.65	10	2
6:D:528:17F:C23	5:D:532:7Q9:C316	0.44	2.95	11	1
6:D:546:17F:H74	6:D:546:17F:H48	0.44	1.90	11	1
6:E:801:17F:H57	6:E:801:17F:H63	0.44	1.86	11	1
5:E:863:7Q9:C35	5:E:863:7Q9:C22	0.44	2.94	15	1
5:A:204:7Q9:C318	6:A:208:17F:H54	0.44	2.42	16	1
5:B:210:7Q9:C312	5:B:210:7Q9:C38	0.44	2.94	16	1
6:D:534:17F:H11	5:D:539:7Q9:C310	0.44	2.42	17	1
5:E:849:7Q9:C32	5:E:863:7Q9:C1	0.44	2.95	17	1
5:E:823:7Q9:C22	5:E:845:7Q9:C14	0.44	2.94	18	1
1:A:31:GLU:HG3	1:B:128:LYS:HB3	0.44	1.86	19	1
6:E:809:17F:H68	6:E:809:17F:H54	0.44	1.90	20	1
6:D:510:17F:C40	5:E:832:7Q9:C315	0.44	2.95	1	1
5:D:506:7Q9:O31	5:D:506:7Q9:C21	0.44	2.65	2	1
6:D:533:17F:C22	6:D:533:17F:H63	0.44	2.42	2	1
5:E:825:7Q9:O13	5:E:825:7Q9:C12	0.44	2.65	18	2
6:D:527:17F:H68	6:D:527:17F:H39	0.44	1.89	3	1
5:E:848:7Q9:C313	5:E:851:7Q9:C35	0.44	2.94	4	1
5:D:505:7Q9:O31	5:D:505:7Q9:O22	0.44	2.35	20	2
5:E:877:7Q9:C1	5:E:877:7Q9:O22	0.44	2.63	8	1
5:B:211:7Q9:P	6:D:501:17F:H5	0.44	2.53	9	1
5:E:853:7Q9:O21	5:E:853:7Q9:O32	0.44	2.36	9	2
5:A:215:7Q9:C3	5:A:215:7Q9:O22	0.44	2.58	10	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:B:208:17F:O10	6:B:208:17F:H4	0.44	2.12	10	2
6:D:501:17F:H53	5:D:525:7Q9:C318	0.44	2.42	10	1
6:E:841:17F:C9	5:E:876:7Q9:O14	0.44	2.55	10	1
5:B:203:7Q9:C12	5:B:204:7Q9:O32	0.44	2.65	17	2
5:A:206:7Q9:O14	5:A:206:7Q9:C12	0.44	2.66	13	1
6:E:818:17F:O2	6:E:818:17F:C2	0.44	2.60	13	1
5:D:537:7Q9:O31	6:D:546:17F:C10	0.44	2.65	20	2
5:E:814:7Q9:C33	5:E:820:7Q9:C36	0.44	2.95	17	1
6:E:874:17F:N1	6:E:874:17F:C10	0.44	2.79	17	1
5:B:211:7Q9:C314	6:B:215:17F:C1Z	0.44	2.95	18	1
5:E:812:7Q9:C12	5:E:827:7Q9:C32	0.44	2.96	18	1
6:D:533:17F:H12	6:D:533:17F:C34	0.44	2.43	19	1
1:B:22:GLN:HG3	1:B:146:ALA:HB1	0.44	1.88	1	1
6:D:501:17F:H38	5:D:508:7Q9:C35	0.44	2.42	1	1
5:D:506:7Q9:C318	6:D:517:17F:H49	0.44	2.43	1	1
5:D:522:7Q9:C1	5:D:545:7Q9:C32	0.44	2.95	1	1
5:E:808:7Q9:O22	5:E:808:7Q9:C1	0.44	2.62	6	5
6:E:872:17F:H62	6:E:872:17F:C31	0.44	2.41	1	3
6:B:208:17F:H5	5:B:212:7Q9:C36	0.44	2.41	2	1
5:B:216:7Q9:O31	5:B:216:7Q9:C21	0.44	2.65	8	7
5:B:216:7Q9:O21	5:B:216:7Q9:O14	0.44	2.36	14	5
5:D:523:7Q9:C14	5:D:523:7Q9:P	0.44	3.05	2	4
6:E:807:17F:H65	6:E:818:17F:H38	0.44	1.88	2	1
6:D:501:17F:H40	6:D:501:17F:H10A	0.44	1.88	4	1
5:D:526:7Q9:C22	5:D:526:7Q9:C38	0.44	2.96	11	3
6:D:546:17F:C1Y	6:D:546:17F:C17	0.44	2.95	4	1
3:B:201:GSP:S1G	3:B:201:GSP:O2A	0.44	2.76	5	1
6:D:527:17F:H32	6:D:527:17F:C6	0.44	2.42	5	1
5:B:209:7Q9:O32	5:D:505:7Q9:C1	0.44	2.66	6	1
6:D:511:17F:H69	6:D:511:17F:H59	0.44	1.89	6	2
5:B:217:7Q9:C23	5:B:217:7Q9:C32	0.44	2.95	7	1
6:D:528:17F:H66	6:D:528:17F:H12A	0.44	1.89	7	1
6:E:855:17F:H59	5:E:867:7Q9:C310	0.44	2.42	7	1
5:E:857:7Q9:O22	5:E:857:7Q9:C1	0.44	2.63	7	4
1:B:101:LYS:HD2	1:B:107:GLU:HG3	0.44	1.90	9	1
5:E:825:7Q9:C14	5:E:825:7Q9:P	0.44	3.05	10	3
6:D:517:17F:H8A	5:D:529:7Q9:O22	0.44	2.12	11	1
6:E:817:17F:C11	5:E:833:7Q9:C32	0.44	2.92	15	1
6:D:528:17F:C6	5:D:532:7Q9:C35	0.44	2.96	16	1
6:D:533:17F:C35	6:D:533:17F:C21	0.44	2.96	16	1
2:E:628:GLU:HA	2:E:631:ARG:HD3	0.44	1.89	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:855:17F:H37	5:E:857:7Q9:C315	0.44	2.42	17	1
5:A:204:7Q9:C23	5:A:209:7Q9:C33	0.44	2.95	18	1
5:E:869:7Q9:O32	5:E:869:7Q9:O21	0.44	2.35	18	1
6:E:855:17F:C31	6:E:855:17F:H40	0.44	2.41	20	1
6:E:870:17F:C32	6:E:870:17F:C2X	0.44	2.95	20	1
1:B:117:LYS:HG2	3:B:201:GSP:C6	0.44	2.47	9	2
6:B:215:17F:O5	5:D:515:7Q9:C13	0.44	2.65	2	2
2:E:722:LEU:HG	2:E:726:LYS:HE3	0.44	1.88	1	1
5:E:803:7Q9:C23	5:E:803:7Q9:C37	0.44	2.94	1	1
5:E:837:7Q9:O32	6:E:841:17F:C19	0.44	2.66	1	1
6:E:841:17F:C8	5:E:876:7Q9:O14	0.44	2.65	1	1
6:D:510:17F:H8A	6:D:516:17F:C18	0.44	2.42	2	1
6:E:807:17F:H50	6:E:809:17F:H62	0.44	1.89	2	1
2:D:429:PHE:CE1	6:D:533:17F:H69	0.44	2.47	3	1
6:E:805:17F:O6	6:E:805:17F:O7	0.44	2.35	3	4
6:E:805:17F:C4	5:E:810:7Q9:C14	0.44	2.91	5	1
5:A:206:7Q9:C35	5:A:212:7Q9:C37	0.44	2.96	6	2
6:D:510:17F:H18	5:D:524:7Q9:C3	0.44	2.43	6	1
5:B:217:7Q9:C15	5:D:522:7Q9:C2	0.44	2.95	7	1
5:D:508:7Q9:C32	5:D:509:7Q9:C23	0.44	2.95	8	1
6:D:510:17F:H60	6:D:516:17F:H37	0.44	1.88	9	1
5:D:513:7Q9:C37	6:D:528:17F:H34	0.44	2.43	10	1
6:E:807:17F:H50	6:E:807:17F:H74	0.44	1.90	10	1
2:E:598:GLN:HA	5:E:876:7Q9:C313	0.44	2.43	11	1
6:D:501:17F:O1	5:D:509:7Q9:C22	0.44	2.65	15	1
6:E:818:17F:H59	6:E:818:17F:H36	0.44	1.89	15	1
6:E:819:17F:C6	5:E:836:7Q9:C21	0.44	2.84	15	1
6:E:819:17F:C7	6:E:819:17F:H20A	0.44	2.42	16	1
5:E:816:7Q9:O32	5:E:816:7Q9:C11	0.44	2.66	20	1
6:B:214:17F:C4	5:B:217:7Q9:O32	0.44	2.59	1	1
6:E:818:17F:O10	6:E:818:17F:C4	0.44	2.65	15	3
5:E:839:7Q9:O32	5:E:839:7Q9:C23	0.44	2.66	15	3
5:D:513:7Q9:C14	5:D:526:7Q9:O13	0.44	2.66	3	1
5:E:846:7Q9:C22	5:E:869:7Q9:O13	0.44	2.65	3	2
5:D:536:7Q9:C1	5:D:547:7Q9:C3	0.44	2.95	4	1
5:E:810:7Q9:C14	5:E:816:7Q9:O32	0.44	2.66	14	4
1:B:82:PHE:HB2	1:B:89:SER:HB2	0.44	1.87	5	3
5:D:529:7Q9:O14	5:D:529:7Q9:C12	0.44	2.66	16	4
2:D:421:VAL:HB	2:E:736:TYR:CE2	0.44	2.47	6	1
5:D:504:7Q9:O31	6:D:516:17F:H18A	0.44	2.13	10	2
5:E:843:7Q9:C3	5:E:859:7Q9:C34	0.44	2.96	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:A:204:7Q9:C315	6:A:208:17F:H48	0.44	2.41	8	1
5:D:535:7Q9:C317	6:E:874:17F:H76	0.44	2.42	8	1
5:A:209:7Q9:C32	5:A:212:7Q9:C37	0.44	2.96	20	2
6:E:872:17F:C32	6:E:872:17F:H44	0.44	2.42	11	1
5:D:514:7Q9:O13	5:D:514:7Q9:C21	0.44	2.66	12	1
5:E:815:7Q9:C1	5:E:815:7Q9:O32	0.44	2.66	20	3
3:B:201:GSP:O2B	3:B:201:GSP:O1A	0.44	2.34	15	2
5:E:821:7Q9:C31	5:E:824:7Q9:C22	0.44	2.95	15	1
6:E:855:17F:H31	5:E:867:7Q9:C39	0.44	2.42	16	1
5:D:514:7Q9:C311	5:D:519:7Q9:C318	0.44	2.96	17	1
6:D:510:17F:C26	6:D:516:17F:C40	0.44	2.95	18	1
5:E:824:7Q9:C38	6:E:841:17F:H69	0.44	2.43	18	1
6:D:510:17F:C27	6:D:516:17F:C22	0.44	2.95	19	1
5:D:519:7Q9:C314	5:D:540:7Q9:C318	0.44	2.95	19	1
5:D:524:7Q9:C12	5:D:526:7Q9:C32	0.44	2.96	19	1
6:D:533:17F:N1	6:D:533:17F:H19	0.44	2.27	19	1
5:A:216:7Q9:C37	5:D:547:7Q9:C32	0.44	2.95	1	1
6:D:510:17F:C25	6:D:510:17F:H36	0.44	2.41	6	2
6:E:807:17F:H38	6:E:809:17F:C20	0.44	2.42	1	1
5:E:821:7Q9:O31	5:E:821:7Q9:C21	0.44	2.66	2	3
5:E:813:7Q9:C23	5:E:829:7Q9:C3	0.44	2.96	2	1
5:A:216:7Q9:O21	5:A:216:7Q9:P	0.44	2.75	5	3
5:E:837:7Q9:C35	6:E:841:17F:H55	0.44	2.43	3	1
5:A:205:7Q9:O22	5:A:205:7Q9:C1	0.44	2.60	4	6
1:B:65:SER:O	1:B:68:ARG:HG2	0.44	2.13	4	1
6:E:819:17F:H52	6:E:819:17F:C38	0.44	2.38	11	2
5:D:506:7Q9:O11	5:D:506:7Q9:C21	0.44	2.66	12	3
6:D:510:17F:C42	6:D:516:17F:H72	0.44	2.43	6	1
5:D:514:7Q9:C37	5:D:519:7Q9:C318	0.44	2.96	6	1
6:D:516:17F:H50	6:D:516:17F:C39	0.44	2.43	6	1
2:E:630:ALA:HB1	5:E:878:7Q9:C317	0.44	2.43	6	1
5:E:853:7Q9:O21	5:E:853:7Q9:O14	0.44	2.35	6	1
1:A:47:ASP:OD1	1:A:161:ARG:HD2	0.44	2.13	9	2
5:B:210:7Q9:O22	5:B:210:7Q9:C3	0.44	2.63	10	2
6:E:801:17F:C23	5:E:804:7Q9:C37	0.44	2.96	8	1
5:E:831:7Q9:O32	5:E:831:7Q9:O21	0.44	2.35	8	1
5:A:205:7Q9:C34	5:D:503:7Q9:O22	0.44	2.66	9	3
5:E:824:7Q9:C37	6:E:841:17F:H39	0.44	2.43	9	1
6:B:219:17F:H62	6:B:219:17F:C31	0.44	2.34	10	2
6:E:807:17F:C28	6:E:807:17F:H74	0.44	2.42	10	1
5:D:541:7Q9:O22	5:D:541:7Q9:C1	0.44	2.62	18	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:B:214:17F:H74	6:B:214:17F:H43	0.44	1.88	12	1
6:B:215:17F:H72	5:E:821:7Q9:C315	0.44	2.42	13	1
1:A:36:ILE:HD11	1:B:135:ARG:HD3	0.44	1.89	14	1
6:D:510:17F:H19	5:D:524:7Q9:C2	0.44	2.43	15	1
5:A:204:7Q9:C314	6:A:208:17F:H71	0.44	2.43	16	1
2:D:414:LEU:O	2:D:418:LEU:HG	0.44	2.13	16	1
6:D:527:17F:H42	6:D:527:17F:H36	0.44	1.88	16	1
6:E:819:17F:H8A	6:E:819:17F:C1Y	0.44	2.43	16	1
5:E:832:7Q9:C13	6:E:838:17F:O2	0.44	2.66	16	1
6:B:215:17F:H70	6:B:215:17F:C30	0.44	2.41	18	1
1:A:59:ALA:HA	3:A:201:GSP:O2G	0.44	2.12	20	1
5:E:836:7Q9:O21	5:E:836:7Q9:O32	0.44	2.36	17	3
6:E:805:17F:C25	5:E:816:7Q9:C317	0.44	2.95	2	3
6:D:501:17F:H9A	6:D:501:17F:C1Y	0.44	2.43	3	1
6:D:533:17F:H65	6:D:533:17F:H58	0.44	1.89	3	1
6:A:208:17F:C31	6:A:208:17F:C35	0.44	2.78	5	1
1:B:133:LEU:HG	1:B:137:TYR:CE2	0.44	2.48	6	1
6:D:510:17F:C19	6:D:527:17F:H19	0.44	2.38	6	1
5:E:869:7Q9:O22	5:E:869:7Q9:C1	0.44	2.63	6	4
5:B:203:7Q9:C313	6:B:208:17F:H74	0.44	2.43	7	1
2:D:306:LYS:O	2:D:310:GLU:HG3	0.44	2.13	7	1
6:E:819:17F:H52	6:E:819:17F:H69	0.44	1.88	18	2
5:E:806:7Q9:C13	6:E:817:17F:O2	0.44	2.66	8	1
5:E:844:7Q9:C13	5:E:877:7Q9:O13	0.44	2.66	14	2
6:E:856:17F:C38	6:E:856:17F:H37	0.44	2.43	8	1
5:D:507:7Q9:C313	5:E:820:7Q9:C318	0.44	2.96	9	1
6:E:819:17F:C20	6:E:819:17F:O9	0.44	2.62	10	1
6:D:546:17F:H61	6:D:546:17F:H46	0.44	1.88	11	1
6:D:517:17F:H51	6:D:517:17F:H75	0.44	1.88	12	1
6:D:546:17F:H9	6:D:546:17F:C31	0.44	2.43	12	1
5:E:836:7Q9:C318	5:E:852:7Q9:C318	0.44	2.95	12	1
2:D:313:GLU:OE1	2:D:316:ARG:HD3	0.44	2.12	15	1
5:E:851:7Q9:C2	5:E:851:7Q9:C11	0.44	2.96	15	1
5:E:862:7Q9:O13	5:E:862:7Q9:C12	0.44	2.65	20	2
6:E:811:17F:O10	5:E:823:7Q9:C11	0.44	2.66	19	2
5:A:203:7Q9:C15	5:B:204:7Q9:C1	0.44	2.96	20	1
5:D:507:7Q9:C34	6:D:516:17F:C31	0.44	2.96	1	1
5:E:863:7Q9:O14	5:E:863:7Q9:C12	0.44	2.65	18	6
6:D:511:17F:H58	6:D:511:17F:H63	0.44	1.52	10	7
6:E:819:17F:H6A	5:E:836:7Q9:O22	0.44	2.12	2	1
5:A:211:7Q9:C318	5:A:213:7Q9:C318	0.44	2.96	16	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:B:214:17F:O10	6:B:219:17F:H8	0.44	2.13	3	1
6:E:870:17F:H59	6:E:870:17F:H62	0.44	1.53	10	3
5:D:537:7Q9:C15	5:D:537:7Q9:P	0.44	3.06	8	5
1:A:32:TYR:CE2	3:A:201:GSP:H4'	0.44	2.48	5	1
6:D:510:17F:C25	6:D:510:17F:C2X	0.44	2.96	9	2
1:A:144:THR:HG22	1:A:151:GLY:HA3	0.44	1.89	7	2
5:B:212:7Q9:C33	5:B:217:7Q9:C34	0.44	2.96	7	2
5:D:521:7Q9:O21	5:D:521:7Q9:C31	0.44	2.66	20	3
5:D:522:7Q9:C35	5:D:545:7Q9:C311	0.44	2.96	9	1
2:E:674:LEU:HD21	6:E:855:17F:C2X	0.44	2.35	9	2
5:A:211:7Q9:C14	6:B:214:17F:O4	0.44	2.66	12	2
6:D:510:17F:C1Y	6:D:527:17F:H20	0.44	2.43	13	1
6:E:817:17F:C22	5:E:833:7Q9:C311	0.44	2.96	13	1
5:E:829:7Q9:C38	5:E:852:7Q9:C314	0.44	2.95	13	1
2:D:308:TRP:CZ3	6:E:856:17F:H75	0.44	2.47	15	1
5:B:212:7Q9:C311	5:B:212:7Q9:C37	0.44	2.96	16	1
6:D:501:17F:H12	6:D:501:17F:C20	0.44	2.43	16	1
6:D:533:17F:C30	6:E:870:17F:H67	0.44	2.43	19	1
6:D:510:17F:C42	6:E:856:17F:H44	0.44	2.42	20	1
5:D:515:7Q9:O13	5:D:519:7Q9:C15	0.44	2.66	20	1
2:E:591:GLU:HB2	5:E:861:7Q9:C39	0.44	2.42	20	1
2:E:595:ALA:HA	2:E:598:GLN:NE2	0.44	2.27	20	1
6:E:818:17F:C41	6:E:818:17F:C26	0.44	2.88	20	1
5:A:207:7Q9:C13	5:D:507:7Q9:O14	0.43	2.66	3	3
5:D:504:7Q9:C13	5:D:507:7Q9:O13	0.43	2.66	1	1
5:E:866:7Q9:O13	5:E:866:7Q9:C2	0.43	2.65	5	6
5:E:822:7Q9:C14	5:E:822:7Q9:P	0.43	3.06	12	3
1:A:6:LEU:HD13	1:A:159:LEU:HD23	0.43	1.88	4	1
5:D:515:7Q9:C3	6:D:517:17F:H19	0.43	2.43	4	1
5:A:211:7Q9:C15	6:B:214:17F:O5	0.43	2.66	6	1
5:E:820:7Q9:P	5:E:820:7Q9:O21	0.43	2.76	6	2
5:E:866:7Q9:C33	5:E:876:7Q9:C33	0.43	2.96	6	1
2:D:374:LEU:HD21	5:D:529:7Q9:C317	0.43	2.43	7	1
6:B:214:17F:O8	6:B:214:17F:H19	0.43	2.12	8	1
2:D:423:GLU:O	2:D:427:VAL:HG23	0.43	2.13	10	1
5:E:820:7Q9:C1	5:E:833:7Q9:O13	0.43	2.66	10	1
5:D:507:7Q9:C3	6:D:516:17F:HN1A	0.43	2.25	11	1
6:A:214:17F:HN1	5:D:539:7Q9:C13	0.43	2.26	12	1
5:E:813:7Q9:C15	5:E:813:7Q9:P	0.43	3.06	13	2
1:A:29:VAL:HG11	1:B:128:LYS:HG2	0.43	1.90	14	1
6:D:501:17F:H35	6:D:501:17F:C24	0.43	2.43	14	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:809:17F:H61	6:E:809:17F:H48	0.43	1.89	16	1
2:D:331:ARG:HD2	2:D:332:GLN:OE1	0.43	2.13	18	1
6:E:838:17F:H70	6:E:874:17F:C30	0.43	2.43	20	1
6:D:501:17F:C22	5:D:508:7Q9:C35	0.43	2.96	1	1
5:D:512:7Q9:C21	5:D:512:7Q9:O32	0.43	2.65	1	1
5:E:871:7Q9:O22	5:E:871:7Q9:C1	0.43	2.63	10	2
5:D:544:7Q9:C35	6:D:546:17F:H32	0.43	2.43	4	1
1:A:4:TYR:CE2	1:A:51:CYS:HB3	0.43	2.48	5	1
6:A:214:17F:H54	5:E:840:7Q9:C313	0.43	2.43	5	1
5:E:803:7Q9:O31	5:E:803:7Q9:C21	0.43	2.66	5	4
5:E:832:7Q9:O13	5:E:851:7Q9:C13	0.43	2.66	5	1
5:A:209:7Q9:O11	5:A:209:7Q9:C21	0.43	2.67	11	5
6:E:872:17F:O2	6:E:872:17F:C8	0.43	2.66	6	1
5:E:873:7Q9:O32	5:E:873:7Q9:C21	0.43	2.65	15	2
5:D:508:7Q9:C313	5:E:813:7Q9:C316	0.43	2.97	7	1
6:D:528:17F:H76	5:E:878:7Q9:C316	0.43	2.43	9	1
5:E:825:7Q9:C12	5:E:825:7Q9:O13	0.43	2.66	11	3
5:E:868:7Q9:C32	5:E:873:7Q9:C13	0.43	2.95	9	2
6:A:208:17F:H43	5:E:822:7Q9:C318	0.43	2.42	13	1
1:B:16:LYS:HB2	3:B:201:GSP:O2B	0.43	2.13	16	1
5:E:865:7Q9:C3	5:E:868:7Q9:C15	0.43	2.95	17	1
5:B:220:7Q9:C22	6:D:533:17F:O8	0.43	2.67	18	1
5:A:210:7Q9:C32	5:A:212:7Q9:C22	0.43	2.96	19	1
5:E:813:7Q9:C314	6:E:818:17F:C30	0.43	2.97	1	3
5:B:209:7Q9:O22	5:D:502:7Q9:C14	0.43	2.66	3	1
6:D:501:17F:H31	6:D:501:17F:H9A	0.43	1.90	3	1
5:D:547:7Q9:C22	5:D:547:7Q9:C13	0.43	2.96	3	1
5:E:837:7Q9:O13	6:E:841:17F:C5	0.43	2.60	5	2
5:E:802:7Q9:O11	5:E:802:7Q9:C21	0.43	2.66	11	5
5:E:826:7Q9:O13	5:E:840:7Q9:C14	0.43	2.66	8	3
1:A:156:PHE:O	1:A:160:VAL:HG23	0.43	2.13	5	1
5:E:863:7Q9:O22	5:E:863:7Q9:C1	0.43	2.63	5	1
6:E:872:17F:H44	6:E:872:17F:C33	0.43	2.43	5	1
1:B:120:LEU:HD11	3:B:201:GSP:N2	0.43	2.28	6	1
6:B:208:17F:C4	6:B:208:17F:O10	0.43	2.62	6	1
5:E:854:7Q9:O12	5:E:854:7Q9:C14	0.43	2.66	6	1
5:D:513:7Q9:C1	6:D:528:17F:H8A	0.43	2.43	8	1
6:E:805:17F:H43	5:E:816:7Q9:C317	0.43	2.42	10	1
5:D:502:7Q9:C313	5:E:813:7Q9:C318	0.43	2.97	12	1
2:E:660:ARG:HD2	6:E:874:17F:H31	0.43	1.89	13	2
1:B:144:THR:HG21	1:B:155:ALA:HB2	0.43	1.89	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:543:7Q9:O31	5:D:543:7Q9:C34	0.43	2.66	14	1
5:D:539:7Q9:C317	5:E:873:7Q9:C318	0.43	2.96	15	1
5:D:547:7Q9:O11	5:D:547:7Q9:C21	0.43	2.66	15	2
1:B:13:GLY:HA2	3:B:201:GSP:H4'	0.43	1.89	16	1
1:A:168:GLU:HG2	1:A:172:LYS:HE2	0.43	1.88	19	1
5:D:524:7Q9:C15	5:D:526:7Q9:C13	0.43	2.96	19	1
5:E:854:7Q9:O14	5:E:854:7Q9:C12	0.43	2.66	20	2
5:D:519:7Q9:O32	5:D:519:7Q9:O21	0.43	2.37	12	2
6:E:855:17F:C3	5:E:857:7Q9:C15	0.43	2.96	1	1
5:D:504:7Q9:C13	6:D:516:17F:O2	0.43	2.66	4	1
6:E:828:17F:C4	6:E:828:17F:H1A	0.43	2.44	4	1
6:E:838:17F:H49	6:E:874:17F:H53	0.43	1.90	5	1
5:B:209:7Q9:C13	5:B:209:7Q9:P	0.43	3.06	6	1
6:D:517:17F:H43	6:D:517:17F:C37	0.43	2.42	6	1
6:E:807:17F:H71	6:E:818:17F:H55	0.43	1.90	6	2
5:E:820:7Q9:C22	5:E:833:7Q9:C32	0.43	2.97	6	1
5:E:829:7Q9:C1	5:E:852:7Q9:C35	0.43	2.95	6	1
6:E:838:17F:H2	6:E:874:17F:O8	0.43	2.14	6	1
6:D:517:17F:H59	6:D:517:17F:H64	0.43	1.90	7	1
5:E:847:7Q9:O21	5:E:847:7Q9:C31	0.43	2.67	7	4
5:E:832:7Q9:C22	6:E:838:17F:H6A	0.43	2.43	8	2
6:D:510:17F:H58	6:D:516:17F:C21	0.43	2.43	10	1
6:D:517:17F:H66	6:D:517:17F:H51	0.43	1.90	10	1
5:D:549:7Q9:C35	6:E:856:17F:H54	0.43	2.44	12	1
1:B:146:ALA:N	3:B:201:GSP:O6	0.43	2.51	20	4
6:B:219:17F:C38	5:D:522:7Q9:C311	0.43	2.90	13	1
5:D:536:7Q9:C15	5:D:547:7Q9:C22	0.43	2.96	14	1
5:A:212:7Q9:C15	6:A:214:17F:O5	0.43	2.66	16	1
1:B:78:PHE:HE2	1:B:104:LYS:HD2	0.43	1.73	16	1
2:E:634:LEU:HD13	5:E:878:7Q9:C315	0.43	2.43	16	1
6:B:214:17F:HN1A	6:B:214:17F:H18A	0.43	1.73	17	1
6:D:516:17F:C25	6:D:527:17F:H41	0.43	2.33	19	1
5:A:215:7Q9:O32	5:D:536:7Q9:C23	0.43	2.67	20	1
6:E:819:17F:H20	5:E:829:7Q9:C22	0.43	2.43	20	1
1:A:72:MET:HE2	1:A:100:ILE:CG1	0.43	2.43	1	1
6:E:809:17F:H34	6:E:818:17F:H68	0.43	1.91	1	2
6:E:818:17F:C42	6:E:818:17F:H45	0.43	2.43	1	1
6:E:838:17F:H36	6:E:838:17F:H69	0.43	1.90	20	2
5:A:204:7Q9:C14	6:B:208:17F:O1	0.43	2.66	3	1
2:E:634:LEU:HG	5:E:862:7Q9:C313	0.43	2.43	3	2
5:E:825:7Q9:C31	5:E:825:7Q9:O21	0.43	2.66	9	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:B:208:17F:C31	6:B:208:17F:H40	0.43	2.43	4	1
2:D:422:LEU:HD13	5:E:875:7Q9:C318	0.43	2.43	7	2
5:B:218:7Q9:O22	5:B:218:7Q9:C1	0.43	2.62	18	3
6:D:511:17F:C30	6:E:828:17F:H48	0.43	2.44	6	1
5:E:837:7Q9:O14	5:E:837:7Q9:O21	0.43	2.36	6	1
1:A:27:HIS:CE1	1:B:127:THR:HG21	0.43	2.48	7	1
5:D:507:7Q9:O12	5:D:507:7Q9:O21	0.43	2.36	8	1
6:A:214:17F:H9A	5:D:539:7Q9:C37	0.43	2.43	9	1
5:E:823:7Q9:C14	5:E:823:7Q9:P	0.43	3.06	13	2
5:A:206:7Q9:C15	5:A:206:7Q9:O11	0.43	2.67	12	1
5:D:519:7Q9:C311	5:D:519:7Q9:C36	0.43	2.97	12	1
2:E:634:LEU:HB2	5:E:878:7Q9:C315	0.43	2.43	12	1
5:E:829:7Q9:C313	5:E:851:7Q9:C37	0.43	2.96	12	1
6:E:855:17F:H48	6:E:855:17F:H72	0.43	1.90	12	1
5:D:515:7Q9:C317	5:E:821:7Q9:C318	0.43	2.97	15	2
5:A:215:7Q9:C3	5:D:536:7Q9:C23	0.43	2.97	15	1
2:E:705:GLU:HG3	2:E:706:LYS:H	0.43	1.72	15	1
5:D:505:7Q9:O31	5:D:505:7Q9:C21	0.43	2.67	20	3
2:E:630:ALA:HB1	5:E:878:7Q9:C314	0.43	2.43	16	1
1:B:146:ALA:HB3	3:B:201:GSP:O6	0.43	2.13	17	1
5:D:522:7Q9:C313	5:D:545:7Q9:C318	0.43	2.97	18	1
6:E:817:17F:H63	6:E:817:17F:H58	0.43	1.57	18	1
6:A:208:17F:H18	5:A:211:7Q9:C3	0.43	2.43	19	1
5:D:537:7Q9:O31	6:D:546:17F:H29	0.43	2.11	19	1
6:D:527:17F:C29	6:E:856:17F:H74	0.43	2.44	20	1
5:D:538:7Q9:C318	5:E:842:7Q9:C318	0.43	2.97	20	1
6:D:511:17F:H77	6:D:511:17F:H50	0.43	1.90	1	1
1:A:26:ASN:ND2	1:A:149:ARG:HH12	0.43	2.11	2	1
2:D:342:SER:HB2	2:D:343:PRO:HD3	0.43	1.90	2	1
6:B:208:17F:C4	6:B:208:17F:H1	0.43	2.43	4	1
5:E:823:7Q9:C38	5:E:865:7Q9:C314	0.43	2.96	4	1
5:E:850:7Q9:C313	6:E:870:17F:C20	0.43	2.96	5	1
5:B:209:7Q9:C36	5:D:503:7Q9:O31	0.43	2.67	6	1
2:E:673:ARG:O	2:E:677:ARG:HG3	0.43	2.12	6	1
1:A:58:THR:HG21	1:A:71:TYR:CE1	0.43	2.47	7	1
5:D:532:7Q9:O31	5:D:532:7Q9:O11	0.43	2.36	7	4
6:E:818:17F:O7	6:E:818:17F:P1	0.43	2.77	7	1
5:E:850:7Q9:C313	6:E:870:17F:H61	0.43	2.43	8	1
5:E:863:7Q9:C32	5:E:873:7Q9:O31	0.43	2.67	9	4
6:B:215:17F:H63	6:B:215:17F:H58	0.43	1.62	11	1
5:E:813:7Q9:O22	5:E:829:7Q9:C14	0.43	2.66	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:870:17F:H62	6:E:870:17F:H59	0.43	1.54	20	4
1:B:99:GLN:O	1:B:103:VAL:HG23	0.43	2.13	14	1
1:B:6:LEU:HD12	1:B:55:ILE:HG12	0.43	1.89	15	1
5:D:518:7Q9:C32	5:D:537:7Q9:C2	0.43	2.96	15	1
5:E:849:7Q9:C3	5:E:863:7Q9:C1	0.43	2.96	16	2
5:A:204:7Q9:C39	6:A:208:17F:H66	0.43	2.44	16	1
5:A:215:7Q9:O11	5:A:215:7Q9:O32	0.43	2.36	16	1
5:B:217:7Q9:C315	5:D:548:7Q9:C312	0.43	2.96	17	1
5:E:834:7Q9:O22	5:E:849:7Q9:C12	0.43	2.67	17	1
5:B:220:7Q9:C2	5:D:543:7Q9:O13	0.43	2.66	18	1
6:D:510:17F:C32	6:D:527:17F:H75	0.43	2.44	18	1
2:D:269:GLN:HG2	6:D:534:17F:C1Z	0.43	2.43	19	1
6:D:511:17F:H55	6:E:828:17F:H48	0.43	1.90	19	1
5:E:820:7Q9:O14	5:E:820:7Q9:O21	0.43	2.36	19	1
2:E:627:GLN:O	2:E:631:ARG:HB2	0.43	2.13	19	2
6:E:807:17F:O8	6:E:807:17F:H10	0.43	2.13	2	1
5:B:213:7Q9:C13	5:B:213:7Q9:O11	0.43	2.67	12	4
2:D:374:LEU:HD23	5:D:529:7Q9:C310	0.43	2.44	3	3
5:D:504:7Q9:C3	6:D:516:17F:HN1	0.43	2.26	3	1
5:D:519:7Q9:C36	5:D:540:7Q9:C310	0.43	2.96	3	1
6:D:533:17F:H5	5:D:543:7Q9:C13	0.43	2.43	3	1
5:D:540:7Q9:C12	5:D:540:7Q9:C21	0.43	2.96	3	1
5:E:863:7Q9:C12	5:E:863:7Q9:O14	0.43	2.66	19	2
6:E:872:17F:O7	6:E:872:17F:O6	0.43	2.36	3	2
5:E:860:7Q9:O21	5:E:860:7Q9:C31	0.43	2.67	11	6
5:D:536:7Q9:C15	5:D:547:7Q9:O22	0.43	2.66	10	2
6:E:874:17F:H49	6:E:874:17F:C40	0.43	2.43	5	1
6:A:208:17F:C1Y	6:B:208:17F:C1X	0.43	2.85	6	1
6:D:510:17F:H31	6:D:516:17F:C9	0.43	2.44	6	1
6:E:818:17F:H45	6:E:818:17F:C42	0.43	2.43	6	1
5:A:211:7Q9:C37	5:A:211:7Q9:C311	0.43	2.94	7	1
6:E:870:17F:C9	5:E:871:7Q9:O13	0.43	2.67	7	1
5:A:206:7Q9:C318	5:A:212:7Q9:C318	0.43	2.96	8	1
6:D:516:17F:H74	6:D:527:17F:H53	0.43	1.91	8	1
6:E:818:17F:H59	6:E:818:17F:H62	0.43	1.54	9	2
6:D:528:17F:H49	5:E:852:7Q9:C316	0.43	2.43	10	1
6:D:546:17F:H41	6:D:546:17F:H70	0.43	1.91	11	1
6:E:819:17F:H18A	5:E:829:7Q9:C11	0.43	2.44	11	1
1:A:5:LYS:HA	1:A:54:ASP:HB3	0.43	1.89	16	2
5:D:507:7Q9:C31	6:D:516:17F:N1	0.43	2.81	12	1
5:A:205:7Q9:O11	5:A:205:7Q9:O31	0.43	2.37	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:E:608:TRP:HE3	5:E:860:7Q9:C318	0.43	2.27	13	1
6:D:501:17F:O5	6:D:501:17F:H4	0.43	2.14	14	1
5:B:220:7Q9:C13	5:B:220:7Q9:O14	0.43	2.66	15	1
5:D:514:7Q9:C15	5:D:514:7Q9:C1	0.43	2.97	16	2
5:E:850:7Q9:O13	5:E:850:7Q9:C12	0.43	2.66	16	1
6:E:819:17F:H71	5:E:852:7Q9:C36	0.43	2.43	17	1
5:D:549:7Q9:C11	5:E:851:7Q9:O13	0.43	2.67	18	1
5:B:216:7Q9:C318	5:D:514:7Q9:C315	0.43	2.96	19	1
5:D:532:7Q9:O13	5:D:532:7Q9:C12	0.43	2.67	19	1
5:D:536:7Q9:C13	5:D:536:7Q9:O21	0.43	2.66	19	1
6:E:841:17F:H35	6:E:841:17F:H39	0.43	1.63	20	1
5:A:204:7Q9:C310	6:A:208:17F:C9	0.43	2.97	1	1
5:A:212:7Q9:C315	6:A:214:17F:H76	0.43	2.44	1	1
6:E:809:17F:H29	6:E:809:17F:H56	0.43	1.90	1	1
6:D:510:17F:H57	6:D:527:17F:H60	0.43	1.89	2	1
6:D:510:17F:C18	6:D:516:17F:C8	0.43	2.92	2	1
6:D:510:17F:H62	6:D:510:17F:H59	0.43	1.54	6	1
6:D:516:17F:H36	6:D:527:17F:C22	0.43	2.43	6	1
5:E:813:7Q9:C313	6:E:819:17F:C30	0.43	2.96	12	2
6:E:872:17F:O2	6:E:872:17F:C2	0.43	2.67	6	2
5:D:525:7Q9:O22	5:D:525:7Q9:C1	0.43	2.62	7	2
5:A:213:7Q9:O12	5:A:213:7Q9:O21	0.43	2.37	13	3
1:B:144:THR:HG22	1:B:151:GLY:HA3	0.43	1.91	9	1
5:E:822:7Q9:C11	5:E:822:7Q9:C1	0.43	2.97	15	2
2:D:337:LEU:HG	2:E:626:LEU:HD13	0.43	1.89	12	1
2:D:309:GLN:HA	6:D:527:17F:H63	0.43	1.90	13	1
5:E:813:7Q9:C1	5:E:829:7Q9:O13	0.43	2.67	13	1
5:B:206:7Q9:C34	5:B:212:7Q9:C3	0.43	2.96	14	1
2:D:373:ARG:HA	2:D:373:ARG:NE	0.43	2.27	15	1
5:D:503:7Q9:C37	5:D:505:7Q9:C35	0.43	2.97	15	1
5:E:842:7Q9:C37	5:E:842:7Q9:C311	0.43	2.94	15	1
5:D:537:7Q9:C2	6:D:546:17F:H29	0.43	2.44	17	1
2:E:671:ARG:HD3	5:E:857:7Q9:C22	0.43	2.44	18	1
6:E:828:17F:H75	5:E:829:7Q9:C35	0.43	2.43	18	1
6:E:874:17F:C2X	6:E:874:17F:C24	0.43	2.87	20	1
5:A:209:7Q9:C35	6:A:214:17F:H60	0.43	2.44	1	1
5:E:852:7Q9:C12	5:E:852:7Q9:O32	0.43	2.67	2	1
6:A:208:17F:H48	6:E:811:17F:H70	0.43	1.91	3	1
5:B:203:7Q9:C14	5:B:205:7Q9:C13	0.43	2.97	3	1
6:E:818:17F:O10	6:E:818:17F:H4	0.43	2.14	20	4
6:D:511:17F:H66	6:D:511:17F:H40	0.43	1.90	13	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:A:205:7Q9:C13	5:A:205:7Q9:O11	0.43	2.67	5	2
5:D:523:7Q9:C14	5:D:547:7Q9:O13	0.43	2.66	5	1
6:E:809:17F:C37	6:E:809:17F:H54	0.43	2.43	6	1
6:D:501:17F:H40	6:D:501:17F:C10	0.43	2.44	7	1
5:E:830:7Q9:O22	5:E:830:7Q9:C1	0.43	2.64	7	3
5:B:211:7Q9:C316	6:B:215:17F:C1Z	0.43	2.92	8	1
6:E:818:17F:H4	6:E:818:17F:O5	0.43	2.12	8	1
5:A:209:7Q9:C317	5:E:822:7Q9:C312	0.43	2.96	9	1
5:D:529:7Q9:O13	5:D:529:7Q9:C2	0.43	2.67	9	1
5:A:209:7Q9:O21	6:A:214:17F:N1	0.43	2.52	10	1
5:D:506:7Q9:C1	6:D:517:17F:O1	0.43	2.66	10	1
5:B:205:7Q9:O11	5:B:205:7Q9:C21	0.43	2.67	11	1
6:D:517:17F:HN1A	5:D:529:7Q9:C13	0.43	2.27	11	1
5:D:536:7Q9:O12	5:D:536:7Q9:O21	0.43	2.37	12	3
5:A:206:7Q9:C15	5:A:206:7Q9:P	0.43	3.07	13	1
2:E:664:ALA:N	2:E:665:PRO:HD2	0.43	2.29	14	1
5:E:868:7Q9:O32	5:E:873:7Q9:C13	0.43	2.66	14	1
5:E:815:7Q9:O32	5:E:815:7Q9:C1	0.43	2.67	15	1
6:E:856:17F:H68	6:E:874:17F:H68	0.43	1.91	15	1
5:A:204:7Q9:C313	6:A:208:17F:H44	0.43	2.44	16	1
1:A:15:GLY:HA3	1:A:116:ASN:ND2	0.43	2.28	18	1
6:E:838:17F:H49	6:E:874:17F:H55	0.43	1.90	18	1
5:E:876:7Q9:O32	5:E:876:7Q9:C23	0.43	2.67	18	1
5:E:824:7Q9:C312	5:E:824:7Q9:C38	0.43	2.94	20	1
5:A:204:7Q9:C15	6:B:208:17F:O5	0.43	2.67	1	1
5:B:212:7Q9:C21	5:B:213:7Q9:C12	0.43	2.97	2	1
5:E:821:7Q9:C13	5:E:821:7Q9:O21	0.43	2.66	2	1
6:E:870:17F:H35	6:E:870:17F:C1Y	0.43	2.43	2	1
6:E:805:17F:H39	6:E:805:17F:C1X	0.43	2.43	6	2
6:E:805:17F:H41	6:E:805:17F:H36	0.43	1.91	3	1
5:E:823:7Q9:O14	5:E:823:7Q9:C12	0.43	2.67	15	2
5:E:857:7Q9:C38	6:E:874:17F:C21	0.43	2.97	3	1
1:A:38:ASP:O	1:A:56:LEU:HG	0.43	2.14	5	1
5:E:864:7Q9:P	5:E:864:7Q9:O21	0.43	2.77	5	5
5:A:205:7Q9:C318	5:E:814:7Q9:C312	0.43	2.97	6	1
6:E:841:17F:C23	6:E:841:17F:C1X	0.43	2.97	7	1
6:E:856:17F:C36	6:E:874:17F:H60	0.43	2.43	7	1
1:A:43:GLN:HB2	1:B:161:ARG:NH1	0.43	2.28	8	1
5:B:207:7Q9:C13	6:D:501:17F:C17	0.43	2.97	8	2
5:D:520:7Q9:C315	5:D:538:7Q9:C314	0.43	2.97	8	1
5:E:831:7Q9:O22	5:E:831:7Q9:C1	0.43	2.62	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:832:7Q9:C313	6:E:856:17F:H55	0.43	2.43	8	1
5:A:205:7Q9:C23	5:A:207:7Q9:C39	0.43	2.96	10	1
6:A:214:17F:H10	6:A:214:17F:O8	0.43	2.14	10	1
6:D:527:17F:HN1	6:D:527:17F:C18	0.43	2.27	10	1
6:A:214:17F:N1	5:D:539:7Q9:C13	0.43	2.82	12	1
1:A:16:LYS:HG2	3:A:201:GSP:O1B	0.43	2.14	13	1
6:D:510:17F:C6	6:D:527:17F:C20	0.43	2.87	14	1
5:A:216:7Q9:O11	5:A:216:7Q9:C21	0.43	2.66	15	1
6:E:807:17F:C30	6:E:818:17F:C42	0.43	2.94	15	1
6:E:828:17F:H40	6:E:828:17F:H59	0.43	1.91	15	1
3:A:201:GSP:S1G	3:A:201:GSP:O3A	0.43	2.77	16	1
6:E:809:17F:C34	6:E:809:17F:H48	0.43	2.44	16	1
6:E:870:17F:H43	6:E:870:17F:C38	0.43	2.44	18	1
5:B:209:7Q9:C32	5:D:503:7Q9:O14	0.43	2.67	19	1
5:B:216:7Q9:O22	5:B:216:7Q9:O31	0.43	2.37	19	1
1:A:147:LYS:HB2	3:A:201:GSP:C6	0.43	2.48	20	1
5:B:205:7Q9:C38	5:B:211:7Q9:C37	0.43	2.96	20	1
5:D:514:7Q9:P	5:D:514:7Q9:O21	0.42	2.77	18	2
6:E:811:17F:H6A	5:E:823:7Q9:C3	0.42	2.44	1	1
6:D:510:17F:C7	6:D:516:17F:H9A	0.42	2.43	2	1
2:E:684:ASN:O	2:E:688:ARG:HD2	0.42	2.13	10	2
5:E:812:7Q9:C14	5:E:816:7Q9:C22	0.42	2.96	8	2
1:B:123:ARG:H	1:B:123:ARG:HD2	0.42	1.74	4	1
6:B:214:17F:C38	6:B:214:17F:H56	0.42	2.44	4	1
5:D:506:7Q9:C34	6:D:517:17F:C21	0.42	2.95	4	1
5:E:823:7Q9:O21	5:E:823:7Q9:C31	0.42	2.66	9	6
5:E:848:7Q9:O22	5:E:848:7Q9:C1	0.42	2.61	7	3
1:A:159:LEU:O	1:A:163:ILE:HG13	0.42	2.14	6	2
5:A:209:7Q9:C315	5:E:822:7Q9:C311	0.42	2.97	6	1
6:E:805:17F:C33	5:E:810:7Q9:C36	0.42	2.97	11	2
2:D:302:ASP:HB2	5:D:535:7Q9:C35	0.42	2.43	7	1
6:B:214:17F:C31	5:B:220:7Q9:C34	0.42	2.98	8	1
5:D:520:7Q9:O11	5:D:525:7Q9:C15	0.42	2.67	8	1
6:A:214:17F:H9A	5:D:539:7Q9:C38	0.42	2.44	9	1
5:D:518:7Q9:C32	5:D:537:7Q9:O22	0.42	2.67	9	1
6:E:838:17F:H65	6:E:838:17F:H11A	0.42	1.83	9	1
5:A:215:7Q9:C36	6:D:534:17F:H45	0.42	2.45	10	1
6:E:818:17F:C1	5:E:835:7Q9:O14	0.42	2.67	11	1
5:E:823:7Q9:C34	5:E:823:7Q9:C23	0.42	2.97	13	1
6:E:838:17F:C35	6:E:838:17F:H57	0.42	2.44	15	1
5:A:210:7Q9:O11	5:A:210:7Q9:C21	0.42	2.66	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:517:17F:H57	6:D:517:17F:C21	0.42	2.44	18	1
2:E:581:GLY:O	2:E:585:GLU:HG2	0.42	2.14	18	1
5:D:504:7Q9:O21	5:D:504:7Q9:C31	0.42	2.67	19	1
2:D:440:LEU:HD22	5:D:537:7Q9:C315	0.42	2.44	20	1
6:E:807:17F:C32	6:E:807:17F:C12	0.42	2.97	20	1
5:D:524:7Q9:C13	5:D:526:7Q9:C32	0.42	2.97	1	1
5:D:520:7Q9:C318	5:E:866:7Q9:C310	0.42	2.97	2	1
6:D:527:17F:H12	6:D:527:17F:H31	0.42	1.91	3	1
5:D:538:7Q9:O32	5:D:538:7Q9:C14	0.42	2.67	3	1
6:D:501:17F:H12A	5:D:509:7Q9:O22	0.42	2.14	5	1
5:D:548:7Q9:C23	5:E:827:7Q9:C34	0.42	2.97	6	1
5:A:205:7Q9:C13	5:A:205:7Q9:P	0.42	3.07	8	1
6:E:811:17F:O6	6:E:811:17F:H2	0.42	2.13	9	1
6:E:817:17F:O8	6:E:817:17F:H5	0.42	2.13	9	1
6:E:841:17F:H11	5:E:876:7Q9:C3	0.42	2.44	9	1
6:D:516:17F:H45	5:D:535:7Q9:C316	0.42	2.44	10	1
5:B:205:7Q9:C22	5:B:211:7Q9:C34	0.42	2.97	11	1
6:B:208:17F:H31	6:B:214:17F:C12	0.42	2.40	12	1
6:D:511:17F:H30	6:D:528:17F:H55	0.42	1.90	12	1
5:E:806:7Q9:C15	5:E:806:7Q9:C22	0.42	2.98	12	1
5:E:852:7Q9:C23	5:E:878:7Q9:C22	0.42	2.96	13	2
6:A:208:17F:H70	6:E:811:17F:C27	0.42	2.41	14	1
6:D:533:17F:O8	5:D:543:7Q9:C13	0.42	2.67	17	1
6:E:838:17F:C31	6:E:838:17F:C19	0.42	2.89	18	1
5:A:205:7Q9:C1	5:B:204:7Q9:C22	0.42	2.97	19	1
5:B:206:7Q9:C311	5:B:212:7Q9:C311	0.42	2.97	19	1
6:D:533:17F:H55	6:E:870:17F:H67	0.42	1.91	19	1
6:D:510:17F:H76	6:D:510:17F:C30	0.42	2.43	1	1
5:E:837:7Q9:C11	6:E:841:17F:C17	0.42	2.97	1	1
5:E:837:7Q9:O11	6:E:841:17F:O10	0.42	2.36	1	1
5:B:205:7Q9:C12	5:B:206:7Q9:C23	0.42	2.97	2	1
6:E:801:17F:H69	5:E:803:7Q9:C312	0.42	2.44	2	1
6:E:818:17F:O5	5:E:824:7Q9:C15	0.42	2.68	3	1
5:E:868:7Q9:O22	5:E:868:7Q9:C3	0.42	2.63	13	3
6:D:527:17F:C1Y	6:D:527:17F:O1	0.42	2.67	4	2
5:E:808:7Q9:C315	6:E:817:17F:H52	0.42	2.44	4	2
6:A:208:17F:H31	6:B:208:17F:C12	0.42	2.44	6	1
5:D:502:7Q9:O21	5:D:502:7Q9:O32	0.42	2.37	6	1
6:E:809:17F:H29	6:E:809:17F:C24	0.42	2.44	6	1
6:D:528:17F:H10A	6:D:528:17F:C34	0.42	2.44	7	1
6:E:807:17F:O2	5:E:813:7Q9:C14	0.42	2.67	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:A:214:17F:C2X	6:A:214:17F:C24	0.42	2.96	10	1
5:B:213:7Q9:C35	5:B:218:7Q9:C39	0.42	2.97	11	1
5:B:216:7Q9:O21	5:B:216:7Q9:C12	0.42	2.67	12	1
5:B:205:7Q9:C317	6:E:805:17F:H51	0.42	2.45	14	1
5:D:505:7Q9:C38	6:E:828:17F:H77	0.42	2.43	15	1
5:E:821:7Q9:O31	5:E:821:7Q9:O22	0.42	2.37	15	1
5:E:830:7Q9:C22	5:E:830:7Q9:C37	0.42	2.97	16	1
1:A:29:VAL:HG12	1:B:127:THR:HB	0.42	1.90	17	1
5:E:810:7Q9:C22	5:E:816:7Q9:C38	0.42	2.97	17	1
6:D:534:17F:C34	6:D:534:17F:C2X	0.42	2.97	18	1
5:B:211:7Q9:C314	6:B:215:17F:H60	0.42	2.44	1	1
5:B:220:7Q9:O11	5:B:220:7Q9:C21	0.42	2.67	3	6
6:E:801:17F:H35	6:E:801:17F:C24	0.42	2.44	2	1
5:D:506:7Q9:O22	5:D:506:7Q9:P	0.42	2.77	3	1
6:D:528:17F:O10	6:D:528:17F:C9	0.42	2.67	3	1
2:E:730:LEU:O	2:E:733:LEU:HB2	0.42	2.14	3	1
2:E:634:LEU:HD22	5:E:878:7Q9:C315	0.42	2.44	11	2
6:D:510:17F:C1	6:D:516:17F:C4	0.42	2.92	7	1
6:E:801:17F:H40	5:E:804:7Q9:C38	0.42	2.45	7	1
5:E:825:7Q9:C39	5:E:844:7Q9:C39	0.42	2.97	7	1
5:E:861:7Q9:O22	5:E:861:7Q9:C1	0.42	2.65	7	1
1:A:15:GLY:HA2	3:A:201:GSP:PB	0.42	2.54	8	1
2:D:430:LEU:CD2	6:D:533:17F:H33	0.42	2.43	8	2
5:D:502:7Q9:C15	5:D:502:7Q9:C1	0.42	2.97	12	2
6:E:805:17F:H68	6:E:805:17F:H55	0.42	1.90	20	2
6:E:874:17F:O7	6:E:874:17F:C10	0.42	2.62	9	1
5:D:547:7Q9:C14	5:D:547:7Q9:O14	0.42	2.68	16	2
5:A:213:7Q9:C318	5:E:830:7Q9:C318	0.42	2.98	11	1
2:D:330:ALA:CB	6:D:528:17F:H78	0.42	2.44	11	1
6:D:534:17F:H10A	5:D:539:7Q9:C39	0.42	2.44	11	1
5:A:211:7Q9:C13	6:B:214:17F:O4	0.42	2.66	12	1
5:B:216:7Q9:C13	5:D:515:7Q9:O14	0.42	2.67	12	1
6:E:811:17F:O8	6:E:811:17F:C4	0.42	2.68	13	2
6:E:818:17F:C9	6:E:819:17F:H9A	0.42	2.45	13	1
5:A:204:7Q9:C314	6:A:208:17F:C26	0.42	2.96	14	2
6:D:527:17F:O9	6:D:527:17F:C7	0.42	2.68	14	1
1:A:15:GLY:O	1:A:19:LEU:HG	0.42	2.15	15	1
6:D:533:17F:C17	6:D:533:17F:O8	0.42	2.67	16	1
6:E:819:17F:H6	5:E:836:7Q9:C2	0.42	2.44	16	1
6:E:828:17F:C8	5:E:832:7Q9:C33	0.42	2.98	17	1
5:D:518:7Q9:C32	5:D:537:7Q9:C1	0.42	2.97	20	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:872:17F:H36	6:E:872:17F:H39	0.42	1.65	2	6
6:E:818:17F:O1	6:E:818:17F:C2	0.42	2.66	2	1
5:E:863:7Q9:C14	5:E:873:7Q9:O13	0.42	2.67	2	1
6:E:874:17F:HN1	6:E:874:17F:C17	0.42	2.27	20	2
6:E:817:17F:H58	6:E:817:17F:H63	0.42	1.64	3	6
5:A:205:7Q9:C316	5:E:820:7Q9:C314	0.42	2.97	5	1
6:B:215:17F:H11	5:D:515:7Q9:C23	0.42	2.44	5	1
2:D:352:ALA:O	2:D:356:VAL:HG23	0.42	2.14	5	2
6:E:841:17F:H37	5:E:876:7Q9:O32	0.42	2.15	5	1
1:A:83:ALA:HB1	1:A:85:ASN:OD1	0.42	2.14	6	1
2:E:615:TYR:O	2:E:619:VAL:HG23	0.42	2.14	9	3
6:E:811:17F:H36	6:E:811:17F:C24	0.42	2.41	6	1
5:D:548:7Q9:O32	5:D:548:7Q9:C21	0.42	2.67	7	1
5:E:814:7Q9:O21	5:E:814:7Q9:O32	0.42	2.37	7	2
6:D:533:17F:H65	6:D:533:17F:H59	0.42	1.90	8	1
5:B:220:7Q9:C21	5:D:543:7Q9:C22	0.42	2.97	9	1
2:D:273:ASP:HB2	6:D:534:17F:H20	0.42	1.91	10	1
6:E:811:17F:C5	5:E:823:7Q9:C11	0.42	2.94	10	1
5:B:216:7Q9:C313	5:D:515:7Q9:C310	0.42	2.98	11	1
6:B:208:17F:C1Y	6:B:214:17F:H12	0.42	2.39	12	1
6:D:501:17F:H9	5:D:506:7Q9:C22	0.42	2.44	12	1
6:E:818:17F:C23	5:E:835:7Q9:C37	0.42	2.97	12	1
6:E:870:17F:H29	5:E:871:7Q9:C23	0.42	2.44	12	1
5:D:515:7Q9:C37	5:D:541:7Q9:C310	0.42	2.97	13	1
5:A:217:7Q9:C14	5:A:217:7Q9:O14	0.42	2.67	14	1
6:E:811:17F:H5	5:E:823:7Q9:C15	0.42	2.44	14	1
5:A:216:7Q9:C13	5:D:547:7Q9:O13	0.42	2.68	16	1
6:D:510:17F:H67	6:D:510:17F:H52	0.42	1.87	16	1
6:E:874:17F:H54	6:E:874:17F:H72	0.42	1.90	16	2
6:E:870:17F:H30	6:E:870:17F:H56	0.42	1.92	17	1
6:D:501:17F:H42	6:D:501:17F:C34	0.42	2.45	18	1
5:B:207:7Q9:C313	5:E:803:7Q9:C318	0.42	2.97	20	1
1:A:117:LYS:NZ	3:A:201:GSP:C5	0.42	2.88	2	2
5:E:844:7Q9:C14	5:E:864:7Q9:O13	0.42	2.67	3	2
6:E:856:17F:H37	6:E:874:17F:C36	0.42	2.45	2	1
5:E:826:7Q9:O22	5:E:826:7Q9:C1	0.42	2.65	3	2
5:E:826:7Q9:C1	5:E:826:7Q9:O22	0.42	2.65	5	2
6:A:208:17F:H39	6:A:208:17F:H35	0.42	1.57	18	2
6:D:533:17F:O10	6:D:533:17F:C6	0.42	2.50	7	1
5:A:205:7Q9:C32	5:D:503:7Q9:C3	0.42	2.97	8	1
5:B:213:7Q9:C37	5:D:514:7Q9:C36	0.42	2.97	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:533:17F:H44	6:D:533:17F:H74	0.42	1.91	8	1
6:D:517:17F:C30	5:E:842:7Q9:C318	0.42	2.97	9	1
5:A:207:7Q9:C35	5:D:504:7Q9:O32	0.42	2.67	10	1
6:A:208:17F:O10	6:A:208:17F:H6A	0.42	2.15	11	2
6:D:533:17F:H39	6:D:533:17F:H35	0.42	1.66	11	2
6:E:809:17F:C10	5:E:810:7Q9:C33	0.42	2.98	11	1
1:A:21:ILE:HG23	1:A:25:GLN:NE2	0.42	2.29	12	1
5:B:211:7Q9:C15	5:B:211:7Q9:C1	0.42	2.97	13	1
5:E:857:7Q9:C21	6:E:874:17F:H2	0.42	2.44	13	1
5:A:212:7Q9:C36	6:A:214:17F:H74	0.42	2.45	14	1
5:D:515:7Q9:C15	6:D:517:17F:H5	0.42	2.45	14	1
5:E:836:7Q9:O14	5:E:854:7Q9:C15	0.42	2.68	14	1
5:D:505:7Q9:C310	6:D:511:17F:H48	0.42	2.45	15	1
5:A:215:7Q9:O32	5:D:536:7Q9:C22	0.42	2.67	16	1
5:D:512:7Q9:C2	5:D:530:7Q9:C13	0.42	2.98	17	1
6:E:828:17F:H40	6:E:828:17F:C34	0.42	2.44	17	1
5:B:203:7Q9:C313	6:B:208:17F:H75	0.42	2.45	20	1
5:D:531:7Q9:C37	5:D:531:7Q9:C311	0.42	2.98	1	2
6:D:510:17F:H20	5:D:524:7Q9:O32	0.42	2.14	4	1
5:D:506:7Q9:C311	6:D:517:17F:H38	0.42	2.44	6	1
1:A:15:GLY:HA2	3:A:201:GSP:O1A	0.42	2.15	7	1
6:E:828:17F:C9	5:E:832:7Q9:C33	0.42	2.98	7	1
6:E:838:17F:HN1	6:E:838:17F:P1	0.42	2.36	17	2
2:E:737:THR:HG21	5:E:875:7Q9:C36	0.42	2.43	8	1
6:E:809:17F:H9A	6:E:809:17F:C18	0.42	2.41	9	1
5:D:531:7Q9:O13	5:D:540:7Q9:C14	0.42	2.68	10	1
6:E:841:17F:C24	6:E:841:17F:H56	0.42	2.45	12	2
6:E:801:17F:H40	6:E:801:17F:H35	0.42	1.61	17	2
5:E:802:7Q9:C38	6:E:807:17F:C24	0.42	2.98	11	1
5:B:218:7Q9:C35	5:D:514:7Q9:C32	0.42	2.97	12	1
2:D:368:ASP:HA	2:D:371:ARG:NE	0.42	2.30	12	1
6:E:807:17F:O2	5:E:813:7Q9:C12	0.42	2.68	12	1
5:B:211:7Q9:C316	6:B:215:17F:H52	0.42	2.44	15	1
5:B:212:7Q9:O14	5:B:217:7Q9:O31	0.42	2.38	15	1
6:E:838:17F:C22	5:E:857:7Q9:C310	0.42	2.97	15	2
5:E:842:7Q9:C21	5:E:842:7Q9:C11	0.42	2.98	15	1
1:A:81:VAL:HG22	1:A:114:VAL:HB	0.42	1.90	17	1
5:A:212:7Q9:C36	5:A:212:7Q9:C312	0.42	2.97	18	1
6:E:801:17F:H36	6:E:801:17F:H20	0.42	1.91	20	1
6:E:819:17F:H19A	5:E:829:7Q9:C23	0.42	2.45	20	1
6:D:527:17F:O2	5:D:535:7Q9:C13	0.42	2.68	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:841:17F:H8A	5:E:876:7Q9:O14	0.42	2.15	1	1
5:B:206:7Q9:C14	5:B:206:7Q9:C23	0.42	2.97	2	1
5:B:204:7Q9:O31	5:B:204:7Q9:O11	0.42	2.38	19	3
2:D:257:PHE:CE2	2:E:706:LYS:HG2	0.42	2.50	4	2
2:D:389:LEU:HD21	5:D:540:7Q9:C313	0.42	2.44	4	1
5:D:503:7Q9:O32	5:D:503:7Q9:O21	0.42	2.36	4	3
6:E:855:17F:H39	6:E:855:17F:H36	0.42	1.59	8	2
5:A:213:7Q9:C312	5:A:213:7Q9:C38	0.42	2.97	5	1
6:D:527:17F:O1	6:D:527:17F:O7	0.42	2.37	9	2
6:E:874:17F:H63	6:E:874:17F:H58	0.42	1.69	8	2
5:E:831:7Q9:O32	5:E:831:7Q9:C34	0.42	2.67	11	3
5:D:508:7Q9:C313	5:E:813:7Q9:C314	0.42	2.98	8	1
6:E:838:17F:O2	6:E:856:17F:H9A	0.42	2.15	8	1
6:B:215:17F:H67	6:B:215:17F:C27	0.42	2.43	10	1
6:D:510:17F:H8	6:D:516:17F:C7	0.42	2.45	12	1
5:E:813:7Q9:C312	6:E:818:17F:H54	0.42	2.45	12	1
6:A:208:17F:H19A	6:B:208:17F:C1X	0.42	2.44	13	1
6:D:501:17F:C22	5:D:509:7Q9:C23	0.42	2.98	13	1
5:D:519:7Q9:C35	5:D:540:7Q9:C310	0.42	2.98	13	1
5:D:518:7Q9:C313	6:D:533:17F:C26	0.42	2.98	14	1
5:D:520:7Q9:O21	5:D:520:7Q9:P	0.42	2.78	16	1
5:A:205:7Q9:O13	5:A:205:7Q9:C12	0.42	2.68	17	1
5:B:218:7Q9:C22	5:D:531:7Q9:C14	0.42	2.98	17	1
5:E:833:7Q9:C15	6:E:855:17F:O5	0.42	2.68	17	1
5:E:834:7Q9:C37	5:E:834:7Q9:C311	0.42	2.97	17	1
6:D:510:17F:P1	6:D:516:17F:C4	0.42	3.07	19	1
5:E:850:7Q9:C38	6:E:870:17F:H19A	0.42	2.45	19	1
2:D:312:MET:HE1	6:D:527:17F:C36	0.42	2.45	1	1
5:E:848:7Q9:C311	5:E:851:7Q9:C35	0.42	2.97	2	2
6:B:214:17F:H76	5:B:217:7Q9:C313	0.42	2.45	3	1
5:D:515:7Q9:C310	6:D:517:17F:H64	0.42	2.45	4	1
5:D:537:7Q9:C31	6:D:546:17F:C10	0.42	2.98	5	1
6:B:215:17F:H52	6:B:215:17F:H60	0.42	1.92	17	2
6:D:517:17F:H55	5:D:538:7Q9:C316	0.42	2.45	6	1
6:E:817:17F:H56	5:E:833:7Q9:C33	0.42	2.45	6	1
1:B:98:GLU:HA	1:B:101:LYS:HE2	0.42	1.91	7	1
2:D:273:ASP:HB2	6:D:534:17F:C31	0.42	2.45	7	2
5:E:835:7Q9:C22	5:E:836:7Q9:C22	0.42	2.98	8	2
5:D:535:7Q9:C14	5:D:535:7Q9:O11	0.42	2.67	10	1
5:E:813:7Q9:O22	5:E:829:7Q9:C11	0.42	2.67	10	1
5:E:857:7Q9:C3	6:E:874:17F:H10A	0.42	2.45	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:VAL:HG13	1:A:79:LEU:HD23	0.42	1.92	12	1
6:B:215:17F:H64	6:B:215:17F:C1X	0.42	2.45	12	1
2:E:634:LEU:HD13	5:E:878:7Q9:C318	0.42	2.44	12	1
1:A:30:ASP:HA	3:A:201:GSP:O2'	0.42	2.13	13	1
5:A:209:7Q9:C316	5:E:839:7Q9:C314	0.42	2.98	13	1
6:E:819:17F:H57	6:E:819:17F:C23	0.42	2.35	13	1
5:D:523:7Q9:O22	5:D:523:7Q9:C1	0.42	2.63	15	1
6:D:528:17F:C21	6:D:528:17F:C38	0.42	2.97	15	1
5:A:204:7Q9:C314	6:A:208:17F:H78	0.42	2.44	16	1
6:E:809:17F:H61	6:E:809:17F:C28	0.42	2.44	16	1
6:E:811:17F:C41	5:E:822:7Q9:C315	0.42	2.95	16	1
5:E:867:7Q9:O32	5:E:867:7Q9:O21	0.42	2.37	16	1
5:D:512:7Q9:C23	5:D:530:7Q9:C33	0.42	2.98	17	1
6:E:807:17F:H63	6:E:807:17F:H59	0.42	1.63	17	2
6:E:819:17F:H70	5:E:852:7Q9:C311	0.42	2.45	17	1
5:D:548:7Q9:O14	5:E:847:7Q9:C12	0.42	2.68	18	1
2:E:620:GLU:HG2	5:E:858:7Q9:C311	0.42	2.44	18	1
6:E:807:17F:H59	6:E:807:17F:H63	0.42	1.68	16	2
5:E:847:7Q9:C32	6:E:872:17F:C11	0.42	2.98	1	1
5:D:503:7Q9:C313	6:D:511:17F:H78	0.42	2.45	2	1
6:D:511:17F:C3	5:D:526:7Q9:C15	0.42	2.98	2	1
5:E:837:7Q9:O32	6:E:841:17F:C12	0.42	2.63	3	1
6:B:208:17F:H44	6:B:214:17F:H50	0.42	1.92	4	1
2:D:320:GLU:HG3	2:D:323:ARG:NH2	0.42	2.29	4	1
6:E:872:17F:O10	6:E:872:17F:C6	0.42	2.58	4	2
2:D:404:SER:CB	5:D:542:7Q9:C312	0.42	2.98	5	1
6:E:807:17F:C22	6:E:809:17F:H20	0.42	2.41	5	1
5:E:816:7Q9:C13	5:E:825:7Q9:O22	0.42	2.68	5	1
6:A:208:17F:H47	5:E:823:7Q9:C316	0.42	2.45	6	1
6:E:819:17F:O10	5:E:836:7Q9:C3	0.42	2.68	6	1
2:D:342:SER:HB3	2:D:343:PRO:HD3	0.42	1.91	7	1
6:D:510:17F:C7	6:D:516:17F:O7	0.42	2.68	8	1
5:D:531:7Q9:O13	5:D:540:7Q9:C22	0.42	2.67	8	1
5:D:513:7Q9:O31	5:D:513:7Q9:C21	0.42	2.68	18	2
5:D:513:7Q9:C39	6:D:528:17F:H71	0.42	2.45	12	1
6:E:809:17F:H30	5:E:810:7Q9:C33	0.42	2.45	12	1
1:B:17:SER:HB2	3:B:201:GSP:O3G	0.42	2.15	14	1
6:D:516:17F:H32	5:D:535:7Q9:C313	0.42	2.45	14	1
6:E:817:17F:C3	5:E:820:7Q9:C13	0.42	2.98	14	1
6:E:818:17F:H10A	6:E:819:17F:H9A	0.42	1.92	14	1
5:D:518:7Q9:C38	6:D:533:17F:H30	0.42	2.44	16	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:818:17F:C10	6:E:819:17F:C9	0.42	2.97	15	1
5:E:832:7Q9:C22	6:E:838:17F:O8	0.42	2.68	15	1
5:E:848:7Q9:C34	5:E:851:7Q9:C35	0.42	2.98	16	1
6:E:874:17F:O7	6:E:874:17F:C17	0.42	2.68	16	2
5:E:834:7Q9:C15	6:E:855:17F:C3	0.42	2.97	17	1
5:B:211:7Q9:C318	6:B:215:17F:H53	0.42	2.45	18	1
5:B:217:7Q9:C12	5:D:522:7Q9:O14	0.42	2.68	19	1
1:B:148:THR:O	1:B:149:ARG:HB3	0.42	2.14	20	1
6:D:516:17F:C42	6:E:838:17F:C41	0.42	2.98	20	1
5:D:523:7Q9:O14	5:D:523:7Q9:C12	0.41	2.68	4	2
2:E:656:VAL:CG1	6:E:856:17F:H64	0.41	2.44	5	2
6:E:818:17F:H46	5:E:835:7Q9:C310	0.41	2.45	2	1
5:E:848:7Q9:C22	5:E:852:7Q9:O12	0.41	2.68	2	1
6:D:510:17F:C17	6:D:527:17F:H18	0.41	2.45	3	1
6:E:807:17F:O4	5:E:813:7Q9:C13	0.41	2.68	3	1
5:B:211:7Q9:O21	5:B:211:7Q9:C31	0.41	2.68	4	1
5:E:832:7Q9:C22	6:E:838:17F:H4	0.41	2.45	4	1
5:E:852:7Q9:O12	5:E:852:7Q9:O21	0.41	2.38	4	1
5:B:203:7Q9:C31	6:B:208:17F:C6	0.41	2.97	5	1
5:D:514:7Q9:C13	5:D:519:7Q9:O22	0.41	2.68	6	1
6:E:801:17F:H5	5:E:803:7Q9:O14	0.41	2.15	8	1
6:E:819:17F:H75	5:E:852:7Q9:C311	0.41	2.45	8	1
2:D:434:GLU:O	2:D:438:LYS:HG3	0.41	2.15	19	2
5:E:837:7Q9:P	5:E:837:7Q9:O21	0.41	2.78	11	1
6:D:511:17F:C1X	6:D:528:17F:H55	0.41	2.45	12	1
2:E:590:LEU:HG	2:E:594:LYS:HE2	0.41	1.92	12	1
1:B:23:LEU:HG	1:B:42:LYS:HE2	0.41	1.92	15	1
5:D:512:7Q9:C318	6:D:528:17F:H35	0.41	2.45	16	1
5:E:853:7Q9:O22	5:E:853:7Q9:C1	0.41	2.65	17	2
5:B:206:7Q9:C12	5:B:210:7Q9:O32	0.41	2.68	17	1
5:A:210:7Q9:O14	5:A:215:7Q9:C13	0.41	2.68	19	1
6:D:516:17F:H59	6:D:516:17F:H63	0.41	1.61	20	1
1:B:144:THR:HB	1:B:152:VAL:HG22	0.41	1.90	1	1
5:E:812:7Q9:O31	5:E:812:7Q9:C21	0.41	2.68	9	2
5:D:502:7Q9:O22	5:D:502:7Q9:C3	0.41	2.60	4	1
6:D:510:17F:O9	6:D:516:17F:C11	0.41	2.68	5	2
6:D:510:17F:C1	6:D:516:17F:O2	0.41	2.67	7	1
5:B:218:7Q9:C2	5:D:531:7Q9:C15	0.41	2.98	8	1
6:D:511:17F:H42	6:D:528:17F:H48	0.41	1.92	8	1
2:D:272:TRP:CZ2	2:E:695:LYS:HB2	0.41	2.50	9	1
5:D:523:7Q9:C310	5:D:535:7Q9:C316	0.41	2.98	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:A:208:17F:O10	6:A:208:17F:H20A	0.41	2.15	10	1
5:A:215:7Q9:C14	5:D:536:7Q9:O22	0.41	2.68	10	1
6:B:208:17F:N1	6:B:214:17F:O2	0.41	2.50	10	1
6:D:528:17F:C21	6:D:528:17F:C37	0.41	2.98	11	1
6:B:214:17F:H51	5:E:827:7Q9:C318	0.41	2.46	12	1
1:B:147:LYS:HB2	3:B:201:GSP:N1	0.41	2.30	17	2
2:D:388:ARG:HG2	2:E:575:LEU:HG	0.41	1.92	13	1
6:D:534:17F:H30	6:D:534:17F:H65	0.41	1.90	13	1
6:E:807:17F:H33	6:E:818:17F:C11	0.41	2.43	13	1
6:D:510:17F:C23	6:D:510:17F:C1X	0.41	2.68	14	1
6:D:516:17F:C11	6:D:527:17F:H31	0.41	2.41	14	1
5:E:810:7Q9:C23	5:E:825:7Q9:C3	0.41	2.98	14	1
5:D:524:7Q9:C21	6:D:527:17F:C19	0.41	2.98	15	1
1:B:97:ARG:O	1:B:101:LYS:HG3	0.41	2.15	16	1
5:D:506:7Q9:C316	5:E:837:7Q9:C316	0.41	2.99	19	1
6:D:533:17F:H55	6:E:870:17F:C37	0.41	2.45	19	1
5:E:854:7Q9:O22	5:E:854:7Q9:C3	0.41	2.64	20	1
6:E:841:17F:H59	6:E:841:17F:H62	0.41	1.53	1	1
6:E:855:17F:H62	6:E:855:17F:H58	0.41	1.66	1	1
5:A:215:7Q9:O32	5:D:536:7Q9:C39	0.41	2.68	2	1
2:E:723:GLU:HA	2:E:726:LYS:HD2	0.41	1.92	3	1
5:E:826:7Q9:C14	5:E:849:7Q9:C13	0.41	2.99	3	1
5:D:503:7Q9:C38	6:D:511:17F:H52	0.41	2.46	4	1
6:B:214:17F:C19	6:B:219:17F:H11A	0.41	2.42	5	1
5:D:520:7Q9:O14	5:D:520:7Q9:C2	0.41	2.69	6	1
5:D:537:7Q9:C318	6:E:870:17F:H53	0.41	2.45	6	1
5:E:834:7Q9:C318	6:E:855:17F:C39	0.41	2.94	6	1
6:B:219:17F:H20	6:B:219:17F:H39	0.41	1.91	7	1
6:D:501:17F:H30	5:D:506:7Q9:C11	0.41	2.45	7	1
5:E:833:7Q9:O32	5:E:834:7Q9:C13	0.41	2.68	7	1
5:E:840:7Q9:O12	5:E:849:7Q9:C22	0.41	2.67	7	1
1:A:158:THR:O	1:A:162:GLU:HG2	0.41	2.15	8	1
5:E:839:7Q9:C22	5:E:865:7Q9:C310	0.41	2.98	8	1
6:B:219:17F:C20	6:B:219:17F:C1X	0.41	2.98	9	1
6:D:501:17F:C31	6:D:501:17F:C35	0.41	2.92	9	1
1:B:47:ASP:HB2	1:B:164:ARG:NH1	0.41	2.28	10	1
1:B:64:TYR:HB2	1:B:67:MET:HB3	0.41	1.92	10	1
5:B:203:7Q9:C12	5:B:204:7Q9:C3	0.41	2.98	20	2
5:D:545:7Q9:O32	5:D:545:7Q9:C34	0.41	2.69	10	1
5:A:211:7Q9:C310	5:E:845:7Q9:C318	0.41	2.99	11	1
5:E:834:7Q9:O13	5:E:849:7Q9:C12	0.41	2.68	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:D:546:17F:H41	6:D:546:17F:H68	0.41	1.92	12	1
6:E:805:17F:H30	6:E:805:17F:C18	0.41	2.45	12	1
6:E:856:17F:N1	6:E:856:17F:P1	0.41	2.94	12	1
5:E:803:7Q9:C23	5:E:806:7Q9:C34	0.41	2.98	13	1
5:E:837:7Q9:C32	6:E:841:17F:H12A	0.41	2.45	13	1
2:D:340:LYS:HB3	2:E:626:LEU:HD11	0.41	1.91	14	1
5:D:504:7Q9:C33	5:D:507:7Q9:O22	0.41	2.68	14	1
6:D:510:17F:H31	6:D:527:17F:H20	0.41	1.91	15	1
5:D:513:7Q9:C33	5:D:513:7Q9:C22	0.41	2.98	15	1
6:D:528:17F:H6A	5:D:532:7Q9:C35	0.41	2.46	16	1
6:E:818:17F:H62	6:E:818:17F:H59	0.41	1.54	16	1
1:B:16:LYS:NZ	3:B:201:GSP:O2G	0.41	2.53	17	1
1:A:79:LEU:HD13	1:A:159:LEU:HD22	0.41	1.92	18	1
5:A:210:7Q9:C23	5:A:216:7Q9:C318	0.41	2.98	18	1
6:B:208:17F:H60	5:B:212:7Q9:C38	0.41	2.45	18	1
2:D:389:LEU:HD21	5:D:540:7Q9:C311	0.41	2.45	19	1
6:D:533:17F:H8	6:D:533:17F:H2	0.41	1.91	19	1
5:E:823:7Q9:C310	5:E:839:7Q9:C312	0.41	2.98	20	1
5:E:824:7Q9:C36	6:E:841:17F:H35	0.41	2.45	20	1
5:D:523:7Q9:C318	5:D:547:7Q9:C318	0.41	2.97	1	1
5:E:876:7Q9:C14	5:E:876:7Q9:P	0.41	3.08	13	2
5:B:210:7Q9:C34	5:B:210:7Q9:O31	0.41	2.68	2	2
5:D:507:7Q9:C13	5:D:507:7Q9:C22	0.41	2.98	3	1
5:E:804:7Q9:O32	6:E:811:17F:C1Y	0.41	2.68	3	1
6:E:828:17F:C2	5:E:851:7Q9:O14	0.41	2.67	3	1
5:A:204:7Q9:C312	6:A:208:17F:C36	0.41	2.93	4	1
6:E:807:17F:C41	6:E:818:17F:H54	0.41	2.25	17	2
6:B:214:17F:H40	6:B:214:17F:C35	0.41	2.46	5	1
2:D:322:LEU:HD22	2:E:644:LEU:HD22	0.41	1.91	6	1
6:D:511:17F:H63	6:D:511:17F:H58	0.41	1.59	7	1
6:E:801:17F:O4	5:E:808:7Q9:C14	0.41	2.68	7	1
5:B:210:7Q9:O31	5:B:210:7Q9:C34	0.41	2.68	8	1
6:E:818:17F:H40	6:E:819:17F:C24	0.41	2.38	8	1
2:D:368:ASP:O	2:D:371:ARG:HG2	0.41	2.16	9	1
6:E:872:17F:C20	6:E:872:17F:C23	0.41	2.98	9	1
6:D:534:17F:H36	6:D:534:17F:H39	0.41	1.63	10	1
5:D:543:7Q9:C38	5:D:545:7Q9:C38	0.41	2.98	10	1
2:D:298:GLN:HB3	2:D:299:PRO:HD3	0.41	1.90	11	1
6:D:546:17F:C40	6:D:546:17F:H45	0.41	2.45	11	1
6:D:517:17F:H49	5:D:520:7Q9:C317	0.41	2.45	12	1
6:A:214:17F:C30	5:E:840:7Q9:C318	0.41	2.92	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:308:TRP:CZ3	6:D:527:17F:H73	0.41	2.50	15	1
5:D:509:7Q9:C312	5:D:525:7Q9:C317	0.41	2.98	16	1
6:E:872:17F:O6	6:E:872:17F:C2	0.41	2.65	16	1
6:D:501:17F:N1	5:D:508:7Q9:O13	0.41	2.54	17	1
1:B:83:ALA:HB1	1:B:85:ASN:OD1	0.41	2.16	19	1
6:D:527:17F:H30	6:D:527:17F:C38	0.41	2.45	19	1
6:D:534:17F:C1X	6:D:534:17F:C36	0.41	2.97	19	1
2:E:623:ARG:HD2	5:E:858:7Q9:C315	0.41	2.45	19	1
6:B:208:17F:H58	6:B:208:17F:H62	0.41	1.57	20	1
5:D:505:7Q9:C312	6:D:511:17F:H52	0.41	2.46	20	1
6:D:510:17F:C41	6:E:856:17F:H48	0.41	2.46	1	1
6:A:214:17F:O5	5:D:539:7Q9:C14	0.41	2.68	2	1
6:B:219:17F:H39	6:B:219:17F:H36	0.41	1.58	17	2
1:A:81:VAL:HA	1:A:114:VAL:O	0.41	2.16	4	1
5:A:205:7Q9:O22	5:B:204:7Q9:C14	0.41	2.69	4	1
6:A:208:17F:H47	5:E:823:7Q9:C315	0.41	2.45	6	1
5:D:519:7Q9:C1	5:D:541:7Q9:C23	0.41	2.98	6	1
1:A:31:GLU:OE1	3:A:201:GSP:O3G	0.41	2.38	7	1
5:D:523:7Q9:O21	5:D:523:7Q9:C31	0.41	2.69	9	3
1:A:32:TYR:HA	3:A:201:GSP:H5'2	0.41	1.92	8	1
5:E:813:7Q9:C39	6:E:819:17F:H37	0.41	2.45	8	3
5:E:823:7Q9:O13	5:E:845:7Q9:C14	0.41	2.68	8	1
5:D:529:7Q9:C13	5:D:529:7Q9:P	0.41	3.09	16	3
6:A:208:17F:H19	6:B:208:17F:C12	0.41	2.45	10	1
5:B:212:7Q9:O21	5:B:212:7Q9:P	0.41	2.79	10	1
6:E:841:17F:H56	6:E:841:17F:H42	0.41	1.91	12	2
5:A:204:7Q9:C311	6:A:208:17F:C36	0.41	2.98	11	2
5:D:509:7Q9:C36	5:D:525:7Q9:C312	0.41	2.99	11	1
5:A:205:7Q9:C14	5:B:204:7Q9:O14	0.41	2.68	12	1
6:E:872:17F:H41	6:E:872:17F:H34	0.41	1.91	12	1
1:B:17:SER:HB2	3:B:201:GSP:PA	0.41	2.55	13	1
5:E:814:7Q9:O11	5:E:814:7Q9:C21	0.41	2.69	20	2
6:E:872:17F:O2	6:E:872:17F:H2	0.41	2.15	14	1
6:A:208:17F:O2	6:A:208:17F:H2	0.41	2.15	15	1
5:E:848:7Q9:C37	5:E:851:7Q9:C34	0.41	2.98	15	1
3:A:201:GSP:O1A	3:A:201:GSP:O2B	0.41	2.39	16	1
5:A:204:7Q9:C310	6:A:208:17F:C35	0.41	2.98	16	1
1:A:139:ILE:HB	1:A:140:PRO:HD2	0.41	1.92	17	1
6:D:510:17F:H55	6:D:527:17F:H55	0.41	1.89	17	1
5:E:850:7Q9:C315	6:E:870:17F:H61	0.41	2.44	17	1
6:E:856:17F:H57	6:E:856:17F:C23	0.41	2.45	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:LEU:HD12	1:A:112:VAL:HB	0.41	1.92	19	1
5:B:204:7Q9:C315	5:B:207:7Q9:C312	0.41	2.99	19	1
6:D:517:17F:H63	6:D:517:17F:H33	0.41	1.92	19	1
5:E:857:7Q9:C3	6:E:874:17F:C9	0.41	2.98	1	1
6:D:534:17F:C39	5:D:539:7Q9:C318	0.41	2.99	2	1
1:B:163:ILE:O	1:B:167:LYS:HG3	0.41	2.15	3	1
5:E:834:7Q9:O21	5:E:834:7Q9:C31	0.41	2.68	4	2
5:B:213:7Q9:C35	5:B:218:7Q9:C38	0.41	2.98	5	1
5:B:217:7Q9:C15	5:D:522:7Q9:O22	0.41	2.68	5	1
5:D:544:7Q9:O11	5:D:544:7Q9:C21	0.41	2.68	8	4
6:D:510:17F:C32	6:D:516:17F:H29	0.41	2.45	6	1
6:E:855:17F:H58	6:E:855:17F:H62	0.41	1.60	6	2
5:D:512:7Q9:O11	5:D:512:7Q9:C21	0.41	2.68	7	1
5:D:520:7Q9:C315	5:D:538:7Q9:C315	0.41	2.99	9	2
6:E:809:17F:C34	6:E:809:17F:H52	0.41	2.45	9	1
5:E:845:7Q9:O11	5:E:845:7Q9:C21	0.41	2.68	9	1
5:D:537:7Q9:C318	5:E:871:7Q9:C314	0.41	2.98	19	2
2:D:368:ASP:O	2:D:372:GLN:HG3	0.41	2.15	11	1
6:D:510:17F:H63	6:D:510:17F:H58	0.41	1.64	11	1
5:E:864:7Q9:C21	5:E:864:7Q9:O13	0.41	2.69	11	2
6:B:219:17F:H36	6:B:219:17F:H39	0.41	1.60	12	1
5:D:549:7Q9:C35	6:E:856:17F:C30	0.41	2.98	12	1
6:D:510:17F:H36	6:D:510:17F:H40	0.41	1.54	13	1
5:B:213:7Q9:C21	5:B:213:7Q9:C12	0.41	2.98	15	1
5:E:813:7Q9:C31	5:E:813:7Q9:O21	0.41	2.69	15	1
2:D:272:TRP:CE3	6:D:534:17F:H71	0.41	2.51	16	1
5:D:520:7Q9:C315	5:D:538:7Q9:C313	0.41	2.98	18	1
5:D:548:7Q9:C13	5:D:548:7Q9:P	0.41	3.09	18	1
6:E:807:17F:H46	6:E:809:17F:H65	0.41	1.91	18	1
5:A:213:7Q9:O14	5:A:217:7Q9:C15	0.41	2.68	19	1
5:E:846:7Q9:C33	5:E:850:7Q9:O22	0.41	2.69	1	1
6:E:818:17F:H12	6:E:819:17F:H10A	0.41	1.90	3	1
5:E:863:7Q9:C23	5:E:867:7Q9:C22	0.41	2.98	3	1
5:B:205:7Q9:C34	5:B:211:7Q9:C39	0.41	2.98	5	1
1:A:97:ARG:HG3	1:A:111:MET:HE1	0.41	1.93	7	1
5:A:204:7Q9:C310	6:A:208:17F:H56	0.41	2.45	7	1
5:E:806:7Q9:C31	5:E:806:7Q9:O21	0.41	2.69	12	2
5:E:824:7Q9:C36	6:E:841:17F:H56	0.41	2.45	9	1
2:E:694:ALA:O	2:E:698:GLU:HG2	0.41	2.16	10	1
6:E:807:17F:C38	5:E:813:7Q9:C310	0.41	2.98	10	1
2:E:711:LEU:HD22	5:E:865:7Q9:C311	0.41	2.45	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:E:818:17F:H36	6:E:818:17F:H41	0.41	1.92	13	1
2:D:333:LYS:HD3	2:E:633:LYS:HG2	0.41	1.92	15	1
5:B:209:7Q9:C318	5:D:503:7Q9:C37	0.41	2.98	16	1
2:D:334:LEU:HD13	5:D:532:7Q9:C317	0.41	2.45	16	1
1:B:18:ALA:O	1:B:22:GLN:HG2	0.41	2.15	17	1
6:B:214:17F:H33	6:B:219:17F:C11	0.41	2.46	17	1
6:D:533:17F:H47	5:D:543:7Q9:C23	0.41	2.45	17	1
2:E:715:ARG:HG2	2:E:716:GLN:N	0.41	2.29	17	1
5:A:206:7Q9:O32	5:A:206:7Q9:C34	0.41	2.69	18	1
5:E:826:7Q9:C13	5:E:849:7Q9:C13	0.41	2.99	18	1
6:B:214:17F:H9	5:B:217:7Q9:C36	0.41	2.45	19	1
5:B:216:7Q9:C33	5:D:515:7Q9:O22	0.41	2.69	20	1
2:D:384:ASN:O	2:D:388:ARG:HD3	0.41	2.16	20	1
6:D:533:17F:O6	6:D:533:17F:O7	0.41	2.39	1	2
5:E:871:7Q9:O21	5:E:871:7Q9:C31	0.41	2.69	1	3
2:D:355:HIS:CE1	2:E:608:TRP:HB2	0.41	2.51	2	1
6:E:841:17F:C8	5:E:876:7Q9:C12	0.41	2.96	3	1
5:A:215:7Q9:C1	5:A:215:7Q9:O32	0.41	2.69	6	1
5:E:836:7Q9:C310	5:E:852:7Q9:C318	0.41	2.99	6	1
5:B:216:7Q9:C31	5:D:519:7Q9:C15	0.41	2.99	7	1
5:D:549:7Q9:C317	2:E:648:MET:HE1	0.41	2.46	7	1
1:B:25:GLN:HB3	1:B:27:HIS:CE1	0.41	2.51	8	1
6:E:856:17F:H68	6:E:856:17F:H37	0.41	1.92	13	1
6:D:517:17F:H43	6:D:517:17F:H63	0.41	1.93	15	1
5:D:549:7Q9:C1	5:D:549:7Q9:O22	0.41	2.63	16	1
5:E:840:7Q9:C33	5:E:849:7Q9:C22	0.41	2.98	16	1
5:A:207:7Q9:C14	5:D:507:7Q9:O13	0.41	2.68	17	1
2:E:591:GLU:HG2	5:E:861:7Q9:C39	0.41	2.46	17	1
5:E:815:7Q9:C31	5:E:815:7Q9:C1	0.41	2.99	19	2
6:E:818:17F:H1	5:E:835:7Q9:O14	0.41	2.16	19	1
5:E:834:7Q9:C38	5:E:849:7Q9:C313	0.41	2.98	19	1
6:D:510:17F:C42	6:E:856:17F:H48	0.41	2.44	20	1
2:D:305:GLN:NE2	6:D:527:17F:H29	0.41	2.31	1	1
5:D:515:7Q9:C316	5:E:821:7Q9:C318	0.41	2.99	1	1
5:D:539:7Q9:C3	5:D:539:7Q9:O22	0.41	2.61	1	2
5:D:505:7Q9:C23	5:D:513:7Q9:C12	0.41	2.99	2	1
6:E:856:17F:H68	6:E:874:17F:C35	0.41	2.46	11	2
5:B:220:7Q9:C22	5:D:543:7Q9:C22	0.41	2.99	3	1
5:D:509:7Q9:C33	5:D:525:7Q9:C32	0.41	2.98	3	1
1:A:17:SER:N	3:A:201:GSP:O1A	0.41	2.54	4	1
1:A:123:ARG:HD3	1:A:125:VAL:O	0.41	2.16	7	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:B:203:7Q9:C32	6:B:208:17F:H8A	0.41	2.46	4	1
5:E:852:7Q9:O32	5:E:858:7Q9:C13	0.41	2.69	4	1
6:D:528:17F:H76	5:D:532:7Q9:C314	0.41	2.46	5	1
5:E:823:7Q9:O13	5:E:845:7Q9:C13	0.41	2.69	10	2
5:E:837:7Q9:C15	5:E:837:7Q9:O21	0.41	2.69	5	1
6:E:838:17F:C28	6:E:874:17F:H53	0.41	2.46	5	1
5:E:864:7Q9:O32	5:E:864:7Q9:C34	0.41	2.68	16	2
1:A:116:ASN:OD1	1:A:145:SER:HA	0.41	2.15	6	1
1:B:160:VAL:HA	1:B:163:ILE:HD12	0.41	1.93	6	1
6:E:805:17F:C39	5:E:810:7Q9:C317	0.41	2.99	6	1
5:E:868:7Q9:C34	5:E:873:7Q9:C38	0.41	2.99	6	1
5:B:210:7Q9:C316	6:B:215:17F:H44	0.41	2.46	7	1
6:D:510:17F:C12	6:D:516:17F:C7	0.41	2.84	7	1
6:D:527:17F:H39	6:D:527:17F:H36	0.41	1.58	8	1
6:E:807:17F:H38	6:E:809:17F:H32	0.41	1.93	8	1
5:E:829:7Q9:C1	5:E:852:7Q9:C33	0.41	2.99	8	1
5:A:215:7Q9:C14	5:D:536:7Q9:C2	0.41	2.99	10	1
6:E:819:17F:O6	6:E:819:17F:C17	0.41	2.68	10	1
5:A:205:7Q9:C33	5:D:503:7Q9:C3	0.41	2.99	11	1
6:A:214:17F:O2	5:A:217:7Q9:C13	0.41	2.69	11	1
6:B:219:17F:H10A	6:B:219:17F:O8	0.41	2.16	11	1
6:D:516:17F:H1A	6:D:516:17F:O9	0.41	2.15	11	1
5:E:840:7Q9:C2	5:E:840:7Q9:O13	0.41	2.69	15	2
1:B:68:ARG:HG3	1:B:71:TYR:OH	0.41	2.16	12	1
5:B:207:7Q9:C316	6:E:801:17F:C38	0.41	2.99	12	1
6:D:511:17F:C37	6:D:511:17F:H39	0.41	2.46	12	1
5:A:211:7Q9:C311	5:A:213:7Q9:C39	0.41	2.99	13	1
5:B:210:7Q9:C13	5:B:210:7Q9:P	0.41	3.09	13	1
5:D:513:7Q9:O14	5:D:513:7Q9:O21	0.41	2.38	13	1
5:D:548:7Q9:O21	5:D:548:7Q9:C31	0.41	2.69	16	2
5:E:857:7Q9:O32	6:E:874:17F:C10	0.41	2.58	13	1
5:D:548:7Q9:O31	5:E:831:7Q9:C32	0.41	2.69	14	1
2:D:408:LYS:HE2	5:D:542:7Q9:C33	0.41	2.46	15	1
5:D:524:7Q9:O21	5:D:524:7Q9:O32	0.41	2.38	15	1
5:D:543:7Q9:C318	5:E:875:7Q9:C316	0.41	2.99	15	1
5:E:840:7Q9:C22	5:E:868:7Q9:C35	0.41	2.99	15	1
5:E:850:7Q9:C37	5:E:850:7Q9:C311	0.41	2.97	15	2
5:E:861:7Q9:O31	5:E:861:7Q9:O11	0.41	2.39	15	1
5:A:212:7Q9:C32	6:A:214:17F:H18A	0.41	2.46	16	1
6:E:809:17F:C33	6:E:809:17F:H41	0.41	2.46	16	1
6:E:838:17F:H38	6:E:874:17F:H51	0.41	1.92	16	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:B:203:7Q9:C14	5:B:204:7Q9:C31	0.41	2.99	17	1
5:B:206:7Q9:C3	5:B:206:7Q9:O22	0.41	2.63	17	1
6:D:527:17F:H32	6:D:527:17F:O10	0.41	2.16	17	1
2:E:605:GLN:HG3	5:E:866:7Q9:C313	0.41	2.46	17	1
1:A:17:SER:HA	1:A:20:THR:OG1	0.41	2.15	18	1
1:B:90:PHE:HE1	1:B:130:ALA:HA	0.41	1.76	18	1
5:D:529:7Q9:C315	5:D:541:7Q9:C316	0.41	2.99	18	1
6:E:819:17F:O1	5:E:829:7Q9:C13	0.41	2.68	18	1
5:E:847:7Q9:O21	5:E:847:7Q9:O32	0.41	2.38	18	1
6:D:517:17F:C38	6:D:517:17F:H47	0.41	2.46	19	1
6:E:801:17F:H31	5:E:803:7Q9:C22	0.41	2.46	20	1
6:E:817:17F:C8	5:E:820:7Q9:C22	0.41	2.90	20	1
5:E:837:7Q9:O12	5:E:837:7Q9:C15	0.41	2.69	20	1
5:D:514:7Q9:O21	5:D:514:7Q9:O13	0.41	2.38	1	1
6:A:208:17F:O1	6:A:208:17F:H5	0.41	2.16	2	1
6:D:517:17F:O10	6:D:517:17F:C6	0.41	2.59	2	1
5:D:536:7Q9:O14	5:D:536:7Q9:C21	0.41	2.69	2	1
5:D:512:7Q9:C34	6:D:528:17F:C6	0.41	2.99	3	1
6:E:801:17F:O8	6:E:801:17F:C10	0.41	2.69	6	1
6:E:872:17F:O6	6:E:872:17F:O7	0.41	2.39	8	2
6:D:501:17F:H66	6:D:501:17F:H50	0.41	1.91	9	1
5:E:824:7Q9:C37	6:E:841:17F:C23	0.41	2.98	9	1
5:D:507:7Q9:C13	5:D:507:7Q9:O21	0.41	2.68	10	1
6:E:874:17F:O10	6:E:874:17F:C4	0.41	2.57	10	1
1:B:97:ARG:HD3	1:B:98:GLU:OE1	0.41	2.16	11	1
5:D:502:7Q9:C34	5:D:505:7Q9:O31	0.41	2.69	11	1
6:D:517:17F:H51	6:D:517:17F:C41	0.41	2.46	12	1
5:E:827:7Q9:O21	5:E:827:7Q9:O32	0.41	2.39	12	1
5:B:204:7Q9:O21	5:B:204:7Q9:C31	0.41	2.69	14	2
6:D:517:17F:H57	6:D:517:17F:C23	0.41	2.45	14	1
5:E:827:7Q9:O21	5:E:827:7Q9:C31	0.41	2.69	15	1
6:D:527:17F:O10	6:D:527:17F:C1Z	0.41	2.69	17	1
5:D:537:7Q9:C11	6:D:546:17F:H12A	0.41	2.46	17	1
3:A:201:GSP:O2A	3:A:201:GSP:O2G	0.41	2.38	18	1
6:B:214:17F:H6A	5:B:217:7Q9:C31	0.41	2.46	18	1
5:D:515:7Q9:C310	5:E:821:7Q9:C318	0.41	2.99	18	1
5:E:852:7Q9:C15	5:E:852:7Q9:P	0.41	3.09	18	1
1:A:142:ILE:CD1	1:A:155:ALA:HA	0.41	2.46	19	1
6:D:501:17F:H36	6:D:501:17F:H39	0.41	1.63	20	1
5:D:548:7Q9:O11	5:D:548:7Q9:C21	0.40	2.69	1	3
5:A:203:7Q9:C14	5:A:203:7Q9:P	0.40	3.09	8	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
6:B:215:17F:H65	6:B:215:17F:C26	0.40	2.46	2	1
6:D:546:17F:H35	6:D:546:17F:H39	0.40	1.62	2	2
5:A:204:7Q9:C316	6:A:208:17F:H65	0.40	2.46	3	1
6:D:533:17F:O8	6:D:533:17F:H60	0.40	2.17	3	1
5:E:853:7Q9:C15	5:E:877:7Q9:O14	0.40	2.69	3	1
5:B:217:7Q9:C12	5:B:217:7Q9:O14	0.40	2.70	4	1
5:E:823:7Q9:O21	5:E:823:7Q9:O32	0.40	2.38	4	1
5:A:212:7Q9:C3	5:A:212:7Q9:O22	0.40	2.64	5	1
5:E:825:7Q9:O21	5:E:825:7Q9:O32	0.40	2.39	5	1
5:E:851:7Q9:O22	5:E:851:7Q9:C3	0.40	2.66	6	1
5:B:209:7Q9:O21	5:B:209:7Q9:C31	0.40	2.68	8	1
5:E:815:7Q9:O31	5:E:815:7Q9:C34	0.40	2.70	9	2
6:E:817:17F:C28	5:E:820:7Q9:C318	0.40	2.91	9	1
5:A:204:7Q9:C312	6:A:208:17F:C35	0.40	2.99	10	1
5:D:513:7Q9:C14	5:D:526:7Q9:P	0.40	3.09	11	1
6:E:818:17F:C24	5:E:835:7Q9:C311	0.40	2.93	13	1
5:A:204:7Q9:C39	6:A:208:17F:H10A	0.40	2.46	14	1
5:B:211:7Q9:C15	5:B:211:7Q9:O11	0.40	2.69	14	1
5:B:218:7Q9:C31	5:B:218:7Q9:C1	0.40	2.99	15	1
2:D:374:LEU:HD23	5:D:529:7Q9:C38	0.40	2.45	15	1
5:A:204:7Q9:C310	6:A:208:17F:C36	0.40	2.99	16	1
1:A:168:GLU:HG3	1:A:172:LYS:NZ	0.40	2.31	18	1
6:D:510:17F:C26	6:D:516:17F:H73	0.40	2.46	18	1
5:E:862:7Q9:C38	5:E:862:7Q9:C313	0.40	2.98	18	1
5:A:215:7Q9:O22	5:D:536:7Q9:C35	0.40	2.69	19	1
6:E:841:17F:O7	6:E:841:17F:C10	0.40	2.68	19	1
5:B:216:7Q9:C36	5:D:515:7Q9:C22	0.40	2.99	20	1
6:D:533:17F:H62	6:D:533:17F:H59	0.40	1.76	20	1
5:A:209:7Q9:C315	5:E:822:7Q9:C314	0.40	2.98	2	1
5:D:537:7Q9:C31	6:D:546:17F:C1X	0.40	3.00	3	1
5:D:505:7Q9:C33	6:D:511:17F:H9	0.40	2.46	4	1
6:E:819:17F:H58	6:E:819:17F:H62	0.40	1.62	4	1
5:E:812:7Q9:O22	5:E:812:7Q9:O31	0.40	2.39	5	1
5:E:831:7Q9:C35	5:E:853:7Q9:O32	0.40	2.69	5	1
2:D:287:SER:O	2:D:291:GLU:HG3	0.40	2.17	6	1
6:D:510:17F:O6	6:D:516:17F:H6	0.40	2.17	6	1
6:D:510:17F:C1X	6:D:516:17F:C8	0.40	2.99	6	1
5:D:521:7Q9:O21	5:D:521:7Q9:O32	0.40	2.39	6	1
5:B:205:7Q9:C32	5:B:211:7Q9:C39	0.40	2.99	7	1
6:E:807:17F:H47	6:E:807:17F:H78	0.40	1.92	7	1
5:E:822:7Q9:O14	5:E:839:7Q9:P	0.40	2.79	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:A:211:7Q9:C38	5:A:213:7Q9:C310	0.40	2.99	8	1
6:D:517:17F:O6	6:D:517:17F:C7	0.40	2.68	8	1
6:E:811:17F:H75	5:E:822:7Q9:C317	0.40	2.46	9	1
1:A:78:PHE:HE2	1:A:104:LYS:HD2	0.40	1.75	12	1
6:D:527:17F:H11	5:D:535:7Q9:C35	0.40	2.47	12	1
6:E:872:17F:O1	6:E:872:17F:O9	0.40	2.39	12	1
3:B:201:GSP:O2G	3:B:201:GSP:O2B	0.40	2.39	13	1
1:B:97:ARG:HG3	1:B:111:MET:SD	0.40	2.56	14	1
6:B:214:17F:O10	6:B:219:17F:C10	0.40	2.69	14	1
6:D:546:17F:H1A	6:D:546:17F:C4	0.40	2.45	14	1
5:E:846:7Q9:C12	5:E:846:7Q9:O13	0.40	2.70	14	2
6:E:807:17F:H40	6:E:807:17F:H35	0.40	1.62	15	1
6:E:828:17F:H39	5:E:832:7Q9:C38	0.40	2.46	15	1
5:E:837:7Q9:O31	5:E:837:7Q9:C21	0.40	2.69	15	1
1:B:80:CYS:HB2	1:B:93:ILE:HD12	0.40	1.93	16	1
6:E:818:17F:C25	5:E:835:7Q9:C311	0.40	2.99	16	1
5:D:545:7Q9:C15	5:D:545:7Q9:C32	0.40	2.99	17	1
6:E:856:17F:C35	6:E:856:17F:C31	0.40	2.96	20	1
1:A:13:GLY:HA2	3:A:201:GSP:C5'	0.40	2.46	3	1
5:A:215:7Q9:C11	6:D:534:17F:H29	0.40	2.47	4	1
6:B:214:17F:H76	5:B:217:7Q9:C38	0.40	2.46	4	1
2:D:269:GLN:HG2	6:D:534:17F:H20	0.40	1.93	4	1
2:D:389:LEU:HD21	5:D:540:7Q9:C38	0.40	2.47	4	1
3:B:201:GSP:S1G	3:B:201:GSP:PA	0.40	3.19	5	1
6:D:501:17F:H10	6:D:501:17F:H62	0.40	1.93	5	1
5:D:522:7Q9:O32	5:D:545:7Q9:C37	0.40	2.69	5	1
5:E:834:7Q9:O32	5:E:834:7Q9:O21	0.40	2.40	5	1
6:B:215:17F:C20	6:D:517:17F:H60	0.40	2.46	6	1
5:D:505:7Q9:P	5:D:505:7Q9:O21	0.40	2.80	6	1
6:D:517:17F:H59	6:D:517:17F:H63	0.40	1.60	6	1
6:D:501:17F:C24	6:D:501:17F:H61	0.40	2.47	7	2
5:E:825:7Q9:C39	5:E:844:7Q9:C310	0.40	2.99	8	1
5:B:218:7Q9:C1	5:B:218:7Q9:C31	0.40	2.99	9	1
5:D:537:7Q9:O13	5:D:537:7Q9:C12	0.40	2.69	9	1
5:E:802:7Q9:C315	6:E:809:17F:C37	0.40	2.98	9	1
5:E:853:7Q9:C310	5:E:877:7Q9:C35	0.40	2.99	9	1
6:E:856:17F:C38	6:E:874:17F:H68	0.40	2.45	9	1
5:A:203:7Q9:C23	5:A:207:7Q9:C22	0.40	3.00	10	1
6:B:208:17F:C1Z	6:B:214:17F:H10A	0.40	2.47	10	1
5:D:538:7Q9:C21	5:D:538:7Q9:O14	0.40	2.68	12	1
6:D:546:17F:H56	6:D:546:17F:C9	0.40	2.46	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:GLY:HA3	3:A:201:GSP:C8	0.40	2.52	13	1
5:B:211:7Q9:O31	5:B:211:7Q9:C34	0.40	2.68	14	1
5:D:525:7Q9:C21	5:D:525:7Q9:O14	0.40	2.69	14	1
1:A:80:CYS:HB2	1:A:93:ILE:HD12	0.40	1.93	15	1
6:B:214:17F:H19A	6:B:219:17F:C12	0.40	2.46	15	1
6:A:214:17F:C36	6:A:214:17F:H59	0.40	2.46	16	1
5:E:862:7Q9:C11	5:E:862:7Q9:C23	0.40	2.99	16	1
6:E:872:17F:O9	6:E:872:17F:P1	0.40	2.79	16	1
5:B:213:7Q9:C38	5:D:514:7Q9:C310	0.40	3.00	17	1
6:D:533:17F:C40	5:D:543:7Q9:O32	0.40	2.69	17	1
6:D:533:17F:H43	6:D:533:17F:C40	0.40	2.47	19	1
5:E:802:7Q9:C315	6:E:809:17F:C39	0.40	2.95	19	1
5:B:206:7Q9:C314	6:E:805:17F:C41	0.40	2.95	20	1
2:D:297:VAL:O	2:D:301:LEU:HG	0.40	2.17	20	1
2:E:620:GLU:HG3	5:E:858:7Q9:C38	0.40	2.47	20	1
2:E:726:LYS:CD	6:E:870:17F:H11	0.40	2.44	20	1
5:E:837:7Q9:C34	6:E:841:17F:H12A	0.40	2.46	20	1
5:D:524:7Q9:C35	5:D:526:7Q9:C34	0.40	2.99	1	1
6:B:214:17F:H31	5:B:220:7Q9:C33	0.40	2.47	2	1
6:B:215:17F:H35	6:B:215:17F:H39	0.40	1.58	2	1
6:D:517:17F:H43	6:D:517:17F:H59	0.40	1.91	2	1
6:D:527:17F:H49	6:E:856:17F:C42	0.40	2.46	2	1
6:E:828:17F:H64	5:E:829:7Q9:C318	0.40	2.46	3	1
5:E:853:7Q9:C12	5:E:853:7Q9:O11	0.40	2.69	3	1
6:B:215:17F:H54	6:B:215:17F:C37	0.40	2.27	4	1
6:D:534:17F:O10	6:D:534:17F:C4	0.40	2.67	4	1
6:E:874:17F:H58	6:E:874:17F:H63	0.40	1.64	4	1
5:E:803:7Q9:C313	5:E:814:7Q9:C38	0.40	3.00	5	1
6:E:801:17F:O6	6:E:801:17F:O7	0.40	2.38	7	1
5:E:857:7Q9:O21	5:E:857:7Q9:C31	0.40	2.70	7	1
6:D:501:17F:C1Y	6:D:501:17F:C8	0.40	2.89	8	1
5:A:204:7Q9:O11	5:A:204:7Q9:O32	0.40	2.39	10	1
6:D:528:17F:C2X	5:D:532:7Q9:C315	0.40	2.97	10	1
5:E:815:7Q9:O22	5:E:815:7Q9:C1	0.40	2.63	10	1
6:E:872:17F:H44	6:E:872:17F:H59	0.40	1.92	11	1
5:B:220:7Q9:C12	5:B:220:7Q9:O14	0.40	2.70	12	1
6:D:517:17F:H77	5:D:541:7Q9:C318	0.40	2.46	12	1
5:D:538:7Q9:C317	5:E:876:7Q9:C315	0.40	2.99	15	1
5:E:867:7Q9:O31	5:E:867:7Q9:C34	0.40	2.69	15	1
6:B:219:17F:H46	5:D:543:7Q9:C39	0.40	2.47	17	1
6:D:533:17F:H35	6:D:533:17F:H39	0.40	1.67	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:E:815:7Q9:C318	5:E:827:7Q9:C318	0.40	2.99	18	1
5:A:204:7Q9:C314	6:A:208:17F:C25	0.40	3.00	19	1
5:E:813:7Q9:C34	5:E:829:7Q9:C22	0.40	2.99	19	1
5:D:547:7Q9:C13	5:D:547:7Q9:C22	0.40	2.99	2	1
6:D:511:17F:C23	6:D:511:17F:H66	0.40	2.46	3	1
6:E:870:17F:O1	6:E:870:17F:H5	0.40	2.17	3	1
2:D:429:PHE:CD1	6:D:533:17F:H66	0.40	2.51	4	1
5:E:803:7Q9:C3	5:E:813:7Q9:C22	0.40	3.00	4	1
5:A:216:7Q9:C13	5:D:536:7Q9:C1	0.40	3.00	5	1
6:B:208:17F:H67	6:B:208:17F:C26	0.40	2.47	5	1
5:D:523:7Q9:O32	5:D:523:7Q9:O21	0.40	2.40	6	1
6:E:809:17F:C17	6:E:809:17F:O7	0.40	2.69	6	1
6:E:817:17F:O10	6:E:817:17F:H4	0.40	2.16	7	1
6:B:214:17F:O8	6:B:214:17F:C19	0.40	2.69	8	1
5:B:218:7Q9:C14	5:B:218:7Q9:P	0.40	3.09	9	1
6:D:510:17F:O3	6:D:516:17F:H6	0.40	2.13	9	1
5:E:853:7Q9:C14	5:E:877:7Q9:O14	0.40	2.70	11	1
6:D:510:17F:H59	6:D:510:17F:H62	0.40	1.71	12	1
5:A:209:7Q9:O32	5:A:209:7Q9:C34	0.40	2.69	13	1
6:D:510:17F:C7	6:D:516:17F:O9	0.40	2.69	13	2
6:D:516:17F:H44	5:D:535:7Q9:C313	0.40	2.47	13	1
6:B:219:17F:H45	5:D:545:7Q9:C310	0.40	2.47	14	1
5:E:839:7Q9:O13	5:E:845:7Q9:C13	0.40	2.69	14	1
5:D:502:7Q9:O32	5:D:502:7Q9:C21	0.40	2.69	15	1
5:D:507:7Q9:C31	6:D:516:17F:H32	0.40	2.46	15	1
5:D:532:7Q9:O11	5:D:532:7Q9:O31	0.40	2.39	15	1
5:E:813:7Q9:O31	5:E:829:7Q9:C21	0.40	2.69	15	1
5:E:857:7Q9:C31	6:E:874:17F:H9	0.40	2.46	15	1
6:E:874:17F:H78	6:E:874:17F:C30	0.40	2.47	16	1
6:E:872:17F:H76	6:E:872:17F:H54	0.40	1.93	18	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	171/185 (92%)	160±2 (93±1%)	10±2 (6±1%)	1±1 (0±1%)	31	76
1	B	161/185 (87%)	152±2 (95±1%)	9±2 (5±1%)	0±0 (0±0%)	49	83
2	D	185/200 (92%)	181±1 (98±1%)	4±1 (2±1%)	0±0 (0±0%)	44	80
2	E	185/200 (92%)	180±2 (97±1%)	4±2 (2±1%)	0±1 (0±0%)	49	83
All	All	14040/15400 (91%)	13467 (96%)	543 (4%)	30 (0%)	44	80

