



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 02:09 PM UTC

PDB ID : 6CCX / pdb_00006ccx
BMRB ID : 30403
Title : NMR data-driven model of GTPase KRas-GMPPNP:Cmpd2 complex tethered to a nanodisc
Authors : Fang, Z.; Marshall, C.B.; Nishikawa, T.; Gossert, A.D.; Jansen, J.M.; Jahnke, W.; Ikura, M.
Deposited on : 2018-02-07

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

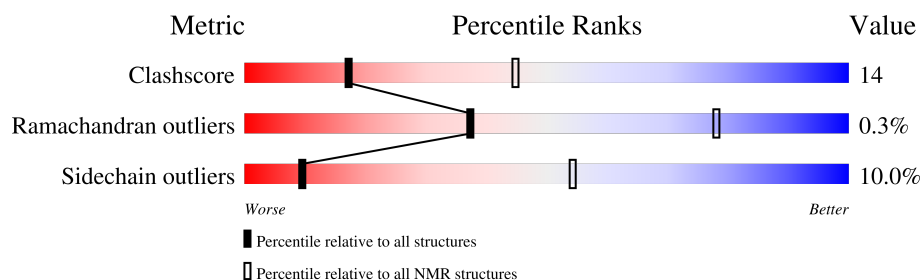
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 3%.

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	200	84% 13% ...
1	C	200	83% 14% ..
2	B	187	80% 11% • 7% •

2 Ensemble composition and analysis

This entry contains 10 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:201-A:396, C:401-C:596 (392)	0.45	10
2	B:2-B:172 (171)	0.70	3

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4
2	5, 6, 8, 9
3	7, 10

3 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9535 atoms, of which 429 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	A	198	Total	C	H	N	O	S	0
			1645	1019	22	287	314	3	
1	C	198	Total	C	H	N	O	S	0
			1646	1019	22	287	315	3	

There are 4 discrepancies between the modelled and reference sequences:

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

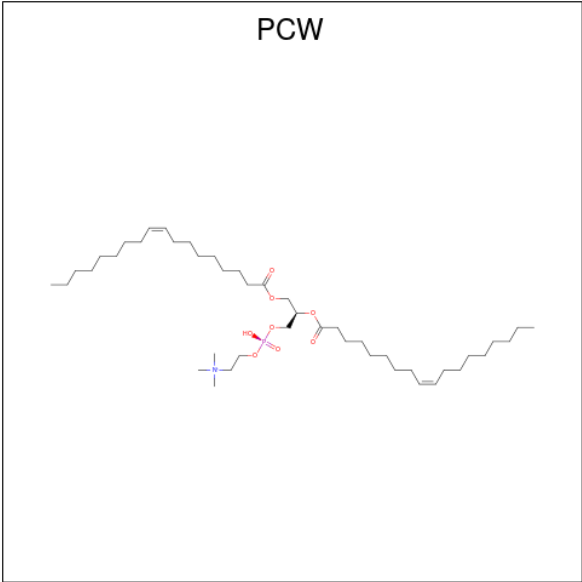
- Molecule 2 is a protein called GTPase KRas.

Mol	Chain	Residues	Atoms						Trace
2	B	185	Total	C	H	N	O	S	0
			1842	926	363	257	287	9	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P01116
B	0	SER	-	expression tag	UNP P01116
B	12	VAL	GLY	engineered mutation	UNP P01116

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



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

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

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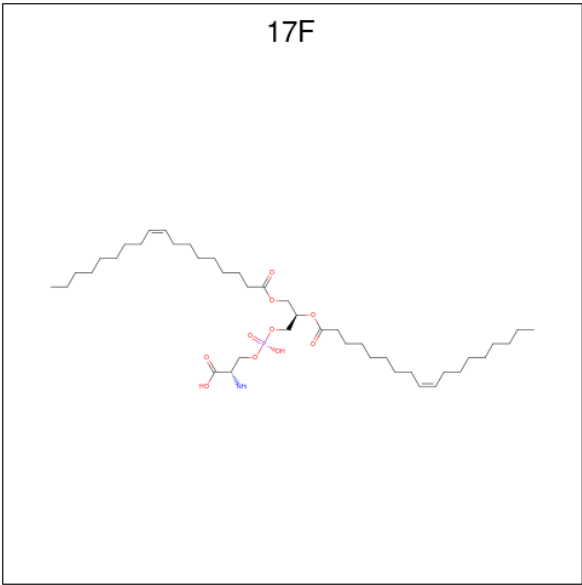
Mol	Chain	Residues	Atoms				
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44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

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

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



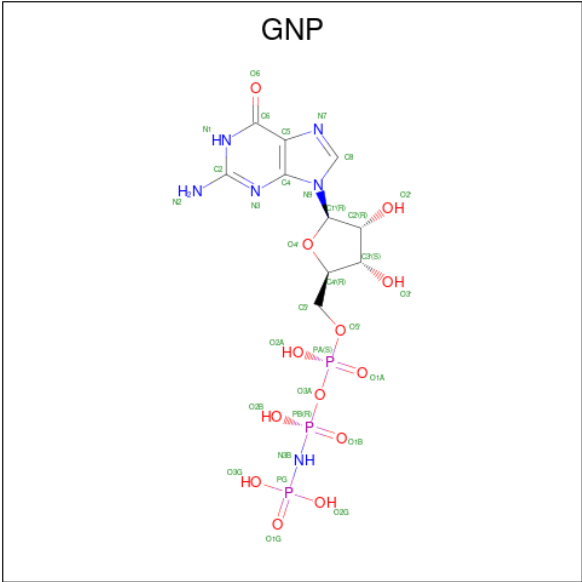
Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	B	1	Total	C	N	O	P
			54	42	1	10	1
4	B	1	Total	C	N	O	P
			54	42	1	10	1

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Mol	Chain	Residues	Atoms				
4	B	1	Total	C	N	O	P
			54	42	1	10	1
4	B	1	Total	C	N	O	P
			54	42	1	10	1
4	B	1	Total	C	N	O	P
			54	42	1	10	1
4	B	1	Total	C	N	O	P
			54	42	1	10	1
4	B	1	Total	C	N	O	P
			54	42	1	10	1
4	B	1	Total	C	N	O	P
			54	42	1	10	1
4	C	1	Total	C	N	O	P
			54	42	1	10	1
4	C	1	Total	C	N	O	P
			54	42	1	10	1
4	C	1	Total	C	N	O	P
			54	42	1	10	1
4	C	1	Total	C	N	O	P
			54	42	1	10	1
4	C	1	Total	C	N	O	P
			54	42	1	10	1

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

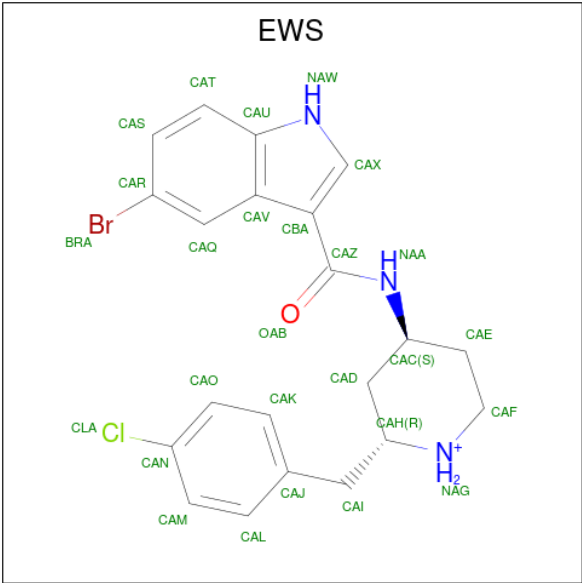


Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
5	B	1	32	10	6	13	3

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

Mol	Chain	Residues	Atoms	
			Total	Mg
6	B	1	1	1

- Molecule 7 is (2R,4S)-4-[(5-bromo-1H-indole-3-carbonyl)amino]-2-[(4-chlorophenyl)methyl]piperidin-1-ium (CCD ID: EWS) (formula: C₂₁H₂₂BrClN₃O).



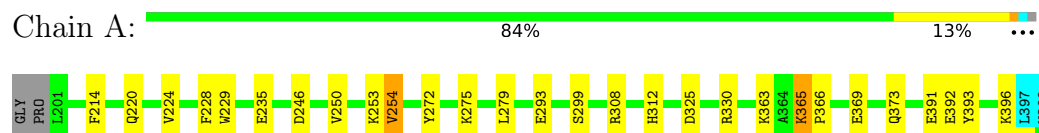
Mol	Chain	Residues	Atoms						
			Total	Br	C	Cl	H	N	O
7	B	1	49	1	21	1	22	3	1

4 Residue-property plots [i](#)

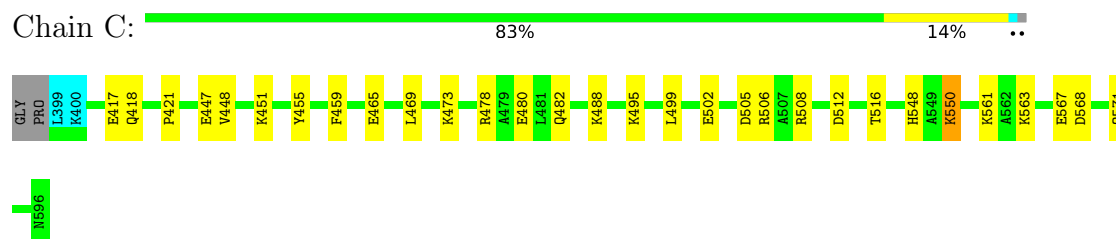
4.1 Average score per residue in the NMR ensemble

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.

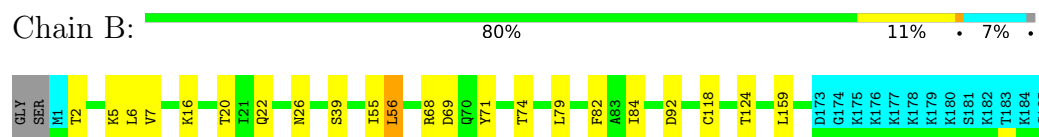
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas

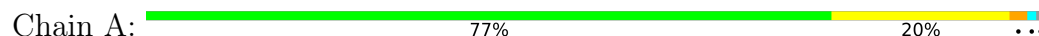


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

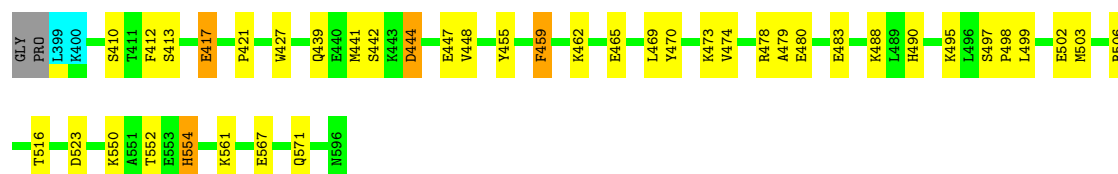
- Molecule 1: Apolipoprotein A-I





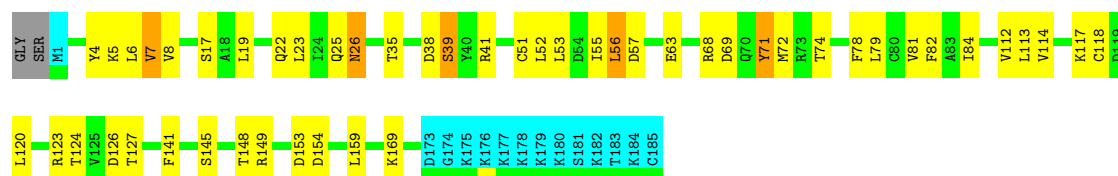
• Molecule 1: Apolipoprotein A-I

Chain C: 78% 18% ...



• Molecule 2: GTPase KRas

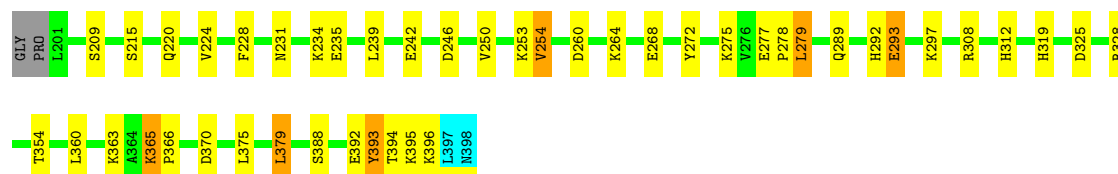
Chain B: 65% 24% 7% ...



4.2.2 Score per residue for model 2

• Molecule 1: Apolipoprotein A-I

Chain A: 76% 20% ...

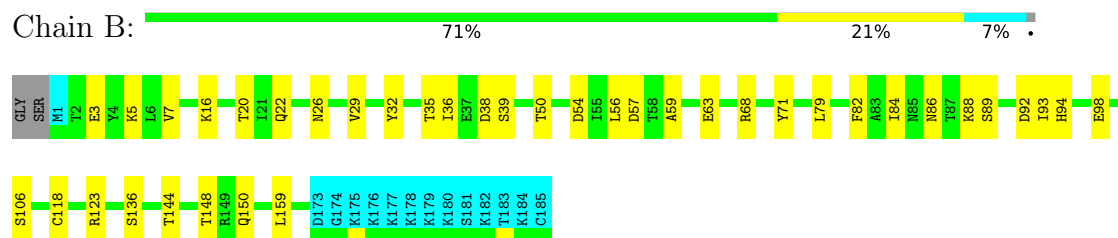


• Molecule 1: Apolipoprotein A-I

Chain C: 78% 20% ...

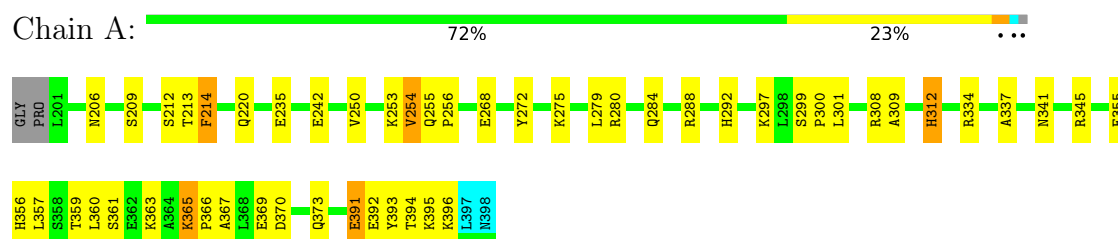


• Molecule 2: GTPase KRas

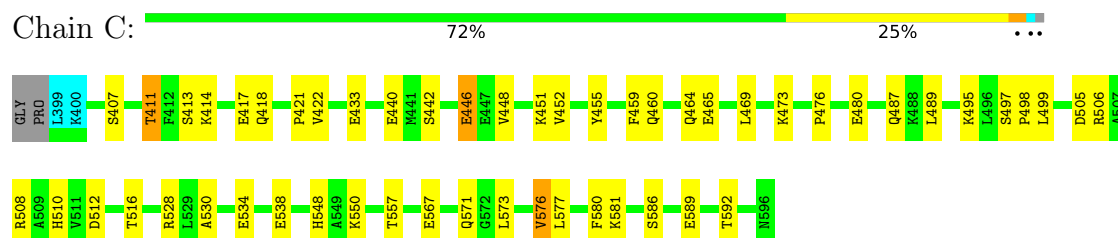


4.2.3 Score per residue for model 3

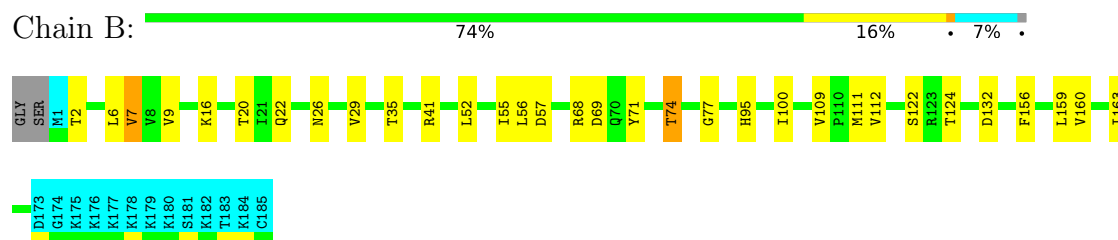
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I

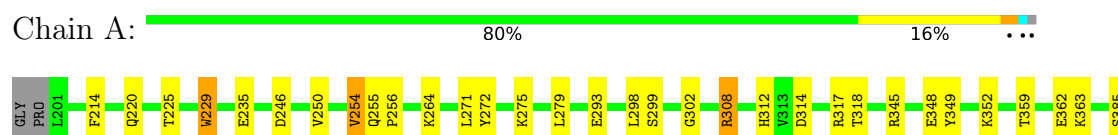


- Molecule 2: GTPase KRas



4.2.4 Score per residue for model 4

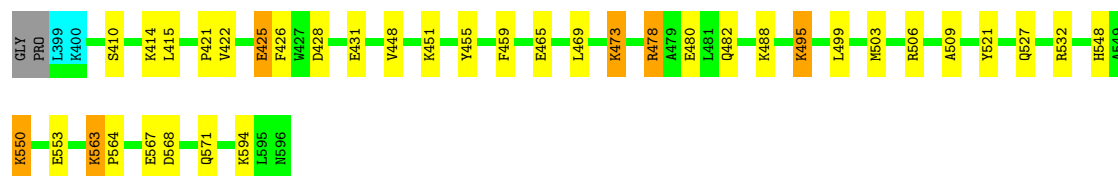
- Molecule 1: Apolipoprotein A-I





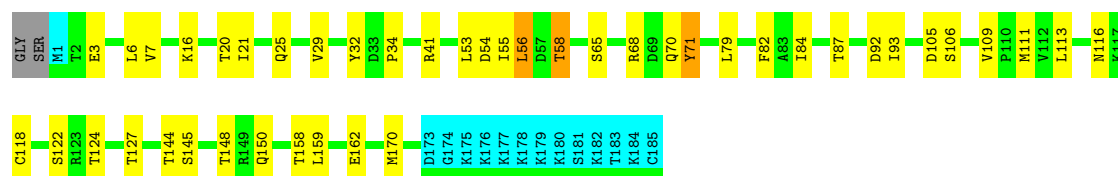
• Molecule 1: Apolipoprotein A-I

Chain C: 80% 16%



• Molecule 2: GTPase KRas

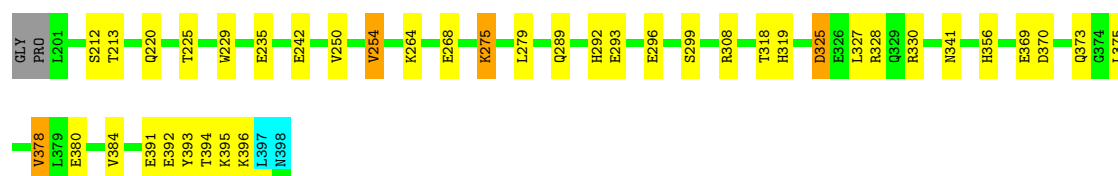
Chain B: 68% 22% 7%



4.2.5 Score per residue for model 5

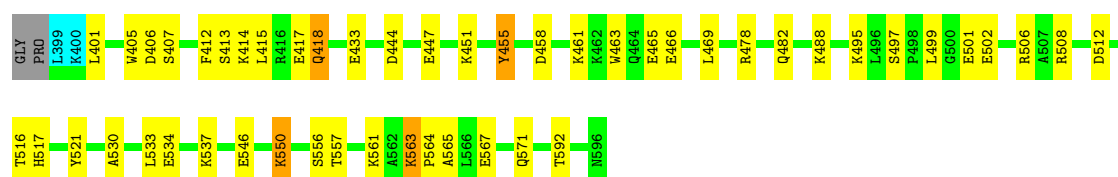
• Molecule 1: Apolipoprotein A-I

Chain A: 78% 18%



• Molecule 1: Apolipoprotein A-I

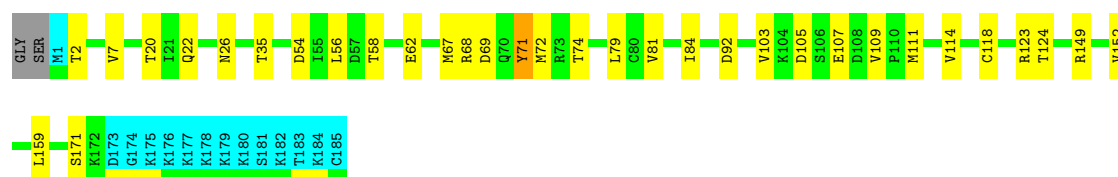
Chain C: 73% 23%



• Molecule 2: GTPase KRas

Chain B: 74% 17% 7%

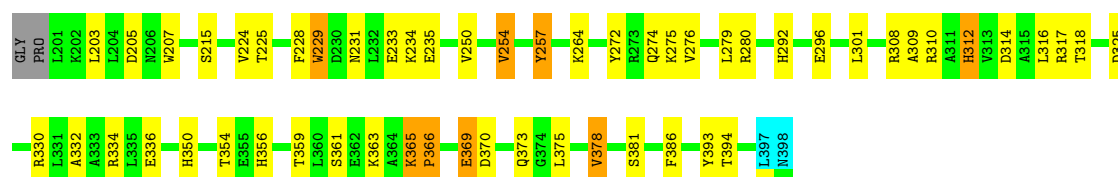




4.2.6 Score per residue for model 6

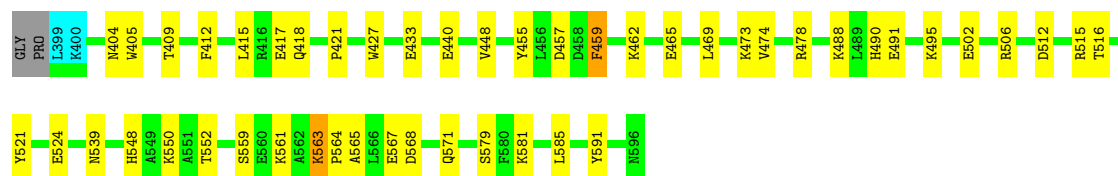
- Molecule 1: Apolipoprotein A-I

Chain A: 70% 24%



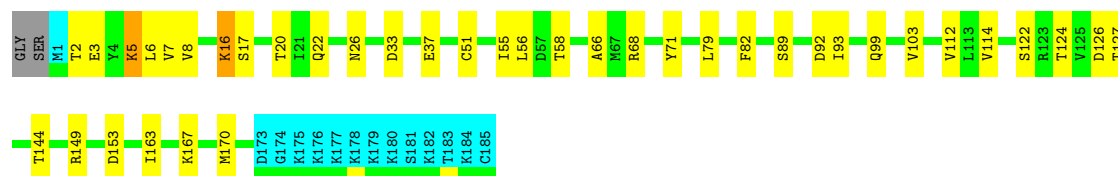
- Molecule 1: Apolipoprotein A-I

Chain C: 74% 23%



- Molecule 2: GTPase KRas

Chain B: 71% 20% 7%



4.2.7 Score per residue for model 7

- Molecule 1: Apolipoprotein A-I

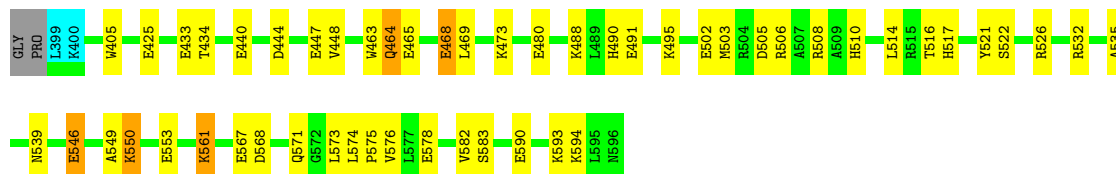
Chain A: 75% 20%





• Molecule 1: Apolipoprotein A-I

Chain C: 72% 24% ...



• Molecule 2: GTPase KRas

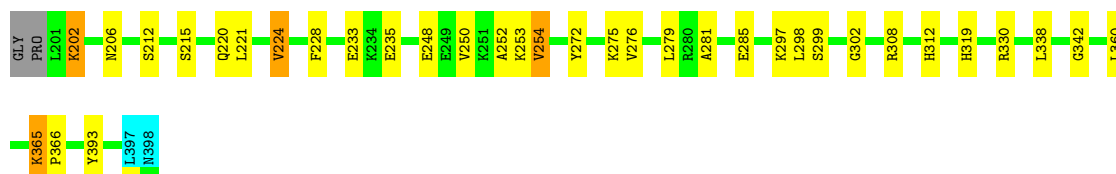
Chain B: 74% 17% 7% .



4.2.8 Score per residue for model 8

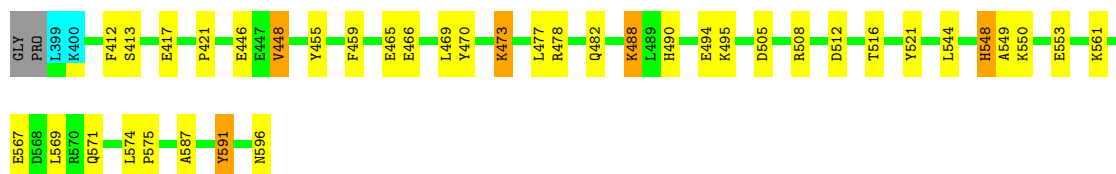
• Molecule 1: Apolipoprotein A-I

Chain A: 80% 16% ...



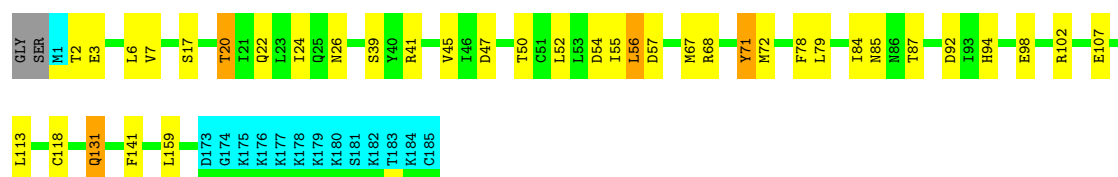
• Molecule 1: Apolipoprotein A-I

Chain C: 78% 17% ...



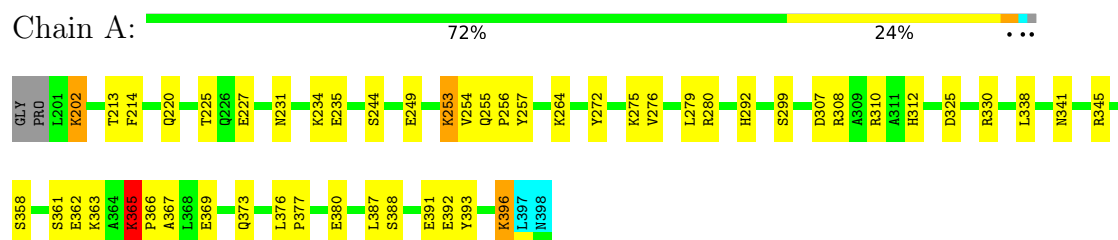
• Molecule 2: GTPase KRas

Chain B: 71% 18% 7% .

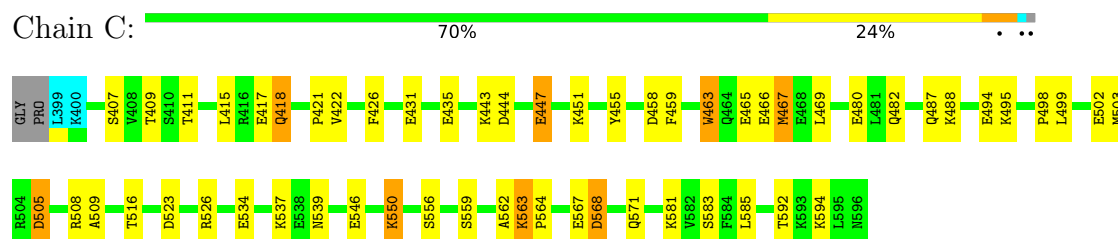


4.2.9 Score per residue for model 9

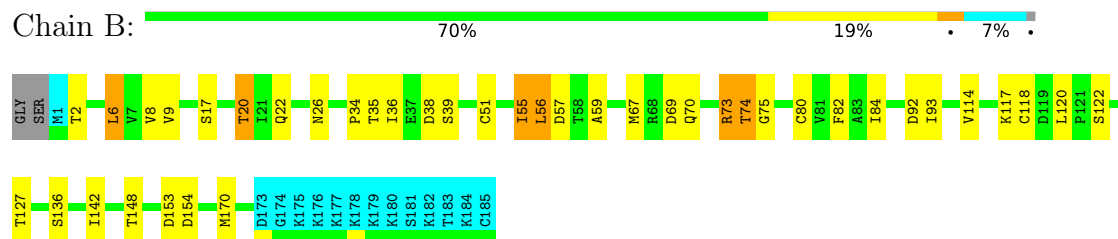
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I

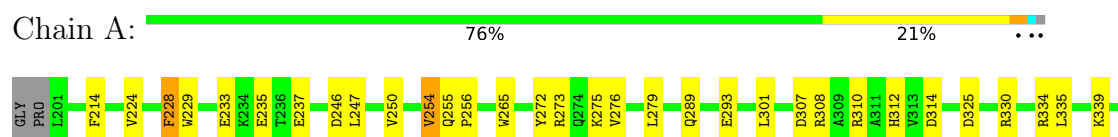


- Molecule 2: GTPase KRas



4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Apolipoprotein A-I





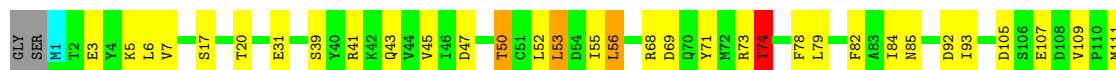
• Molecule 1: Apolipoprotein A-I

Chain C: 75% 20% ...



• Molecule 2: GTPase KRas

Chain B: 70% 20% 7% ..



5 Refinement protocol and experimental data overview

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

Of the 3000 calculated structures, 10 were deposited, based on the following criterion: *10 structures for lowest energy*.

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

Software name	Classification	Version
HADDOCK	structure calculation	
HADDOCK	refinement	
CNS	refinement	

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	268
Number of shifts mapped to atoms	193
Number of unparsed shifts	0
Number of shifts with mapping errors	75
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	3%

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: MG, EWS, GNP, PCW, 17F

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	0.39±0.01	0±0/1635 (0.0± 0.0%)	0.78±0.01	0±0/2199 (0.0± 0.0%)
1	C	0.40±0.01	0±0/1634 (0.0± 0.0%)	0.79±0.01	0±0/2196 (0.0± 0.0%)
2	B	0.33±0.00	0±0/1390 (0.0± 0.0%)	0.70±0.04	1±1/1875 (0.0± 0.1%)
All	All	0.38	0/46590 (0.0%)	0.76	6/62700 (0.0%)

There are no bond-length outliers.

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
2	B	74	THR	CA-CB-OG1	-14.22	88.28	109.60	10	1
2	B	74	THR	CB-CA-C	-9.37	91.26	110.38	10	1
2	B	74	THR	N-CA-CB	9.18	124.44	110.30	10	1
2	B	55	ILE	N-CA-C	5.29	114.40	106.42	9	1
2	B	63	GLU	CB-CA-C	-5.22	109.55	117.07	2	1
2	B	63	GLU	CA-C-O	5.19	120.95	117.94	2	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	1607	22	1609	34±7
1	C	1607	22	1603	35±9
2	B	1368	322	1354	26±5
3	A	540	0	840	45±4
3	B	1350	0	2100	97±6
3	C	1566	0	2436	89±10
4	A	54	0	76	4±1
4	B	486	0	684	50±8
4	C	324	0	456	21±4
5	B	32	0	13	1±1
7	B	27	22	0	17±4
All	All	89620	3880	111707	2760

