



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 03:37 PM UTC

PDB ID : 8SR2 / pdb_00008sr2
EMDB ID : EMD-40718
Title : particulate methane monooxygenase incubated with 4,4,4-trifluorobutanol
Authors : Tucci, F.J.; Rosenzweig, A.C.
Deposited on : 2023-05-05
Resolution : 2.36 Å (reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

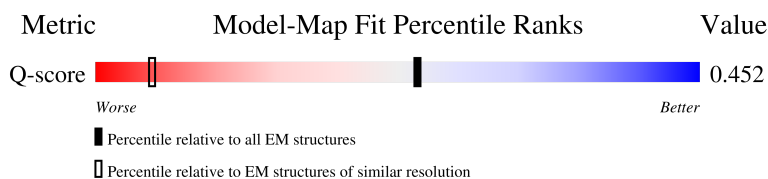
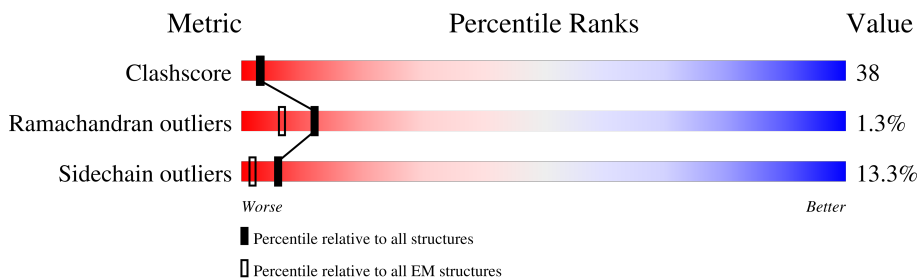
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.36 Å.

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.





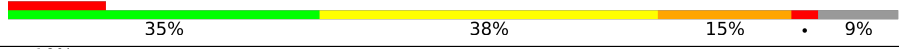
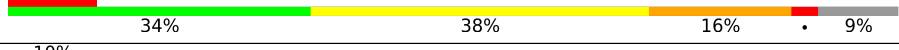

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4686 (1.86 - 2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	414	<p>67% 22% 8%</p>
1	E	414	<p>68% 21% 8%</p>
1	I	414	<p>65% 23% 8%</p>
2	B	247	<p>5% 50% 42% 5%</p>

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Mol	Chain	Length	Quality of chain
2	F	247	
2	J	247	
3	C	260	
3	G	260	
3	K	260	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	D10	A	503	-	-	X	-
5	D10	B	305	-	-	X	-
5	D10	E	503	-	-	X	-
5	D10	F	307	-	-	X	-
5	D10	I	503	-	-	X	-
5	D10	J	304	-	-	X	-
6	PLC	C	306	-	-	X	-
6	PLC	G	308	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 25361 atoms, of which 2479 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Particulate methane monooxygenase alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	S			
1	A	382	3017	1938	513	551	15	0	0	
1	E	382	3036	1938	19	513	551	15	0	0
1	I	382	3017	1938	513	551	15	0	0	

- Molecule 2 is a protein called Particulate methane monooxygenase beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	241	1977	1329	315	322	11	0	0
2	J	241	1976	1329	315	321	11	0	0
2	F	241	1977	1329	315	322	11	0	0

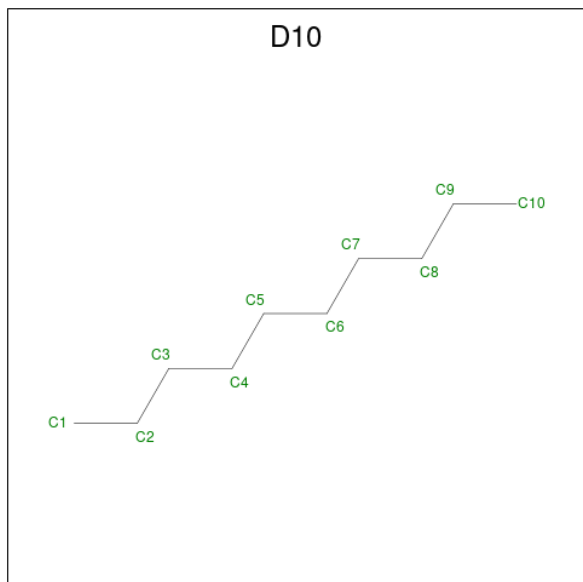
- Molecule 3 is a protein called Ammonia monooxygenase/methane monooxygenase, subunit C family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	236	1972	1339	299	329	5	0	0
3	G	236	1972	1339	299	329	5	0	0
3	K	236	1972	1339	299	329	5	0	0

- Molecule 4 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
4	A	2	Total Cu 2 2	0
4	C	1	Total Cu 1 1	0
4	E	2	Total Cu 2 2	0
4	I	2	Total Cu 2 2	0
4	G	1	Total Cu 1 1	0
4	K	1	Total Cu 1 1	0

- Molecule 5 is DECANE (CCD ID: D10) (formula: C₁₀H₂₂).



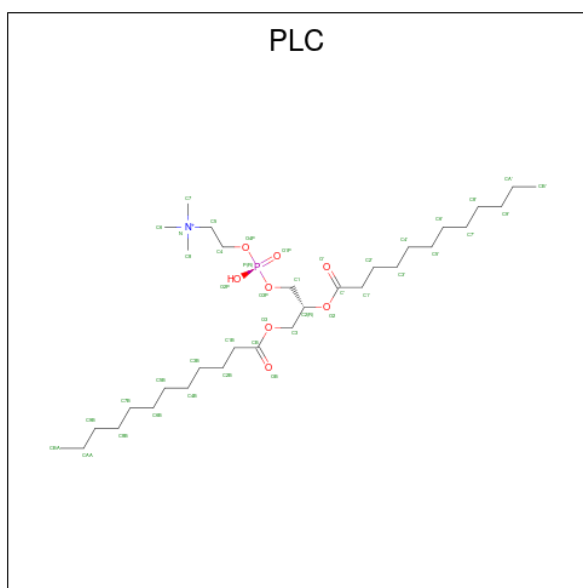
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C H 32 10 22	0
5	B	1	Total C H 32 10 22	0
5	B	1	Total C H 32 10 22	0
5	B	1	Total C H 32 10 22	0
5	B	1	Total C H 32 10 22	0
5	C	1	Total C H 32 10 22	0

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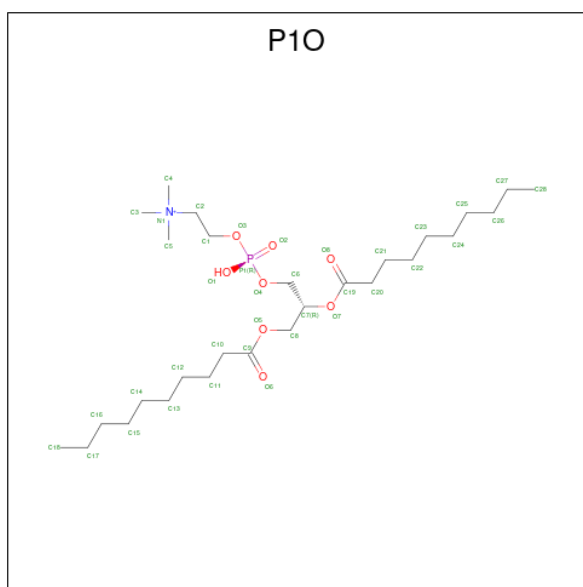
Mol	Chain	Residues	Atoms			AltConf
5	E	1	Total	C	H	0
			32	10	22	
5	I	1	Total	C	H	0
			32	10	22	
5	J	1	Total	C	H	0
			32	10	22	
5	J	1	Total	C	H	0
			32	10	22	
5	J	1	Total	C	H	0
			32	10	22	
5	J	1	Total	C	H	0
			32	10	22	
5	F	1	Total	C	H	0
			32	10	22	
5	F	1	Total	C	H	0
			32	10	22	
5	F	1	Total	C	H	0
			32	10	22	
5	F	1	Total	C	H	0
			32	10	22	
5	G	1	Total	C	H	0
			32	10	22	
5	K	1	Total	C	H	0
			32	10	22	

- Molecule 6 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: $C_{32}H_{65}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf	
6	B	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	J	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	J	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	F	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	F	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	G	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	G	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	G	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	G	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	K	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	K	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	K	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	K	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	

- Molecule 7 is 1,2-DIDECANOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: P1O) (formula: C₂₈H₅₇NO₈P).

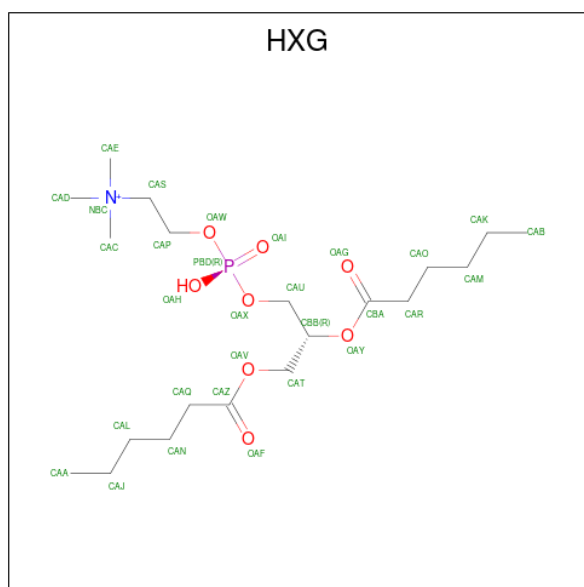


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
7	B	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
7	B	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
7	C	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
7	C	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
7	J	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
7	J	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
7	F	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
7	F	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
7	G	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
7	G	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
7	K	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
7	K	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	AltConf
8	C	1	Total Cl 1 1	0
8	G	1	Total Cl 1 1	0
8	K	1	Total Cl 1 1	0

- Molecule 9 is 1,2-dihexanoyl-sn-glycero-3-phosphocholine (CCD ID: HXG) (formula: $C_{20}H_{41}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf	
9	C	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
9	C	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
9	G	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
9	G	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
9	K	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
9	K	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	AltConf
10	A	79	Total O 79 79	0
10	B	43	Total O 43 43	0
10	C	12	Total O 12 12	0
10	E	81	Total O 81 81	0
10	I	79	Total O 79 79	0
10	J	43	Total O 43 43	0
10	F	43	Total O 43 43	0
10	G	10	Total O 10 10	0
10	K	11	Total O 11 11	0

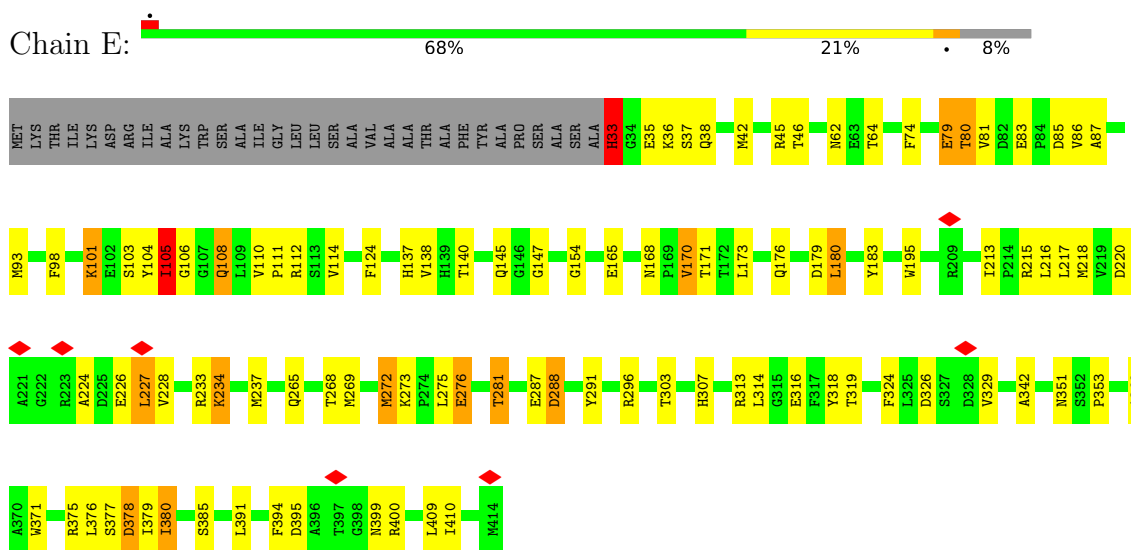
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

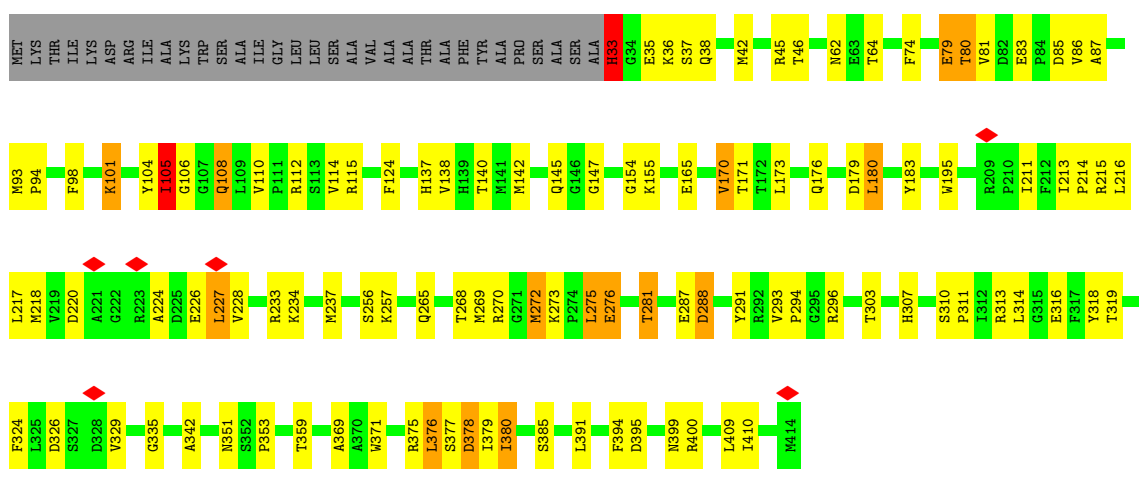
- Molecule 1: Particulate methane monooxygenase alpha subunit



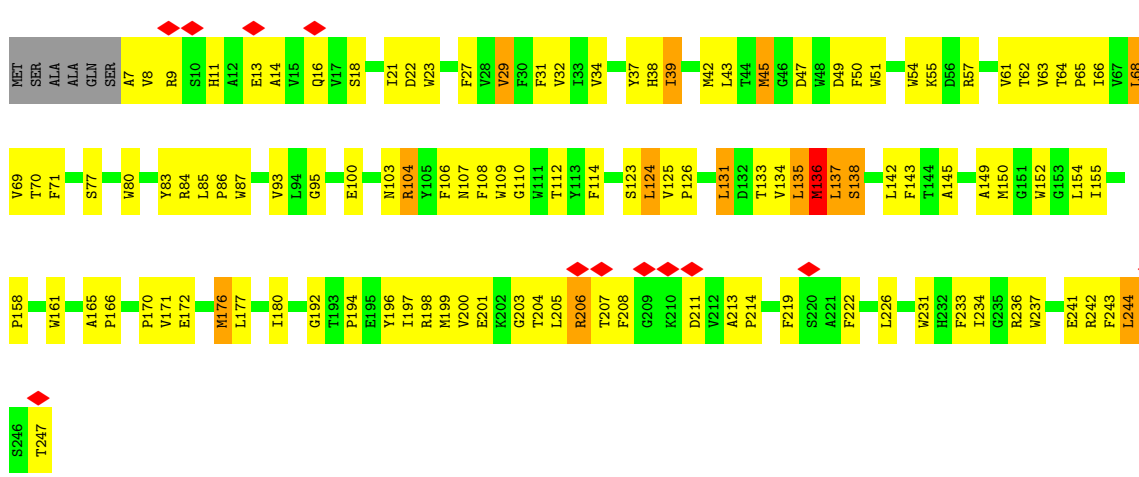
- Molecule 1: Particulate methane monooxygenase alpha subunit



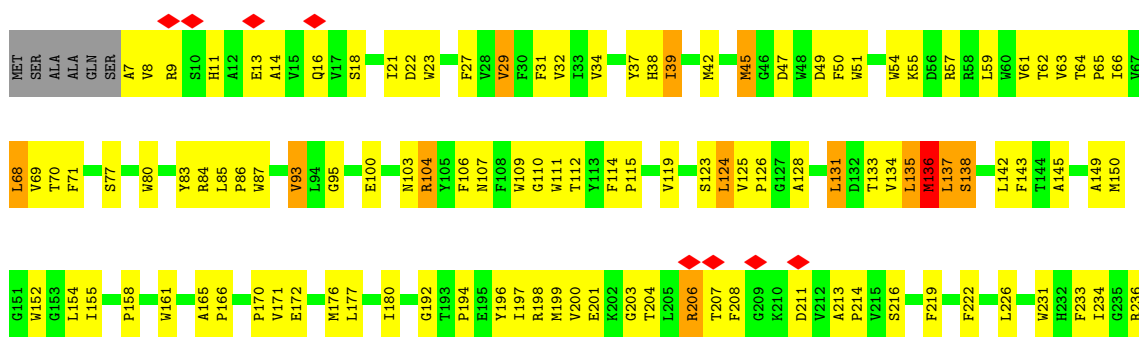
- Molecule 1: Particulate methane monooxygenase alpha subunit



• Molecule 2: Particulate methane monooxygenase beta subunit

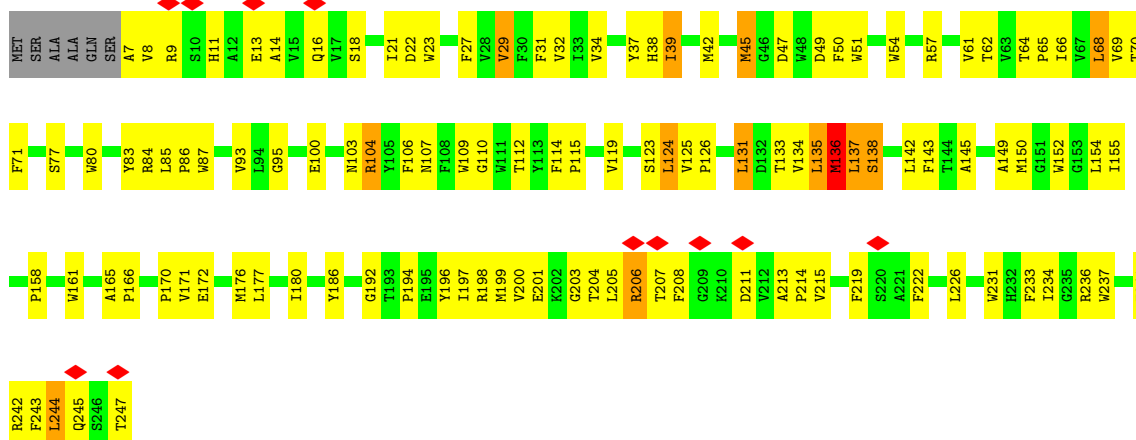


• Molecule 2: Particulate methane monooxygenase beta subunit

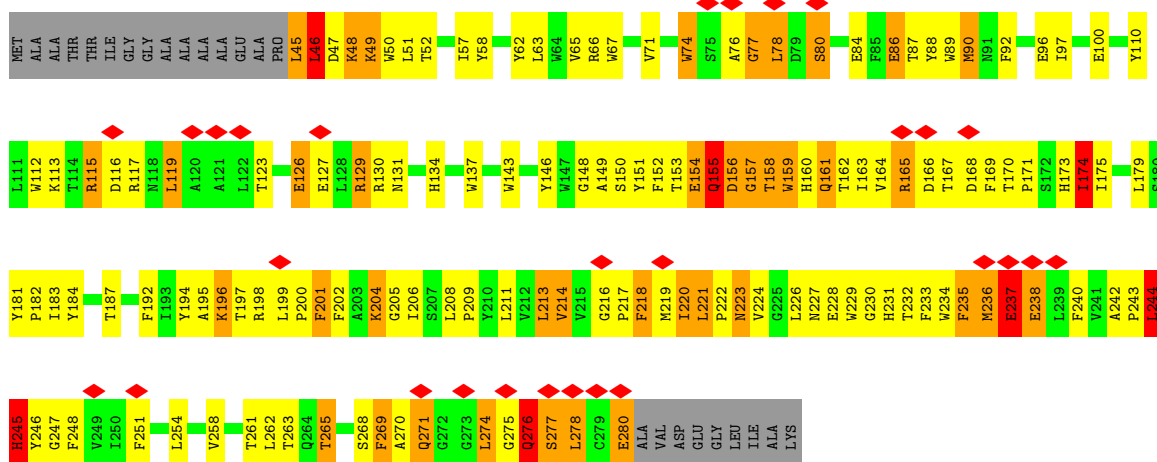




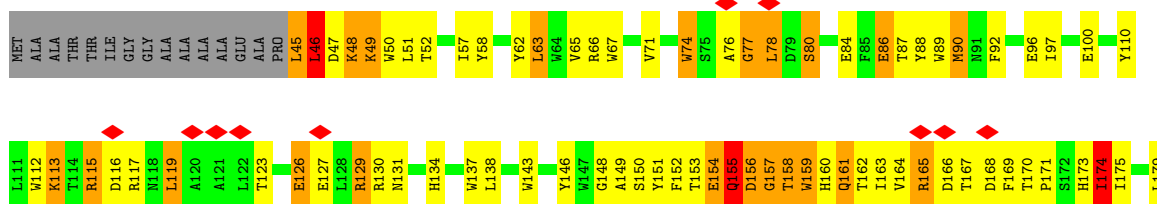
• Molecule 2: Particulate methane monooxygenase beta subunit



• Molecule 3: Ammonia monooxygenase/methane monooxygenase, subunit C family protein



• Molecule 3: Ammonia monooxygenase/methane monooxygenase, subunit C family protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	615783	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52.57	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.903	Depositor
Minimum map value	-0.699	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	273.7152, 273.7152, 273.7152	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5346, 0.5346, 0.5346	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: HXG, D10, CU, PLC, P1O, CL

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 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	0.22	0/3099	0.55	2/4215 (0.0%)
1	E	0.22	0/3099	0.55	2/4215 (0.0%)
1	I	0.22	0/3099	0.55	2/4215 (0.0%)
2	B	0.27	0/2053	0.64	2/2810 (0.1%)
2	F	0.27	0/2053	0.64	2/2810 (0.1%)
2	J	0.25	0/2052	0.62	2/2808 (0.1%)
3	C	0.44	0/2051	0.84	6/2810 (0.2%)
3	G	0.44	0/2051	0.84	6/2810 (0.2%)
3	K	0.44	0/2051	0.84	6/2810 (0.2%)
All	All	0.31	0/21608	0.67	30/29503 (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 outliers	#Planarity outliers
2	B	0	1
2	F	0	1
2	J	0	1
3	C	0	1
3	G	0	1
3	K	0	1
All	All	0	6

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	136	MET	N-CA-C	-8.78	101.40	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	136	MET	N-CA-C	-8.75	101.43	110.97
2	J	136	MET	N-CA-C	-8.69	101.50	110.97
3	K	156	ASP	CA-CB-CG	-7.80	104.80	112.60
3	G	156	ASP	CA-CB-CG	-7.78	104.82	112.60
3	C	156	ASP	CA-CB-CG	-7.77	104.83	112.60
2	F	137	LEU	N-CA-C	-7.74	98.21	109.59
2	B	137	LEU	N-CA-C	-7.73	98.22	109.59
2	J	137	LEU	N-CA-C	-7.65	98.34	109.59
3	G	245	HIS	CB-CG-CD2	-7.23	121.81	131.20
3	C	245	HIS	CB-CG-CD2	-7.22	121.81	131.20
3	K	245	HIS	CB-CG-CD2	-7.21	121.83	131.20
1	A	105	ILE	N-CA-C	-6.50	98.37	107.80
1	I	105	ILE	N-CA-C	-6.48	98.41	107.80
1	E	105	ILE	N-CA-C	-6.43	98.48	107.80
3	G	155	GLN	N-CA-C	-6.29	103.70	111.75
3	K	155	GLN	N-CA-C	-6.28	103.72	111.75
3	C	155	GLN	N-CA-C	-6.27	103.72	111.75
3	C	46	LEU	CB-CA-C	-5.25	110.50	116.54
3	K	46	LEU	CB-CA-C	-5.24	110.51	116.54
3	G	46	LEU	CB-CA-C	-5.22	110.53	116.54
3	C	174	ILE	CA-C-N	-5.21	117.61	122.66
3	C	174	ILE	C-N-CA	-5.21	117.61	122.66
3	K	174	ILE	CA-C-N	-5.19	117.63	122.66
3	K	174	ILE	C-N-CA	-5.19	117.63	122.66
3	G	174	ILE	CA-C-N	-5.18	117.64	122.66
3	G	174	ILE	C-N-CA	-5.18	117.64	122.66
1	I	33	HIS	N-CA-C	-5.09	96.75	111.00
1	E	33	HIS	N-CA-C	-5.08	96.78	111.00
1	A	33	HIS	N-CA-C	-5.07	96.80	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	7	ALA	Peptide
3	C	276	GLN	Peptide
2	F	7	ALA	Peptide
3	G	276	GLN	Peptide
2	J	7	ALA	Peptide
3	K	276	GLN	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3017	0	2980	118	0
1	E	3017	19	2980	111	0
1	I	3017	0	2980	120	0
2	B	1977	0	1936	204	0
2	F	1977	0	1936	196	0
2	J	1976	0	1936	186	0
3	C	1972	0	1904	301	0
3	G	1972	0	1904	292	0
3	K	1972	0	1904	285	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
4	E	2	0	0	0	0
4	G	1	0	0	0	0
4	I	2	0	0	0	0
4	K	1	0	0	0	0
5	A	10	22	22	11	0
5	B	40	88	88	14	0
5	C	10	22	22	2	0
5	E	10	22	22	10	0
5	F	40	88	88	12	0
5	G	10	22	22	2	0
5	I	10	22	22	14	0
5	J	40	88	88	12	0
5	K	10	22	22	3	0
6	B	42	64	64	15	0
6	C	168	256	256	53	0
6	F	84	128	128	29	0
6	G	210	320	320	64	0
6	J	84	128	128	23	0
6	K	168	256	256	52	0
7	B	76	112	112	17	0
7	C	76	112	112	28	0
7	F	76	112	112	18	0
7	G	76	112	112	23	0
7	J	76	112	112	17	0
7	K	76	112	112	23	0
8	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	1	0	0	0	0
8	K	1	0	0	0	0
9	C	60	80	80	28	0
9	G	60	80	80	28	0
9	K	60	80	80	28	0
10	A	79	0	0	11	0
10	B	43	0	0	15	0
10	C	12	0	0	4	0
10	E	81	0	0	13	0
10	F	43	0	0	13	0
10	G	10	0	0	3	0
10	I	79	0	0	11	0
10	J	43	0	0	13	0
10	K	11	0	0	4	0
All	All	22882	2479	22920	1723	0

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 38.