All 20 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	36	ILE	4
2	D	419	LEU	3
1	A	173	ASP	2
2	E	598	GLN	2
2	E	718	LEU	2
1	A	29	VAL	2
1	B	122	SER	2
1	A	26	ASN	1
1	A	28	PHE	1
2	D	404	SER	1
1	A	21	ILE	1
1	B	121	PRO	1
2	D	420	PRO	1
2	D	342	SER	1
1	A	30	ASP	1
2	D	265	GLY	1
1	A	37	GLU	1
1	A	60	GLY	1
2	D	405	GLU	1
2	E	642	SER	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	153/165 (93%)	138±3 (90±2%)	15±3 (10±2%)	10	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	143/165 (87%)	128±2 (90±2%)	15±2 (10±2%)	9	52
2	D	163/175 (93%)	151±3 (93±2%)	12±3 (7±2%)	15	64
2	E	163/175 (93%)	151±2 (93±1%)	12±2 (7±1%)	15	63
All	All	12440/13600 (91%)	11372 (91%)	1068 (9%)	12	58

All 260 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)
2	E	556	THR	18
1	B	65	SER	17
1	A	65	SER	16
2	D	258	SER	16
2	D	402	THR	16
1	B	87	THR	15
1	B	124	THR	15
2	D	268	THR	15
1	A	87	THR	15
1	B	2	THR	13
1	B	128	LYS	13
1	A	74	THR	13
1	B	74	THR	13
2	D	256	THR	12
2	E	702	THR	12
2	E	705	GLU	12
2	D	373	ARG	12
2	E	555	SER	12
1	A	161	ARG	12
1	A	50	THR	11
1	A	128	LYS	11
1	B	35	THR	11
1	B	127	THR	11
1	A	92	ASP	10
1	A	132	ASP	10
1	B	58	THR	10
1	B	69	ASP	10
2	E	579	THR	10
1	A	62	GLU	9
2	D	388	ARG	9
2	E	653	ARG	9
1	A	2	THR	9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	50	THR	9
1	A	63	GLU	9
1	A	35	THR	8
1	A	68	ARG	8
1	A	124	THR	8
2	D	257	PHE	8
2	E	623	ARG	8
1	A	39	SER	8
1	B	12	ASP	8
1	B	68	ARG	8
1	B	80	CYS	8
1	B	161	ARG	8
1	A	148	THR	8
1	B	63	GLU	8
1	B	148	THR	8
2	E	558	SER	8
2	E	688	ARG	8
2	D	377	ARG	8
2	E	661	THR	8
2	E	733	LEU	8
2	D	255	SER	8
2	E	561	ARG	8
1	B	92	ASP	7
2	D	401	SER	7
2	E	594	LYS	7
2	D	279	THR	7
1	B	132	ASP	7
2	E	737	THR	7
2	D	437	THR	6
2	E	619	VAL	6
2	E	655	HIS	6
1	A	25	GLN	6
2	D	316	ARG	6
2	E	704	SER	6
1	A	89	SER	6
1	A	172	LYS	6
2	D	335	HIS	6
1	A	20	THR	6
1	A	58	THR	6
1	A	145	SER	6
1	B	149	ARG	6
2	D	361	THR	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	12	ASP	5
1	A	31	GLU	5
1	B	119	ASP	5
2	D	428	SER	5
2	E	613	GLU	5
1	A	126	ASP	5
1	B	64	TYR	5
2	D	421	VAL	5
2	E	637	LEU	5
1	A	38	ASP	5
1	B	20	THR	5
1	A	108	ASP	5
1	A	153	ASP	5
2	D	320	GLU	5
1	B	153	ASP	4
2	E	604	PHE	4
2	E	724	SER	4
1	A	41	ARG	4
1	B	62	GLU	4
2	D	346	GLU	4
2	E	568	THR	4
2	E	691	GLU	4
1	A	43	GLN	4
2	D	431	SER	4
2	E	569	GLN	4
2	D	440	LEU	4
1	A	127	THR	4
2	D	261	ARG	4
1	A	69	ASP	3
1	A	173	ASP	3
2	D	397	THR	3
2	E	684	ASN	3
1	A	51	CYS	3
1	A	123	ARG	3
1	B	39	SER	3
1	B	97	ARG	3
2	D	360	ARG	3
1	B	41	ARG	3
2	D	280	GLU	3
1	B	118	CYS	3
1	B	142	ILE	3
1	B	38	ASP	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	89	SER	3
2	D	308	TRP	3
2	D	351	ARG	3
2	E	657	ASP	3
1	A	119	ASP	3
1	B	47	ASP	3
2	D	404	SER	3
1	B	145	SER	3
1	B	143	GLU	3
1	B	27	HIS	2
1	B	44	VAL	2
2	D	311	GLU	2
2	E	728	SER	2
1	A	29	VAL	2
1	A	47	ASP	2
1	B	36	ILE	2
1	B	51	CYS	2
2	E	660	ARG	2
1	B	9	VAL	2
1	B	17	SER	2
2	E	646	GLU	2
1	A	8	VAL	2
2	D	435	GLU	2
2	E	575	LEU	2
1	B	16	LYS	2
2	D	328	GLU	2
2	E	641	LEU	2
1	A	36	ILE	2
1	B	70	GLN	2
2	D	333	LYS	2
2	E	721	VAL	2
2	E	701	SER	2
2	E	642	SER	2
1	B	108	ASP	2
2	E	597	VAL	2
1	A	80	CYS	2
1	A	17	SER	2
1	A	23	LEU	2
2	D	424	SER	2
1	B	43	GLN	2
1	A	136	SER	2
2	D	305	GLN	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	D	304	PHE	2
2	D	389	LEU	2
2	E	734	GLU	2
1	A	37	GLU	2
1	A	27	HIS	1
1	A	56	LEU	1
1	B	22	GLN	1
1	B	112	VAL	1
1	B	131	GLN	1
2	D	275	LEU	1
1	A	99	GLN	1
1	B	163	ILE	1
2	D	391	GLU	1
2	E	667	SER	1
1	A	55	ILE	1
1	B	26	ASN	1
2	D	369	GLU	1
2	E	592	GLU	1
2	E	740	LEU	1
1	A	22	GLN	1
1	A	109	VAL	1
1	A	154	ASP	1
1	B	5	LYS	1
1	B	122	SER	1
1	B	123	ARG	1
2	E	563	GLN	1
2	E	598	GLN	1
2	E	640	LYS	1
1	A	26	ASN	1
1	A	33	ASP	1
1	A	142	ILE	1
1	B	49	GLU	1
2	D	282	LEU	1
2	E	589	ASP	1
1	A	21	ILE	1
1	B	144	THR	1
2	D	313	GLU	1
2	D	367	SER	1
2	D	382	LYS	1
2	E	668	ASP	1
2	E	679	GLU	1
1	A	6	LEU	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	D	303	ASP	1
2	D	339	GLU	1
2	E	628	GLU	1
2	E	678	LEU	1
1	A	107	GLU	1
1	B	28	PHE	1
1	B	150	GLN	1
1	B	158	THR	1
1	B	168	GLU	1
2	D	403	LEU	1
2	D	312	MET	1
2	E	559	LYS	1
2	E	697	THR	1
2	E	736	TYR	1
1	A	64	TYR	1
1	A	171	SER	1
1	B	129	GLN	1
2	D	262	GLU	1
2	D	383	GLU	1
2	D	412	GLU	1
2	E	578	GLU	1
2	E	656	VAL	1
1	A	147	LYS	1
1	B	154	ASP	1
2	D	342	SER	1
2	E	713	ASP	1
1	A	16	LYS	1
2	D	439	LYS	1
2	E	620	GLU	1
2	E	712	GLU	1
1	A	81	VAL	1
1	B	101	LYS	1
2	D	414	LEU	1
2	E	587	SER	1
2	E	608	TRP	1
1	B	55	ILE	1
2	D	264	LEU	1
2	D	372	GLN	1
2	D	405	GLU	1
1	A	149	ARG	1
2	D	309	GLN	1
2	E	590	LEU	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	E	632	GLN	1
1	B	8	VAL	1
1	B	46	ILE	1
2	D	291	GLU	1
2	E	601	LEU	1
2	E	617	GLN	1
2	E	715	ARG	1
1	A	57	ASP	1
2	D	384	ASN	1
1	A	143	GLU	1
1	A	170	MET	1
1	B	169	LYS	1
2	D	363	LEU	1
2	D	314	LEU	1
2	D	331	ARG	1
2	E	580	GLU	1
2	E	635	HIS	1
2	E	741	ASN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 164 ligands modelled in this entry, 2 are monoatomic - leaving 162 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	7Q9	D	513	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	834	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	866	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	E	805	-	52,53,53	0.83±0.00	0±0 (0±0%)
6	17F	E	855	-	52,53,53	0.82±0.00	0±0 (0±0%)
5	7Q9	E	843	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	839	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	831	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	B	206	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	514	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	862	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	812	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	D	516	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	E	836	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	A	213	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	B	214	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	E	827	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	B	203	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	523	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	830	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	849	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	B	215	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	B	220	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	844	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	525	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	539	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	535	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	832	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	825	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	851	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	D	533	-	52,53,53	0.82±0.00	0±0 (0±0%)
5	7Q9	D	515	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	544	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	859	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	821	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	D	546	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	E	815	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	B	211	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	A	214	-	52,53,53	0.83±0.00	0±0 (0±0%)
6	17F	E	856	-	52,53,53	0.83±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
5	7Q9	B	210	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	837	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	541	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	835	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	871	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	876	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	816	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	B	207	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	858	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	A	203	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	503	-	38,38,38	0.80±0.00	0±0 (0±0%)
3	GSP	B	201	4	33,34,34	1.18±0.01	1±0 (3±0%)
5	7Q9	E	813	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	877	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	A	212	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	861	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	E	828	-	52,53,53	0.83±0.00	0±0 (0±0%)
6	17F	E	838	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	B	218	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	521	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	A	208	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	E	869	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	531	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	A	205	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	A	217	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	518	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	537	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	810	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	D	527	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	E	854	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	847	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	E	819	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	D	519	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	878	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	860	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	505	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	A	215	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	833	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	536	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	865	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	E	811	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	E	845	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	848	-	38,38,38	0.80±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
5	7Q9	D	545	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	A	210	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	803	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	857	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	868	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	512	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	529	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	526	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	542	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	863	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	D	501	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	D	506	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	B	205	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	549	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	808	-	38,38,38	0.80±0.00	0±0 (0±0%)
3	GSP	A	201	4	33,34,34	1.17±0.01	1±0 (3±0%)
6	17F	E	818	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	D	540	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	509	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	804	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	508	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	842	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	824	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	E	809	-	52,53,53	0.83±0.00	0±0 (0±0%)
6	17F	B	208	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	B	217	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	823	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	B	204	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	543	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	840	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	B	213	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	B	209	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	B	212	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	D	511	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	A	204	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	D	517	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	A	207	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	507	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	522	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	820	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	E	817	-	52,53,53	0.82±0.00	0±0 (0±0%)
5	7Q9	D	520	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	A	216	-	38,38,38	0.81±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
5	7Q9	E	853	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	A	209	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	873	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	814	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	852	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	864	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	875	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	D	528	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	D	538	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	524	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	D	530	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	E	872	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	D	502	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	504	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	E	867	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	B	216	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	822	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	826	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	806	-	38,38,38	0.80±0.00	0±0 (0±0%)
5	7Q9	D	532	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	A	206	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	D	510	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	D	547	-	38,38,38	0.81±0.00	0±0 (0±0%)
6	17F	E	870	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	E	802	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	E	874	-	52,53,53	0.83±0.00	0±0 (0±0%)
6	17F	E	807	-	52,53,53	0.83±0.00	0±0 (0±0%)
6	17F	E	841	-	52,53,53	0.82±0.00	0±0 (0±0%)
5	7Q9	E	829	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	D	534	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	D	548	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	B	219	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	E	846	-	38,38,38	0.80±0.00	0±0 (0±0%)
6	17F	E	801	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	7Q9	A	211	-	38,38,38	0.81±0.00	0±0 (0±0%)
5	7Q9	E	850	-	38,38,38	0.80±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	Counts	Bond angles	
						RMSZ	#Z>2
5	7Q9	D	513	-	44,46,46	1.02±0.02	4±0 (8±0%)
5	7Q9	E	834	-	44,46,46	1.01±0.02	3±0 (7±0%)
5	7Q9	E	866	-	44,46,46	0.98±0.02	3±0 (6±0%)
6	17F	E	805	-	54,60,60	1.11±0.04	4±0 (7±0%)
6	17F	E	855	-	54,60,60	1.10±0.02	4±0 (7±0%)
5	7Q9	E	843	-	44,46,46	1.02±0.02	3±0 (7±1%)
5	7Q9	E	839	-	44,46,46	1.00±0.02	3±0 (7±1%)
5	7Q9	E	831	-	44,46,46	1.00±0.02	3±0 (7±1%)
5	7Q9	B	206	-	44,46,46	0.99±0.02	3±0 (6±0%)
5	7Q9	D	514	-	44,46,46	0.99±0.02	3±0 (7±1%)
5	7Q9	E	862	-	44,46,46	1.01±0.02	3±0 (7±1%)
5	7Q9	E	812	-	44,46,46	1.04±0.02	4±0 (9±0%)
6	17F	D	516	-	54,60,60	1.07±0.03	4±0 (7±0%)
5	7Q9	E	836	-	44,46,46	0.99±0.02	3±0 (7±1%)
5	7Q9	A	213	-	44,46,46	1.01±0.03	3±0 (7±0%)
6	17F	B	214	-	54,60,60	1.11±0.05	4±0 (8±0%)
5	7Q9	E	827	-	44,46,46	1.03±0.02	3±0 (7±0%)
5	7Q9	B	203	-	44,46,46	1.00±0.02	3±0 (7±0%)
5	7Q9	D	523	-	44,46,46	1.02±0.02	3±0 (6±0%)
5	7Q9	E	830	-	44,46,46	1.01±0.02	3±0 (6±0%)
5	7Q9	E	849	-	44,46,46	1.00±0.01	3±0 (6±0%)
6	17F	B	215	-	54,60,60	1.11±0.02	4±0 (7±0%)
5	7Q9	B	220	-	44,46,46	1.01±0.01	3±0 (6±0%)
5	7Q9	E	844	-	44,46,46	1.01±0.01	3±0 (7±1%)
5	7Q9	D	525	-	44,46,46	0.97±0.02	3±0 (6±0%)
5	7Q9	D	539	-	44,46,46	0.99±0.02	3±0 (7±0%)
5	7Q9	D	535	-	44,46,46	1.01±0.02	3±0 (7±1%)
5	7Q9	E	832	-	44,46,46	1.00±0.02	3±0 (6±0%)
5	7Q9	E	825	-	44,46,46	1.00±0.02	3±0 (7±0%)
5	7Q9	E	851	-	44,46,46	0.98±0.02	3±0 (6±0%)
6	17F	D	533	-	54,60,60	1.12±0.03	4±0 (7±0%)
5	7Q9	D	515	-	44,46,46	1.01±0.02	3±0 (7±0%)
5	7Q9	D	544	-	44,46,46	1.01±0.01	3±0 (7±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
5	7Q9	E	859	-	44,46,46	1.01±0.02	3±0 (6±0%)
5	7Q9	E	821	-	44,46,46	1.05±0.02	4±0 (9±0%)
6	17F	D	546	-	54,60,60	1.12±0.03	5±0 (8±0%)
5	7Q9	E	815	-	44,46,46	0.97±0.04	3±0 (7±0%)
5	7Q9	B	211	-	44,46,46	0.99±0.03	3±0 (7±0%)
6	17F	A	214	-	54,60,60	1.12±0.02	4±0 (7±0%)
6	17F	E	856	-	54,60,60	1.17±0.05	4±0 (7±0%)
5	7Q9	B	210	-	44,46,46	1.02±0.01	4±0 (8±1%)
5	7Q9	E	837	-	44,46,46	1.03±0.03	4±0 (8±0%)
5	7Q9	D	541	-	44,46,46	0.98±0.02	3±0 (6±0%)
5	7Q9	E	835	-	44,46,46	0.97±0.02	3±0 (6±0%)
5	7Q9	E	871	-	44,46,46	0.99±0.02	3±0 (6±0%)
5	7Q9	E	876	-	44,46,46	1.01±0.02	3±0 (7±0%)
5	7Q9	E	816	-	44,46,46	0.98±0.03	3±0 (7±0%)
5	7Q9	B	207	-	44,46,46	0.99±0.02	3±0 (7±1%)
5	7Q9	E	858	-	44,46,46	1.00±0.02	3±0 (7±0%)
5	7Q9	A	203	-	44,46,46	1.01±0.02	3±0 (7±0%)
5	7Q9	D	503	-	44,46,46	1.01±0.02	3±0 (7±1%)
3	GSP	B	201	4	47,54,54	1.72±0.03	11±1 (23±1%)
5	7Q9	E	813	-	44,46,46	1.02±0.02	3±0 (7±0%)
5	7Q9	E	877	-	44,46,46	1.00±0.02	4±0 (8±1%)
5	7Q9	A	212	-	44,46,46	0.99±0.02	3±0 (7±0%)
5	7Q9	E	861	-	44,46,46	0.99±0.02	3±0 (7±1%)
6	17F	E	828	-	54,60,60	1.09±0.02	4±0 (7±0%)
6	17F	E	838	-	54,60,60	1.12±0.04	5±0 (8±0%)
5	7Q9	B	218	-	44,46,46	0.98±0.03	3±0 (7±0%)
5	7Q9	D	521	-	44,46,46	1.00±0.02	3±0 (7±0%)
6	17F	A	208	-	54,60,60	1.09±0.03	4±0 (7±0%)
5	7Q9	E	869	-	44,46,46	1.01±0.01	4±0 (8±0%)
5	7Q9	D	531	-	44,46,46	1.00±0.03	4±0 (8±1%)
5	7Q9	A	205	-	44,46,46	1.02±0.03	3±0 (7±0%)
5	7Q9	A	217	-	44,46,46	1.00±0.01	3±0 (6±0%)
5	7Q9	D	518	-	44,46,46	1.00±0.02	3±0 (6±0%)
5	7Q9	D	537	-	44,46,46	1.01±0.02	3±0 (7±0%)
5	7Q9	E	810	-	44,46,46	1.01±0.02	3±0 (7±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
6	17F	D	527	-	54,60,60	1.14±0.03	4±0 (8±0%)
5	7Q9	E	854	-	44,46,46	0.99±0.01	3±0 (6±0%)
5	7Q9	E	847	-	44,46,46	1.01±0.01	3±0 (6±0%)
6	17F	E	819	-	54,60,60	1.07±0.05	4±0 (7±0%)
5	7Q9	D	519	-	44,46,46	1.01±0.02	3±1 (7±1%)
5	7Q9	E	878	-	44,46,46	1.01±0.01	3±0 (7±0%)
5	7Q9	E	860	-	44,46,46	1.02±0.02	3±0 (7±0%)
5	7Q9	D	505	-	44,46,46	1.00±0.02	3±0 (7±0%)
5	7Q9	A	215	-	44,46,46	1.00±0.02	3±0 (7±0%)
5	7Q9	E	833	-	44,46,46	0.99±0.02	4±0 (7±1%)
5	7Q9	D	536	-	44,46,46	1.00±0.02	3±0 (7±0%)
5	7Q9	E	865	-	44,46,46	1.00±0.02	3±0 (6±0%)
6	17F	E	811	-	54,60,60	1.08±0.03	4±0 (7±0%)
5	7Q9	E	845	-	44,46,46	1.02±0.02	4±0 (8±1%)
5	7Q9	E	848	-	44,46,46	1.00±0.01	3±0 (7±0%)
5	7Q9	D	545	-	44,46,46	1.02±0.02	4±0 (8±0%)
5	7Q9	A	210	-	44,46,46	0.99±0.02	3±0 (7±0%)
5	7Q9	E	803	-	44,46,46	0.99±0.03	3±0 (7±1%)
5	7Q9	E	857	-	44,46,46	0.99±0.02	3±0 (6±0%)
5	7Q9	E	868	-	44,46,46	1.01±0.02	4±0 (7±1%)
5	7Q9	D	512	-	44,46,46	1.01±0.02	3±0 (6±0%)
5	7Q9	D	529	-	44,46,46	1.01±0.02	4±0 (8±1%)
5	7Q9	D	526	-	44,46,46	1.09±0.02	4±0 (9±0%)
5	7Q9	D	542	-	44,46,46	1.02±0.02	4±0 (8±0%)
5	7Q9	E	863	-	44,46,46	1.01±0.02	3±0 (7±1%)
6	17F	D	501	-	54,60,60	1.11±0.07	5±0 (8±0%)
5	7Q9	D	506	-	44,46,46	1.04±0.03	4±0 (8±1%)
5	7Q9	B	205	-	44,46,46	0.97±0.02	3±0 (7±0%)
5	7Q9	D	549	-	44,46,46	1.01±0.01	3±0 (6±0%)
5	7Q9	E	808	-	44,46,46	0.96±0.02	3±0 (6±0%)
3	GSP	A	201	4	47,54,54	1.72±0.02	11±1 (24±1%)
6	17F	E	818	-	54,60,60	1.06±0.04	4±0 (7±0%)
5	7Q9	D	540	-	44,46,46	1.03±0.01	4±0 (8±0%)
5	7Q9	D	509	-	44,46,46	1.03±0.03	4±0 (8±0%)
5	7Q9	E	804	-	44,46,46	1.01±0.02	4±0 (8±1%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
5	7Q9	D	508	-	44,46,46	1.00±0.02	3±0 (6±0%)
5	7Q9	E	842	-	44,46,46	0.98±0.02	3±0 (7±0%)
5	7Q9	E	824	-	44,46,46	0.98±0.03	3±0 (7±0%)
6	17F	E	809	-	54,60,60	1.17±0.03	5±0 (9±0%)
6	17F	B	208	-	54,60,60	1.07±0.03	4±0 (7±0%)
5	7Q9	B	217	-	44,46,46	1.02±0.02	3±0 (7±1%)
5	7Q9	E	823	-	44,46,46	1.01±0.01	3±0 (7±0%)
5	7Q9	B	204	-	44,46,46	1.00±0.02	3±0 (6±0%)
5	7Q9	D	543	-	44,46,46	1.00±0.02	3±0 (7±1%)
5	7Q9	E	840	-	44,46,46	0.96±0.03	3±0 (7±0%)
5	7Q9	B	213	-	44,46,46	1.00±0.02	3±0 (7±0%)
5	7Q9	B	209	-	44,46,46	1.00±0.02	3±0 (7±0%)
5	7Q9	B	212	-	44,46,46	1.01±0.02	4±0 (8±1%)
6	17F	D	511	-	54,60,60	1.10±0.03	4±0 (8±0%)
5	7Q9	A	204	-	44,46,46	1.01±0.03	4±0 (8±1%)
6	17F	D	517	-	54,60,60	1.12±0.03	4±0 (7±0%)
5	7Q9	A	207	-	44,46,46	1.01±0.02	3±0 (7±1%)
5	7Q9	D	507	-	44,46,46	1.02±0.02	3±0 (6±0%)
5	7Q9	D	522	-	44,46,46	1.02±0.01	4±0 (8±0%)
5	7Q9	E	820	-	44,46,46	1.00±0.02	3±0 (7±1%)
6	17F	E	817	-	54,60,60	1.10±0.03	4±0 (7±0%)
5	7Q9	D	520	-	44,46,46	1.04±0.02	4±0 (9±0%)
5	7Q9	A	216	-	44,46,46	1.01±0.02	3±0 (7±0%)
5	7Q9	E	853	-	44,46,46	1.01±0.01	3±0 (6±0%)
5	7Q9	A	209	-	44,46,46	1.01±0.02	3±0 (7±1%)
5	7Q9	E	873	-	44,46,46	0.99±0.01	3±0 (6±0%)
5	7Q9	E	814	-	44,46,46	1.01±0.02	3±0 (7±1%)
5	7Q9	E	852	-	44,46,46	1.03±0.02	4±0 (8±0%)
5	7Q9	E	864	-	44,46,46	1.01±0.02	3±0 (7±1%)
5	7Q9	E	875	-	44,46,46	0.99±0.02	3±0 (7±0%)
6	17F	D	528	-	54,60,60	1.11±0.02	5±0 (9±0%)
5	7Q9	D	538	-	44,46,46	1.00±0.02	3±0 (6±0%)
5	7Q9	D	524	-	44,46,46	0.97±0.02	3±0 (7±0%)
5	7Q9	D	530	-	44,46,46	1.00±0.02	3±0 (7±1%)
6	17F	E	872	-	54,60,60	1.16±0.02	4±0 (8±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
5	7Q9	D	502	-	44,46,46	1.00±0.01	3±0 (6±0%)
5	7Q9	D	504	-	44,46,46	1.01±0.03	3±0 (7±0%)
5	7Q9	E	867	-	44,46,46	1.00±0.02	3±0 (6±0%)
5	7Q9	B	216	-	44,46,46	1.01±0.03	3±0 (7±1%)
5	7Q9	E	822	-	44,46,46	0.99±0.02	3±0 (6±0%)
5	7Q9	E	826	-	44,46,46	0.99±0.02	3±0 (6±0%)
5	7Q9	E	806	-	44,46,46	1.05±0.02	4±0 (8±0%)
5	7Q9	D	532	-	44,46,46	0.99±0.02	3±0 (6±0%)
5	7Q9	A	206	-	44,46,46	1.00±0.01	3±0 (7±0%)
6	17F	D	510	-	54,60,60	1.06±0.07	4±1 (6±1%)
5	7Q9	D	547	-	44,46,46	1.01±0.03	3±0 (7±1%)
6	17F	E	870	-	54,60,60	1.13±0.02	4±0 (7±0%)
5	7Q9	E	802	-	44,46,46	1.03±0.02	3±0 (7±0%)
6	17F	E	874	-	54,60,60	1.12±0.02	5±0 (8±0%)
6	17F	E	807	-	54,60,60	1.10±0.02	4±0 (8±0%)
6	17F	E	841	-	54,60,60	1.11±0.02	4±0 (7±0%)
5	7Q9	E	829	-	44,46,46	0.99±0.02	4±0 (7±1%)
6	17F	D	534	-	54,60,60	1.14±0.02	4±0 (8±0%)
5	7Q9	D	548	-	44,46,46	0.99±0.03	3±0 (6±0%)
6	17F	B	219	-	54,60,60	1.15±0.04	5±0 (8±0%)
5	7Q9	E	846	-	44,46,46	1.03±0.01	4±0 (8±1%)
6	17F	E	801	-	54,60,60	1.13±0.04	4±0 (7±0%)
5	7Q9	A	211	-	44,46,46	1.03±0.02	4±0 (8±1%)
5	7Q9	E	850	-	44,46,46	1.00±0.02	3±0 (7±1%)

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
6	17F	E	855	-	-	0±0,59,59,59	-
5	7Q9	E	843	-	-	0±0,42,42,42	-
5	7Q9	B	203	-	-	0±0,42,42,42	-
5	7Q9	B	206	-	-	0±0,42,42,42	-
5	7Q9	B	218	-	-	0±0,42,42,42	-
5	7Q9	D	521	-	-	0±0,42,42,42	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	7Q9	D	519	-	-	0±0,42,42,42	-
6	17F	E	838	-	-	0±0,59,59,59	-
5	7Q9	D	545	-	-	0±0,42,42,42	-
6	17F	D	516	-	-	0±0,59,59,59	-
5	7Q9	B	209	-	-	0±0,42,42,42	-
5	7Q9	E	853	-	-	0±0,42,42,42	-
5	7Q9	A	209	-	-	0±0,42,42,42	-
5	7Q9	A	216	-	-	0±0,42,42,42	-
5	7Q9	E	849	-	-	0±0,42,42,42	-
6	17F	B	214	-	-	0±0,59,59,59	-
6	17F	D	546	-	-	0±0,59,59,59	-
5	7Q9	E	822	-	-	0±0,42,42,42	-
5	7Q9	B	220	-	-	0±0,42,42,42	-
5	7Q9	E	804	-	-	0±0,42,42,42	-
6	17F	D	527	-	-	0±0,59,59,59	-
5	7Q9	D	532	-	-	0±0,42,42,42	-
6	17F	D	501	-	-	0±0,59,59,59	-
5	7Q9	E	842	-	-	0±0,42,42,42	-
5	7Q9	B	210	-	-	0±0,42,42,42	-
5	7Q9	A	207	-	-	0±0,42,42,42	-
5	7Q9	E	861	-	-	0±0,42,42,42	-
5	7Q9	D	505	-	-	0±0,42,42,42	-
5	7Q9	D	504	-	-	0±0,42,42,42	-
6	17F	E	807	-	-	0±0,59,59,59	-
5	7Q9	E	831	-	-	0±0,42,42,42	-
6	17F	D	528	-	-	0±0,59,59,59	-
5	7Q9	D	518	-	-	0±0,42,42,42	-
5	7Q9	E	824	-	-	0±0,42,42,42	-
5	7Q9	B	212	-	-	0±0,42,42,42	-
5	7Q9	B	217	-	-	0±0,42,42,42	-
5	7Q9	D	544	-	-	0±0,42,42,42	-
6	17F	E	819	-	-	0±0,59,59,59	-
5	7Q9	E	810	-	-	0±0,42,42,42	-
5	7Q9	E	866	-	-	0±0,42,42,42	-
5	7Q9	E	846	-	-	0±0,42,42,42	-
5	7Q9	E	878	-	-	0±0,42,42,42	-
6	17F	E	805	-	-	0±0,59,59,59	-
5	7Q9	A	204	-	-	0±0,42,42,42	-
5	7Q9	E	813	-	-	0±0,42,42,42	-
5	7Q9	E	834	-	-	0±0,42,42,42	-
5	7Q9	E	875	-	-	0±0,42,42,42	-
5	7Q9	D	507	-	-	0±0,42,42,42	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	7Q9	D	548	-	-	0±0,42,42,42	-
6	17F	E	809	-	-	0±0,59,59,59	-
5	7Q9	D	524	-	-	0±0,42,42,42	-
5	7Q9	D	537	-	-	0±0,42,42,42	-
5	7Q9	D	522	-	-	0±0,42,42,42	-
6	17F	E	817	-	-	0±0,59,59,59	-
5	7Q9	E	868	-	-	0±0,42,42,42	-
5	7Q9	E	871	-	-	0±0,42,42,42	-
5	7Q9	E	847	-	-	0±0,42,42,42	-
3	GSP	B	201	4	-	0±0,21,38,38	0±0,3,3,3
5	7Q9	E	820	-	-	0±0,42,42,42	-
5	7Q9	E	806	-	-	0±0,42,42,42	-
6	17F	A	208	-	-	0±0,59,59,59	-
5	7Q9	E	827	-	-	0±0,42,42,42	-
5	7Q9	B	207	-	-	0±0,42,42,42	-
6	17F	D	517	-	-	0±0,59,59,59	-
6	17F	E	841	-	-	0±0,59,59,59	-
5	7Q9	D	520	-	-	0±0,42,42,42	-
6	17F	E	811	-	-	0±0,59,59,59	-
5	7Q9	A	203	-	-	0±0,42,42,42	-
6	17F	E	870	-	-	0±0,59,59,59	-
5	7Q9	D	543	-	-	0±0,42,42,42	-
6	17F	E	801	-	-	0±0,59,59,59	-
5	7Q9	E	877	-	-	0±0,42,42,42	-
5	7Q9	D	542	-	-	0±0,42,42,42	-
6	17F	D	534	-	-	0±0,59,59,59	-
6	17F	E	874	-	-	0±0,59,59,59	-
5	7Q9	D	525	-	-	0±0,42,42,42	-
5	7Q9	D	514	-	-	0±0,42,42,42	-
5	7Q9	E	862	-	-	0±0,42,42,42	-
5	7Q9	D	526	-	-	0±0,42,42,42	-
5	7Q9	D	549	-	-	0±0,42,42,42	-
6	17F	E	872	-	-	0±0,59,59,59	-
5	7Q9	E	823	-	-	0±0,42,42,42	-
5	7Q9	E	852	-	-	0±0,42,42,42	-
5	7Q9	E	844	-	-	0±0,42,42,42	-
6	17F	E	856	-	-	0±0,59,59,59	-
5	7Q9	D	538	-	-	0±0,42,42,42	-
6	17F	E	818	-	-	0±0,59,59,59	-
5	7Q9	E	815	-	-	0±0,42,42,42	-
6	17F	D	511	-	-	0±0,59,59,59	-
5	7Q9	E	832	-	-	0±0,42,42,42	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	7Q9	D	502	-	-	0±0,42,42,42	-
3	GSP	A	201	4	-	0±0,21,38,38	0±0,3,3,3
5	7Q9	E	863	-	-	0±0,42,42,42	-
5	7Q9	D	513	-	-	0±0,42,42,42	-
5	7Q9	D	530	-	-	0±0,42,42,42	-
5	7Q9	E	851	-	-	0±0,42,42,42	-
5	7Q9	E	869	-	-	0±0,42,42,42	-
5	7Q9	E	833	-	-	0±0,42,42,42	-
5	7Q9	D	503	-	-	0±0,42,42,42	-
5	7Q9	E	835	-	-	0±0,42,42,42	-
5	7Q9	E	873	-	-	0±0,42,42,42	-
5	7Q9	E	865	-	-	0±0,42,42,42	-
6	17F	D	533	-	-	0±0,59,59,59	-
5	7Q9	E	808	-	-	0±0,42,42,42	-
5	7Q9	B	205	-	-	0±0,42,42,42	-
5	7Q9	E	816	-	-	0±0,42,42,42	-
5	7Q9	E	840	-	-	0±0,42,42,42	-
5	7Q9	D	512	-	-	0±0,42,42,42	-
5	7Q9	D	536	-	-	0±0,42,42,42	-
6	17F	D	510	-	-	0±0,59,59,59	-
5	7Q9	A	211	-	-	0±0,42,42,42	-
5	7Q9	E	830	-	-	0±0,42,42,42	-
5	7Q9	E	857	-	-	0±0,42,42,42	-
6	17F	B	215	-	-	0±0,59,59,59	-
5	7Q9	D	508	-	-	0±0,42,42,42	-
5	7Q9	B	216	-	-	0±0,42,42,42	-
5	7Q9	E	876	-	-	0±0,42,42,42	-
5	7Q9	B	204	-	-	0±0,42,42,42	-
5	7Q9	D	539	-	-	0±0,42,42,42	-
5	7Q9	A	217	-	-	0±0,42,42,42	-
5	7Q9	E	867	-	-	0±0,42,42,42	-
5	7Q9	A	206	-	-	0±0,42,42,42	-
5	7Q9	E	837	-	-	0±0,42,42,42	-
5	7Q9	E	845	-	-	0±0,42,42,42	-
5	7Q9	A	213	-	-	0±0,42,42,42	-
5	7Q9	E	860	-	-	0±0,42,42,42	-
5	7Q9	D	515	-	-	0±0,42,42,42	-
6	17F	B	219	-	-	0±0,59,59,59	-
5	7Q9	D	509	-	-	0±0,42,42,42	-
5	7Q9	E	839	-	-	0±0,42,42,42	-
6	17F	A	214	-	-	0±0,59,59,59	-
5	7Q9	D	535	-	-	0±0,42,42,42	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	7Q9	D	547	-	-	0±0,42,42,42	-
5	7Q9	A	205	-	-	0±0,42,42,42	-
5	7Q9	A	210	-	-	0±0,42,42,42	-
5	7Q9	B	213	-	-	0±0,42,42,42	-
6	17F	B	208	-	-	0±0,59,59,59	-
5	7Q9	E	859	-	-	0±0,42,42,42	-
5	7Q9	D	523	-	-	0±0,42,42,42	-
5	7Q9	E	829	-	-	0±0,42,42,42	-
5	7Q9	D	506	-	-	0±0,42,42,42	-
5	7Q9	D	529	-	-	0±0,42,42,42	-
5	7Q9	E	826	-	-	0±0,42,42,42	-
5	7Q9	E	850	-	-	0±0,42,42,42	-
5	7Q9	E	812	-	-	0±0,42,42,42	-
5	7Q9	E	825	-	-	0±0,42,42,42	-
5	7Q9	D	541	-	-	0±0,42,42,42	-
5	7Q9	E	854	-	-	0±0,42,42,42	-
5	7Q9	E	821	-	-	0±0,42,42,42	-
5	7Q9	E	858	-	-	0±0,42,42,42	-
5	7Q9	B	211	-	-	0±0,42,42,42	-
5	7Q9	A	212	-	-	0±0,42,42,42	-
5	7Q9	D	531	-	-	0±0,42,42,42	-
5	7Q9	A	215	-	-	0±0,42,42,42	-
5	7Q9	E	803	-	-	0±0,42,42,42	-
5	7Q9	E	836	-	-	0±0,42,42,42	-
5	7Q9	E	848	-	-	0±0,42,42,42	-
5	7Q9	E	864	-	-	0±0,42,42,42	-
5	7Q9	E	814	-	-	0±0,42,42,42	-
6	17F	E	828	-	-	0±0,59,59,59	-
5	7Q9	D	540	-	-	0±0,42,42,42	-
5	7Q9	E	802	-	-	0±0,42,42,42	-

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	B	201	GSP	C5-N7	2.99	1.33	1.39	8	20
3	A	201	GSP	C5-N7	2.98	1.33	1.39	6	20
3	B	201	GSP	PB-O3A	2.02	1.61	1.59	17	1
3	A	201	GSP	PB-O3B	2.01	1.61	1.59	15	1
3	B	201	GSP	PG-O2G	2.00	1.48	1.54	7	1

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	A	201	GSP	C2-N3-C4	5.36	121.53	112.30	14	20
3	B	201	GSP	C2-N3-C4	5.34	121.50	112.30	14	20
6	E	805	17F	O3-C1-C2	5.20	112.59	108.06	6	20
6	E	856	17F	O3-C1-C2	5.08	112.49	108.06	20	20
3	A	201	GSP	C5-C4-N3	5.01	120.42	128.39	2	20
6	D	501	17F	O3-C1-C2	4.93	112.36	108.06	11	20
3	B	201	GSP	C5-C4-N3	4.93	120.54	128.39	14	20
6	B	208	17F	O3-C1-C2	4.71	112.17	108.06	6	20
6	D	510	17F	O3-C1-C2	4.53	112.01	108.06	20	20
6	E	841	17F	O3-C1-C2	4.43	111.92	108.06	20	20
6	D	546	17F	O3-C1-C2	4.43	111.92	108.06	7	20
6	E	818	17F	O3-C1-C2	4.42	111.91	108.06	18	20
6	E	838	17F	O3-C1-C2	4.41	111.90	108.06	2	20
6	D	527	17F	O3-C1-C2	4.36	111.86	108.06	17	20
6	E	801	17F	O3-C1-C2	4.36	111.86	108.06	2	20
6	D	510	17F	O9-C17-C18	4.35	120.89	111.48	8	20
6	E	870	17F	O3-C1-C2	4.35	111.85	108.06	16	20
6	E	828	17F	O3-C1-C2	4.33	111.83	108.06	10	20
6	E	809	17F	O3-C1-C2	4.28	111.79	108.06	1	20
6	D	501	17F	O9-C17-C18	4.25	120.67	111.48	2	20
6	D	527	17F	O9-C17-C18	4.24	120.66	111.48	8	20
6	B	214	17F	O3-C1-C2	4.22	111.74	108.06	3	20
6	A	214	17F	O3-C1-C2	4.17	111.69	108.06	20	20
6	E	819	17F	O3-C1-C2	4.16	111.69	108.06	4	20
6	D	533	17F	O3-C1-C2	4.15	111.68	108.06	12	20
6	E	872	17F	O3-C1-C2	4.15	111.68	108.06	1	20
3	B	201	GSP	C4'-O4'-C1'	4.15	100.31	109.47	10	3
3	A	201	GSP	PB-O3B-PG	4.14	118.01	133.17	11	20
6	E	817	17F	O3-C1-C2	4.13	111.66	108.06	16	20
6	E	807	17F	O3-C1-C2	4.12	111.65	108.06	18	20
6	E	801	17F	C5-O9-C17	4.09	108.00	117.80	10	20
6	E	805	17F	C5-O9-C17	4.09	108.01	117.80	13	20
6	E	872	17F	O9-C17-C18	4.06	120.27	111.48	14	20
6	E	856	17F	O9-C17-C18	4.06	120.26	111.48	1	20
6	E	811	17F	O3-C1-C2	4.06	111.59	108.06	7	20
3	B	201	GSP	PB-O3B-PG	4.04	118.39	133.17	3	20
6	E	801	17F	O9-C17-C18	4.04	120.21	111.48	10	20
6	B	214	17F	O9-C17-C18	4.03	120.21	111.48	6	20
6	D	511	17F	O3-C1-C2	4.03	111.57	108.06	4	20
6	B	219	17F	O3-C1-C2	4.02	111.57	108.06	17	20
6	B	215	17F	O3-C1-C2	4.02	111.56	108.06	11	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
6	B	219	17F	O9-C17-C18	4.02	120.17	111.48	16	20
6	D	534	17F	O9-C17-C18	4.00	120.14	111.48	8	20
5	E	863	7Q9	C2-O21-C21	3.98	108.26	117.80	12	20
6	E	809	17F	O9-C17-C18	3.98	120.10	111.48	16	20
6	D	516	17F	O3-C1-C2	3.97	111.52	108.06	16	20
5	D	526	7Q9	C2-O21-C21	3.97	108.30	117.80	10	20
6	D	528	17F	O3-C1-C2	3.96	111.51	108.06	12	20
6	D	528	17F	O9-C17-C18	3.96	120.04	111.48	3	20
6	E	807	17F	O9-C17-C18	3.95	120.03	111.48	2	20
6	B	215	17F	O9-C17-C18	3.95	120.02	111.48	18	20
6	E	872	17F	C5-O9-C17	3.95	108.35	117.80	14	20
6	A	214	17F	O9-C17-C18	3.93	119.97	111.48	8	20
6	A	208	17F	O3-C1-C2	3.92	111.48	108.06	10	20
6	D	517	17F	O9-C17-C18	3.92	119.96	111.48	20	20
6	D	534	17F	O3-C1-C2	3.92	111.47	108.06	20	20
6	E	805	17F	O9-C17-C18	3.91	119.95	111.48	1	20
6	E	874	17F	O3-C1-C2	3.91	111.47	108.06	5	20
6	E	856	17F	C5-O9-C17	3.89	108.48	117.80	4	20
6	A	208	17F	O9-C17-C18	3.89	119.89	111.48	16	20
6	D	533	17F	O9-C17-C18	3.88	119.87	111.48	18	20
6	E	874	17F	O9-C17-C18	3.86	119.82	111.48	10	20
6	D	501	17F	C5-O9-C17	3.85	108.58	117.80	2	20
6	E	818	17F	O9-C17-C18	3.85	119.81	111.48	2	20
6	D	534	17F	C5-O9-C17	3.85	108.58	117.80	8	20
6	E	870	17F	O9-C17-C18	3.85	119.80	111.48	10	20
6	E	819	17F	O9-C17-C18	3.84	119.80	111.48	13	20
5	A	213	7Q9	C2-O21-C21	3.84	108.61	117.80	20	20
6	E	841	17F	O9-C17-C18	3.83	119.77	111.48	11	20
5	D	507	7Q9	C2-O21-C21	3.82	108.66	117.80	15	20
6	D	516	17F	O9-C17-C18	3.81	119.73	111.48	18	20
6	D	517	17F	O3-C1-C2	3.81	111.38	108.06	15	20
6	E	811	17F	O9-C17-C18	3.79	119.68	111.48	10	20
6	D	517	17F	C5-O9-C17	3.79	108.73	117.80	7	20
5	B	216	7Q9	C2-O21-C21	3.78	108.75	117.80	5	20
5	D	508	7Q9	C2-O21-C21	3.77	108.77	117.80	17	20
5	E	858	7Q9	C2-O21-C21	3.77	108.77	117.80	14	20
6	B	219	17F	C5-O9-C17	3.77	108.78	117.80	2	20
5	A	205	7Q9	C2-O21-C21	3.77	108.78	117.80	6	20
5	E	854	7Q9	C2-O21-C21	3.77	108.78	117.80	4	20
6	E	855	17F	O3-C1-C2	3.75	111.33	108.06	5	20
6	A	214	17F	C5-O9-C17	3.75	108.83	117.80	9	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
6	E	817	17F	O9-C17-C18	3.74	119.58	111.48	12	20
5	D	502	7Q9	C2-O21-C21	3.74	108.85	117.80	8	20
6	E	809	17F	C5-O9-C17	3.74	108.85	117.80	3	20
5	E	876	7Q9	C2-O21-C21	3.72	108.89	117.80	3	20
5	D	532	7Q9	C2-O21-C21	3.72	108.89	117.80	14	20
6	E	855	17F	O9-C17-C18	3.72	119.53	111.48	10	20
5	E	843	7Q9	C2-O21-C21	3.72	108.90	117.80	15	20
5	D	530	7Q9	C2-O21-C21	3.71	108.91	117.80	10	20
5	D	512	7Q9	C2-O21-C21	3.71	108.92	117.80	7	20
5	B	204	7Q9	C2-O21-C21	3.71	108.92	117.80	10	20
6	B	214	17F	C5-O9-C17	3.71	108.92	117.80	2	19
5	D	523	7Q9	C2-O21-C21	3.70	108.94	117.80	2	20
5	E	865	7Q9	C2-O21-C21	3.70	108.94	117.80	20	20
5	D	506	7Q9	C2-O21-C21	3.70	108.95	117.80	6	20
5	E	806	7Q9	C2-O21-C21	3.70	108.95	117.80	7	20
6	D	511	17F	O9-C17-C18	3.69	119.46	111.48	18	20
5	E	827	7Q9	C2-O21-C21	3.69	108.97	117.80	8	20
5	D	515	7Q9	C2-O21-C21	3.68	108.98	117.80	9	20
5	D	513	7Q9	C2-O21-C21	3.68	108.99	117.80	4	20
5	E	837	7Q9	C2-O21-C21	3.68	108.99	117.80	9	20
5	B	213	7Q9	C2-O21-C21	3.67	109.00	117.80	16	20
6	D	533	17F	C5-O9-C17	3.67	109.00	117.80	18	20
5	D	518	7Q9	C2-O21-C21	3.67	109.01	117.80	14	20
5	E	830	7Q9	C2-O21-C21	3.67	109.01	117.80	2	20
6	E	838	17F	O9-C17-C18	3.67	119.42	111.48	20	20
6	E	828	17F	O9-C17-C18	3.66	119.41	111.48	20	20
5	B	210	7Q9	C2-O21-C21	3.66	109.04	117.80	8	20
5	E	852	7Q9	C2-O21-C21	3.65	109.05	117.80	11	20
6	B	208	17F	O9-C17-C18	3.65	119.38	111.48	2	20
5	E	821	7Q9	C2-O21-C21	3.65	109.06	117.80	1	20
5	E	873	7Q9	C2-O21-C21	3.65	109.06	117.80	11	20
5	E	813	7Q9	C2-O21-C21	3.64	109.07	117.80	13	20
5	E	851	7Q9	C2-O21-C21	3.65	109.07	117.80	11	20
5	E	834	7Q9	C2-O21-C21	3.64	109.08	117.80	13	20
6	D	510	17F	C5-O9-C17	3.64	109.09	117.80	8	9
5	A	217	7Q9	C2-O21-C21	3.63	109.11	117.80	10	20
5	D	505	7Q9	C2-O21-C21	3.63	109.12	117.80	8	20
5	E	802	7Q9	C2-O21-C21	3.63	109.12	117.80	11	20
5	E	859	7Q9	C2-O21-C21	3.62	109.14	117.80	10	20
6	D	546	17F	O9-C17-C18	3.62	119.31	111.48	1	20
5	D	537	7Q9	C2-O21-C21	3.61	109.14	117.80	17	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	D	549	7Q9	C2-O21-C21	3.61	109.15	117.80	2	20
5	D	545	7Q9	C2-O21-C21	3.61	109.16	117.80	7	20
5	E	839	7Q9	C2-O21-C21	3.60	109.18	117.80	9	20
5	E	878	7Q9	C2-O21-C21	3.60	109.19	117.80	18	20
6	E	819	17F	C5-O9-C17	3.60	109.19	117.80	13	20
5	D	542	7Q9	C2-O21-C21	3.59	109.20	117.80	3	20
5	E	864	7Q9	C2-O21-C21	3.59	109.20	117.80	15	20
5	B	206	7Q9	C2-O21-C21	3.59	109.20	117.80	1	20
5	D	503	7Q9	C2-O21-C21	3.59	109.21	117.80	6	20
5	D	529	7Q9	C2-O21-C21	3.59	109.21	117.80	8	20
5	A	207	7Q9	C2-O21-C21	3.59	109.21	117.80	7	20
5	A	206	7Q9	C2-O21-C21	3.58	109.22	117.80	19	20
5	A	216	7Q9	C2-O21-C21	3.58	109.23	117.80	5	20
5	D	514	7Q9	C2-O21-C21	3.58	109.23	117.80	12	20
5	D	536	7Q9	C2-O21-C21	3.58	109.24	117.80	15	20
5	E	877	7Q9	C2-O21-C21	3.58	109.24	117.80	12	20
5	E	822	7Q9	C2-O21-C21	3.57	109.24	117.80	4	20
5	E	824	7Q9	C2-O21-C21	3.57	109.24	117.80	5	20
5	D	547	7Q9	C2-O21-C21	3.57	109.25	117.80	5	20
5	D	548	7Q9	C2-O21-C21	3.56	109.27	117.80	7	20
5	D	519	7Q9	C2-O21-C21	3.56	109.27	117.80	7	20
5	E	844	7Q9	C2-O21-C21	3.56	109.28	117.80	20	20
5	E	867	7Q9	C2-O21-C21	3.56	109.28	117.80	16	20
5	D	544	7Q9	C2-O21-C21	3.56	109.28	117.80	18	20
5	D	541	7Q9	C2-O21-C21	3.55	109.29	117.80	12	20
5	E	810	7Q9	C2-O21-C21	3.55	109.30	117.80	5	20
5	D	504	7Q9	C2-O21-C21	3.55	109.31	117.80	19	20
5	E	845	7Q9	C2-O21-C21	3.54	109.32	117.80	15	20
5	E	846	7Q9	C2-O21-C21	3.54	109.33	117.80	19	20
5	E	814	7Q9	C2-O21-C21	3.54	109.33	117.80	13	20
6	E	841	17F	C5-O9-C17	3.54	109.33	117.80	11	20
6	B	215	17F	C5-O9-C17	3.53	109.34	117.80	18	20
5	A	203	7Q9	C2-O21-C21	3.53	109.35	117.80	3	20
5	A	212	7Q9	C2-O21-C21	3.52	109.36	117.80	18	20
5	E	804	7Q9	C2-O21-C21	3.52	109.37	117.80	10	20
6	D	527	17F	C5-O9-C17	3.52	109.37	117.80	9	20
5	D	531	7Q9	C2-O21-C21	3.51	109.39	117.80	7	20
5	E	803	7Q9	C2-O21-C21	3.51	109.39	117.80	19	20
5	E	868	7Q9	C2-O21-C21	3.51	109.40	117.80	1	20
5	E	823	7Q9	C2-O21-C21	3.50	109.41	117.80	14	20
5	E	875	7Q9	C2-O21-C21	3.50	109.41	117.80	7	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	E	826	7Q9	C2-O21-C21	3.50	109.42	117.80	14	20
5	B	209	7Q9	C2-O21-C21	3.50	109.42	117.80	8	20
5	E	850	7Q9	C2-O21-C21	3.50	109.43	117.80	6	20
6	A	208	17F	C5-O9-C17	3.50	109.43	117.80	16	20
5	E	825	7Q9	C2-O21-C21	3.49	109.44	117.80	5	20
5	E	861	7Q9	C2-O21-C21	3.49	109.44	117.80	5	20
5	E	853	7Q9	C2-O21-C21	3.49	109.45	117.80	9	20
6	E	818	17F	C5-O9-C17	3.49	109.45	117.80	2	20
5	D	521	7Q9	C2-O21-C21	3.49	109.45	117.80	3	20
5	E	840	7Q9	C2-O21-C21	3.48	109.46	117.80	10	20
5	E	812	7Q9	C2-O21-C21	3.48	109.47	117.80	3	20
5	E	831	7Q9	C2-O21-C21	3.47	109.49	117.80	20	20
5	D	535	7Q9	C2-O21-C21	3.47	109.49	117.80	17	20
5	D	543	7Q9	C2-O21-C21	3.46	109.51	117.80	3	20
5	E	849	7Q9	C2-O21-C21	3.46	109.52	117.80	16	20
5	D	525	7Q9	C2-O21-C21	3.46	109.52	117.80	9	20
6	D	516	17F	C5-O9-C17	3.46	109.52	117.80	2	20
5	A	211	7Q9	C2-O21-C21	3.46	109.53	117.80	15	20
6	E	870	17F	C5-O9-C17	3.46	109.53	117.80	3	20
5	E	871	7Q9	C2-O21-C21	3.45	109.54	117.80	18	20
5	B	212	7Q9	C2-O21-C21	3.45	109.54	117.80	5	20
5	A	210	7Q9	C2-O21-C21	3.45	109.55	117.80	2	20
5	D	540	7Q9	C2-O21-C21	3.45	109.55	117.80	12	20
6	E	874	17F	C5-O9-C17	3.45	109.55	117.80	10	20
5	B	203	7Q9	C2-O21-C21	3.44	109.56	117.80	5	20
5	E	815	7Q9	C2-O21-C21	3.44	109.57	117.80	10	20
5	E	866	7Q9	C2-O21-C21	3.44	109.57	117.80	15	20
5	D	538	7Q9	C2-O21-C21	3.43	109.58	117.80	8	20
5	E	860	7Q9	C2-O21-C21	3.43	109.58	117.80	17	20
5	E	857	7Q9	C2-O21-C21	3.43	109.59	117.80	4	20
6	E	807	17F	C5-O9-C17	3.42	109.60	117.80	2	20
5	E	832	7Q9	C2-O21-C21	3.42	109.62	117.80	19	20
5	E	835	7Q9	C2-O21-C21	3.42	109.62	117.80	10	20
5	E	848	7Q9	C2-O21-C21	3.42	109.62	117.80	8	20
5	D	520	7Q9	C2-O21-C21	3.41	109.63	117.80	7	20
5	E	816	7Q9	C2-O21-C21	3.41	109.63	117.80	11	20
5	B	218	7Q9	C2-O21-C21	3.41	109.64	117.80	7	20
6	E	811	17F	C5-O9-C17	3.40	109.65	117.80	14	20
6	E	855	17F	C5-O9-C17	3.40	109.65	117.80	16	20
5	E	862	7Q9	C2-O21-C21	3.40	109.66	117.80	13	20
5	B	220	7Q9	C2-O21-C21	3.39	109.69	117.80	17	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	E	808	7Q9	C2-O21-C21	3.39	109.69	117.80	3	20
5	B	207	7Q9	C2-O21-C21	3.38	109.70	117.80	1	20
5	E	820	7Q9	C2-O21-C21	3.38	109.70	117.80	1	20
5	E	836	7Q9	C2-O21-C21	3.38	109.70	117.80	18	20
5	E	847	7Q9	C2-O21-C21	3.38	109.70	117.80	11	20
5	B	211	7Q9	C2-O21-C21	3.38	109.70	117.80	8	20
5	A	209	7Q9	C2-O21-C21	3.38	109.71	117.80	5	20
5	A	204	7Q9	C2-O21-C21	3.37	109.72	117.80	18	20
5	B	217	7Q9	C2-O21-C21	3.36	109.75	117.80	2	20
5	E	869	7Q9	C2-O21-C21	3.36	109.75	117.80	6	20
5	D	509	7Q9	C2-O21-C21	3.36	109.75	117.80	6	20
6	E	828	17F	C5-O9-C17	3.36	109.75	117.80	16	20
5	D	539	7Q9	C2-O21-C21	3.35	109.77	117.80	8	20
3	A	201	GSP	C2-N1-C6	3.35	119.04	125.11	2	20
3	B	201	GSP	N9-C4-N3	3.35	132.64	125.95	4	20
3	B	201	GSP	C2-N1-C6	3.34	119.05	125.11	4	20
3	A	201	GSP	N9-C4-N3	3.34	132.63	125.95	2	20
5	D	522	7Q9	C2-O21-C21	3.34	109.81	117.80	2	20
5	B	205	7Q9	C2-O21-C21	3.34	109.81	117.80	1	20
6	E	817	17F	C5-O9-C17	3.30	109.89	117.80	4	20
6	D	511	17F	C5-O9-C17	3.28	109.94	117.80	19	20
5	E	833	7Q9	C2-O21-C21	3.28	109.95	117.80	18	20
5	D	524	7Q9	C2-O21-C21	3.27	109.96	117.80	5	20
5	A	215	7Q9	C2-O21-C21	3.27	109.96	117.80	17	20
5	E	829	7Q9	C2-O21-C21	3.27	109.98	117.80	19	20
6	B	208	17F	C5-O9-C17	3.23	110.06	117.80	2	20
6	D	546	17F	C5-O9-C17	3.20	110.14	117.80	8	20
5	E	842	7Q9	C2-O21-C21	3.18	110.19	117.80	8	20
6	D	528	17F	C5-O9-C17	3.13	110.31	117.80	2	20
5	D	526	7Q9	O31-C31-C32	3.04	121.09	111.83	12	20
6	E	838	17F	C5-O9-C17	3.01	110.58	117.80	2	20
6	E	809	17F	O7-C7-C8	3.00	121.00	111.83	15	20
5	A	211	7Q9	O31-C31-C32	2.99	120.94	111.83	16	20
6	E	838	17F	O7-C7-C8	2.93	120.77	111.83	14	20
5	D	509	7Q9	O31-C31-C32	2.92	120.74	111.83	10	20
5	E	816	7Q9	O31-C31-C32	2.91	120.70	111.83	20	20
6	D	501	17F	O7-C7-C8	2.89	120.65	111.83	9	20
5	E	837	7Q9	O31-C31-C32	2.86	120.57	111.83	9	20
5	D	506	7Q9	O31-C31-C32	2.83	120.47	111.83	18	20
5	B	209	7Q9	O31-C31-C32	2.83	120.46	111.83	3	20
5	E	812	7Q9	O31-C31-C32	2.83	120.45	111.83	6	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
6	E	818	17F	O7-C7-C8	2.83	120.45	111.83	2	20
5	E	863	7Q9	O31-C31-C32	2.81	120.41	111.83	8	20
5	B	212	7Q9	O31-C31-C32	2.81	120.39	111.83	3	20
5	D	531	7Q9	O31-C31-C32	2.81	120.40	111.83	7	20
6	E	819	17F	O7-C7-C8	2.80	120.39	111.83	10	20
6	B	219	17F	O7-C7-C8	2.79	120.34	111.83	5	20
5	D	520	7Q9	O31-C31-C32	2.79	120.33	111.83	9	20
6	D	510	17F	O7-C7-C8	2.77	120.29	111.83	14	20
5	E	806	7Q9	O31-C31-C32	2.77	120.28	111.83	15	20
5	D	540	7Q9	O31-C31-C32	2.76	120.25	111.83	19	20
6	D	528	17F	O7-C7-C8	2.75	120.21	111.83	7	20
5	E	839	7Q9	O31-C31-C32	2.74	120.20	111.83	11	20
6	D	534	17F	O7-C7-C8	2.74	120.20	111.83	16	20
5	D	542	7Q9	O31-C31-C32	2.74	120.18	111.83	14	20
5	E	821	7Q9	O31-C31-C32	2.74	120.18	111.83	19	20
5	E	846	7Q9	O31-C31-C32	2.74	120.18	111.83	12	20
5	D	522	7Q9	O31-C31-C32	2.72	120.14	111.83	7	20
5	B	207	7Q9	O31-C31-C32	2.72	120.13	111.83	20	20
5	E	836	7Q9	O31-C31-C32	2.71	120.10	111.83	12	20
5	E	845	7Q9	O31-C31-C32	2.71	120.11	111.83	1	20
6	E	811	17F	O7-C7-C8	2.71	120.11	111.83	12	20
5	A	204	7Q9	O31-C31-C32	2.71	120.09	111.83	18	20
5	E	852	7Q9	O31-C31-C32	2.71	120.09	111.83	15	20
6	B	214	17F	O7-C7-C8	2.71	120.09	111.83	8	20
5	A	213	7Q9	O31-C31-C32	2.71	120.09	111.83	13	20
6	D	546	17F	O7-C7-C8	2.70	120.08	111.83	4	20
5	B	210	7Q9	O31-C31-C32	2.70	120.06	111.83	10	20
5	D	529	7Q9	O31-C31-C32	2.70	120.07	111.83	16	20
5	E	803	7Q9	O31-C31-C32	2.70	120.06	111.83	19	20
5	E	833	7Q9	O31-C31-C32	2.70	120.05	111.83	13	20
6	D	511	17F	O7-C7-C8	2.69	120.05	111.83	15	20
6	E	856	17F	O7-C7-C8	2.69	120.05	111.83	13	20
5	D	536	7Q9	O31-C31-C32	2.69	120.03	111.83	2	20
5	E	862	7Q9	O31-C31-C32	2.68	120.02	111.83	2	20
6	E	801	17F	O7-C7-C8	2.68	120.02	111.83	20	20
5	D	530	7Q9	O31-C31-C32	2.68	120.01	111.83	1	20
6	E	872	17F	O7-C7-C8	2.68	120.00	111.83	2	20
5	D	513	7Q9	O31-C31-C32	2.67	119.99	111.83	8	20
5	D	504	7Q9	O31-C31-C32	2.67	119.98	111.83	19	20
5	D	519	7Q9	O31-C31-C32	2.67	119.97	111.83	6	20
5	E	814	7Q9	O31-C31-C32	2.67	119.97	111.83	12	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	E	869	7Q9	O31-C31-C32	2.67	119.98	111.83	19	20
5	E	831	7Q9	O31-C31-C32	2.67	119.97	111.83	11	20
5	D	514	7Q9	O31-C31-C32	2.67	119.97	111.83	3	20
6	E	874	17F	O7-C7-C8	2.67	119.96	111.83	7	20
5	A	207	7Q9	O31-C31-C32	2.66	119.95	111.83	9	20
5	E	847	7Q9	O31-C31-C32	2.66	119.95	111.83	15	20
5	D	524	7Q9	O31-C31-C32	2.66	119.93	111.83	12	20
5	D	548	7Q9	O31-C31-C32	2.66	119.93	111.83	20	20
5	E	823	7Q9	O31-C31-C32	2.65	119.93	111.83	5	20
5	E	848	7Q9	O31-C31-C32	2.65	119.93	111.83	15	20
6	E	807	17F	O7-C7-C8	2.66	119.93	111.83	9	20
5	B	206	7Q9	O31-C31-C32	2.65	119.92	111.83	6	20
5	E	858	7Q9	O31-C31-C32	2.65	119.92	111.83	20	20
6	D	527	17F	O7-C7-C8	2.65	119.92	111.83	14	20
5	D	539	7Q9	O31-C31-C32	2.65	119.91	111.83	10	20
5	D	547	7Q9	O31-C31-C32	2.65	119.91	111.83	6	20
5	E	840	7Q9	O31-C31-C32	2.65	119.92	111.83	4	20
5	D	515	7Q9	O31-C31-C32	2.65	119.91	111.83	13	20
5	D	509	7Q9	C3-O31-C31	2.64	107.46	117.12	10	17
5	D	545	7Q9	O31-C31-C32	2.64	119.89	111.83	16	20
5	E	810	7Q9	O31-C31-C32	2.64	119.89	111.83	16	20
5	E	844	7Q9	O31-C31-C32	2.64	119.89	111.83	6	20
5	A	216	7Q9	O31-C31-C32	2.64	119.88	111.83	7	20
5	D	543	7Q9	O31-C31-C32	2.64	119.88	111.83	19	20
5	E	834	7Q9	O31-C31-C32	2.63	119.87	111.83	4	20
5	E	877	7Q9	O31-C31-C32	2.64	119.87	111.83	16	20
5	E	878	7Q9	O31-C31-C32	2.64	119.87	111.83	9	20
6	A	208	17F	O7-C7-C8	2.64	119.87	111.83	2	20
5	E	820	7Q9	O31-C31-C32	2.63	119.86	111.83	19	20
5	E	843	7Q9	O31-C31-C32	2.63	119.85	111.83	13	20
5	E	813	7Q9	O31-C31-C32	2.63	119.84	111.83	15	20
5	D	521	7Q9	O31-C31-C32	2.62	119.83	111.83	2	20
5	A	212	7Q9	O31-C31-C32	2.62	119.82	111.83	14	20
5	E	868	7Q9	O31-C31-C32	2.62	119.82	111.83	5	20
6	D	517	17F	O7-C7-C8	2.62	119.82	111.83	7	20
5	E	827	7Q9	O31-C31-C32	2.62	119.81	111.83	4	20
5	B	213	7Q9	O31-C31-C32	2.61	119.81	111.83	4	20
5	B	216	7Q9	O31-C31-C32	2.61	119.81	111.83	1	20
5	E	802	7Q9	O31-C31-C32	2.61	119.81	111.83	9	20
5	E	804	7Q9	O31-C31-C32	2.61	119.80	111.83	10	20
5	B	217	7Q9	O31-C31-C32	2.61	119.80	111.83	5	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	E	815	7Q9	O31-C31-C32	2.61	119.79	111.83	13	20
5	B	220	7Q9	O31-C31-C32	2.61	119.79	111.83	3	20
5	A	211	7Q9	C3-O31-C31	2.61	107.59	117.12	16	13
5	D	538	7Q9	O31-C31-C32	2.61	119.79	111.83	9	20
5	B	211	7Q9	O31-C31-C32	2.61	119.78	111.83	4	20
5	D	535	7Q9	O31-C31-C32	2.60	119.77	111.83	4	20
5	B	218	7Q9	O31-C31-C32	2.60	119.77	111.83	14	20
5	E	853	7Q9	O31-C31-C32	2.60	119.77	111.83	12	20
6	B	215	17F	O7-C7-C8	2.60	119.77	111.83	1	20
5	A	205	7Q9	O31-C31-C32	2.60	119.75	111.83	5	20
5	A	215	7Q9	O31-C31-C32	2.59	119.75	111.83	7	20
5	D	505	7Q9	O31-C31-C32	2.59	119.74	111.83	3	20
5	E	825	7Q9	O31-C31-C32	2.59	119.75	111.83	1	20
5	D	503	7Q9	O31-C31-C32	2.59	119.73	111.83	7	20
5	E	860	7Q9	O31-C31-C32	2.59	119.73	111.83	3	20
3	B	201	GSP	O4'-C1'-N9	2.59	114.22	108.36	10	18
6	E	817	17F	O7-C7-C8	2.59	119.72	111.83	12	20
5	D	544	7Q9	O31-C31-C32	2.58	119.71	111.83	11	20
5	E	832	7Q9	O31-C31-C32	2.58	119.71	111.83	10	20
5	E	876	7Q9	O31-C31-C32	2.58	119.70	111.83	8	20
5	D	537	7Q9	O31-C31-C32	2.58	119.70	111.83	7	20
5	E	859	7Q9	O31-C31-C32	2.58	119.70	111.83	19	20
5	E	861	7Q9	O31-C31-C32	2.58	119.70	111.83	17	20
6	E	828	17F	O7-C7-C8	2.58	119.70	111.83	16	20
5	A	210	7Q9	O31-C31-C32	2.58	119.69	111.83	1	20
5	E	829	7Q9	O31-C31-C32	2.58	119.69	111.83	6	20
5	A	209	7Q9	O31-C31-C32	2.57	119.68	111.83	8	20
6	E	838	17F	C6-O7-C7	2.57	107.72	117.12	14	17
5	D	507	7Q9	O31-C31-C32	2.57	119.67	111.83	4	20
5	D	523	7Q9	O31-C31-C32	2.57	119.67	111.83	9	20
5	E	850	7Q9	O31-C31-C32	2.57	119.66	111.83	2	20
5	E	864	7Q9	O31-C31-C32	2.57	119.66	111.83	2	20
6	D	533	17F	O7-C7-C8	2.57	119.66	111.83	19	20
6	E	841	17F	O7-C7-C8	2.57	119.66	111.83	9	20
6	E	809	17F	C6-O7-C7	2.56	107.76	117.12	15	18
5	A	217	7Q9	O31-C31-C32	2.56	119.64	111.83	17	20
5	E	822	7Q9	O31-C31-C32	2.56	119.64	111.83	13	20
5	E	871	7Q9	O31-C31-C32	2.56	119.63	111.83	17	20
5	E	842	7Q9	O31-C31-C32	2.55	119.62	111.83	10	20
6	A	214	17F	O7-C7-C8	2.55	119.62	111.83	11	20
5	D	532	7Q9	O31-C31-C32	2.55	119.61	111.83	20	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	A	203	7Q9	O31-C31-C32	2.55	119.60	111.83	18	20
6	D	516	17F	O7-C7-C8	2.55	119.60	111.83	2	20
5	D	526	7Q9	C3-O31-C31	2.54	107.82	117.12	8	20
5	E	875	7Q9	O31-C31-C32	2.54	119.58	111.83	9	20
6	E	870	17F	O7-C7-C8	2.54	119.57	111.83	11	20
5	D	525	7Q9	O31-C31-C32	2.53	119.56	111.83	1	20
6	D	501	17F	C6-O7-C7	2.53	107.86	117.12	20	16
6	E	855	17F	O7-C7-C8	2.53	119.55	111.83	10	20
5	A	206	7Q9	O31-C31-C32	2.53	119.54	111.83	18	20
5	D	520	7Q9	C3-O31-C31	2.53	107.88	117.12	9	20
5	B	203	7Q9	O31-C31-C32	2.52	119.53	111.83	7	20
5	D	508	7Q9	O31-C31-C32	2.52	119.53	111.83	6	20
5	E	837	7Q9	C3-O31-C31	2.52	107.90	117.12	9	15
6	B	208	17F	O7-C7-C8	2.52	119.53	111.83	4	20
5	E	867	7Q9	O31-C31-C32	2.52	119.52	111.83	16	20
5	D	512	7Q9	O31-C31-C32	2.52	119.51	111.83	6	20
5	B	204	7Q9	O31-C31-C32	2.51	119.50	111.83	16	20
5	E	865	7Q9	O31-C31-C32	2.51	119.50	111.83	9	20
5	D	518	7Q9	O31-C31-C32	2.51	119.50	111.83	10	20
5	E	824	7Q9	O31-C31-C32	2.51	119.50	111.83	3	20
5	E	849	7Q9	O31-C31-C32	2.51	119.49	111.83	14	20
5	D	502	7Q9	O31-C31-C32	2.51	119.48	111.83	10	20
5	D	549	7Q9	O31-C31-C32	2.50	119.46	111.83	20	20
5	E	851	7Q9	O31-C31-C32	2.50	119.47	111.83	11	20
5	E	830	7Q9	O31-C31-C32	2.49	119.44	111.83	8	20
5	E	839	7Q9	C3-O31-C31	2.49	108.00	117.12	11	6
5	E	863	7Q9	O21-C21-C22	2.49	120.09	110.93	2	20
5	D	526	7Q9	O21-C21-C22	2.49	120.07	110.93	3	20
5	D	548	7Q9	O21-C21-C22	2.49	120.07	110.93	16	20
5	E	866	7Q9	O31-C31-C32	2.49	119.42	111.83	7	20
5	D	506	7Q9	C3-O31-C31	2.48	108.04	117.12	18	13
5	D	541	7Q9	O31-C31-C32	2.47	119.38	111.83	16	20
5	A	213	7Q9	O21-C21-C22	2.47	120.01	110.93	13	20
5	A	204	7Q9	C3-O31-C31	2.47	108.09	117.12	20	11
5	E	835	7Q9	O31-C31-C32	2.47	119.36	111.83	19	20
5	D	537	7Q9	O21-C21-C22	2.46	119.98	110.93	4	20
5	E	854	7Q9	O31-C31-C32	2.46	119.35	111.83	16	20
5	D	505	7Q9	O21-C21-C22	2.46	119.97	110.93	9	20
5	D	523	7Q9	O21-C21-C22	2.46	119.97	110.93	10	20
5	E	878	7Q9	O21-C21-C22	2.46	119.97	110.93	13	20
5	D	540	7Q9	O21-C21-C22	2.46	119.97	110.93	9	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	E	852	7Q9	C3-O31-C31	2.46	108.13	117.12	19	18
5	E	868	7Q9	O21-C21-C22	2.46	119.95	110.93	1	20
5	E	821	7Q9	O21-C21-C22	2.45	119.94	110.93	13	20
5	E	873	7Q9	O21-C21-C22	2.45	119.95	110.93	11	20
5	A	216	7Q9	O21-C21-C22	2.45	119.93	110.93	5	20
5	D	545	7Q9	O21-C21-C22	2.45	119.94	110.93	4	20
5	E	857	7Q9	O31-C31-C32	2.45	119.31	111.83	2	20
6	E	805	17F	O7-C7-C8	2.45	119.31	111.83	5	20
5	B	205	7Q9	O21-C21-C22	2.45	119.93	110.93	1	20
5	A	217	7Q9	O21-C21-C22	2.45	119.92	110.93	10	20
5	B	203	7Q9	O21-C21-C22	2.45	119.92	110.93	1	20
5	D	507	7Q9	O21-C21-C22	2.45	119.92	110.93	8	20
3	A	201	GSP	O4'-C1'-N9	2.45	113.90	108.36	4	14
5	A	204	7Q9	O21-C21-C22	2.45	119.92	110.93	14	20
5	D	541	7Q9	O21-C21-C22	2.45	119.92	110.93	6	20
5	B	212	7Q9	C3-O31-C31	2.44	108.18	117.12	13	14
5	D	503	7Q9	O21-C21-C22	2.44	119.91	110.93	14	20
5	D	518	7Q9	O21-C21-C22	2.44	119.90	110.93	13	20
5	E	806	7Q9	O21-C21-C22	2.44	119.90	110.93	17	20
5	E	820	7Q9	O21-C21-C22	2.44	119.90	110.93	1	20
5	E	858	7Q9	O21-C21-C22	2.44	119.90	110.93	19	20
5	B	216	7Q9	O21-C21-C22	2.44	119.89	110.93	5	20
5	D	502	7Q9	O21-C21-C22	2.44	119.89	110.93	18	20
5	B	213	7Q9	O21-C21-C22	2.44	119.89	110.93	16	20
5	D	513	7Q9	O21-C21-C22	2.44	119.89	110.93	5	20
5	B	218	7Q9	O21-C21-C22	2.44	119.88	110.93	7	20
5	E	821	7Q9	C3-O31-C31	2.44	108.21	117.12	9	20
5	E	854	7Q9	O21-C21-C22	2.44	119.88	110.93	17	20
5	B	205	7Q9	O31-C31-C32	2.43	119.26	111.83	7	20
5	D	506	7Q9	O21-C21-C22	2.43	119.87	110.93	6	20
5	E	826	7Q9	O31-C31-C32	2.43	119.26	111.83	8	20
5	B	217	7Q9	O21-C21-C22	2.43	119.87	110.93	4	20
5	D	544	7Q9	O21-C21-C22	2.43	119.87	110.93	18	20
5	E	873	7Q9	O31-C31-C32	2.43	119.25	111.83	7	20
5	E	875	7Q9	O21-C21-C22	2.43	119.86	110.93	10	20
5	E	859	7Q9	O21-C21-C22	2.43	119.86	110.93	20	20
5	A	205	7Q9	O21-C21-C22	2.43	119.85	110.93	6	20
5	D	531	7Q9	O21-C21-C22	2.43	119.85	110.93	18	20
5	A	206	7Q9	O21-C21-C22	2.43	119.84	110.93	13	20
5	A	207	7Q9	O21-C21-C22	2.43	119.84	110.93	15	20
5	D	542	7Q9	O21-C21-C22	2.43	119.84	110.93	13	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	D	549	7Q9	O21-C21-C22	2.43	119.84	110.93	2	20
5	B	210	7Q9	O21-C21-C22	2.42	119.83	110.93	16	20
5	D	519	7Q9	O21-C21-C22	2.42	119.84	110.93	7	20
5	E	834	7Q9	O21-C21-C22	2.43	119.84	110.93	13	20
5	E	857	7Q9	O21-C21-C22	2.43	119.84	110.93	1	20
5	E	850	7Q9	O21-C21-C22	2.42	119.83	110.93	1	20
5	D	532	7Q9	O21-C21-C22	2.42	119.83	110.93	6	20
5	E	851	7Q9	O21-C21-C22	2.42	119.83	110.93	7	20
5	E	865	7Q9	O21-C21-C22	2.42	119.82	110.93	20	20
6	B	219	17F	C6-O7-C7	2.42	108.27	117.12	20	14
5	B	209	7Q9	O21-C21-C22	2.42	119.82	110.93	9	20
5	E	830	7Q9	O21-C21-C22	2.42	119.82	110.93	18	20
5	E	843	7Q9	O21-C21-C22	2.42	119.82	110.93	16	20
5	E	836	7Q9	O21-C21-C22	2.42	119.82	110.93	18	20
5	E	860	7Q9	O21-C21-C22	2.42	119.82	110.93	5	20
5	E	864	7Q9	O21-C21-C22	2.42	119.82	110.93	12	20
5	D	512	7Q9	O21-C21-C22	2.42	119.81	110.93	17	20
5	D	536	7Q9	O21-C21-C22	2.42	119.81	110.93	4	20
5	B	220	7Q9	O21-C21-C22	2.41	119.80	110.93	15	20
5	D	543	7Q9	O21-C21-C22	2.42	119.80	110.93	1	20
5	E	802	7Q9	O21-C21-C22	2.42	119.81	110.93	18	20
5	E	845	7Q9	O21-C21-C22	2.42	119.80	110.93	12	20
5	D	535	7Q9	O21-C21-C22	2.41	119.80	110.93	16	20
5	E	812	7Q9	O21-C21-C22	2.41	119.80	110.93	3	20
5	E	832	7Q9	O21-C21-C22	2.41	119.80	110.93	19	20
5	E	852	7Q9	O21-C21-C22	2.41	119.80	110.93	6	20
5	E	862	7Q9	O21-C21-C22	2.42	119.80	110.93	13	20
5	E	835	7Q9	O21-C21-C22	2.41	119.80	110.93	16	20
5	E	867	7Q9	O21-C21-C22	2.41	119.80	110.93	20	20
5	E	871	7Q9	O21-C21-C22	2.41	119.80	110.93	8	20
5	B	206	7Q9	O21-C21-C22	2.41	119.79	110.93	4	20
5	D	539	7Q9	O21-C21-C22	2.41	119.79	110.93	8	20
5	E	823	7Q9	O21-C21-C22	2.41	119.78	110.93	13	20
5	D	522	7Q9	O21-C21-C22	2.41	119.78	110.93	17	20
5	E	812	7Q9	C3-O31-C31	2.41	108.31	117.12	6	20
5	E	877	7Q9	O21-C21-C22	2.41	119.78	110.93	12	20
5	A	203	7Q9	O21-C21-C22	2.41	119.77	110.93	10	20
5	D	521	7Q9	O21-C21-C22	2.41	119.78	110.93	3	20
5	D	531	7Q9	C3-O31-C31	2.41	108.31	117.12	7	13
5	B	204	7Q9	O21-C21-C22	2.41	119.77	110.93	8	20
5	D	508	7Q9	O21-C21-C22	2.41	119.77	110.93	3	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	E	824	7Q9	O21-C21-C22	2.41	119.77	110.93	7	20
5	E	813	7Q9	O21-C21-C22	2.41	119.77	110.93	10	20
5	E	822	7Q9	O21-C21-C22	2.41	119.77	110.93	9	20
5	E	861	7Q9	O21-C21-C22	2.41	119.77	110.93	6	20
5	D	509	7Q9	O21-C21-C22	2.40	119.76	110.93	20	20
5	D	514	7Q9	O21-C21-C22	2.40	119.76	110.93	7	20
5	E	804	7Q9	O21-C21-C22	2.40	119.76	110.93	5	20
5	E	844	7Q9	O21-C21-C22	2.40	119.76	110.93	19	20
5	E	866	7Q9	O21-C21-C22	2.40	119.76	110.93	13	20
5	E	806	7Q9	C3-O31-C31	2.40	108.33	117.12	12	19
5	E	816	7Q9	O21-C21-C22	2.40	119.75	110.93	11	20
5	E	827	7Q9	O21-C21-C22	2.40	119.75	110.93	3	20
5	D	504	7Q9	O21-C21-C22	2.40	119.75	110.93	14	20
5	E	846	7Q9	O21-C21-C22	2.40	119.75	110.93	19	20
5	E	848	7Q9	O21-C21-C22	2.40	119.75	110.93	7	20
5	D	530	7Q9	O21-C21-C22	2.40	119.74	110.93	13	20
5	E	833	7Q9	O21-C21-C22	2.40	119.74	110.93	17	20
5	E	815	7Q9	O21-C21-C22	2.40	119.74	110.93	10	20
5	A	211	7Q9	O21-C21-C22	2.40	119.73	110.93	5	20
5	E	803	7Q9	O21-C21-C22	2.40	119.73	110.93	2	20
5	E	814	7Q9	O21-C21-C22	2.40	119.73	110.93	6	20
5	E	853	7Q9	O21-C21-C22	2.40	119.74	110.93	15	20
5	E	847	7Q9	O21-C21-C22	2.40	119.73	110.93	12	20
5	D	524	7Q9	O21-C21-C22	2.39	119.72	110.93	19	20
5	D	520	7Q9	O21-C21-C22	2.39	119.72	110.93	7	20
5	E	825	7Q9	O21-C21-C22	2.39	119.72	110.93	5	20
5	E	840	7Q9	O21-C21-C22	2.39	119.72	110.93	16	20
5	E	849	7Q9	O21-C21-C22	2.39	119.71	110.93	8	20
5	E	826	7Q9	O21-C21-C22	2.39	119.71	110.93	17	20
5	B	207	7Q9	O21-C21-C22	2.39	119.70	110.93	17	20
5	D	515	7Q9	O21-C21-C22	2.39	119.70	110.93	11	20
5	D	529	7Q9	O21-C21-C22	2.39	119.70	110.93	18	20
5	D	538	7Q9	O21-C21-C22	2.39	119.70	110.93	12	20
5	E	842	7Q9	O21-C21-C22	2.39	119.71	110.93	17	20
5	A	212	7Q9	O21-C21-C22	2.39	119.69	110.93	8	20
5	E	810	7Q9	O21-C21-C22	2.39	119.69	110.93	7	20
5	E	831	7Q9	O21-C21-C22	2.38	119.69	110.93	19	20
5	E	839	7Q9	O21-C21-C22	2.38	119.69	110.93	11	20
5	A	209	7Q9	O21-C21-C22	2.38	119.68	110.93	18	20
5	E	876	7Q9	O21-C21-C22	2.38	119.68	110.93	12	20
5	E	837	7Q9	O21-C21-C22	2.38	119.67	110.93	6	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
6	E	807	17F	C6-O7-C7	2.38	108.41	117.12	16	9
5	B	212	7Q9	O21-C21-C22	2.38	119.67	110.93	15	20
5	D	547	7Q9	O21-C21-C22	2.38	119.67	110.93	10	20
5	E	808	7Q9	O21-C21-C22	2.38	119.67	110.93	11	20
5	D	525	7Q9	O21-C21-C22	2.38	119.66	110.93	1	20
5	A	215	7Q9	O21-C21-C22	2.37	119.65	110.93	16	20
5	A	210	7Q9	O21-C21-C22	2.37	119.65	110.93	18	20
5	E	869	7Q9	O21-C21-C22	2.37	119.63	110.93	9	20
5	B	211	7Q9	O21-C21-C22	2.36	119.61	110.93	9	20
5	E	808	7Q9	O31-C31-C32	2.36	119.03	111.83	18	20
5	E	829	7Q9	O21-C21-C22	2.35	119.56	110.93	12	20
5	D	522	7Q9	C3-O31-C31	2.34	108.57	117.12	15	19
5	D	543	7Q9	C3-O31-C31	2.33	108.60	117.12	5	7
3	A	201	GSP	O6-C6-C5	2.32	120.41	126.53	3	20
5	D	519	7Q9	C3-O31-C31	2.32	108.65	117.12	6	6
5	E	803	7Q9	C3-O31-C31	2.32	108.65	117.12	19	6
5	E	846	7Q9	C3-O31-C31	2.31	108.66	117.12	12	13
6	E	818	17F	C6-O7-C7	2.31	108.69	117.12	2	2
5	B	216	7Q9	C3-O31-C31	2.30	108.69	117.12	1	8
6	D	546	17F	C6-O7-C7	2.30	108.70	117.12	4	12
5	D	503	7Q9	C3-O31-C31	2.30	108.72	117.12	7	6
5	D	540	7Q9	C3-O31-C31	2.29	108.73	117.12	2	17
6	D	528	17F	C6-O7-C7	2.29	108.75	117.12	7	19
5	E	802	7Q9	C3-O31-C31	2.29	108.76	117.12	9	2
5	E	863	7Q9	C3-O31-C31	2.28	108.77	117.12	8	8
3	B	201	GSP	O6-C6-C5	2.28	120.50	126.53	6	20
5	D	545	7Q9	C3-O31-C31	2.28	108.78	117.12	14	16
5	D	542	7Q9	C3-O31-C31	2.28	108.79	117.12	14	18
5	A	213	7Q9	C3-O31-C31	2.27	108.82	117.12	13	5
6	E	874	17F	C6-O7-C7	2.27	108.81	117.12	15	12
5	D	529	7Q9	C3-O31-C31	2.27	108.82	117.12	16	14
3	B	201	GSP	C4-C5-N7	2.27	107.08	110.67	9	16
5	E	831	7Q9	C3-O31-C31	2.27	108.83	117.12	11	9
5	D	513	7Q9	C3-O31-C31	2.26	108.84	117.12	4	16
5	D	530	7Q9	C3-O31-C31	2.26	108.84	117.12	1	6
6	D	510	17F	C6-O7-C7	2.26	108.85	117.12	8	2
3	B	201	GSP	N9-C8-N7	2.26	109.21	113.40	4	20
5	A	205	7Q9	C3-O31-C31	2.26	108.86	117.12	7	5
5	E	861	7Q9	C3-O31-C31	2.26	108.87	117.12	6	7
5	B	203	7Q9	C3-O31-C31	2.26	108.87	117.12	16	2
3	A	201	GSP	C3'-C2'-C1'	2.25	97.20	101.46	3	14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	B	209	7Q9	C3-O31-C31	2.25	108.88	117.12	3	4
6	E	872	17F	C6-O7-C7	2.25	108.89	117.12	19	9
5	E	820	7Q9	C3-O31-C31	2.25	108.90	117.12	10	6
5	E	876	7Q9	C3-O31-C31	2.25	108.90	117.12	5	5
5	E	869	7Q9	C3-O31-C31	2.25	108.91	117.12	19	15
3	A	201	GSP	N9-C8-N7	2.24	109.24	113.40	6	20
5	D	535	7Q9	C3-O31-C31	2.24	108.92	117.12	4	7
5	B	211	7Q9	C3-O31-C31	2.24	108.93	117.12	3	5
5	E	877	7Q9	C3-O31-C31	2.23	108.95	117.12	15	14
5	D	524	7Q9	C3-O31-C31	2.23	108.96	117.12	12	2
6	D	517	17F	C6-O7-C7	2.23	108.95	117.12	7	5
5	E	829	7Q9	C3-C2-C1	2.23	106.59	111.78	1	5
5	E	804	7Q9	C3-O31-C31	2.23	108.98	117.12	20	14
5	E	833	7Q9	C3-O31-C31	2.23	108.98	117.12	13	10
6	E	811	17F	C6-O7-C7	2.22	109.00	117.12	20	5
5	E	816	7Q9	C3-O31-C31	2.22	109.01	117.12	20	2
5	B	210	7Q9	C3-O31-C31	2.22	109.02	117.12	5	13
3	A	201	GSP	C8-N7-C5	2.21	108.19	104.26	6	20
5	B	217	7Q9	C3-O31-C31	2.21	109.05	117.12	4	8
3	A	201	GSP	C4-C5-N7	2.20	107.18	110.67	1	19
3	B	201	GSP	C3'-C2'-C1'	2.20	97.30	101.46	1	9
5	B	217	7Q9	C3-C2-C1	2.20	106.66	111.78	15	1
5	D	504	7Q9	C3-O31-C31	2.20	109.09	117.12	19	3
3	B	201	GSP	C8-N7-C5	2.20	108.17	104.26	9	20
5	D	547	7Q9	C3-O31-C31	2.19	109.10	117.12	10	8
5	E	822	7Q9	C3-O31-C31	2.19	109.09	117.12	13	1
5	E	845	7Q9	C3-O31-C31	2.19	109.10	117.12	1	12
5	B	207	7Q9	C3-O31-C31	2.19	109.12	117.12	20	6
5	B	206	7Q9	C3-O31-C31	2.19	109.12	117.12	6	1
3	B	201	GSP	C5-C6-N1	2.18	118.81	113.25	4	19
5	E	844	7Q9	C3-O31-C31	2.18	109.13	117.12	6	8
6	E	856	17F	C6-O7-C7	2.18	109.14	117.12	11	5
5	D	536	7Q9	C3-O31-C31	2.18	109.17	117.12	2	4
5	E	827	7Q9	C3-O31-C31	2.18	109.16	117.12	4	3
5	E	868	7Q9	C3-O31-C31	2.18	109.16	117.12	20	10
5	A	207	7Q9	C3-O31-C31	2.17	109.18	117.12	9	7
5	E	864	7Q9	C3-O31-C31	2.17	109.18	117.12	2	6
5	E	829	7Q9	C3-O31-C31	2.17	109.19	117.12	6	5
5	E	836	7Q9	C3-O31-C31	2.17	109.20	117.12	19	9
6	D	511	17F	C6-O7-C7	2.17	109.20	117.12	15	9
5	A	206	7Q9	C3-O31-C31	2.16	109.21	117.12	13	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	201	GSP	O4'-C1'-C2'	2.16	101.99	106.62	12	2
3	A	201	GSP	C5-C6-N1	2.15	118.73	113.25	2	19
5	E	840	7Q9	C3-O31-C31	2.15	109.25	117.12	4	2
5	E	853	7Q9	C3-O31-C31	2.15	109.26	117.12	5	1
5	B	205	7Q9	C3-O31-C31	2.15	109.28	117.12	7	1
5	A	209	7Q9	C3-O31-C31	2.14	109.29	117.12	8	9
5	E	862	7Q9	C3-O31-C31	2.14	109.30	117.12	9	8
5	E	850	7Q9	C3-O31-C31	2.14	109.30	117.12	1	6
5	B	220	7Q9	C3-O31-C31	2.14	109.31	117.12	3	1
6	D	534	17F	C6-O7-C7	2.14	109.31	117.12	16	8
5	D	514	7Q9	C3-O31-C31	2.13	109.31	117.12	2	8
5	E	860	7Q9	C3-O31-C31	2.13	109.32	117.12	3	4
6	E	819	17F	C6-O7-C7	2.13	109.33	117.12	17	2
5	E	802	7Q9	C3-C2-C1	2.13	106.82	111.78	6	2
6	B	214	17F	C6-O7-C7	2.13	109.33	117.12	18	11
5	E	843	7Q9	C3-O31-C31	2.13	109.34	117.12	3	8
5	E	814	7Q9	C3-O31-C31	2.12	109.38	117.12	4	8
6	D	527	17F	C6-O7-C7	2.12	109.39	117.12	14	10
5	A	210	7Q9	C3-O31-C31	2.11	109.40	117.12	20	4
5	E	858	7Q9	C3-O31-C31	2.11	109.41	117.12	20	1
5	D	547	7Q9	C3-C2-C1	2.10	106.88	111.78	7	1
5	E	842	7Q9	C3-O31-C31	2.10	109.42	117.12	1	3
5	D	504	7Q9	C3-C2-C1	2.10	106.89	111.78	6	1
5	A	216	7Q9	C3-O31-C31	2.10	109.45	117.12	19	4
5	D	537	7Q9	C3-O31-C31	2.10	109.45	117.12	12	2
5	A	203	7Q9	C3-O31-C31	2.09	109.46	117.12	4	5
6	E	841	17F	C6-C5-C4	2.09	106.92	111.78	20	1
5	E	878	7Q9	C3-O31-C31	2.09	109.50	117.12	6	4
5	D	523	7Q9	C3-O31-C31	2.08	109.50	117.12	9	1
5	E	824	7Q9	C3-O31-C31	2.08	109.50	117.12	7	3
6	B	215	17F	C6-O7-C7	2.08	109.50	117.12	4	2
5	E	848	7Q9	C3-O31-C31	2.08	109.51	117.12	12	3
5	D	539	7Q9	C3-O31-C31	2.08	109.51	117.12	10	3
5	E	815	7Q9	C3-O31-C31	2.08	109.51	117.12	16	2
5	E	834	7Q9	C3-O31-C31	2.08	109.53	117.12	8	2
5	B	218	7Q9	C3-O31-C31	2.07	109.53	117.12	3	5
6	E	801	17F	C6-O7-C7	2.07	109.56	117.12	2	1
5	D	507	7Q9	C3-O31-C31	2.07	109.56	117.12	17	1
5	A	215	7Q9	C3-O31-C31	2.07	109.57	117.12	4	4
5	E	825	7Q9	C3-O31-C31	2.07	109.56	117.12	4	3
5	E	875	7Q9	C3-O31-C31	2.06	109.60	117.12	9	5