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:393:TYR:CE1	3:A:407:PCW:C28	1.61	1.83	8	2
1:A:393:TYR:CE1	3:A:407:PCW:C27	1.59	1.82	8	2
1:C:488:LYS:CE	3:C:623:PCW:C28	1.54	1.81	4	2
1:C:488:LYS:CE	3:C:623:PCW:H283	1.54	1.15	4	1
1:C:488:LYS:HD3	3:C:623:PCW:C27	1.53	1.04	4	2
1:C:488:LYS:HE2	3:C:623:PCW:C28	1.51	1.27	4	1
1:C:488:LYS:CD	3:C:623:PCW:H271	1.46	1.38	4	1
1:C:488:LYS:HD3	3:C:623:PCW:C28	1.46	1.36	5	7
1:A:308:ARG:CG	1:C:469:LEU:HD11	1.45	1.42	4	2
1:A:393:TYR:CZ	3:A:407:PCW:H271	1.42	1.48	6	4
1:A:393:TYR:CE1	3:A:407:PCW:H271	1.42	1.46	3	3
1:A:396:LYS:NZ	3:A:407:PCW:H271	1.41	1.22	5	1
1:C:488:LYS:CD	3:C:623:PCW:C28	1.39	1.95	4	4
1:C:488:LYS:CD	3:C:623:PCW:C27	1.38	1.92	4	1
3:B:207:PCW:H72	7:B:237:EWS:BRA	1.38	1.73	10	1
1:C:488:LYS:CD	3:C:623:PCW:H281	1.37	1.48	5	5
1:A:393:TYR:CZ	3:A:407:PCW:C27	1.35	1.97	3	3
2:B:75:GLY:N	7:B:237:EWS:BRA	1.35	2.14	9	1
1:A:393:TYR:CD1	3:A:407:PCW:C28	1.33	2.12	8	2
1:A:393:TYR:CD1	3:A:407:PCW:C27	1.32	2.11	8	2
1:A:393:TYR:CE1	3:A:407:PCW:H281	1.32	1.44	8	1
3:B:201:PCW:H32	7:B:237:EWS:CLA	1.31	1.60	5	1
1:A:393:TYR:CD1	3:A:407:PCW:H281	1.31	1.58	8	2
3:B:207:PCW:C7	7:B:237:EWS:BRA	1.31	2.32	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:393:TYR:OH	3:A:407:PCW:H271	1.30	1.14	2	2
1:A:393:TYR:CZ	3:A:407:PCW:H272	1.29	1.53	3	2
1:C:465:GLU:O	1:C:469:LEU:CG	1.27	1.82	10	8
1:A:308:ARG:HG2	1:C:469:LEU:CD1	1.25	1.60	4	1
1:A:396:LYS:CD	3:A:407:PCW:H281	1.25	1.61	5	1
1:A:396:LYS:HD3	3:A:407:PCW:C28	1.24	1.63	5	1
2:B:56:LEU:HD22	7:B:237:EWS:OAB	1.22	1.28	1	7
1:C:465:GLU:O	1:C:469:LEU:HG	1.22	1.00	10	10
2:B:74:THR:HB	7:B:237:EWS:BRA	1.21	1.90	9	1
1:A:396:LYS:NZ	3:A:407:PCW:C27	1.19	2.06	5	1
1:A:393:TYR:OH	3:A:407:PCW:C27	1.19	1.91	2	2
1:A:393:TYR:OH	3:A:407:PCW:C26	1.19	1.91	6	1
3:B:220:PCW:H52	7:B:237:EWS:BRA	1.19	1.93	8	1
3:B:208:PCW:H81	7:B:237:EWS:BRA	1.17	1.93	4	1
3:B:220:PCW:H42	7:B:237:EWS:BRA	1.17	1.93	8	1
3:B:220:PCW:C4	7:B:237:EWS:BRA	1.15	2.49	8	1
3:B:207:PCW:C6	7:B:237:EWS:BRA	1.14	2.50	10	1
1:C:488:LYS:CG	3:C:623:PCW:H281	1.13	1.73	4	2
1:A:393:TYR:HE1	3:A:407:PCW:C28	1.13	1.25	8	1
3:B:207:PCW:H63	7:B:237:EWS:BRA	1.12	1.99	10	1
2:B:56:LEU:CD2	7:B:237:EWS:OAB	1.12	1.96	1	7
1:A:214:PHE:CZ	3:A:404:PCW:H162	1.12	1.79	4	2
1:A:393:TYR:OH	3:A:407:PCW:H262	1.12	1.43	6	1
3:B:220:PCW:C5	7:B:237:EWS:BRA	1.11	2.53	8	1
1:A:391:GLU:O	1:A:395:LYS:HG3	1.09	1.46	5	1
1:A:393:TYR:CD1	3:A:407:PCW:H272	1.08	1.79	8	1
1:C:488:LYS:HG2	3:C:623:PCW:H281	1.07	1.23	4	1
2:B:56:LEU:HD13	7:B:237:EWS:CAZ	1.07	1.79	1	1
1:C:455:TYR:OH	3:C:601:PCW:C21	1.07	2.03	3	4
2:B:74:THR:C	7:B:237:EWS:BRA	1.07	2.53	9	1
2:B:56:LEU:HD13	7:B:237:EWS:OAB	1.04	1.49	9	5
1:C:567:GLU:O	1:C:571:GLN:HG3	1.04	1.50	8	10
1:C:488:LYS:CE	3:C:623:PCW:H281	1.03	1.83	9	3
2:B:5:LYS:HB3	7:B:237:EWS:CAT	1.03	1.84	1	3
3:A:408:PCW:H341	3:B:231:PCW:H39	1.02	1.30	4	7
1:A:396:LYS:HZ2	3:A:407:PCW:C27	1.02	1.63	5	1
2:B:71:TYR:HB3	7:B:237:EWS:CAF	1.02	1.84	5	1
3:B:221:PCW:H51	7:B:237:EWS:BRA	1.01	2.10	1	1
1:C:455:TYR:OH	3:C:601:PCW:H211	1.01	1.56	4	4
2:B:56:LEU:CD1	7:B:237:EWS:OAB	1.01	2.08	9	5
1:A:308:ARG:CD	1:C:469:LEU:HD21	1.00	1.86	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:71:TYR:HA	7:B:237:EWS:CAC	1.00	1.86	1	1
4:B:228:17F:H4	4:B:228:17F:H1	0.99	1.29	10	3
1:A:308:ARG:HG3	1:C:469:LEU:HD21	0.99	1.32	9	7
3:B:221:PCW:C5	7:B:237:EWS:BRA	0.99	2.65	1	1
1:A:393:TYR:HD1	3:A:407:PCW:H281	0.99	1.18	10	1
3:B:201:PCW:C3	7:B:237:EWS:CLA	0.98	2.47	5	1
1:C:488:LYS:HD3	3:C:623:PCW:H281	0.98	1.01	10	7
1:A:396:LYS:HD3	3:A:407:PCW:H281	0.98	1.01	5	1
3:B:201:PCW:O3P	7:B:237:EWS:CAO	0.97	2.13	5	1
3:B:202:PCW:H31	3:B:212:PCW:H322	0.97	1.34	10	2
2:B:56:LEU:HD23	7:B:237:EWS:OAB	0.97	1.59	5	1
1:A:214:PHE:CZ	3:A:404:PCW:H171	0.97	1.94	1	2
3:B:221:PCW:H32	7:B:237:EWS:CLA	0.96	1.96	9	1
1:A:392:GLU:OE1	1:A:395:LYS:HD2	0.94	1.62	5	1
1:C:488:LYS:HD3	3:C:623:PCW:H283	0.93	1.39	5	1
2:B:7:VAL:HG13	7:B:237:EWS:NAW	0.92	1.79	7	2
1:C:455:TYR:OH	3:C:601:PCW:C22	0.92	2.18	9	2
1:C:455:TYR:OH	3:C:601:PCW:H232	0.92	1.65	8	2
1:C:567:GLU:O	1:C:571:GLN:CG	0.91	2.17	8	3
1:A:369:GLU:OE1	1:A:373:GLN:NE2	0.91	2.02	1	1
2:B:74:THR:CB	7:B:237:EWS:BRA	0.91	2.73	9	1
1:A:393:TYR:HE1	3:A:407:PCW:H271	0.90	1.16	3	1
1:A:396:LYS:CE	3:A:407:PCW:H281	0.90	1.98	5	1
3:B:208:PCW:H71	7:B:237:EWS:BRA	0.89	2.22	4	1
1:A:392:GLU:CD	1:A:395:LYS:HD2	0.89	1.93	5	1
1:A:308:ARG:HD2	1:C:469:LEU:HD21	0.89	1.43	6	1
1:A:369:GLU:O	1:A:373:GLN:HG3	0.89	1.67	9	7
1:C:488:LYS:NZ	3:C:623:PCW:H281	0.89	1.82	9	2
3:B:210:PCW:H162	4:B:227:17F:H11A	0.88	1.43	8	1
3:B:210:PCW:H332	4:B:224:17F:H19	0.88	1.45	9	1
1:C:455:TYR:OH	3:C:601:PCW:C20	0.88	2.22	3	3
3:C:607:PCW:H412	3:C:611:PCW:H31	0.88	1.45	9	3
2:B:75:GLY:CA	7:B:237:EWS:BRA	0.88	2.76	9	1
1:C:488:LYS:HD3	3:C:623:PCW:H272	0.87	1.41	9	1
3:B:217:PCW:H11	7:B:237:EWS:CAM	0.87	2.00	7	1
3:A:407:PCW:H342	4:B:225:17F:H9	0.87	1.44	6	5
3:A:410:PCW:H372	4:C:633:17F:H36	0.87	1.46	4	1
3:B:221:PCW:H63	7:B:237:EWS:BRA	0.86	2.25	1	2
3:B:210:PCW:C7	7:B:237:EWS:CAO	0.86	2.53	10	1
1:A:396:LYS:HZ3	3:A:407:PCW:H271	0.86	1.04	5	1
1:A:214:PHE:HZ	3:A:404:PCW:H162	0.85	1.12	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:618:PCW:H121	3:C:620:PCW:H381	0.85	1.47	10	1
3:A:410:PCW:H331	4:C:633:17F:H37	0.85	1.49	1	2
1:A:214:PHE:HZ	3:A:404:PCW:H171	0.85	1.27	1	2
4:B:223:17F:H35	4:B:225:17F:H20A	0.84	1.46	6	1
1:A:308:ARG:HG3	1:C:469:LEU:CD2	0.84	2.01	9	3
3:B:219:PCW:O2P	7:B:237:EWS:CAI	0.84	2.25	9	1
3:C:621:PCW:H361	3:C:629:PCW:H212	0.84	1.50	10	3
4:A:411:17F:H35	3:C:624:PCW:H482	0.84	1.47	3	2
3:B:208:PCW:H61	7:B:237:EWS:BRA	0.84	2.28	4	1
3:B:207:PCW:H71	7:B:237:EWS:BRA	0.84	2.28	10	1
1:A:392:GLU:OE1	1:A:395:LYS:CD	0.83	2.25	5	1
3:A:410:PCW:H121	4:C:633:17F:H30	0.83	1.47	8	8
3:B:207:PCW:O3P	7:B:237:EWS:CAK	0.83	2.26	6	1
3:B:231:PCW:H341	3:C:604:PCW:H322	0.83	1.50	6	7
3:A:407:PCW:H122	4:B:223:17F:H20	0.83	1.48	3	2
1:C:488:LYS:NZ	3:C:623:PCW:H283	0.83	1.87	4	1
2:B:56:LEU:HD22	7:B:237:EWS:CAZ	0.82	2.03	8	4
1:C:465:GLU:O	1:C:469:LEU:CB	0.82	2.27	6	3
3:A:407:PCW:H342	4:B:225:17F:H8A	0.82	1.49	9	1
2:B:70:GLN:HG3	3:B:220:PCW:H41	0.82	1.51	9	1
4:B:234:17F:H57	3:C:625:PCW:H141	0.82	1.52	1	6
4:C:633:17F:H2	4:C:633:17F:H4A	0.82	1.49	2	2
1:A:393:TYR:HD1	3:A:407:PCW:C28	0.82	1.86	8	2
1:A:314:ASP:HA	1:A:317:ARG:HD2	0.81	1.52	1	3
2:B:84:ILE:HD11	2:B:118:CYS:HA	0.81	1.49	4	6
3:B:201:PCW:H411	3:B:219:PCW:H452	0.81	1.50	5	3
1:A:365:LYS:HB2	1:A:366:PRO:HD3	0.81	1.52	1	8
3:B:208:PCW:H371	4:B:226:17F:H18A	0.81	1.48	10	1
2:B:7:VAL:CG2	7:B:237:EWS:CAX	0.81	2.58	8	3
3:A:410:PCW:H362	4:C:633:17F:H36	0.80	1.53	6	2
3:A:407:PCW:H331	4:B:223:17F:H20	0.80	1.52	10	1
3:B:208:PCW:H321	7:B:237:EWS:CAO	0.80	2.05	4	1
1:A:214:PHE:CZ	3:A:404:PCW:H161	0.80	2.11	10	1
3:B:207:PCW:H12	7:B:237:EWS:CAO	0.80	2.06	6	1
3:C:617:PCW:H212	4:C:632:17F:H41	0.80	1.50	6	2
3:C:607:PCW:H252	4:C:631:17F:H39	0.80	1.53	3	3
3:B:219:PCW:H73	7:B:237:EWS:NAA	0.80	1.91	9	1
3:B:221:PCW:C4	7:B:237:EWS:BRA	0.80	2.84	1	1
1:A:308:ARG:CB	1:C:469:LEU:HD11	0.80	2.06	4	2
3:B:202:PCW:H12	3:B:212:PCW:H322	0.80	1.52	8	1
3:A:401:PCW:H40	3:C:613:PCW:H251	0.79	1.52	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:232:PCW:H122	3:C:625:PCW:H171	0.79	1.54	7	4
4:A:411:17F:H47	3:C:617:PCW:H422	0.79	1.52	8	1
3:C:618:PCW:H122	3:C:620:PCW:H381	0.79	1.52	1	3
1:A:279:LEU:HD22	1:C:495:LYS:HG2	0.79	1.51	6	2
3:C:617:PCW:H222	4:C:635:17F:H39	0.79	1.54	10	3
3:C:618:PCW:H381	3:C:619:PCW:H121	0.79	1.54	4	1
1:A:393:TYR:HE1	3:A:407:PCW:H283	0.79	1.35	8	1
1:A:396:LYS:HZ2	3:A:407:PCW:H271	0.79	1.00	5	1
3:A:410:PCW:H352	4:C:633:17F:H36	0.78	1.54	3	5
3:B:202:PCW:H442	4:B:226:17F:H12A	0.78	1.53	6	4
2:B:71:TYR:CB	7:B:237:EWS:CAF	0.78	2.60	5	1
3:A:408:PCW:H422	3:B:204:PCW:H451	0.78	1.54	3	1
3:B:205:PCW:H83	7:B:237:EWS:BRA	0.78	2.33	6	2
3:B:208:PCW:H31	3:B:221:PCW:H141	0.78	1.56	8	2
3:A:402:PCW:H39	3:B:214:PCW:H232	0.78	1.54	2	1
3:B:217:PCW:H152	3:B:218:PCW:H141	0.77	1.55	10	2
1:C:455:TYR:OH	3:C:601:PCW:H222	0.77	1.78	9	1
3:B:221:PCW:C3	7:B:237:EWS:CLA	0.77	2.69	9	1
3:B:210:PCW:H52	7:B:237:EWS:CAK	0.77	2.10	10	1
1:A:391:GLU:O	1:A:395:LYS:CG	0.77	2.31	5	1
3:B:211:PCW:H382	4:B:229:17F:H10A	0.77	1.55	3	4
1:A:393:TYR:CE1	3:A:407:PCW:H272	0.77	2.14	2	2
3:C:605:PCW:H182	3:C:626:PCW:H151	0.77	1.56	2	3
1:A:393:TYR:HH	3:A:407:PCW:H271	0.77	0.97	2	1
1:C:465:GLU:O	1:C:469:LEU:CD1	0.76	2.32	6	3
1:A:393:TYR:HD1	1:A:396:LYS:HE3	0.76	1.39	5	1
2:B:54:ASP:OD2	7:B:237:EWS:BRA	0.76	2.58	7	1
2:B:56:LEU:HD22	7:B:237:EWS:CAX	0.76	2.10	9	2
2:B:38:ASP:HB3	2:B:57:ASP:HB3	0.76	1.58	2	2
1:A:392:GLU:O	1:A:396:LYS:HG3	0.76	1.80	5	1
1:A:308:ARG:HD3	1:C:469:LEU:HD21	0.76	1.57	6	1
3:B:221:PCW:H72	7:B:237:EWS:BRA	0.76	2.36	1	1
3:B:203:PCW:H11	3:B:220:PCW:H81	0.76	1.57	9	1
3:A:410:PCW:H381	4:C:633:17F:H36	0.76	1.58	10	3
3:A:406:PCW:H182	3:A:409:PCW:H261	0.76	1.55	7	1
3:A:406:PCW:H152	4:B:226:17F:H34	0.75	1.55	5	1
3:A:406:PCW:H40	4:B:226:17F:H69	0.75	1.59	10	1
3:B:202:PCW:H421	4:B:226:17F:H40	0.75	1.57	7	4
1:A:297:LYS:HE2	1:C:476:PRO:HB2	0.75	1.56	3	2
3:A:408:PCW:H422	3:B:204:PCW:H472	0.75	1.58	9	1
3:A:410:PCW:H331	4:C:633:17F:H12A	0.75	1.59	10	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:201:PCW:H251	4:B:228:17F:H64	0.75	1.57	5	1
3:B:210:PCW:H161	4:B:224:17F:H18A	0.75	1.58	8	1
3:C:611:PCW:H242	3:C:617:PCW:H421	0.75	1.58	9	1
3:B:208:PCW:C8	7:B:237:EWS:BRA	0.75	2.83	4	1
4:B:226:17F:HN1	7:B:237:EWS:CAL	0.75	1.93	4	1
1:C:563:LYS:HB2	1:C:564:PRO:HD3	0.75	1.55	4	4
3:A:410:PCW:H332	4:C:633:17F:H12A	0.75	1.56	1	2
4:B:226:17F:H12	4:B:230:17F:H11	0.75	1.58	5	1
3:C:611:PCW:H381	3:C:617:PCW:H412	0.74	1.58	2	3
1:A:396:LYS:CE	3:A:407:PCW:C28	0.74	2.63	5	1
3:C:611:PCW:H482	4:C:635:17F:H42	0.74	1.59	1	3
4:B:234:17F:H56	3:C:625:PCW:H19	0.74	1.59	10	1
1:A:308:ARG:CG	1:C:469:LEU:CD1	0.74	2.39	4	1
3:B:217:PCW:H2	7:B:237:EWS:CLA	0.74	2.18	7	1
1:A:214:PHE:CZ	3:A:404:PCW:C16	0.74	2.69	4	3
4:A:411:17F:H29	4:C:631:17F:H65	0.74	1.59	1	1
3:C:618:PCW:H121	3:C:620:PCW:H382	0.74	1.57	5	3
1:A:393:TYR:CD1	1:A:396:LYS:HE3	0.73	2.18	5	1
2:B:7:VAL:HG21	7:B:237:EWS:CAX	0.73	2.13	6	2
4:B:223:17F:H1	4:B:223:17F:H4	0.73	1.58	3	1
2:B:71:TYR:HB2	7:B:237:EWS:CAC	0.73	2.12	8	1
3:A:407:PCW:H121	4:B:223:17F:H20A	0.73	1.59	10	2
4:B:234:17F:H31	3:C:625:PCW:H19	0.73	1.60	8	1
3:C:619:PCW:H322	3:C:621:PCW:H172	0.73	1.60	3	1
3:C:621:PCW:H31	3:C:629:PCW:H151	0.73	1.59	3	1
2:B:56:LEU:CD2	7:B:237:EWS:CAZ	0.73	2.65	5	1
3:C:606:PCW:H471	3:C:622:PCW:H39	0.73	1.58	6	1
3:B:215:PCW:H221	3:C:609:PCW:H483	0.73	1.58	8	1
3:C:617:PCW:H241	4:C:635:17F:H44	0.73	1.57	10	1
4:B:228:17F:H1	4:B:228:17F:C4	0.73	2.12	10	3
4:B:225:17F:H63	3:C:626:PCW:H262	0.73	1.61	2	1
3:A:407:PCW:H331	4:B:223:17F:H31	0.73	1.60	9	3
1:C:455:TYR:HE2	3:C:601:PCW:H231	0.73	1.43	3	1
1:A:393:TYR:HD1	1:A:396:LYS:CE	0.73	1.96	5	1
3:B:219:PCW:H212	3:C:605:PCW:H281	0.73	1.58	10	1
3:A:410:PCW:H121	4:C:633:17F:H29	0.73	1.61	1	2
4:C:631:17F:H60	4:C:631:17F:H37	0.73	1.60	2	1
3:C:608:PCW:H31	3:C:628:PCW:H332	0.73	1.58	8	3
3:B:220:PCW:H62	3:B:220:PCW:H2	0.73	1.60	9	1
3:B:210:PCW:H72	7:B:237:EWS:CAO	0.73	2.13	10	1
3:B:209:PCW:H252	3:B:213:PCW:H431	0.72	1.61	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:231:PCW:H341	3:C:604:PCW:H331	0.72	1.60	9	1
3:A:406:PCW:H182	3:A:409:PCW:H242	0.72	1.61	5	2
3:A:410:PCW:H132	4:C:633:17F:H11A	0.72	1.60	2	4
3:C:613:PCW:H162	3:C:626:PCW:H451	0.72	1.60	7	4
4:B:234:17F:H9A	4:B:234:17F:H20A	0.72	1.62	5	2
3:C:613:PCW:H162	3:C:622:PCW:H161	0.72	1.59	9	3
3:B:209:PCW:H122	3:B:213:PCW:H122	0.72	1.61	3	3
3:B:217:PCW:H42	3:B:217:PCW:H321	0.72	1.61	5	2
3:C:617:PCW:H211	4:C:632:17F:H41	0.72	1.58	5	1
3:C:611:PCW:H372	3:C:617:PCW:H412	0.72	1.62	4	1
3:A:409:PCW:H481	3:B:208:PCW:H462	0.72	1.62	6	1
3:B:207:PCW:H20	3:B:232:PCW:H483	0.72	1.60	1	1
3:C:610:PCW:H341	3:C:614:PCW:H121	0.72	1.60	1	2
2:B:7:VAL:CG1	7:B:237:EWS:NAW	0.71	2.53	7	2
4:B:223:17F:H1	4:B:223:17F:C4	0.71	2.15	3	1
3:B:210:PCW:H172	4:B:224:17F:H18	0.71	1.60	5	3
1:A:308:ARG:CG	1:C:469:LEU:HD21	0.71	2.14	9	2
3:A:403:PCW:H332	3:B:204:PCW:H32	0.71	1.62	10	2
4:B:234:17F:H9	4:B:234:17F:H20	0.71	1.60	9	1
2:B:54:ASP:CG	7:B:237:EWS:BRA	0.71	2.89	7	2
3:A:408:PCW:H342	3:C:604:PCW:H232	0.71	1.61	4	1
3:C:618:PCW:H122	3:C:620:PCW:H382	0.71	1.63	7	2
4:B:234:17F:H12	4:C:631:17F:H38	0.71	1.61	6	1
3:A:403:PCW:H351	3:A:403:PCW:H161	0.71	1.62	2	1
3:B:210:PCW:H361	4:B:224:17F:H19A	0.71	1.63	8	1
3:C:607:PCW:H332	3:C:611:PCW:H131	0.71	1.61	3	1
3:A:407:PCW:H352	4:B:223:17F:H56	0.71	1.61	10	3
3:C:613:PCW:H151	3:C:626:PCW:H431	0.71	1.63	7	4
2:B:74:THR:HB	4:B:230:17F:H1A	0.70	1.61	1	1
3:A:407:PCW:H331	4:B:223:17F:H32	0.70	1.62	8	4
4:A:411:17F:H1A	4:C:631:17F:H6A	0.70	1.63	4	6
3:C:627:PCW:H331	3:C:628:PCW:H121	0.70	1.63	6	7
3:B:217:PCW:C2	7:B:237:EWS:CLA	0.70	2.76	7	1
3:B:220:PCW:H122	3:B:220:PCW:H361	0.70	1.63	8	1
4:B:228:17F:H4	4:B:228:17F:C1	0.70	2.17	2	3
3:B:210:PCW:H372	4:B:224:17F:H20A	0.70	1.62	7	2
3:B:210:PCW:H73	7:B:237:EWS:CAO	0.70	2.15	10	1
1:A:369:GLU:OE1	1:A:373:GLN:CD	0.70	2.34	1	1
3:B:233:PCW:H411	3:C:604:PCW:H39	0.70	1.63	2	2
1:A:392:GLU:OE2	1:A:395:LYS:NZ	0.70	2.24	5	1
2:B:39:SER:HB2	7:B:237:EWS:BRA	0.70	2.42	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:209:PCW:H331	3:B:213:PCW:H121	0.70	1.63	3	1
3:A:407:PCW:H151	4:B:223:17F:H33	0.70	1.63	9	2
3:B:210:PCW:H331	4:B:224:17F:H19	0.70	1.62	7	1
3:B:217:PCW:C1	7:B:237:EWS:CLA	0.70	2.77	7	1
2:B:56:LEU:HD13	7:B:237:EWS:CBA	0.70	2.16	1	1
3:B:231:PCW:H371	3:C:604:PCW:H212	0.70	1.64	10	4
4:B:223:17F:H51	3:C:626:PCW:H231	0.70	1.64	7	1
3:B:208:PCW:H331	3:B:221:PCW:H19	0.70	1.63	7	2
3:A:402:PCW:H341	3:B:213:PCW:H321	0.70	1.62	3	1
3:B:212:PCW:H332	3:B:212:PCW:H131	0.70	1.63	4	2
3:B:201:PCW:H371	4:B:226:17F:H42	0.70	1.63	9	1
3:C:609:PCW:H162	4:C:632:17F:H18	0.69	1.62	8	2
3:C:615:PCW:H132	3:C:622:PCW:H382	0.69	1.63	3	3
3:B:202:PCW:H331	4:B:228:17F:H4A	0.69	1.62	8	1
3:B:205:PCW:H232	3:B:220:PCW:H412	0.69	1.64	8	1
2:B:7:VAL:HG22	7:B:237:EWS:NAW	0.69	2.03	1	2
1:A:396:LYS:CD	3:A:407:PCW:C28	0.69	2.41	5	1
2:B:71:TYR:HB2	7:B:237:EWS:CAE	0.69	2.17	5	2
3:B:207:PCW:H162	3:B:232:PCW:H281	0.69	1.63	10	1
3:B:210:PCW:H131	3:B:216:PCW:H2	0.69	1.63	2	2
3:B:217:PCW:H11	7:B:237:EWS:CLA	0.69	2.24	7	1
3:B:211:PCW:H412	4:B:229:17F:H60	0.69	1.65	2	1
3:B:209:PCW:H181	3:B:213:PCW:H19	0.69	1.64	3	2
3:C:611:PCW:H341	3:C:617:PCW:H341	0.69	1.64	4	1
3:A:407:PCW:H121	4:B:223:17F:H33	0.69	1.65	5	4
1:C:458:ASP:HA	1:C:461:LYS:HE2	0.69	1.63	5	1
3:C:611:PCW:H171	3:C:617:PCW:H352	0.69	1.65	5	1
2:B:7:VAL:HG23	7:B:237:EWS:NAW	0.69	2.03	8	1
3:C:611:PCW:H181	3:C:617:PCW:H351	0.69	1.63	9	1
1:A:308:ARG:HG2	1:C:469:LEU:HD11	0.69	0.70	4	1
4:B:228:17F:H63	3:C:615:PCW:H472	0.69	1.64	5	1
3:B:231:PCW:H472	3:C:604:PCW:H271	0.69	1.63	10	1
1:A:255:GLN:HB2	1:A:256:PRO:HD3	0.68	1.65	3	3
3:B:202:PCW:H451	4:B:226:17F:H10A	0.68	1.64	5	1
3:B:219:PCW:H342	4:B:226:17F:H37	0.68	1.63	1	1
3:B:218:PCW:H262	3:C:625:PCW:H421	0.68	1.63	4	1
3:A:406:PCW:H151	4:B:226:17F:H34	0.68	1.64	8	1
4:B:234:17F:H69	4:C:631:17F:H77	0.68	1.65	2	1
3:A:408:PCW:H372	3:B:204:PCW:H481	0.68	1.64	10	1
3:C:621:PCW:H412	3:C:629:PCW:H19	0.68	1.62	3	1
3:B:202:PCW:H483	3:B:208:PCW:H411	0.68	1.64	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:79:LEU:HG	2:B:159:LEU:HD22	0.68	1.65	7	7
3:B:207:PCW:H321	3:B:220:PCW:H372	0.68	1.64	4	1
1:A:396:LYS:HD3	3:A:407:PCW:C27	0.68	2.17	5	1
4:B:234:17F:H10	4:C:631:17F:H41	0.68	1.64	9	1
3:A:407:PCW:H131	4:B:223:17F:H33	0.68	1.65	6	2
3:B:205:PCW:H62	7:B:237:EWS:BRA	0.68	2.43	6	1
3:C:619:PCW:H411	3:C:621:PCW:H472	0.68	1.64	3	1
3:B:211:PCW:H121	4:B:229:17F:H9A	0.68	1.66	9	3
3:B:209:PCW:H351	3:B:213:PCW:H132	0.68	1.65	7	1
3:A:406:PCW:H441	3:A:409:PCW:H20	0.68	1.64	2	2
1:A:308:ARG:HD3	1:C:469:LEU:HD11	0.68	1.65	6	2
1:C:590:GLU:HA	1:C:593:LYS:HE3	0.68	1.62	7	2
1:C:488:LYS:CE	3:C:623:PCW:C27	0.68	2.52	4	1
2:B:67:MET:HE1	7:B:237:EWS:CAF	0.68	2.19	5	1
3:B:209:PCW:H141	3:B:213:PCW:H332	0.67	1.65	10	1
3:B:201:PCW:H242	4:B:228:17F:H59	0.67	1.65	4	1
3:C:611:PCW:H152	3:C:617:PCW:H321	0.67	1.66	5	6
3:B:202:PCW:H422	4:B:226:17F:H12A	0.67	1.63	9	1
3:B:233:PCW:H32	3:C:604:PCW:H11	0.67	1.65	9	3
1:A:276:VAL:O	1:A:280:ARG:HB2	0.67	1.88	7	3
2:B:5:LYS:CB	7:B:237:EWS:CAT	0.67	2.69	1	2
3:B:203:PCW:H142	4:B:229:17F:H20	0.67	1.66	5	1
3:B:216:PCW:H73	4:B:224:17F:HN1A	0.67	1.49	6	1
3:A:406:PCW:H431	3:A:409:PCW:H241	0.67	1.65	7	1
1:A:279:LEU:HB3	1:C:495:LYS:HE3	0.67	1.65	9	3
3:C:627:PCW:H351	3:C:628:PCW:H121	0.67	1.66	1	7
3:B:203:PCW:H142	3:B:211:PCW:H39	0.67	1.67	7	1
3:C:607:PCW:H332	3:C:611:PCW:H122	0.67	1.67	10	1
1:A:388:SER:HB2	1:C:594:LYS:HE2	0.67	1.66	2	1
1:C:455:TYR:OH	3:C:601:PCW:C23	0.67	2.40	8	2
1:A:396:LYS:CD	3:A:407:PCW:C27	0.67	2.72	5	1
3:A:403:PCW:H332	3:B:204:PCW:H31	0.67	1.66	8	1
3:B:213:PCW:H332	3:B:216:PCW:H122	0.67	1.67	9	1
2:B:56:LEU:CG	7:B:237:EWS:OAB	0.67	2.43	1	2
4:B:229:17F:H1	4:B:229:17F:H4	0.67	1.65	6	1
3:B:215:PCW:H252	3:C:609:PCW:H472	0.67	1.66	3	1
3:B:207:PCW:H39	3:B:211:PCW:H381	0.67	1.66	6	1
4:B:234:17F:H34	4:B:234:17F:H10A	0.66	1.66	7	2
1:A:393:TYR:CD1	1:A:396:LYS:NZ	0.66	2.62	5	1
4:B:224:17F:H11	4:B:230:17F:H59	0.66	1.67	5	1
4:B:229:17F:H45	3:C:604:PCW:H481	0.66	1.66	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:201:PCW:H222	4:B:225:17F:H65	0.66	1.65	8	1
1:C:503:MET:HA	1:C:506:ARG:HD2	0.66	1.67	1	4
3:A:409:PCW:H441	3:C:627:PCW:H441	0.66	1.65	2	1
1:A:275:LYS:O	1:A:279:LEU:HG	0.66	1.90	5	9
3:B:218:PCW:H261	3:C:629:PCW:H283	0.66	1.66	3	1
3:B:202:PCW:H361	3:B:212:PCW:H331	0.66	1.67	5	1
3:B:207:PCW:C1	7:B:237:EWS:CAK	0.66	2.72	6	1
3:B:220:PCW:H472	3:B:233:PCW:H283	0.66	1.67	6	1
3:C:619:PCW:H40	3:C:629:PCW:H252	0.66	1.67	8	2
3:C:606:PCW:H232	3:C:615:PCW:H181	0.66	1.65	5	1
3:A:408:PCW:H451	3:B:204:PCW:H452	0.66	1.68	6	1
3:C:613:PCW:H351	3:C:626:PCW:H411	0.66	1.65	8	3
1:A:214:PHE:CE1	3:A:404:PCW:H162	0.66	2.25	4	1
3:C:611:PCW:H161	3:C:617:PCW:H351	0.66	1.67	4	2
3:C:621:PCW:H381	3:C:629:PCW:H171	0.66	1.66	9	6
3:C:614:PCW:H63	3:C:629:PCW:H32	0.66	1.67	9	1
3:A:402:PCW:H341	3:B:213:PCW:H322	0.65	1.67	4	1
3:B:210:PCW:H483	4:B:224:17F:H49	0.65	1.68	4	1
3:B:233:PCW:H172	3:C:625:PCW:H232	0.65	1.66	5	1
3:B:210:PCW:H331	4:B:224:17F:H5	0.65	1.65	6	2
3:B:201:PCW:H42	3:B:219:PCW:H322	0.65	1.66	7	1
3:B:220:PCW:H52	7:B:237:EWS:CAR	0.65	2.22	8	1
3:B:210:PCW:H121	4:B:224:17F:H18A	0.65	1.66	10	1
1:C:497:SER:HB2	1:C:498:PRO:HD3	0.65	1.68	3	2
1:A:396:LYS:CE	3:A:407:PCW:C27	0.65	2.74	5	1
4:B:234:17F:H40	4:B:234:17F:H64	0.65	1.68	5	1
1:A:214:PHE:HZ	3:A:404:PCW:C17	0.65	2.04	1	1
3:C:611:PCW:H411	3:C:617:PCW:H432	0.65	1.68	1	1
3:C:616:PCW:H412	3:C:622:PCW:H221	0.65	1.66	4	1
3:B:212:PCW:H121	4:B:226:17F:H6	0.65	1.68	3	1
3:B:221:PCW:C6	7:B:237:EWS:BRA	0.65	2.98	1	1
4:B:226:17F:H6A	7:B:237:EWS:CAM	0.65	2.22	2	1
1:C:455:TYR:HH	3:C:601:PCW:H211	0.65	1.50	4	2
3:A:402:PCW:H362	3:B:214:PCW:H161	0.65	1.68	1	1
3:C:611:PCW:H32	3:C:617:PCW:H62	0.65	1.68	5	3
2:B:35:THR:HG21	2:B:57:ASP:HB3	0.65	1.68	3	1
4:B:225:17F:H62	4:B:225:17F:H12A	0.65	1.68	3	1
3:C:611:PCW:H442	4:C:635:17F:H43	0.65	1.66	7	2
3:C:617:PCW:H221	4:C:635:17F:H44	0.65	1.67	9	1
3:B:209:PCW:H282	3:B:213:PCW:H431	0.65	1.69	5	1
1:A:393:TYR:OH	3:A:403:PCW:H281	0.65	1.91	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:512:ASP:HA	1:C:515:ARG:HD2	0.65	1.68	6	2
3:A:403:PCW:H431	3:C:618:PCW:H482	0.65	1.68	7	1
3:A:401:PCW:H472	3:C:626:PCW:H482	0.65	1.67	1	2
3:C:608:PCW:H31	3:C:628:PCW:H331	0.65	1.68	6	1
2:B:7:VAL:HB	2:B:78:PHE:CD1	0.65	2.26	8	2
3:B:207:PCW:H381	3:B:232:PCW:H242	0.64	1.69	3	1
3:C:628:PCW:H362	3:C:628:PCW:H142	0.64	1.68	7	3
3:B:203:PCW:H371	3:B:220:PCW:H151	0.64	1.68	8	1
3:B:207:PCW:H61	7:B:237:EWS:BRA	0.64	2.44	10	1
3:B:231:PCW:H362	3:C:604:PCW:H181	0.64	1.70	8	4
3:A:407:PCW:H341	4:B:225:17F:H11	0.64	1.69	9	2
3:B:203:PCW:H141	3:B:207:PCW:H351	0.64	1.68	1	1
4:B:230:17F:H76	4:C:631:17F:H54	0.64	1.70	3	2
4:C:633:17F:H2	4:C:633:17F:C4	0.64	2.23	2	1
3:C:601:PCW:H421	4:C:630:17F:H54	0.64	1.67	4	1
1:C:573:LEU:HA	1:C:576:VAL:HG12	0.64	1.69	7	3
3:B:205:PCW:H211	3:B:219:PCW:H141	0.64	1.69	1	1
3:C:611:PCW:H151	3:C:617:PCW:H352	0.64	1.67	2	1
1:A:308:ARG:CD	1:C:469:LEU:HD11	0.64	2.23	7	1
3:B:205:PCW:H161	3:B:219:PCW:H122	0.64	1.68	5	1
3:A:409:PCW:H481	3:B:208:PCW:H441	0.63	1.68	1	1
2:B:84:ILE:HD12	2:B:123:ARG:HG3	0.63	1.68	2	3
2:B:71:TYR:CB	7:B:237:EWS:CAE	0.63	2.76	5	1
3:A:406:PCW:H231	3:A:409:PCW:H261	0.63	1.69	1	1
3:B:213:PCW:H232	3:C:611:PCW:H422	0.63	1.67	9	1
3:C:621:PCW:H372	3:C:629:PCW:H152	0.63	1.69	10	5
3:B:202:PCW:H431	3:B:212:PCW:H172	0.63	1.69	2	1
3:C:613:PCW:H161	3:C:622:PCW:H19	0.63	1.71	5	2
1:A:376:LEU:HB2	1:A:377:PRO:HD3	0.63	1.68	9	1
3:B:204:PCW:H483	3:B:231:PCW:H422	0.63	1.70	6	1
1:A:264:LYS:HE2	1:C:509:ALA:HB1	0.63	1.69	9	1
3:B:204:PCW:H232	3:C:618:PCW:H481	0.63	1.69	1	1
3:B:231:PCW:H412	3:C:604:PCW:H432	0.63	1.69	1	1
3:B:207:PCW:H20	3:B:232:PCW:H481	0.63	1.69	2	1
3:C:606:PCW:H182	3:C:615:PCW:H142	0.63	1.70	2	1
3:B:213:PCW:H441	3:B:216:PCW:H251	0.63	1.70	5	1
3:B:209:PCW:H171	3:B:216:PCW:H162	0.63	1.70	7	1
4:B:227:17F:H75	3:C:602:PCW:H431	0.63	1.71	1	1
3:B:203:PCW:H322	3:B:220:PCW:H121	0.63	1.70	6	3
3:A:408:PCW:H371	3:A:410:PCW:H361	0.63	1.69	6	1
1:C:470:TYR:CE1	4:C:632:17F:H76	0.63	2.28	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:209:PCW:H251	3:C:611:PCW:H483	0.63	1.69	3	2
3:B:209:PCW:H382	3:B:213:PCW:H152	0.63	1.71	6	2
4:B:227:17F:H39	4:B:227:17F:H29	0.63	1.70	8	1
1:A:393:TYR:CD1	1:A:396:LYS:CE	0.62	2.80	5	1
1:A:301:LEU:HD22	1:C:473:LYS:HG2	0.62	1.69	7	2
3:B:219:PCW:H232	4:B:230:17F:H73	0.62	1.69	1	1
3:C:611:PCW:H182	3:C:617:PCW:H351	0.62	1.71	3	3
3:B:205:PCW:H251	3:B:219:PCW:H422	0.62	1.69	7	1
3:B:203:PCW:H481	3:B:233:PCW:H481	0.62	1.72	8	1
3:C:617:PCW:H221	4:C:635:17F:H40	0.62	1.70	2	1
3:A:403:PCW:H352	3:A:403:PCW:H122	0.62	1.71	5	1
3:C:608:PCW:H361	3:C:628:PCW:H212	0.62	1.71	7	2
1:C:505:ASP:HA	1:C:508:ARG:HD2	0.62	1.71	7	3
3:B:201:PCW:H483	3:C:627:PCW:H252	0.62	1.71	10	1
4:B:234:17F:H10	4:C:631:17F:H38	0.62	1.71	4	2
1:A:392:GLU:HA	1:A:395:LYS:HB2	0.62	1.71	5	1
2:B:56:LEU:HD11	3:B:219:PCW:H61	0.62	1.68	6	1
3:B:233:PCW:H171	3:C:625:PCW:H232	0.62	1.70	6	1
3:C:615:PCW:H372	3:C:622:PCW:H351	0.62	1.71	10	1
1:A:308:ARG:CB	1:C:469:LEU:CD1	0.62	2.76	4	1
2:B:54:ASP:HB3	7:B:237:EWS:BRA	0.62	2.49	2	1
1:A:393:TYR:CE2	3:A:407:PCW:H272	0.62	2.25	3	1
3:A:407:PCW:H152	4:B:223:17F:H33	0.62	1.72	5	3
3:B:232:PCW:H371	3:B:232:PCW:H152	0.62	1.70	3	1
3:A:406:PCW:H431	3:A:409:PCW:H251	0.62	1.71	8	1
3:A:407:PCW:C34	4:B:225:17F:H11	0.62	2.25	9	1
3:B:202:PCW:H341	3:B:212:PCW:H351	0.62	1.71	1	1
4:C:631:17F:H60	4:C:631:17F:C21	0.62	2.25	2	1
3:C:608:PCW:H352	3:C:609:PCW:H352	0.62	1.72	6	1
3:B:221:PCW:H2	4:B:230:17F:H18A	0.62	1.71	7	1
3:A:409:PCW:H371	3:C:627:PCW:H341	0.61	1.72	5	3
3:B:232:PCW:H331	3:C:619:PCW:H341	0.61	1.71	3	2
3:C:611:PCW:H181	3:C:617:PCW:H341	0.61	1.70	10	1
3:B:220:PCW:H142	3:B:220:PCW:H39	0.61	1.73	1	1
3:B:210:PCW:H352	4:B:224:17F:H19	0.61	1.71	6	2
3:C:605:PCW:H351	3:C:605:PCW:H122	0.61	1.69	2	2
3:C:610:PCW:H461	3:C:614:PCW:H19	0.61	1.70	5	1
3:B:202:PCW:H322	3:B:212:PCW:H371	0.61	1.71	8	1
3:B:210:PCW:H362	4:B:224:17F:H8	0.61	1.71	9	1
4:B:230:17F:H49	3:C:613:PCW:H452	0.61	1.70	2	2
3:B:205:PCW:H231	3:B:219:PCW:H412	0.61	1.71	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:201:PCW:H342	3:B:219:PCW:H362	0.61	1.72	7	1
4:B:226:17F:H6A	7:B:237:EWS:CLA	0.61	2.32	1	1
3:B:208:PCW:H151	3:B:215:PCW:H171	0.61	1.73	2	1
1:A:334:ARG:HD2	1:C:440:GLU:OE1	0.61	1.96	6	2
1:C:418:GLN:O	1:C:422:VAL:HB	0.61	1.95	9	2
3:A:401:PCW:H61	4:B:226:17F:H1A	0.61	1.72	8	1
1:A:330:ARG:HH21	1:C:447:GLU:HB2	0.61	1.56	5	1
3:B:218:PCW:H482	3:C:629:PCW:H281	0.61	1.72	9	2
3:B:217:PCW:H172	3:B:218:PCW:H161	0.61	1.70	6	1
3:B:203:PCW:H232	3:C:621:PCW:H481	0.61	1.72	9	1
3:B:219:PCW:H341	4:B:226:17F:H37	0.61	1.73	10	1
2:B:6:LEU:HB2	2:B:55:ILE:HG13	0.61	1.71	1	1
3:A:409:PCW:H442	3:C:605:PCW:H231	0.61	1.70	8	1
3:B:209:PCW:H241	3:C:611:PCW:H461	0.61	1.71	5	1
3:B:202:PCW:H122	4:B:228:17F:H9	0.61	1.72	10	3
3:B:219:PCW:H422	3:B:220:PCW:H182	0.61	1.72	3	1
3:B:218:PCW:H372	3:C:603:PCW:H372	0.61	1.71	8	1
3:B:209:PCW:H161	3:B:216:PCW:H182	0.61	1.71	10	1
3:B:201:PCW:H362	3:B:219:PCW:H351	0.60	1.71	4	1
3:A:401:PCW:H462	3:C:613:PCW:H251	0.60	1.71	7	1
4:B:225:17F:H75	3:C:615:PCW:H242	0.60	1.71	8	1
3:B:210:PCW:H472	4:B:227:17F:H44	0.60	1.73	9	1
3:A:410:PCW:H121	4:C:633:17F:C1X	0.60	2.25	1	4
3:B:220:PCW:H371	3:B:220:PCW:H122	0.60	1.73	1	1
3:B:205:PCW:H39	4:B:224:17F:H59	0.60	1.73	3	1
3:C:607:PCW:H242	4:C:631:17F:H39	0.60	1.73	6	1
3:A:407:PCW:H331	4:B:223:17F:C1Y	0.60	2.27	3	4
3:A:408:PCW:H322	3:B:231:PCW:H372	0.60	1.72	3	1
3:B:210:PCW:H231	4:B:227:17F:H44	0.60	1.74	4	1
3:A:407:PCW:H451	4:B:223:17F:H71	0.60	1.73	5	2
3:B:201:PCW:O2P	7:B:237:EWS:CAK	0.60	2.49	5	1
3:B:219:PCW:N	7:B:237:EWS:BRA	0.60	2.89	6	1
3:B:210:PCW:H332	4:B:224:17F:H5	0.60	1.74	7	1
3:B:232:PCW:H151	3:C:625:PCW:H171	0.60	1.73	3	2
1:C:561:LYS:HA	1:C:565:ALA:HB3	0.60	1.73	6	2
3:B:206:PCW:H372	3:B:215:PCW:H412	0.60	1.72	3	1
3:B:209:PCW:H122	3:B:213:PCW:H132	0.60	1.74	8	1
1:A:365:LYS:O	1:A:369:GLU:HB2	0.60	1.97	1	2
3:B:207:PCW:H471	3:B:232:PCW:H39	0.60	1.71	2	1
2:B:109:VAL:HB	2:B:111:MET:HE2	0.60	1.73	10	3
3:B:211:PCW:H342	4:B:229:17F:H11	0.60	1.73	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:203:PCW:H162	3:B:211:PCW:H39	0.60	1.73	1	1
3:B:231:PCW:C34	3:C:604:PCW:H322	0.60	2.25	3	3
3:C:621:PCW:H352	3:C:629:PCW:H162	0.60	1.72	8	1
3:B:219:PCW:H221	3:B:233:PCW:H272	0.60	1.71	10	1
3:C:629:PCW:H242	4:C:634:17F:H45	0.60	1.72	10	1
2:B:144:THR:HA	2:B:150:GLN:O	0.60	1.97	4	2
3:B:211:PCW:H212	3:B:217:PCW:H411	0.60	1.73	2	1
4:B:223:17F:H43	3:C:626:PCW:H271	0.60	1.72	2	1
2:B:38:ASP:HB2	2:B:57:ASP:HB3	0.60	1.73	1	1
3:B:213:PCW:H231	4:C:635:17F:H47	0.60	1.73	1	1
3:C:613:PCW:H73	3:C:627:PCW:H61	0.60	1.74	2	1
3:C:602:PCW:H271	4:C:630:17F:H52	0.60	1.74	3	1
3:B:201:PCW:P	7:B:237:EWS:CAK	0.60	2.90	5	1
2:B:56:LEU:HD22	7:B:237:EWS:CBA	0.60	2.27	9	2
3:C:610:PCW:H372	3:C:614:PCW:H221	0.60	1.73	10	1
4:A:411:17F:H54	3:C:607:PCW:H222	0.60	1.71	7	2
3:B:209:PCW:H171	3:B:213:PCW:H171	0.60	1.73	5	1
3:B:205:PCW:H171	4:B:224:17F:H37	0.60	1.73	6	1
3:B:231:PCW:H461	3:C:604:PCW:H461	0.60	1.72	6	1
1:A:250:VAL:O	1:A:254:VAL:HB	0.59	1.97	1	9
3:B:233:PCW:H351	3:C:626:PCW:H121	0.59	1.74	8	3
3:B:233:PCW:H12	3:C:605:PCW:H71	0.59	1.72	2	1
3:B:220:PCW:H442	3:B:232:PCW:H251	0.59	1.71	4	1
3:C:615:PCW:H151	3:C:615:PCW:H382	0.59	1.74	5	1
3:B:208:PCW:H372	4:B:226:17F:H20A	0.59	1.72	9	1
2:B:8:VAL:HG12	2:B:79:LEU:HB2	0.59	1.74	1	1
3:B:201:PCW:H221	4:B:225:17F:H68	0.59	1.73	7	1
3:A:405:PCW:H19	3:B:222:PCW:H242	0.59	1.72	8	1
3:C:619:PCW:H352	3:C:621:PCW:H141	0.59	1.73	8	1
3:C:619:PCW:H411	3:C:621:PCW:H461	0.59	1.74	8	1
3:B:210:PCW:H412	4:B:224:17F:H8	0.59	1.73	10	1
4:B:234:17F:H73	4:C:631:17F:H68	0.59	1.73	3	3
2:B:6:LEU:O	2:B:55:ILE:HA	0.59	1.96	9	6
3:B:202:PCW:H331	4:B:228:17F:H6	0.59	1.75	4	2
1:A:214:PHE:HZ	3:A:404:PCW:C16	0.59	2.10	3	1
3:C:606:PCW:H412	3:C:622:PCW:H412	0.59	1.73	3	1
3:A:407:PCW:H361	4:B:225:17F:H11	0.59	1.73	5	1
3:B:218:PCW:H242	3:C:629:PCW:H283	0.59	1.72	10	1
1:C:451:LYS:O	1:C:455:TYR:HB2	0.59	1.98	4	6
3:C:627:PCW:H39	3:C:628:PCW:H382	0.59	1.72	5	1
1:A:393:TYR:HH	3:A:407:PCW:H262	0.59	1.54	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:39:SER:CB	7:B:237:EWS:BRA	0.59	3.06	7	1
3:C:609:PCW:H272	4:C:632:17F:H48	0.59	1.75	8	1
2:B:32:TYR:HD1	5:B:235:GNP:H5'1	0.59	1.58	4	2
2:B:82:PHE:HB3	2:B:93:ILE:HD11	0.59	1.74	4	5
3:B:233:PCW:H371	3:C:606:PCW:H351	0.59	1.75	2	1
3:C:619:PCW:H381	3:C:629:PCW:H20	0.59	1.73	4	1
3:C:610:PCW:H362	3:C:614:PCW:H351	0.59	1.74	7	1
3:C:611:PCW:H341	3:C:617:PCW:H352	0.59	1.74	10	1
1:A:231:ASN:HA	1:A:234:LYS:HE2	0.59	1.73	2	3
4:A:411:17F:H58	3:C:624:PCW:H431	0.59	1.74	2	3
3:B:205:PCW:H11	3:B:207:PCW:H82	0.59	1.73	7	1
3:B:210:PCW:H341	4:B:224:17F:H5	0.59	1.75	8	2
3:C:601:PCW:H411	3:C:602:PCW:H212	0.59	1.72	8	1
3:B:220:PCW:H451	3:B:233:PCW:H271	0.59	1.75	9	1
3:C:617:PCW:H211	4:C:632:17F:H42	0.59	1.74	9	1
2:B:45:VAL:HG22	2:B:50:THR:HB	0.59	1.73	10	1
3:B:218:PCW:H411	3:C:603:PCW:H421	0.59	1.74	10	1
3:A:407:PCW:H341	4:B:225:17F:H9	0.59	1.73	1	1
3:B:201:PCW:O3P	7:B:237:EWS:CAN	0.59	2.50	5	1
3:B:203:PCW:H451	3:B:220:PCW:H20	0.59	1.74	6	1
3:B:209:PCW:H261	3:B:213:PCW:H461	0.59	1.74	7	1
3:C:609:PCW:H371	4:C:630:17F:H56	0.59	1.73	10	1
3:B:211:PCW:H132	4:B:229:17F:H6A	0.59	1.75	9	4
3:A:404:PCW:H411	3:B:217:PCW:H421	0.59	1.75	10	4
3:B:201:PCW:H352	4:B:225:17F:H31	0.59	1.73	2	1
3:A:403:PCW:H483	4:B:229:17F:H71	0.59	1.75	4	1
1:A:375:LEU:HA	1:A:378:VAL:HG12	0.59	1.75	5	2
1:C:466:GLU:HA	1:C:469:LEU:HD12	0.59	1.73	5	2
3:C:617:PCW:H232	4:C:632:17F:H45	0.59	1.75	5	1
3:B:232:PCW:H181	3:C:625:PCW:H182	0.59	1.74	6	1
1:A:345:ARG:HG2	1:C:429:ASN:OD1	0.59	1.97	10	1
3:C:614:PCW:H72	3:C:629:PCW:H32	0.59	1.74	10	1
3:B:211:PCW:H351	4:B:229:17F:H8A	0.58	1.73	10	4
3:B:202:PCW:H121	3:B:202:PCW:H172	0.58	1.74	3	1
3:C:621:PCW:H331	3:C:629:PCW:H172	0.58	1.73	3	1
4:B:229:17F:H64	3:C:619:PCW:H281	0.58	1.75	4	1
3:B:205:PCW:H172	3:B:219:PCW:H122	0.58	1.74	6	1
3:B:211:PCW:H331	4:B:229:17F:H8A	0.58	1.74	2	2
4:B:223:17F:H75	3:C:606:PCW:H252	0.58	1.75	5	1
3:B:231:PCW:H412	3:C:604:PCW:H422	0.58	1.75	8	1
3:A:407:PCW:H351	4:B:223:17F:H56	0.58	1.74	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:201:PCW:H252	4:B:228:17F:H64	0.58	1.75	3	1
3:A:406:PCW:H412	4:B:226:17F:H62	0.58	1.74	6	1
3:B:205:PCW:C8	7:B:237:EWS:BRA	0.58	3.07	6	2
4:C:633:17F:H4A	4:C:633:17F:N1	0.58	2.13	6	2
2:B:74:THR:CA	7:B:237:EWS:BRA	0.58	3.06	9	1
1:A:214:PHE:CZ	3:A:404:PCW:C17	0.58	2.80	1	1
3:B:233:PCW:H212	3:C:625:PCW:H251	0.58	1.74	1	1
3:B:219:PCW:H232	4:B:230:17F:H74	0.58	1.75	8	1
3:A:410:PCW:H351	4:C:633:17F:H12A	0.58	1.73	6	1
3:B:212:PCW:H472	3:C:613:PCW:H451	0.58	1.76	6	1
3:B:205:PCW:H371	4:B:224:17F:H34	0.58	1.74	9	1
3:B:220:PCW:H161	3:B:220:PCW:H39	0.58	1.73	2	1
3:B:231:PCW:H39	3:C:604:PCW:H232	0.58	1.76	5	1
3:B:218:PCW:H452	3:C:603:PCW:H451	0.58	1.74	6	1
3:B:210:PCW:H361	4:B:224:17F:H18A	0.58	1.73	9	2
3:B:209:PCW:H121	3:B:213:PCW:H321	0.58	1.76	8	1
4:B:234:17F:H41	4:B:234:17F:H71	0.58	1.74	8	1
4:B:234:17F:H71	4:C:631:17F:H68	0.58	1.75	1	2
3:C:606:PCW:H39	3:C:613:PCW:H361	0.58	1.74	2	4
2:B:6:LEU:HB2	2:B:55:ILE:HG12	0.58	1.75	3	2
3:B:221:PCW:H132	4:B:230:17F:H6	0.58	1.74	7	1
3:B:210:PCW:H371	4:B:224:17F:H11A	0.58	1.75	9	2
3:B:205:PCW:H461	4:B:224:17F:H73	0.58	1.75	9	1
3:A:401:PCW:H482	3:C:616:PCW:H20	0.58	1.76	10	1
2:B:38:ASP:O	2:B:56:LEU:HG	0.58	1.97	1	1
3:B:209:PCW:H221	3:C:611:PCW:H483	0.58	1.75	1	1
3:B:221:PCW:C7	7:B:237:EWS:BRA	0.58	3.07	1	1
4:A:411:17F:H53	3:C:607:PCW:H222	0.58	1.74	2	1
2:B:36:ILE:HA	2:B:59:ALA:HB2	0.58	1.74	9	2
4:B:228:17F:H66	3:C:615:PCW:H452	0.58	1.74	3	2
4:A:411:17F:H6	3:C:624:PCW:H152	0.58	1.75	5	3
3:B:202:PCW:H451	4:B:230:17F:H48	0.58	1.75	4	1
3:C:624:PCW:H212	4:C:634:17F:H19	0.58	1.76	4	1
3:B:233:PCW:H421	3:C:604:PCW:H39	0.58	1.76	6	1
2:B:7:VAL:HG13	7:B:237:EWS:CAU	0.58	2.29	7	1
3:C:621:PCW:H331	3:C:629:PCW:H182	0.58	1.76	7	1
3:B:203:PCW:H151	3:B:211:PCW:H39	0.58	1.73	8	1
3:C:611:PCW:H341	3:C:617:PCW:H362	0.58	1.75	2	3
3:B:231:PCW:H421	3:C:604:PCW:H261	0.58	1.74	6	2
3:B:203:PCW:H142	3:B:207:PCW:H351	0.58	1.76	10	3
3:C:613:PCW:H382	3:C:626:PCW:H422	0.58	1.76	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:402:PCW:H212	3:B:214:PCW:H242	0.58	1.75	3	4
3:C:607:PCW:H222	4:C:631:17F:H35	0.58	1.75	8	1
3:B:202:PCW:H482	3:B:212:PCW:H212	0.58	1.75	10	1
3:A:410:PCW:C33	4:C:633:17F:H12A	0.57	2.29	1	1
3:B:208:PCW:C7	7:B:237:EWS:BRA	0.57	3.05	4	1
3:B:205:PCW:H172	3:B:219:PCW:H142	0.57	1.73	1	1
1:A:308:ARG:HG3	1:C:469:LEU:HD11	0.57	1.72	7	2
4:B:223:17F:C4	4:B:223:17F:H1	0.57	2.29	9	5
3:A:403:PCW:H431	4:B:229:17F:H73	0.57	1.76	10	1
3:B:205:PCW:H121	3:B:220:PCW:H342	0.57	1.77	1	1
2:B:7:VAL:CG2	7:B:237:EWS:NAW	0.57	2.67	6	4
4:B:226:17F:N1	7:B:237:EWS:CAL	0.57	2.65	4	1
3:A:408:PCW:H332	3:A:410:PCW:H341	0.57	1.75	7	2
3:B:202:PCW:H122	4:B:228:17F:H9A	0.57	1.76	2	1
3:B:207:PCW:H12	7:B:237:EWS:CAK	0.57	2.27	6	1
3:A:408:PCW:H341	3:B:231:PCW:H371	0.57	1.76	8	2
2:B:80:CYS:HB3	2:B:93:ILE:HD12	0.57	1.76	9	1
3:B:209:PCW:H122	3:B:213:PCW:H131	0.57	1.74	10	1
3:B:221:PCW:H281	4:B:226:17F:H72	0.57	1.76	1	1
3:B:207:PCW:H481	3:B:232:PCW:H141	0.57	1.76	3	1
1:C:478:ARG:O	1:C:482:GLN:HB2	0.57	1.99	10	4
3:A:402:PCW:H341	3:A:402:PCW:H122	0.57	1.75	10	3
3:A:401:PCW:H411	3:B:212:PCW:H471	0.57	1.75	6	2
3:A:403:PCW:H461	3:C:618:PCW:H452	0.57	1.76	8	1
3:A:401:PCW:H42	4:B:226:17F:O2	0.57	2.00	3	1
3:B:207:PCW:H212	4:C:631:17F:H76	0.57	1.76	9	2
3:B:203:PCW:H39	3:B:220:PCW:H172	0.57	1.76	7	1
3:B:203:PCW:H121	3:B:207:PCW:H342	0.57	1.77	10	1
3:B:208:PCW:H471	3:C:627:PCW:H471	0.57	1.76	2	1
3:B:205:PCW:H281	3:B:233:PCW:H232	0.57	1.77	3	1
3:C:614:PCW:H132	3:C:614:PCW:H341	0.57	1.75	6	1
3:C:611:PCW:H411	3:C:617:PCW:H442	0.57	1.76	9	1
3:A:408:PCW:H39	3:A:410:PCW:H412	0.57	1.74	2	1
3:C:607:PCW:H262	4:C:631:17F:H39	0.57	1.76	5	2
3:C:613:PCW:H132	3:C:622:PCW:H151	0.57	1.76	7	1
3:A:406:PCW:H352	3:B:215:PCW:H412	0.57	1.75	8	1
3:B:217:PCW:H262	3:C:619:PCW:H461	0.57	1.76	8	3
3:A:407:PCW:H481	3:A:410:PCW:H211	0.57	1.75	5	1
3:C:611:PCW:H121	3:C:617:PCW:H342	0.57	1.76	8	1
3:C:617:PCW:H231	4:C:635:17F:H44	0.57	1.75	4	2
3:C:614:PCW:H132	3:C:614:PCW:H331	0.57	1.75	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:401:PCW:H462	3:C:613:PCW:H241	0.57	1.77	9	1
1:A:214:PHE:HE1	3:A:404:PCW:H171	0.57	1.60	10	1
3:B:209:PCW:H242	3:C:611:PCW:H481	0.56	1.78	2	1
1:A:327:LEU:HD23	1:A:330:ARG:HD2	0.56	1.77	5	1
3:B:201:PCW:O3P	7:B:237:EWS:CAK	0.56	2.52	5	1
3:B:203:PCW:H40	3:B:231:PCW:H281	0.56	1.76	6	1
3:C:607:PCW:H231	4:C:631:17F:H39	0.56	1.76	2	1
3:B:207:PCW:H182	3:B:232:PCW:H283	0.56	1.77	5	1
3:B:203:PCW:H261	3:B:217:PCW:H442	0.56	1.77	1	1
4:B:228:17F:H61	3:C:615:PCW:H462	0.56	1.77	1	1
3:B:218:PCW:H461	3:C:629:PCW:H281	0.56	1.77	2	2
3:B:210:PCW:H351	4:B:224:17F:H19	0.56	1.78	3	1
3:B:219:PCW:H132	3:B:219:PCW:H331	0.56	1.77	6	1
3:B:208:PCW:H31	3:B:221:PCW:H131	0.56	1.78	7	1
4:B:227:17F:O2	3:C:602:PCW:H73	0.56	2.00	7	1
3:A:402:PCW:H342	3:B:214:PCW:H152	0.56	1.77	1	1
3:A:408:PCW:H11	3:B:231:PCW:H321	0.56	1.77	3	3
3:A:408:PCW:H141	3:C:620:PCW:H141	0.56	1.77	6	1
2:B:45:VAL:HA	2:B:50:THR:HA	0.56	1.78	8	2
3:C:610:PCW:H182	3:C:614:PCW:H171	0.56	1.78	9	2
3:B:202:PCW:H483	3:B:208:PCW:H381	0.56	1.76	1	1
3:B:216:PCW:H481	3:C:603:PCW:H412	0.56	1.76	2	1
3:B:217:PCW:H282	3:C:619:PCW:H482	0.56	1.78	5	3
3:C:602:PCW:H462	3:C:609:PCW:H252	0.56	1.76	2	1
3:C:610:PCW:H382	3:C:614:PCW:H371	0.56	1.77	2	2
3:B:213:PCW:H482	4:C:635:17F:H66	0.56	1.77	3	1
1:C:414:LYS:O	1:C:418:GLN:HG3	0.56	2.00	3	2
3:A:409:PCW:H431	3:C:627:PCW:H231	0.56	1.77	6	1
3:C:613:PCW:H39	3:C:627:PCW:H242	0.56	1.76	8	1
3:B:206:PCW:H262	3:C:602:PCW:H411	0.56	1.78	3	1
3:B:207:PCW:H19	4:B:234:17F:H45	0.56	1.77	5	1
3:B:232:PCW:H341	3:C:625:PCW:H151	0.56	1.78	7	1
3:B:203:PCW:H212	3:B:217:PCW:H211	0.56	1.78	9	1
3:C:611:PCW:H162	3:C:628:PCW:H271	0.56	1.76	4	1
1:A:396:LYS:HZ3	3:A:407:PCW:C27	0.56	1.90	5	1
1:A:242:GLU:HB3	1:C:532:ARG:HH21	0.56	1.61	7	1
3:A:402:PCW:H272	3:B:209:PCW:H283	0.56	1.76	10	1
3:C:609:PCW:H161	4:C:630:17F:H34	0.56	1.76	2	1
2:B:7:VAL:HG13	7:B:237:EWS:CAX	0.56	2.31	3	1
3:B:201:PCW:H221	4:B:225:17F:H69	0.56	1.75	3	1
3:C:605:PCW:H62	3:C:605:PCW:H331	0.56	1.78	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:406:PCW:H341	3:B:206:PCW:H342	0.56	1.76	5	1
3:A:402:PCW:H322	3:A:402:PCW:H83	0.56	1.78	9	1
3:C:615:PCW:H132	3:C:622:PCW:H371	0.56	1.77	5	1
3:B:210:PCW:H222	4:B:227:17F:H43	0.56	1.76	6	1
1:A:279:LEU:HB3	1:C:495:LYS:HD3	0.56	1.78	7	1
4:B:230:17F:H38	3:C:605:PCW:H282	0.56	1.77	7	1
3:B:220:PCW:H271	3:B:231:PCW:H452	0.56	1.78	8	1
3:B:213:PCW:H272	4:C:630:17F:H74	0.56	1.78	9	1
3:B:202:PCW:H131	3:B:202:PCW:H342	0.56	1.77	1	1
3:C:618:PCW:H142	3:C:620:PCW:H431	0.56	1.77	1	1
3:A:408:PCW:H171	3:A:408:PCW:H381	0.56	1.77	2	1
3:B:217:PCW:H261	3:C:619:PCW:H461	0.56	1.76	4	1
4:B:228:17F:H19	4:B:228:17F:H9	0.56	1.78	4	1
3:A:401:PCW:H261	3:C:622:PCW:H281	0.56	1.77	8	1
3:A:408:PCW:H40	3:A:410:PCW:H441	0.56	1.78	8	1
3:B:209:PCW:H351	3:B:213:PCW:H141	0.56	1.76	10	2
4:A:411:17F:H37	3:C:624:PCW:H461	0.55	1.77	1	2
1:A:308:ARG:HG2	1:C:469:LEU:CG	0.55	2.29	4	1
3:A:407:PCW:H121	4:B:223:17F:H57	0.55	1.78	4	1
3:C:622:PCW:H151	3:C:622:PCW:H381	0.55	1.76	5	3
3:C:607:PCW:H161	3:C:607:PCW:H342	0.55	1.77	10	2
3:C:621:PCW:H352	3:C:629:PCW:H172	0.55	1.76	6	1
4:B:225:17F:H10	3:C:626:PCW:H281	0.55	1.78	9	1
3:B:207:PCW:N	7:B:237:EWS:BRA	0.55	2.94	10	1
3:B:213:PCW:H221	4:B:227:17F:H46	0.55	1.78	5	2
1:C:455:TYR:HH	3:C:601:PCW:C20	0.55	2.12	3	1
3:A:407:PCW:H2	4:B:223:17F:H18	0.55	1.78	4	1
2:B:7:VAL:HG23	7:B:237:EWS:CAX	0.55	2.29	8	1
3:A:408:PCW:H181	3:C:604:PCW:H252	0.55	1.78	10	1
3:B:212:PCW:H40	3:C:613:PCW:H482	0.55	1.77	3	1
3:C:610:PCW:H122	3:C:614:PCW:H212	0.55	1.79	3	1
1:C:488:LYS:HE2	3:C:623:PCW:H283	0.55	0.58	4	1
3:B:217:PCW:H11	7:B:237:EWS:CAN	0.55	2.31	7	1
3:A:401:PCW:H411	3:B:212:PCW:H452	0.55	1.79	2	1
2:B:116:ASN:HA	2:B:144:THR:O	0.55	2.02	4	1
3:B:203:PCW:H352	3:B:220:PCW:H132	0.55	1.78	4	1
3:B:205:PCW:H231	3:B:219:PCW:H411	0.55	1.77	6	1
3:C:622:PCW:H142	3:C:622:PCW:H381	0.55	1.79	6	1
2:B:70:GLN:CG	3:B:220:PCW:H41	0.55	2.29	9	1
1:C:466:GLU:OE1	1:C:469:LEU:HD12	0.55	2.01	10	1
4:B:234:17F:H70	3:C:607:PCW:H262	0.55	1.79	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:618:PCW:H2	3:C:620:PCW:H352	0.55	1.79	1	3
3:C:621:PCW:H122	3:C:629:PCW:H181	0.55	1.78	8	4
2:B:5:LYS:HG3	7:B:237:EWS:CAT	0.55	2.31	6	1
3:A:401:PCW:H341	3:B:212:PCW:H371	0.55	1.78	3	1
1:A:214:PHE:CE1	3:A:404:PCW:C16	0.55	2.88	4	2
3:C:624:PCW:H421	4:C:634:17F:H60	0.55	1.78	5	1
3:A:406:PCW:H432	4:B:226:17F:H70	0.55	1.78	7	1
3:B:210:PCW:H152	4:B:224:17F:H4	0.55	1.78	8	1
3:A:407:PCW:H472	4:B:223:17F:H72	0.55	1.79	9	1
3:B:201:PCW:H351	4:B:226:17F:H38	0.55	1.79	9	1
3:B:202:PCW:H272	3:C:622:PCW:H262	0.55	1.77	10	1
4:B:225:17F:H59	3:C:626:PCW:H282	0.55	1.79	2	2
1:A:277:GLU:HB2	1:A:278:PRO:HD3	0.55	1.78	7	2
3:A:409:PCW:H412	3:C:627:PCW:H432	0.55	1.77	4	1
4:B:226:17F:H10	4:B:230:17F:H8	0.55	1.77	8	3
3:B:210:PCW:H121	4:B:224:17F:H19A	0.55	1.79	9	1
3:B:207:PCW:C1	7:B:237:EWS:CAO	0.55	2.83	6	1
3:B:219:PCW:H20	3:B:233:PCW:H272	0.55	1.78	8	1
3:A:408:PCW:H352	3:A:410:PCW:H341	0.55	1.79	3	1
3:C:613:PCW:H322	3:C:622:PCW:H122	0.55	1.78	6	2
1:C:447:GLU:OE1	1:C:451:LYS:HE2	0.55	2.01	9	2
3:B:211:PCW:H151	4:B:229:17F:C6	0.55	2.32	2	1
4:A:411:17F:H10	4:A:411:17F:H31	0.55	1.78	3	1
3:A:401:PCW:H83	4:B:226:17F:O2	0.55	2.01	4	1
4:B:234:17F:H48	4:B:234:17F:H77	0.55	1.78	4	1
4:B:229:17F:H1	4:B:229:17F:C4	0.55	2.32	6	1
3:B:209:PCW:H271	3:C:611:PCW:H483	0.55	1.78	7	1
3:A:409:PCW:H351	3:C:627:PCW:H341	0.55	1.78	9	1
3:B:201:PCW:H342	3:B:219:PCW:H351	0.54	1.79	1	1
3:B:217:PCW:C1	7:B:237:EWS:CAM	0.54	2.83	7	1
4:B:229:17F:H10A	4:B:229:17F:H58	0.54	1.79	9	1
2:B:41:ARG:HD2	2:B:52:LEU:HG	0.54	1.78	3	1
1:C:455:TYR:OH	3:C:601:PCW:H20	0.54	2.00	3	2
3:C:621:PCW:H331	3:C:629:PCW:H181	0.54	1.79	5	1
3:B:220:PCW:H281	3:C:625:PCW:H222	0.54	1.79	4	1
3:C:609:PCW:H181	4:C:630:17F:H34	0.54	1.79	4	1
3:B:209:PCW:H142	3:B:213:PCW:H151	0.54	1.79	6	1
2:B:22:GLN:O	2:B:26:ASN:HA	0.54	2.03	5	8
3:B:215:PCW:H481	4:B:226:17F:H75	0.54	1.78	3	1
1:A:330:ARG:NH2	1:C:444:ASP:HA	0.54	2.17	5	1
3:B:220:PCW:H452	3:B:233:PCW:H252	0.54	1.80	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:203:PCW:P	7:B:237:EWS:CAO	0.54	2.96	8	1
3:C:609:PCW:H171	4:C:632:17F:H20A	0.54	1.79	8	1
4:B:234:17F:H34	3:C:625:PCW:H141	0.54	1.79	10	1
1:A:239:LEU:HA	1:A:242:GLU:HB2	0.54	1.79	2	1
3:B:202:PCW:H152	3:B:212:PCW:H412	0.54	1.78	2	1
3:B:211:PCW:H362	4:B:229:17F:H10A	0.54	1.78	2	1
1:A:288:ARG:O	1:A:292:HIS:HB2	0.54	2.03	3	1
3:A:407:PCW:H122	4:B:223:17F:C20	0.54	2.33	6	2
3:A:402:PCW:H372	3:B:214:PCW:H182	0.54	1.78	7	1
3:B:219:PCW:H231	4:B:224:17F:H43	0.54	1.80	8	1
3:B:232:PCW:H351	3:C:619:PCW:H341	0.54	1.80	9	2
3:A:406:PCW:H441	3:A:409:PCW:H231	0.54	1.80	1	1
4:B:234:17F:H69	4:B:234:17F:H40	0.54	1.77	10	2
3:B:205:PCW:H122	3:B:207:PCW:H131	0.54	1.79	6	3
3:A:408:PCW:H351	3:A:410:PCW:H351	0.54	1.80	1	1
3:C:611:PCW:H461	4:C:635:17F:H41	0.54	1.78	4	1
3:C:611:PCW:H252	3:C:617:PCW:H441	0.54	1.80	6	1
1:A:307:ASP:HA	1:A:310:ARG:HD2	0.54	1.80	9	2
3:A:407:PCW:H371	4:B:223:17F:H56	0.54	1.80	9	1
3:C:607:PCW:H483	3:C:611:PCW:H371	0.54	1.79	4	1
2:B:39:SER:HA	2:B:56:LEU:HG	0.54	1.79	9	1
1:A:312:HIS:HE1	1:C:465:GLU:HB2	0.54	1.63	2	3
1:C:469:LEU:HD22	1:C:473:LYS:HZ2	0.54	1.62	2	1
2:B:163:ILE:HG22	2:B:167:LYS:HE3	0.54	1.80	6	1
3:B:209:PCW:H122	3:B:213:PCW:C13	0.54	2.32	8	1
3:B:217:PCW:H283	3:B:218:PCW:H272	0.54	1.77	8	1
3:B:201:PCW:H211	4:B:225:17F:H61	0.54	1.79	10	1
1:C:519:ALA:HB3	1:C:520:PRO:HD3	0.54	1.79	10	1
1:A:301:LEU:HD13	1:C:473:LYS:HG2	0.53	1.79	10	2
2:B:41:ARG:HD2	2:B:52:LEU:HD21	0.53	1.80	1	1
2:B:117:LYS:HB3	2:B:120:LEU:HD13	0.53	1.81	1	1
2:B:109:VAL:HB	2:B:111:MET:HE3	0.53	1.78	7	2
1:C:401:LEU:O	1:C:405:TRP:HB2	0.53	2.03	5	1
3:C:614:PCW:H331	3:C:614:PCW:C13	0.53	2.33	5	1
3:C:617:PCW:H212	4:C:632:17F:H42	0.53	1.79	7	1
4:A:411:17F:H4A	3:C:624:PCW:H132	0.53	1.78	8	2
3:B:212:PCW:H422	3:C:613:PCW:H481	0.53	1.80	9	1
3:B:212:PCW:H181	4:B:226:17F:H10A	0.53	1.80	9	1
2:B:4:TYR:HB2	2:B:53:LEU:HD23	0.53	1.79	1	1
3:B:208:PCW:H31	3:B:221:PCW:H121	0.53	1.79	2	1
3:C:611:PCW:H161	3:C:628:PCW:H282	0.53	1.79	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:218:PCW:H441	3:C:629:PCW:H281	0.53	1.81	3	1
3:A:405:PCW:H251	4:C:634:17F:H55	0.53	1.79	8	1
3:B:231:PCW:H361	3:C:604:PCW:H352	0.53	1.81	9	3
1:C:469:LEU:HD22	1:C:473:LYS:NZ	0.53	2.18	2	1
3:B:220:PCW:H483	3:B:232:PCW:H442	0.53	1.80	3	1
1:C:491:GLU:O	1:C:495:LYS:HG3	0.53	2.03	6	2
3:B:203:PCW:H321	3:B:211:PCW:H332	0.53	1.80	10	1
2:B:71:TYR:CA	7:B:237:EWS:CAC	0.53	2.76	1	1
2:B:84:ILE:CD1	2:B:118:CYS:HA	0.53	2.32	2	3
3:B:208:PCW:C6	7:B:237:EWS:BRA	0.53	3.09	4	1
3:B:208:PCW:H142	3:B:221:PCW:H212	0.53	1.81	6	1
1:C:474:VAL:O	1:C:478:ARG:HB2	0.53	2.04	1	2
3:B:204:PCW:H352	4:B:223:17F:H29	0.53	1.81	6	1
3:B:231:PCW:H482	3:C:604:PCW:H482	0.53	1.78	6	1
3:A:402:PCW:H351	3:B:213:PCW:H322	0.53	1.80	7	1
3:B:207:PCW:O4P	7:B:237:EWS:CAL	0.53	2.57	7	1
3:C:606:PCW:H211	3:C:615:PCW:H142	0.53	1.80	7	1
1:C:567:GLU:O	1:C:571:GLN:CB	0.53	2.57	8	1
1:A:369:GLU:O	1:A:373:GLN:CG	0.53	2.50	9	1
3:A:401:PCW:H73	3:B:212:PCW:H12	0.53	1.78	10	1
3:B:206:PCW:H71	3:B:215:PCW:H12	0.53	1.78	2	1
4:B:223:17F:H46	3:C:626:PCW:H252	0.53	1.80	2	1
3:B:212:PCW:H20	3:B:212:PCW:H432	0.53	1.79	7	2
1:C:544:LEU:O	1:C:548:HIS:HB2	0.53	2.03	8	1
3:C:612:PCW:H31	4:C:634:17F:H6	0.53	1.79	8	2
2:B:74:THR:HG23	7:B:237:EWS:CAD	0.53	2.34	10	1
1:A:301:LEU:HB3	1:C:473:LYS:HE3	0.53	1.81	3	1
3:B:203:PCW:H331	3:B:211:PCW:H322	0.53	1.80	3	1
3:A:404:PCW:H381	3:B:217:PCW:H432	0.53	1.81	9	1
3:C:613:PCW:H141	3:C:622:PCW:H19	0.53	1.78	9	1
3:A:406:PCW:H212	3:A:409:PCW:H241	0.53	1.81	1	1
2:B:82:PHE:HE2	2:B:113:LEU:HG	0.53	1.64	1	2
3:A:402:PCW:H181	3:B:214:PCW:H231	0.53	1.81	6	1
3:B:217:PCW:H221	4:C:634:17F:H54	0.53	1.81	6	1
3:C:607:PCW:H421	3:C:611:PCW:H11	0.53	1.80	6	1
3:B:213:PCW:H342	3:B:216:PCW:H122	0.53	1.80	7	1
3:A:409:PCW:O31	3:C:627:PCW:H362	0.53	2.04	1	1
3:C:613:PCW:H411	3:C:613:PCW:H19	0.53	1.79	1	1
4:B:234:17F:H56	3:C:625:PCW:H181	0.53	1.81	3	1
3:C:618:PCW:H322	3:C:620:PCW:H39	0.53	1.79	4	1
1:A:243:MET:HA	1:A:246:ASP:HB2	0.53	1.79	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:84:ILE:HD13	2:B:118:CYS:HA	0.53	1.81	8	1
3:B:218:PCW:H432	3:B:218:PCW:H232	0.53	1.79	8	1
3:C:627:PCW:H371	3:C:628:PCW:H382	0.53	1.81	8	1
3:B:213:PCW:H283	3:C:611:PCW:H412	0.53	1.81	9	1
3:A:403:PCW:H172	3:A:403:PCW:H351	0.53	1.79	1	1
3:B:209:PCW:H232	3:B:213:PCW:H421	0.53	1.81	3	1
3:B:215:PCW:H251	3:C:609:PCW:H482	0.53	1.81	4	1
3:C:606:PCW:H461	3:C:615:PCW:H172	0.53	1.80	5	1
1:C:465:GLU:O	1:C:469:LEU:HD12	0.53	2.02	6	1
3:A:406:PCW:H162	3:A:409:PCW:H271	0.53	1.80	8	1
3:C:611:PCW:H182	3:C:617:PCW:H362	0.53	1.81	10	1
4:B:234:17F:H33	3:C:625:PCW:H19	0.52	1.80	1	1
3:C:607:PCW:H342	3:C:607:PCW:H172	0.52	1.80	1	1
2:B:68:ARG:HA	2:B:71:TYR:CE2	0.52	2.39	8	4
1:C:455:TYR:HE2	3:C:601:PCW:C23	0.52	2.16	3	1
3:A:406:PCW:H232	3:A:409:PCW:H262	0.52	1.80	7	1
3:A:408:PCW:H422	3:A:410:PCW:H441	0.52	1.81	10	1
3:C:611:PCW:H252	3:C:617:PCW:H431	0.52	1.80	10	1
3:B:220:PCW:H251	3:C:604:PCW:H471	0.52	1.81	2	1
3:C:619:PCW:H411	3:C:621:PCW:H211	0.52	1.81	2	1
3:B:205:PCW:H251	3:B:220:PCW:H211	0.52	1.80	3	1
3:B:219:PCW:O31	4:B:230:17F:H20	0.52	2.04	4	1
3:C:609:PCW:H283	4:C:632:17F:H48	0.52	1.80	6	2
3:B:201:PCW:H232	3:C:613:PCW:H483	0.52	1.81	7	1
3:B:208:PCW:H472	4:B:226:17F:H65	0.52	1.80	8	1
3:C:610:PCW:H372	3:C:614:PCW:H211	0.52	1.81	1	2
3:B:201:PCW:H182	4:B:228:17F:H18	0.52	1.80	3	1
3:B:209:PCW:H81	4:B:227:17F:H1	0.52	1.82	3	1
3:B:216:PCW:H171	4:B:227:17F:H37	0.52	1.80	3	1
3:A:408:PCW:H331	3:A:408:PCW:H131	0.52	1.79	8	2
3:B:208:PCW:H121	3:B:221:PCW:H162	0.52	1.82	4	1
3:B:212:PCW:H483	3:C:613:PCW:H451	0.52	1.80	4	1
3:B:218:PCW:H362	3:B:218:PCW:H162	0.52	1.80	5	1
3:B:203:PCW:H262	3:B:217:PCW:H161	0.52	1.80	7	1
3:A:406:PCW:H361	3:A:406:PCW:H141	0.52	1.82	10	1
3:B:213:PCW:H483	4:C:635:17F:H66	0.52	1.82	4	2
3:B:220:PCW:H251	3:B:232:PCW:H211	0.52	1.81	4	1
3:B:214:PCW:O3P	3:C:603:PCW:H71	0.52	2.05	5	1
3:A:406:PCW:H12	4:B:226:17F:O1	0.52	2.05	10	2
3:B:203:PCW:H481	3:B:233:PCW:H483	0.52	1.80	7	1
3:B:205:PCW:C1	3:B:207:PCW:H82	0.52	2.34	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:232:PCW:H151	3:C:625:PCW:H182	0.52	1.81	8	1
3:A:406:PCW:H242	3:A:409:PCW:H241	0.52	1.82	9	1
3:B:212:PCW:H461	3:C:613:PCW:H462	0.52	1.80	1	1
3:B:222:PCW:H461	4:C:634:17F:H47	0.52	1.81	1	2
1:C:417:GLU:O	1:C:421:PRO:HD2	0.52	2.04	8	5
3:C:619:PCW:H39	3:C:629:PCW:H221	0.52	1.81	2	2
3:C:621:PCW:H382	3:C:629:PCW:H161	0.52	1.79	3	1
3:B:221:PCW:H52	3:B:221:PCW:H31	0.52	1.82	4	1
3:B:203:PCW:O3P	3:B:220:PCW:H81	0.52	2.04	5	1
3:B:209:PCW:H182	3:B:213:PCW:H361	0.52	1.81	5	1
3:C:609:PCW:H83	3:C:611:PCW:H141	0.52	1.82	6	1
3:C:627:PCW:H372	3:C:628:PCW:H141	0.52	1.80	9	5
3:A:410:PCW:H251	4:C:633:17F:H53	0.52	1.80	7	1
1:A:363:LYS:HE2	1:C:411:THR:HB	0.52	1.80	2	1
1:A:392:GLU:CD	1:A:395:LYS:CD	0.52	2.76	5	1
1:C:510:HIS:O	1:C:514:LEU:HG	0.52	2.04	7	1
3:B:215:PCW:H271	3:C:608:PCW:H451	0.52	1.81	8	1
2:B:7:VAL:CG1	7:B:237:EWS:CAX	0.52	2.88	3	2
3:B:211:PCW:H271	3:C:619:PCW:H272	0.52	1.81	4	2
3:A:405:PCW:H352	3:A:405:PCW:H122	0.52	1.81	5	1
3:C:618:PCW:H181	3:C:620:PCW:H451	0.52	1.82	5	1
4:B:223:17F:H50	3:C:626:PCW:H251	0.52	1.81	6	1
3:A:407:PCW:H121	4:B:223:17F:H20	0.52	1.80	7	1
3:B:221:PCW:H283	4:B:226:17F:H69	0.52	1.82	7	1
3:C:613:PCW:H83	3:C:626:PCW:H322	0.52	1.82	7	1
3:B:213:PCW:H462	4:C:635:17F:H69	0.52	1.82	10	1
3:C:611:PCW:H151	3:C:617:PCW:H321	0.52	1.82	7	1
3:B:210:PCW:H151	4:B:227:17F:H10	0.52	1.81	2	3
1:C:589:GLU:HG2	1:C:593:LYS:HE2	0.52	1.80	2	1
3:A:405:PCW:H332	3:B:222:PCW:H122	0.52	1.81	4	1
2:B:105:ASP:HB3	3:B:203:PCW:H72	0.52	1.82	5	1
1:C:465:GLU:O	1:C:469:LEU:HB2	0.52	2.01	6	1
2:B:24:ILE:HG13	2:B:40:TYR:HB3	0.52	1.82	7	1
4:B:228:17F:H70	3:C:622:PCW:H451	0.52	1.81	7	1
3:A:409:PCW:H422	3:C:605:PCW:H20	0.52	1.82	8	1
1:C:568:ASP:OD1	1:C:571:GLN:OE1	0.52	2.28	9	1
3:C:607:PCW:H231	4:C:631:17F:H35	0.52	1.80	9	1
3:B:205:PCW:H252	3:B:220:PCW:H171	0.52	1.80	10	1
3:B:219:PCW:H31	3:B:220:PCW:H12	0.51	1.81	2	1
2:B:74:THR:HA	4:B:230:17F:HN1A	0.51	1.65	3	1
2:B:41:ARG:HA	2:B:53:LEU:O	0.51	2.04	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:488:LYS:HD3	3:C:623:PCW:H271	0.51	0.52	4	1
3:B:205:PCW:C6	7:B:237:EWS:BRA	0.51	3.12	6	1
3:B:209:PCW:H162	3:B:213:PCW:H161	0.51	1.83	7	1
3:B:207:PCW:H281	3:C:625:PCW:H461	0.51	1.82	6	2
3:B:210:PCW:H182	4:B:227:17F:H30	0.51	1.82	3	1
3:B:204:PCW:H361	4:B:223:17F:H10A	0.51	1.82	4	1
3:B:203:PCW:H452	4:B:223:17F:H44	0.51	1.81	5	1
3:B:213:PCW:H39	3:B:214:PCW:H212	0.51	1.82	5	1
3:C:613:PCW:H162	3:C:626:PCW:H452	0.51	1.81	5	1
3:C:606:PCW:H222	3:C:615:PCW:H172	0.51	1.82	6	1
3:B:201:PCW:H261	3:B:212:PCW:H452	0.51	1.80	8	1
1:A:214:PHE:CZ	3:A:404:PCW:H172	0.51	2.41	9	1
3:B:206:PCW:H282	3:B:215:PCW:H161	0.51	1.81	3	1
3:C:621:PCW:H352	3:C:629:PCW:H182	0.51	1.82	4	1
3:B:219:PCW:H331	3:B:219:PCW:H152	0.51	1.82	9	1
3:A:410:PCW:H331	4:C:633:17F:C12	0.51	2.35	10	1
4:B:228:17F:C1	4:B:228:17F:C4	0.51	2.87	2	1
2:B:79:LEU:HD23	2:B:112:VAL:HB	0.51	1.81	7	2
1:C:559:SER:HA	1:C:562:ALA:HB3	0.51	1.82	9	1
4:B:234:17F:H62	4:C:631:17F:H63	0.51	1.81	10	1
3:A:408:PCW:H32	3:C:620:PCW:H63	0.51	1.82	5	5
3:C:616:PCW:H172	3:C:616:PCW:H411	0.51	1.81	5	1
3:B:211:PCW:H61	4:B:229:17F:O2	0.51	2.06	3	2
3:B:203:PCW:H212	3:B:217:PCW:H181	0.51	1.82	2	1
3:B:233:PCW:H382	3:C:606:PCW:H351	0.51	1.80	3	1
3:B:216:PCW:H19	3:C:617:PCW:H481	0.51	1.82	5	1
3:A:409:PCW:H451	3:C:605:PCW:H231	0.51	1.82	10	1
3:B:206:PCW:H242	3:B:215:PCW:H20	0.51	1.83	10	1
3:B:231:PCW:H412	3:C:604:PCW:H421	0.51	1.82	2	3
1:C:469:LEU:O	1:C:473:LYS:HB2	0.51	2.05	4	2
3:A:407:PCW:H121	4:B:223:17F:C1Z	0.51	2.34	9	3
1:A:308:ARG:HD3	1:C:469:LEU:CD2	0.51	2.32	6	1
3:A:406:PCW:H432	3:A:409:PCW:H251	0.51	1.80	6	1
3:B:203:PCW:H483	4:B:223:17F:H48	0.51	1.83	7	1
1:A:338:LEU:HA	1:A:341:ASN:HB3	0.51	1.82	9	1
1:A:221:LEU:HA	1:A:224:VAL:HG12	0.51	1.83	8	2
3:B:211:PCW:H332	4:B:229:17F:H8A	0.51	1.83	1	2
3:B:210:PCW:H382	4:B:224:17F:H10	0.51	1.81	5	1
4:B:227:17F:H66	3:C:602:PCW:H421	0.51	1.82	7	1
3:C:611:PCW:H461	4:C:635:17F:H39	0.51	1.81	8	1
3:A:407:PCW:C34	4:B:225:17F:H9	0.51	2.28	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:610:PCW:H351	3:C:614:PCW:H382	0.51	1.83	10	3
2:B:3:GLU:OE2	3:B:221:PCW:H63	0.51	2.05	4	1
3:B:219:PCW:H20	3:C:605:PCW:H281	0.51	1.81	4	1
3:B:206:PCW:H351	3:B:215:PCW:H412	0.51	1.81	5	1
1:C:491:GLU:HB3	1:C:495:LYS:HE2	0.51	1.83	7	1
3:B:206:PCW:H142	3:B:208:PCW:H181	0.51	1.83	8	1
3:C:613:PCW:H362	3:C:613:PCW:H171	0.51	1.82	8	1
3:A:408:PCW:H351	3:A:410:PCW:H362	0.51	1.82	9	1
3:B:205:PCW:H41	3:B:205:PCW:H31	0.51	1.82	9	1
4:B:225:17F:H59	3:C:626:PCW:H283	0.51	1.82	5	1
4:C:635:17F:H30	4:C:635:17F:H57	0.51	1.82	5	1
3:B:221:PCW:H281	3:C:627:PCW:H482	0.51	1.83	7	1
3:B:202:PCW:H261	4:B:228:17F:H65	0.50	1.82	3	1
3:A:405:PCW:H141	3:A:405:PCW:H372	0.50	1.83	5	1
4:A:411:17F:H49	3:C:607:PCW:H242	0.50	1.82	7	1
3:C:615:PCW:H281	3:C:626:PCW:H251	0.50	1.81	9	1
3:B:211:PCW:H262	3:B:217:PCW:H451	0.50	1.83	1	1
3:A:406:PCW:H142	3:A:409:PCW:H252	0.50	1.82	3	1
3:B:201:PCW:H171	4:B:225:17F:H60	0.50	1.83	3	1
3:A:402:PCW:H81	3:B:214:PCW:H132	0.50	1.83	4	1
3:C:615:PCW:O1P	3:C:622:PCW:H11	0.50	2.06	6	2
4:B:223:17F:H55	3:C:626:PCW:H232	0.50	1.83	6	1
1:A:310:ARG:O	1:A:314:ASP:HB2	0.50	2.07	10	2
3:B:220:PCW:H482	3:C:625:PCW:H232	0.50	1.83	7	1
3:B:202:PCW:H362	3:B:212:PCW:H372	0.50	1.82	9	1
4:B:234:17F:H35	3:C:625:PCW:H272	0.50	1.83	9	1
3:B:203:PCW:H242	3:B:211:PCW:H451	0.50	1.83	1	1
3:B:211:PCW:H151	4:B:229:17F:H6A	0.50	1.82	2	1
1:A:330:ARG:HH21	1:C:447:GLU:HB3	0.50	1.67	10	2
3:B:207:PCW:H362	3:B:211:PCW:H372	0.50	1.83	7	1
1:A:202:LYS:HZ3	1:A:202:LYS:HB3	0.50	1.66	9	1
3:B:213:PCW:H232	4:B:227:17F:H51	0.50	1.82	2	1
3:A:407:PCW:H122	4:B:223:17F:H33	0.50	1.82	3	1
3:A:408:PCW:H372	3:A:410:PCW:H351	0.50	1.83	3	1
3:B:211:PCW:H421	4:B:229:17F:H60	0.50	1.83	3	1
3:B:219:PCW:H461	4:B:223:17F:H45	0.50	1.82	3	1
3:A:406:PCW:H172	4:B:226:17F:H64	0.50	1.83	4	1
3:B:211:PCW:H171	4:B:229:17F:H33	0.50	1.83	8	1
4:B:223:17F:H43	3:C:626:PCW:H272	0.50	1.84	8	2
3:B:220:PCW:H462	3:B:232:PCW:H481	0.50	1.83	10	1
3:B:208:PCW:H141	3:B:215:PCW:H372	0.50	1.83	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:218:PCW:H182	3:B:218:PCW:H362	0.50	1.83	4	2
4:B:223:17F:H46	3:C:626:PCW:H251	0.50	1.82	4	1
3:B:202:PCW:H321	3:B:212:PCW:H81	0.50	1.84	8	1
3:A:406:PCW:H2	4:B:226:17F:O10	0.50	2.07	10	1
3:B:221:PCW:H42	7:B:237:EWS:BRA	0.50	2.59	1	1
3:B:202:PCW:H362	3:B:212:PCW:H381	0.50	1.83	7	3
3:C:611:PCW:C15	3:C:617:PCW:H321	0.50	2.36	3	1
3:B:221:PCW:H39	4:B:230:17F:H71	0.50	1.83	5	1
3:A:407:PCW:C15	4:B:223:17F:H33	0.50	2.35	7	1
3:B:203:PCW:H362	3:B:204:PCW:H122	0.50	1.83	7	1
3:C:621:PCW:H342	3:C:629:PCW:H371	0.50	1.82	7	1
4:B:226:17F:H72	3:C:628:PCW:H451	0.50	1.82	9	1
1:C:443:LYS:O	1:C:447:GLU:HB2	0.50	2.07	9	2
3:A:407:PCW:H152	4:B:223:17F:H20	0.50	1.84	1	1
3:A:406:PCW:H141	3:A:406:PCW:H382	0.50	1.84	2	1
3:B:212:PCW:H171	3:B:212:PCW:H371	0.50	1.84	2	1
3:C:621:PCW:H122	3:C:629:PCW:H182	0.50	1.82	2	1
1:C:442:SER:O	1:C:446:GLU:HB2	0.50	2.07	3	1
1:C:427:TRP:HA	1:C:427:TRP:CE3	0.50	2.40	6	1
3:C:603:PCW:H483	3:C:624:PCW:H252	0.50	1.84	6	1
3:B:219:PCW:H221	3:B:233:PCW:H282	0.50	1.84	9	1
4:B:225:17F:H76	3:C:606:PCW:C48	0.50	2.37	9	1
3:B:205:PCW:H161	3:B:207:PCW:H171	0.50	1.82	10	1
3:B:209:PCW:H161	3:B:216:PCW:H181	0.50	1.83	6	1
3:B:220:PCW:H142	3:B:220:PCW:H382	0.50	1.84	9	2
4:B:228:17F:H11A	4:B:228:17F:H31	0.50	1.83	1	1
4:B:234:17F:H70	3:C:607:PCW:H283	0.50	1.83	2	1
3:B:220:PCW:H472	3:B:233:PCW:H282	0.50	1.83	10	2
3:B:231:PCW:H141	3:C:604:PCW:H19	0.50	1.83	5	2
3:B:205:PCW:H83	7:B:237:EWS:CAR	0.50	2.36	6	1
3:B:217:PCW:H261	3:B:218:PCW:H241	0.50	1.84	10	1
3:B:219:PCW:H421	4:B:223:17F:H38	0.50	1.84	10	1
1:A:275:LYS:O	1:A:279:LEU:HB2	0.49	2.06	2	1
3:B:201:PCW:H20	4:B:228:17F:H34	0.49	1.83	4	1
3:C:613:PCW:H222	3:C:622:PCW:H242	0.49	1.83	5	1
3:A:406:PCW:H432	3:A:409:PCW:H221	0.49	1.82	8	1
2:B:7:VAL:HB	2:B:78:PHE:CE1	0.49	2.41	8	1
3:A:406:PCW:H382	4:B:226:17F:H60	0.49	1.83	9	1
3:C:611:PCW:H152	3:C:617:PCW:H332	0.49	1.84	10	1
1:A:214:PHE:CE2	3:A:404:PCW:H171	0.49	2.39	1	1
2:B:63:GLU:O	2:B:68:ARG:HG2	0.49	2.06	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:218:PCW:H432	3:B:222:PCW:H421	0.49	1.84	1	1
1:C:470:TYR:CD1	4:C:632:17F:H76	0.49	2.41	1	1
4:B:229:17F:H55	3:B:231:PCW:H182	0.49	1.83	3	1
1:C:421:PRO:O	1:C:425:GLU:HG3	0.49	2.07	4	1
3:A:409:PCW:H441	3:C:605:PCW:H222	0.49	1.83	1	1
3:B:217:PCW:H321	3:B:217:PCW:H41	0.49	1.83	1	1
3:A:405:PCW:H42	3:B:222:PCW:H32	0.49	1.84	4	1
1:A:253:LYS:O	1:A:257:TYR:HB2	0.49	2.07	7	1
3:B:209:PCW:H432	3:C:617:PCW:H252	0.49	1.84	9	1
3:C:608:PCW:H62	4:C:630:17F:H2	0.49	1.83	10	1
3:C:616:PCW:H412	3:C:622:PCW:H212	0.49	1.83	1	3
2:B:56:LEU:HD23	2:B:58:THR:HG23	0.49	1.83	4	1
1:A:393:TYR:OH	3:A:407:PCW:C25	0.49	2.57	6	1
4:A:411:17F:H69	3:C:624:PCW:H421	0.49	1.85	9	1
1:C:441:MET:HA	1:C:444:ASP:HB2	0.49	1.84	1	1
3:A:408:PCW:H12	3:B:231:PCW:H352	0.49	1.84	3	1
1:C:489:LEU:CD2	3:C:623:PCW:H261	0.49	2.37	3	1
2:B:149:ARG:HG2	2:B:152:VAL:HB	0.49	1.82	5	1
1:A:334:ARG:HD2	1:C:440:GLU:OE2	0.49	2.07	7	1
2:B:74:THR:HG21	7:B:237:EWS:NAA	0.49	2.23	7	1
3:A:402:PCW:H39	3:B:214:PCW:H262	0.49	1.83	8	1
3:B:211:PCW:H241	3:B:217:PCW:H431	0.49	1.84	9	1
1:A:224:VAL:O	1:A:228:PHE:HB2	0.49	2.08	1	3
3:C:608:PCW:H63	4:C:630:17F:H2	0.49	1.85	1	1
3:A:408:PCW:H242	3:C:618:PCW:H483	0.49	1.83	2	1
4:B:223:17F:H1	4:B:223:17F:H4A	0.49	1.85	9	3
3:C:617:PCW:H232	4:C:632:17F:H42	0.49	1.83	3	1
1:A:298:LEU:O	1:A:302:GLY:HA3	0.49	2.07	8	2
3:B:208:PCW:H181	3:B:215:PCW:H411	0.49	1.84	4	1
4:B:228:17F:H72	3:C:622:PCW:H252	0.49	1.85	4	1
1:A:341:ASN:ND2	1:C:433:GLU:HA	0.49	2.22	7	2
3:C:610:PCW:H431	3:C:614:PCW:H172	0.49	1.84	5	1
3:C:610:PCW:H161	3:C:619:PCW:H172	0.49	1.82	5	1
2:B:66:ALA:HB3	4:B:229:17F:HN1	0.49	1.68	6	1
3:A:401:PCW:H452	3:C:616:PCW:H272	0.49	1.84	1	1
2:B:113:LEU:HB3	2:B:141:PHE:HD1	0.49	1.67	1	1
1:A:325:ASP:HA	1:A:328:ARG:HD2	0.49	1.84	5	2
3:A:407:PCW:C12	4:B:223:17F:H20A	0.49	2.38	4	2
3:B:231:PCW:H361	3:C:604:PCW:H382	0.49	1.83	5	2
1:A:332:ALA:O	1:A:336:GLU:HG2	0.49	2.07	7	1
3:A:407:PCW:H132	4:B:223:17F:H20	0.49	1.83	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:202:PCW:H471	4:B:226:17F:H10A	0.49	1.84	1	1
3:B:209:PCW:H171	3:B:216:PCW:H181	0.49	1.85	4	1
4:B:225:17F:H71	3:C:615:PCW:H242	0.49	1.85	9	2
3:B:231:PCW:H252	3:C:604:PCW:H271	0.49	1.83	4	1
3:B:204:PCW:H483	3:C:604:PCW:H261	0.49	1.85	5	1
3:B:215:PCW:H451	3:B:221:PCW:H252	0.49	1.85	6	1
3:B:218:PCW:H472	3:C:603:PCW:H471	0.49	1.84	7	1
3:B:219:PCW:H131	4:B:230:17F:H34	0.49	1.85	7	1
3:B:209:PCW:H132	3:B:216:PCW:H122	0.49	1.84	8	1
3:B:232:PCW:H352	3:B:232:PCW:H122	0.49	1.85	10	1
3:C:603:PCW:H441	3:C:625:PCW:H472	0.49	1.83	3	1
3:B:205:PCW:H242	3:B:219:PCW:H431	0.49	1.85	4	1
3:C:621:PCW:H471	4:C:634:17F:H53	0.49	1.85	6	1
1:A:388:SER:HB2	1:C:594:LYS:CE	0.49	2.38	9	1
1:C:523:ASP:HA	1:C:526:ARG:HD2	0.49	1.84	9	1
1:A:363:LYS:HA	1:A:367:ALA:HB3	0.49	1.84	10	1
3:A:409:PCW:H372	3:C:627:PCW:H361	0.49	1.83	10	1
3:B:221:PCW:N	7:B:237:EWS:BRA	0.49	3.00	1	1
1:C:508:ARG:O	1:C:512:ASP:HB2	0.49	2.07	2	3
1:C:455:TYR:CE2	3:C:601:PCW:H231	0.49	2.34	3	1
4:B:226:17F:H51	4:B:230:17F:H50	0.49	1.85	4	1
3:B:209:PCW:H261	3:C:611:PCW:H482	0.49	1.83	5	1
3:B:201:PCW:H62	3:B:220:PCW:O2P	0.49	2.08	6	1
3:C:606:PCW:H462	3:C:615:PCW:H171	0.49	1.85	6	1
3:B:202:PCW:H20	4:B:228:17F:H12	0.49	1.83	7	1
3:B:212:PCW:H141	4:B:226:17F:H18	0.49	1.84	7	1
3:C:611:PCW:H472	4:C:635:17F:H45	0.49	1.85	10	1
2:B:72:MET:HG2	2:B:78:PHE:CE1	0.48	2.43	1	1
3:B:214:PCW:H461	3:C:612:PCW:H283	0.48	1.85	1	1
1:C:455:TYR:O	1:C:459:PHE:HB2	0.48	2.07	9	3
3:B:203:PCW:H31	3:B:211:PCW:H321	0.48	1.85	3	1
3:B:231:PCW:H362	3:C:604:PCW:H171	0.48	1.84	4	1
3:A:403:PCW:H461	3:C:618:PCW:H461	0.48	1.85	5	1
3:C:611:PCW:H361	3:C:617:PCW:H381	0.48	1.85	5	1
1:C:502:GLU:HG2	1:C:506:ARG:HE	0.48	1.68	7	2
3:C:605:PCW:H182	3:C:626:PCW:H132	0.48	1.84	7	1
3:C:612:PCW:H12	4:C:634:17F:H6	0.48	1.85	7	1
1:C:534:GLU:HA	1:C:537:LYS:HE3	0.48	1.85	9	1
3:C:616:PCW:H412	3:C:616:PCW:H171	0.48	1.83	9	1
3:C:615:PCW:H132	3:C:622:PCW:H362	0.48	1.85	10	2
1:A:392:GLU:O	1:A:396:LYS:HG2	0.48	2.07	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:327:LEU:HA	1:A:330:ARG:HG2	0.48	1.84	5	1
3:B:201:PCW:H441	4:B:226:17F:H55	0.48	1.85	5	1
3:B:203:PCW:H471	4:B:223:17F:H48	0.48	1.84	5	2
1:C:546:GLU:O	1:C:550:LYS:HD2	0.48	2.08	5	3
3:A:410:PCW:O2P	3:C:620:PCW:H52	0.48	2.08	8	1
4:A:411:17F:H75	4:C:634:17F:H71	0.48	1.83	8	1
3:B:201:PCW:H72	7:B:237:EWS:BRA	0.48	2.63	8	1
3:B:219:PCW:H283	4:C:631:17F:H52	0.48	1.84	1	1
4:B:229:17F:H47	3:B:231:PCW:H212	0.48	1.85	1	1
4:B:227:17F:O2	3:C:602:PCW:H82	0.48	2.07	9	2
3:B:231:PCW:H19	3:C:618:PCW:H39	0.48	1.85	10	3
3:B:203:PCW:H141	3:B:207:PCW:H322	0.48	1.84	7	1
3:B:204:PCW:H81	3:B:220:PCW:H52	0.48	1.85	9	1
4:B:225:17F:H72	4:B:228:17F:H68	0.48	1.84	6	1
3:C:626:PCW:H19	3:C:627:PCW:H282	0.48	1.86	6	1
3:B:205:PCW:H171	3:B:207:PCW:H141	0.48	1.85	7	1
2:B:94:HIS:O	2:B:98:GLU:HG2	0.48	2.07	2	2
4:B:225:17F:H74	4:B:228:17F:H62	0.48	1.86	2	1
3:C:607:PCW:H481	3:C:611:PCW:H372	0.48	1.84	2	1
3:B:209:PCW:H282	3:B:209:PCW:H20	0.48	1.85	4	1
3:B:201:PCW:C1	7:B:237:EWS:CAN	0.48	2.91	5	1
3:B:203:PCW:H20	3:B:217:PCW:H252	0.48	1.86	5	1
3:C:615:PCW:H381	3:C:622:PCW:H371	0.48	1.84	7	1
3:A:402:PCW:H361	3:A:402:PCW:H141	0.48	1.86	9	1
3:B:209:PCW:H483	3:C:617:PCW:H232	0.48	1.85	10	1
4:C:631:17F:H1A	4:C:631:17F:H4	0.48	1.86	10	1
1:A:322:PRO:O	1:A:326:GLU:HG3	0.48	2.09	1	1
3:A:408:PCW:H172	3:A:408:PCW:H362	0.48	1.84	1	2
4:A:411:17F:H61	4:C:635:17F:H68	0.48	1.84	7	2
1:C:455:TYR:HH	3:C:601:PCW:C21	0.48	2.15	3	1
3:C:614:PCW:H132	3:C:614:PCW:H342	0.48	1.85	3	1
3:A:402:PCW:H382	3:B:213:PCW:H372	0.48	1.86	4	1
1:C:488:LYS:CG	3:C:623:PCW:C28	0.48	2.51	4	1
1:A:396:LYS:NZ	3:A:407:PCW:C28	0.48	2.70	5	1
3:A:407:PCW:H342	4:B:225:17F:C9	0.48	2.31	6	1
4:B:234:17F:H58	4:B:234:17F:H12A	0.48	1.84	6	1
3:C:621:PCW:H362	3:C:629:PCW:H411	0.48	1.84	6	1
3:B:219:PCW:H261	3:C:625:PCW:H281	0.48	1.85	7	1
3:C:618:PCW:H182	3:C:620:PCW:H452	0.48	1.84	9	1
3:C:622:PCW:H152	3:C:622:PCW:H361	0.48	1.84	9	1
1:A:214:PHE:CE1	3:A:404:PCW:H171	0.48	2.43	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:479:ALA:O	1:C:483:GLU:HG2	0.48	2.09	1	1
1:A:365:LYS:CB	1:A:366:PRO:HD3	0.48	2.35	3	4
3:A:408:PCW:H352	3:A:410:PCW:C34	0.48	2.38	3	1
3:B:216:PCW:H172	4:B:224:17F:H61	0.48	1.86	3	1
2:B:65:SER:HB3	2:B:68:ARG:HB3	0.48	1.86	4	1
3:B:203:PCW:H482	3:B:231:PCW:H452	0.48	1.86	5	1
3:B:219:PCW:H251	3:C:605:PCW:H271	0.48	1.85	7	1
3:B:211:PCW:H442	3:C:621:PCW:H232	0.48	1.86	8	1
1:C:411:THR:O	1:C:415:LEU:HG	0.48	2.09	9	1
1:A:214:PHE:HZ	3:A:404:PCW:H161	0.48	1.62	10	1
3:B:213:PCW:H241	3:C:611:PCW:H422	0.48	1.86	10	1
3:B:205:PCW:O2P	3:B:210:PCW:H51	0.48	2.09	1	1
4:B:230:17F:H37	3:C:605:PCW:H282	0.48	1.84	1	1
3:C:621:PCW:H431	3:C:621:PCW:H162	0.48	1.85	1	1
3:A:406:PCW:H12	3:B:206:PCW:H322	0.48	1.84	2	1
1:A:299:SER:HB2	1:A:300:PRO:HD3	0.48	1.84	3	1
4:B:224:17F:H77	4:C:631:17F:H73	0.48	1.85	5	1
3:B:220:PCW:H232	3:C:604:PCW:H482	0.48	1.85	8	1
3:C:607:PCW:H19	3:C:628:PCW:H272	0.48	1.85	9	1
3:B:206:PCW:H251	3:C:601:PCW:H39	0.48	1.86	10	1
1:A:231:ASN:HA	1:A:234:LYS:CE	0.48	2.38	9	2
3:B:219:PCW:H32	3:B:220:PCW:H322	0.48	1.85	7	1
3:C:613:PCW:H52	3:C:613:PCW:H12	0.48	1.84	7	1
3:B:208:PCW:C3	3:B:221:PCW:H141	0.48	2.39	1	1
3:B:209:PCW:H152	3:B:216:PCW:H162	0.48	1.85	1	1
1:C:495:LYS:O	1:C:499:LEU:HB2	0.48	2.09	5	7
2:B:54:ASP:CB	7:B:237:EWS:BRA	0.48	3.15	2	1
3:B:201:PCW:H39	3:C:626:PCW:H251	0.48	1.86	2	1
3:B:207:PCW:H83	3:B:217:PCW:O1P	0.48	2.09	3	1
3:B:208:PCW:H361	4:B:226:17F:H8A	0.48	1.86	3	1
3:B:219:PCW:C6	7:B:237:EWS:BRA	0.48	3.17	6	1
3:B:209:PCW:H151	4:B:227:17F:H12A	0.48	1.85	9	1
2:B:133:LEU:HG	2:B:137:TYR:CE2	0.48	2.44	10	1
3:B:205:PCW:H171	4:B:224:17F:H29	0.48	1.85	10	1
3:C:606:PCW:H211	3:C:615:PCW:H171	0.48	1.86	10	1
3:C:615:PCW:H31	3:C:615:PCW:O31	0.47	2.08	3	7
1:A:355:GLU:OE1	1:A:355:GLU:HA	0.47	2.08	3	1
3:A:401:PCW:H372	3:B:202:PCW:H171	0.47	1.84	3	1
3:B:211:PCW:H472	3:C:621:PCW:H471	0.47	1.85	3	1
3:B:209:PCW:H442	3:C:617:PCW:H252	0.47	1.85	4	1
3:B:222:PCW:H472	4:C:634:17F:H47	0.47	1.86	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:234:17F:H35	3:C:625:PCW:H283	0.47	1.84	7	2
3:C:610:PCW:H162	3:C:614:PCW:H171	0.47	1.85	5	1
4:B:234:17F:H45	4:B:234:17F:H74	0.47	1.85	7	1
3:C:611:PCW:H182	3:C:617:PCW:H361	0.47	1.85	1	1
3:B:205:PCW:H272	3:B:220:PCW:H241	0.47	1.86	4	1
4:A:411:17F:H34	3:C:624:PCW:H422	0.47	1.86	6	1
3:B:206:PCW:H172	3:B:208:PCW:H232	0.47	1.86	6	1
3:B:211:PCW:H172	4:B:229:17F:H19	0.47	1.85	6	1
3:C:601:PCW:H422	4:C:630:17F:H54	0.47	1.86	10	1
3:C:617:PCW:H252	4:C:635:17F:H41	0.47	1.85	1	1
3:C:616:PCW:H412	3:C:622:PCW:H20	0.47	1.84	2	1
3:A:401:PCW:H73	2:B:70:GLN:OE1	0.47	2.09	4	1
3:B:219:PCW:C34	4:B:226:17F:H37	0.47	2.38	10	2
3:B:210:PCW:C37	4:B:224:17F:H11A	0.47	2.39	8	2
3:B:204:PCW:H62	3:B:211:PCW:O2P	0.47	2.08	10	1
3:B:205:PCW:H32	3:B:207:PCW:O1P	0.47	2.10	10	1
4:B:227:17F:H70	3:C:602:PCW:H422	0.47	1.86	10	1
2:B:72:MET:HG2	2:B:78:PHE:HE1	0.47	1.69	1	1
2:B:79:LEU:CD2	2:B:112:VAL:HB	0.47	2.40	1	1
4:B:225:17F:H40	3:C:615:PCW:H232	0.47	1.87	1	1
4:A:411:17F:H53	3:C:607:PCW:H242	0.47	1.85	2	1
3:B:205:PCW:H42	3:B:205:PCW:H31	0.47	1.84	2	1
3:C:610:PCW:H481	3:C:614:PCW:H282	0.47	1.85	3	1
2:B:67:MET:SD	3:B:211:PCW:H63	0.47	2.49	8	1
1:A:316:LEU:HG	1:C:462:LYS:HE3	0.47	1.86	6	2
2:B:39:SER:HA	2:B:55:ILE:O	0.47	2.09	1	1
3:B:201:PCW:H63	3:B:219:PCW:O2P	0.47	2.09	1	1
3:A:410:PCW:H51	3:A:410:PCW:H11	0.47	1.87	2	2
1:A:225:THR:O	1:A:229:TRP:HB2	0.47	2.09	5	3
3:B:215:PCW:H282	3:C:609:PCW:H421	0.47	1.87	4	1
3:A:406:PCW:H472	3:A:409:PCW:H242	0.47	1.84	8	3
3:A:401:PCW:H41	3:B:212:PCW:O11	0.47	2.10	7	1
1:A:363:LYS:O	1:A:367:ALA:HB3	0.47	2.10	3	3
3:B:212:PCW:H41	3:B:212:PCW:H31	0.47	1.86	1	1
3:B:202:PCW:H322	3:B:212:PCW:H331	0.47	1.87	2	1
3:B:212:PCW:H161	3:B:212:PCW:H361	0.47	1.86	3	1
3:C:628:PCW:H52	3:C:628:PCW:O11	0.47	2.10	3	1
3:A:403:PCW:H451	3:C:618:PCW:H461	0.47	1.86	4	1
3:C:616:PCW:H171	3:C:616:PCW:H351	0.47	1.87	5	1
3:B:231:PCW:H411	3:C:604:PCW:H421	0.47	1.87	7	1
3:B:216:PCW:H232	3:C:611:PCW:H451	0.47	1.85	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:408:PCW:H362	3:A:408:PCW:H171	0.47	1.85	9	1
1:C:421:PRO:O	1:C:425:GLU:HG2	0.47	2.10	10	1
3:C:601:PCW:H381	3:C:602:PCW:H141	0.47	1.84	10	1
3:A:401:PCW:H39	3:B:202:PCW:H242	0.47	1.87	1	1
3:A:403:PCW:H82	4:B:223:17F:O4	0.47	2.09	2	1
2:B:32:TYR:CD1	5:B:235:GNP:H5'1	0.47	2.45	2	1
1:C:570:ARG:O	1:C:574:LEU:HG	0.47	2.09	2	1
1:A:309:ALA:HA	1:A:312:HIS:HB2	0.47	1.85	6	2
1:A:391:GLU:O	1:A:395:LYS:HB2	0.47	2.09	3	1
3:B:208:PCW:H31	3:B:221:PCW:H152	0.47	1.86	3	1
3:C:625:PCW:H73	3:C:625:PCW:H331	0.47	1.87	3	1
3:B:206:PCW:H221	3:C:601:PCW:H371	0.47	1.85	5	1
3:A:402:PCW:H283	3:B:209:PCW:H272	0.47	1.85	6	1
3:A:405:PCW:H83	3:B:222:PCW:H32	0.47	1.87	6	1
3:A:409:PCW:H382	3:C:627:PCW:H382	0.47	1.86	6	1
3:B:205:PCW:H161	3:B:207:PCW:H162	0.47	1.86	6	1
3:A:406:PCW:H212	3:A:409:PCW:H232	0.47	1.86	7	1
3:C:609:PCW:H172	4:C:632:17F:H20A	0.47	1.85	7	1
3:A:401:PCW:H382	3:B:212:PCW:H451	0.47	1.86	8	1
3:B:231:PCW:H131	3:C:619:PCW:H11	0.47	1.85	8	1
3:B:231:PCW:H121	3:C:604:PCW:H19	0.47	1.86	8	1
4:A:411:17F:H55	3:C:617:PCW:H39	0.47	1.85	9	1
3:B:202:PCW:H471	4:B:230:17F:H12A	0.47	1.87	9	1
3:B:203:PCW:H482	3:B:231:PCW:H451	0.47	1.85	7	2
4:B:224:17F:H29	4:B:230:17F:H59	0.47	1.85	2	1
1:C:534:GLU:O	1:C:538:GLU:HG2	0.47	2.10	3	1
3:C:609:PCW:H172	4:C:632:17F:H18	0.47	1.86	3	1
3:B:232:PCW:C48	4:B:234:17F:H42	0.47	2.40	4	1
3:C:606:PCW:H181	3:C:615:PCW:H122	0.47	1.85	4	1
2:B:68:ARG:HA	2:B:71:TYR:CD2	0.47	2.44	8	2
3:C:614:PCW:H132	3:C:614:PCW:C34	0.47	2.40	6	1
4:C:630:17F:H71	4:C:632:17F:H53	0.47	1.87	7	1
3:C:610:PCW:H362	3:C:614:PCW:H362	0.47	1.87	9	1
3:A:406:PCW:H222	3:A:409:PCW:H241	0.47	1.85	10	1
4:B:226:17F:H78	3:C:628:PCW:H451	0.47	1.87	4	1
3:A:407:PCW:C33	4:B:223:17F:H31	0.47	2.38	5	1
4:B:234:17F:H70	3:C:607:PCW:H261	0.47	1.87	9	2
1:C:466:GLU:HA	1:C:469:LEU:HB2	0.47	1.87	9	1
3:B:202:PCW:H452	4:B:226:17F:H12A	0.47	1.86	1	1
3:C:621:PCW:H371	3:C:629:PCW:H412	0.47	1.86	9	2
3:A:407:PCW:C35	4:B:223:17F:H56	0.47	2.38	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:201:PCW:H341	3:B:219:PCW:H361	0.47	1.87	3	2
4:B:234:17F:H70	3:C:607:PCW:H271	0.47	1.87	3	2
1:A:255:GLN:HB2	1:A:256:PRO:CD	0.47	2.39	10	3
3:B:205:PCW:H452	3:B:207:PCW:H241	0.47	1.85	4	1
3:B:232:PCW:H40	3:C:619:PCW:H452	0.47	1.87	4	1
3:C:617:PCW:H222	4:C:635:17F:H35	0.47	1.86	4	1
3:C:617:PCW:C22	4:C:632:17F:H42	0.47	2.40	4	1
3:B:210:PCW:H352	4:B:224:17F:H31	0.46	1.87	1	1
3:C:606:PCW:H62	4:C:633:17F:O5	0.46	2.10	1	1
3:C:609:PCW:H211	4:C:630:17F:H37	0.46	1.86	1	1
4:B:224:17F:H44	4:B:234:17F:H43	0.46	1.86	2	1
2:B:6:LEU:HD23	2:B:159:LEU:HD23	0.46	1.87	3	1
3:B:201:PCW:H232	3:C:613:PCW:H471	0.46	1.87	3	1
3:C:606:PCW:H181	3:C:615:PCW:H341	0.46	1.87	5	1
3:B:202:PCW:H481	4:B:226:17F:H20	0.46	1.85	6	1
4:B:227:17F:H41	4:B:227:17F:H30	0.46	1.87	6	1
3:C:629:PCW:H231	4:C:634:17F:H40	0.46	1.86	6	1
3:B:213:PCW:H462	4:C:635:17F:H70	0.46	1.87	7	1
3:A:410:PCW:H332	4:C:633:17F:C12	0.46	2.36	8	1
4:C:635:17F:H18	4:C:635:17F:H9A	0.46	1.86	10	1
3:B:205:PCW:H251	3:B:220:PCW:H181	0.46	1.87	2	1
1:A:299:SER:HB2	1:A:300:PRO:CD	0.46	2.39	3	1
3:A:406:PCW:H182	3:A:409:PCW:H252	0.46	1.87	8	1
2:B:113:LEU:O	2:B:141:PHE:HA	0.46	2.10	8	1
3:B:201:PCW:H151	4:B:225:17F:O8	0.46	2.11	9	1
2:B:118:CYS:HB3	2:B:143:GLU:HG2	0.46	1.86	10	1
3:B:207:PCW:H341	3:B:220:PCW:H372	0.46	1.86	2	1
3:C:608:PCW:H63	4:C:630:17F:HN1A	0.46	1.70	2	1
3:B:231:PCW:H461	3:C:604:PCW:H271	0.46	1.87	3	1
3:C:613:PCW:H411	3:C:622:PCW:H441	0.46	1.87	4	1
3:A:401:PCW:H62	3:B:212:PCW:H11	0.46	1.86	5	1
4:A:411:17F:H53	3:C:607:PCW:H221	0.46	1.85	6	1
4:B:225:17F:H71	3:C:615:PCW:H222	0.46	1.86	6	1
3:C:611:PCW:C37	4:C:635:17F:H34	0.46	2.40	6	1
3:B:209:PCW:H61	4:B:224:17F:O1	0.46	2.10	9	1
3:C:619:PCW:H39	3:C:629:PCW:H232	0.46	1.87	3	2
1:A:234:LYS:HE3	1:C:539:ASN:OD1	0.46	2.11	2	3
1:A:293:GLU:O	1:A:297:LYS:HB2	0.46	2.09	2	1
3:C:626:PCW:H39	3:C:626:PCW:H131	0.46	1.86	3	1
3:A:409:PCW:H483	3:B:208:PCW:H471	0.46	1.86	4	1
3:A:405:PCW:H261	3:C:621:PCW:H412	0.46	1.87	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:219:PCW:H432	3:B:219:PCW:H381	0.46	1.86	5	1
3:C:621:PCW:H42	3:C:629:PCW:H41	0.46	1.88	5	1
3:B:205:PCW:H282	3:B:220:PCW:H241	0.46	1.86	6	1
3:B:207:PCW:H142	3:B:232:PCW:H281	0.46	1.85	6	1
1:A:358:SER:O	1:A:362:GLU:HG3	0.46	2.09	9	2
3:B:212:PCW:H261	4:B:226:17F:H59	0.46	1.87	7	1
1:C:470:TYR:CE1	4:C:632:17F:C42	0.46	2.98	1	1
1:A:253:LYS:C	1:A:256:PRO:HD2	0.46	2.36	3	1
4:B:226:17F:H49	3:C:626:PCW:H241	0.46	1.86	3	1
3:B:232:PCW:H372	3:B:232:PCW:H411	0.46	1.86	3	1
1:C:422:VAL:HA	1:C:425:GLU:OE2	0.46	2.11	4	1
3:B:203:PCW:H442	3:B:204:PCW:H39	0.46	1.86	8	1
3:C:606:PCW:H262	3:C:615:PCW:H181	0.46	1.86	8	1
3:A:404:PCW:O2P	3:B:211:PCW:H141	0.46	2.10	9	1
3:B:215:PCW:H52	3:B:215:PCW:H2	0.46	1.86	9	1
3:A:401:PCW:H483	3:C:613:PCW:H271	0.46	1.86	10	1
1:A:203:LEU:O	1:A:207:TRP:HB2	0.46	2.10	6	2
3:B:216:PCW:H221	3:C:611:PCW:H452	0.46	1.86	5	1
1:A:330:ARG:O	1:A:334:ARG:HG2	0.46	2.11	6	2
3:B:217:PCW:H283	3:B:218:PCW:H262	0.46	1.87	6	1
3:B:221:PCW:H81	4:B:224:17F:O2	0.46	2.10	6	1
3:B:218:PCW:H261	3:C:625:PCW:H40	0.46	1.87	7	1
4:B:234:17F:H41	4:B:234:17F:H69	0.46	1.87	9	1
1:C:456:LEU:O	1:C:460:GLN:HB2	0.46	2.10	2	1
3:B:232:PCW:H122	3:C:625:PCW:C17	0.46	2.41	3	1
1:C:563:LYS:HB2	1:C:564:PRO:CD	0.46	2.41	5	2
3:C:627:PCW:H351	3:C:628:PCW:C12	0.46	2.41	5	1
3:C:607:PCW:H371	4:C:631:17F:H6	0.46	1.87	7	1
3:B:212:PCW:H152	3:B:212:PCW:H341	0.46	1.88	10	2
3:A:405:PCW:H83	3:B:222:PCW:H11	0.46	1.87	1	1
3:A:410:PCW:H382	4:C:633:17F:H36	0.46	1.87	1	1
3:C:613:PCW:H382	3:C:613:PCW:H171	0.46	1.88	2	1
4:B:226:17F:H10	4:B:230:17F:H10A	0.46	1.86	3	1
1:C:530:ALA:O	1:C:534:GLU:HG3	0.46	2.11	3	2
3:C:619:PCW:H271	3:C:621:PCW:H242	0.46	1.88	4	1
1:A:308:ARG:HD3	1:C:469:LEU:CD1	0.46	2.38	6	1
4:B:234:17F:H66	4:C:631:17F:H63	0.46	1.88	6	1
3:B:221:PCW:H52	3:B:221:PCW:H12	0.46	1.87	3	1
2:B:41:ARG:HD3	2:B:54:ASP:OD2	0.46	2.11	4	2
3:A:410:PCW:H121	4:C:633:17F:H11A	0.46	1.86	7	1
2:B:5:LYS:HE3	3:B:219:PCW:H72	0.46	1.87	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:499:LEU:O	1:C:503:MET:HB2	0.46	2.11	9	1
3:C:623:PCW:H131	4:C:635:17F:H18A	0.46	1.88	10	1
3:A:406:PCW:H172	4:B:226:17F:H59	0.46	1.87	1	1
3:C:626:PCW:H31	3:C:627:PCW:H161	0.46	1.87	1	3
3:B:203:PCW:H162	3:B:207:PCW:H351	0.46	1.87	4	1
3:C:611:PCW:H482	4:C:635:17F:H45	0.46	1.88	4	1
3:B:213:PCW:H421	3:B:216:PCW:H272	0.46	1.87	5	1
4:B:234:17F:H73	4:B:234:17F:H43	0.46	1.87	6	1
3:A:408:PCW:H431	3:C:604:PCW:H281	0.46	1.86	7	1
3:C:628:PCW:H83	3:C:628:PCW:O11	0.46	2.11	8	2
3:B:213:PCW:H242	3:C:611:PCW:H422	0.45	1.88	1	1
3:C:611:PCW:H172	3:C:617:PCW:H331	0.45	1.88	2	1
3:B:231:PCW:H382	3:C:604:PCW:H432	0.45	1.87	3	1
3:B:219:PCW:H222	4:B:224:17F:H42	0.45	1.87	4	1
3:B:206:PCW:H461	3:B:208:PCW:H271	0.45	1.87	5	1
4:B:226:17F:H43	4:B:230:17F:H42	0.45	1.87	6	1
3:B:210:PCW:H121	4:B:224:17F:H32	0.45	1.87	9	2
2:B:131:GLN:HG2	2:B:141:PHE:CD2	0.45	2.45	8	1
3:C:602:PCW:H283	4:C:630:17F:H52	0.45	1.88	8	1
3:C:616:PCW:H482	3:C:616:PCW:H222	0.45	1.87	8	1
1:A:387:LEU:O	1:A:391:GLU:HG3	0.45	2.09	10	2
3:A:408:PCW:C33	3:A:410:PCW:H341	0.45	2.41	9	1
3:B:203:PCW:H271	4:C:634:17F:H55	0.45	1.87	2	1
1:A:363:LYS:HG2	1:C:411:THR:HG22	0.45	1.88	3	1
1:C:460:GLN:O	1:C:464:GLN:HG3	0.45	2.11	3	1
3:C:605:PCW:O1P	3:C:605:PCW:H31	0.45	2.11	6	1
3:B:203:PCW:P	7:B:237:EWS:CAK	0.45	3.04	8	1
3:B:210:PCW:H242	3:B:210:PCW:H422	0.45	1.88	8	1
3:C:611:PCW:H282	3:C:617:PCW:H452	0.45	1.87	9	2
4:B:227:17F:H30	4:B:227:17F:H39	0.45	1.89	9	1
3:B:211:PCW:H221	3:B:217:PCW:H412	0.45	1.87	10	1
1:A:268:GLU:OE1	1:C:506:ARG:HD3	0.45	2.12	3	1
3:B:205:PCW:H221	3:B:233:PCW:H283	0.45	1.87	4	1
1:C:561:LYS:O	1:C:565:ALA:HB3	0.45	2.11	5	1
3:A:406:PCW:H331	3:B:208:PCW:H352	0.45	1.87	7	1
3:B:209:PCW:H131	4:B:227:17F:H10A	0.45	1.89	9	1
1:C:488:LYS:CD	3:C:623:PCW:H272	0.45	2.29	9	1
1:A:335:LEU:O	1:A:339:LYS:HB2	0.45	2.12	10	1
2:B:71:TYR:HB2	7:B:237:EWS:OAB	0.45	2.11	6	2
1:A:264:LYS:CE	1:C:509:ALA:HB1	0.45	2.41	4	1
4:A:411:17F:H32	4:A:411:17F:H8A	0.45	1.87	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:204:PCW:H251	3:C:618:PCW:H483	0.45	1.87	6	1
3:B:216:PCW:H451	4:C:634:17F:H74	0.45	1.87	6	1
3:A:407:PCW:H342	4:B:225:17F:H11A	0.45	1.88	7	1
3:B:201:PCW:H212	4:B:228:17F:H34	0.45	1.88	9	1
3:A:406:PCW:H372	3:B:208:PCW:H39	0.45	1.89	2	2
3:B:211:PCW:H171	4:B:229:17F:H59	0.45	1.87	1	1
3:C:611:PCW:H63	4:C:635:17F:HN1	0.45	1.71	2	1
1:A:345:ARG:O	1:A:349:TYR:HB2	0.45	2.12	4	1
3:A:410:PCW:H371	3:A:410:PCW:H412	0.45	1.87	4	1
3:B:209:PCW:H251	4:C:635:17F:H38	0.45	1.87	4	1
3:C:621:PCW:H361	3:C:629:PCW:H221	0.45	1.87	4	1
3:C:613:PCW:H171	3:C:613:PCW:H381	0.45	1.89	5	1
3:B:207:PCW:H442	3:C:621:PCW:H222	0.45	1.89	6	1
3:A:403:PCW:H332	3:B:204:PCW:C3	0.45	2.39	8	1
3:B:205:PCW:H172	3:B:220:PCW:H352	0.45	1.89	9	1
1:A:393:TYR:OH	3:A:403:PCW:C28	0.45	2.64	2	1
3:C:626:PCW:H19	3:C:627:PCW:H271	0.45	1.87	2	1
2:B:77:GLY:HA3	2:B:163:ILE:HD11	0.45	1.89	3	1
1:A:308:ARG:HG3	1:C:465:GLU:HB3	0.45	1.88	4	1
4:B:228:17F:H55	3:C:615:PCW:H483	0.45	1.89	5	1
3:C:615:PCW:H151	3:C:615:PCW:C38	0.45	2.41	5	1
3:A:408:PCW:H422	3:B:204:PCW:H461	0.45	1.87	7	1
4:B:224:17F:H51	4:B:230:17F:H74	0.45	1.87	7	1
3:C:619:PCW:H282	3:C:621:PCW:H252	0.45	1.88	7	1
1:C:550:LYS:O	1:C:554:HIS:HB2	0.45	2.12	1	1
3:C:607:PCW:H20	4:C:631:17F:H44	0.45	1.88	3	1
4:A:411:17F:H54	3:C:607:PCW:H241	0.45	1.88	4	1
4:B:229:17F:H50	3:B:231:PCW:H181	0.45	1.89	4	1
3:A:401:PCW:H41	3:B:212:PCW:H2	0.45	1.88	6	1
3:B:219:PCW:H482	4:B:223:17F:H49	0.45	1.89	6	2
3:B:201:PCW:H172	4:B:225:17F:H60	0.45	1.88	7	1
3:B:231:PCW:H441	3:C:604:PCW:H261	0.45	1.87	7	1
1:C:549:ALA:O	1:C:553:GLU:HG3	0.45	2.12	7	2
3:B:202:PCW:H271	4:B:228:17F:H66	0.45	1.89	10	1
2:B:118:CYS:SG	2:B:145:SER:HB2	0.45	2.52	4	2
3:C:609:PCW:H211	4:C:630:17F:H58	0.45	1.89	2	1
4:C:631:17F:H37	4:C:631:17F:H57	0.45	1.87	2	1
3:B:219:PCW:H283	3:C:625:PCW:H252	0.45	1.87	4	1
3:B:203:PCW:H483	3:B:220:PCW:H262	0.45	1.88	5	1
1:A:310:ARG:O	1:A:314:ASP:HB3	0.45	2.11	6	1
3:C:607:PCW:C24	4:C:631:17F:H39	0.45	2.41	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:201:PCW:H381	3:B:219:PCW:H441	0.45	1.88	7	1
3:B:219:PCW:H483	3:B:233:PCW:H241	0.45	1.89	10	1
3:C:611:PCW:H282	3:C:617:PCW:H422	0.45	1.88	10	1
3:A:410:PCW:H461	3:C:620:PCW:H283	0.45	1.88	2	1
3:B:201:PCW:H342	3:B:219:PCW:H361	0.45	1.88	2	1
3:B:202:PCW:H432	4:B:226:17F:H43	0.45	1.89	10	2
3:C:615:PCW:H132	3:C:622:PCW:C38	0.45	2.40	3	1
3:B:216:PCW:H73	4:B:224:17F:N1	0.45	2.24	6	1
1:A:202:LYS:HE3	1:C:576:VAL:HG21	0.45	1.89	7	1
3:A:406:PCW:H371	4:B:226:17F:H60	0.45	1.89	7	1
3:B:205:PCW:H272	3:B:233:PCW:H262	0.45	1.89	8	1
3:B:221:PCW:H341	3:B:221:PCW:H121	0.45	1.87	9	1
1:A:247:LEU:HA	1:A:250:VAL:HG12	0.45	1.87	10	1
3:B:205:PCW:H212	3:B:220:PCW:H412	0.45	1.88	10	1
3:B:203:PCW:H171	3:B:217:PCW:H132	0.45	1.89	2	1
3:C:621:PCW:O3	3:C:629:PCW:H171	0.45	2.12	3	1
4:C:630:17F:H35	4:C:630:17F:H42	0.45	1.89	4	2
3:B:215:PCW:H471	3:C:608:PCW:H482	0.45	1.89	5	1
4:A:411:17F:H63	3:B:216:PCW:H251	0.45	1.87	6	1
1:C:415:LEU:HA	1:C:418:GLN:NE2	0.45	2.27	6	1
3:A:401:PCW:H51	3:B:212:PCW:H2	0.45	1.88	8	1
3:B:201:PCW:H242	3:B:212:PCW:H422	0.45	1.88	8	1
3:A:401:PCW:H411	3:B:212:PCW:H472	0.44	1.89	1	1
3:B:202:PCW:H122	4:B:228:17F:C9	0.44	2.41	2	1
3:B:204:PCW:H482	3:B:231:PCW:H422	0.44	1.89	3	1
3:C:609:PCW:H483	4:C:630:17F:H55	0.44	1.89	3	1
4:A:411:17F:H61	4:C:635:17F:H72	0.44	1.89	5	1
2:B:56:LEU:HD12	7:B:237:EWS:CAQ	0.44	2.42	7	1
3:B:201:PCW:C22	4:B:225:17F:H65	0.44	2.37	8	1
3:B:203:PCW:O11	4:B:229:17F:H18A	0.44	2.11	8	1
1:A:376:LEU:O	1:A:380:GLU:HG3	0.44	2.12	9	1
1:C:585:LEU:O	1:C:589:GLU:HB2	0.44	2.12	10	1
1:A:268:GLU:O	1:A:272:TYR:HB2	0.44	2.13	2	1
2:B:68:ARG:HA	2:B:71:TYR:CZ	0.44	2.47	2	1
3:B:202:PCW:H52	3:B:202:PCW:O31	0.44	2.12	3	2
3:C:629:PCW:O31	3:C:629:PCW:H41	0.44	2.12	2	1
3:A:403:PCW:H251	3:A:407:PCW:H231	0.44	1.88	3	1
4:B:234:17F:H10A	4:B:234:17F:C1Z	0.44	2.42	4	1
3:B:205:PCW:H40	3:B:216:PCW:H372	0.44	1.88	5	1
4:B:226:17F:H49	3:C:613:PCW:H462	0.44	1.88	6	1
4:B:227:17F:O2	3:C:602:PCW:H81	0.44	2.13	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:405:PCW:H162	3:B:222:PCW:H372	0.44	1.88	7	1
3:B:201:PCW:H442	4:B:230:17F:H77	0.44	1.89	8	1
3:B:207:PCW:H341	3:B:232:PCW:H282	0.44	1.89	9	1
3:B:203:PCW:H341	3:B:220:PCW:H132	0.44	1.88	10	1
4:B:223:17F:H50	3:C:626:PCW:H232	0.44	1.90	10	1
3:C:603:PCW:H471	3:C:625:PCW:H452	0.44	1.88	10	1
3:A:409:PCW:H432	3:C:605:PCW:H20	0.44	1.89	3	1
3:B:212:PCW:H20	3:B:212:PCW:H421	0.44	1.88	3	1
3:A:407:PCW:H442	3:C:606:PCW:H271	0.44	1.89	8	1
3:C:607:PCW:H321	3:C:609:PCW:C8	0.44	2.43	8	1
1:A:249:GLU:O	1:A:253:LYS:HB2	0.44	2.12	9	1
3:A:407:PCW:H442	4:B:223:17F:H71	0.44	1.89	1	1
3:B:201:PCW:H483	3:C:605:PCW:H222	0.44	1.88	2	1
3:B:220:PCW:H272	3:B:233:PCW:H212	0.44	1.89	2	1
1:A:359:THR:O	1:A:363:LYS:HG3	0.44	2.12	6	2
3:C:607:PCW:H451	3:C:611:PCW:H321	0.44	1.88	4	1
3:B:209:PCW:H31	4:B:227:17F:H10A	0.44	1.88	5	1
1:A:292:HIS:O	1:A:296:GLU:HG2	0.44	2.13	6	1
3:B:203:PCW:H442	3:B:231:PCW:H451	0.44	1.89	6	1
3:B:203:PCW:H41	4:B:229:17F:O1	0.44	2.13	2	1
3:C:611:PCW:H262	3:C:617:PCW:H441	0.44	1.87	3	1
3:C:606:PCW:H283	3:C:615:PCW:H182	0.44	1.90	5	1
3:C:613:PCW:H151	3:C:626:PCW:H432	0.44	1.89	10	1
3:C:602:PCW:H452	4:C:630:17F:H40	0.44	1.89	1	1
3:C:614:PCW:H83	3:C:629:PCW:H32	0.44	1.88	2	1
1:A:242:GLU:OE1	1:C:528:ARG:HB3	0.44	2.12	3	1
3:B:218:PCW:H442	3:B:222:PCW:H441	0.44	1.90	8	2
3:B:203:PCW:H381	3:B:204:PCW:H142	0.44	1.88	4	1
2:B:62:GLU:HB3	2:B:68:ARG:NH1	0.44	2.28	5	1
3:B:201:PCW:H82	3:B:219:PCW:C1	0.44	2.43	5	1
3:B:207:PCW:H472	4:B:229:17F:H51	0.44	1.88	6	1
3:B:201:PCW:H39	3:C:626:PCW:H242	0.44	1.88	7	1
3:B:212:PCW:H422	3:C:613:PCW:H482	0.44	1.90	7	1
3:A:401:PCW:H471	3:C:613:PCW:H232	0.44	1.90	8	1
3:B:203:PCW:H483	3:B:231:PCW:H432	0.44	1.89	10	1
3:B:209:PCW:H161	3:B:213:PCW:H361	0.44	1.90	1	1
3:B:201:PCW:H422	3:B:219:PCW:H472	0.44	1.88	2	1
4:B:229:17F:H43	3:C:621:PCW:H252	0.44	1.89	6	1
3:B:203:PCW:H481	3:B:233:PCW:C48	0.44	2.43	7	1
1:A:202:LYS:O	1:A:206:ASN:HB2	0.44	2.13	8	1
3:C:607:PCW:H241	3:C:611:PCW:H283	0.44	1.88	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:209:PCW:H182	3:C:611:PCW:H471	0.44	1.89	1	1
3:B:213:PCW:H20	3:C:611:PCW:H441	0.44	1.90	2	1
3:C:613:PCW:H171	3:C:613:PCW:C38	0.44	2.43	5	2
1:C:448:VAL:O	1:C:452:VAL:HB	0.44	2.12	3	1
3:A:409:PCW:H371	3:C:627:PCW:C34	0.44	2.42	5	1
3:B:205:PCW:H272	3:B:219:PCW:H482	0.44	1.88	5	1
4:B:234:17F:H64	4:B:234:17F:C23	0.44	2.42	5	1
3:C:608:PCW:C3	3:C:628:PCW:H331	0.44	2.41	6	1
3:B:205:PCW:H252	3:B:220:PCW:H421	0.44	1.87	7	1
3:C:626:PCW:H161	3:C:627:PCW:H252	0.44	1.89	7	1
4:B:234:17F:C1Y	3:C:625:PCW:H172	0.44	2.43	9	1
3:B:219:PCW:H261	3:C:625:PCW:H282	0.44	1.90	1	1
3:C:618:PCW:H121	3:C:620:PCW:H412	0.44	1.89	2	2
4:B:223:17F:HN1	4:B:223:17F:P1	0.44	2.36	4	1
3:B:202:PCW:H452	3:B:212:PCW:H162	0.44	1.88	5	1
1:C:533:LEU:O	1:C:537:LYS:HG3	0.44	2.13	5	1
3:A:401:PCW:H472	3:C:626:PCW:H483	0.44	1.89	7	1
3:A:407:PCW:H63	4:B:228:17F:N1	0.44	2.27	7	1
3:B:205:PCW:H181	3:B:219:PCW:H122	0.44	1.89	7	1
3:B:208:PCW:H452	4:B:226:17F:H61	0.44	1.88	8	1
3:C:609:PCW:H83	3:C:611:PCW:H142	0.44	1.89	10	1
1:A:271:LEU:O	1:A:275:LYS:HG2	0.43	2.13	1	2
3:A:410:PCW:H352	4:C:633:17F:C2X	0.43	2.40	5	2
3:A:406:PCW:H152	3:A:406:PCW:H362	0.43	1.87	3	1
3:C:618:PCW:H122	3:C:620:PCW:C38	0.43	2.43	6	2
2:B:72:MET:HB3	2:B:103:VAL:HG21	0.43	1.91	5	1
3:B:207:PCW:H182	3:B:232:PCW:C28	0.43	2.41	5	1
1:C:517:HIS:O	1:C:521:TYR:HB2	0.43	2.13	5	2
3:A:408:PCW:H151	3:C:604:PCW:H221	0.43	1.91	6	1
3:B:210:PCW:H482	4:B:227:17F:H41	0.43	1.89	8	1
3:B:212:PCW:H362	3:B:212:PCW:H171	0.43	1.90	10	2
2:B:53:LEU:HD12	2:B:55:ILE:HD11	0.43	1.90	10	1
3:B:209:PCW:H20	3:C:611:PCW:H471	0.43	1.90	10	1
3:C:613:PCW:H62	3:C:627:PCW:C7	0.43	2.43	1	1
1:C:491:GLU:HB3	1:C:495:LYS:HZ2	0.43	1.73	2	1
1:C:563:LYS:CB	1:C:564:PRO:HD3	0.43	2.39	9	2
1:A:337:ALA:O	1:A:341:ASN:HB2	0.43	2.12	3	1
3:C:613:PCW:H332	3:C:626:PCW:H411	0.43	1.90	3	1
2:B:8:VAL:HG12	2:B:16:LYS:HD2	0.43	1.88	6	1
3:C:602:PCW:H231	4:C:630:17F:H49	0.43	1.89	6	1
3:B:209:PCW:H151	3:B:213:PCW:H171	0.43	1.90	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:201:PCW:H251	3:C:613:PCW:H482	0.43	1.89	1	1
3:C:611:PCW:H63	4:C:635:17F:N1	0.43	2.28	2	1
3:A:406:PCW:H11	4:B:226:17F:O1	0.43	2.13	3	1
3:A:402:PCW:H331	3:A:402:PCW:H83	0.43	1.90	4	1
3:B:212:PCW:O11	4:B:226:17F:H6	0.43	2.14	4	1
1:C:550:LYS:HA	1:C:553:GLU:OE1	0.43	2.13	4	1
1:C:412:PHE:HA	1:C:415:LEU:HD12	0.43	1.90	5	1
3:A:408:PCW:H341	3:B:231:PCW:C39	0.43	2.44	7	1
3:B:202:PCW:H451	4:B:230:17F:H10A	0.43	1.90	7	1
3:B:219:PCW:H11	3:B:220:PCW:O1P	0.43	2.14	8	1
2:B:114:VAL:HG12	2:B:142:ILE:HB	0.43	1.91	9	1
3:A:406:PCW:H211	3:A:409:PCW:H282	0.43	1.91	10	1
4:B:228:17F:C4	4:B:228:17F:C1	0.43	2.90	10	1
3:B:208:PCW:H152	3:B:215:PCW:H372	0.43	1.90	1	1
2:B:54:ASP:OD1	3:B:208:PCW:H73	0.43	2.12	2	1
3:B:205:PCW:H422	4:B:224:17F:H70	0.43	1.91	2	1
1:A:280:ARG:O	1:A:284:GLN:HB2	0.43	2.13	3	1
3:B:233:PCW:H351	3:C:626:PCW:C12	0.43	2.42	5	1
3:B:205:PCW:H251	3:B:220:PCW:H171	0.43	1.91	6	2
3:A:403:PCW:H142	3:A:403:PCW:H382	0.43	1.89	7	1
3:B:212:PCW:C42	3:C:613:PCW:H482	0.43	2.43	7	1
3:B:210:PCW:H481	3:C:617:PCW:H461	0.43	1.88	9	1
3:B:211:PCW:C34	4:B:229:17F:H11	0.43	2.44	9	1
3:B:231:PCW:H441	3:C:604:PCW:H452	0.43	1.89	9	1
3:B:210:PCW:H73	7:B:237:EWS:CAN	0.43	2.43	10	1
3:C:606:PCW:H282	3:C:615:PCW:H211	0.43	1.90	10	1
3:B:202:PCW:H141	4:B:228:17F:H9A	0.43	1.89	4	1
3:C:606:PCW:H283	3:C:615:PCW:H181	0.43	1.89	4	1
1:A:393:TYR:HD1	1:A:396:LYS:NZ	0.43	2.03	5	1
3:C:619:PCW:H362	3:C:621:PCW:H142	0.43	1.90	5	1
1:A:229:TRP:O	1:A:233:GLU:HG3	0.43	2.13	6	1
3:B:213:PCW:H39	3:B:214:PCW:H221	0.43	1.90	7	1
3:C:618:PCW:H211	3:C:620:PCW:H471	0.43	1.90	7	1
3:B:215:PCW:H252	3:C:609:PCW:H432	0.43	1.90	8	1
1:C:473:LYS:O	1:C:477:LEU:HB2	0.43	2.12	8	1
3:C:601:PCW:H362	3:C:602:PCW:H121	0.43	1.89	8	1
4:B:225:17F:H44	3:C:615:PCW:H20	0.43	1.90	1	1
3:A:403:PCW:O3P	3:B:204:PCW:H12	0.43	2.12	2	1
4:B:224:17F:H42	4:B:230:17F:H66	0.43	1.91	3	1
1:C:577:LEU:O	1:C:581:LYS:HB2	0.43	2.14	3	1
3:B:232:PCW:H481	4:B:234:17F:H41	0.43	1.90	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:607:PCW:H262	4:C:631:17F:C23	0.43	2.43	5	1
3:C:622:PCW:H142	3:C:622:PCW:H361	0.43	1.90	6	1
3:B:231:PCW:H471	3:C:604:PCW:H283	0.43	1.91	8	1
1:C:587:ALA:O	1:C:591:TYR:HB2	0.43	2.14	8	1
3:A:405:PCW:H481	3:C:629:PCW:H481	0.43	1.89	9	1
3:B:205:PCW:H162	3:B:219:PCW:H122	0.43	1.91	9	1
3:B:211:PCW:H151	4:B:229:17F:H8	0.43	1.91	9	1
1:A:273:ARG:HA	1:A:276:VAL:HG12	0.43	1.91	10	1
4:A:411:17F:H31	4:A:411:17F:H8A	0.43	1.90	10	1
3:B:207:PCW:C16	3:B:232:PCW:H281	0.43	2.41	10	1
4:B:234:17F:H34	3:C:625:PCW:H162	0.43	1.90	10	1
3:A:408:PCW:H351	3:A:410:PCW:C35	0.43	2.43	1	1
1:A:301:LEU:HD13	1:C:473:LYS:HG3	0.43	1.91	3	1
3:B:213:PCW:H212	4:B:227:17F:H42	0.43	1.90	3	1
3:B:201:PCW:H51	3:B:220:PCW:O2P	0.43	2.13	4	1
2:B:171:SER:HA	3:B:218:PCW:H82	0.43	1.90	5	1
3:C:624:PCW:H341	4:C:635:17F:H76	0.43	1.91	5	1
3:B:207:PCW:H282	3:B:218:PCW:H212	0.43	1.90	6	1
3:B:207:PCW:H212	4:C:631:17F:H78	0.43	1.90	8	1
3:B:215:PCW:H241	3:C:609:PCW:H472	0.43	1.89	10	1
4:B:234:17F:O8	3:C:605:PCW:H342	0.43	2.12	10	1
1:A:266:GLN:O	1:A:270:GLU:HG3	0.43	2.13	1	1
1:A:393:TYR:CZ	3:A:403:PCW:H281	0.43	2.48	2	1
3:B:213:PCW:H482	3:C:611:PCW:H483	0.43	1.91	2	1
3:A:406:PCW:H162	3:A:409:PCW:H252	0.43	1.89	4	1
3:B:208:PCW:C32	7:B:237:EWS:CAO	0.43	2.90	4	1
3:C:626:PCW:H421	3:C:627:PCW:H20	0.43	1.90	5	1
3:A:406:PCW:H12	4:B:226:17F:P1	0.43	2.53	10	2
3:C:617:PCW:H221	4:C:635:17F:H36	0.43	1.90	6	1
1:C:522:SER:O	1:C:526:ARG:HG3	0.43	2.13	7	1
1:C:561:LYS:HA	1:C:561:LYS:HE3	0.43	1.90	7	1
3:B:211:PCW:H132	4:B:229:17F:C6	0.43	2.42	9	1
3:C:602:PCW:H211	4:C:630:17F:H49	0.43	1.91	9	1
4:B:229:17F:H20A	4:B:229:17F:H8	0.43	1.90	10	1
3:A:406:PCW:H52	3:B:206:PCW:O2P	0.43	2.14	2	1
3:B:211:PCW:H482	3:C:621:PCW:H451	0.43	1.91	2	1
3:B:219:PCW:H241	3:B:233:PCW:H262	0.43	1.91	2	1
3:C:601:PCW:H372	3:C:602:PCW:H141	0.43	1.91	3	1
3:A:408:PCW:H172	3:A:408:PCW:H382	0.43	1.91	4	1
2:B:68:ARG:HA	2:B:71:TYR:CE1	0.43	2.48	4	1
3:B:212:PCW:H121	4:B:226:17F:O9	0.43	2.14	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:210:PCW:H352	4:B:224:17F:C19	0.43	2.40	6	1
3:C:606:PCW:H2	3:C:606:PCW:O1P	0.43	2.14	6	1
2:B:20:THR:O	2:B:24:ILE:HG12	0.43	2.13	8	1
3:B:205:PCW:H251	3:B:220:PCW:H431	0.43	1.91	8	1
3:A:408:PCW:H332	3:A:410:PCW:C34	0.43	2.43	4	1
2:B:171:SER:HA	3:B:218:PCW:H63	0.43	1.90	5	1
3:B:221:PCW:H83	4:B:224:17F:H6	0.43	1.91	5	1
3:B:220:PCW:H232	3:C:604:PCW:H483	0.43	1.91	7	1
1:A:248:GLU:O	1:A:252:ALA:HB3	0.43	2.14	8	1
3:A:406:PCW:H182	3:A:409:PCW:H232	0.43	1.90	9	1
3:B:219:PCW:H322	4:B:226:17F:H37	0.43	1.91	9	1
1:A:362:GLU:HB3	1:C:414:LYS:HD3	0.42	1.90	4	1
3:B:203:PCW:H462	3:B:205:PCW:H282	0.42	1.91	6	1
3:B:207:PCW:H341	3:B:220:PCW:H39	0.42	1.91	7	1
1:C:498:PRO:O	1:C:502:GLU:HB2	0.42	2.14	9	1
4:A:411:17F:H8A	4:A:411:17F:C1Y	0.42	2.44	10	1
2:B:112:VAL:HG23	2:B:159:LEU:HD13	0.42	1.90	3	1
1:C:508:ARG:O	1:C:512:ASP:HB3	0.42	2.14	3	1
3:A:404:PCW:H222	3:C:610:PCW:H261	0.42	1.91	4	1
4:B:234:17F:H65	4:C:631:17F:H77	0.42	1.92	4	1
1:C:422:VAL:O	1:C:426:PHE:HB2	0.42	2.14	4	1
3:A:406:PCW:H172	4:B:226:17F:H58	0.42	1.90	5	1
3:B:219:PCW:H222	4:B:230:17F:H73	0.42	1.90	5	1
3:B:211:PCW:H282	3:C:619:PCW:H251	0.42	1.90	6	1
3:A:402:PCW:C35	3:B:213:PCW:H322	0.42	2.44	7	1
1:C:578:GLU:O	1:C:582:VAL:HG23	0.42	2.14	7	1
3:B:219:PCW:H411	3:B:220:PCW:H172	0.42	1.92	9	1
2:B:74:THR:HB	3:B:201:PCW:H71	0.42	1.90	1	1
2:B:81:VAL:HA	2:B:114:VAL:HB	0.42	1.91	1	1
4:B:224:17F:H46	4:B:230:17F:H70	0.42	1.90	1	1
3:B:203:PCW:H121	3:B:207:PCW:H322	0.42	1.91	3	1
3:B:217:PCW:H262	3:C:619:PCW:H472	0.42	1.91	3	1
1:C:576:VAL:O	1:C:580:PHE:HB2	0.42	2.14	3	1
3:B:209:PCW:H152	3:B:216:PCW:H142	0.42	1.91	4	1
3:C:607:PCW:H331	3:C:611:PCW:H131	0.42	1.91	4	1
3:B:202:PCW:H242	3:B:202:PCW:H211	0.42	1.67	5	1
4:B:234:17F:H57	3:C:625:PCW:H161	0.42	1.91	5	1
3:B:210:PCW:C33	4:B:224:17F:H5	0.42	2.42	7	1
1:C:464:GLN:O	1:C:468:GLU:HB2	0.42	2.13	7	1
3:C:613:PCW:H331	3:C:613:PCW:H152	0.42	1.91	8	1
3:B:208:PCW:H2	3:B:208:PCW:O2P	0.42	2.14	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:210:PCW:H42	7:B:237:EWS:CAJ	0.42	2.44	10	1
3:C:601:PCW:H422	4:C:630:17F:C30	0.42	2.44	10	1
3:C:607:PCW:H411	4:C:631:17F:H9A	0.42	1.90	5	2
3:B:214:PCW:H421	4:C:634:17F:H76	0.42	1.91	2	1
3:B:219:PCW:H232	3:C:605:PCW:H271	0.42	1.90	2	1
3:B:219:PCW:H252	3:C:605:PCW:H271	0.42	1.90	4	1
3:B:221:PCW:H2	4:B:230:17F:H19	0.42	1.91	4	1
3:C:603:PCW:H451	3:C:625:PCW:H472	0.42	1.92	4	1
3:C:626:PCW:H40	3:C:627:PCW:H241	0.42	1.92	5	1
3:C:610:PCW:H411	3:C:614:PCW:H181	0.42	1.90	6	1
3:B:203:PCW:H321	3:B:211:PCW:H341	0.42	1.91	7	1
3:B:220:PCW:H251	3:C:604:PCW:H461	0.42	1.90	8	1
3:B:209:PCW:H272	3:C:611:PCW:H483	0.42	1.91	9	1
4:B:225:17F:H76	3:C:606:PCW:H483	0.42	1.91	9	1
3:A:406:PCW:H2	4:B:226:17F:O1	0.42	2.15	1	1
4:B:234:17F:H72	4:C:631:17F:H72	0.42	1.89	1	2
4:B:225:17F:H63	3:C:626:PCW:C26	0.42	2.39	2	1
3:B:233:PCW:H61	3:C:604:PCW:H332	0.42	1.90	4	1
3:C:619:PCW:H342	3:C:621:PCW:H141	0.42	1.91	4	1
3:B:216:PCW:C24	4:C:635:17F:H65	0.42	2.45	5	1
1:C:413:SER:O	1:C:417:GLU:HG3	0.42	2.15	5	1
1:C:581:LYS:O	1:C:585:LEU:HG	0.42	2.14	9	2
2:B:7:VAL:HB	2:B:78:PHE:HD1	0.42	1.73	10	2
1:A:253:LYS:HE2	1:A:257:TYR:OH	0.42	2.15	9	1
1:A:224:VAL:HG22	1:C:550:LYS:HD3	0.42	1.90	10	1
3:B:202:PCW:C15	3:B:212:PCW:H412	0.42	2.44	2	1
3:A:403:PCW:H31	3:A:403:PCW:O1P	0.42	2.14	4	1
3:B:208:PCW:H161	3:B:215:PCW:H372	0.42	1.91	4	1
3:B:203:PCW:N	3:B:203:PCW:O2P	0.42	2.52	5	1
2:B:22:GLN:CG	2:B:149:ARG:HG3	0.42	2.44	6	1
3:B:205:PCW:H451	3:B:207:PCW:H283	0.42	1.90	6	1
3:A:410:PCW:H251	4:C:633:17F:C30	0.42	2.45	7	1
3:B:211:PCW:H172	4:B:229:17F:H33	0.42	1.92	7	1
1:A:393:TYR:HE1	3:A:407:PCW:C27	0.42	1.61	8	1
3:A:406:PCW:H151	3:A:409:PCW:H252	0.42	1.91	9	1
3:A:408:PCW:H441	3:B:204:PCW:H451	0.42	1.92	9	1
3:B:202:PCW:H321	3:B:212:PCW:H83	0.42	1.90	10	1
3:B:219:PCW:H262	4:C:631:17F:H54	0.42	1.90	1	1
1:A:357:LEU:HA	1:A:360:LEU:HB2	0.42	1.91	3	1
1:C:455:TYR:CE2	3:C:601:PCW:C23	0.42	3.00	3	1
1:A:348:GLU:O	1:A:352:LYS:HG3	0.42	2.13	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:601:PCW:H441	3:C:602:PCW:H211	0.42	1.92	4	1
4:B:223:17F:H50	3:C:626:PCW:H231	0.42	1.91	5	1
3:B:232:PCW:H412	3:C:619:PCW:H441	0.42	1.90	7	1
3:B:220:PCW:H422	3:B:232:PCW:H251	0.42	1.91	9	1
1:C:431:GLU:O	1:C:435:GLU:HG3	0.42	2.14	9	1
3:B:203:PCW:H481	4:B:223:17F:H48	0.42	1.91	3	1
3:B:231:PCW:H232	3:B:231:PCW:H483	0.42	1.90	4	1
3:B:231:PCW:H461	3:C:604:PCW:C46	0.42	2.45	4	1
1:A:312:HIS:HA	1:C:462:LYS:HD3	0.42	1.91	6	1
4:B:234:17F:H33	3:C:625:PCW:C19	0.42	2.44	6	1
3:A:408:PCW:H441	3:B:204:PCW:H432	0.42	1.91	7	1
3:B:203:PCW:H412	3:B:204:PCW:H371	0.42	1.92	10	1
2:B:74:THR:CB	3:B:201:PCW:H71	0.42	2.45	1	1
3:B:208:PCW:C34	7:B:237:EWS:CLA	0.42	3.05	2	1
3:C:626:PCW:H40	3:C:627:PCW:H231	0.42	1.90	2	1
3:C:601:PCW:H262	3:C:602:PCW:H282	0.42	1.91	3	1
3:C:610:PCW:H121	3:C:614:PCW:H212	0.42	1.89	4	1
2:B:81:VAL:HG12	2:B:114:VAL:HB	0.42	1.91	5	1
1:A:307:ASP:O	1:A:310:ARG:HB2	0.42	2.14	10	1
3:A:402:PCW:H211	3:B:214:PCW:H232	0.42	1.91	1	1
3:B:205:PCW:H272	3:B:220:PCW:H261	0.42	1.90	1	1
1:C:502:GLU:O	1:C:506:ARG:HG3	0.42	2.15	10	3
3:B:202:PCW:H222	4:B:228:17F:H59	0.42	1.92	3	1
2:B:34:PRO:HA	5:B:235:GNP:O3G	0.42	2.15	7	2
3:B:201:PCW:H141	4:B:225:17F:H56	0.42	1.91	5	1
3:B:211:PCW:H20	3:B:217:PCW:H361	0.42	1.92	5	1
4:B:226:17F:H12	4:B:230:17F:H8	0.42	1.92	7	1
3:B:231:PCW:C12	3:C:604:PCW:H19	0.42	2.45	8	1
3:C:606:PCW:H211	3:C:615:PCW:H161	0.42	1.92	8	1
3:B:207:PCW:H442	3:C:619:PCW:H452	0.42	1.91	9	1
3:C:620:PCW:O11	3:C:620:PCW:H41	0.42	2.15	10	1
2:B:71:TYR:HA	7:B:237:EWS:CAD	0.41	2.42	1	1
3:B:203:PCW:C40	3:B:204:PCW:H151	0.41	2.45	2	1
3:B:231:PCW:H442	3:B:233:PCW:H483	0.41	1.92	2	1
3:C:616:PCW:H181	3:C:616:PCW:H411	0.41	1.92	2	1
3:B:232:PCW:H241	3:C:619:PCW:H482	0.41	1.92	3	1
3:B:222:PCW:H19	3:C:603:PCW:H142	0.41	1.92	4	1
3:C:621:PCW:H122	3:C:629:PCW:C18	0.41	2.44	6	1
3:C:618:PCW:H182	3:C:620:PCW:H451	0.41	1.92	7	1
1:A:376:LEU:CB	1:A:377:PRO:HD3	0.41	2.44	9	1
3:C:606:PCW:H471	3:C:615:PCW:H182	0.41	1.91	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:202:PCW:H321	3:B:212:PCW:C8	0.41	2.45	10	1
3:B:232:PCW:H142	3:C:625:PCW:H181	0.41	1.92	10	1
3:B:208:PCW:H342	7:B:237:EWS:CLA	0.41	2.52	2	1
3:B:202:PCW:H72	4:B:228:17F:H9A	0.41	1.92	3	1
3:C:601:PCW:H152	3:C:601:PCW:H451	0.41	1.92	3	1
3:A:407:PCW:H121	4:B:223:17F:C31	0.41	2.45	4	1
3:C:617:PCW:H221	4:C:632:17F:H42	0.41	1.91	4	1
3:B:216:PCW:H171	4:B:224:17F:H61	0.41	1.92	6	1
1:A:308:ARG:HG3	1:C:469:LEU:CD1	0.41	2.41	7	1
2:B:32:TYR:HA	5:B:235:GNP:H5'1	0.41	1.91	7	1
3:B:203:PCW:H151	4:B:229:17F:H20	0.41	1.92	7	1
3:C:610:PCW:H372	3:C:614:PCW:H241	0.41	1.92	7	1
4:B:229:17F:H55	3:B:231:PCW:H162	0.41	1.90	8	1
3:A:401:PCW:H41	3:B:212:PCW:H11	0.41	1.93	10	1
4:B:229:17F:H51	3:B:231:PCW:H181	0.41	1.92	1	1
1:A:268:GLU:OE2	1:C:510:HIS:NE2	0.41	2.53	3	1
3:B:205:PCW:H262	3:B:220:PCW:H421	0.41	1.92	3	1
1:A:264:LYS:HE3	1:C:509:ALA:HB1	0.41	1.92	4	1
2:B:21:ILE:HG23	2:B:25:GLN:HE21	0.41	1.75	4	1
4:B:224:17F:H41	4:B:230:17F:H66	0.41	1.90	4	1
3:B:233:PCW:H351	3:C:626:PCW:H331	0.41	1.90	4	1
3:B:201:PCW:H282	3:C:613:PCW:H221	0.41	1.92	5	1
2:B:37:GLU:OE2	3:B:220:PCW:H83	0.41	2.15	6	1
3:B:218:PCW:H412	3:B:222:PCW:H421	0.41	1.91	7	1
3:C:610:PCW:H431	3:C:614:PCW:H181	0.41	1.91	7	1
4:B:223:17F:H35	4:B:225:17F:H19	0.41	1.90	8	1
1:A:334:ARG:HD3	1:C:440:GLU:OE1	0.41	2.15	10	1
3:B:209:PCW:H172	3:B:213:PCW:H151	0.41	1.93	10	1
3:A:402:PCW:H381	3:B:213:PCW:H351	0.41	1.91	1	1
3:B:211:PCW:H81	4:B:229:17F:O2	0.41	2.16	2	1
3:B:231:PCW:H461	3:C:604:PCW:H462	0.41	1.92	4	1
3:B:232:PCW:H31	3:C:604:PCW:H122	0.41	1.92	5	1
4:B:234:17F:C31	3:C:625:PCW:H141	0.41	2.42	5	1
1:C:521:TYR:HA	1:C:524:GLU:OE1	0.41	2.16	6	1
3:C:617:PCW:H171	4:C:635:17F:H12	0.41	1.90	6	1
3:B:219:PCW:O2	3:B:219:PCW:H352	0.41	2.16	8	1
3:C:611:PCW:C44	4:C:635:17F:H43	0.41	2.46	8	1
3:B:203:PCW:H161	3:B:207:PCW:H372	0.41	1.91	9	1
3:B:216:PCW:H221	3:C:611:PCW:H421	0.41	1.92	9	1
2:B:5:LYS:HD2	2:B:74:THR:O	0.41	2.16	10	1
3:B:207:PCW:H83	3:B:217:PCW:O2P	0.41	2.15	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:220:PCW:H452	3:B:233:PCW:H251	0.41	1.92	1	1
1:A:393:TYR:HE1	3:A:407:PCW:H272	0.41	1.69	2	1
2:B:86:ASN:OD1	2:B:88:LYS:HB3	0.41	2.15	2	1
3:B:208:PCW:H131	3:B:215:PCW:H122	0.41	1.92	2	1
3:A:401:PCW:H442	3:C:613:PCW:H251	0.41	1.92	3	1
3:B:217:PCW:H251	3:C:619:PCW:H442	0.41	1.92	3	1
3:B:233:PCW:C34	3:C:626:PCW:H331	0.41	2.45	3	1
3:A:406:PCW:H362	3:A:406:PCW:H122	0.41	1.92	4	1
1:A:330:ARG:NH2	1:C:447:GLU:HB2	0.41	2.27	5	1
4:B:234:17F:H9A	4:B:234:17F:C20	0.41	2.41	5	1
3:A:402:PCW:H142	3:B:214:PCW:H172	0.41	1.93	7	1
3:A:403:PCW:H282	3:A:407:PCW:H252	0.41	1.91	2	1
3:B:201:PCW:H232	3:C:613:PCW:H482	0.41	1.93	4	1
3:B:212:PCW:H422	3:C:613:PCW:H483	0.41	1.90	4	1
3:C:618:PCW:H122	3:C:620:PCW:H361	0.41	1.92	4	1
2:B:71:TYR:CD1	2:B:71:TYR:C	0.41	2.99	5	1
1:C:427:TRP:HA	1:C:427:TRP:HE3	0.41	1.74	6	1
3:B:203:PCW:H371	3:B:220:PCW:H181	0.41	1.92	9	1
3:C:608:PCW:H172	3:C:608:PCW:H142	0.41	1.71	10	1
3:B:217:PCW:H252	3:B:218:PCW:H282	0.41	1.92	1	1
1:A:375:LEU:O	1:A:379:LEU:HB2	0.41	2.16	2	1
1:A:341:ASN:O	1:A:345:ARG:HG3	0.41	2.16	3	1
3:A:408:PCW:C1	3:B:231:PCW:H321	0.41	2.44	3	1
1:C:521:TYR:CE2	3:C:603:PCW:H281	0.41	2.51	4	1
3:A:407:PCW:C13	4:B:223:17F:H33	0.41	2.44	6	1
3:B:201:PCW:H422	3:C:626:PCW:H231	0.41	1.91	6	1
3:B:204:PCW:H482	3:C:604:PCW:H282	0.41	1.93	7	1
4:B:224:17F:H46	4:B:230:17F:H71	0.41	1.93	7	1
1:C:469:LEU:O	1:C:473:LYS:HE2	0.41	2.16	8	1
2:B:117:LYS:HB3	2:B:120:LEU:HD12	0.41	1.92	9	1
2:B:3:GLU:HA	2:B:52:LEU:O	0.41	2.15	10	1
3:B:203:PCW:H421	3:B:204:PCW:H19	0.41	1.91	1	1
1:A:388:SER:O	1:A:392:GLU:HG2	0.41	2.16	2	1
3:B:210:PCW:H442	3:B:221:PCW:H381	0.41	1.93	2	1
1:C:574:LEU:HB2	1:C:575:PRO:CD	0.41	2.46	8	2
3:C:614:PCW:H261	3:C:614:PCW:H222	0.41	1.91	2	1
3:B:203:PCW:H182	3:B:211:PCW:H40	0.41	1.91	4	1
2:B:54:ASP:HB3	7:B:237:EWS:CAS	0.41	2.45	5	1
2:B:3:GLU:OE2	3:B:205:PCW:H71	0.41	2.16	6	1
3:B:209:PCW:H73	4:B:224:17F:O1	0.41	2.15	6	1
3:B:213:PCW:H212	4:B:227:17F:H40	0.41	1.92	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:574:LEU:HB2	1:C:575:PRO:HD3	0.41	1.93	7	2
3:B:214:PCW:H40	4:C:634:17F:H76	0.41	1.93	8	1
3:C:607:PCW:H482	3:C:611:PCW:H371	0.41	1.92	8	1
2:B:67:MET:SD	3:B:204:PCW:H63	0.41	2.56	9	1
3:B:233:PCW:H39	3:C:606:PCW:H372	0.41	1.92	9	1
3:A:406:PCW:H141	3:A:406:PCW:H171	0.41	1.81	1	1
3:B:208:PCW:H451	3:C:627:PCW:H483	0.41	1.93	1	1
3:B:219:PCW:H52	3:B:220:PCW:O1P	0.41	2.15	1	1
3:C:602:PCW:H482	3:C:609:PCW:H241	0.41	1.92	1	1
2:B:5:LYS:NZ	4:B:230:17F:H1	0.41	2.31	2	1
4:B:226:17F:H73	3:C:628:PCW:H451	0.41	1.93	2	1
4:B:234:17F:H48	4:B:234:17F:H76	0.41	1.93	2	1
3:C:607:PCW:O1P	3:C:609:PCW:H73	0.41	2.16	2	1
3:A:408:PCW:C34	3:B:231:PCW:H39	0.41	2.40	3	1
3:A:410:PCW:H132	4:C:633:17F:H8A	0.41	1.93	3	1
2:B:156:PHE:O	2:B:160:VAL:HG23	0.41	2.16	3	1
3:B:201:PCW:C41	3:B:219:PCW:H20	0.41	2.46	3	1
1:A:348:GLU:HB3	1:A:352:LYS:HE2	0.41	1.91	4	1
1:A:264:LYS:O	1:A:268:GLU:HG3	0.41	2.14	5	1
3:B:201:PCW:H152	4:B:225:17F:H8	0.41	1.92	5	1
4:B:234:17F:H59	4:B:234:17F:H65	0.41	1.93	5	1
2:B:99:GLN:O	2:B:103:VAL:HG13	0.41	2.16	6	1
3:C:615:PCW:H162	3:C:615:PCW:H422	0.41	1.93	6	1
1:A:228:PHE:O	1:A:232:LEU:HG	0.41	2.16	7	1
1:A:376:LEU:HB2	1:A:377:PRO:CD	0.41	2.46	7	1
3:C:607:PCW:C43	3:C:611:PCW:H11	0.41	2.46	7	1
3:C:613:PCW:H19	3:C:622:PCW:H432	0.41	1.91	7	1
1:A:281:ALA:O	1:A:285:GLU:HG2	0.41	2.16	8	1
3:B:202:PCW:C33	4:B:228:17F:H4A	0.41	2.40	8	1
2:B:17:SER:HA	2:B:20:THR:OG1	0.41	2.16	9	1
2:B:84:ILE:HG12	2:B:118:CYS:HA	0.41	1.91	9	1
3:C:611:PCW:H152	3:C:617:PCW:H342	0.41	1.92	9	1
3:B:203:PCW:O1P	3:B:211:PCW:H12	0.41	2.16	10	1
3:B:231:PCW:H382	3:C:604:PCW:H421	0.41	1.93	10	1
3:B:209:PCW:H441	4:B:227:17F:H72	0.41	1.92	1	1
3:C:625:PCW:H352	3:C:625:PCW:H322	0.41	1.72	3	1
2:B:7:VAL:HG22	2:B:56:LEU:HB3	0.41	1.92	5	1
3:B:217:PCW:H283	3:B:218:PCW:H251	0.41	1.93	5	1
1:A:254:VAL:HA	1:A:257:TYR:HB2	0.41	1.93	6	1
3:A:408:PCW:H322	3:B:231:PCW:H371	0.41	1.93	7	1
3:C:618:PCW:H122	3:C:620:PCW:H412	0.41	1.93	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:609:PCW:H451	4:C:630:17F:H53	0.41	1.92	8	1
3:A:406:PCW:H231	3:A:409:PCW:H262	0.41	1.93	9	1
2:B:34:PRO:HA	5:B:235:GNP:O1G	0.41	2.16	9	1
3:A:409:PCW:H171	3:C:616:PCW:H251	0.41	1.93	10	1
3:C:624:PCW:H211	4:C:634:17F:H31	0.41	1.91	10	1
3:B:202:PCW:H282	4:B:228:17F:H66	0.40	1.93	1	1
1:A:253:LYS:O	1:A:256:PRO:HD2	0.40	2.17	3	1
3:A:408:PCW:H322	3:B:231:PCW:C37	0.40	2.46	4	1
3:B:205:PCW:H51	3:B:210:PCW:H341	0.40	1.92	4	1
1:C:561:LYS:HA	1:C:565:ALA:CB	0.40	2.45	6	1
3:C:601:PCW:H351	3:C:602:PCW:H152	0.40	1.93	7	1
1:A:330:ARG:HH22	1:C:448:VAL:HG23	0.40	1.76	8	1
4:B:227:17F:H73	3:C:602:PCW:H371	0.40	1.92	8	1
3:A:408:PCW:H242	3:C:618:PCW:H461	0.40	1.92	9	1
3:B:202:PCW:H412	4:B:226:17F:H40	0.40	1.93	10	1
4:B:234:17F:H73	4:C:631:17F:H72	0.40	1.93	10	1
3:A:410:PCW:H331	4:C:633:17F:C21	0.40	2.33	1	1
3:B:217:PCW:H251	3:C:619:PCW:H441	0.40	1.92	2	1
3:B:218:PCW:H441	3:B:218:PCW:H241	0.40	1.93	2	1
3:A:407:PCW:H351	3:A:407:PCW:H322	0.40	1.48	4	1
2:B:158:THR:O	2:B:162:GLU:HG2	0.40	2.16	4	1
3:C:610:PCW:H361	3:C:614:PCW:H132	0.40	1.92	4	1
3:B:201:PCW:H283	3:C:613:PCW:H241	0.40	1.93	6	1
3:B:202:PCW:H241	4:B:228:17F:H62	0.40	1.92	7	1
3:A:403:PCW:C33	3:B:204:PCW:H31	0.40	2.43	8	1
3:C:601:PCW:H452	3:C:602:PCW:H262	0.40	1.93	8	1
3:B:231:PCW:H261	3:B:231:PCW:H482	0.40	1.94	9	1
3:C:613:PCW:H62	3:C:627:PCW:H71	0.40	1.92	1	1
1:A:260:ASP:O	1:A:264:LYS:HD3	0.40	2.16	2	1
3:A:406:PCW:H421	4:B:226:17F:H71	0.40	1.94	2	1
4:B:234:17F:H35	3:C:625:PCW:H282	0.40	1.92	2	1
3:C:611:PCW:H172	3:C:617:PCW:C33	0.40	2.46	2	1
2:B:9:VAL:HG21	2:B:100:ILE:HD11	0.40	1.93	3	1
3:C:601:PCW:H411	3:C:602:PCW:H181	0.40	1.93	3	1
4:B:224:17F:H44	4:B:234:17F:H47	0.40	1.93	4	1
3:B:220:PCW:H483	4:B:234:17F:H38	0.40	1.93	6	1
3:A:402:PCW:H39	3:B:213:PCW:H372	0.40	1.92	7	1
4:B:230:17F:H19	4:B:230:17F:H33	0.40	1.71	7	1
1:A:279:LEU:HD22	1:C:495:LYS:HE3	0.40	1.93	10	1
3:B:203:PCW:H222	3:B:211:PCW:H441	0.40	1.92	2	1
3:B:201:PCW:H382	4:B:226:17F:H42	0.40	1.92	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:402:PCW:H362	3:B:214:PCW:C16	0.40	2.46	4	1
1:C:428:ASP:O	1:C:431:GLU:HB2	0.40	2.17	4	1
3:C:602:PCW:H271	4:C:630:17F:H47	0.40	1.93	4	1
1:A:380:GLU:O	1:A:384:VAL:HG23	0.40	2.16	5	1
3:B:201:PCW:H251	4:B:228:17F:C36	0.40	2.38	5	1
3:B:221:PCW:C3	4:B:230:17F:H4A	0.40	2.46	5	1
3:B:232:PCW:H452	3:C:619:PCW:H481	0.40	1.92	6	1
3:C:626:PCW:H371	3:C:627:PCW:H182	0.40	1.93	6	1
2:B:7:VAL:CG2	2:B:75:GLY:HA3	0.40	2.46	7	1
2:B:22:GLN:NE2	2:B:28:PHE:HB2	0.40	2.30	7	1
1:C:535:ALA:O	1:C:539:ASN:HB2	0.40	2.16	7	1
1:A:338:LEU:O	1:A:342:GLY:HA3	0.40	2.15	8	1
1:A:233:GLU:O	1:A:237:GLU:HB2	0.40	2.15	10	1
3:B:209:PCW:H332	3:B:213:PCW:H122	0.40	1.93	1	1
3:A:402:PCW:H342	3:B:213:PCW:H322	0.40	1.93	2	1
3:B:218:PCW:H483	3:C:624:PCW:H283	0.40	1.92	2	1
3:B:217:PCW:H232	3:B:218:PCW:H241	0.40	1.93	3	1
3:B:221:PCW:H71	4:B:227:17F:O5	0.40	2.16	3	1
3:B:233:PCW:H231	3:C:625:PCW:H251	0.40	1.94	5	1
1:A:332:ALA:O	1:A:336:GLU:HG3	0.40	2.16	6	1
3:B:203:PCW:H262	3:B:217:PCW:H442	0.40	1.94	6	1
3:B:207:PCW:H272	3:B:218:PCW:H252	0.40	1.92	6	1
3:B:218:PCW:H272	3:C:629:PCW:H262	0.40	1.92	6	1
2:B:15:GLY:O	2:B:19:LEU:HG	0.40	2.15	7	1
3:B:202:PCW:H332	4:B:228:17F:O1	0.40	2.17	7	1
3:B:212:PCW:H152	3:B:212:PCW:H182	0.40	1.71	7	1
1:C:463:TRP:O	1:C:467:MET:HB2	0.40	2.17	9	1
3:B:211:PCW:H241	3:B:217:PCW:H432	0.40	1.92	10	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	195/200 (98%)	190±2 (98±1%)	4±1 (2±1%)	1±1 (0±0%)	26	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	195/200 (98%)	191±2 (98±1%)	4±2 (2±1%)	0±0 (0±0%)	37	78
2	B	171/187 (91%)	162±3 (95±2%)	8±3 (5±2%)	0±0 (0±0%)	49	83
All	All	5610/5870 (96%)	5439 (97%)	155 (3%)	16 (0%)	37	78

