



Full wwPDB EM Validation Report ⓘ

Nov 10, 2024 – 03:48 pm GMT

PDB ID : 8AB7
EMDB ID : EMD-15313
Title : Complex III₂ from *Yarrowia lipolytica*, atovaquone and antimycin A bound
Authors : Wieferig, J.P.; Kuhlbrandt, W.
Deposited on : 2022-07-04
Resolution : 3.30 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

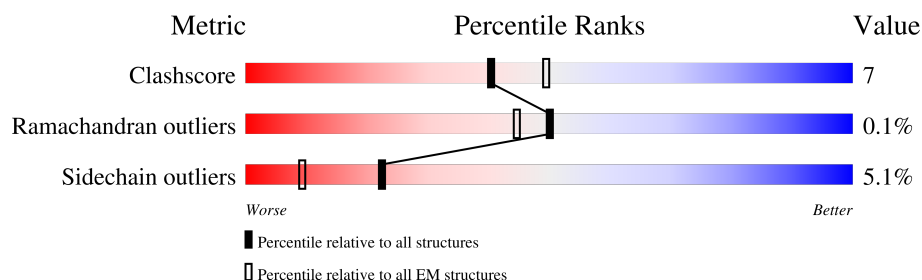
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	C	385	
1	N	385	
2	E	225	
2	P	225	
3	G	128	
3	R	128	
4	F	137	
4	Q	137	

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Mol	Chain	Length	Quality of chain
5	A	474	
5	L	474	
6	B	417	
6	M	417	
7	D	330	
7	O	330	
8	H	93	
8	S	93	
9	I	69	
9	T	69	
10	J	82	
10	U	82	

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
17	AOQ	N	509	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 33654 atoms, of which 0 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 Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	383	Total	C	N	O	S	0	0
			3052	2064	474	496	18		
1	N	383	Total	C	N	O	S	0	0
			3052	2064	474	496	18		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	186	Total	C	N	O	S	0	0
			1445	920	248	268	9		
2	E	186	Total	C	N	O	S	0	0
			1445	920	248	268	9		

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	124	Total	C	N	O	S	0	0
			994	640	162	190	2		
3	R	124	Total	C	N	O	S	0	0
			994	640	162	190	2		

- Molecule 4 is a protein called YALI0F24673p.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	71	Total	C	N	O	S	0	0
			579	361	99	115	4		
4	Q	71	Total	C	N	O	S	0	0
			579	361	99	115	4		

- Molecule 5 is a protein called YALI0A14806p.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	438	Total	C	N	O	S	0	0
			3446	2154	603	682	7		
5	L	438	Total	C	N	O	S	0	0
			3446	2154	603	682	7		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	402	Total	C	N	O	S	0	0
			3008	1907	516	583	2		
6	M	402	Total	C	N	O	S	0	0
			3008	1907	516	583	2		

- Molecule 7 is a protein called YALI0A17468p.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	244	Total	C	N	O	S	0	0
			1893	1210	323	352	8		
7	O	244	Total	C	N	O	S	0	0
			1893	1210	323	352	8		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	85	Total	C	N	O	S	0	0
			690	459	118	111	2		
8	S	85	Total	C	N	O	S	0	0
			690	459	118	111	2		

- Molecule 9 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	54	Total	C	N	O	S	0	0
			452	297	76	78	1		
9	T	54	Total	C	N	O	S	0	0
			452	297	76	78	1		

- Molecule 10 is a protein called YALI0C12210p.

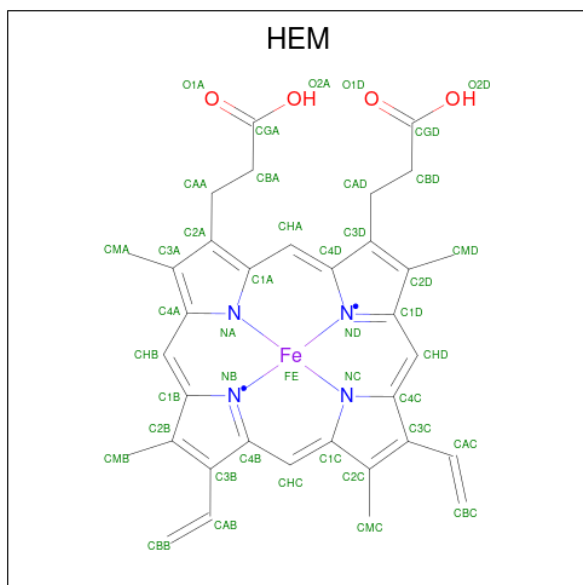
Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	75	Total	C	N	O	0	0
			598	403	99	96		

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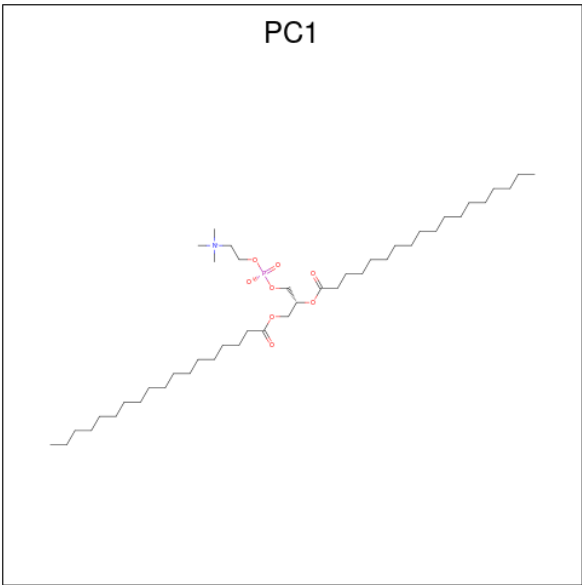
Mol	Chain	Residues	Atoms				AltConf	Trace
10	U	75	Total	C	N	O	0	0
			598	403	99	96		

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



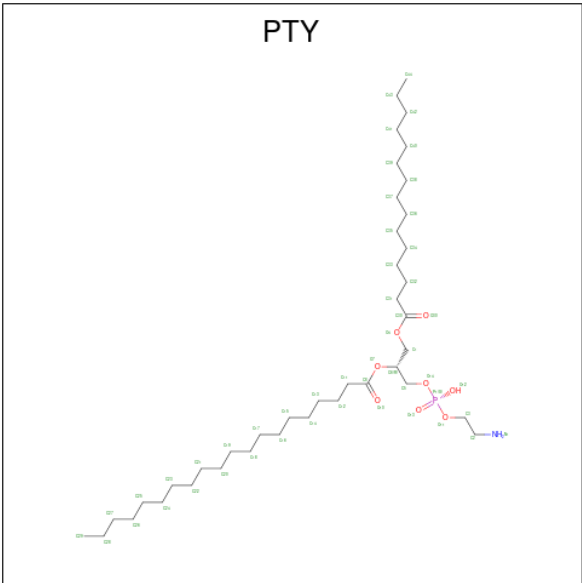
Mol	Chain	Residues	Atoms				AltConf
11	C	1	Total	C	Fe	N	O
			43	34	1	4	4
11	C	1	Total	C	Fe	N	O
			43	34	1	4	4
11	N	1	Total	C	Fe	N	O
			43	34	1	4	4
11	N	1	Total	C	Fe	N	O
			43	34	1	4	4

- Molecule 12 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



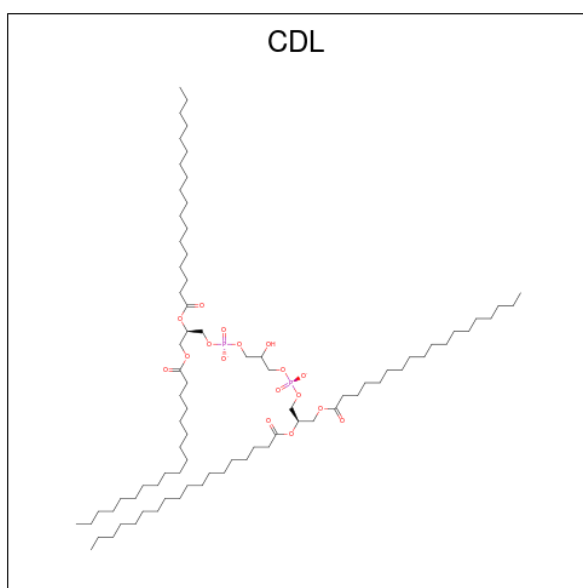
Mol	Chain	Residues	Atoms					AltConf
12	C	1	Total	C	N	O	P	0
			38	28	1	8	1	
12	I	1	Total	C	N	O	P	0
			32	22	1	8	1	
12	N	1	Total	C	N	O	P	0
			38	28	1	8	1	
12	T	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 13 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: C₄₀H₈₀NO₈P).



Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			41	31	1	8	1	
13	P	1	Total	C	N	O	P	0
			41	31	1	8	1	
13	D	1	Total	C	N	O	P	0
			41	31	1	8	1	
13	N	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



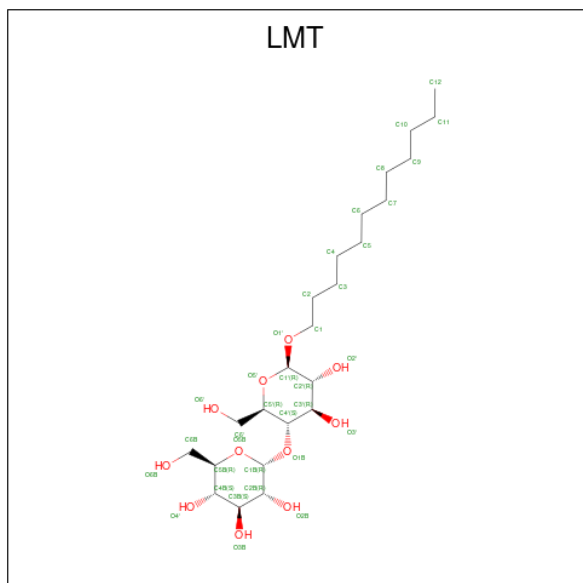
Mol	Chain	Residues	Atoms				AltConf
14	C	1	Total	C	O	P	0
			48	29	17	2	
14	A	1	Total	C	O	P	0
			42	25	15	2	
14	A	1	Total	C	O	P	0
			47	30	15	2	
14	H	1	Total	C	O	P	0
			50	31	17	2	
14	H	1	Total	C	O	P	0
			39	20	17	2	
14	N	1	Total	C	O	P	0
			50	31	17	2	
14	N	1	Total	C	O	P	0
			48	29	17	2	
14	L	1	Total	C	O	P	0
			42	25	15	2	

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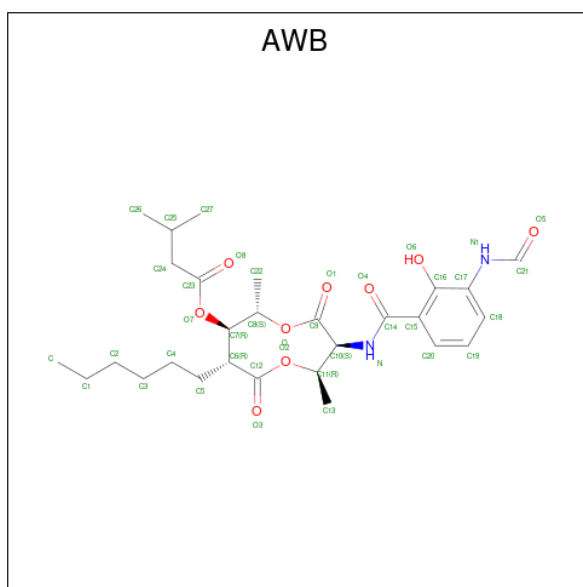
Mol	Chain	Residues	Atoms				AltConf
14	L	1	Total	C	O	P	0
			47	30	15	2	
14	S	1	Total	C	O	P	0
			39	20	17	2	

- Molecule 15 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



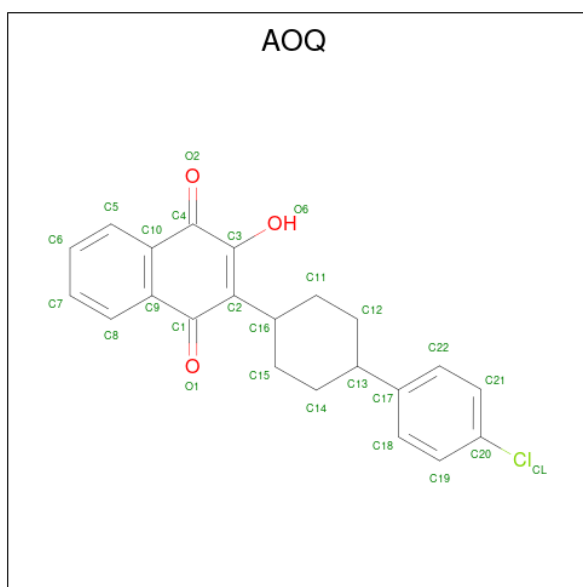
Mol	Chain	Residues	Atoms			AltConf
15	C	1	Total	C	O	0
			35	24	11	
15	J	1	Total	C	O	0
			35	24	11	
15	N	1	Total	C	O	0
			35	24	11	
15	U	1	Total	C	O	0
			35	24	11	

- Molecule 16 is [(2R,3S,6S,7R,8R)-3-[(3-formamido-2-oxidanyl-phenyl)carbonylamino]-8-hexyl-2,6-dimethyl-4,9-bis(oxidanylidene)-1,5-dioxonan-7-yl] 3-methylbutanoate (three-letter code: AWB) (formula: $C_{28}H_{40}N_2O_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
16	C	1	Total	C	N	O	0
			39	28	2	9	
16	N	1	Total	C	N	O	0
			39	28	2	9	

- Molecule 17 is 2-[trans-4-(4-chlorophenyl)cyclohexyl]-3-hydroxynaphthalene-1,4-dione (three-letter code: AOQ) (formula: $C_{22}H_{19}ClO_3$) (labeled as "Ligand of Interest" by depositor).



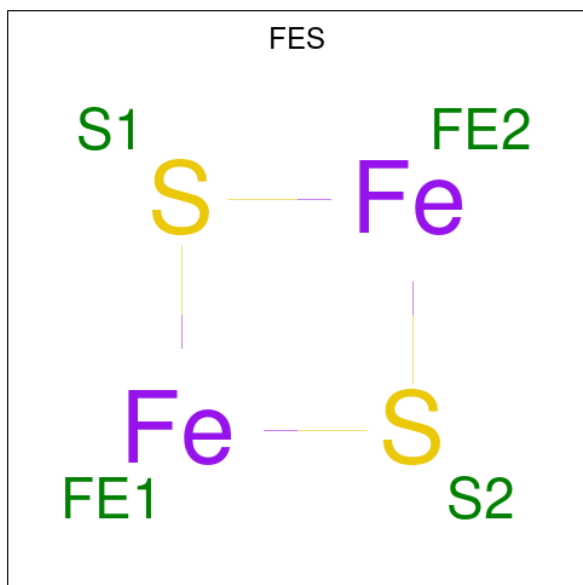
Mol	Chain	Residues	Atoms				AltConf
17	C	1	Total	C	Cl	O	0
			26	22	1	3	

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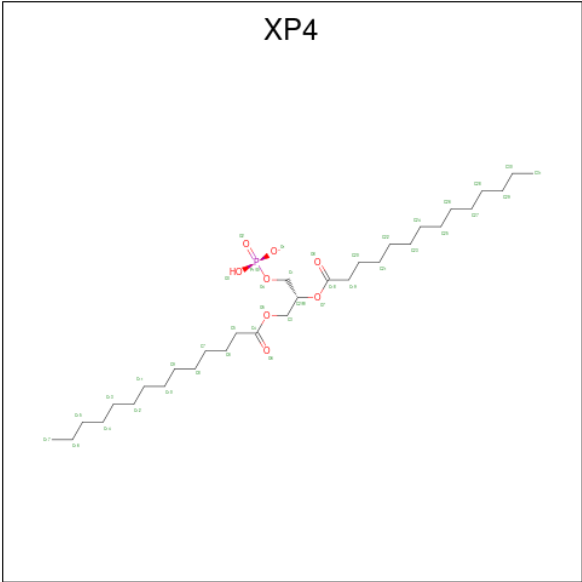
Mol	Chain	Residues	Atoms				AltConf
17	N	1	Total	C	Cl	O	0
			26	22	1	3	

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



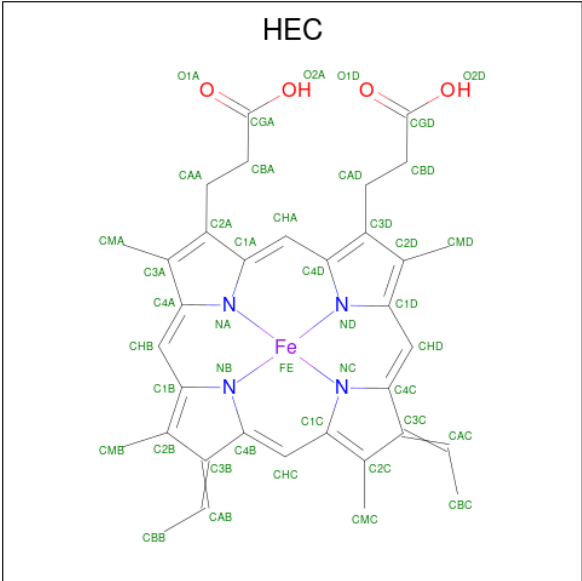
Mol	Chain	Residues	Atoms			AltConf
18	P	1	Total	Fe	S	0
			4	2	2	
18	E	1	Total	Fe	S	0
			4	2	2	

- Molecule 19 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: XP4) (formula: $\text{C}_{31}\text{H}_{60}\text{O}_8\text{P}$).



Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			24	15	8	1	
19	L	1	Total	C	O	P	0
			24	15	8	1	

- Molecule 20 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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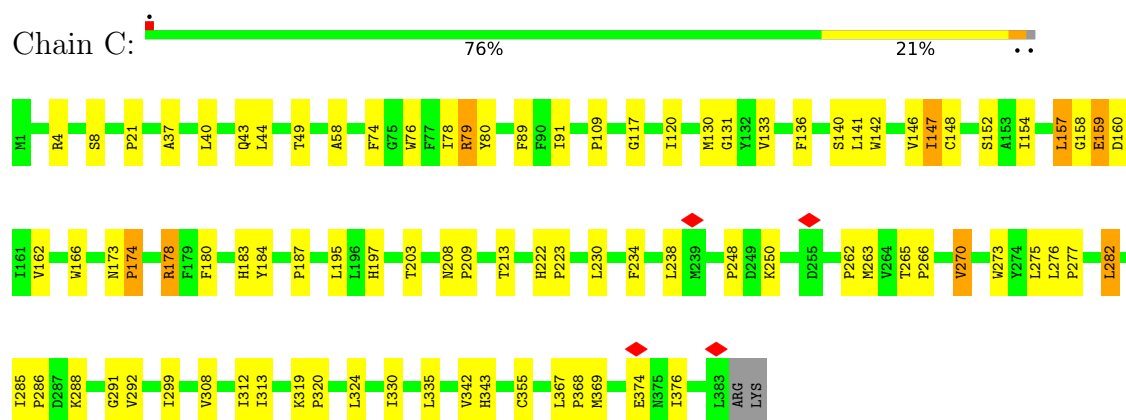
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
20	O	1	43	34	1	4	4	0

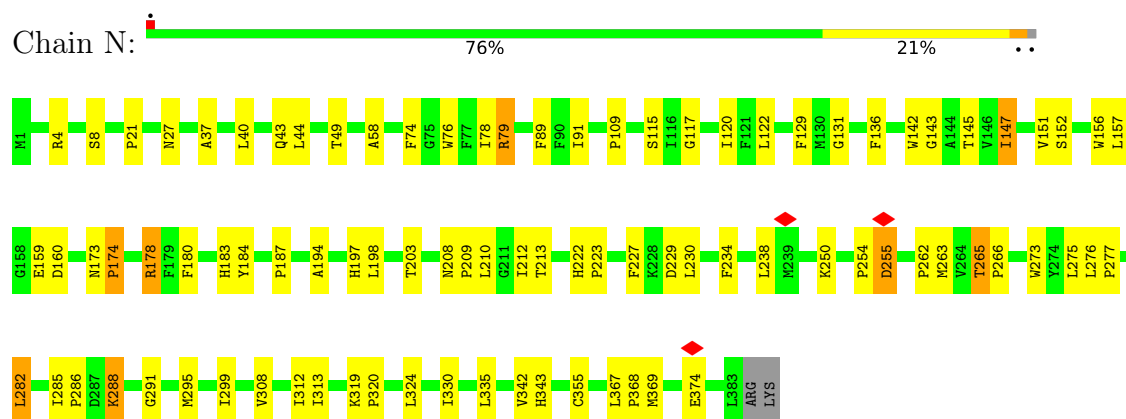
3 Residue-property plots

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.

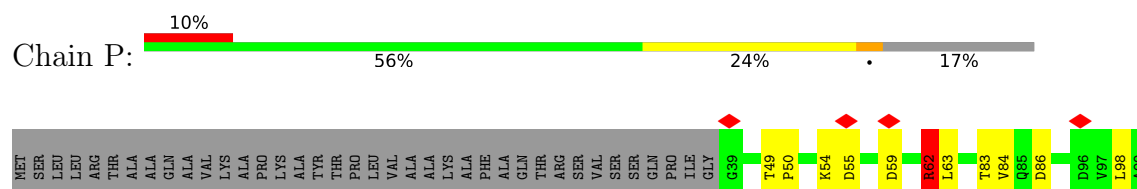
• Molecule 1: Cytochrome b

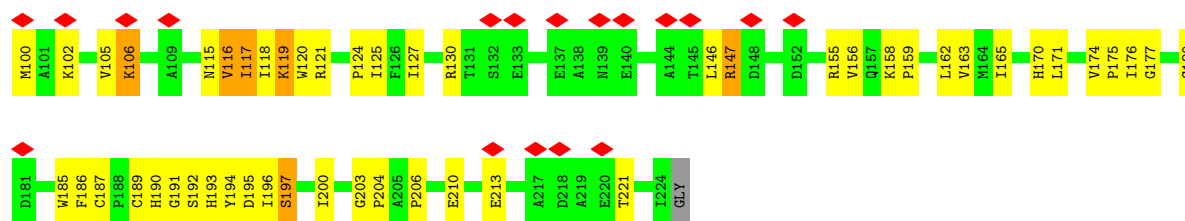


• Molecule 1: Cytochrome b

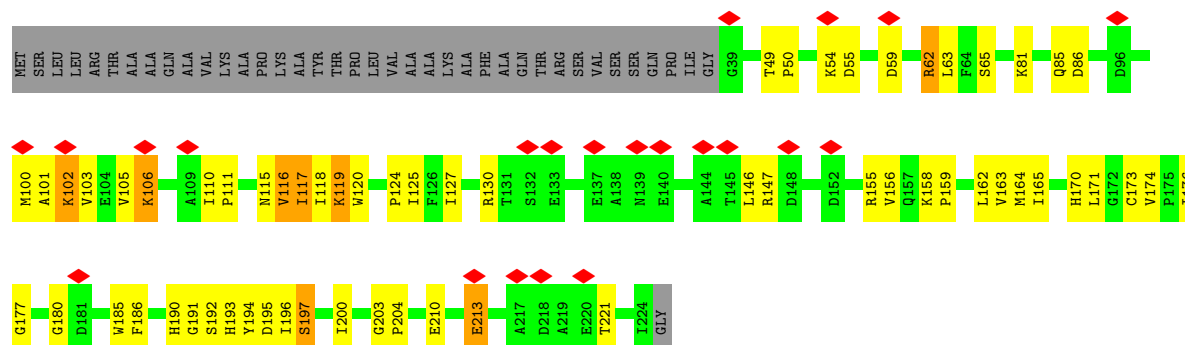


• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

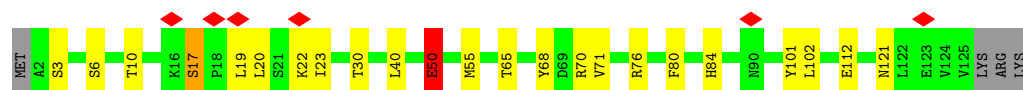
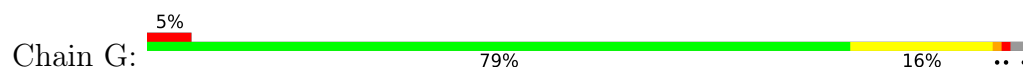




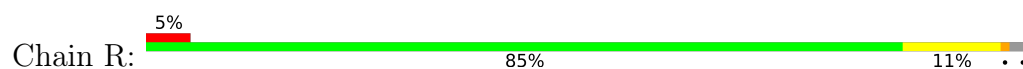
• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial



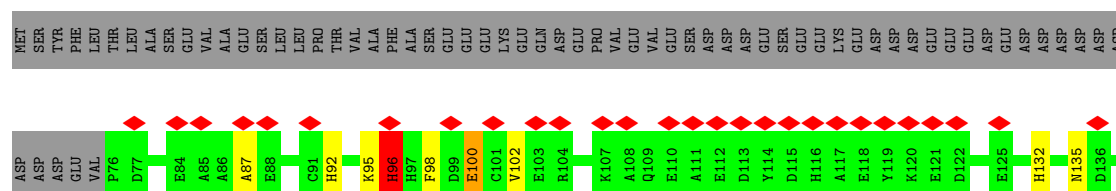
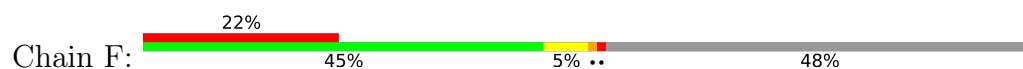
• Molecule 3: Cytochrome b-c1 complex subunit 7



• Molecule 3: Cytochrome b-c1 complex subunit 7

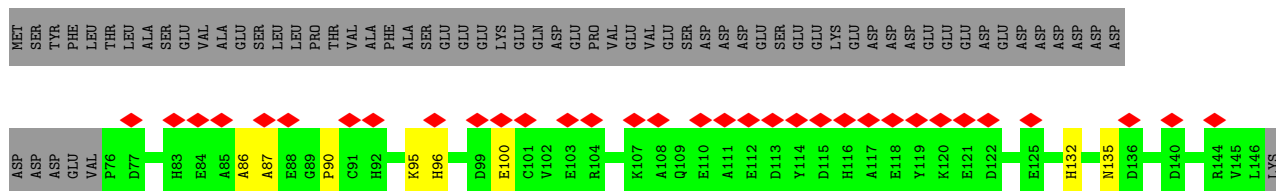


• Molecule 4: YALI0F24673p

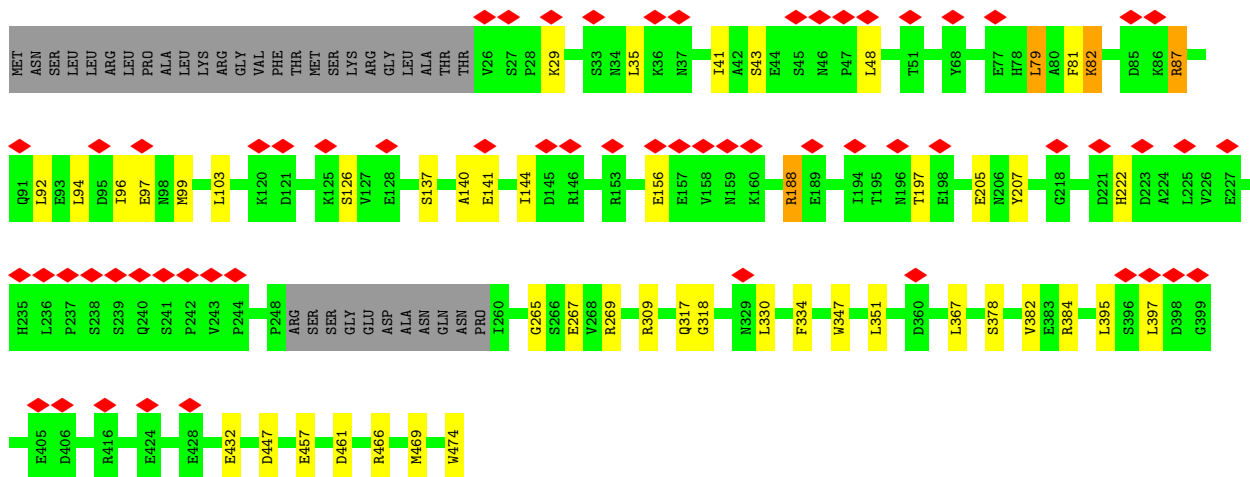
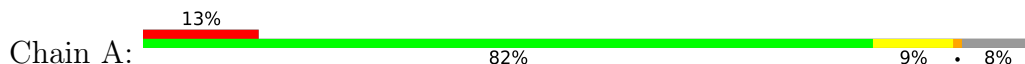