Continued on next page...

Continued from previous page...

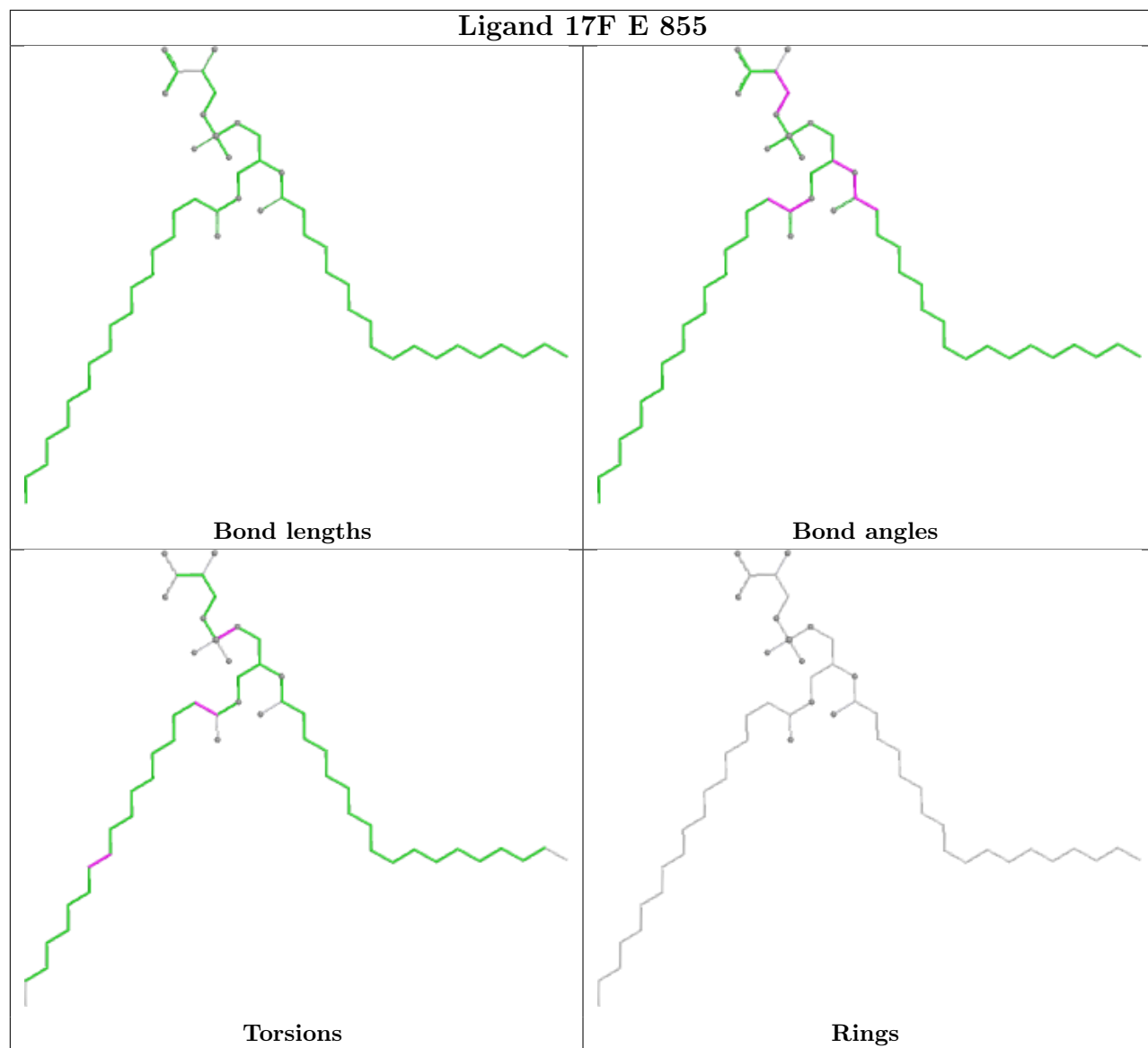
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	E	813	7Q9	C3-O31-C31	2.05	109.61	117.12	11	3
6	E	841	17F	C6-O7-C7	2.05	109.62	117.12	9	2
5	E	810	7Q9	C3-O31-C31	2.05	109.62	117.12	16	4
5	D	521	7Q9	C3-O31-C31	2.05	109.63	117.12	13	4
5	D	515	7Q9	C3-O31-C31	2.04	109.64	117.12	13	2
5	D	544	7Q9	C3-C2-C1	2.04	107.02	111.78	7	2
5	E	858	7Q9	C11-C12-N	2.04	109.27	115.82	12	1
6	E	828	17F	C6-O7-C7	2.04	109.66	117.12	14	4
6	A	214	17F	C6-O7-C7	2.04	109.66	117.12	16	1
5	B	205	7Q9	C3-C2-C1	2.03	107.04	111.78	12	1
5	E	832	7Q9	C3-O31-C31	2.03	109.69	117.12	19	1
5	E	823	7Q9	C3-O31-C31	2.03	109.70	117.12	5	2
5	B	213	7Q9	C3-O31-C31	2.03	109.71	117.12	4	2
5	D	519	7Q9	C11-C12-N	2.02	109.32	115.82	17	1
5	D	505	7Q9	C3-O31-C31	2.02	109.72	117.12	15	2
5	A	212	7Q9	C3-O31-C31	2.01	109.77	117.12	8	2
6	B	208	17F	C6-O7-C7	2.01	109.77	117.12	8	1
6	E	817	17F	C6-O7-C7	2.00	109.80	117.12	16	1
5	D	505	7Q9	C3-C2-C1	2.00	107.12	111.78	2	1
5	D	538	7Q9	C3-O31-C31	2.00	109.80	117.12	4	1
5	D	502	7Q9	C11-C12-N	2.00	109.40	115.82	16	1

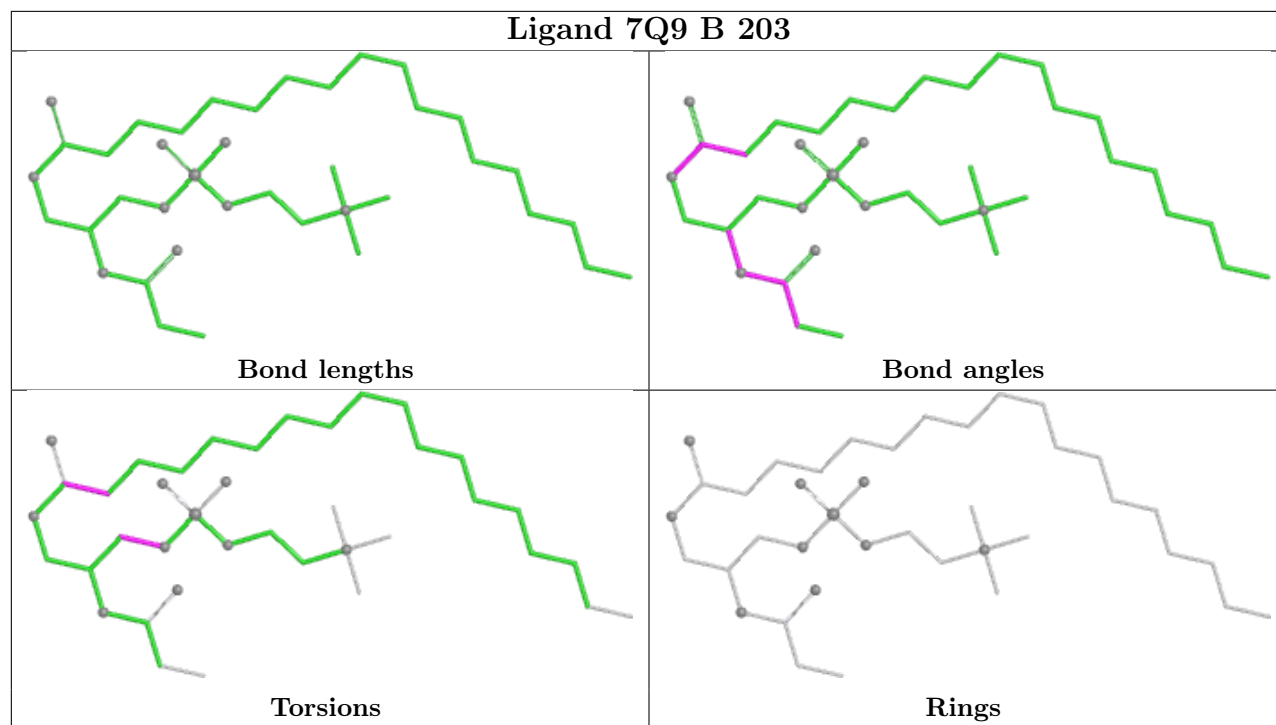
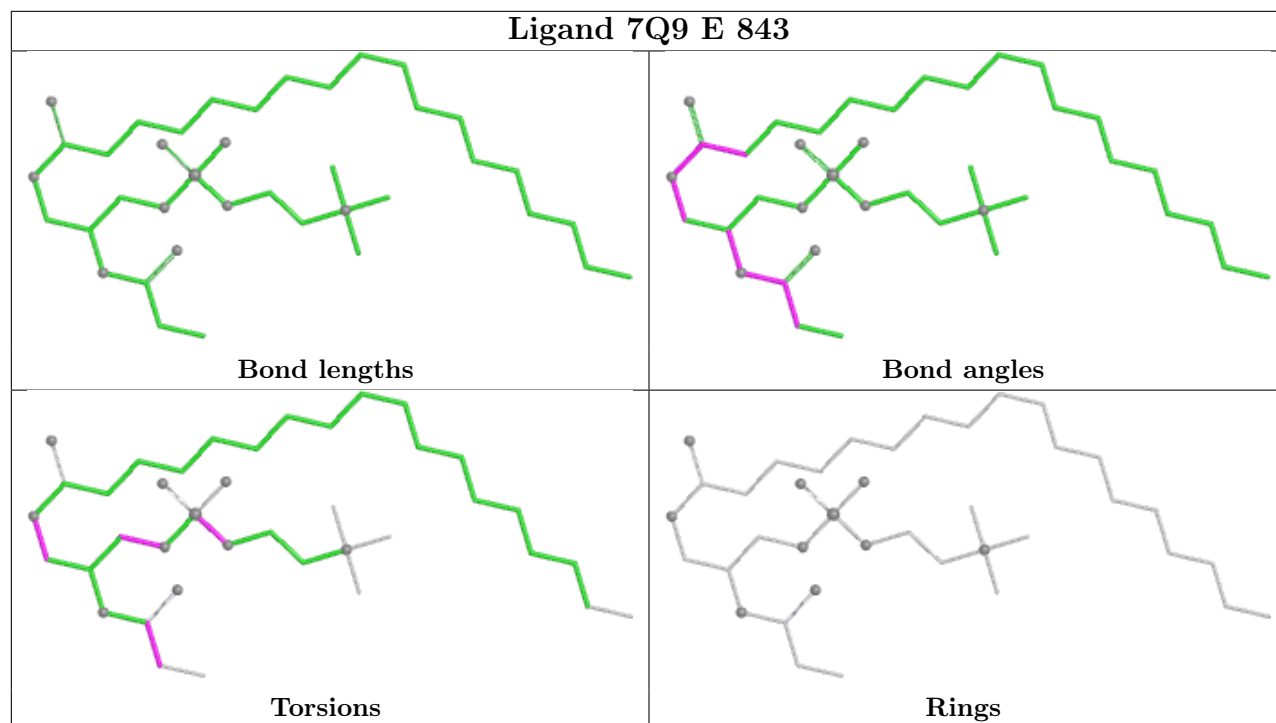
There are no chirality outliers.

There are no torsion outliers.

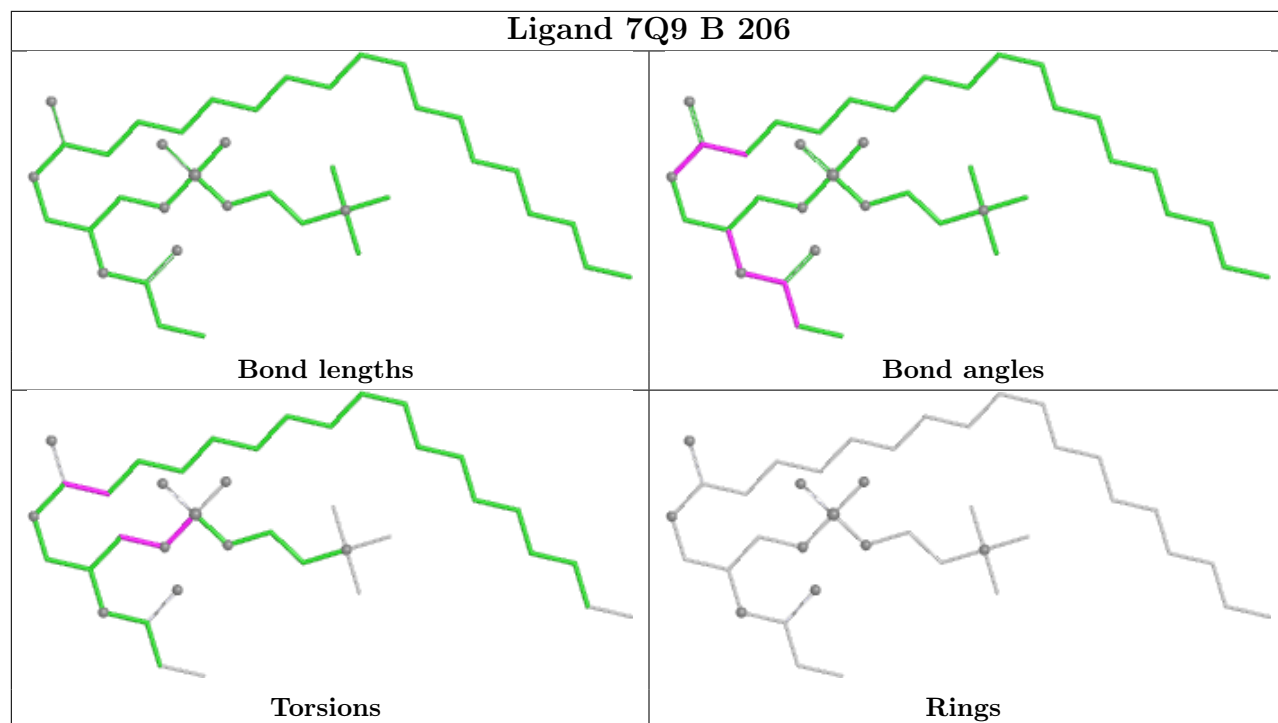
There are no ring outliers.

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.

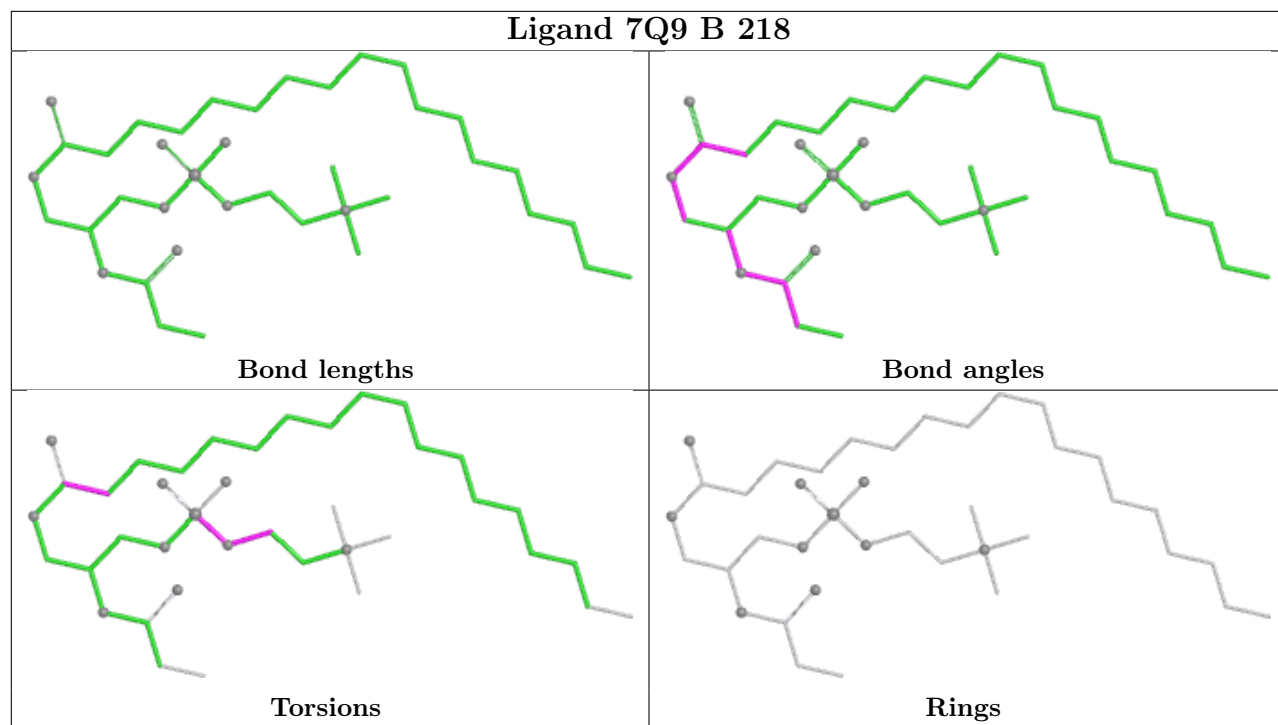


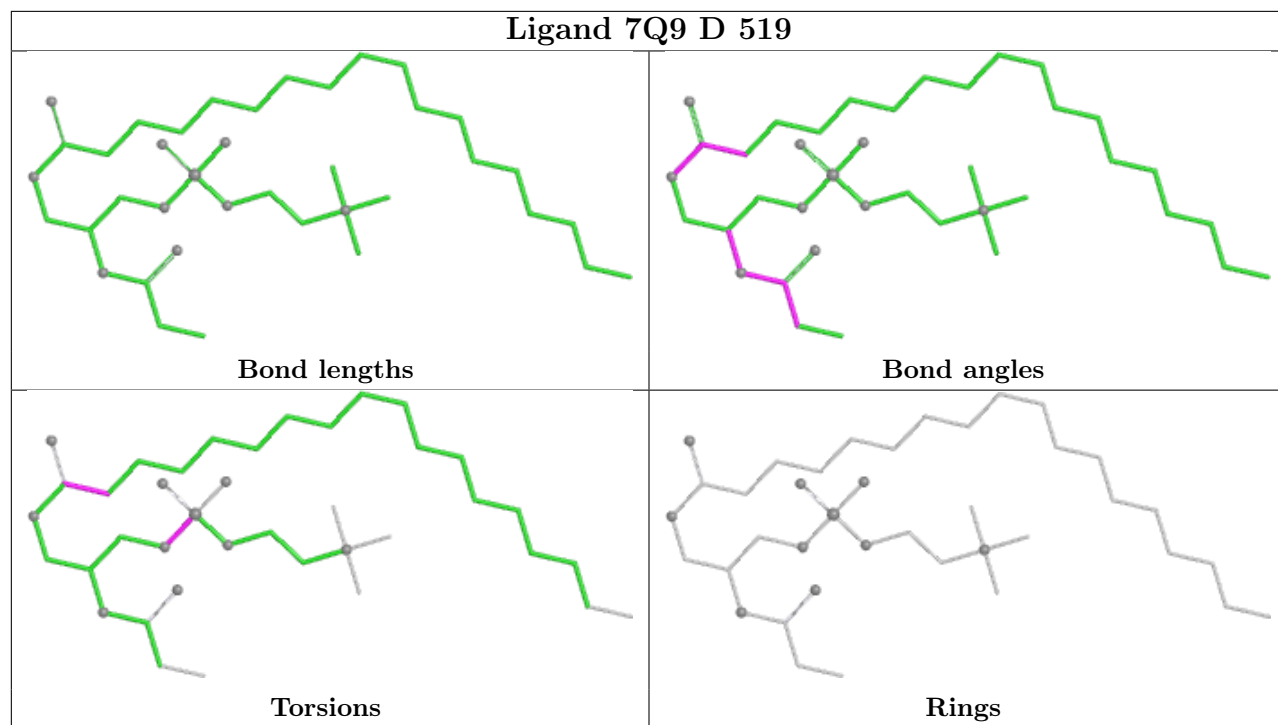
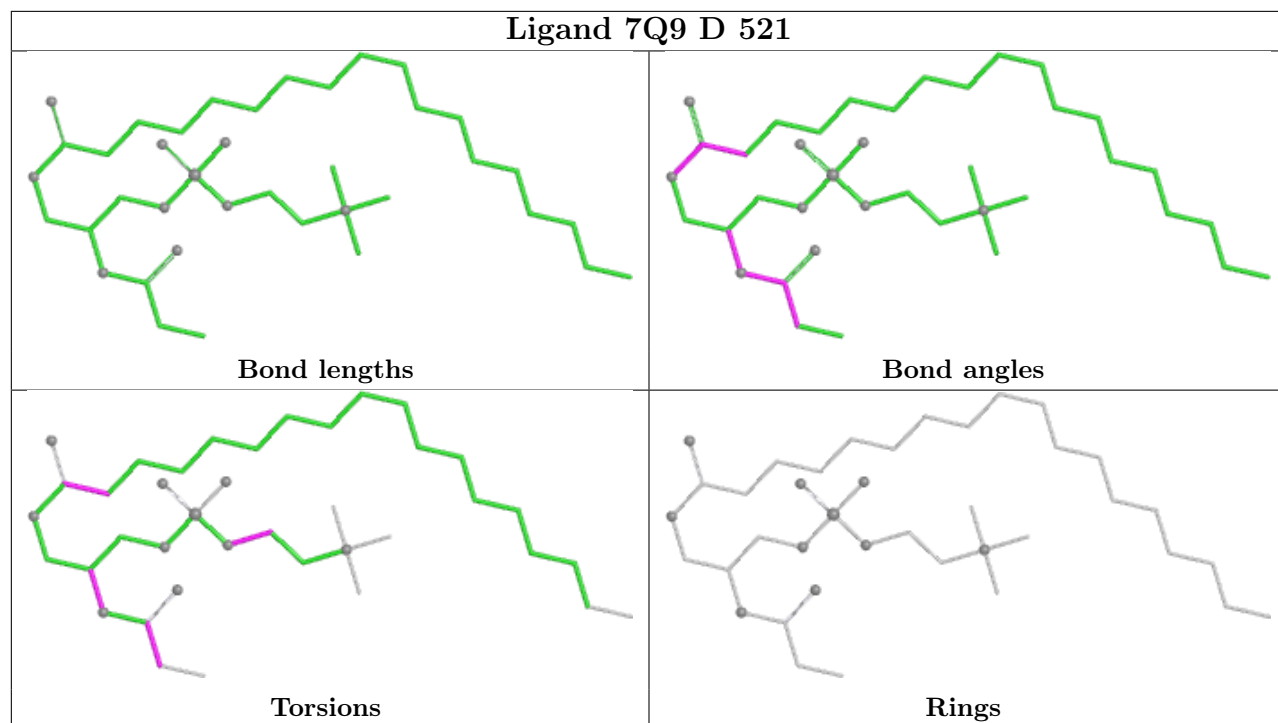


Ligand 7Q9 B 206

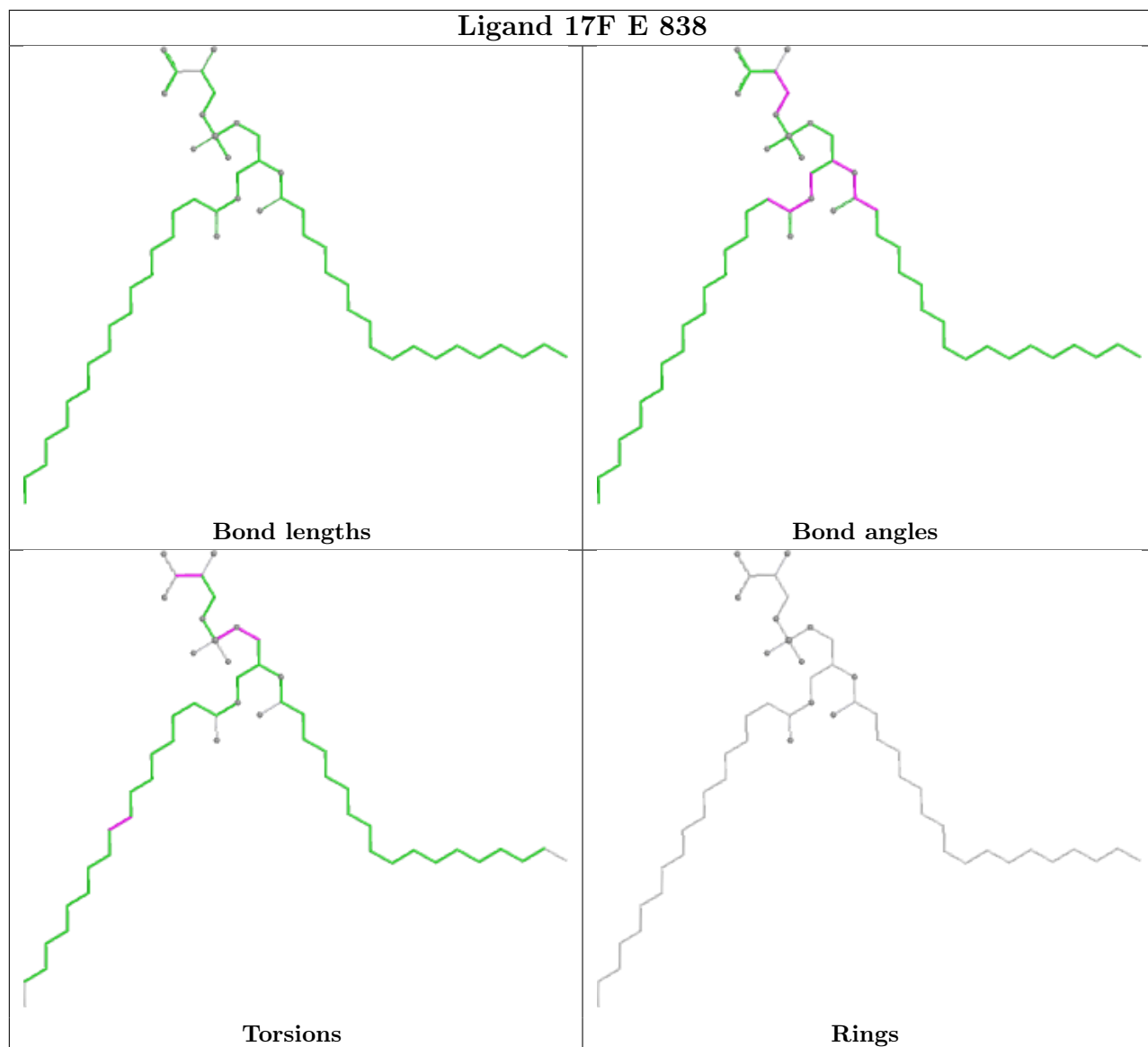


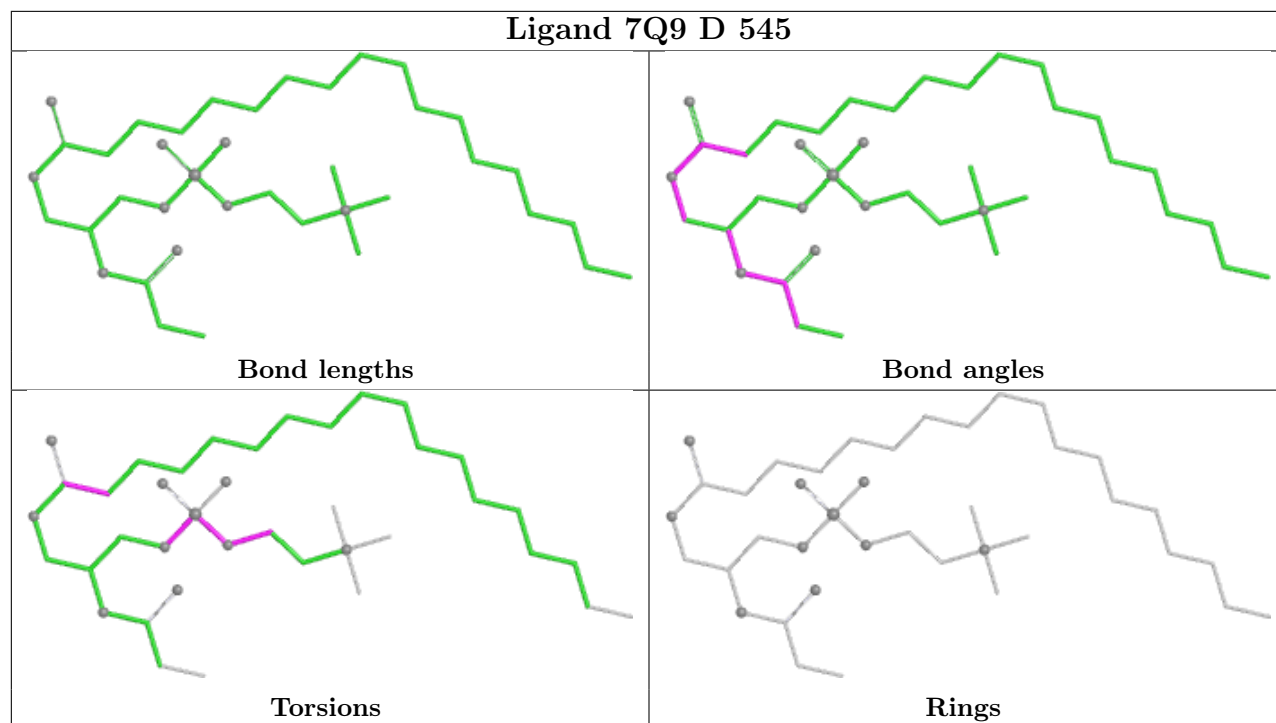
Ligand 7Q9 B 218

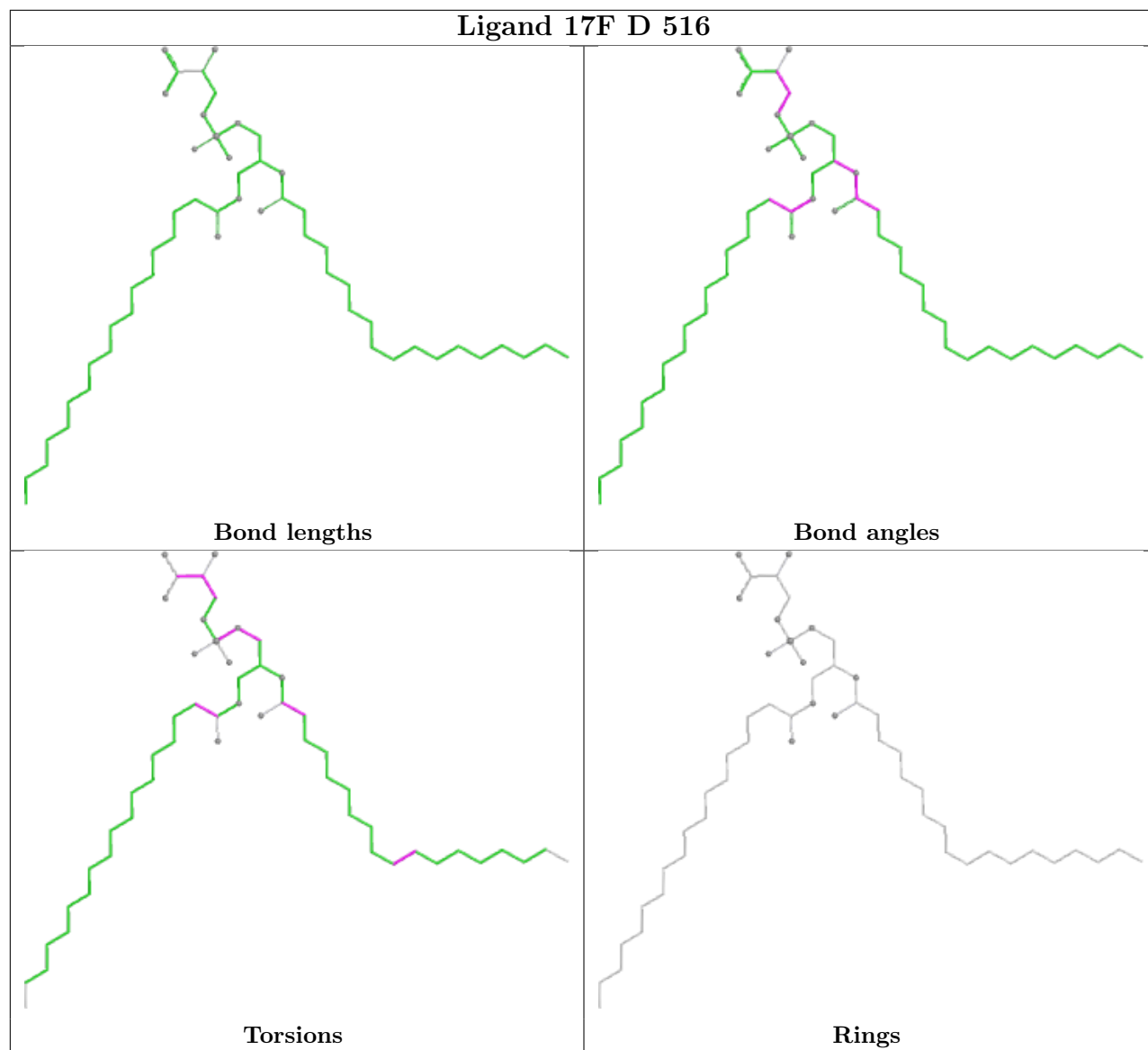


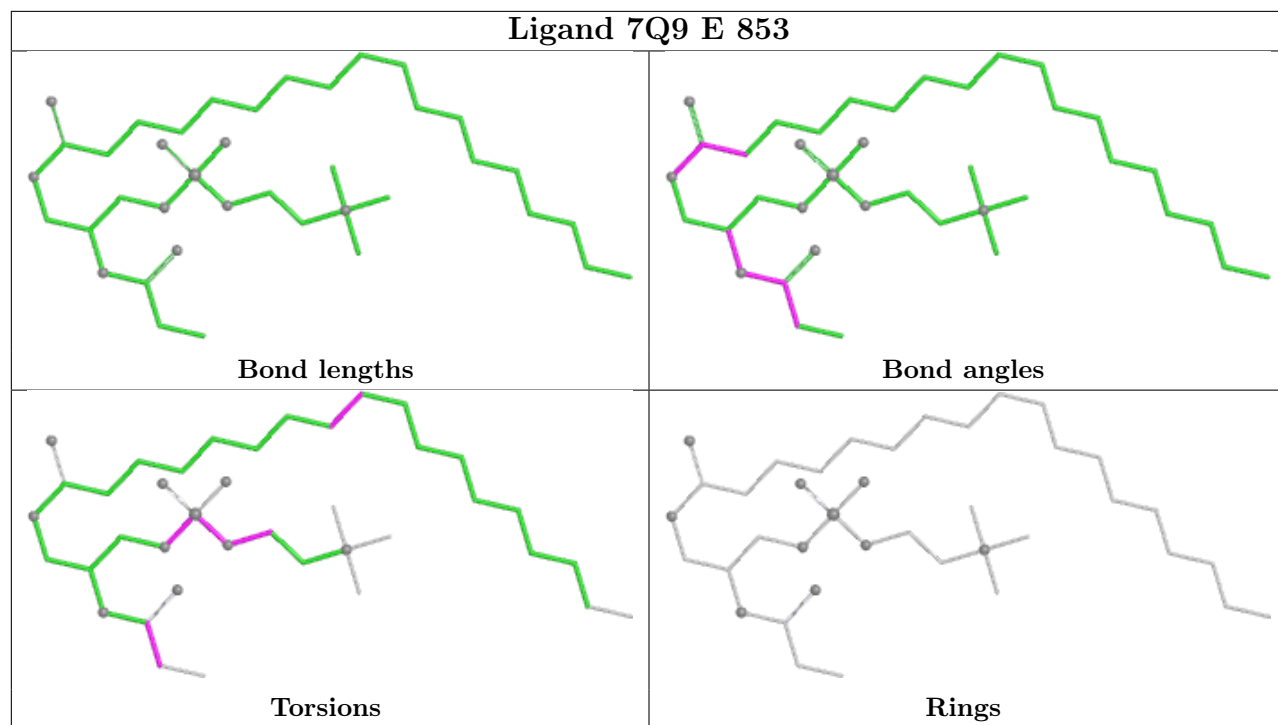
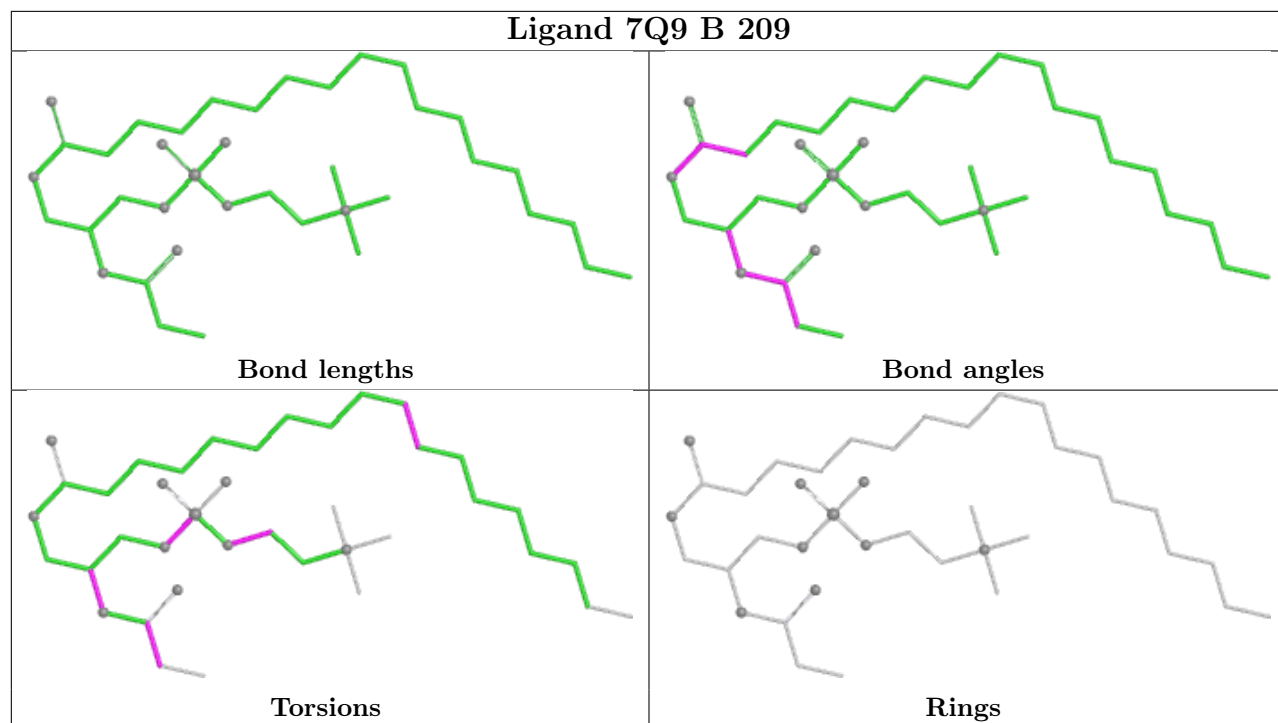


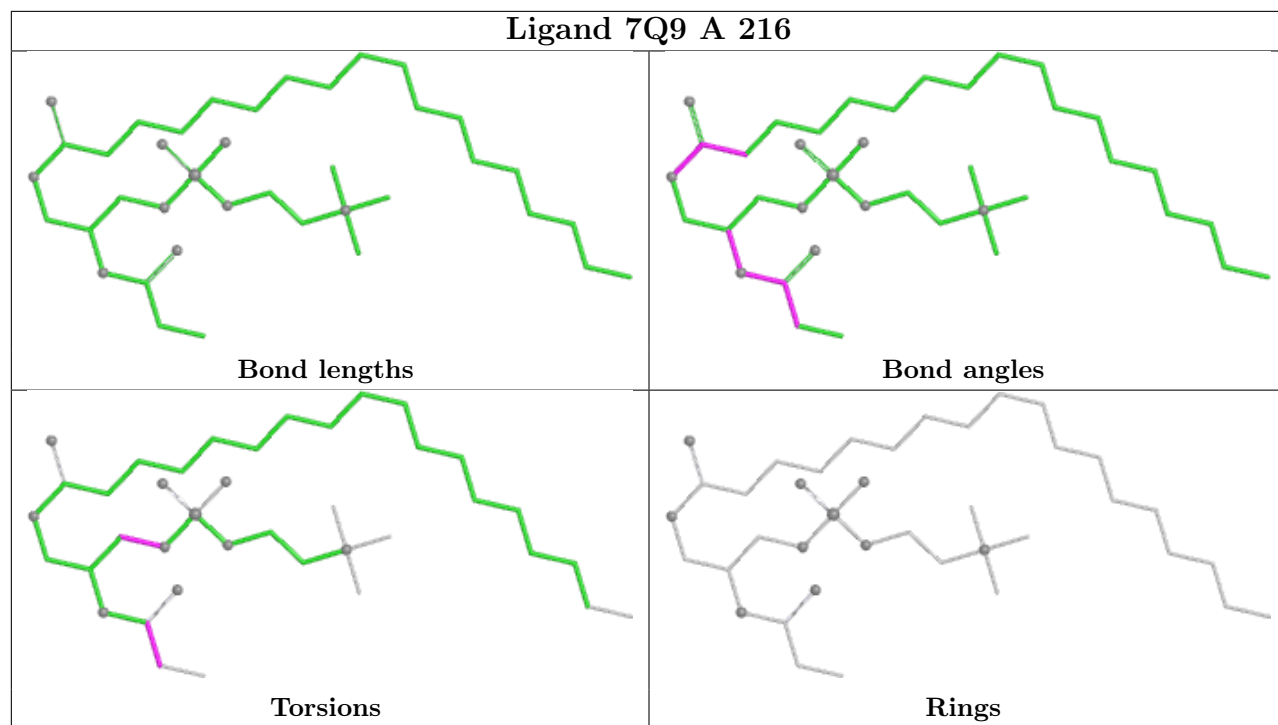
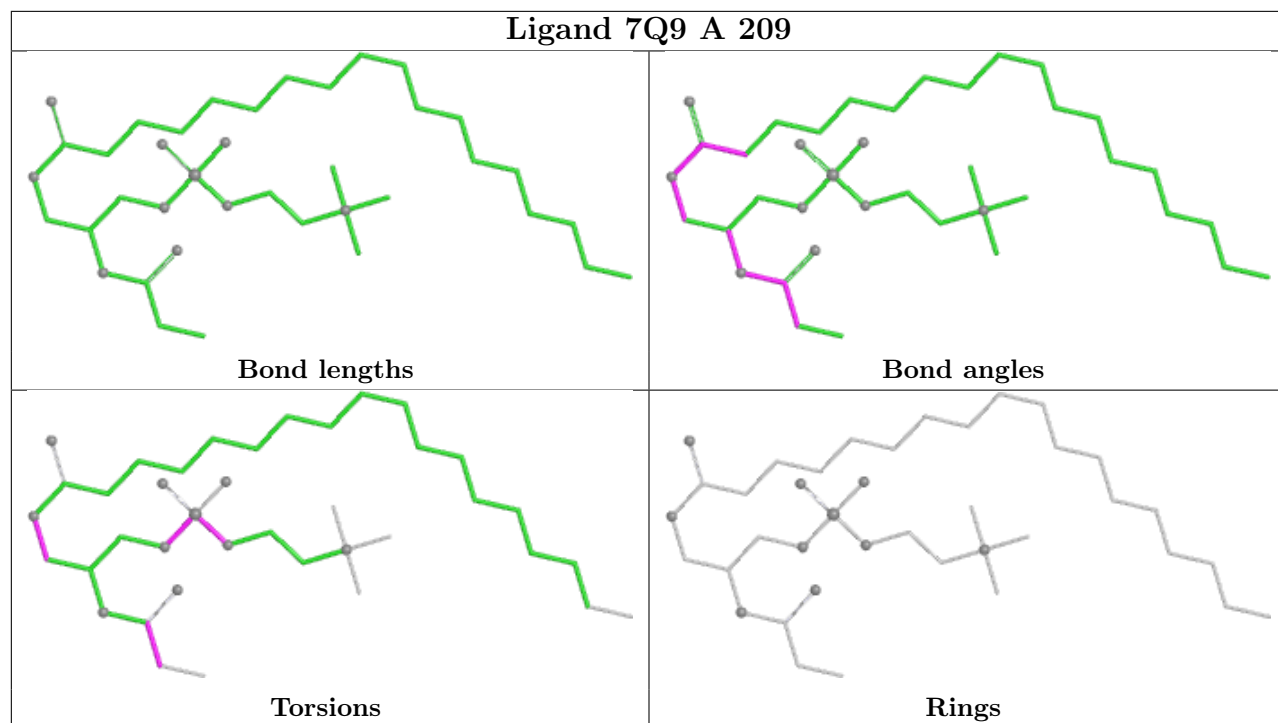
Ligand 17F E 838

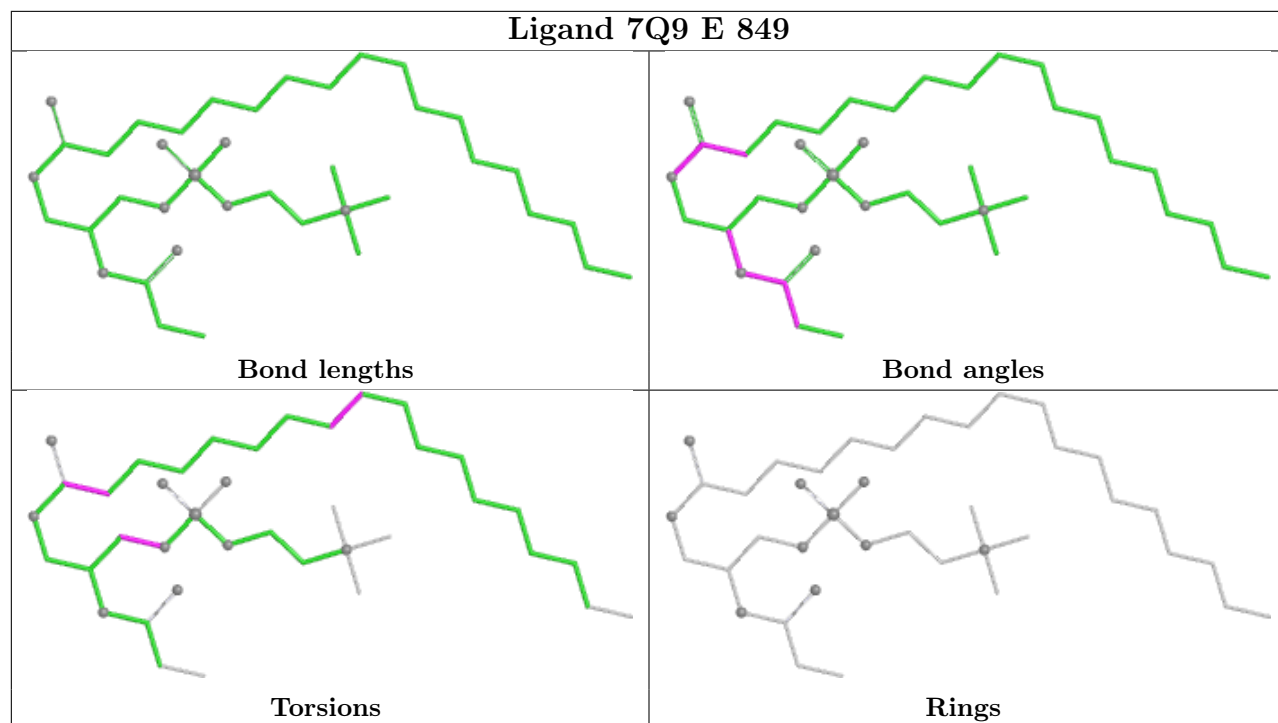


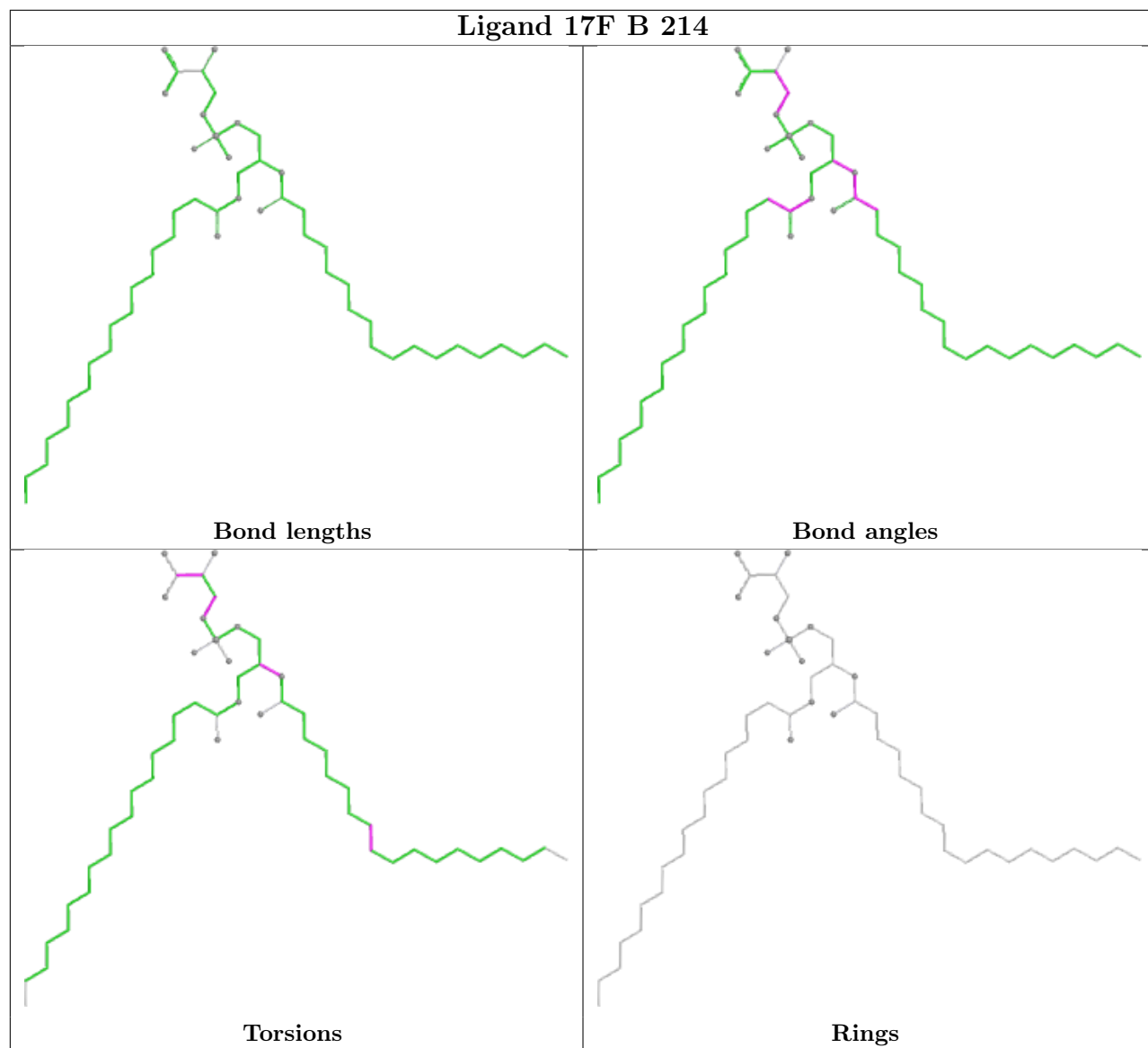


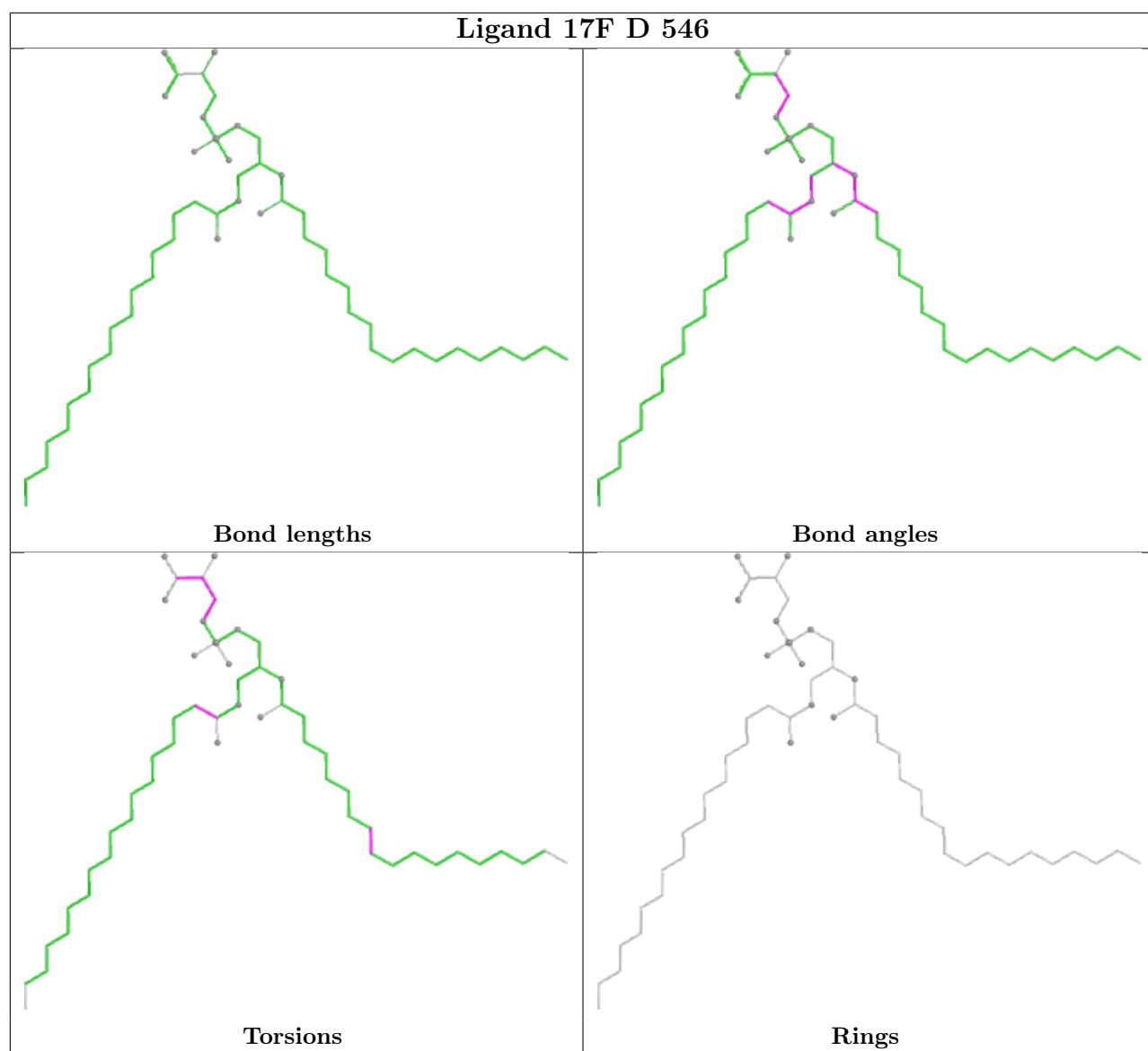


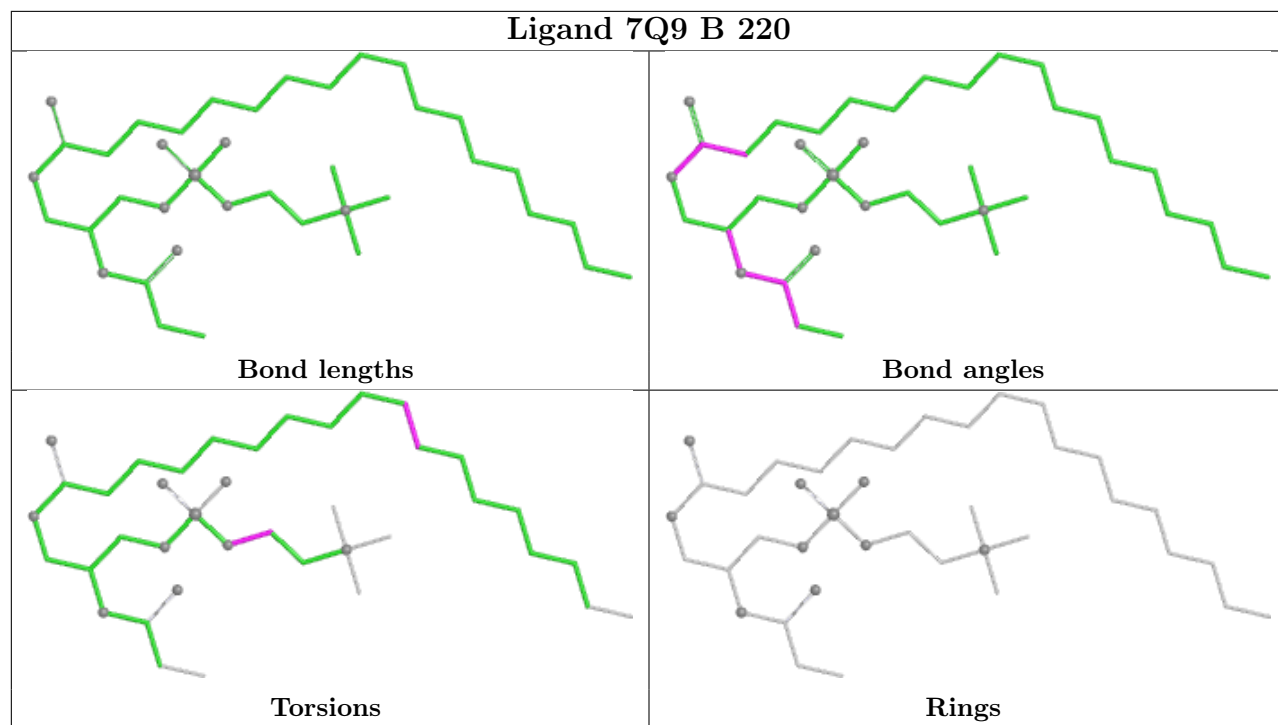
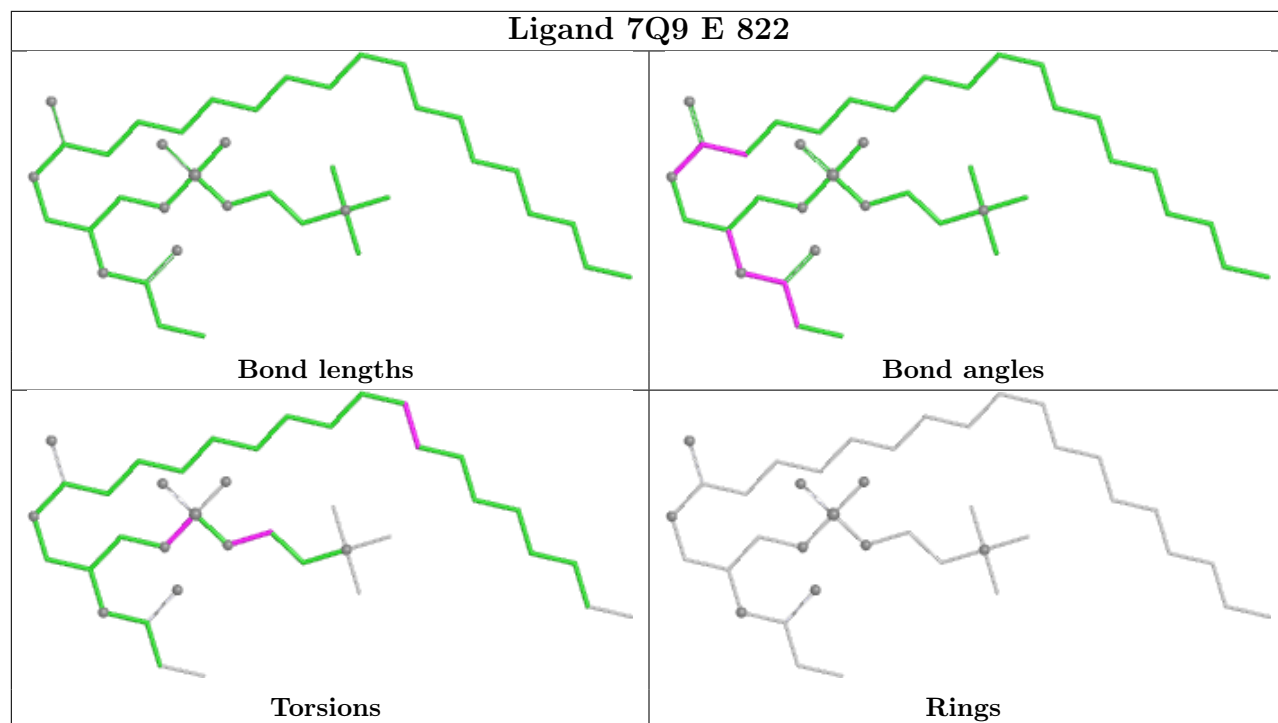


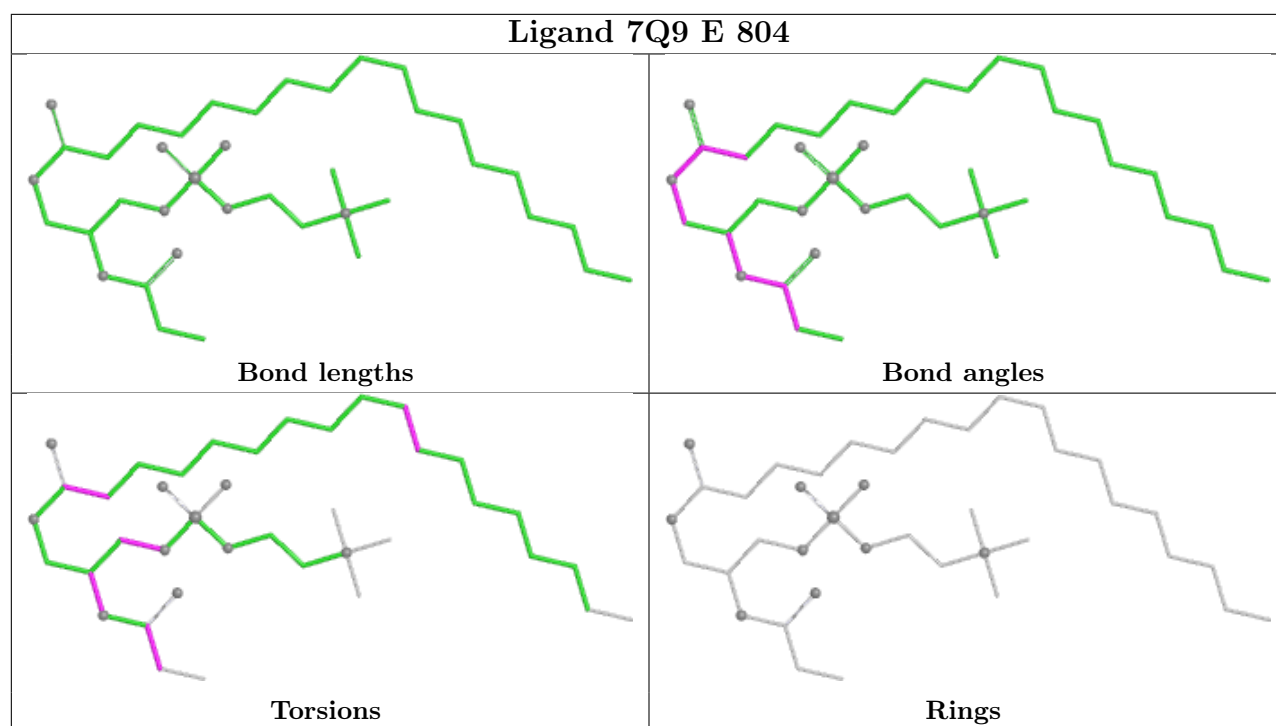


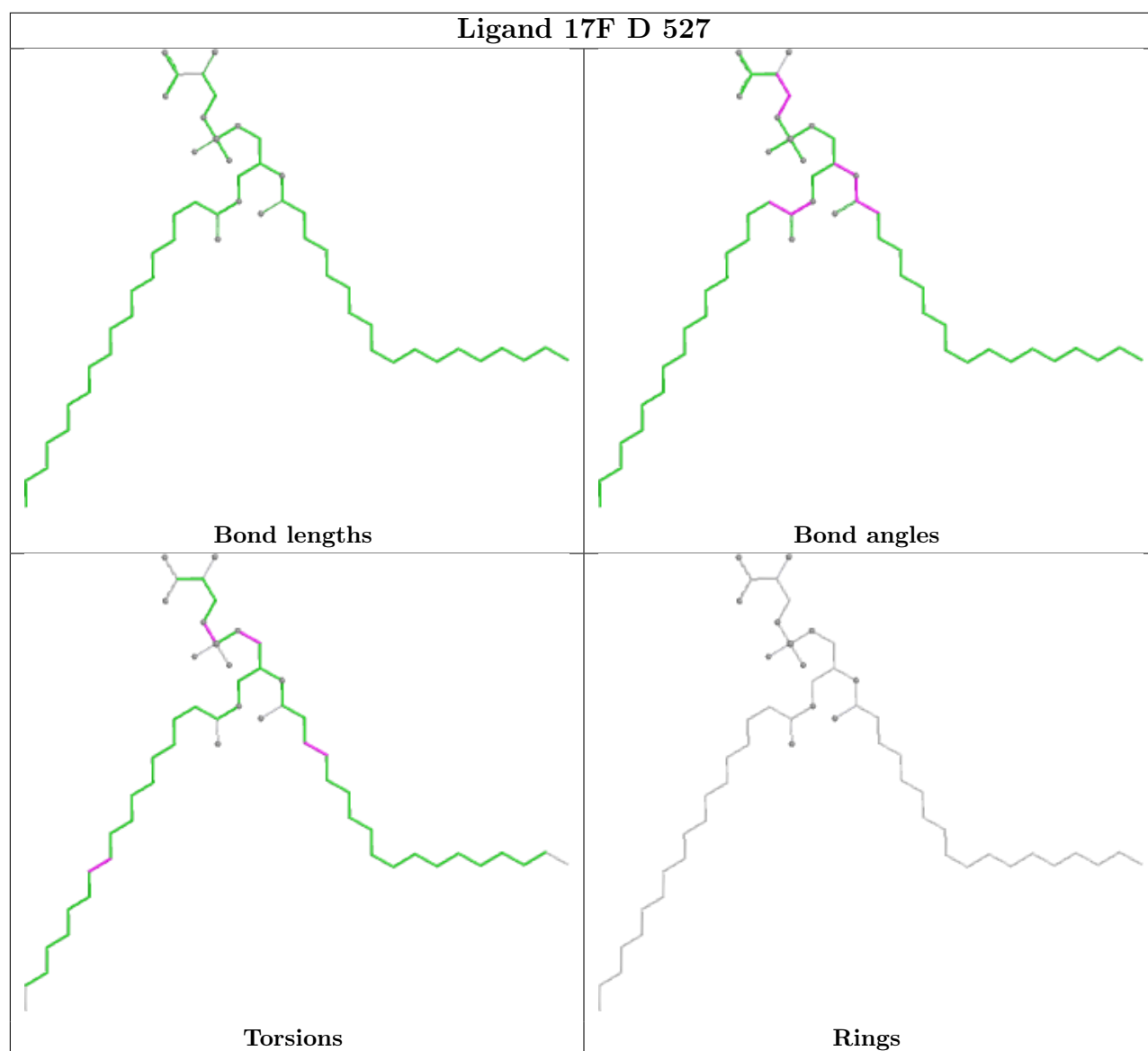


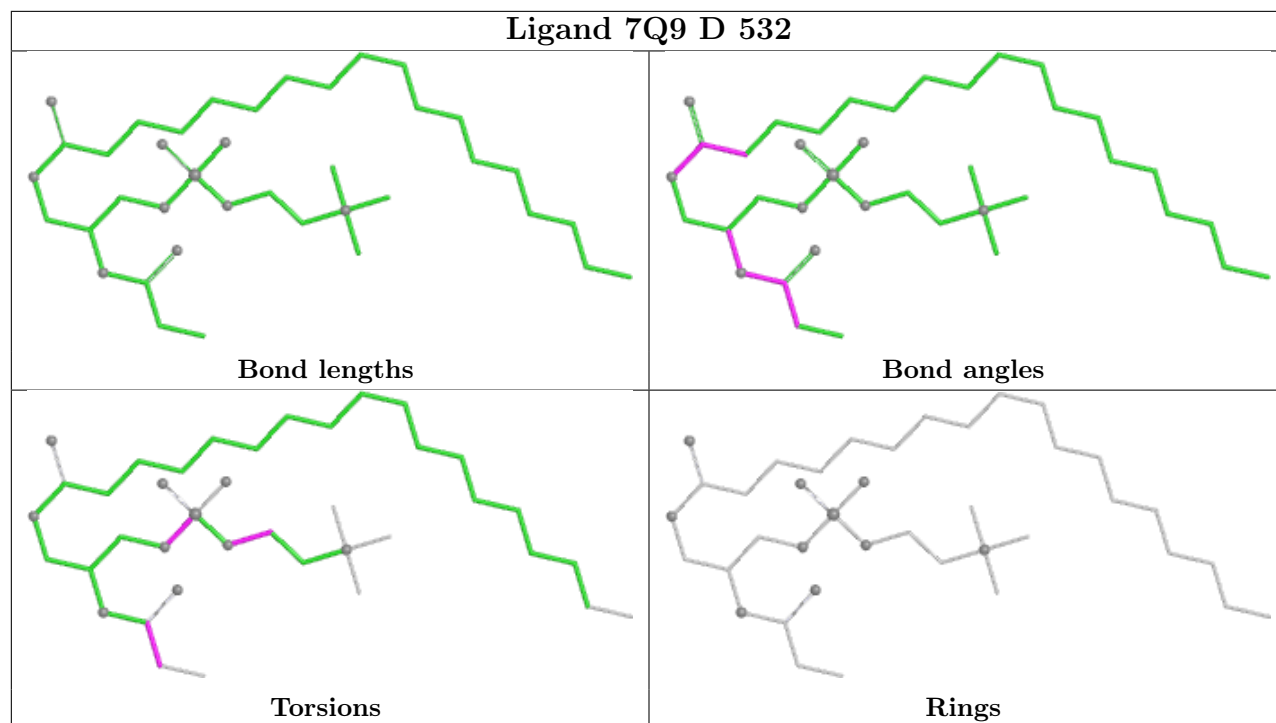




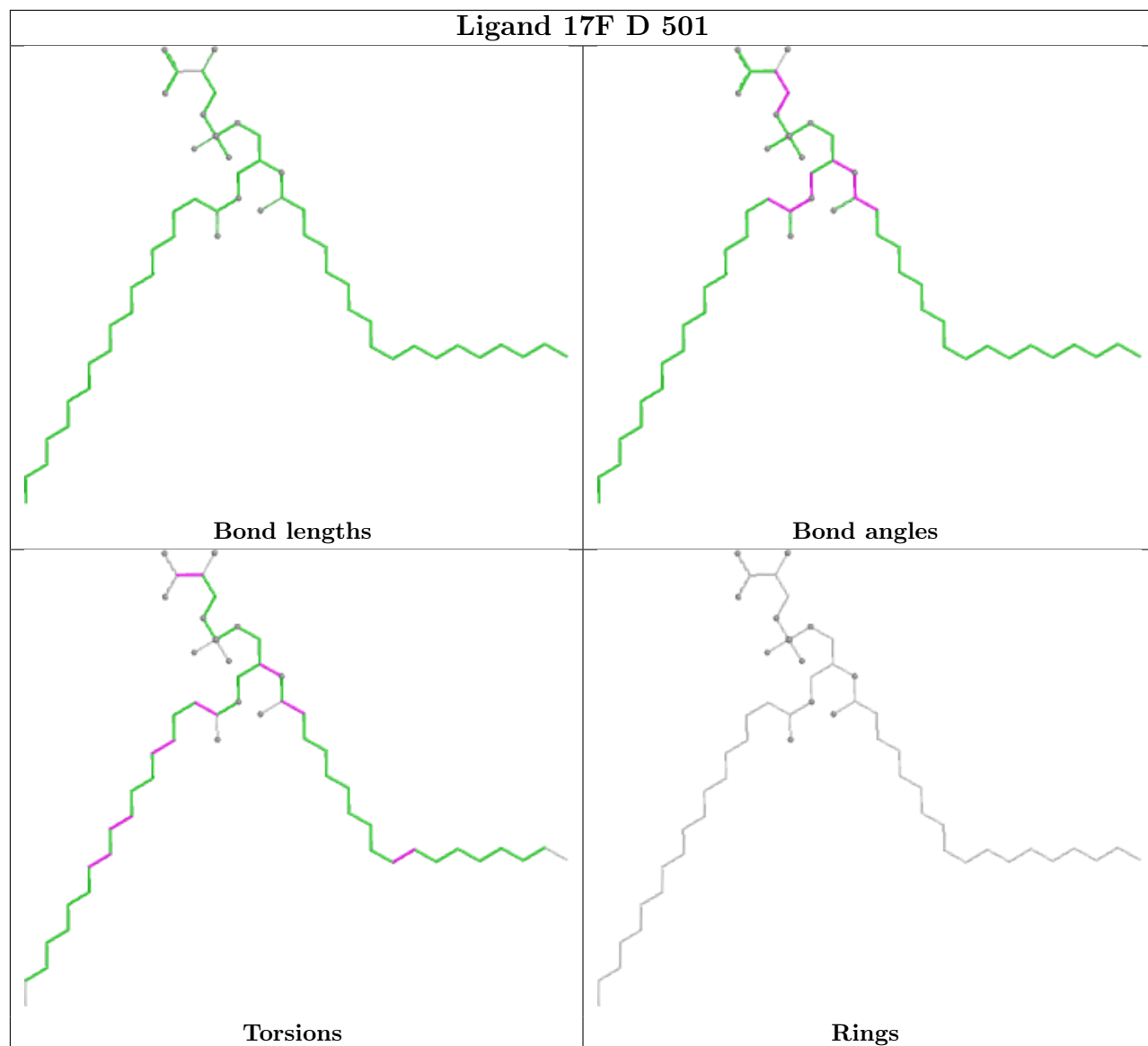




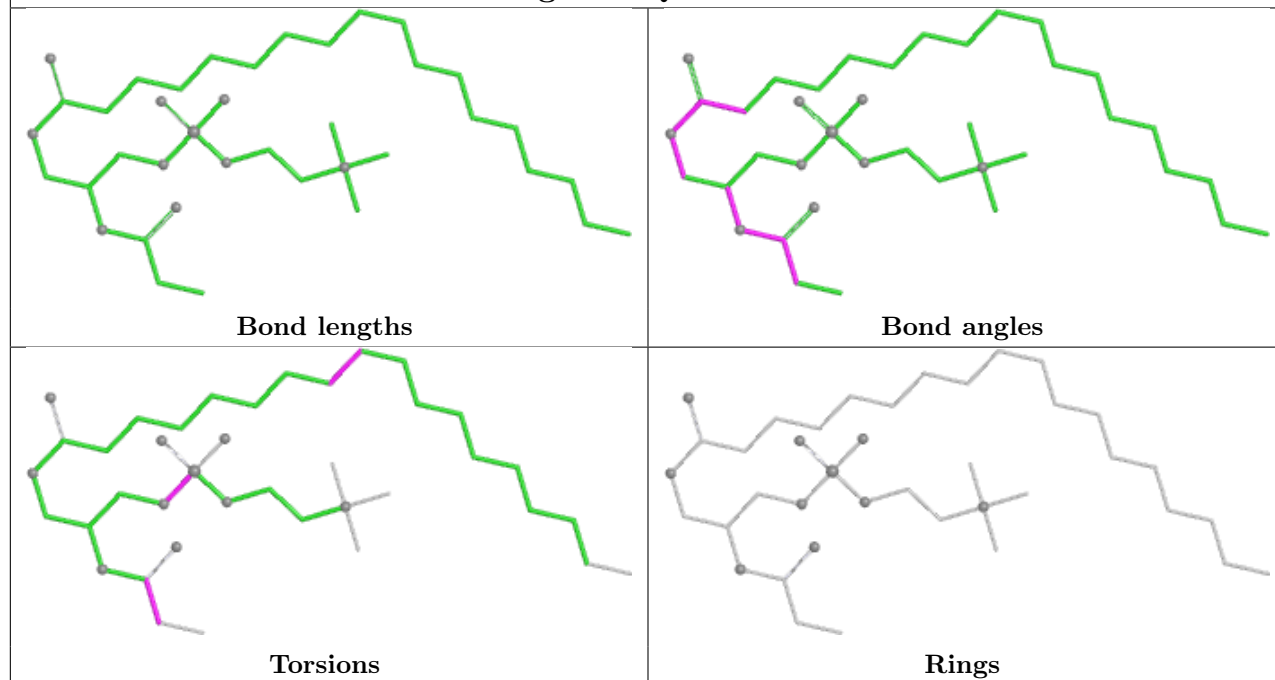




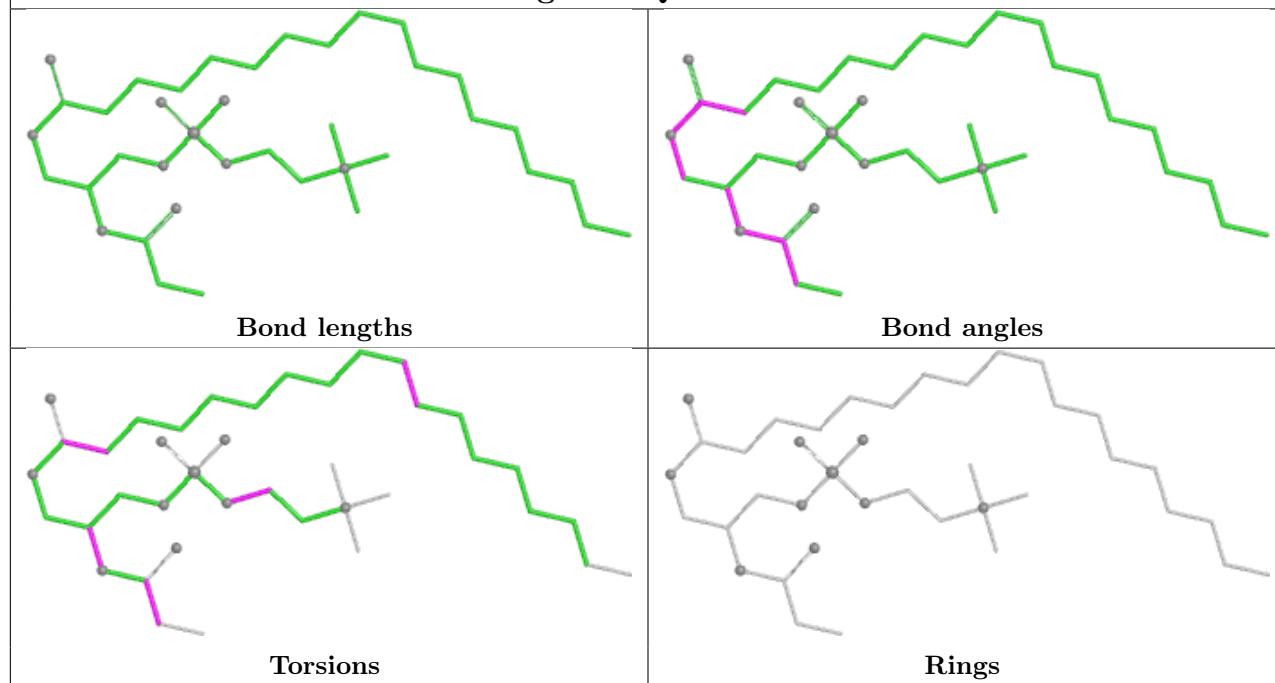
Ligand 17F D 501

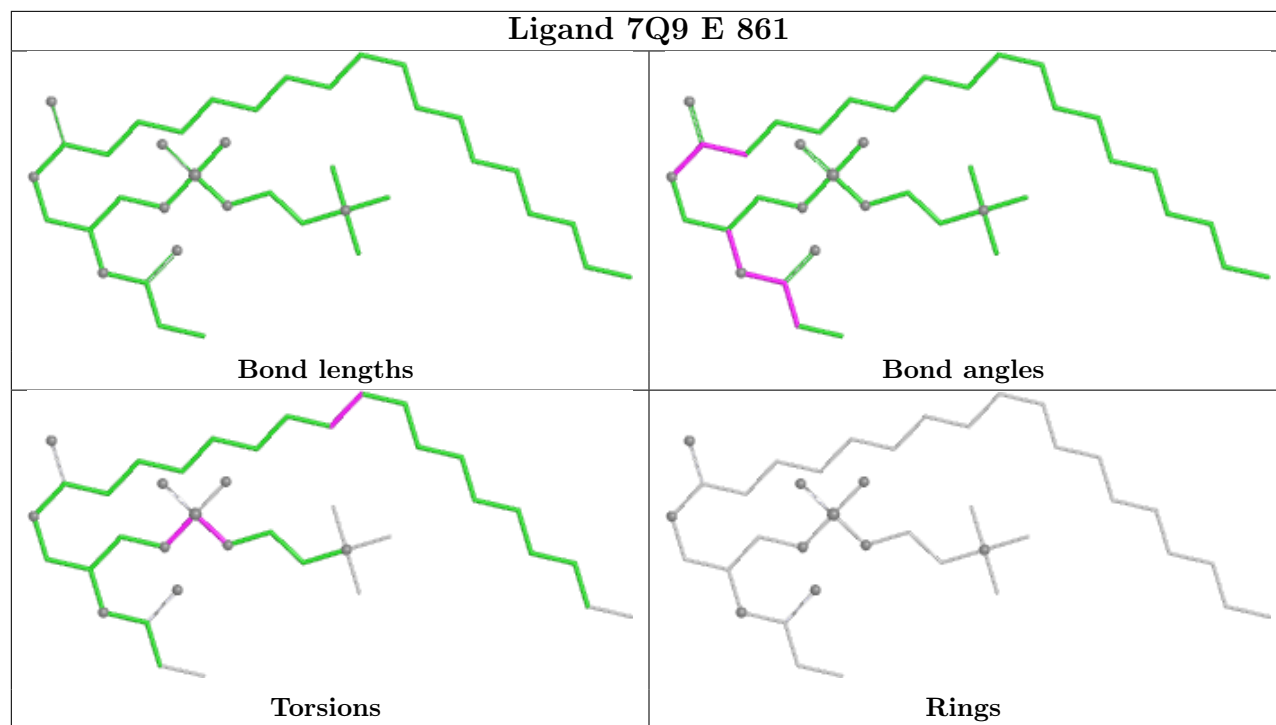
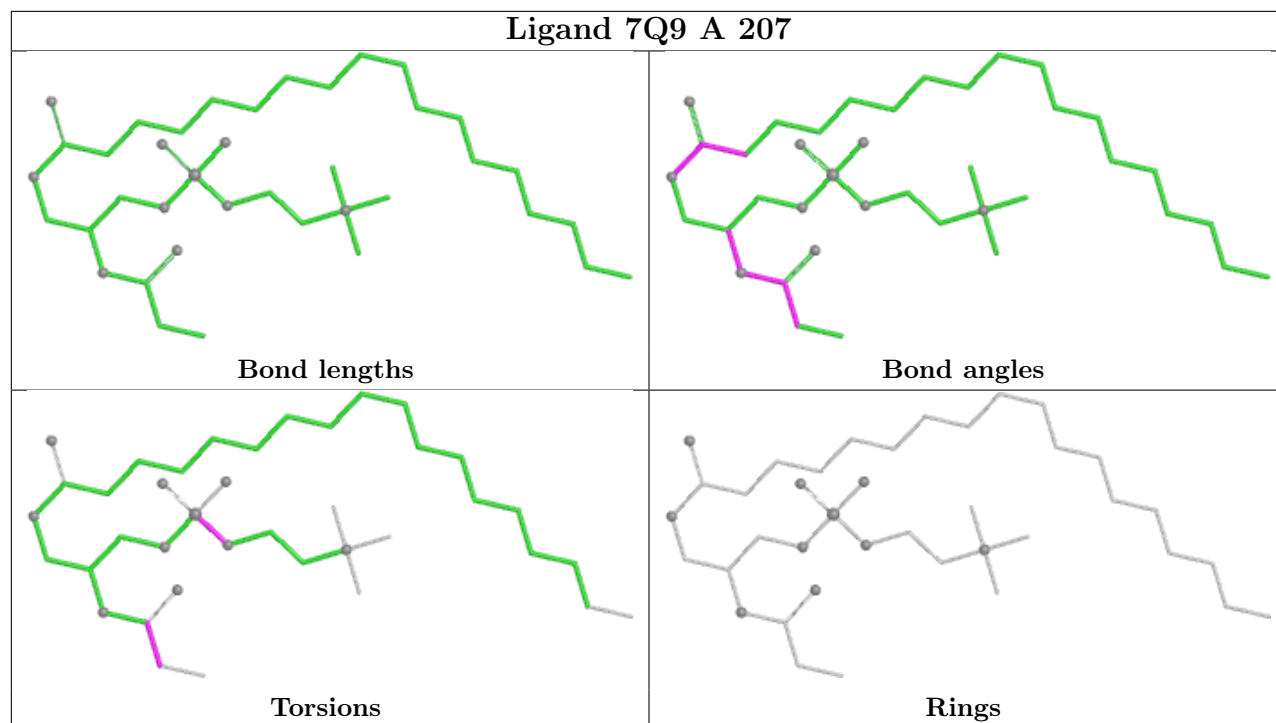


