



Full wwPDB NMR Structure Validation Report ⓘ

Mar 27, 2026 – 08:35 AM UTC

PDB ID : 6PTW / pdb_00006ptw
BMRB ID : 30640
Title : NMR data-driven model of KRas-GMPPNP:RBD-CRD complex tethered to a nanodisc (state B)
Authors : Fang, Z.; Lee, K.; Gasmi-Seabrook, G.; Ikura, M.; Marshall, C.B.
Deposited on : 2019-07-16

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

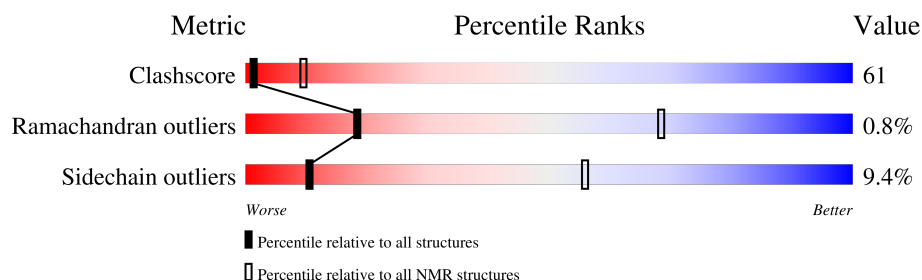
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 6%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	198	80% 12% 8%
1	C	198	83% 16% .
2	B	185	78% 16% 5%
3	D	132	79% 18% .

2 Ensemble composition and analysis

This entry contains 10 models. Model 2 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:205-A:387, C:400-C:596 (380)	0.35	2
2	B:1-B:175, D:356-D:487 (307)	1.90	8

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11566 atoms, of which 1424 are hydrogens and 0 are deuteriums.

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

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

- Molecule 2 is a protein called GTPase KRas.

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

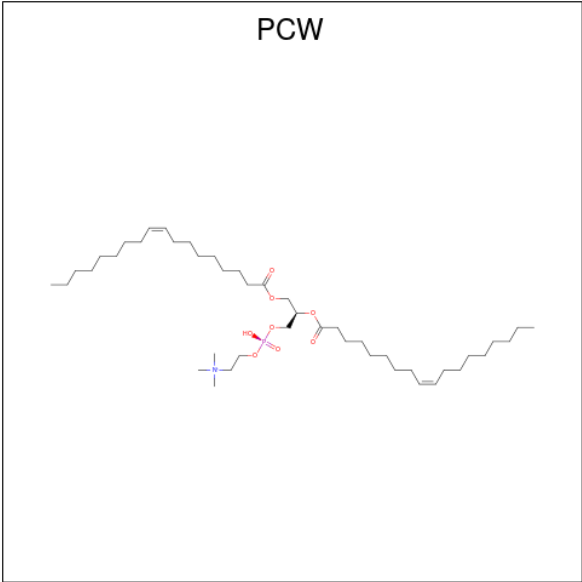
- Molecule 3 is a protein called RAF proto-oncogene serine/threonine-protein kinase.

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

There is a discrepancy between the modelled and reference sequences:

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

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



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

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

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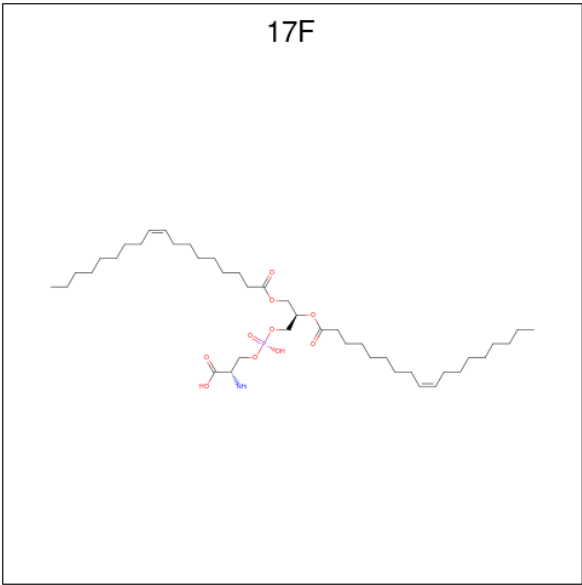
Mol	Chain	Residues	Atoms				
4	C	1	Total	C	N	O	P
			54	44	1	8	1
4	C	1	Total	C	N	O	P
			54	44	1	8	1
4	C	1	Total	C	N	O	P
			54	44	1	8	1
4	C	1	Total	C	N	O	P
			54	44	1	8	1
4	B	1	Total	C	N	O	P
			54	44	1	8	1
4	B	1	Total	C	N	O	P
			54	44	1	8	1
4	B	1	Total	C	N	O	P
			54	44	1	8	1
4	B	1	Total	C	N	O	P
			54	44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

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

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



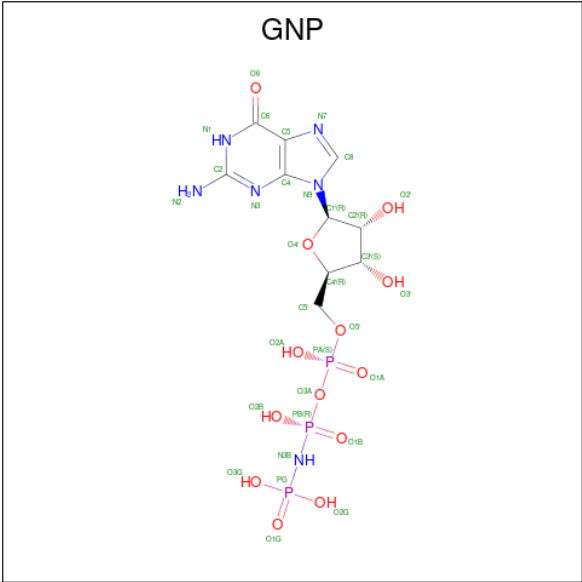
Mol	Chain	Residues	Atoms					
5	A	1	Total	C	H	N	O	P
			57	42	3	1	10	1
5	C	1	Total	C	H	N	O	P
			57	42	3	1	10	1
5	C	1	Total	C	H	N	O	P
			57	42	3	1	10	1

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

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



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

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

Mol	Chain	Residues	Atoms	
7	B	1	Total	Mg
			1	1

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

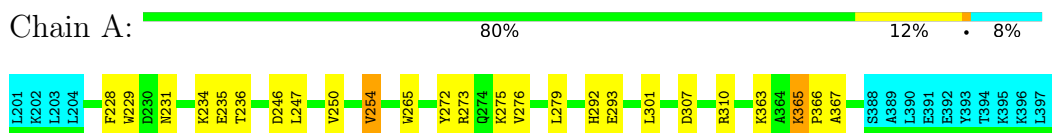
Mol	Chain	Residues	Atoms	
8	D	2	Total	Zn
			2	2

4 Residue-property plots

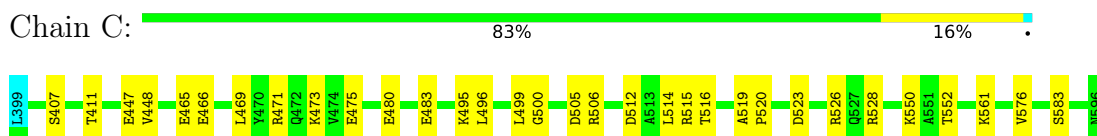
4.1 Average score per residue in the NMR ensemble

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

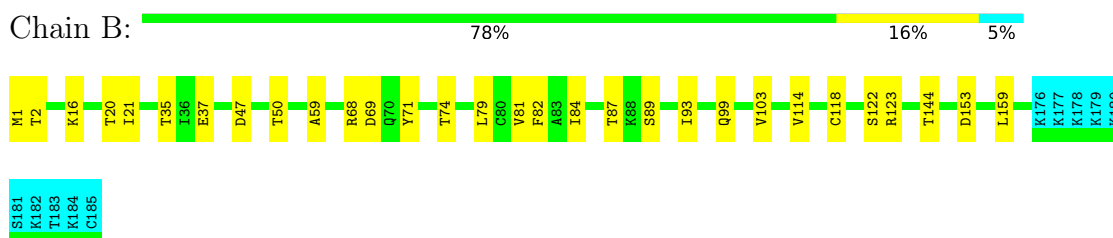
- Molecule 1: Apolipoprotein A-I



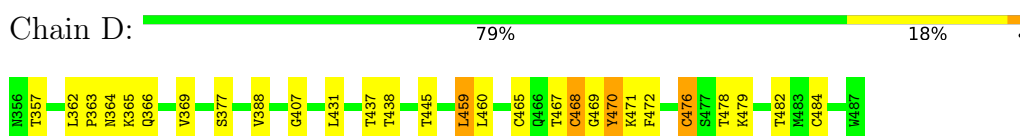
- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas



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

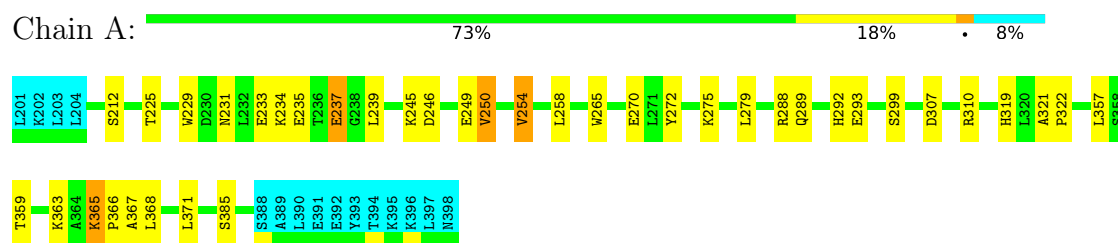


4.2 Scores per residue for each member of the ensemble

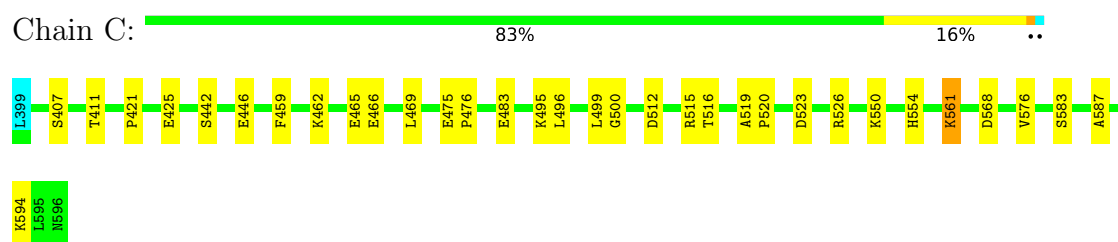
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

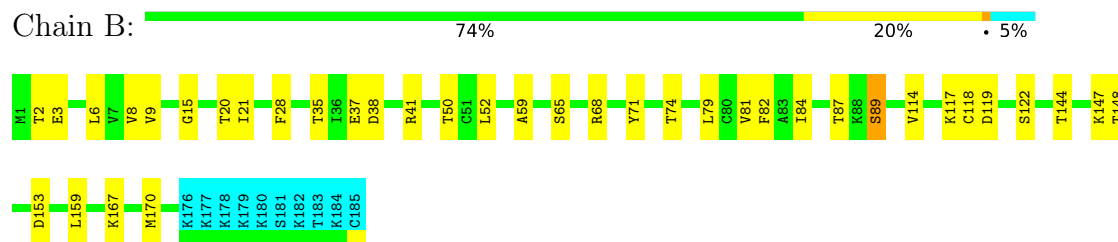
• Molecule 1: Apolipoprotein A-I



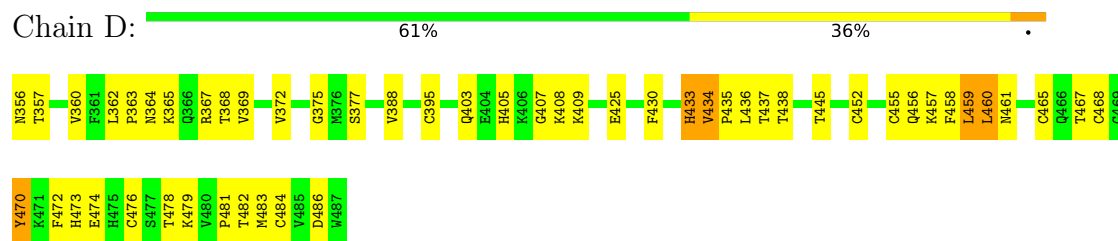
• Molecule 1: Apolipoprotein A-I



• Molecule 2: GTPase KRas

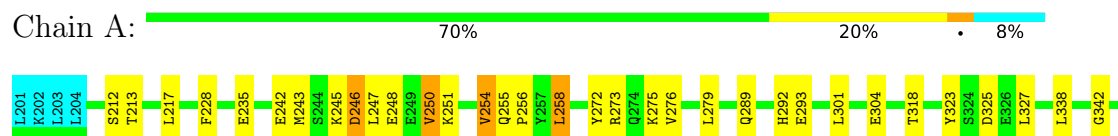


• Molecule 3: RAF proto-oncogene serine/threonine-protein kinase



4.2.2 Score per residue for model 2 (medoid)

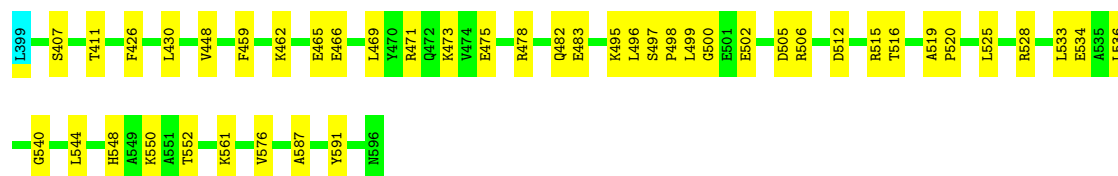
• Molecule 1: Apolipoprotein A-I





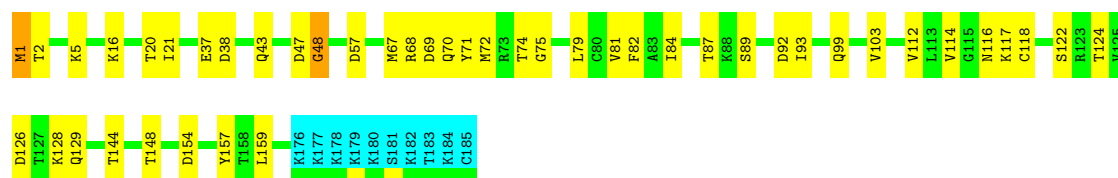
• Molecule 1: Apolipoprotein A-I

Chain C: 77% 22%



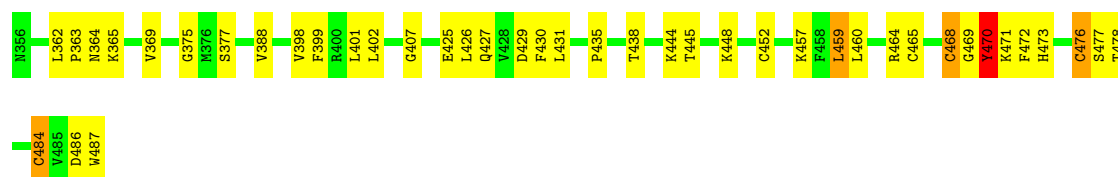
• Molecule 2: GTPase KRas

Chain B: 70% 23% 5%



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

Chain D: 68% 28%



4.2.3 Score per residue for model 3

• Molecule 1: Apolipoprotein A-I

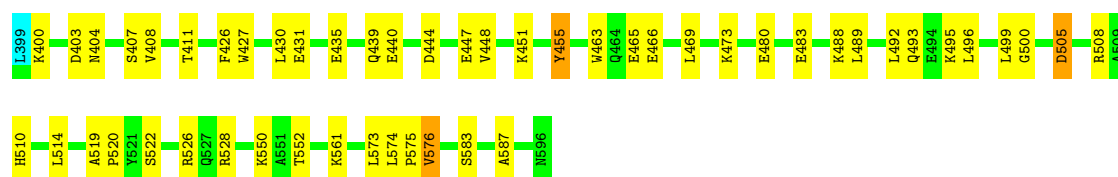
Chain A: 70% 21% 8%



• Molecule 1: Apolipoprotein A-I

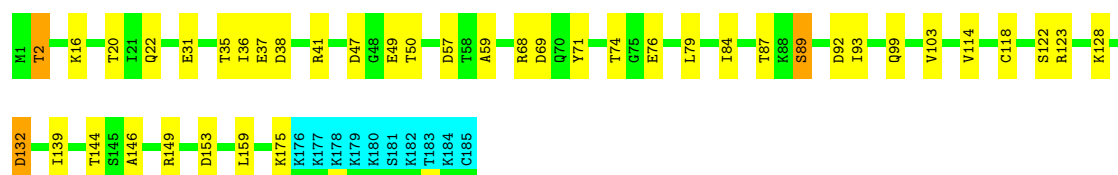
Chain C: 74% 24%





- Molecule 2: GTPase KRas

Chain B: 72% 21% 5%



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

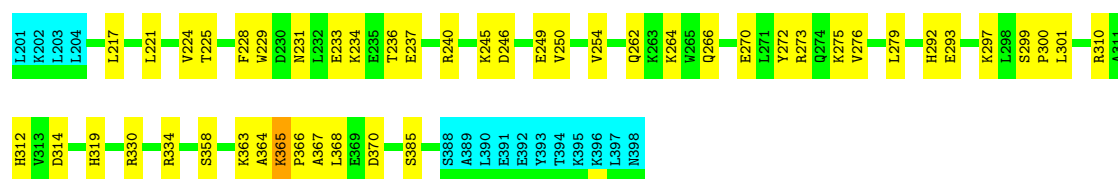
Chain D: 73% 23% 5%



4.2.4 Score per residue for model 4

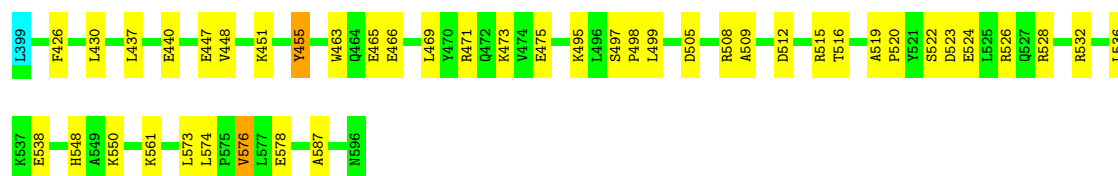
- Molecule 1: Apolipoprotein A-I

Chain A: 69% 23% 8%



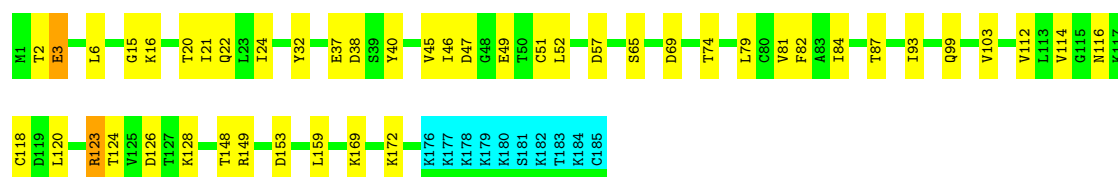
- Molecule 1: Apolipoprotein A-I

Chain C: 78% 21% 2%



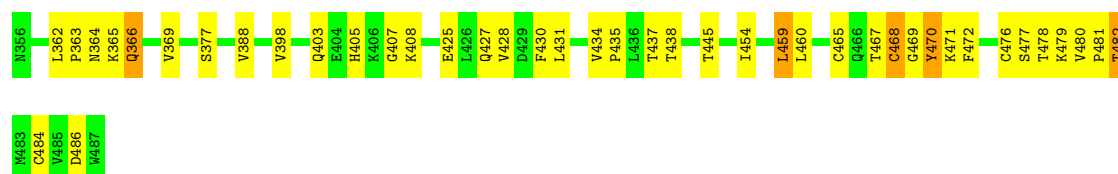
- Molecule 2: GTPase KRas

Chain B: 70% 24% 5%



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

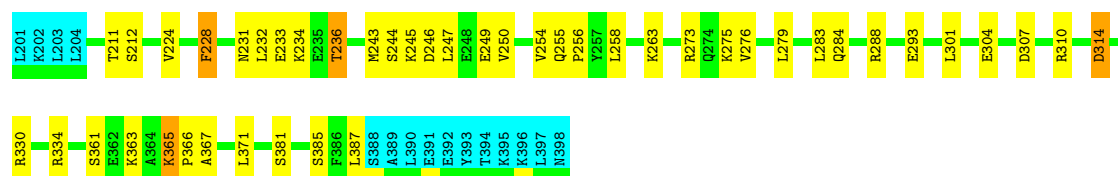
Chain D: 68% 28%



4.2.5 Score per residue for model 5

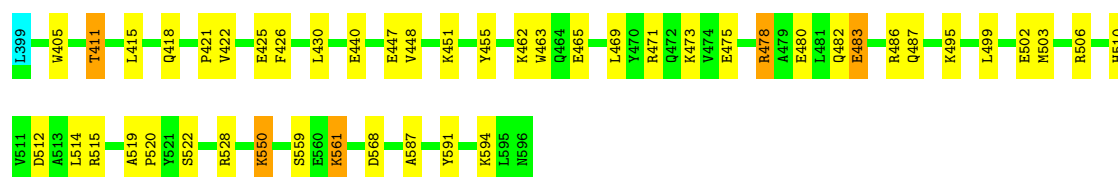
- Molecule 1: Apolipoprotein A-I

Chain A: 70% 21% 8%



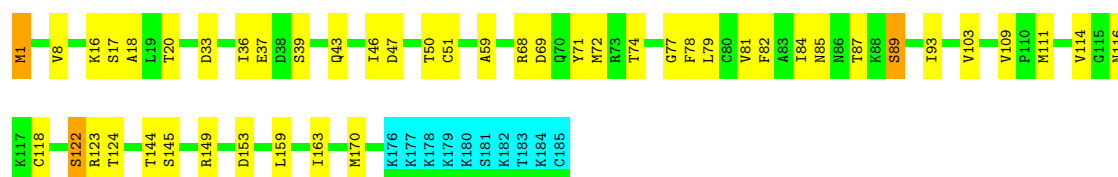
- Molecule 1: Apolipoprotein A-I

Chain C: 76% 21%

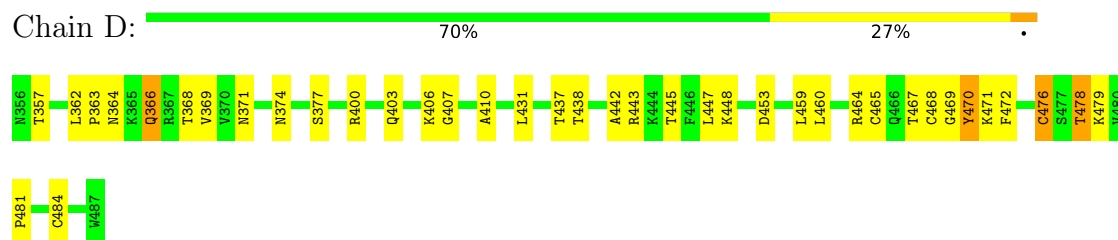


- Molecule 2: GTPase KRas

Chain B: 69% 24% 5%

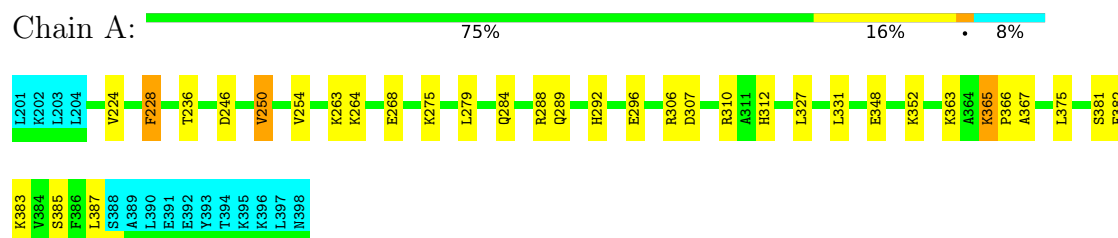


- Molecule 3: RAF proto-oncogene serine/threonine-protein kinase

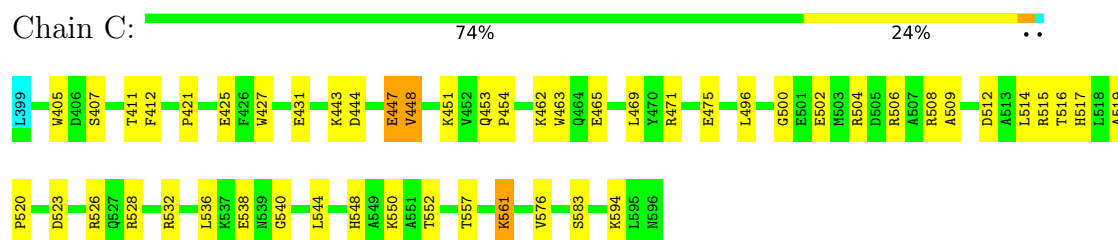


4.2.6 Score per residue for model 6

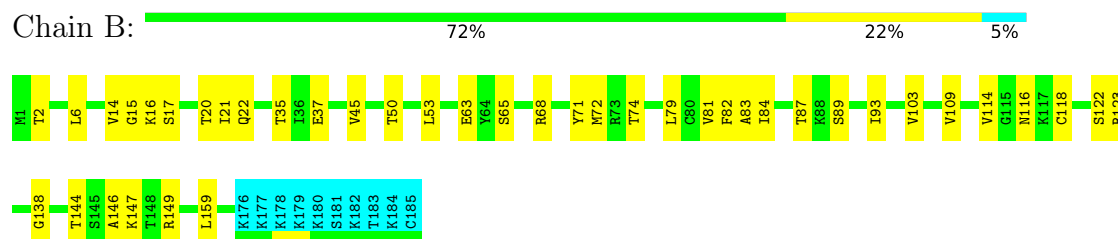
- Molecule 1: Apolipoprotein A-I



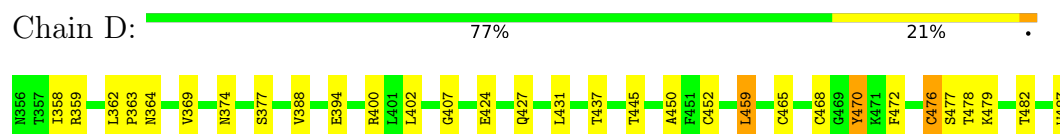
- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas

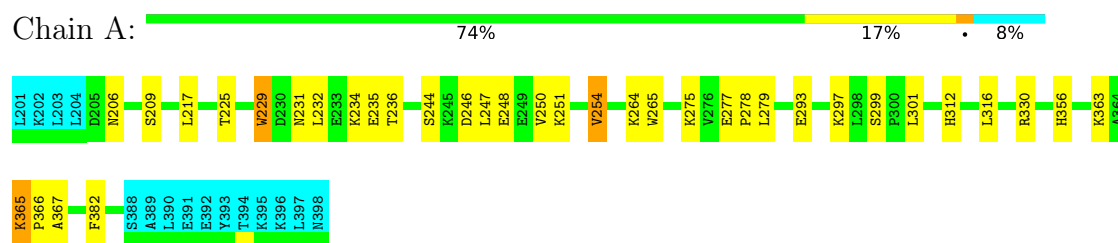


- Molecule 3: RAF proto-oncogene serine/threonine-protein kinase

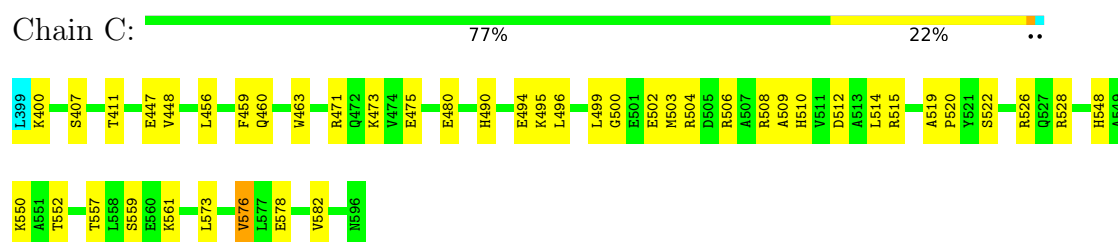


4.2.7 Score per residue for model 7

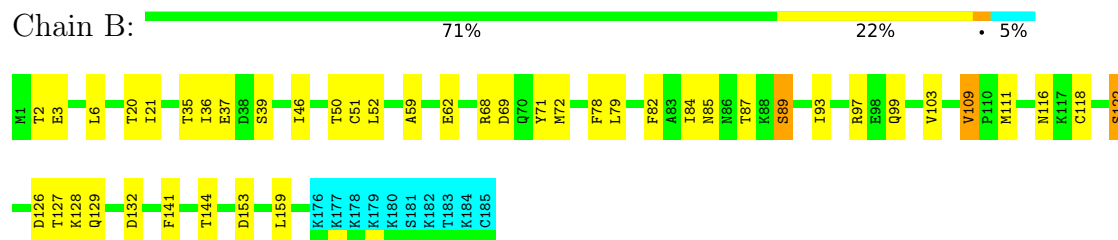
• Molecule 1: Apolipoprotein A-I



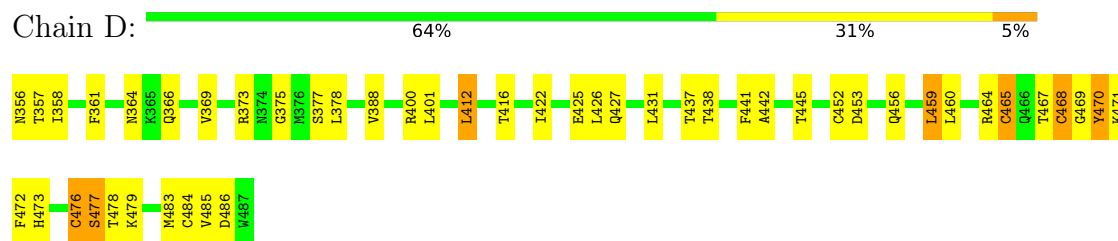
• Molecule 1: Apolipoprotein A-I



• Molecule 2: GTPase KRas

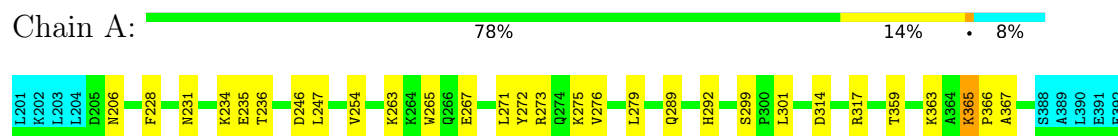


• Molecule 3: RAF proto-oncogene serine/threonine-protein kinase



4.2.8 Score per residue for model 8

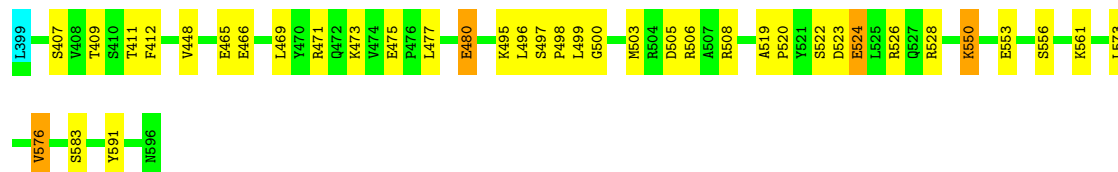
• Molecule 1: Apolipoprotein A-I



Y393
T394
K395
K396
L397
N398

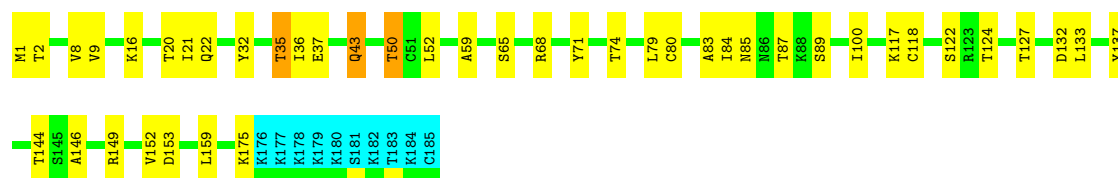
• Molecule 1: Apolipoprotein A-I

Chain C: 80% 17% ..



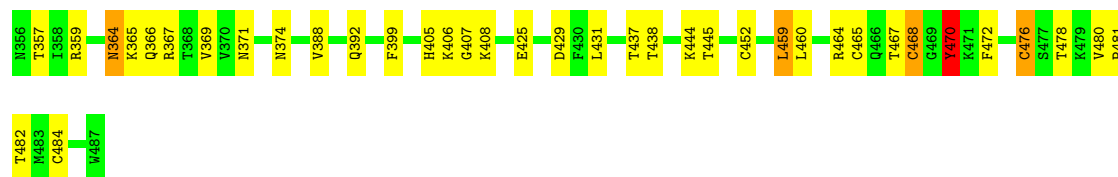
• Molecule 2: GTPase KRas

Chain B: 71% 22% • 5%



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

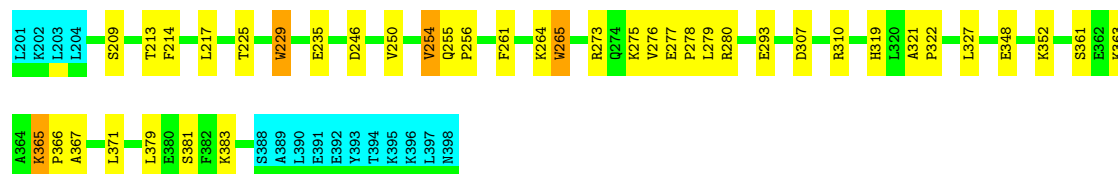
Chain D: 71% 25% ..



4.2.9 Score per residue for model 9

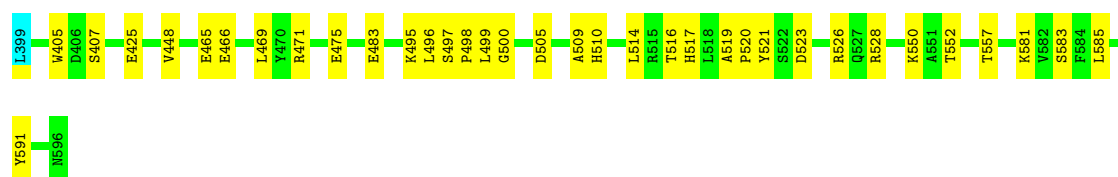
• Molecule 1: Apolipoprotein A-I

Chain A: 72% 18% • 8%



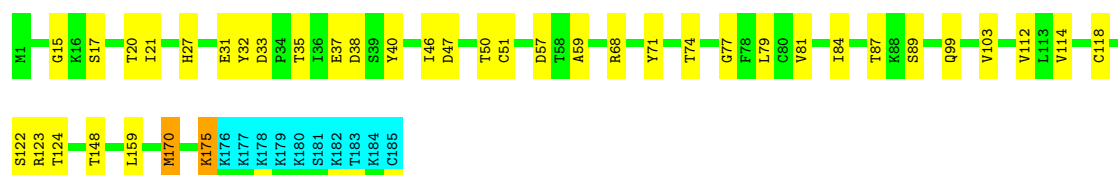
• Molecule 1: Apolipoprotein A-I

Chain C: 82% 18% .



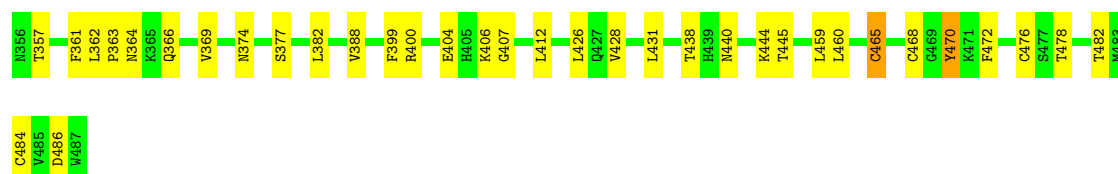
- Molecule 2: GTPase KRas

Chain B: 74% 20% 5%



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

Chain D: 73% 25% 2%



4.2.10 Score per residue for model 10

- Molecule 1: Apolipoprotein A-I

Chain A: 73% 17% 8%

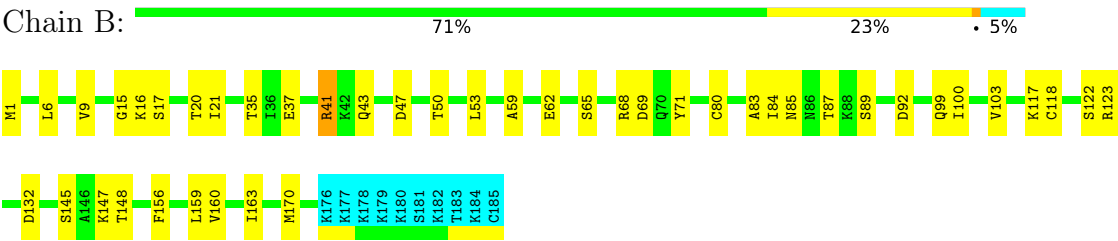


- Molecule 1: Apolipoprotein A-I

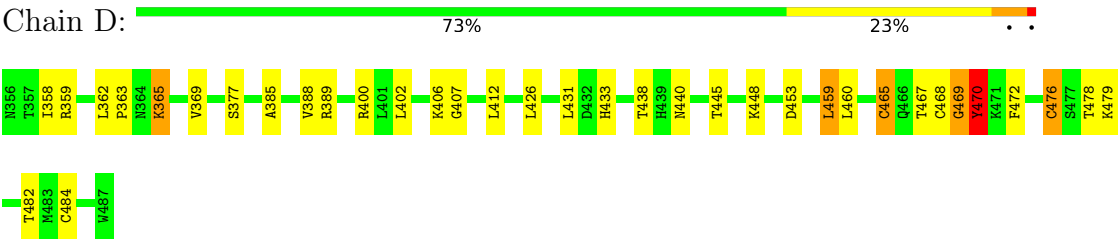
Chain C: 78% 21% 1%



- Molecule 2: GTPase KRas



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



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
CNS	refinement	
HADDOCK	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	557
Number of shifts mapped to atoms	437
Number of unparsed shifts	0
Number of shifts with mapping errors	120
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	6%

6 Model quality

6.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.39±0.01	0±0/1527 (0.0± 0.0%)	0.78±0.01	0±0/2055 (0.0± 0.0%)
1	C	0.39±0.00	0±0/1642 (0.0± 0.0%)	0.82±0.00	0±0/2207 (0.0± 0.0%)
2	B	0.35±0.01	0±0/1416 (0.0± 0.0%)	0.70±0.01	0±0/1907 (0.0± 0.0%)
3	D	0.46±0.01	2±0/1088 (0.2± 0.0%)	2.30±0.01	7±0/1466 (0.5± 0.0%)
All	All	0.39	20/56730 (0.0%)	1.22	70/76350 (0.1%)

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

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	D	470	TYR	CB-CG	6.78	1.66	1.51	7	10
3	D	470	TYR	CZ-OH	5.85	1.50	1.38	8	10

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	D	470	TYR	CD1-CG-CD2	-41.83	55.36	118.10	8	10
3	D	470	TYR	CG-CD1-CE1	-36.94	65.79	121.20	4	10
3	D	470	TYR	CG-CD2-CE2	-32.67	72.19	121.20	2	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	D	470	TYR	CE1-CZ-CE2	-31.53	57.24	120.30	10	10
3	D	470	TYR	CZ-CE2-CD2	-30.80	64.17	119.60	2	10
3	D	470	TYR	CD1-CE1-CZ	-27.60	69.93	119.60	8	10
3	D	470	TYR	CB-CG-CD1	9.64	135.26	120.80	2	10

There are no chirality outliers.

All unique planar outliers are listed below.

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

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1500	352	1489	22±6
1	C	1615	378	1616	20±5
2	B	1394	325	1379	24±2
3	D	1065	251	1070	21±5
4	A	756	0	1120	267±30
4	B	216	0	320	103±9
4	C	1350	0	2000	520±18
4	D	1134	0	1680	494±41
5	A	54	3	76	11±3
5	C	324	18	456	132±12
5	D	486	27	684	202±17
6	B	32	6	13	5±2
7	B	1	0	0	1±0
All	All	99290	13600	119030	13215