• Molecule 4: YALI0F24673p

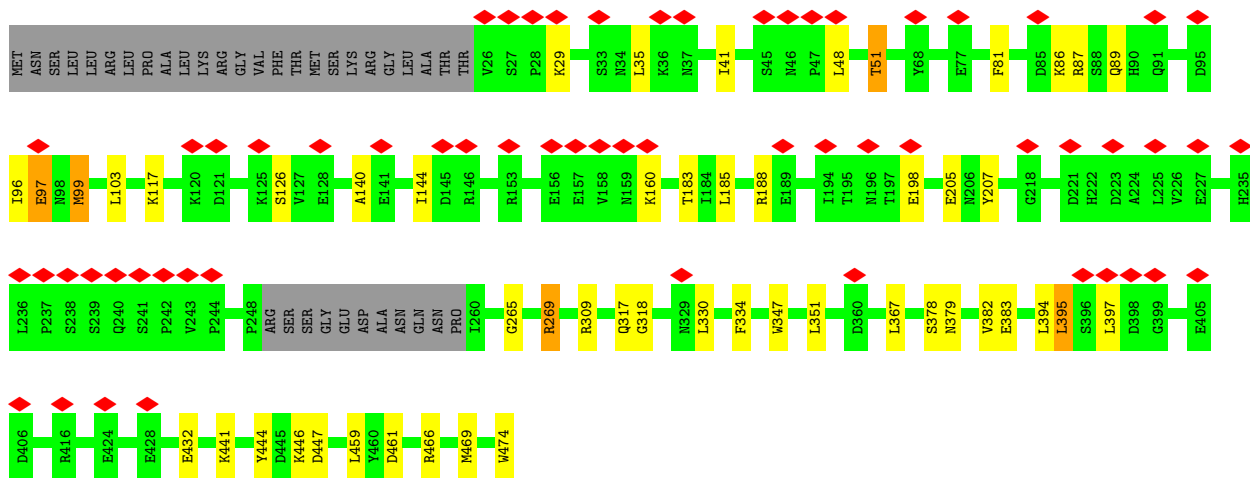
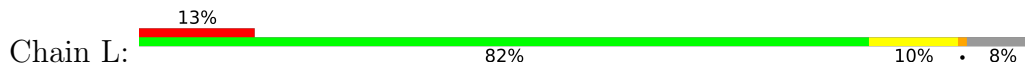




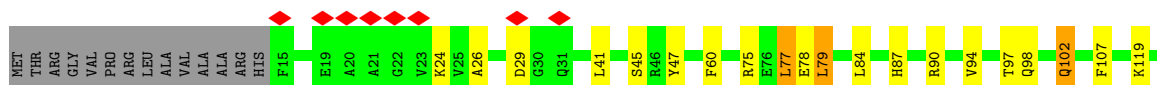
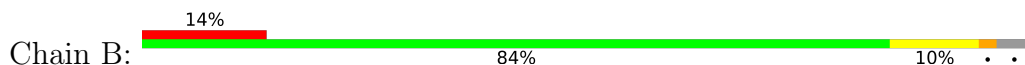
- Molecule 5: YALI0A14806p

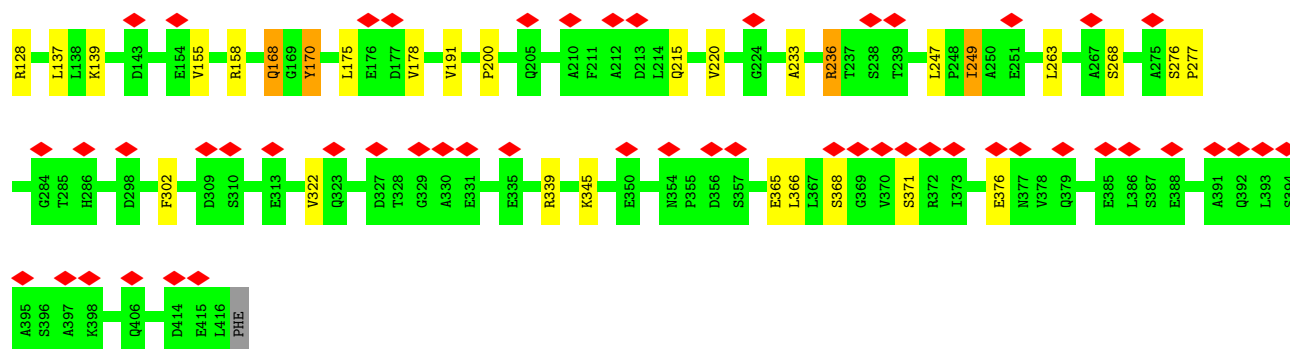


- Molecule 5: YALI0A14806p

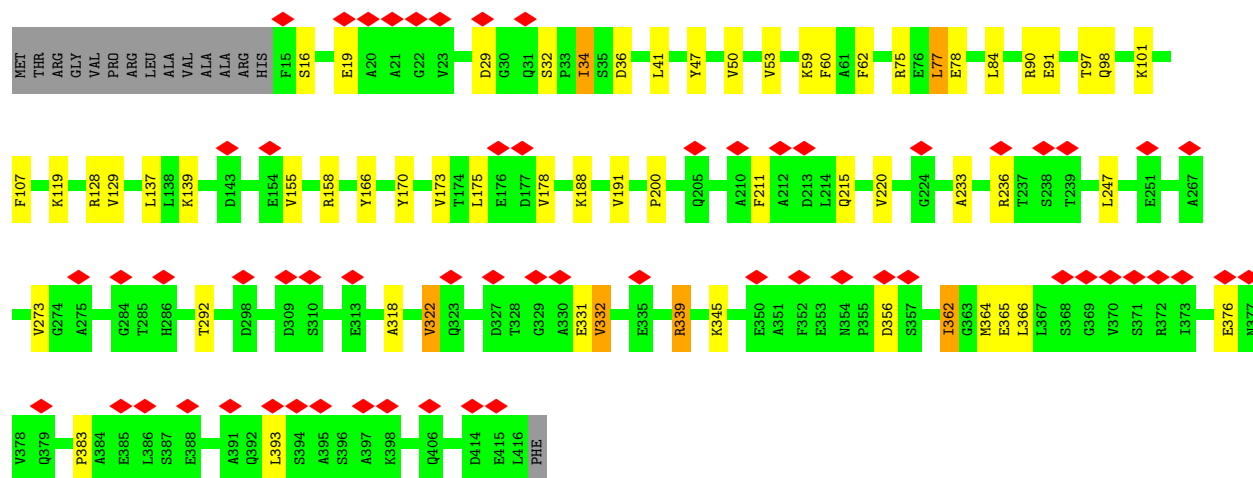
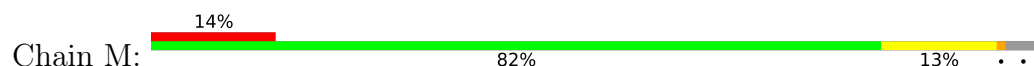


- Molecule 6: Cytochrome b-c1 complex subunit 2, mitochondrial

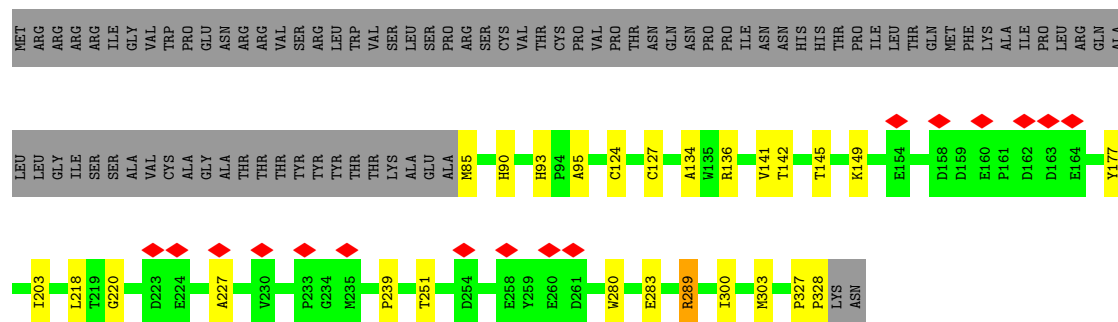




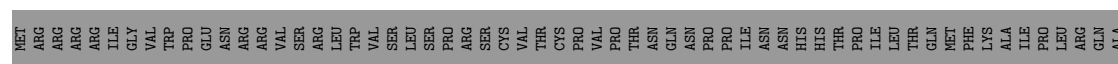
- Molecule 6: Cytochrome b-c1 complex subunit 2, mitochondrial



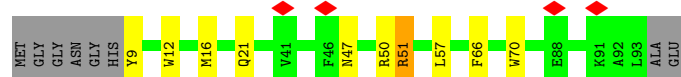
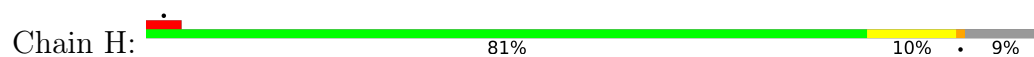
- Molecule 7: YALI0A17468p



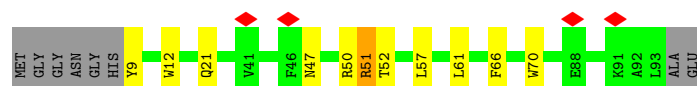
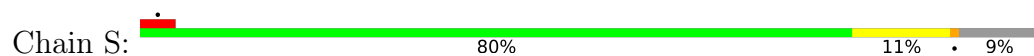
- Molecule 7: YALI0A17468p



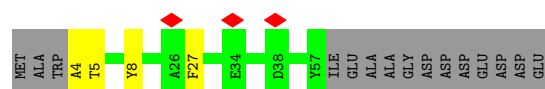
- Molecule 8: Cytochrome b-c1 complex subunit 8



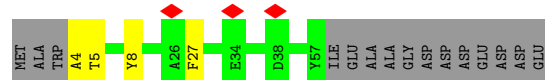
- Molecule 8: Cytochrome b-c1 complex subunit 8



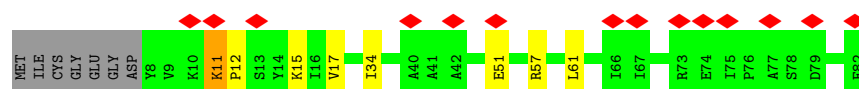
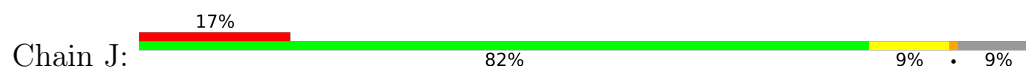
- Molecule 9: Complex III subunit 9



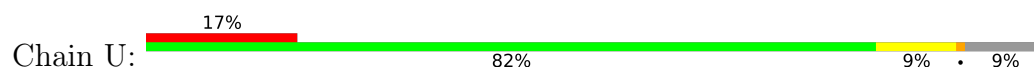
- Molecule 9: Complex III subunit 9

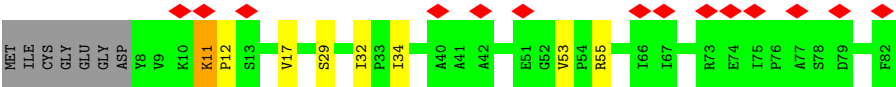


- Molecule 10: YALI0C12210p



- Molecule 10: YALI0C12210p





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	35394	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	301.32, 301.32, 301.32	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, PTY, CDL, HEC, HEM, PC1, AWB, AOQ, FES, XP4

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	C	0.59	1/3153 (0.0%)	0.99	3/4305 (0.1%)
1	N	0.58	1/3153 (0.0%)	0.99	3/4305 (0.1%)
2	E	0.43	0/1479	0.87	1/2003 (0.0%)
2	P	0.46	0/1479	0.96	4/2003 (0.2%)
3	G	0.50	1/1012 (0.1%)	0.84	0/1373
3	R	0.47	0/1012	0.85	0/1373
4	F	0.51	1/595 (0.2%)	0.84	3/805 (0.4%)
4	Q	0.61	1/595 (0.2%)	0.93	3/805 (0.4%)
5	A	0.49	0/3510	0.89	4/4768 (0.1%)
5	L	0.50	1/3510 (0.0%)	0.92	8/4768 (0.2%)
6	B	0.46	1/3069 (0.0%)	0.89	6/4178 (0.1%)
6	M	0.49	1/3069 (0.0%)	0.90	5/4178 (0.1%)
7	D	0.48	1/1950 (0.1%)	0.92	3/2656 (0.1%)
7	O	0.52	2/1950 (0.1%)	0.93	4/2656 (0.2%)
8	H	0.47	1/717 (0.1%)	0.84	0/975
8	S	0.47	1/717 (0.1%)	0.83	0/975
9	I	0.46	1/465 (0.2%)	0.75	0/629
9	T	0.47	1/465 (0.2%)	0.75	0/629
10	J	0.39	0/620	0.78	0/846
10	U	0.39	0/620	0.78	0/846
All	All	0.50	15/33140 (0.0%)	0.91	47/45076 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	100	GLU	CD-OE2	-10.44	1.14	1.25
6	M	365	GLU	CD-OE2	-8.61	1.16	1.25
7	O	283	GLU	CD-OE2	-8.47	1.16	1.25
3	G	50	GLU	CD-OE2	-6.73	1.18	1.25
6	B	365	GLU	CD-OE2	-6.41	1.18	1.25
7	O	283	GLU	CD-OE1	-6.01	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	100	GLU	CD-OE2	-5.98	1.19	1.25
1	C	159	GLU	CD-OE2	5.96	1.32	1.25
8	H	9	TYR	N-CA	5.61	1.57	1.46
8	S	9	TYR	N-CA	5.56	1.57	1.46
7	D	283	GLU	CD-OE2	-5.54	1.19	1.25
5	L	198	GLU	CD-OE2	-5.33	1.19	1.25
9	I	4	ALA	N-CA	5.28	1.56	1.46
9	T	4	ALA	N-CA	5.25	1.56	1.46
1	N	115	SER	CA-CB	-5.00	1.45	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	62	ARG	CG-CD-NE	12.04	137.08	111.80
6	B	90	ARG	CG-CD-NE	-10.18	90.42	111.80
4	Q	96	HIS	CB-CA-C	-9.95	90.50	110.40
6	M	90	ARG	CG-CD-NE	-9.62	91.61	111.80
2	P	62	ARG	NE-CZ-NH2	9.53	125.06	120.30
2	P	62	ARG	NE-CZ-NH1	-9.16	115.72	120.30
4	Q	100	GLU	CB-CA-C	-8.27	93.87	110.40
6	M	215	GLN	CB-CA-C	-8.25	93.90	110.40
6	B	215	GLN	CB-CA-C	-8.11	94.18	110.40
5	A	269	ARG	CG-CD-NE	-7.87	95.27	111.80
5	L	269	ARG	CG-CD-NE	-7.30	96.47	111.80
7	D	289	ARG	CG-CD-NE	-7.29	96.48	111.80
4	F	96	HIS	CB-CA-C	7.26	124.92	110.40
7	D	283	GLU	CB-CA-C	-7.15	96.09	110.40
7	O	289	ARG	NE-CZ-NH1	-6.97	116.81	120.30
5	L	309	ARG	CG-CD-NE	-6.96	97.19	111.80
5	A	309	ARG	CG-CD-NE	-6.92	97.26	111.80
4	F	96	HIS	N-CA-CB	-6.88	98.21	110.60
7	O	283	GLU	CB-CA-C	-6.82	96.76	110.40
5	L	188	ARG	NE-CZ-NH1	-6.81	116.89	120.30
4	Q	100	GLU	CB-CG-CD	-6.63	96.30	114.20
5	L	188	ARG	CG-CD-NE	-6.61	97.91	111.80
7	O	289	ARG	CG-CD-NE	-6.51	98.13	111.80
1	N	147	ILE	CA-CB-CG1	-6.42	98.80	111.00
1	N	4	ARG	CG-CD-NE	-6.27	98.64	111.80
5	L	269	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	C	4	ARG	CG-CD-NE	-6.19	98.80	111.80
6	B	170	TYR	CB-CG-CD1	6.05	124.63	121.00
6	B	158	ARG	CG-CD-NE	-5.99	99.22	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	158	ARG	CG-CD-NE	-5.88	99.44	111.80
1	C	142	TRP	CA-CB-CG	-5.88	102.53	113.70
2	E	62	ARG	CB-CG-CD	-5.83	96.44	111.60
5	L	198	GLU	CB-CA-C	-5.81	98.79	110.40
2	P	62	ARG	CB-CA-C	-5.80	98.79	110.40
1	C	265	THR	OG1-CB-CG2	-5.69	96.91	110.00
7	D	136	ARG	CG-CD-NE	-5.62	100.00	111.80
6	B	236	ARG	CG-CD-NE	5.41	123.15	111.80
5	L	89	GLN	CB-CG-CD	5.35	125.51	111.60
6	B	339	ARG	CG-CD-NE	5.22	122.76	111.80
1	N	142	TRP	CA-CB-CG	-5.18	103.86	113.70
7	O	136	ARG	CG-CD-NE	-5.17	100.93	111.80
5	A	347	TRP	C-N-CA	-5.14	111.51	122.30
5	L	347	TRP	C-N-CA	-5.13	111.52	122.30
4	F	100	GLU	CB-CA-C	5.11	120.62	110.40
5	A	188	ARG	CG-CD-NE	-5.11	101.07	111.80
6	M	128	ARG	CG-CD-NE	-5.09	101.12	111.80
6	M	339	ARG	CG-CD-NE	5.07	122.45	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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	C	3052	0	3113	69	0
1	N	3052	0	3113	72	0
2	E	1445	0	1426	39	0
2	P	1445	0	1426	49	0
3	G	994	0	1022	10	0
3	R	994	0	1022	9	0
4	F	579	0	511	7	0
4	Q	579	0	511	4	0
5	A	3446	0	3369	29	0
5	L	3446	0	3369	33	0
6	B	3008	0	2991	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	3008	0	2991	39	0
7	D	1893	0	1834	29	0
7	O	1893	0	1834	30	0
8	H	690	0	673	10	0
8	S	690	0	673	12	0
9	I	452	0	435	2	0
9	T	452	0	435	5	0
10	J	598	0	615	5	0
10	U	598	0	615	6	0
11	C	86	0	60	13	0
11	N	86	0	60	11	0
12	C	38	0	50	2	0
12	I	32	0	38	1	0
12	N	38	0	50	2	0
12	T	32	0	38	0	0
13	C	41	0	58	2	0
13	D	41	0	58	2	0
13	N	41	0	58	7	0
13	P	41	0	58	13	0
14	A	89	0	85	4	0
14	C	48	0	40	1	0
14	H	89	0	66	2	0
14	L	89	0	85	5	0
14	N	98	0	84	7	0
14	S	39	0	22	1	0
15	C	35	0	46	4	0
15	J	35	0	46	3	0
15	N	35	0	46	2	0
15	U	35	0	46	0	0
16	C	39	0	39	5	0
16	N	39	0	39	5	0
17	C	26	0	18	4	0
17	N	26	0	17	13	0
18	E	4	0	0	0	0
18	P	4	0	0	0	0
19	A	24	0	22	0	0
19	L	24	0	22	0	0
20	D	43	0	32	14	0
20	O	43	0	32	14	0
All	All	33654	0	33293	454	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 7.