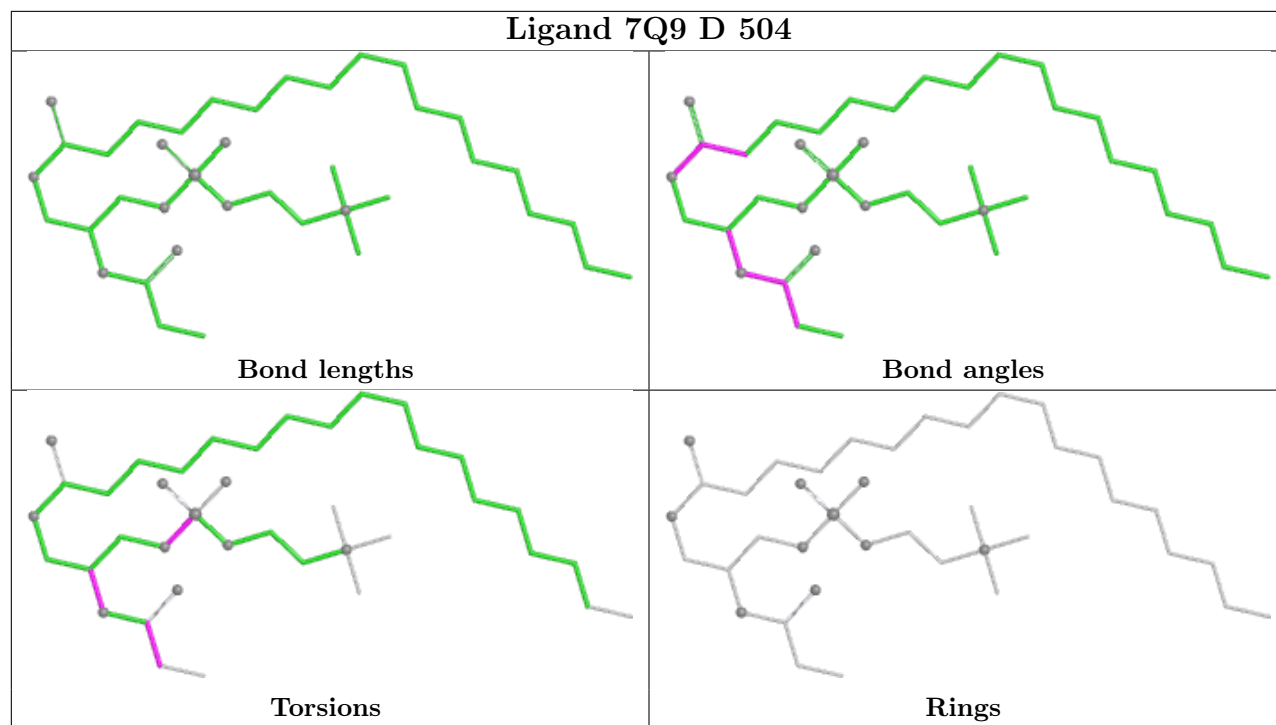
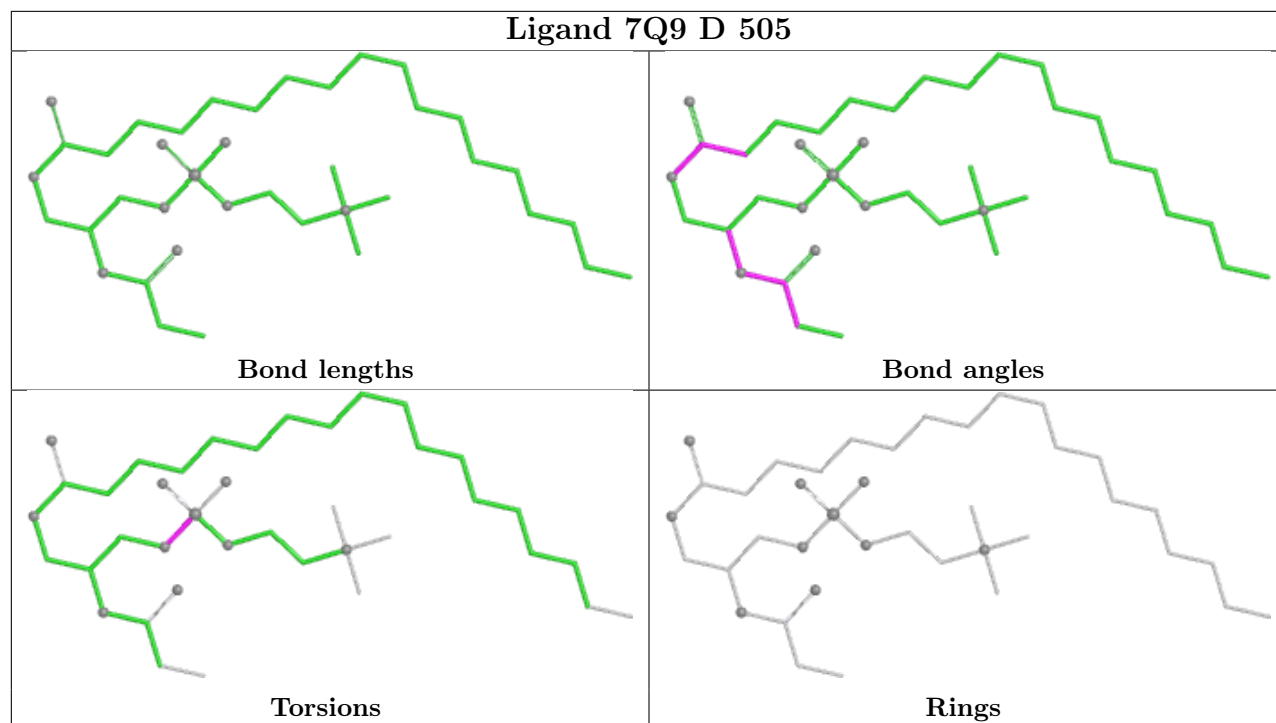
Ligand 7Q9 E 842

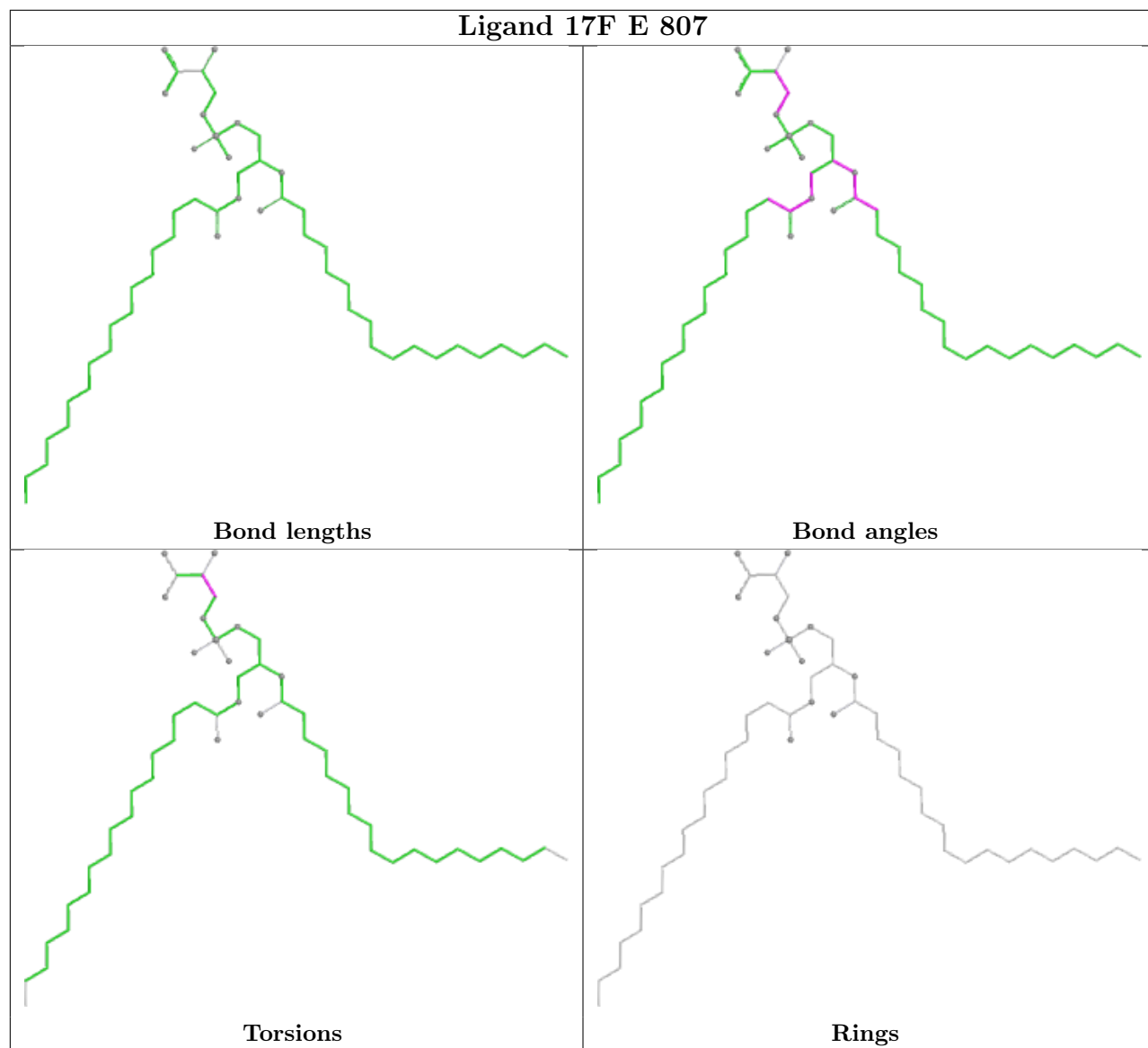


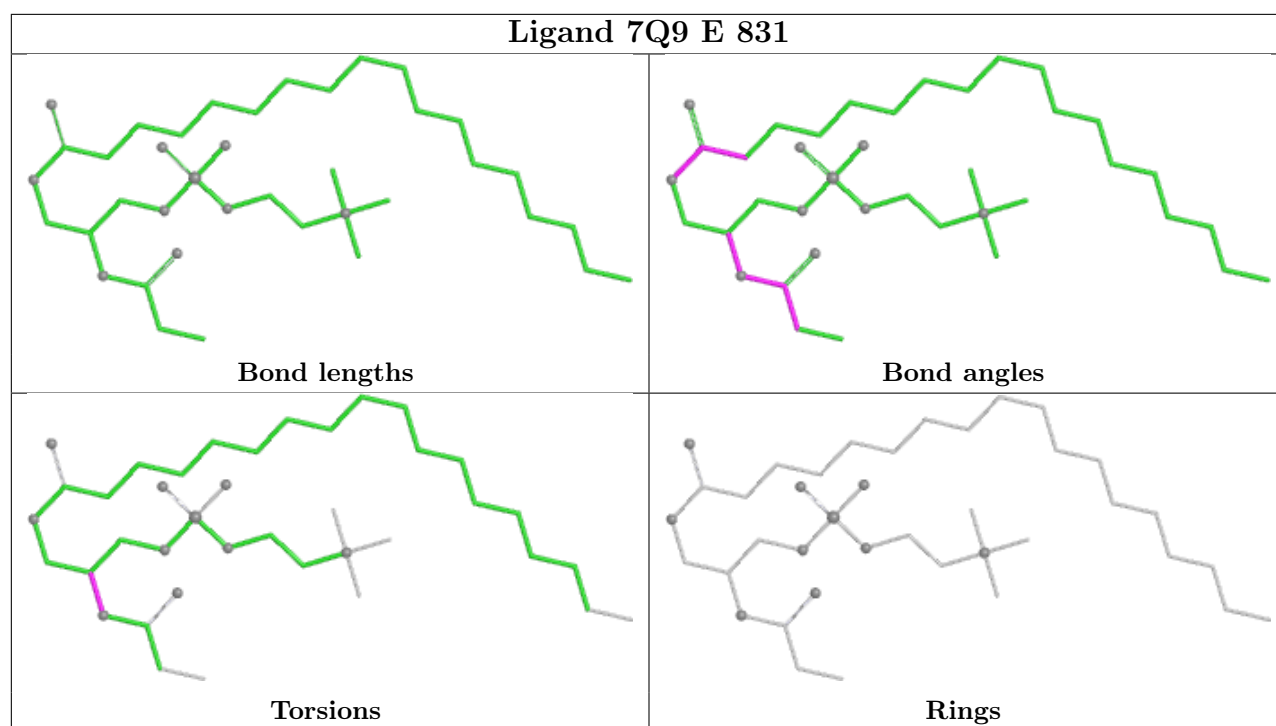
Ligand 7Q9 B 210

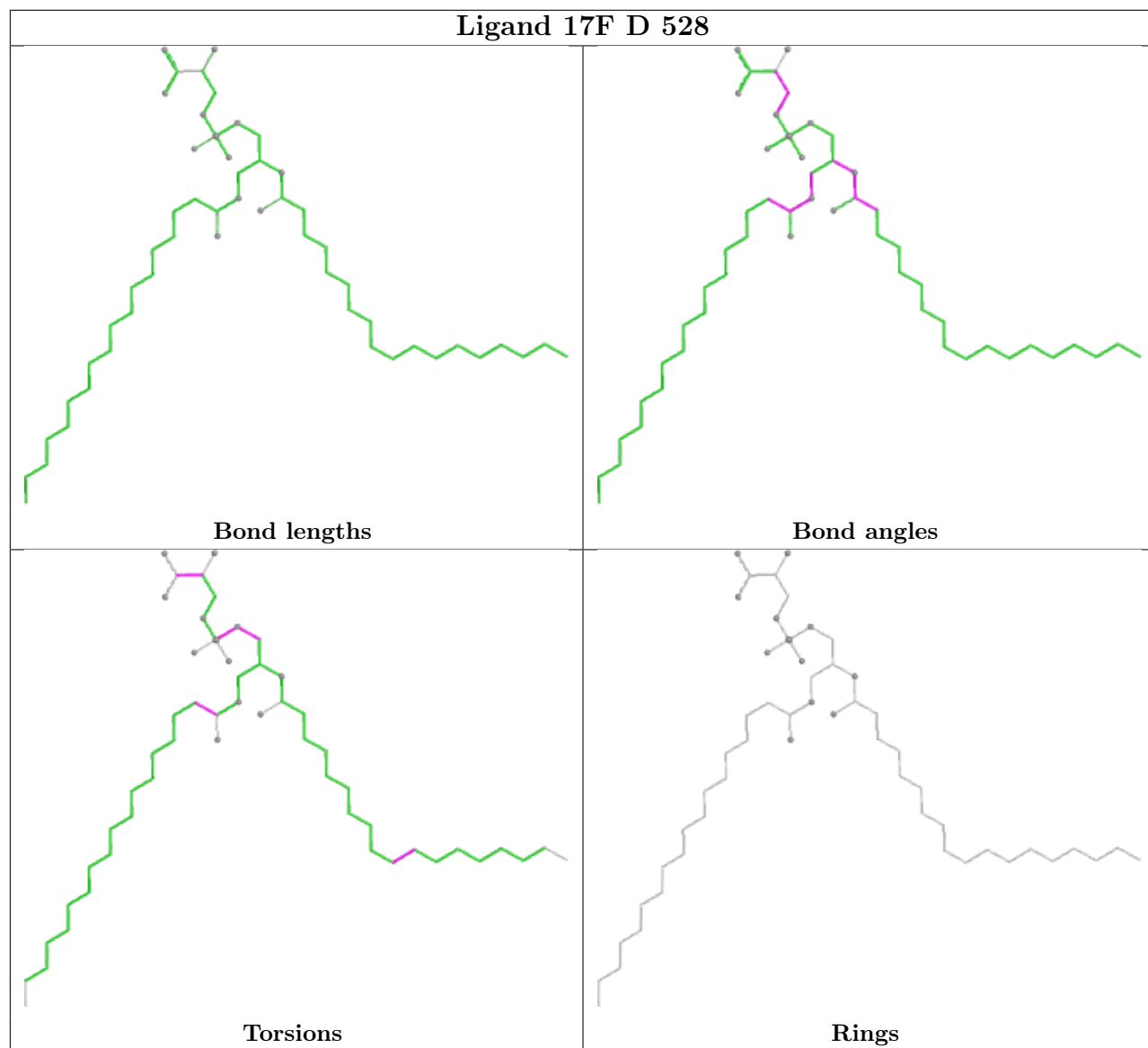


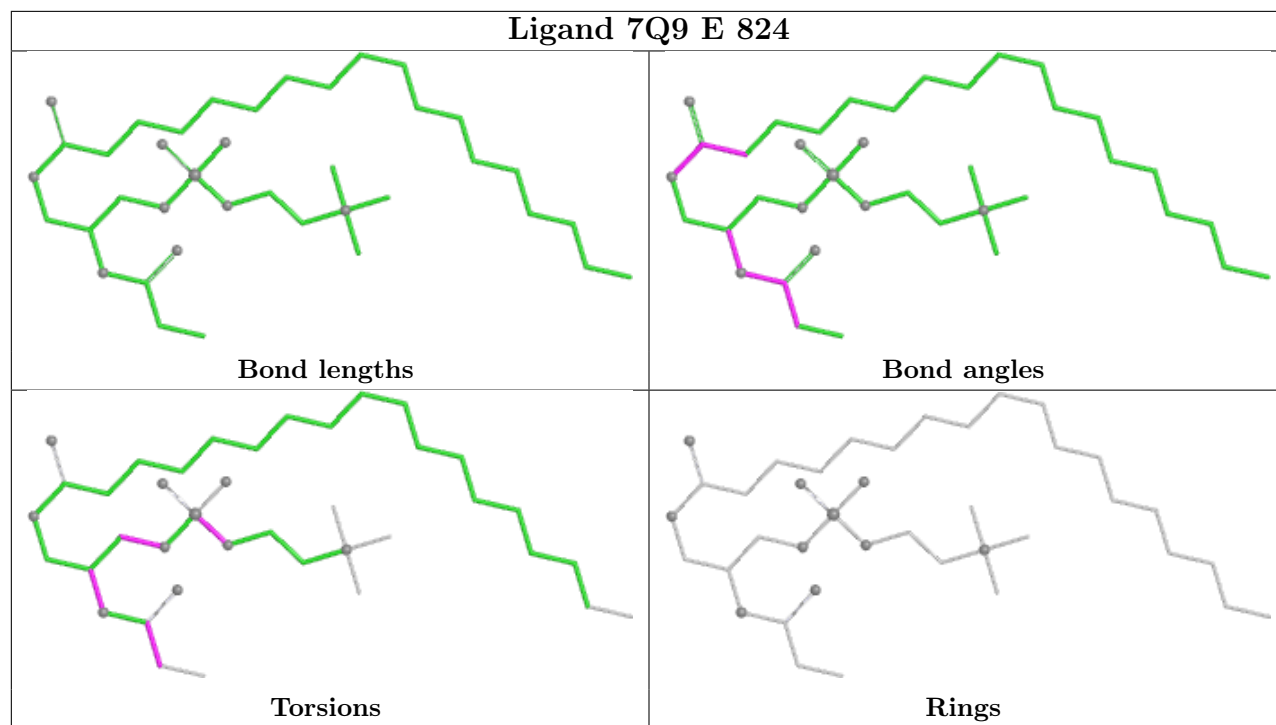
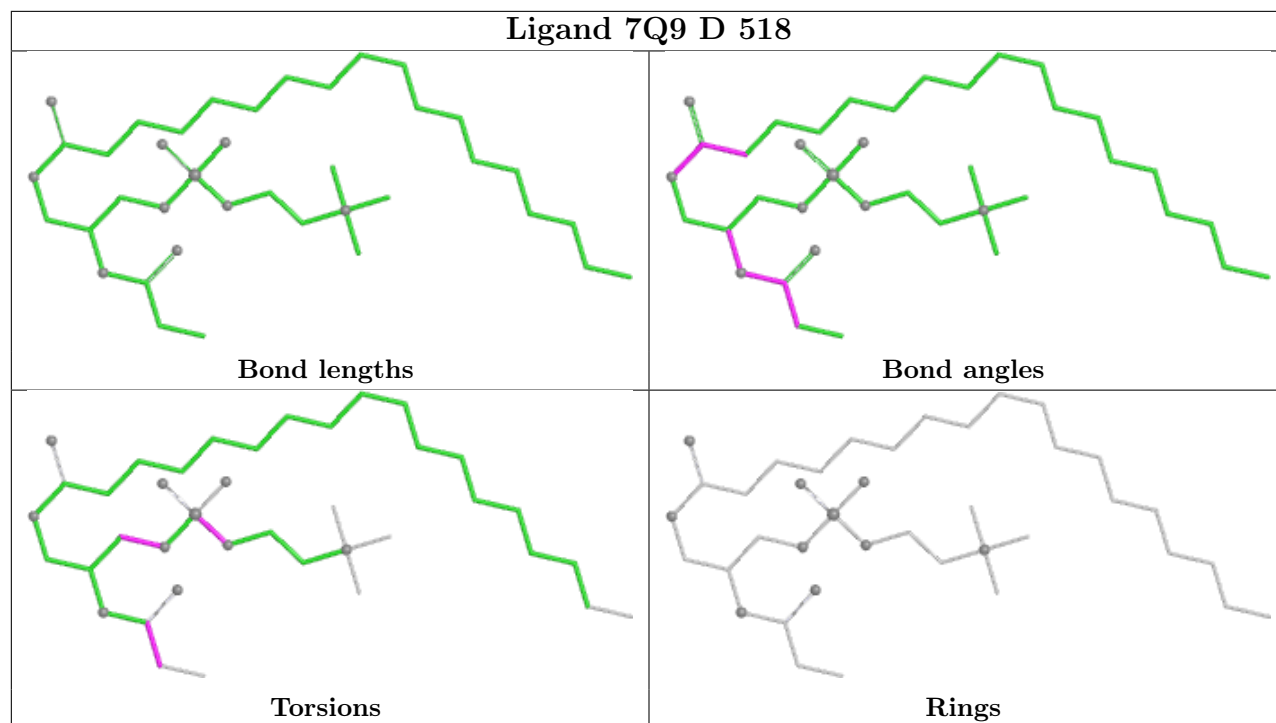


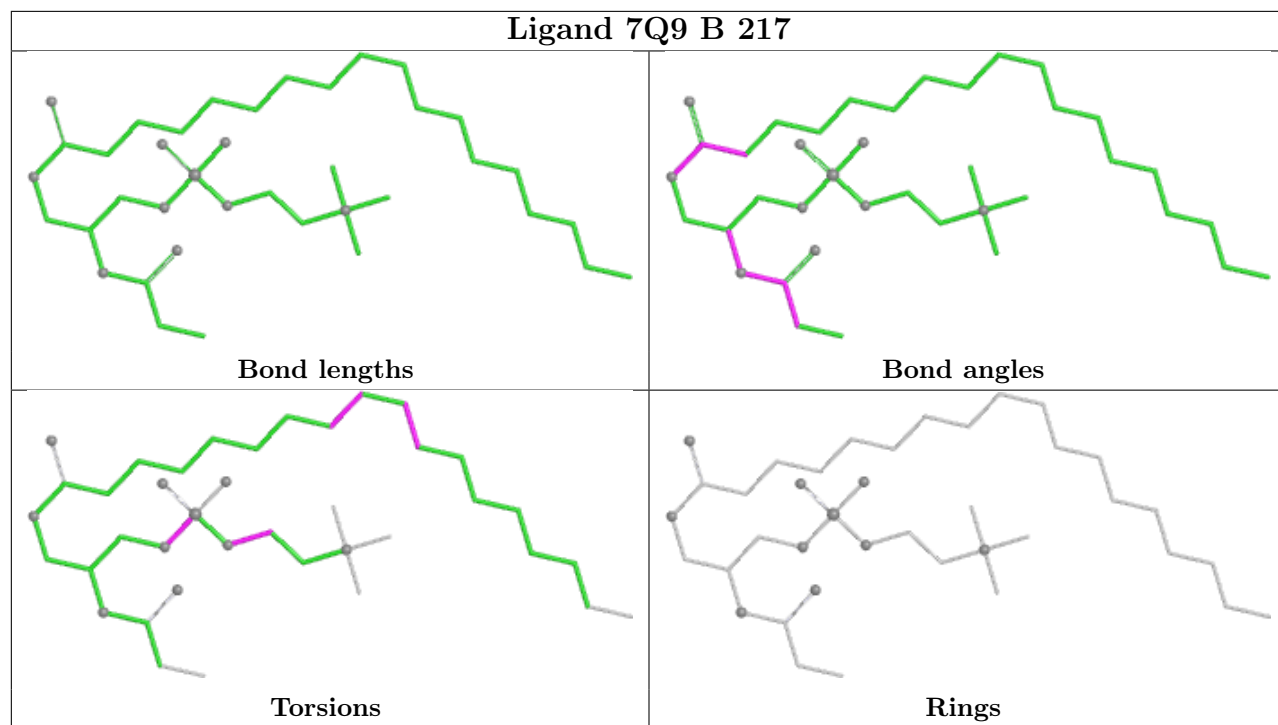
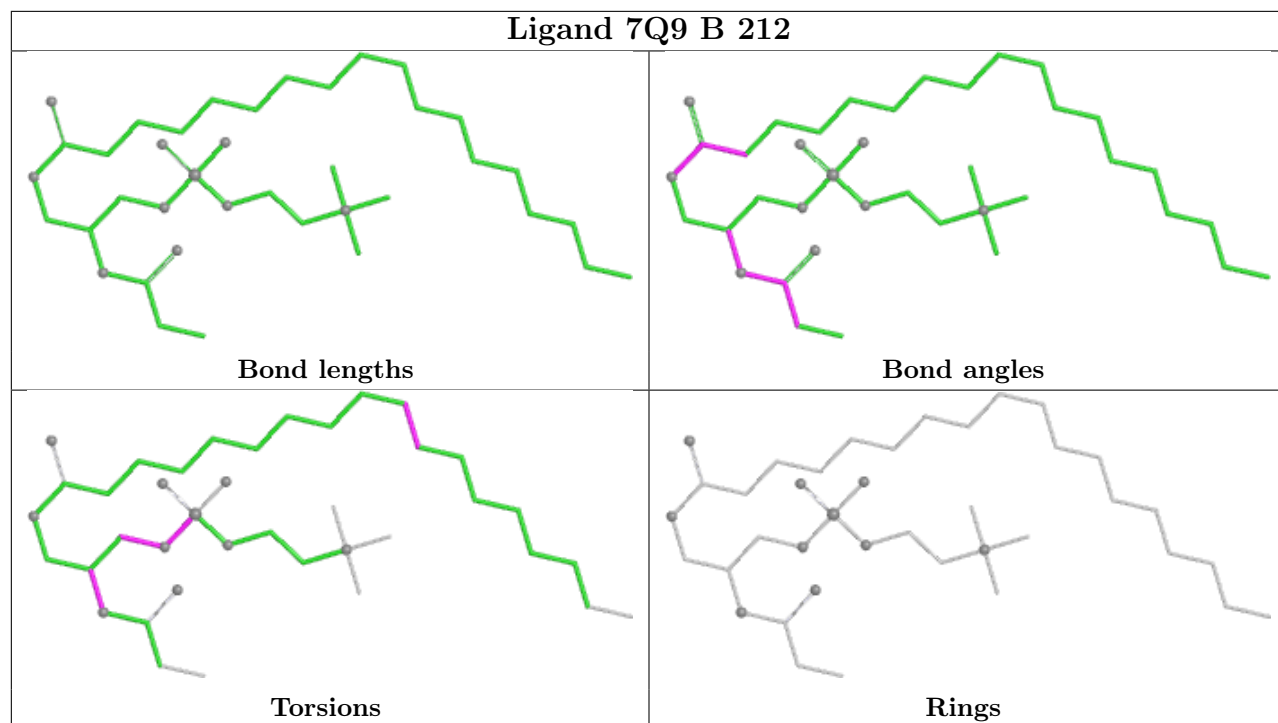


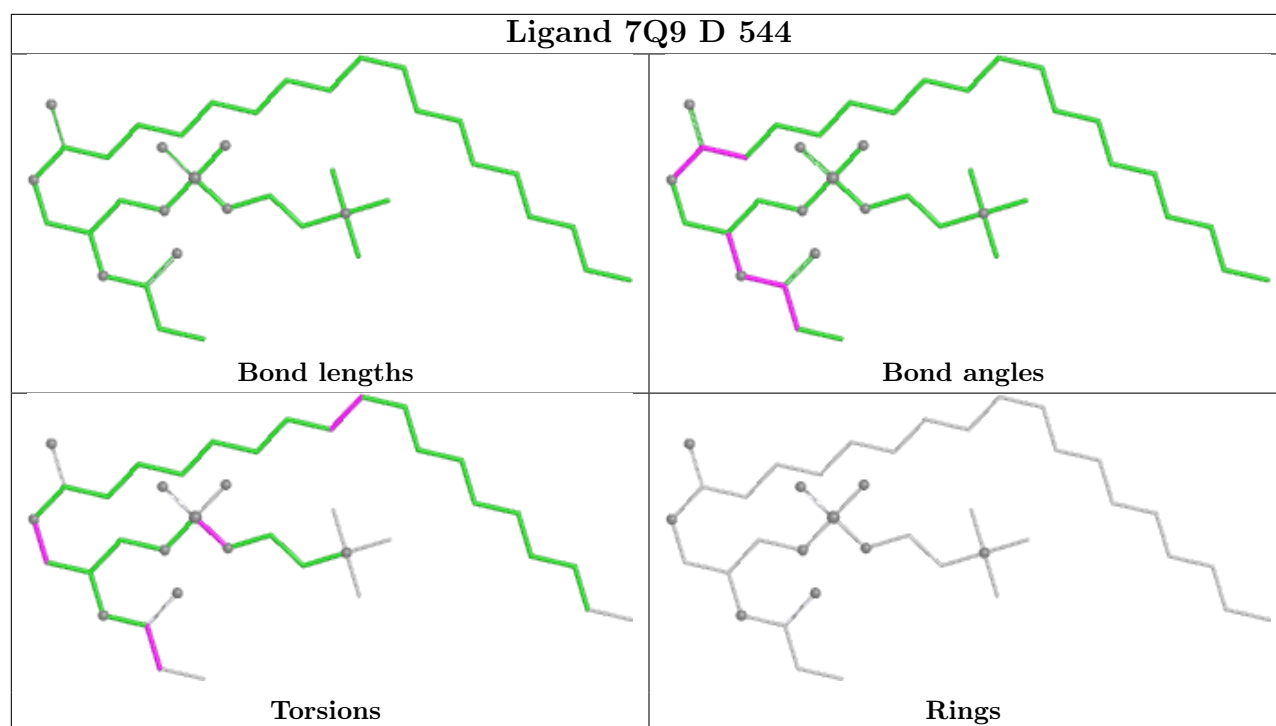


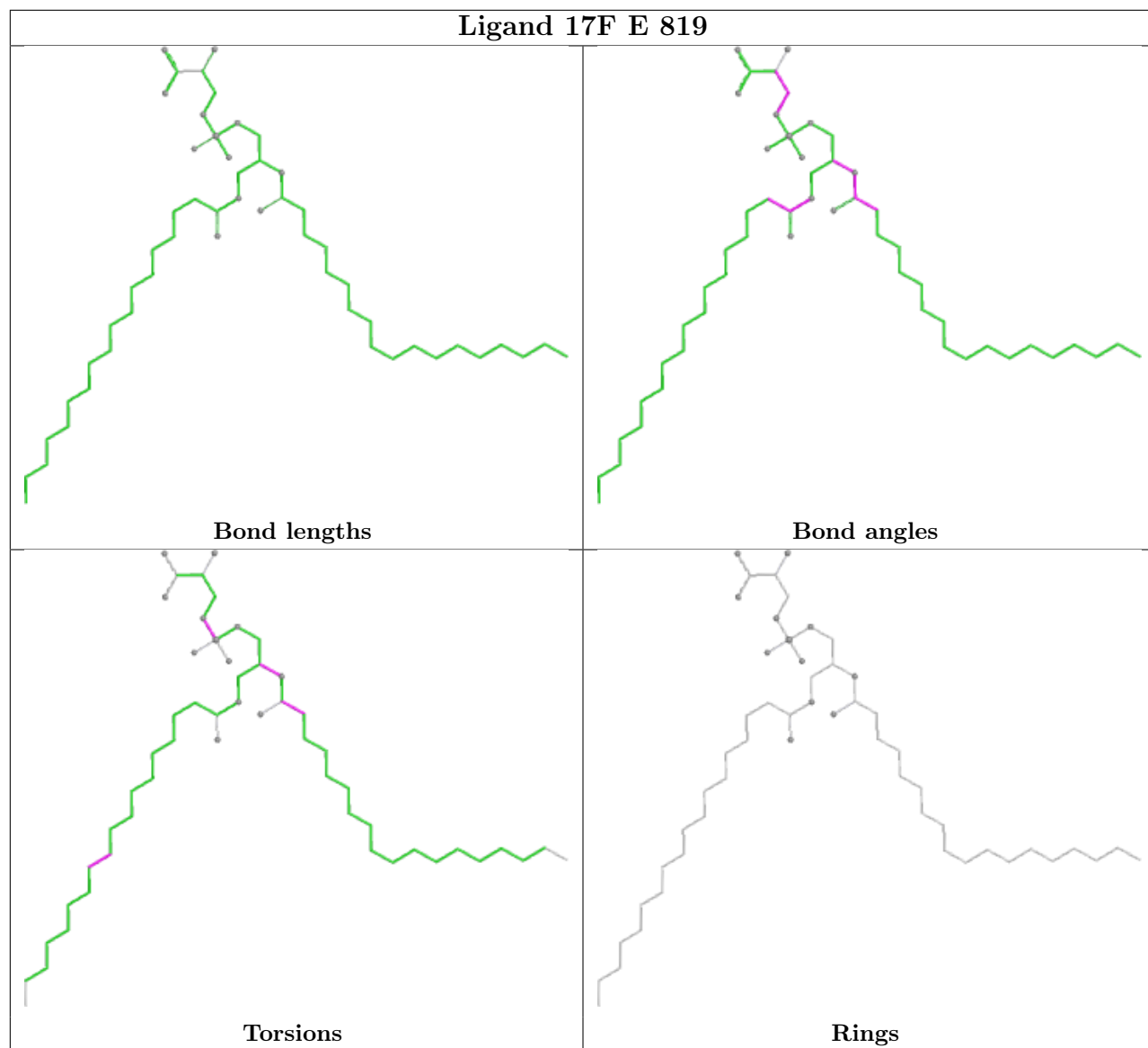


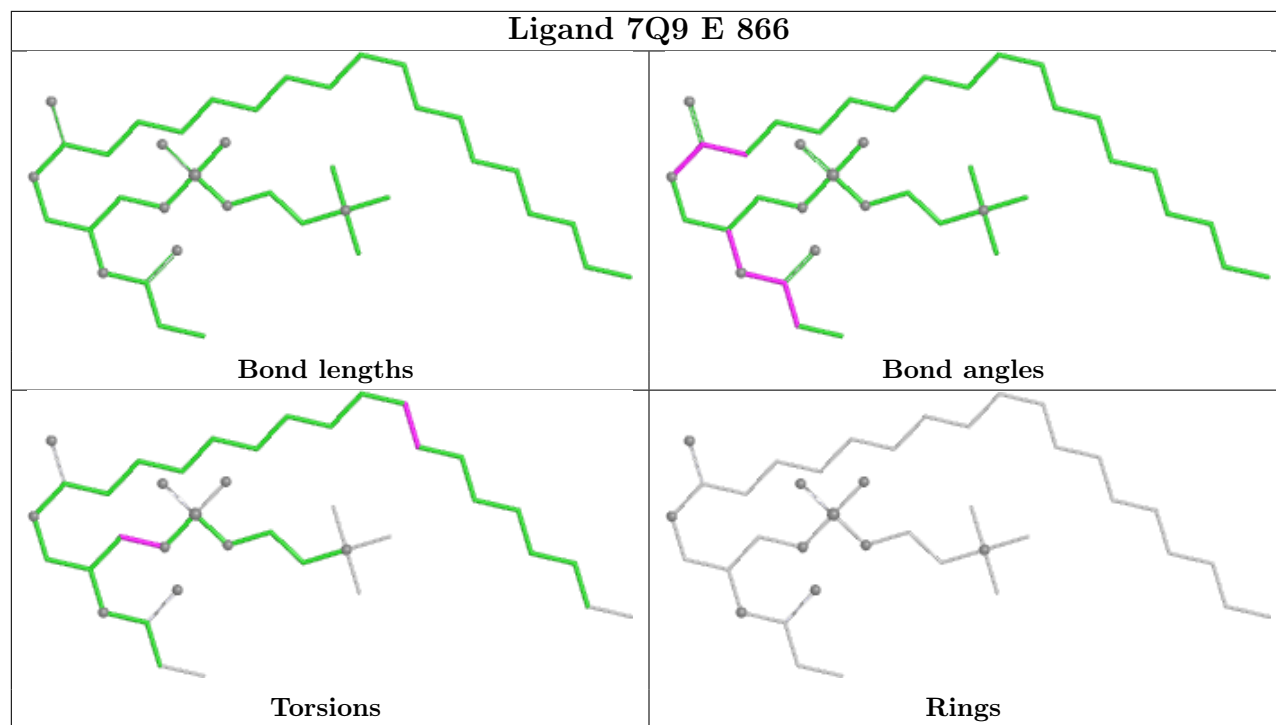
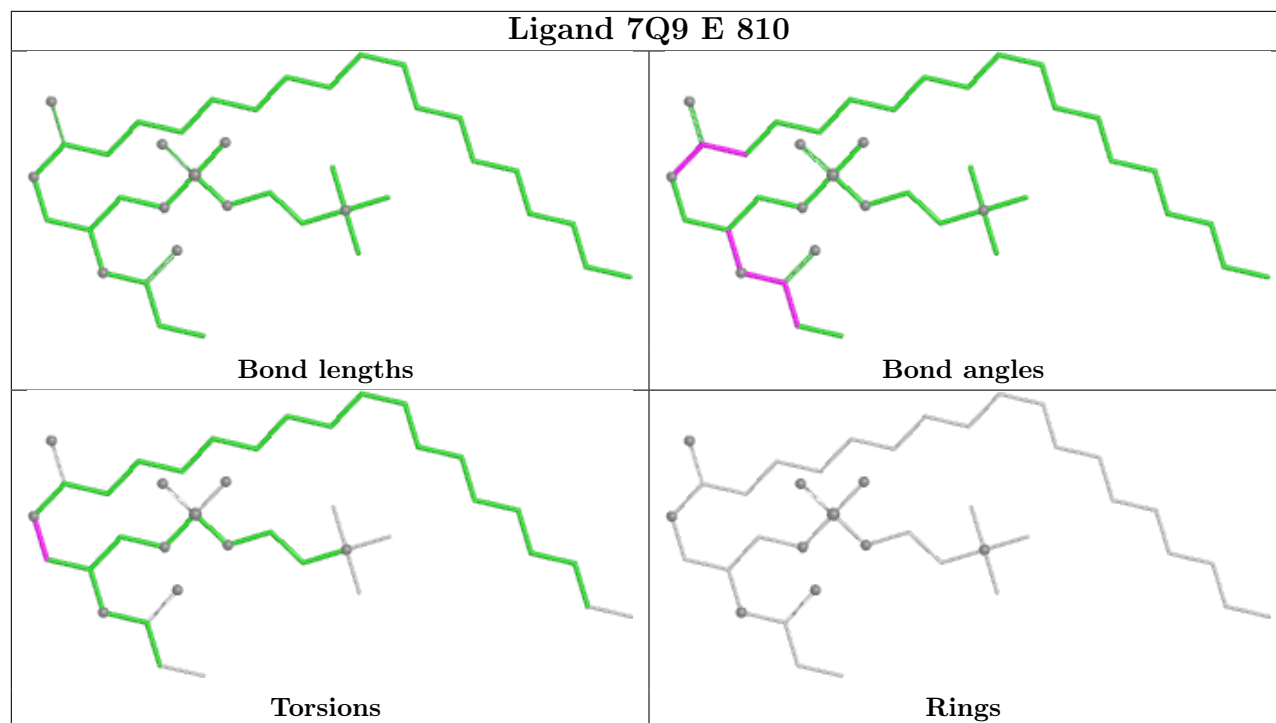


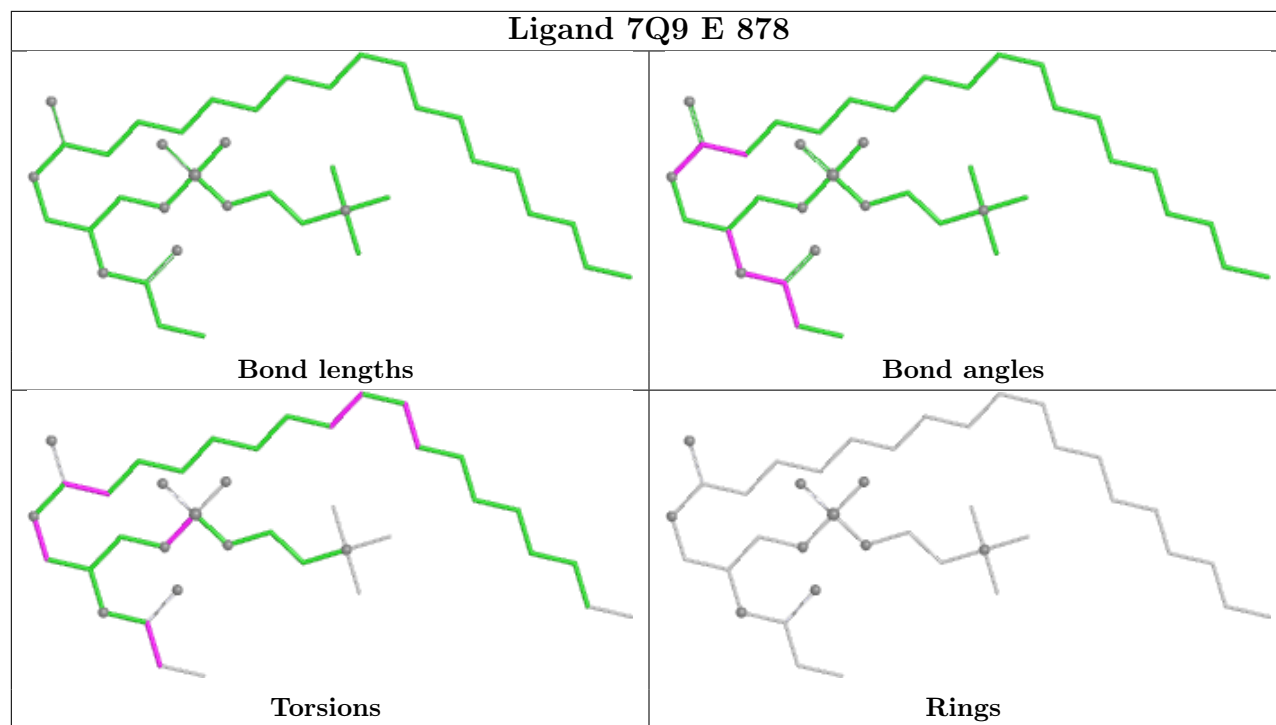
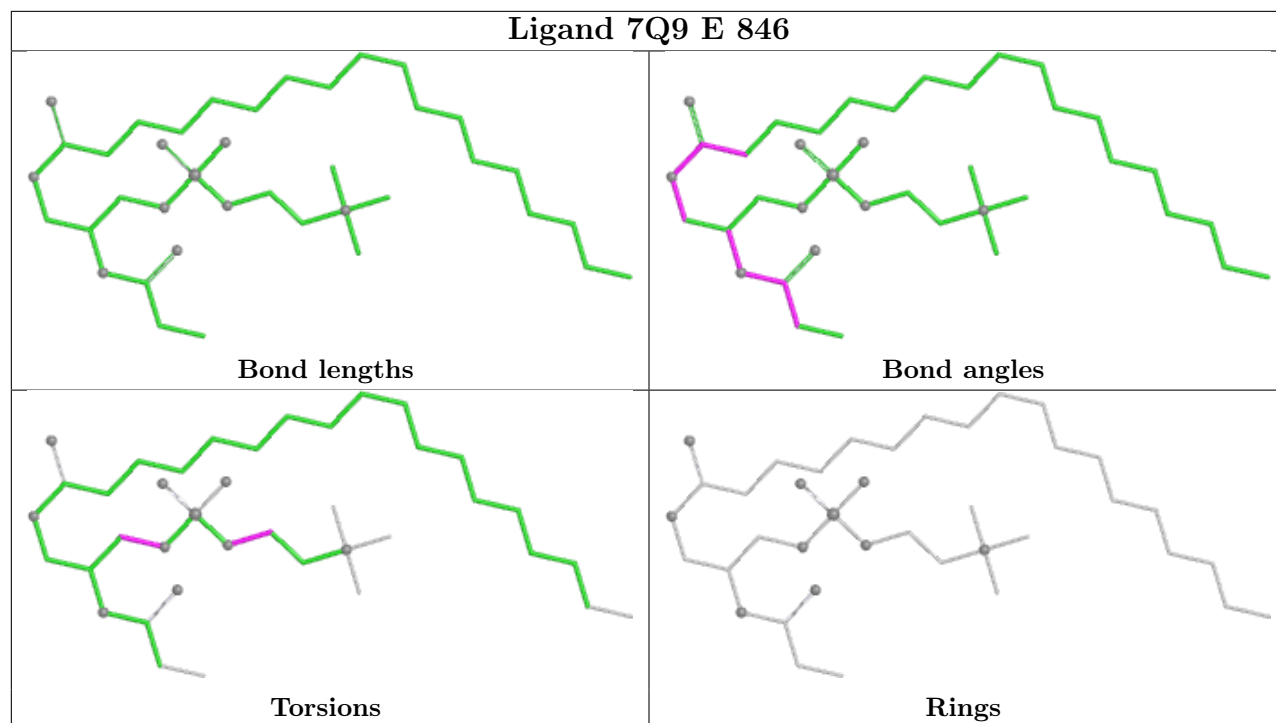


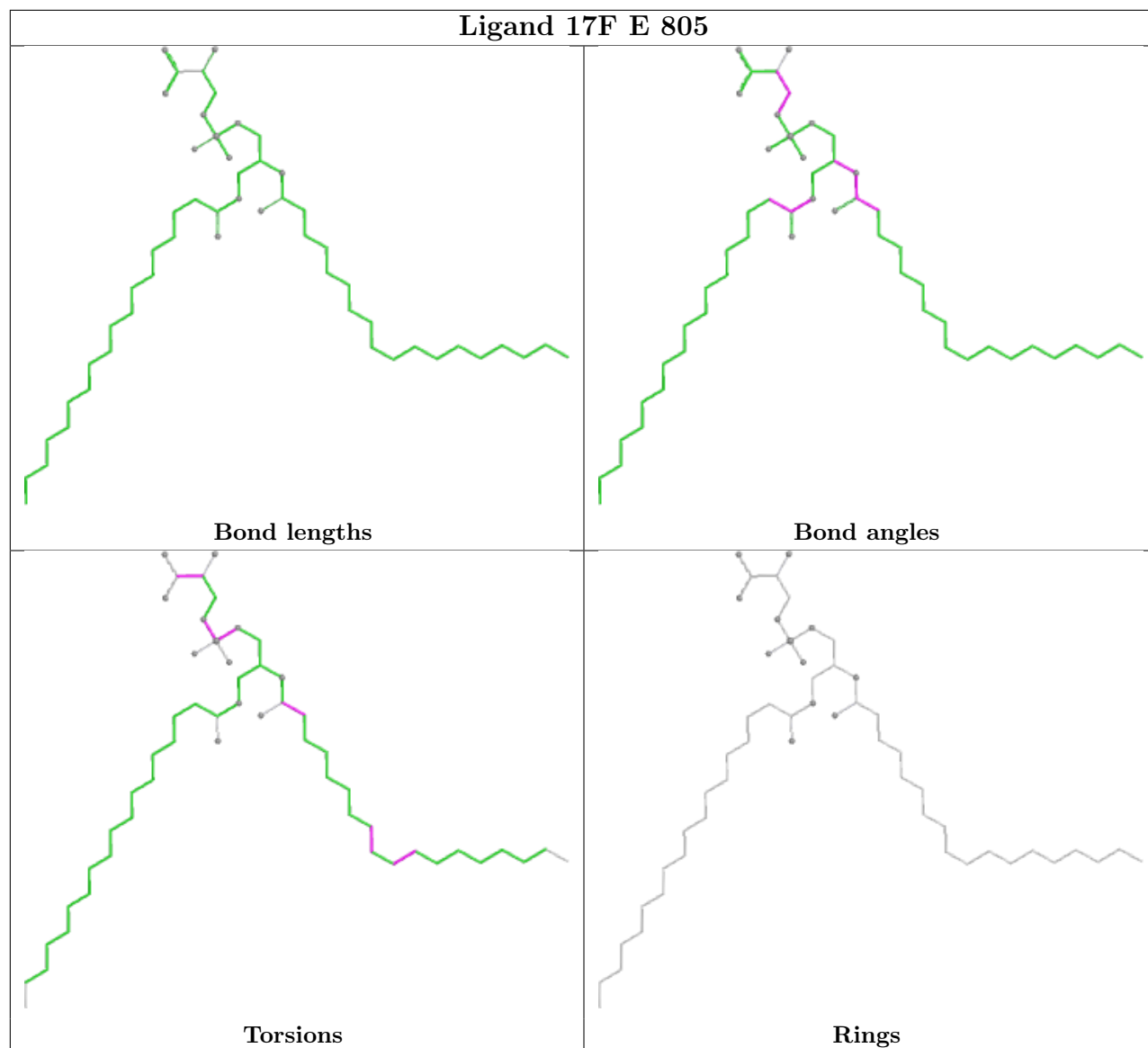


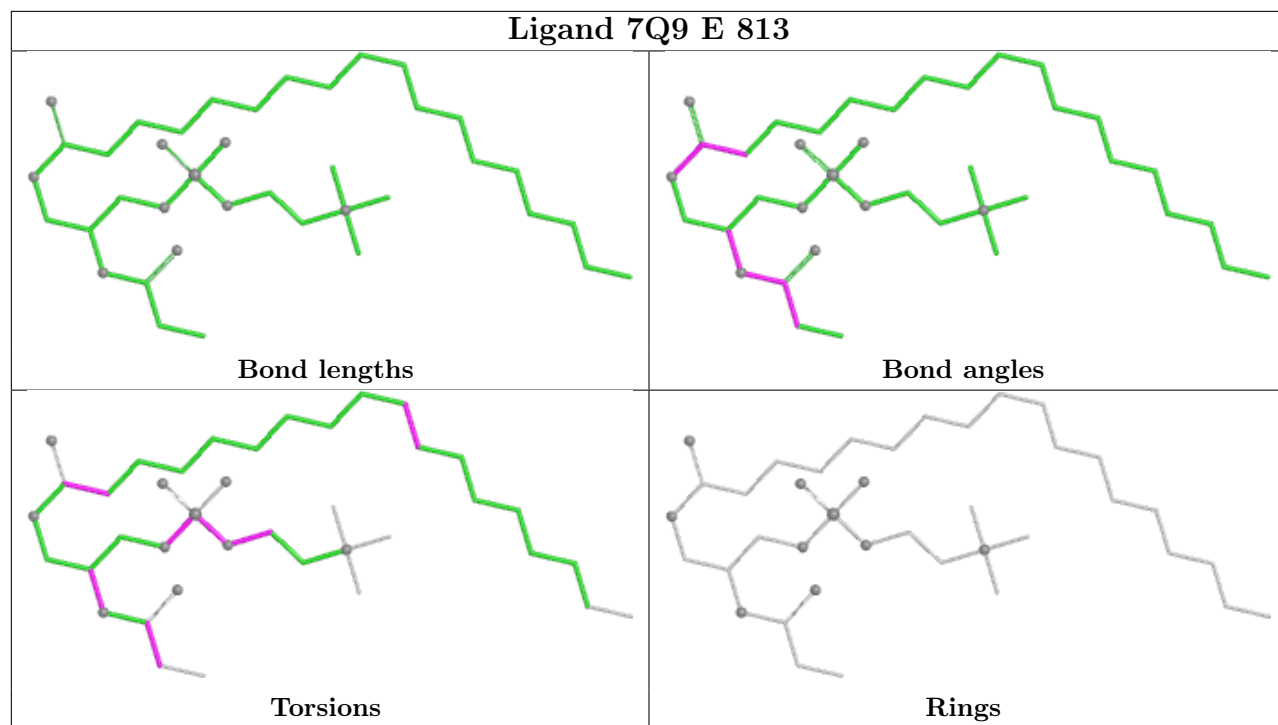
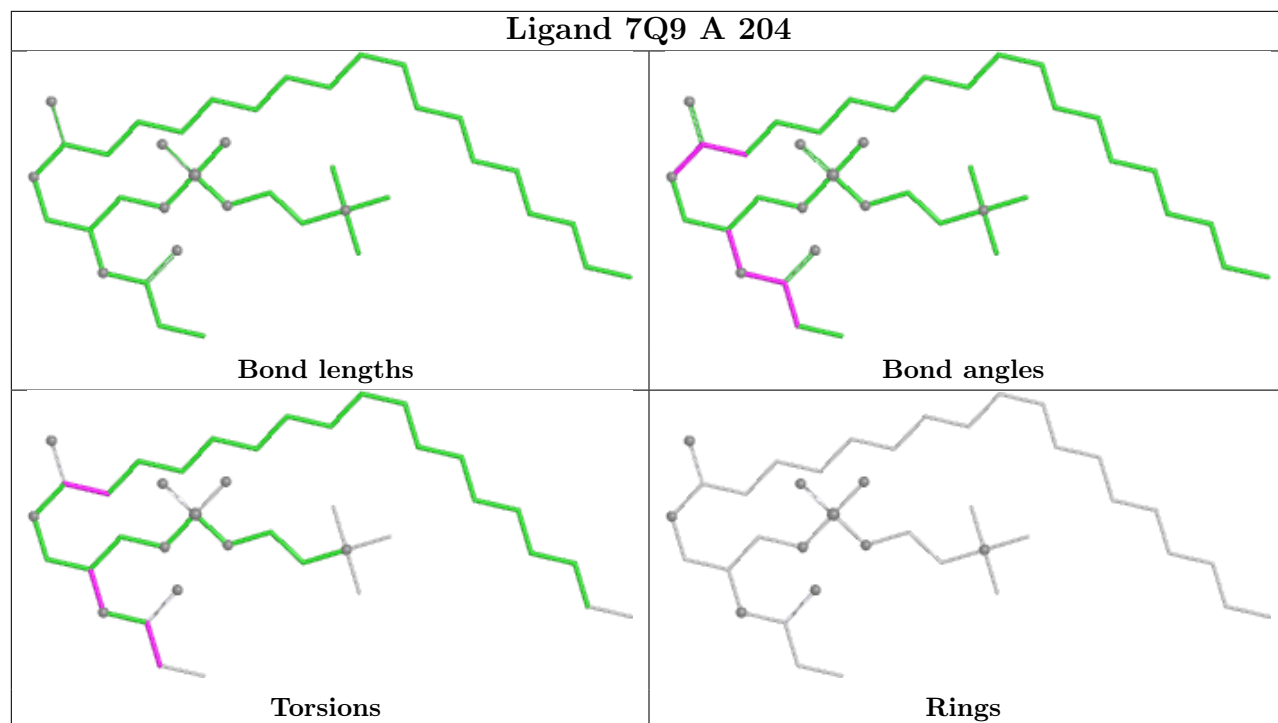


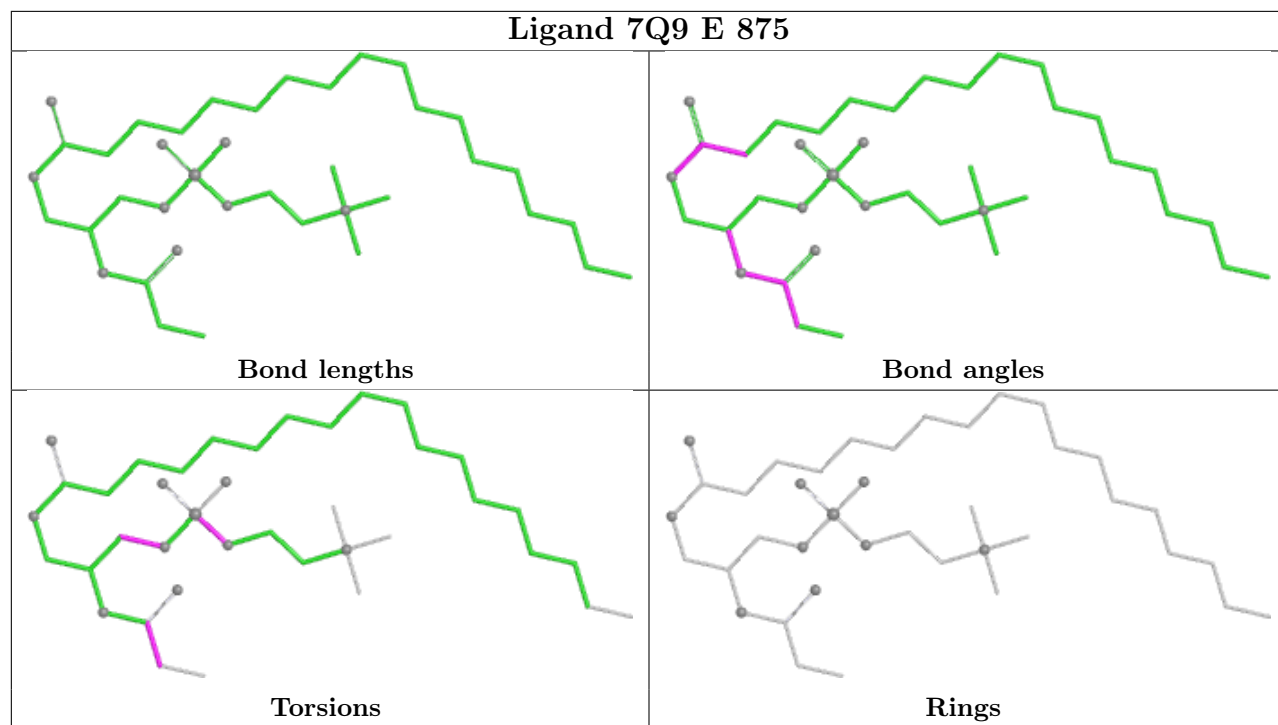
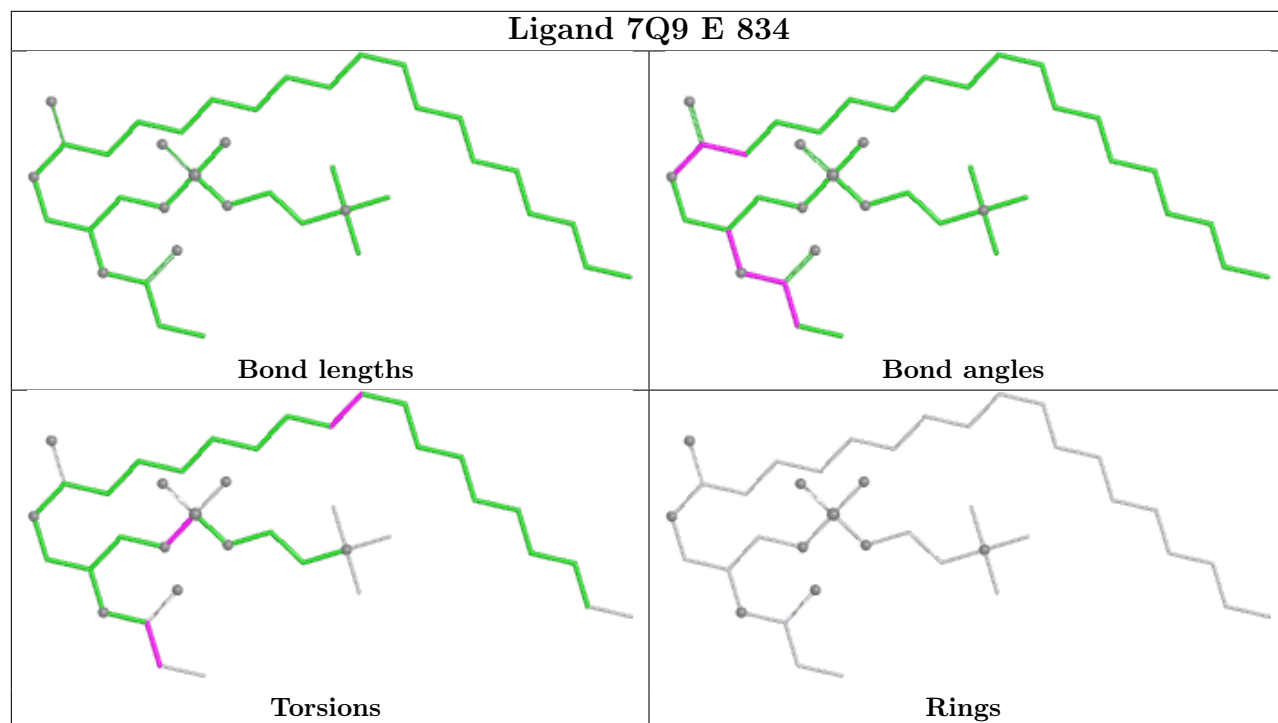


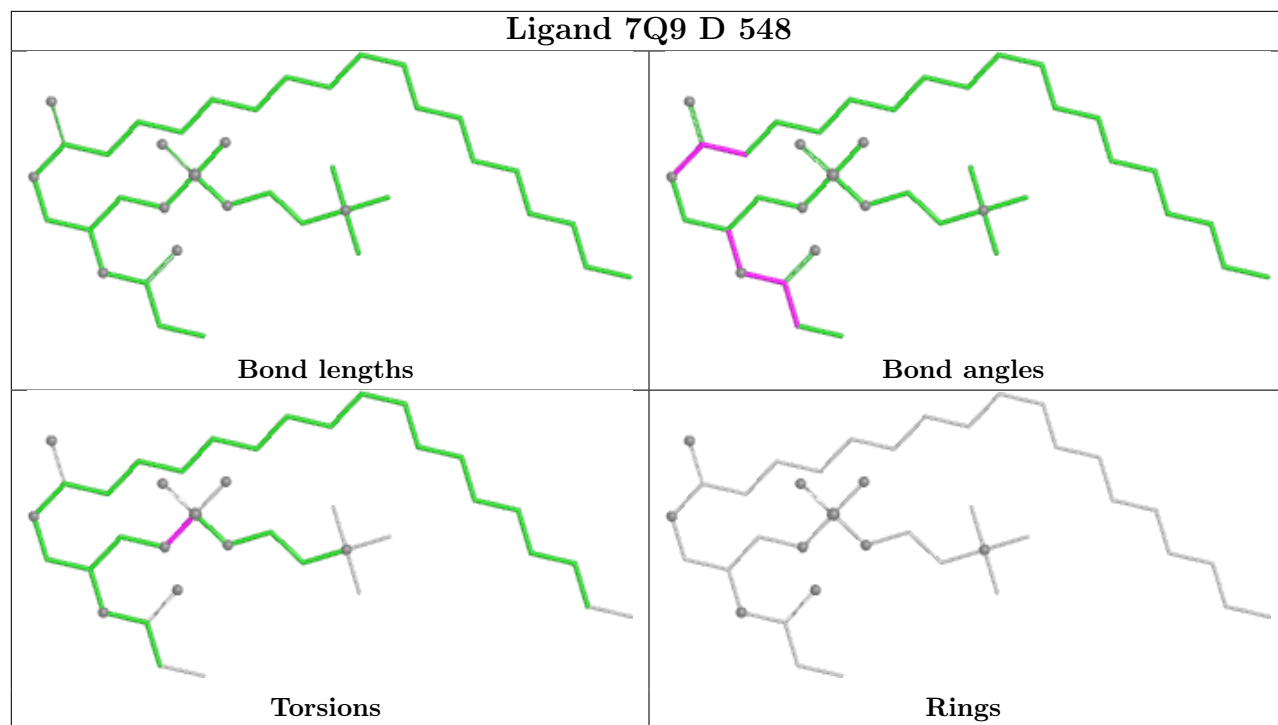
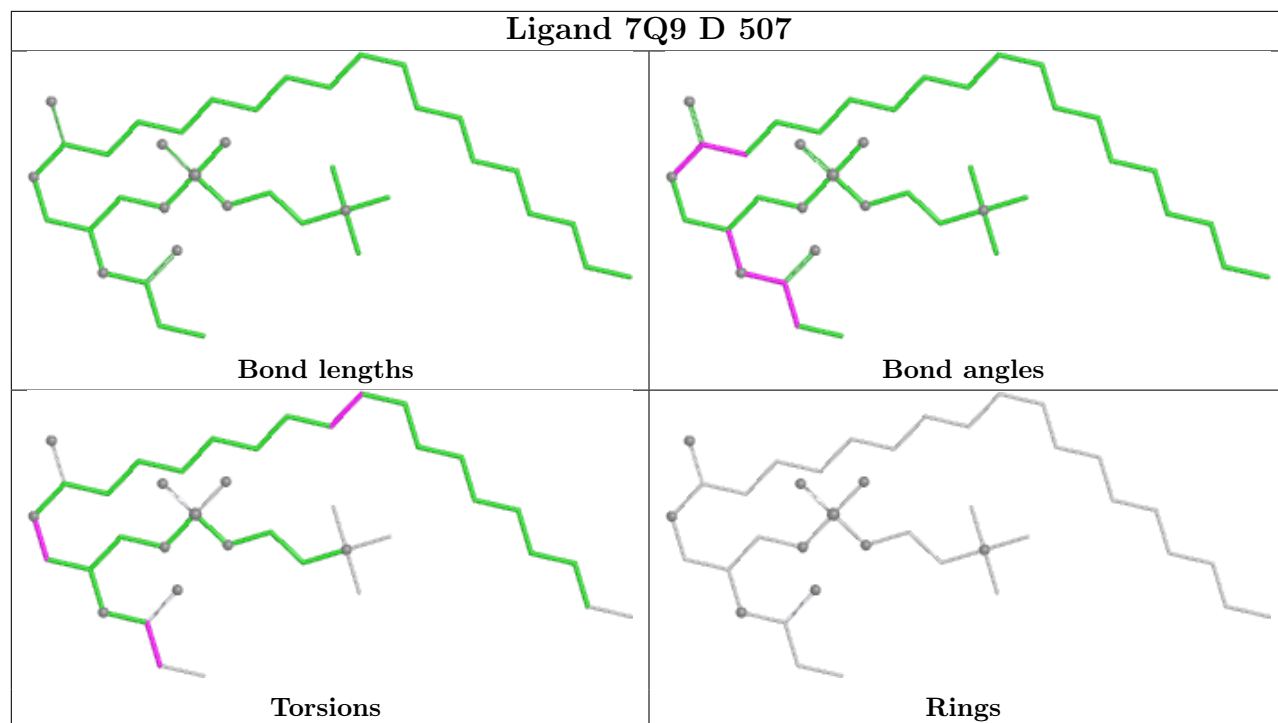


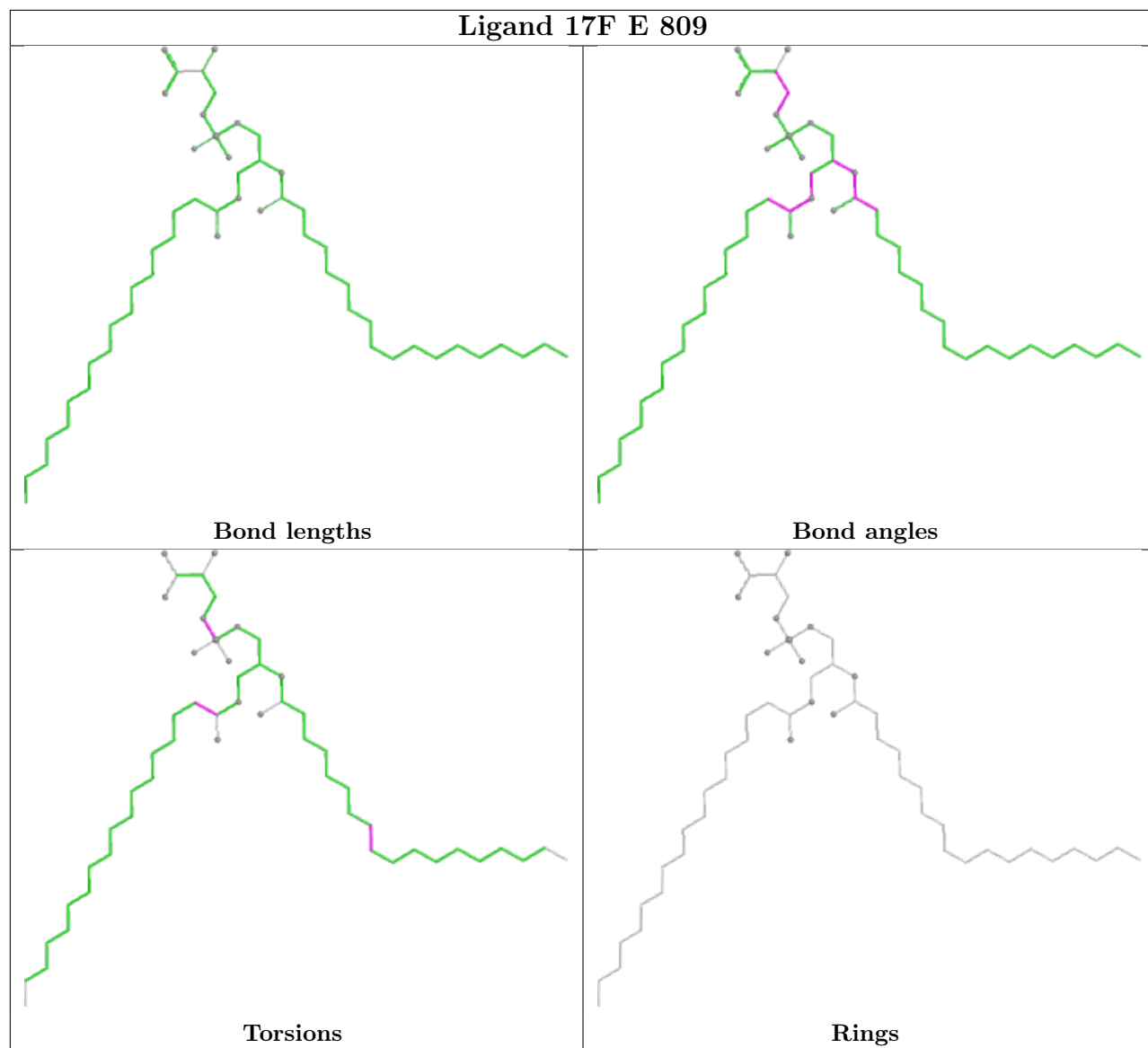


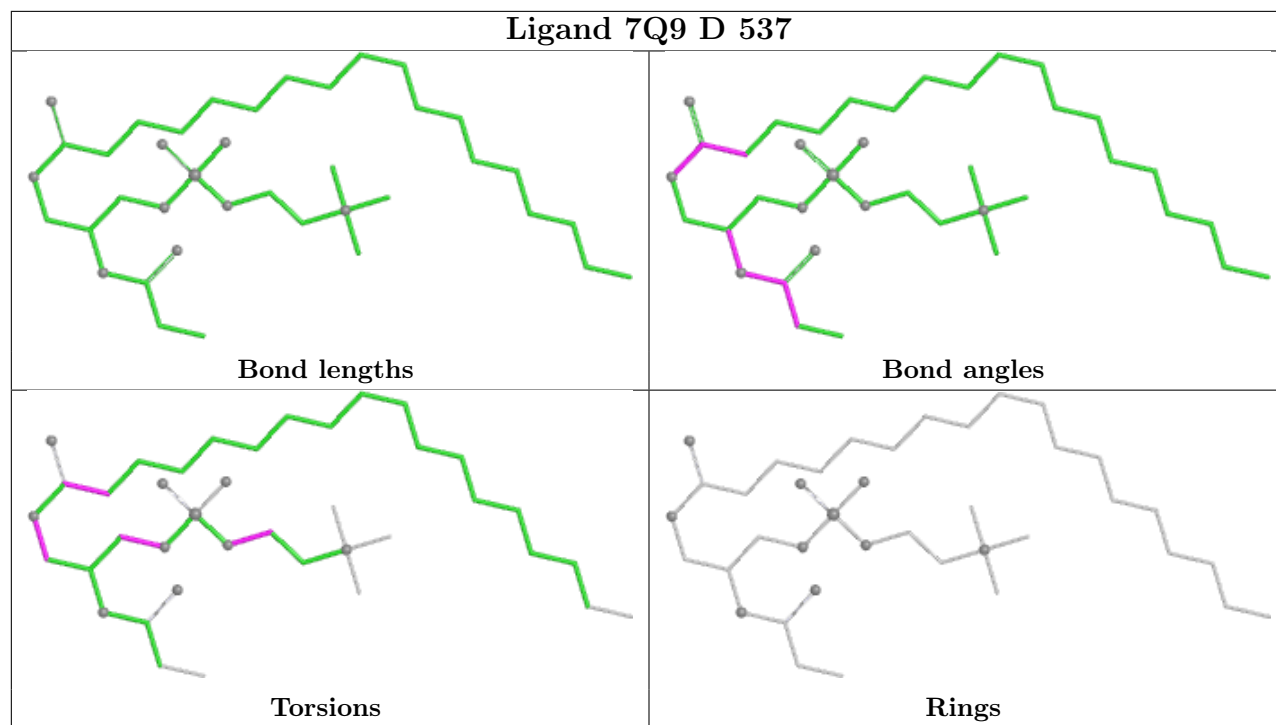
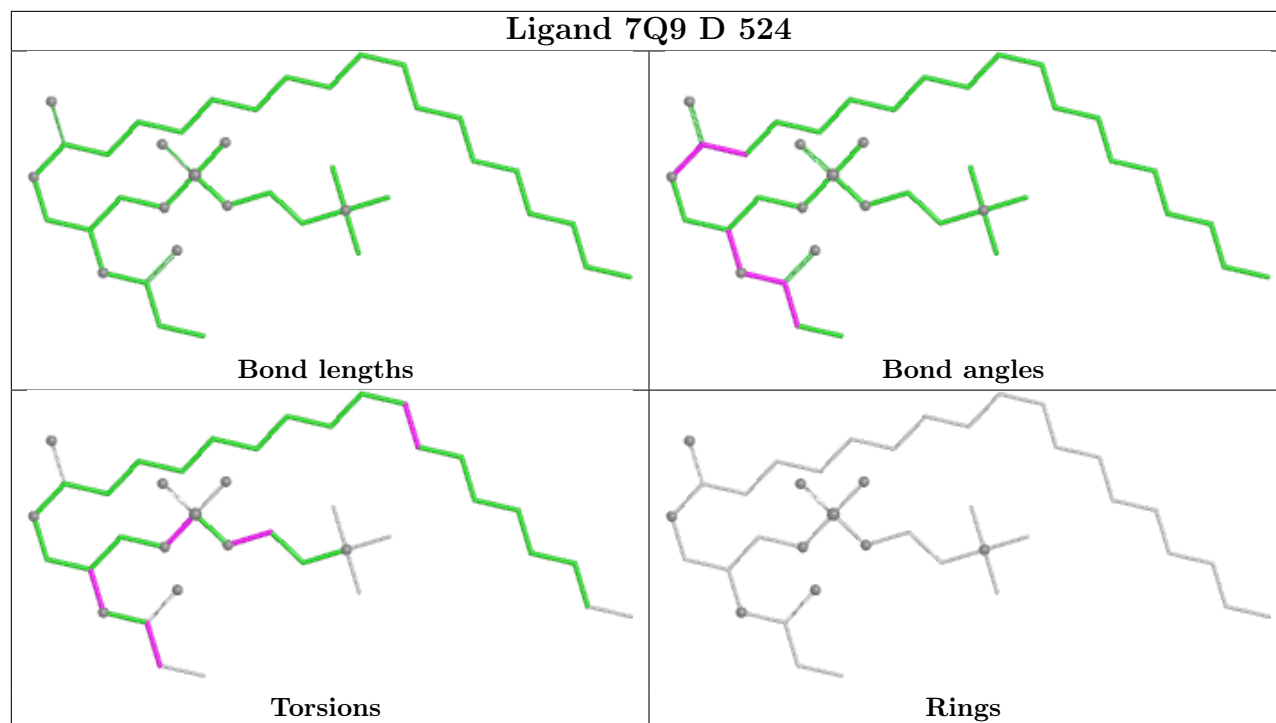


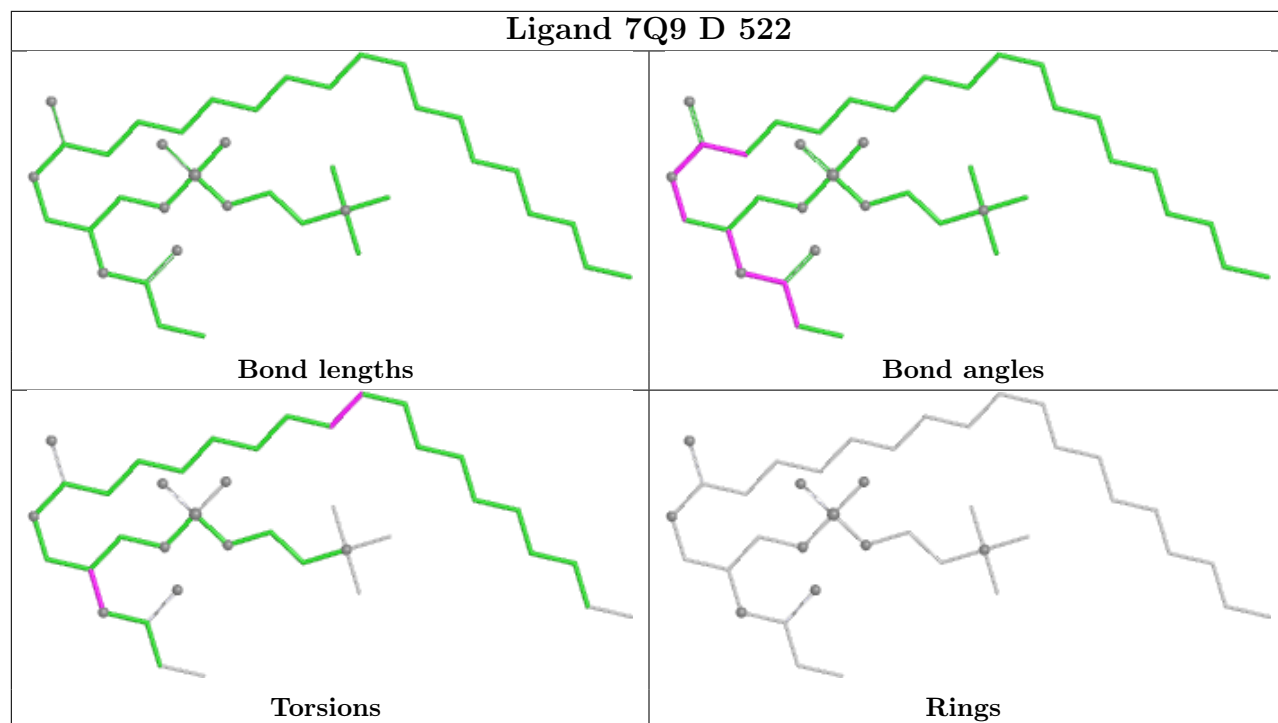


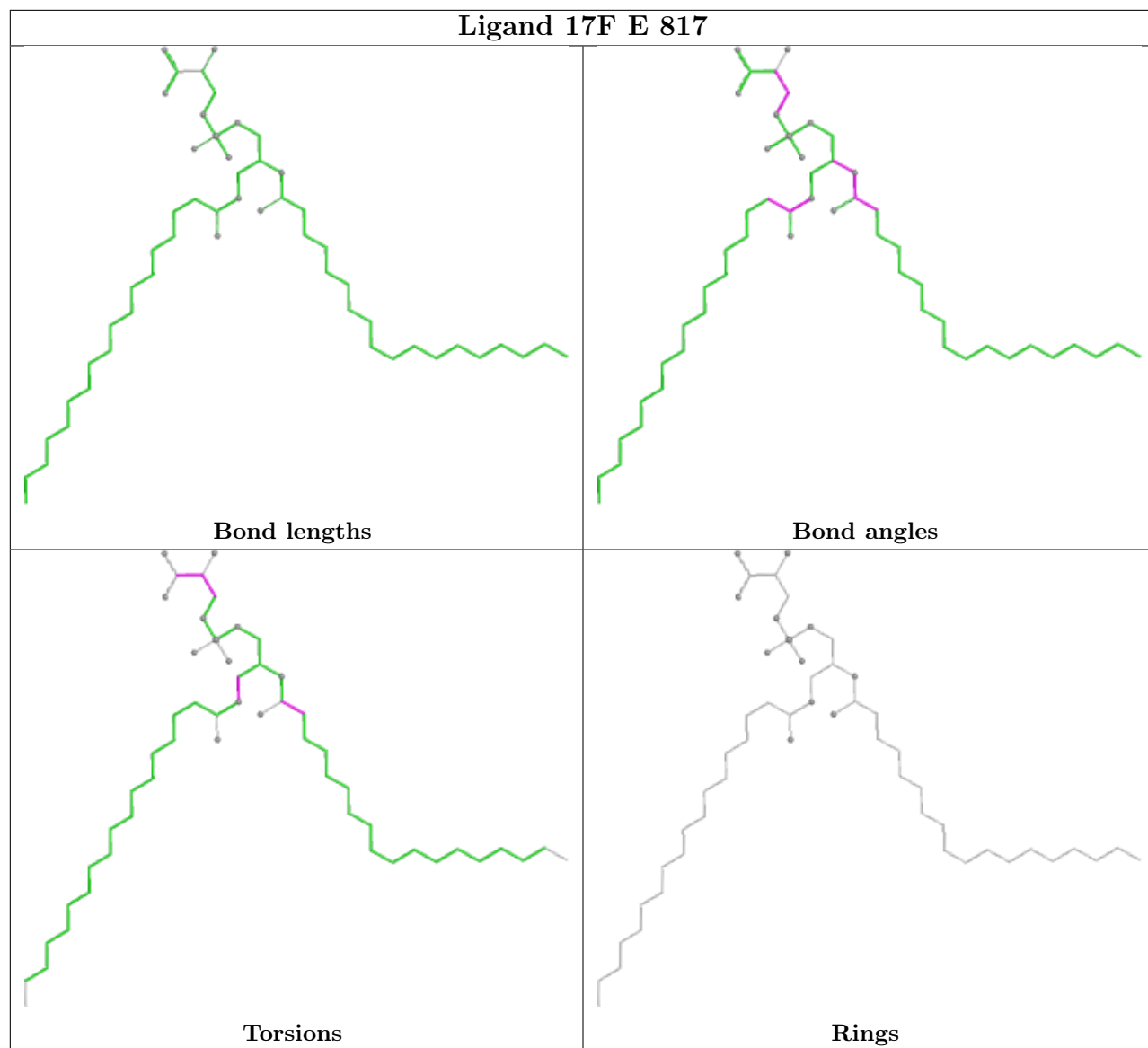


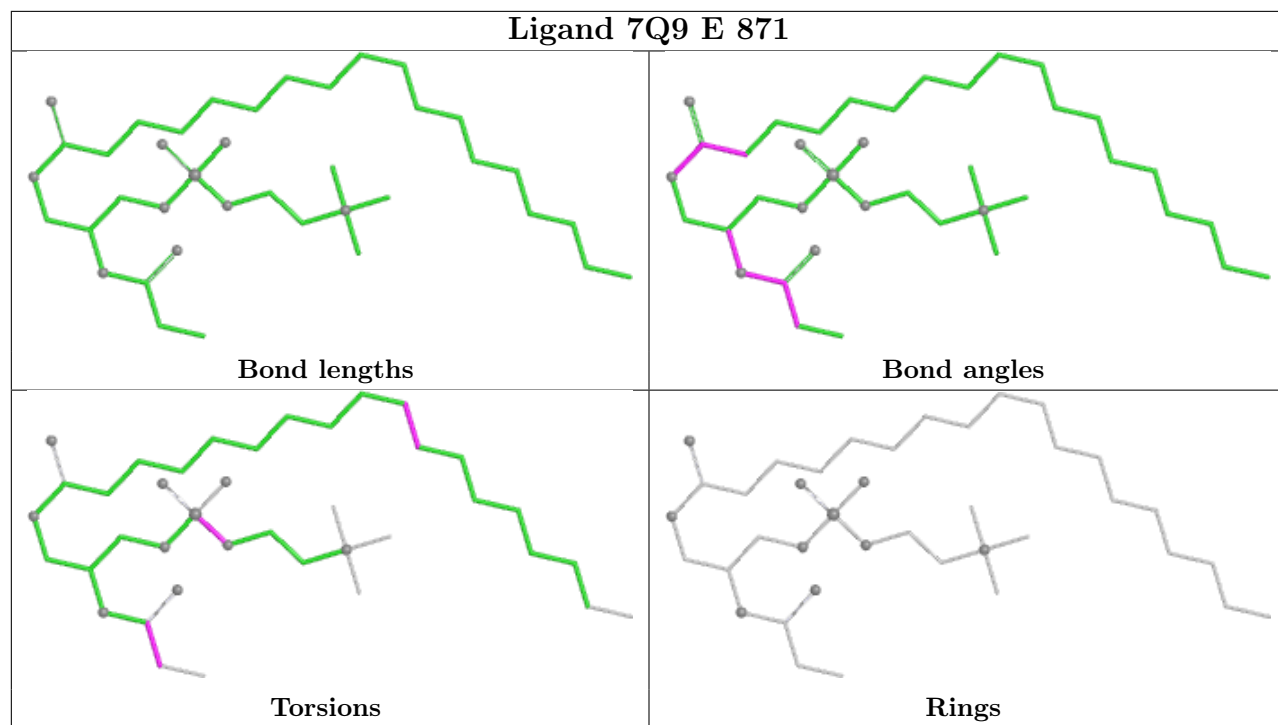
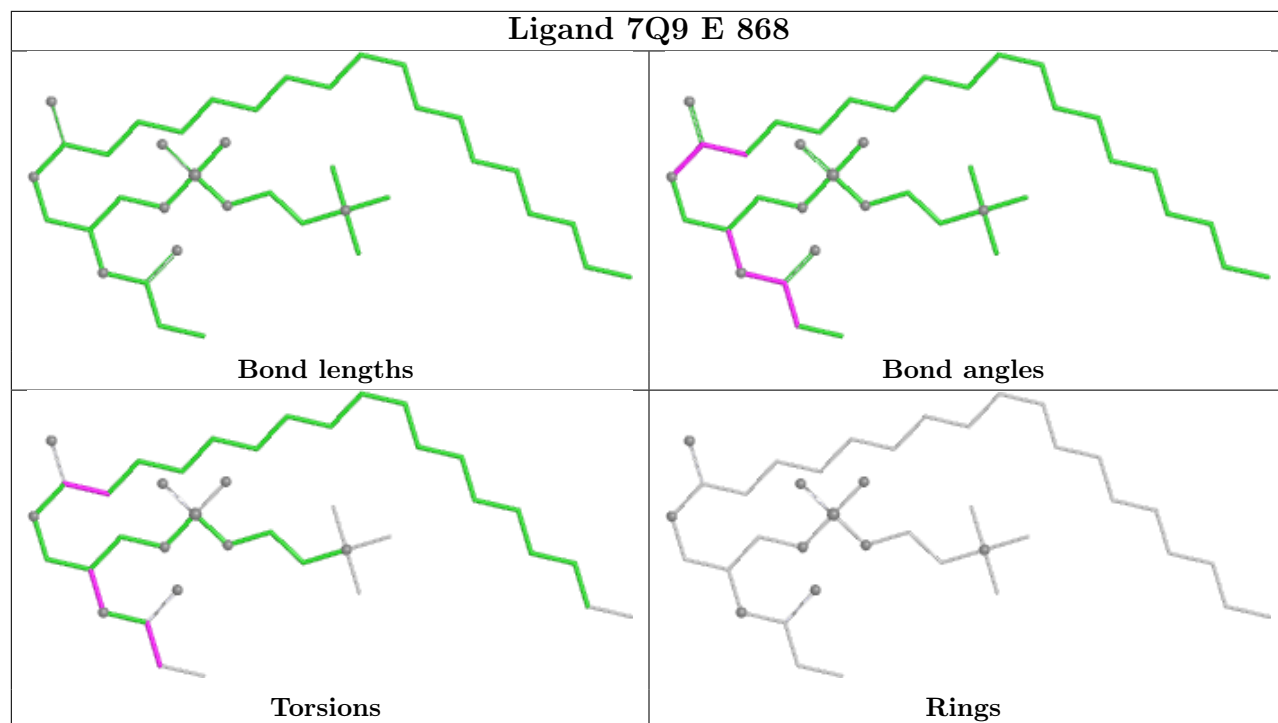


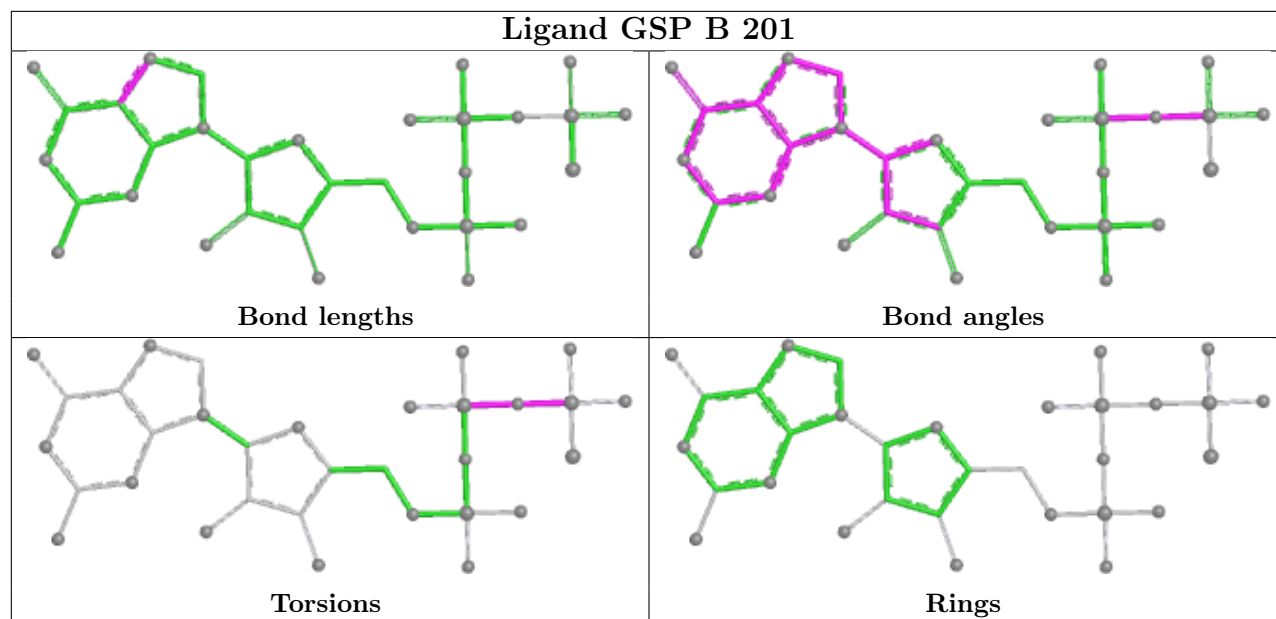
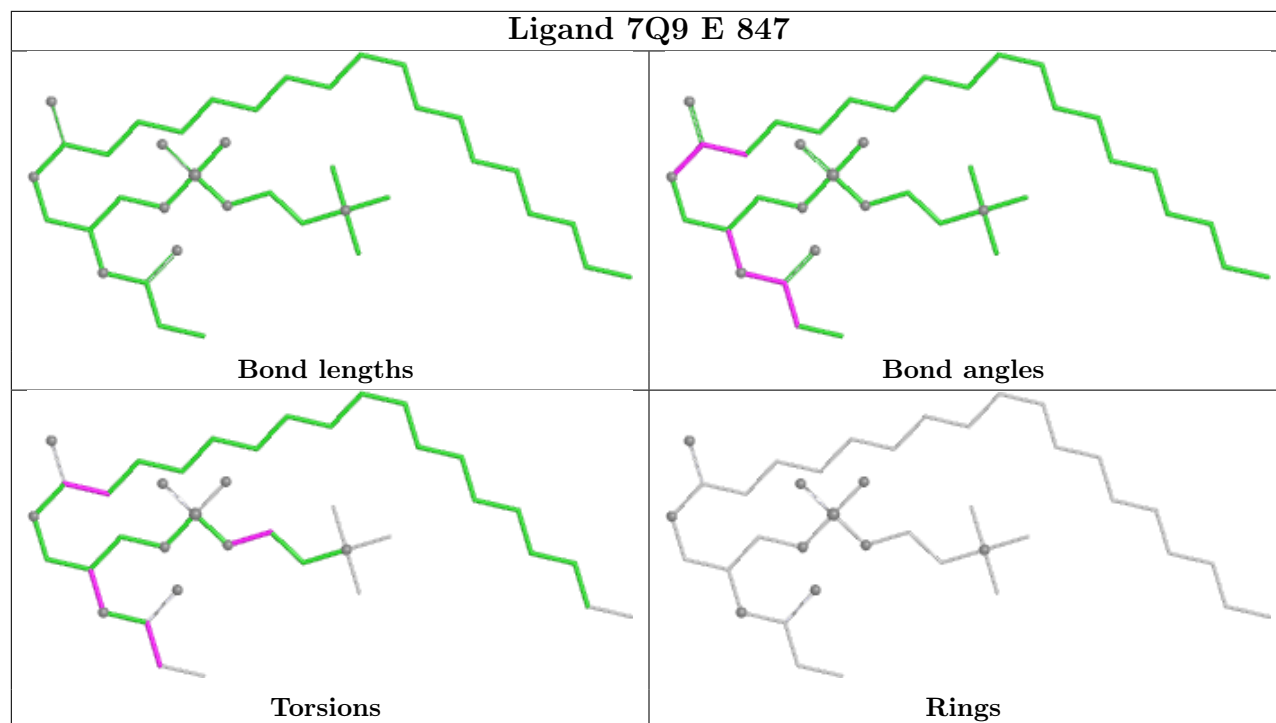