All (1723) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:GLY:O	2:F:205:LEU:CD1	1.67	1.42
2:B:205:LEU:CD1	1:I:147:GLY:O	1.64	1.41
2:J:206:ARG:CG	3:G:236:MET:CE	2.13	1.24
6:G:310:PLC:CBA	7:G:311:P1O:H54	1.68	1.24
6:C:308:PLC:CBA	7:C:309:P1O:H54	1.68	1.23
6:K:309:PLC:CBA	7:K:310:P1O:H54	1.68	1.23
2:B:206:ARG:CG	3:K:236:MET:CE	2.18	1.21
5:I:503:D10:C9	6:G:308:PLC:H61	1.69	1.20
3:K:261:THR:O	3:K:265:THR:HG23	1.43	1.19
5:A:503:D10:C9	6:K:307:PLC:H61	1.74	1.18
3:G:261:THR:O	3:G:265:THR:HG23	1.43	1.18
1:A:81:VAL:HG13	1:A:147:GLY:HA3	1.18	1.18
3:C:96:GLU:OE1	3:C:179:LEU:HB2	1.44	1.17
3:G:96:GLU:OE1	3:G:179:LEU:HB2	1.44	1.17
1:A:213:ILE:HG22	3:C:278:LEU:CD1	1.75	1.17
3:C:261:THR:O	3:C:265:THR:HG23	1.43	1.15
6:C:306:PLC:H5A1	6:F:301:PLC:H8A2	1.28	1.15
1:I:213:ILE:HG22	3:K:278:LEU:CD1	1.76	1.15
6:C:306:PLC:H61	5:E:503:D10:H92	1.28	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:306:PLC:H8A2	6:K:307:PLC:H5A1	1.28	1.15
1:I:81:VAL:HG13	1:I:147:GLY:CA	1.78	1.14
2:B:197:ILE:HD11	3:C:237:GLU:HG2	1.15	1.14
1:E:81:VAL:HG13	1:E:147:GLY:CA	1.78	1.14
3:C:67:TRP:HA	9:C:307:HXG:H39	1.18	1.14
3:K:96:GLU:OE1	3:K:179:LEU:HB2	1.44	1.13
6:C:306:PLC:H61	5:E:503:D10:C9	1.77	1.13
1:A:81:VAL:HG13	1:A:147:GLY:CA	1.78	1.12
1:I:81:VAL:CG1	1:I:147:GLY:HA3	1.80	1.12
1:E:81:VAL:CG1	1:E:147:GLY:HA3	1.80	1.12
6:K:303:PLC:H73	9:K:304:HXG:H36	1.32	1.11
2:B:112:THR:HG21	3:C:162:THR:HG21	1.13	1.11
2:B:206:ARG:HB2	3:K:236:MET:HE1	1.17	1.11
6:G:307:PLC:H8A2	6:G:308:PLC:H5A1	1.28	1.11
1:E:213:ILE:HG22	3:G:278:LEU:CD1	1.81	1.10
1:A:81:VAL:CG1	1:A:147:GLY:HA3	1.80	1.10
2:J:206:ARG:CB	3:G:236:MET:HE1	1.80	1.10
2:J:206:ARG:HG3	3:G:236:MET:CE	1.79	1.10
1:E:81:VAL:HG13	1:E:147:GLY:HA3	1.18	1.10
2:B:161:TRP:CZ2	6:B:301:PLC:H73	1.87	1.09
2:J:206:ARG:HB2	3:G:236:MET:HE1	1.10	1.09
3:G:67:TRP:HA	9:G:309:HXG:H39	1.18	1.09
3:K:67:TRP:HA	9:K:308:HXG:H39	1.18	1.09
3:C:92:PHE:CD2	6:C:308:PLC:OB	2.06	1.09
3:C:236:MET:CE	2:F:206:ARG:CG	2.31	1.09
2:J:161:TRP:CZ2	6:J:307:PLC:H73	1.87	1.09
2:F:161:TRP:CZ2	6:F:303:PLC:H73	1.87	1.09
3:G:92:PHE:CD2	6:G:310:PLC:OB	2.06	1.08
3:K:92:PHE:CD2	6:K:309:PLC:OB	2.06	1.08
1:I:213:ILE:HG22	3:K:278:LEU:HD11	1.31	1.08
2:J:197:ILE:HD11	3:K:237:GLU:HG2	1.16	1.08
1:I:81:VAL:HG13	1:I:147:GLY:HA3	1.18	1.07
2:B:206:ARG:HG3	3:K:236:MET:CE	1.83	1.06
6:C:303:PLC:H73	9:C:304:HXG:H36	1.33	1.06
6:G:304:PLC:H73	9:G:305:HXG:H36	1.32	1.05
2:B:206:ARG:HG3	3:K:236:MET:HE3	1.37	1.05
2:B:237:TRP:HE1	5:B:305:D10:H32	1.22	1.05
3:C:236:MET:HE1	2:F:206:ARG:HB2	1.39	1.05
2:F:197:ILE:HD11	3:G:237:GLU:HG2	1.09	1.05
5:I:503:D10:H92	6:G:308:PLC:H61	1.36	1.05
2:J:112:THR:HG21	3:K:162:THR:HG21	1.06	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:206:ARG:HG3	3:G:236:MET:HE3	1.32	1.04
2:B:206:ARG:CB	3:K:236:MET:HE1	1.86	1.04
2:J:206:ARG:HG2	3:G:236:MET:HE2	1.36	1.03
5:I:503:D10:H91	6:G:308:PLC:H61	1.39	1.03
2:J:237:TRP:HE1	5:J:304:D10:H32	1.22	1.03
6:K:309:PLC:CBA	7:K:310:P1O:C28	2.36	1.02
6:C:308:PLC:CBA	7:C:309:P1O:C28	2.36	1.02
2:F:237:TRP:HE1	5:F:307:D10:H32	1.22	1.02
6:G:310:PLC:CBA	7:G:311:P1O:C28	2.36	1.02
2:B:206:ARG:HG2	3:K:236:MET:HE2	1.41	1.01
3:C:236:MET:HE3	3:C:236:MET:HA	1.42	1.01
3:K:130:ARG:C	3:K:199:LEU:HD21	1.85	1.01
1:E:213:ILE:HG22	3:G:278:LEU:HD11	1.38	1.01
1:E:80:THR:HG21	2:J:203:GLY:O	1.61	1.01
3:G:236:MET:HE3	3:G:236:MET:HA	1.42	1.01
2:B:197:ILE:CD1	3:C:237:GLU:HG2	1.90	1.01
3:C:130:ARG:C	3:C:199:LEU:HD21	1.85	1.01
1:A:213:ILE:HG22	3:C:278:LEU:HD11	1.36	1.00
5:A:503:D10:H92	6:K:307:PLC:H61	1.37	1.00
3:G:130:ARG:C	3:G:199:LEU:HD21	1.85	1.00
3:C:67:TRP:CD1	9:C:307:HXG:H41	1.96	1.00
3:C:236:MET:CE	2:F:206:ARG:HG3	1.90	1.00
2:F:197:ILE:CD1	3:G:237:GLU:HG2	1.91	1.00
2:J:206:ARG:CG	3:G:236:MET:HE2	1.86	1.00
3:K:67:TRP:CD1	9:K:308:HXG:H41	1.96	1.00
2:F:112:THR:HG21	3:G:162:THR:CG2	1.92	1.00
2:F:112:THR:CG2	3:G:162:THR:HG21	1.91	0.99
3:G:67:TRP:CD1	9:G:309:HXG:H41	1.96	0.99
5:I:503:D10:H92	6:G:308:PLC:C6	1.91	0.99
5:A:503:D10:H91	6:K:307:PLC:H61	1.45	0.98
6:C:308:PLC:HEA3	7:C:309:P1O:H54	1.46	0.98
5:I:503:D10:C9	6:G:308:PLC:C6	2.41	0.98
1:A:80:THR:HG21	2:F:203:GLY:O	1.63	0.97
3:K:236:MET:HE3	3:K:236:MET:HA	1.42	0.97
6:G:310:PLC:HEA3	7:G:311:P1O:H54	1.46	0.97
5:A:503:D10:H92	6:K:307:PLC:C6	1.95	0.96
2:B:203:GLY:O	1:I:80:THR:HG21	1.65	0.96
1:I:213:ILE:CG2	3:K:278:LEU:HD11	1.96	0.96
3:G:67:TRP:CD1	9:G:309:HXG:CAC	2.49	0.96
2:J:197:ILE:CD1	3:K:237:GLU:HG2	1.96	0.96
6:G:310:PLC:HEA2	7:G:311:P1O:H54	1.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:112:THR:HG21	3:G:162:THR:HG21	0.97	0.95
6:C:308:PLC:HEA2	7:C:309:P1O:H54	1.48	0.95
3:K:67:TRP:CD1	9:K:308:HXG:CAC	2.49	0.95
1:A:147:GLY:C	2:F:205:LEU:HD12	1.92	0.95
2:B:161:TRP:CZ2	6:B:301:PLC:C7	2.50	0.95
6:K:309:PLC:HEA2	7:K:310:P1O:H54	1.48	0.95
2:B:205:LEU:HD12	1:I:147:GLY:C	1.91	0.94
3:C:67:TRP:CD1	9:C:307:HXG:CAC	2.49	0.94
6:K:309:PLC:HEA3	7:K:310:P1O:H54	1.46	0.94
1:I:124:PHE:CE2	1:I:140:THR:HG21	2.02	0.94
2:J:161:TRP:CZ2	6:J:307:PLC:C7	2.50	0.94
2:F:161:TRP:CZ2	6:F:303:PLC:C7	2.50	0.94
6:C:306:PLC:C6	5:E:503:D10:H92	1.97	0.94
2:J:206:ARG:CB	3:G:236:MET:CE	2.43	0.94
2:J:206:ARG:NH2	3:G:237:GLU:O	1.99	0.94
3:K:261:THR:O	3:K:265:THR:CG2	2.16	0.94
1:A:213:ILE:CG2	3:C:278:LEU:HD11	1.97	0.94
3:C:261:THR:O	3:C:265:THR:CG2	2.16	0.93
3:G:86:GLU:HA	3:G:90:MET:HB2	1.49	0.93
5:A:503:D10:C9	6:K:307:PLC:C6	2.46	0.93
3:K:67:TRP:HA	9:K:308:HXG:CAC	1.99	0.93
1:A:124:PHE:CE2	1:A:140:THR:HG21	2.02	0.93
2:J:206:ARG:HB2	3:G:236:MET:CE	1.97	0.93
3:G:261:THR:O	3:G:265:THR:CG2	2.16	0.93
1:E:124:PHE:CE2	1:E:140:THR:HG21	2.02	0.93
3:G:67:TRP:HA	9:G:309:HXG:CAC	1.99	0.93
3:C:86:GLU:HA	3:C:90:MET:HB2	1.49	0.92
1:E:108:GLN:OE1	1:E:269:MET:HE1	1.69	0.92
3:K:270:ALA:HB1	3:K:274:LEU:HB2	1.51	0.92
3:C:236:MET:HE3	2:F:206:ARG:HG3	1.51	0.92
1:I:108:GLN:OE1	1:I:269:MET:HE1	1.69	0.92
3:K:86:GLU:HA	3:K:90:MET:HB2	1.49	0.91
3:G:270:ALA:HB1	3:G:274:LEU:HB2	1.51	0.91
2:B:206:ARG:CG	3:K:236:MET:HE2	1.92	0.91
3:C:67:TRP:HA	9:C:307:HXG:CAC	1.99	0.91
1:E:213:ILE:CG2	3:G:278:LEU:HD11	2.01	0.91
1:I:217:LEU:HD12	3:K:278:LEU:HD13	1.50	0.91
2:B:197:ILE:HD11	3:C:237:GLU:CG	2.00	0.90
3:C:236:MET:HE2	2:F:206:ARG:HG2	1.54	0.90
2:F:197:ILE:HD11	3:G:237:GLU:CG	1.99	0.90
3:G:49:LYS:NZ	3:G:49:LYS:HB3	1.86	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:LYS:HB3	3:C:49:LYS:NZ	1.86	0.90
3:C:270:ALA:HB1	3:C:274:LEU:HB2	1.52	0.90
2:B:237:TRP:HE1	5:B:305:D10:C3	1.83	0.90
2:J:237:TRP:HE1	5:J:304:D10:C3	1.84	0.90
2:F:237:TRP:HE1	5:F:307:D10:C3	1.84	0.90
2:B:206:ARG:NH2	3:K:237:GLU:O	2.04	0.90
2:F:244:LEU:HD21	3:G:208:LEU:HD13	1.54	0.90
1:A:108:GLN:OE1	1:A:269:MET:HE1	1.69	0.90
1:A:147:GLY:O	2:F:205:LEU:HD12	0.72	0.89
1:I:217:LEU:HD12	3:K:278:LEU:CD1	2.02	0.89
3:K:49:LYS:NZ	3:K:49:LYS:HB3	1.86	0.88
9:C:304:HXG:H9	5:C:305:D10:H42	1.56	0.88
3:G:235:PHE:HD2	3:G:244:LEU:HD13	1.39	0.88
2:B:206:ARG:CB	3:K:236:MET:CE	2.50	0.88
2:B:205:LEU:HD12	1:I:147:GLY:O	0.70	0.87
3:C:235:PHE:HD2	3:C:244:LEU:HD13	1.39	0.87
3:K:235:PHE:HD2	3:K:244:LEU:HD13	1.39	0.87
9:K:304:HXG:H9	5:K:305:D10:H42	1.56	0.87
1:E:217:LEU:HD12	3:G:278:LEU:HD13	1.54	0.87
9:G:305:HXG:H9	5:G:306:D10:H42	1.56	0.87
3:C:236:MET:HE1	2:F:206:ARG:CB	2.05	0.86
9:G:309:HXG:H37	9:G:309:HXG:H26	1.57	0.86
10:B:419:HOH:O	3:K:232:THR:HB	1.73	0.86
3:K:74:TRP:HA	3:K:78:LEU:HD22	1.57	0.85
3:C:74:TRP:HA	3:C:78:LEU:HD22	1.57	0.85
10:J:419:HOH:O	3:G:232:THR:HB	1.77	0.85
3:G:74:TRP:HA	3:G:78:LEU:HD22	1.57	0.84
2:J:165:ALA:HB3	2:J:166:PRO:HD3	1.60	0.84
9:K:308:HXG:H26	9:K:308:HXG:H37	1.57	0.84
2:B:165:ALA:HB3	2:B:166:PRO:HD3	1.59	0.84
2:J:112:THR:CG2	3:K:162:THR:HG21	2.00	0.84
1:A:213:ILE:CG2	3:C:278:LEU:CD1	2.55	0.84
2:B:245:GLN:HA	3:C:205:GLY:HA2	1.60	0.84
3:G:230:GLY:HA3	3:G:244:LEU:HD12	1.58	0.84
9:C:307:HXG:H26	9:C:307:HXG:H37	1.58	0.84
1:E:237:MET:HG3	2:F:137:LEU:HD11	1.59	0.84
2:F:237:TRP:NE1	5:F:307:D10:H51	1.92	0.84
1:E:217:LEU:HD12	3:G:278:LEU:CD1	2.08	0.84
2:B:237:TRP:NE1	5:B:305:D10:H51	1.92	0.84
2:B:237:TRP:NE1	5:B:305:D10:H32	1.93	0.83
3:G:156:ASP:C	3:G:158:THR:H	1.86	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:230:GLY:HA3	3:K:244:LEU:HD12	1.59	0.83
3:C:230:GLY:HA3	3:C:244:LEU:HD12	1.58	0.83
2:J:197:ILE:HD11	3:K:237:GLU:CG	2.05	0.83
2:J:237:TRP:NE1	5:J:304:D10:H51	1.93	0.83
7:J:301:P1O:O8	7:J:301:P1O:H20	1.79	0.83
3:K:156:ASP:C	3:K:158:THR:H	1.87	0.83
3:C:130:ARG:O	3:C:199:LEU:HD21	1.79	0.83
6:C:306:PLC:C6	5:E:503:D10:C9	2.56	0.83
3:G:230:GLY:CA	3:G:244:LEU:HD12	2.09	0.83
1:A:237:MET:HG3	2:B:137:LEU:HD11	1.61	0.82
2:F:165:ALA:HB3	2:F:166:PRO:HD3	1.59	0.82
3:C:67:TRP:CA	9:C:307:HGX:H39	2.07	0.82
2:J:237:TRP:NE1	5:J:304:D10:H32	1.94	0.82
3:C:204:LYS:O	3:C:204:LYS:HD2	1.80	0.82
3:C:230:GLY:CA	3:C:244:LEU:HD12	2.09	0.82
2:F:237:TRP:NE1	5:F:307:D10:H32	1.93	0.82
3:K:230:GLY:CA	3:K:244:LEU:HD12	2.09	0.82
1:I:93:MET:HE1	1:I:98:PHE:HB2	1.62	0.82
7:F:304:P1O:O8	7:F:304:P1O:H20	1.79	0.82
3:K:130:ARG:O	3:K:199:LEU:HD21	1.79	0.82
7:B:302:P1O:O8	7:B:302:P1O:H20	1.79	0.82
1:A:217:LEU:HD12	3:C:278:LEU:HD13	1.61	0.82
3:G:130:ARG:O	3:G:199:LEU:HD21	1.79	0.82
2:B:206:ARG:HB2	3:K:236:MET:CE	2.04	0.82
2:J:112:THR:HG21	3:K:162:THR:CG2	2.01	0.82
3:G:204:LYS:HD2	3:G:204:LYS:O	1.80	0.81
3:G:129:ARG:HH11	3:G:129:ARG:HG3	1.45	0.81
3:G:67:TRP:CA	9:G:309:HGX:H39	2.07	0.81
3:K:204:LYS:O	3:K:204:LYS:HD2	1.80	0.81
2:B:143:PHE:CD2	7:B:302:P1O:H26	2.16	0.81
6:C:306:PLC:H61	5:E:503:D10:H91	1.63	0.81
2:J:143:PHE:CD2	7:J:301:P1O:H26	2.16	0.81
1:E:93:MET:HE1	1:E:98:PHE:HB2	1.62	0.81
2:B:244:LEU:HD12	3:C:206:ILE:HG22	1.62	0.81
1:E:215:ARG:HG2	1:E:227:LEU:HD22	1.63	0.81
1:A:93:MET:HE1	1:A:98:PHE:HB2	1.62	0.81
1:A:215:ARG:HG2	1:A:227:LEU:HD22	1.63	0.81
3:K:58:TYR:HH	3:K:187:THR:HG1	1.29	0.80
3:C:129:ARG:HH11	3:C:129:ARG:HG3	1.45	0.80
2:F:143:PHE:CD2	7:F:304:P1O:H26	2.16	0.80
2:F:206:ARG:HB3	2:F:206:ARG:HH11	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:156:ASP:C	3:C:158:THR:H	1.87	0.80
1:I:237:MET:HG3	2:J:137:LEU:HD11	1.62	0.80
2:J:206:ARG:HB3	2:J:206:ARG:HH11	1.46	0.80
3:K:129:ARG:HG3	3:K:129:ARG:HH11	1.45	0.80
2:B:213:ALA:HB3	6:B:301:PLC:H11	1.63	0.80
3:C:67:TRP:HD1	9:C:307:HXG:H41	1.48	0.79
1:I:215:ARG:HG2	1:I:227:LEU:HD22	1.63	0.79
2:J:213:ALA:HB3	6:J:307:PLC:H11	1.63	0.79
2:B:206:ARG:HH11	2:B:206:ARG:HB3	1.46	0.78
6:C:306:PLC:C5B	6:F:301:PLC:H8A2	2.13	0.78
2:F:213:ALA:HB3	6:F:303:PLC:H11	1.63	0.78
2:J:66:ILE:HG22	6:G:304:PLC:H9A2	1.65	0.78
3:C:67:TRP:HD1	9:C:307:HXG:CAC	1.96	0.78
7:J:301:P1O:H48	7:J:301:P1O:H38	1.66	0.78
1:A:217:LEU:HD12	3:C:278:LEU:CD1	2.12	0.78
1:I:213:ILE:CG2	3:K:278:LEU:CD1	2.57	0.78
3:K:130:ARG:C	3:K:199:LEU:CD2	2.57	0.78
3:K:67:TRP:HD1	9:K:308:HXG:CAC	1.96	0.78
3:K:67:TRP:HD1	9:K:308:HXG:H41	1.48	0.78
2:F:245:GLN:HA	3:G:205:GLY:HA2	1.66	0.77
3:C:130:ARG:C	3:C:199:LEU:CD2	2.57	0.77
3:G:67:TRP:HD1	9:G:309:HXG:CAC	1.96	0.77
3:G:130:ARG:C	3:G:199:LEU:CD2	2.57	0.77
7:B:302:P1O:H48	7:B:302:P1O:H38	1.66	0.76
1:A:79:GLU:HB2	1:E:268:THR:HB	1.67	0.76
5:I:503:D10:C7	6:G:308:PLC:OB	2.33	0.76
1:A:33:HIS:HD2	3:C:78:LEU:HB3	1.50	0.76
2:B:244:LEU:HD21	3:C:208:LEU:HD13	1.66	0.76
7:F:304:P1O:H38	7:F:304:P1O:H48	1.66	0.76
3:C:236:MET:HE2	2:F:206:ARG:CG	2.07	0.76
3:C:89:TRP:HB3	3:C:174:ILE:HD13	1.68	0.76
1:A:268:THR:HB	1:I:79:GLU:HB2	1.66	0.76
3:K:67:TRP:CA	9:K:308:HXG:H39	2.07	0.76
2:B:112:THR:CG2	3:C:162:THR:HG21	2.07	0.75
3:K:89:TRP:HB3	3:K:174:ILE:HD13	1.68	0.75
2:B:192:GLY:O	3:C:238:GLU:HB2	1.86	0.75
6:C:308:PLC:HEA3	7:C:309:P1O:C28	2.11	0.75
6:G:307:PLC:H8A2	6:G:308:PLC:C5B	2.12	0.75
1:E:79:GLU:HB2	1:I:268:THR:HB	1.67	0.75
1:A:176:GLN:NE2	10:A:605:HOH:O	2.19	0.74
3:C:236:MET:HE3	3:C:236:MET:CA	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:50:TRP:CE3	7:K:310:P1O:H39	2.22	0.74
2:B:29:VAL:HG23	3:C:262:LEU:HD12	1.69	0.74
1:I:176:GLN:NE2	10:I:606:HOH:O	2.19	0.74
3:G:50:TRP:CE3	7:G:311:P1O:H39	2.22	0.74
3:C:134:HIS:CB	3:C:199:LEU:HD11	2.17	0.74
2:J:45:MET:HG2	2:J:45:MET:O	1.86	0.74
5:I:503:D10:H71	6:G:308:PLC:OB	1.87	0.74
3:C:201:PHE:CE1	3:C:268:SER:HB2	2.23	0.74
2:J:135:LEU:O	2:J:135:LEU:HD22	1.88	0.74
6:G:310:PLC:HEA3	7:G:311:P1O:C28	2.11	0.74
2:B:241:GLU:OE2	10:B:401:HOH:O	2.06	0.74
7:B:307:P1O:O6	7:B:307:P1O:H43	1.88	0.74
2:F:45:MET:O	2:F:45:MET:HG2	1.86	0.74
3:G:242:ALA:O	3:G:245:HIS:HB2	1.88	0.74
3:K:88:TYR:CE1	6:K:309:PLC:O1P	2.41	0.74
3:C:156:ASP:O	3:C:158:THR:N	2.21	0.74
7:F:302:P1O:O6	7:F:302:P1O:H43	1.88	0.74
3:K:201:PHE:CE1	3:K:268:SER:HB2	2.23	0.74
3:C:88:TYR:CE1	6:C:308:PLC:O1P	2.41	0.74
1:E:176:GLN:NE2	10:E:607:HOH:O	2.20	0.74
3:G:89:TRP:HB3	3:G:174:ILE:HD13	1.68	0.74
3:G:134:HIS:CB	3:G:199:LEU:HD11	2.17	0.74
3:K:274:LEU:O	3:K:274:LEU:HD12	1.88	0.73
3:C:50:TRP:CE3	7:C:309:P1O:H39	2.22	0.73
3:C:242:ALA:O	3:C:245:HIS:HB2	1.88	0.73
1:E:213:ILE:CG2	3:G:278:LEU:CD1	2.60	0.73
3:G:271:GLN:OE1	3:G:271:GLN:HA	1.88	0.73
3:G:156:ASP:O	3:G:158:THR:N	2.21	0.73
2:B:66:ILE:HG22	6:K:303:PLC:H9A2	1.68	0.73
3:C:232:THR:HB	10:F:417:HOH:O	1.88	0.73
2:F:135:LEU:O	2:F:135:LEU:HD22	1.88	0.73
3:G:45:LEU:N	3:G:45:LEU:HD23	2.04	0.73
6:K:306:PLC:H8A2	6:K:307:PLC:C5B	2.12	0.73
2:B:45:MET:HG2	2:B:45:MET:O	1.86	0.73
3:C:274:LEU:O	3:C:274:LEU:HD12	1.88	0.73
3:G:88:TYR:CE1	6:G:310:PLC:O1P	2.41	0.73
3:C:45:LEU:HD23	3:C:45:LEU:N	2.04	0.73
3:K:242:ALA:O	3:K:245:HIS:HB2	1.88	0.73
3:G:274:LEU:HD12	3:G:274:LEU:O	1.88	0.73
3:K:271:GLN:OE1	3:K:271:GLN:HA	1.88	0.72
6:K:309:PLC:HEA3	7:K:310:P1O:C28	2.11	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:LEU:O	2:B:135:LEU:HD22	1.88	0.72
3:G:49:LYS:HB3	3:G:49:LYS:HZ1	1.52	0.72
3:K:134:HIS:CB	3:K:199:LEU:HD11	2.17	0.72
3:K:236:MET:HE3	3:K:236:MET:CA	2.17	0.72
5:A:503:D10:C7	6:K:307:PLC:OB	2.37	0.72
7:J:308:P1O:O6	7:J:308:P1O:H43	1.88	0.72
2:J:213:ALA:HB3	6:J:307:PLC:C1	2.19	0.72
1:E:35:GLU:OE2	10:E:601:HOH:O	2.07	0.72
3:G:201:PHE:CE1	3:G:268:SER:HB2	2.23	0.72
3:G:234:TRP:O	3:G:235:PHE:HB2	1.90	0.72
1:A:81:VAL:HG13	1:A:147:GLY:HA2	1.71	0.72
2:F:213:ALA:HB3	6:F:303:PLC:C1	2.19	0.72
3:K:234:TRP:O	3:K:235:PHE:HB2	1.90	0.72
2:B:213:ALA:HB3	6:B:301:PLC:C1	2.19	0.72
2:B:65:PRO:O	2:B:69:VAL:HG13	1.90	0.71
2:B:244:LEU:HD12	3:C:206:ILE:CG2	2.18	0.71
3:C:234:TRP:O	3:C:235:PHE:HB2	1.90	0.71
3:C:237:GLU:O	2:F:206:ARG:NH2	2.22	0.71
3:K:45:LEU:HD23	3:K:45:LEU:N	2.04	0.71
1:E:81:VAL:HG13	1:E:147:GLY:HA2	1.71	0.71
2:F:192:GLY:O	3:G:238:GLU:HB2	1.91	0.71
3:G:156:ASP:C	3:G:158:THR:N	2.46	0.71
3:K:156:ASP:O	3:K:158:THR:N	2.21	0.71
3:C:156:ASP:C	3:C:158:THR:N	2.46	0.71
3:G:67:TRP:HD1	9:G:309:HXG:H41	1.48	0.71
3:C:271:GLN:OE1	3:C:271:GLN:HA	1.88	0.71
1:A:220:ASP:OD1	10:A:601:HOH:O	2.08	0.71
2:F:65:PRO:O	2:F:69:VAL:HG13	1.90	0.71
2:F:69:VAL:HG12	2:F:152:TRP:CE2	2.26	0.71
1:I:35:GLU:H	1:I:35:GLU:CD	1.99	0.71
2:F:247:THR:HG22	3:G:211:LEU:HD22	1.73	0.71
1:A:35:GLU:H	1:A:35:GLU:CD	1.99	0.71
2:J:47:ASP:HB3	2:J:54:TRP:CZ3	2.26	0.71
3:K:156:ASP:C	3:K:158:THR:N	2.46	0.71
3:K:112:TRP:CH2	7:K:311:P1O:H2	2.26	0.70
1:I:81:VAL:HG13	1:I:147:GLY:HA2	1.71	0.70
1:I:217:LEU:CD1	3:K:278:LEU:HD12	2.21	0.70
2:B:47:ASP:HB3	2:B:54:TRP:CZ3	2.26	0.70
2:J:65:PRO:O	2:J:69:VAL:HG13	1.90	0.70
3:G:112:TRP:CH2	7:G:312:P1O:H2	2.27	0.70
2:J:241:GLU:OE2	10:J:401:HOH:O	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:270:ALA:CB	3:G:274:LEU:HB2	2.22	0.70
3:K:270:ALA:CB	3:K:274:LEU:HB2	2.22	0.70
6:K:309:PLC:H1'1	6:K:309:PLC:H72	1.74	0.70
3:C:274:LEU:HD12	3:C:274:LEU:C	2.17	0.70
1:E:35:GLU:CD	1:E:35:GLU:H	1.99	0.70
1:E:220:ASP:OD1	10:E:602:HOH:O	2.09	0.70
2:F:47:ASP:HB3	2:F:54:TRP:CZ3	2.26	0.70
2:F:241:GLU:OE2	10:F:401:HOH:O	2.08	0.70
2:B:18:SER:OG	10:B:402:HOH:O	2.10	0.70
3:C:270:ALA:CB	3:C:274:LEU:HB2	2.22	0.70
2:J:69:VAL:HG12	2:J:152:TRP:CE2	2.26	0.70
3:K:274:LEU:HD12	3:K:274:LEU:C	2.17	0.70
1:A:276:GLU:OE1	1:A:276:GLU:HA	1.92	0.69
2:B:69:VAL:HG12	2:B:152:TRP:CE2	2.26	0.69
6:C:306:PLC:OB	5:E:503:D10:H72	1.92	0.69
6:C:308:PLC:H72	6:C:308:PLC:H1'1	1.74	0.69
1:E:272:MET:HE2	1:E:272:MET:CA	2.23	0.69
6:C:306:PLC:OB	5:E:503:D10:C7	2.41	0.69
2:J:18:SER:OG	10:J:402:HOH:O	2.09	0.69
5:A:503:D10:H71	6:K:307:PLC:OB	1.92	0.69
3:C:112:TRP:CH2	7:C:310:P1O:H2	2.27	0.69
6:C:306:PLC:H5A1	6:F:301:PLC:C8B	2.17	0.69
3:K:221:LEU:HB3	3:K:222:PRO:HD3	1.75	0.69
3:C:168:ASP:OD2	2:F:211:ASP:OD2	2.11	0.69
3:G:221:LEU:HB3	3:G:222:PRO:HD3	1.75	0.69
3:G:274:LEU:HD12	3:G:274:LEU:C	2.17	0.69
3:C:58:TYR:HH	3:C:187:THR:HG1	1.37	0.69
3:C:221:LEU:HB3	3:C:222:PRO:HD3	1.75	0.69
1:E:371:TRP:NE1	1:E:377:SER:HB3	2.08	0.69
1:I:220:ASP:OD1	10:I:601:HOH:O	2.09	0.69
1:I:276:GLU:OE1	1:I:276:GLU:HA	1.92	0.69
1:I:371:TRP:NE1	1:I:377:SER:HB3	2.08	0.69
2:J:192:GLY:O	3:K:238:GLU:HB2	1.93	0.69
6:G:310:PLC:H1'1	6:G:310:PLC:H72	1.73	0.69
3:G:130:ARG:HB3	3:G:199:LEU:HD23	1.75	0.69
2:B:199:MET:SD	6:C:311:PLC:H2	2.33	0.68
3:C:117:ARG:HG2	3:C:117:ARG:HH11	1.58	0.68
3:G:117:ARG:HG2	3:G:117:ARG:HH11	1.58	0.68
3:K:117:ARG:HG2	3:K:117:ARG:HH11	1.58	0.68
3:C:127:GLU:CD	3:C:200:PRO:CG	2.66	0.68
3:G:58:TYR:HH	3:G:187:THR:HG1	1.33	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:ARG:HB3	3:C:199:LEU:HD23	1.75	0.68
2:F:18:SER:OG	10:F:402:HOH:O	2.10	0.68
2:B:39:ILE:HA	2:B:42:MET:HE3	1.76	0.68
3:K:127:GLU:CD	3:K:200:PRO:CG	2.66	0.68
1:I:272:MET:CA	1:I:272:MET:HE2	2.23	0.68
1:A:371:TRP:NE1	1:A:377:SER:HB3	2.08	0.68
3:C:236:MET:HE1	2:F:206:ARG:CG	2.21	0.68
1:E:276:GLU:HA	1:E:276:GLU:OE1	1.92	0.68
2:J:39:ILE:HA	2:J:42:MET:HE3	1.75	0.68
1:A:272:MET:CA	1:A:272:MET:HE2	2.23	0.68
2:B:226:LEU:HD11	3:K:251:PHE:HZ	1.59	0.68
3:C:216:GLY:HA2	3:C:254:LEU:HD12	1.76	0.68
1:I:35:GLU:OE2	10:I:602:HOH:O	2.10	0.67
2:J:199:MET:SD	6:J:306:PLC:H2	2.33	0.67
2:B:112:THR:HG21	3:C:162:THR:CG2	2.08	0.67
1:I:33:HIS:HD2	3:K:78:LEU:HB3	1.59	0.67
3:G:127:GLU:CD	3:G:200:PRO:CG	2.66	0.67
3:K:223:ASN:OD1	3:K:226:LEU:HD23	1.95	0.67
3:G:134:HIS:HB2	3:G:199:LEU:HD11	1.77	0.67
3:K:216:GLY:HA2	3:K:254:LEU:HD12	1.76	0.67
3:K:235:PHE:CE2	3:K:243:PRO:HD2	2.30	0.67
2:F:194:PRO:HD2	2:F:197:ILE:HD12	1.77	0.67
3:G:223:ASN:OD1	3:G:226:LEU:HD23	1.95	0.67
3:K:49:LYS:HB3	3:K:49:LYS:HZ1	1.56	0.67
3:K:130:ARG:HB3	3:K:199:LEU:HD23	1.75	0.67
3:C:134:HIS:HB2	3:C:199:LEU:HD11	1.77	0.67
3:C:223:ASN:OD1	3:C:226:LEU:HD23	1.95	0.67
1:A:35:GLU:OE2	10:A:602:HOH:O	2.12	0.67
2:F:29:VAL:HG23	3:G:262:LEU:HD12	1.77	0.67
3:C:152:PHE:HA	3:C:155:GLN:HB3	1.77	0.67
3:G:216:GLY:HA2	3:G:254:LEU:HD12	1.76	0.67
3:K:134:HIS:HB2	3:K:199:LEU:HD11	1.77	0.67
1:I:217:LEU:CD1	3:K:278:LEU:CD1	2.72	0.67
2:J:29:VAL:HG23	3:K:262:LEU:HD12	1.76	0.67
2:F:39:ILE:HA	2:F:42:MET:HE3	1.76	0.67
2:F:244:LEU:HD12	3:G:206:ILE:HG22	1.77	0.67
3:C:126:GLU:OE1	3:C:126:GLU:HA	1.95	0.66
3:C:235:PHE:CE2	3:C:243:PRO:HD2	2.30	0.66
1:E:237:MET:HG3	2:F:137:LEU:CD1	2.25	0.66
2:J:143:PHE:HD2	7:J:301:P1O:H26	1.61	0.66
3:G:119:LEU:HD11	3:G:198:ARG:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:152:PHE:HA	3:G:155:GLN:HB3	1.77	0.66
3:C:119:LEU:HD11	3:C:198:ARG:O	1.96	0.66
1:I:35:GLU:C	1:I:37:SER:H	2.03	0.66
2:F:22:ASP:OD1	10:F:403:HOH:O	2.13	0.66
6:K:306:PLC:H6A1	6:K:307:PLC:H4A2	1.77	0.66
2:J:133:THR:O	2:J:137:LEU:HB2	1.96	0.66
3:K:126:GLU:OE1	3:K:126:GLU:HA	1.95	0.66
2:B:194:PRO:HD2	2:B:197:ILE:HD12	1.77	0.66
10:B:416:HOH:O	2:J:247:THR:C	2.38	0.66
2:F:237:TRP:NE1	5:F:307:D10:C3	2.56	0.66
3:K:129:ARG:HG3	3:K:129:ARG:NH1	2.11	0.66
6:G:301:PLC:H32	6:G:301:PLC:H1'2	1.78	0.66
3:K:119:LEU:HD11	3:K:198:ARG:O	1.96	0.66
2:B:133:THR:O	2:B:137:LEU:HB2	1.96	0.66
3:C:129:ARG:HG3	3:C:129:ARG:NH1	2.11	0.66
3:C:224:VAL:O	3:C:228:GLU:HG3	1.95	0.66
1:E:79:GLU:O	1:E:79:GLU:HG2	1.96	0.66
1:E:93:MET:CE	1:E:98:PHE:HB2	2.26	0.66
1:I:93:MET:CE	1:I:98:PHE:HB2	2.26	0.66
2:F:133:THR:O	2:F:137:LEU:HB2	1.96	0.66
3:G:235:PHE:CE2	3:G:243:PRO:HD2	2.30	0.66
2:J:22:ASP:OD1	10:J:403:HOH:O	2.14	0.66
3:K:224:VAL:O	3:K:228:GLU:HG3	1.95	0.66
2:B:11:HIS:CE1	3:C:277:SER:HA	2.32	0.65
1:E:35:GLU:C	1:E:37:SER:H	2.03	0.65
2:J:226:LEU:HD11	3:G:251:PHE:HZ	1.60	0.65
9:G:309:HXG:H37	9:G:309:HXG:CAU	2.26	0.65
3:C:234:TRP:HH2	3:C:243:PRO:HG2	1.62	0.65
3:G:129:ARG:HG3	3:G:129:ARG:NH1	2.11	0.65
3:G:224:VAL:O	3:G:228:GLU:HG3	1.95	0.65
3:C:67:TRP:CD1	9:C:307:HXG:H40	2.31	0.65
6:C:306:PLC:H4A2	6:F:301:PLC:H6A1	1.77	0.65
1:I:79:GLU:O	1:I:79:GLU:HG2	1.96	0.65
6:J:306:PLC:H1'2	6:J:306:PLC:H32	1.78	0.65
3:G:236:MET:H	9:G:305:HXG:H37	1.61	0.65
6:G:307:PLC:H6A1	6:G:308:PLC:H4A2	1.77	0.65
3:K:230:GLY:C	3:K:244:LEU:HD12	2.21	0.65
6:K:306:PLC:C8B	6:K:307:PLC:H5A1	2.17	0.65
1:A:106:GLY:O	10:A:603:HOH:O	2.15	0.65
2:J:194:PRO:HD2	2:J:197:ILE:HD12	1.77	0.65
2:F:107:ASN:HB3	3:G:158:THR:HG21	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:ASP:OD1	10:B:403:HOH:O	2.15	0.65
2:B:233:PHE:CG	5:B:303:D10:H51	2.32	0.65
3:C:230:GLY:C	3:C:244:LEU:HD12	2.21	0.65
1:I:145:GLN:HG2	10:I:679:HOH:O	1.97	0.65
2:B:204:THR:O	1:I:42:MET:HE1	1.96	0.65
6:C:311:PLC:H32	6:C:311:PLC:H1'2	1.78	0.65
1:E:145:GLN:HG2	10:E:681:HOH:O	1.96	0.65
1:A:35:GLU:C	1:A:37:SER:H	2.03	0.65
3:C:236:MET:H	9:C:304:HXG:H37	1.61	0.65
1:E:217:LEU:CD1	3:G:278:LEU:HD12	2.26	0.65
3:G:126:GLU:OE1	3:G:126:GLU:HA	1.95	0.65
2:B:237:TRP:NE1	5:B:305:D10:C3	2.56	0.65
2:J:57:ARG:HG3	10:J:435:HOH:O	1.96	0.65
3:G:230:GLY:C	3:G:244:LEU:HD12	2.21	0.65
9:K:308:HXG:H37	9:K:308:HXG:CAU	2.26	0.65
9:C:307:HXG:H37	9:C:307:HXG:CAU	2.26	0.64
1:E:33:HIS:HD2	3:G:78:LEU:HB3	1.62	0.64
1:E:106:GLY:O	10:E:603:HOH:O	2.14	0.64
2:F:143:PHE:HD2	7:F:304:P1O:H26	1.61	0.64
3:G:236:MET:HE3	3:G:236:MET:CA	2.17	0.64
3:C:127:GLU:OE2	3:C:200:PRO:HG2	1.97	0.64
1:E:42:MET:HE1	2:J:204:THR:O	1.96	0.64
3:K:127:GLU:CD	3:K:200:PRO:HG2	2.22	0.64
3:K:92:PHE:CG	6:K:309:PLC:OB	2.50	0.64
3:K:152:PHE:HA	3:K:155:GLN:HB3	1.77	0.64
2:B:143:PHE:HD2	7:B:302:P1O:H26	1.61	0.64
6:G:307:PLC:C8B	6:G:308:PLC:H5A1	2.17	0.64
3:K:67:TRP:CD1	9:K:308:HXG:H40	2.31	0.64
1:A:108:GLN:OE1	1:A:269:MET:CE	2.45	0.64
2:J:233:PHE:CG	5:J:302:D10:H51	2.32	0.64
7:F:302:P1O:H12	7:F:302:P1O:O3	1.98	0.64
3:K:80:SER:N	3:K:166:ASP:OD2	2.29	0.64
3:K:236:MET:H	9:K:304:HXG:H37	1.61	0.64
3:G:92:PHE:CG	6:G:310:PLC:OB	2.50	0.64
3:C:92:PHE:CG	6:C:308:PLC:OB	2.50	0.64
3:G:127:GLU:CD	3:G:200:PRO:HG2	2.22	0.64
7:J:308:P1O:H12	7:J:308:P1O:O3	1.98	0.64
3:K:127:GLU:OE2	3:K:200:PRO:HG2	1.97	0.64
3:K:131:ASN:N	3:K:199:LEU:CD2	2.61	0.64
3:C:131:ASN:N	3:C:199:LEU:CD2	2.61	0.64
1:I:326:ASP:OD2	1:I:351:ASN:ND2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:213:ALA:HB1	6:F:303:PLC:O'	1.98	0.64
1:I:108:GLN:OE1	1:I:269:MET:CE	2.45	0.64
2:F:194:PRO:HG2	2:F:197:ILE:HG13	1.80	0.64
2:B:213:ALA:HB1	6:B:301:PLC:O'	1.98	0.63
3:K:234:TRP:HH2	3:K:243:PRO:HG2	1.62	0.63
1:A:93:MET:CE	1:A:98:PHE:HB2	2.26	0.63
1:A:237:MET:HG3	2:B:137:LEU:CD1	2.27	0.63
7:B:307:P1O:H12	7:B:307:P1O:O3	1.98	0.63
3:C:116:ASP:HB3	3:C:119:LEU:HD13	1.80	0.63
1:E:375:ARG:NH1	1:E:378:ASP:OD2	2.32	0.63
1:I:237:MET:HG3	2:J:137:LEU:CD1	2.29	0.63
2:J:213:ALA:CB	6:J:307:PLC:H12	2.29	0.63
3:G:80:SER:N	3:G:166:ASP:OD2	2.29	0.63
3:G:127:GLU:OE2	3:G:200:PRO:HG2	1.98	0.63
1:A:326:ASP:OD2	1:A:351:ASN:ND2	2.31	0.63
2:F:233:PHE:CG	5:F:305:D10:H51	2.32	0.63
5:A:503:D10:H72	6:K:307:PLC:OB	1.99	0.63
2:J:213:ALA:HB1	6:J:307:PLC:O'	1.98	0.63
2:F:107:ASN:ND2	3:G:155:GLN:HA	2.13	0.63
1:A:375:ARG:NH1	1:A:378:ASP:OD2	2.32	0.63
2:B:213:ALA:CB	6:B:301:PLC:H12	2.29	0.63
3:C:234:TRP:CH2	3:C:243:PRO:HG2	2.34	0.63
1:I:375:ARG:NH1	1:I:378:ASP:OD2	2.32	0.63
1:A:79:GLU:O	1:A:79:GLU:HG2	1.96	0.63
2:B:194:PRO:HG2	2:B:197:ILE:HG13	1.80	0.63
3:C:127:GLU:CD	3:C:200:PRO:HG2	2.22	0.63
5:I:503:D10:H72	6:G:308:PLC:OB	1.97	0.63
3:G:115:ARG:HB2	3:G:197:THR:HB	1.81	0.63
1:A:145:GLN:HG2	10:A:679:HOH:O	1.98	0.63
3:C:80:SER:N	3:C:166:ASP:OD2	2.29	0.63
2:F:237:TRP:CD1	5:F:307:D10:H51	2.34	0.63
3:G:131:ASN:N	3:G:199:LEU:CD2	2.61	0.63
3:G:234:TRP:HH2	3:G:243:PRO:HG2	1.62	0.63
3:C:50:TRP:CZ3	7:C:309:P1O:H39	2.34	0.63
1:E:217:LEU:CD1	3:G:278:LEU:CD1	2.77	0.63
1:E:326:ASP:OD2	1:E:351:ASN:ND2	2.31	0.63
2:J:237:TRP:CD2	5:J:304:D10:H72	2.34	0.63
3:G:168:ASP:HB3	3:G:228:GLU:OE2	1.99	0.63
3:K:168:ASP:HB3	3:K:228:GLU:OE2	1.99	0.63
2:J:68:LEU:HD12	2:J:124:LEU:HD22	1.81	0.63
2:J:194:PRO:HG2	2:J:197:ILE:HG13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:237:TRP:CD1	5:J:304:D10:H51	2.34	0.63
3:G:116:ASP:HB3	3:G:119:LEU:HD13	1.80	0.63
3:K:235:PHE:HA	9:K:304:HXG:H37	1.81	0.63
2:B:237:TRP:CD2	5:B:305:D10:H72	2.34	0.62
3:G:50:TRP:CZ3	7:G:311:P1O:H39	2.34	0.62
2:J:34:VAL:HG22	2:J:95:GLY:CA	2.29	0.62
2:J:237:TRP:NE1	5:J:304:D10:C3	2.56	0.62
2:F:213:ALA:CB	6:F:303:PLC:H12	2.29	0.62
2:F:68:LEU:HD12	2:F:124:LEU:HD22	1.81	0.62
3:K:96:GLU:OE1	3:K:179:LEU:CB	2.35	0.62
2:B:51:TRP:HZ2	3:C:161:GLN:HG3	1.65	0.62
2:B:57:ARG:HG3	10:B:429:HOH:O	1.99	0.62
3:C:115:ARG:HB2	3:C:197:THR:HB	1.81	0.62
6:C:306:PLC:H73	5:E:503:D10:H101	1.81	0.62
2:F:34:VAL:HG22	2:F:95:GLY:CA	2.29	0.62
7:G:311:P1O:H24	7:G:311:P1O:H18	1.82	0.62
1:A:105:ILE:HD12	1:A:114:VAL:HG21	1.81	0.62
2:B:237:TRP:CD1	5:B:305:D10:H51	2.34	0.62
3:K:116:ASP:HB3	3:K:119:LEU:HD13	1.80	0.62
3:C:168:ASP:HB3	3:C:228:GLU:OE2	1.99	0.62
1:I:105:ILE:HD12	1:I:114:VAL:HG21	1.81	0.62
2:J:123:SER:OG	10:J:404:HOH:O	2.16	0.62
3:K:50:TRP:CZ3	7:K:310:P1O:H39	2.34	0.62
2:B:219:PHE:HE1	3:K:226:LEU:HD13	1.63	0.62
1:E:108:GLN:OE1	1:E:269:MET:CE	2.45	0.62
2:J:69:VAL:CG1	2:J:152:TRP:NE1	2.63	0.62
2:F:69:VAL:CG1	2:F:152:TRP:NE1	2.63	0.62
3:K:234:TRP:CH2	3:K:243:PRO:HG2	2.34	0.62
3:C:244:LEU:HD23	3:C:244:LEU:C	2.25	0.62
3:G:67:TRP:CD1	9:G:309:HXG:H40	2.31	0.62
3:G:100:GLU:OE2	3:G:179:LEU:HA	2.00	0.62
3:G:235:PHE:HA	9:G:305:HXG:H37	1.81	0.62
2:B:34:VAL:HG22	2:B:95:GLY:CA	2.29	0.62
2:F:237:TRP:CD2	5:F:307:D10:H72	2.34	0.62
7:G:312:P1O:O8	7:G:312:P1O:H7	1.99	0.62
3:K:115:ARG:HB2	3:K:197:THR:HB	1.81	0.62
1:A:213:ILE:HG22	3:C:278:LEU:HD13	1.79	0.61
2:B:68:LEU:HD12	2:B:124:LEU:HD22	1.81	0.61
2:B:69:VAL:CG1	2:B:152:TRP:NE1	2.63	0.61
1:E:237:MET:CG	2:F:137:LEU:HD11	2.30	0.61
2:J:86:PRO:HG3	2:J:136:MET:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:234:TRP:CH2	3:G:243:PRO:HG2	2.34	0.61
3:C:170:THR:HB	3:C:171:PRO:HD2	1.82	0.61
3:C:196:LYS:HG3	3:C:196:LYS:O	2.01	0.61
3:C:238:GLU:OE1	3:C:238:GLU:HA	1.99	0.61
7:C:309:P1O:H18	7:C:309:P1O:H24	1.82	0.61
3:K:170:THR:HB	3:K:171:PRO:HD2	1.82	0.61
7:K:311:P1O:O8	7:K:311:P1O:H7	1.99	0.61
2:B:86:PRO:HG3	2:B:136:MET:HG3	1.83	0.61
2:B:237:TRP:CE2	5:B:305:D10:H51	2.36	0.61
1:E:291:TYR:HA	10:E:653:HOH:O	2.00	0.61
7:C:310:P1O:O8	7:C:310:P1O:H7	1.99	0.61
1:I:287:GLU:OE1	1:I:303:THR:OG1	2.19	0.61
2:J:219:PHE:HE1	3:G:226:LEU:HD13	1.64	0.61
1:A:217:LEU:CD1	3:C:278:LEU:HD12	2.31	0.61
2:B:106:PHE:O	2:B:110:GLY:HA3	2.01	0.61
3:K:244:LEU:HD23	3:K:244:LEU:C	2.25	0.61
7:K:310:P1O:H24	7:K:310:P1O:H18	1.82	0.61
1:A:42:MET:HE1	2:F:204:THR:O	2.00	0.61
1:A:291:TYR:HA	10:A:647:HOH:O	1.99	0.61
2:B:123:SER:OG	10:B:404:HOH:O	2.16	0.61
3:C:235:PHE:HA	9:C:304:HXC:H37	1.81	0.61
2:F:11:HIS:CE1	3:G:277:SER:HA	2.35	0.61
1:E:228:VAL:O	1:E:228:VAL:HG12	2.01	0.60
3:K:196:LYS:HG3	3:K:196:LYS:O	2.01	0.60
2:B:243:PHE:HD2	3:C:205:GLY:O	1.84	0.60
6:C:308:PLC:HEA1	7:C:309:P1O:C28	2.31	0.60
1:E:371:TRP:HE1	1:E:377:SER:HB3	1.66	0.60
1:I:291:TYR:HA	10:I:654:HOH:O	2.01	0.60
3:C:117:ARG:HH11	3:C:117:ARG:CG	2.14	0.60
1:E:105:ILE:HD12	1:E:114:VAL:HG21	1.81	0.60
3:C:100:GLU:OE2	3:C:179:LEU:HA	2.00	0.60
1:I:145:GLN:HB3	10:I:631:HOH:O	2.01	0.60
3:K:100:GLU:OE2	3:K:179:LEU:HA	2.00	0.60
2:F:154:LEU:HD22	6:F:303:PLC:H5'1	1.83	0.60
2:F:247:THR:HG22	3:G:211:LEU:CD2	2.30	0.60
3:G:244:LEU:HD23	3:G:244:LEU:C	2.25	0.60
3:K:243:PRO:C	3:K:245:HIS:H	2.09	0.60
1:A:145:GLN:HB3	10:A:628:HOH:O	2.02	0.60
6:C:306:PLC:H63	6:C:306:PLC:O3	2.02	0.60
3:G:170:THR:HB	3:G:171:PRO:HD2	1.82	0.60
2:F:86:PRO:HG3	2:F:136:MET:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:117:ARG:HH11	3:G:117:ARG:CG	2.14	0.60
3:G:196:LYS:HG3	3:G:196:LYS:O	2.01	0.60
3:G:243:PRO:C	3:G:245:HIS:H	2.09	0.60
6:K:307:PLC:H63	6:K:307:PLC:O3	2.02	0.60
1:A:287:GLU:OE1	1:A:303:THR:OG1	2.19	0.60
5:C:305:D10:H92	5:K:305:D10:H92	1.83	0.60
1:E:145:GLN:HB3	10:E:630:HOH:O	2.01	0.60
3:G:130:ARG:CB	3:G:199:LEU:HD23	2.32	0.60
3:C:201:PHE:CD1	3:C:268:SER:HB2	2.37	0.60
3:C:251:PHE:HZ	2:F:226:LEU:HD11	1.66	0.60
7:C:309:P1O:O2	7:C:309:P1O:H4	2.02	0.60
2:J:237:TRP:CE2	5:J:304:D10:H51	2.36	0.60
7:K:310:P1O:O2	7:K:310:P1O:H4	2.02	0.60
2:B:154:LEU:HD22	6:B:301:PLC:H5'1	1.83	0.60
1:E:287:GLU:OE1	1:E:303:THR:OG1	2.19	0.60
2:F:237:TRP:CE2	5:F:307:D10:H51	2.36	0.60
7:G:311:P1O:O2	7:G:311:P1O:H4	2.02	0.60
3:K:201:PHE:CD1	3:K:268:SER:HB2	2.37	0.60
2:B:247:THR:HG22	3:C:211:LEU:HD22	1.84	0.59
3:C:243:PRO:C	3:C:245:HIS:H	2.09	0.59
1:I:228:VAL:O	1:I:228:VAL:HG12	2.01	0.59
3:G:89:TRP:HB3	3:G:174:ILE:CD1	2.32	0.59
3:G:173:HIS:C	3:G:175:ILE:N	2.60	0.59
3:K:165:ARG:HD2	3:K:238:GLU:OE2	2.02	0.59
7:B:307:P1O:H15	7:B:307:P1O:H39	1.83	0.59
1:E:110:VAL:HG23	1:E:110:VAL:O	2.03	0.59
1:I:371:TRP:HE1	1:I:377:SER:HB3	1.66	0.59
3:K:238:GLU:OE1	3:K:238:GLU:HA	1.99	0.59
2:J:106:PHE:O	2:J:110:GLY:HA3	2.01	0.59
2:J:154:LEU:HD22	6:J:307:PLC:H5'1	1.83	0.59
7:J:308:P1O:H15	7:J:308:P1O:H39	1.83	0.59
2:F:134:VAL:C	2:F:137:LEU:O	2.46	0.59
3:G:165:ARG:HD2	3:G:238:GLU:OE2	2.02	0.59
1:A:371:TRP:HE1	1:A:377:SER:HB3	1.66	0.59
2:J:206:ARG:CB	2:J:206:ARG:HH11	2.14	0.59
3:G:238:GLU:OE1	3:G:238:GLU:HA	1.99	0.59
3:K:243:PRO:O	3:K:245:HIS:N	2.31	0.59
1:A:110:VAL:O	1:A:110:VAL:HG23	2.03	0.59
1:A:170:VAL:HG11	1:A:180:LEU:HG	1.85	0.59
2:B:14:ALA:HB3	3:C:277:SER:HB2	1.83	0.59
1:I:170:VAL:HG11	1:I:180:LEU:HG	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:117:ARG:HH11	3:K:117:ARG:CG	2.14	0.59
1:A:237:MET:CG	2:B:137:LEU:HD11	2.32	0.59
2:B:245:GLN:CA	3:C:205:GLY:HA2	2.32	0.59
3:C:243:PRO:O	3:C:245:HIS:N	2.31	0.59
2:J:213:ALA:CB	6:J:307:PLC:C1	2.81	0.59
2:F:106:PHE:O	2:F:110:GLY:HA3	2.01	0.59
2:F:213:ALA:CB	6:F:303:PLC:C1	2.81	0.59
3:G:201:PHE:CD1	3:G:268:SER:HB2	2.37	0.59
2:B:134:VAL:C	2:B:137:LEU:O	2.46	0.59
3:C:164:VAL:HG13	10:F:443:HOH:O	2.01	0.59
2:J:66:ILE:CG2	6:G:304:PLC:H9A2	2.32	0.59
7:F:302:P1O:H15	7:F:302:P1O:H39	1.84	0.59
1:E:170:VAL:HG11	1:E:180:LEU:HG	1.85	0.59
3:C:165:ARG:HD2	3:C:238:GLU:OE2	2.02	0.58
2:J:107:ASN:HB3	3:K:158:THR:HG21	1.85	0.58
3:G:131:ASN:N	3:G:199:LEU:HD21	2.18	0.58
6:G:308:PLC:O3	6:G:308:PLC:H63	2.02	0.58
3:K:89:TRP:HB3	3:K:174:ILE:CD1	2.32	0.58
3:C:130:ARG:CB	3:C:199:LEU:HD23	2.32	0.58
3:K:130:ARG:CB	3:K:199:LEU:HD23	2.32	0.58
3:K:235:PHE:CD2	3:K:244:LEU:HD13	2.30	0.58
2:F:123:SER:OG	10:F:404:HOH:O	2.17	0.58
3:K:131:ASN:N	3:K:199:LEU:HD21	2.18	0.58
2:F:245:GLN:HG3	2:F:245:GLN:O	2.04	0.58
3:C:67:TRP:CA	9:C:307:HXG:CAC	2.76	0.58
3:C:131:ASN:N	3:C:199:LEU:HD21	2.18	0.58
2:J:134:VAL:C	2:J:137:LEU:O	2.46	0.58
3:K:173:HIS:C	3:K:175:ILE:N	2.60	0.58
1:A:228:VAL:HG12	1:A:228:VAL:O	2.01	0.58
2:B:206:ARG:CB	2:B:206:ARG:HH11	2.14	0.58
1:E:45:ARG:HB3	1:E:74:PHE:CD2	2.39	0.58
1:I:106:GLY:O	10:I:603:HOH:O	2.16	0.58
1:I:110:VAL:O	1:I:110:VAL:HG23	2.02	0.58
2:F:206:ARG:CB	2:F:206:ARG:HH11	2.14	0.58
7:B:307:P1O:H39	7:B:307:P1O:H17	1.85	0.58
7:C:309:P1O:O2	7:C:309:P1O:H6	2.04	0.58
1:E:124:PHE:CZ	1:E:140:THR:HG21	2.39	0.58
2:F:161:TRP:CE2	6:F:303:PLC:C7	2.87	0.58
7:F:302:P1O:H39	7:F:302:P1O:H17	1.85	0.58
2:B:135:LEU:HD22	2:B:135:LEU:C	2.29	0.58
3:C:89:TRP:HB3	3:C:174:ILE:CD1	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:173:HIS:C	3:C:175:ILE:N	2.60	0.58
1:I:124:PHE:CZ	1:I:140:THR:HG21	2.39	0.58
2:F:57:ARG:HG3	10:F:430:HOH:O	2.03	0.58
1:A:45:ARG:HB3	1:A:74:PHE:CD2	2.39	0.58
1:A:81:VAL:O	10:A:604:HOH:O	2.17	0.58
2:B:161:TRP:CE2	6:B:301:PLC:C7	2.87	0.58
6:K:309:PLC:HEA1	7:K:310:P1O:C28	2.31	0.58
2:B:245:GLN:HG3	2:B:245:GLN:O	2.03	0.57
3:C:62:TYR:CD1	3:C:152:PHE:HE2	2.22	0.57
3:G:67:TRP:CB	9:G:309:HXG:H40	2.34	0.57
3:C:62:TYR:OH	10:C:402:HOH:O	2.17	0.57
1:E:281:THR:O	1:E:307:HIS:HB2	2.04	0.57
2:J:135:LEU:HD22	2:J:135:LEU:C	2.29	0.57
3:K:62:TYR:CD1	3:K:152:PHE:HE2	2.22	0.57
2:B:213:ALA:CB	6:B:301:PLC:C1	2.81	0.57
2:J:11:HIS:HD1	2:J:11:HIS:C	2.13	0.57
7:J:308:P1O:H39	7:J:308:P1O:H17	1.85	0.57
2:F:135:LEU:HD22	2:F:135:LEU:C	2.29	0.57
2:B:11:HIS:HD1	2:B:11:HIS:C	2.13	0.57
2:F:51:TRP:HZ2	3:G:161:GLN:HG3	1.69	0.57
3:C:76:ALA:HB2	3:C:84:GLU:HG3	1.86	0.57
1:E:81:VAL:O	10:E:604:HOH:O	2.18	0.57
2:F:11:HIS:C	2:F:11:HIS:HD1	2.13	0.57
3:G:234:TRP:HA	6:G:304:PLC:H72	1.87	0.57
3:G:236:MET:N	9:G:305:HXG:H37	2.20	0.57
7:G:311:P1O:O2	7:G:311:P1O:H6	2.04	0.57
3:C:67:TRP:CB	9:C:307:HXG:H40	2.34	0.57
1:I:45:ARG:HB3	1:I:74:PHE:CD2	2.39	0.57
3:K:67:TRP:CB	9:K:308:HXG:H40	2.34	0.57
3:K:67:TRP:CG	9:K:308:HXG:CAC	2.88	0.57
3:K:76:ALA:HB2	3:K:84:GLU:HG3	1.86	0.57
7:K:310:P1O:O2	7:K:310:P1O:H6	2.04	0.57
2:B:66:ILE:CG2	6:K:303:PLC:H9A2	2.35	0.57
2:B:114:PHE:HE2	3:C:162:THR:HG22	1.70	0.57
2:J:161:TRP:CE2	6:J:307:PLC:C7	2.87	0.57
3:G:76:ALA:HB2	3:G:84:GLU:HG3	1.86	0.57
3:G:112:TRP:CH2	7:G:312:P1O:C1	2.87	0.57
6:G:307:PLC:C6B	6:G:308:PLC:H4A2	2.35	0.57
3:K:112:TRP:CH2	7:K:311:P1O:C1	2.87	0.57
3:C:49:LYS:HB3	3:C:49:LYS:HZ1	1.65	0.57
3:C:234:TRP:HA	6:C:303:PLC:H72	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:281:THR:O	1:I:307:HIS:HB2	2.04	0.57
2:J:199:MET:SD	6:J:306:PLC:C2	2.93	0.57
2:J:219:PHE:CE1	3:G:226:LEU:HD13	2.40	0.57
1:A:124:PHE:CZ	1:A:140:THR:HG21	2.39	0.56
3:C:112:TRP:CH2	7:C:310:P1O:C1	2.87	0.56
3:G:67:TRP:CG	9:G:309:HXG:CAC	2.88	0.56
3:G:243:PRO:C	3:G:245:HIS:N	2.63	0.56
2:J:45:MET:HE3	2:J:49:ASP:HB2	1.88	0.56
2:J:63:VAL:HG22	6:G:304:PLC:H3A2	1.87	0.56
2:F:161:TRP:CE2	6:F:303:PLC:H73	2.40	0.56
1:A:217:LEU:CD1	3:C:278:LEU:CD1	2.83	0.56
1:A:281:THR:O	1:A:307:HIS:HB2	2.04	0.56
2:B:211:ASP:OD2	3:K:168:ASP:OD2	2.24	0.56
3:C:97:ILE:HG21	6:F:301:PLC:H7A1	1.87	0.56
1:I:81:VAL:O	10:I:604:HOH:O	2.18	0.56
2:F:14:ALA:HB3	3:G:277:SER:HB2	1.87	0.56
2:F:45:MET:HE3	2:F:49:ASP:HB2	1.88	0.56
2:F:103:ASN:CG	3:G:154:GLU:HB3	2.30	0.56
3:G:62:TYR:CD1	3:G:152:PHE:HE2	2.22	0.56
3:C:67:TRP:CG	9:C:307:HXG:CAC	2.88	0.56
1:E:215:ARG:NH2	2:F:84:ARG:O	2.38	0.56
1:I:237:MET:CG	2:J:137:LEU:HD11	2.33	0.56
3:K:243:PRO:C	3:K:245:HIS:N	2.63	0.56
5:I:503:D10:H101	6:G:308:PLC:H73	1.87	0.56
3:G:173:HIS:C	3:G:175:ILE:H	2.14	0.56
2:B:219:PHE:CE1	3:K:226:LEU:HD13	2.39	0.56
3:G:219:MET:C	3:G:222:PRO:HD2	2.31	0.56
6:G:310:PLC:HEA1	7:G:311:P1O:C28	2.31	0.56
3:K:173:HIS:C	3:K:175:ILE:H	2.14	0.56
2:F:34:VAL:HG22	2:F:95:GLY:C	2.31	0.56
2:F:37:TYR:OH	2:F:68:LEU:O	2.24	0.56
3:G:127:GLU:CD	3:G:200:PRO:HG3	2.31	0.56
6:G:301:PLC:O4P	6:G:301:PLC:H63	2.06	0.56
6:K:306:PLC:C6B	6:K:307:PLC:H4A2	2.35	0.56
2:B:143:PHE:CE2	7:B:302:P1O:H26	2.41	0.56
2:B:197:ILE:CG1	3:C:237:GLU:HG2	2.35	0.56
2:B:244:LEU:O	2:B:245:GLN:HB3	2.06	0.56
3:C:219:MET:C	3:C:222:PRO:HD2	2.31	0.56
2:F:50:PHE:HD1	2:F:104:ARG:NH2	2.04	0.56
2:B:45:MET:HE3	2:B:49:ASP:HB2	1.88	0.55
2:B:50:PHE:HD1	2:B:104:ARG:NH2	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:173:HIS:C	3:C:175:ILE:H	2.14	0.55
3:C:208:LEU:N	3:C:209:PRO:HD2	2.22	0.55
2:J:107:ASN:ND2	3:K:155:GLN:HA	2.21	0.55
1:A:94:PRO:CB	3:C:74:TRP:HD1	2.20	0.55
2:B:199:MET:SD	6:C:311:PLC:C2	2.93	0.55
3:C:236:MET:N	9:C:304:HXG:H37	2.20	0.55
6:C:306:PLC:C7	5:E:503:D10:H101	2.36	0.55
3:G:67:TRP:CA	9:G:309:HXG:CAC	2.76	0.55
3:G:208:LEU:N	3:G:209:PRO:HD2	2.22	0.55
3:K:219:MET:C	3:K:222:PRO:HD2	2.31	0.55
3:K:234:TRP:HA	6:K:303:PLC:H72	1.87	0.55
3:K:236:MET:N	9:K:304:HXG:H37	2.20	0.55
2:B:39:ILE:HG13	3:C:149:ALA:HB1	1.87	0.55
1:E:35:GLU:N	1:E:35:GLU:OE1	2.40	0.55
3:C:48:LYS:HD2	3:C:50:TRP:HD1	1.72	0.55
3:C:127:GLU:CD	3:C:200:PRO:HG3	2.31	0.55
3:C:169:PHE:HE2	6:F:301:PLC:C3	2.19	0.55
1:I:35:GLU:OE1	1:I:35:GLU:N	2.40	0.55
6:C:306:PLC:H4A2	6:F:301:PLC:C6B	2.35	0.55
1:E:145:GLN:HA	2:F:196:TYR:CE1	2.41	0.55
2:B:63:VAL:HG22	6:K:303:PLC:H3A2	1.88	0.55
3:C:96:GLU:OE1	3:C:179:LEU:CB	2.35	0.55
3:C:243:PRO:C	3:C:245:HIS:N	2.63	0.55
1:I:213:ILE:HG22	3:K:278:LEU:HD13	1.82	0.55
2:B:34:VAL:HG22	2:B:95:GLY:C	2.31	0.55
3:C:67:TRP:HB2	9:C:307:HXG:H40	1.88	0.55
3:G:169:PHE:HE2	6:G:307:PLC:C3	2.19	0.55
1:A:215:ARG:NH2	2:B:84:ARG:O	2.39	0.55
2:J:34:VAL:HG22	2:J:95:GLY:C	2.31	0.55
2:J:143:PHE:CE2	7:J:301:P1O:H26	2.41	0.55
3:G:112:TRP:CZ2	7:G:312:P1O:H7	2.42	0.55
3:K:97:ILE:HG21	6:K:306:PLC:H7A1	1.87	0.55
3:K:127:GLU:CD	3:K:200:PRO:HG3	2.31	0.55
3:C:148:GLY:O	3:C:181:TYR:HE1	1.90	0.55
6:C:306:PLC:OB	5:E:503:D10:H71	2.06	0.55
3:G:97:ILE:HG21	6:G:307:PLC:H7A1	1.87	0.55
3:G:151:TYR:O	3:G:155:GLN:N	2.28	0.55
3:K:169:PHE:HE2	6:K:306:PLC:C3	2.19	0.55
2:F:244:LEU:O	2:F:245:GLN:HB3	2.06	0.54
3:K:208:LEU:N	3:K:209:PRO:HD2	2.22	0.54
3:G:67:TRP:HB2	9:G:309:HXG:H40	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:201:PHE:CD1	3:G:201:PHE:C	2.86	0.54
3:G:235:PHE:H	6:G:304:PLC:C7	2.20	0.54
3:K:201:PHE:CD1	3:K:201:PHE:C	2.86	0.54
3:K:235:PHE:H	6:K:303:PLC:C7	2.20	0.54
3:C:213:LEU:HG	3:C:213:LEU:O	2.08	0.54
3:C:223:ASN:O	3:C:226:LEU:HB3	2.07	0.54
2:J:11:HIS:CE1	3:K:277:SER:HA	2.41	0.54
2:J:50:PHE:HD1	2:J:104:ARG:NH2	2.04	0.54
2:J:51:TRP:HZ2	3:K:161:GLN:HG3	1.73	0.54
2:J:150:MET:HE1	10:J:424:HOH:O	2.07	0.54
3:K:48:LYS:HD2	3:K:50:TRP:HD1	1.72	0.54
3:K:160:HIS:C	3:K:162:THR:H	2.15	0.54
1:A:272:MET:HE2	1:A:272:MET:N	2.23	0.54
3:C:112:TRP:CZ2	7:C:310:P1O:C1	2.91	0.54
3:C:235:PHE:H	6:C:303:PLC:C7	2.20	0.54
6:C:311:PLC:O4P	6:C:311:PLC:H63	2.06	0.54
3:G:48:LYS:HD2	3:G:50:TRP:HD1	1.72	0.54
6:J:306:PLC:O4P	6:J:306:PLC:H63	2.06	0.54
2:F:143:PHE:CE2	7:F:304:P1O:H26	2.41	0.54
3:G:67:TRP:CB	9:G:309:HXG:CAC	2.86	0.54
1:I:272:MET:HE2	1:I:272:MET:N	2.23	0.54
3:K:223:ASN:O	3:K:226:LEU:HB3	2.07	0.54
3:C:67:TRP:CB	9:C:307:HXG:CAC	2.86	0.54
3:C:236:MET:CE	2:F:206:ARG:CB	2.71	0.54
3:G:148:GLY:O	3:G:181:TYR:HE1	1.90	0.54
3:G:223:ASN:O	3:G:226:LEU:HB3	2.07	0.54
3:G:235:PHE:CD2	3:G:244:LEU:HD13	2.30	0.54
3:K:112:TRP:CZ2	7:K:311:P1O:C1	2.91	0.54