All (454) 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)
14:L:3002:CDL:C55	14:L:3002:CDL:C56	1.74	1.59
14:A:3001:CDL:C34	14:A:3001:CDL:C35	1.76	1.57
14:N:504:CDL:C14	14:N:504:CDL:C15	1.76	1.55
7:D:124:CYS:SG	20:D:401:HEC:HBB3	1.54	1.47
7:O:124:CYS:SG	20:O:401:HEC:HBB3	1.54	1.46
2:P:84:VAL:CG2	13:P:302:PTY:H441	1.62	1.26
1:C:299:ILE:HD12	17:C:508:AOQ:CL	1.72	1.26
7:D:124:CYS:SG	20:D:401:HEC:CBB	2.25	1.25
7:O:124:CYS:SG	20:O:401:HEC:CBB	2.25	1.24
2:P:84:VAL:HG23	13:P:302:PTY:C44	1.72	1.19
1:N:299:ILE:HD12	17:N:509:AOQ:CL	1.81	1.17
7:O:127:CYS:SG	20:O:401:HEC:HBC3	1.93	1.08
1:N:152:SER:OG	1:N:288:LYS:NZ	1.87	1.06
7:D:127:CYS:SG	20:D:401:HEC:HBC3	1.94	1.06
7:O:127:CYS:SG	20:O:401:HEC:CAC	2.44	1.06
1:N:299:ILE:CD1	17:N:509:AOQ:CL	2.41	1.05
7:D:127:CYS:SG	20:D:401:HEC:CAC	2.43	1.05
7:D:124:CYS:SG	20:D:401:HEC:CAB	2.48	1.01
7:D:127:CYS:SG	20:D:401:HEC:CBC	2.48	1.01
7:O:127:CYS:SG	20:O:401:HEC:CBC	2.47	1.01
7:O:124:CYS:SG	20:O:401:HEC:CAB	2.48	1.01
2:P:84:VAL:HG23	13:P:302:PTY:H441	1.00	1.00
1:C:330:ILE:HD12	12:C:503:PC1:H2A1	1.50	0.93
1:N:330:ILE:HD12	12:N:503:PC1:H2A1	1.50	0.91
1:C:299:ILE:CD1	17:C:508:AOQ:CL	2.57	0.89
1:C:58:ALA:H	1:C:173:ASN:HD22	1.22	0.88
1:N:122:LEU:HD23	17:N:509:AOQ:CL	2.11	0.87
6:B:170:TYR:CE2	6:M:236:ARG:HD3	2.10	0.87
11:N:501:HEM:HBB2	11:N:501:HEM:CMB	2.04	0.86
1:C:286:PRO:O	2:P:204:PRO:HA	1.75	0.86
4:Q:135:ASN:HB3	7:O:95:ALA:HB2	1.59	0.84
4:F:135:ASN:HB3	7:D:95:ALA:HB2	1.58	0.84
11:C:501:HEM:CMB	11:C:501:HEM:HBB2	2.07	0.84
3:R:71:VAL:HG11	8:S:21:GLN:HG2	1.61	0.83
2:P:62:ARG:NH1	9:T:8:TYR:CZ	2.47	0.82
11:N:501:HEM:HBB2	11:N:501:HEM:HMB1	1.61	0.82
1:C:40:LEU:HD23	16:C:507:AWB:H27	1.60	0.82
1:N:299:ILE:HD11	17:N:509:AOQ:H17	1.58	0.82
6:B:84:LEU:HD12	6:B:97:THR:HG22	1.60	0.81
1:N:122:LEU:CD2	17:N:509:AOQ:CL	2.66	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:71:VAL:HG11	8:H:21:GLN:HG2	1.61	0.80
5:L:395:LEU:CD2	6:M:98:GLN:HG2	2.13	0.79
2:P:84:VAL:HG22	13:P:302:PTY:H441	1.64	0.78
5:A:156:GLU:OE2	5:A:188:ARG:NH1	2.16	0.78
11:C:501:HEM:HBB2	11:C:501:HEM:HMB1	1.64	0.78
11:N:501:HEM:HBC2	11:N:501:HEM:HHD	1.66	0.78
11:C:501:HEM:HBC2	11:C:501:HEM:HHD	1.65	0.77
10:U:11:LYS:HG2	10:U:12:PRO:HD2	1.67	0.75
5:A:395:LEU:CD2	6:B:98:GLN:HG2	2.17	0.75
2:P:84:VAL:HG23	13:P:302:PTY:C43	2.17	0.73
5:A:43:SER:HB3	5:A:222:HIS:HD2	1.54	0.73
2:P:84:VAL:CG2	13:P:302:PTY:C44	2.48	0.72
11:N:501:HEM:HBC2	11:N:501:HEM:CHD	2.19	0.72
11:C:501:HEM:HBC2	11:C:501:HEM:CHD	2.19	0.71
3:G:17:SER:HB2	3:G:20:LEU:HB2	1.72	0.70
3:R:17:SER:HB2	3:R:20:LEU:HB2	1.73	0.70
1:C:157:LEU:HD11	10:U:53:VAL:HG11	1.74	0.69
7:O:218:LEU:HD11	20:O:401:HEC:HMB2	1.75	0.69
1:N:299:ILE:CD1	17:N:509:AOQ:H17	2.23	0.69
5:L:395:LEU:HD23	6:M:98:GLN:HG2	1.73	0.69
1:C:147:ILE:HD11	17:C:508:AOQ:H11	1.73	0.68
6:B:41:LEU:CD2	6:B:191:VAL:HG22	2.22	0.68
1:C:146:VAL:HG13	2:P:171:LEU:HD13	1.76	0.68
7:D:218:LEU:HD11	20:D:401:HEC:HMB2	1.75	0.66
5:A:382:VAL:HG21	5:A:432:GLU:HA	1.78	0.65
20:D:401:HEC:HBA2	20:D:401:HEC:HHA	1.78	0.65
20:O:401:HEC:HBA2	20:O:401:HEC:HHA	1.79	0.65
5:L:395:LEU:HD21	6:M:98:GLN:HG2	1.79	0.65
5:L:395:LEU:HA	6:M:34:ILE:HD12	1.79	0.65
1:N:129:PHE:CD2	1:N:147:ILE:HD13	2.32	0.64
1:N:299:ILE:HD13	17:N:509:AOQ:CL	2.31	0.64
15:C:506:LMT:H22	15:N:507:LMT:H32	1.79	0.64
1:N:238:LEU:HD13	7:O:300:ILE:HG22	1.80	0.63
1:C:213:THR:HB	3:G:50:GLU:OE2	1.98	0.63
4:F:102:VAL:HG13	7:D:227:ALA:HB2	1.80	0.63
2:E:180:GLY:HA2	2:E:186:PHE:HB2	1.81	0.63
6:M:41:LEU:CD2	6:M:191:VAL:HG22	2.29	0.63
7:O:124:CYS:SG	20:O:401:HEC:C3B	2.87	0.63
7:D:124:CYS:SG	20:D:401:HEC:C3B	2.87	0.62
1:N:44:LEU:HD23	11:N:501:HEM:HMC2	1.81	0.62
1:C:238:LEU:HD13	7:D:300:ILE:HG22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:265:THR:HG21	2:E:173:CYS:HB3	1.80	0.62
1:N:265:THR:CG2	2:E:174:VAL:H	2.13	0.62
1:N:229:ASP:HB2	13:N:505:PTY:H382	1.80	0.62
2:P:180:GLY:HA2	2:P:186:PHE:HB2	1.81	0.62
1:N:147:ILE:HD11	17:N:509:AOQ:H6	1.82	0.62
5:L:382:VAL:HG21	5:L:432:GLU:HA	1.82	0.62
1:C:37:ALA:HB2	16:C:507:AWB:C22	2.30	0.62
1:C:76:TRP:CZ3	7:D:289:ARG:HG3	2.35	0.61
1:N:213:THR:HB	3:R:50:GLU:OE2	2.00	0.61
11:N:502:HEM:HBC2	11:N:502:HEM:HMC2	1.82	0.61
15:N:507:LMT:H62	16:N:508:AWB:H3	1.81	0.61
1:N:129:PHE:CE2	1:N:147:ILE:HD13	2.36	0.60
1:C:343:HIS:NE2	7:D:90:HIS:CE1	2.69	0.60
2:E:155:ARG:NH1	2:E:197:SER:O	2.35	0.60
1:C:335:LEU:HD22	8:H:66:PHE:HD1	1.66	0.60
1:N:335:LEU:HD22	8:S:66:PHE:HD1	1.67	0.59
11:C:502:HEM:HBC2	11:C:502:HEM:HMC2	1.83	0.59
5:L:81:PHE:HE1	5:L:103:LEU:HD23	1.67	0.59
1:N:343:HIS:NE2	7:O:90:HIS:CE1	2.71	0.59
8:H:47:ASN:O	8:H:51:ARG:HG2	2.03	0.59
1:N:76:TRP:CZ3	7:O:289:ARG:HG3	2.37	0.59
13:C:504:PTY:H112	13:C:504:PTY:HC12	1.83	0.59
2:P:62:ARG:NH1	9:T:8:TYR:CE2	2.68	0.59
7:D:251:THR:HG21	20:D:401:HEC:HMC2	1.84	0.58
8:S:47:ASN:O	8:S:51:ARG:HG2	2.02	0.58
14:A:3001:CDL:C34	14:A:3001:CDL:C36	2.78	0.58
2:P:155:ARG:NH1	2:P:197:SER:O	2.35	0.58
6:B:170:TYR:CZ	6:M:236:ARG:HD3	2.38	0.58
14:N:504:CDL:C15	14:N:504:CDL:C13	2.76	0.58
7:O:251:THR:HG21	20:O:401:HEC:HMC2	1.84	0.58
1:C:44:LEU:HD23	11:C:501:HEM:HMC3	1.87	0.57
5:A:81:PHE:HE1	5:A:103:LEU:HD23	1.68	0.57
5:A:79:LEU:HD21	5:A:144:ILE:HD13	1.86	0.57
2:E:124:PRO:HG2	2:E:174:VAL:HG11	1.86	0.57
4:F:98:PHE:O	4:F:102:VAL:HG23	2.05	0.57
14:A:3001:CDL:OB9	14:A:3001:CDL:HB4	2.03	0.57
7:O:203:ILE:HG12	20:O:401:HEC:HMA3	1.87	0.56
10:U:29:SER:HA	10:U:32:ILE:HG12	1.87	0.56
6:B:236:ARG:HD3	6:M:170:TYR:CE2	2.41	0.56
7:D:127:CYS:SG	20:D:401:HEC:C3C	2.94	0.56
2:P:124:PRO:HG2	2:P:174:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:127:CYS:HG	20:D:401:HEC:HBC3	1.69	0.56
6:M:36:ASP:OD1	6:M:98:GLN:HG3	2.06	0.56
1:C:180:PHE:HE2	1:N:180:PHE:HE2	1.53	0.55
1:C:133:VAL:HA	1:C:140:SER:HB3	1.88	0.55
7:D:203:ILE:HG12	20:D:401:HEC:HMA3	1.89	0.55
6:M:41:LEU:HD23	6:M:191:VAL:HG22	1.88	0.55
1:N:255:ASP:OD2	1:N:266:PRO:HB3	2.06	0.55
5:L:474:TRP:CD1	10:U:34:ILE:HG13	2.42	0.55
5:A:43:SER:CB	5:A:222:HIS:HD2	2.19	0.55
5:A:378:SER:HA	5:A:432:GLU:OE1	2.07	0.55
1:C:154:ILE:O	1:C:158:GLY:HA3	2.07	0.55
13:N:505:PTY:H361	14:L:3001:CDL:H362	1.89	0.55
14:L:3002:CDL:C56	14:L:3002:CDL:C54	2.76	0.55
7:O:127:CYS:SG	20:O:401:HEC:C3C	2.93	0.55
1:C:343:HIS:NE2	7:D:90:HIS:HE1	2.05	0.54
5:L:334:PHE:HB3	5:L:351:LEU:HD23	1.89	0.54
6:B:170:TYR:CE2	6:M:236:ARG:CD	2.87	0.54
10:J:17:VAL:HG22	3:R:121:ASN:O	2.07	0.54
1:C:335:LEU:HD23	1:C:355:CYS:SG	2.48	0.54
3:G:121:ASN:O	10:U:17:VAL:HG22	2.07	0.54
14:N:504:CDL:OB3	14:S:101:CDL:O1	2.26	0.54
1:C:44:LEU:HD23	11:C:501:HEM:CMC	2.38	0.54
1:N:342:VAL:HG11	8:S:70:TRP:HH2	1.73	0.54
5:A:334:PHE:HB3	5:A:351:LEU:HD23	1.89	0.54
5:L:379:ASN:HB2	5:L:383:GLU:HG2	1.89	0.54
15:J:101:LMT:H31	2:E:85:GLN:HG3	1.90	0.54
1:C:367:LEU:HB3	1:C:368:PRO:HD3	1.90	0.53
11:C:501:HEM:HHD	11:C:501:HEM:CBC	2.38	0.53
2:P:118:ILE:HD13	2:P:127:ILE:HD12	1.91	0.53
5:A:265:GLY:HA3	5:A:447:ASP:HB3	1.90	0.53
1:N:27:ASN:HB2	14:N:504:CDL:OB4	2.08	0.53
1:C:37:ALA:HB2	16:C:507:AWB:H22B	1.89	0.53
3:G:68:TYR:CD2	7:D:328:PRO:HG2	2.43	0.53
1:N:263:MET:HE3	2:E:119:LYS:HB3	1.90	0.53
2:E:118:ILE:HD13	2:E:127:ILE:HD12	1.90	0.53
1:C:91:ILE:HG13	1:C:273:TRP:CZ2	2.44	0.53
1:C:152:SER:OG	1:C:288:LYS:NZ	2.35	0.53
1:N:44:LEU:HD23	11:N:501:HEM:CMC	2.38	0.53
1:N:335:LEU:HD23	1:N:355:CYS:SG	2.48	0.53
7:D:145:THR:O	7:D:149:LYS:HG3	2.09	0.53
1:N:295:MET:SD	17:N:509:AOQ:H10	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:263:MET:SD	2:E:124:PRO:HG3	2.49	0.53
5:L:334:PHE:CB	5:L:351:LEU:HD23	2.39	0.53
6:M:53:VAL:HG12	6:M:173:VAL:HG13	1.91	0.53
1:N:122:LEU:HD21	17:N:509:AOQ:CL	2.44	0.52
5:L:395:LEU:HD23	6:M:98:GLN:CG	2.39	0.52
5:A:474:TRP:CD1	10:J:34:ILE:HG13	2.44	0.52
1:N:91:ILE:HG13	1:N:273:TRP:CZ2	2.45	0.52
3:R:68:TYR:CD2	7:O:328:PRO:HG2	2.44	0.52
5:L:97:GLU:HB3	6:M:339:ARG:HD3	1.91	0.52
1:C:342:VAL:HG11	8:H:70:TRP:HH2	1.74	0.52
5:A:334:PHE:CB	5:A:351:LEU:HD23	2.39	0.52
1:N:367:LEU:HB3	1:N:368:PRO:HD3	1.91	0.52
5:L:265:GLY:HA3	5:L:447:ASP:HB3	1.92	0.52
6:B:26:ALA:HB2	6:B:366:LEU:HD11	1.92	0.51
11:N:501:HEM:HHD	11:N:501:HEM:CBC	2.38	0.51
1:C:157:LEU:CD1	10:U:53:VAL:HG11	2.40	0.51
20:D:401:HEC:CBB	20:D:401:HEC:HMB1	2.41	0.51
20:O:401:HEC:CBB	20:O:401:HEC:HMB1	2.40	0.51
2:P:186:PHE:CE1	2:P:191:GLY:HA2	2.46	0.51
1:N:129:PHE:HZ	1:N:143:GLY:HA3	1.76	0.51
11:N:501:HEM:HMB1	11:N:501:HEM:CBB	2.36	0.51
2:E:186:PHE:CE1	2:E:191:GLY:HA2	2.46	0.51
1:N:234:PHE:CZ	7:O:303:MET:HE2	2.46	0.51
2:P:62:ARG:HH21	5:L:446:LYS:HD3	1.76	0.51
2:P:83:THR:HA	13:P:302:PTY:H121	1.93	0.50
6:B:24:LYS:HB3	6:B:366:LEU:HD22	1.93	0.50
6:M:84:LEU:HD12	6:M:97:THR:HG22	1.92	0.50
6:M:91:GLU:HG2	6:M:364:MET:HE1	1.93	0.50
1:C:222:HIS:CG	1:C:223:PRO:HA	2.46	0.50
6:M:77:LEU:HD12	6:M:107:PHE:HE1	1.76	0.50
2:P:130:ARG:HD2	2:P:162:LEU:HB2	1.94	0.50
1:N:343:HIS:NE2	7:O:90:HIS:HE1	2.08	0.50
5:L:99:MET:SD	5:L:126:SER:HB3	2.52	0.50
6:M:50:VAL:HB	6:M:53:VAL:HG13	1.93	0.50
1:C:276:LEU:N	1:C:277:PRO:CD	2.75	0.50
2:P:62:ARG:NH2	5:L:446:LYS:HD3	2.27	0.50
2:P:84:VAL:CG2	13:P:302:PTY:C43	2.87	0.50
13:P:302:PTY:HC52	7:O:295:LYS:HD3	1.94	0.50
5:A:96:ILE:HG12	5:A:103:LEU:HD13	1.92	0.50
1:N:222:HIS:CG	1:N:223:PRO:HA	2.47	0.50
6:B:41:LEU:HD23	6:B:191:VAL:HG22	1.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:130:ARG:HD2	2:E:162:LEU:HB2	1.93	0.49
3:G:55:MET:HE1	3:G:102:LEU:HD21	1.93	0.49
6:M:318:ALA:O	6:M:322:VAL:HG23	2.12	0.49
3:R:76:ARG:HD3	3:R:80:PHE:CE2	2.48	0.49
15:C:506:LMT:H31	15:C:506:LMT:H61	1.56	0.49
14:H:701:CDL:OB3	14:H:702:CDL:O1	2.31	0.49
2:P:117:ILE:HG22	2:P:124:PRO:HB3	1.95	0.49
1:C:79:ARG:HD3	1:C:79:ARG:C	2.33	0.49
1:C:8:SER:HB3	1:N:203:THR:CG2	2.43	0.49
1:C:58:ALA:H	1:C:173:ASN:ND2	1.98	0.49
14:A:3001:CDL:H1	14:A:3002:CDL:HA4	1.95	0.48
5:L:394:LEU:O	6:M:34:ILE:CD1	2.61	0.48
1:C:203:THR:CG2	1:N:8:SER:HB3	2.43	0.48
3:G:76:ARG:HD3	3:G:80:PHE:CE2	2.47	0.48
16:C:507:AWB:H27B	16:C:507:AWB:H22	1.94	0.48
1:N:79:ARG:HD3	1:N:79:ARG:C	2.33	0.48
1:N:227:PHE:HZ	13:N:505:PTY:HC6	1.78	0.48
1:N:276:LEU:N	1:N:277:PRO:CD	2.76	0.48
13:D:402:PTY:H132	13:D:402:PTY:H161	1.55	0.48
1:C:230:LEU:HD11	13:C:504:PTY:H332	1.96	0.48
1:C:21:PRO:HD3	8:H:12:TRP:CZ3	2.49	0.48
6:B:137:LEU:HD22	6:B:168:GLN:HG3	1.96	0.48
5:L:395:LEU:HD23	6:M:98:GLN:OE1	2.14	0.47
11:C:501:HEM:HMB1	11:C:501:HEM:CBB	2.39	0.47
14:N:504:CDL:HA21	8:S:51:ARG:HH21	1.79	0.47
11:C:501:HEM:CHD	11:C:501:HEM:CBC	2.92	0.47
14:C:505:CDL:H142	14:C:505:CDL:H331	1.97	0.47
2:P:192:SER:HB3	2:P:204:PRO:HD2	1.97	0.47
5:A:82:LYS:HD3	5:A:82:LYS:HA	1.57	0.47
5:L:160:LYS:HA	5:L:160:LYS:HD2	1.76	0.47
1:C:263:MET:HE1	2:P:119:LYS:HB3	1.97	0.47
5:A:317:GLN:HG2	6:B:78:GLU:OE1	2.15	0.47
1:C:195:LEU:HD22	15:C:506:LMT:H102	1.97	0.47
7:D:141:VAL:HG12	7:D:142:THR:HG23	1.96	0.47
2:E:105:VAL:HG21	2:E:118:ILE:HG12	1.96	0.47
1:N:37:ALA:HB2	16:N:508:AWB:H22B	1.97	0.47
2:E:117:ILE:HG22	2:E:124:PRO:HB3	1.95	0.47
2:P:62:ARG:NH2	5:L:444:TYR:O	2.48	0.47
4:F:102:VAL:HG13	7:D:227:ALA:CB	2.45	0.47
1:N:131:GLY:HA3	1:N:183:HIS:CE1	2.50	0.47
7:O:141:VAL:HG12	7:O:142:THR:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:21:PRO:HD3	8:S:12:TRP:CZ3	2.49	0.46
1:N:43:GLN:OE1	1:N:43:GLN:HA	2.15	0.46
1:C:21:PRO:HD3	8:H:12:TRP:CH2	2.51	0.46
2:P:105:VAL:HG21	2:P:118:ILE:HG12	1.98	0.46
13:P:302:PTY:H132	13:P:302:PTY:H161	1.76	0.46
4:F:92:HIS:O	4:F:96:HIS:HB3	2.16	0.46
4:Q:87:ALA:HB1	4:Q:95:LYS:HD3	1.97	0.46
1:C:141:LEU:HD21	1:C:262:PRO:HA	1.98	0.46
1:C:184:TYR:CD2	11:C:501:HEM:HBC1	2.51	0.46
13:N:505:PTY:H311	13:N:505:PTY:H342	1.33	0.46
1:N:21:PRO:HD3	8:S:12:TRP:CH2	2.51	0.46
15:C:506:LMT:H72	16:C:507:AWB:H2A	1.98	0.46
2:P:147:ARG:HE	2:P:147:ARG:HB2	1.06	0.46
11:C:501:HEM:CMB	11:C:501:HEM:CBB	2.88	0.46
2:P:63:LEU:HD13	9:T:8:TYR:HB2	1.98	0.46
1:N:286:PRO:O	2:E:204:PRO:HA	2.15	0.46
1:N:342:VAL:CG1	8:S:70:TRP:HH2	2.28	0.46
2:E:165:ILE:HD12	2:E:210:GLU:HB2	1.98	0.46
1:N:184:TYR:CD2	11:N:501:HEM:HBC1	2.51	0.45
17:N:509:AOQ:H19	17:N:509:AOQ:H8	1.66	0.45
6:M:362:ILE:HG22	6:M:366:LEU:HD13	1.96	0.45
5:A:99:MET:SD	5:A:126:SER:HB3	2.56	0.45
7:D:134:ALA:HA	7:D:177:TYR:HA	1.98	0.45
9:I:8:TYR:HB2	2:E:63:LEU:HD13	1.98	0.45
2:E:192:SER:HB3	2:E:204:PRO:HD2	1.97	0.45
2:E:101:ALA:HB1	2:E:103:VAL:HG13	1.98	0.45
6:M:137:LEU:HD13	6:M:166:TYR:HB2	1.98	0.45
6:M:155:VAL:CG2	6:M:233:ALA:HB2	2.47	0.45
1:C:208:ASN:HB2	1:C:209:PRO:HD2	1.99	0.45
1:C:234:PHE:CZ	7:D:303:MET:HE2	2.51	0.45
5:L:51:THR:HG21	5:L:117:LYS:HE3	1.99	0.45
2:P:127:ILE:HG12	2:P:163:VAL:HG22	1.99	0.45
5:A:43:SER:HB3	5:A:222:HIS:CD2	2.42	0.45
5:A:367:LEU:HD13	5:A:469:MET:SD	2.57	0.45
6:M:91:GLU:HG2	6:M:364:MET:CE	2.45	0.45
1:C:178:ARG:HE	1:C:178:ARG:HB3	1.50	0.45
2:E:106:LYS:HA	2:E:221:THR:HG22	1.98	0.45
5:L:207:TYR:N	5:L:207:TYR:CD1	2.84	0.45
1:C:43:GLN:HA	1:C:43:GLN:OE1	2.15	0.45
1:C:275:LEU:HB3	17:C:508:AOQ:H8	1.98	0.45
1:C:342:VAL:CG1	8:H:70:TRP:HH2	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:506:CDL:H142	14:N:506:CDL:H331	1.99	0.45
2:E:127:ILE:HG12	2:E:163:VAL:HG22	1.99	0.45
1:C:285:ILE:HB	1:C:291:GLY:HA2	1.99	0.45
1:N:117:GLY:HA2	1:N:120:ILE:HD12	1.99	0.45
13:N:505:PTY:H331	13:N:505:PTY:H362	1.42	0.45
1:C:152:SER:HB3	1:C:162:VAL:HG21	1.99	0.44
15:J:101:LMT:H52	15:J:101:LMT:H21	1.65	0.44
1:N:173:ASN:N	1:N:174:PRO:CD	2.80	0.44
7:O:134:ALA:HA	7:O:177:TYR:HA	1.99	0.44
1:C:58:ALA:HB2	1:C:173:ASN:HA	2.00	0.44
13:P:302:PTY:H331	13:P:302:PTY:H361	1.73	0.44
6:M:47:TYR:HB3	6:M:220:VAL:CG1	2.47	0.44
2:P:189:CYS:HB3	2:P:190:HIS:CE1	2.53	0.44
13:P:302:PTY:H381	13:P:302:PTY:H352	1.80	0.44
5:L:35:LEU:HG	5:L:41:ILE:HD11	1.99	0.44
1:C:312:ILE:HG13	1:C:313:ILE:HG13	1.99	0.44
2:P:59:ASP:OD2	9:T:5:THR:HG23	2.18	0.44
1:C:117:GLY:HA2	1:C:120:ILE:HD12	2.00	0.44
1:C:173:ASN:N	1:C:174:PRO:CD	2.80	0.44
7:O:220:GLY:O	7:O:239:PRO:HD2	2.18	0.44
2:P:165:ILE:HD12	2:P:210:GLU:HB2	1.98	0.44
1:N:208:ASN:HB2	1:N:209:PRO:HD2	1.98	0.44
2:E:213:GLU:H	2:E:213:GLU:HG3	1.56	0.44
5:A:207:TYR:CD1	5:A:207:TYR:N	2.85	0.44
6:B:87:HIS:CE1	6:B:94:VAL:HB	2.53	0.44
15:J:101:LMT:H41	15:J:101:LMT:H71	1.61	0.43
6:M:332:VAL:O	6:M:383:PRO:HB3	2.18	0.43
6:B:47:TYR:HB3	6:B:220:VAL:CG1	2.48	0.43
6:B:249:ILE:HD11	6:B:302:PHE:HB2	2.00	0.43
2:E:156:VAL:HG21	2:E:159:PRO:HA	2.01	0.43
1:N:299:ILE:CD1	17:N:509:AOQ:C19	2.96	0.43
13:N:505:PTY:H112	13:N:505:PTY:HC12	1.99	0.43
5:L:269:ARG:NH2	5:L:459:LEU:HG	2.33	0.43
1:N:285:ILE:HB	1:N:291:GLY:HA2	2.00	0.43
13:N:505:PTY:H372	13:N:505:PTY:H402	1.54	0.43
6:M:247:LEU:HD13	6:M:393:LEU:HB3	2.00	0.43
12:C:503:PC1:O13	12:C:503:PC1:H133	2.18	0.43
2:P:117:ILE:CG2	2:P:124:PRO:HB3	2.49	0.43
1:C:308:VAL:HB	1:C:368:PRO:HG3	2.01	0.43
6:B:263:LEU:HA	6:B:277:PRO:HG2	1.99	0.43
5:L:367:LEU:HD13	5:L:469:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:106:LYS:HA	2:P:221:THR:HG22	2.00	0.43
5:A:384:ARG:HG2	6:B:79:LEU:HD11	2.00	0.43
5:A:87:ARG:HD3	5:A:92:LEU:HD13	2.00	0.43
7:D:220:GLY:O	7:D:239:PRO:HD2	2.18	0.43
1:N:194:ALA:HB3	16:N:508:AWB:H27A	2.01	0.43
5:L:96:ILE:O	5:L:99:MET:HB2	2.19	0.43
5:L:395:LEU:HG	6:M:34:ILE:HG21	1.99	0.43
14:L:3002:CDL:H112	14:L:3002:CDL:H141	1.78	0.43
2:P:156:VAL:HG21	2:P:159:PRO:HA	2.01	0.43
2:P:177:GLY:HA2	2:P:185:TRP:CD1	2.54	0.43
5:A:457:GLU:OE2	8:H:16:MET:N	2.47	0.43
7:D:327:PRO:HA	7:D:328:PRO:HD3	1.83	0.43
1:N:262:PRO:HB2	1:N:263:MET:HE1	2.00	0.43
1:N:282:LEU:HD23	2:E:190:HIS:CD2	2.54	0.43
2:E:117:ILE:CG2	2:E:124:PRO:HB3	2.49	0.43
6:B:155:VAL:CG2	6:B:233:ALA:HB2	2.48	0.42
1:N:198:LEU:HA	1:N:198:LEU:HD23	1.74	0.42
11:N:502:HEM:HBC2	11:N:502:HEM:CMC	2.48	0.42
5:L:207:TYR:N	5:L:207:TYR:HD1	2.17	0.42
1:C:173:ASN:HB3	1:C:174:PRO:HD3	2.01	0.42
1:N:312:ILE:HG13	1:N:313:ILE:HG13	1.99	0.42
2:E:116:VAL:HG23	2:E:127:ILE:O	2.19	0.42
2:E:177:GLY:HA2	2:E:185:TRP:CD1	2.54	0.42
14:N:504:CDL:H131	8:S:52:THR:HG23	2.00	0.42
2:P:62:ARG:NH1	9:T:8:TYR:OH	2.52	0.42
2:P:116:VAL:HG23	2:P:127:ILE:O	2.19	0.42
4:F:132:HIS:CE1	7:D:93:HIS:NE2	2.87	0.42
1:N:230:LEU:HD23	1:N:230:LEU:HA	1.85	0.42
14:L:3001:CDL:H1	14:L:3002:CDL:HA4	2.01	0.42
1:C:74:PHE:CE2	2:E:86:ASP:HB3	2.54	0.42
6:B:168:GLN:HB3	6:B:170:TYR:CD1	2.54	0.42
13:D:402:PTY:H352	13:D:402:PTY:H381	1.32	0.42
12:I:201:PC1:H351	12:I:201:PC1:H322	1.63	0.42
1:N:275:LEU:HB3	17:N:509:AOQ:H12	2.00	0.42
1:N:319:LYS:HB3	1:N:374:GLU:OE2	2.20	0.42
6:M:175:LEU:HA	6:M:178:VAL:HG12	2.02	0.42
7:O:218:LEU:HD11	20:O:401:HEC:CMB	2.47	0.42
1:N:308:VAL:HB	1:N:368:PRO:HG3	2.02	0.42
6:M:29:ASP:HB2	6:M:200:PRO:HD3	2.02	0.42
1:C:270:VAL:HG23	1:C:276:LEU:HD21	2.02	0.42
2:P:49:THR:N	2:P:50:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:29:ASP:HB2	6:B:200:PRO:HD3	2.02	0.42
10:J:57:ARG:HA	10:J:61:LEU:HB2	2.00	0.42
2:E:102:LYS:HA	2:E:102:LYS:HD2	1.53	0.42
2:E:193:HIS:O	2:E:200:ILE:HD12	2.20	0.42
8:S:61:LEU:HD23	8:S:61:LEU:HA	1.82	0.42
13:P:302:PTY:H141	13:P:302:PTY:H311	2.01	0.42
6:B:77:LEU:HD12	6:B:107:PHE:HE1	1.85	0.42
2:E:49:THR:N	2:E:50:PRO:CD	2.83	0.42
5:L:96:ILE:HG12	5:L:103:LEU:HD13	2.01	0.42
1:C:158:GLY:O	1:C:162:VAL:HG23	2.20	0.42
14:H:701:CDL:HA21	14:H:701:CDL:OB7	2.20	0.42
1:N:40:LEU:HD23	16:N:508:AWB:H27	2.01	0.42
2:P:193:HIS:O	2:P:200:ILE:HD12	2.20	0.42
2:E:110:ILE:HA	2:E:111:PRO:HD3	1.92	0.42
6:M:59:LYS:HB3	6:M:129:VAL:HG13	2.01	0.42
1:C:152:SER:C	1:C:288:LYS:HE2	2.40	0.41
5:A:35:LEU:HG	5:A:41:ILE:HD11	2.01	0.41
5:A:207:TYR:N	5:A:207:TYR:HD1	2.19	0.41
10:J:11:LYS:HD2	10:J:12:PRO:HD2	2.02	0.41
2:E:185:TRP:HB2	2:E:194:TYR:HB2	2.01	0.41
5:L:317:GLN:HG2	6:M:78:GLU:OE1	2.19	0.41
1:C:49:THR:HG21	1:C:78:ILE:HD13	2.02	0.41
1:C:319:LYS:HB3	1:C:374:GLU:OE2	2.20	0.41
3:R:84:HIS:O	8:S:50:ARG:NH2	2.53	0.41
2:P:185:TRP:HB2	2:P:194:TYR:HB2	2.01	0.41
6:B:102:GLN:H	6:B:102:GLN:HG3	1.53	0.41
1:N:178:ARG:HE	1:N:178:ARG:HB3	1.66	0.41
2:P:174:VAL:O	2:P:174:VAL:HG23	2.19	0.41
5:A:79:LEU:HD12	5:A:79:LEU:HA	1.79	0.41
6:B:236:ARG:HD3	6:M:170:TYR:CZ	2.55	0.41
10:J:51:GLU:OE1	2:E:81:LYS:NZ	2.49	0.41
2:E:170:HIS:CE1	2:E:171:LEU:HG	2.55	0.41
1:C:282:LEU:HD23	2:P:190:HIS:CD2	2.56	0.41
1:C:342:VAL:HG11	8:H:70:TRP:CH2	2.55	0.41
2:P:86:ASP:HB3	1:N:74:PHE:CE2	2.56	0.41
6:B:128:ARG:NH2	3:R:112:GLU:OE2	2.51	0.41
1:N:342:VAL:HG11	8:S:70:TRP:CH2	2.54	0.41
12:N:503:PC1:O13	12:N:503:PC1:H133	2.19	0.41
2:E:174:VAL:O	2:E:174:VAL:HG23	2.20	0.41
5:L:330:LEU:HD23	5:L:330:LEU:HA	1.89	0.41
5:A:330:LEU:HD23	5:A:330:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:508:AWB:HB27B	16:N:508:AWB:H22	2.02	0.41
2:E:120:TRP:CE3	2:E:125:ILE:HD11	2.56	0.41
6:M:62:PHE:CE2	6:M:84:LEU:HD11	2.56	0.41
2:P:192:SER:HA	2:P:203:GLY:HA3	2.03	0.41
9:I:5:THR:HG23	2:E:59:ASP:OD2	2.21	0.41
1:N:210:LEU:HB2	1:N:212:ILE:HG12	2.02	0.41
2:E:192:SER:HA	2:E:203:GLY:HA3	2.03	0.41
4:Q:86:ALA:HA	4:Q:90:PRO:HD2	2.03	0.41
5:L:318:GLY:HA2	6:M:75:ARG:CZ	2.51	0.41
1:C:76:TRP:CH2	7:D:289:ARG:HA	2.56	0.41
11:C:502:HEM:HBC2	11:C:502:HEM:CMC	2.49	0.41
2:P:120:TRP:O	2:P:121:ARG:HB2	2.21	0.41
5:A:318:GLY:HA2	6:B:75:ARG:CZ	2.50	0.41
6:B:26:ALA:CB	6:B:366:LEU:HD11	2.51	0.41
1:N:76:TRP:CH2	7:O:289:ARG:HA	2.55	0.41
7:O:141:VAL:HG11	7:O:280:TRP:CE2	2.56	0.41
7:O:297:ILE:HD13	7:O:297:ILE:HA	2.01	0.41
2:P:147:ARG:HD2	2:P:206:PRO:HA	2.03	0.41
4:F:87:ALA:HB1	4:F:95:LYS:HD3	2.02	0.41
1:C:80:TYR:CD1	1:C:248:PRO:HB2	2.56	0.40
2:P:125:ILE:HD13	2:P:165:ILE:HA	2.02	0.40
2:P:175:PRO:HA	2:P:187:CYS:HA	2.03	0.40
6:M:84:LEU:CD1	6:M:97:THR:HG22	2.50	0.40
7:O:327:PRO:HA	7:O:328:PRO:HD3	1.83	0.40
5:A:140:ALA:O	5:A:144:ILE:HG12	2.22	0.40
6:B:175:LEU:HA	6:B:178:VAL:HG12	2.03	0.40
7:D:141:VAL:HG11	7:D:280:TRP:CE2	2.57	0.40
3:R:20:LEU:HD23	3:R:20:LEU:HA	1.89	0.40
4:Q:132:HIS:CE1	7:O:93:HIS:NE2	2.89	0.40
6:M:188:LYS:HE2	6:M:211:PHE:O	2.21	0.40
1:C:148:CYS:HB2	1:C:166:TRP:HE1	1.86	0.40
2:P:170:HIS:CE1	2:P:171:LEU:HG	2.56	0.40
5:L:140:ALA:O	5:L:144:ILE:HG12	2.21	0.40
1:C:131:GLY:HA3	1:C:183:HIS:CE1	2.56	0.40
1:C:288:LYS:O	1:C:292:VAL:HG23	2.21	0.40
3:G:84:HIS:O	8:H:50:ARG:NH2	2.54	0.40
5:A:144:ILE:HG12	5:A:144:ILE:H	1.76	0.40
1:C:376:ILE:HD11	3:G:10:THR:HG21	2.03	0.40
3:G:70:ARG:HD2	3:G:101:TYR:OH	2.22	0.40
1:N:49:THR:HG21	1:N:78:ILE:HD13	2.03	0.40
1:N:58:ALA:HB2	1:N:173:ASN:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:164:MET:HE3	2:E:164:MET:HB2	1.98	0.40
6:M:77:LEU:HD12	6:M:107:PHE:CE1	2.55	0.40
7:O:173:LYS:HB2	7:O:173:LYS:HE3	1.82	0.40
7:O:202:LEU:HD23	7:O:202:LEU:HA	1.96	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	C	381/385 (99%)	372 (98%)	9 (2%)	0	100	100
1	N	381/385 (99%)	371 (97%)	9 (2%)	1 (0%)	37	66
2	E	184/225 (82%)	171 (93%)	13 (7%)	0	100	100
2	P	184/225 (82%)	168 (91%)	14 (8%)	2 (1%)	12	40
3	G	122/128 (95%)	122 (100%)	0	0	100	100
3	R	122/128 (95%)	122 (100%)	0	0	100	100
4	F	69/137 (50%)	67 (97%)	2 (3%)	0	100	100
4	Q	69/137 (50%)	67 (97%)	2 (3%)	0	100	100
5	A	434/474 (92%)	423 (98%)	11 (2%)	0	100	100
5	L	434/474 (92%)	420 (97%)	14 (3%)	0	100	100
6	B	400/417 (96%)	385 (96%)	14 (4%)	1 (0%)	37	66
6	M	400/417 (96%)	386 (96%)	14 (4%)	0	100	100
7	D	242/330 (73%)	238 (98%)	4 (2%)	0	100	100
7	O	242/330 (73%)	238 (98%)	4 (2%)	0	100	100
8	H	83/93 (89%)	82 (99%)	1 (1%)	0	100	100
8	S	83/93 (89%)	82 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	52/69 (75%)	50 (96%)	2 (4%)	0	100	100
9	T	52/69 (75%)	50 (96%)	2 (4%)	0	100	100
10	J	73/82 (89%)	71 (97%)	2 (3%)	0	100	100
10	U	73/82 (89%)	71 (97%)	2 (3%)	0	100	100
All	All	4080/4680 (87%)	3956 (97%)	120 (3%)	4 (0%)	50	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	98	LEU
1	N	156	TRP
2	P	102	LYS
6	B	368	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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	C	331/333 (99%)	311 (94%)	20 (6%)	16	42
1	N	331/333 (99%)	309 (93%)	22 (7%)	14	40
2	E	154/182 (85%)	135 (88%)	19 (12%)	4	16
2	P	154/182 (85%)	137 (89%)	17 (11%)	5	20
3	G	113/117 (97%)	102 (90%)	11 (10%)	6	25
3	R	113/117 (97%)	107 (95%)	6 (5%)	19	47
4	F	61/123 (50%)	59 (97%)	2 (3%)	33	60
4	Q	61/123 (50%)	61 (100%)	0	100	100
5	A	377/407 (93%)	362 (96%)	15 (4%)	27	55
5	L	377/407 (93%)	361 (96%)	16 (4%)	25	53
6	B	311/322 (97%)	295 (95%)	16 (5%)	20	48
6	M	311/322 (97%)	293 (94%)	18 (6%)	17	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	D	192/268 (72%)	190 (99%)	2 (1%)	73	84
7	O	192/268 (72%)	191 (100%)	1 (0%)	86	91
8	H	67/71 (94%)	65 (97%)	2 (3%)	36	62
8	S	67/71 (94%)	65 (97%)	2 (3%)	36	62
9	I	46/57 (81%)	45 (98%)	1 (2%)	47	69
9	T	46/57 (81%)	45 (98%)	1 (2%)	47	69
10	J	63/68 (93%)	61 (97%)	2 (3%)	34	61
10	U	63/68 (93%)	61 (97%)	2 (3%)	34	61
All	All	3430/3896 (88%)	3255 (95%)	175 (5%)	22	48