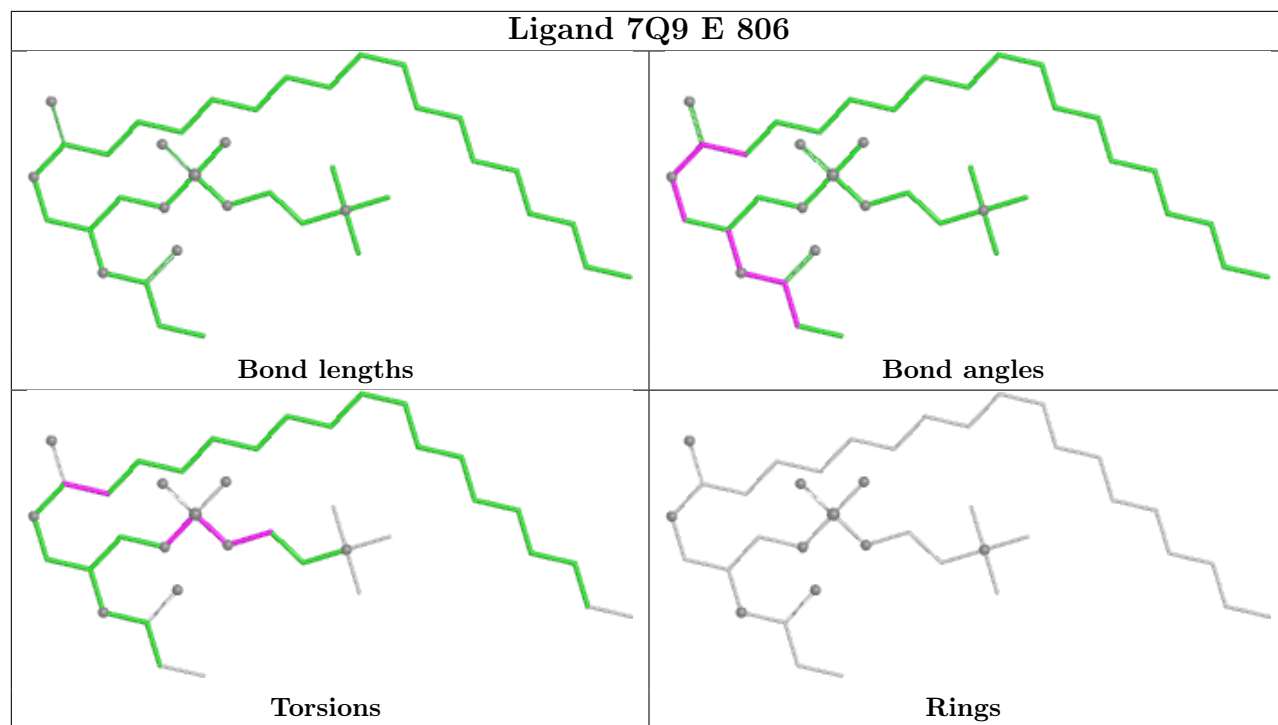
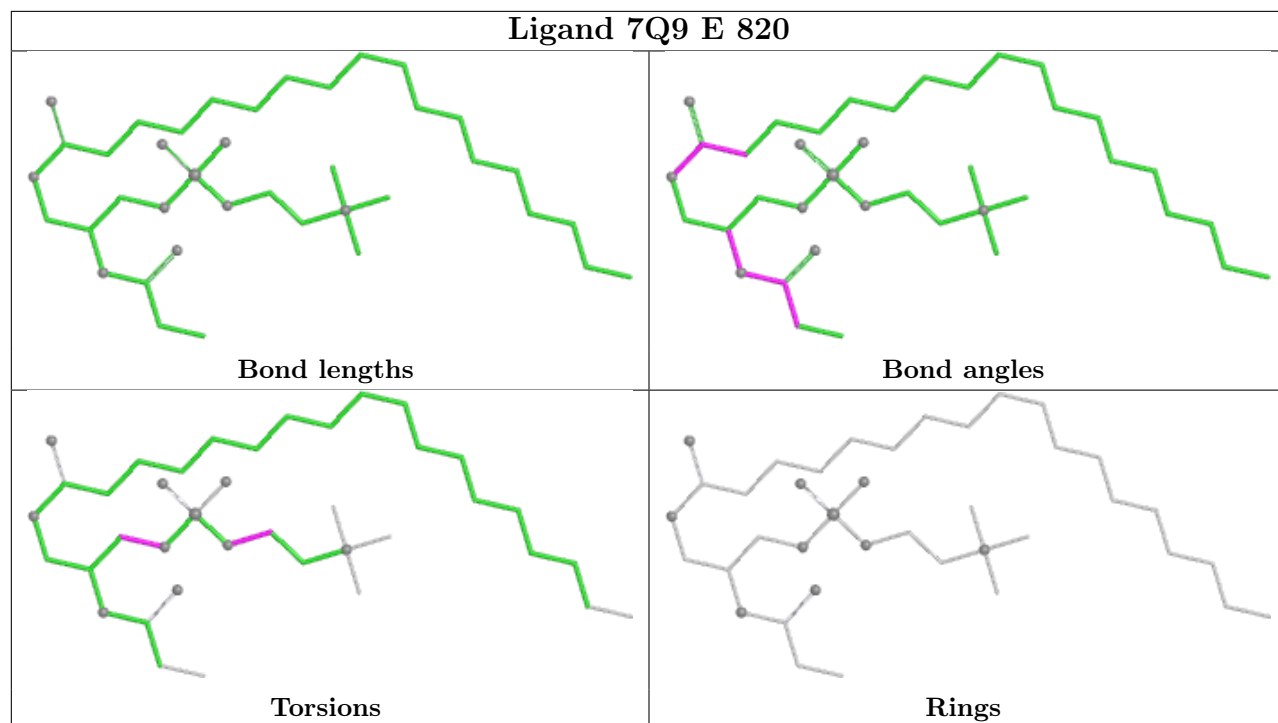


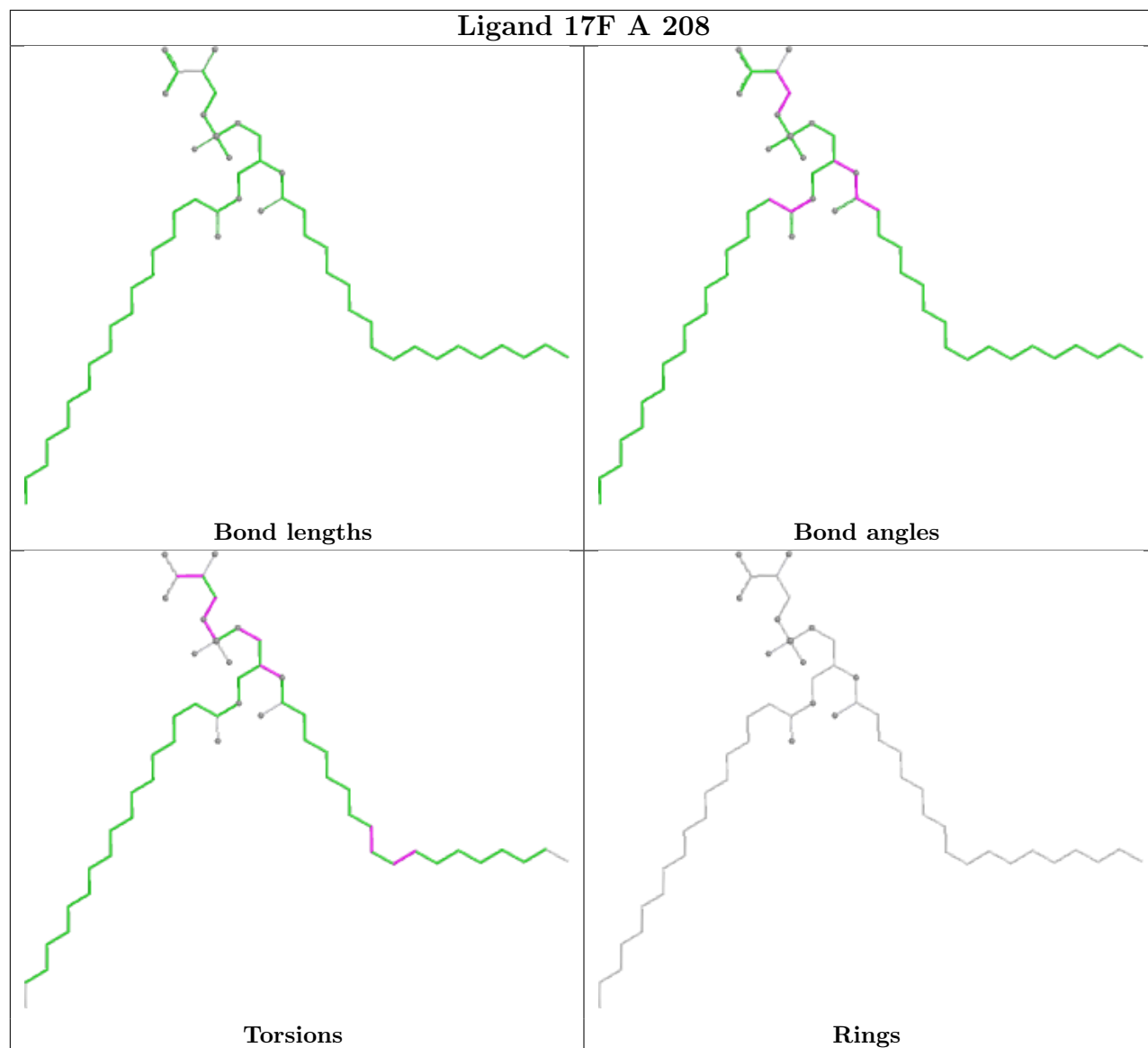


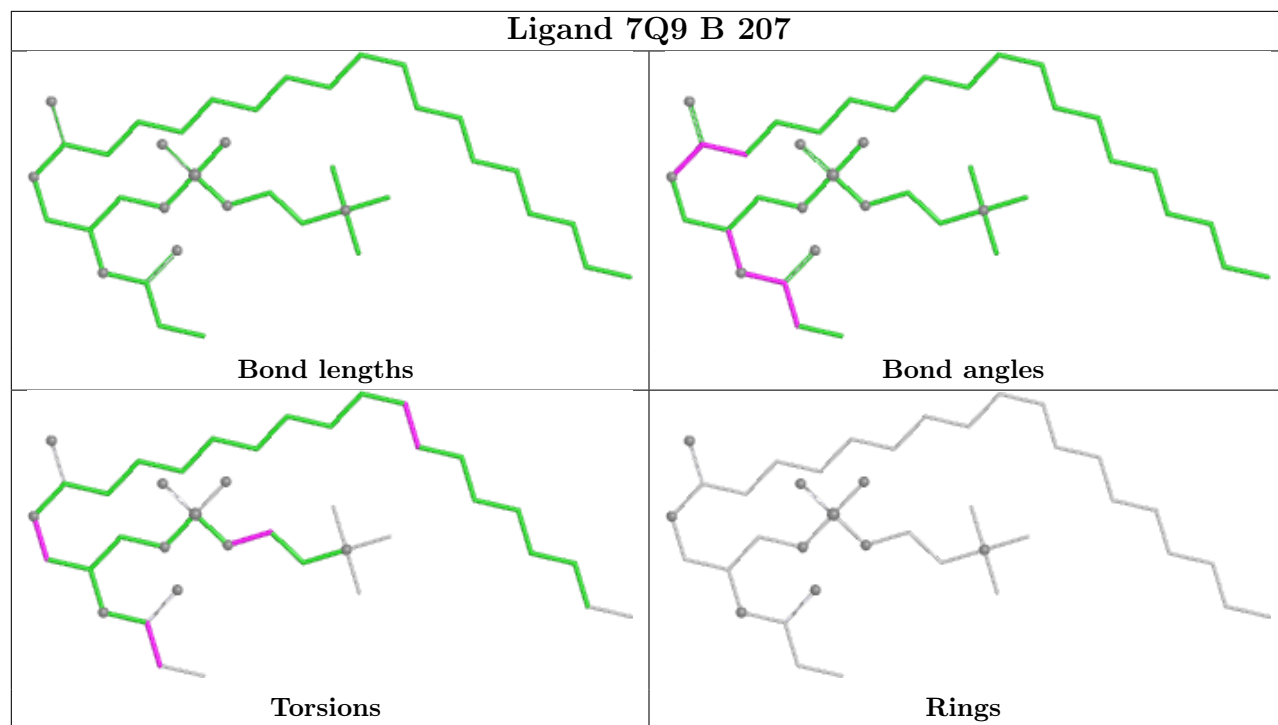
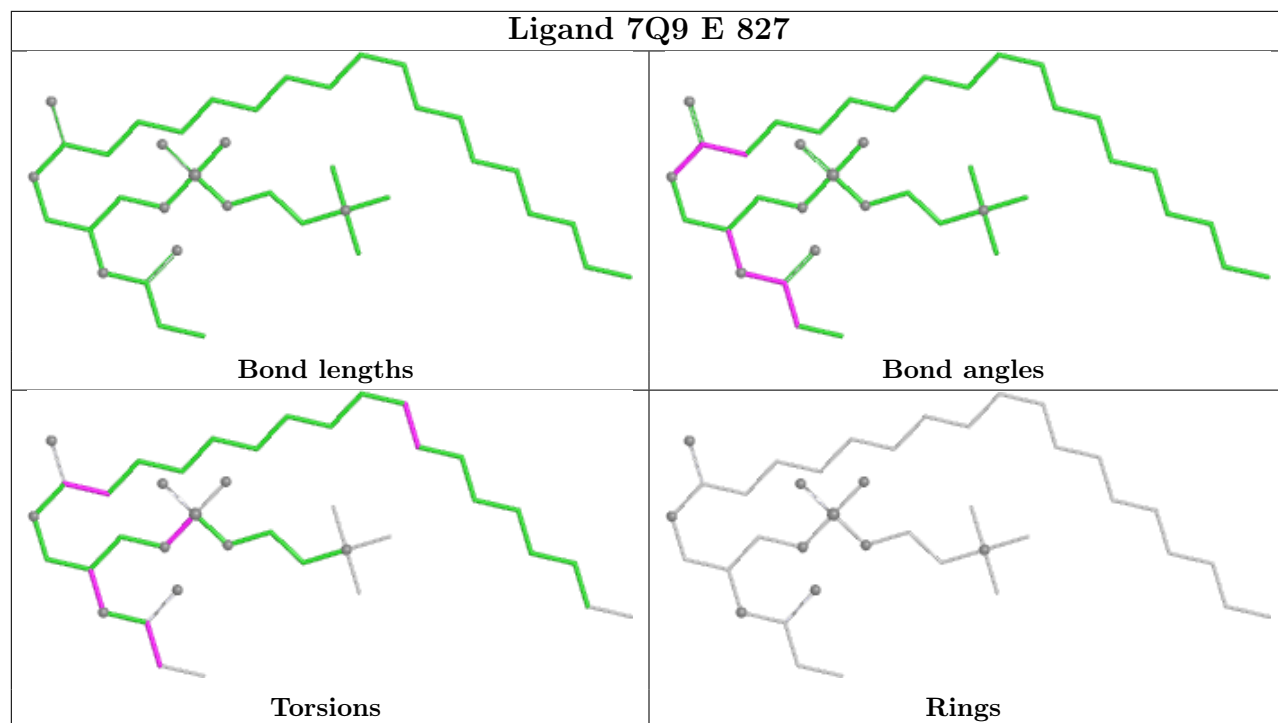


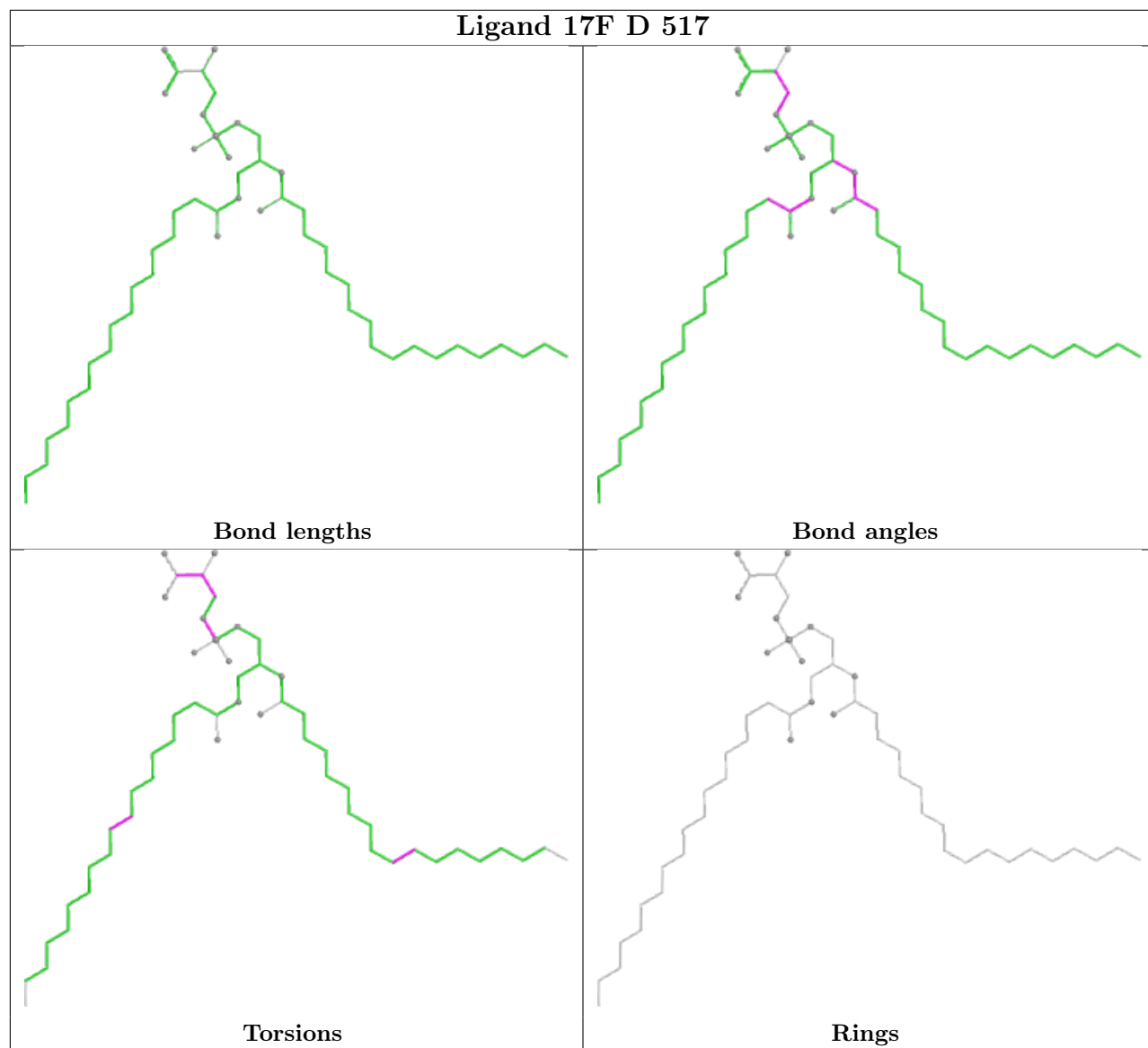


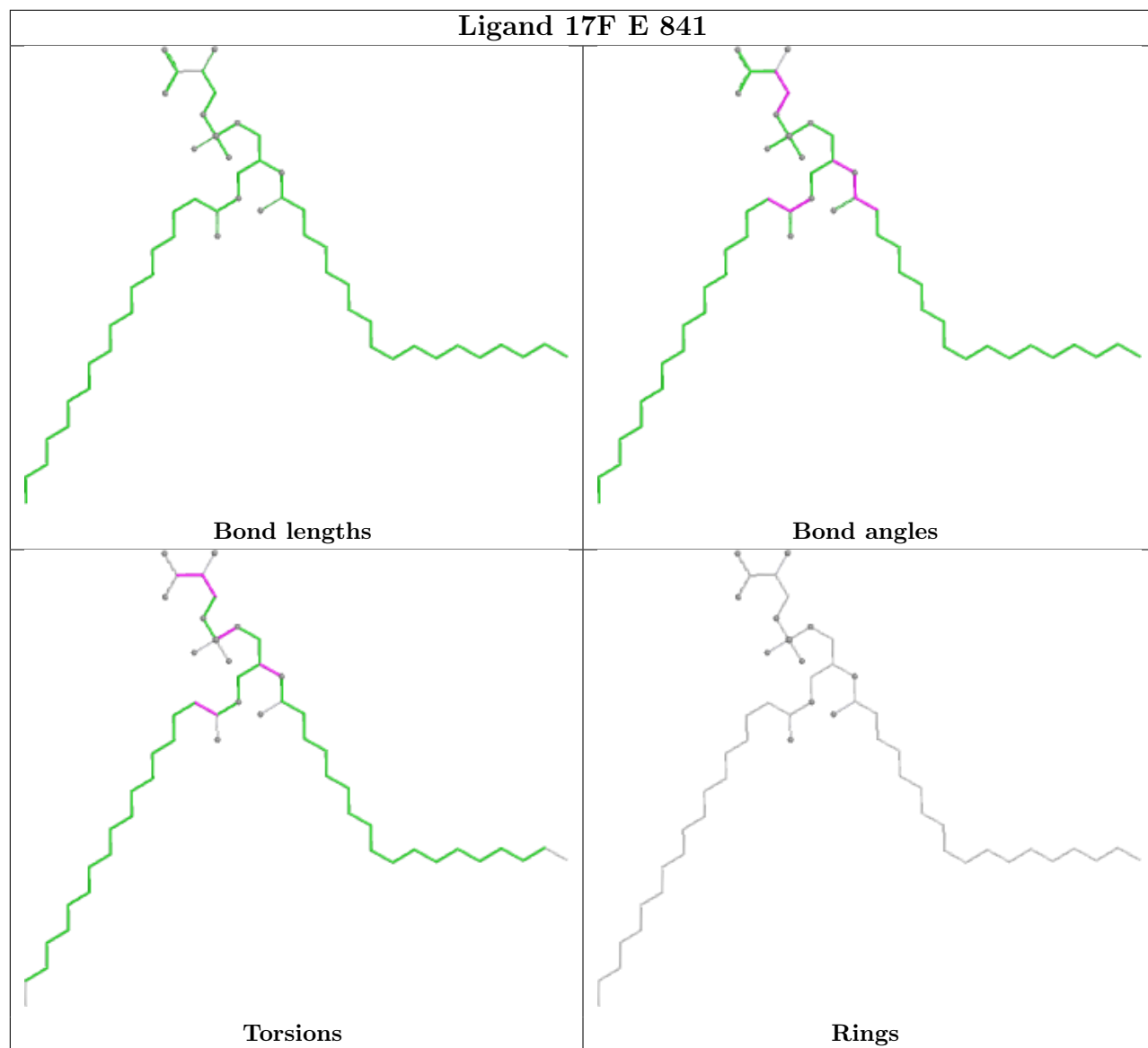


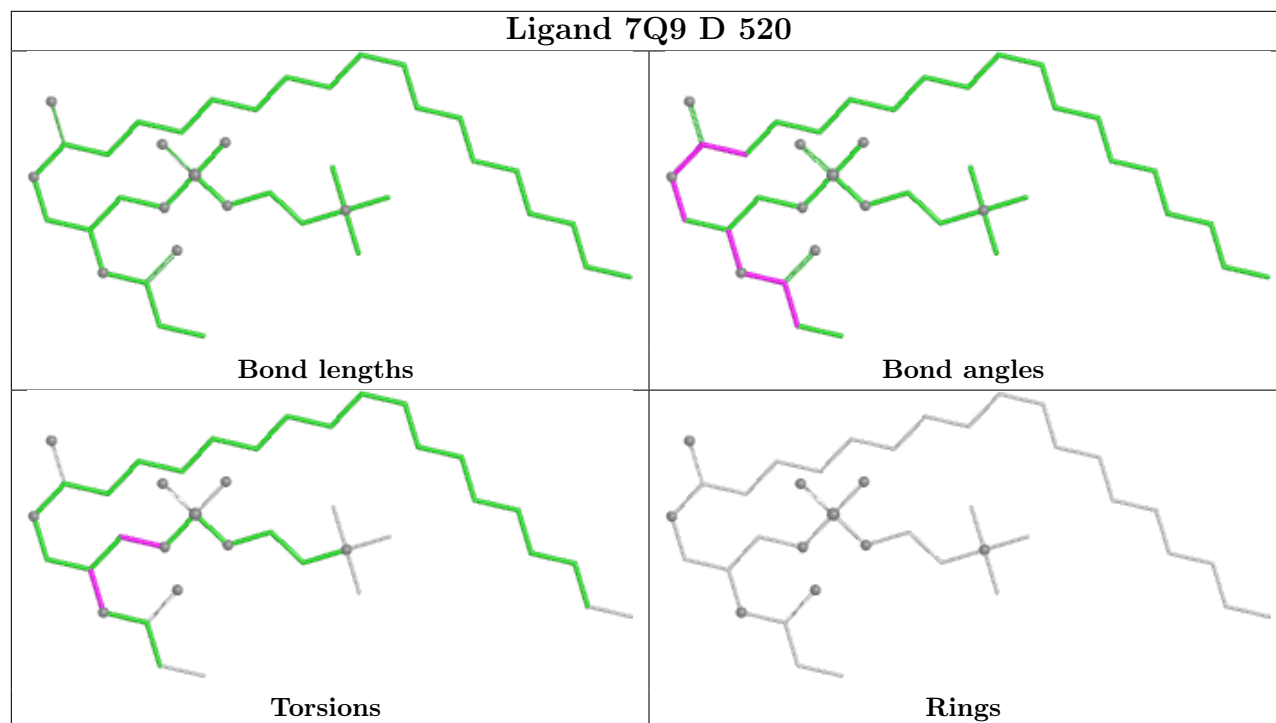


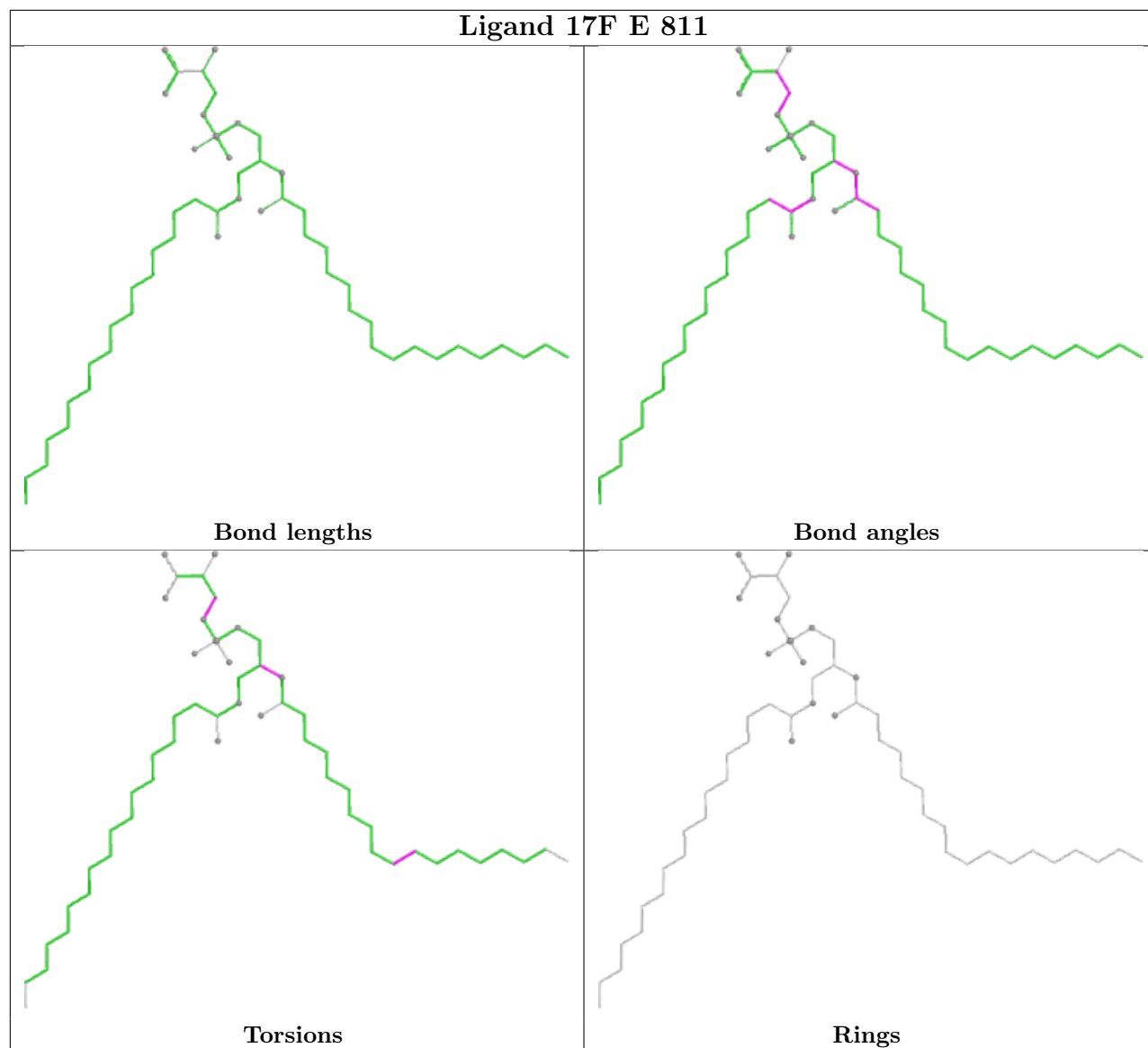


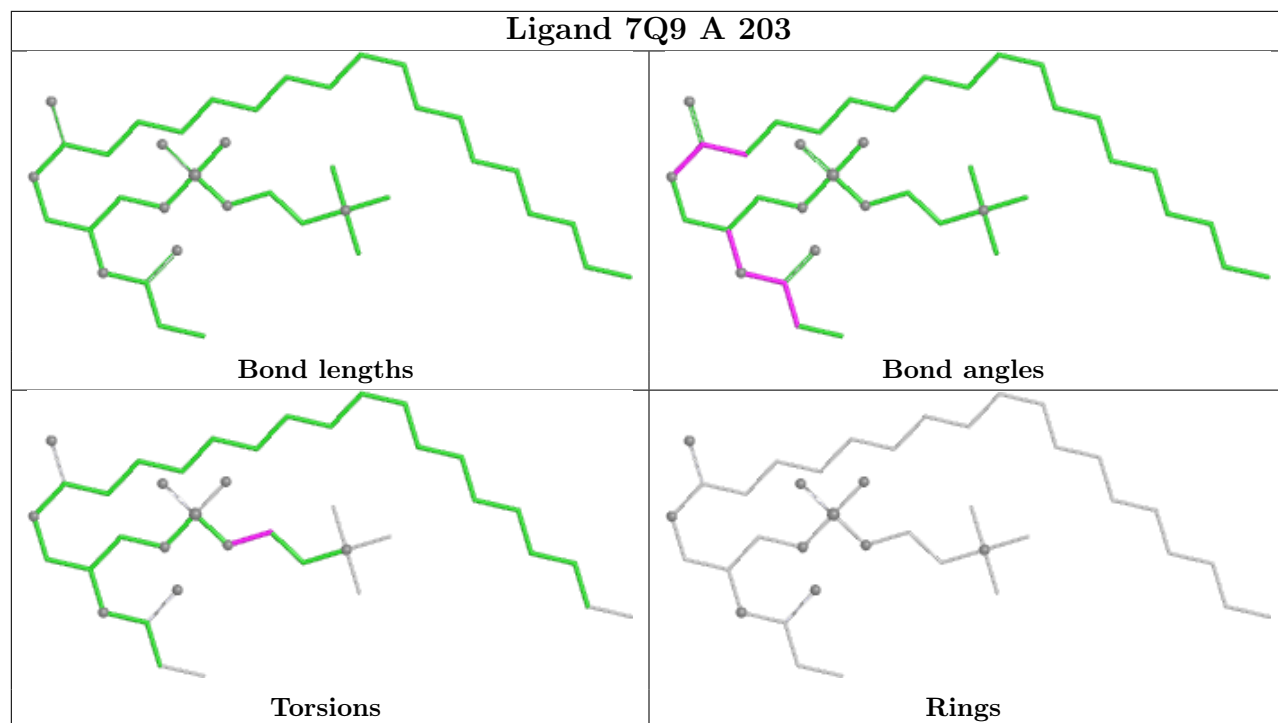


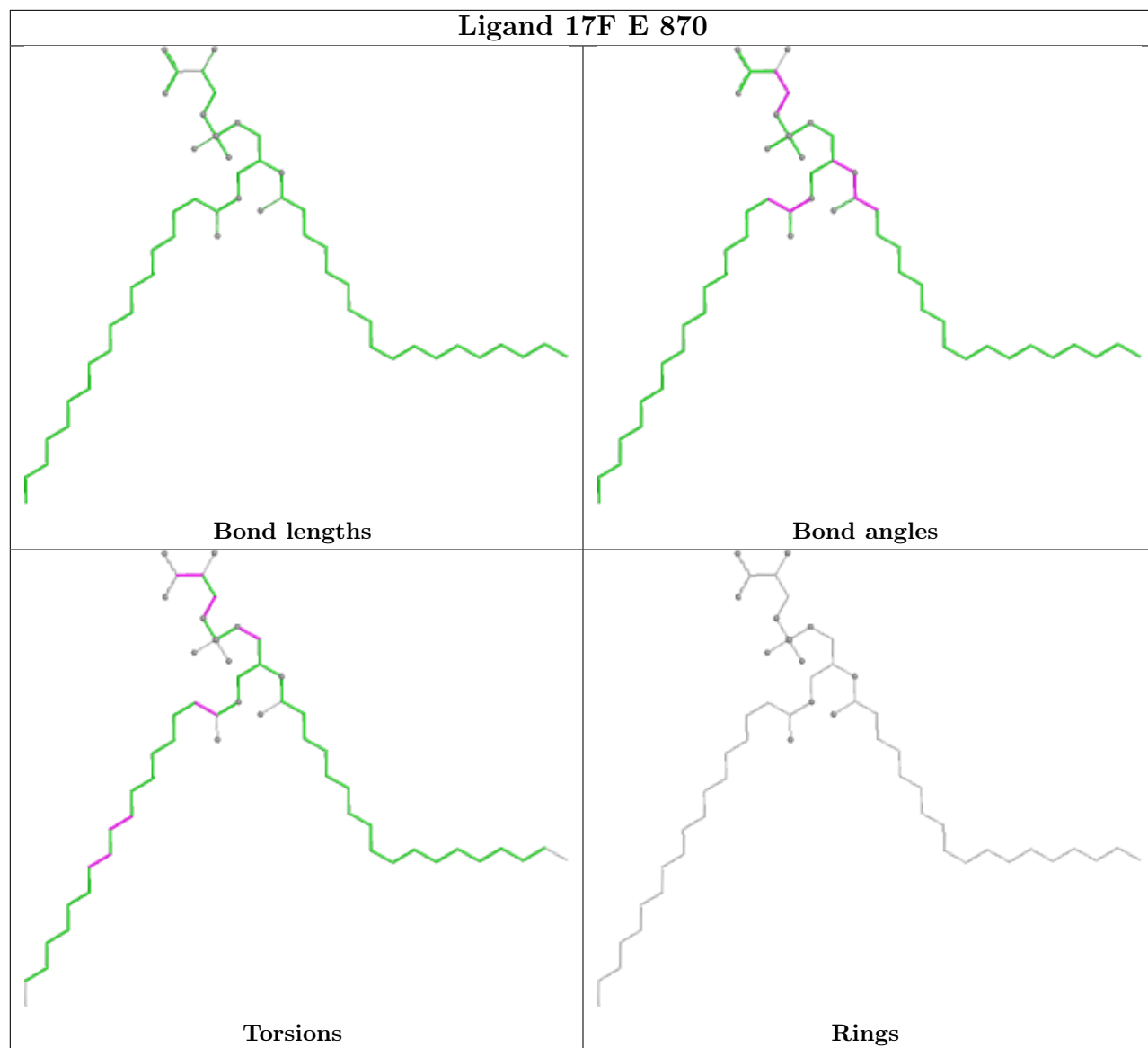


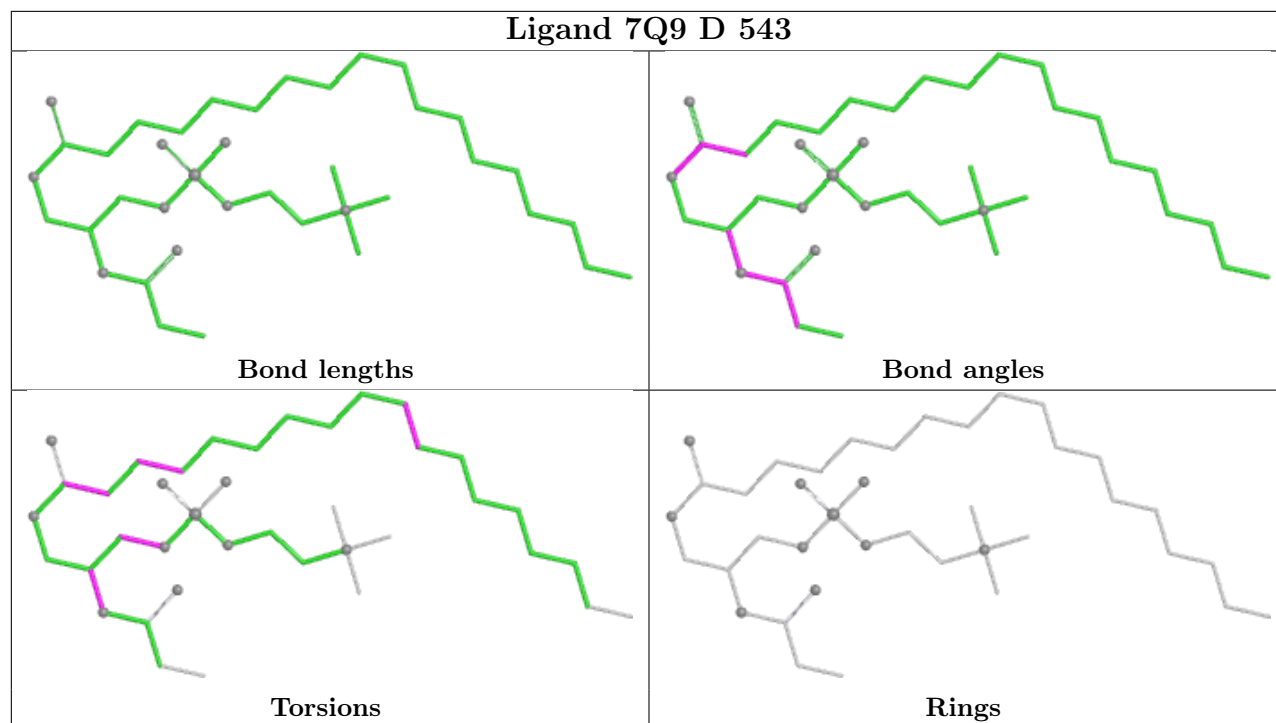




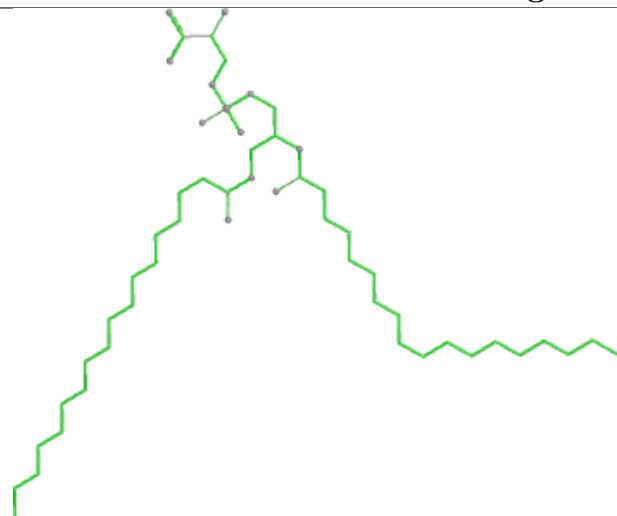




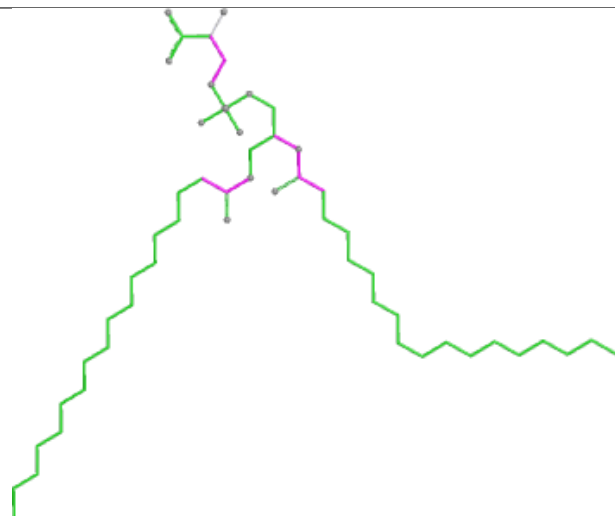




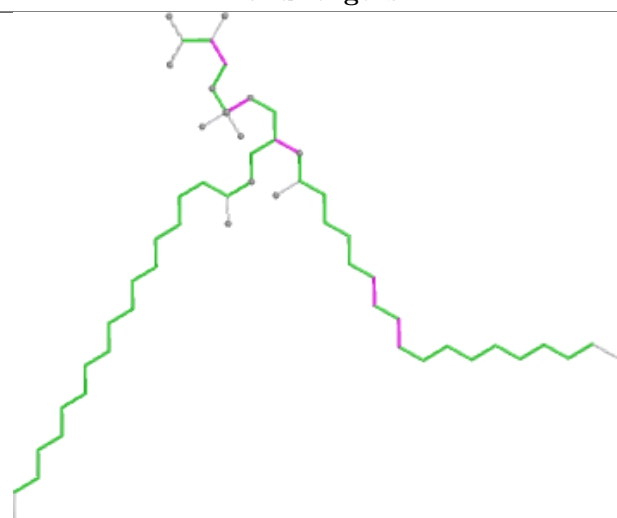
Ligand 17F E 801



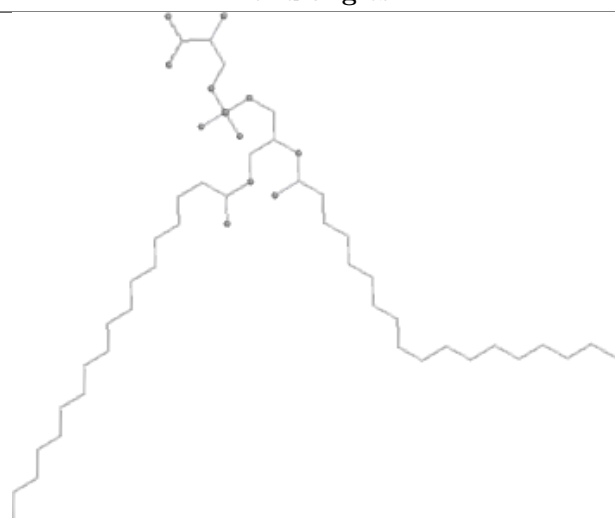
Bond lengths



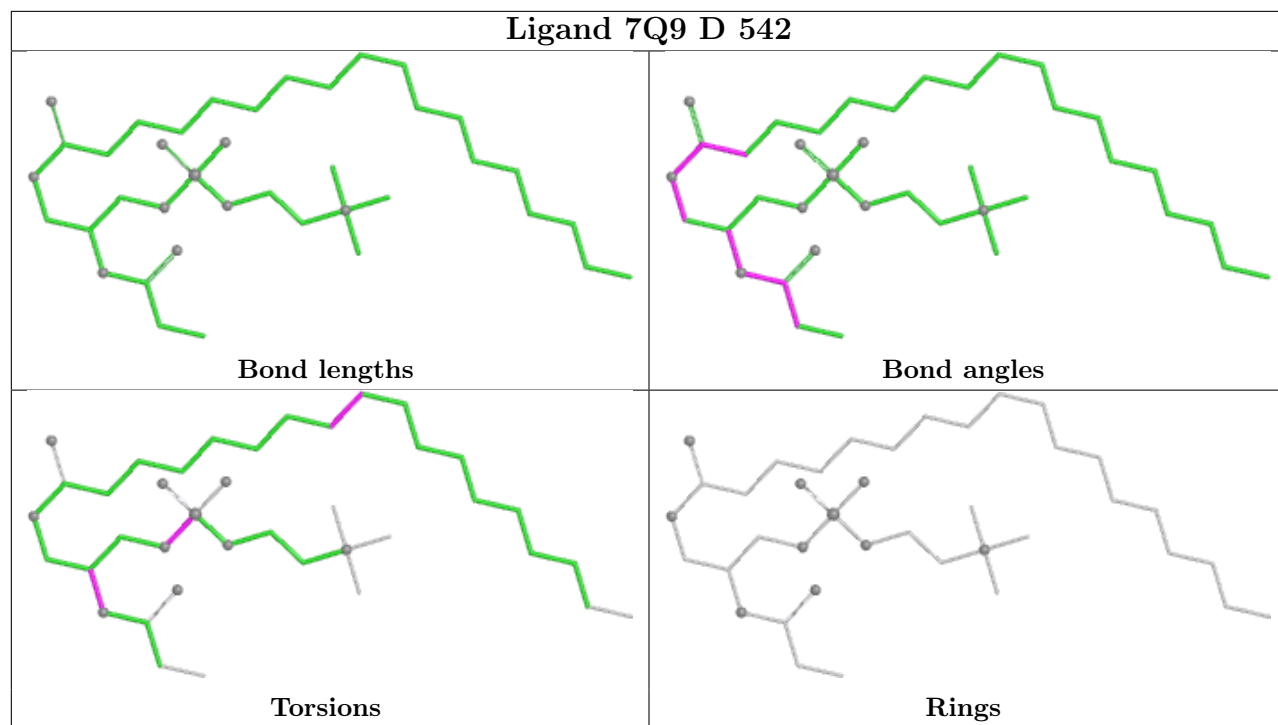
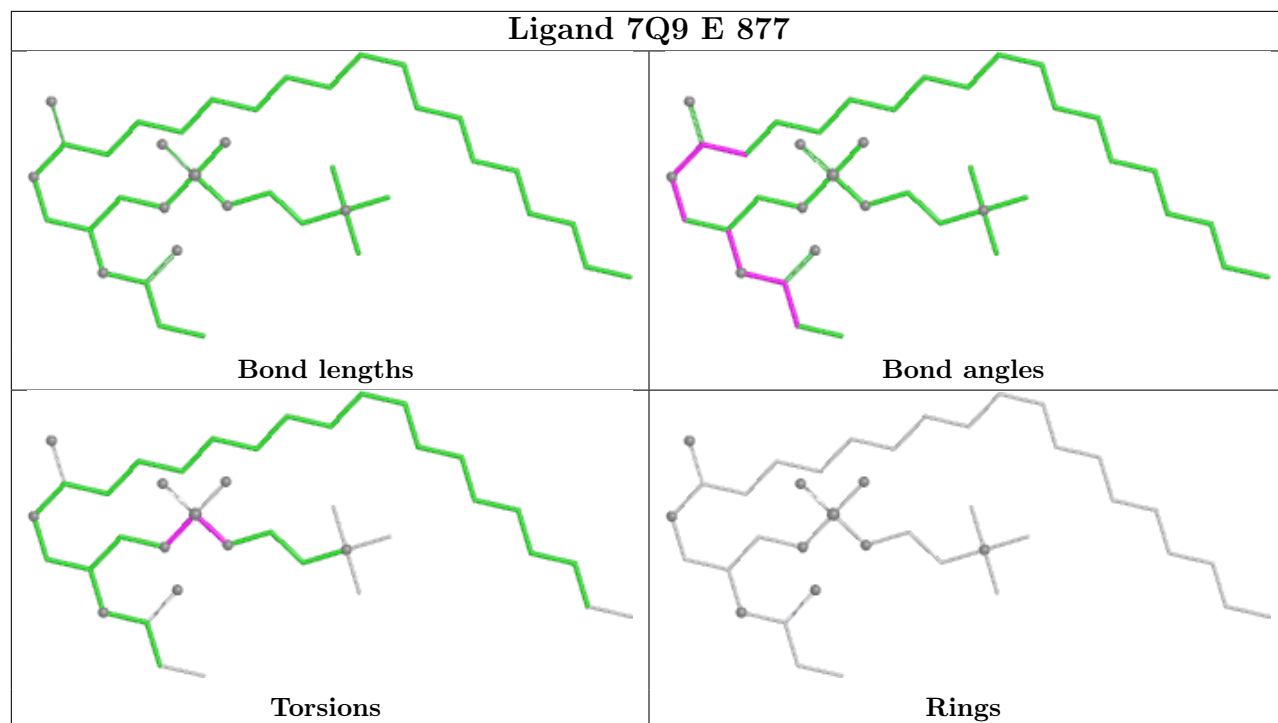
Bond angles



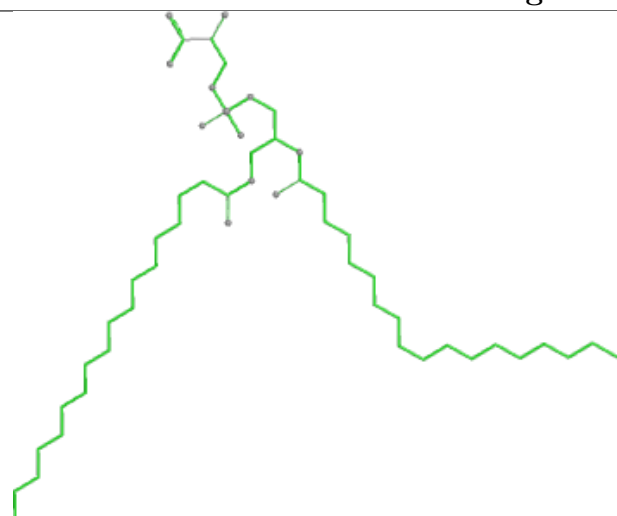
Torsions



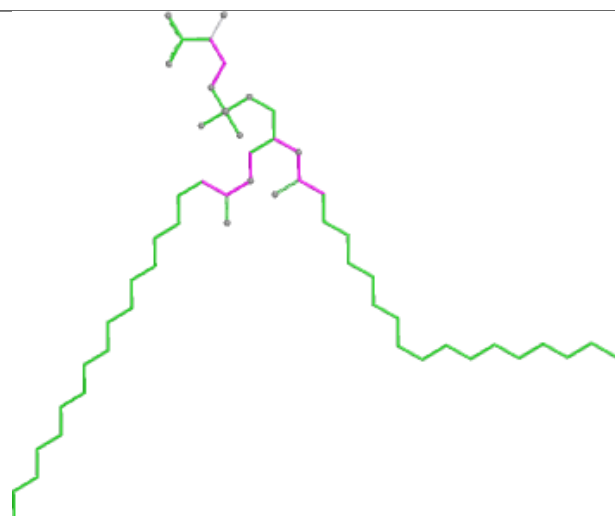
Rings



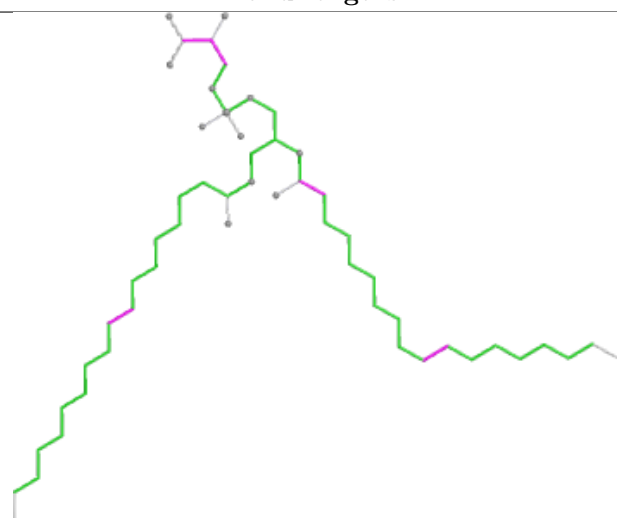
Ligand 17F D 534



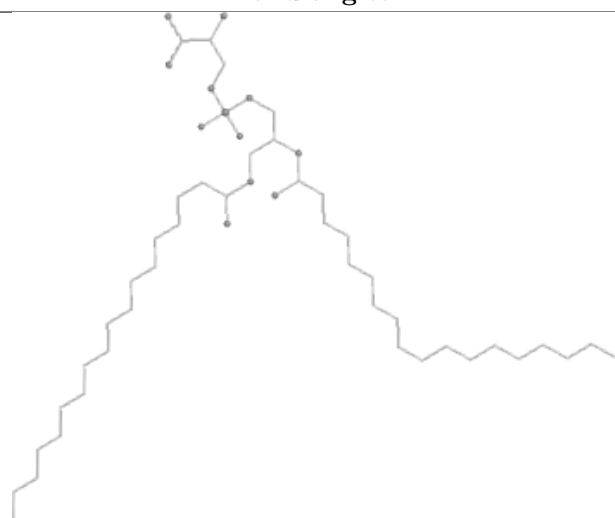
Bond lengths



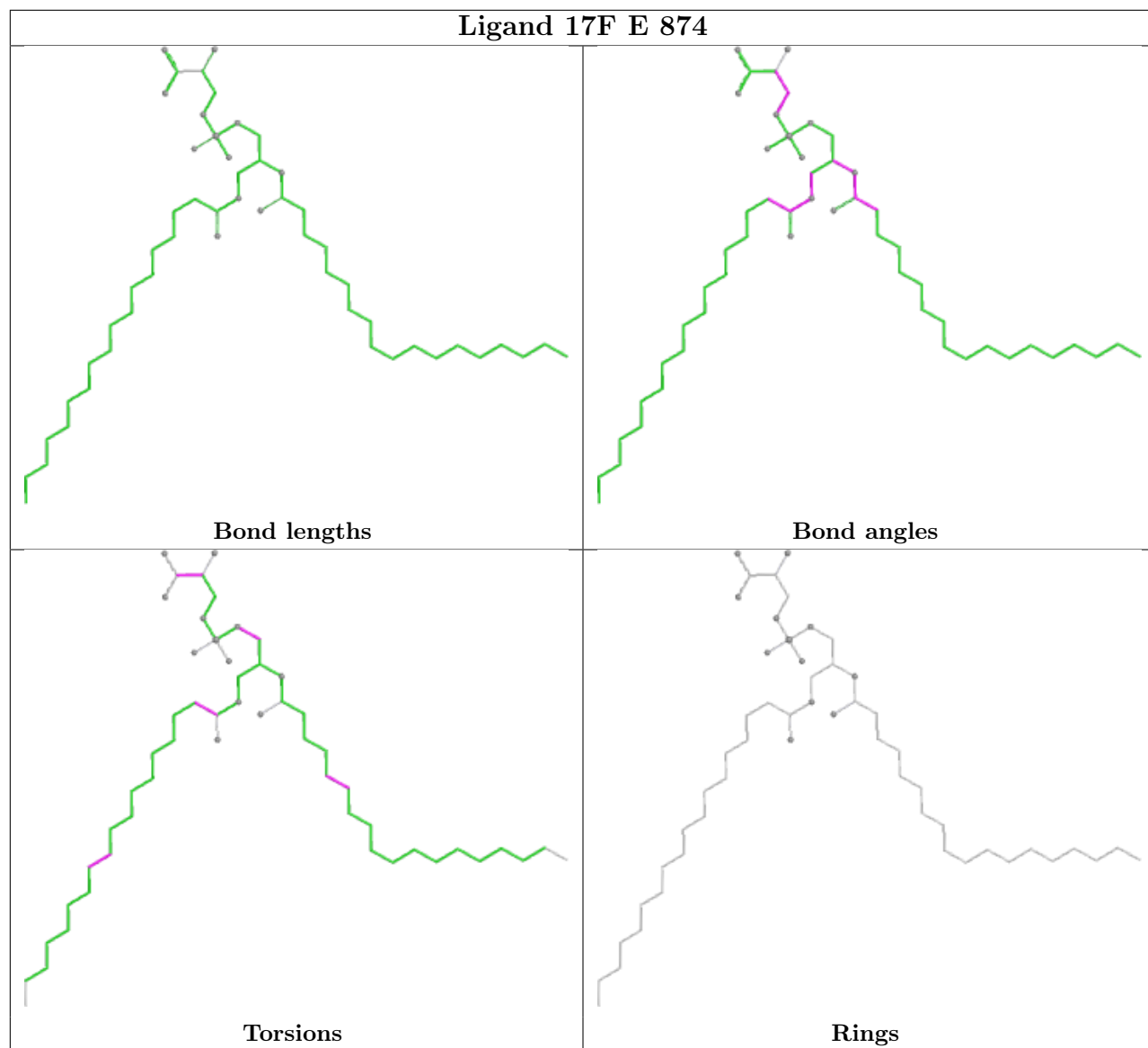
Bond angles

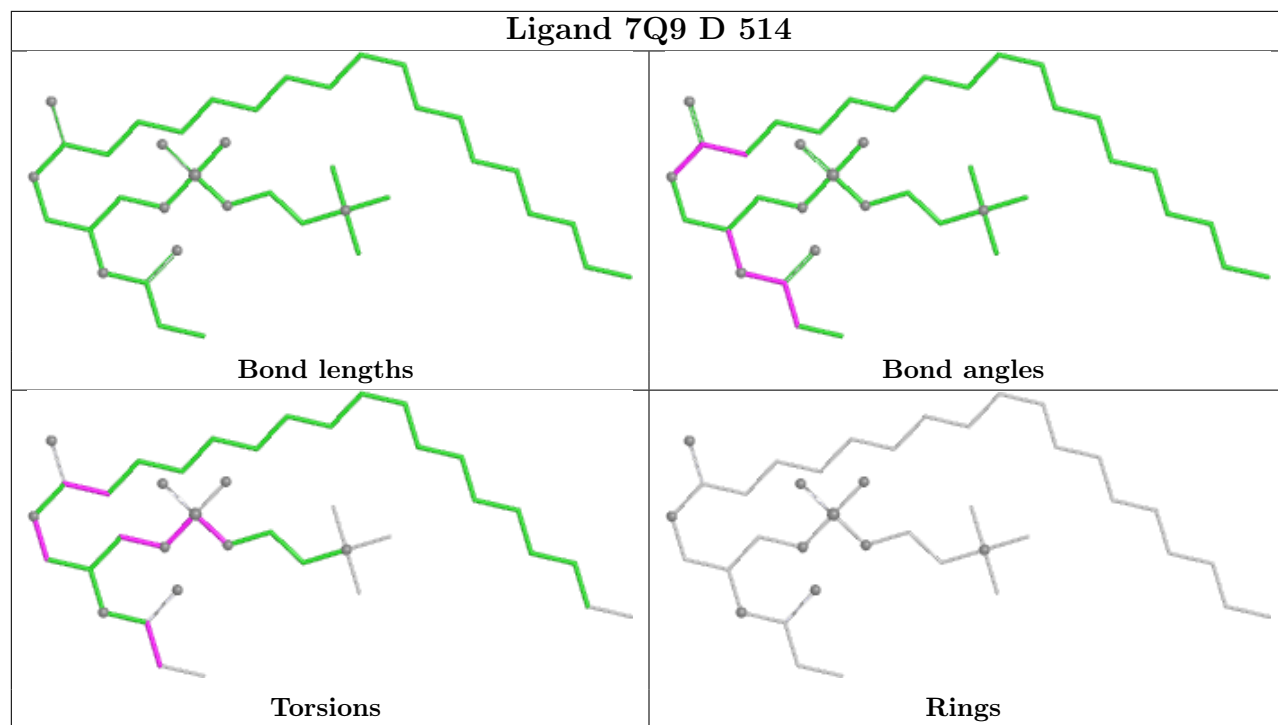
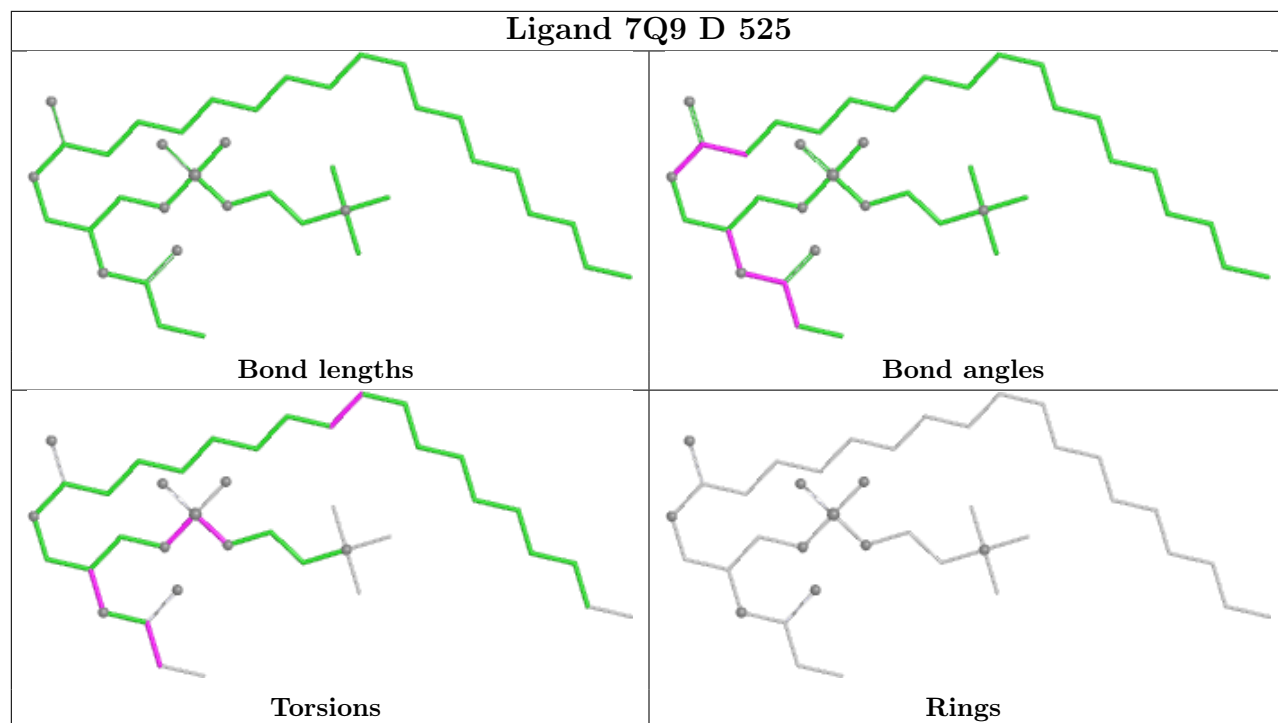


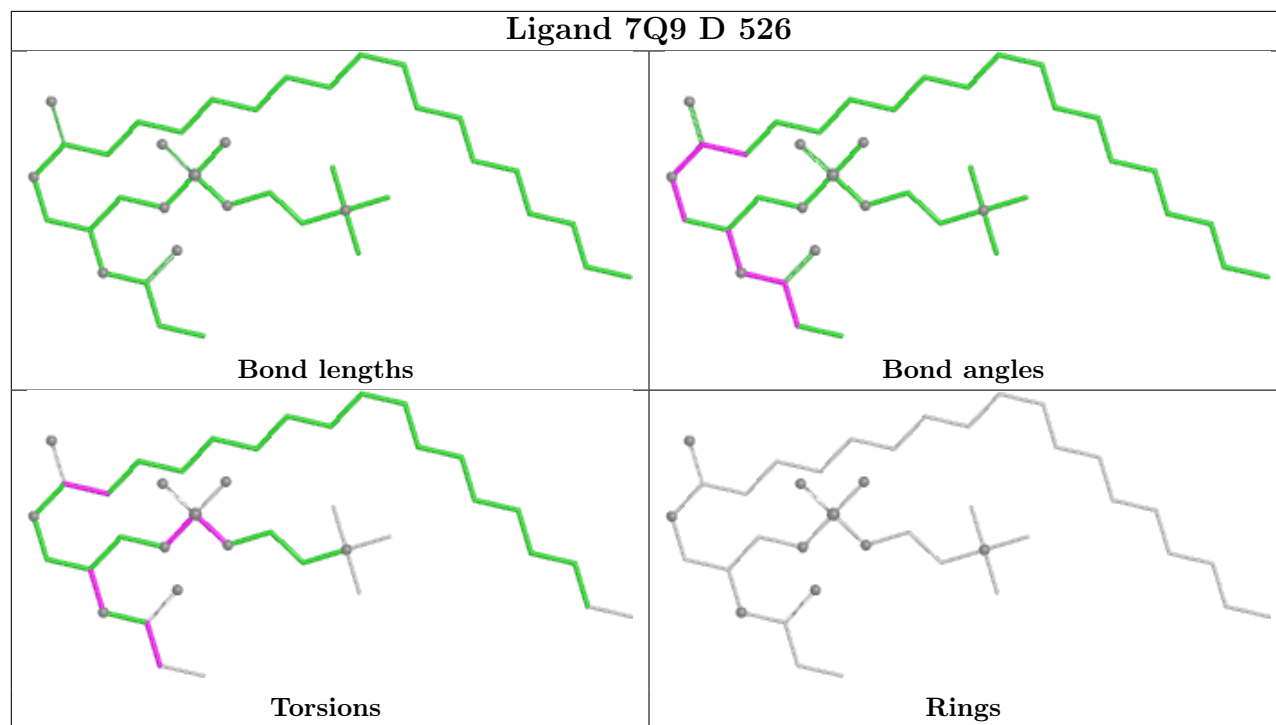
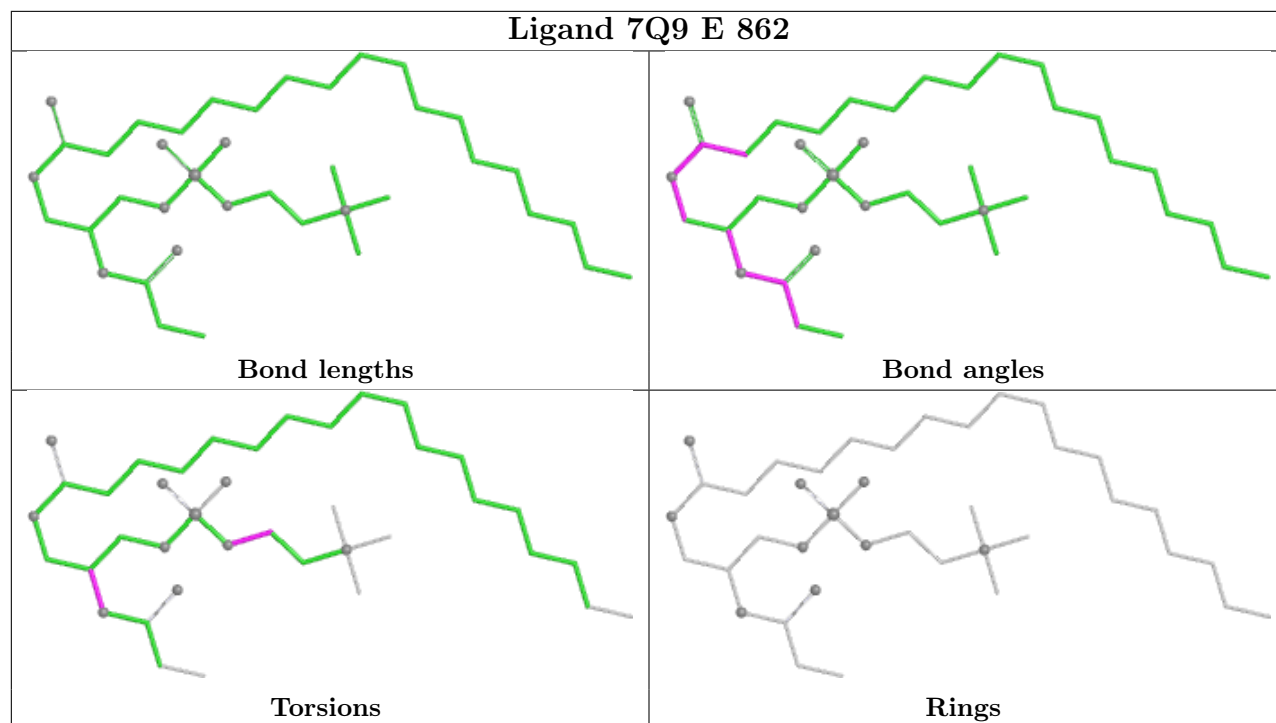
Torsions

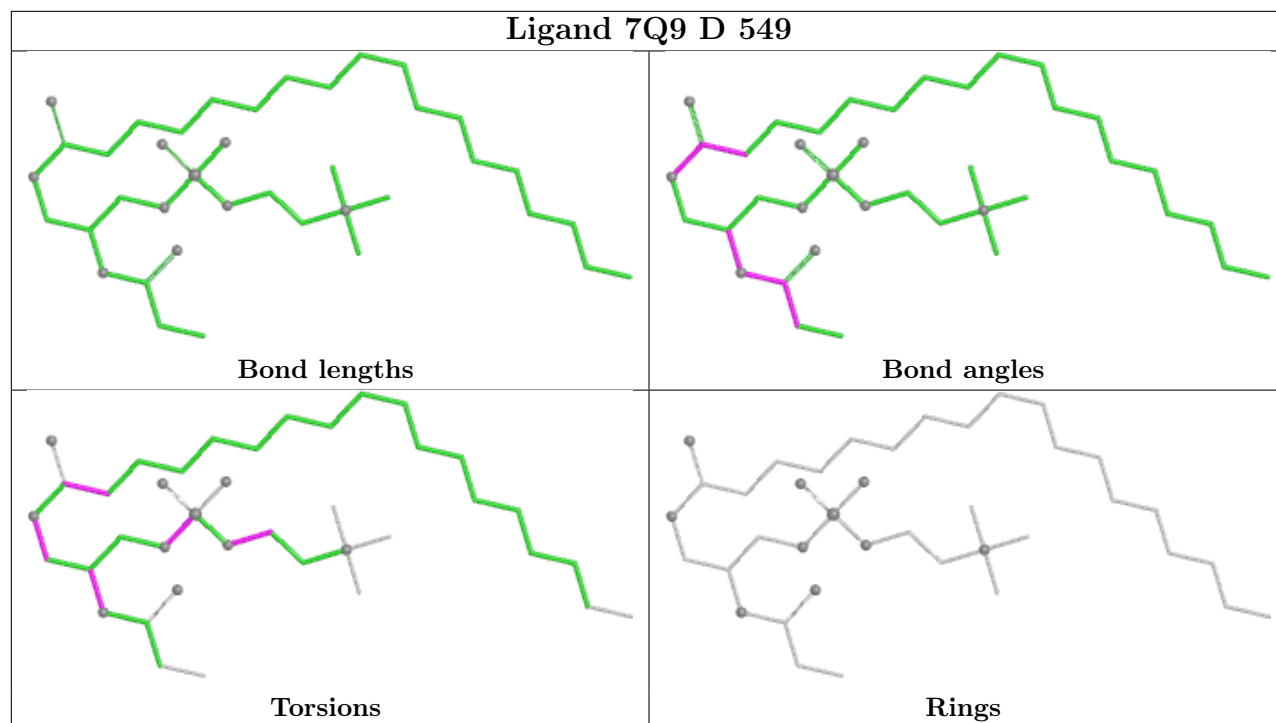


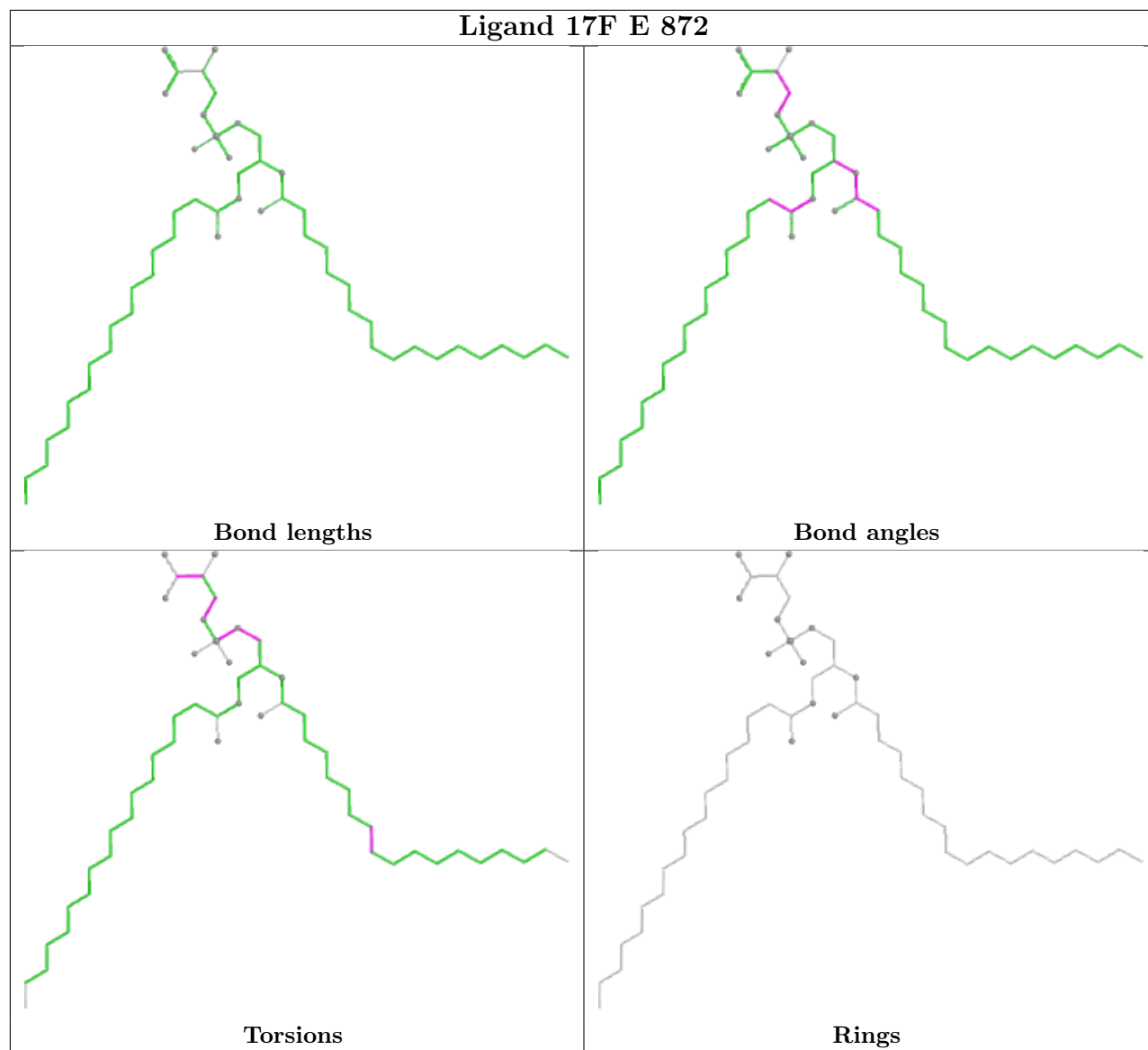
Rings

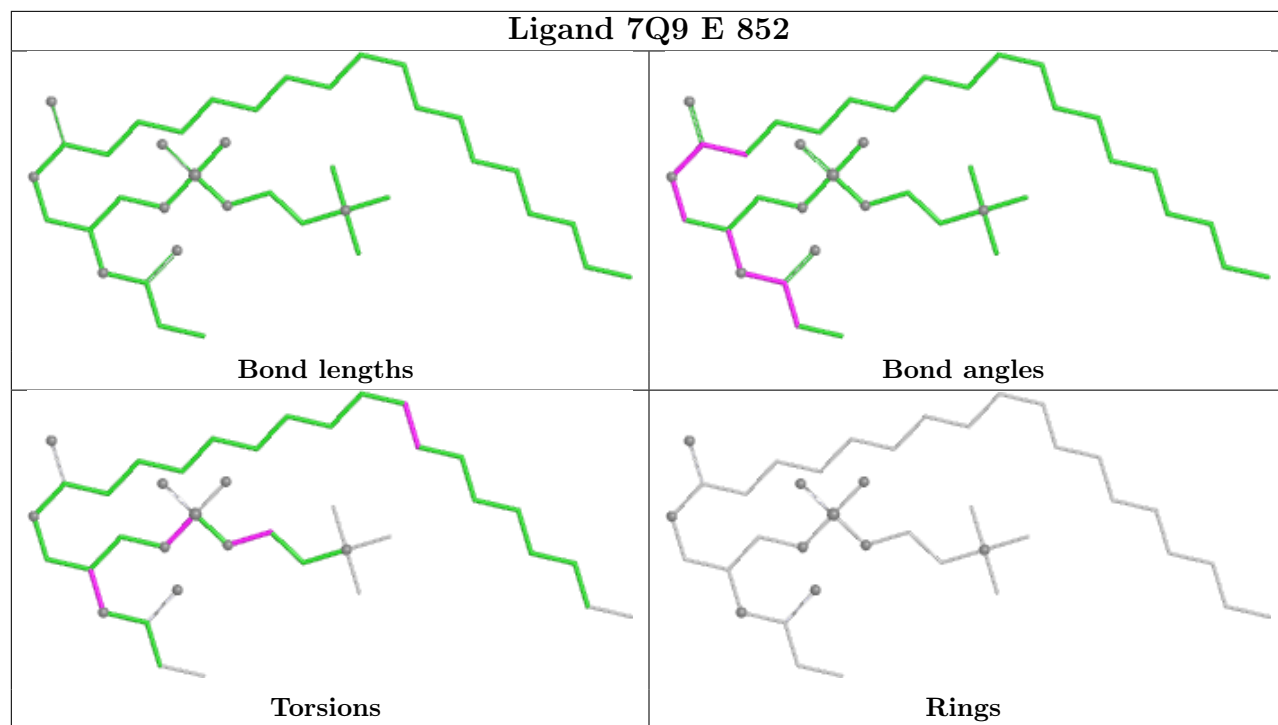
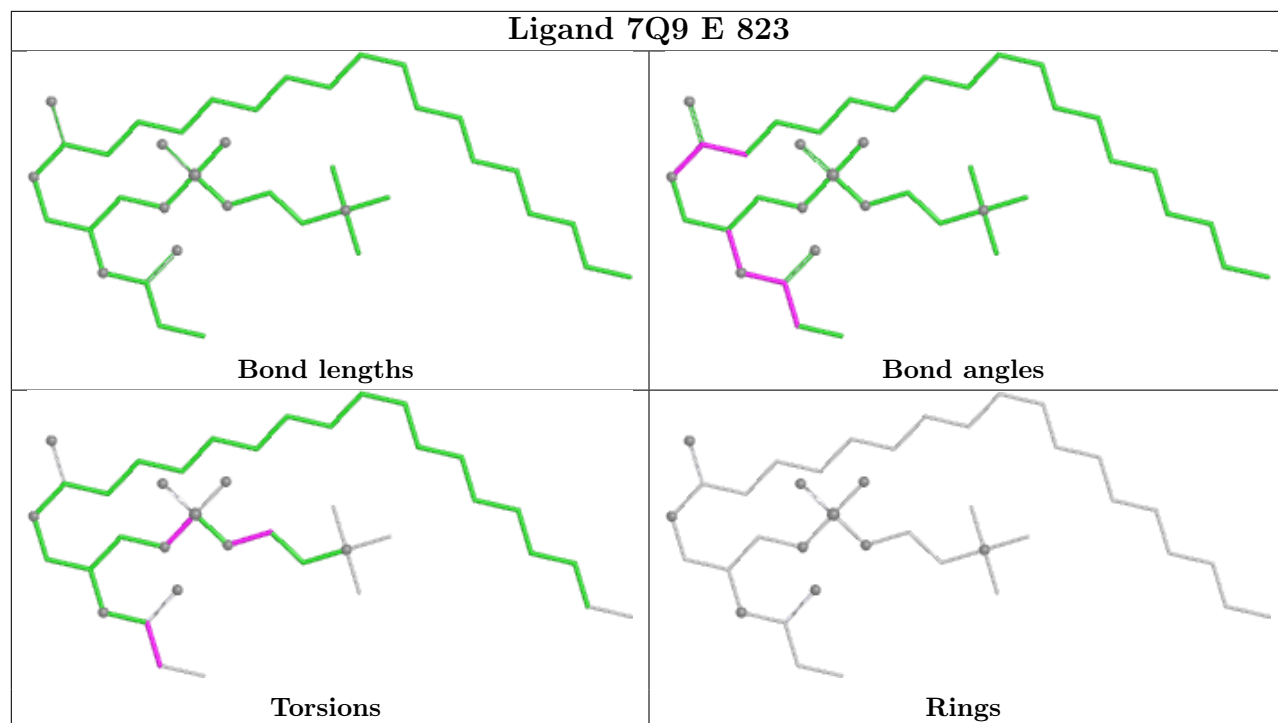


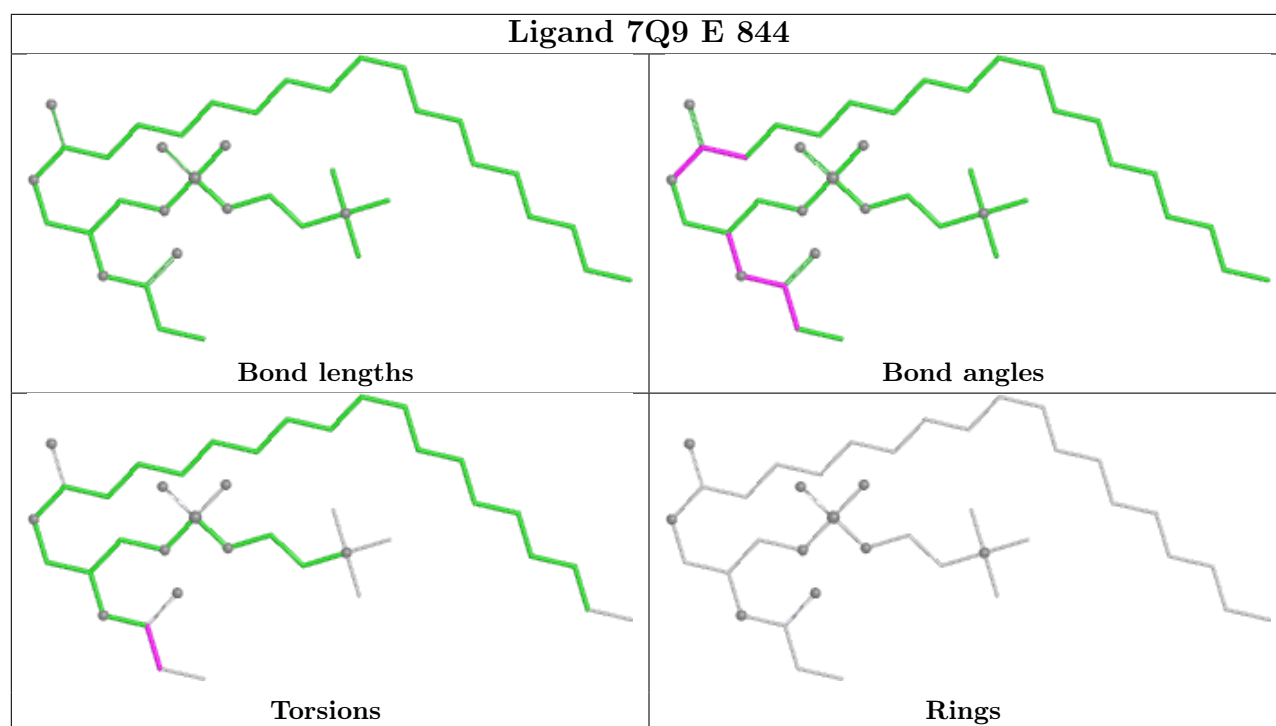




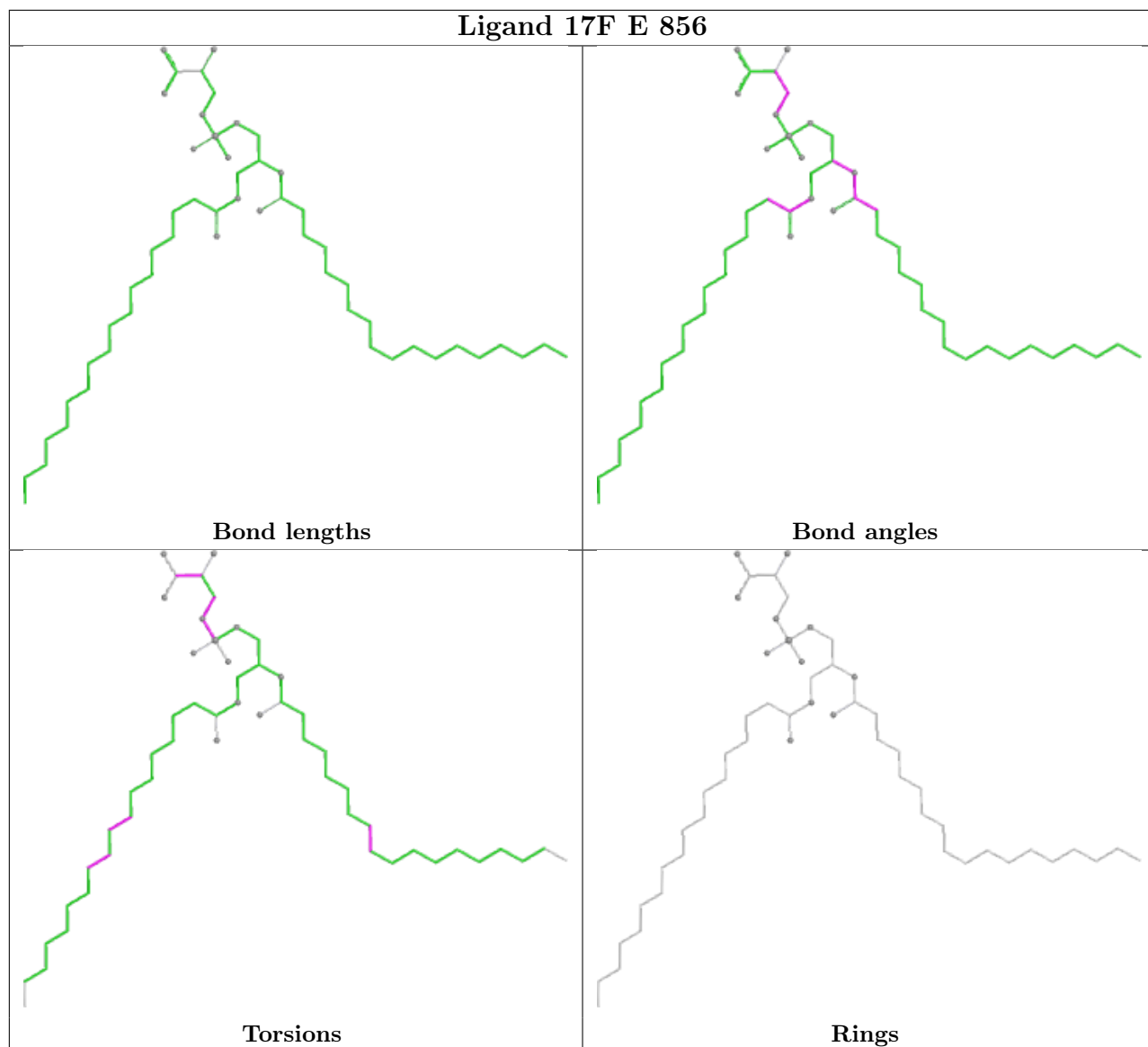


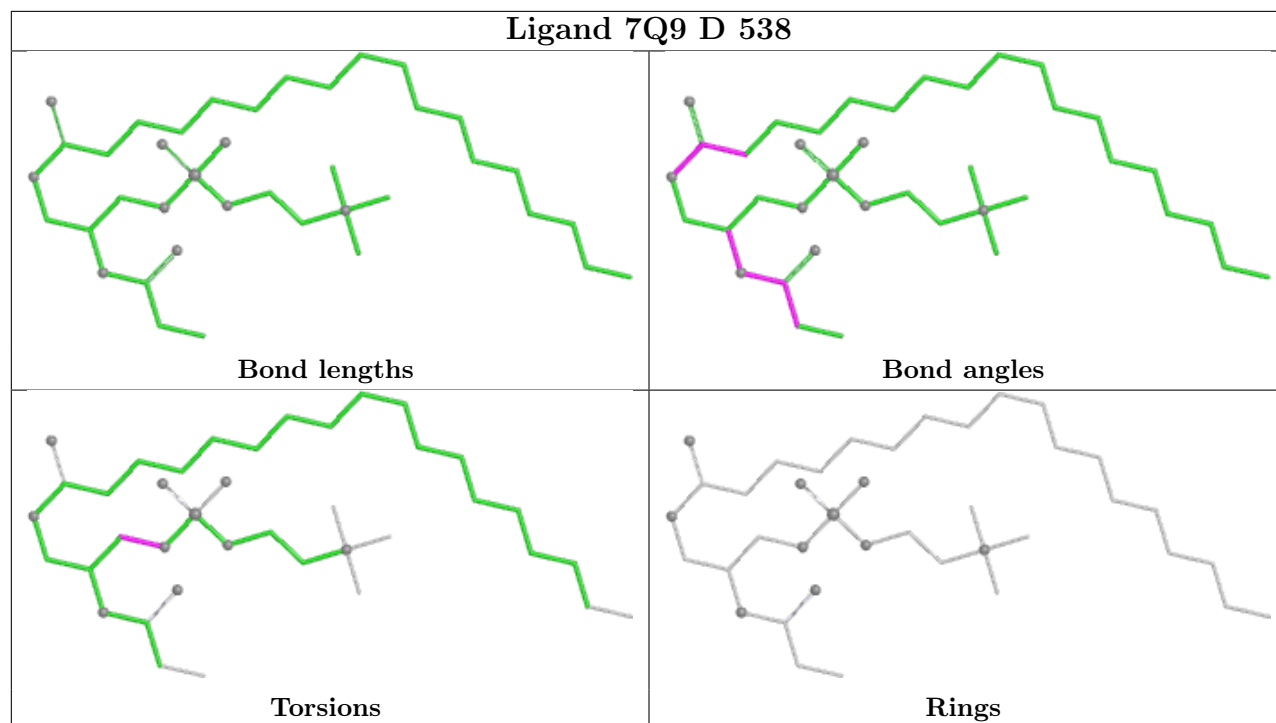


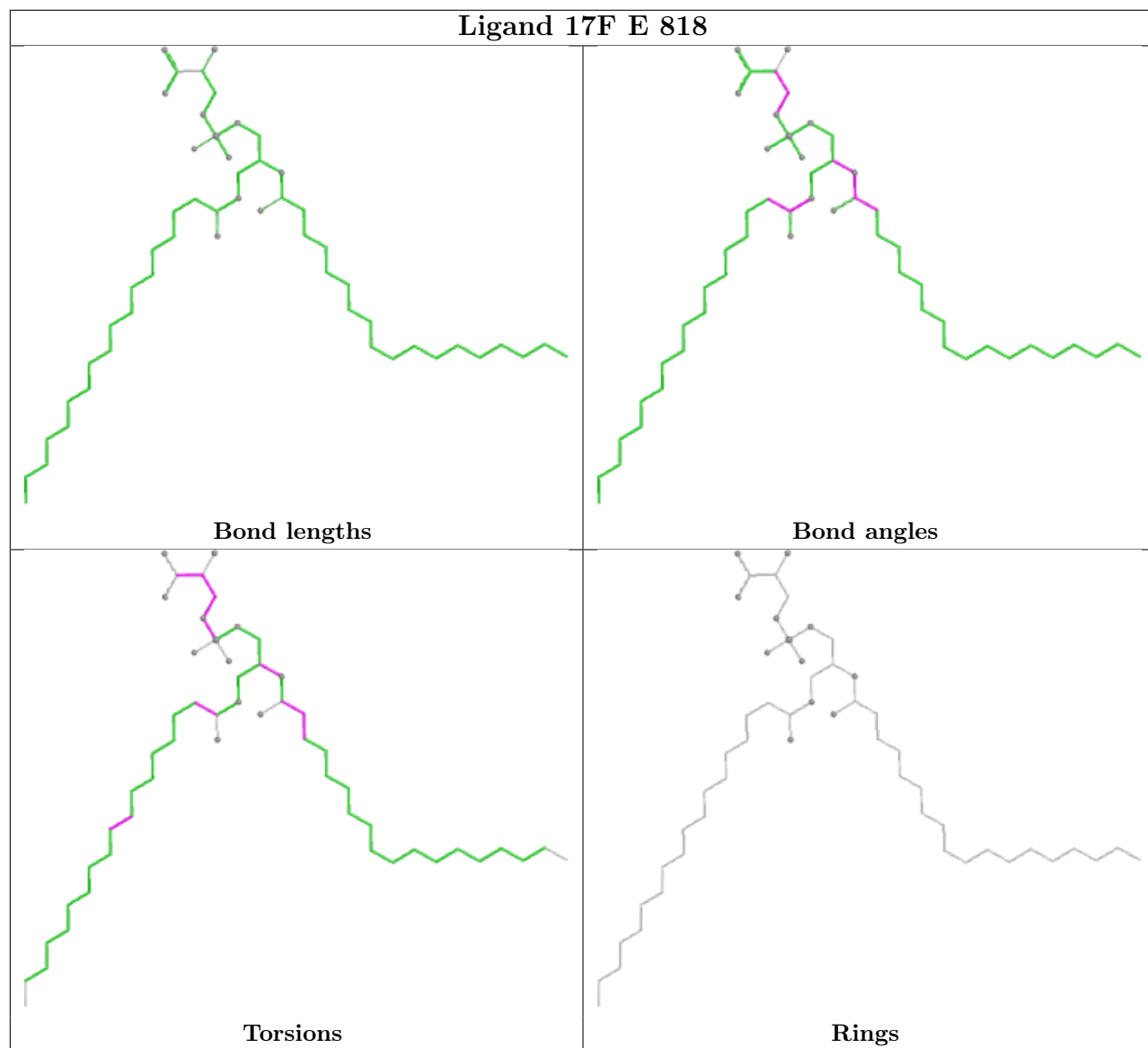


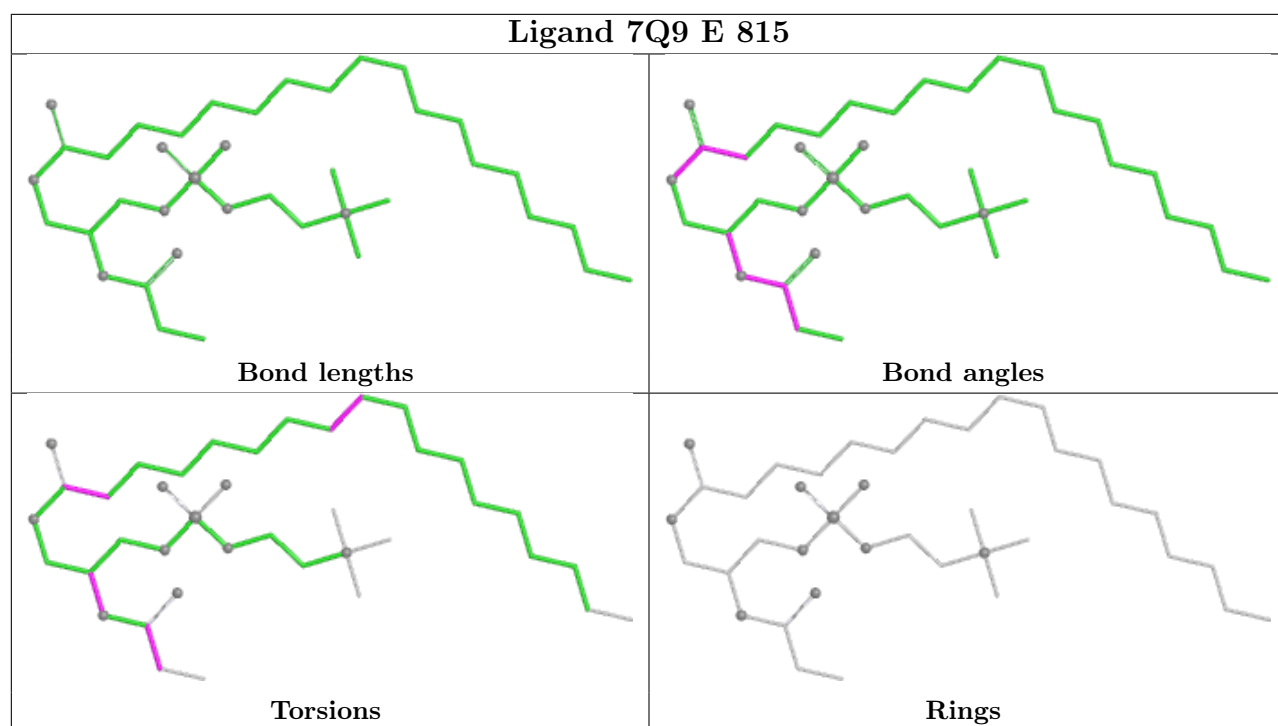


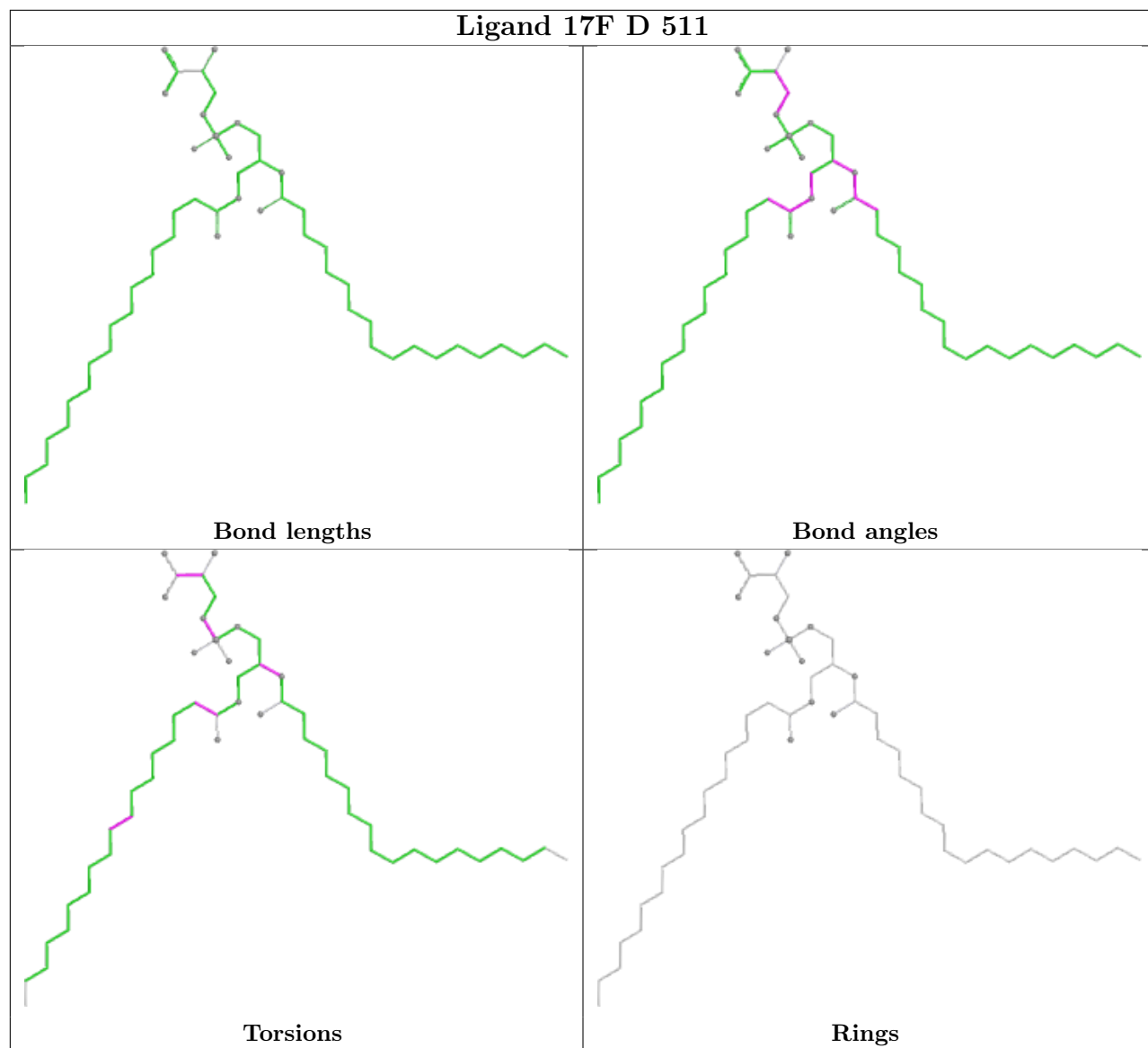
Ligand 17F E 856

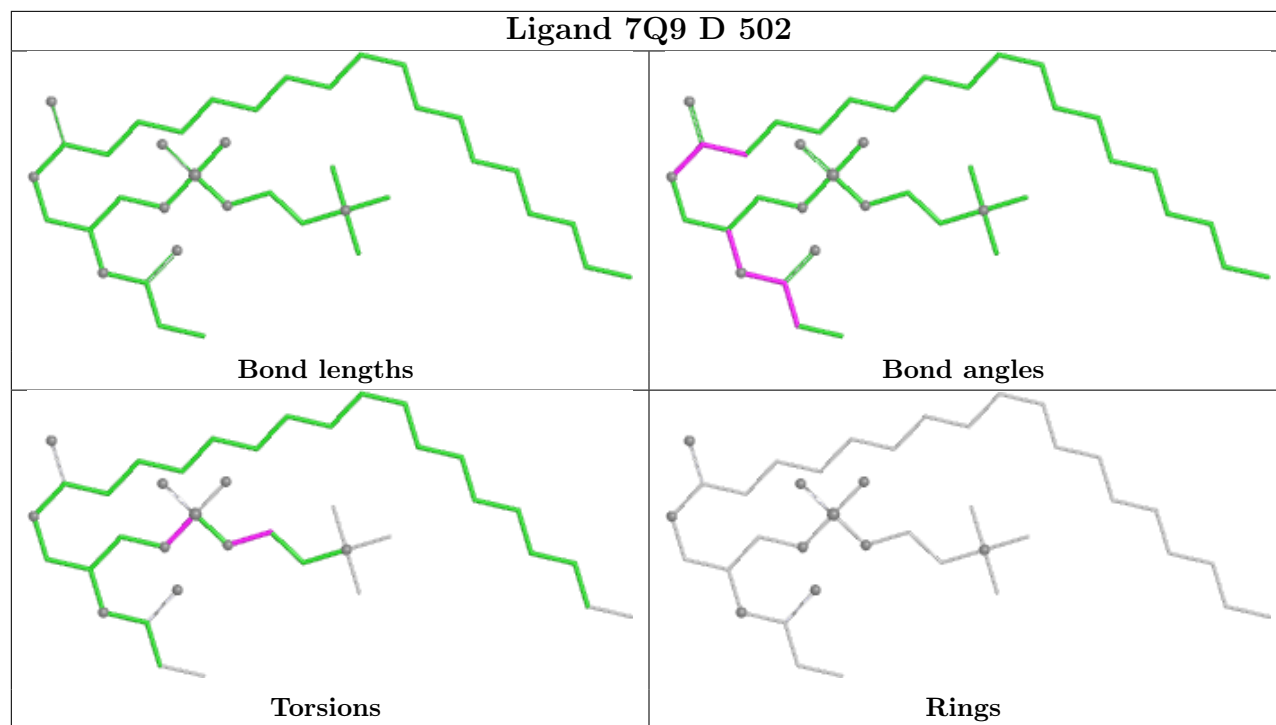
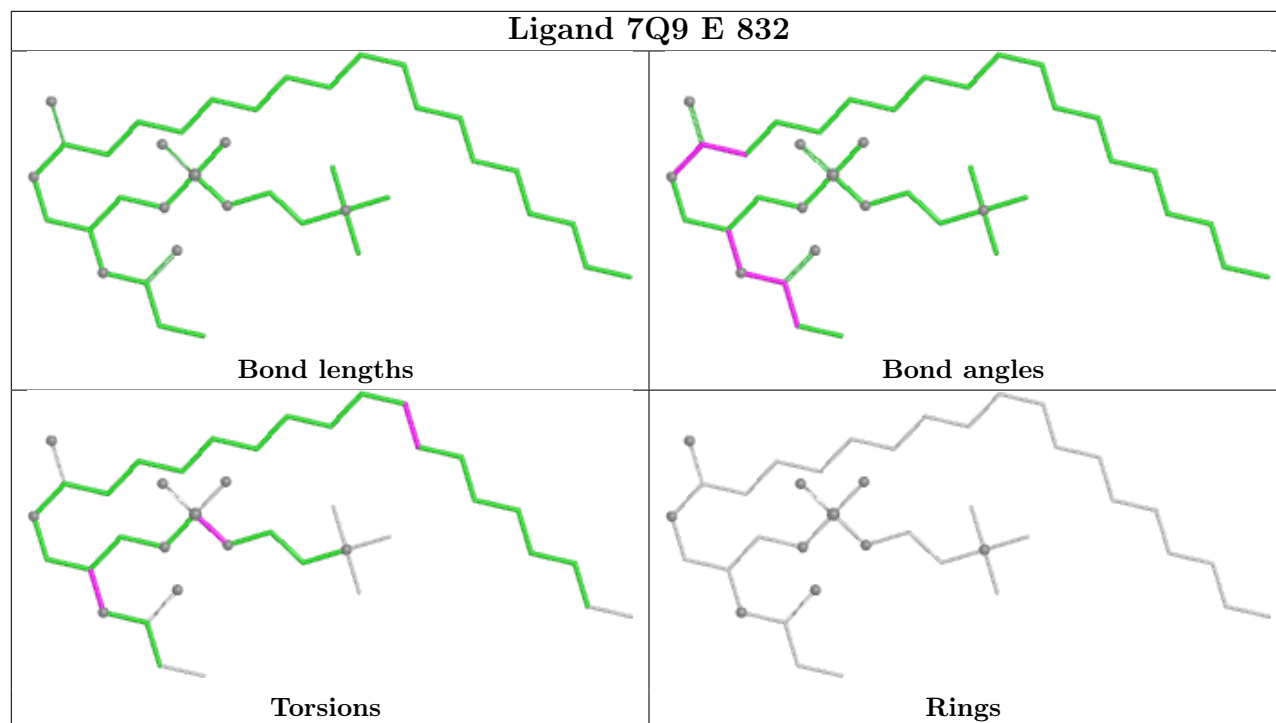