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	365	LYS	8
1	C	563	LYS	5
2	B	73	ARG	2
1	A	366	PRO	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/175 (98%)	154±3 (90±2%)	18±3 (10±2%)	9	53
1	C	172/175 (98%)	155±3 (90±1%)	17±3 (10±1%)	10	55
2	B	152/166 (92%)	137±4 (90±2%)	15±4 (10±2%)	10	54
All	All	4960/5160 (96%)	4464 (90%)	496 (10%)	9	54

All 198 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	235	GLU	10
1	A	254	VAL	10
1	C	516	THR	9
2	B	20	THR	9
1	C	550	LYS	9
1	A	220	GLN	8
1	A	272	TYR	8
1	A	312	HIS	7
1	C	480	GLU	7

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Mol	Chain	Res	Type	Models (Total)
2	B	92	ASP	7
1	A	293	GLU	6
2	B	69	ASP	6
2	B	124	THR	6
1	C	448	VAL	6
1	C	459	PHE	6
2	B	2	THR	6
1	A	246	ASP	5
2	B	56	LEU	5
1	A	370	ASP	5
1	A	394	THR	5
2	B	16	LYS	5
1	C	548	HIS	5
1	A	299	SER	5
1	C	568	ASP	5
1	A	213	THR	4
1	A	289	GLN	4
1	A	318	THR	4
2	B	7	VAL	4
2	B	17	SER	4
2	B	35	THR	4
2	B	39	SER	4
2	B	51	CYS	4
2	B	71	TYR	4
2	B	127	THR	4
2	B	148	THR	4
1	C	490	HIS	4
1	C	561	LYS	4
1	A	228	PHE	4
1	A	396	LYS	4
1	C	405	TRP	4
1	C	487	GLN	4
2	B	74	THR	4
2	B	122	SER	4
2	B	170	MET	4
1	A	325	ASP	4
1	A	381	SER	3
2	B	153	ASP	3
2	B	154	ASP	3
1	C	412	PHE	3
1	C	413	SER	3
1	C	444	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	C	447	GLU	3
1	C	552	THR	3
1	A	215	SER	3
1	A	253	LYS	3
1	A	292	HIS	3
1	A	319	HIS	3
2	B	29	VAL	3
1	C	409	THR	3
1	A	212	SER	3
1	A	356	HIS	3
1	A	361	SER	3
1	C	407	SER	3
1	C	505	ASP	3
1	C	592	THR	3
1	A	229	TRP	3
2	B	58	THR	3
2	B	87	THR	3
2	B	107	GLU	3
1	C	463	TRP	3
1	C	583	SER	3
1	A	205	ASP	2
1	A	207	TRP	2
1	A	296	GLU	2
2	B	26	ASN	2
2	B	126	ASP	2
2	B	149	ARG	2
1	C	410	SER	2
1	C	427	TRP	2
1	C	554	HIS	2
1	A	209	SER	2
1	A	224	VAL	2
1	A	354	THR	2
1	A	360	LEU	2
2	B	3	GLU	2
2	B	50	THR	2
2	B	89	SER	2
2	B	106	SER	2
2	B	136	SER	2
1	C	455	TYR	2
1	C	467	MET	2
1	C	532	ARG	2
1	C	559	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	A	214	PHE	2
1	A	391	GLU	2
1	C	433	GLU	2
1	C	446	GLU	2
1	C	557	THR	2
1	C	576	VAL	2
1	A	385	SER	2
1	A	392	GLU	2
2	B	105	ASP	2
1	C	415	LEU	2
1	C	425	GLU	2
1	C	473	LYS	2
1	C	594	LYS	2
1	A	378	VAL	2
1	C	418	GLN	2
1	C	556	SER	2
1	C	591	TYR	2
1	A	244	SER	2
1	A	202	LYS	2
2	B	47	ASP	2
2	B	85	ASN	2
1	C	466	GLU	2
1	C	494	GLU	2
1	C	596	ASN	2
1	C	482	GLN	2
1	A	211	THR	1
1	A	237	GLU	1
1	A	245	LYS	1
1	A	303	GLU	1
2	B	19	LEU	1
2	B	23	LEU	1
2	B	25	GLN	1
2	B	169	LYS	1
1	C	417	GLU	1
1	C	439	GLN	1
1	C	442	SER	1
1	C	523	ASP	1
1	A	279	LEU	1
1	A	379	LEU	1
1	A	393	TYR	1
1	A	395	LYS	1
1	C	401	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	206	ASN	1
1	A	359	THR	1
2	B	95	HIS	1
2	B	132	ASP	1
1	C	411	THR	1
1	C	586	SER	1
1	C	589	GLU	1
1	A	308	ARG	1
1	C	478	ARG	1
1	C	495	LYS	1
1	C	527	GLN	1
1	A	242	GLU	1
1	A	275	LYS	1
1	C	406	ASP	1
1	C	497	SER	1
1	C	501	GLU	1
1	A	257	TYR	1
1	A	264	LYS	1
1	A	274	GLN	1
1	A	350	HIS	1
1	A	369	GLU	1
1	A	386	PHE	1
2	B	5	LYS	1
2	B	33	ASP	1
2	B	114	VAL	1
2	B	144	THR	1
1	C	404	ASN	1
1	C	457	ASP	1
1	C	579	SER	1
1	A	261	PHE	1
1	A	349	TYR	1
2	B	14	VAL	1
1	C	434	THR	1
1	C	464	GLN	1
1	C	468	GLU	1
1	C	546	GLU	1
1	A	233	GLU	1
1	A	276	VAL	1
1	A	297	LYS	1
2	B	57	ASP	1
2	B	72	MET	1
2	B	102	ARG	1

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Mol	Chain	Res	Type	Models (Total)
2	B	131	GLN	1
1	C	488	LYS	1
1	C	521	TYR	1
1	C	569	LEU	1
1	A	225	THR	1
1	A	227	GLU	1
1	A	330	ARG	1
1	A	345	ARG	1
1	A	365	LYS	1
2	B	6	LEU	1
2	B	8	VAL	1
2	B	9	VAL	1
2	B	73	ARG	1
1	C	426	PHE	1
1	C	458	ASP	1
1	A	265	TRP	1
2	B	31	GLU	1
2	B	41	ARG	1
2	B	43	GLN	1
2	B	53	LEU	1
1	C	483	GLU	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 83 ligands modelled in this entry, 1 is monoatomic - leaving 82 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types,

if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	17F	B	226	-	52,53,53	0.92±0.01	1±0 (1±0%)
4	17F	C	631	-	52,53,53	0.90±0.01	0±0 (0±0%)
3	PCW	C	610	-	53,53,53	1.04±0.01	4±0 (8±0%)
4	17F	C	635	-	52,53,53	0.91±0.01	1±0 (1±0%)
3	PCW	C	615	-	53,53,53	1.08±0.01	5±1 (9±1%)
3	PCW	A	402	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	C	604	-	53,53,53	1.06±0.01	4±0 (7±0%)
3	PCW	C	628	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	B	209	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	B	215	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	C	624	-	53,53,53	1.05±0.02	5±1 (9±1%)
3	PCW	C	612	-	53,53,53	1.05±0.01	4±1 (8±1%)
3	PCW	A	406	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	B	202	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	B	208	-	53,53,53	1.05±0.02	5±1 (8±1%)
3	PCW	C	622	-	53,53,53	1.04±0.01	3±0 (6±0%)
3	PCW	C	606	-	53,53,53	1.05±0.02	4±0 (7±0%)
3	PCW	B	205	-	53,53,53	1.05±0.01	5±0 (9±0%)
3	PCW	B	214	-	53,53,53	1.05±0.01	5±0 (9±0%)
3	PCW	C	603	-	53,53,53	1.05±0.01	4±1 (7±1%)
3	PCW	C	616	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	404	-	53,53,53	1.05±0.01	5±0 (9±0%)
3	PCW	C	626	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	B	218	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	C	605	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	B	213	-	53,53,53	1.05±0.01	4±1 (7±1%)
3	PCW	C	619	-	53,53,53	1.04±0.01	3±0 (6±0%)
4	17F	B	230	-	52,53,53	0.92±0.01	0±0 (0±0%)
3	PCW	A	409	-	53,53,53	1.05±0.01	4±0 (6±0%)
4	17F	B	234	-	52,53,53	0.93±0.00	1±0 (1±0%)
4	17F	C	632	-	52,53,53	0.92±0.01	1±0 (1±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	17F	C	630	-	52,53,53	0.92±0.01	0±0 (0±0%)
3	PCW	A	401	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	C	627	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	C	625	-	53,53,53	1.06±0.01	4±0 (6±0%)
3	PCW	C	614	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	B	216	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	B	211	-	53,53,53	1.06±0.02	5±0 (9±0%)
4	17F	B	227	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	A	410	-	53,53,53	1.07±0.01	4±0 (7±0%)
3	PCW	B	220	-	53,53,53	1.05±0.01	4±0 (6±0%)
4	17F	B	229	-	52,53,53	0.92±0.01	1±0 (1±0%)
4	17F	C	634	-	52,53,53	0.91±0.01	1±0 (1±0%)
3	PCW	A	405	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	17F	B	225	-	52,53,53	0.93±0.01	1±0 (1±0%)
3	PCW	B	210	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	C	609	-	53,53,53	1.05±0.01	5±1 (8±1%)
3	PCW	A	407	-	53,53,53	1.07±0.01	5±0 (9±0%)
3	PCW	B	204	-	53,53,53	1.04±0.01	4±0 (8±0%)
3	PCW	B	219	-	53,53,53	1.04±0.01	4±0 (6±0%)
4	17F	A	411	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	B	201	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	C	602	-	53,53,53	1.07±0.01	5±0 (9±0%)
7	EWS	B	237	-	30,30,30	2.27±0.00	10±0 (33±0%)
5	GNP	B	235	-	34,34,34	1.50±0.01	5±0 (14±0%)
3	PCW	C	613	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	408	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	A	403	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	B	207	-	53,53,53	1.04±0.01	4±1 (8±1%)
3	PCW	C	629	-	53,53,53	1.05±0.01	5±0 (9±0%)
3	PCW	B	212	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	C	611	-	53,53,53	1.05±0.02	4±1 (7±1%)
4	17F	B	224	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	B	203	-	53,53,53	1.04±0.01	3±0 (6±0%)
4	17F	B	223	-	52,53,53	0.92±0.01	1±0 (1±0%)
3	PCW	C	623	-	53,53,53	1.04±0.01	5±0 (8±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PCW	B	222	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	B	221	-	53,53,53	1.04±0.01	5±0 (8±0%)
3	PCW	C	601	-	53,53,53	1.05±0.01	5±0 (8±0%)
3	PCW	B	231	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	C	620	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	B	217	-	53,53,53	1.05±0.01	4±0 (6±0%)
3	PCW	B	233	-	53,53,53	1.04±0.01	4±0 (6±0%)
4	17F	B	228	-	52,53,53	0.91±0.01	0±0 (0±0%)
3	PCW	C	621	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	B	206	-	53,53,53	1.04±0.01	4±0 (6±0%)
3	PCW	C	618	-	53,53,53	1.06±0.01	4±0 (7±0%)
3	PCW	C	607	-	53,53,53	1.05±0.01	4±0 (7±0%)
3	PCW	B	232	-	53,53,53	1.04±0.01	4±0 (7±0%)
3	PCW	C	608	-	53,53,53	1.05±0.01	4±0 (7±0%)
4	17F	C	633	-	52,53,53	0.92±0.01	0±0 (0±0%)
3	PCW	C	617	-	53,53,53	1.04±0.01	4±0 (7±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	17F	B	226	-	54,60,60	1.09±0.02	5±0 (9±0%)
4	17F	C	631	-	54,60,60	1.11±0.02	6±0 (10±0%)
3	PCW	C	610	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	17F	C	635	-	54,60,60	1.04±0.01	4±0 (7±0%)
3	PCW	C	615	-	59,61,61	0.83±0.01	1±0 (1±0%)
3	PCW	A	402	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	604	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	628	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	B	209	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	B	215	-	59,61,61	2.32±0.00	5±0 (8±0%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
3	PCW	C	624	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	C	612	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	A	406	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	B	202	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	B	208	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	C	622	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	606	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	B	205	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	B	214	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	C	603	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	616	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	A	404	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	C	626	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	B	218	-	59,61,61	2.33±0.00	5±0 (8±0%)
3	PCW	C	605	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	B	213	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	C	619	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	B	230	-	54,60,60	1.06±0.02	5±0 (9±0%)
3	PCW	A	409	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	17F	B	234	-	54,60,60	1.03±0.02	5±0 (9±0%)
4	17F	C	632	-	54,60,60	1.03±0.01	5±0 (9±0%)
4	17F	C	630	-	54,60,60	1.06±0.04	5±0 (9±0%)
3	PCW	A	401	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	C	627	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	625	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	614	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	B	216	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	B	211	-	59,61,61	0.84±0.01	1±0 (1±0%)
4	17F	B	227	-	54,60,60	1.05±0.03	5±0 (9±0%)
3	PCW	A	410	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	B	220	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	B	229	-	54,60,60	1.08±0.02	5±0 (9±0%)
4	17F	C	634	-	54,60,60	1.06±0.02	5±0 (9±0%)
3	PCW	A	405	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	B	225	-	54,60,60	1.06±0.02	5±0 (9±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PCW	B	210	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	C	609	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	A	407	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	B	204	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	B	219	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	17F	A	411	-	54,60,60	1.06±0.02	5±0 (9±0%)
3	PCW	B	201	-	59,61,61	2.33±0.01	5±0 (8±0%)
3	PCW	C	602	-	59,61,61	0.84±0.01	1±0 (1±0%)
7	EWS	B	237	-	37,42,42	1.38±0.01	2±0 (5±0%)
5	GNP	B	235	-	47,54,54	0.81±0.01	1±0 (2±0%)
3	PCW	C	613	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	A	408	-	59,61,61	2.33±0.01	5±0 (8±0%)
3	PCW	A	403	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	B	207	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	C	629	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	B	212	-	59,61,61	2.33±0.01	5±0 (8±0%)
3	PCW	C	611	-	59,61,61	2.32±0.00	5±0 (8±0%)
4	17F	B	224	-	54,60,60	1.05±0.02	5±0 (9±0%)
3	PCW	B	203	-	59,61,61	2.77±0.01	9±0 (15±0%)
4	17F	B	223	-	54,60,60	1.77±0.02	9±0 (16±0%)
3	PCW	C	623	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	B	222	-	59,61,61	2.33±0.01	5±0 (8±0%)
3	PCW	B	221	-	59,61,61	0.85±0.01	1±0 (1±0%)
3	PCW	C	601	-	59,61,61	0.84±0.01	1±0 (1±0%)
3	PCW	B	231	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	620	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	B	217	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	B	233	-	59,61,61	2.32±0.01	5±0 (8±0%)
4	17F	B	228	-	54,60,60	1.06±0.03	5±1 (8±1%)
3	PCW	C	621	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	B	206	-	59,61,61	2.32±0.00	5±0 (8±0%)
3	PCW	C	618	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	C	607	-	59,61,61	2.32±0.01	5±0 (8±0%)
3	PCW	B	232	-	59,61,61	2.77±0.00	9±0 (15±0%)
3	PCW	C	608	-	59,61,61	2.32±0.01	5±0 (8±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	17F	C	633	-	54,60,60	1.80±0.03	10±0 (18±0%)
3	PCW	C	617	-	59,61,61	2.32±0.00	5±0 (8±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	C	604	-	-	0±0,57,57,57	-
3	PCW	C	606	-	-	0±0,57,57,57	-
3	PCW	C	616	-	-	0±0,57,57,57	-
4	17F	C	635	-	-	0±0,59,59,59	-
4	17F	B	230	-	-	0±0,59,59,59	-
4	17F	C	630	-	-	0±0,59,59,59	-
3	PCW	A	404	-	-	0±0,57,57,57	-
3	PCW	B	218	-	-	0±0,57,57,57	-
3	PCW	B	220	-	-	0±0,57,57,57	-
3	PCW	A	403	-	-	0±0,57,57,57	-
3	PCW	C	627	-	-	0±0,57,57,57	-
5	GNP	B	235	-	-	1±0,18,38,38	0±0,3,3,3
3	PCW	B	203	-	-	0±0,57,57,57	-
3	PCW	B	221	-	-	0±0,57,57,57	-
3	PCW	C	615	-	-	0±0,57,57,57	-
3	PCW	B	233	-	-	0±0,57,57,57	-
3	PCW	C	618	-	-	0±0,57,57,57	-
3	PCW	C	601	-	-	0±0,57,57,57	-
3	PCW	B	206	-	-	0±0,57,57,57	-
4	17F	B	225	-	-	0±0,59,59,59	-
4	17F	B	223	-	-	0±0,59,59,59	-
3	PCW	A	401	-	-	0±0,57,57,57	-
3	PCW	C	605	-	-	0±0,57,57,57	-
3	PCW	A	409	-	-	0±0,57,57,57	-
3	PCW	B	213	-	-	0±0,57,57,57	-
3	PCW	B	216	-	-	0±0,57,57,57	-
4	17F	B	226	-	-	0±0,59,59,59	-
3	PCW	A	402	-	-	0±0,57,57,57	-
4	17F	B	229	-	-	0±0,59,59,59	-
3	PCW	C	610	-	-	0±0,57,57,57	-
3	PCW	A	406	-	-	0±0,57,57,57	-
7	EWS	B	237	-	-	0±0,12,22,22	1±0,4,4,4
3	PCW	C	603	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	B	214	-	-	0±0,57,57,57	-
3	PCW	C	626	-	-	0±0,57,57,57	-
3	PCW	B	222	-	-	0±0,57,57,57	-
3	PCW	C	612	-	-	0±0,57,57,57	-
3	PCW	B	201	-	-	0±0,57,57,57	-
3	PCW	C	609	-	-	0±0,57,57,57	-
3	PCW	B	215	-	-	0±0,57,57,57	-
3	PCW	B	208	-	-	0±0,57,57,57	-
3	PCW	B	231	-	-	0±0,57,57,57	-
3	PCW	C	617	-	-	0±0,57,57,57	-
3	PCW	B	212	-	-	0±0,57,57,57	-
3	PCW	B	205	-	-	0±0,57,57,57	-
3	PCW	B	204	-	-	0±0,57,57,57	-
3	PCW	B	232	-	-	0±0,57,57,57	-
3	PCW	B	202	-	-	0±0,57,57,57	-
3	PCW	B	211	-	-	0±0,57,57,57	-
3	PCW	C	620	-	-	0±0,57,57,57	-
3	PCW	A	405	-	-	0±0,57,57,57	-
3	PCW	C	621	-	-	0±0,57,57,57	-
4	17F	C	633	-	-	0±0,59,59,59	-
4	17F	B	234	-	-	0±0,59,59,59	-
3	PCW	A	410	-	-	0±0,57,57,57	-
3	PCW	C	624	-	-	0±0,57,57,57	-
3	PCW	C	614	-	-	0±0,57,57,57	-
3	PCW	B	210	-	-	0±0,57,57,57	-
3	PCW	C	629	-	-	0±0,57,57,57	-
3	PCW	C	602	-	-	0±0,57,57,57	-
3	PCW	C	622	-	-	0±0,57,57,57	-
3	PCW	B	207	-	-	0±0,57,57,57	-
3	PCW	A	407	-	-	0±0,57,57,57	-
4	17F	C	631	-	-	0±0,59,59,59	-
3	PCW	C	607	-	-	0±0,57,57,57	-
3	PCW	C	619	-	-	0±0,57,57,57	-
3	PCW	C	613	-	-	0±0,57,57,57	-
3	PCW	B	219	-	-	0±0,57,57,57	-
3	PCW	C	625	-	-	0±0,57,57,57	-
4	17F	C	634	-	-	0±0,59,59,59	-
4	17F	A	411	-	-	0±0,59,59,59	-
3	PCW	A	408	-	-	0±0,57,57,57	-
4	17F	C	632	-	-	0±0,59,59,59	-
3	PCW	C	608	-	-	0±0,57,57,57	-
3	PCW	C	623	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	B	209	-	-	0±0,57,57,57	-
3	PCW	B	217	-	-	0±0,57,57,57	-
3	PCW	C	611	-	-	0±0,57,57,57	-
4	17F	B	224	-	-	0±0,59,59,59	-
3	PCW	C	628	-	-	0±0,57,57,57	-
4	17F	B	227	-	-	0±0,59,59,59	-
4	17F	B	228	-	-	0±0,59,59,59	-

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
7	B	237	EWS	CAV-CBA	6.57	1.34	1.45	4	10
7	B	237	EWS	CAI-CAJ	5.03	1.39	1.51	8	10
5	B	235	GNP	PG-O1G	4.69	1.53	1.46	7	10
5	B	235	GNP	PB-O2B	4.10	1.45	1.56	10	10
7	B	237	EWS	CAV-CAU	3.90	1.36	1.41	7	10
5	B	235	GNP	PG-O3G	3.36	1.47	1.56	1	10
7	B	237	EWS	CAX-CBA	3.15	1.33	1.38	5	10
3	C	607	PCW	C5-N	2.91	1.42	1.51	9	10
3	C	618	PCW	C5-N	2.89	1.42	1.51	6	10
3	C	606	PCW	C5-N	2.89	1.42	1.51	4	10
3	C	625	PCW	C5-N	2.88	1.42	1.51	1	10
3	B	219	PCW	C5-N	2.86	1.42	1.51	10	10
5	B	235	GNP	PB-O3A	2.86	1.55	1.59	2	10
3	B	201	PCW	C5-N	2.85	1.42	1.51	1	10
3	C	628	PCW	C5-N	2.85	1.42	1.51	6	10
3	B	220	PCW	C5-N	2.84	1.42	1.51	4	10
3	B	202	PCW	C5-N	2.83	1.42	1.51	1	10
3	B	212	PCW	C5-N	2.83	1.42	1.51	7	10
3	B	203	PCW	C5-N	2.82	1.42	1.51	8	10
3	B	231	PCW	C5-N	2.82	1.42	1.51	3	10
3	B	209	PCW	C5-N	2.82	1.42	1.51	1	10
3	C	608	PCW	C5-N	2.81	1.42	1.51	9	10
5	B	235	GNP	PG-O2G	2.81	1.49	1.56	8	10
3	B	206	PCW	C5-N	2.81	1.42	1.51	8	10
3	C	627	PCW	C5-N	2.81	1.42	1.51	3	10
3	C	614	PCW	C5-N	2.80	1.42	1.51	2	10
3	C	626	PCW	C5-N	2.80	1.42	1.51	8	10
3	C	611	PCW	C5-N	2.80	1.43	1.51	3	10
3	A	402	PCW	C5-N	2.79	1.43	1.51	8	10
3	B	215	PCW	C5-N	2.79	1.43	1.51	3	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	410	PCW	C5-N	2.79	1.43	1.51	7	10
3	C	620	PCW	C5-N	2.78	1.43	1.51	6	10
3	C	605	PCW	C5-N	2.78	1.43	1.51	3	10
3	C	621	PCW	C5-N	2.78	1.43	1.51	9	10
3	A	406	PCW	C5-N	2.77	1.43	1.51	7	10
3	C	604	PCW	C5-N	2.77	1.43	1.51	8	10
3	B	211	PCW	C1-C2	2.76	1.59	1.50	10	10
3	B	213	PCW	C5-N	2.76	1.43	1.51	5	10
3	B	216	PCW	C5-N	2.75	1.43	1.51	6	10
3	B	210	PCW	C5-N	2.74	1.43	1.51	3	10
3	B	217	PCW	C5-N	2.74	1.43	1.51	5	10
3	C	616	PCW	C5-N	2.74	1.43	1.51	3	10
3	C	622	PCW	C5-N	2.73	1.43	1.51	3	10
3	C	619	PCW	C5-N	2.73	1.43	1.51	8	10
3	B	233	PCW	C5-N	2.73	1.43	1.51	4	10
3	C	603	PCW	C5-N	2.73	1.43	1.51	4	10
3	C	615	PCW	C1-C2	2.72	1.59	1.50	6	10
3	C	613	PCW	C5-N	2.72	1.43	1.51	9	10
3	C	617	PCW	C5-N	2.72	1.43	1.51	9	10
3	C	611	PCW	C1-C2	2.71	1.59	1.50	3	10
3	A	401	PCW	C5-N	2.71	1.43	1.51	6	10
3	A	409	PCW	C5-N	2.71	1.43	1.51	2	10
3	C	603	PCW	C1-C2	2.71	1.59	1.50	10	10
3	A	403	PCW	C5-N	2.70	1.43	1.51	7	10
3	C	625	PCW	C1-C2	2.70	1.59	1.50	6	10
3	B	218	PCW	C5-N	2.70	1.43	1.51	10	10
3	C	604	PCW	C1-C2	2.70	1.59	1.50	1	10
3	A	405	PCW	C5-N	2.70	1.43	1.51	1	10
3	A	407	PCW	C1-C2	2.70	1.59	1.50	9	10
3	A	402	PCW	C1-C2	2.68	1.59	1.50	3	10
3	B	208	PCW	C1-C2	2.68	1.59	1.50	7	10
3	B	203	PCW	C1-C2	2.67	1.59	1.50	10	10
3	A	408	PCW	C5-N	2.67	1.43	1.51	7	10
7	B	237	EWS	CAT-CAU	2.67	1.35	1.39	3	10
7	B	237	EWS	CBA-CAZ	2.66	1.34	1.51	5	10
3	C	613	PCW	C1-C2	2.65	1.59	1.50	5	10
3	A	409	PCW	C1-C2	2.65	1.59	1.50	5	10
3	B	231	PCW	C1-C2	2.64	1.59	1.50	6	10
3	B	232	PCW	C5-N	2.64	1.43	1.51	3	10
3	A	408	PCW	C1-C2	2.64	1.59	1.50	1	10
3	C	622	PCW	C1-C2	2.64	1.59	1.50	5	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	210	PCW	C1-C2	2.63	1.59	1.50	2	10
3	B	205	PCW	C1-C2	2.63	1.59	1.50	8	10
3	B	222	PCW	C5-N	2.62	1.43	1.51	8	10
3	B	221	PCW	C1-C2	2.62	1.59	1.50	4	10
3	B	213	PCW	C1-C2	2.62	1.59	1.50	9	10
3	C	620	PCW	C1-C2	2.62	1.59	1.50	7	10
3	C	602	PCW	C1-C2	2.62	1.59	1.50	7	10
3	C	628	PCW	C1-C2	2.61	1.59	1.50	2	10
3	A	403	PCW	C1-C2	2.60	1.59	1.50	9	10
3	C	618	PCW	C1-C2	2.60	1.59	1.50	2	10
3	C	626	PCW	C1-C2	2.60	1.59	1.50	1	10
3	C	606	PCW	C1-C2	2.60	1.58	1.50	5	10
3	A	410	PCW	C1-C2	2.60	1.58	1.50	4	10
3	A	401	PCW	C1-C2	2.59	1.58	1.50	6	10
3	C	617	PCW	C1-C2	2.59	1.58	1.50	5	10
3	C	601	PCW	C1-C2	2.58	1.58	1.50	7	10
3	C	609	PCW	C5-N	2.58	1.43	1.51	1	10
3	B	216	PCW	C1-C2	2.57	1.58	1.50	7	10
3	C	619	PCW	C1-C2	2.58	1.58	1.50	8	10
3	B	232	PCW	C1-C2	2.56	1.58	1.50	7	10
3	C	607	PCW	C1-C2	2.56	1.58	1.50	1	10
3	B	206	PCW	C1-C2	2.56	1.58	1.50	9	10
3	C	608	PCW	C1-C2	2.56	1.58	1.50	10	10
3	C	622	PCW	C33-C32	2.56	1.61	1.52	2	10
3	B	204	PCW	C5-N	2.56	1.43	1.51	5	10
3	C	602	PCW	C5-N	2.56	1.43	1.51	3	10
3	A	406	PCW	C1-C2	2.56	1.58	1.50	7	10
3	B	218	PCW	C1-C2	2.55	1.58	1.50	6	10
3	C	601	PCW	C5-N	2.55	1.43	1.51	4	10
3	C	610	PCW	C1-C2	2.55	1.58	1.50	8	10
3	C	624	PCW	C1-C2	2.55	1.58	1.50	9	10
3	B	222	PCW	C1-C2	2.55	1.58	1.50	5	10
3	C	629	PCW	C5-N	2.55	1.43	1.51	4	10
3	B	212	PCW	C1-C2	2.54	1.58	1.50	3	10
3	B	217	PCW	C1-C2	2.54	1.58	1.50	4	10
3	B	208	PCW	C5-N	2.54	1.43	1.51	10	10
3	A	405	PCW	C1-C2	2.53	1.58	1.50	5	10
3	B	201	PCW	C1-C2	2.54	1.58	1.50	5	10
3	B	210	PCW	C33-C32	2.54	1.61	1.52	6	10
3	C	609	PCW	C1-C2	2.54	1.58	1.50	3	10
3	C	610	PCW	C5-N	2.53	1.43	1.51	4	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	623	PCW	C5-N	2.53	1.43	1.51	2	10
3	B	207	PCW	C1-C2	2.53	1.58	1.50	2	10
3	B	207	PCW	C5-N	2.53	1.43	1.51	9	10
3	B	209	PCW	C1-C2	2.53	1.58	1.50	10	10
3	B	211	PCW	C5-N	2.53	1.43	1.51	9	10
3	C	605	PCW	C1-C2	2.53	1.58	1.50	9	10
3	B	219	PCW	C1-C2	2.52	1.58	1.50	3	10
3	C	616	PCW	C1-C2	2.52	1.58	1.50	6	10
3	A	404	PCW	C1-C2	2.52	1.58	1.50	5	10
3	B	201	PCW	C33-C32	2.52	1.61	1.52	7	10
3	C	629	PCW	C1-C2	2.52	1.58	1.50	1	10
7	B	237	EWS	CAU-NAW	2.52	1.33	1.37	8	10
3	B	214	PCW	C5-N	2.52	1.43	1.51	2	10
3	B	233	PCW	C1-C2	2.52	1.58	1.50	8	10
3	B	215	PCW	C1-C2	2.52	1.58	1.50	2	10
3	B	220	PCW	C1-C2	2.51	1.58	1.50	7	10
7	B	237	EWS	CAX-NAW	2.51	1.33	1.37	2	10
3	B	211	PCW	C33-C32	2.50	1.61	1.52	9	10
3	B	232	PCW	C33-C32	2.50	1.61	1.52	5	10
3	B	205	PCW	C5-N	2.50	1.43	1.51	3	10
3	C	607	PCW	C33-C32	2.50	1.61	1.52	4	10
3	C	621	PCW	C1-C2	2.50	1.58	1.50	1	10
3	A	404	PCW	C5-N	2.49	1.43	1.51	5	10
3	C	615	PCW	C5-N	2.49	1.43	1.51	2	10
3	C	614	PCW	C1-C2	2.49	1.58	1.50	5	10
3	B	220	PCW	C33-C32	2.49	1.61	1.52	10	10
3	C	629	PCW	C33-C32	2.49	1.61	1.52	4	10
3	A	407	PCW	C5-N	2.49	1.43	1.51	8	10
3	A	402	PCW	C33-C32	2.49	1.61	1.52	9	10
3	C	612	PCW	C5-N	2.48	1.43	1.51	8	10
3	C	627	PCW	C1-C2	2.48	1.58	1.50	7	10
3	B	202	PCW	C1-C2	2.48	1.58	1.50	6	10
3	C	612	PCW	C1-C2	2.48	1.58	1.50	3	10
3	A	407	PCW	C33-C32	2.48	1.61	1.52	8	10
3	B	203	PCW	C33-C32	2.47	1.61	1.52	9	10
3	C	614	PCW	C33-C32	2.47	1.61	1.52	10	10
3	C	623	PCW	C1-C2	2.47	1.58	1.50	1	10
3	A	405	PCW	C33-C32	2.47	1.61	1.52	8	10
3	B	221	PCW	C5-N	2.46	1.44	1.51	10	10
3	B	214	PCW	C1-C2	2.46	1.58	1.50	6	10
3	C	624	PCW	C33-C32	2.46	1.61	1.52	9	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	214	PCW	C33-C32	2.45	1.61	1.52	5	10
3	B	204	PCW	C1-C2	2.45	1.58	1.50	7	10
3	B	217	PCW	C33-C32	2.45	1.61	1.52	1	10
3	B	206	PCW	C33-C32	2.45	1.61	1.52	10	10
3	C	610	PCW	C33-C32	2.45	1.61	1.52	10	10
3	C	617	PCW	C33-C32	2.45	1.61	1.52	7	10
3	C	627	PCW	C33-C32	2.45	1.61	1.52	10	10
3	C	628	PCW	C33-C32	2.44	1.61	1.52	7	10
3	C	618	PCW	C33-C32	2.44	1.61	1.52	8	10
3	C	619	PCW	C33-C32	2.44	1.61	1.52	2	10
3	C	609	PCW	C33-C32	2.44	1.61	1.52	2	10
3	C	621	PCW	C33-C32	2.44	1.61	1.52	5	10
3	C	626	PCW	C33-C32	2.44	1.61	1.52	8	10
3	B	222	PCW	C33-C32	2.44	1.61	1.52	6	10
3	C	601	PCW	C33-C32	2.43	1.61	1.52	8	10
3	A	404	PCW	C33-C32	2.43	1.61	1.52	2	10
3	C	605	PCW	C33-C32	2.43	1.61	1.52	3	10
3	C	604	PCW	C33-C32	2.43	1.61	1.52	1	10
3	A	409	PCW	C33-C32	2.42	1.61	1.52	8	10
3	B	231	PCW	C33-C32	2.42	1.61	1.52	1	10
3	C	625	PCW	C33-C32	2.42	1.61	1.52	2	10
3	C	606	PCW	C33-C32	2.42	1.61	1.52	4	10
3	B	209	PCW	C33-C32	2.41	1.61	1.52	7	10
3	A	410	PCW	C3-C2	2.41	1.58	1.50	8	10
3	B	213	PCW	C33-C32	2.41	1.61	1.52	9	10
3	A	410	PCW	C33-C32	2.41	1.61	1.52	5	10
3	C	623	PCW	C33-C32	2.41	1.61	1.52	1	10
3	B	204	PCW	C33-C32	2.41	1.61	1.52	10	10
3	C	624	PCW	C5-N	2.41	1.44	1.51	10	10
3	A	403	PCW	C33-C32	2.41	1.61	1.52	4	10
3	A	401	PCW	C33-C32	2.40	1.61	1.52	7	10
3	B	219	PCW	C33-C32	2.40	1.61	1.52	10	10
3	C	613	PCW	C33-C32	2.40	1.61	1.52	10	10
3	B	232	PCW	C3-C2	2.40	1.58	1.50	7	9
3	B	208	PCW	C33-C32	2.40	1.61	1.52	3	10
3	B	233	PCW	C33-C32	2.40	1.61	1.52	7	10
3	C	612	PCW	C33-C32	2.40	1.61	1.52	2	10
3	B	215	PCW	C33-C32	2.40	1.61	1.52	2	10
3	B	207	PCW	C33-C32	2.39	1.60	1.52	10	10
3	B	216	PCW	C33-C32	2.39	1.60	1.52	10	10
3	B	218	PCW	C33-C32	2.39	1.60	1.52	3	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	202	PCW	C33-C32	2.39	1.60	1.52	10	10
3	B	205	PCW	C33-C32	2.39	1.60	1.52	8	10
3	B	212	PCW	C33-C32	2.39	1.60	1.52	5	10
3	C	602	PCW	C33-C32	2.38	1.60	1.52	8	10
3	C	603	PCW	C33-C32	2.38	1.60	1.52	3	10
3	C	620	PCW	C33-C32	2.38	1.60	1.52	7	10
3	C	611	PCW	C33-C32	2.38	1.60	1.52	8	10
3	C	615	PCW	C33-C32	2.38	1.60	1.52	9	10
3	C	616	PCW	C33-C32	2.37	1.60	1.52	1	10
3	C	608	PCW	C33-C32	2.36	1.60	1.52	5	10
3	A	408	PCW	C33-C32	2.35	1.60	1.52	4	10
3	B	221	PCW	C33-C32	2.34	1.60	1.52	1	10
3	C	624	PCW	C7-N	2.33	1.43	1.50	2	10
3	A	406	PCW	C33-C32	2.32	1.60	1.52	3	10
3	B	205	PCW	C7-N	2.32	1.43	1.50	6	10
3	B	211	PCW	C7-N	2.32	1.43	1.50	9	10
3	C	609	PCW	C7-N	2.31	1.43	1.50	5	9
3	A	407	PCW	C7-N	2.31	1.43	1.50	3	10
3	C	615	PCW	O2-C2	2.30	1.52	1.46	9	3
3	C	623	PCW	C7-N	2.28	1.43	1.50	6	9
3	C	615	PCW	C3-C2	2.28	1.57	1.50	6	9
3	C	629	PCW	C7-N	2.28	1.43	1.50	6	10
3	B	221	PCW	C7-N	2.28	1.43	1.50	1	10
3	C	612	PCW	C7-N	2.27	1.43	1.50	9	9
3	B	208	PCW	C7-N	2.27	1.43	1.50	10	9
3	C	602	PCW	C7-N	2.27	1.43	1.50	3	10
3	C	602	PCW	C3-C2	2.26	1.57	1.50	4	10
3	B	214	PCW	C7-N	2.26	1.43	1.50	7	10
3	A	407	PCW	C3-C2	2.25	1.57	1.50	7	10
4	B	234	17F	C1X-C2X	2.25	1.61	1.52	7	9
3	C	601	PCW	C7-N	2.25	1.43	1.50	10	9
7	B	237	EWS	CAO-CAN	2.25	1.42	1.38	9	10
3	C	603	PCW	C3-C2	2.24	1.57	1.50	10	8
3	C	604	PCW	C3-C2	2.24	1.57	1.50	1	9
3	B	216	PCW	C3-C2	2.24	1.57	1.50	4	7
3	B	203	PCW	C3-C2	2.23	1.57	1.50	1	4
3	C	610	PCW	C7-N	2.23	1.43	1.50	6	9
3	C	613	PCW	C3-C2	2.23	1.57	1.50	8	7
3	B	204	PCW	C7-N	2.23	1.43	1.50	9	10
3	A	403	PCW	C3-C2	2.22	1.57	1.50	1	8
3	C	616	PCW	C3-C2	2.22	1.57	1.50	3	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	215	PCW	C3-C2	2.22	1.57	1.50	1	7
3	A	404	PCW	C7-N	2.21	1.43	1.50	3	10
3	C	606	PCW	C3-C2	2.22	1.57	1.50	8	9
3	A	409	PCW	C3-C2	2.21	1.57	1.50	7	7
3	C	612	PCW	C3-C2	2.21	1.57	1.50	3	6
3	B	207	PCW	C7-N	2.21	1.43	1.50	10	9
3	C	618	PCW	C3-C2	2.21	1.57	1.50	6	9
3	B	212	PCW	C3-C2	2.19	1.57	1.50	10	7
3	B	218	PCW	C3-C2	2.19	1.57	1.50	6	9
3	C	615	PCW	C7-N	2.19	1.43	1.50	10	10
3	A	401	PCW	C3-C2	2.19	1.57	1.50	6	8
3	B	231	PCW	C3-C2	2.19	1.57	1.50	4	8
3	C	614	PCW	C3-C2	2.18	1.57	1.50	4	8
3	A	405	PCW	C3-C2	2.18	1.57	1.50	7	9
3	B	221	PCW	C3-C2	2.18	1.57	1.50	4	6
3	C	611	PCW	C3-C2	2.17	1.57	1.50	5	7
3	A	406	PCW	C3-C2	2.17	1.57	1.50	1	8
4	B	227	17F	C1X-C2X	2.17	1.61	1.52	10	9
3	B	209	PCW	C3-C2	2.17	1.57	1.50	8	7
3	B	214	PCW	C3-C2	2.17	1.57	1.50	6	8
3	B	210	PCW	C3-C2	2.16	1.57	1.50	10	9
3	B	220	PCW	C3-C2	2.16	1.57	1.50	2	7
3	B	206	PCW	C3-C2	2.16	1.57	1.50	3	7
3	C	620	PCW	C3-C2	2.16	1.57	1.50	10	7
3	B	202	PCW	C3-C2	2.16	1.57	1.50	2	5
3	C	624	PCW	C3-C2	2.16	1.57	1.50	8	8
4	A	411	17F	C1X-C2X	2.16	1.61	1.52	3	9
3	B	211	PCW	C3-C2	2.15	1.57	1.50	1	9
4	B	224	17F	C1X-C2X	2.15	1.61	1.52	4	9
3	C	610	PCW	C3-C2	2.15	1.57	1.50	4	6
3	C	605	PCW	C3-C2	2.15	1.57	1.50	9	7
3	C	627	PCW	C3-C2	2.15	1.57	1.50	5	6
3	B	213	PCW	C3-C2	2.14	1.57	1.50	9	8
3	A	402	PCW	C3-C2	2.14	1.57	1.50	5	7
3	B	222	PCW	C3-C2	2.14	1.57	1.50	10	7
3	C	623	PCW	C3-C2	2.14	1.57	1.50	4	8
3	C	609	PCW	C3-C2	2.14	1.57	1.50	3	7
3	C	626	PCW	C3-C2	2.13	1.57	1.50	3	8
3	B	201	PCW	C3-C2	2.13	1.57	1.50	7	7
3	B	204	PCW	C3-C2	2.13	1.57	1.50	3	4
3	C	621	PCW	C3-C2	2.13	1.57	1.50	9	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	622	PCW	C3-C2	2.13	1.57	1.50	2	4
3	B	219	PCW	C3-C2	2.12	1.57	1.50	5	5
3	C	629	PCW	C3-C2	2.12	1.57	1.50	6	8
4	B	225	17F	C1X-C2X	2.12	1.61	1.52	3	10
3	B	207	PCW	C3-C2	2.12	1.57	1.50	10	6
3	B	208	PCW	C3-C2	2.12	1.57	1.50	7	7
3	C	601	PCW	C3-C2	2.12	1.57	1.50	2	8
3	C	607	PCW	C3-C2	2.12	1.57	1.50	1	9
4	C	632	17F	C1X-C2X	2.12	1.61	1.52	7	8
3	A	404	PCW	C3-C2	2.11	1.57	1.50	5	8
3	B	217	PCW	C3-C2	2.11	1.57	1.50	5	5
3	C	608	PCW	C3-C2	2.11	1.57	1.50	3	8
3	B	205	PCW	C3-C2	2.11	1.57	1.50	4	9
3	A	408	PCW	C3-C2	2.11	1.57	1.50	9	5
3	C	625	PCW	C3-C2	2.11	1.57	1.50	5	6
3	C	617	PCW	C3-C2	2.11	1.57	1.50	5	9
3	C	609	PCW	P-O4P	2.10	1.51	1.59	1	1
7	B	237	EWS	CAQ-CAV	2.10	1.36	1.39	10	10
4	B	229	17F	C1X-C2X	2.10	1.61	1.52	6	6
3	C	628	PCW	C3-C2	2.10	1.57	1.50	4	5
4	B	223	17F	C1X-C2X	2.10	1.61	1.52	5	9
4	B	228	17F	C1X-C2X	2.09	1.61	1.52	1	5
4	B	226	17F	C1X-C2X	2.09	1.61	1.52	8	6
4	C	630	17F	C1X-C2X	2.09	1.61	1.52	8	4
4	C	635	17F	C1X-C2X	2.08	1.61	1.52	10	9
3	B	233	PCW	C3-C2	2.08	1.57	1.50	8	7
4	C	634	17F	C1X-C2X	2.08	1.61	1.52	10	7
4	B	230	17F	C1X-C2X	2.07	1.61	1.52	10	4
3	C	619	PCW	C3-C2	2.06	1.57	1.50	9	4
3	C	620	PCW	P-O4P	2.03	1.51	1.59	6	2
4	C	633	17F	C1X-C2X	2.03	1.60	1.52	5	3
3	C	611	PCW	P-O4P	2.03	1.51	1.59	4	1
3	C	603	PCW	C42-C41	2.02	1.60	1.52	10	1
3	A	407	PCW	P-O4P	2.01	1.51	1.59	4	1
3	B	213	PCW	P-O4P	2.01	1.51	1.59	9	1
3	B	211	PCW	P-O4P	2.01	1.51	1.59	9	1
3	C	624	PCW	P-O4P	2.01	1.51	1.59	10	1
3	C	606	PCW	P-O4P	2.00	1.51	1.59	8	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	B	222	PCW	C8-N-C7	12.09	77.21	108.98	1	10
3	B	219	PCW	C8-N-C7	12.08	77.23	108.98	1	10
3	C	618	PCW	C8-N-C7	12.04	77.35	108.98	9	10
3	C	616	PCW	C8-N-C7	12.04	77.36	108.98	3	10
3	C	625	PCW	C8-N-C7	12.03	77.38	108.98	5	10
3	A	408	PCW	C8-N-C7	12.02	77.39	108.98	6	10
3	A	410	PCW	C8-N-C7	12.01	77.42	108.98	8	10
3	C	627	PCW	C8-N-C7	12.01	77.42	108.98	6	10
3	B	212	PCW	C8-N-C7	12.01	77.42	108.98	1	10
3	B	232	PCW	C8-N-C7	12.01	77.42	108.98	1	10
3	B	206	PCW	C8-N-C7	12.01	77.43	108.98	1	10
3	C	606	PCW	C8-N-C7	12.00	77.46	108.98	6	10
3	C	608	PCW	C8-N-C7	11.99	77.48	108.98	5	10
3	A	401	PCW	C8-N-C7	11.99	77.49	108.98	7	10
3	B	217	PCW	C8-N-C7	11.98	77.51	108.98	9	10
3	B	218	PCW	C8-N-C7	11.98	77.52	108.98	6	10
3	B	231	PCW	C8-N-C7	11.97	77.55	108.98	9	10
3	C	620	PCW	C8-N-C7	11.97	77.54	108.98	10	10
3	B	220	PCW	C8-N-C7	11.96	77.56	108.98	7	10
3	B	202	PCW	C8-N-C7	11.96	77.56	108.98	10	10
3	A	403	PCW	C8-N-C7	11.96	77.57	108.98	4	10
3	C	605	PCW	C8-N-C7	11.95	77.59	108.98	2	10
3	C	614	PCW	C8-N-C7	11.95	77.59	108.98	10	10
3	B	233	PCW	C8-N-C7	11.95	77.60	108.98	1	10
3	C	611	PCW	C8-N-C7	11.94	77.60	108.98	2	10
3	A	406	PCW	C8-N-C7	11.94	77.61	108.98	7	10
3	C	622	PCW	C8-N-C7	11.94	77.60	108.98	7	10
3	A	402	PCW	C8-N-C7	11.94	77.62	108.98	2	10
3	B	209	PCW	C8-N-C7	11.94	77.62	108.98	3	10
3	C	619	PCW	C8-N-C7	11.94	77.62	108.98	5	10
3	C	604	PCW	C8-N-C7	11.93	77.63	108.98	10	10
3	B	216	PCW	C8-N-C7	11.93	77.64	108.98	8	10
3	C	617	PCW	C8-N-C7	11.93	77.65	108.98	9	10
3	B	213	PCW	C8-N-C7	11.92	77.66	108.98	5	10
3	B	203	PCW	C8-N-C7	11.92	77.67	108.98	5	10
3	C	628	PCW	C8-N-C7	11.92	77.67	108.98	5	10
3	B	210	PCW	C8-N-C7	11.92	77.68	108.98	7	10
3	B	201	PCW	C8-N-C7	11.91	77.68	108.98	5	10
3	A	405	PCW	C8-N-C7	11.91	77.69	108.98	3	10
3	C	607	PCW	C8-N-C7	11.91	77.70	108.98	4	10
3	C	626	PCW	C8-N-C7	11.91	77.70	108.98	9	10
3	B	215	PCW	C8-N-C7	11.90	77.71	108.98	9	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	C	613	PCW	C8-N-C7	11.90	77.73	108.98	2	10
3	C	621	PCW	C8-N-C7	11.89	77.74	108.98	5	10
3	C	603	PCW	C8-N-C7	11.87	77.81	108.98	9	10
3	A	409	PCW	C8-N-C7	11.86	77.81	108.98	5	10
3	B	212	PCW	C8-N-C6	10.21	82.16	108.98	9	10
3	C	608	PCW	C8-N-C6	10.20	82.19	108.98	3	10
3	C	606	PCW	C8-N-C6	10.20	82.19	108.98	1	10
3	B	218	PCW	C8-N-C6	10.18	82.24	108.98	1	10
3	C	604	PCW	C8-N-C6	10.16	82.30	108.98	5	10
3	C	625	PCW	C8-N-C6	10.15	82.32	108.98	2	10
3	C	607	PCW	C8-N-C6	10.12	82.38	108.98	6	10
3	B	217	PCW	C8-N-C6	10.12	82.39	108.98	3	10
3	B	209	PCW	C8-N-C6	10.12	82.41	108.98	7	10
3	C	626	PCW	C8-N-C6	10.11	82.42	108.98	8	10
3	B	215	PCW	C8-N-C6	10.10	82.44	108.98	10	10
3	B	233	PCW	C8-N-C6	10.10	82.45	108.98	3	10
3	C	605	PCW	C8-N-C6	10.09	82.46	108.98	1	10
3	A	409	PCW	C8-N-C6	10.09	82.47	108.98	5	10
3	C	622	PCW	C8-N-C6	10.07	82.52	108.98	4	10
3	B	219	PCW	C8-N-C6	10.07	82.52	108.98	4	10
3	C	627	PCW	C8-N-C6	10.07	82.53	108.98	2	10
3	B	206	PCW	C8-N-C6	10.07	82.53	108.98	5	10
3	C	628	PCW	C8-N-C6	10.07	82.53	108.98	9	10
3	A	410	PCW	C8-N-C6	10.06	82.54	108.98	7	10
3	B	220	PCW	C8-N-C6	10.06	82.55	108.98	5	10
3	B	213	PCW	C8-N-C6	10.06	82.56	108.98	6	10
3	C	603	PCW	C8-N-C6	10.05	82.57	108.98	8	10
3	C	613	PCW	C8-N-C6	10.05	82.57	108.98	7	10
3	C	620	PCW	C8-N-C6	10.05	82.57	108.98	2	10
3	B	222	PCW	C8-N-C6	10.05	82.58	108.98	9	10
3	C	616	PCW	C8-N-C6	10.05	82.58	108.98	6	10
3	B	210	PCW	C8-N-C6	10.05	82.58	108.98	6	10
3	B	216	PCW	C8-N-C6	10.05	82.59	108.98	6	10
3	A	401	PCW	C8-N-C6	10.04	82.59	108.98	9	10
3	C	614	PCW	C8-N-C6	10.04	82.59	108.98	2	10
3	C	621	PCW	C8-N-C6	10.04	82.59	108.98	10	10
3	A	408	PCW	C8-N-C6	10.03	82.64	108.98	1	10
3	A	406	PCW	C8-N-C6	10.03	82.64	108.98	6	10
3	B	232	PCW	C8-N-C6	10.02	82.66	108.98	6	10
3	C	618	PCW	C8-N-C6	10.02	82.67	108.98	1	10
3	B	231	PCW	C8-N-C6	10.01	82.67	108.98	1	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	B	201	PCW	C8-N-C6	10.01	82.67	108.98	8	10
3	A	403	PCW	C8-N-C6	10.01	82.69	108.98	5	10
3	C	617	PCW	C8-N-C6	10.01	82.69	108.98	7	10
3	C	619	PCW	C8-N-C6	10.01	82.69	108.98	9	10
3	B	202	PCW	C8-N-C6	10.00	82.70	108.98	8	10
3	B	203	PCW	C8-N-C6	9.99	82.73	108.98	1	10
3	A	405	PCW	C8-N-C6	9.99	82.75	108.98	1	10
3	C	611	PCW	C8-N-C6	9.98	82.75	108.98	8	10
3	A	402	PCW	C8-N-C6	9.98	82.77	108.98	7	10
3	B	203	PCW	O4P-P-O2P	7.71	78.39	108.94	6	10
3	B	232	PCW	O4P-P-O2P	7.57	78.94	108.94	6	10
4	B	223	17F	O2-P1-O6	6.34	78.83	107.57	5	10
4	B	223	17F	O2-P1-O3	6.28	79.10	107.57	3	10
4	C	633	17F	O2-P1-O6	6.24	79.29	107.57	1	10
4	C	633	17F	O2-P1-O3	6.11	79.87	107.57	5	10
3	B	232	PCW	O1P-P-O2P	5.87	85.12	112.44	7	10
3	B	203	PCW	O1P-P-O2P	5.87	85.16	112.44	2	10
3	B	232	PCW	O3P-P-O2P	5.80	85.93	108.94	4	10
3	B	203	PCW	O3P-P-O2P	5.77	86.07	108.94	8	10
7	B	237	EWS	CAV-CBA-CAX	5.75	109.32	106.15	4	10
4	C	633	17F	O3-C1-C2	5.72	113.05	108.06	1	10
3	A	403	PCW	C8-N-C5	5.53	87.94	109.91	7	10
3	B	203	PCW	C8-N-C5	5.47	88.15	109.91	6	10
3	C	608	PCW	C8-N-C5	5.48	88.15	109.91	8	10
3	C	614	PCW	C8-N-C5	5.47	88.18	109.91	4	10
3	B	231	PCW	C8-N-C5	5.45	88.26	109.91	5	10
3	B	219	PCW	C8-N-C5	5.43	88.32	109.91	10	10
3	C	621	PCW	C8-N-C5	5.42	88.35	109.91	6	10
3	C	618	PCW	C8-N-C5	5.42	88.37	109.91	10	10
3	A	401	PCW	C8-N-C5	5.42	88.38	109.91	10	10
3	B	201	PCW	C8-N-C5	5.42	88.38	109.91	6	10
3	C	606	PCW	C8-N-C5	5.41	88.41	109.91	8	10
3	B	210	PCW	C8-N-C5	5.41	88.41	109.91	9	10
3	A	405	PCW	C8-N-C5	5.41	88.42	109.91	2	10
3	B	216	PCW	C8-N-C5	5.41	88.42	109.91	7	10
3	C	605	PCW	C8-N-C5	5.41	88.42	109.91	7	10
3	C	626	PCW	C8-N-C5	5.41	88.42	109.91	3	10
3	C	607	PCW	C8-N-C5	5.40	88.43	109.91	3	10
3	C	625	PCW	C8-N-C5	5.40	88.43	109.91	7	10
3	C	619	PCW	C8-N-C5	5.40	88.45	109.91	6	10
3	B	202	PCW	C8-N-C5	5.40	88.46	109.91	2	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	B	220	PCW	C8-N-C5	5.40	88.46	109.91	8	10
3	C	604	PCW	C8-N-C5	5.40	88.46	109.91	7	10
3	C	617	PCW	C8-N-C5	5.39	88.48	109.91	2	10
3	C	620	PCW	C8-N-C5	5.39	88.47	109.91	6	10
3	B	212	PCW	C8-N-C5	5.39	88.48	109.91	10	10
3	A	408	PCW	C8-N-C5	5.39	88.50	109.91	7	10
3	B	209	PCW	C8-N-C5	5.38	88.52	109.91	4	10
3	B	215	PCW	C8-N-C5	5.38	88.52	109.91	6	10
3	C	627	PCW	C8-N-C5	5.38	88.52	109.91	3	10
3	A	402	PCW	C8-N-C5	5.38	88.53	109.91	1	10
3	C	603	PCW	C8-N-C5	5.38	88.53	109.91	10	10
3	B	213	PCW	C8-N-C5	5.37	88.55	109.91	3	10
3	C	613	PCW	C8-N-C5	5.37	88.56	109.91	9	10
3	A	406	PCW	C8-N-C5	5.37	88.57	109.91	4	10
3	B	233	PCW	C8-N-C5	5.37	88.56	109.91	6	10
3	C	628	PCW	C8-N-C5	5.37	88.56	109.91	6	10
3	A	410	PCW	C8-N-C5	5.37	88.57	109.91	6	10
3	B	206	PCW	C8-N-C5	5.37	88.57	109.91	9	10
3	C	611	PCW	C8-N-C5	5.37	88.58	109.91	10	10
3	C	622	PCW	C8-N-C5	5.36	88.59	109.91	7	10
3	B	232	PCW	C8-N-C5	5.36	88.59	109.91	4	10
3	B	218	PCW	C8-N-C5	5.36	88.60	109.91	7	10
3	C	616	PCW	C8-N-C5	5.36	88.60	109.91	8	10
3	A	409	PCW	C8-N-C5	5.36	88.62	109.91	8	10
3	B	217	PCW	C8-N-C5	5.34	88.69	109.91	5	10
3	B	222	PCW	C8-N-C5	5.30	88.83	109.91	6	10
4	B	223	17F	O2-P1-O1	4.80	90.12	112.44	8	10
4	C	633	17F	O2-P1-O1	4.76	90.30	112.44	4	10
4	B	226	17F	O3-C1-C2	4.11	111.64	108.06	7	10
4	C	630	17F	O3-C1-C2	4.11	111.64	108.06	5	10
4	B	223	17F	O3-C1-C2	4.10	111.64	108.06	1	9
7	B	237	EWS	CBA-CAX-NAW	4.03	107.49	110.22	4	10
4	B	230	17F	O3-C1-C2	3.83	111.39	108.06	1	10
4	B	229	17F	O3-C1-C2	3.82	111.39	108.06	4	10
4	C	631	17F	O3-C1-C2	3.80	111.37	108.06	7	10
4	A	411	17F	O3-C1-C2	3.76	111.33	108.06	8	10
3	B	203	PCW	O1P-P-O4P	3.68	124.23	107.57	3	10
4	C	634	17F	O3-C1-C2	3.66	111.25	108.06	1	10
4	B	225	17F	O3-C1-C2	3.66	111.25	108.06	3	10
4	B	227	17F	O3-C1-C2	3.65	111.24	108.06	7	10
3	B	232	PCW	O1P-P-O4P	3.54	123.62	107.57	7	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	B	224	17F	O3-C1-C2	3.49	111.11	108.06	10	10
4	B	228	17F	O3-C1-C2	3.48	111.09	108.06	3	9
4	C	631	17F	O7-C7-O8	3.46	132.28	123.63	2	10
4	B	224	17F	O5-C3-O4	3.42	116.33	124.08	10	10
4	B	229	17F	O5-C3-O4	3.40	116.36	124.08	5	10
4	C	634	17F	O5-C3-O4	3.39	116.39	124.08	9	10
3	C	627	PCW	C6-N-C5	3.38	123.33	109.91	1	10
4	B	226	17F	O5-C3-O4	3.38	116.42	124.08	8	10
3	B	206	PCW	C6-N-C5	3.37	123.31	109.91	4	10
3	B	209	PCW	C6-N-C5	3.36	123.28	109.91	5	10
3	B	201	PCW	C6-N-C5	3.36	123.27	109.91	6	10
3	C	621	PCW	C6-N-C5	3.36	123.27	109.91	6	10
3	C	616	PCW	C6-N-C5	3.36	123.26	109.91	9	10
3	A	410	PCW	C6-N-C5	3.36	123.26	109.91	9	10
4	B	223	17F	O5-C3-O4	3.36	116.46	124.08	7	10
4	B	230	17F	O5-C3-O4	3.36	116.46	124.08	4	10
3	C	613	PCW	C6-N-C5	3.36	123.25	109.91	8	10
3	C	604	PCW	C6-N-C5	3.35	123.24	109.91	5	10
3	C	626	PCW	C6-N-C5	3.35	123.24	109.91	4	10
4	B	227	17F	O5-C3-O4	3.35	116.47	124.08	7	10
4	C	632	17F	O5-C3-O4	3.35	116.47	124.08	3	10
3	B	218	PCW	C6-N-C5	3.35	123.22	109.91	1	10
3	A	403	PCW	C6-N-C5	3.35	123.21	109.91	7	10
3	A	409	PCW	C6-N-C5	3.35	123.21	109.91	3	10
3	B	215	PCW	C6-N-C5	3.34	123.20	109.91	10	10
3	C	608	PCW	C6-N-C5	3.35	123.21	109.91	8	10
4	C	635	17F	O5-C3-O4	3.34	116.49	124.08	4	10
3	B	202	PCW	C6-N-C5	3.34	123.19	109.91	9	10
3	C	619	PCW	C6-N-C5	3.34	123.18	109.91	5	10
3	A	402	PCW	C6-N-C5	3.33	123.16	109.91	5	10
3	B	219	PCW	C6-N-C5	3.33	123.16	109.91	10	10
4	B	228	17F	O5-C3-O4	3.33	116.52	124.08	10	10
4	C	635	17F	O3-C1-C2	3.33	110.96	108.06	2	10
3	B	203	PCW	C6-N-C5	3.33	123.14	109.91	6	10
4	B	225	17F	O5-C3-O4	3.33	116.53	124.08	6	10
3	B	222	PCW	C6-N-C5	3.33	123.14	109.91	2	10
3	C	606	PCW	C6-N-C5	3.33	123.13	109.91	8	10
3	C	614	PCW	C6-N-C5	3.33	123.13	109.91	2	10
3	C	607	PCW	C6-N-C5	3.32	123.12	109.91	6	10
4	C	630	17F	O5-C3-O4	3.32	116.54	124.08	5	10
3	B	212	PCW	C6-N-C5	3.32	123.12	109.91	6	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	411	17F	O5-C3-O4	3.32	116.54	124.08	8	10
3	A	408	PCW	C6-N-C5	3.32	123.10	109.91	7	10
3	B	216	PCW	C6-N-C5	3.32	123.09	109.91	4	10
4	C	631	17F	O5-C3-O4	3.32	116.55	124.08	7	10
3	C	625	PCW	C6-N-C5	3.31	123.09	109.91	9	10
4	B	234	17F	O5-C3-O4	3.31	116.57	124.08	5	10
3	C	603	PCW	C6-N-C5	3.31	123.07	109.91	10	10
4	C	633	17F	O5-C3-O4	3.31	116.57	124.08	9	10
3	A	401	PCW	C6-N-C5	3.30	123.03	109.91	3	10
3	C	617	PCW	C6-N-C5	3.30	123.03	109.91	7	10
3	C	611	PCW	C6-N-C5	3.30	123.02	109.91	7	10
3	B	213	PCW	C6-N-C5	3.29	123.01	109.91	3	10
3	C	622	PCW	C6-N-C5	3.30	123.01	109.91	10	10
3	C	628	PCW	C6-N-C5	3.30	123.01	109.91	2	10
3	B	231	PCW	C6-N-C5	3.29	122.98	109.91	1	10
3	C	605	PCW	C6-N-C5	3.29	122.98	109.91	6	10
3	A	405	PCW	C6-N-C5	3.29	122.98	109.91	2	10
3	B	232	PCW	C6-N-C5	3.29	122.98	109.91	10	10
3	A	406	PCW	C6-N-C5	3.29	122.97	109.91	5	10
3	B	233	PCW	C6-N-C5	3.28	122.95	109.91	2	10
3	C	620	PCW	C6-N-C5	3.28	122.95	109.91	1	10
3	B	220	PCW	C6-N-C5	3.28	122.93	109.91	1	10
3	B	217	PCW	C6-N-C5	3.27	122.90	109.91	4	10
3	C	618	PCW	C6-N-C5	3.26	122.88	109.91	1	10
3	B	210	PCW	C6-N-C5	3.25	122.81	109.91	3	10
4	B	234	17F	O3-C1-C2	3.23	110.88	108.06	6	10
4	C	634	17F	O7-C7-O8	3.14	131.48	123.63	6	10
4	B	228	17F	O7-C7-O8	3.13	131.47	123.63	10	10
4	C	632	17F	O3-C1-C2	3.12	110.78	108.06	3	10
4	B	234	17F	O7-C7-O8	3.00	131.14	123.63	6	10
4	B	223	17F	O3-P1-O1	2.99	120.80	108.94	10	10
4	C	635	17F	O7-C7-O8	2.99	131.10	123.63	5	10
4	C	630	17F	O7-C7-O8	2.98	131.08	123.63	6	10
4	B	230	17F	O7-C7-O8	2.97	131.05	123.63	10	10
4	C	632	17F	O7-C7-O8	2.97	131.05	123.63	9	10
4	B	229	17F	O7-C7-O8	2.95	131.01	123.63	3	10
4	B	223	17F	O7-C7-O8	2.94	130.97	123.63	8	10
4	B	224	17F	O7-C7-O8	2.93	130.94	123.63	10	10
4	C	633	17F	O7-C7-O8	2.92	130.93	123.63	5	10
4	B	227	17F	O7-C7-O8	2.89	130.87	123.63	6	10
4	A	411	17F	O7-C7-O8	2.89	130.84	123.63	8	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	B	226	17F	O7-C7-O8	2.88	130.84	123.63	10	10
4	C	633	17F	O3-P1-O1	2.88	120.36	108.94	10	10
4	B	225	17F	O7-C7-O8	2.80	130.64	123.63	9	10
3	C	624	PCW	C8-N-C7	2.72	101.84	108.98	5	10
3	C	615	PCW	C8-N-C7	2.72	101.84	108.98	6	10
3	B	205	PCW	C8-N-C7	2.71	101.85	108.98	5	10
3	B	221	PCW	C8-N-C7	2.71	101.86	108.98	8	10
4	C	634	17F	C5-O9-C17	2.71	111.31	117.80	3	10
3	C	601	PCW	C8-N-C7	2.70	101.89	108.98	8	10
3	A	404	PCW	C8-N-C7	2.69	101.90	108.98	8	10
3	C	609	PCW	C8-N-C7	2.68	101.93	108.98	7	10
3	C	623	PCW	C8-N-C7	2.68	101.94	108.98	7	10
3	C	612	PCW	C8-N-C7	2.67	101.97	108.98	9	10
3	B	208	PCW	C8-N-C7	2.66	101.99	108.98	3	10
3	B	214	PCW	C8-N-C7	2.66	101.99	108.98	1	10
3	C	629	PCW	C8-N-C7	2.66	101.99	108.98	7	10
3	A	407	PCW	C8-N-C7	2.65	102.02	108.98	1	10
3	B	211	PCW	C8-N-C7	2.64	102.03	108.98	2	10
3	C	610	PCW	C8-N-C7	2.64	102.03	108.98	10	10
3	B	207	PCW	C8-N-C7	2.64	102.03	108.98	3	10
3	C	602	PCW	C8-N-C7	2.63	102.06	108.98	1	10
4	C	631	17F	C5-O9-C17	2.62	111.54	117.80	10	10
3	B	204	PCW	C8-N-C7	2.61	102.13	108.98	9	10
4	C	635	17F	O9-C17-O10	2.58	129.74	123.70	6	10
4	B	225	17F	C5-O9-C17	2.56	111.67	117.80	4	9
3	A	401	PCW	C7-N-C5	2.56	120.07	109.91	10	10
4	B	224	17F	C5-O9-C17	2.54	111.72	117.80	2	10
3	B	217	PCW	C7-N-C5	2.53	119.96	109.91	2	10
4	B	226	17F	C5-O9-C17	2.52	111.75	117.80	2	9
4	B	229	17F	C5-O9-C17	2.53	111.75	117.80	6	10
5	B	235	GNP	O1G-PG-N3B	2.52	108.05	111.77	8	10
3	C	627	PCW	C7-N-C5	2.52	119.93	109.91	5	10
3	C	625	PCW	C7-N-C5	2.52	119.92	109.91	5	10
3	C	606	PCW	C7-N-C5	2.51	119.89	109.91	10	10
3	C	613	PCW	C7-N-C5	2.51	119.89	109.91	1	10
4	C	633	17F	O6-P1-O1	2.51	118.87	108.94	2	10
3	B	203	PCW	C7-N-C5	2.50	119.86	109.91	5	10
3	C	619	PCW	C7-N-C5	2.50	119.86	109.91	2	10
3	B	216	PCW	C7-N-C5	2.50	119.85	109.91	2	10
4	B	230	17F	C5-O9-C17	2.50	111.82	117.80	4	10
4	A	411	17F	C5-O9-C17	2.49	111.83	117.80	3	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	B	228	17F	O9-C17-O10	2.49	129.53	123.70	2	10
3	C	611	PCW	C7-N-C5	2.49	119.81	109.91	4	10
3	C	622	PCW	C7-N-C5	2.49	119.81	109.91	7	10
3	B	220	PCW	C7-N-C5	2.49	119.80	109.91	9	10
3	B	222	PCW	C7-N-C5	2.49	119.79	109.91	7	10
3	C	604	PCW	C7-N-C5	2.49	119.79	109.91	3	10
3	B	212	PCW	C7-N-C5	2.48	119.78	109.91	8	10
3	B	231	PCW	C7-N-C5	2.48	119.77	109.91	5	10
3	B	232	PCW	C7-N-C5	2.48	119.77	109.91	9	10
3	C	605	PCW	C7-N-C5	2.48	119.75	109.91	3	10
4	C	630	17F	C5-O9-C17	2.47	111.89	117.80	5	10
3	B	202	PCW	C7-N-C5	2.46	119.70	109.91	10	10
3	B	233	PCW	C7-N-C5	2.46	119.70	109.91	8	10
3	C	617	PCW	C7-N-C5	2.46	119.70	109.91	5	10
3	C	618	PCW	C7-N-C5	2.46	119.71	109.91	6	10
3	A	408	PCW	C7-N-C5	2.46	119.70	109.91	10	10
3	C	616	PCW	C7-N-C5	2.46	119.70	109.91	3	10
4	B	226	17F	O9-C17-O10	2.46	129.46	123.70	8	10
3	A	403	PCW	C7-N-C5	2.46	119.68	109.91	9	10
3	C	621	PCW	C7-N-C5	2.45	119.67	109.91	1	10
3	C	603	PCW	C7-N-C5	2.45	119.66	109.91	10	10
3	B	210	PCW	C7-N-C5	2.45	119.65	109.91	5	10
3	C	620	PCW	C7-N-C5	2.45	119.66	109.91	10	10
3	A	402	PCW	C7-N-C5	2.45	119.65	109.91	1	10
3	A	405	PCW	C7-N-C5	2.44	119.63	109.91	5	10
3	B	213	PCW	C7-N-C5	2.45	119.63	109.91	9	10
3	B	201	PCW	C7-N-C5	2.44	119.62	109.91	9	10
3	C	626	PCW	C7-N-C5	2.44	119.61	109.91	3	10
3	B	215	PCW	C7-N-C5	2.44	119.60	109.91	9	10
3	B	218	PCW	C7-N-C5	2.44	119.59	109.91	10	10
4	C	632	17F	C5-O9-C17	2.44	111.97	117.80	7	10
3	B	206	PCW	C7-N-C5	2.43	119.56	109.91	3	10
3	B	209	PCW	C7-N-C5	2.43	119.56	109.91	3	10
3	A	406	PCW	C7-N-C5	2.42	119.53	109.91	10	10
4	B	224	17F	O9-C17-O10	2.42	129.36	123.70	8	10
3	A	409	PCW	C7-N-C5	2.41	119.51	109.91	10	10
3	B	219	PCW	C7-N-C5	2.41	119.51	109.91	1	10
3	C	608	PCW	C7-N-C5	2.41	119.50	109.91	2	10
3	C	614	PCW	C7-N-C5	2.41	119.50	109.91	10	10
4	B	223	17F	O6-P1-O1	2.41	118.50	108.94	8	10
3	C	607	PCW	C7-N-C5	2.41	119.48	109.91	1	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	B	225	17F	O9-C17-O10	2.41	129.33	123.70	10	10
4	C	632	17F	O9-C17-O10	2.41	129.33	123.70	3	10
4	B	227	17F	C5-O9-C17	2.39	112.07	117.80	1	10
4	C	630	17F	O9-C17-O10	2.39	129.29	123.70	8	10
3	A	410	PCW	C7-N-C5	2.39	119.39	109.91	3	10
4	C	633	17F	C5-O9-C17	2.38	112.09	117.80	4	9
3	C	628	PCW	C7-N-C5	2.38	119.36	109.91	5	10
4	B	223	17F	O9-C17-O10	2.36	129.23	123.70	4	10
4	B	234	17F	O9-C17-O10	2.36	129.22	123.70	7	10
4	B	229	17F	O9-C17-O10	2.35	129.19	123.70	10	10
4	C	633	17F	O9-C17-O10	2.33	129.14	123.70	5	10
4	A	411	17F	O9-C17-O10	2.31	129.11	123.70	4	10
4	B	227	17F	O9-C17-O10	2.31	129.11	123.70	5	10
4	B	228	17F	C5-O9-C17	2.31	112.28	117.80	7	8
4	C	631	17F	O7-C7-C8	2.30	104.81	111.83	2	8
4	B	234	17F	C5-O9-C17	2.30	112.29	117.80	2	10
4	C	633	17F	C6-C5-C4	2.27	106.50	111.78	10	1
4	B	230	17F	O9-C17-O10	2.26	128.99	123.70	2	10
4	C	631	17F	O9-C17-O10	2.24	128.95	123.70	1	8
4	B	223	17F	C5-O9-C17	2.24	112.44	117.80	10	2
4	C	634	17F	O9-C17-O10	2.18	128.79	123.70	3	10
3	C	625	PCW	C7-N-C6	2.11	114.52	108.98	1	2
3	B	217	PCW	C7-N-C6	2.08	114.43	108.98	9	1
3	C	604	PCW	C7-N-C6	2.06	114.40	108.98	10	1
3	B	203	PCW	O1P-P-O3P	2.06	116.91	107.57	2	4
3	C	611	PCW	C7-N-C6	2.06	114.38	108.98	2	1
3	C	605	PCW	C7-N-C6	2.06	114.38	108.98	10	2
3	B	233	PCW	C7-N-C6	2.04	114.34	108.98	9	1
3	C	618	PCW	C7-N-C6	2.04	114.34	108.98	7	2
3	B	222	PCW	C7-N-C6	2.03	114.31	108.98	1	1
3	C	628	PCW	C7-N-C6	2.03	114.31	108.98	3	2
3	B	212	PCW	C7-N-C6	2.03	114.31	108.98	7	3
3	C	603	PCW	C7-N-C6	2.03	114.30	108.98	9	1
3	C	626	PCW	C7-N-C6	2.02	114.28	108.98	8	1
3	B	206	PCW	C7-N-C6	2.02	114.28	108.98	3	1
3	A	408	PCW	C7-N-C6	2.02	114.27	108.98	6	1
3	C	620	PCW	C7-N-C6	2.01	114.27	108.98	2	1
3	B	220	PCW	C7-N-C6	2.01	114.26	108.98	2	1
3	C	606	PCW	C7-N-C6	2.01	114.26	108.98	6	1
3	C	616	PCW	C7-N-C6	2.01	114.25	108.98	1	1
3	A	401	PCW	C7-N-C6	2.01	114.25	108.98	9	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	B	201	PCW	C7-N-C6	2.01	114.25	108.98	1	1