3:K:151:TYR:O	3:K:155:GLN:N	2.28	0.54
2:B:103:ASN:CG	3:C:154:GLU:HB3	2.33	0.54
3:C:201:PHE:CD1	3:C:201:PHE:C	2.86	0.54
1:E:233:ARG:HA	2:F:136:MET:HE1	1.90	0.54
3:K:67:TRP:CA	9:K:308:HXG:CAC	2.76	0.54
1:E:272:MET:HE2	1:E:272:MET:N	2.23	0.54
3:G:160:HIS:C	3:G:162:THR:H	2.15	0.54
3:K:112:TRP:CZ2	7:K:311:P1O:H7	2.43	0.54
3:C:112:TRP:CZ2	7:C:310:P1O:H7	2.42	0.53
3:C:158:THR:O	3:C:162:THR:HG23	2.08	0.53
1:I:215:ARG:NH2	2:J:84:ARG:O	2.40	0.53
3:G:158:THR:O	3:G:162:THR:HG23	2.08	0.53
3:G:218:PHE:CD1	3:G:218:PHE:C	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLU:OE1	1:A:35:GLU:N	2.40	0.53
3:C:160:HIS:C	3:C:162:THR:H	2.15	0.53
3:C:218:PHE:C	3:C:218:PHE:CD1	2.86	0.53
3:G:112:TRP:CZ2	7:G:312:P1O:C1	2.91	0.53
3:K:67:TRP:HB2	9:K:308:HXG:H40	1.88	0.53
3:G:213:LEU:O	3:G:213:LEU:HG	2.08	0.53
3:G:234:TRP:O	3:G:235:PHE:CB	2.57	0.53
3:C:219:MET:O	3:C:222:PRO:HD2	2.09	0.53
2:J:134:VAL:O	2:J:137:LEU:O	2.27	0.53
2:J:243:PHE:HD2	3:K:205:GLY:O	1.92	0.53
3:K:67:TRP:CB	9:K:308:HXG:CAC	2.86	0.53
5:A:503:D10:H101	6:K:307:PLC:H73	1.89	0.53
2:B:37:TYR:OH	2:B:68:LEU:O	2.24	0.53
3:C:234:TRP:O	3:C:235:PHE:CB	2.57	0.53
1:E:79:GLU:CB	1:I:268:THR:HB	2.39	0.53
2:J:100:GLU:HG2	2:J:104:ARG:HH12	1.74	0.53
2:F:244:LEU:HD12	3:G:206:ILE:CG2	2.38	0.53
5:G:306:D10:H92	5:K:305:D10:H92	1.89	0.53
1:A:272:MET:HE2	1:A:272:MET:HA	1.91	0.53
3:K:158:THR:O	3:K:162:THR:HG23	2.08	0.53
6:C:308:PLC:H1'1	6:C:308:PLC:H51	1.90	0.53
2:F:134:VAL:O	2:F:137:LEU:O	2.27	0.53
3:K:148:GLY:O	3:K:181:TYR:HE1	1.90	0.53
3:K:235:PHE:CA	9:K:304:HXG:H37	2.39	0.53
2:B:107:ASN:HB3	3:C:158:THR:HG21	1.91	0.53
2:J:37:TYR:OH	2:J:68:LEU:O	2.24	0.53
2:F:100:GLU:HG2	2:F:104:ARG:HH12	1.74	0.53
2:B:63:VAL:CG2	6:K:303:PLC:H3A2	2.40	0.52
3:C:134:HIS:CD2	3:C:195:ALA:HB2	2.44	0.52
3:C:226:LEU:HD13	2:F:219:PHE:HE1	1.73	0.52
2:B:100:GLU:HG2	2:B:104:ARG:HH12	1.74	0.52
5:I:503:D10:H92	6:G:308:PLC:H62	1.84	0.52
3:K:112:TRP:CZ2	7:K:311:P1O:H2	2.45	0.52
3:K:213:LEU:HG	3:K:213:LEU:O	2.08	0.52
3:K:216:GLY:O	3:K:251:PHE:HB3	2.10	0.52
2:B:134:VAL:O	2:B:137:LEU:O	2.27	0.52
3:C:216:GLY:O	3:C:251:PHE:HB3	2.09	0.52
3:G:62:TYR:CD1	3:G:152:PHE:CE2	2.98	0.52
6:G:310:PLC:H1'1	6:G:310:PLC:H51	1.90	0.52
3:K:134:HIS:CD2	3:K:195:ALA:HB2	2.44	0.52
3:K:219:MET:O	3:K:222:PRO:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:VAL:HG12	2:B:152:TRP:NE1	2.25	0.52
2:B:107:ASN:ND2	3:C:155:GLN:HA	2.24	0.52
3:C:160:HIS:C	3:C:162:THR:N	2.68	0.52
1:E:394:PHE:CD2	1:E:400:ARG:HB3	2.45	0.52
2:J:211:ASP:OD2	3:G:168:ASP:OD2	2.28	0.52
2:F:62:THR:HG23	2:F:219:PHE:CD2	2.44	0.52
3:G:96:GLU:OE1	3:G:179:LEU:CB	2.36	0.52
3:G:216:GLY:O	3:G:251:PHE:HB3	2.09	0.52
3:G:219:MET:O	3:G:222:PRO:HD2	2.09	0.52
2:B:125:VAL:HB	2:B:126:PRO:HD3	1.92	0.52
3:C:234:TRP:HB2	6:C:303:PLC:H1'1	1.91	0.52
3:C:235:PHE:CA	9:C:304:HGX:H37	2.39	0.52
2:B:62:THR:HG23	2:B:219:PHE:CD2	2.44	0.52
2:J:62:THR:HG23	2:J:219:PHE:CD2	2.44	0.52
2:J:125:VAL:HB	2:J:126:PRO:HD3	1.92	0.52
2:F:134:VAL:O	2:F:134:VAL:HG12	2.10	0.52
3:G:134:HIS:CD2	3:G:195:ALA:HB2	2.44	0.52
1:A:394:PHE:CD2	1:A:400:ARG:HB3	2.45	0.52
2:F:114:PHE:HE2	3:G:162:THR:HG22	1.74	0.52
2:F:244:LEU:HD11	3:G:208:LEU:HA	1.91	0.52
3:K:218:PHE:C	3:K:218:PHE:CD1	2.86	0.52
2:J:34:VAL:HG22	2:J:95:GLY:HA3	1.92	0.52
2:J:161:TRP:CE2	6:J:307:PLC:H73	2.40	0.52
9:K:304:HGX:H17	9:K:304:HGX:H10	1.92	0.52
3:C:226:LEU:HA	2:F:219:PHE:CD1	2.44	0.52
2:J:199:MET:SD	6:J:306:PLC:O2	2.67	0.52
3:K:62:TYR:OH	10:K:402:HOH:O	2.18	0.52
3:K:234:TRP:HB2	6:K:303:PLC:H1'1	1.91	0.52
1:A:38:GLN:HA	10:F:421:HOH:O	2.10	0.52
1:I:145:GLN:HA	2:J:196:TYR:CE1	2.44	0.52
3:G:235:PHE:CA	9:G:305:HGX:H37	2.39	0.52
2:B:199:MET:SD	6:C:311:PLC:O2	2.68	0.51
6:C:311:PLC:H9'1	6:K:303:PLC:HTA1	1.92	0.51
1:E:265:GLN:HG3	2:F:177:LEU:O	2.10	0.51
1:I:272:MET:HE2	1:I:272:MET:HA	1.91	0.51
2:J:14:ALA:HB3	3:K:277:SER:HB2	1.91	0.51
2:F:125:VAL:HB	2:F:126:PRO:HD3	1.92	0.51
3:G:236:MET:HG2	9:G:305:HGX:CAE	2.40	0.51
2:B:11:HIS:O	2:B:11:HIS:ND1	2.38	0.51
3:C:49:LYS:HB3	3:C:49:LYS:HZ2	1.72	0.51
3:C:235:PHE:CD2	3:C:244:LEU:HD13	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:303:PLC:HTA1	6:G:301:PLC:H9'1	1.92	0.51
2:J:244:LEU:HD21	3:K:208:LEU:HD13	1.93	0.51
3:G:112:TRP:CZ2	7:G:312:P1O:H2	2.45	0.51
3:G:234:TRP:HB2	6:G:304:PLC:H1'1	1.91	0.51
9:G:305:HXG:H10	9:G:305:HXG:H17	1.92	0.51
1:A:87:ALA:O	1:A:114:VAL:N	2.31	0.51
1:A:233:ARG:HA	2:B:136:MET:HE1	1.92	0.51
1:E:213:ILE:HG22	3:G:278:LEU:HD13	1.84	0.51
1:E:272:MET:HE2	1:E:272:MET:HA	1.91	0.51
2:B:107:ASN:ND2	3:C:155:GLN:HB2	2.26	0.51
3:C:62:TYR:CD1	3:C:152:PHE:CE2	2.98	0.51
3:C:151:TYR:O	3:C:155:GLN:N	2.28	0.51
3:C:270:ALA:C	3:C:274:LEU:HB3	2.36	0.51
6:K:309:PLC:H1'1	6:K:309:PLC:H51	1.90	0.51
2:B:45:MET:HG3	2:B:64:THR:HG23	1.92	0.51
3:C:112:TRP:CZ2	7:C:310:P1O:H2	2.45	0.51
3:C:117:ARG:CG	3:C:117:ARG:NH1	2.73	0.51
2:F:150:MET:HE1	10:F:423:HOH:O	2.09	0.51
3:K:159:TRP:HA	3:K:159:TRP:CE3	2.44	0.51
2:J:231:TRP:HA	2:J:234:ILE:HB	1.93	0.51
2:F:86:PRO:HA	10:F:429:HOH:O	2.11	0.51
2:F:231:TRP:HA	2:F:234:ILE:HB	1.93	0.51
3:K:62:TYR:CD1	3:K:152:PHE:CE2	2.98	0.51
1:A:410:ILE:HG21	2:F:172:GLU:HG2	1.93	0.51
2:B:34:VAL:HG22	2:B:95:GLY:HA3	1.92	0.51
2:B:85:LEU:HD22	2:B:87:TRP:HE1	1.75	0.51
2:B:231:TRP:HA	2:B:234:ILE:HB	1.93	0.51
2:B:237:TRP:HB2	5:B:304:D10:H51	1.93	0.51
3:C:159:TRP:HA	3:C:159:TRP:CE3	2.44	0.51
3:C:221:LEU:HD23	3:C:222:PRO:CD	2.41	0.51
1:I:87:ALA:O	1:I:114:VAL:N	2.31	0.51
2:J:11:HIS:O	2:J:11:HIS:ND1	2.38	0.51
2:J:219:PHE:HB2	3:G:229:TRP:HB2	1.92	0.51
6:J:306:PLC:H9'1	6:G:304:PLC:HTA1	1.93	0.51
2:F:138:SER:O	2:F:138:SER:OG	2.28	0.51
3:G:243:PRO:O	3:G:245:HIS:N	2.31	0.51
3:K:236:MET:HG2	9:K:304:HXG:CAE	2.40	0.51
2:B:134:VAL:O	2:B:134:VAL:HG12	2.10	0.51
7:C:310:P1O:H12	7:C:310:P1O:H16	1.93	0.51
2:J:63:VAL:CG2	6:G:304:PLC:H3A2	2.40	0.51
2:J:85:LEU:HD22	2:J:87:TRP:HE1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:86:PRO:HA	10:J:430:HOH:O	2.10	0.51
2:J:103:ASN:CG	3:K:154:GLU:HB3	2.36	0.51
2:F:197:ILE:HG12	3:G:237:GLU:OE2	2.11	0.51
2:F:233:PHE:CD2	5:F:305:D10:H51	2.46	0.51
3:G:159:TRP:CE3	3:G:159:TRP:HA	2.45	0.51
3:G:221:LEU:HD23	3:G:222:PRO:CD	2.41	0.51
1:A:145:GLN:HA	2:B:196:TYR:CE1	2.46	0.51
2:B:219:PHE:CD1	3:K:226:LEU:HA	2.46	0.51
9:C:304:HXG:H17	9:C:304:HXG:H10	1.92	0.51
2:F:57:ARG:HH21	2:F:201:GLU:CD	2.19	0.51
2:F:85:LEU:HD22	2:F:87:TRP:HE1	1.75	0.51
3:K:117:ARG:CG	3:K:117:ARG:NH1	2.73	0.51
3:K:220:ILE:HG23	3:K:248:PHE:CD2	2.46	0.51
3:K:234:TRP:O	3:K:235:PHE:CB	2.57	0.51
2:B:61:VAL:HG12	10:B:423:HOH:O	2.11	0.50
1:I:217:LEU:HD11	3:K:278:LEU:HD12	1.91	0.50
1:I:233:ARG:HA	2:J:136:MET:HE1	1.93	0.50
1:I:394:PHE:CD2	1:I:400:ARG:HB3	2.45	0.50
2:J:70:THR:HB	2:J:231:TRP:CE2	2.46	0.50
2:J:247:THR:HG23	3:K:206:ILE:HD13	1.92	0.50
2:F:34:VAL:HG22	2:F:95:GLY:HA3	1.92	0.50
2:F:45:MET:HG3	2:F:64:THR:HG23	1.92	0.50
2:F:237:TRP:HB2	5:F:306:D10:H51	1.93	0.50
3:K:88:TYR:CD1	6:K:309:PLC:O1P	2.64	0.50
3:K:221:LEU:HD23	3:K:222:PRO:CD	2.41	0.50
1:A:173:LEU:HD12	2:B:170:PRO:HB2	1.93	0.50
3:C:236:MET:HG2	9:C:304:HXG:CAE	2.40	0.50
2:J:242:ARG:HH21	7:J:308:P1O:C5	2.24	0.50
2:F:61:VAL:HG12	10:F:422:HOH:O	2.11	0.50
2:B:233:PHE:CD2	5:B:303:D10:H51	2.46	0.50
6:C:303:PLC:C7	9:C:304:HXG:H36	2.24	0.50
2:F:80:TRP:O	2:F:84:ARG:NH1	2.44	0.50
3:K:270:ALA:C	3:K:274:LEU:HB3	2.36	0.50
2:B:57:ARG:HH21	2:B:201:GLU:CD	2.19	0.50
2:B:70:THR:HB	2:B:231:TRP:CE2	2.47	0.50
1:E:179:ASP:O	1:E:183:TYR:HB2	2.11	0.50
2:J:237:TRP:HB2	5:J:303:D10:H51	1.93	0.50
3:G:156:ASP:O	3:G:156:ASP:OD1	2.29	0.50
3:C:146:TYR:O	3:C:150:SER:HB3	2.12	0.50
2:J:80:TRP:O	2:J:84:ARG:NH1	2.44	0.50
3:G:270:ALA:C	3:G:274:LEU:HB3	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:ILE:HG12	3:C:237:GLU:OE2	2.11	0.50
1:E:385:SER:OG	10:E:606:HOH:O	2.20	0.50
2:J:134:VAL:O	2:J:134:VAL:HG12	2.09	0.50
3:G:160:HIS:C	3:G:162:THR:N	2.68	0.50
7:K:311:P1O:H12	7:K:311:P1O:H16	1.93	0.50
1:A:179:ASP:O	1:A:183:TYR:HB2	2.11	0.50
2:B:161:TRP:CE2	6:B:301:PLC:H73	2.40	0.50
6:C:308:PLC:CBA	7:C:309:P1O:H56	2.38	0.50
1:E:38:GLN:HA	10:E:638:HOH:O	2.10	0.50
2:J:61:VAL:HG12	10:J:423:HOH:O	2.11	0.50
2:F:69:VAL:CG1	2:F:152:TRP:CD1	2.95	0.50
3:G:62:TYR:OH	10:G:402:HOH:O	2.20	0.50
7:G:312:P1O:H12	7:G:312:P1O:H16	1.93	0.50
2:B:242:ARG:HH21	7:B:307:P1O:C5	2.25	0.50
3:C:88:TYR:CD1	6:C:308:PLC:O1P	2.64	0.50
3:C:220:ILE:HG23	3:C:248:PHE:CD2	2.46	0.50
3:C:236:MET:CE	3:C:236:MET:CA	2.89	0.50
2:J:45:MET:HG3	2:J:64:THR:HG23	1.92	0.50
2:J:69:VAL:CG1	2:J:152:TRP:CD1	2.95	0.50
2:F:32:VAL:HG11	3:G:258:VAL:HG11	1.94	0.50
2:F:69:VAL:HG12	2:F:152:TRP:NE1	2.25	0.50
3:G:146:TYR:O	3:G:150:SER:HB3	2.12	0.50
3:K:208:LEU:HB3	3:K:209:PRO:CD	2.42	0.50
2:B:219:PHE:HD1	3:K:226:LEU:HA	1.77	0.50
1:I:105:ILE:HG13	1:I:110:VAL:HG21	1.93	0.50
1:I:385:SER:OG	10:I:605:HOH:O	2.19	0.50
2:J:69:VAL:HG12	2:J:152:TRP:NE1	2.25	0.50
2:J:233:PHE:CD2	5:J:302:D10:H51	2.46	0.50
2:F:103:ASN:OD1	2:F:107:ASN:ND2	2.29	0.50
3:K:112:TRP:CZ2	7:K:311:P1O:C3	2.95	0.50
2:B:39:ILE:HG12	3:C:149:ALA:O	2.12	0.49
2:B:80:TRP:O	2:B:84:ARG:NH1	2.44	0.49
3:G:112:TRP:CZ2	7:G:312:P1O:C3	2.95	0.49
2:B:55:LYS:NZ	10:B:411:HOH:O	2.43	0.49
2:B:69:VAL:CG1	2:B:152:TRP:CD1	2.95	0.49
2:B:247:THR:HG21	7:C:310:P1O:H22	1.93	0.49
3:C:112:TRP:CZ2	7:C:310:P1O:C3	2.95	0.49
3:C:156:ASP:O	3:C:156:ASP:OD1	2.30	0.49
6:J:306:PLC:OB	6:J:306:PLC:H81	2.12	0.49
3:G:233:PHE:CG	3:G:234:TRP:N	2.79	0.49
3:G:242:ALA:HB3	3:G:244:LEU:CD2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:146:TYR:O	3:K:150:SER:HB3	2.12	0.49
3:K:221:LEU:CB	3:K:222:PRO:HD3	2.42	0.49
1:A:105:ILE:HG13	1:A:110:VAL:HG21	1.93	0.49
2:B:103:ASN:OD1	2:B:107:ASN:ND2	2.29	0.49
10:B:422:HOH:O	1:I:38:GLN:HA	2.11	0.49
3:C:242:ALA:HB3	3:C:244:LEU:CD2	2.43	0.49
1:E:168:ASN:OD1	10:E:605:HOH:O	2.19	0.49
1:I:265:GLN:HG3	2:J:177:LEU:O	2.13	0.49
2:J:39:ILE:HG13	3:K:149:ALA:HB1	1.94	0.49
2:F:62:THR:HG23	2:F:219:PHE:HD2	1.78	0.49
2:F:70:THR:HB	2:F:231:TRP:CE2	2.47	0.49
3:K:76:ALA:CB	3:K:84:GLU:HB2	2.43	0.49
1:E:105:ILE:HG13	1:E:110:VAL:HG21	1.93	0.49
2:F:107:ASN:ND2	3:G:155:GLN:HB2	2.27	0.49
3:G:220:ILE:HG23	3:G:248:PHE:CD2	2.46	0.49
6:G:301:PLC:OB	6:G:301:PLC:H81	2.12	0.49
3:K:46:LEU:H	3:K:129:ARG:HE	1.60	0.49
3:K:160:HIS:C	3:K:162:THR:N	2.68	0.49
2:B:150:MET:HE1	10:K:404:HOH:O	2.12	0.49
2:B:219:PHE:HB2	3:K:229:TRP:HB2	1.94	0.49
3:C:164:VAL:HG12	10:C:411:HOH:O	2.11	0.49
3:C:208:LEU:HB3	3:C:209:PRO:CD	2.42	0.49
1:E:318:TYR:CD1	1:E:318:TYR:C	2.90	0.49
2:J:57:ARG:HH21	2:J:201:GLU:CD	2.19	0.49
3:G:171:PRO:HA	3:G:174:ILE:HD12	1.95	0.49
3:K:169:PHE:HE2	6:K:306:PLC:H32	1.78	0.49
2:B:172:GLU:HG2	1:I:410:ILE:HG21	1.95	0.49
6:C:306:PLC:H3A2	6:F:303:PLC:H8'1	1.94	0.49
1:I:179:ASP:O	1:I:183:TYR:HB2	2.11	0.49
10:J:443:HOH:O	3:G:164:VAL:HG13	2.11	0.49
3:G:88:TYR:CD1	6:G:310:PLC:O1P	2.64	0.49
3:G:208:LEU:HB3	3:G:209:PRO:CD	2.42	0.49
3:G:234:TRP:HA	6:G:304:PLC:C7	2.43	0.49
3:K:92:PHE:HB3	3:K:174:ILE:HG21	1.95	0.49
3:K:156:ASP:O	3:K:156:ASP:OD1	2.29	0.49
3:C:233:PHE:CG	3:C:234:TRP:N	2.79	0.49
3:K:233:PHE:CG	3:K:234:TRP:N	2.79	0.49
3:K:234:TRP:HA	6:K:303:PLC:C7	2.43	0.49
1:A:62:ASN:ND2	1:A:165:GLU:O	2.41	0.49
5:A:503:D10:H92	6:K:307:PLC:H62	1.89	0.49
6:C:303:PLC:H9A2	2:F:66:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:311:PLC:OB	6:C:311:PLC:H81	2.12	0.49
1:E:410:ILE:HG21	2:J:172:GLU:HG2	1.94	0.49
1:I:318:TYR:CD1	1:I:318:TYR:C	2.90	0.49
2:F:215:VAL:HG23	6:F:301:PLC:H2'1	1.93	0.49
3:K:171:PRO:HA	3:K:174:ILE:HD12	1.95	0.49
2:B:62:THR:HG23	2:B:219:PHE:HD2	1.78	0.49
3:C:76:ALA:CB	3:C:84:GLU:HB2	2.43	0.49
3:C:171:PRO:HA	3:C:174:ILE:HD12	1.95	0.49
3:C:242:ALA:HB3	3:C:244:LEU:HD21	1.95	0.49
1:I:173:LEU:HD12	2:J:170:PRO:HB2	1.94	0.49
3:G:221:LEU:CB	3:G:222:PRO:HD3	2.42	0.49
3:K:242:ALA:HB3	3:K:244:LEU:CD2	2.43	0.49
1:A:318:TYR:CD1	1:A:318:TYR:C	2.90	0.48
1:E:324:PHE:HA	1:E:342:ALA:HB3	1.95	0.48
2:J:114:PHE:HE2	3:K:162:THR:HG22	1.77	0.48
1:A:94:PRO:HB3	3:C:74:TRP:HD1	1.78	0.48
2:B:11:HIS:HA	3:C:276:GLN:O	2.13	0.48
1:I:62:ASN:ND2	1:I:165:GLU:O	2.41	0.48
3:G:242:ALA:HB3	3:G:244:LEU:HD21	1.95	0.48
1:A:324:PHE:HA	1:A:342:ALA:HB3	1.95	0.48
3:C:221:LEU:CB	3:C:222:PRO:HD3	2.42	0.48
1:I:324:PHE:HA	1:I:342:ALA:HB3	1.95	0.48
2:J:138:SER:O	2:J:138:SER:OG	2.28	0.48
3:G:76:ALA:CB	3:G:84:GLU:HB2	2.42	0.48
2:B:247:THR:HG22	3:C:211:LEU:CD2	2.43	0.48
3:C:92:PHE:HB3	3:C:174:ILE:HG21	1.95	0.48
3:G:221:LEU:HD23	3:G:222:PRO:HD3	1.96	0.48
5:B:306:D10:H103	5:F:308:D10:H103	1.95	0.48
1:E:173:LEU:HD12	2:F:170:PRO:HB2	1.95	0.48
2:F:244:LEU:HD21	3:G:208:LEU:CD1	2.37	0.48
3:G:92:PHE:HB3	3:G:174:ILE:HG21	1.95	0.48
6:G:304:PLC:H2A2	6:G:304:PLC:H4'1	1.96	0.48
3:K:242:ALA:HB3	3:K:244:LEU:HD21	1.95	0.48
6:K:303:PLC:H4'1	6:K:303:PLC:H2A2	1.95	0.48
1:A:79:GLU:CB	1:E:268:THR:HB	2.40	0.48
3:C:223:ASN:OD1	3:C:247:GLY:HA3	2.14	0.48
2:J:219:PHE:CD1	3:G:226:LEU:HA	2.49	0.48
3:G:181:TYR:HA	3:G:184:TYR:CE2	2.49	0.48
3:C:153:THR:O	3:C:156:ASP:HB3	2.14	0.48
1:E:86:VAL:HB	1:E:145:GLN:HB2	1.96	0.48
2:F:198:ARG:HG2	2:F:200:VAL:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:46:LEU:H	3:G:129:ARG:HE	1.60	0.48
3:G:223:ASN:OD1	3:G:247:GLY:HA3	2.14	0.48
3:K:46:LEU:HB3	3:K:47:ASP:H	1.50	0.48
3:K:153:THR:O	3:K:156:ASP:HB3	2.14	0.48
1:A:195:TRP:HB3	2:B:125:VAL:HB	1.96	0.48
1:A:268:THR:HB	1:I:79:GLU:CB	2.38	0.48
2:B:213:ALA:CB	6:B:301:PLC:O'	2.62	0.48
3:C:169:PHE:HE2	6:F:301:PLC:H32	1.78	0.48
3:C:234:TRP:HA	6:C:303:PLC:C7	2.43	0.48
1:A:86:VAL:HB	1:A:145:GLN:HB2	1.96	0.48
2:B:161:TRP:HZ2	6:B:301:PLC:C7	2.21	0.48
1:I:35:GLU:C	1:I:37:SER:N	2.71	0.48
2:J:219:PHE:HD1	3:G:226:LEU:HA	1.78	0.48
3:K:110:TYR:CD1	3:K:110:TYR:C	2.92	0.48
3:K:156:ASP:OD2	3:K:160:HIS:CE1	2.67	0.48
3:K:244:LEU:CD2	3:K:244:LEU:N	2.77	0.48
1:A:101:LYS:HD2	1:A:101:LYS:HA	1.44	0.48
2:J:62:THR:HG23	2:J:219:PHE:HD2	1.78	0.48
2:J:213:ALA:CB	6:J:307:PLC:O'	2.62	0.48
3:G:110:TYR:C	3:G:110:TYR:CD1	2.92	0.48
3:G:236:MET:CE	3:G:236:MET:CA	2.89	0.48
3:K:113:LYS:HD2	3:K:113:LYS:HA	1.71	0.48
3:K:221:LEU:HD23	3:K:222:PRO:HD3	1.96	0.48
1:A:265:GLN:HG3	2:B:177:LEU:O	2.13	0.47
1:E:380:ILE:HA	10:E:606:HOH:O	2.13	0.47
2:J:206:ARG:O	3:G:232:THR:HA	2.14	0.47
3:G:169:PHE:HE2	6:G:307:PLC:H32	1.78	0.47
3:G:220:ILE:HG23	3:G:248:PHE:HD2	1.79	0.47
1:I:380:ILE:HA	10:I:605:HOH:O	2.13	0.47
3:G:223:ASN:O	3:G:226:LEU:N	2.47	0.47
2:B:86:PRO:HA	10:B:431:HOH:O	2.13	0.47
2:B:242:ARG:HH21	7:B:307:P1O:C4	2.28	0.47
3:C:181:TYR:HA	3:C:184:TYR:CE2	2.49	0.47
3:C:244:LEU:CD2	3:C:244:LEU:N	2.77	0.47
3:K:45:LEU:HG	3:K:129:ARG:HH21	1.80	0.47
3:K:58:TYR:HB2	3:K:143:TRP:HD1	1.80	0.47
3:G:156:ASP:OD2	3:G:160:HIS:CE1	2.67	0.47
1:A:385:SER:OG	10:A:606:HOH:O	2.20	0.47
3:C:110:TYR:CD1	3:C:110:TYR:C	2.92	0.47
2:J:198:ARG:HG2	2:J:200:VAL:HG13	1.95	0.47
3:K:223:ASN:OD1	3:K:247:GLY:HA3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:223:ASN:O	3:K:226:LEU:N	2.47	0.47
1:A:380:ILE:HA	10:A:606:HOH:O	2.12	0.47
2:B:206:ARG:O	3:K:232:THR:HA	2.14	0.47
3:C:156:ASP:OD2	3:C:160:HIS:CE1	2.67	0.47
2:F:11:HIS:O	2:F:11:HIS:ND1	2.38	0.47
2:F:213:ALA:CB	6:F:303:PLC:O'	2.62	0.47
2:F:242:ARG:HH21	7:F:302:P1O:C4	2.26	0.47
3:C:46:LEU:H	3:C:129:ARG:HE	1.60	0.47
3:C:58:TYR:HB2	3:C:143:TRP:HD1	1.80	0.47
3:C:221:LEU:HD23	3:C:222:PRO:HD3	1.96	0.47
1:E:104:TYR:O	1:E:124:PHE:HA	2.15	0.47
1:I:93:MET:SD	1:I:98:PHE:HB2	2.55	0.47
2:F:11:HIS:C	2:F:11:HIS:ND1	2.73	0.47
2:F:199:MET:SD	6:G:301:PLC:H2	2.54	0.47
3:G:153:THR:O	3:G:156:ASP:HB3	2.14	0.47
3:K:181:TYR:HA	3:K:184:TYR:CE2	2.49	0.47
3:K:220:ILE:HG23	3:K:248:PHE:HD2	1.79	0.47
1:A:35:GLU:C	1:A:37:SER:N	2.71	0.47
1:A:104:TYR:O	1:A:124:PHE:HA	2.15	0.47
1:A:218:MET:HE3	1:A:218:MET:HB3	1.83	0.47
10:B:443:HOH:O	3:K:164:VAL:HG13	2.14	0.47
3:C:226:LEU:HD13	2:F:219:PHE:CE1	2.50	0.47
3:G:244:LEU:CD2	3:G:244:LEU:N	2.77	0.47
1:A:93:MET:SD	1:A:98:PHE:HB2	2.55	0.47
2:B:198:ARG:HG2	2:B:200:VAL:HG13	1.96	0.47
3:C:131:ASN:HA	3:C:199:LEU:CD2	2.45	0.47
1:I:104:TYR:O	1:I:124:PHE:HA	2.15	0.47
3:G:45:LEU:HG	3:G:129:ARG:HH21	1.80	0.47
3:G:58:TYR:HB2	3:G:143:TRP:HD1	1.80	0.47
2:B:204:THR:C	1:I:42:MET:HE1	2.40	0.47
3:C:198:ARG:HE	7:C:309:P1O:H13	1.80	0.47
3:C:220:ILE:HG23	3:C:248:PHE:HD2	1.79	0.47
1:E:395:ASP:OD2	1:E:399:ASN:ND2	2.48	0.47
5:I:503:D10:H91	6:G:308:PLC:C6	2.23	0.47
3:G:198:ARG:HE	7:G:311:P1O:H13	1.80	0.47
3:K:78:LEU:HD12	3:K:78:LEU:HA	1.78	0.47
2:B:222:PHE:CE1	3:K:223:ASN:HB2	2.49	0.46
6:C:303:PLC:H4'1	6:C:303:PLC:H2A2	1.95	0.46
2:J:45:MET:HE3	2:J:49:ASP:CB	2.45	0.46
3:G:119:LEU:HD12	3:G:119:LEU:HA	1.77	0.46
3:G:131:ASN:HA	3:G:199:LEU:CD2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:198:ARG:HE	7:K:310:P1O:H13	1.80	0.46
1:A:395:ASP:OD2	1:A:399:ASN:ND2	2.48	0.46
2:B:11:HIS:C	2:B:11:HIS:ND1	2.73	0.46
2:B:108:PHE:CE2	3:C:158:THR:HG22	2.50	0.46
3:C:230:GLY:HA3	3:C:244:LEU:CD1	2.38	0.46
3:C:232:THR:HA	2:F:206:ARG:O	2.15	0.46
1:E:45:ARG:HB3	1:E:74:PHE:CE2	2.50	0.46
1:E:216:LEU:HB2	2:F:83:TYR:CE2	2.49	0.46
2:J:32:VAL:HG11	3:K:258:VAL:HG11	1.96	0.46
2:F:45:MET:HE3	2:F:49:ASP:CB	2.45	0.46
2:F:242:ARG:HH21	7:F:302:P1O:C5	2.28	0.46
3:K:131:ASN:HA	3:K:199:LEU:CD2	2.45	0.46
6:K:309:PLC:CBA	7:K:310:P1O:H56	2.38	0.46
3:C:45:LEU:HG	3:C:129:ARG:HH21	1.80	0.46
3:C:76:ALA:HB1	3:C:84:GLU:HB2	1.98	0.46
3:C:77:GLY:HA2	3:C:89:TRP:CD1	2.51	0.46
3:C:100:GLU:CD	3:C:182:PRO:HB2	2.41	0.46
1:E:93:MET:SD	1:E:98:PHE:HB2	2.55	0.46
2:J:39:ILE:HG12	3:K:149:ALA:O	2.15	0.46
2:J:50:PHE:CD1	2:J:104:ARG:NH2	2.84	0.46
2:J:107:ASN:ND2	3:K:155:GLN:HB2	2.31	0.46
2:F:236:ARG:HD3	2:F:236:ARG:HA	1.67	0.46
2:F:243:PHE:HD2	3:G:205:GLY:O	1.99	0.46
3:G:76:ALA:HB1	3:G:84:GLU:HB2	1.98	0.46
6:K:303:PLC:C7	9:K:304:HXG:H36	2.24	0.46
3:C:155:GLN:O	3:C:158:THR:HG23	2.16	0.46
3:C:174:ILE:O	3:C:175:ILE:HD13	2.16	0.46
1:I:395:ASP:OD2	1:I:399:ASN:ND2	2.48	0.46
2:J:34:VAL:CG2	2:J:95:GLY:HA3	2.46	0.46
2:J:206:ARG:HG3	3:G:236:MET:HA	1.97	0.46
1:A:45:ARG:HB3	1:A:74:PHE:CE2	2.50	0.46
3:C:208:LEU:HB3	3:C:209:PRO:HD3	1.98	0.46
1:E:101:LYS:HE2	10:E:605:HOH:O	2.15	0.46
1:I:275:LEU:HD12	1:I:275:LEU:HA	1.76	0.46
2:J:55:LYS:NZ	10:J:412:HOH:O	2.48	0.46
2:F:247:THR:CG2	3:G:211:LEU:CD2	2.93	0.46
3:G:155:GLN:O	3:G:158:THR:HG23	2.16	0.46
3:G:230:GLY:HA3	3:G:244:LEU:CD1	2.38	0.46
6:G:310:PLC:CBA	7:G:311:P1O:H56	2.38	0.46
3:K:100:GLU:CD	3:K:182:PRO:HB2	2.41	0.46
2:B:45:MET:HE3	2:B:49:ASP:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:103:ASN:OD1	2:J:107:ASN:ND2	2.29	0.46
3:G:77:GLY:HA2	3:G:89:TRP:CD1	2.51	0.46
3:G:245:HIS:C	3:G:247:GLY:N	2.74	0.46
3:K:58:TYR:HE1	3:K:183:ILE:CG2	2.29	0.46
1:A:93:MET:HE1	1:A:98:PHE:CB	2.41	0.46
2:B:138:SER:O	2:B:138:SER:OG	2.28	0.46
1:E:314:LEU:HD11	1:E:391:LEU:HD22	1.98	0.46
1:I:314:LEU:HD11	1:I:391:LEU:HD22	1.98	0.46
2:F:50:PHE:CD1	2:F:104:ARG:NH2	2.84	0.46
3:C:164:VAL:CG1	10:C:411:HOH:O	2.63	0.46
3:C:245:HIS:C	3:C:247:GLY:N	2.74	0.46
1:E:237:MET:CG	2:F:137:LEU:CD1	2.92	0.46
1:I:45:ARG:HB3	1:I:74:PHE:CE2	2.50	0.46
1:I:86:VAL:HB	1:I:145:GLN:HB2	1.96	0.46
3:G:80:SER:HB3	3:G:166:ASP:HB3	1.98	0.46
3:G:100:GLU:CD	3:G:182:PRO:HB2	2.41	0.46
3:G:234:TRP:CZ2	3:G:235:PHE:CZ	3.05	0.46
3:K:77:GLY:HA2	3:K:89:TRP:CD1	2.51	0.46
1:A:94:PRO:HB2	3:C:74:TRP:HD1	1.82	0.45
1:A:313:ARG:HG3	1:A:353:PRO:HA	1.98	0.45
2:B:145:ALA:O	2:B:149:ALA:HB3	2.16	0.45
1:E:217:LEU:HD11	3:G:278:LEU:HD12	1.97	0.45
1:I:218:MET:HE3	1:I:218:MET:HB3	1.83	0.45
2:F:161:TRP:HZ2	6:F:303:PLC:C7	2.21	0.45
2:F:244:LEU:O	2:F:245:GLN:CB	2.64	0.45
1:A:314:LEU:HD11	1:A:391:LEU:HD22	1.98	0.45
3:C:181:TYR:HA	3:C:184:TYR:CD2	2.52	0.45
2:F:34:VAL:CG2	2:F:95:GLY:HA3	2.46	0.45
2:F:214:PRO:HA	6:F:303:PLC:H2'1	1.98	0.45
3:G:58:TYR:HE1	3:G:183:ILE:CG2	2.29	0.45
3:K:238:GLU:HG2	10:K:409:HOH:O	2.16	0.45
2:J:222:PHE:CE1	3:G:223:ASN:HB2	2.51	0.45
3:C:58:TYR:HE1	3:C:183:ILE:CG2	2.28	0.45
3:C:80:SER:HB3	3:C:166:ASP:HB3	1.98	0.45
3:C:223:ASN:HB2	2:F:222:PHE:CE1	2.50	0.45
2:F:145:ALA:O	2:F:149:ALA:HB3	2.17	0.45
3:K:155:GLN:O	3:K:158:THR:HG23	2.16	0.45
1:I:216:LEU:HB2	2:J:83:TYR:CE2	2.51	0.45
2:J:161:TRP:HZ2	6:J:307:PLC:C7	2.21	0.45
3:G:181:TYR:HA	3:G:184:TYR:CD2	2.52	0.45
3:K:274:LEU:C	3:K:274:LEU:CD1	2.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:ARG:HB3	3:C:199:LEU:CD2	2.46	0.45
2:J:34:VAL:O	2:J:38:HIS:HB2	2.17	0.45
2:J:214:PRO:HA	6:J:307:PLC:H2'1	1.99	0.45
10:J:401:HOH:O	3:K:263:THR:HG21	2.16	0.45
2:F:77:SER:HB3	10:F:424:HOH:O	2.15	0.45
3:G:174:ILE:O	3:G:175:ILE:HD13	2.16	0.45
6:K:306:PLC:H1A2	6:K:306:PLC:H31	1.80	0.45
1:A:171:THR:O	2:B:171:VAL:HG13	2.17	0.45
1:A:216:LEU:HB2	2:B:83:TYR:CE2	2.52	0.45
2:B:34:VAL:CG2	2:B:95:GLY:HA3	2.46	0.45
2:B:34:VAL:O	2:B:38:HIS:HB2	2.17	0.45
2:B:205:LEU:CG	1:I:147:GLY:O	2.55	0.45
2:B:214:PRO:HA	6:B:301:PLC:H2'1	1.98	0.45
2:B:244:LEU:O	2:B:245:GLN:CB	2.64	0.45
2:J:27:PHE:CE2	2:J:31:PHE:CE2	3.05	0.45
2:F:47:ASP:OD2	3:G:241:VAL:HG22	2.17	0.45
2:F:242:ARG:NH2	7:F:302:P1O:H8	2.31	0.45
6:G:310:PLC:H1A2	6:G:310:PLC:H31	1.79	0.45
1:I:101:LYS:HD2	1:I:101:LYS:HA	1.44	0.45
1:I:394:PHE:CE2	1:I:400:ARG:HB3	2.52	0.45
2:F:161:TRP:O	2:F:165:ALA:HB2	2.17	0.45
2:B:27:PHE:CE2	2:B:31:PHE:CE2	3.05	0.45
2:B:155:ILE:HA	2:B:158:PRO:HG2	1.99	0.45
5:B:306:D10:H103	5:J:305:D10:H103	1.98	0.45
1:E:313:ARG:HG3	1:E:353:PRO:HA	1.98	0.45
1:I:195:TRP:HB3	2:J:125:VAL:HB	1.98	0.45
3:G:63:LEU:HD23	3:G:63:LEU:HA	1.81	0.45
3:K:80:SER:HB3	3:K:166:ASP:HB3	1.98	0.45
3:K:234:TRP:CZ2	3:K:235:PHE:CZ	3.04	0.45
1:I:108:GLN:O	1:I:108:GLN:HG3	2.17	0.45
1:I:313:ARG:HG3	1:I:353:PRO:HA	1.98	0.45
5:I:503:D10:C9	6:G:308:PLC:H62	2.37	0.45
2:J:145:ALA:O	2:J:149:ALA:HB3	2.17	0.45
3:G:234:TRP:HZ2	9:G:305:HXG:H14	1.82	0.45
3:K:76:ALA:HB1	3:K:84:GLU:HB2	1.98	0.45
3:K:181:TYR:HA	3:K:184:TYR:CD2	2.52	0.45
3:K:236:MET:CE	3:K:236:MET:CA	2.89	0.45
3:K:262:LEU:HD23	3:K:262:LEU:HA	1.77	0.45
2:B:50:PHE:CD1	2:B:104:ARG:NH2	2.84	0.44
3:C:194:TYR:C	3:C:194:TYR:CD1	2.96	0.44
3:C:234:TRP:CZ2	3:C:235:PHE:CZ	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:236:ARG:HD3	2:J:236:ARG:HA	1.67	0.44
2:F:109:TRP:CG	2:F:109:TRP:O	2.70	0.44
3:G:130:ARG:HB3	3:G:199:LEU:CD2	2.46	0.44
3:G:208:LEU:HB3	3:G:209:PRO:HD3	1.98	0.44
3:G:238:GLU:HG2	10:G:408:HOH:O	2.16	0.44
3:K:234:TRP:HZ2	9:K:304:HXG:H14	1.82	0.44
6:K:309:PLC:HEA2	7:K:310:P1O:C28	2.29	0.44
1:A:394:PHE:CE2	1:A:400:ARG:HB3	2.52	0.44
3:C:226:LEU:HA	2:F:219:PHE:HD1	1.81	0.44
1:E:62:ASN:ND2	1:E:165:GLU:O	2.41	0.44
1:E:195:TRP:HB3	2:F:125:VAL:HB	1.98	0.44
1:I:237:MET:CG	2:J:137:LEU:CD1	2.95	0.44
3:K:245:HIS:C	3:K:247:GLY:N	2.74	0.44
3:K:276:GLN:HG2	3:K:280:GLU:HG3	2.00	0.44
1:A:42:MET:HE1	2:F:204:THR:C	2.42	0.44
2:B:109:TRP:O	2:B:109:TRP:CG	2.70	0.44
3:C:129:ARG:NH1	3:C:129:ARG:CG	2.79	0.44
3:C:134:HIS:HB3	3:C:199:LEU:HD11	1.99	0.44
3:C:237:GLU:HB3	3:C:238:GLU:H	1.52	0.44
3:C:246:TYR:CD1	3:C:246:TYR:N	2.85	0.44
3:C:275:GLY:HA3	3:C:276:GLN:NE2	2.33	0.44
2:J:37:TYR:CE1	2:J:71:PHE:HB2	2.53	0.44
2:J:161:TRP:O	2:J:165:ALA:HB2	2.17	0.44
2:J:197:ILE:HG12	3:K:237:GLU:OE2	2.16	0.44
2:J:242:ARG:HH21	7:J:308:P1O:C4	2.30	0.44
6:G:310:PLC:H72	6:G:310:PLC:C1'	2.46	0.44
3:K:174:ILE:O	3:K:175:ILE:HD13	2.16	0.44
3:K:208:LEU:HB3	3:K:209:PRO:HD3	1.98	0.44
2:B:43:LEU:HD12	3:C:248:PHE:HB2	2.00	0.44
2:B:161:TRP:O	2:B:165:ALA:HB2	2.17	0.44
3:C:58:TYR:OH	3:C:187:THR:OG1	2.12	0.44
3:C:223:ASN:O	3:C:226:LEU:N	2.48	0.44
6:C:306:PLC:H62	6:C:306:PLC:H41	1.85	0.44
2:F:131:LEU:HD23	2:F:131:LEU:HA	1.78	0.44
3:G:117:ARG:CG	3:G:117:ARG:NH1	2.73	0.44
3:G:160:HIS:CE1	10:G:401:HOH:O	2.70	0.44
3:G:163:ILE:C	3:G:163:ILE:HD12	2.43	0.44
3:K:167:THR:HG23	3:K:169:PHE:H	1.82	0.44
3:C:154:GLU:C	3:C:156:ASP:N	2.73	0.44
3:C:160:HIS:CE1	10:C:401:HOH:O	2.70	0.44
3:C:244:LEU:O	3:C:245:HIS:CD2	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:ILE:HG21	3:G:278:LEU:HD11	1.96	0.44
2:F:34:VAL:O	2:F:38:HIS:HB2	2.17	0.44
3:G:46:LEU:HB3	3:G:47:ASP:H	1.50	0.44
3:K:58:TYR:HB2	3:K:143:TRP:CD1	2.53	0.44
3:K:154:GLU:C	3:K:156:ASP:N	2.73	0.44
3:K:275:GLY:HA3	3:K:276:GLN:NE2	2.33	0.44
6:K:309:PLC:H72	6:K:309:PLC:H2'2	2.00	0.44
3:C:234:TRP:HZ2	9:C:304:HXG:H14	1.82	0.44
2:J:199:MET:HE3	2:J:199:MET:HB2	1.93	0.44
1:A:108:GLN:O	1:A:108:GLN:HG3	2.17	0.44
2:B:247:THR:HG21	7:C:310:P1O:C10	2.48	0.44
3:C:163:ILE:C	3:C:163:ILE:HD12	2.43	0.44
3:C:167:THR:HG23	3:C:169:PHE:H	1.82	0.44
1:E:379:ILE:HG21	1:E:409:LEU:HD23	2.00	0.44
2:F:107:ASN:HD21	3:G:155:GLN:HB2	1.83	0.44
3:K:50:TRP:CD2	7:K:310:P1O:H16	2.53	0.44
2:B:32:VAL:HG11	3:C:258:VAL:HG11	1.99	0.44
2:J:155:ILE:HA	2:J:158:PRO:HG2	1.99	0.44
2:F:155:ILE:HA	2:F:158:PRO:HG2	1.99	0.44
3:G:246:TYR:N	3:G:246:TYR:CD1	2.85	0.44
3:K:66:ARG:HH11	3:K:66:ARG:HG3	1.82	0.44
2:B:68:LEU:HD12	2:B:124:LEU:CD2	2.48	0.44
2:B:204:THR:HB	3:K:236:MET:SD	2.58	0.44
3:C:65:VAL:HG11	3:C:175:ILE:HG23	2.00	0.44
3:C:66:ARG:HH11	3:C:66:ARG:HG3	1.82	0.44
3:C:74:TRP:CD2	3:C:74:TRP:N	2.83	0.44
3:C:234:TRP:CH2	9:C:304:HXG:H18	2.53	0.44
1:E:80:THR:HG21	2:J:204:THR:HA	2.00	0.44
2:J:109:TRP:O	2:J:109:TRP:CG	2.70	0.44
2:J:131:LEU:HD23	2:J:131:LEU:HA	1.78	0.44
2:J:207:THR:O	2:J:207:THR:HG22	2.18	0.44
2:F:11:HIS:HA	3:G:276:GLN:O	2.18	0.44
2:F:27:PHE:CE2	2:F:31:PHE:CE2	3.05	0.44
2:F:213:ALA:HB1	6:F:303:PLC:H12	1.99	0.44
3:K:163:ILE:C	3:K:163:ILE:HD12	2.43	0.44
2:B:37:TYR:CE1	2:B:71:PHE:HB2	2.53	0.43
6:C:308:PLC:H31	6:C:308:PLC:H1A2	1.79	0.43
1:E:111:PRO:HA	2:F:186:TYR:CE1	2.53	0.43
1:I:272:MET:CA	1:I:272:MET:CE	2.95	0.43
3:G:66:ARG:HH11	3:G:66:ARG:HG3	1.82	0.43
3:C:50:TRP:CD2	7:C:309:P1O:H16	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:223:ASN:HB2	2:F:222:PHE:CZ	2.53	0.43
3:C:246:TYR:N	3:C:246:TYR:HD1	2.17	0.43
1:I:379:ILE:HG21	1:I:409:LEU:HD23	2.00	0.43
3:G:194:TYR:CD1	3:G:194:TYR:C	2.96	0.43
2:B:242:ARG:NH2	7:B:307:P1O:H8	2.32	0.43
3:C:78:LEU:HD12	3:C:78:LEU:HA	1.78	0.43
1:E:35:GLU:C	1:E:37:SER:N	2.71	0.43
3:G:50:TRP:CD2	7:G:311:P1O:H16	2.53	0.43
3:G:167:THR:HG23	3:G:169:PHE:H	1.82	0.43
3:G:237:GLU:HB3	3:G:238:GLU:H	1.52	0.43
3:G:246:TYR:N	3:G:246:TYR:HD1	2.17	0.43
3:K:156:ASP:O	3:K:157:GLY:C	2.61	0.43
3:K:194:TYR:C	3:K:194:TYR:CD1	2.96	0.43
3:K:234:TRP:CH2	9:K:304:HXG:H18	2.53	0.43
3:K:244:LEU:O	3:K:245:HIS:CD2	2.71	0.43
1:I:313:ARG:CZ	1:I:329:VAL:HG22	2.49	0.43
7:J:308:P1O:H15	7:J:308:P1O:C20	2.47	0.43
2:F:37:TYR:CE1	2:F:71:PHE:HB2	2.53	0.43
1:A:147:GLY:O	2:F:205:LEU:CG	2.55	0.43
2:B:34:VAL:CG2	2:B:95:GLY:CA	2.97	0.43
3:C:45:LEU:N	3:C:45:LEU:CD2	2.73	0.43
3:C:276:GLN:HG2	3:C:280:GLU:HG3	2.00	0.43
6:C:308:PLC:H72	6:C:308:PLC:H2'2	2.00	0.43
1:E:93:MET:HE1	1:E:98:PHE:CB	2.41	0.43
1:E:394:PHE:CE2	1:E:400:ARG:HB3	2.52	0.43
2:J:213:ALA:HB1	6:J:307:PLC:H12	1.99	0.43
3:G:244:LEU:O	3:G:245:HIS:CD2	2.71	0.43
1:A:83:GLU:O	1:A:85:ASP:N	2.47	0.43
3:C:58:TYR:HB2	3:C:143:TRP:CD1	2.53	0.43
3:G:65:VAL:HG11	3:G:175:ILE:HG23	2.00	0.43
3:G:217:PRO:HA	3:G:220:ILE:HD13	2.01	0.43
3:G:275:GLY:HA3	3:G:276:GLN:NE2	2.33	0.43
3:K:246:TYR:N	3:K:246:TYR:CD1	2.85	0.43
3:K:276:GLN:HG2	3:K:280:GLU:CG	2.49	0.43
1:E:42:MET:HE1	2:J:204:THR:C	2.43	0.43
1:E:108:GLN:O	1:E:108:GLN:HG3	2.17	0.43
1:I:214:PRO:HB3	3:K:278:LEU:HD22	2.01	0.43
2:F:34:VAL:CG2	2:F:95:GLY:CA	2.97	0.43
6:G:304:PLC:C7	9:G:305:HXG:H36	2.24	0.43
6:G:310:PLC:H72	6:G:310:PLC:H2'2	2.00	0.43
3:K:160:HIS:CE1	10:K:401:HOH:O	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:235:PHE:HA	9:G:305:HXG:H41	2.01	0.43
3:G:276:GLN:HG2	3:G:280:GLU:CG	2.48	0.43
1:E:103:SER:OG	2:F:186:TYR:OH	2.15	0.43
2:J:204:THR:HB	3:G:236:MET:SD	2.59	0.43
3:G:131:ASN:CA	3:G:199:LEU:CD2	2.97	0.43
3:G:276:GLN:HG2	3:G:280:GLU:HG3	1.99	0.43
3:K:246:TYR:N	3:K:246:TYR:HD1	2.17	0.43
1:A:237:MET:CG	2:B:137:LEU:CD1	2.94	0.43
1:A:313:ARG:CZ	1:A:329:VAL:HG22	2.49	0.43
2:B:236:ARG:HD3	2:B:236:ARG:HA	1.67	0.43
6:C:308:PLC:H72	6:C:308:PLC:C1'	2.46	0.43
1:E:313:ARG:CZ	1:E:329:VAL:HG22	2.49	0.43
1:E:385:SER:HB2	2:J:177:LEU:HD23	2.01	0.43
1:I:94:PRO:CB	3:K:74:TRP:HD1	2.32	0.43
2:J:136:MET:HE2	2:J:136:MET:HB3	1.89	0.43
2:F:242:ARG:NH2	7:F:302:P1O:C4	2.82	0.43
3:G:46:LEU:HD12	3:G:129:ARG:HG2	2.01	0.43
3:G:58:TYR:HB2	3:G:143:TRP:CD1	2.53	0.43
3:G:156:ASP:O	3:G:157:GLY:C	2.61	0.43
6:K:307:PLC:H31	6:K:307:PLC:H1'1	2.01	0.43
1:A:379:ILE:HG21	1:A:409:LEU:HD23	2.00	0.42
2:B:237:TRP:HE1	5:B:305:D10:H31	1.79	0.42
7:B:307:P1O:H43	7:B:307:P1O:H17	2.01	0.42
3:C:46:LEU:HD12	3:C:129:ARG:HG2	2.01	0.42
3:C:156:ASP:O	3:C:157:GLY:C	2.61	0.42
3:C:235:PHE:HA	9:C:304:HXG:H41	2.01	0.42
1:E:83:GLU:O	1:E:85:ASP:N	2.47	0.42
7:J:308:P1O:H43	7:J:308:P1O:H17	2.01	0.42
3:G:234:TRP:CH2	9:G:305:HXG:H18	2.53	0.42
3:K:131:ASN:CA	3:K:199:LEU:CD2	2.97	0.42
3:K:217:PRO:HA	3:K:220:ILE:HD13	2.01	0.42
2:B:135:LEU:HD12	10:B:431:HOH:O	2.19	0.42
2:B:207:THR:O	2:B:207:THR:HG22	2.18	0.42
2:B:247:THR:HG21	7:C:310:P1O:C11	2.48	0.42
2:F:11:HIS:NE2	3:G:277:SER:HA	2.35	0.42
2:F:247:THR:CG2	3:G:211:LEU:HD22	2.47	0.42
3:G:154:GLU:C	3:G:156:ASP:N	2.73	0.42
1:A:138:VAL:O	1:A:154:GLY:HA2	2.19	0.42
3:C:270:ALA:CA	3:C:274:LEU:CB	2.98	0.42
2:J:59:LEU:HD11	6:G:304:PLC:H32	2.01	0.42
2:J:142:LEU:HD22	7:F:302:P1O:H48	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:78:LEU:HD12	3:G:78:LEU:HA	1.78	0.42
2:B:213:ALA:HB1	6:B:301:PLC:H12	1.99	0.42
3:C:217:PRO:HA	3:C:220:ILE:HD13	2.01	0.42
6:C:306:PLC:H31	6:C:306:PLC:H1'1	2.01	0.42
1:E:101:LYS:HD2	1:E:101:LYS:HA	1.44	0.42
7:F:302:P1O:H43	7:F:302:P1O:H17	2.01	0.42
3:G:134:HIS:HB3	3:G:199:LEU:HD11	1.99	0.42
3:G:192:PHE:HB2	3:G:214:VAL:HG21	2.01	0.42
3:K:217:PRO:HA	3:K:220:ILE:CD1	2.49	0.42
3:K:235:PHE:HA	9:K:304:HXG:H41	2.01	0.42
6:K:309:PLC:H72	6:K:309:PLC:C1'	2.46	0.42
6:K:309:PLC:H31	6:K:309:PLC:H1A2	1.79	0.42
1:A:213:ILE:HG21	3:C:278:LEU:HD11	1.93	0.42
2:B:204:THR:HA	1:I:80:THR:HG21	2.01	0.42
2:B:226:LEU:HD11	3:K:251:PHE:CZ	2.46	0.42
6:C:306:PLC:H1A1	6:F:303:PLC:H7'2	2.00	0.42
1:E:218:MET:HE3	1:E:218:MET:HB3	1.83	0.42
1:I:213:ILE:HG21	3:K:278:LEU:HD11	1.93	0.42
1:I:376:LEU:HD23	1:I:376:LEU:HA	1.81	0.42
5:I:503:D10:H101	6:G:308:PLC:C7	2.50	0.42
2:J:204:THR:CG2	6:G:304:PLC:H61	2.50	0.42
3:K:46:LEU:HD12	3:K:129:ARG:HG2	2.01	0.42
3:K:65:VAL:HG11	3:K:175:ILE:HG23	2.00	0.42
3:K:230:GLY:HA3	3:K:244:LEU:CD1	2.38	0.42
3:K:235:PHE:HE2	3:K:243:PRO:HD2	1.79	0.42
3:C:156:ASP:C	3:C:156:ASP:OD1	2.61	0.42
3:C:276:GLN:HG2	3:C:280:GLU:CG	2.49	0.42
2:F:107:ASN:ND2	3:G:155:GLN:CA	2.81	0.42
3:G:113:LYS:HD2	3:G:113:LYS:HA	1.71	0.42
3:G:217:PRO:HA	3:G:220:ILE:CD1	2.49	0.42
3:G:275:GLY:HA3	3:G:276:GLN:CD	2.45	0.42
6:G:308:PLC:H1'1	6:G:308:PLC:H31	2.01	0.42
3:C:76:ALA:CB	3:C:84:GLU:HG3	2.50	0.42
3:C:211:LEU:HD21	2:F:142:LEU:CD2	2.49	0.42
3:C:217:PRO:HA	3:C:220:ILE:CD1	2.49	0.42
3:C:262:LEU:HD23	3:C:262:LEU:HA	1.77	0.42
2:F:21:ILE:HD11	3:G:269:PHE:CE1	2.54	0.42
2:F:124:LEU:HB3	10:F:441:HOH:O	2.20	0.42
2:B:11:HIS:NE2	3:C:277:SER:HA	2.35	0.42
2:B:176:MET:HE2	2:B:176:MET:HB3	1.72	0.42
2:B:204:THR:O	1:I:42:MET:CE	2.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:77:SER:HB3	10:J:425:HOH:O	2.19	0.42
2:J:111:TRP:CD1	3:K:74:TRP:CH2	3.08	0.42
3:G:76:ALA:CB	3:G:84:GLU:HG3	2.50	0.42
7:B:307:P1O:H48	2:F:142:LEU:HD22	2.01	0.42
3:C:216:GLY:HA3	3:C:254:LEU:CB	2.50	0.42
1:I:310:SER:HA	1:I:311:PRO:HD3	1.96	0.42
6:J:307:PLC:H62	6:J:307:PLC:P	2.60	0.42
6:F:303:PLC:H62	6:F:303:PLC:P	2.60	0.42
3:G:278:LEU:N	3:G:278:LEU:HD23	2.35	0.42
1:A:214:PRO:HB3	3:C:278:LEU:HD22	2.01	0.42
1:A:217:LEU:HD11	3:C:278:LEU:HD12	2.01	0.42
6:B:301:PLC:P	6:B:301:PLC:H62	2.60	0.42
3:C:46:LEU:HB3	3:C:47:ASP:H	1.50	0.42
1:E:215:ARG:NH1	1:E:227:LEU:HB3	2.34	0.42
1:I:35:GLU:HG2	1:I:36:LYS:HG3	2.02	0.42
2:F:207:THR:O	2:F:207:THR:HG22	2.18	0.42
1:A:215:ARG:NH1	1:A:227:LEU:HB3	2.35	0.41
1:A:385:SER:HB2	2:F:177:LEU:HD23	2.01	0.41
2:B:69:VAL:HG13	2:B:152:TRP:NE1	2.34	0.41
2:B:237:TRP:HH2	7:B:307:P1O:H27	1.85	0.41
3:C:131:ASN:CA	3:C:199:LEU:CD2	2.97	0.41
6:F:301:PLC:H41	6:F:301:PLC:H73	1.83	0.41
3:G:216:GLY:HA3	3:G:254:LEU:CB	2.50	0.41
3:G:245:HIS:O	3:G:248:PHE:HD1	2.03	0.41
3:K:278:LEU:N	3:K:278:LEU:HD23	2.35	0.41
1:A:35:GLU:HG2	1:A:36:LYS:HG3	2.02	0.41
2:B:77:SER:HB3	10:B:426:HOH:O	2.19	0.41
2:B:142:LEU:HD22	7:J:308:P1O:H48	2.01	0.41
1:E:138:VAL:O	1:E:154:GLY:HA2	2.19	0.41
3:G:270:ALA:CA	3:G:274:LEU:CB	2.97	0.41
6:G:304:PLC:H1A1	6:G:304:PLC:H31	1.83	0.41
3:K:262:LEU:HA	3:K:265:THR:HG23	2.02	0.41
2:B:21:ILE:HD11	3:C:269:PHE:CE1	2.55	0.41
2:J:68:LEU:HD12	2:J:124:LEU:CD2	2.48	0.41
2:F:68:LEU:HD12	2:F:124:LEU:CD2	2.48	0.41
3:K:245:HIS:O	3:K:248:PHE:HD1	2.03	0.41
3:K:270:ALA:CA	3:K:274:LEU:CB	2.98	0.41
3:C:275:GLY:HA3	3:C:276:GLN:CD	2.45	0.41
7:C:309:P1O:H7	7:C:309:P1O:H1	1.85	0.41
1:E:35:GLU:HG2	1:E:36:LYS:HG3	2.02	0.41
1:I:138:VAL:O	1:I:154:GLY:HA2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:142:MET:HE2	1:I:142:MET:HB2	1.86	0.41
2:J:115:PRO:O	2:J:119:VAL:HG22	2.21	0.41
2:F:69:VAL:CG1	2:F:152:TRP:CE2	3.02	0.41
2:F:115:PRO:O	2:F:119:VAL:HG22	2.21	0.41
9:K:304:HXG:H40	9:K:304:HXG:OAW	2.21	0.41
1:A:42:MET:CE	2:F:204:THR:O	2.68	0.41
3:C:181:TYR:HB2	3:C:182:PRO:HD3	2.03	0.41
6:C:306:PLC:H5A1	6:F:301:PLC:HTA1	2.03	0.41
1:I:170:VAL:CG1	1:I:180:LEU:HG	2.50	0.41
1:A:142:MET:HE2	1:A:142:MET:HB2	1.86	0.41
3:C:270:ALA:HB1	3:C:274:LEU:CB	2.38	0.41
2:J:197:ILE:CG1	3:K:237:GLU:HG2	2.49	0.41
2:F:39:ILE:HG13	3:G:149:ALA:HB1	2.02	0.41
3:G:181:TYR:HB2	3:G:182:PRO:HD3	2.03	0.41
6:G:310:PLC:H42	6:G:310:PLC:H63	1.81	0.41
3:K:49:LYS:HB3	3:K:49:LYS:HZ2	1.80	0.41
3:K:76:ALA:CB	3:K:84:GLU:HG3	2.50	0.41
5:A:503:D10:H101	6:K:307:PLC:C7	2.51	0.41
3:C:192:PHE:HZ	3:C:206:ILE:HG23	1.86	0.41
3:C:192:PHE:HB2	3:C:214:VAL:HG21	2.02	0.41
1:E:42:MET:CE	2:J:204:THR:O	2.66	0.41
1:E:80:THR:CG2	2:J:203:GLY:O	2.51	0.41
1:I:293:VAL:HA	1:I:294:PRO:HA	1.92	0.41
2:J:21:ILE:HD11	3:K:269:PHE:CE1	2.56	0.41
9:G:305:HXG:OAW	9:G:305:HXG:H40	2.21	0.41
3:K:134:HIS:HB3	3:K:199:LEU:HD11	1.99	0.41
6:K:306:PLC:HTA1	6:K:307:PLC:H5A1	2.03	0.41
2:B:14:ALA:CB	3:C:277:SER:CB	2.99	0.41
2:B:131:LEU:HA	2:B:131:LEU:HD23	1.77	0.41
2:B:206:ARG:HG3	3:K:236:MET:HA	2.03	0.41
2:B:244:LEU:HG	3:C:206:ILE:O	2.21	0.41
9:C:304:HXG:H40	9:C:304:HXG:OAW	2.21	0.41
1:I:256:SER:OG	1:I:257:LYS:N	2.54	0.41
2:J:34:VAL:CG2	2:J:95:GLY:CA	2.97	0.41
3:G:127:GLU:OE1	3:G:200:PRO:HG3	2.21	0.41
3:G:138:LEU:HD23	3:G:138:LEU:HA	1.92	0.41
3:K:119:LEU:HD12	3:K:119:LEU:HA	1.77	0.41
3:K:192:PHE:HB2	3:K:214:VAL:HG21	2.01	0.41
1:A:296:ARG:NH1	1:A:369:ALA:HB2	2.36	0.41
1:A:376:LEU:HD23	1:A:376:LEU:HA	1.81	0.41
2:B:242:ARG:NH2	7:B:307:P1O:C4	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:251:PHE:CZ	2:F:226:LEU:HD11	2.50	0.41
1:I:145:GLN:HB3	10:I:679:HOH:O	2.21	0.41
1:I:211:ILE:O	1:I:215:ARG:HD3	2.21	0.41
1:I:215:ARG:NH1	1:I:227:LEU:HB3	2.35	0.41
5:I:503:D10:H101	6:G:308:PLC:H62	2.03	0.41
2:J:216:SER:HA	3:G:229:TRP:CD1	2.56	0.41
7:F:302:P1O:H15	7:F:302:P1O:C20	2.47	0.41
7:F:302:P1O:H17	7:F:302:P1O:C20	2.51	0.41
3:G:137:TRP:HZ2	7:G:311:P1O:H19	1.86	0.41
6:G:307:PLC:H31	6:G:307:PLC:H1A2	1.81	0.41
6:G:307:PLC:HTA1	6:G:308:PLC:H5A1	2.03	0.41
3:K:127:GLU:OE1	3:K:200:PRO:HG3	2.21	0.41
3:K:181:TYR:HB2	3:K:182:PRO:HD3	2.03	0.41
3:K:275:GLY:HA3	3:K:276:GLN:CD	2.45	0.41
1:A:371:TRP:CD1	1:A:377:SER:HB3	2.56	0.41
7:B:307:P1O:H15	7:B:307:P1O:C20	2.47	0.41
3:C:137:TRP:HZ2	7:C:309:P1O:H19	1.86	0.41
3:C:278:LEU:N	3:C:278:LEU:HD23	2.35	0.41
1:I:83:GLU:O	1:I:85:ASP:N	2.47	0.41
1:I:115:ARG:HD2	1:I:270:ARG:HG2	2.03	0.41
2:J:242:ARG:NH2	7:J:308:P1O:H8	2.35	0.41
2:J:242:ARG:NH2	7:J:308:P1O:C4	2.84	0.41
2:F:103:ASN:HB3	3:G:154:GLU:OE1	2.20	0.41
3:K:216:GLY:HA3	3:K:254:LEU:CB	2.50	0.41
3:K:244:LEU:HD22	3:K:244:LEU:H	1.86	0.41
1:A:121:THR:HG21	1:A:277:LEU:HD11	2.03	0.40
1:A:310:SER:HA	1:A:311:PRO:HD3	1.96	0.40
1:I:155:LYS:NZ	1:I:335:GLY:O	2.42	0.40
1:I:296:ARG:NH1	1:I:369:ALA:HB2	2.36	0.40
6:F:301:PLC:H31	6:F:301:PLC:H1A2	1.81	0.40
2:B:247:THR:CG2	7:C:310:P1O:C10	2.99	0.40
3:C:245:HIS:O	3:C:248:PHE:HD1	2.03	0.40
1:E:87:ALA:O	1:E:114:VAL:N	2.31	0.40
1:E:170:VAL:CG1	1:E:180:LEU:HG	2.50	0.40
1:E:234:LYS:HA	1:E:237:MET:HE2	2.04	0.40
2:J:161:TRP:CZ2	6:J:307:PLC:H72	2.50	0.40
7:F:302:P1O:C20	7:F:302:P1O:C6	2.99	0.40
1:A:170:VAL:CG1	1:A:180:LEU:HG	2.50	0.40
2:B:23:TRP:HA	2:B:23:TRP:CE3	2.56	0.40
3:C:216:GLY:CA	3:C:254:LEU:HD12	2.49	0.40
3:C:229:TRP:HB2	2:F:219:PHE:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:244:LEU:HD22	3:C:244:LEU:H	1.86	0.40
2:J:93:VAL:HG21	2:J:128:ALA:HB2	2.03	0.40
7:J:308:P1O:H17	7:J:308:P1O:C20	2.51	0.40
2:F:133:THR:O	2:F:137:LEU:N	2.53	0.40
3:G:274:LEU:C	3:G:274:LEU:CD1	2.86	0.40
3:K:270:ALA:HA	3:K:274:LEU:CB	2.51	0.40
1:A:215:ARG:CZ	1:A:227:LEU:HB3	2.52	0.40
2:B:177:LEU:HD23	1:I:385:SER:HB2	2.04	0.40
2:B:244:LEU:CD1	3:C:206:ILE:HG22	2.44	0.40
1:E:215:ARG:CZ	1:E:227:LEU:HB3	2.52	0.40
1:I:171:THR:O	2:J:171:VAL:HG13	2.21	0.40
2:J:23:TRP:CE3	2:J:23:TRP:HA	2.56	0.40
3:G:156:ASP:C	3:G:156:ASP:OD1	2.61	0.40
3:G:270:ALA:HA	3:G:274:LEU:CB	2.51	0.40
3:K:156:ASP:C	3:K:156:ASP:OD1	2.61	0.40
3:K:175:ILE:O	3:K:179:LEU:HB3	2.22	0.40
1:A:96:PRO:HD2	10:A:631:HOH:O	2.22	0.40
10:B:401:HOH:O	3:C:263:THR:HG21	2.21	0.40
1:E:171:THR:O	2:F:171:VAL:HG13	2.22	0.40
1:E:296:ARG:NH1	1:E:369:ALA:HB2	2.36	0.40
2:J:59:LEU:HD11	6:G:304:PLC:C3	2.51	0.40
2:F:23:TRP:HA	2:F:23:TRP:CE3	2.57	0.40
2:F:69:VAL:HG13	2:F:152:TRP:NE1	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 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 EM 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	380/414 (92%)	355 (93%)	23 (6%)	2 (0%)	24 27
1	E	380/414 (92%)	355 (93%)	23 (6%)	2 (0%)	24 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	380/414 (92%)	355 (93%)	23 (6%)	2 (0%)	24	27
2	B	239/247 (97%)	221 (92%)	17 (7%)	1 (0%)	30	34
2	F	239/247 (97%)	221 (92%)	17 (7%)	1 (0%)	30	34
2	J	239/247 (97%)	223 (93%)	15 (6%)	1 (0%)	30	34
3	C	234/260 (90%)	192 (82%)	34 (14%)	8 (3%)	3	1
3	G	234/260 (90%)	192 (82%)	34 (14%)	8 (3%)	3	1
3	K	234/260 (90%)	192 (82%)	34 (14%)	8 (3%)	3	1
All	All	2559/2763 (93%)	2306 (90%)	220 (9%)	33 (1%)	12	8