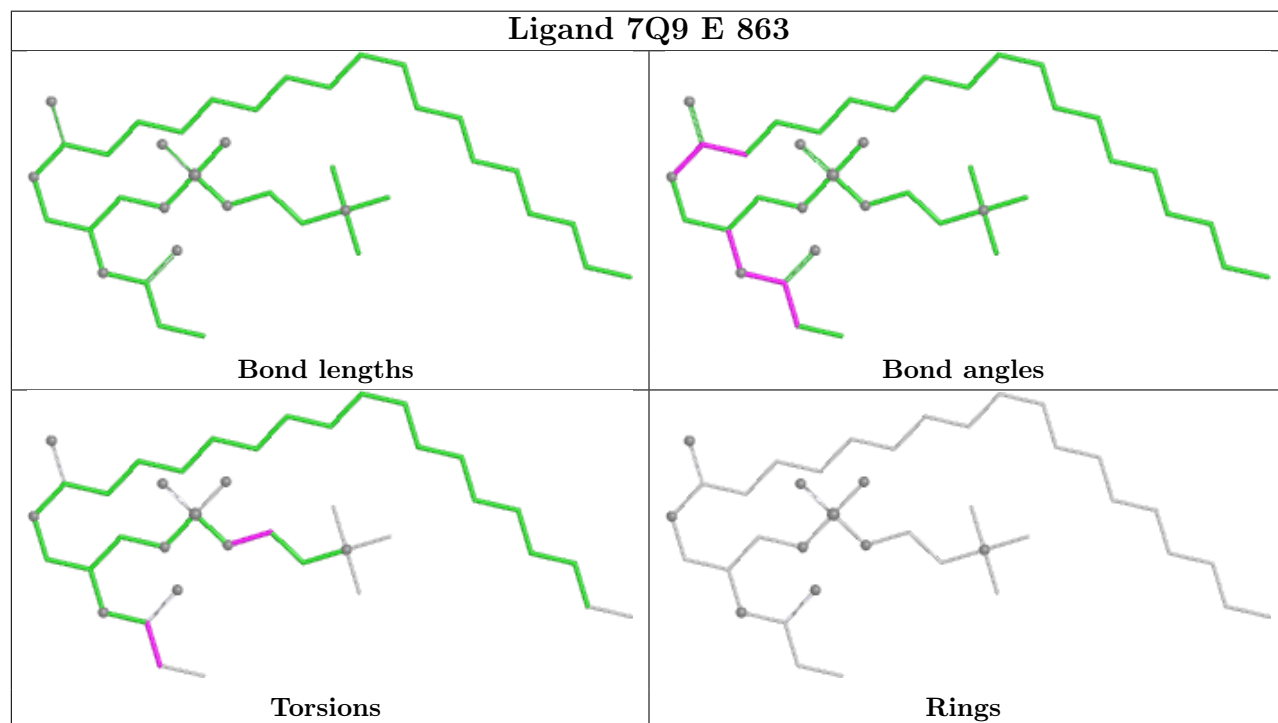
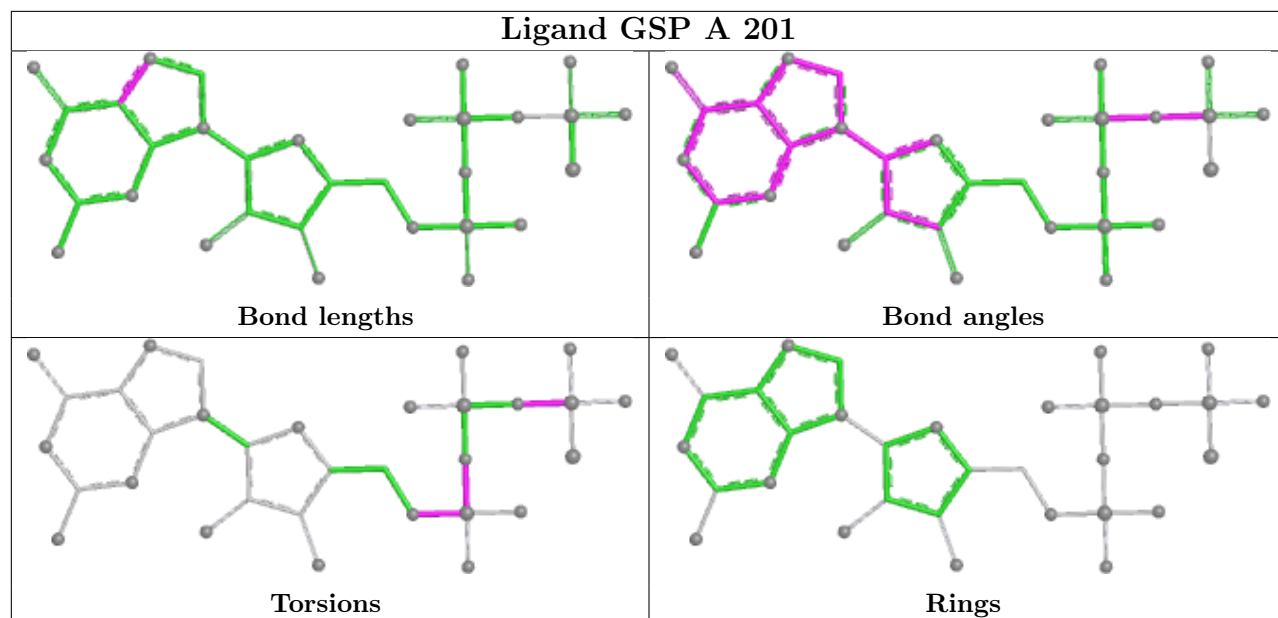


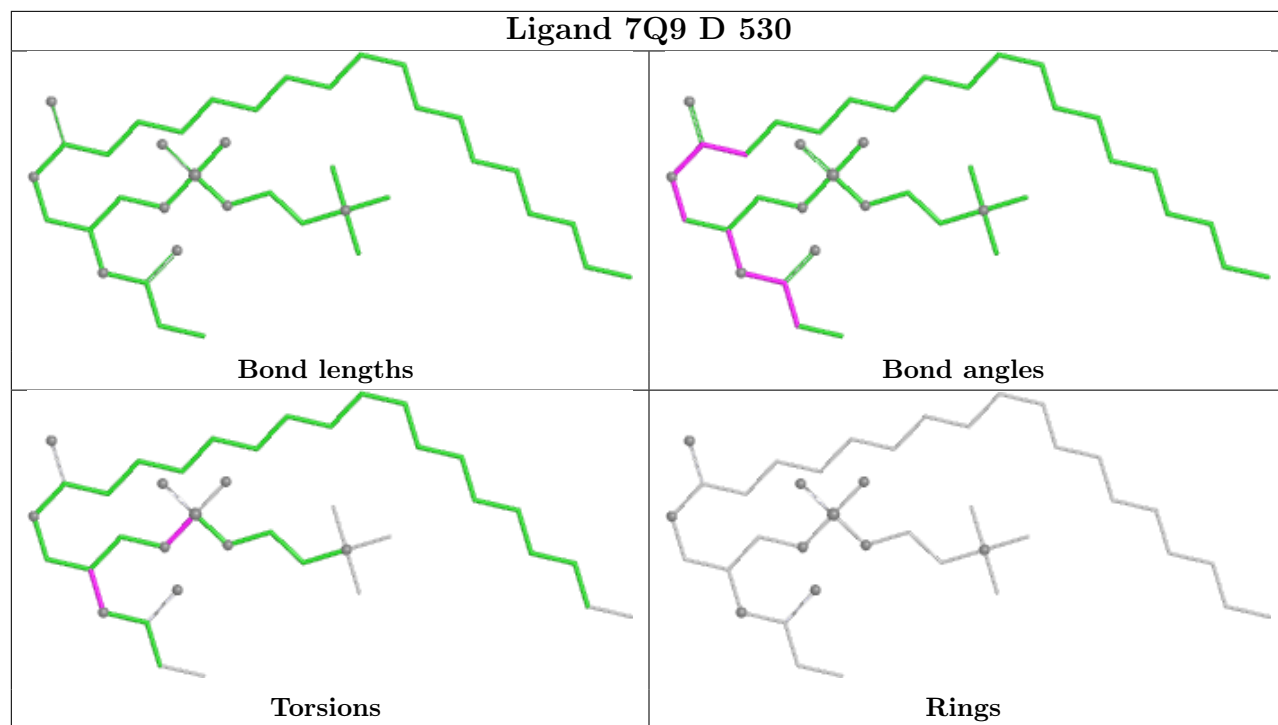
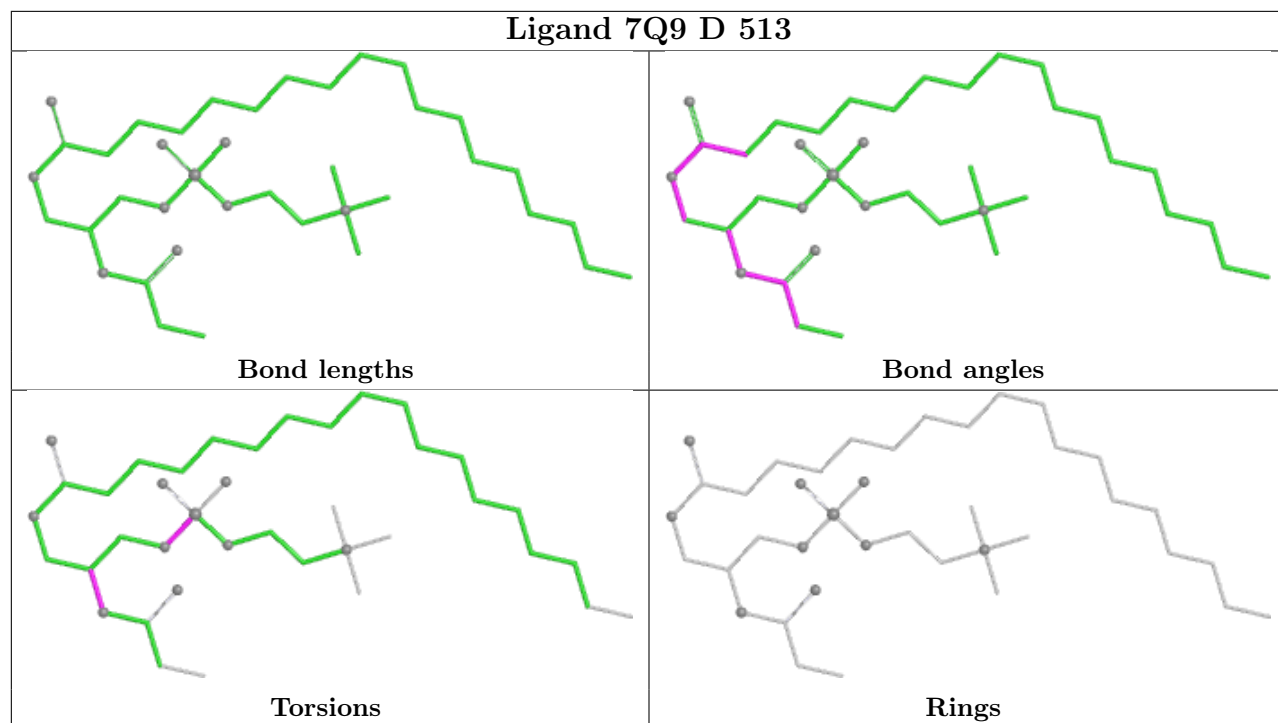


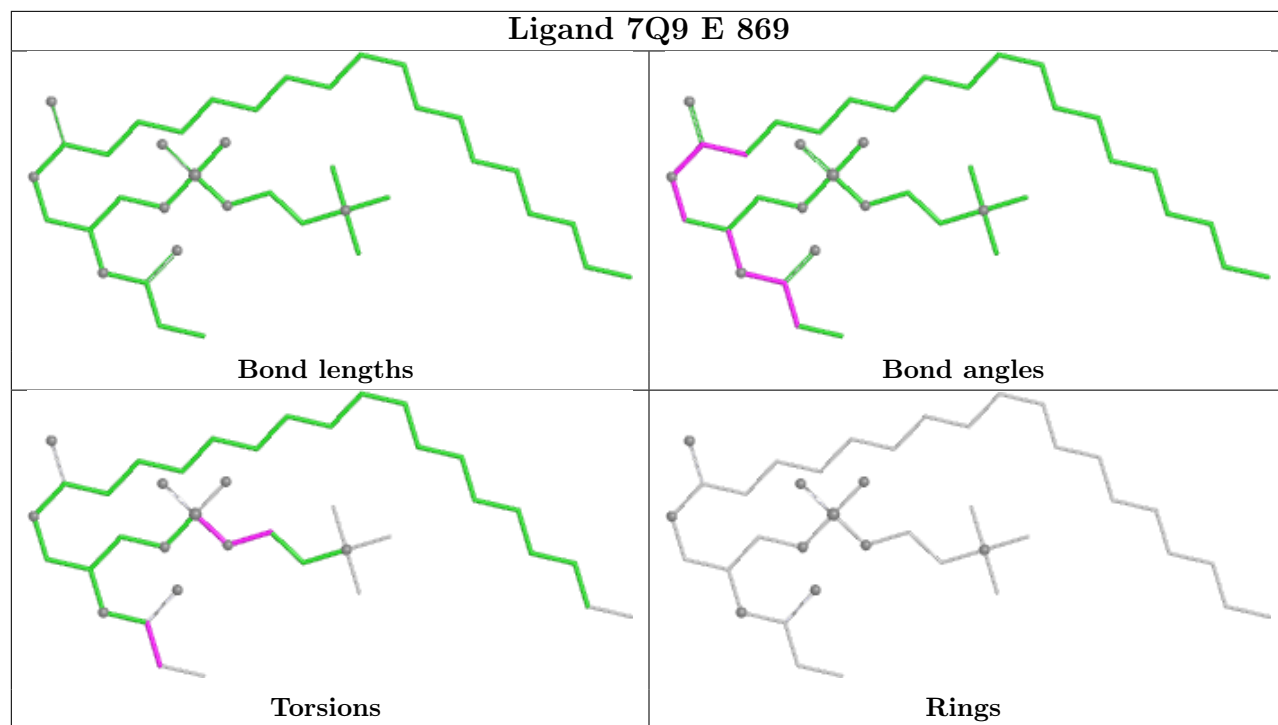
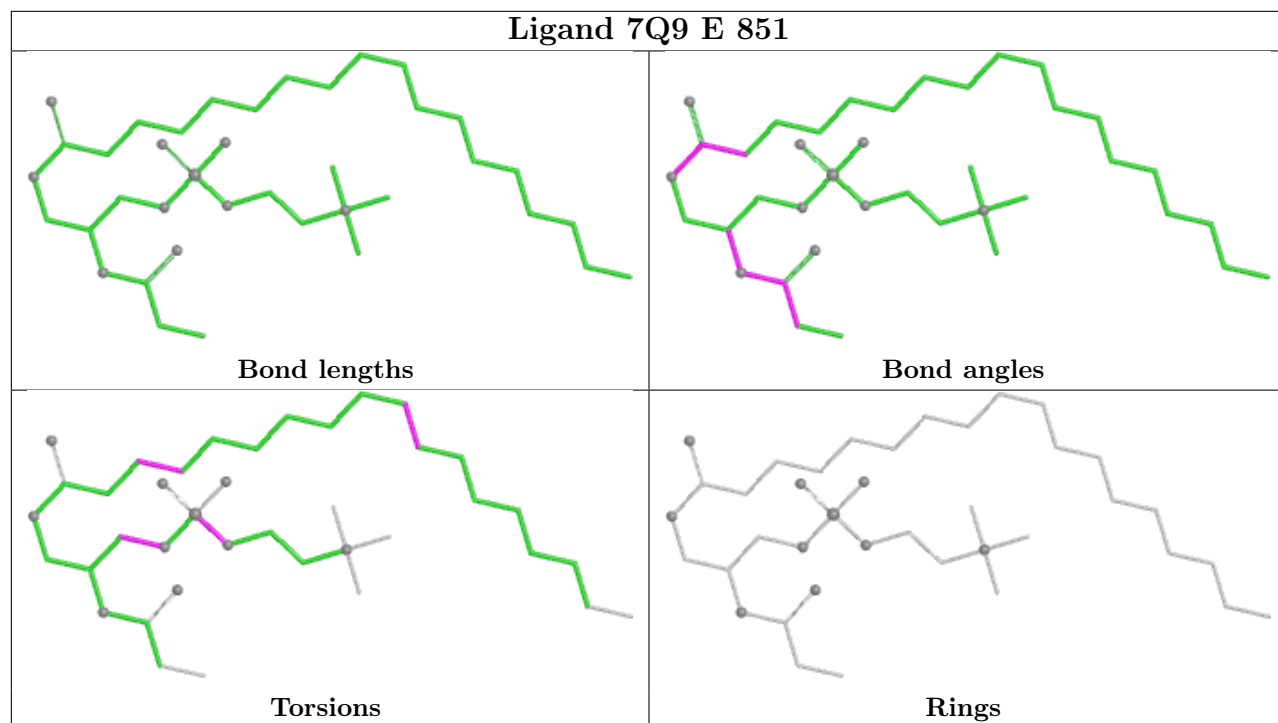


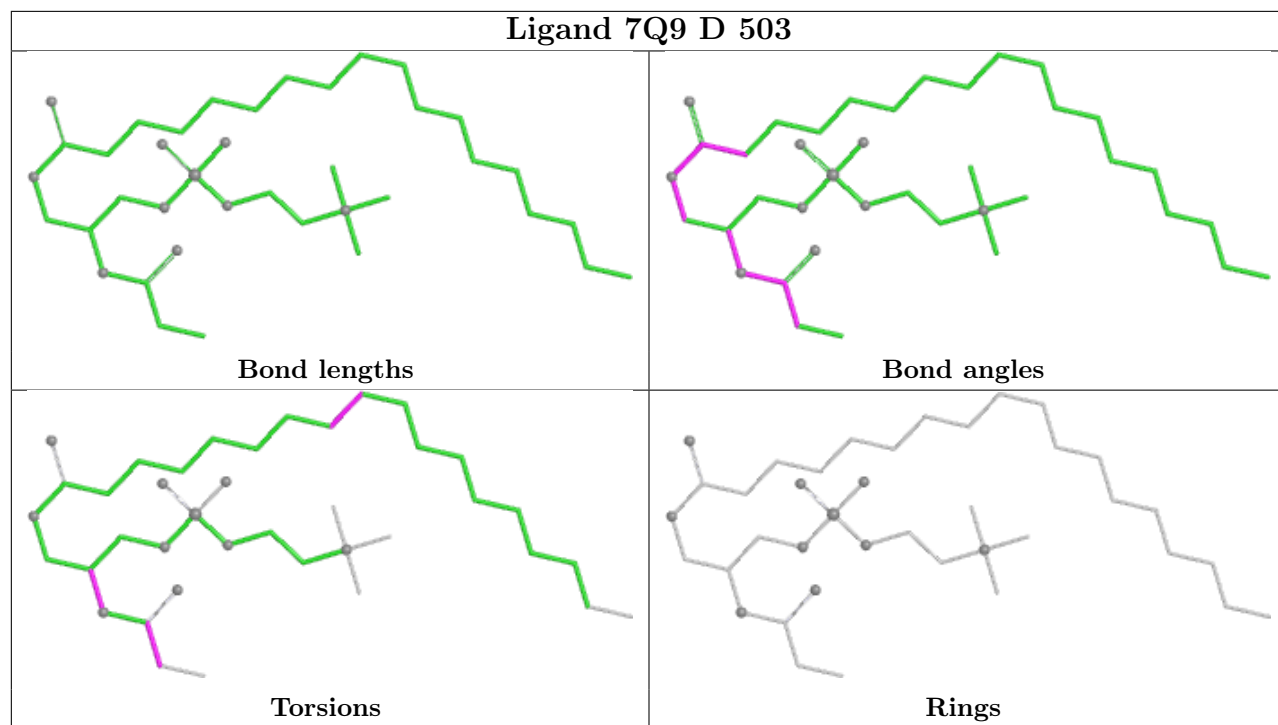
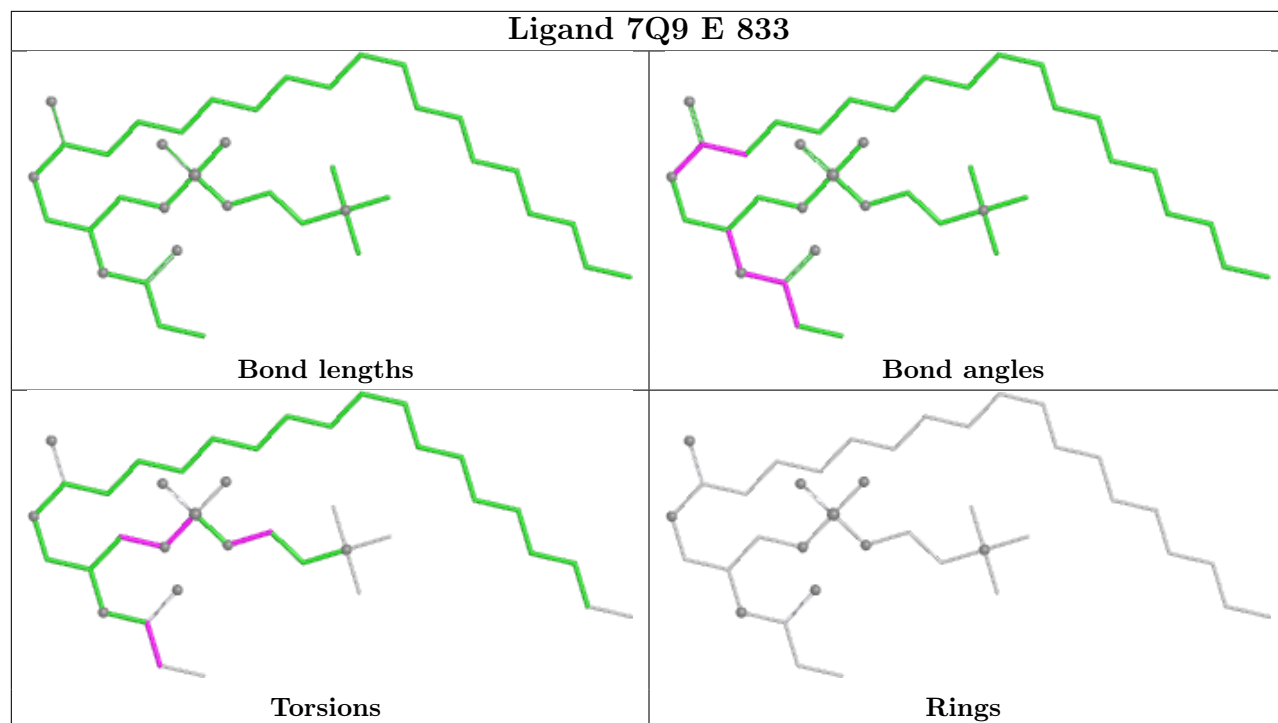


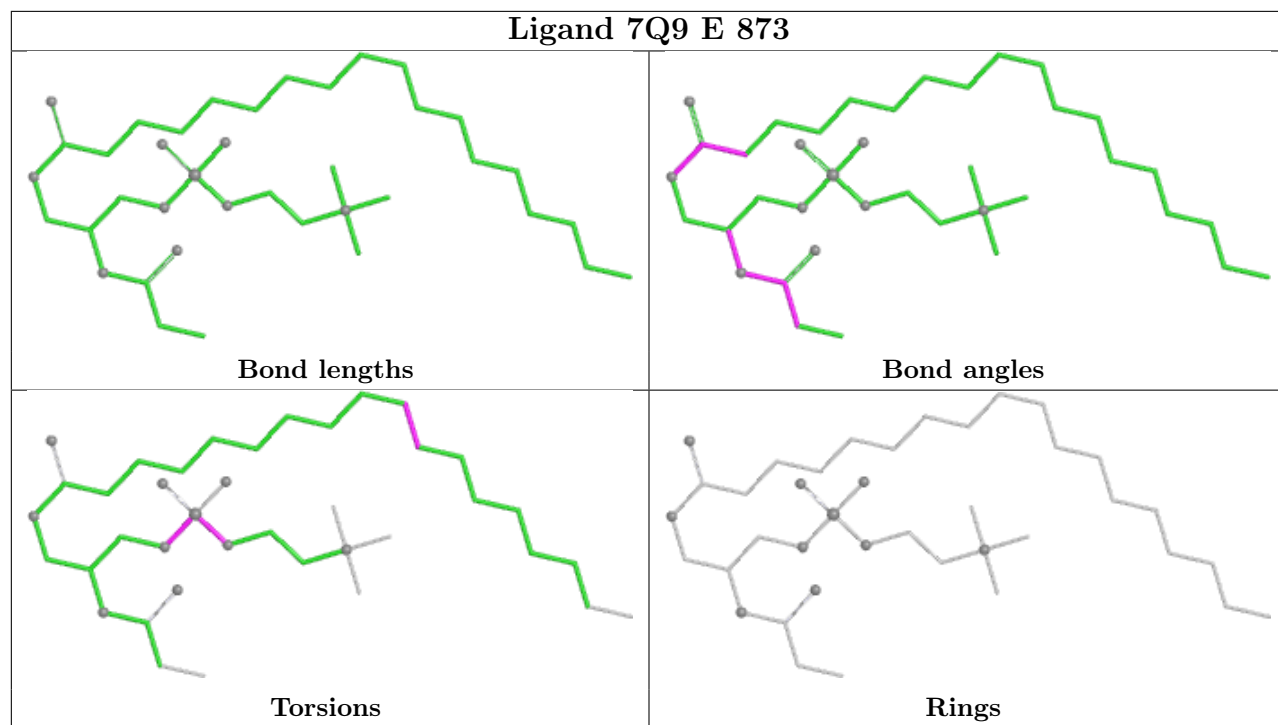
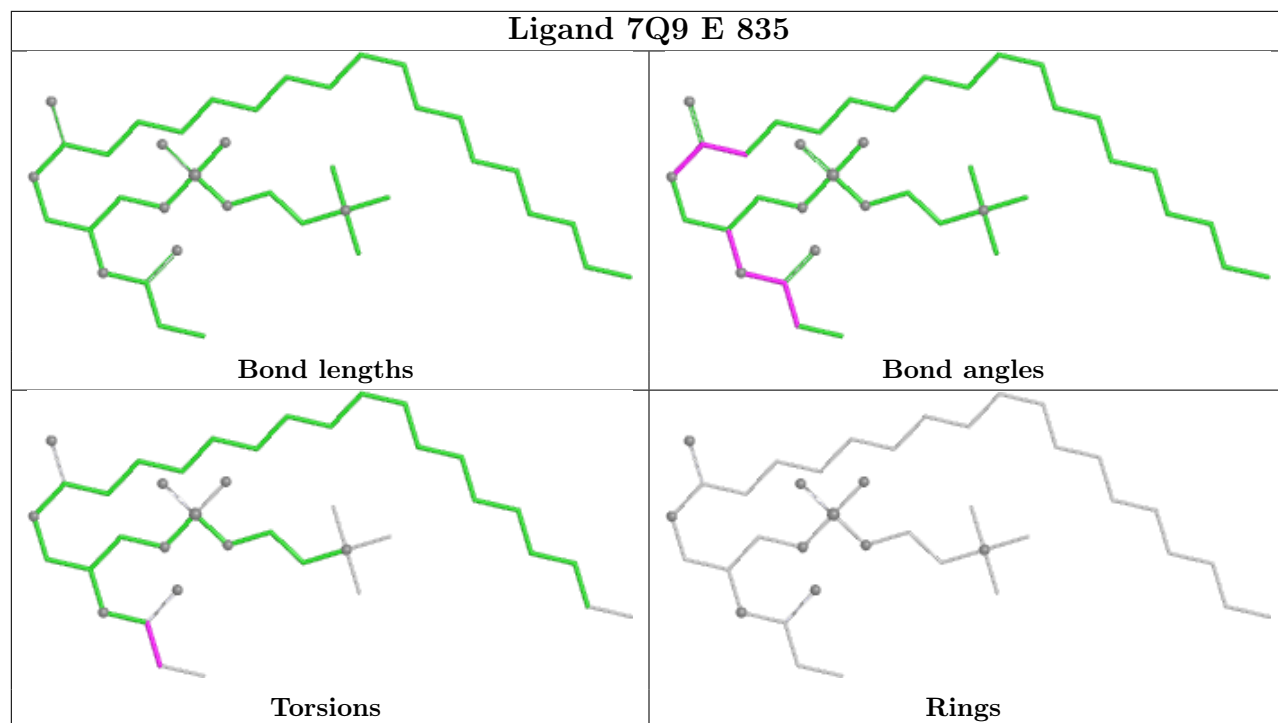


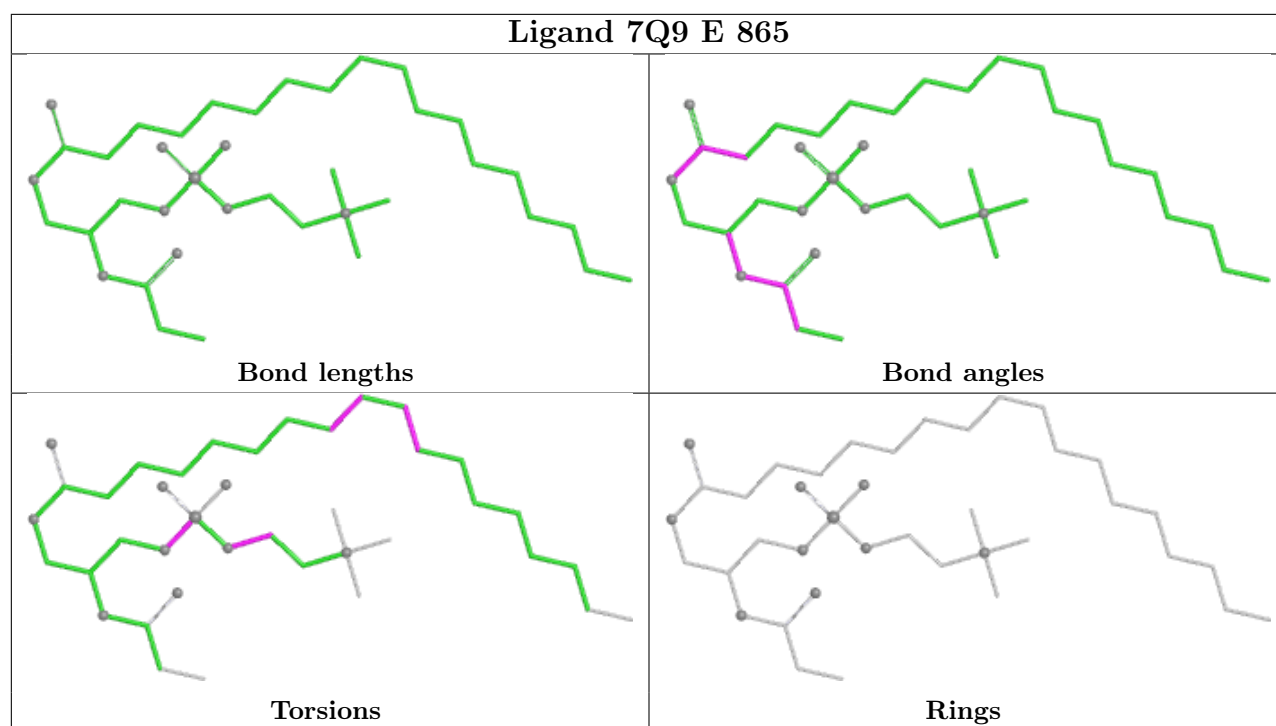


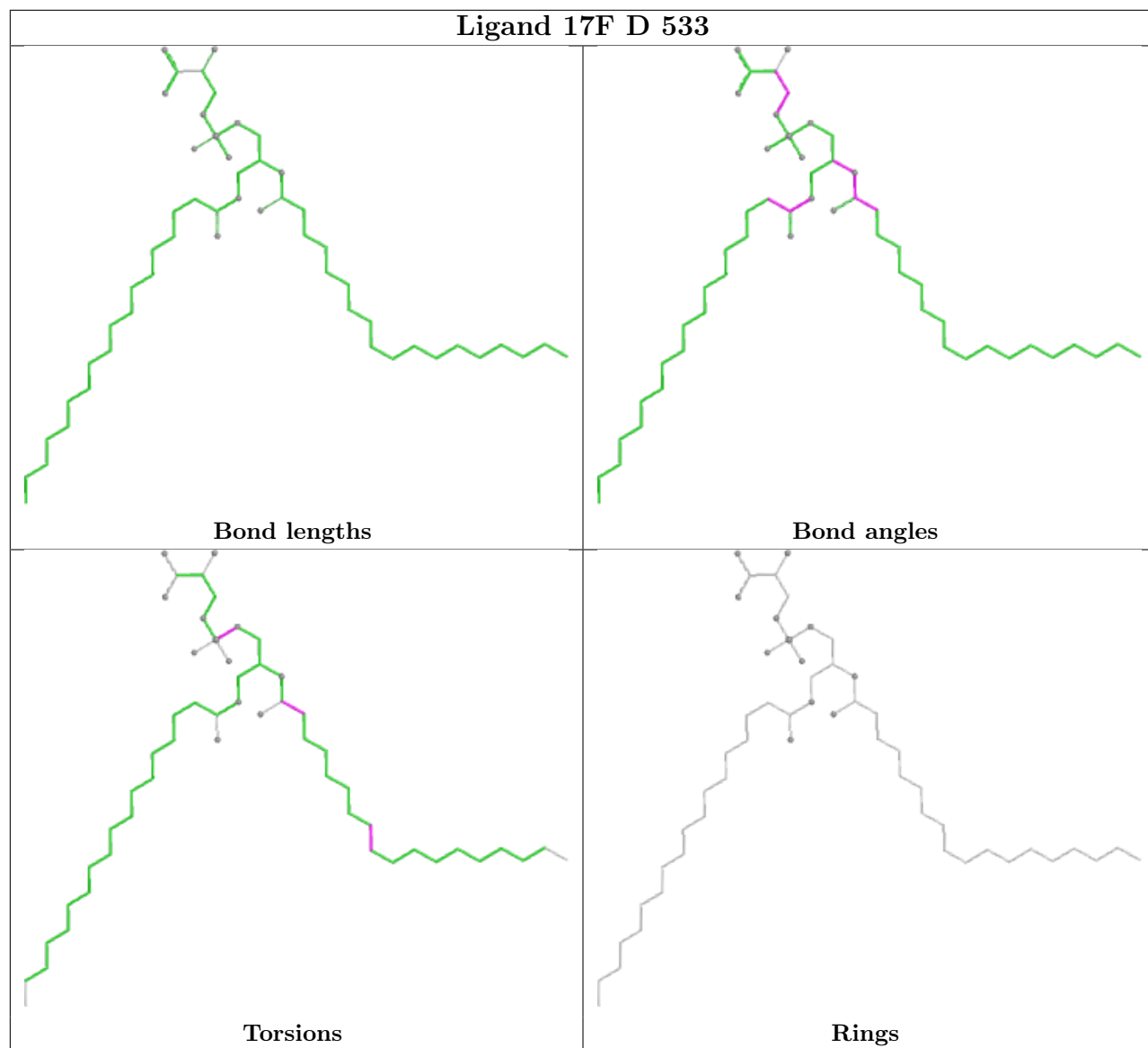


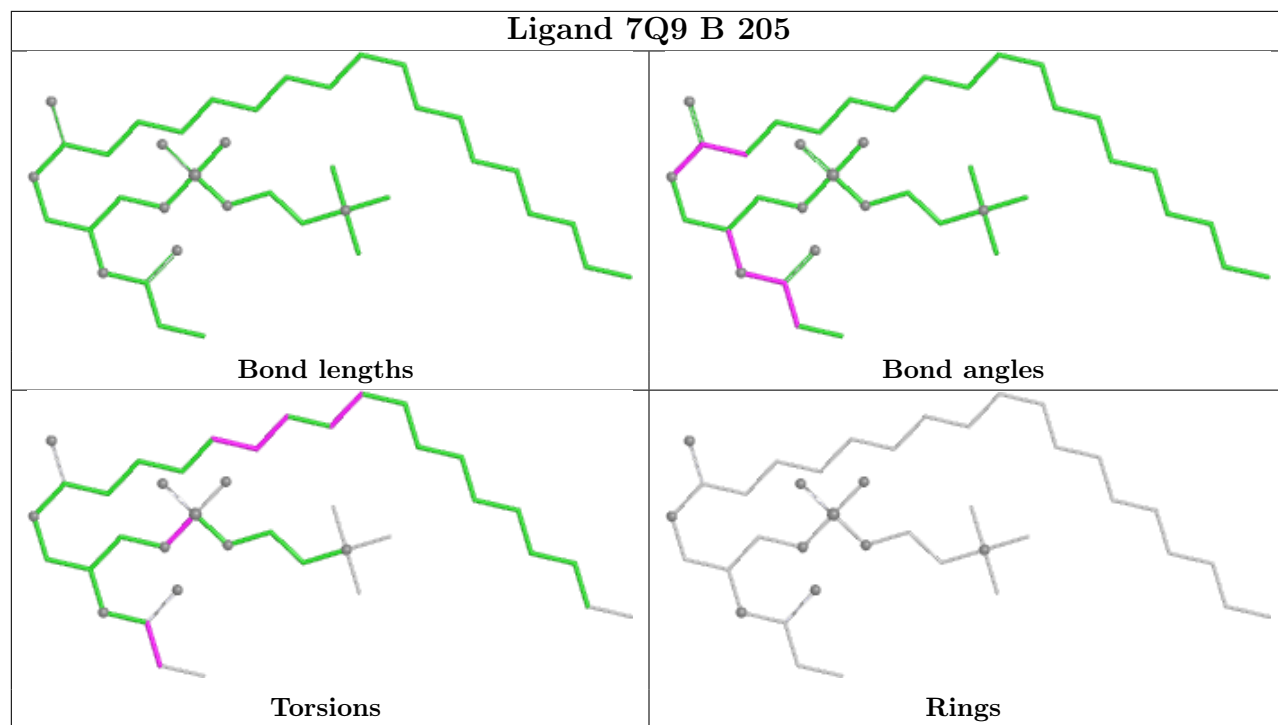
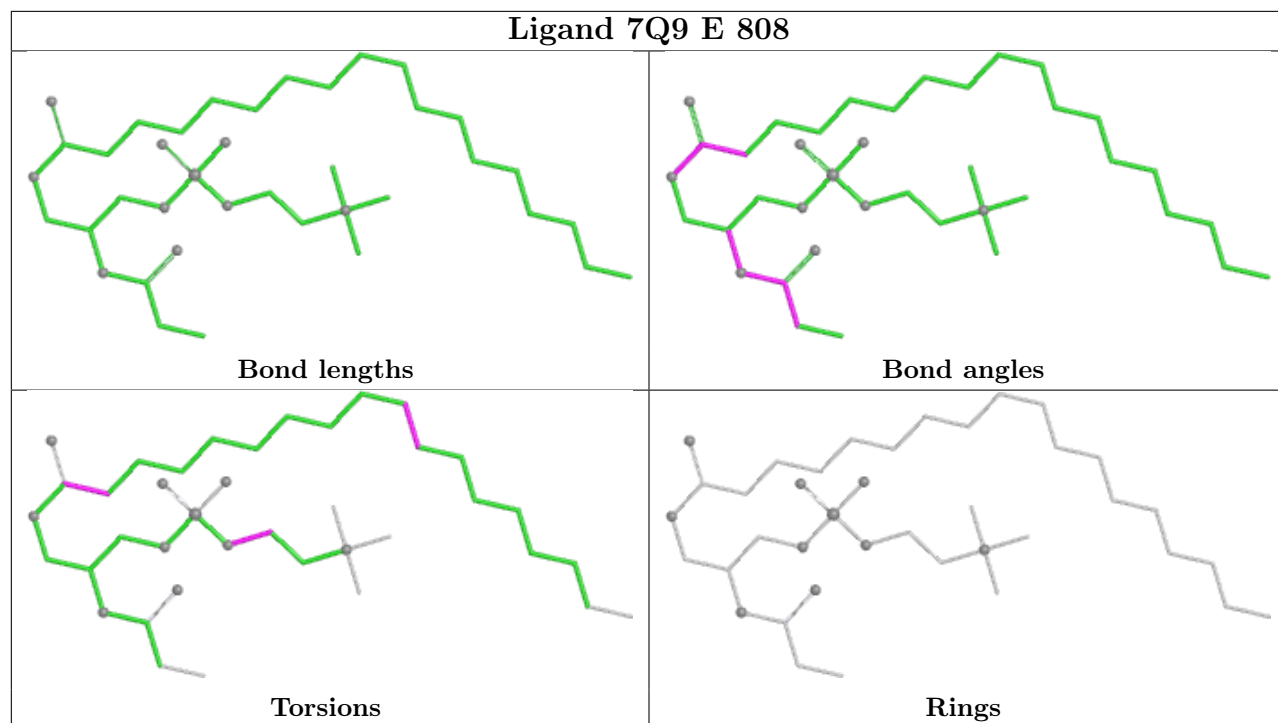


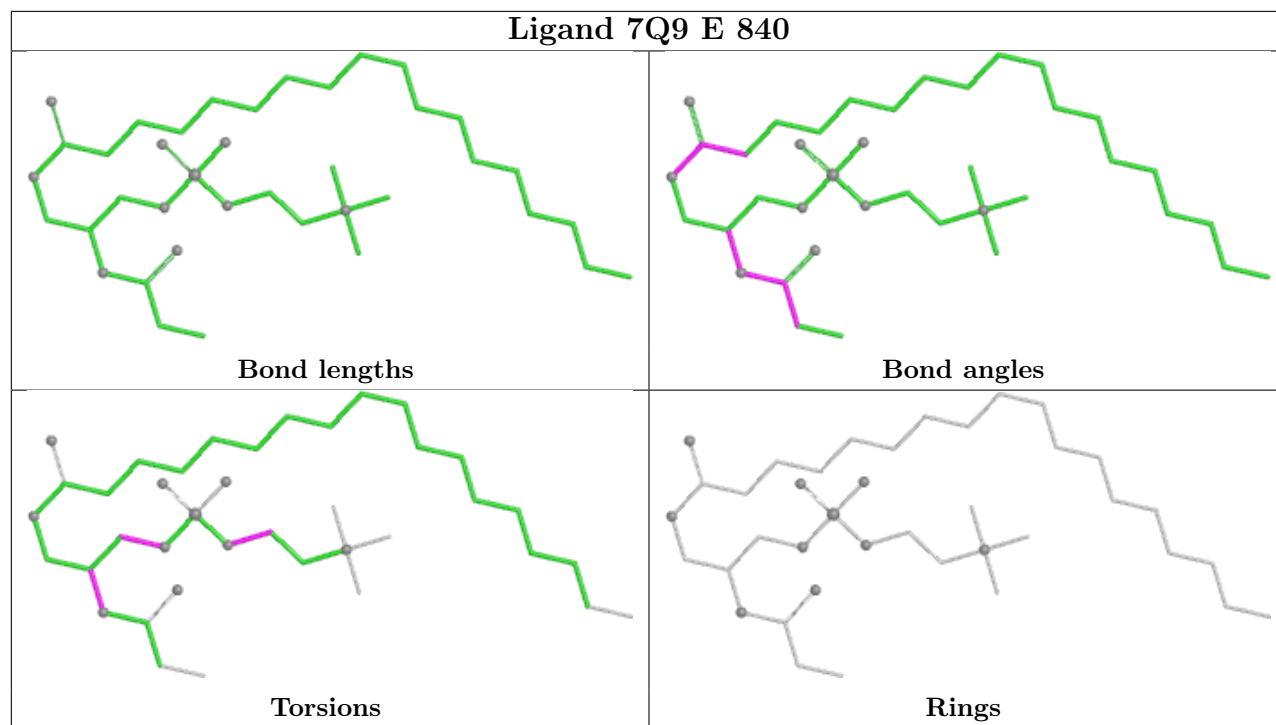
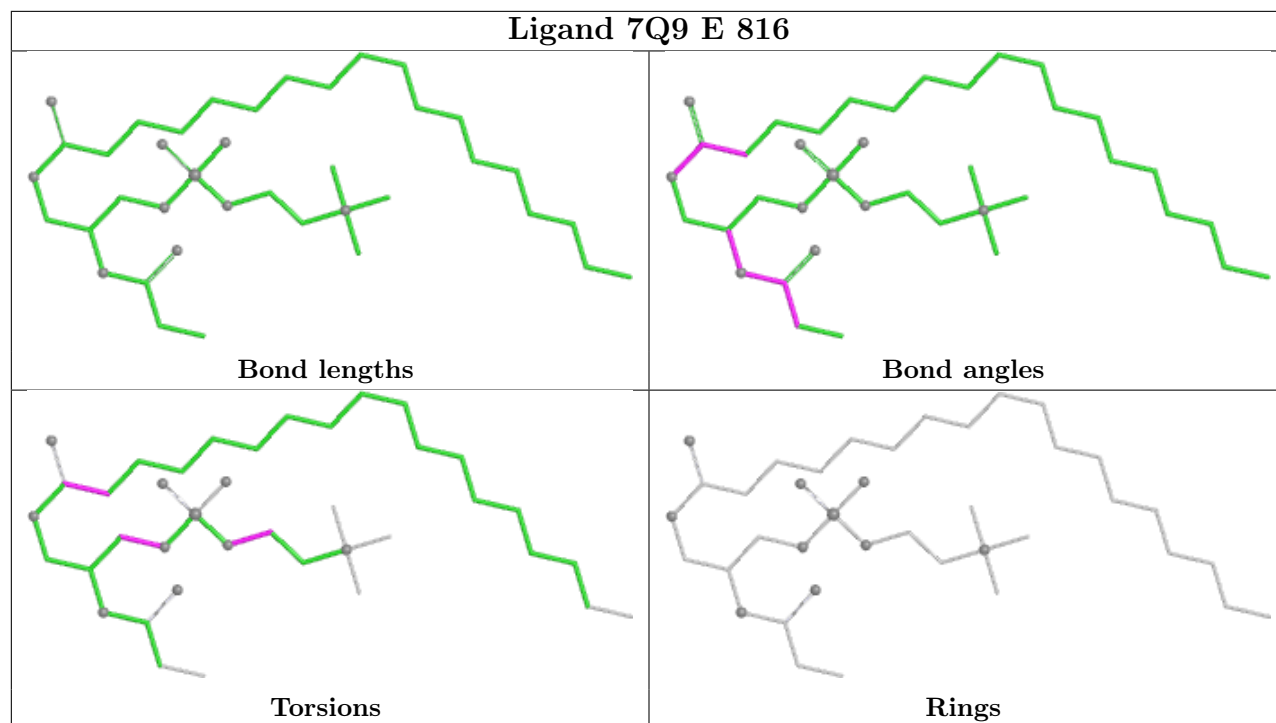


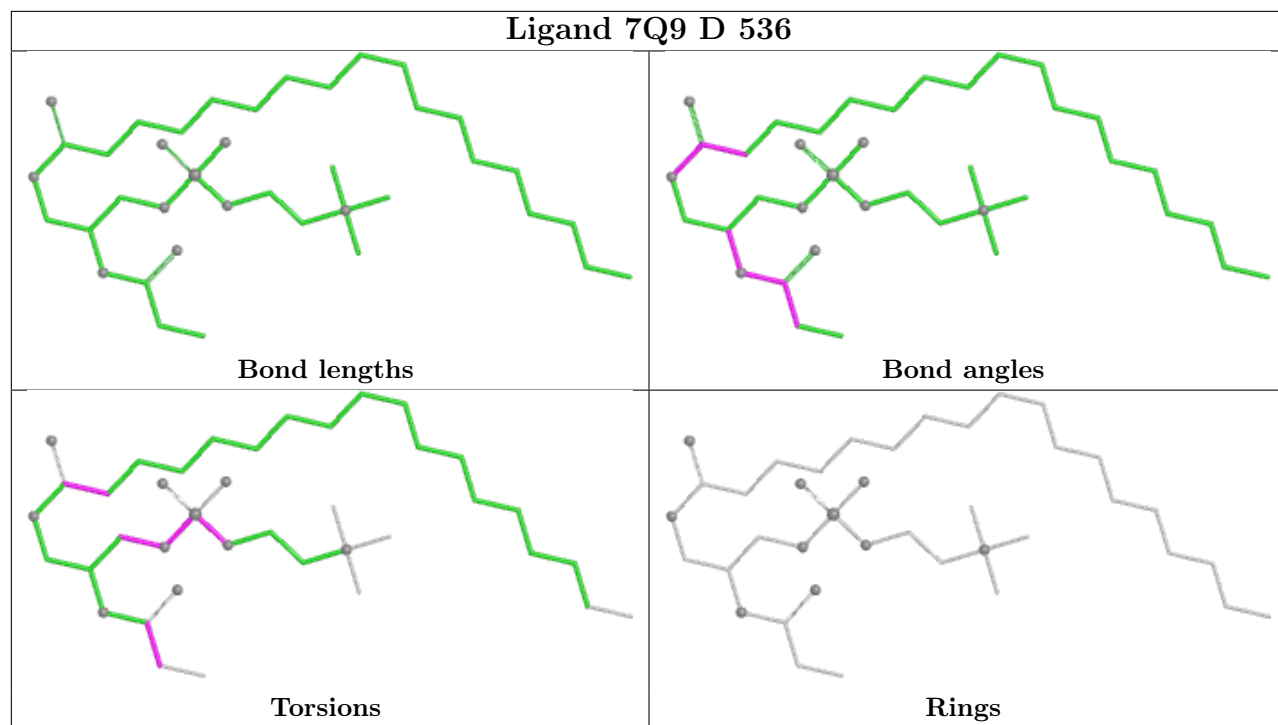
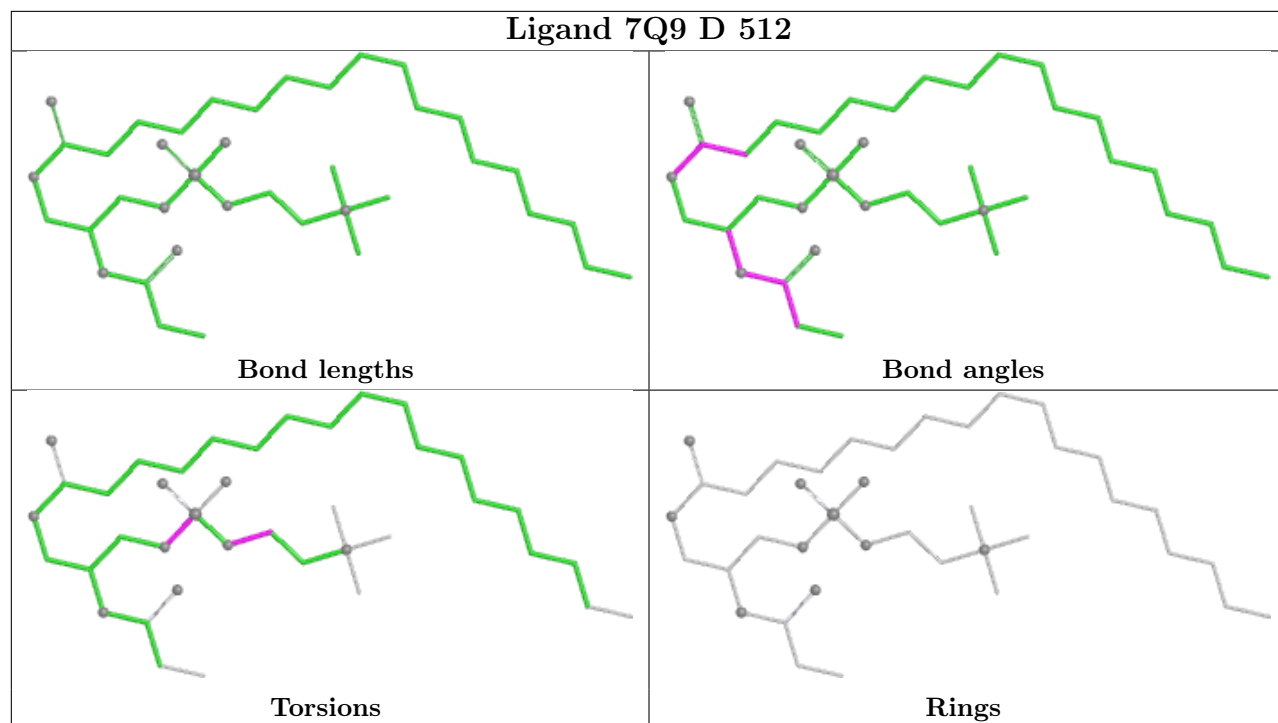


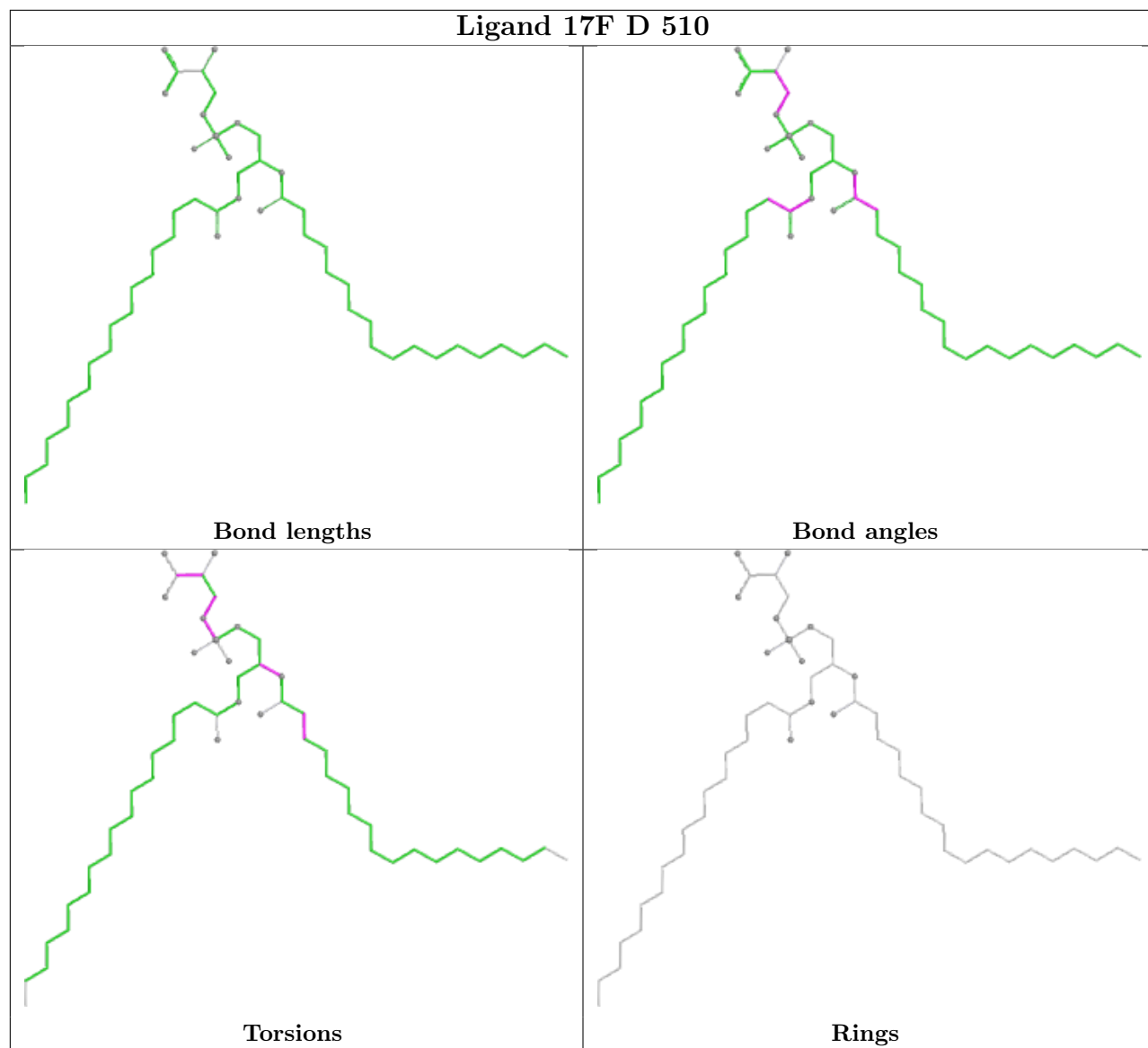


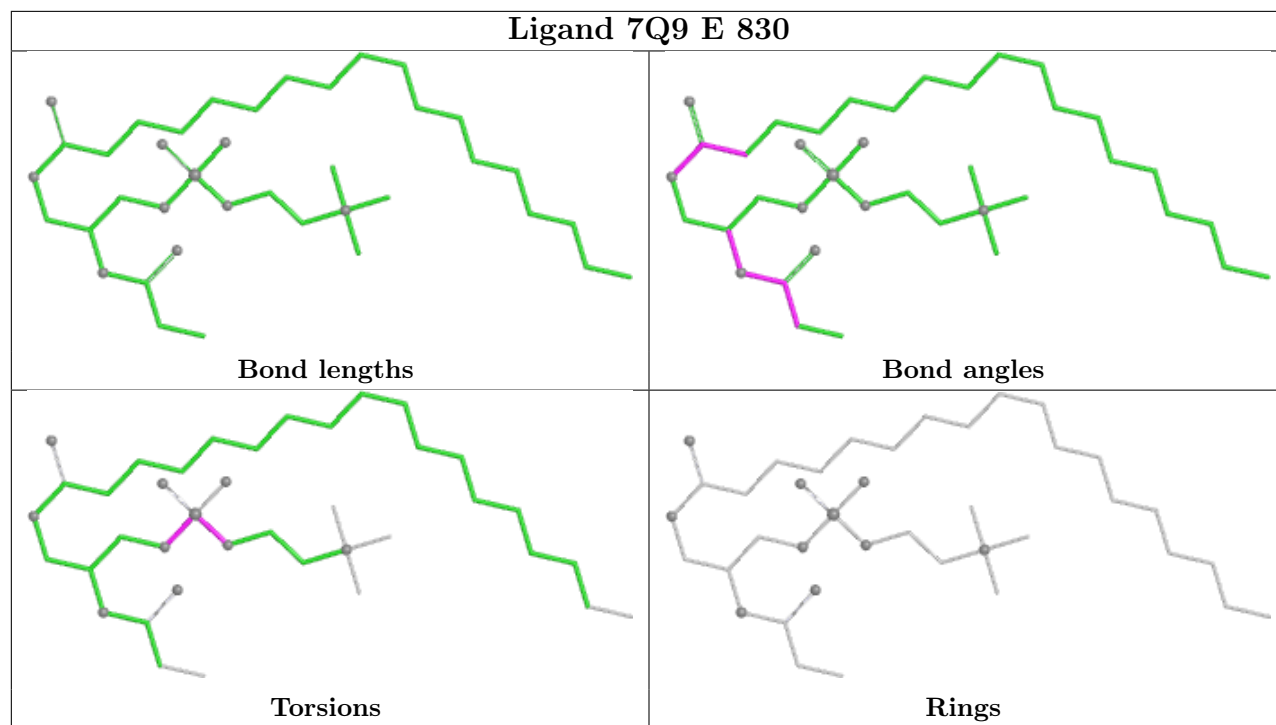
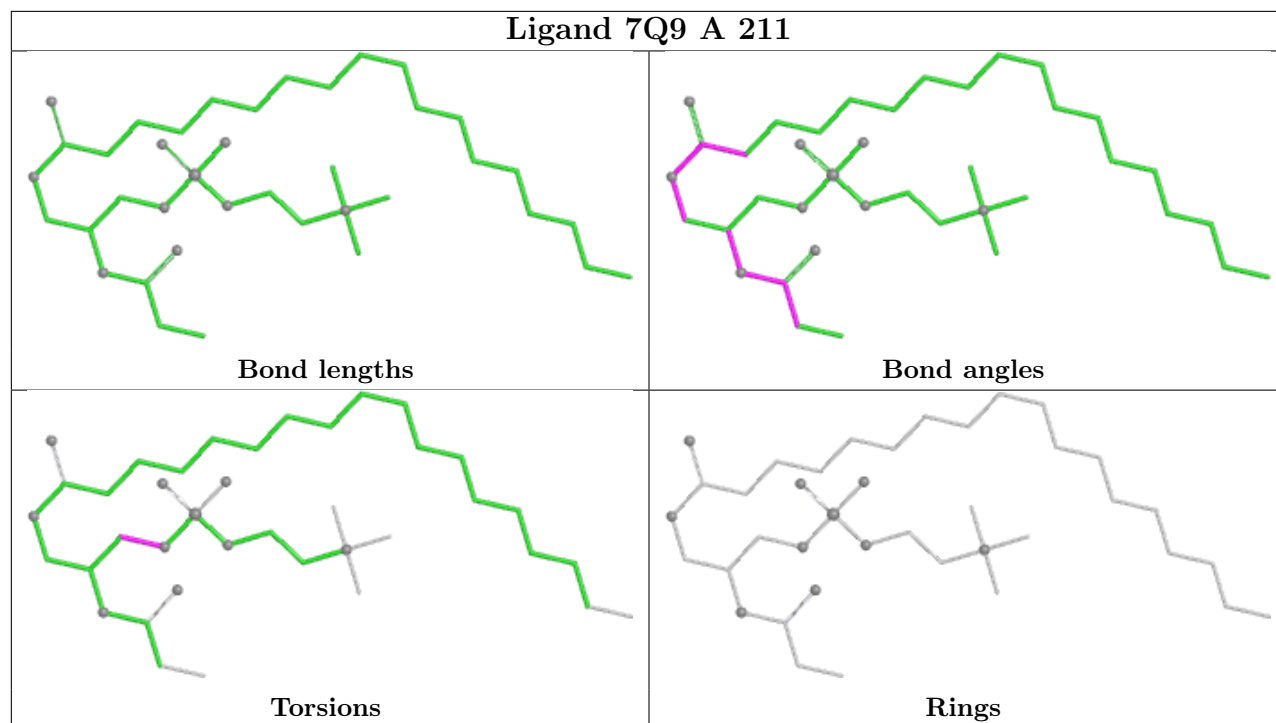


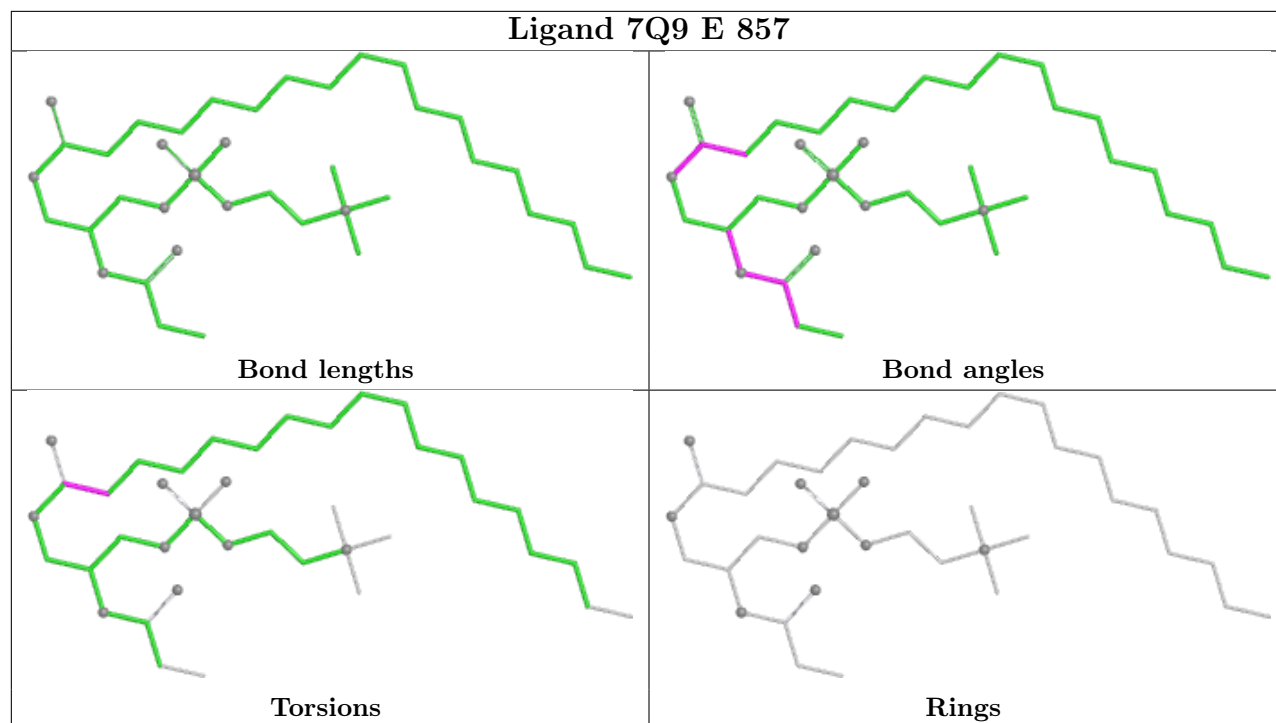


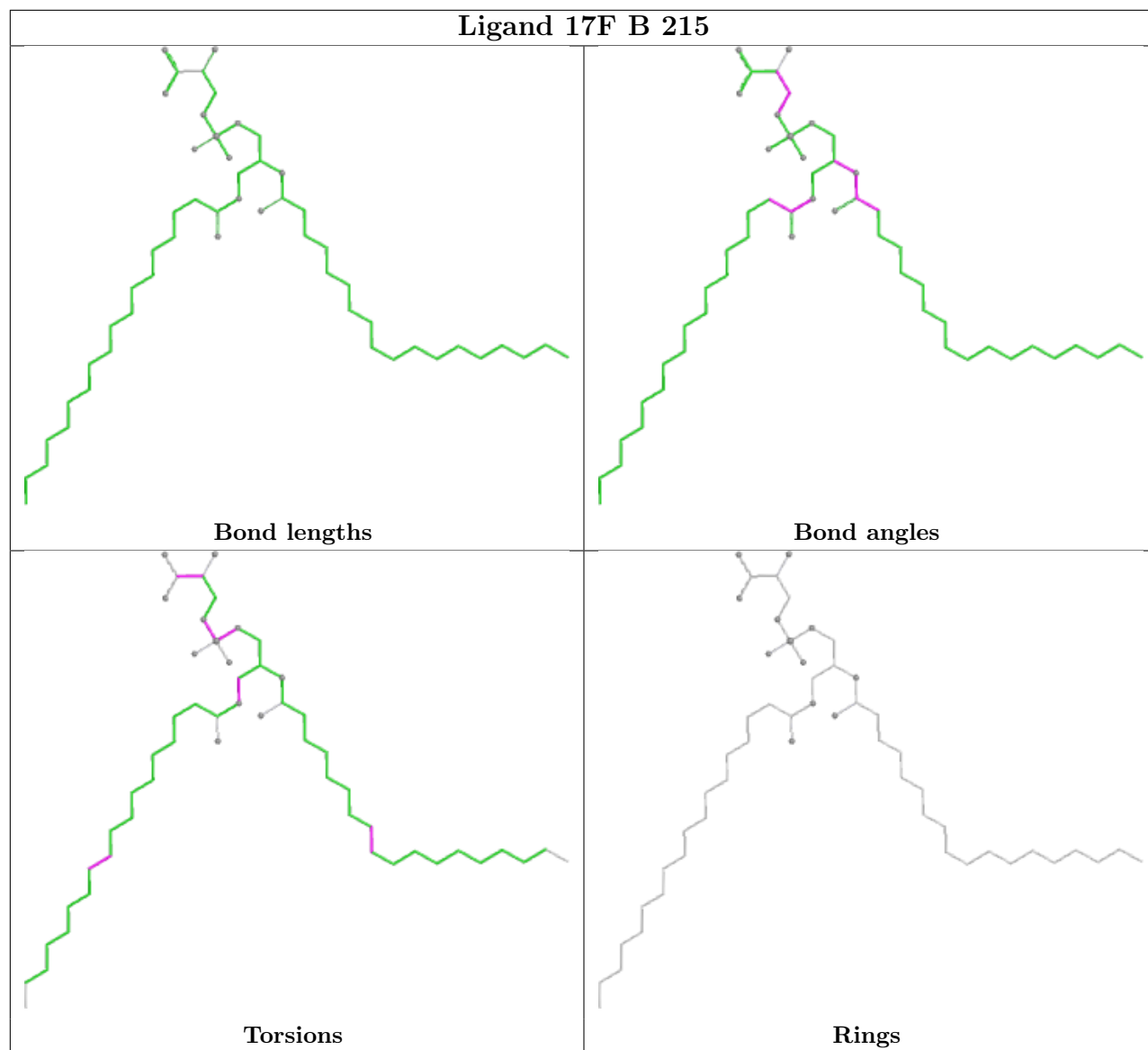


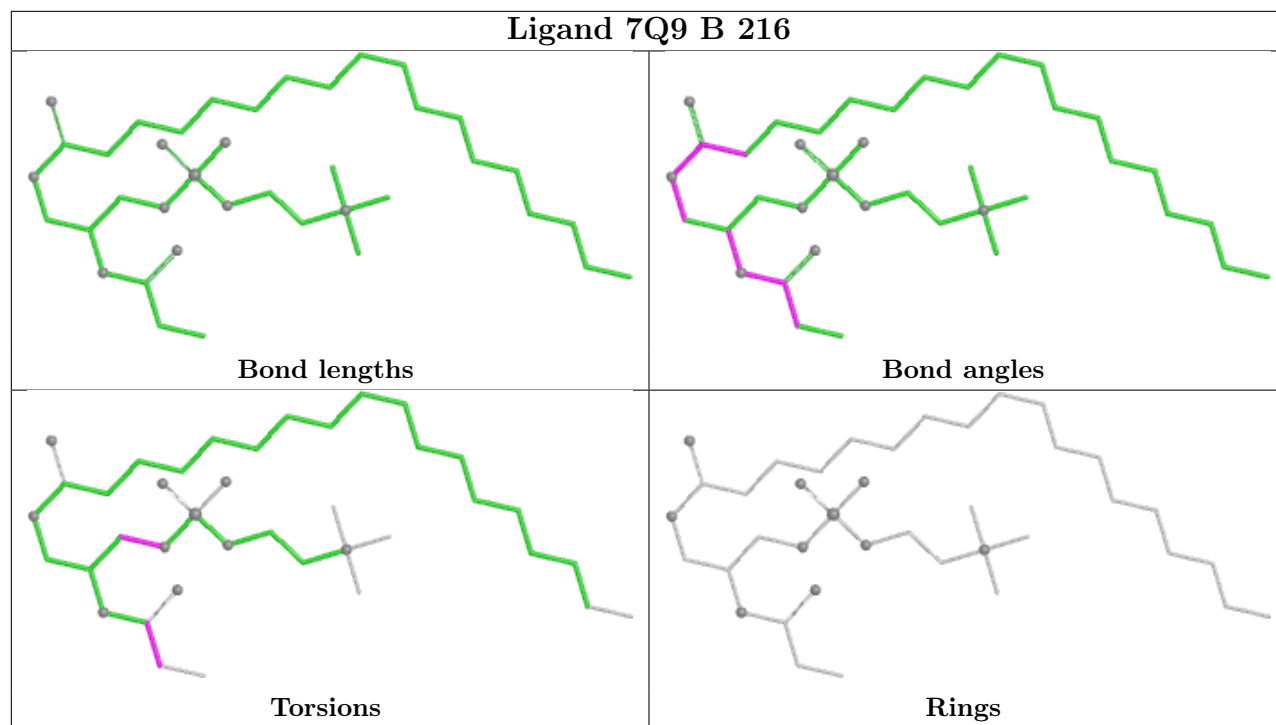
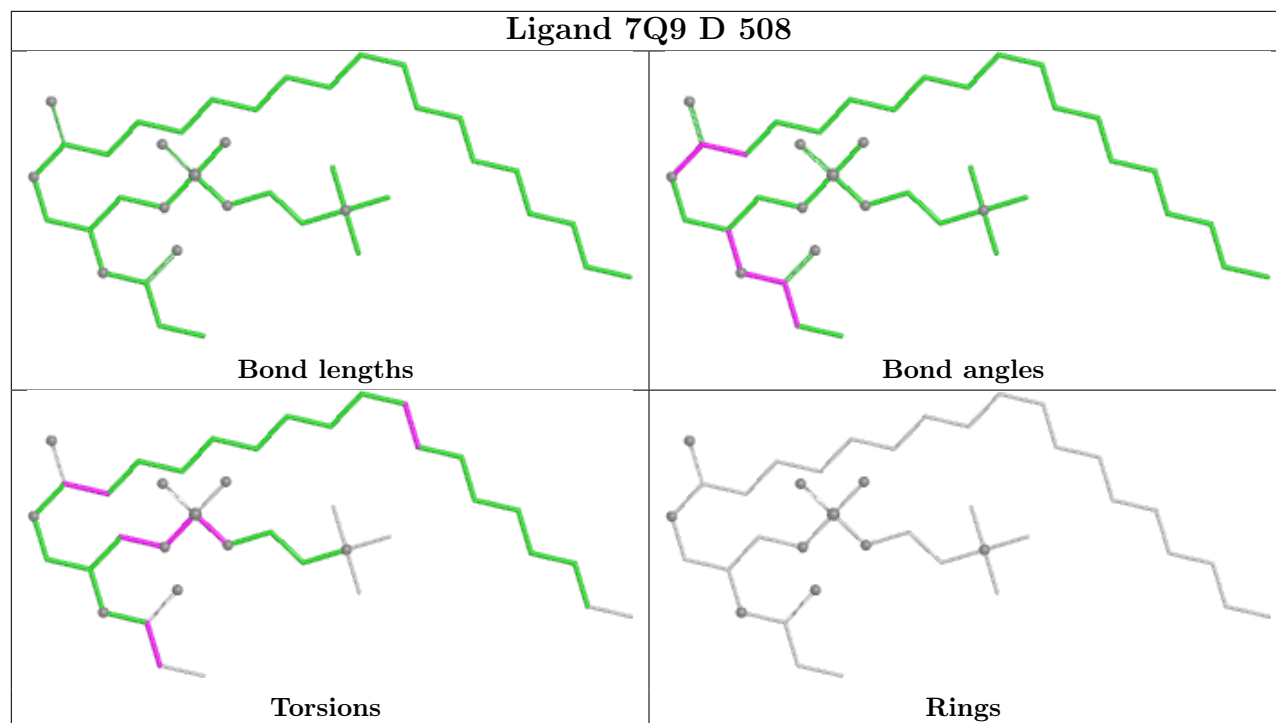


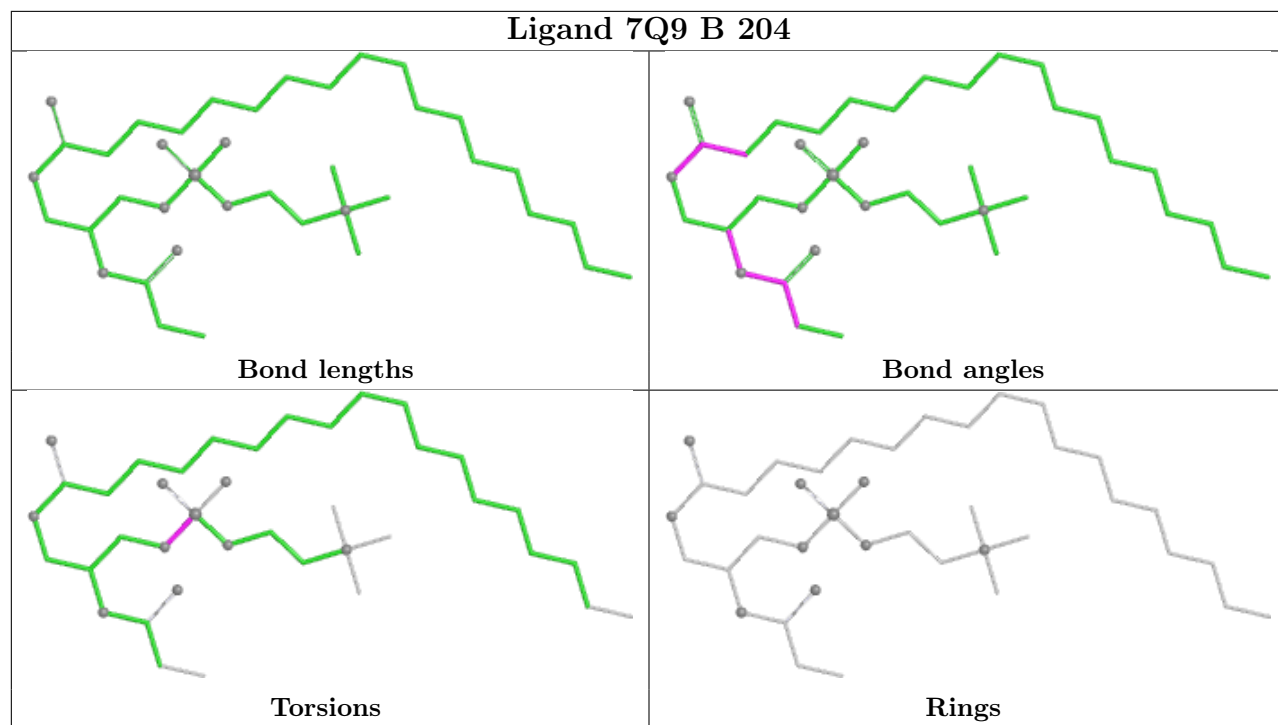
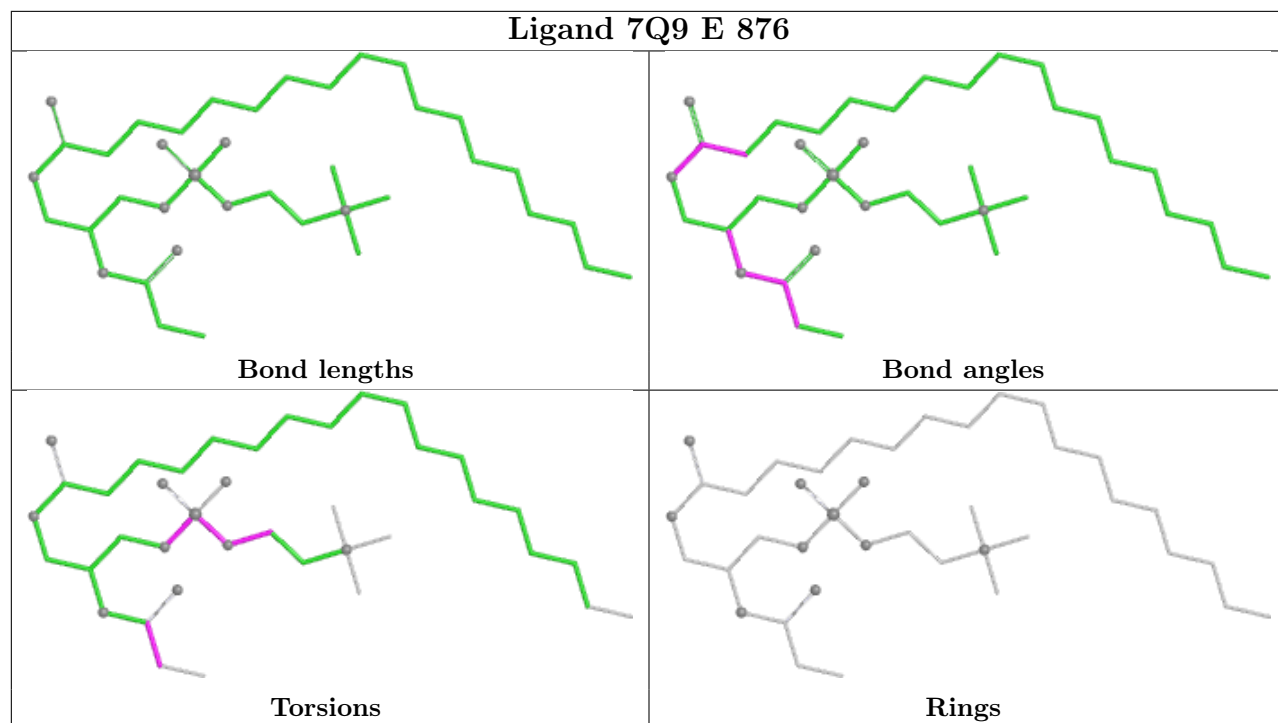


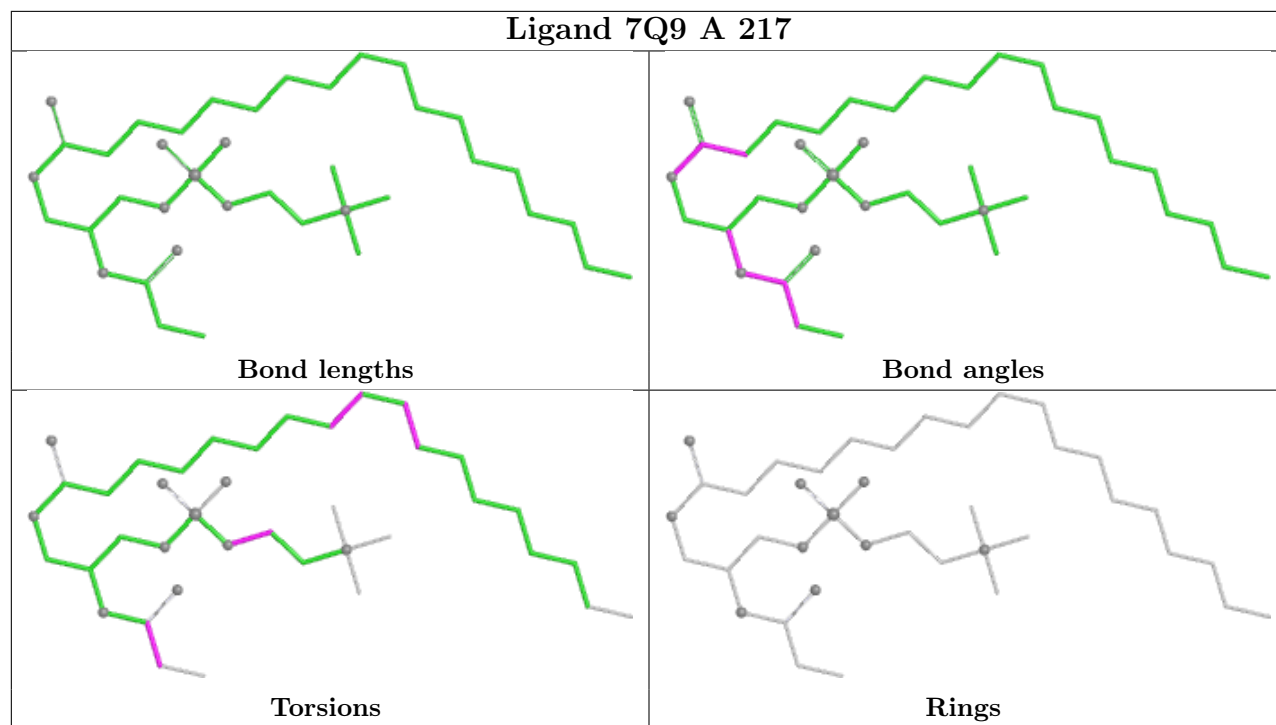
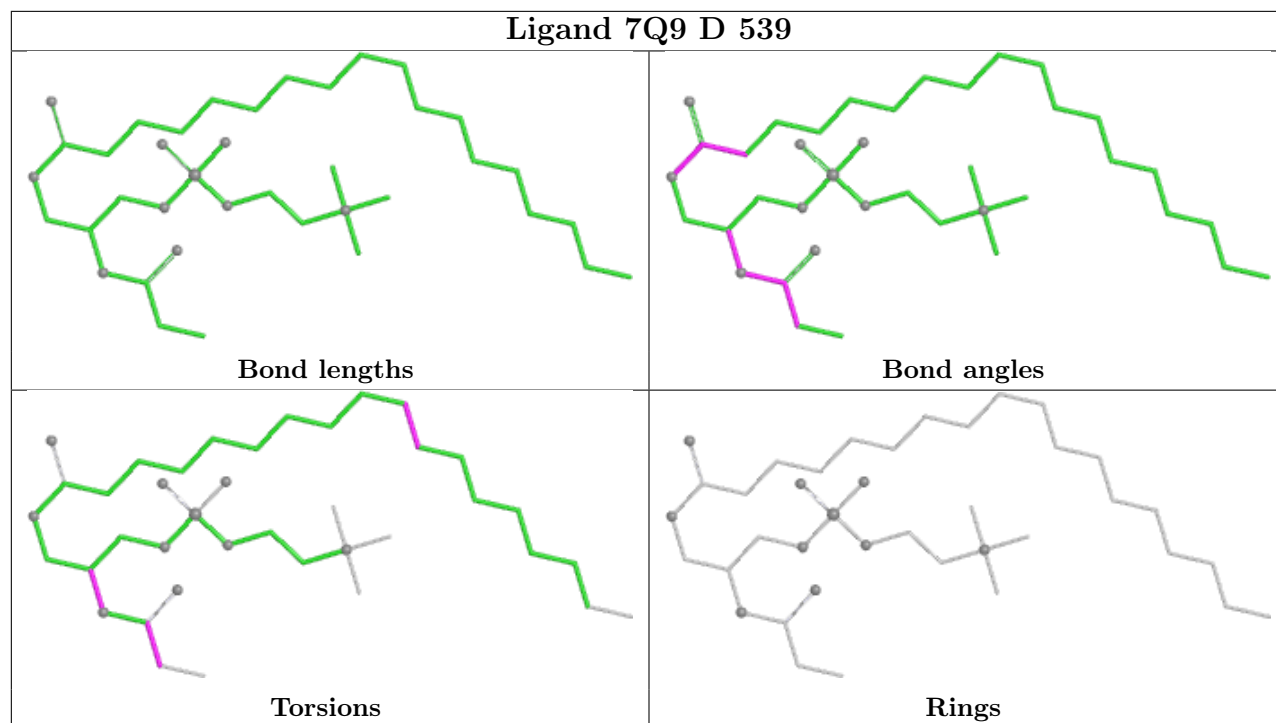