There are no chirality outliers.

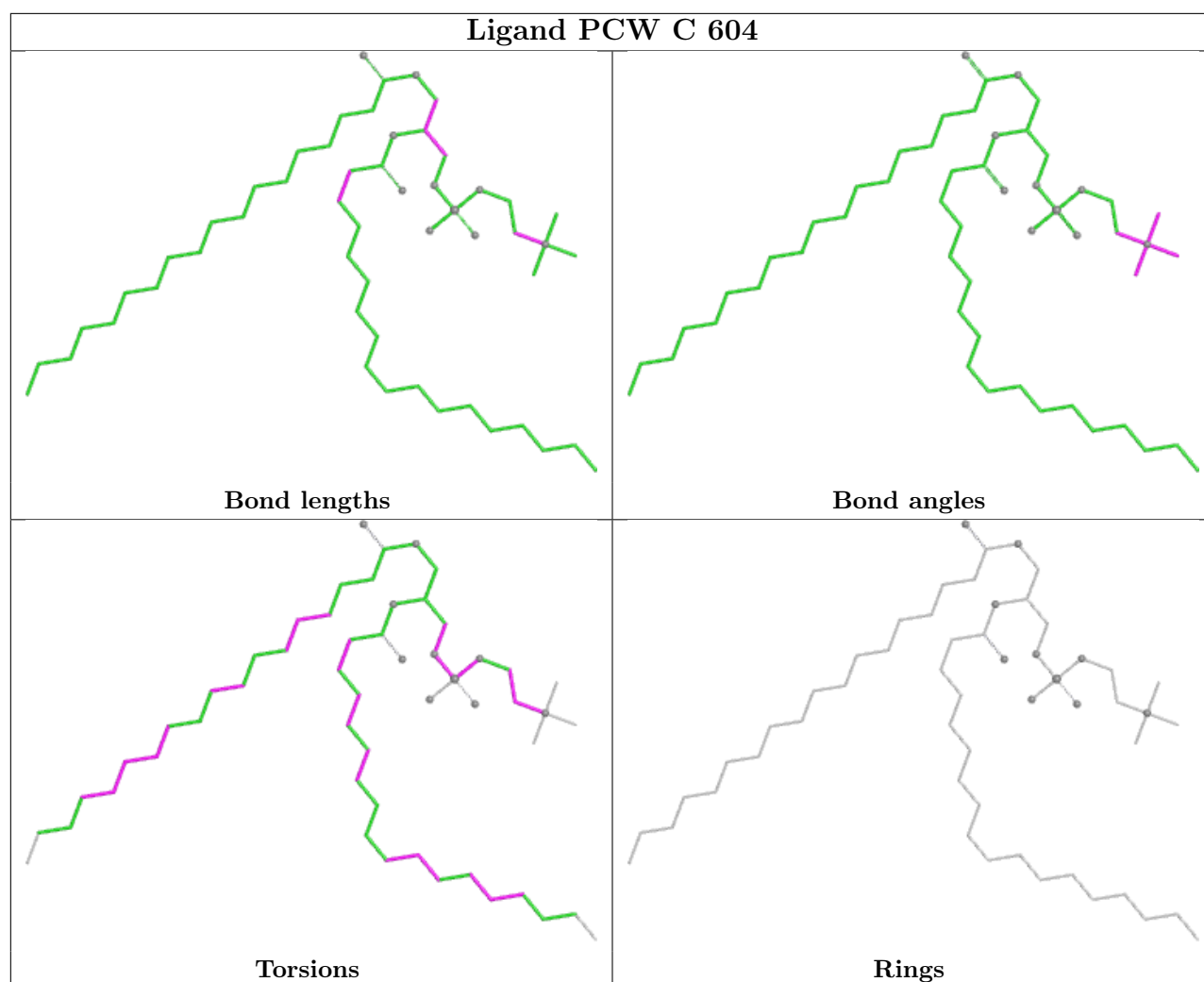
All unique torsion outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

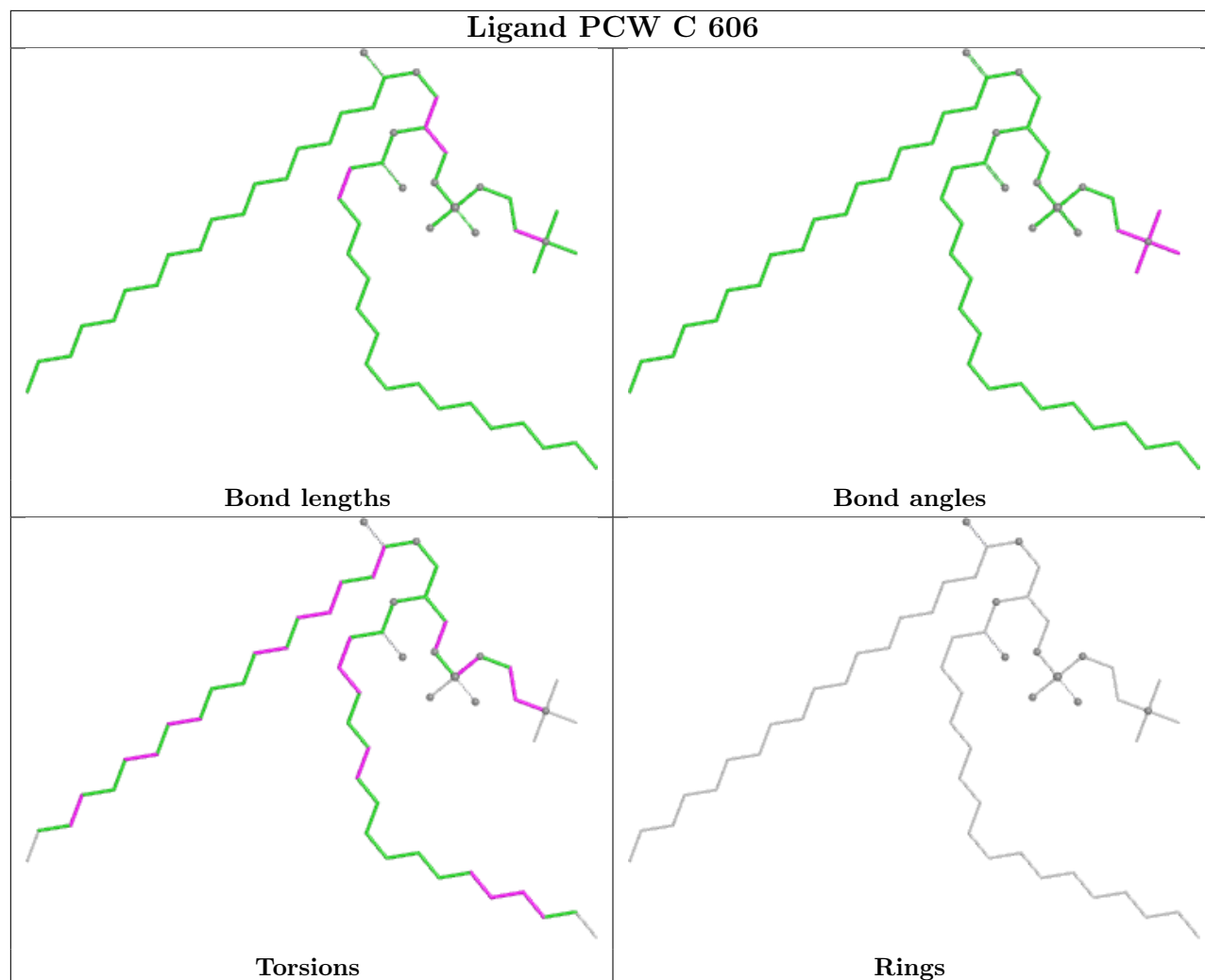
Mol	Chain	Res	Type	Atoms	Models (Total)
3	B	203	PCW	C5-C4-O4P-P	1
5	B	235	GNP	PG-N3B-PB-O1B	1

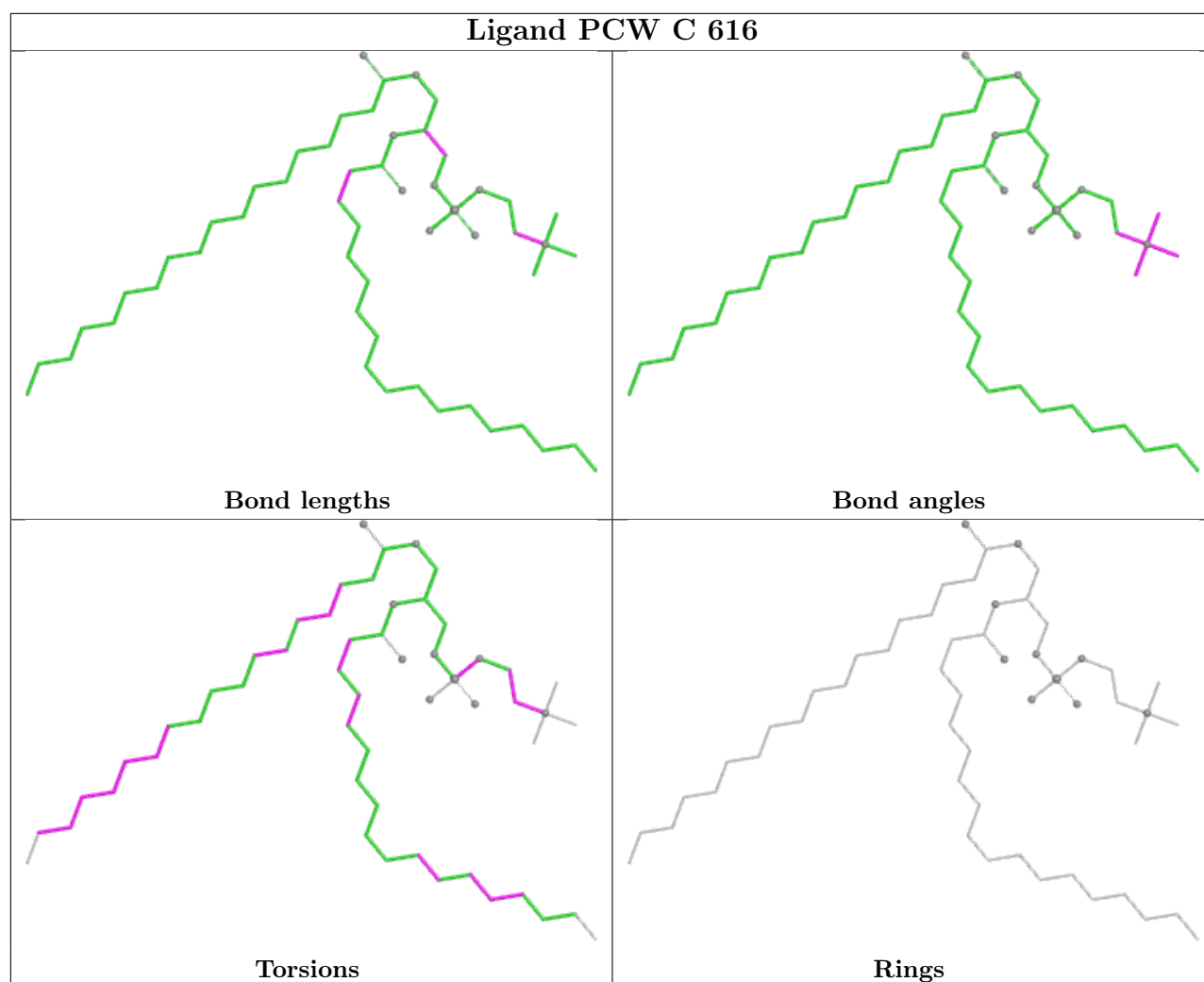
All unique ring outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
7	B	237	EWS	CAC-CAD-CAE-CAF-CAH-NAG	10

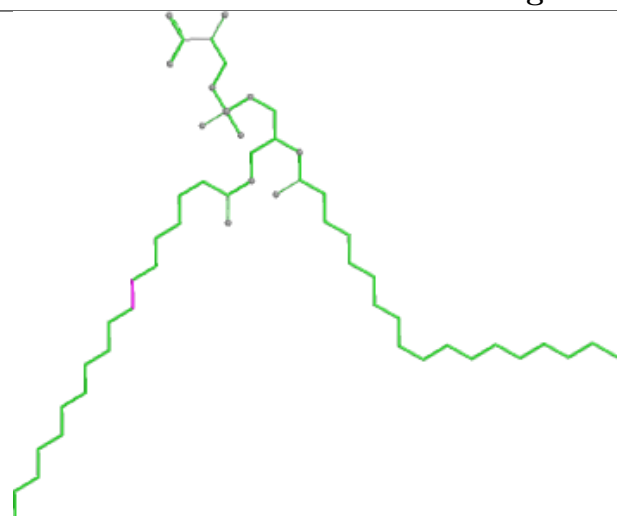
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