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 61.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:511:PCW:H222	4:D:511:PCW:C27	1.20	1.65	2	5
4:D:509:PCW:H231	4:D:509:PCW:C28	1.17	1.69	1	1
4:D:509:PCW:H283	4:D:509:PCW:C23	1.16	1.70	1	1
4:A:413:PCW:H11	4:C:617:PCW:H411	1.14	1.17	5	10
4:B:203:PCW:H121	4:B:203:PCW:H371	1.14	1.19	1	9
4:B:203:PCW:H261	4:B:203:PCW:H221	1.14	1.16	1	10
4:A:407:PCW:C19	4:A:407:PCW:H142	1.14	1.71	7	10
4:D:518:PCW:H472	4:D:518:PCW:H432	1.14	1.19	6	10
4:D:511:PCW:H272	4:D:511:PCW:C22	1.14	1.73	4	5
4:D:513:PCW:H262	4:D:513:PCW:H222	1.14	1.20	5	10
4:D:505:PCW:H182	4:D:505:PCW:H221	1.14	1.17	7	6
4:C:617:PCW:H272	4:C:617:PCW:H232	1.13	1.19	9	10
4:A:413:PCW:H372	4:C:617:PCW:H431	1.13	1.21	10	9
4:D:516:PCW:H472	4:D:516:PCW:H432	1.13	1.18	9	10
4:A:415:PCW:H242	4:D:528:PCW:H242	1.13	1.16	7	9
4:C:623:PCW:H412	4:C:624:PCW:H412	1.13	1.17	8	8
4:D:513:PCW:H472	4:D:513:PCW:H432	1.13	1.18	2	10
4:D:504:PCW:H251	4:D:504:PCW:H211	1.12	1.15	6	10
4:C:603:PCW:H222	4:D:526:PCW:H351	1.12	1.17	1	7
4:C:621:PCW:H132	5:C:630:17F:H4A	1.12	1.16	2	10
4:C:616:PCW:H39	4:C:618:PCW:H142	1.12	1.14	8	8
4:C:614:PCW:H461	4:C:614:PCW:H421	1.11	1.19	1	10
4:C:601:PCW:H461	4:C:601:PCW:H421	1.11	1.16	10	8
4:C:621:PCW:H362	5:C:629:17F:H59	1.11	1.14	9	2
4:D:506:PCW:H252	4:D:506:PCW:H212	1.11	1.17	9	10
4:B:201:PCW:H461	4:B:201:PCW:H421	1.11	1.16	7	8
4:D:507:PCW:H141	4:D:513:PCW:H321	1.11	1.22	5	6
5:D:522:17F:H12	5:D:522:17F:H41	1.11	1.23	2	4
4:C:613:PCW:H482	4:C:619:PCW:H211	1.10	1.22	6	7
4:A:415:PCW:H20	4:A:415:PCW:H241	1.10	1.20	9	10
4:C:606:PCW:H212	4:C:606:PCW:H172	1.10	1.23	4	10
4:C:621:PCW:H19	5:C:629:17F:H5	1.10	1.20	2	9
4:C:602:PCW:H42	5:D:523:17F:H19	1.10	1.20	4	1
4:D:503:PCW:H422	5:D:522:17F:H44	1.10	1.20	6	1
4:D:518:PCW:H31	4:D:518:PCW:H371	1.10	1.16	4	9
4:D:508:PCW:H161	4:D:512:PCW:C17	1.10	1.76	3	6
4:C:606:PCW:H182	4:C:606:PCW:H142	1.10	1.14	4	10
4:C:611:PCW:H472	4:D:501:PCW:H271	1.10	1.16	3	1
4:C:608:PCW:H41	4:C:624:PCW:H222	1.10	1.23	9	6
4:C:621:PCW:H141	5:C:630:17F:H6	1.09	1.14	7	10
4:C:624:PCW:H271	4:C:624:PCW:H231	1.09	1.18	9	10
4:A:411:PCW:H422	4:C:612:PCW:H231	1.09	1.15	4	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:602:PCW:H261	5:C:627:17F:H76	1.09	1.18	8	3
4:D:513:PCW:H172	4:D:513:PCW:H211	1.09	1.18	9	2
5:D:524:17F:H12	5:D:524:17F:H65	1.09	1.19	2	2
4:D:515:PCW:H412	4:D:515:PCW:H371	1.09	1.16	9	6
4:A:405:PCW:H171	4:A:405:PCW:H212	1.09	1.19	2	8
4:C:602:PCW:H212	4:C:602:PCW:H172	1.09	1.15	7	5
4:D:506:PCW:H171	4:D:506:PCW:H132	1.09	1.20	7	9
4:D:517:PCW:H20	4:D:517:PCW:H241	1.09	1.23	8	10
5:D:529:17F:H42	5:D:530:17F:H73	1.09	1.23	8	2
4:C:616:PCW:H451	4:B:201:PCW:H452	1.09	1.22	5	1
4:C:618:PCW:H381	4:C:625:PCW:H161	1.09	1.23	5	8
5:D:521:17F:H57	5:D:521:17F:H19A	1.09	1.22	9	8
4:C:612:PCW:H212	4:C:612:PCW:H172	1.09	1.13	7	6
5:C:626:17F:H19A	5:C:626:17F:H57	1.08	1.25	5	10
4:D:510:PCW:H471	5:D:524:17F:H57	1.08	1.16	2	2
4:C:604:PCW:H461	4:C:624:PCW:H282	1.08	1.12	4	8
4:C:608:PCW:H431	5:C:626:17F:H34	1.08	1.17	4	7
4:D:528:PCW:H19	5:D:530:17F:H20	1.08	1.13	5	3
4:D:508:PCW:H332	4:D:512:PCW:H121	1.08	1.25	5	1
4:C:604:PCW:H2	4:C:606:PCW:H82	1.08	1.12	10	4
4:D:510:PCW:H471	5:D:524:17F:H60	1.08	1.25	8	3
4:C:611:PCW:H39	4:C:622:PCW:H462	1.08	1.26	7	5
4:A:413:PCW:H451	4:D:526:PCW:H211	1.07	1.24	1	5
4:C:611:PCW:H63	4:C:622:PCW:H321	1.07	1.11	9	10
4:D:507:PCW:H221	4:D:513:PCW:H242	1.07	1.23	4	5
4:D:511:PCW:H272	4:D:511:PCW:H222	1.07	1.13	6	2
4:C:622:PCW:H362	4:C:622:PCW:H322	1.07	1.14	3	5
4:D:505:PCW:H351	4:D:505:PCW:O31	1.07	1.49	7	7
5:C:631:17F:H52	4:D:512:PCW:H172	1.07	1.15	5	1
5:D:522:17F:H68	5:D:522:17F:H77	1.07	1.17	6	1
4:D:504:PCW:H412	4:D:516:PCW:H82	1.06	1.21	2	1
4:B:201:PCW:H161	4:D:506:PCW:H461	1.06	1.11	6	4
4:D:515:PCW:P	4:D:515:PCW:H62	1.06	1.91	3	1
4:A:403:PCW:H241	4:D:513:PCW:H122	1.06	1.20	7	3
4:D:515:PCW:H431	4:D:516:PCW:H31	1.06	1.20	9	1
4:C:601:PCW:H472	4:C:601:PCW:H432	1.06	1.21	1	2
4:C:610:PCW:H63	5:C:629:17F:H6A	1.06	1.10	9	7
4:C:611:PCW:H321	4:C:622:PCW:H352	1.06	1.10	10	8
4:C:611:PCW:H371	4:C:611:PCW:H19	1.06	1.07	1	2
4:B:203:PCW:H20	4:D:506:PCW:H451	1.06	1.21	5	5
4:C:608:PCW:H261	5:C:627:17F:H62	1.06	1.28	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:616:PCW:H471	4:B:201:PCW:H452	1.06	1.26	8	3
4:D:508:PCW:H182	4:D:512:PCW:C17	1.06	1.81	6	1
4:A:414:PCW:H61	5:C:628:17F:H4	1.06	1.26	7	3
4:D:505:PCW:H161	4:D:505:PCW:H421	1.06	1.21	9	2
4:C:603:PCW:H2	4:C:603:PCW:H41	1.05	1.08	10	9
4:A:411:PCW:H341	4:C:612:PCW:H132	1.05	1.26	3	2
4:C:601:PCW:H152	4:C:601:PCW:H451	1.05	1.23	4	1
4:C:608:PCW:H181	5:C:627:17F:H11	1.05	1.27	1	8
5:D:529:17F:H18A	5:D:529:17F:O7	1.05	1.51	3	6
4:C:604:PCW:H482	4:C:624:PCW:H282	1.05	1.28	5	6
4:C:615:PCW:H472	4:D:512:PCW:H222	1.05	1.27	10	2
4:C:622:PCW:C36	4:C:622:PCW:H322	1.05	1.81	10	1
5:D:529:17F:H46	5:D:530:17F:H73	1.05	1.20	1	6
4:D:509:PCW:H19	5:D:520:17F:H57	1.05	1.17	8	3
4:D:511:PCW:H41	4:D:511:PCW:H31	1.05	1.29	3	6
4:D:510:PCW:H131	5:D:524:17F:H71	1.05	1.27	6	1
4:A:401:PCW:H321	4:D:511:PCW:H382	1.05	1.22	10	1
4:A:401:PCW:H442	4:C:614:PCW:H262	1.05	1.28	1	5
4:C:608:PCW:H461	5:C:626:17F:H61	1.05	1.27	2	8
4:A:405:PCW:H162	4:A:405:PCW:H212	1.05	1.28	9	1
4:A:410:PCW:H283	4:A:413:PCW:H251	1.04	1.29	1	5
4:C:613:PCW:H251	5:D:521:17F:H47	1.04	1.27	8	8
4:D:510:PCW:H351	5:D:524:17F:H9	1.04	1.27	7	7
4:D:508:PCW:H20	4:D:512:PCW:H431	1.04	1.29	9	2
4:C:622:PCW:H322	4:C:622:PCW:C36	1.04	1.83	5	9
4:D:502:PCW:H342	4:D:505:PCW:H11	1.04	1.29	1	1
4:D:511:PCW:H222	4:D:511:PCW:H272	1.04	1.04	1	3
4:D:509:PCW:H142	5:D:520:17F:H60	1.04	1.10	2	1
4:D:509:PCW:H211	5:D:520:17F:H57	1.04	1.20	5	2
4:A:402:PCW:H431	4:D:508:PCW:H262	1.04	1.23	9	1
4:D:512:PCW:H271	4:D:512:PCW:H231	1.04	1.18	5	1
4:C:611:PCW:H222	4:C:619:PCW:H442	1.04	1.07	8	1
4:A:414:PCW:H122	5:C:628:17F:H9	1.04	1.28	10	9
4:C:621:PCW:H351	5:C:630:17F:H33	1.04	1.26	10	8
4:D:506:PCW:H62	5:D:520:17F:H6A	1.04	1.21	5	1
4:D:502:PCW:H332	4:D:510:PCW:H11	1.04	1.30	7	2
4:D:506:PCW:H42	4:D:509:PCW:H331	1.04	1.19	1	1
4:D:508:PCW:H151	4:D:512:PCW:H151	1.04	1.22	1	1
4:C:622:PCW:H421	4:C:623:PCW:H261	1.04	1.26	2	4
4:C:611:PCW:H221	4:C:619:PCW:H461	1.04	1.29	9	1
4:D:501:PCW:H461	5:D:525:17F:H47	1.03	1.25	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:512:PCW:H232	4:D:512:PCW:H271	1.03	1.21	9	1
4:D:516:PCW:H39	4:D:527:PCW:H271	1.03	1.04	1	1
4:C:625:PCW:H2	4:C:625:PCW:H42	1.03	1.26	3	3
4:D:502:PCW:O4P	4:D:502:PCW:H31	1.03	1.52	8	3
4:D:502:PCW:H132	4:D:505:PCW:H12	1.03	1.21	1	1
4:A:405:PCW:H212	4:A:405:PCW:C17	1.03	1.78	10	8
4:A:403:PCW:H422	4:D:513:PCW:H40	1.03	1.24	5	2
5:D:522:17F:C12	5:D:522:17F:H41	1.03	1.84	4	3
4:A:403:PCW:H272	4:D:507:PCW:H19	1.03	1.24	10	4
4:A:402:PCW:H162	4:A:405:PCW:H211	1.03	1.29	10	2
4:D:503:PCW:H231	4:D:503:PCW:H272	1.03	1.17	8	1
4:D:514:PCW:H182	4:D:514:PCW:C25	1.03	1.82	9	1
4:A:414:PCW:H162	5:C:628:17F:H57	1.03	1.28	4	10
4:C:616:PCW:H451	4:B:201:PCW:H472	1.03	1.25	1	5
4:C:616:PCW:H282	4:D:510:PCW:H272	1.03	1.25	5	1
4:D:512:PCW:H61	5:D:520:17F:H1A	1.03	1.05	10	3
4:C:611:PCW:H351	4:C:611:PCW:H172	1.03	1.20	10	3
4:D:506:PCW:H122	5:D:520:17F:H29	1.03	1.24	4	1
4:A:408:PCW:H442	4:D:506:PCW:H412	1.02	1.19	4	3
4:A:405:PCW:H212	4:A:405:PCW:C16	1.02	1.82	9	1
4:C:615:PCW:H452	4:D:512:PCW:H241	1.02	1.13	9	2
4:D:513:PCW:H241	4:D:513:PCW:H481	1.02	1.25	9	1
4:D:514:PCW:H182	4:D:514:PCW:H252	1.02	1.04	9	1
4:D:517:PCW:H462	5:D:525:17F:H41	1.02	1.31	9	1
5:D:530:17F:H12A	5:D:530:17F:H59	1.02	1.25	9	7
4:A:411:PCW:H431	4:C:612:PCW:H172	1.02	1.24	10	4
4:D:501:PCW:H132	4:D:503:PCW:H342	1.02	1.28	3	1
4:D:515:PCW:H32	5:D:525:17F:H31	1.02	1.25	10	2
4:A:401:PCW:H421	4:C:611:PCW:H271	1.02	1.26	9	1
4:C:604:PCW:H381	5:D:529:17F:H36	1.02	1.30	7	4
4:C:611:PCW:C32	4:C:622:PCW:H352	1.02	1.85	10	7
4:B:201:PCW:H142	4:D:506:PCW:H361	1.02	1.24	2	3
4:D:507:PCW:H421	4:D:517:PCW:H222	1.02	1.13	2	1
4:D:510:PCW:H20	5:D:524:17F:H31	1.02	1.29	8	5
4:C:606:PCW:H73	4:C:624:PCW:H19	1.02	1.31	5	5
4:C:610:PCW:H12	5:C:629:17F:H6	1.02	1.30	3	1
4:B:201:PCW:H482	4:D:527:PCW:H232	1.02	1.26	1	3
4:D:508:PCW:H181	4:D:512:PCW:H362	1.02	1.28	10	6
4:D:511:PCW:H381	4:D:511:PCW:H242	1.02	1.27	1	1
5:D:529:17F:H18A	5:D:529:17F:C7	1.02	1.85	1	4
4:D:513:PCW:H32	4:D:513:PCW:O4P	1.02	1.55	7	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:515:PCW:H271	4:D:528:PCW:H281	1.02	1.32	3	1
4:A:405:PCW:H212	4:A:405:PCW:H171	1.02	1.06	10	1
5:D:529:17F:H47	5:D:530:17F:H39	1.01	1.17	4	9
4:C:601:PCW:H40	4:C:602:PCW:H251	1.01	1.31	10	1
4:C:614:PCW:H51	4:C:623:PCW:O1P	1.01	1.54	8	4
4:D:513:PCW:H451	4:D:517:PCW:H472	1.01	1.26	5	3
4:A:403:PCW:H252	4:D:507:PCW:H171	1.01	1.23	9	6
4:D:508:PCW:C16	4:D:512:PCW:H171	1.01	1.86	3	3
4:D:502:PCW:H171	4:D:505:PCW:H122	1.01	1.27	5	4
4:D:517:PCW:H371	5:D:525:17F:H59	1.01	1.31	10	2
4:A:413:PCW:H482	4:C:616:PCW:H271	1.01	1.32	1	2
4:C:602:PCW:H362	5:D:523:17F:H67	1.01	1.30	7	6
4:C:624:PCW:H342	4:C:624:PCW:H122	1.01	1.30	2	1
4:C:607:PCW:H471	4:D:513:PCW:H483	1.01	1.31	6	1
5:D:524:17F:H65	5:D:524:17F:H30	1.01	1.28	6	1
4:A:403:PCW:H42	4:A:403:PCW:H31	1.01	1.28	2	3
4:A:410:PCW:H141	4:A:413:PCW:H341	1.01	1.31	6	7
4:C:625:PCW:H20	4:D:528:PCW:H352	1.01	1.25	4	4
4:C:605:PCW:H172	4:C:613:PCW:H132	1.01	1.26	9	5
5:C:630:17F:H74	4:D:514:PCW:H252	1.01	1.26	7	1
4:D:508:PCW:H73	5:D:520:17F:H2	1.01	1.31	7	2
4:D:508:PCW:H73	5:D:520:17F:O1	1.01	1.55	1	5
4:B:201:PCW:H51	4:B:202:PCW:H31	1.01	1.30	6	1
4:D:512:PCW:C6	5:D:520:17F:H1A	1.01	1.86	6	2
4:C:617:PCW:H471	4:C:617:PCW:H431	1.01	1.23	8	1
4:D:509:PCW:H411	4:D:509:PCW:H372	1.01	1.18	9	1
4:D:509:PCW:H282	5:D:520:17F:H19	1.00	1.29	1	1
4:A:413:PCW:H481	5:D:524:17F:H37	1.00	1.27	4	1
5:D:521:17F:H56	5:D:521:17F:H62	1.00	1.30	6	1
4:D:514:PCW:H252	4:D:514:PCW:C18	1.00	1.85	9	1
4:C:611:PCW:H20	4:C:611:PCW:H412	1.00	1.32	1	3
4:C:622:PCW:H362	4:C:622:PCW:C32	1.00	1.87	10	10
4:D:508:PCW:H161	4:D:512:PCW:H171	1.00	1.01	10	5
4:D:517:PCW:H421	5:D:525:17F:H12	1.00	1.33	8	1
4:B:203:PCW:H132	4:B:204:PCW:H322	1.00	1.31	7	6
4:A:413:PCW:H382	4:D:526:PCW:H231	1.00	1.33	5	1
4:A:415:PCW:H321	4:A:415:PCW:H73	1.00	1.31	5	2
4:D:504:PCW:H331	4:D:510:PCW:H321	1.00	1.27	8	1
4:C:606:PCW:H161	5:D:529:17F:H11A	1.00	1.27	7	8
4:D:513:PCW:H19	5:D:523:17F:H40	1.00	1.34	1	1
4:D:506:PCW:H141	5:D:520:17F:H36	1.00	1.32	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:481:PRO:HA	4:D:509:PCW:H52	1.00	1.33	8	1
4:D:518:PCW:H321	5:D:519:17F:H20	1.00	1.08	9	1
4:A:403:PCW:H242	4:D:513:PCW:H82	1.00	1.34	9	1
4:A:406:PCW:H242	4:B:202:PCW:H221	1.00	1.29	9	2
4:D:508:PCW:H182	4:D:512:PCW:H172	1.00	1.00	6	1
4:D:509:PCW:C4	4:D:509:PCW:H31	1.00	1.87	1	2
4:D:517:PCW:H441	5:D:525:17F:H10	1.00	1.25	3	1
4:C:603:PCW:H222	4:D:526:PCW:C33	1.00	1.85	5	6
4:A:414:PCW:H51	4:A:414:PCW:O11	1.00	1.57	10	1
4:C:621:PCW:H181	4:C:621:PCW:H142	0.99	1.33	6	10
4:A:411:PCW:H431	4:C:612:PCW:C17	0.99	1.85	10	6
4:C:622:PCW:H382	4:C:623:PCW:H171	0.99	1.34	4	9
4:B:204:PCW:H132	4:B:204:PCW:H341	0.99	1.33	5	10
4:C:612:PCW:H212	4:C:612:PCW:C17	0.99	1.87	7	6
4:D:504:PCW:H342	4:D:510:PCW:H341	0.99	1.32	9	4
4:A:403:PCW:H141	4:A:403:PCW:H362	0.99	1.32	1	2
4:C:623:PCW:H19	4:C:623:PCW:H151	0.99	1.35	4	10
4:D:507:PCW:H432	4:D:517:PCW:C23	0.99	1.86	5	1
4:A:410:PCW:H39	4:A:410:PCW:H151	0.99	1.25	6	3
4:A:411:PCW:H431	4:C:612:PCW:H181	0.99	1.32	9	2
4:D:516:PCW:H451	5:D:529:17F:H49	0.99	1.33	1	1
4:C:602:PCW:H461	4:C:608:PCW:H472	0.99	1.34	2	3
4:D:502:PCW:H441	4:D:502:PCW:H232	0.99	1.34	7	4
4:D:507:PCW:H221	4:D:513:PCW:H271	0.99	1.33	9	1
4:B:201:PCW:H11	4:D:504:PCW:H151	0.99	1.34	3	2
4:D:502:PCW:H271	4:D:518:PCW:H222	0.99	1.33	5	1
4:D:507:PCW:C43	4:D:517:PCW:H231	0.99	1.88	5	1
5:C:631:17F:H53	4:D:512:PCW:H161	0.99	1.34	4	4
4:D:510:PCW:H352	5:D:524:17F:H8A	0.99	1.04	6	1
4:C:607:PCW:C1	4:C:624:PCW:H372	0.99	1.88	5	7
5:A:409:17F:H58	4:D:503:PCW:H242	0.99	1.35	8	1
4:C:616:PCW:H341	4:D:527:PCW:H341	0.98	1.32	8	9
4:D:527:PCW:H152	4:D:528:PCW:H162	0.98	1.34	3	5
4:A:414:PCW:H122	5:C:628:17F:H11	0.98	1.29	8	5
4:C:611:PCW:C16	4:C:619:PCW:H171	0.98	1.88	1	7
4:A:411:PCW:H422	4:C:612:PCW:C23	0.98	1.88	10	7
4:B:203:PCW:H162	4:B:203:PCW:H422	0.98	1.35	4	2
4:A:406:PCW:H482	4:B:204:PCW:H232	0.98	1.27	9	2
4:D:508:PCW:H131	4:D:509:PCW:H222	0.98	1.32	4	2
4:D:501:PCW:H222	5:D:521:17F:H19	0.98	1.34	5	2
4:C:621:PCW:H421	5:C:630:17F:H62	0.98	1.26	2	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:623:PCW:H451	4:C:624:PCW:H482	0.98	1.31	7	7
4:B:201:PCW:H161	4:D:506:PCW:H411	0.98	1.32	3	1
4:A:414:PCW:H122	5:C:628:17F:C9	0.98	1.88	10	10
4:C:603:PCW:H441	4:C:603:PCW:H212	0.98	1.28	3	7
4:C:625:PCW:H20	4:D:528:PCW:C35	0.98	1.86	4	8
4:A:402:PCW:H431	4:D:508:PCW:H251	0.98	1.30	7	2
4:C:620:PCW:H283	5:C:631:17F:H35	0.98	1.34	8	6
5:D:524:17F:H12	5:D:524:17F:H66	0.98	1.30	5	1
4:B:201:PCW:H161	4:D:506:PCW:H442	0.98	1.28	4	3
4:C:608:PCW:H20	5:C:627:17F:H46	0.98	1.30	1	4
4:C:609:PCW:H211	4:C:615:PCW:H372	0.98	1.36	5	3
4:D:528:PCW:H141	5:D:530:17F:H33	0.98	1.32	6	4
4:C:602:PCW:H483	5:C:627:17F:H47	0.98	1.30	3	4
4:D:513:PCW:H171	5:D:523:17F:H30	0.98	1.26	5	1
4:A:401:PCW:H322	4:D:511:PCW:H382	0.97	1.29	8	4
4:C:603:PCW:H462	4:D:526:PCW:H432	0.97	1.35	4	5
4:D:518:PCW:H352	5:D:519:17F:H66	0.97	1.36	6	2
4:C:601:PCW:H482	5:C:626:17F:H47	0.97	1.28	2	1
4:D:518:PCW:H331	5:D:519:17F:H32	0.97	1.36	7	1
4:D:518:PCW:C12	5:D:519:17F:H66	0.97	1.89	2	1
4:C:604:PCW:H361	5:D:529:17F:H36	0.97	1.28	3	2
4:A:408:PCW:H422	4:D:506:PCW:H432	0.97	1.33	6	2
4:A:407:PCW:H271	4:A:412:PCW:H271	0.97	1.36	4	3
4:D:511:PCW:H31	4:D:511:PCW:C4	0.97	1.89	8	7
4:C:615:PCW:H483	4:D:509:PCW:H241	0.97	1.35	9	1
4:D:504:PCW:H331	4:D:516:PCW:H141	0.97	1.37	7	1
4:D:518:PCW:H31	4:D:518:PCW:C37	0.97	1.90	10	6
4:D:507:PCW:H442	5:D:522:17F:H60	0.97	1.37	3	1
4:D:513:PCW:H451	4:D:517:PCW:H283	0.97	1.36	4	1
4:C:605:PCW:O31	4:C:613:PCW:H51	0.97	1.59	10	3
4:C:622:PCW:H322	4:C:622:PCW:H362	0.97	0.97	10	5
4:D:509:PCW:H31	4:D:509:PCW:H41	0.97	1.36	1	2
4:D:510:PCW:H351	5:D:524:17F:H10A	0.97	1.32	6	2
4:B:201:PCW:C23	4:B:203:PCW:H20	0.97	1.90	7	2
4:C:621:PCW:C14	5:C:630:17F:H6	0.96	1.90	7	10
4:D:506:PCW:H172	4:D:516:PCW:H362	0.96	1.37	1	3
4:D:507:PCW:C18	4:D:513:PCW:H221	0.96	1.90	8	6
4:C:621:PCW:C13	5:C:630:17F:H4A	0.96	1.89	2	6
5:C:626:17F:H69	5:C:627:17F:H48	0.96	1.30	5	2
4:C:605:PCW:C31	4:C:613:PCW:H51	0.96	1.90	1	3
4:B:201:PCW:H73	4:D:504:PCW:H51	0.96	1.33	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:503:PCW:H172	4:D:511:PCW:H40	0.96	1.35	10	1
4:C:625:PCW:H241	4:D:527:PCW:H451	0.96	1.37	4	7
4:A:408:PCW:H431	4:B:203:PCW:H182	0.96	1.33	2	2
4:D:504:PCW:H482	4:D:516:PCW:H20	0.96	1.34	6	1
4:D:518:PCW:H341	5:D:519:17F:H57	0.96	1.34	8	1
4:A:413:PCW:H422	4:C:616:PCW:H232	0.96	1.32	9	5
4:D:509:PCW:H171	4:D:514:PCW:H122	0.96	1.32	6	1
4:B:203:PCW:H352	4:B:203:PCW:O31	0.96	1.60	3	10
4:B:201:PCW:H151	4:D:516:PCW:H422	0.96	1.37	6	1
4:D:507:PCW:H132	4:D:513:PCW:H122	0.96	1.00	9	1
4:C:621:PCW:H371	5:C:629:17F:H63	0.96	1.34	8	4
4:D:502:PCW:H331	4:D:510:PCW:H52	0.96	1.36	1	1
4:D:515:PCW:H342	4:D:516:PCW:H11	0.96	1.35	3	2
4:A:408:PCW:H411	4:B:203:PCW:H182	0.96	1.33	5	1
4:D:513:PCW:H211	4:D:513:PCW:C17	0.96	1.89	9	2
4:C:605:PCW:O1P	4:C:613:PCW:H52	0.96	1.61	3	7
4:D:504:PCW:H362	4:D:510:PCW:H321	0.96	1.34	9	2
4:D:518:PCW:H141	5:D:519:17F:H63	0.96	1.36	8	1
4:A:410:PCW:H362	4:A:414:PCW:H371	0.95	1.36	5	3
4:B:202:PCW:H32	4:D:504:PCW:H131	0.95	1.38	6	1
4:A:402:PCW:H442	4:D:508:PCW:H231	0.95	1.38	7	1
4:A:411:PCW:H332	4:C:612:PCW:H132	0.95	1.37	4	5
4:D:508:PCW:H52	5:D:523:17F:H9	0.95	1.31	2	1
5:C:630:17F:H29	5:D:529:17F:H68	0.95	1.35	8	3
4:A:402:PCW:H121	4:A:405:PCW:H132	0.95	1.36	6	5
4:D:503:PCW:H412	4:D:511:PCW:H431	0.95	1.34	2	1
4:D:517:PCW:H341	5:D:520:17F:H8	0.95	1.37	6	1
4:A:405:PCW:H162	4:A:405:PCW:C21	0.95	1.90	9	1
4:D:515:PCW:H431	4:D:516:PCW:C3	0.95	1.91	9	1
5:A:409:17F:H56	4:D:503:PCW:H162	0.95	1.36	2	3
4:D:518:PCW:H371	4:D:518:PCW:C3	0.95	1.91	10	9
4:A:411:PCW:H351	4:C:612:PCW:H152	0.95	1.34	9	2
4:C:603:PCW:H2	4:C:603:PCW:C4	0.95	1.91	10	6
4:D:515:PCW:H221	4:D:515:PCW:H181	0.95	1.34	7	2
4:D:516:PCW:H232	5:D:519:17F:H50	0.95	1.36	10	1
4:C:603:PCW:H222	4:D:526:PCW:C35	0.95	1.91	1	7
4:D:509:PCW:H231	4:D:509:PCW:H283	0.95	0.96	1	1
4:D:527:PCW:H442	4:D:528:PCW:H341	0.95	1.33	6	7
4:C:612:PCW:H232	4:C:612:PCW:H471	0.95	1.38	2	3
4:D:513:PCW:H52	4:D:513:PCW:O11	0.95	1.62	6	4
4:D:506:PCW:H61	4:D:517:PCW:H11	0.95	1.38	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:401:PCW:H182	4:A:401:PCW:H221	0.95	1.33	6	5
4:D:506:PCW:H281	4:D:515:PCW:H382	0.95	1.38	1	1
4:D:509:PCW:H19	5:D:520:17F:H31	0.95	1.33	6	2
4:A:404:PCW:H281	4:A:411:PCW:H221	0.95	1.35	10	3
4:D:509:PCW:C19	5:D:520:17F:H31	0.95	1.91	6	1
4:B:203:PCW:H232	4:B:204:PCW:H431	0.94	1.36	7	4
4:C:621:PCW:H412	5:C:631:17F:H77	0.94	1.37	4	2
4:D:505:PCW:H171	4:D:505:PCW:H221	0.94	1.37	3	3
4:C:624:PCW:H122	4:C:624:PCW:C34	0.94	1.92	2	1
4:D:501:PCW:H421	5:D:521:17F:H77	0.94	1.38	3	1
4:C:615:PCW:H221	4:D:512:PCW:H261	0.94	1.34	4	3
5:A:409:17F:H57	4:D:503:PCW:H211	0.94	1.35	2	3
4:D:506:PCW:H42	4:D:509:PCW:C33	0.94	1.91	1	1
4:C:604:PCW:H41	4:C:604:PCW:H31	0.94	1.37	9	1
4:A:401:PCW:H51	4:D:503:PCW:O2P	0.94	1.63	1	1
4:D:510:PCW:H451	5:D:524:17F:H58	0.94	1.40	7	4
4:A:411:PCW:C33	4:C:612:PCW:H132	0.94	1.93	4	3
4:B:201:PCW:H422	5:D:524:17F:H43	0.94	1.37	4	1
4:C:606:PCW:H422	4:C:609:PCW:H31	0.94	1.36	6	6
5:A:409:17F:H71	4:D:501:PCW:H272	0.94	1.36	4	1
5:A:409:17F:O5	4:D:503:PCW:H51	0.94	1.62	5	2
4:D:515:PCW:C15	5:D:525:17F:H61	0.94	1.92	10	1
4:A:412:PCW:H40	4:C:623:PCW:H441	0.94	1.36	3	8
4:C:603:PCW:H472	4:C:603:PCW:H231	0.94	1.39	10	2
4:C:607:PCW:H472	4:D:513:PCW:H483	0.94	1.36	7	4
4:D:505:PCW:H421	4:D:505:PCW:C16	0.94	1.92	9	3
4:A:410:PCW:H211	4:C:617:PCW:H472	0.94	1.40	9	1
4:C:606:PCW:H252	5:D:529:17F:H38	0.93	1.37	3	5
4:D:507:PCW:H182	4:D:513:PCW:H221	0.93	1.38	7	3
4:B:203:PCW:H2	4:B:204:PCW:H82	0.93	1.39	10	4
4:D:502:PCW:H31	4:D:502:PCW:H41	0.93	1.40	1	1
4:C:611:PCW:H51	4:C:622:PCW:H342	0.93	1.37	3	2
4:C:603:PCW:H271	4:D:526:PCW:H212	0.93	1.36	8	8
4:D:502:PCW:H381	5:D:524:17F:H76	0.93	1.40	2	1
4:D:501:PCW:H122	5:D:519:17F:H35	0.93	1.41	7	1
4:D:514:PCW:H242	4:D:514:PCW:H181	0.93	1.40	6	5
4:D:507:PCW:H432	4:D:517:PCW:H231	0.93	0.96	5	1
4:C:612:PCW:H321	4:C:618:PCW:H132	0.93	1.39	10	5
4:A:403:PCW:H31	4:A:403:PCW:C4	0.93	1.94	2	4
4:C:605:PCW:H472	4:C:619:PCW:H432	0.93	1.41	10	5
4:D:517:PCW:H471	5:D:525:17F:H72	0.93	1.39	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:515:PCW:H2	5:D:525:17F:H19A	0.93	1.40	10	2
4:D:514:PCW:H212	4:D:514:PCW:H251	0.93	1.39	9	1
4:C:616:PCW:C39	4:C:618:PCW:H142	0.93	1.94	8	6
4:C:625:PCW:H381	4:C:625:PCW:H421	0.93	1.41	9	6
4:D:510:PCW:H161	5:D:524:17F:H19A	0.93	1.41	6	2
5:D:522:17F:H41	5:D:522:17F:C12	0.93	1.94	2	3
4:A:405:PCW:H321	4:D:514:PCW:H372	0.93	1.37	3	3
4:A:403:PCW:H452	4:D:507:PCW:H262	0.93	1.39	9	1
5:D:524:17F:H11	5:D:524:17F:H65	0.93	1.41	10	1
4:D:508:PCW:C18	4:D:512:PCW:H172	0.93	1.92	6	1
5:C:630:17F:H11	5:D:529:17F:C38	0.93	1.94	9	5
4:C:608:PCW:H19	5:C:627:17F:H46	0.93	1.37	8	7
4:C:623:PCW:H12	4:C:624:PCW:H32	0.92	1.40	2	2
4:D:508:PCW:H222	4:D:512:PCW:H411	0.92	1.34	3	3
4:D:508:PCW:H131	4:D:509:PCW:C22	0.92	1.93	4	2
4:C:610:PCW:C11	5:C:629:17F:H18	0.92	1.94	7	6
4:D:507:PCW:H132	4:D:513:PCW:C12	0.92	1.93	9	1
5:D:525:17F:O6	5:D:525:17F:H18A	0.92	1.64	2	5
4:C:607:PCW:H31	4:C:624:PCW:H372	0.92	1.37	2	4
4:C:622:PCW:H12	4:C:623:PCW:H161	0.92	1.38	4	4
4:D:513:PCW:H51	4:D:513:PCW:O11	0.92	1.64	1	2
5:D:522:17F:H41	5:D:522:17F:H12	0.92	1.37	5	3
4:D:528:PCW:H172	5:D:530:17F:H32	0.92	1.42	7	4
4:C:606:PCW:H341	4:C:606:PCW:H132	0.92	1.37	2	6
4:B:203:PCW:H11	4:B:204:PCW:H12	0.92	1.42	1	1
4:B:201:PCW:H40	4:D:527:PCW:H242	0.92	1.42	2	2
4:D:507:PCW:H141	4:D:513:PCW:C32	0.92	1.92	4	3
4:A:412:PCW:C40	4:C:623:PCW:H441	0.92	1.95	3	10
4:C:604:PCW:H182	5:D:525:17F:H53	0.92	1.41	2	1
4:A:401:PCW:H381	4:D:503:PCW:H20	0.92	1.37	7	1
4:B:202:PCW:H472	4:D:510:PCW:H221	0.92	1.39	8	2
4:C:625:PCW:H222	4:D:528:PCW:H352	0.92	1.42	7	2
4:D:528:PCW:H172	5:D:530:17F:C1Z	0.92	1.95	6	2
4:D:508:PCW:H152	4:D:509:PCW:C22	0.92	1.94	6	1
4:D:507:PCW:H32	4:D:513:PCW:H152	0.92	1.42	7	2
4:D:517:PCW:H171	4:D:517:PCW:H381	0.92	1.41	8	1
4:C:604:PCW:H31	4:C:604:PCW:O4P	0.92	1.64	4	8
4:C:612:PCW:C32	4:C:618:PCW:H132	0.92	1.94	10	8
4:C:623:PCW:C41	4:C:624:PCW:H412	0.92	1.94	6	6
4:D:503:PCW:H121	4:D:511:PCW:H39	0.92	1.40	1	2
4:D:503:PCW:H432	4:D:511:PCW:H20	0.92	1.38	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:406:PCW:H241	4:B:203:PCW:H242	0.91	1.41	1	2
4:C:607:PCW:H12	4:C:624:PCW:C37	0.91	1.96	1	7
5:C:630:17F:H39	5:D:530:17F:H67	0.91	1.41	4	9
4:D:516:PCW:C39	4:D:527:PCW:H271	0.91	1.94	1	1
3:D:425:GLU:HB3	4:D:502:PCW:H73	0.91	1.35	2	1
4:C:609:PCW:H452	4:D:512:PCW:H231	0.91	1.40	7	5
4:C:611:PCW:H371	4:C:611:PCW:C19	0.91	1.95	1	1
4:C:611:PCW:O2P	4:C:619:PCW:H41	0.91	1.64	2	3
4:C:611:PCW:H19	4:C:611:PCW:C37	0.91	1.94	1	1
4:C:611:PCW:H161	4:C:619:PCW:H171	0.91	1.38	5	5
4:A:406:PCW:C7	4:B:204:PCW:H11	0.91	1.94	5	2
4:A:403:PCW:P	4:A:403:PCW:H31	0.91	2.06	6	4
4:D:510:PCW:C35	5:D:524:17F:H8A	0.91	1.94	6	2
4:D:515:PCW:H51	4:D:515:PCW:H12	0.91	1.42	8	4
4:D:509:PCW:H31	4:D:509:PCW:O1P	0.91	1.65	7	5
4:D:518:PCW:H232	5:D:519:17F:H59	0.91	1.38	5	2
4:A:411:PCW:H431	4:C:612:PCW:C18	0.91	1.95	9	2
4:C:606:PCW:H212	4:C:606:PCW:C17	0.91	1.91	9	10
4:D:510:PCW:C20	5:D:524:17F:H31	0.91	1.94	8	2
4:A:402:PCW:H283	4:D:508:PCW:H281	0.91	1.38	3	1
4:C:620:PCW:O1P	4:C:621:PCW:H51	0.91	1.65	8	1
4:D:508:PCW:H182	4:D:512:PCW:H151	0.91	1.42	8	1
4:C:604:PCW:H222	4:D:515:PCW:H282	0.91	1.40	9	1
4:C:616:PCW:H39	4:C:618:PCW:C14	0.91	1.94	6	8
4:C:624:PCW:H231	4:C:624:PCW:C27	0.91	1.96	6	10
4:C:609:PCW:C18	4:C:615:PCW:H352	0.91	1.94	10	5
4:C:605:PCW:C18	4:C:613:PCW:H362	0.91	1.96	7	10
4:D:507:PCW:H421	4:D:517:PCW:C22	0.91	1.95	2	1
4:B:201:PCW:H342	4:D:510:PCW:H381	0.91	1.40	8	2
4:A:405:PCW:H171	4:A:405:PCW:C21	0.91	1.96	3	9
4:A:407:PCW:H142	4:A:407:PCW:C20	0.91	1.96	10	10
4:C:611:PCW:C8	4:C:623:PCW:H141	0.91	1.96	2	3
4:D:517:PCW:H432	4:D:517:PCW:H181	0.91	1.39	5	1
4:D:511:PCW:H61	5:D:522:17F:H6	0.91	1.41	8	1
4:C:603:PCW:H261	4:D:526:PCW:H142	0.91	1.41	10	8
4:C:611:PCW:C22	4:C:619:PCW:H461	0.91	1.96	9	2
5:C:630:17F:H8A	5:D:529:17F:H69	0.91	1.43	2	3
4:A:403:PCW:H341	4:A:407:PCW:C32	0.91	1.96	10	1
4:C:604:PCW:H451	4:C:606:PCW:H181	0.91	1.40	10	4
4:B:202:PCW:H482	4:D:510:PCW:H221	0.91	1.43	1	1
4:C:618:PCW:H411	4:C:625:PCW:H181	0.91	1.43	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:407:PCW:H272	4:A:407:PCW:H472	0.90	1.43	1	5
4:D:505:PCW:H272	5:D:524:17F:H73	0.90	1.41	5	1
4:B:201:PCW:H362	4:D:510:PCW:H381	0.90	1.42	1	3
4:A:406:PCW:H73	4:B:204:PCW:H11	0.90	1.41	5	2
4:D:517:PCW:H281	5:D:522:17F:H71	0.90	1.42	8	1
4:D:509:PCW:H19	5:D:520:17F:C1Y	0.90	1.97	6	1
4:D:504:PCW:H361	4:D:510:PCW:H321	0.90	1.40	10	1
4:A:405:PCW:H331	4:D:514:PCW:H352	0.90	1.43	6	4
4:A:413:PCW:H372	4:C:617:PCW:C43	0.90	1.97	2	9
4:C:623:PCW:H412	4:C:624:PCW:C41	0.90	1.95	8	5
5:C:630:17F:H36	5:D:530:17F:H67	0.90	1.42	4	3
4:B:203:PCW:H121	4:B:203:PCW:C37	0.90	1.95	4	7
4:C:610:PCW:H63	5:C:629:17F:O8	0.90	1.67	3	5
4:D:515:PCW:H152	4:D:517:PCW:H122	0.90	1.42	6	1
4:C:618:PCW:H261	4:D:510:PCW:H281	0.90	1.42	8	1
4:D:516:PCW:H261	4:D:526:PCW:H462	0.90	1.40	9	3
4:C:621:PCW:C36	5:C:629:17F:H59	0.90	1.95	9	1
1:C:471:ARG:HA	1:C:475:GLU:HG3	0.90	1.43	9	7
4:D:504:PCW:H152	4:D:510:PCW:H39	0.90	1.42	2	3
4:A:403:PCW:H212	4:D:513:PCW:H351	0.90	1.41	9	1
4:C:625:PCW:C20	4:D:528:PCW:H352	0.90	1.97	4	8
4:D:509:PCW:H19	5:D:520:17F:C31	0.90	1.97	8	2
4:B:201:PCW:H482	4:D:527:PCW:H231	0.90	1.41	10	2
4:D:504:PCW:H361	4:D:516:PCW:C8	0.90	1.96	8	1
4:A:410:PCW:H19	4:A:413:PCW:H431	0.90	1.44	3	6
4:C:623:PCW:H12	4:C:624:PCW:H12	0.90	1.41	6	7
4:C:616:PCW:O4P	4:C:616:PCW:H31	0.90	1.65	4	4
4:D:506:PCW:H2	4:D:515:PCW:H62	0.90	1.43	2	1
5:D:521:17F:H57	5:D:521:17F:C19	0.90	1.95	5	8
4:C:625:PCW:H2	4:C:625:PCW:C4	0.90	1.95	10	2
4:D:511:PCW:H381	4:D:511:PCW:H231	0.90	1.40	10	1
4:B:202:PCW:H11	4:D:504:PCW:H131	0.90	1.43	2	2
4:A:410:PCW:H141	4:A:413:PCW:C34	0.90	1.97	9	2
4:D:508:PCW:H162	4:D:509:PCW:H242	0.90	1.44	10	1
4:C:621:PCW:H132	5:C:630:17F:C4	0.89	1.97	2	7
4:D:506:PCW:H212	4:D:506:PCW:C25	0.89	1.97	10	10
4:C:609:PCW:H271	5:C:626:17F:H73	0.89	1.40	8	5
4:A:403:PCW:H231	4:D:507:PCW:H151	0.89	1.43	9	3
4:A:414:PCW:O1P	4:C:617:PCW:H82	0.89	1.67	9	4
4:C:611:PCW:C22	4:C:619:PCW:H442	0.89	1.97	8	1
4:C:609:PCW:H251	5:C:626:17F:H70	0.89	1.41	7	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:504:PCW:O31	4:D:516:PCW:H61	0.89	1.68	1	1
4:D:516:PCW:H452	5:D:529:17F:H49	0.89	1.44	5	1
4:B:202:PCW:O2P	4:D:504:PCW:H32	0.89	1.67	10	1
4:D:506:PCW:O11	4:D:515:PCW:H62	0.89	1.67	10	1
4:B:202:PCW:H322	4:B:202:PCW:H42	0.89	1.44	4	5
4:D:511:PCW:H41	4:D:511:PCW:C3	0.89	1.96	8	3
4:C:616:PCW:H19	4:C:617:PCW:H461	0.89	1.44	6	1
4:C:604:PCW:H461	4:C:624:PCW:C28	0.89	1.96	4	2
4:A:415:PCW:H441	4:C:605:PCW:H451	0.89	1.43	7	5
4:D:513:PCW:H162	5:D:523:17F:H11A	0.89	1.44	5	2
4:B:204:PCW:H52	4:B:204:PCW:O31	0.89	1.67	10	1
4:A:406:PCW:H242	4:B:202:PCW:H252	0.89	1.45	8	1
4:A:410:PCW:H161	4:A:413:PCW:H331	0.89	1.39	7	6
4:C:606:PCW:H42	4:C:624:PCW:H19	0.89	1.45	10	2
4:C:607:PCW:H431	4:C:624:PCW:H481	0.89	1.44	6	2
4:C:611:PCW:C6	4:C:622:PCW:H321	0.89	1.97	8	8
4:D:527:PCW:H462	4:D:528:PCW:H361	0.89	1.42	1	3
4:A:403:PCW:H422	4:D:513:PCW:C40	0.89	1.98	4	4
5:C:629:17F:H8	4:D:528:PCW:C7	0.89	1.96	5	5
4:A:414:PCW:O2P	4:C:617:PCW:H42	0.89	1.67	5	1
4:B:201:PCW:H41	4:D:504:PCW:H132	0.89	1.42	6	1
4:D:506:PCW:H271	4:D:516:PCW:H161	0.89	1.44	7	2
4:C:611:PCW:H222	4:C:619:PCW:C44	0.88	1.96	8	1
4:D:507:PCW:H51	5:D:523:17F:O8	0.88	1.68	10	1
4:D:518:PCW:H162	5:D:519:17F:H33	0.88	1.42	2	1
4:C:618:PCW:H442	4:C:625:PCW:H261	0.88	1.44	4	1
4:B:202:PCW:H172	4:B:202:PCW:H211	0.88	1.41	10	1
4:C:601:PCW:H421	4:C:601:PCW:C46	0.88	1.99	10	8
4:A:406:PCW:H31	4:B:204:PCW:O3	0.88	1.68	10	2
3:D:472:PHE:HB2	3:D:476:CYS:HB2	0.88	1.45	5	9
4:C:606:PCW:H61	4:C:624:PCW:H281	0.88	1.43	7	5
4:A:412:PCW:H483	4:D:517:PCW:H283	0.88	1.43	6	1
4:B:201:PCW:H51	4:D:504:PCW:O11	0.88	1.67	10	1
4:C:620:PCW:H141	5:C:631:17F:O9	0.88	1.67	6	9
4:A:403:PCW:H42	4:D:507:PCW:H341	0.88	1.42	3	1
4:C:606:PCW:H31	5:D:529:17F:O1	0.88	1.67	4	1
4:C:604:PCW:H2	4:C:606:PCW:C8	0.88	1.97	10	3
4:A:415:PCW:H481	5:D:521:17F:H55	0.88	1.43	8	2
5:C:630:17F:H11	5:D:529:17F:H69	0.88	1.43	9	2
4:D:504:PCW:H451	4:D:505:PCW:H39	0.88	1.44	10	2
4:D:504:PCW:H211	4:D:504:PCW:C25	0.88	1.99	4	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:513:PCW:H432	4:D:513:PCW:C47	0.88	1.99	7	10
4:D:517:PCW:H281	5:D:522:17F:H67	0.88	1.43	3	2
4:A:411:PCW:H341	4:C:612:PCW:C13	0.88	1.98	3	2
4:D:503:PCW:H461	4:D:507:PCW:H471	0.88	1.42	10	1
4:A:402:PCW:H352	4:A:402:PCW:O31	0.88	1.69	2	8
4:A:415:PCW:C24	4:D:528:PCW:H242	0.88	1.98	7	8
4:C:609:PCW:H483	4:D:512:PCW:H472	0.88	1.45	3	3
4:D:513:PCW:H41	4:D:513:PCW:O31	0.88	1.69	1	2
4:A:401:PCW:H322	4:D:511:PCW:H39	0.88	1.45	6	1
4:C:607:PCW:C3	4:C:624:PCW:H372	0.87	1.99	2	4
4:C:608:PCW:H262	5:C:627:17F:H35	0.87	1.43	2	2
4:A:404:PCW:H222	4:A:411:PCW:H262	0.87	1.43	4	2
4:D:518:PCW:H471	5:D:521:17F:H12A	0.87	1.46	10	2
4:C:605:PCW:H232	4:C:613:PCW:H161	0.87	1.45	8	1
4:B:201:PCW:H181	4:D:506:PCW:H422	0.87	1.43	1	1
4:D:528:PCW:H141	5:D:530:17F:C1Z	0.87	1.99	4	9
4:D:507:PCW:C14	4:D:513:PCW:H321	0.87	1.95	4	6
5:C:626:17F:H57	5:C:627:17F:H51	0.87	1.46	3	6
4:C:616:PCW:H461	4:C:625:PCW:H262	0.87	1.43	7	2
4:C:617:PCW:H41	4:C:617:PCW:O31	0.87	1.68	9	1
4:C:623:PCW:H19	4:C:623:PCW:C15	0.87	1.99	5	10
4:A:411:PCW:C42	4:C:612:PCW:H231	0.87	1.96	10	5
4:D:509:PCW:C19	5:D:520:17F:H57	0.87	1.99	8	3
4:D:507:PCW:C13	4:D:513:PCW:H122	0.87	1.95	9	1
4:A:403:PCW:H212	4:D:513:PCW:O31	0.87	1.70	8	4
5:C:630:17F:H48	5:D:529:17F:H10	0.87	1.45	5	2
4:C:603:PCW:H52	4:C:603:PCW:O31	0.87	1.70	9	1
4:C:601:PCW:H472	4:C:601:PCW:C43	0.87	2.00	6	2
4:B:203:PCW:H52	4:B:203:PCW:C32	0.87	1.98	1	2
4:C:620:PCW:H132	5:C:631:17F:H18	0.87	1.46	5	4
4:A:406:PCW:H152	4:B:202:PCW:H222	0.87	1.44	7	2
4:D:503:PCW:H231	4:D:503:PCW:C27	0.87	2.00	8	1
4:D:508:PCW:H161	4:D:512:PCW:H172	0.87	1.45	9	1
4:A:415:PCW:H20	4:A:415:PCW:C24	0.87	1.99	10	10
4:C:614:PCW:H421	4:C:614:PCW:C46	0.87	2.00	7	10
4:B:203:PCW:H221	4:B:203:PCW:C26	0.87	1.99	3	10
4:D:506:PCW:H371	4:D:509:PCW:H332	0.87	1.46	2	1
4:D:509:PCW:H411	4:D:509:PCW:C37	0.87	1.97	9	2
4:B:201:PCW:H321	4:D:504:PCW:H151	0.87	1.43	5	1
4:D:506:PCW:O1P	4:D:515:PCW:H52	0.87	1.70	5	1
4:A:408:PCW:H442	4:D:506:PCW:H451	0.87	1.45	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:503:PCW:H172	4:D:511:PCW:C40	0.87	1.99	10	1
4:B:203:PCW:H261	4:B:203:PCW:C22	0.87	2.00	3	10
4:D:518:PCW:H121	5:D:519:17F:H66	0.87	1.44	2	4
4:A:406:PCW:C4	4:B:204:PCW:H32	0.87	2.00	7	4
4:D:508:PCW:H121	4:D:512:PCW:H142	0.87	1.47	5	1
4:B:203:PCW:H19	4:D:506:PCW:H471	0.87	1.45	6	2
4:B:201:PCW:C14	4:D:506:PCW:H361	0.86	2.00	2	2
4:D:501:PCW:H122	4:D:515:PCW:C39	0.86	2.00	2	1
4:D:502:PCW:H281	4:D:518:PCW:H242	0.86	1.44	5	2
4:B:203:PCW:H422	4:B:203:PCW:H142	0.86	1.46	7	1
4:A:414:PCW:H122	5:C:628:17F:C11	0.86	2.00	8	7
4:C:603:PCW:H371	4:C:603:PCW:H412	0.86	1.45	2	9
4:D:504:PCW:C32	4:D:510:PCW:H332	0.86	1.99	1	1
4:A:401:PCW:H483	4:C:614:PCW:H471	0.86	1.44	4	1
4:C:603:PCW:H222	4:D:526:PCW:H332	0.86	1.46	5	3
4:C:606:PCW:C34	4:C:606:PCW:H132	0.86	2.00	7	4
4:C:609:PCW:H232	4:C:615:PCW:H381	0.86	1.46	1	2
4:A:402:PCW:H51	4:A:402:PCW:O11	0.86	1.70	5	3
4:D:502:PCW:H422	4:D:502:PCW:H212	0.86	1.47	7	3
4:D:517:PCW:H73	5:D:520:17F:H4A	0.86	1.44	6	1
4:C:616:PCW:C39	4:C:618:PCW:H162	0.86	2.00	4	8
4:B:203:PCW:H371	4:B:203:PCW:C12	0.86	1.98	4	6
4:A:403:PCW:H42	4:A:403:PCW:C3	0.86	2.00	2	3
4:C:605:PCW:H182	4:C:613:PCW:H362	0.86	1.47	2	10
4:C:608:PCW:C20	5:C:627:17F:H46	0.86	2.00	1	9
4:D:503:PCW:H122	4:D:511:PCW:H39	0.86	1.44	2	2
4:D:507:PCW:H181	4:D:513:PCW:H221	0.86	1.46	8	3
4:C:602:PCW:H212	4:C:602:PCW:C17	0.86	1.98	7	6
4:A:411:PCW:H411	4:A:411:PCW:H371	0.86	1.47	8	4
4:D:507:PCW:H231	4:D:513:PCW:H40	0.86	1.45	9	1
4:C:610:PCW:C6	5:C:629:17F:H6A	0.86	1.98	9	4
4:C:613:PCW:H221	5:D:521:17F:H47	0.86	1.45	5	2
4:A:406:PCW:H152	4:B:202:PCW:H232	0.86	1.46	8	2
5:A:409:17F:H76	5:D:521:17F:H73	0.86	1.46	10	1
4:D:517:PCW:H20	4:D:517:PCW:C24	0.86	1.99	10	10
4:C:612:PCW:H63	4:C:618:PCW:H12	0.86	1.47	7	4
4:B:202:PCW:H11	4:D:504:PCW:C13	0.86	2.01	2	1
4:D:504:PCW:H321	4:D:510:PCW:H361	0.86	1.45	9	2
4:A:413:PCW:C37	4:C:617:PCW:H431	0.86	1.99	1	8
4:C:605:PCW:H211	4:C:613:PCW:H382	0.86	1.48	3	10
4:D:508:PCW:H171	4:D:512:PCW:H342	0.86	1.46	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:513:PCW:C17	5:D:523:17F:H30	0.86	2.00	5	1
4:D:510:PCW:H352	5:D:524:17F:C8	0.86	1.98	6	1
5:D:522:17F:H68	5:D:522:17F:C42	0.86	2.01	6	1
4:D:509:PCW:O3	5:D:520:17F:H4	0.86	1.71	9	4
4:A:401:PCW:H321	4:D:511:PCW:C38	0.86	2.00	10	1
4:C:606:PCW:H73	4:C:624:PCW:H281	0.86	1.46	2	1
4:D:516:PCW:C48	4:D:527:PCW:H252	0.86	2.01	2	1
4:D:504:PCW:H172	4:D:510:PCW:H40	0.86	1.44	7	2
4:C:607:PCW:H342	4:C:624:PCW:H422	0.86	1.45	10	1
4:C:611:PCW:H39	4:C:622:PCW:H471	0.86	1.48	4	1
4:A:403:PCW:H422	4:D:513:PCW:H39	0.86	1.45	8	2
4:D:513:PCW:H451	5:D:522:17F:H78	0.86	1.47	9	1
4:D:515:PCW:H151	5:D:525:17F:H61	0.86	1.45	10	1
4:C:608:PCW:H42	4:C:624:PCW:H242	0.85	1.44	1	2
5:C:630:17F:H29	5:D:529:17F:H71	0.85	1.47	1	2
4:A:405:PCW:C32	4:A:408:PCW:H351	0.85	2.00	9	1
4:A:413:PCW:C1	4:C:617:PCW:H411	0.85	2.01	5	10
4:C:609:PCW:H241	4:C:615:PCW:H381	0.85	1.47	8	4
4:A:406:PCW:C23	4:A:406:PCW:H182	0.85	2.00	6	4
4:C:607:PCW:H12	4:C:624:PCW:H372	0.85	1.44	9	7
4:C:618:PCW:H422	4:C:625:PCW:H261	0.85	1.48	10	3
4:B:201:PCW:H51	4:B:202:PCW:H12	0.85	1.43	5	3
4:D:502:PCW:H141	4:D:505:PCW:C1	0.85	2.01	6	1
4:D:505:PCW:H161	4:D:505:PCW:C42	0.85	1.99	7	3
4:C:615:PCW:H452	4:D:512:PCW:C24	0.85	2.00	9	1
4:D:503:PCW:H381	4:D:511:PCW:H352	0.85	1.46	4	2
4:B:202:PCW:H322	4:B:202:PCW:H41	0.85	1.48	2	1
4:D:505:PCW:H352	5:D:519:17F:H9A	0.85	1.47	8	1
4:D:507:PCW:H232	4:D:513:PCW:H281	0.85	1.48	9	1
4:D:511:PCW:H51	4:D:511:PCW:C1	0.85	2.02	1	1
4:D:513:PCW:H262	4:D:513:PCW:C22	0.85	2.02	2	10
4:D:516:PCW:H432	4:D:516:PCW:C47	0.85	2.02	3	10
4:C:618:PCW:H151	4:C:625:PCW:H142	0.85	1.46	5	8
4:C:606:PCW:C6	4:C:624:PCW:H281	0.85	2.01	10	5
4:C:608:PCW:H41	4:C:624:PCW:C22	0.85	2.01	9	4
4:D:505:PCW:H221	4:D:505:PCW:C18	0.85	2.00	9	4
4:A:414:PCW:O31	4:C:617:PCW:H52	0.85	1.70	6	5
4:C:606:PCW:H182	4:C:606:PCW:C14	0.85	2.00	4	10
4:D:504:PCW:H351	4:D:516:PCW:H141	0.85	1.49	6	1
4:A:402:PCW:H411	4:D:512:PCW:H361	0.85	1.47	7	5
4:A:411:PCW:H422	4:C:612:PCW:H212	0.85	1.48	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:615:PCW:H211	5:C:631:17F:H41	0.85	1.46	5	4
4:D:508:PCW:H63	4:D:517:PCW:H321	0.85	1.47	9	2
4:D:501:PCW:H461	5:D:525:17F:H43	0.85	1.47	9	1
4:A:412:PCW:H431	4:C:623:PCW:C46	0.85	2.02	1	8
4:D:511:PCW:H51	4:D:511:PCW:H12	0.85	1.47	1	1
4:D:504:PCW:H262	4:D:510:PCW:H40	0.85	1.46	3	2
5:D:521:17F:H10	5:D:521:17F:H59	0.85	1.46	7	3
4:D:503:PCW:C40	5:D:522:17F:H9A	0.85	2.01	8	1
4:D:507:PCW:H11	5:D:523:17F:H8A	0.85	1.48	3	3
4:C:618:PCW:H251	4:B:201:PCW:H442	0.85	1.48	5	2
4:D:505:PCW:H182	4:D:505:PCW:C22	0.85	2.02	7	4
1:A:365:LYS:HB2	1:A:366:PRO:HD3	0.85	1.49	5	10
4:A:406:PCW:O4P	4:A:406:PCW:H31	0.85	1.72	5	4
5:C:626:17F:C32	5:C:627:17F:H51	0.85	2.02	2	6
4:C:615:PCW:H2	4:C:615:PCW:H42	0.85	1.49	7	7
4:C:618:PCW:H361	4:C:625:PCW:H172	0.85	1.47	7	5
4:C:608:PCW:H461	5:C:626:17F:C34	0.85	2.02	3	4
4:D:502:PCW:C17	4:D:505:PCW:H122	0.84	2.01	5	4
4:D:509:PCW:C16	5:D:520:17F:H56	0.84	2.03	7	1
4:C:602:PCW:H341	5:D:523:17F:H61	0.84	1.46	3	3
4:C:606:PCW:H142	4:C:606:PCW:C18	0.84	1.99	6	10
4:D:503:PCW:H471	4:D:511:PCW:H281	0.84	1.45	2	1
4:D:504:PCW:H483	5:D:519:17F:H45	0.84	1.48	10	1
4:A:415:PCW:H82	4:C:605:PCW:O2P	0.84	1.71	10	8
5:C:631:17F:H52	4:D:512:PCW:H181	0.84	1.48	4	5
5:D:530:17F:H36	5:D:530:17F:H65	0.84	1.47	1	4
5:C:630:17F:C8	5:D:529:17F:H69	0.84	2.02	2	3
4:B:203:PCW:C31	4:B:203:PCW:H352	0.84	2.02	9	2
4:C:607:PCW:H341	4:C:624:PCW:H372	0.84	1.49	8	1
4:D:515:PCW:C43	4:D:516:PCW:H31	0.84	2.03	9	1
4:B:201:PCW:H461	4:B:201:PCW:C42	0.84	2.02	7	8
5:D:522:17F:H6A	5:D:525:17F:H2	0.84	1.47	1	1
4:C:610:PCW:H63	5:C:629:17F:C6	0.84	2.00	9	4
4:A:413:PCW:H362	4:C:617:PCW:H412	0.84	1.48	3	8
4:C:616:PCW:C34	4:D:527:PCW:H341	0.84	2.01	8	8
4:C:618:PCW:H131	4:C:625:PCW:H151	0.84	1.47	10	4
4:C:622:PCW:H382	4:C:623:PCW:C17	0.84	2.02	4	5
5:D:519:17F:H61	5:D:521:17F:H37	0.84	1.50	2	1
4:D:508:PCW:C13	4:D:509:PCW:H222	0.84	2.02	4	2
4:A:401:PCW:H62	4:D:511:PCW:H32	0.84	1.48	6	1
4:D:509:PCW:H142	5:D:520:17F:C33	0.84	2.01	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:602:PCW:C4	5:D:523:17F:H19	0.84	2.03	4	1
4:C:614:PCW:C45	4:C:619:PCW:H20	0.84	2.03	6	2
4:A:403:PCW:H61	4:A:407:PCW:O2P	0.84	1.72	5	1
4:D:528:PCW:H19	5:D:530:17F:C20	0.84	2.00	5	2
4:D:508:PCW:H19	4:D:509:PCW:H221	0.84	1.50	8	1
4:A:413:PCW:H451	4:D:526:PCW:C21	0.84	2.01	1	5
4:C:621:PCW:H412	5:C:631:17F:H75	0.84	1.47	3	5
4:A:411:PCW:H332	4:C:612:PCW:O11	0.84	1.71	10	1
4:D:503:PCW:H361	4:D:511:PCW:C37	0.84	2.02	1	2
4:D:506:PCW:H252	4:D:506:PCW:C21	0.84	2.01	10	10
4:D:513:PCW:H52	5:D:523:17F:H4	0.84	1.49	9	2
4:D:515:PCW:H161	5:D:520:17F:H41	0.84	1.47	1	1
4:D:506:PCW:O11	4:D:506:PCW:H2	0.84	1.73	10	2
4:D:507:PCW:O2P	4:D:517:PCW:H31	0.84	1.72	5	1
4:D:504:PCW:C48	4:D:516:PCW:H20	0.84	2.02	6	2
4:D:510:PCW:H351	5:D:524:17F:H8	0.84	1.48	10	1
5:D:529:17F:H19	5:D:529:17F:H5	0.84	1.49	4	4
4:C:622:PCW:H371	4:C:622:PCW:O3	0.84	1.72	4	1
4:D:509:PCW:H351	5:D:520:17F:H66	0.84	1.50	5	1
4:D:516:PCW:H41	4:D:516:PCW:O31	0.84	1.71	6	2
4:D:507:PCW:H421	4:D:517:PCW:H231	0.84	1.46	8	2
4:A:412:PCW:H82	4:C:624:PCW:H362	0.83	1.48	3	2
4:D:512:PCW:H231	4:D:512:PCW:C27	0.83	2.02	5	1
4:C:613:PCW:H142	4:C:619:PCW:C39	0.83	2.03	8	1
4:D:502:PCW:H19	4:D:505:PCW:H142	0.83	1.50	8	1
4:D:518:PCW:H341	5:D:519:17F:H33	0.83	1.50	9	1
4:D:508:PCW:H52	5:D:523:17F:C9	0.83	2.02	2	1
4:C:611:PCW:H472	4:D:501:PCW:C27	0.83	2.00	3	1
4:D:509:PCW:H142	5:D:520:17F:H20A	0.83	1.46	9	2
4:B:202:PCW:H251	4:D:504:PCW:H281	0.83	1.49	8	1
4:C:604:PCW:H372	4:C:604:PCW:H422	0.83	1.47	6	8
5:C:626:17F:H78	5:D:523:17F:H53	0.83	1.48	6	3
4:D:502:PCW:H351	4:D:502:PCW:C31	0.83	2.03	7	10
4:A:405:PCW:H63	4:D:514:PCW:H371	0.83	1.50	3	4
4:C:620:PCW:H372	4:C:620:PCW:H412	0.83	1.50	8	6
4:D:508:PCW:H332	4:D:512:PCW:C12	0.83	2.01	5	1
4:C:604:PCW:H482	4:C:624:PCW:C28	0.83	2.03	7	7
4:D:504:PCW:H251	4:D:504:PCW:C21	0.83	2.01	6	10
4:A:408:PCW:H351	4:D:514:PCW:H40	0.83	1.48	4	1
4:D:508:PCW:H19	4:D:509:PCW:C22	0.83	2.03	8	2
5:C:631:17F:H52	4:D:512:PCW:H211	0.83	1.49	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:617:PCW:H232	4:C:617:PCW:C27	0.83	2.03	8	10
4:A:412:PCW:H483	4:D:517:PCW:H471	0.83	1.49	7	2
5:D:519:17F:H61	5:D:521:17F:C21	0.83	2.04	2	1
5:A:409:17F:H77	4:C:611:PCW:H471	0.83	1.50	2	1
4:C:616:PCW:H31	4:C:616:PCW:O2P	0.83	1.71	9	4
4:A:402:PCW:H441	4:D:512:PCW:H121	0.83	1.50	9	1
4:B:202:PCW:H2	5:D:524:17F:H18A	0.83	1.49	10	1
4:C:602:PCW:H221	4:C:602:PCW:H172	0.83	1.51	2	3
4:A:403:PCW:H272	4:D:507:PCW:C19	0.83	2.03	10	5
4:C:607:PCW:H11	4:C:624:PCW:H372	0.83	1.51	5	3
4:A:411:PCW:C43	4:C:612:PCW:H181	0.83	2.03	9	1
4:C:608:PCW:C19	5:C:627:17F:H46	0.83	2.03	8	10
4:B:201:PCW:C48	4:D:527:PCW:H232	0.83	2.03	1	1
4:C:605:PCW:C31	4:C:613:PCW:H62	0.83	2.04	6	6
4:D:507:PCW:H132	4:D:513:PCW:H131	0.83	1.50	7	4
4:D:515:PCW:H412	4:D:515:PCW:C37	0.83	1.98	9	2
4:A:407:PCW:H461	4:A:412:PCW:H272	0.83	1.50	9	4
4:C:605:PCW:H461	4:C:619:PCW:H483	0.83	1.49	5	1
4:D:508:PCW:C7	5:D:520:17F:H2	0.83	2.03	7	1
4:C:621:PCW:H20	4:D:528:PCW:H82	0.83	1.51	9	7
4:C:615:PCW:H63	5:C:631:17F:H2	0.83	1.49	10	1
4:A:414:PCW:O3	5:C:628:17F:H9	0.83	1.72	9	6
4:D:505:PCW:H461	4:D:518:PCW:H282	0.83	1.48	3	1
4:C:607:PCW:H31	4:C:624:PCW:H411	0.83	1.48	10	2
4:D:518:PCW:H162	5:D:519:17F:C32	0.83	2.04	8	1
4:D:502:PCW:H232	4:D:502:PCW:H431	0.83	1.48	9	1
4:D:503:PCW:H461	4:D:511:PCW:H442	0.82	1.51	1	1
4:D:516:PCW:H472	4:D:516:PCW:C43	0.82	2.04	4	9
4:A:402:PCW:H181	4:A:405:PCW:H211	0.82	1.50	3	3
5:C:626:17F:H8	5:C:627:17F:H33	0.82	1.49	10	2
4:A:414:PCW:H381	4:C:617:PCW:H151	0.82	1.51	7	1
4:D:509:PCW:H182	4:D:512:PCW:H331	0.82	1.49	7	2
4:D:506:PCW:C22	4:D:516:PCW:H351	0.82	2.03	1	2
4:D:501:PCW:H211	5:D:521:17F:H19	0.82	1.48	9	2
4:D:503:PCW:H432	5:D:522:17F:C17	0.82	2.04	5	1
4:C:603:PCW:H41	4:C:603:PCW:C2	0.82	1.99	3	8
4:D:517:PCW:H422	5:D:525:17F:H10	0.82	1.49	2	1
4:A:403:PCW:H241	4:D:507:PCW:H171	0.82	1.51	2	3
4:A:413:PCW:C36	4:C:617:PCW:H412	0.82	2.05	6	8
4:C:621:PCW:H142	4:C:621:PCW:C18	0.82	2.04	6	10
4:A:404:PCW:C27	4:A:411:PCW:H241	0.82	2.04	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:516:PCW:H481	4:D:527:PCW:H252	0.82	1.49	2	1
4:D:502:PCW:H283	4:D:505:PCW:H121	0.82	1.51	4	1
4:D:502:PCW:H342	4:D:505:PCW:H12	0.82	1.50	9	2
4:C:613:PCW:H261	5:D:521:17F:H71	0.82	1.51	9	2
4:D:505:PCW:H372	5:D:519:17F:H11	0.82	1.48	8	1
4:C:613:PCW:H31	4:C:619:PCW:H2	0.82	1.49	6	6
4:C:618:PCW:H131	4:C:625:PCW:C15	0.82	2.04	10	3
4:D:506:PCW:C20	4:D:516:PCW:H362	0.82	2.05	5	2
4:D:515:PCW:H32	4:D:517:PCW:H12	0.82	1.50	6	1
4:C:617:PCW:H431	4:C:617:PCW:C47	0.82	2.04	8	1
4:C:624:PCW:H271	4:C:624:PCW:C23	0.82	2.03	6	9
4:D:503:PCW:O3P	4:D:503:PCW:H73	0.82	1.75	4	7
4:C:613:PCW:H251	5:D:521:17F:C27	0.82	2.04	9	6
4:C:622:PCW:H211	4:D:515:PCW:H251	0.82	1.50	2	1
4:A:403:PCW:C21	4:D:513:PCW:H351	0.82	2.03	9	1
4:D:514:PCW:C25	4:D:514:PCW:H212	0.82	2.03	9	1
4:A:401:PCW:H472	4:C:611:PCW:H232	0.82	1.50	10	1
4:A:411:PCW:H442	4:C:612:PCW:H242	0.82	1.50	10	4
4:B:201:PCW:H421	4:B:201:PCW:C46	0.82	2.03	7	8
4:D:502:PCW:H472	4:D:505:PCW:H283	0.82	1.47	10	3
4:D:506:PCW:H271	4:D:516:PCW:H122	0.82	1.49	2	1
4:C:614:PCW:H142	4:C:622:PCW:H481	0.82	1.50	5	1
4:B:201:PCW:H362	4:D:510:PCW:C38	0.82	2.04	8	1
4:A:413:PCW:C45	4:D:526:PCW:H211	0.82	2.05	10	5
4:B:203:PCW:H141	4:B:204:PCW:H382	0.82	1.49	10	5
4:A:406:PCW:H242	4:B:202:PCW:H231	0.82	1.51	6	2
4:D:506:PCW:C6	5:D:520:17F:H6A	0.82	2.03	5	1
4:D:504:PCW:H332	4:D:516:PCW:H82	0.82	1.52	6	1
4:D:511:PCW:H171	5:D:522:17F:O10	0.82	1.74	3	3
4:A:411:PCW:H471	4:C:612:PCW:H271	0.82	1.50	10	4
4:D:505:PCW:H352	4:D:505:PCW:H51	0.82	1.52	5	1
4:C:603:PCW:H421	4:D:526:PCW:H362	0.82	1.51	6	7
4:B:201:PCW:H422	5:D:524:17F:H48	0.82	1.52	5	1
4:A:411:PCW:H2	4:A:411:PCW:H42	0.82	1.49	7	1
5:C:630:17F:C41	4:D:514:PCW:H252	0.82	2.05	7	1
4:B:203:PCW:H282	4:D:506:PCW:H452	0.81	1.51	4	1
5:D:524:17F:H12	5:D:524:17F:C37	0.81	2.05	5	1
4:D:518:PCW:H432	4:D:518:PCW:C47	0.81	2.04	9	10
4:A:402:PCW:H82	4:A:405:PCW:H32	0.81	1.52	6	2
4:C:621:PCW:H222	5:C:629:17F:H31	0.81	1.50	4	4
4:C:622:PCW:C23	4:D:501:PCW:H481	0.81	2.05	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:515:PCW:H82	4:D:516:PCW:H41	0.81	1.52	10	1
4:A:403:PCW:H31	4:A:403:PCW:O1P	0.81	1.73	9	9
4:C:622:PCW:C24	4:D:501:PCW:H381	0.81	2.05	1	1
4:D:518:PCW:O3	4:D:518:PCW:H351	0.81	1.75	4	8
5:D:529:17F:C26	5:D:530:17F:H73	0.81	2.05	1	5
4:A:402:PCW:H321	4:D:514:PCW:O3	0.81	1.75	2	1
4:C:603:PCW:C22	4:D:526:PCW:H351	0.81	2.04	4	5
4:B:201:PCW:H73	4:B:202:PCW:O1P	0.81	1.75	2	1
4:D:508:PCW:H222	4:D:512:PCW:H431	0.81	1.50	2	4
4:D:517:PCW:C42	5:D:525:17F:H10	0.81	2.05	2	1
4:A:402:PCW:H331	4:D:514:PCW:H31	0.81	1.53	3	1
4:D:508:PCW:C22	4:D:512:PCW:H411	0.81	2.05	3	2
4:D:517:PCW:H142	5:D:525:17F:H9A	0.81	1.49	5	1
4:C:618:PCW:H131	4:C:625:PCW:C13	0.81	2.06	7	1
4:A:403:PCW:H283	5:D:523:17F:H20	0.81	1.50	10	3
4:D:509:PCW:H122	5:D:520:17F:C17	0.81	2.04	9	1
4:C:606:PCW:H172	4:C:606:PCW:C21	0.81	2.06	3	10
4:B:201:PCW:C40	4:D:527:PCW:H242	0.81	2.05	2	1
4:B:203:PCW:O2P	4:B:204:PCW:H51	0.81	1.75	8	4
5:D:520:17F:H69	5:D:520:17F:C34	0.81	2.06	6	1
4:A:401:PCW:H181	4:A:401:PCW:H221	0.81	1.49	10	3
4:D:510:PCW:H351	5:D:524:17F:C8	0.81	2.05	10	2
4:C:602:PCW:H362	5:D:523:17F:H61	0.81	1.50	6	3
4:C:620:PCW:C12	5:C:631:17F:H4A	0.81	2.05	1	2
4:A:407:PCW:H2	5:D:522:17F:H33	0.81	1.51	10	1
4:C:604:PCW:H31	4:C:604:PCW:C4	0.81	2.06	3	2
4:D:515:PCW:H62	4:D:515:PCW:O3P	0.81	1.74	3	1
4:A:406:PCW:H42	4:B:204:PCW:H32	0.81	1.49	7	1
4:C:621:PCW:H19	5:C:629:17F:C5	0.81	2.03	2	2
4:D:512:PCW:H61	5:D:520:17F:C1	0.81	1.99	10	1
4:A:414:PCW:P	4:C:617:PCW:H42	0.81	2.15	8	3
4:A:406:PCW:H482	4:B:204:PCW:C25	0.81	2.05	10	1
4:C:620:PCW:H152	5:C:631:17F:H18	0.81	1.51	3	2
4:D:509:PCW:H142	5:D:520:17F:H56	0.81	1.52	4	1
4:B:201:PCW:H242	4:B:203:PCW:H482	0.81	1.51	6	1
4:D:511:PCW:H342	4:D:511:PCW:H182	0.81	1.53	3	4
4:D:506:PCW:H51	5:D:520:17F:O8	0.81	1.75	4	1
4:D:508:PCW:C33	4:D:512:PCW:H121	0.81	2.05	5	1
5:C:626:17F:H57	5:C:626:17F:C19	0.80	2.06	4	10
4:D:502:PCW:C13	4:D:505:PCW:H12	0.80	2.06	1	1
4:A:402:PCW:H73	4:D:514:PCW:O2P	0.80	1.74	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:616:PCW:H31	4:C:616:PCW:C4	0.80	2.05	4	5
5:D:529:17F:C27	5:D:530:17F:H39	0.80	2.04	4	4
4:C:621:PCW:H362	5:C:629:17F:C32	0.80	2.03	9	1
4:D:501:PCW:H161	5:D:521:17F:H20A	0.80	1.53	9	1
5:C:630:17F:H39	5:D:530:17F:C37	0.80	2.06	4	3
5:D:524:17F:H69	5:D:524:17F:H30	0.80	1.51	4	2
4:D:506:PCW:H171	4:D:506:PCW:C13	0.80	2.04	7	8
4:D:512:PCW:H271	4:D:512:PCW:C23	0.80	2.04	9	2
4:D:503:PCW:H272	4:D:503:PCW:C23	0.80	2.05	8	1
4:C:615:PCW:C45	4:D:512:PCW:H241	0.80	2.04	9	1
4:A:401:PCW:H221	4:A:401:PCW:C18	0.80	2.03	6	3
4:D:506:PCW:H20	4:D:516:PCW:H362	0.80	1.50	2	2
4:D:506:PCW:H382	4:D:509:PCW:C33	0.80	2.05	3	1
4:C:623:PCW:C28	5:D:525:17F:H50	0.80	2.07	6	1
4:A:401:PCW:O3P	4:D:511:PCW:H161	0.80	1.77	10	1
4:B:201:PCW:H62	4:D:504:PCW:H51	0.80	1.53	10	1
4:A:401:PCW:H411	4:D:503:PCW:H262	0.80	1.53	1	1
4:C:603:PCW:H261	4:D:526:PCW:H171	0.80	1.52	4	9
4:C:614:PCW:H461	4:C:614:PCW:C42	0.80	2.06	8	10
4:C:616:PCW:C45	4:B:201:PCW:H472	0.80	2.06	2	4
4:C:608:PCW:H262	5:C:627:17F:C2X	0.80	2.06	2	5
5:D:520:17F:H42	5:D:529:17F:H55	0.80	1.51	9	2
4:A:403:PCW:H283	5:D:523:17F:C20	0.80	2.06	10	2
4:C:604:PCW:C2	4:C:606:PCW:H82	0.80	2.03	10	1
4:C:621:PCW:H141	5:C:630:17F:C6	0.80	2.03	7	7
4:A:402:PCW:H421	4:D:512:PCW:H152	0.80	1.52	7	1
4:D:505:PCW:H372	5:D:519:17F:C11	0.80	2.06	8	1
4:D:515:PCW:H472	4:D:515:PCW:H122	0.80	1.50	9	1
4:C:617:PCW:H272	4:C:617:PCW:C23	0.80	2.02	8	10
4:C:612:PCW:H172	4:C:612:PCW:C21	0.80	2.06	5	5
4:C:620:PCW:H121	5:C:631:17F:H4A	0.80	1.50	1	5
4:D:506:PCW:H132	4:D:506:PCW:C17	0.80	2.06	7	9
4:C:603:PCW:H82	4:C:603:PCW:O31	0.80	1.76	2	4
4:C:607:PCW:H431	4:C:623:PCW:H471	0.80	1.50	5	7
4:B:201:PCW:H41	4:D:504:PCW:O11	0.80	1.76	5	1
4:A:403:PCW:H232	4:D:513:PCW:C31	0.80	2.07	10	2
5:D:522:17F:H77	5:D:522:17F:C38	0.80	2.05	6	1
4:A:402:PCW:H352	4:A:402:PCW:C31	0.80	2.07	1	10
4:C:604:PCW:H19	5:D:525:17F:H76	0.80	1.52	1	1
4:D:513:PCW:H472	4:D:513:PCW:C43	0.80	2.05	10	10
4:D:518:PCW:H472	4:D:518:PCW:C43	0.80	2.05	2	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:603:PCW:H242	4:D:526:PCW:H352	0.80	1.54	7	7
4:C:618:PCW:H131	4:C:625:PCW:H132	0.80	1.54	7	2
5:C:630:17F:H29	5:D:529:17F:C38	0.80	2.06	7	2
4:A:412:PCW:O1P	4:C:623:PCW:H322	0.80	1.77	1	2
4:B:201:PCW:C48	4:D:527:PCW:H231	0.80	2.06	10	2
4:D:501:PCW:H431	4:D:515:PCW:H161	0.80	1.53	7	1
4:C:616:PCW:H451	4:B:201:PCW:C47	0.80	2.04	1	4
4:C:620:PCW:O1P	4:C:621:PCW:H52	0.80	1.76	2	7
4:C:625:PCW:C4	4:C:625:PCW:H2	0.80	2.07	1	1
2:B:21:ILE:HD13	3:D:388:VAL:HG11	0.80	1.54	6	3
4:D:527:PCW:H462	5:D:529:17F:H76	0.80	1.52	8	2
4:A:412:PCW:H40	4:C:623:PCW:H461	0.79	1.52	1	3
4:D:505:PCW:H452	4:D:518:PCW:H261	0.79	1.53	1	2
4:C:607:PCW:H12	4:C:624:PCW:C36	0.79	2.07	10	5
5:C:626:17F:H36	5:C:627:17F:H75	0.79	1.54	3	3
4:A:404:PCW:H372	4:D:510:PCW:H182	0.79	1.54	1	1
4:C:601:PCW:H432	4:C:601:PCW:C47	0.79	2.06	6	2
4:D:503:PCW:H482	4:D:511:PCW:H462	0.79	1.54	1	1
4:A:412:PCW:O1P	4:C:614:PCW:H41	0.79	1.77	2	2
4:C:601:PCW:H461	4:C:601:PCW:C42	0.79	2.05	10	8
4:D:527:PCW:C46	5:D:529:17F:H76	0.79	2.07	8	3
4:D:507:PCW:H322	4:D:517:PCW:H121	0.79	1.54	5	1
4:B:202:PCW:H11	4:D:504:PCW:H32	0.79	1.52	3	2
4:D:517:PCW:H241	4:D:517:PCW:C20	0.79	2.07	4	10
4:C:605:PCW:H442	4:C:619:PCW:H451	0.79	1.51	3	1
4:A:401:PCW:H381	4:D:503:PCW:H231	0.79	1.55	6	2
4:B:201:PCW:C16	4:D:506:PCW:H442	0.79	2.08	5	4
4:A:413:PCW:H362	4:C:617:PCW:C38	0.79	2.06	7	4
4:D:509:PCW:H162	5:D:520:17F:H60	0.79	1.54	7	1
4:A:415:PCW:H471	5:D:521:17F:H51	0.79	1.53	1	1
4:C:625:PCW:H2	4:C:625:PCW:H41	0.79	1.55	1	1
4:C:605:PCW:H421	4:C:619:PCW:H141	0.79	1.52	5	6
4:B:203:PCW:H372	4:B:204:PCW:C8	0.79	2.07	2	2
4:B:203:PCW:H161	4:B:204:PCW:H382	0.79	1.54	3	5
4:A:402:PCW:C12	4:A:405:PCW:H132	0.79	2.07	6	3
4:A:401:PCW:C24	4:C:614:PCW:H281	0.79	2.08	6	1
4:D:504:PCW:H31	4:D:510:PCW:H352	0.79	1.53	10	1
4:A:406:PCW:H272	4:C:618:PCW:H452	0.79	1.55	1	1
4:C:602:PCW:H462	5:C:626:17F:C36	0.79	2.07	1	2
4:C:614:PCW:H63	4:C:623:PCW:O1P	0.79	1.77	3	6
4:D:502:PCW:H332	4:D:510:PCW:O4P	0.79	1.77	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:518:PCW:H442	5:D:519:17F:H68	0.79	1.51	4	2
4:D:504:PCW:H271	4:D:504:PCW:H161	0.79	1.52	4	1
4:D:513:PCW:H121	5:D:523:17F:O9	0.79	1.77	10	4
4:A:401:PCW:H462	4:C:614:PCW:H242	0.79	1.52	10	2
4:B:201:PCW:H212	4:D:506:PCW:H452	0.79	1.53	10	1
4:B:202:PCW:H2	5:D:524:17F:C18	0.79	2.08	10	1
4:D:506:PCW:H12	4:D:515:PCW:H62	0.79	1.54	1	2
4:D:527:PCW:H422	4:D:528:PCW:C33	0.79	2.07	6	5
4:A:402:PCW:C33	4:D:514:PCW:H31	0.79	2.08	3	1
4:A:415:PCW:C7	4:C:605:PCW:H332	0.79	2.07	3	3
5:D:530:17F:H60	5:D:530:17F:H10A	0.79	1.54	6	3
4:D:508:PCW:H151	4:D:512:PCW:H171	0.79	1.53	6	1
4:D:517:PCW:H442	5:D:525:17F:H40	0.79	1.53	10	1
5:C:626:17F:H40	5:C:627:17F:H78	0.79	1.54	1	2
4:A:403:PCW:C8	4:D:507:PCW:H341	0.79	2.08	4	1
4:C:607:PCW:C47	4:D:513:PCW:H462	0.79	2.08	4	1
4:B:202:PCW:H62	5:D:524:17F:C3	0.79	2.08	10	3
4:A:413:PCW:H461	4:C:616:PCW:H251	0.79	1.54	1	2
4:C:602:PCW:O2	5:D:523:17F:H56	0.79	1.78	4	2
4:D:508:PCW:H141	4:D:509:PCW:C22	0.79	2.06	2	1
4:A:402:PCW:C44	4:D:512:PCW:H132	0.79	2.08	3	1
4:D:518:PCW:H252	5:D:519:17F:C33	0.79	2.08	3	1
4:A:403:PCW:C39	4:A:407:PCW:H371	0.79	2.08	1	1
4:C:611:PCW:H162	4:C:619:PCW:H171	0.79	1.55	1	3
4:C:617:PCW:O31	4:C:617:PCW:H12	0.79	1.78	4	10
2:B:84:ILE:HD11	2:B:118:CYS:HA	0.79	1.54	3	10
5:D:525:17F:H72	5:D:525:17F:H44	0.79	1.54	9	3
4:A:411:PCW:H332	4:C:612:PCW:C13	0.79	2.07	4	3
4:B:201:PCW:H272	4:D:528:PCW:H421	0.79	1.52	8	3
4:B:201:PCW:H431	4:D:510:PCW:H411	0.79	1.52	4	1
4:A:413:PCW:H382	4:D:526:PCW:C23	0.79	2.07	5	1
4:A:415:PCW:H321	4:A:415:PCW:C7	0.79	2.07	5	2
4:D:511:PCW:H19	5:D:522:17F:O10	0.79	1.77	9	1
4:A:407:PCW:C19	4:A:407:PCW:C14	0.78	2.60	7	10
4:D:513:PCW:H222	4:D:513:PCW:C26	0.78	2.07	5	9
4:D:504:PCW:H12	4:D:504:PCW:O31	0.78	1.78	9	6
4:D:515:PCW:H12	4:D:515:PCW:C5	0.78	2.07	2	3
4:D:511:PCW:C11	4:D:511:PCW:H73	0.78	2.08	3	4
5:D:530:17F:H10A	5:D:530:17F:H56	0.78	1.55	4	2
4:A:411:PCW:H331	4:C:612:PCW:H132	0.78	1.54	6	1
4:D:503:PCW:H411	4:D:511:PCW:H352	0.78	1.54	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:513:PCW:H241	4:D:513:PCW:C48	0.78	2.07	9	1
4:A:403:PCW:H31	4:A:403:PCW:O4P	0.78	1.77	6	6
4:C:606:PCW:H132	4:C:606:PCW:H341	0.78	1.54	7	4
4:B:203:PCW:H52	4:B:203:PCW:H321	0.78	1.55	1	1
4:D:503:PCW:H361	4:D:511:PCW:H371	0.78	1.53	4	2
4:A:405:PCW:H51	4:D:514:PCW:H321	0.78	1.56	9	6
5:C:630:17F:C28	5:D:529:17F:H10	0.78	2.08	10	4
4:C:603:PCW:H222	4:D:526:PCW:H331	0.78	1.52	5	5
4:C:618:PCW:H261	4:D:510:PCW:H483	0.78	1.55	5	2
4:D:518:PCW:C32	5:D:519:17F:H20	0.78	2.02	9	1
4:C:616:PCW:H282	4:D:510:PCW:C27	0.78	2.08	5	1
4:A:412:PCW:H431	4:C:623:PCW:H462	0.78	1.54	5	7
4:D:516:PCW:H232	5:D:519:17F:H42	0.78	1.52	6	1
4:A:414:PCW:H61	5:C:628:17F:C4	0.78	2.08	7	2
3:D:465:CYS:HB2	3:D:469:GLY:H	0.78	1.38	7	1
4:D:507:PCW:C3	4:D:513:PCW:H152	0.78	2.08	7	1
4:A:406:PCW:H41	4:B:204:PCW:H32	0.78	1.52	1	3
4:C:614:PCW:H452	4:C:619:PCW:H222	0.78	1.56	2	4
4:C:621:PCW:H283	4:D:528:PCW:H61	0.78	1.54	9	5
4:A:401:PCW:H452	4:C:611:PCW:H251	0.78	1.54	10	3
4:A:403:PCW:H341	4:A:407:PCW:H321	0.78	1.52	10	3
4:A:404:PCW:H222	4:A:411:PCW:C26	0.78	2.08	4	1
4:C:613:PCW:H241	5:D:521:17F:H71	0.78	1.54	7	1
4:A:411:PCW:H411	4:C:612:PCW:H181	0.78	1.55	1	2
4:D:516:PCW:H40	4:D:527:PCW:H252	0.78	1.55	3	1
4:A:401:PCW:H322	4:D:511:PCW:C39	0.78	2.08	6	3
4:D:518:PCW:H422	5:D:519:17F:H70	0.78	1.53	5	1
4:D:509:PCW:H52	4:D:514:PCW:O1P	0.78	1.77	6	1
4:C:606:PCW:H63	4:C:624:PCW:H281	0.78	1.56	8	1
4:C:611:PCW:H221	4:C:619:PCW:C46	0.78	2.08	9	1
4:D:506:PCW:C33	4:D:509:PCW:H371	0.78	2.08	1	1
4:C:618:PCW:C38	4:C:625:PCW:H161	0.78	2.07	2	7
4:B:202:PCW:H472	4:D:510:PCW:H481	0.78	1.53	2	1
4:C:606:PCW:H62	4:C:624:PCW:H19	0.78	1.53	8	2
4:C:608:PCW:C43	5:C:626:17F:H34	0.78	2.03	4	3
4:C:611:PCW:H321	4:C:622:PCW:C35	0.78	2.01	10	4
4:D:515:PCW:C23	4:D:515:PCW:H181	0.78	2.08	9	1
4:C:610:PCW:H241	4:C:610:PCW:C20	0.78	2.09	8	10
4:D:528:PCW:H141	5:D:530:17F:H32	0.78	1.54	3	6
4:C:606:PCW:H411	5:C:630:17F:H55	0.78	1.56	5	2
4:D:508:PCW:H221	4:D:512:PCW:H19	0.78	1.54	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:518:PCW:C14	5:D:519:17F:H66	0.78	2.09	9	1
4:A:407:PCW:H162	4:A:412:PCW:H283	0.78	1.56	2	1
4:A:401:PCW:H472	4:C:611:PCW:H461	0.78	1.54	3	1
4:A:403:PCW:H141	4:A:403:PCW:C40	0.78	2.09	3	1
4:A:401:PCW:C42	4:C:611:PCW:H271	0.78	2.06	9	1
4:A:410:PCW:H61	5:C:628:17F:O4	0.78	1.79	1	1
4:C:620:PCW:H283	5:C:631:17F:H37	0.78	1.55	1	1
4:C:625:PCW:H20	4:D:528:PCW:H351	0.78	1.56	10	8
4:B:202:PCW:C48	4:D:510:PCW:H221	0.78	2.09	1	1
4:C:606:PCW:H51	4:C:606:PCW:O11	0.78	1.77	3	1
4:A:405:PCW:H181	4:A:405:PCW:H39	0.78	1.56	4	1
4:C:613:PCW:H221	5:D:521:17F:H43	0.78	1.54	7	4
5:D:530:17F:H59	5:D:530:17F:C12	0.77	2.08	9	6
4:B:201:PCW:H232	4:D:506:PCW:C44	0.77	2.09	3	1
4:C:615:PCW:H261	5:C:631:17F:H45	0.77	1.55	7	1
4:C:603:PCW:H261	4:D:526:PCW:C14	0.77	2.09	6	8
4:C:622:PCW:H232	4:D:501:PCW:H481	0.77	1.53	4	1
4:C:611:PCW:O2P	4:C:619:PCW:H63	0.77	1.78	1	3
4:D:516:PCW:H51	4:D:516:PCW:O11	0.77	1.79	3	2
4:D:515:PCW:H32	5:D:525:17F:H56	0.77	1.54	4	1
4:D:503:PCW:H421	4:D:511:PCW:H19	0.77	1.54	8	1
5:C:626:17F:H19A	5:C:626:17F:C31	0.77	2.09	9	10
4:C:611:PCW:H63	4:C:622:PCW:C32	0.77	2.09	6	7
4:C:616:PCW:H31	4:C:616:PCW:P	0.77	2.20	9	9
4:D:505:PCW:O2P	4:D:510:PCW:H52	0.77	1.80	6	3
4:A:403:PCW:H352	4:A:407:PCW:H322	0.77	1.56	6	1
4:A:414:PCW:C12	5:C:628:17F:H9	0.77	2.09	1	7
4:C:604:PCW:H482	4:C:624:PCW:H281	0.77	1.55	1	3
4:C:605:PCW:H181	4:C:613:PCW:H362	0.77	1.54	10	7
4:C:606:PCW:H161	5:D:529:17F:C11	0.77	2.10	7	5
4:D:508:PCW:H151	4:D:512:PCW:C15	0.77	2.08	1	1
4:A:407:PCW:C18	4:A:412:PCW:H261	0.77	2.09	2	1
4:A:412:PCW:H452	4:C:623:PCW:H462	0.77	1.56	2	6
4:C:608:PCW:C4	4:C:624:PCW:H222	0.77	2.08	9	3
4:A:406:PCW:H222	4:B:204:PCW:H452	0.77	1.57	10	2
2:B:15:GLY:HA3	6:B:205:GNP:H8	0.77	1.57	9	4
4:B:203:PCW:H422	4:B:203:PCW:C16	0.77	2.08	4	1
4:A:405:PCW:H82	4:D:514:PCW:H351	0.77	1.56	2	5
4:C:604:PCW:H412	4:C:606:PCW:H241	0.77	1.55	9	3
4:D:509:PCW:C28	5:D:520:17F:H19	0.77	2.10	1	1
4:D:504:PCW:C41	4:D:516:PCW:H82	0.77	2.09	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:513:PCW:H32	4:D:513:PCW:P	0.77	2.20	8	7
4:A:406:PCW:H351	4:B:204:PCW:C15	0.77	2.09	3	3
4:D:508:PCW:H372	4:D:512:PCW:H141	0.77	1.56	3	1
4:C:606:PCW:H73	4:C:624:PCW:H171	0.77	1.57	10	2
4:C:624:PCW:H411	4:C:624:PCW:H372	0.77	1.55	4	1
4:C:601:PCW:H11	4:D:513:PCW:H82	0.77	1.55	6	1
4:B:201:PCW:H232	4:D:506:PCW:H452	0.77	1.54	10	2
4:D:509:PCW:H2	5:D:520:17F:H4	0.77	1.56	8	1
4:A:415:PCW:H241	4:A:415:PCW:C20	0.77	2.08	3	10
4:C:622:PCW:H422	5:D:525:17F:H55	0.77	1.57	1	1
5:C:630:17F:C23	5:D:530:17F:H67	0.77	2.10	9	5
4:D:506:PCW:C3	4:D:515:PCW:H31	0.77	2.10	1	1
4:C:606:PCW:C7	4:C:624:PCW:H281	0.77	2.08	2	1
4:C:613:PCW:H283	5:D:521:17F:H63	0.77	1.56	3	1
4:D:516:PCW:H32	4:D:516:PCW:P	0.77	2.20	8	2
3:D:482:THR:HG22	4:D:504:PCW:H62	0.77	1.57	4	1
4:D:502:PCW:H171	4:D:505:PCW:C12	0.77	2.07	5	4
4:D:518:PCW:H141	5:D:519:17F:H72	0.77	1.57	7	1
4:A:413:PCW:H412	4:D:526:PCW:H181	0.77	1.57	8	1
4:D:504:PCW:C33	4:D:510:PCW:H321	0.77	2.10	8	1
4:C:618:PCW:C35	4:C:625:PCW:H341	0.77	2.10	10	1
4:A:412:PCW:H472	4:C:623:PCW:H483	0.77	1.53	9	4
4:A:407:PCW:H2	5:D:522:17F:H31	0.77	1.55	5	3
4:C:602:PCW:H462	5:C:626:17F:H64	0.77	1.56	1	3
4:C:624:PCW:H342	4:C:624:PCW:C12	0.77	2.09	2	1
4:A:405:PCW:H241	4:D:508:PCW:H271	0.77	1.55	10	2
4:A:410:PCW:H452	4:A:414:PCW:H421	0.77	1.55	3	2
4:D:503:PCW:C40	5:D:522:17F:H10A	0.77	2.10	6	3
4:A:401:PCW:H483	4:C:614:PCW:H222	0.77	1.57	9	1
4:D:508:PCW:H61	4:D:517:PCW:O2P	0.77	1.80	1	1
4:D:510:PCW:H331	5:D:524:17F:H11	0.77	1.52	1	1
4:A:407:PCW:H271	4:A:412:PCW:H262	0.77	1.54	2	1
4:B:202:PCW:H51	5:D:524:17F:H1A	0.77	1.57	2	2
4:A:412:PCW:H381	4:C:623:PCW:H251	0.77	1.56	3	6
4:B:203:PCW:H132	4:B:204:PCW:C32	0.77	2.09	7	4
4:D:508:PCW:H73	4:D:517:PCW:O2P	0.77	1.79	4	1
5:C:630:17F:H39	5:D:530:17F:H71	0.77	1.53	6	2
4:D:502:PCW:H161	4:D:505:PCW:H31	0.77	1.56	6	1
4:A:404:PCW:H241	4:A:411:PCW:H262	0.77	1.55	8	1
4:C:606:PCW:H62	4:C:624:PCW:C19	0.77	2.10	8	1
4:A:410:PCW:H451	4:C:617:PCW:C25	0.76	2.09	6	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:623:PCW:H151	4:C:623:PCW:C19	0.76	2.10	5	10
4:C:623:PCW:H41	4:C:623:PCW:O31	0.76	1.80	10	5
4:D:516:PCW:H39	4:D:527:PCW:C27	0.76	1.99	1	1
5:D:519:17F:H65	5:D:519:17F:H58	0.76	1.57	1	2
5:C:630:17F:H11	5:D:529:17F:H68	0.76	1.56	2	4
4:C:622:PCW:H421	4:C:623:PCW:C26	0.76	2.08	2	3
4:A:411:PCW:H441	4:C:612:PCW:H272	0.76	1.58	3	4
4:C:602:PCW:H232	5:C:626:17F:H44	0.76	1.55	3	1
4:C:617:PCW:H51	4:C:617:PCW:C1	0.76	2.09	10	6
4:D:516:PCW:H32	4:D:516:PCW:O4P	0.76	1.79	8	2
4:A:415:PCW:H451	5:D:521:17F:H75	0.76	1.54	10	2
4:C:616:PCW:H451	4:B:201:PCW:C45	0.76	2.08	5	2
4:D:518:PCW:C33	5:D:519:17F:H32	0.76	2.10	7	1
4:C:615:PCW:H211	5:C:631:17F:H38	0.76	1.57	3	2
4:B:201:PCW:H161	4:D:506:PCW:C41	0.76	2.10	3	1
4:D:512:PCW:H351	4:D:514:PCW:H141	0.76	1.56	5	1
4:C:615:PCW:H212	4:C:615:PCW:H171	0.76	1.56	7	1
4:C:601:PCW:H482	5:C:626:17F:H51	0.76	1.57	10	1
4:A:407:PCW:H432	4:A:412:PCW:H241	0.76	1.55	4	5
4:A:411:PCW:H411	4:C:612:PCW:C18	0.76	2.11	1	2
4:C:606:PCW:H132	4:C:606:PCW:C34	0.76	2.09	8	5
4:A:415:PCW:H82	4:C:605:PCW:O3P	0.76	1.80	5	2
4:D:507:PCW:H432	5:D:525:17F:H8	0.76	1.57	3	1
4:D:508:PCW:H141	4:D:509:PCW:C18	0.76	2.10	3	2
4:D:508:PCW:H141	4:D:509:PCW:H182	0.76	1.57	3	2
4:C:613:PCW:C48	4:C:619:PCW:H211	0.76	2.09	6	5
5:C:630:17F:H74	4:D:514:PCW:H232	0.76	1.54	5	1
4:D:508:PCW:H152	4:D:509:PCW:H222	0.76	1.55	6	1
4:C:616:PCW:H39	4:C:618:PCW:H162	0.76	1.55	5	4
4:C:618:PCW:H381	4:C:625:PCW:H181	0.76	1.55	8	3
4:A:403:PCW:H382	4:A:403:PCW:H141	0.76	1.56	6	1
4:A:403:PCW:C27	4:D:507:PCW:H19	0.76	2.10	7	4
4:C:603:PCW:H242	4:D:526:PCW:C35	0.76	2.10	10	2
4:D:502:PCW:H62	5:D:519:17F:C3	0.76	2.09	7	1
4:A:406:PCW:C4	4:A:406:PCW:H31	0.76	2.11	8	1
4:A:414:PCW:H372	4:C:617:PCW:H141	0.76	1.56	9	1
6:B:205:GNP:O2G	7:B:206:MG:MG	0.76	1.29	3	7
4:D:509:PCW:H412	5:D:520:17F:H11A	0.76	1.57	7	3
4:C:601:PCW:C48	5:C:626:17F:H47	0.76	2.10	2	1
4:B:201:PCW:H212	4:D:506:PCW:H442	0.76	1.56	3	1
4:B:201:PCW:H232	4:D:506:PCW:C45	0.76	2.11	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:608:PCW:H452	5:C:626:17F:H60	0.76	1.58	8	5
5:C:628:17F:H5	5:C:628:17F:O8	0.76	1.78	1	5
4:D:502:PCW:H382	4:D:502:PCW:H151	0.76	1.57	2	4
4:B:203:PCW:H211	4:B:204:PCW:H40	0.76	1.57	2	1
4:C:610:PCW:H42	5:C:629:17F:O8	0.76	1.79	9	8
5:A:409:17F:H75	4:D:501:PCW:H281	0.76	1.57	2	1
4:D:517:PCW:H451	5:D:525:17F:H68	0.76	1.56	4	1
4:C:619:PCW:H481	5:D:521:17F:H74	0.76	1.57	5	1
4:C:608:PCW:H63	4:C:624:PCW:H242	0.76	1.58	9	2
4:D:503:PCW:H452	4:D:511:PCW:H20	0.76	1.58	8	1
4:D:508:PCW:H61	4:D:517:PCW:O1P	0.76	1.81	10	1
4:C:608:PCW:C18	5:C:627:17F:H11	0.76	2.10	1	5
4:C:618:PCW:H422	4:C:625:PCW:H231	0.76	1.55	1	3
3:D:476:CYS:HA	3:D:479:LYS:HB2	0.76	1.58	1	1
4:A:407:PCW:H371	5:D:522:17F:H65	0.76	1.55	2	1
4:C:613:PCW:H471	4:C:619:PCW:H422	0.76	1.58	7	1
4:D:508:PCW:H212	4:D:512:PCW:C15	0.76	2.11	8	1
5:D:530:17F:H12A	5:D:530:17F:C32	0.76	2.09	9	8
5:C:630:17F:H49	5:D:529:17F:H10	0.76	1.57	9	3
4:D:517:PCW:H411	4:D:517:PCW:H181	0.76	1.57	2	2
4:A:415:PCW:C8	4:C:605:PCW:H332	0.76	2.11	5	3
4:D:516:PCW:H231	5:D:519:17F:H54	0.76	1.57	3	1
4:C:602:PCW:H351	5:D:523:17F:H77	0.76	1.57	7	1
4:C:618:PCW:H351	4:C:625:PCW:H341	0.76	1.57	10	1
4:C:605:PCW:O31	4:C:605:PCW:P	0.75	2.44	1	10
4:C:625:PCW:C28	5:C:629:17F:H51	0.75	2.11	1	7
4:D:509:PCW:H412	5:D:520:17F:H8	0.75	1.58	8	2
4:B:203:PCW:H412	4:B:203:PCW:H162	0.75	1.58	5	2
4:D:528:PCW:C14	5:D:530:17F:H33	0.75	2.09	6	5
4:A:403:PCW:H52	4:D:507:PCW:H341	0.75	1.57	5	3
4:A:413:PCW:C42	4:C:616:PCW:H232	0.75	2.10	7	3
4:D:509:PCW:O11	4:D:509:PCW:H82	0.75	1.81	6	2
4:D:517:PCW:H352	5:D:520:17F:H11A	0.75	1.58	6	1
4:D:504:PCW:H39	4:D:505:PCW:H51	0.75	1.57	8	1
4:C:608:PCW:C19	5:C:627:17F:H39	0.75	2.11	8	4
4:C:622:PCW:C38	4:C:623:PCW:H171	0.75	2.10	3	4
4:C:608:PCW:H232	5:C:626:17F:H10A	0.75	1.58	3	1
4:A:413:PCW:H481	5:D:524:17F:C21	0.75	2.09	4	1
4:C:620:PCW:H141	5:C:631:17F:H18	0.75	1.57	8	2
4:D:509:PCW:C18	4:D:512:PCW:H331	0.75	2.10	7	2
4:D:507:PCW:O31	4:D:513:PCW:H32	0.75	1.81	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:529:17F:H52	5:D:530:17F:H43	0.75	1.59	4	3
4:C:604:PCW:C45	4:C:606:PCW:H181	0.75	2.10	3	5
4:C:618:PCW:O1P	4:C:625:PCW:H51	0.75	1.80	7	1
4:C:602:PCW:H232	5:C:626:17F:H48	0.75	1.59	8	1
4:D:517:PCW:H432	4:D:517:PCW:C21	0.75	2.11	8	1
4:C:616:PCW:H341	4:D:527:PCW:C34	0.75	2.10	8	3
4:C:621:PCW:H481	5:C:630:17F:H12	0.75	1.58	9	2
4:D:508:PCW:C17	4:D:512:PCW:H362	0.75	2.11	6	1
4:B:204:PCW:H283	4:B:204:PCW:H421	0.75	1.59	3	1
4:D:504:PCW:H483	4:D:516:PCW:C17	0.75	2.12	3	1
4:D:505:PCW:H51	4:D:505:PCW:C35	0.75	2.11	5	1
4:D:518:PCW:C34	5:D:519:17F:H57	0.75	2.09	8	1
4:A:410:PCW:H451	4:C:617:PCW:H242	0.75	1.59	6	8
4:C:618:PCW:H131	4:C:625:PCW:C14	0.75	2.12	7	4
4:D:503:PCW:H121	4:D:511:PCW:C39	0.75	2.10	1	1
4:D:508:PCW:H222	4:D:512:PCW:C41	0.75	2.12	3	3
4:D:508:PCW:H142	4:D:512:PCW:H151	0.75	1.57	6	1
4:A:402:PCW:H442	4:D:508:PCW:H272	0.75	1.58	8	1
4:D:505:PCW:H471	5:D:519:17F:H53	0.75	1.56	9	1
4:D:505:PCW:H442	4:D:518:PCW:H261	0.75	1.56	10	1
4:C:610:PCW:C6	5:C:629:17F:H4A	0.75	2.11	1	1
4:D:509:PCW:H261	5:D:520:17F:H32	0.75	1.59	2	1
4:D:517:PCW:H441	4:D:517:PCW:H222	0.75	1.57	4	1
5:D:530:17F:H10A	5:D:530:17F:C33	0.75	2.12	6	4
4:A:413:PCW:C38	4:D:526:PCW:H231	0.75	2.11	5	1
4:C:607:PCW:O2	4:C:624:PCW:H371	0.75	1.81	6	2
4:C:613:PCW:H142	4:C:619:PCW:H39	0.75	1.58	8	1
4:D:507:PCW:H332	4:D:513:PCW:H332	0.75	1.57	8	1
4:A:406:PCW:C35	4:B:204:PCW:H152	0.75	2.12	1	1
4:A:401:PCW:H322	4:D:511:PCW:C38	0.75	2.12	8	4
4:A:414:PCW:H321	4:C:617:PCW:H51	0.75	1.58	2	1
4:B:203:PCW:H142	4:B:203:PCW:C39	0.75	2.11	6	4
4:D:515:PCW:H282	4:D:528:PCW:H281	0.75	1.59	2	1
5:D:522:17F:H41	5:D:522:17F:H12A	0.75	1.59	4	3
4:C:606:PCW:O31	4:C:606:PCW:H41	0.75	1.82	7	1
4:C:625:PCW:O1P	4:C:625:PCW:H52	0.75	1.81	10	1
4:D:504:PCW:C3	4:D:510:PCW:H352	0.75	2.11	10	1
1:A:307:ASP:HA	1:A:310:ARG:HD2	0.75	1.56	3	6
4:C:601:PCW:H39	4:C:602:PCW:H171	0.75	1.58	4	2
4:B:201:PCW:H272	4:D:528:PCW:H472	0.75	1.57	3	2
4:D:504:PCW:C16	4:D:510:PCW:H39	0.75	2.11	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:A:409:17F:H73	4:D:503:PCW:H282	0.75	1.59	7	1
4:B:203:PCW:H452	4:B:204:PCW:H412	0.75	1.58	7	1
4:D:515:PCW:H321	4:D:516:PCW:C1	0.75	2.12	8	2
4:C:621:PCW:O1P	4:C:621:PCW:H52	0.75	1.82	8	1
4:D:507:PCW:H432	5:D:522:17F:H30	0.75	1.55	8	1
4:B:202:PCW:H281	4:D:506:PCW:H481	0.75	1.58	9	1
4:C:609:PCW:H2	4:C:615:PCW:H61	0.74	1.57	6	5
4:C:618:PCW:H362	5:C:629:17F:C22	0.74	2.11	1	4
4:C:602:PCW:H261	5:C:627:17F:C42	0.74	2.12	2	3
4:B:201:PCW:C1	4:D:504:PCW:H151	0.74	2.10	3	1
4:D:502:PCW:H472	4:D:505:PCW:C28	0.74	2.12	9	3
4:D:508:PCW:H142	4:D:509:PCW:C20	0.74	2.12	7	1
4:D:506:PCW:H221	4:D:516:PCW:H351	0.74	1.57	1	2
4:A:402:PCW:H283	4:D:508:PCW:C28	0.74	2.11	3	1
4:C:608:PCW:H431	5:C:626:17F:C1Z	0.74	2.12	3	4
4:C:616:PCW:C34	4:D:527:PCW:H362	0.74	2.11	3	6
4:A:403:PCW:H332	4:A:407:PCW:H332	0.74	1.59	9	1
4:D:509:PCW:H19	5:D:520:17F:H56	0.74	1.58	1	1
4:A:406:PCW:H261	5:C:629:17F:H54	0.74	1.57	2	2
4:C:603:PCW:H212	4:C:603:PCW:C44	0.74	2.10	3	3
4:C:615:PCW:C21	4:D:512:PCW:H282	0.74	2.11	9	2
4:D:516:PCW:H40	4:D:527:PCW:H283	0.74	1.57	7	5
4:D:502:PCW:H141	4:D:505:PCW:H12	0.74	1.59	6	1
4:D:509:PCW:C17	4:D:512:PCW:H331	0.74	2.12	7	2
4:D:515:PCW:H61	4:D:516:PCW:O31	0.74	1.82	7	1
4:A:404:PCW:H283	4:A:411:PCW:H241	0.74	1.58	8	1
4:A:402:PCW:H442	4:D:512:PCW:H132	0.74	1.56	3	1
4:C:606:PCW:H62	4:C:624:PCW:H281	0.74	1.57	10	2
4:D:510:PCW:H351	5:D:524:17F:C9	0.74	2.12	4	5
4:A:403:PCW:H271	4:D:507:PCW:H19	0.74	1.57	7	1
4:D:516:PCW:C45	5:D:529:17F:H49	0.74	2.11	1	1
4:C:613:PCW:H212	5:D:521:17F:H51	0.74	1.58	5	3
5:D:521:17F:H19A	5:D:521:17F:C31	0.74	2.08	9	6
5:C:626:17F:C22	5:C:627:17F:H75	0.74	2.13	5	2
4:A:411:PCW:H371	4:C:612:PCW:H182	0.74	1.58	9	1
4:D:518:PCW:H181	4:D:518:PCW:H221	0.74	1.58	1	5
4:C:614:PCW:C44	4:C:619:PCW:H20	0.74	2.13	6	4
4:D:501:PCW:H482	5:D:525:17F:H51	0.74	1.60	4	2
4:A:406:PCW:C24	4:B:202:PCW:H231	0.74	2.13	6	1
3:D:479:LYS:HA	4:D:517:PCW:H73	0.74	1.57	7	1
4:D:504:PCW:H121	4:D:510:PCW:H39	0.74	1.58	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:407:PCW:C39	5:D:522:17F:H65	0.74	2.13	1	2
4:C:606:PCW:C16	5:D:529:17F:H11A	0.74	2.12	7	8
4:D:513:PCW:H19	5:D:523:17F:C23	0.74	2.11	1	1
4:C:605:PCW:H171	4:C:613:PCW:H342	0.74	1.59	5	4
4:C:611:PCW:H221	4:C:619:PCW:H482	0.74	1.57	2	2
4:D:513:PCW:H422	4:D:517:PCW:H271	0.74	1.60	2	2
4:C:615:PCW:C47	4:D:512:PCW:H222	0.74	2.09	10	2
4:A:412:PCW:H63	4:C:624:PCW:H2	0.74	1.57	8	3
4:C:604:PCW:C22	4:D:515:PCW:H282	0.74	2.12	9	1
4:D:510:PCW:H351	5:D:524:17F:H8A	0.74	1.59	9	1
4:A:403:PCW:H321	4:A:407:PCW:H52	0.74	1.57	10	1
4:C:618:PCW:H412	5:C:629:17F:H45	0.74	1.58	2	1
4:D:501:PCW:H421	5:D:521:17F:C42	0.74	2.12	3	1
4:D:508:PCW:H211	4:D:512:PCW:H411	0.74	1.59	7	1
4:A:410:PCW:H451	4:C:617:PCW:C24	0.74	2.13	4	8
4:C:621:PCW:C42	5:C:630:17F:H62	0.74	2.11	9	6
4:C:613:PCW:C25	5:D:521:17F:H47	0.74	2.11	9	3
3:D:476:CYS:HA	3:D:479:LYS:HB3	0.74	1.59	5	4
4:A:415:PCW:H242	4:D:528:PCW:C24	0.74	2.07	7	7
4:C:605:PCW:O31	4:C:613:PCW:H62	0.74	1.83	7	6
4:C:605:PCW:C17	4:C:613:PCW:H132	0.74	2.09	9	5
4:D:510:PCW:H471	5:D:524:17F:C31	0.74	2.08	2	2
4:A:405:PCW:C33	4:D:514:PCW:H352	0.74	2.12	6	3
4:C:617:PCW:H382	4:D:526:PCW:C16	0.74	2.12	5	1
4:D:504:PCW:C36	4:D:510:PCW:H321	0.74	2.13	10	2
4:C:617:PCW:H471	4:C:617:PCW:C43	0.74	2.11	8	1
4:B:201:PCW:H212	4:D:506:PCW:H422	0.73	1.60	1	1
4:D:504:PCW:H321	4:D:510:PCW:H332	0.73	1.56	1	1
4:C:605:PCW:H152	4:C:613:PCW:O2	0.73	1.84	3	8
3:D:359:ARG:HG2	3:D:369:VAL:HG22	0.73	1.58	6	1
4:A:415:PCW:H221	4:D:528:PCW:C23	0.73	2.14	4	6
4:C:606:PCW:H63	4:C:606:PCW:O11	0.73	1.83	7	5
4:C:616:PCW:H432	4:C:625:PCW:H232	0.73	1.60	2	3
4:C:603:PCW:C31	4:C:603:PCW:H42	0.73	2.13	4	4
4:C:613:PCW:H272	5:D:521:17F:H46	0.73	1.57	7	5
4:A:405:PCW:H82	4:D:514:PCW:H371	0.73	1.59	4	1
4:A:410:PCW:C14	4:A:413:PCW:H341	0.73	2.12	6	2
4:C:601:PCW:H462	4:C:601:PCW:H152	0.73	1.60	6	1
4:D:505:PCW:C8	4:D:505:PCW:H321	0.73	2.12	6	1
4:D:510:PCW:H131	5:D:524:17F:C39	0.73	2.11	6	1
4:D:504:PCW:O3	4:D:510:PCW:H372	0.73	1.83	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:524:17F:H65	5:D:524:17F:C11	0.73	2.13	10	1
4:C:605:PCW:C40	4:C:619:PCW:H141	0.73	2.13	9	3
5:C:626:17F:H66	5:C:627:17F:H52	0.73	1.58	5	2
4:C:604:PCW:H31	4:C:604:PCW:H41	0.73	1.58	3	1
4:C:623:PCW:H51	4:C:623:PCW:O11	0.73	1.84	4	2
4:C:616:PCW:H441	4:C:625:PCW:H261	0.73	1.57	7	1
4:A:406:PCW:C24	4:B:202:PCW:H221	0.73	2.13	9	1
4:A:413:PCW:H432	4:D:526:PCW:H211	0.73	1.58	8	3
4:D:517:PCW:H39	5:D:520:17F:H49	0.73	1.58	3	1
4:C:604:PCW:C11	4:C:604:PCW:C31	0.73	2.66	4	3
4:C:618:PCW:H412	5:C:629:17F:H41	0.73	1.59	4	1
4:A:414:PCW:C6	5:C:628:17F:H4	0.73	2.10	7	3
4:C:621:PCW:H371	5:C:629:17F:C35	0.73	2.13	8	3
4:D:506:PCW:H20	4:D:516:PCW:H331	0.73	1.57	9	1
4:D:512:PCW:H232	4:D:512:PCW:C27	0.73	2.09	9	1
4:A:401:PCW:H412	4:D:511:PCW:H482	0.73	1.61	10	1
4:C:604:PCW:O31	4:C:606:PCW:H82	0.73	1.82	1	3
4:D:513:PCW:H451	4:D:517:PCW:C47	0.73	2.13	3	1
4:D:510:PCW:H131	5:D:524:17F:C41	0.73	2.14	4	1
4:C:604:PCW:O11	4:C:604:PCW:H73	0.73	1.84	3	2
4:A:406:PCW:H171	4:B:202:PCW:H222	0.73	1.58	9	1
5:D:525:17F:H48	5:D:525:17F:H77	0.73	1.60	10	1
5:D:522:17F:H40	5:D:522:17F:C12	0.73	2.14	1	2
4:B:203:PCW:H20	4:D:506:PCW:C45	0.73	2.13	4	4
4:D:506:PCW:O1P	4:D:515:PCW:H73	0.73	1.83	4	3
4:A:404:PCW:H283	4:A:411:PCW:H482	0.73	1.59	6	2
5:D:521:17F:H62	5:D:521:17F:C31	0.73	2.04	6	1
4:D:513:PCW:H172	4:D:513:PCW:C21	0.73	2.07	9	1
4:A:402:PCW:C41	4:D:512:PCW:H381	0.73	2.13	7	3
4:B:203:PCW:H461	4:B:204:PCW:H421	0.73	1.58	2	2
5:D:529:17F:H29	5:D:530:17F:H8	0.73	1.60	3	3
4:C:602:PCW:C21	4:C:602:PCW:H172	0.73	2.12	6	2
4:C:602:PCW:C16	4:C:602:PCW:H221	0.73	2.14	6	1
4:A:407:PCW:H39	5:D:522:17F:H72	0.73	1.58	10	1
1:A:279:LEU:HD22	1:C:495:LYS:HE3	0.73	1.59	3	8
4:A:406:PCW:H162	4:B:204:PCW:C41	0.73	2.14	3	1
4:A:405:PCW:H62	4:A:408:PCW:O1P	0.73	1.83	4	1
4:A:407:PCW:H272	4:A:407:PCW:H482	0.73	1.60	6	1
4:D:509:PCW:C20	5:D:520:17F:H31	0.73	2.13	6	1
4:D:509:PCW:C6	4:D:514:PCW:H32	0.73	2.14	6	1
4:B:201:PCW:C34	4:D:510:PCW:H381	0.73	2.14	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:403:PCW:C23	4:D:507:PCW:H151	0.73	2.12	10	2
4:C:608:PCW:O1P	4:C:624:PCW:H221	0.73	1.84	9	8
4:D:502:PCW:O31	4:D:502:PCW:H11	0.73	1.84	8	10
4:A:402:PCW:H331	4:D:514:PCW:H332	0.73	1.61	2	1
4:A:412:PCW:H63	4:C:624:PCW:C31	0.73	2.13	7	5
4:D:510:PCW:H141	5:D:524:17F:H8	0.73	1.59	2	1
5:D:519:17F:H2	5:D:519:17F:O1	0.73	1.83	8	6
4:A:412:PCW:C8	4:C:624:PCW:H331	0.73	2.14	3	2
3:D:362:LEU:HB2	3:D:366:GLN:HB3	0.73	1.61	5	4
4:B:202:PCW:H271	4:B:204:PCW:H39	0.73	1.60	10	1
4:C:604:PCW:H31	4:C:604:PCW:P	0.72	2.24	10	8
4:A:415:PCW:H141	4:C:603:PCW:H382	0.72	1.60	3	7
4:C:605:PCW:H371	4:C:611:PCW:H322	0.72	1.58	3	1
4:D:527:PCW:H152	4:D:528:PCW:C16	0.72	2.12	3	3
4:C:608:PCW:H141	4:C:609:PCW:H171	0.72	1.60	9	3
4:C:611:PCW:C4	4:C:622:PCW:H342	0.72	2.14	7	5
4:A:413:PCW:O1P	4:C:617:PCW:H372	0.72	1.83	6	2
4:B:201:PCW:C16	4:D:506:PCW:H461	0.72	2.13	9	3
4:D:502:PCW:H161	4:D:505:PCW:H322	0.72	1.59	7	2
4:A:415:PCW:H282	4:D:528:PCW:H283	0.72	1.59	7	4
4:C:625:PCW:C28	5:C:629:17F:H46	0.72	2.14	4	3
5:D:522:17F:H40	5:D:522:17F:H12	0.72	1.61	1	3
4:C:607:PCW:H12	4:C:624:PCW:H362	0.72	1.61	4	3
4:D:508:PCW:C16	4:D:512:PCW:H151	0.72	2.13	4	3
4:A:412:PCW:H472	4:C:607:PCW:H471	0.72	1.60	3	4
4:B:203:PCW:H231	4:B:204:PCW:H40	0.72	1.60	3	3
4:C:605:PCW:H471	4:C:613:PCW:H162	0.72	1.59	6	4
5:C:630:17F:H29	5:D:530:17F:H62	0.72	1.61	4	2
4:D:510:PCW:C35	5:D:524:17F:H9	0.72	2.13	4	1
5:D:529:17F:H47	5:D:530:17F:C23	0.72	2.10	7	3
5:D:524:17F:H2	5:D:524:17F:O2	0.72	1.83	2	6
4:A:407:PCW:H39	5:D:522:17F:H65	0.72	1.61	5	1
4:A:410:PCW:H382	4:C:617:PCW:H141	0.72	1.60	5	1
4:D:503:PCW:C41	4:D:511:PCW:H352	0.72	2.15	6	1
4:C:615:PCW:H51	5:C:631:17F:O4	0.72	1.85	6	3
4:C:621:PCW:H262	4:D:528:PCW:C8	0.72	2.13	4	3
4:D:504:PCW:H122	4:D:510:PCW:H372	0.72	1.61	2	1
4:A:402:PCW:C28	4:D:508:PCW:H281	0.72	2.14	3	1
4:A:408:PCW:H442	4:D:506:PCW:H441	0.72	1.57	7	1
4:D:515:PCW:H40	5:D:519:17F:H38	0.72	1.61	7	1
4:A:405:PCW:H162	4:A:405:PCW:H231	0.72	1.61	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:516:PCW:H462	5:D:529:17F:H49	0.72	1.59	9	1
4:C:613:PCW:O31	4:C:613:PCW:H12	0.72	1.84	8	10
4:D:502:PCW:H31	4:D:502:PCW:C4	0.72	2.13	1	1
4:A:407:PCW:H331	5:D:522:17F:H34	0.72	1.61	3	1
4:A:414:PCW:C16	5:C:628:17F:H57	0.72	2.15	5	5
4:C:606:PCW:H261	5:D:530:17F:H74	0.72	1.61	5	1
4:A:413:PCW:H382	4:D:526:PCW:C16	0.72	2.13	6	3
4:C:616:PCW:C36	4:D:527:PCW:H362	0.72	2.14	8	2
5:D:524:17F:H65	5:D:524:17F:C1X	0.72	2.10	6	1
2:B:37:GLU:HB2	3:D:369:VAL:HB	0.72	1.61	10	1
5:D:521:17F:C19	5:D:521:17F:C31	0.72	2.68	5	8
4:A:406:PCW:C35	4:B:204:PCW:H162	0.72	2.15	7	3
4:C:622:PCW:C1	4:C:623:PCW:H161	0.72	2.14	4	2
4:D:501:PCW:C21	5:D:521:17F:H19	0.72	2.14	4	1
4:D:518:PCW:H162	5:D:519:17F:H58	0.72	1.62	8	1
4:A:403:PCW:C45	4:D:507:PCW:H262	0.72	2.14	9	1
4:D:516:PCW:C26	4:D:526:PCW:H462	0.72	2.12	9	1
4:D:515:PCW:H151	5:D:525:17F:C34	0.72	2.14	10	1
4:D:514:PCW:O11	4:D:514:PCW:H2	0.72	1.85	6	10
4:A:405:PCW:C6	4:D:514:PCW:H371	0.72	2.14	2	2
4:C:605:PCW:P	4:C:613:PCW:H52	0.72	2.24	3	5
4:C:605:PCW:H382	4:C:611:PCW:O2	0.72	1.85	6	6
4:D:509:PCW:C14	5:D:520:17F:H60	0.72	2.05	2	1
4:C:606:PCW:H31	5:D:529:17F:H1	0.72	1.59	3	1
4:C:602:PCW:H52	5:D:523:17F:O10	0.72	1.85	4	2
4:B:202:PCW:H42	4:B:202:PCW:C32	0.72	2.15	10	4
4:D:505:PCW:C31	4:D:505:PCW:H351	0.72	2.13	5	3
4:D:508:PCW:H142	4:D:512:PCW:H321	0.72	1.62	4	1
4:D:518:PCW:O31	5:D:519:17F:H32	0.72	1.84	6	1
4:C:607:PCW:H12	4:C:624:PCW:H371	0.72	1.61	1	2
4:D:506:PCW:C28	4:D:515:PCW:H471	0.72	2.14	4	1
4:A:403:PCW:C25	4:D:507:PCW:H171	0.72	2.12	10	4
5:A:409:17F:H57	4:D:503:PCW:C21	0.72	2.15	1	2
4:D:517:PCW:H432	5:D:520:17F:H55	0.72	1.61	1	1
4:A:401:PCW:H452	4:C:611:PCW:H271	0.72	1.61	2	2
4:C:610:PCW:H283	5:C:629:17F:H68	0.72	1.62	10	7
4:C:609:PCW:H51	5:C:631:17F:O2	0.72	1.85	3	2
5:C:626:17F:H19A	5:C:627:17F:H51	0.72	1.59	8	2
4:C:611:PCW:H39	4:C:622:PCW:C47	0.72	2.15	4	1
4:D:515:PCW:C3	5:D:525:17F:H56	0.72	2.14	4	1
4:C:618:PCW:H151	4:C:625:PCW:C14	0.72	2.14	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:518:PCW:H52	5:D:519:17F:O10	0.72	1.85	6	1
5:D:520:17F:H47	5:D:525:17F:H71	0.72	1.62	7	1
4:A:405:PCW:H322	4:A:408:PCW:H351	0.72	1.59	9	1
4:D:510:PCW:H432	5:D:524:17F:H12	0.72	1.60	10	1
4:C:618:PCW:H63	4:D:528:PCW:P	0.72	2.25	3	3
4:D:517:PCW:H61	5:D:520:17F:O5	0.72	1.85	1	1
4:C:604:PCW:H52	4:C:604:PCW:O11	0.72	1.83	4	1
4:C:607:PCW:H471	4:D:513:PCW:C48	0.72	2.14	6	1
3:D:487:TRP:CH2	4:D:510:PCW:H42	0.72	2.20	6	1
4:D:513:PCW:H42	5:D:523:17F:O2	0.72	1.84	6	1
5:C:630:17F:H76	4:D:514:PCW:H222	0.72	1.61	7	1
4:D:517:PCW:H371	5:D:525:17F:C32	0.72	2.15	7	2
4:D:501:PCW:C7	5:D:525:17F:H2	0.72	2.15	10	1
4:A:403:PCW:H141	4:A:403:PCW:C36	0.71	2.13	1	1
4:D:510:PCW:H271	4:D:510:PCW:H483	0.71	1.61	2	2
4:B:202:PCW:H262	4:D:504:PCW:H271	0.71	1.62	8	1
4:C:606:PCW:H162	5:D:529:17F:H30	0.71	1.62	7	5
4:C:607:PCW:H31	4:C:624:PCW:C39	0.71	2.14	8	3
4:A:402:PCW:H122	4:A:405:PCW:O11	0.71	1.85	5	3
5:C:630:17F:H8A	5:D:529:17F:C38	0.71	2.15	2	1
4:C:608:PCW:H261	5:C:627:17F:C35	0.71	2.13	7	4
1:A:250:VAL:HG11	4:A:408:PCW:H271	0.71	1.63	4	1
4:A:410:PCW:H282	4:A:413:PCW:H251	0.71	1.60	9	2
4:D:504:PCW:H482	4:D:516:PCW:C20	0.71	2.15	6	1
4:A:404:PCW:H361	4:B:202:PCW:H441	0.71	1.61	9	1
4:C:601:PCW:C7	4:C:602:PCW:H32	0.71	2.16	8	3
4:C:602:PCW:C48	5:C:627:17F:H47	0.71	2.14	9	3
4:C:604:PCW:H272	4:C:623:PCW:H481	0.71	1.62	3	2
4:B:201:PCW:C16	4:D:506:PCW:H411	0.71	2.13	3	1
4:D:515:PCW:C27	4:D:528:PCW:H281	0.71	2.14	3	1
4:B:201:PCW:H151	4:D:516:PCW:C42	0.71	2.16	6	1
5:C:629:17F:H11A	4:D:528:PCW:C7	0.71	2.16	7	6
4:B:201:PCW:H342	4:D:510:PCW:H382	0.71	1.61	2	1
4:B:203:PCW:C20	4:D:506:PCW:H471	0.71	2.16	2	1
4:D:506:PCW:H222	4:D:506:PCW:H181	0.71	1.61	7	3
4:C:613:PCW:C14	4:C:619:PCW:H382	0.71	2.16	5	2
4:B:203:PCW:H19	4:D:506:PCW:H451	0.71	1.62	10	2
4:D:503:PCW:H122	4:D:511:PCW:H411	0.71	1.62	7	1
4:D:509:PCW:H372	4:D:509:PCW:C41	0.71	2.08	9	1
4:B:203:PCW:H161	4:B:204:PCW:C39	0.71	2.16	3	4
2:B:37:GLU:HB3	3:D:369:VAL:HG23	0.71	1.63	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:415:PCW:C45	4:C:622:PCW:H281	0.71	2.15	5	1
4:D:509:PCW:C21	5:D:520:17F:H57	0.71	2.09	5	1
4:D:517:PCW:H461	4:D:517:PCW:H262	0.71	1.59	5	1
4:C:618:PCW:C26	4:D:510:PCW:H281	0.71	2.15	8	1
4:C:608:PCW:H172	5:C:627:17F:O10	0.71	1.86	1	4
4:C:616:PCW:O2P	4:D:527:PCW:H51	0.71	1.84	1	1
4:C:609:PCW:H73	4:C:620:PCW:O11	0.71	1.86	5	8
4:B:203:PCW:H161	4:B:204:PCW:C38	0.71	2.14	3	2
4:D:513:PCW:O31	4:D:513:PCW:H12	0.71	1.86	6	3
4:A:413:PCW:O2P	4:A:413:PCW:H32	0.71	1.85	5	2
4:D:503:PCW:H40	5:D:522:17F:H10A	0.71	1.62	10	3
4:C:602:PCW:H31	4:C:602:PCW:O31	0.71	1.86	4	7
4:C:603:PCW:H62	4:D:527:PCW:P	0.71	2.25	3	4
4:C:604:PCW:C46	4:C:624:PCW:H282	0.71	2.06	4	6
4:D:504:PCW:O11	4:D:504:PCW:H2	0.71	1.86	1	6
4:A:414:PCW:H19	5:C:628:17F:H57	0.71	1.60	10	5
4:A:403:PCW:C41	4:D:513:PCW:H39	0.71	2.15	6	2
4:A:411:PCW:H371	4:A:411:PCW:C41	0.71	2.15	8	4
4:C:623:PCW:H12	4:C:624:PCW:C1	0.71	2.16	6	1
4:C:602:PCW:H172	4:C:602:PCW:C21	0.71	2.13	3	4
4:C:610:PCW:H12	5:C:629:17F:C6	0.71	2.14	3	1
4:A:412:PCW:H63	4:C:624:PCW:C2	0.71	2.16	4	2
4:A:413:PCW:C48	5:D:524:17F:H37	0.71	2.14	4	1
4:A:403:PCW:H362	4:A:403:PCW:H121	0.71	1.62	6	2
4:D:509:PCW:H412	4:D:517:PCW:H321	0.71	1.61	6	1
4:A:403:PCW:C24	4:D:513:PCW:H122	0.71	2.08	7	2
4:D:501:PCW:C39	4:D:515:PCW:H421	0.71	2.16	8	1
4:C:609:PCW:H251	5:C:626:17F:C40	0.71	2.15	9	2
4:B:202:PCW:H62	5:D:524:17F:O4	0.71	1.85	9	3
4:D:501:PCW:H431	5:D:525:17F:H47	0.71	1.60	1	1
4:D:513:PCW:C5	5:D:523:17F:H4	0.71	2.15	1	1
4:C:614:PCW:H52	4:C:623:PCW:O1P	0.71	1.85	2	5
2:B:72:MET:HE3	2:B:103:VAL:HG21	0.71	1.62	7	4
4:D:505:PCW:O31	4:D:505:PCW:C35	0.71	2.36	7	6
5:D:520:17F:H2	5:D:520:17F:O2	0.71	1.86	2	2
4:D:513:PCW:C45	4:D:517:PCW:H472	0.71	2.12	5	2
4:C:623:PCW:C1	4:C:624:PCW:H12	0.71	2.14	6	1
4:C:616:PCW:H361	4:D:527:PCW:H362	0.71	1.61	8	1
4:A:402:PCW:C44	4:D:512:PCW:H152	0.71	2.16	1	1
4:D:503:PCW:H73	4:D:503:PCW:C1	0.71	2.16	5	6
4:A:412:PCW:H52	4:C:624:PCW:O31	0.71	1.85	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:612:PCW:H332	4:C:625:PCW:H131	0.71	1.61	7	3
4:D:503:PCW:H40	5:D:522:17F:H9A	0.71	1.61	8	1
4:A:402:PCW:H82	4:D:514:PCW:O2P	0.71	1.85	9	1
1:A:250:VAL:O	1:A:254:VAL:HB	0.70	1.86	6	9
4:D:514:PCW:O1P	4:D:514:PCW:H52	0.70	1.85	1	10
4:C:608:PCW:H63	4:C:624:PCW:H222	0.70	1.63	2	4
4:C:621:PCW:H181	4:C:621:PCW:C14	0.70	2.16	6	7
4:C:622:PCW:C42	4:C:623:PCW:H261	0.70	2.15	9	4
4:D:501:PCW:H122	4:D:515:PCW:C38	0.70	2.16	2	1
4:C:611:PCW:O2P	4:C:613:PCW:H73	0.70	1.86	4	1
4:C:615:PCW:H121	5:C:631:17F:O7	0.70	1.85	6	1
4:B:201:PCW:C33	4:D:510:PCW:H382	0.70	2.15	6	1
4:D:508:PCW:H73	5:D:520:17F:H6	0.70	1.63	9	2
4:B:202:PCW:H73	5:D:524:17F:O5	0.70	1.86	10	1
4:A:412:PCW:C39	4:C:623:PCW:H441	0.70	2.16	5	6
4:A:401:PCW:C7	4:D:511:PCW:H2	0.70	2.16	2	1
4:D:513:PCW:H42	5:D:523:17F:H4	0.70	1.63	10	3
4:A:412:PCW:C8	4:C:624:PCW:H362	0.70	2.17	9	2
4:B:201:PCW:H272	4:D:528:PCW:C47	0.70	2.16	3	1
4:C:612:PCW:H321	4:C:618:PCW:H152	0.70	1.62	5	2
4:D:510:PCW:O3	5:D:524:17F:H75	0.70	1.86	9	2
5:D:525:17F:H30	5:D:525:17F:H61	0.70	1.63	5	1
4:D:513:PCW:C47	4:D:513:PCW:H272	0.70	2.16	10	1
4:D:516:PCW:C23	5:D:519:17F:H50	0.70	2.15	10	1
4:C:618:PCW:C15	4:C:625:PCW:H142	0.70	2.15	6	6
4:C:616:PCW:H452	4:B:201:PCW:C46	0.70	2.16	3	1
2:B:41:ARG:HD3	3:D:365:LYS:HD2	0.70	1.61	10	2
2:B:84:ILE:HD12	2:B:123:ARG:HG3	0.70	1.61	6	4
4:C:603:PCW:H441	4:C:603:PCW:H181	0.70	1.62	4	1
4:B:202:PCW:H42	4:B:202:PCW:H322	0.70	1.62	10	2
5:D:525:17F:H73	5:D:525:17F:H44	0.70	1.60	7	1
4:C:609:PCW:C48	4:D:512:PCW:H472	0.70	2.15	3	2
4:D:510:PCW:H371	4:D:510:PCW:H412	0.70	1.64	6	2
4:D:518:PCW:H73	5:D:519:17F:H8A	0.70	1.61	1	1
4:C:610:PCW:C17	5:C:629:17F:H61	0.70	2.16	2	2
5:D:529:17F:O7	5:D:529:17F:C18	0.70	2.38	3	6
4:A:411:PCW:H361	4:C:612:PCW:H131	0.70	1.61	3	2
4:C:612:PCW:C17	4:C:612:PCW:C21	0.70	2.67	6	6
4:C:618:PCW:H322	4:C:625:PCW:H121	0.70	1.63	3	2
4:C:609:PCW:H431	4:D:512:PCW:H242	0.70	1.63	6	2
4:D:511:PCW:H281	5:D:522:17F:H56	0.70	1.63	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:509:PCW:H2	5:D:520:17F:C4	0.70	2.16	8	3
4:A:403:PCW:H352	4:A:407:PCW:H361	0.70	1.64	9	1
4:D:517:PCW:C39	5:D:525:17F:H63	0.70	2.17	10	1
4:A:404:PCW:O11	4:A:404:PCW:H2	0.70	1.85	5	8
4:A:407:PCW:H352	5:D:522:17F:H62	0.70	1.61	2	1
1:C:497:SER:HB2	1:C:498:PRO:HD3	0.70	1.61	4	4
4:C:605:PCW:H39	4:C:611:PCW:H341	0.70	1.61	3	6
4:C:610:PCW:H241	4:C:610:PCW:H20	0.70	1.63	6	4
4:C:614:PCW:H442	4:C:619:PCW:H20	0.70	1.61	6	4
4:D:506:PCW:C8	5:D:525:17F:H20	0.70	2.17	4	1
4:C:606:PCW:H161	5:D:529:17F:C8	0.70	2.16	5	1
4:D:515:PCW:C3	4:D:517:PCW:H12	0.70	2.15	6	1
4:D:502:PCW:C33	4:D:510:PCW:H11	0.70	2.14	7	2
5:D:524:17F:O10	5:D:524:17F:H6A	0.70	1.86	10	2
4:C:615:PCW:H221	4:D:512:PCW:H251	0.70	1.64	1	1
4:D:508:PCW:O4P	5:D:523:17F:H10A	0.70	1.86	1	1
5:C:631:17F:H5	5:C:631:17F:O8	0.70	1.86	9	9
4:A:405:PCW:H321	4:D:514:PCW:C37	0.70	2.16	8	4
4:C:612:PCW:H321	4:C:618:PCW:C14	0.70	2.17	6	2
5:C:631:17F:C29	4:D:512:PCW:H172	0.70	2.09	5	1
5:C:631:17F:H52	4:D:512:PCW:C21	0.70	2.17	10	1
4:A:411:PCW:H361	4:C:612:PCW:H152	0.70	1.62	1	2
4:A:413:PCW:C35	4:C:617:PCW:H412	0.70	2.17	8	4
4:C:622:PCW:C23	4:D:501:PCW:H381	0.70	2.16	1	1
4:B:201:PCW:H232	4:B:203:PCW:H20	0.70	1.63	7	3
4:B:203:PCW:C21	4:B:204:PCW:H40	0.70	2.16	2	1
4:D:518:PCW:H121	5:D:519:17F:H71	0.70	1.60	3	2
4:C:615:PCW:H431	5:D:523:17F:H54	0.70	1.62	4	1
4:C:625:PCW:H281	5:C:629:17F:H46	0.70	1.64	8	2
4:D:515:PCW:C3	5:D:525:17F:H31	0.70	2.15	7	2
4:D:515:PCW:H321	4:D:516:PCW:O3P	0.70	1.86	10	3
4:D:515:PCW:H181	4:D:515:PCW:H231	0.70	1.62	9	2
4:C:613:PCW:H121	4:C:619:PCW:H382	0.70	1.63	4	1
4:C:621:PCW:H421	5:C:630:17F:H59	0.70	1.64	4	2
4:D:509:PCW:H371	5:D:520:17F:H70	0.70	1.62	5	1
4:D:517:PCW:H432	4:D:517:PCW:C18	0.70	2.15	5	1
4:D:507:PCW:C15	4:D:513:PCW:H321	0.70	2.17	6	1
4:D:513:PCW:H442	4:D:517:PCW:H271	0.70	1.64	10	2
4:D:515:PCW:H132	5:D:525:17F:H58	0.70	1.62	8	1
4:A:401:PCW:H411	4:D:503:PCW:H283	0.70	1.64	9	1
4:A:404:PCW:H231	4:A:411:PCW:H262	0.70	1.63	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:513:PCW:H272	4:D:513:PCW:C40	0.70	2.16	9	1
4:A:414:PCW:C12	5:C:628:17F:H11	0.70	2.12	8	3
4:C:606:PCW:O11	4:C:606:PCW:H2	0.70	1.86	6	9
5:D:529:17F:H70	5:D:530:17F:H63	0.70	1.64	3	3
2:B:82:PHE:HB3	2:B:93:ILE:HD11	0.70	1.64	6	5
4:A:406:PCW:H162	4:B:204:PCW:H411	0.70	1.64	3	1
4:C:613:PCW:H431	4:C:619:PCW:C39	0.70	2.16	10	2
5:D:520:17F:C30	5:D:525:17F:H71	0.70	2.17	4	1
4:A:407:PCW:H472	4:A:407:PCW:C28	0.70	2.17	5	1
4:A:408:PCW:H482	4:D:528:PCW:C47	0.70	2.16	1	1
4:D:511:PCW:H381	4:D:511:PCW:C24	0.70	2.13	1	1
4:A:415:PCW:H222	4:C:603:PCW:H182	0.70	1.62	8	5
4:D:516:PCW:H40	4:D:527:PCW:C25	0.70	2.17	3	1
4:D:526:PCW:H82	4:D:527:PCW:H73	0.70	1.61	3	1
4:B:201:PCW:H51	4:B:202:PCW:C3	0.70	2.13	6	1
4:C:606:PCW:H41	4:C:606:PCW:H2	0.70	1.63	7	1
4:C:617:PCW:H62	4:C:617:PCW:H2	0.70	1.63	10	2
4:D:510:PCW:H20	5:D:524:17F:H20	0.70	1.62	7	1
4:A:405:PCW:H162	4:A:405:PCW:C23	0.70	2.17	9	1
4:D:502:PCW:C34	4:D:505:PCW:H11	0.69	2.13	1	1
4:A:415:PCW:C27	4:D:516:PCW:H251	0.69	2.17	2	1
4:C:622:PCW:H242	4:D:501:PCW:H451	0.69	1.63	6	2
4:D:508:PCW:H51	5:D:520:17F:H9A	0.69	1.64	6	1
4:A:404:PCW:C34	4:D:510:PCW:H212	0.69	2.16	9	1
4:A:406:PCW:H31	4:A:406:PCW:P	0.69	2.27	5	8
4:D:502:PCW:H342	4:D:505:PCW:C1	0.69	2.14	1	1
4:D:513:PCW:C22	4:D:513:PCW:C26	0.69	2.70	5	10
4:D:515:PCW:H321	4:D:516:PCW:H322	0.69	1.63	1	1
4:C:618:PCW:O2P	4:C:625:PCW:H51	0.69	1.87	6	2
4:D:509:PCW:H161	5:D:520:17F:H56	0.69	1.63	7	3
4:D:502:PCW:H452	4:D:505:PCW:H271	0.69	1.62	9	1
4:D:505:PCW:H472	4:D:518:PCW:H282	0.69	1.62	1	1
4:D:527:PCW:C15	4:D:528:PCW:H162	0.69	2.15	3	4
4:C:603:PCW:H73	4:D:527:PCW:O3P	0.69	1.88	2	2
4:D:508:PCW:C18	4:D:512:PCW:H362	0.69	2.15	4	4
4:D:517:PCW:H281	5:D:522:17F:C37	0.69	2.17	3	1
4:A:405:PCW:O1P	4:A:408:PCW:H42	0.69	1.86	4	1
4:D:515:PCW:C15	5:D:525:17F:H62	0.69	2.17	4	1
4:C:615:PCW:H63	5:C:631:17F:C2	0.69	2.16	10	1
4:D:502:PCW:H421	4:D:505:PCW:H271	0.69	1.64	10	1
5:A:409:17F:H77	4:D:501:PCW:H272	0.69	1.63	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:413:PCW:H451	4:D:526:PCW:H231	0.69	1.65	3	2
4:C:606:PCW:H252	5:D:529:17F:H41	0.69	1.64	4	5
2:B:37:GLU:HB3	3:D:369:VAL:CG2	0.69	2.18	6	9
4:D:509:PCW:O1P	4:D:509:PCW:C3	0.69	2.40	9	3
4:D:511:PCW:H41	4:D:511:PCW:O11	0.69	1.88	9	6
4:D:509:PCW:H151	5:D:520:17F:H60	0.69	1.63	4	1
5:C:630:17F:C33	5:C:631:17F:H74	0.69	2.17	7	3
4:D:511:PCW:O1P	4:D:511:PCW:C3	0.69	2.41	6	4
4:A:406:PCW:H32	4:B:202:PCW:H152	0.69	1.62	9	1
4:C:612:PCW:O11	4:C:612:PCW:H2	0.69	1.86	3	9
4:C:625:PCW:C24	4:D:527:PCW:H451	0.69	2.16	4	3
4:D:506:PCW:H321	4:D:509:PCW:H39	0.69	1.63	1	1
4:B:202:PCW:H252	4:D:504:PCW:H252	0.69	1.64	4	1
4:A:406:PCW:H31	4:A:406:PCW:H42	0.69	1.64	8	1
5:C:626:17F:H40	5:C:627:17F:H74	0.69	1.65	9	3
4:D:513:PCW:H121	5:D:523:17F:H6	0.69	1.64	8	1
4:A:404:PCW:C23	4:A:411:PCW:H262	0.69	2.17	9	1
4:D:516:PCW:H73	4:D:516:PCW:O11	0.69	1.88	10	1
4:A:403:PCW:H362	4:A:403:PCW:C14	0.69	2.16	1	1
4:A:406:PCW:H242	4:B:202:PCW:C23	0.69	2.17	1	2
4:C:622:PCW:H231	4:D:501:PCW:H381	0.69	1.65	1	1
5:C:631:17F:O10	5:C:631:17F:H6	0.69	1.87	10	10
2:B:15:GLY:CA	6:B:205:GNP:H8	0.69	2.16	9	4
4:B:201:PCW:H51	4:B:202:PCW:C1	0.69	2.17	2	1
4:C:617:PCW:O31	4:C:617:PCW:H73	0.69	1.88	5	3
4:C:608:PCW:H212	5:C:627:17F:C1X	0.69	2.18	3	7
4:A:414:PCW:H19	5:C:628:17F:C31	0.69	2.17	2	3
4:A:412:PCW:H40	4:C:623:PCW:C44	0.69	2.15	3	1
4:C:616:PCW:H62	4:D:526:PCW:O11	0.69	1.88	3	2
4:D:507:PCW:H422	5:D:522:17F:H20	0.69	1.63	5	1
4:B:202:PCW:H252	4:B:204:PCW:C40	0.69	2.17	10	1
4:A:408:PCW:H462	4:B:201:PCW:H271	0.69	1.63	3	2
4:C:609:PCW:H452	4:D:512:PCW:H20	0.69	1.64	1	1
4:C:614:PCW:C5	4:C:623:PCW:O1P	0.69	2.40	3	8
4:C:620:PCW:H121	5:C:631:17F:C4	0.69	2.18	1	2
4:D:502:PCW:H31	4:D:502:PCW:P	0.69	2.28	9	9
4:D:510:PCW:H471	5:D:524:17F:H32	0.69	1.65	4	2
5:D:523:17F:H5	5:D:523:17F:O8	0.69	1.88	9	7
4:C:603:PCW:O1P	4:C:603:PCW:O2	0.69	2.11	2	4
5:C:626:17F:H58	5:C:627:17F:H51	0.69	1.64	2	2
4:D:501:PCW:H261	5:D:521:17F:H64	0.69	1.65	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:403:PCW:H362	4:A:407:PCW:H361	0.69	1.65	3	1
4:C:611:PCW:H20	4:C:611:PCW:H432	0.69	1.63	7	6
5:C:631:17F:H52	4:D:512:PCW:C17	0.69	2.07	5	2
2:B:22:GLN:HG3	2:B:149:ARG:HG3	0.69	1.64	6	4
4:D:502:PCW:H52	4:D:502:PCW:O11	0.69	1.87	8	3
4:A:403:PCW:H252	4:D:507:PCW:C17	0.69	2.15	10	3
4:D:510:PCW:C13	5:D:524:17F:H71	0.69	2.15	6	1
5:D:520:17F:C34	5:D:520:17F:C38	0.69	2.71	6	1
4:A:406:PCW:H152	4:B:202:PCW:C22	0.69	2.17	10	3
4:C:605:PCW:H212	4:C:613:PCW:H152	0.69	1.64	8	1
4:D:515:PCW:C13	5:D:525:17F:H58	0.69	2.18	8	1
4:A:402:PCW:H442	4:D:512:PCW:H172	0.69	1.64	10	1
4:B:202:PCW:H252	4:B:204:PCW:C39	0.69	2.18	10	1
4:D:509:PCW:H31	4:D:509:PCW:H42	0.69	1.64	6	2
4:D:502:PCW:H212	4:D:502:PCW:C42	0.69	2.18	9	4
4:D:518:PCW:H122	5:D:519:17F:H66	0.69	1.65	2	1
4:D:504:PCW:H332	4:D:516:PCW:C8	0.69	2.18	7	3
4:D:509:PCW:H19	5:D:520:17F:C20	0.69	2.18	6	2
4:D:509:PCW:H431	5:D:520:17F:H12	0.69	1.65	9	1
4:C:621:PCW:H141	5:C:630:17F:O8	0.69	1.87	2	3
5:C:626:17F:C19	5:C:626:17F:C31	0.69	2.71	4	6
4:D:507:PCW:H212	4:D:507:PCW:H172	0.69	1.65	9	2
4:D:503:PCW:C47	4:D:511:PCW:H281	0.69	2.18	2	1
4:B:202:PCW:H121	5:D:524:17F:H18	0.69	1.65	3	1
4:D:507:PCW:H442	5:D:522:17F:C33	0.69	2.17	3	1
4:D:518:PCW:C31	4:D:518:PCW:H351	0.69	2.18	3	2
4:C:611:PCW:O1P	4:C:622:PCW:H332	0.69	1.88	4	1
4:C:602:PCW:H483	5:C:626:17F:H65	0.69	1.65	8	2
4:D:507:PCW:H372	5:D:525:17F:C7	0.69	2.18	5	1
4:B:201:PCW:H211	4:D:506:PCW:H472	0.69	1.63	6	1
4:B:201:PCW:H342	4:D:510:PCW:H411	0.69	1.63	6	2
4:D:508:PCW:H182	4:D:512:PCW:H362	0.69	1.64	7	1
4:D:504:PCW:H381	4:D:510:PCW:O1P	0.69	1.87	8	1
4:C:607:PCW:H481	4:D:513:PCW:H483	0.69	1.64	10	1
4:C:611:PCW:H141	4:C:619:PCW:H19	0.68	1.64	1	2
4:C:613:PCW:H31	4:C:613:PCW:O31	0.68	1.86	3	6
4:D:506:PCW:C27	4:D:516:PCW:H122	0.68	2.17	2	1
4:A:415:PCW:H41	4:C:622:PCW:H331	0.68	1.65	4	1
4:D:506:PCW:H122	5:D:520:17F:C1X	0.68	2.14	4	1
4:D:508:PCW:H152	4:D:509:PCW:C19	0.68	2.17	5	1
4:B:201:PCW:C4	4:D:504:PCW:H132	0.68	2.18	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:201:PCW:H73	4:B:202:PCW:O2P	0.68	1.88	7	1
4:D:511:PCW:H31	4:D:511:PCW:O4P	0.68	1.86	7	1
4:C:601:PCW:H382	5:C:626:17F:H52	0.68	1.64	10	1
4:C:605:PCW:H462	5:D:521:17F:H53	0.68	1.65	2	2
4:B:201:PCW:H231	4:B:203:PCW:H282	0.68	1.64	5	3
4:B:201:PCW:H171	4:D:527:PCW:H281	0.68	1.64	5	1
4:D:505:PCW:H352	4:D:505:PCW:C7	0.68	2.18	5	1
5:D:529:17F:H42	5:D:530:17F:C40	0.68	2.13	8	3
4:B:202:PCW:H182	4:D:504:PCW:H282	0.68	1.65	6	1
5:A:409:17F:C32	4:D:503:PCW:H242	0.68	2.18	8	1
4:D:517:PCW:C28	5:D:522:17F:H71	0.68	2.18	8	1
4:A:406:PCW:H482	4:B:204:PCW:H252	0.68	1.65	10	1
4:A:403:PCW:H31	4:A:403:PCW:P	0.68	2.28	10	6
4:C:602:PCW:H462	5:C:626:17F:H65	0.68	1.65	9	5
4:B:201:PCW:C3	4:B:201:PCW:O1P	0.68	2.41	4	9
4:D:506:PCW:C1	4:D:515:PCW:H62	0.68	2.19	4	2
4:C:611:PCW:H2	4:C:619:PCW:H63	0.68	1.64	10	4
4:C:621:PCW:H412	5:C:631:17F:C41	0.68	2.19	8	2
4:C:608:PCW:H19	5:C:627:17F:C26	0.68	2.18	6	5
4:D:506:PCW:H141	5:D:520:17F:C2X	0.68	2.16	4	1
4:A:405:PCW:O1P	4:A:408:PCW:H11	0.68	1.89	7	1
4:C:603:PCW:H42	4:C:603:PCW:H2	0.68	1.65	9	1
4:D:501:PCW:H19	4:D:503:PCW:H362	0.68	1.65	10	1
4:A:406:PCW:H351	4:B:204:PCW:H152	0.68	1.66	1	3
4:A:406:PCW:H182	4:A:406:PCW:H231	0.68	1.62	6	4
4:A:405:PCW:H82	4:D:514:PCW:C35	0.68	2.17	2	4
4:C:616:PCW:H31	4:C:616:PCW:O4P	0.68	1.89	7	5
4:C:621:PCW:C22	5:C:629:17F:H31	0.68	2.18	8	4
4:D:506:PCW:H152	5:D:520:17F:H41	0.68	1.65	4	1
4:A:407:PCW:H122	4:D:511:PCW:C28	0.68	2.18	6	1
5:A:409:17F:H72	4:D:501:PCW:H242	0.68	1.66	7	1
4:C:607:PCW:H321	4:C:607:PCW:H51	0.68	1.65	8	1
5:D:522:17F:H35	5:D:525:17F:H12A	0.68	1.65	8	1
5:D:525:17F:H35	5:D:525:17F:H64	0.68	1.65	8	1
4:A:411:PCW:C41	4:C:612:PCW:H181	0.68	2.17	9	2
5:D:529:17F:H9A	5:D:529:17F:H20A	0.68	1.64	1	2
4:A:412:PCW:H483	4:D:517:PCW:C47	0.68	2.19	7	2
4:D:504:PCW:H321	4:D:510:PCW:C36	0.68	2.18	3	1
4:D:505:PCW:H181	4:D:505:PCW:H442	0.68	1.66	3	1
4:C:615:PCW:H2	4:C:615:PCW:C4	0.68	2.18	5	4
4:D:501:PCW:H61	5:D:525:17F:O5	0.68	1.87	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:509:PCW:H171	4:D:514:PCW:H142	0.68	1.65	5	1
4:D:516:PCW:H40	4:D:527:PCW:C27	0.68	2.18	9	2
4:A:402:PCW:H141	4:A:405:PCW:H162	0.68	1.63	7	2
4:D:513:PCW:H121	5:D:523:17F:C17	0.68	2.19	7	2
4:D:518:PCW:H73	5:D:521:17F:HN1A	0.68	1.49	7	1
4:A:415:PCW:H441	5:D:521:17F:H51	0.68	1.65	1	1
4:C:620:PCW:H283	5:C:631:17F:C21	0.68	2.18	1	5
4:D:510:PCW:H331	5:D:524:17F:C11	0.68	2.19	1	1
4:A:410:PCW:C45	4:C:617:PCW:H242	0.68	2.17	4	7
4:D:502:PCW:H422	4:D:502:PCW:C21	0.68	2.19	6	4
4:D:518:PCW:H452	5:D:521:17F:H12A	0.68	1.66	2	1
4:A:412:PCW:H82	4:C:624:PCW:H331	0.68	1.64	3	4
4:C:616:PCW:H452	4:B:201:PCW:C47	0.68	2.18	3	1
5:C:626:17F:H36	5:C:627:17F:H70	0.68	1.65	4	1
4:A:411:PCW:H411	4:C:612:PCW:H151	0.68	1.64	5	1
4:C:609:PCW:H231	5:C:626:17F:H70	0.68	1.65	5	1
5:C:630:17F:H65	5:C:631:17F:H71	0.68	1.65	6	2
4:D:504:PCW:H172	4:D:510:PCW:C39	0.68	2.19	6	1
4:D:501:PCW:O1P	4:D:515:PCW:H352	0.68	1.89	7	1
4:D:503:PCW:H421	4:D:511:PCW:C19	0.68	2.18	8	1
4:A:402:PCW:C41	4:D:512:PCW:H361	0.68	2.19	9	1
4:A:403:PCW:C16	4:D:513:PCW:H352	0.68	2.19	9	1
4:A:406:PCW:H32	4:B:202:PCW:H141	0.68	1.66	10	1
4:A:414:PCW:H441	4:C:617:PCW:H211	0.68	1.64	1	1
4:A:414:PCW:C32	4:C:617:PCW:H52	0.68	2.19	8	2
4:C:611:PCW:C47	4:D:501:PCW:H251	0.68	2.18	1	1
4:D:506:PCW:H382	4:D:509:PCW:H331	0.68	1.64	3	1
4:A:401:PCW:C48	4:C:614:PCW:H471	0.68	2.19	4	1
5:D:529:17F:H51	5:D:530:17F:C42	0.68	2.19	4	1
4:A:407:PCW:H261	4:A:412:PCW:H271	0.68	1.64	9	1
4:D:504:PCW:H451	4:D:505:PCW:C39	0.68	2.19	9	2
4:D:507:PCW:H152	4:D:513:PCW:C38	0.68	2.18	9	1
4:D:513:PCW:H451	5:D:522:17F:C42	0.68	2.18	9	1
4:D:516:PCW:H232	5:D:519:17F:C28	0.68	2.18	10	1
1:C:523:ASP:HA	1:C:526:ARG:HD2	0.68	1.65	8	6
4:C:625:PCW:H20	4:D:528:PCW:H321	0.68	1.66	1	3
5:C:631:17F:C30	4:D:508:PCW:H39	0.68	2.19	3	2
2:B:21:ILE:HD13	3:D:388:VAL:CG1	0.68	2.18	1	6
4:D:527:PCW:O31	4:D:527:PCW:H11	0.68	1.89	9	10
4:D:527:PCW:H172	4:D:528:PCW:H162	0.68	1.65	9	4
4:C:609:PCW:H182	4:C:615:PCW:H352	0.68	1.65	10	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:513:PCW:H442	4:D:517:PCW:H283	0.68	1.63	3	1
4:A:403:PCW:H422	4:D:513:PCW:C39	0.68	2.19	8	3
4:D:513:PCW:H12	4:D:513:PCW:O31	0.68	1.89	10	4
5:D:524:17F:H69	5:D:524:17F:H35	0.68	1.66	5	1
4:D:506:PCW:H251	4:D:515:PCW:H471	0.68	1.64	6	1
4:D:511:PCW:O11	4:D:511:PCW:H41	0.68	1.88	7	1
4:C:615:PCW:H212	4:D:512:PCW:H272	0.68	1.65	8	1
4:C:601:PCW:H121	4:C:601:PCW:H451	0.68	1.65	9	1
4:A:415:PCW:H282	4:D:528:PCW:H271	0.68	1.64	10	1
4:C:615:PCW:H483	4:D:509:PCW:H271	0.68	1.65	10	1
4:B:203:PCW:C31	4:B:203:PCW:C35	0.68	2.71	9	7
4:D:502:PCW:H322	4:D:505:PCW:O2P	0.68	1.89	7	3
4:D:508:PCW:H51	5:D:520:17F:O1	0.68	1.89	2	1
4:D:517:PCW:H411	4:D:517:PCW:C18	0.68	2.19	10	2
4:C:611:PCW:H283	4:C:619:PCW:H272	0.68	1.64	3	1
4:C:625:PCW:H251	4:B:201:PCW:H481	0.68	1.66	3	1
4:C:622:PCW:H362	4:C:622:PCW:O2	0.68	1.89	4	1
4:B:201:PCW:H362	4:D:510:PCW:H382	0.68	1.66	8	1
4:D:508:PCW:H212	4:D:512:PCW:H152	0.68	1.66	8	1
4:D:508:PCW:H12	5:D:523:17F:C11	0.68	2.18	8	1
4:D:513:PCW:H121	5:D:523:17F:C6	0.68	2.18	8	1
4:A:403:PCW:H341	4:A:407:PCW:H322	0.68	1.66	10	1
4:C:621:PCW:C15	5:C:630:17F:H6	0.68	2.19	2	8
4:D:506:PCW:H283	4:D:516:PCW:H122	0.68	1.64	1	1
5:D:529:17F:H51	5:D:530:17F:H78	0.68	1.64	4	3
4:C:603:PCW:H142	4:D:528:PCW:H221	0.68	1.64	7	2
4:A:401:PCW:H241	4:C:614:PCW:H281	0.68	1.66	6	1
4:C:625:PCW:H281	5:C:629:17F:H51	0.68	1.65	6	3
4:D:517:PCW:C7	5:D:520:17F:H4A	0.68	2.18	6	1
4:A:408:PCW:H451	4:B:203:PCW:H182	0.68	1.63	8	1
4:A:404:PCW:C36	4:B:202:PCW:H441	0.68	2.18	9	1
4:D:502:PCW:H232	4:D:502:PCW:C43	0.68	2.19	9	1
4:A:403:PCW:C31	4:A:407:PCW:H82	0.68	2.19	10	1
4:A:406:PCW:O31	4:A:406:PCW:H11	0.67	1.88	5	5
4:C:617:PCW:C4	4:C:617:PCW:H2	0.67	2.19	9	2
4:A:406:PCW:H261	5:C:629:17F:C30	0.67	2.19	2	2
4:C:606:PCW:H152	5:D:529:17F:H11A	0.67	1.65	4	2
4:C:614:PCW:H452	4:C:619:PCW:C22	0.67	2.20	2	2
5:C:630:17F:H19A	5:C:630:17F:H9	0.67	1.66	9	3
4:B:201:PCW:H161	4:D:506:PCW:H422	0.67	1.66	2	1
4:D:503:PCW:C41	4:D:511:PCW:H431	0.67	2.18	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:410:PCW:H283	4:A:413:PCW:C25	0.67	2.19	3	3
4:C:617:PCW:H51	4:C:617:PCW:O3P	0.67	1.89	10	6
4:C:606:PCW:H161	5:D:529:17F:C12	0.67	2.19	9	2
4:D:517:PCW:H162	4:D:517:PCW:H211	0.67	1.65	10	3
4:A:406:PCW:H121	4:B:204:PCW:H121	0.67	1.65	8	2
4:C:607:PCW:C47	4:D:513:PCW:H483	0.67	2.15	7	3
4:D:502:PCW:H212	4:D:502:PCW:H422	0.67	1.66	9	1
4:C:607:PCW:C34	4:C:624:PCW:H422	0.67	2.17	10	1
4:A:411:PCW:C44	4:C:612:PCW:H271	0.67	2.19	9	2
4:C:608:PCW:H42	4:C:624:PCW:C24	0.67	2.19	3	2
4:C:620:PCW:O1P	4:C:621:PCW:C5	0.67	2.42	6	3
4:C:625:PCW:H381	4:C:625:PCW:C42	0.67	2.13	9	7
4:D:506:PCW:H222	4:D:516:PCW:H351	0.67	1.66	9	2
4:D:511:PCW:H272	4:D:511:PCW:C23	0.67	2.19	6	5
4:D:508:PCW:C17	4:D:512:PCW:H151	0.67	2.20	4	3
4:D:526:PCW:H82	4:D:527:PCW:C7	0.67	2.19	3	1
4:D:506:PCW:H352	4:D:509:PCW:H382	0.67	1.65	5	1
4:A:405:PCW:O31	4:A:405:PCW:H51	0.67	1.90	5	3
4:C:603:PCW:C46	4:D:526:PCW:H432	0.67	2.16	4	4
4:A:414:PCW:H442	4:C:617:PCW:C20	0.67	2.20	5	4
4:C:604:PCW:H452	4:C:606:PCW:C18	0.67	2.19	2	4
4:C:607:PCW:C43	4:C:624:PCW:H472	0.67	2.19	2	1
4:A:412:PCW:H31	4:C:614:PCW:C11	0.67	2.19	3	2
4:A:404:PCW:H73	5:D:524:17F:O4	0.67	1.89	4	1
4:D:517:PCW:C45	5:D:525:17F:H68	0.67	2.19	4	1
4:A:414:PCW:H62	5:C:628:17F:O8	0.67	1.90	5	3
4:A:411:PCW:H411	4:A:411:PCW:C37	0.67	2.18	8	3
5:D:521:17F:H56	5:D:521:17F:C35	0.67	2.17	6	1
4:C:607:PCW:H452	4:C:624:PCW:H481	0.67	1.67	8	1
4:C:601:PCW:H451	4:C:601:PCW:H152	0.67	1.66	9	1
4:A:404:PCW:H361	4:B:202:PCW:H461	0.67	1.64	10	1
3:D:362:LEU:HB3	3:D:363:PRO:HD2	0.67	1.66	3	8
4:A:415:PCW:C22	4:C:603:PCW:H162	0.67	2.19	8	5
4:C:602:PCW:C46	4:C:608:PCW:H472	0.67	2.19	10	3
4:C:618:PCW:H251	4:D:510:PCW:H461	0.67	1.66	3	1
4:D:501:PCW:H132	4:D:503:PCW:C34	0.67	2.14	3	1
4:D:507:PCW:H11	5:D:523:17F:C8	0.67	2.19	3	1
4:D:515:PCW:H362	4:D:516:PCW:O2P	0.67	1.89	3	2
4:D:527:PCW:H461	5:D:529:17F:H76	0.67	1.65	3	2
4:A:410:PCW:H282	4:A:413:PCW:C25	0.67	2.19	9	2
4:D:517:PCW:H52	4:D:517:PCW:C1	0.67	2.18	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:413:PCW:H382	4:D:526:PCW:H161	0.67	1.64	6	3
4:D:509:PCW:H441	5:D:520:17F:H33	0.67	1.67	6	3
4:D:518:PCW:H471	5:D:521:17F:C12	0.67	2.19	10	1
4:C:608:PCW:H20	5:C:627:17F:C26	0.67	2.16	1	2
4:C:609:PCW:H483	4:D:512:PCW:C47	0.67	2.19	3	2
4:D:518:PCW:H351	4:D:518:PCW:C31	0.67	2.19	9	8
4:D:528:PCW:H141	5:D:530:17F:C1Y	0.67	2.20	7	7
4:A:410:PCW:C45	4:A:414:PCW:H421	0.67	2.19	3	1
4:D:501:PCW:H182	4:D:511:PCW:H422	0.67	1.64	3	1
3:D:382:LEU:HD21	3:D:428:VAL:HG21	0.67	1.66	9	1
4:C:604:PCW:C8	5:D:530:17F:H4A	0.67	2.19	1	2
4:C:608:PCW:O1P	4:C:624:PCW:H241	0.67	1.89	1	4
4:D:516:PCW:H451	5:D:529:17F:C28	0.67	2.18	1	1
4:C:621:PCW:H371	5:C:629:17F:C34	0.67	2.19	5	4
4:D:517:PCW:H421	4:D:517:PCW:H212	0.67	1.66	2	3
4:C:602:PCW:H172	4:C:602:PCW:H212	0.67	1.64	6	2
4:C:609:PCW:H41	5:C:631:17F:O10	0.67	1.90	5	1
4:C:620:PCW:O1P	4:C:621:PCW:H73	0.67	1.88	10	3
4:B:202:PCW:H282	4:D:504:PCW:H212	0.67	1.66	7	1
4:A:411:PCW:H39	4:C:612:PCW:H451	0.67	1.65	9	1
4:A:402:PCW:H39	4:A:405:PCW:H261	0.67	1.64	1	1
4:C:622:PCW:H231	4:D:501:PCW:C38	0.67	2.19	1	1
4:A:404:PCW:H272	4:A:411:PCW:H241	0.67	1.67	7	3
4:D:505:PCW:H351	4:D:505:PCW:C31	0.67	2.20	2	1
3:D:479:LYS:HE2	5:D:525:17F:H1A	0.67	1.66	4	1
4:D:508:PCW:H132	4:D:512:PCW:H122	0.67	1.66	5	1
4:A:406:PCW:H272	4:C:618:PCW:H462	0.67	1.65	6	1
4:B:201:PCW:H161	4:D:506:PCW:C46	0.67	2.05	6	2
4:D:506:PCW:H172	4:D:516:PCW:H342	0.67	1.66	10	1
4:C:601:PCW:C39	4:C:602:PCW:H171	0.67	2.19	1	2
4:D:509:PCW:H281	5:D:520:17F:H31	0.67	1.64	1	1
4:D:527:PCW:C44	4:D:528:PCW:H341	0.67	2.18	6	3
4:C:612:PCW:H321	4:C:618:PCW:H141	0.67	1.67	6	2
4:D:501:PCW:H39	4:D:515:PCW:H441	0.67	1.66	4	1
4:C:610:PCW:H20	4:C:610:PCW:C24	0.67	2.19	6	1
4:A:404:PCW:H52	4:D:510:PCW:O11	0.67	1.89	9	1
4:B:201:PCW:C21	4:D:506:PCW:H452	0.67	2.20	10	1
4:C:602:PCW:O31	4:C:602:PCW:H12	0.67	1.88	2	10
4:C:602:PCW:H172	4:C:602:PCW:C22	0.67	2.19	6	4
4:D:508:PCW:H141	4:D:509:PCW:H222	0.67	1.66	2	1
4:D:516:PCW:H451	5:D:530:17F:H42	0.67	1.67	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:522:17F:H12A	5:D:522:17F:H41	0.67	1.67	6	1
4:D:508:PCW:H12	5:D:523:17F:C12	0.67	2.19	8	1
4:C:605:PCW:C47	4:C:619:PCW:H432	0.67	2.19	9	2
4:B:203:PCW:H232	4:B:204:PCW:H451	0.67	1.66	9	2
4:C:605:PCW:H61	5:C:628:17F:O4	0.67	1.90	10	1
1:C:462:LYS:HB3	4:C:602:PCW:H281	0.67	1.65	5	2
4:B:203:PCW:C23	4:B:204:PCW:H431	0.67	2.20	9	4
4:B:204:PCW:H132	4:B:204:PCW:C34	0.67	2.20	9	6
4:C:602:PCW:H73	5:D:523:17F:H19A	0.67	1.67	3	3
4:C:618:PCW:O2P	4:C:625:PCW:H82	0.67	1.90	3	1
4:D:518:PCW:H351	4:D:518:PCW:O3	0.67	1.89	3	2
4:D:507:PCW:H422	5:D:522:17F:C20	0.67	2.18	5	1
4:B:201:PCW:H162	5:D:520:17F:C42	0.67	2.20	8	1
4:A:414:PCW:H12	4:C:617:PCW:C4	0.67	2.19	10	1
4:D:506:PCW:H271	4:D:516:PCW:H142	0.66	1.66	1	1
4:D:510:PCW:C33	5:D:524:17F:H11	0.66	2.20	1	1
5:D:525:17F:O2	5:D:525:17F:N1	0.66	2.27	2	10
5:C:626:17F:H59	5:C:627:17F:H51	0.66	1.67	2	1
4:B:202:PCW:C48	5:D:524:17F:H31	0.66	2.20	4	1
4:A:411:PCW:C40	4:C:612:PCW:H231	0.66	2.20	5	1
4:D:517:PCW:H211	4:D:517:PCW:C16	0.66	2.20	5	4
4:D:509:PCW:C44	5:D:520:17F:H33	0.66	2.21	7	2
4:D:515:PCW:H152	5:D:525:17F:H61	0.66	1.66	10	2
4:C:618:PCW:H442	4:C:625:PCW:H282	0.66	1.66	9	1
4:D:516:PCW:C23	5:D:519:17F:H55	0.66	2.19	9	1
1:A:363:LYS:HA	1:A:367:ALA:HB3	0.66	1.65	6	9
4:C:608:PCW:H261	5:C:627:17F:C34	0.66	2.20	8	4
5:C:630:17F:H29	5:D:529:17F:C39	0.66	2.20	1	3
4:D:509:PCW:H11	4:D:509:PCW:O31	0.66	1.90	6	10
4:C:605:PCW:H231	4:C:613:PCW:C39	0.66	2.20	6	7
4:D:508:PCW:C22	4:D:512:PCW:H431	0.66	2.19	10	2
4:D:509:PCW:H152	4:D:514:PCW:H122	0.66	1.67	2	1
4:D:517:PCW:H421	4:D:517:PCW:C21	0.66	2.20	2	2
5:D:522:17F:H2	5:D:522:17F:O2	0.66	1.91	7	7
4:A:405:PCW:H51	4:D:514:PCW:H351	0.66	1.65	10	3
4:A:412:PCW:C47	4:C:607:PCW:H471	0.66	2.20	3	4
4:C:616:PCW:H11	4:D:527:PCW:H342	0.66	1.65	4	3
4:D:528:PCW:H172	5:D:530:17F:C1Y	0.66	2.20	6	3
4:D:508:PCW:H171	4:D:512:PCW:H382	0.66	1.67	6	1
4:B:203:PCW:C23	4:B:204:PCW:H40	0.66	2.19	7	1
4:D:502:PCW:H161	4:D:505:PCW:C32	0.66	2.20	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:501:PCW:H411	4:D:515:PCW:H182	0.66	1.66	10	1
5:C:631:17F:C29	4:D:512:PCW:H161	0.66	2.21	1	1
4:C:615:PCW:H212	4:D:512:PCW:H282	0.66	1.65	2	2
4:B:203:PCW:C26	4:B:203:PCW:C22	0.66	2.73	8	7
4:D:503:PCW:H431	5:D:522:17F:H9A	0.66	1.67	4	1
4:D:518:PCW:H381	5:D:521:17F:H9A	0.66	1.67	5	1
5:D:524:17F:H62	5:D:524:17F:H56	0.66	1.65	6	1
4:D:515:PCW:H32	5:D:525:17F:C1Y	0.66	2.14	10	2
4:C:613:PCW:C20	5:D:521:17F:H48	0.66	2.21	8	2
4:D:509:PCW:O1P	4:D:509:PCW:H31	0.66	1.89	9	1
4:D:501:PCW:H461	5:D:525:17F:H50	0.66	1.66	10	1
4:A:410:PCW:H52	4:A:410:PCW:O1P	0.66	1.90	1	10
4:D:501:PCW:H431	5:D:525:17F:H51	0.66	1.67	1	1
4:D:502:PCW:H221	4:D:505:PCW:H251	0.66	1.65	2	2
4:C:616:PCW:H461	4:C:625:PCW:C26	0.66	2.20	7	2
4:C:623:PCW:H282	5:D:525:17F:H50	0.66	1.67	6	1
5:D:529:17F:C24	5:D:530:17F:H73	0.66	2.13	8	2
4:A:403:PCW:H161	4:D:513:PCW:H352	0.66	1.66	9	1
4:D:516:PCW:H452	5:D:529:17F:H54	0.66	1.67	9	1
4:B:201:PCW:H261	4:D:528:PCW:H421	0.66	1.66	1	1
4:A:405:PCW:O31	4:D:514:PCW:H321	0.66	1.91	10	4
4:C:604:PCW:H281	4:C:607:PCW:H483	0.66	1.67	3	2
1:A:299:SER:HB2	1:A:300:PRO:HD3	0.66	1.67	4	1
4:D:509:PCW:C6	4:D:514:PCW:H12	0.66	2.21	6	1
4:D:511:PCW:H182	4:D:511:PCW:C34	0.66	2.21	8	3
4:A:405:PCW:H152	4:D:512:PCW:C39	0.66	2.19	9	1
4:A:414:PCW:C37	4:C:617:PCW:H141	0.66	2.20	9	1
4:D:503:PCW:H461	4:D:507:PCW:C47	0.66	2.18	10	1
4:D:505:PCW:H421	4:D:505:PCW:H162	0.66	1.66	10	1
4:C:615:PCW:O1P	4:C:615:PCW:H52	0.66	1.91	10	9
4:D:502:PCW:H331	4:D:510:PCW:C5	0.66	2.19	1	1
4:C:611:PCW:H222	4:C:619:PCW:H461	0.66	1.66	2	1
4:A:408:PCW:H351	4:D:514:PCW:H39	0.66	1.67	3	2
4:C:604:PCW:H272	4:C:623:PCW:C48	0.66	2.20	7	2
4:B:201:PCW:H482	4:D:527:PCW:C23	0.66	2.20	4	3
4:A:408:PCW:C41	4:B:203:PCW:H182	0.66	2.18	5	1
4:C:616:PCW:H381	4:C:618:PCW:H162	0.66	1.68	5	1
4:C:615:PCW:H82	5:C:631:17F:O4	0.66	1.91	10	3
4:D:515:PCW:C15	4:D:517:PCW:H122	0.66	2.18	6	1
4:D:506:PCW:H351	4:D:509:PCW:H351	0.66	1.67	8	1
4:D:508:PCW:H12	5:D:523:17F:H12A	0.66	1.66	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:617:PCW:H51	4:C:617:PCW:O11	0.66	1.91	1	2
5:D:525:17F:H77	5:D:525:17F:C27	0.66	2.20	1	2
3:D:430:PHE:HB2	3:D:435:PRO:HA	0.66	1.68	4	2
4:D:509:PCW:H31	4:D:509:PCW:P	0.66	2.31	5	4
4:C:613:PCW:O31	4:C:619:PCW:H2	0.66	1.90	8	3
4:C:620:PCW:C7	4:C:620:PCW:H11	0.66	2.21	4	2
4:C:606:PCW:H161	5:D:529:17F:H8	0.66	1.66	5	1
4:D:502:PCW:H141	4:D:505:PCW:H11	0.66	1.66	6	1
4:D:515:PCW:H63	4:D:516:PCW:H321	0.66	1.68	10	3
4:C:625:PCW:H42	4:C:625:PCW:C2	0.66	2.16	10	1
4:D:506:PCW:C25	4:D:506:PCW:C21	0.66	2.69	10	8
4:A:410:PCW:C44	4:C:617:PCW:H242	0.66	2.20	5	3
4:C:607:PCW:O3	4:C:624:PCW:H422	0.66	1.91	3	2
4:C:607:PCW:H361	4:C:624:PCW:H431	0.66	1.68	4	2
5:C:630:17F:H65	5:C:631:17F:H72	0.66	1.67	9	2
4:D:504:PCW:C7	4:D:516:PCW:H63	0.66	2.21	4	1
4:C:613:PCW:H141	4:C:619:PCW:C39	0.66	2.21	7	2
5:C:626:17F:H20A	5:C:626:17F:O9	0.66	1.89	6	1
4:A:401:PCW:H62	4:D:511:PCW:O31	0.66	1.91	9	2
4:D:506:PCW:H12	4:D:515:PCW:C6	0.66	2.21	8	1
4:D:501:PCW:H431	4:D:515:PCW:H221	0.66	1.67	10	1
4:A:407:PCW:H272	4:A:407:PCW:C47	0.66	2.21	2	5
4:A:412:PCW:H63	4:C:624:PCW:O31	0.66	1.91	1	3
4:C:606:PCW:H252	5:D:529:17F:C22	0.66	2.21	9	4
4:D:502:PCW:C31	4:D:502:PCW:C35	0.66	2.73	3	10
5:D:530:17F:H11	5:D:530:17F:H56	0.66	1.66	1	4
4:C:601:PCW:C5	4:D:513:PCW:H61	0.66	2.21	2	2
4:C:604:PCW:C18	5:D:525:17F:H53	0.66	2.19	2	1
4:D:502:PCW:H82	4:D:505:PCW:O1P	0.66	1.91	7	3
4:A:411:PCW:C8	4:C:617:PCW:H40	0.66	2.21	7	2
4:C:615:PCW:H181	5:C:631:17F:C21	0.66	2.21	5	3
4:D:517:PCW:O3P	4:D:517:PCW:H82	0.66	1.90	5	1
4:C:604:PCW:H451	4:C:606:PCW:H141	0.66	1.68	9	1
4:B:203:PCW:C19	4:D:506:PCW:H451	0.66	2.20	10	1
4:C:621:PCW:H422	5:C:630:17F:H66	0.66	1.66	9	3
4:C:623:PCW:C45	4:C:624:PCW:H482	0.66	2.20	5	5
4:D:516:PCW:O11	4:D:516:PCW:H2	0.66	1.90	3	7
4:C:621:PCW:C14	5:C:630:17F:H4A	0.66	2.21	2	3
4:D:513:PCW:H442	4:D:517:PCW:H262	0.66	1.67	2	2
4:C:618:PCW:H151	4:C:625:PCW:H151	0.66	1.67	4	1
4:A:407:PCW:H151	4:D:511:PCW:H283	0.66	1.65	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:611:PCW:C20	4:C:619:PCW:H482	0.66	2.21	6	2
4:D:503:PCW:H31	4:D:511:PCW:H11	0.66	1.66	6	1
4:D:505:PCW:H411	5:D:519:17F:H56	0.66	1.66	6	1
4:D:508:PCW:H172	4:D:512:PCW:H362	0.66	1.67	6	1
4:D:518:PCW:H341	5:D:519:17F:H62	0.66	1.68	6	1
4:D:503:PCW:H211	4:D:503:PCW:H172	0.66	1.66	8	1
4:B:202:PCW:H11	4:D:504:PCW:C11	0.66	2.21	9	1
4:D:503:PCW:H422	5:D:522:17F:C24	0.66	2.22	10	1
1:A:231:ASN:HA	1:A:234:LYS:HD2	0.65	1.68	4	6
4:C:618:PCW:H382	5:C:629:17F:H41	0.65	1.67	1	4
5:C:629:17F:O7	5:C:629:17F:O10	0.65	2.14	9	10
5:D:522:17F:O8	5:D:525:17F:H6A	0.65	1.91	1	1
4:D:508:PCW:H181	4:D:512:PCW:C36	0.65	2.15	10	3
4:C:625:PCW:H182	4:C:625:PCW:H221	0.65	1.66	5	3
4:B:201:PCW:C42	5:D:524:17F:H48	0.65	2.21	5	1
4:D:509:PCW:H62	4:D:514:PCW:H12	0.65	1.66	6	1
4:A:402:PCW:H411	4:D:512:PCW:C36	0.65	2.21	7	1
4:A:403:PCW:H481	4:C:607:PCW:H262	0.65	1.66	7	2
4:B:201:PCW:H341	4:D:510:PCW:H361	0.65	1.68	8	1
4:D:502:PCW:H472	4:D:505:PCW:H271	0.65	1.68	8	1
5:D:525:17F:H64	5:D:525:17F:C2X	0.65	2.21	8	2
4:A:414:PCW:H442	4:C:617:PCW:H20	0.65	1.68	2	1
4:B:203:PCW:O31	4:B:204:PCW:H82	0.65	1.91	2	3
4:D:528:PCW:H121	5:D:530:17F:C1Y	0.65	2.21	2	1
4:C:602:PCW:H321	5:D:523:17F:H60	0.65	1.68	9	2
4:C:610:PCW:H132	4:C:610:PCW:H342	0.65	1.68	6	2
4:D:517:PCW:C34	5:D:520:17F:H8	0.65	2.18	6	1
4:C:613:PCW:H212	5:D:521:17F:H47	0.65	1.66	7	1
4:D:518:PCW:H341	5:D:519:17F:C31	0.65	2.19	8	1
4:D:518:PCW:H141	5:D:519:17F:H66	0.65	1.68	9	1
4:A:414:PCW:H321	4:C:617:PCW:H52	0.65	1.65	8	3
4:A:404:PCW:H271	4:A:411:PCW:H241	0.65	1.66	10	5
4:A:407:PCW:O31	5:D:522:17F:H33	0.65	1.91	4	3
4:C:625:PCW:H211	4:D:528:PCW:H372	0.65	1.66	7	5
4:B:202:PCW:H19	4:B:202:PCW:H431	0.65	1.67	4	1
4:D:501:PCW:H432	5:D:522:17F:H36	0.65	1.69	5	1
4:D:516:PCW:O31	4:D:516:PCW:C4	0.65	2.44	10	3
4:D:515:PCW:H232	5:D:525:17F:H43	0.65	1.69	7	1
4:C:616:PCW:H471	4:B:201:PCW:C45	0.65	2.15	8	1
4:C:602:PCW:C36	5:D:523:17F:H61	0.65	2.21	6	3
4:C:616:PCW:H341	4:D:527:PCW:H362	0.65	1.65	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:504:PCW:H452	4:D:505:PCW:H141	0.65	1.65	3	1
4:D:511:PCW:H141	5:D:522:17F:C17	0.65	2.21	3	1
4:D:509:PCW:C19	5:D:520:17F:H19	0.65	2.21	4	1
4:D:508:PCW:O4P	5:D:523:17F:H12A	0.65	1.91	6	1
4:D:507:PCW:H40	5:D:522:17F:H11A	0.65	1.68	8	1
4:A:408:PCW:H342	4:D:514:PCW:H451	0.65	1.67	4	2
4:C:610:PCW:H241	4:C:610:PCW:C19	0.65	2.22	4	3
4:D:504:PCW:H362	4:D:510:PCW:O2P	0.65	1.92	1	1
4:A:414:PCW:H32	4:A:414:PCW:H41	0.65	1.67	3	1
5:C:626:17F:C31	5:C:627:17F:H51	0.65	2.20	10	5
4:D:504:PCW:C25	4:D:504:PCW:C21	0.65	2.71	4	3
4:A:411:PCW:H431	4:C:612:PCW:C16	0.65	2.21	5	2
4:D:517:PCW:H52	4:D:517:PCW:H11	0.65	1.68	5	1
4:C:613:PCW:H482	4:C:619:PCW:C21	0.65	2.14	6	2
4:A:413:PCW:H362	4:C:617:PCW:H381	0.65	1.68	8	4
4:A:415:PCW:C48	5:D:521:17F:H55	0.65	2.20	8	1
4:C:607:PCW:H362	4:C:624:PCW:C43	0.65	2.21	10	1
4:A:410:PCW:C41	4:A:410:PCW:H371	0.65	2.22	6	6
4:A:401:PCW:H472	4:C:611:PCW:C26	0.65	2.22	2	3
4:C:602:PCW:H141	5:C:626:17F:H54	0.65	1.67	2	2
4:A:402:PCW:H331	4:D:514:PCW:C3	0.65	2.21	3	1
4:D:518:PCW:H471	5:D:521:17F:H9A	0.65	1.68	3	1
4:C:606:PCW:H73	4:C:624:PCW:C19	0.65	2.16	5	2
4:C:616:PCW:C38	4:C:618:PCW:H162	0.65	2.21	5	1
4:C:618:PCW:C14	4:C:625:PCW:H142	0.65	2.21	7	1
4:D:515:PCW:H321	4:D:516:PCW:H12	0.65	1.67	7	1
4:A:404:PCW:H241	4:A:411:PCW:C26	0.65	2.21	8	1
4:A:406:PCW:O1P	4:B:202:PCW:H361	0.65	1.92	1	1
4:D:508:PCW:H82	5:D:523:17F:H10	0.65	1.67	6	2
4:C:604:PCW:H231	5:D:525:17F:H76	0.65	1.66	2	3
5:D:523:17F:O8	5:D:523:17F:H5	0.65	1.91	10	2
4:C:604:PCW:H411	5:D:529:17F:H36	0.65	1.69	8	3
4:D:513:PCW:O11	4:D:513:PCW:C5	0.65	2.43	6	4
4:A:404:PCW:H362	4:D:510:PCW:H232	0.65	1.67	9	2
4:D:518:PCW:H162	5:D:519:17F:H59	0.65	1.68	9	2
4:C:607:PCW:H432	4:C:624:PCW:C47	0.65	2.22	7	2
4:D:527:PCW:H372	4:D:527:PCW:H142	0.65	1.66	1	1
4:A:415:PCW:H211	4:C:603:PCW:H161	0.65	1.68	10	2
4:C:620:PCW:C14	5:C:631:17F:H18	0.65	2.22	8	4
5:D:519:17F:C34	5:D:521:17F:H37	0.65	2.21	2	1
4:D:506:PCW:C13	4:D:506:PCW:C17	0.65	2.73	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:202:PCW:C28	4:D:506:PCW:H481	0.65	2.21	9	1
4:A:413:PCW:O2	4:C:617:PCW:H411	0.65	1.91	6	3
4:C:606:PCW:H252	5:D:529:17F:C24	0.65	2.22	9	5
4:D:501:PCW:H472	5:D:525:17F:H42	0.65	1.67	2	1
4:A:410:PCW:H431	4:A:414:PCW:C40	0.65	2.22	3	1
4:B:202:PCW:H362	4:B:202:PCW:H122	0.65	1.67	3	1
4:D:508:PCW:H73	5:D:520:17F:O8	0.65	1.91	6	1
4:A:405:PCW:H321	4:A:408:PCW:H351	0.65	1.67	9	1
4:C:610:PCW:C20	4:C:610:PCW:C24	0.65	2.75	8	10
4:B:203:PCW:O31	4:B:203:PCW:H73	0.65	1.92	7	3
4:D:506:PCW:H20	4:D:516:PCW:H342	0.65	1.67	4	2
4:C:608:PCW:H461	5:C:626:17F:C33	0.65	2.22	3	1
4:C:612:PCW:C32	4:C:618:PCW:H152	0.65	2.22	4	2
4:C:617:PCW:H382	4:D:526:PCW:H161	0.65	1.68	5	1
4:D:501:PCW:H432	5:D:522:17F:C2X	0.65	2.22	5	1
4:C:604:PCW:H251	4:D:517:PCW:H472	0.65	1.69	6	1
4:A:403:PCW:H231	4:D:507:PCW:C15	0.65	2.20	9	2
4:A:412:PCW:H2	4:A:412:PCW:O11	0.64	1.92	9	2
4:C:616:PCW:H39	4:C:618:PCW:C16	0.64	2.22	10	4
3:D:427:GLN:HB2	4:D:502:PCW:C6	0.64	2.22	2	1
4:A:414:PCW:C11	4:A:414:PCW:H63	0.64	2.22	3	1
4:D:505:PCW:O31	4:D:505:PCW:H51	0.64	1.92	6	2
4:D:511:PCW:H31	4:D:511:PCW:P	0.64	2.33	7	5
4:C:611:PCW:H161	4:C:619:PCW:C17	0.64	2.19	5	1
4:D:507:PCW:H41	5:D:523:17F:HN1A	0.64	1.52	5	1
4:C:609:PCW:H452	4:D:512:PCW:C23	0.64	2.22	6	3
4:D:515:PCW:O3	4:D:517:PCW:H32	0.64	1.92	6	1
4:D:518:PCW:H122	5:D:519:17F:H67	0.64	1.67	8	1
4:D:511:PCW:H231	4:D:511:PCW:C38	0.64	2.18	10	1
4:A:410:PCW:C28	4:A:413:PCW:H251	0.64	2.22	9	3
4:C:609:PCW:H122	4:C:615:PCW:C7	0.64	2.22	5	5
4:C:614:PCW:C46	4:C:614:PCW:C42	0.64	2.72	10	10
4:D:505:PCW:O31	4:D:505:PCW:O3	0.64	2.16	2	7
4:A:407:PCW:H182	4:A:412:PCW:H261	0.64	1.70	2	1
4:C:620:PCW:H283	5:C:631:17F:C2X	0.64	2.18	8	4
5:D:525:17F:H51	5:D:525:17F:H77	0.64	1.67	3	1
4:A:408:PCW:H452	4:B:203:PCW:H472	0.64	1.70	6	2
4:C:618:PCW:H381	4:C:625:PCW:C16	0.64	2.20	9	5
4:D:513:PCW:C45	4:D:517:PCW:H283	0.64	2.18	4	1
4:C:603:PCW:H52	4:C:603:PCW:C31	0.64	2.21	9	1
4:D:507:PCW:H221	4:D:513:PCW:C27	0.64	2.20	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:507:PCW:H63	4:D:517:PCW:O2P	0.64	1.92	10	1
4:A:402:PCW:C8	4:A:405:PCW:H32	0.64	2.22	5	5
4:D:504:PCW:C21	4:D:504:PCW:C25	0.64	2.72	6	7
1:C:574:LEU:HB2	1:C:575:PRO:HD3	0.64	1.68	3	1
4:D:516:PCW:H242	4:D:526:PCW:H461	0.64	1.69	3	1
5:D:529:17F:C20	5:D:529:17F:H9A	0.64	2.23	7	1
4:B:201:PCW:C27	4:D:528:PCW:H421	0.64	2.23	8	1
4:B:201:PCW:H252	4:D:506:PCW:H441	0.64	1.69	9	1
4:A:411:PCW:H441	4:C:612:PCW:H271	0.64	1.69	1	2
4:C:601:PCW:C43	4:C:601:PCW:C47	0.64	2.71	6	2
4:C:623:PCW:H31	4:C:624:PCW:H32	0.64	1.68	10	4
4:C:613:PCW:C22	5:D:521:17F:H47	0.64	2.23	5	2
4:D:504:PCW:H321	4:D:510:PCW:C35	0.64	2.21	3	1
4:C:603:PCW:C22	4:D:526:PCW:H331	0.64	2.23	10	4
4:C:606:PCW:C7	4:C:624:PCW:H19	0.64	2.17	5	1
4:D:509:PCW:H211	5:D:520:17F:C31	0.64	2.12	5	1