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	235	PHE
3	C	244	LEU
3	C	277	SER
3	G	235	PHE
3	G	244	LEU
3	G	277	SER
3	K	235	PHE
3	K	244	LEU
3	K	277	SER
3	C	157	GLY
3	G	157	GLY
3	K	157	GLY
3	C	237	GLU
3	G	237	GLU
3	K	237	GLU
3	C	77	GLY
3	G	77	GLY
3	K	77	GLY
1	A	224	ALA
1	A	288	ASP
2	B	9	ARG
3	C	231	HIS
1	E	224	ALA
1	E	288	ASP
1	I	224	ALA
1	I	288	ASP
2	J	9	ARG
2	F	9	ARG

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Mol	Chain	Res	Type
3	G	231	HIS
3	K	231	HIS
3	C	174	ILE
3	G	174	ILE
3	K	174	ILE

5.3.2 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 EM 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	323/345 (94%)	297 (92%)	26 (8%)	11	12
1	E	323/345 (94%)	297 (92%)	26 (8%)	11	12
1	I	323/345 (94%)	296 (92%)	27 (8%)	10	11
2	B	206/210 (98%)	187 (91%)	19 (9%)	8	9
2	F	206/210 (98%)	187 (91%)	19 (9%)	8	9
2	J	206/210 (98%)	186 (90%)	20 (10%)	8	7
3	C	200/212 (94%)	149 (74%)	51 (26%)	0	0
3	G	200/212 (94%)	149 (74%)	51 (26%)	0	0
3	K	200/212 (94%)	149 (74%)	51 (26%)	0	0
All	All	2187/2301 (95%)	1897 (87%)	290 (13%)	6	3

All (290) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	46	THR
1	A	64	THR
1	A	79	GLU
1	A	80	THR
1	A	101	LYS
1	A	105	ILE
1	A	108	GLN
1	A	112	ARG

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Mol	Chain	Res	Type
1	A	137	HIS
1	A	170	VAL
1	A	180	LEU
1	A	226	GLU
1	A	227	LEU
1	A	234	LYS
1	A	272	MET
1	A	273	LYS
1	A	275	LEU
1	A	276	GLU
1	A	281	THR
1	A	288	ASP
1	A	316	GLU
1	A	319	THR
1	A	376	LEU
1	A	378	ASP
1	A	380	ILE
2	B	8	VAL
2	B	13	GLU
2	B	16	GLN
2	B	29	VAL
2	B	39	ILE
2	B	45	MET
2	B	68	LEU
2	B	93	VAL
2	B	104	ARG
2	B	124	LEU
2	B	131	LEU
2	B	135	LEU
2	B	136	MET
2	B	138	SER
2	B	176	MET
2	B	180	ILE
2	B	206	ARG
2	B	208	PHE
2	B	244	LEU
3	C	45	LEU
3	C	46	LEU
3	C	48	LYS
3	C	49	LYS
3	C	51	LEU
3	C	52	THR

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Mol	Chain	Res	Type
3	C	57	ILE
3	C	63	LEU
3	C	71	VAL
3	C	74	TRP
3	C	78	LEU
3	C	80	SER
3	C	86	GLU
3	C	87	THR
3	C	90	MET
3	C	113	LYS
3	C	115	ARG
3	C	119	LEU
3	C	123	THR
3	C	126	GLU
3	C	129	ARG
3	C	154	GLU
3	C	155	GLN
3	C	158	THR
3	C	159	TRP
3	C	161	GLN
3	C	165	ARG
3	C	196	LYS
3	C	201	PHE
3	C	202	PHE
3	C	204	LYS
3	C	213	LEU
3	C	214	VAL
3	C	218	PHE
3	C	220	ILE
3	C	221	LEU
3	C	223	ASN
3	C	227	ASN
3	C	236	MET
3	C	237	GLU
3	C	238	GLU
3	C	240	PHE
3	C	244	LEU
3	C	245	HIS
3	C	265	THR
3	C	269	PHE
3	C	271	GLN
3	C	274	LEU

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Mol	Chain	Res	Type
3	C	276	GLN
3	C	278	LEU
3	C	280	GLU
1	E	33	HIS
1	E	46	THR
1	E	64	THR
1	E	79	GLU
1	E	80	THR
1	E	101	LYS
1	E	105	ILE
1	E	108	GLN
1	E	112	ARG
1	E	137	HIS
1	E	170	VAL
1	E	180	LEU
1	E	226	GLU
1	E	227	LEU
1	E	234	LYS
1	E	272	MET
1	E	273	LYS
1	E	275	LEU
1	E	276	GLU
1	E	281	THR
1	E	288	ASP
1	E	316	GLU
1	E	319	THR
1	E	376	LEU
1	E	378	ASP
1	E	380	ILE
1	I	33	HIS
1	I	46	THR
1	I	64	THR
1	I	79	GLU
1	I	80	THR
1	I	101	LYS
1	I	105	ILE
1	I	108	GLN
1	I	112	ARG
1	I	137	HIS
1	I	170	VAL
1	I	180	LEU
1	I	226	GLU

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Mol	Chain	Res	Type
1	I	227	LEU
1	I	234	LYS
1	I	272	MET
1	I	273	LYS
1	I	275	LEU
1	I	276	GLU
1	I	281	THR
1	I	288	ASP
1	I	316	GLU
1	I	319	THR
1	I	359	THR
1	I	376	LEU
1	I	378	ASP
1	I	380	ILE
2	J	8	VAL
2	J	13	GLU
2	J	16	GLN
2	J	29	VAL
2	J	39	ILE
2	J	45	MET
2	J	68	LEU
2	J	93	VAL
2	J	104	ARG
2	J	124	LEU
2	J	131	LEU
2	J	135	LEU
2	J	136	MET
2	J	138	SER
2	J	176	MET
2	J	180	ILE
2	J	206	ARG
2	J	208	PHE
2	J	244	LEU
2	J	245	GLN
2	F	8	VAL
2	F	13	GLU
2	F	16	GLN
2	F	29	VAL
2	F	39	ILE
2	F	45	MET
2	F	68	LEU
2	F	93	VAL

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Mol	Chain	Res	Type
2	F	104	ARG
2	F	124	LEU
2	F	131	LEU
2	F	135	LEU
2	F	136	MET
2	F	138	SER
2	F	176	MET
2	F	180	ILE
2	F	206	ARG
2	F	208	PHE
2	F	244	LEU
3	G	45	LEU
3	G	46	LEU
3	G	48	LYS
3	G	49	LYS
3	G	51	LEU
3	G	52	THR
3	G	57	ILE
3	G	63	LEU
3	G	71	VAL
3	G	74	TRP
3	G	78	LEU
3	G	80	SER
3	G	86	GLU
3	G	87	THR
3	G	90	MET
3	G	113	LYS
3	G	115	ARG
3	G	119	LEU
3	G	123	THR
3	G	126	GLU
3	G	129	ARG
3	G	154	GLU
3	G	155	GLN
3	G	158	THR
3	G	159	TRP
3	G	161	GLN
3	G	165	ARG
3	G	196	LYS
3	G	201	PHE
3	G	202	PHE
3	G	204	LYS

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Mol	Chain	Res	Type
3	G	213	LEU
3	G	214	VAL
3	G	218	PHE
3	G	220	ILE
3	G	221	LEU
3	G	223	ASN
3	G	227	ASN
3	G	236	MET
3	G	237	GLU
3	G	238	GLU
3	G	240	PHE
3	G	244	LEU
3	G	245	HIS
3	G	265	THR
3	G	269	PHE
3	G	271	GLN
3	G	274	LEU
3	G	276	GLN
3	G	278	LEU
3	G	280	GLU
3	K	45	LEU
3	K	46	LEU
3	K	48	LYS
3	K	49	LYS
3	K	51	LEU
3	K	52	THR
3	K	57	ILE
3	K	63	LEU
3	K	71	VAL
3	K	74	TRP
3	K	78	LEU
3	K	80	SER
3	K	86	GLU
3	K	87	THR
3	K	90	MET
3	K	113	LYS
3	K	115	ARG
3	K	119	LEU
3	K	123	THR
3	K	126	GLU
3	K	129	ARG
3	K	154	GLU

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Mol	Chain	Res	Type
3	K	155	GLN
3	K	158	THR
3	K	159	TRP
3	K	161	GLN
3	K	165	ARG
3	K	196	LYS
3	K	201	PHE
3	K	202	PHE
3	K	204	LYS
3	K	213	LEU
3	K	214	VAL
3	K	218	PHE
3	K	220	ILE
3	K	221	LEU
3	K	223	ASN
3	K	227	ASN
3	K	236	MET
3	K	237	GLU
3	K	238	GLU
3	K	240	PHE
3	K	244	LEU
3	K	245	HIS
3	K	265	THR
3	K	269	PHE
3	K	271	GLN
3	K	274	LEU
3	K	276	GLN
3	K	278	LEU
3	K	280	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	A	168	ASN
2	B	16	GLN
2	B	174	ASN
2	B	187	ASN
3	C	160	HIS
3	C	227	ASN
3	C	245	HIS
1	E	143	ASN

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Mol	Chain	Res	Type
1	E	168	ASN
1	I	143	ASN
1	I	168	ASN
2	J	16	GLN
2	J	174	ASN
2	J	187	ASN
2	F	174	ASN
2	F	187	ASN
3	G	160	HIS
3	G	227	ASN
3	G	245	HIS
3	G	276	GLN
3	K	160	HIS
3	K	227	ASN
3	K	245	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 66 ligands modelled in this entry, 12 are monoatomic - leaving 54 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PLC	C	311	-	41,41,41	1.05	2 (4%)	47,49,49	1.05	4 (8%)
6	PLC	G	307	-	41,41,41	1.07	2 (4%)	47,49,49	1.08	3 (6%)
6	PLC	C	308	-	41,41,41	1.06	2 (4%)	47,49,49	1.09	3 (6%)
5	D10	F	307	-	9,9,9	0.22	0	8,8,8	0.56	0
6	PLC	K	309	-	41,41,41	1.06	2 (4%)	47,49,49	1.09	3 (6%)
7	P1O	J	301	-	37,37,37	1.12	2 (5%)	43,45,45	1.12	3 (6%)
5	D10	F	305	-	9,9,9	0.20	0	8,8,8	0.57	0
7	P1O	G	312	-	37,37,37	1.12	2 (5%)	43,45,45	1.13	3 (6%)
7	P1O	C	310	-	37,37,37	1.12	2 (5%)	43,45,45	1.13	3 (6%)
5	D10	I	503	-	9,9,9	0.21	0	8,8,8	0.56	0
5	D10	E	503	-	9,9,9	0.20	0	8,8,8	0.56	0
5	D10	B	306	-	9,9,9	0.20	0	8,8,8	0.56	0
9	HXG	C	304	-	29,29,29	0.35	0	35,37,37	0.36	0
5	D10	B	305	-	9,9,9	0.22	0	8,8,8	0.56	0
5	D10	J	303	-	9,9,9	0.20	0	8,8,8	0.55	0
7	P1O	K	311	-	37,37,37	1.11	2 (5%)	43,45,45	1.13	3 (6%)
5	D10	B	304	-	9,9,9	0.21	0	8,8,8	0.56	0
5	D10	J	304	-	9,9,9	0.21	0	8,8,8	0.55	0
5	D10	G	306	-	9,9,9	0.20	0	8,8,8	0.56	0
5	D10	F	308	-	9,9,9	0.20	0	8,8,8	0.56	0
6	PLC	F	301	-	41,41,41	1.07	2 (4%)	47,49,49	1.08	3 (6%)
6	PLC	B	301	-	41,41,41	1.06	2 (4%)	47,49,49	1.14	3 (6%)
7	P1O	F	302	-	37,37,37	1.12	2 (5%)	43,45,45	1.10	3 (6%)
5	D10	J	305	-	9,9,9	0.21	0	8,8,8	0.57	0
9	HXG	K	308	-	29,29,29	0.34	0	35,37,37	0.37	0
7	P1O	C	309	-	37,37,37	1.11	2 (5%)	43,45,45	1.13	4 (9%)
7	P1O	B	307	-	37,37,37	1.12	2 (5%)	43,45,45	1.10	3 (6%)
6	PLC	J	306	-	41,41,41	1.05	2 (4%)	47,49,49	1.05	3 (6%)
6	PLC	C	303	-	41,41,41	1.06	2 (4%)	47,49,49	1.10	4 (8%)
6	PLC	K	303	-	41,41,41	1.06	2 (4%)	47,49,49	1.10	4 (8%)
9	HXG	G	309	-	29,29,29	0.35	0	35,37,37	0.36	0
6	PLC	K	306	-	41,41,41	1.07	2 (4%)	47,49,49	1.08	3 (6%)
9	HXG	G	305	-	29,29,29	0.35	0	35,37,37	0.36	0
9	HXG	K	304	-	29,29,29	0.35	0	35,37,37	0.36	0
6	PLC	G	301	-	41,41,41	1.05	2 (4%)	47,49,49	1.05	4 (8%)
5	D10	C	305	-	9,9,9	0.20	0	8,8,8	0.56	0
5	D10	A	503	-	9,9,9	0.20	0	8,8,8	0.56	0
6	PLC	G	308	-	41,41,41	1.06	2 (4%)	47,49,49	1.08	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	D10	K	305	-	9,9,9	0.21	0	8,8,8	0.56	0
6	PLC	F	303	-	41,41,41	1.06	2 (4%)	47,49,49	1.14	3 (6%)
6	PLC	C	306	-	41,41,41	1.06	2 (4%)	47,49,49	1.08	3 (6%)
5	D10	F	306	-	9,9,9	0.21	0	8,8,8	0.56	0
7	P1O	J	308	-	37,37,37	1.12	2 (5%)	43,45,45	1.10	3 (6%)
5	D10	J	302	-	9,9,9	0.20	0	8,8,8	0.56	0
6	PLC	K	307	-	41,41,41	1.06	2 (4%)	47,49,49	1.08	3 (6%)
7	P1O	F	304	-	37,37,37	1.12	2 (5%)	43,45,45	1.12	4 (9%)
6	PLC	G	304	-	41,41,41	1.05	2 (4%)	47,49,49	1.10	4 (8%)
7	P1O	K	310	-	37,37,37	1.11	2 (5%)	43,45,45	1.13	4 (9%)
7	P1O	B	302	-	37,37,37	1.12	2 (5%)	43,45,45	1.12	3 (6%)
6	PLC	J	307	-	41,41,41	1.06	2 (4%)	47,49,49	1.14	3 (6%)
7	P1O	G	311	-	37,37,37	1.11	2 (5%)	43,45,45	1.14	4 (9%)
9	HXG	C	307	-	29,29,29	0.34	0	35,37,37	0.36	0
6	PLC	G	310	-	41,41,41	1.06	2 (4%)	47,49,49	1.09	3 (6%)
5	D10	B	303	-	9,9,9	0.20	0	8,8,8	0.56	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
6	PLC	C	311	-	-	25/45/45/45	-
6	PLC	G	307	-	-	23/45/45/45	-
6	PLC	C	308	-	-	27/45/45/45	-
5	D10	F	307	-	-	6/7/7/7	-
6	PLC	K	309	-	-	27/45/45/45	-
7	P1O	J	301	-	-	26/41/41/41	-
5	D10	F	305	-	-	0/7/7/7	-
7	P1O	G	312	-	-	26/41/41/41	-
7	P1O	C	310	-	-	26/41/41/41	-
5	D10	I	503	-	-	0/7/7/7	-
5	D10	E	503	-	-	0/7/7/7	-
5	D10	B	306	-	-	5/7/7/7	-
9	HXG	C	304	-	-	9/33/33/33	-
5	D10	B	305	-	-	6/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	D10	J	303	-	-	2/7/7/7	-
7	P1O	K	311	-	-	26/41/41/41	-
5	D10	B	304	-	-	2/7/7/7	-
5	D10	J	304	-	-	6/7/7/7	-
5	D10	G	306	-	-	0/7/7/7	-
5	D10	F	308	-	-	5/7/7/7	-
6	PLC	F	301	-	-	23/45/45/45	-
6	PLC	B	301	-	-	26/45/45/45	-
7	P1O	F	302	-	-	20/41/41/41	-
5	D10	J	305	-	-	5/7/7/7	-
9	HXG	K	308	-	-	7/33/33/33	-
7	P1O	C	309	-	-	19/41/41/41	-
7	P1O	B	307	-	-	20/41/41/41	-
6	PLC	J	306	-	-	25/45/45/45	-
6	PLC	C	303	-	-	22/45/45/45	-
6	PLC	K	303	-	-	22/45/45/45	-
9	HXG	G	309	-	-	7/33/33/33	-
6	PLC	K	306	-	-	23/45/45/45	-
9	HXG	G	305	-	-	9/33/33/33	-
9	HXG	K	304	-	-	9/33/33/33	-
6	PLC	G	301	-	-	25/45/45/45	-
5	D10	C	305	-	-	0/7/7/7	-
5	D10	A	503	-	-	0/7/7/7	-
6	PLC	G	308	-	-	30/45/45/45	-
5	D10	K	305	-	-	0/7/7/7	-
6	PLC	F	303	-	-	27/45/45/45	-
6	PLC	C	306	-	-	30/45/45/45	-
5	D10	F	306	-	-	2/7/7/7	-
7	P1O	J	308	-	-	20/41/41/41	-
5	D10	J	302	-	-	0/7/7/7	-
6	PLC	K	307	-	-	30/45/45/45	-
7	P1O	F	304	-	-	26/41/41/41	-
6	PLC	G	304	-	-	22/45/45/45	-
7	P1O	K	310	-	-	19/41/41/41	-
7	P1O	B	302	-	-	26/41/41/41	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PLC	J	307	-	-	26/45/45/45	-
7	P1O	G	311	-	-	19/41/41/41	-
9	HXG	C	307	-	-	7/33/33/33	-
6	PLC	G	310	-	-	27/45/45/45	-
5	D10	B	303	-	-	0/7/7/7	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	307	PLC	O3-CB	4.31	1.45	1.33
6	G	308	PLC	O3-CB	4.31	1.45	1.33
7	J	301	P1O	O5-C9	4.30	1.45	1.33
6	C	306	PLC	O3-CB	4.29	1.45	1.33
6	F	301	PLC	O3-CB	4.29	1.45	1.33
6	J	307	PLC	O3-CB	4.28	1.45	1.33
6	K	306	PLC	O3-CB	4.28	1.45	1.33
6	G	307	PLC	O3-CB	4.28	1.45	1.33
6	F	303	PLC	O3-CB	4.28	1.45	1.33
7	F	304	P1O	O5-C9	4.28	1.45	1.33
6	K	303	PLC	O3-CB	4.27	1.45	1.33
6	B	301	PLC	O3-CB	4.27	1.45	1.33
7	K	310	P1O	O5-C9	4.27	1.45	1.33
7	C	309	P1O	O5-C9	4.27	1.45	1.33
7	B	302	P1O	O5-C9	4.27	1.45	1.33
6	J	306	PLC	O3-CB	4.27	1.45	1.33
6	G	301	PLC	O3-CB	4.26	1.45	1.33
7	F	302	P1O	O5-C9	4.26	1.45	1.33
7	G	312	P1O	O5-C9	4.26	1.45	1.33
6	C	303	PLC	O3-CB	4.25	1.45	1.33
7	J	308	P1O	O5-C9	4.25	1.45	1.33
7	G	311	P1O	O5-C9	4.25	1.45	1.33
7	K	311	P1O	O5-C9	4.25	1.45	1.33
7	B	307	P1O	O5-C9	4.25	1.45	1.33
7	C	310	P1O	O5-C9	4.25	1.45	1.33
6	C	308	PLC	O3-CB	4.25	1.45	1.33
6	G	310	PLC	O3-CB	4.24	1.45	1.33
6	G	304	PLC	O3-CB	4.24	1.45	1.33
6	C	311	PLC	O3-CB	4.24	1.45	1.33
6	K	309	PLC	O3-CB	4.24	1.45	1.33
7	B	307	P1O	O7-C19	4.19	1.46	1.34
7	J	308	P1O	O7-C19	4.17	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	307	PLC	O2-C'	4.16	1.46	1.34
7	F	302	P1O	O7-C19	4.15	1.46	1.34
6	F	301	PLC	O2-C'	4.14	1.46	1.34
6	G	310	PLC	O2-C'	4.13	1.46	1.34
6	K	306	PLC	O2-C'	4.12	1.45	1.34
7	G	312	P1O	O7-C19	4.12	1.45	1.34
7	C	310	P1O	O7-C19	4.12	1.45	1.34
6	J	307	PLC	O2-C'	4.12	1.45	1.34
6	C	311	PLC	O2-C'	4.12	1.45	1.34
6	C	308	PLC	O2-C'	4.10	1.45	1.34
6	B	301	PLC	O2-C'	4.10	1.45	1.34
7	J	301	P1O	O7-C19	4.10	1.45	1.34
6	K	309	PLC	O2-C'	4.10	1.45	1.34
6	G	301	PLC	O2-C'	4.09	1.45	1.34
7	B	302	P1O	O7-C19	4.08	1.45	1.34
7	F	304	P1O	O7-C19	4.08	1.45	1.34
6	F	303	PLC	O2-C'	4.08	1.45	1.34
7	G	311	P1O	O7-C19	4.08	1.45	1.34
7	K	311	P1O	O7-C19	4.08	1.45	1.34
6	J	306	PLC	O2-C'	4.07	1.45	1.34
6	K	307	PLC	O2-C'	4.06	1.45	1.34
6	K	303	PLC	O2-C'	4.06	1.45	1.34
6	C	306	PLC	O2-C'	4.06	1.45	1.34
6	G	308	PLC	O2-C'	4.06	1.45	1.34
6	C	303	PLC	O2-C'	4.06	1.45	1.34
7	C	309	P1O	O7-C19	4.05	1.45	1.34
6	G	304	PLC	O2-C'	4.04	1.45	1.34
7	K	310	P1O	O7-C19	4.02	1.45	1.34

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	308	P1O	O7-C19-C20	4.24	120.65	111.48
7	B	307	P1O	O7-C19-C20	4.23	120.62	111.48
7	F	302	P1O	O7-C19-C20	4.20	120.57	111.48
7	K	311	P1O	O7-C19-C20	4.18	120.53	111.48
7	K	310	P1O	O7-C19-C20	4.18	120.52	111.48
7	C	310	P1O	O7-C19-C20	4.17	120.50	111.48
7	C	309	P1O	O7-C19-C20	4.16	120.48	111.48
7	G	312	P1O	O7-C19-C20	4.16	120.48	111.48
7	G	311	P1O	O7-C19-C20	4.15	120.47	111.48
7	F	304	P1O	O7-C19-C20	4.15	120.46	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	302	P1O	O7-C19-C20	4.13	120.42	111.48
6	G	304	PLC	O2-C'-C1'	4.12	120.40	111.48
6	K	303	PLC	O2-C'-C1'	4.12	120.40	111.48
7	J	301	P1O	O7-C19-C20	4.12	120.39	111.48
6	C	303	PLC	O2-C'-C1'	4.11	120.38	111.48
6	K	309	PLC	O2-C'-C1'	4.11	120.37	111.48
6	C	308	PLC	O2-C'-C1'	4.10	120.35	111.48
6	K	306	PLC	O2-C'-C1'	4.08	120.30	111.48
6	G	310	PLC	O2-C'-C1'	4.08	120.30	111.48
6	J	306	PLC	O2-C'-C1'	4.08	120.30	111.48
6	G	301	PLC	O2-C'-C1'	4.07	120.29	111.48
6	C	311	PLC	O2-C'-C1'	4.07	120.28	111.48
6	F	301	PLC	O2-C'-C1'	4.07	120.28	111.48
6	K	307	PLC	O2-C'-C1'	4.04	120.23	111.48
6	G	307	PLC	O2-C'-C1'	4.04	120.22	111.48
6	G	308	PLC	O2-C'-C1'	4.04	120.21	111.48
6	C	306	PLC	O2-C'-C1'	4.03	120.20	111.48
6	F	303	PLC	O2-C'-C1'	3.97	120.06	111.48
6	B	301	PLC	O2-C'-C1'	3.96	120.05	111.48
6	J	307	PLC	O2-C'-C1'	3.96	120.05	111.48
6	F	303	PLC	CB'-CA'-C9'	3.15	134.65	113.36
6	B	301	PLC	CB'-CA'-C9'	3.15	134.60	113.36
6	J	307	PLC	CB'-CA'-C9'	3.13	134.51	113.36
6	G	304	PLC	O3-CB-C1B	2.83	120.47	111.83
6	C	303	PLC	O3-CB-C1B	2.83	120.46	111.83
6	K	303	PLC	O3-CB-C1B	2.83	120.45	111.83
6	G	310	PLC	O3-CB-C1B	2.82	120.45	111.83
6	C	308	PLC	O3-CB-C1B	2.81	120.42	111.83
6	K	306	PLC	O3-CB-C1B	2.81	120.39	111.83
7	F	304	P1O	O5-C9-C10	2.80	120.38	111.83
6	K	309	PLC	O3-CB-C1B	2.80	120.38	111.83
7	J	301	P1O	O5-C9-C10	2.80	120.37	111.83
6	G	307	PLC	O3-CB-C1B	2.80	120.37	111.83
6	F	301	PLC	O3-CB-C1B	2.80	120.37	111.83
6	F	303	PLC	O3-CB-C1B	2.80	120.36	111.83
7	J	308	P1O	O5-C9-C10	2.80	120.36	111.83
7	F	302	P1O	O5-C9-C10	2.80	120.36	111.83
7	B	302	P1O	O5-C9-C10	2.79	120.35	111.83
7	B	307	P1O	O5-C9-C10	2.79	120.35	111.83
6	B	301	PLC	O3-CB-C1B	2.79	120.34	111.83
7	G	311	P1O	O5-C9-C10	2.79	120.34	111.83
6	J	307	PLC	O3-CB-C1B	2.79	120.33	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	311	PLC	O3-CB-C1B	2.77	120.29	111.83
7	C	309	P1O	O5-C9-C10	2.77	120.28	111.83
6	G	301	PLC	O3-CB-C1B	2.77	120.28	111.83
7	K	310	P1O	O5-C9-C10	2.76	120.25	111.83
6	J	306	PLC	O3-CB-C1B	2.76	120.25	111.83
7	K	311	P1O	O5-C9-C10	2.69	120.05	111.83
7	C	310	P1O	O5-C9-C10	2.69	120.05	111.83
7	G	312	P1O	O5-C9-C10	2.69	120.03	111.83
6	G	308	PLC	O3-CB-C1B	2.68	120.00	111.83
6	C	306	PLC	O3-CB-C1B	2.67	119.98	111.83
6	K	307	PLC	O3-CB-C1B	2.65	119.93	111.83
7	G	312	P1O	C7-O7-C19	-2.45	111.94	117.80
7	C	310	P1O	C7-O7-C19	-2.45	111.94	117.80
7	K	311	P1O	C7-O7-C19	-2.44	111.96	117.80
6	K	307	PLC	C2-O2-C'	-2.43	111.98	117.80
6	C	303	PLC	C2-O2-C'	-2.43	111.99	117.80
6	K	303	PLC	C2-O2-C'	-2.42	112.00	117.80
6	G	304	PLC	C2-O2-C'	-2.42	112.01	117.80
6	G	308	PLC	C2-O2-C'	-2.42	112.01	117.80
6	C	306	PLC	C2-O2-C'	-2.41	112.03	117.80
7	J	301	P1O	C7-O7-C19	-2.40	112.06	117.80
7	B	302	P1O	C7-O7-C19	-2.38	112.10	117.80
7	F	304	P1O	C7-O7-C19	-2.36	112.15	117.80
7	G	311	P1O	C7-O7-C19	-2.31	112.26	117.80
7	C	309	P1O	C7-O7-C19	-2.31	112.26	117.80
7	K	310	P1O	C7-O7-C19	-2.30	112.28	117.80
6	G	310	PLC	C2-O2-C'	-2.21	112.50	117.80
6	K	309	PLC	C2-O2-C'	-2.21	112.50	117.80
6	C	308	PLC	C2-O2-C'	-2.21	112.51	117.80
6	J	306	PLC	C2-O2-C'	-2.16	112.62	117.80
6	C	311	PLC	C2-O2-C'	-2.16	112.62	117.80
6	G	301	PLC	C2-O2-C'	-2.16	112.63	117.80
7	J	308	P1O	O7-C19-O8	-2.09	118.83	123.70
7	B	307	P1O	O7-C19-O8	-2.08	118.84	123.70
6	F	301	PLC	C2-O2-C'	-2.08	112.82	117.80
6	K	306	PLC	C2-O2-C'	-2.08	112.83	117.80
6	G	307	PLC	C2-O2-C'	-2.07	112.84	117.80
7	F	302	P1O	O7-C19-O8	-2.06	118.89	123.70
7	F	304	P1O	O7-C19-O8	-2.03	118.95	123.70
6	G	304	PLC	O2-C'-O'	-2.03	118.96	123.70
7	K	310	P1O	C1-C2-N1	-2.01	109.36	115.82
6	C	311	PLC	O2-C'-O'	-2.01	119.00	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	303	PLC	O2-C'-O'	-2.01	119.00	123.70
6	C	303	PLC	O2-C'-O'	-2.01	119.00	123.70
7	G	311	P1O	C1-C2-N1	-2.01	109.37	115.82
7	C	309	P1O	C1-C2-N1	-2.01	109.38	115.82
6	G	301	PLC	O2-C'-O'	-2.01	119.02	123.70

There are no chirality outliers.

All (820) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	301	PLC	C4-O4P-P-O2P
6	B	301	PLC	C4-O4P-P-O3P
6	C	303	PLC	O4P-C4-C5-N
6	C	303	PLC	C1'-C'-O2-C2
6	C	303	PLC	C1B-CB-O3-C3
6	C	303	PLC	OB-CB-O3-C3
6	C	303	PLC	C1-O3P-P-O2P
6	C	303	PLC	C1-O3P-P-O4P
6	C	303	PLC	C4-O4P-P-O2P
6	C	303	PLC	C4-O4P-P-O3P
6	C	306	PLC	C1'-C'-O2-C2
6	C	306	PLC	C1B-CB-O3-C3
6	C	306	PLC	OB-CB-O3-C3
6	C	306	PLC	C1-O3P-P-O1P
6	C	306	PLC	C1-O3P-P-O2P
6	C	306	PLC	C1-O3P-P-O4P
6	C	306	PLC	C4-O4P-P-O1P
6	C	306	PLC	C4-O4P-P-O2P
6	C	308	PLC	C1'-C'-O2-C2
6	C	308	PLC	C1B-CB-O3-C3
6	C	308	PLC	OB-CB-O3-C3
6	C	308	PLC	C1-O3P-P-O1P
6	C	308	PLC	C1-O3P-P-O2P
6	C	308	PLC	C1-O3P-P-O4P
6	C	311	PLC	C1'-C'-O2-C2
6	J	306	PLC	C1'-C'-O2-C2
6	J	307	PLC	C4-O4P-P-O2P
6	J	307	PLC	C4-O4P-P-O3P
6	F	301	PLC	O4P-C4-C5-N
6	F	301	PLC	C1B-CB-O3-C3
6	F	301	PLC	OB-CB-O3-C3
6	F	301	PLC	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
6	F	301	PLC	C4-O4P-P-O1P
6	F	301	PLC	C4-O4P-P-O2P
6	F	301	PLC	C4-O4P-P-O3P
6	F	303	PLC	C4-O4P-P-O2P
6	F	303	PLC	C4-O4P-P-O3P
6	G	301	PLC	C1'-C'-O2-C2
6	G	304	PLC	O4P-C4-C5-N
6	G	304	PLC	C1'-C'-O2-C2
6	G	304	PLC	C1B-CB-O3-C3
6	G	304	PLC	OB-CB-O3-C3
6	G	304	PLC	C1-O3P-P-O2P
6	G	304	PLC	C1-O3P-P-O4P
6	G	304	PLC	C4-O4P-P-O2P
6	G	304	PLC	C4-O4P-P-O3P
6	G	307	PLC	O4P-C4-C5-N
6	G	307	PLC	C1B-CB-O3-C3
6	G	307	PLC	OB-CB-O3-C3
6	G	307	PLC	C1-O3P-P-O1P
6	G	307	PLC	C4-O4P-P-O1P
6	G	307	PLC	C4-O4P-P-O2P
6	G	307	PLC	C4-O4P-P-O3P
6	G	308	PLC	C1'-C'-O2-C2
6	G	308	PLC	C1B-CB-O3-C3
6	G	308	PLC	OB-CB-O3-C3
6	G	308	PLC	C1-O3P-P-O1P
6	G	308	PLC	C1-O3P-P-O2P
6	G	308	PLC	C1-O3P-P-O4P
6	G	308	PLC	C4-O4P-P-O1P
6	G	308	PLC	C4-O4P-P-O2P
6	G	310	PLC	C1'-C'-O2-C2
6	G	310	PLC	C1B-CB-O3-C3
6	G	310	PLC	OB-CB-O3-C3
6	G	310	PLC	C1-O3P-P-O1P
6	G	310	PLC	C1-O3P-P-O2P
6	G	310	PLC	C1-O3P-P-O4P
6	K	303	PLC	O4P-C4-C5-N
6	K	303	PLC	C1'-C'-O2-C2
6	K	303	PLC	C1B-CB-O3-C3
6	K	303	PLC	OB-CB-O3-C3
6	K	303	PLC	C1-O3P-P-O2P
6	K	303	PLC	C1-O3P-P-O4P
6	K	303	PLC	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
6	K	303	PLC	C4-O4P-P-O3P
6	K	306	PLC	O4P-C4-C5-N
6	K	306	PLC	C1B-CB-O3-C3
6	K	306	PLC	OB-CB-O3-C3
6	K	306	PLC	C1-O3P-P-O1P
6	K	306	PLC	C4-O4P-P-O1P
6	K	306	PLC	C4-O4P-P-O2P
6	K	306	PLC	C4-O4P-P-O3P
6	K	307	PLC	C1'-C'-O2-C2
6	K	307	PLC	C1B-CB-O3-C3
6	K	307	PLC	OB-CB-O3-C3
6	K	307	PLC	C1-O3P-P-O1P
6	K	307	PLC	C1-O3P-P-O2P
6	K	307	PLC	C1-O3P-P-O4P
6	K	307	PLC	C4-O4P-P-O1P
6	K	307	PLC	C4-O4P-P-O2P
6	K	309	PLC	C1'-C'-O2-C2
6	K	309	PLC	C1B-CB-O3-C3
6	K	309	PLC	OB-CB-O3-C3
6	K	309	PLC	C1-O3P-P-O1P
6	K	309	PLC	C1-O3P-P-O2P
6	K	309	PLC	C1-O3P-P-O4P
7	B	302	P1O	C1-O3-P1-O1
7	B	302	P1O	C1-O3-P1-O2
7	B	302	P1O	C1-O3-P1-O4
7	B	302	P1O	C6-O4-P1-O1
7	B	302	P1O	C6-O4-P1-O2
7	B	302	P1O	C6-O4-P1-O3
7	B	307	P1O	C6-O4-P1-O1
7	B	307	P1O	C6-O4-P1-O2
7	B	307	P1O	C6-O4-P1-O3
7	B	307	P1O	O8-C19-O7-C7
7	C	309	P1O	C1-O3-P1-O1
7	C	309	P1O	C1-O3-P1-O4
7	C	309	P1O	C6-O4-P1-O3
7	C	309	P1O	C2-C1-O3-P1
7	C	309	P1O	O3-C1-C2-N1
7	C	309	P1O	O6-C9-O5-C8
7	C	309	P1O	C10-C9-O5-C8
7	C	309	P1O	O8-C19-O7-C7
7	C	310	P1O	C1-O3-P1-O1
7	C	310	P1O	C1-O3-P1-O2

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Mol	Chain	Res	Type	Atoms
7	C	310	P1O	C6-O4-P1-O1
7	C	310	P1O	C6-O4-P1-O2
7	C	310	P1O	C6-O4-P1-O3
7	J	301	P1O	C1-O3-P1-O1
7	J	301	P1O	C1-O3-P1-O2
7	J	301	P1O	C1-O3-P1-O4
7	J	301	P1O	C6-O4-P1-O1
7	J	301	P1O	C6-O4-P1-O2
7	J	301	P1O	C6-O4-P1-O3
7	J	308	P1O	C6-O4-P1-O1
7	J	308	P1O	C6-O4-P1-O2
7	J	308	P1O	C6-O4-P1-O3
7	J	308	P1O	O8-C19-O7-C7
7	F	302	P1O	C6-O4-P1-O1
7	F	302	P1O	C6-O4-P1-O2
7	F	302	P1O	C6-O4-P1-O3
7	F	302	P1O	O8-C19-O7-C7
7	F	304	P1O	C1-O3-P1-O1
7	F	304	P1O	C1-O3-P1-O2
7	F	304	P1O	C1-O3-P1-O4
7	F	304	P1O	C6-O4-P1-O1
7	F	304	P1O	C6-O4-P1-O2
7	F	304	P1O	C6-O4-P1-O3
7	G	311	P1O	C1-O3-P1-O1
7	G	311	P1O	C1-O3-P1-O4
7	G	311	P1O	C6-O4-P1-O3
7	G	311	P1O	C2-C1-O3-P1
7	G	311	P1O	O3-C1-C2-N1
7	G	311	P1O	O6-C9-O5-C8
7	G	311	P1O	C10-C9-O5-C8
7	G	311	P1O	O8-C19-O7-C7
7	G	312	P1O	C1-O3-P1-O1
7	G	312	P1O	C1-O3-P1-O2
7	G	312	P1O	C6-O4-P1-O1
7	G	312	P1O	C6-O4-P1-O2
7	G	312	P1O	C6-O4-P1-O3
7	K	310	P1O	C1-O3-P1-O1
7	K	310	P1O	C1-O3-P1-O4
7	K	310	P1O	C6-O4-P1-O3
7	K	310	P1O	C2-C1-O3-P1
7	K	310	P1O	O3-C1-C2-N1
7	K	310	P1O	O6-C9-O5-C8