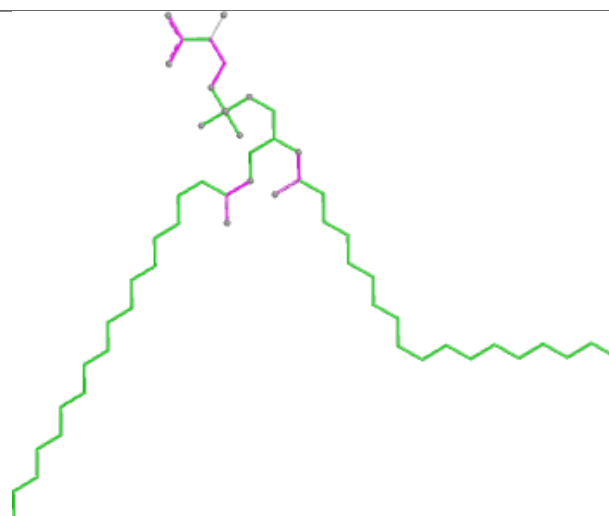




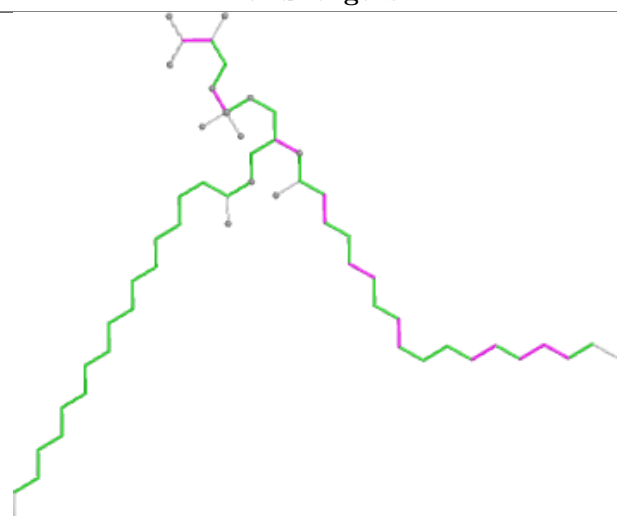
Ligand 17F C 635



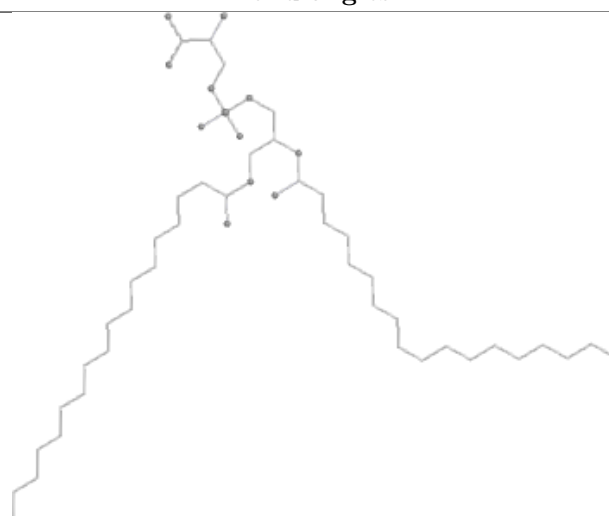
Bond lengths



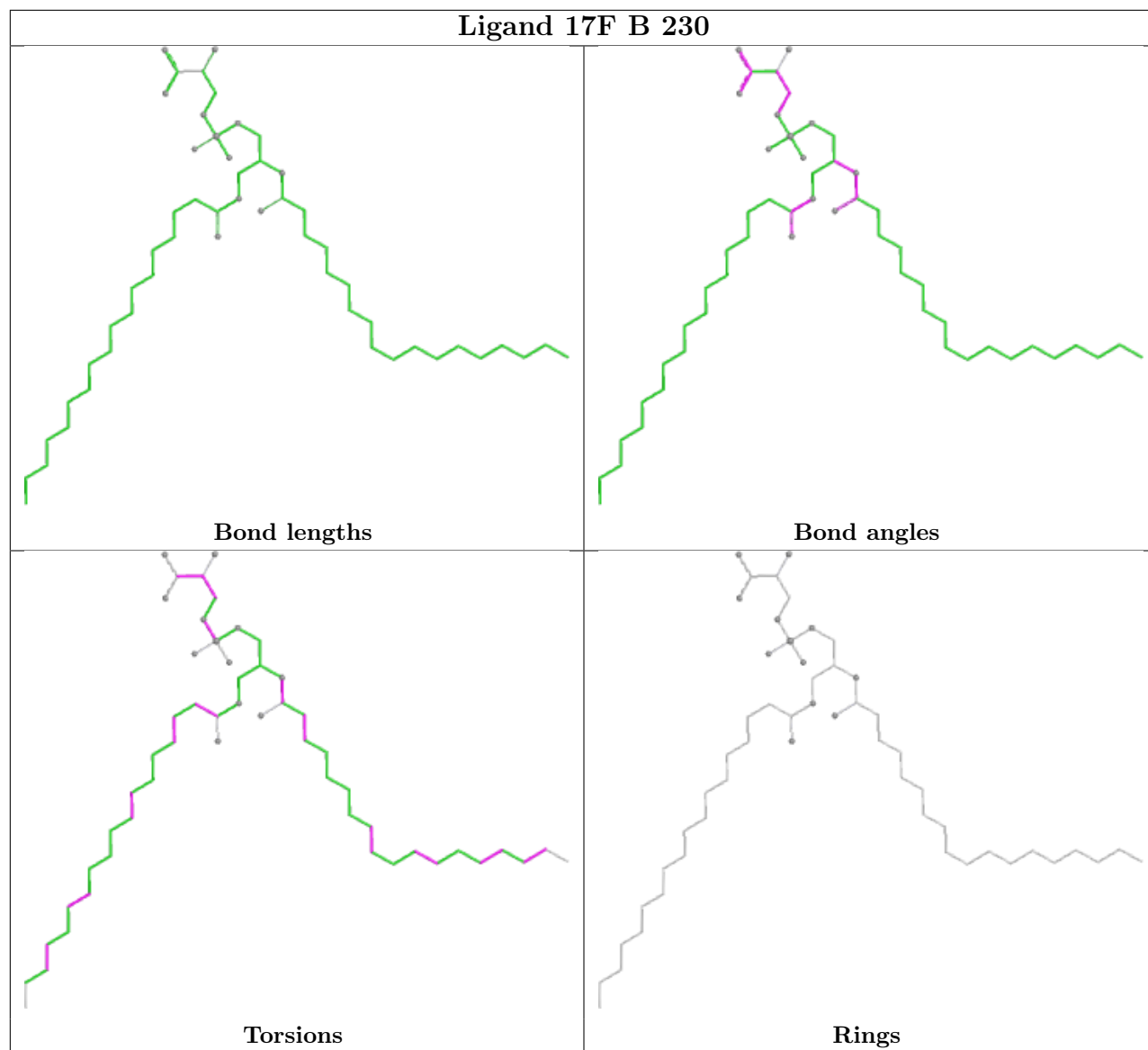
Bond angles

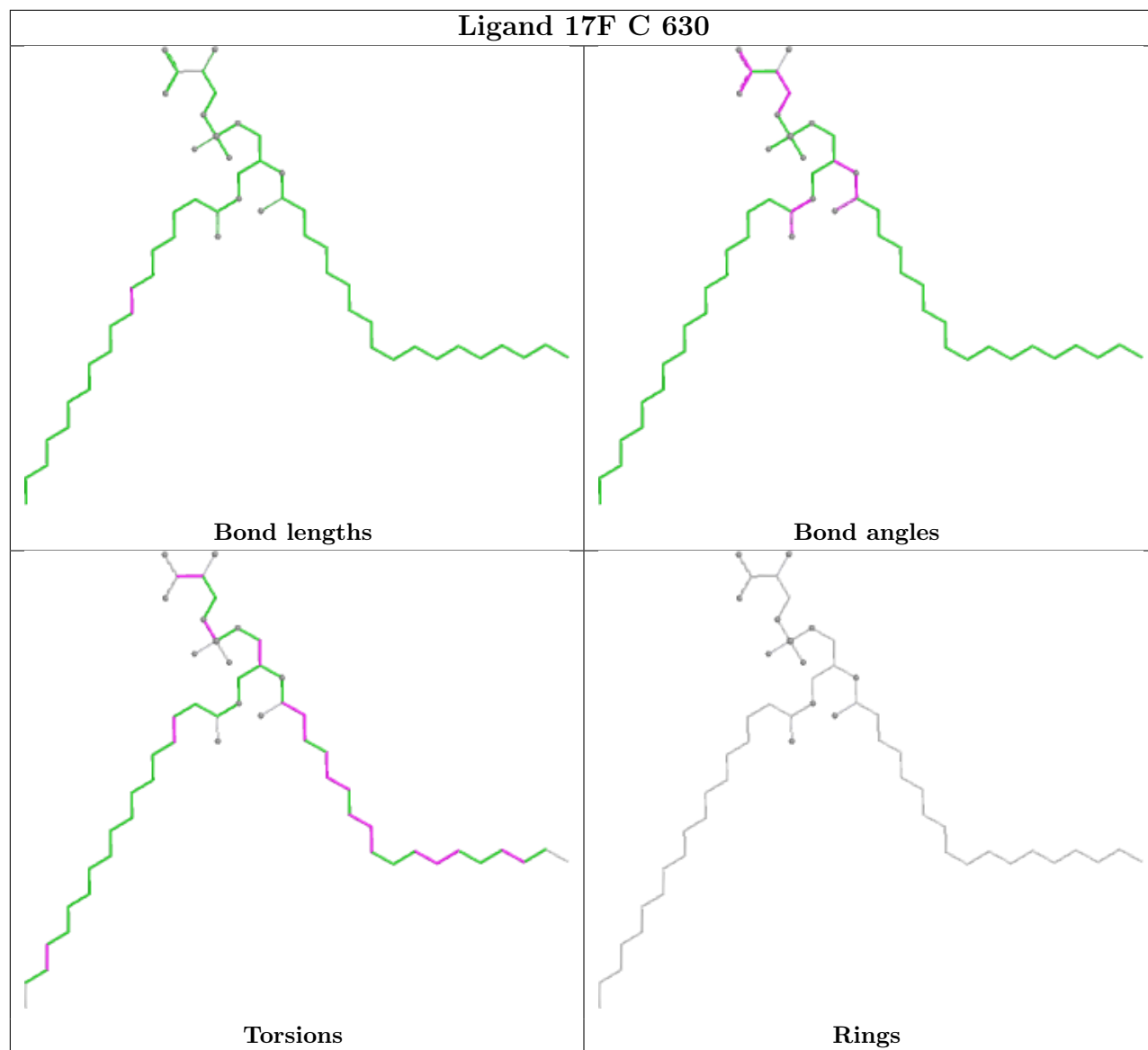


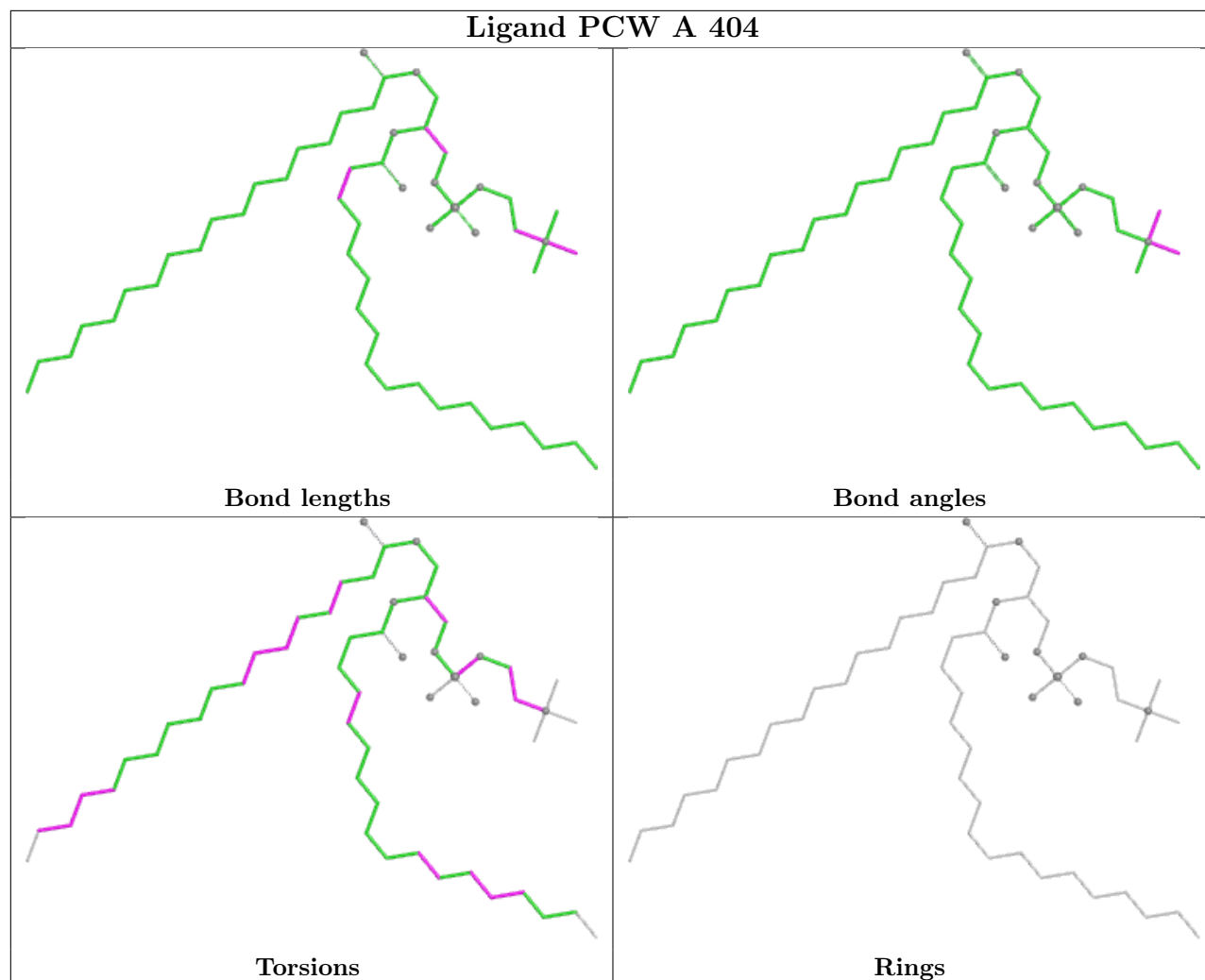
Torsions

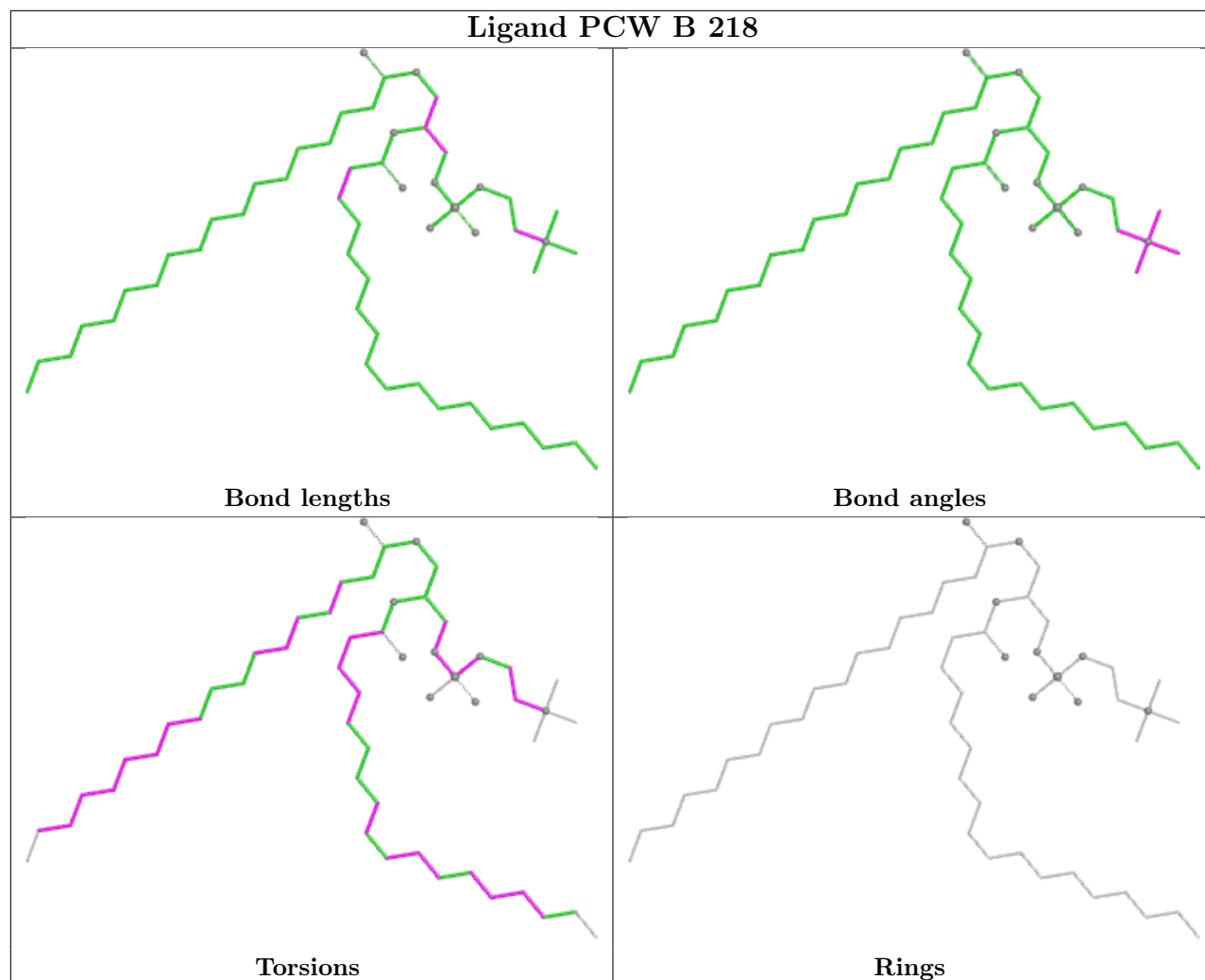


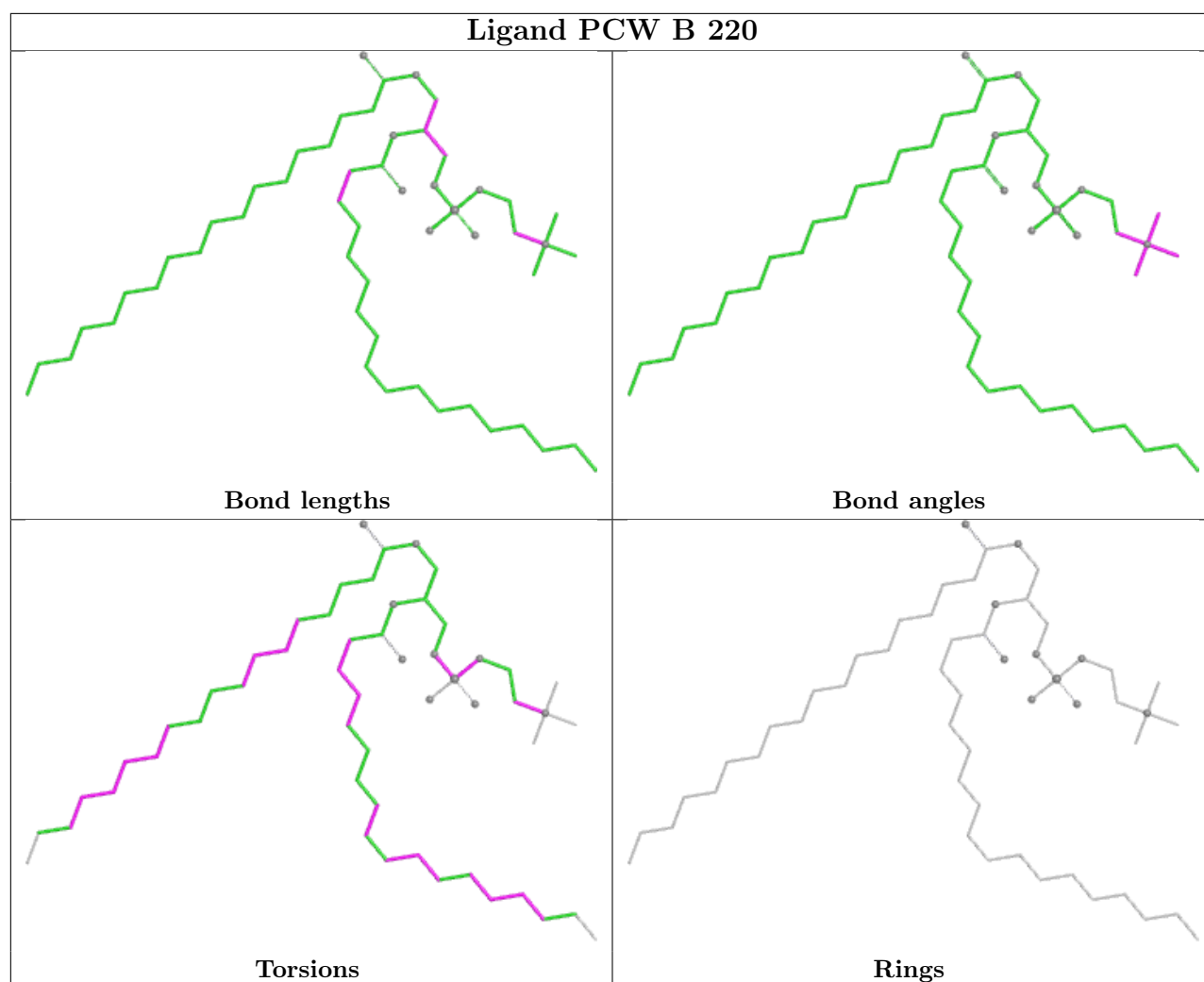
Rings

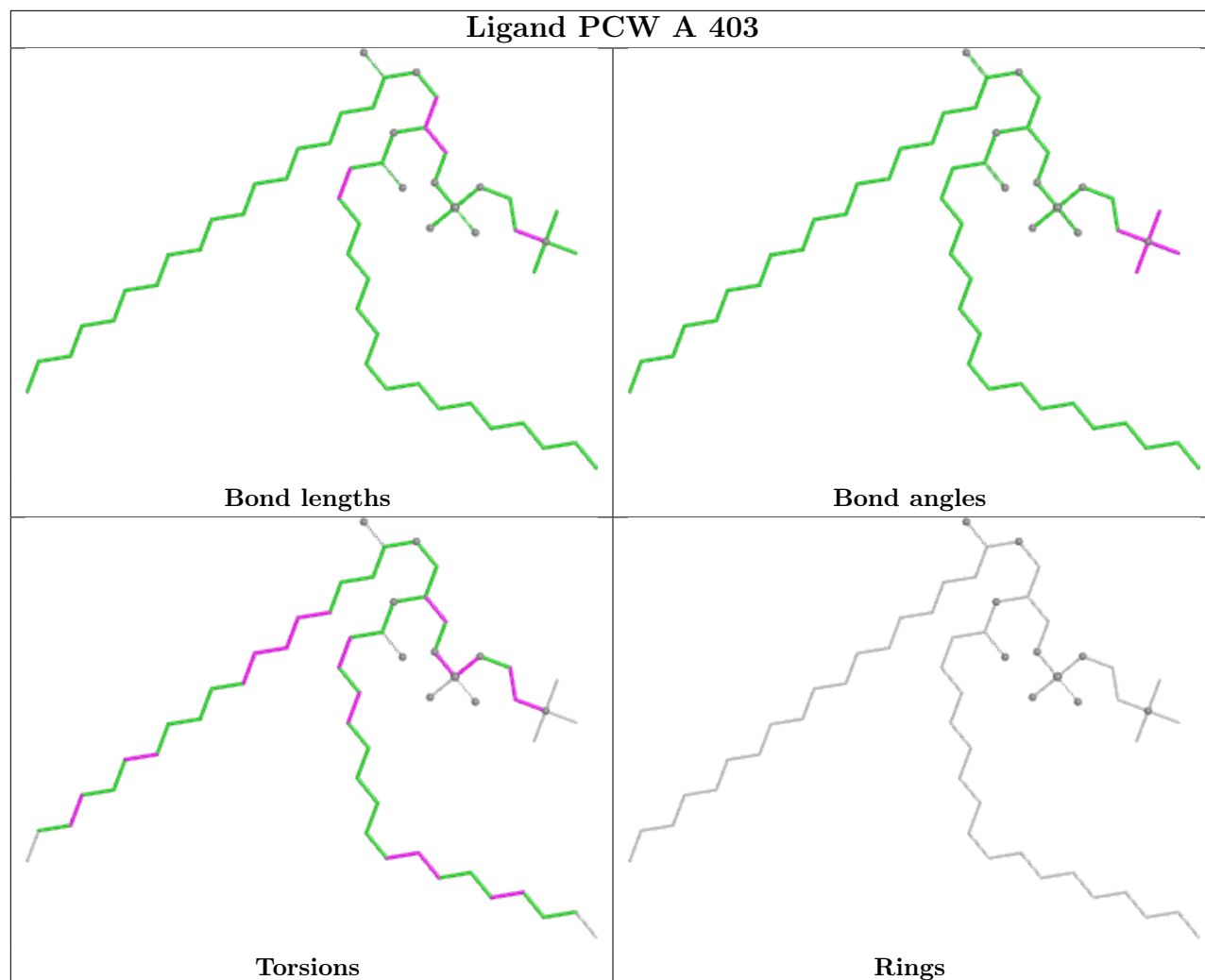


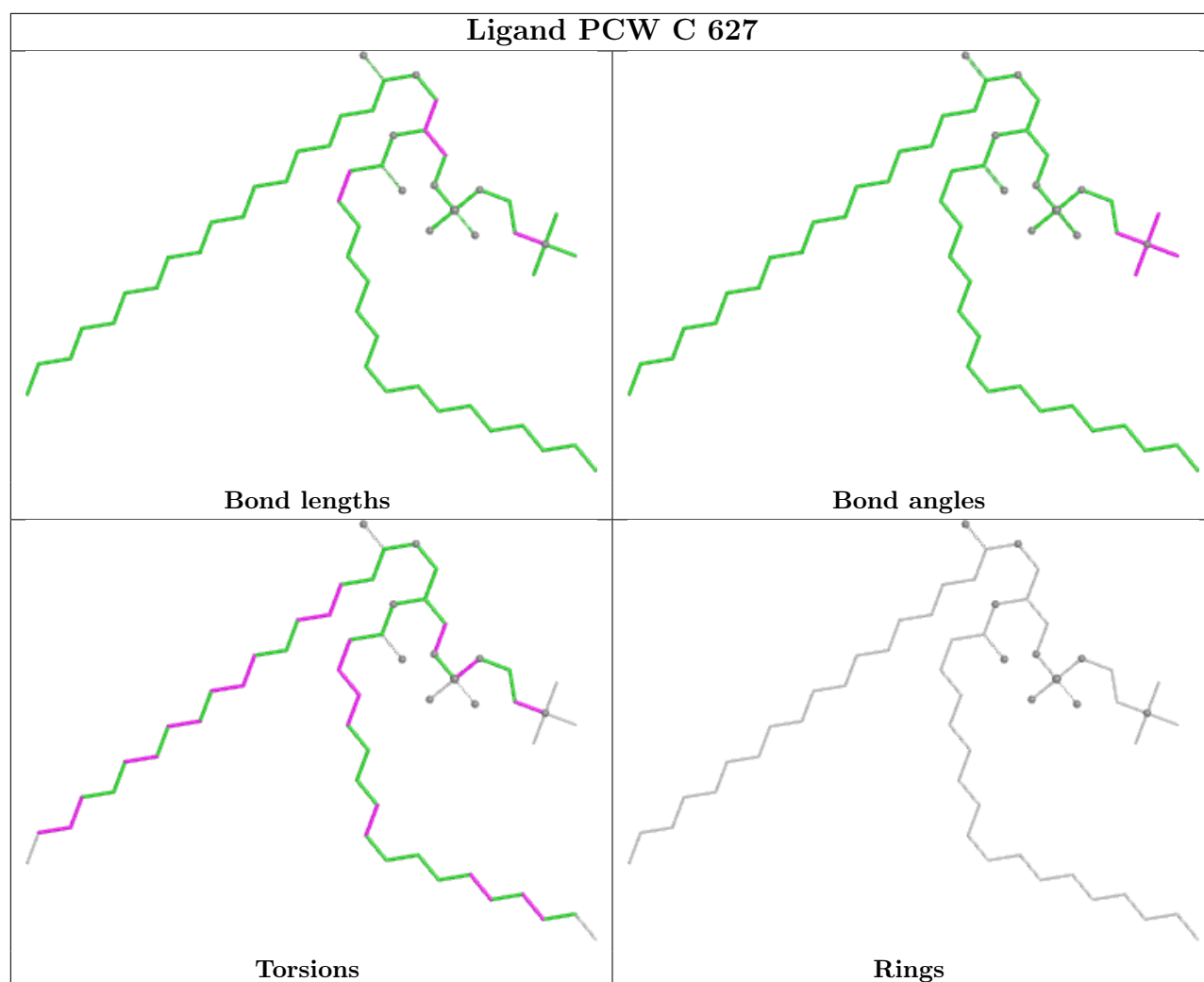


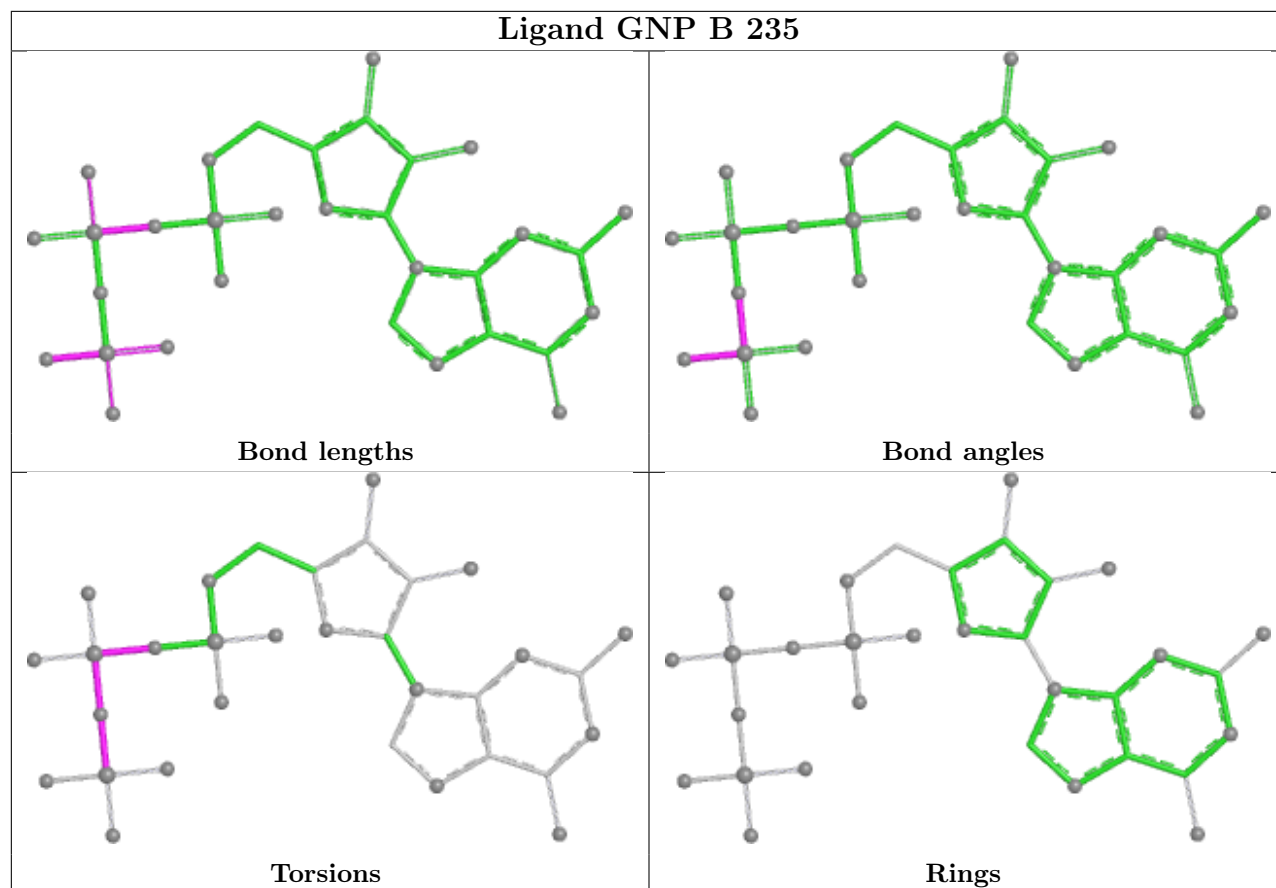


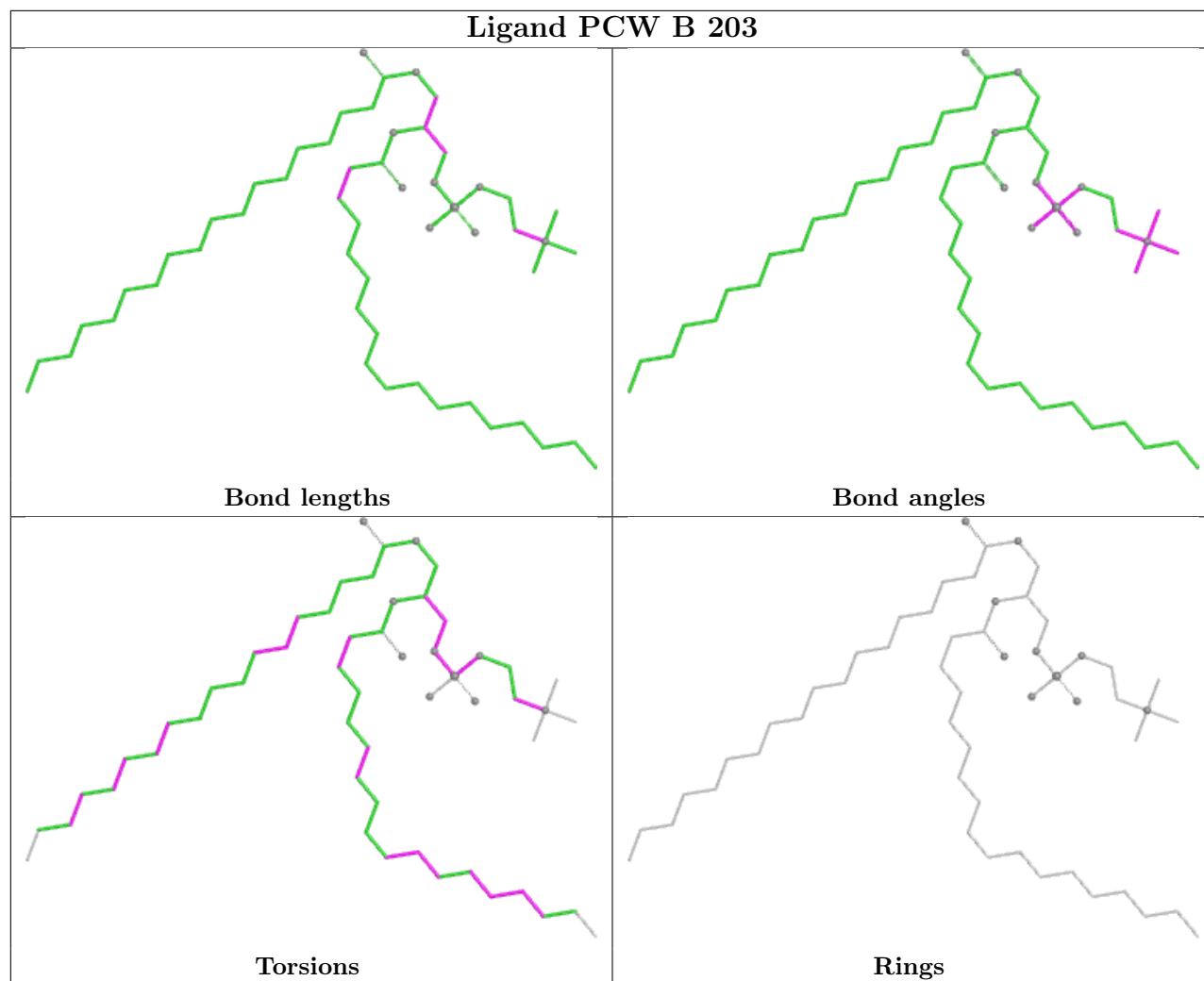


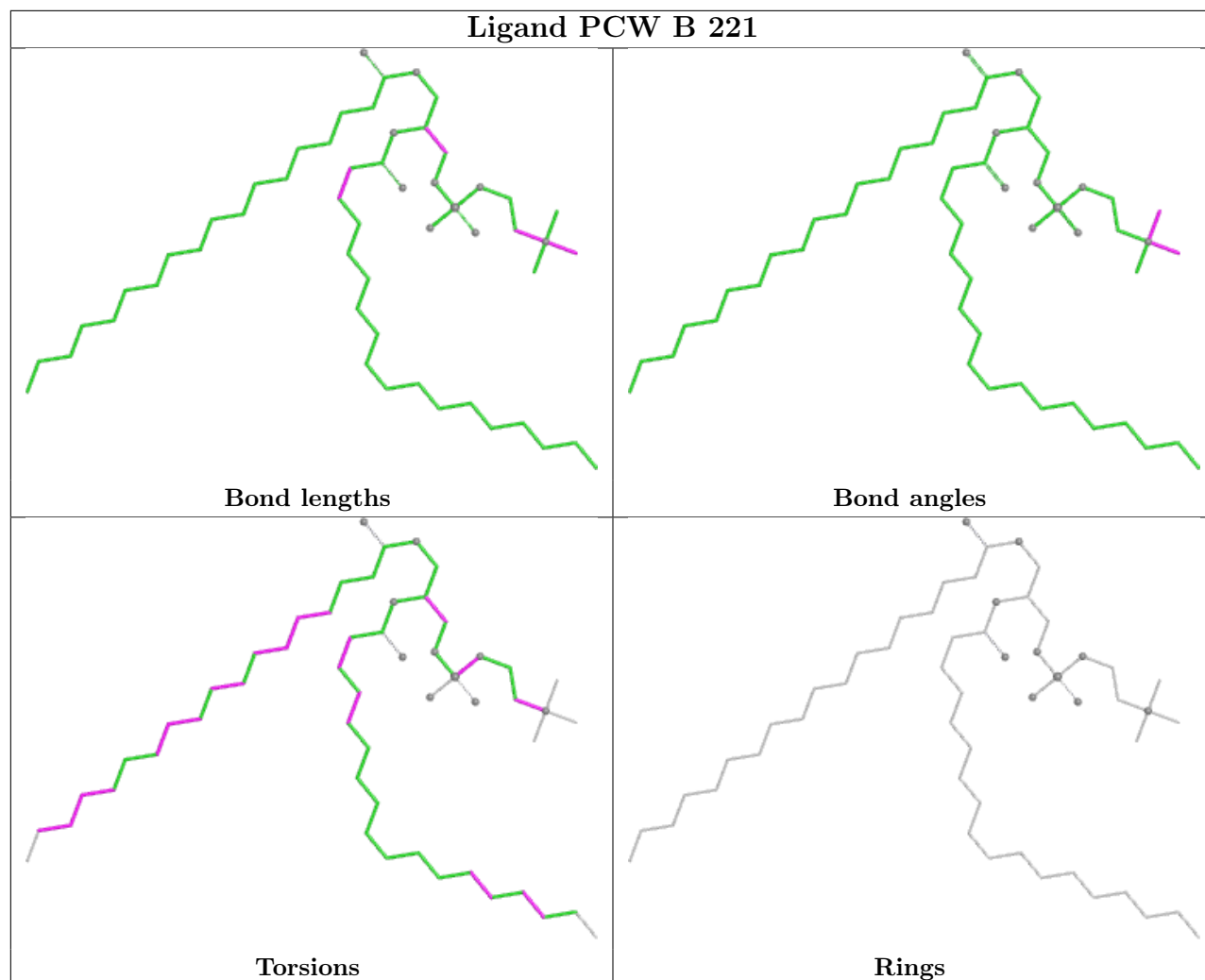


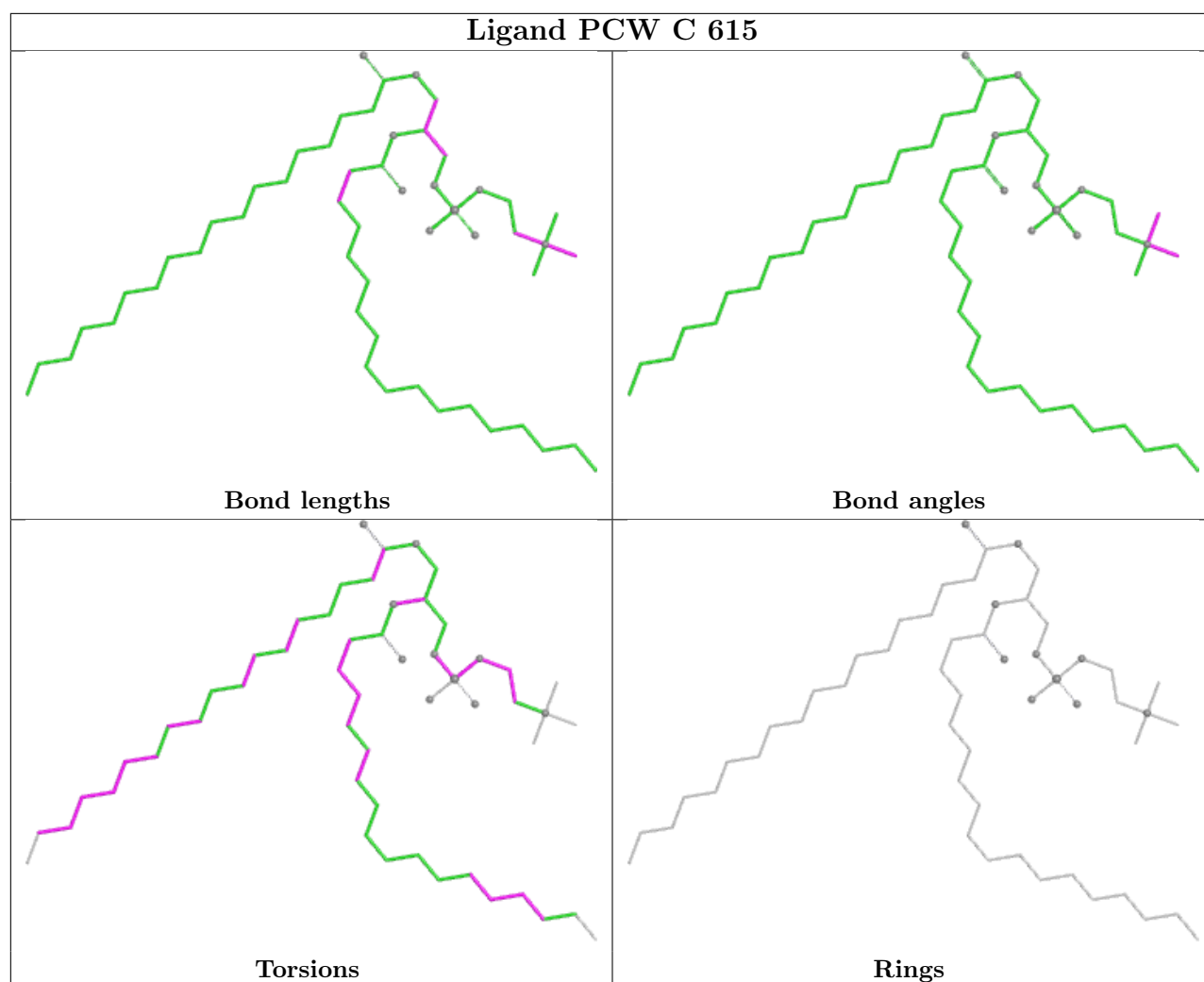


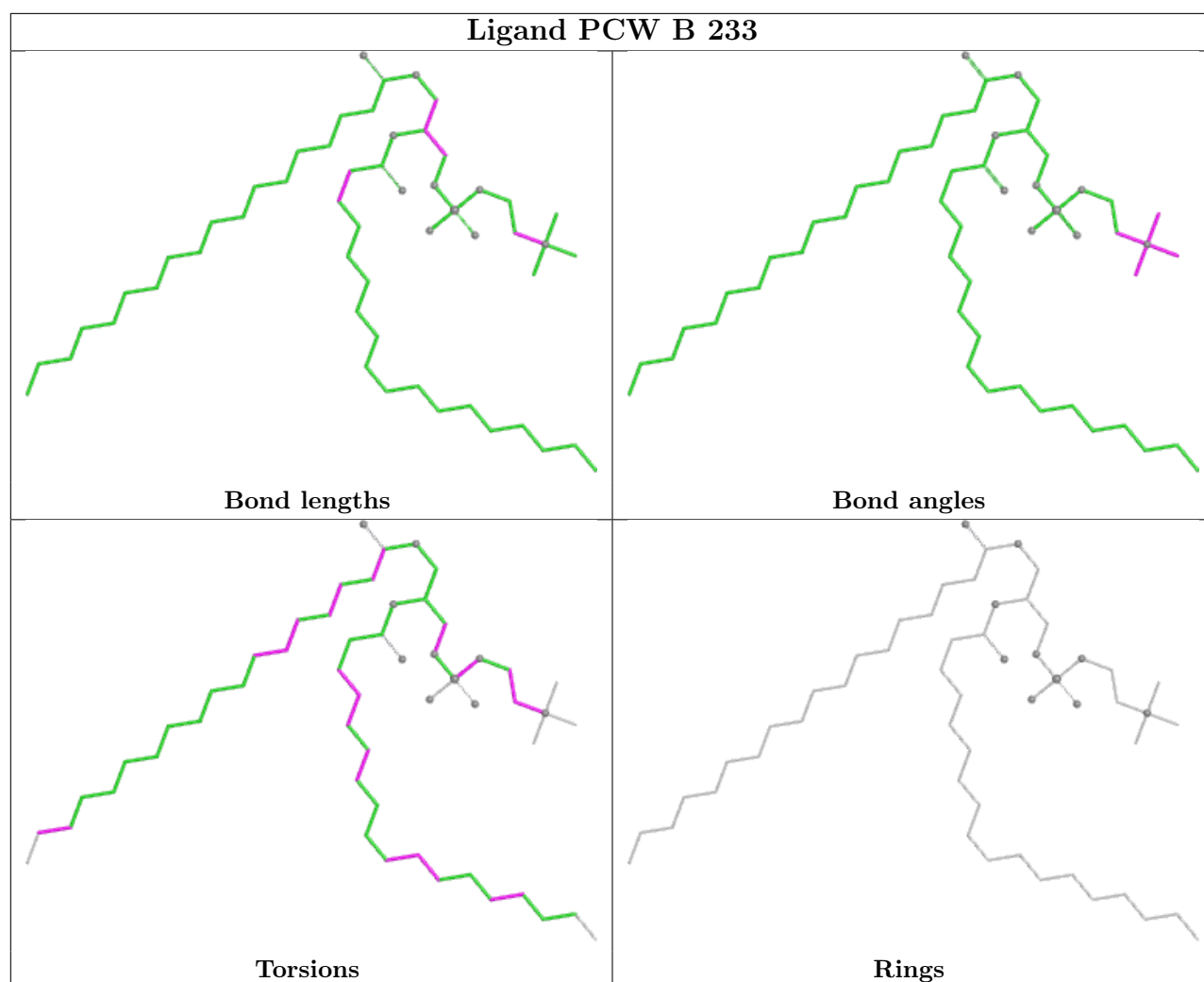


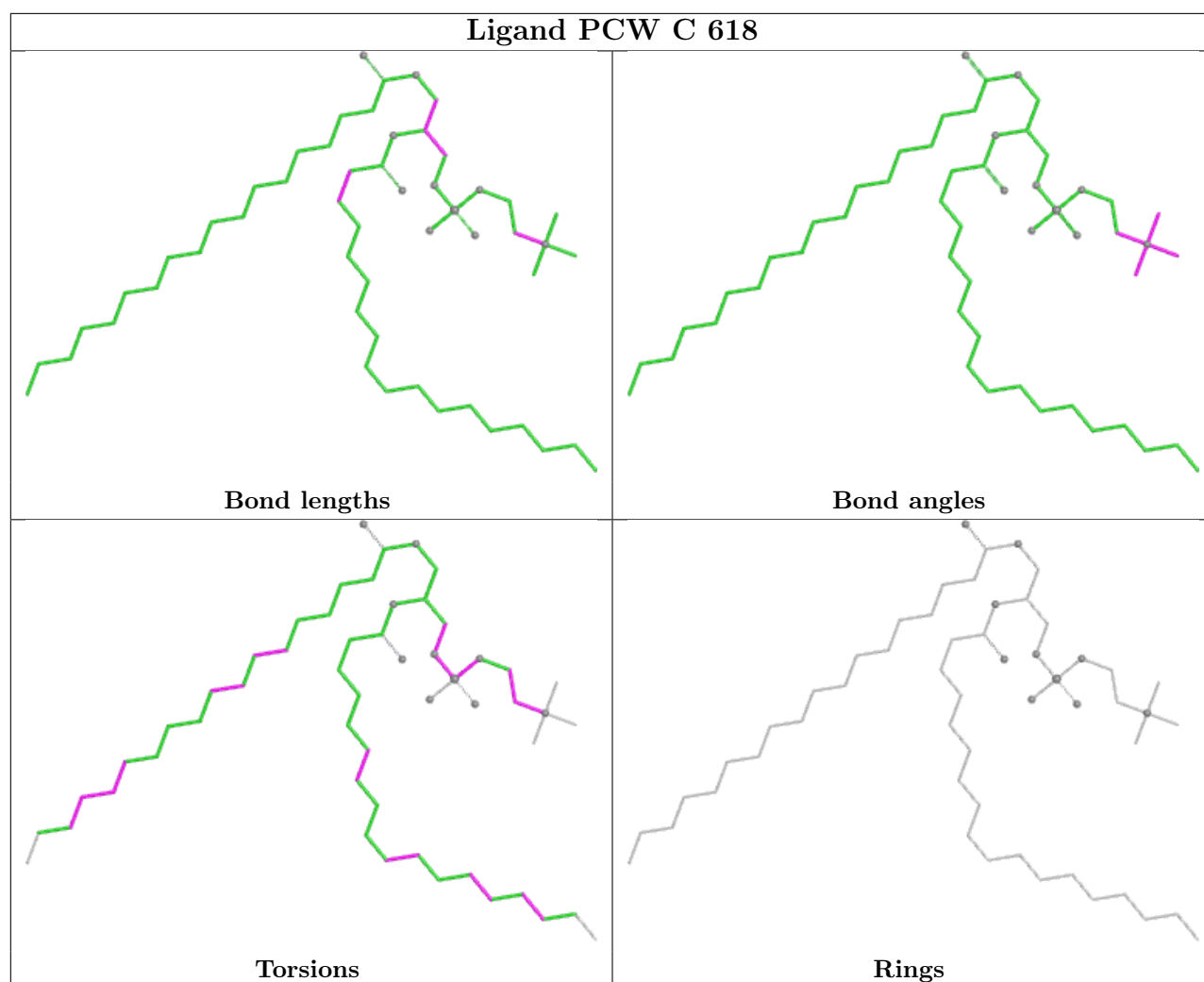


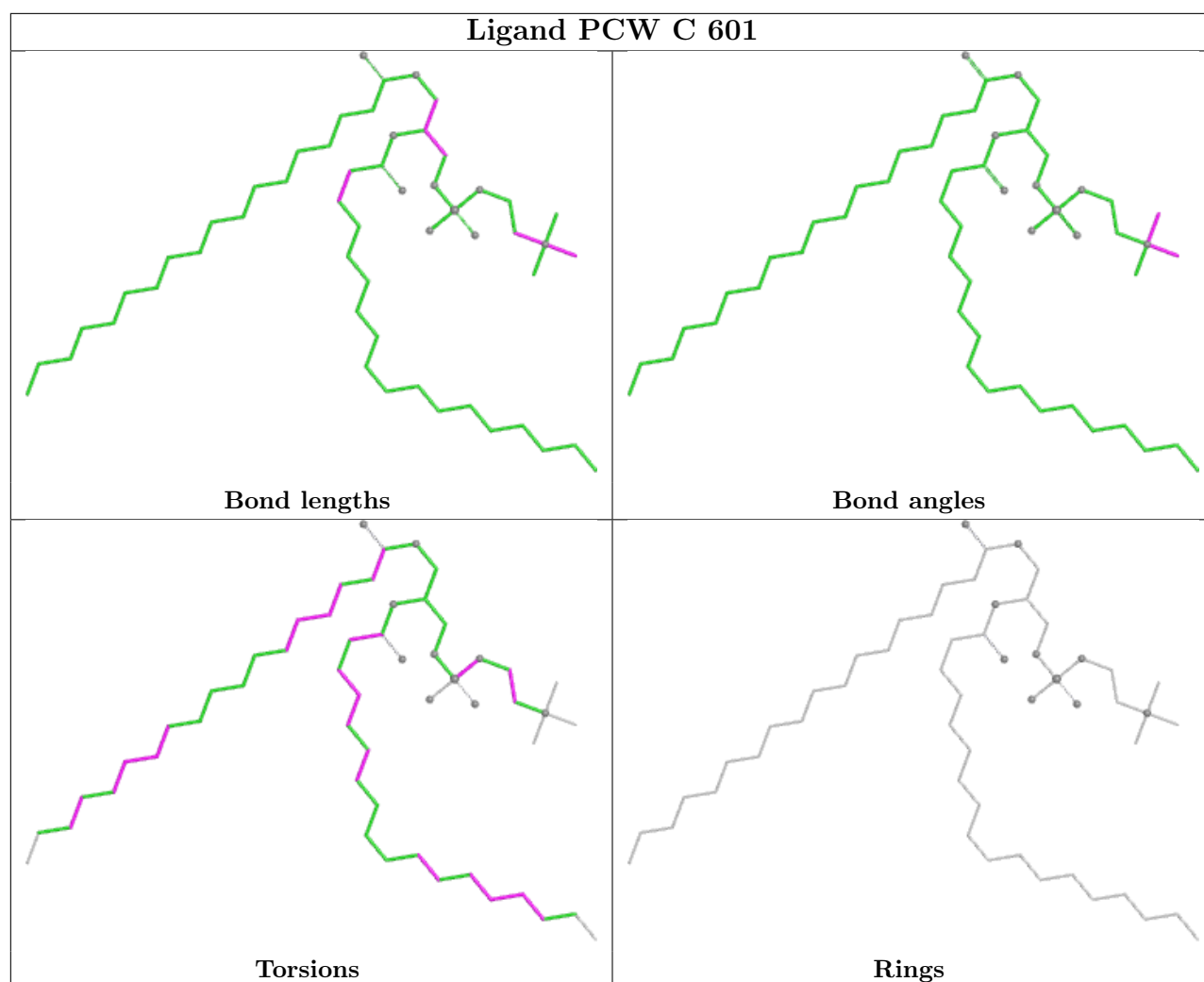


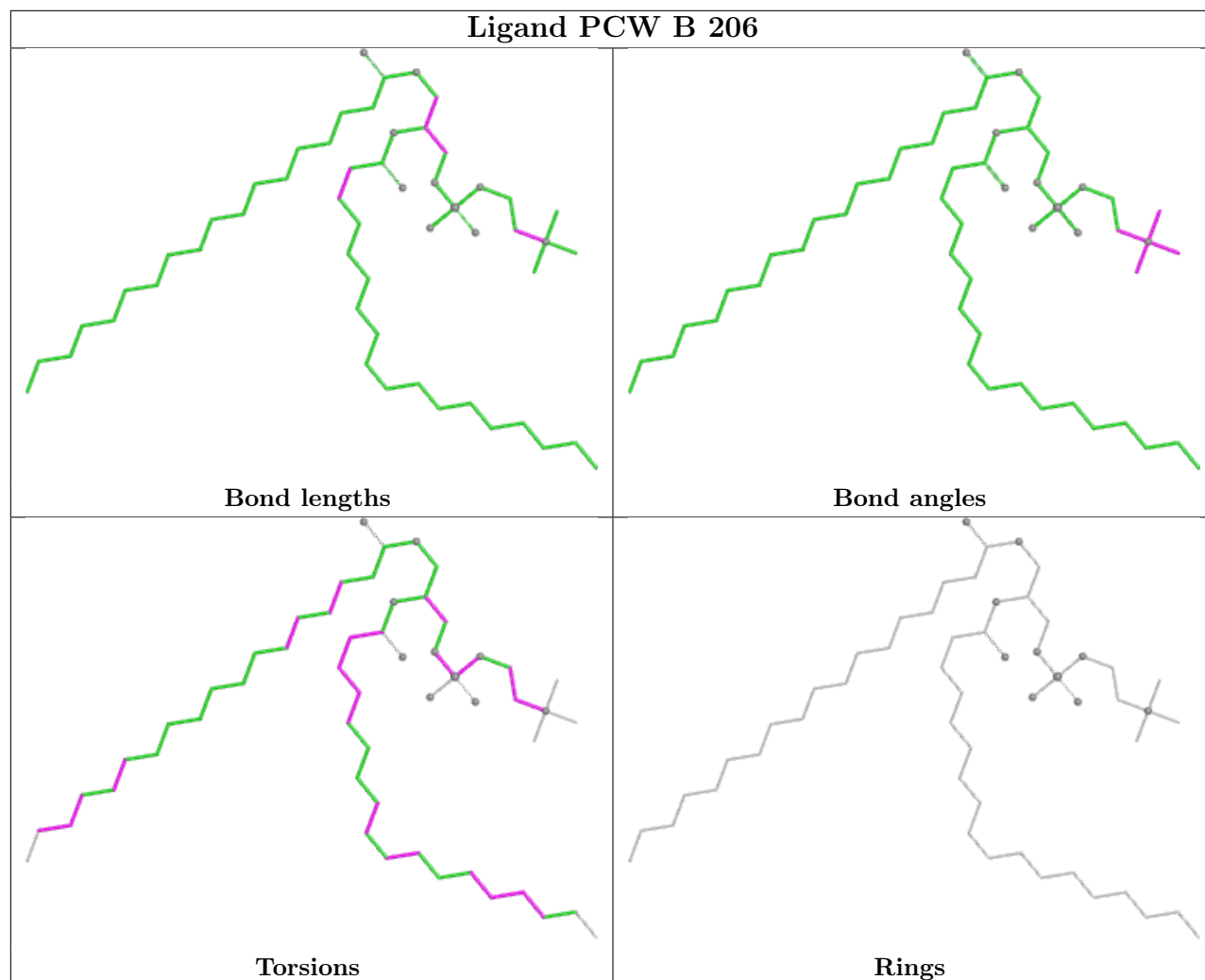


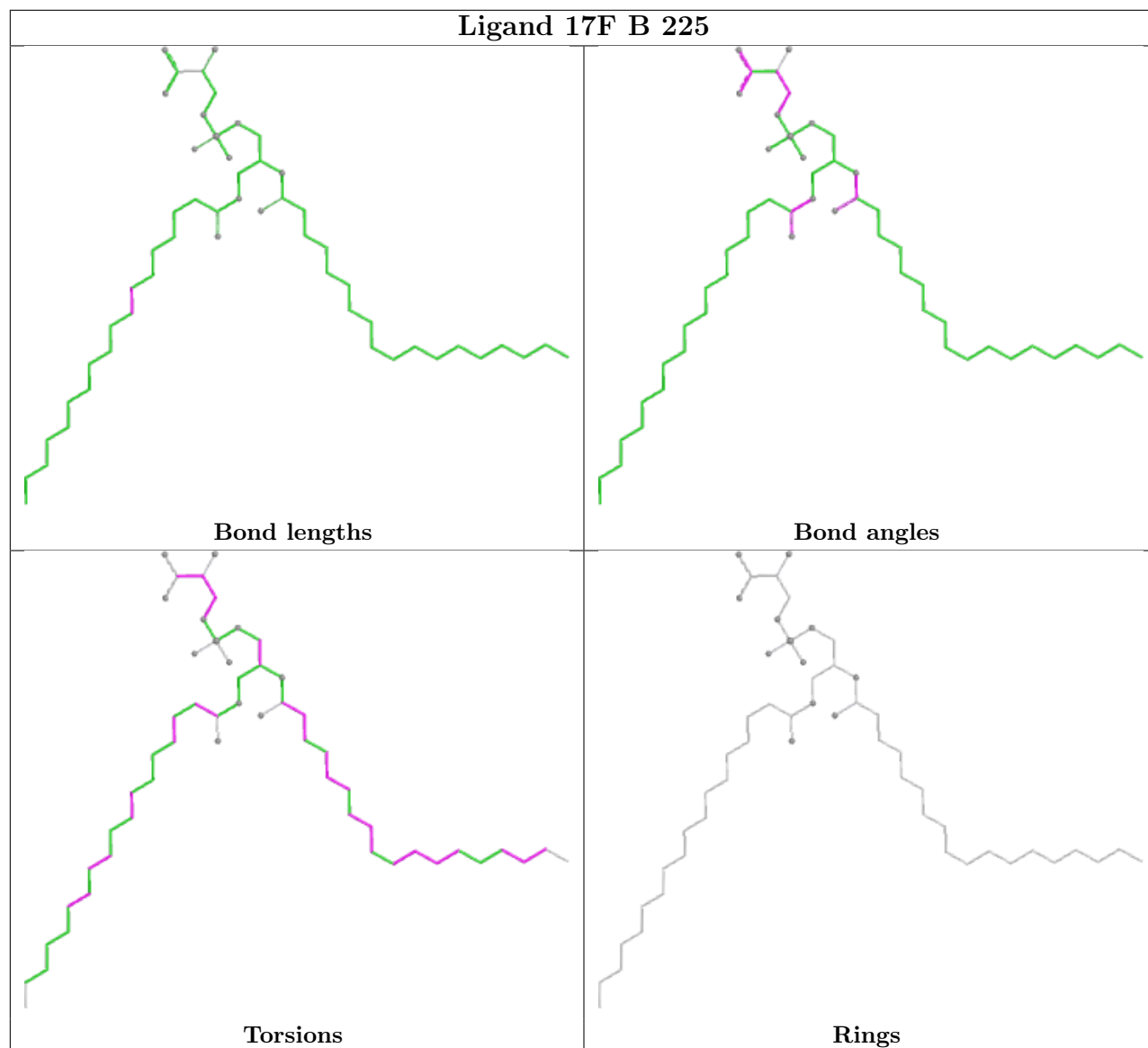


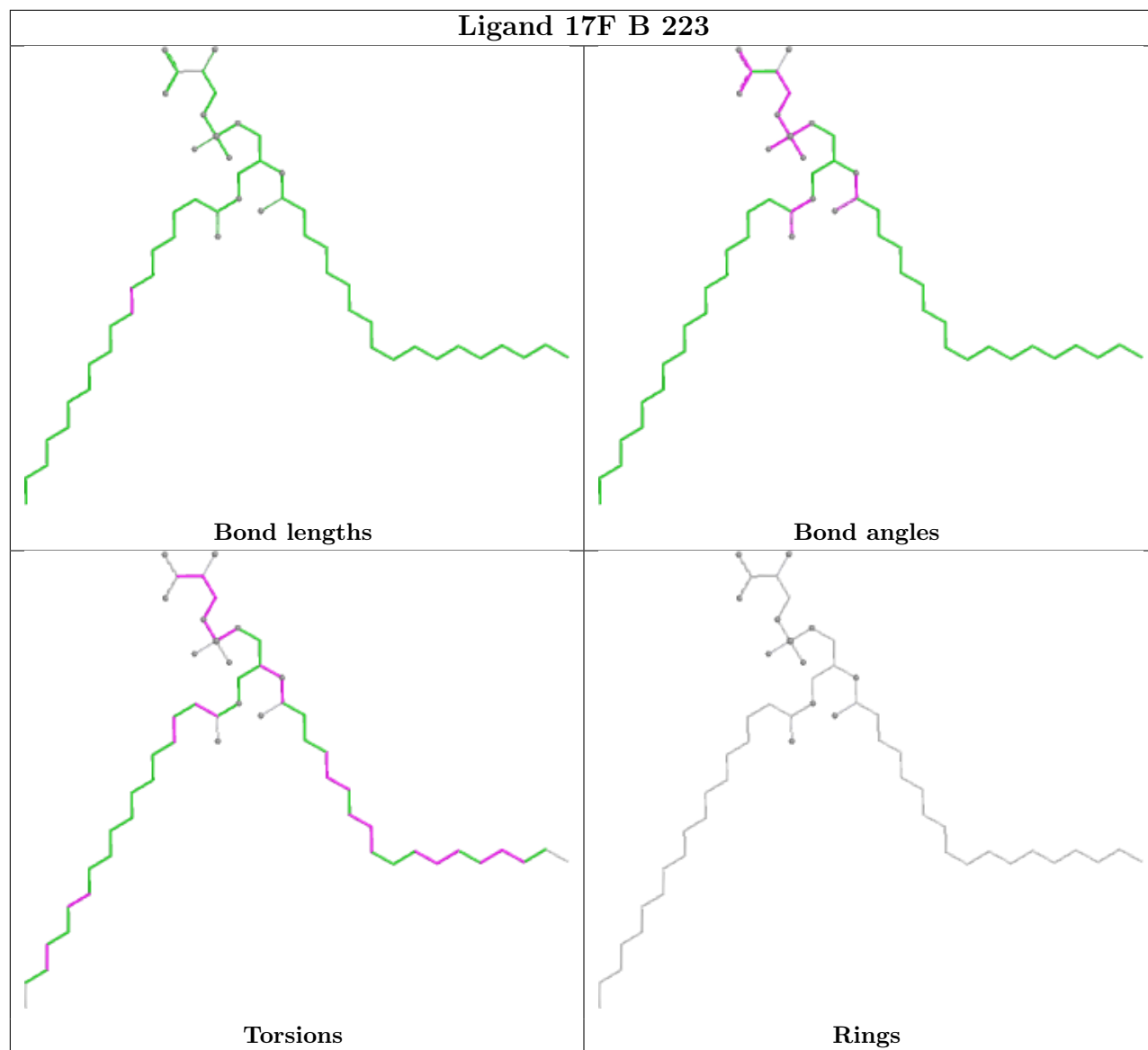


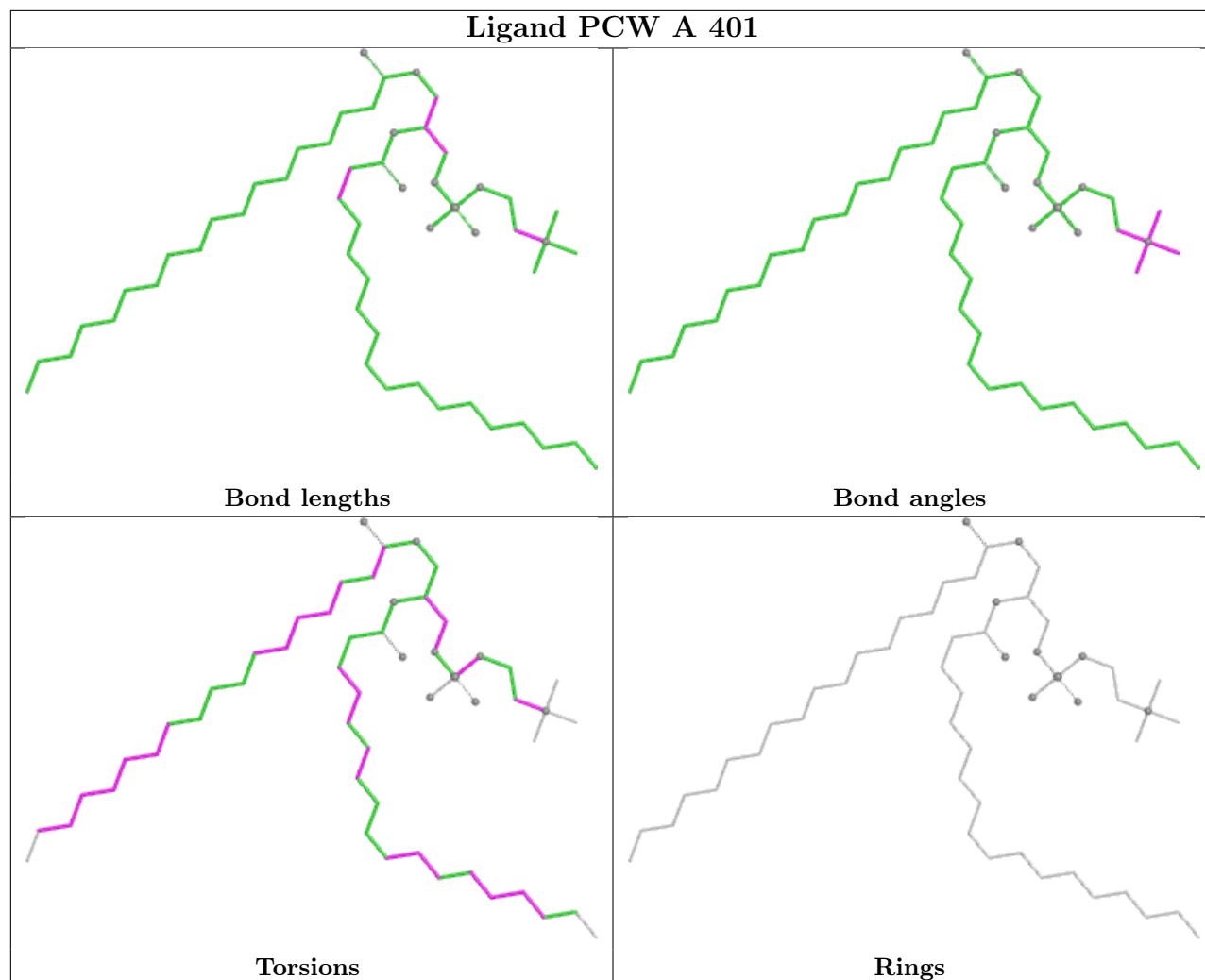


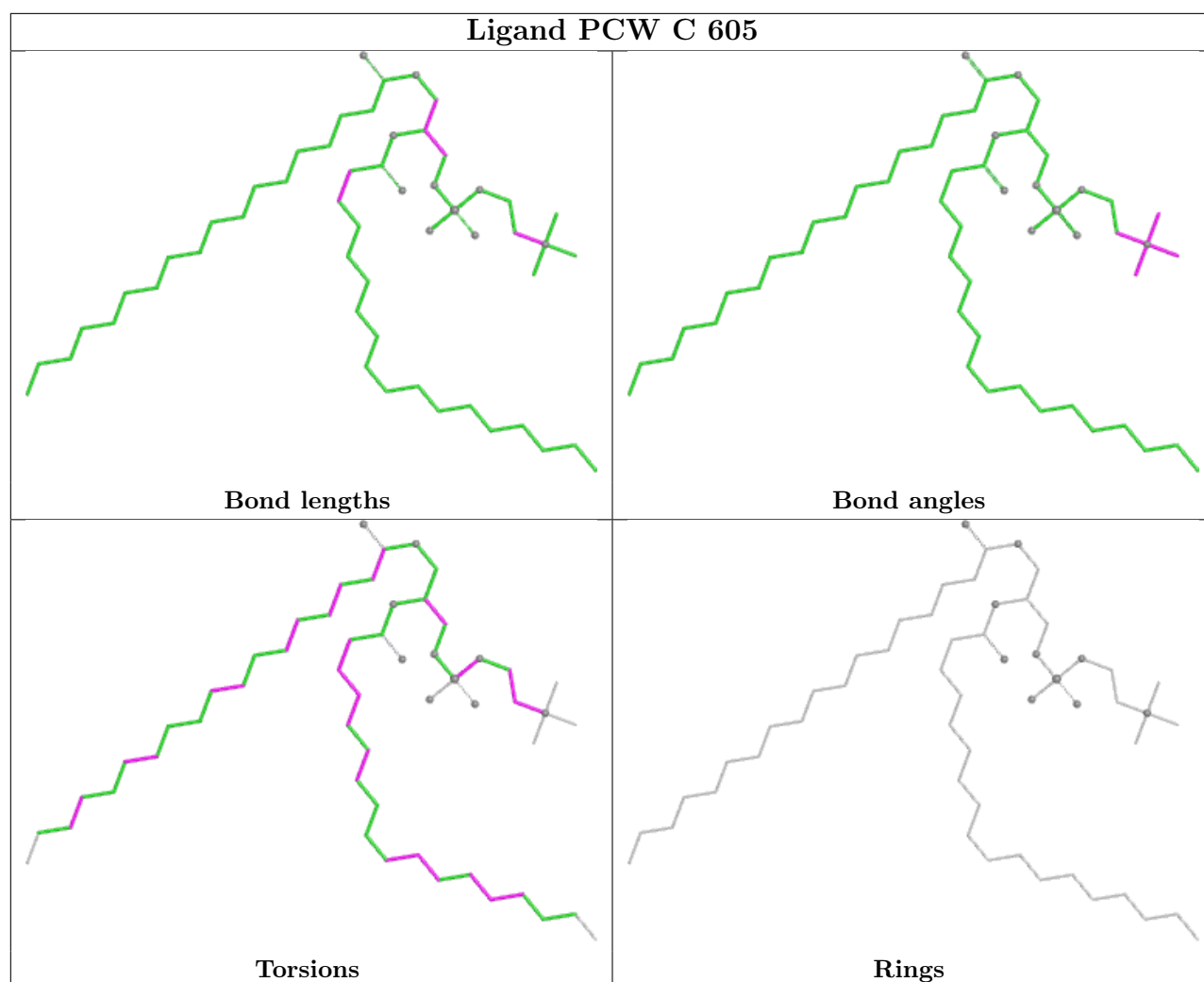


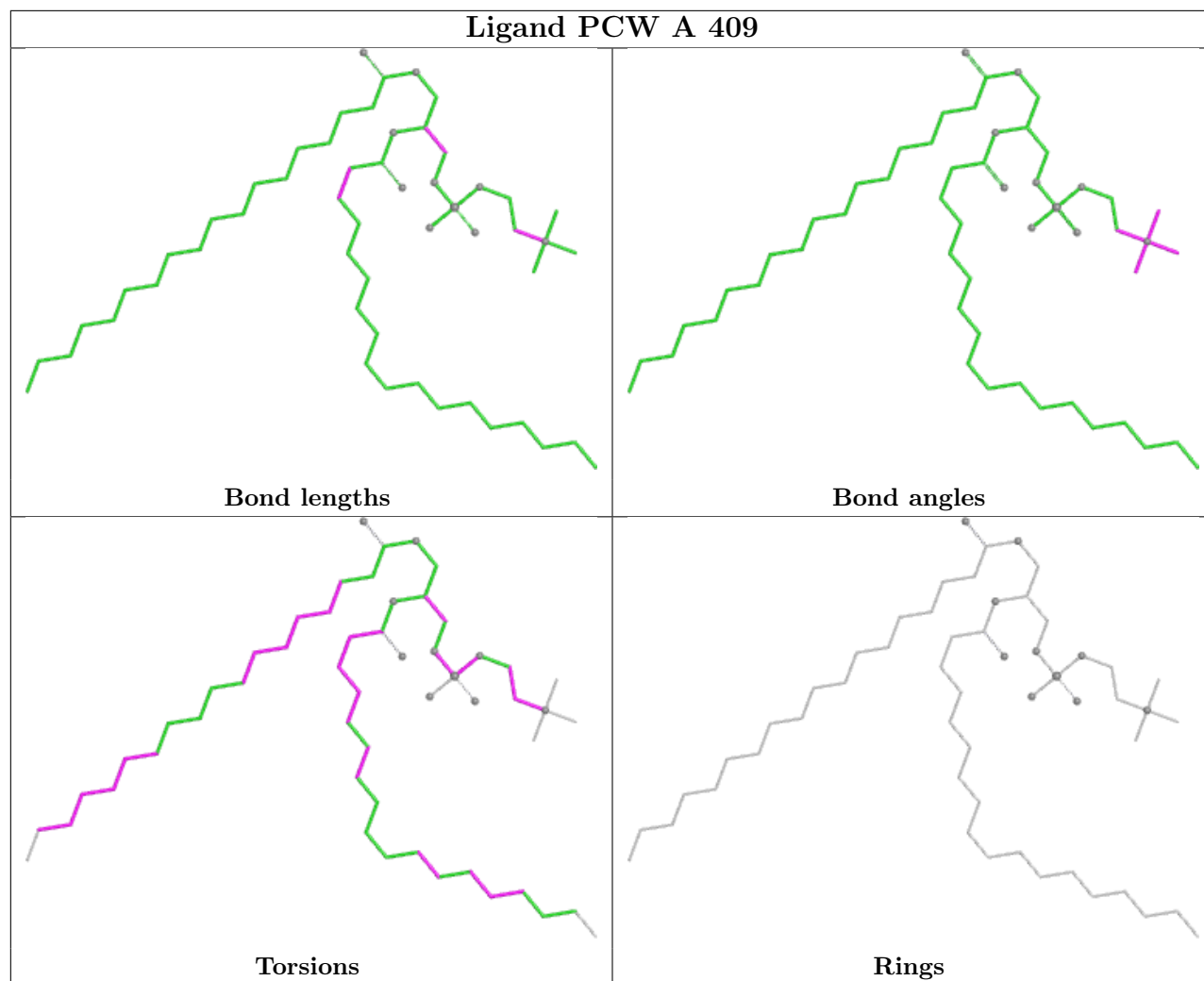


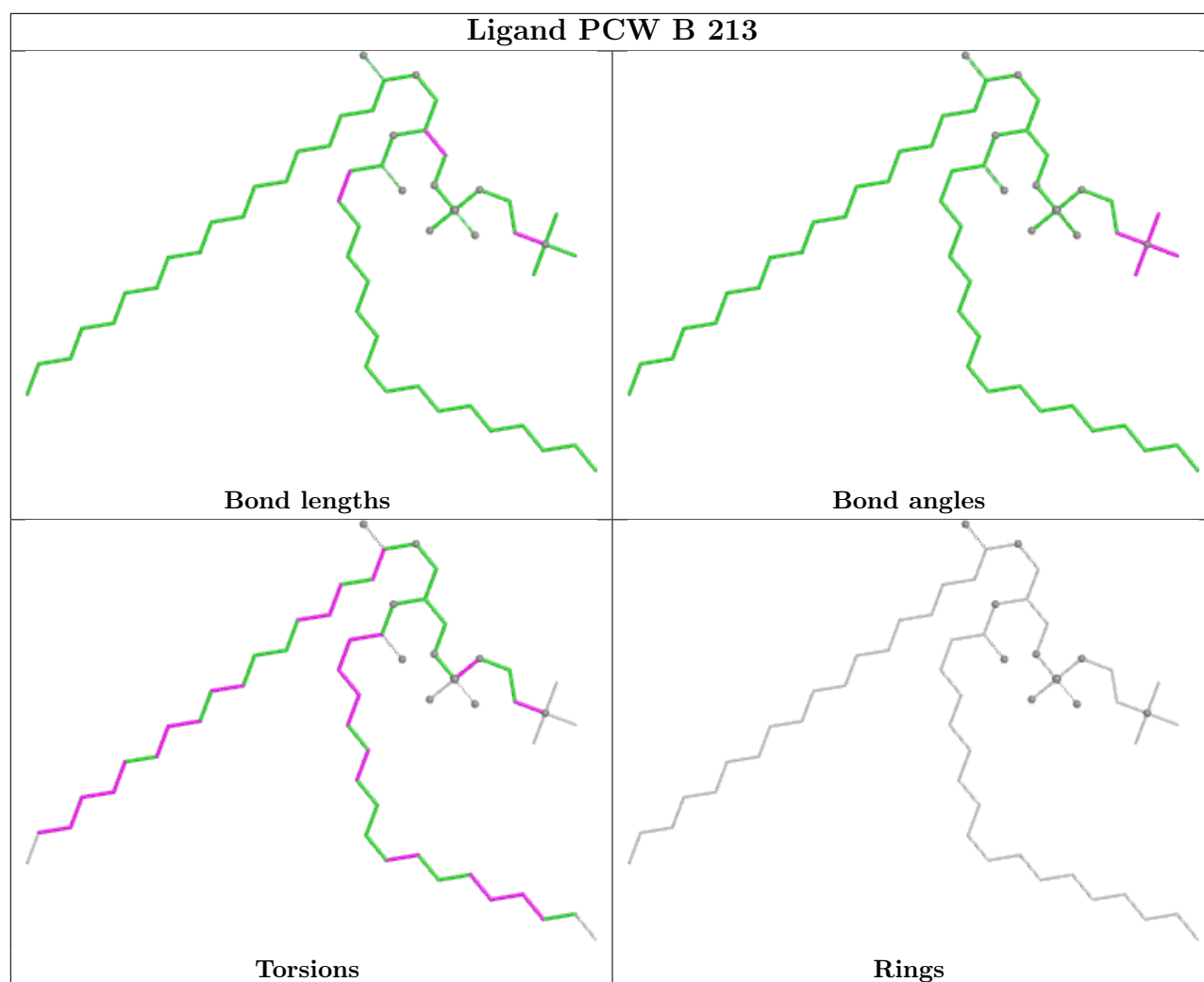


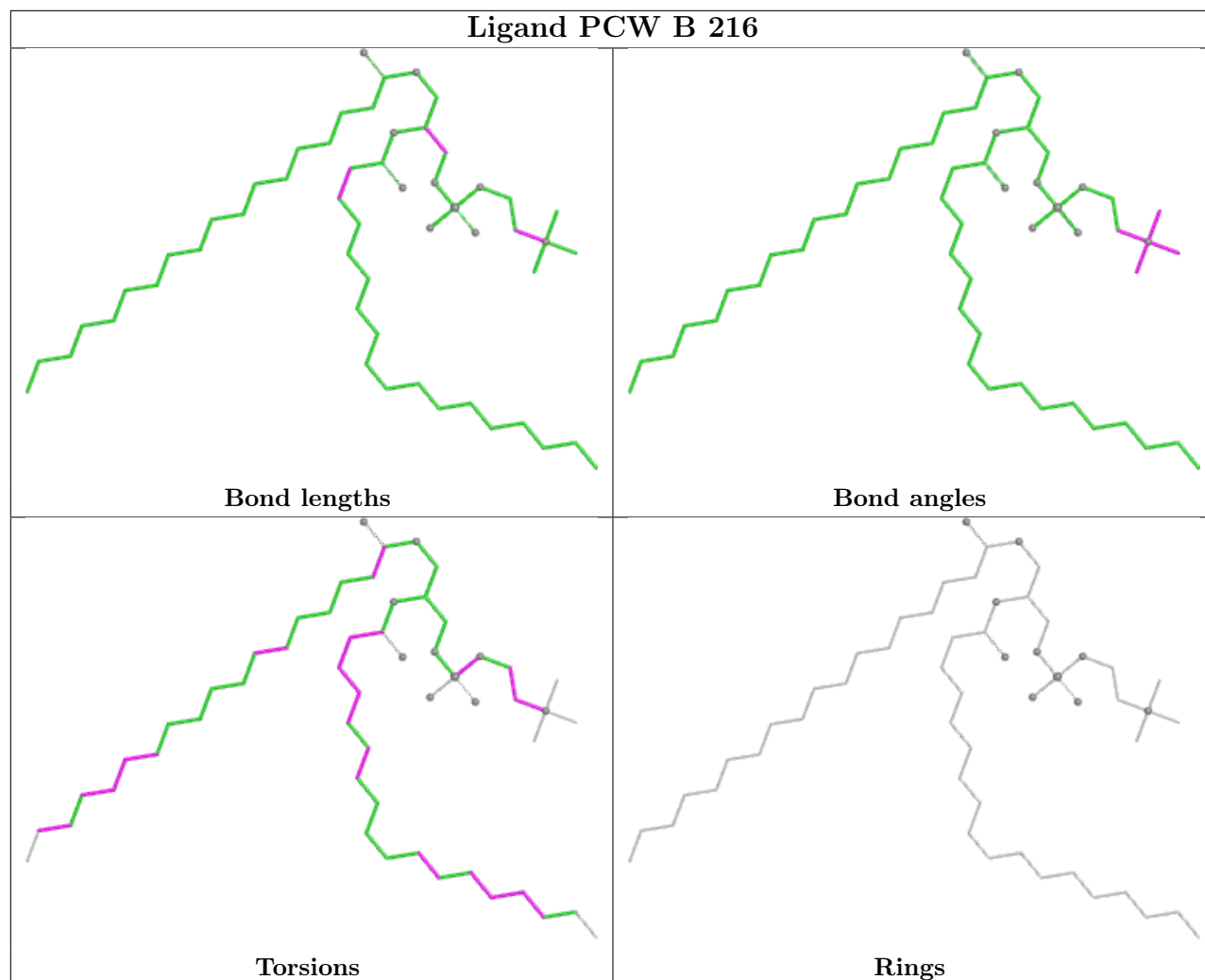


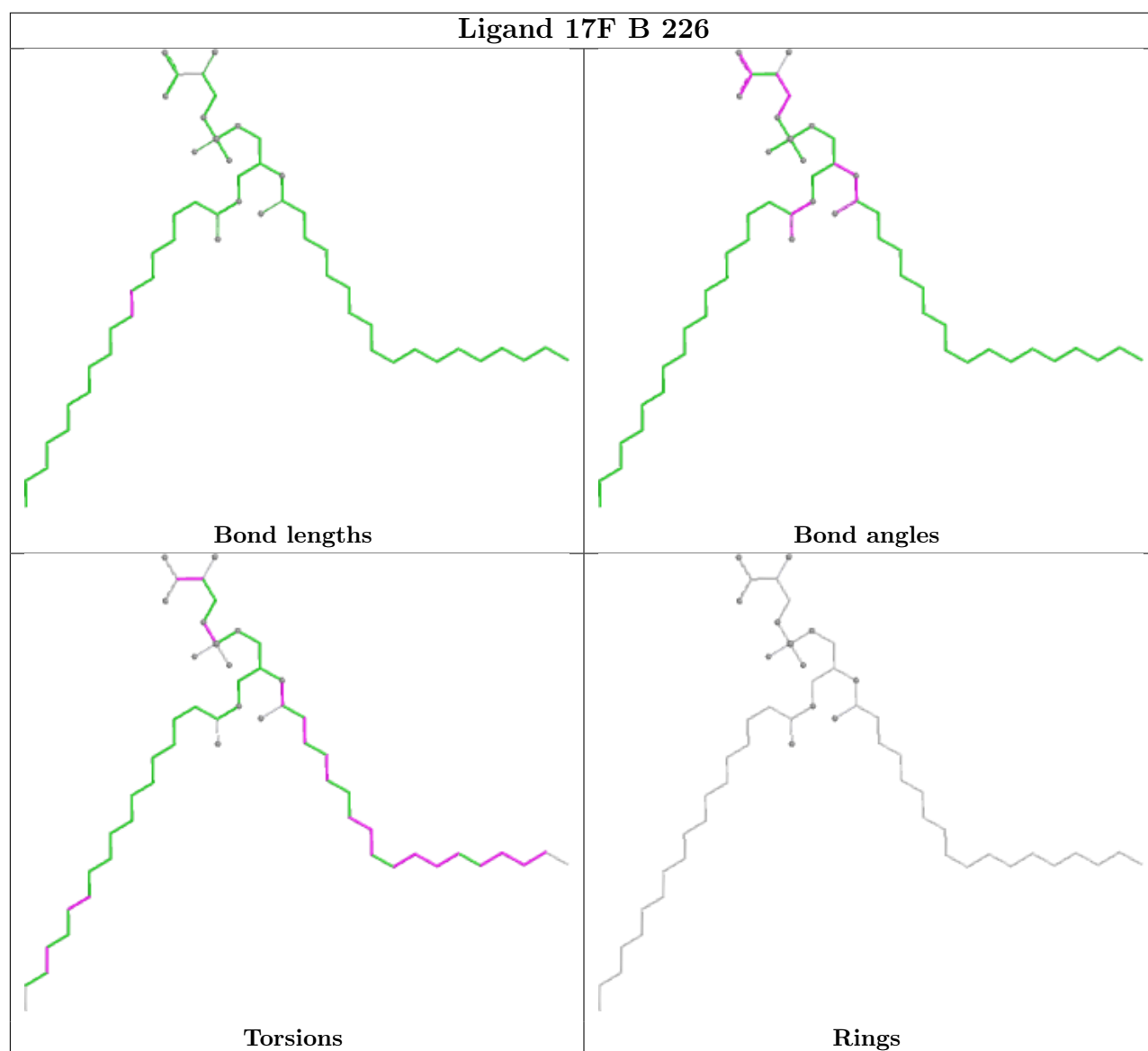


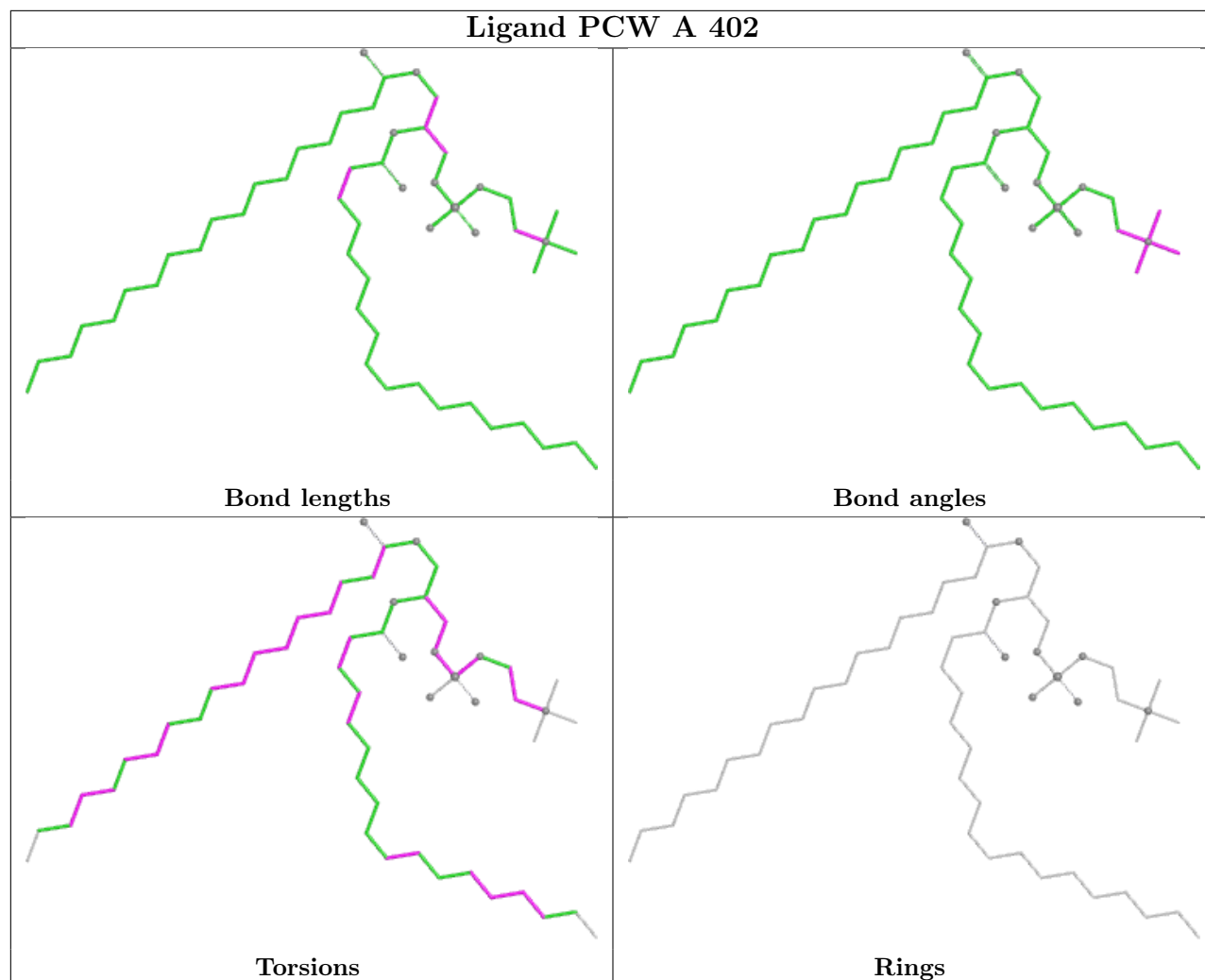


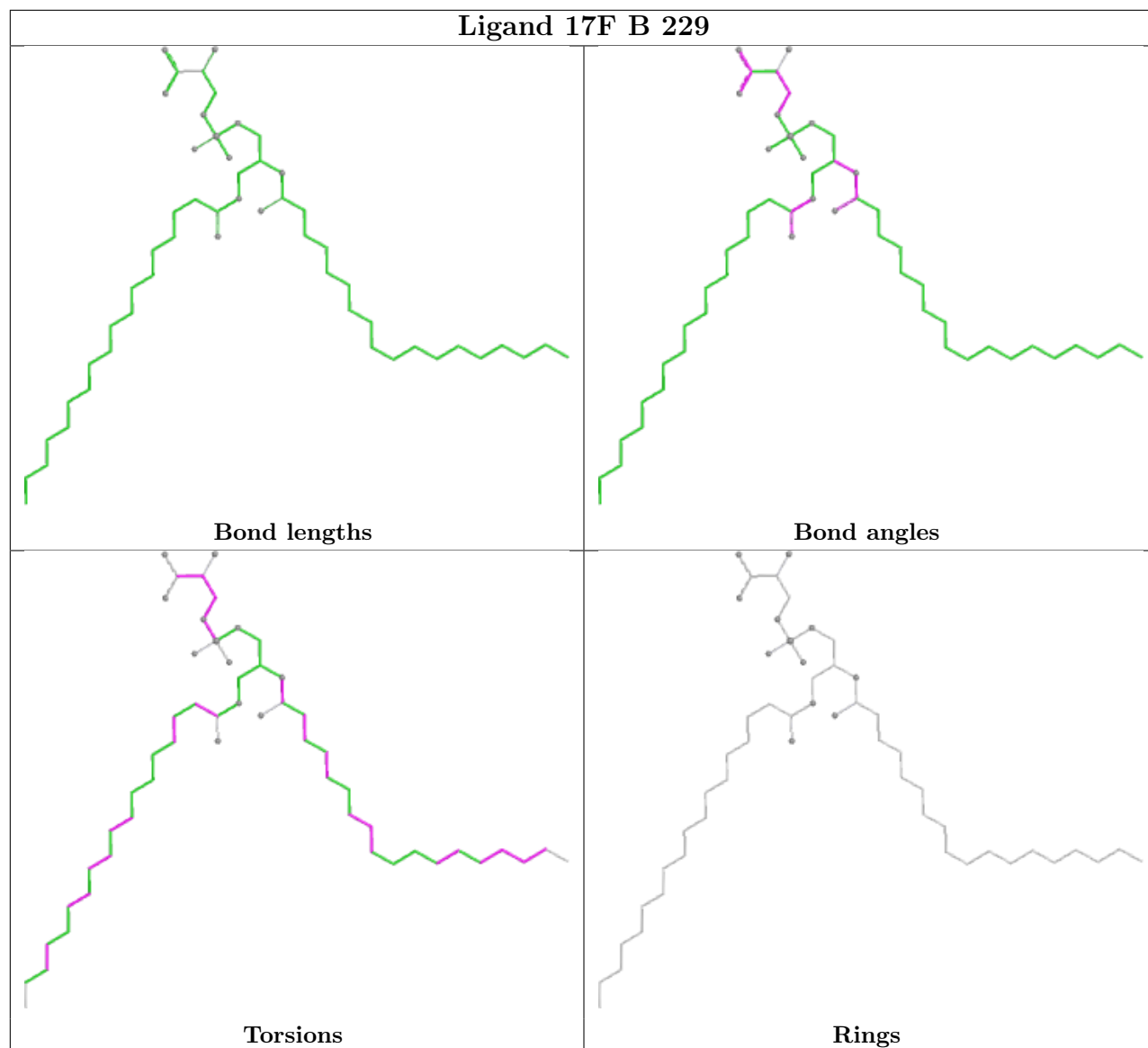


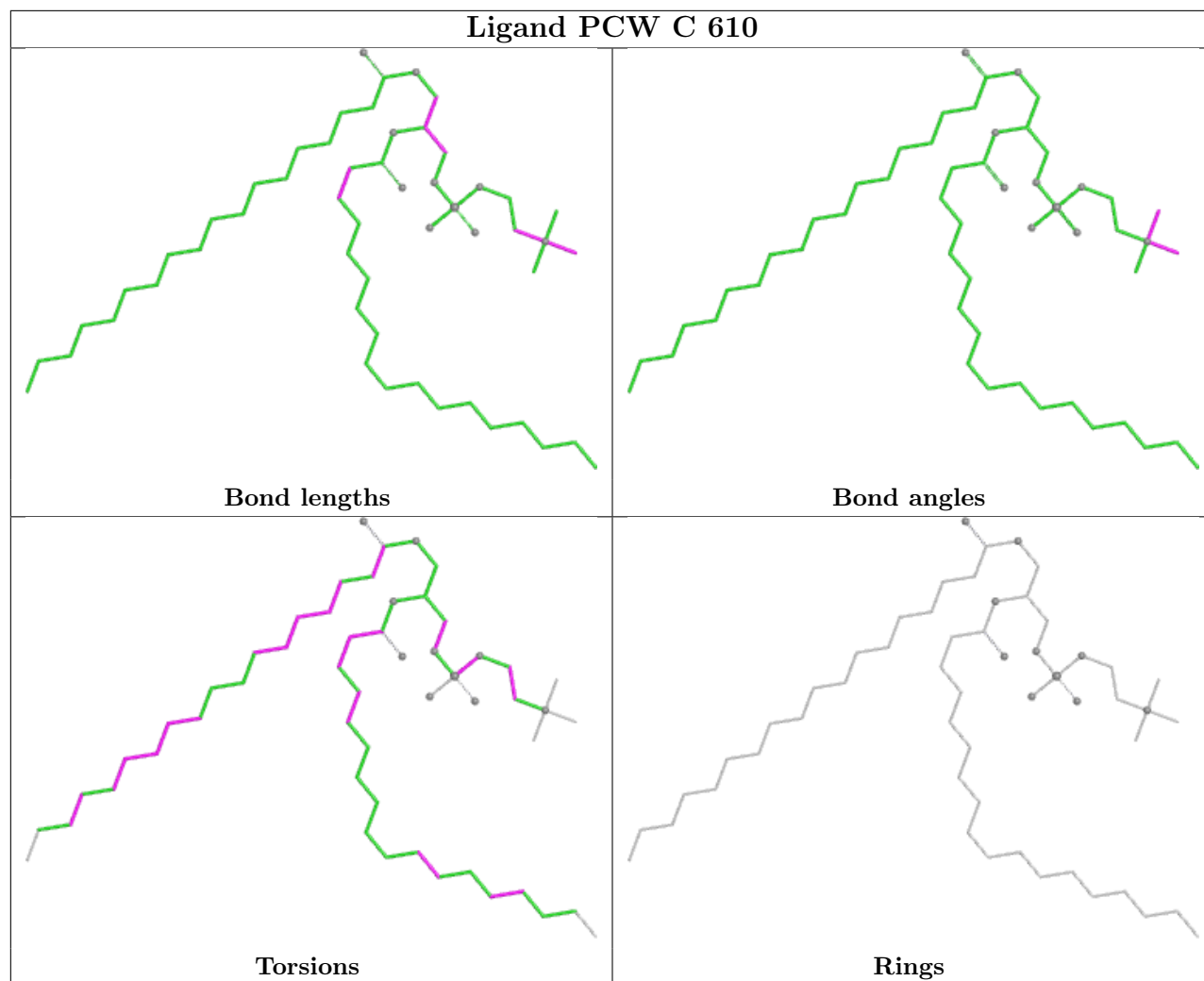


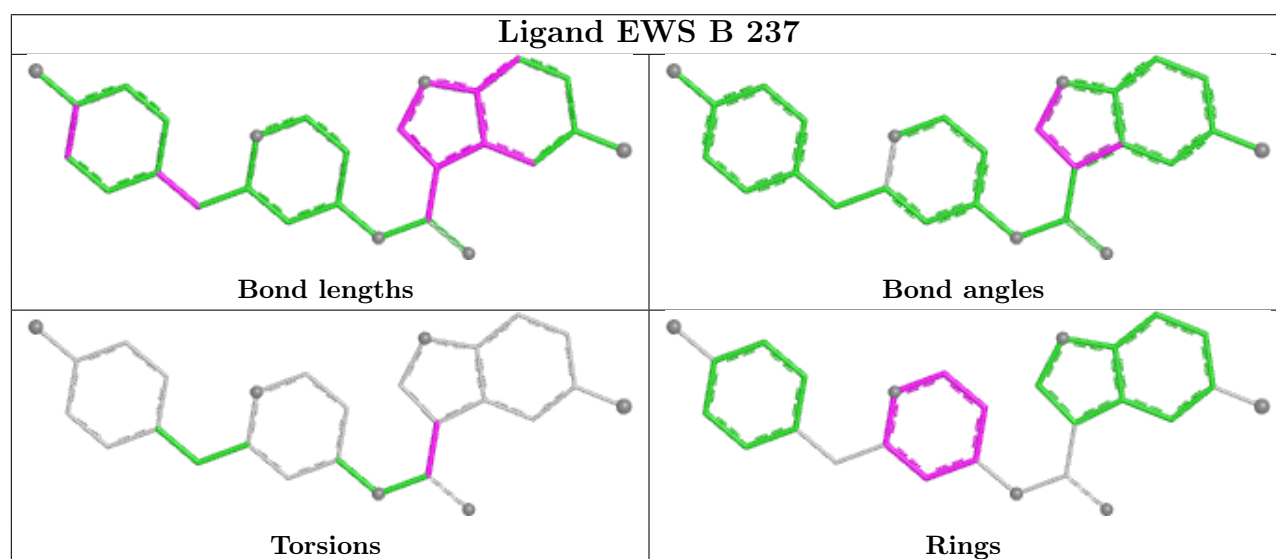
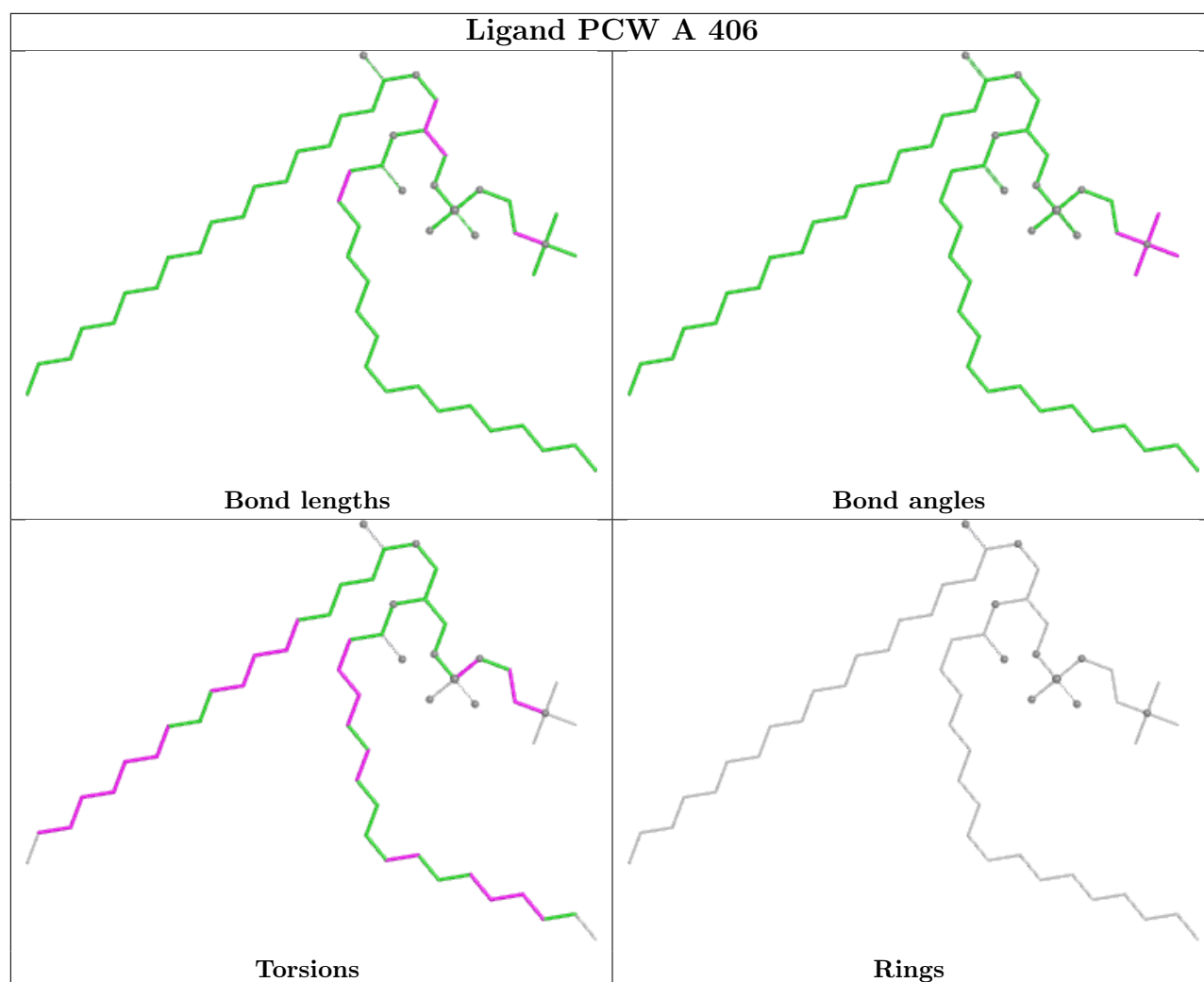