4:A:411:PCW:H351	4:C:612:PCW:C15	0.64	2.22	6	2
4:A:406:PCW:H262	4:D:504:PCW:H241	0.64	1.69	7	1
4:D:502:PCW:H212	4:D:502:PCW:C41	0.64	2.21	9	1
4:C:619:PCW:H11	4:C:619:PCW:O31	0.64	1.91	4	10
4:C:618:PCW:H251	4:B:201:PCW:H441	0.64	1.68	2	1
4:D:508:PCW:H62	5:D:520:17F:O1	0.64	1.92	2	1
4:C:605:PCW:H322	4:C:611:PCW:O3P	0.64	1.93	4	3
4:D:512:PCW:C27	4:D:512:PCW:C23	0.64	2.74	5	1
4:A:403:PCW:C35	4:A:407:PCW:H322	0.64	2.21	6	1
4:A:406:PCW:H2	4:B:202:PCW:H381	0.64	1.70	6	1
4:D:512:PCW:H371	4:D:512:PCW:H411	0.64	1.67	9	1
4:C:615:PCW:H432	4:D:512:PCW:H262	0.64	1.68	10	1
4:B:204:PCW:O31	4:B:204:PCW:C5	0.64	2.44	10	1
1:C:512:ASP:HA	1:C:515:ARG:HD2	0.64	1.70	10	7
4:C:610:PCW:H62	5:C:629:17F:H4A	0.64	1.68	1	1
4:A:415:PCW:H272	4:D:516:PCW:H272	0.64	1.68	2	1
5:A:409:17F:H2	5:A:409:17F:O2	0.64	1.92	10	4
5:C:630:17F:C1X	5:D:530:17F:H62	0.64	2.23	4	3
4:D:518:PCW:H212	5:D:519:17F:H34	0.64	1.69	3	2
4:B:203:PCW:C20	4:D:506:PCW:H451	0.64	2.23	9	3
4:D:517:PCW:C40	5:D:525:17F:H59	0.64	2.23	4	1
4:A:411:PCW:H431	4:C:612:PCW:H162	0.64	1.69	5	1
4:A:410:PCW:O11	4:D:526:PCW:H121	0.64	1.93	6	2
4:A:413:PCW:H362	4:C:617:PCW:H382	0.64	1.68	7	3
4:A:406:PCW:C15	4:B:202:PCW:H222	0.64	2.21	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:509:PCW:C28	4:D:509:PCW:H483	0.64	2.23	8	1
4:D:513:PCW:H361	5:D:522:17F:H64	0.64	1.68	8	1
4:A:402:PCW:C31	4:A:402:PCW:C35	0.64	2.76	8	10
4:A:413:PCW:C46	4:C:616:PCW:H251	0.64	2.23	1	1
4:C:608:PCW:C46	5:C:626:17F:H61	0.64	2.15	2	3
4:C:621:PCW:H381	5:C:631:17F:C42	0.64	2.23	1	1
5:C:631:17F:O10	5:C:631:17F:H4	0.64	1.91	1	8
4:D:503:PCW:H471	4:D:511:PCW:C28	0.64	2.22	2	1
4:D:510:PCW:C47	5:D:524:17F:H57	0.64	2.10	2	2
4:D:518:PCW:H122	5:D:519:17F:C37	0.64	2.23	8	2
4:D:518:PCW:H172	5:D:519:17F:H20A	0.64	1.68	3	2
4:A:412:PCW:H471	4:C:607:PCW:H471	0.64	1.68	4	1
4:D:504:PCW:C33	4:D:516:PCW:H141	0.64	2.18	7	2
4:D:528:PCW:H19	5:D:530:17F:H19A	0.64	1.69	10	2
4:D:502:PCW:H481	4:D:505:PCW:H283	0.64	1.68	8	1
4:D:515:PCW:C6	4:D:516:PCW:H321	0.64	2.23	9	1
4:B:201:PCW:H32	4:B:201:PCW:P	0.64	2.33	1	5
4:D:528:PCW:H172	5:D:530:17F:H34	0.64	1.67	6	3
4:A:401:PCW:C45	4:C:611:PCW:H271	0.64	2.22	2	2
4:C:610:PCW:H172	5:C:629:17F:H61	0.64	1.67	2	2
2:B:47:ASP:HA	3:D:448:LYS:HD2	0.64	1.69	2	4
2:B:16:LYS:HB3	6:B:205:GNP:O1G	0.64	1.91	3	3
4:D:516:PCW:H40	4:D:527:PCW:C26	0.64	2.23	3	2
4:C:602:PCW:H51	4:C:602:PCW:O1P	0.64	1.92	4	1
4:B:203:PCW:H482	4:B:203:PCW:H212	0.64	1.68	4	1
4:A:406:PCW:C17	4:B:202:PCW:H232	0.64	2.22	6	2
4:D:508:PCW:H42	5:D:520:17F:H6	0.64	1.69	9	1
4:D:518:PCW:C47	5:D:521:17F:H12A	0.64	2.23	10	1
4:A:413:PCW:H422	4:C:616:PCW:C23	0.64	2.21	7	6
4:C:605:PCW:C32	4:C:613:PCW:H51	0.64	2.23	1	2
4:C:617:PCW:C27	4:C:617:PCW:C23	0.64	2.75	6	9
4:D:517:PCW:H441	4:D:517:PCW:H212	0.64	1.68	1	1
5:D:522:17F:C6	5:D:525:17F:H2	0.64	2.22	1	1
4:C:615:PCW:H221	4:D:512:PCW:C26	0.64	2.16	4	3
4:D:506:PCW:H82	4:D:515:PCW:O1P	0.64	1.93	2	1
4:D:509:PCW:H421	4:D:509:PCW:H372	0.64	1.70	10	2
4:A:405:PCW:O3P	4:A:405:PCW:O31	0.64	2.15	3	2
4:C:616:PCW:H281	4:C:618:PCW:H282	0.64	1.68	3	1
4:D:505:PCW:H411	5:D:519:17F:H39	0.64	1.70	5	1
4:C:606:PCW:O11	4:C:606:PCW:H63	0.64	1.92	6	1
4:D:509:PCW:H161	5:D:520:17F:C31	0.64	2.23	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:527:PCW:C16	4:D:528:PCW:H162	0.64	2.22	6	2
4:D:511:PCW:H362	4:D:511:PCW:H221	0.64	1.68	7	2
4:D:506:PCW:H142	5:D:520:17F:H41	0.64	1.68	8	1
4:A:405:PCW:H152	4:D:512:PCW:H39	0.64	1.68	9	1
4:C:615:PCW:H472	4:D:512:PCW:C22	0.64	2.16	10	1
4:A:402:PCW:H441	4:D:512:PCW:H152	0.64	1.70	1	2
4:A:403:PCW:H39	4:A:407:PCW:H371	0.64	1.68	1	1
4:C:621:PCW:O3P	4:C:621:PCW:O31	0.64	2.16	1	10
4:D:509:PCW:H41	4:D:509:PCW:C3	0.64	2.18	1	1
3:D:425:GLU:O	4:D:502:PCW:H62	0.64	1.93	2	1
4:A:410:PCW:O3P	4:A:410:PCW:O31	0.64	2.16	3	2
4:C:604:PCW:H452	4:C:606:PCW:H181	0.64	1.70	3	3
4:D:508:PCW:C14	4:D:509:PCW:H182	0.64	2.23	3	1
4:D:506:PCW:C7	4:D:517:PCW:H332	0.64	2.23	4	1
4:D:507:PCW:H41	5:D:523:17F:O4	0.64	1.93	4	1
4:A:405:PCW:H122	4:D:514:PCW:H322	0.64	1.69	5	1
4:A:413:PCW:H31	4:C:617:PCW:C42	0.64	2.23	8	3
4:C:606:PCW:C25	5:D:529:17F:H38	0.64	2.23	9	2
4:C:624:PCW:C27	4:C:624:PCW:C23	0.63	2.73	6	10
4:D:509:PCW:H441	5:D:520:17F:C1Y	0.63	2.23	1	1
4:C:606:PCW:H52	4:C:624:PCW:H19	0.63	1.70	2	1
4:B:201:PCW:H422	5:D:524:17F:H47	0.63	1.70	8	3
4:C:611:PCW:H51	4:C:622:PCW:C34	0.63	2.20	3	1
4:D:506:PCW:H222	4:D:516:PCW:H371	0.63	1.70	3	1
4:D:515:PCW:H371	4:D:515:PCW:C41	0.63	2.07	9	2
4:B:201:PCW:H11	4:D:504:PCW:C15	0.63	2.20	6	1
4:C:616:PCW:H281	4:D:510:PCW:H282	0.63	1.69	8	1
4:A:406:PCW:H131	4:B:202:PCW:H211	0.63	1.70	9	1
4:C:625:PCW:H283	5:C:629:17F:H51	0.63	1.70	8	3
5:C:630:17F:H36	5:D:530:17F:H62	0.63	1.69	7	3
4:A:410:PCW:H371	4:A:410:PCW:H411	0.63	1.70	2	3
4:D:507:PCW:H39	5:D:522:17F:H6A	0.63	1.71	2	1
4:C:604:PCW:H242	5:D:525:17F:H76	0.63	1.69	7	2
4:B:203:PCW:C31	4:B:203:PCW:H52	0.63	2.22	3	1
4:D:505:PCW:H171	4:D:505:PCW:C22	0.63	2.20	3	1
4:A:415:PCW:H322	4:C:622:PCW:O31	0.63	1.93	10	2
4:A:415:PCW:H261	4:D:528:PCW:H262	0.63	1.70	9	1
4:B:203:PCW:H441	4:B:204:PCW:H382	0.63	1.69	9	1
4:B:201:PCW:C23	4:D:506:PCW:H452	0.63	2.22	10	1
4:A:403:PCW:H261	4:D:507:PCW:H19	0.63	1.71	1	1
4:A:407:PCW:H142	4:A:407:PCW:C18	0.63	2.24	9	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:611:PCW:H172	4:C:611:PCW:C35	0.63	2.23	1	2
4:C:602:PCW:O31	4:C:602:PCW:H31	0.63	1.92	8	3
4:C:614:PCW:C6	4:C:623:PCW:O1P	0.63	2.47	6	7
4:B:201:PCW:H212	4:D:506:PCW:H441	0.63	1.69	2	1
4:D:506:PCW:C19	4:D:516:PCW:H362	0.63	2.23	3	3
4:D:509:PCW:H441	5:D:520:17F:C1Z	0.63	2.23	6	2
4:D:505:PCW:H441	4:D:518:PCW:H251	0.63	1.67	7	1
4:D:506:PCW:H262	4:D:516:PCW:H161	0.63	1.70	9	1
4:D:511:PCW:C11	4:D:511:PCW:C31	0.63	2.77	10	2
4:A:407:PCW:C38	5:D:522:17F:H65	0.63	2.23	1	1
4:A:415:PCW:C6	4:A:415:PCW:O4P	0.63	2.47	7	7
5:C:630:17F:C27	5:D:529:17F:H10	0.63	2.20	5	2
4:D:506:PCW:H222	4:D:516:PCW:H411	0.63	1.70	2	1
4:A:415:PCW:H62	4:A:415:PCW:O4P	0.63	1.92	9	3
4:C:601:PCW:C7	4:C:602:PCW:H11	0.63	2.23	4	1
4:D:501:PCW:C22	5:D:521:17F:H19	0.63	2.17	5	1
4:D:517:PCW:H283	4:D:517:PCW:H482	0.63	1.70	5	1
4:A:406:PCW:O1P	4:A:406:PCW:H51	0.63	1.93	10	3
4:B:201:PCW:C15	4:D:516:PCW:H422	0.63	2.19	6	1
4:D:515:PCW:H481	4:D:516:PCW:H481	0.63	1.69	6	1
4:B:201:PCW:C25	4:D:506:PCW:H441	0.63	2.24	9	1
4:A:415:PCW:C24	4:A:415:PCW:C20	0.63	2.72	9	10
4:C:613:PCW:H431	4:C:619:PCW:H39	0.63	1.71	10	3
2:B:167:LYS:HB3	4:B:203:PCW:H63	0.63	1.68	1	1
4:C:604:PCW:H41	4:C:604:PCW:O11	0.63	1.93	9	2
4:C:617:PCW:H62	4:C:617:PCW:C31	0.63	2.24	7	4
4:A:410:PCW:H211	4:A:413:PCW:H411	0.63	1.70	5	1
4:D:508:PCW:C13	4:D:509:PCW:H242	0.63	2.23	6	1
4:D:506:PCW:O3	4:D:509:PCW:H381	0.63	1.93	10	1
4:A:406:PCW:H432	4:B:204:PCW:H19	0.63	1.69	1	1
4:C:603:PCW:H172	4:C:603:PCW:H211	0.63	1.70	10	7
4:B:203:PCW:C22	4:B:203:PCW:C26	0.63	2.76	4	3
4:D:514:PCW:O31	4:D:514:PCW:H11	0.63	1.93	3	4
4:C:603:PCW:H62	4:D:527:PCW:O3P	0.63	1.92	3	2
4:D:504:PCW:C32	4:D:510:PCW:H361	0.63	2.22	3	1
4:C:601:PCW:H121	4:C:601:PCW:C45	0.63	2.23	4	2
4:C:609:PCW:H431	4:D:512:PCW:H241	0.63	1.68	1	1
4:D:506:PCW:C4	4:D:509:PCW:H331	0.63	2.12	1	1
4:D:513:PCW:C47	4:D:513:PCW:C43	0.63	2.76	2	10
4:D:517:PCW:H483	5:D:525:17F:C10	0.63	2.23	1	1
4:A:405:PCW:H321	4:D:514:PCW:H352	0.63	1.71	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:615:PCW:H471	4:D:512:PCW:H232	0.63	1.69	2	1
4:B:201:PCW:C7	4:B:202:PCW:H31	0.63	2.24	3	1
5:C:626:17F:C31	5:C:626:17F:C19	0.63	2.76	6	4
4:A:401:PCW:H182	4:A:401:PCW:C22	0.63	2.17	6	1
4:B:203:PCW:C13	4:B:204:PCW:H322	0.63	2.17	7	1
4:D:509:PCW:H422	5:D:520:17F:H32	0.63	1.69	9	1
4:D:509:PCW:O4P	4:D:514:PCW:H82	0.63	1.93	9	1
4:D:517:PCW:H462	5:D:525:17F:C24	0.63	2.18	9	1
4:C:605:PCW:H382	4:C:611:PCW:H12	0.63	1.69	1	1
4:C:618:PCW:O2P	4:C:625:PCW:H52	0.63	1.93	1	1
5:C:627:17F:O10	5:C:627:17F:O7	0.63	2.17	1	1
4:D:502:PCW:C11	4:D:502:PCW:H73	0.63	2.24	1	1
5:A:409:17F:H77	4:C:611:PCW:C47	0.63	2.24	2	1
4:A:415:PCW:C31	4:A:415:PCW:H62	0.63	2.24	3	2
4:C:606:PCW:O4P	4:C:606:PCW:C6	0.63	2.47	3	2
4:A:407:PCW:H272	4:A:407:PCW:H452	0.63	1.71	5	1
4:A:406:PCW:H31	4:A:406:PCW:O4P	0.63	1.94	8	2
4:D:513:PCW:H382	4:D:513:PCW:H422	0.63	1.71	7	1
4:C:620:PCW:H141	5:C:631:17F:C18	0.63	2.23	8	1
4:B:202:PCW:C4	4:B:202:PCW:H322	0.63	2.24	8	2
4:D:512:PCW:C23	4:D:512:PCW:C27	0.63	2.75	9	1
4:C:622:PCW:H441	4:C:623:PCW:H261	0.63	1.71	1	2
4:A:401:PCW:H73	4:D:511:PCW:H2	0.63	1.71	2	1
4:A:405:PCW:C32	4:D:514:PCW:H352	0.63	2.23	4	6
4:B:201:PCW:C42	4:B:201:PCW:C46	0.63	2.73	2	5
4:D:511:PCW:H322	4:D:511:PCW:H63	0.63	1.70	2	1
4:D:507:PCW:O31	4:D:513:PCW:H31	0.63	1.94	3	1
4:D:509:PCW:H132	4:D:514:PCW:H122	0.63	1.70	4	1
4:D:508:PCW:H241	4:D:512:PCW:H431	0.63	1.68	5	1
4:D:502:PCW:H472	4:D:505:PCW:H281	0.63	1.69	7	2
4:D:501:PCW:H451	4:D:515:PCW:H232	0.63	1.69	10	1
4:C:604:PCW:O31	4:C:604:PCW:O3	0.62	2.17	1	2
4:D:508:PCW:C7	5:D:520:17F:O1	0.62	2.47	3	4
4:D:513:PCW:O31	4:D:513:PCW:O3P	0.62	2.17	9	2
4:A:407:PCW:C37	5:D:522:17F:H65	0.62	2.23	2	1
4:C:621:PCW:H222	5:C:629:17F:H19A	0.62	1.71	8	2
4:D:501:PCW:H122	4:D:515:PCW:H381	0.62	1.70	2	1
4:D:511:PCW:H432	4:D:511:PCW:H232	0.62	1.70	2	2
4:D:506:PCW:H73	4:D:517:PCW:H332	0.62	1.71	4	1
5:C:630:17F:C41	4:D:514:PCW:H232	0.62	2.23	5	1
4:D:515:PCW:H61	4:D:516:PCW:H321	0.62	1.70	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:519:17F:H64	5:D:521:17F:H29	0.62	1.70	5	1
4:C:608:PCW:C14	4:C:609:PCW:H171	0.62	2.23	9	1
4:D:504:PCW:H483	5:D:519:17F:H49	0.62	1.71	9	1
4:D:508:PCW:H222	4:D:512:PCW:H422	0.62	1.70	9	1
4:C:610:PCW:H62	5:C:629:17F:O1	0.62	1.94	1	4
4:D:509:PCW:C19	5:D:520:17F:H60	0.62	2.24	1	1
5:D:525:17F:H77	5:D:525:17F:H48	0.62	1.71	1	1
4:C:607:PCW:H431	4:C:624:PCW:C48	0.62	2.22	6	2
4:D:503:PCW:H40	5:D:522:17F:H10	0.62	1.71	2	1
4:C:601:PCW:C39	5:C:626:17F:H52	0.62	2.24	10	2
4:C:613:PCW:H471	4:C:619:PCW:C42	0.62	2.24	7	1
4:D:505:PCW:C37	5:D:519:17F:H11	0.62	2.24	8	1
4:B:201:PCW:H141	4:D:506:PCW:H482	0.62	1.69	9	1
4:A:402:PCW:C44	4:D:512:PCW:H172	0.62	2.23	10	1
4:B:202:PCW:C2	5:D:524:17F:H18A	0.62	2.23	10	1
4:A:413:PCW:O2P	4:A:413:PCW:H52	0.62	1.95	6	4
4:A:414:PCW:C11	5:C:628:17F:H9	0.62	2.24	5	5
4:C:602:PCW:H73	5:D:523:17F:C19	0.62	2.24	5	4
4:C:606:PCW:H132	4:C:606:PCW:H342	0.62	1.72	7	5
4:C:609:PCW:O1P	5:C:631:17F:H18A	0.62	1.93	1	1
4:C:621:PCW:H32	5:C:630:17F:O2	0.62	1.94	1	1
4:C:625:PCW:O1P	4:C:625:PCW:H51	0.62	1.93	9	3
4:D:503:PCW:C39	5:D:522:17F:H42	0.62	2.23	2	1
4:D:513:PCW:C44	4:D:517:PCW:H283	0.62	2.24	3	1
4:D:527:PCW:H121	4:D:528:PCW:H171	0.62	1.70	10	3
4:C:608:PCW:O1P	4:C:624:PCW:C22	0.62	2.47	4	4
4:C:609:PCW:H62	4:C:620:PCW:O11	0.62	1.94	9	5
4:C:617:PCW:H51	4:C:617:PCW:H2	0.62	1.71	7	4
4:B:201:PCW:H242	4:B:203:PCW:C48	0.62	2.23	6	1
4:D:510:PCW:C20	5:D:524:17F:H20	0.62	2.24	7	2
4:D:518:PCW:H352	4:D:518:PCW:H121	0.62	1.70	8	2
4:A:412:PCW:C48	4:C:604:PCW:H271	0.62	2.24	7	1
4:D:503:PCW:C12	4:D:511:PCW:H39	0.62	2.23	5	4
4:D:518:PCW:C43	4:D:518:PCW:C47	0.62	2.74	1	2
4:A:404:PCW:H73	5:D:524:17F:O5	0.62	1.94	3	1
4:C:611:PCW:C28	4:C:619:PCW:H272	0.62	2.25	3	1
3:D:478:THR:HB	4:D:517:PCW:H52	0.62	1.71	3	1
4:C:601:PCW:H371	4:C:602:PCW:H171	0.62	1.70	8	2
4:D:507:PCW:H141	4:D:513:PCW:H342	0.62	1.71	6	1
4:D:504:PCW:H322	4:D:510:PCW:H341	0.62	1.69	8	1
4:D:515:PCW:H2	5:D:525:17F:H57	0.62	1.72	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:A:409:17F:C42	5:D:521:17F:H73	0.62	2.24	10	1
4:C:605:PCW:O31	4:C:605:PCW:O3P	0.62	2.18	1	9
5:D:519:17F:H58	5:D:519:17F:C36	0.62	2.24	1	2
5:D:525:17F:H77	5:D:525:17F:C28	0.62	2.25	1	1
4:C:601:PCW:C46	4:C:601:PCW:C42	0.62	2.75	9	8
5:C:626:17F:C2X	5:C:627:17F:H75	0.62	2.25	3	2
2:B:2:THR:HG22	4:D:510:PCW:H61	0.62	1.70	3	1
4:D:506:PCW:O31	4:D:506:PCW:H11	0.62	1.93	3	6
4:C:622:PCW:H12	4:C:623:PCW:C16	0.62	2.23	4	1
4:D:503:PCW:H372	4:D:511:PCW:H321	0.62	1.71	5	1
4:C:612:PCW:H321	4:C:618:PCW:C13	0.62	2.23	10	4
4:D:508:PCW:C12	4:D:509:PCW:H242	0.62	2.25	6	1
5:A:409:17F:H58	4:D:503:PCW:C24	0.62	2.20	8	1
4:D:510:PCW:H2	5:D:524:17F:O1	0.62	1.95	10	1
4:C:609:PCW:C45	4:D:512:PCW:H20	0.62	2.23	1	1
4:C:625:PCW:C21	4:D:528:PCW:H352	0.62	2.24	1	4
4:D:516:PCW:O3P	4:D:516:PCW:O31	0.62	2.17	5	4
4:D:508:PCW:O1P	4:D:508:PCW:H2	0.62	1.95	5	7
1:A:330:ARG:HH21	1:C:447:GLU:HB3	0.62	1.54	10	4
4:D:502:PCW:H31	4:D:502:PCW:O4P	0.62	1.94	3	4
4:D:511:PCW:H372	4:D:511:PCW:H412	0.62	1.70	4	2
2:B:78:PHE:HB2	2:B:111:MET:HG2	0.62	1.72	7	2
4:C:621:PCW:C20	4:D:528:PCW:H82	0.62	2.25	10	2
4:D:501:PCW:H381	4:D:515:PCW:H421	0.62	1.71	8	1
2:B:79:LEU:HG	2:B:159:LEU:HD22	0.62	1.70	8	9
4:D:502:PCW:O1P	4:D:502:PCW:C3	0.62	2.46	1	6
4:A:405:PCW:H51	4:A:405:PCW:O31	0.62	1.95	7	4
4:C:611:PCW:O2P	4:C:619:PCW:C4	0.62	2.47	2	2
4:C:614:PCW:C45	4:C:619:PCW:H222	0.62	2.25	3	2
5:C:631:17F:H4	5:C:631:17F:O10	0.62	1.94	2	1
4:C:604:PCW:C24	5:D:525:17F:H76	0.62	2.24	3	2
4:C:616:PCW:O2P	4:C:616:PCW:C3	0.62	2.48	9	4
4:C:616:PCW:C48	4:D:504:PCW:H221	0.62	2.25	3	1
4:D:505:PCW:O3	4:D:505:PCW:O31	0.62	2.18	8	2
4:B:203:PCW:H231	4:B:204:PCW:H431	0.62	1.70	9	3
4:A:410:PCW:H39	4:A:410:PCW:C15	0.62	2.16	6	1
5:C:630:17F:H49	5:D:529:17F:H12	0.62	1.71	6	1
4:D:511:PCW:H63	4:D:511:PCW:O11	0.62	1.94	6	1
4:D:509:PCW:H182	4:D:512:PCW:C33	0.62	2.24	7	1
4:C:613:PCW:H261	5:D:521:17F:C39	0.62	2.24	8	2
4:C:616:PCW:H452	4:C:625:PCW:H251	0.62	1.71	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:601:PCW:H39	4:C:602:PCW:H151	0.62	1.70	1	1
4:C:608:PCW:H431	5:C:626:17F:C33	0.62	2.25	1	4
4:D:507:PCW:H40	5:D:525:17F:H6	0.62	1.70	1	1
4:C:604:PCW:C48	4:C:624:PCW:H282	0.62	2.23	2	4
4:D:516:PCW:C47	4:D:516:PCW:C43	0.62	2.73	3	8
4:A:408:PCW:H342	4:D:514:PCW:H40	0.62	1.70	3	1
1:C:463:TRP:CD1	5:C:627:17F:H71	0.62	2.29	3	2
4:D:501:PCW:H11	4:D:515:PCW:H352	0.62	1.72	4	2
5:C:629:17F:H52	4:B:204:PCW:H462	0.62	1.71	6	2
4:D:518:PCW:H52	5:D:519:17F:H5	0.62	1.71	6	1
4:A:411:PCW:H2	4:A:411:PCW:C4	0.62	2.23	7	1
4:D:513:PCW:H421	5:D:522:17F:C42	0.62	2.24	10	1
4:A:401:PCW:C38	4:D:503:PCW:H231	0.62	2.24	6	2
4:C:603:PCW:H261	4:D:526:PCW:H141	0.62	1.71	6	3
4:C:615:PCW:H51	5:C:631:17F:C3	0.62	2.24	8	4
4:A:406:PCW:H2	4:A:406:PCW:O11	0.62	1.94	7	2
4:C:604:PCW:C36	5:D:529:17F:H36	0.62	2.17	3	2
4:A:404:PCW:H371	4:B:202:PCW:H442	0.62	1.70	5	1
4:A:405:PCW:H122	4:D:514:PCW:H331	0.62	1.70	6	3
4:A:406:PCW:H171	4:B:202:PCW:H232	0.62	1.70	6	2
4:A:404:PCW:H62	4:D:510:PCW:O11	0.62	1.95	7	1
4:C:625:PCW:C22	4:D:528:PCW:H352	0.62	2.22	7	1
4:D:518:PCW:H352	5:D:519:17F:H62	0.62	1.70	8	1
4:C:614:PCW:C4	4:C:623:PCW:O1P	0.62	2.48	10	1
4:D:504:PCW:H483	5:D:519:17F:C26	0.62	2.24	10	1
1:A:275:LYS:O	1:A:279:LEU:HG	0.62	1.95	4	10
4:C:604:PCW:O31	4:C:606:PCW:C8	0.62	2.48	1	3
2:B:15:GLY:HA3	6:B:205:GNP:C8	0.62	2.25	9	5
4:D:501:PCW:H61	5:D:525:17F:H2	0.62	1.71	2	1
4:D:501:PCW:H19	4:D:503:PCW:C33	0.62	2.25	2	1
4:A:403:PCW:H63	4:A:403:PCW:O3P	0.62	1.95	3	2
4:D:504:PCW:H483	4:D:516:PCW:H172	0.62	1.70	3	1
5:C:630:17F:H36	5:D:530:17F:C37	0.62	2.21	4	1
4:D:503:PCW:H381	4:D:511:PCW:C35	0.62	2.22	4	1
5:D:529:17F:H5	5:D:529:17F:C19	0.62	2.16	4	2
5:C:626:17F:H74	5:D:523:17F:H53	0.62	1.71	5	1
4:D:509:PCW:C23	5:D:520:17F:H31	0.62	2.25	5	1
4:D:517:PCW:H122	5:D:525:17F:O8	0.62	1.95	5	1
4:C:607:PCW:C1	4:C:624:PCW:H371	0.62	2.24	6	1
5:D:520:17F:H2	5:D:520:17F:O1	0.62	1.95	7	2
4:C:603:PCW:H242	4:D:526:PCW:H372	0.61	1.71	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:516:PCW:C43	4:D:516:PCW:C47	0.61	2.74	1	2
4:D:501:PCW:H61	5:D:525:17F:C3	0.61	2.25	2	1
4:D:508:PCW:H181	4:D:512:PCW:H342	0.61	1.70	9	2
4:A:408:PCW:H20	4:D:514:PCW:H472	0.61	1.71	3	1
4:D:505:PCW:H441	4:D:518:PCW:H272	0.61	1.72	3	1
4:C:622:PCW:H20	5:D:525:17F:H53	0.61	1.72	4	1
4:B:201:PCW:H211	4:B:203:PCW:H282	0.61	1.72	4	1
4:C:605:PCW:H461	4:C:619:PCW:C48	0.61	2.24	5	1
4:B:203:PCW:O2P	4:B:204:PCW:H63	0.61	1.95	10	2
4:D:504:PCW:C17	4:D:510:PCW:H39	0.61	2.25	6	1
4:A:406:PCW:C15	4:B:202:PCW:H232	0.61	2.22	8	2
4:D:503:PCW:H73	4:D:503:PCW:O31	0.61	1.93	8	1
4:D:513:PCW:H141	5:D:523:17F:O7	0.61	1.95	8	1
4:A:402:PCW:H421	4:D:512:PCW:C11	0.61	2.25	9	1
4:C:617:PCW:H41	4:C:617:PCW:H2	0.61	1.72	9	1
5:D:524:17F:H65	5:D:524:17F:H11A	0.61	1.71	9	1
4:C:603:PCW:C26	4:D:526:PCW:H171	0.61	2.25	7	6
4:C:605:PCW:O1P	4:C:605:PCW:H2	0.61	1.95	3	5
4:D:517:PCW:C24	4:D:517:PCW:C20	0.61	2.75	1	7
4:A:406:PCW:H482	4:B:204:PCW:C23	0.61	2.15	9	2
4:D:508:PCW:H222	4:D:512:PCW:C42	0.61	2.25	10	3
4:D:515:PCW:H62	4:D:515:PCW:O1P	0.61	1.95	3	1
4:A:406:PCW:C23	4:B:202:PCW:H231	0.61	2.25	6	1
4:D:509:PCW:H142	5:D:520:17F:C20	0.61	2.22	9	1
4:A:406:PCW:H482	4:B:204:PCW:H251	0.61	1.69	10	1
4:A:414:PCW:C4	4:A:414:PCW:H32	0.61	2.25	10	1
4:C:601:PCW:C48	5:C:626:17F:H51	0.61	2.24	10	1
4:D:509:PCW:H181	4:D:514:PCW:H142	0.61	1.72	10	1
2:B:170:MET:HE2	2:B:170:MET:HA	0.61	1.72	1	2
4:D:501:PCW:H63	4:D:515:PCW:H371	0.61	1.71	1	1
4:D:502:PCW:H41	4:D:502:PCW:O11	0.61	1.94	1	1
4:D:503:PCW:H412	4:D:511:PCW:H212	0.61	1.72	1	1
4:C:604:PCW:O3	4:C:604:PCW:O31	0.61	2.17	10	5
4:C:618:PCW:H361	4:C:625:PCW:C17	0.61	2.25	10	4
4:D:518:PCW:C44	5:D:519:17F:H68	0.61	2.25	4	2
4:C:607:PCW:H361	4:C:624:PCW:C43	0.61	2.26	4	1
4:C:606:PCW:C16	5:D:529:17F:H8	0.61	2.25	5	1
4:D:517:PCW:H283	4:D:517:PCW:C48	0.61	2.25	5	1
4:C:604:PCW:H381	5:D:529:17F:C2X	0.61	2.17	7	1
4:B:201:PCW:H431	4:D:510:PCW:H431	0.61	1.72	8	1
4:D:509:PCW:C3	4:D:509:PCW:O2P	0.61	2.47	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:603:PCW:H82	5:D:530:17F:H1	0.61	1.72	9	1
4:C:602:PCW:O4P	4:C:602:PCW:C6	0.61	2.49	6	10
4:D:506:PCW:H281	4:D:515:PCW:C38	0.61	2.22	1	1
4:D:507:PCW:O31	4:D:507:PCW:O3	0.61	2.17	1	2
4:B:202:PCW:C1	4:D:504:PCW:H131	0.61	2.23	2	1
4:A:403:PCW:C4	4:D:507:PCW:H341	0.61	2.22	3	1
4:C:622:PCW:H381	4:C:623:PCW:C17	0.61	2.25	3	1
4:D:518:PCW:H252	5:D:519:17F:H60	0.61	1.71	3	2
4:B:203:PCW:C28	4:D:506:PCW:H472	0.61	2.25	4	1
4:D:509:PCW:H171	4:D:512:PCW:H331	0.61	1.73	4	2
4:D:515:PCW:O3P	4:D:515:PCW:O31	0.61	2.17	8	3
4:D:508:PCW:C12	4:D:512:PCW:H171	0.61	2.25	6	1
4:C:604:PCW:O1P	4:C:604:PCW:C3	0.61	2.48	7	3
4:D:507:PCW:H182	4:D:513:PCW:C22	0.61	2.21	7	1
4:A:401:PCW:H361	4:D:503:PCW:C20	0.61	2.24	8	1
5:D:529:17F:C7	5:D:529:17F:C18	0.61	2.78	8	1
4:A:401:PCW:H421	4:C:611:PCW:C27	0.61	2.16	9	1
4:D:501:PCW:C16	5:D:521:17F:H20A	0.61	2.25	9	1
4:D:508:PCW:H73	5:D:520:17F:C6	0.61	2.25	9	1
4:A:406:PCW:H232	4:A:406:PCW:H171	0.61	1.71	10	1
4:D:503:PCW:H482	4:D:507:PCW:H483	0.61	1.71	10	1
4:D:511:PCW:H222	4:D:511:PCW:C26	0.61	2.26	5	5
4:A:401:PCW:H472	4:C:611:PCW:H262	0.61	1.70	2	2
2:B:1:MET:SD	4:D:504:PCW:H52	0.61	2.36	2	1
4:C:607:PCW:H412	4:C:624:PCW:H472	0.61	1.72	5	2
4:A:407:PCW:H272	4:A:407:PCW:C48	0.61	2.26	6	2
4:B:201:PCW:H31	4:B:201:PCW:O1P	0.61	1.94	8	1
4:D:504:PCW:O31	4:D:504:PCW:H11	0.61	1.94	8	1
4:D:505:PCW:H483	4:D:505:PCW:H171	0.61	1.70	8	1
4:D:513:PCW:H381	5:D:522:17F:H68	0.61	1.70	8	1
4:A:403:PCW:H232	4:D:513:PCW:H121	0.61	1.72	9	1
4:B:201:PCW:H73	4:D:504:PCW:C5	0.61	2.20	9	1
4:D:516:PCW:H232	5:D:519:17F:H55	0.61	1.73	9	1
4:D:513:PCW:H272	4:D:513:PCW:H471	0.61	1.72	10	1
4:D:505:PCW:O2P	4:D:510:PCW:H62	0.61	1.96	4	1
4:D:504:PCW:H351	4:D:516:PCW:C14	0.61	2.23	6	1
4:D:501:PCW:C38	4:D:515:PCW:H421	0.61	2.24	8	1
4:D:509:PCW:H51	4:D:509:PCW:O2	0.61	1.94	9	1
4:B:202:PCW:C7	5:D:524:17F:O5	0.61	2.48	10	1
4:C:608:PCW:H212	5:C:627:17F:H29	0.61	1.73	3	7
4:D:511:PCW:H372	4:D:511:PCW:C41	0.61	2.25	4	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:602:PCW:H261	5:C:627:17F:H77	0.61	1.72	2	1
4:D:503:PCW:C7	4:D:503:PCW:H2	0.61	2.26	3	1
4:A:406:PCW:H372	4:B:204:PCW:H162	0.61	1.73	4	2
4:A:415:PCW:H452	4:C:622:PCW:H281	0.61	1.71	5	1
4:C:607:PCW:C2	4:C:624:PCW:H371	0.61	2.26	6	1
4:B:203:PCW:O31	4:B:203:PCW:O4P	0.61	2.19	7	2
4:D:509:PCW:H161	5:D:520:17F:H60	0.61	1.73	8	1
3:D:400:ARG:HB3	3:D:412:LEU:HD11	0.61	1.72	10	1
4:A:402:PCW:C5	4:A:402:PCW:H322	0.61	2.25	1	1
4:C:610:PCW:O1P	4:C:610:PCW:H52	0.61	1.96	1	7
4:C:621:PCW:H421	5:C:630:17F:C35	0.61	2.16	2	4
4:D:515:PCW:H161	5:D:520:17F:C24	0.61	2.24	1	1
4:C:620:PCW:C13	5:C:631:17F:H18	0.61	2.26	7	2
4:B:202:PCW:H51	5:D:524:17F:C1	0.61	2.25	9	2
4:B:203:PCW:H372	4:B:204:PCW:C7	0.61	2.25	2	2
4:A:403:PCW:O1P	4:A:403:PCW:C3	0.61	2.49	4	7
4:C:603:PCW:C31	4:C:603:PCW:C4	0.61	2.79	6	3
4:A:414:PCW:H63	5:C:628:17F:O8	0.61	1.95	8	2
4:D:504:PCW:O31	4:D:516:PCW:H82	0.61	1.95	7	2
4:D:515:PCW:C6	4:D:515:PCW:O4P	0.61	2.48	9	2
4:C:603:PCW:H412	4:C:603:PCW:C37	0.61	2.21	1	8
4:D:503:PCW:H2	4:D:503:PCW:H73	0.61	1.71	3	1
4:A:403:PCW:H212	4:D:513:PCW:C37	0.61	2.26	1	1
4:A:406:PCW:O4P	4:A:406:PCW:C6	0.61	2.49	5	4
4:C:613:PCW:O31	4:C:613:PCW:C1	0.61	2.47	2	6
5:C:627:17F:O7	5:C:627:17F:O10	0.61	2.18	3	9
3:D:487:TRP:CZ2	5:D:524:17F:H6A	0.61	2.30	2	1
4:A:412:PCW:H31	4:C:614:PCW:O3	0.61	1.96	3	1
4:D:516:PCW:H222	5:D:519:17F:H49	0.61	1.73	3	1
4:A:406:PCW:H472	4:B:204:PCW:H221	0.61	1.71	4	1
4:A:413:PCW:C39	4:C:617:PCW:H451	0.61	2.26	5	2
4:B:201:PCW:O1P	4:B:201:PCW:H32	0.61	1.96	4	4
4:B:201:PCW:H331	4:D:516:PCW:C8	0.61	2.25	4	1
4:D:507:PCW:C42	5:D:522:17F:H20	0.61	2.26	5	1
4:A:407:PCW:H412	4:A:412:PCW:H251	0.61	1.72	8	3
4:C:601:PCW:H462	4:C:601:PCW:C15	0.61	2.25	6	1
4:B:201:PCW:C5	4:B:202:PCW:H31	0.61	2.18	6	1
4:A:407:PCW:H181	4:A:407:PCW:H222	0.61	1.73	8	1
4:D:513:PCW:C45	5:D:522:17F:H78	0.61	2.26	9	1
4:C:618:PCW:H322	4:C:625:PCW:H152	0.61	1.73	10	1
4:B:201:PCW:C46	4:B:201:PCW:C42	0.60	2.75	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:513:PCW:O11	4:D:513:PCW:H2	0.60	1.96	7	10
5:A:409:17F:C31	4:D:503:PCW:H211	0.60	2.21	2	2
4:B:202:PCW:H322	4:B:202:PCW:C4	0.60	2.24	2	1
4:A:405:PCW:O2	4:A:405:PCW:H342	0.60	1.96	9	2
5:A:409:17F:O5	4:D:503:PCW:H82	0.60	1.96	4	2
4:B:201:PCW:H211	4:B:203:PCW:C28	0.60	2.25	4	1
4:C:617:PCW:H282	4:D:502:PCW:H221	0.60	1.71	5	1
4:B:201:PCW:H431	4:D:510:PCW:H441	0.60	1.71	5	1
4:D:503:PCW:O11	4:D:503:PCW:H2	0.60	1.97	9	1
4:A:411:PCW:H371	4:C:612:PCW:H151	0.60	1.71	10	1
4:C:618:PCW:H241	4:B:201:PCW:H442	0.60	1.73	10	1
4:B:202:PCW:H73	5:D:524:17F:O4	0.60	1.96	1	1
4:C:611:PCW:H39	4:C:622:PCW:C46	0.60	2.17	7	5
4:D:515:PCW:P	4:D:515:PCW:C6	0.60	2.82	3	1
4:D:506:PCW:H282	4:D:515:PCW:H471	0.60	1.72	10	2
4:A:407:PCW:H122	4:D:511:PCW:H283	0.60	1.71	6	1
4:B:203:PCW:C19	4:D:506:PCW:H471	0.60	2.26	8	3
4:D:502:PCW:H332	4:D:510:PCW:C1	0.60	2.25	8	2
4:D:504:PCW:H232	4:D:510:PCW:H422	0.60	1.73	8	1
4:D:509:PCW:C2	5:D:520:17F:H4	0.60	2.25	8	1
4:D:517:PCW:C46	5:D:525:17F:H41	0.60	2.19	9	1
4:D:518:PCW:H321	5:D:519:17F:C20	0.60	2.04	9	1
4:B:201:PCW:C23	4:B:203:PCW:H282	0.60	2.26	10	1
4:A:415:PCW:H281	4:C:622:PCW:H251	0.60	1.71	1	1
1:A:246:ASP:HA	1:C:528:ARG:NH1	0.60	2.11	3	8
4:D:518:PCW:C47	4:D:518:PCW:C43	0.60	2.75	7	8
4:D:503:PCW:H31	4:D:511:PCW:H322	0.60	1.73	3	1
4:C:612:PCW:H321	4:C:618:PCW:C15	0.60	2.26	4	2
4:C:613:PCW:O31	4:C:613:PCW:H31	0.60	1.96	8	4
4:D:510:PCW:H131	5:D:524:17F:H75	0.60	1.73	4	1
4:D:506:PCW:C35	4:D:509:PCW:H382	0.60	2.26	5	1
4:D:510:PCW:C35	5:D:524:17F:H10A	0.60	2.19	6	1
4:B:201:PCW:H231	4:B:203:PCW:H20	0.60	1.72	7	2
4:A:404:PCW:C24	4:A:411:PCW:H262	0.60	2.24	8	1
4:C:607:PCW:C48	4:D:513:PCW:H483	0.60	2.26	10	2
4:D:509:PCW:O11	4:D:509:PCW:C8	0.60	2.49	9	1
5:D:524:17F:O2	5:D:524:17F:H5	0.60	1.96	10	2
4:C:605:PCW:H412	4:C:619:PCW:H121	0.60	1.74	10	1
4:C:606:PCW:H42	4:C:624:PCW:C19	0.60	2.24	10	1
4:A:406:PCW:C24	4:B:203:PCW:H242	0.60	2.24	1	1
4:D:501:PCW:H212	5:D:521:17F:C34	0.60	2.26	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:604:PCW:H251	5:D:525:17F:H75	0.60	1.72	4	2
4:C:615:PCW:H211	5:C:631:17F:C22	0.60	2.25	3	2
2:B:146:ALA:HB3	6:B:205:GNP:N7	0.60	2.11	3	3
4:D:507:PCW:H11	5:D:523:17F:C7	0.60	2.26	4	3
4:D:510:PCW:H412	5:D:524:17F:H10A	0.60	1.72	4	1
1:C:591:TYR:HB3	5:C:628:17F:H48	0.60	1.72	9	3
5:D:522:17F:C42	5:D:522:17F:C38	0.60	2.73	6	1
1:A:316:LEU:HD11	4:C:602:PCW:H283	0.60	1.71	7	1
4:C:603:PCW:C6	4:D:527:PCW:P	0.60	2.89	1	1
4:C:613:PCW:H282	5:D:521:17F:H11	0.60	1.74	1	1
3:D:436:LEU:HD21	4:D:502:PCW:H52	0.60	1.72	1	1
4:D:509:PCW:H231	4:D:509:PCW:C27	0.60	2.27	1	1
5:D:520:17F:H20	5:D:520:17F:O10	0.60	1.95	9	5
5:D:524:17F:C7	5:D:524:17F:C17	0.60	2.79	7	2
4:C:606:PCW:O11	4:C:606:PCW:C5	0.60	2.49	3	4
4:D:513:PCW:H73	5:D:523:17F:C4	0.60	2.25	3	1
4:A:401:PCW:H252	4:C:614:PCW:H281	0.60	1.74	4	1
4:C:617:PCW:H51	4:C:617:PCW:C2	0.60	2.27	7	4
4:C:622:PCW:H371	4:C:622:PCW:C11	0.60	2.27	4	1
5:C:627:17F:C17	5:C:627:17F:O7	0.60	2.49	4	6
4:D:505:PCW:H39	5:D:519:17F:H10A	0.60	1.73	6	1
4:D:517:PCW:C20	4:D:517:PCW:C24	0.60	2.79	7	2
4:C:605:PCW:C17	4:C:613:PCW:H131	0.60	2.26	8	1
4:B:201:PCW:H171	4:D:516:PCW:H422	0.60	1.72	10	1
4:B:203:PCW:H262	4:D:504:PCW:H232	0.60	1.72	10	1
4:C:614:PCW:C6	4:C:614:PCW:O4P	0.60	2.49	1	1
4:A:401:PCW:H2	4:A:401:PCW:O2P	0.60	1.95	4	3
4:D:518:PCW:H321	5:D:519:17F:C19	0.60	2.26	2	1
4:C:603:PCW:H442	4:D:526:PCW:H351	0.60	1.72	3	4
4:C:620:PCW:H132	5:C:631:17F:C18	0.60	2.26	9	4
4:D:504:PCW:H31	5:D:524:17F:H6	0.60	1.74	3	1
4:C:618:PCW:H151	4:C:625:PCW:C15	0.60	2.26	4	1
4:A:413:PCW:H412	4:D:526:PCW:H231	0.60	1.73	5	1
4:D:517:PCW:H142	5:D:525:17F:C9	0.60	2.27	5	1
4:C:616:PCW:H19	4:C:617:PCW:C46	0.60	2.24	6	1
4:A:415:PCW:O4P	4:A:415:PCW:C6	0.60	2.49	8	2
4:B:202:PCW:H271	4:B:203:PCW:H231	0.60	1.72	8	1
4:D:510:PCW:H471	5:D:524:17F:C33	0.60	2.17	8	2
4:D:510:PCW:C47	5:D:524:17F:H60	0.60	2.16	8	1
4:A:411:PCW:H61	4:C:617:PCW:H40	0.60	1.73	10	1
4:C:602:PCW:H62	4:C:602:PCW:O4P	0.60	1.96	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:503:PCW:H411	4:D:511:PCW:C22	0.60	2.26	10	1
4:D:503:PCW:C11	4:D:503:PCW:O31	0.60	2.50	2	8
4:D:505:PCW:H341	4:D:505:PCW:O31	0.60	1.96	1	1
4:A:401:PCW:C44	4:C:614:PCW:H262	0.60	2.26	7	3
4:A:406:PCW:H31	4:A:406:PCW:C4	0.60	2.26	5	2
5:C:630:17F:O7	5:D:529:17F:H65	0.60	1.97	2	1
4:D:513:PCW:P	4:D:513:PCW:C3	0.60	2.89	8	7
4:C:616:PCW:H452	4:B:201:PCW:H462	0.60	1.72	3	1
4:C:622:PCW:H381	4:C:623:PCW:H171	0.60	1.71	3	1
4:D:507:PCW:O11	4:D:513:PCW:H152	0.60	1.95	4	2
4:D:508:PCW:C7	5:D:520:17F:O8	0.60	2.50	6	1
2:B:9:VAL:HG21	2:B:100:ILE:HD11	0.60	1.72	8	2
4:D:514:PCW:H251	4:D:514:PCW:C21	0.60	2.20	9	1
4:D:515:PCW:H222	5:D:525:17F:H73	0.60	1.73	9	1
4:A:401:PCW:H12	4:D:511:PCW:H162	0.60	1.74	1	1
4:A:405:PCW:H171	4:A:405:PCW:C22	0.60	2.26	1	2
4:C:625:PCW:H20	4:D:528:PCW:C32	0.60	2.26	1	1
4:C:602:PCW:H483	5:C:627:17F:C27	0.60	2.17	3	2
4:C:604:PCW:H211	4:C:604:PCW:H162	0.60	1.73	5	1
4:C:619:PCW:H481	5:D:521:17F:C41	0.60	2.26	5	1
4:D:506:PCW:C21	4:D:506:PCW:C25	0.60	2.77	6	2
4:A:414:PCW:H442	4:C:617:PCW:H211	0.60	1.73	6	1
4:C:616:PCW:H441	4:C:625:PCW:C23	0.60	2.27	6	1
4:D:510:PCW:C16	5:D:524:17F:H19A	0.60	2.23	6	1
4:D:512:PCW:H62	5:D:520:17F:H1A	0.60	1.70	6	1
4:D:516:PCW:O31	4:D:516:PCW:O3P	0.60	2.19	7	2
4:A:411:PCW:H42	4:A:411:PCW:C2	0.60	2.25	7	1
4:C:614:PCW:H442	4:C:619:PCW:C19	0.60	2.26	7	4
4:D:506:PCW:H281	4:D:515:PCW:H451	0.60	1.73	7	1
4:C:604:PCW:H372	4:C:604:PCW:C42	0.60	2.24	6	6
4:C:608:PCW:H261	5:C:627:17F:C33	0.60	2.27	1	1
5:C:631:17F:C30	4:D:512:PCW:H161	0.60	2.26	1	3
4:C:608:PCW:H19	5:C:627:17F:H50	0.60	1.72	6	2
4:C:620:PCW:H412	4:C:620:PCW:C37	0.60	2.26	2	6
4:A:406:PCW:C35	4:B:204:PCW:C15	0.60	2.79	3	2
4:A:408:PCW:H20	4:D:514:PCW:C47	0.60	2.26	3	1
1:A:361:SER:HB3	1:A:365:LYS:HE3	0.60	1.74	9	2
4:A:403:PCW:H152	4:A:403:PCW:H431	0.60	1.73	6	1
4:C:613:PCW:H482	4:C:619:PCW:H231	0.60	1.72	7	1
4:D:507:PCW:H152	4:D:513:PCW:H382	0.60	1.72	9	1
4:C:607:PCW:H362	4:C:624:PCW:C42	0.60	2.27	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:37:GLU:HB2	3:D:369:VAL:CB	0.60	2.27	10	1
4:A:414:PCW:H351	4:C:617:PCW:H151	0.60	1.74	5	4
4:C:608:PCW:O11	4:C:608:PCW:H2	0.60	1.97	10	10
4:D:506:PCW:H2	4:D:506:PCW:O11	0.60	1.96	9	7
4:C:604:PCW:H372	4:C:604:PCW:C41	0.60	2.26	8	2
4:C:613:PCW:C3	4:C:619:PCW:H2	0.60	2.25	10	3
4:C:616:PCW:H39	4:C:618:PCW:C15	0.60	2.25	6	3
5:C:630:17F:H65	5:C:631:17F:C39	0.60	2.26	6	5
4:C:608:PCW:H452	5:C:626:17F:C34	0.60	2.26	5	1
5:A:409:17F:H65	4:D:503:PCW:H272	0.60	1.73	6	1
4:C:604:PCW:H82	5:D:530:17F:O1	0.60	1.97	7	1
4:C:608:PCW:C45	5:C:626:17F:H60	0.60	2.27	8	1
4:A:410:PCW:H472	4:C:617:PCW:H252	0.59	1.74	7	5
5:D:529:17F:H46	5:D:530:17F:C40	0.59	2.12	1	3
4:A:405:PCW:C17	4:A:405:PCW:C21	0.59	2.63	3	5
4:B:201:PCW:C21	4:D:506:PCW:H442	0.59	2.27	3	1
4:A:413:PCW:H40	4:C:616:PCW:H232	0.59	1.72	4	1
4:C:609:PCW:H2	4:C:615:PCW:C6	0.59	2.27	6	3
4:B:201:PCW:H282	4:B:204:PCW:H482	0.59	1.72	7	1
4:D:503:PCW:H172	4:D:503:PCW:C21	0.59	2.27	8	1
4:D:517:PCW:C28	5:D:522:17F:H77	0.59	2.27	8	1
5:A:409:17F:O9	5:A:409:17F:H20	0.59	1.96	9	5
4:D:518:PCW:H181	4:D:518:PCW:C22	0.59	2.26	8	4
4:C:617:PCW:O11	4:C:617:PCW:H2	0.59	1.96	5	4
4:C:621:PCW:C19	5:C:629:17F:O10	0.59	2.50	9	4
4:D:505:PCW:C44	4:D:518:PCW:H261	0.59	2.25	10	2
4:A:406:PCW:H351	4:B:204:PCW:H162	0.59	1.74	7	1
4:D:516:PCW:H421	4:D:527:PCW:H271	0.59	1.74	7	1
4:A:408:PCW:H381	4:B:203:PCW:H361	0.59	1.74	8	1
4:C:611:PCW:H321	4:C:622:PCW:C36	0.59	2.27	9	1
4:D:507:PCW:H31	4:D:507:PCW:O31	0.59	1.97	9	1
4:C:613:PCW:H481	4:C:619:PCW:H211	0.59	1.72	1	1
5:C:627:17F:O7	5:C:627:17F:C17	0.59	2.50	3	4
4:C:605:PCW:O31	4:C:613:PCW:H52	0.59	1.96	2	1
4:D:506:PCW:H11	4:D:515:PCW:H73	0.59	1.75	2	1
4:A:411:PCW:H361	4:C:612:PCW:C13	0.59	2.27	5	1
4:B:201:PCW:H2	4:D:516:PCW:H372	0.59	1.74	6	1
4:D:505:PCW:H381	5:D:519:17F:H9A	0.59	1.74	6	1
4:A:402:PCW:O2P	4:D:514:PCW:H73	0.59	1.97	8	1
4:A:413:PCW:C31	4:A:413:PCW:O3	0.59	2.50	5	10
4:A:415:PCW:O4P	4:A:415:PCW:H62	0.59	1.97	7	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:504:PCW:H262	4:D:510:PCW:H452	0.59	1.75	2	1
4:D:508:PCW:H172	4:D:512:PCW:H151	0.59	1.75	10	3
4:D:510:PCW:H122	5:D:524:17F:O7	0.59	1.97	2	1
4:A:406:PCW:H352	4:B:204:PCW:H162	0.59	1.73	3	3
4:A:410:PCW:H61	5:C:628:17F:O5	0.59	1.97	5	2
2:B:36:ILE:HA	2:B:59:ALA:HB2	0.59	1.73	5	3
4:A:413:PCW:H39	4:C:617:PCW:H451	0.59	1.73	5	2
4:C:604:PCW:H271	5:D:520:17F:H53	0.59	1.75	5	1
4:C:611:PCW:H41	4:C:622:PCW:H342	0.59	1.72	7	4
4:A:406:PCW:H271	4:C:618:PCW:H462	0.59	1.74	10	2
4:D:505:PCW:C47	5:D:519:17F:H53	0.59	2.28	9	1
4:D:510:PCW:H451	5:D:524:17F:C33	0.59	2.27	9	1
4:C:615:PCW:H63	5:C:631:17F:C3	0.59	2.26	10	1
4:D:517:PCW:H462	5:D:525:17F:H44	0.59	1.73	10	1
4:A:410:PCW:H61	5:C:628:17F:C3	0.59	2.27	1	1
4:C:606:PCW:C18	4:C:606:PCW:C14	0.59	2.76	5	6
4:B:203:PCW:H211	4:B:204:PCW:C40	0.59	2.26	2	1
4:D:516:PCW:O11	4:D:516:PCW:C2	0.59	2.49	3	2
4:A:403:PCW:O2P	4:A:403:PCW:H51	0.59	1.98	6	3
4:A:407:PCW:O3	4:A:407:PCW:O31	0.59	2.18	3	1
5:C:630:17F:H65	5:C:631:17F:H70	0.59	1.73	8	4
4:B:201:PCW:C40	4:D:527:PCW:H251	0.59	2.27	4	2
4:D:503:PCW:H432	5:D:522:17F:O10	0.59	1.98	5	1
4:C:616:PCW:C19	4:C:617:PCW:H461	0.59	2.24	6	1
4:D:518:PCW:H322	5:D:519:17F:H19A	0.59	1.74	7	1
4:D:506:PCW:O1P	4:D:515:PCW:H41	0.59	1.98	9	1
4:C:623:PCW:C15	4:C:623:PCW:C19	0.59	2.81	6	7
5:C:630:17F:H40	5:C:630:17F:H30	0.59	1.75	4	5
4:D:501:PCW:H472	5:D:525:17F:C24	0.59	2.26	2	1
4:A:410:PCW:O31	4:A:410:PCW:P	0.59	2.60	7	4
5:D:519:17F:O1	5:D:519:17F:C2	0.59	2.50	6	4
4:C:606:PCW:H442	4:C:609:PCW:O2	0.59	1.97	10	3
4:C:613:PCW:H20	5:D:521:17F:H48	0.59	1.72	8	2
4:D:505:PCW:C35	4:D:505:PCW:O31	0.59	2.50	5	1
4:D:510:PCW:H351	5:D:524:17F:C10	0.59	2.20	6	1
4:C:619:PCW:H481	5:D:521:17F:H76	0.59	1.73	8	1
4:C:601:PCW:C38	5:C:626:17F:H52	0.59	2.27	10	1
4:D:509:PCW:H171	4:D:514:PCW:H131	0.59	1.73	10	1
1:A:321:ALA:HB3	1:A:322:PRO:HD3	0.59	1.74	9	2
4:A:410:PCW:H481	4:D:505:PCW:H19	0.59	1.74	8	3
4:C:601:PCW:H341	4:C:601:PCW:O31	0.59	1.97	9	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:506:PCW:C20	4:D:516:PCW:H342	0.59	2.27	8	3
4:A:405:PCW:C5	4:D:514:PCW:H321	0.59	2.28	8	4
4:D:506:PCW:H371	4:D:509:PCW:C33	0.59	2.26	2	1
4:D:511:PCW:H141	5:D:522:17F:O10	0.59	1.97	3	1
4:D:516:PCW:H242	4:D:526:PCW:C46	0.59	2.28	3	1
4:D:511:PCW:H332	4:D:511:PCW:H132	0.59	1.75	8	2
4:C:605:PCW:O31	4:C:613:PCW:C5	0.59	2.49	1	3
5:D:522:17F:O6	5:D:522:17F:H18A	0.59	1.98	1	2
5:C:626:17F:H36	5:C:627:17F:H74	0.59	1.74	2	2
4:D:528:PCW:H362	5:D:529:17F:H76	0.59	1.73	10	2
4:C:610:PCW:H62	5:C:629:17F:P1	0.59	2.37	3	1
4:C:605:PCW:H171	4:C:613:PCW:C34	0.59	2.27	5	3
4:C:614:PCW:O1P	4:C:614:PCW:H51	0.59	1.97	6	2
4:C:617:PCW:H2	4:C:617:PCW:O11	0.59	1.98	10	2
4:D:515:PCW:H152	5:D:525:17F:C34	0.59	2.26	7	1
4:D:504:PCW:C34	4:D:510:PCW:H341	0.59	2.28	10	2
4:C:615:PCW:C48	4:D:509:PCW:H252	0.59	2.27	10	1
4:D:517:PCW:C37	5:D:525:17F:H59	0.59	2.20	10	1
4:A:412:PCW:H431	4:C:623:PCW:H461	0.59	1.72	1	3
5:C:631:17F:H55	4:D:508:PCW:H39	0.59	1.74	3	2
4:A:415:PCW:H242	4:D:528:PCW:C23	0.59	2.27	2	2
4:C:602:PCW:C7	5:D:523:17F:H4A	0.59	2.27	2	2
4:A:405:PCW:C24	4:D:508:PCW:H271	0.59	2.27	10	2
4:A:411:PCW:O3P	4:A:411:PCW:O31	0.59	2.20	3	6
4:C:608:PCW:H181	5:C:627:17F:C11	0.59	2.17	8	3
4:C:618:PCW:H251	4:D:510:PCW:C46	0.59	2.26	3	1
4:D:509:PCW:H371	5:D:520:17F:H66	0.59	1.75	3	1
4:D:515:PCW:H342	4:D:516:PCW:C1	0.59	2.27	7	2
4:D:507:PCW:H452	5:D:525:17F:C6	0.59	2.28	6	1
4:D:508:PCW:H152	4:D:509:PCW:H221	0.59	1.75	6	1
4:D:508:PCW:N	5:D:520:17F:O8	0.59	2.36	6	1
4:D:515:PCW:H32	4:D:517:PCW:C1	0.59	2.27	6	1
4:B:203:PCW:H422	4:B:203:PCW:C14	0.59	2.25	7	1
4:D:511:PCW:H221	4:D:511:PCW:C36	0.59	2.27	7	1
4:C:610:PCW:H322	5:C:629:17F:H8A	0.59	1.75	1	1
4:D:502:PCW:H31	4:D:502:PCW:O1P	0.59	1.98	1	5
4:D:508:PCW:O1P	5:D:520:17F:N1	0.59	2.36	1	1
4:A:408:PCW:H412	4:B:203:PCW:H412	0.59	1.74	6	2
4:C:605:PCW:H2	4:C:613:PCW:H62	0.59	1.73	5	2
4:C:607:PCW:H432	4:C:624:PCW:C48	0.59	2.27	7	1
4:A:403:PCW:H212	4:D:513:PCW:C31	0.59	2.27	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:406:PCW:H152	4:B:202:PCW:H211	0.59	1.74	9	1
4:D:505:PCW:H451	5:D:519:17F:C30	0.59	2.28	9	1
4:D:518:PCW:H471	5:D:521:17F:C1X	0.59	2.27	9	1
4:C:620:PCW:O1P	4:C:621:PCW:H42	0.59	1.98	10	1
4:A:410:PCW:H472	4:C:617:PCW:C25	0.58	2.28	2	2
4:C:605:PCW:H39	4:C:611:PCW:C34	0.58	2.28	3	5
4:C:616:PCW:H452	4:B:201:PCW:H471	0.58	1.74	3	1
4:D:511:PCW:H61	5:D:522:17F:O7	0.58	1.97	3	2
4:A:413:PCW:O2P	4:A:413:PCW:C3	0.58	2.51	5	1
4:A:408:PCW:C44	4:D:506:PCW:H451	0.58	2.25	6	1
4:D:504:PCW:H172	4:D:510:PCW:H39	0.58	1.75	6	1
4:D:511:PCW:O1P	4:D:511:PCW:H31	0.58	1.98	6	1
4:D:527:PCW:C17	4:D:528:PCW:H162	0.58	2.27	6	1
4:A:401:PCW:C38	4:D:503:PCW:H20	0.58	2.20	7	1
4:B:201:PCW:H241	4:B:203:PCW:H282	0.58	1.72	7	2
4:B:201:PCW:O1P	4:B:201:PCW:C3	0.58	2.51	8	1
4:A:403:PCW:C23	4:D:513:PCW:H121	0.58	2.28	9	1
4:A:404:PCW:H281	4:A:411:PCW:H241	0.58	1.75	1	1
4:D:508:PCW:H172	4:D:512:PCW:H342	0.58	1.74	1	2
4:C:605:PCW:H462	5:D:521:17F:C30	0.58	2.28	10	2
3:D:402:LEU:HD22	4:D:502:PCW:H122	0.58	1.74	2	1
4:D:515:PCW:H181	4:D:515:PCW:C23	0.58	2.28	3	1
4:D:515:PCW:H152	5:D:525:17F:C35	0.58	2.28	4	1
4:A:411:PCW:H381	4:C:612:PCW:H151	0.58	1.75	5	1
4:C:605:PCW:O3P	4:C:605:PCW:O31	0.58	2.21	5	1
4:C:614:PCW:H171	4:C:622:PCW:H481	0.58	1.75	5	1
4:D:503:PCW:H462	4:D:507:PCW:H462	0.58	1.73	5	1
4:A:414:PCW:P	4:C:617:PCW:H82	0.58	2.38	6	1
4:D:509:PCW:H422	5:D:520:17F:O7	0.58	1.98	6	1
4:C:604:PCW:O1P	4:C:604:PCW:H31	0.58	1.98	7	1
4:C:606:PCW:C16	5:D:529:17F:H30	0.58	2.27	7	2
4:A:406:PCW:H162	4:B:204:PCW:H372	0.58	1.74	8	1
4:A:407:PCW:H371	5:D:522:17F:H66	0.58	1.74	8	1
4:A:414:PCW:O3P	4:C:617:PCW:H42	0.58	1.98	8	1
4:A:403:PCW:O31	4:A:407:PCW:H82	0.58	1.97	10	1
4:A:403:PCW:O4P	4:A:403:PCW:C6	0.58	2.51	9	10
4:A:411:PCW:O2	4:A:411:PCW:H342	0.58	1.98	2	3
4:A:415:PCW:H211	4:C:603:PCW:C16	0.58	2.29	2	1
4:B:201:PCW:H342	4:D:510:PCW:C38	0.58	2.28	2	4
4:D:508:PCW:H19	4:D:509:PCW:H181	0.58	1.75	2	1
4:D:503:PCW:C3	4:D:511:PCW:H322	0.58	2.28	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:506:PCW:H371	4:D:509:PCW:H362	0.58	1.74	5	2
4:C:605:PCW:C47	4:C:613:PCW:H162	0.58	2.29	6	2
5:C:626:17F:C37	5:C:627:17F:H52	0.58	2.28	5	1
4:A:406:PCW:H182	4:A:406:PCW:H232	0.58	1.72	6	1
4:D:509:PCW:H62	4:D:514:PCW:H32	0.58	1.73	9	2
4:C:602:PCW:H483	5:C:626:17F:H69	0.58	1.73	8	1
5:D:525:17F:H44	5:D:525:17F:C40	0.58	2.26	9	2
5:D:529:17F:H18	5:D:529:17F:H9A	0.58	1.75	8	1
4:A:415:PCW:H62	4:A:415:PCW:O31	0.58	1.97	9	1
4:C:601:PCW:H482	5:C:626:17F:C29	0.58	2.27	10	1
2:B:37:GLU:HB2	3:D:369:VAL:CG2	0.58	2.28	10	1
4:A:414:PCW:O31	4:A:414:PCW:O3P	0.58	2.20	5	7
4:C:616:PCW:C48	4:B:203:PCW:H281	0.58	2.29	1	1
4:C:621:PCW:C14	4:C:621:PCW:H181	0.58	2.28	7	3
4:D:504:PCW:H441	4:D:516:PCW:H171	0.58	1.75	1	1
4:C:623:PCW:C1	4:C:624:PCW:H32	0.58	2.23	2	1
2:B:38:ASP:HB3	2:B:57:ASP:HB3	0.58	1.75	3	4
4:B:203:PCW:H222	4:D:506:PCW:H471	0.58	1.74	2	2
4:D:517:PCW:H12	4:D:517:PCW:H41	0.58	1.74	2	1
4:A:403:PCW:O1P	4:A:403:PCW:H32	0.58	1.98	3	1
4:A:406:PCW:C6	4:A:406:PCW:O4P	0.58	2.51	3	6
4:A:411:PCW:H62	4:A:411:PCW:O4P	0.58	1.98	3	1
4:C:605:PCW:C47	4:C:619:PCW:H441	0.58	2.28	3	1
4:D:505:PCW:H272	5:D:524:17F:H78	0.58	1.75	4	1
4:A:411:PCW:C41	4:A:411:PCW:C37	0.58	2.79	8	2
4:C:602:PCW:H221	4:C:602:PCW:C17	0.58	2.28	6	1
5:C:626:17F:H5	5:C:626:17F:O8	0.58	1.96	6	1
4:D:505:PCW:O2P	4:D:510:PCW:C5	0.58	2.51	6	1
4:A:401:PCW:H62	4:D:511:PCW:C31	0.58	2.28	7	1
3:D:456:GLN:OE1	4:D:509:PCW:H73	0.58	1.98	7	1
4:D:528:PCW:H19	5:D:530:17F:C19	0.58	2.29	7	1
4:A:406:PCW:H42	4:A:406:PCW:O11	0.58	1.97	8	1
4:C:623:PCW:H412	4:C:624:PCW:C40	0.58	2.28	10	2
5:C:631:17F:C37	5:C:631:17F:C32	0.58	2.81	9	1
4:D:506:PCW:C26	4:D:516:PCW:H161	0.58	2.27	9	1
4:D:507:PCW:O31	4:D:507:PCW:H12	0.58	1.98	9	1
4:C:625:PCW:H242	4:D:528:PCW:H372	0.58	1.74	10	1
4:C:607:PCW:C11	4:C:607:PCW:O31	0.58	2.51	7	10
4:C:625:PCW:H421	4:C:625:PCW:C38	0.58	2.27	6	4
4:D:513:PCW:H152	5:D:523:17F:H18	0.58	1.75	1	1
5:D:525:17F:H20A	5:D:525:17F:O10	0.58	1.98	5	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:401:PCW:H472	4:C:611:PCW:C27	0.58	2.29	2	2
4:D:501:PCW:H122	4:D:515:PCW:H39	0.58	1.73	2	1
4:A:404:PCW:H242	4:A:411:PCW:H241	0.58	1.76	3	2
4:D:517:PCW:H483	5:D:525:17F:H40	0.58	1.74	3	1
4:D:514:PCW:O11	4:D:514:PCW:C2	0.58	2.50	9	5
4:C:617:PCW:H2	4:C:617:PCW:H62	0.58	1.75	5	1
4:D:505:PCW:H361	5:D:519:17F:H9A	0.58	1.74	5	1
4:D:508:PCW:C15	4:D:509:PCW:H222	0.58	2.28	6	1
4:A:402:PCW:H412	4:D:512:PCW:H381	0.58	1.75	7	1
4:C:603:PCW:H142	4:D:528:PCW:C22	0.58	2.28	7	1
4:D:503:PCW:H31	4:D:511:PCW:H352	0.58	1.74	7	2
4:A:403:PCW:H212	4:D:513:PCW:H372	0.58	1.74	1	1
4:A:408:PCW:H483	4:B:201:PCW:C27	0.58	2.28	1	1
4:C:604:PCW:O3	4:C:604:PCW:C31	0.58	2.51	10	4
4:D:506:PCW:C15	4:D:516:PCW:H411	0.58	2.29	1	1
5:D:524:17F:O7	5:D:524:17F:C17	0.58	2.52	3	6
4:B:201:PCW:H62	4:D:504:PCW:H42	0.58	1.74	2	1
4:D:506:PCW:H20	4:D:516:PCW:C36	0.58	2.25	2	1
4:D:518:PCW:H172	5:D:519:17F:C20	0.58	2.29	3	1
4:A:410:PCW:H271	4:D:502:PCW:H483	0.58	1.74	4	1
4:A:415:PCW:C47	5:D:521:17F:H55	0.58	2.28	7	2
4:D:513:PCW:C47	4:D:513:PCW:H281	0.58	2.28	5	1
4:D:511:PCW:H162	5:D:522:17F:C17	0.58	2.28	6	1
4:D:516:PCW:C26	4:D:526:PCW:H483	0.58	2.28	6	3
4:D:516:PCW:H262	4:D:526:PCW:H483	0.58	1.73	8	3
4:D:504:PCW:H331	4:D:516:PCW:C14	0.58	2.21	7	1
4:A:407:PCW:H171	4:D:511:PCW:H281	0.58	1.75	8	1
4:C:613:PCW:H283	5:D:521:17F:H66	0.58	1.74	9	2
4:D:503:PCW:C27	4:D:503:PCW:C23	0.58	2.73	8	1
4:D:509:PCW:H171	4:D:514:PCW:C13	0.58	2.28	10	1
4:A:414:PCW:H362	4:C:617:PCW:H141	0.58	1.75	1	1
4:C:607:PCW:H432	4:C:624:PCW:H472	0.58	1.73	7	2
4:D:510:PCW:O11	5:D:524:17F:H75	0.58	1.99	1	1
4:D:528:PCW:H121	5:D:530:17F:H33	0.58	1.75	1	3
4:C:604:PCW:C23	5:D:525:17F:H76	0.58	2.28	2	3
4:A:410:PCW:H442	4:C:617:PCW:H242	0.58	1.74	5	2
4:A:415:PCW:C31	4:A:415:PCW:C6	0.58	2.82	3	1
4:D:506:PCW:H40	4:D:528:PCW:C48	0.58	2.28	3	1
4:D:511:PCW:C3	4:D:511:PCW:O1P	0.58	2.51	3	2
4:D:518:PCW:H121	5:D:519:17F:C39	0.58	2.28	3	1
4:A:415:PCW:H283	4:D:515:PCW:H20	0.58	1.76	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:612:PCW:H332	4:C:625:PCW:C13	0.58	2.28	7	5
4:C:617:PCW:O31	4:C:617:PCW:H62	0.58	1.99	7	3
4:C:608:PCW:H452	5:C:626:17F:H61	0.58	1.74	5	1
5:C:630:17F:H39	5:D:530:17F:C39	0.58	2.29	6	1
4:A:415:PCW:H62	4:A:415:PCW:C31	0.58	2.29	10	1
4:C:606:PCW:H352	5:D:529:17F:O8	0.58	1.97	10	1
4:D:501:PCW:H431	4:D:515:PCW:C22	0.58	2.28	10	1
5:D:524:17F:H11	5:D:524:17F:C36	0.58	2.22	10	1
4:C:606:PCW:H2	4:C:606:PCW:H41	0.58	1.74	1	3
3:D:434:VAL:CG1	4:D:518:PCW:H63	0.58	2.29	1	1
4:D:507:PCW:C40	5:D:525:17F:H6	0.58	2.29	1	1
4:C:610:PCW:C4	5:C:629:17F:O8	0.58	2.52	9	5
4:D:503:PCW:H40	5:D:522:17F:C10	0.58	2.29	10	3
4:C:620:PCW:C15	5:C:631:17F:H18	0.58	2.26	3	2
4:D:506:PCW:H382	4:D:509:PCW:H332	0.58	1.73	3	1
4:D:515:PCW:O1P	4:D:515:PCW:C6	0.58	2.52	3	1
4:A:405:PCW:H39	4:A:405:PCW:C18	0.58	2.28	4	1
4:A:406:PCW:H73	4:B:204:PCW:O2P	0.58	1.99	7	2
4:D:517:PCW:H122	5:D:525:17F:O9	0.58	1.98	4	1
4:A:405:PCW:H172	4:D:512:PCW:H39	0.58	1.76	5	1
4:C:607:PCW:H12	4:C:624:PCW:H351	0.58	1.74	5	2
4:D:507:PCW:H372	5:D:525:17F:H8	0.58	1.76	5	1
4:D:511:PCW:H252	4:D:511:PCW:H451	0.58	1.75	5	1
4:B:201:PCW:H171	4:D:516:PCW:C44	0.58	2.29	6	1
4:C:617:PCW:H2	4:C:617:PCW:C6	0.58	2.28	10	2
4:D:503:PCW:H471	4:D:511:PCW:H271	0.58	1.75	7	1
4:D:515:PCW:H342	4:D:516:PCW:O1P	0.58	1.98	8	1
4:D:501:PCW:H412	4:D:515:PCW:H171	0.58	1.76	9	1
4:D:515:PCW:C23	4:D:515:PCW:C18	0.58	2.82	9	1
4:A:411:PCW:H441	4:C:612:PCW:C27	0.58	2.28	1	3
4:C:606:PCW:C21	4:C:606:PCW:C17	0.58	2.76	3	5
4:B:201:PCW:O1P	4:B:201:PCW:H31	0.58	1.99	1	6
3:D:460:LEU:HG	3:D:461:ASN:H	0.58	1.57	1	1
4:D:503:PCW:H361	4:D:511:PCW:H372	0.58	1.76	1	1
4:D:506:PCW:C32	4:D:509:PCW:H371	0.58	2.28	1	1
4:C:601:PCW:H52	4:D:513:PCW:H61	0.58	1.75	2	1
4:C:609:PCW:H272	5:D:523:17F:H54	0.58	1.76	5	2
4:C:602:PCW:H481	4:C:608:PCW:H231	0.58	1.75	3	3
4:D:516:PCW:P	4:D:516:PCW:C3	0.58	2.92	8	2
4:C:606:PCW:C7	4:C:624:PCW:H171	0.58	2.29	4	1
4:A:403:PCW:C5	4:D:507:PCW:H341	0.58	2.26	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:525:17F:H64	5:D:525:17F:H36	0.58	1.76	5	3
4:C:605:PCW:H212	4:C:613:PCW:C15	0.58	2.29	8	1
4:D:518:PCW:H121	5:D:519:17F:C35	0.58	2.29	8	1
4:A:403:PCW:C24	4:D:513:PCW:H121	0.58	2.28	9	1
4:A:403:PCW:H261	4:D:507:PCW:C19	0.58	2.29	1	1
4:A:408:PCW:H482	4:D:528:PCW:H471	0.58	1.76	1	1
4:A:410:PCW:H161	4:A:413:PCW:H352	0.58	1.74	9	2
4:C:612:PCW:O2	4:C:612:PCW:H342	0.58	1.99	4	9
5:C:628:17F:O10	5:C:628:17F:H20A	0.58	1.98	5	9
3:D:458:PHE:HB3	4:D:517:PCW:C1	0.58	2.29	1	1
4:D:510:PCW:H331	5:D:524:17F:C10	0.58	2.29	1	1
4:D:512:PCW:O31	4:D:512:PCW:O3	0.58	2.22	5	9
4:B:201:PCW:H142	4:D:506:PCW:C36	0.58	2.16	2	1
4:A:415:PCW:H221	4:D:528:PCW:H231	0.58	1.74	4	4
4:D:518:PCW:H442	5:D:519:17F:C38	0.58	2.27	3	2
4:D:526:PCW:O31	4:D:526:PCW:H341	0.58	1.99	10	7
5:A:409:17F:C3	4:D:503:PCW:H82	0.58	2.28	4	2
4:C:603:PCW:H73	4:D:527:PCW:P	0.58	2.39	4	1
5:D:530:17F:H56	5:D:530:17F:C10	0.58	2.27	4	2
4:D:513:PCW:H281	4:D:513:PCW:H471	0.58	1.76	5	1
4:A:403:PCW:H141	4:A:403:PCW:C38	0.58	2.28	6	1
4:A:403:PCW:H321	4:A:407:PCW:C8	0.58	2.29	6	1
5:C:631:17F:H65	4:D:512:PCW:H482	0.58	1.74	6	1
4:D:509:PCW:O11	4:D:509:PCW:H41	0.58	1.99	6	1
4:D:508:PCW:C18	4:D:512:PCW:H151	0.58	2.25	8	1
4:A:405:PCW:H162	4:A:405:PCW:C22	0.58	2.28	9	1
4:D:518:PCW:C7	5:D:519:17F:H8A	0.57	2.29	1	1
4:C:608:PCW:C6	4:C:624:PCW:H222	0.57	2.28	2	3
4:A:411:PCW:H422	4:C:612:PCW:C24	0.57	2.28	6	3
4:D:505:PCW:H352	4:D:505:PCW:C5	0.57	2.28	5	1
4:C:606:PCW:C25	5:D:529:17F:H41	0.57	2.28	6	1
4:D:501:PCW:H411	4:D:515:PCW:C18	0.57	2.28	10	1
4:C:616:PCW:O2P	4:C:616:PCW:O2	0.57	2.22	1	2
4:C:603:PCW:O31	4:C:603:PCW:O3	0.57	2.22	9	5
5:D:524:17F:H50	4:D:527:PCW:H212	0.57	1.75	4	1
4:C:606:PCW:C15	5:D:529:17F:H8	0.57	2.29	5	1
4:D:508:PCW:H131	4:D:509:PCW:H242	0.57	1.74	6	1
4:D:508:PCW:H122	4:D:512:PCW:H171	0.57	1.75	6	1
4:D:508:PCW:H73	5:D:520:17F:C2	0.57	2.21	7	1
4:D:509:PCW:H161	5:D:520:17F:H20A	0.57	1.75	7	1
4:D:509:PCW:C41	5:D:520:17F:H8A	0.57	2.28	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:407:PCW:H39	5:D:522:17F:C40	0.57	2.27	10	1
4:C:611:PCW:H222	4:C:619:PCW:H482	0.57	1.75	10	1
4:C:606:PCW:C14	4:C:606:PCW:C18	0.57	2.78	7	4
4:C:616:PCW:H482	4:B:203:PCW:H281	0.57	1.73	1	1
4:C:616:PCW:H121	4:D:526:PCW:H151	0.57	1.76	1	1
4:A:401:PCW:H472	4:C:611:PCW:H271	0.57	1.76	5	3
4:C:618:PCW:H251	4:B:201:PCW:C44	0.57	2.27	5	2
4:D:515:PCW:H51	4:D:515:PCW:C1	0.57	2.24	8	2
4:C:607:PCW:H451	4:C:623:PCW:C48	0.57	2.29	9	3
4:C:621:PCW:H281	5:C:629:17F:H35	0.57	1.76	3	1
4:A:401:PCW:C45	4:C:611:PCW:H251	0.57	2.30	4	2
4:D:517:PCW:H122	5:D:525:17F:C17	0.57	2.29	4	1
4:C:616:PCW:C45	4:B:201:PCW:H452	0.57	2.15	5	1
4:C:617:PCW:O31	4:C:617:PCW:C7	0.57	2.52	5	1
4:B:202:PCW:C18	4:D:504:PCW:H282	0.57	2.28	6	1
4:C:604:PCW:H411	4:C:604:PCW:H372	0.57	1.75	8	1
4:D:515:PCW:H483	4:D:516:PCW:C22	0.57	2.30	8	1
4:A:406:PCW:H372	4:B:204:PCW:H171	0.57	1.75	1	1
4:A:413:PCW:C2	4:C:617:PCW:H411	0.57	2.29	6	5
4:C:620:PCW:O3P	4:C:620:PCW:O31	0.57	2.21	3	4
5:C:631:17F:H52	4:D:512:PCW:H161	0.57	1.75	1	1
4:A:414:PCW:C32	4:C:617:PCW:H51	0.57	2.29	2	1
4:A:415:PCW:H211	4:C:603:PCW:H162	0.57	1.74	4	2
2:B:126:ASP:HB3	2:B:129:GLN:HG3	0.57	1.75	7	2
4:B:201:PCW:C38	5:D:524:17F:H48	0.57	2.29	2	1
4:A:410:PCW:H431	4:A:414:PCW:H40	0.57	1.77	3	1
4:C:610:PCW:H52	5:C:629:17F:O1	0.57	1.99	3	2
4:A:401:PCW:C46	4:C:611:PCW:H251	0.57	2.29	4	2
4:C:606:PCW:H161	5:D:529:17F:H12	0.57	1.76	4	1
4:D:508:PCW:C17	4:D:512:PCW:H342	0.57	2.26	4	1
4:C:622:PCW:H282	5:D:521:17F:H77	0.57	1.76	5	1
4:D:513:PCW:H471	4:D:513:PCW:C28	0.57	2.29	5	1
4:D:504:PCW:O31	4:D:516:PCW:C8	0.57	2.52	6	2
4:A:410:PCW:H141	4:A:413:PCW:C33	0.57	2.30	7	1
4:A:404:PCW:H342	4:D:510:PCW:H212	0.57	1.76	9	1
4:A:405:PCW:H322	4:A:408:PCW:C35	0.57	2.29	9	1
4:C:602:PCW:C21	4:C:602:PCW:C17	0.57	2.78	6	3
4:C:607:PCW:H362	4:C:624:PCW:H431	0.57	1.77	10	2
4:B:203:PCW:O31	4:B:204:PCW:C8	0.57	2.53	6	3
4:D:509:PCW:C26	5:D:520:17F:H32	0.57	2.27	2	1
4:A:411:PCW:O4P	4:A:411:PCW:C6	0.57	2.51	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:24:ILE:HG13	2:B:40:TYR:HB3	0.57	1.75	4	1
4:C:604:PCW:H52	5:D:530:17F:H4A	0.57	1.74	7	1
4:D:513:PCW:C42	5:D:522:17F:H72	0.57	2.29	8	1
4:A:401:PCW:C41	4:D:511:PCW:H482	0.57	2.28	10	1
4:C:608:PCW:H431	5:C:626:17F:H60	0.57	1.77	10	1
4:A:406:PCW:H51	4:A:406:PCW:O2P	0.57	1.99	1	4
4:C:616:PCW:C43	4:C:625:PCW:H232	0.57	2.29	10	2
4:C:623:PCW:O11	4:C:623:PCW:H2	0.57	1.99	6	7
4:D:501:PCW:H211	4:D:501:PCW:H172	0.57	1.76	1	2
4:D:506:PCW:H20	4:D:516:PCW:C34	0.57	2.29	4	2
4:D:508:PCW:H222	4:D:512:PCW:C43	0.57	2.28	10	3
4:D:511:PCW:O11	4:D:511:PCW:O2	0.57	2.22	5	5
4:D:504:PCW:H452	4:D:505:PCW:C14	0.57	2.30	3	1
4:D:503:PCW:H442	5:D:522:17F:H9A	0.57	1.75	5	1
4:A:411:PCW:H351	4:C:612:PCW:C13	0.57	2.29	6	2
4:C:604:PCW:H451	4:C:606:PCW:C14	0.57	2.29	6	2
4:D:509:PCW:O1P	4:D:509:PCW:H32	0.57	2.00	6	1
4:C:615:PCW:H121	5:C:631:17F:H8	0.57	1.76	7	1
5:C:631:17F:C29	4:D:512:PCW:H181	0.57	2.28	7	1
4:A:413:PCW:C3	4:C:617:PCW:H422	0.57	2.29	8	1
4:D:504:PCW:H332	4:D:516:PCW:H141	0.57	1.77	8	1
4:A:401:PCW:C18	4:A:401:PCW:C22	0.57	2.73	6	3
4:C:602:PCW:O4P	4:C:602:PCW:H62	0.57	2.00	1	8
4:C:618:PCW:H451	5:C:629:17F:H55	0.57	1.77	1	3
4:D:502:PCW:O31	4:D:510:PCW:H73	0.57	1.99	1	1
4:D:503:PCW:H482	4:D:511:PCW:C46	0.57	2.27	1	1
4:D:506:PCW:C27	4:D:516:PCW:H142	0.57	2.29	1	1
4:A:410:PCW:H371	4:A:410:PCW:C41	0.57	2.29	2	1
4:A:414:PCW:H141	5:C:628:17F:H11A	0.57	1.75	10	2
4:C:618:PCW:O31	4:C:618:PCW:O3P	0.57	2.22	3	4
2:B:43:GLN:O	3:D:469:GLY:HA3	0.57	2.00	5	3
4:D:518:PCW:O11	5:D:519:17F:H71	0.57	2.00	2	1
4:A:403:PCW:H141	4:A:403:PCW:C39	0.57	2.29	3	1
4:A:411:PCW:H421	4:C:612:PCW:H251	0.57	1.75	3	1
4:D:513:PCW:H481	4:D:513:PCW:H282	0.57	1.76	3	1
5:D:529:17F:H6	5:D:529:17F:O1	0.57	2.00	3	1
4:C:601:PCW:H51	4:D:513:PCW:H61	0.57	1.76	4	1
4:D:507:PCW:C13	4:D:513:PCW:H131	0.57	2.28	4	1
4:C:617:PCW:H361	4:D:526:PCW:H152	0.57	1.76	5	1
4:D:517:PCW:C42	5:D:525:17F:H12	0.57	2.30	5	1
4:A:408:PCW:H40	4:D:506:PCW:H412	0.57	1.76	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:415:PCW:H222	4:C:603:PCW:C18	0.57	2.30	8	4
4:A:415:PCW:C7	4:C:622:PCW:H332	0.57	2.29	8	2
4:C:604:PCW:H281	4:C:607:PCW:C46	0.57	2.29	6	1
4:C:601:PCW:H471	4:C:601:PCW:H162	0.57	1.76	7	1
4:D:511:PCW:H362	4:D:511:PCW:C22	0.57	2.30	7	1
4:B:201:PCW:H483	5:D:524:17F:H50	0.57	1.76	8	1
4:B:201:PCW:C11	4:D:506:PCW:H322	0.57	2.30	8	1
4:D:505:PCW:H432	4:D:518:PCW:H252	0.57	1.76	10	1
4:D:511:PCW:H342	4:D:511:PCW:H162	0.57	1.77	10	1
4:C:602:PCW:O31	4:C:602:PCW:C3	0.57	2.51	10	5
4:B:203:PCW:H352	4:B:203:PCW:C31	0.57	2.29	3	8
4:C:618:PCW:O2P	4:C:625:PCW:H41	0.57	2.00	2	1
4:D:504:PCW:H411	4:D:505:PCW:C7	0.57	2.29	2	1
4:D:505:PCW:H161	4:D:505:PCW:H462	0.57	1.74	2	1
4:A:403:PCW:H232	4:D:513:PCW:H82	0.57	1.76	3	1
4:C:610:PCW:C1	5:C:629:17F:H6	0.57	2.20	3	1
4:C:609:PCW:C7	4:C:620:PCW:O11	0.57	2.53	5	5
4:A:415:PCW:H452	4:C:622:PCW:C28	0.57	2.30	5	1
4:C:618:PCW:P	4:C:625:PCW:H51	0.57	2.40	8	2
4:D:516:PCW:H431	5:D:529:17F:H54	0.57	1.76	5	1
4:B:201:PCW:H181	4:D:506:PCW:H461	0.57	1.77	7	1
4:D:507:PCW:H152	4:D:513:PCW:C37	0.57	2.30	9	1
4:C:602:PCW:H73	5:D:523:17F:H19	0.57	1.77	2	3
4:C:618:PCW:C42	4:C:625:PCW:H231	0.57	2.30	1	1
4:D:504:PCW:O4P	4:D:504:PCW:H82	0.57	2.00	9	10
5:D:523:17F:O8	5:D:523:17F:C5	0.57	2.49	4	5
4:C:623:PCW:H19	4:C:623:PCW:C14	0.57	2.29	5	3
4:A:414:PCW:H162	5:C:628:17F:H20	0.57	1.76	3	2
4:C:615:PCW:H451	5:D:523:17F:C30	0.57	2.30	7	2
4:D:507:PCW:O3	4:D:507:PCW:O31	0.57	2.22	7	5
4:D:503:PCW:H442	4:D:507:PCW:H481	0.57	1.76	6	1
4:D:516:PCW:C40	4:D:527:PCW:H283	0.57	2.30	10	3
4:A:413:PCW:H362	4:C:617:PCW:C39	0.57	2.29	8	1
3:D:486:ASP:CG	4:D:501:PCW:H62	0.57	2.24	9	1
4:A:401:PCW:H342	4:D:511:PCW:H242	0.57	1.75	10	1
4:A:401:PCW:O3	4:A:401:PCW:O31	0.57	2.23	2	10
4:C:625:PCW:C20	4:D:528:PCW:C35	0.57	2.83	9	7
5:C:626:17F:O10	5:C:626:17F:C7	0.57	2.53	10	9
4:D:508:PCW:C8	5:D:523:17F:H10	0.57	2.29	1	2
4:D:515:PCW:O31	4:D:515:PCW:O3	0.57	2.23	1	1
4:D:527:PCW:O31	4:D:527:PCW:C1	0.57	2.50	2	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:529:17F:H9A	5:D:529:17F:C20	0.57	2.30	1	2
4:A:414:PCW:H63	4:A:414:PCW:O11	0.57	2.00	2	1
4:C:612:PCW:O11	4:C:612:PCW:C2	0.57	2.51	4	3
4:D:507:PCW:H52	5:D:523:17F:O4	0.57	2.00	2	1
4:D:516:PCW:O31	4:D:516:PCW:O4P	0.57	2.23	7	3
4:C:601:PCW:H371	4:C:602:PCW:H121	0.57	1.75	6	1
4:B:202:PCW:C5	5:D:524:17F:O5	0.57	2.52	6	2
4:B:201:PCW:H162	5:D:520:17F:H77	0.57	1.76	8	1
4:D:517:PCW:H431	5:D:525:17F:H71	0.57	1.77	9	1
4:C:620:PCW:H20	5:C:631:17F:H10A	0.56	1.76	1	2
4:A:410:PCW:C8	5:C:628:17F:H1	0.56	2.30	3	3
4:C:607:PCW:C43	4:C:624:PCW:H481	0.56	2.29	5	4
4:D:507:PCW:C44	5:D:522:17F:H60	0.56	2.24	3	1
4:A:410:PCW:H161	4:A:413:PCW:H341	0.56	1.77	5	1
2:B:46:ILE:HA	3:D:447:LEU:HD12	0.56	1.77	5	1
4:B:203:PCW:H342	4:D:506:PCW:H382	0.56	1.76	6	1
4:A:401:PCW:C32	4:D:511:PCW:H382	0.56	2.14	10	2
4:B:202:PCW:C26	4:D:504:PCW:H271	0.56	2.28	8	1
4:A:412:PCW:O1P	4:C:623:PCW:C32	0.56	2.52	10	1
4:C:618:PCW:H341	5:C:629:17F:C21	0.56	2.29	10	1
4:C:604:PCW:H82	5:D:530:17F:H6	0.56	1.77	1	1
5:D:521:17F:O10	5:D:521:17F:H20	0.56	1.99	7	8
4:A:407:PCW:H271	4:A:412:PCW:C27	0.56	2.22	4	3
4:C:609:PCW:C24	4:C:615:PCW:H381	0.56	2.27	8	6
4:D:503:PCW:H152	4:D:511:PCW:H39	0.56	1.77	3	1
4:D:506:PCW:H172	4:D:516:PCW:H382	0.56	1.77	3	1
4:D:510:PCW:H432	5:D:524:17F:H12A	0.56	1.78	3	1
5:D:529:17F:H70	5:D:530:17F:C35	0.56	2.29	3	1
4:C:609:PCW:H181	4:C:615:PCW:H352	0.56	1.76	10	2
4:C:618:PCW:C26	4:D:510:PCW:H483	0.56	2.27	5	1
4:D:505:PCW:H19	4:D:505:PCW:H462	0.56	1.77	6	1
4:C:615:PCW:H283	4:D:508:PCW:H482	0.56	1.77	7	1
4:A:402:PCW:H361	4:D:512:PCW:O11	0.56	2.00	8	1
5:A:409:17F:H8A	3:D:404:GLU:HG2	0.56	1.77	9	1
2:B:68:ARG:HA	2:B:71:TYR:CE2	0.56	2.35	9	1
4:D:507:PCW:H51	5:D:523:17F:C7	0.56	2.30	10	1
1:A:371:LEU:HD13	5:A:409:17F:H45	0.56	1.77	1	1
5:A:409:17F:O10	5:A:409:17F:O6	0.56	2.23	6	7
4:A:411:PCW:C42	4:C:612:PCW:H181	0.56	2.31	9	3
1:C:465:GLU:O	1:C:469:LEU:HG	0.56	2.00	3	8
4:C:609:PCW:H251	5:C:626:17F:C39	0.56	2.30	9	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:614:PCW:O31	4:C:614:PCW:H11	0.56	2.00	5	8
2:B:81:VAL:HG12	2:B:114:VAL:HB	0.56	1.76	5	6
4:B:203:PCW:H52	4:B:203:PCW:C31	0.56	2.29	1	1
4:B:203:PCW:C48	4:B:204:PCW:H472	0.56	2.30	1	1
4:D:502:PCW:C4	4:D:502:PCW:O11	0.56	2.52	1	1
5:D:525:17F:O6	5:D:525:17F:C18	0.56	2.50	2	5
4:C:606:PCW:H132	4:C:606:PCW:O31	0.56	2.00	2	1
4:C:606:PCW:O4P	4:C:606:PCW:H62	0.56	2.00	3	2
4:C:620:PCW:H121	5:C:631:17F:C17	0.56	2.30	7	4
4:D:506:PCW:H221	4:D:516:PCW:H371	0.56	1.76	2	2
4:D:509:PCW:C35	5:D:520:17F:H63	0.56	2.30	2	1
4:D:513:PCW:H442	4:D:517:PCW:C26	0.56	2.30	2	2
4:A:412:PCW:O31	4:A:412:PCW:O3	0.56	2.23	3	4
4:C:625:PCW:H20	4:D:528:PCW:C37	0.56	2.30	9	2
4:B:201:PCW:H261	4:D:528:PCW:H441	0.56	1.76	3	1
4:C:602:PCW:H151	5:C:626:17F:H54	0.56	1.76	4	1
4:D:517:PCW:H221	5:D:525:17F:H10A	0.56	1.76	4	1
5:C:628:17F:O8	5:C:628:17F:H5	0.56	2.00	9	3
4:C:615:PCW:C5	5:C:631:17F:O4	0.56	2.53	6	1
4:A:401:PCW:H181	4:A:401:PCW:C22	0.56	2.28	7	3
4:D:509:PCW:H162	5:D:520:17F:H56	0.56	1.77	7	1
4:D:527:PCW:H422	4:D:528:PCW:H341	0.56	1.77	9	2
5:D:522:17F:H11	5:D:525:17F:H8	0.56	1.77	8	1
4:A:404:PCW:C7	5:D:524:17F:H2	0.56	2.29	10	1
4:C:602:PCW:H462	5:C:626:17F:C34	0.56	2.30	10	1
4:B:201:PCW:C6	4:D:504:PCW:H51	0.56	2.30	10	1
4:D:506:PCW:H151	4:D:516:PCW:C34	0.56	2.30	10	1
5:D:522:17F:O8	5:D:522:17F:H5	0.56	1.99	10	1
4:A:414:PCW:C12	5:C:628:17F:C9	0.56	2.82	4	4
4:C:603:PCW:H61	4:D:527:PCW:O2P	0.56	2.00	1	1
4:D:507:PCW:H82	4:D:507:PCW:O4P	0.56	2.00	9	9
3:D:487:TRP:HZ2	5:D:524:17F:H6A	0.56	1.58	2	1
4:D:504:PCW:H483	4:D:516:PCW:H171	0.56	1.77	3	1
4:D:513:PCW:H421	5:D:522:17F:H72	0.56	1.77	8	2
4:D:517:PCW:O1P	5:D:520:17F:N1	0.56	2.39	4	1
4:C:604:PCW:H482	4:C:606:PCW:H61	0.56	1.76	6	1
4:D:504:PCW:H472	4:D:505:PCW:H161	0.56	1.76	6	1
5:D:530:17F:H59	5:D:530:17F:H12A	0.56	1.77	8	1
4:B:201:PCW:H141	4:D:506:PCW:H461	0.56	1.76	9	1
4:D:513:PCW:O2P	5:D:523:17F:H1A	0.56	1.99	9	1
4:D:501:PCW:H482	5:D:525:17F:H55	0.56	1.76	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:408:PCW:H483	4:B:201:PCW:H272	0.56	1.78	1	1
4:A:410:PCW:O11	4:A:410:PCW:H2	0.56	1.99	2	1
4:B:202:PCW:C12	5:D:524:17F:H18	0.56	2.31	3	1
3:D:409:LYS:HE2	4:D:503:PCW:H41	0.56	1.77	3	1
4:A:412:PCW:C5	4:C:624:PCW:O31	0.56	2.54	4	1
4:B:203:PCW:O2P	4:B:204:PCW:C5	0.56	2.53	7	4
4:A:401:PCW:C32	4:D:511:PCW:H39	0.56	2.25	6	2
4:A:414:PCW:O31	4:C:617:PCW:H82	0.56	2.01	10	3
4:C:606:PCW:H61	4:C:624:PCW:C28	0.56	2.25	7	1
4:D:515:PCW:C32	4:D:516:PCW:H12	0.56	2.30	7	1
4:A:402:PCW:H39	4:A:405:PCW:H272	0.56	1.76	8	1
4:C:605:PCW:H211	4:C:613:PCW:C38	0.56	2.29	8	1
4:B:202:PCW:C4	5:D:524:17F:H1A	0.56	2.31	8	1
4:A:405:PCW:H221	4:D:508:PCW:H271	0.56	1.75	1	1
4:A:405:PCW:H2	4:A:405:PCW:O4P	0.56	1.99	8	8
4:A:406:PCW:O4P	4:A:406:PCW:H62	0.56	1.99	1	9
4:C:603:PCW:H281	4:D:526:PCW:H232	0.56	1.77	3	5
4:C:606:PCW:H2	4:C:606:PCW:C4	0.56	2.29	7	4
2:B:68:ARG:HA	2:B:71:TYR:CZ	0.56	2.36	10	8
1:C:525:LEU:HD23	1:C:528:ARG:HD2	0.56	1.76	2	1
4:D:510:PCW:C27	5:D:524:17F:H60	0.56	2.30	2	1
4:A:415:PCW:O31	4:A:415:PCW:O3	0.56	2.24	5	3
4:B:201:PCW:H332	4:D:510:PCW:H382	0.56	1.77	6	1
4:D:511:PCW:C28	5:D:522:17F:H56	0.56	2.30	6	1
4:C:615:PCW:H121	5:C:631:17F:C8	0.56	2.31	7	1
4:C:606:PCW:C6	4:C:624:PCW:H19	0.56	2.28	8	1
4:A:401:PCW:H31	4:D:511:PCW:H231	0.56	1.76	9	1
4:A:405:PCW:H241	4:D:508:PCW:H261	0.56	1.78	9	1
4:A:402:PCW:H422	4:D:508:PCW:H182	0.56	1.76	10	1
4:A:402:PCW:H63	4:A:402:PCW:O11	0.56	2.01	1	1
4:A:411:PCW:H422	4:C:612:PCW:C21	0.56	2.30	1	2
4:D:508:PCW:H42	5:D:520:17F:O1	0.56	2.00	3	2
5:D:525:17F:O9	5:D:525:17F:O8	0.56	2.24	2	7
1:A:276:VAL:O	1:A:280:ARG:HB2	0.56	2.01	9	2
4:C:611:PCW:C47	4:D:501:PCW:H271	0.56	2.10	3	1
4:C:622:PCW:H211	4:D:515:PCW:H242	0.56	1.76	3	1
4:B:203:PCW:H161	4:B:204:PCW:H39	0.56	1.76	3	1
4:D:510:PCW:H20	5:D:524:17F:H19A	0.56	1.78	5	2
4:C:602:PCW:H172	4:C:602:PCW:H221	0.56	1.77	4	1
4:C:616:PCW:H361	4:D:527:PCW:H382	0.56	1.76	4	1
4:C:618:PCW:H381	4:C:625:PCW:C17	0.56	2.31	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:510:PCW:H20	5:D:524:17F:H56	0.56	1.78	4	1
4:D:507:PCW:H372	5:D:525:17F:C8	0.56	2.31	5	1
4:B:203:PCW:H331	4:D:506:PCW:H362	0.56	1.78	6	1
4:C:622:PCW:H242	4:D:501:PCW:H381	0.56	1.78	1	1
4:D:510:PCW:O3P	4:D:510:PCW:O31	0.56	2.24	1	7
4:C:618:PCW:H242	4:B:201:PCW:H451	0.56	1.76	2	1
4:C:605:PCW:H472	4:C:619:PCW:H441	0.56	1.77	3	1
4:B:201:PCW:H232	4:D:506:PCW:H441	0.56	1.76	3	1
4:C:605:PCW:C31	4:C:613:PCW:C6	0.56	2.83	5	3
4:C:621:PCW:C21	5:C:629:17F:H31	0.56	2.31	6	2
4:A:413:PCW:H351	4:C:617:PCW:H412	0.56	1.78	8	2
1:C:514:LEU:HA	1:C:517:HIS:HB2	0.56	1.77	6	2
4:D:508:PCW:H62	5:D:520:17F:O8	0.56	2.01	6	1
3:D:486:ASP:OD1	4:D:501:PCW:H63	0.56	2.01	7	1
4:C:620:PCW:P	4:C:621:PCW:H51	0.56	2.40	8	1
4:B:203:PCW:O2P	4:B:204:PCW:H82	0.56	2.00	9	3
4:A:404:PCW:H61	5:D:524:17F:O1	0.56	2.01	9	1
4:C:617:PCW:H73	4:C:617:PCW:C31	0.56	2.31	9	1
4:D:518:PCW:H142	5:D:519:17F:H66	0.56	1.77	9	1
4:D:503:PCW:H432	4:D:511:PCW:C20	0.56	2.23	10	1
4:C:611:PCW:H162	4:C:619:PCW:C17	0.56	2.28	1	2
4:C:613:PCW:H20	5:D:521:17F:H42	0.56	1.77	1	1
4:D:501:PCW:C43	5:D:525:17F:H51	0.56	2.30	1	1
4:D:507:PCW:H462	5:D:522:17F:H60	0.56	1.77	1	1
4:D:518:PCW:C16	5:D:519:17F:H20	0.56	2.31	2	1
4:A:401:PCW:H272	4:C:614:PCW:H281	0.56	1.77	3	1
4:A:406:PCW:C3	4:A:406:PCW:O1P	0.56	2.53	7	4
4:B:202:PCW:C36	4:B:202:PCW:H141	0.56	2.31	3	1
4:D:507:PCW:C19	4:D:513:PCW:H221	0.56	2.31	3	1
4:D:518:PCW:H442	5:D:519:17F:H73	0.56	1.78	3	1
4:C:616:PCW:C36	4:D:527:PCW:H382	0.56	2.31	4	1
4:D:517:PCW:H421	4:D:517:PCW:H181	0.56	1.78	6	1
4:C:614:PCW:H432	4:C:619:PCW:H20	0.56	1.77	7	1
4:D:518:PCW:C16	5:D:519:17F:H33	0.56	2.31	8	1
4:D:509:PCW:O11	4:D:509:PCW:H63	0.56	2.01	9	1
4:D:501:PCW:O2P	5:D:525:17F:H6A	0.56	2.01	10	1
4:D:514:PCW:H162	5:D:520:17F:H61	0.56	1.78	10	1
1:C:519:ALA:HB3	1:C:520:PRO:HD3	0.56	1.78	7	10
4:D:513:PCW:O31	4:D:513:PCW:C4	0.56	2.51	1	2
4:A:401:PCW:O3	4:A:401:PCW:C31	0.56	2.54	2	3
4:A:411:PCW:H422	4:C:612:PCW:H181	0.56	1.78	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:426:PHE:O	1:C:430:LEU:HG	0.56	2.01	5	4
4:D:501:PCW:C11	4:D:501:PCW:O31	0.56	2.53	7	8
4:D:502:PCW:O31	4:D:502:PCW:C1	0.56	2.53	2	4
4:D:515:PCW:O11	4:D:515:PCW:O2	0.56	2.24	6	4
4:C:605:PCW:H481	4:C:619:PCW:H421	0.56	1.78	4	2
4:C:621:PCW:H222	5:C:629:17F:C1Y	0.56	2.29	4	3
4:D:501:PCW:H211	5:D:521:17F:C19	0.56	2.31	4	1
1:A:334:ARG:HA	1:C:440:GLU:OE1	0.56	2.01	5	1
4:C:602:PCW:H422	5:C:626:17F:C26	0.56	2.31	6	1
4:D:517:PCW:H341	5:D:520:17F:C8	0.56	2.25	6	1
4:A:403:PCW:H241	5:D:523:17F:H18	0.56	1.78	7	1
4:A:403:PCW:C3	4:A:403:PCW:O1P	0.55	2.53	2	2
4:A:413:PCW:H451	4:D:526:PCW:C23	0.55	2.30	3	2
1:C:475:GLU:HB2	1:C:476:PRO:HD3	0.55	1.78	1	2
4:C:606:PCW:O11	4:C:606:PCW:H51	0.55	2.01	9	5
4:C:609:PCW:O11	4:C:615:PCW:C7	0.55	2.54	1	2
4:C:609:PCW:H251	5:C:626:17F:H73	0.55	1.77	9	2
4:C:610:PCW:C28	5:C:629:17F:H72	0.55	2.31	2	3
4:C:616:PCW:C40	4:C:618:PCW:H162	0.55	2.31	10	3
4:C:610:PCW:C24	4:C:610:PCW:H20	0.55	2.31	3	5
4:C:614:PCW:H442	4:C:619:PCW:C20	0.55	2.32	3	5
3:D:427:GLN:HB2	4:D:502:PCW:H61	0.55	1.78	4	2
4:D:517:PCW:H181	4:D:517:PCW:C41	0.55	2.31	10	2
2:B:37:GLU:HB3	3:D:369:VAL:HG21	0.55	1.76	6	2
4:B:202:PCW:H382	4:B:202:PCW:H151	0.55	1.78	4	1
4:C:614:PCW:H452	4:C:619:PCW:H20	0.55	1.78	6	2
4:D:505:PCW:H342	5:D:519:17F:C7	0.55	2.30	5	1
4:D:513:PCW:H52	4:D:513:PCW:H2	0.55	1.78	5	3
5:A:409:17F:H77	4:D:501:PCW:H252	0.55	1.78	6	1
4:D:511:PCW:O11	4:D:511:PCW:H73	0.55	2.00	7	1
4:D:510:PCW:H20	5:D:524:17F:C1Y	0.55	2.19	8	2
5:D:522:17F:H29	5:D:525:17F:H10A	0.55	1.78	8	1
4:A:405:PCW:C16	4:A:405:PCW:H231	0.55	2.32	9	1
4:A:415:PCW:O11	4:A:415:PCW:H2	0.55	2.01	9	1
4:C:615:PCW:C48	4:D:509:PCW:H241	0.55	2.23	9	1
4:D:506:PCW:H151	4:D:516:PCW:H342	0.55	1.77	10	1
4:A:407:PCW:H331	5:D:522:17F:H33	0.55	1.78	1	1
5:D:519:17F:O10	5:D:519:17F:H4	0.55	2.01	10	7
4:D:513:PCW:H442	4:D:517:PCW:C27	0.55	2.30	7	2
4:A:413:PCW:C48	5:D:524:17F:H38	0.55	2.32	3	1
4:D:502:PCW:C8	4:D:505:PCW:O1P	0.55	2.54	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:201:PCW:H161	4:D:506:PCW:C44	0.55	2.27	5	2
4:A:405:PCW:H63	4:A:405:PCW:C32	0.55	2.31	5	1
4:A:411:PCW:H422	4:C:612:PCW:H251	0.55	1.77	7	1
4:C:611:PCW:C31	4:C:622:PCW:H352	0.55	2.31	9	3
3:D:400:ARG:HD2	3:D:412:LEU:HG	0.55	1.78	7	1
4:D:516:PCW:H231	5:D:519:17F:H55	0.55	1.78	7	2
4:C:604:PCW:O11	4:C:604:PCW:C5	0.55	2.55	9	1
4:C:609:PCW:C45	4:D:512:PCW:H231	0.55	2.31	10	1
4:A:406:PCW:C43	4:B:204:PCW:H19	0.55	2.31	1	1
4:C:604:PCW:H451	4:C:606:PCW:C18	0.55	2.32	1	2
4:C:606:PCW:H41	4:C:606:PCW:O31	0.55	2.02	1	1
4:B:203:PCW:H141	4:B:204:PCW:C38	0.55	2.31	1	1
4:D:503:PCW:H171	4:D:503:PCW:C21	0.55	2.32	2	2
4:C:601:PCW:H451	4:C:601:PCW:C15	0.55	2.15	4	1
4:C:618:PCW:H431	5:C:629:17F:H45	0.55	1.78	4	1
4:C:624:PCW:H182	4:C:624:PCW:H82	0.55	1.78	6	1
5:D:519:17F:O1	5:D:519:17F:H2	0.55	2.01	6	1
4:A:415:PCW:C28	4:D:528:PCW:H283	0.55	2.31	7	1
4:D:507:PCW:H421	4:D:517:PCW:C23	0.55	2.26	8	1
4:D:517:PCW:H171	4:D:517:PCW:C38	0.55	2.26	8	1
5:D:520:17F:H58	5:D:520:17F:H65	0.55	1.78	8	1
4:A:414:PCW:C36	4:C:617:PCW:H141	0.55	2.30	9	1
4:C:608:PCW:H121	4:C:609:PCW:C16	0.55	2.32	9	1
4:D:502:PCW:H41	4:D:502:PCW:C3	0.55	2.26	1	1
4:C:610:PCW:C28	5:C:629:17F:H68	0.55	2.31	9	3
4:D:506:PCW:H40	5:D:520:17F:H70	0.55	1.79	9	2
4:C:620:PCW:H141	5:C:631:17F:C17	0.55	2.32	6	3
3:D:465:CYS:HB3	3:D:468:CYS:SG	0.55	2.41	8	2
5:A:409:17F:O2	4:D:503:PCW:C8	0.55	2.55	9	1
4:A:411:PCW:H442	4:C:612:PCW:H271	0.55	1.76	9	1
4:C:604:PCW:H222	4:D:515:PCW:C28	0.55	2.24	9	1
4:D:509:PCW:H412	5:D:520:17F:H8A	0.55	1.76	9	1
5:C:631:17F:O10	5:C:631:17F:C6	0.55	2.51	3	5
3:D:436:LEU:HD21	4:D:502:PCW:C5	0.55	2.32	1	1
4:D:507:PCW:H332	4:D:513:PCW:H31	0.55	1.79	1	1
4:D:510:PCW:O31	4:D:510:PCW:P	0.55	2.65	1	1
4:A:401:PCW:C48	4:C:611:PCW:H441	0.55	2.32	3	1
4:C:601:PCW:H162	4:C:601:PCW:H451	0.55	1.76	3	1
4:D:513:PCW:H471	4:D:513:PCW:H272	0.55	1.76	7	3
4:A:402:PCW:H421	4:D:512:PCW:H132	0.55	1.77	4	1
4:C:602:PCW:H42	5:D:523:17F:C19	0.55	2.13	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:613:PCW:H221	5:D:521:17F:C25	0.55	2.32	8	2
4:C:622:PCW:H362	4:C:622:PCW:C31	0.55	2.31	4	1
4:C:622:PCW:O2	4:C:622:PCW:C36	0.55	2.55	4	1
4:B:201:PCW:H40	4:D:527:PCW:H251	0.55	1.78	4	1
4:D:501:PCW:O11	4:D:501:PCW:H2	0.55	2.02	5	1
4:D:506:PCW:H231	4:D:516:PCW:H412	0.55	1.79	6	1
4:A:401:PCW:H51	4:D:511:PCW:O31	0.55	2.00	9	2
4:C:613:PCW:C26	5:D:521:17F:H71	0.55	2.28	8	2
4:B:202:PCW:H281	4:D:506:PCW:C48	0.55	2.30	9	1
4:D:528:PCW:H181	5:D:530:17F:H37	0.55	1.77	9	1
4:D:505:PCW:H61	5:D:519:17F:O8	0.55	2.01	1	1
4:D:517:PCW:H252	5:D:525:17F:H8	0.55	1.78	1	1
4:C:605:PCW:O1P	4:C:613:PCW:C5	0.55	2.53	2	2
5:A:409:17F:H60	4:D:501:PCW:H241	0.55	1.78	4	1
4:C:609:PCW:C6	4:C:620:PCW:O11	0.55	2.55	9	4
1:C:453:GLN:HB2	1:C:454:PRO:HD3	0.55	1.78	6	1
4:C:607:PCW:O2	4:C:624:PCW:C37	0.55	2.54	6	1
4:D:502:PCW:H322	4:D:510:PCW:C7	0.55	2.32	6	1
4:A:401:PCW:H381	4:D:503:PCW:C20	0.55	2.23	7	1
4:C:622:PCW:C38	4:C:623:PCW:H182	0.55	2.32	7	2
4:D:509:PCW:H162	5:D:520:17F:C33	0.55	2.31	7	1
5:A:409:17F:H2	5:A:409:17F:O1	0.55	2.01	8	1
4:B:202:PCW:H251	4:D:504:PCW:C28	0.55	2.28	8	1
4:D:513:PCW:C12	5:D:523:17F:H6	0.55	2.31	8	1
4:D:506:PCW:H242	5:D:524:17F:C25	0.55	2.32	9	1
4:D:511:PCW:O11	4:D:511:PCW:C4	0.55	2.54	9	1
4:A:405:PCW:O31	4:D:514:PCW:C32	0.55	2.55	10	1
4:C:619:PCW:H82	4:C:619:PCW:O4P	0.55	2.02	6	10
4:A:406:PCW:H272	4:C:618:PCW:H451	0.55	1.78	2	1
4:A:408:PCW:H431	4:B:203:PCW:C18	0.55	2.23	2	1
4:A:411:PCW:C42	4:C:612:PCW:H251	0.55	2.31	7	2
4:C:606:PCW:O31	4:C:606:PCW:P	0.55	2.65	3	1
4:A:410:PCW:H482	4:D:518:PCW:H281	0.55	1.78	7	1
4:A:411:PCW:C33	4:C:612:PCW:C13	0.55	2.83	9	1
5:C:631:17F:O8	5:C:631:17F:C5	0.55	2.53	9	1
4:C:612:PCW:C33	4:C:618:PCW:H132	0.55	2.32	10	1
4:C:605:PCW:C48	4:C:619:PCW:H441	0.55	2.31	3	2
4:C:618:PCW:H131	4:C:625:PCW:H142	0.55	1.77	7	3
4:C:618:PCW:O1P	4:C:625:PCW:H63	0.55	2.02	1	2
4:C:620:PCW:O4P	4:C:620:PCW:H73	0.55	2.02	4	5
5:C:630:17F:C2X	5:D:530:17F:H62	0.55	2.32	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:203:PCW:H482	4:B:204:PCW:H472	0.55	1.77	1	2
4:D:505:PCW:H73	4:D:505:PCW:H342	0.55	1.78	1	1
4:D:506:PCW:H321	4:D:509:PCW:H371	0.55	1.77	1	1
4:D:509:PCW:O11	4:D:509:PCW:O2	0.55	2.25	2	8
5:D:524:17F:O2	5:D:524:17F:C2	0.55	2.55	2	2
4:C:608:PCW:C26	5:C:627:17F:H62	0.55	2.22	7	3
4:C:616:PCW:C47	4:B:201:PCW:H452	0.55	2.22	4	2
4:D:502:PCW:H161	4:D:505:PCW:C3	0.55	2.28	6	1
4:A:404:PCW:H242	4:A:411:PCW:H262	0.55	1.77	7	1
4:A:405:PCW:C8	4:D:514:PCW:O31	0.55	2.55	7	2
4:D:508:PCW:H211	4:D:512:PCW:C41	0.55	2.30	7	1
4:A:406:PCW:H152	4:B:202:PCW:C23	0.55	2.31	9	2
4:A:406:PCW:H271	5:C:629:17F:H55	0.55	1.77	8	1
4:C:614:PCW:H42	4:C:623:PCW:H62	0.55	1.79	8	1
4:C:617:PCW:C47	4:C:617:PCW:C43	0.55	2.77	8	1
4:C:618:PCW:H431	4:C:625:PCW:H282	0.55	1.78	8	2
4:B:201:PCW:C48	5:D:524:17F:H50	0.55	2.32	8	1
4:A:404:PCW:H52	4:D:510:PCW:C11	0.55	2.30	9	1
4:B:201:PCW:H181	4:D:506:PCW:H442	0.55	1.78	10	1
4:C:604:PCW:P	4:C:604:PCW:C3	0.55	2.95	1	8
4:C:605:PCW:H231	4:C:613:PCW:C38	0.55	2.31	6	4
4:C:613:PCW:O11	4:C:613:PCW:H2	0.55	2.02	6	6
4:C:625:PCW:H282	5:C:629:17F:H46	0.55	1.79	1	3
4:B:201:PCW:H11	4:D:504:PCW:H132	0.55	1.77	1	2
4:D:511:PCW:C27	4:D:511:PCW:C22	0.55	2.56	2	3
1:A:301:LEU:HD13	1:C:473:LYS:HG2	0.55	1.78	4	4
4:A:405:PCW:H372	4:A:405:PCW:H411	0.55	1.78	9	2
4:C:605:PCW:C21	4:C:613:PCW:H382	0.55	2.31	4	3
4:C:609:PCW:H282	4:C:615:PCW:H422	0.55	1.78	2	1
4:B:201:PCW:H422	5:D:524:17F:C27	0.55	2.28	5	2
3:D:468:CYS:HB3	3:D:484:CYS:HB2	0.55	1.77	2	1
4:D:516:PCW:H481	4:D:527:PCW:C25	0.55	2.28	2	1
4:C:607:PCW:H471	4:D:513:PCW:H462	0.55	1.78	4	1
4:D:515:PCW:H151	5:D:525:17F:H62	0.55	1.79	4	1
5:D:530:17F:H10A	5:D:530:17F:C31	0.55	2.30	4	1
4:A:406:PCW:H151	4:B:202:PCW:H172	0.55	1.77	5	1
1:C:418:GLN:O	1:C:422:VAL:HB	0.55	2.02	5	1
4:D:504:PCW:C47	4:D:505:PCW:H161	0.55	2.32	6	1
4:A:401:PCW:O2	4:D:511:PCW:H231	0.55	2.02	7	1
4:A:404:PCW:C6	4:D:510:PCW:H121	0.55	2.30	9	1
4:D:509:PCW:H161	5:D:520:17F:H57	0.55	1.79	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:412:PCW:O31	4:A:412:PCW:O3P	0.55	2.24	7	5
4:B:201:PCW:P	4:B:201:PCW:C3	0.55	2.94	1	2
4:B:204:PCW:H341	4:B:204:PCW:O31	0.55	2.02	1	5
4:A:410:PCW:O31	4:A:410:PCW:O3P	0.55	2.25	7	3
4:D:501:PCW:H61	5:D:525:17F:C2	0.55	2.31	2	1
4:C:606:PCW:H73	4:C:624:PCW:C17	0.55	2.32	4	2
4:D:513:PCW:C11	5:D:523:17F:H6	0.55	2.32	4	1
4:D:501:PCW:O31	4:D:501:PCW:H11	0.55	2.01	5	1
4:D:507:PCW:H422	4:D:507:PCW:C38	0.55	2.32	6	1
4:D:504:PCW:C17	4:D:510:PCW:H40	0.55	2.25	7	1
5:D:523:17F:C7	5:D:523:17F:O10	0.55	2.55	7	1
4:A:406:PCW:H171	4:B:202:PCW:C23	0.55	2.32	8	1
4:A:407:PCW:O1P	5:D:522:17F:N1	0.54	2.40	1	1
1:C:561:LYS:HA	1:C:561:LYS:HE3	0.54	1.79	6	2
4:C:618:PCW:H282	5:D:524:17F:H61	0.54	1.79	6	2
4:C:623:PCW:C46	4:C:624:PCW:H482	0.54	2.32	1	3
3:D:452:CYS:HA	3:D:459:LEU:HD23	0.54	1.79	7	5
3:D:456:GLN:HB3	4:D:517:PCW:H351	0.54	1.79	1	1
4:C:603:PCW:C4	4:C:603:PCW:C31	0.54	2.85	2	1
4:D:515:PCW:H271	4:D:528:PCW:C28	0.54	2.21	3	1
4:C:615:PCW:C22	4:D:512:PCW:H261	0.54	2.22	4	1
4:D:515:PCW:H362	4:D:516:PCW:O3P	0.54	2.02	5	1
5:C:626:17F:H78	5:D:523:17F:C30	0.54	2.27	6	1
4:D:513:PCW:C3	4:D:513:PCW:O2P	0.54	2.55	8	1
4:B:201:PCW:C24	4:B:203:PCW:H282	0.54	2.32	10	1
4:A:408:PCW:O31	4:A:408:PCW:O3	0.54	2.25	2	7
1:C:495:LYS:O	1:C:499:LEU:HB2	0.54	2.02	7	8
4:D:506:PCW:C17	4:D:506:PCW:C13	0.54	2.84	2	7
5:D:522:17F:H6A	5:D:525:17F:C2	0.54	2.29	1	1
4:C:606:PCW:H341	4:C:606:PCW:O31	0.54	2.02	2	1
4:C:621:PCW:H362	5:C:629:17F:C33	0.54	2.32	2	3
4:D:504:PCW:H431	4:D:505:PCW:C8	0.54	2.32	2	1
4:A:406:PCW:C27	4:C:618:PCW:H462	0.54	2.33	9	4
4:A:401:PCW:H482	4:C:611:PCW:H232	0.54	1.79	5	1
4:D:511:PCW:O11	4:D:511:PCW:H63	0.54	2.02	5	1
4:D:517:PCW:H181	4:D:517:PCW:C43	0.54	2.25	5	1
4:D:501:PCW:H39	4:D:515:PCW:H421	0.54	1.79	8	1
4:D:516:PCW:O4P	4:D:516:PCW:H2	0.54	2.02	9	1
4:A:407:PCW:H162	4:A:412:PCW:H261	0.54	1.78	1	1
4:D:506:PCW:O2P	4:D:506:PCW:H331	0.54	2.03	1	1
4:D:507:PCW:H332	4:D:513:PCW:C3	0.54	2.33	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:508:PCW:C7	4:D:517:PCW:O2P	0.54	2.56	1	1
4:D:501:PCW:H19	4:D:503:PCW:H332	0.54	1.80	2	1
4:D:505:PCW:H2	4:D:505:PCW:O1P	0.54	2.02	2	1
4:D:506:PCW:H11	4:D:506:PCW:O31	0.54	2.02	2	1
4:D:508:PCW:H161	4:D:512:PCW:H151	0.54	1.79	4	3
4:D:527:PCW:O11	4:D:527:PCW:O2	0.54	2.26	8	9
4:A:401:PCW:H361	4:D:503:PCW:H172	0.54	1.80	3	1
4:C:602:PCW:H471	5:C:627:17F:H43	0.54	1.77	3	2
4:A:413:PCW:O1P	4:A:413:PCW:H52	0.54	2.02	5	2
4:C:603:PCW:H271	4:D:526:PCW:C21	0.54	2.23	8	2
4:C:621:PCW:H19	5:C:629:17F:O10	0.54	2.01	9	2
4:A:412:PCW:H63	4:C:624:PCW:C32	0.54	2.32	5	1
4:A:414:PCW:H122	5:C:628:17F:H9A	0.54	1.76	5	3
4:C:616:PCW:H482	4:B:203:PCW:H271	0.54	1.78	5	1
4:D:508:PCW:H142	4:D:512:PCW:H131	0.54	1.78	5	1
5:A:409:17F:H2	4:D:503:PCW:H82	0.54	1.78	6	1
4:C:602:PCW:C26	5:C:627:17F:H76	0.54	2.12	8	1
4:C:618:PCW:C38	4:C:625:PCW:H181	0.54	2.29	8	1
4:A:404:PCW:H321	4:D:510:PCW:C18	0.54	2.32	9	1
4:D:509:PCW:C43	5:D:520:17F:H12	0.54	2.31	9	1
4:C:622:PCW:H52	4:C:622:PCW:O1P	0.54	2.03	10	7
5:D:530:17F:H12A	5:D:530:17F:C33	0.54	2.32	2	6
4:C:618:PCW:H482	4:B:201:PCW:H442	0.54	1.79	2	1
4:D:506:PCW:O31	4:D:515:PCW:C7	0.54	2.55	2	1
5:A:409:17F:O8	5:A:409:17F:O9	0.54	2.26	4	5
4:C:605:PCW:H182	4:C:613:PCW:C36	0.54	2.31	8	3
5:D:519:17F:C17	5:D:519:17F:O2	0.54	2.56	8	2
5:D:529:17F:O3	5:D:529:17F:O9	0.54	2.25	3	2
4:A:404:PCW:C37	4:B:202:PCW:H442	0.54	2.32	5	1
4:A:415:PCW:H73	4:A:415:PCW:C32	0.54	2.21	5	1
4:D:502:PCW:C28	4:D:518:PCW:H242	0.54	2.27	5	2
4:D:505:PCW:C35	4:D:505:PCW:C31	0.54	2.84	5	1
5:A:409:17F:H73	4:D:503:PCW:C28	0.54	2.31	7	1
4:C:609:PCW:C27	5:C:626:17F:H73	0.54	2.33	7	3
4:A:406:PCW:H222	4:B:204:PCW:H432	0.54	1.79	8	1
5:D:525:17F:H40	5:D:525:17F:H68	0.54	1.79	9	2
4:A:404:PCW:H341	4:D:510:PCW:H212	0.54	1.80	9	1
4:C:613:PCW:H282	5:D:521:17F:H40	0.54	1.78	9	1
4:B:202:PCW:H51	5:D:524:17F:C3	0.54	2.33	9	1
4:C:607:PCW:H31	4:C:624:PCW:C41	0.54	2.27	10	1
4:A:407:PCW:H382	5:D:522:17F:H65	0.54	1.79	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:611:PCW:O31	4:C:611:PCW:C11	0.54	2.55	10	4
4:C:615:PCW:H272	5:C:631:17F:H45	0.54	1.80	4	2
4:A:406:PCW:H63	4:A:406:PCW:O2P	0.54	2.02	5	3
4:A:410:PCW:H121	4:C:617:PCW:H331	0.54	1.80	7	3
4:B:203:PCW:H441	4:B:204:PCW:H412	0.54	1.79	2	1
4:A:403:PCW:C36	4:A:407:PCW:H361	0.54	2.33	3	1
4:B:204:PCW:C11	4:B:204:PCW:O31	0.54	2.56	3	4
4:A:403:PCW:C42	4:D:513:PCW:H40	0.54	2.31	4	1
4:A:415:PCW:C33	4:C:622:PCW:H122	0.54	2.33	9	2
4:D:510:PCW:C11	4:D:510:PCW:O31	0.54	2.56	4	1
4:B:202:PCW:H42	4:B:202:PCW:C31	0.54	2.33	10	2
4:D:508:PCW:C6	5:D:520:17F:O8	0.54	2.55	6	1
4:B:202:PCW:H261	4:D:504:PCW:H252	0.54	1.80	7	1
4:A:401:PCW:C5	4:D:511:PCW:O31	0.54	2.56	9	2
4:C:604:PCW:O1P	4:C:622:PCW:H73	0.54	2.02	8	2
4:D:504:PCW:H40	5:D:519:17F:H37	0.54	1.79	8	1
4:D:515:PCW:H63	4:D:516:PCW:C32	0.54	2.33	8	1
4:D:518:PCW:H141	5:D:519:17F:C35	0.54	2.25	8	1
4:D:507:PCW:C15	4:D:513:PCW:H382	0.54	2.31	9	1
4:D:515:PCW:H11	4:D:515:PCW:O31	0.54	2.01	9	1
4:B:201:PCW:H171	4:D:516:PCW:C42	0.54	2.32	10	1
4:A:406:PCW:H121	4:B:204:PCW:O3	0.54	2.02	1	1
5:C:628:17F:O8	5:C:628:17F:C5	0.54	2.48	4	4
5:D:522:17F:C12	5:D:522:17F:C23	0.54	2.84	1	1
4:C:603:PCW:H62	4:D:527:PCW:O2P	0.54	2.03	2	1
4:C:615:PCW:C22	4:D:512:PCW:H282	0.54	2.33	2	1
5:A:409:17F:O4	4:D:503:PCW:H82	0.54	2.03	3	1
4:C:616:PCW:H481	4:D:504:PCW:H221	0.54	1.78	3	1
4:D:506:PCW:O4P	4:D:506:PCW:H82	0.54	2.02	5	1
4:A:415:PCW:H222	4:C:603:PCW:H181	0.54	1.78	7	1
2:B:3:GLU:HG3	2:B:52:LEU:HD22	0.54	1.79	7	1
4:C:605:PCW:H262	4:C:613:PCW:H181	0.54	1.80	8	1
4:D:502:PCW:H321	4:D:510:PCW:O4P	0.54	2.02	8	1
4:A:406:PCW:H152	4:B:202:PCW:C21	0.54	2.32	9	1
4:A:403:PCW:H62	4:A:403:PCW:O4P	0.54	2.03	10	1
4:A:414:PCW:H32	4:A:414:PCW:O4P	0.54	2.03	10	1
1:A:365:LYS:HB2	1:A:366:PRO:CD	0.54	2.29	5	6
4:A:403:PCW:H212	4:D:513:PCW:C35	0.54	2.32	1	1
4:D:518:PCW:O3	4:D:518:PCW:O31	0.54	2.26	1	9
4:D:507:PCW:H351	5:D:522:17F:O1	0.54	2.03	4	2
4:C:622:PCW:H272	4:D:501:PCW:H442	0.54	1.80	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:201:PCW:O31	4:B:201:PCW:H12	0.54	2.01	10	5
4:D:517:PCW:H432	4:D:517:PCW:H212	0.54	1.78	3	1
4:C:605:PCW:C32	4:C:611:PCW:O3P	0.54	2.56	4	1
4:C:607:PCW:H472	4:D:513:PCW:H462	0.54	1.76	4	1
5:C:626:17F:O7	5:C:626:17F:O10	0.54	2.26	4	1
4:D:517:PCW:H231	5:D:525:17F:C22	0.54	2.33	4	1
4:D:518:PCW:H122	5:D:519:17F:H71	0.54	1.79	4	2
1:C:451:LYS:HB3	4:C:601:PCW:H271	0.54	1.77	5	2
4:D:506:PCW:H182	4:D:516:PCW:H481	0.54	1.80	5	1
4:D:509:PCW:H272	5:D:520:17F:H10A	0.54	1.77	6	1
4:D:508:PCW:C22	4:D:512:PCW:H172	0.54	2.32	8	1
4:B:201:PCW:H341	4:D:506:PCW:H231	0.54	1.80	9	1
4:D:504:PCW:H452	4:D:505:PCW:H132	0.54	1.80	10	2
4:C:617:PCW:C23	4:C:617:PCW:C27	0.54	2.78	10	1
4:C:621:PCW:H122	5:C:629:17F:H20	0.54	1.79	1	1
5:C:628:17F:O10	5:C:628:17F:O6	0.54	2.24	4	9
4:D:505:PCW:H472	4:D:518:PCW:C28	0.54	2.31	1	1
4:C:617:PCW:O31	4:C:617:PCW:C1	0.54	2.49	5	4
4:D:502:PCW:H362	4:D:502:PCW:C13	0.54	2.32	10	3
4:C:621:PCW:H283	5:C:629:17F:C1X	0.54	2.33	3	1
5:C:626:17F:O10	5:C:626:17F:O7	0.54	2.26	8	2
3:D:363:PRO:HD3	3:D:428:VAL:O	0.54	2.02	4	1
4:D:507:PCW:H41	5:D:523:17F:N1	0.54	2.18	5	1
4:D:512:PCW:C35	4:D:514:PCW:H121	0.54	2.33	6	1
4:A:401:PCW:C6	4:D:511:PCW:O31	0.54	2.55	8	2
4:D:509:PCW:O11	4:D:509:PCW:C6	0.54	2.56	9	1
2:B:82:PHE:HB2	2:B:89:SER:HB2	0.54	1.78	1	3
4:A:408:PCW:C41	4:B:203:PCW:H412	0.54	2.33	2	1
4:C:612:PCW:H322	4:C:618:PCW:H132	0.54	1.79	2	3
4:B:201:PCW:O2P	3:D:456:GLN:HB3	0.54	2.03	3	1
4:D:511:PCW:C37	4:D:511:PCW:H412	0.54	2.33	4	1
4:A:405:PCW:H63	4:A:405:PCW:H321	0.54	1.78	5	1
4:A:412:PCW:C48	4:D:517:PCW:H283	0.54	2.27	6	1
4:A:411:PCW:C8	4:C:617:PCW:H421	0.54	2.32	8	1
4:D:508:PCW:C19	4:D:509:PCW:H221	0.54	2.29	8	1
4:B:202:PCW:H41	5:D:524:17F:O5	0.54	2.03	9	1
5:C:629:17F:H78	4:D:514:PCW:H281	0.54	1.79	10	1
3:D:457:LYS:NZ	4:D:517:PCW:H122	0.54	2.18	1	1
4:C:602:PCW:H381	4:C:602:PCW:H142	0.54	1.80	2	1
4:C:606:PCW:C15	5:D:529:17F:H11A	0.54	2.33	2	2
4:C:613:PCW:O4P	4:C:613:PCW:H63	0.54	2.03	5	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:505:PCW:O31	4:D:505:PCW:C36	0.54	2.56	5	3
5:D:519:17F:H61	5:D:521:17F:H29	0.54	1.79	2	1
4:C:621:PCW:H262	4:D:528:PCW:H82	0.54	1.78	4	1
4:D:515:PCW:H11	5:D:525:17F:H31	0.54	1.79	4	1
4:B:201:PCW:O2	4:D:504:PCW:H171	0.54	2.02	6	1
4:C:616:PCW:C37	4:C:618:PCW:H141	0.54	2.33	7	1
4:C:621:PCW:H121	5:C:630:17F:O9	0.54	2.02	7	2
4:B:203:PCW:H141	4:B:204:PCW:H362	0.54	1.79	7	1
4:D:516:PCW:H40	4:D:527:PCW:H262	0.54	1.78	9	2
4:D:517:PCW:H222	4:D:517:PCW:H421	0.54	1.80	9	1
4:D:503:PCW:C17	4:D:511:PCW:H40	0.54	2.23	10	1
4:A:407:PCW:H162	4:A:412:PCW:C28	0.53	2.30	2	1
4:C:602:PCW:H39	4:C:602:PCW:C20	0.53	2.32	2	1
4:C:605:PCW:O31	4:C:613:PCW:C6	0.53	2.56	5	4
1:C:447:GLU:OE1	1:C:451:LYS:HE2	0.53	2.03	4	1
3:D:479:LYS:HA	4:D:517:PCW:C7	0.53	2.32	7	1
1:A:277:GLU:HB2	1:A:278:PRO:HD3	0.53	1.79	9	1
4:A:412:PCW:H82	4:C:624:PCW:O31	0.53	2.02	9	2
4:C:606:PCW:H161	5:D:529:17F:H30	0.53	1.79	9	1
4:C:607:PCW:H342	4:C:624:PCW:C42	0.53	2.28	10	1
4:D:501:PCW:H271	4:D:511:PCW:H441	0.53	1.80	10	1
4:A:403:PCW:O4P	4:A:403:PCW:H62	0.53	2.03	5	7
4:A:411:PCW:O3	4:A:411:PCW:O31	0.53	2.26	1	1
4:C:608:PCW:H262	5:C:627:17F:H30	0.53	1.80	8	5
4:C:611:PCW:H471	4:D:501:PCW:H251	0.53	1.79	1	1
4:C:618:PCW:H282	5:D:524:17F:C34	0.53	2.34	1	1
4:D:510:PCW:H211	4:D:510:PCW:H162	0.53	1.78	1	3
4:A:412:PCW:O1P	4:C:614:PCW:C4	0.53	2.55	2	2
4:C:607:PCW:H431	4:C:624:PCW:H472	0.53	1.79	2	1
3:D:426:LEU:C	4:D:502:PCW:H61	0.53	2.28	2	1
4:C:603:PCW:C27	4:D:526:PCW:H212	0.53	2.24	8	3
4:C:622:PCW:C24	4:D:501:PCW:H451	0.53	2.34	3	1
4:D:516:PCW:C23	5:D:519:17F:H54	0.53	2.31	3	1
4:A:405:PCW:C8	4:D:514:PCW:H371	0.53	2.31	4	1
4:A:411:PCW:H82	4:C:617:PCW:H40	0.53	1.79	5	1
4:C:606:PCW:H422	4:C:609:PCW:C3	0.53	2.28	5	1
4:C:608:PCW:H452	5:C:626:17F:C33	0.53	2.33	5	1
4:A:414:PCW:C39	4:C:617:PCW:H152	0.53	2.32	10	2
4:D:510:PCW:H371	5:D:524:17F:H8A	0.53	1.79	7	1
4:D:502:PCW:H19	4:D:505:PCW:C14	0.53	2.30	8	1
4:A:406:PCW:H52	4:B:204:PCW:H11	0.53	1.79	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:507:PCW:C14	4:D:513:PCW:H382	0.53	2.32	9	1
4:D:516:PCW:C45	5:D:529:17F:H54	0.53	2.31	9	1
4:C:612:PCW:H372	4:C:625:PCW:O11	0.53	2.03	10	1
4:D:510:PCW:C35	5:D:524:17F:H8	0.53	2.29	10	1
4:C:609:PCW:C27	5:D:523:17F:H54	0.53	2.34	2	3
4:D:517:PCW:O31	4:D:517:PCW:O3	0.53	2.26	1	7
4:C:609:PCW:O3	4:C:609:PCW:O31	0.53	2.26	7	6
4:C:615:PCW:O3	4:C:615:PCW:O31	0.53	2.25	8	5
4:D:508:PCW:O31	4:D:508:PCW:O3	0.53	2.27	4	8
4:D:509:PCW:H151	4:D:514:PCW:H142	0.53	1.79	2	1
4:C:616:PCW:P	4:C:616:PCW:C3	0.53	2.97	10	7
3:D:454:ILE:HD11	3:D:480:VAL:HG23	0.53	1.80	4	1
4:A:412:PCW:H63	4:C:624:PCW:H321	0.53	1.81	5	1
4:D:503:PCW:H12	4:D:511:PCW:H12	0.53	1.80	6	1
4:C:613:PCW:H471	4:C:619:PCW:C43	0.53	2.34	7	1
5:C:630:17F:H40	5:D:530:17F:H67	0.53	1.79	10	3
4:D:503:PCW:O31	4:D:503:PCW:C11	0.53	2.56	8	1
4:A:404:PCW:C36	4:B:202:PCW:H461	0.53	2.32	10	1
4:C:615:PCW:C31	4:C:615:PCW:O3	0.53	2.57	2	6
4:C:625:PCW:H211	4:D:528:PCW:H352	0.53	1.79	1	1
4:D:506:PCW:C28	4:D:515:PCW:H382	0.53	2.23	1	1
1:C:540:GLY:O	1:C:544:LEU:HG	0.53	2.04	2	2
4:C:602:PCW:C14	5:C:626:17F:H54	0.53	2.33	2	2
4:C:606:PCW:C3	5:D:529:17F:H1	0.53	2.33	3	1
4:C:625:PCW:C21	4:D:528:PCW:H372	0.53	2.33	3	1
4:B:202:PCW:O2P	4:B:202:PCW:H52	0.53	2.03	3	1
4:D:511:PCW:C22	4:D:511:PCW:C27	0.53	2.60	6	2
4:D:508:PCW:H352	4:D:512:PCW:H121	0.53	1.81	5	1
4:C:623:PCW:H281	5:D:525:17F:H50	0.53	1.80	6	1
4:B:203:PCW:H161	4:B:203:PCW:H451	0.53	1.81	7	1
4:D:507:PCW:C11	4:D:513:PCW:H152	0.53	2.33	7	1
4:D:513:PCW:H422	4:D:513:PCW:C38	0.53	2.32	7	1
4:B:201:PCW:C36	4:D:510:PCW:H381	0.53	2.33	8	1
4:D:513:PCW:H381	5:D:522:17F:C38	0.53	2.34	8	1
4:D:507:PCW:H231	4:D:513:PCW:C40	0.53	2.27	9	1
4:D:505:PCW:H421	4:D:505:PCW:H161	0.53	1.79	10	1
4:D:509:PCW:C18	4:D:514:PCW:H142	0.53	2.33	10	1
4:C:612:PCW:O3P	4:C:612:PCW:O31	0.53	2.25	9	8
4:D:509:PCW:H283	4:D:509:PCW:C24	0.53	2.29	1	1
5:D:520:17F:O10	5:D:520:17F:O7	0.53	2.26	9	5
4:C:614:PCW:O4P	4:C:614:PCW:H73	0.53	2.03	8	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:518:PCW:H162	5:D:519:17F:C1Z	0.53	2.33	8	2
4:A:402:PCW:H442	4:D:512:PCW:C13	0.53	2.32	3	1
4:C:605:PCW:C44	4:C:619:PCW:H451	0.53	2.30	3	1
5:C:630:17F:O7	5:C:630:17F:O10	0.53	2.26	7	5
4:D:502:PCW:P	4:D:502:PCW:C3	0.53	2.97	6	7
4:C:622:PCW:H131	4:C:622:PCW:H372	0.53	1.79	4	1
4:D:515:PCW:H251	5:D:525:17F:H47	0.53	1.80	7	1
4:C:607:PCW:H341	4:C:624:PCW:C37	0.53	2.31	8	1
4:C:606:PCW:H161	5:D:529:17F:C1X	0.53	2.34	9	1
4:C:606:PCW:H232	5:D:529:17F:H38	0.53	1.80	9	1
4:A:410:PCW:H451	4:C:617:PCW:H252	0.53	1.81	4	5
5:C:626:17F:C22	5:C:627:17F:H72	0.53	2.34	1	1
4:D:501:PCW:H431	5:D:525:17F:C27	0.53	2.34	1	1
5:D:530:17F:O7	5:D:530:17F:O10	0.53	2.26	9	6
4:A:401:PCW:H272	4:C:614:PCW:H271	0.53	1.81	4	1
4:A:415:PCW:H331	4:C:622:PCW:H122	0.53	1.80	4	1
4:A:408:PCW:H442	4:D:506:PCW:C44	0.53	2.31	7	1
4:A:414:PCW:H381	4:C:617:PCW:C15	0.53	2.31	7	1
4:D:518:PCW:C12	5:D:519:17F:C37	0.53	2.86	8	1
4:C:616:PCW:C38	4:C:618:PCW:H142	0.53	2.32	9	1
4:B:201:PCW:C47	4:D:527:PCW:H231	0.53	2.33	9	1
4:D:504:PCW:H31	5:D:524:17F:H4	0.53	1.78	10	2
4:A:411:PCW:H351	4:C:612:PCW:H132	0.53	1.80	10	1
4:A:415:PCW:H242	4:D:528:PCW:H262	0.53	1.79	1	1
4:A:415:PCW:C47	5:D:521:17F:H51	0.53	2.30	1	1
4:C:605:PCW:C31	4:C:613:PCW:C5	0.53	2.80	1	1
4:B:202:PCW:C7	5:D:524:17F:O4	0.53	2.57	1	1
4:C:614:PCW:O4P	4:C:614:PCW:C7	0.53	2.56	8	7
4:C:621:PCW:C37	5:C:629:17F:H63	0.53	2.32	10	2
4:D:510:PCW:C16	4:D:510:PCW:C21	0.53	2.86	3	1
5:D:519:17F:O2	5:D:519:17F:O9	0.53	2.27	6	2
1:A:310:ARG:O	1:A:314:ASP:HB2	0.53	2.04	10	3
3:D:405:HIS:CE1	3:D:408:LYS:HB3	0.53	2.39	4	2
4:A:405:PCW:H172	4:D:512:PCW:C39	0.53	2.34	5	1
4:C:604:PCW:H211	4:C:604:PCW:C16	0.53	2.34	5	1
4:C:608:PCW:O1P	4:C:624:PCW:C24	0.53	2.57	7	1
4:C:606:PCW:H352	5:D:529:17F:O7	0.53	2.04	8	1
4:B:203:PCW:H39	4:B:204:PCW:C7	0.53	2.33	9	1
5:C:626:17F:H36	5:C:627:17F:H73	0.53	1.80	10	1
4:A:402:PCW:H42	4:D:514:PCW:O2P	0.53	2.04	2	2
4:D:513:PCW:H51	4:D:513:PCW:O3P	0.53	2.04	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:526:PCW:O11	4:D:526:PCW:O2	0.53	2.27	2	2
4:C:603:PCW:H73	4:D:527:PCW:H31	0.53	1.80	3	2
5:C:630:17F:H5	5:C:630:17F:O1	0.53	2.04	5	2
4:C:606:PCW:O3P	4:C:606:PCW:O31	0.53	2.27	5	5
4:D:504:PCW:H262	5:D:524:17F:H20A	0.53	1.80	4	1
4:C:622:PCW:H131	4:C:622:PCW:H371	0.53	1.78	5	1
1:A:250:VAL:HG21	4:A:408:PCW:H281	0.53	1.79	7	1
3:D:361:PHE:HB3	3:D:427:GLN:HA	0.53	1.80	7	1
4:D:503:PCW:H461	4:D:507:PCW:H481	0.53	1.79	7	1
4:A:410:PCW:H151	4:C:603:PCW:H272	0.53	1.81	8	1
4:A:401:PCW:C31	4:A:401:PCW:O3	0.53	2.57	6	7
4:C:614:PCW:H51	4:C:623:PCW:P	0.53	2.44	1	1
3:D:458:PHE:HB3	4:D:517:PCW:H12	0.53	1.81	1	1
4:D:517:PCW:H483	5:D:525:17F:H10A	0.53	1.80	1	1
1:A:243:MET:HG3	1:A:247:LEU:HD12	0.53	1.79	5	3
4:A:414:PCW:O31	4:C:617:PCW:C5	0.53	2.54	10	2
4:C:620:PCW:H372	4:C:620:PCW:C41	0.53	2.29	8	2
4:D:505:PCW:C31	4:D:505:PCW:C35	0.53	2.87	8	3
4:C:603:PCW:H441	4:C:603:PCW:C21	0.53	2.27	7	2
4:C:615:PCW:C21	5:C:631:17F:H38	0.53	2.32	3	1
4:C:616:PCW:C6	4:D:526:PCW:O11	0.53	2.57	3	1
5:D:529:17F:C25	5:D:530:17F:H73	0.53	2.33	9	3
4:A:408:PCW:H342	4:D:514:PCW:C45	0.53	2.34	4	1
4:A:415:PCW:H322	4:C:622:PCW:C31	0.53	2.34	7	2
4:D:504:PCW:C35	4:D:516:PCW:H141	0.53	2.29	6	1
4:A:404:PCW:H61	5:D:524:17F:P1	0.53	2.44	7	1
4:A:415:PCW:H471	5:D:521:17F:H55	0.53	1.80	7	1
4:D:511:PCW:H182	4:D:511:PCW:H342	0.53	1.79	8	1
2:B:59:ALA:HB3	2:B:62:GLU:HB2	0.53	1.81	10	1
4:D:506:PCW:H73	5:D:520:17F:O2	0.53	2.04	10	1
4:A:402:PCW:H411	4:D:512:PCW:H381	0.53	1.80	7	3
4:A:405:PCW:H171	4:A:405:PCW:H221	0.53	1.79	1	1
4:A:406:PCW:P	4:A:406:PCW:C3	0.53	2.97	1	6
4:C:620:PCW:O4P	4:C:620:PCW:C7	0.53	2.56	1	4
5:C:630:17F:O8	5:C:630:17F:O9	0.53	2.26	1	2
4:D:502:PCW:H281	4:D:518:PCW:H211	0.53	1.80	1	1
4:A:404:PCW:C28	4:A:411:PCW:H221	0.53	2.33	3	1
4:C:607:PCW:H432	4:C:624:PCW:H481	0.53	1.81	7	4
4:C:621:PCW:H283	5:C:629:17F:H30	0.53	1.80	3	3
4:B:203:PCW:H283	4:D:506:PCW:H472	0.53	1.80	4	1
4:C:609:PCW:C11	4:C:609:PCW:O31	0.53	2.57	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:604:PCW:H281	4:C:607:PCW:H471	0.53	1.81	7	1
4:D:502:PCW:H171	4:D:505:PCW:C11	0.53	2.34	7	2
4:C:613:PCW:H261	5:D:521:17F:H69	0.53	1.79	10	1
4:D:504:PCW:O31	4:D:504:PCW:H12	0.52	2.03	7	2
4:D:506:PCW:H151	4:D:516:PCW:H382	0.52	1.80	1	1
4:D:527:PCW:C46	4:D:528:PCW:H361	0.52	2.28	1	1
4:D:513:PCW:C42	4:D:517:PCW:H271	0.52	2.31	2	1
4:C:610:PCW:H62	5:C:629:17F:O6	0.52	2.04	3	1
4:A:413:PCW:C38	4:D:526:PCW:H161	0.52	2.34	6	2
4:C:601:PCW:C48	4:C:601:PCW:H121	0.52	2.34	6	1
4:C:610:PCW:H52	4:C:610:PCW:O1P	0.52	2.03	6	1
4:D:508:PCW:C5	5:D:520:17F:H9A	0.52	2.35	6	1
4:D:513:PCW:H32	4:D:513:PCW:C4	0.52	2.34	6	1
4:D:528:PCW:C17	5:D:530:17F:H32	0.52	2.33	6	2
4:D:513:PCW:H121	5:D:523:17F:C5	0.52	2.34	8	1
4:A:411:PCW:C39	4:C:612:PCW:H451	0.52	2.33	9	1
1:C:433:GLU:O	1:C:437:LEU:HG	0.52	2.03	10	1
4:C:603:PCW:H242	4:D:526:PCW:C37	0.52	2.34	1	1
4:C:622:PCW:C36	4:C:622:PCW:C32	0.52	2.70	1	6
4:C:611:PCW:H2	4:C:619:PCW:C6	0.52	2.32	10	6
4:C:625:PCW:C38	4:C:625:PCW:H421	0.52	2.34	2	1
3:D:468:CYS:CB	3:D:484:CYS:HB2	0.52	2.34	2	1
4:D:504:PCW:H381	4:D:516:PCW:H82	0.52	1.80	2	1
4:D:509:PCW:C41	4:D:509:PCW:H372	0.52	2.33	7	4
4:B:202:PCW:C25	4:D:504:PCW:H252	0.52	2.34	4	1
4:D:506:PCW:H61	5:D:525:17F:O1	0.52	2.04	4	1
4:D:508:PCW:H172	4:D:512:PCW:C15	0.52	2.34	9	2
4:D:507:PCW:C48	5:D:522:17F:H48	0.52	2.34	5	1
4:C:605:PCW:H482	4:C:619:PCW:H471	0.52	1.80	8	1
4:A:407:PCW:C26	4:A:412:PCW:H271	0.52	2.34	9	1
4:D:502:PCW:H141	4:D:505:PCW:H322	0.52	1.80	9	1
4:D:509:PCW:O11	4:D:509:PCW:N	0.52	2.43	9	1
4:B:201:PCW:C5	4:D:504:PCW:O11	0.52	2.49	10	1
4:C:602:PCW:C7	5:D:523:17F:O10	0.52	2.58	9	4
4:C:616:PCW:C44	4:B:201:PCW:H472	0.52	2.35	2	1
4:B:203:PCW:C22	4:D:506:PCW:H471	0.52	2.34	2	2
4:D:518:PCW:H341	5:D:519:17F:C1Y	0.52	2.34	2	1
4:C:605:PCW:O2P	4:C:613:PCW:H63	0.52	2.04	3	1
4:C:601:PCW:H451	4:C:601:PCW:H121	0.52	1.79	4	1
4:C:616:PCW:H441	4:C:625:PCW:H232	0.52	1.81	4	2
4:D:501:PCW:H411	4:D:515:PCW:H162	0.52	1.80	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:601:PCW:C1	4:D:513:PCW:H82	0.52	2.32	6	1
4:D:509:PCW:H61	4:D:514:PCW:H32	0.52	1.82	6	1
5:D:522:17F:C2X	5:D:525:17F:H12A	0.52	2.33	8	1
5:D:523:17F:H30	5:D:523:17F:H39	0.52	1.81	8	1
4:C:614:PCW:H42	4:C:623:PCW:H42	0.52	1.81	10	1
4:A:403:PCW:H212	4:D:513:PCW:H352	0.52	1.81	1	1
4:C:609:PCW:H232	4:C:615:PCW:C38	0.52	2.29	1	1
4:C:617:PCW:H2	4:C:617:PCW:H41	0.52	1.80	1	1
4:C:622:PCW:H441	4:C:623:PCW:C26	0.52	2.34	3	2
1:A:273:ARG:HA	1:A:276:VAL:HG12	0.52	1.79	8	6
4:C:620:PCW:H132	5:C:631:17F:H18A	0.52	1.80	3	1
4:A:407:PCW:H462	4:A:412:PCW:H221	0.52	1.81	4	1
4:C:610:PCW:H162	5:C:629:17F:C34	0.52	2.34	4	2
4:C:615:PCW:H281	4:D:508:PCW:H482	0.52	1.81	4	1
4:C:620:PCW:C7	4:C:620:PCW:O4P	0.52	2.57	4	1
4:C:621:PCW:O11	4:C:621:PCW:O2	0.52	2.27	6	5
2:B:49:GLU:HG2	4:B:203:PCW:H63	0.52	1.80	4	1
4:C:608:PCW:C20	5:C:627:17F:H50	0.52	2.34	9	2
4:C:621:PCW:H262	4:D:528:PCW:H61	0.52	1.80	10	2
1:A:348:GLU:HB3	1:A:352:LYS:HE2	0.52	1.82	6	1
1:A:348:GLU:O	1:A:352:LYS:HG3	0.52	2.05	9	3
4:C:604:PCW:H281	4:C:607:PCW:H462	0.52	1.81	6	1
4:C:609:PCW:H261	4:C:615:PCW:H411	0.52	1.81	8	3
4:B:202:PCW:H51	5:D:524:17F:O5	0.52	2.04	6	1
4:D:508:PCW:C5	5:D:520:17F:O8	0.52	2.56	6	1
4:C:606:PCW:O11	4:C:606:PCW:C6	0.52	2.55	7	2
5:D:530:17F:H56	5:D:530:17F:H10A	0.52	1.80	7	1
4:D:509:PCW:C40	5:D:520:17F:H11A	0.52	2.35	9	1
4:A:403:PCW:H42	4:A:403:PCW:O11	0.52	2.04	1	1
4:A:415:PCW:H472	5:D:521:17F:H47	0.52	1.80	1	1
4:C:602:PCW:C34	5:D:523:17F:H61	0.52	2.34	1	1
4:A:405:PCW:H82	4:D:514:PCW:C36	0.52	2.34	2	3
3:D:486:ASP:OD2	5:D:524:17F:N1	0.52	2.42	2	1
4:D:502:PCW:O11	4:D:502:PCW:O2	0.52	2.28	8	4
4:D:508:PCW:H162	4:D:509:PCW:H212	0.52	1.81	2	1
4:C:620:PCW:O31	4:C:620:PCW:H41	0.52	2.04	3	1
4:C:610:PCW:H171	5:C:629:17F:H61	0.52	1.80	5	2
4:D:511:PCW:O11	4:D:511:PCW:C6	0.52	2.58	6	2
4:D:507:PCW:H40	5:D:525:17F:N1	0.52	2.19	6	1
4:C:614:PCW:H52	4:C:623:PCW:O31	0.52	2.04	8	1
4:B:201:PCW:H372	4:D:506:PCW:H242	0.52	1.81	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:404:PCW:H412	4:B:202:PCW:H442	0.52	1.81	9	1
4:A:406:PCW:H32	4:B:202:PCW:C15	0.52	2.34	9	1
3:D:486:ASP:OD2	4:D:501:PCW:H62	0.52	2.05	9	1
4:C:607:PCW:H362	4:C:624:PCW:H422	0.52	1.81	10	1
4:D:508:PCW:C31	4:D:508:PCW:O3	0.52	2.58	1	1
4:B:201:PCW:H331	4:D:510:PCW:H39	0.52	1.82	3	1
4:B:204:PCW:C31	4:B:204:PCW:H52	0.52	2.34	4	3
4:D:501:PCW:H39	4:D:515:PCW:C44	0.52	2.34	4	1
4:A:406:PCW:C16	4:B:202:PCW:H232	0.52	2.34	6	1
4:B:202:PCW:H472	5:D:524:17F:H32	0.52	1.81	6	1
4:D:503:PCW:H452	4:D:511:PCW:C20	0.52	2.33	8	1
4:C:609:PCW:C3	4:C:615:PCW:H61	0.52	2.35	9	1
4:D:510:PCW:H451	5:D:524:17F:H30	0.52	1.80	10	1
4:C:613:PCW:H32	4:C:619:PCW:C11	0.52	2.35	1	1
4:C:621:PCW:C19	5:C:629:17F:C17	0.52	2.88	3	3
4:C:605:PCW:O1P	4:C:605:PCW:H52	0.52	2.05	8	3
4:C:621:PCW:H231	4:D:528:PCW:H82	0.52	1.82	2	2
1:A:214:PHE:HZ	4:A:404:PCW:H142	0.52	1.65	3	1
4:C:601:PCW:O31	4:C:601:PCW:O3	0.52	2.27	3	1
4:C:611:PCW:C39	4:C:622:PCW:H462	0.52	2.18	7	2
4:A:401:PCW:H461	4:C:611:PCW:H251	0.52	1.82	4	1
4:C:620:PCW:H11	4:C:620:PCW:H73	0.52	1.80	4	1
1:C:503:MET:HA	1:C:506:ARG:HD2	0.52	1.80	5	3
4:B:201:PCW:C15	4:D:506:PCW:H442	0.52	2.35	5	1
5:D:529:17F:H43	5:D:530:17F:H35	0.52	1.81	5	1
4:A:415:PCW:H332	4:C:622:PCW:H122	0.52	1.80	6	3
2:B:17:SER:HB2	6:B:205:GNP:O1A	0.52	2.03	6	1
4:D:517:PCW:H371	5:D:525:17F:H58	0.52	1.80	7	1
4:C:623:PCW:O31	4:C:623:PCW:O3P	0.52	2.28	9	2
4:D:515:PCW:H483	4:D:516:PCW:H221	0.52	1.80	8	1
4:A:401:PCW:H62	4:D:511:PCW:H2	0.52	1.82	9	1
4:D:502:PCW:H212	4:D:502:PCW:H412	0.52	1.81	9	1
4:C:603:PCW:O4P	5:D:530:17F:O1	0.52	2.28	3	4
4:C:618:PCW:C42	4:C:625:PCW:H261	0.52	2.33	1	1
4:A:405:PCW:H372	4:A:405:PCW:C41	0.52	2.34	2	2
4:A:415:PCW:H242	4:D:528:PCW:H232	0.52	1.79	2	2
4:B:203:PCW:O31	4:B:203:PCW:C35	0.52	2.48	3	6
4:D:501:PCW:H282	5:D:521:17F:H68	0.52	1.80	2	1
5:D:520:17F:H4	5:D:520:17F:O10	0.52	2.05	3	2
4:C:603:PCW:C28	4:D:526:PCW:H232	0.52	2.35	3	1
4:C:606:PCW:H211	5:C:630:17F:C30	0.52	2.34	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:624:PCW:O2	4:C:624:PCW:O2P	0.52	2.27	7	2
4:D:508:PCW:C14	4:D:512:PCW:H321	0.52	2.33	4	1
4:B:201:PCW:H431	4:D:510:PCW:C44	0.52	2.35	5	1
4:D:517:PCW:H372	5:D:520:17F:H30	0.52	1.82	6	1
4:C:618:PCW:C13	4:C:625:PCW:H142	0.52	2.34	7	2
4:D:509:PCW:O31	4:D:509:PCW:C1	0.52	2.51	9	3
4:D:502:PCW:H481	4:D:505:PCW:C28	0.52	2.35	8	1
4:D:509:PCW:C3	5:D:520:17F:H4	0.52	2.34	8	3
4:A:403:PCW:H283	5:D:523:17F:C1Z	0.52	2.35	10	1
4:C:604:PCW:C38	5:D:529:17F:H40	0.52	2.35	10	1
4:B:202:PCW:N	5:D:524:17F:O5	0.52	2.43	10	1
1:A:319:HIS:O	1:A:322:PRO:HD2	0.52	2.05	1	2
4:A:405:PCW:O31	4:A:405:PCW:O3	0.52	2.27	5	5
4:A:407:PCW:H182	4:A:412:PCW:H283	0.52	1.82	7	2
4:D:514:PCW:O31	4:D:514:PCW:C1	0.52	2.57	2	1
4:D:516:PCW:H19	4:D:526:PCW:H462	0.52	1.82	2	1
5:D:519:17F:H61	5:D:521:17F:C1X	0.52	2.34	2	1
4:A:403:PCW:H11	4:A:403:PCW:O31	0.52	2.05	3	1
4:C:603:PCW:P	5:D:530:17F:O1	0.52	2.67	3	1
4:C:604:PCW:H381	5:D:529:17F:C22	0.52	2.35	3	1
4:C:618:PCW:C39	4:C:625:PCW:H161	0.52	2.35	4	1
4:D:515:PCW:H152	5:D:525:17F:H62	0.52	1.80	4	1
4:A:403:PCW:H481	4:C:607:PCW:H242	0.52	1.80	5	1
5:D:525:17F:H78	5:D:525:17F:H52	0.52	1.80	5	1
4:A:403:PCW:C34	4:A:407:PCW:H322	0.52	2.34	10	2
4:C:604:PCW:H231	4:D:517:PCW:C47	0.52	2.34	6	1
4:C:607:PCW:C34	4:C:624:PCW:H372	0.52	2.30	8	1
4:D:517:PCW:H432	4:D:517:PCW:H211	0.52	1.79	8	1
4:C:604:PCW:H412	4:C:606:PCW:C24	0.52	2.31	9	1
5:D:522:17F:H8A	5:D:525:17F:O7	0.52	2.05	9	1
1:A:341:ASN:HD21	1:C:432:LYS:HB3	0.52	1.65	10	1
4:A:410:PCW:O31	4:A:410:PCW:O3	0.52	2.28	4	3
4:C:616:PCW:O31	4:C:616:PCW:O3	0.52	2.28	9	8
4:D:507:PCW:C46	5:D:522:17F:H60	0.52	2.35	1	2
4:B:203:PCW:H461	4:B:204:PCW:C42	0.52	2.31	2	1
4:D:516:PCW:H171	4:D:526:PCW:H483	0.52	1.80	2	1
4:D:502:PCW:H441	4:D:502:PCW:C23	0.52	2.22	7	2
4:D:511:PCW:H342	4:D:511:PCW:C18	0.52	2.32	9	2
4:D:507:PCW:H63	5:D:523:17F:C3	0.52	2.35	4	1
4:C:615:PCW:H221	4:D:512:PCW:H272	0.52	1.81	5	2
4:D:516:PCW:H40	4:D:527:PCW:C28	0.52	2.35	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:410:PCW:C16	4:A:413:PCW:H331	0.52	2.23	7	2
4:A:402:PCW:C44	4:D:508:PCW:H231	0.52	2.26	7	1
4:C:604:PCW:O11	4:C:604:PCW:C4	0.52	2.58	9	1
4:D:502:PCW:C5	4:D:502:PCW:O11	0.52	2.58	9	1
4:A:407:PCW:H181	4:A:412:PCW:H261	0.51	1.82	2	1
3:D:401:LEU:HD13	3:D:425:GLU:HB2	0.51	1.82	2	1
5:D:529:17F:H42	5:D:530:17F:H70	0.51	1.82	5	2
5:A:409:17F:C42	4:C:619:PCW:H422	0.51	2.35	3	1
4:D:511:PCW:C17	5:D:522:17F:O10	0.51	2.58	10	2
4:C:603:PCW:H172	4:C:603:PCW:C21	0.51	2.35	5	2
4:D:509:PCW:H19	5:D:520:17F:H19	0.51	1.82	4	1
5:D:521:17F:C31	5:D:521:17F:C35	0.51	2.78	6	1
4:A:402:PCW:H181	4:A:405:PCW:H231	0.51	1.81	8	1
4:C:602:PCW:H483	5:C:626:17F:C36	0.51	2.34	8	1
4:C:615:PCW:H172	4:C:615:PCW:H132	0.51	1.80	8	1
4:D:507:PCW:H2	5:D:523:17F:O7	0.51	2.05	9	1
4:A:401:PCW:H442	4:C:614:PCW:C26	0.51	2.33	5	4
4:A:415:PCW:H121	4:C:603:PCW:H331	0.51	1.81	1	1
4:D:509:PCW:C42	5:D:520:17F:H32	0.51	2.35	1	1
4:A:405:PCW:C8	4:D:514:PCW:H351	0.51	2.34	2	1
4:A:407:PCW:H39	5:D:522:17F:H69	0.51	1.80	2	1
4:D:501:PCW:O1P	4:D:501:PCW:H52	0.51	2.04	2	1
4:D:504:PCW:H152	4:D:510:PCW:C39	0.51	2.27	2	1
4:D:507:PCW:H481	5:D:522:17F:C27	0.51	2.34	2	2
4:A:410:PCW:H442	4:C:617:PCW:H211	0.51	1.80	5	2
4:C:618:PCW:H351	4:C:625:PCW:C36	0.51	2.36	3	1
4:C:608:PCW:H171	5:C:627:17F:H18A	0.51	1.82	6	2
4:C:609:PCW:C2	4:C:615:PCW:H61	0.51	2.33	4	1
4:D:503:PCW:H212	4:D:503:PCW:H171	0.51	1.82	4	3
4:D:505:PCW:H441	4:D:518:PCW:H261	0.51	1.82	4	1
4:D:510:PCW:H31	5:D:524:17F:H75	0.51	1.81	5	1
4:A:403:PCW:H241	4:D:513:PCW:C12	0.51	2.35	6	2
4:B:201:PCW:H382	4:B:201:PCW:H422	0.51	1.80	6	1
4:A:401:PCW:O2	4:D:511:PCW:C23	0.51	2.58	7	1
4:C:603:PCW:H271	4:D:526:PCW:C18	0.51	2.34	10	2
4:C:615:PCW:H451	5:D:523:17F:H54	0.51	1.80	7	1
4:D:502:PCW:H232	4:D:502:PCW:C44	0.51	2.23	7	1
4:C:602:PCW:C48	5:C:626:17F:H65	0.51	2.35	8	1
4:D:511:PCW:C6	5:D:522:17F:H6	0.51	2.28	8	1
4:D:511:PCW:H132	4:D:511:PCW:C32	0.51	2.35	10	2
5:D:520:17F:C24	5:D:529:17F:H55	0.51	2.30	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:C:626:17F:C8	5:C:627:17F:H33	0.51	2.30	10	1
4:D:501:PCW:H271	4:D:511:PCW:C44	0.51	2.35	10	1
4:A:404:PCW:H372	4:D:510:PCW:C18	0.51	2.31	1	1
4:A:411:PCW:C37	4:C:612:PCW:H182	0.51	2.36	1	1
4:C:621:PCW:H151	5:C:630:17F:H4A	0.51	1.82	4	2
4:D:508:PCW:H61	4:D:517:PCW:H321	0.51	1.81	3	1
4:D:510:PCW:C20	5:D:524:17F:H19A	0.51	2.36	5	2
4:C:608:PCW:H62	4:C:624:PCW:H20	0.51	1.82	4	1
4:C:609:PCW:H281	5:D:523:17F:H49	0.51	1.82	5	1
4:D:505:PCW:H461	4:D:518:PCW:H261	0.51	1.82	6	1
4:D:507:PCW:O1P	5:D:523:17F:N1	0.51	2.40	7	2
4:C:621:PCW:C19	5:C:629:17F:H5	0.51	2.32	7	1
4:C:609:PCW:H281	5:D:523:17F:C30	0.51	2.34	10	1
4:D:502:PCW:H283	4:D:518:PCW:H241	0.51	1.83	10	1
4:D:504:PCW:H40	4:D:505:PCW:C7	0.51	2.36	10	1
4:A:402:PCW:H331	4:D:514:PCW:O2	0.51	2.05	6	2
5:C:630:17F:H9	5:C:630:17F:C19	0.51	2.34	9	3
4:B:203:PCW:H422	4:B:204:PCW:H382	0.51	1.83	2	1
4:D:507:PCW:C4	5:D:523:17F:HN1A	0.51	2.18	5	2
4:C:615:PCW:H471	4:D:512:PCW:H222	0.51	1.83	3	2
4:C:616:PCW:C48	4:B:203:PCW:H271	0.51	2.35	3	1
4:B:201:PCW:C26	4:D:528:PCW:H441	0.51	2.36	3	1
4:C:605:PCW:C48	4:C:613:PCW:H162	0.51	2.36	4	2
4:C:611:PCW:H82	4:C:623:PCW:H141	0.51	1.82	4	1
5:C:626:17F:C21	5:C:627:17F:H75	0.51	2.36	4	1
4:B:201:PCW:H11	4:D:504:PCW:C13	0.51	2.36	5	1
4:A:406:PCW:H212	4:B:204:PCW:H411	0.51	1.83	8	1
4:C:609:PCW:H232	4:C:615:PCW:H361	0.51	1.82	8	1
4:B:201:PCW:C12	4:D:506:PCW:H322	0.51	2.35	8	1
4:C:621:PCW:H20	4:D:528:PCW:C8	0.51	2.31	9	2
4:D:506:PCW:C20	4:D:516:PCW:H331	0.51	2.34	9	1
4:D:515:PCW:H482	4:D:515:PCW:H172	0.51	1.80	9	1
4:C:618:PCW:O2	4:C:625:PCW:H121	0.51	2.05	1	1
4:D:503:PCW:O2P	4:D:511:PCW:H11	0.51	2.05	1	2
5:D:530:17F:H56	5:D:530:17F:C11	0.51	2.35	2	3
4:D:509:PCW:P	4:D:509:PCW:C3	0.51	2.98	10	3
4:A:406:PCW:H41	4:B:204:PCW:H11	0.51	1.82	3	1
4:A:411:PCW:C34	4:C:612:PCW:H132	0.51	2.17	3	1
4:A:415:PCW:C28	4:D:515:PCW:H20	0.51	2.34	4	1
4:D:508:PCW:H241	4:D:512:PCW:C43	0.51	2.36	5	1
4:A:403:PCW:C42	4:D:513:PCW:H39	0.51	2.35	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:203:PCW:C33	4:D:506:PCW:H362	0.51	2.36	6	1
4:D:504:PCW:H40	5:D:519:17F:C21	0.51	2.35	8	1
4:A:410:PCW:C21	4:C:617:PCW:H472	0.51	2.27	9	1
4:A:401:PCW:C36	4:D:511:PCW:H452	0.51	2.35	10	1
1:C:546:GLU:O	1:C:550:LYS:HD2	0.51	2.05	10	1
4:A:414:PCW:C31	4:C:617:PCW:H52	0.51	2.35	8	3
4:C:616:PCW:O11	4:D:526:PCW:H151	0.51	2.06	1	2
5:A:409:17F:H56	4:D:503:PCW:C16	0.51	2.25	2	1
4:C:602:PCW:C15	5:C:626:17F:H54	0.51	2.36	5	2
4:D:504:PCW:C12	4:D:510:PCW:H372	0.51	2.34	2	1
4:D:505:PCW:H51	4:D:510:PCW:H42	0.51	1.82	2	1
4:D:518:PCW:H422	5:D:519:17F:H69	0.51	1.82	2	1
1:A:301:LEU:HB3	1:C:473:LYS:HE3	0.51	1.81	3	1
4:C:605:PCW:C31	4:C:613:PCW:H82	0.51	2.36	3	1
4:D:518:PCW:H232	5:D:519:17F:C32	0.51	2.25	5	2
4:A:404:PCW:C7	5:D:524:17F:O4	0.51	2.58	4	1
4:B:202:PCW:H472	5:D:524:17F:H20	0.51	1.81	4	1
4:D:501:PCW:C48	5:D:525:17F:H51	0.51	2.34	4	1
4:D:504:PCW:H442	4:D:505:PCW:O4P	0.51	2.04	5	1
4:A:406:PCW:O2P	4:A:406:PCW:C3	0.51	2.59	6	1
4:B:201:PCW:H381	5:D:524:17F:H47	0.51	1.80	6	1
4:D:509:PCW:H20	5:D:520:17F:H31	0.51	1.82	6	1
4:D:517:PCW:C7	5:D:520:17F:O2	0.51	2.59	6	1
4:D:517:PCW:H421	4:D:517:PCW:C18	0.51	2.36	6	1
5:A:409:17F:H68	4:D:501:PCW:H241	0.51	1.82	7	1
3:D:480:VAL:O	4:D:509:PCW:H82	0.51	2.06	8	1
4:D:511:PCW:H182	4:D:511:PCW:H341	0.51	1.83	8	1
4:A:413:PCW:H31	4:C:617:PCW:H411	0.51	1.81	9	1
4:A:403:PCW:H361	4:A:407:PCW:H332	0.51	1.83	10	1
4:A:410:PCW:H172	4:A:413:PCW:H381	0.51	1.83	10	1
4:C:621:PCW:C34	5:C:630:17F:H20A	0.51	2.36	10	1
4:D:510:PCW:H442	5:D:524:17F:H35	0.51	1.81	10	1
4:A:415:PCW:H141	4:C:603:PCW:H351	0.51	1.81	1	1
3:D:460:LEU:HD23	3:D:460:LEU:H	0.51	1.66	1	1
5:D:524:17F:O7	5:D:524:17F:O10	0.51	2.28	1	4
4:A:413:PCW:O3	4:A:413:PCW:O31	0.51	2.28	7	9
4:D:510:PCW:H2	4:D:510:PCW:O11	0.51	2.06	3	3
2:B:116:ASN:ND2	6:B:205:GNP:N7	0.51	2.59	4	1
5:D:530:17F:H10A	5:D:530:17F:H60	0.51	1.82	4	2
4:D:517:PCW:C35	5:D:520:17F:H11A	0.51	2.33	6	1
4:D:516:PCW:C19	5:D:519:17F:H46	0.51	2.36	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:518:PCW:C12	5:D:519:17F:H67	0.51	2.34	8	1
4:D:509:PCW:H412	5:D:520:17F:C10	0.51	2.36	9	1
4:A:404:PCW:H62	5:D:524:17F:O2	0.51	2.06	10	1
4:C:614:PCW:C5	4:C:623:PCW:O31	0.51	2.59	1	2
4:D:516:PCW:H19	4:D:526:PCW:C46	0.51	2.35	2	1
4:B:201:PCW:H231	4:B:203:PCW:H272	0.51	1.82	4	1
4:D:506:PCW:H181	4:D:506:PCW:C22	0.51	2.31	7	2
4:D:513:PCW:H141	5:D:523:17F:O9	0.51	2.05	6	1
1:A:275:LYS:HG2	1:C:499:LEU:HD21	0.51	1.83	7	1
4:A:412:PCW:H322	4:C:623:PCW:C34	0.51	2.35	7	2
4:D:509:PCW:H2	5:D:520:17F:H4A	0.51	1.80	10	2
4:C:616:PCW:H40	4:C:618:PCW:H162	0.51	1.81	10	1
4:A:404:PCW:O1P	4:A:404:PCW:C31	0.51	2.59	2	5
4:C:609:PCW:O31	4:C:609:PCW:C11	0.51	2.58	7	4
1:C:478:ARG:O	1:C:482:GLN:HB2	0.51	2.06	10	3
3:D:426:LEU:O	4:D:502:PCW:H61	0.51	2.05	2	1
4:A:404:PCW:C22	4:A:411:PCW:H262	0.51	2.28	4	2
4:A:406:PCW:C48	4:B:204:PCW:H232	0.51	2.32	3	1
5:A:409:17F:H74	4:C:605:PCW:C28	0.51	2.35	3	1
4:C:608:PCW:H171	5:C:627:17F:C18	0.51	2.35	6	2
4:C:611:PCW:O31	4:C:611:PCW:O3	0.51	2.29	9	4
3:D:409:LYS:HE2	4:D:503:PCW:C4	0.51	2.36	3	1
4:A:413:PCW:H11	4:C:617:PCW:C41	0.51	2.12	5	2
4:C:604:PCW:H432	4:C:606:PCW:H181	0.51	1.82	6	2
4:C:611:PCW:H131	4:C:619:PCW:H171	0.51	1.82	5	1
5:C:626:17F:C41	5:D:523:17F:H53	0.51	2.36	5	1
4:D:504:PCW:H161	4:D:510:PCW:H39	0.51	1.81	6	1
4:D:511:PCW:H11	4:D:511:PCW:O31	0.51	2.06	6	1
4:A:406:PCW:H351	4:B:204:PCW:C16	0.51	2.35	7	1
4:A:411:PCW:H341	4:C:612:PCW:H131	0.51	1.79	7	1
4:C:614:PCW:H442	4:C:619:PCW:H19	0.51	1.82	7	2
4:C:613:PCW:C14	4:C:619:PCW:H39	0.51	2.34	8	1
4:D:516:PCW:H261	4:D:526:PCW:C46	0.51	2.28	9	1
4:B:201:PCW:C22	4:D:506:PCW:H452	0.51	2.36	10	1
4:C:604:PCW:H283	5:D:520:17F:H53	0.51	1.83	1	1
4:C:625:PCW:H241	4:D:527:PCW:C45	0.51	2.26	4	2
4:D:527:PCW:H442	4:D:528:PCW:C34	0.51	2.25	1	2
4:C:612:PCW:H51	4:C:618:PCW:O11	0.51	2.06	2	1
5:C:630:17F:H19A	5:C:630:17F:C9	0.51	2.36	2	2
5:D:520:17F:H55	5:D:525:17F:C39	0.51	2.36	2	1
4:A:414:PCW:C36	4:C:617:PCW:H151	0.51	2.36	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:604:PCW:H73	4:C:604:PCW:C11	0.51	2.35	3	1
4:D:516:PCW:H231	5:D:519:17F:C30	0.51	2.33	3	1
4:A:413:PCW:C36	4:C:617:PCW:H431	0.51	2.35	4	1
4:C:621:PCW:C28	5:C:629:17F:H30	0.51	2.36	6	3
4:D:516:PCW:C11	4:D:516:PCW:O31	0.51	2.59	4	1
4:D:517:PCW:H442	5:D:525:17F:H64	0.51	1.82	4	1
4:C:613:PCW:H272	5:D:521:17F:H50	0.51	1.82	6	2
4:D:502:PCW:H422	4:D:502:PCW:C18	0.51	2.36	5	1
4:D:513:PCW:H382	4:D:513:PCW:C42	0.51	2.34	7	1
4:A:410:PCW:H442	4:C:617:PCW:H212	0.51	1.82	8	2
3:D:444:LYS:HG3	3:D:464:ARG:HD3	0.51	1.81	8	1
4:D:504:PCW:H19	4:D:506:PCW:H481	0.51	1.83	8	1
4:D:516:PCW:H482	4:D:527:PCW:H221	0.51	1.80	8	1
5:C:631:17F:C37	5:C:631:17F:H59	0.51	2.36	9	1
4:D:518:PCW:H471	5:D:521:17F:H29	0.51	1.84	9	1
4:C:615:PCW:C48	4:D:509:PCW:H271	0.51	2.35	10	1
4:B:203:PCW:O2P	4:B:204:PCW:C6	0.51	2.59	10	1
4:A:401:PCW:H472	4:C:611:PCW:H251	0.50	1.83	1	2
4:A:406:PCW:O1P	4:A:406:PCW:C3	0.50	2.59	1	1
4:C:624:PCW:O31	4:C:624:PCW:O3	0.50	2.28	3	4
4:B:202:PCW:C5	5:D:524:17F:H1A	0.50	2.35	8	2
4:D:503:PCW:H122	4:D:511:PCW:C39	0.50	2.29	2	1
4:A:405:PCW:O31	4:A:405:PCW:P	0.50	2.69	3	2
4:A:405:PCW:H462	4:D:514:PCW:H262	0.50	1.82	3	1
4:A:412:PCW:H381	4:C:623:PCW:C25	0.50	2.34	3	4
1:A:245:LYS:HA	1:A:249:GLU:HG3	0.50	1.83	5	2
4:A:405:PCW:H42	4:A:408:PCW:O1P	0.50	2.06	4	1
1:A:367:ALA:O	1:A:371:LEU:HG	0.50	2.06	10	3
4:C:609:PCW:H431	4:D:512:PCW:C24	0.50	2.36	6	2
4:D:502:PCW:C14	4:D:505:PCW:H12	0.50	2.33	6	1
4:D:506:PCW:C23	4:D:516:PCW:H412	0.50	2.36	6	1
4:D:516:PCW:C23	5:D:519:17F:H42	0.50	2.30	6	1
4:A:404:PCW:O1P	4:D:510:PCW:H171	0.50	2.06	10	2
4:D:504:PCW:H381	4:D:510:PCW:P	0.50	2.46	8	1
4:A:403:PCW:H241	4:D:513:PCW:H121	0.50	1.81	9	1
4:B:201:PCW:C8	4:D:504:PCW:O11	0.50	2.60	9	1
4:C:625:PCW:H20	4:D:528:PCW:C33	0.50	2.35	1	1
2:B:99:GLN:O	2:B:103:VAL:HG23	0.50	2.06	4	6
4:D:517:PCW:H2	5:D:525:17F:O1	0.50	2.05	2	1
4:C:620:PCW:O31	4:C:620:PCW:C4	0.50	2.59	3	1
4:D:503:PCW:H73	4:D:503:PCW:C2	0.50	2.35	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:515:PCW:H211	5:D:525:17F:H69	0.50	1.83	3	1
4:C:602:PCW:C36	5:D:523:17F:H67	0.50	2.36	6	2
4:C:622:PCW:H422	4:C:623:PCW:H261	0.50	1.81	4	1
4:B:201:PCW:H152	4:D:506:PCW:H461	0.50	1.81	4	1
4:D:506:PCW:H152	5:D:520:17F:C24	0.50	2.36	4	1
5:A:409:17F:C31	4:D:503:PCW:H162	0.50	2.36	5	1
3:D:478:THR:HB	4:D:501:PCW:H51	0.50	1.82	5	1
4:D:503:PCW:H431	5:D:522:17F:C8	0.50	2.36	5	1
4:D:513:PCW:H171	5:D:523:17F:C1X	0.50	2.18	5	1
4:D:513:PCW:C40	5:D:522:17F:H68	0.50	2.36	5	1
4:A:415:PCW:H451	5:D:521:17F:H76	0.50	1.84	7	3
4:C:612:PCW:C7	4:C:618:PCW:H31	0.50	2.36	8	1
5:C:630:17F:C1X	5:D:529:17F:H68	0.50	2.24	8	1
4:D:501:PCW:H451	4:D:515:PCW:H221	0.50	1.83	8	1
4:D:518:PCW:H141	5:D:519:17F:H58	0.50	1.84	8	1
4:C:605:PCW:C32	4:C:611:PCW:H12	0.50	2.36	9	1
4:D:512:PCW:H411	4:D:512:PCW:C37	0.50	2.30	9	1
5:A:409:17F:H69	4:D:501:PCW:H252	0.50	1.83	10	1
4:C:608:PCW:H241	5:C:627:17F:C1X	0.50	2.36	1	2
3:D:436:LEU:HG	4:D:505:PCW:O1P	0.50	2.07	1	1
4:A:403:PCW:H321	4:A:407:PCW:O2P	0.50	2.07	3	1
4:D:506:PCW:H40	4:D:528:PCW:H482	0.50	1.82	3	1
4:D:528:PCW:C12	5:D:530:17F:H33	0.50	2.36	3	1
4:A:405:PCW:O3	4:A:405:PCW:O31	0.50	2.30	8	2
4:A:413:PCW:H371	4:D:526:PCW:C16	0.50	2.37	4	1
5:C:630:17F:H40	5:D:530:17F:H62	0.50	1.82	5	1
4:D:507:PCW:H472	4:D:517:PCW:H282	0.50	1.82	5	1
1:C:444:ASP:O	1:C:448:VAL:HB	0.50	2.07	6	1
4:C:621:PCW:C14	4:C:621:PCW:C18	0.50	2.81	6	3
4:D:518:PCW:H121	5:D:519:17F:C37	0.50	2.37	6	1
4:C:613:PCW:C21	5:D:521:17F:H47	0.50	2.37	10	2
5:C:630:17F:C42	4:D:514:PCW:C22	0.50	2.89	7	1
4:D:514:PCW:H181	4:D:514:PCW:H231	0.50	1.82	7	1
4:A:406:PCW:H242	4:B:202:PCW:C22	0.50	2.21	9	1
4:D:506:PCW:H242	5:D:524:17F:H44	0.50	1.83	9	1
4:D:509:PCW:C17	4:D:514:PCW:H142	0.50	2.36	10	1
4:A:414:PCW:H372	4:A:414:PCW:H411	0.50	1.84	1	1
4:A:415:PCW:H221	4:D:528:PCW:C24	0.50	2.36	4	2
3:D:409:LYS:HG3	4:D:502:PCW:H42	0.50	1.84	1	1
4:D:501:PCW:H451	5:D:525:17F:C22	0.50	2.36	2	1
4:A:407:PCW:H321	5:D:522:17F:H33	0.50	1.82	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:515:PCW:H132	5:D:525:17F:C33	0.50	2.37	3	1
4:A:415:PCW:C21	4:C:603:PCW:H162	0.50	2.36	4	1
4:D:518:PCW:C12	5:D:519:17F:H71	0.50	2.36	4	1
4:C:613:PCW:H132	4:C:619:PCW:H382	0.50	1.82	7	2
4:D:511:PCW:C20	5:D:522:17F:O10	0.50	2.59	5	1
4:C:624:PCW:H82	4:C:624:PCW:C18	0.50	2.36	6	1
4:C:615:PCW:C26	5:C:631:17F:H45	0.50	2.34	7	1
4:C:615:PCW:O3	4:C:615:PCW:C31	0.50	2.59	9	2
4:D:515:PCW:H52	4:D:516:PCW:O31	0.50	2.05	8	1
1:A:246:ASP:HB2	1:C:528:ARG:HD3	0.50	1.81	10	1
5:D:522:17F:H35	5:D:525:17F:C34	0.50	2.37	1	1
4:A:401:PCW:C6	4:D:511:PCW:H2	0.50	2.36	2	1
4:C:602:PCW:H161	4:C:602:PCW:C39	0.50	2.36	2	1
4:A:402:PCW:C31	4:A:402:PCW:O2P	0.50	2.59	3	1
5:A:409:17F:H64	4:D:501:PCW:H241	0.50	1.82	3	1
4:A:414:PCW:H372	4:C:617:PCW:C15	0.50	2.36	3	1
4:C:625:PCW:H82	4:C:625:PCW:O4P	0.50	2.06	3	1
4:D:505:PCW:C46	4:D:518:PCW:H282	0.50	2.31	3	1
1:A:224:VAL:O	1:A:228:PHE:HB2	0.50	2.06	6	3
1:A:233:GLU:HA	1:A:236:THR:OG1	0.50	2.07	4	2
4:D:508:PCW:C13	4:D:509:PCW:C22	0.50	2.75	4	1
5:C:626:17F:C21	5:C:627:17F:H70	0.50	2.36	5	1
5:D:525:17F:H61	5:D:525:17F:C1X	0.50	2.34	5	1
5:A:409:17F:H72	4:D:501:PCW:C24	0.50	2.35	7	1
4:D:511:PCW:H31	4:D:511:PCW:H41	0.50	1.82	7	1
4:D:518:PCW:H212	5:D:519:17F:H58	0.50	1.83	7	1
4:C:605:PCW:C26	4:C:613:PCW:H181	0.50	2.37	8	1
4:C:609:PCW:C11	4:C:615:PCW:H61	0.50	2.37	8	1
2:B:1:MET:SD	2:B:50:THR:HB	0.50	2.46	8	1
4:D:513:PCW:H32	4:D:513:PCW:O2P	0.50	2.07	8	1
4:D:518:PCW:H371	4:D:518:PCW:C11	0.50	2.37	9	1
4:A:411:PCW:C47	4:C:612:PCW:H271	0.50	2.29	10	1
4:C:605:PCW:C18	4:C:613:PCW:C36	0.50	2.84	10	1
4:B:201:PCW:H212	4:D:506:PCW:C45	0.50	2.30	10	1
4:B:202:PCW:H211	4:B:202:PCW:C17	0.50	2.16	10	1
4:C:609:PCW:C23	4:C:615:PCW:H381	0.50	2.30	1	2
4:D:508:PCW:C8	5:D:523:17F:C10	0.50	2.89	1	2
4:D:518:PCW:H62	5:D:519:17F:O8	0.50	2.07	1	1
4:A:402:PCW:C18	4:A:405:PCW:H211	0.50	2.31	3	1
4:A:412:PCW:C40	4:C:623:PCW:C44	0.50	2.83	3	1
4:D:515:PCW:O3	5:D:525:17F:H56	0.50	2.06	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:605:PCW:H472	4:C:619:PCW:C43	0.50	2.32	4	1
4:C:615:PCW:H451	5:D:523:17F:H55	0.50	1.83	4	1
4:C:621:PCW:H412	5:C:631:17F:C42	0.50	2.26	4	1
2:B:21:ILE:HD11	3:D:388:VAL:CG1	0.50	2.37	4	1
5:D:529:17F:H42	5:D:530:17F:C39	0.50	2.36	5	1
4:C:602:PCW:H221	4:C:602:PCW:H161	0.50	1.84	6	1
4:C:602:PCW:C42	5:C:626:17F:H41	0.50	2.37	6	1
4:C:602:PCW:H421	5:C:626:17F:H41	0.50	1.83	6	1
4:D:517:PCW:H352	5:D:520:17F:H30	0.50	1.83	6	1
4:D:502:PCW:H331	4:D:510:PCW:H11	0.50	1.81	8	1
4:A:404:PCW:H321	4:D:510:PCW:H181	0.50	1.84	9	1
5:C:630:17F:O9	5:C:630:17F:O8	0.50	2.29	9	1
4:C:608:PCW:H63	4:C:624:PCW:C22	0.50	2.35	10	1
4:B:203:PCW:C2	4:B:204:PCW:H82	0.50	2.27	10	1
4:D:517:PCW:C44	5:D:525:17F:H40	0.50	2.32	10	1
4:C:614:PCW:O4P	4:C:614:PCW:H62	0.50	2.06	1	1
4:B:204:PCW:O31	4:B:204:PCW:C11	0.50	2.59	5	2
5:D:522:17F:H35	5:D:525:17F:H61	0.50	1.82	1	1
5:C:630:17F:O10	5:C:630:17F:P1	0.50	2.70	2	1
4:C:611:PCW:P	4:C:613:PCW:H73	0.50	2.47	4	1
4:C:622:PCW:C32	4:C:622:PCW:C36	0.50	2.90	4	1
4:D:508:PCW:H152	4:D:509:PCW:C20	0.50	2.37	5	1
4:C:602:PCW:H282	5:C:627:17F:C42	0.50	2.37	6	1
4:C:615:PCW:H212	4:C:615:PCW:C17	0.50	2.26	7	1
4:D:509:PCW:C16	5:D:520:17F:C31	0.50	2.84	7	1
4:D:515:PCW:H232	5:D:525:17F:C25	0.50	2.36	7	1
4:D:509:PCW:O2P	4:D:509:PCW:H31	0.50	2.07	8	1
4:A:407:PCW:H461	4:A:412:PCW:C27	0.50	2.31	9	1
4:C:620:PCW:O4P	4:C:620:PCW:H2	0.50	2.07	10	1
1:C:496:LEU:O	1:C:500:GLY:HA3	0.50	2.06	2	8
4:C:611:PCW:H481	4:D:503:PCW:H283	0.50	1.83	1	1
4:C:618:PCW:O3	4:C:625:PCW:H151	0.50	2.07	1	1
4:D:510:PCW:H331	5:D:524:17F:H9	0.50	1.83	1	1
4:C:605:PCW:C42	4:C:619:PCW:H141	0.50	2.32	5	5
4:D:513:PCW:O11	4:D:513:PCW:H52	0.50	2.07	2	1
4:D:516:PCW:H482	4:D:527:PCW:H252	0.50	1.82	2	1
1:C:505:ASP:HA	1:C:508:ARG:HD2	0.50	1.82	8	3
4:C:616:PCW:H281	4:C:618:PCW:C28	0.50	2.36	3	1
4:C:616:PCW:H472	4:B:201:PCW:H471	0.50	1.83	3	1
4:D:504:PCW:O31	4:D:504:PCW:C1	0.50	2.54	4	2
4:C:617:PCW:C28	4:D:502:PCW:H221	0.50	2.37	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:509:PCW:H372	4:D:509:PCW:C42	0.50	2.37	7	2
4:C:618:PCW:H422	4:C:625:PCW:H282	0.50	1.83	6	2
4:D:517:PCW:H352	5:D:520:17F:C11	0.50	2.32	6	1
4:A:414:PCW:H422	4:C:617:PCW:C20	0.50	2.36	7	2
4:C:610:PCW:O11	5:C:629:17F:H18	0.50	2.07	7	1
5:D:521:17F:H10	5:D:521:17F:C32	0.50	2.29	7	2
4:A:401:PCW:C31	4:D:511:PCW:H231	0.50	2.37	8	1
4:D:515:PCW:H472	4:D:515:PCW:C12	0.50	2.33	9	1
4:D:518:PCW:C11	4:D:518:PCW:C37	0.50	2.89	9	1
4:A:406:PCW:H351	4:B:204:PCW:H161	0.50	1.82	10	1
4:C:603:PCW:H371	4:C:603:PCW:C41	0.50	2.28	10	1
4:C:614:PCW:H12	4:C:623:PCW:C6	0.50	2.36	10	1
4:A:412:PCW:O11	4:A:412:PCW:C2	0.50	2.55	1	1
4:D:505:PCW:C47	4:D:518:PCW:H282	0.50	2.35	1	1
4:A:414:PCW:C44	4:C:617:PCW:H20	0.50	2.37	2	1
4:C:606:PCW:O31	4:C:606:PCW:C11	0.50	2.60	2	1
4:C:611:PCW:H31	4:C:619:PCW:O11	0.50	2.07	10	3
4:B:201:PCW:C21	4:D:506:PCW:H441	0.50	2.36	2	1
4:D:506:PCW:O31	4:D:506:PCW:C1	0.50	2.54	3	3
4:D:508:PCW:H42	5:D:520:17F:P1	0.50	2.47	3	1
4:C:604:PCW:C43	4:C:606:PCW:H181	0.50	2.37	4	2
4:A:411:PCW:H361	4:C:612:PCW:H132	0.50	1.82	5	1
4:A:414:PCW:C7	5:C:628:17F:H4	0.50	2.36	5	1
4:C:621:PCW:H212	5:C:629:17F:H31	0.50	1.83	6	1
5:A:409:17F:O4	3:D:401:LEU:HA	0.50	2.05	7	1
4:A:408:PCW:H482	4:D:528:PCW:H481	0.50	1.83	8	1
4:D:503:PCW:O31	4:D:503:PCW:C7	0.50	2.60	9	1
1:A:353:ALA:O	1:A:357:LEU:HG	0.50	2.06	10	1
4:A:401:PCW:C34	4:D:511:PCW:H242	0.50	2.36	10	1
4:A:406:PCW:H171	4:A:406:PCW:C23	0.50	2.35	10	1
4:A:406:PCW:C18	4:B:204:PCW:H283	0.50	2.37	10	1
4:A:414:PCW:H421	4:C:617:PCW:H211	0.50	1.83	10	1
4:A:415:PCW:C21	4:C:603:PCW:H161	0.50	2.37	10	1
4:A:413:PCW:H451	4:D:526:PCW:C22	0.49	2.37	1	2
4:C:603:PCW:H61	4:D:527:PCW:P	0.49	2.46	1	1
4:D:509:PCW:C3	4:D:509:PCW:O1P	0.49	2.60	1	1
4:D:510:PCW:H211	4:D:510:PCW:C16	0.49	2.37	1	2
4:A:404:PCW:O1P	4:A:404:PCW:O2	0.49	2.30	2	1
4:C:616:PCW:H221	4:C:616:PCW:H172	0.49	1.83	6	3
4:D:518:PCW:H232	5:D:519:17F:C31	0.49	2.36	3	1
2:B:1:MET:HA	2:B:50:THR:HB	0.49	1.82	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:201:PCW:H272	4:D:528:PCW:H441	0.49	1.84	5	1
4:A:415:PCW:C18	4:C:603:PCW:H141	0.49	2.37	6	2
4:A:401:PCW:H122	4:D:511:PCW:H272	0.49	1.82	8	1
4:C:619:PCW:H481	5:D:521:17F:C42	0.49	2.37	8	1
4:D:517:PCW:H422	5:D:525:17F:H67	0.49	1.83	9	1
4:C:604:PCW:H381	5:D:529:17F:H40	0.49	1.84	10	1
4:D:506:PCW:H52	4:D:509:PCW:H11	0.49	1.84	10	1
4:D:508:PCW:H63	4:D:517:PCW:C32	0.49	2.37	10	1
4:A:411:PCW:C42	4:C:612:PCW:H212	0.49	2.32	2	3
4:C:609:PCW:H131	4:C:609:PCW:O31	0.49	2.07	1	1
2:B:52:LEU:HD13	4:D:504:PCW:H61	0.49	1.83	1	1
4:D:507:PCW:H162	4:D:513:PCW:H122	0.49	1.84	1	1
5:D:525:17F:H77	5:D:525:17F:H49	0.49	1.84	1	1
5:A:409:17F:H75	4:D:501:PCW:C28	0.49	2.34	2	1