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	79	ARG
1	C	89	PHE
1	C	109	PRO
1	C	130	MET
1	C	136	PHE
1	C	147	ILE
1	C	157	LEU
1	C	159	GLU
1	C	160	ASP
1	C	174	PRO
1	C	178	ARG
1	C	187	PRO
1	C	197	HIS
1	C	250	LYS
1	C	266	PRO
1	C	270	VAL
1	C	282	LEU
1	C	320	PRO
1	C	324	LEU
1	C	369	MET
2	P	54	LYS
2	P	55	ASP
2	P	62	ARG
2	P	100	MET
2	P	106	LYS
2	P	115	ASN

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Mol	Chain	Res	Type
2	P	116	VAL
2	P	117	ILE
2	P	119	LYS
2	P	146	LEU
2	P	147	ARG
2	P	158	LYS
2	P	176	ILE
2	P	195	ASP
2	P	196	ILE
2	P	197	SER
2	P	213	GLU
3	G	3	SER
3	G	6	SER
3	G	17	SER
3	G	19	LEU
3	G	22	LYS
3	G	23	ILE
3	G	30	THR
3	G	40	LEU
3	G	50	GLU
3	G	65	THR
3	G	112	GLU
4	F	96	HIS
4	F	100	GLU
5	A	29	LYS
5	A	48	LEU
5	A	79	LEU
5	A	82	LYS
5	A	87	ARG
5	A	94	LEU
5	A	97	GLU
5	A	137	SER
5	A	141	GLU
5	A	197	THR
5	A	205	GLU
5	A	267	GLU
5	A	397	LEU
5	A	461	ASP
5	A	466	ARG
6	B	45	SER
6	B	60	PHE
6	B	77	LEU

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Mol	Chain	Res	Type
6	B	79	LEU
6	B	102	GLN
6	B	119	LYS
6	B	139	LYS
6	B	168	GLN
6	B	247	LEU
6	B	249	ILE
6	B	268	SER
6	B	276	SER
6	B	322	VAL
6	B	345	LYS
6	B	371	SER
6	B	376	GLU
7	D	85	MET
7	D	193	GLN
8	H	51	ARG
8	H	57	LEU
9	I	27	PHE
10	J	11	LYS
10	J	15	LYS
1	N	79	ARG
1	N	89	PHE
1	N	109	PRO
1	N	136	PHE
1	N	145	THR
1	N	151	VAL
1	N	157	LEU
1	N	159	GLU
1	N	160	ASP
1	N	174	PRO
1	N	178	ARG
1	N	187	PRO
1	N	197	HIS
1	N	250	LYS
1	N	254	PRO
1	N	255	ASP
1	N	265	THR
1	N	282	LEU
1	N	288	LYS
1	N	320	PRO
1	N	324	LEU
1	N	369	MET

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Mol	Chain	Res	Type
2	E	54	LYS
2	E	55	ASP
2	E	62	ARG
2	E	65	SER
2	E	100	MET
2	E	102	LYS
2	E	106	LYS
2	E	115	ASN
2	E	116	VAL
2	E	117	ILE
2	E	119	LYS
2	E	146	LEU
2	E	147	ARG
2	E	158	LYS
2	E	176	ILE
2	E	195	ASP
2	E	196	ILE
2	E	197	SER
2	E	213	GLU
3	R	17	SER
3	R	19	LEU
3	R	22	LYS
3	R	23	ILE
3	R	30	THR
3	R	65	THR
5	L	29	LYS
5	L	48	LEU
5	L	51	THR
5	L	86	LYS
5	L	87	ARG
5	L	97	GLU
5	L	99	MET
5	L	183	THR
5	L	185	LEU
5	L	205	GLU
5	L	378	SER
5	L	395	LEU
5	L	397	LEU
5	L	441	LYS
5	L	461	ASP
5	L	466	ARG
6	M	16	SER

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Mol	Chain	Res	Type
6	M	19	GLU
6	M	32	SER
6	M	34	ILE
6	M	60	PHE
6	M	77	LEU
6	M	101	LYS
6	M	119	LYS
6	M	139	LYS
6	M	273	VAL
6	M	292	THR
6	M	322	VAL
6	M	331	GLU
6	M	332	VAL
6	M	345	LYS
6	M	356	ASP
6	M	362	ILE
6	M	376	GLU
7	O	193	GLN
8	S	51	ARG
8	S	57	LEU
9	T	27	PHE
10	U	11	LYS
10	U	55	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	14	ASN
1	C	173	ASN
1	C	332	ASN
2	P	90	ASN
2	P	193	HIS
3	G	54	ASN
3	G	84	HIS
4	F	132	HIS
5	A	74	HIS
5	A	222	HIS
6	B	87	HIS
6	B	215	GLN
7	D	90	HIS
10	J	70	HIS
1	N	14	ASN

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Mol	Chain	Res	Type
1	N	332	ASN
2	E	85	GLN
2	E	90	ASN
2	E	193	HIS
3	R	84	HIS
4	Q	132	HIS
5	L	192	GLN
6	M	92	HIS
6	M	184	GLN
6	M	215	GLN
7	O	90	HIS
10	U	70	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](#)

36 ligands are modelled in this entry.

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	$\# Z > 2$
20	HEC	D	401	7	32,50,50	1.66	7 (21%)	24,82,82	3.08	8 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	HEM	C	502	1	41,50,50	1.47	6 (14%)	45,82,82	2.21	24 (53%)
19	XP4	A	3003	-	23,23,39	1.61	2 (8%)	27,28,44	2.45	6 (22%)
13	PTY	P	302	-	40,40,49	0.48	0	43,45,54	0.67	0
14	CDL	A	3001	-	41,41,99	1.12	3 (7%)	45,51,111	0.78	1 (2%)
12	PC1	C	503	-	37,37,53	0.61	0	43,45,61	1.07	3 (6%)
15	LMT	C	506	-	36,36,36	0.48	0	47,47,47	1.07	3 (6%)
11	HEM	C	501	1	41,50,50	1.78	9 (21%)	45,82,82	2.70	17 (37%)
16	AWB	C	507	-	40,40,40	0.57	0	36,54,54	1.20	2 (5%)
14	CDL	A	3002	-	46,46,99	0.47	0	51,56,111	0.84	2 (3%)
17	AOQ	N	509	-	29,29,29	1.86	6 (20%)	40,42,42	2.45	21 (52%)
18	FES	E	301	2	0,4,4	-	-	-	-	-
19	XP4	L	3003	-	23,23,39	1.63	2 (8%)	27,28,44	2.34	7 (25%)
14	CDL	N	506	-	47,47,99	0.49	0	53,59,111	0.87	2 (3%)
15	LMT	N	507	-	36,36,36	0.60	0	47,47,47	1.04	3 (6%)
14	CDL	L	3001	-	41,41,99	0.69	1 (2%)	45,51,111	0.75	1 (2%)
15	LMT	U	101	-	36,36,36	0.55	0	47,47,47	1.01	3 (6%)
14	CDL	S	101	-	38,38,99	0.47	0	44,50,111	1.08	4 (9%)
11	HEM	N	501	1	41,50,50	1.79	9 (21%)	45,82,82	2.79	17 (37%)
14	CDL	C	505	-	47,47,99	0.48	0	53,59,111	0.88	3 (5%)
15	LMT	J	101	-	36,36,36	0.50	0	47,47,47	1.17	4 (8%)
13	PTY	N	505	-	40,40,49	0.42	0	43,45,54	0.62	1 (2%)
12	PC1	I	201	-	31,31,53	0.39	0	37,39,61	0.70	1 (2%)
14	CDL	H	701	-	49,49,99	0.40	0	55,61,111	0.74	0
11	HEM	N	502	1	41,50,50	1.54	6 (14%)	45,82,82	2.31	21 (46%)
12	PC1	T	201	-	31,31,53	0.40	0	37,39,61	0.75	1 (2%)
14	CDL	L	3002	-	46,46,99	0.65	1 (2%)	51,56,111	0.87	2 (3%)
18	FES	P	301	2	0,4,4	-	-	-	-	-
14	CDL	N	504	-	49,49,99	0.62	1 (2%)	55,61,111	0.71	0
20	HEC	O	401	7	32,50,50	1.65	7 (21%)	24,82,82	3.06	8 (33%)
14	CDL	H	702	-	38,38,99	0.48	0	44,50,111	1.09	4 (9%)
13	PTY	C	504	-	40,40,49	0.43	0	43,45,54	0.66	1 (2%)
17	AOQ	C	508	-	29,29,29	2.06	6 (20%)	40,42,42	2.10	11 (27%)
13	PTY	D	402	-	40,40,49	0.45	0	43,45,54	0.58	0
16	AWB	N	508	-	40,40,40	0.61	0	36,54,54	1.38	4 (11%)
12	PC1	N	503	-	37,37,53	0.59	0	43,45,61	0.92	3 (6%)

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
20	HEC	D	401	7	-	6/10/54/54	-
11	HEM	C	502	1	-	5/12/54/54	-
19	XP4	A	3003	-	-	1/24/24/41	-
13	PTY	P	302	-	-	25/44/44/53	-
14	CDL	A	3001	-	-	15/48/48/110	-
12	PC1	C	503	-	-	13/41/41/57	-
15	LMT	C	506	-	-	14/21/61/61	0/2/2/2
11	HEM	C	501	1	-	5/12/54/54	-
16	AWB	C	507	-	-	9/38/53/53	0/1/2/2
14	CDL	A	3002	-	-	23/54/54/110	-
17	AOQ	N	509	-	-	0/8/38/38	0/4/4/4
19	XP4	L	3003	-	-	1/24/24/41	-
18	FES	E	301	2	-	-	0/1/1/1
14	CDL	N	506	-	-	29/57/57/110	-
15	LMT	N	507	-	-	17/21/61/61	0/2/2/2
14	CDL	L	3001	-	-	19/48/48/110	-
15	LMT	U	101	-	-	8/21/61/61	0/2/2/2
14	CDL	S	101	-	-	28/48/48/110	-
11	HEM	N	501	1	-	5/12/54/54	-
14	CDL	C	505	-	-	30/57/57/110	-
15	LMT	J	101	-	-	10/21/61/61	0/2/2/2
13	PTY	N	505	-	-	31/44/44/53	-
12	PC1	I	201	-	-	18/35/35/57	-
14	CDL	H	701	-	-	32/59/59/110	-
11	HEM	N	502	1	-	4/12/54/54	-
12	PC1	T	201	-	-	14/35/35/57	-
14	CDL	L	3002	-	-	25/54/54/110	-
20	HEC	O	401	7	-	6/10/54/54	-
14	CDL	N	504	-	-	38/59/59/110	-
18	FES	P	301	2	-	-	0/1/1/1
14	CDL	H	702	-	-	28/48/48/110	-
13	PTY	C	504	-	-	30/44/44/53	-
17	AOQ	C	508	-	-	0/8/38/38	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	PTY	D	402	-	-	29/44/44/53	-
16	AWB	N	508	-	-	8/38/53/53	0/1/2/2
12	PC1	N	503	-	-	14/41/41/57	-

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	508	AOQ	C3-C2	7.36	1.45	1.35
19	L	3003	XP4	O7-C18	5.86	1.48	1.35
11	C	501	HEM	C3C-C2C	-5.76	1.32	1.40
11	N	501	HEM	C3C-C2C	-5.76	1.32	1.40
19	A	3003	XP4	O7-C18	5.72	1.48	1.35
17	N	509	AOQ	C3-C2	5.59	1.43	1.35
14	A	3001	CDL	C35-C34	4.49	1.76	1.51
11	N	501	HEM	C1B-NB	-4.05	1.33	1.40
11	N	502	HEM	C1B-NB	-4.02	1.33	1.40
19	A	3003	XP4	O5-C4	4.01	1.45	1.33
11	C	501	HEM	C1B-NB	-3.93	1.33	1.40
19	L	3003	XP4	O5-C4	3.92	1.44	1.33
11	C	502	HEM	C1B-NB	-3.84	1.33	1.40
17	N	509	AOQ	O2-C4	-3.63	1.15	1.23
20	D	401	HEC	CAA-C2A	-3.60	1.45	1.52
11	N	502	HEM	C4D-ND	-3.57	1.34	1.40
20	O	401	HEC	CAA-C2A	-3.52	1.46	1.52
11	N	502	HEM	C4B-NB	-3.49	1.31	1.38
11	C	501	HEM	C4B-NB	-3.45	1.31	1.38
11	N	501	HEM	C1D-ND	-3.45	1.31	1.38
11	N	501	HEM	C4B-NB	-3.44	1.31	1.38
14	A	3001	CDL	C33-C32	3.44	1.70	1.51
11	C	501	HEM	C1D-ND	-3.39	1.31	1.38
11	C	502	HEM	C4B-NB	-3.32	1.32	1.38
14	N	504	CDL	C15-C14	3.29	1.76	1.49
20	D	401	HEC	CAD-C3D	-3.24	1.47	1.52
20	O	401	HEC	CAD-C3D	-3.19	1.47	1.52
11	N	501	HEM	C4D-ND	-3.17	1.34	1.40
11	C	501	HEM	C4D-ND	-3.12	1.34	1.40
11	C	502	HEM	C4D-ND	-3.09	1.35	1.40
14	L	3002	CDL	C56-C55	3.03	1.74	1.49
20	O	401	HEC	C3C-C2C	2.98	1.43	1.40
11	N	502	HEM	C1D-ND	-2.97	1.32	1.38
20	D	401	HEC	C3C-C2C	2.93	1.43	1.40
17	C	508	AOQ	C2-C1	-2.83	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	502	HEM	C1D-ND	-2.65	1.33	1.38
17	N	509	AOQ	C14-C13	2.60	1.60	1.53
17	C	508	AOQ	O2-C4	-2.59	1.17	1.23
20	D	401	HEC	C1B-NB	-2.59	1.30	1.36
20	O	401	HEC	C1B-NB	-2.59	1.30	1.36
20	D	401	HEC	C2B-C3B	2.52	1.43	1.40
11	C	502	HEM	CHB-C1B	2.48	1.41	1.35
14	L	3001	CDL	C31-CA7	2.45	1.57	1.50
17	C	508	AOQ	C20-CL	2.45	1.79	1.74
20	O	401	HEC	C2B-C3B	2.42	1.43	1.40
17	N	509	AOQ	C9-C1	2.39	1.52	1.48
11	N	501	HEM	O2D-CGD	-2.32	1.22	1.30
17	C	508	AOQ	C7-C8	2.31	1.43	1.38
11	C	501	HEM	O2D-CGD	-2.31	1.23	1.30
11	N	502	HEM	CHB-C1B	2.29	1.40	1.35
20	O	401	HEC	C1C-NC	-2.28	1.31	1.36
20	D	401	HEC	C1C-NC	-2.25	1.31	1.36
11	N	501	HEM	FE-ND	-2.21	1.85	1.96
11	N	502	HEM	FE-ND	-2.21	1.85	1.96
17	N	509	AOQ	C12-C13	-2.20	1.47	1.53
11	C	501	HEM	FE-ND	-2.18	1.86	1.96
11	C	502	HEM	FE-NB	2.17	2.07	1.96
14	A	3001	CDL	C32-C31	2.14	1.60	1.52
20	D	401	HEC	C4D-CHA	2.11	1.46	1.41
11	N	501	HEM	CAA-C2A	-2.10	1.49	1.52
11	N	501	HEM	CHC-C4B	-2.10	1.35	1.41
11	C	501	HEM	CAA-C2A	-2.09	1.49	1.52
20	O	401	HEC	C4D-CHA	2.08	1.46	1.41
11	C	501	HEM	CHC-C4B	-2.08	1.35	1.41
17	C	508	AOQ	C22-C17	2.03	1.42	1.39
17	N	509	AOQ	C7-C8	2.01	1.43	1.38

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	N	501	HEM	CHC-C4B-NB	9.14	134.37	124.43
11	C	501	HEM	CHC-C4B-NB	8.64	133.82	124.43
19	A	3003	XP4	O7-C18-C19	8.55	126.82	111.09
19	L	3003	XP4	O7-C18-C19	8.15	126.08	111.09
11	N	501	HEM	CBA-CAA-C2A	-8.11	98.78	112.62
11	C	501	HEM	CBA-CAA-C2A	-7.93	99.09	112.62
20	O	401	HEC	C1D-C2D-C3D	-7.69	101.64	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	D	401	HEC	C1D-C2D-C3D	-7.67	101.66	107.00
20	D	401	HEC	CMB-C2B-C3B	6.85	133.87	125.82
20	O	401	HEC	CMB-C2B-C3B	6.77	133.79	125.82
20	D	401	HEC	CAA-CBA-CGA	-6.75	94.84	113.76
20	O	401	HEC	CAA-CBA-CGA	-6.74	94.88	113.76
17	N	509	AOQ	O6-C3-C2	-5.40	114.70	122.05
19	A	3003	XP4	O7-C18-O8	-5.38	112.28	122.96
11	N	502	HEM	CHC-C4B-NB	5.27	130.16	124.43
11	N	501	HEM	C1B-NB-C4B	5.15	110.39	105.07
19	L	3003	XP4	O7-C18-O8	-5.04	112.95	122.96
16	N	508	AWB	C18-C17-C16	4.94	123.01	119.79
20	D	401	HEC	CMC-C2C-C3C	4.82	131.49	125.82
11	C	501	HEM	C1B-NB-C4B	4.76	109.99	105.07
11	N	501	HEM	CAD-CBD-CGD	-4.74	103.39	113.60
11	C	501	HEM	CAD-CBD-CGD	-4.72	103.44	113.60
20	O	401	HEC	CMC-C2C-C3C	4.71	131.36	125.82
17	N	509	AOQ	C15-C16-C11	4.64	119.78	109.97
17	C	508	AOQ	C14-C13-C17	-4.62	101.96	112.79
11	N	502	HEM	CHD-C1D-C2D	-4.50	117.95	124.98
11	C	502	HEM	CHD-C1D-C2D	-4.33	118.22	124.98
17	N	509	AOQ	C22-C17-C18	4.20	123.53	118.29
11	N	501	HEM	CHD-C1D-ND	4.11	128.90	124.43
17	C	508	AOQ	C15-C14-C13	4.11	118.25	110.52
20	O	401	HEC	CBD-CAD-C3D	-4.10	105.62	112.62
20	D	401	HEC	CBD-CAD-C3D	-4.07	105.68	112.62
11	N	502	HEM	CBD-CAD-C3D	-4.06	101.35	112.63
11	N	501	HEM	CHC-C4B-C3B	-4.04	118.38	124.57
19	A	3003	XP4	O4-P1-O2	-4.01	95.23	106.47
11	C	502	HEM	CHC-C4B-NB	3.99	128.76	124.43
11	C	502	HEM	CBD-CAD-C3D	-3.97	101.61	112.63
17	C	508	AOQ	C21-C22-C17	-3.93	117.25	121.20
15	U	101	LMT	C1-O1'-C1'	-3.90	107.37	113.84
11	C	501	HEM	CHD-C1D-ND	3.85	128.62	124.43
17	N	509	AOQ	C14-C15-C16	3.85	117.64	111.18
17	N	509	AOQ	C8-C9-C1	-3.84	114.47	120.10
11	C	501	HEM	CHC-C4B-C3B	-3.84	118.69	124.57
11	C	501	HEM	C3B-C2B-C1B	-3.77	103.69	106.49
17	N	509	AOQ	C5-C10-C9	3.75	123.43	119.26
12	C	503	PC1	O21-C21-C22	-3.73	103.46	111.50
17	C	508	AOQ	C5-C10-C9	3.59	123.26	119.26
11	N	501	HEM	C3B-C2B-C1B	-3.58	103.83	106.49
11	N	502	HEM	CHD-C1D-ND	3.53	128.27	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	502	HEM	CAD-C3D-C4D	3.52	130.81	124.66
17	C	508	AOQ	C15-C16-C11	3.51	117.38	109.97
11	N	501	HEM	CHD-C1D-C2D	-3.50	119.51	124.98
11	N	502	HEM	CAD-C3D-C4D	3.47	130.71	124.66
15	J	101	LMT	C1-O1'-C1'	-3.46	108.09	113.84
11	N	502	HEM	C4C-CHD-C1D	-3.44	118.02	122.56
17	C	508	AOQ	C8-C9-C1	-3.43	115.08	120.10
16	C	507	AWB	C18-C17-N1	-3.41	117.46	122.59
11	C	501	HEM	CHD-C1D-C2D	-3.40	119.67	124.98
11	N	502	HEM	C2C-C3C-C4C	3.38	109.26	106.90
17	C	508	AOQ	C11-C16-C2	3.33	121.42	113.97
11	C	502	HEM	CHD-C1D-ND	3.28	127.99	124.43
11	C	502	HEM	C2C-C3C-C4C	3.25	109.17	106.90
12	C	503	PC1	O22-C21-C22	3.23	136.35	123.73
11	N	502	HEM	CHC-C4B-C3B	-3.23	119.62	124.57
11	C	502	HEM	C4C-CHD-C1D	-3.23	118.30	122.56
17	C	508	AOQ	C22-C17-C18	3.21	122.30	118.29
15	C	506	LMT	C2'-C3'-C4'	3.21	117.00	109.68
17	C	508	AOQ	C6-C7-C8	3.20	125.07	120.19
11	N	501	HEM	CBB-CAB-C3B	-3.20	111.71	127.62
19	L	3003	XP4	P1-O4-C1	3.18	127.06	118.30
11	C	502	HEM	C2D-C1D-ND	3.17	113.68	109.88
17	N	509	AOQ	C15-C16-C2	3.17	121.05	113.97
11	N	502	HEM	C2D-C1D-ND	3.16	113.67	109.88
17	N	509	AOQ	C2-C3-C4	3.13	126.65	123.34
17	N	509	AOQ	C21-C22-C17	-3.12	118.06	121.20
14	S	101	CDL	CB4-OB6-CB5	3.11	123.68	117.90
14	H	702	CDL	CB4-OB6-CB5	3.10	123.67	117.90
16	N	508	AWB	C17-N1-C21	-3.10	120.77	126.63
11	N	501	HEM	CHB-C1B-NB	3.09	128.20	124.38
11	N	502	HEM	C1B-NB-C4B	3.07	108.24	105.07
11	C	501	HEM	CBB-CAB-C3B	-3.05	112.42	127.62
15	N	507	LMT	C1-O1'-C1'	-3.03	108.82	113.84
11	N	502	HEM	CMB-C2B-C1B	3.02	129.63	125.04
11	C	502	HEM	C1B-NB-C4B	2.97	108.14	105.07
16	N	508	AWB	C18-C17-N1	-2.93	118.19	122.59
11	C	502	HEM	CAD-C3D-C2D	-2.93	122.43	127.88
11	N	502	HEM	CAD-C3D-C2D	-2.88	122.52	127.88
11	N	501	HEM	CHA-C4D-C3D	-2.87	119.94	125.33
17	C	508	AOQ	C7-C8-C9	-2.86	114.41	119.81
11	N	501	HEM	CHA-C4D-ND	2.85	127.91	124.38
11	C	501	HEM	CHB-C1B-NB	2.84	127.89	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	501	HEM	CHA-C4D-C3D	-2.83	120.01	125.33
19	A	3003	XP4	P1-O4-C1	2.82	126.07	118.30
11	C	502	HEM	CHA-C4D-ND	2.82	127.86	124.38
16	C	507	AWB	C18-C17-C16	2.82	121.63	119.79
11	C	502	HEM	CMC-C2C-C3C	2.82	129.95	124.68
20	D	401	HEC	CMD-C2D-C1D	2.78	132.73	128.46
17	N	509	AOQ	C19-C18-C17	-2.78	118.40	121.20
11	N	501	HEM	C4B-CHC-C1C	-2.77	118.90	122.56
11	N	502	HEM	CMC-C2C-C3C	2.77	129.86	124.68
20	O	401	HEC	CMD-C2D-C1D	2.71	132.63	128.46
11	C	502	HEM	O2D-CGD-CBD	2.71	122.73	114.03
14	L	3002	CDL	OA5-PA1-OA3	-2.70	98.51	109.07
19	L	3003	XP4	O4-P1-O2	-2.70	98.91	106.47
11	N	501	HEM	CMB-C2B-C1B	2.68	129.12	125.04
15	J	101	LMT	C1'-O5'-C5'	-2.67	108.44	113.69
11	C	501	HEM	CMB-C2B-C1B	2.67	129.10	125.04
11	C	501	HEM	CHA-C4D-ND	2.67	127.68	124.38
16	N	508	AWB	O5-C21-N1	-2.66	122.41	125.80
11	C	501	HEM	C4B-CHC-C1C	-2.63	119.08	122.56
17	N	509	AOQ	C21-C20-C19	2.61	124.63	121.24
12	N	503	PC1	O21-C21-C22	-2.61	105.88	111.50
14	A	3001	CDL	OB8-CB6-CB4	2.60	118.34	105.77
14	L	3001	CDL	OB6-CB4-CB3	-2.60	100.42	109.56
19	A	3003	XP4	O5-C3-C2	-2.60	100.86	108.43
14	A	3002	CDL	OA2-PA1-OA3	2.59	119.19	109.07
14	C	505	CDL	OB6-CB4-CB3	2.58	117.73	108.40
14	N	506	CDL	OB6-CB4-CB3	2.57	117.69	108.40
11	N	502	HEM	CHA-C4D-ND	2.55	127.53	124.38
11	N	502	HEM	C1D-C2D-C3D	-2.55	104.28	106.96
17	N	509	AOQ	C7-C8-C9	-2.54	115.02	119.81
14	L	3002	CDL	OA2-PA1-OA3	2.52	118.93	109.07
17	C	508	AOQ	C8-C9-C10	2.52	122.06	119.26
11	C	502	HEM	CMA-C3A-C4A	-2.51	124.61	128.46
11	C	502	HEM	O1D-CGD-CBD	-2.49	115.08	123.08
17	N	509	AOQ	C10-C9-C1	2.49	123.37	120.68
14	H	702	CDL	OB6-CB5-C51	2.47	115.63	111.09
17	N	509	AOQ	C6-C7-C8	2.47	123.95	120.19
19	L	3003	XP4	O1-P1-O4	2.44	113.23	106.73
19	L	3003	XP4	O5-C3-C2	-2.44	101.34	108.43
19	A	3003	XP4	O1-P1-O4	2.43	113.19	106.73
11	C	502	HEM	O2A-CGA-O1A	-2.40	117.33	123.30
11	N	502	HEM	C4B-CHC-C1C	-2.39	119.40	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	3002	CDL	OA5-PA1-OA3	-2.39	99.72	109.07
15	N	507	LMT	C2'-C3'-C4'	2.39	115.13	109.68
15	J	101	LMT	O5B-C5B-C4B	2.38	114.03	109.69
14	S	101	CDL	OB6-CB5-C51	2.38	115.47	111.09
11	N	502	HEM	CHB-C1B-NB	2.38	127.32	124.38
12	N	503	PC1	O22-C21-C22	2.38	133.00	123.73
11	N	502	HEM	CBA-CAA-C2A	-2.37	108.57	112.62
14	H	702	CDL	OB6-CB4-CB6	2.36	116.96	108.40
11	C	502	HEM	C1D-C2D-C3D	-2.34	104.50	106.96
11	C	502	HEM	CHC-C4B-C3B	-2.32	121.01	124.57
17	N	509	AOQ	O1-C1-C2	2.32	124.34	120.78
14	S	101	CDL	OB6-CB4-CB6	2.31	116.78	108.40
17	N	509	AOQ	C8-C9-C10	2.31	121.83	119.26
15	N	507	LMT	C4B-C3B-C2B	2.29	114.83	110.82
15	J	101	LMT	C1'-C2'-C3'	-2.29	105.24	110.00
20	D	401	HEC	CAD-CBD-CGD	-2.28	107.38	113.76
14	H	702	CDL	OA5-PA1-OA3	-2.27	100.22	109.07
14	N	506	CDL	CB4-OB6-CB5	2.26	123.36	117.79
20	D	401	HEC	O1D-CGD-CBD	-2.26	115.81	123.08
15	U	101	LMT	C2'-C3'-C4'	2.25	114.82	109.68
20	O	401	HEC	O1D-CGD-CBD	-2.25	115.86	123.08
20	O	401	HEC	CAD-CBD-CGD	-2.23	107.50	113.76
11	N	502	HEM	O2D-CGD-CBD	2.23	121.20	114.03
14	C	505	CDL	CB4-OB6-CB5	2.22	123.27	117.79
11	C	502	HEM	C3C-C4C-NC	-2.22	106.75	110.94
11	C	502	HEM	CMB-C2B-C1B	2.21	128.40	125.04
14	S	101	CDL	OA5-PA1-OA3	-2.21	100.44	109.07
11	N	502	HEM	C3C-C4C-NC	-2.19	106.81	110.94
17	N	509	AOQ	C19-C20-CL	-2.19	115.94	119.35
15	C	506	LMT	O5'-C1'-C2'	2.18	114.97	110.35
15	C	506	LMT	C1B-O1B-C4'	-2.17	112.58	117.96
17	N	509	AOQ	C14-C13-C17	2.17	117.89	112.79
11	N	501	HEM	O2D-CGD-O1D	-2.17	117.89	123.30
12	C	503	PC1	O12-P-O14	2.16	122.91	112.24
11	C	502	HEM	CHA-C4D-C3D	-2.15	121.28	125.33
11	C	502	HEM	C4B-C3B-C2B	-2.15	105.41	107.11
13	C	504	PTY	O7-C8-C11	2.15	116.13	111.50
17	N	509	AOQ	O1-C1-C9	-2.15	118.08	121.56
12	T	201	PC1	O11-P-O14	-2.13	100.76	109.07
12	N	503	PC1	O12-P-O14	2.11	122.67	112.24
11	C	501	HEM	O1A-CGA-CBA	-2.11	116.32	123.08
11	C	502	HEM	CBA-CAA-C2A	-2.10	109.04	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	501	HEM	O2D-CGD-O1D	-2.08	118.11	123.30
11	C	502	HEM	CHB-C1B-NB	2.08	126.95	124.38
11	N	501	HEM	CAA-C2A-C3A	-2.05	121.36	127.25
11	N	501	HEM	O1A-CGA-CBA	-2.05	116.50	123.08
17	N	509	AOQ	C12-C11-C16	2.05	114.61	111.18
14	C	505	CDL	OB6-CB4-CB6	2.05	115.81	108.40
13	N	505	PTY	O12-P1-O13	2.04	122.31	112.24
12	I	201	PC1	O12-P-O14	2.03	122.26	112.24
19	L	3003	XP4	O5-C4-O6	-2.03	118.48	123.59
15	U	101	LMT	O5B-C5B-C4B	2.02	113.36	109.69
17	N	509	AOQ	C15-C14-C13	-2.02	106.73	110.52
11	N	502	HEM	O1D-CGD-CBD	-2.01	116.62	123.08
11	C	501	HEM	CAA-C2A-C3A	-2.00	121.49	127.25

There are no chirality outliers.