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Mol	Chain	Res	Type	Atoms
7	K	310	P1O	C10-C9-O5-C8
7	K	310	P1O	O8-C19-O7-C7
7	K	311	P1O	C1-O3-P1-O1
7	K	311	P1O	C1-O3-P1-O2
7	K	311	P1O	C6-O4-P1-O1
7	K	311	P1O	C6-O4-P1-O2
7	K	311	P1O	C6-O4-P1-O3
9	C	304	HXG	CAU-OAX-PBD-OAH
9	C	304	HXG	CAU-OAX-PBD-OAW
9	C	304	HXG	CAP-OAW-PBD-OAX
9	C	307	HXG	OAW-CAP-CAS-NBC
9	G	305	HXG	CAU-OAX-PBD-OAH
9	G	305	HXG	CAU-OAX-PBD-OAW
9	G	305	HXG	CAP-OAW-PBD-OAX
9	G	309	HXG	OAW-CAP-CAS-NBC
9	K	304	HXG	CAU-OAX-PBD-OAH
9	K	304	HXG	CAU-OAX-PBD-OAW
9	K	304	HXG	CAP-OAW-PBD-OAX
9	K	308	HXG	OAW-CAP-CAS-NBC
6	B	301	PLC	OB-CB-O3-C3
6	J	307	PLC	OB-CB-O3-C3
6	F	303	PLC	OB-CB-O3-C3
6	B	301	PLC	C1B-CB-O3-C3
6	J	307	PLC	C1B-CB-O3-C3
6	F	303	PLC	C1B-CB-O3-C3
7	B	302	P1O	C10-C9-O5-C8
7	J	301	P1O	C10-C9-O5-C8
7	F	304	P1O	C10-C9-O5-C8
7	B	302	P1O	O6-C9-O5-C8
7	J	301	P1O	O6-C9-O5-C8
7	F	304	P1O	O6-C9-O5-C8
6	C	303	PLC	O'-C'-O2-C2
6	C	306	PLC	O'-C'-O2-C2
6	C	308	PLC	O'-C'-O2-C2
6	C	311	PLC	O'-C'-O2-C2
6	J	306	PLC	O'-C'-O2-C2
6	G	301	PLC	O'-C'-O2-C2
6	G	304	PLC	O'-C'-O2-C2
6	G	308	PLC	O'-C'-O2-C2
6	G	310	PLC	O'-C'-O2-C2
6	K	303	PLC	O'-C'-O2-C2
6	K	307	PLC	O'-C'-O2-C2

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Mol	Chain	Res	Type	Atoms
6	K	309	PLC	O'-C'-O2-C2
7	B	307	P1O	C20-C19-O7-C7
7	C	309	P1O	C20-C19-O7-C7
7	J	308	P1O	C20-C19-O7-C7
7	F	302	P1O	C20-C19-O7-C7
7	G	311	P1O	C20-C19-O7-C7
7	K	310	P1O	C20-C19-O7-C7
6	J	306	PLC	C4-C5-N-C6
6	F	301	PLC	C1'-C'-O2-C2
6	G	307	PLC	C1'-C'-O2-C2
6	K	306	PLC	C1'-C'-O2-C2
6	C	311	PLC	C1B-CB-O3-C3
6	J	306	PLC	C1B-CB-O3-C3
6	G	301	PLC	C1B-CB-O3-C3
6	C	311	PLC	C4-C5-N-C6
6	G	301	PLC	C4-C5-N-C6
7	C	309	P1O	C9-C10-C11-C12
7	G	311	P1O	C9-C10-C11-C12
7	K	310	P1O	C9-C10-C11-C12
6	F	301	PLC	O'-C'-O2-C2
6	G	307	PLC	O'-C'-O2-C2
6	K	306	PLC	O'-C'-O2-C2
7	C	310	P1O	C10-C9-O5-C8
7	G	312	P1O	C10-C9-O5-C8
7	K	311	P1O	C10-C9-O5-C8
9	C	304	HXG	CAL-CAN-CAQ-CAZ
9	G	305	HXG	CAL-CAN-CAQ-CAZ
9	K	304	HXG	CAL-CAN-CAQ-CAZ
6	F	301	PLC	CB-C1B-C2B-C3B
6	G	307	PLC	CB-C1B-C2B-C3B
6	K	306	PLC	CB-C1B-C2B-C3B
6	C	311	PLC	OB-CB-O3-C3
7	C	310	P1O	C7-C6-O4-P1
7	G	312	P1O	C7-C6-O4-P1
7	K	311	P1O	C7-C6-O4-P1
6	C	308	PLC	C'-C1'-C2'-C3'
6	G	310	PLC	C'-C1'-C2'-C3'
6	K	309	PLC	C'-C1'-C2'-C3'
7	B	307	P1O	C19-C20-C21-C22
7	J	308	P1O	C19-C20-C21-C22
7	F	302	P1O	C19-C20-C21-C22
9	C	307	HXG	CAM-CAO-CAR-CBA

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Mol	Chain	Res	Type	Atoms
9	G	309	HXG	CAM-CAO-CAR-CBA
9	K	308	HXG	CAM-CAO-CAR-CBA
6	J	306	PLC	OB-CB-O3-C3
6	G	301	PLC	OB-CB-O3-C3
6	B	301	PLC	CB-C1B-C2B-C3B
6	J	307	PLC	CB-C1B-C2B-C3B
6	F	303	PLC	CB-C1B-C2B-C3B
6	C	311	PLC	C4-C5-N-C7
6	J	306	PLC	C4-C5-N-C7
6	G	301	PLC	C4-C5-N-C7
7	B	302	P1O	C20-C19-O7-C7
7	J	301	P1O	C20-C19-O7-C7
7	F	304	P1O	C20-C19-O7-C7
7	B	302	P1O	O8-C19-O7-C7
7	J	301	P1O	O8-C19-O7-C7
7	F	304	P1O	O8-C19-O7-C7
6	C	311	PLC	CB-C1B-C2B-C3B
6	G	301	PLC	CB-C1B-C2B-C3B
6	J	306	PLC	CB-C1B-C2B-C3B
7	C	310	P1O	O6-C9-O5-C8
7	G	312	P1O	O6-C9-O5-C8
7	K	311	P1O	O6-C9-O5-C8
6	B	301	PLC	C1'-C'-O2-C2
6	J	307	PLC	C1'-C'-O2-C2
6	F	303	PLC	C1'-C'-O2-C2
6	C	311	PLC	C4-C5-N-C8
6	J	306	PLC	C4-C5-N-C8
6	G	301	PLC	C4-C5-N-C8
6	C	311	PLC	C2B-C3B-C4B-C5B
6	J	306	PLC	C2B-C3B-C4B-C5B
6	G	301	PLC	C2B-C3B-C4B-C5B
7	C	309	P1O	C21-C22-C23-C24
7	C	310	P1O	C13-C14-C15-C16
7	G	311	P1O	C21-C22-C23-C24
7	G	312	P1O	C13-C14-C15-C16
7	K	310	P1O	C21-C22-C23-C24
7	K	311	P1O	C13-C14-C15-C16
6	C	306	PLC	C1B-C2B-C3B-C4B
6	C	306	PLC	C3B-C4B-C5B-C6B
6	G	308	PLC	C1B-C2B-C3B-C4B
6	G	308	PLC	C3B-C4B-C5B-C6B
6	K	307	PLC	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
6	K	307	PLC	C3B-C4B-C5B-C6B
7	F	304	P1O	C11-C12-C13-C14
7	B	302	P1O	C11-C12-C13-C14
7	J	301	P1O	C11-C12-C13-C14
6	C	303	PLC	C6B-C7B-C8B-C9B
6	G	304	PLC	C6B-C7B-C8B-C9B
6	B	301	PLC	O'-C'-O2-C2
6	J	307	PLC	O'-C'-O2-C2
6	F	303	PLC	O'-C'-O2-C2
6	K	303	PLC	C6B-C7B-C8B-C9B
6	B	301	PLC	C3B-C4B-C5B-C6B
6	J	307	PLC	C3B-C4B-C5B-C6B
6	F	303	PLC	C3B-C4B-C5B-C6B
6	B	301	PLC	C7'-C8'-C9'-CA'
6	J	307	PLC	C7'-C8'-C9'-CA'
6	F	303	PLC	C7'-C8'-C9'-CA'
9	C	304	HXG	CAR-CBA-OAY-CBB
9	G	305	HXG	CAR-CBA-OAY-CBB
9	K	304	HXG	CAR-CBA-OAY-CBB
7	B	307	P1O	C9-C10-C11-C12
7	J	308	P1O	C9-C10-C11-C12
6	C	308	PLC	C3'-C4'-C5'-C6'
6	C	311	PLC	C4B-C5B-C6B-C7B
6	G	301	PLC	C4B-C5B-C6B-C7B
6	G	310	PLC	C3'-C4'-C5'-C6'
6	K	309	PLC	C3'-C4'-C5'-C6'
7	B	307	P1O	C23-C24-C25-C26
7	J	308	P1O	C23-C24-C25-C26
7	F	302	P1O	C23-C24-C25-C26
6	J	306	PLC	C4B-C5B-C6B-C7B
6	G	307	PLC	C3B-C4B-C5B-C6B
6	K	306	PLC	C3B-C4B-C5B-C6B
6	C	311	PLC	C3B-C4B-C5B-C6B
6	J	306	PLC	C3B-C4B-C5B-C6B
6	F	301	PLC	C3B-C4B-C5B-C6B
6	G	301	PLC	C3B-C4B-C5B-C6B
6	G	310	PLC	C6B-C7B-C8B-C9B
5	B	305	D10	C5-C6-C7-C8
6	C	308	PLC	C2B-C3B-C4B-C5B
6	C	308	PLC	C6B-C7B-C8B-C9B
6	G	310	PLC	C2B-C3B-C4B-C5B
6	K	309	PLC	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
6	K	309	PLC	C6B-C7B-C8B-C9B
7	B	307	P1O	C14-C15-C16-C17
7	J	308	P1O	C14-C15-C16-C17
7	F	302	P1O	C14-C15-C16-C17
7	F	302	P1O	C9-C10-C11-C12
5	F	307	D10	C5-C6-C7-C8
5	J	304	D10	C5-C6-C7-C8
6	C	306	PLC	C1'-C2'-C3'-C4'
6	G	308	PLC	C1'-C2'-C3'-C4'
6	K	307	PLC	C1'-C2'-C3'-C4'
6	C	303	PLC	C1'-C2'-C3'-C4'
7	B	302	P1O	C21-C22-C23-C24
7	F	304	P1O	C21-C22-C23-C24
6	G	304	PLC	C1'-C2'-C3'-C4'
6	K	303	PLC	C1'-C2'-C3'-C4'
6	K	309	PLC	C6'-C7'-C8'-C9'
7	B	302	P1O	C13-C14-C15-C16
7	F	304	P1O	C13-C14-C15-C16
6	C	308	PLC	C6'-C7'-C8'-C9'
7	C	310	P1O	C24-C25-C26-C27
7	J	301	P1O	C13-C14-C15-C16
7	J	301	P1O	C21-C22-C23-C24
7	G	312	P1O	C24-C25-C26-C27
7	K	311	P1O	C24-C25-C26-C27
6	G	310	PLC	C6'-C7'-C8'-C9'
7	C	310	P1O	C21-C22-C23-C24
7	G	312	P1O	C21-C22-C23-C24
7	K	311	P1O	C21-C22-C23-C24
6	C	308	PLC	CB-C1B-C2B-C3B
6	G	310	PLC	CB-C1B-C2B-C3B
6	K	309	PLC	CB-C1B-C2B-C3B
6	F	301	PLC	C5B-C6B-C7B-C8B
6	G	307	PLC	C5B-C6B-C7B-C8B
6	K	306	PLC	C5B-C6B-C7B-C8B
7	C	310	P1O	C20-C19-O7-C7
7	G	312	P1O	C20-C19-O7-C7
7	K	311	P1O	C20-C19-O7-C7
9	C	304	HXG	OAG-CBA-OAY-CBB
9	G	305	HXG	OAG-CBA-OAY-CBB
9	K	304	HXG	OAG-CBA-OAY-CBB
6	C	311	PLC	C4'-C5'-C6'-C7'
6	J	306	PLC	C4'-C5'-C6'-C7'

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Mol	Chain	Res	Type	Atoms
6	G	301	PLC	C4'-C5'-C6'-C7'
7	B	307	P1O	C13-C14-C15-C16
7	J	308	P1O	C13-C14-C15-C16
7	F	302	P1O	C13-C14-C15-C16
6	F	301	PLC	C7B-C8B-C9B-CAA
6	G	307	PLC	C7B-C8B-C9B-CAA
6	K	306	PLC	C7B-C8B-C9B-CAA
6	C	303	PLC	CB-C1B-C2B-C3B
6	G	304	PLC	CB-C1B-C2B-C3B
6	K	303	PLC	CB-C1B-C2B-C3B
6	B	301	PLC	C1'-C2'-C3'-C4'
6	C	311	PLC	C6'-C7'-C8'-C9'
6	C	303	PLC	C3B-C4B-C5B-C6B
6	J	306	PLC	C6'-C7'-C8'-C9'
6	F	303	PLC	C1'-C2'-C3'-C4'
6	G	301	PLC	C6'-C7'-C8'-C9'
6	G	304	PLC	C3B-C4B-C5B-C6B
6	K	303	PLC	C3B-C4B-C5B-C6B
6	J	307	PLC	C1'-C2'-C3'-C4'
5	J	305	D10	C5-C6-C7-C8
5	B	306	D10	C5-C6-C7-C8
5	F	308	D10	C5-C6-C7-C8
7	C	310	P1O	C12-C13-C14-C15
7	K	311	P1O	C12-C13-C14-C15
6	C	303	PLC	C4B-C5B-C6B-C7B
6	K	303	PLC	C4B-C5B-C6B-C7B
7	G	312	P1O	C12-C13-C14-C15
6	G	304	PLC	C4B-C5B-C6B-C7B
6	B	301	PLC	C1B-C2B-C3B-C4B
6	C	308	PLC	C1B-C2B-C3B-C4B
6	J	307	PLC	C1B-C2B-C3B-C4B
6	F	303	PLC	C1B-C2B-C3B-C4B
6	G	310	PLC	C1B-C2B-C3B-C4B
6	K	309	PLC	C1B-C2B-C3B-C4B
6	C	303	PLC	C6'-C7'-C8'-C9'
6	G	304	PLC	C6'-C7'-C8'-C9'
6	K	303	PLC	C6'-C7'-C8'-C9'
7	J	301	P1O	C23-C24-C25-C26
7	F	304	P1O	C23-C24-C25-C26
7	B	302	P1O	C23-C24-C25-C26
9	C	304	HXG	OAX-CAU-CBB-CAT
9	G	305	HXG	OAX-CAU-CBB-CAT

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Mol	Chain	Res	Type	Atoms
9	K	304	HXG	OAX-CAU-CBB-CAT
7	C	310	P1O	O8-C19-O7-C7
7	K	311	P1O	O8-C19-O7-C7
6	C	308	PLC	C4'-C5'-C6'-C7'
6	G	310	PLC	C4'-C5'-C6'-C7'
6	K	309	PLC	C4'-C5'-C6'-C7'
7	C	310	P1O	C10-C11-C12-C13
7	G	312	P1O	C10-C11-C12-C13
7	K	311	P1O	C10-C11-C12-C13
7	F	302	P1O	C12-C13-C14-C15
7	B	307	P1O	C12-C13-C14-C15
7	J	308	P1O	C12-C13-C14-C15
7	B	307	P1O	C22-C23-C24-C25
7	C	309	P1O	C22-C23-C24-C25
7	J	301	P1O	C20-C21-C22-C23
7	J	308	P1O	C22-C23-C24-C25
7	F	302	P1O	C22-C23-C24-C25
7	G	311	P1O	C22-C23-C24-C25
7	K	310	P1O	C22-C23-C24-C25
7	B	302	P1O	C20-C21-C22-C23
7	F	304	P1O	C20-C21-C22-C23
7	G	312	P1O	O8-C19-O7-C7
6	C	308	PLC	C7B-C8B-C9B-CAA
6	G	310	PLC	C7B-C8B-C9B-CAA
6	K	309	PLC	C7B-C8B-C9B-CAA
6	C	306	PLC	C3-C2-O2-C'
6	F	301	PLC	C3-C2-O2-C'
6	G	307	PLC	C3-C2-O2-C'
6	G	308	PLC	C3-C2-O2-C'
6	K	306	PLC	C3-C2-O2-C'
6	K	307	PLC	C3-C2-O2-C'
7	B	307	P1O	C6-C7-O7-C19
7	J	308	P1O	C6-C7-O7-C19
7	F	302	P1O	C6-C7-O7-C19
5	B	304	D10	C5-C6-C7-C8
5	F	306	D10	C5-C6-C7-C8
5	F	308	D10	C4-C5-C6-C7
5	B	305	D10	C4-C5-C6-C7
5	B	306	D10	C4-C5-C6-C7
5	J	303	D10	C5-C6-C7-C8
5	J	304	D10	C4-C5-C6-C7
5	J	305	D10	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
5	F	307	D10	C4-C5-C6-C7
6	C	306	PLC	C7'-C8'-C9'-CA'
6	G	308	PLC	C7'-C8'-C9'-CA'
6	K	307	PLC	C7'-C8'-C9'-CA'
7	B	307	P10	C15-C16-C17-C18
7	J	308	P10	C15-C16-C17-C18
7	F	302	P10	C15-C16-C17-C18
5	J	305	D10	C6-C7-C8-C9
5	F	308	D10	C6-C7-C8-C9
6	F	303	PLC	C2'-C3'-C4'-C5'
5	B	306	D10	C6-C7-C8-C9
6	B	301	PLC	C2'-C3'-C4'-C5'
6	J	307	PLC	C2'-C3'-C4'-C5'
6	C	303	PLC	O2-C2-C3-O3
6	G	304	PLC	O2-C2-C3-O3
6	K	303	PLC	O2-C2-C3-O3
6	C	311	PLC	C6B-C7B-C8B-C9B
6	J	306	PLC	C6B-C7B-C8B-C9B
6	G	301	PLC	C6B-C7B-C8B-C9B
6	K	307	PLC	C2B-C3B-C4B-C5B
6	C	308	PLC	C8'-C9'-CA'-CB'
6	F	301	PLC	C8B-C9B-CAA-CBA
6	K	306	PLC	C8B-C9B-CAA-CBA
6	C	306	PLC	C2B-C3B-C4B-C5B
6	G	308	PLC	C2B-C3B-C4B-C5B
6	G	307	PLC	C8B-C9B-CAA-CBA
6	G	310	PLC	C8'-C9'-CA'-CB'
6	K	309	PLC	C8'-C9'-CA'-CB'
6	J	307	PLC	C5'-C6'-C7'-C8'
6	B	301	PLC	C5'-C6'-C7'-C8'
6	F	303	PLC	C5'-C6'-C7'-C8'
5	J	305	D10	C2-C3-C4-C5
5	B	305	D10	C2-C3-C4-C5
5	F	307	D10	C2-C3-C4-C5
5	B	306	D10	C2-C3-C4-C5
5	J	304	D10	C2-C3-C4-C5
5	F	308	D10	C2-C3-C4-C5
6	F	301	PLC	C4B-C5B-C6B-C7B
6	G	307	PLC	C4B-C5B-C6B-C7B
6	K	306	PLC	C4B-C5B-C6B-C7B
6	C	311	PLC	C7B-C8B-C9B-CAA
6	J	306	PLC	C7B-C8B-C9B-CAA

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Mol	Chain	Res	Type	Atoms
6	G	301	PLC	C7B-C8B-C9B-CAA
6	B	301	PLC	O3P-C1-C2-C3
6	C	308	PLC	O3P-C1-C2-C3
6	J	307	PLC	O3P-C1-C2-C3
6	F	301	PLC	O3P-C1-C2-C3
6	F	303	PLC	O3P-C1-C2-C3
6	G	307	PLC	O3P-C1-C2-C3
6	G	310	PLC	O3P-C1-C2-C3
6	K	306	PLC	O3P-C1-C2-C3
6	K	309	PLC	O3P-C1-C2-C3
7	C	310	P1O	O4-C6-C7-C8
7	G	312	P1O	O4-C6-C7-C8
7	K	311	P1O	O4-C6-C7-C8
5	B	305	D10	C6-C7-C8-C9
5	J	304	D10	C6-C7-C8-C9
5	F	307	D10	C6-C7-C8-C9
6	C	303	PLC	C8B-C9B-CAA-CBA
6	G	304	PLC	C8B-C9B-CAA-CBA
6	K	303	PLC	C8B-C9B-CAA-CBA
6	G	308	PLC	CB-C1B-C2B-C3B
6	G	308	PLC	C3'-C4'-C5'-C6'
6	K	307	PLC	C3'-C4'-C5'-C6'
6	C	306	PLC	C3'-C4'-C5'-C6'
6	C	306	PLC	CB-C1B-C2B-C3B
6	K	307	PLC	CB-C1B-C2B-C3B
7	B	302	P1O	C12-C13-C14-C15
7	J	301	P1O	C12-C13-C14-C15
7	F	304	P1O	C12-C13-C14-C15
6	B	301	PLC	C4'-C5'-C6'-C7'
6	J	307	PLC	C4'-C5'-C6'-C7'
6	F	303	PLC	C4'-C5'-C6'-C7'
6	C	303	PLC	C8'-C9'-CA'-CB'
6	G	304	PLC	C8'-C9'-CA'-CB'
6	K	303	PLC	C8'-C9'-CA'-CB'
7	C	310	P1O	C19-C20-C21-C22
7	G	312	P1O	C19-C20-C21-C22
7	K	311	P1O	C19-C20-C21-C22
7	C	310	P1O	C15-C16-C17-C18
7	G	312	P1O	C15-C16-C17-C18
7	K	311	P1O	C15-C16-C17-C18
5	J	304	D10	C3-C4-C5-C6
6	G	304	PLC	C3'-C4'-C5'-C6'

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Mol	Chain	Res	Type	Atoms
5	B	305	D10	C3-C4-C5-C6
5	F	307	D10	C3-C4-C5-C6
6	K	303	PLC	C1B-C2B-C3B-C4B
6	C	303	PLC	C3'-C4'-C5'-C6'
6	K	303	PLC	C3'-C4'-C5'-C6'
6	C	306	PLC	O3P-C1-C2-C3
6	C	311	PLC	O3P-C1-C2-C3
6	J	306	PLC	O3P-C1-C2-C3
6	G	301	PLC	O3P-C1-C2-C3
6	G	308	PLC	O3P-C1-C2-C3
6	K	307	PLC	O3P-C1-C2-C3
6	C	303	PLC	C1B-C2B-C3B-C4B
6	G	304	PLC	C1B-C2B-C3B-C4B
6	F	301	PLC	C8'-C9'-CA'-CB'
6	G	307	PLC	C8'-C9'-CA'-CB'
6	K	306	PLC	C8'-C9'-CA'-CB'
6	C	308	PLC	C3-C2-O2-C'
6	C	311	PLC	C3-C2-O2-C'
6	J	306	PLC	C3-C2-O2-C'
6	G	301	PLC	C3-C2-O2-C'
6	G	310	PLC	C3-C2-O2-C'
6	K	309	PLC	C3-C2-O2-C'
9	C	307	HXG	CAT-CBB-OAY-CBA
9	G	309	HXG	CAT-CBB-OAY-CBA
9	K	308	HXG	CAT-CBB-OAY-CBA
6	B	301	PLC	O3P-C1-C2-O2
6	C	311	PLC	O3P-C1-C2-O2
6	J	306	PLC	O3P-C1-C2-O2
6	J	307	PLC	O3P-C1-C2-O2
6	F	301	PLC	O3P-C1-C2-O2
6	F	303	PLC	O3P-C1-C2-O2
6	G	301	PLC	O3P-C1-C2-O2
6	G	307	PLC	O3P-C1-C2-O2
6	K	306	PLC	O3P-C1-C2-O2
7	C	310	P10	O4-C6-C7-O7
7	G	312	P10	O4-C6-C7-O7
7	K	311	P10	O4-C6-C7-O7
9	C	304	HXG	OAX-CAU-CBB-OAY
9	K	304	HXG	OAX-CAU-CBB-OAY
6	C	306	PLC	C4'-C5'-C6'-C7'
6	G	308	PLC	C4'-C5'-C6'-C7'
6	K	307	PLC	C4'-C5'-C6'-C7'

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Mol	Chain	Res	Type	Atoms
6	C	306	PLC	C8'-C9'-CA'-CB'
6	G	308	PLC	C8'-C9'-CA'-CB'
6	K	307	PLC	C8'-C9'-CA'-CB'
7	K	311	P1O	C14-C15-C16-C17
7	C	310	P1O	C14-C15-C16-C17
7	C	310	P1O	C22-C23-C24-C25
7	G	312	P1O	C14-C15-C16-C17
7	C	310	P1O	O7-C7-C8-O5
7	G	312	P1O	O7-C7-C8-O5
7	K	311	P1O	O7-C7-C8-O5
7	G	312	P1O	C22-C23-C24-C25
7	C	309	P1O	C11-C12-C13-C14
7	G	311	P1O	C11-C12-C13-C14
7	K	310	P1O	C11-C12-C13-C14
7	K	311	P1O	C22-C23-C24-C25
7	J	301	P1O	C1-C2-N1-C5
6	C	306	PLC	O4P-C4-C5-N
6	G	308	PLC	O4P-C4-C5-N
6	K	307	PLC	O4P-C4-C5-N
7	B	302	P1O	C24-C25-C26-C27
7	J	301	P1O	C24-C25-C26-C27
7	F	304	P1O	C24-C25-C26-C27
7	J	301	P1O	C9-C10-C11-C12
7	B	302	P1O	C1-C2-N1-C4
7	B	302	P1O	C1-C2-N1-C5
7	F	304	P1O	C1-C2-N1-C4
7	F	304	P1O	C1-C2-N1-C5
7	B	302	P1O	C9-C10-C11-C12
7	F	304	P1O	C9-C10-C11-C12
7	B	302	P1O	C15-C16-C17-C18
7	J	301	P1O	C15-C16-C17-C18
7	F	304	P1O	C15-C16-C17-C18
6	C	306	PLC	O3P-C1-C2-O2
6	C	308	PLC	O3P-C1-C2-O2
6	G	308	PLC	O3P-C1-C2-O2
6	G	310	PLC	O3P-C1-C2-O2
6	K	307	PLC	O3P-C1-C2-O2
6	K	309	PLC	O3P-C1-C2-O2
9	G	305	HXG	OAX-CAU-CBB-OAY
7	J	301	P1O	C1-C2-N1-C4
6	K	309	PLC	C3B-C4B-C5B-C6B
6	C	308	PLC	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
6	G	310	PLC	C3B-C4B-C5B-C6B
7	B	307	P1O	C21-C22-C23-C24
7	J	308	P1O	C21-C22-C23-C24
7	F	302	P1O	C21-C22-C23-C24
6	B	301	PLC	O2-C2-C3-O3
6	J	307	PLC	O2-C2-C3-O3
6	F	303	PLC	O2-C2-C3-O3
6	B	301	PLC	C1-C2-C3-O3
6	C	303	PLC	C1-C2-C3-O3
6	J	307	PLC	C1-C2-C3-O3
6	F	303	PLC	C1-C2-C3-O3
6	G	304	PLC	C1-C2-C3-O3
6	K	303	PLC	C1-C2-C3-O3
5	B	306	D10	C3-C4-C5-C6
5	J	305	D10	C3-C4-C5-C6
5	F	308	D10	C3-C4-C5-C6
7	J	301	P1O	C10-C11-C12-C13
6	C	306	PLC	C5B-C6B-C7B-C8B
6	G	308	PLC	C5B-C6B-C7B-C8B
7	B	302	P1O	C10-C11-C12-C13
6	K	307	PLC	C5B-C6B-C7B-C8B
6	K	309	PLC	C5'-C6'-C7'-C8'
7	F	304	P1O	C10-C11-C12-C13
6	G	310	PLC	C5'-C6'-C7'-C8'
6	C	308	PLC	C5'-C6'-C7'-C8'
6	B	301	PLC	C4-O4P-P-O1P
6	C	306	PLC	C4-O4P-P-O3P
6	C	311	PLC	C4-O4P-P-O2P
6	C	311	PLC	C4-O4P-P-O3P
6	J	306	PLC	C4-O4P-P-O2P
6	J	306	PLC	C4-O4P-P-O3P
6	J	307	PLC	C4-O4P-P-O1P
6	F	301	PLC	C1-O3P-P-O4P
6	F	303	PLC	C4-O4P-P-O1P
6	G	301	PLC	C4-O4P-P-O2P
6	G	301	PLC	C4-O4P-P-O3P
6	G	307	PLC	C1-O3P-P-O4P
6	G	308	PLC	C4-O4P-P-O3P
6	K	306	PLC	C1-O3P-P-O4P
6	K	307	PLC	C4-O4P-P-O3P
7	B	307	P1O	C1-O3-P1-O1
7	C	309	P1O	C6-O4-P1-O2

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Mol	Chain	Res	Type	Atoms
7	C	310	P1O	C1-O3-P1-O4
7	J	308	P1O	C1-O3-P1-O1
7	F	302	P1O	C1-O3-P1-O1
7	G	311	P1O	C6-O4-P1-O2
7	G	312	P1O	C1-O3-P1-O4
7	K	310	P1O	C6-O4-P1-O2
7	K	311	P1O	C1-O3-P1-O4
9	C	304	HXG	CAP-OAW-PBD-OAI
9	C	307	HXG	CAU-OAX-PBD-OAI
9	G	305	HXG	CAP-OAW-PBD-OAI
9	G	309	HXG	CAU-OAX-PBD-OAI
9	K	304	HXG	CAP-OAW-PBD-OAI
9	K	308	HXG	CAU-OAX-PBD-OAI
6	J	306	PLC	C3'-C4'-C5'-C6'
6	G	301	PLC	C3'-C4'-C5'-C6'
6	C	311	PLC	C3'-C4'-C5'-C6'
6	K	307	PLC	C6'-C7'-C8'-C9'
6	C	306	PLC	C6'-C7'-C8'-C9'
6	G	308	PLC	C6'-C7'-C8'-C9'
7	C	310	P1O	C6-C7-C8-O5
7	G	312	P1O	C6-C7-C8-O5
7	K	311	P1O	C6-C7-C8-O5
7	G	311	P1O	C24-C25-C26-C27
7	C	309	P1O	C24-C25-C26-C27
7	K	310	P1O	C24-C25-C26-C27
6	B	301	PLC	C6'-C7'-C8'-C9'
6	F	303	PLC	C6'-C7'-C8'-C9'
6	J	307	PLC	C6'-C7'-C8'-C9'
6	C	308	PLC	C5B-C6B-C7B-C8B
6	G	310	PLC	C5B-C6B-C7B-C8B
6	K	309	PLC	C5B-C6B-C7B-C8B
6	K	303	PLC	C5B-C6B-C7B-C8B
6	C	303	PLC	C5B-C6B-C7B-C8B
6	G	304	PLC	C5B-C6B-C7B-C8B
7	B	302	P1O	O7-C7-C8-O5
7	J	301	P1O	O7-C7-C8-O5
7	F	304	P1O	O7-C7-C8-O5
9	C	307	HXG	OAV-CAT-CBB-OAY
9	G	309	HXG	OAV-CAT-CBB-OAY
9	K	308	HXG	OAV-CAT-CBB-OAY
9	C	307	HXG	CBB-CAU-OAX-PBD
9	G	309	HXG	CBB-CAU-OAX-PBD

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Mol	Chain	Res	Type	Atoms
9	K	308	HXG	CBB-CAU-OAX-PBD
6	G	307	PLC	C3'-C4'-C5'-C6'
6	K	306	PLC	C3'-C4'-C5'-C6'
5	B	305	D10	C7-C8-C9-C10
5	F	307	D10	C7-C8-C9-C10
6	G	301	PLC	C5'-C6'-C7'-C8'
7	B	302	P1O	C1-C2-N1-C3
7	J	301	P1O	C1-C2-N1-C3
7	F	304	P1O	C1-C2-N1-C3
6	J	306	PLC	C5'-C6'-C7'-C8'
5	J	304	D10	C7-C8-C9-C10
6	F	301	PLC	C3'-C4'-C5'-C6'
6	C	311	PLC	C5'-C6'-C7'-C8'
6	B	301	PLC	C3-C2-O2-C'
6	J	307	PLC	C3-C2-O2-C'
6	F	303	PLC	C3-C2-O2-C'
6	C	308	PLC	C7'-C8'-C9'-CA'
6	G	310	PLC	C7'-C8'-C9'-CA'
6	K	309	PLC	C7'-C8'-C9'-CA'
7	K	311	P1O	C23-C24-C25-C26
7	C	310	P1O	C23-C24-C25-C26
7	G	312	P1O	C23-C24-C25-C26
6	J	307	PLC	C4B-C5B-C6B-C7B
6	B	301	PLC	C4B-C5B-C6B-C7B
6	F	303	PLC	C4B-C5B-C6B-C7B
6	G	308	PLC	C2'-C3'-C4'-C5'
6	K	307	PLC	C2'-C3'-C4'-C5'
6	C	306	PLC	C2'-C3'-C4'-C5'
6	C	306	PLC	O2-C2-C3-O3
6	G	308	PLC	O2-C2-C3-O3
6	K	307	PLC	O2-C2-C3-O3
6	C	308	PLC	C2-C1-O3P-P
6	G	310	PLC	C2-C1-O3P-P
6	K	309	PLC	C2-C1-O3P-P
6	B	301	PLC	C4-C5-N-C6
6	J	307	PLC	C4-C5-N-C6
6	F	303	PLC	C4-C5-N-C6
6	J	307	PLC	C3'-C4'-C5'-C6'
6	F	303	PLC	C3'-C4'-C5'-C6'
6	B	301	PLC	C3'-C4'-C5'-C6'
6	C	306	PLC	C1-C2-C3-O3
6	G	308	PLC	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	K	307	PLC	C1-C2-C3-O3
6	C	306	PLC	C5-C4-O4P-P
6	G	308	PLC	C5-C4-O4P-P
6	K	307	PLC	C5-C4-O4P-P
7	C	310	P1O	C9-C10-C11-C12
7	G	312	P1O	C9-C10-C11-C12
7	K	311	P1O	C9-C10-C11-C12
6	C	308	PLC	O2-C'-C1'-C2'
6	G	310	PLC	O2-C'-C1'-C2'
6	K	309	PLC	O2-C'-C1'-C2'
6	C	306	PLC	C7B-C8B-C9B-CAA
6	K	307	PLC	C7B-C8B-C9B-CAA
7	B	307	P1O	O7-C19-C20-C21
7	J	308	P1O	O7-C19-C20-C21
7	F	302	P1O	O7-C19-C20-C21
6	G	308	PLC	C7B-C8B-C9B-CAA
5	B	304	D10	C7-C8-C9-C10
5	F	306	D10	C7-C8-C9-C10
6	C	311	PLC	C2B-C1B-CB-O3
6	J	306	PLC	C2B-C1B-CB-O3
6	G	301	PLC	C2B-C1B-CB-O3
5	J	303	D10	C7-C8-C9-C10
6	F	301	PLC	C2B-C1B-CB-O3
6	G	307	PLC	C2B-C1B-CB-O3
6	K	306	PLC	C2B-C1B-CB-O3
7	G	311	P1O	C10-C11-C12-C13
7	K	310	P1O	C10-C11-C12-C13
7	B	307	P1O	C25-C26-C27-C28
7	C	309	P1O	C10-C11-C12-C13
7	J	308	P1O	C25-C26-C27-C28
7	F	302	P1O	C25-C26-C27-C28
6	B	301	PLC	C4-C5-N-C8
6	J	307	PLC	C4-C5-N-C8
6	F	303	PLC	C4-C5-N-C8
9	K	308	HXG	OAG-CBA-OAY-CBB
6	J	307	PLC	O2-C'-C1'-C2'
7	C	309	P1O	C7-C6-O4-P1
7	G	311	P1O	C7-C6-O4-P1
7	K	310	P1O	C7-C6-O4-P1
6	F	303	PLC	O2-C'-C1'-C2'
6	B	301	PLC	O2-C'-C1'-C2'
9	G	309	HXG	OAG-CBA-OAY-CBB

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Mol	Chain	Res	Type	Atoms
7	C	309	P1O	C11-C10-C9-O5
7	G	311	P1O	C11-C10-C9-O5
7	K	310	P1O	C11-C10-C9-O5
9	C	307	HXG	OAG-CBA-OAY-CBB
7	B	302	P1O	C6-C7-C8-O5
7	J	301	P1O	C6-C7-C8-O5
7	F	304	P1O	C6-C7-C8-O5
6	F	301	PLC	C2B-C1B-CB-OB
6	G	307	PLC	C2B-C1B-CB-OB
6	G	310	PLC	O'-C'-C1'-C2'
6	K	306	PLC	C2B-C1B-CB-OB
7	B	307	P1O	O4-C6-C7-C8
7	J	308	P1O	O4-C6-C7-C8
7	F	302	P1O	O4-C6-C7-C8
6	C	308	PLC	O'-C'-C1'-C2'
6	J	306	PLC	C2B-C1B-CB-OB
6	K	309	PLC	O'-C'-C1'-C2'
7	B	307	P1O	O8-C19-C20-C21
7	F	302	P1O	O8-C19-C20-C21
6	J	306	PLC	O2-C'-C1'-C2'
6	C	311	PLC	C2B-C1B-CB-OB
6	G	301	PLC	C2B-C1B-CB-OB
7	C	309	P1O	C11-C10-C9-O6
7	J	308	P1O	O8-C19-C20-C21
7	G	311	P1O	C11-C10-C9-O6
7	K	310	P1O	C11-C10-C9-O6
6	C	311	PLC	O2-C'-C1'-C2'
6	G	301	PLC	O2-C'-C1'-C2'
7	B	302	P1O	C11-C10-C9-O5
7	J	301	P1O	C11-C10-C9-O5
7	F	304	P1O	C11-C10-C9-O5
6	F	303	PLC	O'-C'-C1'-C2'

There are no ring outliers.

54 monomers are involved in 445 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	311	PLC	7	0
6	G	307	PLC	10	0
6	C	308	PLC	16	0
5	F	307	D10	8	0
6	K	309	PLC	17	0

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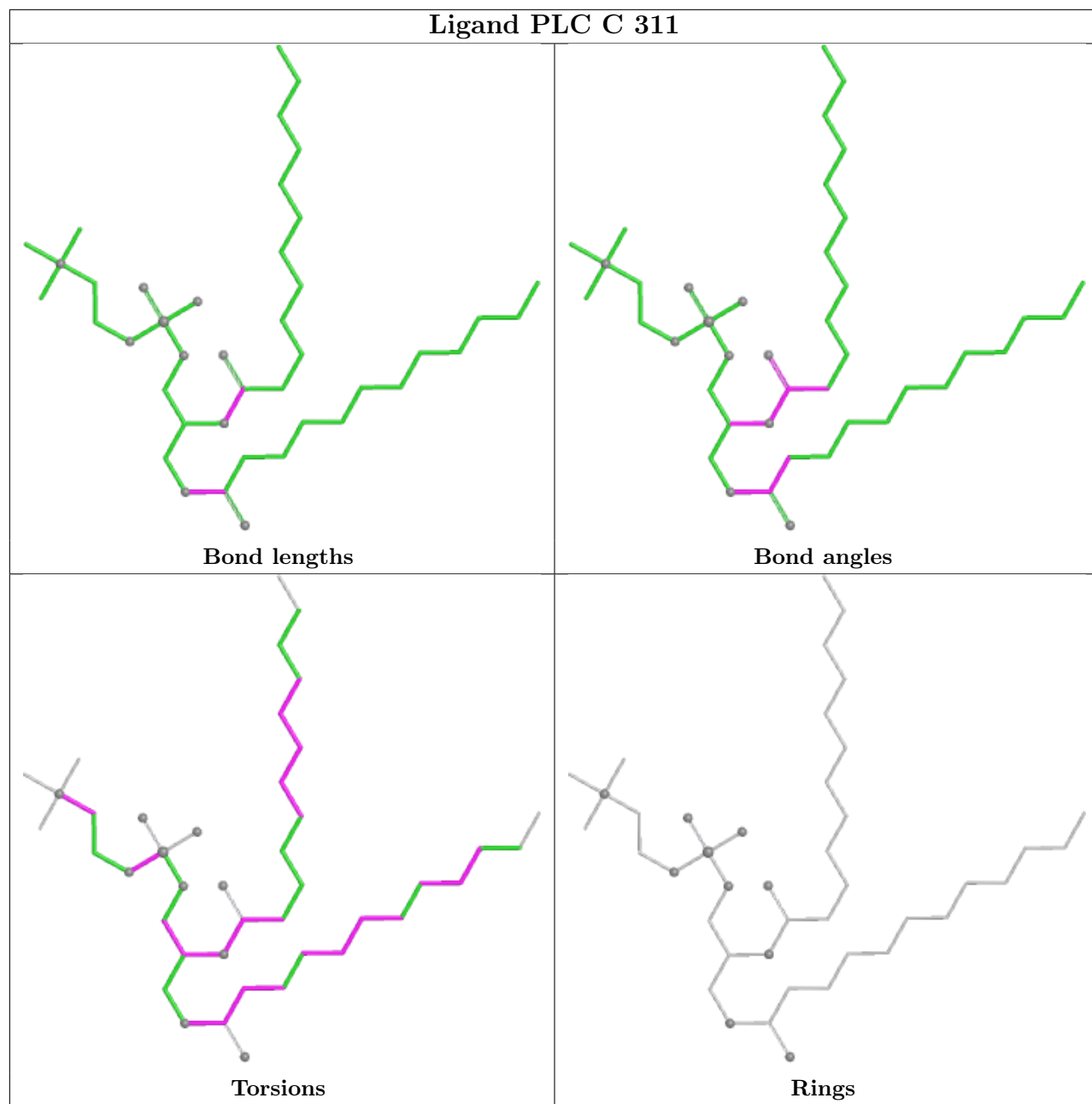
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	301	P1O	5	0
5	F	305	D10	2	0
7	G	312	P1O	8	0
7	C	310	P1O	12	0
5	I	503	D10	14	0
5	E	503	D10	10	0
5	B	306	D10	2	0
9	C	304	HXG	13	0
5	B	305	D10	9	0
5	J	303	D10	1	0
7	K	311	P1O	8	0
5	B	304	D10	1	0
5	J	304	D10	8	0
5	G	306	D10	2	0
5	F	308	D10	1	0
6	F	301	PLC	12	0
6	B	301	PLC	15	0
7	F	302	P1O	13	0
5	J	305	D10	1	0
9	K	308	HXG	15	0
7	C	309	P1O	16	0
7	B	307	P1O	12	0
6	J	306	PLC	7	0
6	C	303	PLC	9	0
6	K	303	PLC	12	0
9	G	309	HXG	15	0
6	K	306	PLC	10	0
9	G	305	HXG	13	0
9	K	304	HXG	13	0
6	G	301	PLC	5	0
5	C	305	D10	2	0
5	A	503	D10	11	0
6	G	308	PLC	22	0
5	K	305	D10	3	0
6	F	303	PLC	17	0
6	C	306	PLC	21	0
5	F	306	D10	1	0
7	J	308	P1O	12	0
5	J	302	D10	2	0
6	K	307	PLC	19	0
7	F	304	P1O	5	0
6	G	304	PLC	16	0

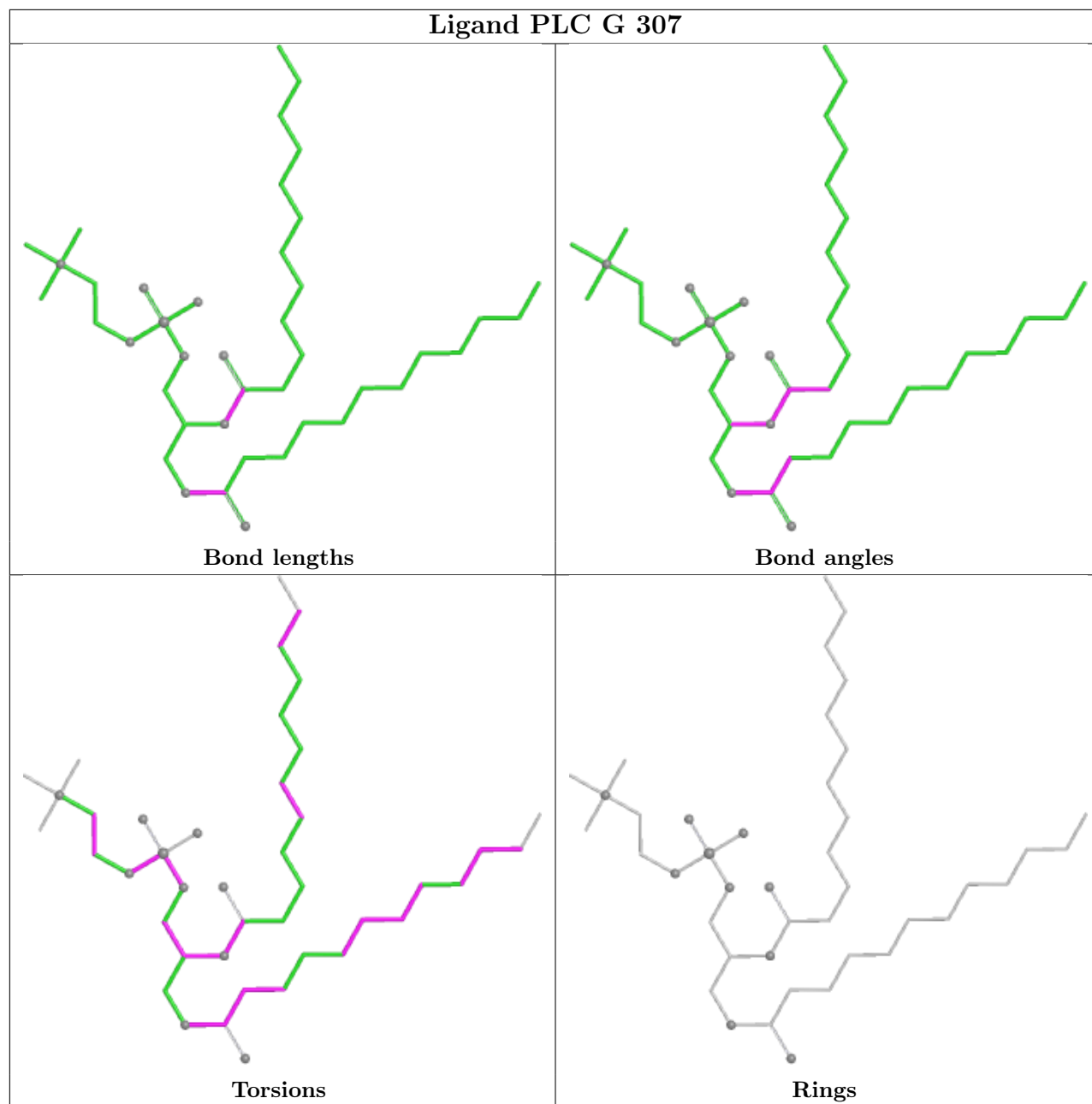
Continued on next page...

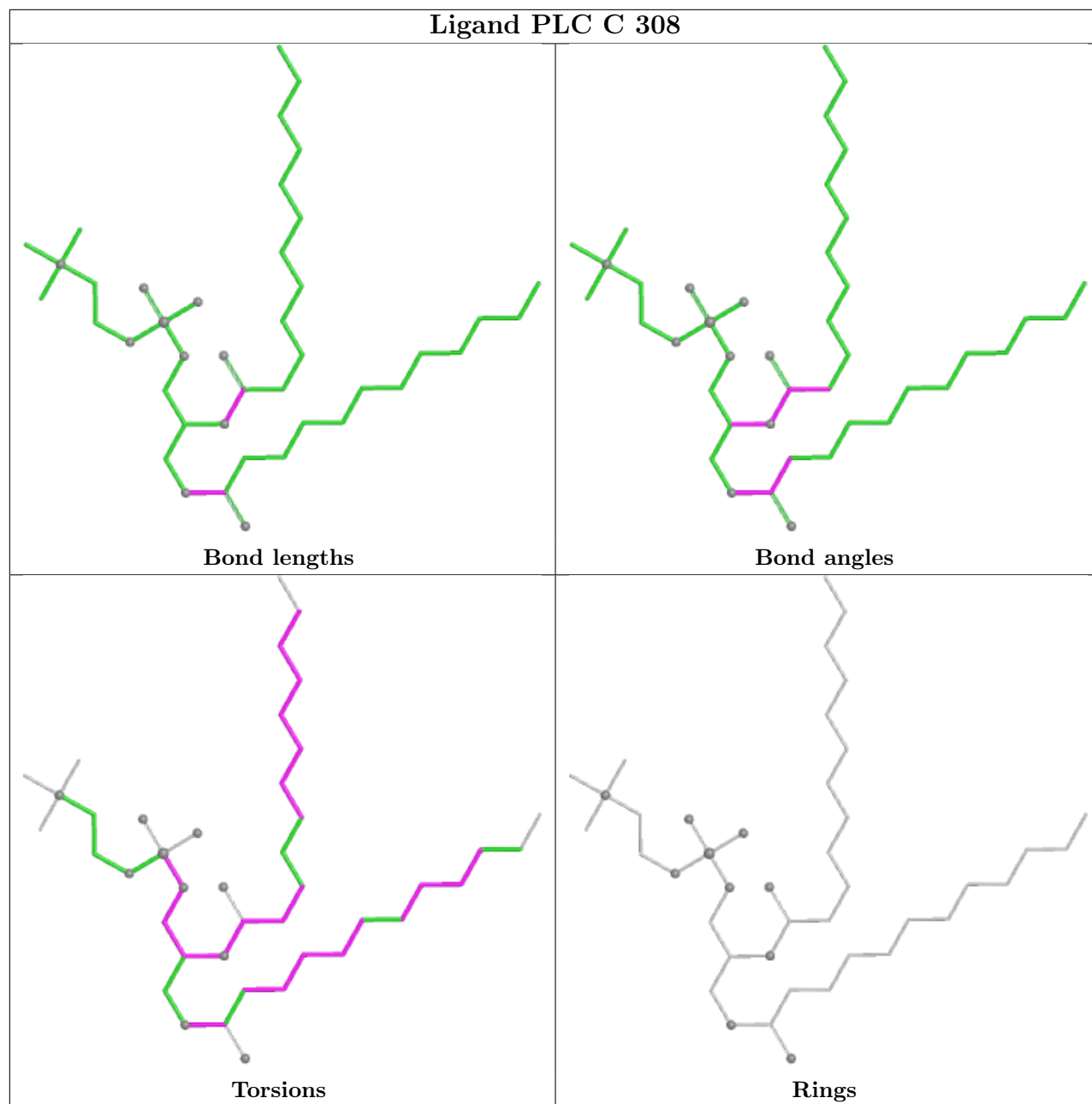
Continued from previous page...