5:A:409:17F:H68	4:D:501:PCW:H242	0.49	1.82	3	1
4:C:605:PCW:O31	4:C:613:PCW:H82	0.49	2.07	3	1
4:B:202:PCW:O31	4:B:202:PCW:O3	0.49	2.29	10	5
3:D:478:THR:HB	4:D:517:PCW:C5	0.49	2.37	3	1
4:D:513:PCW:O11	4:D:513:PCW:C2	0.49	2.58	10	4
4:C:609:PCW:O1P	5:C:631:17F:H20A	0.49	2.06	4	1
4:B:201:PCW:H483	5:D:524:17F:H49	0.49	1.84	4	1
4:A:402:PCW:O31	4:A:402:PCW:H11	0.49	2.07	9	4
4:C:615:PCW:H161	5:C:631:17F:H11A	0.49	1.83	5	1
2:B:36:ILE:HD11	3:D:371:ASN:HB2	0.49	1.82	5	2
2:B:85:ASN:HB2	2:B:122:SER:HB2	0.49	1.84	5	2
4:D:516:PCW:O31	4:D:516:PCW:P	0.49	2.70	5	4
4:D:517:PCW:H422	5:D:525:17F:H64	0.49	1.83	5	1
4:A:414:PCW:H442	4:C:617:PCW:C21	0.49	2.36	6	1
5:D:522:17F:C23	5:D:522:17F:C12	0.49	2.90	6	1
4:A:406:PCW:C4	4:B:204:PCW:H11	0.49	2.37	7	1
4:D:518:PCW:C16	5:D:519:17F:C1Z	0.49	2.90	8	1
4:D:504:PCW:H483	5:D:519:17F:C28	0.49	2.36	9	1
4:A:403:PCW:C28	5:D:523:17F:H33	0.49	2.36	10	1
4:A:402:PCW:O11	4:A:402:PCW:O2	0.49	2.29	10	3
4:C:607:PCW:O31	4:C:607:PCW:O3	0.49	2.30	6	3
4:D:513:PCW:H52	5:D:523:17F:C4	0.49	2.31	1	1
4:C:601:PCW:O31	4:C:601:PCW:O3P	0.49	2.30	8	5
4:C:608:PCW:O11	4:C:608:PCW:C2	0.49	2.59	6	6
4:C:616:PCW:H431	4:B:201:PCW:C47	0.49	2.37	2	1
4:D:501:PCW:H331	4:D:511:PCW:C7	0.49	2.37	2	1
4:D:509:PCW:H231	5:D:520:17F:H31	0.49	1.83	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:402:PCW:C32	4:D:514:PCW:H31	0.49	2.38	3	1
4:A:403:PCW:O11	4:A:403:PCW:O2	0.49	2.30	3	1
3:D:468:CYS:SG	3:D:484:CYS:HB3	0.49	2.48	7	2
4:D:505:PCW:C31	4:D:505:PCW:O3	0.49	2.60	8	3
4:D:510:PCW:H471	5:D:524:17F:C1Y	0.49	2.36	4	1
4:A:405:PCW:H331	4:D:514:PCW:H331	0.49	1.83	5	1
4:B:203:PCW:H181	4:B:203:PCW:H441	0.49	1.83	6	1
4:D:507:PCW:C15	4:D:513:PCW:C32	0.49	2.91	6	1
4:D:503:PCW:C42	4:D:511:PCW:H19	0.49	2.32	8	1
4:D:509:PCW:H483	4:D:509:PCW:H281	0.49	1.83	8	1
4:D:516:PCW:C3	4:D:516:PCW:O2P	0.49	2.60	8	1
4:A:404:PCW:H52	4:D:510:PCW:C12	0.49	2.37	9	1
4:B:202:PCW:H51	5:D:524:17F:H1	0.49	1.84	10	2
4:B:201:PCW:H411	5:D:524:17F:H39	0.49	1.82	10	1
4:D:509:PCW:H461	5:D:520:17F:H33	0.49	1.84	10	1
4:C:618:PCW:O1P	4:C:625:PCW:C6	0.49	2.60	1	1
4:D:506:PCW:O11	4:D:506:PCW:C2	0.49	2.43	10	2
4:D:510:PCW:H432	5:D:524:17F:H58	0.49	1.84	1	1
1:A:213:THR:O	1:A:217:LEU:HG	0.49	2.06	2	2
4:D:503:PCW:H441	4:D:507:PCW:H471	0.49	1.82	2	1
4:D:518:PCW:C31	4:D:518:PCW:C35	0.49	2.90	3	7
4:A:403:PCW:C3	4:A:403:PCW:P	0.49	3.00	3	1
4:B:202:PCW:H472	5:D:524:17F:C20	0.49	2.38	6	2
4:C:618:PCW:H481	4:D:510:PCW:H482	0.49	1.84	5	1
4:D:505:PCW:C38	5:D:519:17F:H9A	0.49	2.37	6	1
4:D:518:PCW:C34	5:D:519:17F:H62	0.49	2.37	6	1
5:D:519:17F:H65	5:D:521:17F:H29	0.49	1.85	6	1
5:D:522:17F:C12	5:D:522:17F:H40	0.49	2.37	6	1
4:A:402:PCW:H441	4:D:512:PCW:C16	0.49	2.37	7	1
4:C:615:PCW:H121	5:C:631:17F:C7	0.49	2.38	7	1
4:B:203:PCW:H11	4:B:204:PCW:O3P	0.49	2.07	7	1
4:C:625:PCW:H283	4:B:203:PCW:C27	0.49	2.38	9	1
4:B:201:PCW:H483	4:D:527:PCW:H40	0.49	1.84	9	1
4:C:615:PCW:C8	5:C:631:17F:O4	0.49	2.59	10	1
4:A:406:PCW:H352	4:B:204:PCW:H152	0.49	1.81	1	1
4:D:502:PCW:O11	4:D:502:PCW:C5	0.49	2.60	1	1
4:D:506:PCW:H31	4:D:515:PCW:H31	0.49	1.83	1	1
4:D:507:PCW:H40	5:D:525:17F:C6	0.49	2.37	1	1
5:D:521:17F:O7	5:D:521:17F:O10	0.49	2.31	1	2
4:A:402:PCW:H82	4:A:405:PCW:C3	0.49	2.36	2	1
4:C:608:PCW:C19	5:C:627:17F:H50	0.49	2.38	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:201:PCW:H122	4:D:506:PCW:C34	0.49	2.38	2	1
4:D:516:PCW:H19	4:D:526:PCW:C47	0.49	2.36	2	1
4:A:403:PCW:O4P	4:A:403:PCW:H31	0.49	2.08	3	1
4:D:513:PCW:H73	5:D:523:17F:H4	0.49	1.83	3	1
1:A:264:LYS:HE2	1:C:509:ALA:HB1	0.49	1.83	7	4
4:A:408:PCW:C44	4:D:506:PCW:H412	0.49	2.14	4	1
4:C:623:PCW:O3P	4:C:623:PCW:O31	0.49	2.31	5	2
4:D:510:PCW:C47	5:D:524:17F:H32	0.49	2.36	4	1
4:A:414:PCW:C44	4:C:617:PCW:H211	0.49	2.37	6	1
4:C:601:PCW:O2	4:C:601:PCW:O2P	0.49	2.30	6	1
4:D:502:PCW:H63	4:D:505:PCW:O1P	0.49	2.07	6	1
4:D:504:PCW:H152	4:D:510:PCW:H381	0.49	1.84	6	1
4:D:509:PCW:C14	5:D:520:17F:H18	0.49	2.37	9	2
5:D:519:17F:O2	5:D:519:17F:C17	0.49	2.60	6	1
4:B:203:PCW:C45	4:B:204:PCW:H382	0.49	2.36	7	1
4:C:612:PCW:C8	4:C:618:PCW:H31	0.49	2.38	8	1
4:D:504:PCW:H362	4:D:510:PCW:O1P	0.49	2.07	8	1
4:D:509:PCW:C20	5:D:520:17F:H60	0.49	2.37	10	1
4:A:403:PCW:O2P	4:A:403:PCW:H63	0.49	2.07	1	1
5:A:409:17F:O1	5:D:521:17F:H1A	0.49	2.07	1	1
4:A:413:PCW:C45	4:D:526:PCW:H231	0.49	2.38	1	2
4:A:414:PCW:H321	4:C:617:PCW:C5	0.49	2.37	1	1
4:D:509:PCW:C44	5:D:520:17F:H32	0.49	2.37	1	2
4:C:604:PCW:H11	4:C:606:PCW:H51	0.49	1.83	3	1
4:B:202:PCW:H141	4:B:202:PCW:C38	0.49	2.37	3	1
4:D:508:PCW:C21	4:D:512:PCW:H411	0.49	2.38	3	1
4:D:510:PCW:C21	4:D:510:PCW:H162	0.49	2.37	3	1
4:A:406:PCW:O31	4:A:406:PCW:C1	0.49	2.51	5	1
4:B:201:PCW:C5	4:B:202:PCW:H12	0.49	2.28	5	1
4:D:509:PCW:H372	4:D:509:PCW:H421	0.49	1.84	7	2
4:C:618:PCW:C42	4:C:625:PCW:H282	0.49	2.38	6	1
4:C:602:PCW:H252	5:C:627:17F:H76	0.49	1.85	7	1
5:D:524:17F:H59	5:D:524:17F:H12	0.49	1.84	7	1
4:D:505:PCW:H471	5:D:519:17F:C30	0.49	2.33	9	1
4:C:603:PCW:C6	4:D:527:PCW:O2P	0.49	2.61	10	1
3:D:434:VAL:HG11	4:D:518:PCW:H63	0.49	1.83	1	1
4:A:407:PCW:H241	4:A:412:PCW:H262	0.49	1.84	2	1
4:C:606:PCW:C5	4:C:624:PCW:H19	0.49	2.38	2	1
4:D:507:PCW:H42	5:D:523:17F:HN1A	0.49	1.68	2	1
4:A:404:PCW:O11	4:A:404:PCW:C2	0.49	2.51	5	4
4:C:603:PCW:H271	4:D:526:PCW:H182	0.49	1.85	9	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:616:PCW:O2P	4:D:527:PCW:H62	0.49	2.08	4	1
4:D:509:PCW:C27	5:D:520:17F:H10A	0.49	2.38	6	1
4:B:201:PCW:C24	4:B:203:PCW:H20	0.49	2.35	7	1
4:A:413:PCW:C3	4:C:617:PCW:C42	0.49	2.90	8	1
4:D:518:PCW:C14	5:D:519:17F:H63	0.49	2.23	8	1
5:D:521:17F:H12	5:D:521:17F:C35	0.49	2.37	9	1
4:A:410:PCW:H19	4:A:413:PCW:H411	0.49	1.85	10	1
4:D:503:PCW:H422	5:D:522:17F:H42	0.49	1.85	10	1
4:A:413:PCW:H452	4:C:616:PCW:H232	0.49	1.83	1	1
4:A:415:PCW:C6	4:A:415:PCW:C31	0.49	2.90	2	3
4:C:618:PCW:O1P	4:C:625:PCW:H82	0.49	2.07	5	2
3:D:474:GLU:OE2	4:D:511:PCW:H62	0.49	2.08	1	1
4:A:415:PCW:H19	4:D:516:PCW:H271	0.49	1.83	2	1
4:C:607:PCW:C1	4:C:624:PCW:C37	0.49	2.86	10	2
4:D:518:PCW:H341	5:D:519:17F:H32	0.49	1.84	2	2
4:D:502:PCW:H211	4:D:502:PCW:H422	0.49	1.84	3	1
4:D:528:PCW:O3P	4:D:528:PCW:O31	0.49	2.31	6	4
4:D:518:PCW:H212	4:D:518:PCW:H172	0.49	1.84	5	1
4:D:528:PCW:C19	5:D:530:17F:H20	0.49	2.09	5	1
4:D:507:PCW:H422	4:D:507:PCW:H381	0.49	1.83	6	1
4:D:508:PCW:H151	4:D:512:PCW:C17	0.49	2.34	6	1
4:D:518:PCW:H431	5:D:521:17F:H10A	0.49	1.84	6	1
4:C:624:PCW:O2	4:C:624:PCW:P	0.49	2.71	8	2
4:D:501:PCW:O1P	4:D:515:PCW:C35	0.49	2.61	7	1
4:D:503:PCW:H461	4:D:507:PCW:C48	0.49	2.38	7	1
4:A:407:PCW:H331	5:D:522:17F:C32	0.49	2.38	8	1
4:A:411:PCW:H352	4:C:612:PCW:H131	0.49	1.85	8	1
4:C:607:PCW:H472	4:D:513:PCW:C48	0.49	2.38	8	1
4:A:405:PCW:O31	4:A:405:PCW:C4	0.49	2.61	9	1
4:C:609:PCW:H172	4:C:615:PCW:H331	0.49	1.84	10	1
1:A:239:LEU:HD13	4:A:406:PCW:H451	0.49	1.85	1	1
2:B:38:ASP:HA	3:D:367:ARG:O	0.49	2.07	1	1
4:C:602:PCW:H481	4:C:608:PCW:H232	0.49	1.85	2	1
4:C:620:PCW:P	4:C:621:PCW:H52	0.49	2.47	5	2
4:C:624:PCW:H51	4:C:624:PCW:O11	0.49	2.08	2	1
4:D:506:PCW:C22	4:D:516:PCW:H371	0.49	2.38	2	1
1:C:451:LYS:O	1:C:455:TYR:HB2	0.49	2.08	4	3
4:C:624:PCW:C31	4:C:624:PCW:O3	0.49	2.61	3	4
4:D:501:PCW:C8	4:D:501:PCW:O4P	0.49	2.61	9	3
4:D:513:PCW:O3P	4:D:513:PCW:O31	0.49	2.29	3	1
4:A:413:PCW:H372	4:C:617:PCW:H451	0.49	1.85	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:120:LEU:HD21	6:B:205:GNP:N2	0.49	2.23	4	1
3:D:425:GLU:O	4:D:502:PCW:H82	0.49	2.08	4	1
4:D:517:PCW:H471	5:D:525:17F:C40	0.49	2.26	4	1
5:A:409:17F:C2	4:D:503:PCW:H82	0.49	2.38	6	1
4:B:201:PCW:H42	4:B:202:PCW:O11	0.49	2.08	6	1
4:A:402:PCW:H441	4:D:512:PCW:H161	0.49	1.85	7	1
4:A:403:PCW:O2	4:A:407:PCW:H52	0.49	2.07	7	1
5:C:630:17F:H76	4:D:514:PCW:C22	0.49	2.37	7	1
2:B:62:GLU:HB3	2:B:68:ARG:NH2	0.49	2.23	7	2
4:D:502:PCW:C47	4:D:505:PCW:H281	0.49	2.38	7	1
4:A:411:PCW:C35	4:C:612:PCW:H131	0.49	2.37	8	1
4:D:501:PCW:H222	5:D:521:17F:C19	0.49	2.35	8	1
4:D:508:PCW:H231	4:D:512:PCW:H172	0.49	1.83	8	1
4:D:504:PCW:C3	5:D:524:17F:H4	0.49	2.38	9	1
4:A:414:PCW:H341	4:C:617:PCW:H132	0.49	1.85	1	1
2:B:117:LYS:HG2	6:B:205:GNP:C6	0.49	2.38	1	2
4:D:506:PCW:C28	4:D:515:PCW:H362	0.49	2.37	1	1
4:C:608:PCW:C22	5:C:626:17F:H8A	0.49	2.38	3	1
4:C:607:PCW:O3	4:C:624:PCW:C42	0.49	2.61	4	1
4:D:516:PCW:H241	5:D:519:17F:H46	0.49	1.82	6	1
4:A:402:PCW:H40	4:A:405:PCW:H282	0.49	1.83	8	1
4:A:413:PCW:H381	4:C:617:PCW:H481	0.49	1.85	8	1
4:D:502:PCW:C33	4:D:510:PCW:C1	0.49	2.90	8	1
4:A:412:PCW:H82	4:C:624:PCW:C36	0.49	2.35	9	1
4:C:601:PCW:H73	5:D:523:17F:O2	0.49	2.07	9	1
4:B:201:PCW:H19	4:D:516:PCW:H422	0.49	1.85	9	1
4:A:402:PCW:H422	4:D:508:PCW:C18	0.49	2.38	10	1
4:D:505:PCW:C39	4:D:505:PCW:H141	0.49	2.38	10	1
5:A:409:17F:H77	4:D:501:PCW:C27	0.48	2.38	1	1
4:C:611:PCW:O2P	4:C:619:PCW:C6	0.48	2.61	2	3
4:C:604:PCW:H182	5:D:525:17F:C30	0.48	2.28	2	1
4:C:605:PCW:H63	5:C:628:17F:HN1A	0.48	1.68	2	1
5:C:629:17F:O7	5:C:629:17F:C17	0.48	2.61	4	4
5:D:524:17F:H12	5:D:524:17F:C36	0.48	2.38	8	3
4:C:604:PCW:H381	5:D:529:17F:C23	0.48	2.38	3	1
4:D:504:PCW:H262	4:D:510:PCW:C40	0.48	2.30	3	1
1:A:297:LYS:O	1:A:301:LEU:HB2	0.48	2.08	7	2
4:C:601:PCW:O4P	4:D:513:PCW:H61	0.48	2.07	4	1
4:C:611:PCW:H41	4:C:622:PCW:C32	0.48	2.38	4	1
4:A:410:PCW:C38	4:C:617:PCW:H141	0.48	2.35	5	1
4:C:608:PCW:H19	5:C:627:17F:C28	0.48	2.37	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:618:PCW:H152	4:C:625:PCW:H142	0.48	1.82	6	1
4:D:508:PCW:H152	4:D:509:PCW:C24	0.48	2.38	6	1
4:D:509:PCW:C28	5:D:520:17F:H10A	0.48	2.38	6	1
4:C:607:PCW:H431	4:C:623:PCW:C47	0.48	2.36	7	2
5:A:409:17F:O7	5:A:409:17F:O10	0.48	2.31	8	1
4:C:607:PCW:C35	4:C:624:PCW:H422	0.48	2.38	10	1
4:C:618:PCW:H251	4:D:510:PCW:H483	0.48	1.85	10	1
4:D:507:PCW:O2P	4:D:507:PCW:O2	0.48	2.31	1	1
5:D:530:17F:H11	5:D:530:17F:C31	0.48	2.38	1	1
1:A:254:VAL:O	1:A:258:LEU:HB2	0.48	2.07	5	2
5:A:409:17F:H57	4:D:503:PCW:H182	0.48	1.85	2	2
4:D:507:PCW:H481	5:D:522:17F:H48	0.48	1.85	2	1
4:D:526:PCW:H51	4:D:527:PCW:H73	0.48	1.85	6	3
4:A:406:PCW:H162	4:B:204:PCW:H412	0.48	1.85	3	1
4:C:602:PCW:C17	4:C:602:PCW:C21	0.48	2.77	7	3
4:C:621:PCW:C21	5:C:629:17F:H19A	0.48	2.38	3	1
4:D:527:PCW:H422	4:D:528:PCW:H332	0.48	1.81	6	1
4:D:504:PCW:H461	4:D:516:PCW:H19	0.48	1.84	7	1
4:D:511:PCW:P	4:D:511:PCW:C3	0.48	3.01	7	1
4:D:518:PCW:O3	4:D:518:PCW:C35	0.48	2.58	9	1
5:D:524:17F:H11A	5:D:524:17F:C36	0.48	2.37	9	1
4:A:406:PCW:C48	4:B:204:PCW:H252	0.48	2.36	10	1
4:C:614:PCW:H41	4:C:623:PCW:O1P	0.48	2.07	10	1
4:C:616:PCW:C39	4:C:618:PCW:C16	0.48	2.90	10	1
4:B:204:PCW:H2	4:B:204:PCW:O11	0.48	2.08	10	1
4:D:515:PCW:H82	4:D:516:PCW:C4	0.48	2.34	10	1
4:D:517:PCW:H40	5:D:525:17F:H67	0.48	1.84	10	1
4:A:408:PCW:C34	4:D:514:PCW:H451	0.48	2.37	1	2
5:C:630:17F:C33	5:C:631:17F:H75	0.48	2.38	1	1
3:D:481:PRO:CD	4:D:515:PCW:H381	0.48	2.38	1	1
4:D:513:PCW:H421	4:D:513:PCW:H272	0.48	1.85	1	1
4:C:625:PCW:H241	4:D:527:PCW:H431	0.48	1.86	2	2
2:B:79:LEU:HD23	2:B:112:VAL:HB	0.48	1.86	9	3
2:B:117:LYS:HE2	6:B:205:GNP:C4	0.48	2.39	10	2
4:A:414:PCW:O1P	4:A:414:PCW:H2	0.48	2.08	3	1
4:C:612:PCW:H52	4:C:618:PCW:O11	0.48	2.08	4	1
5:D:522:17F:H12A	5:D:522:17F:C24	0.48	2.35	6	2
4:A:413:PCW:O2	4:C:617:PCW:H422	0.48	2.08	5	1
4:C:615:PCW:H231	4:D:512:PCW:H261	0.48	1.84	6	1
4:D:509:PCW:H62	4:D:514:PCW:C1	0.48	2.38	6	1
4:C:602:PCW:H351	5:D:523:17F:C42	0.48	2.36	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:C:630:17F:C42	4:D:514:PCW:H222	0.48	2.36	7	1
4:B:201:PCW:H483	5:D:524:17F:C28	0.48	2.38	8	1
4:D:510:PCW:H352	5:D:524:17F:O8	0.48	2.09	8	1
4:D:518:PCW:H121	5:D:519:17F:H62	0.48	1.85	8	1
4:B:201:PCW:C18	4:D:506:PCW:H442	0.48	2.37	9	1
4:C:615:PCW:H272	5:C:631:17F:H46	0.48	1.83	10	1
4:B:201:PCW:H151	4:D:516:PCW:C40	0.48	2.39	10	1
4:D:507:PCW:C5	5:D:523:17F:H9	0.48	2.37	10	1
4:A:401:PCW:C47	4:C:611:PCW:H251	0.48	2.38	1	1
4:C:620:PCW:O1P	4:C:621:PCW:H62	0.48	2.08	1	1
4:C:605:PCW:P	4:C:613:PCW:C5	0.48	3.02	9	3
4:C:612:PCW:C32	4:C:618:PCW:C13	0.48	2.91	6	2
4:C:602:PCW:C32	5:D:523:17F:H60	0.48	2.38	9	2
5:C:628:17F:O6	5:C:628:17F:C17	0.48	2.61	5	5
4:D:503:PCW:H73	4:D:503:PCW:O3P	0.48	2.09	5	2
4:A:414:PCW:H161	5:C:628:17F:C33	0.48	2.38	4	1
4:C:608:PCW:H20	5:C:627:17F:H50	0.48	1.85	5	2
4:B:203:PCW:H121	4:B:203:PCW:H351	0.48	1.85	8	3
4:D:517:PCW:H181	4:D:517:PCW:C42	0.48	2.38	6	2
4:A:401:PCW:N	4:D:511:PCW:O31	0.48	2.47	8	2
4:C:602:PCW:H483	5:C:626:17F:C38	0.48	2.37	8	1
4:C:607:PCW:H51	4:C:607:PCW:C32	0.48	2.38	8	1
4:D:506:PCW:H20	4:D:516:PCW:H322	0.48	1.85	8	1
4:D:508:PCW:C1	5:D:523:17F:H12A	0.48	2.35	8	1
4:A:405:PCW:C32	4:A:408:PCW:C35	0.48	2.85	9	1
5:D:524:17F:H11A	5:D:524:17F:H69	0.48	1.84	9	1
4:A:402:PCW:H431	4:D:508:PCW:H242	0.48	1.85	10	1
4:A:411:PCW:H82	4:A:411:PCW:O4P	0.48	2.09	10	1
4:B:204:PCW:H52	4:B:204:PCW:C31	0.48	2.38	10	1
4:D:503:PCW:H431	5:D:522:17F:H10	0.48	1.85	10	1
4:C:616:PCW:H281	4:C:618:PCW:H281	0.48	1.86	1	1
4:D:505:PCW:H412	4:D:505:PCW:H371	0.48	1.84	1	2
4:D:511:PCW:O3P	4:D:511:PCW:O31	0.48	2.32	1	2
4:A:407:PCW:H352	5:D:522:17F:C35	0.48	2.33	2	1
1:C:533:LEU:HA	1:C:536:LEU:HD12	0.48	1.84	2	1
4:C:613:PCW:H411	4:C:619:PCW:H39	0.48	1.85	9	4
1:A:214:PHE:CZ	4:A:404:PCW:H142	0.48	2.42	3	1
4:A:410:PCW:O11	4:C:617:PCW:H332	0.48	2.08	7	2
4:C:604:PCW:H11	4:C:606:PCW:C5	0.48	2.38	3	1
4:D:507:PCW:H142	4:D:513:PCW:H362	0.48	1.85	3	1
4:D:511:PCW:H31	4:D:511:PCW:O1P	0.48	2.09	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:407:PCW:C27	4:A:412:PCW:H271	0.48	2.39	8	2
4:C:622:PCW:H371	4:C:622:PCW:C3	0.48	2.38	4	1
2:B:46:ILE:HB	2:B:51:CYS:SG	0.48	2.48	9	4
4:A:415:PCW:H221	4:D:528:PCW:H232	0.48	1.84	5	1
4:C:614:PCW:H171	4:C:622:PCW:C48	0.48	2.39	5	1
4:C:619:PCW:O31	4:C:619:PCW:C1	0.48	2.59	6	2
4:D:504:PCW:H242	4:D:510:PCW:H422	0.48	1.85	6	1
4:D:506:PCW:H32	4:D:515:PCW:C6	0.48	2.39	6	1
4:D:511:PCW:H281	5:D:522:17F:C31	0.48	2.37	6	1
4:A:406:PCW:H42	4:B:204:PCW:C3	0.48	2.33	7	1
4:A:406:PCW:C24	4:B:202:PCW:H252	0.48	2.31	8	1
4:C:621:PCW:O1P	4:C:621:PCW:C5	0.48	2.59	8	1
4:A:403:PCW:H241	4:D:513:PCW:H141	0.48	1.85	9	1
4:C:607:PCW:C36	4:C:624:PCW:H422	0.48	2.39	10	1
4:D:503:PCW:H411	4:D:511:PCW:H222	0.48	1.85	10	1
4:C:602:PCW:O31	4:C:602:PCW:C1	0.48	2.53	2	4
4:C:604:PCW:H372	4:C:604:PCW:H411	0.48	1.86	2	1
4:C:605:PCW:C39	4:C:611:PCW:H341	0.48	2.35	3	2
4:A:405:PCW:O3	4:D:514:PCW:H322	0.48	2.09	3	1
4:A:406:PCW:C4	4:B:204:PCW:C3	0.48	2.90	3	1
4:D:502:PCW:C3	4:D:502:PCW:O1P	0.48	2.61	3	1
4:B:202:PCW:H322	4:B:202:PCW:C8	0.48	2.37	10	2
4:C:616:PCW:H442	4:C:618:PCW:H472	0.48	1.86	5	1
4:B:201:PCW:H171	4:D:516:PCW:H441	0.48	1.86	6	1
4:A:402:PCW:C43	4:D:508:PCW:H251	0.48	2.19	7	1
4:A:408:PCW:H372	4:B:203:PCW:H382	0.48	1.84	7	1
4:D:501:PCW:H19	4:D:503:PCW:H342	0.48	1.85	7	1
4:D:528:PCW:C19	5:D:530:17F:H19A	0.48	2.38	7	1
4:C:604:PCW:O1P	4:C:622:PCW:C7	0.48	2.62	8	1
4:A:415:PCW:H282	4:D:528:PCW:C27	0.48	2.37	10	1
4:D:504:PCW:H452	4:D:505:PCW:C13	0.48	2.39	10	1
4:A:403:PCW:P	4:A:403:PCW:C3	0.48	2.88	6	6
4:A:413:PCW:C45	4:C:616:PCW:H232	0.48	2.39	1	1
4:A:413:PCW:H371	4:D:526:PCW:H152	0.48	1.84	1	1
4:B:201:PCW:H212	4:D:506:PCW:C42	0.48	2.36	1	1
4:D:510:PCW:H152	5:D:524:17F:O10	0.48	2.08	1	1
1:A:217:LEU:HD21	4:A:404:PCW:H252	0.48	1.83	2	1
4:A:401:PCW:H481	4:C:614:PCW:H471	0.48	1.84	2	1
4:C:602:PCW:C48	4:C:608:PCW:H232	0.48	2.38	2	1
4:C:621:PCW:C15	5:C:630:17F:H4A	0.48	2.37	2	2
4:C:625:PCW:H421	4:C:625:PCW:H381	0.48	1.84	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:247:LEU:O	1:A:250:VAL:HG12	0.48	2.09	3	2
1:C:573:LEU:HA	1:C:576:VAL:HG12	0.48	1.85	4	4
1:A:225:THR:O	1:A:229:TRP:HB2	0.48	2.09	4	3
4:C:612:PCW:H332	4:C:625:PCW:H132	0.48	1.85	4	2
4:C:622:PCW:H231	4:D:501:PCW:H481	0.48	1.84	4	1
4:C:610:PCW:H151	5:C:629:17F:C34	0.48	2.39	5	1
4:B:201:PCW:H172	4:B:201:PCW:H212	0.48	1.85	5	1
4:A:406:PCW:O31	4:A:406:PCW:O3P	0.48	2.32	9	2
4:A:411:PCW:C43	4:C:612:PCW:C17	0.48	2.90	9	1
4:D:502:PCW:H161	4:D:505:PCW:C33	0.48	2.38	9	1
4:C:609:PCW:H211	4:C:615:PCW:C37	0.48	2.36	10	1
4:C:615:PCW:H483	4:D:509:PCW:C27	0.48	2.36	10	1
1:A:288:ARG:O	1:A:292:HIS:HB2	0.48	2.09	1	2
4:A:402:PCW:H211	4:A:405:PCW:C21	0.48	2.38	1	1
4:A:407:PCW:C19	4:A:407:PCW:C15	0.48	2.92	8	9
4:C:621:PCW:H381	5:C:631:17F:H77	0.48	1.84	1	1
5:C:630:17F:O10	5:C:630:17F:O6	0.48	2.31	1	3
4:D:501:PCW:H172	4:D:501:PCW:C21	0.48	2.38	1	1
4:D:509:PCW:H421	5:D:520:17F:H32	0.48	1.86	1	1
4:A:404:PCW:H281	4:A:411:PCW:C22	0.48	2.27	2	2
4:A:413:PCW:C43	4:D:526:PCW:H211	0.48	2.39	2	1
4:C:615:PCW:H221	4:D:512:PCW:H282	0.48	1.85	2	1
4:C:605:PCW:H82	5:C:628:17F:O4	0.48	2.08	3	1
4:C:609:PCW:H271	5:C:626:17F:H70	0.48	1.85	3	1
4:A:408:PCW:H381	4:B:203:PCW:H412	0.48	1.85	10	3
4:C:613:PCW:H251	5:D:521:17F:C26	0.48	2.39	4	3
5:D:520:17F:H55	5:D:525:17F:H71	0.48	1.86	4	1
4:D:511:PCW:H221	5:D:522:17F:O10	0.48	2.09	5	1
3:D:400:ARG:HB2	3:D:424:GLU:OE1	0.48	2.09	6	1
1:A:217:LEU:HD11	4:A:404:PCW:H251	0.48	1.85	7	1
4:B:203:PCW:H461	4:B:204:PCW:H422	0.48	1.84	8	2
4:D:501:PCW:O1P	5:D:525:17F:H19A	0.48	2.07	8	1
4:D:506:PCW:O11	4:D:516:PCW:H341	0.48	2.08	8	1
4:C:616:PCW:C48	4:D:504:PCW:H222	0.48	2.39	10	1
4:B:201:PCW:H362	4:D:510:PCW:H431	0.48	1.85	10	1
4:D:501:PCW:H472	4:D:515:PCW:H251	0.48	1.84	10	1
4:D:506:PCW:O2	4:D:509:PCW:H382	0.48	2.08	10	1
4:A:404:PCW:C37	4:D:510:PCW:H182	0.48	2.35	1	1
1:C:442:SER:O	1:C:446:GLU:HG2	0.48	2.09	1	1
2:B:8:VAL:HG12	2:B:79:LEU:HB2	0.48	1.85	8	2
4:A:408:PCW:H381	4:B:203:PCW:H411	0.48	1.85	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:610:PCW:C6	5:C:629:17F:O8	0.48	2.62	2	3
3:D:427:GLN:HB2	4:D:502:PCW:H63	0.48	1.85	2	1
4:C:602:PCW:C15	5:C:626:17F:H49	0.48	2.38	4	1
2:B:21:ILE:HD11	3:D:388:VAL:HG11	0.48	1.85	4	1
4:B:202:PCW:H481	5:D:524:17F:H31	0.48	1.84	4	1
4:D:502:PCW:H283	4:D:505:PCW:C12	0.48	2.34	4	1
4:D:511:PCW:H32	4:D:511:PCW:O1P	0.48	2.09	6	1
4:A:401:PCW:H472	4:C:611:PCW:H283	0.48	1.86	8	1
4:B:202:PCW:H472	4:D:510:PCW:C22	0.48	2.29	8	2
4:D:517:PCW:H222	4:D:517:PCW:C42	0.48	2.39	9	1
4:C:623:PCW:O31	4:C:623:PCW:C4	0.48	2.58	10	1
4:D:507:PCW:H42	5:D:523:17F:H9	0.48	1.86	10	1
4:D:511:PCW:H132	4:D:511:PCW:H321	0.48	1.86	10	1
4:C:605:PCW:H39	4:C:611:PCW:O2	0.48	2.09	5	2
4:C:618:PCW:O1P	4:C:625:PCW:C8	0.48	2.62	10	2
4:D:507:PCW:H161	4:D:513:PCW:H262	0.48	1.86	1	1
4:D:513:PCW:H421	4:D:513:PCW:C28	0.48	2.39	1	1
3:D:399:PHE:CE2	3:D:429:ASP:HB3	0.48	2.44	8	2
5:D:529:17F:O9	5:D:529:17F:P1	0.48	2.72	4	2
4:A:415:PCW:C6	4:C:605:PCW:O2P	0.48	2.61	4	1
4:D:507:PCW:H63	5:D:523:17F:H2	0.48	1.84	4	1
4:C:603:PCW:H12	4:C:603:PCW:O31	0.48	2.09	5	1
4:C:616:PCW:C44	4:C:625:PCW:H232	0.48	2.39	6	1
4:D:509:PCW:C7	4:D:514:PCW:H12	0.48	2.38	6	1
5:D:524:17F:H12	5:D:524:17F:H62	0.48	1.84	8	1
1:C:581:LYS:O	1:C:585:LEU:HG	0.48	2.09	10	2
4:D:506:PCW:H82	4:D:515:PCW:O2P	0.48	2.09	9	1
4:D:509:PCW:H412	5:D:520:17F:H10	0.48	1.84	9	1
4:C:603:PCW:H242	4:D:526:PCW:H351	0.48	1.85	10	1
4:C:612:PCW:O31	4:C:612:PCW:O3	0.48	2.32	10	1
4:C:604:PCW:C19	5:D:525:17F:H76	0.47	2.34	1	1
1:A:242:GLU:HA	1:A:245:LYS:HD2	0.47	1.86	2	1
4:C:616:PCW:H431	4:B:201:PCW:H472	0.47	1.85	2	1
4:C:625:PCW:H282	5:C:629:17F:H51	0.47	1.84	2	1
4:D:527:PCW:H422	4:D:528:PCW:H331	0.47	1.86	2	2
5:A:409:17F:H74	4:C:605:PCW:H281	0.47	1.84	3	1
1:C:510:HIS:O	1:C:514:LEU:HG	0.47	2.08	3	4
4:C:605:PCW:H472	4:C:619:PCW:C44	0.47	2.38	3	1
4:B:203:PCW:H412	4:B:203:PCW:C16	0.47	2.36	5	2
4:D:505:PCW:C8	5:D:519:17F:O8	0.47	2.62	3	1
4:D:517:PCW:O2	4:D:517:PCW:O1P	0.47	2.32	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:415:PCW:H73	4:C:622:PCW:H332	0.47	1.85	6	1
4:D:510:PCW:H272	5:D:524:17F:C34	0.47	2.38	6	1
4:C:603:PCW:H162	4:D:528:PCW:H231	0.47	1.85	7	1
4:D:509:PCW:H162	5:D:520:17F:C31	0.47	2.39	7	1
4:D:506:PCW:H51	4:D:515:PCW:O1P	0.47	2.09	8	1
4:D:502:PCW:O4P	4:D:502:PCW:O11	0.47	2.32	9	1
4:D:507:PCW:C23	4:D:513:PCW:H40	0.47	2.30	9	1
4:D:510:PCW:H451	5:D:524:17F:H60	0.47	1.85	9	1
4:C:603:PCW:H442	4:D:526:PCW:C36	0.47	2.38	10	1
4:A:403:PCW:H141	4:A:403:PCW:H382	0.47	1.86	1	1
4:D:511:PCW:H372	4:D:511:PCW:H411	0.47	1.86	2	2
4:C:607:PCW:H451	4:C:624:PCW:H481	0.47	1.86	2	1
4:A:414:PCW:H12	4:A:414:PCW:O31	0.47	2.09	3	1
4:B:202:PCW:H283	4:B:203:PCW:H172	0.47	1.85	3	1
4:C:602:PCW:H362	5:D:523:17F:C37	0.47	2.39	9	3
2:B:169:LYS:HA	2:B:172:LYS:HE2	0.47	1.86	4	1
4:B:203:PCW:H20	4:D:506:PCW:C46	0.47	2.38	4	1
4:D:517:PCW:H351	5:D:520:17F:C8	0.47	2.39	4	1
4:D:517:PCW:H421	5:D:525:17F:C12	0.47	2.38	5	1
4:D:513:PCW:O11	4:D:513:PCW:C7	0.47	2.62	6	1
4:A:410:PCW:H121	4:C:617:PCW:C33	0.47	2.38	7	1
4:A:412:PCW:C32	4:C:623:PCW:H342	0.47	2.39	7	1
4:C:614:PCW:C43	4:C:619:PCW:H20	0.47	2.39	7	1
4:B:201:PCW:C34	4:D:510:PCW:H361	0.47	2.36	8	1
4:B:201:PCW:H122	4:D:506:PCW:H322	0.47	1.85	8	1
4:D:516:PCW:H32	4:D:516:PCW:O2P	0.47	2.09	8	1
5:D:529:17F:C18	5:D:529:17F:H9A	0.47	2.38	8	1
4:A:401:PCW:H332	3:D:406:LYS:HD2	0.47	1.86	9	2
4:A:406:PCW:H31	4:B:204:PCW:C11	0.47	2.38	9	1
4:D:515:PCW:O4P	4:D:515:PCW:H62	0.47	2.09	9	1
5:D:530:17F:O9	5:D:530:17F:P1	0.47	2.72	9	1
4:C:624:PCW:O2P	4:C:624:PCW:C31	0.47	2.62	10	1
4:B:202:PCW:N	5:D:524:17F:O4	0.47	2.48	1	1
4:C:625:PCW:C25	4:D:527:PCW:H451	0.47	2.40	2	1
4:D:509:PCW:C27	5:D:520:17F:H10	0.47	2.38	2	1
4:A:403:PCW:H272	4:D:507:PCW:H171	0.47	1.84	3	1
4:B:202:PCW:H481	4:D:510:PCW:H271	0.47	1.85	3	1
3:D:478:THR:HB	4:D:501:PCW:C5	0.47	2.40	5	1
4:D:506:PCW:C15	5:D:529:17F:H55	0.47	2.39	5	1
4:C:609:PCW:O31	4:C:609:PCW:O3	0.47	2.32	6	1
4:C:611:PCW:C3	4:C:619:PCW:H63	0.47	2.39	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:623:PCW:H411	4:C:624:PCW:H412	0.47	1.79	6	1
4:D:507:PCW:H151	4:D:513:PCW:H321	0.47	1.83	6	1
4:D:518:PCW:C31	5:D:519:17F:H32	0.47	2.38	6	1
4:A:411:PCW:O4P	4:A:411:PCW:O31	0.47	2.32	7	1
4:C:603:PCW:H32	4:C:604:PCW:C8	0.47	2.39	7	1
4:D:518:PCW:H161	5:D:519:17F:H33	0.47	1.86	8	1
5:C:631:17F:H59	5:C:631:17F:H67	0.47	1.86	9	1
2:B:77:GLY:HA3	2:B:159:LEU:HD21	0.47	1.86	9	1
4:B:201:PCW:C14	4:D:506:PCW:H461	0.47	2.39	9	1
4:D:507:PCW:H181	4:D:513:PCW:H271	0.47	1.84	9	1
4:D:514:PCW:H231	4:D:514:PCW:H161	0.47	1.86	9	1
4:A:412:PCW:O2P	4:C:623:PCW:H321	0.47	2.10	1	1
4:C:605:PCW:H382	4:C:611:PCW:C1	0.47	2.39	1	1
4:A:407:PCW:H371	5:D:522:17F:C36	0.47	2.33	2	1
4:C:606:PCW:O4P	4:C:606:PCW:H2	0.47	2.09	3	1
4:C:609:PCW:C12	4:C:615:PCW:C7	0.47	2.92	5	4
4:C:620:PCW:O31	4:C:620:PCW:P	0.47	2.73	3	1
4:B:201:PCW:H232	4:D:506:PCW:H442	0.47	1.82	3	1
4:D:511:PCW:H73	4:D:511:PCW:O11	0.47	2.09	3	1
4:D:517:PCW:C39	5:D:520:17F:H49	0.47	2.37	3	1
4:D:513:PCW:C48	5:D:522:17F:H78	0.47	2.39	5	1
4:A:406:PCW:C23	4:A:406:PCW:C18	0.47	2.86	6	1
5:A:409:17F:C36	4:D:503:PCW:H272	0.47	2.39	6	1
4:D:504:PCW:C15	4:D:510:PCW:H39	0.47	2.39	6	1
4:D:507:PCW:H141	4:D:513:PCW:C34	0.47	2.39	6	1
4:A:412:PCW:H481	4:C:604:PCW:H271	0.47	1.84	7	1
4:A:414:PCW:O3P	4:A:414:PCW:O31	0.47	2.32	8	1
4:D:512:PCW:H371	4:D:512:PCW:C41	0.47	2.38	9	1
4:A:401:PCW:H51	4:D:511:PCW:H131	0.47	1.86	10	1
4:B:203:PCW:H262	4:D:504:PCW:C23	0.47	2.38	10	1
1:C:421:PRO:O	1:C:425:GLU:HG2	0.47	2.09	1	3
4:A:401:PCW:C39	4:D:503:PCW:H231	0.47	2.39	6	2
5:C:626:17F:H40	5:C:627:17F:C42	0.47	2.34	2	1
4:C:617:PCW:O3P	4:C:617:PCW:C5	0.47	2.62	10	2
5:C:630:17F:O7	5:C:630:17F:C17	0.47	2.63	3	6
3:D:425:GLU:HB2	4:D:502:PCW:H52	0.47	1.85	4	1
4:D:511:PCW:O1P	4:D:511:PCW:H32	0.47	2.10	10	2
4:B:203:PCW:C34	4:D:506:PCW:H382	0.47	2.40	6	1
4:D:510:PCW:C19	5:D:524:17F:H20	0.47	2.40	6	1
4:D:511:PCW:C27	5:D:522:17F:H56	0.47	2.39	6	1
1:C:463:TRP:CD1	5:C:627:17F:H68	0.47	2.45	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:405:PCW:O3	4:D:514:PCW:H331	0.47	2.09	9	1
4:D:513:PCW:O31	4:D:513:PCW:P	0.47	2.72	9	1
4:D:506:PCW:H441	4:D:528:PCW:H481	0.47	1.85	10	1
4:A:401:PCW:H12	4:D:511:PCW:C16	0.47	2.38	1	1
4:C:619:PCW:H472	4:D:501:PCW:C28	0.47	2.39	1	1
4:C:625:PCW:C31	4:C:625:PCW:O3	0.47	2.62	1	2
4:B:201:PCW:H41	4:D:504:PCW:H142	0.47	1.86	3	1
4:D:501:PCW:C21	5:D:521:17F:C19	0.47	2.91	4	1
4:D:503:PCW:C41	4:D:511:PCW:H331	0.47	2.39	5	1
4:A:403:PCW:H411	4:D:513:PCW:H39	0.47	1.83	6	1
4:A:412:PCW:O1P	4:C:623:PCW:H321	0.47	2.08	6	1
4:D:508:PCW:C11	4:D:509:PCW:H261	0.47	2.40	6	1
4:D:513:PCW:O4P	4:D:513:PCW:C3	0.47	2.47	6	1
4:A:402:PCW:C42	4:D:512:PCW:H152	0.47	2.33	7	1
4:B:202:PCW:H252	4:B:204:PCW:H39	0.47	1.86	7	1
4:B:203:PCW:H451	4:B:203:PCW:C16	0.47	2.40	7	1
4:A:413:PCW:C39	4:C:617:PCW:H472	0.47	2.40	8	1
4:A:414:PCW:C34	4:C:617:PCW:H132	0.47	2.40	8	1
4:A:401:PCW:H51	4:D:511:PCW:C31	0.47	2.40	9	1
4:D:507:PCW:C23	4:D:513:PCW:H281	0.47	2.30	9	1
5:D:524:17F:C30	4:D:527:PCW:H212	0.47	2.39	10	1
4:D:506:PCW:H151	4:D:516:PCW:H411	0.47	1.87	3	2
5:D:520:17F:O7	5:D:520:17F:C17	0.47	2.62	1	3
4:A:403:PCW:O1P	4:A:403:PCW:H51	0.47	2.10	4	2
4:A:406:PCW:C5	4:B:204:PCW:H32	0.47	2.39	2	1
4:A:407:PCW:O4P	4:A:407:PCW:C8	0.47	2.62	2	5
4:A:412:PCW:H483	4:D:517:PCW:H472	0.47	1.86	2	1
4:C:602:PCW:H39	4:C:602:PCW:H161	0.47	1.85	2	1
4:C:615:PCW:C20	5:C:631:17F:H38	0.47	2.40	2	1
4:C:625:PCW:H252	4:D:527:PCW:H451	0.47	1.87	2	1
4:D:512:PCW:H441	4:D:514:PCW:H251	0.47	1.86	2	1
4:C:604:PCW:H361	5:D:529:17F:C2X	0.47	2.20	3	1
4:C:608:PCW:H461	5:C:626:17F:H60	0.47	1.87	3	1
4:B:202:PCW:H262	4:B:204:PCW:H39	0.47	1.87	3	1
4:D:508:PCW:O3	4:D:508:PCW:C31	0.47	2.62	4	5
4:C:607:PCW:H361	4:C:624:PCW:C44	0.47	2.40	4	1
4:C:617:PCW:O31	4:C:617:PCW:C6	0.47	2.62	7	3
4:B:202:PCW:H62	3:D:486:ASP:HB2	0.47	1.86	4	1
4:D:503:PCW:C39	5:D:522:17F:H10A	0.47	2.39	4	2
4:D:506:PCW:H281	4:D:515:PCW:H471	0.47	1.86	4	1
4:D:510:PCW:H131	5:D:524:17F:C42	0.47	2.39	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:611:PCW:H12	4:C:619:PCW:O11	0.47	2.10	5	1
4:C:622:PCW:H20	5:D:525:17F:H78	0.47	1.86	6	1
4:D:518:PCW:H442	5:D:519:17F:H70	0.47	1.87	7	1
1:A:267:GLU:O	1:A:271:LEU:HG	0.47	2.09	8	1
4:A:402:PCW:H442	4:D:508:PCW:C27	0.47	2.36	8	1
4:A:404:PCW:H283	4:A:411:PCW:C24	0.47	2.37	8	1
4:A:405:PCW:C32	4:D:514:PCW:H372	0.47	2.35	8	1
2:B:43:GLN:HG3	2:B:52:LEU:HG	0.47	1.87	8	1
4:B:203:PCW:H19	4:D:506:PCW:C47	0.47	2.38	8	1
4:D:516:PCW:H482	4:D:527:PCW:C22	0.47	2.40	8	1
4:D:517:PCW:H281	5:D:522:17F:H77	0.47	1.86	8	1
4:A:405:PCW:O31	4:A:405:PCW:O4P	0.47	2.33	9	1
4:A:407:PCW:C43	4:A:412:PCW:H281	0.47	2.40	9	1
4:C:609:PCW:H73	4:C:620:PCW:H31	0.47	1.87	9	1
4:D:513:PCW:H272	4:D:513:PCW:C41	0.47	2.39	9	1
4:D:515:PCW:C18	4:D:515:PCW:H232	0.47	2.39	9	1
4:C:611:PCW:O11	4:C:619:PCW:C6	0.47	2.62	10	1
4:C:612:PCW:C6	4:C:618:PCW:H12	0.47	2.38	10	1
1:A:365:LYS:CB	1:A:366:PRO:HD3	0.47	2.39	2	7
4:A:402:PCW:C39	4:A:405:PCW:H261	0.47	2.38	1	1
5:C:631:17F:H52	4:D:512:PCW:C18	0.47	2.39	3	3
4:A:402:PCW:H332	4:A:405:PCW:H121	0.47	1.86	5	2
4:C:611:PCW:C22	4:C:619:PCW:H482	0.47	2.40	10	2
4:C:613:PCW:H32	4:C:619:PCW:C3	0.47	2.39	2	2
4:D:502:PCW:H381	5:D:524:17F:C42	0.47	2.27	2	1
4:C:605:PCW:H482	4:C:619:PCW:H441	0.47	1.86	4	2
4:C:602:PCW:C5	5:D:523:17F:O10	0.47	2.62	4	1
4:D:510:PCW:H20	5:D:524:17F:C31	0.47	2.40	4	1
4:D:506:PCW:H222	4:D:516:PCW:H412	0.47	1.87	5	1
4:C:610:PCW:C31	4:C:610:PCW:O3	0.47	2.62	10	2
4:B:201:PCW:C32	4:D:510:PCW:H382	0.47	2.39	6	1
4:A:401:PCW:H322	4:D:511:PCW:H232	0.47	1.86	7	1
4:A:406:PCW:H31	4:A:406:PCW:O1P	0.47	2.09	7	1
4:A:407:PCW:H131	4:A:407:PCW:C34	0.47	2.40	7	1
4:D:503:PCW:H431	5:D:522:17F:C9	0.47	2.39	8	1
4:D:508:PCW:H12	5:D:523:17F:H11	0.47	1.85	8	1
4:D:502:PCW:C32	4:D:505:PCW:O2P	0.47	2.62	9	1
4:A:411:PCW:C35	4:C:612:PCW:C13	0.47	2.92	10	1
3:D:402:LEU:HD13	4:D:503:PCW:C6	0.47	2.40	10	1
4:D:502:PCW:C28	4:D:518:PCW:H211	0.47	2.39	1	1
4:D:503:PCW:C38	4:D:511:PCW:H352	0.47	2.35	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:517:PCW:H73	5:D:520:17F:O2	0.47	2.10	1	1
4:A:412:PCW:H431	4:C:623:PCW:C44	0.47	2.40	2	1
4:C:621:PCW:H151	5:C:630:17F:C4	0.47	2.40	4	2
3:D:464:ARG:HA	3:D:470:TYR:O	0.47	2.10	2	1
4:D:506:PCW:H271	4:D:516:PCW:C12	0.47	2.32	2	1
2:B:128:LYS:O	2:B:132:ASP:HB2	0.47	2.10	3	2
4:D:508:PCW:H62	4:D:517:PCW:O3P	0.47	2.09	4	1
1:A:224:VAL:HG22	1:C:550:LYS:HD3	0.47	1.87	5	1
4:C:616:PCW:H421	4:C:625:PCW:H232	0.47	1.87	5	1
4:D:504:PCW:H172	4:D:510:PCW:C40	0.47	2.40	5	1
4:D:506:PCW:H152	5:D:520:17F:C22	0.47	2.40	5	1
4:C:611:PCW:H41	4:C:622:PCW:H321	0.47	1.87	6	1
4:C:611:PCW:O4P	4:C:622:PCW:H342	0.47	2.10	6	1
4:A:415:PCW:H451	5:D:521:17F:C42	0.47	2.40	8	1
4:D:508:PCW:C23	4:D:512:PCW:H172	0.47	2.39	8	1
4:D:509:PCW:H483	4:D:509:PCW:H282	0.47	1.87	8	1
4:C:609:PCW:C26	4:C:615:PCW:H411	0.47	2.40	9	2
4:C:618:PCW:P	4:C:625:PCW:H42	0.47	2.50	9	1
4:D:515:PCW:H2	5:D:525:17F:C31	0.47	2.40	9	1
5:D:524:17F:H11A	5:D:524:17F:C37	0.47	2.40	9	1
4:A:411:PCW:C43	4:C:612:PCW:H172	0.47	2.18	10	1
4:C:602:PCW:H341	5:D:523:17F:C34	0.47	2.39	1	1
4:C:603:PCW:H461	4:D:526:PCW:H412	0.47	1.86	1	3
4:C:606:PCW:H63	4:C:606:PCW:H131	0.47	1.87	1	1
4:A:407:PCW:H432	4:A:412:PCW:H242	0.47	1.86	2	1
4:C:609:PCW:O31	4:C:609:PCW:H131	0.47	2.10	2	3
2:B:1:MET:SD	4:B:201:PCW:H61	0.47	2.49	2	1
4:D:509:PCW:H40	5:D:520:17F:H30	0.47	1.87	2	1
4:D:509:PCW:H222	4:D:509:PCW:H182	0.47	1.87	3	1
4:C:615:PCW:H2	4:C:615:PCW:O4P	0.47	2.10	5	1
4:B:202:PCW:H281	4:B:203:PCW:H172	0.47	1.87	8	2
4:D:508:PCW:H162	4:D:512:PCW:H362	0.47	1.86	5	1
4:A:406:PCW:C7	4:B:204:PCW:O2P	0.47	2.64	7	1
4:C:613:PCW:C13	4:C:613:PCW:H361	0.47	2.40	8	1
4:B:201:PCW:C3	4:B:201:PCW:P	0.47	3.03	8	1
4:C:608:PCW:H63	4:C:624:PCW:C24	0.47	2.37	9	1
2:B:32:TYR:HD1	6:B:205:GNP:H5'1	0.47	1.70	9	1
4:B:204:PCW:C7	4:B:204:PCW:H321	0.47	2.40	9	1
4:D:505:PCW:H451	5:D:519:17F:H53	0.47	1.87	9	1
4:D:505:PCW:H432	4:D:518:PCW:C25	0.47	2.39	10	1
4:D:511:PCW:H412	4:D:511:PCW:C23	0.47	2.40	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:501:PCW:H212	5:D:521:17F:H61	0.46	1.87	1	1
5:D:519:17F:H65	5:D:519:17F:C32	0.46	2.37	1	1
4:A:403:PCW:H41	4:A:407:PCW:O1P	0.46	2.10	2	1
4:A:406:PCW:H52	4:B:204:PCW:H32	0.46	1.87	2	1
4:C:609:PCW:C8	4:C:609:PCW:O4P	0.46	2.63	2	6
4:D:513:PCW:H461	5:D:522:17F:H78	0.46	1.87	2	1
5:D:525:17F:O9	5:D:525:17F:C7	0.46	2.63	10	4
4:B:201:PCW:H162	4:D:506:PCW:C37	0.46	2.41	3	1
4:B:202:PCW:O4P	4:B:202:PCW:O2	0.46	2.33	3	1
4:D:501:PCW:O3	4:D:503:PCW:H351	0.46	2.11	3	1
4:D:503:PCW:H40	5:D:522:17F:H41	0.46	1.87	3	1
4:A:408:PCW:H351	4:D:514:PCW:H431	0.46	1.85	4	1
4:C:601:PCW:H382	5:C:626:17F:H53	0.46	1.87	4	1
4:C:618:PCW:P	4:C:625:PCW:H52	0.46	2.50	4	1
4:D:501:PCW:O31	4:D:501:PCW:O3	0.46	2.34	7	5
4:C:613:PCW:C14	4:C:619:PCW:C38	0.46	2.91	5	1
4:D:510:PCW:O3P	4:D:510:PCW:C31	0.46	2.63	6	2
4:A:406:PCW:H232	4:A:406:PCW:C18	0.46	2.39	6	1
4:A:410:PCW:H151	4:A:410:PCW:C39	0.46	2.18	6	1
4:D:505:PCW:O3	4:D:505:PCW:C31	0.46	2.63	9	2
4:C:603:PCW:H162	4:D:528:PCW:C23	0.46	2.39	7	1
4:C:618:PCW:H362	5:C:629:17F:C21	0.46	2.40	8	1
4:D:502:PCW:H62	5:D:519:17F:O4	0.46	2.10	9	1
4:D:507:PCW:H152	4:D:513:PCW:H371	0.46	1.86	9	1
4:A:403:PCW:O31	4:A:403:PCW:H11	0.46	2.10	10	1
4:D:517:PCW:H411	4:D:517:PCW:C17	0.46	2.40	10	1
5:D:522:17F:H1	5:D:522:17F:C4	0.46	2.40	10	1
4:D:527:PCW:H142	4:D:527:PCW:C37	0.46	2.39	1	1
4:A:410:PCW:O11	4:A:410:PCW:C2	0.46	2.57	2	1
4:A:415:PCW:H261	4:D:528:PCW:H242	0.46	1.86	2	2
4:D:511:PCW:C19	5:D:522:17F:O10	0.46	2.63	2	3
4:C:621:PCW:H212	5:C:629:17F:H19A	0.46	1.87	3	1
4:D:516:PCW:O2P	4:D:516:PCW:H32	0.46	2.09	3	1
1:A:330:ARG:O	1:A:334:ARG:HG2	0.46	2.09	4	1
4:A:406:PCW:O11	4:B:202:PCW:C14	0.46	2.63	4	1
3:D:459:LEU:HG	3:D:471:LYS:HB2	0.46	1.87	4	1
4:D:508:PCW:H82	5:D:523:17F:H9	0.46	1.87	4	1
4:C:608:PCW:C17	5:C:627:17F:C18	0.46	2.93	6	1
4:C:614:PCW:N	4:C:623:PCW:O1P	0.46	2.48	6	1
4:D:510:PCW:O11	4:D:510:PCW:H2	0.46	2.11	6	1
4:D:511:PCW:H182	5:D:522:17F:H19A	0.46	1.87	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:411:PCW:O31	4:A:411:PCW:O4P	0.46	2.34	8	1
4:C:611:PCW:O4P	4:C:619:PCW:H62	0.46	2.11	8	1
4:C:608:PCW:H121	4:C:609:PCW:H161	0.46	1.86	9	1
4:D:501:PCW:C41	4:D:515:PCW:H171	0.46	2.40	9	1
4:D:511:PCW:O11	4:D:511:PCW:C5	0.46	2.63	9	1
4:A:408:PCW:C40	4:B:203:PCW:H362	0.46	2.40	10	1
5:C:631:17F:C29	4:D:512:PCW:H211	0.46	2.34	10	1
4:D:513:PCW:C12	5:D:523:17F:H18	0.46	2.40	10	1
4:D:517:PCW:H351	5:D:525:17F:H57	0.46	1.87	10	1
4:A:403:PCW:H241	4:D:507:PCW:C17	0.46	2.34	2	2
4:A:408:PCW:C48	4:D:528:PCW:H471	0.46	2.40	1	1
4:A:414:PCW:H162	5:C:628:17F:C31	0.46	2.20	4	2
4:A:415:PCW:H281	4:C:622:PCW:C25	0.46	2.41	1	1
4:A:415:PCW:H321	4:A:415:PCW:H61	0.46	1.88	1	1
4:C:614:PCW:O1P	4:C:623:PCW:H73	0.46	2.10	1	1
2:B:3:GLU:OE1	4:B:201:PCW:H62	0.46	2.09	1	1
3:D:405:HIS:CE1	3:D:408:LYS:HB2	0.46	2.45	1	1
4:D:503:PCW:C41	4:D:511:PCW:H212	0.46	2.40	1	1
4:C:604:PCW:H251	5:D:525:17F:C41	0.46	2.39	4	2
5:C:630:17F:H47	5:D:529:17F:H12	0.46	1.87	2	1
4:D:510:PCW:H272	5:D:524:17F:H60	0.46	1.87	2	1
4:A:402:PCW:H82	4:A:405:PCW:O11	0.46	2.10	3	1
4:A:403:PCW:H141	4:A:403:PCW:H40	0.46	1.82	3	1
1:C:435:GLU:O	1:C:439:GLN:HG3	0.46	2.09	3	1
4:C:605:PCW:O1P	4:C:605:PCW:O31	0.46	2.34	3	1
4:C:616:PCW:C33	4:D:527:PCW:H341	0.46	2.40	7	4
4:B:201:PCW:H332	4:D:504:PCW:H172	0.46	1.86	3	1
4:B:203:PCW:H63	4:B:203:PCW:O4P	0.46	2.10	3	1
1:C:574:LEU:O	1:C:578:GLU:HG2	0.46	2.10	10	2
4:D:503:PCW:H411	4:D:511:PCW:H221	0.46	1.87	10	2
4:D:518:PCW:H422	5:D:519:17F:H68	0.46	1.87	4	1
4:B:201:PCW:H212	4:B:201:PCW:C17	0.46	2.40	5	1
3:D:442:ALA:HB3	3:D:464:ARG:O	0.46	2.11	5	2
4:B:201:PCW:C21	4:D:506:PCW:H472	0.46	2.39	6	1
4:D:504:PCW:H161	4:D:504:PCW:H271	0.46	1.87	6	1
4:D:508:PCW:H122	4:D:509:PCW:H242	0.46	1.88	6	1
4:A:406:PCW:H261	4:B:203:PCW:H242	0.46	1.86	8	2
4:C:607:PCW:C3	4:C:624:PCW:H371	0.46	2.41	8	1
4:A:415:PCW:O11	4:A:415:PCW:C2	0.46	2.60	9	1
4:C:605:PCW:H322	4:C:611:PCW:C1	0.46	2.41	9	1
4:D:507:PCW:C22	4:D:513:PCW:H271	0.46	2.23	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:509:PCW:C14	5:D:520:17F:H20A	0.46	2.32	9	1
4:D:510:PCW:H20	5:D:524:17F:C20	0.46	2.40	9	1
4:D:515:PCW:C16	4:D:515:PCW:H212	0.46	2.41	9	1
4:A:415:PCW:H481	5:D:521:17F:C30	0.46	2.41	10	1
4:C:601:PCW:H382	5:C:626:17F:C29	0.46	2.37	10	1
4:C:608:PCW:H63	4:C:624:PCW:C23	0.46	2.41	10	1
4:A:413:PCW:C44	4:D:526:PCW:H231	0.46	2.40	1	1
4:A:415:PCW:H221	4:D:528:PCW:H242	0.46	1.87	4	2
4:C:605:PCW:O1P	4:C:613:PCW:H42	0.46	2.11	4	2
4:A:415:PCW:H472	5:D:521:17F:H55	0.46	1.88	2	1
4:C:615:PCW:C21	5:C:631:17F:C22	0.46	2.94	3	1
4:C:622:PCW:H241	4:D:501:PCW:H472	0.46	1.87	3	1
4:B:204:PCW:H283	4:B:204:PCW:C42	0.46	2.36	3	1
4:C:609:PCW:N	4:C:620:PCW:O11	0.46	2.48	9	4
4:D:506:PCW:C15	5:D:520:17F:H41	0.46	2.37	4	1
4:D:507:PCW:H481	5:D:522:17F:H47	0.46	1.87	4	1
4:D:508:PCW:C17	4:D:512:PCW:C15	0.46	2.93	4	1
4:A:415:PCW:C18	4:C:603:PCW:C14	0.46	2.94	6	1
4:C:604:PCW:H231	4:D:517:PCW:H472	0.46	1.85	6	1
4:C:616:PCW:H441	4:C:625:PCW:H231	0.46	1.87	6	1
2:B:84:ILE:CD1	2:B:118:CYS:HA	0.46	2.36	6	1
4:D:512:PCW:C6	5:D:520:17F:O4	0.46	2.63	7	1
4:A:413:PCW:H40	4:C:616:PCW:H172	0.46	1.87	8	1
4:A:403:PCW:H161	4:D:513:PCW:H372	0.46	1.87	9	1
4:C:606:PCW:C40	4:C:609:PCW:H31	0.46	2.40	10	1
4:D:501:PCW:C21	5:D:521:17F:C33	0.46	2.93	1	1
4:D:506:PCW:C22	4:D:516:PCW:C35	0.46	2.88	1	1
4:C:605:PCW:H421	4:C:619:PCW:C14	0.46	2.35	6	5
3:D:425:GLU:CB	4:D:502:PCW:H73	0.46	2.26	2	1
4:A:413:PCW:H482	5:D:524:17F:H38	0.46	1.87	3	1
4:B:201:PCW:H331	4:D:510:PCW:C39	0.46	2.40	3	1
4:C:610:PCW:H31	5:C:629:17F:O9	0.46	2.11	4	2
3:D:425:GLU:CB	4:D:502:PCW:H52	0.46	2.41	4	1
5:C:626:17F:C23	5:C:627:17F:H75	0.46	2.40	5	1
4:D:505:PCW:O2P	4:D:510:PCW:O4P	0.46	2.34	5	1
5:D:522:17F:C4	5:D:522:17F:H18A	0.46	2.41	5	1
4:C:602:PCW:H221	4:C:602:PCW:C15	0.46	2.40	6	1
4:D:508:PCW:H121	4:D:512:PCW:C16	0.46	2.40	6	1
4:B:201:PCW:H62	4:D:504:PCW:H52	0.46	1.87	7	1
3:D:483:MET:HG3	3:D:485:VAL:H	0.46	1.71	7	1
4:D:514:PCW:C23	4:D:514:PCW:C18	0.46	2.93	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:520:17F:C27	5:D:525:17F:H71	0.46	2.37	7	1
4:C:605:PCW:H321	4:C:611:PCW:H12	0.46	1.88	9	2
4:C:615:PCW:H483	4:D:509:PCW:C24	0.46	2.24	9	1
4:C:616:PCW:H482	4:B:203:PCW:C28	0.46	2.41	9	1
4:A:404:PCW:O31	4:A:404:PCW:H11	0.46	2.09	4	2
4:A:407:PCW:O31	4:A:407:PCW:H11	0.46	2.10	8	4
4:D:506:PCW:O2P	4:D:506:PCW:C31	0.46	2.64	1	1
4:C:613:PCW:H281	5:D:521:17F:H35	0.46	1.88	2	1
4:D:502:PCW:H422	4:D:502:PCW:H211	0.46	1.87	2	1
4:A:410:PCW:C19	4:A:413:PCW:H431	0.46	2.40	9	2
4:C:602:PCW:H152	5:C:626:17F:H49	0.46	1.87	4	1
4:D:506:PCW:H141	5:D:520:17F:H29	0.46	1.88	5	1
5:D:522:17F:H12	5:D:522:17F:C24	0.46	2.25	5	1
4:D:508:PCW:C15	4:D:512:PCW:H171	0.46	2.33	6	1
4:C:606:PCW:H63	4:C:606:PCW:C11	0.46	2.39	7	1
2:B:97:ARG:HG2	2:B:111:MET:HE1	0.46	1.87	7	1
3:D:441:PHE:HE1	3:D:477:SER:HB3	0.46	1.71	7	1
4:A:406:PCW:H121	4:B:204:PCW:C12	0.46	2.39	8	1
4:C:609:PCW:H271	5:C:626:17F:C40	0.46	2.26	8	2
5:C:626:17F:H18A	5:C:627:17F:H55	0.46	1.85	8	1
1:A:249:GLU:O	1:A:253:LYS:HB2	0.46	2.10	10	1
4:D:515:PCW:C22	4:D:515:PCW:H181	0.46	2.41	10	1
4:A:412:PCW:O1P	4:C:623:PCW:H351	0.46	2.11	1	1
4:A:413:PCW:C44	4:C:616:PCW:H232	0.46	2.41	1	1
4:A:413:PCW:H31	4:C:617:PCW:H421	0.46	1.86	1	1
4:C:621:PCW:H352	5:C:631:17F:C42	0.46	2.40	1	1
4:D:504:PCW:H441	4:D:516:PCW:C17	0.46	2.40	1	1
5:D:530:17F:H59	5:D:530:17F:C1X	0.46	2.41	1	1
4:A:401:PCW:H63	4:D:503:PCW:O2P	0.46	2.10	2	1
4:D:509:PCW:H442	5:D:520:17F:H33	0.46	1.86	2	2
4:D:527:PCW:H422	4:D:528:PCW:C34	0.46	2.41	9	3
1:A:342:GLY:O	1:A:346:LEU:HG	0.46	2.10	3	1
4:C:625:PCW:H20	4:D:528:PCW:H371	0.46	1.88	3	1
4:D:502:PCW:H152	4:D:505:PCW:H31	0.46	1.86	3	1
4:A:401:PCW:C25	4:C:614:PCW:H281	0.46	2.39	4	1
5:C:631:17F:H48	4:D:512:PCW:H211	0.46	1.88	4	1
4:D:504:PCW:H262	5:D:524:17F:C20	0.46	2.41	4	1
4:D:511:PCW:C27	4:D:511:PCW:C23	0.46	2.92	6	2
4:C:618:PCW:C48	4:D:510:PCW:H482	0.46	2.41	5	1
4:D:517:PCW:H252	5:D:522:17F:H60	0.46	1.86	5	1
1:A:383:LYS:O	1:A:387:LEU:HG	0.46	2.09	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:618:PCW:C43	4:C:625:PCW:H282	0.46	2.41	6	1
4:D:511:PCW:C36	4:D:511:PCW:C22	0.46	2.94	7	1
4:B:202:PCW:O4P	5:D:524:17F:H1A	0.46	2.10	8	1
4:D:515:PCW:C12	5:D:525:17F:H58	0.46	2.41	8	1
4:A:403:PCW:H31	4:A:403:PCW:H42	0.46	1.86	9	1
4:C:621:PCW:H481	5:C:630:17F:C12	0.46	2.37	9	1
4:B:201:PCW:C7	4:D:504:PCW:H51	0.46	2.24	9	1
5:D:520:17F:H42	5:D:529:17F:C30	0.46	2.34	9	1
5:D:524:17F:O2	5:D:524:17F:H2	0.46	2.09	10	2
4:C:623:PCW:C41	4:C:624:PCW:C39	0.46	2.94	10	1
4:A:410:PCW:C19	4:A:413:PCW:H411	0.46	2.41	10	2
4:C:604:PCW:H19	5:D:525:17F:C42	0.46	2.33	1	1
4:C:614:PCW:O31	4:C:614:PCW:C1	0.46	2.59	5	3
5:C:626:17F:C21	5:C:627:17F:H72	0.46	2.40	1	1
4:D:517:PCW:H341	5:D:520:17F:O8	0.46	2.10	1	1
4:C:607:PCW:C43	4:C:624:PCW:C47	0.46	2.92	2	1
4:B:204:PCW:H132	4:B:204:PCW:O31	0.46	2.10	3	1
4:A:410:PCW:H271	4:D:502:PCW:C48	0.46	2.40	4	1
4:B:201:PCW:H442	4:D:510:PCW:H431	0.46	1.87	4	1
4:D:506:PCW:H281	4:D:516:PCW:H142	0.46	1.87	4	1
4:A:413:PCW:H412	4:D:526:PCW:C23	0.46	2.40	5	1
4:C:604:PCW:C8	5:D:530:17F:O2	0.46	2.64	6	1
4:A:405:PCW:C12	4:D:514:PCW:H331	0.46	2.40	7	1
4:A:406:PCW:H42	4:B:204:PCW:H11	0.46	1.87	7	1
4:C:603:PCW:O11	4:C:604:PCW:C8	0.46	2.64	7	1
4:C:615:PCW:C24	5:C:631:17F:H41	0.46	2.40	7	1
4:D:512:PCW:H51	4:D:512:PCW:H322	0.46	1.87	8	1
4:C:609:PCW:H281	5:D:523:17F:H54	0.46	1.87	10	1
1:A:233:GLU:O	1:A:237:GLU:HB2	0.46	2.11	1	1
1:A:245:LYS:O	1:A:249:GLU:HB2	0.46	2.11	5	2
3:D:457:LYS:HZ2	4:D:517:PCW:H122	0.46	1.70	1	1
4:D:527:PCW:O4P	4:D:527:PCW:C8	0.46	2.64	7	8
4:D:506:PCW:C26	4:D:516:PCW:H122	0.46	2.40	2	1
5:A:409:17F:O4	4:D:503:PCW:H51	0.46	2.10	3	1
4:C:612:PCW:H471	4:C:612:PCW:H252	0.46	1.87	3	1
4:C:606:PCW:C17	4:C:606:PCW:C21	0.46	2.78	4	2
4:C:606:PCW:H152	5:D:529:17F:H8	0.46	1.87	5	1
4:D:501:PCW:O11	4:D:501:PCW:C2	0.46	2.62	5	1
4:A:401:PCW:H342	4:D:511:PCW:H39	0.46	1.88	6	1
4:A:407:PCW:H2	5:D:522:17F:C1Y	0.46	2.41	6	1
4:A:408:PCW:H442	4:D:506:PCW:C45	0.46	2.30	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:601:PCW:H121	4:C:601:PCW:H483	0.46	1.86	6	1
4:A:406:PCW:H42	4:A:406:PCW:C3	0.46	2.38	8	1
4:B:202:PCW:C27	4:B:204:PCW:H39	0.46	2.41	8	2
5:D:520:17F:H72	5:D:530:17F:H54	0.46	1.88	8	1
5:C:631:17F:H40	4:D:512:PCW:H281	0.46	1.87	9	1
5:D:524:17F:H69	5:D:524:17F:C11	0.46	2.40	9	1
4:B:204:PCW:O1P	4:B:204:PCW:H51	0.46	2.11	10	1
4:D:511:PCW:H132	4:D:511:PCW:C33	0.46	2.41	10	1
4:A:408:PCW:H451	4:B:203:PCW:C19	0.46	2.41	1	1
4:C:616:PCW:O3	4:C:616:PCW:C31	0.46	2.64	4	5
4:D:507:PCW:H161	4:D:513:PCW:H222	0.46	1.88	1	1
4:D:510:PCW:H331	5:D:524:17F:C9	0.46	2.41	1	1
5:D:520:17F:O2	5:D:520:17F:C2	0.46	2.61	2	1
4:D:503:PCW:H40	5:D:522:17F:H8	0.46	1.88	4	1
4:A:410:PCW:H382	4:C:617:PCW:C14	0.46	2.39	5	1
4:C:613:PCW:H141	4:C:619:PCW:H382	0.46	1.88	5	1
5:C:629:17F:H53	4:B:203:PCW:C25	0.46	2.41	5	1
4:D:509:PCW:H232	5:D:520:17F:H31	0.46	1.87	5	1
5:A:409:17F:O5	4:D:503:PCW:C5	0.46	2.64	6	1
4:A:415:PCW:H181	4:C:603:PCW:C14	0.46	2.40	6	1
1:C:443:LYS:O	1:C:447:GLU:HB2	0.46	2.11	6	1
4:D:504:PCW:C38	4:D:516:PCW:H151	0.46	2.41	6	1
5:A:409:17F:H65	4:D:503:PCW:C21	0.46	2.41	7	1
3:D:441:PHE:CE1	3:D:477:SER:HB3	0.46	2.46	7	1
4:D:508:PCW:H211	4:D:512:PCW:H382	0.46	1.87	7	1
4:D:514:PCW:H231	4:D:514:PCW:C18	0.46	2.41	7	1
5:A:409:17F:H68	4:D:501:PCW:H252	0.46	1.87	8	1
4:C:615:PCW:C21	4:D:512:PCW:H272	0.46	2.40	8	1
4:B:201:PCW:P	4:B:201:PCW:H32	0.46	2.51	8	1
4:D:513:PCW:H381	5:D:522:17F:H64	0.46	1.87	8	1
4:A:402:PCW:H342	4:A:405:PCW:H121	0.46	1.88	9	1
5:C:631:17F:C29	4:D:512:PCW:C16	0.46	2.94	9	1
4:D:506:PCW:C26	4:D:516:PCW:C16	0.46	2.93	9	1
4:C:621:PCW:H342	5:C:630:17F:H20A	0.46	1.87	10	1
4:D:506:PCW:O3	4:D:509:PCW:C38	0.46	2.62	10	1
4:A:402:PCW:H442	4:D:512:PCW:H152	0.45	1.83	1	1
4:C:613:PCW:O31	4:C:613:PCW:C3	0.45	2.55	1	2
4:C:620:PCW:C20	5:C:631:17F:H10A	0.45	2.41	1	1
4:D:506:PCW:H371	5:D:520:17F:H75	0.45	1.87	1	1
4:B:201:PCW:C22	4:D:506:PCW:H442	0.45	2.42	3	1
4:D:513:PCW:H481	4:D:513:PCW:C28	0.45	2.41	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:515:PCW:O1P	4:D:515:PCW:C7	0.45	2.64	3	1
4:D:516:PCW:O2P	4:D:516:PCW:C3	0.45	2.64	3	1
4:C:622:PCW:O3P	4:C:622:PCW:O31	0.45	2.33	9	2
4:A:406:PCW:H73	4:B:204:PCW:C1	0.45	2.30	5	1
1:C:463:TRP:NE1	5:C:627:17F:H71	0.45	2.26	5	1
4:D:504:PCW:H412	4:D:516:PCW:H171	0.45	1.88	6	1
4:D:509:PCW:H141	5:D:520:17F:H18	0.45	1.86	6	1
4:D:506:PCW:H61	4:D:517:PCW:C1	0.45	2.28	7	1
4:A:407:PCW:H331	5:D:522:17F:H59	0.45	1.88	8	1
5:D:524:17F:H12	5:D:524:17F:C35	0.45	2.41	8	1
5:D:529:17F:H9A	5:D:529:17F:H20	0.45	1.87	8	1
4:A:413:PCW:H382	4:D:526:PCW:H162	0.45	1.88	10	2
4:C:605:PCW:C32	4:C:613:PCW:H62	0.45	2.41	2	1
4:C:611:PCW:H31	4:C:619:PCW:C11	0.45	2.42	2	1
4:C:612:PCW:H471	4:C:612:PCW:C23	0.45	2.27	2	1
4:D:506:PCW:H221	4:D:516:PCW:C35	0.45	2.41	2	1
4:C:604:PCW:H411	5:D:529:17F:C21	0.45	2.41	3	2
4:C:606:PCW:H31	5:D:529:17F:C1	0.45	2.37	3	1
4:D:514:PCW:C20	5:D:520:17F:H64	0.45	2.40	4	1
4:A:403:PCW:C6	4:A:403:PCW:O2	0.45	2.64	5	1
4:A:404:PCW:C36	4:B:202:PCW:H442	0.45	2.41	5	1
4:A:405:PCW:C19	4:D:512:PCW:H40	0.45	2.41	5	1
4:B:201:PCW:H231	4:B:203:PCW:C28	0.45	2.40	5	1
4:D:503:PCW:C44	5:D:522:17F:H9A	0.45	2.40	5	1
4:C:603:PCW:C7	4:D:527:PCW:H31	0.45	2.40	6	1
4:C:606:PCW:O11	4:C:606:PCW:C2	0.45	2.51	6	2
4:D:509:PCW:H431	4:D:517:PCW:H341	0.45	1.88	6	1
4:D:527:PCW:H442	4:D:528:PCW:H361	0.45	1.88	7	1
4:C:605:PCW:H172	4:C:613:PCW:H131	0.45	1.87	8	1
4:C:608:PCW:H42	4:C:624:PCW:C22	0.45	2.41	8	1
4:C:618:PCW:H381	4:C:625:PCW:C18	0.45	2.36	8	1
4:A:402:PCW:H342	4:A:405:PCW:C13	0.45	2.40	9	1
4:B:201:PCW:H261	4:D:528:PCW:H472	0.45	1.87	9	1
4:D:508:PCW:C17	4:D:512:PCW:H152	0.45	2.41	9	1
4:D:513:PCW:O2	4:D:513:PCW:H342	0.45	2.11	9	1
4:C:606:PCW:C6	4:C:606:PCW:O11	0.45	2.61	10	1
4:C:618:PCW:H321	4:C:625:PCW:H332	0.45	1.88	10	1
4:D:509:PCW:H281	5:D:520:17F:C1Y	0.45	2.40	1	1
1:A:255:GLN:HB2	1:A:256:PRO:CD	0.45	2.41	3	4
4:A:401:PCW:H322	4:D:511:PCW:H381	0.45	1.88	2	1
4:C:605:PCW:C6	5:C:628:17F:N1	0.45	2.79	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:607:PCW:H431	4:C:624:PCW:C47	0.45	2.40	2	1
5:D:519:17F:C34	5:D:521:17F:H29	0.45	2.41	2	1
4:C:608:PCW:H42	4:C:624:PCW:H222	0.45	1.88	8	2
2:B:89:SER:O	2:B:93:ILE:HG12	0.45	2.11	3	3
4:A:401:PCW:H272	4:C:614:PCW:C27	0.45	2.40	4	1
4:A:410:PCW:H362	4:A:414:PCW:C37	0.45	2.42	4	2
1:C:532:ARG:O	1:C:536:LEU:HG	0.45	2.11	4	2
4:A:410:PCW:C41	4:A:410:PCW:C37	0.45	2.87	6	2
4:C:623:PCW:H12	4:C:624:PCW:C3	0.45	2.42	6	1
2:B:45:VAL:HG11	3:D:450:ALA:HB2	0.45	1.87	6	1
4:C:610:PCW:C11	5:C:629:17F:C18	0.45	2.84	7	1
4:C:615:PCW:H141	5:C:631:17F:H9A	0.45	1.88	7	1
4:C:616:PCW:H31	4:C:616:PCW:O1P	0.45	2.10	7	1
4:A:407:PCW:H432	4:A:412:PCW:C28	0.45	2.42	8	1
2:B:21:ILE:HG23	3:D:388:VAL:HG13	0.45	1.88	8	1
4:A:401:PCW:H40	4:C:611:PCW:H281	0.45	1.87	9	1
4:A:404:PCW:H73	5:D:524:17F:H2	0.45	1.87	10	1
4:C:610:PCW:H62	5:C:629:17F:C4	0.45	2.41	1	1
4:D:509:PCW:C28	4:D:509:PCW:C23	0.45	2.56	1	1
4:D:509:PCW:H441	5:D:520:17F:H32	0.45	1.89	1	1
4:C:604:PCW:C47	4:C:624:PCW:H282	0.45	2.41	2	1
4:D:507:PCW:H51	4:D:507:PCW:O1P	0.45	2.11	2	1
4:B:202:PCW:H481	4:D:510:PCW:C27	0.45	2.42	3	1
4:D:516:PCW:O31	4:D:516:PCW:H12	0.45	2.10	3	2
4:D:513:PCW:H421	5:D:522:17F:H68	0.45	1.87	4	1
1:A:284:GLN:O	1:A:288:ARG:HG3	0.45	2.11	6	2
4:A:414:PCW:O31	4:A:414:PCW:P	0.45	2.75	5	1
3:D:437:THR:HG21	3:D:467:THR:HG21	0.45	1.87	5	1
4:D:503:PCW:C48	4:D:507:PCW:H483	0.45	2.42	5	1
5:D:525:17F:H36	5:D:525:17F:C36	0.45	2.40	5	1
4:A:404:PCW:C28	4:A:411:PCW:H482	0.45	2.36	6	1
4:C:618:PCW:H132	4:C:625:PCW:H132	0.45	1.89	6	1
4:C:618:PCW:H63	4:D:528:PCW:O2P	0.45	2.10	6	1
4:D:508:PCW:H82	5:D:523:17F:C10	0.45	2.39	6	1
4:A:402:PCW:C38	4:D:512:PCW:H361	0.45	2.41	7	1
4:A:414:PCW:C39	4:C:617:PCW:C15	0.45	2.94	10	2
4:C:623:PCW:H412	4:C:624:PCW:H432	0.45	1.87	7	1
4:B:202:PCW:H262	4:B:203:PCW:H241	0.45	1.89	7	1
4:A:405:PCW:C1	4:A:408:PCW:C7	0.45	2.95	8	1
4:D:515:PCW:O3	5:D:525:17F:H57	0.45	2.12	8	1
4:A:410:PCW:H211	4:C:617:PCW:C47	0.45	2.29	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:610:PCW:C17	5:C:629:17F:C34	0.45	2.95	9	1
4:B:202:PCW:H241	4:B:204:PCW:C39	0.45	2.42	9	1
4:D:508:PCW:H172	4:D:512:PCW:H152	0.45	1.87	9	1
4:A:402:PCW:O2	4:A:402:PCW:O4P	0.45	2.34	10	1
4:D:507:PCW:C4	5:D:523:17F:H9	0.45	2.42	10	1
4:D:517:PCW:H39	5:D:525:17F:H63	0.45	1.84	10	1
4:D:518:PCW:H481	5:D:521:17F:H10A	0.45	1.88	10	1
2:B:28:PHE:CE1	2:B:147:LYS:HA	0.45	2.46	1	1
4:D:509:PCW:C28	5:D:520:17F:H31	0.45	2.37	1	1
5:C:631:17F:O10	5:C:631:17F:C4	0.45	2.63	6	2
1:A:363:LYS:HE2	1:C:411:THR:HG23	0.45	1.86	3	1
4:B:202:PCW:H362	4:B:202:PCW:H141	0.45	1.88	3	1
4:C:606:PCW:H411	5:C:630:17F:C30	0.45	2.36	5	1
4:C:607:PCW:C36	4:C:624:PCW:H452	0.45	2.42	5	1
4:C:613:PCW:C14	4:C:619:PCW:C39	0.45	2.94	5	1
4:C:613:PCW:C13	4:C:619:PCW:H382	0.45	2.41	5	2
5:D:529:17F:H47	5:D:530:17F:C22	0.45	2.41	5	3
2:B:6:LEU:HD11	2:B:53:LEU:HD22	0.45	1.88	6	2
4:D:512:PCW:H352	4:D:514:PCW:H121	0.45	1.89	6	1
3:D:356:ASN:HA	3:D:422:ILE:HD12	0.45	1.87	7	1
4:D:507:PCW:C11	4:D:513:PCW:C15	0.45	2.94	7	1
4:A:413:PCW:H362	4:C:617:PCW:C40	0.45	2.42	8	1
4:D:506:PCW:H172	4:D:506:PCW:H222	0.45	1.88	8	1
5:D:523:17F:H39	5:D:523:17F:C1X	0.45	2.42	8	1
1:A:279:LEU:HB3	1:C:495:LYS:HE3	0.45	1.89	9	1
4:C:608:PCW:H221	5:C:626:17F:H19	0.45	1.89	9	1
4:D:504:PCW:C48	5:D:519:17F:H49	0.45	2.40	9	1
4:A:403:PCW:H283	5:D:523:17F:H33	0.45	1.87	10	1
4:A:405:PCW:O31	4:D:514:PCW:C35	0.45	2.64	10	1
4:B:202:PCW:C6	5:D:524:17F:O5	0.45	2.64	10	1
4:A:415:PCW:H222	4:C:603:PCW:C16	0.45	2.42	1	2
4:C:608:PCW:C20	5:C:627:17F:H39	0.45	2.42	1	1
4:C:614:PCW:O11	4:C:614:PCW:O2	0.45	2.34	8	2
4:C:616:PCW:C12	4:D:526:PCW:H151	0.45	2.41	1	1
4:D:503:PCW:O31	4:D:503:PCW:H132	0.45	2.12	1	2
5:D:525:17F:H48	5:D:525:17F:C42	0.45	2.40	1	1
4:D:503:PCW:C12	4:D:511:PCW:C39	0.45	2.91	2	1
4:D:505:PCW:O1P	4:D:505:PCW:C2	0.45	2.65	2	1
4:B:201:PCW:H171	5:D:530:17F:H53	0.45	1.87	3	1
4:C:601:PCW:H121	4:C:601:PCW:H452	0.45	1.87	4	1
5:D:524:17F:H55	4:D:527:PCW:H182	0.45	1.88	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:510:PCW:O3	5:D:524:17F:C39	0.45	2.64	6	1
4:D:526:PCW:H421	4:D:526:PCW:H262	0.45	1.89	6	1
1:A:277:GLU:HB2	1:A:278:PRO:CD	0.45	2.42	7	1
4:B:201:PCW:H342	4:D:510:PCW:C39	0.45	2.41	7	1
4:B:203:PCW:H19	4:D:506:PCW:C45	0.45	2.42	7	1
4:C:613:PCW:C48	4:C:619:PCW:H181	0.45	2.41	8	1
4:D:504:PCW:H322	4:D:510:PCW:C34	0.45	2.39	8	1
4:D:505:PCW:H372	5:D:519:17F:C10	0.45	2.41	8	1
4:D:508:PCW:O4P	4:D:508:PCW:C8	0.45	2.64	8	2
4:D:517:PCW:C43	5:D:525:17F:H71	0.45	2.42	9	1
4:C:617:PCW:O11	4:C:617:PCW:H63	0.45	2.11	10	1
4:D:510:PCW:C35	5:D:524:17F:C8	0.45	2.90	10	1
1:A:229:TRP:CH2	4:A:404:PCW:H471	0.45	2.46	1	1
4:A:415:PCW:H222	4:C:603:PCW:H161	0.45	1.87	1	1
4:C:604:PCW:C3	4:C:604:PCW:O1P	0.45	2.65	1	2
4:C:615:PCW:H63	5:C:631:17F:HN1A	0.45	1.72	1	1
4:D:504:PCW:O4P	4:D:504:PCW:C8	0.45	2.64	9	4
4:D:508:PCW:O4P	4:D:508:PCW:C7	0.45	2.63	1	1
4:D:509:PCW:H82	4:D:509:PCW:C11	0.45	2.42	1	1
4:A:402:PCW:H361	4:D:512:PCW:C36	0.45	2.41	2	1
4:C:605:PCW:H63	5:C:628:17F:N1	0.45	2.26	2	1
2:B:16:LYS:NZ	6:B:205:GNP:O1G	0.45	2.47	8	2
4:B:202:PCW:C4	4:B:202:PCW:O2	0.45	2.64	2	1
4:D:507:PCW:C8	4:D:508:PCW:C8	0.45	2.94	2	1
5:D:523:17F:H4A	5:D:523:17F:O10	0.45	2.11	2	1
4:C:610:PCW:C5	5:C:629:17F:O1	0.45	2.64	3	1
4:C:618:PCW:H351	4:C:625:PCW:H362	0.45	1.88	3	1
2:B:37:GLU:O	3:D:368:THR:HA	0.45	2.12	5	2
4:C:613:PCW:H472	4:C:619:PCW:H231	0.45	1.87	4	1
4:A:401:PCW:C6	4:D:511:PCW:H32	0.45	2.33	6	1
4:A:415:PCW:H161	4:C:603:PCW:H121	0.45	1.88	6	1
4:A:410:PCW:O31	4:A:410:PCW:O4P	0.45	2.34	7	1
4:A:411:PCW:C41	4:C:612:PCW:C18	0.45	2.87	9	1
4:B:201:PCW:H141	4:D:506:PCW:C48	0.45	2.39	9	1
4:C:625:PCW:O1P	4:C:625:PCW:C5	0.45	2.59	10	1
4:D:506:PCW:C26	4:D:516:PCW:H142	0.45	2.42	1	1
4:B:201:PCW:H182	4:D:506:PCW:H422	0.45	1.88	3	1
4:D:506:PCW:C20	4:D:516:PCW:H351	0.45	2.42	3	1
4:A:405:PCW:O3	4:A:405:PCW:C31	0.45	2.65	4	3
4:C:617:PCW:H382	4:D:526:PCW:H162	0.45	1.87	5	1
5:D:524:17F:H62	5:D:524:17F:H30	0.45	1.89	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:405:PCW:C24	4:D:508:PCW:H261	0.45	2.41	9	1
5:C:631:17F:H53	4:D:512:PCW:H162	0.45	1.87	9	1
4:D:514:PCW:H151	5:D:520:17F:H61	0.45	1.89	9	1
1:A:247:LEU:HG	4:A:408:PCW:C28	0.45	2.42	10	1
5:A:409:17F:H65	4:D:501:PCW:H252	0.45	1.87	10	1
4:B:204:PCW:O31	4:B:204:PCW:C4	0.45	2.64	10	1
4:D:516:PCW:O11	4:D:516:PCW:C7	0.45	2.61	10	1
4:A:412:PCW:O2P	4:C:614:PCW:H52	0.45	2.12	1	1
4:A:413:PCW:O2	4:C:617:PCW:C41	0.45	2.64	1	4
4:C:623:PCW:O11	4:C:623:PCW:C2	0.45	2.63	1	4
4:B:204:PCW:H52	4:B:204:PCW:O2	0.45	2.12	1	1
3:D:473:HIS:HB2	3:D:476:CYS:SG	0.45	2.51	1	3
4:D:504:PCW:H472	4:D:505:PCW:H252	0.45	1.88	1	1
4:D:511:PCW:O11	4:D:511:PCW:H82	0.45	2.11	1	1
4:A:401:PCW:H341	4:D:503:PCW:H172	0.45	1.88	2	1
4:A:411:PCW:H332	4:C:612:PCW:C14	0.45	2.42	2	1
4:A:414:PCW:O3P	4:C:617:PCW:H52	0.45	2.11	2	1
1:C:502:GLU:O	1:C:506:ARG:HG3	0.45	2.12	10	4
5:C:628:17F:O7	5:C:628:17F:O10	0.45	2.35	2	1
5:C:630:17F:C34	5:C:631:17F:H74	0.45	2.42	2	2
2:B:116:ASN:HA	2:B:144:THR:O	0.45	2.11	7	4
4:A:414:PCW:H41	4:A:414:PCW:C2	0.45	2.42	6	1
4:A:403:PCW:H262	5:D:523:17F:H20	0.45	1.88	7	1
4:A:408:PCW:H461	4:D:506:PCW:C45	0.45	2.42	8	1
4:A:411:PCW:H431	4:C:612:PCW:H212	0.45	1.89	8	1
4:C:613:PCW:H261	5:D:521:17F:C38	0.45	2.42	8	1
4:B:202:PCW:C48	4:D:510:PCW:H242	0.45	2.42	8	1
4:D:503:PCW:H211	4:D:503:PCW:C17	0.45	2.33	8	1
1:A:261:PHE:O	1:A:265:TRP:HB2	0.45	2.11	9	1
4:D:511:PCW:C19	5:D:522:17F:H19A	0.45	2.42	9	1
4:A:405:PCW:C12	4:D:514:PCW:C33	0.45	2.95	10	1
4:C:616:PCW:C48	4:D:504:PCW:C22	0.45	2.95	10	1
2:B:41:ARG:CD	3:D:365:LYS:HD2	0.45	2.40	10	1
4:D:518:PCW:H172	4:D:518:PCW:H212	0.45	1.88	10	1
4:C:601:PCW:H421	5:C:626:17F:C29	0.45	2.42	1	1
4:D:502:PCW:H41	4:D:502:PCW:C11	0.45	2.42	1	1
4:C:604:PCW:H231	5:D:525:17F:C42	0.45	2.41	2	1
5:C:630:17F:H8	5:D:529:17F:H69	0.45	1.87	2	1
4:D:526:PCW:O2	4:D:526:PCW:C11	0.45	2.65	4	2
4:C:607:PCW:C43	4:C:624:PCW:C48	0.45	2.95	7	2
4:D:511:PCW:H61	5:D:522:17F:C6	0.45	2.42	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:607:PCW:H452	4:D:513:PCW:H483	0.45	1.88	4	1
4:C:605:PCW:C17	4:C:613:PCW:H342	0.45	2.39	5	1
4:C:617:PCW:O11	4:C:617:PCW:C2	0.45	2.59	5	1
4:B:203:PCW:H371	4:B:203:PCW:H142	0.45	1.87	5	1
1:C:463:TRP:HE1	5:C:627:17F:H75	0.45	1.72	6	1
4:C:602:PCW:H351	5:D:523:17F:H73	0.45	1.89	6	1
2:B:14:VAL:HA	2:B:83:ALA:HB2	0.45	1.89	6	1
4:D:516:PCW:H421	4:D:527:PCW:C28	0.45	2.41	8	1
1:C:517:HIS:O	1:C:521:TYR:HB2	0.45	2.11	9	1
4:C:603:PCW:H261	4:D:526:PCW:C17	0.45	2.37	9	1
4:D:509:PCW:C7	4:D:514:PCW:O11	0.45	2.65	9	1
4:D:517:PCW:H211	4:D:517:PCW:H162	0.45	1.88	9	1
4:A:411:PCW:C35	4:C:612:PCW:H132	0.45	2.42	10	1
4:C:603:PCW:H271	4:D:526:PCW:C17	0.45	2.42	10	1
4:C:606:PCW:O1P	4:C:624:PCW:H20	0.45	2.12	10	1
3:D:459:LEU:HD21	3:D:472:PHE:HA	0.45	1.87	10	1
4:A:411:PCW:H431	4:C:612:PCW:H171	0.44	1.86	1	1
4:D:507:PCW:C41	5:D:525:17F:H6	0.44	2.42	1	1
4:A:404:PCW:H342	4:D:510:PCW:C18	0.44	2.42	2	1
4:C:624:PCW:C31	4:C:624:PCW:C11	0.44	2.95	2	1
4:C:608:PCW:H212	5:C:627:17F:H30	0.44	1.84	3	2
4:D:513:PCW:H442	4:D:517:PCW:C28	0.44	2.38	3	1
4:A:406:PCW:C23	4:B:202:PCW:H241	0.44	2.42	4	1
4:C:608:PCW:H41	4:C:624:PCW:C21	0.44	2.41	4	1
4:B:202:PCW:C31	4:B:202:PCW:O3	0.44	2.64	4	2
3:D:481:PRO:HB3	4:D:515:PCW:C8	0.44	2.40	5	1
4:D:515:PCW:O2P	4:D:515:PCW:H51	0.44	2.12	5	1
4:C:602:PCW:H422	5:C:626:17F:H45	0.44	1.89	6	1
4:C:608:PCW:H19	5:C:627:17F:C27	0.44	2.42	6	1
4:A:403:PCW:H481	4:C:607:PCW:C26	0.44	2.40	7	1
4:C:616:PCW:C39	4:C:618:PCW:C14	0.44	2.80	9	2
4:B:201:PCW:H212	4:D:506:PCW:H461	0.44	1.89	7	1
4:A:407:PCW:H272	4:A:412:PCW:H271	0.44	1.89	8	1
4:C:605:PCW:H141	4:C:613:PCW:C13	0.44	2.42	9	1
4:B:203:PCW:O2P	4:B:204:PCW:C8	0.44	2.65	9	1
4:D:513:PCW:H412	4:D:513:PCW:H251	0.44	1.87	9	1
4:C:602:PCW:H481	4:C:608:PCW:C23	0.44	2.42	10	1
4:B:202:PCW:H62	5:D:524:17F:O5	0.44	2.11	10	1
4:A:410:PCW:O31	4:C:617:PCW:H61	0.44	2.13	1	1
4:A:410:PCW:H442	4:C:617:PCW:C21	0.44	2.42	9	2
3:D:356:ASN:ND2	3:D:372:VAL:HG23	0.44	2.27	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:501:PCW:H431	5:D:525:17F:C29	0.44	2.39	1	1
5:D:522:17F:H30	5:D:525:17F:H11A	0.44	1.88	1	1
4:A:414:PCW:O1P	4:C:617:PCW:H52	0.44	2.12	2	2
4:C:609:PCW:O31	4:C:609:PCW:C13	0.44	2.65	7	3
4:C:616:PCW:O3P	4:D:527:PCW:H51	0.44	2.12	4	2
4:C:625:PCW:O31	4:C:625:PCW:H12	0.44	2.11	2	1
2:B:154:ASP:HA	2:B:157:TYR:CD2	0.44	2.48	2	1
4:D:527:PCW:O2	4:D:527:PCW:C11	0.44	2.64	8	7
4:C:616:PCW:H41	4:D:526:PCW:O11	0.44	2.11	3	1
4:A:410:PCW:H371	4:A:410:PCW:H412	0.44	1.88	4	2
4:D:506:PCW:H11	4:D:515:PCW:C6	0.44	2.43	4	1
4:A:406:PCW:C40	4:B:204:PCW:H19	0.44	2.42	5	1
4:A:414:PCW:O31	4:A:414:PCW:O1P	0.44	2.35	5	2
4:C:605:PCW:O31	4:C:613:PCW:H73	0.44	2.12	5	2
4:C:615:PCW:O31	4:C:615:PCW:H12	0.44	2.11	5	1
4:D:505:PCW:O2P	4:D:510:PCW:P	0.44	2.76	5	1
4:D:517:PCW:C42	5:D:525:17F:C12	0.44	2.95	5	1
4:A:401:PCW:O2	4:D:511:PCW:H382	0.44	2.12	6	1
4:C:604:PCW:C48	4:C:606:PCW:H61	0.44	2.42	6	1
4:D:506:PCW:H141	5:D:520:17F:C21	0.44	2.41	8	1
4:A:403:PCW:C44	4:D:507:PCW:H262	0.44	2.42	9	1
4:A:404:PCW:H52	4:D:510:PCW:H121	0.44	1.88	9	1
4:A:412:PCW:C45	4:C:623:PCW:H462	0.44	2.39	9	1
4:A:403:PCW:C24	4:D:507:PCW:H151	0.44	2.42	10	1
4:C:618:PCW:C25	4:D:510:PCW:H483	0.44	2.42	10	1
4:A:407:PCW:H382	5:D:522:17F:C36	0.44	2.42	1	1
4:C:604:PCW:C45	4:C:606:PCW:C18	0.44	2.89	3	2
4:B:202:PCW:C6	5:D:524:17F:O4	0.44	2.65	1	1
4:D:508:PCW:C15	4:D:512:PCW:H151	0.44	2.16	1	1
4:C:604:PCW:H411	4:C:604:PCW:C37	0.44	2.36	8	2
4:D:509:PCW:H352	5:D:520:17F:H63	0.44	1.89	2	1
3:D:478:THR:CB	4:D:517:PCW:H52	0.44	2.42	3	1
4:D:511:PCW:C11	4:D:511:PCW:O2	0.44	2.65	3	2
5:C:629:17F:C11	4:D:528:PCW:C7	0.44	2.93	4	1
4:D:502:PCW:O1P	4:D:502:PCW:H31	0.44	2.12	4	1
4:D:515:PCW:H442	4:D:516:PCW:H162	0.44	1.88	4	1
5:D:519:17F:O10	5:D:519:17F:C4	0.44	2.61	4	2
4:D:503:PCW:H73	4:D:503:PCW:H11	0.44	1.87	5	1
1:C:502:GLU:HG2	1:C:506:ARG:HE	0.44	1.72	6	1
4:A:402:PCW:O4P	4:A:402:PCW:O2	0.44	2.35	8	1
4:A:413:PCW:H362	4:C:617:PCW:C41	0.44	2.42	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:401:PCW:H321	4:D:511:PCW:C39	0.44	2.41	10	1
4:D:504:PCW:H341	4:D:510:PCW:H341	0.44	1.89	10	1
4:A:406:PCW:H242	4:B:202:PCW:H232	0.44	1.89	1	1
4:A:415:PCW:C28	4:C:622:PCW:H251	0.44	2.39	1	1
4:D:505:PCW:H221	4:D:505:PCW:C17	0.44	2.40	1	1
4:A:412:PCW:C6	4:C:624:PCW:O31	0.44	2.63	2	1
4:D:511:PCW:C22	4:D:511:PCW:C26	0.44	2.95	5	2
4:A:407:PCW:H461	4:A:412:PCW:H241	0.44	1.88	3	1
4:C:605:PCW:O2P	4:C:613:PCW:C5	0.44	2.65	3	1
4:C:611:PCW:H451	4:D:511:PCW:H481	0.44	1.88	3	1
4:C:613:PCW:O4P	4:C:613:PCW:C8	0.44	2.65	3	1
2:B:35:THR:HG21	2:B:38:ASP:HB2	0.44	1.89	3	1
4:B:203:PCW:H412	4:B:203:PCW:H142	0.44	1.89	3	1
4:D:501:PCW:H441	5:D:521:17F:H76	0.44	1.89	3	1
4:D:508:PCW:H62	5:D:520:17F:H6	0.44	1.90	3	1
5:D:522:17F:H52	5:D:525:17F:H35	0.44	1.90	3	1
5:A:409:17F:O5	4:D:503:PCW:C8	0.44	2.66	6	2
4:D:509:PCW:H19	5:D:520:17F:C19	0.44	2.42	4	1
1:A:334:ARG:HD3	1:C:440:GLU:CD	0.44	2.37	5	1
4:D:511:PCW:C23	4:D:511:PCW:H432	0.44	2.42	5	1
4:C:602:PCW:C22	4:C:602:PCW:C17	0.44	2.90	6	1
4:C:613:PCW:C21	5:D:521:17F:H51	0.44	2.41	6	1
4:D:503:PCW:C21	4:D:503:PCW:C17	0.44	2.90	8	1
5:D:522:17F:H29	5:D:525:17F:C10	0.44	2.41	8	1
4:A:405:PCW:H322	4:A:408:PCW:H332	0.44	1.89	9	1
4:A:414:PCW:C6	5:C:628:17F:O8	0.44	2.65	9	1
4:C:621:PCW:C36	5:C:629:17F:C32	0.44	2.82	9	1
4:A:415:PCW:C20	4:D:528:PCW:H232	0.44	2.43	10	1
4:C:611:PCW:H161	4:C:619:PCW:H151	0.44	1.89	10	1
4:C:616:PCW:C42	4:C:625:PCW:H232	0.44	2.42	10	1
4:B:203:PCW:C14	4:B:204:PCW:H382	0.44	2.33	10	1
4:C:601:PCW:H39	4:C:602:PCW:C15	0.44	2.41	1	1
5:C:630:17F:O9	5:C:630:17F:C7	0.44	2.65	9	3
4:A:410:PCW:H411	4:A:410:PCW:C37	0.44	2.33	2	3
4:C:612:PCW:H232	4:C:612:PCW:C47	0.44	2.28	2	1
1:A:237:GLU:HG2	1:A:241:GLN:HE21	0.44	1.73	3	1
4:C:606:PCW:H211	5:C:630:17F:H54	0.44	1.88	3	1
4:B:201:PCW:H161	4:D:506:PCW:C42	0.44	2.43	3	1
4:B:201:PCW:H341	4:D:504:PCW:H332	0.44	1.88	4	1
4:C:605:PCW:O31	4:C:613:PCW:C7	0.44	2.66	5	1
4:B:201:PCW:O2	4:D:504:PCW:H132	0.44	2.12	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:D:525:17F:H4	5:D:525:17F:H2	0.44	1.89	5	1
5:C:626:17F:O8	5:C:626:17F:C5	0.44	2.58	6	1
1:A:330:ARG:NH2	1:C:447:GLU:HB3	0.44	2.28	7	2
4:A:402:PCW:H381	4:D:512:PCW:H361	0.44	1.89	7	1
4:C:609:PCW:H131	4:C:615:PCW:C7	0.44	2.43	7	1
4:C:607:PCW:C34	4:C:624:PCW:C37	0.44	2.95	8	1
4:B:201:PCW:H462	5:D:524:17F:H49	0.44	1.90	8	1
4:D:504:PCW:C40	5:D:519:17F:H37	0.44	2.42	8	1
5:A:409:17F:C42	4:D:501:PCW:H272	0.44	2.40	9	1
4:B:201:PCW:H172	4:D:527:PCW:C28	0.44	2.43	9	1
4:D:508:PCW:C18	4:D:512:PCW:H342	0.44	2.41	9	1
4:D:501:PCW:H382	4:D:515:PCW:H182	0.44	1.87	10	1
4:D:504:PCW:H40	4:D:505:PCW:H73	0.44	1.89	10	1
4:D:516:PCW:H241	5:D:519:17F:H55	0.44	1.87	10	1
4:A:410:PCW:O3	4:A:410:PCW:C31	0.44	2.66	1	2
1:A:364:ALA:HA	1:A:368:LEU:HD12	0.44	1.90	2	2
4:A:407:PCW:H472	4:A:407:PCW:C27	0.44	2.38	7	2
4:C:624:PCW:H122	4:C:624:PCW:H341	0.44	1.85	2	1
4:D:517:PCW:H332	5:D:525:17F:C1Y	0.44	2.42	2	1
1:C:488:LYS:O	1:C:492:LEU:HG	0.44	2.13	3	1
4:A:406:PCW:O11	4:B:202:PCW:H142	0.44	2.12	4	1
4:A:408:PCW:H12	4:A:408:PCW:H41	0.44	1.90	4	1
4:D:501:PCW:H482	5:D:525:17F:C29	0.44	2.37	4	1
4:C:613:PCW:H20	5:D:521:17F:C27	0.44	2.43	5	1
5:C:626:17F:H40	5:C:627:17F:H75	0.44	1.89	5	1
4:C:601:PCW:H483	4:C:601:PCW:C12	0.44	2.43	6	1
4:C:606:PCW:H442	4:C:609:PCW:H12	0.44	1.88	6	1
4:C:610:PCW:H12	5:C:629:17F:H4	0.44	1.88	6	1
4:C:624:PCW:O3	4:C:624:PCW:O31	0.44	2.34	7	1
4:D:507:PCW:C43	5:D:522:17F:H30	0.44	2.34	8	1
5:D:524:17F:H11A	5:D:524:17F:H66	0.44	1.88	8	1
4:A:403:PCW:H212	4:D:513:PCW:H321	0.44	1.88	9	1
2:B:21:ILE:HD13	3:D:388:VAL:HG22	0.44	1.90	9	1
3:D:385:ALA:O	3:D:389:ARG:HG2	0.44	2.13	10	1
4:D:504:PCW:H472	4:D:505:PCW:H152	0.44	1.88	10	1
2:B:48:GLY:O	3:D:471:LYS:HE2	0.44	2.12	2	1
4:A:412:PCW:C6	4:C:624:PCW:C31	0.44	2.94	3	1
4:C:602:PCW:C23	5:C:626:17F:H44	0.44	2.37	3	1
4:C:603:PCW:C46	4:D:526:PCW:H412	0.44	2.42	3	1
4:A:405:PCW:C4	4:A:408:PCW:O1P	0.44	2.66	4	1
4:A:408:PCW:C45	4:B:203:PCW:H472	0.44	2.42	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:607:PCW:C3	4:C:624:PCW:H411	0.44	2.35	4	2
4:D:503:PCW:H40	5:D:522:17F:O7	0.44	2.12	5	1
1:C:463:TRP:CD1	5:C:627:17F:H70	0.44	2.48	6	1
4:C:615:PCW:C22	4:D:512:PCW:H272	0.44	2.43	7	1
4:D:515:PCW:C6	4:D:516:PCW:O1P	0.44	2.66	7	1
4:A:413:PCW:O3	4:C:617:PCW:H422	0.44	2.13	8	1
4:D:501:PCW:H211	5:D:521:17F:H20A	0.44	1.88	8	1
4:D:509:PCW:H32	5:D:520:17F:O3	0.44	2.12	8	1
1:A:214:PHE:HA	1:A:217:LEU:HD12	0.44	1.90	9	1
4:A:405:PCW:C16	4:A:405:PCW:C21	0.44	2.67	9	1
4:D:509:PCW:H412	5:D:520:17F:C8	0.44	2.42	9	1
4:A:401:PCW:C42	4:D:511:PCW:H482	0.44	2.42	10	1
4:A:415:PCW:C22	4:C:603:PCW:C16	0.44	2.95	10	1
4:A:415:PCW:C45	5:D:521:17F:H75	0.44	2.34	10	1
4:C:619:PCW:O4P	4:C:619:PCW:C8	0.44	2.66	1	6
5:C:631:17F:O8	5:C:631:17F:H5	0.44	2.13	1	1
4:D:506:PCW:H31	4:D:515:PCW:C3	0.44	2.43	1	1
4:A:407:PCW:C33	5:D:522:17F:H34	0.44	2.38	3	1
4:A:412:PCW:C3	4:C:614:PCW:C11	0.44	2.95	3	1
4:C:609:PCW:H271	5:C:626:17F:C39	0.44	2.42	3	1
4:B:202:PCW:C6	5:D:524:17F:HN1	0.44	2.25	3	1
4:D:503:PCW:C40	5:D:522:17F:H41	0.44	2.43	3	1
4:C:612:PCW:H63	4:C:618:PCW:H31	0.44	1.90	4	1
4:B:201:PCW:H231	4:B:203:PCW:C27	0.44	2.42	4	1
4:B:204:PCW:H321	4:B:204:PCW:C7	0.44	2.42	4	1
1:A:279:LEU:O	1:A:283:LEU:HG	0.44	2.13	5	2
4:C:621:PCW:H351	5:C:630:17F:C1Z	0.44	2.31	5	1
4:D:506:PCW:H152	5:D:529:17F:H55	0.44	1.89	5	1
4:C:603:PCW:O31	4:C:603:PCW:C4	0.44	2.66	6	1
5:D:524:17F:H62	5:D:524:17F:C31	0.44	2.35	6	1
4:D:505:PCW:H331	5:D:519:17F:H20A	0.44	1.89	7	1
4:D:515:PCW:C34	4:D:516:PCW:C1	0.44	2.95	7	1
4:A:407:PCW:H432	4:A:412:PCW:H282	0.44	1.89	8	1
1:C:550:LYS:HA	1:C:553:GLU:OE1	0.44	2.13	8	1
4:A:411:PCW:C43	4:C:612:PCW:C18	0.44	2.80	9	1
4:C:608:PCW:C6	4:C:624:PCW:H242	0.44	2.40	9	1
5:C:631:17F:C32	5:C:631:17F:H67	0.44	2.42	9	1
4:D:515:PCW:C13	5:D:525:17F:H60	0.44	2.42	10	1
4:D:501:PCW:O3	4:D:501:PCW:O31	0.44	2.35	1	1
4:D:506:PCW:H321	4:D:509:PCW:C39	0.44	2.39	1	1
5:D:522:17F:O6	5:D:522:17F:C18	0.44	2.64	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:5:LYS:HB3	2:B:75:GLY:HA2	0.44	1.90	2	1
4:A:411:PCW:H422	4:C:612:PCW:H242	0.44	1.90	5	1
4:C:609:PCW:O4P	4:C:609:PCW:C8	0.44	2.66	9	2
4:C:610:PCW:H121	5:C:629:17F:H18	0.44	1.90	5	1
4:D:507:PCW:C42	5:D:522:17F:C20	0.44	2.91	5	1
4:D:511:PCW:H412	4:D:511:PCW:C37	0.44	2.43	5	1
1:A:268:GLU:OE1	1:C:506:ARG:HD3	0.44	2.13	6	1
4:D:502:PCW:H19	4:D:505:PCW:C12	0.44	2.43	7	1
4:A:403:PCW:H481	4:C:607:PCW:H241	0.44	1.89	8	1
4:A:407:PCW:C43	4:A:412:PCW:H282	0.44	2.43	8	1
4:C:618:PCW:H261	4:D:510:PCW:C28	0.44	2.29	8	1
4:D:518:PCW:H221	4:D:518:PCW:C18	0.44	2.40	8	1
4:A:404:PCW:H272	4:A:411:PCW:H221	0.44	1.88	9	1
4:A:405:PCW:H322	4:A:408:PCW:C34	0.44	2.42	9	1
4:C:605:PCW:C48	4:C:619:PCW:H432	0.44	2.43	9	1
4:C:621:PCW:C37	5:C:629:17F:H59	0.44	2.42	9	1
4:B:201:PCW:H341	4:D:506:PCW:C23	0.44	2.42	9	1
4:C:605:PCW:C6	5:C:628:17F:O4	0.44	2.64	10	1
4:C:625:PCW:C20	4:D:528:PCW:H321	0.44	2.42	10	1
4:D:510:PCW:H351	5:D:524:17F:C7	0.44	2.43	10	1
5:D:519:17F:H68	5:D:521:17F:H29	0.44	1.90	10	1
4:C:609:PCW:O1P	5:C:631:17F:C18	0.43	2.64	1	1
5:C:630:17F:H9	5:C:630:17F:H19A	0.43	1.90	1	2
4:A:414:PCW:H422	4:C:617:PCW:C19	0.43	2.43	2	1
4:A:402:PCW:C8	4:A:405:PCW:O11	0.43	2.66	3	1
4:C:605:PCW:H322	4:C:613:PCW:H82	0.43	1.90	3	1
4:C:603:PCW:C19	4:C:603:PCW:H472	0.43	2.43	4	1
4:A:410:PCW:H172	4:D:526:PCW:H242	0.43	1.90	5	1
4:A:414:PCW:O2P	4:C:617:PCW:C8	0.43	2.66	5	1
4:C:608:PCW:O3P	4:C:608:PCW:O31	0.43	2.36	5	2
4:D:506:PCW:O4P	4:D:506:PCW:C8	0.43	2.66	5	1
4:D:507:PCW:H421	5:D:522:17F:H57	0.43	1.89	5	1
4:A:403:PCW:O4P	4:A:403:PCW:C3	0.43	2.58	6	1
5:D:529:17F:H52	5:D:530:17F:H39	0.43	1.89	6	1
4:C:615:PCW:H171	4:C:615:PCW:C21	0.43	2.35	7	1
4:D:518:PCW:C14	5:D:519:17F:H67	0.43	2.43	8	1
4:A:402:PCW:H141	4:A:405:PCW:H222	0.43	1.90	9	1
4:C:620:PCW:C28	5:C:631:17F:H35	0.43	2.34	10	1
4:D:505:PCW:C22	4:D:505:PCW:C18	0.43	2.86	10	1
4:C:623:PCW:C28	5:D:525:17F:H46	0.43	2.43	1	1
4:D:507:PCW:O4P	4:D:507:PCW:C8	0.43	2.66	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:602:PCW:H161	4:C:602:PCW:C38	0.43	2.43	2	1
4:C:604:PCW:H341	5:D:530:17F:H8	0.43	1.90	2	1
4:C:610:PCW:O3P	4:C:610:PCW:O31	0.43	2.36	2	1
4:D:508:PCW:H352	4:D:512:PCW:H122	0.43	1.88	4	2
4:C:601:PCW:H381	4:C:601:PCW:H412	0.43	1.55	5	2
4:A:402:PCW:H162	4:A:405:PCW:H212	0.43	1.89	4	1
4:D:511:PCW:H361	4:D:511:PCW:H231	0.43	1.90	4	1
4:A:402:PCW:C18	4:A:405:PCW:H39	0.43	2.42	5	1
1:C:561:LYS:HB2	1:C:561:LYS:NZ	0.43	2.28	5	1
4:C:608:PCW:C45	5:C:626:17F:H61	0.43	2.41	5	1
5:D:520:17F:O1	5:D:520:17F:H2	0.43	2.12	5	1
4:A:402:PCW:H162	4:A:405:PCW:C21	0.43	2.43	7	3
4:C:609:PCW:C5	5:C:631:17F:O3	0.43	2.66	6	1
4:C:609:PCW:O11	4:C:615:PCW:H61	0.43	2.13	6	2
4:D:527:PCW:H172	4:D:528:PCW:C16	0.43	2.41	6	1
2:B:32:TYR:HD1	6:B:205:GNP:H5'2	0.43	1.73	8	1
2:B:85:ASN:OD1	2:B:117:LYS:HD2	0.43	2.12	8	1
4:A:410:PCW:O4P	4:A:410:PCW:O31	0.43	2.36	9	1
4:A:411:PCW:H411	4:C:612:PCW:H182	0.43	1.90	9	1
4:C:609:PCW:H272	4:C:615:PCW:H431	0.43	1.90	9	1
4:B:202:PCW:H262	4:D:504:PCW:H252	0.43	1.90	9	1
4:D:511:PCW:H321	4:D:511:PCW:C13	0.43	2.43	10	1
4:A:406:PCW:H352	4:B:204:PCW:C15	0.43	2.43	1	1
4:A:414:PCW:H351	4:C:617:PCW:C15	0.43	2.43	1	1
4:C:611:PCW:C7	4:C:623:PCW:C8	0.43	2.96	1	1
4:C:620:PCW:H121	5:C:631:17F:C5	0.43	2.43	1	1
2:B:35:THR:O	2:B:59:ALA:HA	0.43	2.14	1	3
4:B:201:PCW:H283	4:B:204:PCW:H482	0.43	1.91	1	1
4:A:406:PCW:O11	4:A:406:PCW:H42	0.43	2.14	5	2
4:C:618:PCW:C48	4:B:201:PCW:H442	0.43	2.43	2	1
4:C:621:PCW:C18	4:C:621:PCW:C14	0.43	2.90	9	4
4:D:509:PCW:C15	4:D:514:PCW:H122	0.43	2.39	2	1
4:D:517:PCW:C8	4:D:517:PCW:O4P	0.43	2.67	9	7
5:D:530:17F:O7	5:D:530:17F:C17	0.43	2.66	4	4
4:C:618:PCW:H482	4:D:504:PCW:H232	0.43	1.90	3	1
4:D:518:PCW:C43	5:D:519:17F:H68	0.43	2.44	4	1
4:A:401:PCW:H472	4:C:611:PCW:C25	0.43	2.43	6	1
4:C:624:PCW:C18	4:C:624:PCW:C8	0.43	2.95	6	1
4:A:415:PCW:H342	4:C:605:PCW:H341	0.43	1.90	8	1
4:C:613:PCW:H361	4:C:613:PCW:H141	0.43	1.90	8	1
4:D:509:PCW:C41	5:D:520:17F:H8	0.43	2.39	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:D:399:PHE:O	3:D:426:LEU:HG	0.43	2.14	9	1
4:D:518:PCW:H162	5:D:519:17F:H34	0.43	1.91	9	1
5:D:521:17F:H10	5:D:521:17F:H62	0.43	1.90	9	1
4:C:608:PCW:H181	5:C:627:17F:H29	0.43	1.89	10	1
4:D:511:PCW:H381	4:D:511:PCW:H412	0.43	1.55	10	1
4:C:621:PCW:H372	4:C:621:PCW:H411	0.43	1.90	10	3
4:C:624:PCW:O3	4:C:624:PCW:C31	0.43	2.66	5	2
4:D:502:PCW:C3	4:D:502:PCW:P	0.43	3.07	2	2
1:A:338:LEU:O	1:A:342:GLY:HA3	0.43	2.14	10	3
4:A:401:PCW:C47	4:C:611:PCW:H271	0.43	2.43	2	1
4:A:414:PCW:C31	4:C:617:PCW:H51	0.43	2.42	2	1
1:C:440:GLU:O	1:C:444:ASP:HB2	0.43	2.14	3	1
4:C:625:PCW:H421	4:C:625:PCW:H372	0.43	1.89	3	2
4:D:515:PCW:O1P	4:D:515:PCW:H73	0.43	2.12	3	1
4:C:623:PCW:O31	4:C:623:PCW:H41	0.43	2.13	4	1
4:A:413:PCW:H412	4:D:526:PCW:C24	0.43	2.43	5	1
4:C:620:PCW:O4P	4:C:620:PCW:C8	0.43	2.67	5	1
4:D:526:PCW:H281	4:D:526:PCW:H472	0.43	1.89	5	1
5:A:409:17F:H69	4:D:503:PCW:H272	0.43	1.88	6	1
2:B:147:LYS:HB2	6:B:205:GNP:N1	0.43	2.28	6	2
4:B:201:PCW:C17	4:D:516:PCW:H442	0.43	2.43	6	1
4:A:403:PCW:O3	4:A:403:PCW:O31	0.43	2.37	7	1
4:C:604:PCW:C28	4:C:607:PCW:H483	0.43	2.43	7	1
4:C:623:PCW:H412	4:C:624:PCW:C43	0.43	2.43	7	1
4:C:606:PCW:H321	4:C:608:PCW:C8	0.43	2.44	8	1
4:C:607:PCW:H31	4:C:624:PCW:H371	0.43	1.90	8	1
5:A:409:17F:O9	5:A:409:17F:O8	0.43	2.36	9	1
4:D:506:PCW:H261	4:D:516:PCW:H131	0.43	1.90	9	1
4:A:401:PCW:C40	4:D:503:PCW:H241	0.43	2.43	1	1
4:C:621:PCW:H352	5:C:631:17F:H76	0.43	1.90	1	1
2:B:28:PHE:HE1	2:B:147:LYS:HA	0.43	1.73	1	1
4:A:406:PCW:H272	4:C:618:PCW:H483	0.43	1.89	3	1
1:C:522:SER:O	1:C:526:ARG:HG3	0.43	2.14	8	3
4:B:203:PCW:H141	4:B:204:PCW:C37	0.43	2.44	3	1
4:D:514:PCW:H381	4:D:514:PCW:H412	0.43	1.59	7	3
4:D:507:PCW:O11	4:D:513:PCW:C15	0.43	2.65	4	1
4:D:527:PCW:C32	4:D:527:PCW:H52	0.43	2.44	4	1
5:A:409:17F:H68	4:D:501:PCW:H272	0.43	1.89	5	1
4:A:413:PCW:C39	4:D:526:PCW:H231	0.43	2.43	5	1
4:D:517:PCW:O3P	4:D:517:PCW:C8	0.43	2.65	5	1
5:A:409:17F:H35	5:A:409:17F:H40	0.43	1.60	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:504:ARG:O	1:C:508:ARG:HG3	0.43	2.13	6	2
4:A:415:PCW:H332	4:C:622:PCW:O3	0.43	2.14	7	1
4:C:618:PCW:C13	4:C:625:PCW:C14	0.43	2.92	7	1
4:C:621:PCW:C27	4:D:528:PCW:H61	0.43	2.43	7	1
3:D:479:LYS:O	4:D:517:PCW:H42	0.43	2.12	7	1
3:D:483:MET:HB3	5:D:525:17F:O5	0.43	2.13	7	1
4:D:501:PCW:H431	4:D:515:PCW:C16	0.43	2.35	7	1
2:B:133:LEU:HG	2:B:137:TYR:CE2	0.43	2.48	8	1
4:B:201:PCW:H272	4:D:528:PCW:C42	0.43	2.35	8	1
4:D:502:PCW:H332	4:D:510:PCW:H12	0.43	1.89	8	1
5:D:529:17F:H11	5:D:530:17F:H8	0.43	1.91	8	1
4:C:606:PCW:C23	5:D:529:17F:H38	0.43	2.43	9	1
4:A:402:PCW:H422	4:D:508:PCW:H211	0.43	1.90	10	1
5:C:629:17F:C30	4:B:204:PCW:H462	0.43	2.42	10	1
1:A:363:LYS:HA	1:A:367:ALA:CB	0.43	2.42	6	2
4:C:613:PCW:H32	4:C:619:PCW:O3	0.43	2.12	1	1
4:D:509:PCW:C44	5:D:520:17F:C1Y	0.43	2.94	1	1
4:A:408:PCW:O3	4:A:408:PCW:C31	0.43	2.67	7	4
4:D:504:PCW:H412	4:D:516:PCW:C8	0.43	2.15	2	1
4:D:528:PCW:C19	5:D:530:17F:H30	0.43	2.43	2	1
1:A:246:ASP:HA	1:C:528:ARG:CZ	0.43	2.44	4	2
2:B:49:GLU:OE2	5:D:524:17F:N1	0.43	2.52	3	1
4:D:508:PCW:H241	4:D:512:PCW:C39	0.43	2.44	3	1
5:A:409:17F:H67	4:D:501:PCW:H252	0.43	1.90	5	2
4:A:413:PCW:H371	4:D:526:PCW:H161	0.43	1.89	4	1
4:C:623:PCW:H132	4:C:623:PCW:H82	0.43	1.91	4	1
4:D:506:PCW:C7	5:D:520:17F:O8	0.43	2.66	4	1
4:C:610:PCW:C12	5:C:629:17F:H18	0.43	2.43	5	1
4:C:612:PCW:O3P	4:C:612:PCW:C31	0.43	2.66	6	3
4:C:613:PCW:H352	4:C:619:PCW:H351	0.43	1.89	8	2
4:D:517:PCW:H412	4:D:517:PCW:H381	0.43	1.61	6	1
4:D:501:PCW:O2	4:D:501:PCW:H341	0.43	2.13	7	1
4:D:517:PCW:H39	5:D:520:17F:H50	0.43	1.90	7	1
2:B:83:ALA:HB1	2:B:85:ASN:OD1	0.43	2.14	10	2
4:D:510:PCW:H271	4:D:510:PCW:C48	0.43	2.43	8	1
4:A:408:PCW:H382	4:D:514:PCW:C40	0.43	2.43	9	1
4:C:611:PCW:C31	4:C:611:PCW:O3	0.43	2.66	9	1
4:A:405:PCW:H122	4:D:514:PCW:C33	0.43	2.43	10	1
4:A:406:PCW:H12	4:B:204:PCW:C3	0.43	2.44	10	1
4:A:406:PCW:H181	4:B:204:PCW:H283	0.43	1.88	10	1
4:B:201:PCW:H151	4:D:516:PCW:C39	0.43	2.43	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:415:PCW:H442	5:D:521:17F:H75	0.43	1.91	1	1
4:C:616:PCW:H121	4:D:526:PCW:C15	0.43	2.44	1	1
4:B:202:PCW:O2	4:B:202:PCW:P	0.43	2.77	7	3
4:D:518:PCW:H321	5:D:519:17F:H19A	0.43	1.89	2	1
1:A:250:VAL:HG11	4:A:408:PCW:C27	0.43	2.42	4	1
4:A:408:PCW:H19	4:D:514:PCW:H481	0.43	1.91	4	1
5:C:626:17F:H8A	5:C:627:17F:H33	0.43	1.89	6	1
4:A:403:PCW:H262	5:D:523:17F:C20	0.43	2.44	7	1
4:D:527:PCW:C12	4:D:528:PCW:H171	0.43	2.43	7	1
4:A:401:PCW:H361	4:D:503:PCW:H212	0.43	1.91	8	1
4:A:401:PCW:C46	4:C:611:PCW:H271	0.43	2.43	8	1
4:A:402:PCW:H422	4:D:512:PCW:H141	0.43	1.89	8	1
4:A:413:PCW:H412	4:D:526:PCW:C18	0.43	2.38	8	1
4:C:611:PCW:O11	4:C:619:PCW:H132	0.43	2.13	9	1
4:A:414:PCW:H12	4:C:617:PCW:H42	0.43	1.87	10	1
4:C:604:PCW:H482	4:C:624:PCW:C27	0.43	2.43	10	1
4:C:612:PCW:H322	4:C:618:PCW:O11	0.43	2.14	10	1
5:C:626:17F:H8	5:C:627:17F:C1Z	0.43	2.35	10	1
4:D:506:PCW:C40	5:D:520:17F:H70	0.43	2.44	10	1
4:A:403:PCW:H42	4:A:403:PCW:C11	0.43	2.43	1	1
4:A:404:PCW:H261	1:C:554:HIS:CE1	0.43	2.48	1	1
4:A:405:PCW:C21	4:A:405:PCW:C17	0.43	2.88	1	1
4:A:406:PCW:C23	4:B:202:PCW:H232	0.43	2.44	1	1
2:B:6:LEU:HD22	2:B:159:LEU:HD23	0.43	1.90	1	3
4:B:201:PCW:H181	4:D:506:PCW:C42	0.43	2.30	1	1
4:A:410:PCW:H19	4:A:413:PCW:C43	0.43	2.44	2	2
3:D:402:LEU:HD22	4:D:502:PCW:C12	0.43	2.43	2	1
4:D:510:PCW:H272	5:D:524:17F:C33	0.43	2.44	2	1
5:D:520:17F:H55	5:D:525:17F:H70	0.43	1.90	2	1
4:D:502:PCW:H281	4:D:518:PCW:H222	0.43	1.89	3	1
4:A:407:PCW:P	4:A:407:PCW:O2	0.43	2.76	4	1
4:D:505:PCW:H272	5:D:524:17F:C42	0.43	2.43	4	1
4:D:509:PCW:H372	4:D:509:PCW:H411	0.43	1.89	7	3
4:A:402:PCW:H162	4:A:405:PCW:H252	0.43	1.89	5	1
4:D:503:PCW:H431	5:D:522:17F:H8	0.43	1.90	5	1
4:D:508:PCW:C35	4:D:512:PCW:H121	0.43	2.43	5	1
4:D:528:PCW:C12	5:D:529:17F:H62	0.43	2.44	5	1
4:C:611:PCW:O3	4:C:619:PCW:H63	0.43	2.14	6	1
3:D:479:LYS:CA	4:D:517:PCW:H73	0.43	2.35	7	1
4:C:621:PCW:C13	5:C:630:17F:H6	0.43	2.42	8	1
5:D:520:17F:H72	5:D:530:17F:C30	0.43	2.44	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:404:PCW:C37	4:B:202:PCW:H441	0.43	2.42	9	1
5:D:520:17F:C17	5:D:520:17F:O7	0.43	2.66	9	1
5:D:523:17F:O10	5:D:523:17F:H4A	0.43	2.12	9	1
4:C:611:PCW:H11	4:C:613:PCW:H61	0.43	1.89	2	1
4:C:616:PCW:C1	4:D:527:PCW:H342	0.43	2.41	3	2
4:C:603:PCW:C2	4:C:603:PCW:C4	0.43	2.95	4	2
4:C:605:PCW:H331	4:C:622:PCW:H341	0.43	1.89	4	1
4:C:610:PCW:H162	5:C:629:17F:H61	0.43	1.90	4	1
4:B:202:PCW:O3	4:B:202:PCW:O31	0.43	2.37	4	1
4:D:510:PCW:O3	4:D:510:PCW:O31	0.43	2.37	4	1
4:C:610:PCW:H82	5:C:629:17F:O8	0.43	2.12	5	1
3:D:478:THR:OG1	4:D:501:PCW:H63	0.43	2.13	5	1
4:D:514:PCW:C41	4:D:514:PCW:H372	0.43	2.44	5	1
1:A:246:ASP:O	1:A:250:VAL:HB	0.43	2.13	6	1
4:A:412:PCW:H382	4:A:412:PCW:H412	0.43	1.56	6	1
4:B:203:PCW:H441	4:B:203:PCW:C18	0.43	2.44	6	1
4:B:202:PCW:O11	4:D:504:PCW:H281	0.43	2.14	7	1
4:D:516:PCW:H482	4:D:527:PCW:H20	0.43	1.90	7	1
4:D:517:PCW:C40	5:D:520:17F:H55	0.43	2.44	7	1
4:A:411:PCW:H382	4:C:612:PCW:H221	0.43	1.90	8	1
4:C:604:PCW:H432	4:C:606:PCW:H221	0.43	1.90	8	1
4:C:608:PCW:H241	5:C:627:17F:H30	0.43	1.91	8	1
4:C:621:PCW:C20	5:C:629:17F:O10	0.43	2.67	8	2
4:A:406:PCW:C16	4:B:204:PCW:H282	0.43	2.43	9	1
4:C:602:PCW:H483	5:C:626:17F:H58	0.43	1.91	9	1
4:B:201:PCW:H471	4:D:527:PCW:H231	0.43	1.90	9	1
5:D:521:17F:O10	5:D:521:17F:O7	0.43	2.36	9	1
4:D:506:PCW:H52	4:D:509:PCW:C1	0.43	2.44	10	1
4:A:404:PCW:H281	4:A:411:PCW:C24	0.43	2.44	1	1
4:A:402:PCW:H411	4:A:402:PCW:H381	0.43	1.55	3	1
2:B:76:GLU:OE1	4:D:502:PCW:H73	0.43	2.14	3	1
4:D:507:PCW:H132	4:D:513:PCW:O3	0.43	2.14	3	1
4:D:515:PCW:C21	5:D:525:17F:H69	0.43	2.44	3	2
4:A:401:PCW:C43	4:C:614:PCW:H262	0.43	2.44	4	1
5:A:409:17F:C39	4:D:501:PCW:H272	0.43	2.25	4	1
5:A:409:17F:C36	4:D:503:PCW:H281	0.43	2.44	4	1
4:C:621:PCW:C48	5:C:630:17F:H12	0.43	2.42	4	1
4:D:518:PCW:C34	5:D:519:17F:H32	0.43	2.44	4	1
4:C:620:PCW:C14	5:C:631:17F:O9	0.43	2.64	5	1
4:B:201:PCW:H122	4:D:506:PCW:C36	0.43	2.44	5	1
4:B:203:PCW:H482	4:B:204:PCW:C47	0.43	2.44	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:203:PCW:H321	4:B:203:PCW:C7	0.43	2.43	5	1
4:D:508:PCW:H152	4:D:509:PCW:C18	0.43	2.44	5	1
4:D:518:PCW:H352	5:D:519:17F:C37	0.43	2.41	5	1
4:A:407:PCW:H131	4:A:407:PCW:H342	0.43	1.90	7	1
4:A:411:PCW:H422	4:C:612:PCW:C25	0.43	2.43	7	1
4:D:506:PCW:H221	4:D:516:PCW:H362	0.43	1.89	8	1
5:D:530:17F:H65	5:D:530:17F:H12A	0.43	1.90	8	1
4:D:502:PCW:H283	4:D:518:PCW:H222	0.43	1.91	9	1
5:D:522:17F:H8A	5:D:525:17F:C6	0.43	2.43	9	1
4:B:201:PCW:H342	4:D:510:PCW:C41	0.43	2.41	10	1
4:D:517:PCW:O31	4:D:517:PCW:H11	0.43	2.13	10	1
4:A:402:PCW:H211	4:A:405:PCW:C20	0.42	2.44	6	2
4:A:402:PCW:C8	4:A:405:PCW:C3	0.42	2.97	1	1
4:C:605:PCW:H322	4:C:613:PCW:H51	0.42	1.91	1	1
4:D:509:PCW:C41	5:D:520:17F:H11A	0.42	2.37	1	1
4:D:513:PCW:H462	4:D:517:PCW:H251	0.42	1.91	1	1
1:A:323:TYR:O	1:A:327:LEU:HG	0.42	2.13	2	1
4:A:406:PCW:H272	4:C:618:PCW:C45	0.42	2.43	2	1
4:D:501:PCW:C19	4:D:503:PCW:H332	0.42	2.43	2	1
1:A:228:PHE:CE1	4:A:404:PCW:H483	0.42	2.49	3	1
3:D:459:LEU:HG	3:D:471:LYS:HB3	0.42	1.91	3	1
1:C:497:SER:HB2	1:C:498:PRO:CD	0.42	2.41	4	2
4:D:515:PCW:H442	4:D:516:PCW:C16	0.42	2.44	4	1
4:C:609:PCW:H471	4:D:508:PCW:H221	0.42	1.90	5	1
5:C:628:17F:H39	5:C:628:17F:H36	0.42	1.60	7	3
1:A:327:LEU:O	1:A:331:LEU:HG	0.42	2.13	6	1
4:A:410:PCW:H461	4:D:518:PCW:C28	0.42	2.43	6	1
4:A:415:PCW:C44	4:C:605:PCW:H451	0.42	2.36	6	1
5:D:522:17F:H12A	5:D:522:17F:C23	0.42	2.44	6	1
4:A:403:PCW:C31	4:A:407:PCW:H52	0.42	2.44	7	1
4:D:513:PCW:C38	4:D:513:PCW:C42	0.42	2.95	7	1
4:A:401:PCW:C36	4:D:503:PCW:H212	0.42	2.44	8	1
4:D:504:PCW:H482	4:D:516:PCW:C19	0.42	2.44	9	1
1:A:217:LEU:HD11	4:A:404:PCW:H232	0.42	1.91	10	1
4:A:405:PCW:C5	4:D:514:PCW:H351	0.42	2.39	10	1
4:C:605:PCW:H40	4:C:619:PCW:H141	0.42	1.91	10	1
4:C:620:PCW:O31	4:C:620:PCW:O3	0.42	2.37	10	1
4:A:405:PCW:C18	4:A:405:PCW:H39	0.42	2.45	1	1
4:A:415:PCW:C27	4:D:516:PCW:H272	0.42	2.43	2	1
4:C:603:PCW:O11	4:C:604:PCW:C6	0.42	2.67	4	2
4:C:615:PCW:H472	4:D:512:PCW:H20	0.42	1.90	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:608:PCW:H152	5:C:627:17F:O10	0.42	2.14	3	1
4:D:527:PCW:H372	4:D:527:PCW:H141	0.42	1.91	3	1
5:A:409:17F:H39	5:A:409:17F:H35	0.42	1.56	4	2
4:A:415:PCW:H73	4:A:415:PCW:O4P	0.42	2.13	4	1
4:C:624:PCW:H211	4:C:624:PCW:H181	0.42	1.52	5	2
4:A:402:PCW:H151	4:A:405:PCW:H382	0.42	1.89	5	1
4:D:515:PCW:O3P	4:D:515:PCW:C31	0.42	2.67	8	2
4:A:408:PCW:C46	4:B:201:PCW:H232	0.42	2.45	6	1
4:B:202:PCW:H472	5:D:524:17F:C1Y	0.42	2.44	6	1
2:B:109:VAL:HG23	2:B:111:MET:HE2	0.42	1.91	7	1
5:D:522:17F:H40	5:D:522:17F:H36	0.42	1.65	9	2
3:D:359:ARG:HA	3:D:369:VAL:HG22	0.42	1.91	10	1
4:C:620:PCW:H121	5:C:631:17F:O9	0.42	2.14	1	1
4:C:613:PCW:H212	5:D:521:17F:C29	0.42	2.43	2	1
4:C:616:PCW:C43	4:B:201:PCW:H472	0.42	2.44	2	1
5:C:631:17F:H39	5:C:631:17F:H36	0.42	1.61	2	3
4:D:510:PCW:H483	4:D:510:PCW:C27	0.42	2.37	2	1
4:D:512:PCW:C7	5:D:520:17F:O5	0.42	2.68	2	1
4:A:414:PCW:C7	5:C:628:17F:O2	0.42	2.67	3	1
3:D:453:ASP:OD2	4:D:504:PCW:H61	0.42	2.13	3	1
4:D:508:PCW:H161	4:D:512:PCW:C16	0.42	2.39	3	1
4:D:515:PCW:C40	5:D:519:17F:H42	0.42	2.44	3	1
5:D:521:17F:O10	5:D:521:17F:C20	0.42	2.67	4	3
1:A:237:GLU:HA	1:A:240:ARG:HD2	0.42	1.91	4	1
3:D:482:THR:CG2	4:D:504:PCW:H62	0.42	2.38	4	1
4:D:504:PCW:H321	4:D:510:PCW:H352	0.42	1.90	4	1
4:D:517:PCW:H351	5:D:520:17F:H8A	0.42	1.90	4	1
4:D:518:PCW:H351	4:D:518:PCW:C3	0.42	2.44	4	1
4:A:412:PCW:H412	4:A:412:PCW:H382	0.42	1.56	5	1
4:C:607:PCW:H362	4:C:624:PCW:H452	0.42	1.89	5	1
4:C:613:PCW:H141	4:C:619:PCW:C38	0.42	2.44	5	1
4:D:505:PCW:C7	5:D:519:17F:H8	0.42	2.44	5	1
4:B:201:PCW:C34	4:D:510:PCW:H382	0.42	2.44	6	1
4:D:508:PCW:H121	4:D:512:PCW:H162	0.42	1.91	6	1
4:D:514:PCW:H242	4:D:514:PCW:C18	0.42	2.29	6	1
4:B:202:PCW:H272	4:B:204:PCW:H39	0.42	1.91	8	1
5:D:525:17F:C7	5:D:525:17F:O9	0.42	2.67	8	1
4:A:408:PCW:C31	4:A:408:PCW:O3	0.42	2.67	9	1
4:B:201:PCW:H172	4:D:527:PCW:H281	0.42	1.91	9	1
4:D:513:PCW:H40	4:D:513:PCW:H272	0.42	1.86	9	1
4:C:611:PCW:C21	4:C:619:PCW:H482	0.42	2.44	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:620:PCW:O1P	4:C:621:PCW:C4	0.42	2.66	10	1
4:B:201:PCW:O31	4:B:201:PCW:C1	0.42	2.63	10	1
4:A:410:PCW:C47	4:C:617:PCW:H252	0.42	2.45	2	2
4:D:507:PCW:O3P	4:D:507:PCW:O31	0.42	2.37	2	1
4:D:508:PCW:C8	4:D:508:PCW:O4P	0.42	2.66	2	1
5:D:523:17F:H62	5:D:523:17F:H59	0.42	1.59	2	1
4:A:402:PCW:C42	4:D:512:PCW:H132	0.42	2.45	3	1
5:A:409:17F:O4	4:D:503:PCW:C8	0.42	2.65	3	1
5:D:525:17F:H18	5:D:525:17F:H5	0.42	1.65	3	2
4:A:407:PCW:C14	4:A:407:PCW:C18	0.42	2.94	9	2
4:A:402:PCW:H162	4:A:405:PCW:C25	0.42	2.44	5	1
4:C:606:PCW:H162	5:D:529:17F:H11A	0.42	1.92	5	1
4:C:615:PCW:H211	5:C:631:17F:C24	0.42	2.33	5	1
4:B:203:PCW:H2	4:B:203:PCW:O2P	0.42	2.14	5	1
4:D:528:PCW:O3P	4:D:528:PCW:C31	0.42	2.66	5	2
4:A:401:PCW:H62	4:D:511:PCW:C3	0.42	2.34	6	1
4:A:415:PCW:H182	4:A:415:PCW:H211	0.42	1.59	6	2
4:C:602:PCW:H461	4:C:608:PCW:C47	0.42	2.32	6	1
4:D:513:PCW:C4	5:D:523:17F:O2	0.42	2.62	6	1
4:C:611:PCW:H452	4:C:611:PCW:H221	0.42	1.91	7	1
4:A:402:PCW:O2P	4:D:514:PCW:C7	0.42	2.67	8	1
4:C:608:PCW:C27	5:C:627:17F:H62	0.42	2.45	9	1
4:C:615:PCW:H211	4:D:512:PCW:H282	0.42	1.88	9	1
4:C:618:PCW:P	4:C:625:PCW:C4	0.42	3.07	9	1
3:D:440:ASN:O	3:D:465:CYS:HA	0.42	2.14	10	2
4:C:609:PCW:C17	4:C:615:PCW:H352	0.42	2.43	10	1
4:C:610:PCW:H281	5:C:629:17F:H72	0.42	1.92	10	1
4:B:203:PCW:C35	4:B:203:PCW:C31	0.42	2.98	10	1
4:C:615:PCW:H212	4:C:615:PCW:H182	0.42	1.58	10	2
3:D:360:VAL:HB	3:D:368:THR:O	0.42	2.14	1	1
4:D:506:PCW:H222	4:D:516:PCW:C35	0.42	2.42	1	1
1:A:251:LYS:O	1:A:254:VAL:HG12	0.42	2.14	2	2
4:A:402:PCW:H42	4:D:514:PCW:P	0.42	2.55	2	1
4:A:407:PCW:C16	4:A:412:PCW:H283	0.42	2.38	2	1
4:C:618:PCW:H341	5:C:629:17F:H36	0.42	1.92	2	1
4:C:609:PCW:H483	4:D:512:PCW:C46	0.42	2.44	3	1
5:C:626:17F:O8	5:C:627:17F:H31	0.42	2.14	3	1
4:D:508:PCW:O11	4:D:509:PCW:H242	0.42	2.14	3	1
1:A:217:LEU:O	1:A:221:LEU:HG	0.42	2.13	4	1
4:B:202:PCW:H171	4:B:202:PCW:C43	0.42	2.44	4	1
4:B:202:PCW:H271	4:B:203:PCW:H241	0.42	1.92	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:403:PCW:H182	4:A:403:PCW:H211	0.42	1.59	6	1
4:A:406:PCW:H162	4:B:202:PCW:H232	0.42	1.92	6	1
4:B:201:PCW:C42	4:B:201:PCW:H382	0.42	2.43	6	1
4:D:501:PCW:H282	5:D:522:17F:H55	0.42	1.90	7	1
4:A:402:PCW:H40	4:A:405:PCW:C28	0.42	2.45	8	1
4:C:606:PCW:H62	4:C:624:PCW:C20	0.42	2.43	8	1
4:C:612:PCW:C7	4:C:618:PCW:C3	0.42	2.97	8	1
4:C:612:PCW:H61	4:C:625:PCW:H32	0.42	1.91	1	1
4:B:202:PCW:H482	4:D:510:PCW:C22	0.42	2.30	1	1
4:A:411:PCW:O3P	4:A:411:PCW:C31	0.42	2.67	9	4
4:C:604:PCW:H41	4:C:604:PCW:C3	0.42	2.38	3	1
4:C:610:PCW:H172	5:C:629:17F:C34	0.42	2.45	9	2
4:D:508:PCW:H141	4:D:509:PCW:H181	0.42	1.88	3	2
4:A:404:PCW:O2	4:A:404:PCW:O2P	0.42	2.36	4	1
4:A:407:PCW:H342	4:A:407:PCW:H131	0.42	1.90	4	1
2:B:3:GLU:HA	2:B:52:LEU:O	0.42	2.13	4	1
4:D:504:PCW:O11	4:D:504:PCW:C2	0.42	2.61	4	1
4:D:507:PCW:H63	5:D:523:17F:C2	0.42	2.44	4	1
1:A:255:GLN:HB2	1:A:256:PRO:HD3	0.42	1.90	5	2
4:C:616:PCW:H461	4:C:625:PCW:H261	0.42	1.88	6	1
4:B:201:PCW:H131	4:D:516:PCW:C39	0.42	2.45	6	1
4:C:613:PCW:H251	5:D:521:17F:H43	0.42	1.91	7	1
4:C:616:PCW:C3	4:C:616:PCW:O1P	0.42	2.68	7	1
4:C:624:PCW:H381	4:C:624:PCW:H411	0.42	1.61	8	1
4:D:504:PCW:H331	4:D:510:PCW:C32	0.42	2.20	8	1
4:D:504:PCW:C39	4:D:505:PCW:H51	0.42	2.38	8	1
4:D:506:PCW:H272	4:D:515:PCW:C47	0.42	2.44	8	1
4:D:509:PCW:O2P	4:D:509:PCW:H32	0.42	2.11	8	1
5:D:529:17F:H18A	5:D:529:17F:O8	0.42	2.15	8	1
4:A:404:PCW:C32	4:D:510:PCW:H181	0.42	2.44	9	1
4:C:617:PCW:H41	4:C:617:PCW:C2	0.42	2.42	9	1
4:D:508:PCW:H241	4:D:512:PCW:H382	0.42	1.91	9	1
4:C:618:PCW:H342	4:C:625:PCW:C34	0.42	2.44	10	1
4:D:509:PCW:C46	5:D:520:17F:H33	0.42	2.44	10	1
4:A:406:PCW:H241	4:B:203:PCW:C24	0.42	2.29	1	1
4:A:415:PCW:H211	4:A:415:PCW:H182	0.42	1.57	9	2
5:C:626:17F:H35	5:C:626:17F:H39	0.42	1.65	1	1
4:A:403:PCW:H261	4:D:507:PCW:C20	0.42	2.45	2	1
4:C:601:PCW:O31	4:C:601:PCW:C34	0.42	2.67	9	2
4:A:406:PCW:C35	4:B:204:PCW:C16	0.42	2.98	3	1
4:D:506:PCW:H181	4:D:506:PCW:H211	0.42	1.63	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:410:PCW:H2	4:A:410:PCW:O2P	0.42	2.13	4	1
4:D:501:PCW:H461	5:D:525:17F:H51	0.42	1.90	4	1
4:C:609:PCW:O11	4:C:615:PCW:C8	0.42	2.67	5	1
4:D:507:PCW:H452	4:D:517:PCW:H261	0.42	1.90	5	1
4:A:411:PCW:O31	4:A:411:PCW:O3P	0.42	2.38	7	1
1:C:524:GLU:O	1:C:528:ARG:HG3	0.42	2.15	8	1
4:C:609:PCW:O31	4:C:615:PCW:C6	0.42	2.68	8	1
4:D:508:PCW:H212	4:D:512:PCW:H151	0.42	1.88	8	1
5:D:522:17F:O8	5:D:525:17F:H6	0.42	2.14	9	1
1:A:279:LEU:HD11	1:C:499:LEU:HD11	0.42	1.91	10	1
5:A:409:17F:H75	5:D:521:17F:H68	0.42	1.90	10	1
4:A:402:PCW:H441	4:D:512:PCW:C15	0.42	2.44	1	1
4:D:508:PCW:H242	4:D:512:PCW:C38	0.42	2.44	1	1
4:D:511:PCW:H341	4:D:511:PCW:H182	0.42	1.90	1	1
4:D:515:PCW:O3	4:D:515:PCW:C31	0.42	2.68	1	1
1:A:372:ARG:O	1:A:376:LEU:HG	0.42	2.15	2	1
4:C:605:PCW:C38	4:C:611:PCW:H31	0.42	2.45	2	1
4:D:507:PCW:H82	4:D:508:PCW:C8	0.42	2.45	2	1
4:A:414:PCW:H372	4:C:617:PCW:H152	0.42	1.90	3	1
4:A:415:PCW:C11	4:A:415:PCW:O31	0.42	2.67	3	1
4:D:503:PCW:O1P	4:D:503:PCW:H52	0.42	2.14	4	1
1:C:483:GLU:OE2	1:C:486:ARG:HD2	0.42	2.14	5	1
4:D:508:PCW:H241	4:D:512:PCW:C42	0.42	2.45	5	1
4:D:513:PCW:H482	5:D:522:17F:H78	0.42	1.90	5	1
4:D:505:PCW:C46	4:D:518:PCW:H261	0.42	2.44	6	1
4:C:611:PCW:H41	4:C:622:PCW:C34	0.42	2.45	8	2
4:D:515:PCW:H63	4:D:516:PCW:O1P	0.42	2.15	7	1
4:A:402:PCW:C39	4:A:405:PCW:H272	0.42	2.44	8	1
3:D:406:LYS:HG3	5:D:523:17F:H76	0.42	1.90	8	1
4:A:404:PCW:H42	4:D:510:PCW:H151	0.42	1.92	9	1
4:A:411:PCW:H39	4:C:612:PCW:C45	0.42	2.39	9	1
4:C:614:PCW:H12	4:C:623:PCW:H61	0.42	1.91	10	1
5:D:529:17F:H35	5:D:530:17F:H10	0.42	1.92	10	1
5:A:409:17F:H57	4:D:503:PCW:H212	0.42	1.89	1	1
4:D:507:PCW:H432	5:D:525:17F:C7	0.42	2.45	1	1
4:D:507:PCW:H411	5:D:525:17F:H6	0.42	1.92	1	1
4:A:406:PCW:H41	4:B:204:PCW:C11	0.42	2.45	2	1
4:A:414:PCW:O31	4:C:617:PCW:H51	0.42	2.14	2	1
4:A:415:PCW:C28	4:D:516:PCW:H251	0.42	2.43	2	1
4:C:621:PCW:H471	5:C:630:17F:H63	0.42	1.91	2	1
1:C:404:ASN:O	1:C:408:VAL:HG23	0.42	2.15	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:508:PCW:C14	4:D:509:PCW:C18	0.42	2.91	3	1
1:A:217:LEU:HD11	4:A:404:PCW:H231	0.42	1.90	4	1
1:A:246:ASP:O	4:A:408:PCW:H281	0.42	2.15	4	1
1:A:262:GLN:O	1:A:266:GLN:HG3	0.42	2.14	4	1
4:A:415:PCW:C32	4:C:622:PCW:H351	0.42	2.45	4	1
4:B:201:PCW:H431	4:D:510:PCW:C41	0.42	2.37	4	1
4:D:509:PCW:C35	5:D:520:17F:H59	0.42	2.44	4	1
4:A:415:PCW:O31	4:A:415:PCW:C11	0.42	2.68	5	1
1:A:375:LEU:CD1	5:A:409:17F:H41	0.42	2.45	6	1
4:D:511:PCW:H221	5:D:522:17F:H19A	0.42	1.90	6	1
4:D:518:PCW:H122	5:D:519:17F:H72	0.42	1.90	6	1
4:A:402:PCW:O1P	4:D:514:PCW:H73	0.42	2.14	7	1
4:A:403:PCW:C24	5:D:523:17F:H18	0.42	2.44	7	1
4:A:404:PCW:H412	4:B:202:PCW:H461	0.42	1.92	7	1
4:A:408:PCW:H431	4:B:203:PCW:H19	0.42	1.91	7	1
4:A:412:PCW:H322	4:C:623:PCW:H341	0.42	1.92	7	1
4:A:404:PCW:H62	5:D:524:17F:H5	0.42	1.91	8	1
4:C:616:PCW:H361	4:D:527:PCW:C36	0.42	2.37	8	1
4:A:404:PCW:C5	4:D:510:PCW:O11	0.42	2.67	9	1
4:A:405:PCW:O31	4:A:405:PCW:H41	0.42	2.15	9	1
4:D:514:PCW:C25	4:D:514:PCW:C21	0.42	2.81	9	1
4:D:502:PCW:C28	4:D:518:PCW:H262	0.42	2.45	10	1
4:C:603:PCW:C5	5:D:530:17F:O1	0.42	2.68	1	1
4:D:506:PCW:O1P	4:D:509:PCW:H332	0.42	2.14	1	1
4:D:509:PCW:H20	5:D:520:17F:H57	0.42	1.92	1	1
4:A:408:PCW:H381	4:B:203:PCW:C41	0.42	2.45	2	1
4:C:605:PCW:H382	4:C:611:PCW:H31	0.42	1.91	2	1
4:C:621:PCW:H152	5:C:630:17F:H6	0.42	1.89	2	1
1:A:244:SER:O	1:A:248:GLU:HB2	0.42	2.14	3	1
4:C:605:PCW:C32	4:C:613:PCW:H82	0.42	2.45	3	1
4:C:611:PCW:H461	4:C:611:PCW:H241	0.42	1.90	3	1
4:D:518:PCW:H442	5:D:519:17F:C40	0.42	2.43	3	1
4:C:603:PCW:C31	4:C:603:PCW:O3	0.42	2.67	4	2
4:D:503:PCW:C41	4:D:511:PCW:H221	0.42	2.45	4	1
4:D:504:PCW:H212	4:D:504:PCW:H181	0.42	1.64	5	1
4:A:403:PCW:C31	4:A:403:PCW:O3	0.42	2.68	6	1
4:C:604:PCW:H451	4:C:606:PCW:H142	0.42	1.92	6	1
4:C:609:PCW:H283	5:D:520:17F:H51	0.42	1.92	6	1
4:D:505:PCW:H2	4:D:505:PCW:O4P	0.42	2.14	6	1
4:A:415:PCW:H352	4:C:622:PCW:H122	0.42	1.91	7	1
4:C:618:PCW:H181	4:C:618:PCW:H212	0.42	1.63	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:477:LEU:HA	1:C:480:GLU:HB2	0.42	1.91	8	1
5:D:522:17F:C21	5:D:525:17F:H37	0.42	2.44	8	1
4:A:406:PCW:H411	4:B:204:PCW:H182	0.42	1.91	9	1
4:A:402:PCW:H412	4:D:508:PCW:H262	0.41	1.92	1	2
4:C:616:PCW:H211	4:C:616:PCW:H181	0.41	1.65	9	2
2:B:15:GLY:HA2	6:B:205:GNP:H8	0.41	1.91	1	1
4:B:202:PCW:H271	4:D:506:PCW:H471	0.41	1.91	1	1
3:D:430:PHE:O	3:D:435:PRO:HA	0.41	2.15	1	1
4:D:505:PCW:O31	4:D:505:PCW:C34	0.41	2.68	1	1
5:D:525:17F:H5	5:D:525:17F:H18	0.41	1.39	7	2
4:A:404:PCW:H362	4:D:510:PCW:H212	0.41	1.92	2	1
4:A:414:PCW:C44	4:C:617:PCW:C20	0.41	2.98	2	1
4:C:603:PCW:H41	4:C:603:PCW:C31	0.41	2.44	2	1
4:C:611:PCW:C1	4:C:613:PCW:H61	0.41	2.44	2	1
4:B:201:PCW:H381	5:D:524:17F:H48	0.41	1.91	2	1
4:D:515:PCW:O2	4:D:515:PCW:C11	0.41	2.68	10	3
4:C:605:PCW:O2P	4:C:613:PCW:C6	0.41	2.68	3	1
4:C:610:PCW:O3	4:C:610:PCW:C31	0.41	2.68	3	1
4:C:616:PCW:H341	4:D:527:PCW:C36	0.41	2.39	3	1
4:C:615:PCW:C19	5:C:631:17F:H38	0.41	2.45	4	1
4:D:517:PCW:C39	5:D:525:17F:H59	0.41	2.44	4	1
2:B:16:LYS:N	6:B:205:GNP:O1B	0.41	2.52	10	3
4:D:501:PCW:H19	4:D:503:PCW:C34	0.41	2.45	5	1
4:D:506:PCW:C1	4:D:515:PCW:H73	0.41	2.45	5	1
4:A:413:PCW:O2P	4:A:413:PCW:C5	0.41	2.65	6	1
4:A:415:PCW:H282	4:D:528:PCW:H262	0.41	1.91	6	1
4:C:624:PCW:H182	4:C:624:PCW:C8	0.41	2.45	6	1
3:D:402:LEU:HD13	4:D:502:PCW:H51	0.41	1.92	6	1
4:D:508:PCW:H171	4:D:512:PCW:H362	0.41	1.88	6	1
4:C:613:PCW:C47	4:C:619:PCW:H422	0.41	2.39	7	1
4:C:617:PCW:C2	4:C:617:PCW:O11	0.41	2.60	7	1
4:D:502:PCW:C19	4:D:505:PCW:H142	0.41	2.36	8	1
4:A:406:PCW:C23	4:B:202:PCW:C22	0.41	2.98	9	1
5:C:631:17F:H40	4:D:512:PCW:C28	0.41	2.44	9	1
4:B:201:PCW:H232	4:B:203:PCW:H282	0.41	1.91	9	1
4:A:405:PCW:H82	4:D:514:PCW:H362	0.41	1.92	10	1
4:C:615:PCW:H272	5:C:631:17F:C26	0.41	2.45	10	1
4:C:621:PCW:C26	4:D:528:PCW:H61	0.41	2.44	10	1
4:D:506:PCW:C5	4:D:509:PCW:H11	0.41	2.45	10	1
4:A:404:PCW:H261	1:C:554:HIS:HE1	0.41	1.74	1	1
4:A:410:PCW:O1P	4:A:410:PCW:C5	0.41	2.67	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:606:PCW:H412	4:C:606:PCW:H381	0.41	1.57	1	1
4:C:609:PCW:C11	4:C:615:PCW:C7	0.41	2.97	1	1
4:C:613:PCW:C20	5:D:521:17F:H42	0.41	2.44	1	1
4:C:618:PCW:P	4:C:625:PCW:H63	0.41	2.56	1	1
4:C:624:PCW:H181	4:C:624:PCW:H211	0.41	1.51	2	3
5:C:629:17F:H53	4:B:203:PCW:H252	0.41	1.91	1	1
4:B:204:PCW:O3P	4:B:204:PCW:H51	0.41	2.15	2	1
4:D:503:PCW:O3	4:D:511:PCW:H371	0.41	2.14	2	1
4:C:625:PCW:O4P	4:C:625:PCW:C8	0.41	2.68	3	1
4:D:510:PCW:H351	5:D:524:17F:H11	0.41	1.92	4	1
4:D:510:PCW:H131	5:D:524:17F:H77	0.41	1.92	4	1
4:C:611:PCW:C5	4:C:622:PCW:H342	0.41	2.45	5	1
4:C:614:PCW:H452	4:C:619:PCW:C20	0.41	2.46	5	1
2:B:18:ALA:HB2	6:B:205:GNP:H2'	0.41	1.92	5	1
2:B:77:GLY:HA3	2:B:163:ILE:HD11	0.41	1.91	5	1
4:D:504:PCW:C26	4:D:510:PCW:H40	0.41	2.45	6	1
4:D:509:PCW:H73	4:D:514:PCW:H12	0.41	1.92	6	1
5:D:520:17F:H36	5:D:520:17F:H39	0.41	1.61	6	1
4:C:616:PCW:H372	4:C:618:PCW:H141	0.41	1.92	7	1
4:C:616:PCW:H181	4:C:616:PCW:H211	0.41	1.63	8	1
5:C:626:17F:C23	5:C:627:17F:H74	0.41	2.42	8	1
4:B:203:PCW:H382	4:B:203:PCW:H412	0.41	1.73	8	1
4:A:406:PCW:C11	4:B:204:PCW:H121	0.41	2.46	9	1
4:A:406:PCW:H331	4:B:204:PCW:H122	0.41	1.91	9	1
4:A:407:PCW:C39	5:D:522:17F:C40	0.41	2.97	10	1
4:C:605:PCW:C41	4:C:619:PCW:H121	0.41	2.43	10	1
4:C:625:PCW:O3	4:C:625:PCW:O31	0.41	2.38	10	1
4:D:517:PCW:H442	5:D:525:17F:C23	0.41	2.35	10	1
4:C:611:PCW:C3	4:C:619:PCW:C11	0.41	2.99	1	1
4:D:509:PCW:C23	4:D:509:PCW:C27	0.41	2.98	1	1
4:D:515:PCW:O2	4:D:515:PCW:O11	0.41	2.37	10	2
4:D:517:PCW:H332	5:D:525:17F:H32	0.41	1.92	2	1
1:A:307:ASP:O	1:A:310:ARG:HB2	0.41	2.15	3	2
5:A:409:17F:O4	4:D:503:PCW:C5	0.41	2.68	3	1
4:A:414:PCW:C7	5:C:628:17F:P1	0.41	3.08	3	1
4:B:201:PCW:H161	4:D:506:PCW:H431	0.41	1.92	3	1
4:A:412:PCW:H63	4:C:624:PCW:O2	0.41	2.16	4	1
4:C:618:PCW:H381	4:C:625:PCW:H172	0.41	1.92	4	1
2:B:32:TYR:HA	6:B:205:GNP:O2A	0.41	2.15	4	1
4:D:515:PCW:H462	4:D:516:PCW:H161	0.41	1.92	4	1
5:D:522:17F:C12	5:D:522:17F:C24	0.41	2.77	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:603:PCW:C21	4:C:603:PCW:C17	0.41	2.97	5	1
4:D:503:PCW:H483	4:D:507:PCW:H483	0.41	1.92	5	1
4:D:517:PCW:H412	5:D:525:17F:H12	0.41	1.92	5	1
4:C:601:PCW:H39	4:C:602:PCW:H141	0.41	1.91	6	1
2:B:3:GLU:HA	2:B:52:LEU:HB3	0.41	1.92	7	1
4:D:507:PCW:H32	4:D:513:PCW:C15	0.41	2.31	7	1
4:D:512:PCW:H61	5:D:520:17F:O4	0.41	2.16	7	1
4:C:607:PCW:C31	4:C:624:PCW:H371	0.41	2.44	8	1
4:D:503:PCW:C39	5:D:522:17F:H9A	0.41	2.42	8	1
4:A:403:PCW:C33	4:A:407:PCW:H332	0.41	2.40	9	1
5:A:409:17F:O2	4:D:503:PCW:H82	0.41	2.16	9	1
2:B:21:ILE:HD13	3:D:388:VAL:HG13	0.41	1.91	9	1
2:B:35:THR:OG1	6:B:205:GNP:O2G	0.41	2.38	9	1
4:A:405:PCW:O31	4:D:514:PCW:H352	0.41	2.16	10	1
4:C:606:PCW:C42	4:C:609:PCW:H31	0.41	2.43	10	1
4:B:204:PCW:H181	4:B:204:PCW:H212	0.41	1.70	10	1
4:A:403:PCW:H211	4:A:403:PCW:H182	0.41	1.59	4	2
4:C:604:PCW:C31	4:C:606:PCW:H82	0.41	2.45	1	1
4:C:610:PCW:H481	4:B:203:PCW:C48	0.41	2.45	1	1
4:D:517:PCW:H352	5:D:520:17F:H9A	0.41	1.93	1	1
4:A:403:PCW:H31	4:A:403:PCW:C5	0.41	2.45	2	1
4:A:403:PCW:C5	4:A:403:PCW:O11	0.41	2.68	2	1
4:C:605:PCW:H481	4:C:613:PCW:H162	0.41	1.92	2	1
4:C:606:PCW:C4	4:C:624:PCW:H19	0.41	2.45	2	1
4:D:508:PCW:H352	4:D:512:PCW:H142	0.41	1.91	3	2
4:D:516:PCW:H461	5:D:530:17F:H38	0.41	1.92	3	1
4:D:503:PCW:O31	4:D:503:PCW:O3	0.41	2.38	8	2
4:D:504:PCW:H182	4:D:506:PCW:H481	0.41	1.91	4	1
4:D:506:PCW:O3	5:D:520:17F:H11	0.41	2.15	4	1
5:D:520:17F:C22	5:D:529:17F:H55	0.41	2.45	4	1
5:D:525:17F:H36	5:D:525:17F:H39	0.41	1.62	4	1
1:C:411:THR:O	1:C:415:LEU:HG	0.41	2.14	5	1
4:D:504:PCW:H442	4:D:505:PCW:H52	0.41	1.92	5	1
4:D:510:PCW:H31	5:D:524:17F:C42	0.41	2.45	5	1
4:D:513:PCW:H471	4:D:513:PCW:C27	0.41	2.44	5	1
1:A:306:ARG:O	1:A:310:ARG:HG3	0.41	2.15	6	1
4:A:415:PCW:H182	4:C:603:PCW:H141	0.41	1.91	6	1
1:C:463:TRP:HD1	5:C:627:17F:H70	0.41	1.75	6	1
4:D:512:PCW:O3	4:D:512:PCW:C31	0.41	2.68	6	2
4:D:527:PCW:H152	4:D:528:PCW:C17	0.41	2.46	6	1
5:A:409:17F:H75	5:D:521:17F:C33	0.41	2.44	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:616:PCW:H341	4:D:527:PCW:C35	0.41	2.46	8	1
4:D:506:PCW:C22	4:D:516:PCW:H362	0.41	2.46	8	1
4:A:405:PCW:H231	4:A:405:PCW:C15	0.41	2.45	9	1
4:A:412:PCW:C47	4:C:623:PCW:H483	0.41	2.37	9	1
4:C:618:PCW:H442	4:C:625:PCW:C28	0.41	2.42	9	1
4:B:202:PCW:C1	4:D:504:PCW:C11	0.41	2.96	9	1
4:D:501:PCW:H432	4:D:515:PCW:H171	0.41	1.92	9	1
4:D:502:PCW:C28	4:D:518:PCW:H222	0.41	2.46	9	1
4:D:513:PCW:H272	4:D:513:PCW:H412	0.41	1.92	9	1
4:C:616:PCW:H483	4:D:504:PCW:H222	0.41	1.91	10	1
4:C:613:PCW:C43	4:C:619:PCW:H39	0.41	2.44	3	2
4:D:507:PCW:C16	4:D:513:PCW:H122	0.41	2.46	1	1
1:A:301:LEU:HD13	1:C:473:LYS:HG3	0.41	1.92	3	1
4:B:202:PCW:H362	4:B:202:PCW:C12	0.41	2.41	3	1
4:D:508:PCW:C13	4:D:509:PCW:H182	0.41	2.45	3	1
5:D:519:17F:H36	5:D:519:17F:H39	0.41	1.60	3	1
2:B:126:ASP:OD2	2:B:128:LYS:HB3	0.41	2.15	4	1
3:D:400:ARG:HG2	3:D:410:ALA:HB3	0.41	1.92	5	1
4:D:509:PCW:H182	4:D:512:PCW:H342	0.41	1.91	5	1
4:C:605:PCW:C48	4:C:619:PCW:H421	0.41	2.45	6	1
4:D:501:PCW:H382	4:D:501:PCW:H412	0.41	1.66	6	1
4:D:501:PCW:H281	5:D:522:17F:H50	0.41	1.90	7	1
4:D:509:PCW:H212	4:D:509:PCW:H181	0.41	1.60	7	1
4:D:515:PCW:H61	4:D:516:PCW:O3P	0.41	2.15	7	1
4:D:517:PCW:O2P	5:D:520:17F:O1	0.41	2.38	7	1
4:C:612:PCW:H212	4:C:612:PCW:H181	0.41	1.64	8	1
4:B:204:PCW:H381	4:B:204:PCW:H412	0.41	1.65	8	1
3:D:359:ARG:HD3	3:D:425:GLU:OE2	0.41	2.16	8	1
4:D:513:PCW:H162	5:D:523:17F:H8	0.41	1.93	8	1
5:D:529:17F:H18A	5:D:529:17F:H5	0.41	1.48	8	1
4:A:401:PCW:C3	4:D:511:PCW:H231	0.41	2.45	9	1
4:A:403:PCW:H211	4:D:513:PCW:H371	0.41	1.92	9	1
4:D:508:PCW:H241	4:D:512:PCW:C38	0.41	2.45	9	1
4:D:517:PCW:H73	5:D:520:17F:O1	0.41	2.15	9	1
5:D:521:17F:H12	5:D:521:17F:H63	0.41	1.93	9	1
4:C:602:PCW:H462	5:C:626:17F:C33	0.41	2.45	10	1
4:C:603:PCW:C27	4:D:526:PCW:H171	0.41	2.45	10	1
5:A:409:17F:O6	5:A:409:17F:C17	0.41	2.68	6	2
4:D:511:PCW:C37	4:D:511:PCW:C41	0.41	2.98	1	1
4:D:514:PCW:O1P	4:D:514:PCW:C5	0.41	2.62	1	1
4:D:518:PCW:H51	5:D:519:17F:C7	0.41	2.44	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:402:PCW:H361	4:D:512:PCW:H361	0.41	1.92	2	1
4:D:507:PCW:C42	4:D:517:PCW:H222	0.41	2.09	2	1
5:A:409:17F:H68	4:D:501:PCW:C24	0.41	2.46	3	1
4:C:603:PCW:H212	4:C:603:PCW:H472	0.41	1.91	3	1
4:D:510:PCW:C16	4:D:510:PCW:H211	0.41	2.45	3	1
3:D:479:LYS:O	3:D:481:PRO:HD3	0.41	2.14	4	1
4:D:515:PCW:H132	5:D:525:17F:C34	0.41	2.45	4	1
1:C:483:GLU:O	1:C:487:GLN:HG2	0.41	2.16	5	1
4:C:607:PCW:H12	4:C:624:PCW:C35	0.41	2.45	7	2
4:C:617:PCW:O31	4:C:617:PCW:N	0.41	2.54	5	1
3:D:406:LYS:HE3	4:D:502:PCW:H40	0.41	1.91	5	1
2:B:118:CYS:HB2	2:B:123:ARG:NH2	0.41	2.30	6	1
4:D:518:PCW:H141	5:D:519:17F:C40	0.41	2.39	7	1
4:A:414:PCW:P	4:C:617:PCW:C4	0.41	3.00	8	1
4:A:415:PCW:H462	4:C:622:PCW:H281	0.41	1.92	8	1
4:C:606:PCW:H331	4:C:608:PCW:C7	0.41	2.46	8	1
4:B:201:PCW:H141	4:D:506:PCW:C46	0.41	2.45	9	1
4:D:506:PCW:H381	4:D:506:PCW:H411	0.41	1.53	9	1
1:A:309:ALA:HA	1:A:312:HIS:HB2	0.41	1.93	10	1
4:A:403:PCW:H321	4:A:407:PCW:C5	0.41	2.37	10	1
4:A:410:PCW:C7	5:C:628:17F:O5	0.41	2.69	10	1
4:C:613:PCW:H462	4:C:619:PCW:C39	0.41	2.45	10	1
4:D:502:PCW:H381	4:D:502:PCW:H411	0.41	1.70	10	1
4:D:507:PCW:H52	5:D:523:17F:H9	0.41	1.91	10	1
4:D:512:PCW:H63	5:D:520:17F:O4	0.41	2.15	10	1
4:A:405:PCW:H39	4:A:405:PCW:H182	0.41	1.91	1	1
4:A:401:PCW:H12	4:D:511:PCW:H211	0.41	1.91	2	1
4:C:621:PCW:H181	4:C:621:PCW:H212	0.41	1.58	2	2
4:C:625:PCW:C38	4:C:625:PCW:C42	0.41	2.97	2	1
4:D:511:PCW:C4	4:D:511:PCW:O11	0.41	2.65	3	1
4:D:518:PCW:C44	5:D:519:17F:H73	0.41	2.44	3	1
4:C:608:PCW:H262	5:C:627:17F:C1X	0.41	2.46	9	3
4:B:201:PCW:C23	4:B:203:PCW:H272	0.41	2.46	4	1
4:C:604:PCW:C16	4:C:604:PCW:C21	0.41	2.99	5	1
4:C:611:PCW:C16	4:C:619:PCW:C17	0.41	2.95	5	1
4:C:619:PCW:H411	4:C:619:PCW:H381	0.41	1.64	5	1
4:D:507:PCW:H52	5:D:523:17F:O5	0.41	2.15	5	1
4:A:402:PCW:H40	4:A:405:PCW:C27	0.41	2.45	7	1
4:C:616:PCW:H441	4:C:625:PCW:C26	0.41	2.37	7	1
4:D:507:PCW:O3	4:D:507:PCW:C31	0.41	2.68	8	1
4:A:407:PCW:H432	4:A:412:PCW:H281	0.41	1.91	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:408:PCW:O3	4:A:408:PCW:O31	0.41	2.39	9	1
4:C:614:PCW:H411	4:C:614:PCW:H381	0.41	1.59	9	1
4:D:515:PCW:C43	4:D:516:PCW:C3	0.41	2.82	9	1
1:A:213:THR:HA	1:C:561:LYS:HE2	0.41	1.92	10	1
4:A:411:PCW:O4P	4:A:411:PCW:C8	0.41	2.69	10	1
4:A:412:PCW:C8	4:C:624:PCW:O31	0.41	2.69	10	1
2:B:159:LEU:O	2:B:163:ILE:HG13	0.41	2.16	10	1
4:A:402:PCW:C31	4:A:402:PCW:O4P	0.41	2.69	1	1
4:A:415:PCW:C31	4:A:415:PCW:H61	0.41	2.45	1	1
4:B:203:PCW:H211	4:B:203:PCW:H181	0.41	1.60	1	1
4:D:511:PCW:H412	4:D:511:PCW:H231	0.41	1.91	1	1
4:D:515:PCW:C16	5:D:520:17F:H41	0.41	2.33	1	1
4:A:411:PCW:H332	4:C:612:PCW:H152	0.41	1.91	2	1
4:B:203:PCW:H181	4:B:203:PCW:H211	0.41	1.65	3	1
3:D:487:TRP:HZ2	4:D:515:PCW:H381	0.41	1.75	3	1
4:D:509:PCW:H351	5:D:520:17F:H64	0.41	1.92	3	1
5:D:529:17F:H63	5:D:529:17F:H58	0.41	1.72	3	1
4:C:613:PCW:H482	4:C:619:PCW:H181	0.41	1.91	4	1
4:A:412:PCW:H481	4:C:607:PCW:H471	0.41	1.93	5	1
4:C:605:PCW:H39	4:C:611:PCW:C31	0.41	2.45	5	1
4:D:508:PCW:H352	4:D:512:PCW:C12	0.41	2.46	5	1
4:A:402:PCW:H451	5:C:631:17F:C30	0.41	2.46	7	1
4:C:605:PCW:C8	5:C:628:17F:O4	0.41	2.69	7	1
4:D:501:PCW:H271	4:D:511:PCW:H442	0.41	1.93	7	1
4:D:501:PCW:H472	4:D:515:PCW:H222	0.41	1.91	8	1
4:D:508:PCW:H221	4:D:512:PCW:H172	0.41	1.92	8	1
3:D:400:ARG:HB3	3:D:412:LEU:HG	0.41	1.91	9	1
4:D:516:PCW:H40	4:D:527:PCW:H271	0.41	1.91	9	1
4:D:517:PCW:P	4:D:517:PCW:O2	0.41	2.79	9	1
4:C:607:PCW:C1	4:C:624:PCW:H362	0.41	2.44	10	1
4:A:413:PCW:H351	4:C:617:PCW:C42	0.41	2.46	1	1
4:D:501:PCW:H371	4:D:501:PCW:H412	0.41	1.92	1	1
4:D:507:PCW:C7	4:D:517:PCW:O3P	0.41	2.68	1	1
5:D:523:17F:H39	5:D:523:17F:H36	0.41	1.59	1	3
4:A:402:PCW:C12	4:A:405:PCW:O11	0.41	2.67	2	1
4:A:414:PCW:P	4:C:617:PCW:H52	0.41	2.56	2	1
4:A:415:PCW:C20	4:D:516:PCW:H262	0.41	2.46	2	1
4:B:201:PCW:H122	4:D:506:PCW:H341	0.41	1.93	2	1
4:D:506:PCW:H20	4:D:516:PCW:C35	0.41	2.46	2	1
5:D:525:17F:O10	5:D:525:17F:H20A	0.41	2.13	2	1
5:D:530:17F:H11	5:D:530:17F:H20	0.41	1.93	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:408:PCW:H462	4:B:201:PCW:C27	0.41	2.41	3	1
4:C:601:PCW:O3	4:C:601:PCW:C31	0.41	2.69	3	1
4:C:609:PCW:O3	4:C:609:PCW:C31	0.41	2.69	3	1
4:B:202:PCW:H382	4:B:202:PCW:H411	0.41	1.57	3	1
3:D:487:TRP:CZ2	4:D:515:PCW:H381	0.41	2.51	3	1
4:A:412:PCW:H182	4:A:412:PCW:H211	0.41	1.67	4	1
4:A:415:PCW:C4	4:C:622:PCW:H331	0.41	2.42	4	1
4:C:601:PCW:H39	4:C:602:PCW:C17	0.41	2.37	4	1
4:B:201:PCW:H211	4:D:506:PCW:H452	0.41	1.93	4	1
4:B:202:PCW:H382	4:B:202:PCW:H412	0.41	1.71	4	1
4:D:506:PCW:C1	4:D:515:PCW:C6	0.41	2.97	4	1
4:A:407:PCW:H472	4:A:407:PCW:H281	0.41	1.86	5	1
4:C:603:PCW:H51	5:D:530:17F:O1	0.41	2.16	5	1
4:C:607:PCW:C41	4:C:624:PCW:H472	0.41	2.45	5	1
4:C:610:PCW:H121	5:C:629:17F:C18	0.41	2.45	5	1
2:B:84:ILE:HD13	2:B:123:ARG:HG3	0.41	1.91	5	1
4:D:503:PCW:H412	4:D:511:PCW:H352	0.41	1.92	5	1
4:C:606:PCW:C26	5:D:529:17F:H41	0.41	2.46	6	1
4:D:501:PCW:H242	5:D:521:17F:H68	0.41	1.93	6	1
4:D:506:PCW:H19	4:D:516:PCW:H342	0.41	1.93	6	1
4:D:507:PCW:H381	4:D:507:PCW:C42	0.41	2.41	6	1
5:A:409:17F:O9	5:A:409:17F:C20	0.41	2.69	9	2
5:A:409:17F:N1	3:D:425:GLU:OE1	0.41	2.54	7	1
4:A:412:PCW:C32	4:C:623:PCW:C34	0.41	2.99	7	1
1:C:490:HIS:O	1:C:494:GLU:HG3	0.41	2.15	7	1
4:C:603:PCW:C23	4:D:526:PCW:H351	0.41	2.46	7	1
4:C:606:PCW:O31	4:C:606:PCW:O3P	0.41	2.38	7	1
4:C:610:PCW:H212	4:C:610:PCW:H181	0.41	1.60	7	1
4:C:622:PCW:H212	4:C:622:PCW:H182	0.41	1.69	7	1
4:D:502:PCW:H321	4:D:510:PCW:H51	0.41	1.93	7	1
4:D:505:PCW:H342	5:D:519:17F:C20	0.41	2.46	7	1
4:D:509:PCW:H172	4:D:512:PCW:H322	0.41	1.92	7	1
1:A:314:ASP:HA	1:A:317:ARG:NH1	0.41	2.31	8	1
5:D:519:17F:H40	5:D:519:17F:H36	0.41	1.63	8	1
4:A:404:PCW:H42	4:D:510:PCW:C15	0.41	2.45	9	1
5:C:631:17F:C24	4:D:512:PCW:H281	0.41	2.46	9	1
4:B:202:PCW:C5	5:D:524:17F:C3	0.41	2.98	9	1
4:D:506:PCW:C19	4:D:516:PCW:H342	0.41	2.46	9	1
4:A:401:PCW:H412	4:A:401:PCW:H382	0.41	1.75	10	1
4:A:406:PCW:H31	4:B:204:PCW:C3	0.41	2.43	10	1
4:C:615:PCW:C27	5:C:631:17F:H46	0.41	2.45	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:618:PCW:C34	4:C:625:PCW:H341	0.41	2.46	10	1
2:B:1:MET:HB2	2:B:50:THR:O	0.41	2.15	10	1
4:D:513:PCW:H121	5:D:523:17F:H18	0.41	1.91	10	1
4:A:406:PCW:C21	4:B:204:PCW:H262	0.41	2.46	1	1
4:C:625:PCW:O31	4:C:625:PCW:C5	0.41	2.68	1	1
4:C:605:PCW:H382	4:C:611:PCW:C3	0.41	2.46	2	1
4:D:508:PCW:H372	4:D:512:PCW:H121	0.41	1.93	2	1
4:A:403:PCW:C40	4:A:403:PCW:C14	0.41	2.92	3	1
4:B:201:PCW:C23	4:D:506:PCW:H442	0.41	2.46	3	1
4:D:501:PCW:H19	4:D:511:PCW:H40	0.41	1.93	3	1
4:D:516:PCW:C1	4:D:516:PCW:O31	0.41	2.67	3	1
4:A:407:PCW:C8	4:A:407:PCW:O4P	0.41	2.69	4	1
4:C:616:PCW:O4P	4:C:616:PCW:C3	0.41	2.66	10	2
4:B:203:PCW:H162	4:B:203:PCW:C42	0.41	2.26	4	1
4:D:506:PCW:C7	4:D:517:PCW:O31	0.41	2.69	4	1
4:C:602:PCW:H19	4:C:602:PCW:H39	0.41	1.92	5	1
4:C:605:PCW:H372	4:C:605:PCW:H411	0.41	1.92	5	1
4:C:613:PCW:H482	4:C:619:PCW:C23	0.41	2.43	7	1
4:C:621:PCW:C12	5:C:630:17F:O9	0.41	2.69	7	1
3:D:378:LEU:HD23	3:D:416:THR:HB	0.41	1.91	7	1
4:D:515:PCW:C32	4:D:516:PCW:C1	0.41	2.96	7	1
4:D:515:PCW:C7	4:D:516:PCW:H321	0.41	2.45	7	1
4:A:405:PCW:H212	4:A:405:PCW:H161	0.41	1.79	9	1
4:C:611:PCW:H321	4:C:622:PCW:H372	0.41	1.92	9	1
4:B:202:PCW:O3	4:B:202:PCW:C31	0.41	2.68	9	1
4:A:403:PCW:H63	4:A:403:PCW:O2P	0.41	2.16	10	1
4:A:406:PCW:O3P	4:A:406:PCW:C31	0.41	2.69	10	1
5:C:628:17F:O10	5:C:628:17F:C20	0.41	2.69	10	1
2:B:160:VAL:HA	2:B:163:ILE:HD12	0.41	1.91	10	1
3:D:358:ILE:O	3:D:369:VAL:HG13	0.41	2.16	10	1
4:A:403:PCW:C14	4:A:403:PCW:H382	0.40	2.45	1	1
4:C:608:PCW:H282	5:C:627:17F:H65	0.40	1.93	1	1
4:D:508:PCW:O3	4:D:508:PCW:O31	0.40	2.39	1	1
4:D:528:PCW:C46	5:D:530:17F:H55	0.40	2.45	2	1
1:C:427:TRP:O	1:C:431:GLU:HG3	0.40	2.16	6	2
4:C:607:PCW:C45	4:C:624:PCW:H481	0.40	2.46	3	1
3:D:409:LYS:CE	4:D:503:PCW:H41	0.40	2.46	3	1
4:D:506:PCW:H261	4:D:516:PCW:H161	0.40	1.92	3	1
4:D:516:PCW:C46	5:D:530:17F:H38	0.40	2.46	3	1
4:D:517:PCW:H483	5:D:525:17F:C23	0.40	2.43	3	1
4:C:603:PCW:O11	4:C:604:PCW:H61	0.40	2.16	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:604:PCW:H251	5:D:525:17F:C42	0.40	2.45	4	1
4:D:508:PCW:H131	4:D:509:PCW:H221	0.40	1.82	4	1
4:D:518:PCW:O3	4:D:518:PCW:C31	0.40	2.70	4	1
4:C:602:PCW:H39	4:C:602:PCW:C19	0.40	2.46	5	1
4:D:502:PCW:H422	4:D:502:PCW:C20	0.40	2.45	5	1
4:D:504:PCW:C20	4:D:510:PCW:H422	0.40	2.46	5	1
5:D:522:17F:H59	5:D:522:17F:H62	0.40	1.57	5	2
4:A:401:PCW:H442	4:C:614:PCW:H242	0.40	1.92	6	1
4:A:407:PCW:C46	4:A:412:PCW:H221	0.40	2.46	6	1
4:C:603:PCW:O31	4:C:603:PCW:C8	0.40	2.65	6	1
1:C:578:GLU:O	1:C:582:VAL:HG23	0.40	2.16	7	1
4:C:611:PCW:H20	4:C:611:PCW:C43	0.40	2.42	7	1
4:D:516:PCW:H421	4:D:527:PCW:C27	0.40	2.46	7	1
4:A:402:PCW:H162	4:A:405:PCW:H231	0.40	1.92	8	1
4:D:506:PCW:O1P	4:D:515:PCW:C7	0.40	2.69	8	1
4:D:518:PCW:H142	5:D:519:17F:H67	0.40	1.93	8	1
1:A:379:LEU:O	1:A:383:LYS:HG3	0.40	2.16	9	1
4:A:405:PCW:H52	4:D:514:PCW:O31	0.40	2.16	9	1
4:C:605:PCW:C32	4:C:611:PCW:C1	0.40	3.00	9	1
4:D:507:PCW:H462	4:D:517:PCW:H272	0.40	1.93	9	1
5:D:522:17F:O8	5:D:525:17F:C6	0.40	2.69	9	1
5:D:524:17F:H62	5:D:524:17F:H59	0.40	1.61	9	1
5:C:631:17F:H36	5:C:631:17F:H39	0.40	1.63	1	1
4:B:202:PCW:C5	5:D:524:17F:O4	0.40	2.69	1	1
3:D:433:HIS:O	3:D:434:VAL:HB	0.40	2.17	1	1
4:D:515:PCW:H181	4:D:515:PCW:H212	0.40	1.66	1	1
4:A:414:PCW:H362	4:C:617:PCW:H151	0.40	1.93	3	1
4:B:203:PCW:H20	4:D:506:PCW:C47	0.40	2.46	3	1
4:D:512:PCW:H62	5:D:520:17F:O4	0.40	2.17	3	1
4:D:502:PCW:O2	4:D:502:PCW:C11	0.40	2.70	4	1
4:D:512:PCW:H181	4:D:512:PCW:H212	0.40	1.68	4	1
5:D:529:17F:H46	5:D:530:17F:H78	0.40	1.93	4	1
4:A:411:PCW:H351	4:C:612:PCW:H151	0.40	1.91	6	1
4:A:414:PCW:H411	4:A:414:PCW:H381	0.40	1.68	6	1
4:C:617:PCW:O31	4:C:617:PCW:H41	0.40	2.16	6	1
4:B:201:PCW:H321	4:D:510:PCW:C38	0.40	2.46	6	1
4:D:508:PCW:C12	4:D:512:PCW:C17	0.40	2.98	6	1
4:D:509:PCW:H152	4:D:514:PCW:O11	0.40	2.15	6	1
4:A:415:PCW:C32	4:C:622:PCW:H331	0.40	2.46	7	1
4:D:503:PCW:H152	4:D:511:PCW:H411	0.40	1.91	7	1
4:A:401:PCW:H361	4:D:503:PCW:C21	0.40	2.46	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:401:PCW:H31	4:D:511:PCW:H212	0.40	1.93	8	1
4:A:404:PCW:H362	4:B:202:PCW:H462	0.40	1.91	8	1
4:A:406:PCW:C21	4:B:204:PCW:H411	0.40	2.45	8	1
2:B:2:THR:HG23	5:D:522:17F:O5	0.40	2.16	8	1
4:D:502:PCW:H411	4:D:502:PCW:H382	0.40	1.73	8	1
4:C:604:PCW:C21	4:D:515:PCW:H282	0.40	2.46	9	1
4:D:504:PCW:C45	4:D:505:PCW:H39	0.40	2.46	9	1
4:D:507:PCW:H212	4:D:507:PCW:C17	0.40	2.39	9	1
4:A:412:PCW:H322	4:C:623:PCW:H342	0.40	1.92	10	1
3:D:459:LEU:HD21	3:D:472:PHE:CA	0.40	2.46	10	1
4:C:601:PCW:C40	4:C:602:PCW:H171	0.40	2.46	1	1
3:D:458:PHE:CD1	4:D:517:PCW:H32	0.40	2.52	1	1
4:D:502:PCW:O31	4:D:510:PCW:C7	0.40	2.68	1	1
4:D:502:PCW:H181	4:D:502:PCW:H211	0.40	1.64	1	1
4:D:506:PCW:H39	5:D:520:17F:H72	0.40	1.91	1	1
4:A:415:PCW:H281	4:D:516:PCW:H251	0.40	1.92	2	1
4:C:604:PCW:C41	4:C:604:PCW:C37	0.40	2.96	2	1
5:C:630:17F:C7	5:D:529:17F:H65	0.40	2.46	2	1
3:D:472:PHE:CE1	3:D:477:SER:HA	0.40	2.51	2	1
1:A:215:SER:O	1:A:219:GLU:HG3	0.40	2.17	3	1
4:C:623:PCW:H432	4:C:624:PCW:H432	0.40	1.93	3	1
4:C:620:PCW:C7	4:C:620:PCW:C1	0.40	2.98	4	1
4:B:201:PCW:O31	4:D:516:PCW:H82	0.40	2.16	4	1
4:B:202:PCW:O2	4:B:202:PCW:O1P	0.40	2.39	4	1
4:D:507:PCW:H39	5:D:525:17F:C8	0.40	2.46	5	1
4:D:513:PCW:H482	5:D:522:17F:C42	0.40	2.46	5	1
4:A:407:PCW:C15	4:D:511:PCW:H283	0.40	2.41	6	1
4:A:408:PCW:H462	4:B:201:PCW:H232	0.40	1.92	6	1
4:A:411:PCW:C41	4:C:612:PCW:H231	0.40	2.47	6	1
4:D:505:PCW:O31	4:D:505:PCW:H341	0.40	2.15	6	1
4:D:512:PCW:H371	4:D:514:PCW:H141	0.40	1.94	6	1
1:C:456:LEU:O	1:C:460:GLN:HB2	0.40	2.17	7	1
2:B:127:THR:HG23	2:B:141:PHE:HE2	0.40	1.77	7	1
4:D:518:PCW:C32	5:D:519:17F:H32	0.40	2.46	7	1
3:D:468:CYS:HB3	3:D:484:CYS:HB3	0.40	1.92	8	1
4:D:508:PCW:C21	4:D:512:PCW:H152	0.40	2.43	8	1
4:A:406:PCW:C24	4:B:202:PCW:C22	0.40	2.94	9	1
4:C:605:PCW:H381	4:C:619:PCW:H121	0.40	1.93	9	1
5:C:631:17F:H52	4:D:512:PCW:C16	0.40	2.46	9	1
1:A:254:VAL:HG22	1:A:258:LEU:HG	0.40	1.94	1	1
4:B:201:PCW:H182	4:D:506:PCW:C38	0.40	2.46	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:D:506:PCW:H221	4:D:516:PCW:C37	0.40	2.46	2	1
4:D:510:PCW:H271	5:D:524:17F:H60	0.40	1.92	2	1
4:A:406:PCW:C35	4:B:204:PCW:H151	0.40	2.45	3	1
4:A:410:PCW:C44	4:A:414:PCW:H421	0.40	2.47	3	1
1:C:489:LEU:O	1:C:493:GLN:HG3	0.40	2.16	3	1
1:A:334:ARG:HD2	1:C:440:GLU:OE1	0.40	2.17	4	1
5:A:409:17F:C33	4:D:501:PCW:H241	0.40	2.45	4	1
4:A:413:PCW:H40	4:C:616:PCW:C23	0.40	2.42	4	1
4:C:610:PCW:O31	4:C:610:PCW:O3P	0.40	2.38	7	2
4:D:510:PCW:H131	5:D:524:17F:C40	0.40	2.46	4	1
4:A:401:PCW:H482	4:C:611:PCW:C23	0.40	2.46	5	1
4:D:518:PCW:H372	5:D:519:17F:H69	0.40	1.92	5	1
4:D:510:PCW:O3	5:D:524:17F:H71	0.40	2.15	6	1
5:D:525:17F:C35	5:D:525:17F:H12	0.40	2.47	6	1
4:A:415:PCW:H282	4:D:528:PCW:C28	0.40	2.42	7	1
4:C:603:PCW:C7	4:C:603:PCW:H131	0.40	2.47	7	1
4:C:613:PCW:H63	4:C:613:PCW:O4P	0.40	2.17	7	1
4:D:518:PCW:H211	5:D:519:17F:H59	0.40	1.92	7	1
4:A:402:PCW:H162	4:A:405:PCW:C23	0.40	2.46	8	1
4:B:201:PCW:C42	5:D:524:17F:H47	0.40	2.44	8	1
4:D:515:PCW:H82	4:D:516:PCW:O31	0.40	2.17	8	1
4:A:415:PCW:H31	4:C:603:PCW:H31	0.40	1.93	9	1
4:C:625:PCW:H283	4:B:203:PCW:H272	0.40	1.94	9	1
4:A:401:PCW:H322	4:D:511:PCW:H241	0.40	1.93	10	1
4:D:507:PCW:H381	4:D:507:PCW:H412	0.40	1.62	10	1
4:D:511:PCW:C32	4:D:511:PCW:C13	0.40	3.00	10	1
4:C:612:PCW:H332	4:C:618:PCW:H132	0.40	1.91	1	1
4:A:403:PCW:O11	4:A:403:PCW:H52	0.40	2.16	2	1
4:B:203:PCW:H181	4:B:204:PCW:C40	0.40	2.46	2	1
4:D:506:PCW:H2	4:D:515:PCW:C6	0.40	2.32	2	1
4:D:507:PCW:C35	5:D:522:17F:O1	0.40	2.70	2	1
4:C:621:PCW:C28	5:C:629:17F:H35	0.40	2.44	3	1
4:C:622:PCW:H242	4:D:501:PCW:H431	0.40	1.94	3	1
4:D:517:PCW:H371	5:D:520:17F:C10	0.40	2.47	4	1
4:A:412:PCW:O1P	4:C:614:PCW:C8	0.40	2.70	5	1
5:C:631:17F:H63	5:C:631:17F:H58	0.40	1.58	5	1
4:A:403:PCW:H241	4:D:513:PCW:C11	0.40	2.46	6	1
4:C:602:PCW:H411	4:C:602:PCW:H382	0.40	1.71	6	1
4:D:508:PCW:H352	4:D:512:PCW:C14	0.40	2.47	6	1
4:D:512:PCW:H61	5:D:520:17F:O5	0.40	2.16	6	1
5:D:524:17F:H36	5:D:524:17F:H40	0.40	1.66	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:415:PCW:H222	4:C:603:PCW:H162	0.40	1.92	8	1
3:D:364:ASN:OD1	3:D:365:LYS:HG2	0.40	2.15	8	1
5:C:631:17F:H44	4:D:512:PCW:H281	0.40	1.93	9	1
4:D:509:PCW:H61	4:D:514:PCW:O11	0.40	2.16	9	1
5:A:409:17F:O9	5:A:409:17F:C7	0.40	2.69	10	1
4:C:603:PCW:C22	4:D:526:PCW:C33	0.40	2.99	10	1
4:C:622:PCW:O3	4:C:622:PCW:C31	0.40	2.69	10	1
4:D:516:PCW:H451	5:D:530:17F:H51	0.40	1.94	10	1
5:D:524:17F:H54	4:D:527:PCW:H212	0.40	1.93	10	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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	183/198 (92%)	178±1 (97±1%)	4±1 (2±1%)	1±0 (1±0%)	26	74
1	C	196/198 (99%)	191±1 (97±1%)	5±1 (3±0%)	0±0 (0±0%)	49	83
2	B	174/185 (94%)	165±3 (95±1%)	9±3 (5±1%)	1±0 (0±0%)	37	78
3	D	130/132 (98%)	112±2 (86±2%)	14±2 (11±2%)	4±1 (3±1%)	6	41
All	All	6830/7130 (96%)	6449 (94%)	329 (5%)	52 (1%)	18	68