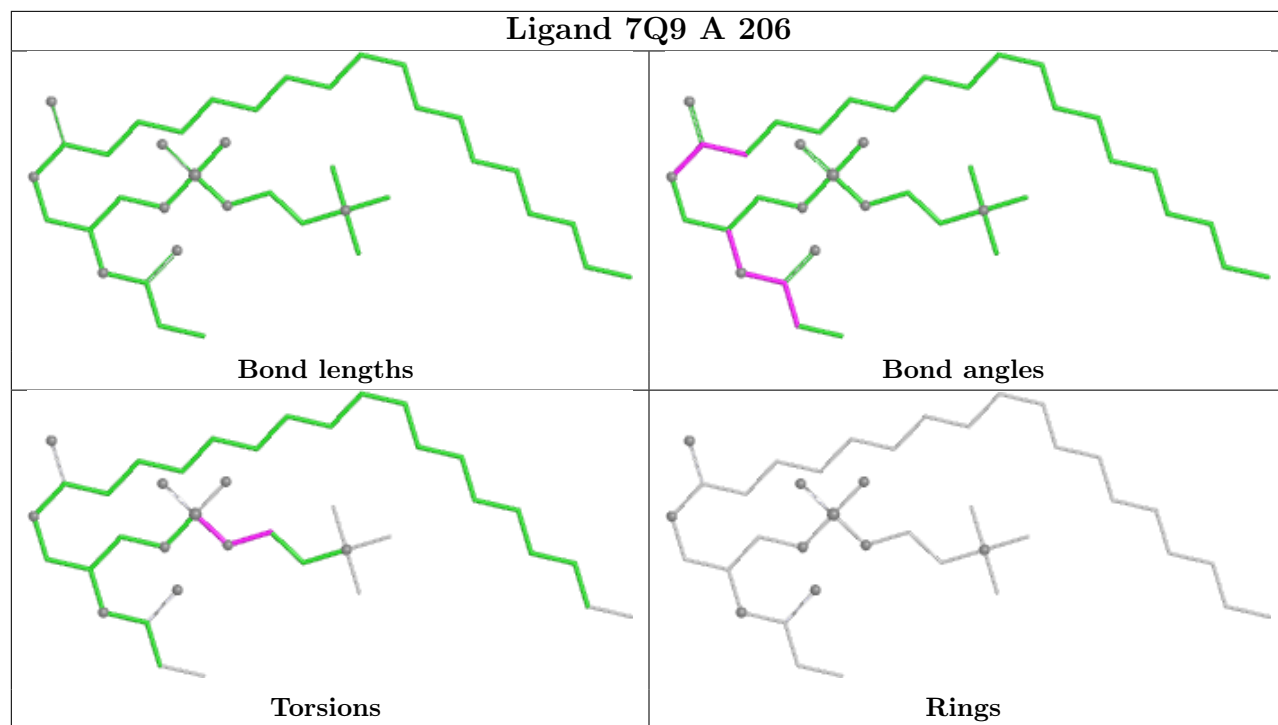
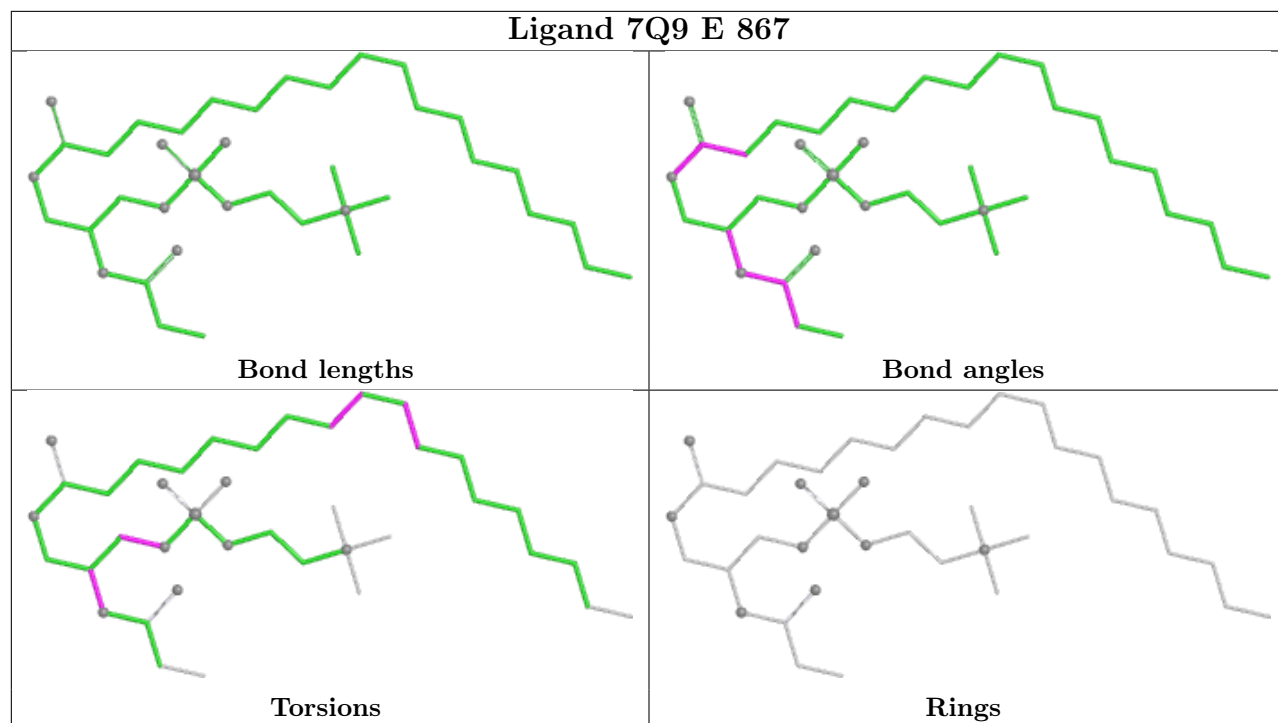


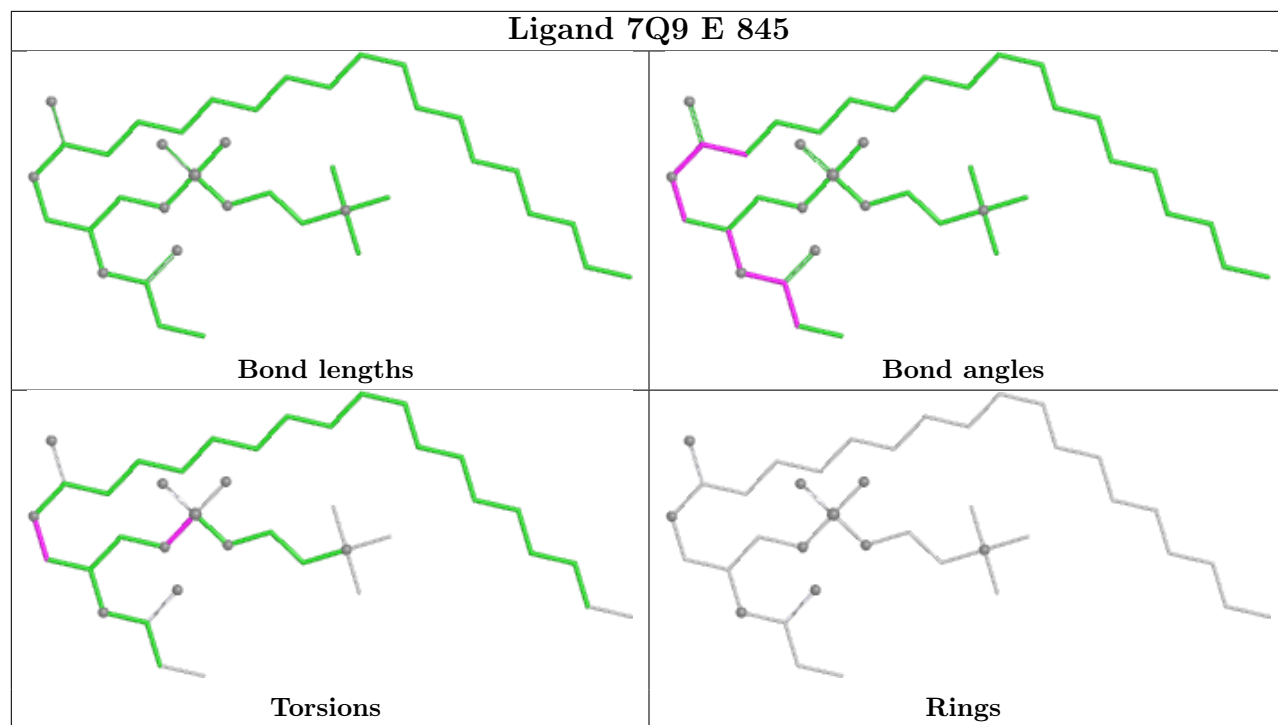
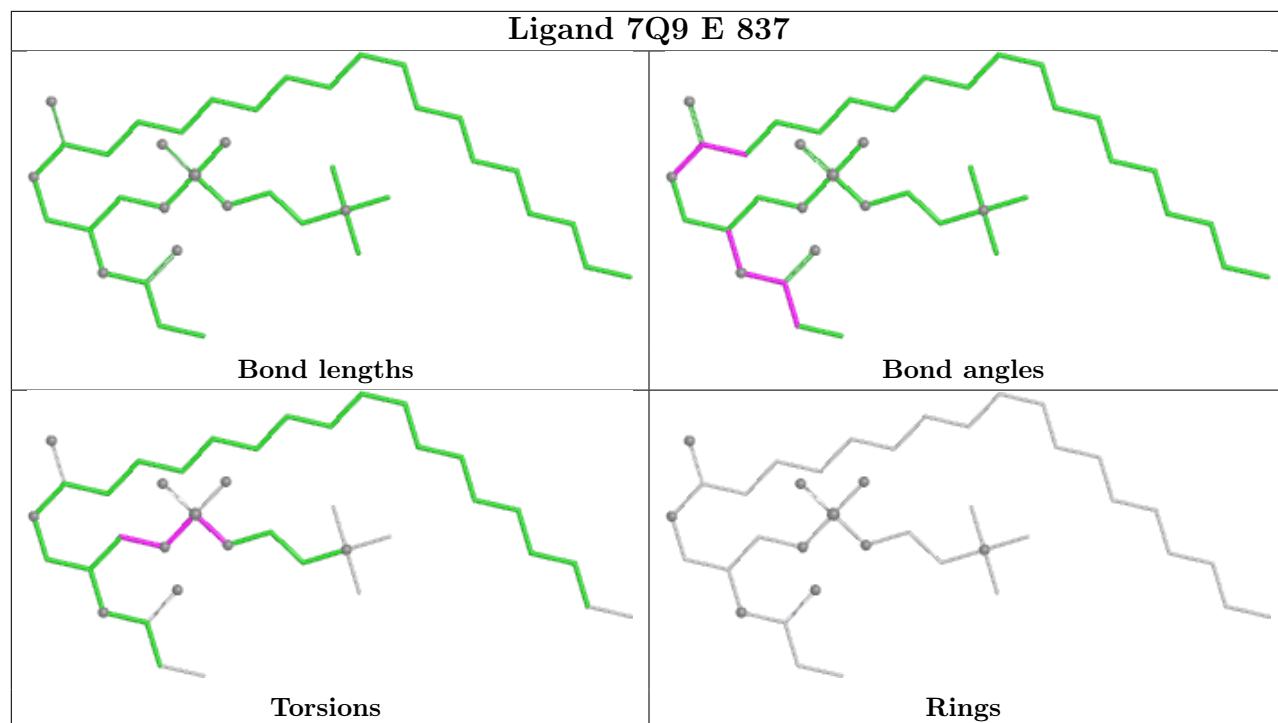


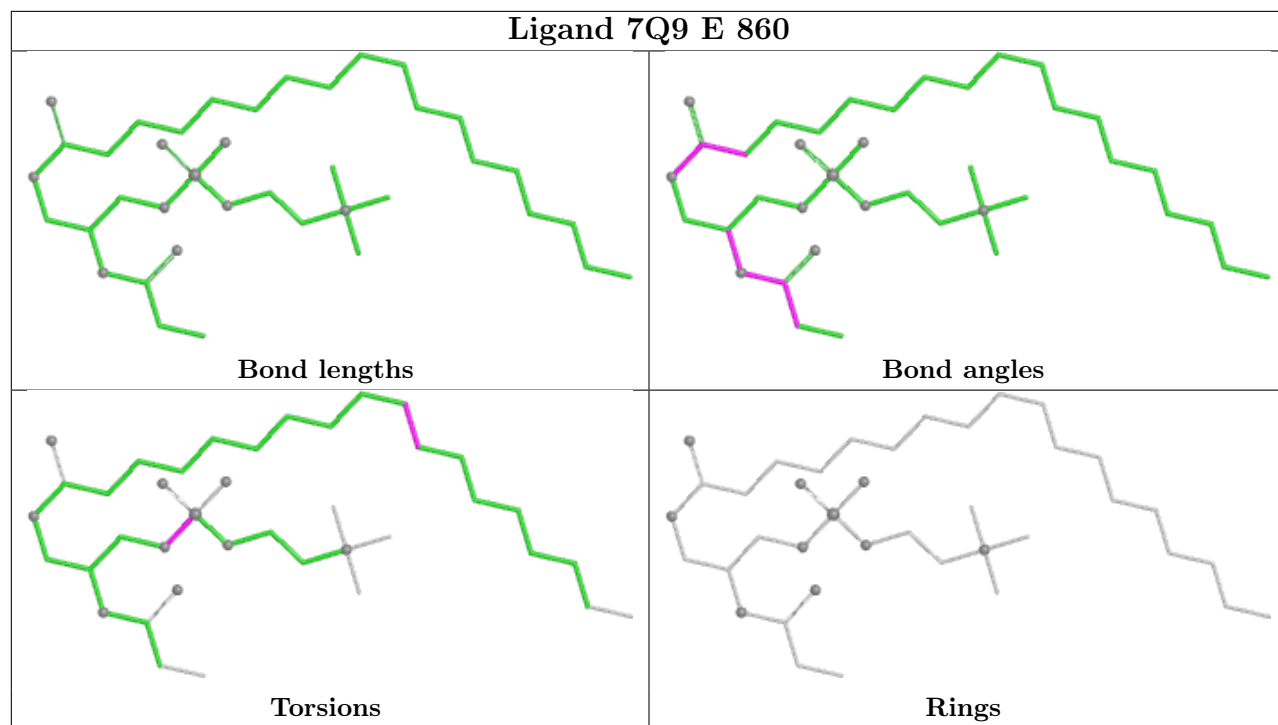
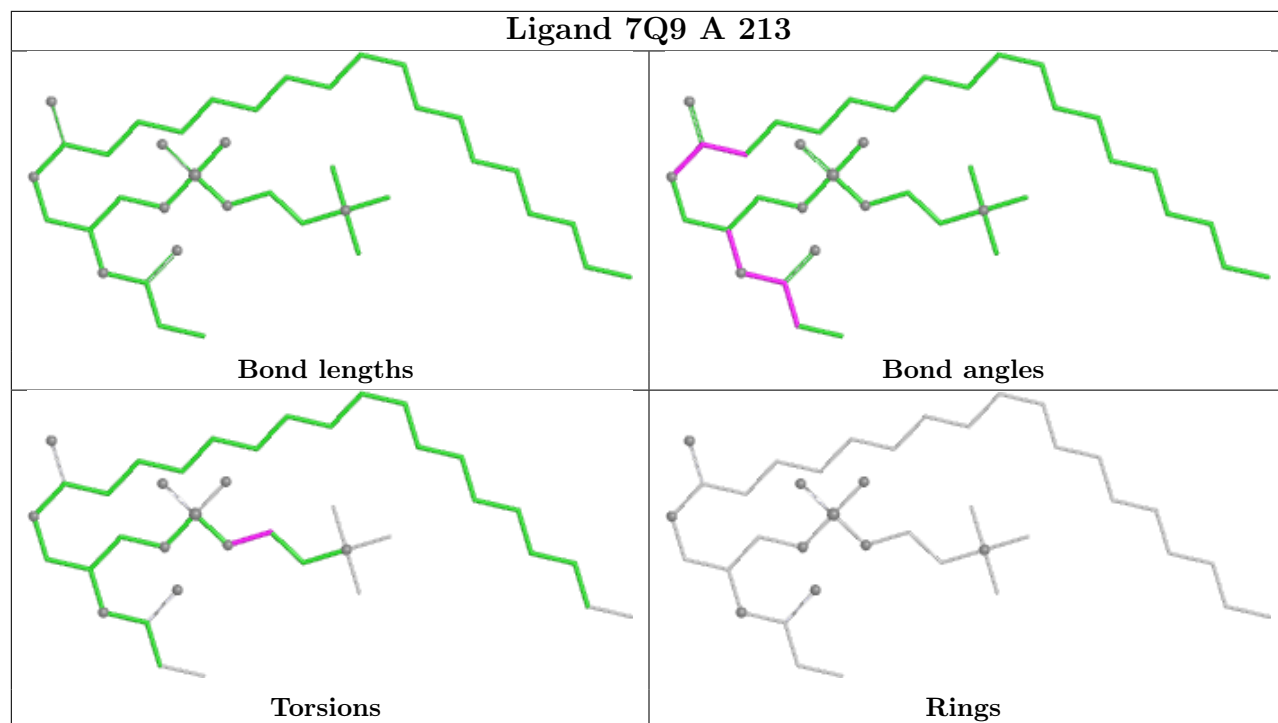


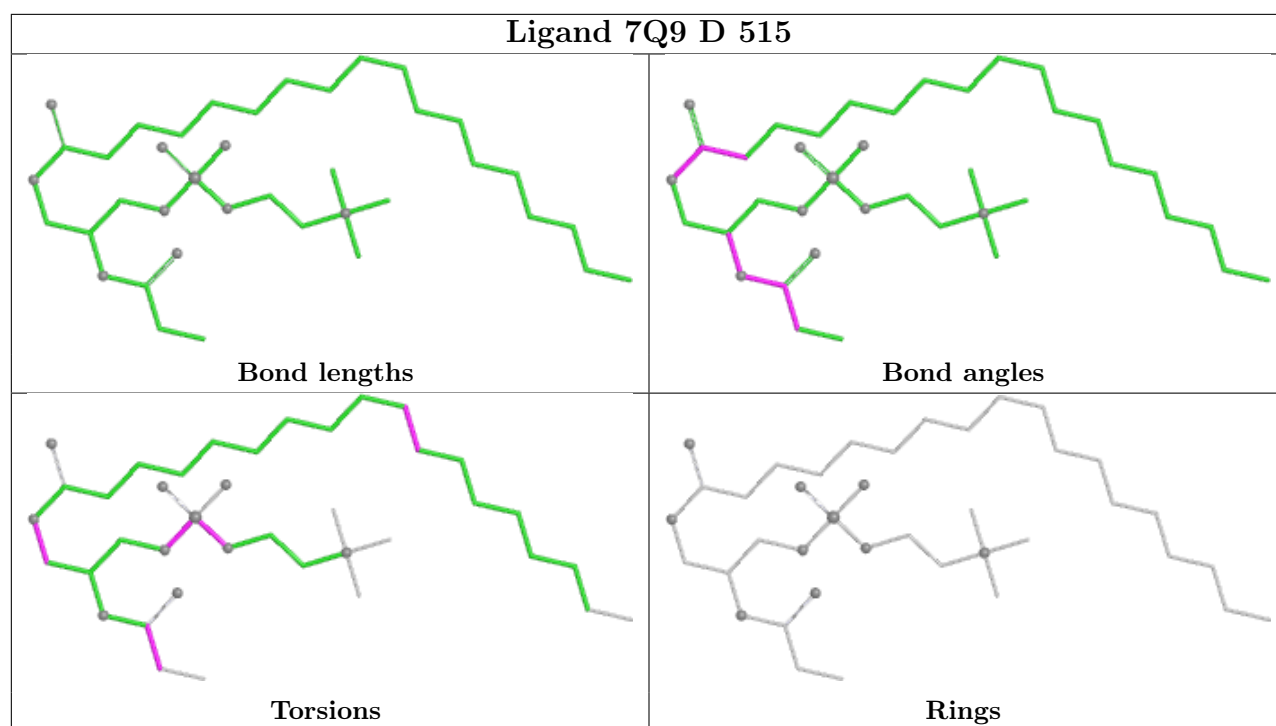




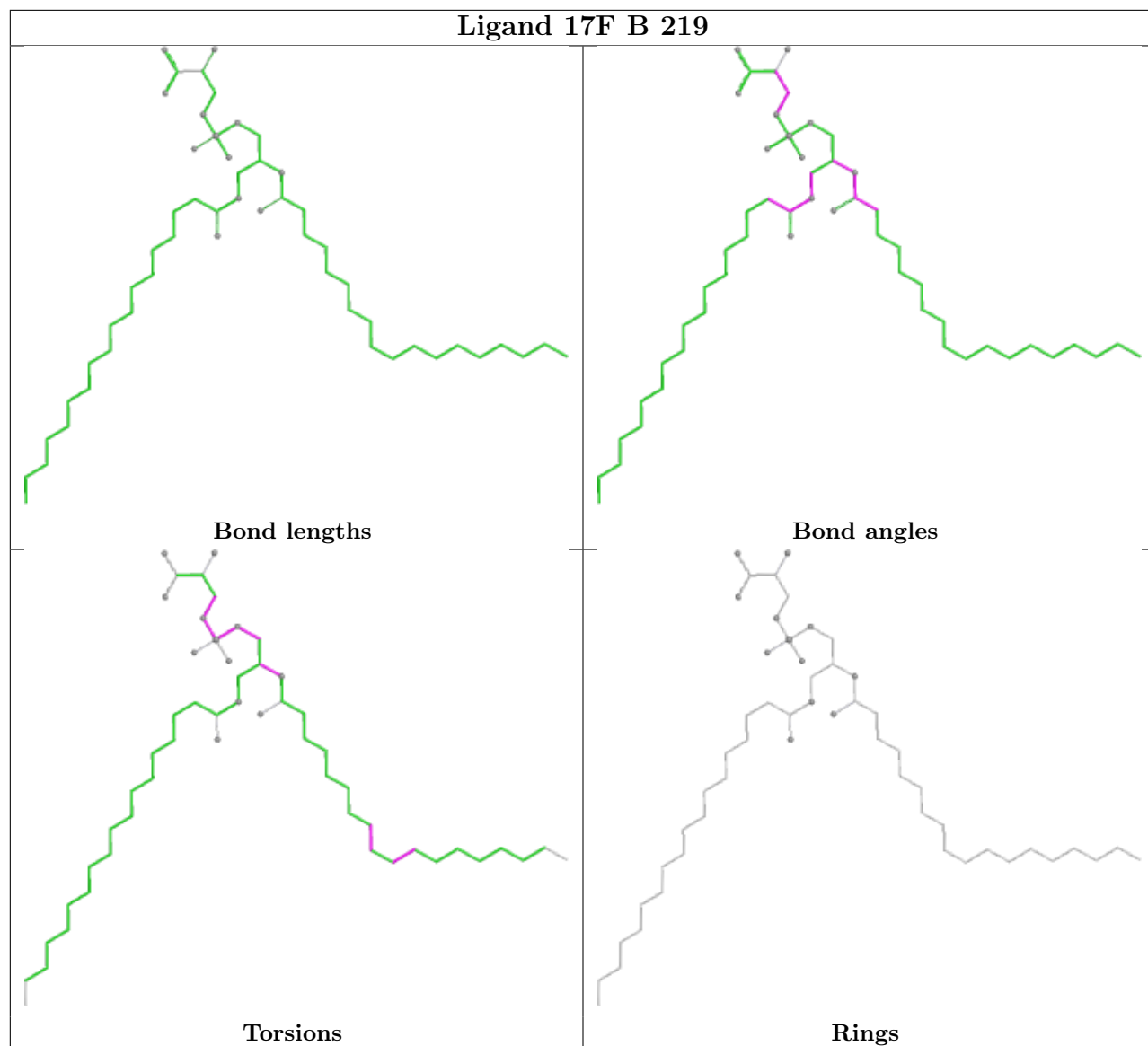


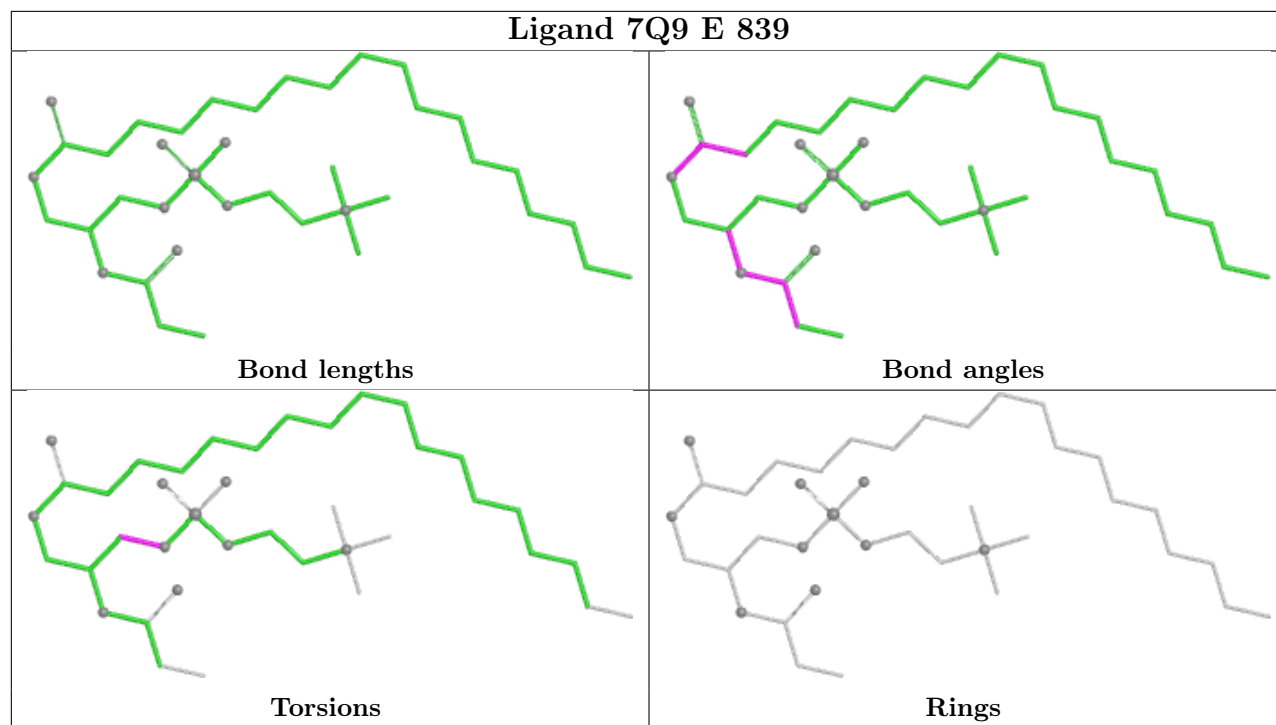
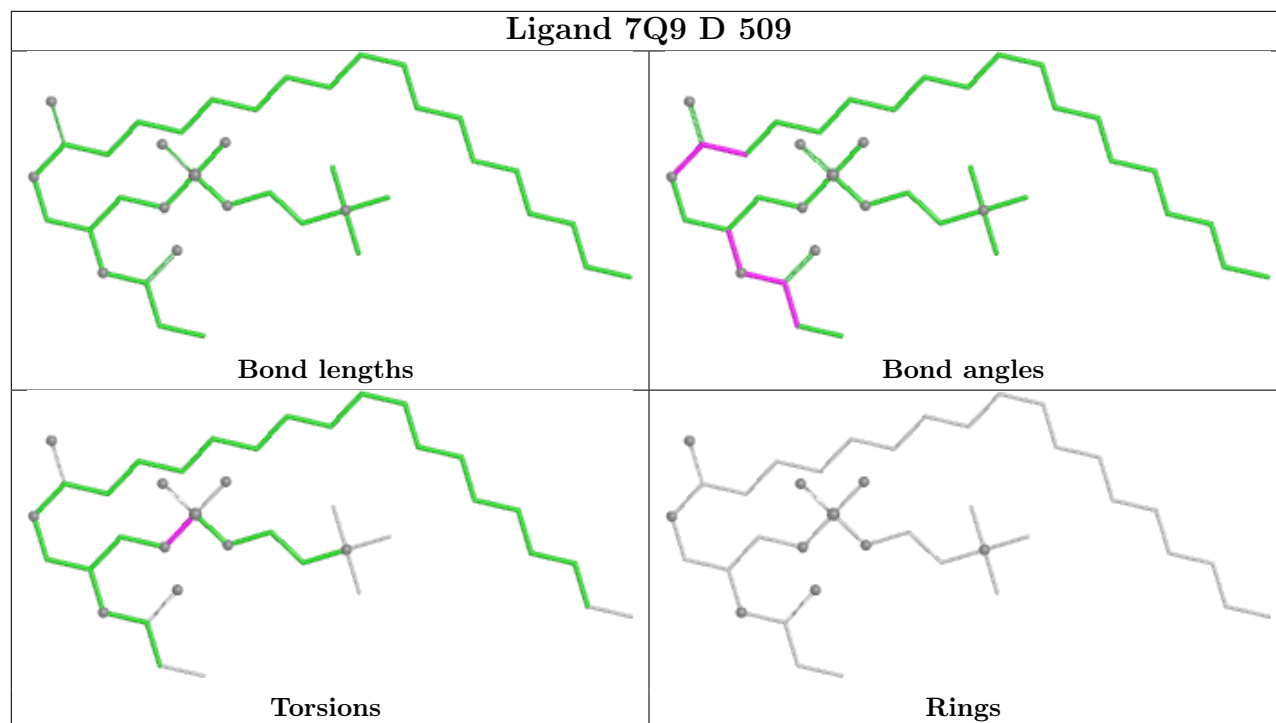


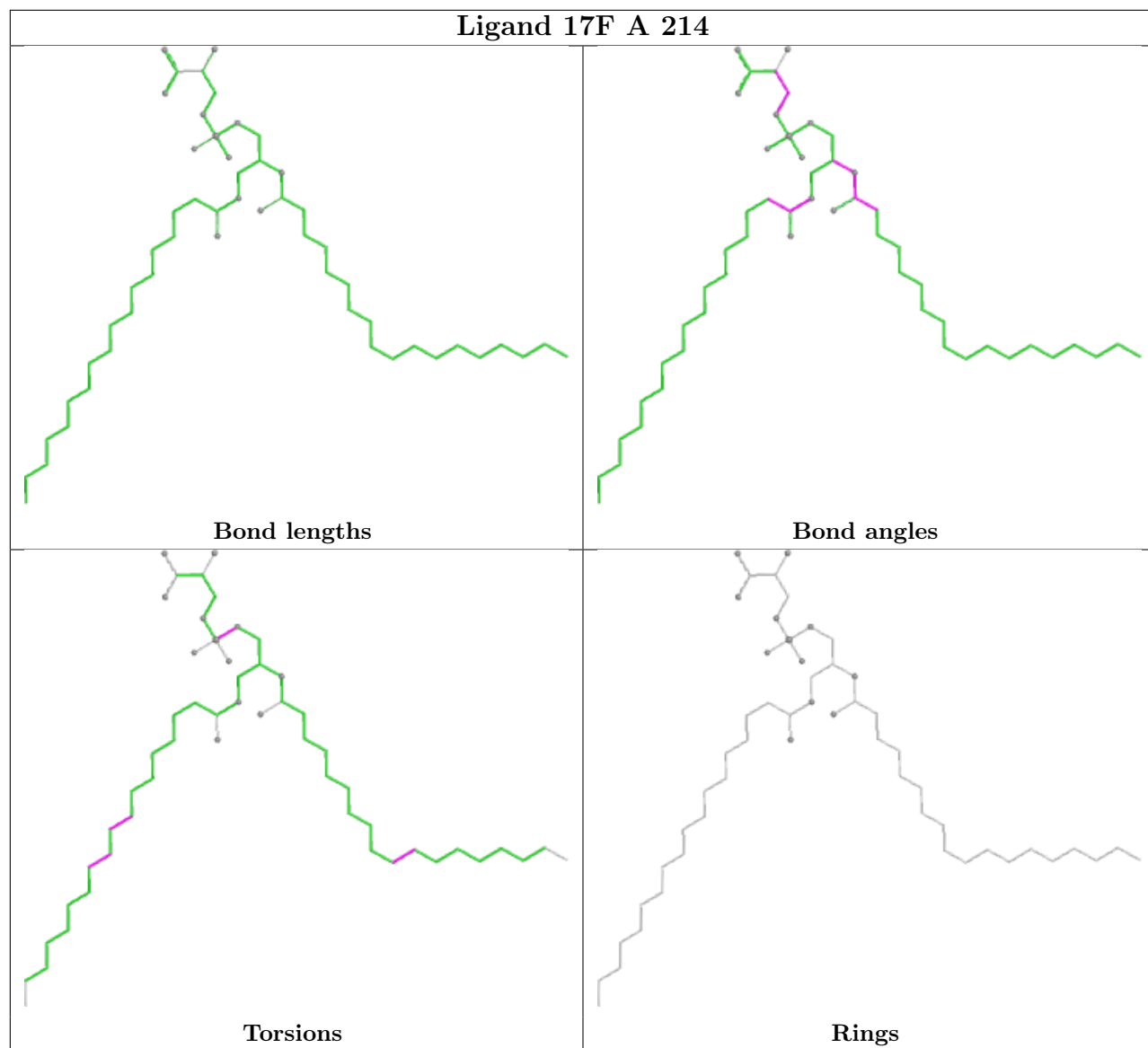


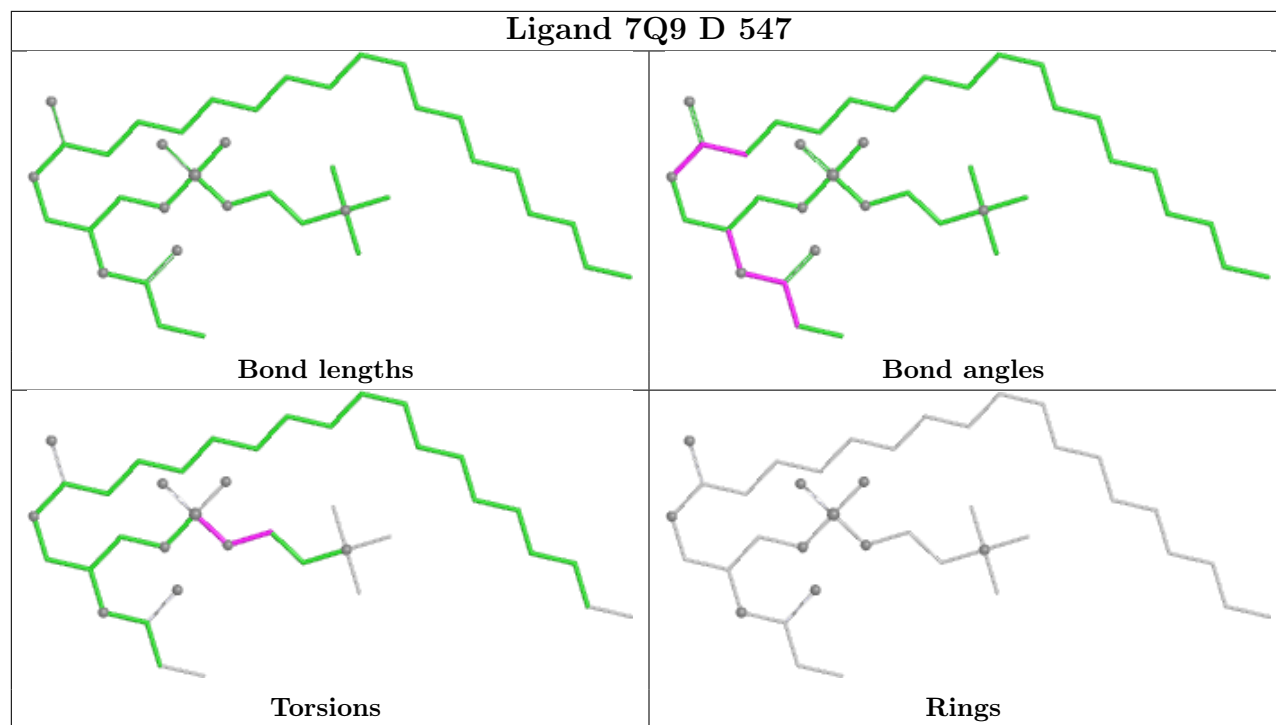
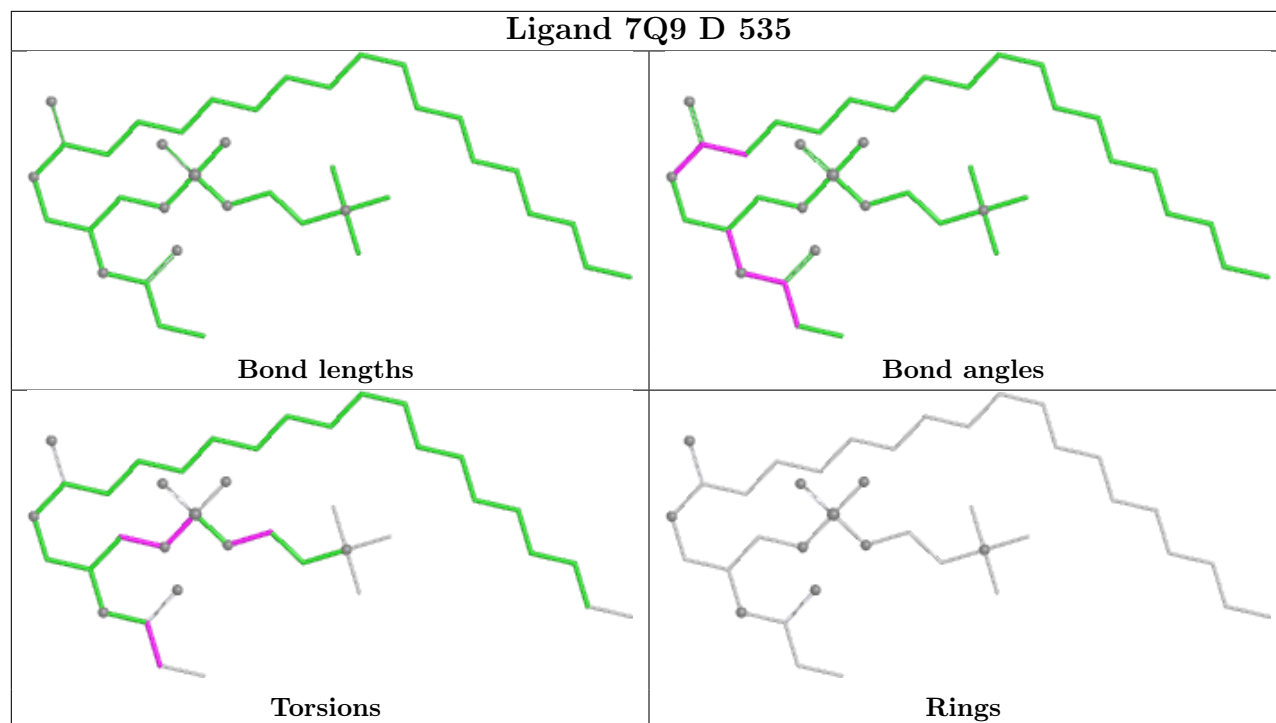


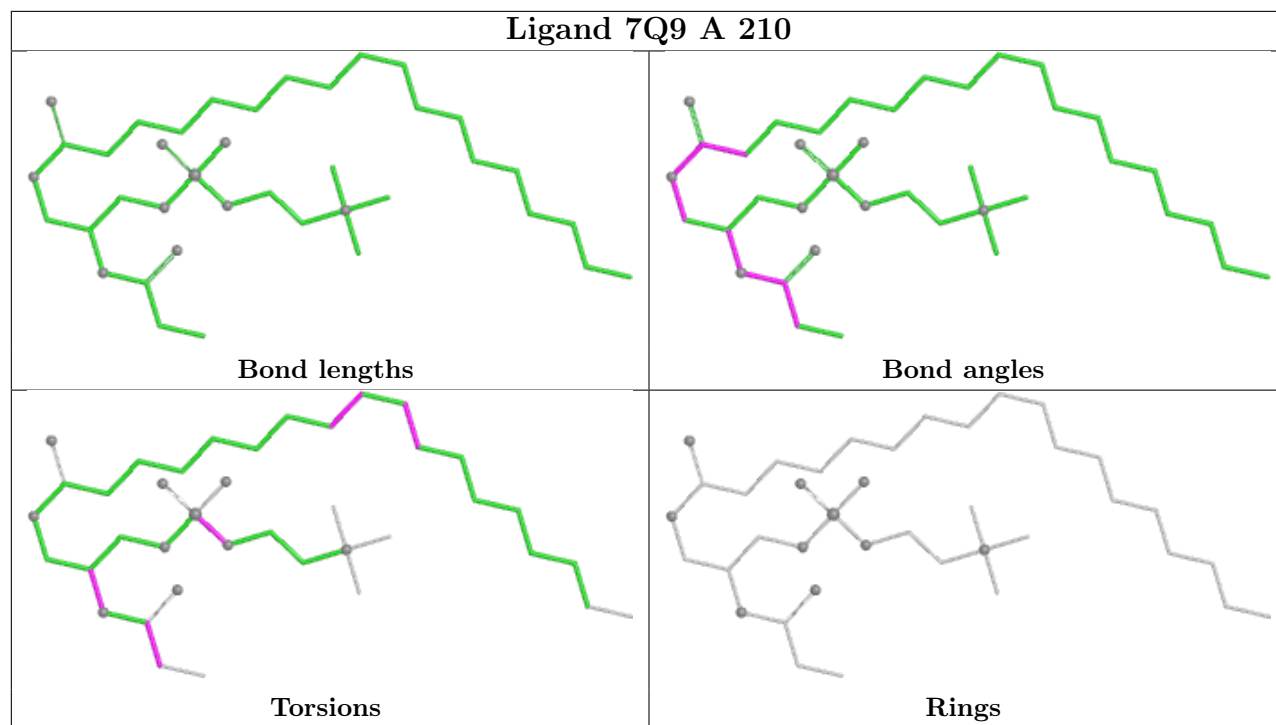
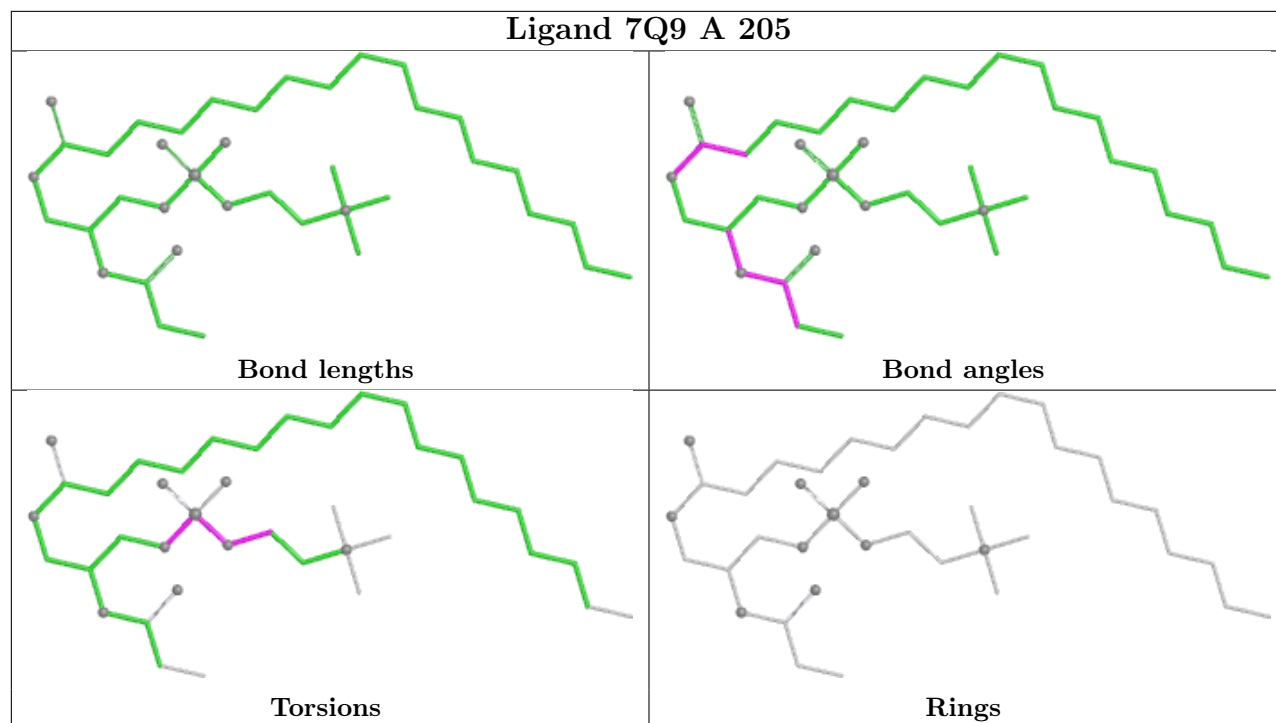
Ligand 17F B 219

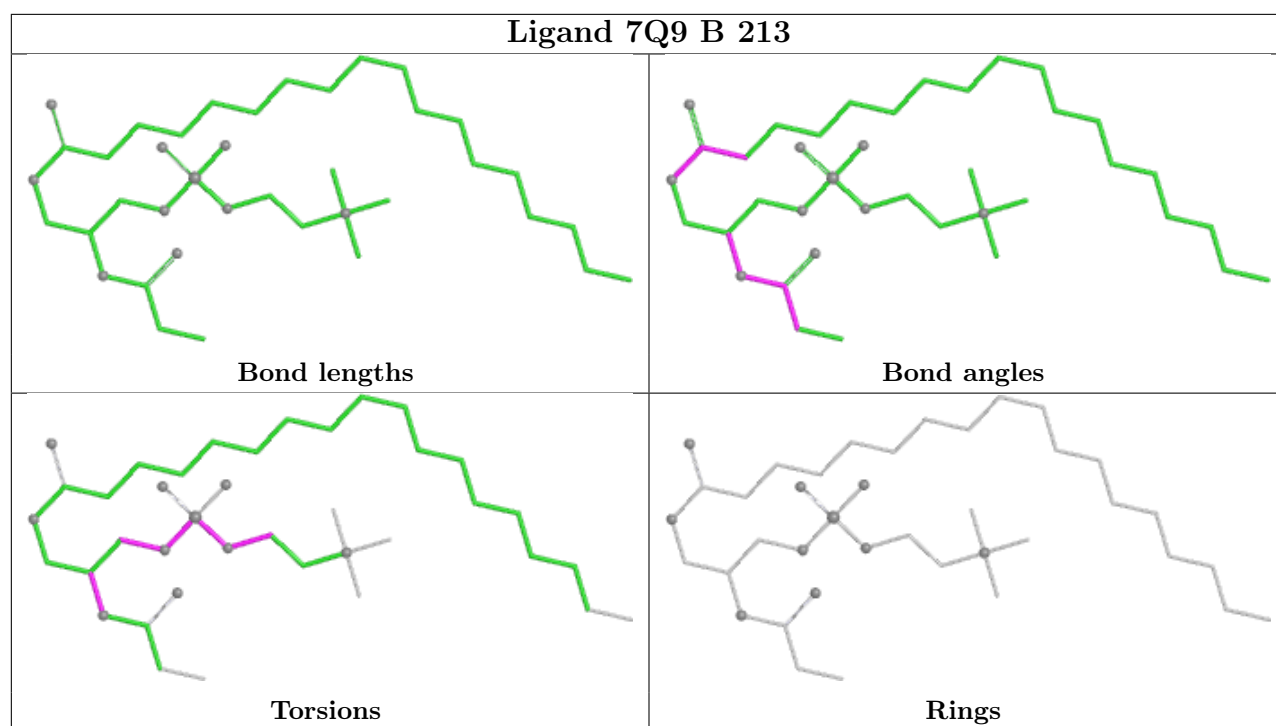




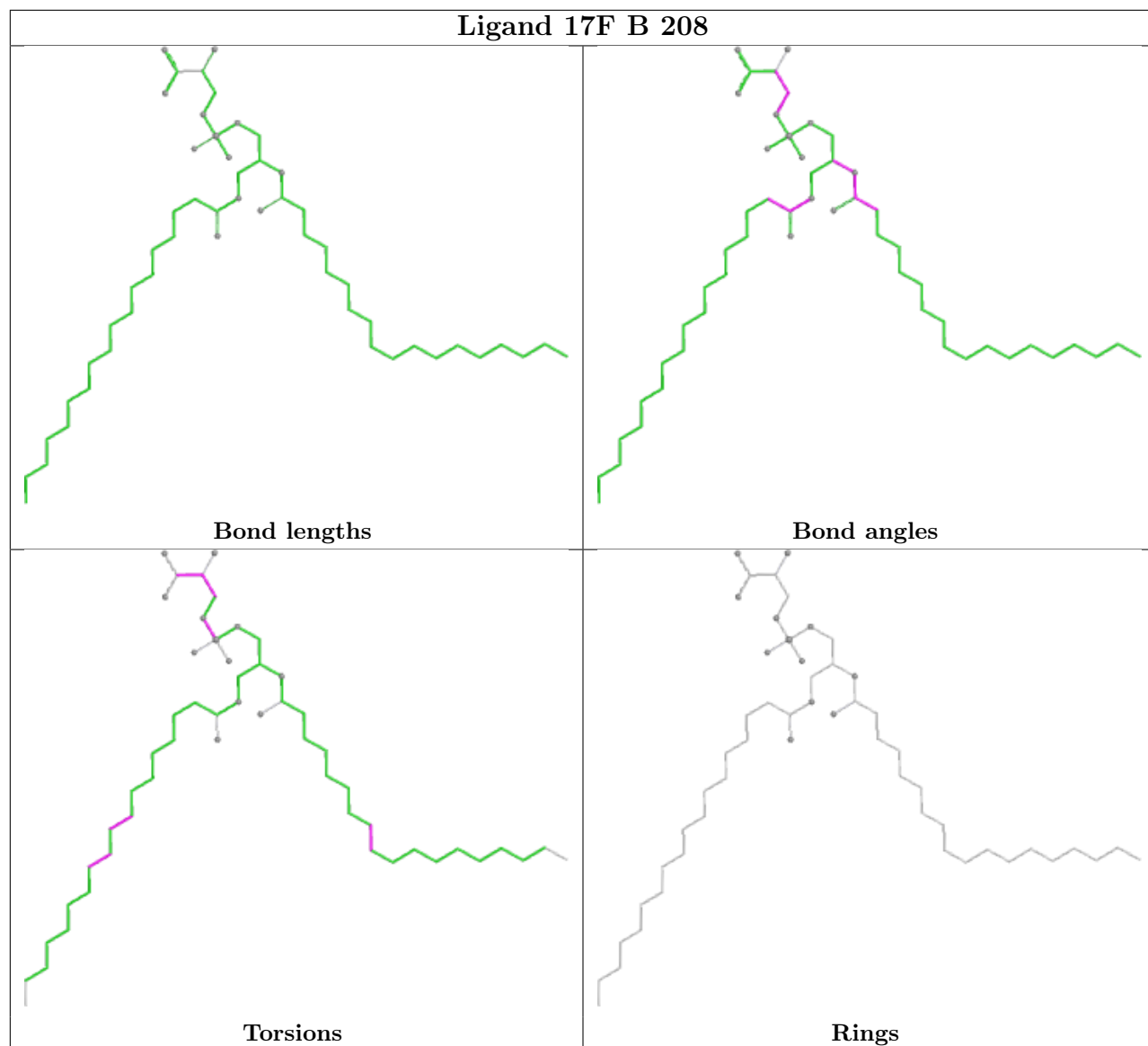


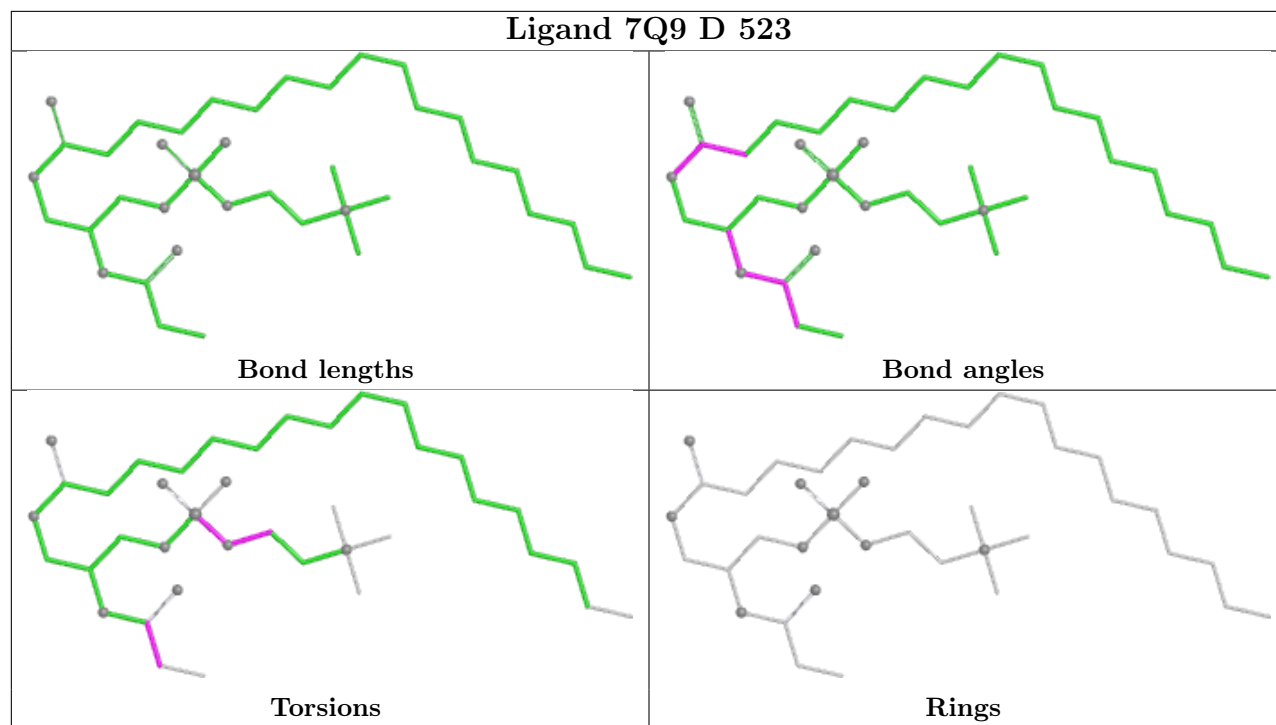
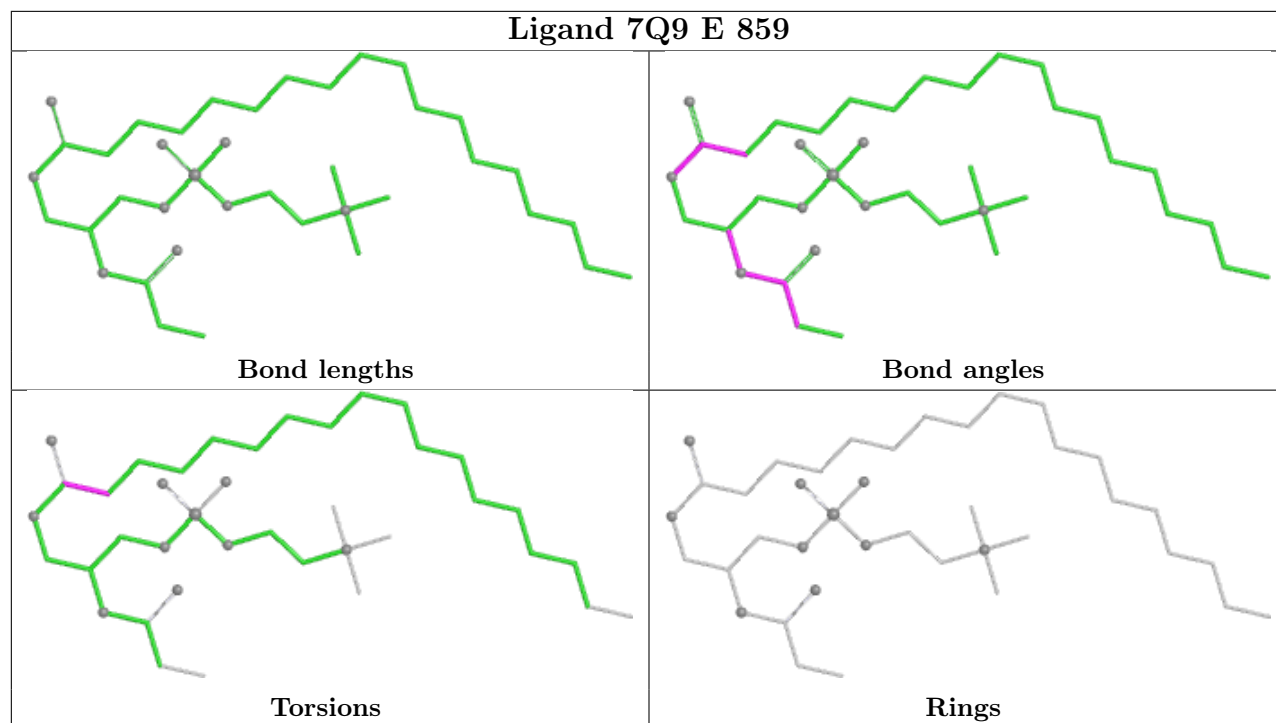


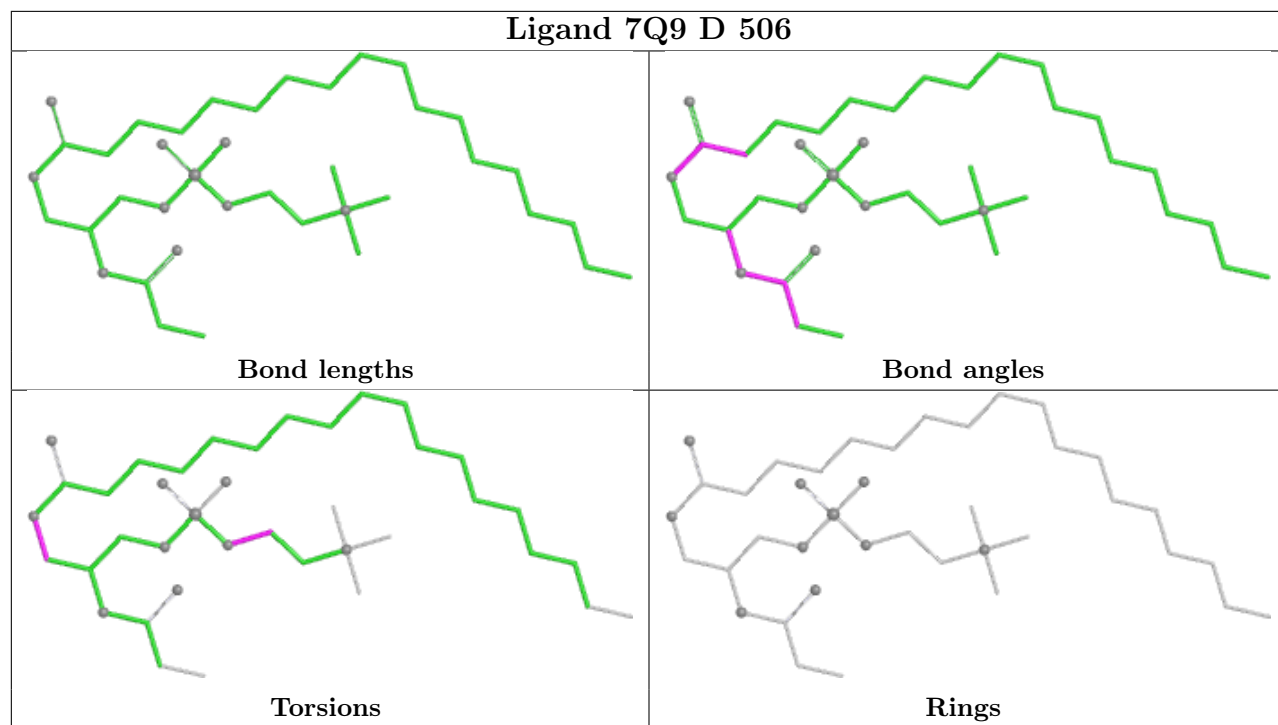
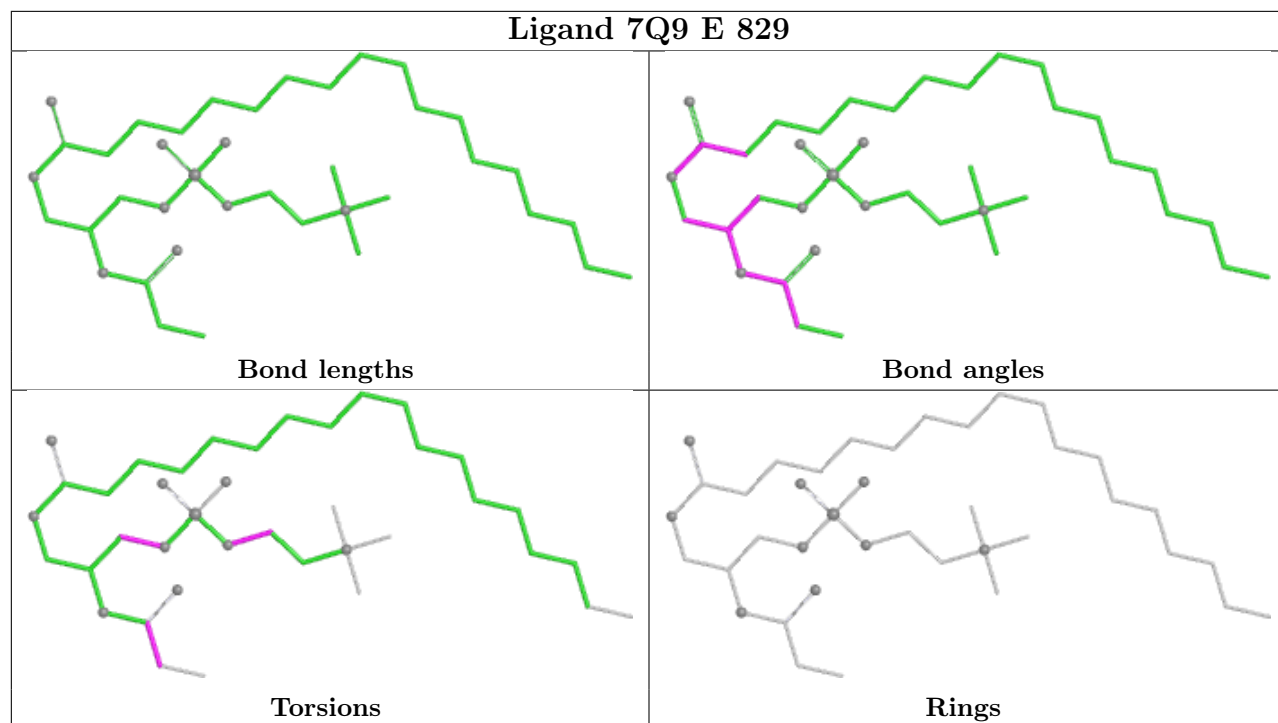


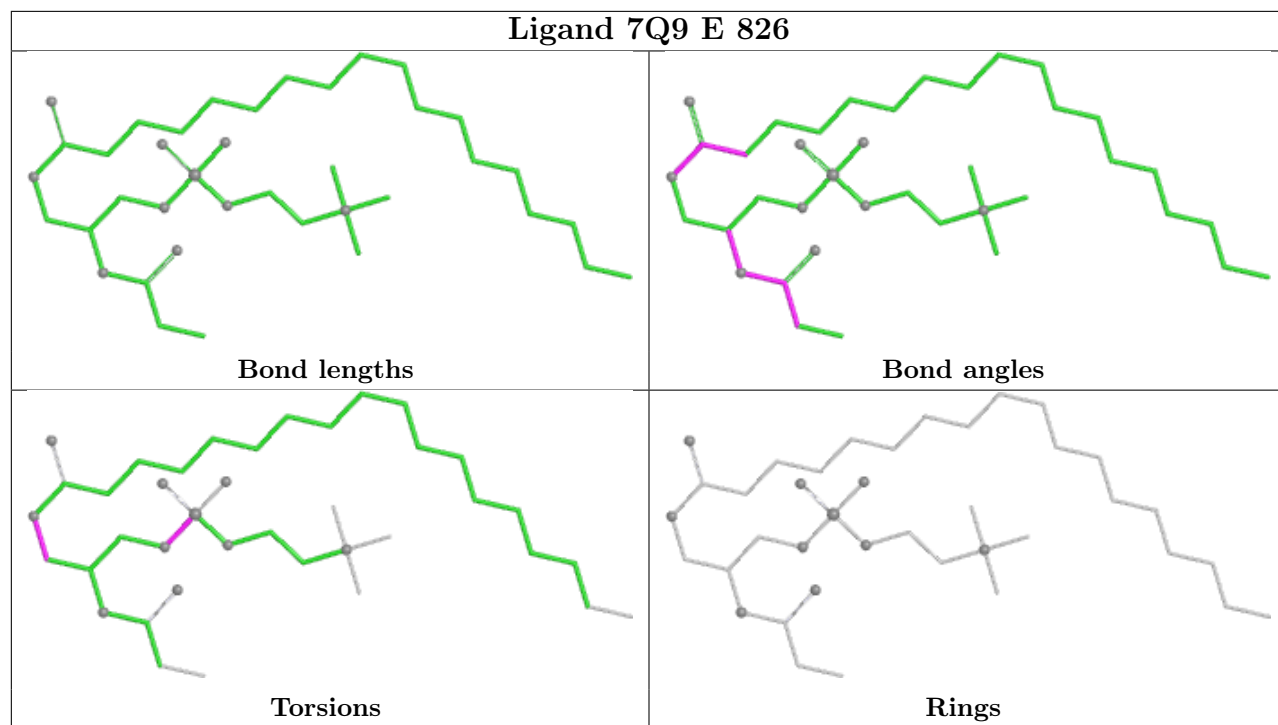
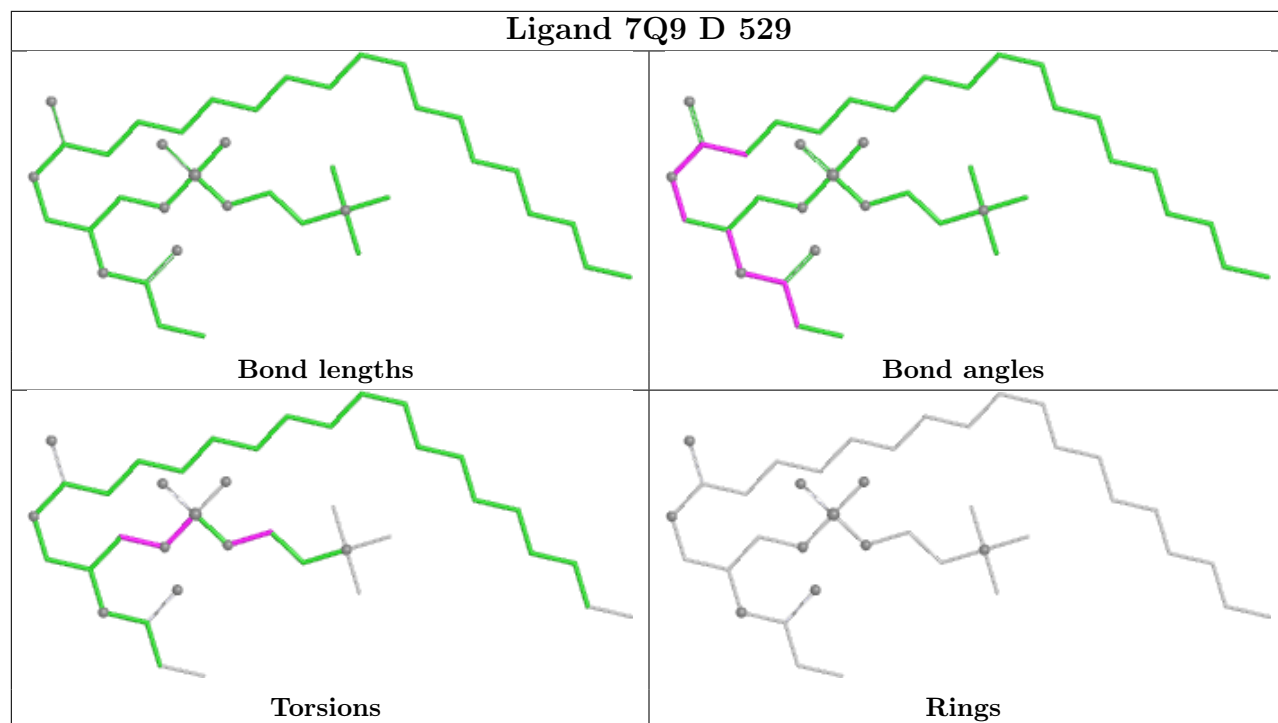


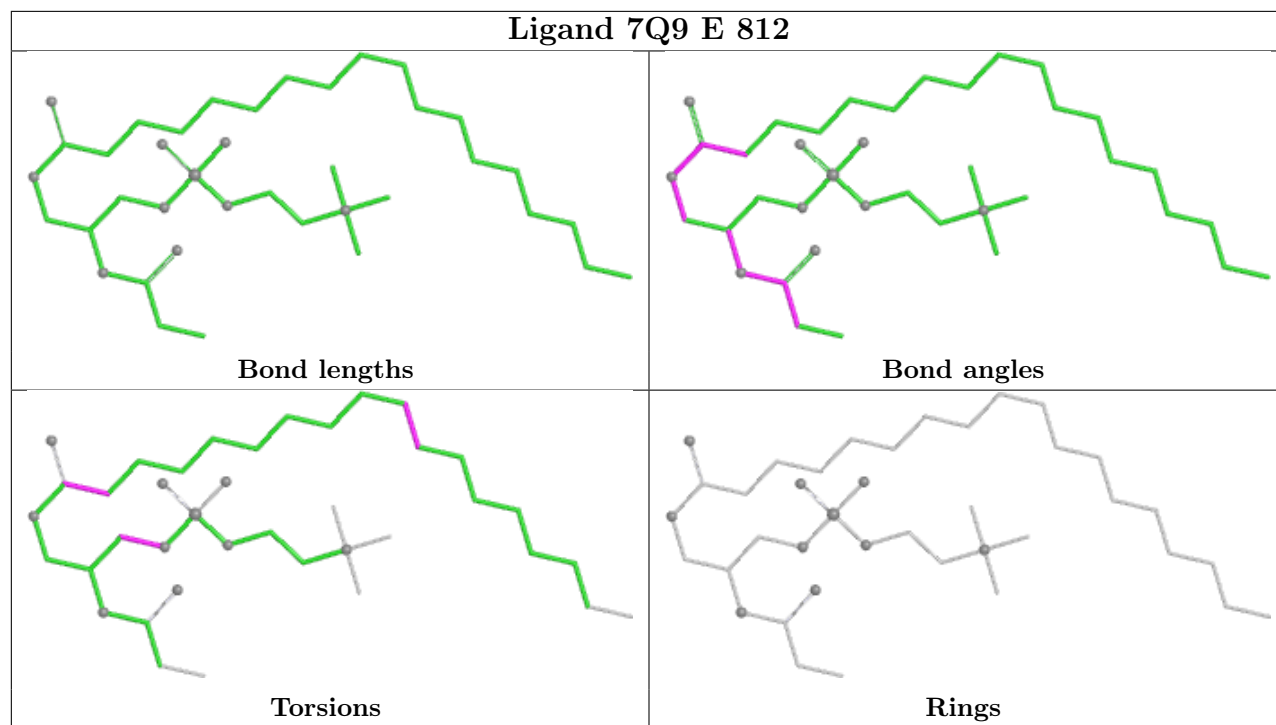
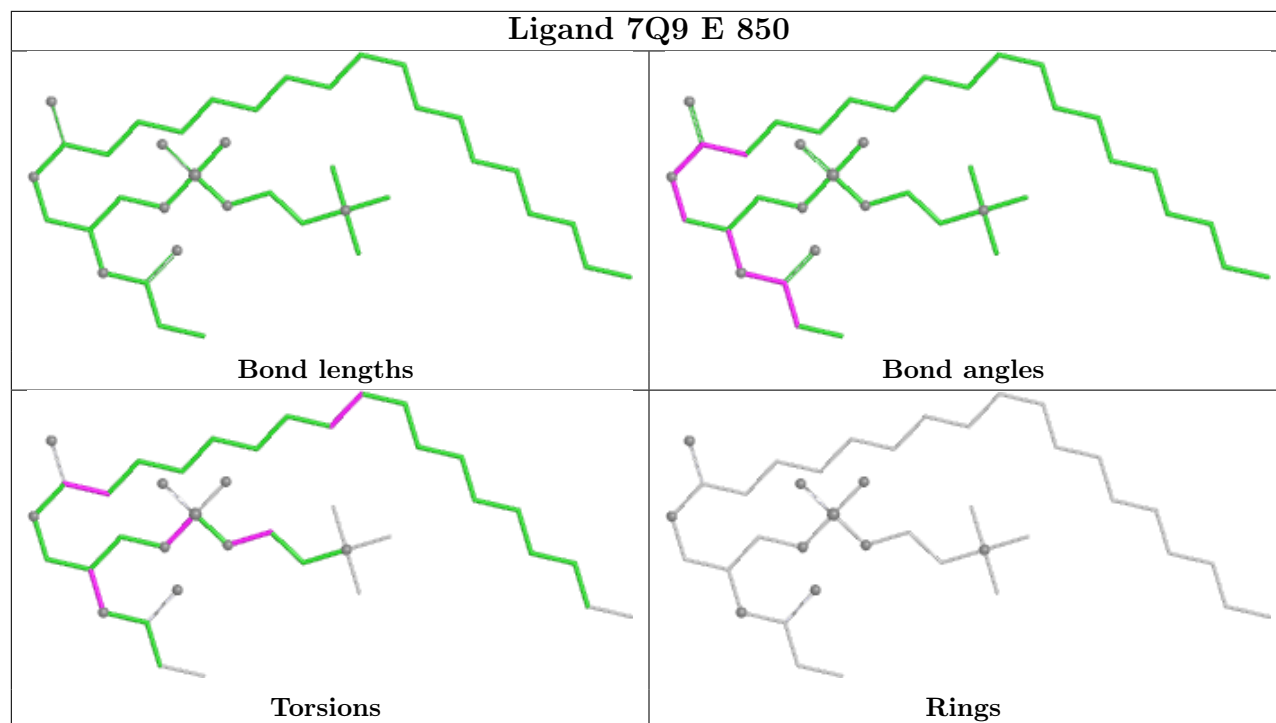
Ligand 17F B 208



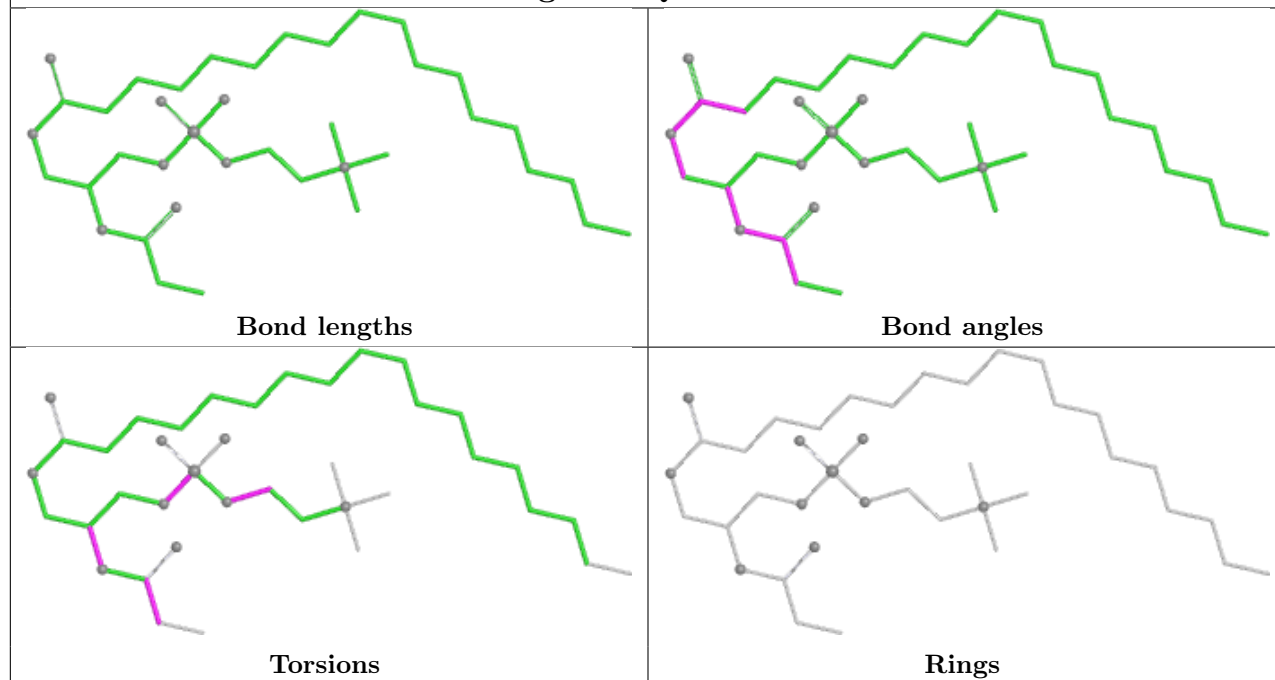




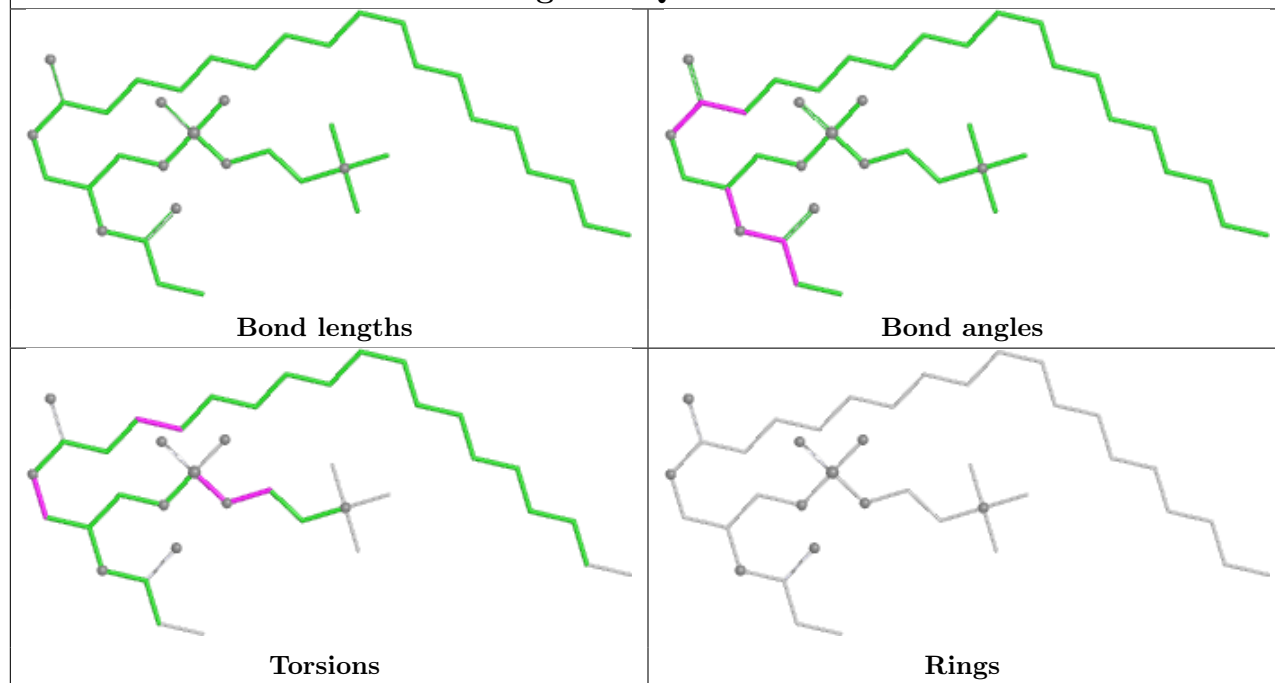


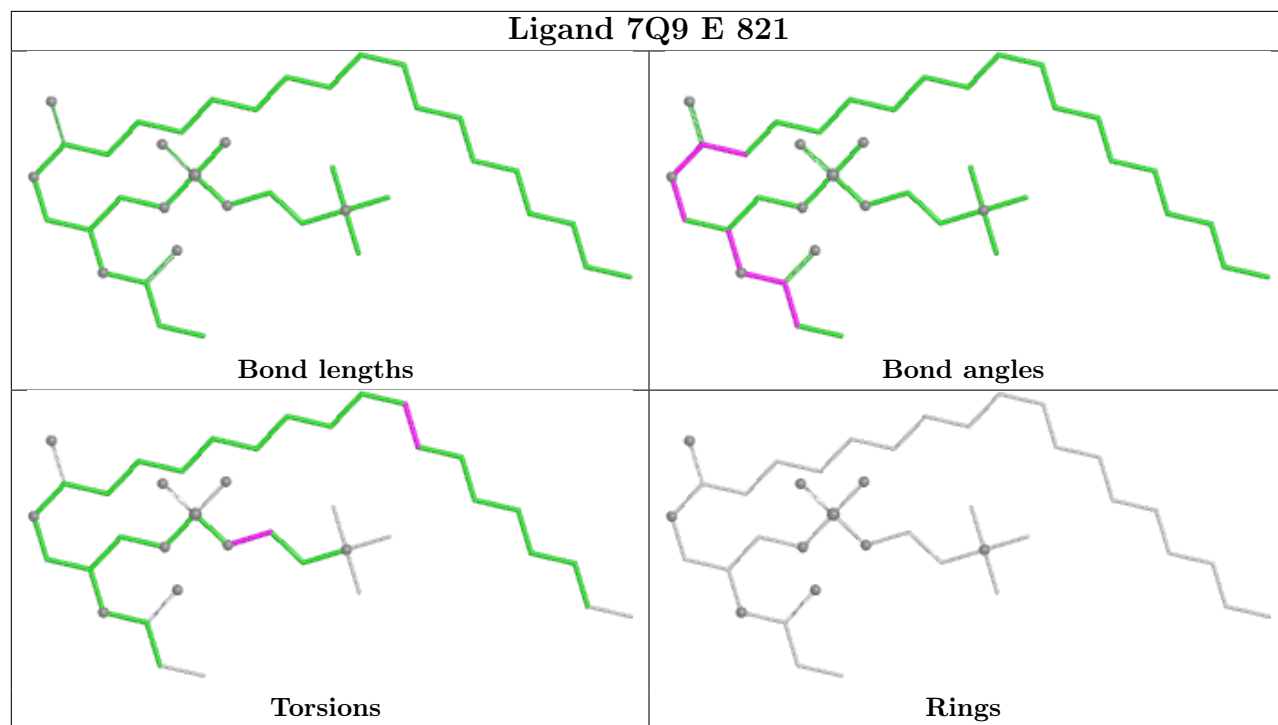
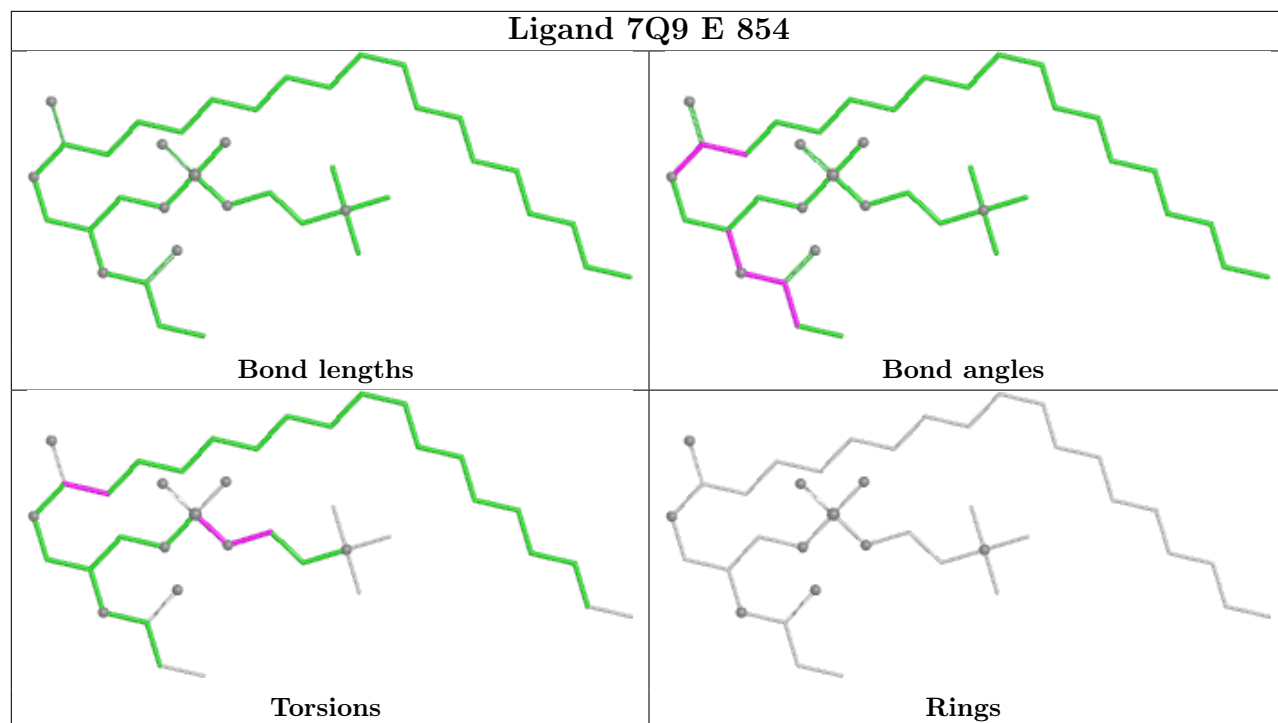


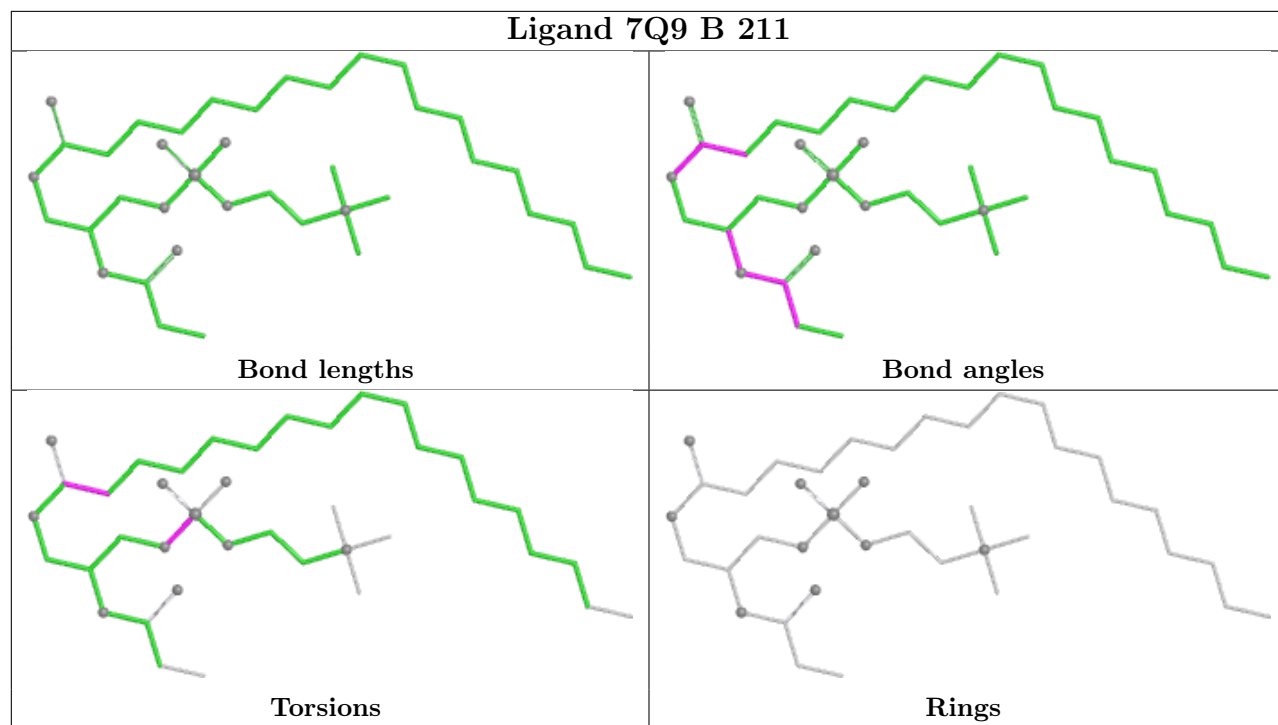
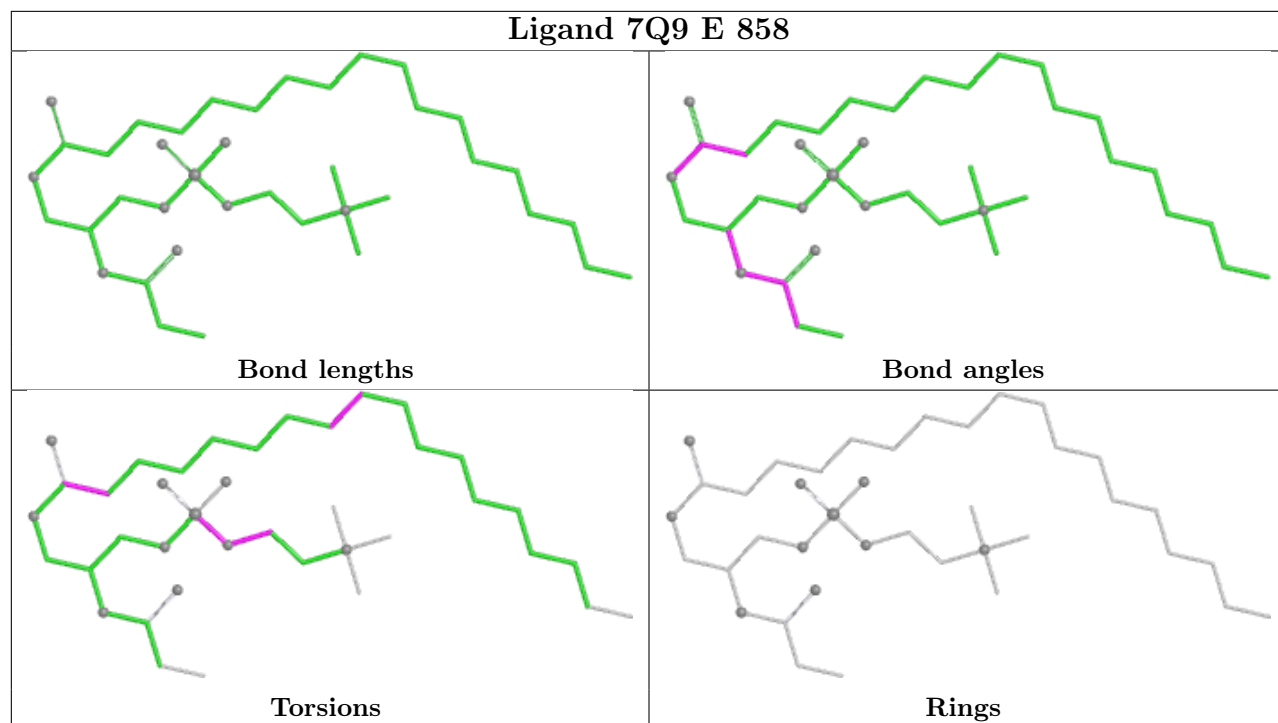
Ligand 7Q9 E 825