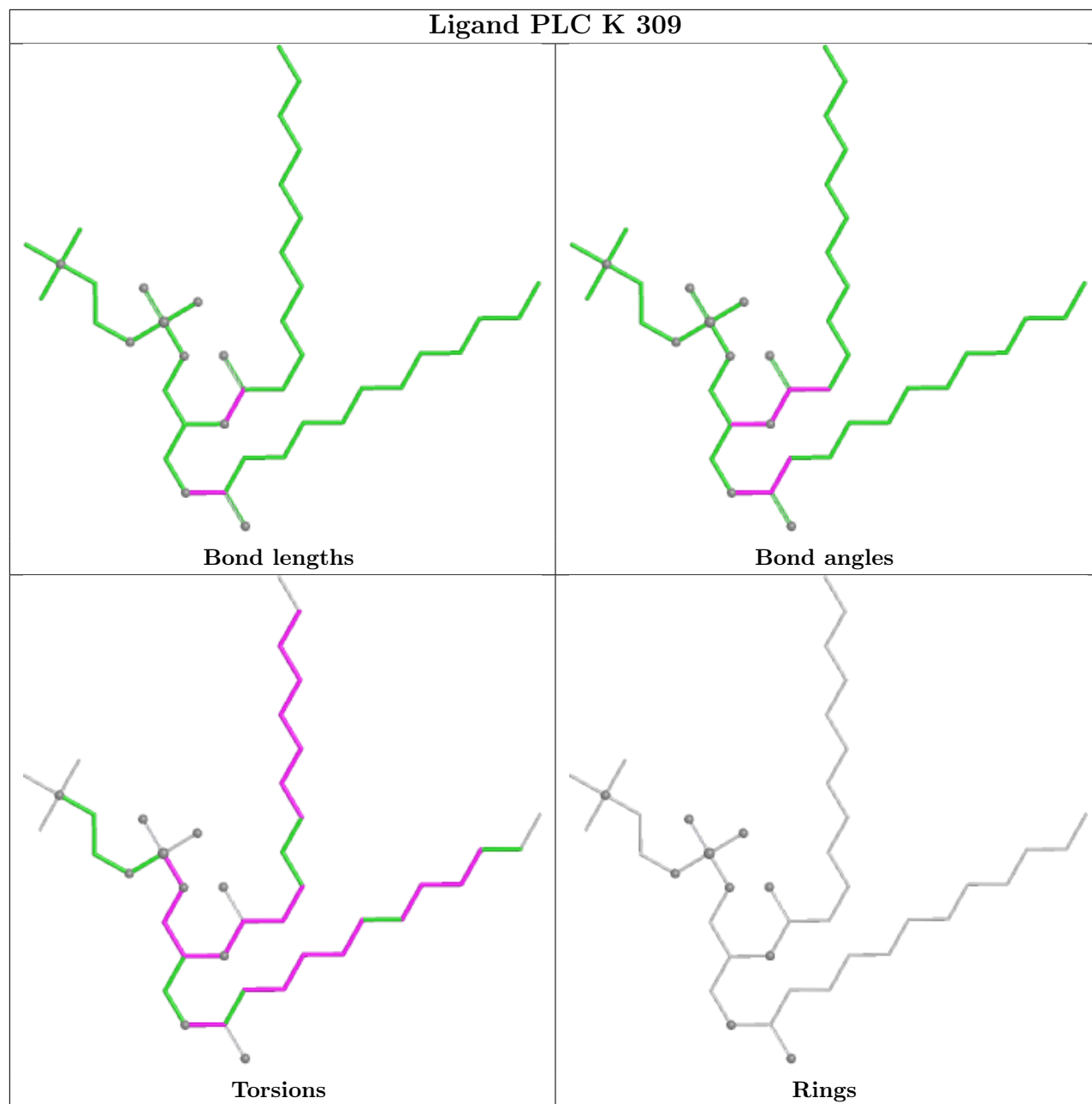
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	K	310	P1O	15	0
7	B	302	P1O	5	0
6	J	307	PLC	16	0
7	G	311	P1O	15	0
9	C	307	HXG	15	0
6	G	310	PLC	17	0
5	B	303	D10	2	0

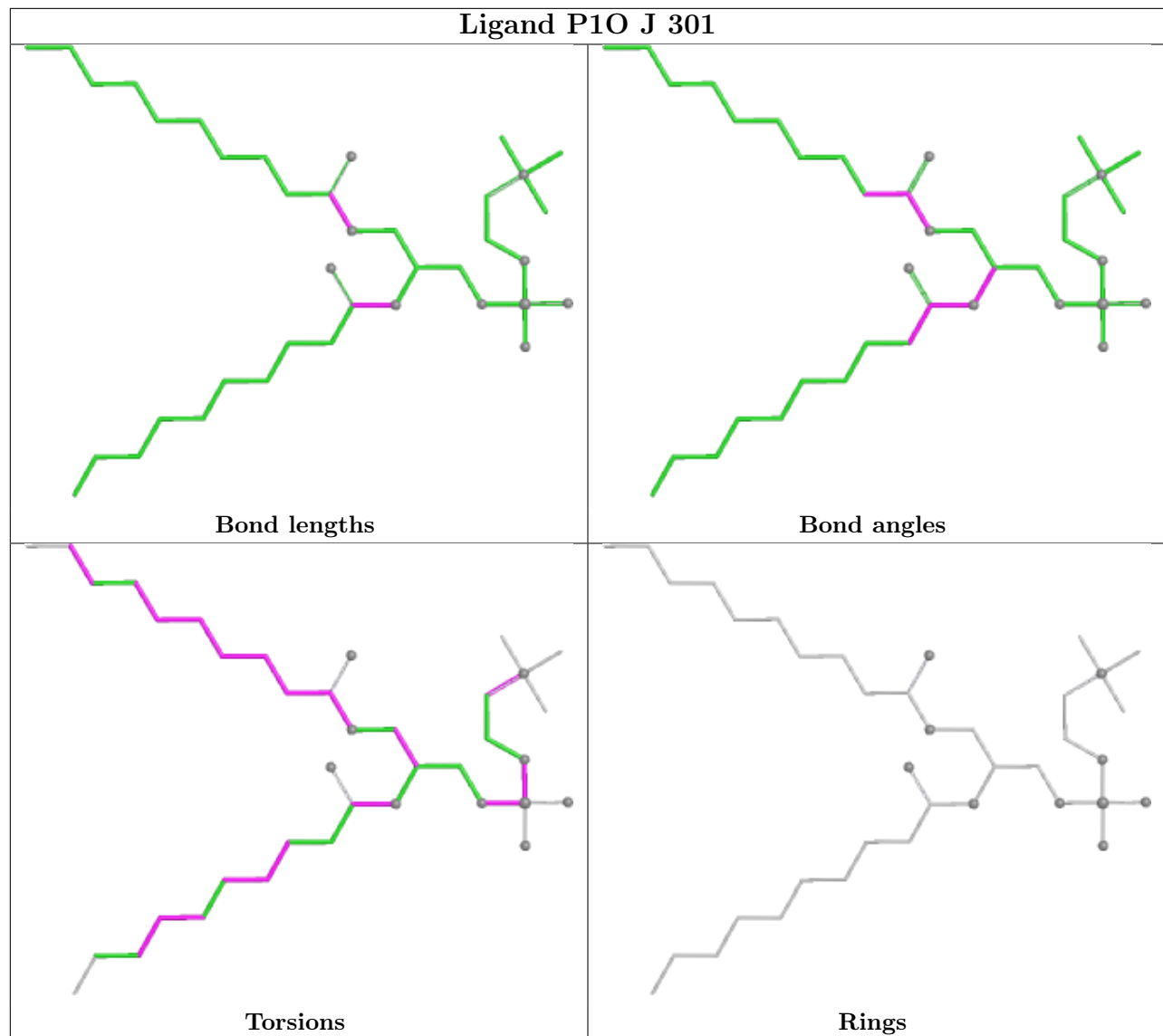
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