All (540) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	I	201	PC1	C11-O13-P-O12
12	I	201	PC1	C11-O13-P-O14
12	I	201	PC1	C11-O13-P-O11
12	T	201	PC1	C11-O13-P-O12
12	T	201	PC1	O21-C2-C3-O31
13	C	504	PTY	N1-C2-C3-O11
13	C	504	PTY	C11-C8-O7-C6
13	C	504	PTY	C3-O11-P1-O13
13	C	504	PTY	C3-O11-P1-O14
13	P	302	PTY	C5-O14-P1-O11
13	P	302	PTY	C5-O14-P1-O12
13	D	402	PTY	N1-C2-C3-O11
13	D	402	PTY	C3-O11-P1-O13
13	D	402	PTY	C5-O14-P1-O12
13	N	505	PTY	C11-C8-O7-C6
13	N	505	PTY	C3-O11-P1-O12
13	N	505	PTY	C3-O11-P1-O13
13	N	505	PTY	C5-O14-P1-O13
14	C	505	CDL	CB2-C1-CA2-OA2
14	C	505	CDL	CA3-OA5-PA1-OA3
14	C	505	CDL	C11-CA5-OA6-CA4
14	C	505	CDL	CB2-OB2-PB2-OB3
14	C	505	CDL	CB2-OB2-PB2-OB4
14	C	505	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
14	C	505	CDL	CB3-OB5-PB2-OB2
14	C	505	CDL	CB3-OB5-PB2-OB3
14	C	505	CDL	CB3-OB5-PB2-OB4
14	A	3001	CDL	OA5-CA3-CA4-OA6
14	A	3001	CDL	OB5-CB3-CB4-CB6
14	A	3001	CDL	CB3-CB4-CB6-OB8
14	A	3002	CDL	CA2-C1-CB2-OB2
14	A	3002	CDL	CA2-OA2-PA1-OA3
14	A	3002	CDL	CA2-OA2-PA1-OA4
14	A	3002	CDL	CA2-OA2-PA1-OA5
14	A	3002	CDL	OB5-CB3-CB4-OB6
14	H	701	CDL	CB3-OB5-PB2-OB3
14	H	702	CDL	CA2-OA2-PA1-OA4
14	H	702	CDL	CB3-OB5-PB2-OB4
14	H	702	CDL	C51-CB5-OB6-CB4
14	N	504	CDL	CA2-OA2-PA1-OA4
14	N	504	CDL	CB3-OB5-PB2-OB3
14	N	504	CDL	C51-CB5-OB6-CB4
14	N	506	CDL	O1-C1-CA2-OA2
14	N	506	CDL	CB2-C1-CA2-OA2
14	N	506	CDL	CA3-OA5-PA1-OA3
14	N	506	CDL	C11-CA5-OA6-CA4
14	N	506	CDL	CB2-OB2-PB2-OB3
14	N	506	CDL	CB2-OB2-PB2-OB4
14	N	506	CDL	CB2-OB2-PB2-OB5
14	N	506	CDL	CB3-OB5-PB2-OB2
14	N	506	CDL	CB3-OB5-PB2-OB3
14	N	506	CDL	CB3-OB5-PB2-OB4
14	L	3001	CDL	CB3-CB4-CB6-OB8
14	L	3002	CDL	CA2-C1-CB2-OB2
14	L	3002	CDL	CA2-OA2-PA1-OA3
14	L	3002	CDL	CA2-OA2-PA1-OA4
14	L	3002	CDL	CA2-OA2-PA1-OA5
14	S	101	CDL	CA2-C1-CB2-OB2
14	S	101	CDL	CA2-OA2-PA1-OA4
14	S	101	CDL	CB3-OB5-PB2-OB4
14	S	101	CDL	C51-CB5-OB6-CB4
15	C	506	LMT	O5'-C1'-O1'-C1
15	C	506	LMT	C2-C1-O1'-C1'
15	J	101	LMT	C2-C1-O1'-C1'
15	N	507	LMT	C2'-C1'-O1'-C1
15	N	507	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
16	C	507	AWB	O5-C21-N1-C17
16	N	508	AWB	O5-C21-N1-C17
20	D	401	HEC	C1A-C2A-CAA-CBA
20	D	401	HEC	C3A-C2A-CAA-CBA
20	O	401	HEC	C1A-C2A-CAA-CBA
20	O	401	HEC	C3A-C2A-CAA-CBA
14	H	702	CDL	OA9-CA7-OA8-CA6
14	H	702	CDL	OB9-CB7-OB8-CB6
14	S	101	CDL	OA9-CA7-OA8-CA6
14	S	101	CDL	OB9-CB7-OB8-CB6
14	A	3001	CDL	CB4-CB6-OB8-CB7
14	H	702	CDL	C31-CA7-OA8-CA6
14	S	101	CDL	C31-CA7-OA8-CA6
12	T	201	PC1	O32-C31-O31-C3
14	A	3001	CDL	OA9-CA7-OA8-CA6
14	H	701	CDL	OB9-CB7-OB8-CB6
14	N	504	CDL	OB9-CB7-OB8-CB6
14	L	3001	CDL	OA9-CA7-OA8-CA6
14	H	702	CDL	OB7-CB5-OB6-CB4
14	S	101	CDL	OB7-CB5-OB6-CB4
15	C	506	LMT	O5B-C5B-C6B-O6B
13	C	504	PTY	O10-C8-O7-C6
13	N	505	PTY	O10-C8-O7-C6
14	C	505	CDL	OA7-CA5-OA6-CA4
14	N	504	CDL	OB7-CB5-OB6-CB4
14	N	506	CDL	OA7-CA5-OA6-CA4
12	T	201	PC1	C32-C31-O31-C3
14	A	3001	CDL	C31-CA7-OA8-CA6
14	H	701	CDL	C71-CB7-OB8-CB6
14	H	702	CDL	C71-CB7-OB8-CB6
14	N	504	CDL	C71-CB7-OB8-CB6
14	L	3001	CDL	C71-CB7-OB8-CB6
14	S	101	CDL	C71-CB7-OB8-CB6
14	H	701	CDL	OA9-CA7-OA8-CA6
15	C	506	LMT	C3-C4-C5-C6
15	J	101	LMT	C2-C3-C4-C5
14	L	3001	CDL	C31-CA7-OA8-CA6
14	H	701	CDL	C31-CA7-OA8-CA6
14	L	3001	CDL	OB9-CB7-OB8-CB6
14	N	504	CDL	OA9-CA7-OA8-CA6
15	N	507	LMT	O5B-C5B-C6B-O6B
14	C	505	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
14	A	3002	CDL	O1-C1-CB2-OB2
14	N	504	CDL	O1-C1-CA2-OA2
14	L	3001	CDL	O1-C1-CA2-OA2
14	L	3001	CDL	OA5-CA3-CA4-OA6
14	L	3001	CDL	OB5-CB3-CB4-OB6
14	L	3002	CDL	O1-C1-CB2-OB2
12	I	201	PC1	C32-C33-C34-C35
13	P	302	PTY	C37-C38-C39-C40
14	A	3002	CDL	C11-CA5-OA6-CA4
14	L	3002	CDL	C11-CA5-OA6-CA4
15	C	506	LMT	C4B-C5B-C6B-O6B
13	C	504	PTY	C31-C32-C33-C34
13	P	302	PTY	C35-C36-C37-C38
13	D	402	PTY	C13-C14-C15-C16
13	N	505	PTY	C33-C34-C35-C36
15	N	507	LMT	C4'-C5'-C6'-O6'
13	C	504	PTY	C35-C36-C37-C38
13	N	505	PTY	C31-C32-C33-C34
13	N	505	PTY	C37-C38-C39-C40
15	N	507	LMT	C4B-C5B-C6B-O6B
13	D	402	PTY	C35-C36-C37-C38
14	N	504	CDL	C31-CA7-OA8-CA6
14	H	702	CDL	CB2-C1-CA2-OA2
14	H	702	CDL	CA2-C1-CB2-OB2
14	N	504	CDL	CA2-C1-CB2-OB2
14	L	3001	CDL	OB5-CB3-CB4-CB6
14	L	3002	CDL	OA7-CA5-OA6-CA4
15	J	101	LMT	C4-C5-C6-C7
12	C	503	PC1	C32-C31-O31-C3
13	P	302	PTY	C31-C30-O4-C1
14	A	3002	CDL	C51-CB5-OB6-CB4
13	P	302	PTY	C13-C14-C15-C16
13	D	402	PTY	O14-C5-C6-O7
14	H	702	CDL	O1-C1-CA2-OA2
14	H	702	CDL	O1-C1-CB2-OB2
14	S	101	CDL	O1-C1-CB2-OB2
15	C	506	LMT	C2'-C1'-O1'-C1
14	L	3001	CDL	OB6-CB4-CB6-OB8
14	A	3001	CDL	CB7-C71-C72-C73
14	L	3002	CDL	CA7-C31-C32-C33
12	I	201	PC1	C32-C31-O31-C3
12	N	503	PC1	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
14	A	3002	CDL	CA7-C31-C32-C33
16	N	508	AWB	C3-C4-C5-C6
12	T	201	PC1	C21-C22-C23-C24
12	T	201	PC1	C31-C32-C33-C34
13	D	402	PTY	C30-C31-C32-C33
14	C	505	CDL	CA7-C31-C32-C33
14	H	701	CDL	CB7-C71-C72-C73
14	N	504	CDL	CA5-C11-C12-C13
14	N	504	CDL	CB7-C71-C72-C73
14	N	506	CDL	CA7-C31-C32-C33
14	A	3002	CDL	OA7-CA5-OA6-CA4
13	P	302	PTY	C30-C31-C32-C33
13	N	505	PTY	C8-C11-C12-C13
14	H	701	CDL	CA5-C11-C12-C13
12	C	503	PC1	O32-C31-O31-C3
13	P	302	PTY	C33-C34-C35-C36
12	I	201	PC1	O32-C31-O31-C3
14	A	3002	CDL	OB7-CB5-OB6-CB4
12	I	201	PC1	C21-C22-C23-C24
13	C	504	PTY	C8-C11-C12-C13
15	N	507	LMT	C5-C6-C7-C8
14	N	504	CDL	O1-C1-CB2-OB2
14	L	3001	CDL	O1-C1-CB2-OB2
14	S	101	CDL	O1-C1-CA2-OA2
12	N	503	PC1	O32-C31-O31-C3
13	P	302	PTY	O30-C30-O4-C1
15	C	506	LMT	C5-C6-C7-C8
15	J	101	LMT	O5B-C5B-C6B-O6B
15	N	507	LMT	O5'-C5'-C6'-O6'
12	T	201	PC1	C11-O13-P-O11
13	D	402	PTY	C5-O14-P1-O11
13	N	505	PTY	C3-O11-P1-O14
13	N	505	PTY	C5-O14-P1-O11
14	H	701	CDL	CB3-OB5-PB2-OB2
14	H	702	CDL	CA2-OA2-PA1-OA5
14	H	702	CDL	CB3-OB5-PB2-OB2
14	N	504	CDL	CA2-OA2-PA1-OA5
14	S	101	CDL	CA2-OA2-PA1-OA5
14	S	101	CDL	CB3-OB5-PB2-OB2
14	A	3001	CDL	OA5-CA3-CA4-CA6
14	L	3001	CDL	CA2-C1-CB2-OB2
14	L	3001	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
14	S	101	CDL	CB2-C1-CA2-OA2
13	P	302	PTY	C41-C42-C43-C44
13	D	402	PTY	C33-C34-C35-C36
14	A	3002	CDL	C12-C13-C14-C15
14	H	701	CDL	C73-C74-C75-C76
13	D	402	PTY	C31-C30-O4-C1
14	L	3002	CDL	C12-C13-C14-C15
15	U	101	LMT	C4-C5-C6-C7
13	P	302	PTY	C34-C35-C36-C37
15	C	506	LMT	C4-C5-C6-C7
15	N	507	LMT	C2-C3-C4-C5
13	D	402	PTY	C8-C11-C12-C13
15	C	506	LMT	C7-C8-C9-C10
13	P	302	PTY	C16-C17-C18-C19
14	H	701	CDL	C11-C12-C13-C14
14	H	701	CDL	C71-C72-C73-C74
14	N	504	CDL	C74-C75-C76-C77
13	N	505	PTY	C32-C33-C34-C35
14	H	701	CDL	C74-C75-C76-C77
14	N	504	CDL	C71-C72-C73-C74
14	N	504	CDL	C73-C74-C75-C76
15	U	101	LMT	C3-C4-C5-C6
16	N	508	AWB	C1-C2-C3-C4
13	P	302	PTY	C40-C41-C42-C43
13	D	402	PTY	C11-C12-C13-C14
13	D	402	PTY	C38-C39-C40-C41
15	J	101	LMT	C6-C7-C8-C9
16	C	507	AWB	C1-C2-C3-C4
13	N	505	PTY	N1-C2-C3-O11
15	N	507	LMT	C7-C8-C9-C10
14	H	701	CDL	CB5-C51-C52-C53
12	C	503	PC1	C28-C29-C2A-C2B
12	N	503	PC1	C26-C27-C28-C29
15	N	507	LMT	C6-C7-C8-C9
13	P	302	PTY	C31-C32-C33-C34
12	N	503	PC1	C28-C29-C2A-C2B
14	H	701	CDL	C11-CA5-OA6-CA4
12	C	503	PC1	C26-C27-C28-C29
12	I	201	PC1	C34-C35-C36-C37
14	A	3001	CDL	C73-C74-C75-C76
13	N	505	PTY	C30-C31-C32-C33
13	C	504	PTY	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
14	C	505	CDL	CA2-C1-CB2-OB2
14	N	506	CDL	CA2-C1-CB2-OB2
14	L	3001	CDL	CB2-C1-CA2-OA2
14	H	701	CDL	OA7-CA5-OA6-CA4
13	D	402	PTY	C14-C15-C16-C17
13	D	402	PTY	C16-C17-C18-C19
13	P	302	PTY	C8-C11-C12-C13
14	L	3001	CDL	CB7-C71-C72-C73
13	C	504	PTY	C11-C12-C13-C14
13	C	504	PTY	C38-C39-C40-C41
13	N	505	PTY	C36-C37-C38-C39
13	D	402	PTY	C12-C13-C14-C15
14	A	3001	CDL	C71-C72-C73-C74
15	C	506	LMT	O1'-C1-C2-C3
16	C	507	AWB	C3-C4-C5-C6
14	N	506	CDL	C11-C12-C13-C14
14	N	504	CDL	OA7-CA5-OA6-CA4
14	N	506	CDL	OB7-CB5-OB6-CB4
12	I	201	PC1	C31-C32-C33-C34
13	P	302	PTY	C14-C15-C16-C17
12	N	503	PC1	C27-C28-C29-C2A
14	L	3002	CDL	CA5-C11-C12-C13
12	C	503	PC1	C27-C28-C29-C2A
12	N	503	PC1	C22-C23-C24-C25
14	C	505	CDL	C51-CB5-OB6-CB4
14	H	701	CDL	C51-CB5-OB6-CB4
14	N	504	CDL	C11-CA5-OA6-CA4
14	N	506	CDL	C51-CB5-OB6-CB4
14	C	505	CDL	OB7-CB5-OB6-CB4
14	H	701	CDL	OB7-CB5-OB6-CB4
12	C	503	PC1	C22-C23-C24-C25
12	C	503	PC1	O21-C2-C3-O31
12	N	503	PC1	O21-C2-C3-O31
12	T	201	PC1	C11-C12-N-C14
14	L	3002	CDL	C11-C12-C13-C14
13	N	505	PTY	C14-C15-C16-C17
13	N	505	PTY	C34-C35-C36-C37
14	L	3001	CDL	C71-C72-C73-C74
15	J	101	LMT	C1-C2-C3-C4
13	D	402	PTY	O30-C30-O4-C1
13	C	504	PTY	C5-O14-P1-O11
14	C	505	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
14	A	3001	CDL	CB3-OB5-PB2-OB2
14	N	506	CDL	CA3-OA5-PA1-OA2
14	L	3001	CDL	C72-C73-C74-C75
15	J	101	LMT	O1'-C1-C2-C3
14	L	3002	CDL	OB5-CB3-CB4-OB6
16	C	507	AWB	C23-C24-C25-C27
16	N	508	AWB	C23-C24-C25-C27
13	D	402	PTY	O14-C5-C6-C1
14	H	701	CDL	OB5-CB3-CB4-CB6
12	T	201	PC1	C33-C34-C35-C36
12	I	201	PC1	C33-C34-C35-C36
15	U	101	LMT	O1'-C1-C2-C3
15	N	507	LMT	C11-C10-C9-C8
14	N	504	CDL	CB2-C1-CA2-OA2
15	U	101	LMT	C2-C3-C4-C5
14	C	505	CDL	C11-C12-C13-C14
15	J	101	LMT	C7-C8-C9-C10
12	T	201	PC1	C11-C12-N-C15
13	N	505	PTY	O4-C1-C6-C5
14	N	504	CDL	CB3-CB4-CB6-OB8
14	A	3002	CDL	C13-C14-C15-C16
13	C	504	PTY	C40-C41-C42-C43
14	N	506	CDL	C13-C14-C15-C16
15	C	506	LMT	C9-C10-C11-C12
15	J	101	LMT	C9-C10-C11-C12
13	C	504	PTY	C41-C42-C43-C44
15	N	507	LMT	C3'-C4'-O1B-C1B
12	N	503	PC1	C22-C21-O21-C2
15	J	101	LMT	C3-C4-C5-C6
13	N	505	PTY	C41-C42-C43-C44
14	C	505	CDL	C13-C14-C15-C16
14	H	701	CDL	C75-C76-C77-C78
14	N	504	CDL	C75-C76-C77-C78
14	L	3002	CDL	CA6-CA4-OA6-CA5
13	D	402	PTY	C41-C42-C43-C44
14	A	3002	CDL	C33-C34-C35-C36
14	L	3002	CDL	C13-C14-C15-C16
16	N	508	AWB	C-C1-C2-C3
14	C	505	CDL	OA5-CA3-CA4-OA6
14	N	506	CDL	OA5-CA3-CA4-OA6
14	C	505	CDL	OB6-CB4-CB6-OB8
15	N	507	LMT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
13	C	504	PTY	C39-C40-C41-C42
14	A	3001	CDL	OB6-CB4-CB6-OB8
15	N	507	LMT	C5'-C4'-O1B-C1B
13	N	505	PTY	O14-C5-C6-C1
14	N	504	CDL	OB5-CB3-CB4-CB6
14	A	3002	CDL	CA5-C11-C12-C13
13	P	302	PTY	C11-C12-C13-C14
12	N	503	PC1	O22-C21-O21-C2
14	L	3002	CDL	C51-CB5-OB6-CB4
15	N	507	LMT	C2-C1-O1'-C1'
11	C	501	HEM	C3D-CAD-CBD-CGD
11	N	501	HEM	C3D-CAD-CBD-CGD
12	C	503	PC1	C1-C2-C3-O31
12	T	201	PC1	C1-C2-C3-O31
14	H	701	CDL	CB3-CB4-CB6-OB8
13	P	302	PTY	C38-C39-C40-C41
15	C	506	LMT	C6-C7-C8-C9
13	D	402	PTY	C34-C35-C36-C37
14	N	506	CDL	CA5-C11-C12-C13
14	N	504	CDL	OA5-CA3-CA4-OA6
14	N	504	CDL	OB5-CB3-CB4-OB6
14	C	505	CDL	O1-C1-CB2-OB2
14	L	3002	CDL	O1-C1-CA2-OA2
13	N	505	PTY	O4-C1-C6-O7
14	H	701	CDL	OA6-CA4-CA6-OA8
14	H	702	CDL	OB6-CB4-CB6-OB8
14	S	101	CDL	OB6-CB4-CB6-OB8
12	C	503	PC1	C22-C21-O21-C2
13	N	505	PTY	C38-C39-C40-C41
13	C	504	PTY	C14-C15-C16-C17
13	D	402	PTY	C32-C33-C34-C35
15	U	101	LMT	C7-C8-C9-C10
14	C	505	CDL	CA5-C11-C12-C13
15	U	101	LMT	C11-C10-C9-C8
13	D	402	PTY	C40-C41-C42-C43
12	C	503	PC1	O22-C21-O21-C2
13	C	504	PTY	C30-C31-C32-C33
14	A	3002	CDL	OA5-CA3-CA4-CA6
14	H	702	CDL	OB5-CB3-CB4-CB6
14	L	3002	CDL	OA5-CA3-CA4-CA6
14	S	101	CDL	OB5-CB3-CB4-CB6
15	C	506	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
13	N	505	PTY	C12-C13-C14-C15
13	D	402	PTY	C31-C32-C33-C34
14	N	506	CDL	C32-C33-C34-C35
14	A	3002	CDL	CA6-CA4-OA6-CA5
15	U	101	LMT	O5'-C1'-O1'-C1
13	C	504	PTY	O4-C1-C6-C5
14	H	702	CDL	CA3-CA4-CA6-OA8
14	H	702	CDL	CB3-CB4-CB6-OB8
14	N	504	CDL	CA3-CA4-CA6-OA8
14	N	506	CDL	CA4-CA3-OA5-PA1
14	S	101	CDL	CA3-CA4-CA6-OA8
14	S	101	CDL	CB3-CB4-CB6-OB8
13	P	302	PTY	O14-C5-C6-O7
13	N	505	PTY	O14-C5-C6-O7
14	H	701	CDL	OA5-CA3-CA4-OA6
14	H	702	CDL	OB5-CB3-CB4-OB6
14	S	101	CDL	OB5-CB3-CB4-OB6
14	N	506	CDL	O1-C1-CB2-OB2
14	N	504	CDL	OA6-CA4-CA6-OA8
14	N	504	CDL	OB6-CB4-CB6-OB8
14	N	506	CDL	OB6-CB4-CB6-OB8
14	C	505	CDL	C32-C33-C34-C35
14	N	504	CDL	CB5-C51-C52-C53
14	L	3002	CDL	C32-C33-C34-C35
15	N	507	LMT	C4-C5-C6-C7
13	N	505	PTY	C17-C18-C19-C20
14	L	3001	CDL	CB2-OB2-PB2-OB5
14	N	504	CDL	C11-C12-C13-C14
13	C	504	PTY	C6-C5-O14-P1
14	C	505	CDL	CA4-CA3-OA5-PA1
13	C	504	PTY	C5-O14-P1-O12
13	C	504	PTY	C5-O14-P1-O13
13	P	302	PTY	C5-O14-P1-O13
13	N	505	PTY	C5-O14-P1-O12
14	C	505	CDL	CA3-OA5-PA1-OA4
14	H	701	CDL	CB3-OB5-PB2-OB4
14	H	702	CDL	CB3-OB5-PB2-OB3
14	N	504	CDL	CA2-OA2-PA1-OA3
14	N	506	CDL	CA3-OA5-PA1-OA4
14	S	101	CDL	CB3-OB5-PB2-OB3
16	C	507	AWB	C23-C24-C25-C26
16	N	508	AWB	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
14	H	701	CDL	OA5-CA3-CA4-CA6
14	H	702	CDL	OA5-CA3-CA4-CA6
14	N	504	CDL	OA5-CA3-CA4-CA6
14	S	101	CDL	OA5-CA3-CA4-CA6
12	I	201	PC1	C22-C23-C24-C25
13	P	302	PTY	C39-C40-C41-C42
14	L	3002	CDL	C33-C34-C35-C36
12	C	503	PC1	C34-C35-C36-C37
14	A	3002	CDL	C32-C33-C34-C35
15	N	507	LMT	O1'-C1-C2-C3
13	C	504	PTY	O14-C5-C6-O7
14	H	702	CDL	OA5-CA3-CA4-OA6
14	S	101	CDL	OA5-CA3-CA4-OA6
19	A	3003	XP4	O4-C1-C2-O7
13	D	402	PTY	C37-C38-C39-C40
12	N	503	PC1	C1-C2-C3-O31
14	H	701	CDL	CA3-CA4-CA6-OA8
13	C	504	PTY	O4-C1-C6-O7
14	H	701	CDL	OB6-CB4-CB6-OB8
13	D	402	PTY	C36-C37-C38-C39
13	C	504	PTY	C31-C30-O4-C1
13	C	504	PTY	O30-C30-O4-C1
14	L	3002	CDL	OB7-CB5-OB6-CB4
16	C	507	AWB	C-C1-C2-C3
13	C	504	PTY	C32-C33-C34-C35
12	T	201	PC1	C11-C12-N-C13
14	H	702	CDL	CB6-CB4-OB6-CB5
14	S	101	CDL	CB6-CB4-OB6-CB5
14	H	701	CDL	OB5-CB3-CB4-OB6
15	U	101	LMT	C6-C7-C8-C9
14	L	3002	CDL	C31-C32-C33-C34
12	I	201	PC1	C22-C21-O21-C2
13	P	302	PTY	C3-O11-P1-O14
13	D	402	PTY	C3-O11-P1-O14
14	A	3002	CDL	CB2-OB2-PB2-OB5
14	H	702	CDL	CB2-OB2-PB2-OB5
14	N	504	CDL	CB3-OB5-PB2-OB2
14	L	3002	CDL	CB2-OB2-PB2-OB5
14	S	101	CDL	CB2-OB2-PB2-OB5
13	C	504	PTY	C33-C34-C35-C36
13	C	504	PTY	C17-C18-C19-C20
14	L	3002	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
11	C	502	HEM	CAD-CBD-CGD-O2D
11	N	502	HEM	CAD-CBD-CGD-O2D
13	C	504	PTY	O14-C5-C6-C1
14	N	504	CDL	C72-C73-C74-C75
16	C	507	AWB	O8-C23-C24-C25
14	A	3001	CDL	OB5-CB3-CB4-OB6
14	A	3002	CDL	O1-C1-CA2-OA2
12	I	201	PC1	O22-C21-O21-C2
14	A	3002	CDL	OA6-CA4-CA6-OA8
13	P	302	PTY	C12-C13-C14-C15
16	C	507	AWB	O7-C23-C24-C25
14	H	702	CDL	CB4-CB3-OB5-PB2
14	S	101	CDL	CB4-CB3-OB5-PB2
13	C	504	PTY	C13-C14-C15-C16
11	N	502	HEM	CAA-CBA-CGA-O1A
11	N	502	HEM	CAD-CBD-CGD-O1D
11	N	501	HEM	CAA-CBA-CGA-O1A
11	N	502	HEM	CAA-CBA-CGA-O2A
11	C	501	HEM	CAA-CBA-CGA-O1A
11	C	502	HEM	CAA-CBA-CGA-O1A
13	N	505	PTY	C1-C6-O7-C8
14	N	504	CDL	C51-C52-C53-C54
11	C	502	HEM	CAA-CBA-CGA-O2A
11	C	502	HEM	CAD-CBD-CGD-O1D
13	N	505	PTY	O30-C30-O4-C1
14	C	505	CDL	OA5-CA3-CA4-CA6
14	H	701	CDL	C72-C73-C74-C75
14	L	3001	CDL	C33-C34-C35-C36
11	N	501	HEM	CAA-CBA-CGA-O2A
11	C	501	HEM	CAA-CBA-CGA-O2A
13	N	505	PTY	C16-C17-C18-C19
14	H	701	CDL	C12-C13-C14-C15
11	C	502	HEM	C3D-CAD-CBD-CGD
12	N	503	PC1	C34-C35-C36-C37
12	T	201	PC1	O11-C1-C2-O21
19	L	3003	XP4	O4-C1-C2-O7
12	I	201	PC1	C11-C12-N-C14
14	N	506	CDL	OA5-CA3-CA4-CA6
13	N	505	PTY	C31-C30-O4-C1
20	O	401	HEC	CAA-CBA-CGA-O1A
14	H	701	CDL	C51-C52-C53-C54
20	D	401	HEC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
20	O	401	HEC	CAA-CBA-CGA-O2A
14	A	3001	CDL	C72-C71-CB7-OB8
14	L	3002	CDL	C34-C35-C36-C37
20	D	401	HEC	CAA-CBA-CGA-O1A
14	N	504	CDL	CB2-OB2-PB2-OB5
12	I	201	PC1	C11-C12-N-C15
14	S	101	CDL	C32-C31-CA7-OA9
14	H	701	CDL	C72-C71-CB7-OB8
11	N	501	HEM	CAD-CBD-CGD-O2D
14	C	505	CDL	CB6-CB4-OB6-CB5
14	N	506	CDL	CB6-CB4-OB6-CB5
13	P	302	PTY	O4-C30-C31-C32
11	C	501	HEM	CAD-CBD-CGD-O2D
12	I	201	PC1	O21-C21-C22-C23
14	N	504	CDL	C72-C71-CB7-OB8
11	C	501	HEM	CAD-CBD-CGD-O1D
11	N	501	HEM	CAD-CBD-CGD-O1D
14	H	702	CDL	C32-C31-CA7-OA9
15	C	506	LMT	C2-C3-C4-C5
14	C	505	CDL	C32-C31-CA7-OA8
16	C	507	AWB	C10-C11-O2-C12
14	N	506	CDL	C32-C31-CA7-OA8
20	D	401	HEC	CAD-CBD-CGD-O1D
20	O	401	HEC	CAD-CBD-CGD-O1D
14	H	702	CDL	C72-C71-CB7-OB8
14	S	101	CDL	C72-C71-CB7-OB8
14	A	3002	CDL	C52-C53-C54-C55
16	N	508	AWB	O7-C23-C24-C25
20	D	401	HEC	CAD-CBD-CGD-O2D
16	N	508	AWB	O8-C23-C24-C25
12	I	201	PC1	O22-C21-C22-C23
13	P	302	PTY	O30-C30-C31-C32
12	I	201	PC1	C35-C36-C37-C38
20	O	401	HEC	CAD-CBD-CGD-O2D
12	N	503	PC1	O31-C31-C32-C33
14	H	701	CDL	C72-C71-CB7-OB9
14	A	3002	CDL	C31-C32-C33-C34
14	C	505	CDL	C32-C31-CA7-OA9
14	C	505	CDL	CA2-OA2-PA1-OA3
14	A	3001	CDL	CB3-OB5-PB2-OB3
14	N	506	CDL	C32-C31-CA7-OA9
12	C	503	PC1	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
14	N	504	CDL	C72-C71-CB7-OB9
12	N	503	PC1	C32-C33-C34-C35
14	L	3002	CDL	CB5-C51-C52-C53
12	T	201	PC1	C12-C11-O13-P
13	D	402	PTY	C2-C3-O11-P1
13	D	402	PTY	O4-C30-C31-C32
14	H	702	CDL	C32-C31-CA7-OA8
14	S	101	CDL	C32-C31-CA7-OA8
12	C	503	PC1	O32-C31-C32-C33
12	N	503	PC1	O32-C31-C32-C33
13	N	505	PTY	C15-C16-C17-C18
13	D	402	PTY	O30-C30-C31-C32