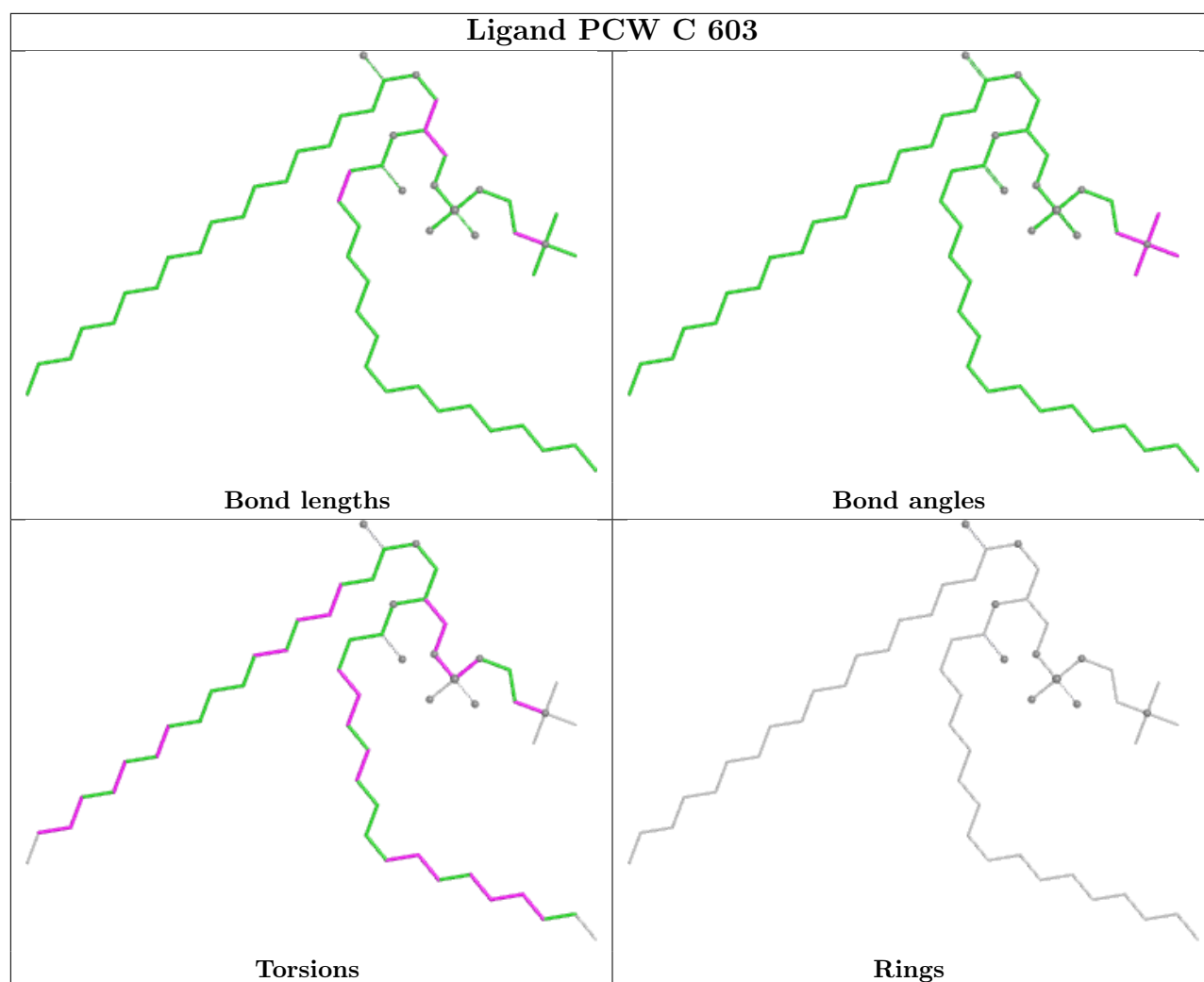


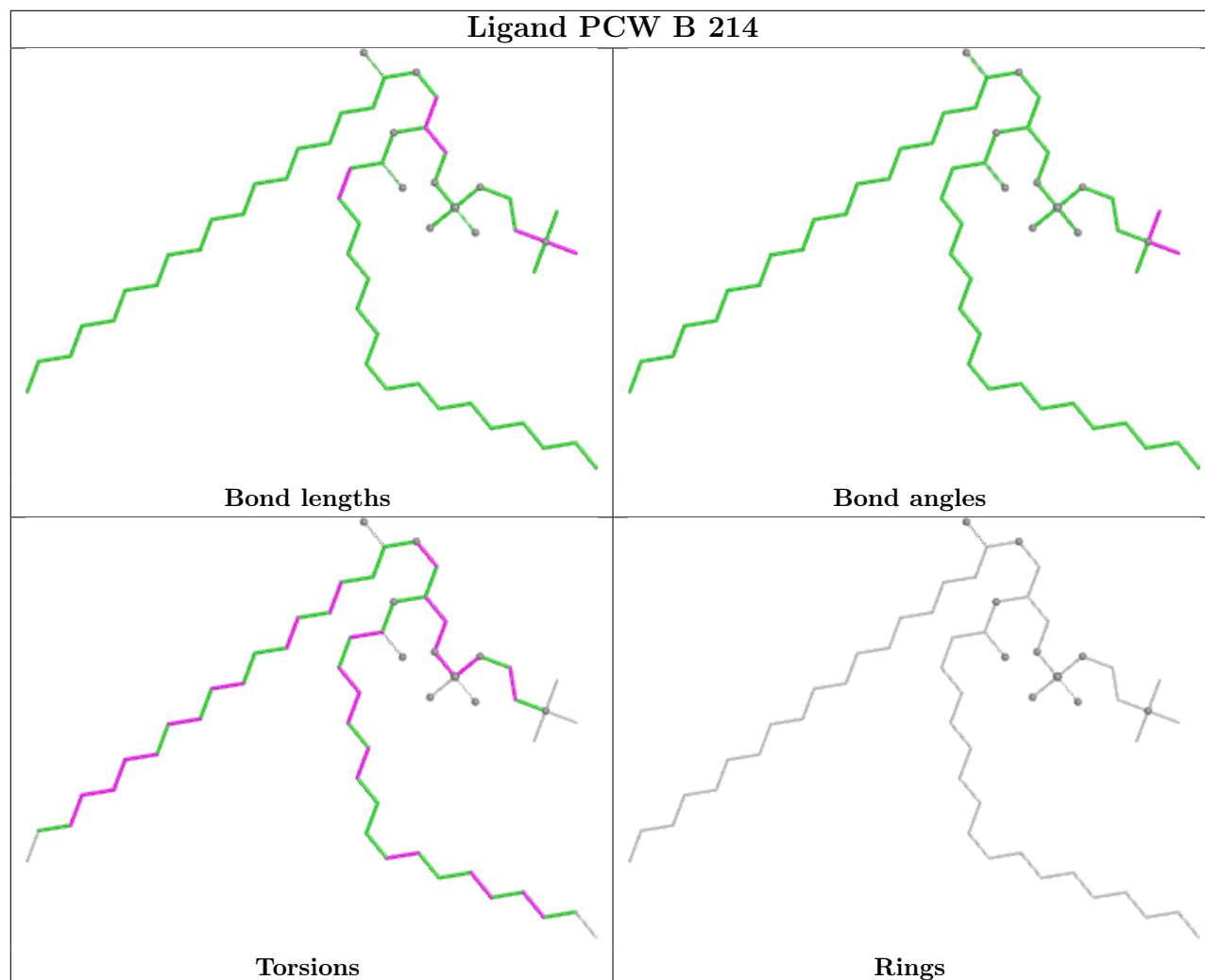


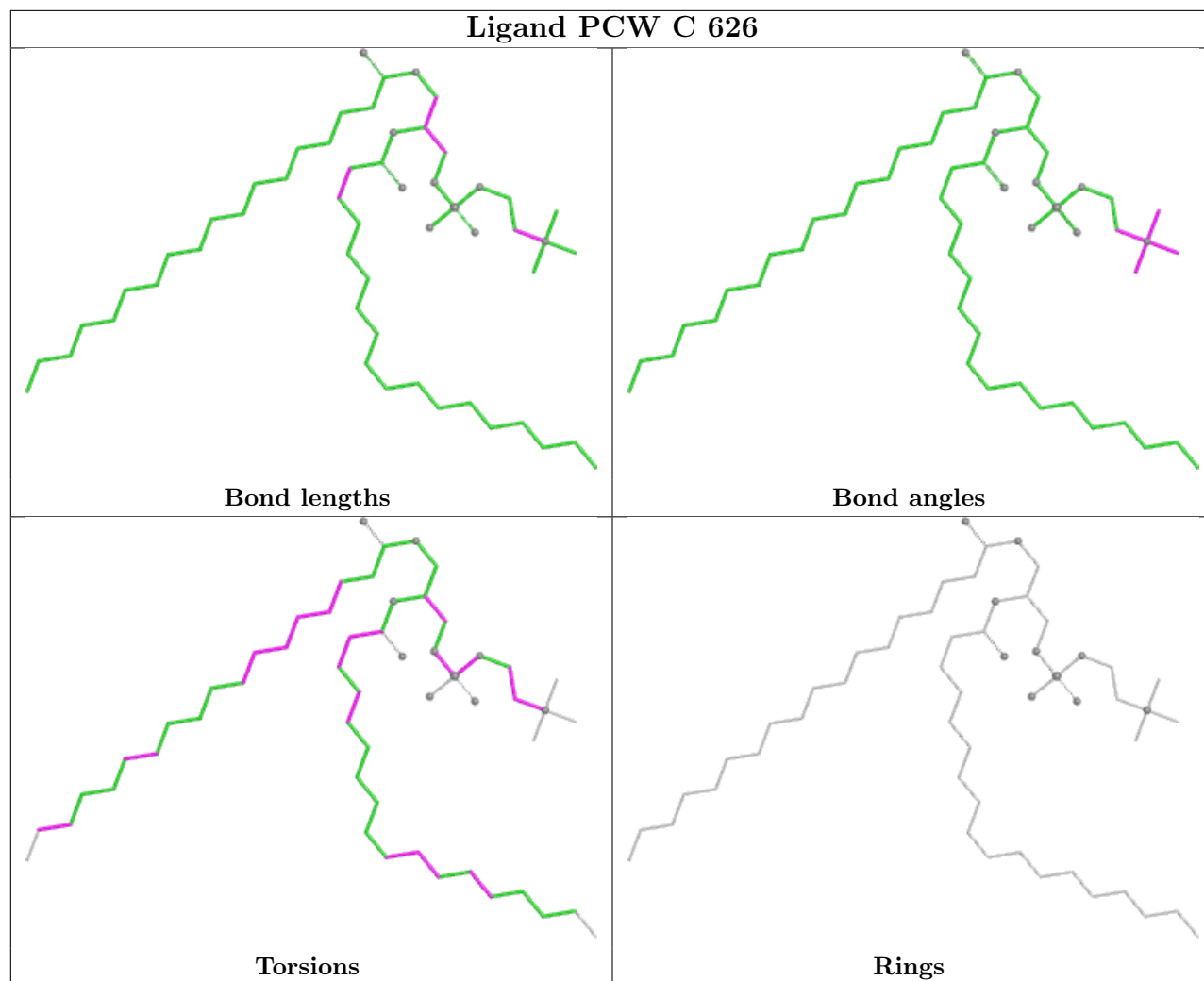


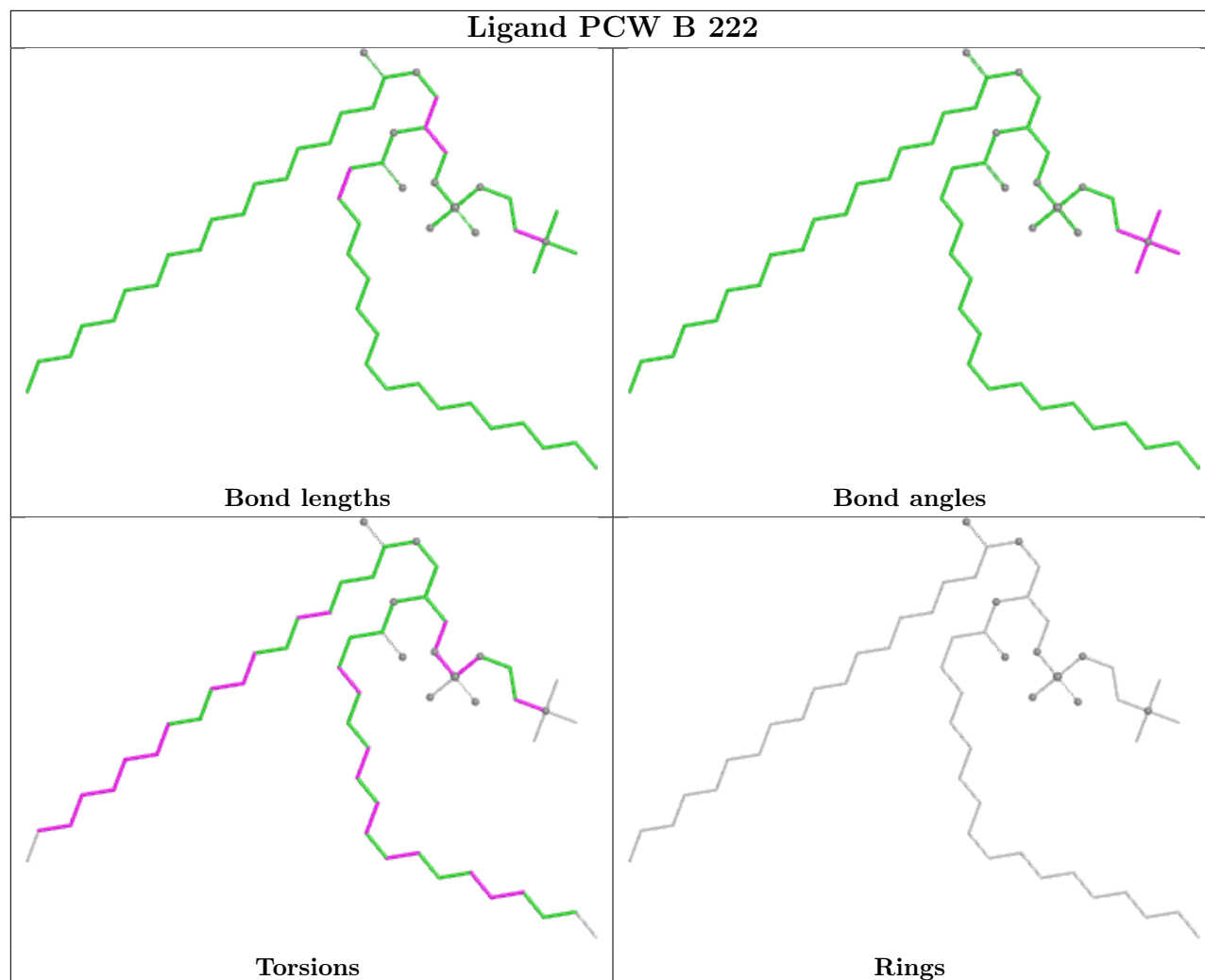


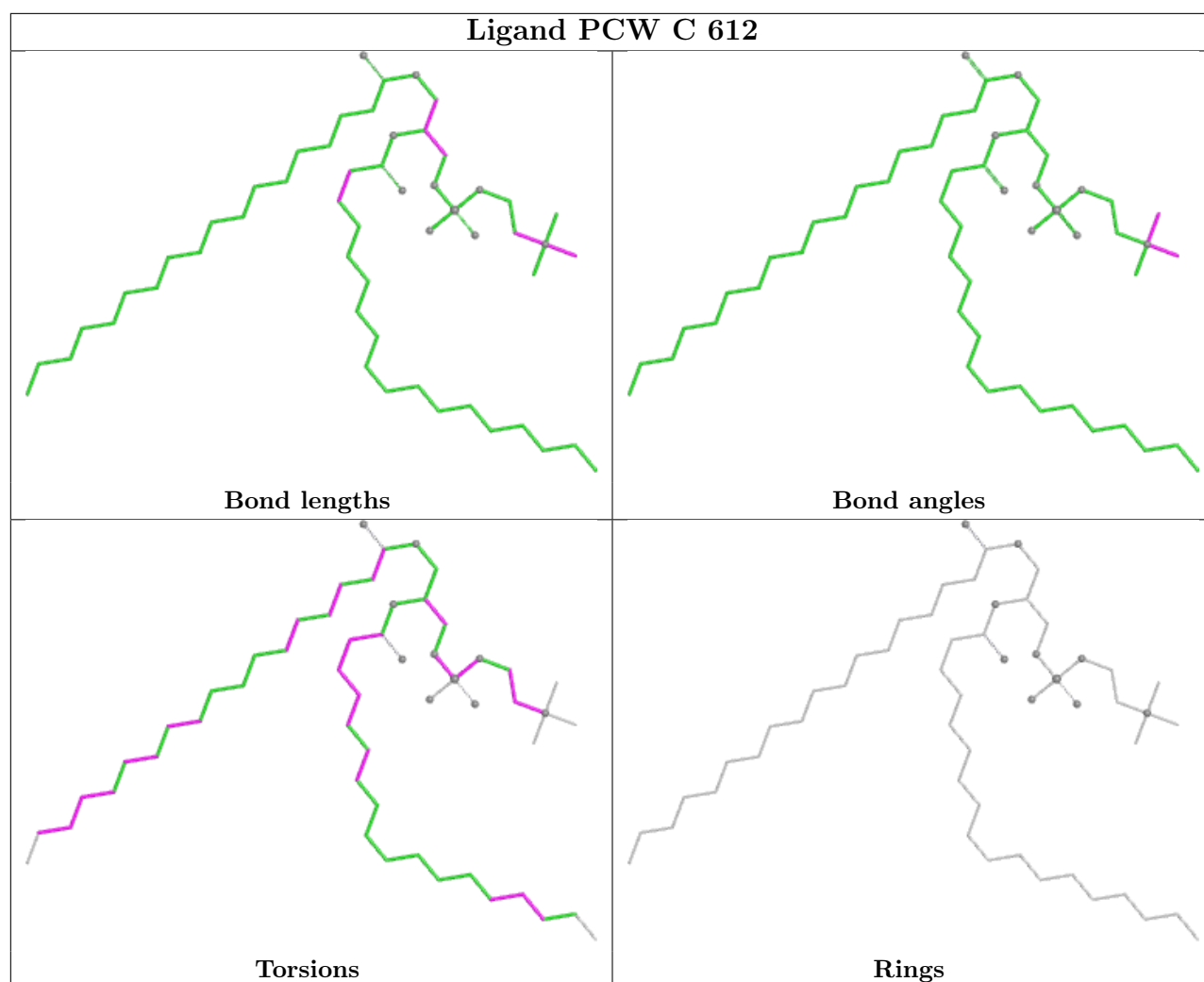


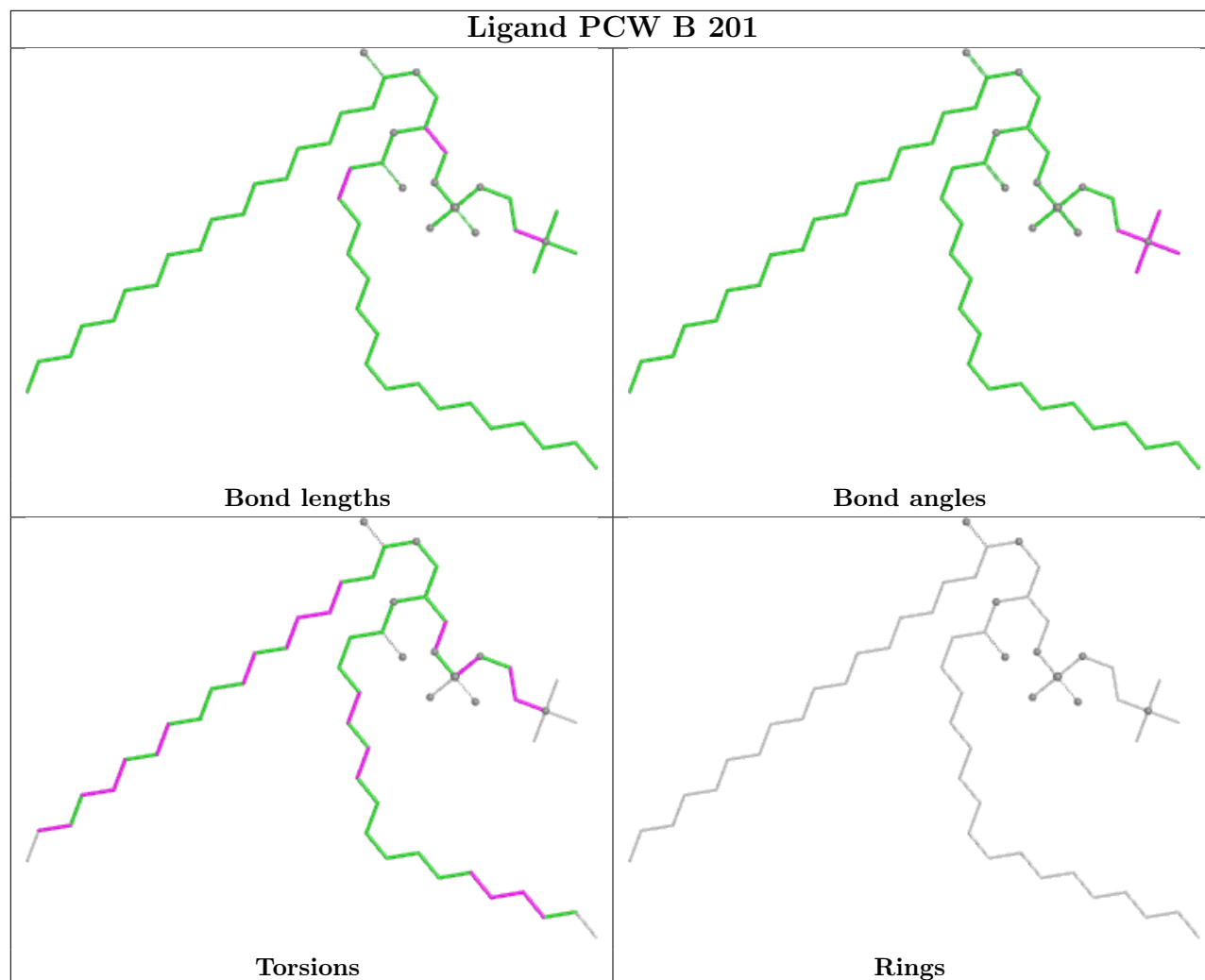


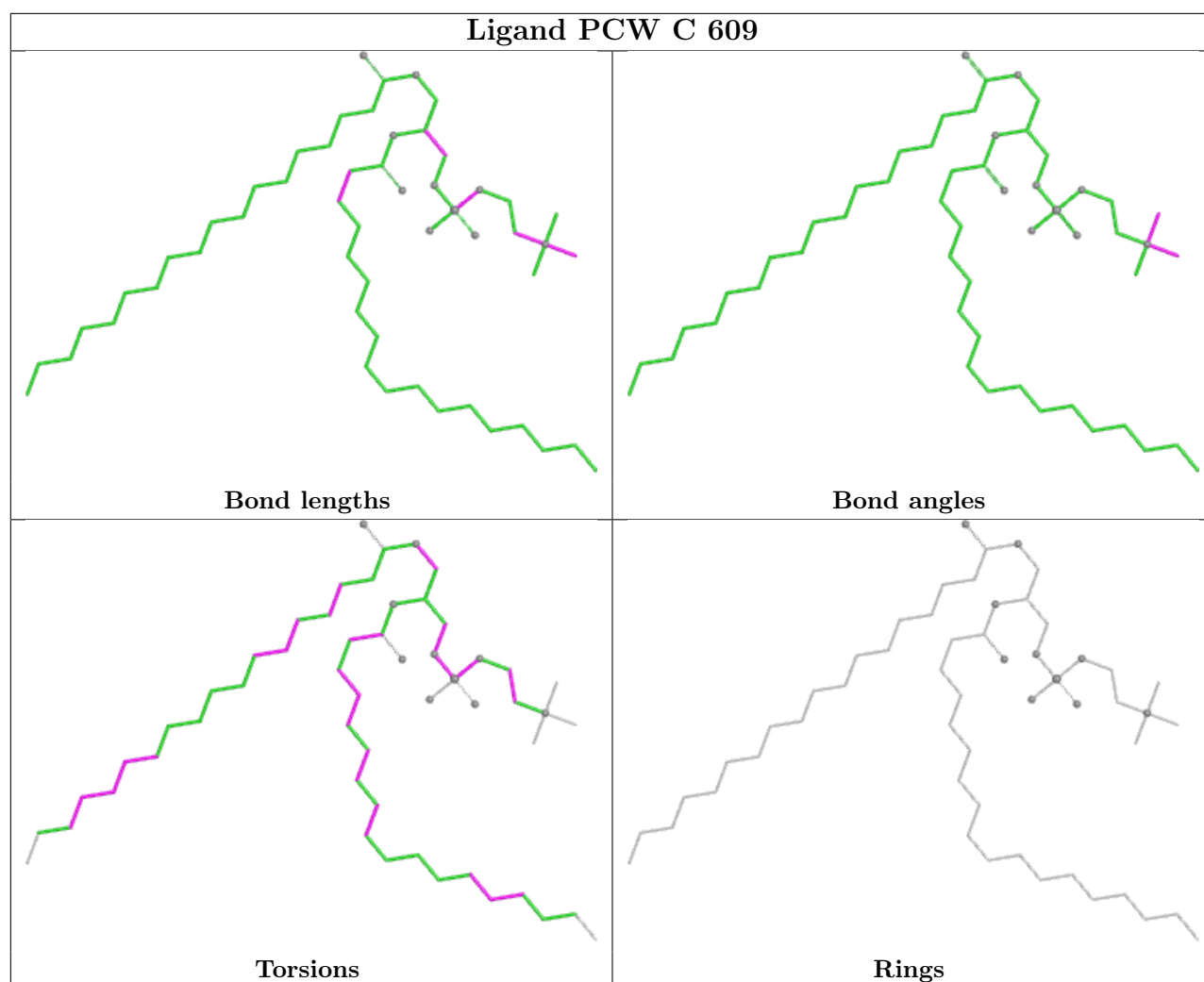


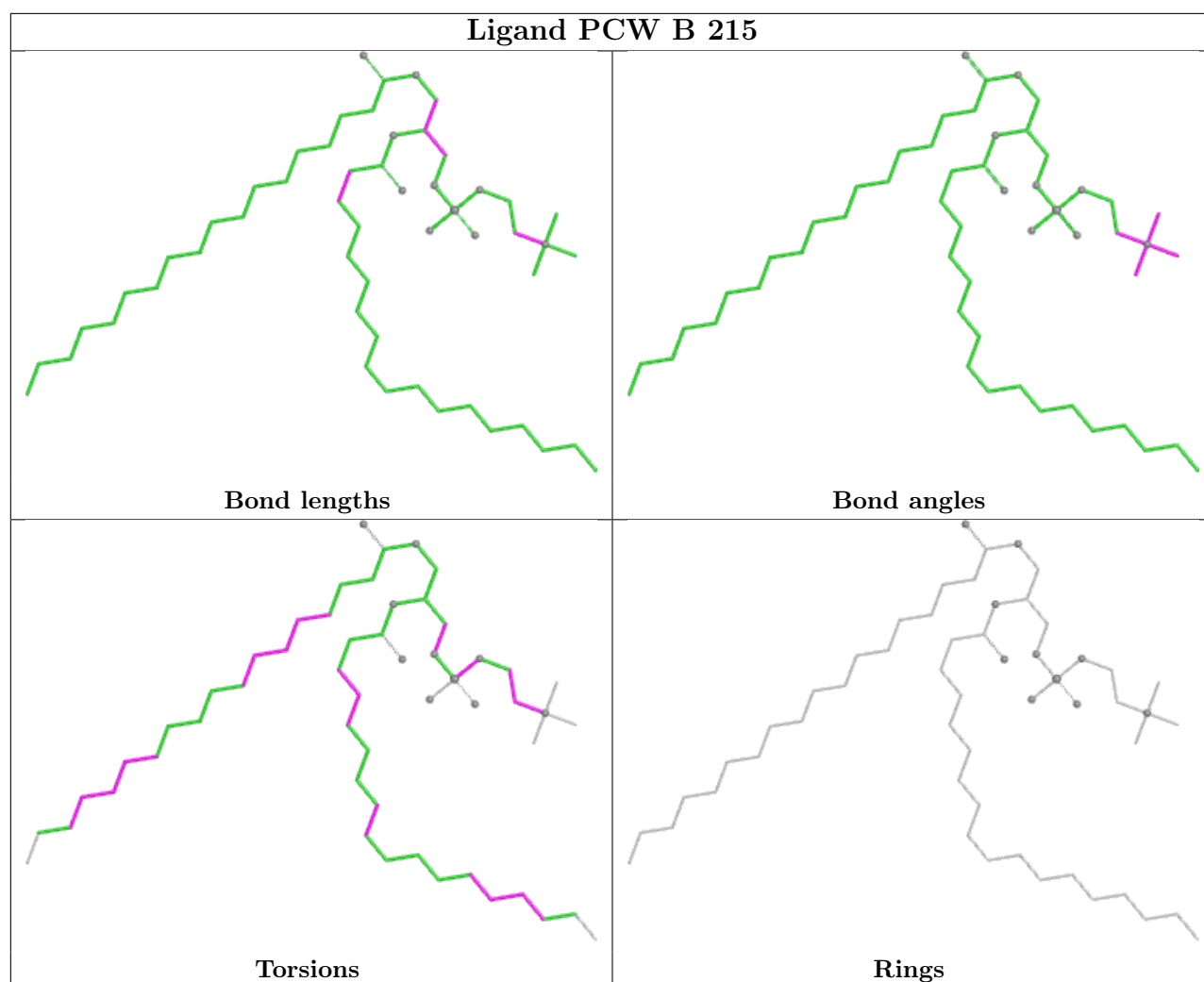


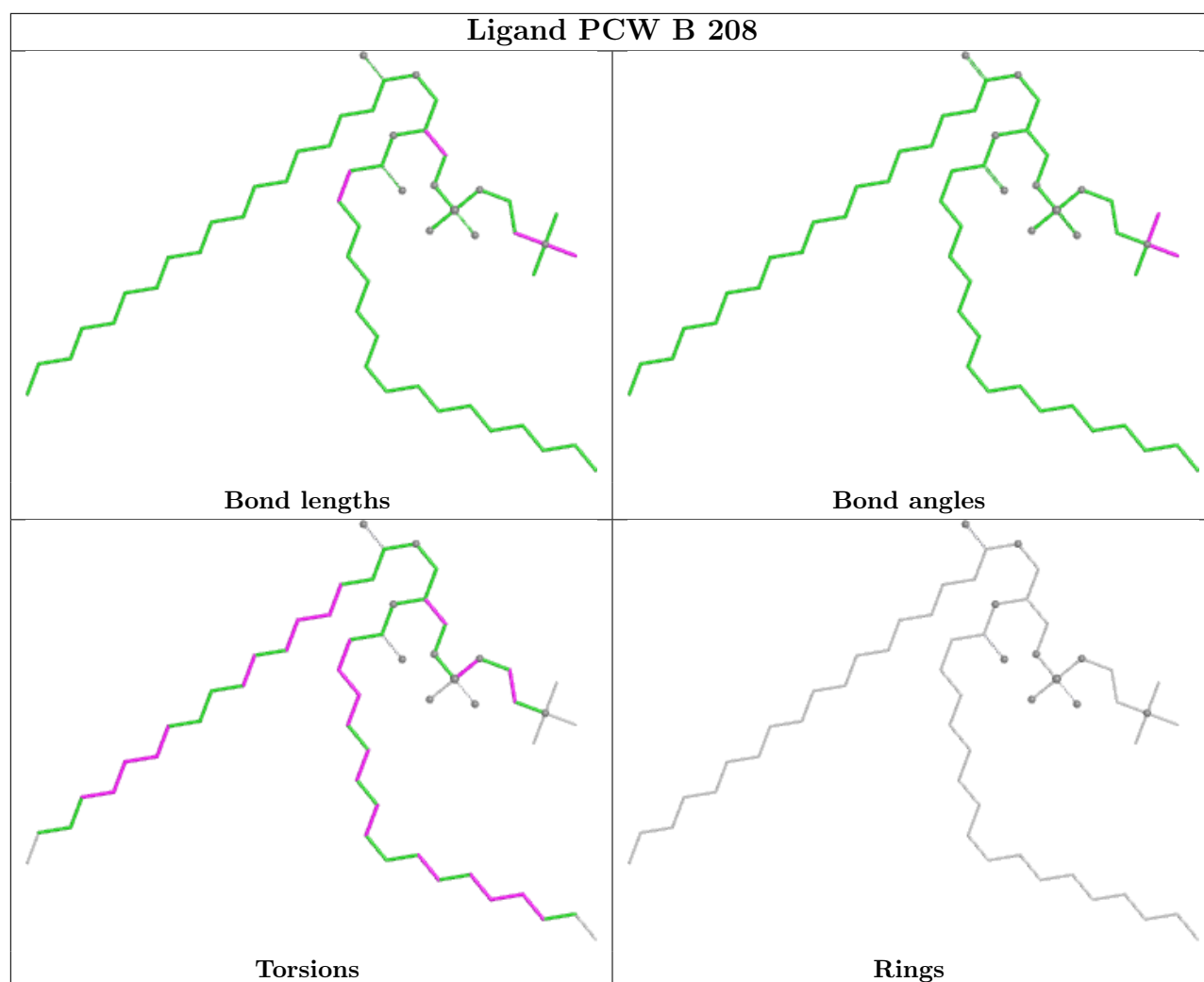


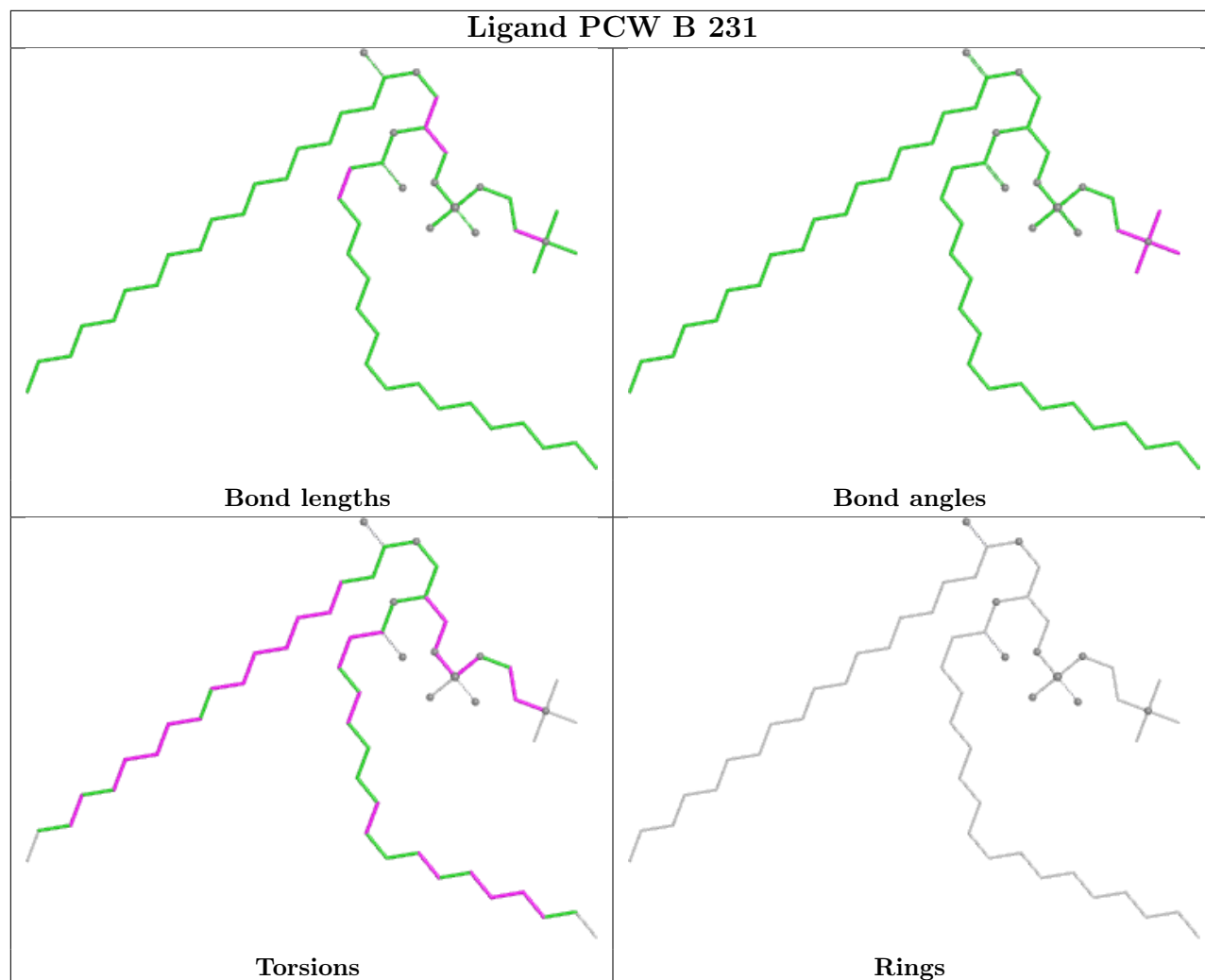


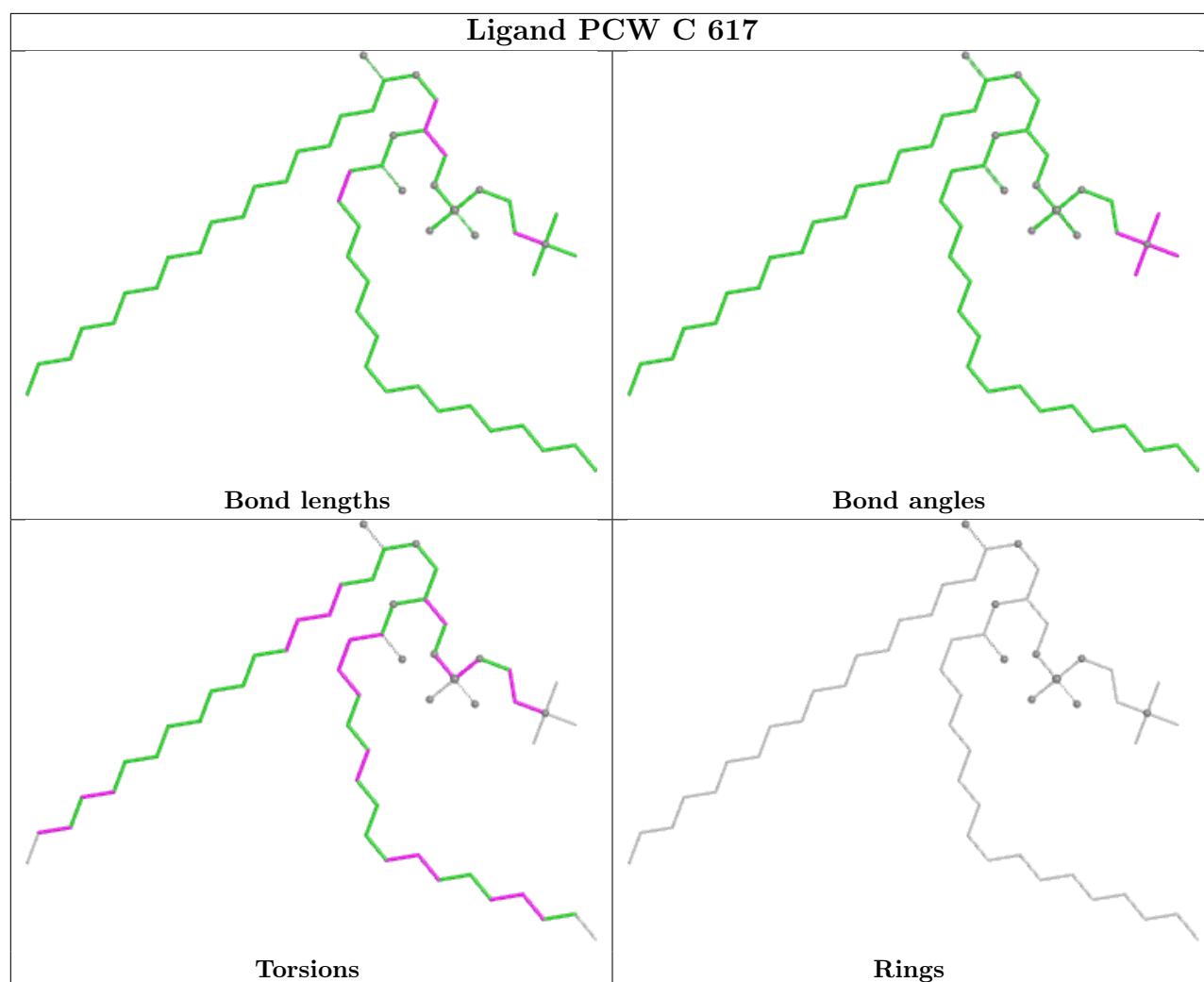


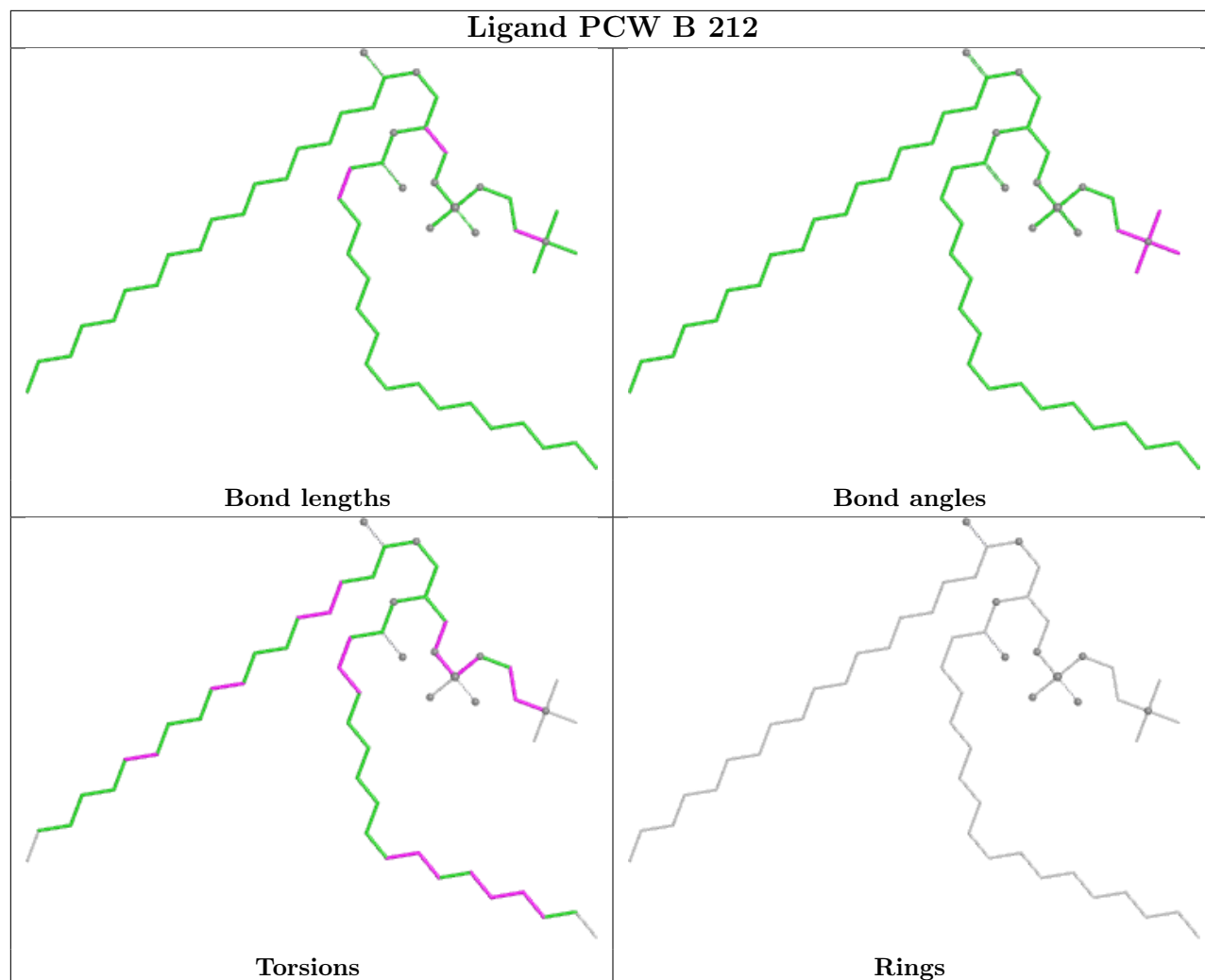


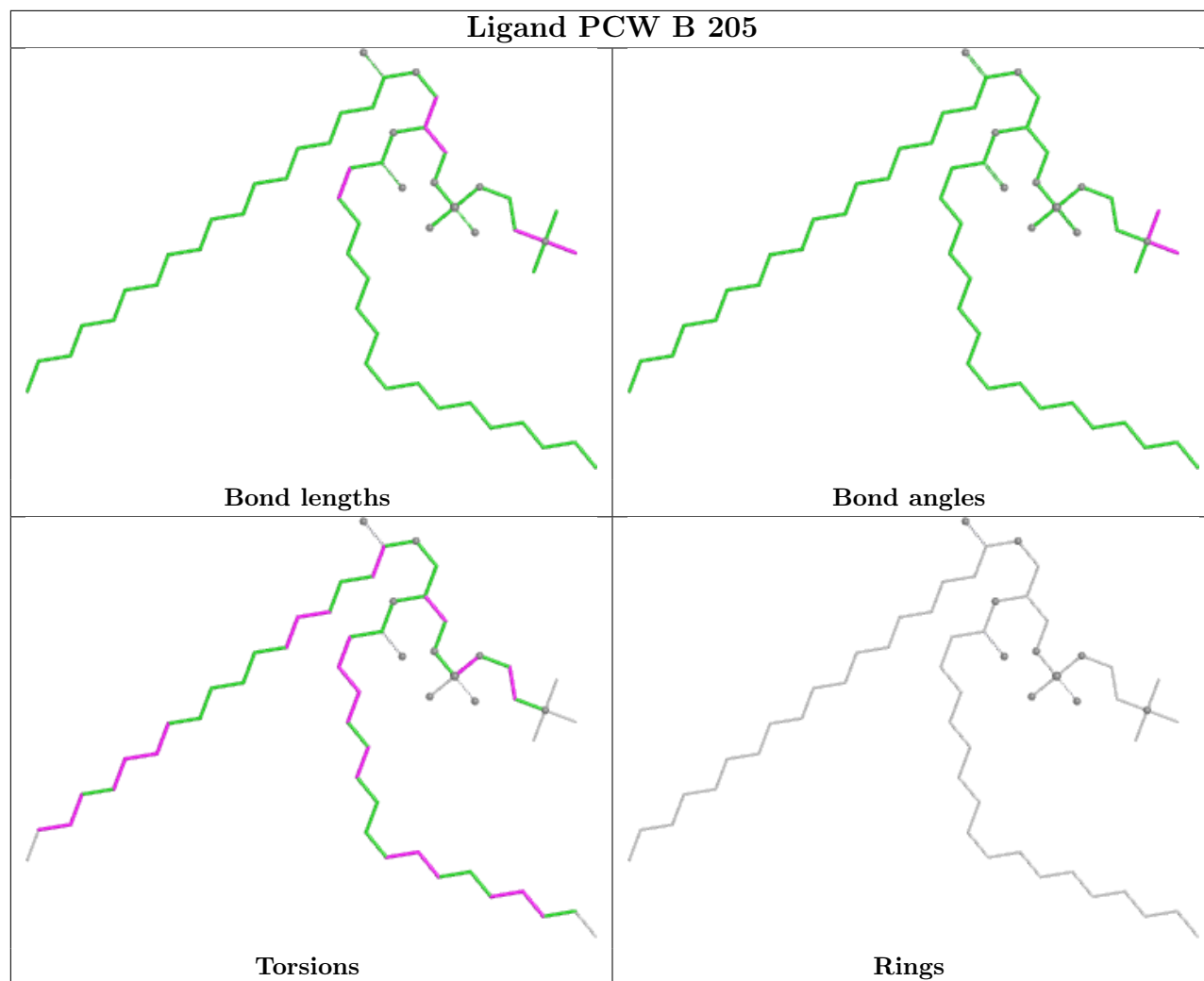


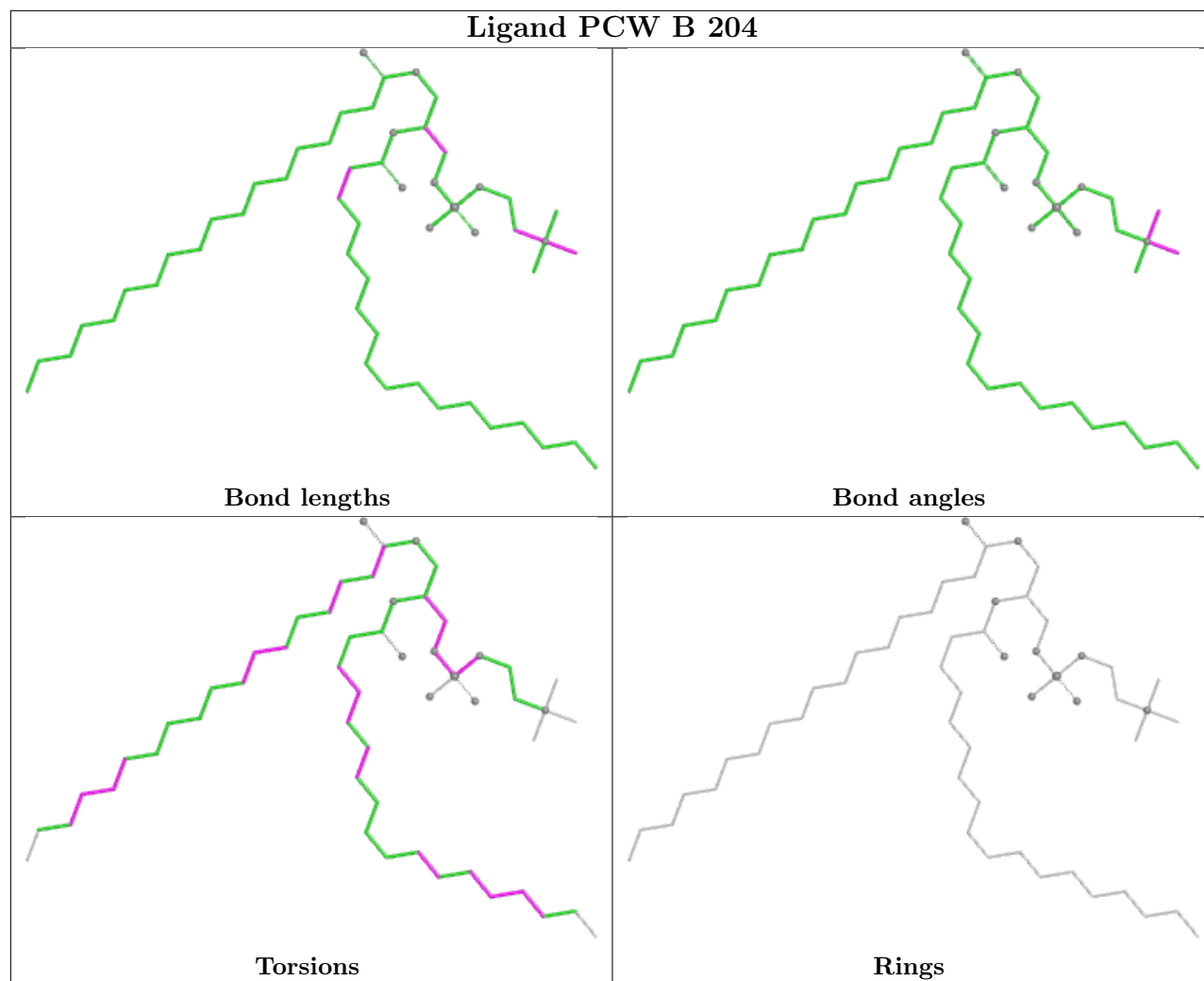


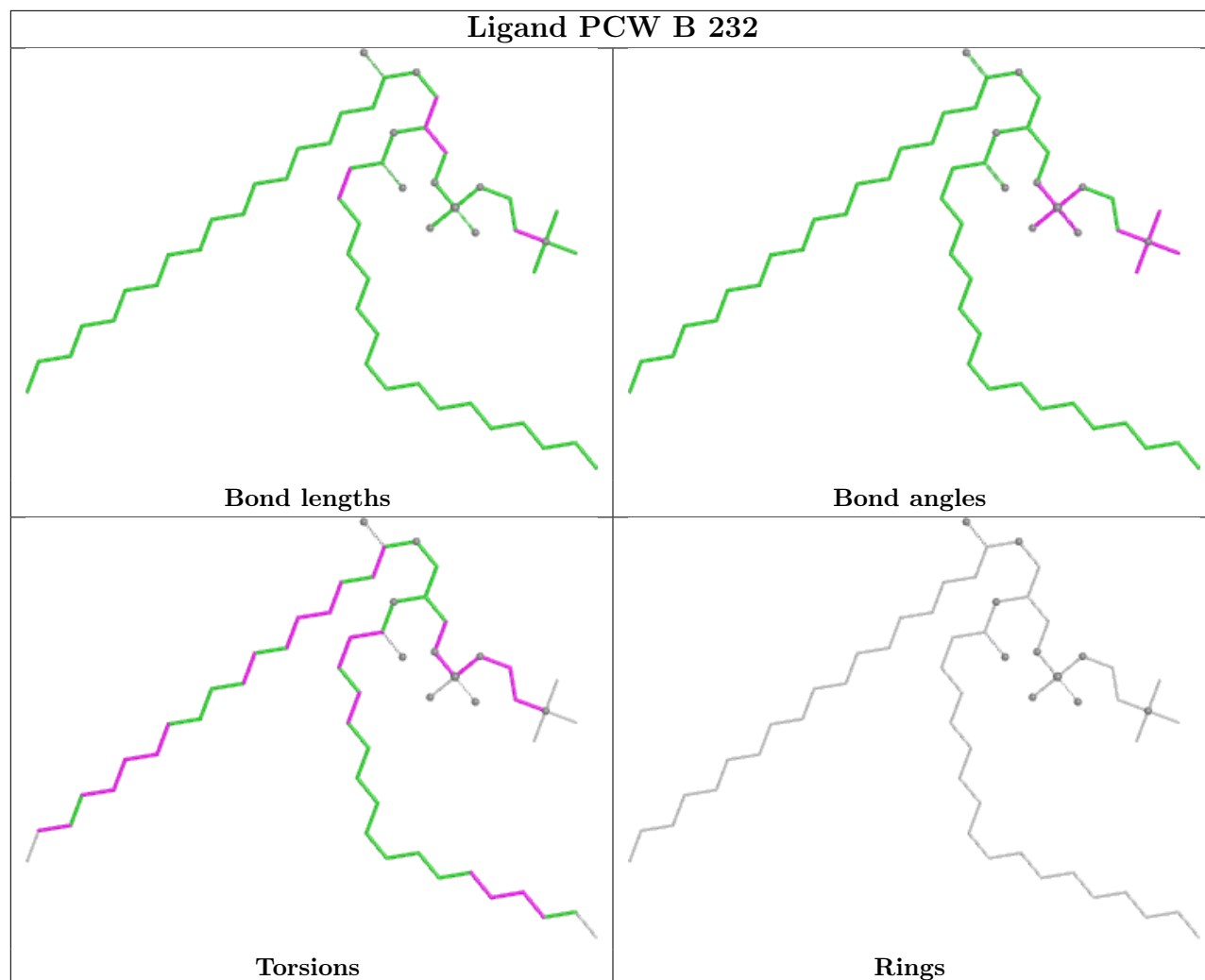


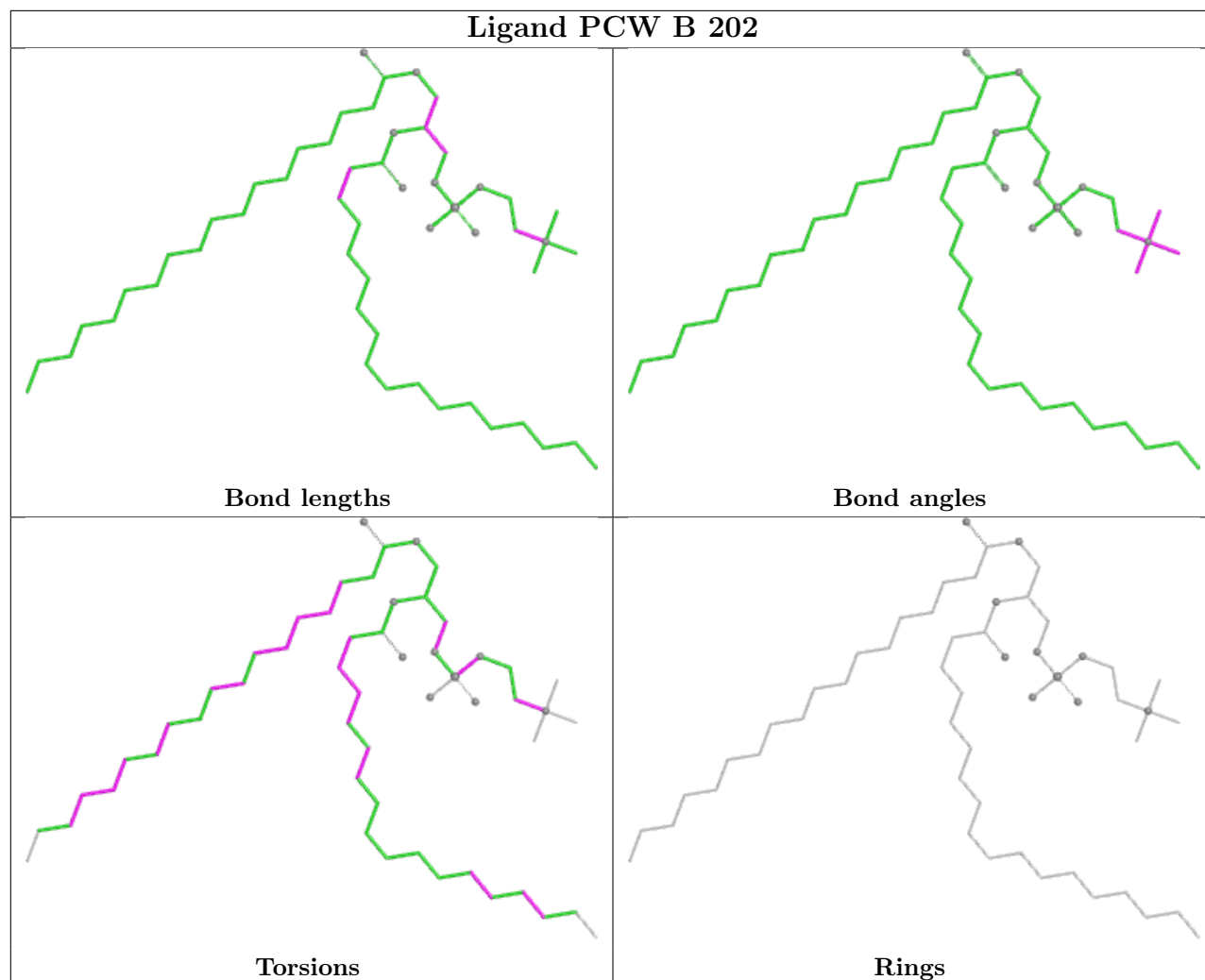


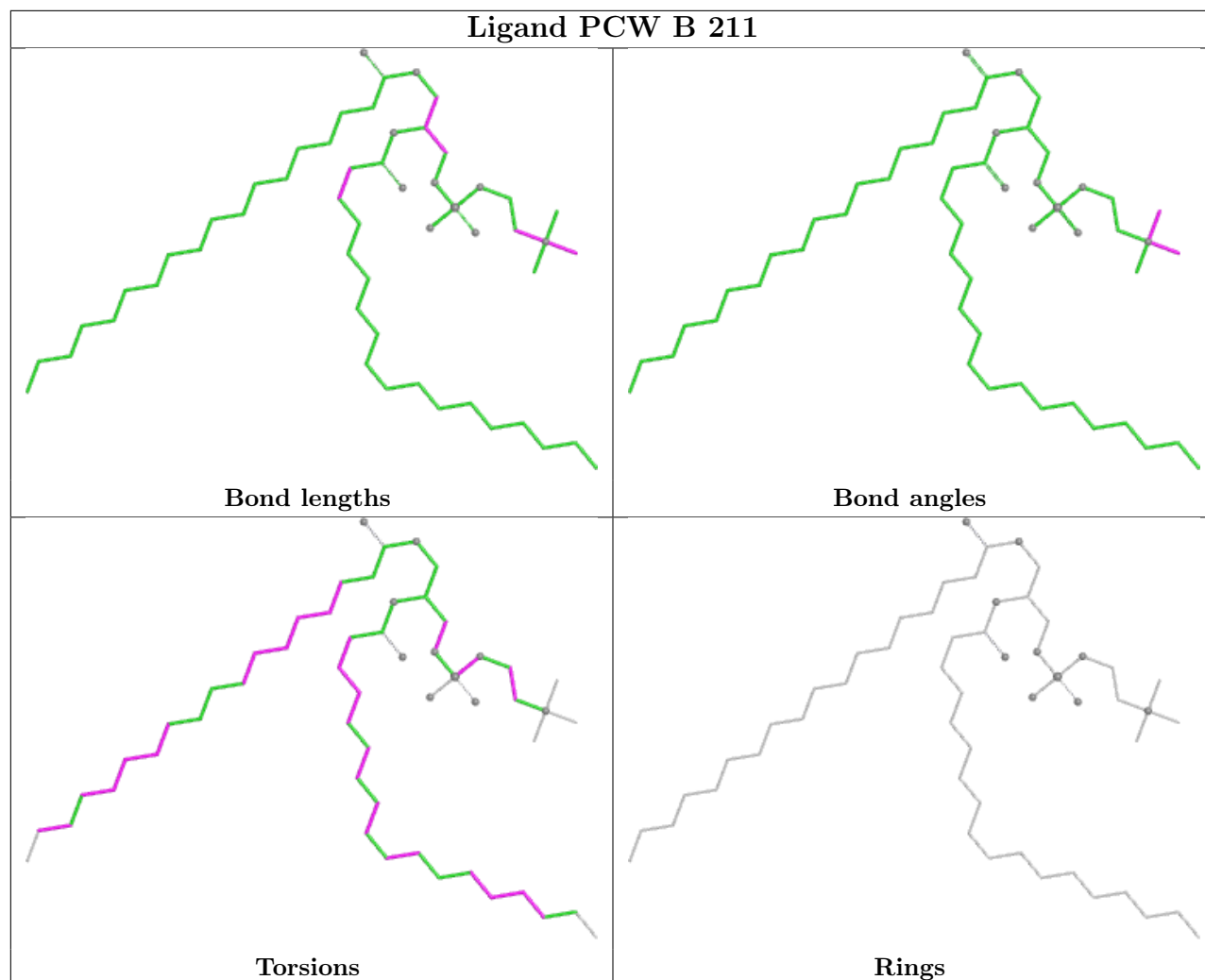


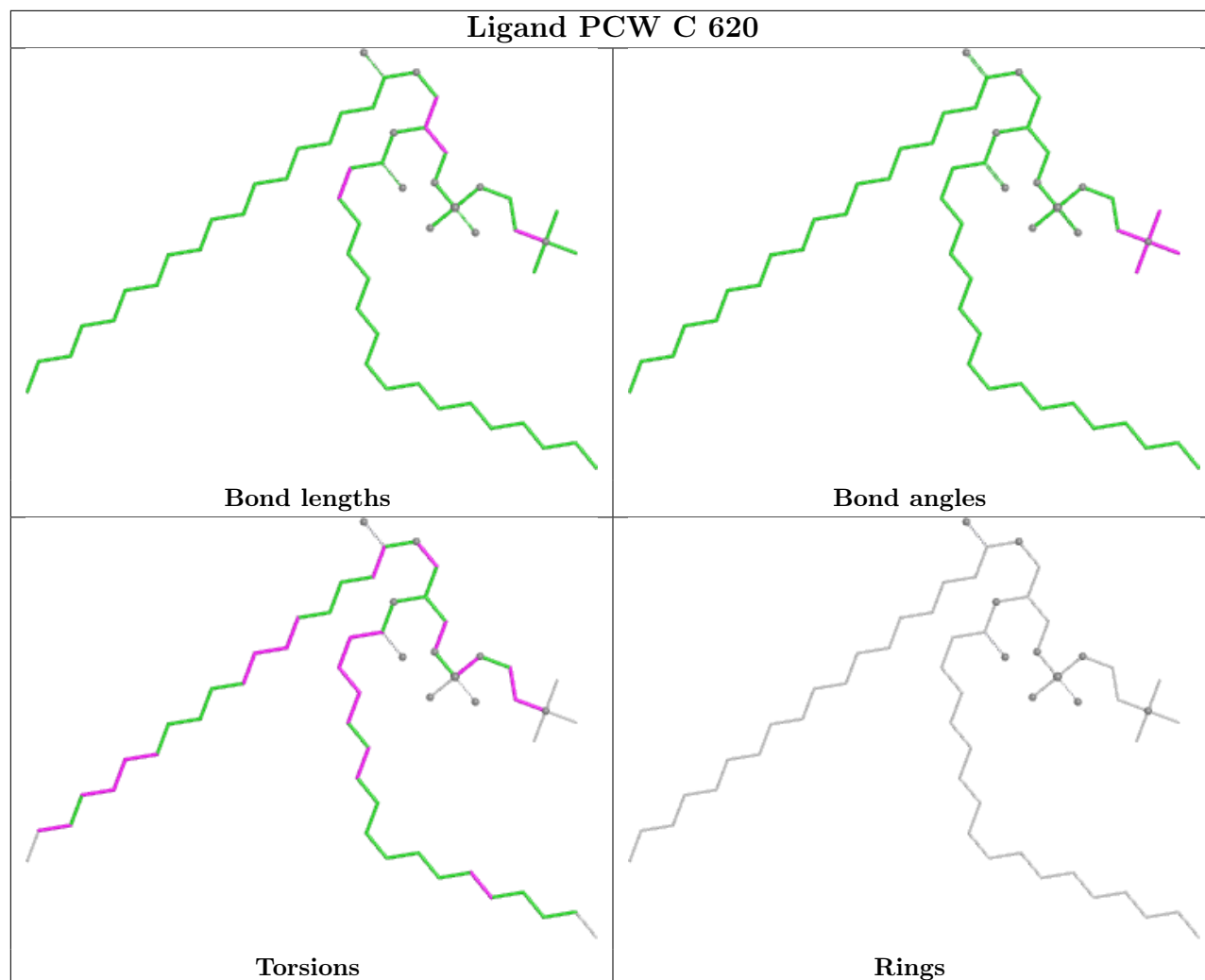


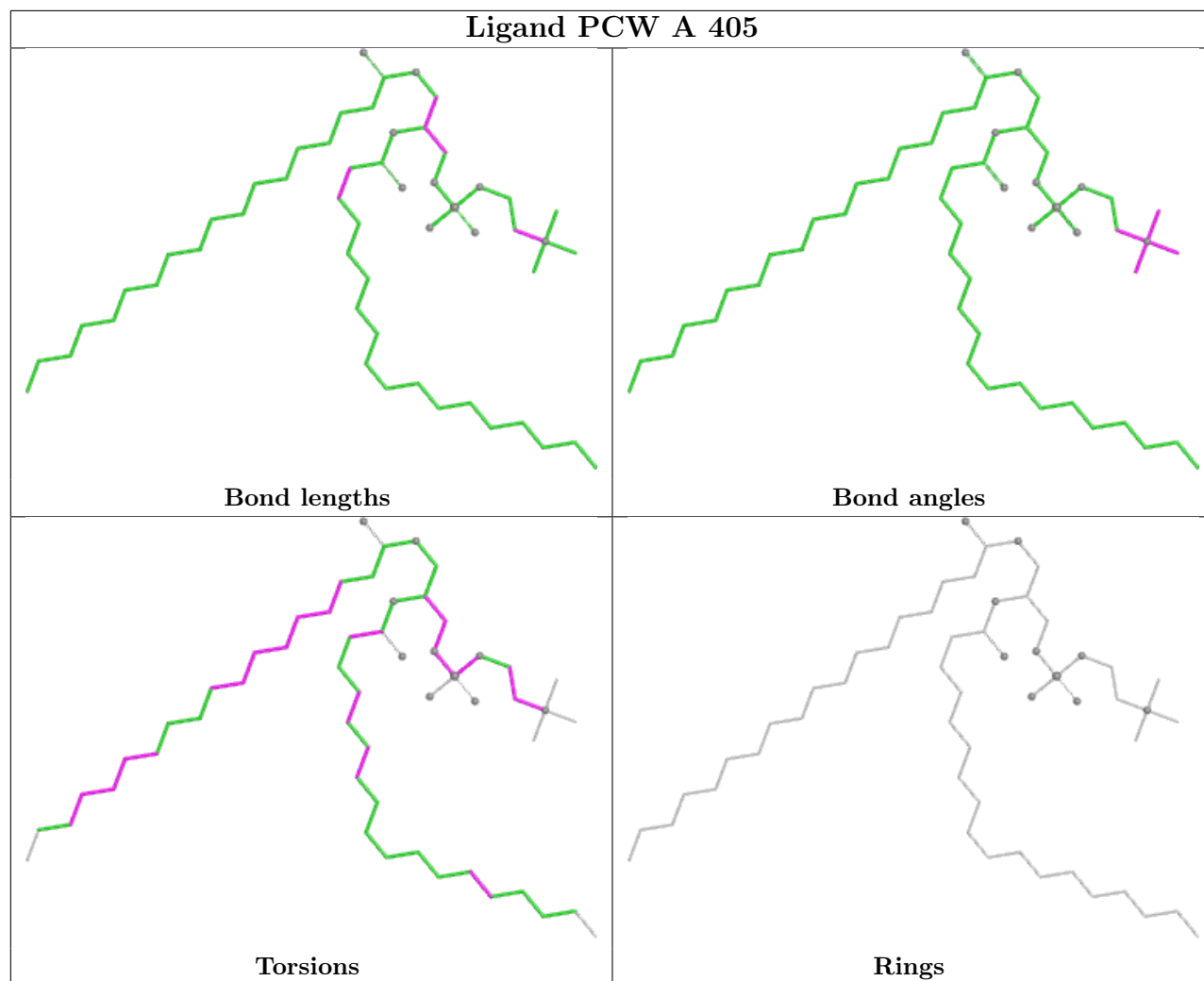


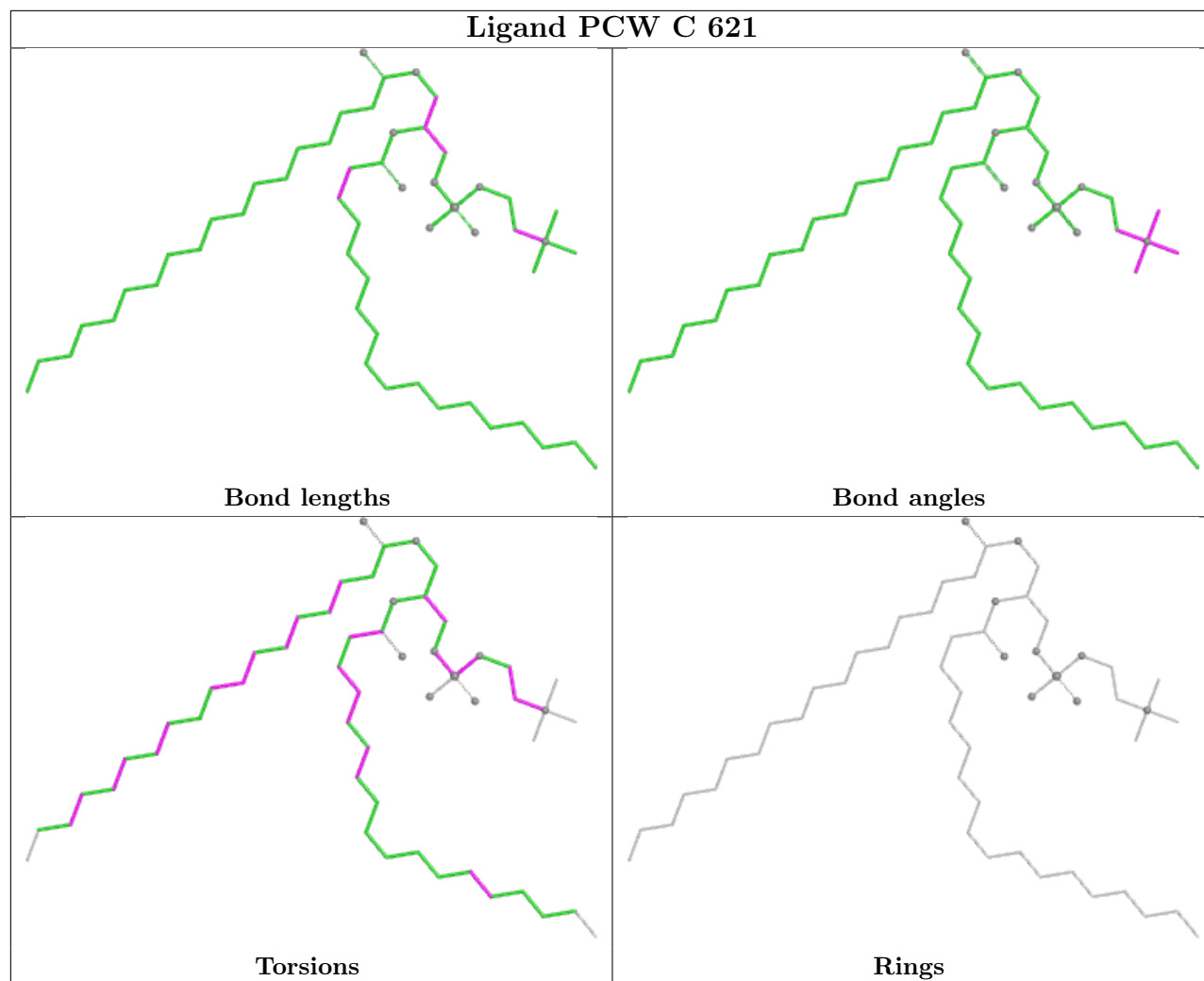


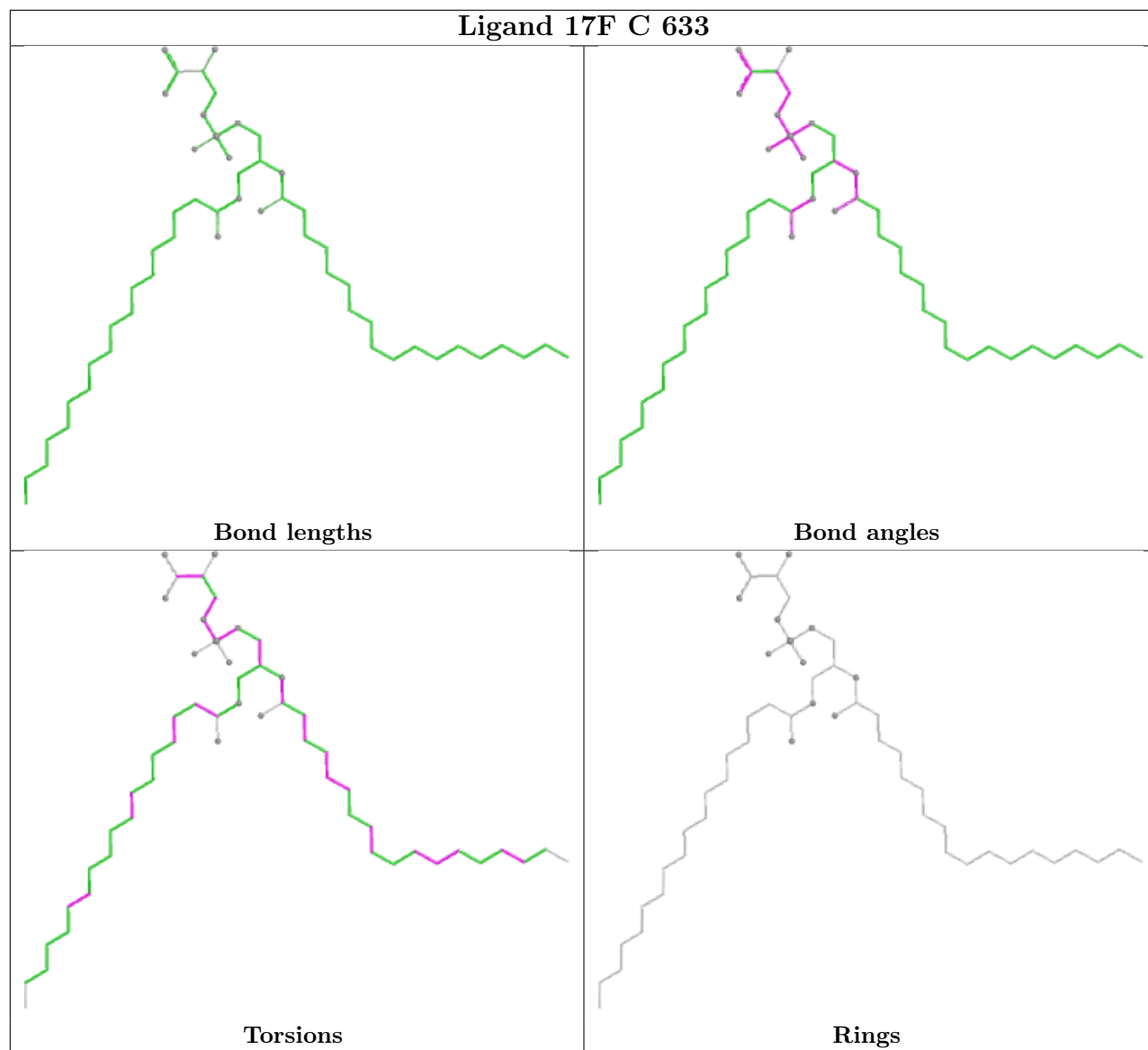


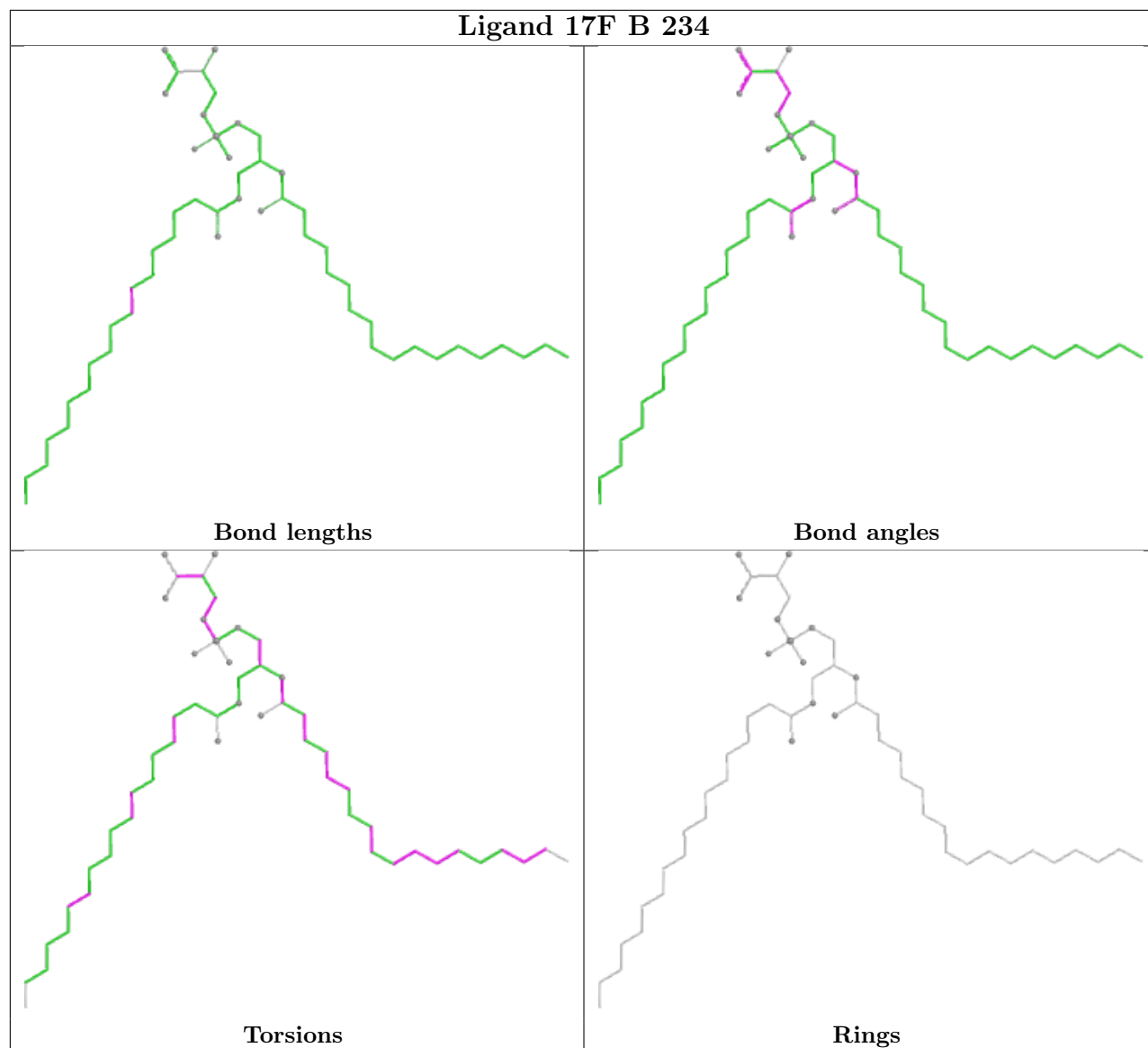


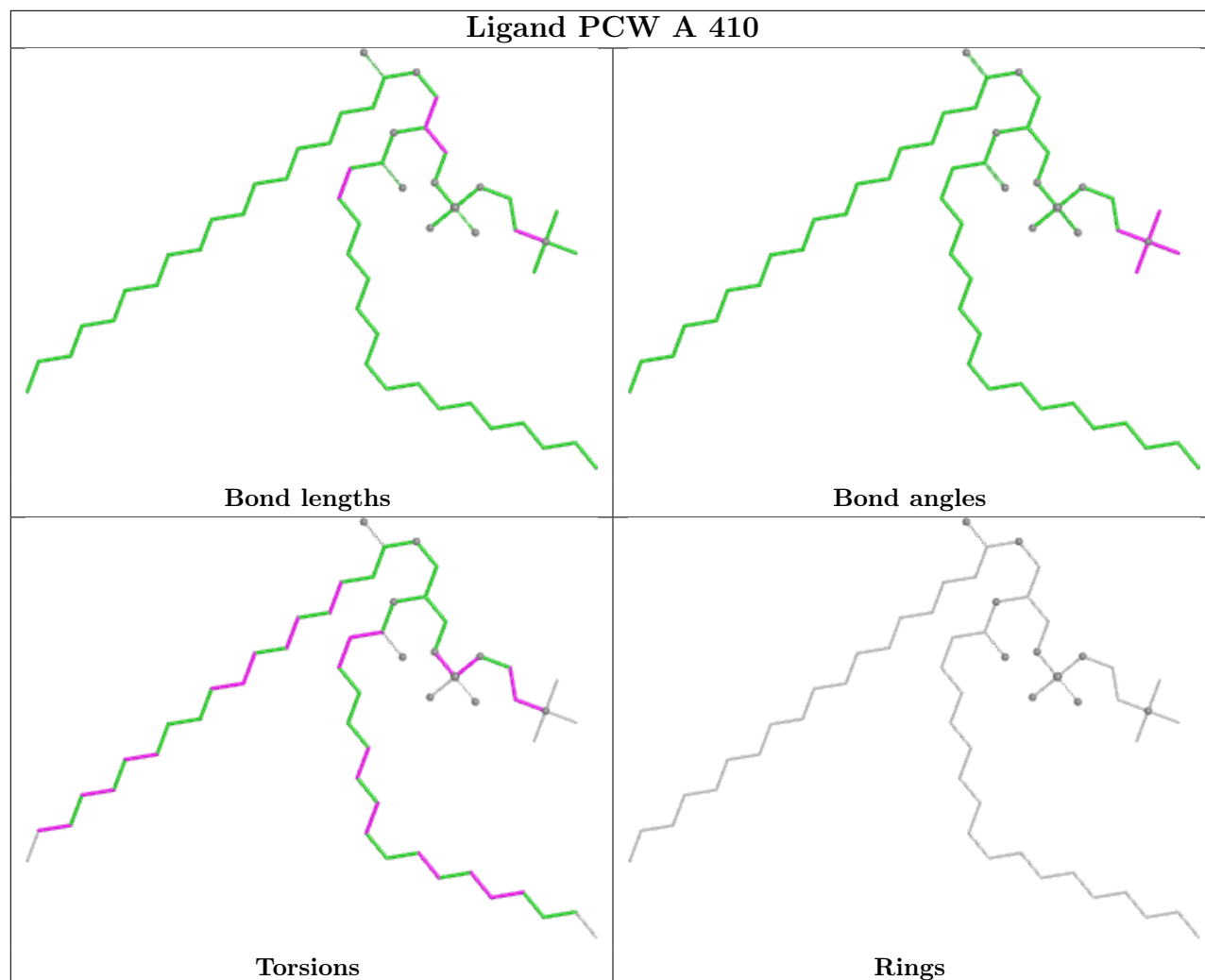


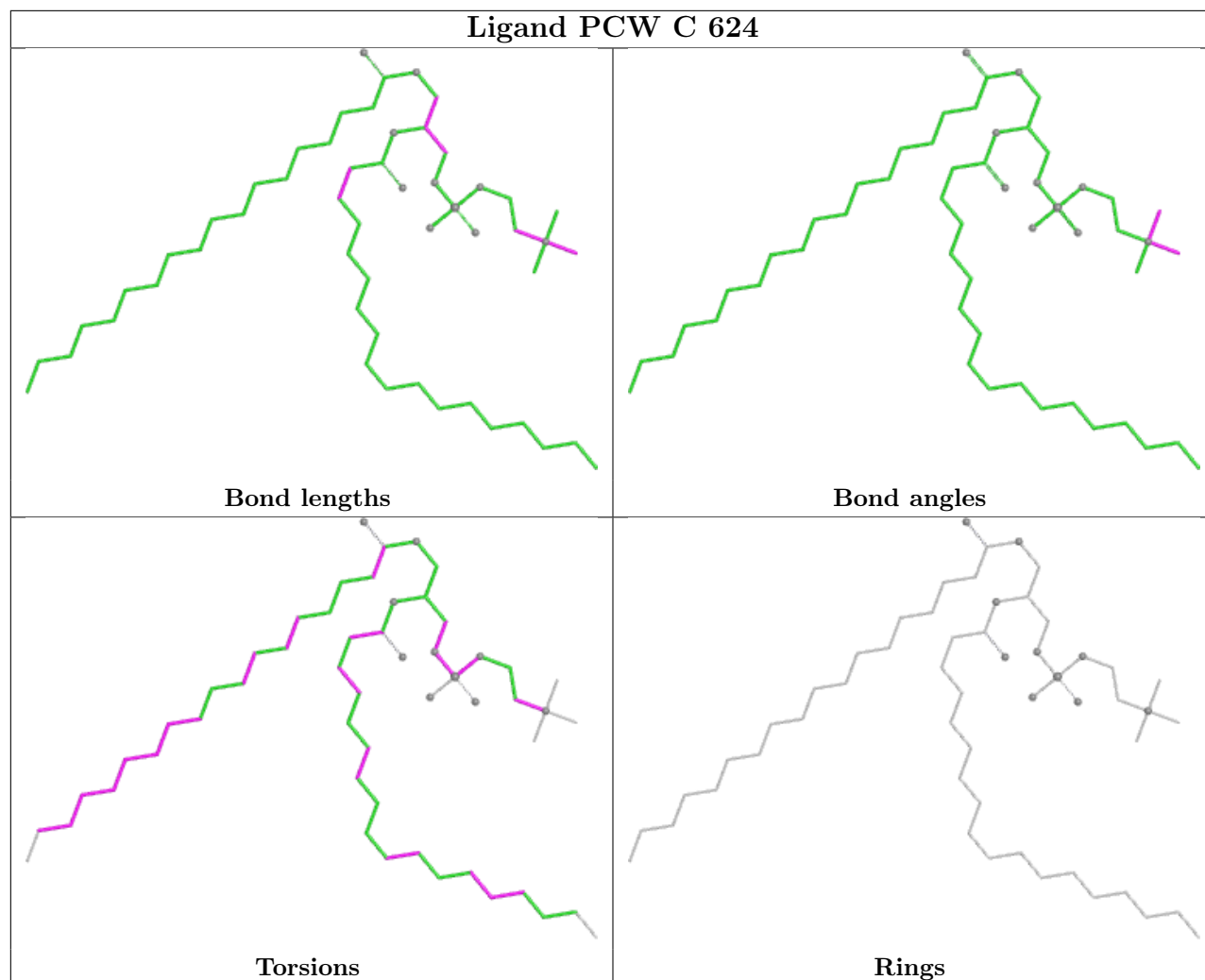


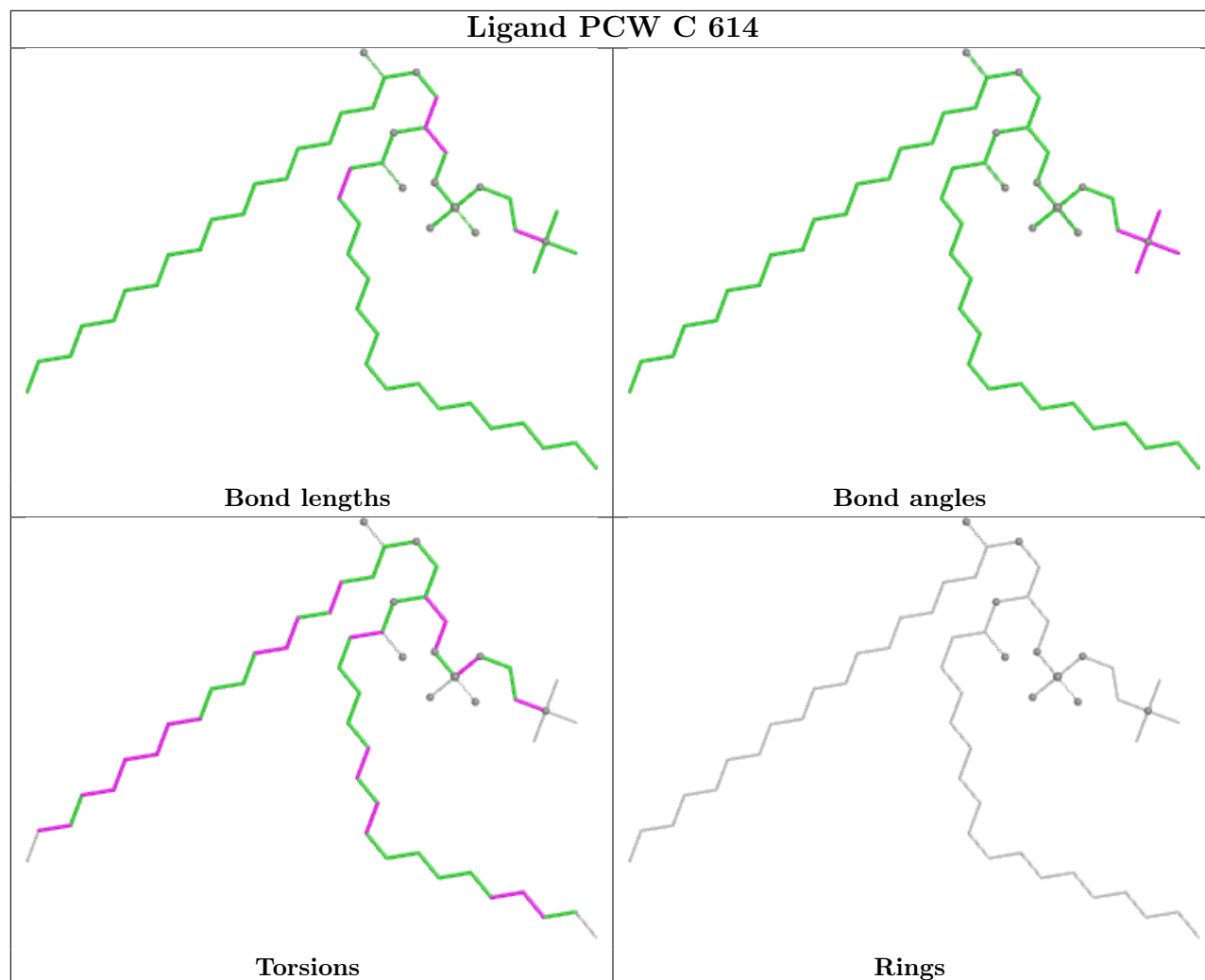


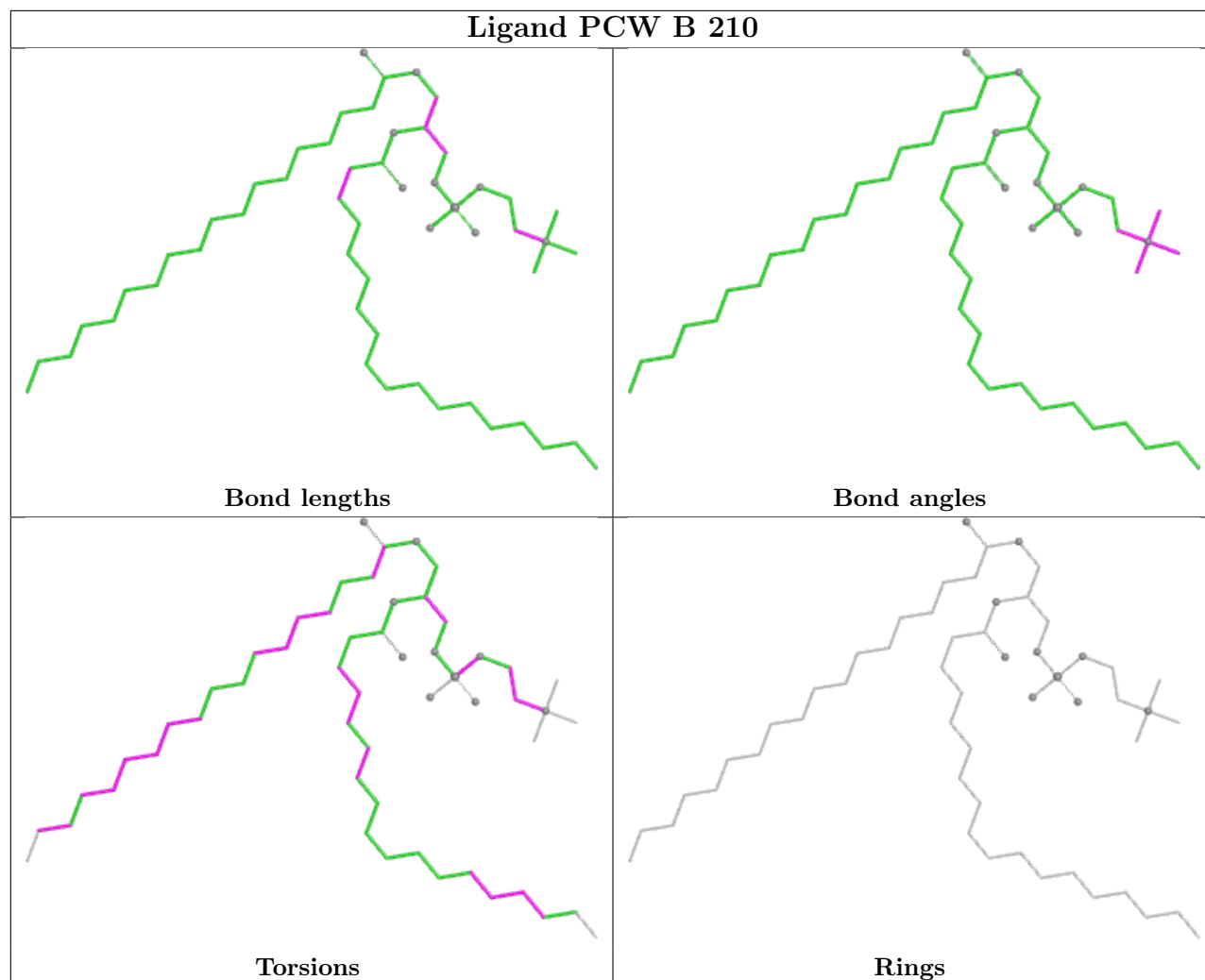


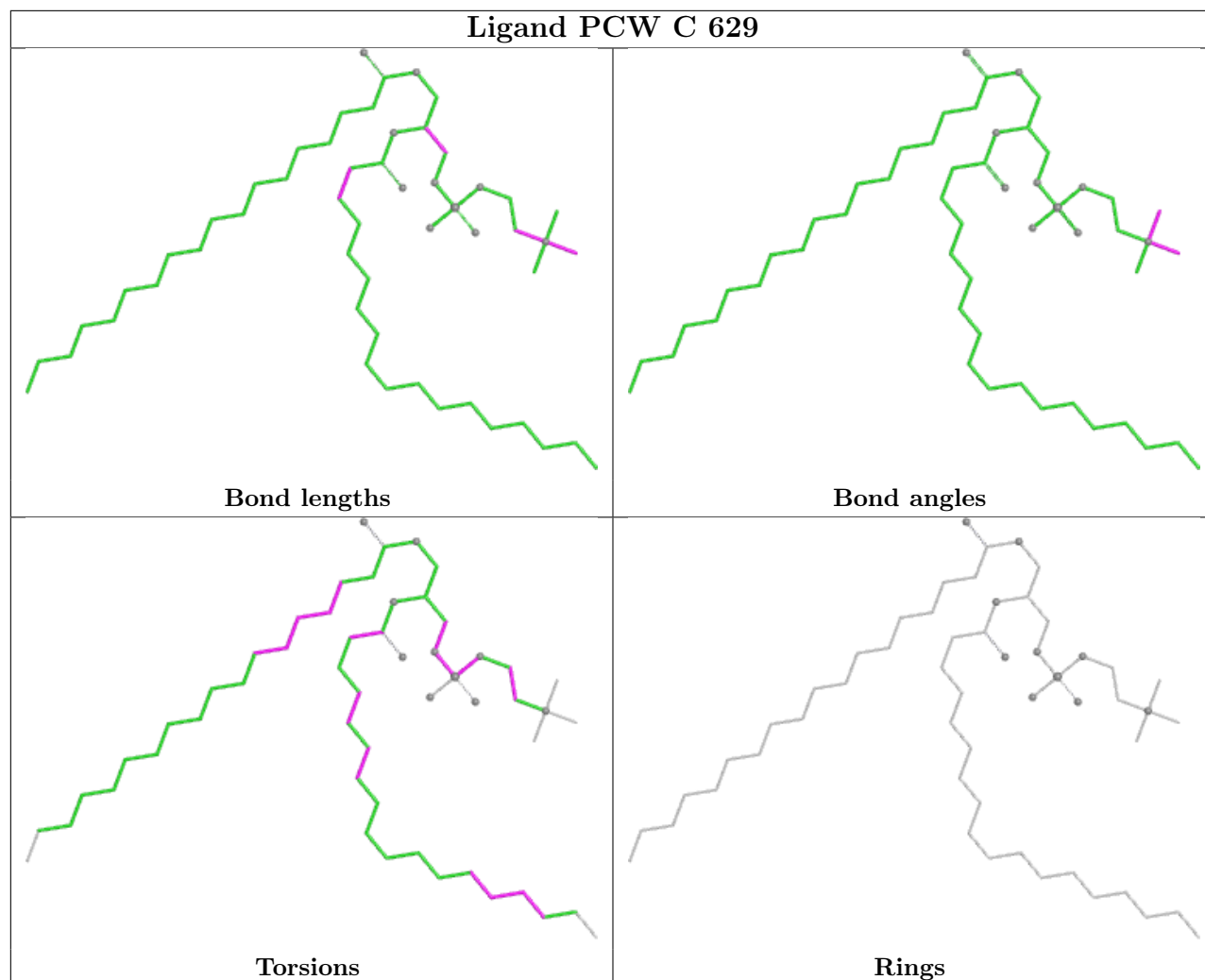


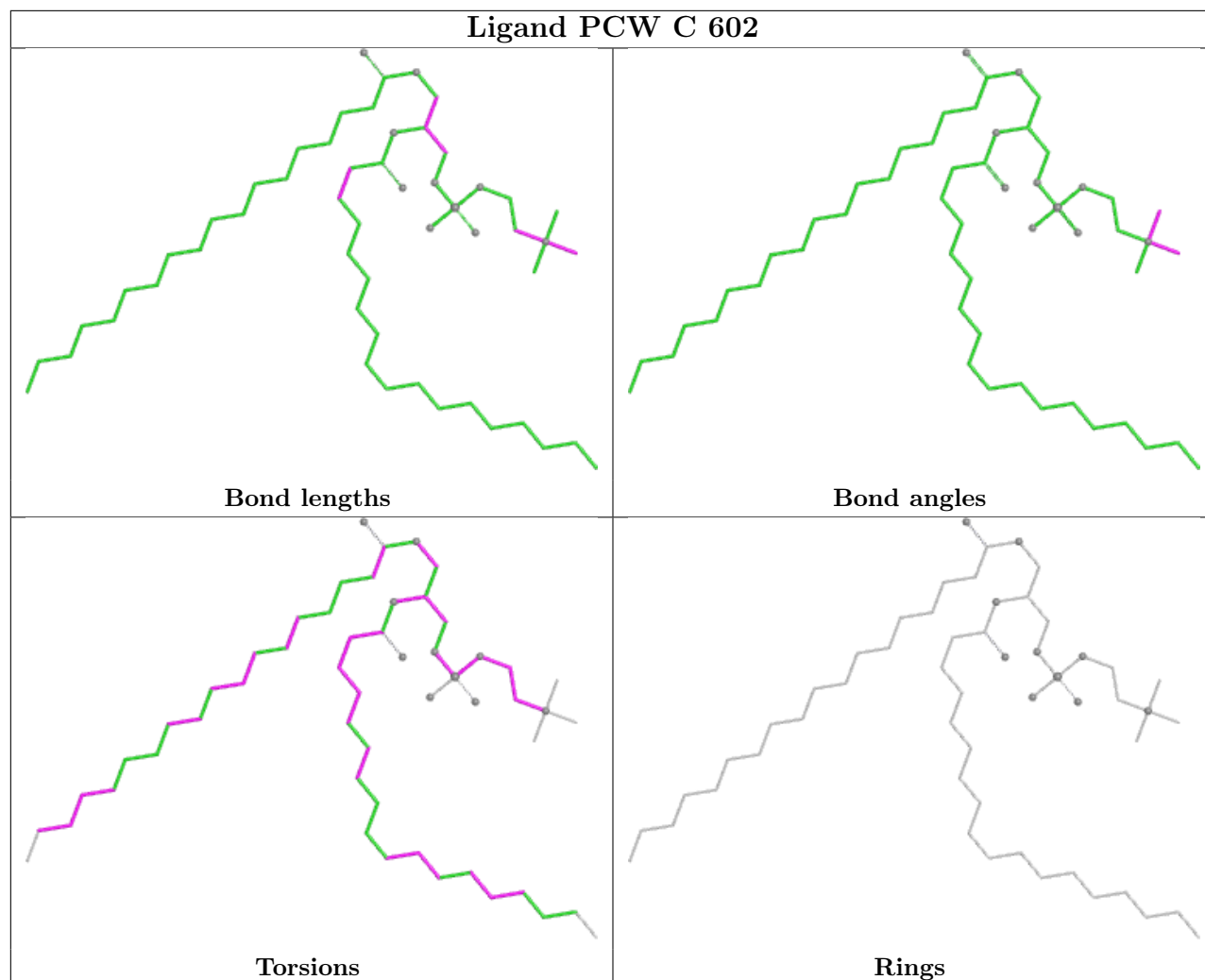


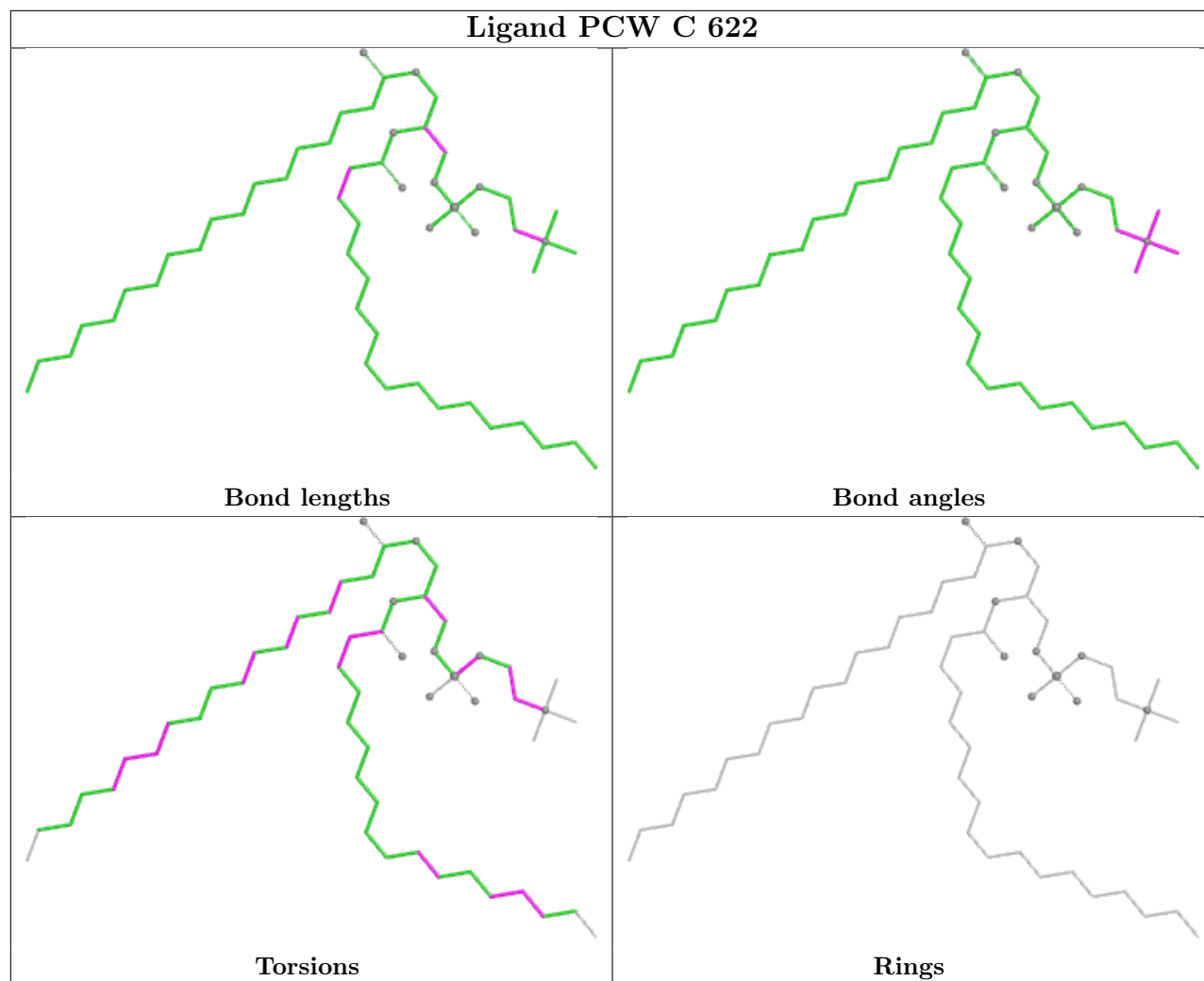


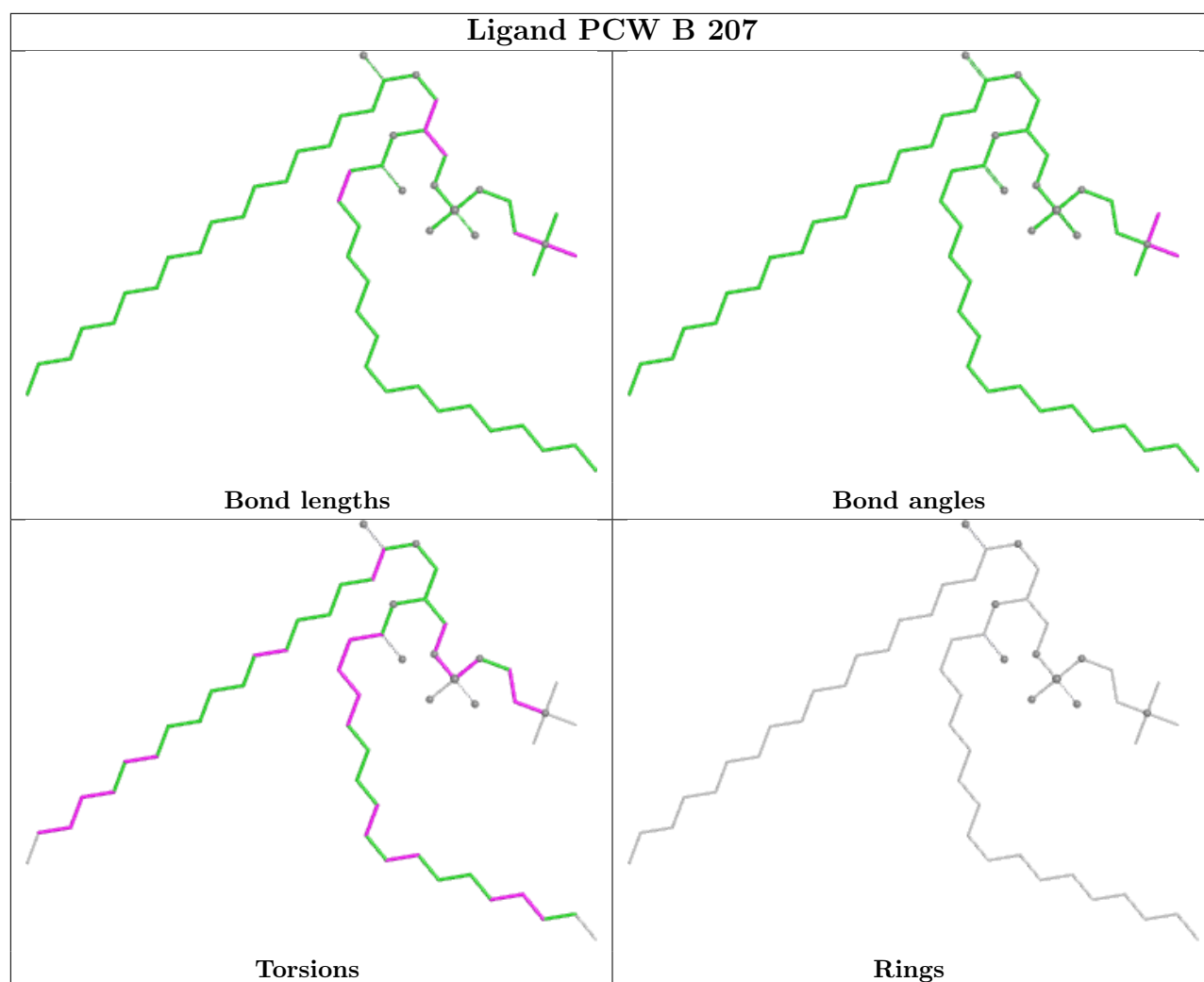


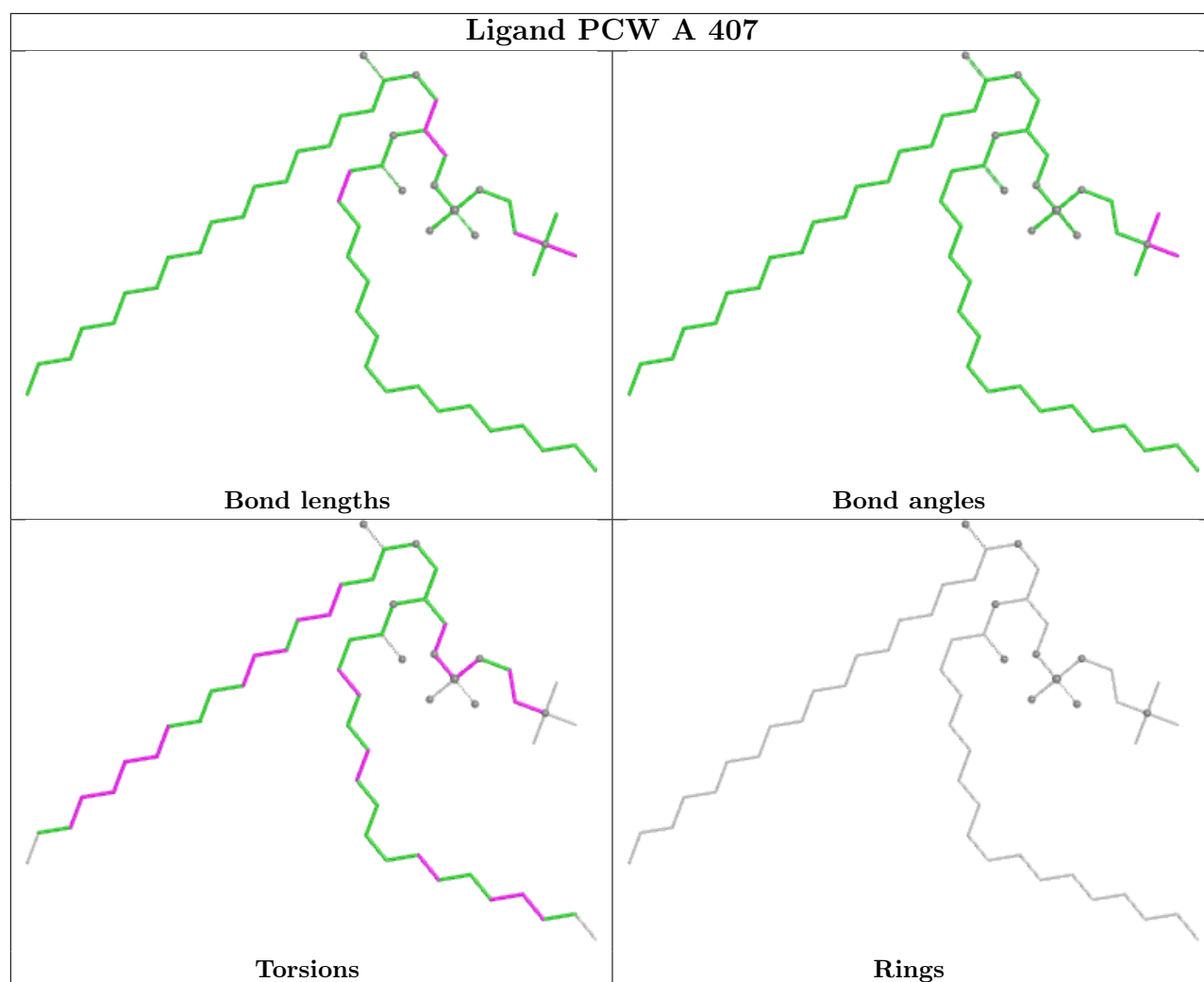


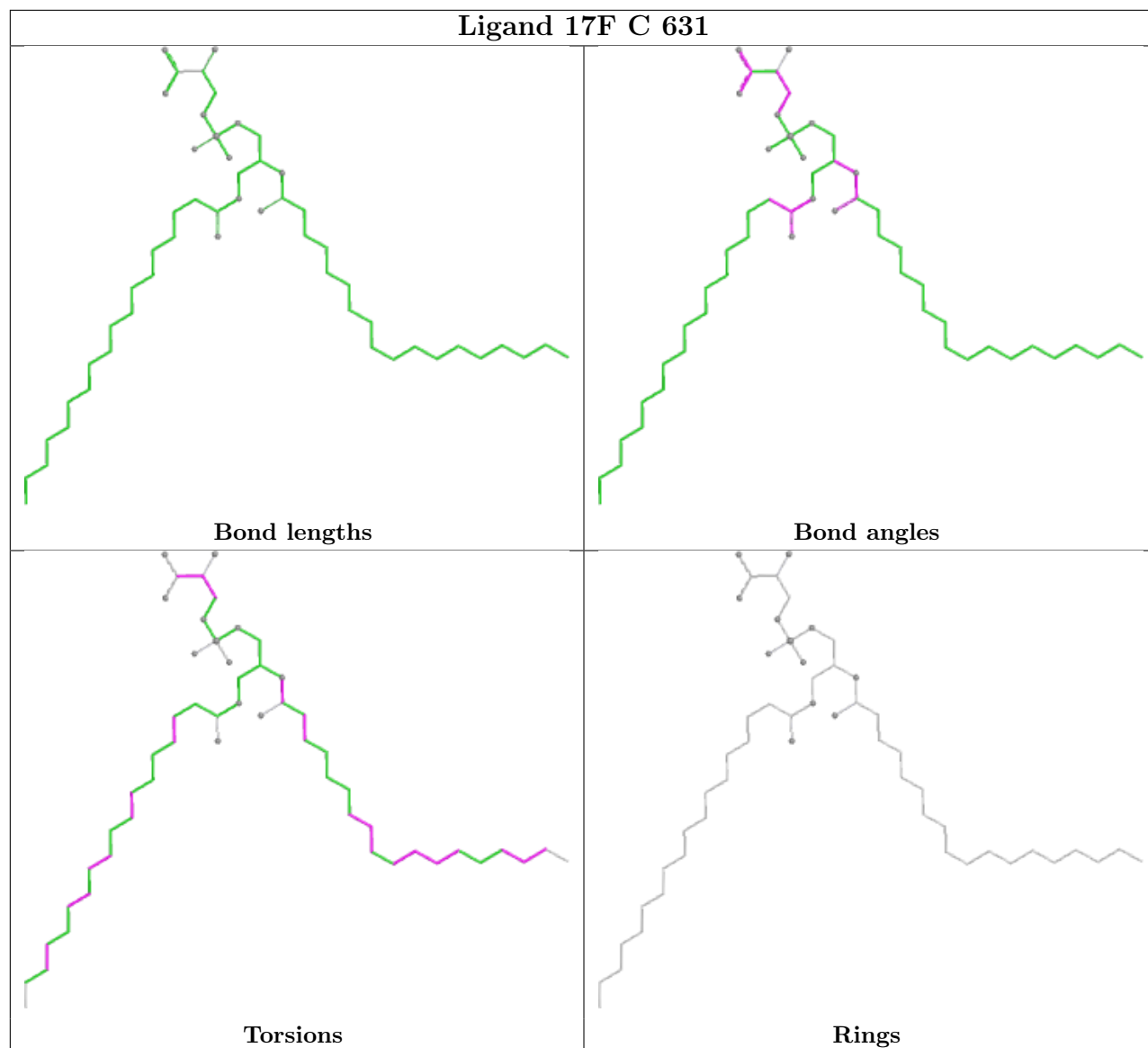


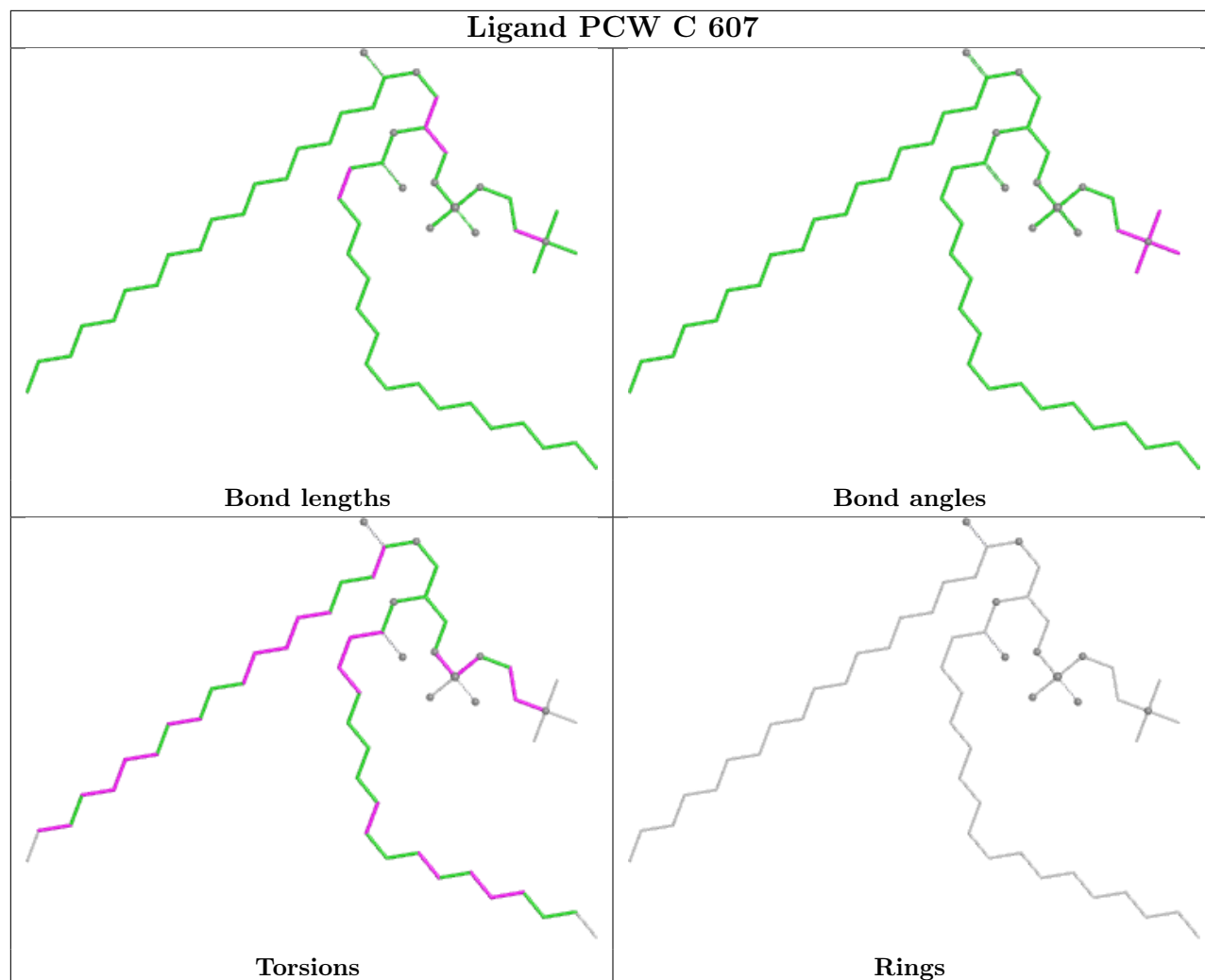


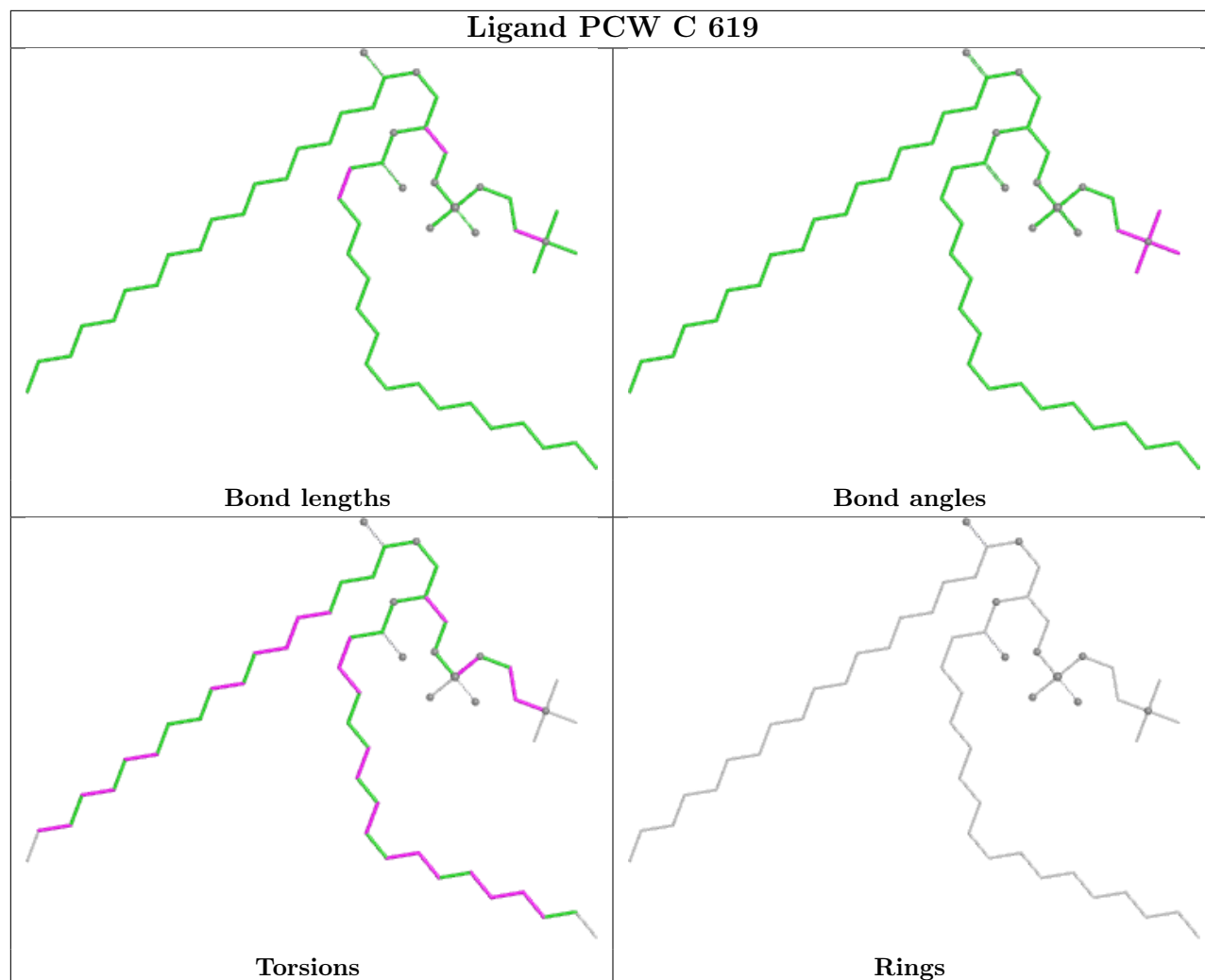


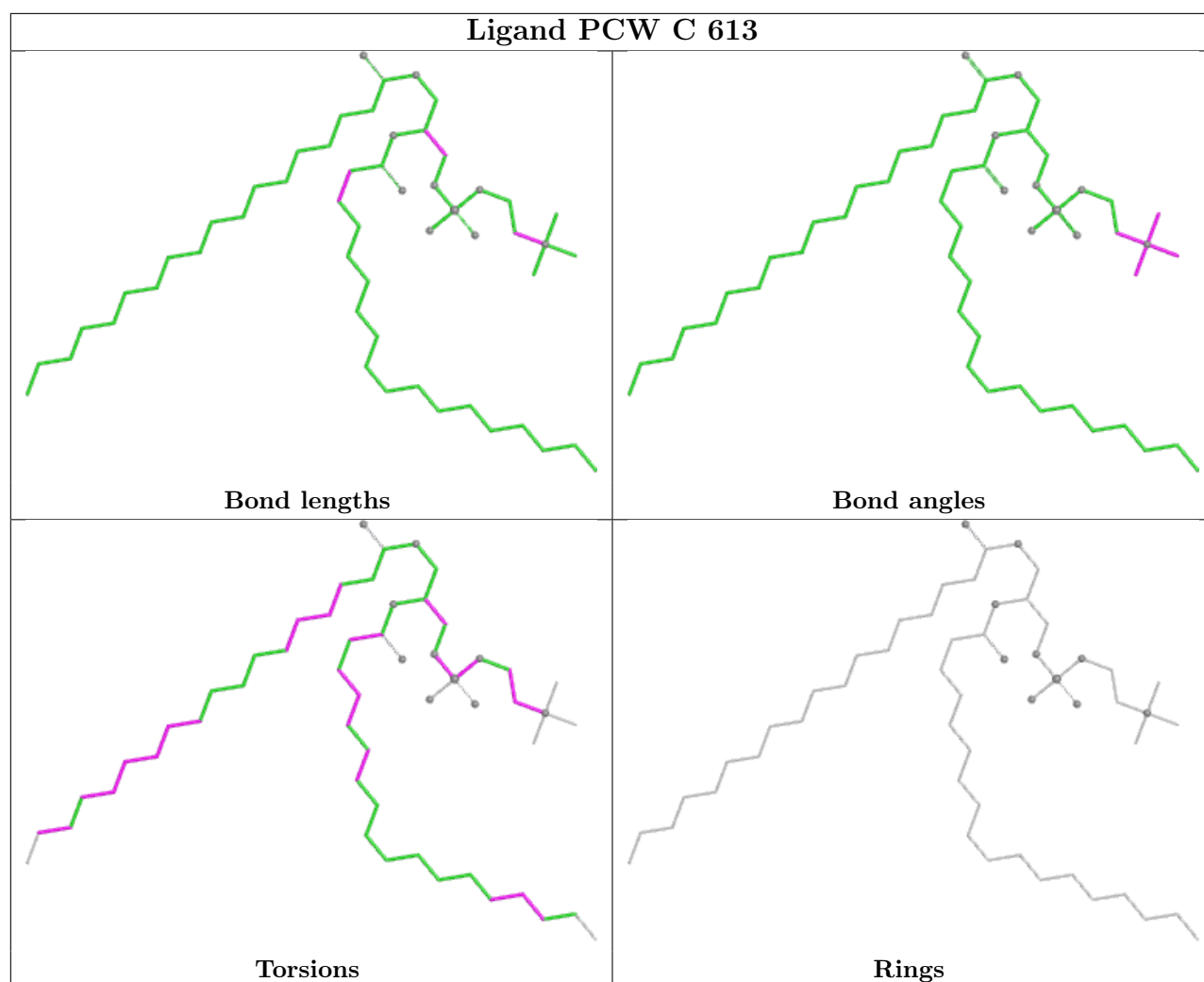


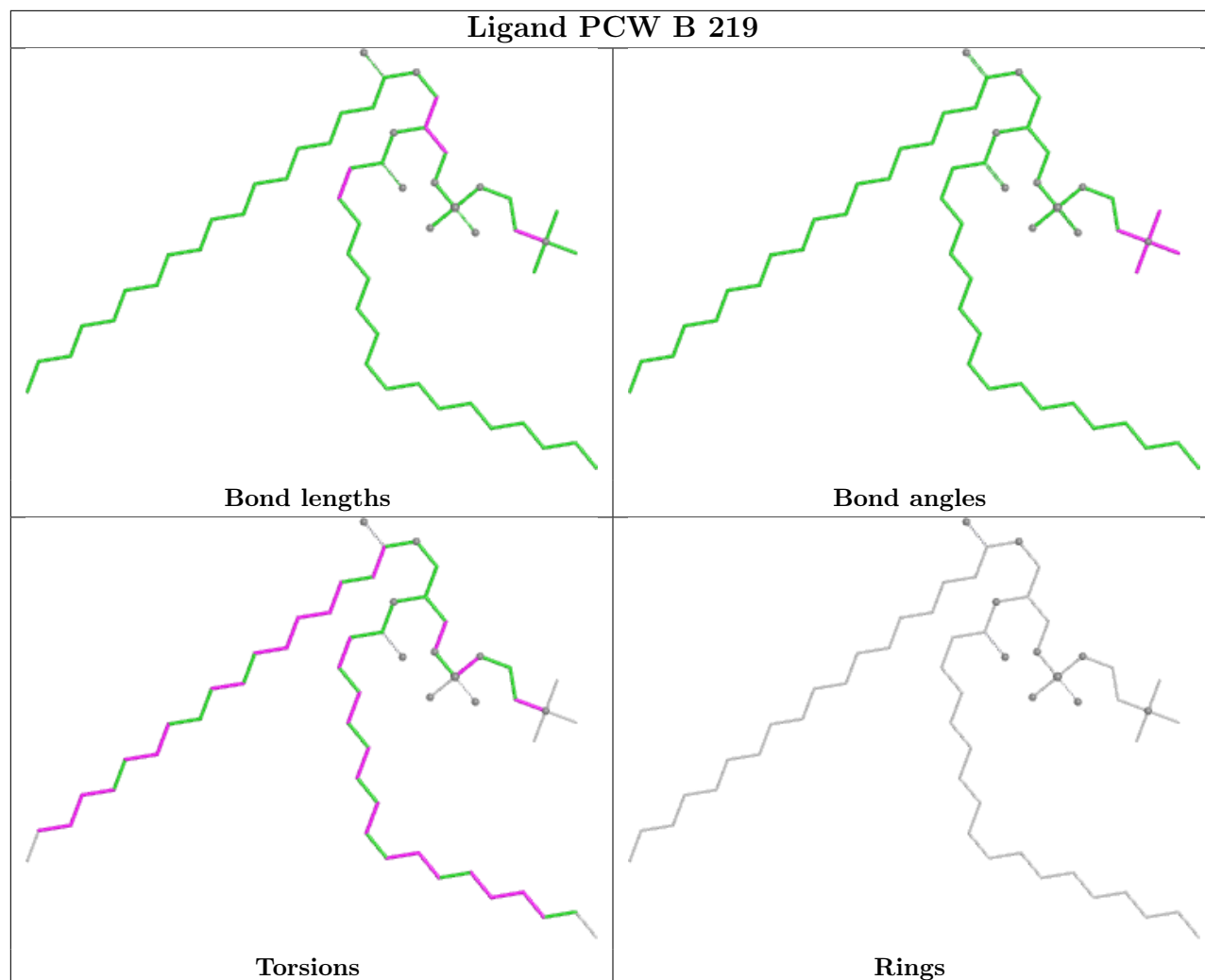


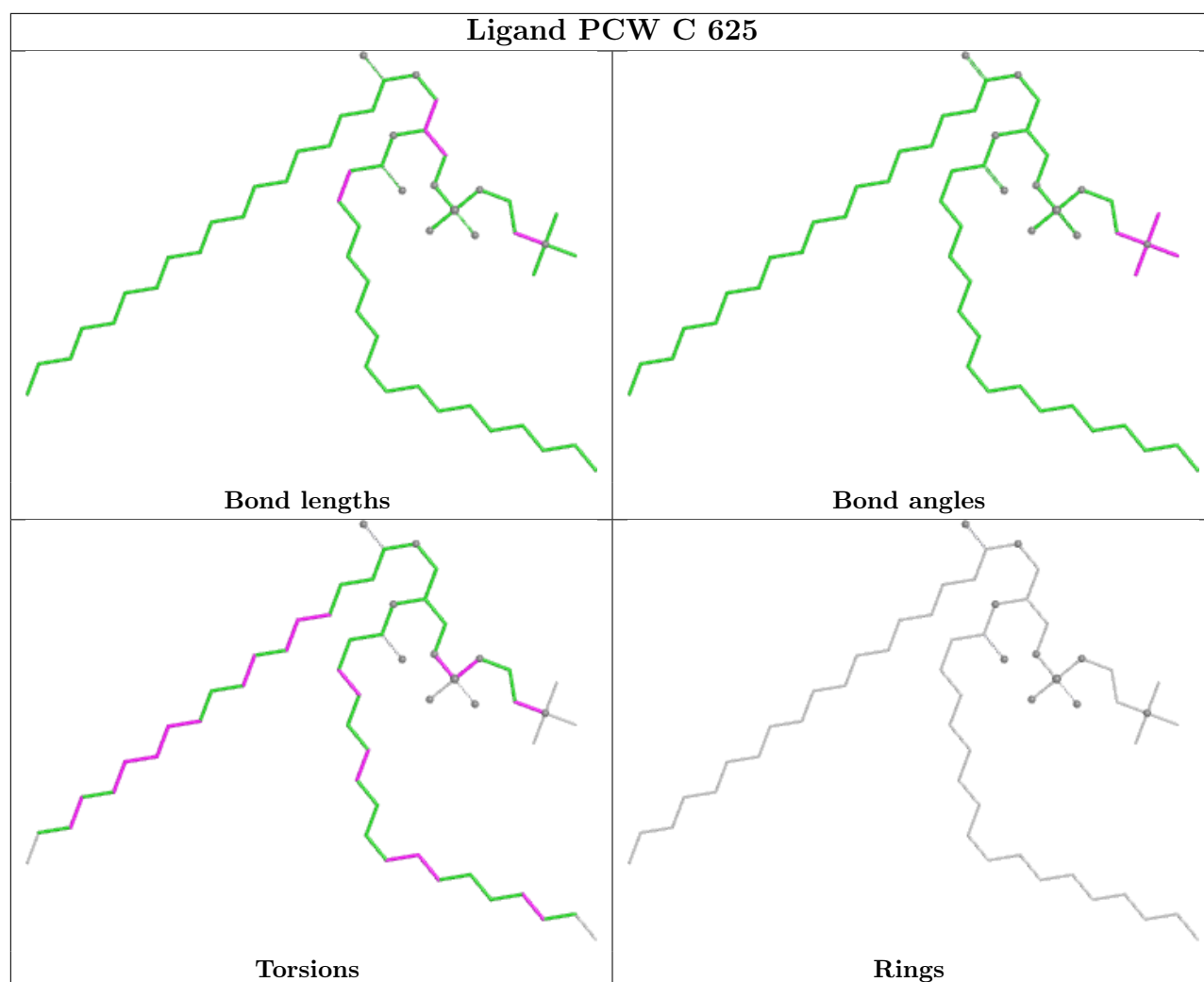




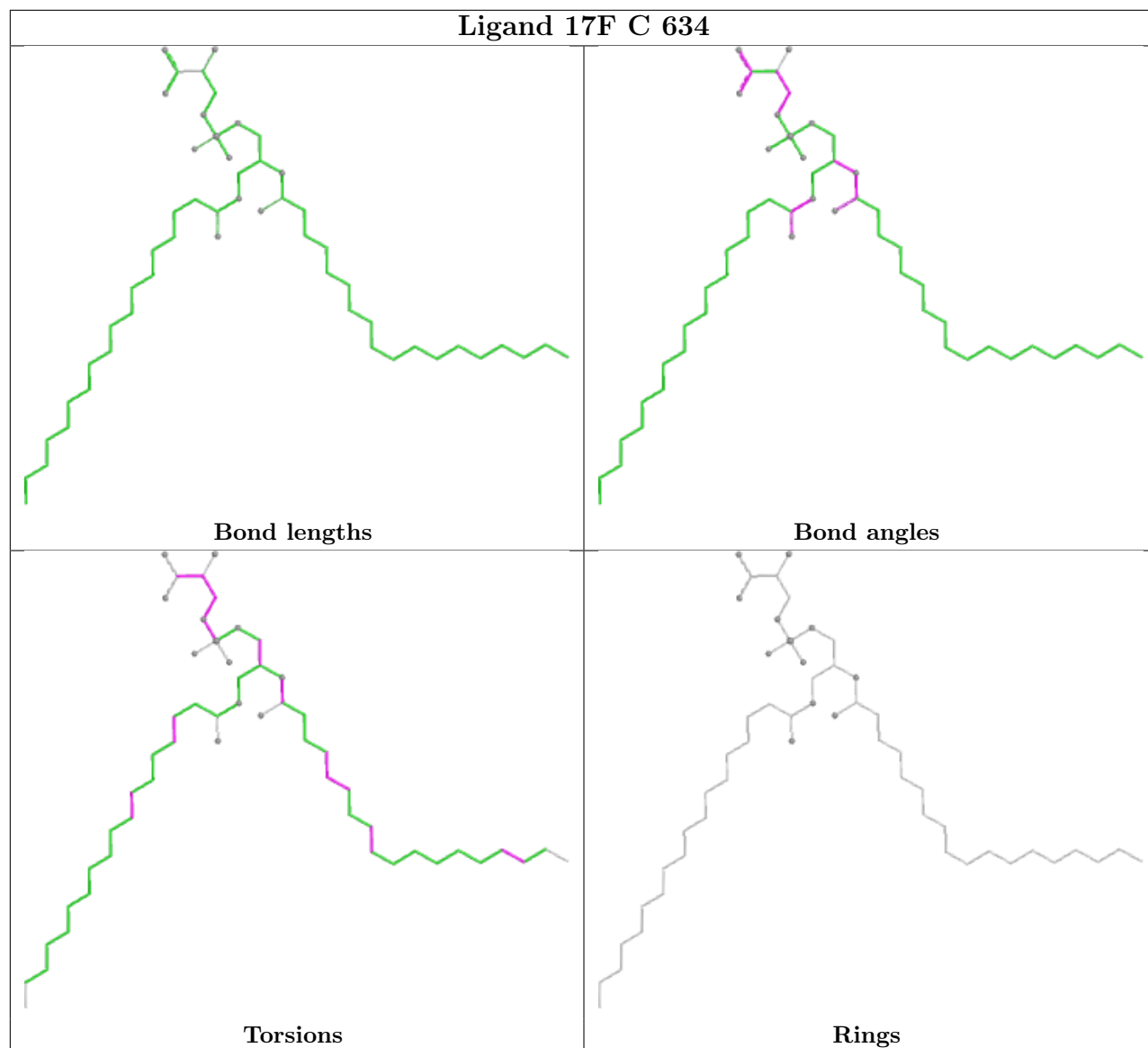


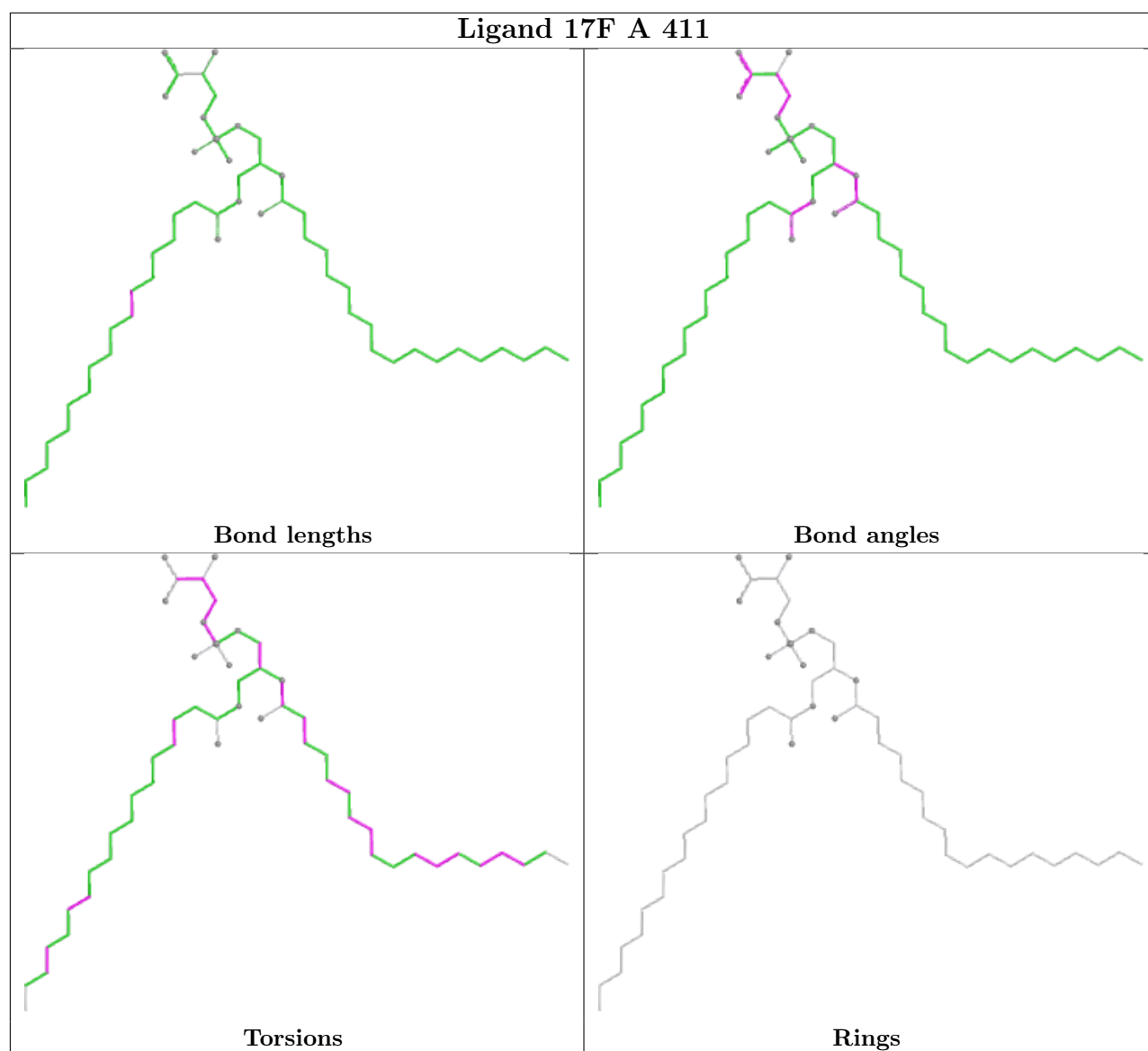


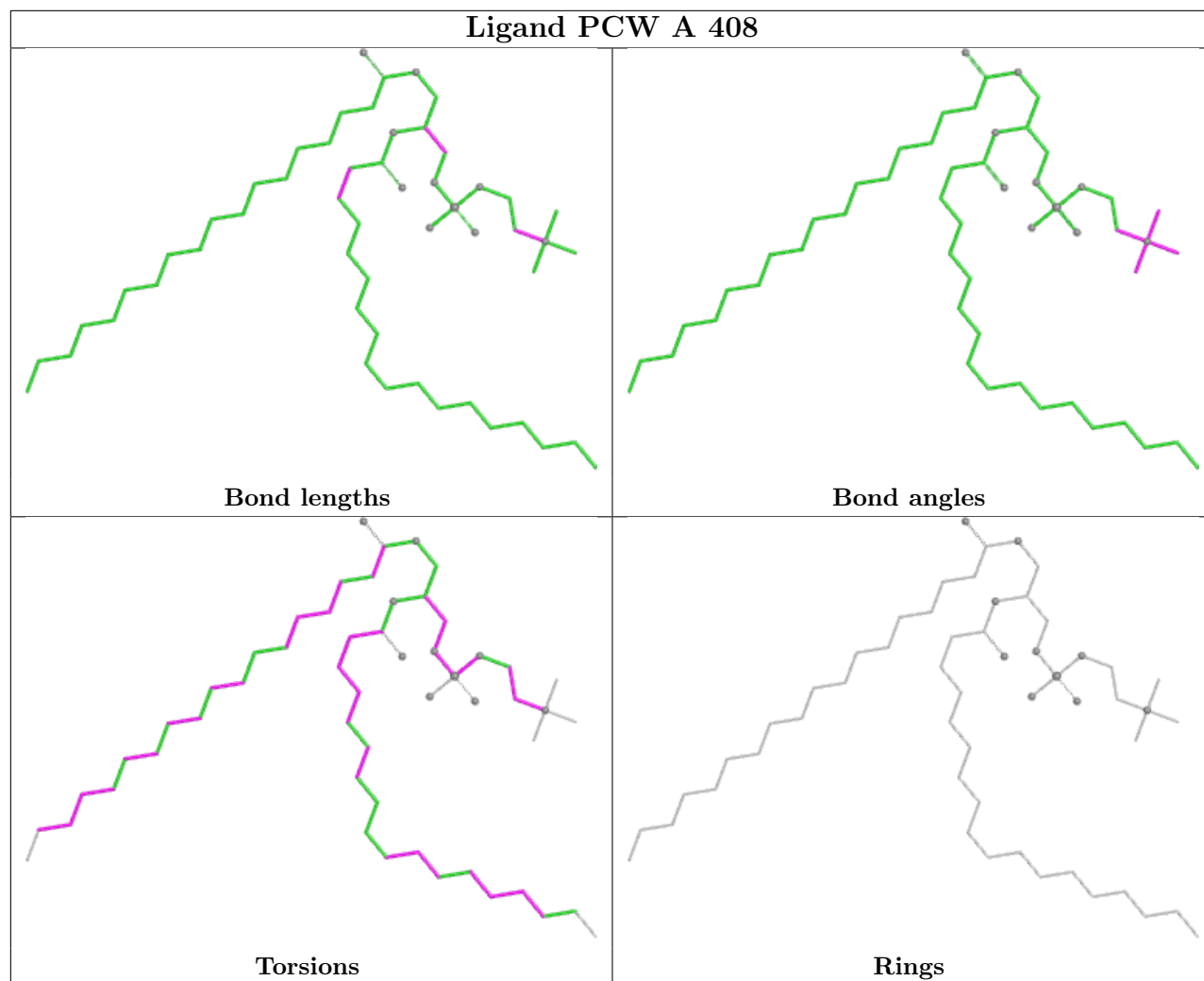




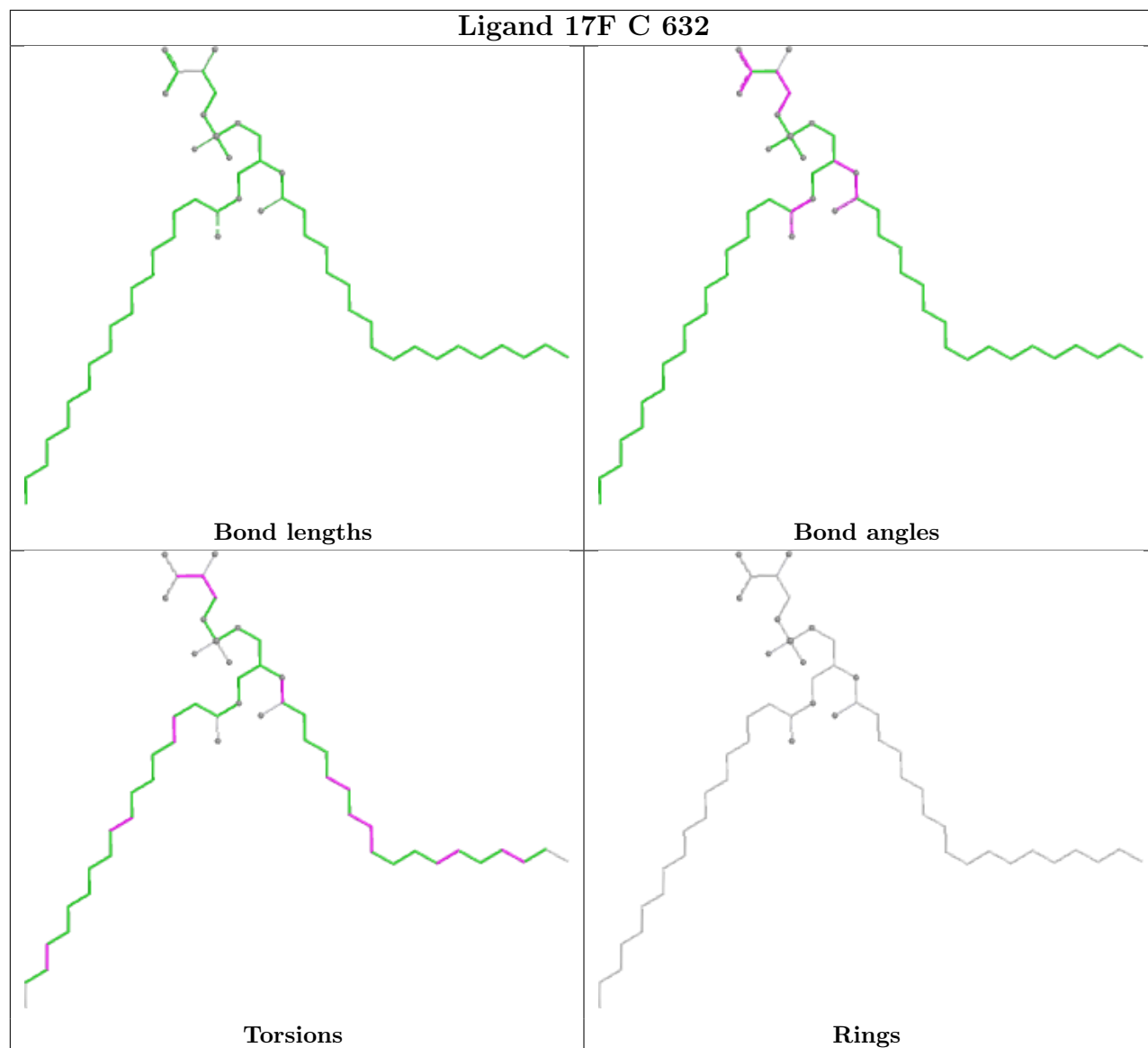
Ligand 17F C 634

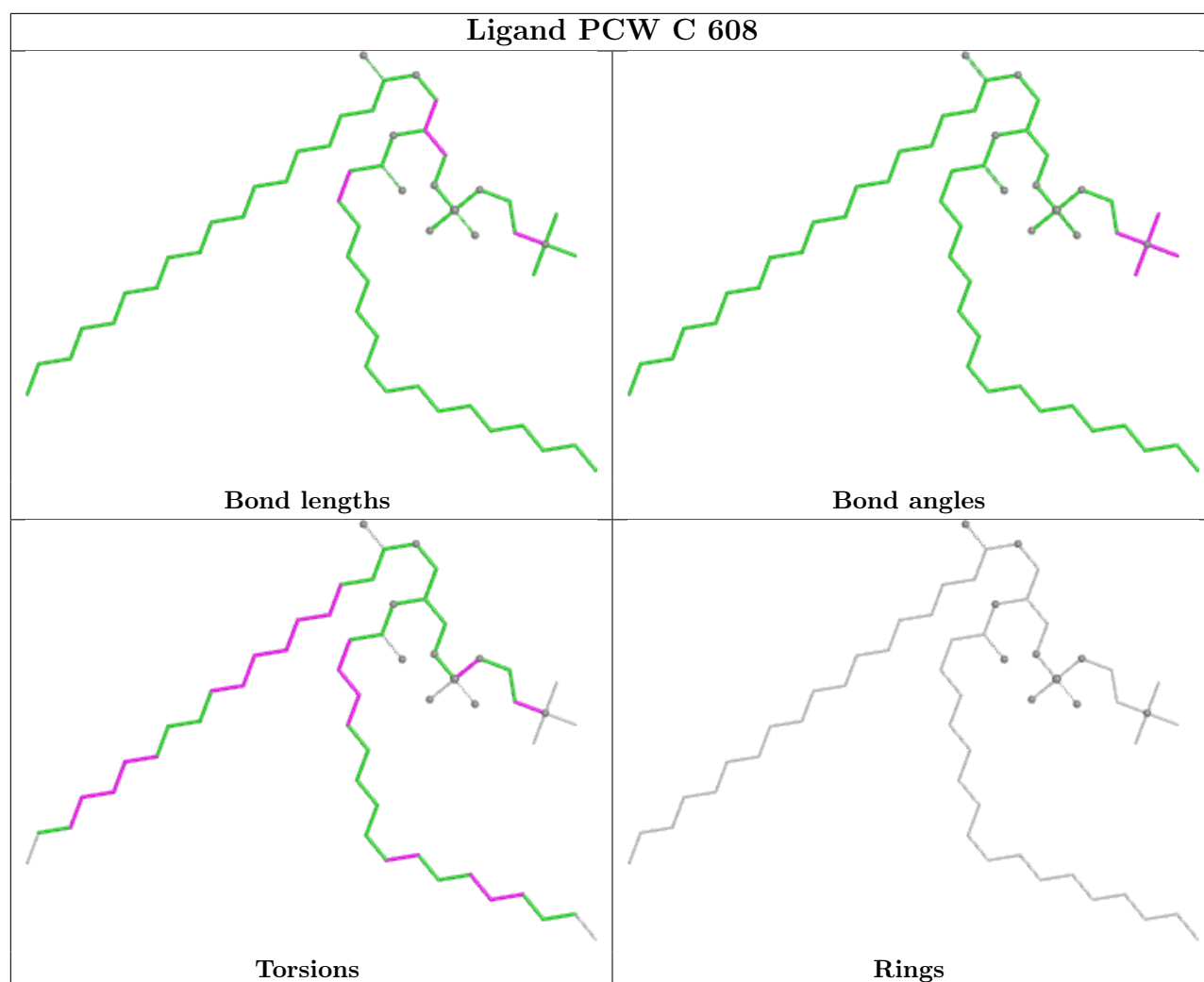


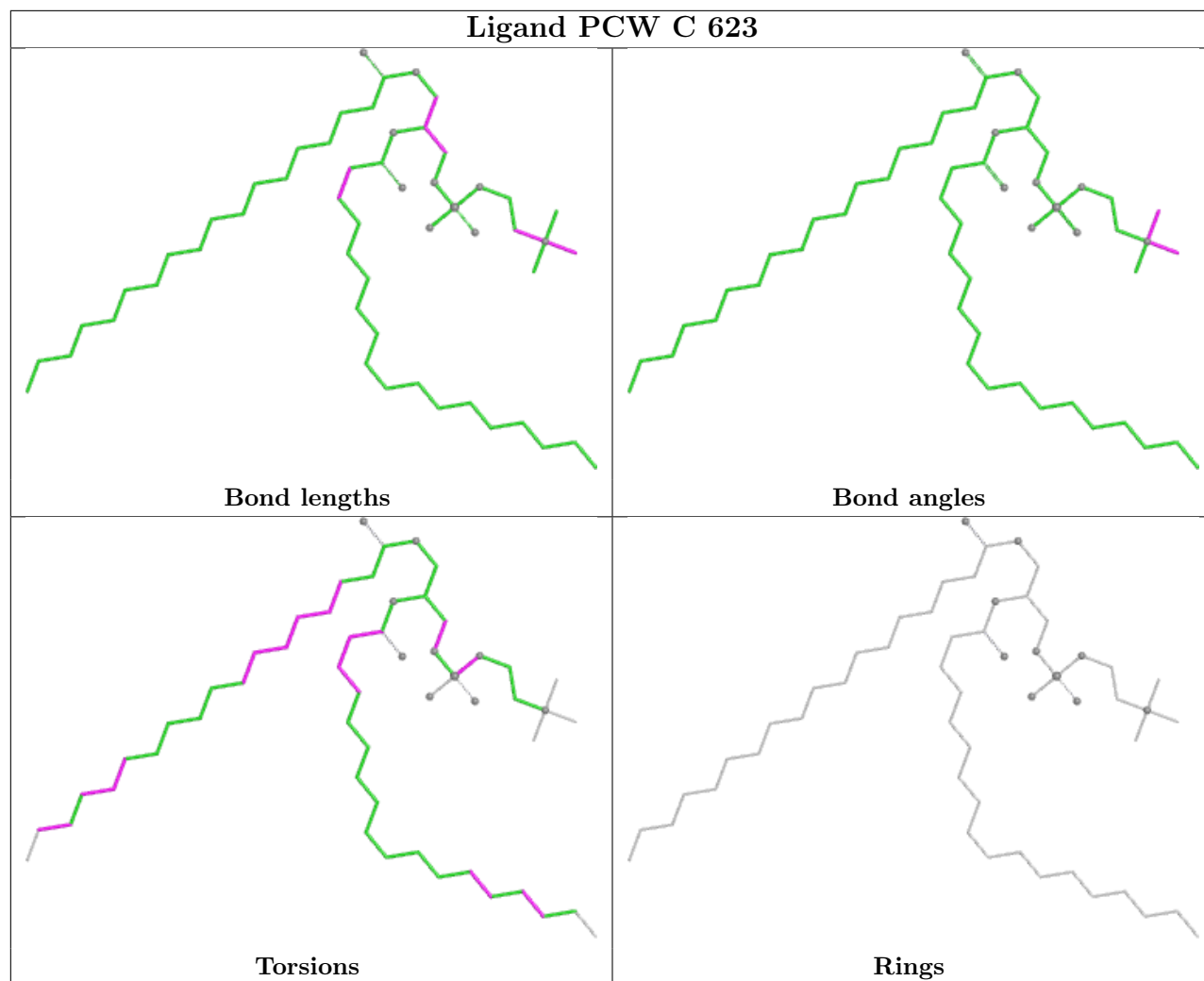


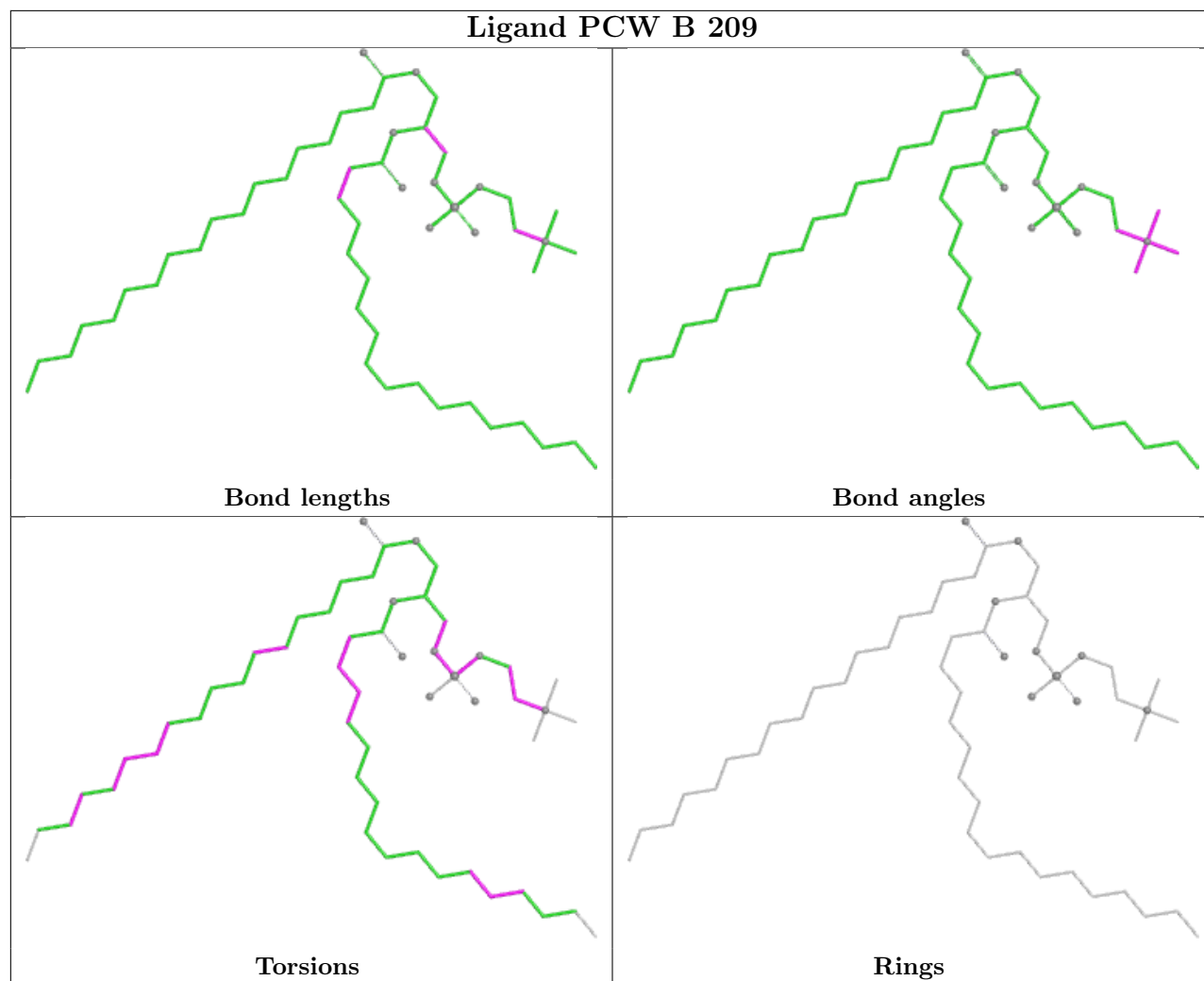


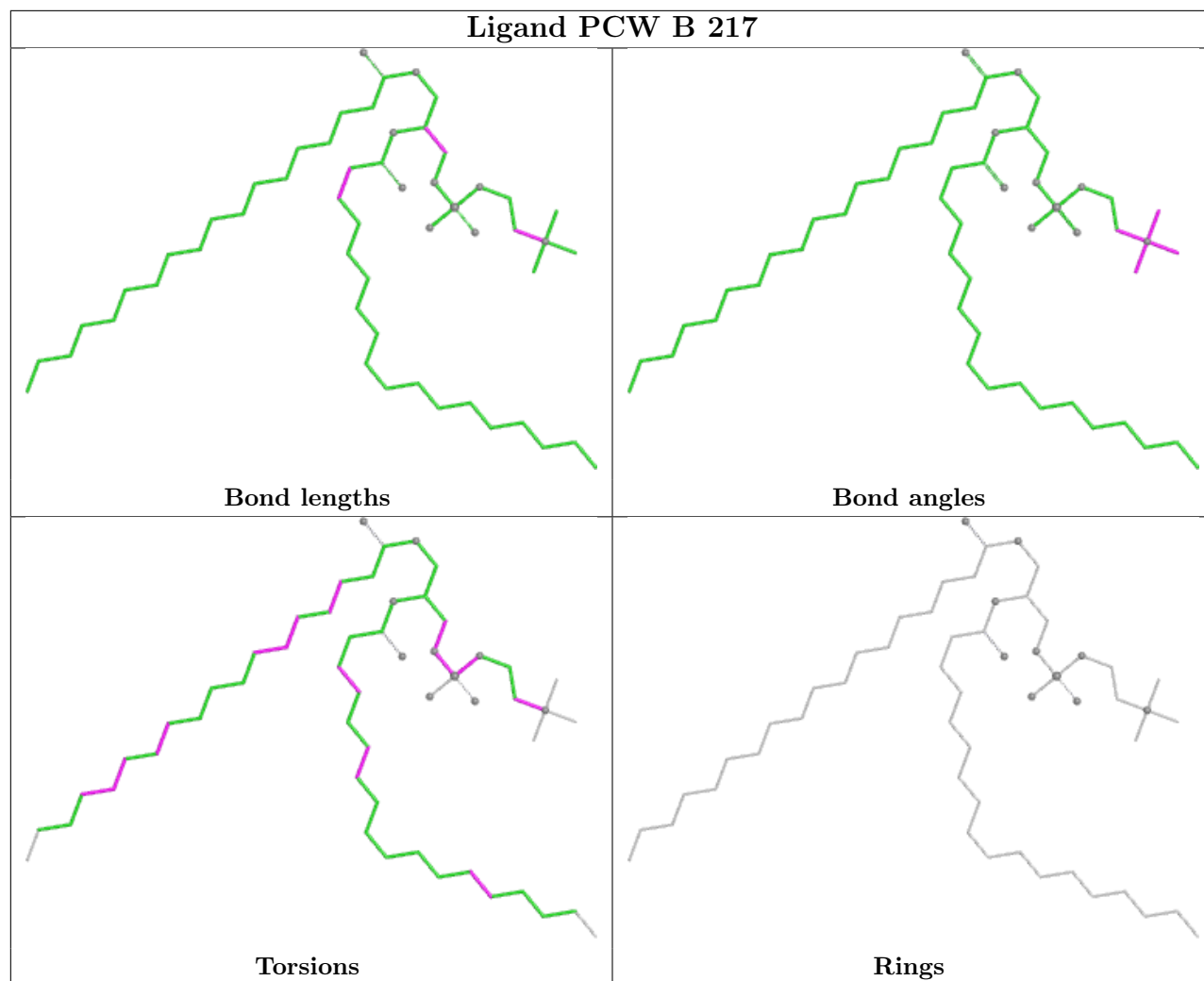
Ligand 17F C 632

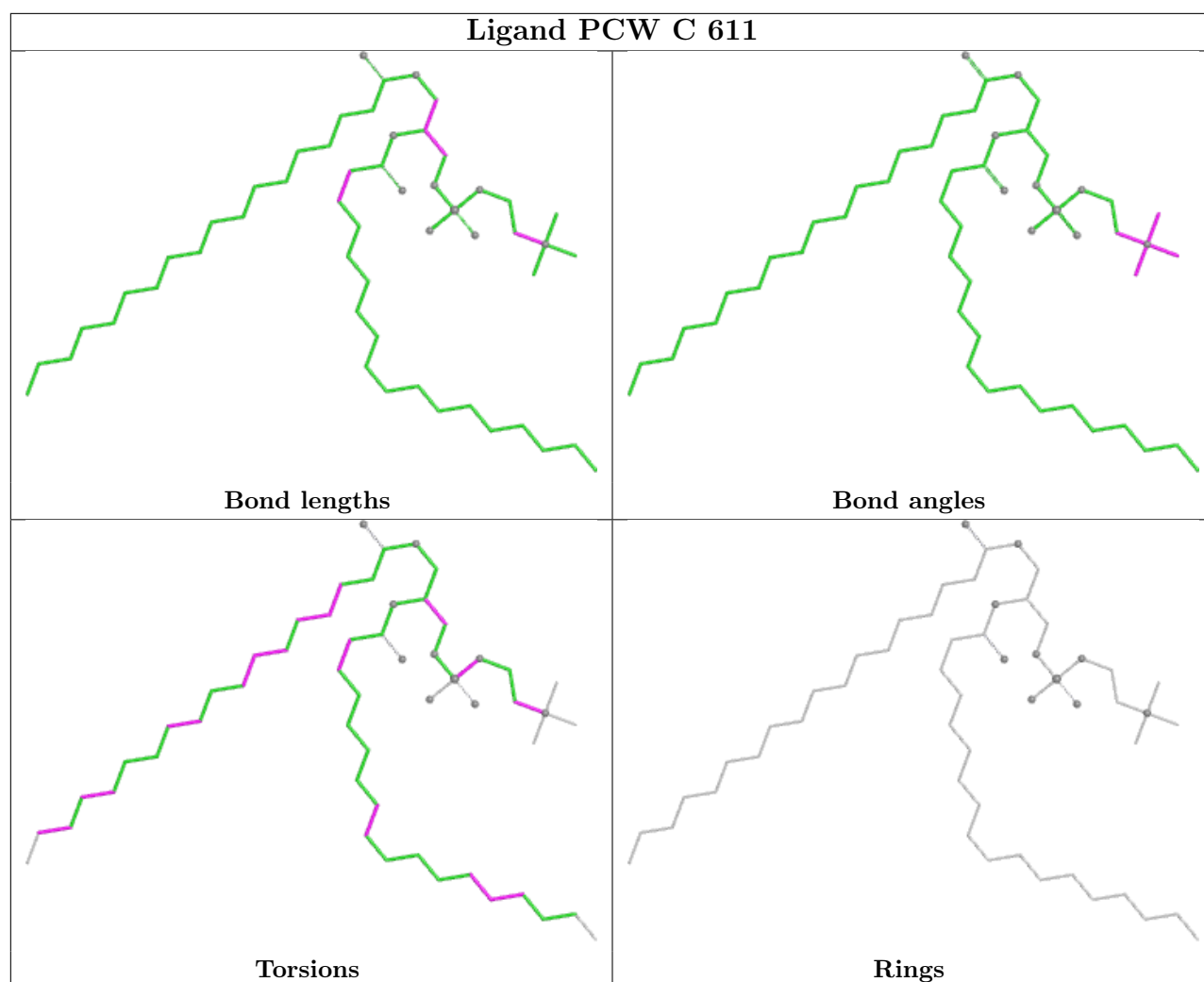


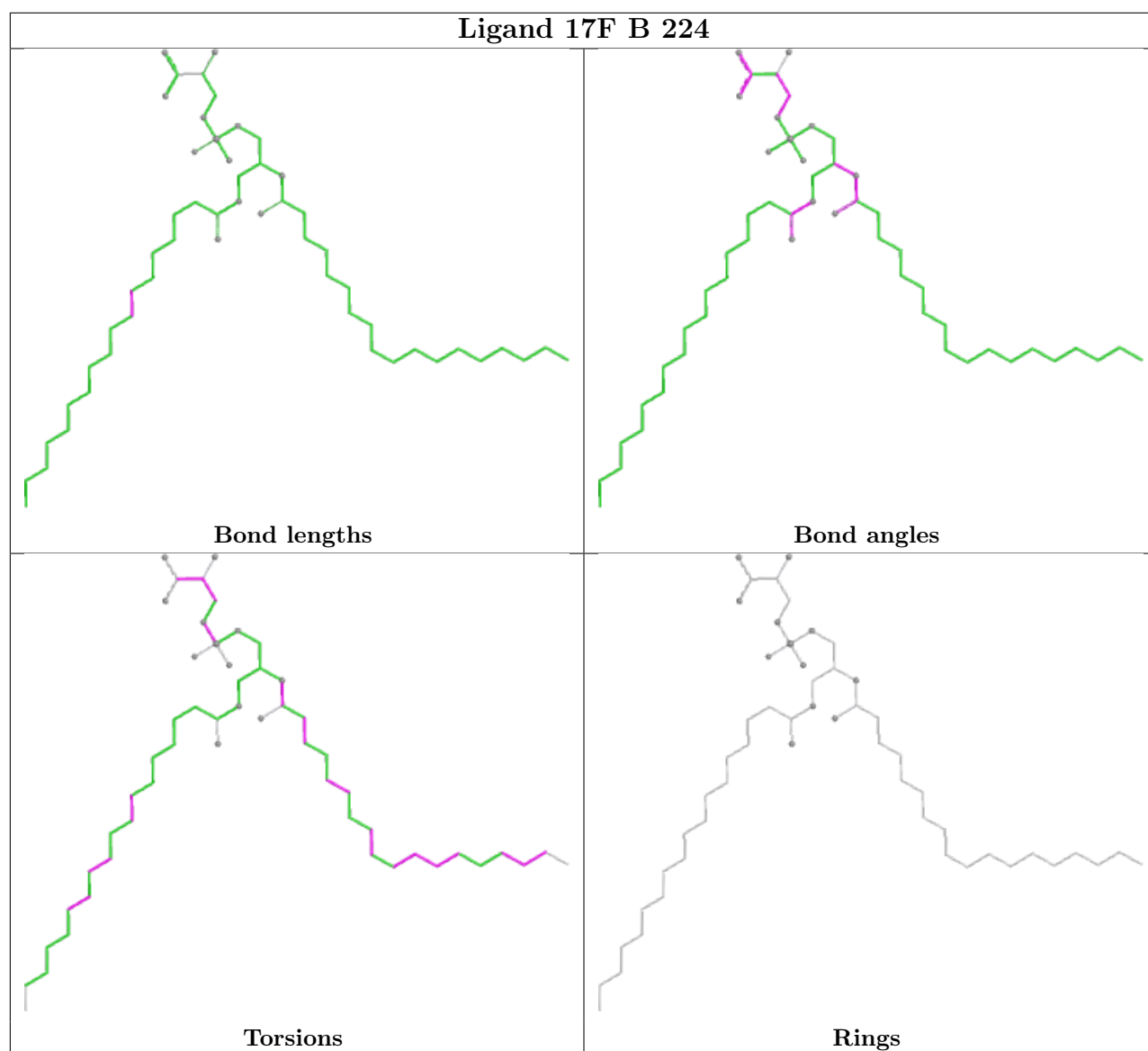


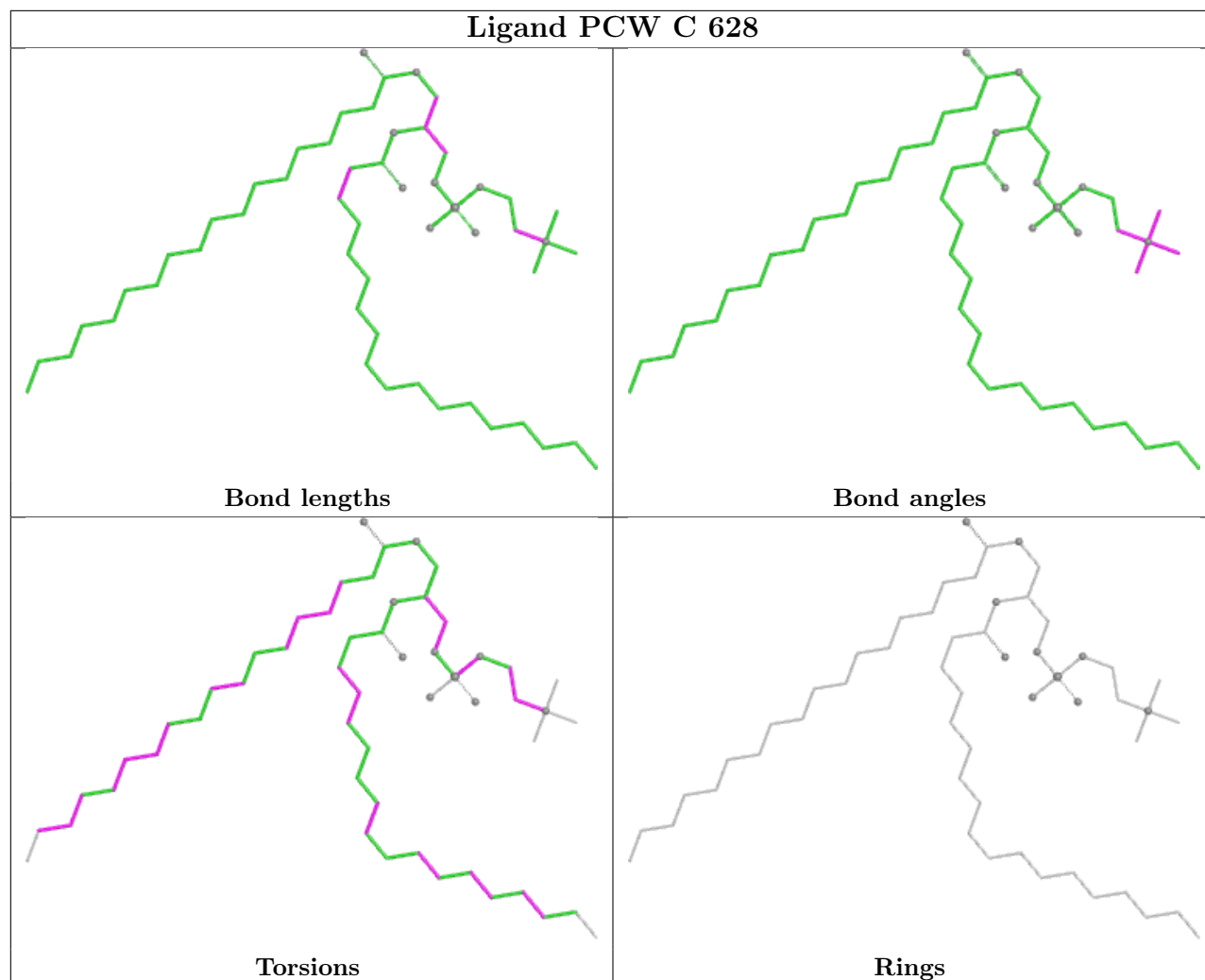


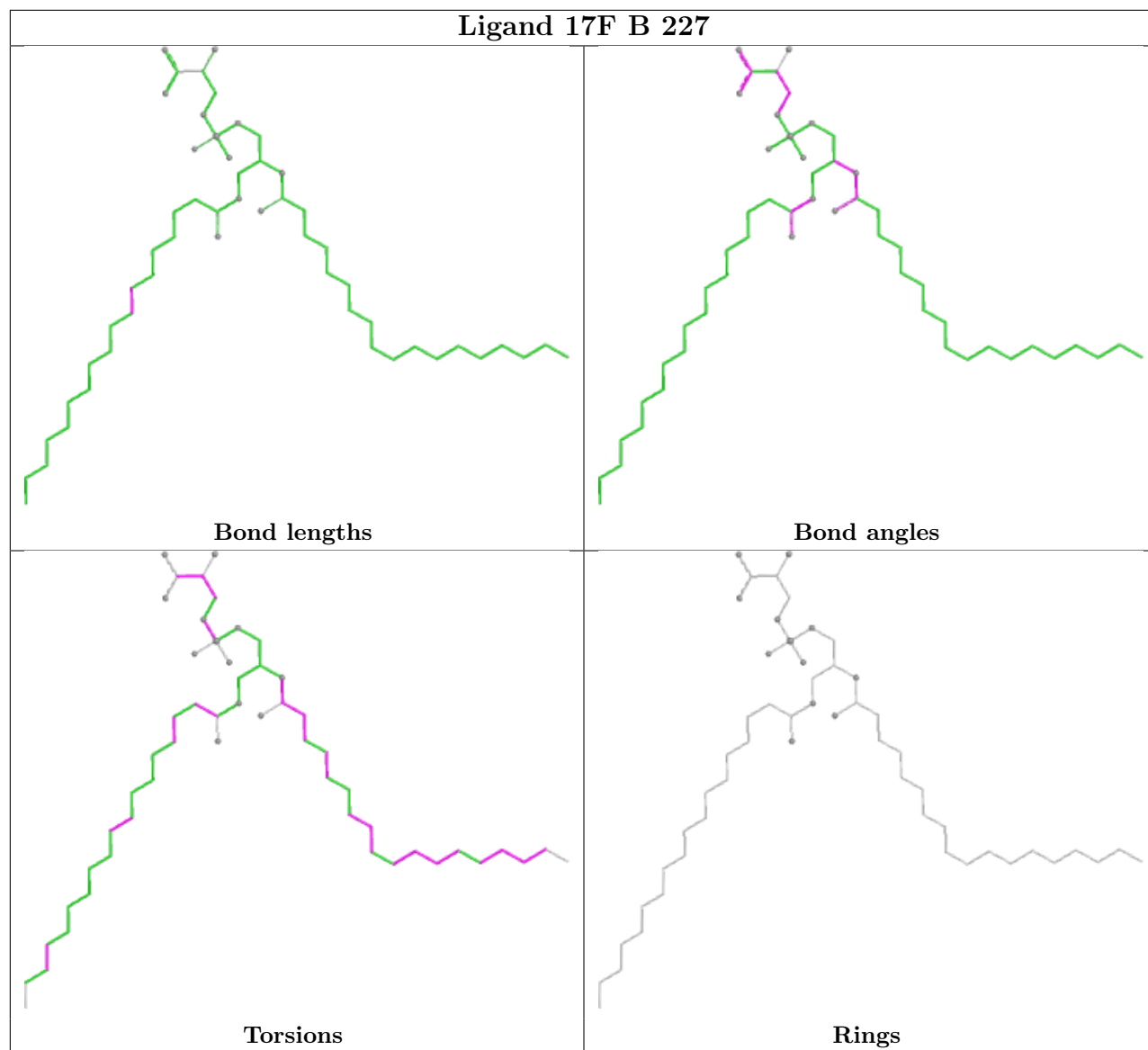


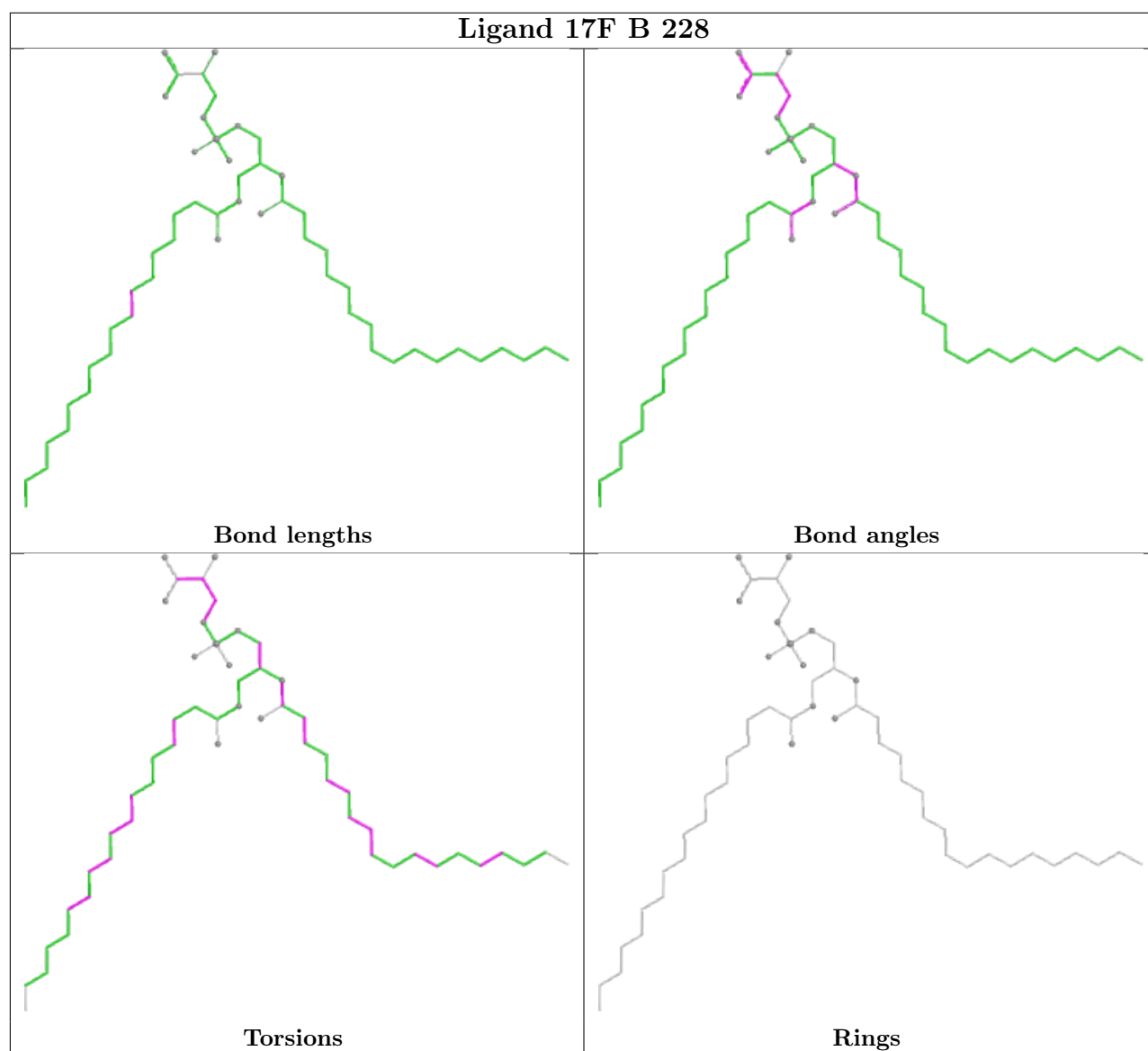












6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 3% for the well-defined parts and 3% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *resonance_list_nmrstar_50_51.txt*

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	268
Number of shifts mapped to atoms	193
Number of unparsed shifts	0
Number of shifts with mapping errors	75
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 75 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	6	LEU	HD21	0.865	.	.
1	B	6	LEU	HD22	0.865	.	.
1	B	6	LEU	HD23	0.865	.	.
1	B	14	VAL	HG11	0.892	.	.
1	B	14	VAL	HG12	0.892	.	.
1	B	14	VAL	HG13	0.892	.	.
1	B	19	LEU	HD11	0.547	.	.
1	B	19	LEU	HD12	0.547	.	.
1	B	19	LEU	HD13	0.547	.	.
1	B	21	ILE	HD11	0.513	.	1
1	B	21	ILE	HD12	0.513	.	1
1	B	21	ILE	HD13	0.513	.	1
1	B	23	LEU	HD11	-0.325	.	.
1	B	23	LEU	HD12	-0.325	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	23	LEU	HD13	-0.325	.	.
1	B	24	ILE	HD11	0.389	.	1
1	B	24	ILE	HD12	0.389	.	1
1	B	24	ILE	HD13	0.389	.	1
1	B	36	ILE	HD11	0.714	.	1
1	B	36	ILE	HD12	0.714	.	1
1	B	36	ILE	HD13	0.714	.	1
1	B	46	ILE	HD11	0.361	.	1
1	B	46	ILE	HD12	0.361	.	1
1	B	46	ILE	HD13	0.361	.	1
1	B	55	ILE	HD11	0.451	.	1
1	B	55	ILE	HD12	0.451	.	1
1	B	55	ILE	HD13	0.451	.	1
1	B	79	LEU	HD11	0.023	.	.
1	B	79	LEU	HD12	0.023	.	.
1	B	79	LEU	HD13	0.023	.	.
1	B	79	LEU	HD21	0.081	.	.
1	B	79	LEU	HD22	0.081	.	.
1	B	79	LEU	HD23	0.081	.	.
1	B	84	ILE	HD11	0.7	.	1
1	B	84	ILE	HD12	0.7	.	1
1	B	84	ILE	HD13	0.7	.	1
1	B	93	ILE	HD11	0.724	.	1
1	B	93	ILE	HD12	0.724	.	1
1	B	93	ILE	HD13	0.724	.	1
1	B	100	ILE	HD11	0.234	.	1
1	B	100	ILE	HD12	0.234	.	1
1	B	100	ILE	HD13	0.234	.	1
1	B	113	LEU	HD11	0.989	.	.
1	B	113	LEU	HD12	0.989	.	.
1	B	113	LEU	HD13	0.989	.	.
1	B	113	LEU	HD21	1.261	.	.
1	B	113	LEU	HD22	1.261	.	.
1	B	113	LEU	HD23	1.261	.	.
1	B	120	LEU	HD21	0.8	.	.
1	B	120	LEU	HD22	0.8	.	.
1	B	120	LEU	HD23	0.8	.	.
1	B	125	VAL	HG11	-0.21	.	.
1	B	125	VAL	HG12	-0.21	.	.
1	B	125	VAL	HG13	-0.21	.	.
1	B	133	LEU	HD11	0.344	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	133	LEU	HD12	0.344	.	.
1	B	133	LEU	HD13	0.344	.	.
1	B	133	LEU	HD21	0.39	.	.
1	B	133	LEU	HD22	0.39	.	.
1	B	133	LEU	HD23	0.39	.	.
1	B	139	ILE	HD11	0.809	.	1
1	B	139	ILE	HD12	0.809	.	1
1	B	139	ILE	HD13	0.809	.	1
1	B	142	ILE	HD11	0.618	.	1
1	B	142	ILE	HD12	0.618	.	1
1	B	142	ILE	HD13	0.618	.	1
1	B	159	LEU	HD11	0.613	.	.
1	B	159	LEU	HD12	0.613	.	.
1	B	159	LEU	HD13	0.613	.	.
1	B	160	VAL	HG11	-0.056	.	.
1	B	160	VAL	HG12	-0.056	.	.
1	B	160	VAL	HG13	-0.056	.	.
1	B	163	ILE	HD11	0.612	.	1
1	B	163	ILE	HD12	0.612	.	1
1	B	163	ILE	HD13	0.612	.	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	84	-0.47 ± 0.76	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 3%, i.e. 254 atoms were assigned a chemical shift out of a possible 7925. 0 out of 107 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	154/2803 (5%)	77/1132 (7%)	0/1126 (0%)	77/545 (14%)

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	Total	¹ H	¹³ C	¹⁵ N
Sidechain	100/4642 (2%)	75/2983 (3%)	25/1453 (2%)	0/206 (0%)
Aromatic	0/480 (0%)	0/244 (0%)	0/228 (0%)	0/8 (0%)
Overall	254/7925 (3%)	152/4359 (3%)	25/2807 (1%)	77/759 (10%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 3%, i.e. 268 atoms were assigned a chemical shift out of a possible 8192. 0 out of 109 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	168/2894 (6%)	84/1169 (7%)	0/1162 (0%)	84/563 (15%)
Sidechain	100/4818 (2%)	75/3094 (2%)	25/1508 (2%)	0/216 (0%)
Aromatic	0/480 (0%)	0/244 (0%)	0/228 (0%)	0/8 (0%)
Overall	268/8192 (3%)	159/4507 (4%)	25/2898 (1%)	84/787 (11%)

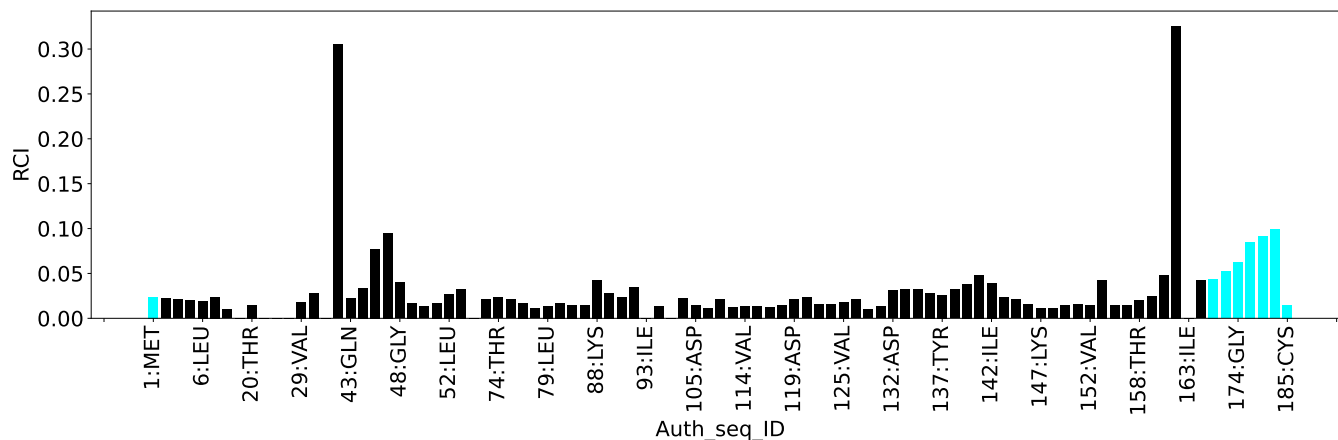
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain B:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	66
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	0
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	0
Inter-chain	66
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.1
Number of long range restraints per residue ¹	0.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	None	None
0.2-0.5 (Medium)	0.3	0.35
>0.5 (Large)	63.5	33.3

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

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

9 Distance violation analysis ⓘ

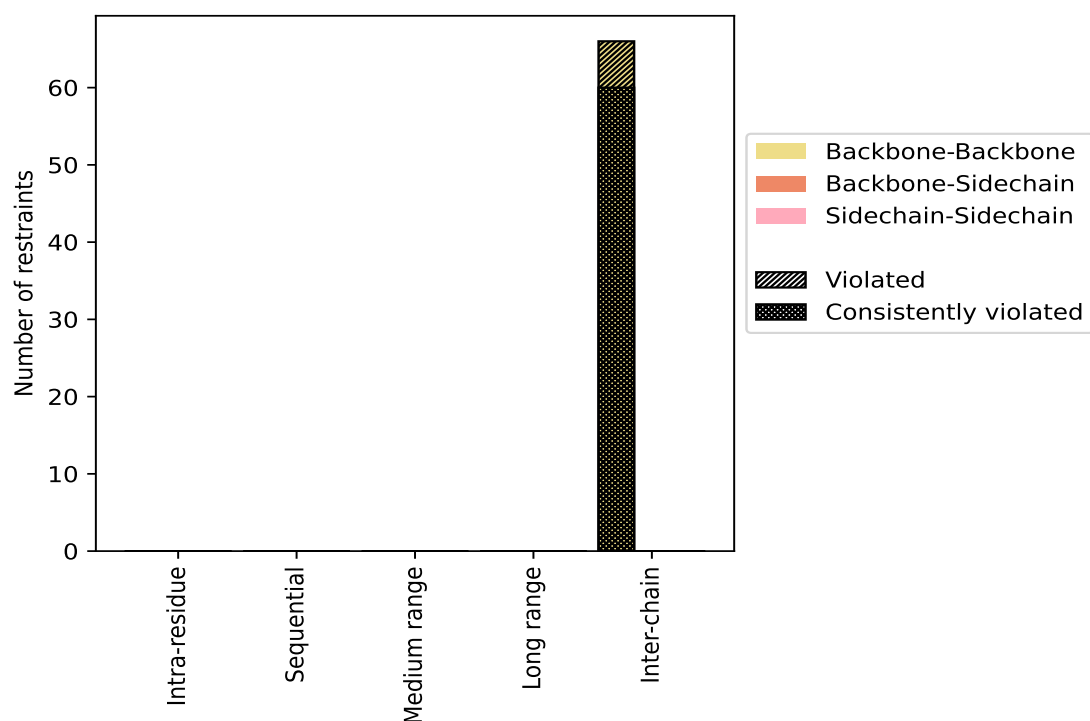
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	66	100.0	66	100.0	100.0	60	90.9	90.9
Backbone-Backbone	66	100.0	66	100.0	100.0	60	90.9	90.9
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
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	66	100.0	66	100.0	100.0	60	90.9	90.9
Backbone-Backbone	66	100.0	66	100.0	100.0	60	90.9	90.9
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

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 disulfid bonds are counted in their appropriate category on the x-axis

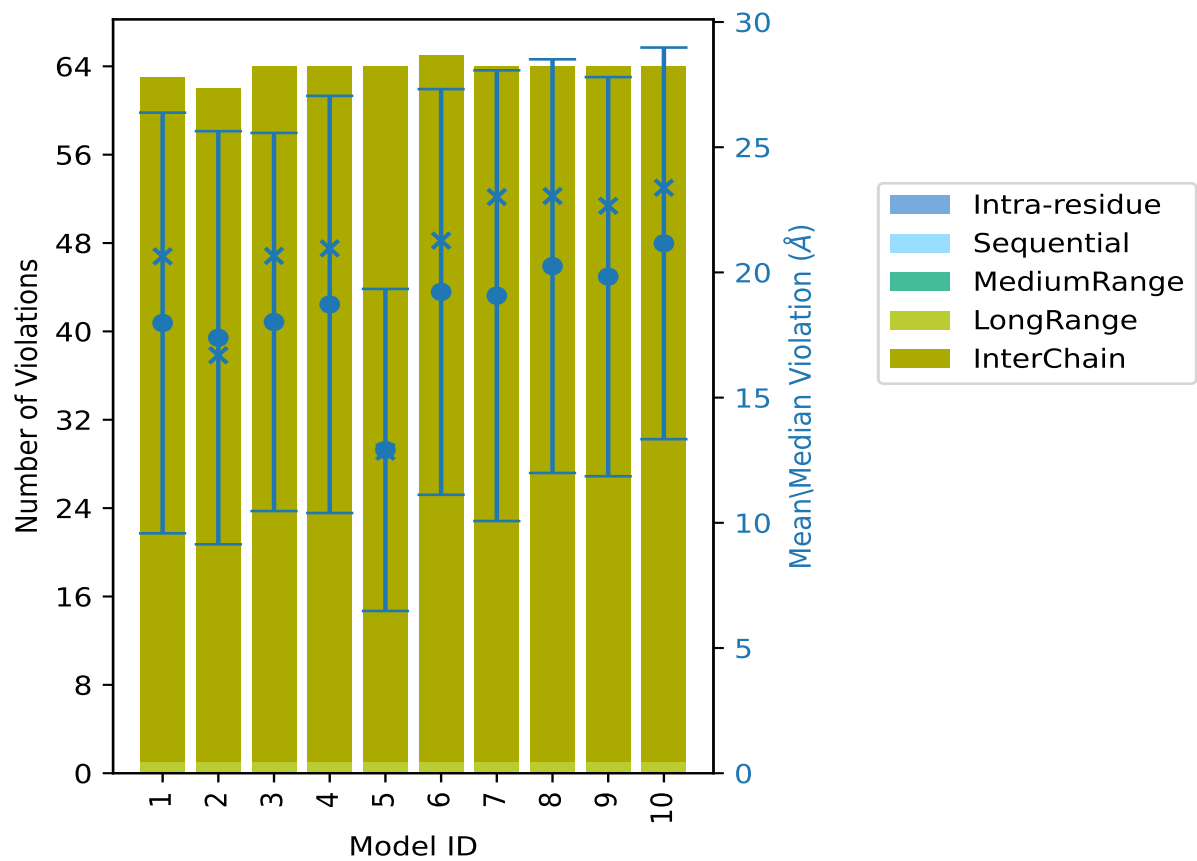
9.2 Distance violation statistics for each model [i](#)

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	1	62	63	17.98	31.68	8.4	20.64
2	0	0	0	1	61	62	17.39	31.77	8.25	16.69
3	0	0	0	1	63	64	18.02	29.36	7.55	20.66
4	0	0	0	1	63	64	18.72	32.85	8.33	20.96
5	0	0	0	1	63	64	12.91	29.74	6.43	12.84
6	0	0	0	1	64	65	19.22	30.98	8.1	21.27
7	0	0	0	1	63	64	19.07	31.96	9.0	23.01
8	0	0	0	1	63	64	20.25	32.25	8.26	23.05
9	0	0	0	1	63	64	19.83	31.38	7.97	22.66
10	0	0	0	1	63	64	21.16	33.3	7.82	23.38

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, 0(IR:0, SQ:0, MR:0, LR:0, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	1	10.0
0	0	0	0	1	1	2	20.0
0	0	0	0	1	1	3	30.0

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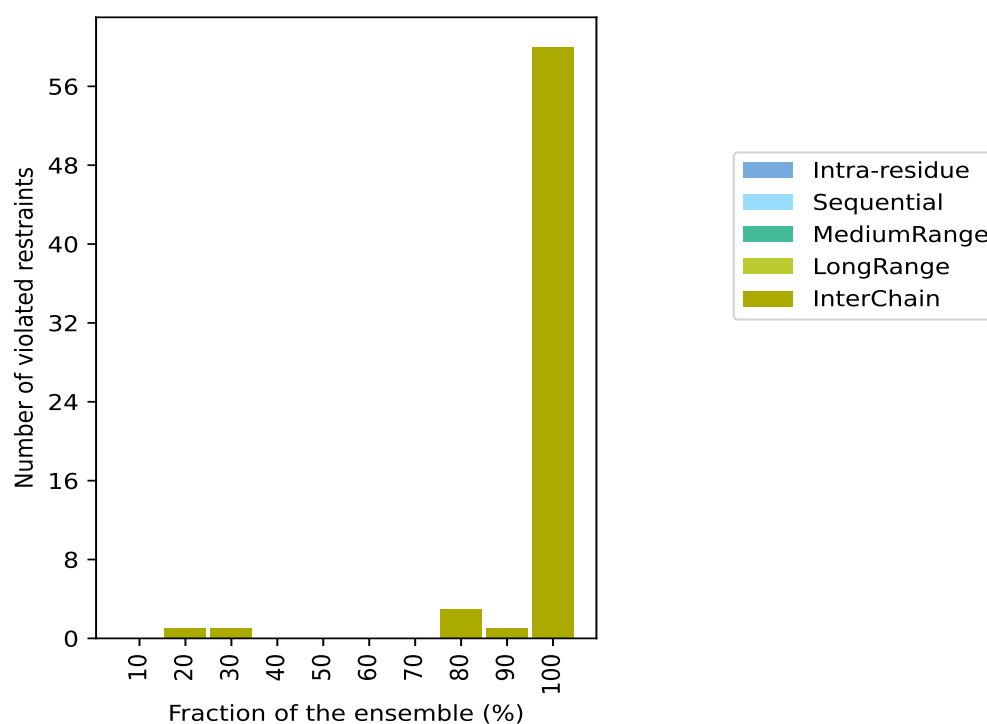
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	4	40.0
0	0	0	0	0	0	5	50.0
0	0	0	0	0	0	6	60.0
0	0	0	0	0	0	7	70.0
0	0	0	0	3	3	8	80.0
0	0	0	0	1	1	9	90.0
0	0	0	0	60	60	10	100.0

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

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

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

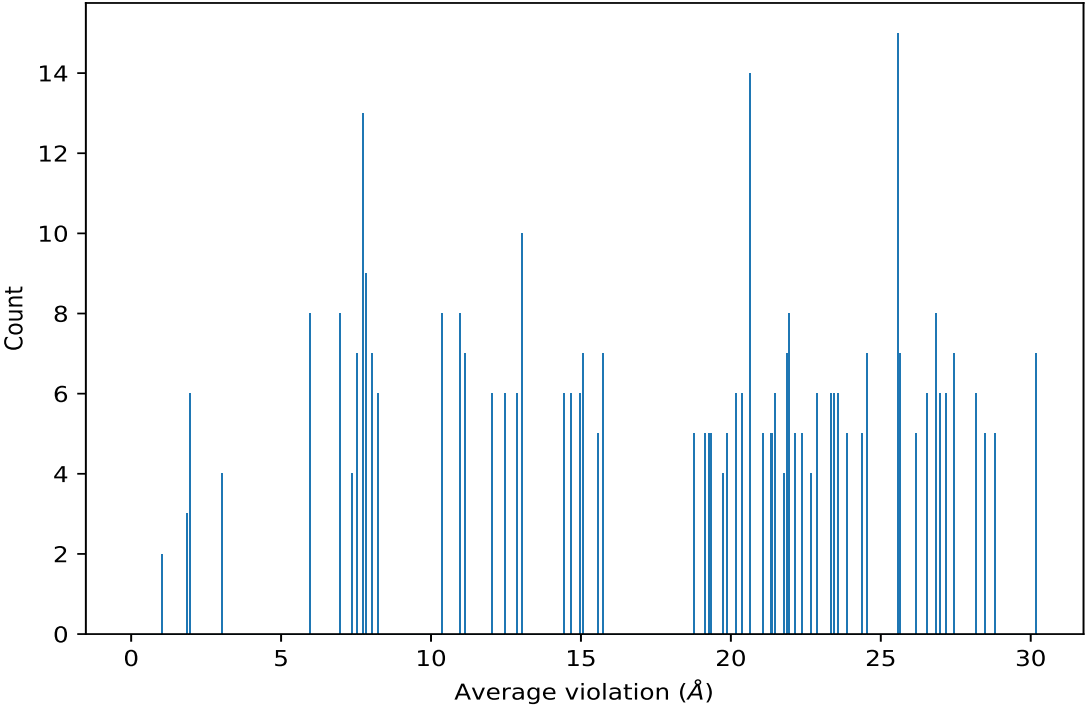


9.4 Most violated distance restraints in the ensemble [i](#)