All 17 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	365	LYS	10
3	D	364	ASN	8
3	D	407	GLY	8
3	D	374	ASN	4
3	D	375	GLY	3
3	D	433	HIS	3
3	D	434	VAL	3
2	B	175	LYS	2
2	B	123	ARG	2

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Mol	Chain	Res	Type	Models (Total)
3	D	469	GLY	2
3	D	365	LYS	1
2	B	48	GLY	1
3	D	435	PRO	1
3	D	468	CYS	1
2	B	63	GLU	1
3	D	431	LEU	1
1	C	420	GLY	1

6.3.2 Protein sidechains [i](#)

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	160/174 (92%)	147±3 (92±2%)	13±3 (8±2%)	13	60
1	C	173/174 (99%)	160±2 (92±1%)	13±2 (8±1%)	14	62
2	B	154/164 (94%)	140±2 (91±2%)	14±2 (9±2%)	11	56
3	D	119/119 (100%)	102±2 (86±2%)	17±2 (14±2%)	5	45
All	All	6060/6310 (96%)	5492 (91%)	568 (9%)	10	56

All 172 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	C	550	LYS	10
2	B	20	THR	10
2	B	87	THR	10
3	D	445	THR	10
3	D	459	LEU	10
3	D	468	CYS	10
3	D	478	THR	10
2	B	89	SER	9
2	B	122	SER	9
3	D	377	SER	9
3	D	438	THR	9
3	D	465	CYS	9
1	C	448	VAL	9

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Mol	Chain	Res	Type	Models (Total)
1	C	561	LYS	8
2	B	74	THR	8
3	D	460	LEU	8
3	D	431	LEU	8
1	A	235	GLU	7
1	A	254	VAL	7
1	A	293	GLU	7
1	C	407	SER	7
1	C	576	VAL	7
3	D	482	THR	7
1	A	265	TRP	6
1	A	272	TYR	6
1	C	411	THR	6
1	C	466	GLU	6
1	C	516	THR	6
1	C	583	SER	6
2	B	2	THR	6
2	B	50	THR	6
2	B	153	ASP	6
3	D	357	THR	6
3	D	437	THR	6
3	D	484	CYS	6
1	C	552	THR	6
2	B	69	ASP	6
3	D	476	CYS	6
1	A	236	THR	6
1	A	212	SER	5
1	A	385	SER	5
1	C	483	GLU	5
2	B	65	SER	5
2	B	148	THR	5
3	D	467	THR	5
1	A	292	HIS	5
1	C	548	HIS	5
2	B	124	THR	5
1	C	480	GLU	5
3	D	366	GLN	5
1	A	250	VAL	4
1	A	289	GLN	4
1	A	359	THR	4
3	D	403	GLN	4
1	A	228	PHE	4

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Mol	Chain	Res	Type	Models (Total)
1	A	312	HIS	4
2	B	35	THR	4
1	A	299	SER	3
1	C	459	PHE	3
1	C	462	LYS	3
2	B	144	THR	3
1	A	248	GLU	3
1	A	382	PHE	3
1	C	505	ASP	3
2	B	92	ASP	3
3	D	365	LYS	3
1	A	209	SER	3
1	A	244	SER	3
1	C	400	LYS	3
2	B	132	ASP	3
3	D	471	LYS	3
3	D	477	SER	3
1	A	263	LYS	3
1	A	381	SER	3
1	C	405	TRP	3
2	B	17	SER	3
2	B	109	VAL	3
2	B	170	MET	3
3	D	453	ASP	3
1	C	557	THR	3
1	A	246	ASP	2
1	A	270	GLU	2
1	C	568	ASP	2
2	B	41	ARG	2
1	A	304	GLU	2
1	A	370	ASP	2
2	B	1	MET	2
3	D	398	VAL	2
3	D	444	LYS	2
1	A	319	HIS	2
1	C	455	TYR	2
2	B	31	GLU	2
1	C	522	SER	2
1	C	524	GLU	2
1	C	538	GLU	2
2	B	47	ASP	2
1	A	232	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	C	559	SER	2
2	B	33	ASP	2
2	B	39	SER	2
2	B	145	SER	2
1	C	412	PHE	2
3	D	358	ILE	2
1	A	206	ASN	2
1	A	229	TRP	2
3	D	426	LEU	2
1	A	247	LEU	2
2	B	80	CYS	2
2	B	175	LYS	2
3	D	470	TYR	2
1	A	225	THR	1
1	A	237	GLU	1
1	A	357	LEU	1
1	A	368	LEU	1
2	B	9	VAL	1
2	B	119	ASP	1
3	D	395	CYS	1
3	D	425	GLU	1
3	D	455	CYS	1
3	D	483	MET	1
3	D	486	ASP	1
1	A	258	LEU	1
1	A	318	THR	1
1	A	325	ASP	1
1	A	350	HIS	1
1	A	386	PHE	1
1	C	499	LEU	1
1	C	534	GLU	1
1	C	591	TYR	1
2	B	67	MET	1
2	B	70	GLN	1
2	B	128	LYS	1
3	D	457	LYS	1
1	A	320	LEU	1
1	C	403	ASP	1
2	B	114	VAL	1
2	B	139	ILE	1
3	D	436	LEU	1
1	A	358	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	C	437	LEU	1
2	B	3	GLU	1
2	B	45	VAL	1
1	A	211	THR	1
1	A	314	ASP	1
1	C	478	ARG	1
2	B	8	VAL	1
2	B	149	ARG	1
3	D	443	ARG	1
1	A	296	GLU	1
1	C	447	GLU	1
3	D	364	ASN	1
3	D	394	GLU	1
3	D	427	GLN	1
1	A	356	HIS	1
1	C	473	LYS	1
3	D	373	ARG	1
3	D	412	LEU	1
1	C	409	THR	1
1	C	556	SER	1
2	B	43	GLN	1
2	B	127	THR	1
2	B	152	VAL	1
3	D	367	ARG	1
3	D	392	GLN	1
1	A	327	LEU	1
1	C	425	GLU	1
2	B	27	HIS	1
2	B	40	TYR	1
3	D	361	PHE	1
1	A	348	GLU	1
1	C	580	PHE	1
2	B	156	PHE	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 84 ligands modelled in this entry, 3 are monoatomic - leaving 81 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PCW	C	618	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	D	524	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	C	605	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	410	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	601	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	412	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	D	521	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	17F	D	529	-	52,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	506	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	413	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	623	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	403	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	625	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	511	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	508	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	D	523	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	A	404	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	518	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	D	522	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	A	401	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	411	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	615	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	C	631	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	17F	D	520	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	C	613	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	405	-	53,53,53	0.82±0.00	0±0 (0±0%)
6	GNP	B	205	-	34,34,34	1.22±0.01	2±0 (6±1%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PCW	C	604	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	501	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	502	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	513	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	606	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	526	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	510	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	516	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	603	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	621	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	402	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	A	409	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	A	407	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	408	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	505	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	619	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	B	203	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	503	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	D	519	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	D	515	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	612	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	509	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	528	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	512	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	620	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	609	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	624	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	610	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	C	629	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	C	614	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	611	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	B	201	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	B	204	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	514	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	607	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	406	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	414	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	507	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	A	415	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	C	626	-	52,53,53	0.83±0.00	0±0 (0±0%)
5	17F	C	630	-	52,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	608	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	D	530	-	52,53,53	0.83±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
5	17F	C	627	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	D	504	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	616	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	B	202	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	527	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	D	517	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	617	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	D	525	-	52,53,53	0.83±0.00	0±0 (0±0%)
4	PCW	C	622	-	53,53,53	0.82±0.00	0±0 (0±0%)
4	PCW	C	602	-	53,53,53	0.82±0.00	0±0 (0±0%)
5	17F	C	628	-	52,53,53	0.83±0.00	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PCW	C	618	-	59,61,61	2.62±0.01	7±0 (12±0%)
5	17F	D	524	-	54,60,60	1.15±0.03	4±0 (7±0%)
4	PCW	C	605	-	59,61,61	2.63±0.01	7±0 (11±0%)
4	PCW	A	410	-	59,61,61	2.59±0.02	7±1 (11±1%)
4	PCW	C	601	-	59,61,61	2.60±0.01	7±0 (11±0%)
4	PCW	A	412	-	59,61,61	2.60±0.02	7±0 (11±0%)
5	17F	D	521	-	54,60,60	1.11±0.03	5±0 (9±0%)
5	17F	D	529	-	54,60,60	1.13±0.02	5±1 (9±0%)
4	PCW	D	506	-	59,61,61	2.60±0.01	6±0 (10±0%)
4	PCW	A	413	-	59,61,61	2.61±0.00	6±0 (10±0%)
4	PCW	C	623	-	59,61,61	2.57±0.01	6±0 (10±0%)
4	PCW	A	403	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	C	625	-	59,61,61	2.59±0.02	7±1 (11±1%)
4	PCW	D	511	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	D	508	-	59,61,61	2.61±0.01	7±0 (11±0%)
5	17F	D	523	-	54,60,60	1.12±0.03	4±0 (7±0%)
4	PCW	A	404	-	59,61,61	2.60±0.01	6±0 (10±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PCW	D	518	-	59,61,61	2.62±0.01	7±0 (11±0%)
5	17F	D	522	-	54,60,60	1.15±0.02	5±1 (8±1%)
4	PCW	A	401	-	59,61,61	2.60±0.01	6±0 (10±0%)
4	PCW	A	411	-	59,61,61	2.61±0.02	7±0 (11±0%)
4	PCW	C	615	-	59,61,61	2.61±0.02	6±0 (10±0%)
5	17F	C	631	-	54,60,60	1.09±0.04	4±0 (7±0%)
5	17F	D	520	-	54,60,60	1.12±0.03	4±0 (8±0%)
4	PCW	C	613	-	59,61,61	2.60±0.01	6±1 (10±1%)
4	PCW	A	405	-	59,61,61	2.59±0.01	6±0 (10±0%)
6	GNP	B	205	-	47,54,54	1.81±0.02	11±1 (23±2%)
4	PCW	C	604	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	D	501	-	59,61,61	2.59±0.01	7±0 (11±0%)
4	PCW	D	502	-	59,61,61	2.60±0.01	6±0 (10±0%)
4	PCW	D	513	-	59,61,61	2.58±0.01	6±0 (10±0%)
4	PCW	C	606	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	D	526	-	59,61,61	2.61±0.01	7±0 (11±0%)
4	PCW	D	510	-	59,61,61	2.60±0.01	6±1 (10±1%)
4	PCW	D	516	-	59,61,61	2.59±0.01	7±1 (11±1%)
4	PCW	C	603	-	59,61,61	2.60±0.01	7±1 (11±1%)
4	PCW	C	621	-	59,61,61	2.57±0.01	6±0 (10±0%)
4	PCW	A	402	-	59,61,61	2.60±0.01	6±0 (10±0%)
5	17F	A	409	-	54,60,60	1.12±0.02	4±0 (7±0%)
4	PCW	A	407	-	59,61,61	2.58±0.01	6±0 (10±0%)
4	PCW	A	408	-	59,61,61	2.60±0.01	6±0 (10±0%)
4	PCW	D	505	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	C	619	-	59,61,61	2.58±0.01	6±0 (10±0%)
4	PCW	B	203	-	59,61,61	2.59±0.01	7±0 (11±0%)
4	PCW	D	503	-	59,61,61	2.60±0.01	6±0 (11±0%)
5	17F	D	519	-	54,60,60	1.35±0.03	8±0 (15±0%)
4	PCW	D	515	-	59,61,61	2.60±0.02	6±1 (11±1%)
4	PCW	C	612	-	59,61,61	2.61±0.01	6±1 (10±1%)
4	PCW	D	509	-	59,61,61	2.58±0.00	6±0 (10±0%)
4	PCW	D	528	-	59,61,61	2.61±0.01	8±1 (12±1%)
4	PCW	D	512	-	59,61,61	2.60±0.01	6±0 (10±0%)
4	PCW	C	620	-	59,61,61	2.59±0.01	7±1 (11±1%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
4	PCW	C	609	-	59,61,61	2.59±0.00	7±1 (11±1%)
4	PCW	C	624	-	59,61,61	2.62±0.01	7±0 (11±0%)
4	PCW	C	610	-	59,61,61	2.59±0.00	7±1 (11±1%)
5	17F	C	629	-	54,60,60	1.13±0.05	4±0 (7±0%)
4	PCW	C	614	-	59,61,61	2.61±0.01	6±1 (11±1%)
4	PCW	C	611	-	59,61,61	2.59±0.01	6±0 (11±0%)
4	PCW	B	201	-	59,61,61	2.59±0.01	7±1 (11±1%)
4	PCW	B	204	-	59,61,61	2.59±0.00	6±0 (10±0%)
4	PCW	D	514	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	C	607	-	59,61,61	2.58±0.01	6±0 (11±0%)
4	PCW	A	406	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	A	414	-	59,61,61	2.59±0.01	7±1 (11±1%)
4	PCW	D	507	-	59,61,61	2.59±0.01	6±0 (10±0%)
4	PCW	A	415	-	59,61,61	2.57±0.01	6±0 (11±0%)
5	17F	C	626	-	54,60,60	1.10±0.02	4±0 (8±0%)
5	17F	C	630	-	54,60,60	1.12±0.03	4±0 (7±0%)
4	PCW	C	608	-	59,61,61	2.60±0.01	7±1 (11±1%)
5	17F	D	530	-	54,60,60	1.09±0.05	4±0 (8±0%)
5	17F	C	627	-	54,60,60	1.12±0.03	4±0 (7±0%)
4	PCW	D	504	-	59,61,61	2.69±0.01	10±0 (17±0%)
4	PCW	C	616	-	59,61,61	2.58±0.01	6±0 (10±0%)
4	PCW	B	202	-	59,61,61	2.61±0.01	7±0 (11±0%)
4	PCW	D	527	-	59,61,61	2.67±0.01	10±0 (16±0%)
4	PCW	D	517	-	59,61,61	2.59±0.01	7±0 (11±0%)
4	PCW	C	617	-	59,61,61	2.61±0.01	7±0 (11±0%)
5	17F	D	525	-	54,60,60	1.24±0.03	4±0 (8±0%)
4	PCW	C	622	-	59,61,61	2.58±0.02	6±0 (10±0%)
4	PCW	C	602	-	59,61,61	2.58±0.01	6±0 (10±0%)
5	17F	C	628	-	54,60,60	1.35±0.03	9±0 (16±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	17F	D	529	-	-	1±0,59,59,59	-
4	PCW	A	403	-	-	0±0,57,57,57	-
4	PCW	A	404	-	-	0±0,57,57,57	-
4	PCW	D	518	-	-	0±0,57,57,57	-
4	PCW	C	613	-	-	0±0,57,57,57	-
4	PCW	A	413	-	-	0±0,57,57,57	-
4	PCW	C	606	-	-	0±0,57,57,57	-
5	17F	D	523	-	-	0±0,59,59,59	-
5	17F	D	522	-	-	1±0,59,59,59	-
4	PCW	D	503	-	-	0±0,57,57,57	-
4	PCW	C	610	-	-	0±0,57,57,57	-
4	PCW	D	513	-	-	0±0,57,57,57	-
4	PCW	B	204	-	-	0±0,57,57,57	-
4	PCW	D	514	-	-	0±0,57,57,57	-
5	17F	C	629	-	-	0±0,59,59,59	-
4	PCW	C	615	-	-	0±0,57,57,57	-
4	PCW	A	415	-	-	0±0,57,57,57	-
5	17F	C	626	-	-	0±0,59,59,59	-
5	17F	D	520	-	-	0±0,59,59,59	-
5	17F	C	627	-	-	0±0,59,59,59	-
4	PCW	D	505	-	-	0±0,57,57,57	-
4	PCW	D	507	-	-	0±0,57,57,57	-
4	PCW	C	612	-	-	0±0,57,57,57	-
5	17F	D	521	-	-	0±0,59,59,59	-
4	PCW	A	401	-	-	0±0,57,57,57	-
4	PCW	A	405	-	-	0±0,57,57,57	-
4	PCW	D	528	-	-	0±0,57,57,57	-
4	PCW	D	512	-	-	0±0,57,57,57	-
5	17F	D	525	-	-	1±0,59,59,59	-
4	PCW	D	508	-	-	0±0,57,57,57	-
4	PCW	C	607	-	-	0±0,57,57,57	-
4	PCW	C	611	-	-	0±0,57,57,57	-
4	PCW	C	614	-	-	0±0,57,57,57	-
4	PCW	A	407	-	-	0±0,57,57,57	-
4	PCW	C	621	-	-	0±0,57,57,57	-
4	PCW	D	527	-	-	0±0,57,57,57	-
4	PCW	A	411	-	-	0±0,57,57,57	-
4	PCW	C	604	-	-	0±0,57,57,57	-
4	PCW	A	402	-	-	0±0,57,57,57	-
5	17F	C	631	-	-	0±0,59,59,59	-
4	PCW	C	623	-	-	0±0,57,57,57	-
4	PCW	C	609	-	-	0±0,57,57,57	-
4	PCW	D	504	-	-	0±0,57,57,57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	C	616	-	-	0±0,57,57,57	-
4	PCW	C	620	-	-	0±0,57,57,57	-
4	PCW	C	601	-	-	0±0,57,57,57	-
4	PCW	D	517	-	-	0±0,57,57,57	-
4	PCW	A	408	-	-	0±0,57,57,57	-
4	PCW	D	502	-	-	0±0,57,57,57	-
4	PCW	D	526	-	-	0±0,57,57,57	-
4	PCW	D	516	-	-	0±0,57,57,57	-
4	PCW	A	412	-	-	0±0,57,57,57	-
4	PCW	B	202	-	-	0±0,57,57,57	-
4	PCW	C	622	-	-	0±0,57,57,57	-
5	17F	C	628	-	-	0±0,59,59,59	-
4	PCW	D	515	-	-	0±0,57,57,57	-
5	17F	D	519	-	-	0±0,59,59,59	-
4	PCW	D	510	-	-	0±0,57,57,57	-
4	PCW	C	624	-	-	0±0,57,57,57	-
4	PCW	C	608	-	-	0±0,57,57,57	-
4	PCW	D	506	-	-	0±0,57,57,57	-
5	17F	D	530	-	-	0±0,59,59,59	-
4	PCW	C	618	-	-	0±0,57,57,57	-
4	PCW	B	203	-	-	0±0,57,57,57	-
5	17F	A	409	-	-	0±0,59,59,59	-
4	PCW	C	625	-	-	0±0,57,57,57	-
4	PCW	C	603	-	-	0±0,57,57,57	-
4	PCW	B	201	-	-	0±0,57,57,57	-
4	PCW	C	617	-	-	0±0,57,57,57	-
4	PCW	C	602	-	-	0±0,57,57,57	-
4	PCW	D	501	-	-	0±0,57,57,57	-
5	17F	D	524	-	-	0±0,59,59,59	-
4	PCW	A	410	-	-	0±0,57,57,57	-
5	17F	C	630	-	-	0±0,59,59,59	-
4	PCW	C	619	-	-	0±0,57,57,57	-
4	PCW	C	605	-	-	0±0,57,57,57	-
4	PCW	D	509	-	-	0±0,57,57,57	-
6	GNP	B	205	-	-	0±0,18,38,38	0±0,3,3,3
4	PCW	D	511	-	-	0±0,57,57,57	-
4	PCW	A	406	-	-	0±0,57,57,57	-
4	PCW	A	414	-	-	0±0,57,57,57	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
6	B	205	GNP	PB-O2B	3.19	1.48	1.56	5	10
6	B	205	GNP	C5-N7	2.96	1.33	1.39	2	10
6	B	205	GNP	PB-O3A	2.24	1.61	1.59	2	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	C	610	PCW	C8-N-C7	17.69	62.50	108.98	10	10
4	C	625	PCW	C8-N-C7	17.69	62.51	108.98	7	10
4	C	613	PCW	C8-N-C7	17.69	62.52	108.98	1	10
4	D	501	PCW	C8-N-C7	17.69	62.52	108.98	7	10
4	C	621	PCW	C8-N-C7	17.69	62.52	108.98	3	10
4	D	511	PCW	C8-N-C7	17.69	62.52	108.98	3	10
4	A	408	PCW	C8-N-C7	17.68	62.52	108.98	6	10
4	D	527	PCW	C8-N-C7	17.69	62.52	108.98	4	10
4	A	406	PCW	C8-N-C7	17.68	62.53	108.98	2	10
4	C	614	PCW	C8-N-C7	17.68	62.53	108.98	2	10
4	D	513	PCW	C8-N-C7	17.68	62.54	108.98	9	10
4	A	407	PCW	C8-N-C7	17.68	62.54	108.98	5	10
4	C	618	PCW	C8-N-C7	17.68	62.54	108.98	5	10
4	C	604	PCW	C8-N-C7	17.68	62.54	108.98	8	10
4	C	606	PCW	C8-N-C7	17.68	62.54	108.98	2	10
4	C	607	PCW	C8-N-C7	17.68	62.55	108.98	1	10
4	C	608	PCW	C8-N-C7	17.68	62.54	108.98	9	10
4	D	512	PCW	C8-N-C7	17.68	62.54	108.98	8	10
4	A	402	PCW	C8-N-C7	17.67	62.55	108.98	8	10
4	A	404	PCW	C8-N-C7	17.67	62.55	108.98	4	10
4	C	611	PCW	C8-N-C7	17.68	62.55	108.98	1	10
4	D	505	PCW	C8-N-C7	17.68	62.55	108.98	1	10
4	D	507	PCW	C8-N-C7	17.68	62.55	108.98	1	10
4	C	616	PCW	C8-N-C7	17.67	62.55	108.98	4	10
4	C	619	PCW	C8-N-C7	17.67	62.55	108.98	4	10
4	C	622	PCW	C8-N-C7	17.67	62.55	108.98	8	10
4	D	503	PCW	C8-N-C7	17.67	62.55	108.98	8	10
4	D	508	PCW	C8-N-C7	17.67	62.55	108.98	3	10
4	C	605	PCW	C8-N-C7	17.67	62.55	108.98	9	10
4	A	410	PCW	C8-N-C7	17.67	62.56	108.98	1	10
4	A	414	PCW	C8-N-C7	17.67	62.56	108.98	4	10
4	A	415	PCW	C8-N-C7	17.67	62.56	108.98	5	10
4	C	601	PCW	C8-N-C7	17.67	62.56	108.98	4	10
4	C	609	PCW	C8-N-C7	17.67	62.56	108.98	8	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	B	201	PCW	C8-N-C7	17.67	62.56	108.98	2	10
4	D	518	PCW	C8-N-C7	17.67	62.56	108.98	1	10
4	D	526	PCW	C8-N-C7	17.67	62.56	108.98	2	10
4	A	401	PCW	C8-N-C7	17.67	62.57	108.98	2	10
4	A	405	PCW	C8-N-C7	17.67	62.56	108.98	7	10
4	C	612	PCW	C8-N-C7	17.67	62.57	108.98	4	10
4	C	615	PCW	C8-N-C7	17.67	62.56	108.98	3	10
4	C	624	PCW	C8-N-C7	17.67	62.56	108.98	1	10
4	B	202	PCW	C8-N-C7	17.67	62.57	108.98	9	10
4	D	515	PCW	C8-N-C7	17.67	62.57	108.98	10	10
4	A	412	PCW	C8-N-C7	17.67	62.57	108.98	6	10
4	C	620	PCW	C8-N-C7	17.67	62.57	108.98	1	10
4	C	623	PCW	C8-N-C7	17.67	62.57	108.98	9	10
4	D	517	PCW	C8-N-C7	17.67	62.57	108.98	7	10
4	A	403	PCW	C8-N-C7	17.66	62.58	108.98	7	10
4	A	411	PCW	C8-N-C7	17.66	62.58	108.98	10	10
4	C	602	PCW	C8-N-C7	17.66	62.58	108.98	7	10
4	C	603	PCW	C8-N-C7	17.66	62.57	108.98	10	10
4	C	617	PCW	C8-N-C7	17.66	62.58	108.98	9	10
4	A	413	PCW	C8-N-C7	17.66	62.58	108.98	6	10
4	D	504	PCW	C8-N-C7	17.66	62.58	108.98	1	10
4	D	516	PCW	C8-N-C7	17.66	62.58	108.98	3	10
4	D	528	PCW	C8-N-C7	17.66	62.58	108.98	4	10
4	B	203	PCW	C8-N-C7	17.66	62.58	108.98	4	10
4	D	510	PCW	C8-N-C7	17.66	62.58	108.98	7	10
4	D	514	PCW	C8-N-C7	17.66	62.58	108.98	9	10
4	D	509	PCW	C8-N-C7	17.66	62.59	108.98	1	10
4	B	204	PCW	C8-N-C7	17.66	62.59	108.98	10	10
4	D	506	PCW	C8-N-C7	17.66	62.60	108.98	3	10
4	D	502	PCW	C8-N-C7	17.66	62.60	108.98	4	10
5	D	525	17F	O3-C1-C2	5.79	113.10	108.06	5	10
6	B	205	GNP	C2-N3-C4	5.29	121.41	112.30	10	10
6	B	205	GNP	C5-C4-N3	4.95	120.52	128.39	1	10
5	C	631	17F	O3-C1-C2	4.56	112.03	108.06	3	10
5	D	529	17F	O9-C17-C18	4.55	121.32	111.48	9	10
5	D	519	17F	O3-C1-C2	4.51	111.99	108.06	6	10
5	C	628	17F	O3-C1-C2	4.47	111.96	108.06	1	10
5	C	630	17F	O3-C1-C2	4.44	111.93	108.06	7	10
5	D	522	17F	O9-C17-C18	4.43	121.07	111.48	4	10
5	D	520	17F	O3-C1-C2	4.42	111.91	108.06	5	10
5	D	523	17F	O3-C1-C2	4.37	111.87	108.06	7	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	411	PCW	O2-C31-C32	4.36	120.91	111.48	10	10
5	C	629	17F	O3-C1-C2	4.27	111.78	108.06	8	10
6	B	205	GNP	C4'-O4'-C1'	4.20	100.18	109.47	3	3
5	D	524	17F	O3-C1-C2	4.18	111.70	108.06	5	10
5	D	525	17F	O9-C17-C18	4.18	120.52	111.48	3	10
4	A	413	PCW	O2-C31-C32	4.17	120.50	111.48	2	10
5	D	524	17F	O9-C17-C18	4.17	120.50	111.48	3	10
5	D	524	17F	C5-O9-C17	4.16	107.84	117.80	4	10
4	C	624	PCW	O2-C31-C32	4.14	120.44	111.48	3	10
4	C	625	PCW	O2-C31-C32	4.11	120.37	111.48	10	10
4	C	612	PCW	O2-C31-C32	4.09	120.34	111.48	9	10
4	A	407	PCW	O2-C31-C32	4.09	120.32	111.48	5	10
5	C	631	17F	O9-C17-C18	4.08	120.31	111.48	1	10
4	C	605	PCW	O2-C31-C32	4.07	120.30	111.48	2	10
5	C	627	17F	O9-C17-C18	4.07	120.29	111.48	1	10
4	C	617	PCW	O2-C31-C32	4.06	120.26	111.48	10	10
4	C	622	PCW	O2-C31-C32	4.06	120.26	111.48	4	10
4	C	625	PCW	C2-O2-C31	4.05	108.10	117.80	1	10
4	C	615	PCW	O2-C31-C32	4.03	120.20	111.48	2	10
4	C	613	PCW	O2-C31-C32	4.03	120.19	111.48	10	10
4	A	403	PCW	O2-C31-C32	4.02	120.17	111.48	6	10
5	D	529	17F	O3-C1-C2	4.00	111.54	108.06	10	10
5	C	629	17F	O9-C17-C18	3.99	120.11	111.48	6	10
4	C	624	PCW	C2-O2-C31	3.97	108.29	117.80	3	10
5	D	530	17F	O9-C17-C18	3.97	120.07	111.48	8	10
4	B	202	PCW	O2-C31-C32	3.96	120.06	111.48	8	10
4	A	401	PCW	O2-C31-C32	3.96	120.05	111.48	6	10
4	C	603	PCW	O2-C31-C32	3.96	120.05	111.48	3	10
4	D	508	PCW	O2-C31-C32	3.95	120.03	111.48	1	10
4	D	518	PCW	O2-C31-C32	3.95	120.03	111.48	6	10
5	C	627	17F	C5-O9-C17	3.95	108.35	117.80	10	10
4	A	413	PCW	C2-O2-C31	3.94	108.36	117.80	5	10
5	C	630	17F	O9-C17-C18	3.94	120.01	111.48	8	10
4	D	515	PCW	O2-C31-C32	3.93	119.98	111.48	5	10
4	C	604	PCW	O2-C31-C32	3.93	119.97	111.48	1	10
4	D	507	PCW	O2-C31-C32	3.92	119.96	111.48	5	10
4	D	514	PCW	O2-C31-C32	3.91	119.94	111.48	1	10
4	D	526	PCW	O2-C31-C32	3.91	119.94	111.48	8	10
5	D	522	17F	O3-C1-C2	3.91	111.47	108.06	6	10
4	A	411	PCW	C2-O2-C31	3.91	108.44	117.80	6	10
4	C	606	PCW	O2-C31-C32	3.90	119.92	111.48	2	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	A	409	17F	O3-C1-C2	3.90	111.46	108.06	8	10
4	C	610	PCW	O2-C31-C32	3.90	119.92	111.48	8	10
4	A	405	PCW	O2-C31-C32	3.90	119.91	111.48	8	10
4	D	511	PCW	O2-C31-C32	3.89	119.91	111.48	7	10
4	A	412	PCW	O2-C31-C32	3.88	119.87	111.48	6	10
4	C	614	PCW	O2-C31-C32	3.88	119.87	111.48	9	10
5	D	530	17F	O3-C1-C2	3.87	111.43	108.06	3	10
4	C	618	PCW	O2-C31-C32	3.87	119.85	111.48	4	10
4	D	512	PCW	O2-C31-C32	3.87	119.84	111.48	1	10
5	A	409	17F	O9-C17-C18	3.85	119.80	111.48	2	10
4	A	415	PCW	O2-C31-C32	3.84	119.80	111.48	9	10
4	D	502	PCW	O2-C31-C32	3.84	119.79	111.48	8	10
5	D	519	17F	O9-C17-C18	3.84	119.79	111.48	2	10
5	D	523	17F	O9-C17-C18	3.84	119.79	111.48	8	10
4	A	404	PCW	O2-C31-C32	3.84	119.78	111.48	2	10
4	A	414	PCW	O2-C31-C32	3.84	119.78	111.48	1	10
6	B	205	GNP	O2B-PB-O1B	3.83	118.09	109.87	5	10
4	D	504	PCW	O2-C31-C32	3.83	119.77	111.48	6	10
4	B	202	PCW	C2-O2-C31	3.82	108.65	117.80	8	10
4	D	501	PCW	O2-C31-C32	3.82	119.75	111.48	1	10
4	A	408	PCW	O2-C31-C32	3.82	119.74	111.48	3	10
5	D	521	17F	O9-C17-C18	3.82	119.74	111.48	1	10
4	D	506	PCW	O2-C31-C32	3.82	119.74	111.48	5	10
4	B	204	PCW	O2-C31-C32	3.82	119.73	111.48	8	10
5	C	628	17F	O9-C17-C18	3.82	119.74	111.48	1	10
5	D	521	17F	O3-C1-C2	3.81	111.38	108.06	2	10
4	D	503	PCW	O2-C31-C32	3.81	119.72	111.48	10	10
4	D	513	PCW	O2-C31-C32	3.81	119.71	111.48	9	10
5	D	520	17F	O9-C17-C18	3.80	119.71	111.48	10	10
4	C	607	PCW	O2-C31-C32	3.80	119.70	111.48	5	10
4	A	407	PCW	C2-O2-C31	3.80	108.71	117.80	5	10
4	C	608	PCW	O2-C31-C32	3.80	119.69	111.48	5	10
4	C	601	PCW	O2-C31-C32	3.79	119.69	111.48	1	10
4	C	602	PCW	O2-C31-C32	3.79	119.67	111.48	8	10
4	B	201	PCW	O2-C31-C32	3.79	119.67	111.48	7	10
5	C	627	17F	O3-C1-C2	3.79	111.36	108.06	1	10
4	D	517	PCW	O2-C31-C32	3.78	119.66	111.48	8	10
4	C	611	PCW	O2-C31-C32	3.78	119.66	111.48	9	10
4	C	612	PCW	C2-O2-C31	3.77	108.77	117.80	4	10
5	D	523	17F	C5-O9-C17	3.77	108.77	117.80	9	10
4	C	620	PCW	O2-C31-C32	3.77	119.63	111.48	3	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	D	509	PCW	O2-C31-C32	3.77	119.63	111.48	9	10
5	C	626	17F	O9-C17-C18	3.76	119.61	111.48	7	10
4	D	528	PCW	O2-C31-C32	3.75	119.60	111.48	6	10
4	A	402	PCW	O2-C31-C32	3.75	119.60	111.48	5	10
4	D	505	PCW	O2-C31-C32	3.75	119.59	111.48	1	10
4	D	526	PCW	C2-O2-C31	3.74	108.85	117.80	6	10
4	D	510	PCW	O2-C31-C32	3.74	119.56	111.48	3	10
5	C	626	17F	O3-C1-C2	3.73	111.31	108.06	10	10
4	A	406	PCW	O2-C31-C32	3.73	119.54	111.48	4	10
5	D	521	17F	C5-O9-C17	3.73	108.88	117.80	1	10
4	A	410	PCW	O2-C31-C32	3.72	119.53	111.48	4	10
5	C	631	17F	C5-O9-C17	3.71	108.92	117.80	1	10
4	D	516	PCW	O2-C31-C32	3.70	119.48	111.48	8	10
5	D	530	17F	C5-O9-C17	3.70	108.95	117.80	6	10
4	A	403	PCW	C2-O2-C31	3.69	108.97	117.80	6	10
4	C	613	PCW	C7-N-C6	3.69	118.66	108.98	7	10
4	C	619	PCW	O2-C31-C32	3.68	119.44	111.48	3	10
4	C	615	PCW	C2-O2-C31	3.67	109.00	117.80	2	10
4	B	203	PCW	O2-C31-C32	3.66	119.39	111.48	7	10
4	D	517	PCW	C2-O2-C31	3.66	109.04	117.80	5	10
4	C	609	PCW	O2-C31-C32	3.65	119.38	111.48	1	10
4	A	404	PCW	C2-O2-C31	3.65	109.06	117.80	2	10
4	C	617	PCW	C2-O2-C31	3.64	109.08	117.80	10	10
4	A	401	PCW	C2-O2-C31	3.62	109.14	117.80	6	10
4	D	504	PCW	C2-O2-C31	3.62	109.14	117.80	1	10
4	D	515	PCW	C7-N-C6	3.60	118.44	108.98	3	10
4	D	507	PCW	C8-N-C6	3.58	118.38	108.98	4	10
4	C	616	PCW	O2-C31-C32	3.57	119.21	111.48	5	10
4	D	527	PCW	O2-C31-C32	3.55	119.17	111.48	5	10
4	C	618	PCW	C2-O2-C31	3.55	109.30	117.80	4	10
4	D	514	PCW	C2-O2-C31	3.55	109.30	117.80	1	10
4	C	620	PCW	C2-O2-C31	3.54	109.32	117.80	7	10
4	D	510	PCW	C2-O2-C31	3.54	109.33	117.80	3	10
5	D	519	17F	C5-O9-C17	3.53	109.36	117.80	2	10
4	A	402	PCW	C2-O2-C31	3.52	109.38	117.80	6	10
4	D	507	PCW	C7-N-C6	3.51	118.20	108.98	3	10
5	C	628	17F	C5-O9-C17	3.50	109.41	117.80	5	10
4	C	621	PCW	O2-C31-C32	3.50	119.06	111.48	2	10
4	D	502	PCW	C2-O2-C31	3.50	109.41	117.80	8	10
4	D	506	PCW	C2-O2-C31	3.50	109.42	117.80	6	10
4	C	610	PCW	C2-O2-C31	3.49	109.43	117.80	7	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	D	518	PCW	C2-O2-C31	3.49	109.45	117.80	4	10
4	D	511	PCW	C2-O2-C31	3.48	109.46	117.80	8	10
5	C	630	17F	C5-O9-C17	3.48	109.47	117.80	8	10
4	D	515	PCW	C2-O2-C31	3.47	109.48	117.80	5	10
4	C	610	PCW	C8-N-C6	3.46	118.08	108.98	10	10
4	C	614	PCW	C2-O2-C31	3.45	109.55	117.80	9	10
4	C	601	PCW	C2-O2-C31	3.44	109.55	117.80	4	10
4	C	622	PCW	C2-O2-C31	3.44	109.55	117.80	5	10
4	D	516	PCW	C2-O2-C31	3.44	109.56	117.80	3	10
5	C	629	17F	C5-O9-C17	3.44	109.56	117.80	8	8
4	C	603	PCW	C2-O2-C31	3.44	109.57	117.80	10	10
4	A	405	PCW	C2-O2-C31	3.43	109.58	117.80	10	10
4	A	415	PCW	C2-O2-C31	3.41	109.64	117.80	9	6
4	C	604	PCW	C2-O2-C31	3.41	109.64	117.80	8	10
4	C	611	PCW	C2-O2-C31	3.41	109.64	117.80	9	10
4	C	623	PCW	O2-C31-C32	3.40	118.83	111.48	7	10
4	C	605	PCW	C2-O2-C31	3.40	109.67	117.80	2	10
4	D	508	PCW	C2-O2-C31	3.40	109.66	117.80	6	10
4	C	614	PCW	C8-N-C6	3.39	117.89	108.98	6	10
6	B	205	GNP	C2-N1-C6	3.39	118.97	125.11	8	10
4	D	507	PCW	C2-O2-C31	3.38	109.70	117.80	6	10
4	A	404	PCW	C7-N-C6	3.38	117.85	108.98	8	10
4	C	608	PCW	C8-N-C6	3.37	117.84	108.98	2	10
4	A	406	PCW	C2-O2-C31	3.37	109.73	117.80	4	10
4	B	203	PCW	C7-N-C6	3.37	117.83	108.98	3	10
4	B	202	PCW	C7-N-C6	3.37	117.82	108.98	10	10
4	A	415	PCW	C7-N-C6	3.37	117.82	108.98	9	10
4	C	625	PCW	C7-N-C6	3.36	117.81	108.98	2	10
5	D	525	17F	C5-O9-C17	3.36	109.75	117.80	5	10
4	C	616	PCW	C7-N-C6	3.36	117.80	108.98	2	10
4	A	412	PCW	C8-N-C6	3.36	117.79	108.98	2	10
5	D	520	17F	C5-O9-C17	3.35	109.77	117.80	9	10
4	C	622	PCW	C8-N-C6	3.35	117.78	108.98	5	10
4	C	602	PCW	C7-N-C6	3.35	117.77	108.98	10	10
4	C	608	PCW	C7-N-C6	3.34	117.76	108.98	2	10
4	D	505	PCW	C8-N-C6	3.34	117.75	108.98	10	10
4	D	512	PCW	C7-N-C6	3.34	117.75	108.98	3	10
4	D	528	PCW	C2-O2-C31	3.34	109.80	117.80	8	10
4	A	408	PCW	C2-O2-C31	3.34	109.81	117.80	9	10
4	C	612	PCW	C8-N-C6	3.34	117.74	108.98	10	10
4	C	619	PCW	C8-N-C6	3.33	117.74	108.98	10	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	B	201	PCW	C8-N-C6	3.34	117.74	108.98	7	10
4	C	603	PCW	C7-N-C6	3.33	117.73	108.98	5	10
4	C	625	PCW	C8-N-C6	3.33	117.73	108.98	3	10
4	C	609	PCW	C7-N-C6	3.33	117.73	108.98	6	10
4	C	621	PCW	C7-N-C6	3.33	117.72	108.98	6	10
4	A	411	PCW	C7-N-C6	3.33	117.72	108.98	3	10
4	C	605	PCW	C8-N-C6	3.33	117.72	108.98	9	10
4	A	401	PCW	C7-N-C6	3.33	117.71	108.98	9	10
4	A	410	PCW	C8-N-C6	3.33	117.71	108.98	9	10
4	C	620	PCW	C7-N-C6	3.32	117.70	108.98	8	10
4	A	405	PCW	C7-N-C6	3.32	117.70	108.98	7	10
4	A	406	PCW	C7-N-C6	3.32	117.69	108.98	1	10
4	A	410	PCW	C2-O2-C31	3.32	109.86	117.80	4	9
4	D	512	PCW	C8-N-C6	3.32	117.69	108.98	8	10
4	A	411	PCW	C8-N-C6	3.32	117.69	108.98	8	10
4	D	509	PCW	C8-N-C6	3.31	117.68	108.98	9	10
4	D	511	PCW	C7-N-C6	3.31	117.68	108.98	10	10
4	D	517	PCW	C7-N-C6	3.31	117.68	108.98	5	10
4	D	526	PCW	C7-N-C6	3.31	117.68	108.98	6	10
4	B	204	PCW	C8-N-C6	3.31	117.67	108.98	10	10
4	C	615	PCW	C7-N-C6	3.31	117.66	108.98	1	10
4	C	622	PCW	C7-N-C6	3.31	117.66	108.98	4	10
4	A	408	PCW	C8-N-C6	3.31	117.66	108.98	7	10
4	A	412	PCW	C2-O2-C31	3.30	109.89	117.80	2	10
4	A	414	PCW	C8-N-C6	3.30	117.66	108.98	4	10
4	B	201	PCW	C7-N-C6	3.30	117.65	108.98	1	10
4	D	502	PCW	C7-N-C6	3.30	117.65	108.98	9	10
4	D	517	PCW	C8-N-C6	3.30	117.65	108.98	1	10
4	C	603	PCW	C8-N-C6	3.30	117.64	108.98	7	10
4	D	503	PCW	C8-N-C6	3.30	117.64	108.98	8	10
4	C	623	PCW	C7-N-C6	3.30	117.63	108.98	10	10
4	D	503	PCW	C7-N-C6	3.29	117.63	108.98	5	10
4	D	506	PCW	C7-N-C6	3.30	117.63	108.98	3	10
4	D	516	PCW	C7-N-C6	3.30	117.63	108.98	5	10
5	C	626	17F	C5-O9-C17	3.29	109.92	117.80	7	10
4	A	408	PCW	C7-N-C6	3.29	117.61	108.98	5	10
4	D	504	PCW	C7-N-C6	3.29	117.61	108.98	5	10
4	C	601	PCW	C8-N-C6	3.29	117.61	108.98	9	10
4	C	617	PCW	C7-N-C6	3.28	117.60	108.98	5	10
4	D	501	PCW	C2-O2-C31	3.29	109.93	117.80	1	10
4	C	606	PCW	C8-N-C6	3.28	117.60	108.98	9	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	C	621	PCW	C8-N-C6	3.28	117.60	108.98	9	10
4	D	518	PCW	C7-N-C6	3.28	117.60	108.98	9	10
4	A	407	PCW	C8-N-C6	3.28	117.60	108.98	4	10
4	D	511	PCW	C8-N-C6	3.28	117.60	108.98	8	10
4	A	403	PCW	C7-N-C6	3.28	117.59	108.98	5	10
4	C	604	PCW	C7-N-C6	3.28	117.59	108.98	7	10
4	C	607	PCW	C8-N-C6	3.28	117.59	108.98	2	10
4	A	402	PCW	C7-N-C6	3.28	117.58	108.98	9	10
4	D	505	PCW	C2-O2-C31	3.27	109.96	117.80	9	10
4	D	509	PCW	C7-N-C6	3.27	117.57	108.98	4	10
4	D	527	PCW	C7-N-C6	3.27	117.57	108.98	10	10
4	A	410	PCW	C7-N-C6	3.27	117.57	108.98	1	10
4	D	512	PCW	C2-O2-C31	3.27	109.97	117.80	1	10
4	C	624	PCW	C8-N-C6	3.27	117.56	108.98	4	10
4	D	501	PCW	C8-N-C6	3.27	117.56	108.98	7	10
4	A	413	PCW	C8-N-C6	3.27	117.56	108.98	7	10
4	C	617	PCW	C8-N-C6	3.27	117.56	108.98	9	10
4	B	203	PCW	C8-N-C6	3.27	117.56	108.98	6	10
4	D	513	PCW	C8-N-C6	3.27	117.56	108.98	4	10
4	D	528	PCW	C7-N-C6	3.27	117.56	108.98	9	10
4	C	601	PCW	C7-N-C6	3.27	117.56	108.98	8	10
4	C	606	PCW	C2-O2-C31	3.27	109.98	117.80	2	10
4	D	510	PCW	C8-N-C6	3.27	117.56	108.98	3	10
4	D	518	PCW	C8-N-C6	3.27	117.56	108.98	7	10
4	C	612	PCW	C7-N-C6	3.26	117.55	108.98	5	10
4	C	616	PCW	C8-N-C6	3.26	117.55	108.98	9	10
4	A	404	PCW	C8-N-C6	3.26	117.55	108.98	7	10
4	C	618	PCW	C7-N-C6	3.26	117.55	108.98	4	10
4	A	413	PCW	C7-N-C6	3.26	117.55	108.98	10	10
4	C	613	PCW	C8-N-C6	3.26	117.54	108.98	1	10
4	C	618	PCW	C8-N-C6	3.26	117.54	108.98	10	10
4	D	514	PCW	C7-N-C6	3.26	117.54	108.98	1	10
4	D	505	PCW	C7-N-C6	3.26	117.54	108.98	7	10
4	D	515	PCW	C8-N-C6	3.26	117.54	108.98	6	10
4	D	526	PCW	C8-N-C6	3.26	117.54	108.98	1	10
4	B	204	PCW	C7-N-C6	3.26	117.53	108.98	4	10
4	A	407	PCW	C7-N-C6	3.26	117.53	108.98	2	10
4	C	604	PCW	C8-N-C6	3.26	117.53	108.98	3	10
5	A	409	17F	C5-O9-C17	3.26	110.00	117.80	1	10
4	D	504	PCW	C8-N-C6	3.25	117.52	108.98	6	10
4	C	615	PCW	C8-N-C6	3.25	117.52	108.98	10	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	D	506	PCW	C8-N-C6	3.25	117.51	108.98	6	10
4	D	508	PCW	C7-N-C6	3.25	117.51	108.98	9	10
4	D	510	PCW	C7-N-C6	3.25	117.51	108.98	4	10
4	D	527	PCW	C8-N-C6	3.25	117.52	108.98	6	10
4	C	607	PCW	C7-N-C6	3.25	117.51	108.98	10	10
4	D	508	PCW	C8-N-C6	3.25	117.51	108.98	7	10
4	C	610	PCW	C7-N-C6	3.25	117.50	108.98	6	10
6	B	205	GNP	N9-C4-N3	3.25	132.45	125.95	1	10
4	A	402	PCW	C8-N-C6	3.25	117.50	108.98	10	10
4	B	201	PCW	C2-O2-C31	3.25	110.03	117.80	3	10
4	D	502	PCW	C8-N-C6	3.25	117.50	108.98	3	10
4	A	412	PCW	C7-N-C6	3.24	117.50	108.98	7	10
4	D	514	PCW	C8-N-C6	3.24	117.50	108.98	3	10
4	D	528	PCW	C8-N-C6	3.24	117.50	108.98	8	10
4	C	623	PCW	C8-N-C6	3.24	117.49	108.98	6	10
4	D	501	PCW	C7-N-C6	3.24	117.50	108.98	1	10
4	C	605	PCW	C7-N-C6	3.24	117.48	108.98	5	10
4	D	516	PCW	C8-N-C6	3.24	117.48	108.98	9	10
4	C	611	PCW	C7-N-C6	3.24	117.48	108.98	4	10
4	C	619	PCW	C7-N-C6	3.23	117.47	108.98	9	10
4	B	202	PCW	C8-N-C6	3.23	117.47	108.98	3	10
4	D	513	PCW	C7-N-C6	3.23	117.47	108.98	2	10
4	C	606	PCW	C7-N-C6	3.23	117.46	108.98	3	10
4	C	602	PCW	C8-N-C6	3.23	117.46	108.98	7	10
4	C	624	PCW	C7-N-C6	3.23	117.46	108.98	1	10
4	A	405	PCW	C8-N-C6	3.23	117.45	108.98	2	10
4	C	620	PCW	C8-N-C6	3.23	117.46	108.98	3	10
4	C	611	PCW	C8-N-C6	3.23	117.45	108.98	1	10
4	C	614	PCW	C7-N-C6	3.23	117.45	108.98	8	10
4	A	403	PCW	C8-N-C6	3.22	117.43	108.98	2	10
4	A	414	PCW	C7-N-C6	3.22	117.43	108.98	5	10
4	A	401	PCW	C8-N-C6	3.21	117.41	108.98	10	10
4	C	608	PCW	C2-O2-C31	3.21	110.11	117.80	8	10
4	C	609	PCW	C8-N-C6	3.21	117.40	108.98	8	10
4	A	415	PCW	C8-N-C6	3.20	117.38	108.98	4	10
4	D	509	PCW	C2-O2-C31	3.19	110.16	117.80	10	10
4	C	613	PCW	C2-O2-C31	3.19	110.17	117.80	8	10
5	C	628	17F	O3-P1-O1	3.17	96.38	108.94	2	10
4	A	406	PCW	C8-N-C6	3.16	117.28	108.98	6	10
4	A	414	PCW	C2-O2-C31	3.16	110.24	117.80	10	10
4	C	616	PCW	C2-O2-C31	3.14	110.28	117.80	1	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	C	602	PCW	C2-O2-C31	3.14	110.28	117.80	8	10
5	D	519	17F	O3-P1-O1	3.12	96.55	108.94	9	10
4	D	513	PCW	C2-O2-C31	3.12	110.33	117.80	2	10
5	D	522	17F	C5-O9-C17	3.12	110.33	117.80	8	10
4	D	503	PCW	C2-O2-C31	3.09	110.39	117.80	9	10
4	C	609	PCW	C2-O2-C31	3.08	110.41	117.80	10	10
4	D	504	PCW	O4P-P-O2P	3.08	96.72	108.94	7	10
4	D	527	PCW	O4P-P-O2P	3.08	96.72	108.94	10	10
4	B	203	PCW	C2-O2-C31	3.07	110.46	117.80	7	10
4	C	607	PCW	C2-O2-C31	3.06	110.47	117.80	5	10
4	C	619	PCW	C2-O2-C31	3.02	110.56	117.80	1	10
4	B	204	PCW	C2-O2-C31	3.01	110.59	117.80	3	10
4	D	518	PCW	O3-C11-C12	3.01	121.02	111.83	8	10
4	C	621	PCW	C2-O2-C31	3.00	110.61	117.80	4	10
4	C	605	PCW	O3-C11-C12	2.90	120.68	111.83	8	10
5	D	521	17F	O7-C7-C8	2.88	120.60	111.83	4	10
4	C	604	PCW	O3-C11-C12	2.87	120.59	111.83	3	10
4	D	527	PCW	C2-O2-C31	2.85	110.98	117.80	7	10
4	C	612	PCW	O3-C11-C12	2.84	120.49	111.83	10	10
4	C	620	PCW	O3-C11-C12	2.83	120.46	111.83	9	10
4	D	506	PCW	O3-C11-C12	2.82	120.44	111.83	10	10
4	C	617	PCW	O3-C11-C12	2.79	120.35	111.83	7	10
4	A	412	PCW	O3-C11-C12	2.78	120.33	111.83	1	10
4	B	203	PCW	O3-C11-C12	2.78	120.32	111.83	1	10
5	C	628	17F	O7-C7-C8	2.78	120.31	111.83	10	10
6	B	205	GNP	C3'-C2'-C1'	2.78	96.21	101.46	10	7
4	D	508	PCW	O3-C11-C12	2.77	120.28	111.83	3	10
6	B	205	GNP	O4'-C1'-C2'	2.76	100.71	106.62	6	4
4	D	527	PCW	O1P-P-O2P	2.75	125.25	112.44	4	10
5	C	628	17F	O2-P1-O1	2.73	125.16	112.44	1	10
4	C	623	PCW	C2-O2-C31	2.73	111.26	117.80	6	10
4	A	414	PCW	O3-C11-C12	2.73	120.15	111.83	8	10
4	A	415	PCW	O3-C11-C12	2.73	120.14	111.83	2	10
4	D	504	PCW	O1P-P-O2P	2.72	125.10	112.44	5	10
4	D	528	PCW	O3-C11-C12	2.72	120.13	111.83	10	10
4	A	406	PCW	O3-C11-C12	2.71	120.10	111.83	3	10
4	B	201	PCW	O3-C11-C12	2.71	120.09	111.83	7	10
5	D	519	17F	O2-P1-O1	2.71	125.04	112.44	10	10
4	C	603	PCW	O3-C11-C12	2.71	120.09	111.83	8	10
4	A	411	PCW	O3-C11-C12	2.71	120.08	111.83	8	10
4	A	410	PCW	O3-C11-C12	2.70	120.06	111.83	4	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	C	615	PCW	O3-C11-C12	2.69	120.03	111.83	3	10
4	C	622	PCW	O3-C11-C12	2.69	120.02	111.83	5	10
4	C	611	PCW	O3-C11-C12	2.68	120.01	111.83	4	10
4	D	526	PCW	O3-C11-C12	2.68	120.01	111.83	10	10
4	C	609	PCW	O3-C11-C12	2.67	119.99	111.83	7	10
4	D	503	PCW	O3-C11-C12	2.67	119.97	111.83	8	10
4	B	202	PCW	O3-C11-C12	2.67	119.97	111.83	10	10
5	D	519	17F	O7-C7-C8	2.66	119.95	111.83	6	10
4	D	515	PCW	O3-C11-C12	2.66	119.94	111.83	10	10
4	C	618	PCW	O3-C11-C12	2.65	119.92	111.83	8	10
4	D	513	PCW	O3-C11-C12	2.65	119.92	111.83	3	10
4	D	516	PCW	O3-C11-C12	2.65	119.92	111.83	3	10
5	C	629	17F	O7-C7-C8	2.65	119.91	111.83	3	10
4	C	624	PCW	O3-C11-C12	2.65	119.90	111.83	7	10
4	D	510	PCW	O3-C11-C12	2.64	119.90	111.83	1	10
5	D	524	17F	O7-C7-C8	2.64	119.90	111.83	6	10
4	C	601	PCW	O3-C11-C12	2.64	119.89	111.83	4	10
4	B	204	PCW	O3-C11-C12	2.63	119.87	111.83	5	10
5	D	529	17F	O7-C7-C8	2.63	119.86	111.83	5	10
4	D	502	PCW	O3-C11-C12	2.63	119.85	111.83	3	10
4	D	501	PCW	O3-C11-C12	2.62	119.83	111.83	10	10
4	D	527	PCW	O3-C11-C12	2.62	119.82	111.83	10	10
4	A	403	PCW	O3-C11-C12	2.62	119.81	111.83	2	10
5	D	525	17F	O7-C7-C8	2.62	119.81	111.83	8	10
5	D	529	17F	C5-O9-C17	2.62	111.53	117.80	5	9
4	A	402	PCW	O3-C11-C12	2.61	119.81	111.83	2	10
4	D	507	PCW	O3-C11-C12	2.61	119.80	111.83	6	10
4	D	517	PCW	O3-C11-C12	2.60	119.75	111.83	2	10
4	D	518	PCW	C3-O3-C11	2.60	107.62	117.12	8	10
5	D	523	17F	O7-C7-C8	2.60	119.75	111.83	3	10
5	C	626	17F	O7-C7-C8	2.59	119.74	111.83	4	10
5	C	631	17F	O7-C7-C8	2.59	119.74	111.83	1	10
4	D	511	PCW	O3-C11-C12	2.59	119.73	111.83	3	10
5	D	522	17F	O7-C7-C8	2.59	119.72	111.83	6	10
4	C	605	PCW	C3-O3-C11	2.58	107.68	117.12	5	10
4	D	514	PCW	O3-C11-C12	2.58	119.71	111.83	6	10
5	D	520	17F	O7-C7-C8	2.58	119.70	111.83	4	10
4	D	509	PCW	O3-C11-C12	2.58	119.69	111.83	7	10
5	C	630	17F	O7-C7-C8	2.58	119.69	111.83	3	10
4	D	512	PCW	O3-C11-C12	2.57	119.67	111.83	8	10
4	C	623	PCW	O3-C11-C12	2.57	119.66	111.83	6	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	A	409	17F	O7-C7-C8	2.56	119.64	111.83	5	10
4	D	504	PCW	O3-C11-C12	2.55	119.62	111.83	3	10
4	A	401	PCW	O3-C11-C12	2.55	119.61	111.83	3	10
4	C	607	PCW	O3-C11-C12	2.55	119.61	111.83	9	10
4	D	505	PCW	O3-C11-C12	2.54	119.58	111.83	1	10
4	A	405	PCW	O3-C11-C12	2.54	119.57	111.83	5	10
4	A	407	PCW	O3-C11-C12	2.53	119.55	111.83	7	10
4	A	414	PCW	C3-O3-C11	2.53	107.88	117.12	8	3
5	D	530	17F	O7-C7-C8	2.52	119.51	111.83	5	10
4	C	606	PCW	O3-C11-C12	2.51	119.48	111.83	5	10
4	A	404	PCW	O3-C11-C12	2.50	119.47	111.83	5	10
4	C	614	PCW	O3-C11-C12	2.49	119.42	111.83	9	10
4	C	602	PCW	O3-C11-C12	2.48	119.41	111.83	5	10
4	C	625	PCW	O3-C11-C12	2.48	119.41	111.83	10	10
4	A	408	PCW	O3-C11-C12	2.48	119.39	111.83	10	10
4	C	610	PCW	O3-C11-C12	2.47	119.38	111.83	1	10
4	C	613	PCW	O3-C11-C12	2.47	119.37	111.83	8	10
4	D	508	PCW	C3-O3-C11	2.47	108.09	117.12	10	10
4	C	620	PCW	C3-O3-C11	2.47	108.09	117.12	2	5
4	D	527	PCW	O1P-P-O4P	2.47	96.37	107.57	3	10
4	C	616	PCW	O3-C11-C12	2.46	119.34	111.83	5	10
4	B	203	PCW	C3-O3-C11	2.46	108.14	117.12	1	8
4	C	608	PCW	O3-C11-C12	2.46	119.32	111.83	8	10
4	D	528	PCW	C3-O3-C11	2.45	108.15	117.12	1	9
4	D	504	PCW	O1P-P-O4P	2.45	96.47	107.57	3	10
5	D	521	17F	C6-O7-C7	2.45	108.17	117.12	4	9
4	C	604	PCW	C3-O3-C11	2.43	108.24	117.12	3	1
4	C	621	PCW	O3-C11-C12	2.42	119.20	111.83	5	10
4	A	412	PCW	C3-O3-C11	2.41	108.31	117.12	2	9
5	D	519	17F	O2-P1-O3	2.40	96.68	107.57	6	10
4	D	504	PCW	O1P-P-O3P	2.38	118.36	107.57	3	10
5	C	628	17F	C6-O7-C7	2.36	108.48	117.12	10	8
4	A	413	PCW	O3-C11-C12	2.36	119.03	111.83	9	10
4	C	618	PCW	C3-O3-C11	2.36	108.50	117.12	6	10
5	C	628	17F	O2-P1-O3	2.36	96.89	107.57	1	10
4	D	527	PCW	O1P-P-O3P	2.34	118.18	107.57	2	10
5	C	631	17F	C6-O7-C7	2.33	108.60	117.12	1	2
5	C	628	17F	O6-P1-O1	2.33	118.15	108.94	10	10
4	D	526	PCW	C3-O3-C11	2.30	108.70	117.12	10	8
4	C	601	PCW	C3-O3-C11	2.29	108.74	117.12	4	7
5	C	627	17F	O7-C7-C8	2.29	118.81	111.83	8	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	D	519	17F	C6-O7-C7	2.28	108.78	117.12	2	4
5	D	530	17F	C6-O7-C7	2.28	108.78	117.12	5	5
4	A	415	PCW	C3-O3-C11	2.28	108.79	117.12	8	9
5	D	519	17F	O6-P1-O1	2.28	117.96	108.94	4	10
4	A	411	PCW	C3-O3-C11	2.26	108.86	117.12	7	5
4	C	619	PCW	O3-C11-C12	2.26	118.72	111.83	6	10
6	B	205	GNP	O6-C6-C5	2.25	120.59	126.53	3	10
4	C	617	PCW	C3-O3-C11	2.25	108.90	117.12	2	8
4	D	513	PCW	C3-O3-C11	2.25	108.89	117.12	3	1
4	A	410	PCW	C3-O3-C11	2.25	108.91	117.12	4	6
4	B	202	PCW	C3-O3-C11	2.25	108.90	117.12	8	8
4	C	612	PCW	C3-O3-C11	2.25	108.91	117.12	10	1
4	D	501	PCW	C3-O3-C11	2.24	108.94	117.12	10	7
6	B	205	GNP	C4-C5-N7	2.23	107.13	110.67	8	8
5	D	529	17F	O9-C17-O10	2.23	118.49	123.70	9	7
4	C	603	PCW	C3-O3-C11	2.22	108.99	117.12	2	6
5	D	529	17F	C6-O7-C7	2.21	109.03	117.12	7	3
6	B	205	GNP	N9-C8-N7	2.21	109.31	113.40	6	10
6	B	205	GNP	C8-N7-C5	2.21	108.20	104.26	6	9
5	C	629	17F	C6-O7-C7	2.21	109.05	117.12	3	5
4	C	624	PCW	C3-O3-C11	2.19	109.11	117.12	8	7
4	D	506	PCW	C3-O3-C11	2.19	109.11	117.12	10	3
4	C	611	PCW	C3-O3-C11	2.19	109.12	117.12	4	5
4	D	517	PCW	C3-O3-C11	2.18	109.13	117.12	4	6
4	C	607	PCW	C3-O3-C11	2.18	109.14	117.12	6	5
4	D	512	PCW	C3-O3-C11	2.18	109.15	117.12	2	3
4	A	406	PCW	C3-O3-C11	2.17	109.17	117.12	3	4
4	C	608	PCW	C8-N-C5	2.17	118.54	109.91	9	3
4	D	515	PCW	C4-C5-N	2.17	108.85	115.82	5	1
4	C	615	PCW	C3-O3-C11	2.17	109.19	117.12	3	4
5	D	525	17F	C6-O7-C7	2.17	109.20	117.12	5	3
6	B	205	GNP	C5-C6-N1	2.17	118.77	113.25	10	9
5	D	524	17F	C6-O7-C7	2.14	109.31	117.12	8	3
4	C	621	PCW	C4-C5-N	2.13	108.97	115.82	8	2
4	B	201	PCW	C3-O3-C11	2.13	109.32	117.12	7	4
4	D	515	PCW	C3-O3-C11	2.13	109.34	117.12	1	3
5	D	520	17F	C6-O7-C7	2.13	109.34	117.12	8	4
4	C	608	PCW	C4-C5-N	2.12	109.00	115.82	7	5
4	C	625	PCW	C8-N-C5	2.12	118.34	109.91	1	2
4	C	625	PCW	C3-O3-C11	2.12	109.37	117.12	3	3
4	D	528	PCW	C4-C5-N	2.12	109.02	115.82	10	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	C	606	PCW	C3-O3-C11	2.12	109.38	117.12	2	2
4	C	610	PCW	C4-C5-N	2.11	109.06	115.82	9	3
4	C	620	PCW	C7-N-C5	2.11	118.28	109.91	9	1
4	C	613	PCW	C4-C5-N	2.10	109.08	115.82	5	2
5	D	522	17F	C6-O7-C7	2.10	109.43	117.12	1	1
5	D	522	17F	O9-C17-O10	2.10	118.79	123.70	1	5
4	C	609	PCW	C3-O3-C11	2.10	109.44	117.12	6	5
4	D	505	PCW	C4-C5-N	2.10	109.08	115.82	7	2
4	C	614	PCW	C3-O3-C11	2.10	109.45	117.12	6	2
5	D	523	17F	C6-O7-C7	2.10	109.45	117.12	3	1
4	D	503	PCW	C3-O3-C11	2.09	109.46	117.12	8	5
4	D	510	PCW	C3-O3-C11	2.10	109.46	117.12	1	1
4	A	411	PCW	C7-N-C5	2.09	118.22	109.91	1	1
5	C	626	17F	C6-O7-C7	2.09	109.48	117.12	5	4
4	A	402	PCW	C3-O3-C11	2.09	109.49	117.12	3	3
4	B	204	PCW	C3-O3-C11	2.09	109.50	117.12	5	3
4	D	504	PCW	C4-C5-N	2.08	109.14	115.82	1	3
5	C	630	17F	C6-O7-C7	2.08	109.53	117.12	3	3
4	A	405	PCW	C3-O3-C11	2.07	109.54	117.12	5	1
4	C	612	PCW	C4-C5-N	2.07	109.19	115.82	10	1
4	C	603	PCW	C4-C5-N	2.06	109.22	115.82	8	4
4	A	401	PCW	C3-O3-C11	2.05	109.62	117.12	7	2
4	C	608	PCW	C3-C2-C1	2.05	107.00	111.78	9	1
4	A	403	PCW	C3-O3-C11	2.05	109.64	117.12	6	4
4	A	412	PCW	C4-C5-N	2.05	109.25	115.82	8	1
4	D	513	PCW	C4-C5-N	2.05	109.25	115.82	7	1
4	D	516	PCW	C4-C5-N	2.05	109.25	115.82	7	2
4	D	516	PCW	C3-O3-C11	2.04	109.64	117.12	5	4
4	D	507	PCW	C8-N-C5	2.04	118.02	109.91	3	1
4	D	510	PCW	C4-C5-N	2.04	109.28	115.82	1	2
4	C	625	PCW	C4-C5-N	2.04	109.28	115.82	9	4
4	C	612	PCW	C3-C2-C1	2.03	107.05	111.78	2	1
4	C	622	PCW	C3-O3-C11	2.03	109.70	117.12	1	2
4	B	201	PCW	C4-C5-N	2.03	109.31	115.82	7	1
6	B	205	GNP	O1G-PG-N3B	2.03	114.76	111.77	9	1
4	A	405	PCW	C7-N-C5	2.03	117.97	109.91	3	1
4	A	410	PCW	C4-C5-N	2.03	109.32	115.82	9	1
4	D	502	PCW	C3-O3-C11	2.03	109.71	117.12	10	2
5	A	409	17F	C6-O7-C7	2.03	109.71	117.12	8	1
4	C	613	PCW	C8-N-C5	2.02	117.96	109.91	1	1
4	C	614	PCW	C8-N-C5	2.03	117.96	109.91	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	C	620	PCW	C8-N-C5	2.03	117.96	109.91	4	1
4	D	506	PCW	C4-C5-N	2.03	109.32	115.82	4	1
5	D	525	17F	O9-C17-O10	2.02	118.97	123.70	9	1
4	A	407	PCW	C3-O3-C11	2.02	109.72	117.12	7	2
4	A	414	PCW	C4-C5-N	2.02	109.33	115.82	7	3
4	D	515	PCW	C7-N-C5	2.02	117.95	109.91	3	1
4	B	201	PCW	C8-N-C5	2.02	117.94	109.91	10	1
4	C	623	PCW	C3-O3-C11	2.02	109.74	117.12	6	2
4	A	402	PCW	C4-C5-N	2.01	109.36	115.82	6	1
4	C	618	PCW	C3-C2-C1	2.02	107.09	111.78	6	1
4	C	609	PCW	C7-N-C5	2.01	117.91	109.91	5	1
4	C	613	PCW	C7-N-C5	2.01	117.91	109.91	1	1
4	C	610	PCW	C7-N-C5	2.01	117.90	109.91	1	1
4	C	610	PCW	C3-O3-C11	2.01	109.77	117.12	6	1
4	C	610	PCW	C8-N-C5	2.01	117.90	109.91	9	1
4	C	614	PCW	C4-C5-N	2.01	109.37	115.82	6	2
4	C	625	PCW	C7-N-C5	2.01	117.88	109.91	4	1
4	D	507	PCW	C3-O3-C11	2.00	109.79	117.12	1	1
4	C	616	PCW	C3-O3-C11	2.00	109.80	117.12	9	1

There are no chirality outliers.