There are no ring outliers.

30 monomers are involved in 132 short contacts:

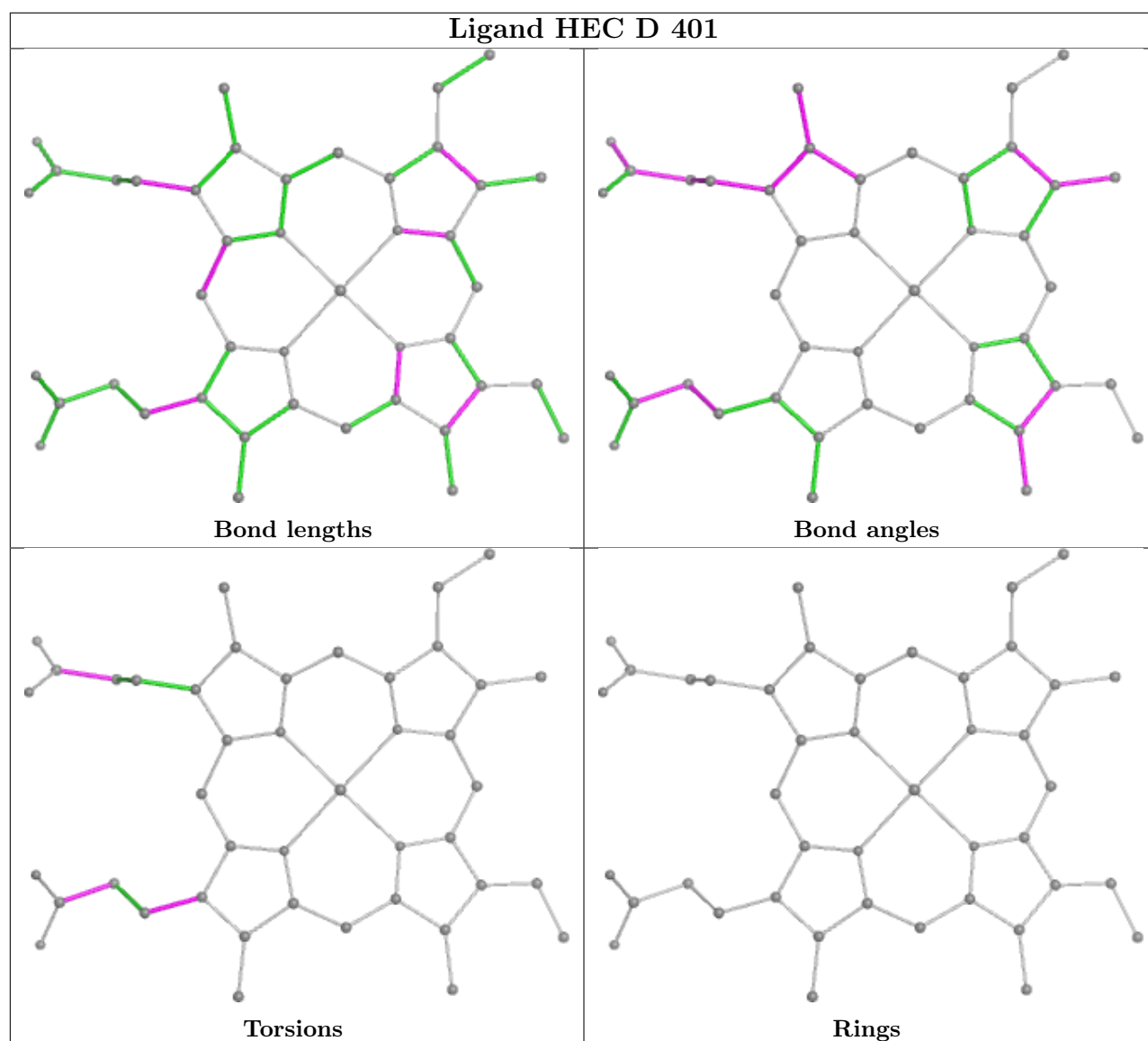
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	D	401	HEC	14	0
11	C	502	HEM	2	0
13	P	302	PTY	13	0
14	A	3001	CDL	4	0
12	C	503	PC1	2	0
15	C	506	LMT	4	0
11	C	501	HEM	11	0
16	C	507	AWB	5	0
14	A	3002	CDL	1	0
17	N	509	AOQ	13	0
14	N	506	CDL	1	0
15	N	507	LMT	2	0
14	L	3001	CDL	2	0
14	S	101	CDL	1	0
11	N	501	HEM	9	0
14	C	505	CDL	1	0
15	J	101	LMT	3	0
13	N	505	PTY	7	0
12	I	201	PC1	1	0
14	H	701	CDL	2	0
11	N	502	HEM	2	0
14	L	3002	CDL	4	0
14	N	504	CDL	6	0
20	O	401	HEC	14	0
14	H	702	CDL	1	0

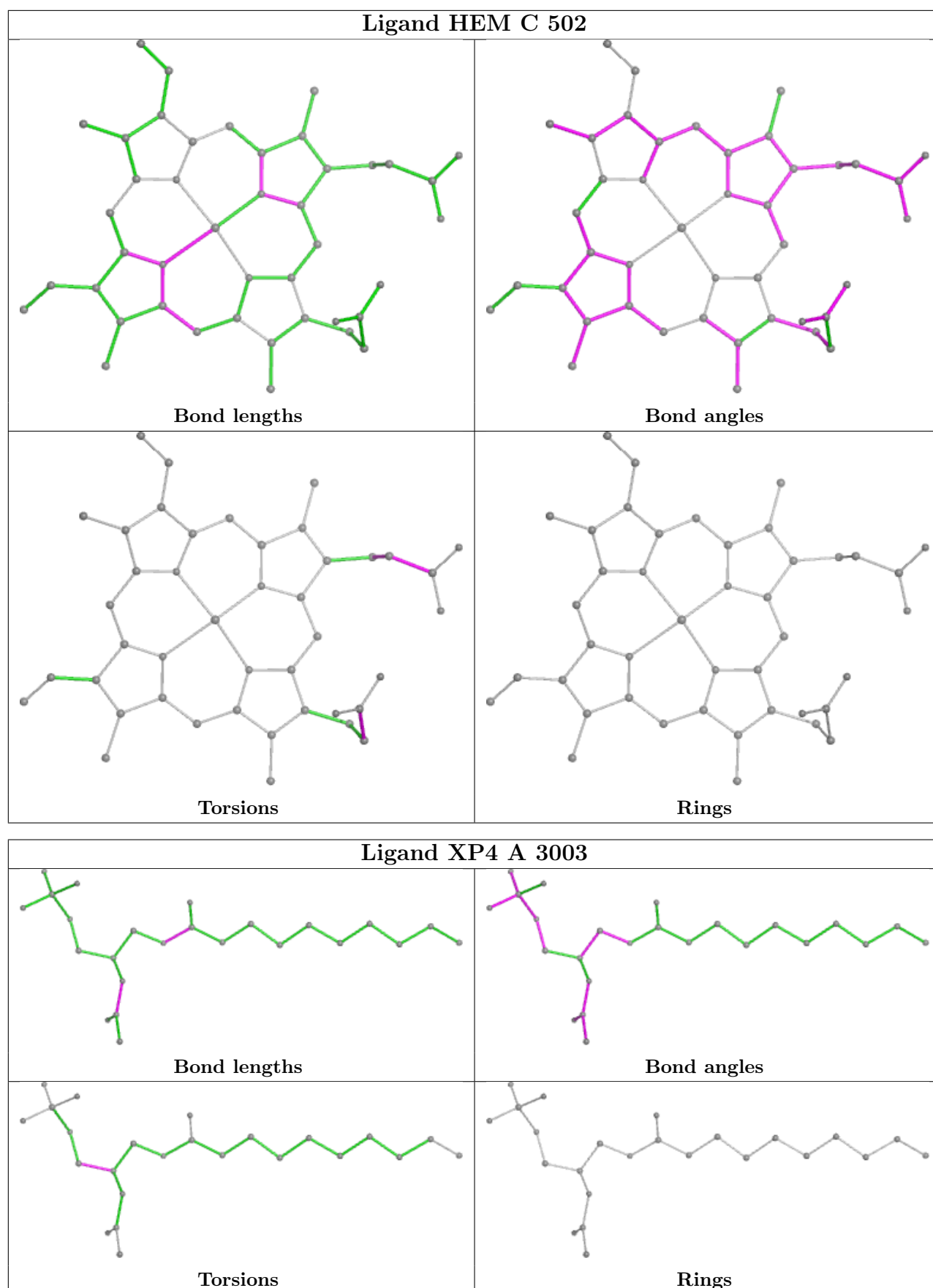
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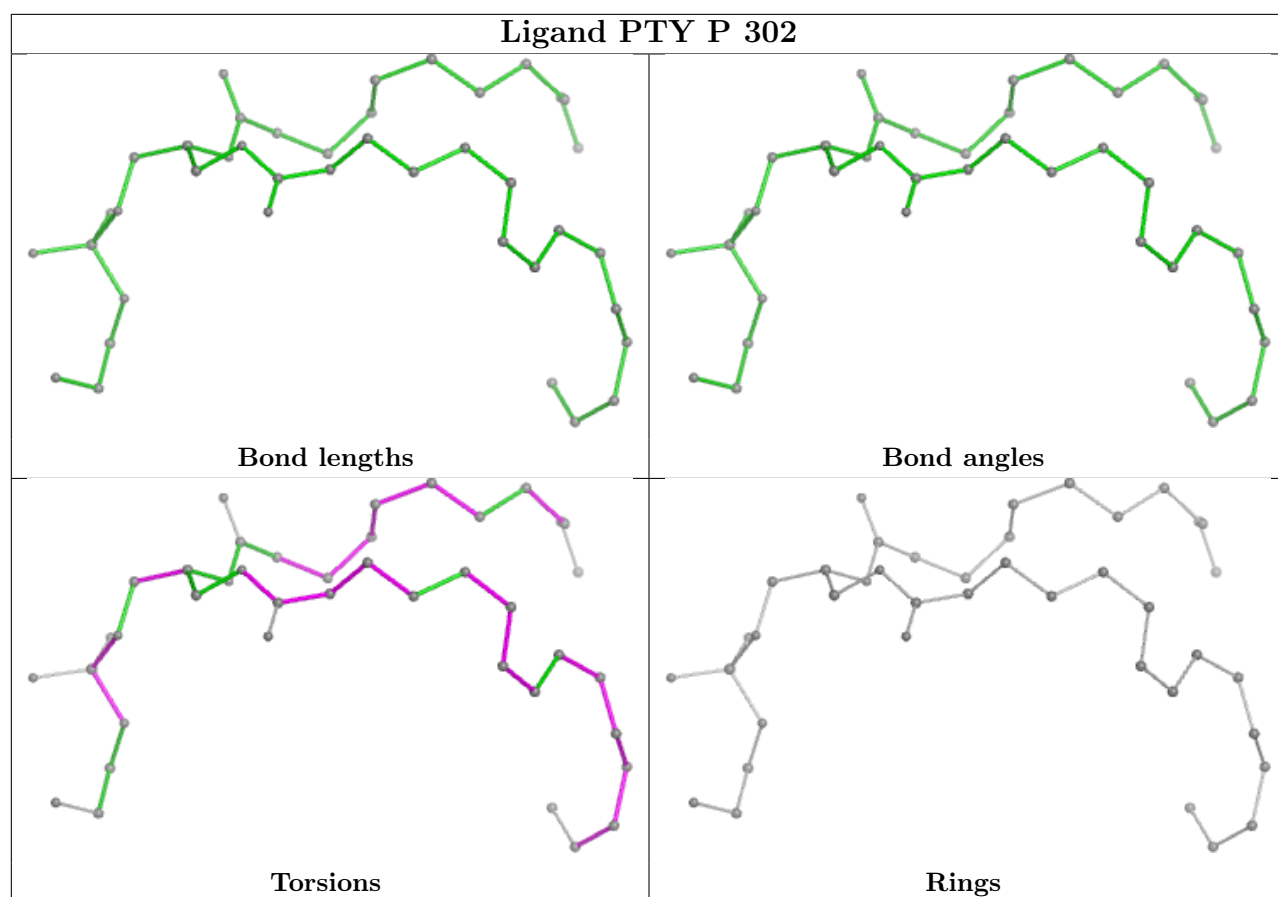
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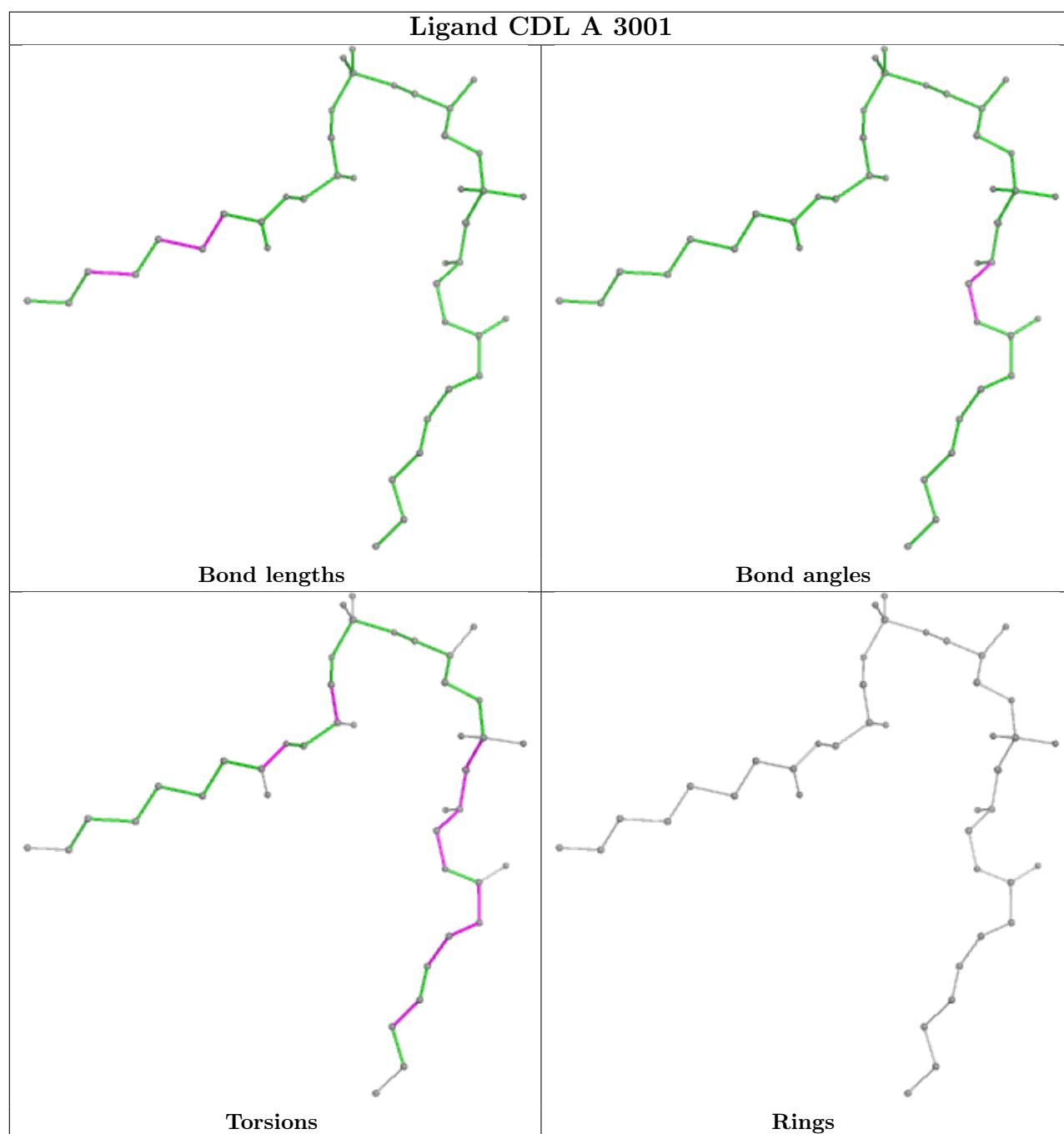
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	504	PTY	2	0
17	C	508	AOQ	4	0
13	D	402	PTY	2	0
16	N	508	AWB	5	0
12	N	503	PC1	2	0

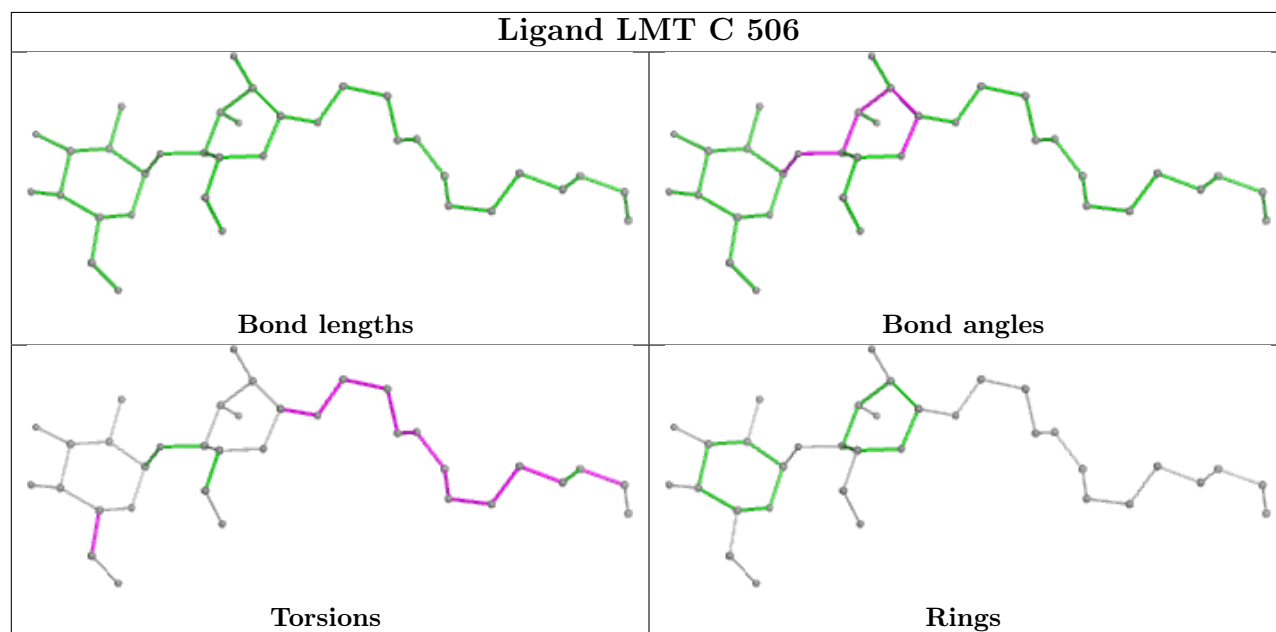
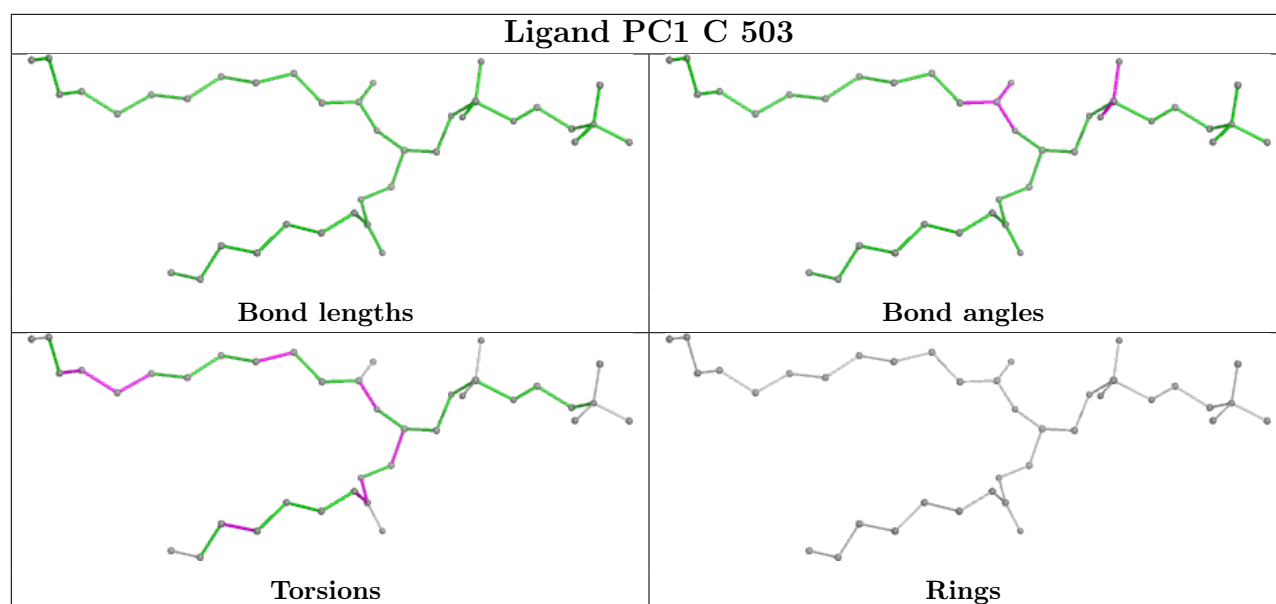
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