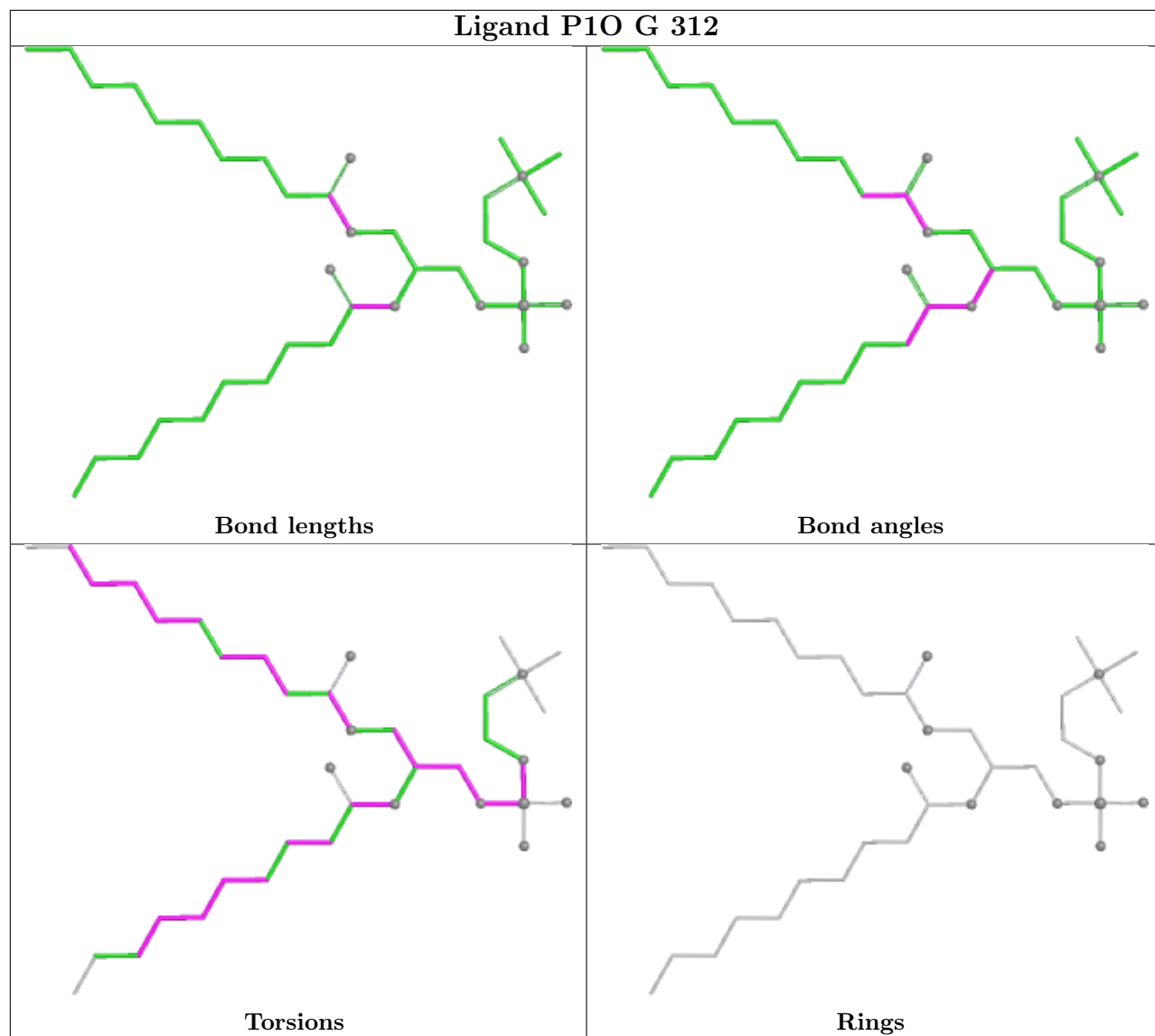


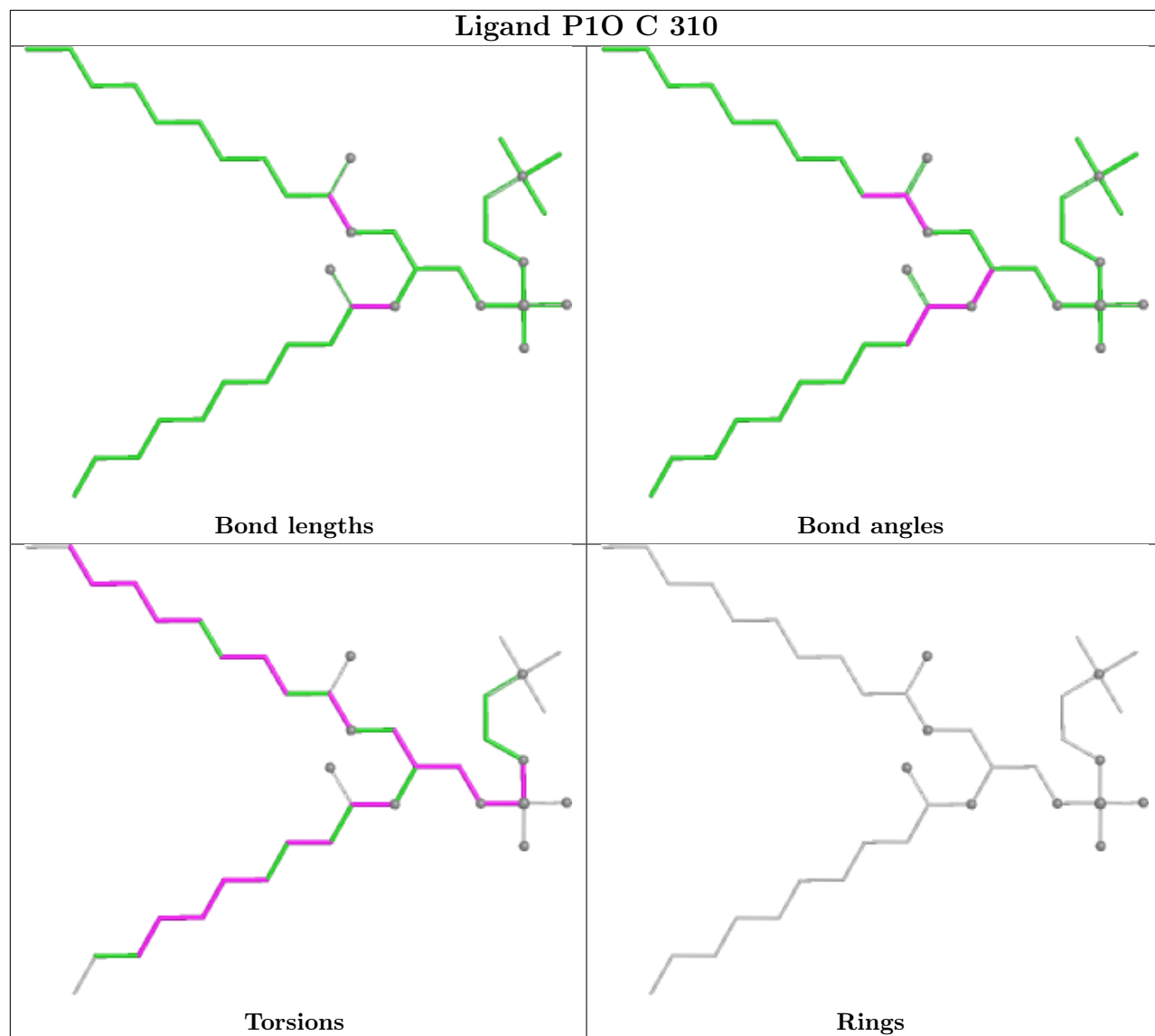


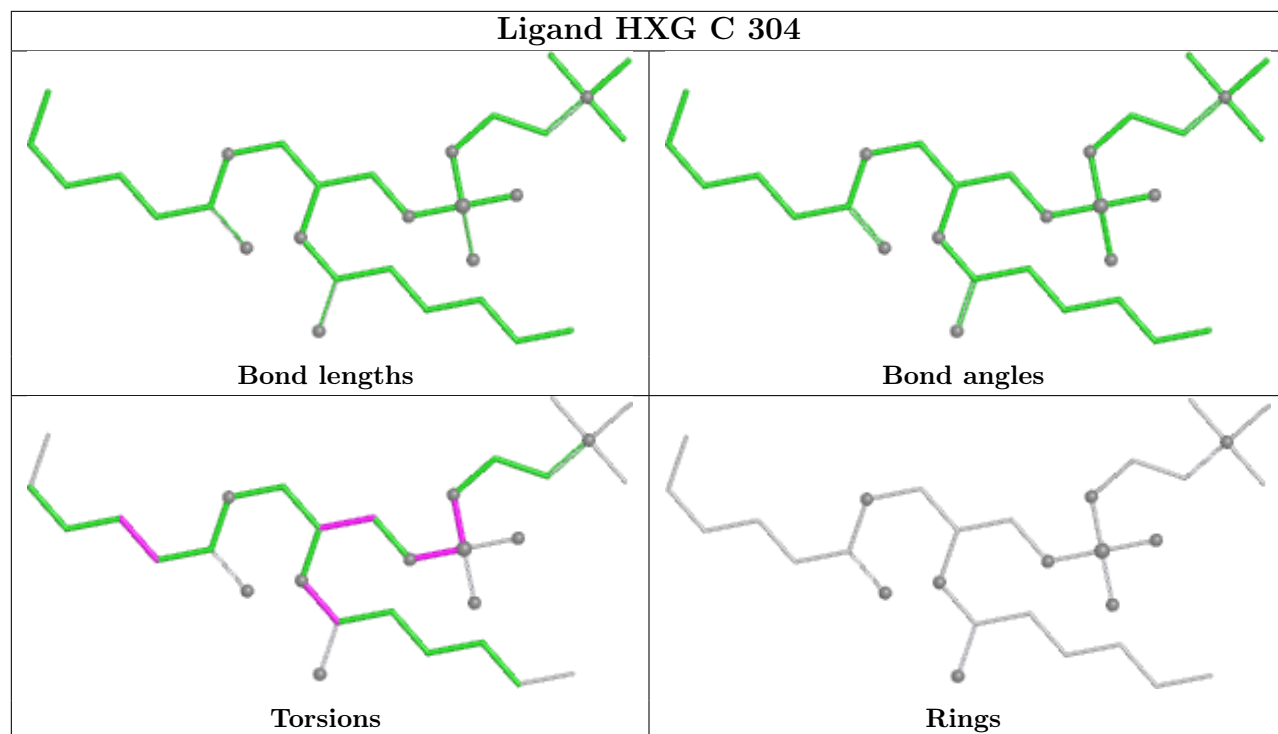


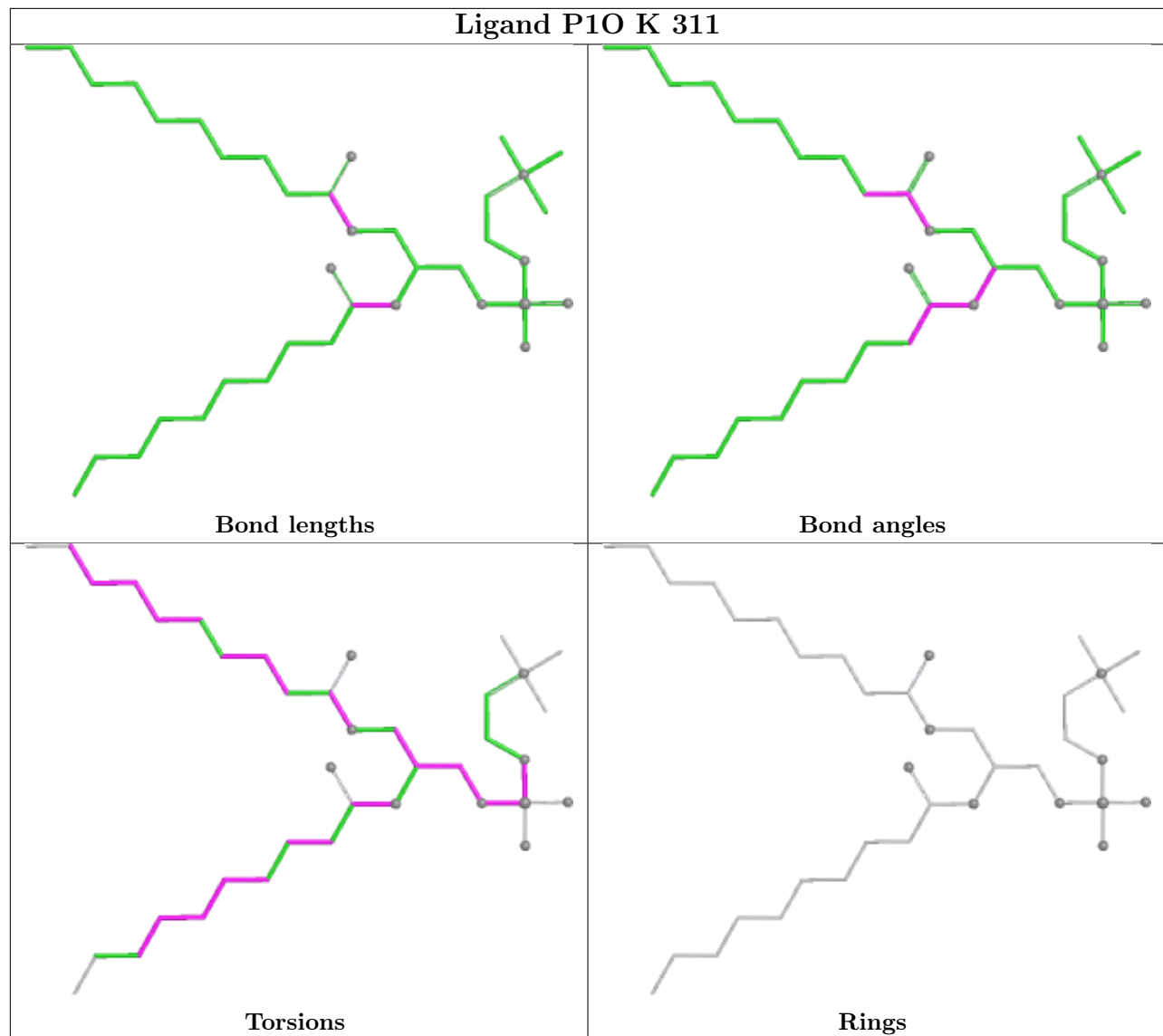


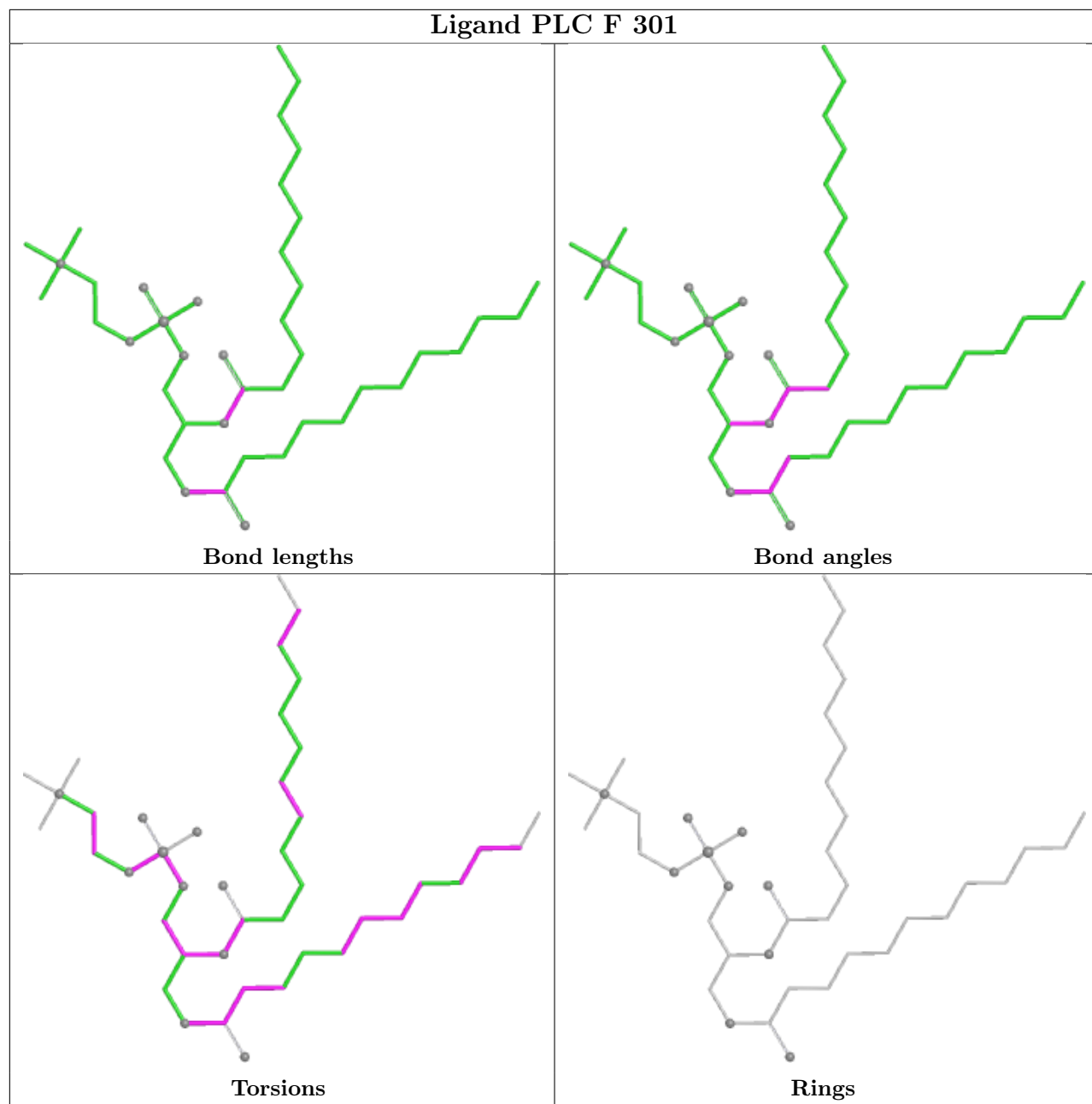


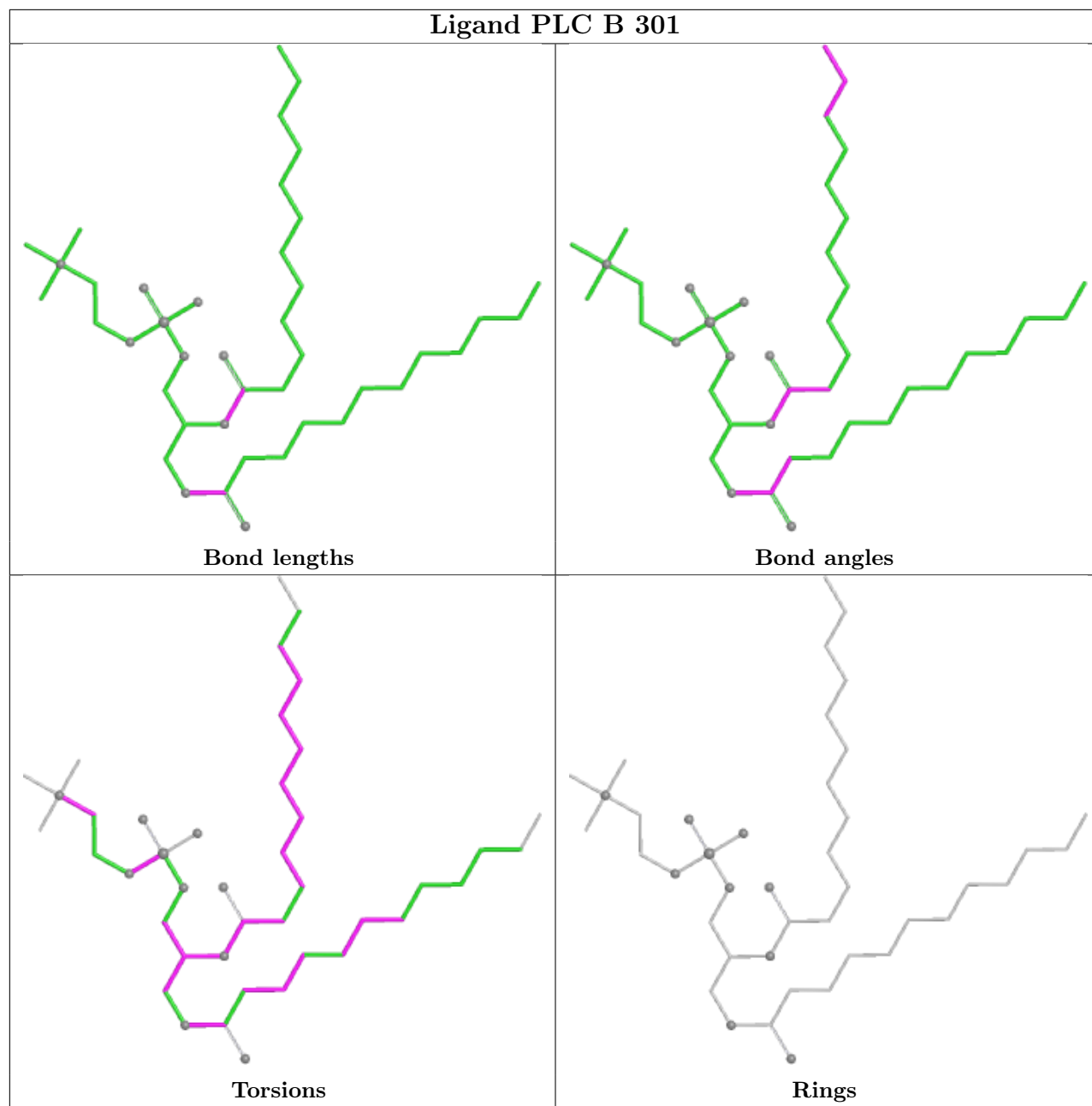


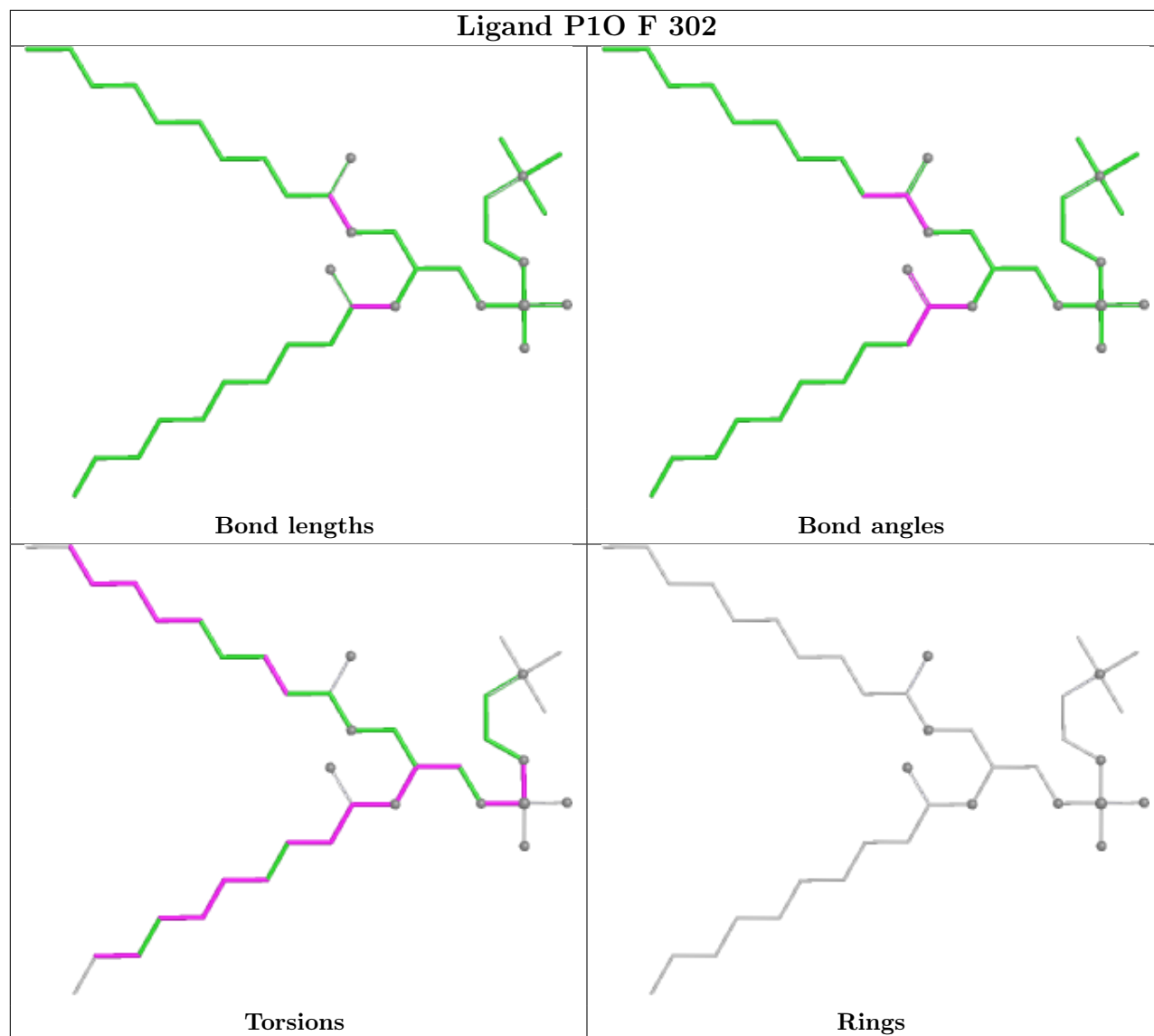


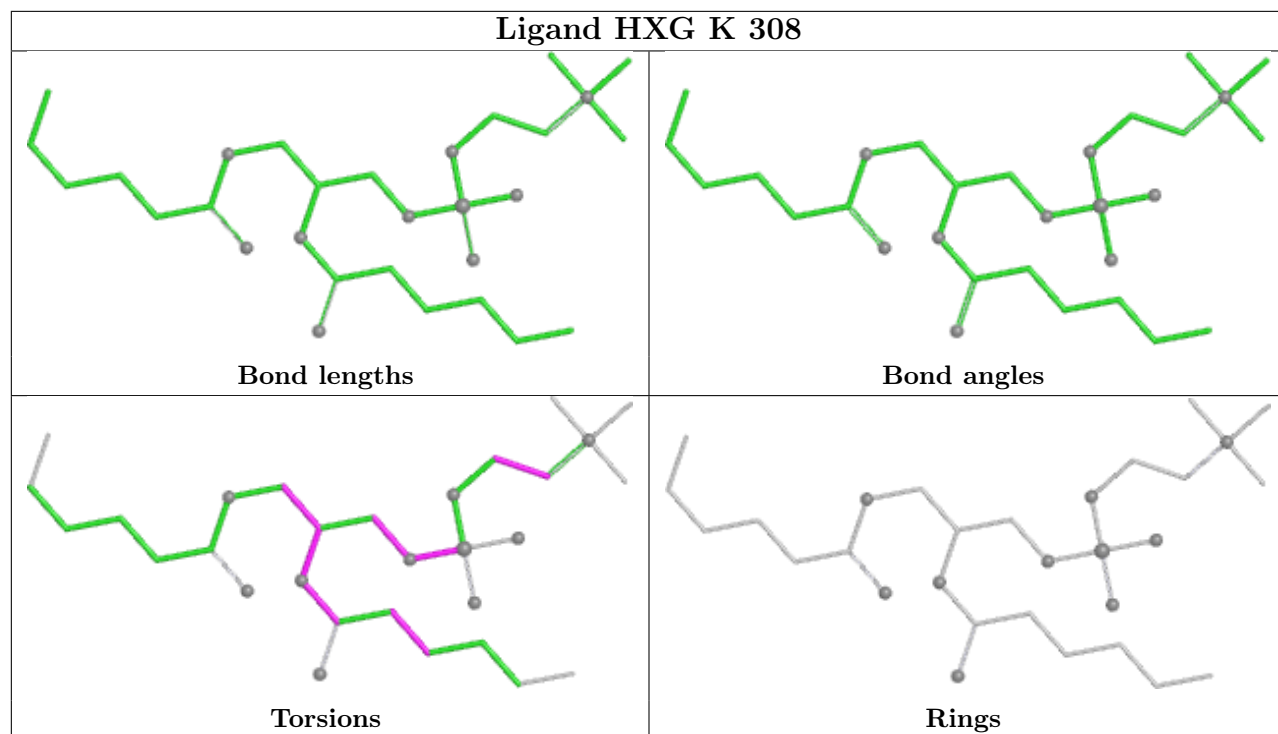


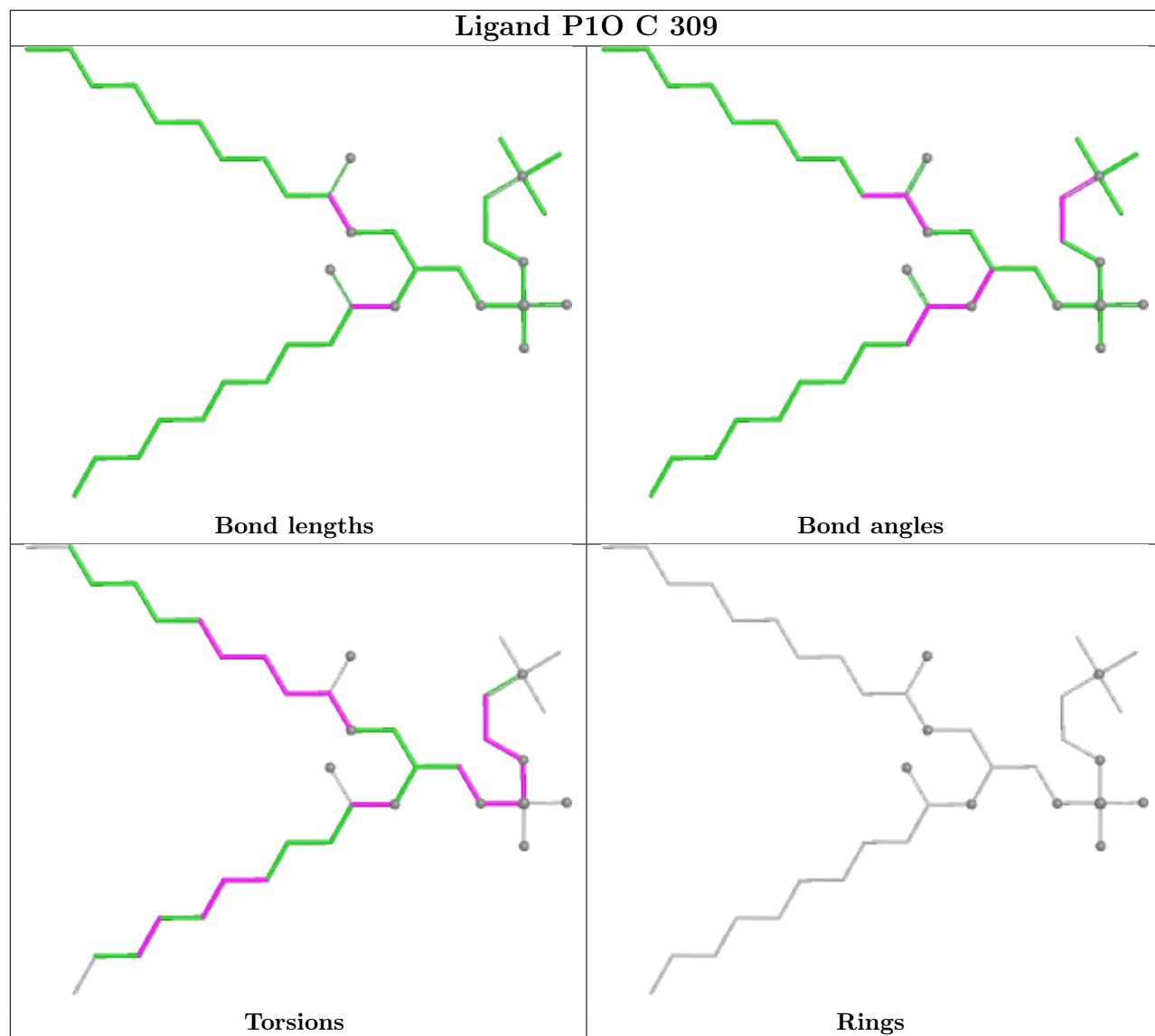


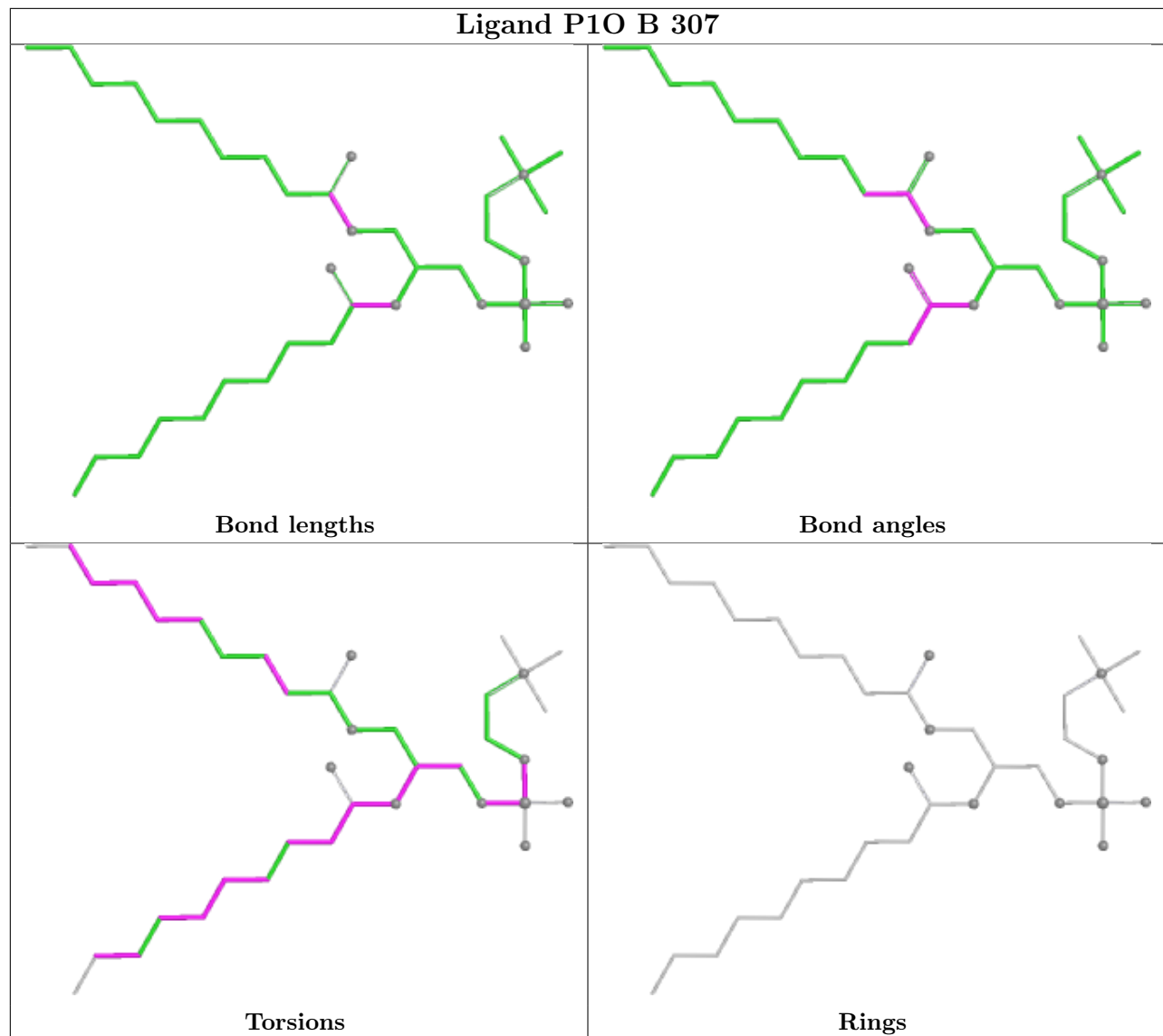


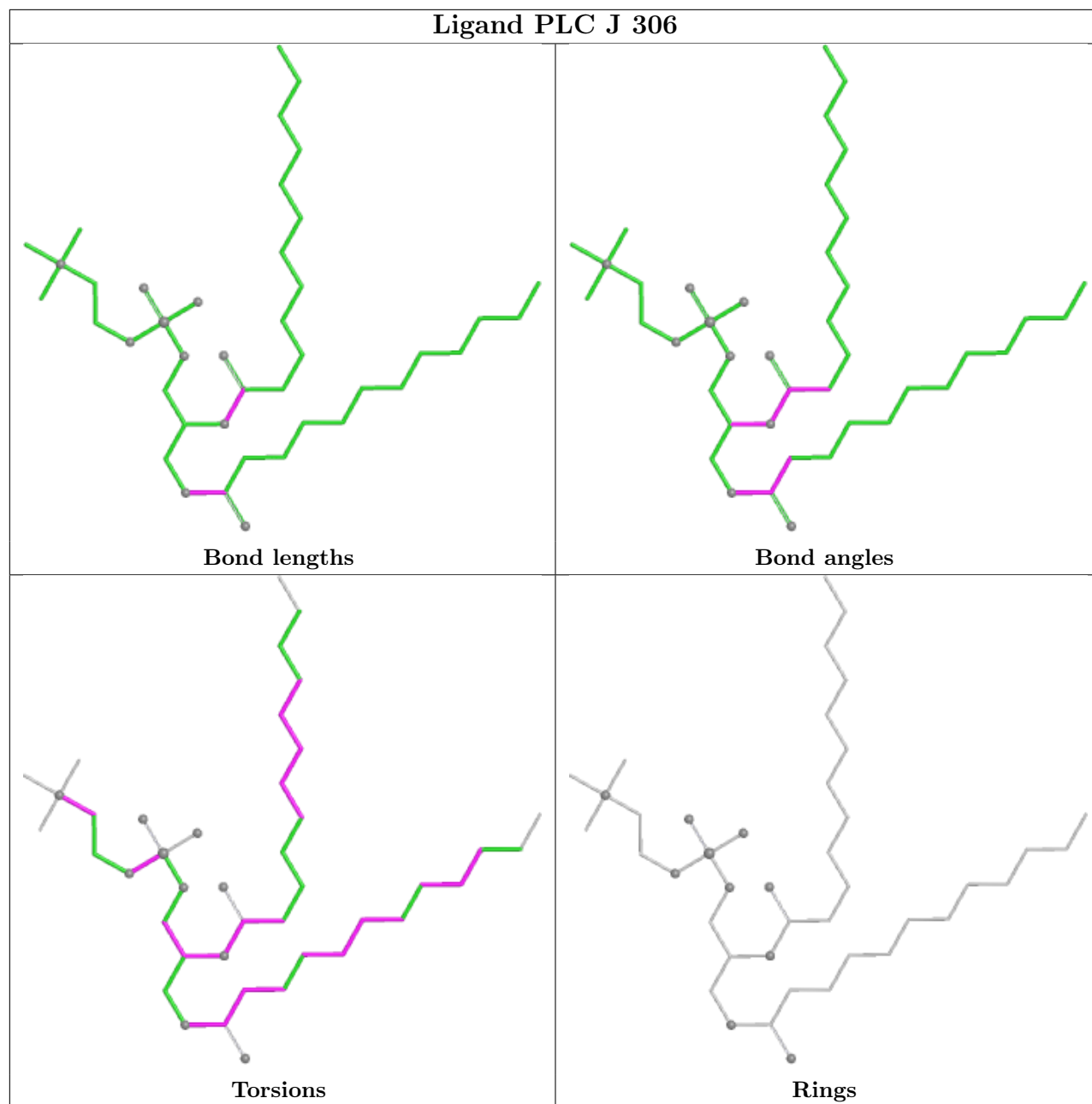


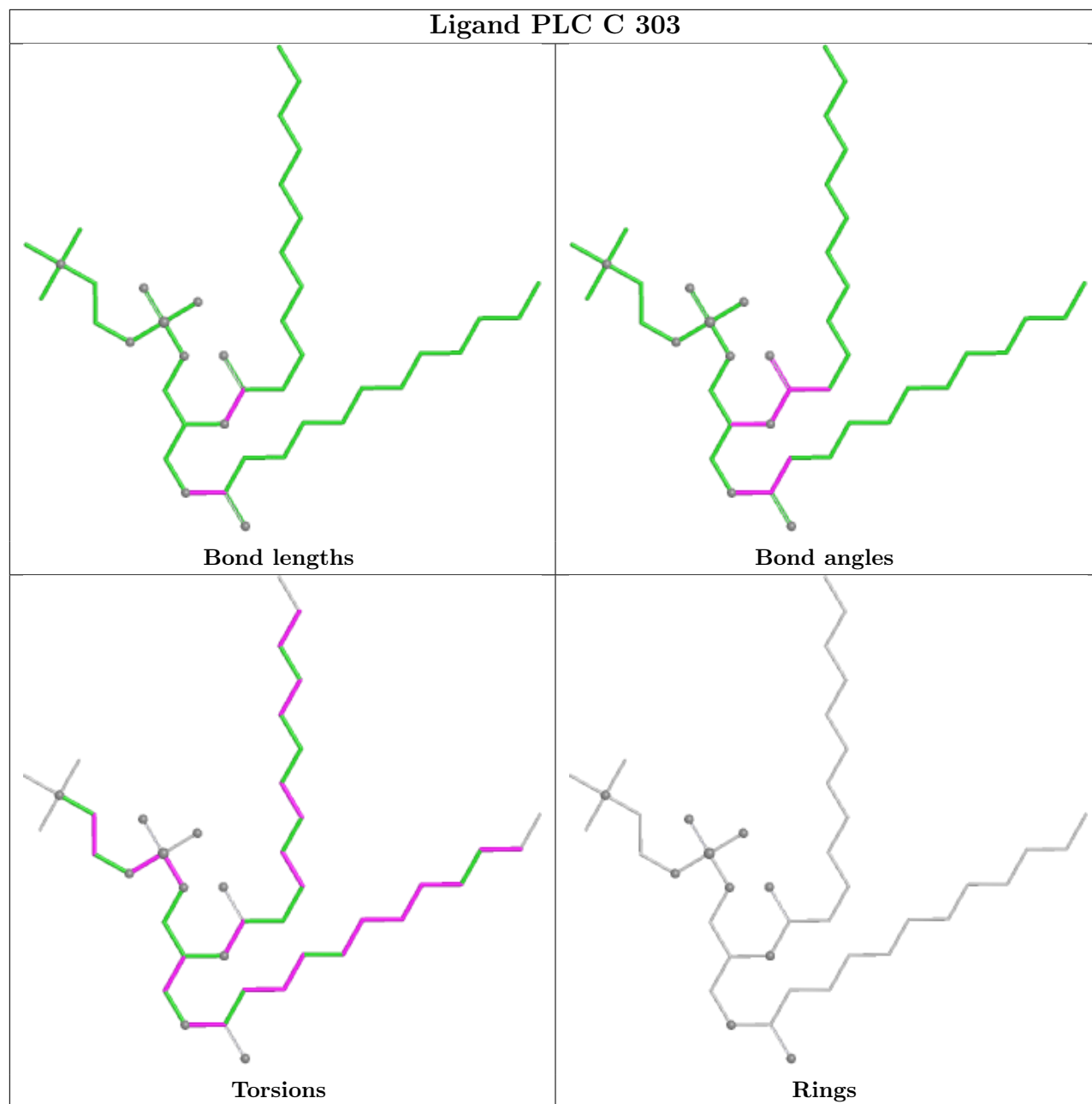


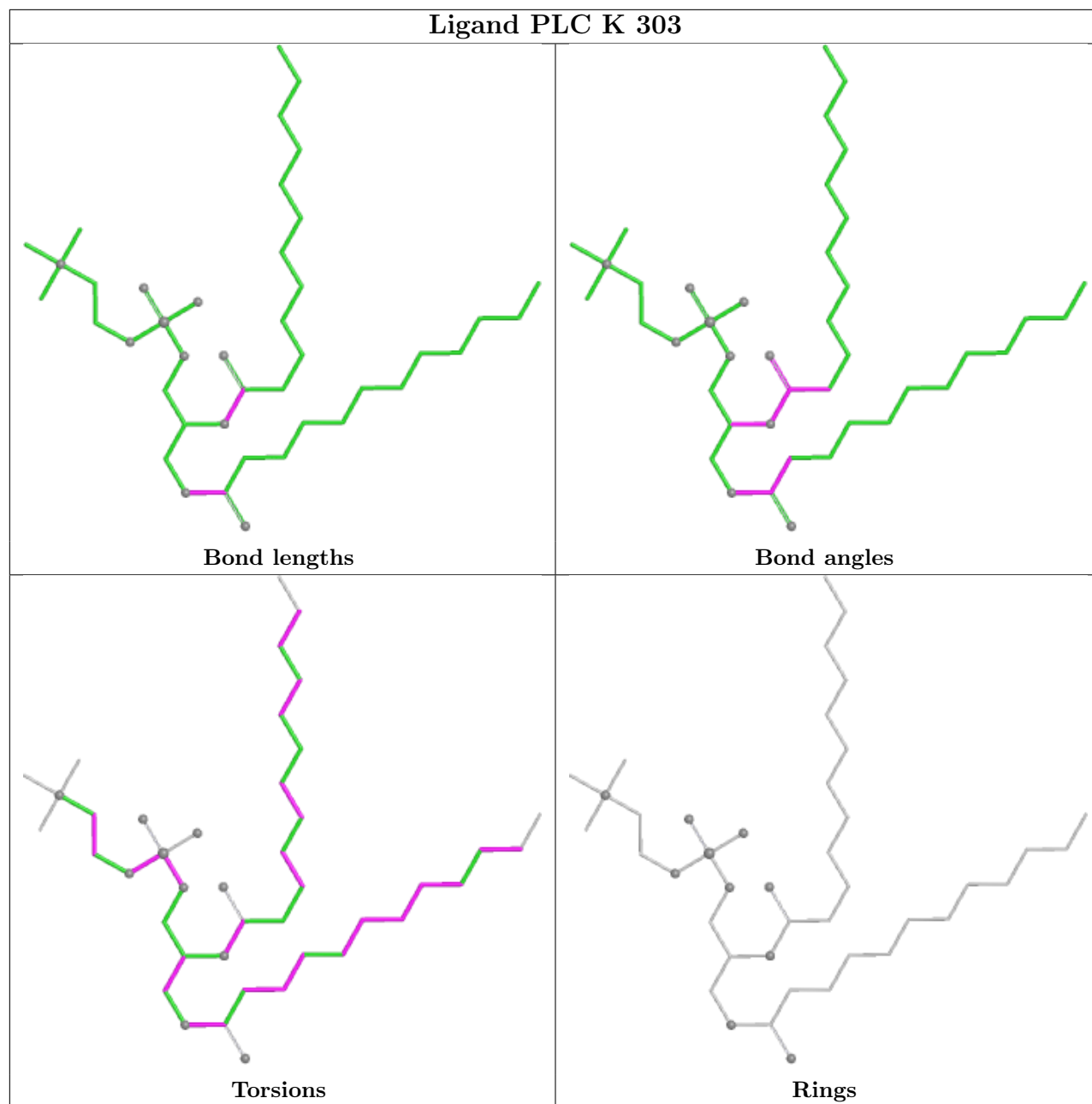


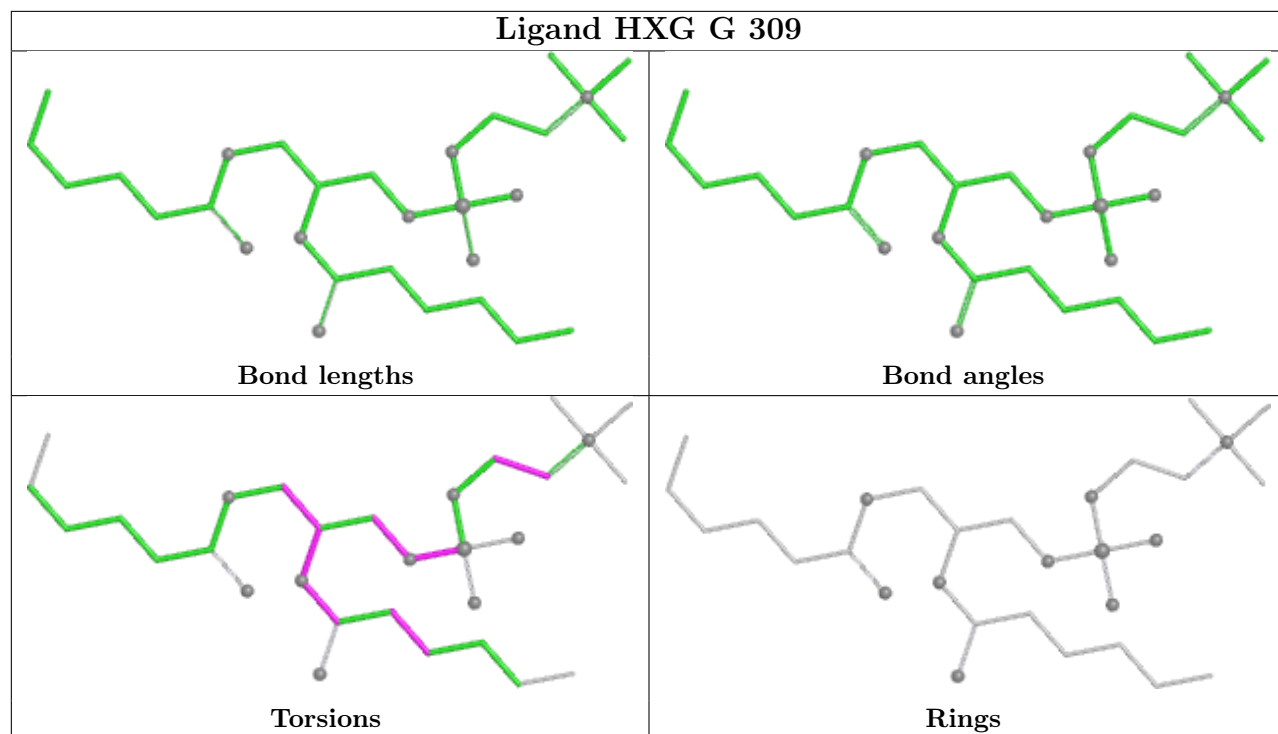


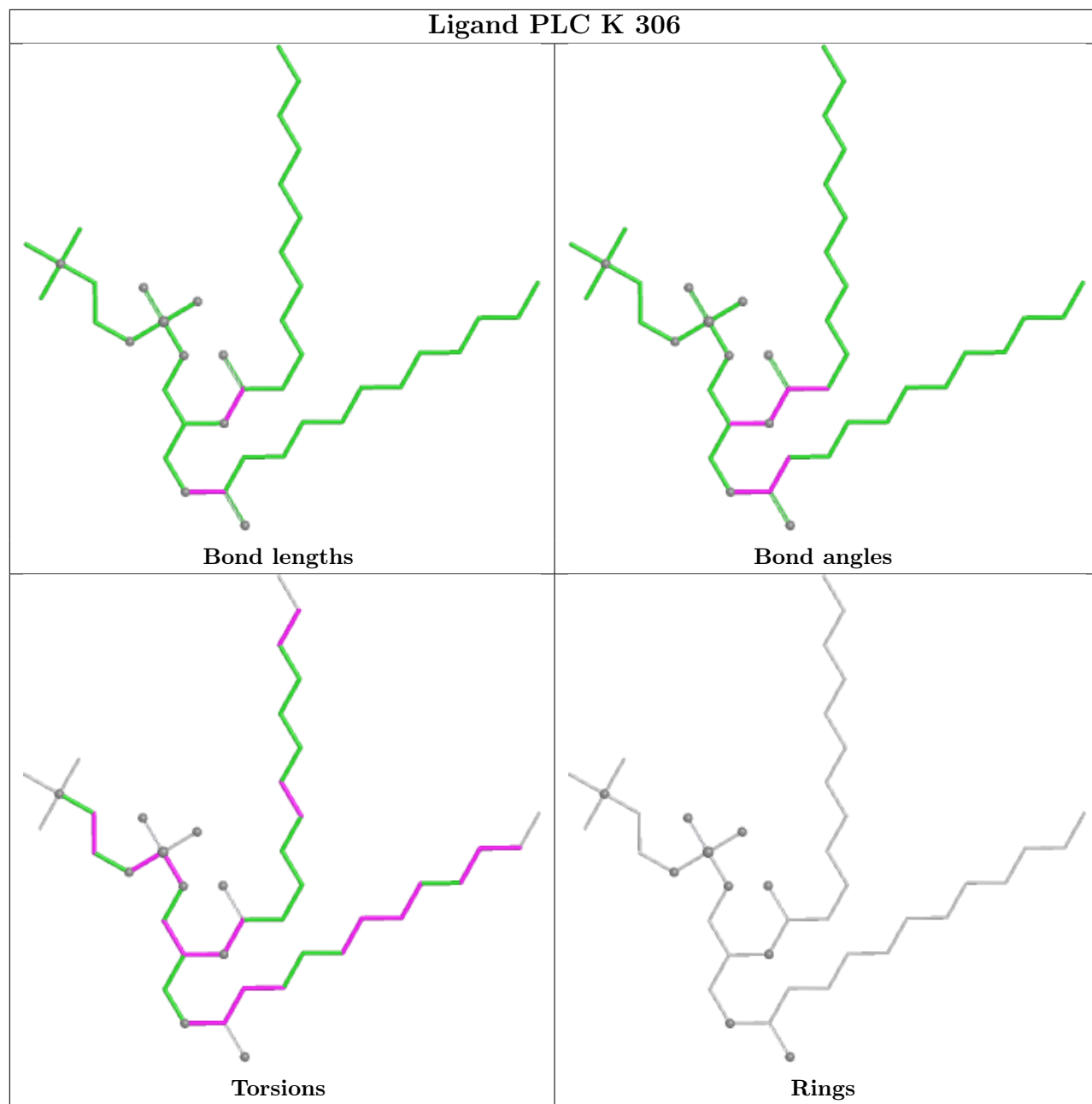


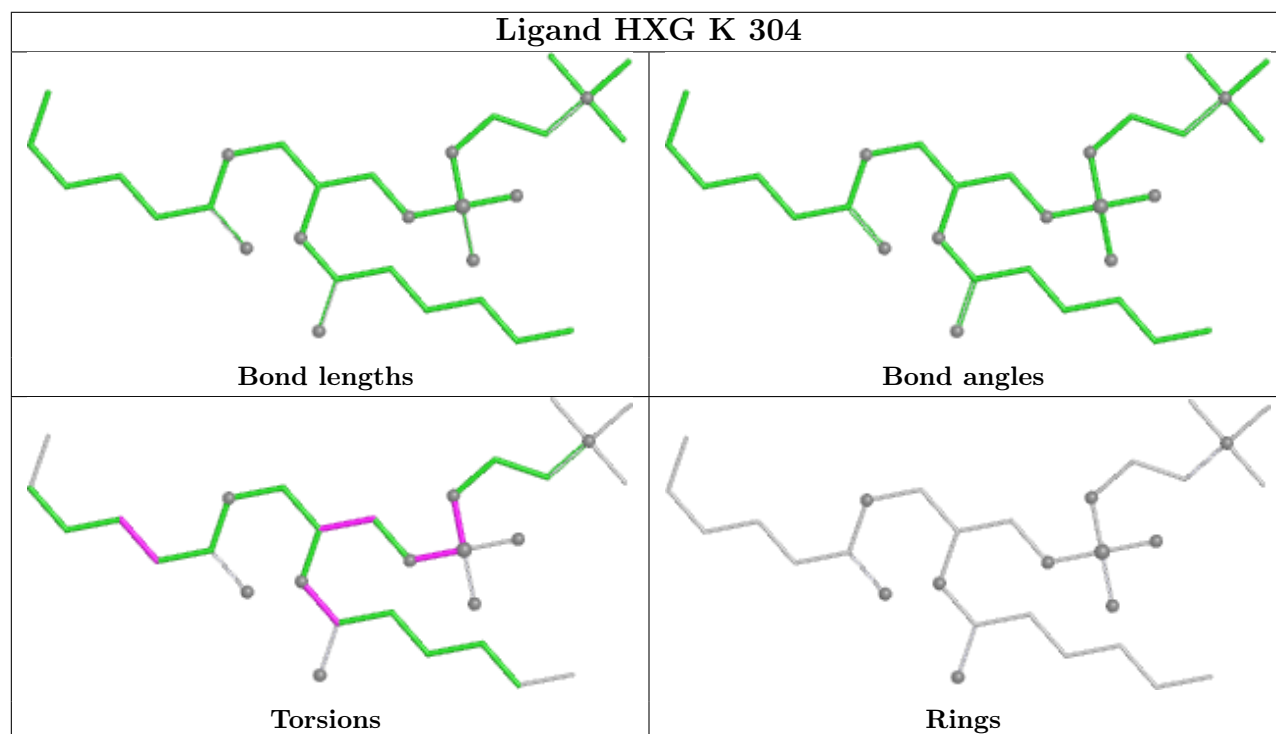
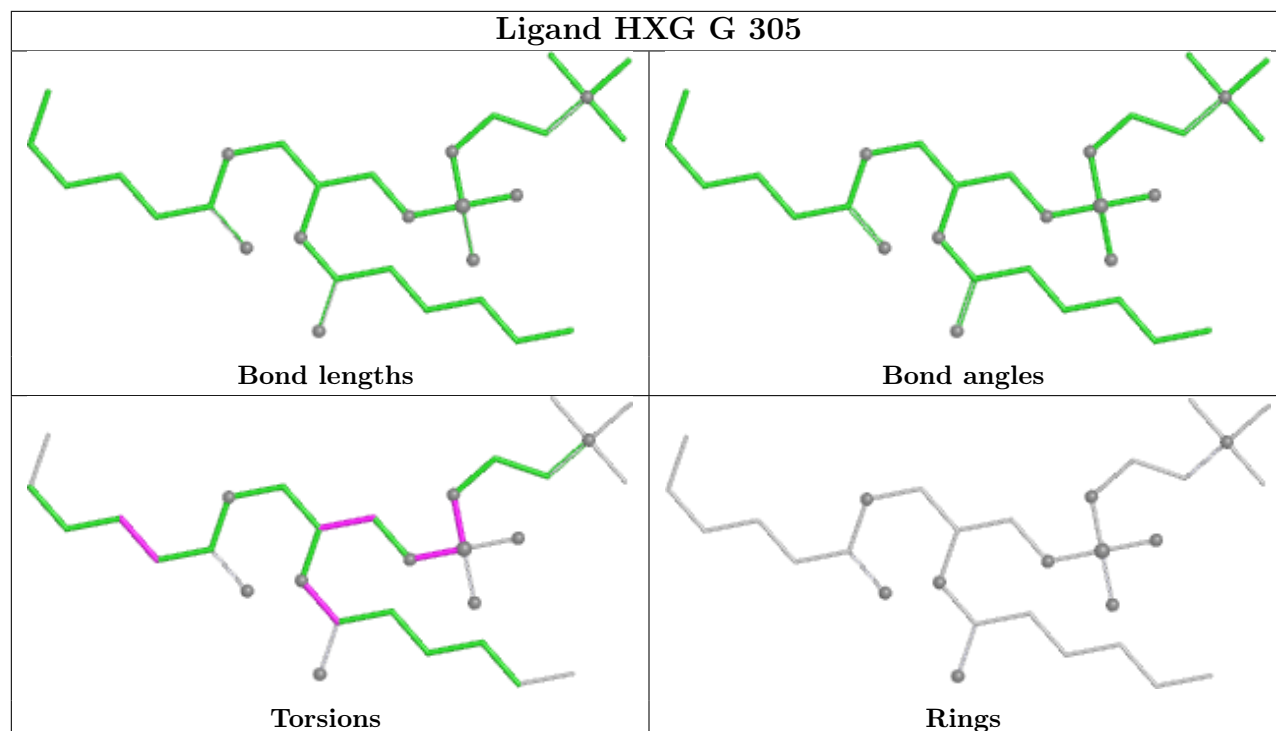