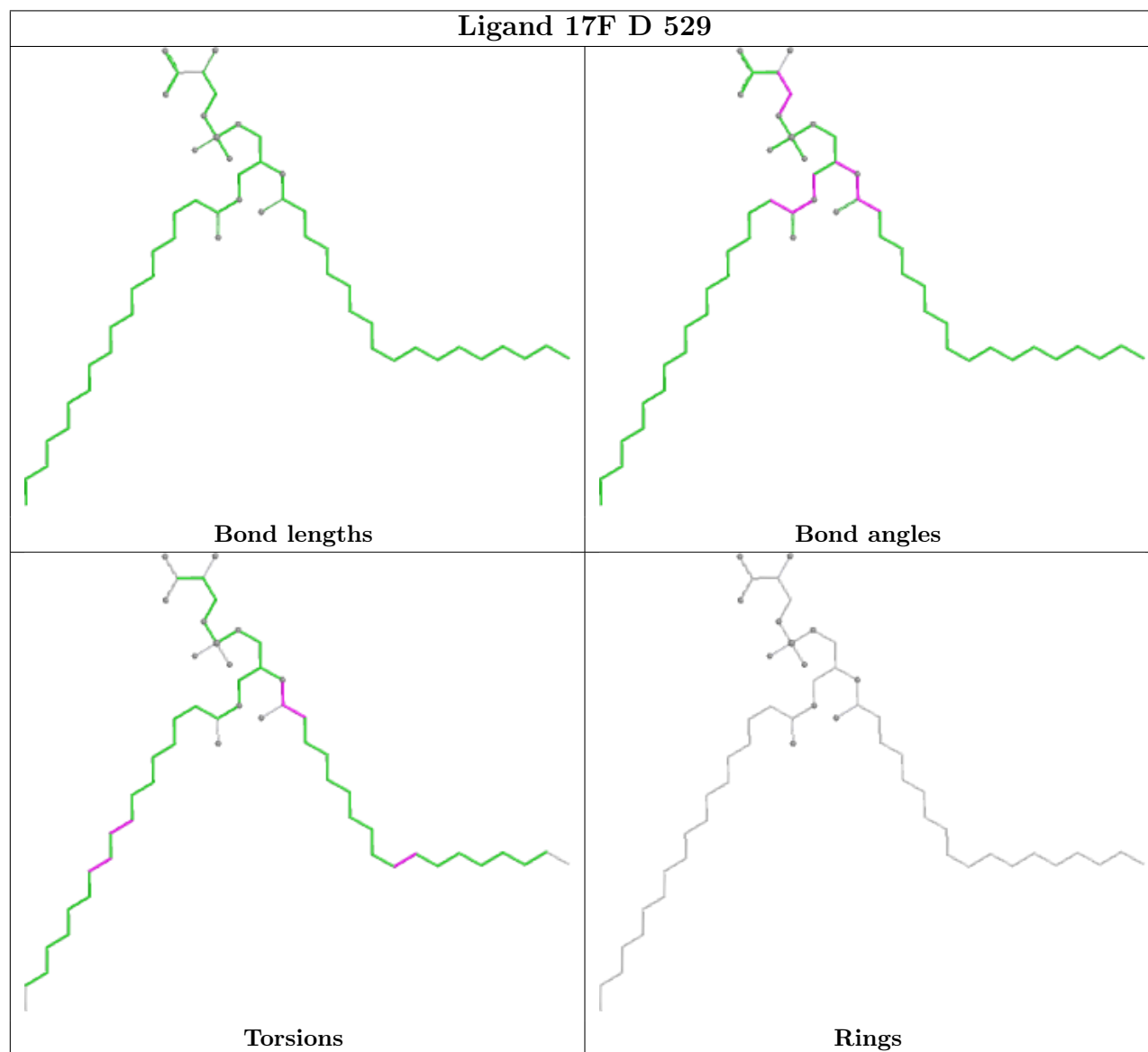
All unique torsion outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

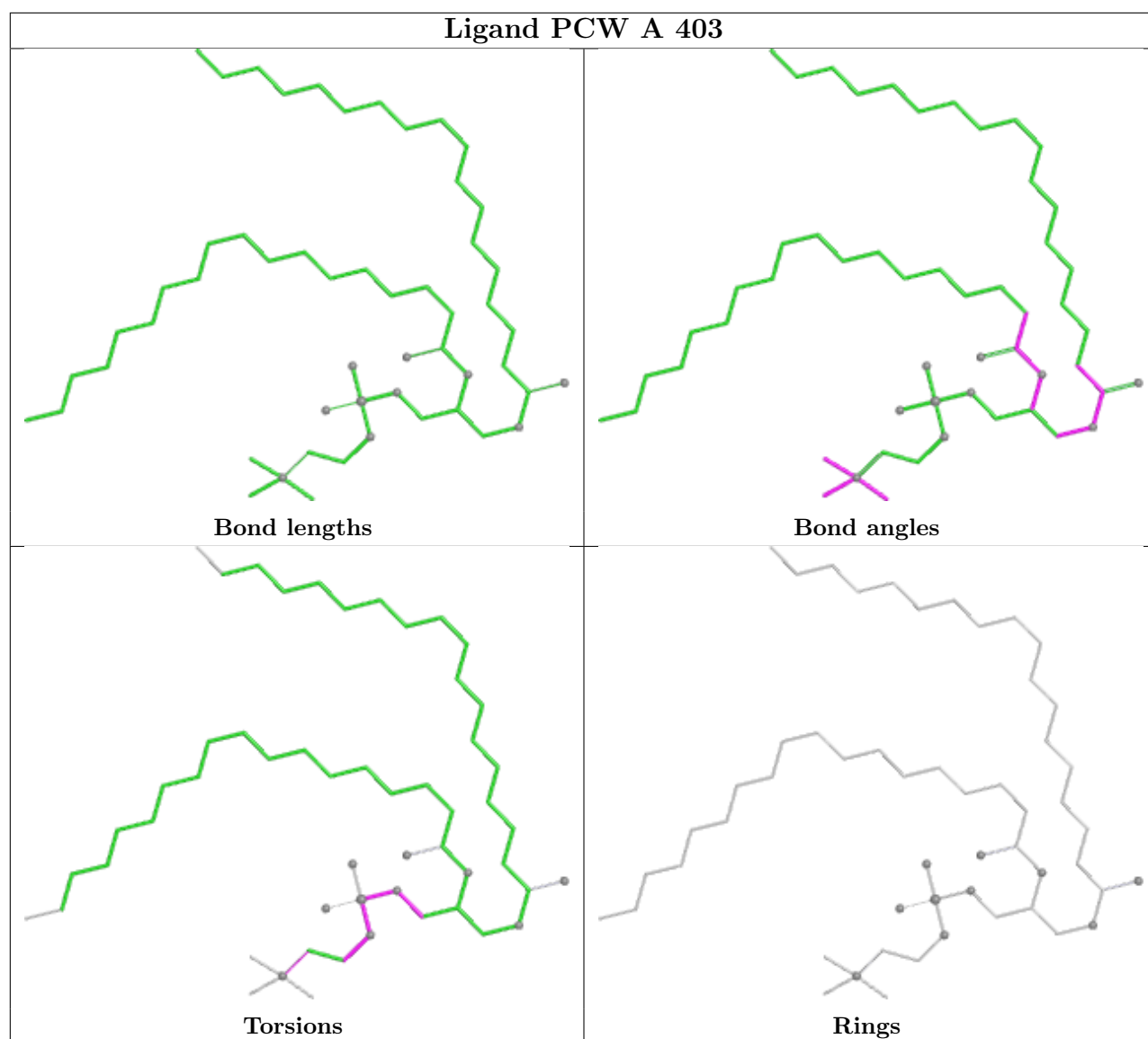
Mol	Chain	Res	Type	Atoms	Models (Total)
5	D	522	17F	O10-C17-O9-C5	10
5	D	525	17F	O10-C17-O9-C5	10
5	D	529	17F	O10-C17-O9-C5	10
5	D	522	17F	C18-C17-O9-C5	2
5	D	525	17F	C18-C17-O9-C5	1
5	D	529	17F	C18-C17-O9-C5	1

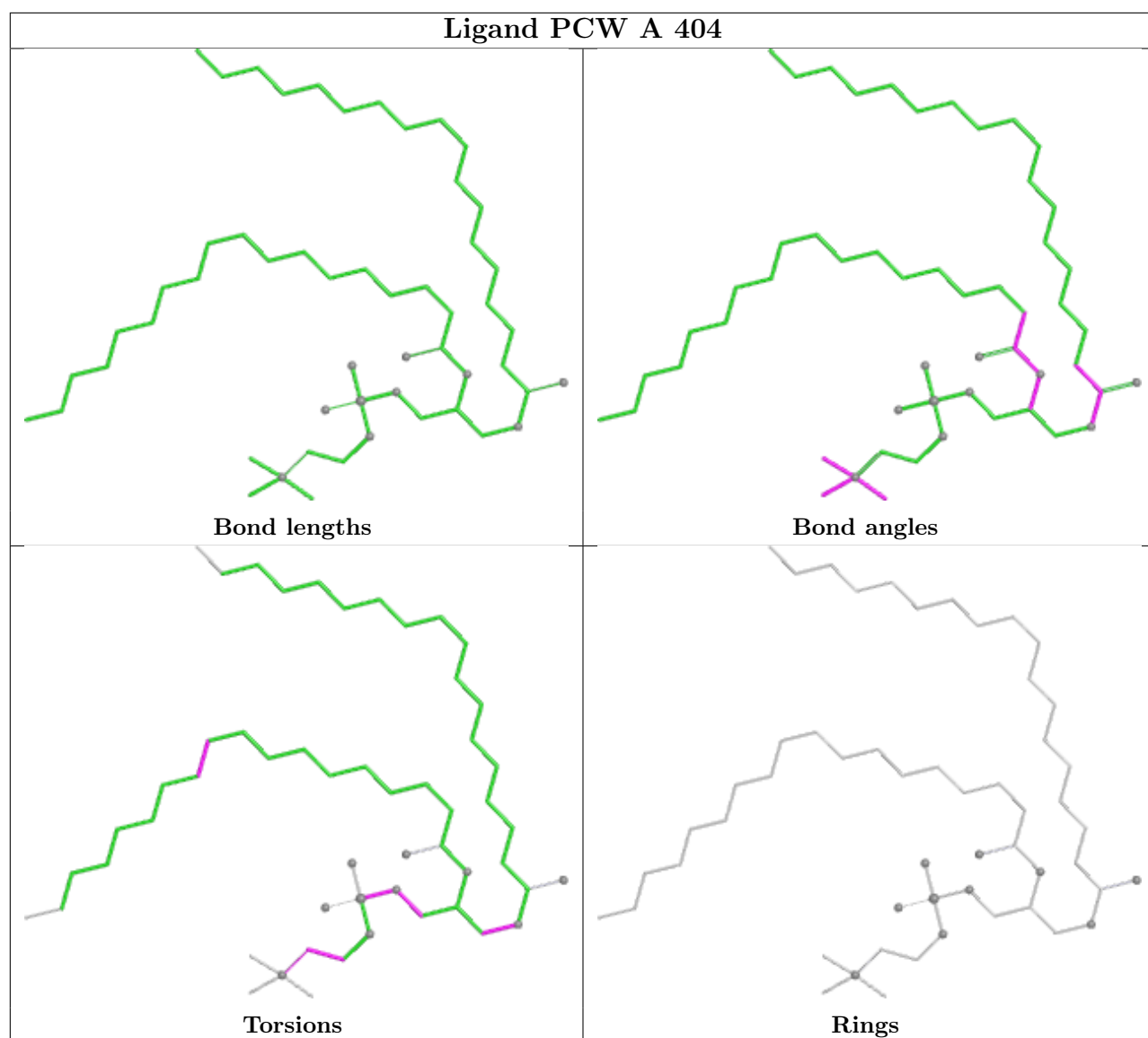
There are no ring outliers.

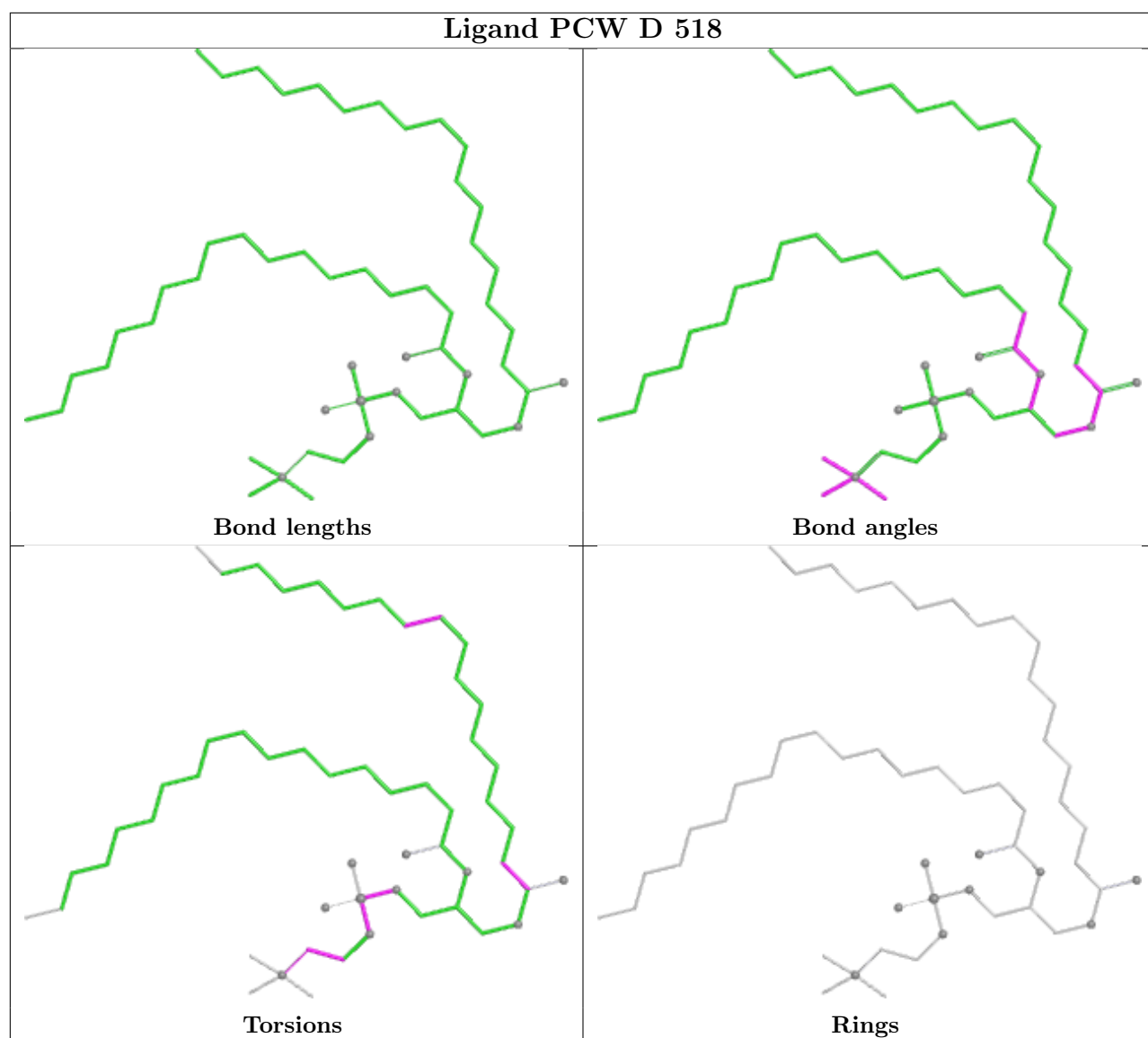
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

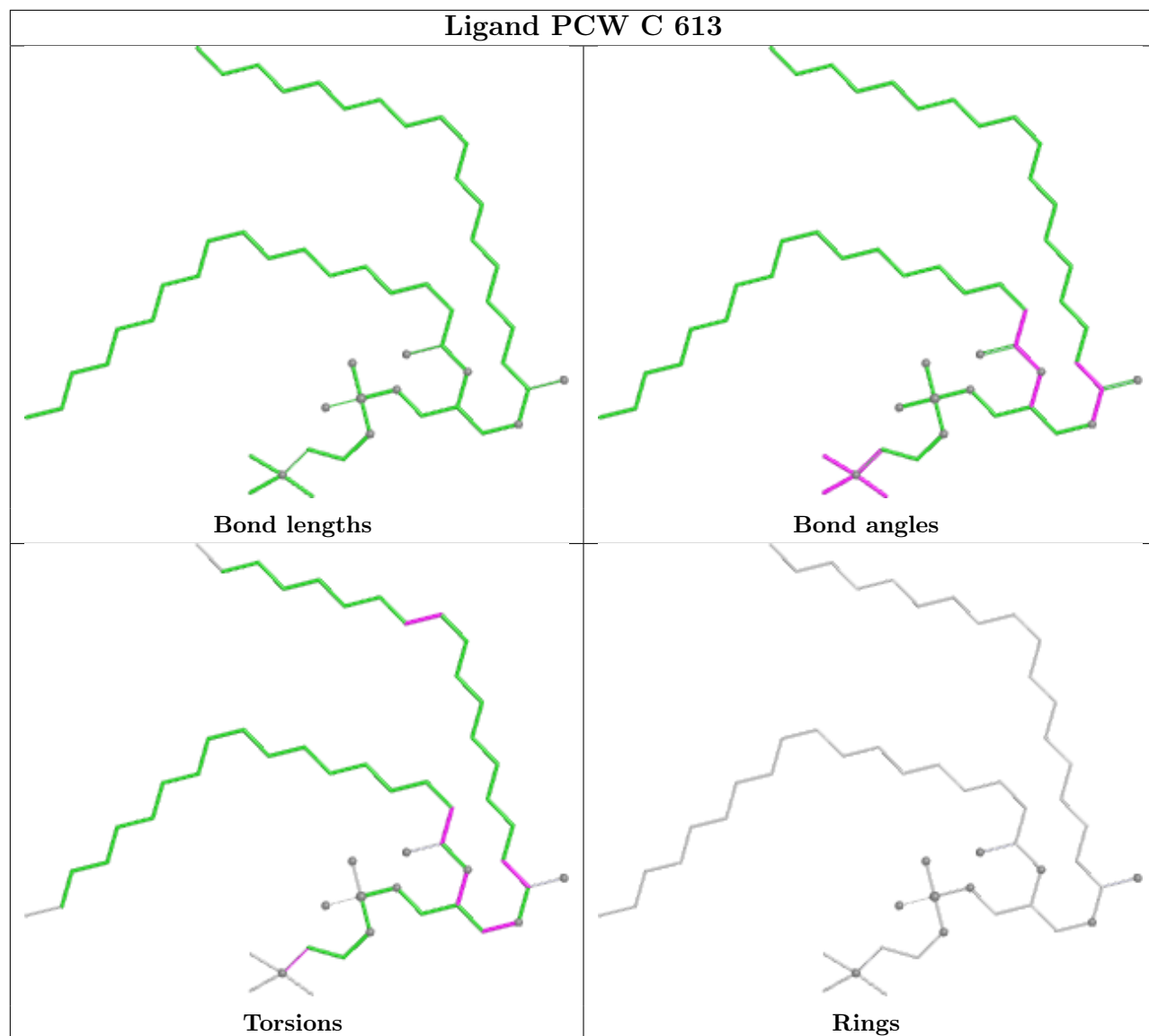
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