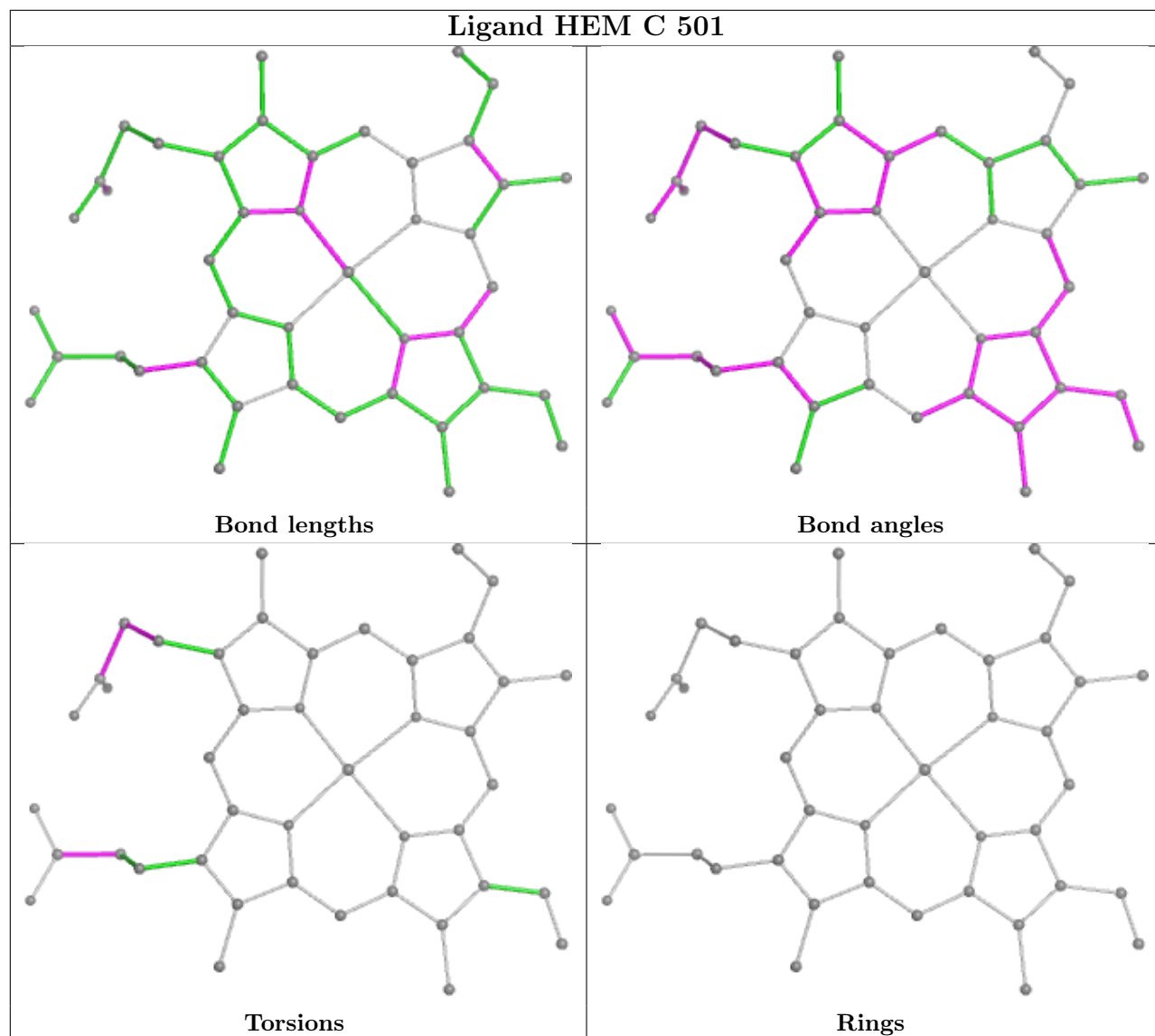


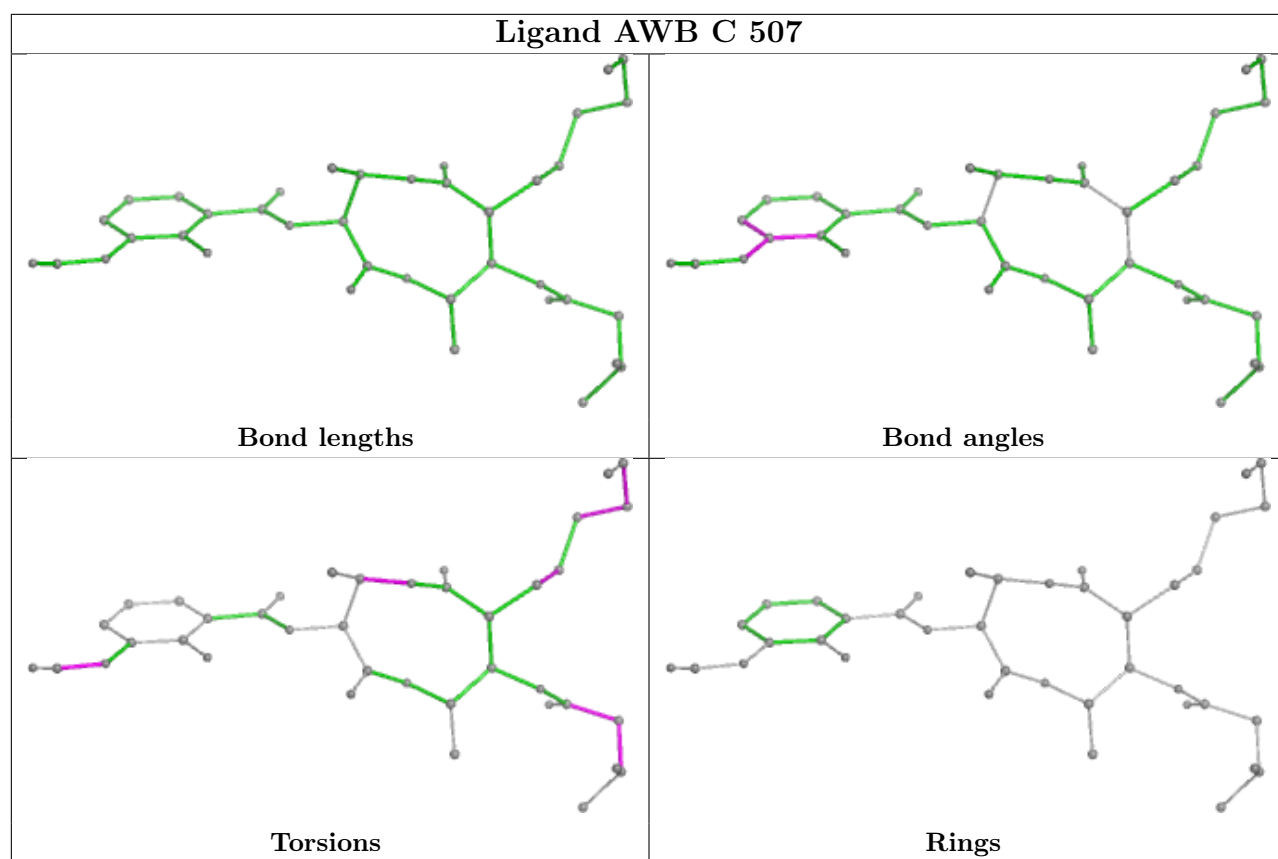


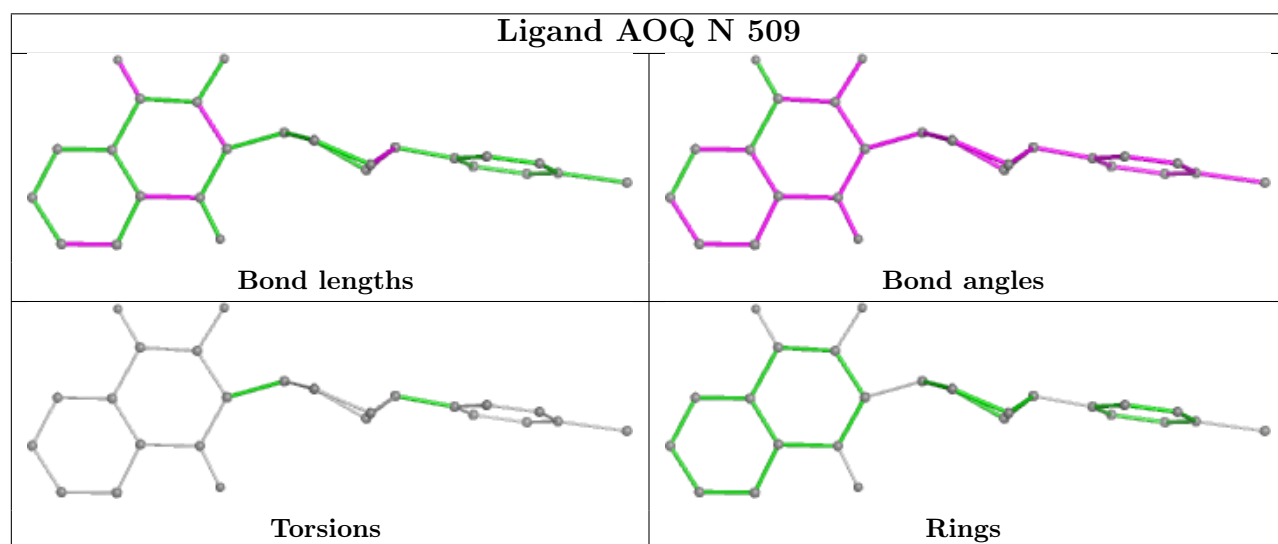
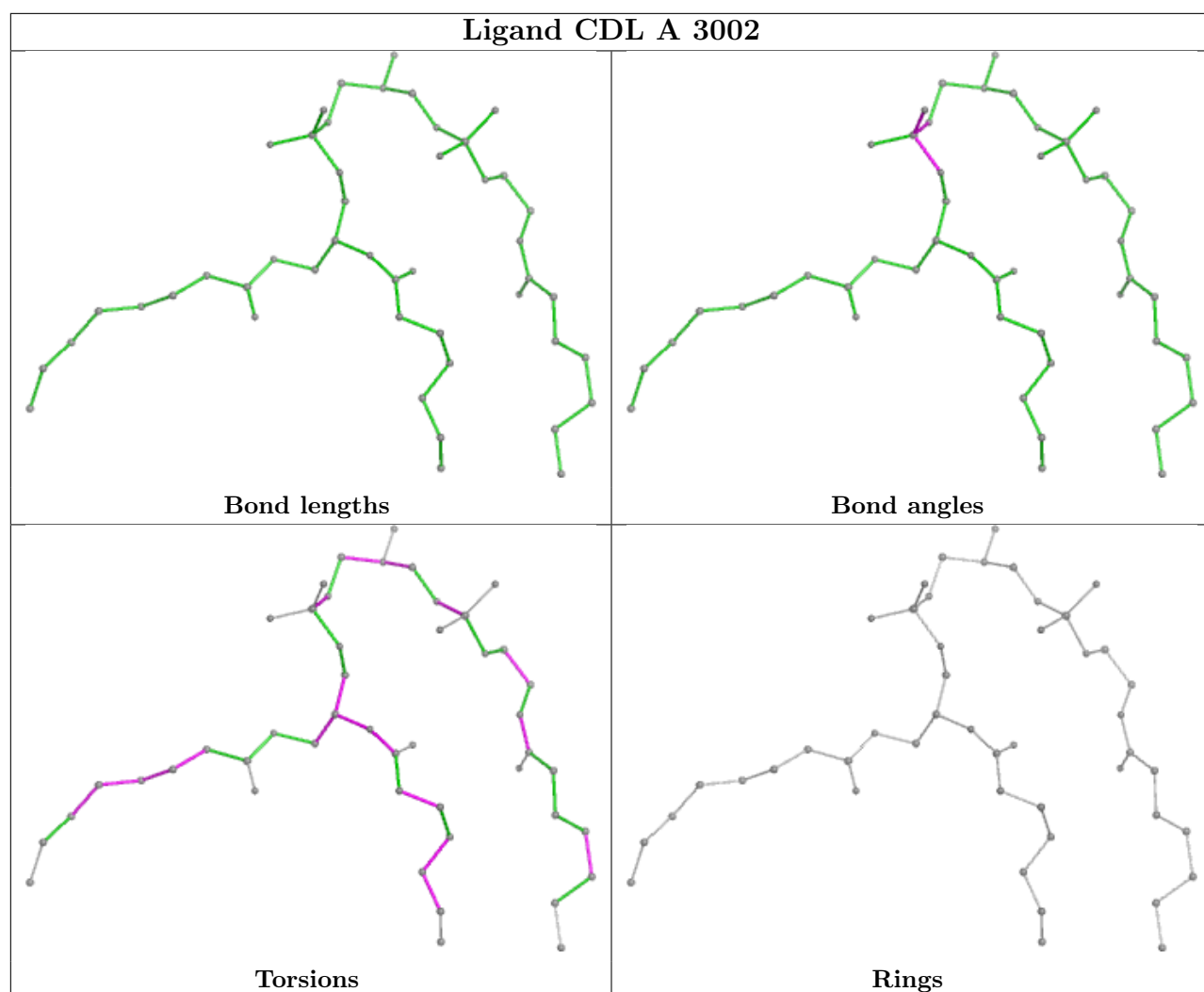


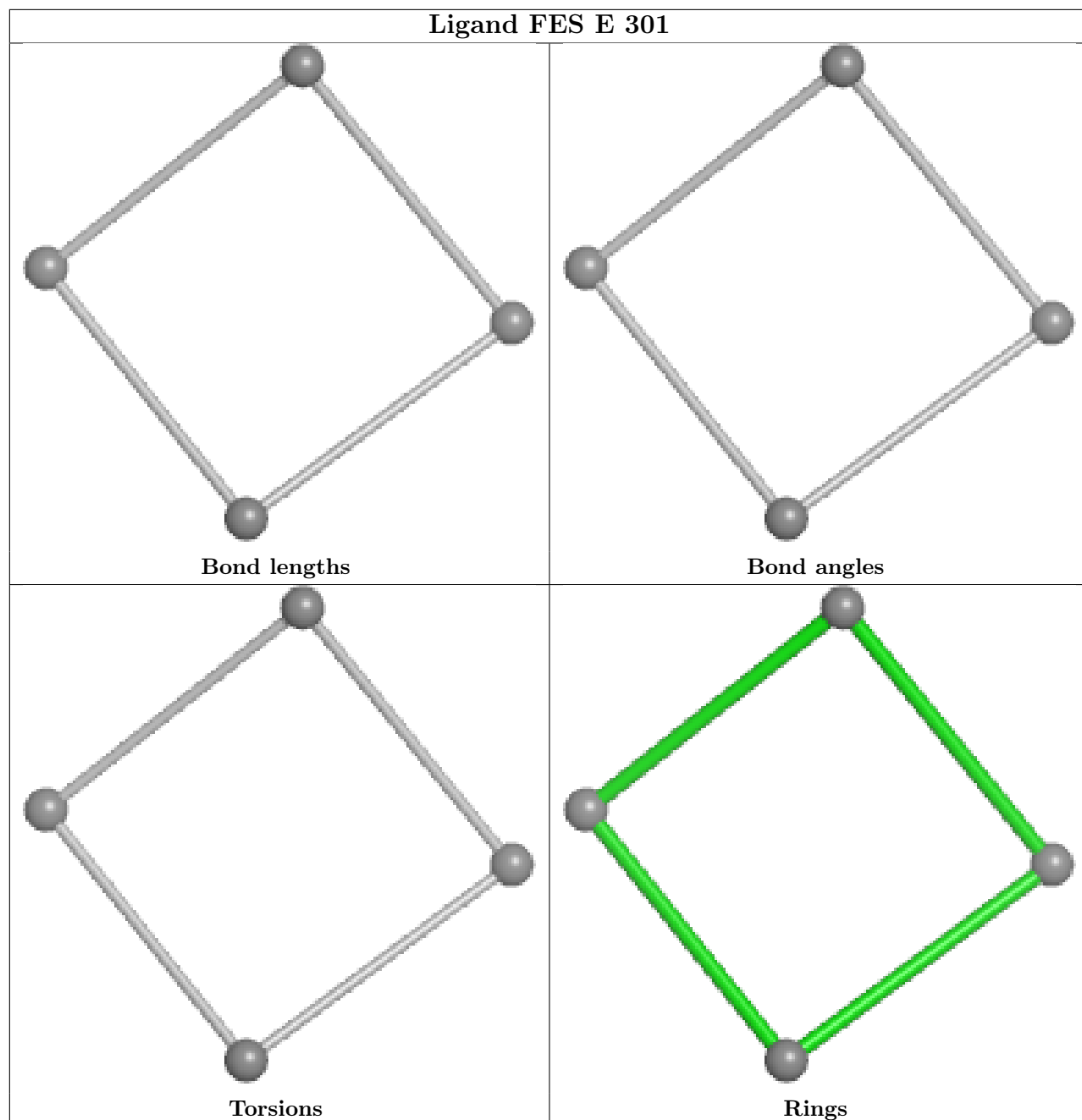


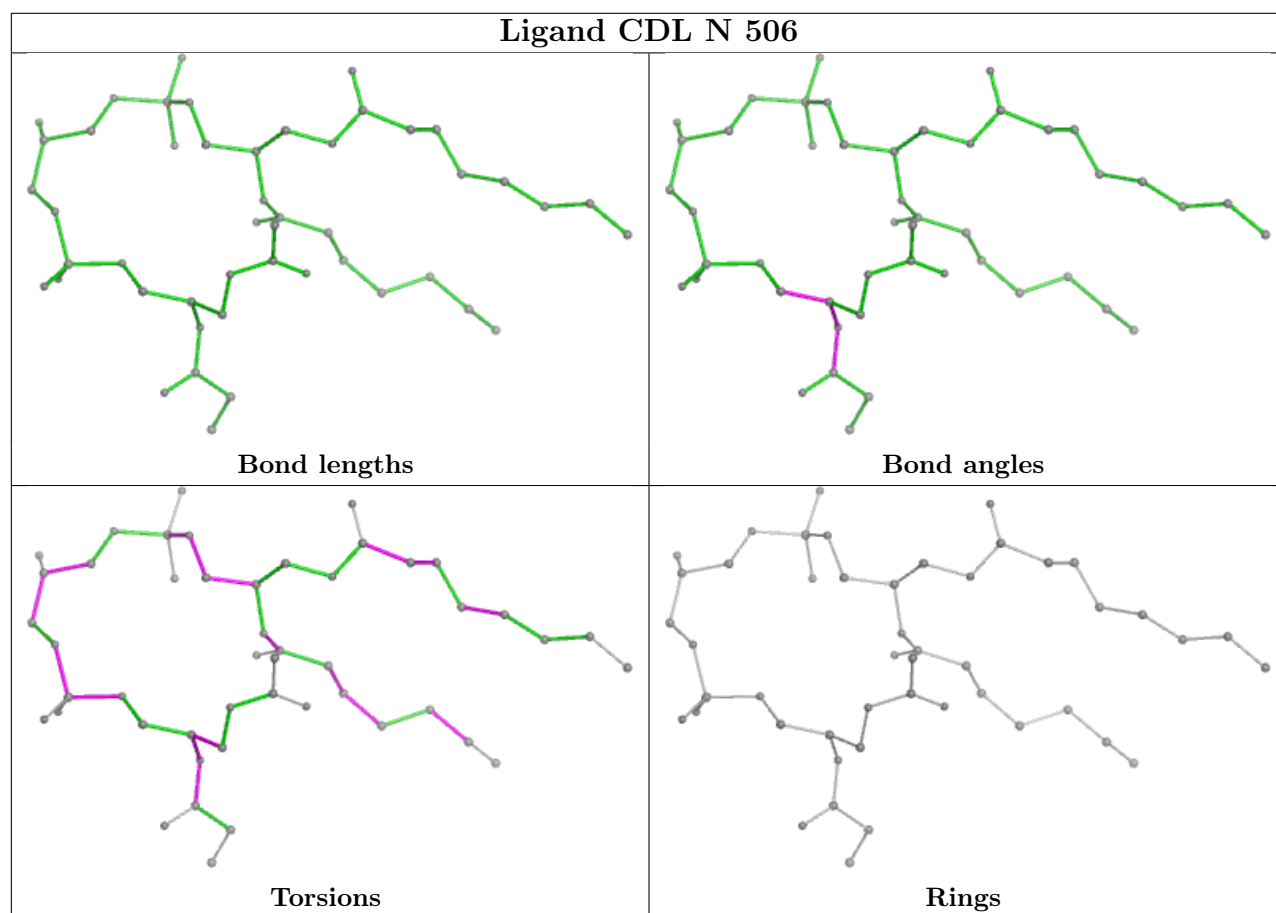
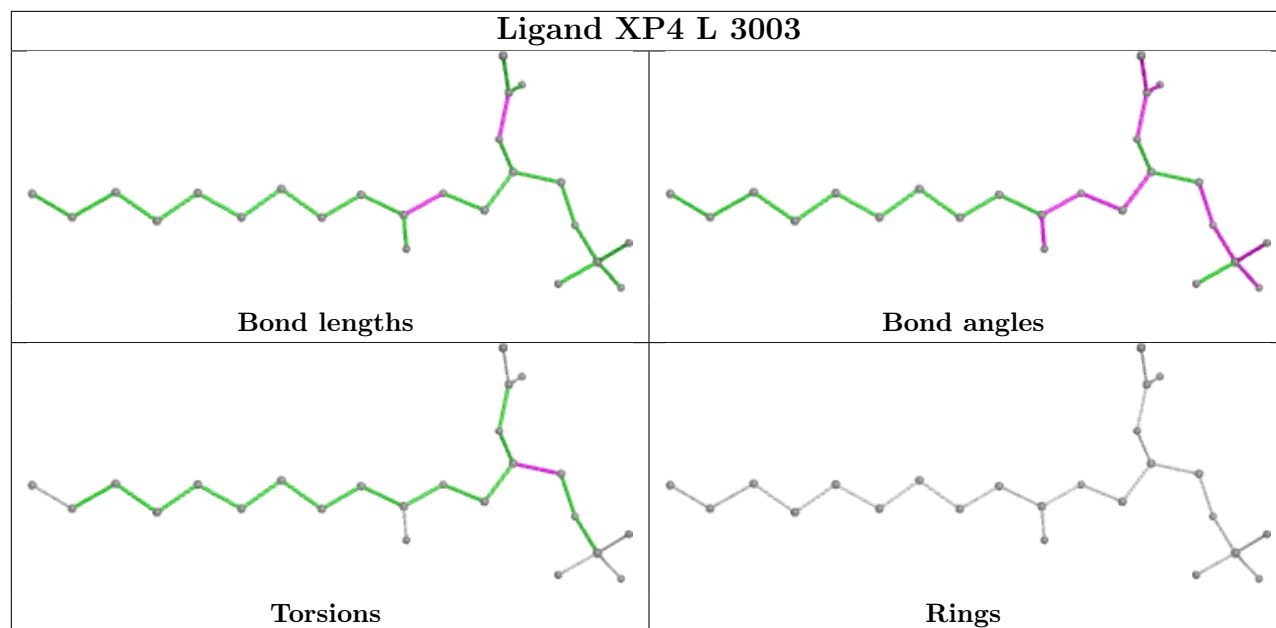


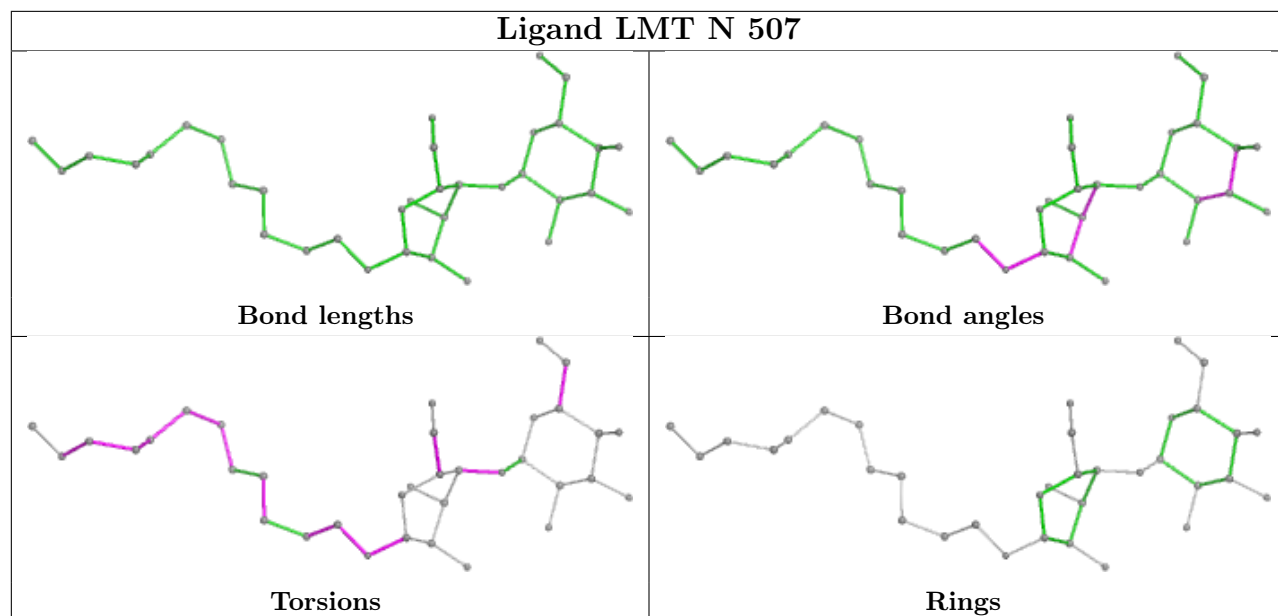


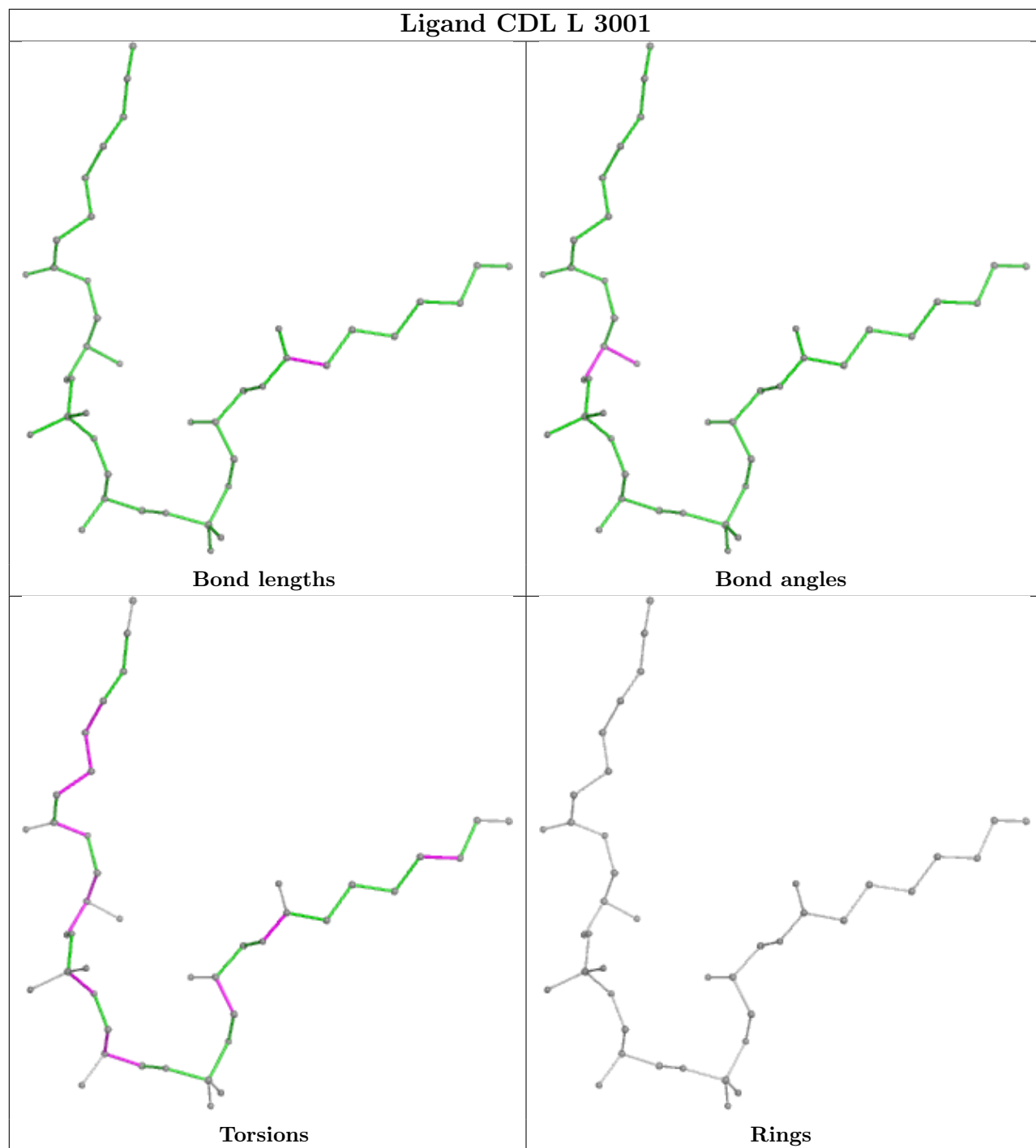


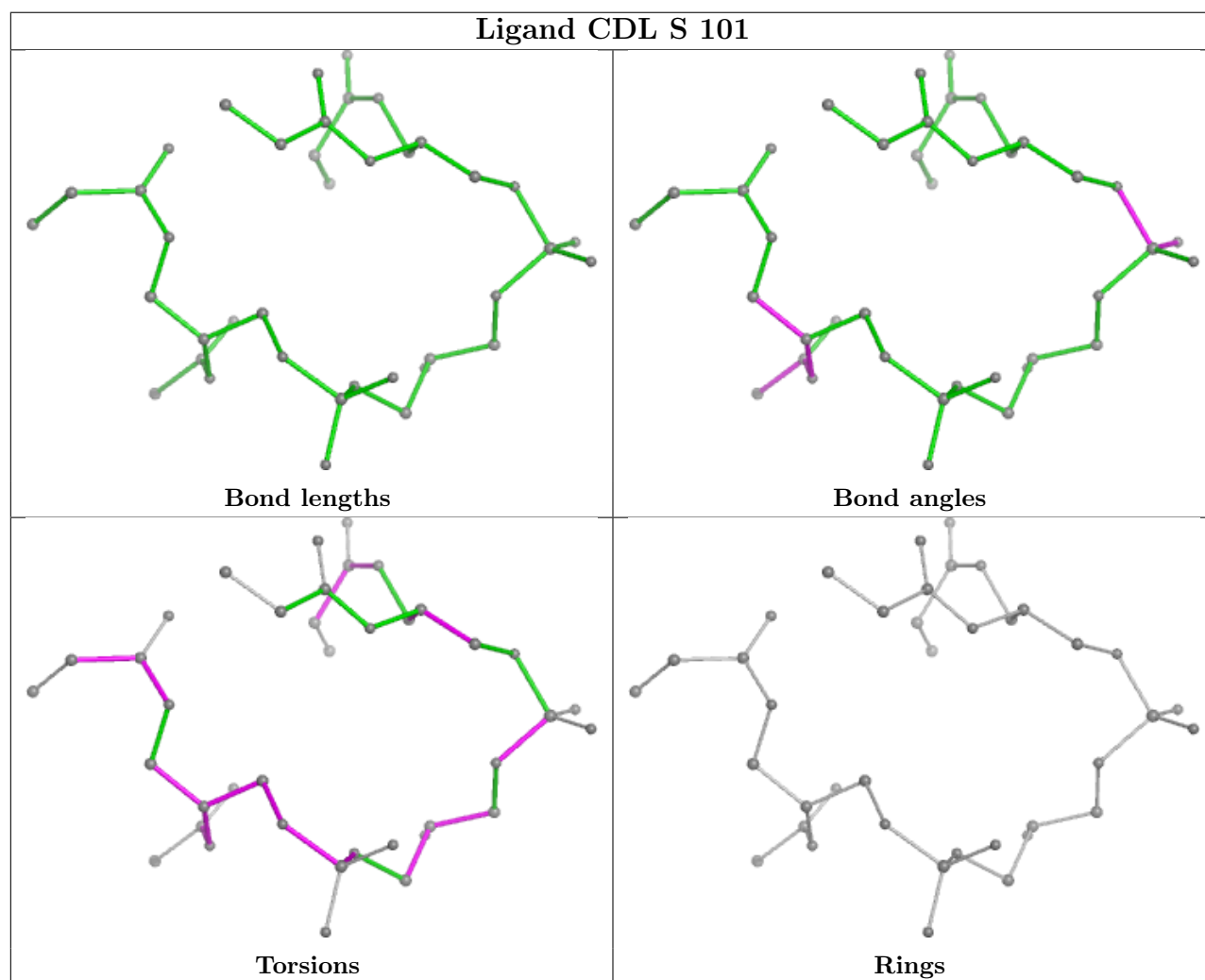
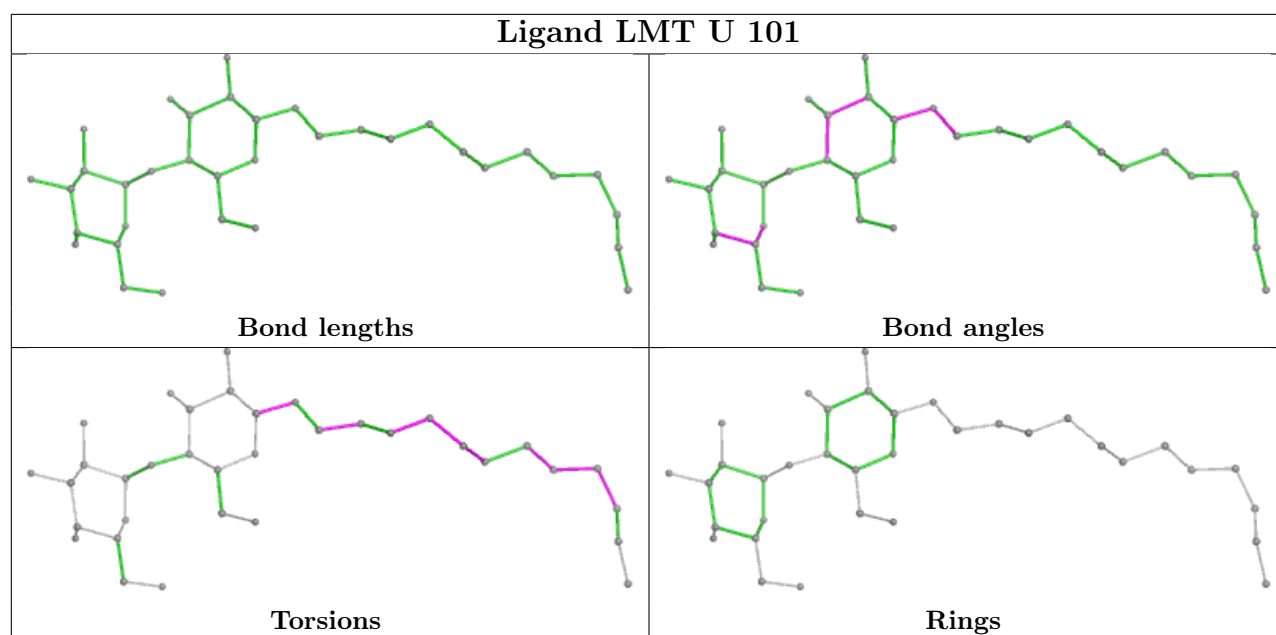