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

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

in the ensemble



9.4.2 Table: Most violated distance restraints ⓘ

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)
(1,38)	1:238:A:GLY:N	4:229:B:17F:O4	10	30.2	3.14	31.71
(1,38)	1:238:A:GLY:N	4:229:B:17F:C5	10	30.2	3.14	31.71
(1,38)	1:238:A:GLY:N	2:184:B:LYS:H	10	30.2	3.14	31.71
(1,38)	1:238:A:GLY:N	2:177:B:LYS:HZ2	10	30.2	3.14	31.71
(1,38)	1:238:A:GLY:N	2:36:B:ILE:CD1	10	30.2	3.14	31.71
(1,38)	1:238:A:GLY:N	4:229:B:17F:O9	10	30.2	3.14	31.71
(1,38)	1:238:A:GLY:N	2:175:B:LYS:HZ1	10	30.2	3.14	31.71
(1,34)	1:234:A:LYS:N	4:229:B:17F:O4	10	28.8	4.05	30.59
(1,34)	1:234:A:LYS:N	4:229:B:17F:C5	10	28.8	4.05	30.59
(1,34)	1:234:A:LYS:N	2:184:B:LYS:CG	10	28.8	4.05	30.59
(1,34)	1:234:A:LYS:N	4:229:B:17F:O9	10	28.8	4.05	30.59
(1,34)	1:234:A:LYS:N	2:36:B:ILE:CD1	10	28.8	4.05	30.59
(1,35)	1:235:A:GLU:N	4:229:B:17F:O4	10	28.47	3.64	29.77
(1,35)	1:235:A:GLU:N	4:229:B:17F:C5	10	28.47	3.64	29.77
(1,35)	1:235:A:GLU:N	2:184:B:LYS:CG	10	28.47	3.64	29.77

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,35)	1:235:A:GLU:N	4:229:B:17F:O9	10	28.47	3.64	29.77
(1,35)	1:235:A:GLU:N	4:229:B:17F:O5	10	28.47	3.64	29.77
(1,37)	1:237:A:GLU:N	4:229:B:17F:O4	10	28.19	3.23	29.39
(1,37)	1:237:A:GLU:N	4:229:B:17F:C5	10	28.19	3.23	29.39
(1,37)	1:237:A:GLU:N	2:184:B:LYS:H	10	28.19	3.23	29.39
(1,37)	1:237:A:GLU:N	2:177:B:LYS:HZ2	10	28.19	3.23	29.39
(1,37)	1:237:A:GLU:N	2:36:B:ILE:CD1	10	28.19	3.23	29.39
(1,37)	1:237:A:GLU:N	2:175:B:LYS:HZ1	10	28.19	3.23	29.39
(1,59)	2:141:B:PHE:N	3:407:A:PCW:N	10	27.44	2.17	27.45
(1,59)	2:141:B:PHE:H	3:407:A:PCW:N	10	27.44	2.17	27.45
(1,59)	2:141:B:PHE:H	3:405:A:PCW:N	10	27.44	2.17	27.45
(1,59)	2:141:B:PHE:N	3:405:A:PCW:N	10	27.44	2.17	27.45
(1,59)	2:141:B:PHE:O	3:407:A:PCW:N	10	27.44	2.17	27.45
(1,59)	2:141:B:PHE:CE1	3:407:A:PCW:N	10	27.44	2.17	27.45
(1,59)	2:141:B:PHE:H	3:402:A:PCW:N	10	27.44	2.17	27.45
(1,31)	1:231:A:ASN:N	4:229:B:17F:O4	10	27.2	4.36	28.79
(1,31)	1:231:A:ASN:N	4:229:B:17F:O8	10	27.2	4.36	28.79
(1,31)	1:231:A:ASN:N	2:184:B:LYS:CG	10	27.2	4.36	28.79
(1,31)	1:231:A:ASN:N	4:229:B:17F:O9	10	27.2	4.36	28.79
(1,31)	1:231:A:ASN:N	4:229:B:17F:C5	10	27.2	4.36	28.79
(1,31)	1:231:A:ASN:N	4:229:B:17F:C8	10	27.2	4.36	28.79
(1,60)	2:142:B:ILE:H	3:407:A:PCW:N	10	26.97	1.54	26.74
(1,60)	2:142:B:ILE:H	3:406:A:PCW:N	10	26.97	1.54	26.74
(1,60)	2:142:B:ILE:CD1	3:407:A:PCW:N	10	26.97	1.54	26.74
(1,60)	2:142:B:ILE:CD1	3:402:A:PCW:N	10	26.97	1.54	26.74
(1,60)	2:142:B:ILE:O	3:407:A:PCW:N	10	26.97	1.54	26.74
(1,60)	2:142:B:ILE:CG2	3:407:A:PCW:N	10	26.97	1.54	26.74
(1,36)	1:236:A:THR:N	4:229:B:17F:O4	10	26.83	3.27	28.0
(1,36)	1:236:A:THR:N	4:229:B:17F:C5	10	26.83	3.27	28.0
(1,36)	1:236:A:THR:N	2:184:B:LYS:H	10	26.83	3.27	28.0
(1,36)	1:236:A:THR:N	2:177:B:LYS:HZ2	10	26.83	3.27	28.0
(1,36)	1:236:A:THR:N	2:37:B:GLU:OE1	10	26.83	3.27	28.0
(1,36)	1:236:A:THR:N	4:229:B:17F:O9	10	26.83	3.27	28.0
(1,36)	1:236:A:THR:N	2:175:B:LYS:HZ1	10	26.83	3.27	28.0
(1,36)	1:236:A:THR:N	2:36:B:ILE:CD1	10	26.83	3.27	28.0
(1,56)	2:133:B:LEU:O	3:407:A:PCW:N	10	26.53	3.88	26.11
(1,56)	2:133:B:LEU:O	3:404:A:PCW:N	10	26.53	3.88	26.11
(1,56)	2:133:B:LEU:O	3:405:A:PCW:N	10	26.53	3.88	26.11
(1,56)	2:133:B:LEU:CD1	3:402:A:PCW:N	10	26.53	3.88	26.11
(1,56)	2:133:B:LEU:CD2	3:404:A:PCW:N	10	26.53	3.88	26.11
(1,56)	2:133:B:LEU:O	3:402:A:PCW:N	10	26.53	3.88	26.11
(1,33)	1:233:A:GLU:N	4:229:B:17F:O4	10	26.2	4.09	28.06

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,33)	1:233:A:GLU:N	4:229:B:17F:C4	10	26.2	4.09	28.06
(1,33)	1:233:A:GLU:N	2:184:B:LYS:CG	10	26.2	4.09	28.06
(1,33)	1:233:A:GLU:N	4:229:B:17F:O9	10	26.2	4.09	28.06
(1,33)	1:233:A:GLU:N	2:36:B:ILE:CD1	10	26.2	4.09	28.06
(1,27)	1:227:A:GLU:N	4:229:B:17F:O4	10	25.64	5.0	27.12
(1,27)	1:227:A:GLU:N	4:229:B:17F:O8	10	25.64	5.0	27.12
(1,27)	1:227:A:GLU:N	2:184:B:LYS:CG	10	25.64	5.0	27.12
(1,27)	1:227:A:GLU:N	4:229:B:17F:O5	10	25.64	5.0	27.12
(1,27)	1:227:A:GLU:N	4:229:B:17F:C5	10	25.64	5.0	27.12
(1,27)	1:227:A:GLU:N	4:229:B:17F:C9	10	25.64	5.0	27.12
(1,27)	1:227:A:GLU:N	4:229:B:17F:C8	10	25.64	5.0	27.12
(1,32)	1:232:A:LEU:N	4:229:B:17F:O4	10	25.58	4.03	27.11
(1,32)	1:232:A:LEU:N	4:229:B:17F:O8	10	25.58	4.03	27.11
(1,32)	1:232:A:LEU:N	2:184:B:LYS:CG	10	25.58	4.03	27.11
(1,32)	1:232:A:LEU:N	4:229:B:17F:O9	10	25.58	4.03	27.11
(1,32)	1:232:A:LEU:N	4:229:B:17F:C5	10	25.58	4.03	27.11
(1,32)	1:232:A:LEU:N	4:229:B:17F:C8	10	25.58	4.03	27.11
(1,55)	2:113:B:LEU:H	3:407:A:PCW:N	10	25.57	2.02	25.59
(1,55)	2:113:B:LEU:N	3:406:A:PCW:N	10	25.57	2.02	25.59
(1,55)	2:113:B:LEU:N	3:407:A:PCW:N	10	25.57	2.02	25.59
(1,55)	2:113:B:LEU:CD1	3:407:A:PCW:N	10	25.57	2.02	25.59
(1,55)	2:113:B:LEU:CD1	3:404:A:PCW:N	10	25.57	2.02	25.59
(1,55)	2:113:B:LEU:C	3:404:A:PCW:N	10	25.57	2.02	25.59
(1,55)	2:113:B:LEU:C	3:407:A:PCW:N	10	25.57	2.02	25.59
(1,55)	2:113:B:LEU:H	3:402:A:PCW:N	10	25.57	2.02	25.59
(1,55)	2:113:B:LEU:C	3:405:A:PCW:N	10	25.57	2.02	25.59
(1,23)	1:223:A:PRO:N	4:229:B:17F:C4	10	24.5	5.48	26.19
(1,23)	1:223:A:PRO:N	4:229:B:17F:O4	10	24.5	5.48	26.19
(1,23)	1:223:A:PRO:N	4:229:B:17F:O8	10	24.5	5.48	26.19
(1,23)	1:223:A:PRO:N	2:184:B:LYS:CG	10	24.5	5.48	26.19
(1,23)	1:223:A:PRO:N	4:229:B:17F:O5	10	24.5	5.48	26.19
(1,23)	1:223:A:PRO:N	4:229:B:17F:C5	10	24.5	5.48	26.19
(1,23)	1:223:A:PRO:N	4:229:B:17F:C9	10	24.5	5.48	26.19
(1,28)	1:228:A:PHE:N	4:229:B:17F:C5	10	24.4	4.56	25.92
(1,28)	1:228:A:PHE:N	4:229:B:17F:O4	10	24.4	4.56	25.92
(1,28)	1:228:A:PHE:N	4:229:B:17F:O8	10	24.4	4.56	25.92
(1,28)	1:228:A:PHE:N	2:184:B:LYS:CG	10	24.4	4.56	25.92
(1,28)	1:228:A:PHE:N	4:229:B:17F:C8	10	24.4	4.56	25.92
(1,24)	1:224:A:VAL:N	4:229:B:17F:C5	10	23.89	5.06	25.36
(1,24)	1:224:A:VAL:N	4:229:B:17F:O4	10	23.89	5.06	25.36
(1,24)	1:224:A:VAL:N	4:229:B:17F:O8	10	23.89	5.06	25.36
(1,24)	1:224:A:VAL:N	2:184:B:LYS:CD	10	23.89	5.06	25.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,24)	1:224:A:VAL:N	4:229:B:17F:C9	10	23.89	5.06	25.36
(1,29)	1:229:A:TRP:N	4:229:B:17F:O4	10	23.56	4.57	25.32
(1,29)	1:229:A:TRP:N	4:229:B:17F:O8	10	23.56	4.57	25.32
(1,29)	1:229:A:TRP:N	2:184:B:LYS:CG	10	23.56	4.57	25.32
(1,29)	1:229:A:TRP:N	4:229:B:17F:O5	10	23.56	4.57	25.32
(1,29)	1:229:A:TRP:N	4:229:B:17F:C5	10	23.56	4.57	25.32
(1,29)	1:229:A:TRP:N	4:229:B:17F:O9	10	23.56	4.57	25.32
(1,26)	1:226:A:GLN:N	4:229:B:17F:O4	10	23.44	5.18	25.06
(1,26)	1:226:A:GLN:N	4:229:B:17F:O8	10	23.44	5.18	25.06
(1,26)	1:226:A:GLN:N	2:184:B:LYS:CG	10	23.44	5.18	25.06
(1,26)	1:226:A:GLN:N	4:229:B:17F:O5	10	23.44	5.18	25.06
(1,26)	1:226:A:GLN:N	4:229:B:17F:C4	10	23.44	5.18	25.06
(1,26)	1:226:A:GLN:N	4:229:B:17F:C5	10	23.44	5.18	25.06
(1,20)	1:220:A:GLN:N	4:229:B:17F:C4	10	23.32	5.21	25.18
(1,20)	1:220:A:GLN:N	4:229:B:17F:C1	10	23.32	5.21	25.18
(1,20)	1:220:A:GLN:N	4:229:B:17F:O4	10	23.32	5.21	25.18
(1,20)	1:220:A:GLN:N	4:229:B:17F:O8	10	23.32	5.21	25.18
(1,20)	1:220:A:GLN:N	2:184:B:LYS:HZ3	10	23.32	5.21	25.18
(1,20)	1:220:A:GLN:N	4:229:B:17F:C9	10	23.32	5.21	25.18
(1,58)	2:139:B:ILE:CG2	3:407:A:PCW:N	10	22.87	4.19	21.92
(1,58)	2:139:B:ILE:N	3:405:A:PCW:N	10	22.87	4.19	21.92
(1,58)	2:139:B:ILE:CG2	3:405:A:PCW:N	10	22.87	4.19	21.92
(1,58)	2:139:B:ILE:C	3:407:A:PCW:N	10	22.87	4.19	21.92
(1,58)	2:139:B:ILE:CD1	3:404:A:PCW:N	10	22.87	4.19	21.92
(1,58)	2:139:B:ILE:CG2	3:402:A:PCW:N	10	22.87	4.19	21.92
(1,57)	2:138:B:GLY:O	3:407:A:PCW:N	10	22.66	4.65	20.61
(1,57)	2:138:B:GLY:O	3:405:A:PCW:N	10	22.66	4.65	20.61
(1,57)	2:138:B:GLY:O	3:406:A:PCW:N	10	22.66	4.65	20.61
(1,57)	2:138:B:GLY:O	3:402:A:PCW:N	10	22.66	4.65	20.61
(1,16)	1:216:A:LYS:N	4:229:B:17F:C9	10	22.39	4.84	23.86
(1,16)	1:216:A:LYS:N	2:184:B:LYS:H	10	22.39	4.84	23.86
(1,16)	1:216:A:LYS:N	4:229:B:17F:O4	10	22.39	4.84	23.86
(1,16)	1:216:A:LYS:N	4:229:B:17F:O8	10	22.39	4.84	23.86
(1,16)	1:216:A:LYS:N	2:184:B:LYS:HZ3	10	22.39	4.84	23.86
(1,5)	1:205:A:ASP:N	2:178:B:LYS:O	10	22.13	4.39	24.35
(1,5)	1:205:A:ASP:N	2:184:B:LYS:H	10	22.13	4.39	24.35
(1,5)	1:205:A:ASP:N	4:229:B:17F:C9	10	22.13	4.39	24.35
(1,5)	1:205:A:ASP:N	2:177:B:LYS:HZ3	10	22.13	4.39	24.35
(1,5)	1:205:A:ASP:N	2:184:B:LYS:HZ2	10	22.13	4.39	24.35
(1,25)	1:225:A:THR:N	4:229:B:17F:C4	10	21.94	5.01	23.39
(1,25)	1:225:A:THR:N	4:229:B:17F:O4	10	21.94	5.01	23.39
(1,25)	1:225:A:THR:N	4:229:B:17F:O8	10	21.94	5.01	23.39