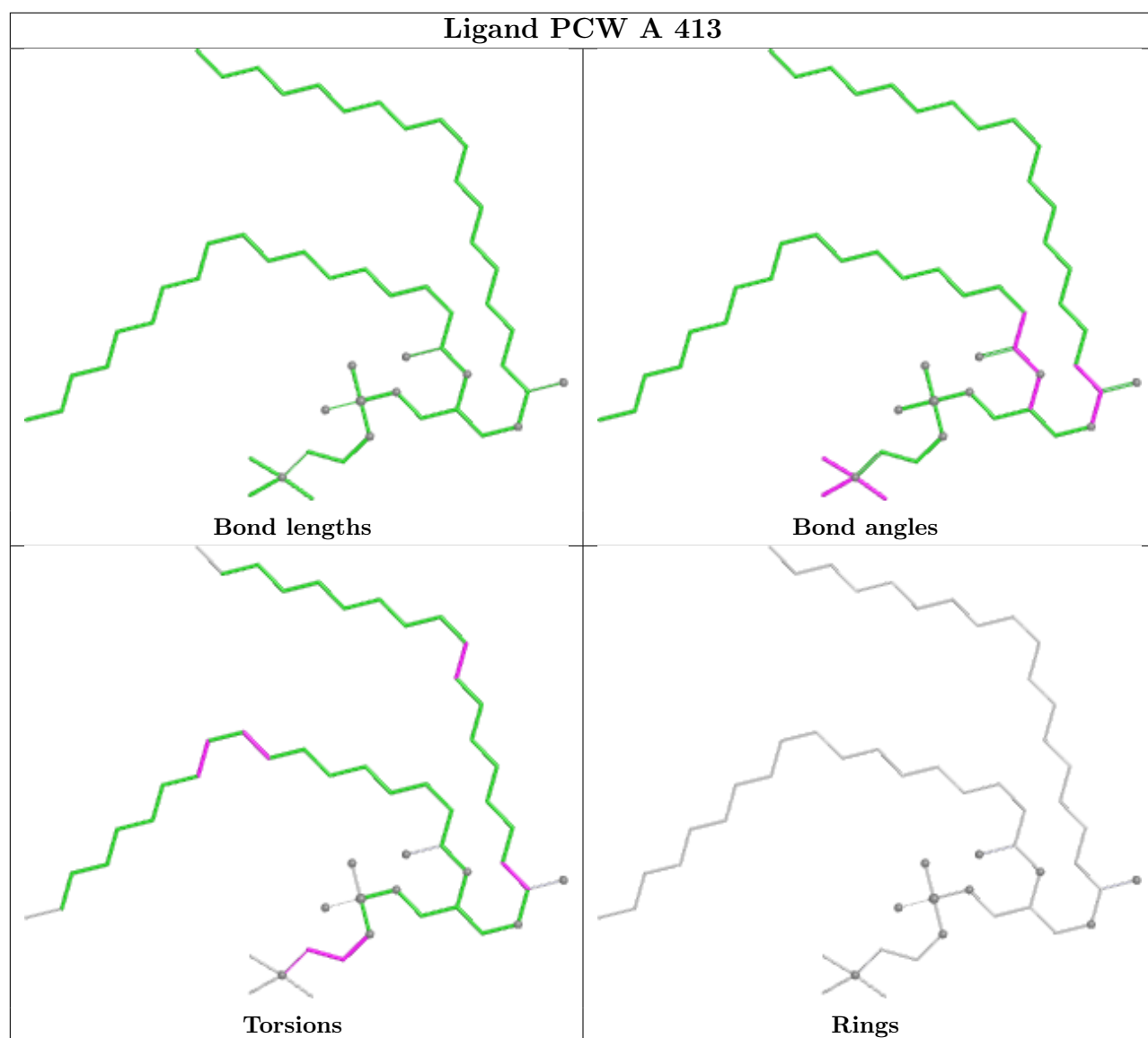


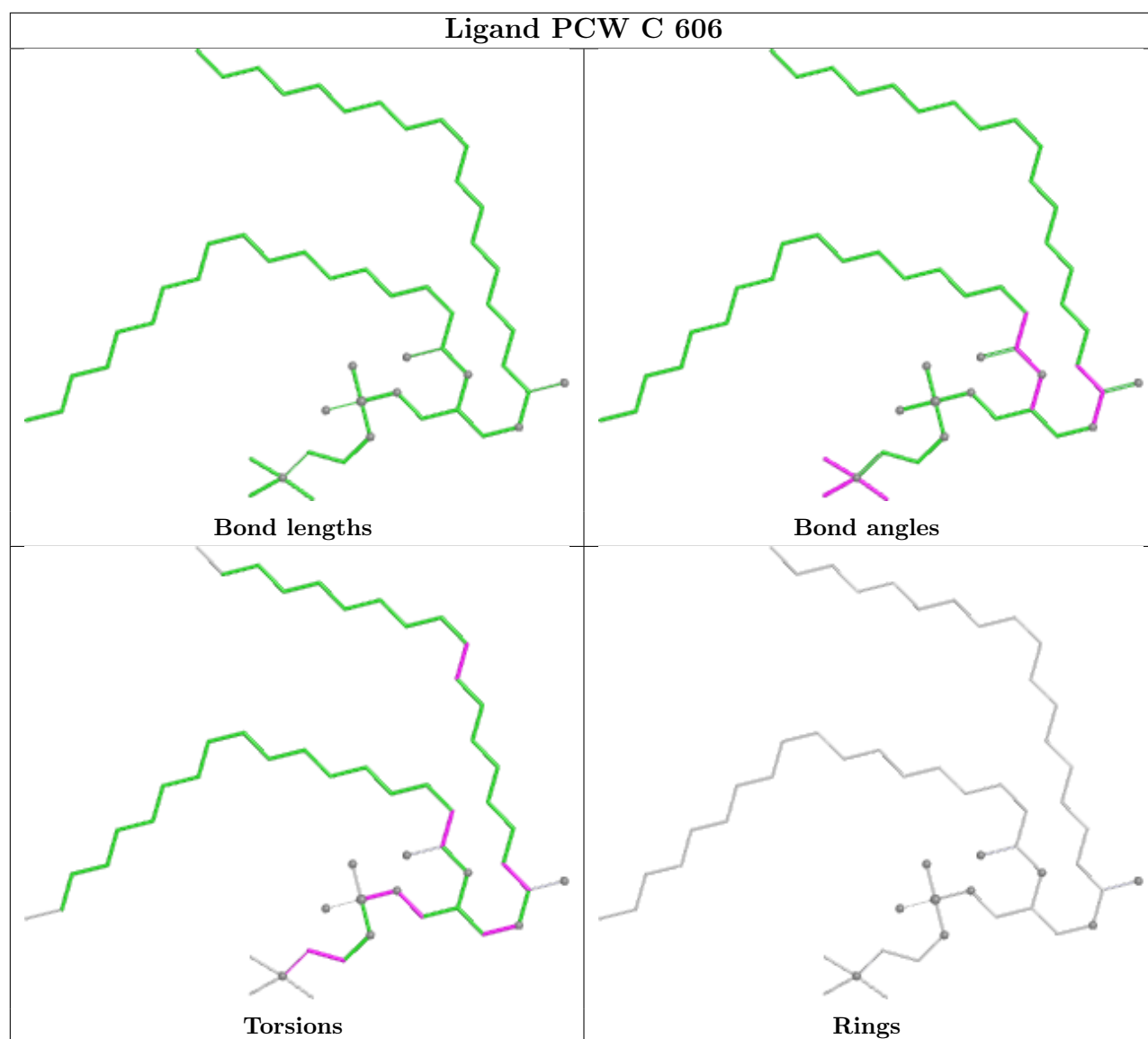


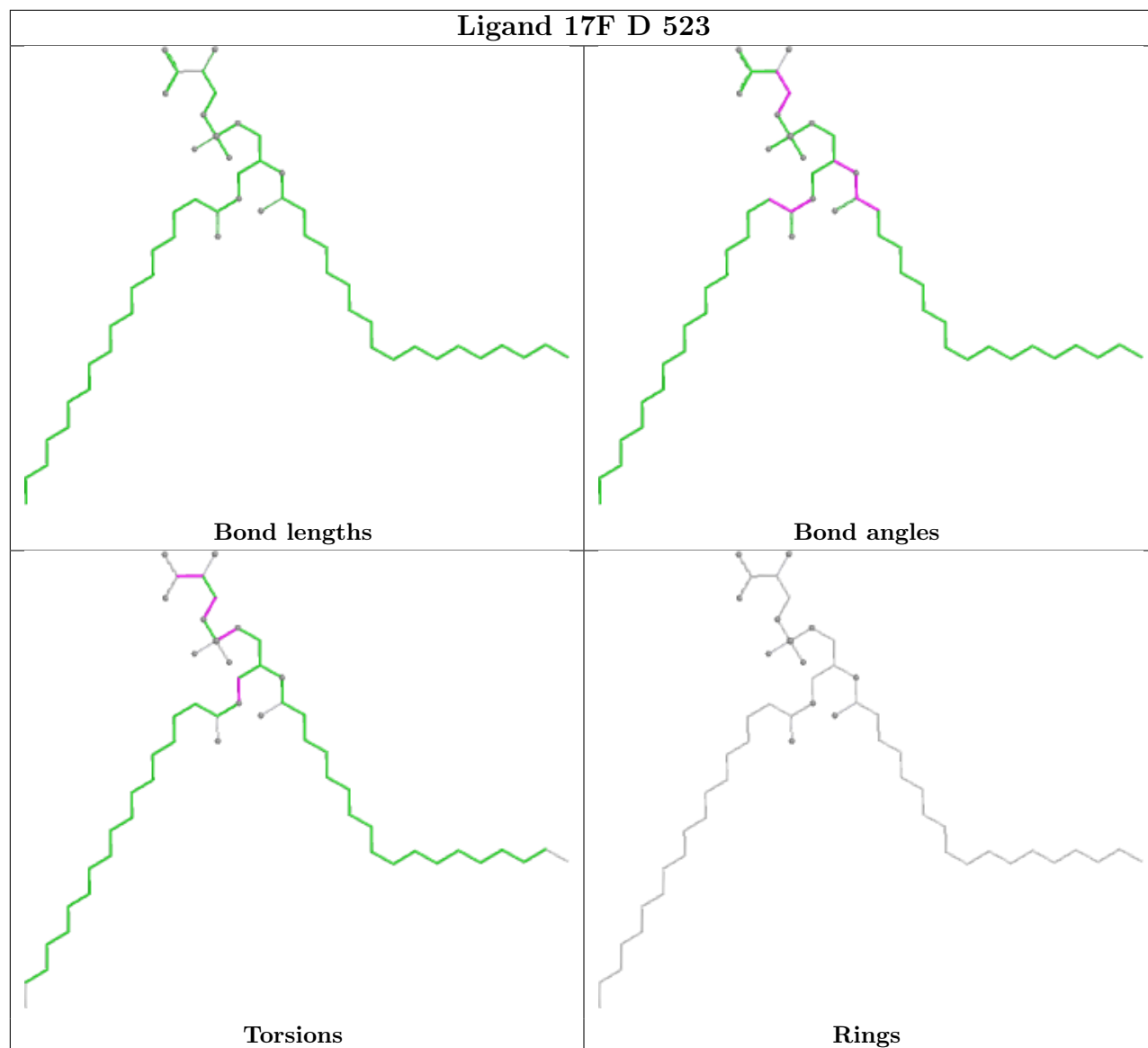


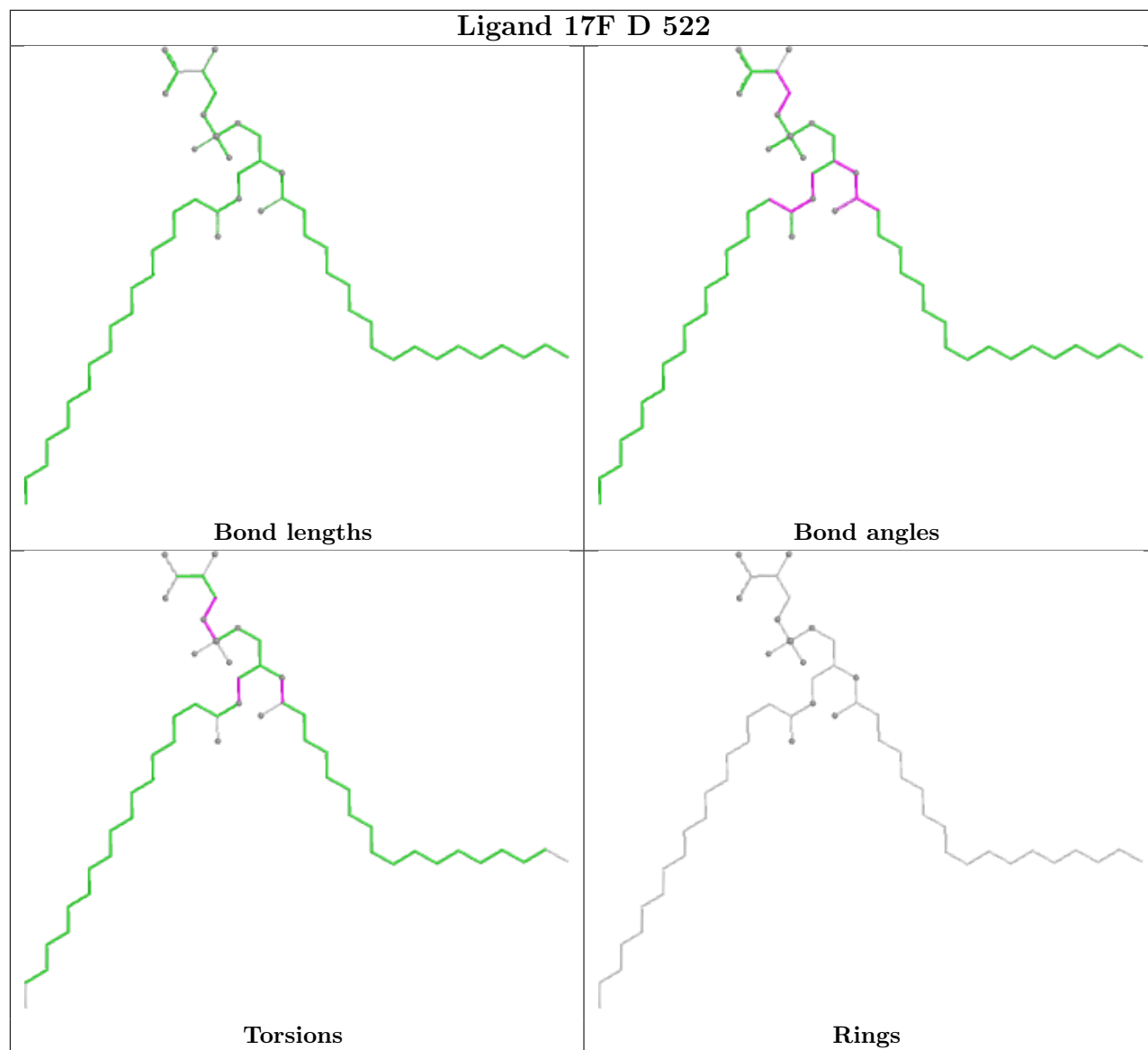


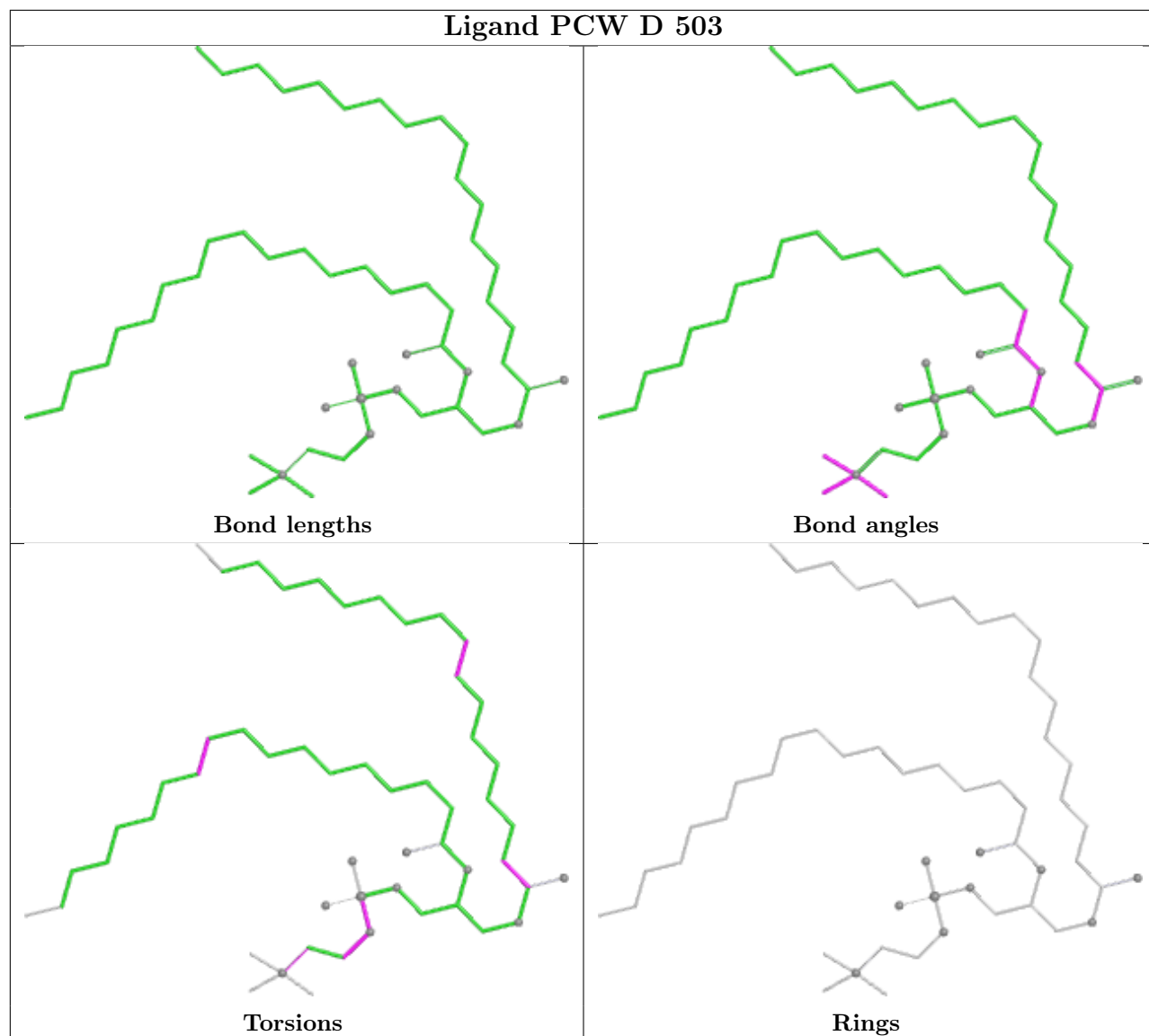


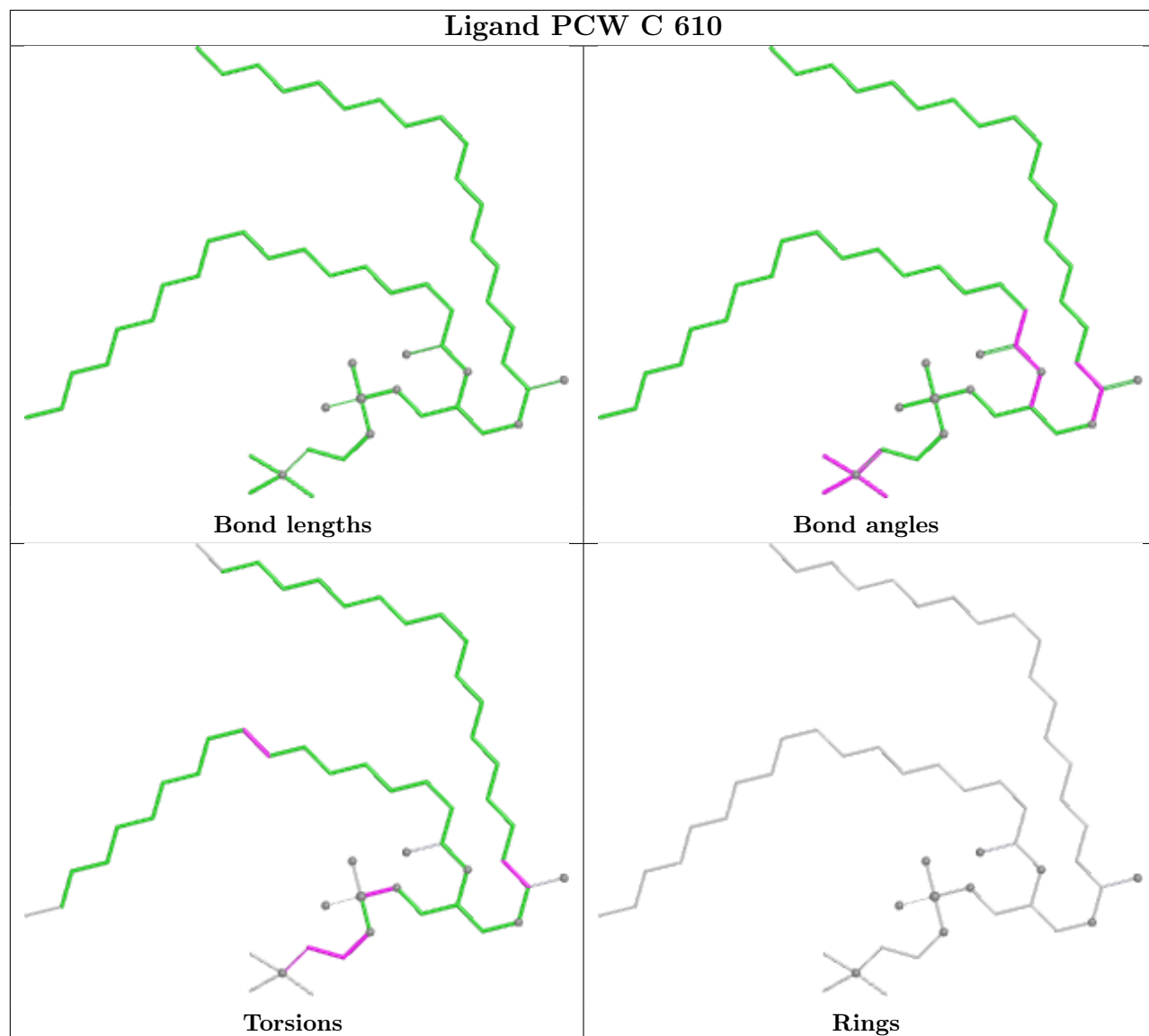


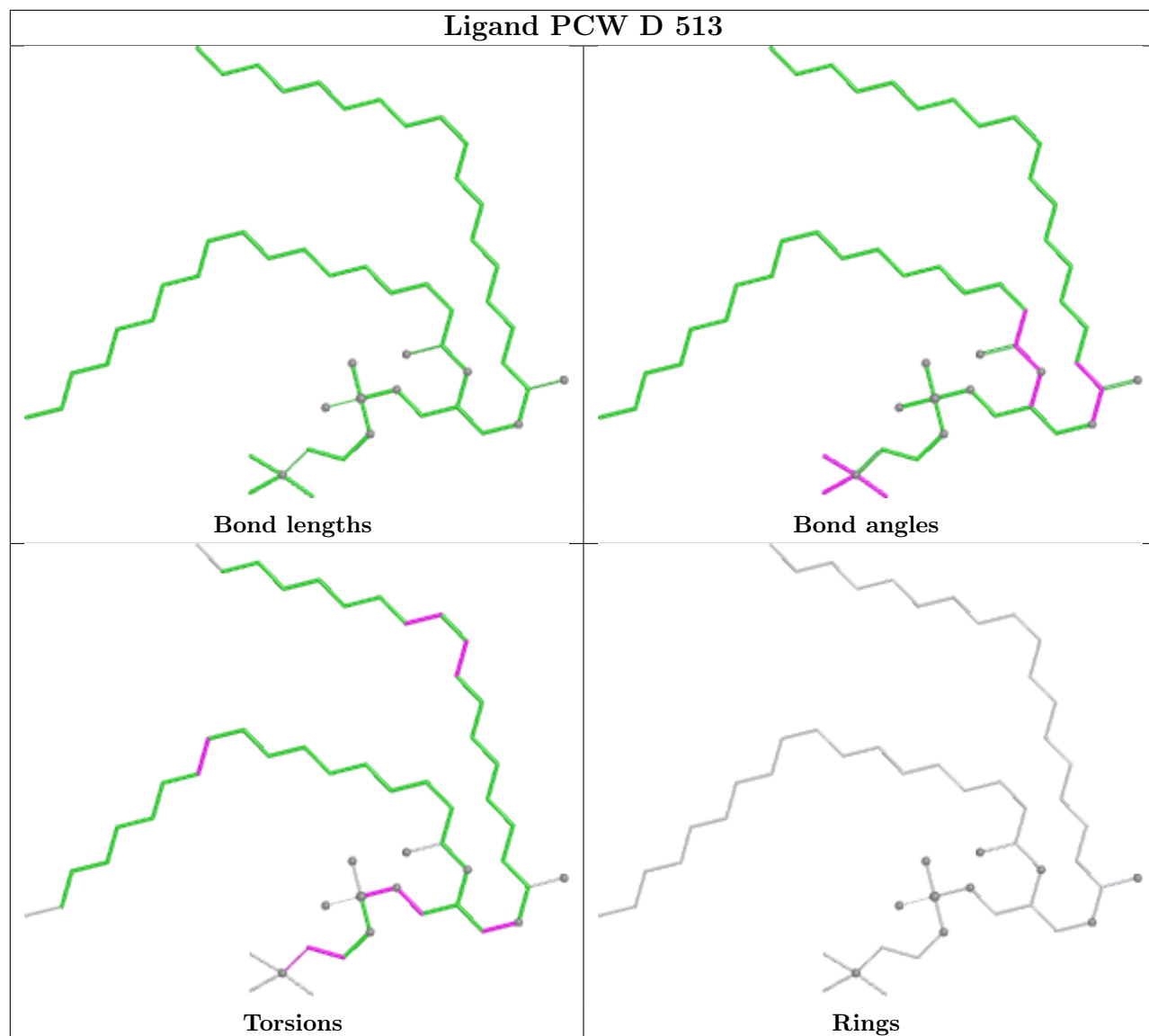


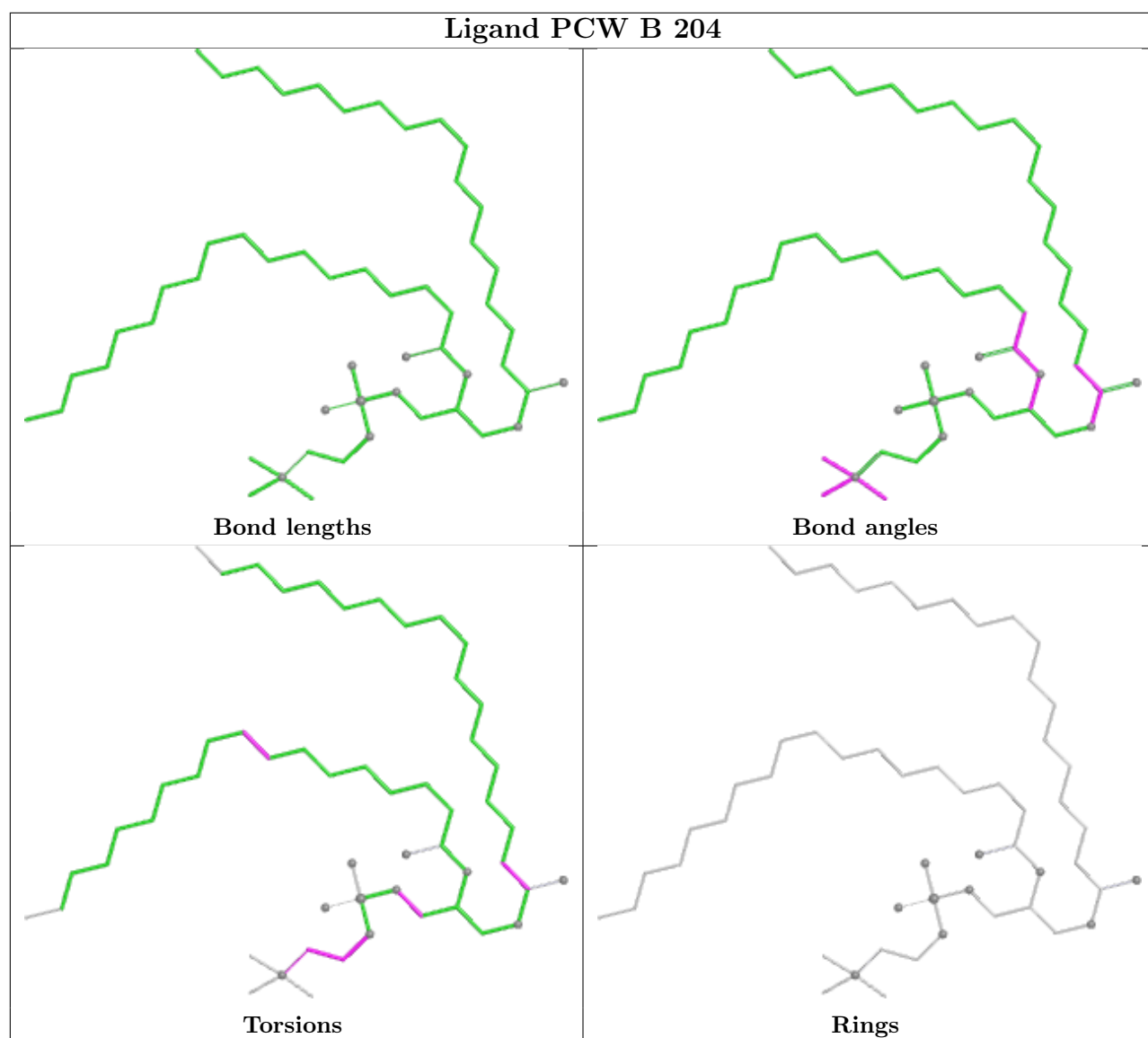


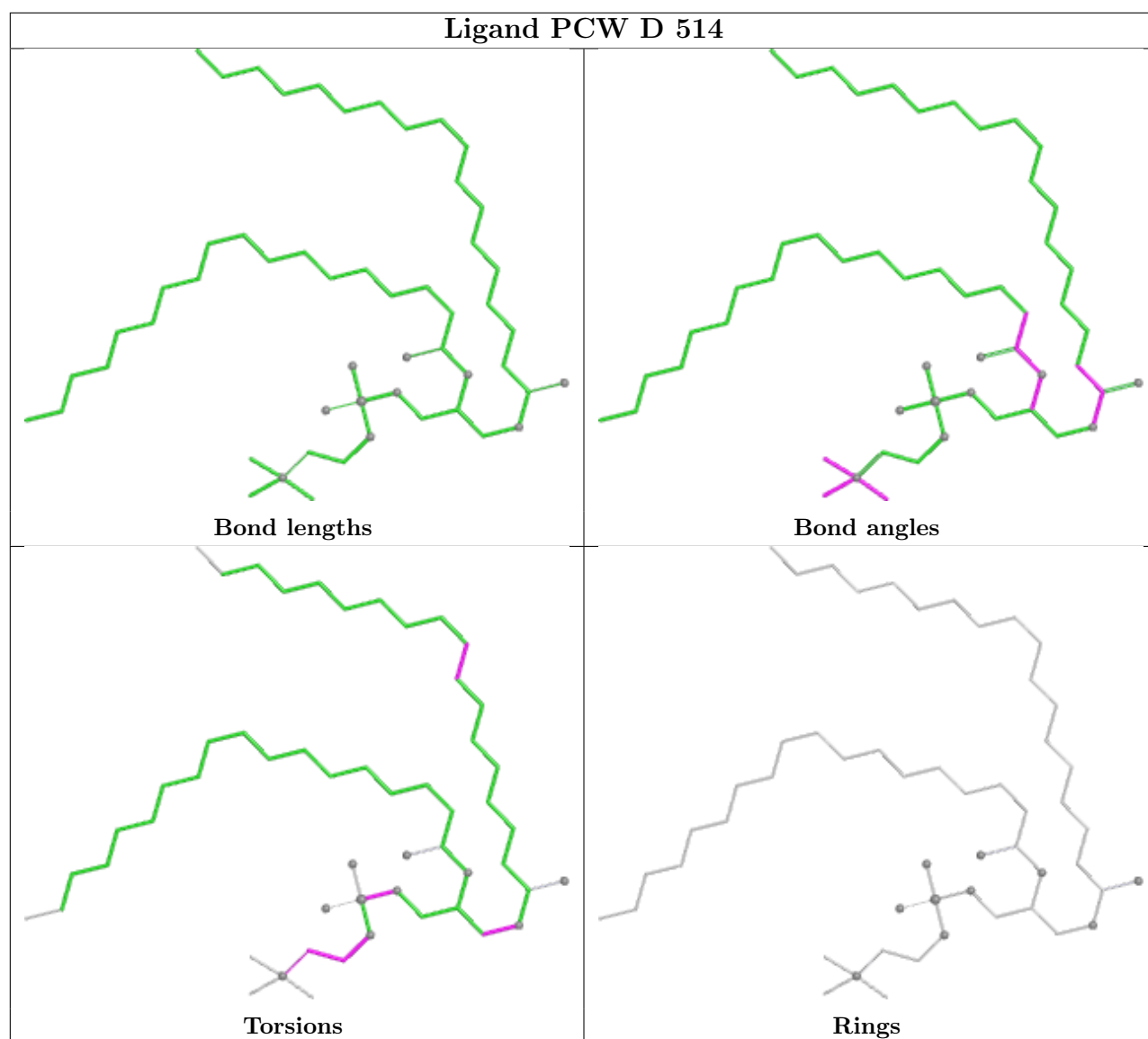




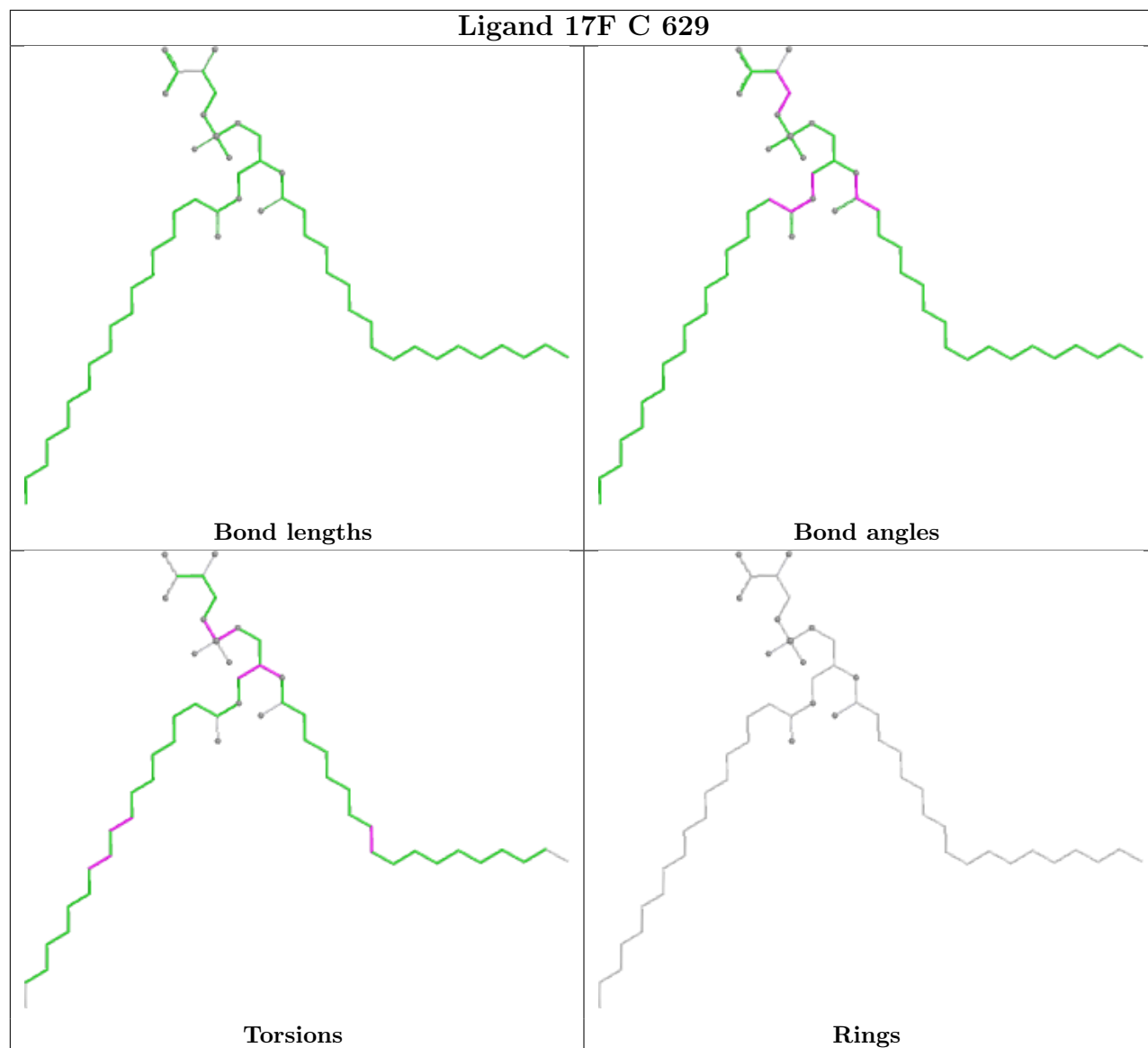


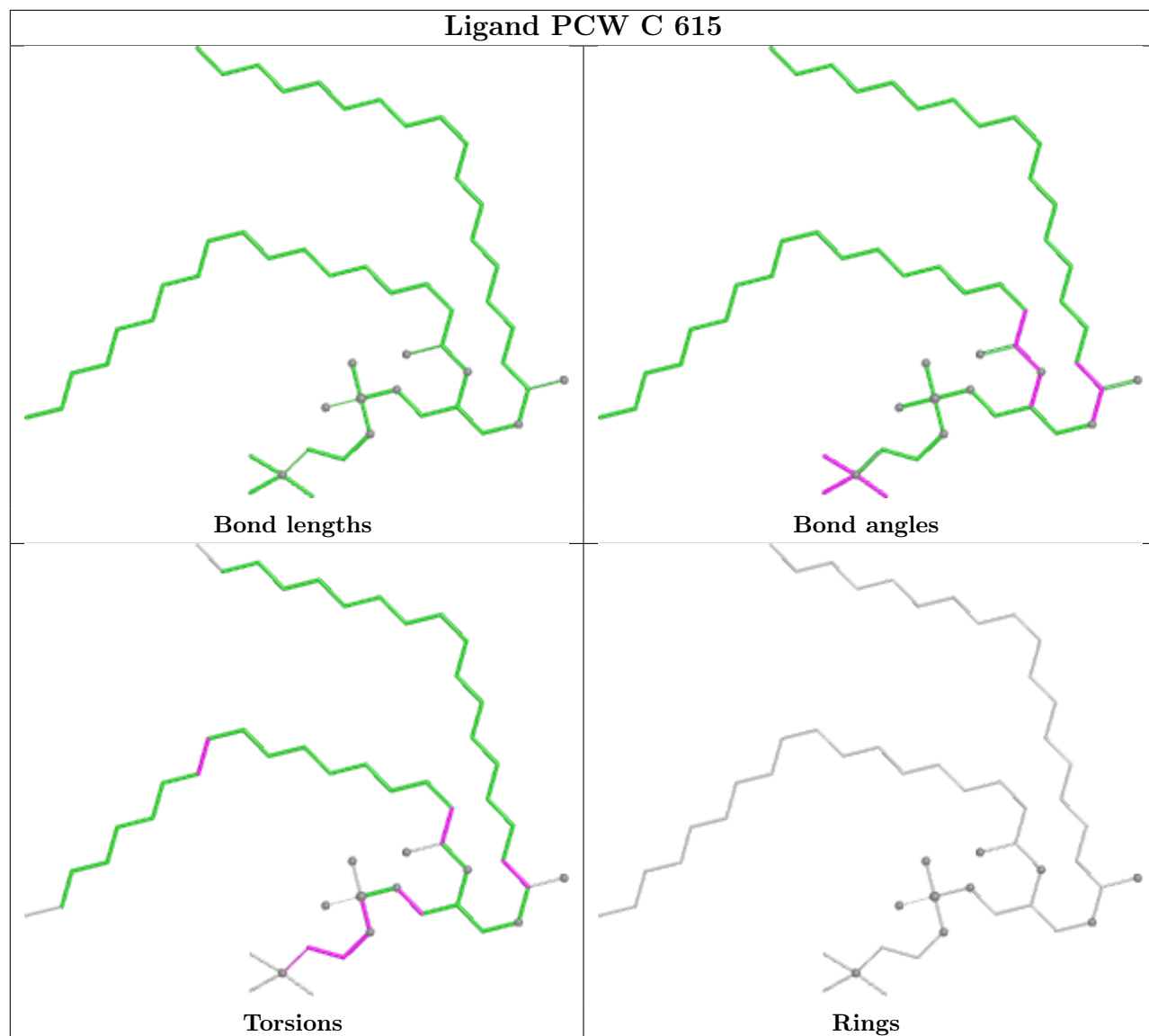


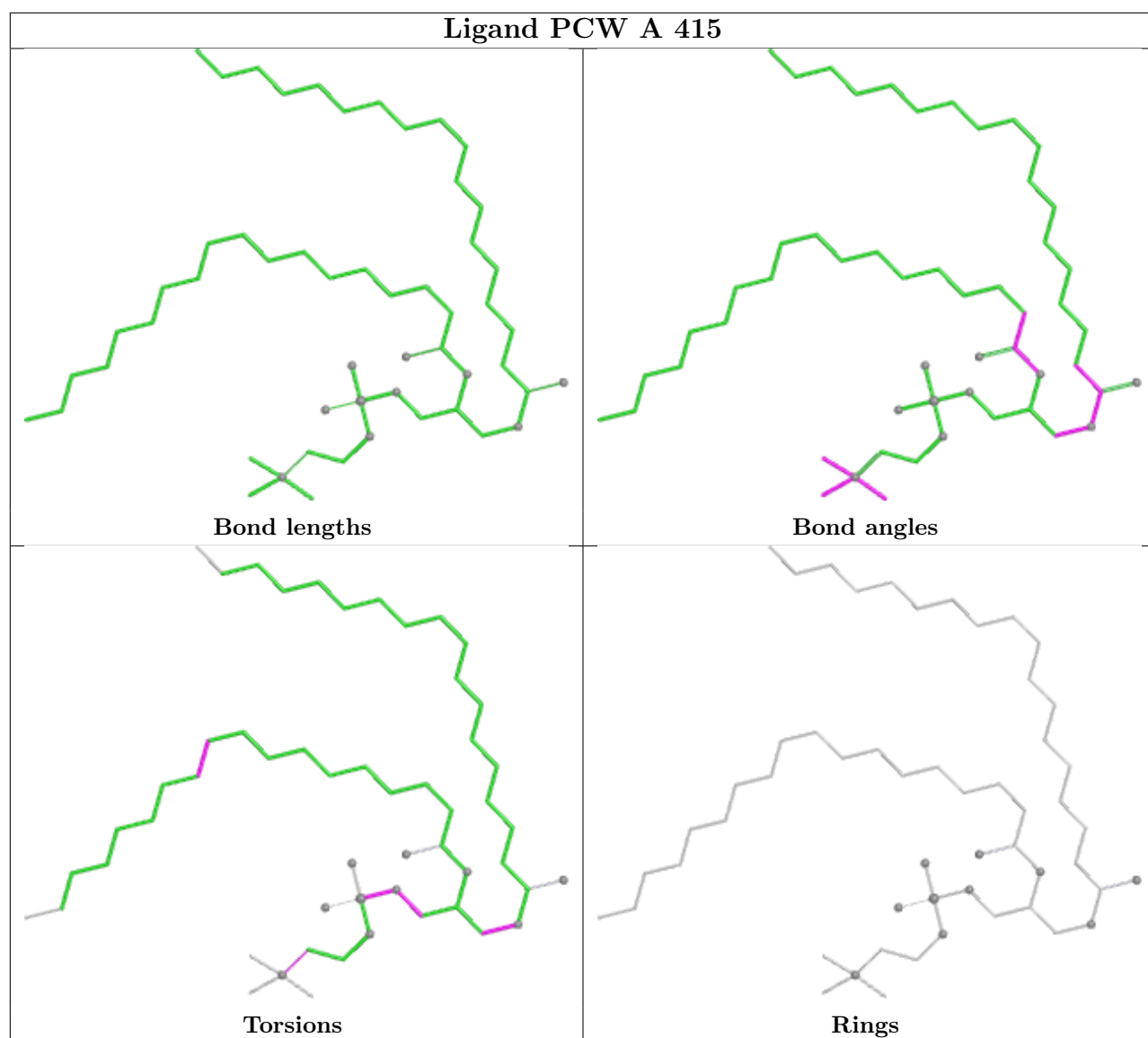


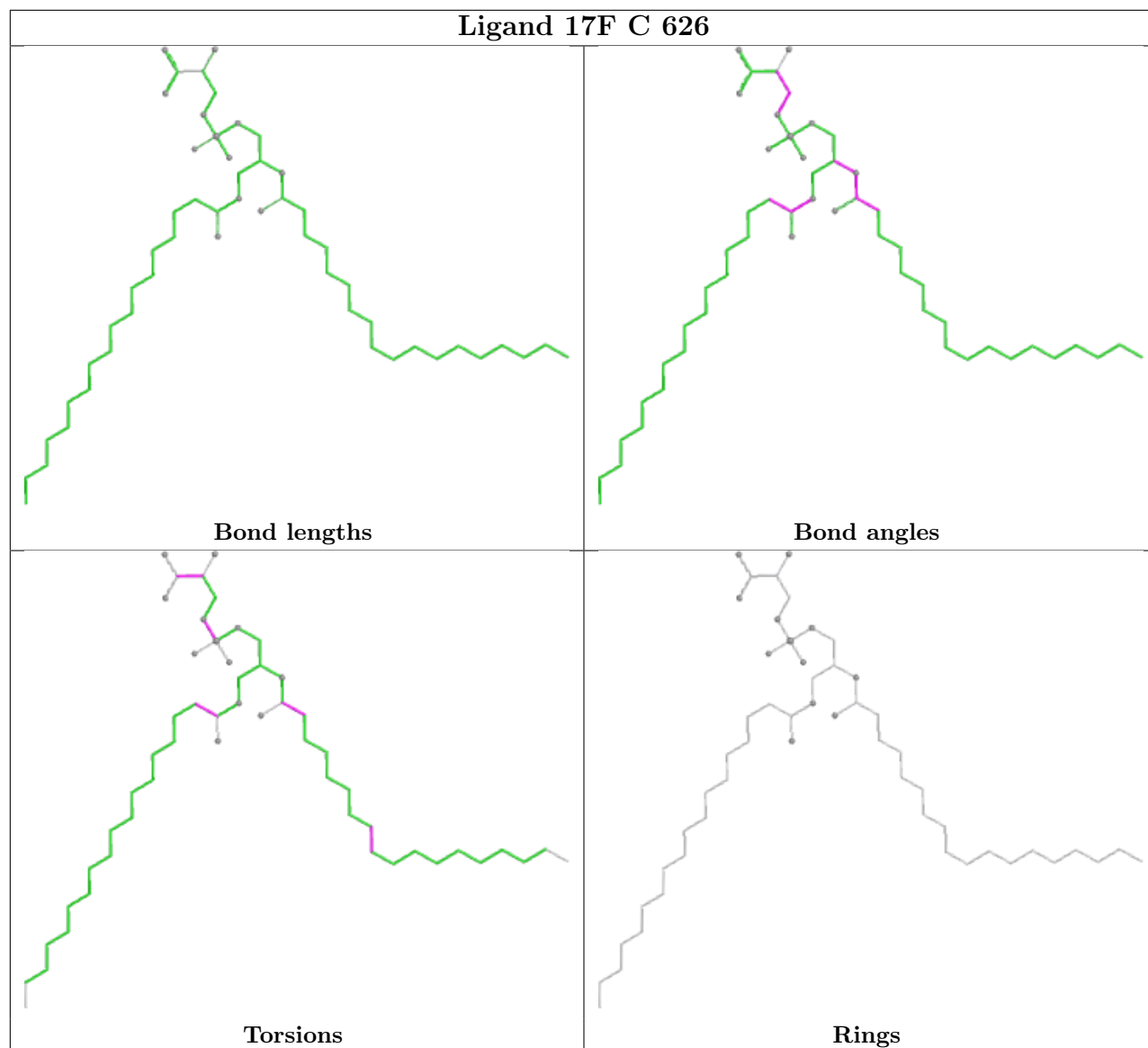


Ligand 17F C 629

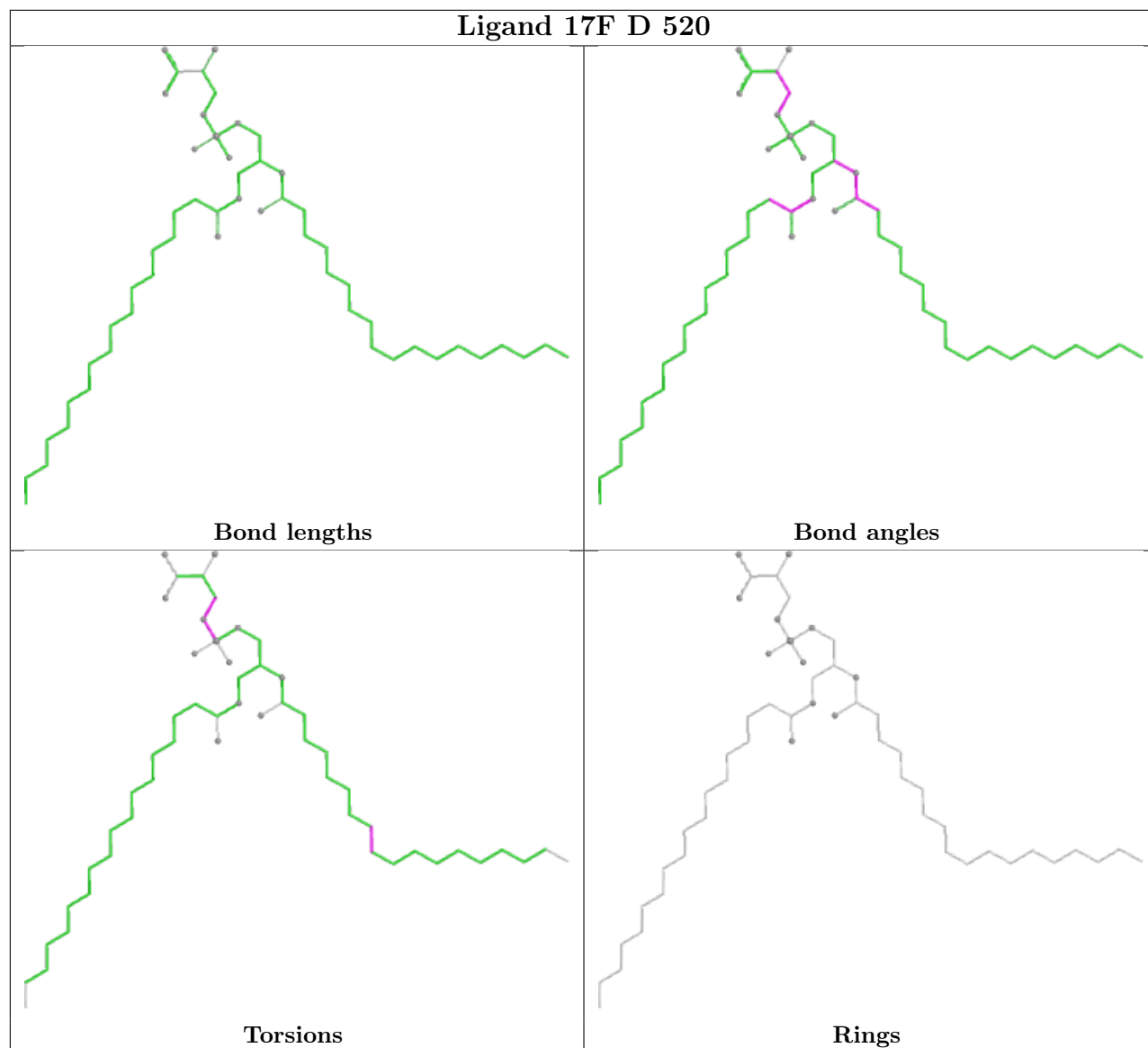




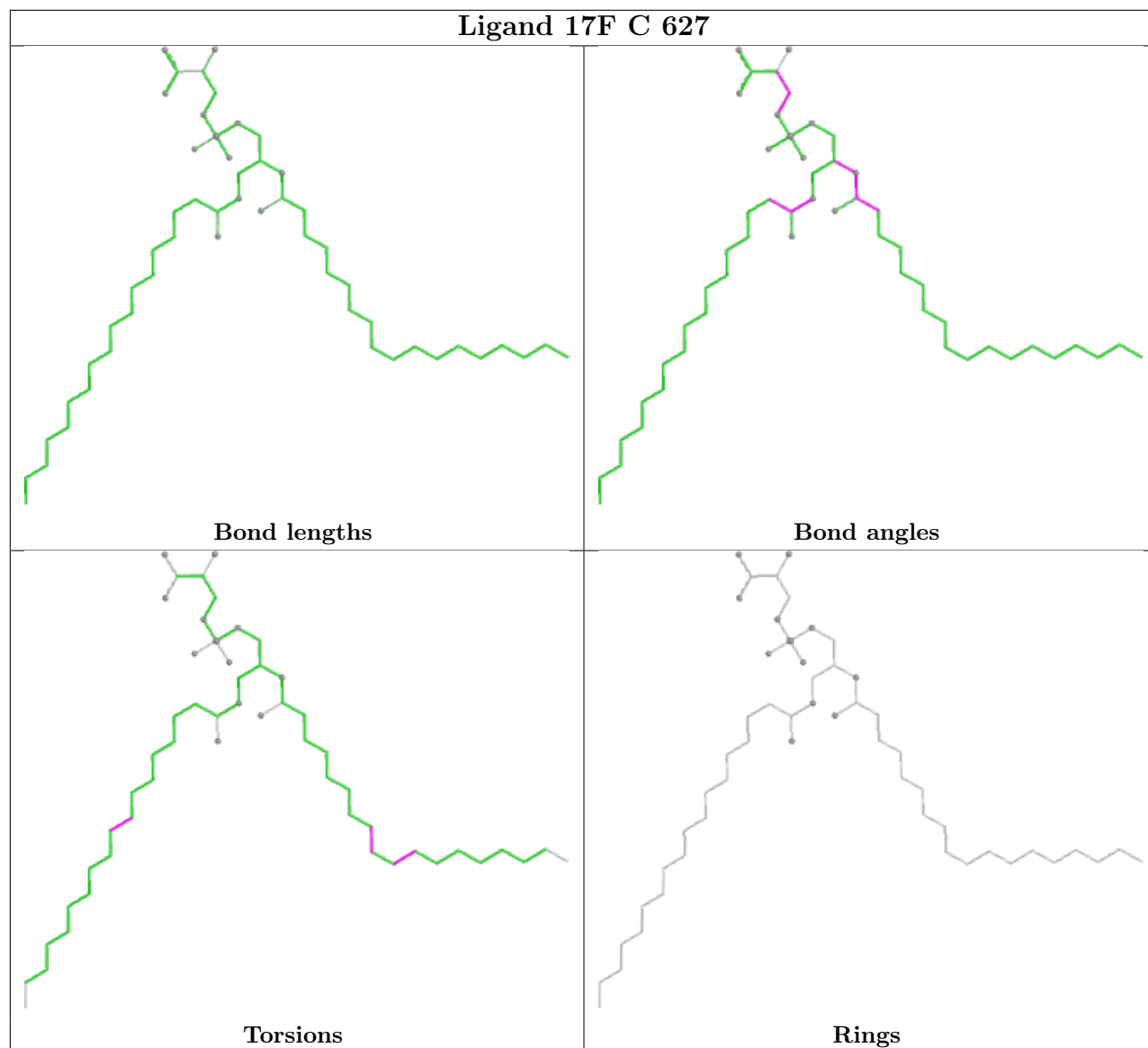


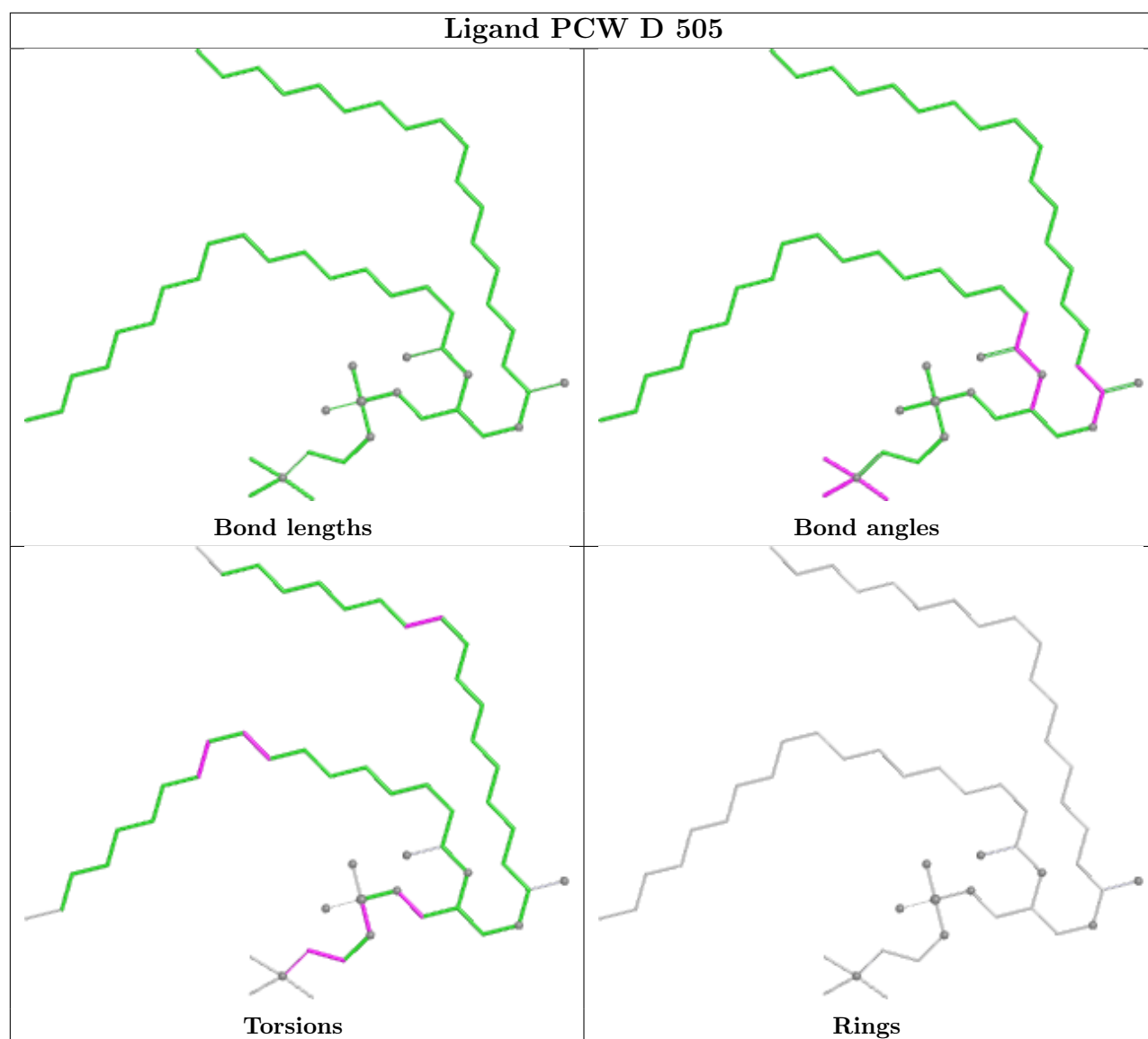


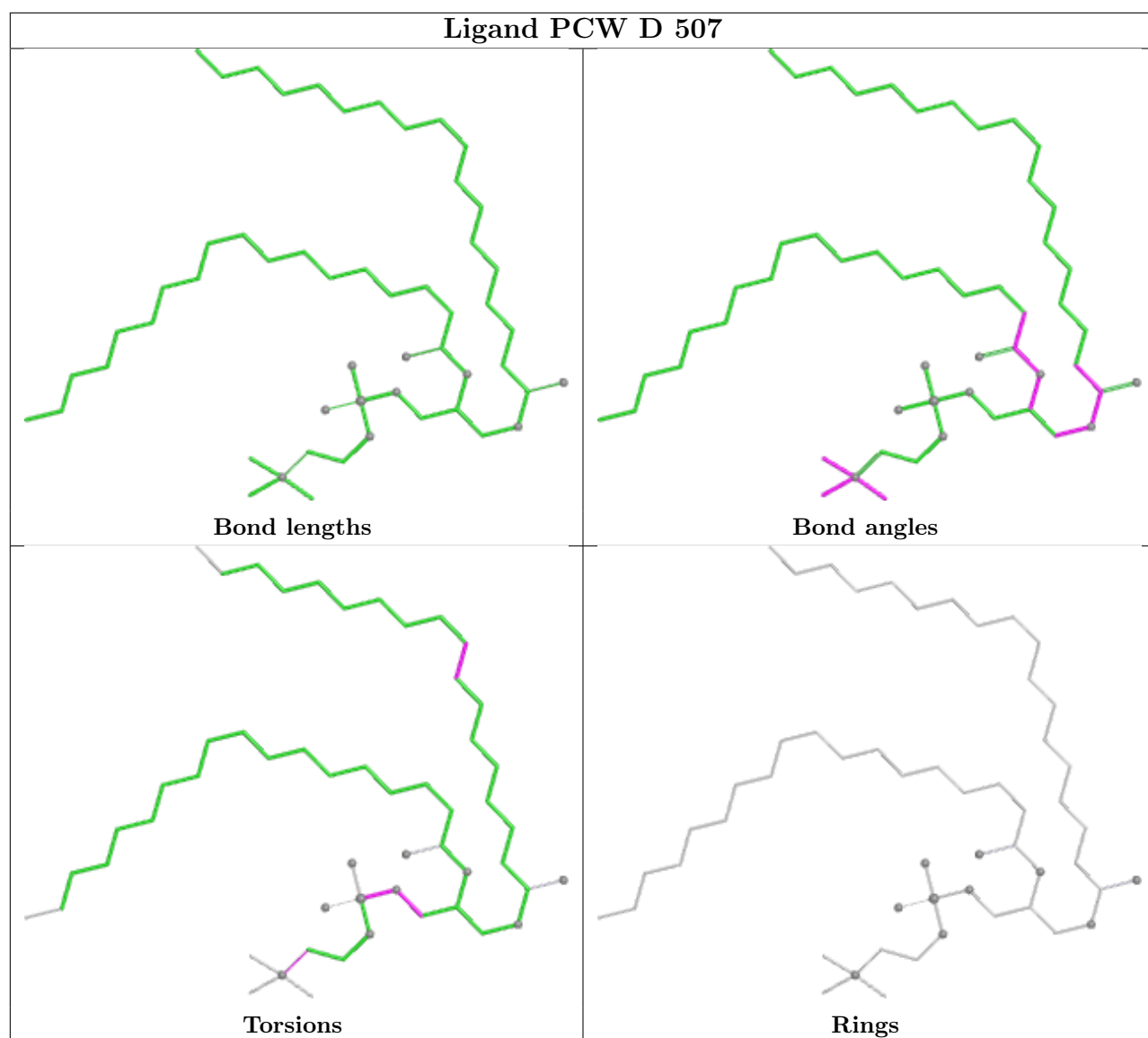
Ligand 17F D 520

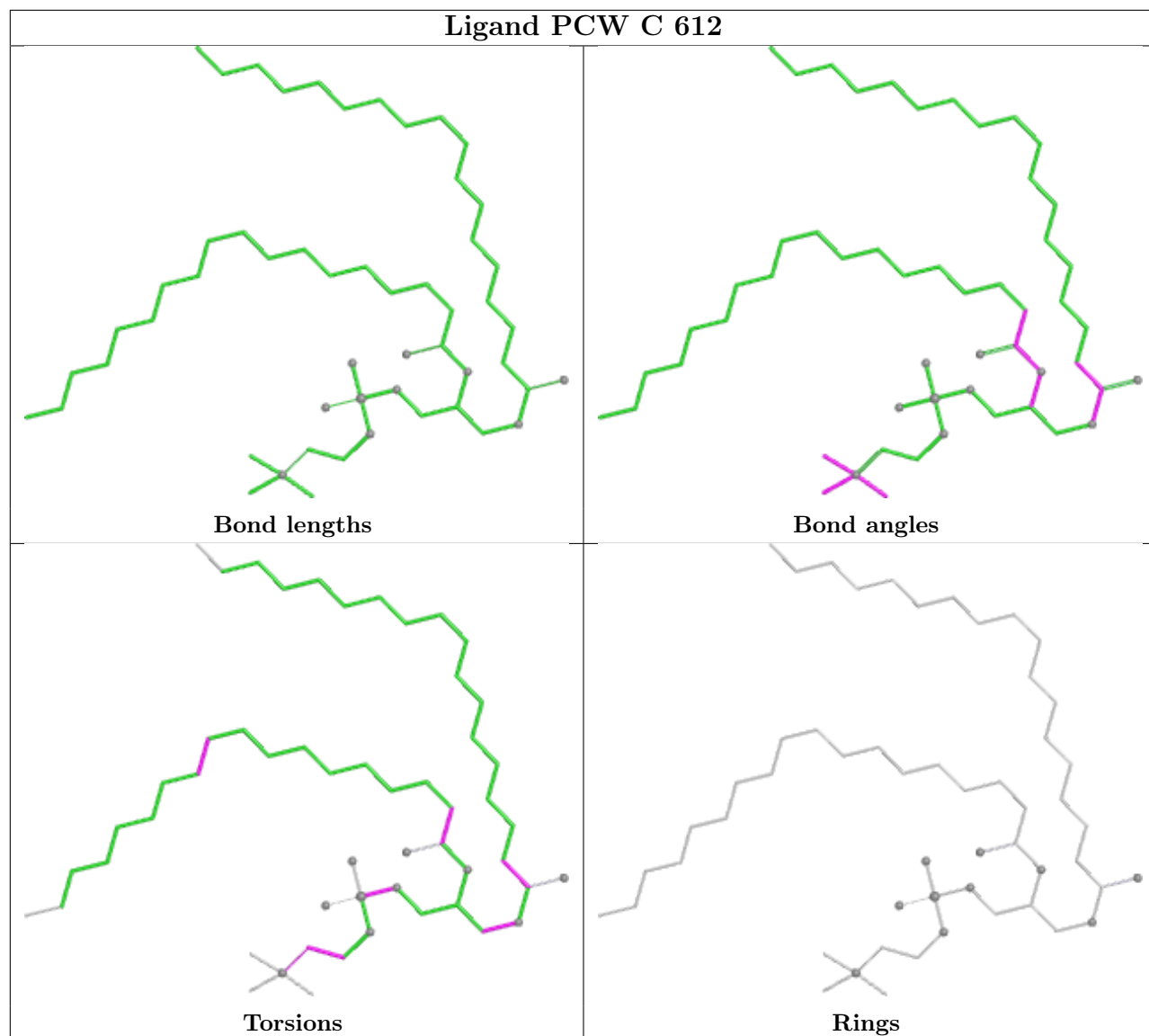


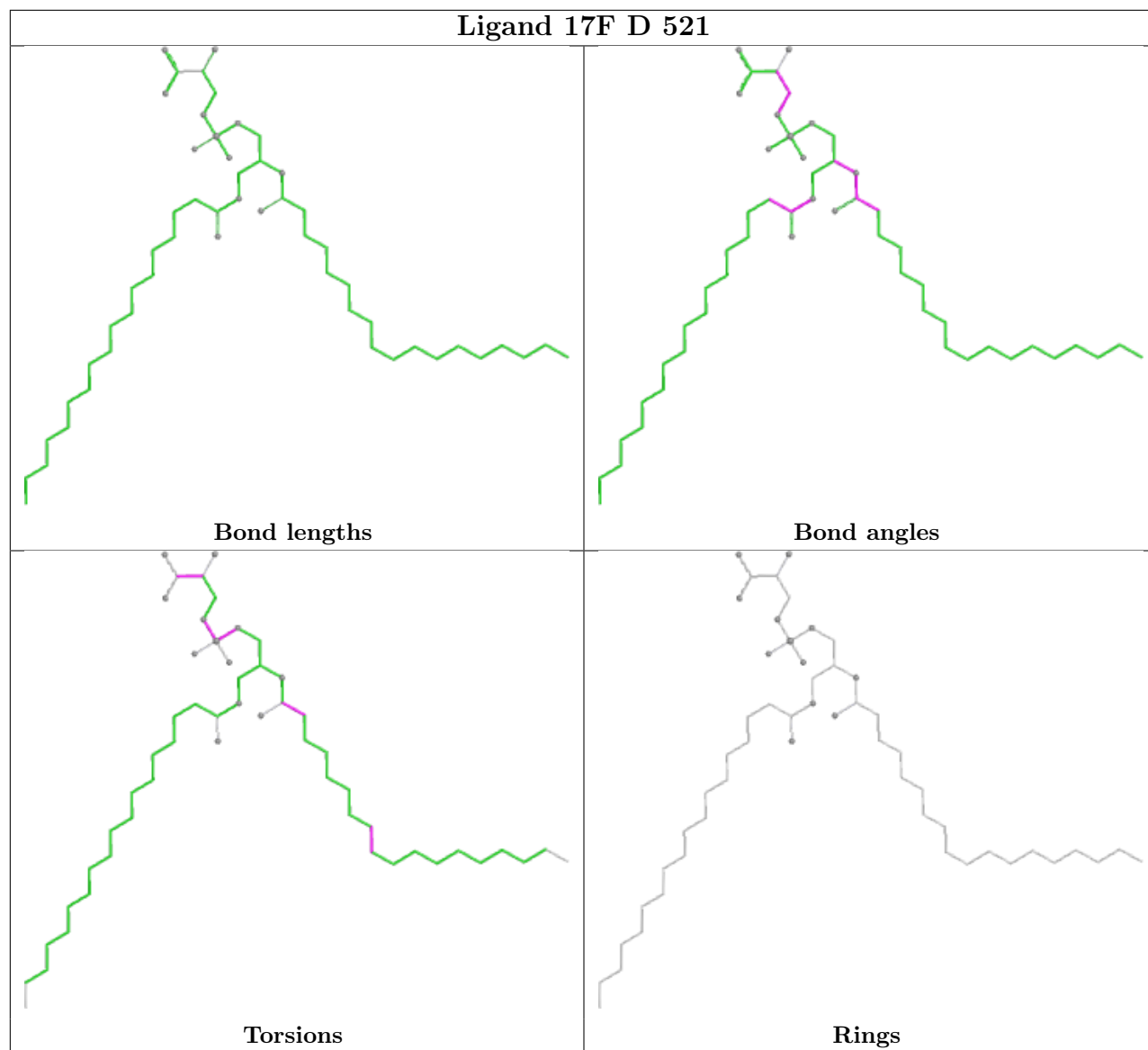
Ligand 17F C 627

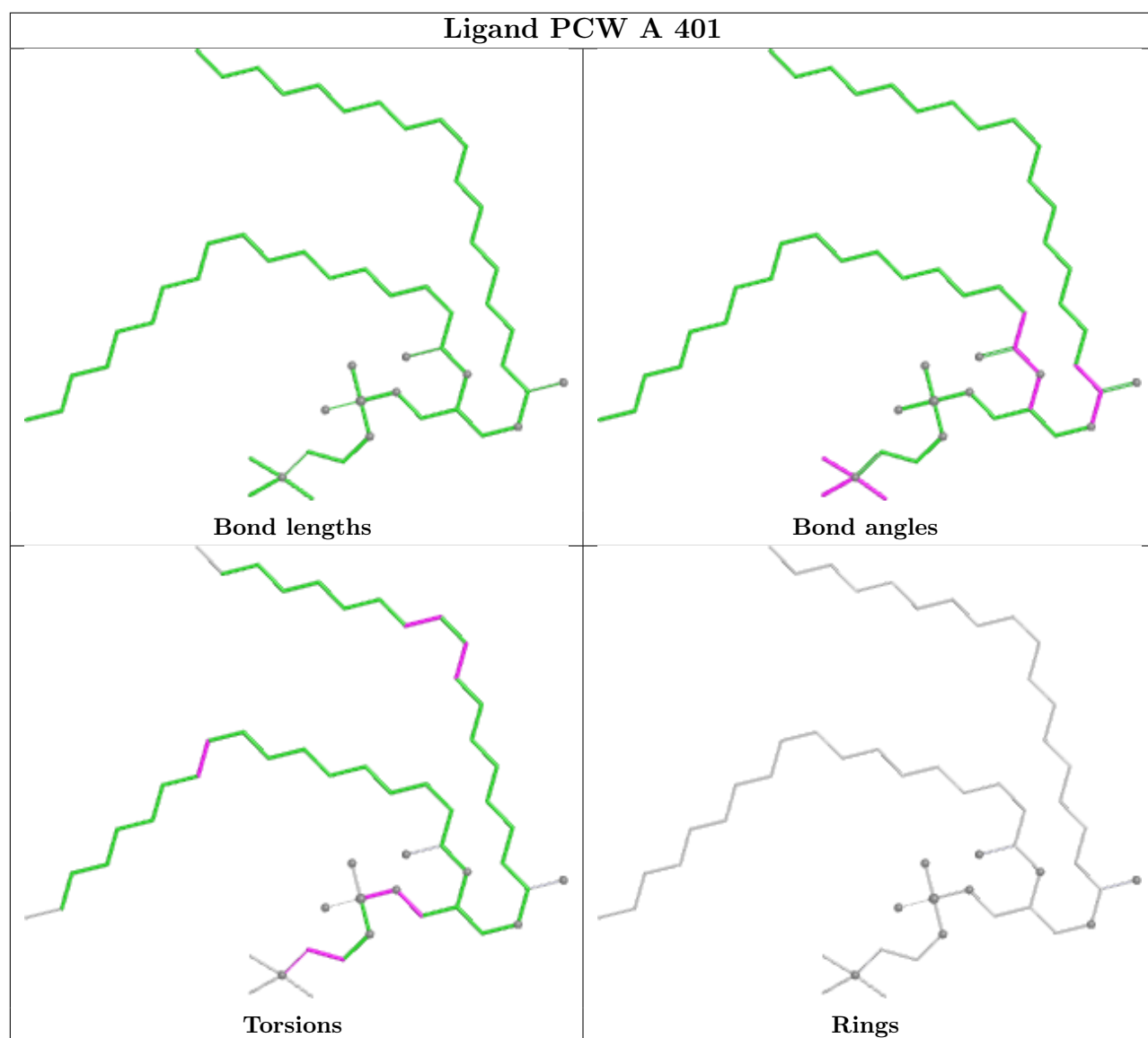


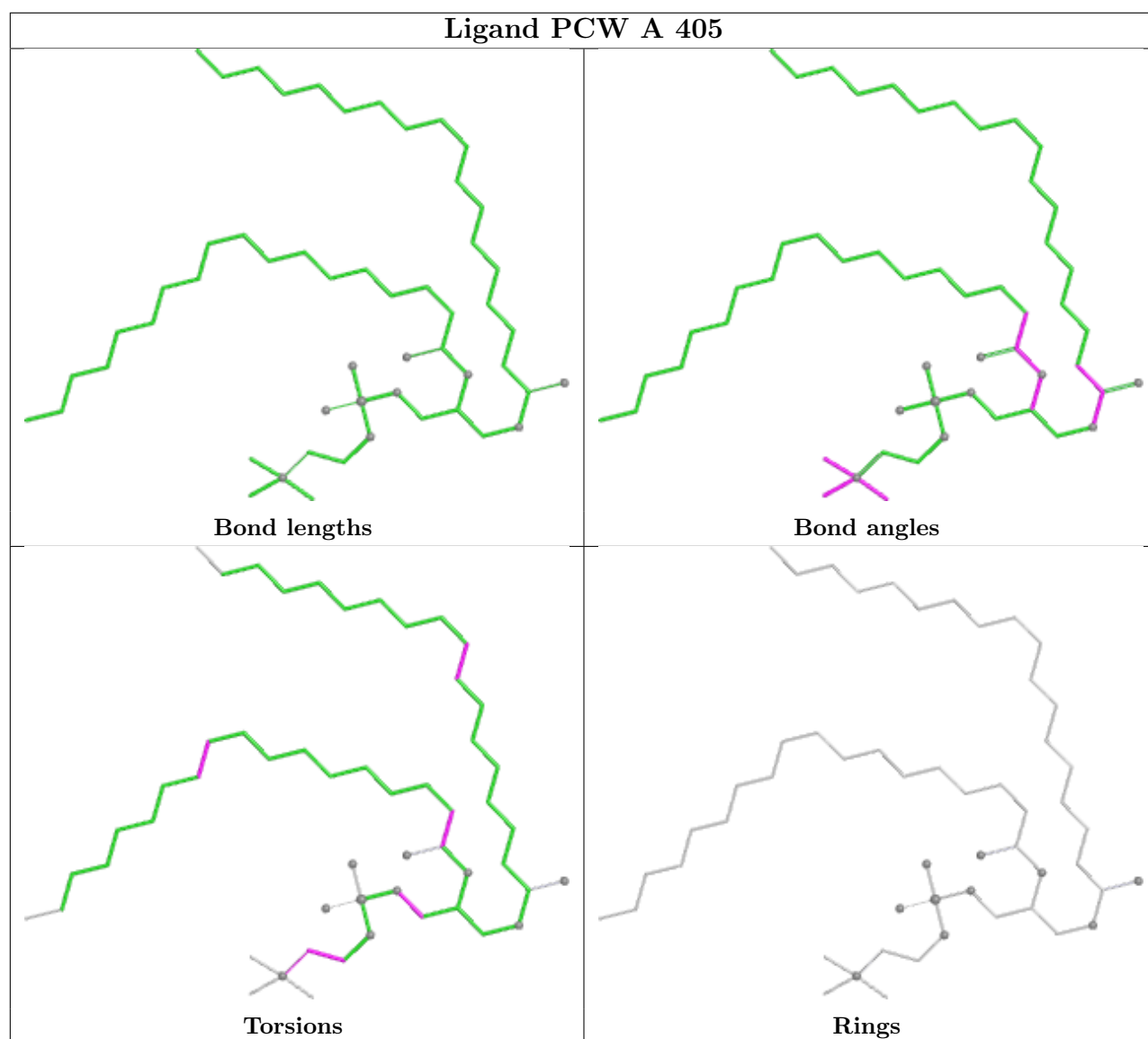


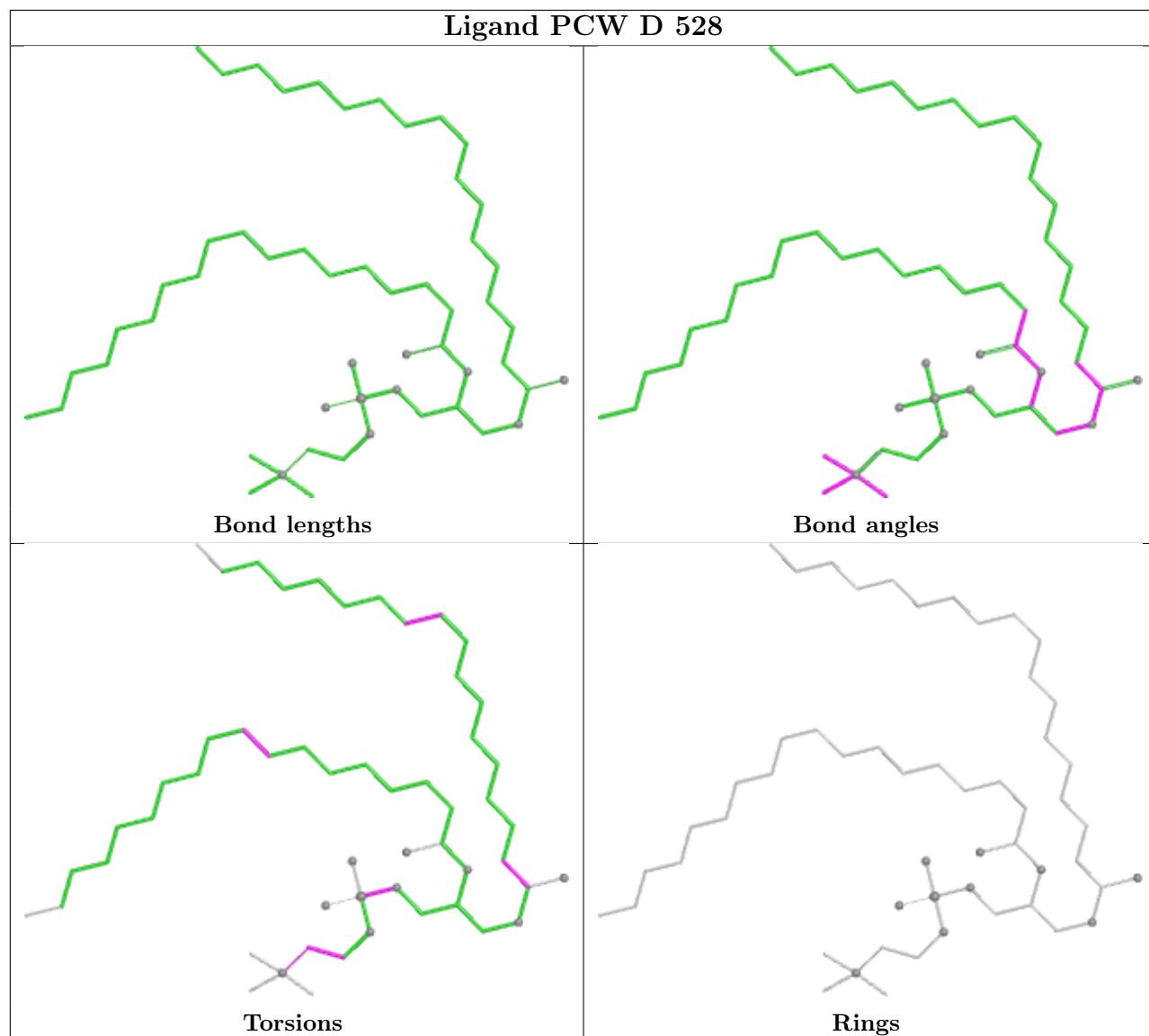


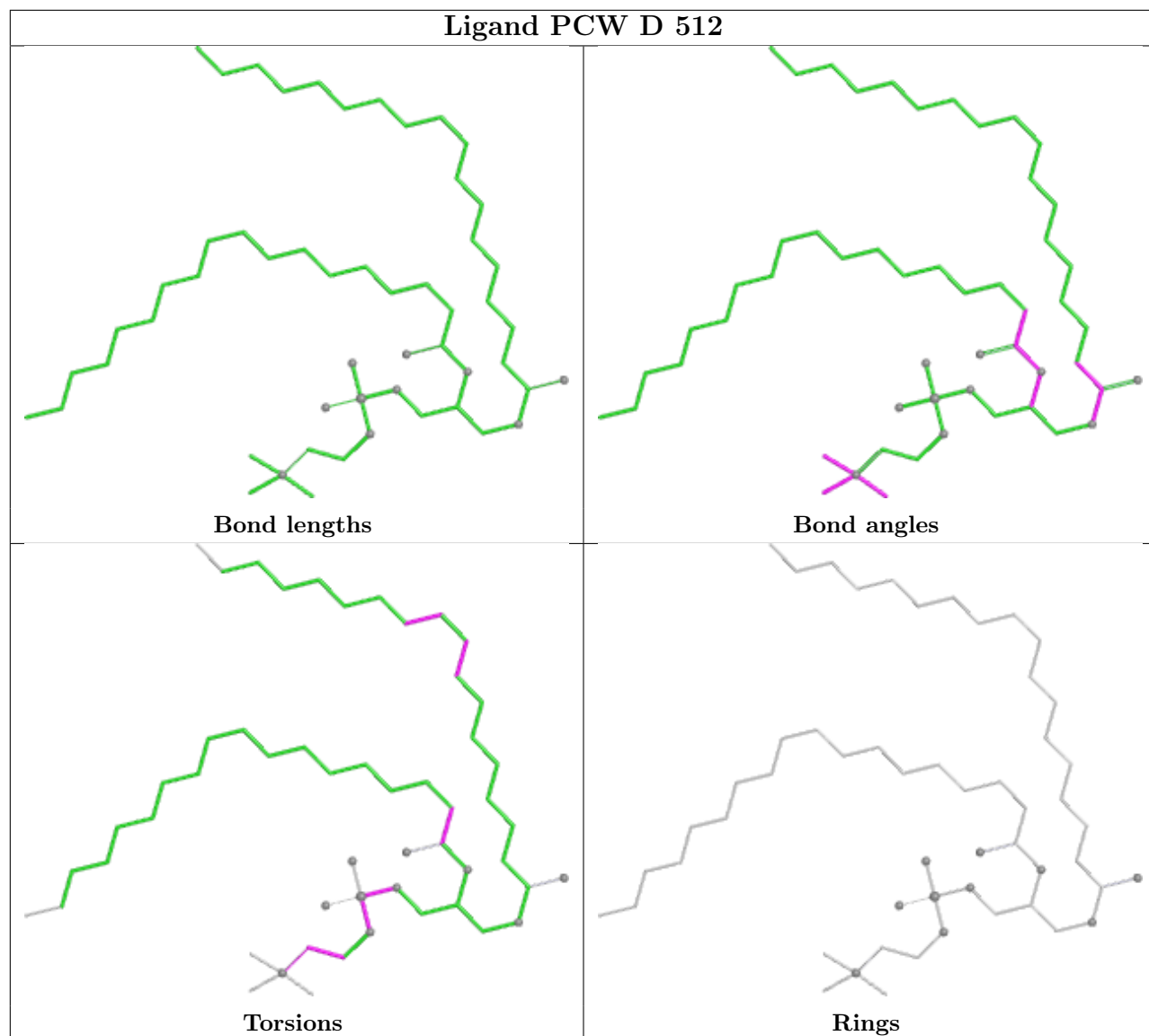


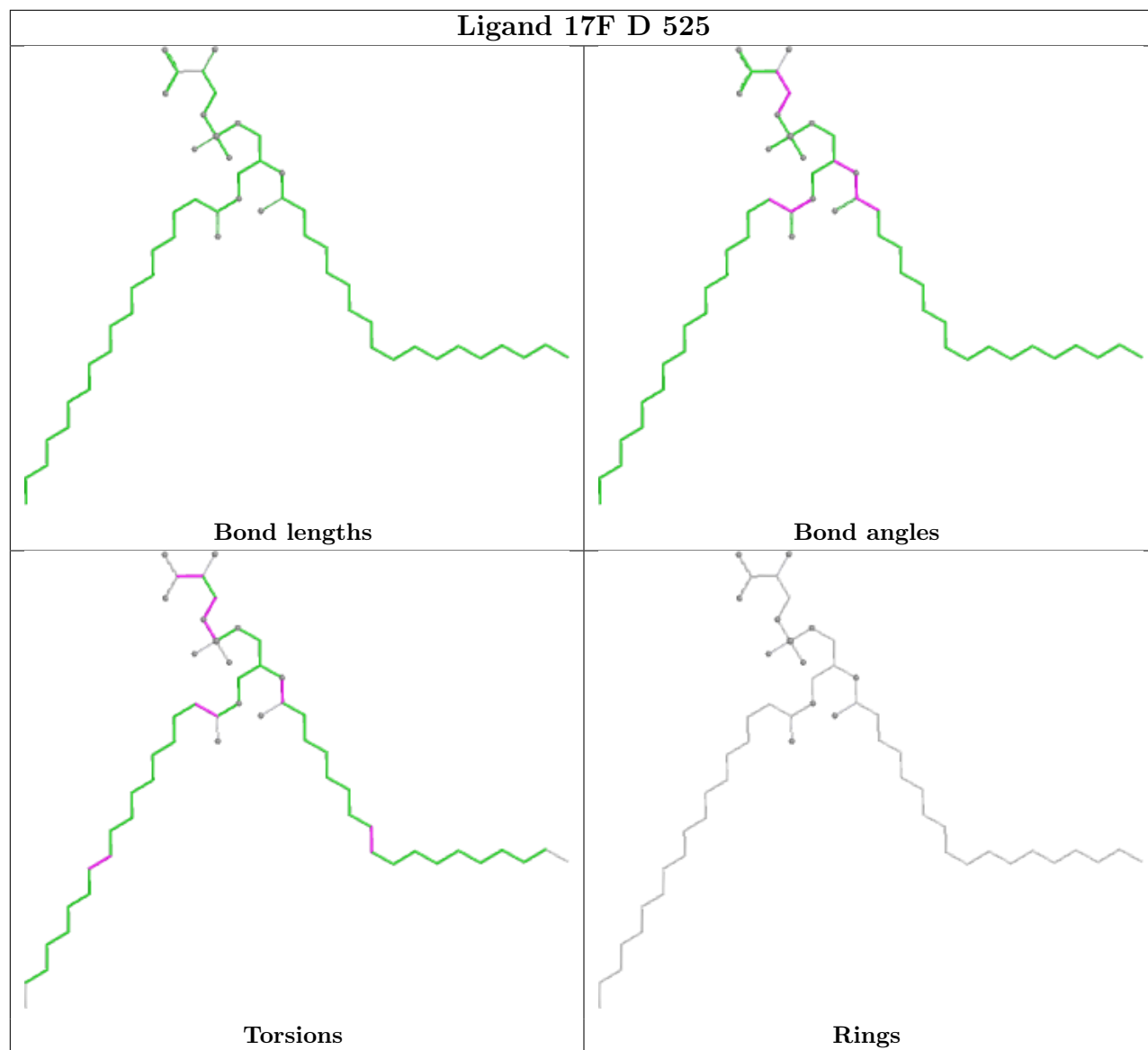


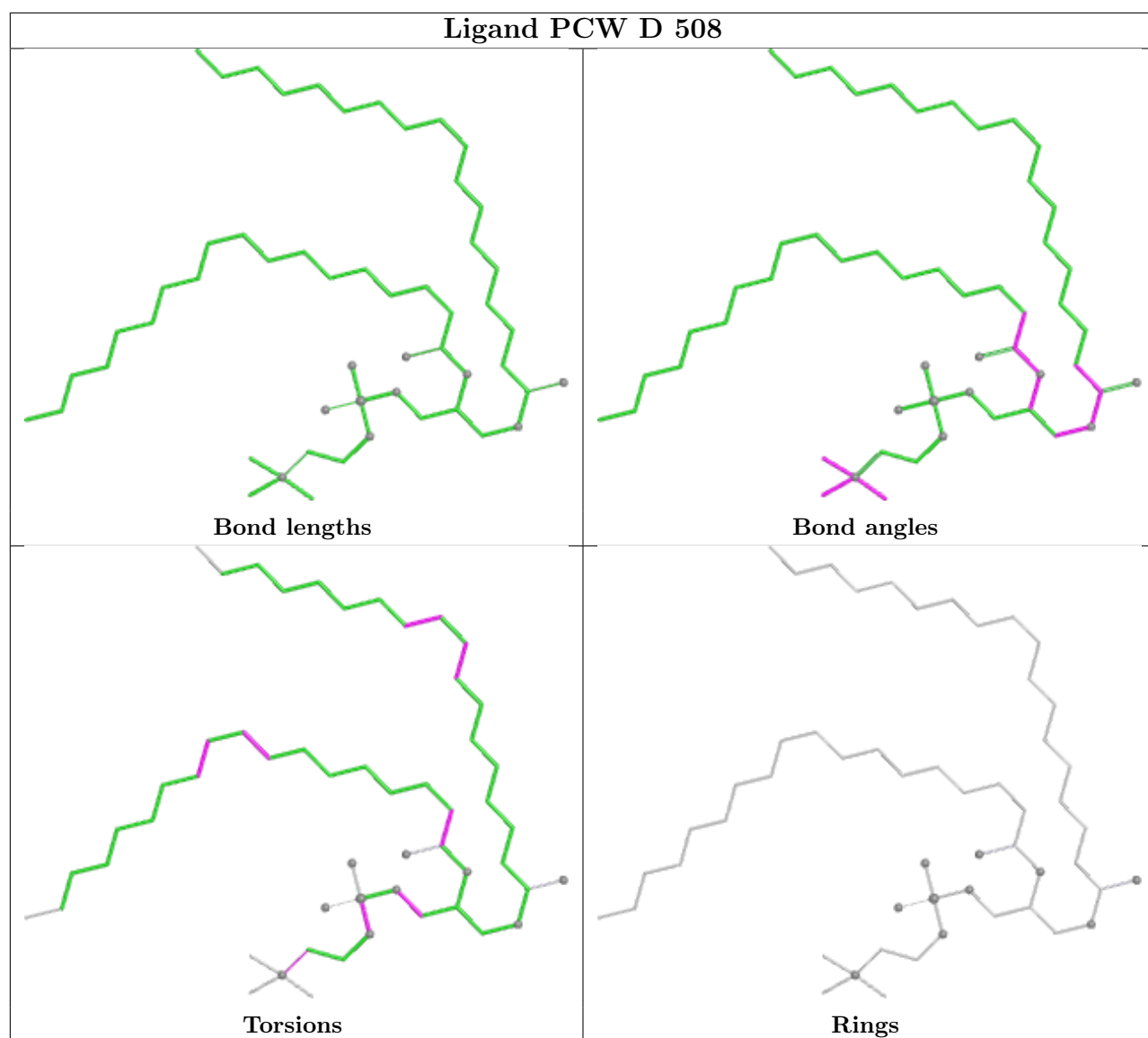


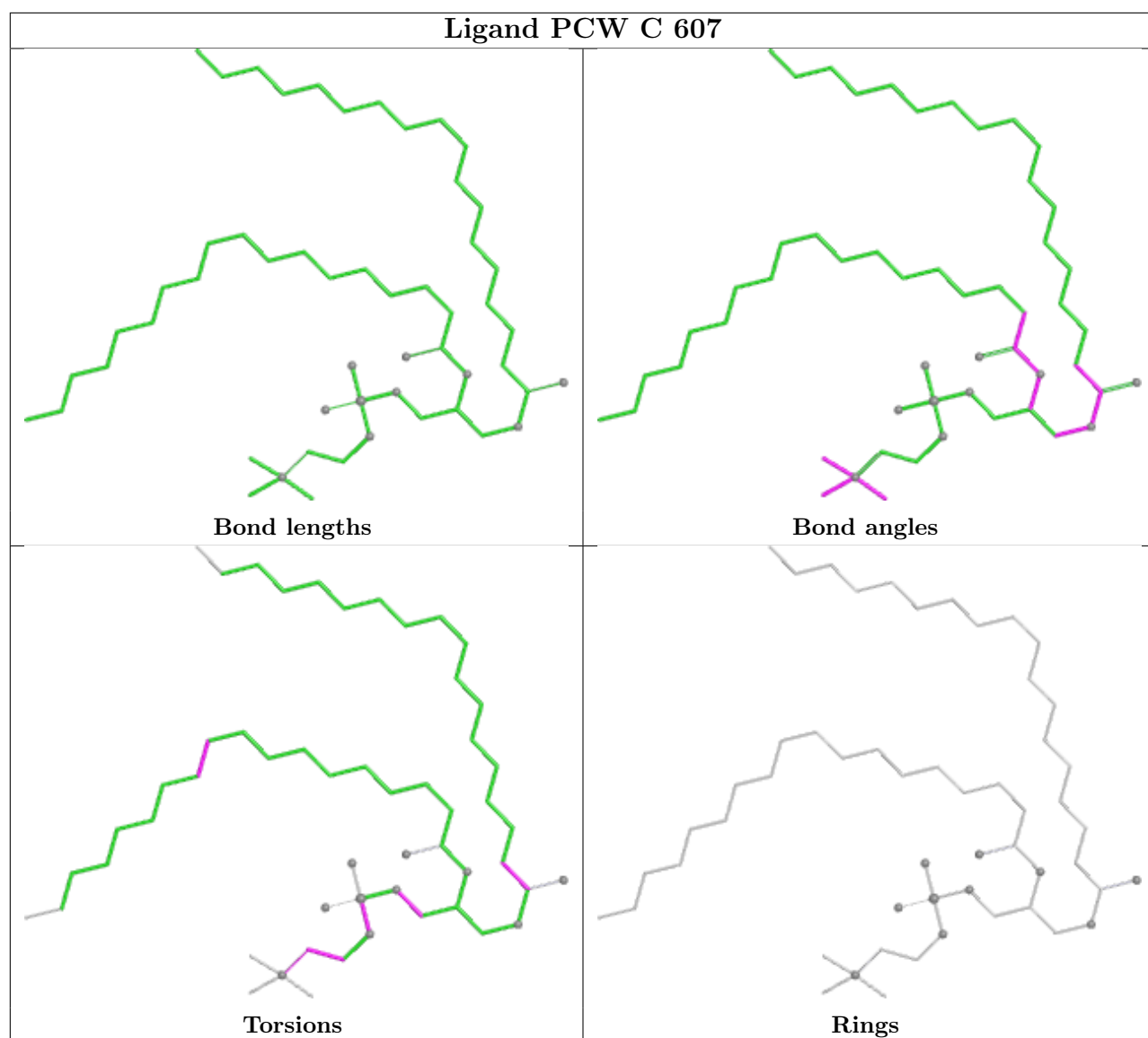


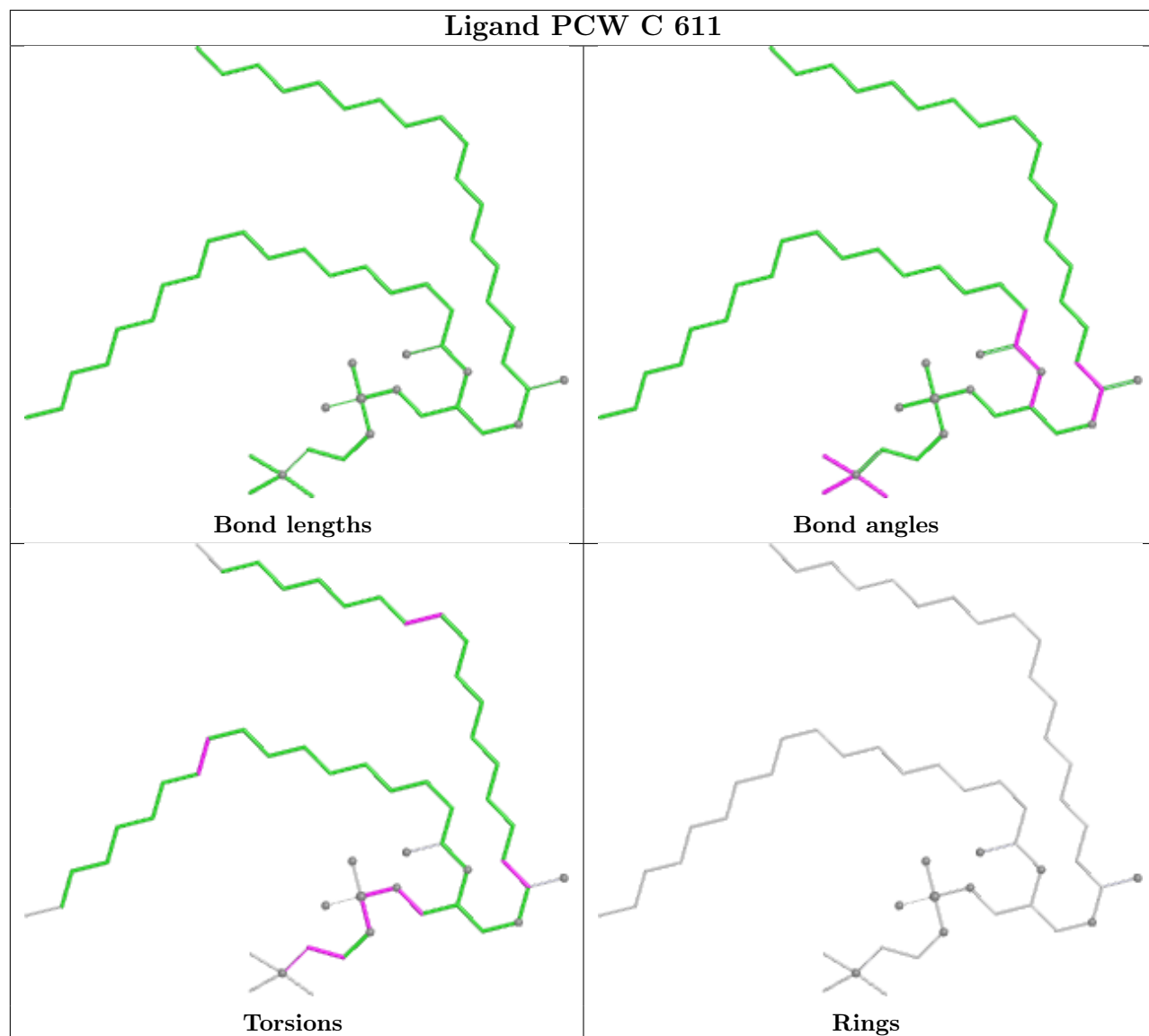


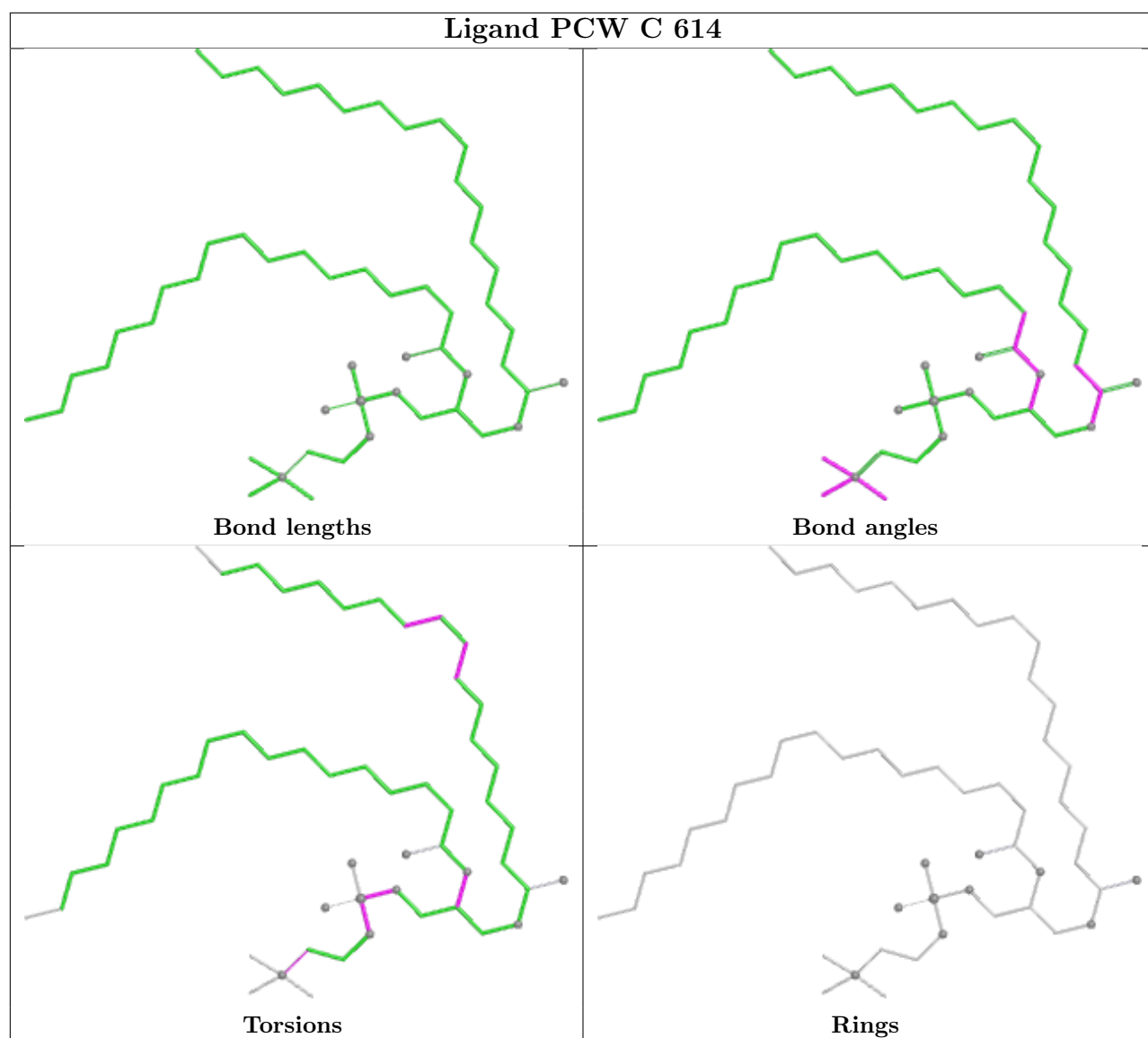


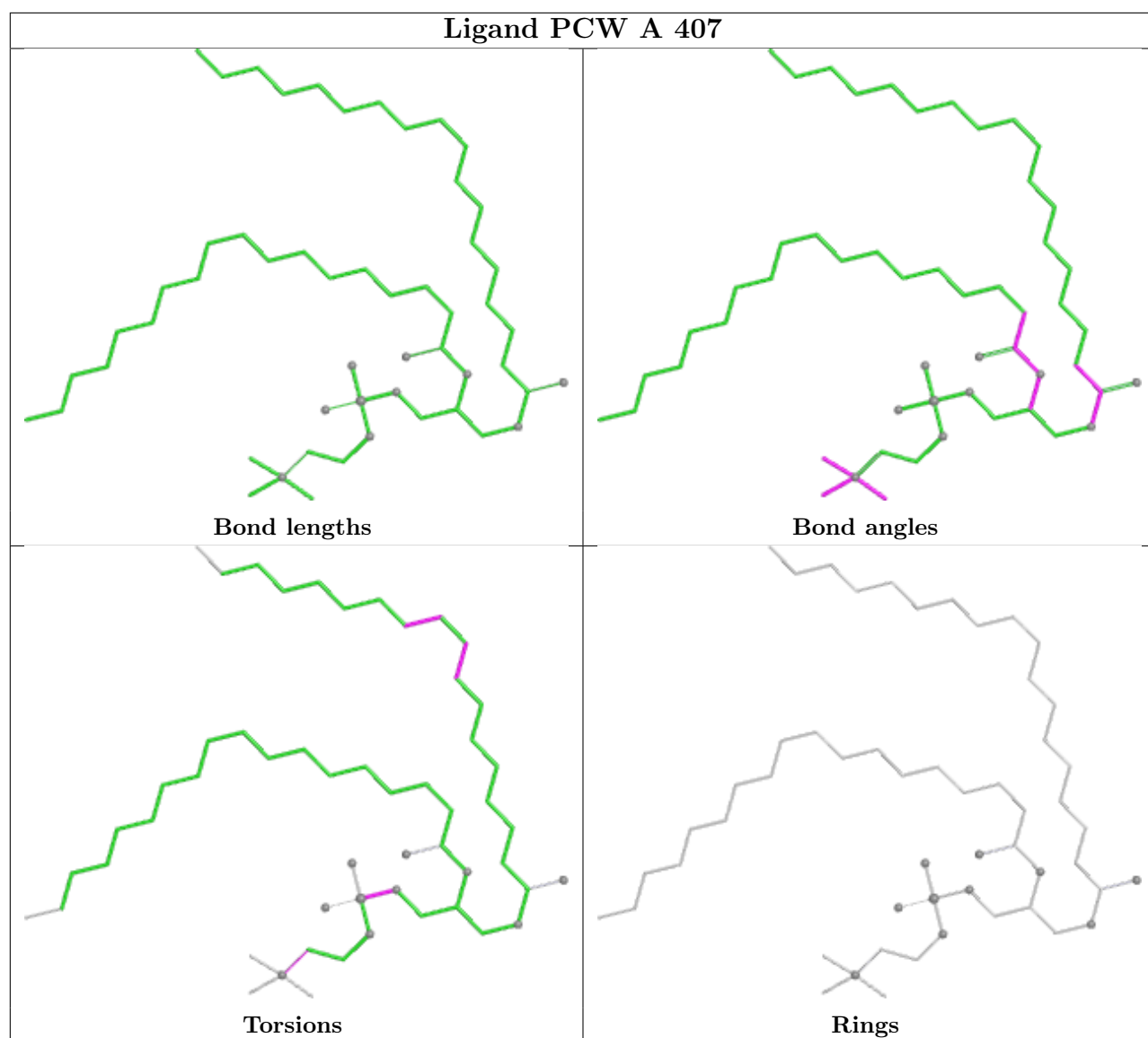


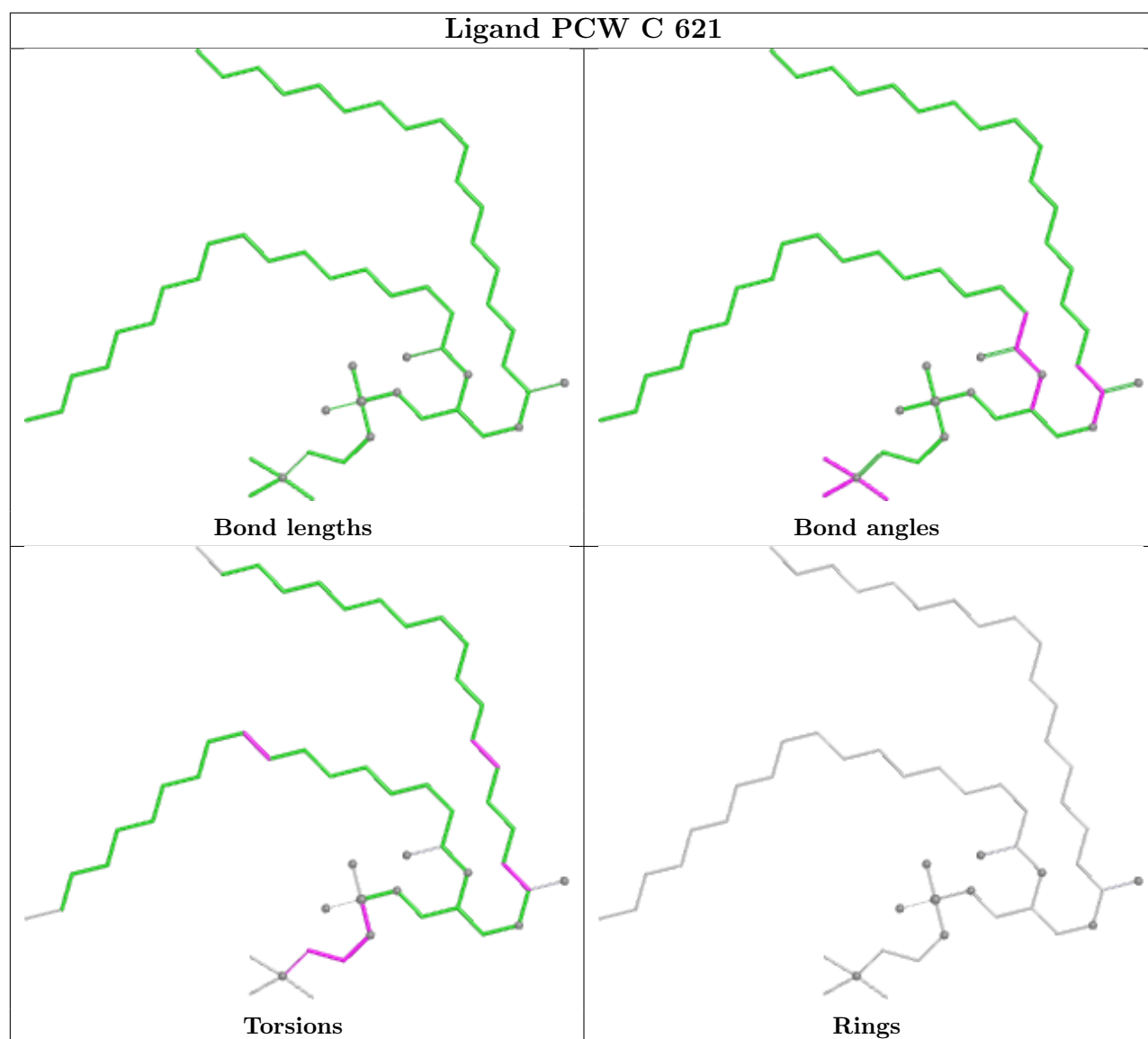


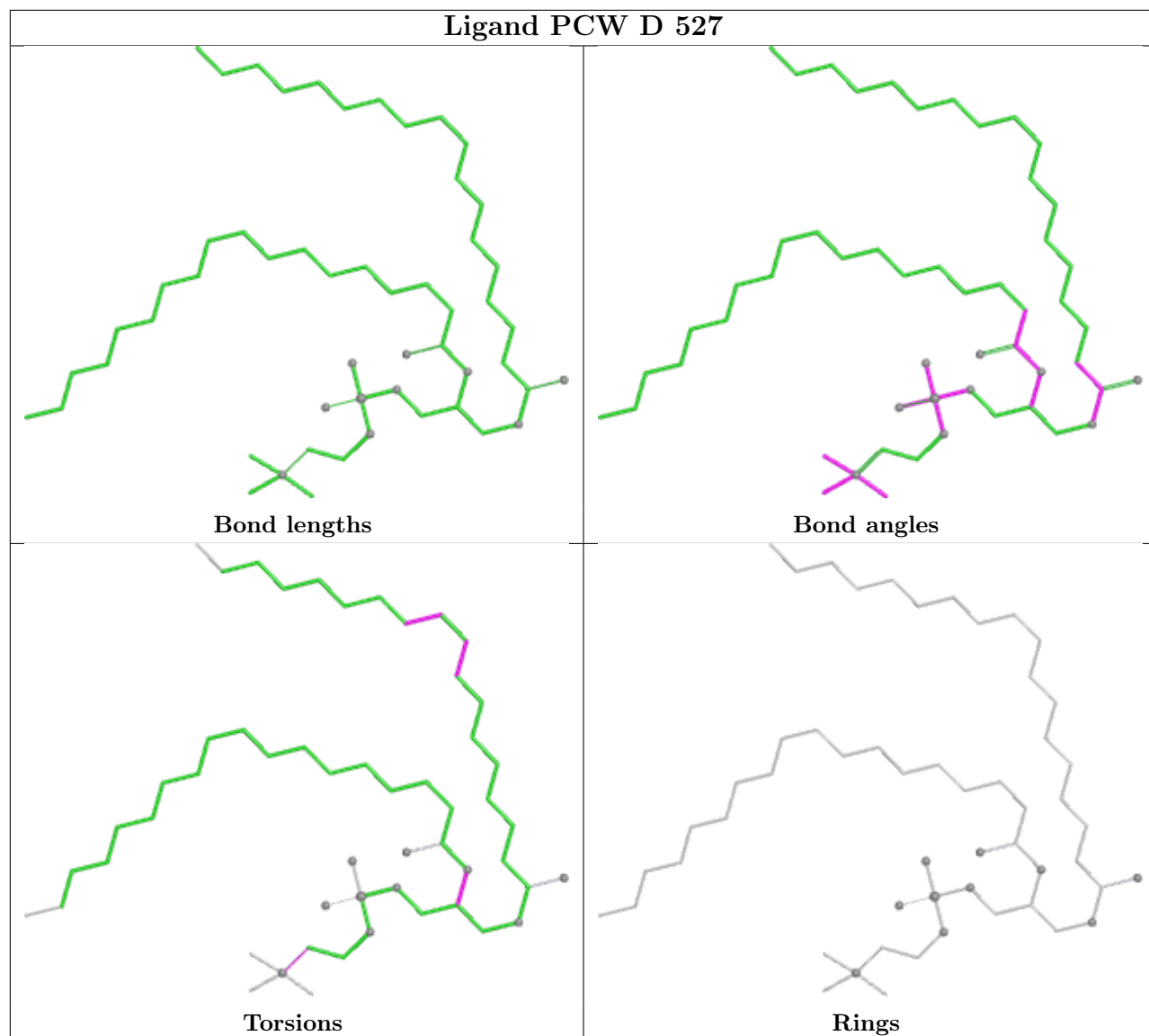


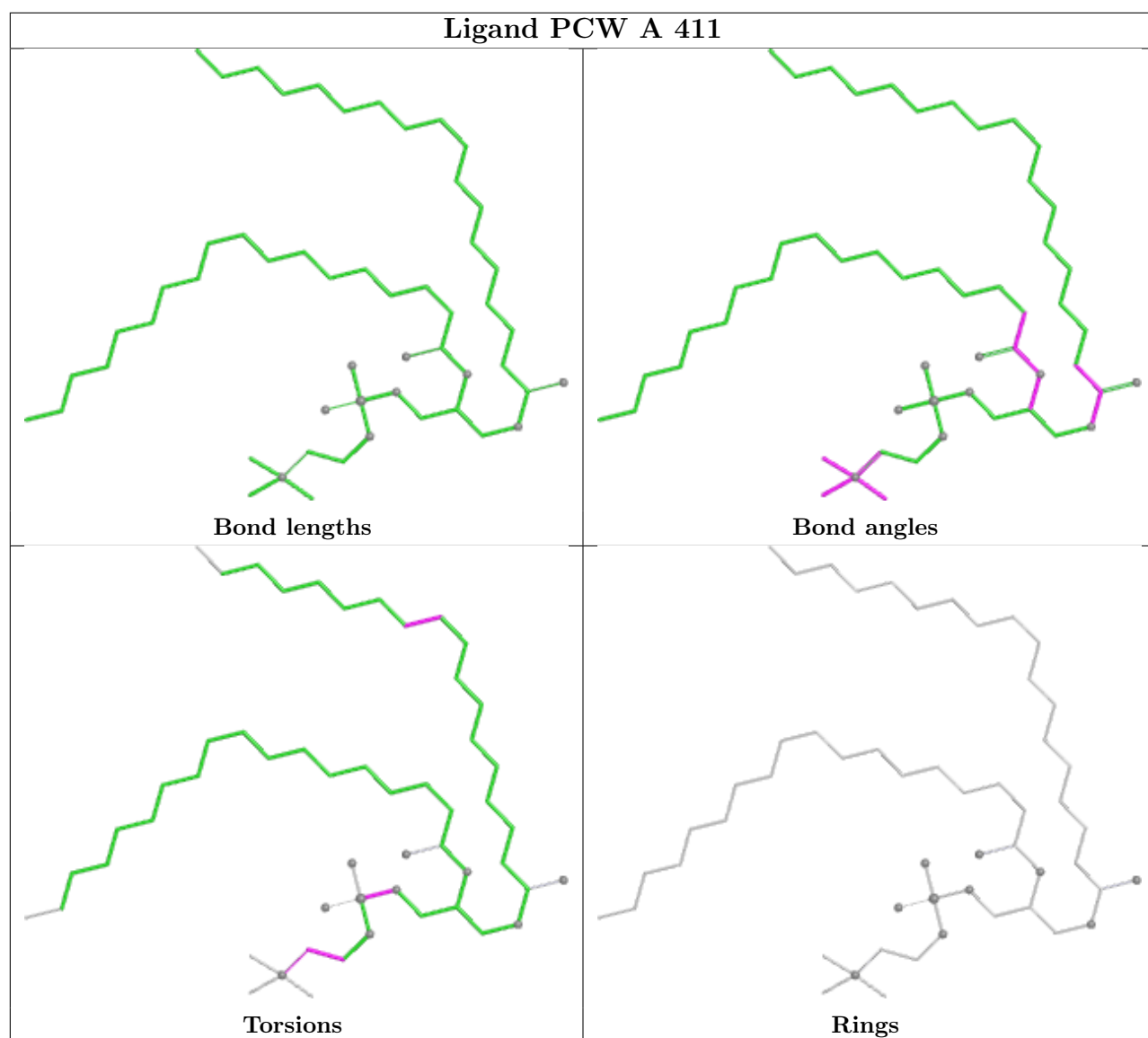


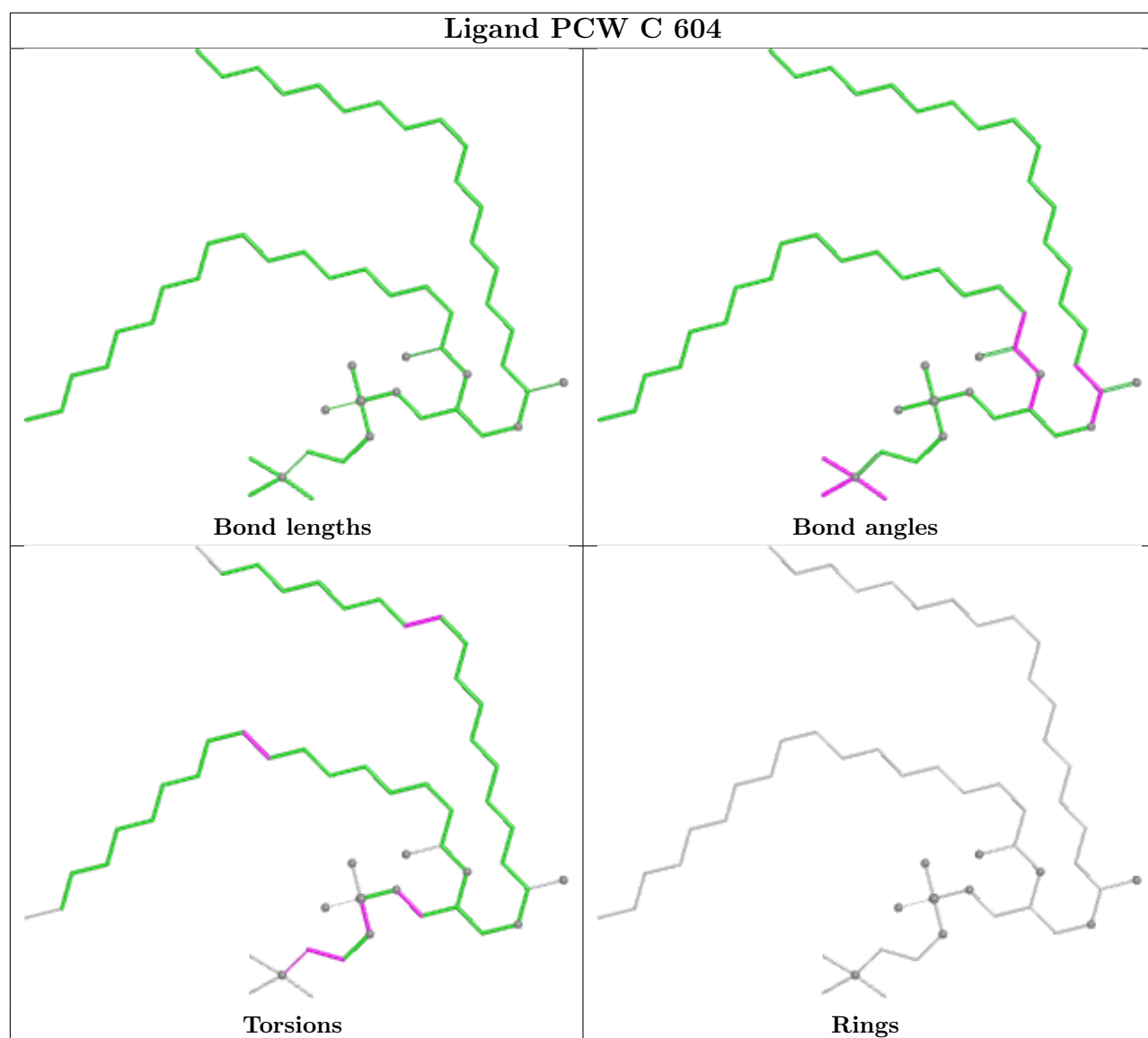


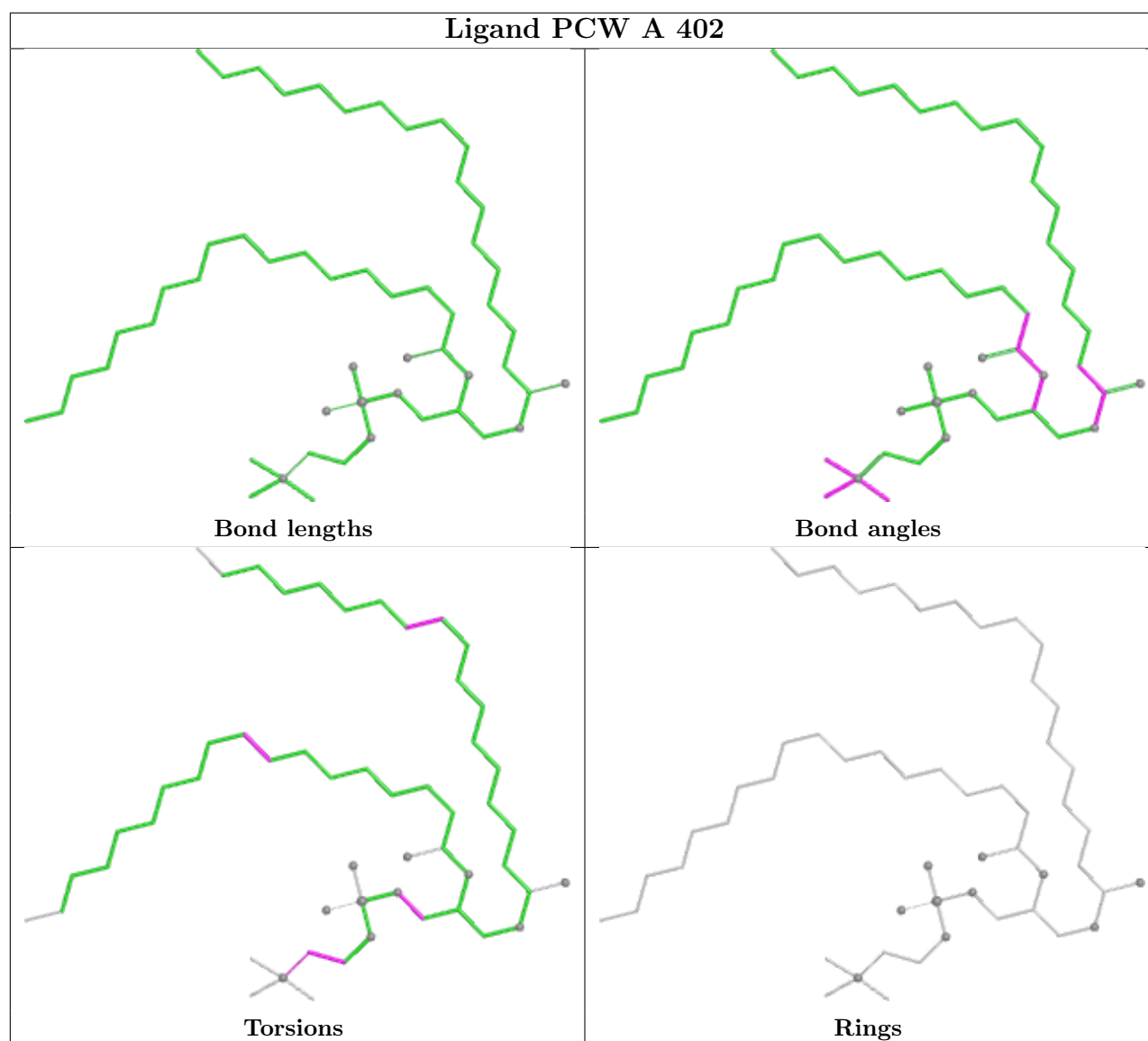


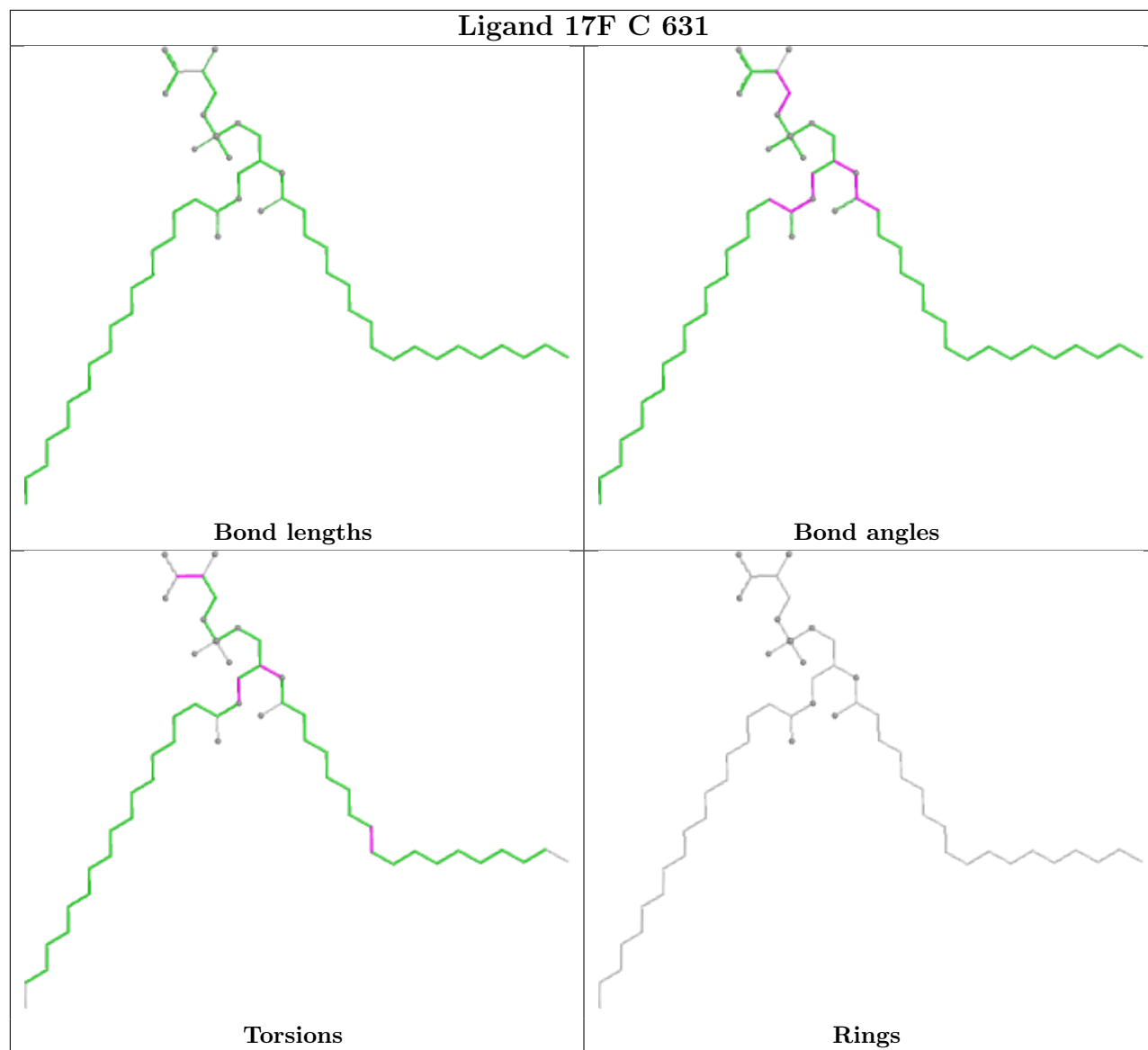


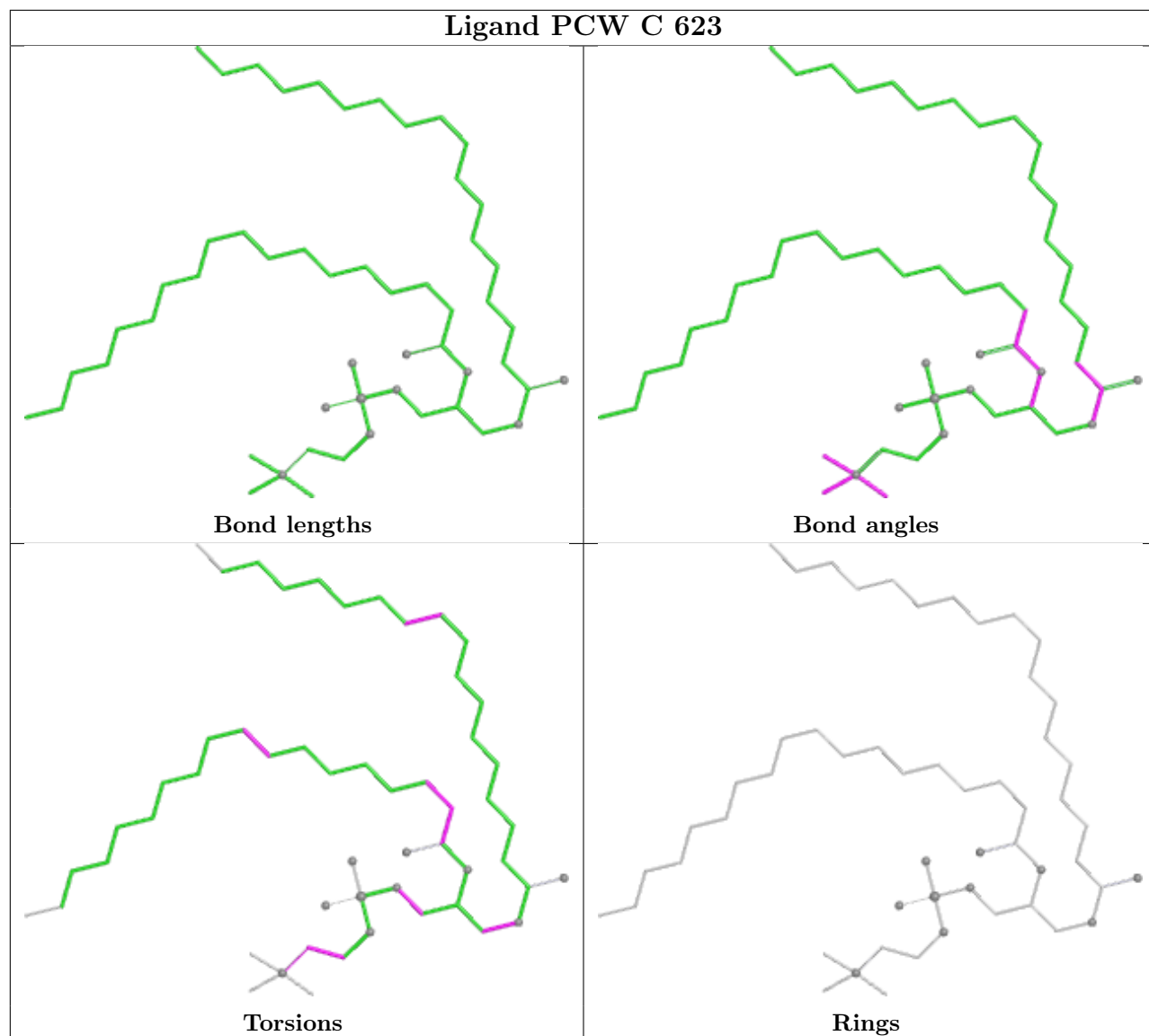


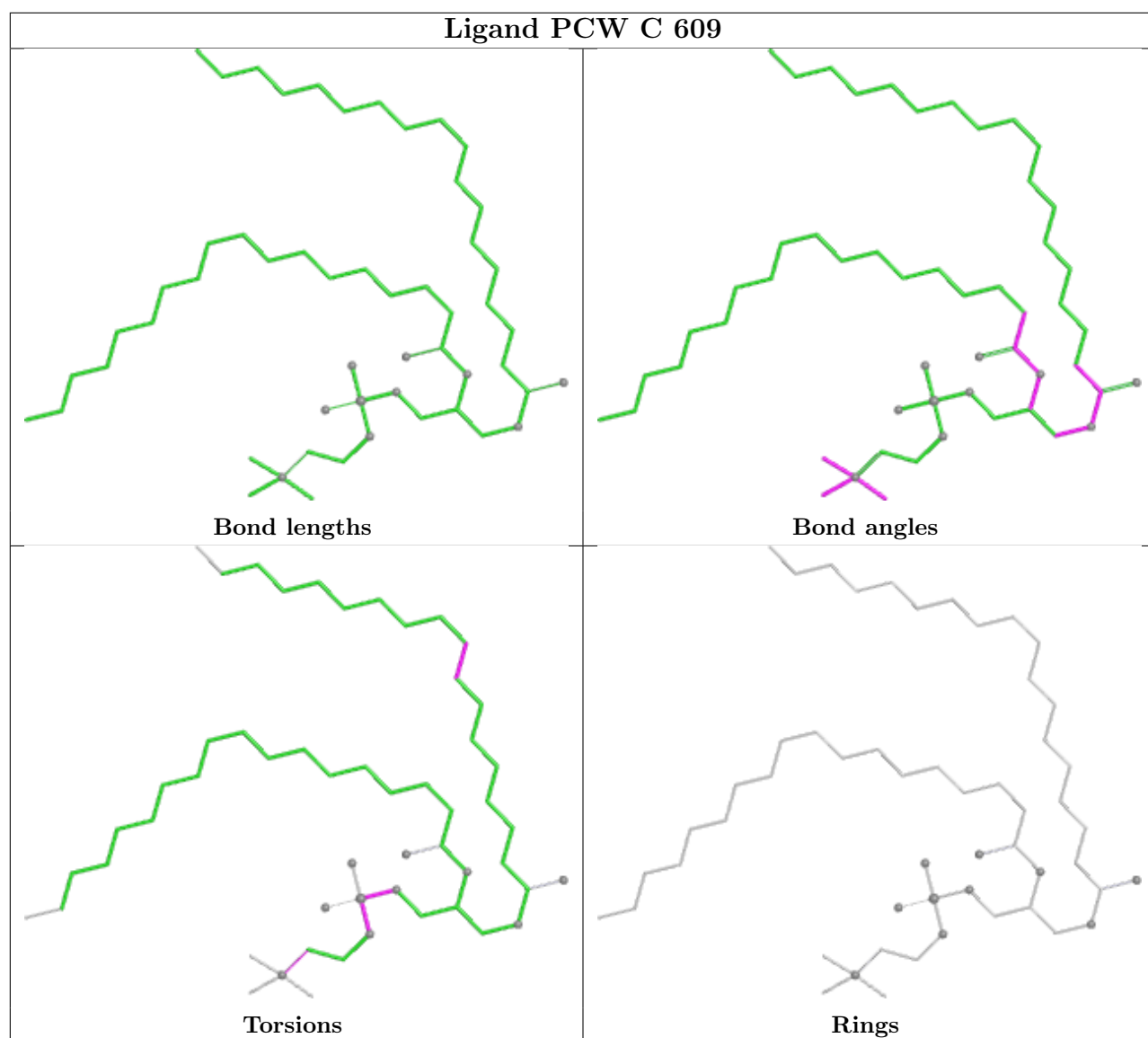


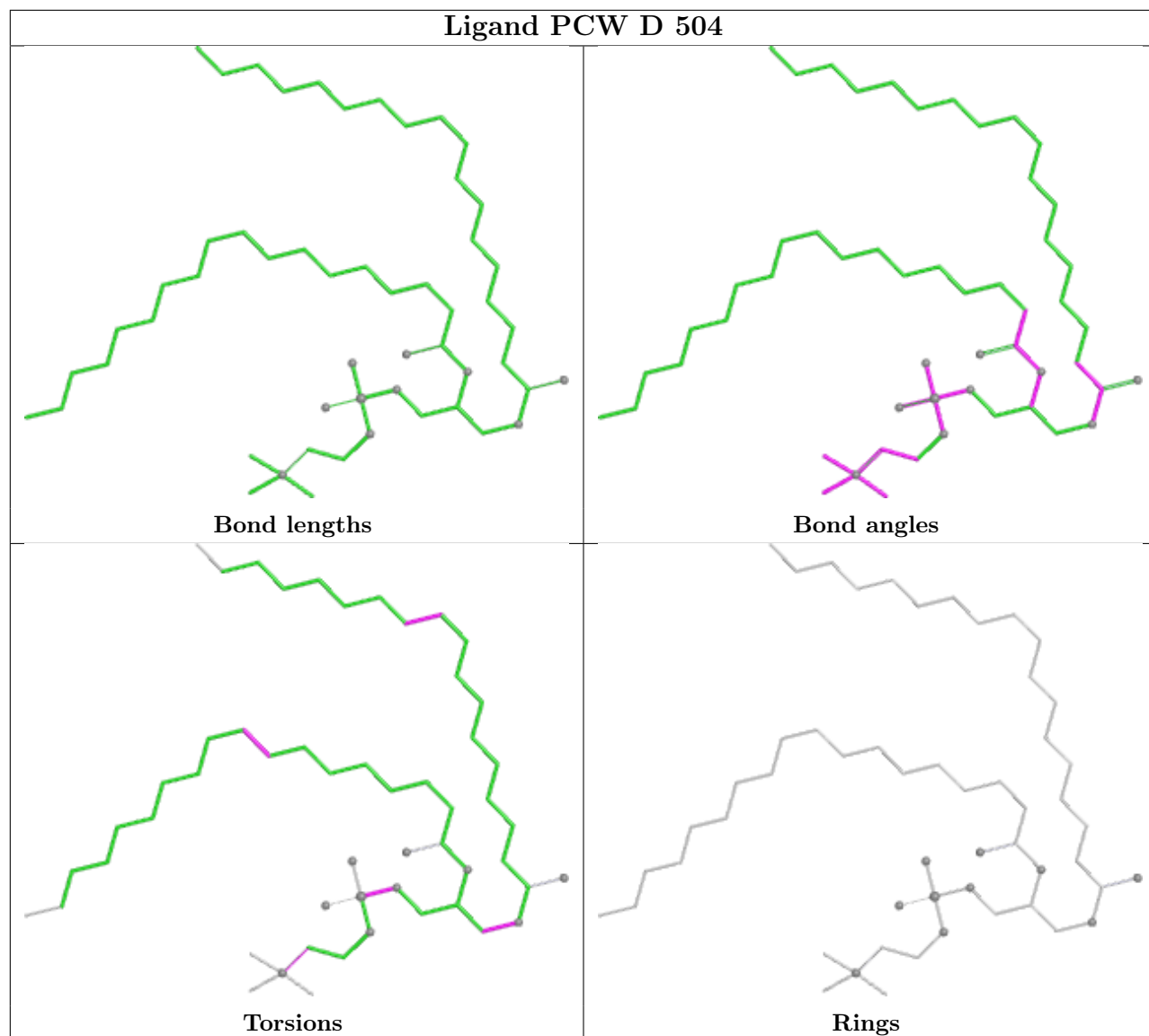


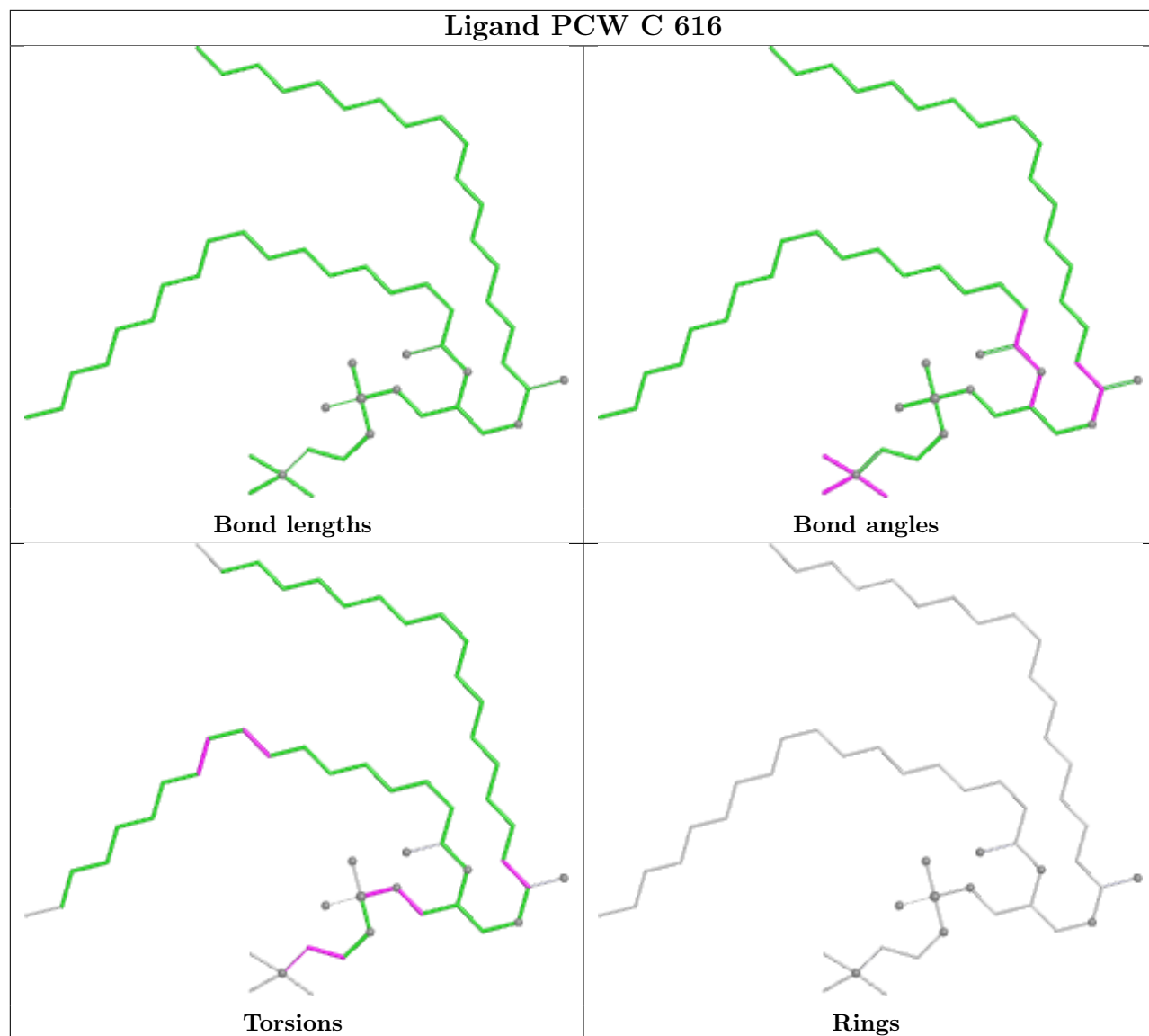


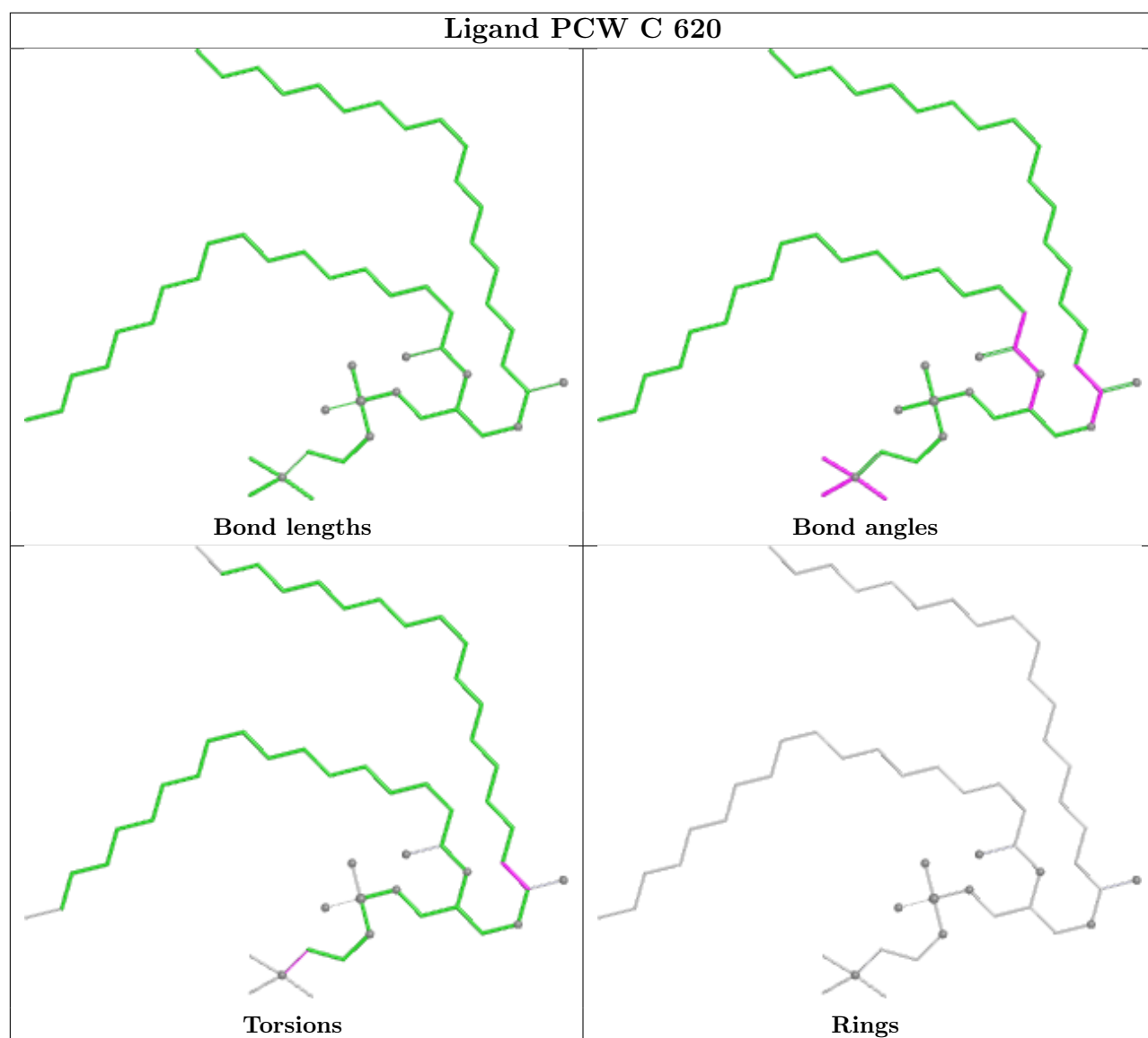


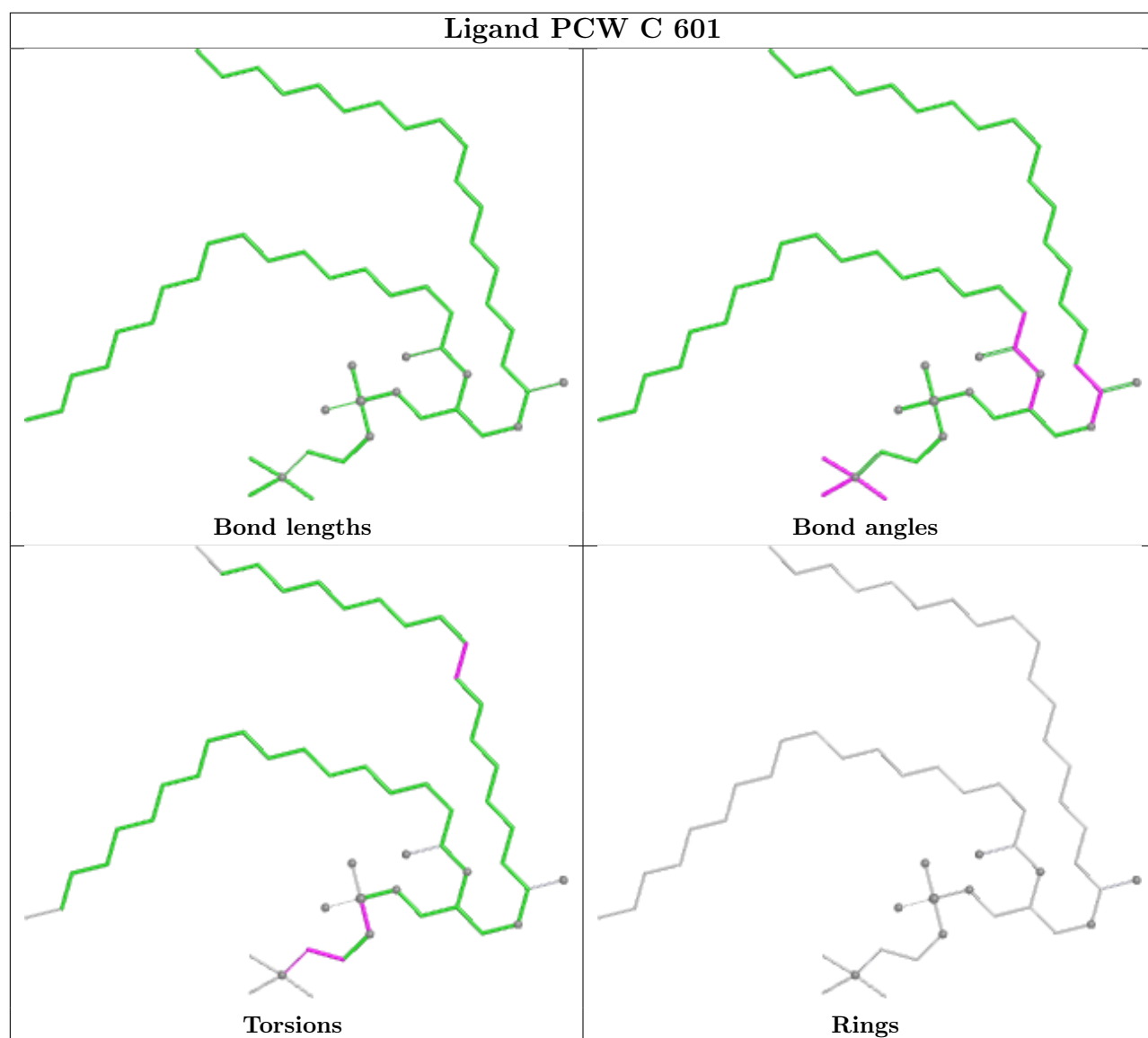


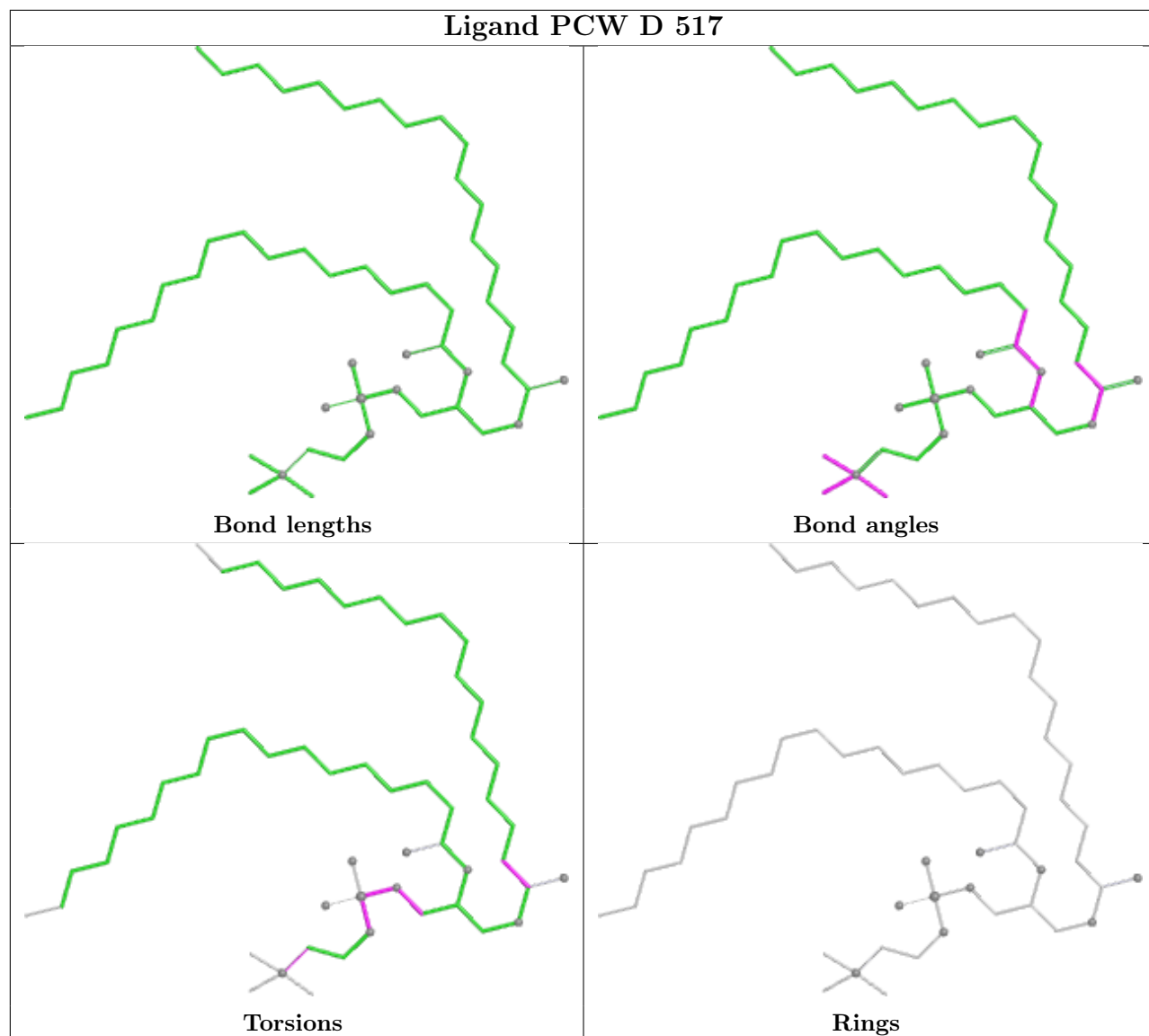


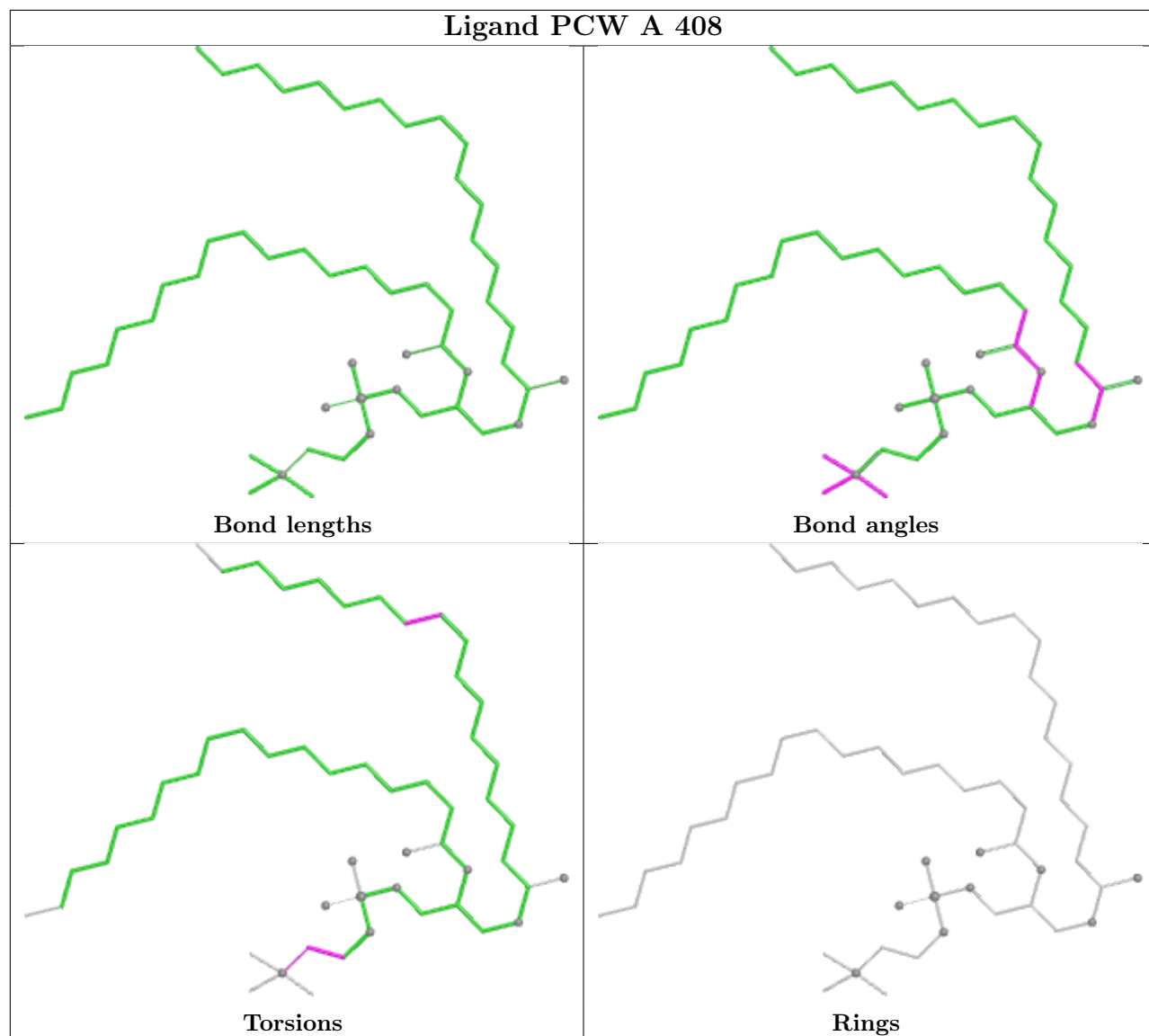


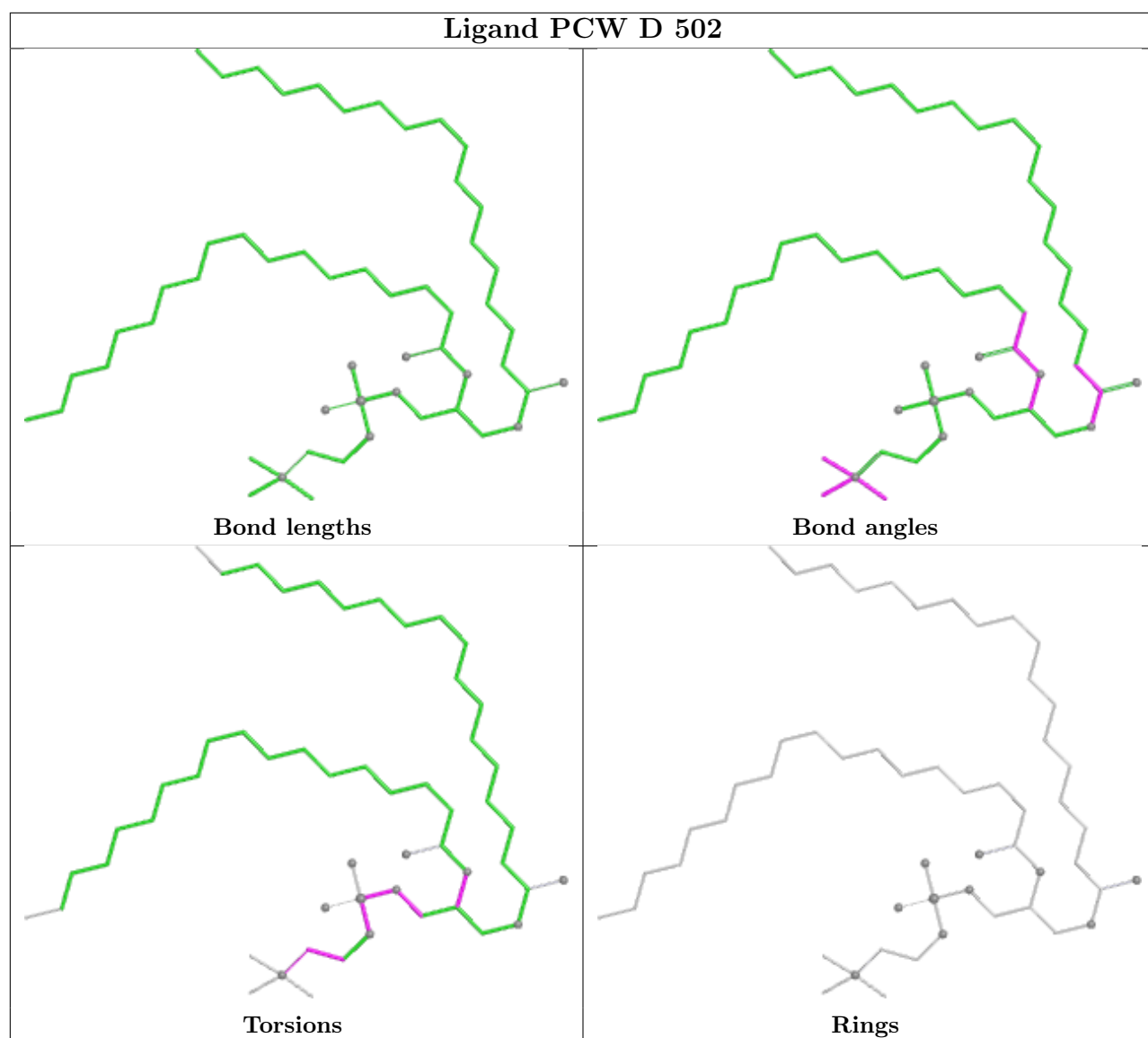


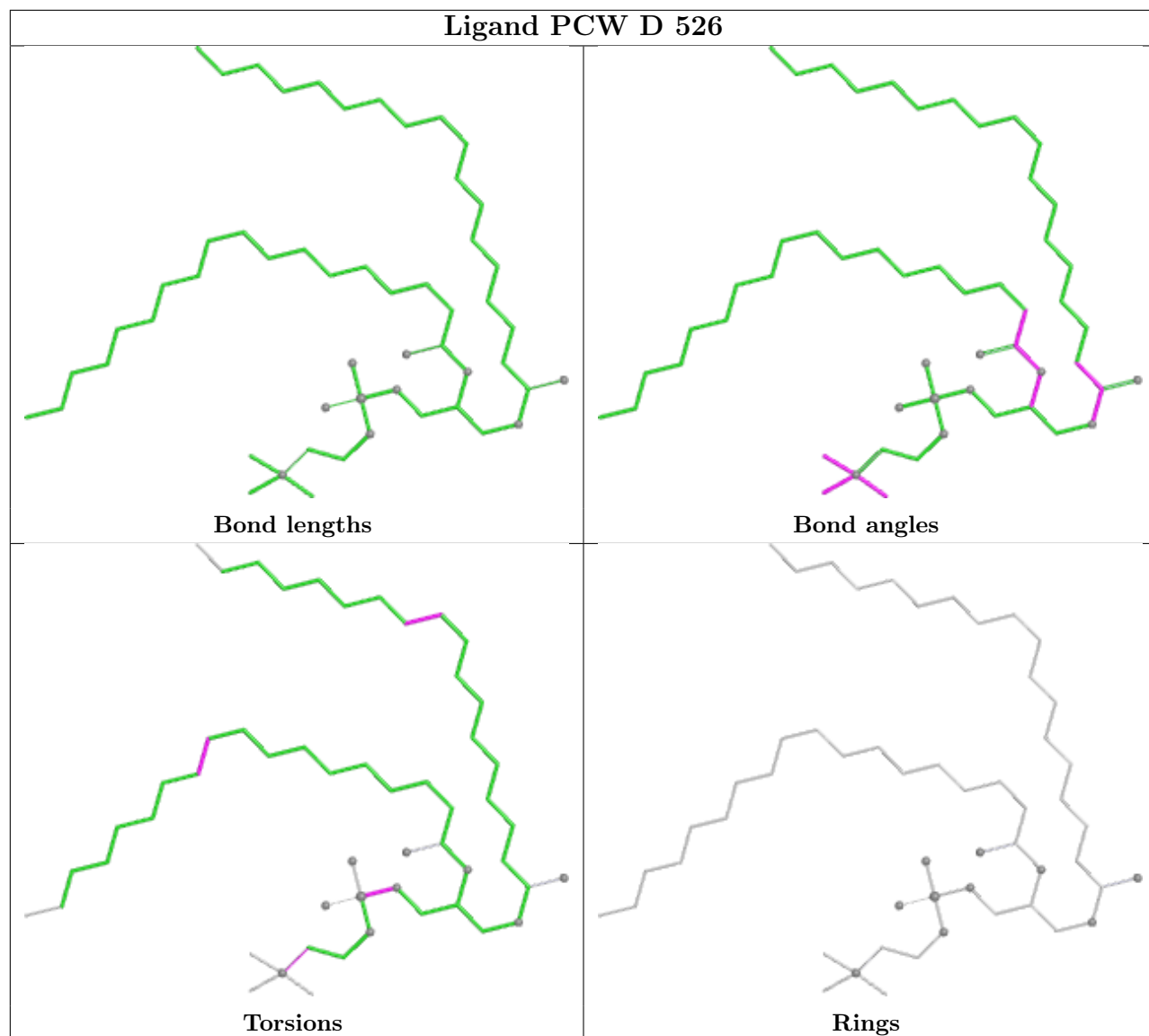


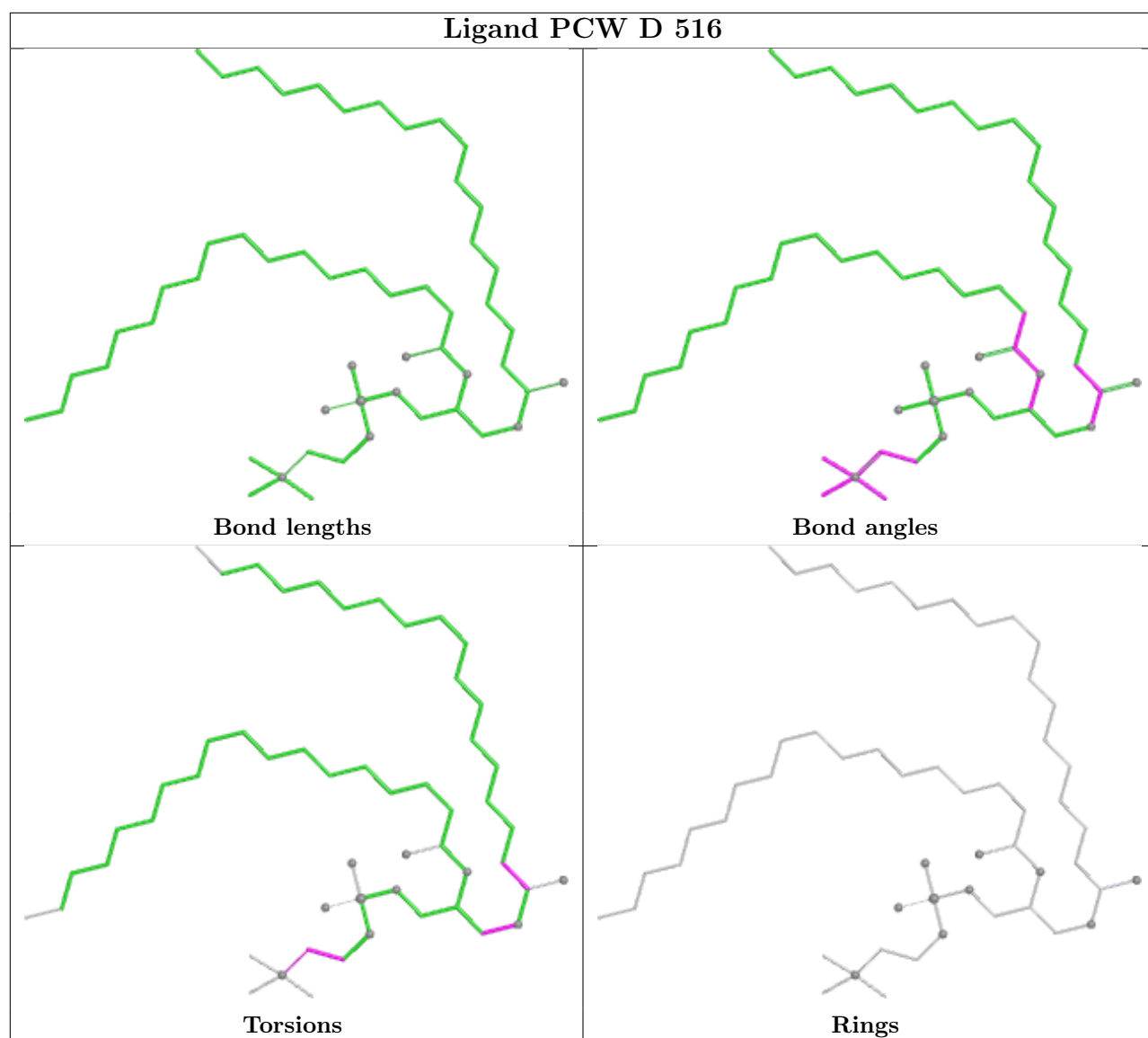


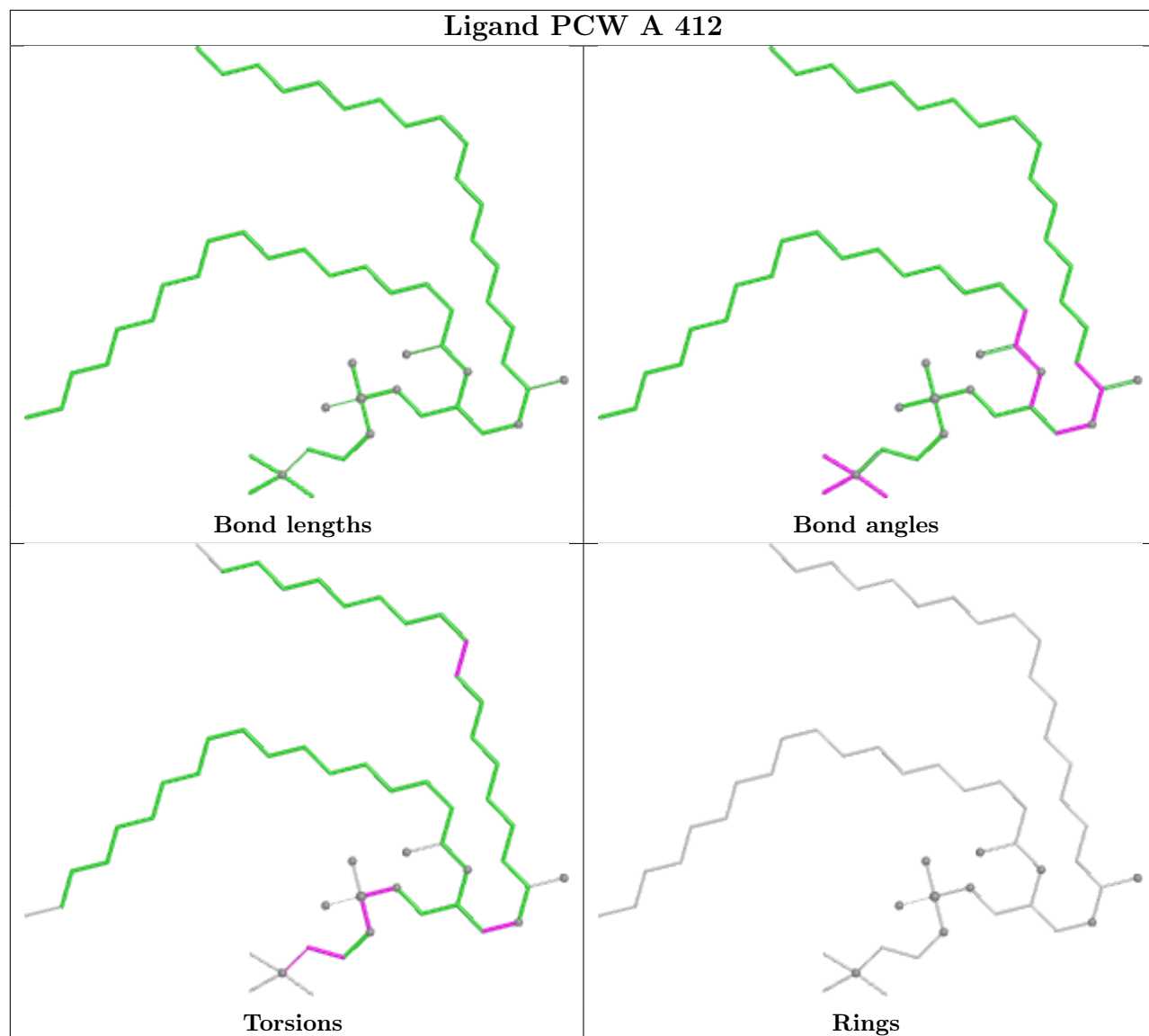


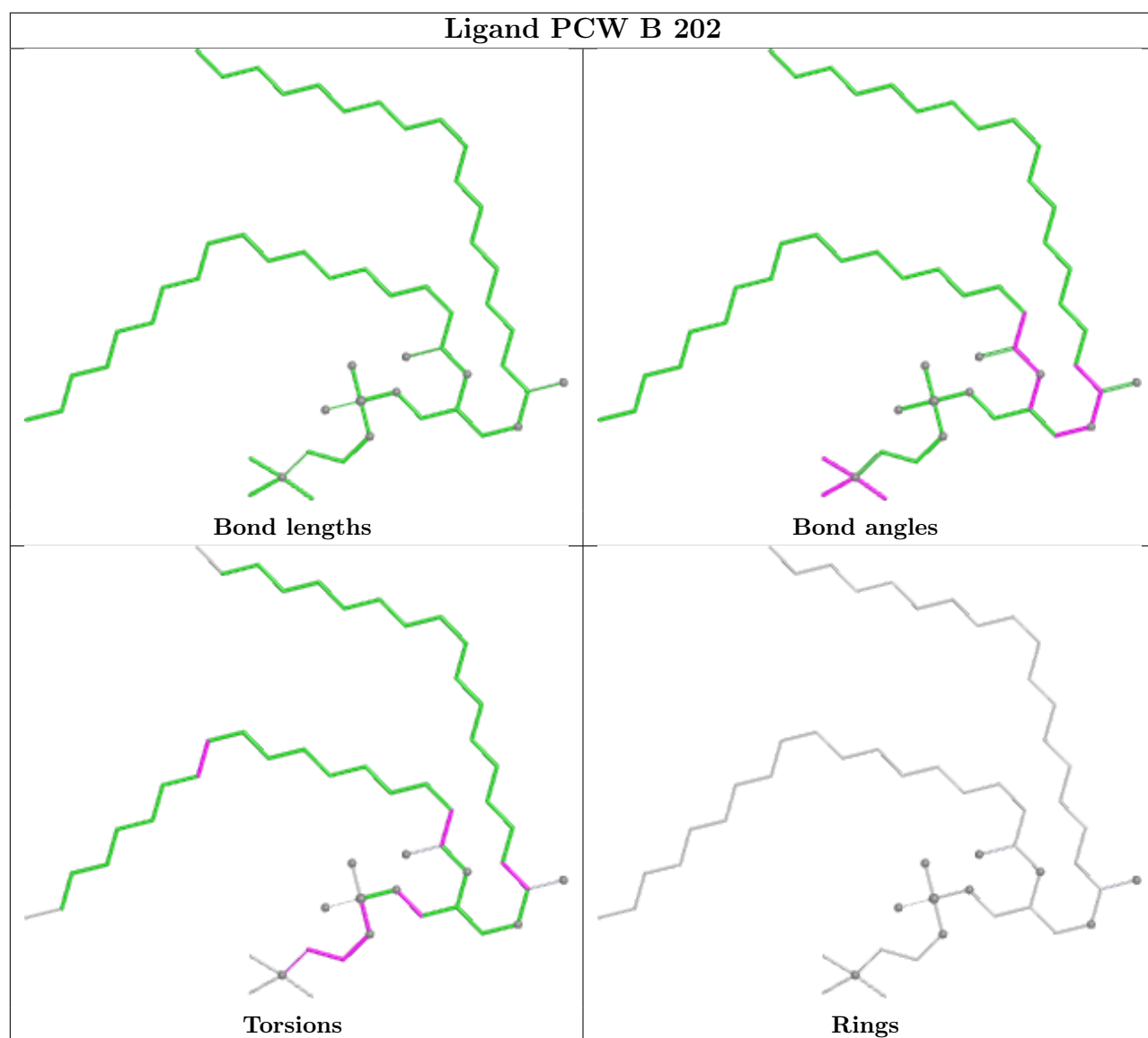


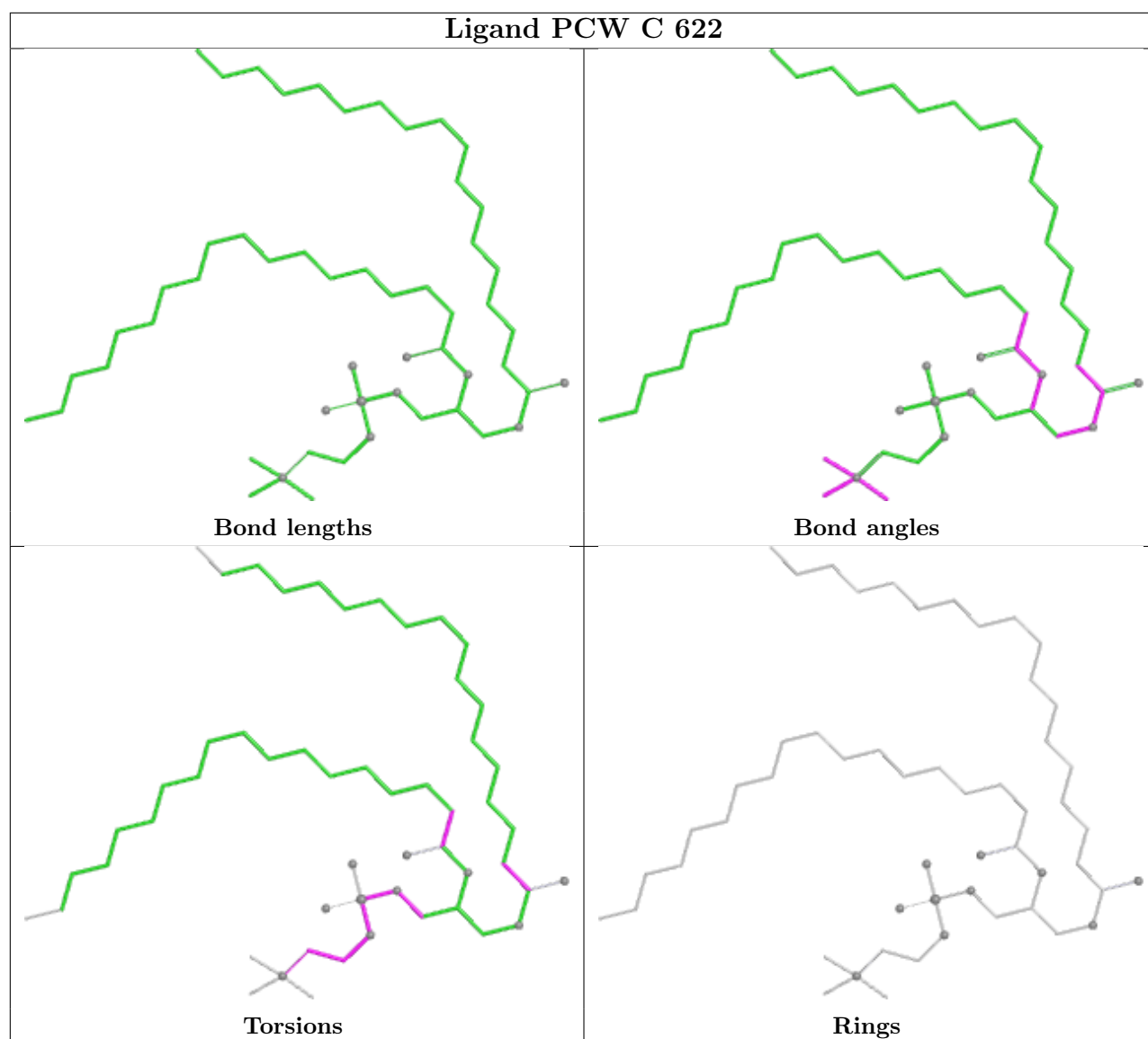


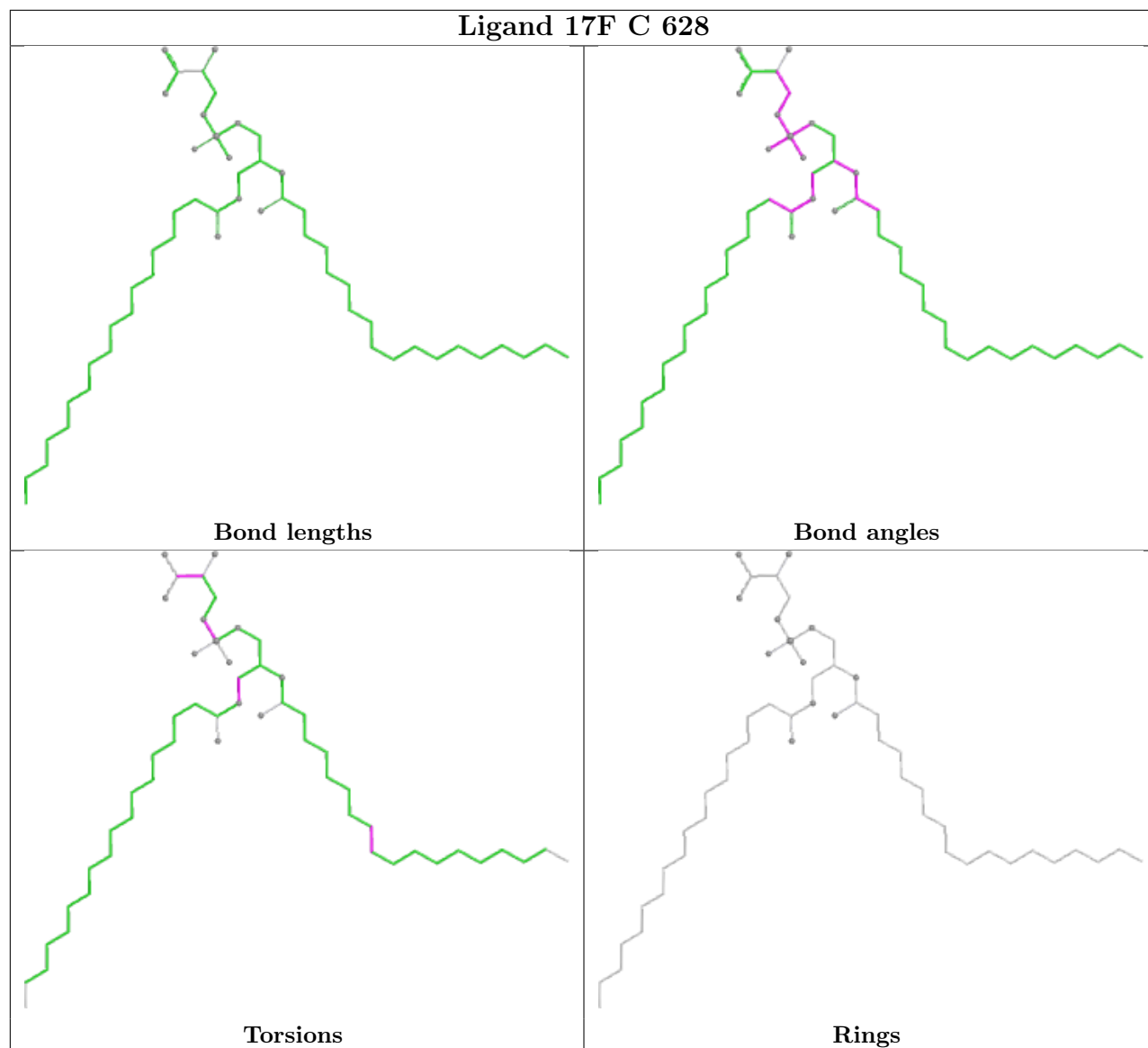


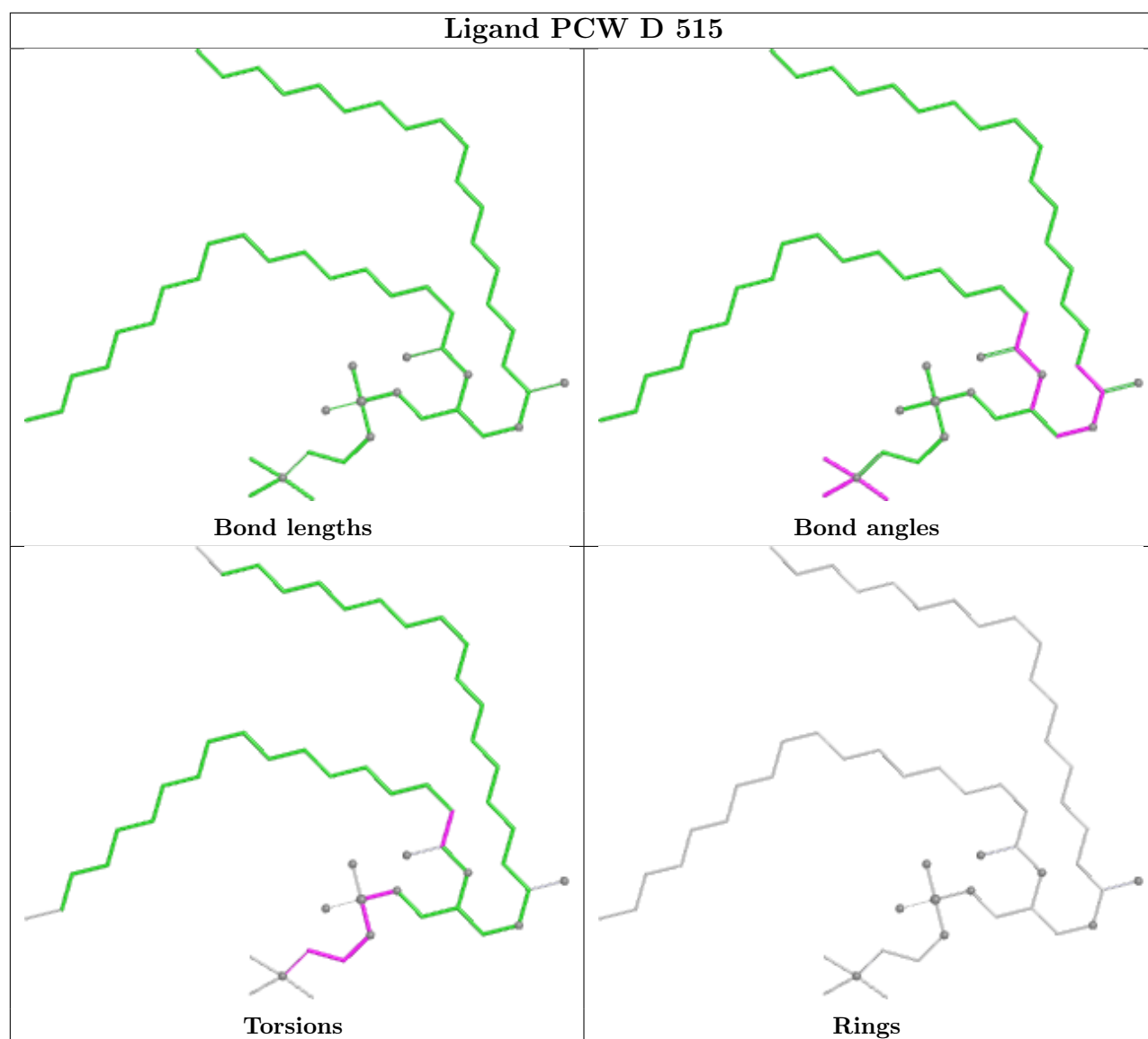


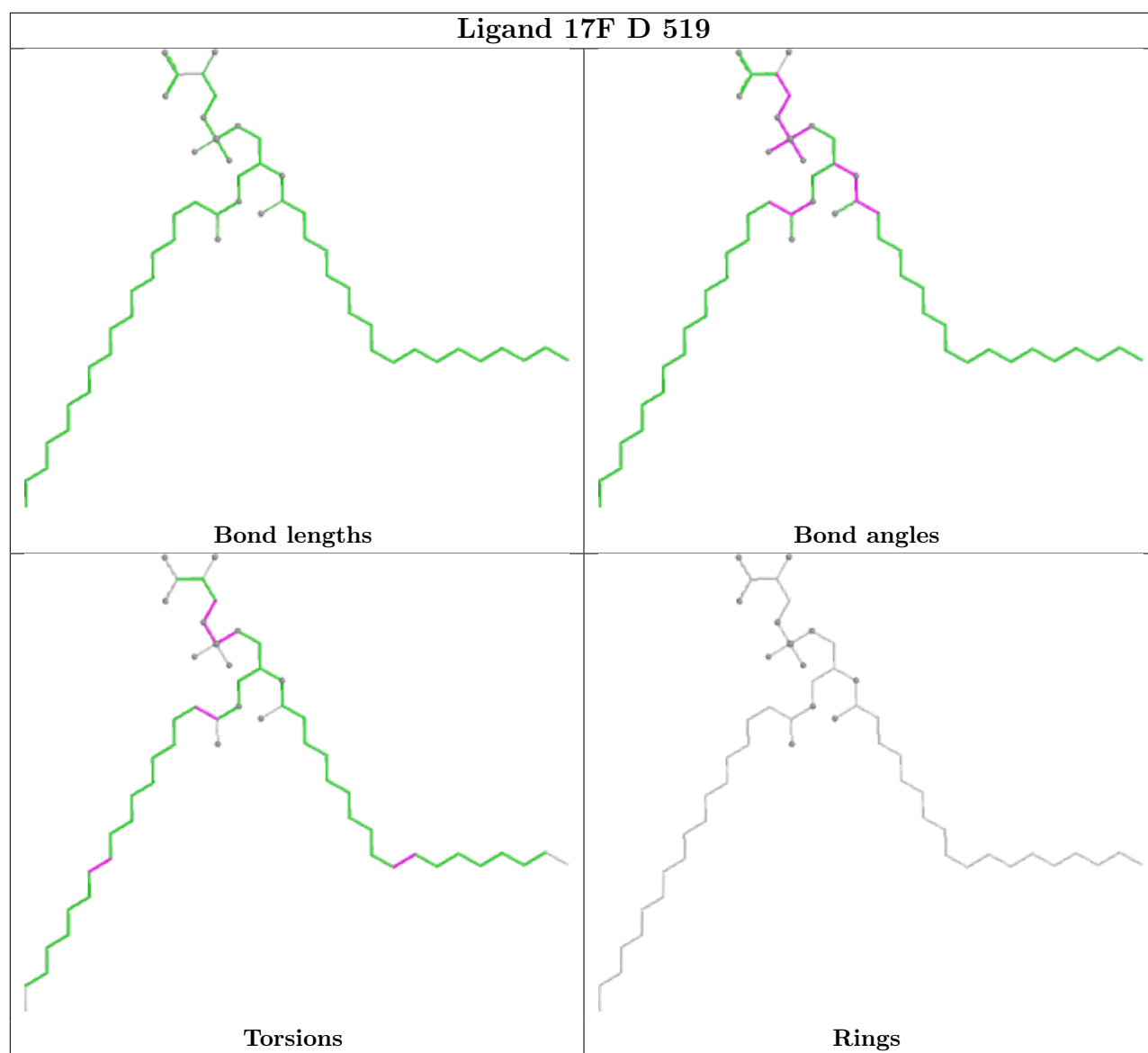


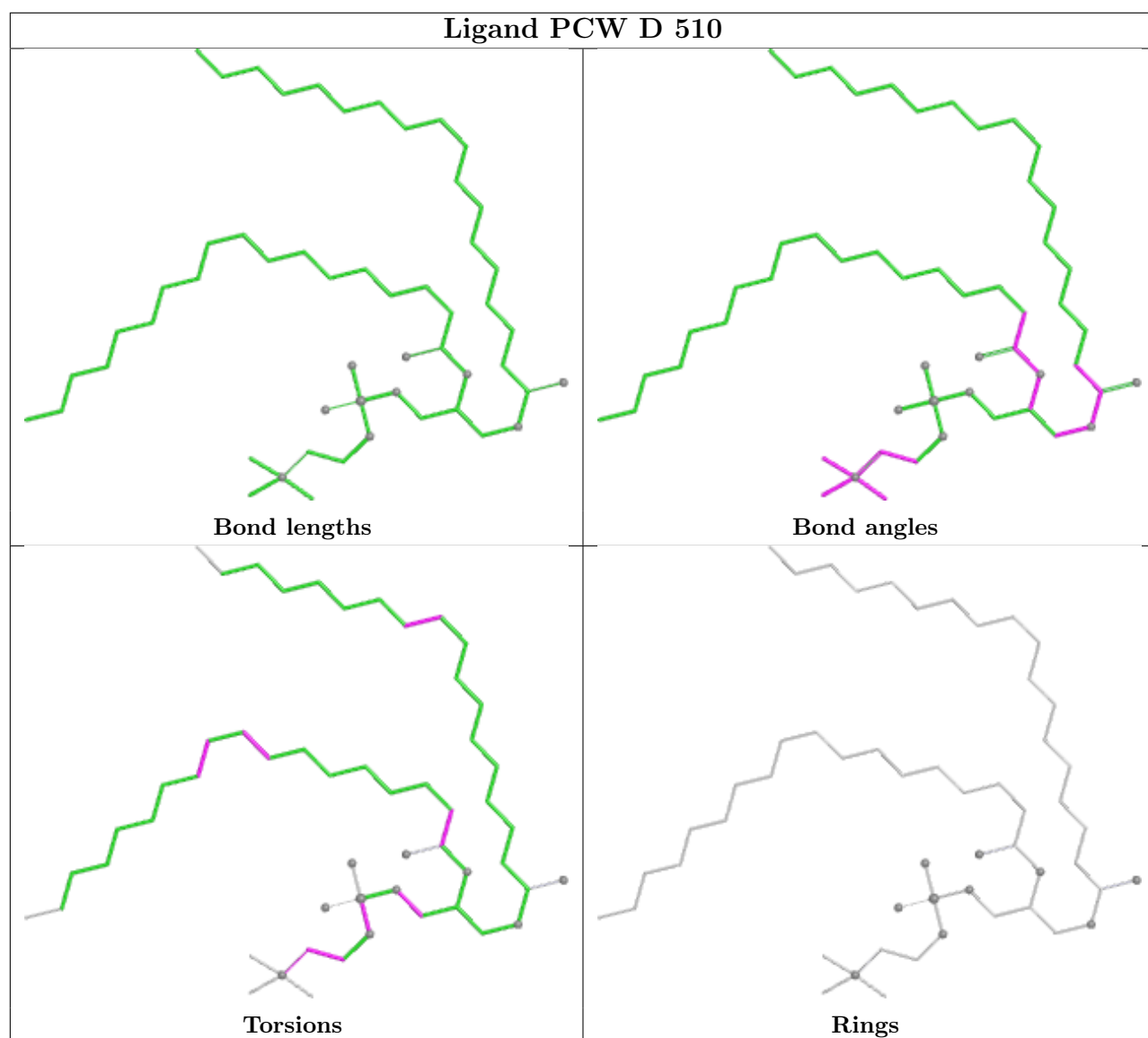


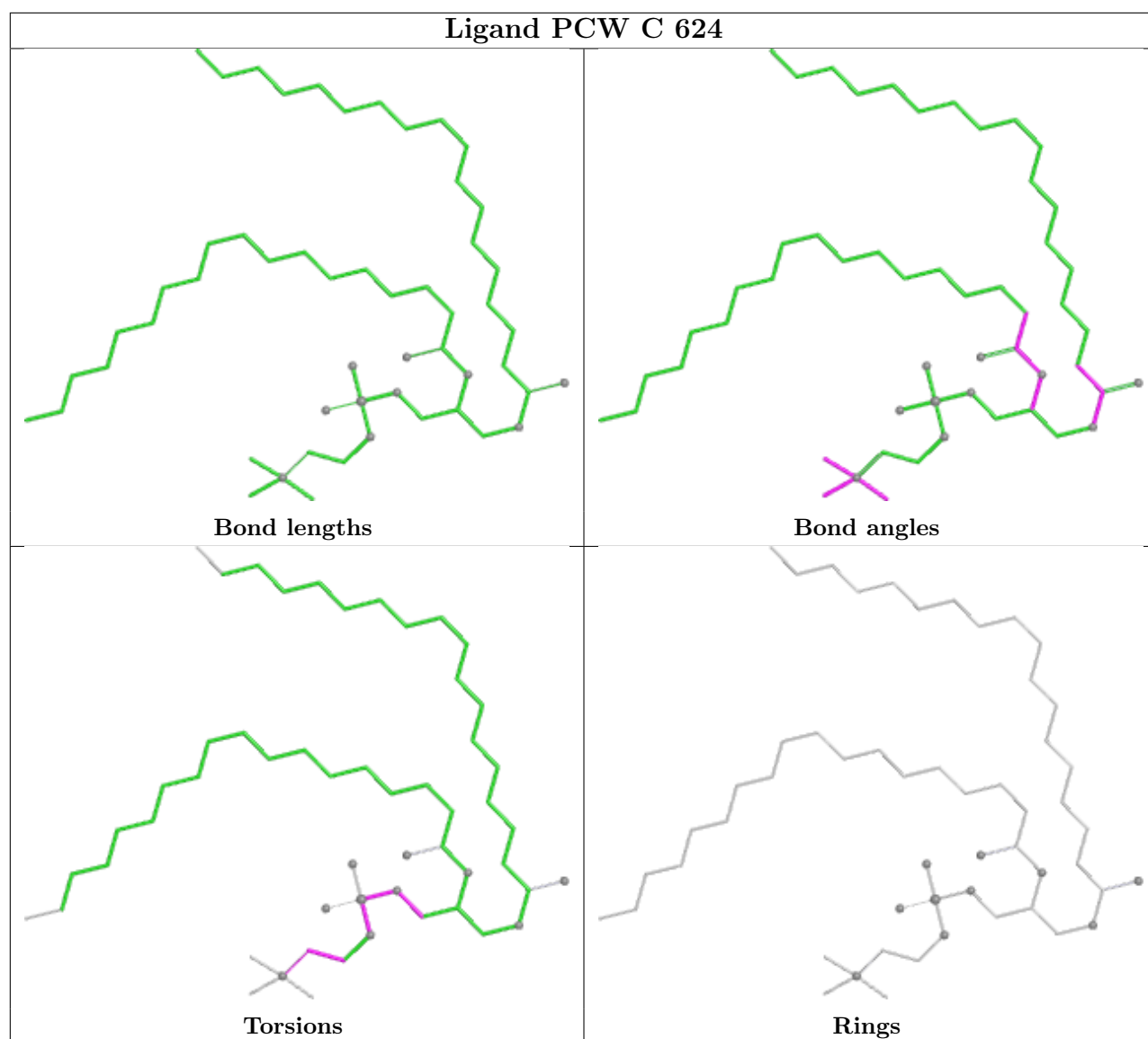


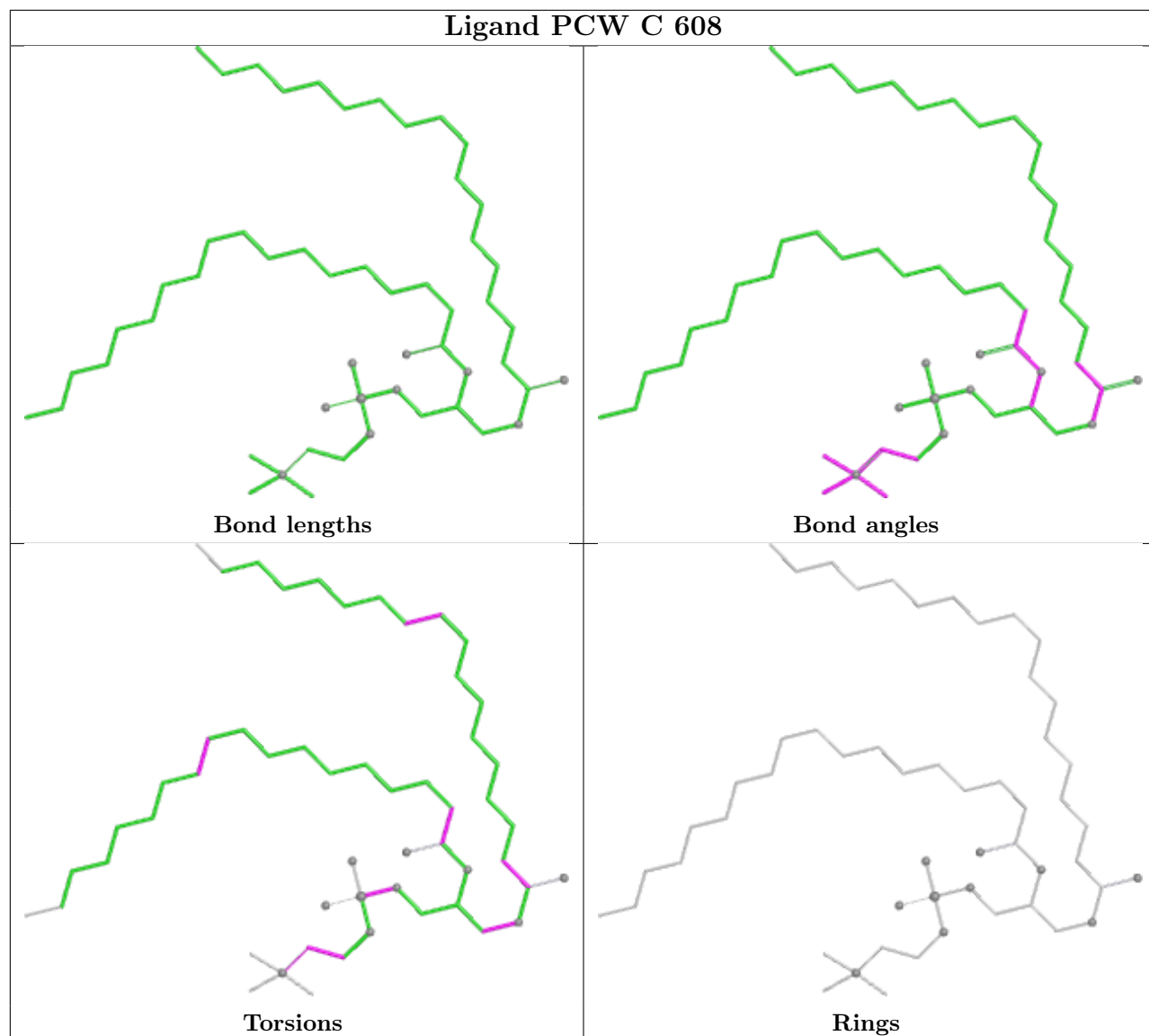


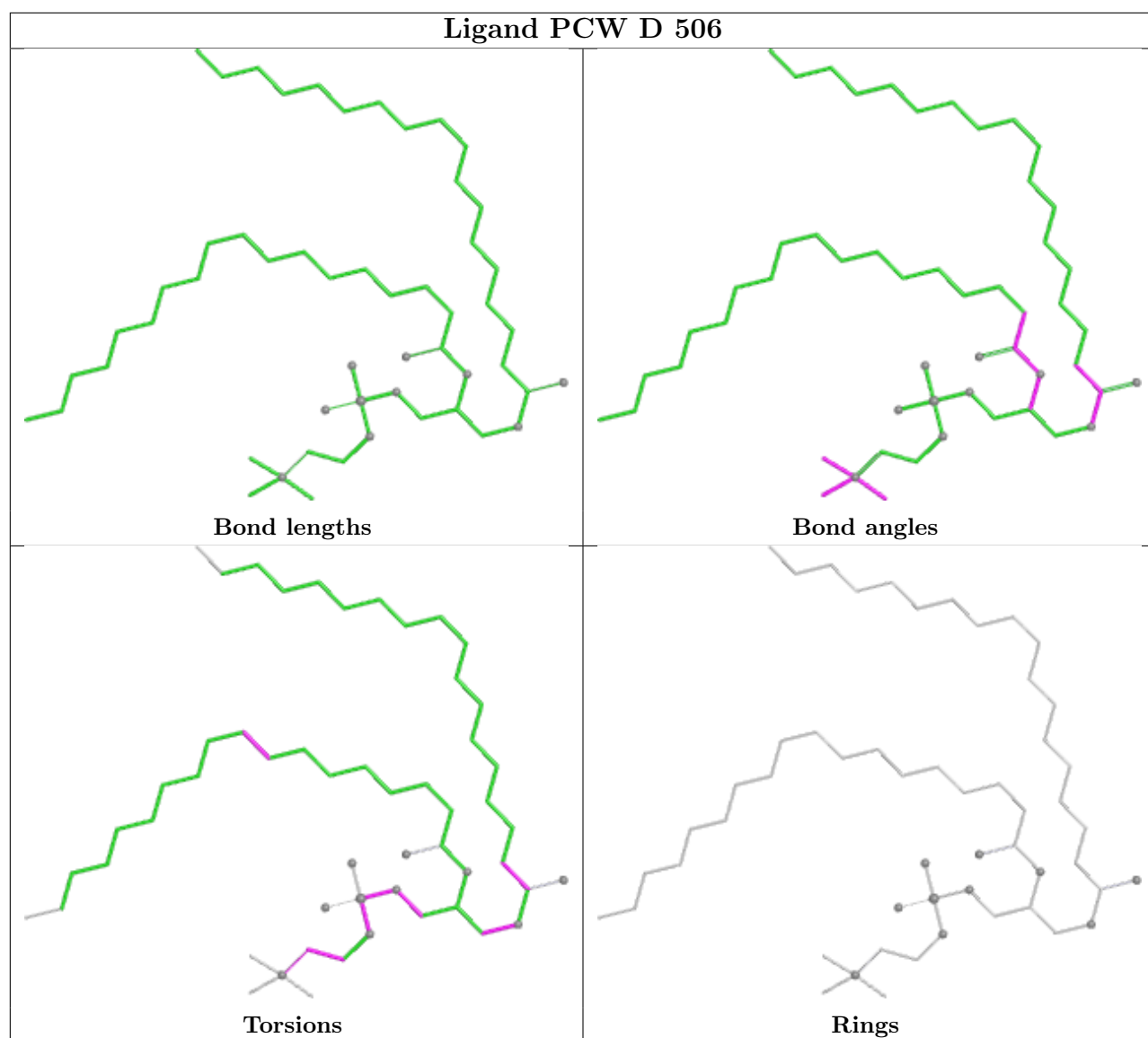




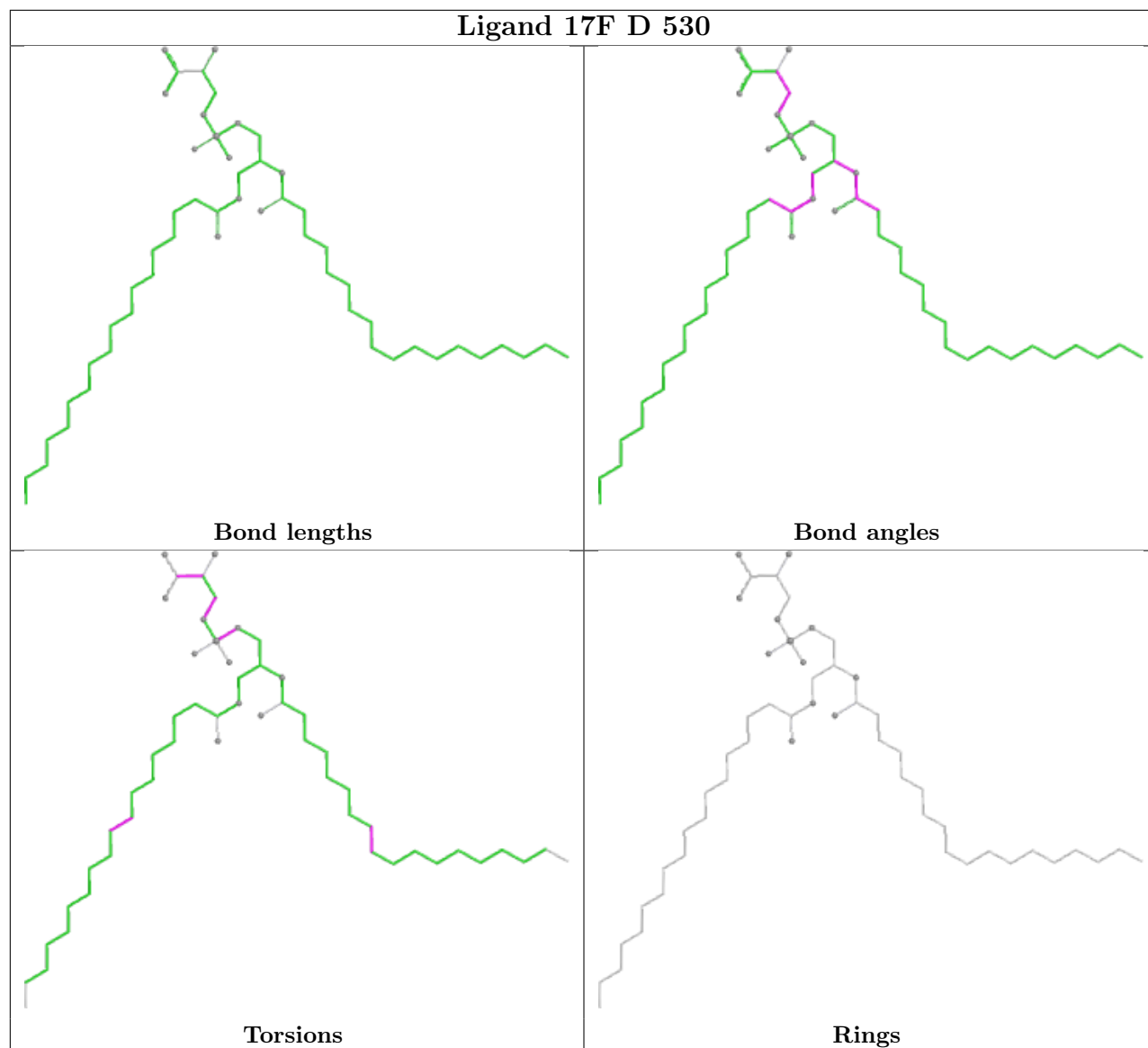


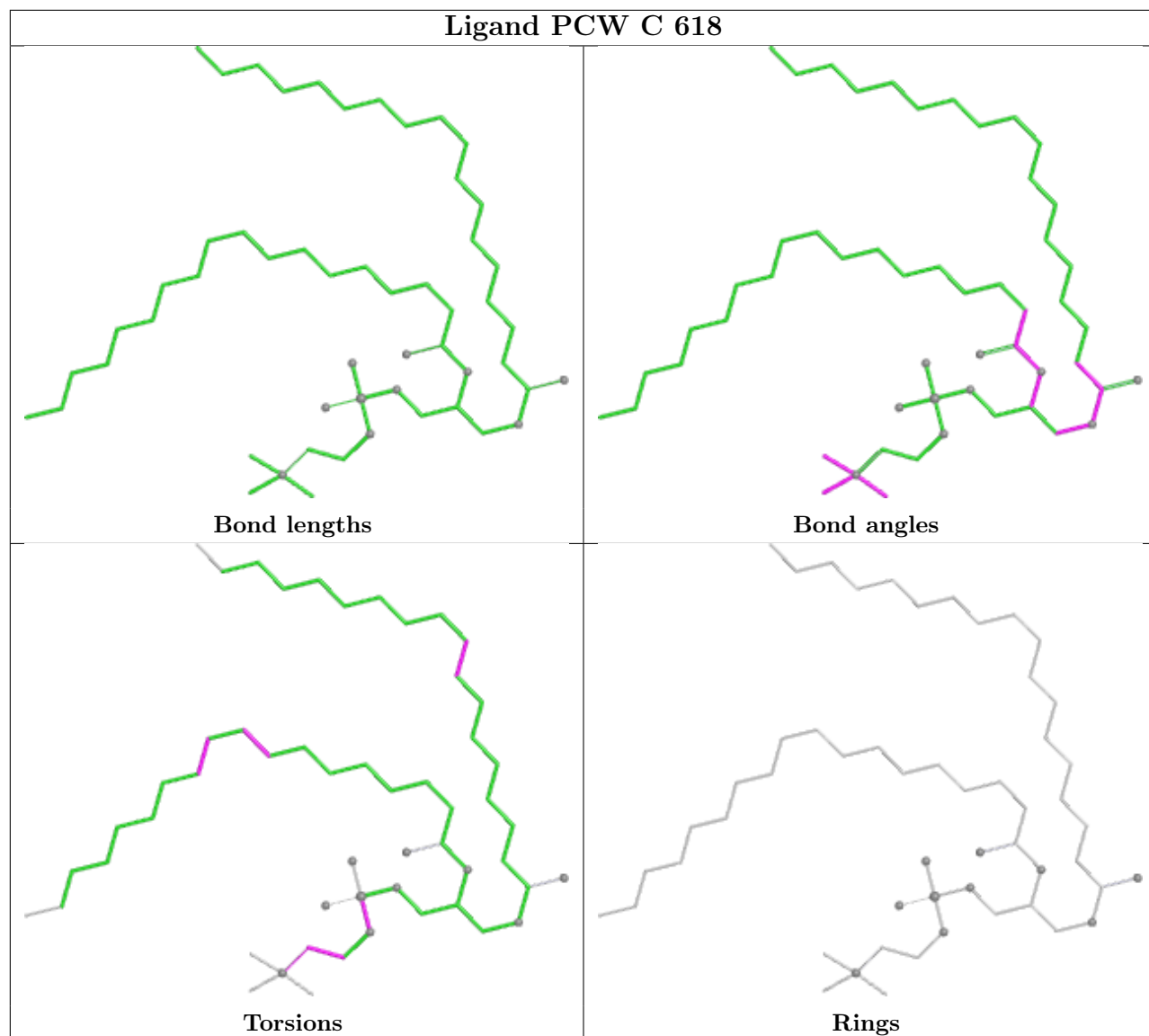


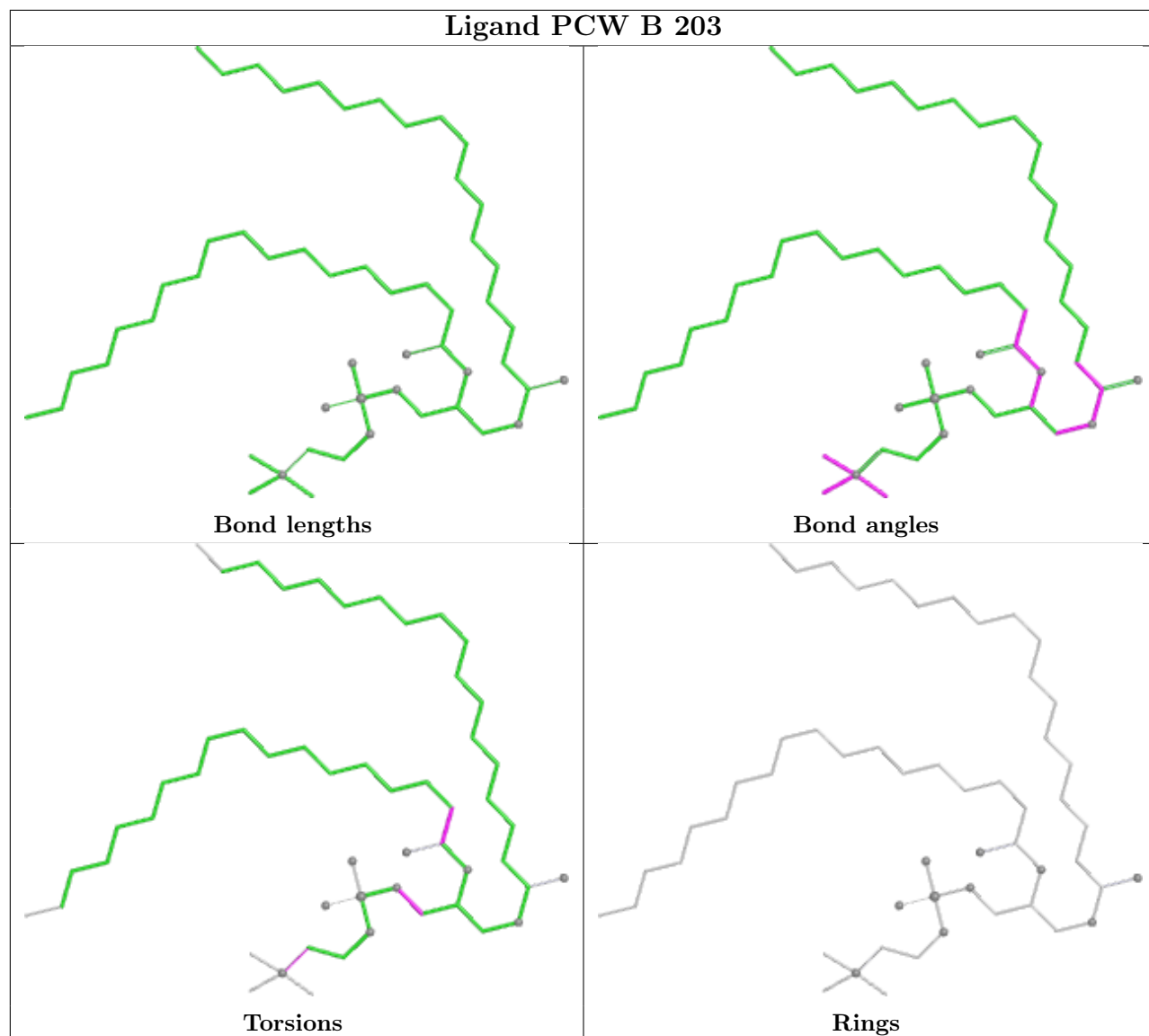


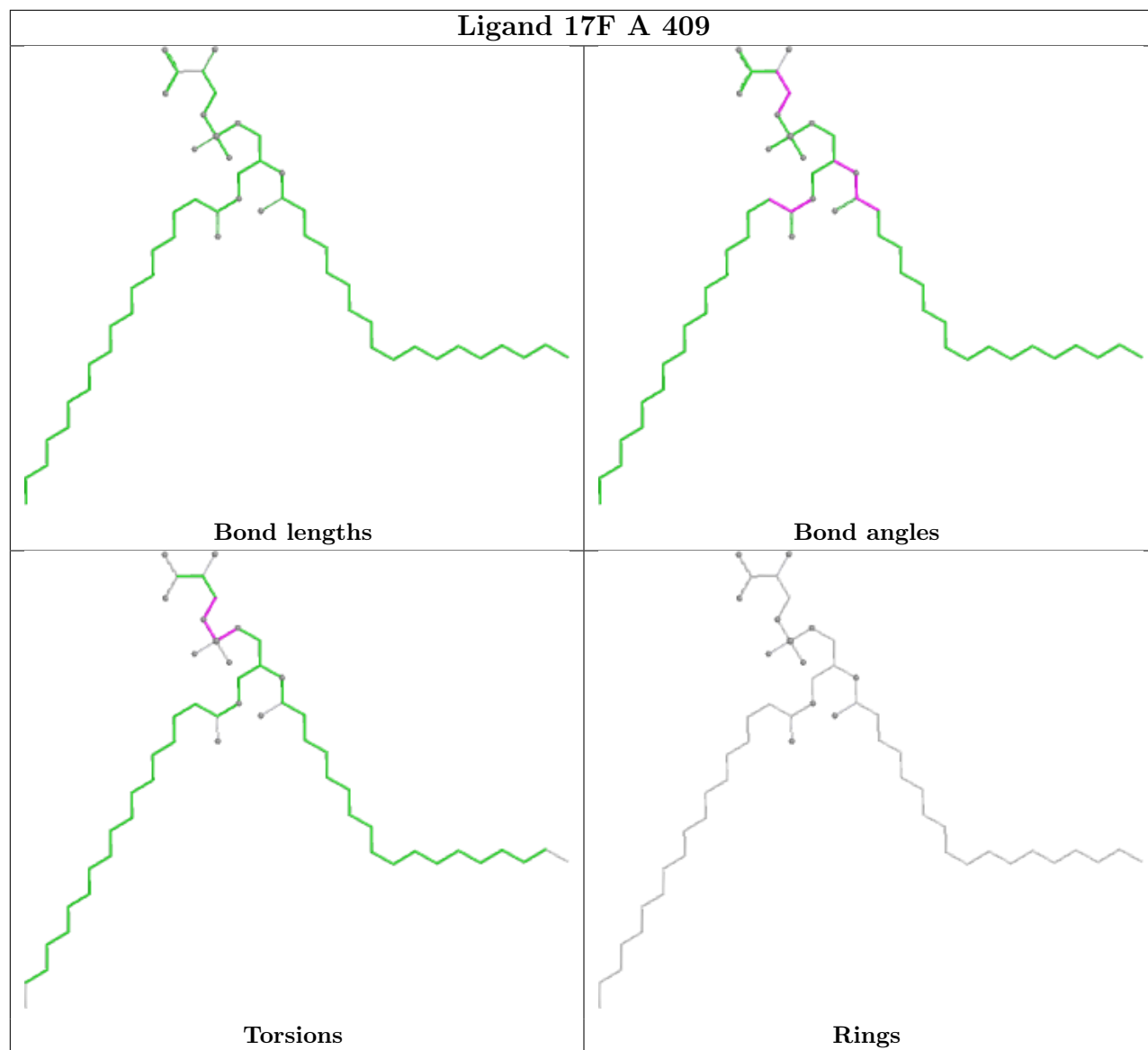


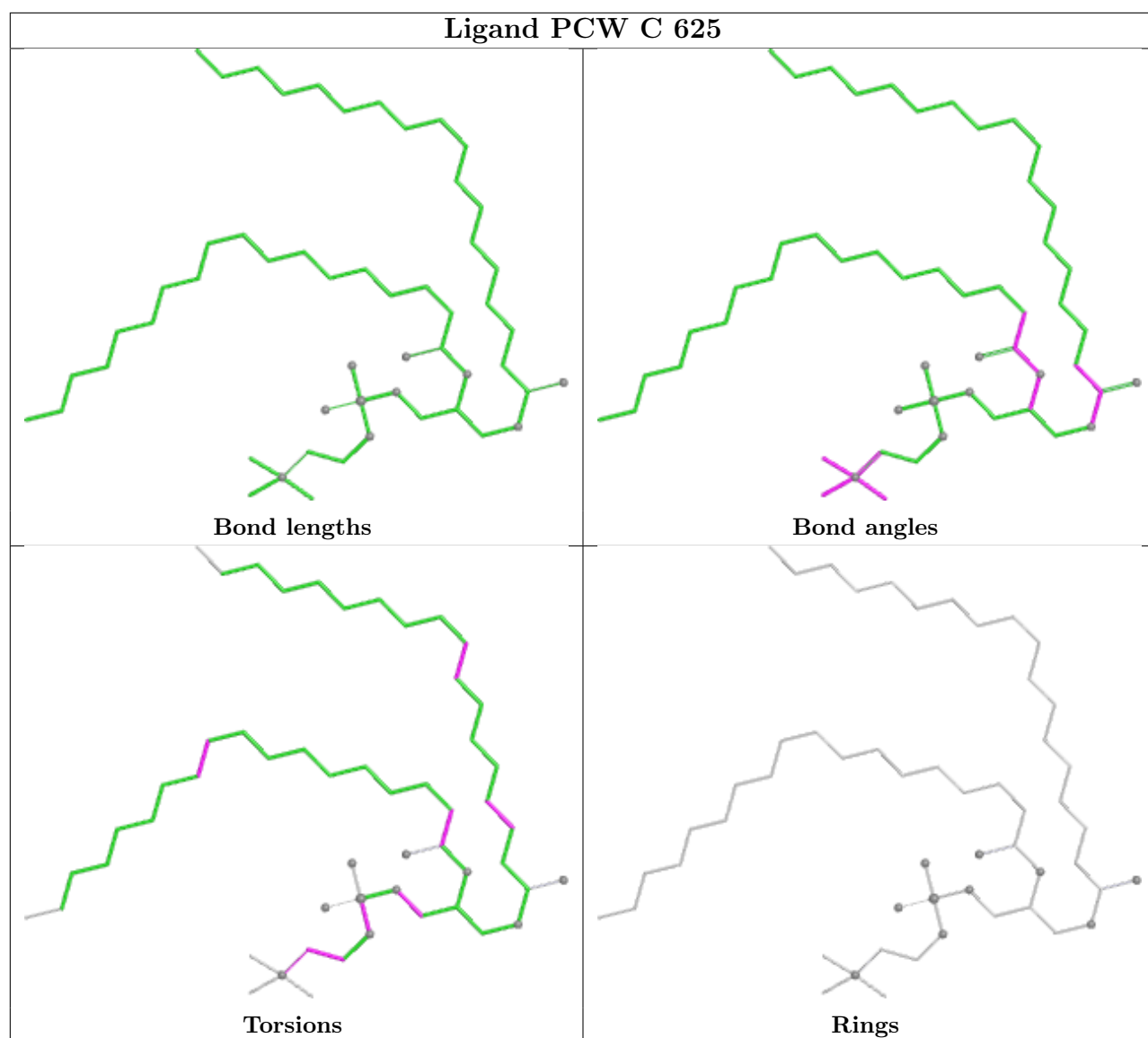
Ligand 17F D 530

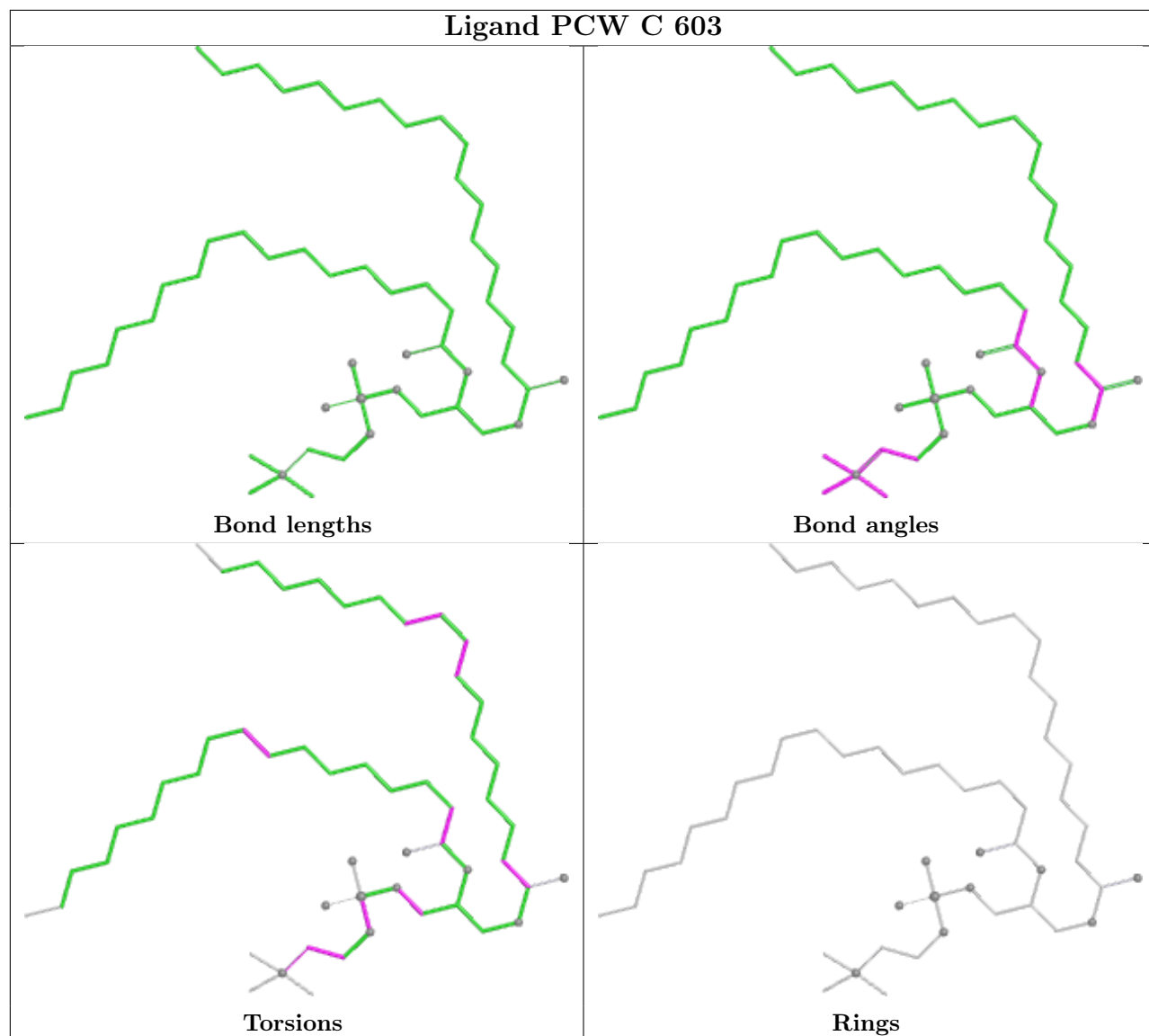


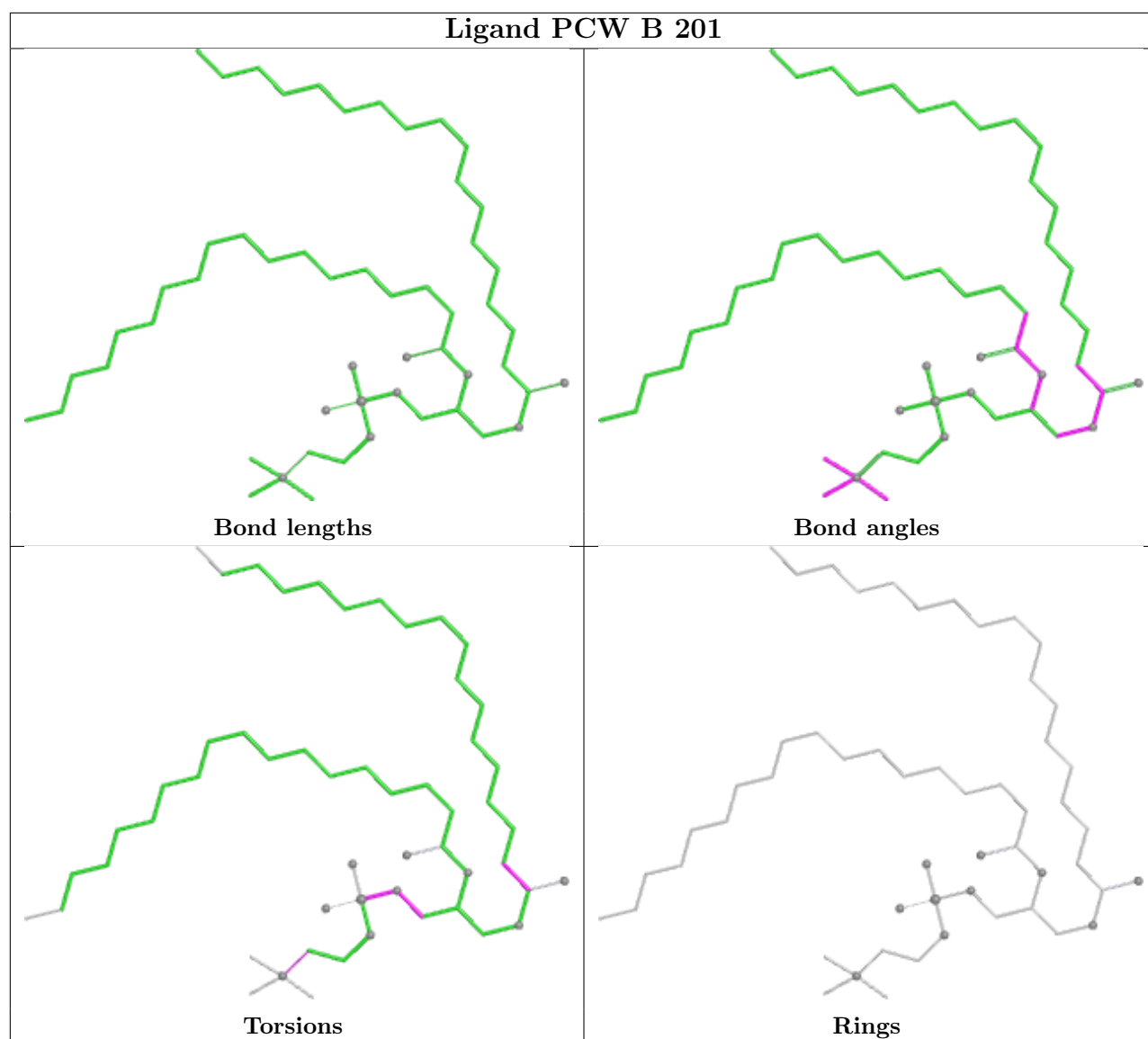


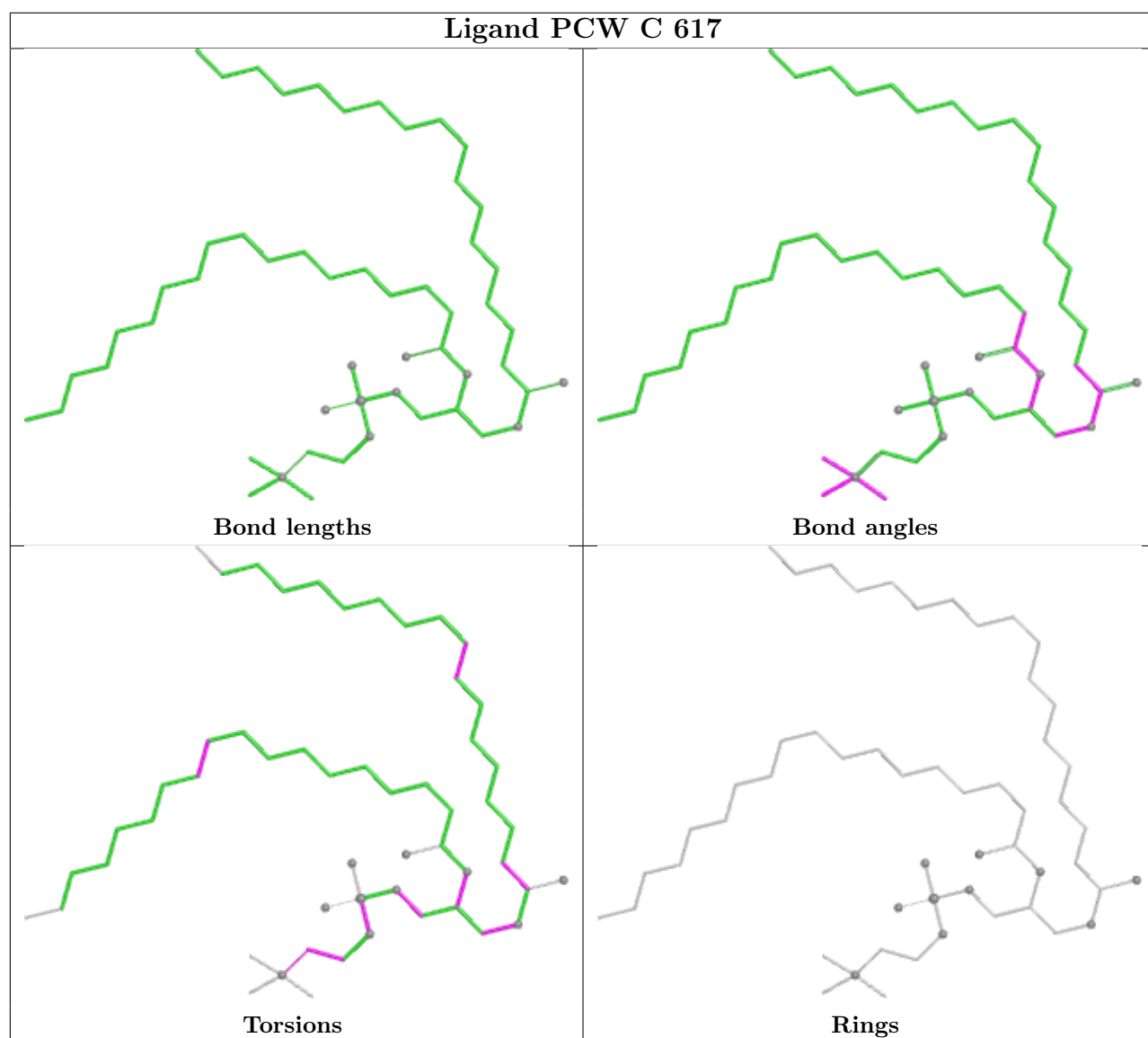


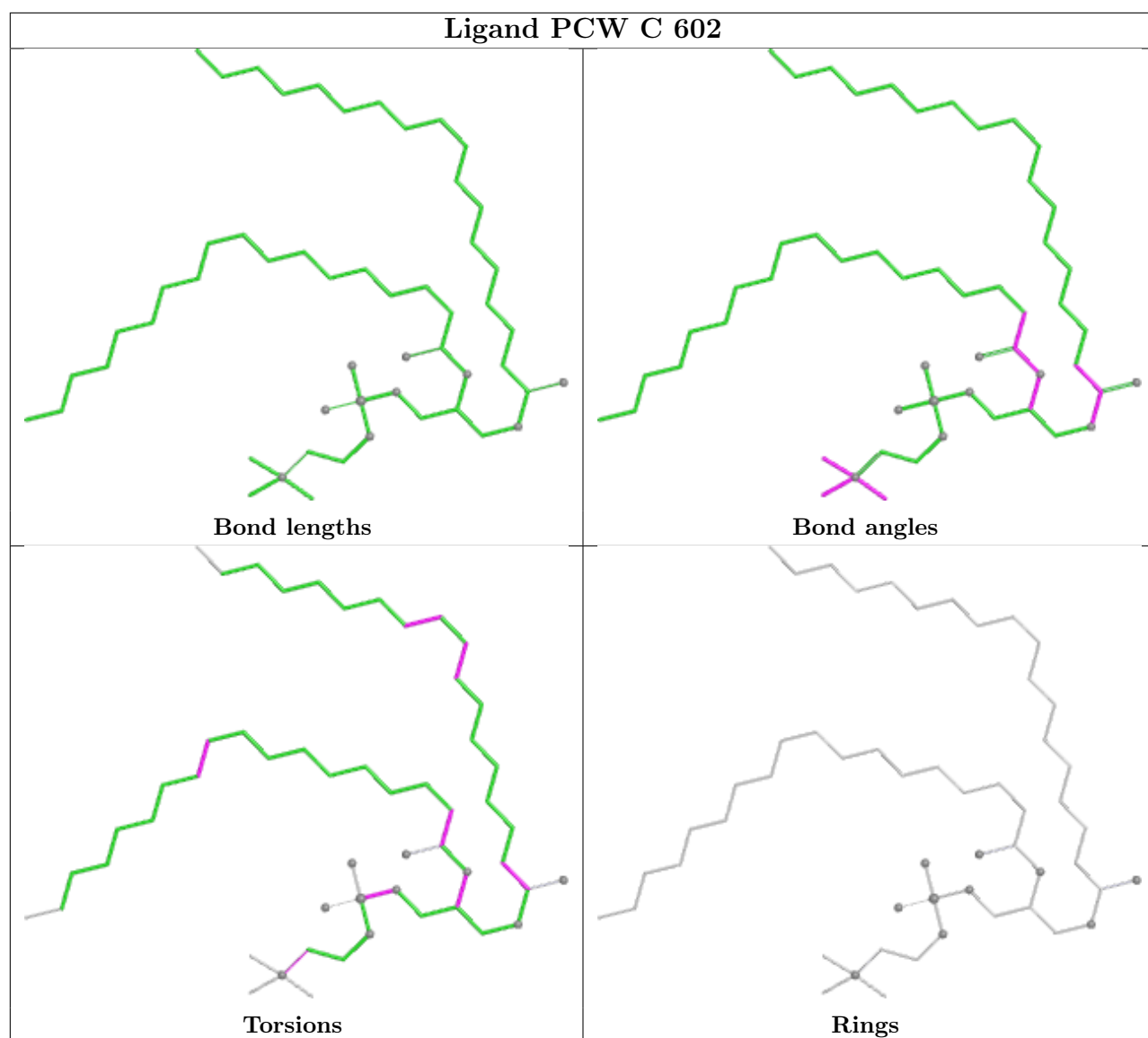


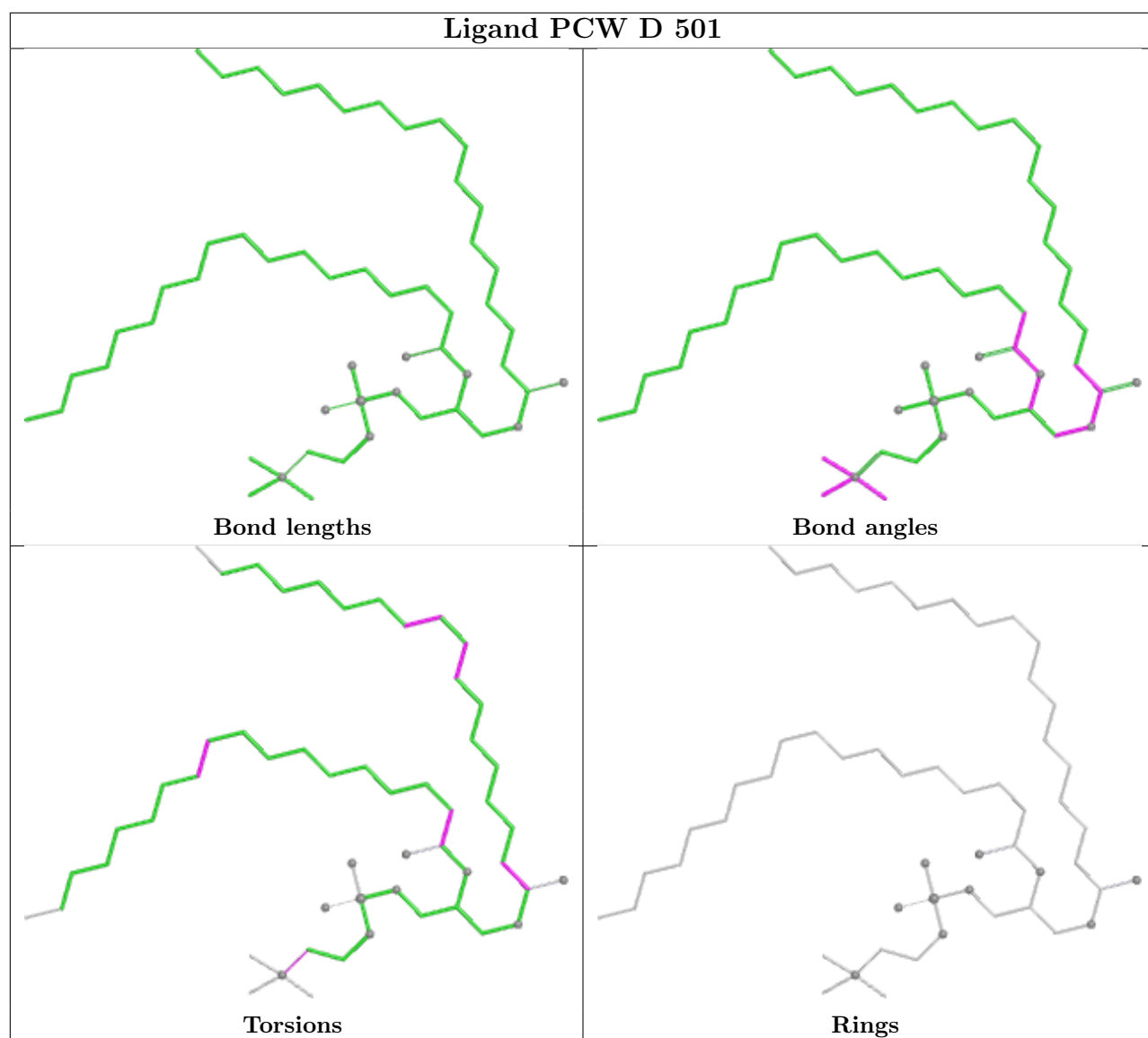


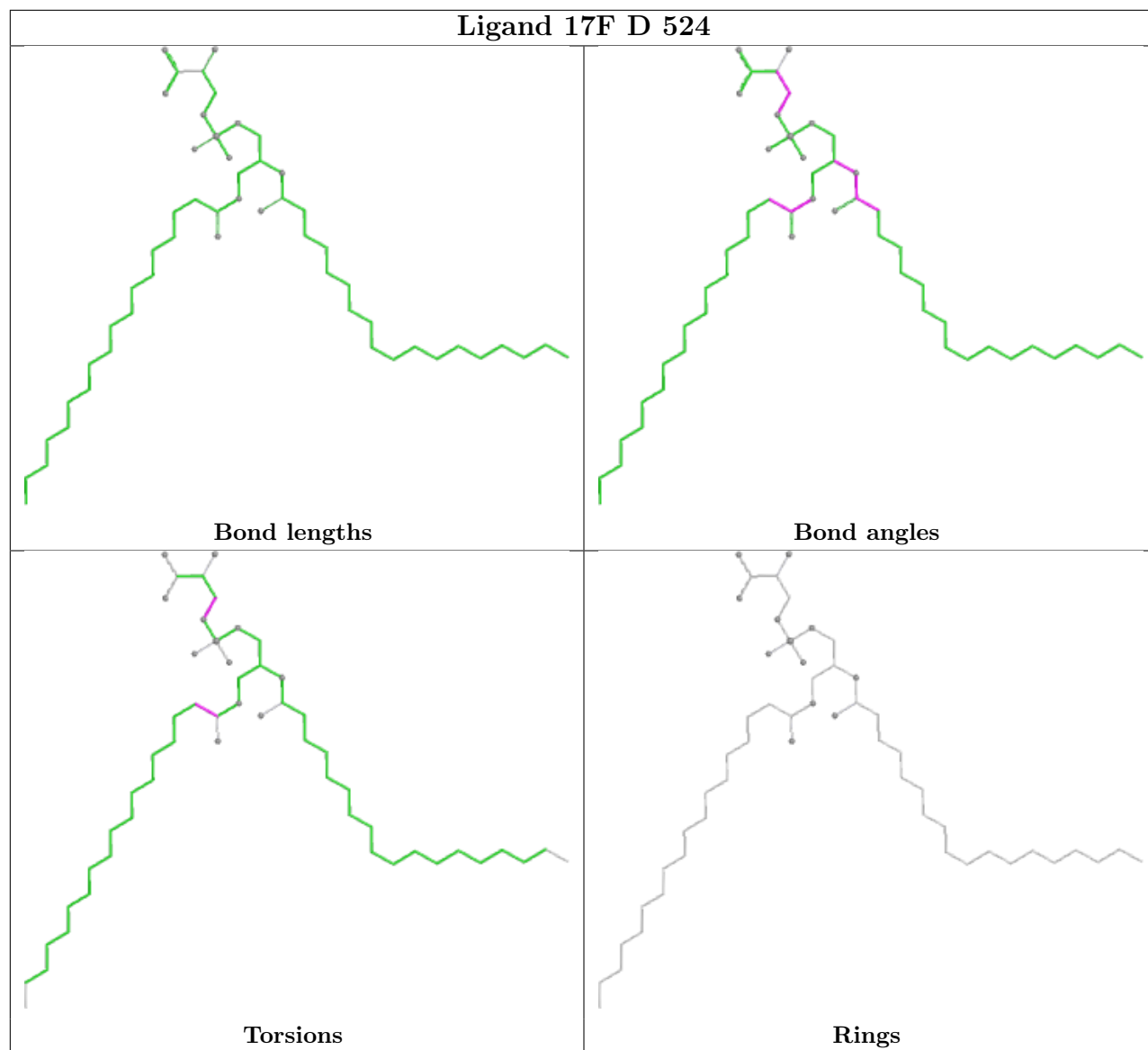


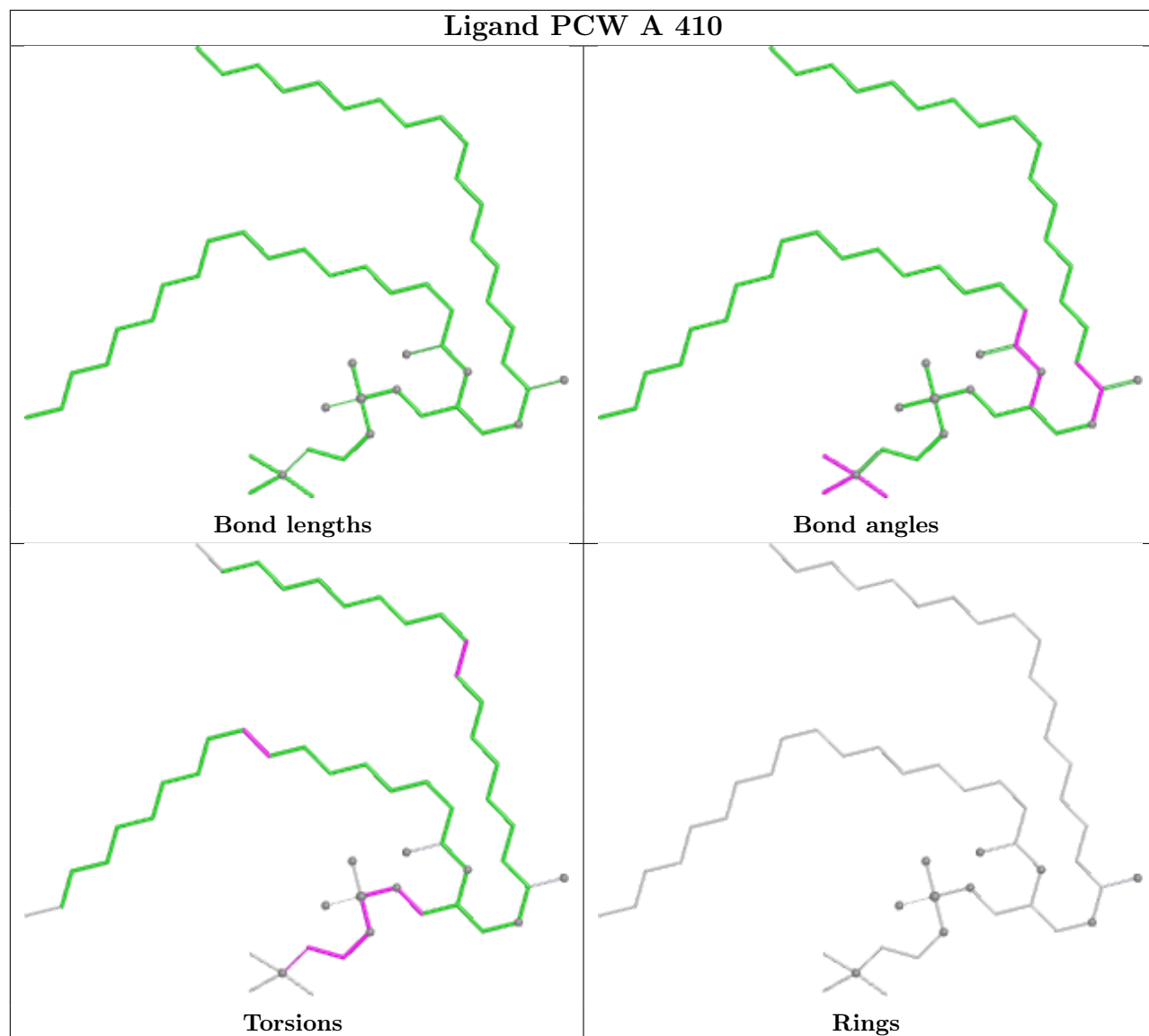


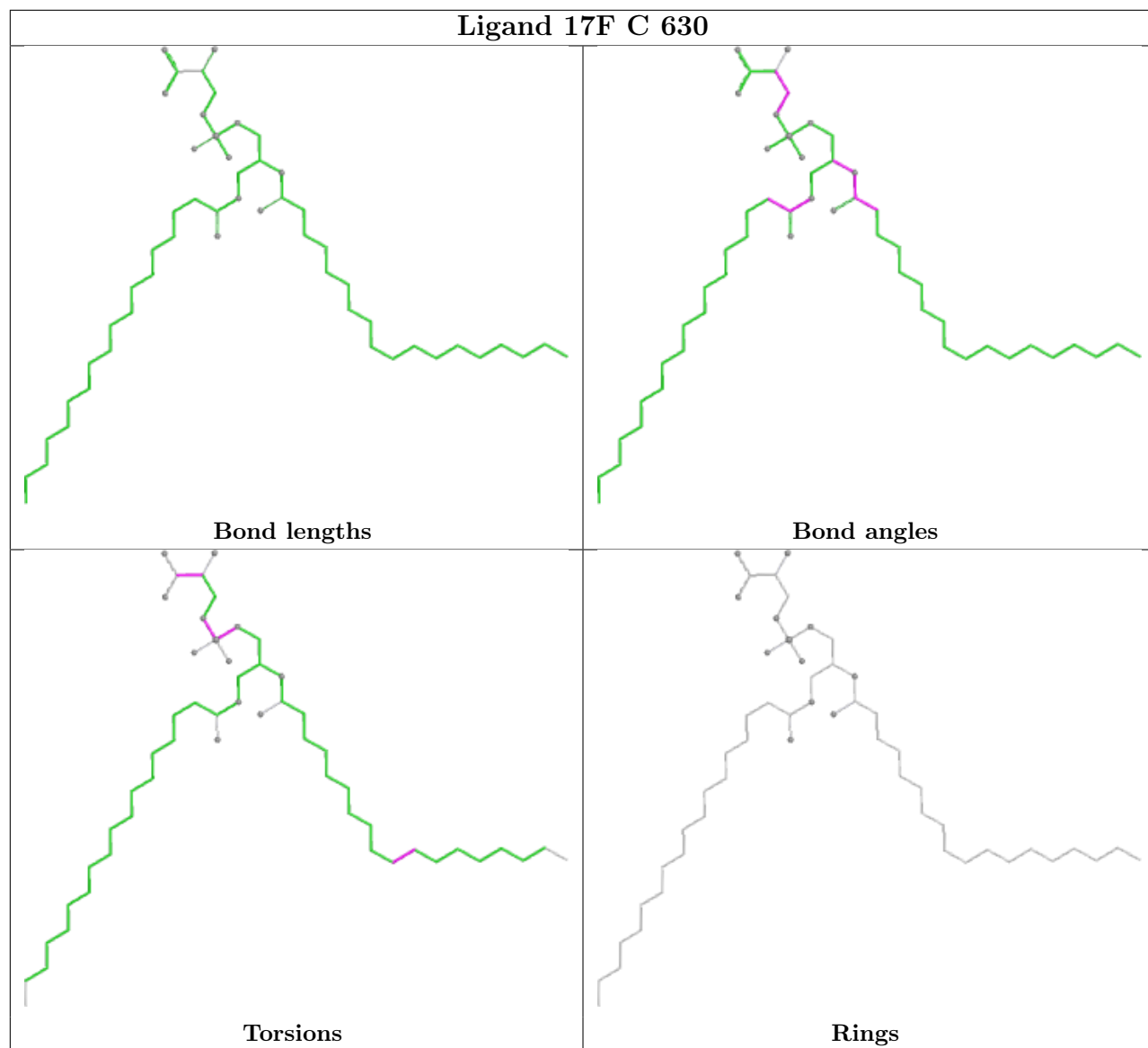


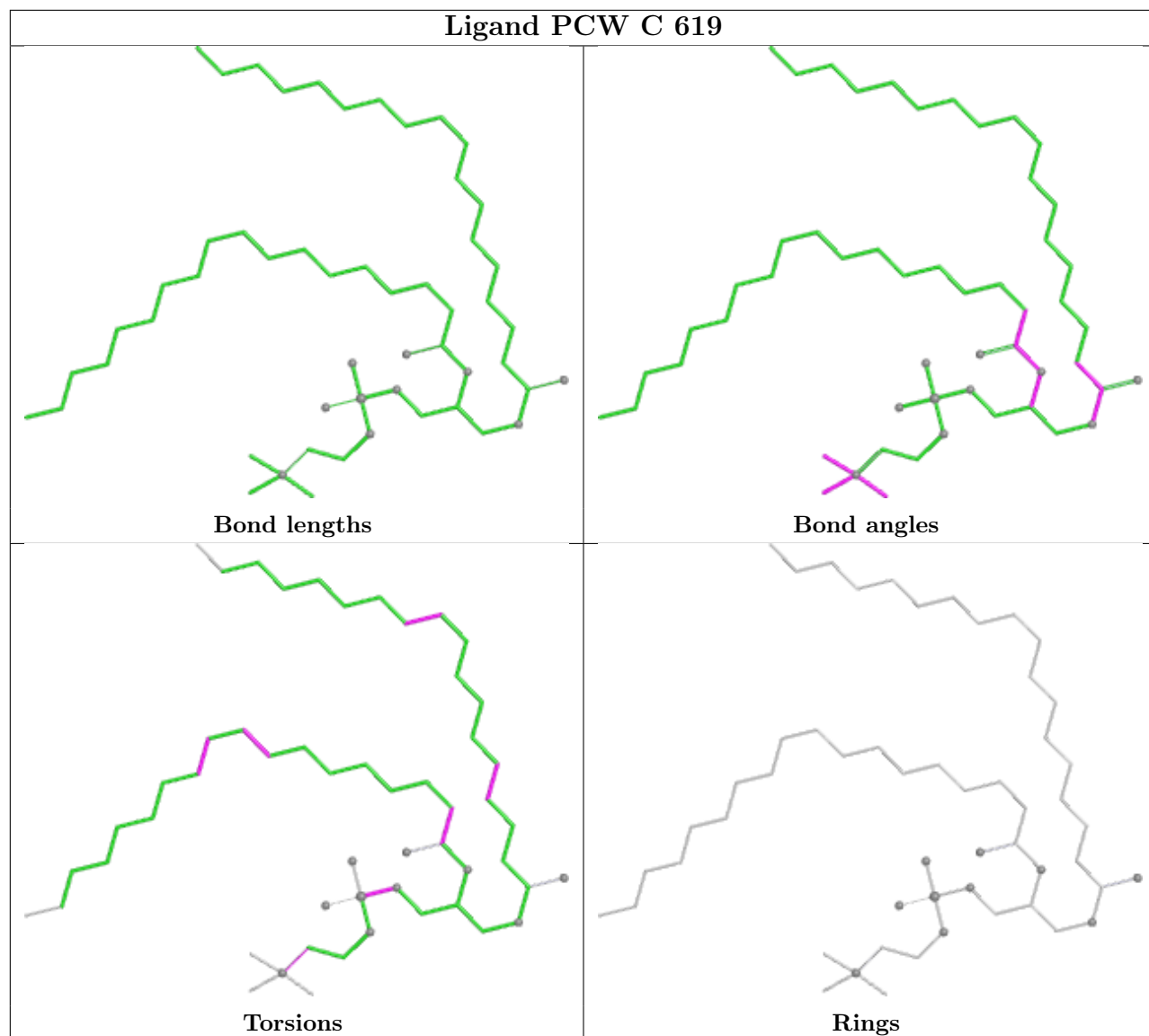


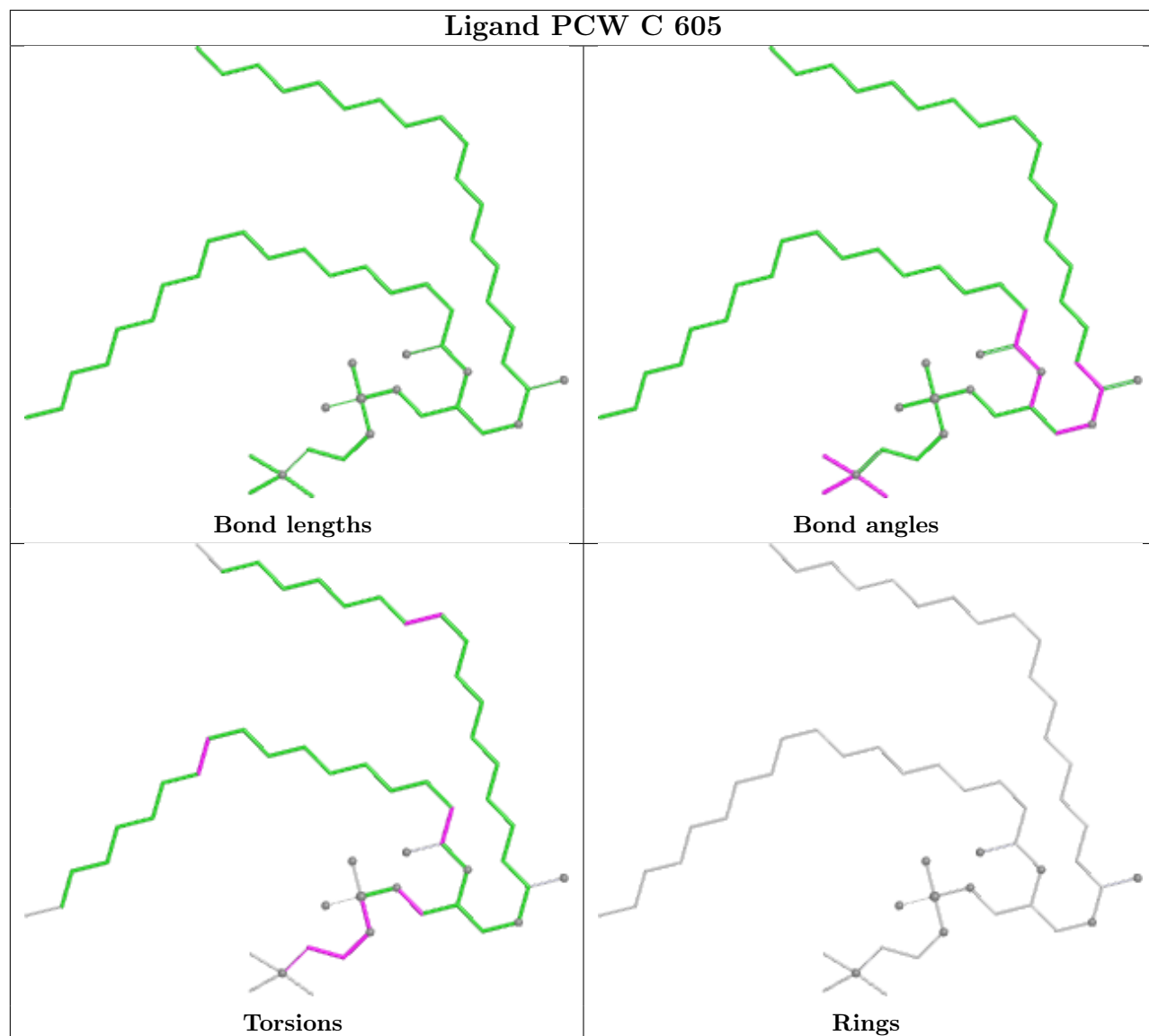


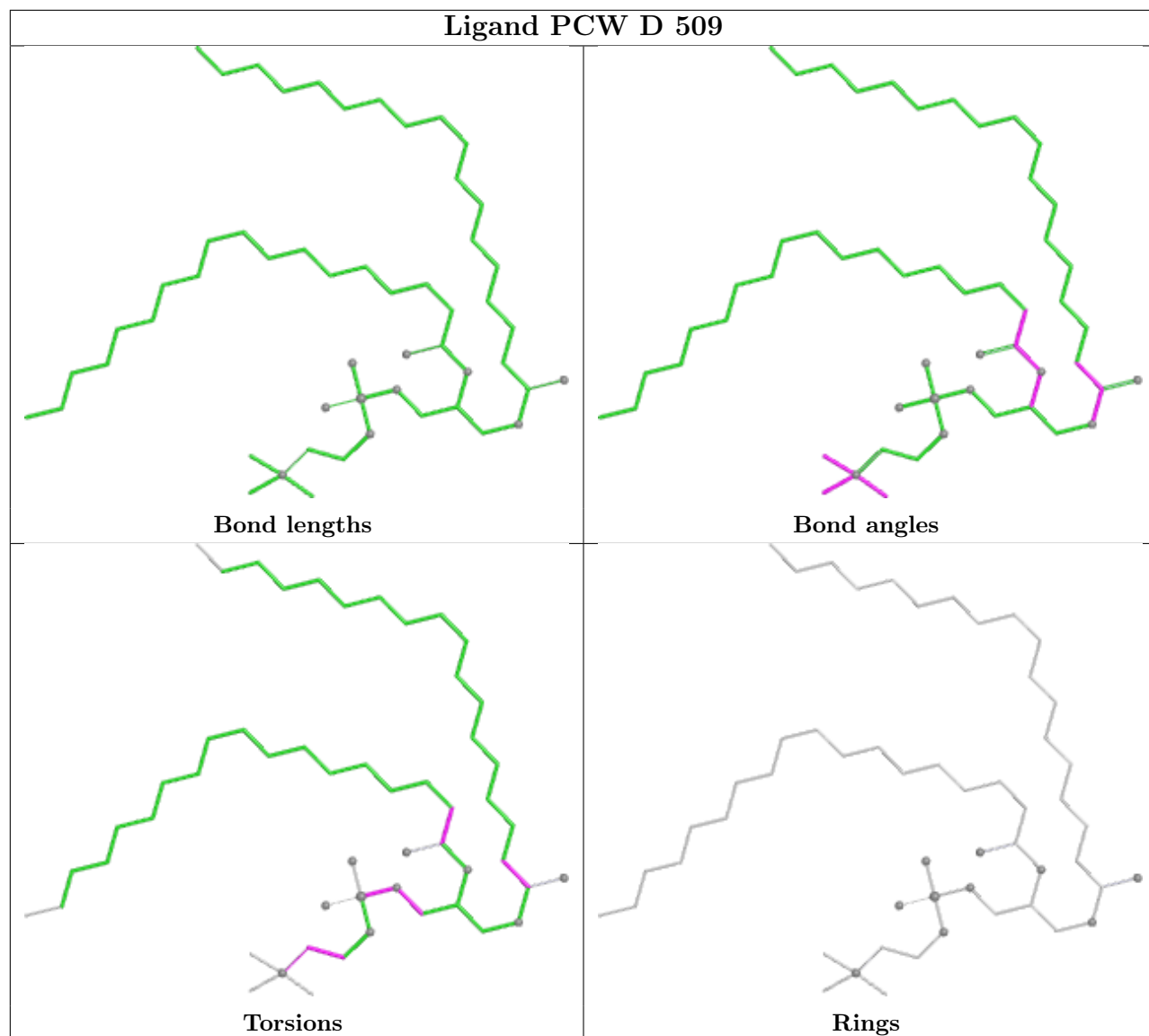


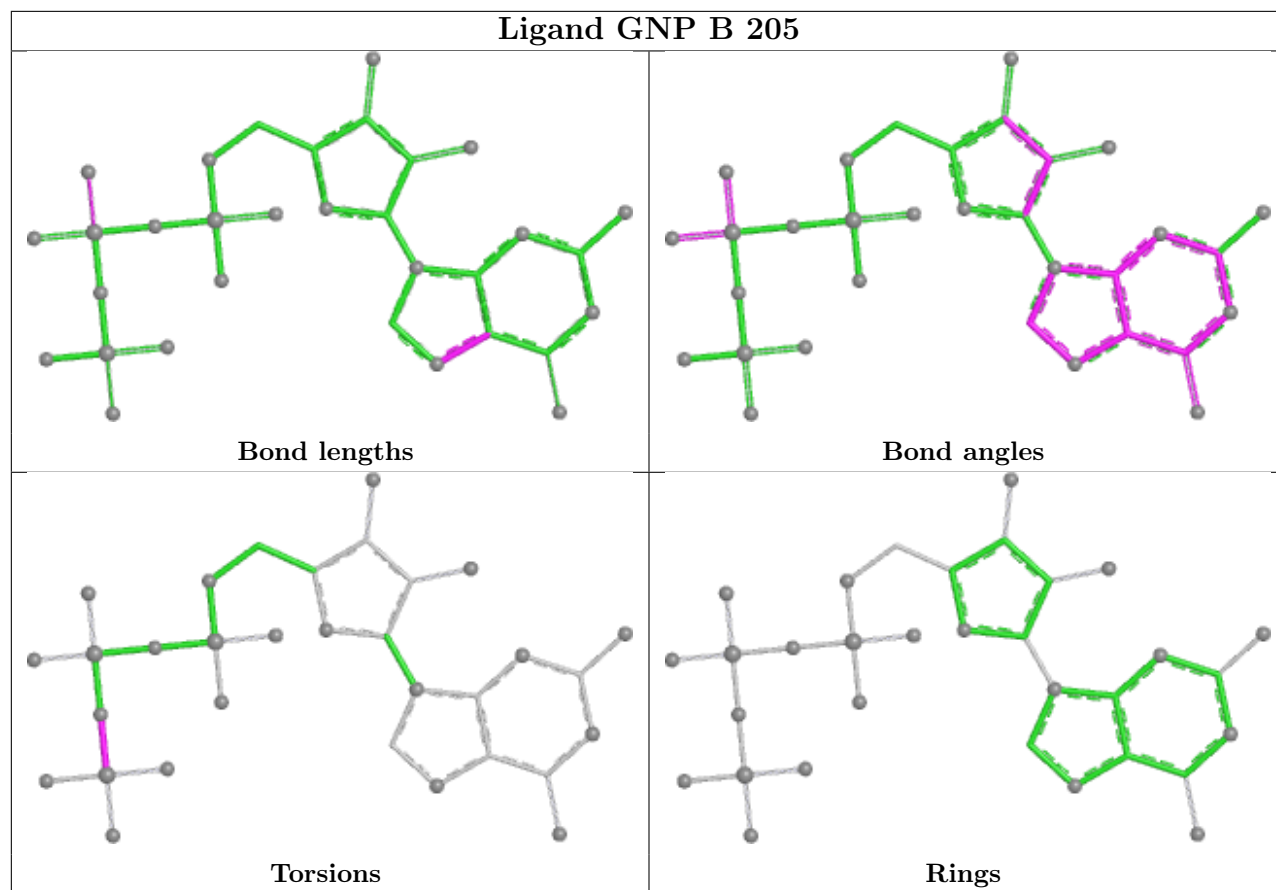


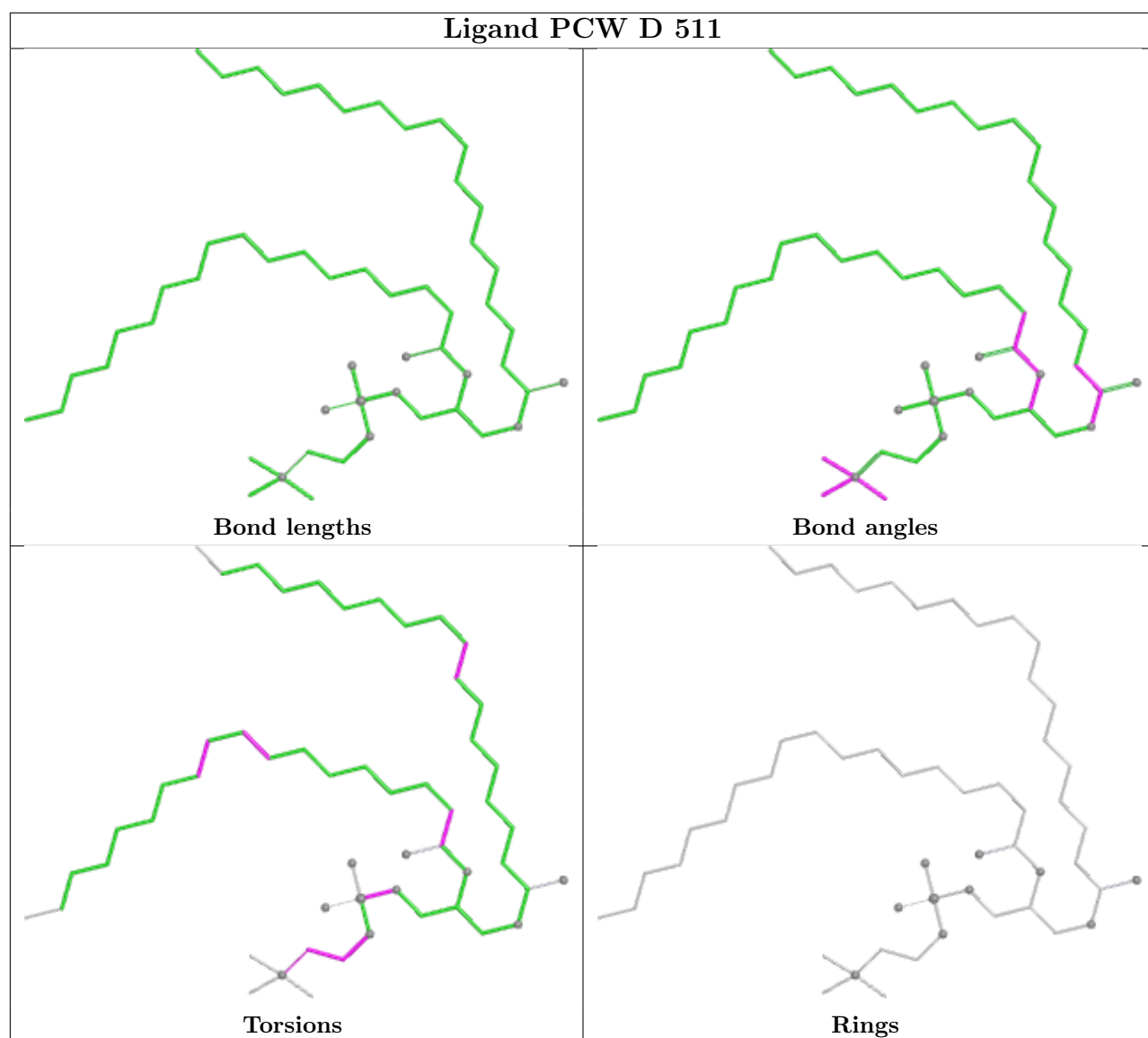


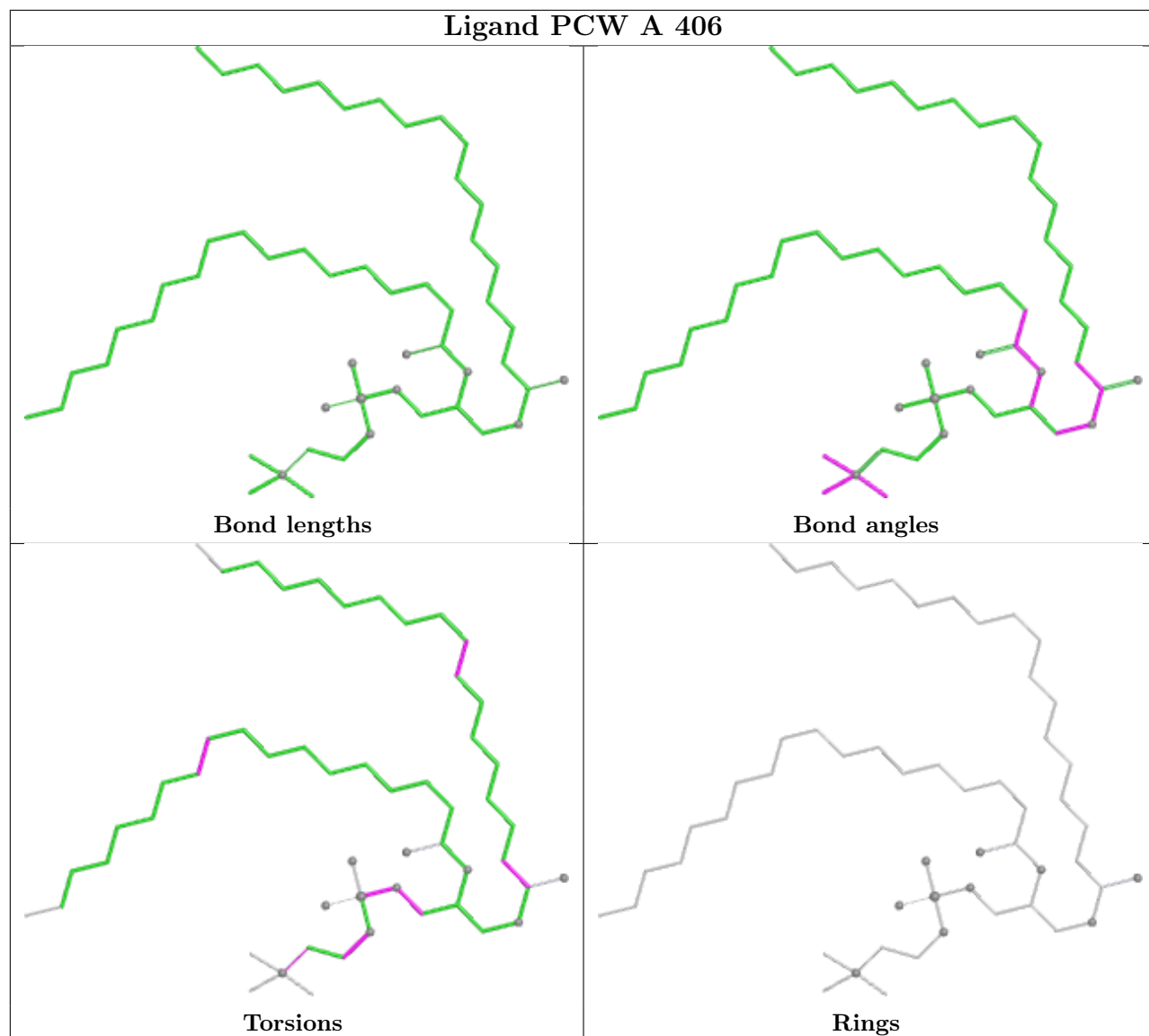


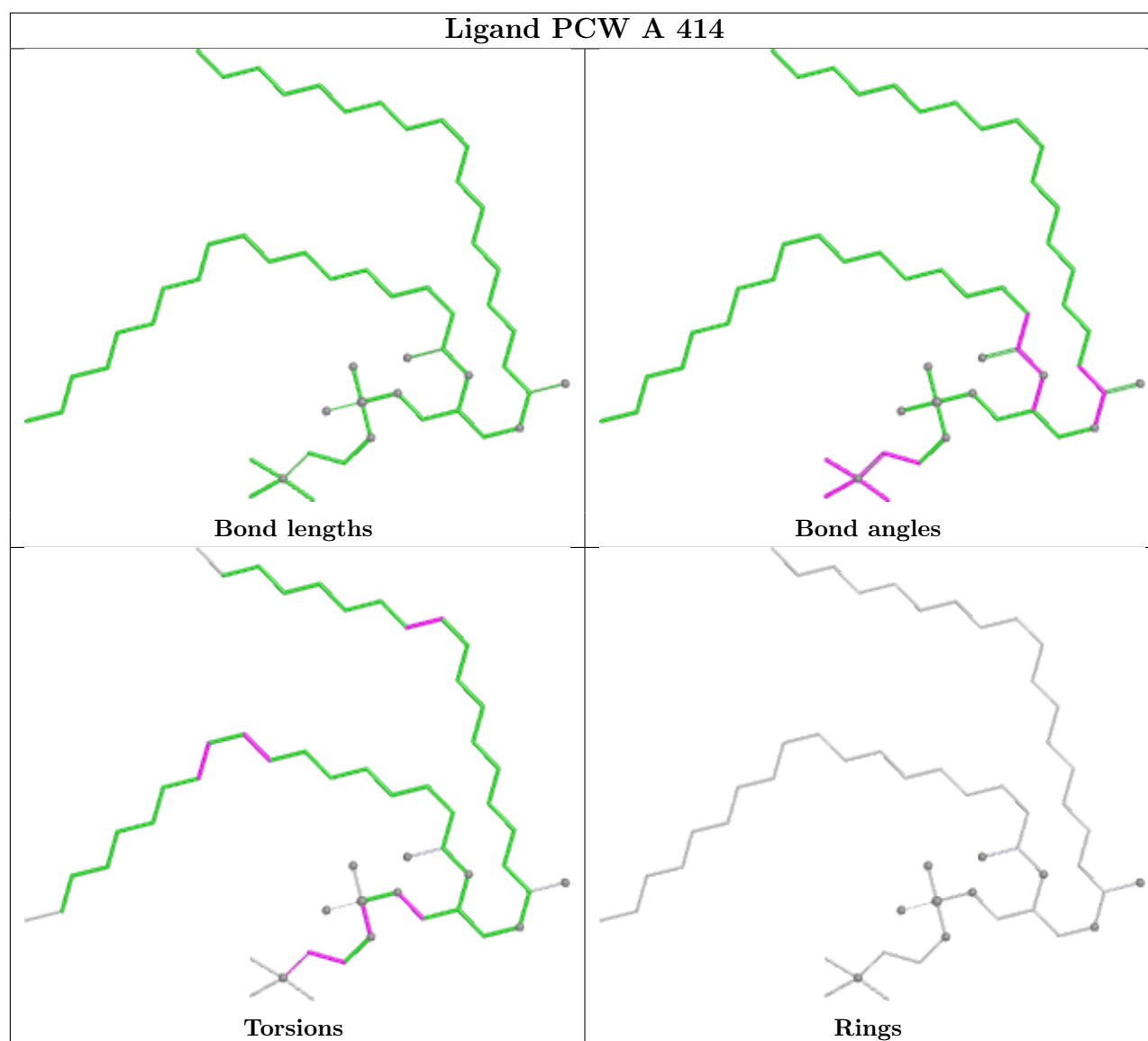












6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 6% for the well-defined parts and 6% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

7.1.1 Bookkeeping

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

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

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

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

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	401	LEU	HD21	0.714	.	.
1	C	401	LEU	HD22	0.714	.	.
1	C	401	LEU	HD23	0.714	.	.
1	B	6	LEU	HD21	0.982	.	.
1	B	6	LEU	HD22	0.982	.	.
1	B	6	LEU	HD23	0.982	.	.
1	B	19	LEU	HD11	0.65	.	.
1	B	19	LEU	HD12	0.65	.	.
1	B	19	LEU	HD13	0.65	.	.
1	B	21	ILE	HD11	0.649	.	1
1	B	21	ILE	HD12	0.649	.	1
1	B	21	ILE	HD13	0.649	.	1
1	B	23	LEU	HD11	-0.175	.	.
1	B	23	LEU	HD12	-0.175	.	.

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

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

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

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

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

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 6%, i.e. 555 atoms were assigned a chemical shift out of a possible 9668. 0 out of 128 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	394/3423 (12%)	197/1384 (14%)	0/1374 (0%)	197/665 (30%)
Sidechain	161/5595 (3%)	120/3599 (3%)	41/1743 (2%)	0/253 (0%)
Aromatic	0/650 (0%)	0/325 (0%)	0/295 (0%)	0/30 (0%)
Overall	555/9668 (6%)	317/5308 (6%)	41/3412 (1%)	197/948 (21%)

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

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

7.1.4 Statistically unusual chemical shifts [i](#)

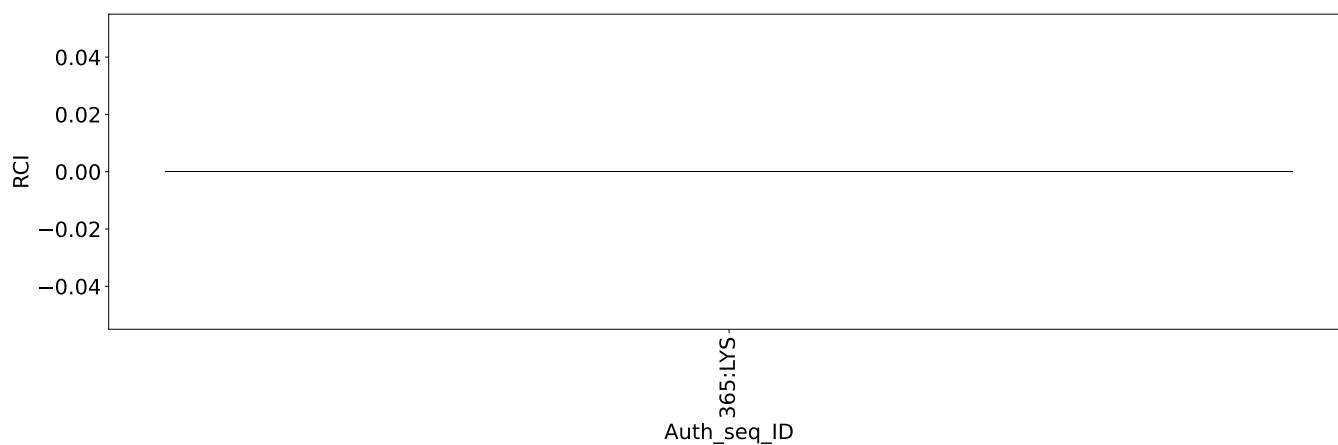
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

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

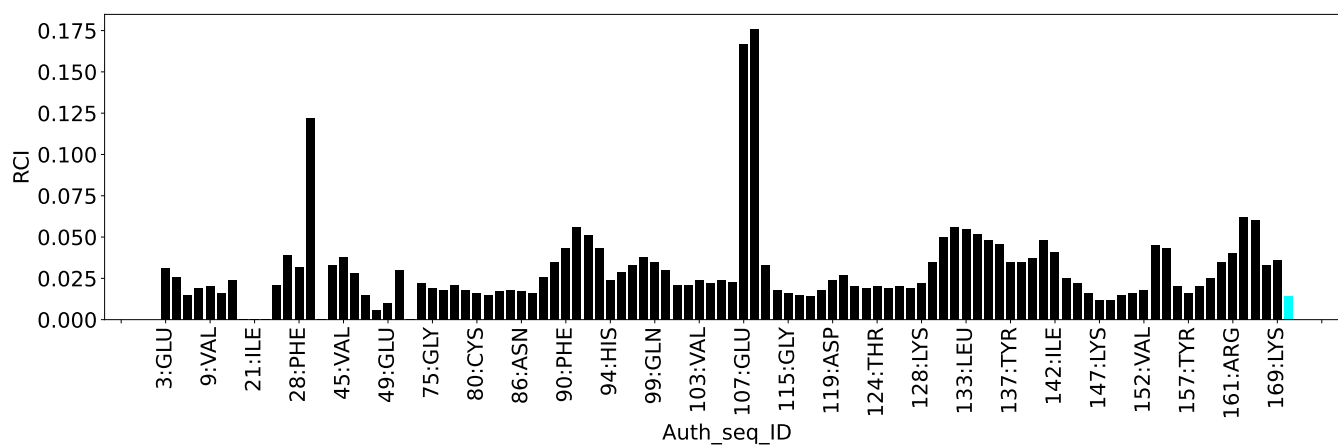
7.1.5 Random Coil Index (RCI) plots [i](#)

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

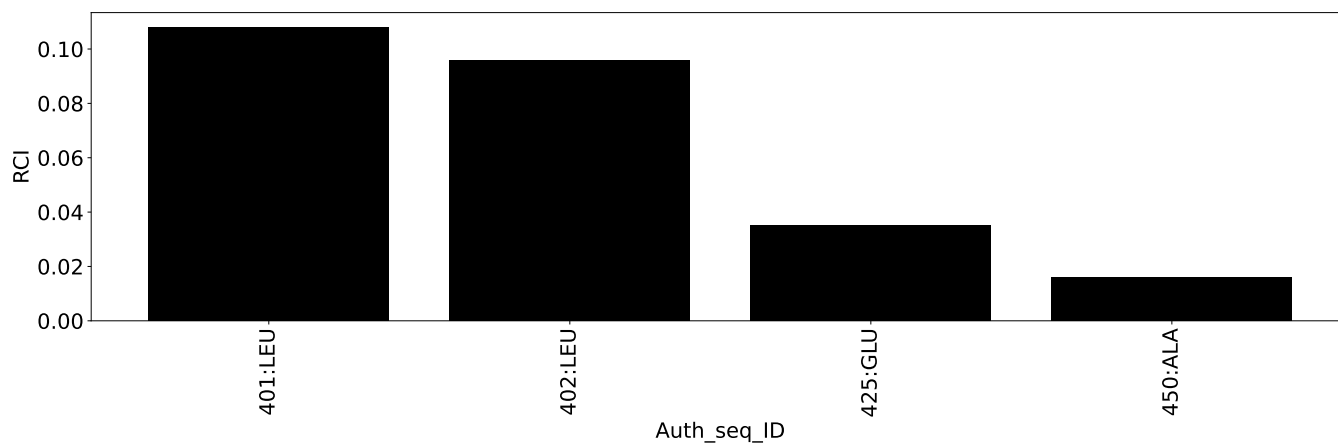
Random coil index (RCI) for chain A:



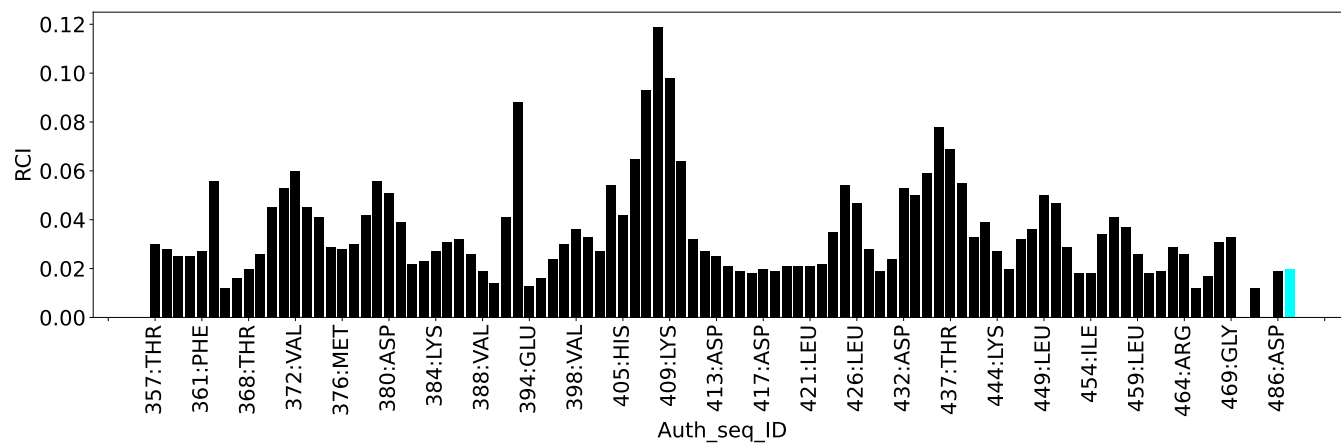
Random coil index (RCI) for chain B:



Random coil index (RCI) for chain C:



Random coil index (RCI) for chain D:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	51
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	2
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	0
Inter-chain	49
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.1
Number of long range restraints per residue ¹	0.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	None	None
0.2-0.5 (Medium)	0.1	0.28
>0.5 (Large)	48.5	33.47

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

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

9 Distance violation analysis ⓘ

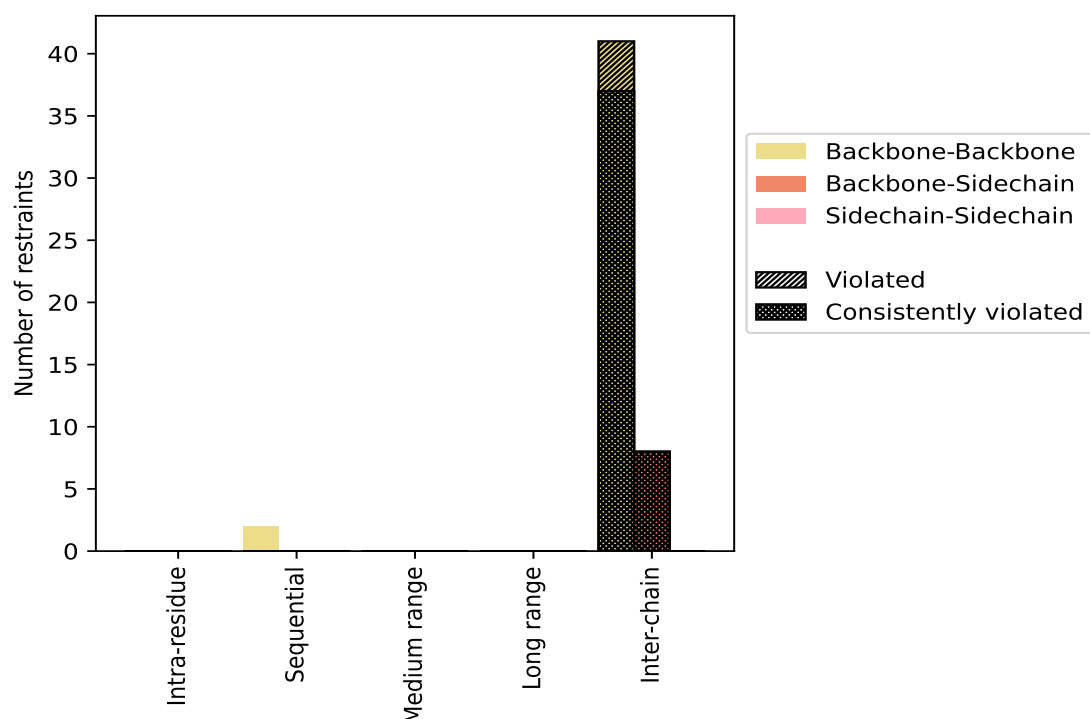
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	2	3.9	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	2	3.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	49	96.1	49	100.0	96.1	45	91.8	88.2
Backbone-Backbone	41	80.4	41	100.0	80.4	37	90.2	72.5
Backbone-Sidechain	8	15.7	8	100.0	15.7	8	100.0	15.7
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	51	100.0	49	96.1	96.1	45	88.2	88.2
Backbone-Backbone	43	84.3	41	95.3	80.4	37	86.0	72.5
Backbone-Sidechain	8	15.7	8	100.0	15.7	8	100.0	15.7
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0

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

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



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

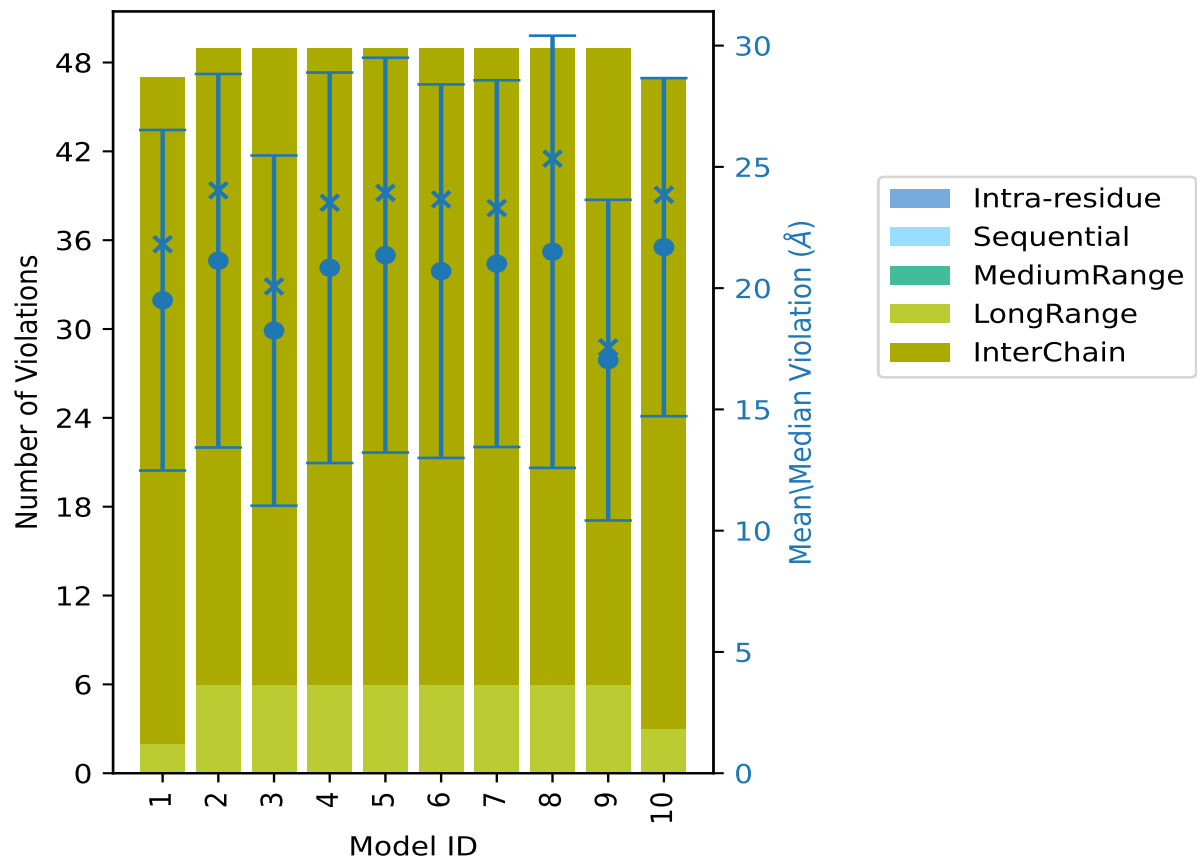
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	0	0	2	45	47	19.5	29.19	7.02	21.81
2	0	0	0	6	43	49	21.13	30.89	7.7	24.03
3	0	0	0	6	43	49	18.25	26.66	7.22	20.07
4	0	0	0	6	43	49	20.84	32.18	8.05	23.52
5	0	0	0	6	43	49	21.36	32.99	8.14	23.93
6	0	0	0	6	43	49	20.7	30.52	7.7	23.66
7	0	0	0	6	43	49	21.01	30.05	7.56	23.3
8	0	0	0	6	43	49	21.5	33.47	8.91	25.34
9	0	0	0	6	43	49	17.03	26.91	6.61	17.56
10	0	0	0	3	44	47	21.69	29.56	6.97	23.85

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, 2(IR:0, SQ:2, 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	0	0	2	20.0
0	0	0	0	0	0	3	30.0

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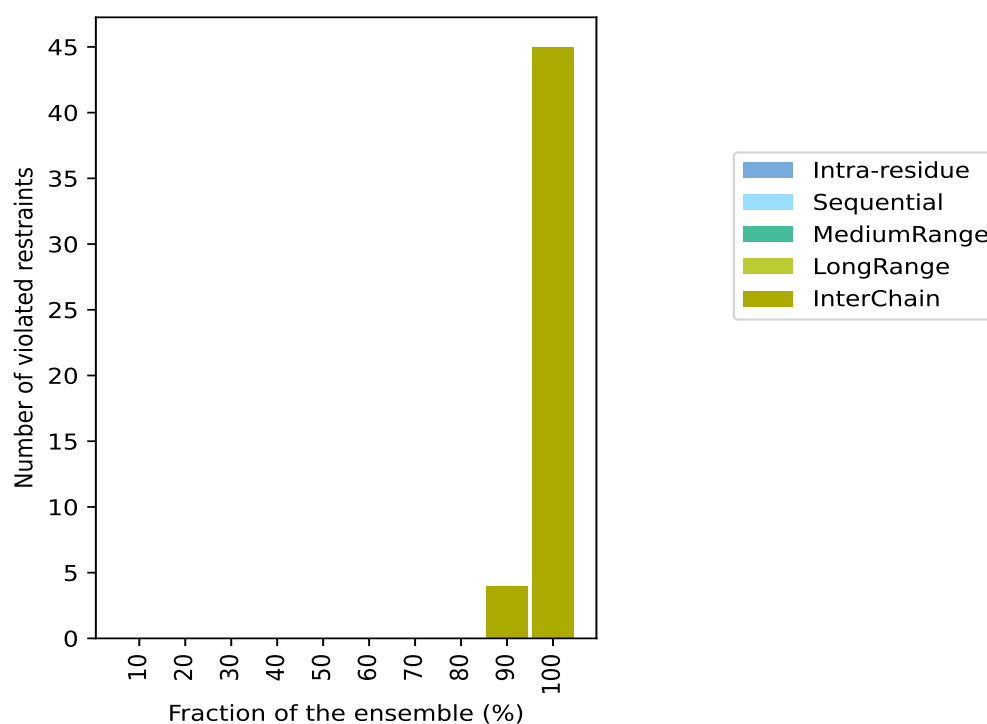
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	4	40.0
0	0	0	0	0	0	5	50.0
0	0	0	0	0	0	6	60.0
0	0	0	0	0	0	7	70.0
0	0	0	0	0	0	8	80.0
0	0	0	0	4	4	9	90.0
0	0	0	0	45	45	10	100.0

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 ⓘ

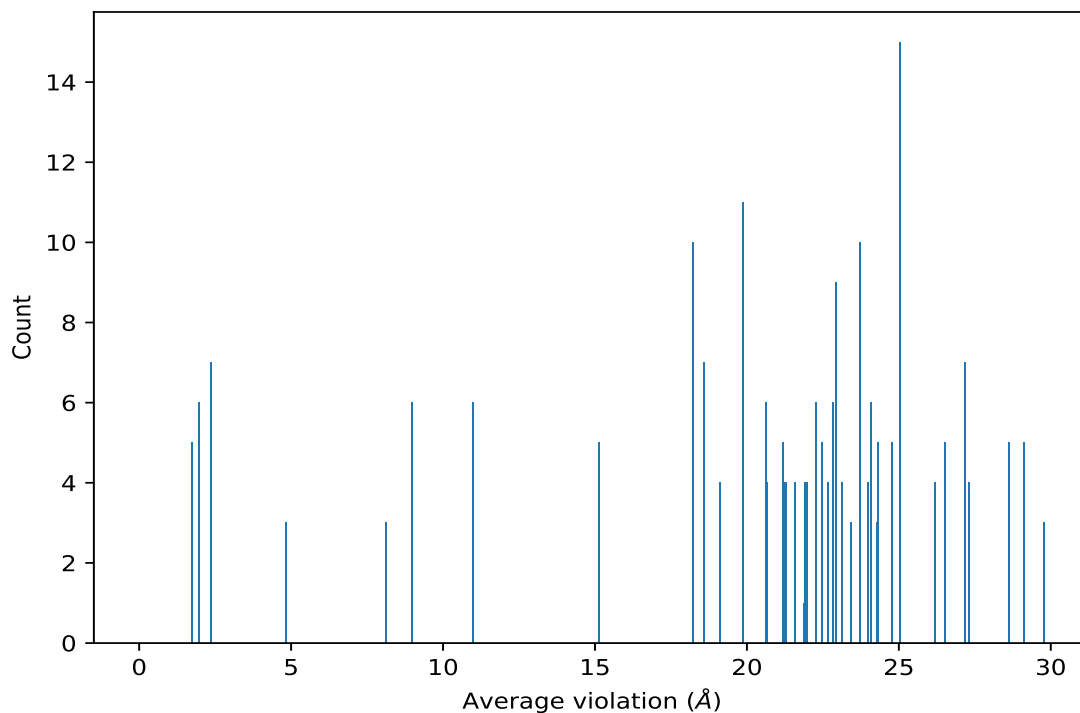


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1)	1:201:A:LEU:N	4:202:B:PCW:C6	10	29.79	2.64	30.04
(1,1)	1:201:A:LEU:N	4:202:B:PCW:C4	10	29.79	2.64	30.04
(1,1)	1:201:A:LEU:N	2:78:B:PHE:CE2	10	29.79	2.64	30.04
(1,5)	1:205:A:ASP:N	4:202:B:PCW:C6	10	29.14	1.72	29.44
(1,5)	1:205:A:ASP:N	4:202:B:PCW:C4	10	29.14	1.72	29.44
(1,5)	1:205:A:ASP:N	2:161:B:ARG:O	10	29.14	1.72	29.44
(1,5)	1:205:A:ASP:N	2:78:B:PHE:CE2	10	29.14	1.72	29.44
(1,5)	1:205:A:ASP:N	2:185:B:CYS:N	10	29.14	1.72	29.44
(1,6)	1:206:A:ASN:N	4:202:B:PCW:C6	10	28.64	1.43	28.82
(1,6)	1:206:A:ASN:N	4:202:B:PCW:C4	10	28.64	1.43	28.82
(1,6)	1:206:A:ASN:N	4:202:B:PCW:O3	10	28.64	1.43	28.82
(1,6)	1:206:A:ASN:N	4:202:B:PCW:C2	10	28.64	1.43	28.82
(1,6)	1:206:A:ASN:N	2:185:B:CYS:N	10	28.64	1.43	28.82
(1,4)	1:204:A:LEU:N	4:202:B:PCW:C6	10	27.3	1.66	27.58
(1,4)	1:204:A:LEU:N	4:202:B:PCW:C4	10	27.3	1.66	27.58

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4)	1:204:A:LEU:N	2:161:B:ARG:O	10	27.3	1.66	27.58
(1,4)	1:204:A:LEU:N	2:78:B:PHE:CE2	10	27.3	1.66	27.58
(1,9)	1:209:A:SER:N	4:202:B:PCW:C6	10	27.2	1.97	27.53
(1,9)	1:209:A:SER:N	4:202:B:PCW:O2	10	27.2	1.97	27.53
(1,9)	1:209:A:SER:N	2:185:B:CYS:H	10	27.2	1.97	27.53
(1,9)	1:209:A:SER:N	4:202:B:PCW:C4	10	27.2	1.97	27.53
(1,9)	1:209:A:SER:N	4:202:B:PCW:O3	10	27.2	1.97	27.53
(1,9)	1:209:A:SER:N	4:202:B:PCW:C2	10	27.2	1.97	27.53
(1,9)	1:209:A:SER:N	2:185:B:CYS:N	10	27.2	1.97	27.53
(1,8)	1:208:A:ASP:N	4:202:B:PCW:C6	10	26.54	1.86	26.95
(1,8)	1:208:A:ASP:N	4:202:B:PCW:C4	10	26.54	1.86	26.95
(1,8)	1:208:A:ASP:N	2:185:B:CYS:H	10	26.54	1.86	26.95
(1,8)	1:208:A:ASP:N	4:202:B:PCW:O3	10	26.54	1.86	26.95
(1,8)	1:208:A:ASP:N	2:185:B:CYS:N	10	26.54	1.86	26.95
(1,7)	1:207:A:TRP:N	4:202:B:PCW:C6	10	26.16	1.48	26.35
(1,7)	1:207:A:TRP:N	4:202:B:PCW:C4	10	26.16	1.48	26.35
(1,7)	1:207:A:TRP:N	4:202:B:PCW:O3	10	26.16	1.48	26.35
(1,7)	1:207:A:TRP:N	2:185:B:CYS:N	10	26.16	1.48	26.35
(1,34)	1:234:A:LYS:O	4:203:B:PCW:C3	10	25.04	1.54	25.54
(1,34)	1:234:A:LYS:O	4:203:B:PCW:O3	10	25.04	1.54	25.54
(1,34)	1:234:A:LYS:O	4:202:B:PCW:O3	10	25.04	1.54	25.54
(1,34)	1:234:A:LYS:O	2:185:B:CYS:HG	10	25.04	1.54	25.54
(1,37)	1:237:A:GLU:O	4:203:B:PCW:C3	10	25.03	1.47	25.27
(1,37)	1:237:A:GLU:O	4:203:B:PCW:O3	10	25.03	1.47	25.27
(1,37)	1:237:A:GLU:O	2:185:B:CYS:HG	10	25.03	1.47	25.27
(1,37)	1:237:A:GLU:O	4:202:B:PCW:O3	10	25.03	1.47	25.27
(1,12)	1:212:A:SER:N	4:202:B:PCW:C6	10	25.0	2.83	25.7
(1,12)	1:212:A:SER:N	4:202:B:PCW:O2	10	25.0	2.83	25.7
(1,12)	1:212:A:SER:N	2:185:B:CYS:H	10	25.0	2.83	25.7
(1,12)	1:212:A:SER:N	4:202:B:PCW:C4	10	25.0	2.83	25.7
(1,12)	1:212:A:SER:N	4:202:B:PCW:C7	10	25.0	2.83	25.7
(1,12)	1:212:A:SER:N	4:202:B:PCW:O3	10	25.0	2.83	25.7
(1,12)	1:212:A:SER:N	2:185:B:CYS:N	10	25.0	2.83	25.7
(1,13)	1:213:A:THR:N	4:202:B:PCW:C4	10	24.78	2.37	25.12
(1,13)	1:213:A:THR:N	4:202:B:PCW:O2	10	24.78	2.37	25.12
(1,13)	1:213:A:THR:N	2:185:B:CYS:H	10	24.78	2.37	25.12
(1,13)	1:213:A:THR:N	4:202:B:PCW:O3	10	24.78	2.37	25.12
(1,13)	1:213:A:THR:N	2:185:B:CYS:N	10	24.78	2.37	25.12
(1,46)	2:133:B:LEU:O	4:406:A:PCW:C8	10	24.31	2.84	24.52
(1,46)	2:133:B:LEU:O	4:404:A:PCW:C7	10	24.31	2.84	24.52
(1,46)	2:133:B:LEU:O	4:406:A:PCW:C6	10	24.31	2.84	24.52
(1,46)	2:133:B:LEU:O	4:406:A:PCW:C7	10	24.31	2.84	24.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,46)	2:133:B:LEU:O	4:407:A:PCW:C6	10	24.31	2.84	24.52
(1,40)	1:240:A:ARG:O	4:203:B:PCW:O3	10	24.26	1.2	24.24
(1,40)	1:240:A:ARG:O	4:203:B:PCW:C6	10	24.26	1.2	24.24
(1,40)	1:240:A:ARG:O	2:185:B:CYS:HG	10	24.26	1.2	24.24
(1,16)	1:216:A:LYS:N	4:202:B:PCW:C7	10	24.07	3.54	25.0
(1,16)	1:216:A:LYS:N	4:202:B:PCW:O2	10	24.07	3.54	25.0
(1,16)	1:216:A:LYS:N	2:185:B:CYS:H	10	24.07	3.54	25.0
(1,16)	1:216:A:LYS:N	4:202:B:PCW:O3	10	24.07	3.54	25.0
(1,16)	1:216:A:LYS:N	4:202:B:PCW:C4	10	24.07	3.54	25.0
(1,16)	1:216:A:LYS:N	2:185:B:CYS:CB	10	24.07	3.54	25.0
(1,31)	1:231:A:ASN:N	4:203:B:PCW:C3	10	23.98	2.33	24.27
(1,31)	1:231:A:ASN:N	4:202:B:PCW:O3	10	23.98	2.33	24.27
(1,31)	1:231:A:ASN:N	4:203:B:PCW:O3	10	23.98	2.33	24.27
(1,31)	1:231:A:ASN:N	2:185:B:CYS:HG	10	23.98	2.33	24.27
(1,33)	1:233:A:GLU:O	4:203:B:PCW:C3	10	23.74	2.02	24.44
(1,33)	1:233:A:GLU:O	4:202:B:PCW:O3	10	23.74	2.02	24.44
(1,33)	1:233:A:GLU:O	4:203:B:PCW:O3	10	23.74	2.02	24.44
(1,33)	1:233:A:GLU:O	2:185:B:CYS:HG	10	23.74	2.02	24.44
(1,11)	1:211:A:THR:N	4:202:B:PCW:C6	10	23.74	1.91	23.94
(1,11)	1:211:A:THR:N	4:202:B:PCW:O2	10	23.74	1.91	23.94
(1,11)	1:211:A:THR:N	2:185:B:CYS:H	10	23.74	1.91	23.94
(1,11)	1:211:A:THR:N	4:202:B:PCW:C4	10	23.74	1.91	23.94
(1,11)	1:211:A:THR:N	4:202:B:PCW:O3	10	23.74	1.91	23.94
(1,11)	1:211:A:THR:N	2:185:B:CYS:N	10	23.74	1.91	23.94
(1,27)	1:227:A:GLU:N	4:202:B:PCW:O3	10	23.42	3.32	24.35
(1,27)	1:227:A:GLU:N	2:185:B:CYS:N	10	23.42	3.32	24.35
(1,27)	1:227:A:GLU:N	2:185:B:CYS:HG	10	23.42	3.32	24.35
(1,23)	1:223:A:PRO:N	4:202:B:PCW:O3	10	23.14	4.29	24.6
(1,23)	1:223:A:PRO:N	2:185:B:CYS:H	10	23.14	4.29	24.6
(1,23)	1:223:A:PRO:N	4:202:B:PCW:C7	10	23.14	4.29	24.6
(1,23)	1:223:A:PRO:N	2:185:B:CYS:HG	10	23.14	4.29	24.6
(1,30)	1:230:A:ASP:N	4:202:B:PCW:O3	10	22.91	2.87	23.4
(1,30)	1:230:A:ASP:N	2:185:B:CYS:O	10	22.91	2.87	23.4
(1,30)	1:230:A:ASP:N	4:203:B:PCW:C3	10	22.91	2.87	23.4
(1,30)	1:230:A:ASP:N	2:185:B:CYS:HG	10	22.91	2.87	23.4
(1,17)	1:217:A:LEU:N	4:202:B:PCW:C4	10	22.91	2.67	23.48
(1,17)	1:217:A:LEU:N	4:202:B:PCW:O3	10	22.91	2.67	23.48
(1,17)	1:217:A:LEU:N	2:185:B:CYS:H	10	22.91	2.67	23.48
(1,17)	1:217:A:LEU:N	4:202:B:PCW:C7	10	22.91	2.67	23.48
(1,17)	1:217:A:LEU:N	2:185:B:CYS:SG	10	22.91	2.67	23.48
(1,10)	4:403:A:PCW:C8	2:47:B:ASP:O	10	22.84	4.46	24.88
(1,10)	1:210:A:VAL:N	4:202:B:PCW:O2	10	22.84	4.46	24.88

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,10)	1:210:A:VAL:N	4:202:B:PCW:O3	10	22.84	4.46	24.88
(1,10)	1:210:A:VAL:N	4:202:B:PCW:C4	10	22.84	4.46	24.88
(1,10)	4:403:A:PCW:C8	2:160:B:VAL:CG1	10	22.84	4.46	24.88
(1,10)	1:210:A:VAL:N	2:185:B:CYS:N	10	22.84	4.46	24.88
(1,24)	1:224:A:VAL:N	4:202:B:PCW:O3	10	22.66	3.15	23.4
(1,24)	1:224:A:VAL:N	2:185:B:CYS:H	10	22.66	3.15	23.4
(1,24)	1:224:A:VAL:N	4:202:B:PCW:C7	10	22.66	3.15	23.4
(1,24)	1:224:A:VAL:N	2:185:B:CYS:HG	10	22.66	3.15	23.4
(1,14)	1:214:A:PHE:N	4:202:B:PCW:C4	10	22.47	2.03	22.58
(1,14)	1:214:A:PHE:N	4:202:B:PCW:O2	10	22.47	2.03	22.58
(1,14)	1:214:A:PHE:N	2:185:B:CYS:H	10	22.47	2.03	22.58
(1,14)	1:214:A:PHE:N	4:202:B:PCW:O3	10	22.47	2.03	22.58
(1,14)	1:214:A:PHE:N	2:185:B:CYS:N	10	22.47	2.03	22.58
(1,28)	1:228:A:PHE:N	4:202:B:PCW:O3	10	22.28	2.4	22.49
(1,28)	1:228:A:PHE:N	2:185:B:CYS:HG	10	22.28	2.4	22.49
(1,35)	1:235:A:GLU:O	4:203:B:PCW:C3	10	22.28	1.16	22.44
(1,35)	1:235:A:GLU:O	4:203:B:PCW:O3	10	22.28	1.16	22.44
(1,35)	1:235:A:GLU:O	2:185:B:CYS:HG	10	22.28	1.16	22.44
(1,35)	1:235:A:GLU:O	4:202:B:PCW:O3	10	22.28	1.16	22.44
(1,32)	1:232:A:LEU:N	4:203:B:PCW:C3	10	21.96	1.78	22.1
(1,32)	1:232:A:LEU:N	4:202:B:PCW:O3	10	21.96	1.78	22.1
(1,32)	1:232:A:LEU:N	4:203:B:PCW:O3	10	21.96	1.78	22.1
(1,32)	1:232:A:LEU:N	2:185:B:CYS:HG	10	21.96	1.78	22.1
(1,36)	1:236:A:THR:O	4:203:B:PCW:C3	10	21.92	1.36	22.07
(1,36)	1:236:A:THR:O	4:203:B:PCW:O3	10	21.92	1.36	22.07
(1,36)	1:236:A:THR:O	2:185:B:CYS:HG	10	21.92	1.36	22.07
(1,36)	1:236:A:THR:O	4:202:B:PCW:O3	10	21.92	1.36	22.07
(1,39)	1:239:A:LEU:O	4:203:B:PCW:O3	10	21.87	1.16	21.88
(1,26)	1:226:A:GLN:N	4:202:B:PCW:O3	10	21.58	3.45	22.55
(1,26)	1:226:A:GLN:N	2:185:B:CYS:H	10	21.58	3.45	22.55
(1,26)	1:226:A:GLN:N	4:202:B:PCW:C7	10	21.58	3.45	22.55
(1,26)	1:226:A:GLN:N	2:185:B:CYS:HG	10	21.58	3.45	22.55
(1,22)	1:222:A:GLY:N	4:202:B:PCW:C7	10	21.27	3.73	22.41
(1,22)	1:222:A:GLY:N	4:202:B:PCW:O3	10	21.27	3.73	22.41
(1,22)	1:222:A:GLY:N	2:185:B:CYS:H	10	21.27	3.73	22.41
(1,22)	1:222:A:GLY:N	2:185:B:CYS:SG	10	21.27	3.73	22.41
(1,2)	4:401:A:PCW:C6	2:45:B:VAL:CG2	10	21.22	6.7	18.97
(1,2)	4:401:A:PCW:C6	2:25:B:GLN:HE22	10	21.22	6.7	18.97
(1,2)	1:202:A:LYS:N	4:202:B:PCW:C4	10	21.22	6.7	18.97
(1,2)	4:401:A:PCW:C6	2:47:B:ASP:O	10	21.22	6.7	18.97
(1,18)	1:218:A:ARG:N	4:202:B:PCW:C7	10	21.17	2.87	21.77
(1,18)	1:218:A:ARG:N	4:202:B:PCW:O3	10	21.17	2.87	21.77

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,18)	1:218:A:ARG:N	2:185:B:CYS:H	10	21.17	2.87	21.77
(1,18)	1:218:A:ARG:N	4:202:B:PCW:C4	10	21.17	2.87	21.77
(1,18)	1:218:A:ARG:N	2:185:B:CYS:SG	10	21.17	2.87	21.77
(1,25)	1:225:A:THR:N	4:202:B:PCW:O3	10	20.66	2.71	21.06
(1,25)	1:225:A:THR:N	2:185:B:CYS:H	10	20.66	2.71	21.06
(1,25)	1:225:A:THR:N	4:202:B:PCW:C7	10	20.66	2.71	21.06
(1,25)	1:225:A:THR:N	2:185:B:CYS:HG	10	20.66	2.71	21.06
(1,47)	2:142:B:ILE:H	4:406:A:PCW:C8	10	20.6	2.24	20.27
(1,47)	2:142:B:ILE:CG1	4:406:A:PCW:C8	10	20.6	2.24	20.27
(1,47)	2:142:B:ILE:CG1	4:404:A:PCW:C7	10	20.6	2.24	20.27
(1,47)	2:142:B:ILE:CG1	4:408:A:PCW:C6	10	20.6	2.24	20.27
(1,47)	2:142:B:ILE:CG1	4:406:A:PCW:C7	10	20.6	2.24	20.27
(1,47)	2:142:B:ILE:CG1	4:407:A:PCW:C6	10	20.6	2.24	20.27
(1,21)	1:221:A:LEU:N	4:202:B:PCW:O3	10	19.89	4.42	21.92
(1,21)	1:221:A:LEU:N	2:185:B:CYS:H	10	19.89	4.42	21.92
(1,21)	1:221:A:LEU:N	4:202:B:PCW:C7	10	19.89	4.42	21.92
(1,21)	4:407:A:PCW:C7	2:160:B:VAL:O	10	19.89	4.42	21.92
(1,21)	1:221:A:LEU:N	2:185:B:CYS:SG	10	19.89	4.42	21.92
(1,38)	5:409:A:17F:O4	2:45:B:VAL:CG1	10	19.85	4.38	19.2
(1,38)	1:238:A:GLY:O	4:203:B:PCW:O3	10	19.85	4.38	19.2
(1,38)	5:409:A:17F:O5	2:25:B:GLN:HE21	10	19.85	4.38	19.2
(1,38)	5:409:A:17F:N1	2:25:B:GLN:HE22	10	19.85	4.38	19.2
(1,38)	5:409:A:17F:O5	2:47:B:ASP:O	10	19.85	4.38	19.2
(1,38)	5:409:A:17F:O4	2:25:B:GLN:HE21	10	19.85	4.38	19.2
(1,45)	2:113:B:LEU:N	4:406:A:PCW:C8	10	19.11	2.7	18.96
(1,45)	2:113:B:LEU:H	4:404:A:PCW:C7	10	19.11	2.7	18.96
(1,45)	2:113:B:LEU:N	4:406:A:PCW:C7	10	19.11	2.7	18.96
(1,45)	2:113:B:LEU:H	4:407:A:PCW:C6	10	19.11	2.7	18.96
(1,41)	2:23:B:LEU:CD2	4:406:A:PCW:C8	10	18.59	3.3	18.8
(1,41)	2:23:B:LEU:O	4:404:A:PCW:C7	10	18.59	3.3	18.8
(1,41)	2:23:B:LEU:CD2	4:404:A:PCW:C7	10	18.59	3.3	18.8
(1,41)	2:23:B:LEU:CD2	4:406:A:PCW:C7	10	18.59	3.3	18.8
(1,41)	2:23:B:LEU:H	5:409:A:17F:O5	10	18.59	3.3	18.8
(1,41)	2:23:B:LEU:CD2	4:407:A:PCW:C7	10	18.59	3.3	18.8
(1,41)	2:23:B:LEU:H	5:409:A:17F:O4	10	18.59	3.3	18.8
(1,49)	2:185:B:CYS:O	4:402:A:PCW:C7	10	18.2	8.65	18.68
(1,49)	2:185:B:CYS:O	4:408:A:PCW:C5	10	18.2	8.65	18.68
(1,49)	2:185:B:CYS:H	1:219:A:GLU:N	10	18.2	8.65	18.68
(1,49)	2:185:B:CYS:O	4:408:A:PCW:C6	10	18.2	8.65	18.68
(1,49)	2:185:B:CYS:N	4:408:A:PCW:C6	10	18.2	8.65	18.68
(1,49)	2:185:B:CYS:H	4:408:A:PCW:C8	10	18.2	8.65	18.68
(1,49)	2:185:B:CYS:O	4:404:A:PCW:C8	10	18.2	8.65	18.68

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,49)	2:185:B:CYS:H	5:409:A:17F:O3	10	18.2	8.65	18.68
(1,49)	2:185:B:CYS:SG	1:222:A:GLY:N	10	18.2	8.65	18.68
(1,49)	2:185:B:CYS:HG	4:406:A:PCW:C8	10	18.2	8.65	18.68
(1,44)	2:79:B:LEU:H	4:406:A:PCW:C8	10	15.11	3.77	14.33
(1,44)	2:79:B:LEU:CD2	4:404:A:PCW:C7	10	15.11	3.77	14.33
(1,44)	2:79:B:LEU:H	4:406:A:PCW:C7	10	15.11	3.77	14.33
(1,44)	2:79:B:LEU:H	4:407:A:PCW:C7	10	15.11	3.77	14.33
(1,44)	2:79:B:LEU:H	4:404:A:PCW:C7	10	15.11	3.77	14.33
(1,43)	2:46:B:ILE:O	4:405:A:PCW:C7	10	10.97	3.09	11.4
(1,43)	2:46:B:ILE:CD1	4:406:A:PCW:C8	10	10.97	3.09	11.4
(1,43)	2:46:B:ILE:O	4:404:A:PCW:C7	10	10.97	3.09	11.4
(1,43)	2:46:B:ILE:O	4:408:A:PCW:C8	10	10.97	3.09	11.4
(1,43)	2:46:B:ILE:CD1	4:406:A:PCW:C7	10	10.97	3.09	11.4
(1,43)	2:46:B:ILE:O	4:401:A:PCW:C6	10	10.97	3.09	11.4
(1,48)	2:160:B:VAL:O	4:406:A:PCW:C8	10	8.96	1.91	8.93
(1,48)	2:160:B:VAL:CG1	4:406:A:PCW:C8	10	8.96	1.91	8.93
(1,48)	2:160:B:VAL:O	4:404:A:PCW:C7	10	8.96	1.91	8.93
(1,48)	2:160:B:VAL:O	4:408:A:PCW:C5	10	8.96	1.91	8.93
(1,48)	2:160:B:VAL:O	4:406:A:PCW:C7	10	8.96	1.91	8.93
(1,48)	2:160:B:VAL:O	4:407:A:PCW:C7	10	8.96	1.91	8.93
(1,29)	4:408:A:PCW:C4	2:185:B:CYS:O	10	4.84	2.48	5.49
(1,29)	4:408:A:PCW:C4	4:203:B:PCW:C8	10	4.84	2.48	5.49
(1,29)	4:408:A:PCW:C4	4:203:B:PCW:C6	10	4.84	2.48	5.49
(1,19)	4:405:A:PCW:C4	2:185:B:CYS:O	10	2.37	1.35	2.13
(1,19)	4:405:A:PCW:C7	4:203:B:PCW:C8	10	2.37	1.35	2.13
(1,19)	4:405:A:PCW:C6	4:203:B:PCW:C7	10	2.37	1.35	2.13
(1,19)	4:405:A:PCW:C6	4:203:B:PCW:C8	10	2.37	1.35	2.13
(1,3)	4:402:A:PCW:C7	4:203:B:PCW:C8	9	8.11	1.9	7.56
(1,3)	4:402:A:PCW:C7	4:203:B:PCW:C7	9	8.11	1.9	7.56
(1,3)	4:402:A:PCW:C8	4:203:B:PCW:C8	9	8.11	1.9	7.56
(1,15)	4:404:A:PCW:C6	4:202:B:PCW:C6	9	2.35	1.1	1.88
(1,15)	4:404:A:PCW:C6	4:202:B:PCW:C4	9	2.35	1.1	1.88
(1,15)	4:404:A:PCW:C6	4:202:B:PCW:C7	9	2.35	1.1	1.88
(1,42)	4:202:B:PCW:C6	4:404:A:PCW:C6	9	1.99	0.67	1.88
(1,42)	4:202:B:PCW:C4	4:404:A:PCW:C6	9	1.99	0.67	1.88
(1,42)	4:202:B:PCW:C7	4:404:A:PCW:C6	9	1.99	0.67	1.88
(1,42)	4:202:B:PCW:C7	4:406:A:PCW:C8	9	1.99	0.67	1.88
(1,42)	4:202:B:PCW:O2	4:406:A:PCW:C5	9	1.99	0.67	1.88
(1,42)	4:202:B:PCW:C8	4:406:A:PCW:C8	9	1.99	0.67	1.88
(1,20)	4:406:A:PCW:C7	4:203:B:PCW:C1	9	1.72	0.6	1.69
(1,20)	4:406:A:PCW:C4	4:203:B:PCW:C3	9	1.72	0.6	1.69
(1,20)	4:406:A:PCW:C5	4:203:B:PCW:C1	9	1.72	0.6	1.69

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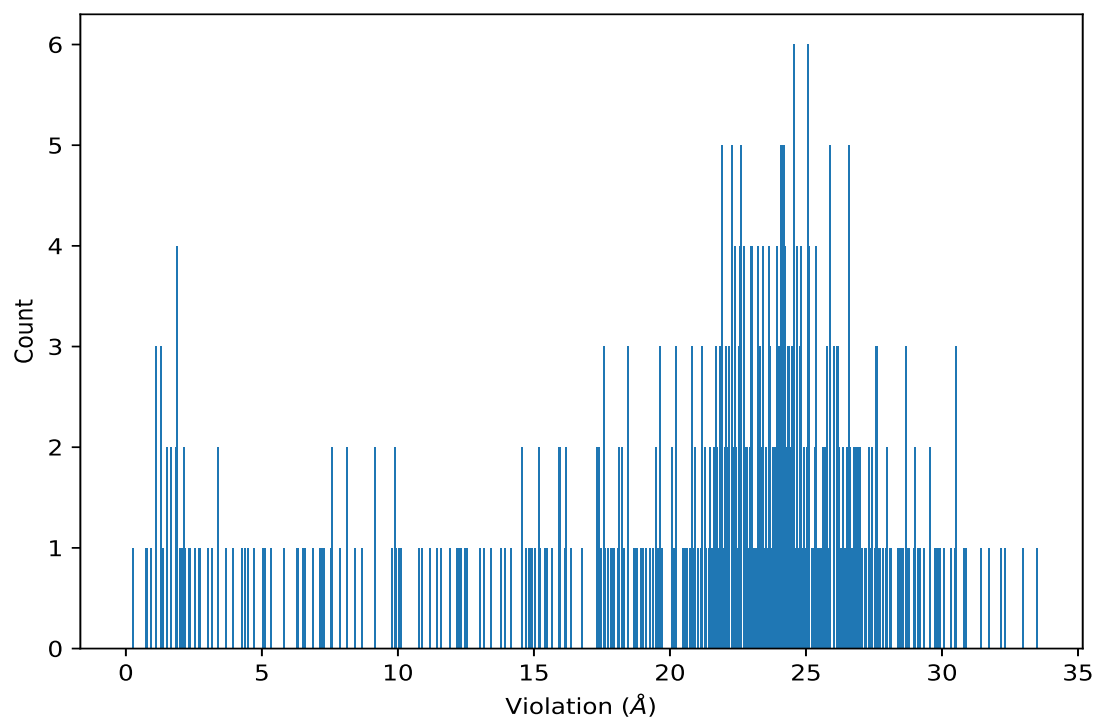
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,20)	4:406:A:PCW:C8	4:203:B:PCW:C1	9	1.72	0.6	1.69
(1,20)	4:406:A:PCW:C8	2:185:B:CYS:HG	9	1.72	0.6	1.69

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:201:A:LEU:N	4:202:B:PCW:C4	8	33.47
(1,1)	1:201:A:LEU:N	4:202:B:PCW:C4	5	32.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:205:A:ASP:N	4:202:B:PCW:C4	8	32.34
(1,1)	1:201:A:LEU:N	4:202:B:PCW:C4	4	32.18
(1,2)	1:202:A:LYS:N	4:202:B:PCW:C4	4	31.71
(1,6)	1:206:A:ASN:N	4:202:B:PCW:C2	8	31.43
(1,1)	1:201:A:LEU:N	4:202:B:PCW:C4	2	30.89
(1,2)	4:401:A:PCW:C6	2:45:B:VAL:CG2	5	30.8
(1,9)	1:209:A:SER:N	4:202:B:PCW:C2	8	30.54
(1,4)	1:204:A:LEU:N	4:202:B:PCW:C4	8	30.54
(1,1)	1:201:A:LEU:N	4:202:B:PCW:C6	6	30.52