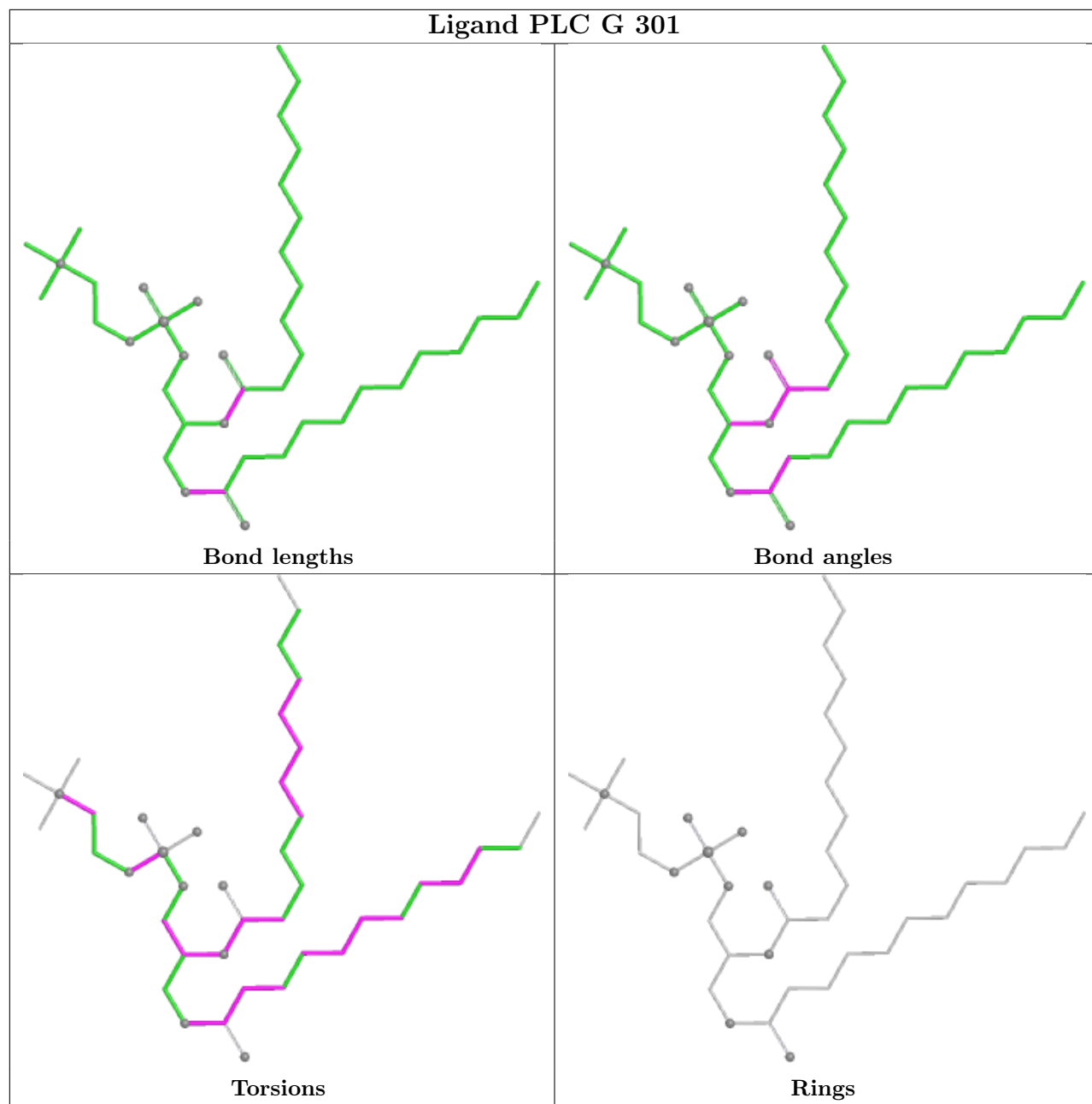


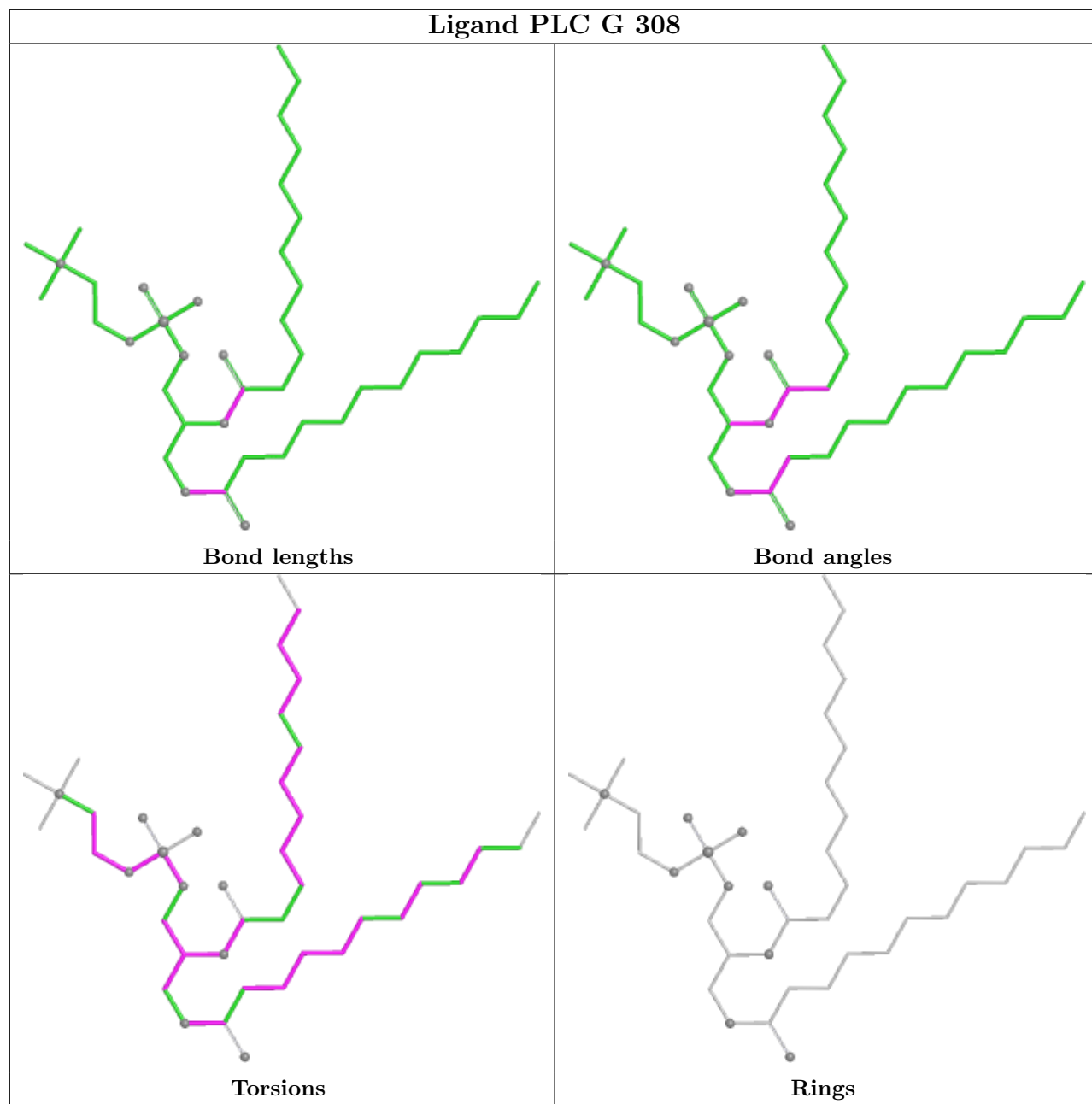


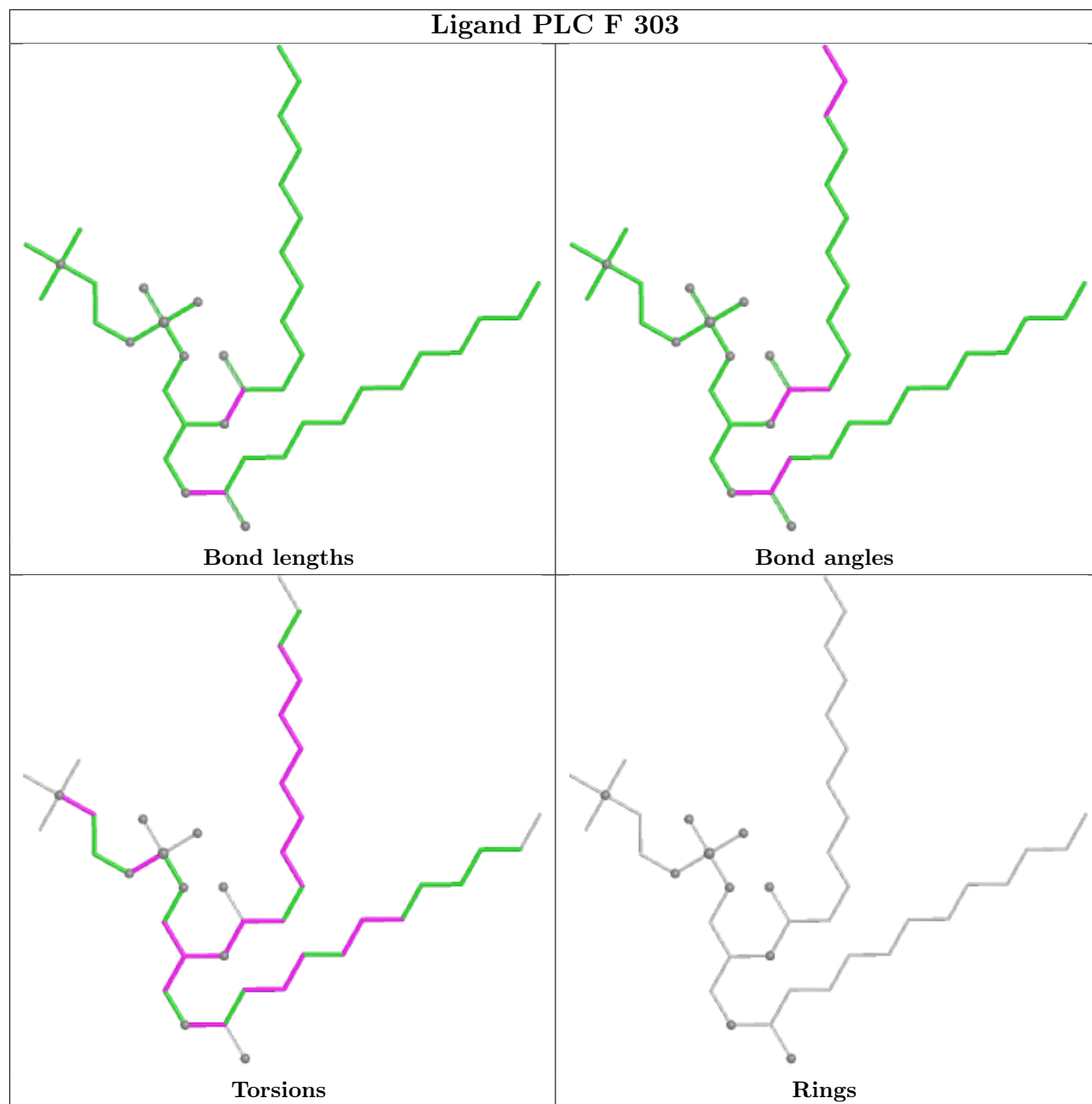


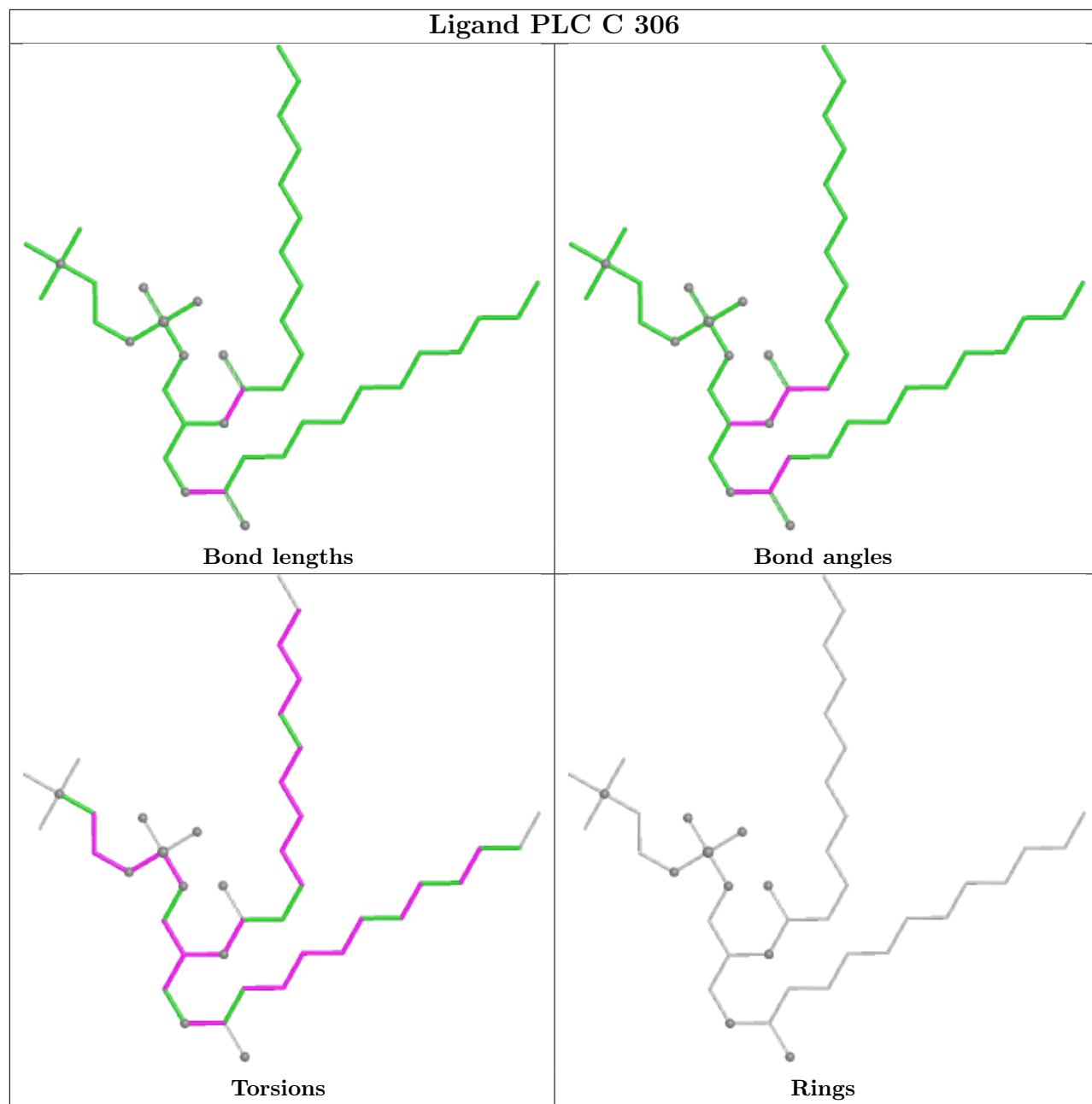


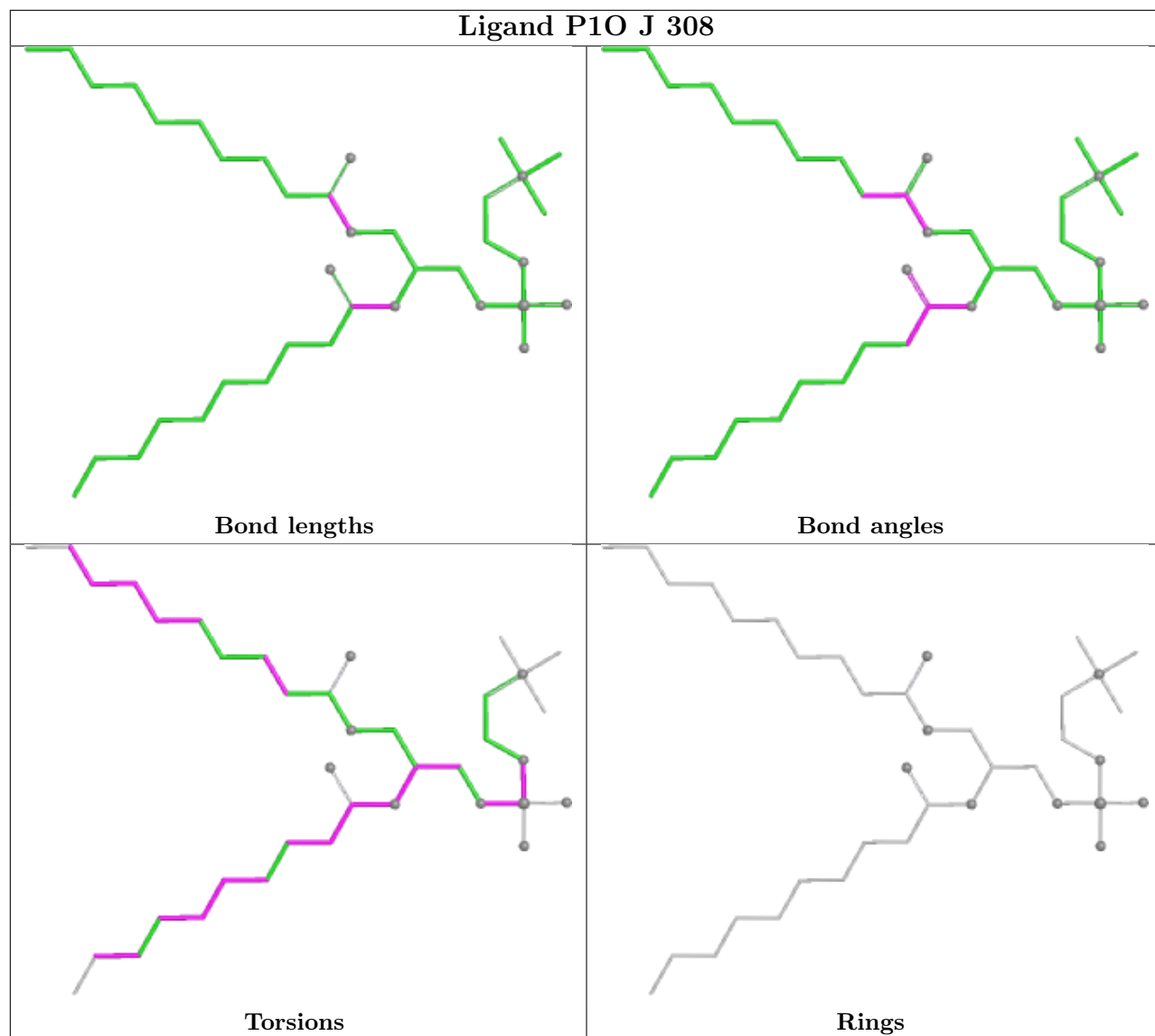


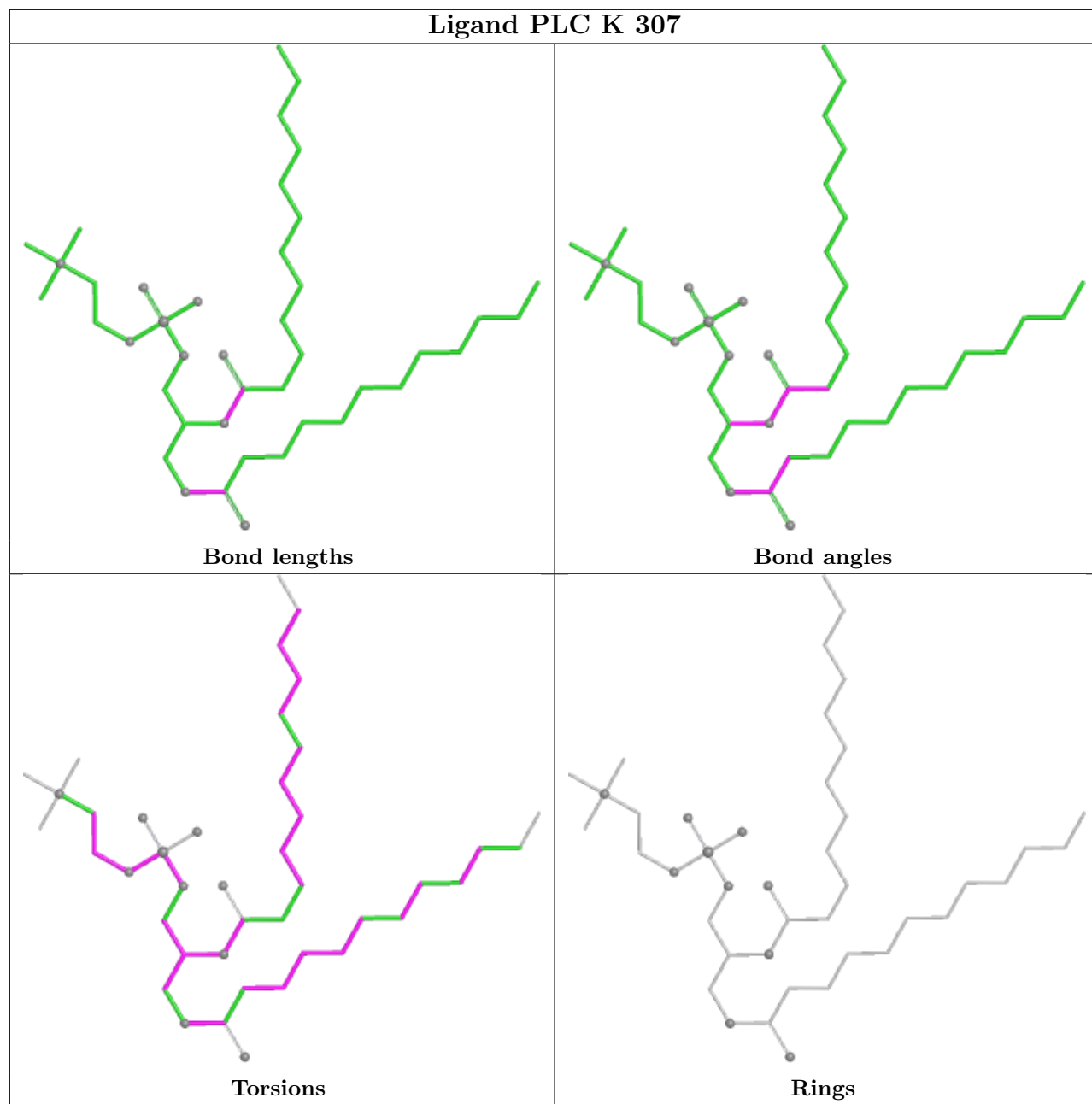


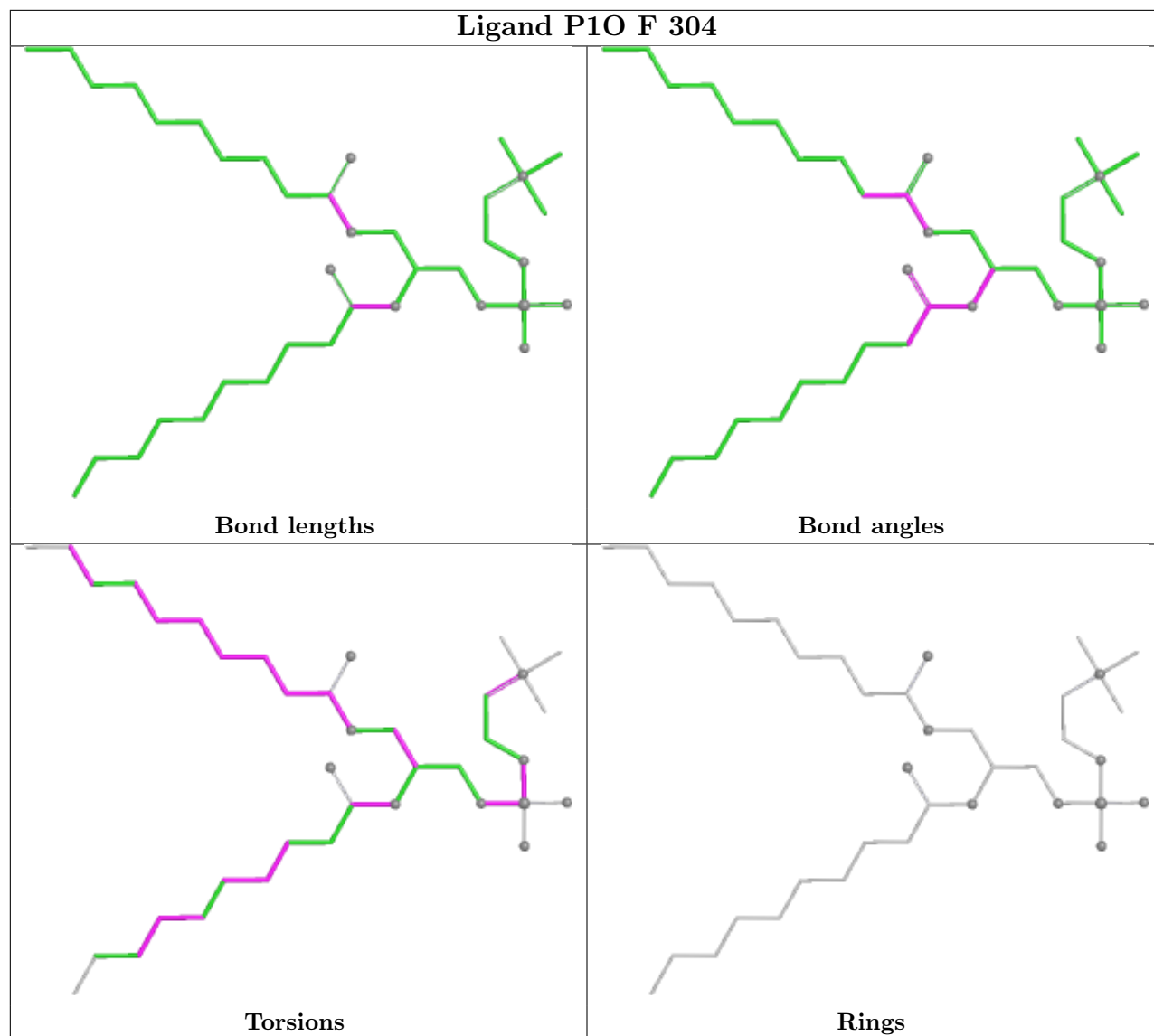


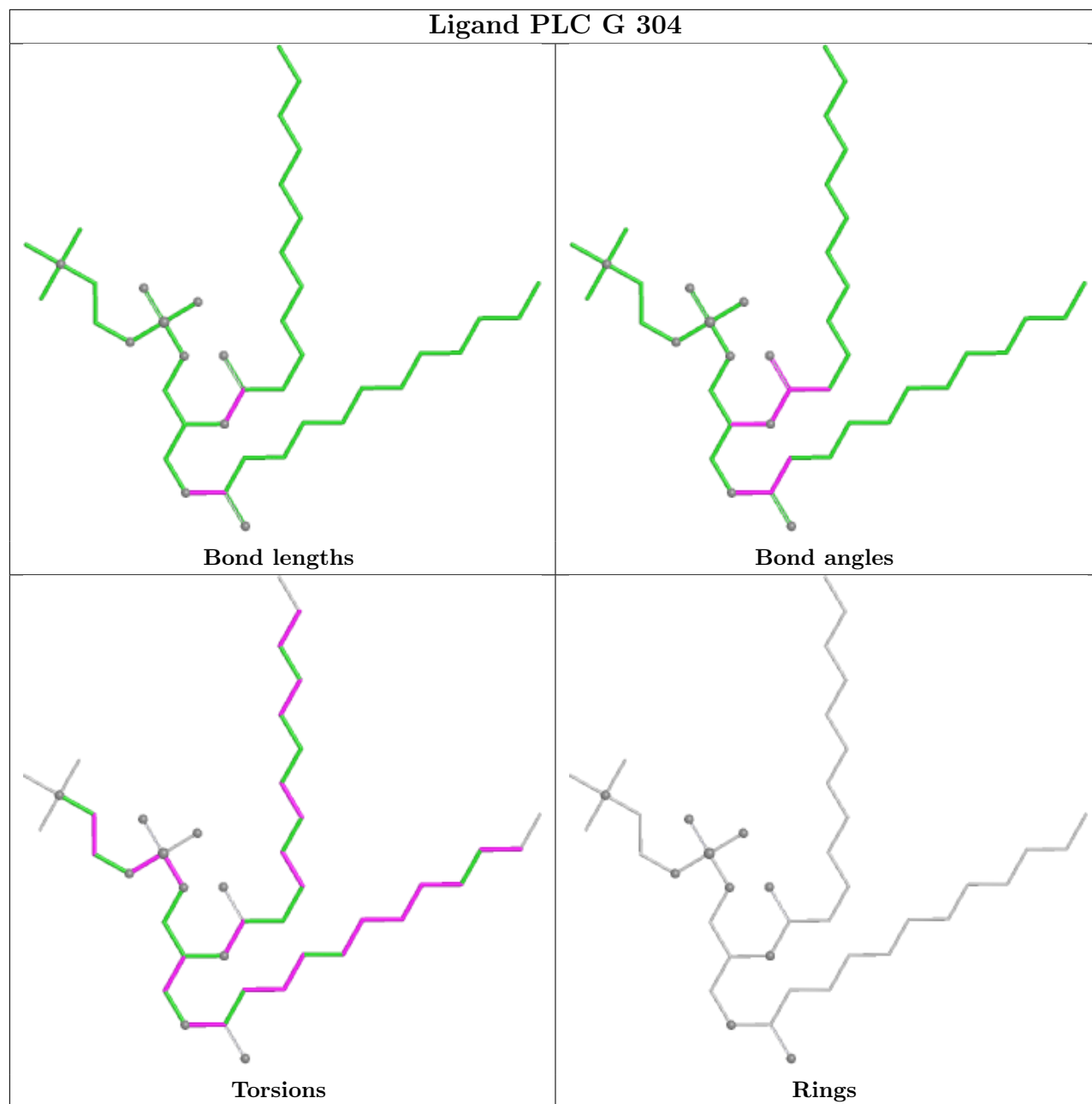


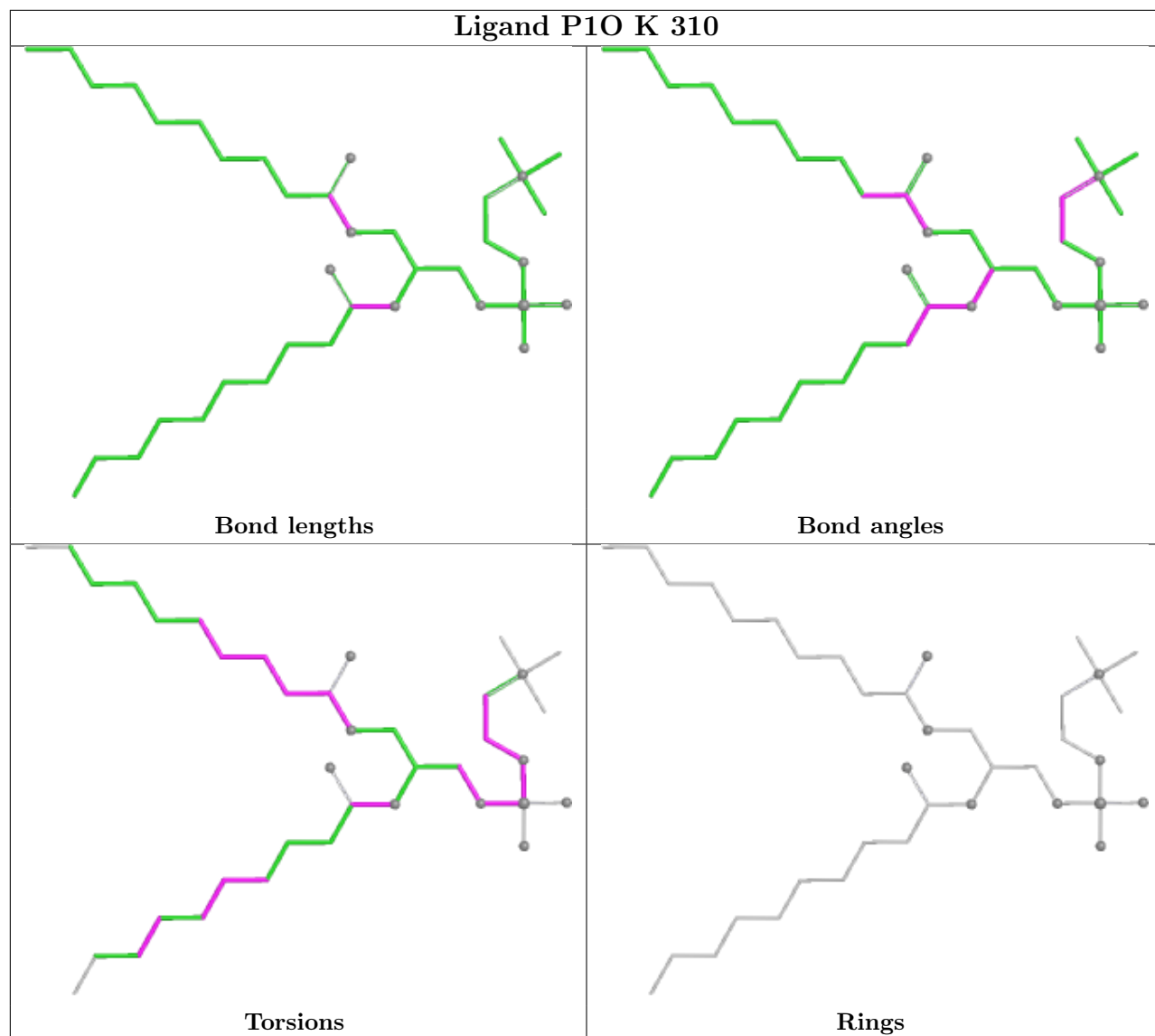


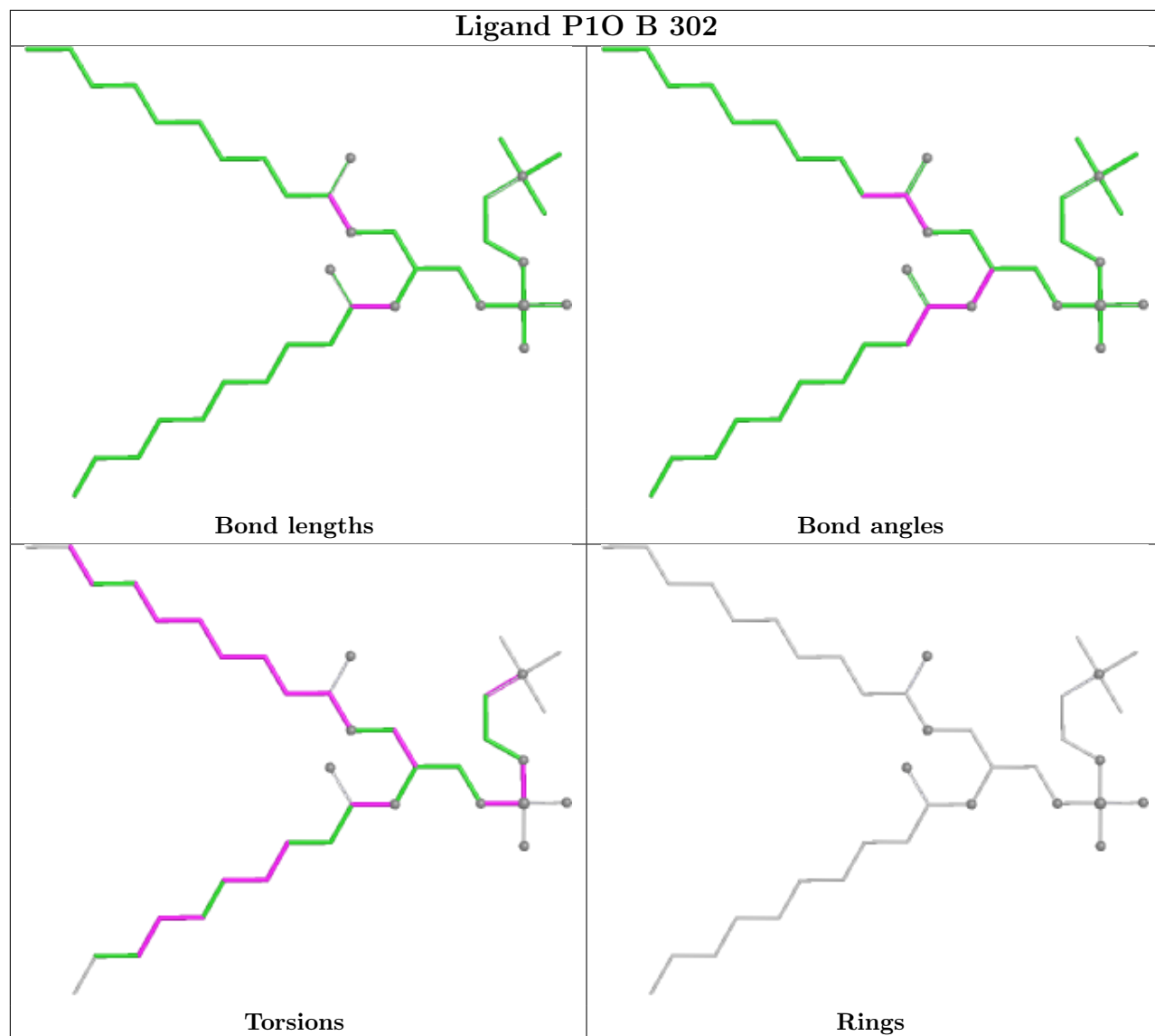


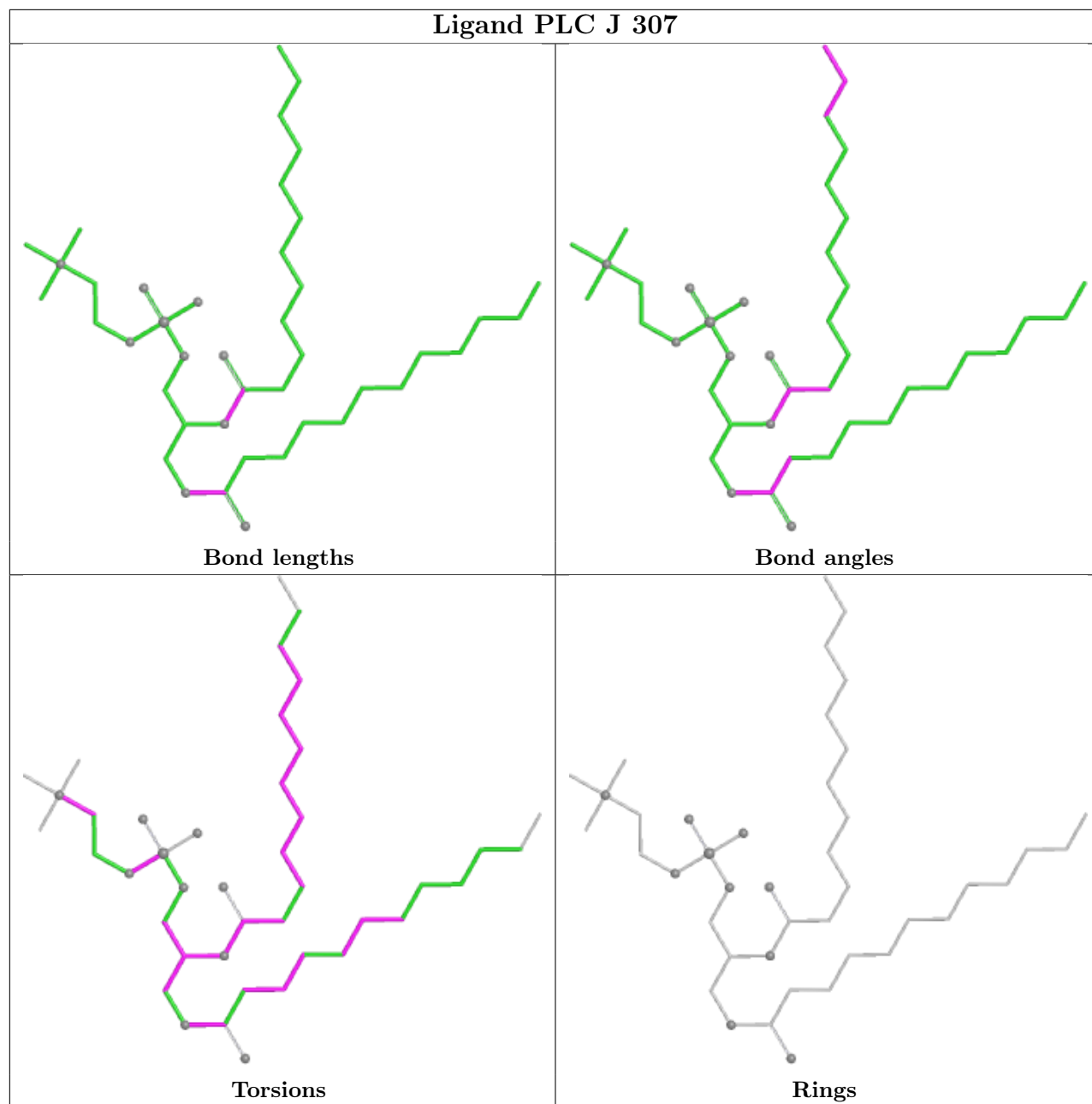


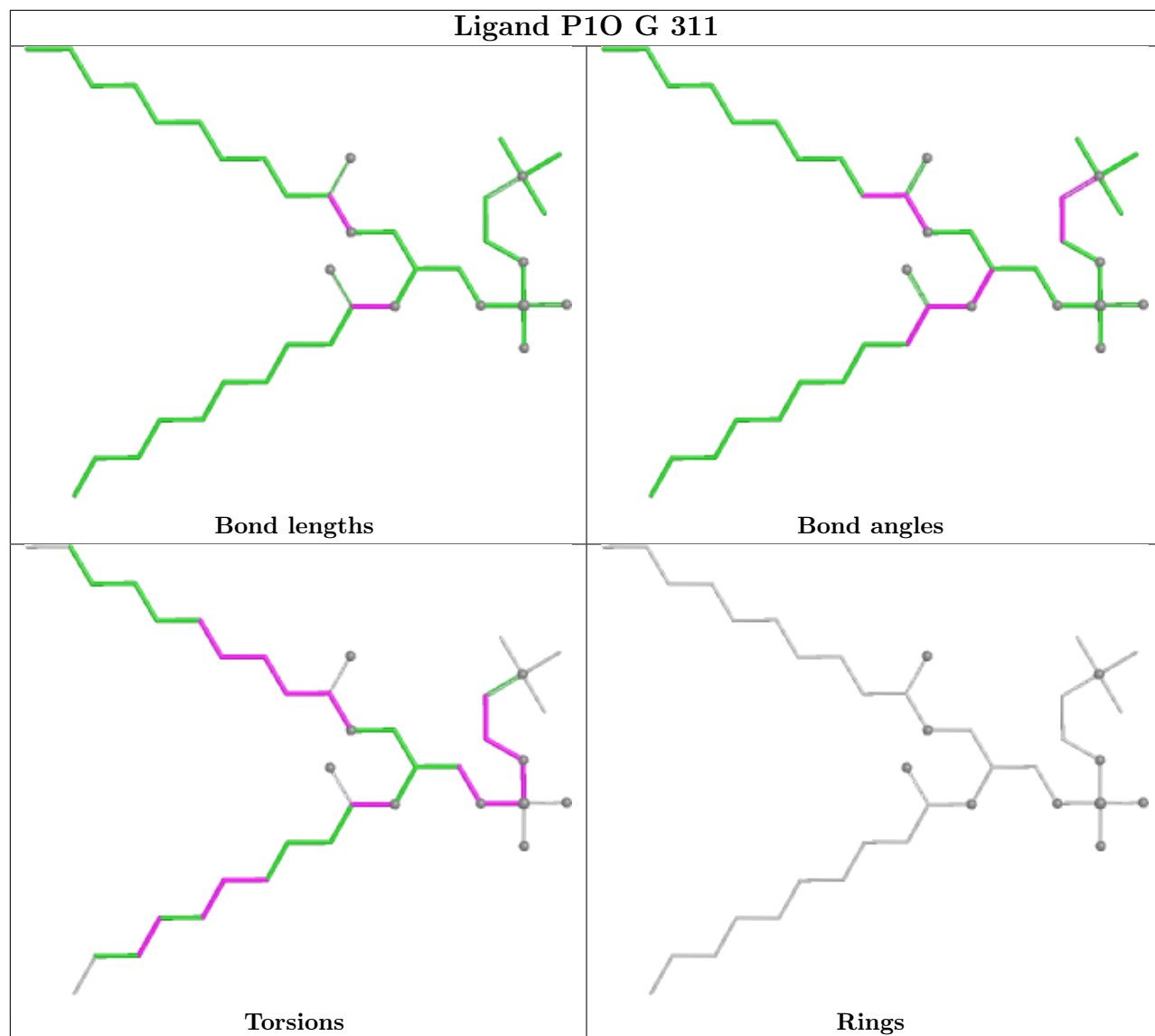


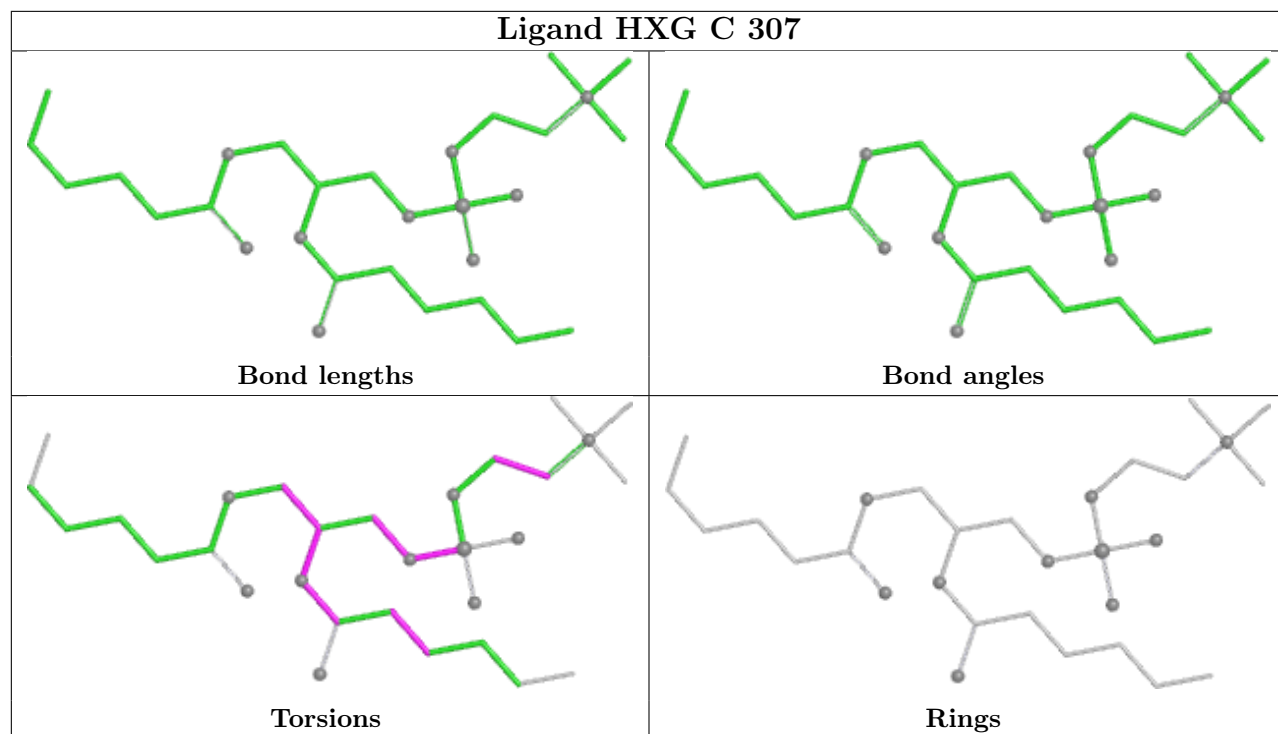


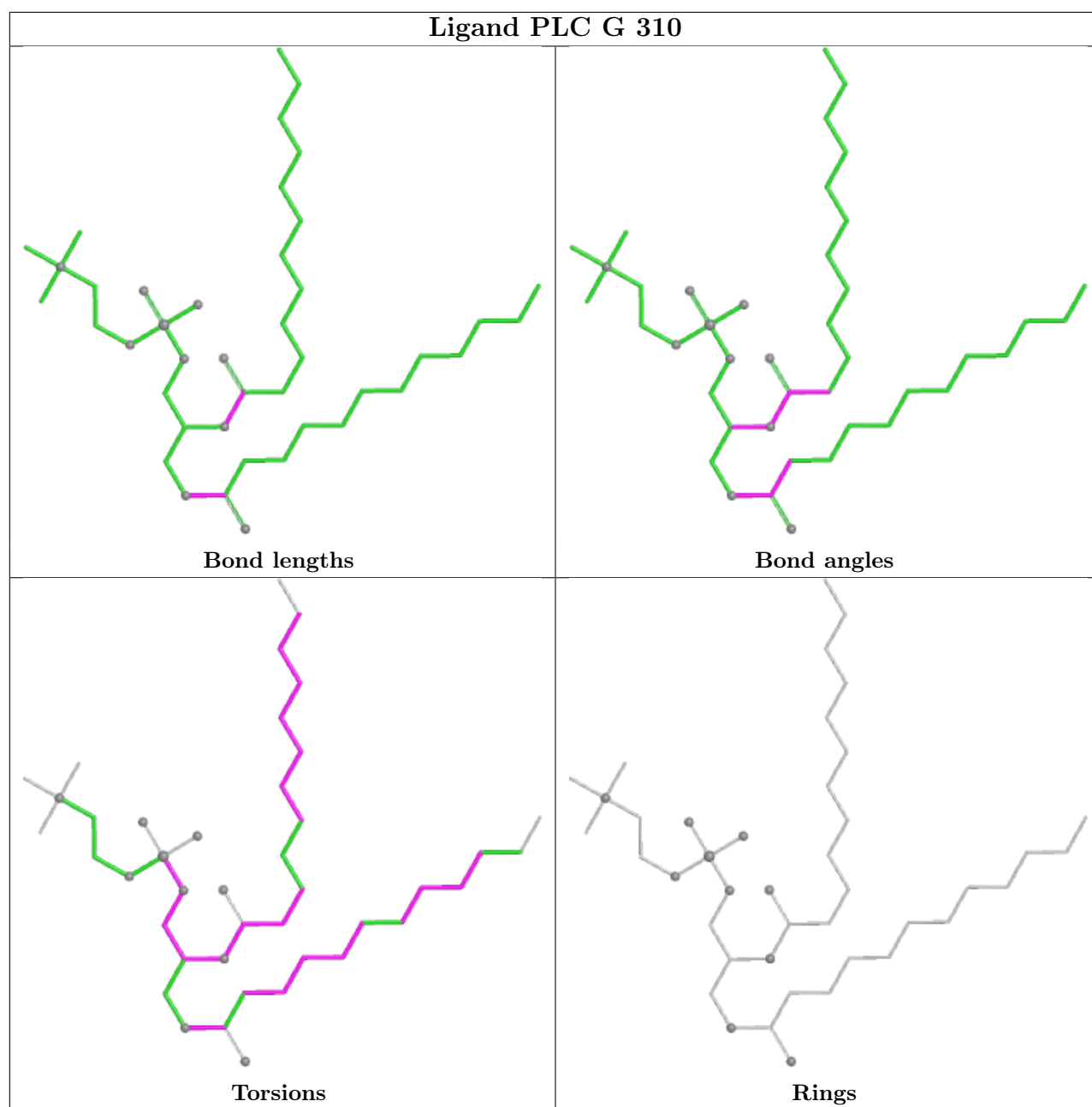












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

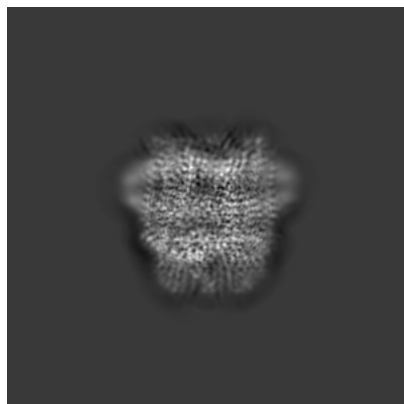
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40718. These allow visual inspection of the internal detail of the map and identification of artifacts.

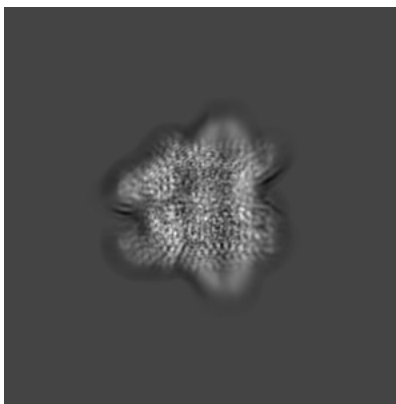
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

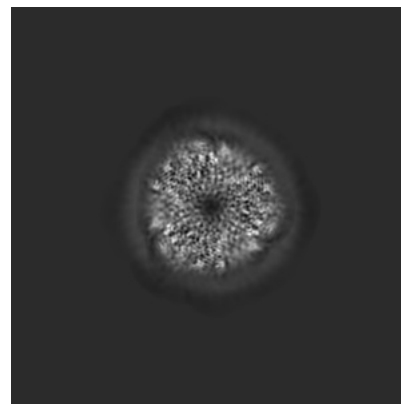
6.1.1 Primary map



X

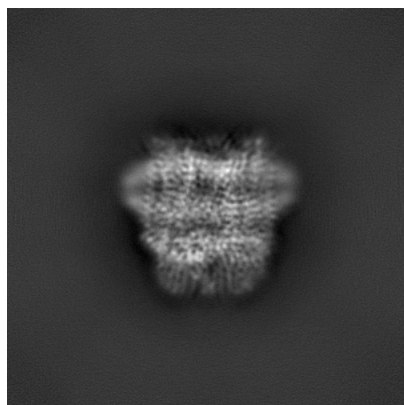


Y

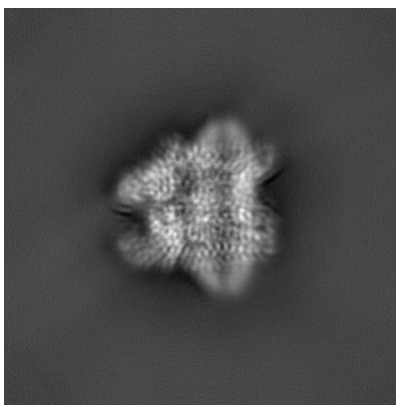


Z

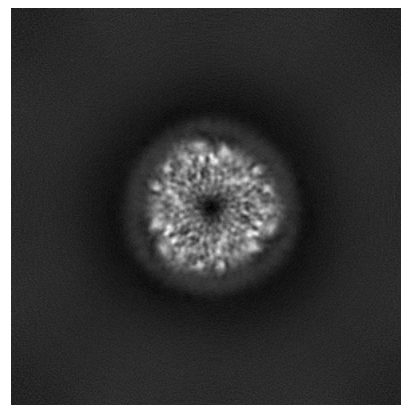
6.1.2 Raw map



X



Y



Z

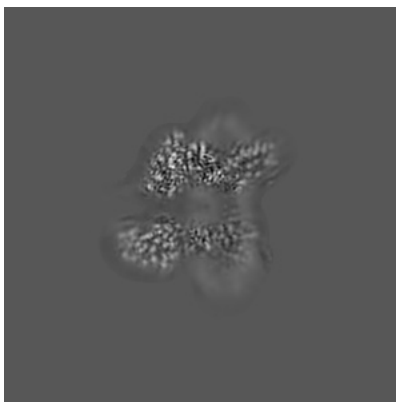
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

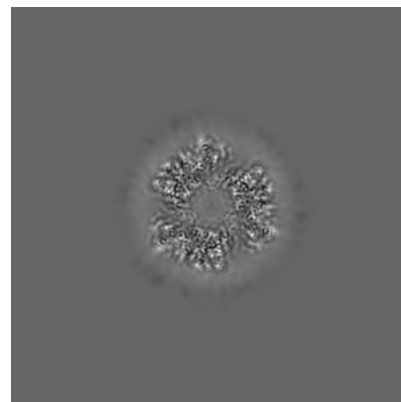
6.2.1 Primary map



X Index: 256

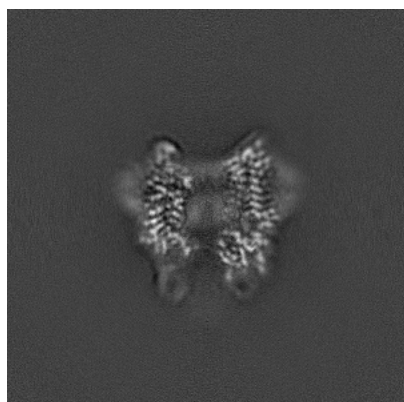


Y Index: 256

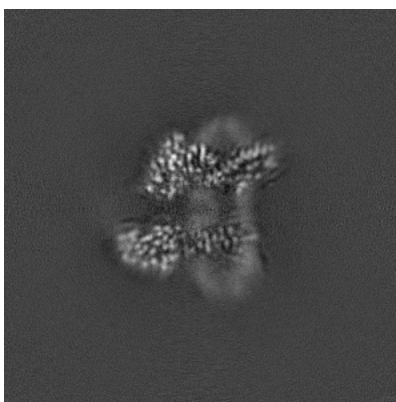


Z Index: 256

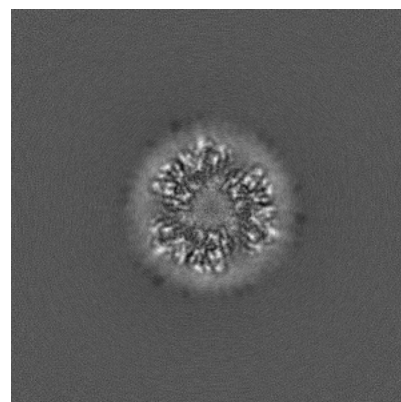
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

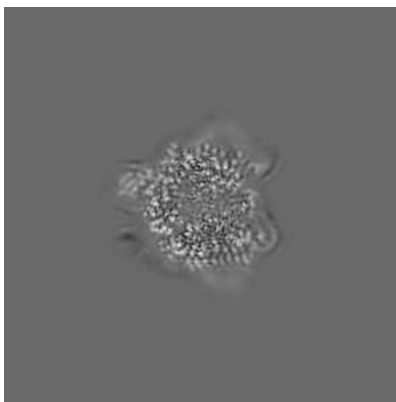
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

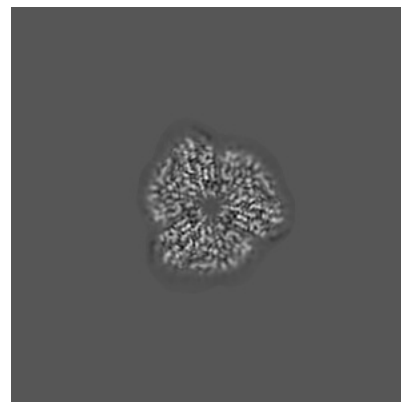
6.3.1 Primary map



X Index: 222

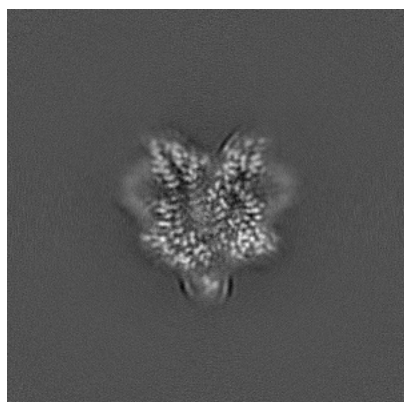


Y Index: 288

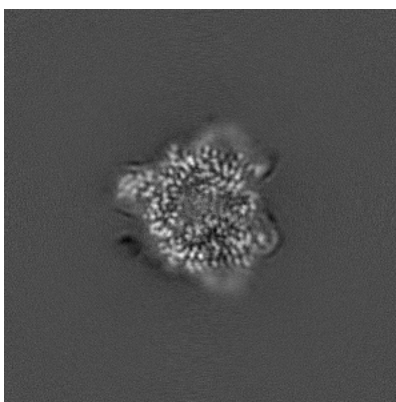


Z Index: 213

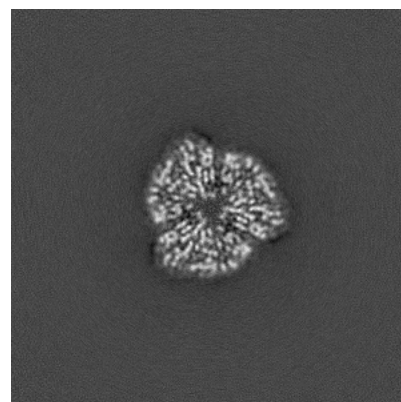
6.3.2 Raw map



X Index: 222



Y Index: 289

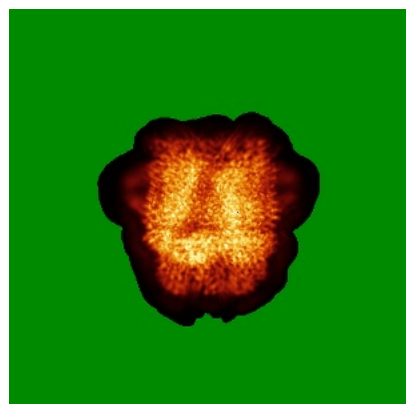


Z Index: 214

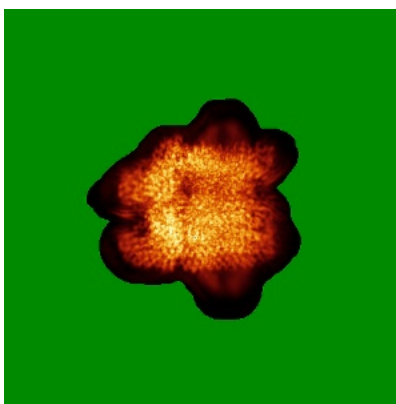
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

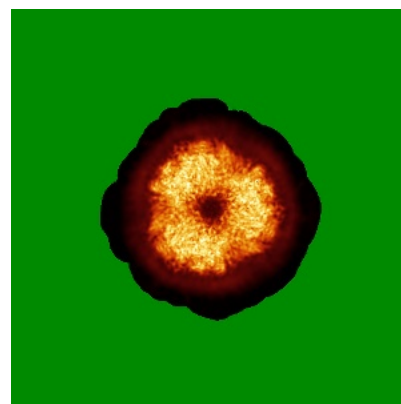
6.4.1 Primary map



X

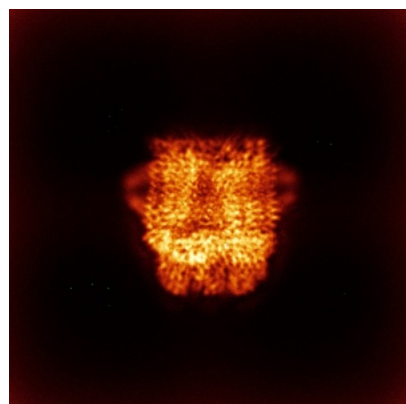


Y

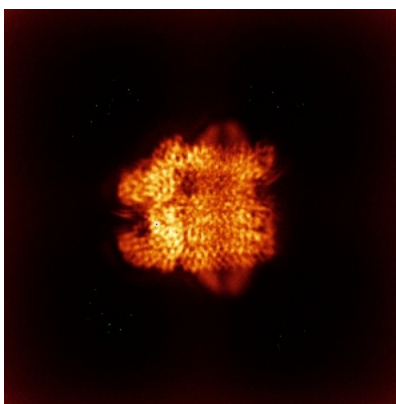


Z

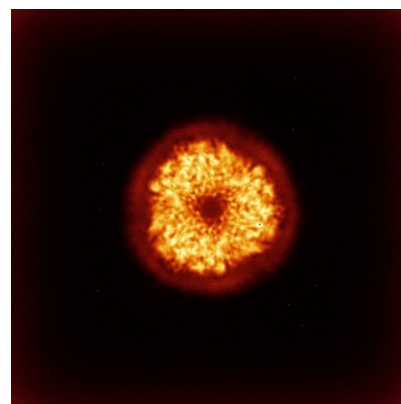
6.4.2 Raw map



X



Y

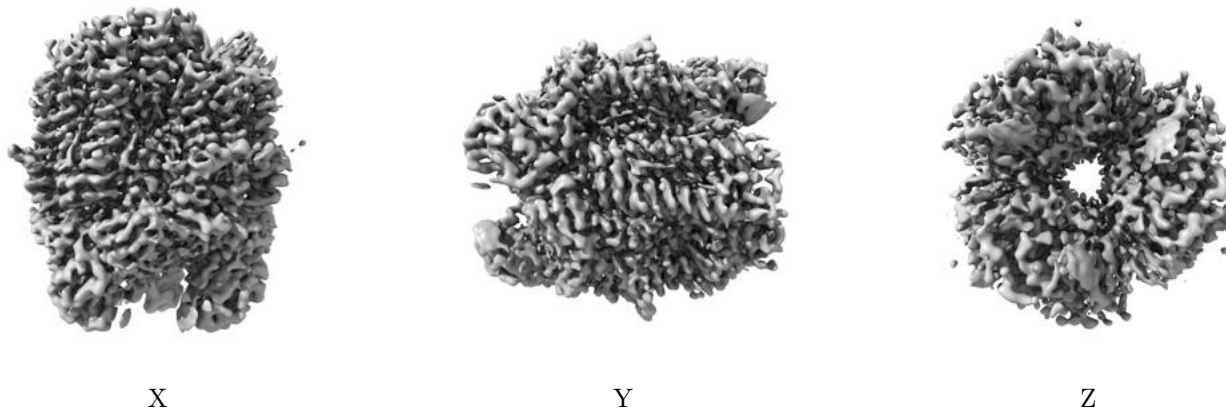


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

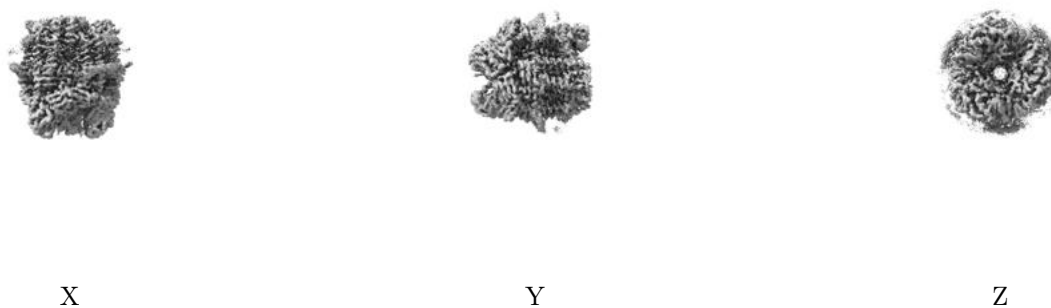
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

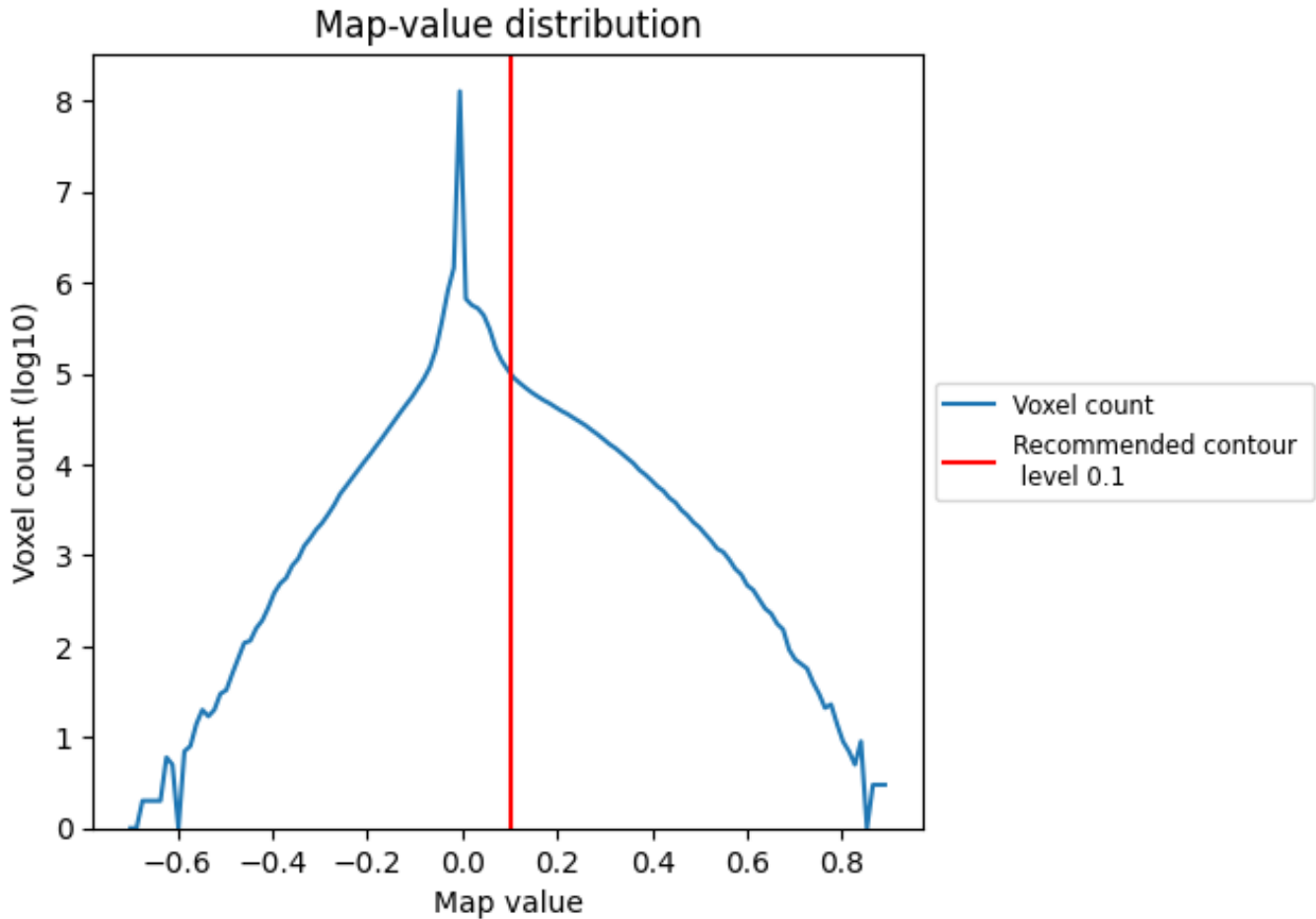
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

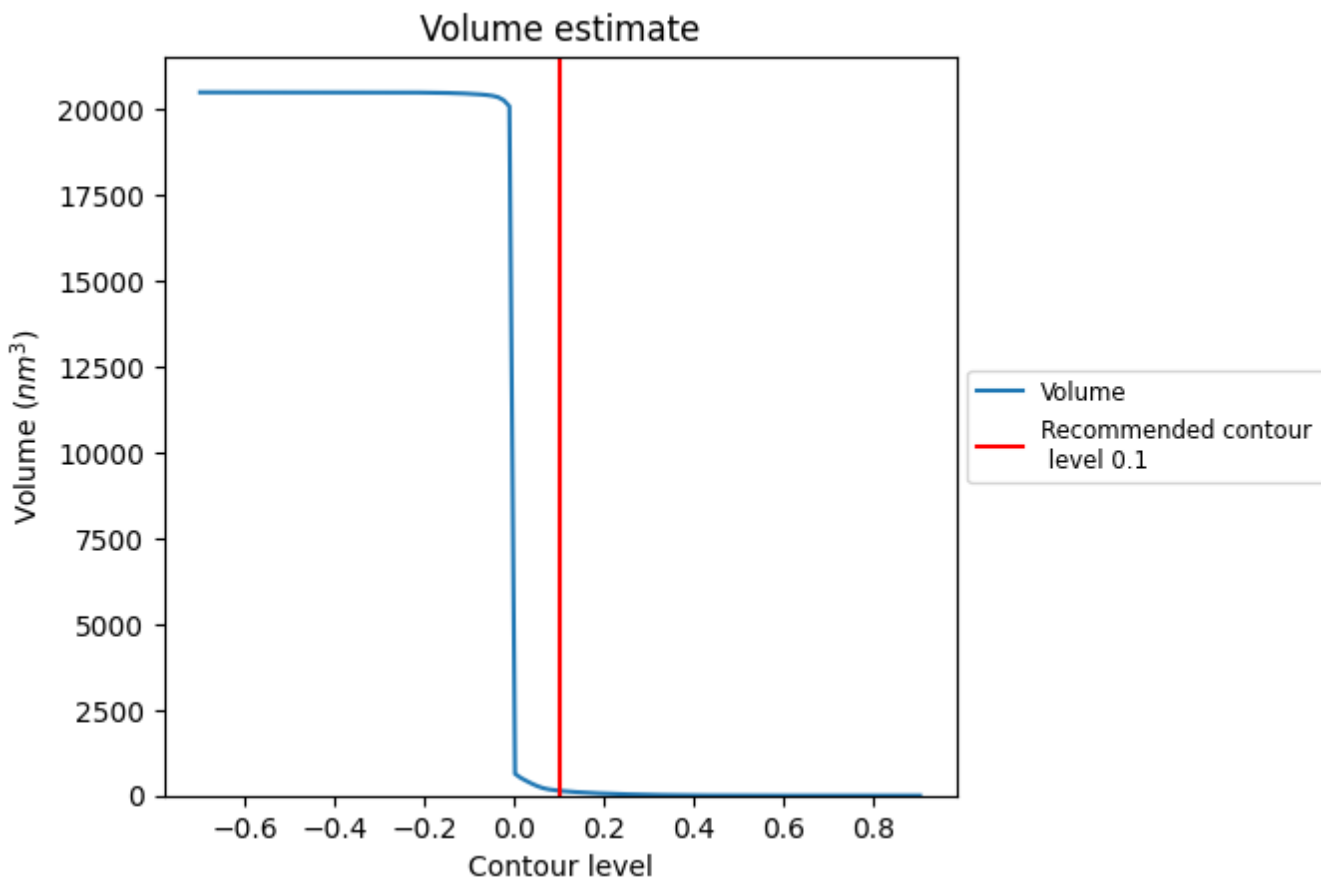
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

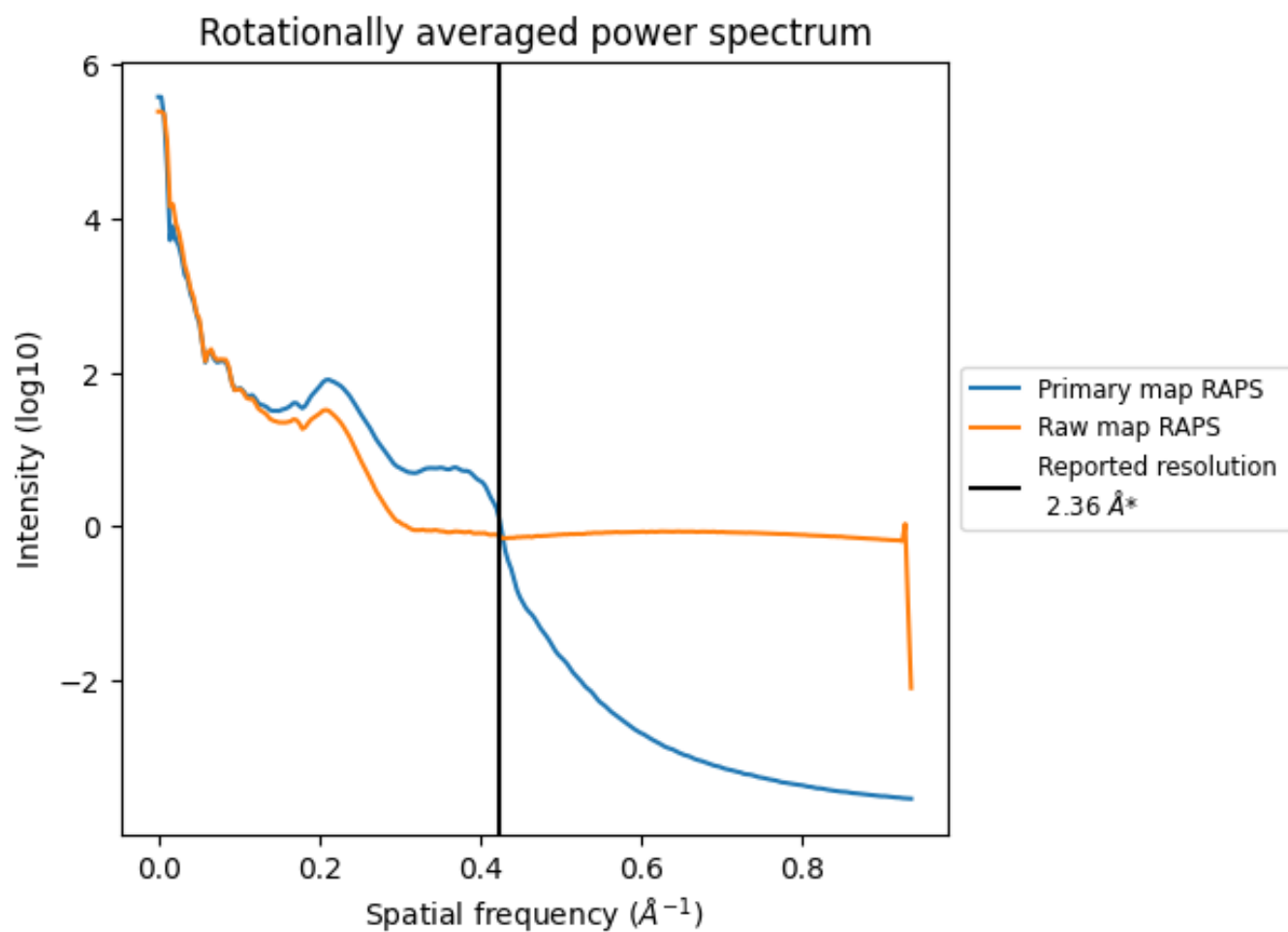
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 141 nm³; this corresponds to an approximate mass of 127 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

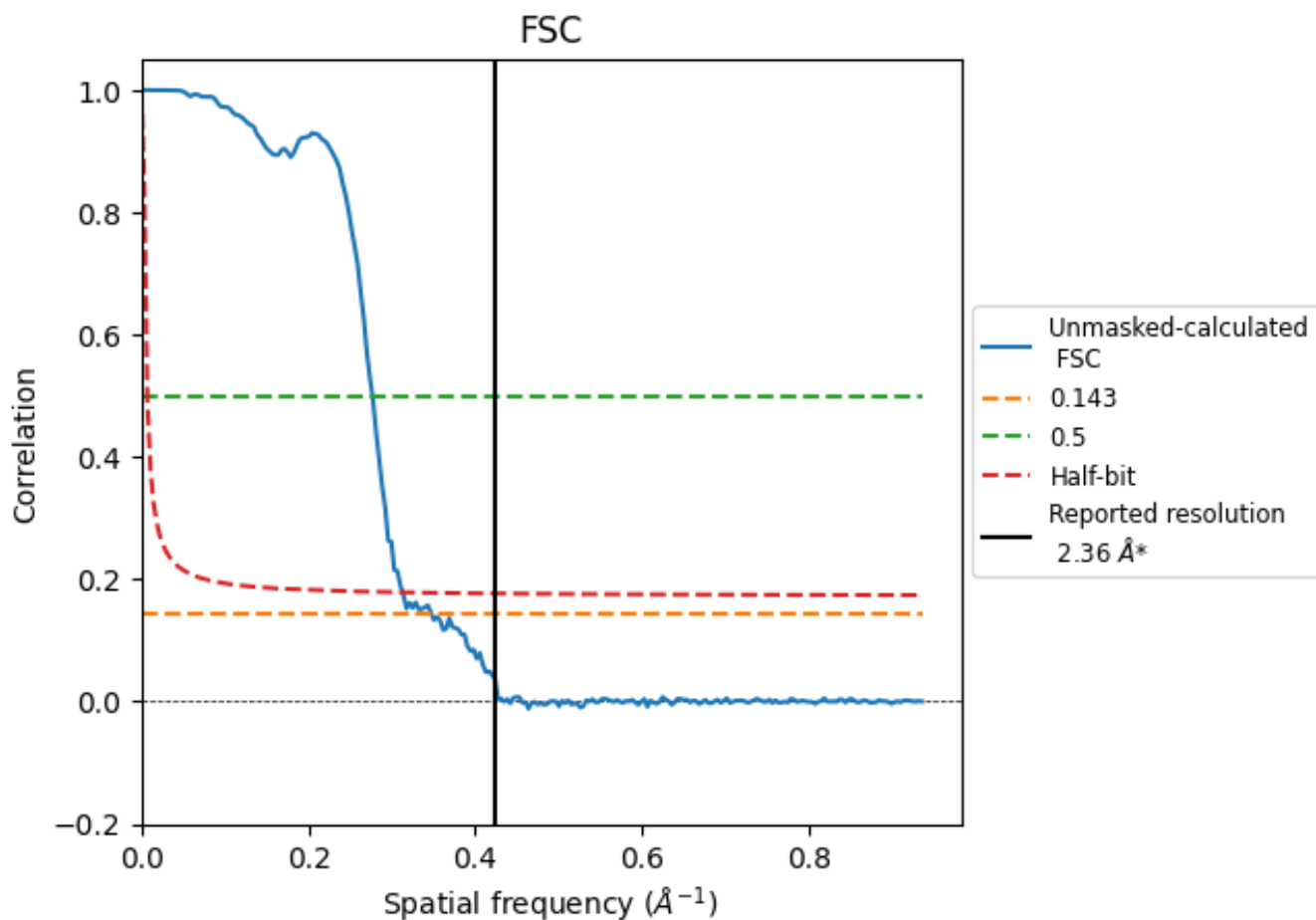


*Reported resolution corresponds to spatial frequency of 0.424 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.424 Å⁻¹

8.2 Resolution estimates [i](#)

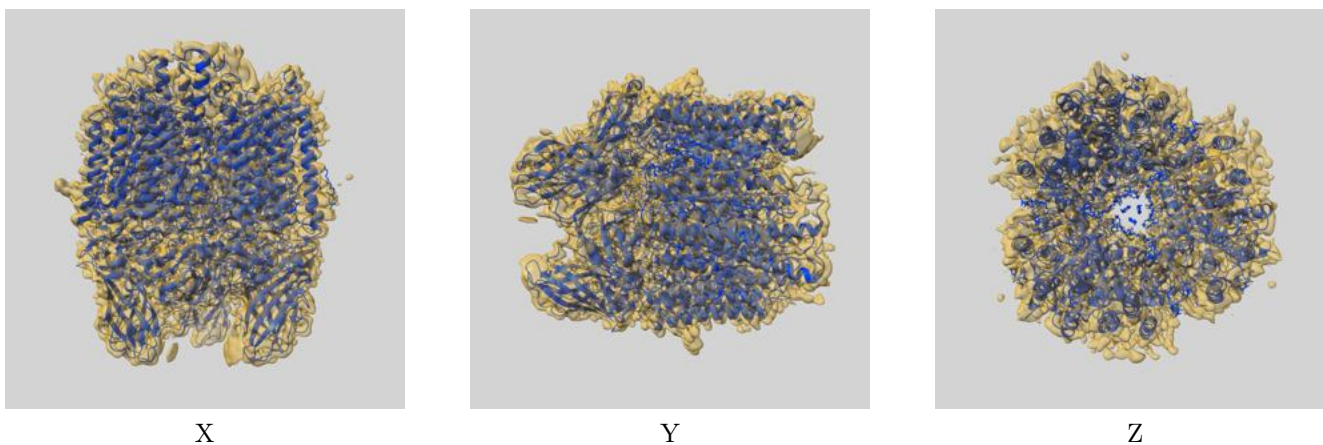
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.36	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.88	3.61	3.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.88 differs from the reported value 2.36 by more than 10 %

9 Map-model fit [i](#)

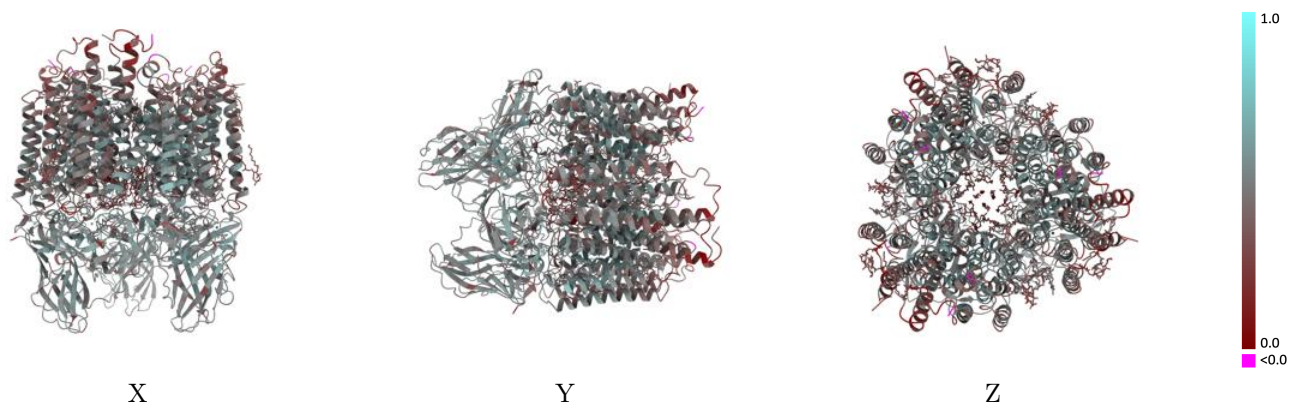
This section contains information regarding the fit between EMDB map EMD-40718 and PDB model 8SR2. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



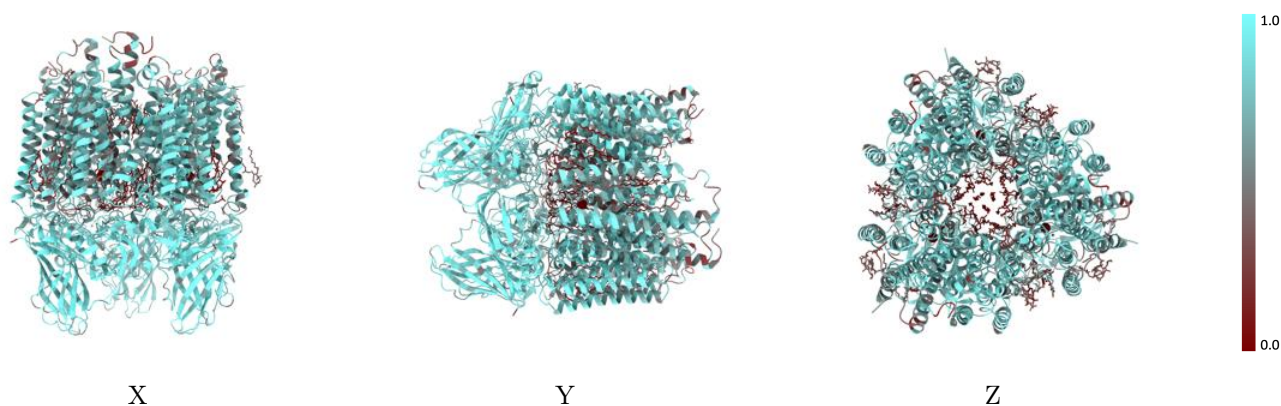
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



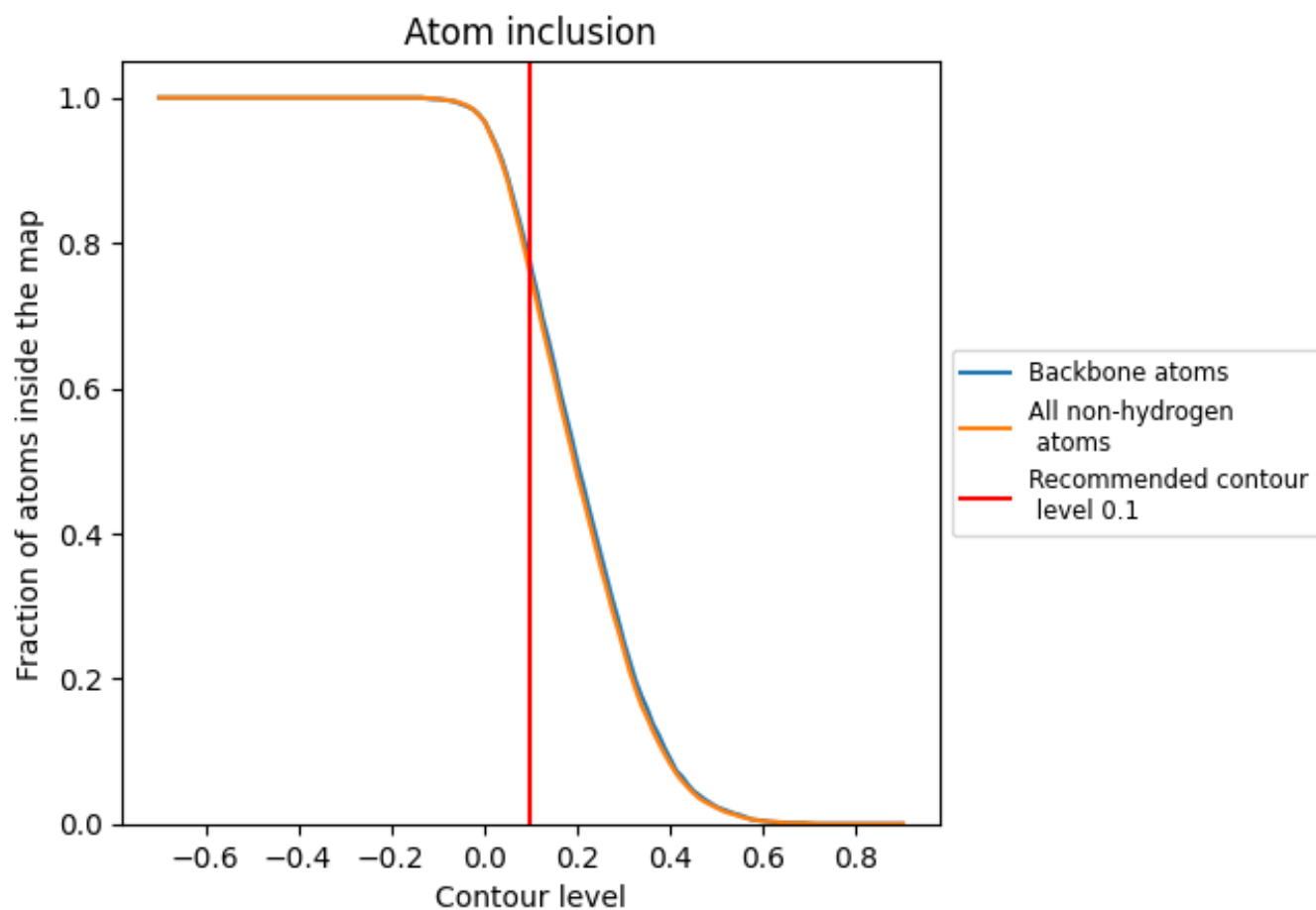
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).





















9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7570	 0.4520
A	 0.8510	 0.4830
B	 0.7690	 0.4690
C	 0.6240	 0.3840
E	 0.8500	 0.4860
F	 0.7520	 0.4680
G	 0.6290	 0.3990
I	 0.8490	 0.4860
J	 0.7550	 0.4690
K	 0.6360	 0.4000