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,25)	1:225:A:THR:N	2:184:B:LYS:CG	10	21.94	5.01	23.39
(1,25)	1:225:A:THR:N	4:229:B:17F:O5	10	21.94	5.01	23.39
(1,25)	1:225:A:THR:N	4:229:B:17F:C5	10	21.94	5.01	23.39
(1,25)	1:225:A:THR:N	4:229:B:17F:C9	10	21.94	5.01	23.39
(1,25)	1:225:A:THR:N	4:229:B:17F:C8	10	21.94	5.01	23.39
(1,22)	1:222:A:GLY:N	4:229:B:17F:C4	10	21.89	5.43	23.58
(1,22)	1:222:A:GLY:N	4:229:B:17F:O4	10	21.89	5.43	23.58
(1,22)	1:222:A:GLY:N	4:229:B:17F:O8	10	21.89	5.43	23.58
(1,22)	1:222:A:GLY:N	2:184:B:LYS:CD	10	21.89	5.43	23.58
(1,22)	1:222:A:GLY:N	4:229:B:17F:O5	10	21.89	5.43	23.58
(1,22)	1:222:A:GLY:N	4:229:B:17F:C5	10	21.89	5.43	23.58
(1,22)	1:222:A:GLY:N	4:229:B:17F:C9	10	21.89	5.43	23.58
(1,9)	1:209:A:SER:N	4:229:B:17F:C9	10	21.77	3.84	23.68
(1,9)	1:209:A:SER:N	2:184:B:LYS:H	10	21.77	3.84	23.68
(1,9)	1:209:A:SER:N	4:229:B:17F:O8	10	21.77	3.84	23.68
(1,9)	1:209:A:SER:N	2:184:B:LYS:HZ2	10	21.77	3.84	23.68
(1,21)	1:221:A:LEU:N	4:229:B:17F:C4	10	21.48	5.15	23.2
(1,21)	1:221:A:LEU:N	4:229:B:17F:O4	10	21.48	5.15	23.2
(1,21)	1:221:A:LEU:N	4:229:B:17F:O8	10	21.48	5.15	23.2
(1,21)	1:221:A:LEU:N	2:184:B:LYS:HZ3	10	21.48	5.15	23.2
(1,21)	1:221:A:LEU:N	4:229:B:17F:C5	10	21.48	5.15	23.2
(1,21)	1:221:A:LEU:N	4:229:B:17F:C9	10	21.48	5.15	23.2
(1,12)	1:212:A:SER:N	4:229:B:17F:C9	10	21.36	4.25	23.1
(1,12)	1:212:A:SER:N	2:184:B:LYS:H	10	21.36	4.25	23.1
(1,12)	1:212:A:SER:N	4:229:B:17F:C2	10	21.36	4.25	23.1
(1,12)	1:212:A:SER:N	4:229:B:17F:O8	10	21.36	4.25	23.1
(1,12)	1:212:A:SER:N	2:184:B:LYS:HZ2	10	21.36	4.25	23.1
(1,6)	1:206:A:ASN:N	2:178:B:LYS:O	10	21.34	3.85	23.16
(1,6)	1:206:A:ASN:N	2:184:B:LYS:H	10	21.34	3.85	23.16
(1,6)	1:206:A:ASN:N	4:229:B:17F:C9	10	21.34	3.85	23.16
(1,6)	1:206:A:ASN:N	2:177:B:LYS:HZ3	10	21.34	3.85	23.16
(1,6)	1:206:A:ASN:N	2:184:B:LYS:HZ2	10	21.34	3.85	23.16
(1,17)	1:217:A:LEU:N	4:229:B:17F:C9	10	21.09	4.8	22.73
(1,17)	1:217:A:LEU:N	4:229:B:17F:C4	10	21.09	4.8	22.73
(1,17)	1:217:A:LEU:N	4:229:B:17F:O4	10	21.09	4.8	22.73
(1,17)	1:217:A:LEU:N	4:229:B:17F:O8	10	21.09	4.8	22.73
(1,17)	1:217:A:LEU:N	2:184:B:LYS:HZ3	10	21.09	4.8	22.73
(1,51)	2:79:B:LEU:N	3:407:A:PCW:N	10	20.65	1.96	20.48
(1,51)	2:79:B:LEU:H	3:406:A:PCW:N	10	20.65	1.96	20.48
(1,51)	2:79:B:LEU:H	3:407:A:PCW:N	10	20.65	1.96	20.48
(1,51)	2:79:B:LEU:O	3:404:A:PCW:N	10	20.65	1.96	20.48
(1,51)	2:79:B:LEU:CD1	3:404:A:PCW:N	10	20.65	1.96	20.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,51)	2:79:B:LEU:CD1	3:407:A:PCW:N	10	20.65	1.96	20.48
(1,51)	2:79:B:LEU:N	3:405:A:PCW:N	10	20.65	1.96	20.48
(1,51)	2:79:B:LEU:H	3:405:A:PCW:N	10	20.65	1.96	20.48
(1,8)	1:208:A:ASP:N	2:178:B:LYS:CB	10	20.61	3.95	22.37
(1,8)	1:208:A:ASP:N	2:184:B:LYS:H	10	20.61	3.95	22.37
(1,8)	1:208:A:ASP:N	4:229:B:17F:C2	10	20.61	3.95	22.37
(1,8)	1:208:A:ASP:N	2:177:B:LYS:HZ3	10	20.61	3.95	22.37
(1,8)	1:208:A:ASP:N	2:184:B:LYS:HZ2	10	20.61	3.95	22.37
(1,8)	1:208:A:ASP:N	4:229:B:17F:C9	10	20.61	3.95	22.37
(1,15)	1:215:A:SER:N	4:229:B:17F:C4	10	20.39	4.79	22.0
(1,15)	1:215:A:SER:N	2:184:B:LYS:H	10	20.39	4.79	22.0
(1,15)	1:215:A:SER:N	4:229:B:17F:O4	10	20.39	4.79	22.0
(1,15)	1:215:A:SER:N	4:229:B:17F:O8	10	20.39	4.79	22.0
(1,15)	1:215:A:SER:N	2:184:B:LYS:HZ2	10	20.39	4.79	22.0
(1,15)	1:215:A:SER:N	4:229:B:17F:C9	10	20.39	4.79	22.0
(1,4)	1:204:A:LEU:N	2:178:B:LYS:O	10	20.18	4.55	22.54
(1,4)	1:204:A:LEU:N	2:184:B:LYS:H	10	20.18	4.55	22.54
(1,4)	1:204:A:LEU:N	4:229:B:17F:O2	10	20.18	4.55	22.54
(1,4)	1:204:A:LEU:N	2:177:B:LYS:HZ3	10	20.18	4.55	22.54
(1,4)	1:204:A:LEU:N	2:184:B:LYS:HZ2	10	20.18	4.55	22.54
(1,4)	1:204:A:LEU:N	4:229:B:17F:C9	10	20.18	4.55	22.54
(1,3)	1:203:A:LEU:N	2:178:B:LYS:O	10	19.89	4.62	21.76
(1,3)	1:203:A:LEU:N	2:184:B:LYS:H	10	19.89	4.62	21.76
(1,3)	1:203:A:LEU:N	4:229:B:17F:C9	10	19.89	4.62	21.76
(1,3)	1:203:A:LEU:N	2:177:B:LYS:HZ3	10	19.89	4.62	21.76
(1,3)	1:203:A:LEU:N	2:184:B:LYS:HZ2	10	19.89	4.62	21.76
(1,10)	1:210:A:VAL:N	4:229:B:17F:C9	10	19.72	3.47	21.32
(1,10)	1:210:A:VAL:N	2:184:B:LYS:H	10	19.72	3.47	21.32
(1,10)	1:210:A:VAL:N	4:229:B:17F:O8	10	19.72	3.47	21.32
(1,10)	1:210:A:VAL:N	2:184:B:LYS:HZ2	10	19.72	3.47	21.32
(1,7)	1:207:A:TRP:N	2:178:B:LYS:CB	10	19.34	3.67	21.08
(1,7)	1:207:A:TRP:N	2:184:B:LYS:H	10	19.34	3.67	21.08
(1,7)	1:207:A:TRP:N	4:229:B:17F:C9	10	19.34	3.67	21.08
(1,7)	1:207:A:TRP:N	2:177:B:LYS:HZ3	10	19.34	3.67	21.08
(1,7)	1:207:A:TRP:N	2:184:B:LYS:HZ2	10	19.34	3.67	21.08
(1,14)	1:214:A:PHE:N	4:229:B:17F:C9	10	19.27	4.19	20.54
(1,14)	1:214:A:PHE:N	2:184:B:LYS:H	10	19.27	4.19	20.54
(1,14)	1:214:A:PHE:N	4:229:B:17F:O4	10	19.27	4.19	20.54
(1,14)	1:214:A:PHE:N	4:229:B:17F:O8	10	19.27	4.19	20.54
(1,14)	1:214:A:PHE:N	2:184:B:LYS:HZ2	10	19.27	4.19	20.54
(1,11)	1:211:A:THR:N	4:229:B:17F:C9	10	19.15	3.86	20.84
(1,11)	1:211:A:THR:N	2:184:B:LYS:H	10	19.15	3.86	20.84

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,11)	1:211:A:THR:N	4:229:B:17F:C2	10	19.15	3.86	20.84
(1,11)	1:211:A:THR:N	4:229:B:17F:O8	10	19.15	3.86	20.84
(1,11)	1:211:A:THR:N	2:184:B:LYS:HZ2	10	19.15	3.86	20.84
(1,61)	2:160:B:VAL:CG1	3:405:A:PCW:N	10	18.79	2.56	18.98
(1,61)	2:160:B:VAL:O	3:407:A:PCW:N	10	18.79	2.56	18.98
(1,61)	2:160:B:VAL:O	3:402:A:PCW:N	10	18.79	2.56	18.98
(1,61)	2:160:B:VAL:CG1	3:407:A:PCW:N	10	18.79	2.56	18.98
(1,61)	2:160:B:VAL:CG2	3:406:A:PCW:N	10	18.79	2.56	18.98
(1,66)	2:185:B:CYS:HG	3:403:A:PCW:N	10	15.72	6.14	15.98
(1,66)	2:185:B:CYS:HG	1:201:A:LEU:N	10	15.72	6.14	15.98
(1,66)	2:185:B:CYS:SG	3:407:A:PCW:N	10	15.72	6.14	15.98
(1,66)	2:185:B:CYS:HG	3:404:A:PCW:N	10	15.72	6.14	15.98
(1,66)	2:185:B:CYS:H	3:402:A:PCW:N	10	15.72	6.14	15.98
(1,66)	2:185:B:CYS:CB	3:402:A:PCW:N	10	15.72	6.14	15.98
(1,66)	2:185:B:CYS:HG	3:402:A:PCW:N	10	15.72	6.14	15.98
(1,54)	2:109:B:VAL:CG2	3:407:A:PCW:N	10	15.55	3.81	15.17
(1,54)	2:109:B:VAL:N	3:407:A:PCW:N	10	15.55	3.81	15.17
(1,54)	2:109:B:VAL:CG2	3:404:A:PCW:N	10	15.55	3.81	15.17
(1,54)	2:109:B:VAL:CG2	3:405:A:PCW:N	10	15.55	3.81	15.17
(1,54)	2:109:B:VAL:CG2	3:402:A:PCW:N	10	15.55	3.81	15.17
(1,50)	2:75:B:GLY:O	3:407:A:PCW:N	10	15.09	2.33	15.47
(1,50)	2:75:B:GLY:H	3:406:A:PCW:N	10	15.09	2.33	15.47
(1,50)	2:75:B:GLY:H	3:407:A:PCW:N	10	15.09	2.33	15.47
(1,50)	2:75:B:GLY:H	3:405:A:PCW:N	10	15.09	2.33	15.47
(1,50)	2:75:B:GLY:H	3:404:A:PCW:N	10	15.09	2.33	15.47
(1,50)	2:75:B:GLY:O	3:405:A:PCW:N	10	15.09	2.33	15.47
(1,50)	2:75:B:GLY:H	3:402:A:PCW:N	10	15.09	2.33	15.47
(1,45)	2:46:B:ILE:O	3:405:A:PCW:N	10	14.99	3.36	16.18
(1,45)	2:46:B:ILE:H	3:402:A:PCW:N	10	14.99	3.36	16.18
(1,45)	2:46:B:ILE:O	3:404:A:PCW:N	10	14.99	3.36	16.18
(1,45)	2:46:B:ILE:O	3:402:A:PCW:N	10	14.99	3.36	16.18
(1,45)	2:46:B:ILE:N	3:406:A:PCW:N	10	14.99	3.36	16.18
(1,45)	2:46:B:ILE:H	3:407:A:PCW:N	10	14.99	3.36	16.18
(1,40)	2:2:B:THR:H	3:405:A:PCW:N	10	14.68	2.87	15.09
(1,40)	2:2:B:THR:H	3:402:A:PCW:N	10	14.68	2.87	15.09
(1,40)	2:2:B:THR:HG1	3:404:A:PCW:N	10	14.68	2.87	15.09
(1,40)	2:2:B:THR:HG1	3:402:A:PCW:N	10	14.68	2.87	15.09
(1,40)	2:2:B:THR:CG2	3:402:A:PCW:N	10	14.68	2.87	15.09
(1,40)	2:2:B:THR:H	3:407:A:PCW:N	10	14.68	2.87	15.09
(1,49)	2:55:B:ILE:H	3:402:A:PCW:N	10	14.41	3.22	14.72
(1,49)	2:55:B:ILE:O	3:406:A:PCW:N	10	14.41	3.22	14.72
(1,49)	2:55:B:ILE:H	3:406:A:PCW:N	10	14.41	3.22	14.72

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,49)	2:55:B:ILE:O	3:407:A:PCW:N	10	14.41	3.22	14.72
(1,49)	2:55:B:ILE:O	3:404:A:PCW:N	10	14.41	3.22	14.72
(1,49)	2:55:B:ILE:O	3:405:A:PCW:N	10	14.41	3.22	14.72
(1,39)	2:1:B:MET:CE	3:402:A:PCW:N	10	13.02	3.07	13.36
(1,39)	2:1:B:MET:H	3:402:A:PCW:N	10	13.02	3.07	13.36
(1,39)	2:1:B:MET:CE	3:405:A:PCW:N	10	13.02	3.07	13.36
(1,39)	2:1:B:MET:CB	3:402:A:PCW:N	10	13.02	3.07	13.36
(1,39)	2:1:B:MET:N	3:402:A:PCW:N	10	13.02	3.07	13.36
(1,39)	2:1:B:MET:O	3:402:A:PCW:N	10	13.02	3.07	13.36
(1,39)	2:1:B:MET:CE	3:407:A:PCW:N	10	13.02	3.07	13.36
(1,39)	2:1:B:MET:SD	3:406:A:PCW:N	10	13.02	3.07	13.36
(1,39)	2:1:B:MET:CE	3:406:A:PCW:N	10	13.02	3.07	13.36
(1,39)	2:1:B:MET:CG	3:407:A:PCW:N	10	13.02	3.07	13.36
(1,46)	2:48:B:GLY:O	3:405:A:PCW:N	10	12.89	4.59	13.14
(1,46)	2:48:B:GLY:O	3:402:A:PCW:N	10	12.89	4.59	13.14
(1,46)	2:48:B:GLY:O	3:404:A:PCW:N	10	12.89	4.59	13.14
(1,46)	2:48:B:GLY:O	3:406:A:PCW:N	10	12.89	4.59	13.14
(1,46)	2:48:B:GLY:O	3:407:A:PCW:N	10	12.89	4.59	13.14
(1,46)	2:48:B:GLY:C	3:402:A:PCW:N	10	12.89	4.59	13.14
(1,47)	2:49:B:GLU:CG	3:405:A:PCW:N	10	12.49	3.53	12.55
(1,47)	2:49:B:GLU:C	3:402:A:PCW:N	10	12.49	3.53	12.55
(1,47)	2:49:B:GLU:CG	3:404:A:PCW:N	10	12.49	3.53	12.55
(1,47)	2:49:B:GLU:OE1	3:402:A:PCW:N	10	12.49	3.53	12.55
(1,47)	2:49:B:GLU:C	3:407:A:PCW:N	10	12.49	3.53	12.55
(1,47)	2:49:B:GLU:C	3:406:A:PCW:N	10	12.49	3.53	12.55
(1,44)	2:45:B:VAL:CG1	3:405:A:PCW:N	10	12.0	4.0	11.74
(1,44)	2:45:B:VAL:CG2	3:402:A:PCW:N	10	12.0	4.0	11.74
(1,44)	2:45:B:VAL:CG2	3:405:A:PCW:N	10	12.0	4.0	11.74
(1,44)	2:45:B:VAL:CG1	3:402:A:PCW:N	10	12.0	4.0	11.74
(1,44)	2:45:B:VAL:CG2	3:406:A:PCW:N	10	12.0	4.0	11.74
(1,44)	2:45:B:VAL:CG2	3:407:A:PCW:N	10	12.0	4.0	11.74
(1,48)	2:50:B:THR:H	3:405:A:PCW:N	10	11.13	3.71	10.94
(1,48)	2:50:B:THR:HG1	3:402:A:PCW:N	10	11.13	3.71	10.94
(1,48)	2:50:B:THR:CG2	3:405:A:PCW:N	10	11.13	3.71	10.94
(1,48)	2:50:B:THR:CG2	3:402:A:PCW:N	10	11.13	3.71	10.94
(1,48)	2:50:B:THR:H	3:402:A:PCW:N	10	11.13	3.71	10.94
(1,48)	2:50:B:THR:HG1	3:406:A:PCW:N	10	11.13	3.71	10.94
(1,48)	2:50:B:THR:CG2	3:407:A:PCW:N	10	11.13	3.71	10.94
(1,53)	2:106:B:SER:HG	3:407:A:PCW:N	10	10.97	3.78	11.11
(1,53)	2:106:B:SER:N	3:407:A:PCW:N	10	10.97	3.78	11.11
(1,53)	2:106:B:SER:HG	3:406:A:PCW:N	10	10.97	3.78	11.11
(1,53)	2:106:B:SER:N	3:404:A:PCW:N	10	10.97	3.78	11.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,53)	2:106:B:SER:HG	3:405:A:PCW:N	10	10.97	3.78	11.11
(1,53)	2:106:B:SER:N	3:402:A:PCW:N	10	10.97	3.78	11.11
(1,53)	2:106:B:SER:N	3:405:A:PCW:N	10	10.97	3.78	11.11
(1,53)	2:106:B:SER:HG	3:402:A:PCW:N	10	10.97	3.78	11.11
(1,43)	2:43:B:GLN:OE1	3:402:A:PCW:N	10	10.36	2.98	11.01
(1,43)	2:43:B:GLN:HE22	3:402:A:PCW:N	10	10.36	2.98	11.01
(1,43)	2:43:B:GLN:OE1	3:405:A:PCW:N	10	10.36	2.98	11.01
(1,43)	2:43:B:GLN:H	3:406:A:PCW:N	10	10.36	2.98	11.01
(1,43)	2:43:B:GLN:OE1	3:406:A:PCW:N	10	10.36	2.98	11.01
(1,43)	2:43:B:GLN:HE22	3:403:A:PCW:N	10	10.36	2.98	11.01
(1,43)	2:43:B:GLN:HE22	3:406:A:PCW:N	10	10.36	2.98	11.01
(1,43)	2:43:B:GLN:HE22	3:407:A:PCW:N	10	10.36	2.98	11.01
(1,63)	2:174:B:GLY:N	3:403:A:PCW:N	10	8.02	5.79	6.92
(1,63)	2:174:B:GLY:C	3:403:A:PCW:N	10	8.02	5.79	6.92
(1,63)	2:174:B:GLY:H	3:407:A:PCW:N	10	8.02	5.79	6.92
(1,63)	2:174:B:GLY:CA	3:405:A:PCW:N	10	8.02	5.79	6.92
(1,63)	2:174:B:GLY:O	3:402:A:PCW:N	10	8.02	5.79	6.92
(1,63)	2:174:B:GLY:H	3:406:A:PCW:N	10	8.02	5.79	6.92
(1,63)	2:174:B:GLY:N	3:402:A:PCW:N	10	8.02	5.79	6.92
(1,1)	3:402:A:PCW:N	4:227:B:17F:C9	10	7.83	4.21	10.08
(1,1)	1:201:A:LEU:N	2:184:B:LYS:O	10	7.83	4.21	10.08
(1,1)	3:402:A:PCW:N	2:43:B:GLN:HE22	10	7.83	4.21	10.08
(1,1)	3:402:A:PCW:N	2:49:B:GLU:OE1	10	7.83	4.21	10.08
(1,1)	3:402:A:PCW:N	2:178:B:LYS:HZ1	10	7.83	4.21	10.08
(1,1)	3:402:A:PCW:N	2:105:B:ASP:OD2	10	7.83	4.21	10.08
(1,1)	3:402:A:PCW:N	2:177:B:LYS:CE	10	7.83	4.21	10.08
(1,1)	3:402:A:PCW:N	2:171:B:SER:O	10	7.83	4.21	10.08
(1,1)	3:402:A:PCW:N	2:105:B:ASP:OD1	10	7.83	4.21	10.08
(1,62)	2:171:B:SER:O	3:403:A:PCW:N	10	7.74	4.51	8.02
(1,62)	2:171:B:SER:O	3:407:A:PCW:N	10	7.74	4.51	8.02
(1,62)	2:171:B:SER:O	3:405:A:PCW:N	10	7.74	4.51	8.02
(1,62)	2:171:B:SER:O	3:402:A:PCW:N	10	7.74	4.51	8.02
(1,62)	2:171:B:SER:O	3:406:A:PCW:N	10	7.74	4.51	8.02
(1,62)	2:171:B:SER:CB	3:406:A:PCW:N	10	7.74	4.51	8.02
(1,18)	3:405:A:PCW:N	2:48:B:GLY:O	10	7.5	2.54	7.44
(1,18)	3:405:A:PCW:N	4:229:B:17F:O4	10	7.5	2.54	7.44
(1,18)	3:405:A:PCW:N	2:177:B:LYS:H	10	7.5	2.54	7.44
(1,18)	3:405:A:PCW:N	2:105:B:ASP:OD1	10	7.5	2.54	7.44
(1,18)	3:405:A:PCW:N	2:37:B:GLU:OE1	10	7.5	2.54	7.44
(1,18)	3:405:A:PCW:N	2:105:B:ASP:OD2	10	7.5	2.54	7.44
(1,18)	3:405:A:PCW:N	2:36:B:ILE:CD1	10	7.5	2.54	7.44
(1,41)	3:202:B:PCW:C8	3:407:A:PCW:N	10	7.38	0.78	7.66

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,41)	3:202:B:PCW:C4	3:407:A:PCW:N	10	7.38	0.78	7.66
(1,41)	3:202:B:PCW:C6	3:407:A:PCW:N	10	7.38	0.78	7.66
(1,41)	3:202:B:PCW:C5	3:407:A:PCW:N	10	7.38	0.78	7.66
(1,52)	2:105:B:ASP:OD1	3:407:A:PCW:N	10	6.95	3.54	7.21
(1,52)	2:105:B:ASP:OD1	3:406:A:PCW:N	10	6.95	3.54	7.21
(1,52)	2:105:B:ASP:OD2	3:407:A:PCW:N	10	6.95	3.54	7.21
(1,52)	2:105:B:ASP:OD1	3:404:A:PCW:N	10	6.95	3.54	7.21
(1,52)	2:105:B:ASP:OD1	3:405:A:PCW:N	10	6.95	3.54	7.21
(1,52)	2:105:B:ASP:OD2	3:402:A:PCW:N	10	6.95	3.54	7.21
(1,52)	2:105:B:ASP:OD2	3:405:A:PCW:N	10	6.95	3.54	7.21
(1,52)	2:105:B:ASP:OD1	3:402:A:PCW:N	10	6.95	3.54	7.21
(1,19)	3:406:A:PCW:N	4:226:B:17F:C2	10	1.97	0.71	2.16
(1,19)	3:406:A:PCW:N	2:37:B:GLU:OE1	10	1.97	0.71	2.16
(1,19)	3:406:A:PCW:N	4:226:B:17F:O4	10	1.97	0.71	2.16
(1,19)	3:406:A:PCW:N	4:226:B:17F:C1	10	1.97	0.71	2.16
(1,19)	3:406:A:PCW:N	4:226:B:17F:N1	10	1.97	0.71	2.16
(1,19)	3:406:A:PCW:N	4:226:B:17F:O1	10	1.97	0.71	2.16
(1,64)	2:176:B:LYS:CB	3:403:A:PCW:N	9	7.72	6.55	5.53
(1,64)	2:176:B:LYS:N	3:407:A:PCW:N	9	7.72	6.55	5.53
(1,64)	2:176:B:LYS:O	3:403:A:PCW:N	9	7.72	6.55	5.53
(1,64)	2:176:B:LYS:CG	3:405:A:PCW:N	9	7.72	6.55	5.53
(1,64)	2:176:B:LYS:CE	3:402:A:PCW:N	9	7.72	6.55	5.53
(1,64)	2:176:B:LYS:O	3:402:A:PCW:N	9	7.72	6.55	5.53
(1,64)	2:176:B:LYS:CE	3:405:A:PCW:N	9	7.72	6.55	5.53
(1,65)	2:177:B:LYS:H	3:407:A:PCW:N	8	8.21	5.58	7.28
(1,65)	2:177:B:LYS:N	3:403:A:PCW:N	8	8.21	5.58	7.28
(1,65)	2:177:B:LYS:H	3:405:A:PCW:N	8	8.21	5.58	7.28
(1,65)	2:177:B:LYS:O	3:402:A:PCW:N	8	8.21	5.58	7.28
(1,65)	2:177:B:LYS:HZ3	3:402:A:PCW:N	8	8.21	5.58	7.28
(1,65)	2:177:B:LYS:CE	3:402:A:PCW:N	8	8.21	5.58	7.28
(1,2)	3:403:A:PCW:N	2:172:B:LYS:HZ1	8	5.97	3.42	5.19
(1,2)	3:403:A:PCW:N	2:176:B:LYS:O	8	5.97	3.42	5.19
(1,2)	3:403:A:PCW:N	4:225:B:17F:O5	8	5.97	3.42	5.19
(1,2)	3:403:A:PCW:N	2:36:B:ILE:CD1	8	5.97	3.42	5.19
(1,2)	3:403:A:PCW:N	2:43:B:GLN:HE22	8	5.97	3.42	5.19
(1,2)	3:403:A:PCW:N	2:36:B:ILE:CG2	8	5.97	3.42	5.19
(1,2)	3:403:A:PCW:N	4:225:B:17F:O4	8	5.97	3.42	5.19
(1,2)	3:403:A:PCW:N	4:229:B:17F:C9	8	5.97	3.42	5.19
(1,13)	3:404:A:PCW:N	4:229:B:17F:O2	8	3.0	1.49	3.14
(1,13)	3:404:A:PCW:N	2:185:B:CYS:HG	8	3.0	1.49	3.14
(1,13)	3:404:A:PCW:N	4:229:B:17F:O4	8	3.0	1.49	3.14
(1,13)	3:404:A:PCW:N	4:229:B:17F:C6	8	3.0	1.49	3.14

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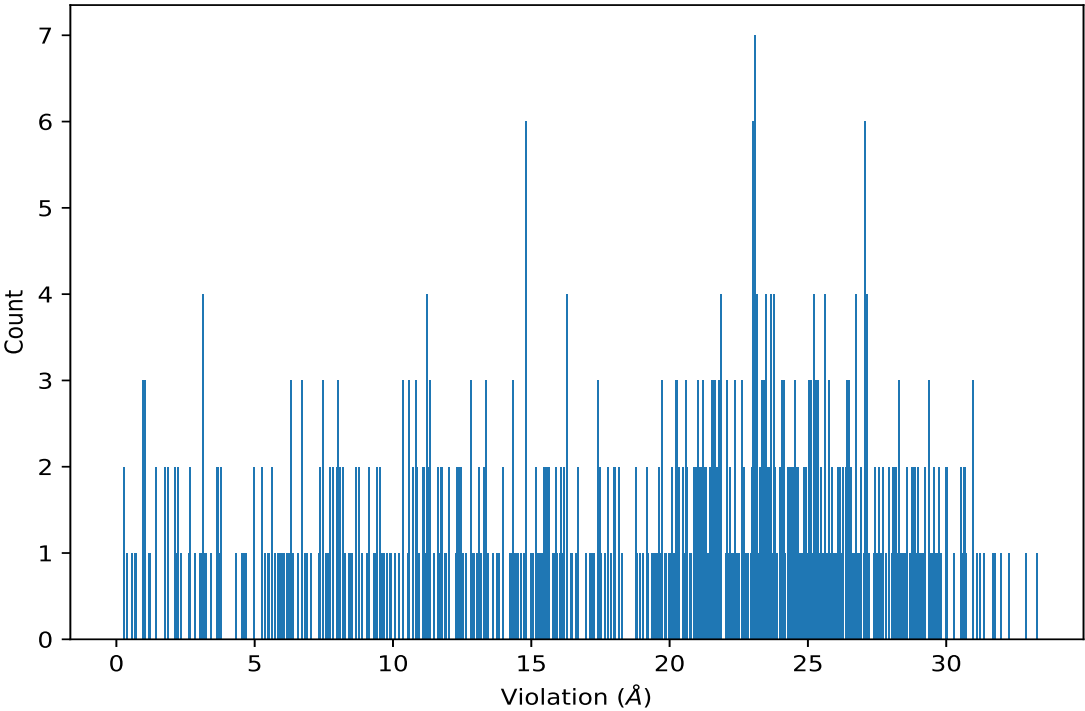
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,42)	4:226:B:17F:C2	3:406:A:PCW:N	3	1.88	0.84	2.22
(1,42)	4:228:B:17F:O5	3:407:A:PCW:N	3	1.88	0.84	2.22
(1,42)	4:226:B:17F:C1	3:406:A:PCW:N	3	1.88	0.84	2.22
(1,30)	3:407:A:PCW:N	2:105:B:ASP:OD1	2	1.02	0.77	1.02
(1,30)	3:407:A:PCW:N	4:225:B:17F:O2	2	1.02	0.77	1.02

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)
(1,56)	2:133:B:LEU:O	3:402:A:PCW:N	10	33.3
(1,38)	1:238:A:GLY:N	4:229:B:17F:C5	4	32.85
(1,38)	1:238:A:GLY:N	4:229:B:17F:O9	8	32.25
(1,38)	1:238:A:GLY:N	2:36:B:ILE:CD1	7	31.96
(1,38)	1:238:A:GLY:N	4:229:B:17F:O4	2	31.77
(1,38)	1:238:A:GLY:N	2:36:B:ILE:CD1	10	31.74
(1,38)	1:238:A:GLY:N	4:229:B:17F:O4	1	31.68
(1,34)	1:234:A:LYS:N	4:229:B:17F:O4	9	31.38
(1,35)	1:235:A:GLU:N	4:229:B:17F:O5	9	31.2
(1,34)	1:234:A:LYS:N	4:229:B:17F:O4	10	31.13
(1,59)	2:141:B:PHE:N	3:405:A:PCW:N	6	30.98
(1,37)	1:237:A:GLU:N	4:229:B:17F:C5	4	30.98
(1,56)	2:133:B:LEU:CD1	3:402:A:PCW:N	7	30.95
(1,34)	1:234:A:LYS:N	2:36:B:ILE:CD1	7	30.71
(1,34)	1:234:A:LYS:N	4:229:B:17F:C5	4	30.69
(1,56)	2:133:B:LEU:CD2	3:404:A:PCW:N	8	30.65
(1,59)	2:141:B:PHE:O	3:407:A:PCW:N	10	30.63
(1,34)	1:234:A:LYS:N	4:229:B:17F:O9	8	30.6
(1,34)	1:234:A:LYS:N	4:229:B:17F:O9	6	30.58
(1,57)	2:138:B:GLY:O	3:405:A:PCW:N	8	30.53
(1,35)	1:235:A:GLU:N	4:229:B:17F:O9	10	30.53
(1,37)	1:237:A:GLU:N	4:229:B:17F:O4	8	30.25
(1,35)	1:235:A:GLU:N	4:229:B:17F:C5	4	30.02
(1,35)	1:235:A:GLU:N	4:229:B:17F:C5	7	30.01
(1,31)	1:231:A:ASN:N	4:229:B:17F:O9	10	29.99
(1,31)	1:231:A:ASN:N	4:229:B:17F:C8	9	29.98
(1,35)	1:235:A:GLU:N	4:229:B:17F:O9	6	29.83
(1,60)	2:142:B:ILE:CD1	3:402:A:PCW:N	5	29.74
(1,35)	1:235:A:GLU:N	4:229:B:17F:O9	8	29.71
(1,38)	1:238:A:GLY:N	2:175:B:LYS:HZ1	9	29.69
(1,57)	2:138:B:GLY:O	3:406:A:PCW:N	10	29.62
(1,37)	1:237:A:GLU:N	2:36:B:ILE:CD1	7	29.58
(1,37)	1:237:A:GLU:N	2:36:B:ILE:CD1	10	29.55
(1,34)	1:234:A:LYS:N	4:229:B:17F:O4	1	29.49
(1,37)	1:237:A:GLU:N	4:229:B:17F:O4	1	29.41
(1,55)	2:113:B:LEU:C	3:405:A:PCW:N	10	29.39
(1,37)	1:237:A:GLU:N	4:229:B:17F:O4	2	29.37
(1,38)	1:238:A:GLY:N	4:229:B:17F:O4	3	29.36
(1,35)	1:235:A:GLU:N	4:229:B:17F:O4	2	29.24
(1,35)	1:235:A:GLU:N	4:229:B:17F:O4	1	29.23
(1,34)	1:234:A:LYS:N	4:229:B:17F:O4	2	29.17
(1,38)	1:238:A:GLY:N	2:177:B:LYS:HZ2	6	29.12
(1,58)	2:139:B:ILE:CD1	3:404:A:PCW:N	8	29.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:231:A:ASN:N	4:229:B:17F:O9	8	29.02
(1,59)	2:141:B:PHE:H	3:405:A:PCW:N	5	28.97
(1,27)	1:227:A:GLU:N	4:229:B:17F:C8	10	28.97
(1,31)	1:231:A:ASN:N	4:229:B:17F:C5	7	28.94
(1,60)	2:142:B:ILE:O	3:407:A:PCW:N	6	28.87
(1,36)	1:236:A:THR:N	2:36:B:ILE:CD1	10	28.87
(1,31)	1:231:A:ASN:N	4:229:B:17F:O9	6	28.82
(1,37)	1:237:A:GLU:N	2:175:B:LYS:HZ1	9	28.81
(1,36)	1:236:A:THR:N	4:229:B:17F:C5	4	28.76
(1,31)	1:231:A:ASN:N	4:229:B:17F:O8	4	28.76
(1,33)	1:233:A:GLU:N	4:229:B:17F:O4	9	28.73
(1,58)	2:139:B:ILE:CG2	3:402:A:PCW:N	10	28.65
(1,27)	1:227:A:GLU:N	4:229:B:17F:C9	9	28.57
(1,33)	1:233:A:GLU:N	4:229:B:17F:O4	10	28.55
(1,36)	1:236:A:THR:N	2:175:B:LYS:HZ1	9	28.53
(1,36)	1:236:A:THR:N	2:37:B:GLU:OE1	7	28.4
(1,31)	1:231:A:ASN:N	4:229:B:17F:O4	1	28.37
(1,36)	1:236:A:THR:N	4:229:B:17F:O9	8	28.29
(1,32)	1:232:A:LEU:N	4:229:B:17F:C8	9	28.29
(1,59)	2:141:B:PHE:CE1	3:407:A:PCW:N	8	28.25
(1,33)	1:233:A:GLU:N	2:36:B:ILE:CD1	7	28.22
(1,33)	1:233:A:GLU:N	4:229:B:17F:C4	4	28.16
(1,27)	1:227:A:GLU:N	4:229:B:17F:C5	8	28.15
(1,32)	1:232:A:LEU:N	4:229:B:17F:O9	10	28.14
(1,60)	2:142:B:ILE:H	3:406:A:PCW:N	2	28.12
(1,33)	1:233:A:GLU:N	4:229:B:17F:O4	8	28.07
(1,33)	1:233:A:GLU:N	4:229:B:17F:O9	6	28.06
(1,58)	2:139:B:ILE:C	3:407:A:PCW:N	7	28.03
(1,31)	1:231:A:ASN:N	4:229:B:17F:O4	2	27.94
(1,37)	1:237:A:GLU:N	2:177:B:LYS:HZ2	6	27.91
(1,23)	1:223:A:PRO:N	4:229:B:17F:C9	10	27.81
(1,27)	1:227:A:GLU:N	4:229:B:17F:C5	7	27.73
(1,36)	1:236:A:THR:N	4:229:B:17F:O4	2	27.72
(1,23)	1:223:A:PRO:N	4:229:B:17F:C5	8	27.61
(1,36)	1:236:A:THR:N	4:229:B:17F:O4	1	27.58
(1,23)	1:223:A:PRO:N	4:229:B:17F:C9	9	27.56
(1,56)	2:133:B:LEU:O	3:405:A:PCW:N	6	27.52
(1,59)	2:141:B:PHE:O	3:407:A:PCW:N	7	27.47
(1,36)	1:236:A:THR:N	2:177:B:LYS:HZ2	6	27.44
(1,59)	2:141:B:PHE:N	3:407:A:PCW:N	2	27.43
(1,28)	1:228:A:PHE:N	4:229:B:17F:C8	10	27.38
(1,32)	1:232:A:LEU:N	4:229:B:17F:C5	7	27.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:232:A:LEU:N	4:229:B:17F:O8	4	27.15
(1,55)	2:113:B:LEU:CD1	3:407:A:PCW:N	5	27.13
(1,32)	1:232:A:LEU:N	4:229:B:17F:O9	8	27.13
(1,27)	1:227:A:GLU:N	4:229:B:17F:O5	6	27.12
(1,27)	1:227:A:GLU:N	4:229:B:17F:O8	4	27.11
(1,60)	2:142:B:ILE:H	3:407:A:PCW:N	4	27.09
(1,32)	1:232:A:LEU:N	4:229:B:17F:O9	6	27.09
(1,37)	1:237:A:GLU:N	4:229:B:17F:O4	3	27.06
(1,34)	1:234:A:LYS:N	4:229:B:17F:O4	3	27.06
(1,27)	1:227:A:GLU:N	4:229:B:17F:O4	1	27.06
(1,60)	2:142:B:ILE:CG2	3:407:A:PCW:N	10	27.05
(1,28)	1:228:A:PHE:N	4:229:B:17F:C8	9	27.01
(1,35)	1:235:A:GLU:N	4:229:B:17F:O4	3	26.91
(1,33)	1:233:A:GLU:N	4:229:B:17F:O4	1	26.9
(1,55)	2:113:B:LEU:C	3:404:A:PCW:N	7	26.89
(1,23)	1:223:A:PRO:N	4:229:B:17F:C4	7	26.81
(1,24)	1:224:A:VAL:N	4:229:B:17F:C5	8	26.74
(1,55)	2:113:B:LEU:CD1	3:404:A:PCW:N	6	26.73
(1,26)	1:226:A:GLN:N	4:229:B:17F:O4	10	26.73
(1,24)	1:224:A:VAL:N	4:229:B:17F:C9	10	26.71
(1,32)	1:232:A:LEU:N	4:229:B:17F:O4	1	26.65
(1,56)	2:133:B:LEU:O	3:404:A:PCW:N	5	26.64
(1,28)	1:228:A:PHE:N	4:229:B:17F:C5	8	26.56
(1,24)	1:224:A:VAL:N	4:229:B:17F:C9	9	26.55
(1,57)	2:138:B:GLY:O	3:406:A:PCW:N	7	26.49
(1,29)	1:229:A:TRP:N	4:229:B:17F:O4	10	26.48
(1,33)	1:233:A:GLU:N	4:229:B:17F:O4	2	26.45
(1,60)	2:142:B:ILE:CD1	3:402:A:PCW:N	9	26.42
(1,26)	1:226:A:GLN:N	4:229:B:17F:O4	9	26.42
(1,27)	1:227:A:GLU:N	4:229:B:17F:O4	2	26.41
(1,60)	2:142:B:ILE:H	3:407:A:PCW:N	1	26.37
(1,29)	1:229:A:TRP:N	4:229:B:17F:O4	9	26.37
(1,23)	1:223:A:PRO:N	4:229:B:17F:C4	1	26.27
(1,26)	1:226:A:GLN:N	4:229:B:17F:C5	8	26.26
(1,32)	1:232:A:LEU:N	4:229:B:17F:O4	2	26.21
(1,28)	1:228:A:PHE:N	4:229:B:17F:C5	6	26.19
(1,28)	1:228:A:PHE:N	4:229:B:17F:C5	7	26.18
(1,23)	1:223:A:PRO:N	4:229:B:17F:O8	4	26.11
(1,20)	1:220:A:GLN:N	4:229:B:17F:C9	10	26.09
(1,60)	2:142:B:ILE:CD1	3:407:A:PCW:N	3	26.06
(1,24)	1:224:A:VAL:N	4:229:B:17F:C5	7	26.03
(1,20)	1:220:A:GLN:N	4:229:B:17F:C9	8	25.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	2:113:B:LEU:C	3:407:A:PCW:N	8	25.89
(1,29)	1:229:A:TRP:N	4:229:B:17F:O9	8	25.88
(1,60)	2:142:B:ILE:O	3:407:A:PCW:N	8	25.83
(1,26)	1:226:A:GLN:N	4:229:B:17F:C4	7	25.79
(1,20)	1:220:A:GLN:N	4:229:B:17F:C9	9	25.79
(1,59)	2:141:B:PHE:H	3:402:A:PCW:N	9	25.78
(1,28)	1:228:A:PHE:N	4:229:B:17F:O8	4	25.66
(1,66)	2:185:B:CYS:CB	3:402:A:PCW:N	10	25.63
(1,23)	1:223:A:PRO:N	4:229:B:17F:O4	2	25.62
(1,31)	1:231:A:ASN:N	4:229:B:17F:O4	3	25.61
(1,28)	1:228:A:PHE:N	4:229:B:17F:C5	1	25.61
(1,56)	2:133:B:LEU:O	3:407:A:PCW:N	3	25.58
(1,20)	1:220:A:GLN:N	4:229:B:17F:C9	7	25.5
(1,29)	1:229:A:TRP:N	4:229:B:17F:C5	7	25.47
(1,23)	1:223:A:PRO:N	4:229:B:17F:O5	6	25.47
(1,24)	1:224:A:VAL:N	4:229:B:17F:C5	1	25.42
(1,59)	2:141:B:PHE:N	3:407:A:PCW:N	4	25.37
(1,20)	1:220:A:GLN:N	4:229:B:17F:C1	2	25.37
(1,29)	1:229:A:TRP:N	4:229:B:17F:O8	4	25.36
(1,5)	1:205:A:ASP:N	4:229:B:17F:C9	10	25.34
(1,24)	1:224:A:VAL:N	4:229:B:17F:O4	6	25.31
(1,36)	1:236:A:THR:N	4:229:B:17F:O4	3	25.3
(1,55)	2:113:B:LEU:H	3:402:A:PCW:N	9	25.29
(1,5)	1:205:A:ASP:N	4:229:B:17F:C9	3	25.29
(1,29)	1:229:A:TRP:N	4:229:B:17F:O5	6	25.27
(1,26)	1:226:A:GLN:N	4:229:B:17F:O8	4	25.24
(1,24)	1:224:A:VAL:N	4:229:B:17F:O4	2	25.23
(1,5)	1:205:A:ASP:N	4:229:B:17F:C9	8	25.23
(1,22)	1:222:A:GLY:N	4:229:B:17F:C9	10	25.2
(1,28)	1:228:A:PHE:N	4:229:B:17F:O4	2	25.15
(1,5)	1:205:A:ASP:N	4:229:B:17F:C9	7	25.13
(1,24)	1:224:A:VAL:N	4:229:B:17F:O8	4	25.11
(1,57)	2:138:B:GLY:O	3:405:A:PCW:N	6	25.1
(1,5)	1:205:A:ASP:N	4:229:B:17F:C9	9	25.08
(1,16)	1:216:A:LYS:N	4:229:B:17F:C9	10	25.06
(1,25)	1:225:A:THR:N	4:229:B:17F:C8	10	25.03
(1,22)	1:222:A:GLY:N	4:229:B:17F:C5	8	25.03
(1,59)	2:141:B:PHE:H	3:407:A:PCW:N	3	25.01
(1,20)	1:220:A:GLN:N	4:229:B:17F:C4	1	24.98
(1,55)	2:113:B:LEU:N	3:406:A:PCW:N	2	24.94
(1,16)	1:216:A:LYS:N	4:229:B:17F:C9	8	24.91
(1,26)	1:226:A:GLN:N	4:229:B:17F:O4	1	24.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:222:A:GLY:N	4:229:B:17F:C9	9	24.87
(1,25)	1:225:A:THR:N	4:229:B:17F:C9	9	24.8
(1,51)	2:79:B:LEU:N	3:405:A:PCW:N	9	24.76
(1,25)	1:225:A:THR:N	4:229:B:17F:C5	8	24.71
(1,20)	1:220:A:GLN:N	4:229:B:17F:O4	6	24.64
(1,26)	1:226:A:GLN:N	4:229:B:17F:O5	6	24.63
(1,16)	1:216:A:LYS:N	4:229:B:17F:C9	7	24.57
(1,59)	2:141:B:PHE:N	3:407:A:PCW:N	1	24.55
(1,66)	2:185:B:CYS:HG	3:403:A:PCW:N	4	24.52
(1,55)	2:113:B:LEU:H	3:407:A:PCW:N	3	24.51
(1,20)	1:220:A:GLN:N	4:229:B:17F:O8	4	24.51
(1,56)	2:133:B:LEU:O	3:407:A:PCW:N	2	24.48
(1,29)	1:229:A:TRP:N	4:229:B:17F:O4	1	24.47
(1,33)	1:233:A:GLU:N	4:229:B:17F:O4	3	24.39
(1,16)	1:216:A:LYS:N	4:229:B:17F:C9	9	24.36
(1,9)	1:209:A:SER:N	4:229:B:17F:C9	10	24.34
(1,21)	1:221:A:LEU:N	4:229:B:17F:C9	10	24.3
(1,26)	1:226:A:GLN:N	4:229:B:17F:O4	2	24.27
(1,6)	1:206:A:ASN:N	4:229:B:17F:C9	10	24.27
(1,21)	1:221:A:LEU:N	4:229:B:17F:C9	8	24.15
(1,22)	1:222:A:GLY:N	4:229:B:17F:C4	7	24.14
(1,27)	1:227:A:GLU:N	4:229:B:17F:O4	3	24.13
(1,60)	2:142:B:ILE:CD1	3:407:A:PCW:N	7	24.11
(1,29)	1:229:A:TRP:N	4:229:B:17F:O4	2	24.06
(1,16)	1:216:A:LYS:N	4:229:B:17F:C9	1	24.05
(1,9)	1:209:A:SER:N	4:229:B:17F:C9	3	24.05
(1,25)	1:225:A:THR:N	4:229:B:17F:C5	7	24.04
(1,9)	1:209:A:SER:N	4:229:B:17F:C9	8	24.04
(1,32)	1:232:A:LEU:N	4:229:B:17F:O4	3	23.99
(1,21)	1:221:A:LEU:N	4:229:B:17F:C9	9	23.96
(1,12)	1:212:A:SER:N	4:229:B:17F:C9	10	23.89
(1,58)	2:139:B:ILE:CG2	3:405:A:PCW:N	6	23.82
(1,9)	1:209:A:SER:N	4:229:B:17F:C9	9	23.81
(1,6)	1:206:A:ASN:N	4:229:B:17F:C9	3	23.79
(1,9)	1:209:A:SER:N	4:229:B:17F:C9	7	23.78
(1,6)	1:206:A:ASN:N	4:229:B:17F:C9	8	23.76
(1,6)	1:206:A:ASN:N	4:229:B:17F:C9	9	23.76
(1,17)	1:217:A:LEU:N	4:229:B:17F:C9	10	23.7
(1,12)	1:212:A:SER:N	4:229:B:17F:C9	8	23.69
(1,22)	1:222:A:GLY:N	4:229:B:17F:C4	1	23.68
(1,21)	1:221:A:LEU:N	4:229:B:17F:C5	7	23.67
(1,16)	1:216:A:LYS:N	4:229:B:17F:O8	4	23.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	1:212:A:SER:N	4:229:B:17F:C9	7	23.63
(1,5)	1:205:A:ASP:N	4:229:B:17F:C9	6	23.63
(1,9)	1:209:A:SER:N	4:229:B:17F:C9	1	23.59
(1,4)	1:204:A:LEU:N	4:229:B:17F:C9	7	23.59
(1,12)	1:212:A:SER:N	4:229:B:17F:C9	9	23.52
(1,25)	1:225:A:THR:N	4:229:B:17F:C4	1	23.5
(1,16)	1:216:A:LYS:N	4:229:B:17F:O4	6	23.49
(1,22)	1:222:A:GLY:N	4:229:B:17F:O8	4	23.48
(1,4)	1:204:A:LEU:N	4:229:B:17F:O2	3	23.46
(1,8)	1:208:A:ASP:N	4:229:B:17F:C9	10	23.45
(1,17)	1:217:A:LEU:N	4:229:B:17F:C9	8	23.43
(1,4)	1:204:A:LEU:N	4:229:B:17F:C9	8	23.41
(1,16)	1:216:A:LYS:N	2:184:B:LYS:H	2	23.4
(1,21)	1:221:A:LEU:N	4:229:B:17F:O4	2	23.37
(1,6)	1:206:A:ASN:N	4:229:B:17F:C9	7	23.32
(1,4)	1:204:A:LEU:N	4:229:B:17F:C9	9	23.31
(1,4)	1:204:A:LEU:N	4:229:B:17F:C9	10	23.31
(1,25)	1:225:A:THR:N	4:229:B:17F:O8	4	23.28
(1,25)	1:225:A:THR:N	4:229:B:17F:O5	6	23.26
(1,9)	1:209:A:SER:N	4:229:B:17F:O8	4	23.24
(1,17)	1:217:A:LEU:N	4:229:B:17F:C4	2	23.19
(1,12)	1:212:A:SER:N	4:229:B:17F:C9	1	23.18
(1,23)	1:223:A:PRO:N	4:229:B:17F:O4	3	23.16
(1,22)	1:222:A:GLY:N	4:229:B:17F:O4	2	23.15
(1,8)	1:208:A:ASP:N	4:229:B:17F:C9	7	23.13
(1,28)	1:228:A:PHE:N	4:229:B:17F:O4	3	23.12
(1,58)	2:139:B:ILE:N	3:405:A:PCW:N	5	23.1
(1,56)	2:133:B:LEU:O	3:405:A:PCW:N	9	23.09
(1,17)	1:217:A:LEU:N	4:229:B:17F:C9	7	23.09
(1,8)	1:208:A:ASP:N	4:229:B:17F:C2	3	23.09
(1,3)	1:203:A:LEU:N	4:229:B:17F:C9	9	23.08
(1,3)	1:203:A:LEU:N	4:229:B:17F:C9	10	23.07
(1,15)	1:215:A:SER:N	4:229:B:17F:C9	8	23.05
(1,8)	1:208:A:ASP:N	4:229:B:17F:C9	8	23.05
(1,3)	1:203:A:LEU:N	4:229:B:17F:C9	3	23.04
(1,12)	1:212:A:SER:N	4:229:B:17F:O8	4	23.03
(1,21)	1:221:A:LEU:N	4:229:B:17F:C4	1	23.02
(1,8)	1:208:A:ASP:N	4:229:B:17F:C9	9	23.02
(1,25)	1:225:A:THR:N	4:229:B:17F:O4	2	23.0
(1,6)	1:206:A:ASN:N	2:177:B:LYS:HZ3	4	23.0
(1,15)	1:215:A:SER:N	4:229:B:17F:C9	10	22.97
(1,17)	1:217:A:LEU:N	4:229:B:17F:C9	9	22.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:203:A:LEU:N	4:229:B:17F:C9	7	22.93
(1,21)	1:221:A:LEU:N	4:229:B:17F:O4	6	22.82
(1,22)	1:222:A:GLY:N	4:229:B:17F:O5	6	22.77
(1,12)	1:212:A:SER:N	4:229:B:17F:C2	3	22.74
(1,24)	1:224:A:VAL:N	4:229:B:17F:O4	3	22.69
(1,55)	2:113:B:LEU:N	3:407:A:PCW:N	4	22.67
(1,5)	1:205:A:ASP:N	2:177:B:LYS:HZ3	4	22.64
(1,21)	1:221:A:LEU:N	4:229:B:17F:O8	4	22.63
(1,15)	1:215:A:SER:N	4:229:B:17F:C9	7	22.6
(1,17)	1:217:A:LEU:N	4:229:B:17F:C9	1	22.5
(1,3)	1:203:A:LEU:N	4:229:B:17F:C9	8	22.45
(1,20)	1:220:A:GLN:N	4:229:B:17F:O4	3	22.43
(1,61)	2:160:B:VAL:CG2	3:406:A:PCW:N	8	22.38
(1,15)	1:215:A:SER:N	4:229:B:17F:C9	9	22.37
(1,9)	1:209:A:SER:N	4:229:B:17F:C9	6	22.35
(1,16)	1:216:A:LYS:N	4:229:B:17F:O4	3	22.31
(1,55)	2:113:B:LEU:H	3:407:A:PCW:N	1	22.29
(1,12)	1:212:A:SER:N	4:229:B:17F:C9	6	22.21
(1,15)	1:215:A:SER:N	4:229:B:17F:C4	1	22.15
(1,6)	1:206:A:ASN:N	4:229:B:17F:C9	6	22.15
(1,56)	2:133:B:LEU:O	3:407:A:PCW:N	4	22.1
(1,17)	1:217:A:LEU:N	4:229:B:17F:C9	6	22.09
(1,7)	1:207:A:TRP:N	4:229:B:17F:C9	10	22.07
(1,10)	1:210:A:VAL:N	4:229:B:17F:C9	10	22.06
(1,17)	1:217:A:LEU:N	4:229:B:17F:O8	4	22.04
(1,51)	2:79:B:LEU:H	3:405:A:PCW:N	10	21.89
(1,29)	1:229:A:TRP:N	4:229:B:17F:O4	3	21.86
(1,15)	1:215:A:SER:N	4:229:B:17F:O8	4	21.86
(1,51)	2:79:B:LEU:H	3:406:A:PCW:N	3	21.85
(1,10)	1:210:A:VAL:N	4:229:B:17F:C9	8	21.76
(1,4)	1:204:A:LEU:N	4:229:B:17F:C9	6	21.76
(1,26)	1:226:A:GLN:N	4:229:B:17F:O4	3	21.75
(1,10)	1:210:A:VAL:N	4:229:B:17F:C9	3	21.74
(1,8)	1:208:A:ASP:N	2:177:B:LYS:HZ3	4	21.72
(1,8)	1:208:A:ASP:N	2:178:B:LYS:CB	1	21.66
(1,51)	2:79:B:LEU:O	3:404:A:PCW:N	6	21.64
(1,7)	1:207:A:TRP:N	4:229:B:17F:C9	3	21.63
(1,7)	1:207:A:TRP:N	4:229:B:17F:C9	9	21.62
(1,10)	1:210:A:VAL:N	4:229:B:17F:C9	9	21.58
(1,61)	2:160:B:VAL:O	3:407:A:PCW:N	2	21.57
(1,38)	1:238:A:GLY:N	2:184:B:LYS:H	5	21.55
(1,7)	1:207:A:TRP:N	4:229:B:17F:C9	8	21.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,11)	1:211:A:THR:N	4:229:B:17F:C9	10	21.51
(1,14)	1:214:A:PHE:N	4:229:B:17F:C9	10	21.5
(1,14)	1:214:A:PHE:N	4:229:B:17F:C9	8	21.49
(1,6)	1:206:A:ASN:N	2:178:B:LYS:O	1	21.47
(1,10)	1:210:A:VAL:N	4:229:B:17F:C9	7	21.39
(1,7)	1:207:A:TRP:N	4:229:B:17F:C9	7	21.31
(1,11)	1:211:A:THR:N	4:229:B:17F:C9	8	21.3
(1,8)	1:208:A:ASP:N	4:229:B:17F:C9	6	21.27
(1,15)	1:215:A:SER:N	4:229:B:17F:O4	6	21.25
(1,10)	1:210:A:VAL:N	4:229:B:17F:C9	1	21.24
(1,11)	1:211:A:THR:N	4:229:B:17F:C9	9	21.21
(1,11)	1:211:A:THR:N	4:229:B:17F:C9	7	21.2
(1,14)	1:214:A:PHE:N	4:229:B:17F:C9	7	21.12
(1,15)	1:215:A:SER:N	2:184:B:LYS:H	2	21.1
(1,3)	1:203:A:LEU:N	4:229:B:17F:C9	6	21.06
(1,57)	2:138:B:GLY:O	3:405:A:PCW:N	5	21.05
(1,51)	2:79:B:LEU:H	3:407:A:PCW:N	5	21.02
(1,14)	1:214:A:PHE:N	4:229:B:17F:C9	9	21.01
(1,17)	1:217:A:LEU:N	4:229:B:17F:O4	3	21.0
(1,3)	1:203:A:LEU:N	2:177:B:LYS:HZ3	4	20.99
(1,56)	2:133:B:LEU:O	3:407:A:PCW:N	1	20.96
(1,11)	1:211:A:THR:N	4:229:B:17F:C9	1	20.94
(1,61)	2:160:B:VAL:O	3:407:A:PCW:N	4	20.93
(1,10)	1:210:A:VAL:N	4:229:B:17F:O8	4	20.89
(1,7)	1:207:A:TRP:N	2:177:B:LYS:HZ3	4	20.85
(1,11)	1:211:A:THR:N	4:229:B:17F:C2	3	20.75
(1,58)	2:139:B:ILE:CG2	3:405:A:PCW:N	9	20.73
(1,5)	1:205:A:ASP:N	2:178:B:LYS:O	1	20.64
(1,14)	1:214:A:PHE:N	4:229:B:17F:C9	1	20.62
(1,11)	1:211:A:THR:N	4:229:B:17F:O8	4	20.59
(1,64)	2:176:B:LYS:O	3:402:A:PCW:N	10	20.57
(1,22)	1:222:A:GLY:N	4:229:B:17F:O4	3	20.56
(1,21)	1:221:A:LEU:N	4:229:B:17F:O4	3	20.52
(1,25)	1:225:A:THR:N	4:229:B:17F:O4	3	20.46
(1,14)	1:214:A:PHE:N	4:229:B:17F:O8	4	20.46
(1,61)	2:160:B:VAL:O	3:402:A:PCW:N	6	20.31
(1,54)	2:109:B:VAL:CG2	3:405:A:PCW:N	8	20.3
(1,54)	2:109:B:VAL:CG2	3:402:A:PCW:N	7	20.29
(1,15)	1:215:A:SER:N	4:229:B:17F:O4	3	20.29
(1,66)	2:185:B:CYS:SG	3:407:A:PCW:N	3	20.25
(1,4)	1:204:A:LEU:N	2:177:B:LYS:HZ3	4	20.24
(1,10)	1:210:A:VAL:N	4:229:B:17F:C9	6	20.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:207:A:TRP:N	2:178:B:LYS:CB	1	20.23
(1,57)	2:138:B:GLY:O	3:407:A:PCW:N	2	20.17
(1,14)	1:214:A:PHE:N	4:229:B:17F:C9	6	20.13
(1,58)	2:139:B:ILE:CG2	3:407:A:PCW:N	2	20.09
(1,58)	2:139:B:ILE:CG2	3:407:A:PCW:N	3	20.05
(1,14)	1:214:A:PHE:N	4:229:B:17F:O4	3	20.0
(1,51)	2:79:B:LEU:N	3:407:A:PCW:N	1	19.95
(1,46)	2:48:B:GLY:C	3:402:A:PCW:N	9	19.86
(1,7)	1:207:A:TRP:N	4:229:B:17F:C9	6	19.84
(1,11)	1:211:A:THR:N	4:229:B:17F:C9	6	19.73
(1,63)	2:174:B:GLY:O	3:402:A:PCW:N	10	19.72
(1,54)	2:109:B:VAL:CG2	3:402:A:PCW:N	10	19.7
(1,51)	2:79:B:LEU:H	3:406:A:PCW:N	4	19.69
(1,57)	2:138:B:GLY:O	3:402:A:PCW:N	9	19.6
(1,46)	2:48:B:GLY:O	3:406:A:PCW:N	6	19.6
(1,14)	1:214:A:PHE:N	2:184:B:LYS:H	2	19.57
(1,45)	2:46:B:ILE:N	3:406:A:PCW:N	6	19.5
(1,50)	2:75:B:GLY:O	3:405:A:PCW:N	9	19.46
(1,51)	2:79:B:LEU:CD1	3:407:A:PCW:N	8	19.41
(1,49)	2:55:B:ILE:H	3:402:A:PCW:N	1	19.35
(1,51)	2:79:B:LEU:CD1	3:404:A:PCW:N	7	19.21
(1,61)	2:160:B:VAL:O	3:402:A:PCW:N	5	19.18
(1,40)	2:2:B:THR:HG1	3:402:A:PCW:N	8	19.15
(1,37)	1:237:A:GLU:N	2:184:B:LYS:H	5	19.02
(1,45)	2:46:B:ILE:O	3:402:A:PCW:N	9	18.93
(1,57)	2:138:B:GLY:O	3:407:A:PCW:N	4	18.8
(1,65)	2:177:B:LYS:CE	3:402:A:PCW:N	10	18.78
(1,61)	2:160:B:VAL:CG1	3:407:A:PCW:N	10	18.77
(1,57)	2:138:B:GLY:O	3:407:A:PCW:N	3	18.25
(1,47)	2:49:B:GLU:OE1	3:402:A:PCW:N	6	18.17
(1,12)	1:212:A:SER:N	2:184:B:LYS:H	2	18.17
(1,49)	2:55:B:ILE:H	3:402:A:PCW:N	3	18.04
(1,35)	1:235:A:GLU:N	2:184:B:LYS:CG	5	18.03
(1,58)	2:139:B:ILE:CG2	3:407:A:PCW:N	4	17.97
(1,54)	2:109:B:VAL:CG2	3:404:A:PCW:N	5	17.97
(1,49)	2:55:B:ILE:H	3:406:A:PCW:N	9	17.89
(1,4)	1:204:A:LEU:N	2:178:B:LYS:O	1	17.77
(1,61)	2:160:B:VAL:CG1	3:405:A:PCW:N	1	17.76
(1,44)	2:45:B:VAL:CG1	3:402:A:PCW:N	5	17.69
(1,44)	2:45:B:VAL:CG2	3:406:A:PCW:N	9	17.52
(1,3)	1:203:A:LEU:N	2:184:B:LYS:HZ2	5	17.47
(1,36)	1:236:A:THR:N	2:184:B:LYS:H	5	17.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,64)	2:176:B:LYS:O	3:402:A:PCW:N	7	17.44
(1,61)	2:160:B:VAL:O	3:407:A:PCW:N	3	17.44
(1,39)	2:1:B:MET:O	3:402:A:PCW:N	6	17.4
(1,3)	1:203:A:LEU:N	2:178:B:LYS:O	1	17.28
(1,58)	2:139:B:ILE:CG2	3:407:A:PCW:N	1	17.21
(1,34)	1:234:A:LYS:N	2:184:B:LYS:CG	5	17.19
(1,51)	2:79:B:LEU:H	3:406:A:PCW:N	2	17.12
(1,57)	2:138:B:GLY:O	3:407:A:PCW:N	1	16.97
(1,5)	1:205:A:ASP:N	2:184:B:LYS:HZ2	5	16.68
(1,50)	2:75:B:GLY:H	3:404:A:PCW:N	8	16.67
(1,50)	2:75:B:GLY:H	3:402:A:PCW:N	10	16.62
(1,66)	2:185:B:CYS:HG	3:403:A:PCW:N	1	16.47
(1,47)	2:49:B:GLU:C	3:406:A:PCW:N	8	16.43
(1,45)	2:46:B:ILE:O	3:402:A:PCW:N	5	16.29
(1,45)	2:46:B:ILE:H	3:402:A:PCW:N	4	16.28
(1,45)	2:46:B:ILE:N	3:406:A:PCW:N	8	16.26
(1,40)	2:2:B:THR:H	3:402:A:PCW:N	2	16.25
(1,4)	1:204:A:LEU:N	2:184:B:LYS:HZ2	5	16.19
(1,66)	2:185:B:CYS:H	3:402:A:PCW:N	6	16.18
(1,40)	2:2:B:THR:CG2	3:402:A:PCW:N	6	16.14
(1,50)	2:75:B:GLY:H	3:405:A:PCW:N	7	16.09
(1,45)	2:46:B:ILE:H	3:402:A:PCW:N	2	16.09
(1,40)	2:2:B:THR:H	3:402:A:PCW:N	4	16.01
(1,61)	2:160:B:VAL:O	3:402:A:PCW:N	9	15.9
(1,50)	2:75:B:GLY:H	3:405:A:PCW:N	6	15.89
(1,48)	2:50:B:THR:HG1	3:406:A:PCW:N	6	15.87
(1,48)	2:50:B:THR:HG1	3:406:A:PCW:N	9	15.8
(1,66)	2:185:B:CYS:CB	3:402:A:PCW:N	7	15.79
(1,11)	1:211:A:THR:N	2:184:B:LYS:H	2	15.64
(1,9)	1:209:A:SER:N	2:184:B:LYS:H	2	15.62
(1,46)	2:48:B:GLY:O	3:406:A:PCW:N	8	15.57
(1,6)	1:206:A:ASN:N	2:184:B:LYS:HZ2	5	15.57
(1,39)	2:1:B:MET:SD	3:406:A:PCW:N	8	15.52
(1,54)	2:109:B:VAL:N	3:407:A:PCW:N	3	15.51
(1,53)	2:106:B:SER:N	3:402:A:PCW:N	7	15.48
(1,10)	1:210:A:VAL:N	2:184:B:LYS:H	2	15.48
(1,53)	2:106:B:SER:HG	3:405:A:PCW:N	8	15.38
(1,49)	2:55:B:ILE:H	3:406:A:PCW:N	5	15.31
(1,40)	2:2:B:THR:HG1	3:404:A:PCW:N	3	15.21
(1,53)	2:106:B:SER:HG	3:402:A:PCW:N	10	15.17
(1,49)	2:55:B:ILE:O	3:405:A:PCW:N	10	15.17
(1,50)	2:75:B:GLY:H	3:407:A:PCW:N	5	15.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,62)	2:171:B:SER:CB	3:406:A:PCW:N	10	15.03
(1,40)	2:2:B:THR:H	3:407:A:PCW:N	10	14.97
(1,63)	2:174:B:GLY:H	3:406:A:PCW:N	7	14.84
(1,54)	2:109:B:VAL:CG2	3:405:A:PCW:N	6	14.83
(1,39)	2:1:B:MET:CB	3:402:A:PCW:N	4	14.83
(1,44)	2:45:B:VAL:CG2	3:406:A:PCW:N	6	14.82
(1,54)	2:109:B:VAL:CG2	3:405:A:PCW:N	9	14.81
(1,43)	2:43:B:GLN:H	3:406:A:PCW:N	5	14.8
(1,40)	2:2:B:THR:CG2	3:402:A:PCW:N	9	14.73
(1,31)	1:231:A:ASN:N	2:184:B:LYS:CG	5	14.61
(1,33)	1:233:A:GLU:N	2:184:B:LYS:CG	5	14.52
(1,47)	2:49:B:GLU:C	3:402:A:PCW:N	4	14.45
(1,39)	2:1:B:MET:N	3:402:A:PCW:N	5	14.44
(1,47)	2:49:B:GLU:C	3:402:A:PCW:N	2	14.34
(1,48)	2:50:B:THR:H	3:402:A:PCW:N	5	14.31
(1,45)	2:46:B:ILE:O	3:404:A:PCW:N	3	14.31
(1,49)	2:55:B:ILE:O	3:407:A:PCW:N	6	14.27
(1,46)	2:48:B:GLY:O	3:402:A:PCW:N	5	14.23
(1,50)	2:75:B:GLY:H	3:406:A:PCW:N	3	13.97
(1,32)	1:232:A:LEU:N	2:184:B:LYS:CG	5	13.97
(1,47)	2:49:B:GLU:OE1	3:402:A:PCW:N	9	13.83
(1,40)	2:2:B:THR:HG1	3:402:A:PCW:N	5	13.79
(1,61)	2:160:B:VAL:CG1	3:407:A:PCW:N	7	13.62
(1,39)	2:1:B:MET:H	3:402:A:PCW:N	2	13.41
(1,62)	2:171:B:SER:O	3:402:A:PCW:N	8	13.37
(1,50)	2:75:B:GLY:O	3:407:A:PCW:N	1	13.36
(1,8)	1:208:A:ASP:N	2:184:B:LYS:H	2	13.35
(1,39)	2:1:B:MET:CE	3:406:A:PCW:N	9	13.32
(1,50)	2:75:B:GLY:O	3:407:A:PCW:N	4	13.27
(1,43)	2:43:B:GLN:OE1	3:406:A:PCW:N	6	13.27
(1,46)	2:48:B:GLY:O	3:402:A:PCW:N	4	13.17
(1,46)	2:48:B:GLY:O	3:402:A:PCW:N	2	13.12
(1,40)	2:2:B:THR:H	3:405:A:PCW:N	1	13.1
(1,53)	2:106:B:SER:N	3:404:A:PCW:N	5	13.02
(1,44)	2:45:B:VAL:CG2	3:402:A:PCW:N	4	12.92
(1,9)	1:209:A:SER:N	2:184:B:LYS:HZ2	5	12.89
(1,49)	2:55:B:ILE:O	3:406:A:PCW:N	4	12.82
(1,48)	2:50:B:THR:HG1	3:406:A:PCW:N	8	12.8
(1,7)	1:207:A:TRP:N	2:184:B:LYS:HZ2	5	12.8
(1,66)	2:185:B:CYS:HG	3:402:A:PCW:N	9	12.63
(1,45)	2:46:B:ILE:O	3:405:A:PCW:N	1	12.5
(1,54)	2:109:B:VAL:CG2	3:407:A:PCW:N	2	12.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,65)	2:177:B:LYS:H	3:405:A:PCW:N	9	12.46
(1,39)	2:1:B:MET:CG	3:407:A:PCW:N	10	12.41
(1,45)	2:46:B:ILE:H	3:407:A:PCW:N	10	12.39
(1,8)	1:208:A:ASP:N	2:184:B:LYS:HZ2	5	12.37
(1,6)	1:206:A:ASN:N	2:184:B:LYS:H	2	12.31
(1,65)	2:177:B:LYS:HZ3	3:402:A:PCW:N	7	12.3
(1,63)	2:174:B:GLY:O	3:402:A:PCW:N	8	12.25
(1,53)	2:106:B:SER:HG	3:406:A:PCW:N	3	12.02
(1,39)	2:1:B:MET:CE	3:405:A:PCW:N	3	12.02
(1,2)	3:403:A:PCW:N	4:229:B:17F:C9	10	11.93
(1,18)	3:405:A:PCW:N	4:229:B:17F:O4	4	11.85
(1,44)	2:45:B:VAL:CG2	3:406:A:PCW:N	8	11.76
(1,1)	3:402:A:PCW:N	4:227:B:17F:C9	3	11.76
(1,44)	2:45:B:VAL:CG2	3:402:A:PCW:N	2	11.73
(1,66)	2:185:B:CYS:HG	1:201:A:LEU:N	2	11.7
(1,43)	2:43:B:GLN:HE22	3:402:A:PCW:N	2	11.69
(1,39)	2:1:B:MET:CE	3:402:A:PCW:N	1	11.62
(1,5)	1:205:A:ASP:N	2:184:B:LYS:H	2	11.6
(1,7)	1:207:A:TRP:N	2:184:B:LYS:H	2	11.48
(1,48)	2:50:B:THR:CG2	3:402:A:PCW:N	4	11.33
(1,52)	2:105:B:ASP:OD1	3:402:A:PCW:N	10	11.32
(1,1)	3:402:A:PCW:N	2:105:B:ASP:OD1	10	11.32
(1,47)	2:49:B:GLU:OE1	3:402:A:PCW:N	5	11.27
(1,1)	3:402:A:PCW:N	2:49:B:GLU:OE1	5	11.27
(1,49)	2:55:B:ILE:O	3:407:A:PCW:N	8	11.23
(1,43)	2:43:B:GLN:HE22	3:406:A:PCW:N	8	11.21
(1,43)	2:43:B:GLN:HE22	3:402:A:PCW:N	4	11.2
(1,1)	3:402:A:PCW:N	2:43:B:GLN:HE22	4	11.2
(1,28)	1:228:A:PHE:N	2:184:B:LYS:CG	5	11.15
(1,52)	2:105:B:ASP:OD1	3:405:A:PCW:N	8	11.14
(1,27)	1:227:A:GLU:N	2:184:B:LYS:CG	5	11.14
(1,47)	2:49:B:GLU:C	3:407:A:PCW:N	10	11.09
(1,44)	2:45:B:VAL:CG1	3:405:A:PCW:N	1	11.08
(1,47)	2:49:B:GLU:CG	3:404:A:PCW:N	3	10.93
(1,49)	2:55:B:ILE:O	3:406:A:PCW:N	2	10.88
(1,44)	2:45:B:VAL:CG2	3:405:A:PCW:N	3	10.87
(1,10)	1:210:A:VAL:N	2:184:B:LYS:HZ2	5	10.84
(1,43)	2:43:B:GLN:HE22	3:406:A:PCW:N	9	10.82
(1,46)	2:48:B:GLY:O	3:404:A:PCW:N	3	10.81
(1,2)	3:403:A:PCW:N	4:225:B:17F:O4	9	10.74
(1,62)	2:171:B:SER:O	3:406:A:PCW:N	7	10.73
(1,52)	2:105:B:ASP:OD2	3:402:A:PCW:N	7	10.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	3:402:A:PCW:N	2:105:B:ASP:OD2	7	10.59
(1,48)	2:50:B:THR:HG1	3:402:A:PCW:N	2	10.56
(1,50)	2:75:B:GLY:H	3:406:A:PCW:N	2	10.5
(1,48)	2:50:B:THR:CG2	3:405:A:PCW:N	3	10.39
(1,29)	1:229:A:TRP:N	2:184:B:LYS:CG	5	10.39
(1,43)	2:43:B:GLN:OE1	3:405:A:PCW:N	3	10.36
(1,53)	2:106:B:SER:HG	3:405:A:PCW:N	6	10.2
(1,46)	2:48:B:GLY:O	3:407:A:PCW:N	10	10.07
(1,54)	2:109:B:VAL:CG2	3:407:A:PCW:N	4	9.92
(1,53)	2:106:B:SER:N	3:405:A:PCW:N	9	9.87
(1,18)	3:405:A:PCW:N	4:229:B:17F:O4	2	9.75
(1,54)	2:109:B:VAL:CG2	3:407:A:PCW:N	1	9.66
(1,43)	2:43:B:GLN:OE1	3:402:A:PCW:N	1	9.63
(1,1)	3:402:A:PCW:N	4:227:B:17F:C9	1	9.57
(1,18)	3:405:A:PCW:N	4:229:B:17F:O4	8	9.54
(1,12)	1:212:A:SER:N	2:184:B:LYS:HZ2	5	9.51
(1,52)	2:105:B:ASP:OD1	3:404:A:PCW:N	5	9.42
(1,64)	2:176:B:LYS:CE	3:405:A:PCW:N	9	9.4
(1,18)	3:405:A:PCW:N	4:229:B:17F:O4	3	9.38
(1,48)	2:50:B:THR:H	3:405:A:PCW:N	1	9.34
(1,49)	2:55:B:ILE:O	3:404:A:PCW:N	7	9.14
(1,63)	2:174:B:GLY:O	3:402:A:PCW:N	6	9.11
(1,24)	1:224:A:VAL:N	2:184:B:LYS:CD	5	9.07
(1,47)	2:49:B:GLU:CG	3:405:A:PCW:N	1	8.87
(1,62)	2:171:B:SER:O	3:405:A:PCW:N	5	8.79
(1,4)	1:204:A:LEU:N	2:184:B:LYS:H	2	8.77
(1,53)	2:106:B:SER:N	3:407:A:PCW:N	2	8.68
(1,11)	1:211:A:THR:N	2:184:B:LYS:HZ2	5	8.67
(1,23)	1:223:A:PRO:N	2:184:B:LYS:CG	5	8.54
(1,66)	2:185:B:CYS:CB	3:402:A:PCW:N	8	8.47
(1,26)	1:226:A:GLN:N	2:184:B:LYS:CG	5	8.44
(1,41)	3:202:B:PCW:C4	3:407:A:PCW:N	3	8.27
(1,62)	2:171:B:SER:O	3:403:A:PCW:N	2	8.24
(1,46)	2:48:B:GLY:O	3:405:A:PCW:N	1	8.16
(1,18)	3:405:A:PCW:N	2:48:B:GLY:O	1	8.16
(1,41)	3:202:B:PCW:C8	3:407:A:PCW:N	1	8.07
(1,16)	1:216:A:LYS:N	2:184:B:LYS:HZ3	5	8.07
(1,41)	3:202:B:PCW:C8	3:407:A:PCW:N	6	8.01
(1,65)	2:177:B:LYS:O	3:402:A:PCW:N	6	8.0
(1,41)	3:202:B:PCW:C8	3:407:A:PCW:N	2	8.0
(1,20)	1:220:A:GLN:N	2:184:B:LYS:HZ3	5	7.99
(1,44)	2:45:B:VAL:CG2	3:407:A:PCW:N	10	7.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	2:50:B:THR:CG2	3:407:A:PCW:N	10	7.82
(1,62)	2:171:B:SER:O	3:402:A:PCW:N	6	7.81
(1,62)	2:171:B:SER:O	3:403:A:PCW:N	4	7.71
(1,52)	2:105:B:ASP:OD1	3:406:A:PCW:N	3	7.71
(1,41)	3:202:B:PCW:C8	3:407:A:PCW:N	9	7.69
(1,41)	3:202:B:PCW:C6	3:407:A:PCW:N	4	7.62
(1,3)	1:203:A:LEU:N	2:184:B:LYS:H	2	7.56
(1,63)	2:174:B:GLY:N	3:402:A:PCW:N	9	7.49
(1,1)	1:201:A:LEU:N	2:184:B:LYS:O	2	7.49
(1,40)	2:2:B:THR:H	3:407:A:PCW:N	7	7.45
(1,45)	2:46:B:ILE:H	3:407:A:PCW:N	7	7.39
(1,25)	1:225:A:THR:N	2:184:B:LYS:CG	5	7.37
(1,41)	3:202:B:PCW:C5	3:407:A:PCW:N	8	7.32
(1,43)	2:43:B:GLN:HE22	3:407:A:PCW:N	10	7.02
(1,17)	1:217:A:LEU:N	2:184:B:LYS:HZ3	5	6.87
(1,14)	1:214:A:PHE:N	2:184:B:LYS:HZ2	5	6.82
(1,41)	3:202:B:PCW:C5	3:407:A:PCW:N	7	6.72
(1,52)	2:105:B:ASP:OD2	3:405:A:PCW:N	9	6.71
(1,18)	3:405:A:PCW:N	2:105:B:ASP:OD2	9	6.71
(1,65)	2:177:B:LYS:H	3:407:A:PCW:N	3	6.55
(1,2)	3:403:A:PCW:N	4:225:B:17F:O5	5	6.39
(1,63)	2:174:B:GLY:N	3:403:A:PCW:N	4	6.34
(1,21)	1:221:A:LEU:N	2:184:B:LYS:HZ3	5	6.34
(1,64)	2:176:B:LYS:O	3:402:A:PCW:N	8	6.32
(1,15)	1:215:A:SER:N	2:184:B:LYS:HZ2	5	6.22
(1,41)	3:202:B:PCW:C8	3:407:A:PCW:N	10	6.18
(1,22)	1:222:A:GLY:N	2:184:B:LYS:CD	5	6.06
(1,41)	3:202:B:PCW:C8	3:407:A:PCW:N	5	5.97
(1,18)	3:405:A:PCW:N	2:37:B:GLU:OE1	7	5.93
(1,13)	3:404:A:PCW:N	4:229:B:17F:C6	10	5.81
(1,2)	3:403:A:PCW:N	2:36:B:ILE:CG2	8	5.74
(1,66)	2:185:B:CYS:HG	3:404:A:PCW:N	5	5.61
(1,18)	3:405:A:PCW:N	2:36:B:ILE:CD1	10	5.6
(1,64)	2:176:B:LYS:N	3:407:A:PCW:N	3	5.53
(1,47)	2:49:B:GLU:C	3:407:A:PCW:N	7	5.49
(1,63)	2:174:B:GLY:CA	3:405:A:PCW:N	5	5.35
(1,39)	2:1:B:MET:CE	3:407:A:PCW:N	7	5.28
(1,53)	2:106:B:SER:N	3:407:A:PCW:N	4	5.27
(1,52)	2:105:B:ASP:OD1	3:405:A:PCW:N	6	4.95
(1,18)	3:405:A:PCW:N	2:105:B:ASP:OD1	6	4.95
(1,52)	2:105:B:ASP:OD1	3:407:A:PCW:N	2	4.68
(1,2)	3:403:A:PCW:N	2:36:B:ILE:CD1	6	4.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	2:106:B:SER:HG	3:407:A:PCW:N	1	4.57
(1,64)	2:176:B:LYS:CE	3:402:A:PCW:N	6	4.54
(1,46)	2:48:B:GLY:O	3:407:A:PCW:N	7	4.33
(1,62)	2:171:B:SER:O	3:403:A:PCW:N	1	3.78
(1,13)	3:404:A:PCW:N	4:229:B:17F:O2	8	3.76
(1,64)	2:176:B:LYS:CG	3:405:A:PCW:N	5	3.7
(1,13)	3:404:A:PCW:N	4:229:B:17F:O4	9	3.67
(1,44)	2:45:B:VAL:CG2	3:407:A:PCW:N	7	3.66
(1,43)	2:43:B:GLN:HE22	3:403:A:PCW:N	7	3.63
(1,2)	3:403:A:PCW:N	2:43:B:GLN:HE22	7	3.63
(1,65)	2:177:B:LYS:N	3:403:A:PCW:N	4	3.44
(1,2)	3:403:A:PCW:N	2:172:B:LYS:HZ1	3	3.24
(1,13)	3:404:A:PCW:N	4:229:B:17F:O2	4	3.16
(1,65)	2:177:B:LYS:H	3:405:A:PCW:N	5	3.14
(1,18)	3:405:A:PCW:N	2:177:B:LYS:H	5	3.14
(1,13)	3:404:A:PCW:N	4:229:B:17F:O2	1	3.13
(1,1)	3:402:A:PCW:N	2:178:B:LYS:HZ1	6	3.12
(1,48)	2:50:B:THR:CG2	3:407:A:PCW:N	7	3.06
(1,63)	2:174:B:GLY:N	3:403:A:PCW:N	1	3.0
(1,19)	3:406:A:PCW:N	4:226:B:17F:C1	10	2.81
(1,42)	4:226:B:17F:C1	3:406:A:PCW:N	6	2.69
(1,19)	3:406:A:PCW:N	4:226:B:17F:C1	6	2.69
(1,13)	3:404:A:PCW:N	2:185:B:CYS:HG	5	2.61
(1,19)	3:406:A:PCW:N	4:226:B:17F:C1	9	2.33
(1,42)	4:226:B:17F:C2	3:406:A:PCW:N	1	2.22
(1,19)	3:406:A:PCW:N	4:226:B:17F:C2	1	2.22
(1,19)	3:406:A:PCW:N	4:226:B:17F:O1	8	2.18
(1,19)	3:406:A:PCW:N	4:226:B:17F:C1	5	2.13
(1,19)	3:406:A:PCW:N	4:226:B:17F:N1	7	2.12
(1,63)	2:174:B:GLY:C	3:403:A:PCW:N	2	1.87
(1,19)	3:406:A:PCW:N	4:226:B:17F:C2	3	1.85
(1,52)	2:105:B:ASP:OD1	3:407:A:PCW:N	1	1.78
(1,30)	3:407:A:PCW:N	2:105:B:ASP:OD1	1	1.78
(1,64)	2:176:B:LYS:O	3:403:A:PCW:N	4	1.43
(1,2)	3:403:A:PCW:N	2:176:B:LYS:O	4	1.43
(1,52)	2:105:B:ASP:OD2	3:407:A:PCW:N	4	1.24
(1,13)	3:404:A:PCW:N	4:229:B:17F:O2	2	1.18
(1,19)	3:406:A:PCW:N	4:226:B:17F:O4	4	1.04
(1,65)	2:177:B:LYS:CE	3:402:A:PCW:N	8	1.03
(1,1)	3:402:A:PCW:N	2:177:B:LYS:CE	8	1.03
(1,62)	2:171:B:SER:O	3:407:A:PCW:N	3	0.95
(1,62)	2:171:B:SER:O	3:402:A:PCW:N	9	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	3:402:A:PCW:N	2:171:B:SER:O	9	0.95
(1,42)	4:228:B:17F:O5	3:407:A:PCW:N	3	0.73
(1,13)	3:404:A:PCW:N	4:229:B:17F:O2	7	0.68
(1,64)	2:176:B:LYS:CB	3:403:A:PCW:N	2	0.55
(1,19)	3:406:A:PCW:N	2:37:B:GLU:OE1	2	0.35
(1,63)	2:174:B:GLY:H	3:407:A:PCW:N	3	0.27
(1,30)	3:407:A:PCW:N	4:225:B:17F:O2	6	0.25

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found