(1,5)	1:205:A:ASP:N	4:202:B:PCW:C4	5	30.46
(1,5)	1:205:A:ASP:N	4:202:B:PCW:C4	4	30.33
(1,5)	1:205:A:ASP:N	2:78:B:PHE:CE2	7	30.05
(1,8)	1:208:A:ASP:N	4:202:B:PCW:C4	8	29.93
(1,6)	1:206:A:ASN:N	4:202:B:PCW:C4	5	29.88
(1,49)	2:185:B:CYS:O	4:404:A:PCW:C8	7	29.82
(1,6)	1:206:A:ASN:N	4:202:B:PCW:C4	4	29.74
(1,5)	1:205:A:ASP:N	4:202:B:PCW:C4	2	29.57
(1,1)	1:201:A:LEU:N	2:78:B:PHE:CE2	10	29.56
(1,5)	1:205:A:ASP:N	4:202:B:PCW:C4	10	29.31
(1,1)	1:201:A:LEU:N	4:202:B:PCW:C6	1	29.19
(1,7)	1:207:A:TRP:N	4:202:B:PCW:C4	8	29.1
(1,12)	1:212:A:SER:N	4:202:B:PCW:O3	8	29.02
(1,6)	1:206:A:ASN:N	4:202:B:PCW:O3	7	29.02
(1,6)	1:206:A:ASN:N	4:202:B:PCW:C4	2	28.96
(1,49)	2:185:B:CYS:H	5:409:A:17F:O3	8	28.77
(1,4)	1:204:A:LEU:N	4:202:B:PCW:C4	5	28.73
(1,16)	1:216:A:LYS:N	4:202:B:PCW:O3	8	28.7
(1,9)	1:209:A:SER:N	4:202:B:PCW:C4	4	28.67
(1,6)	1:206:A:ASN:N	4:202:B:PCW:C4	10	28.67
(1,9)	1:209:A:SER:N	4:202:B:PCW:C4	5	28.58
(1,13)	1:213:A:THR:N	4:202:B:PCW:O3	8	28.49
(1,4)	1:204:A:LEU:N	4:202:B:PCW:C4	4	28.43
(1,5)	1:205:A:ASP:N	4:202:B:PCW:C6	6	28.35
(1,9)	1:209:A:SER:N	4:202:B:PCW:O2	2	28.13
(1,46)	2:133:B:LEU:O	4:404:A:PCW:C7	7	28.07
(1,23)	1:223:A:PRO:N	4:202:B:PCW:O3	8	27.96
(1,8)	1:208:A:ASP:N	4:202:B:PCW:C4	5	27.96
(1,6)	1:206:A:ASN:N	4:202:B:PCW:C4	6	27.94
(1,46)	2:133:B:LEU:O	4:404:A:PCW:C7	10	27.8
(1,8)	1:208:A:ASP:N	4:202:B:PCW:C4	4	27.72
(1,9)	1:209:A:SER:N	4:202:B:PCW:O3	7	27.66
(1,4)	1:204:A:LEU:N	4:202:B:PCW:C4	2	27.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:204:A:LEU:N	4:202:B:PCW:C4	10	27.62
(1,2)	4:401:A:PCW:C6	2:45:B:VAL:CG2	2	27.62
(1,27)	1:227:A:GLU:N	4:202:B:PCW:O3	8	27.57
(1,1)	1:201:A:LEU:N	2:78:B:PHE:CE2	7	27.56
(1,4)	1:204:A:LEU:N	2:78:B:PHE:CE2	7	27.55
(1,5)	1:205:A:ASP:N	4:202:B:PCW:C6	1	27.54
(1,7)	1:207:A:TRP:N	4:202:B:PCW:C4	5	27.44
(1,37)	1:237:A:GLU:O	4:202:B:PCW:O3	10	27.43
(1,9)	1:209:A:SER:N	4:202:B:PCW:O3	10	27.4
(1,8)	1:208:A:ASP:N	4:202:B:PCW:C4	2	27.31
(1,8)	1:208:A:ASP:N	4:202:B:PCW:O3	7	27.3
(1,7)	1:207:A:TRP:N	4:202:B:PCW:C4	4	27.21
(1,6)	1:206:A:ASN:N	4:202:B:PCW:C6	1	27.16
(1,11)	1:211:A:THR:N	4:202:B:PCW:O3	8	27.05
(1,9)	1:209:A:SER:N	4:202:B:PCW:C4	6	26.99
(1,17)	1:217:A:LEU:N	4:202:B:PCW:O3	8	26.97
(1,12)	1:212:A:SER:N	4:202:B:PCW:C4	5	26.91
(1,6)	1:206:A:ASN:N	2:185:B:CYS:N	9	26.91
(1,24)	1:224:A:VAL:N	4:202:B:PCW:O3	8	26.87
(1,12)	1:212:A:SER:N	4:202:B:PCW:C4	4	26.87
(1,5)	1:205:A:ASP:N	2:185:B:CYS:N	9	26.83
(1,46)	2:133:B:LEU:O	4:406:A:PCW:C6	5	26.8
(1,31)	1:231:A:ASN:N	4:203:B:PCW:O3	8	26.79
(1,34)	1:234:A:LYS:O	4:203:B:PCW:O3	6	26.78
(1,6)	1:206:A:ASN:N	4:202:B:PCW:O3	3	26.66
(1,7)	1:207:A:TRP:N	4:202:B:PCW:O3	7	26.64
(1,8)	1:208:A:ASP:N	4:202:B:PCW:C4	10	26.6
(1,5)	1:205:A:ASP:N	2:161:B:ARG:O	3	26.59
(1,7)	1:207:A:TRP:N	4:202:B:PCW:C4	2	26.57
(1,40)	1:240:A:ARG:O	4:203:B:PCW:O3	10	26.56
(1,1)	1:201:A:LEU:N	2:78:B:PHE:CE2	9	26.56
(1,4)	1:204:A:LEU:N	4:202:B:PCW:C6	6	26.55
(1,12)	1:212:A:SER:N	4:202:B:PCW:O2	2	26.54
(1,13)	1:213:A:THR:N	4:202:B:PCW:C4	5	26.5
(1,37)	1:237:A:GLU:O	4:203:B:PCW:O3	6	26.41
(1,16)	1:216:A:LYS:N	4:202:B:PCW:C4	5	26.4
(1,10)	1:210:A:VAL:N	4:202:B:PCW:C4	4	26.37
(1,30)	1:230:A:ASP:N	4:203:B:PCW:C3	8	26.26
(1,9)	1:209:A:SER:N	4:202:B:PCW:C6	1	26.22
(1,13)	1:213:A:THR:N	4:202:B:PCW:O3	4	26.21
(1,34)	1:234:A:LYS:O	4:202:B:PCW:O3	10	26.19
(1,10)	1:210:A:VAL:N	4:202:B:PCW:C4	5	26.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:216:A:LYS:N	4:202:B:PCW:O3	4	26.16
(1,34)	1:234:A:LYS:O	4:203:B:PCW:O3	2	26.13
(1,7)	1:207:A:TRP:N	4:202:B:PCW:C4	10	26.13
(1,37)	1:237:A:GLU:O	4:203:B:PCW:O3	2	26.1
(1,13)	1:213:A:THR:N	4:202:B:PCW:O2	2	26.03
(1,14)	1:214:A:PHE:N	4:202:B:PCW:O3	8	26.02
(1,31)	1:231:A:ASN:N	4:202:B:PCW:O3	6	26.0
(1,34)	1:234:A:LYS:O	4:202:B:PCW:O3	7	25.89
(1,16)	1:216:A:LYS:N	4:202:B:PCW:O2	2	25.89
(1,8)	1:208:A:ASP:N	4:202:B:PCW:C6	6	25.89
(1,27)	1:227:A:GLU:N	4:202:B:PCW:O3	6	25.87
(1,12)	1:212:A:SER:N	4:202:B:PCW:O3	7	25.87
(1,28)	1:228:A:PHE:N	4:202:B:PCW:O3	8	25.8
(1,38)	5:409:A:17F:N1	2:25:B:GLN:HE22	6	25.79
(1,22)	1:222:A:GLY:N	4:202:B:PCW:O3	8	25.78
(1,26)	1:226:A:GLN:N	4:202:B:PCW:O3	8	25.77
(1,10)	1:210:A:VAL:N	4:202:B:PCW:O2	2	25.73
(1,34)	1:234:A:LYS:O	4:203:B:PCW:O3	8	25.71
(1,23)	1:223:A:PRO:N	4:202:B:PCW:O3	5	25.68
(1,4)	1:204:A:LEU:N	4:202:B:PCW:C6	1	25.68
(1,37)	1:237:A:GLU:O	4:203:B:PCW:O3	7	25.61
(1,4)	1:204:A:LEU:N	2:78:B:PHE:CE2	9	25.61
(1,33)	1:233:A:GLU:O	4:203:B:PCW:O3	6	25.57
(1,12)	1:212:A:SER:N	4:202:B:PCW:O3	10	25.53
(1,37)	1:237:A:GLU:O	4:203:B:PCW:O3	8	25.49
(1,40)	1:240:A:ARG:O	4:203:B:PCW:O3	6	25.41
(1,7)	1:207:A:TRP:N	4:202:B:PCW:C4	6	25.38
(1,38)	1:238:A:GLY:O	4:203:B:PCW:O3	2	25.37
(1,34)	1:234:A:LYS:O	4:202:B:PCW:O3	5	25.37
(1,23)	1:223:A:PRO:N	4:202:B:PCW:O3	2	25.36
(1,18)	1:218:A:ARG:N	4:202:B:PCW:O3	8	25.34
(1,46)	2:133:B:LEU:O	4:404:A:PCW:C7	9	25.3
(1,33)	1:233:A:GLU:O	4:202:B:PCW:O3	2	25.25
(1,12)	1:212:A:SER:N	4:202:B:PCW:C7	6	25.21
(1,13)	1:213:A:THR:N	4:202:B:PCW:C4	6	25.15
(1,16)	1:216:A:LYS:N	4:202:B:PCW:O3	7	25.14
(1,10)	1:210:A:VAL:N	4:202:B:PCW:O3	7	25.12
(1,34)	1:234:A:LYS:O	4:203:B:PCW:O3	3	25.11
(1,13)	1:213:A:THR:N	4:202:B:PCW:O3	7	25.09
(1,11)	1:211:A:THR:N	4:202:B:PCW:C4	5	25.09
(1,23)	1:223:A:PRO:N	4:202:B:PCW:C7	6	25.08
(1,40)	1:240:A:ARG:O	4:203:B:PCW:O3	2	25.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,37)	1:237:A:GLU:O	4:203:B:PCW:O3	5	25.05
(1,11)	1:211:A:THR:N	4:202:B:PCW:C4	4	25.05
(1,8)	1:208:A:ASP:N	4:202:B:PCW:C6	1	25.03
(1,1)	1:201:A:LEU:N	2:78:B:PHE:CE2	3	25.02
(1,10)	1:210:A:VAL:N	4:202:B:PCW:O3	10	24.98
(1,13)	1:213:A:THR:N	4:202:B:PCW:O3	10	24.95
(1,30)	1:230:A:ASP:N	4:202:B:PCW:O3	6	24.91
(1,16)	1:216:A:LYS:N	4:202:B:PCW:C7	6	24.85
(1,33)	1:233:A:GLU:O	4:203:B:PCW:O3	8	24.82
(1,31)	1:231:A:ASN:N	4:202:B:PCW:O3	2	24.82
(1,33)	1:233:A:GLU:O	4:202:B:PCW:O3	10	24.8
(1,17)	1:217:A:LEU:N	4:202:B:PCW:C4	5	24.8
(1,37)	1:237:A:GLU:O	4:203:B:PCW:O3	3	24.79
(1,34)	1:234:A:LYS:O	4:203:B:PCW:C3	4	24.78
(1,10)	1:210:A:VAL:N	4:202:B:PCW:C4	6	24.77
(1,16)	1:216:A:LYS:N	4:202:B:PCW:O3	10	24.73
(1,27)	1:227:A:GLU:N	4:202:B:PCW:O3	2	24.69
(1,23)	1:223:A:PRO:N	4:202:B:PCW:O3	4	24.69
(1,11)	1:211:A:THR:N	4:202:B:PCW:O2	2	24.69
(1,24)	1:224:A:VAL:N	4:202:B:PCW:C7	6	24.66
(1,8)	1:208:A:ASP:N	2:185:B:CYS:H	3	24.64
(1,4)	1:204:A:LEU:N	2:161:B:ARG:O	3	24.59
(1,41)	2:23:B:LEU:CD2	4:404:A:PCW:C7	10	24.57
(1,7)	1:207:A:TRP:N	4:202:B:PCW:C6	1	24.56
(1,47)	2:142:B:ILE:CG1	4:404:A:PCW:C7	10	24.55
(1,27)	1:227:A:GLU:N	4:202:B:PCW:O3	4	24.55
(1,27)	1:227:A:GLU:N	4:202:B:PCW:O3	5	24.55
(1,46)	2:133:B:LEU:O	4:404:A:PCW:C7	3	24.53
(1,46)	2:133:B:LEU:O	4:406:A:PCW:C8	2	24.51
(1,23)	1:223:A:PRO:N	4:202:B:PCW:O3	10	24.51
(1,46)	2:133:B:LEU:O	4:406:A:PCW:C8	4	24.49
(1,33)	1:233:A:GLU:O	4:202:B:PCW:O3	7	24.48
(1,38)	1:238:A:GLY:O	4:203:B:PCW:O3	5	24.46
(1,25)	1:225:A:THR:N	4:202:B:PCW:O3	8	24.45
(1,7)	1:207:A:TRP:N	2:185:B:CYS:N	9	24.42
(1,33)	1:233:A:GLU:O	4:203:B:PCW:O3	3	24.39
(1,40)	1:240:A:ARG:O	4:203:B:PCW:O3	7	24.37
(1,31)	1:231:A:ASN:N	4:202:B:PCW:O3	4	24.35
(1,23)	1:223:A:PRO:N	4:202:B:PCW:O3	7	24.34
(1,31)	1:231:A:ASN:N	4:202:B:PCW:O3	10	24.3
(1,12)	1:212:A:SER:N	4:202:B:PCW:C6	1	24.3
(1,40)	1:240:A:ARG:O	4:203:B:PCW:O3	8	24.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:209:A:SER:N	2:185:B:CYS:H	3	24.25
(1,31)	1:231:A:ASN:N	4:202:B:PCW:O3	7	24.24
(1,40)	1:240:A:ARG:O	2:185:B:CYS:HG	9	24.22
(1,40)	1:240:A:ARG:O	4:203:B:PCW:O3	5	24.21
(1,17)	1:217:A:LEU:N	4:202:B:PCW:O3	4	24.21
(1,32)	1:232:A:LEU:N	4:203:B:PCW:O3	8	24.2
(1,13)	1:213:A:THR:N	4:202:B:PCW:C4	1	24.18
(1,7)	1:207:A:TRP:N	4:202:B:PCW:O3	3	24.18
(1,17)	1:217:A:LEU:N	4:202:B:PCW:O3	2	24.17
(1,28)	1:228:A:PHE:N	4:202:B:PCW:O3	6	24.16
(1,27)	1:227:A:GLU:N	4:202:B:PCW:O3	10	24.15
(1,24)	1:224:A:VAL:N	4:202:B:PCW:O3	5	24.14
(1,36)	1:236:A:THR:O	4:202:B:PCW:O3	10	24.11
(1,24)	1:224:A:VAL:N	4:202:B:PCW:O3	2	24.1
(1,23)	1:223:A:PRO:N	4:202:B:PCW:O3	1	24.1
(1,11)	1:211:A:THR:N	4:202:B:PCW:O3	7	24.07
(1,49)	2:185:B:CYS:N	4:408:A:PCW:C6	5	24.06
(1,31)	1:231:A:ASN:N	4:202:B:PCW:O3	3	24.06
(1,27)	1:227:A:GLU:N	4:202:B:PCW:O3	7	24.06
(1,37)	1:237:A:GLU:O	4:203:B:PCW:C3	4	24.05
(1,39)	1:239:A:LEU:O	4:203:B:PCW:O3	10	24.04
(1,30)	1:230:A:ASP:N	4:202:B:PCW:O3	2	24.03
(1,16)	1:216:A:LYS:N	4:202:B:PCW:C7	1	24.02
(1,31)	1:231:A:ASN:N	4:202:B:PCW:O3	5	23.95
(1,47)	2:142:B:ILE:CG1	4:404:A:PCW:C7	7	23.93
(1,33)	1:233:A:GLU:O	4:202:B:PCW:O3	5	23.93
(1,14)	1:214:A:PHE:N	4:202:B:PCW:C4	5	23.93
(1,32)	1:232:A:LEU:N	4:202:B:PCW:O3	6	23.87
(1,35)	1:235:A:GLU:O	4:202:B:PCW:O3	10	23.85
(1,11)	1:211:A:THR:N	4:202:B:PCW:O3	10	23.8
(1,22)	1:222:A:GLY:N	4:202:B:PCW:O3	5	23.78
(1,31)	1:231:A:ASN:N	4:203:B:PCW:C3	1	23.77
(1,2)	4:401:A:PCW:C6	2:45:B:VAL:CG2	6	23.73
(1,38)	1:238:A:GLY:O	4:203:B:PCW:O3	4	23.7
(1,14)	1:214:A:PHE:N	4:202:B:PCW:O3	4	23.7
(1,35)	1:235:A:GLU:O	4:203:B:PCW:O3	6	23.66
(1,27)	1:227:A:GLU:N	4:202:B:PCW:O3	1	23.65
(1,26)	1:226:A:GLN:N	4:202:B:PCW:C7	6	23.63
(1,17)	1:217:A:LEU:N	4:202:B:PCW:C7	6	23.63
(1,9)	1:209:A:SER:N	2:185:B:CYS:N	9	23.61
(1,24)	1:224:A:VAL:N	4:202:B:PCW:O3	4	23.57
(1,30)	1:230:A:ASP:N	4:202:B:PCW:O3	4	23.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,33)	1:233:A:GLU:O	4:203:B:PCW:C3	4	23.52
(1,30)	1:230:A:ASP:N	4:202:B:PCW:O3	7	23.46
(1,21)	1:221:A:LEU:N	4:202:B:PCW:O3	5	23.45
(1,10)	1:210:A:VAL:N	4:202:B:PCW:O3	3	23.43
(1,45)	2:113:B:LEU:H	4:404:A:PCW:C7	10	23.41
(1,14)	1:214:A:PHE:N	4:202:B:PCW:O2	2	23.41
(1,40)	1:240:A:ARG:O	4:203:B:PCW:C6	3	23.38
(1,11)	1:211:A:THR:N	4:202:B:PCW:C4	6	23.35
(1,30)	1:230:A:ASP:N	4:202:B:PCW:O3	10	23.33
(1,17)	1:217:A:LEU:N	4:202:B:PCW:O3	7	23.33
(1,45)	2:113:B:LEU:H	4:404:A:PCW:C7	7	23.3
(1,36)	1:236:A:THR:O	4:203:B:PCW:O3	6	23.24
(1,24)	1:224:A:VAL:N	4:202:B:PCW:O3	10	23.24
(1,22)	1:222:A:GLY:N	4:202:B:PCW:O3	2	23.23
(1,18)	1:218:A:ARG:N	4:202:B:PCW:C4	5	23.21
(1,30)	1:230:A:ASP:N	4:202:B:PCW:O3	5	23.17
(1,24)	1:224:A:VAL:N	4:202:B:PCW:O3	7	23.14
(1,35)	1:235:A:GLU:O	4:203:B:PCW:O3	2	23.09
(1,40)	1:240:A:ARG:O	4:203:B:PCW:O3	4	23.04
(1,8)	1:208:A:ASP:N	2:185:B:CYS:N	9	23.04
(1,26)	1:226:A:GLN:N	4:202:B:PCW:O3	2	23.03
(1,26)	1:226:A:GLN:N	4:202:B:PCW:O3	5	23.02
(1,39)	1:239:A:LEU:O	4:203:B:PCW:O3	6	22.99
(1,36)	1:236:A:THR:O	4:203:B:PCW:O3	2	22.98
(1,30)	1:230:A:ASP:N	4:202:B:PCW:O3	1	22.98
(1,24)	1:224:A:VAL:N	4:202:B:PCW:O3	1	22.97
(1,17)	1:217:A:LEU:N	4:202:B:PCW:O3	10	22.95
(1,34)	1:234:A:LYS:O	4:203:B:PCW:C3	1	22.93
(1,21)	1:221:A:LEU:N	4:202:B:PCW:O3	2	22.89
(1,28)	1:228:A:PHE:N	4:202:B:PCW:O3	4	22.84
(1,28)	1:228:A:PHE:N	4:202:B:PCW:O3	2	22.83
(1,17)	1:217:A:LEU:N	4:202:B:PCW:C4	1	22.79
(1,21)	1:221:A:LEU:N	4:202:B:PCW:C7	6	22.75
(1,37)	1:237:A:GLU:O	4:203:B:PCW:C3	1	22.72
(1,35)	1:235:A:GLU:O	4:203:B:PCW:O3	7	22.72
(1,26)	1:226:A:GLN:N	4:202:B:PCW:O3	4	22.72
(1,32)	1:232:A:LEU:N	4:202:B:PCW:O3	2	22.71
(1,35)	1:235:A:GLU:O	4:203:B:PCW:O3	8	22.63
(1,28)	1:228:A:PHE:N	4:202:B:PCW:O3	5	22.63
(1,39)	1:239:A:LEU:O	4:203:B:PCW:O3	2	22.62
(1,37)	1:237:A:GLU:O	2:185:B:CYS:HG	9	22.62
(1,14)	1:214:A:PHE:N	4:202:B:PCW:C4	6	22.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:218:A:ARG:N	4:202:B:PCW:O3	4	22.59
(1,36)	1:236:A:THR:O	4:203:B:PCW:O3	7	22.58
(1,30)	1:230:A:ASP:N	2:185:B:CYS:O	3	22.57
(1,11)	1:211:A:THR:N	4:202:B:PCW:C6	1	22.56
(1,22)	1:222:A:GLY:N	4:202:B:PCW:C7	6	22.54
(1,14)	1:214:A:PHE:N	4:202:B:PCW:O3	7	22.54
(1,22)	1:222:A:GLY:N	4:202:B:PCW:O3	4	22.52
(1,21)	1:221:A:LEU:N	4:202:B:PCW:O3	4	22.48
(1,33)	1:233:A:GLU:O	4:203:B:PCW:C3	1	22.45
(1,18)	1:218:A:ARG:N	4:202:B:PCW:O3	2	22.45
(1,25)	1:225:A:THR:N	4:202:B:PCW:C7	6	22.4
(1,26)	1:226:A:GLN:N	4:202:B:PCW:O3	10	22.38
(1,28)	1:228:A:PHE:N	4:202:B:PCW:O3	7	22.36
(1,14)	1:214:A:PHE:N	4:202:B:PCW:O3	10	22.35
(1,28)	1:228:A:PHE:N	4:202:B:PCW:O3	10	22.31
(1,22)	1:222:A:GLY:N	4:202:B:PCW:O3	10	22.3
(1,32)	1:232:A:LEU:N	4:202:B:PCW:O3	10	22.28
(1,10)	1:210:A:VAL:N	2:185:B:CYS:N	9	22.28
(1,47)	2:142:B:ILE:CG1	4:404:A:PCW:C7	9	22.26
(1,35)	1:235:A:GLU:O	4:203:B:PCW:O3	5	22.26
(1,36)	1:236:A:THR:O	4:203:B:PCW:O3	8	22.25
(1,26)	1:226:A:GLN:N	4:202:B:PCW:O3	7	22.19
(1,22)	1:222:A:GLY:N	4:202:B:PCW:O3	7	22.18
(1,49)	2:185:B:CYS:O	4:408:A:PCW:C6	4	22.16
(1,32)	1:232:A:LEU:N	4:202:B:PCW:O3	4	22.12
(1,11)	1:211:A:THR:N	2:185:B:CYS:H	3	22.1
(1,32)	1:232:A:LEU:N	4:202:B:PCW:O3	7	22.09
(1,40)	1:240:A:ARG:O	4:203:B:PCW:O3	1	22.06
(1,32)	1:232:A:LEU:N	4:202:B:PCW:O3	3	22.06
(1,39)	1:239:A:LEU:O	4:203:B:PCW:O3	7	22.01
(1,28)	1:228:A:PHE:N	4:202:B:PCW:O3	3	22.01
(1,35)	1:235:A:GLU:O	4:203:B:PCW:O3	3	21.96
(1,28)	1:228:A:PHE:N	4:202:B:PCW:O3	1	21.94
(1,21)	1:221:A:LEU:N	4:202:B:PCW:O3	7	21.94
(1,39)	1:239:A:LEU:O	4:203:B:PCW:O3	8	21.93
(1,26)	1:226:A:GLN:N	4:202:B:PCW:O3	1	21.91
(1,21)	1:221:A:LEU:N	4:202:B:PCW:O3	10	21.91
(1,36)	1:236:A:THR:O	4:203:B:PCW:O3	5	21.89
(1,39)	1:239:A:LEU:O	4:203:B:PCW:O3	9	21.84
(1,18)	1:218:A:ARG:N	4:202:B:PCW:O3	7	21.83
(1,21)	1:221:A:LEU:N	4:202:B:PCW:O3	1	21.81
(1,22)	1:222:A:GLY:N	4:202:B:PCW:C7	1	21.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:239:A:LEU:O	4:203:B:PCW:O3	5	21.72
(1,18)	1:218:A:ARG:N	4:202:B:PCW:C7	6	21.71
(1,46)	2:133:B:LEU:O	4:407:A:PCW:C6	8	21.69
(1,36)	1:236:A:THR:O	4:203:B:PCW:O3	3	21.69
(1,32)	1:232:A:LEU:N	4:202:B:PCW:O3	5	21.69
(1,25)	1:225:A:THR:N	4:202:B:PCW:O3	2	21.65
(1,25)	1:225:A:THR:N	4:202:B:PCW:O3	5	21.65
(1,14)	1:214:A:PHE:N	4:202:B:PCW:C4	1	21.59
(1,34)	1:234:A:LYS:O	2:185:B:CYS:HG	9	21.51
(1,35)	1:235:A:GLU:O	4:203:B:PCW:O3	4	21.47
(1,18)	1:218:A:ARG:N	4:202:B:PCW:O3	10	21.47
(1,35)	1:235:A:GLU:O	2:185:B:CYS:HG	9	21.43
(1,41)	2:23:B:LEU:CD2	4:407:A:PCW:C7	8	21.32
(1,32)	1:232:A:LEU:N	4:203:B:PCW:C3	1	21.25
(1,25)	1:225:A:THR:N	4:202:B:PCW:O3	4	21.25
(1,39)	1:239:A:LEU:O	4:203:B:PCW:O3	3	21.17
(1,44)	2:79:B:LEU:CD2	4:404:A:PCW:C7	7	21.16
(1,41)	2:23:B:LEU:H	5:409:A:17F:O4	9	21.16
(1,47)	2:142:B:ILE:CG1	4:408:A:PCW:C6	5	21.1
(1,46)	2:133:B:LEU:O	4:406:A:PCW:C7	6	21.03
(1,13)	1:213:A:THR:N	2:185:B:CYS:H	3	20.94
(1,18)	1:218:A:ARG:N	4:202:B:PCW:C7	1	20.92
(1,25)	1:225:A:THR:N	4:202:B:PCW:O3	10	20.86
(1,47)	2:142:B:ILE:CG1	4:407:A:PCW:C6	8	20.83
(1,39)	1:239:A:LEU:O	4:203:B:PCW:O3	4	20.82
(1,36)	1:236:A:THR:O	4:203:B:PCW:C3	4	20.81
(1,25)	1:225:A:THR:N	4:202:B:PCW:O3	7	20.74
(1,41)	2:23:B:LEU:H	5:409:A:17F:O5	7	20.64
(1,44)	2:79:B:LEU:H	4:404:A:PCW:C7	10	20.56
(1,25)	1:225:A:THR:N	4:202:B:PCW:O3	1	20.54
(1,14)	1:214:A:PHE:N	2:185:B:CYS:H	3	20.49
(1,45)	2:113:B:LEU:N	4:406:A:PCW:C8	5	20.24
(1,13)	1:213:A:THR:N	2:185:B:CYS:N	9	20.24
(1,36)	1:236:A:THR:O	2:185:B:CYS:HG	9	20.22
(1,45)	2:113:B:LEU:H	4:404:A:PCW:C7	9	20.17
(1,2)	4:401:A:PCW:C6	2:45:B:VAL:CG2	1	20.12
(1,27)	1:227:A:GLU:N	2:185:B:CYS:N	3	20.09
(1,12)	1:212:A:SER:N	2:185:B:CYS:H	3	20.07
(1,47)	2:142:B:ILE:CG1	4:406:A:PCW:C8	2	19.71
(1,35)	1:235:A:GLU:O	4:203:B:PCW:C3	1	19.7
(1,12)	1:212:A:SER:N	2:185:B:CYS:N	9	19.65
(1,11)	1:211:A:THR:N	2:185:B:CYS:N	9	19.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:225:A:THR:N	2:185:B:CYS:H	3	19.63
(1,39)	1:239:A:LEU:O	4:203:B:PCW:O3	1	19.59
(1,45)	2:113:B:LEU:H	4:404:A:PCW:C7	3	19.48
(1,36)	1:236:A:THR:O	4:203:B:PCW:C3	1	19.46
(1,41)	2:23:B:LEU:CD2	4:404:A:PCW:C7	3	19.39
(1,38)	5:409:A:17F:N1	2:25:B:GLN:HE22	10	19.26
(1,38)	5:409:A:17F:O4	2:45:B:VAL:CG1	1	19.14
(1,49)	2:185:B:CYS:O	4:408:A:PCW:C5	2	19.03
(1,17)	1:217:A:LEU:N	2:185:B:CYS:H	3	18.95
(1,46)	2:133:B:LEU:O	4:406:A:PCW:C8	1	18.91
(1,47)	2:142:B:ILE:H	4:406:A:PCW:C8	1	18.78
(1,24)	1:224:A:VAL:N	2:185:B:CYS:H	3	18.72
(1,26)	1:226:A:GLN:N	2:185:B:CYS:H	3	18.66
(1,47)	2:142:B:ILE:CG1	4:404:A:PCW:C7	3	18.49
(1,47)	2:142:B:ILE:CG1	4:406:A:PCW:C7	6	18.45
(1,45)	2:113:B:LEU:N	4:406:A:PCW:C8	2	18.45
(1,49)	2:185:B:CYS:H	1:219:A:GLU:N	3	18.32
(1,33)	1:233:A:GLU:O	2:185:B:CYS:HG	9	18.23
(1,41)	2:23:B:LEU:CD2	4:406:A:PCW:C8	1	18.22
(1,45)	2:113:B:LEU:H	4:407:A:PCW:C6	8	18.15
(1,10)	4:403:A:PCW:C8	2:47:B:ASP:O	1	18.15
(1,14)	1:214:A:PHE:N	2:185:B:CYS:N	9	18.05
(1,21)	1:221:A:LEU:N	2:185:B:CYS:H	3	17.93
(1,47)	2:142:B:ILE:CG1	4:406:A:PCW:C8	4	17.88
(1,2)	4:401:A:PCW:C6	2:25:B:GLN:HE22	10	17.82
(1,49)	2:185:B:CYS:H	4:408:A:PCW:C8	6	17.72
(1,18)	1:218:A:ARG:N	2:185:B:CYS:H	3	17.62
(1,44)	2:79:B:LEU:CD2	4:404:A:PCW:C7	3	17.56
(1,44)	2:79:B:LEU:H	4:404:A:PCW:C7	9	17.56
(1,31)	1:231:A:ASN:N	2:185:B:CYS:HG	9	17.56
(1,16)	1:216:A:LYS:N	2:185:B:CYS:CB	9	17.47
(1,45)	2:113:B:LEU:N	4:406:A:PCW:C8	4	17.42
(1,16)	1:216:A:LYS:N	2:185:B:CYS:H	3	17.37
(1,2)	4:401:A:PCW:C6	2:25:B:GLN:HE22	9	17.37
(1,32)	1:232:A:LEU:N	2:185:B:CYS:HG	9	17.31
(1,17)	1:217:A:LEU:N	2:185:B:CYS:SG	9	17.3
(1,2)	4:401:A:PCW:C6	2:25:B:GLN:HE22	7	16.76
(1,2)	4:401:A:PCW:C6	2:25:B:GLN:HE22	3	16.39
(1,38)	5:409:A:17F:O5	2:47:B:ASP:O	8	16.18
(1,22)	1:222:A:GLY:N	2:185:B:CYS:H	3	16.17
(1,41)	2:23:B:LEU:CD2	4:406:A:PCW:C8	5	16.15
(1,41)	2:23:B:LEU:CD2	4:406:A:PCW:C7	6	15.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	2:46:B:ILE:O	4:405:A:PCW:C7	1	15.96
(1,23)	1:223:A:PRO:N	2:185:B:CYS:H	3	15.94
(1,28)	1:228:A:PHE:N	2:185:B:CYS:HG	9	15.9
(1,45)	2:113:B:LEU:N	4:406:A:PCW:C7	6	15.69
(1,49)	2:185:B:CYS:SG	1:222:A:GLY:N	9	15.48
(1,41)	2:23:B:LEU:O	4:404:A:PCW:C7	2	15.44
(1,38)	5:409:A:17F:O4	2:25:B:GLN:HE21	9	15.24
(1,24)	1:224:A:VAL:N	2:185:B:CYS:HG	9	15.17
(1,38)	5:409:A:17F:O5	2:25:B:GLN:HE21	3	15.15
(1,27)	1:227:A:GLU:N	2:185:B:CYS:HG	9	15.01
(1,43)	2:46:B:ILE:O	4:404:A:PCW:C7	10	14.92
(1,30)	1:230:A:ASP:N	2:185:B:CYS:HG	9	14.87
(1,45)	2:113:B:LEU:N	4:406:A:PCW:C8	1	14.8
(1,44)	2:79:B:LEU:H	4:407:A:PCW:C7	8	14.72
(1,21)	1:221:A:LEU:N	2:185:B:CYS:SG	9	14.6
(1,18)	1:218:A:ARG:N	2:185:B:CYS:SG	9	14.58
(1,38)	5:409:A:17F:O5	2:25:B:GLN:HE21	7	14.18
(1,44)	2:79:B:LEU:H	4:406:A:PCW:C8	5	13.94
(1,23)	1:223:A:PRO:N	2:185:B:CYS:HG	9	13.78
(1,25)	1:225:A:THR:N	2:185:B:CYS:HG	9	13.42
(1,44)	2:79:B:LEU:H	4:406:A:PCW:C8	2	13.18
(1,41)	2:23:B:LEU:CD2	4:406:A:PCW:C8	4	13.01
(1,26)	1:226:A:GLN:N	2:185:B:CYS:HG	9	12.51
(1,22)	1:222:A:GLY:N	2:185:B:CYS:SG	9	12.48
(1,43)	2:46:B:ILE:O	4:404:A:PCW:C7	7	12.35
(1,43)	2:46:B:ILE:O	4:404:A:PCW:C7	9	12.25
(1,44)	2:79:B:LEU:H	4:406:A:PCW:C8	4	12.23
(1,48)	2:160:B:VAL:O	4:404:A:PCW:C7	10	12.16
(1,43)	2:46:B:ILE:CD1	4:406:A:PCW:C7	6	11.92
(1,3)	4:402:A:PCW:C7	4:203:B:PCW:C8	4	11.59
(1,10)	4:403:A:PCW:C8	2:160:B:VAL:CG1	8	11.41
(1,48)	2:160:B:VAL:O	4:404:A:PCW:C7	7	11.2
(1,43)	2:46:B:ILE:O	4:401:A:PCW:C6	8	10.87
(1,43)	2:46:B:ILE:CD1	4:406:A:PCW:C8	2	10.79
(1,44)	2:79:B:LEU:H	4:406:A:PCW:C7	6	10.14
(1,44)	2:79:B:LEU:H	4:406:A:PCW:C8	1	10.07
(1,3)	4:402:A:PCW:C7	4:203:B:PCW:C8	5	10.02
(1,3)	4:402:A:PCW:C7	4:203:B:PCW:C8	8	9.93
(1,2)	4:401:A:PCW:C6	2:47:B:ASP:O	8	9.88
(1,48)	2:160:B:VAL:O	4:406:A:PCW:C8	1	9.86
(1,48)	2:160:B:VAL:O	4:408:A:PCW:C5	5	9.76
(1,48)	2:160:B:VAL:O	4:407:A:PCW:C7	8	9.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	4:407:A:PCW:C7	2:160:B:VAL:O	8	9.18
(1,48)	2:160:B:VAL:O	4:404:A:PCW:C7	9	8.67
(1,48)	2:160:B:VAL:O	4:406:A:PCW:C7	6	8.42
(1,48)	2:160:B:VAL:CG1	4:406:A:PCW:C8	2	8.12
(1,29)	4:408:A:PCW:C4	4:203:B:PCW:C8	4	8.11
(1,3)	4:402:A:PCW:C7	4:203:B:PCW:C7	3	7.87
(1,43)	2:46:B:ILE:O	4:408:A:PCW:C8	5	7.56
(1,3)	4:402:A:PCW:C7	4:203:B:PCW:C8	7	7.56
(1,3)	4:402:A:PCW:C7	4:203:B:PCW:C8	2	7.52
(1,29)	4:408:A:PCW:C4	4:203:B:PCW:C8	10	7.29
(1,48)	2:160:B:VAL:O	4:404:A:PCW:C7	3	7.22
(1,29)	4:408:A:PCW:C4	4:203:B:PCW:C8	6	7.12
(1,3)	4:402:A:PCW:C7	4:203:B:PCW:C8	6	6.88
(1,43)	2:46:B:ILE:CD1	4:406:A:PCW:C8	4	6.59
(1,43)	2:46:B:ILE:O	4:404:A:PCW:C7	3	6.53
(1,29)	4:408:A:PCW:C4	4:203:B:PCW:C8	2	6.33
(1,3)	4:402:A:PCW:C7	4:203:B:PCW:C8	10	6.26
(1,29)	4:408:A:PCW:C4	4:203:B:PCW:C8	8	5.84
(1,3)	4:402:A:PCW:C8	4:203:B:PCW:C8	9	5.34
(1,29)	4:408:A:PCW:C4	2:185:B:CYS:O	1	5.14
(1,48)	2:160:B:VAL:CG1	4:406:A:PCW:C8	4	5.03
(1,19)	4:405:A:PCW:C7	4:203:B:PCW:C8	2	4.7
(1,19)	4:405:A:PCW:C7	4:203:B:PCW:C8	4	4.45
(1,15)	4:404:A:PCW:C6	4:202:B:PCW:C4	7	4.38
(1,29)	4:408:A:PCW:C4	4:203:B:PCW:C6	9	4.27
(1,49)	2:185:B:CYS:HG	4:406:A:PCW:C8	10	3.94
(1,15)	4:404:A:PCW:C6	4:202:B:PCW:C4	5	3.67
(1,19)	4:405:A:PCW:C7	4:203:B:PCW:C8	6	3.37
(1,15)	4:404:A:PCW:C6	4:202:B:PCW:C4	9	3.35
(1,42)	4:202:B:PCW:O2	4:406:A:PCW:C5	7	3.16
(1,42)	4:202:B:PCW:C8	4:406:A:PCW:C8	9	3.05
(1,49)	2:185:B:CYS:O	4:402:A:PCW:C7	1	2.74
(1,20)	4:406:A:PCW:C4	4:203:B:PCW:C3	3	2.69
(1,20)	4:406:A:PCW:C7	4:203:B:PCW:C1	2	2.53
(1,19)	4:405:A:PCW:C6	4:203:B:PCW:C8	8	2.39
(1,29)	4:408:A:PCW:C4	4:203:B:PCW:C6	7	2.31
(1,19)	4:405:A:PCW:C6	4:203:B:PCW:C8	9	2.18
(1,42)	4:202:B:PCW:C6	4:404:A:PCW:C6	6	2.12
(1,15)	4:404:A:PCW:C6	4:202:B:PCW:C6	6	2.12
(1,19)	4:405:A:PCW:C7	4:203:B:PCW:C8	5	2.08
(1,42)	4:202:B:PCW:C7	4:406:A:PCW:C8	5	2.0
(1,20)	4:406:A:PCW:C8	4:203:B:PCW:C1	9	1.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	4:202:B:PCW:C4	4:404:A:PCW:C6	8	1.88
(1,15)	4:404:A:PCW:C6	4:202:B:PCW:C4	8	1.88
(1,42)	4:202:B:PCW:C4	4:404:A:PCW:C6	2	1.85
(1,15)	4:404:A:PCW:C6	4:202:B:PCW:C4	2	1.85
(1,19)	4:405:A:PCW:C7	4:203:B:PCW:C8	7	1.84
(1,20)	4:406:A:PCW:C5	4:203:B:PCW:C1	7	1.82
(1,20)	4:406:A:PCW:C7	4:203:B:PCW:C1	8	1.69
(1,20)	4:406:A:PCW:C7	4:203:B:PCW:C1	5	1.68
(1,42)	4:202:B:PCW:C7	4:404:A:PCW:C6	4	1.5
(1,15)	4:404:A:PCW:C6	4:202:B:PCW:C7	4	1.5
(1,20)	4:406:A:PCW:C5	4:203:B:PCW:C1	4	1.35
(1,29)	4:408:A:PCW:C4	4:203:B:PCW:C8	5	1.3
(1,19)	4:405:A:PCW:C7	4:203:B:PCW:C8	10	1.29
(1,42)	4:202:B:PCW:C6	4:404:A:PCW:C6	3	1.25
(1,15)	4:404:A:PCW:C6	4:202:B:PCW:C6	3	1.25
(1,42)	4:202:B:PCW:C6	4:404:A:PCW:C6	1	1.12
(1,15)	4:404:A:PCW:C6	4:202:B:PCW:C6	1	1.12
(1,19)	4:405:A:PCW:C4	2:185:B:CYS:O	1	1.11
(1,20)	4:406:A:PCW:C8	2:185:B:CYS:HG	10	0.94
(1,20)	4:406:A:PCW:C8	4:203:B:PCW:C1	6	0.79
(1,29)	4:408:A:PCW:C4	4:203:B:PCW:C8	3	0.74
(1,19)	4:405:A:PCW:C6	4:203:B:PCW:C7	3	0.28

10 Dihedral-angle violation analysis

No dihedral-angle restraints found