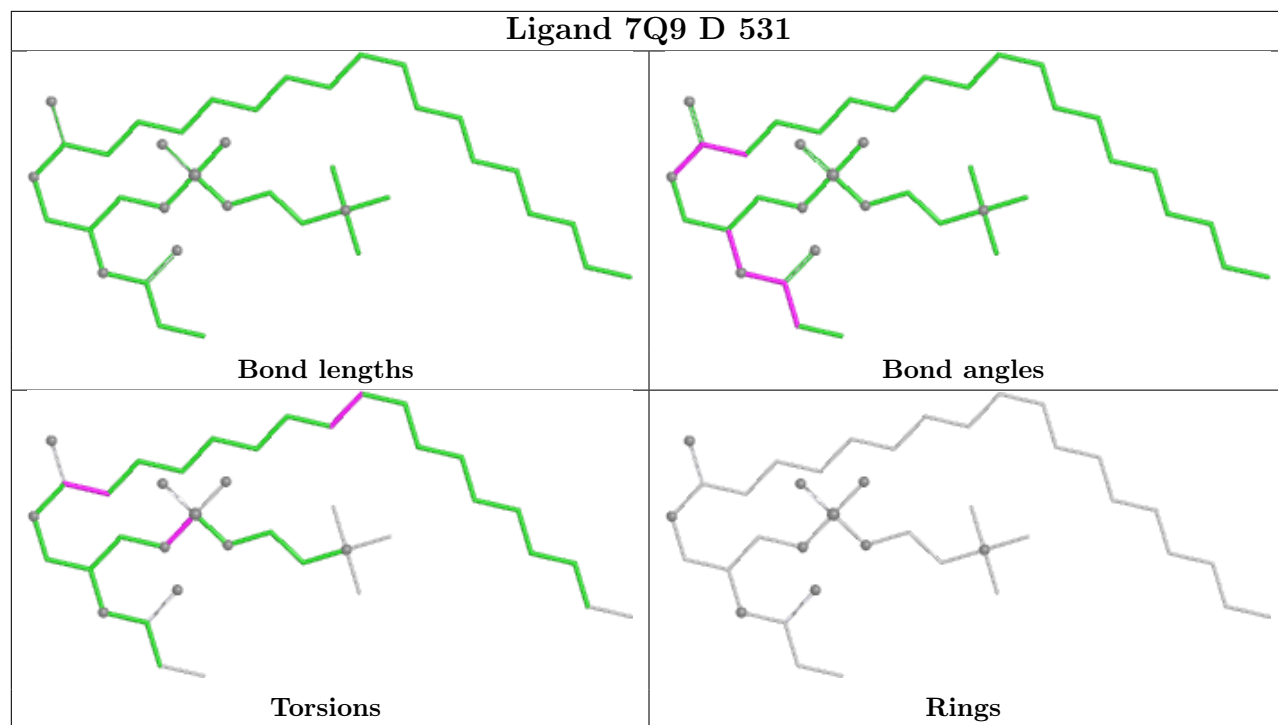
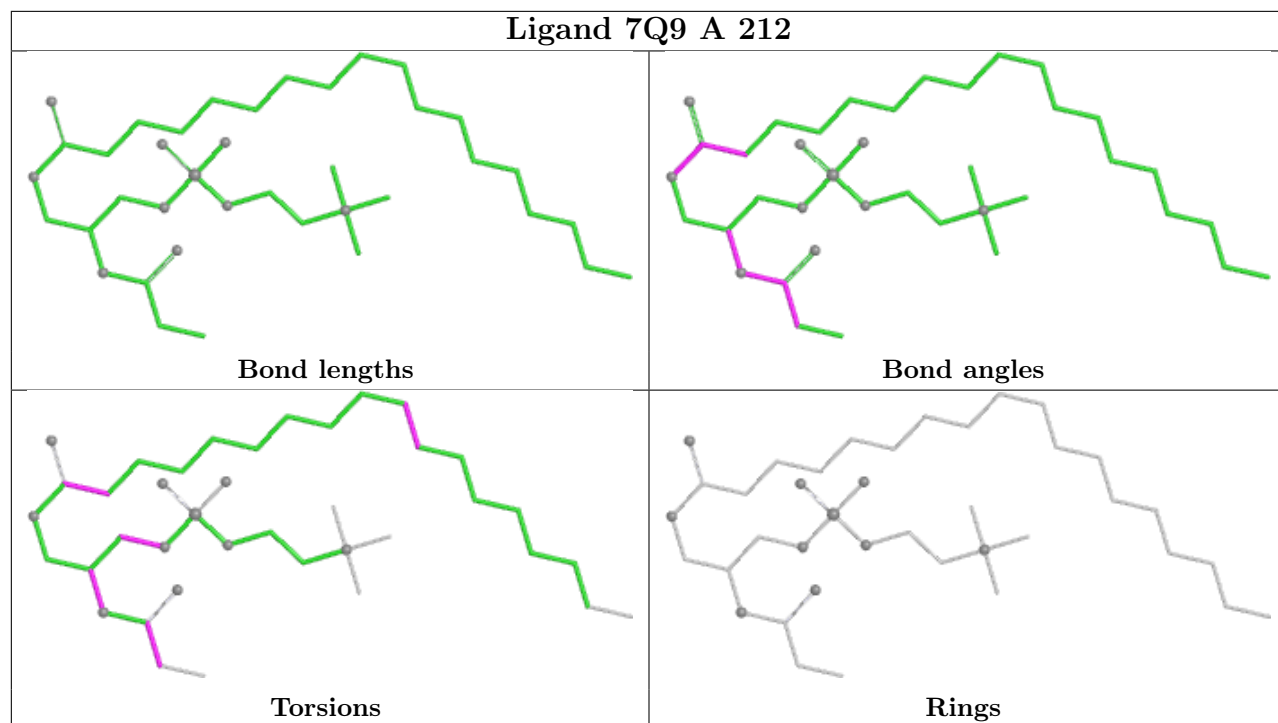


Ligand 7Q9 D 541

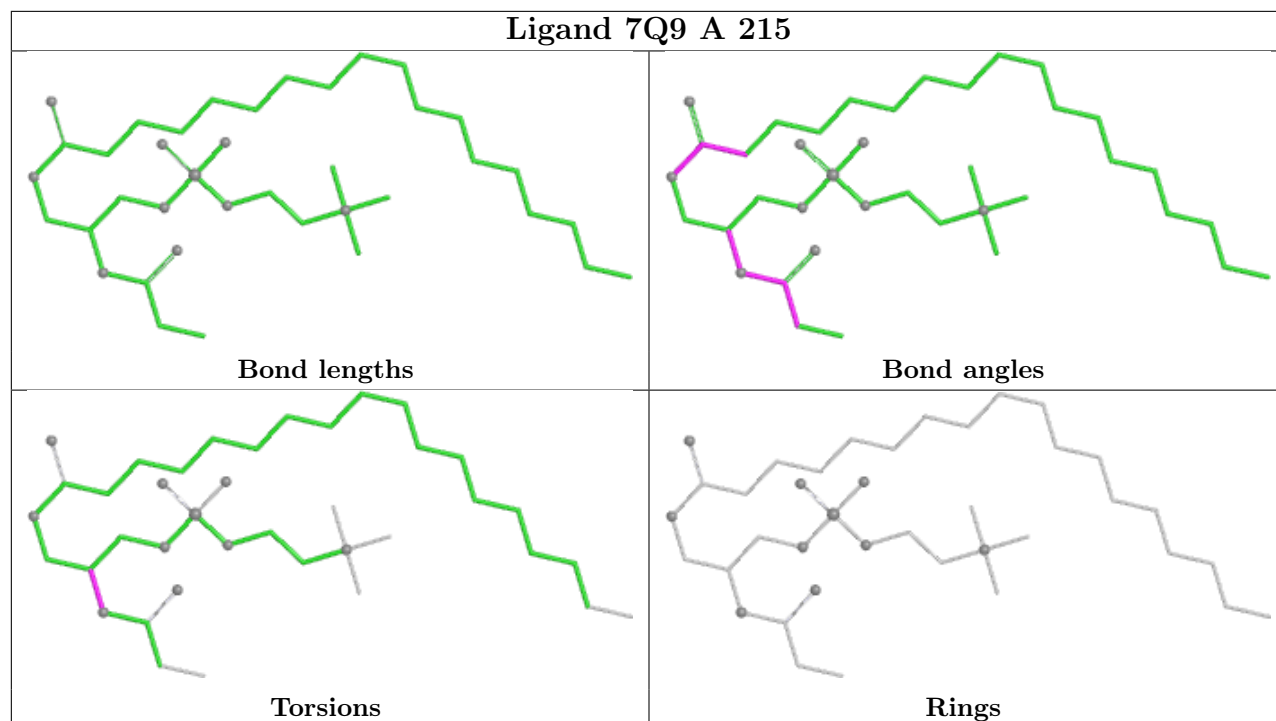




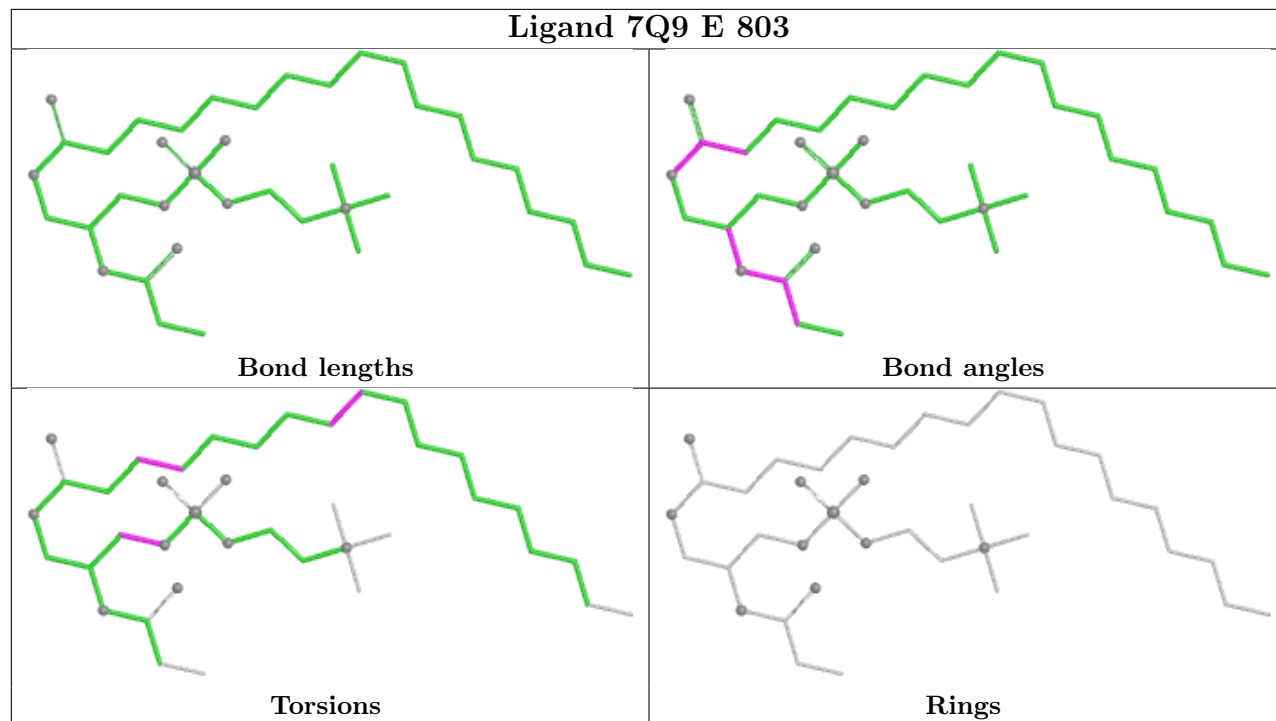


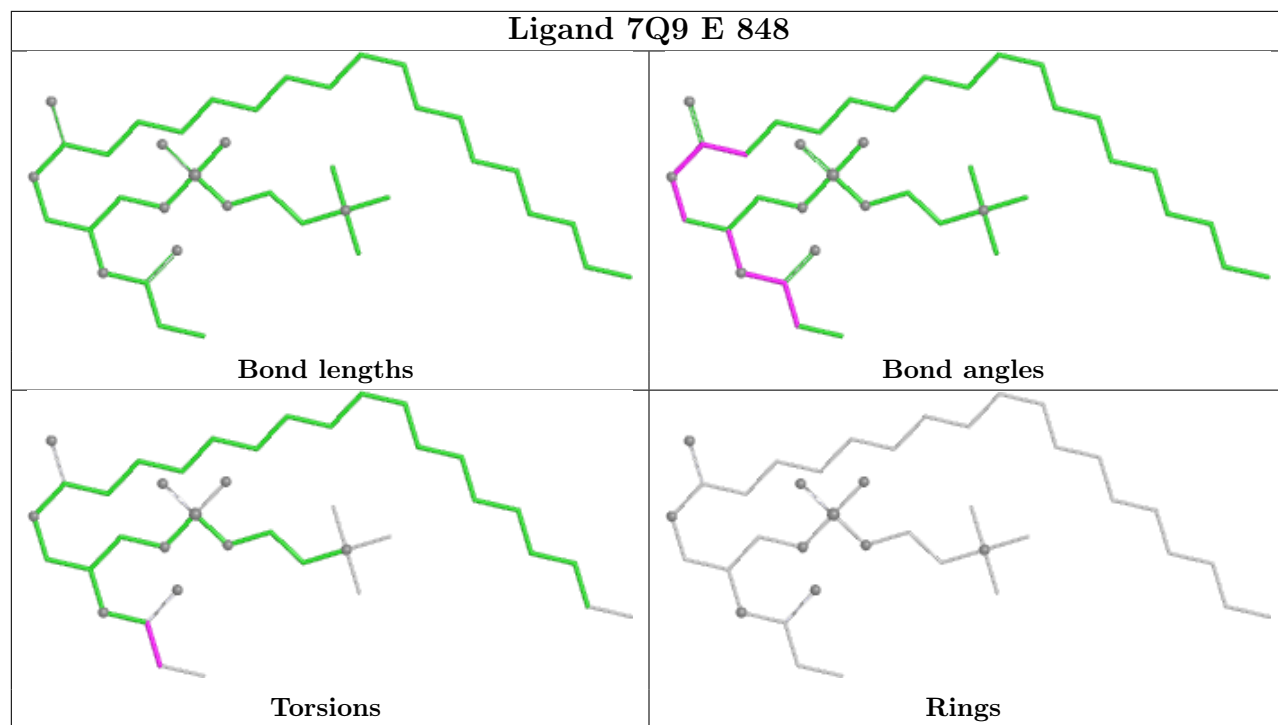
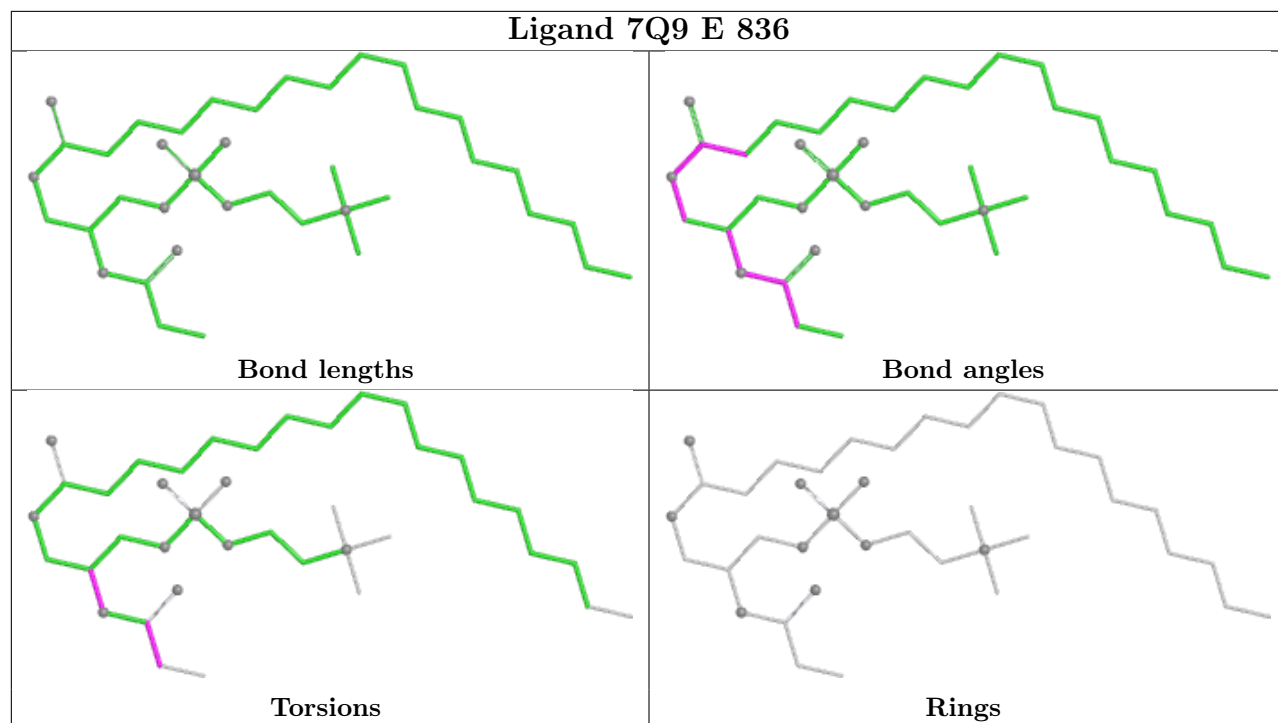


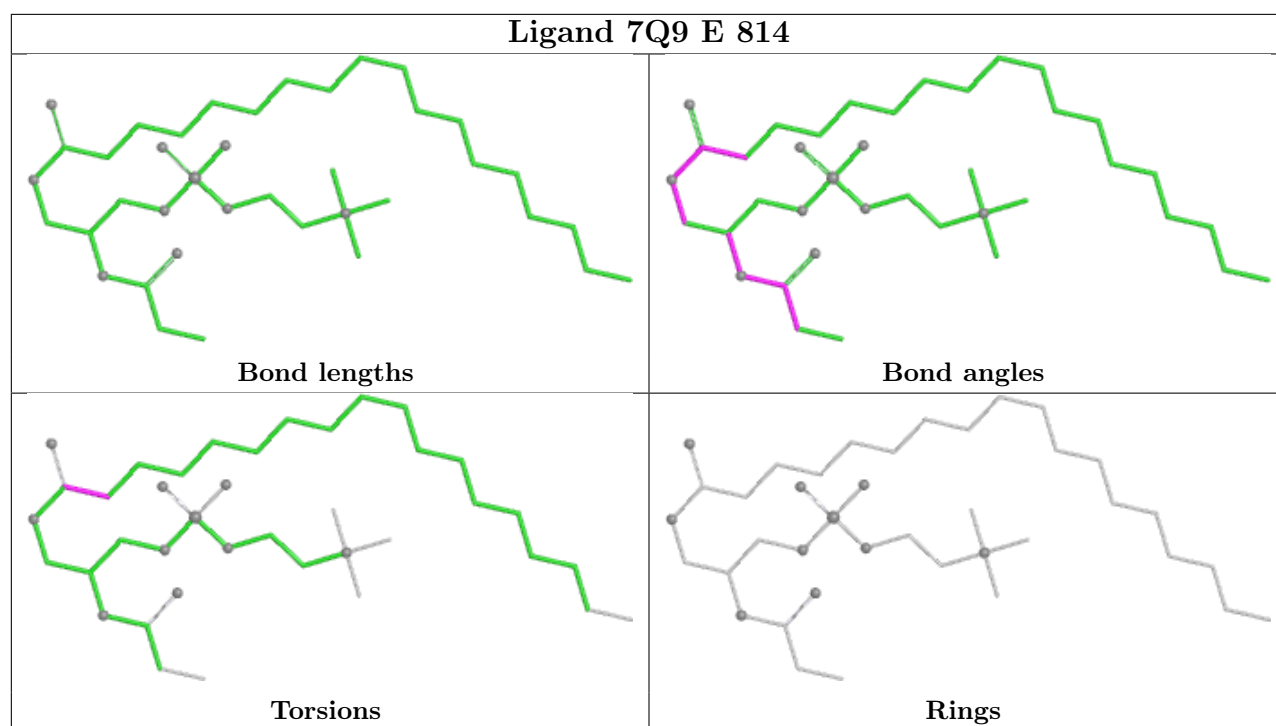
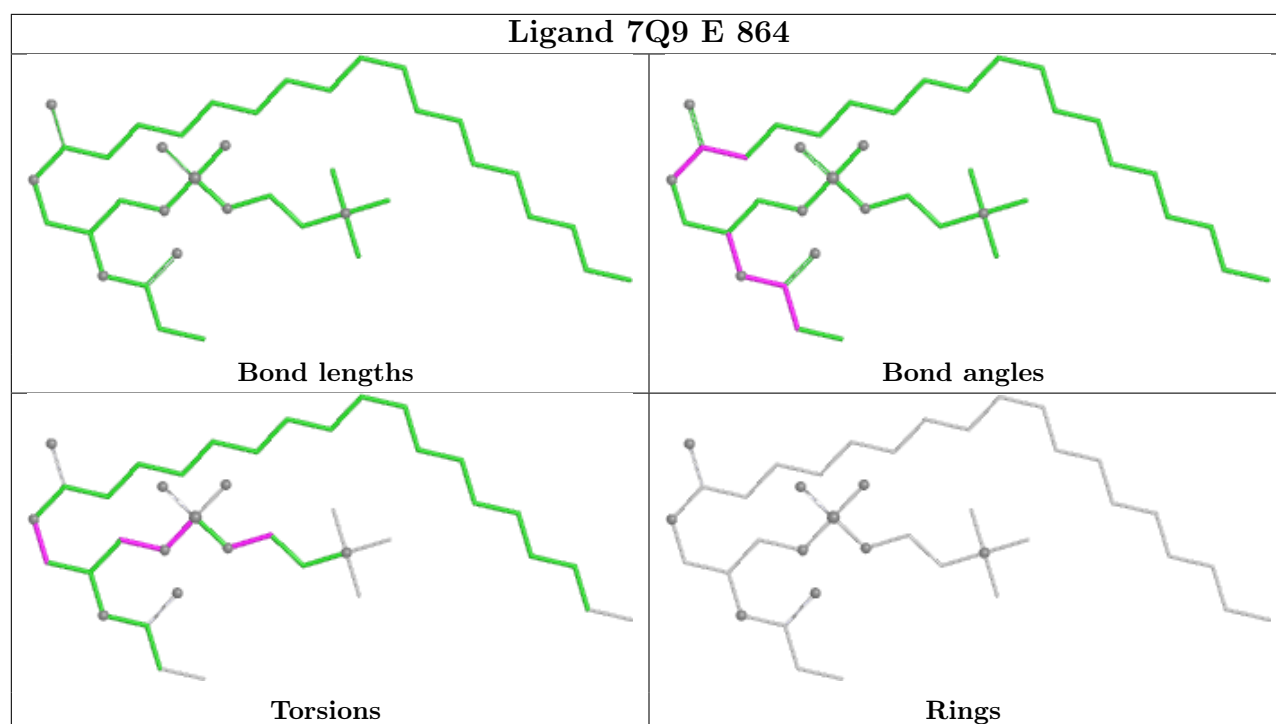
Ligand 7Q9 A 215

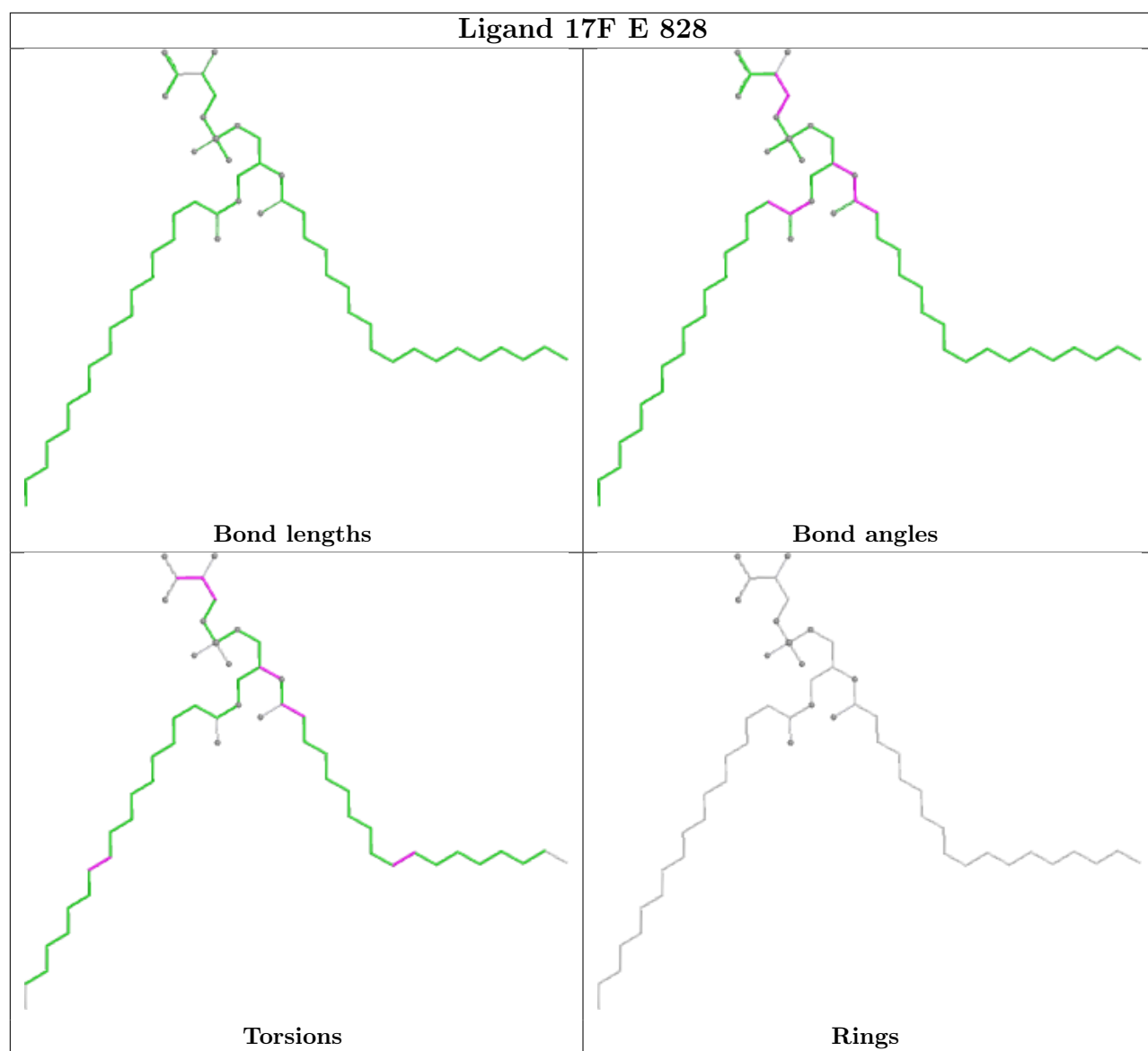


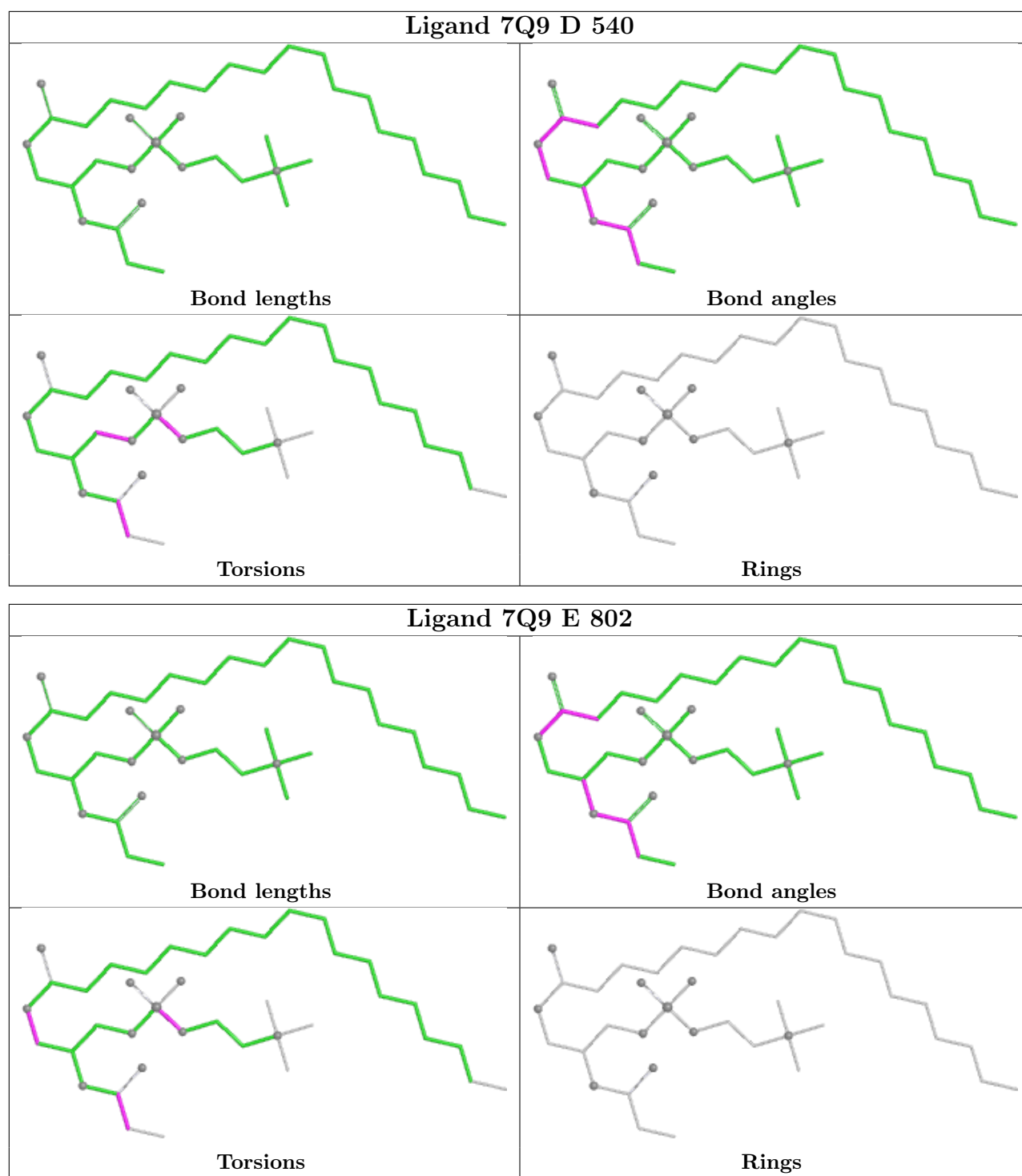
Ligand 7Q9 E 803











6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 1% for the well-defined parts and 1% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	154
Number of shifts mapped to atoms	61
Number of unparsed shifts	0
Number of shifts with mapping errors	93
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. All 93 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	6	LEU	HD11	0.763	.	2
1	A	6	LEU	HD12	0.763	.	2
1	A	6	LEU	HD13	0.763	.	2
1	A	8	VAL	HG21	0.7528	.	2
1	A	8	VAL	HG22	0.7528	.	2
1	A	8	VAL	HG23	0.7528	.	2
1	A	14	VAL	HG21	0.9725	.	2
1	A	14	VAL	HG22	0.9725	.	2
1	A	14	VAL	HG23	0.9725	.	2
1	A	19	LEU	HD11	0.4104	.	2
1	A	19	LEU	HD12	0.4104	.	2
1	A	19	LEU	HD13	0.4104	.	2
1	A	19	LEU	HD21	0.5804	.	2
1	A	19	LEU	HD22	0.5804	.	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	19	LEU	HD23	0.5804	.	2
1	A	21	ILE	HD11	0.4182	.	1
1	A	21	ILE	HD12	0.4182	.	1
1	A	21	ILE	HD13	0.4182	.	1
1	A	23	LEU	HD11	-0.477	.	2
1	A	23	LEU	HD12	-0.477	.	2
1	A	23	LEU	HD13	-0.477	.	2
1	A	24	ILE	HD11	0.2691	.	1
1	A	24	ILE	HD12	0.2691	.	1
1	A	24	ILE	HD13	0.2691	.	1
1	A	36	ILE	HD11	0.5397	.	1
1	A	36	ILE	HD12	0.5397	.	1
1	A	36	ILE	HD13	0.5397	.	1
1	A	44	VAL	HG11	0.5353	.	2
1	A	44	VAL	HG12	0.5353	.	2
1	A	44	VAL	HG13	0.5353	.	2
1	A	45	VAL	HG11	0.4379	.	2
1	A	45	VAL	HG12	0.4379	.	2
1	A	45	VAL	HG13	0.4379	.	2
1	A	46	ILE	HD11	0.2525	.	1
1	A	46	ILE	HD12	0.2525	.	1
1	A	46	ILE	HD13	0.2525	.	1
1	A	55	ILE	HD11	0.3369	.	1
1	A	55	ILE	HD12	0.3369	.	1
1	A	55	ILE	HD13	0.3369	.	1
1	A	56	LEU	HD11	0.5372	.	2
1	A	56	LEU	HD12	0.5372	.	2
1	A	56	LEU	HD13	0.5372	.	2
1	A	79	LEU	HD11	-0.1312	.	2
1	A	79	LEU	HD12	-0.1312	.	2
1	A	79	LEU	HD13	-0.1312	.	2
1	A	79	LEU	HD21	-0.015	.	2
1	A	79	LEU	HD22	-0.015	.	2
1	A	79	LEU	HD23	-0.015	.	2
1	A	81	VAL	HG21	0.4663	.	2
1	A	81	VAL	HG22	0.4663	.	2
1	A	81	VAL	HG23	0.4663	.	2
1	A	84	ILE	HD11	0.5865	.	1
1	A	84	ILE	HD12	0.5865	.	1
1	A	84	ILE	HD13	0.5865	.	1
1	A	93	ILE	HD11	0.6063	.	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	93	ILE	HD12	0.6063	.	1
1	A	93	ILE	HD13	0.6063	.	1
1	A	100	ILE	HD11	0.0964	.	1
1	A	100	ILE	HD12	0.0964	.	1
1	A	100	ILE	HD13	0.0964	.	1
1	A	103	VAL	HG11	0.8243	.	2
1	A	103	VAL	HG12	0.8243	.	2
1	A	103	VAL	HG13	0.8243	.	2
1	A	112	VAL	HG11	0.5953	.	2
1	A	112	VAL	HG12	0.5953	.	2
1	A	112	VAL	HG13	0.5953	.	2
1	A	113	LEU	HD11	0.8748	.	2
1	A	113	LEU	HD12	0.8748	.	2
1	A	113	LEU	HD13	0.8748	.	2
1	A	120	LEU	HD11	0.6958	.	2
1	A	120	LEU	HD12	0.6958	.	2
1	A	120	LEU	HD13	0.6958	.	2
1	A	125	VAL	HG11	-0.3248	.	2
1	A	125	VAL	HG12	-0.3248	.	2
1	A	125	VAL	HG13	-0.3248	.	2
1	A	133	LEU	HD11	0.2014	.	2
1	A	133	LEU	HD12	0.2014	.	2
1	A	133	LEU	HD13	0.2014	.	2
1	A	139	ILE	HD11	0.7118	.	1
1	A	139	ILE	HD12	0.7118	.	1
1	A	139	ILE	HD13	0.7118	.	1
1	A	142	ILE	HD11	0.5035	.	1
1	A	142	ILE	HD12	0.5035	.	1
1	A	142	ILE	HD13	0.5035	.	1
1	A	159	LEU	HD11	0.51	.	2
1	A	159	LEU	HD12	0.51	.	2
1	A	159	LEU	HD13	0.51	.	2
1	A	160	VAL	HG11	-0.2062	.	2
1	A	160	VAL	HG12	-0.2062	.	2
1	A	160	VAL	HG13	-0.2062	.	2
1	A	163	ILE	HD11	0.5261	.	1
1	A	163	ILE	HD12	0.5261	.	1
1	A	163	ILE	HD13	0.5261	.	1

7.1.2 Chemical shift referencing [i](#)

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

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 1%, i.e. 144 atoms were assigned a chemical shift out of a possible 9928. 0 out of 125 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	20/3532 (1%)	10/1429 (1%)	0/1416 (0%)	10/687 (1%)
Sidechain	124/5777 (2%)	93/3712 (3%)	31/1806 (2%)	0/259 (0%)
Aromatic	0/619 (0%)	0/306 (0%)	0/291 (0%)	0/22 (0%)
Overall	144/9928 (1%)	103/5447 (2%)	31/3513 (1%)	10/968 (1%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 1%, i.e. 154 atoms were assigned a chemical shift out of a possible 10390. 0 out of 126 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	30/3692 (1%)	15/1494 (1%)	0/1480 (0%)	15/718 (2%)
Sidechain	124/6070 (2%)	93/3894 (2%)	31/1900 (2%)	0/276 (0%)
Aromatic	0/628 (0%)	0/310 (0%)	0/296 (0%)	0/22 (0%)
Overall	154/10390 (1%)	108/5698 (2%)	31/3676 (1%)	15/1016 (1%)

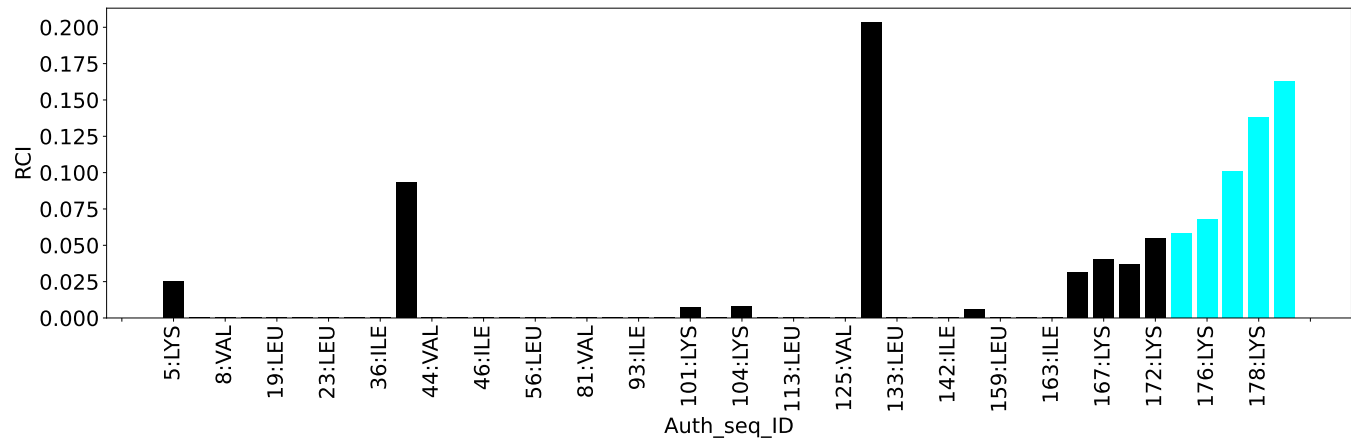
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



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	45
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	0
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	14
Inter-chain	31
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	5
Number of restraints per residue	0.0
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)	0.1	0.48
>0.5 (Large)	21.9	37.39

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

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

9 Distance violation analysis ⓘ

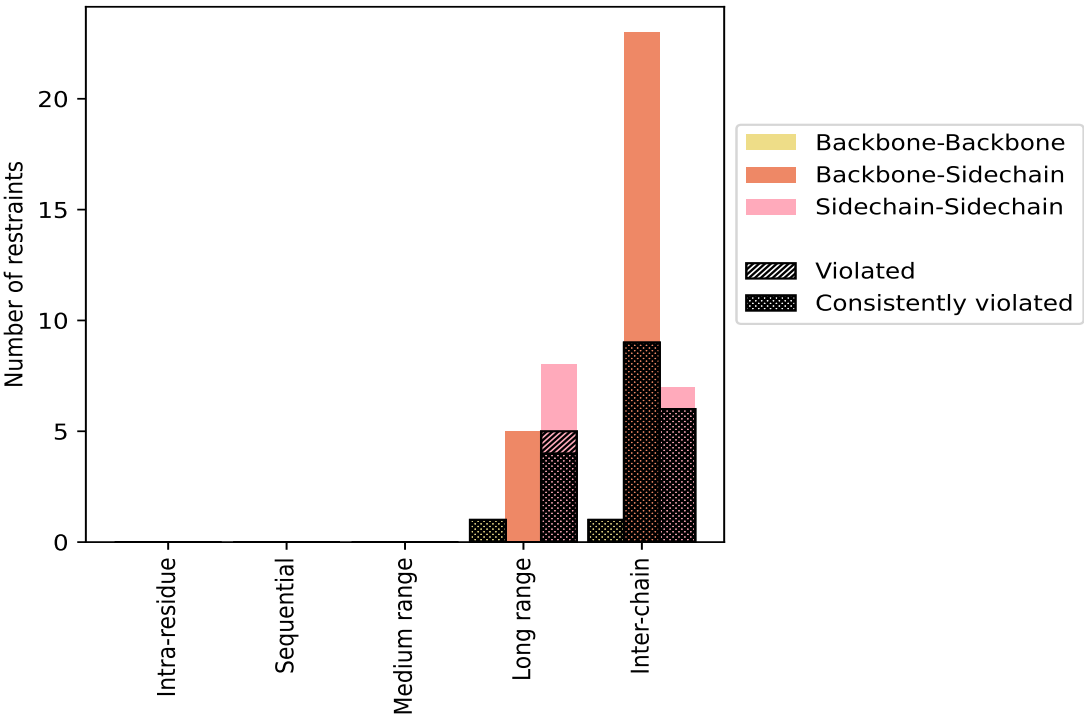
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($ i-j =0$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($ i-j =1$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range ($ i-j >1$ & $ i-j <5$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range ($ i-j \geq 5$)	14	31.1	6	42.9	13.3	5	35.7	11.1
Backbone-Backbone	1	2.2	1	100.0	2.2	1	100.0	2.2
Backbone-Sidechain	5	11.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	8	17.8	5	62.5	11.1	4	50.0	8.9
Inter-chain	31	68.9	16	51.6	35.6	16	51.6	35.6
Backbone-Backbone	1	2.2	1	100.0	2.2	1	100.0	2.2
Backbone-Sidechain	23	51.1	9	39.1	20.0	9	39.1	20.0
Sidechain-Sidechain	7	15.6	6	85.7	13.3	6	85.7	13.3
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	45	100.0	22	48.9	48.9	21	46.7	46.7
Backbone-Backbone	2	4.4	2	100.0	4.4	2	100.0	4.4
Backbone-Sidechain	28	62.2	9	32.1	20.0	9	32.1	20.0
Sidechain-Sidechain	15	33.3	11	73.3	24.4	10	66.7	22.2

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	2	20	22	10.63	20.24	3.97	11.02
2	0	0	0	2	20	22	9.96	15.2	3.83	10.72
3	0	0	0	1	21	22	11.21	24.53	4.62	10.5
4	0	0	0	1	21	22	11.32	37.39	6.42	10.28
5	0	0	0	0	21	21	9.62	14.55	2.5	9.56
6	0	0	0	2	20	22	11.37	28.35	5.17	11.18
7	0	0	0	2	20	22	11.05	26.13	4.59	9.85
8	0	0	0	1	21	22	11.67	35.94	6.41	10.46
9	0	0	0	1	21	22	11.09	30.01	5.21	10.26
10	0	0	0	2	20	22	11.4	27.95	4.73	10.96

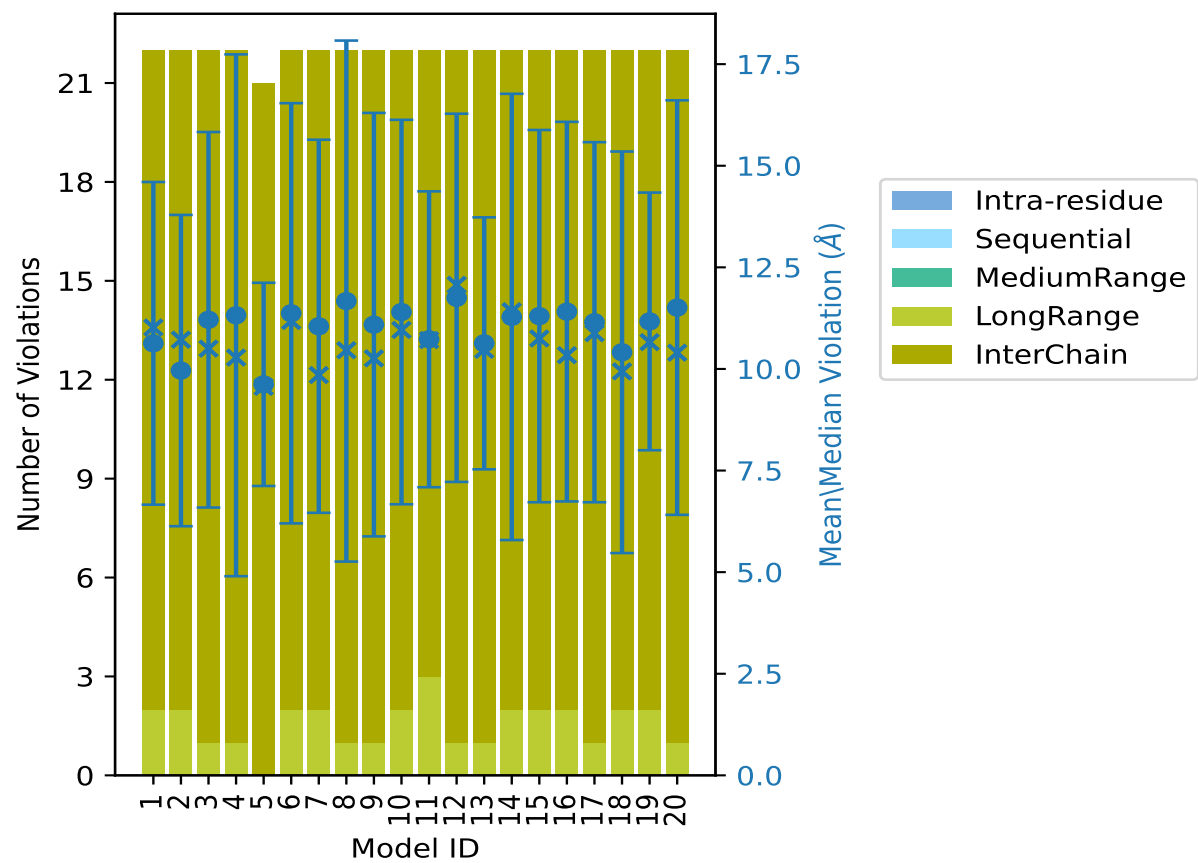
Continued on next page...

Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	0	3	19	22	10.73	18.46	3.64	10.71
12	0	0	0	1	21	22	11.75	24.93	4.53	12.07
13	0	0	0	1	21	22	10.63	15.03	3.1	10.47
14	0	0	0	2	20	22	11.28	29.44	5.49	11.42
15	0	0	0	2	20	22	11.3	26.6	4.58	10.75
16	0	0	0	2	20	22	11.41	28.13	4.67	10.34
17	0	0	0	1	21	22	11.15	24.67	4.43	10.88
18	0	0	0	2	20	22	10.41	26.99	4.94	9.94
19	0	0	0	2	20	22	11.17	16.37	3.17	10.66
20	0	0	0	1	21	22	11.51	29.97	5.1	10.4

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

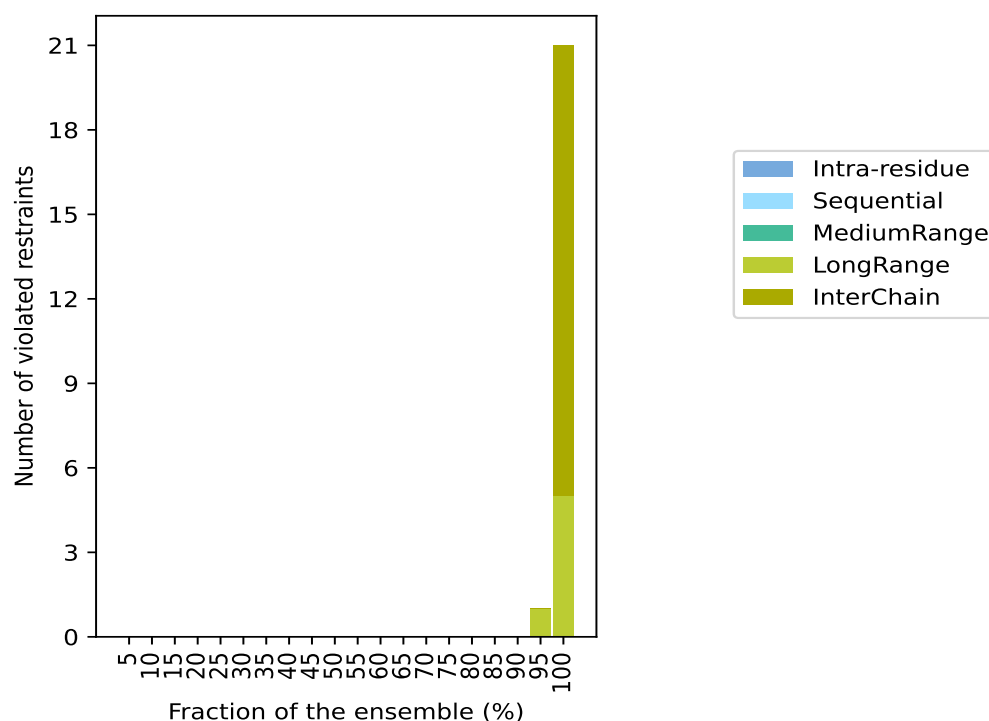
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 23(IR:0, SQ:0, MR:0, LR:8, IC:15) restraints are not violated 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	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	1	0	1	19	95.0
0	0	0	5	16	21	20	100.0

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

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

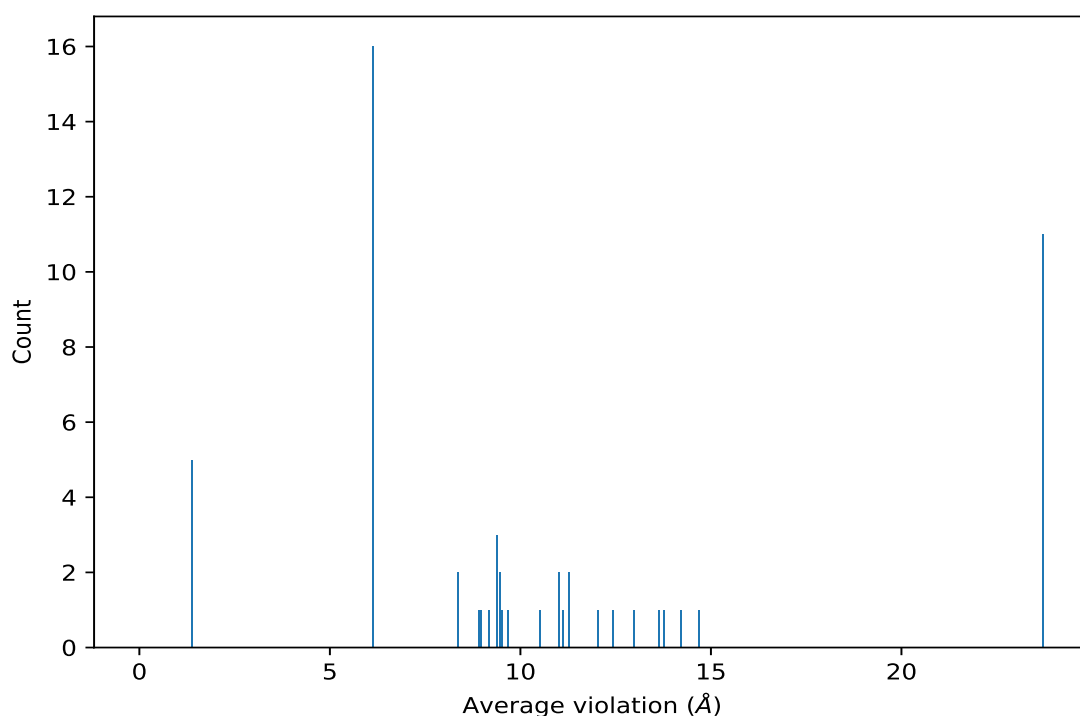
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,21)	1:184:A:LYS:HZ3	5:209:B:7Q9:N	20	23.74	8.95	26.36
(1,21)	1:184:A:LYS:O	5:203:B:7Q9:N	20	23.74	8.95	26.36
(1,21)	1:184:A:LYS:CE	5:209:B:7Q9:N	20	23.74	8.95	26.36
(1,21)	1:184:A:LYS:N	5:203:B:7Q9:N	20	23.74	8.95	26.36
(1,21)	1:184:A:LYS:CE	5:220:B:7Q9:N	20	23.74	8.95	26.36
(1,21)	1:184:A:LYS:HZ2	5:209:B:7Q9:N	20	23.74	8.95	26.36
(1,21)	1:184:A:LYS:HZ1	5:209:B:7Q9:N	20	23.74	8.95	26.36
(1,21)	1:184:A:LYS:N	6:208:B:17F:N1	20	23.74	8.95	26.36
(1,21)	1:184:A:LYS:HZ3	5:220:B:7Q9:N	20	23.74	8.95	26.36
(1,21)	1:184:A:LYS:N	5:216:B:7Q9:N	20	23.74	8.95	26.36
(1,21)	1:184:A:LYS:H	6:208:B:17F:N1	20	23.74	8.95	26.36
(1,5)	1:169:B:LYS:CG	1:36:A:ILE:CD1	20	14.66	0.68	15.04
(1,19)	1:39:A:SER:OG	1:163:B:ILE:CD1	20	14.21	0.73	14.3
(1,8)	1:169:B:LYS:CG	1:42:A:LYS:N	20	13.75	1.57	14.19
(1,7)	1:169:B:LYS:CG	1:5:A:LYS:N	20	13.64	1.42	13.94
(1,4)	1:118:B:CYS:SG	1:42:A:LYS:N	20	12.99	1.43	13.18

Continued on next page...

Continued from previous page...

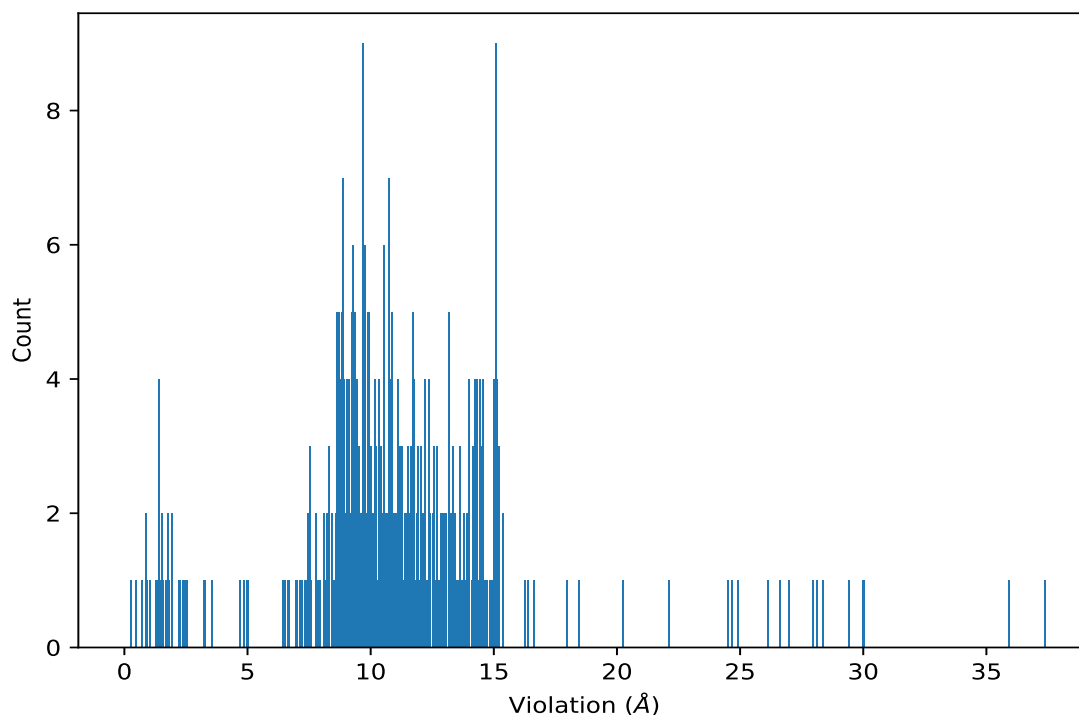
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4)	1:39:A:SER:OG	1:167:B:LYS:N	20	12.44	0.74	12.51
(2,2)	1:39:A:SER:OG	1:128:B:LYS:N	20	12.01	0.88	11.98
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD1	20	11.27	1.09	11.15
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD2	20	11.27	1.09	11.15
(2,5)	1:39:A:SER:OG	1:169:B:LYS:N	20	11.12	0.86	10.84
(1,18)	1:39:A:SER:OG	1:160:A:VAL:CG2	20	11.03	0.71	10.98
(1,18)	1:39:A:SER:OG	1:160:B:VAL:C	20	11.03	0.71	10.98
(1,3)	1:118:B:CYS:SG	1:24:A:ILE:CD1	20	10.53	1.41	10.6
(2,3)	1:39:A:SER:OG	1:165:B:LYS:N	20	9.68	0.86	9.48
(1,1)	1:118:B:CYS:SG	1:21:A:ILE:CD1	20	9.51	1.15	9.66
(1,13)	1:39:A:SER:OG	1:112:B:VAL:CG2	20	9.46	0.51	9.35
(1,13)	1:39:A:SER:OG	1:112:B:VAL:CG1	20	9.46	0.51	9.35
(1,2)	1:118:B:CYS:SG	1:23:A:LEU:O	20	9.35	1.16	9.67
(1,2)	1:118:B:CYS:SG	1:23:A:LEU:C	20	9.35	1.16	9.67
(1,2)	1:118:B:CYS:SG	1:23:B:LEU:CD1	20	9.35	1.16	9.67
(1,14)	1:39:A:SER:OG	1:113:B:LEU:H	20	9.15	0.57	9.07
(1,17)	1:39:A:SER:OG	1:142:B:ILE:CD1	20	8.97	1.13	8.99
(1,16)	1:39:A:SER:OG	1:139:B:ILE:CD1	20	8.93	0.63	8.87
(1,15)	1:39:A:SER:OG	1:133:B:LEU:O	20	8.35	0.87	8.45
(1,15)	1:39:A:SER:OG	1:133:B:LEU:C	20	8.35	0.87	8.45
(1,22)	1:184:B:LYS:HZ1	6:214:B:17F:N1	20	6.14	5.95	3.41
(1,22)	1:184:B:LYS:HZ2	6:219:B:17F:N1	20	6.14	5.95	3.41
(1,22)	1:184:B:LYS:CE	5:218:B:7Q9:N	20	6.14	5.95	3.41
(1,22)	1:184:B:LYS:O	5:210:B:7Q9:N	20	6.14	5.95	3.41
(1,22)	1:184:B:LYS:HZ3	5:205:B:7Q9:N	20	6.14	5.95	3.41
(1,22)	1:184:B:LYS:HZ3	6:208:B:17F:N1	20	6.14	5.95	3.41
(1,22)	1:184:B:LYS:N	6:208:B:17F:N1	20	6.14	5.95	3.41
(1,22)	1:184:B:LYS:N	5:209:B:7Q9:N	20	6.14	5.95	3.41
(1,22)	1:184:B:LYS:HZ3	6:214:B:17F:N1	20	6.14	5.95	3.41
(1,22)	1:184:B:LYS:O	5:212:B:7Q9:N	20	6.14	5.95	3.41
(1,22)	1:184:B:LYS:HZ2	5:205:B:7Q9:N	20	6.14	5.95	3.41
(1,22)	1:184:B:LYS:O	6:219:B:17F:N1	20	6.14	5.95	3.41
(1,22)	1:184:B:LYS:HZ2	6:214:B:17F:N1	20	6.14	5.95	3.41
(1,22)	1:184:B:LYS:C	6:219:B:17F:N1	20	6.14	5.95	3.41
(1,22)	1:184:B:LYS:O	5:203:B:7Q9:N	20	6.14	5.95	3.41
(1,22)	1:184:B:LYS:HZ1	6:208:B:17F:N1	20	6.14	5.95	3.41
(1,20)	1:23:A:LEU:CD2	1:44:A:VAL:CG1	19	1.36	0.54	1.43
(1,20)	1:23:A:LEU:CD1	1:44:A:VAL:CG1	19	1.36	0.54	1.43
(1,20)	1:24:A:ILE:CD1	1:44:A:VAL:CG1	19	1.36	0.54	1.43
(1,20)	1:23:A:LEU:CD2	1:44:A:VAL:CG2	19	1.36	0.54	1.43
(1,20)	1:23:A:LEU:CD1	1:44:A:VAL:CG2	19	1.36	0.54	1.43

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)
(1,21)	1:184:A:LYS:N	5:203:B:7Q9:N	4	37.39
(1,21)	1:184:A:LYS:HZ1	5:209:B:7Q9:N	8	35.94
(1,21)	1:184:A:LYS:N	6:208:B:17F:N1	9	30.01
(1,21)	1:184:A:LYS:N	5:203:B:7Q9:N	20	29.97
(1,21)	1:184:A:LYS:H	6:208:B:17F:N1	14	29.44
(1,21)	1:184:A:LYS:N	5:203:B:7Q9:N	6	28.35
(1,21)	1:184:A:LYS:HZ1	5:209:B:7Q9:N	16	28.13
(1,21)	1:184:A:LYS:N	5:203:B:7Q9:N	10	27.95
(1,21)	1:184:A:LYS:N	5:203:B:7Q9:N	18	26.99
(1,21)	1:184:A:LYS:N	5:203:B:7Q9:N	15	26.6

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:184:A:LYS:HZ2	5:209:B:7Q9:N	7	26.13
(1,21)	1:184:A:LYS:N	5:203:B:7Q9:N	12	24.93
(1,21)	1:184:A:LYS:O	5:203:B:7Q9:N	17	24.67
(1,21)	1:184:A:LYS:CE	5:209:B:7Q9:N	3	24.53
(1,22)	1:184:B:LYS:N	6:208:B:17F:N1	8	22.13
(1,21)	1:184:A:LYS:HZ3	5:209:B:7Q9:N	1	20.24
(1,21)	1:184:A:LYS:HZ3	5:220:B:7Q9:N	11	18.46
(1,22)	1:184:B:LYS:CE	5:218:B:7Q9:N	3	17.98
(1,8)	1:169:B:LYS:CG	1:42:A:LYS:N	3	16.61
(1,22)	1:184:B:LYS:O	5:203:B:7Q9:N	19	16.37
(1,21)	1:184:A:LYS:N	6:208:B:17F:N1	19	16.29
(1,19)	1:39:A:SER:OG	1:163:B:ILE:CD1	10	15.37
(1,7)	1:169:B:LYS:CG	1:5:A:LYS:N	3	15.35
(1,19)	1:39:A:SER:OG	1:163:B:ILE:CD1	14	15.21
(1,7)	1:169:B:LYS:CG	1:5:A:LYS:N	15	15.2
(1,4)	1:118:B:CYS:SG	1:42:A:LYS:N	2	15.2
(1,4)	1:118:B:CYS:SG	1:42:A:LYS:N	12	15.13
(1,5)	1:169:B:LYS:CG	1:36:A:ILE:CD1	7	15.12
(1,19)	1:39:A:SER:OG	1:163:B:ILE:CD1	2	15.11
(1,5)	1:169:B:LYS:CG	1:36:A:ILE:CD1	10	15.1
(1,5)	1:169:B:LYS:CG	1:36:A:ILE:CD1	15	15.09
(1,5)	1:169:B:LYS:CG	1:36:A:ILE:CD1	16	15.09
(1,19)	1:39:A:SER:OG	1:163:B:ILE:CD1	20	15.08
(1,5)	1:169:B:LYS:CG	1:36:A:ILE:CD1	2	15.07
(1,5)	1:169:B:LYS:CG	1:36:A:ILE:CD1	8	15.07
(1,5)	1:169:B:LYS:CG	1:36:A:ILE:CD1	9	15.07
(1,5)	1:169:B:LYS:CG	1:36:A:ILE:CD1	14	15.07
(1,5)	1:169:B:LYS:CG	1:36:A:ILE:CD1	11	15.06
(1,5)	1:169:B:LYS:CG	1:36:A:ILE:CD1	12	15.06
(1,5)	1:169:B:LYS:CG	1:36:A:ILE:CD1	1	15.03
(1,5)	1:169:B:LYS:CG	1:36:A:ILE:CD1	13	15.03
(1,7)	1:169:B:LYS:CG	1:5:A:LYS:N	20	15.02
(1,5)	1:169:B:LYS:CG	1:36:A:ILE:CD1	20	15.02
(1,4)	1:118:B:CYS:SG	1:42:A:LYS:N	11	14.96
(1,7)	1:169:B:LYS:CG	1:5:A:LYS:N	17	14.92
(1,7)	1:169:B:LYS:CG	1:5:A:LYS:N	13	14.88
(1,7)	1:169:B:LYS:CG	1:5:A:LYS:N	12	14.8
(1,19)	1:39:A:SER:OG	1:163:B:ILE:CD1	17	14.73
(1,5)	1:169:B:LYS:CG	1:36:A:ILE:CD1	19	14.6
(1,4)	1:118:B:CYS:SG	1:42:A:LYS:N	14	14.59
(1,8)	1:169:B:LYS:CG	1:42:A:LYS:N	5	14.55
(1,8)	1:169:B:LYS:CG	1:42:A:LYS:N	6	14.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:169:B:LYS:CG	1:5:A:LYS:N	9	14.55
(1,8)	1:169:B:LYS:CG	1:42:A:LYS:N	18	14.53
(1,8)	1:169:B:LYS:CG	1:42:A:LYS:N	15	14.52
(1,19)	1:39:A:SER:OG	1:163:B:ILE:CD1	11	14.46
(1,19)	1:39:A:SER:OG	1:163:B:ILE:CD1	16	14.46
(1,8)	1:169:B:LYS:CG	1:42:A:LYS:N	19	14.46
(1,19)	1:39:A:SER:OG	1:163:B:ILE:CD1	6	14.44
(1,19)	1:39:A:SER:OG	1:163:B:ILE:CD1	19	14.43
(1,8)	1:169:B:LYS:CG	1:42:A:LYS:N	13	14.42
(1,7)	1:169:B:LYS:CG	1:5:A:LYS:N	16	14.4
(1,19)	1:39:A:SER:OG	1:163:B:ILE:CD1	7	14.35
(1,5)	1:169:B:LYS:CG	1:36:A:ILE:CD1	18	14.34
(1,5)	1:169:B:LYS:CG	1:36:A:ILE:CD1	6	14.33
(1,4)	1:118:B:CYS:SG	1:42:A:LYS:N	6	14.33
(1,7)	1:169:B:LYS:CG	1:5:A:LYS:N	10	14.32
(1,8)	1:169:B:LYS:CG	1:42:A:LYS:N	4	14.28
(1,19)	1:39:A:SER:OG	1:163:B:ILE:CD1	15	14.25
(1,19)	1:39:A:SER:OG	1:163:B:ILE:CD1	4	14.24
(1,19)	1:39:A:SER:OG	1:163:B:ILE:CD1	13	14.23
(1,8)	1:169:B:LYS:CG	1:42:A:LYS:N	16	14.22
(1,8)	1:169:B:LYS:CG	1:42:A:LYS:N	9	14.2
(1,5)	1:169:B:LYS:CG	1:36:A:ILE:CD1	5	14.19
(1,8)	1:169:B:LYS:CG	1:42:A:LYS:N	12	14.18
(1,5)	1:169:B:LYS:CG	1:36:A:ILE:CD1	17	14.15
(1,8)	1:169:B:LYS:CG	1:42:A:LYS:N	1	14.14
(1,8)	1:169:B:LYS:CG	1:42:A:LYS:N	20	13.99
(2,4)	1:39:A:SER:OG	1:167:B:LYS:N	10	13.96
(1,8)	1:169:B:LYS:CG	1:42:A:LYS:N	7	13.96
(1,7)	1:169:B:LYS:CG	1:5:A:LYS:N	1	13.95
(1,7)	1:169:B:LYS:CG	1:5:A:LYS:N	19	13.93
(1,4)	1:118:B:CYS:SG	1:42:A:LYS:N	13	13.93
(1,7)	1:169:B:LYS:CG	1:5:A:LYS:N	6	13.87
(1,8)	1:169:B:LYS:CG	1:42:A:LYS:N	17	13.8
(1,19)	1:39:A:SER:OG	1:163:B:ILE:CD1	1	13.79
(1,7)	1:169:B:LYS:CG	1:5:A:LYS:N	14	13.76
(1,19)	1:39:A:SER:OG	1:163:B:ILE:CD1	3	13.73
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD1	17	13.67
(1,19)	1:39:A:SER:OG	1:163:B:ILE:CD1	9	13.62
(1,19)	1:39:A:SER:OG	1:163:B:ILE:CD1	12	13.6
(1,7)	1:169:B:LYS:CG	1:5:A:LYS:N	7	13.6
(2,2)	1:39:A:SER:OG	1:128:B:LYS:N	12	13.59
(1,8)	1:169:B:LYS:CG	1:42:A:LYS:N	8	13.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:39:A:SER:OG	1:163:B:ILE:CD1	18	13.45
(1,19)	1:39:A:SER:OG	1:163:B:ILE:CD1	5	13.41
(1,4)	1:118:B:CYS:SG	1:42:A:LYS:N	16	13.4
(2,2)	1:39:A:SER:OG	1:128:B:LYS:N	20	13.34
(1,4)	1:118:B:CYS:SG	1:42:A:LYS:N	1	13.33
(2,4)	1:39:A:SER:OG	1:167:B:LYS:N	6	13.3
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD1	10	13.28
(1,4)	1:118:B:CYS:SG	1:42:A:LYS:N	15	13.25
(1,4)	1:118:B:CYS:SG	1:42:A:LYS:N	9	13.22
(1,8)	1:169:B:LYS:CG	1:42:A:LYS:N	14	13.19
(2,4)	1:39:A:SER:OG	1:167:B:LYS:N	7	13.17
(2,4)	1:39:A:SER:OG	1:167:B:LYS:N	12	13.17
(2,4)	1:39:A:SER:OG	1:167:B:LYS:N	17	13.17
(1,4)	1:118:B:CYS:SG	1:42:A:LYS:N	20	13.15
(1,4)	1:118:B:CYS:SG	1:42:A:LYS:N	4	13.07
(1,5)	1:169:B:LYS:CG	1:36:A:ILE:CD1	4	13.05
(2,4)	1:39:A:SER:OG	1:167:B:LYS:N	19	13.04
(2,4)	1:39:A:SER:OG	1:167:B:LYS:N	3	13.01
(2,2)	1:39:A:SER:OG	1:128:B:LYS:N	13	12.94
(2,4)	1:39:A:SER:OG	1:167:B:LYS:N	2	12.9
(1,7)	1:169:B:LYS:CG	1:5:A:LYS:N	18	12.87
(1,7)	1:169:B:LYS:CG	1:5:A:LYS:N	4	12.86
(2,2)	1:39:A:SER:OG	1:128:B:LYS:N	15	12.8
(2,2)	1:39:A:SER:OG	1:128:B:LYS:N	9	12.76
(1,5)	1:169:B:LYS:CG	1:36:A:ILE:CD1	3	12.72
(2,4)	1:39:A:SER:OG	1:167:B:LYS:N	11	12.67
(2,4)	1:39:A:SER:OG	1:167:B:LYS:N	14	12.65
(1,8)	1:169:B:LYS:CG	1:42:A:LYS:N	10	12.65
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD1	12	12.63
(2,2)	1:39:A:SER:OG	1:128:B:LYS:N	7	12.59
(2,2)	1:39:A:SER:OG	1:128:B:LYS:N	16	12.59
(2,5)	1:39:A:SER:OG	1:169:B:LYS:N	12	12.55
(1,18)	1:39:A:SER:OG	1:160:A:VAL:CG2	14	12.53
(1,3)	1:118:B:CYS:SG	1:24:A:ILE:CD1	6	12.52
(2,2)	1:39:A:SER:OG	1:128:B:LYS:N	1	12.43
(1,3)	1:118:B:CYS:SG	1:24:A:ILE:CD1	12	12.42
(2,5)	1:39:A:SER:OG	1:169:B:LYS:N	10	12.39
(2,2)	1:39:A:SER:OG	1:128:B:LYS:N	11	12.38
(1,21)	1:184:A:LYS:N	5:216:B:7Q9:N	13	12.38
(2,4)	1:39:A:SER:OG	1:167:B:LYS:N	1	12.37
(1,4)	1:118:B:CYS:SG	1:42:A:LYS:N	19	12.3
(1,19)	1:39:A:SER:OG	1:163:B:ILE:CD1	8	12.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5)	1:39:A:SER:OG	1:169:B:LYS:N	17	12.23
(2,5)	1:39:A:SER:OG	1:169:B:LYS:N	7	12.22
(1,18)	1:39:A:SER:OG	1:160:B:VAL:C	17	12.21
(1,4)	1:118:B:CYS:SG	1:42:A:LYS:N	17	12.21
(1,3)	1:118:B:CYS:SG	1:24:A:ILE:CD1	11	12.17
(1,4)	1:118:B:CYS:SG	1:42:A:LYS:N	18	12.15
(2,4)	1:39:A:SER:OG	1:167:B:LYS:N	15	12.12
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD1	14	12.12
(2,5)	1:39:A:SER:OG	1:169:B:LYS:N	3	12.04
(2,2)	1:39:A:SER:OG	1:128:B:LYS:N	18	12.04
(1,3)	1:118:B:CYS:SG	1:24:A:ILE:CD1	2	12.04
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD2	7	11.99
(2,2)	1:39:A:SER:OG	1:128:B:LYS:N	14	11.93
(2,4)	1:39:A:SER:OG	1:167:B:LYS:N	20	11.92
(1,3)	1:118:B:CYS:SG	1:24:A:ILE:CD1	14	11.91
(2,4)	1:39:A:SER:OG	1:167:B:LYS:N	18	11.88
(2,5)	1:39:A:SER:OG	1:169:B:LYS:N	19	11.87
(2,5)	1:39:A:SER:OG	1:169:B:LYS:N	6	11.82
(2,4)	1:39:A:SER:OG	1:167:B:LYS:N	16	11.79
(1,4)	1:118:B:CYS:SG	1:42:A:LYS:N	10	11.79
(2,4)	1:39:A:SER:OG	1:167:B:LYS:N	4	11.77
(1,18)	1:39:A:SER:OG	1:160:A:VAL:CG2	2	11.77
(2,4)	1:39:A:SER:OG	1:167:B:LYS:N	5	11.74
(1,18)	1:39:A:SER:OG	1:160:B:VAL:C	12	11.71
(1,17)	1:39:A:SER:OG	1:142:B:ILE:CD1	2	11.71
(2,4)	1:39:A:SER:OG	1:167:B:LYS:N	13	11.7
(2,2)	1:39:A:SER:OG	1:128:B:LYS:N	2	11.7
(2,2)	1:39:A:SER:OG	1:128:B:LYS:N	8	11.68
(2,2)	1:39:A:SER:OG	1:128:B:LYS:N	6	11.67
(1,4)	1:118:B:CYS:SG	1:42:A:LYS:N	8	11.65
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD1	3	11.64
(1,1)	1:118:B:CYS:SG	1:21:A:ILE:CD1	12	11.63
(2,2)	1:39:A:SER:OG	1:128:B:LYS:N	3	11.6
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD1	11	11.59
(1,18)	1:39:A:SER:OG	1:160:B:VAL:C	20	11.55
(2,3)	1:39:A:SER:OG	1:165:B:LYS:N	10	11.52
(2,2)	1:39:A:SER:OG	1:128:B:LYS:N	17	11.52
(1,4)	1:118:B:CYS:SG	1:42:A:LYS:N	7	11.51
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD1	15	11.49
(2,5)	1:39:A:SER:OG	1:169:B:LYS:N	1	11.41
(1,18)	1:39:A:SER:OG	1:160:A:VAL:CG2	11	11.4
(1,7)	1:169:B:LYS:CG	1:5:A:LYS:N	8	11.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:118:B:CYS:SG	1:24:A:ILE:CD1	13	11.37
(1,18)	1:39:A:SER:OG	1:160:B:VAL:C	13	11.32
(2,4)	1:39:A:SER:OG	1:167:B:LYS:N	8	11.26
(2,4)	1:39:A:SER:OG	1:167:B:LYS:N	9	11.26
(1,2)	1:118:B:CYS:SG	1:23:A:LEU:O	6	11.26
(1,2)	1:118:B:CYS:SG	1:23:A:LEU:C	2	11.24
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD1	1	11.22
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD1	19	11.2
(1,18)	1:39:A:SER:OG	1:160:A:VAL:CG2	15	11.19
(1,7)	1:169:B:LYS:CG	1:5:A:LYS:N	2	11.17
(1,3)	1:118:B:CYS:SG	1:24:A:ILE:CD1	1	11.15
(2,3)	1:39:A:SER:OG	1:165:B:LYS:N	12	11.13
(1,3)	1:118:B:CYS:SG	1:24:A:ILE:CD1	4	11.11
(1,18)	1:39:A:SER:OG	1:160:A:VAL:CG2	6	11.1
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD1	20	11.1
(1,18)	1:39:A:SER:OG	1:160:A:VAL:CG2	10	11.08
(1,3)	1:118:B:CYS:SG	1:24:A:ILE:CD1	16	11.07
(2,2)	1:39:A:SER:OG	1:128:B:LYS:N	4	11.04
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD1	6	11.01
(1,7)	1:169:B:LYS:CG	1:5:A:LYS:N	5	10.99
(1,7)	1:169:B:LYS:CG	1:5:A:LYS:N	11	10.99
(2,5)	1:39:A:SER:OG	1:169:B:LYS:N	14	10.94
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD1	16	10.91
(2,5)	1:39:A:SER:OG	1:169:B:LYS:N	5	10.89
(1,18)	1:39:A:SER:OG	1:160:B:VAL:C	9	10.89
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD1	9	10.89
(1,18)	1:39:A:SER:OG	1:160:A:VAL:CG2	1	10.88
(1,14)	1:39:A:SER:OG	1:113:B:LEU:H	12	10.87
(1,22)	1:184:B:LYS:N	5:209:B:7Q9:N	10	10.84
(2,5)	1:39:A:SER:OG	1:169:B:LYS:N	15	10.8
(2,2)	1:39:A:SER:OG	1:128:B:LYS:N	19	10.79
(1,18)	1:39:A:SER:OG	1:160:B:VAL:C	4	10.78
(2,5)	1:39:A:SER:OG	1:169:B:LYS:N	8	10.75
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD1	2	10.75
(1,1)	1:118:B:CYS:SG	1:21:A:ILE:CD1	14	10.73
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD2	18	10.72
(2,5)	1:39:A:SER:OG	1:169:B:LYS:N	11	10.71
(2,3)	1:39:A:SER:OG	1:165:B:LYS:N	11	10.71
(2,5)	1:39:A:SER:OG	1:169:B:LYS:N	2	10.7
(2,5)	1:39:A:SER:OG	1:169:B:LYS:N	18	10.7
(1,3)	1:118:B:CYS:SG	1:24:A:ILE:CD1	15	10.7
(1,4)	1:118:B:CYS:SG	1:42:A:LYS:N	3	10.68

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD1	13	10.65
(1,18)	1:39:A:SER:OG	1:160:A:VAL:CG2	18	10.63
(1,1)	1:118:B:CYS:SG	1:21:A:ILE:CD1	4	10.59
(1,18)	1:39:A:SER:OG	1:160:B:VAL:C	5	10.57
(1,13)	1:39:A:SER:OG	1:112:B:VAL:CG1	6	10.54
(2,2)	1:39:A:SER:OG	1:128:B:LYS:N	10	10.53
(1,18)	1:39:A:SER:OG	1:160:A:VAL:CG2	19	10.53
(1,18)	1:39:A:SER:OG	1:160:A:VAL:CG2	16	10.51
(1,3)	1:118:B:CYS:SG	1:24:A:ILE:CD1	9	10.5
(1,1)	1:118:B:CYS:SG	1:21:A:ILE:CD1	8	10.5
(1,2)	1:118:B:CYS:SG	1:23:A:LEU:O	12	10.49
(1,3)	1:118:B:CYS:SG	1:24:A:ILE:CD1	20	10.45
(2,3)	1:39:A:SER:OG	1:165:B:LYS:N	14	10.44
(1,3)	1:118:B:CYS:SG	1:24:A:ILE:CD1	8	10.41
(2,3)	1:39:A:SER:OG	1:165:B:LYS:N	19	10.4
(1,1)	1:118:B:CYS:SG	1:21:A:ILE:CD1	11	10.38
(2,2)	1:39:A:SER:OG	1:128:B:LYS:N	5	10.37
(2,5)	1:39:A:SER:OG	1:169:B:LYS:N	20	10.34
(1,18)	1:39:A:SER:OG	1:160:B:VAL:C	3	10.32
(1,18)	1:39:A:SER:OG	1:160:B:VAL:C	8	10.31
(1,2)	1:118:B:CYS:SG	1:23:A:LEU:O	14	10.31
(2,5)	1:39:A:SER:OG	1:169:B:LYS:N	13	10.29
(2,3)	1:39:A:SER:OG	1:165:B:LYS:N	17	10.24
(1,3)	1:118:B:CYS:SG	1:24:A:ILE:CD1	19	10.22
(1,2)	1:118:B:CYS:SG	1:23:A:LEU:O	13	10.2
(2,3)	1:39:A:SER:OG	1:165:B:LYS:N	6	10.18
(1,13)	1:39:A:SER:OG	1:112:B:VAL:CG2	10	10.18
(2,5)	1:39:A:SER:OG	1:169:B:LYS:N	16	10.17
(1,1)	1:118:B:CYS:SG	1:21:A:ILE:CD1	19	10.15
(1,8)	1:169:B:LYS:CG	1:42:A:LYS:N	11	10.12
(1,16)	1:39:A:SER:OG	1:139:B:ILE:CD1	3	10.06
(1,13)	1:39:A:SER:OG	1:112:B:VAL:CG2	2	10.06
(1,2)	1:118:B:CYS:SG	1:23:B:LEU:CD1	11	10.03
(2,3)	1:39:A:SER:OG	1:165:B:LYS:N	2	10.02
(1,17)	1:39:A:SER:OG	1:142:B:ILE:CD1	9	10.02
(1,13)	1:39:A:SER:OG	1:112:B:VAL:CG2	14	9.99
(1,3)	1:118:B:CYS:SG	1:24:A:ILE:CD1	17	9.97
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD2	4	9.96
(2,3)	1:39:A:SER:OG	1:165:B:LYS:N	7	9.93
(1,15)	1:39:A:SER:OG	1:133:B:LEU:C	3	9.93
(2,5)	1:39:A:SER:OG	1:169:B:LYS:N	9	9.92
(1,1)	1:118:B:CYS:SG	1:21:A:ILE:CD1	6	9.91

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:118:B:CYS:SG	1:42:A:LYS:N	5	9.9
(1,13)	1:39:A:SER:OG	1:112:B:VAL:CG2	11	9.89
(1,14)	1:39:A:SER:OG	1:113:B:LEU:H	2	9.88
(1,13)	1:39:A:SER:OG	1:112:B:VAL:CG2	12	9.87
(1,2)	1:118:B:CYS:SG	1:23:A:LEU:C	9	9.87
(1,17)	1:39:A:SER:OG	1:142:B:ILE:CD1	11	9.85
(1,17)	1:39:A:SER:OG	1:142:B:ILE:CD1	17	9.83
(1,1)	1:118:B:CYS:SG	1:21:A:ILE:CD1	17	9.81
(1,2)	1:118:B:CYS:SG	1:23:A:LEU:O	4	9.79
(1,17)	1:39:A:SER:OG	1:142:B:ILE:CD1	15	9.78
(1,1)	1:118:B:CYS:SG	1:21:A:ILE:CD1	13	9.78
(1,16)	1:39:A:SER:OG	1:139:B:ILE:CD1	7	9.77
(1,16)	1:39:A:SER:OG	1:139:B:ILE:CD1	12	9.77
(1,13)	1:39:A:SER:OG	1:112:B:VAL:CG2	17	9.75
(1,17)	1:39:A:SER:OG	1:142:B:ILE:CD1	10	9.74
(1,2)	1:118:B:CYS:SG	1:23:A:LEU:O	16	9.71
(1,2)	1:118:B:CYS:SG	1:23:A:LEU:O	15	9.69
(1,1)	1:118:B:CYS:SG	1:21:A:ILE:CD1	7	9.69
(2,5)	1:39:A:SER:OG	1:169:B:LYS:N	4	9.68
(1,13)	1:39:A:SER:OG	1:112:B:VAL:CG1	5	9.68
(1,13)	1:39:A:SER:OG	1:112:B:VAL:CG2	7	9.67
(1,16)	1:39:A:SER:OG	1:139:B:ILE:CD1	4	9.66
(1,14)	1:39:A:SER:OG	1:113:B:LEU:H	6	9.66
(1,14)	1:39:A:SER:OG	1:113:B:LEU:H	14	9.65
(1,2)	1:118:B:CYS:SG	1:23:A:LEU:O	19	9.65
(1,1)	1:118:B:CYS:SG	1:21:A:ILE:CD1	20	9.63
(1,17)	1:39:A:SER:OG	1:142:B:ILE:CD1	20	9.62
(2,3)	1:39:A:SER:OG	1:165:B:LYS:N	1	9.58
(1,1)	1:118:B:CYS:SG	1:21:A:ILE:CD1	5	9.56
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD2	8	9.54
(1,1)	1:118:B:CYS:SG	1:21:A:ILE:CD1	2	9.53
(1,17)	1:39:A:SER:OG	1:142:B:ILE:CD1	4	9.5
(1,17)	1:39:A:SER:OG	1:142:B:ILE:CD1	13	9.48
(1,14)	1:39:A:SER:OG	1:113:B:LEU:H	7	9.48
(1,15)	1:39:A:SER:OG	1:133:B:LEU:O	20	9.44
(1,2)	1:118:B:CYS:SG	1:23:A:LEU:O	20	9.43
(1,14)	1:39:A:SER:OG	1:113:B:LEU:H	20	9.42
(1,3)	1:118:B:CYS:SG	1:24:A:ILE:CD1	7	9.4
(2,3)	1:39:A:SER:OG	1:165:B:LYS:N	3	9.38
(1,13)	1:39:A:SER:OG	1:112:B:VAL:CG2	16	9.38
(1,18)	1:39:A:SER:OG	1:160:A:VAL:CG2	7	9.36
(1,15)	1:39:A:SER:OG	1:133:B:LEU:O	7	9.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:118:B:CYS:SG	1:23:A:LEU:O	1	9.36
(1,22)	1:184:B:LYS:N	6:208:B:17F:N1	16	9.34
(1,14)	1:39:A:SER:OG	1:113:B:LEU:H	11	9.34
(1,16)	1:39:A:SER:OG	1:139:B:ILE:CD1	16	9.33
(1,13)	1:39:A:SER:OG	1:112:B:VAL:CG2	20	9.32
(1,13)	1:39:A:SER:OG	1:112:B:VAL:CG2	13	9.31
(1,15)	1:39:A:SER:OG	1:133:B:LEU:O	16	9.29
(1,1)	1:118:B:CYS:SG	1:21:A:ILE:CD1	15	9.29
(1,16)	1:39:A:SER:OG	1:139:B:ILE:CD1	20	9.28
(1,13)	1:39:A:SER:OG	1:112:B:VAL:CG2	15	9.27
(1,3)	1:118:B:CYS:SG	1:24:A:ILE:CD1	18	9.26
(1,16)	1:39:A:SER:OG	1:139:B:ILE:CD1	11	9.25
(1,13)	1:39:A:SER:OG	1:112:B:VAL:CG2	8	9.24
(1,1)	1:118:B:CYS:SG	1:21:A:ILE:CD1	9	9.23
(1,15)	1:39:A:SER:OG	1:133:B:LEU:C	4	9.22
(1,14)	1:39:A:SER:OG	1:113:B:LEU:H	15	9.22
(2,3)	1:39:A:SER:OG	1:165:B:LYS:N	15	9.2
(1,1)	1:118:B:CYS:SG	1:21:A:ILE:CD1	16	9.18
(1,14)	1:39:A:SER:OG	1:113:B:LEU:H	16	9.15
(1,16)	1:39:A:SER:OG	1:139:B:ILE:CD1	5	9.14
(1,14)	1:39:A:SER:OG	1:113:B:LEU:H	10	9.14
(2,3)	1:39:A:SER:OG	1:165:B:LYS:N	5	9.12
(1,17)	1:39:A:SER:OG	1:142:B:ILE:CD1	16	9.1
(1,6)	1:169:B:LYS:CG	1:56:A:LEU:CD1	5	9.09
(1,8)	1:169:B:LYS:CG	1:42:A:LYS:N	2	9.05
(1,15)	1:39:A:SER:OG	1:133:B:LEU:O	12	9.01
(1,14)	1:39:A:SER:OG	1:113:B:LEU:H	4	9.01
(1,13)	1:39:A:SER:OG	1:112:B:VAL:CG2	19	9.01
(2,3)	1:39:A:SER:OG	1:165:B:LYS:N	18	9.0
(2,3)	1:39:A:SER:OG	1:165:B:LYS:N	16	8.96
(1,16)	1:39:A:SER:OG	1:139:B:ILE:CD1	6	8.95
(1,13)	1:39:A:SER:OG	1:112:B:VAL:CG2	4	8.94
(2,3)	1:39:A:SER:OG	1:165:B:LYS:N	20	8.93
(1,1)	1:118:B:CYS:SG	1:21:A:ILE:CD1	1	8.91
(1,14)	1:39:A:SER:OG	1:113:B:LEU:H	17	8.9
(1,14)	1:39:A:SER:OG	1:113:B:LEU:H	13	8.89
(1,17)	1:39:A:SER:OG	1:142:B:ILE:CD1	7	8.88
(1,15)	1:39:A:SER:OG	1:133:B:LEU:O	15	8.88
(1,13)	1:39:A:SER:OG	1:112:B:VAL:CG2	1	8.88
(1,16)	1:39:A:SER:OG	1:139:B:ILE:CD1	15	8.87
(1,16)	1:39:A:SER:OG	1:139:B:ILE:CD1	17	8.87
(2,3)	1:39:A:SER:OG	1:165:B:LYS:N	8	8.85

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	1:39:A:SER:OG	1:165:B:LYS:N	4	8.82
(1,17)	1:39:A:SER:OG	1:142:B:ILE:CD1	19	8.82
(1,16)	1:39:A:SER:OG	1:139:B:ILE:CD1	19	8.82
(1,13)	1:39:A:SER:OG	1:112:B:VAL:CG1	18	8.82
(2,3)	1:39:A:SER:OG	1:165:B:LYS:N	13	8.81
(1,14)	1:39:A:SER:OG	1:113:B:LEU:H	9	8.79
(1,13)	1:39:A:SER:OG	1:112:B:VAL:CG2	3	8.78
(1,2)	1:118:B:CYS:SG	1:23:A:LEU:O	8	8.78
(1,14)	1:39:A:SER:OG	1:113:B:LEU:H	3	8.77
(1,14)	1:39:A:SER:OG	1:113:B:LEU:H	1	8.74
(1,14)	1:39:A:SER:OG	1:113:B:LEU:H	5	8.74
(1,16)	1:39:A:SER:OG	1:139:B:ILE:CD1	13	8.72
(1,17)	1:39:A:SER:OG	1:142:B:ILE:CD1	12	8.7
(1,16)	1:39:A:SER:OG	1:139:B:ILE:CD1	18	8.7
(1,13)	1:39:A:SER:OG	1:112:B:VAL:CG2	9	8.69
(1,3)	1:118:B:CYS:SG	1:24:A:ILE:CD1	10	8.65
(1,14)	1:39:A:SER:OG	1:113:B:LEU:H	19	8.63
(1,2)	1:118:B:CYS:SG	1:23:A:LEU:O	18	8.63
(1,15)	1:39:A:SER:OG	1:133:B:LEU:O	18	8.61
(1,16)	1:39:A:SER:OG	1:139:B:ILE:CD1	10	8.6
(1,15)	1:39:A:SER:OG	1:133:B:LEU:O	9	8.6
(1,15)	1:39:A:SER:OG	1:133:B:LEU:O	13	8.58
(1,16)	1:39:A:SER:OG	1:139:B:ILE:CD1	9	8.55
(1,14)	1:39:A:SER:OG	1:113:B:LEU:H	8	8.53
(1,17)	1:39:A:SER:OG	1:142:B:ILE:CD1	6	8.46
(1,16)	1:39:A:SER:OG	1:139:B:ILE:CD1	1	8.4
(1,16)	1:39:A:SER:OG	1:139:B:ILE:CD1	2	8.4
(1,17)	1:39:A:SER:OG	1:142:B:ILE:CD1	8	8.32
(1,15)	1:39:A:SER:OG	1:133:B:LEU:O	19	8.32
(2,3)	1:39:A:SER:OG	1:165:B:LYS:N	9	8.31
(1,2)	1:118:B:CYS:SG	1:23:A:LEU:O	7	8.28
(1,14)	1:39:A:SER:OG	1:113:B:LEU:H	18	8.25
(1,15)	1:39:A:SER:OG	1:133:B:LEU:O	1	8.24
(1,17)	1:39:A:SER:OG	1:142:B:ILE:CD1	14	8.22
(1,2)	1:118:B:CYS:SG	1:23:A:LEU:O	17	8.17
(1,17)	1:39:A:SER:OG	1:142:B:ILE:CD1	1	8.13
(1,16)	1:39:A:SER:OG	1:139:B:ILE:CD1	8	8.13
(1,3)	1:118:B:CYS:SG	1:24:A:ILE:CD1	3	7.94
(1,15)	1:39:A:SER:OG	1:133:B:LEU:O	2	7.89
(1,15)	1:39:A:SER:OG	1:133:B:LEU:C	5	7.84
(1,15)	1:39:A:SER:OG	1:133:B:LEU:O	11	7.78
(1,15)	1:39:A:SER:OG	1:133:B:LEU:O	6	7.77

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:118:B:CYS:SG	1:21:A:ILE:CD1	18	7.56
(1,2)	1:118:B:CYS:SG	1:23:A:LEU:O	5	7.53
(1,15)	1:39:A:SER:OG	1:133:B:LEU:O	17	7.51
(1,2)	1:118:B:CYS:SG	1:23:A:LEU:C	10	7.51
(1,1)	1:118:B:CYS:SG	1:21:A:ILE:CD1	10	7.48
(1,17)	1:39:A:SER:OG	1:142:B:ILE:CD1	18	7.47
(1,3)	1:118:B:CYS:SG	1:24:A:ILE:CD1	5	7.4
(1,16)	1:39:A:SER:OG	1:139:B:ILE:CD1	14	7.32
(1,17)	1:39:A:SER:OG	1:142:B:ILE:CD1	5	7.24
(1,15)	1:39:A:SER:OG	1:133:B:LEU:O	8	7.12
(1,2)	1:118:B:CYS:SG	1:23:A:LEU:C	3	7.03
(1,15)	1:39:A:SER:OG	1:133:B:LEU:C	10	6.99
(1,15)	1:39:A:SER:OG	1:133:B:LEU:O	14	6.68
(1,1)	1:118:B:CYS:SG	1:21:A:ILE:CD1	3	6.63
(1,17)	1:39:A:SER:OG	1:142:B:ILE:CD1	3	6.51
(1,22)	1:184:B:LYS:HZ1	6:208:B:17F:N1	20	6.44
(1,22)	1:184:B:LYS:O	5:210:B:7Q9:N	5	5.01
(1,21)	1:184:A:LYS:CE	5:220:B:7Q9:N	5	4.96
(1,22)	1:184:B:LYS:HZ2	6:214:B:17F:N1	15	4.89
(1,22)	1:184:B:LYS:HZ2	5:205:B:7Q9:N	13	4.68
(1,22)	1:184:B:LYS:HZ3	6:208:B:17F:N1	9	3.57
(1,22)	1:184:B:LYS:HZ3	6:208:B:17F:N1	7	3.25
(1,22)	1:184:B:LYS:C	6:219:B:17F:N1	17	3.24
(1,22)	1:184:B:LYS:HZ2	6:219:B:17F:N1	2	2.53
(1,20)	1:24:A:ILE:CD1	1:44:A:VAL:CG1	4	2.46
(1,22)	1:184:B:LYS:HZ3	6:214:B:17F:N1	11	2.35
(1,22)	1:184:B:LYS:HZ1	6:214:B:17F:N1	1	2.29
(1,20)	1:23:A:LEU:CD2	1:44:A:VAL:CG1	13	2.2
(1,22)	1:184:B:LYS:HZ1	6:214:B:17F:N1	4	1.93
(1,20)	1:23:A:LEU:CD2	1:44:A:VAL:CG1	19	1.93
(1,20)	1:23:A:LEU:CD2	1:44:A:VAL:CG1	10	1.8
(1,22)	1:184:B:LYS:O	5:212:B:7Q9:N	12	1.79
(1,22)	1:184:B:LYS:HZ3	5:205:B:7Q9:N	6	1.77
(1,20)	1:24:A:ILE:CD1	1:44:A:VAL:CG1	17	1.67
(1,20)	1:23:A:LEU:CD2	1:44:A:VAL:CG1	12	1.55
(1,21)	1:184:A:LYS:O	5:203:B:7Q9:N	2	1.53
(1,20)	1:23:A:LEU:CD2	1:44:A:VAL:CG1	9	1.5
(1,20)	1:23:A:LEU:CD1	1:44:A:VAL:CG1	8	1.45
(1,20)	1:23:A:LEU:CD2	1:44:A:VAL:CG2	11	1.44
(1,20)	1:23:A:LEU:CD2	1:44:A:VAL:CG2	15	1.43
(1,20)	1:23:A:LEU:CD2	1:44:A:VAL:CG1	3	1.42
(1,22)	1:184:B:LYS:HZ1	6:214:B:17F:N1	18	1.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:23:A:LEU:CD2	1:44:A:VAL:CG1	7	1.38
(1,20)	1:23:A:LEU:CD2	1:44:A:VAL:CG1	1	1.29
(1,20)	1:23:A:LEU:CD1	1:44:A:VAL:CG1	18	1.04
(1,20)	1:23:A:LEU:CD1	1:44:A:VAL:CG1	2	0.9
(1,22)	1:184:B:LYS:O	6:219:B:17F:N1	14	0.89
(1,20)	1:23:A:LEU:CD1	1:44:A:VAL:CG1	16	0.87
(1,20)	1:23:A:LEU:CD1	1:44:A:VAL:CG2	20	0.7
(1,20)	1:23:A:LEU:CD1	1:44:A:VAL:CG1	14	0.48
(1,20)	1:23:A:LEU:CD1	1:44:A:VAL:CG1	6	0.27

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found