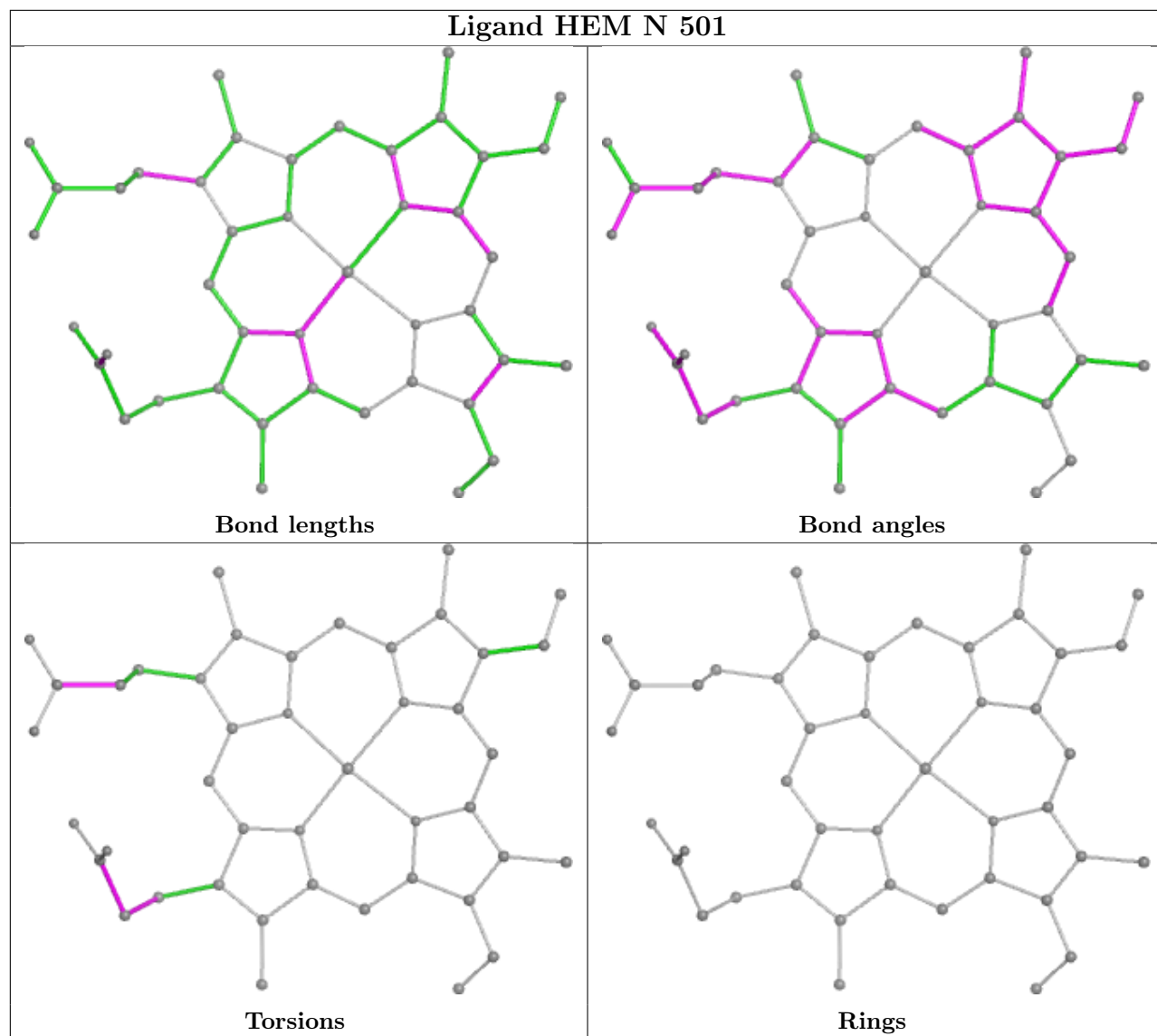


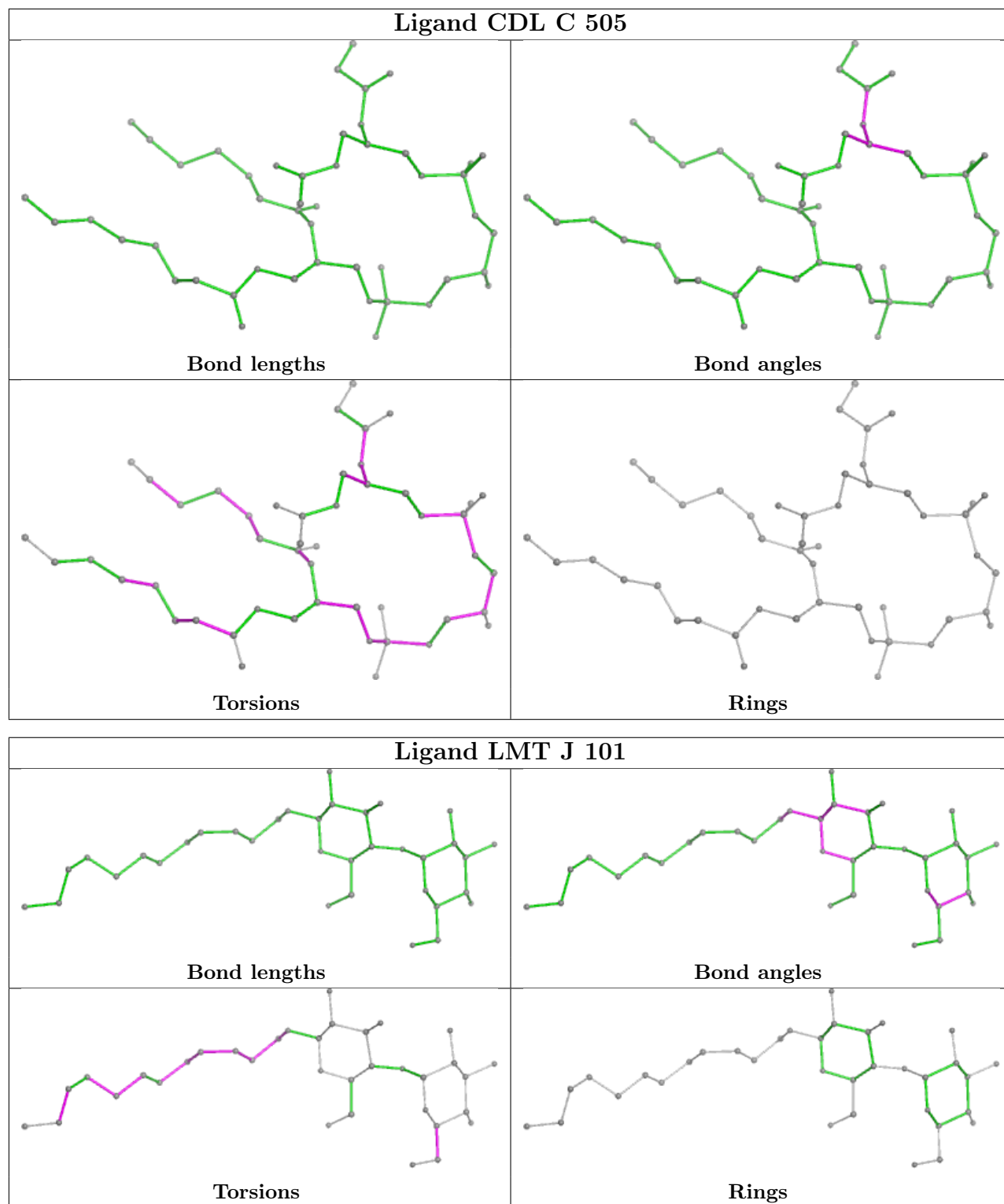


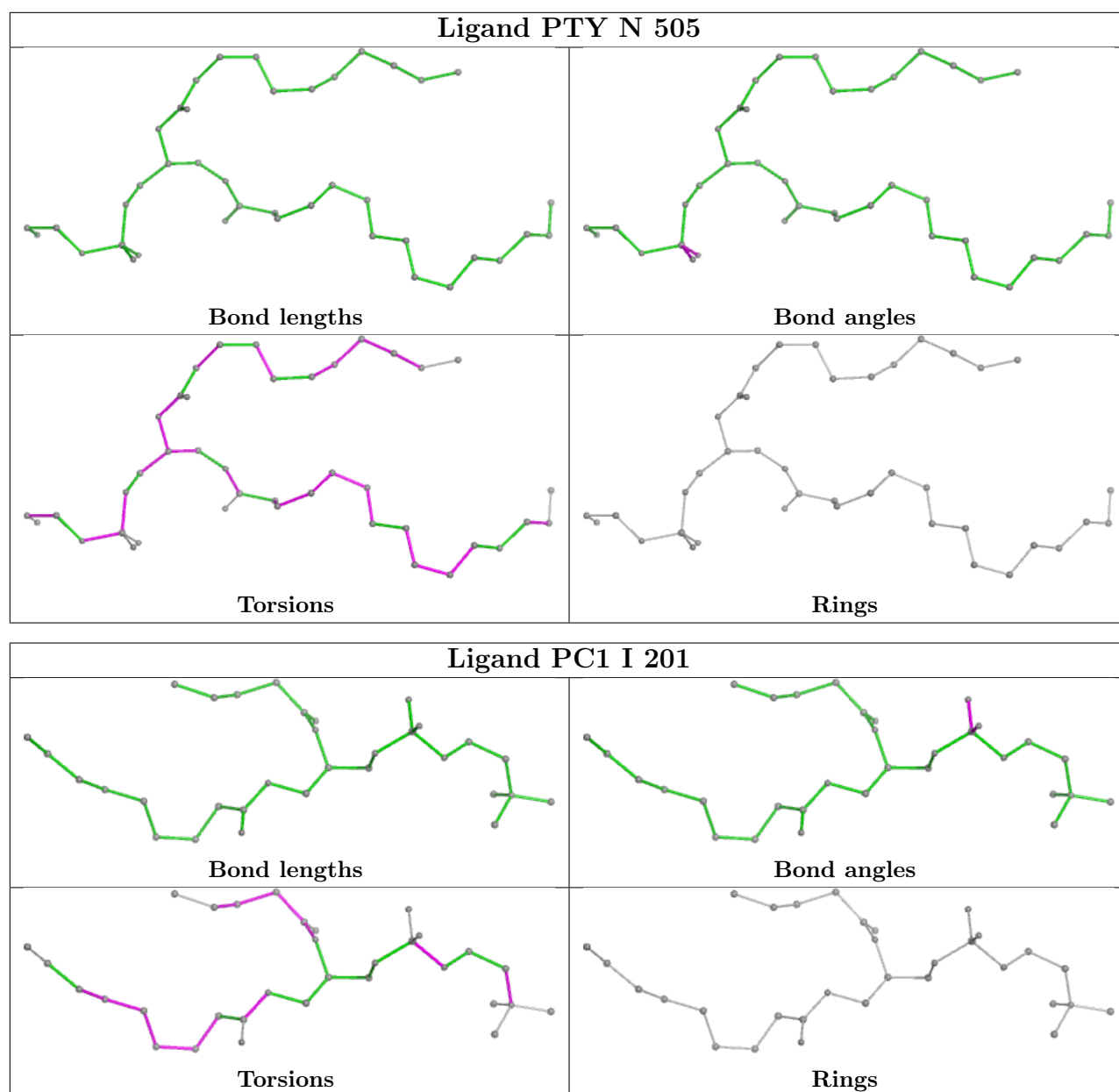


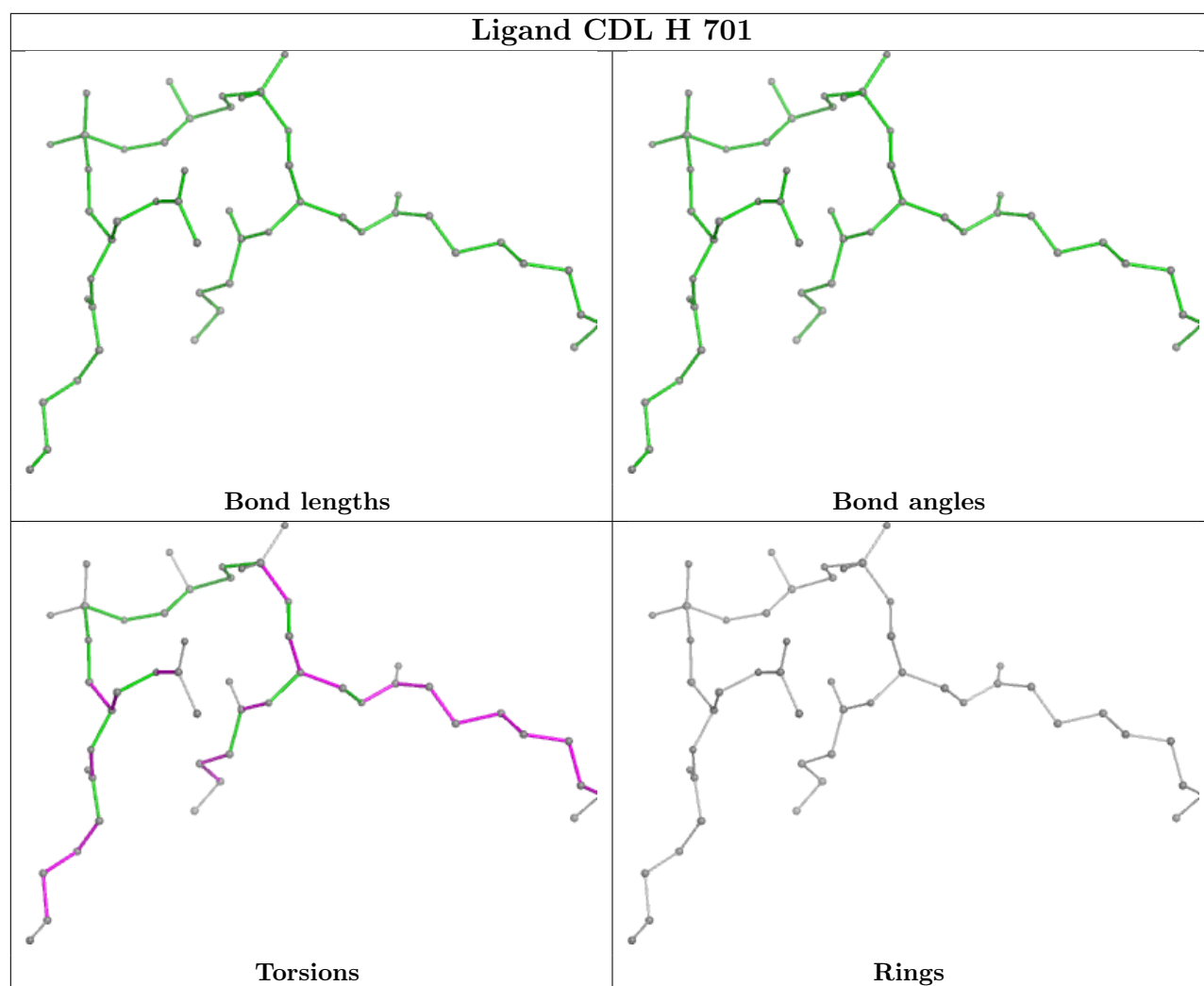


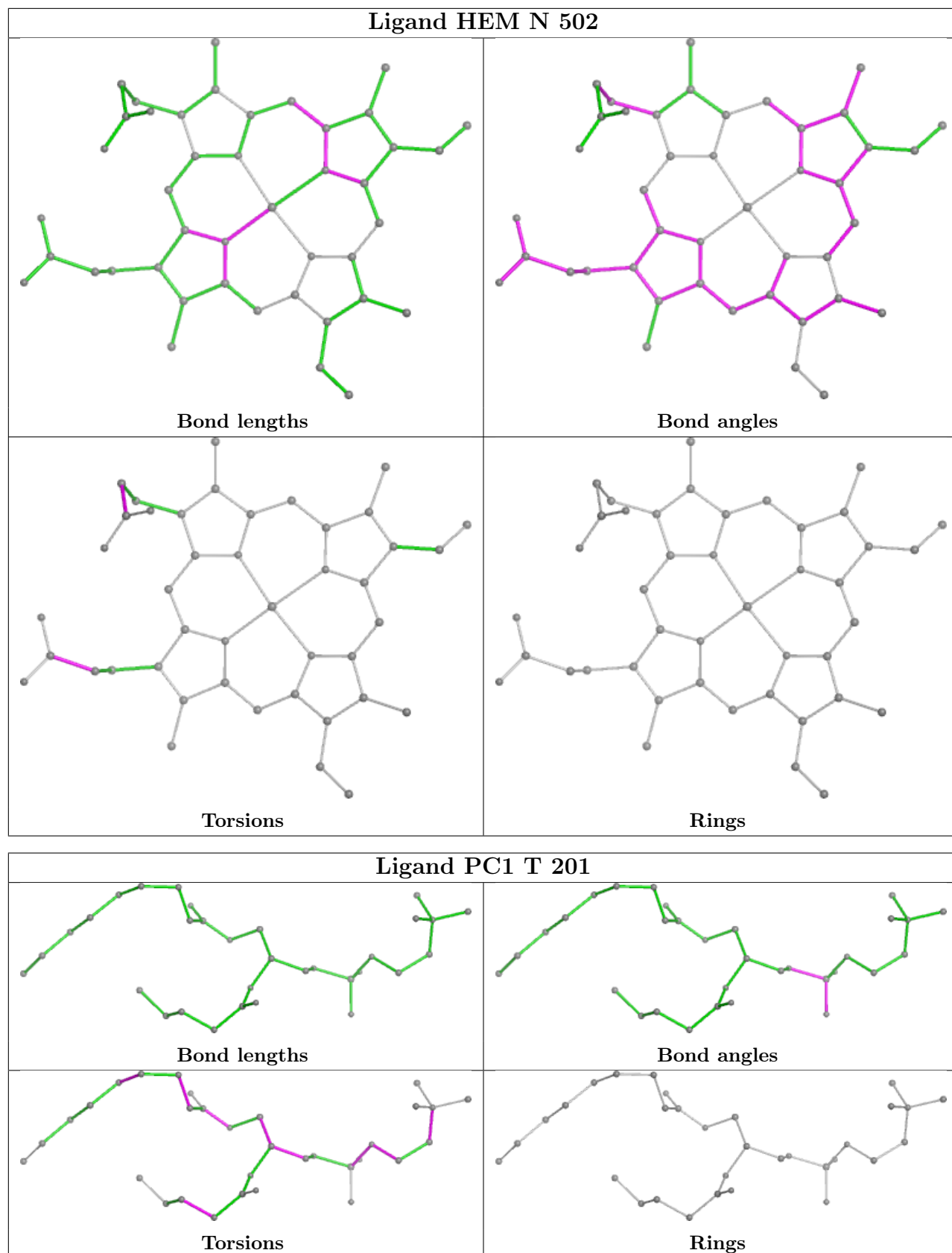


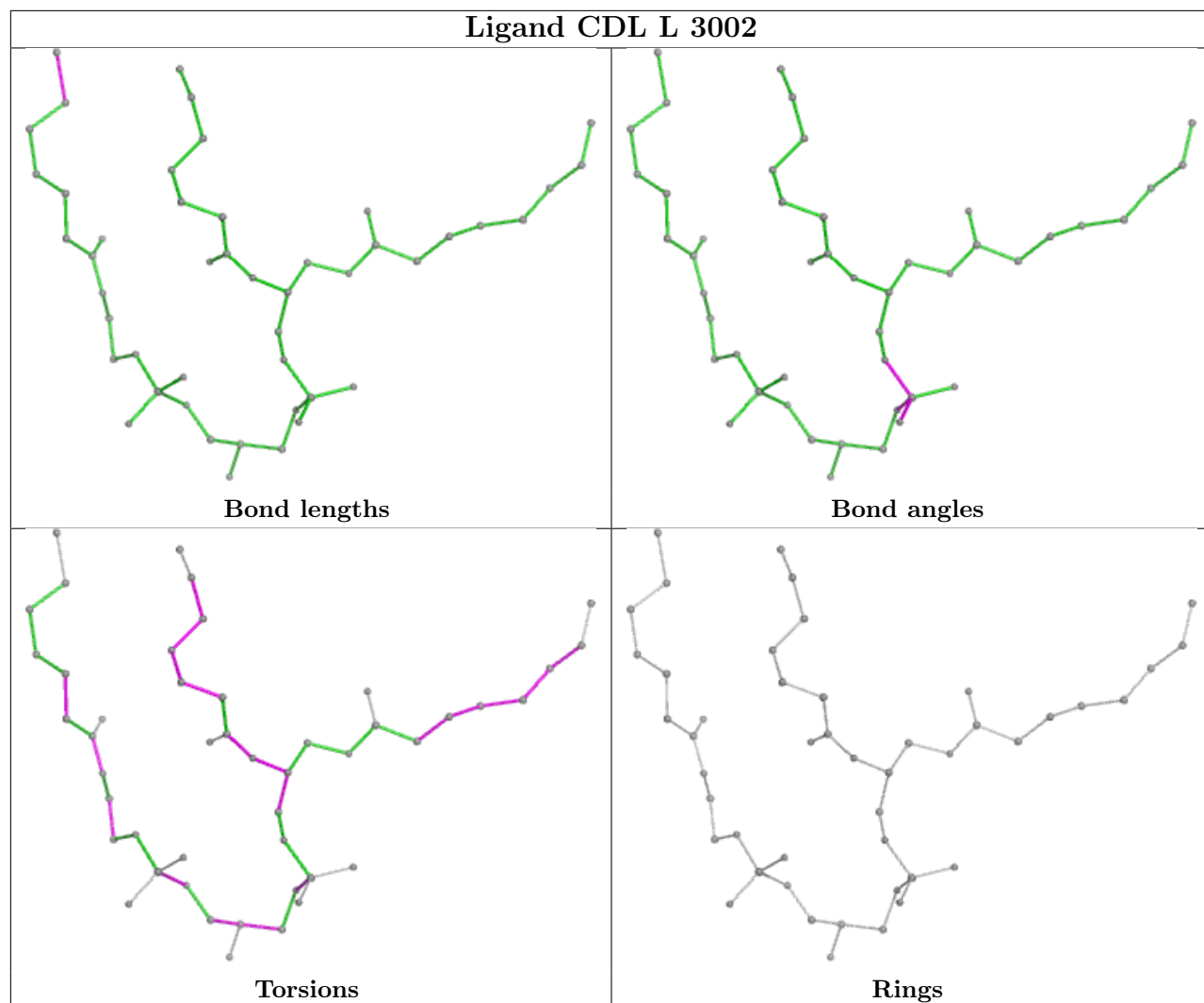


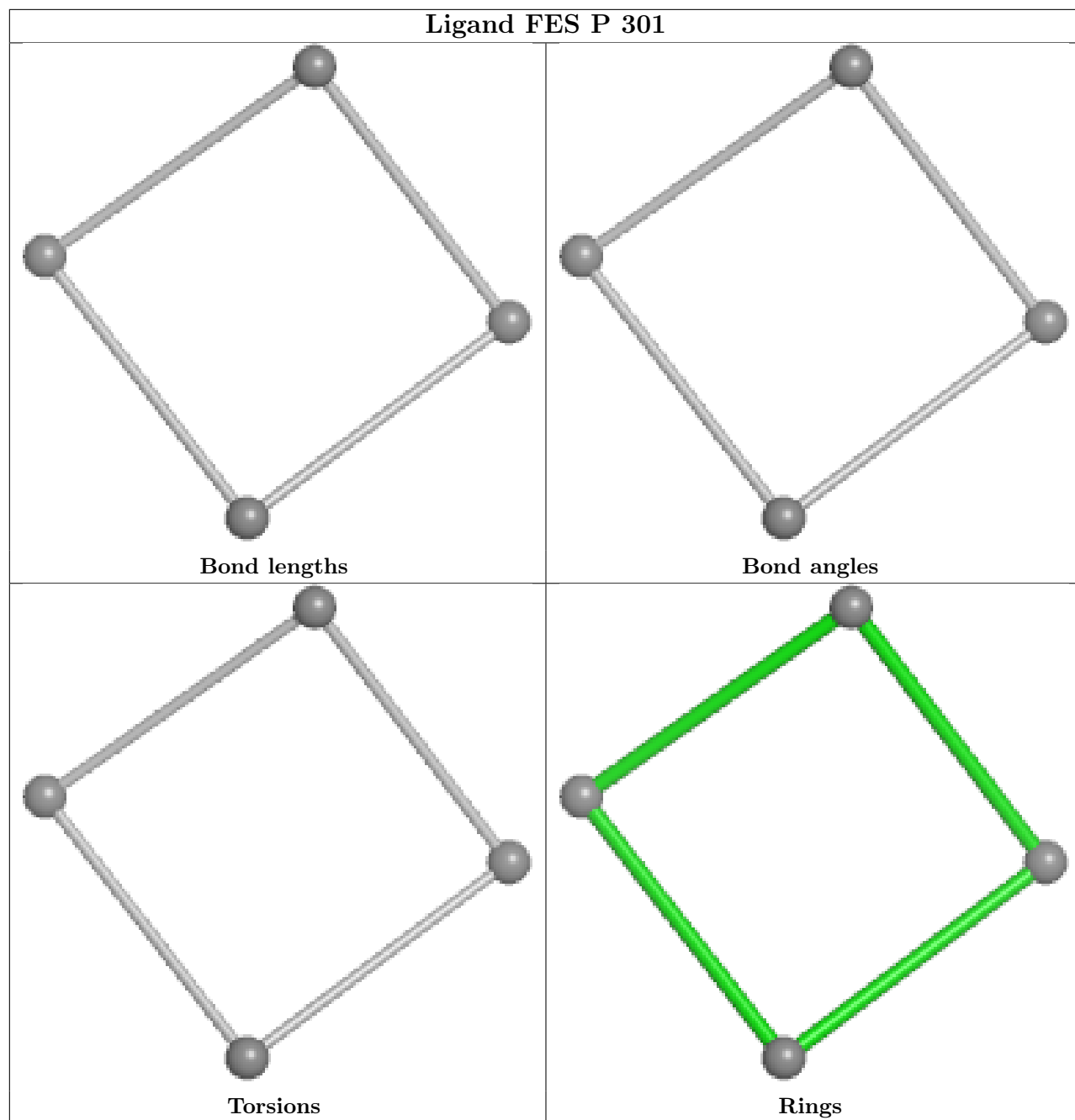


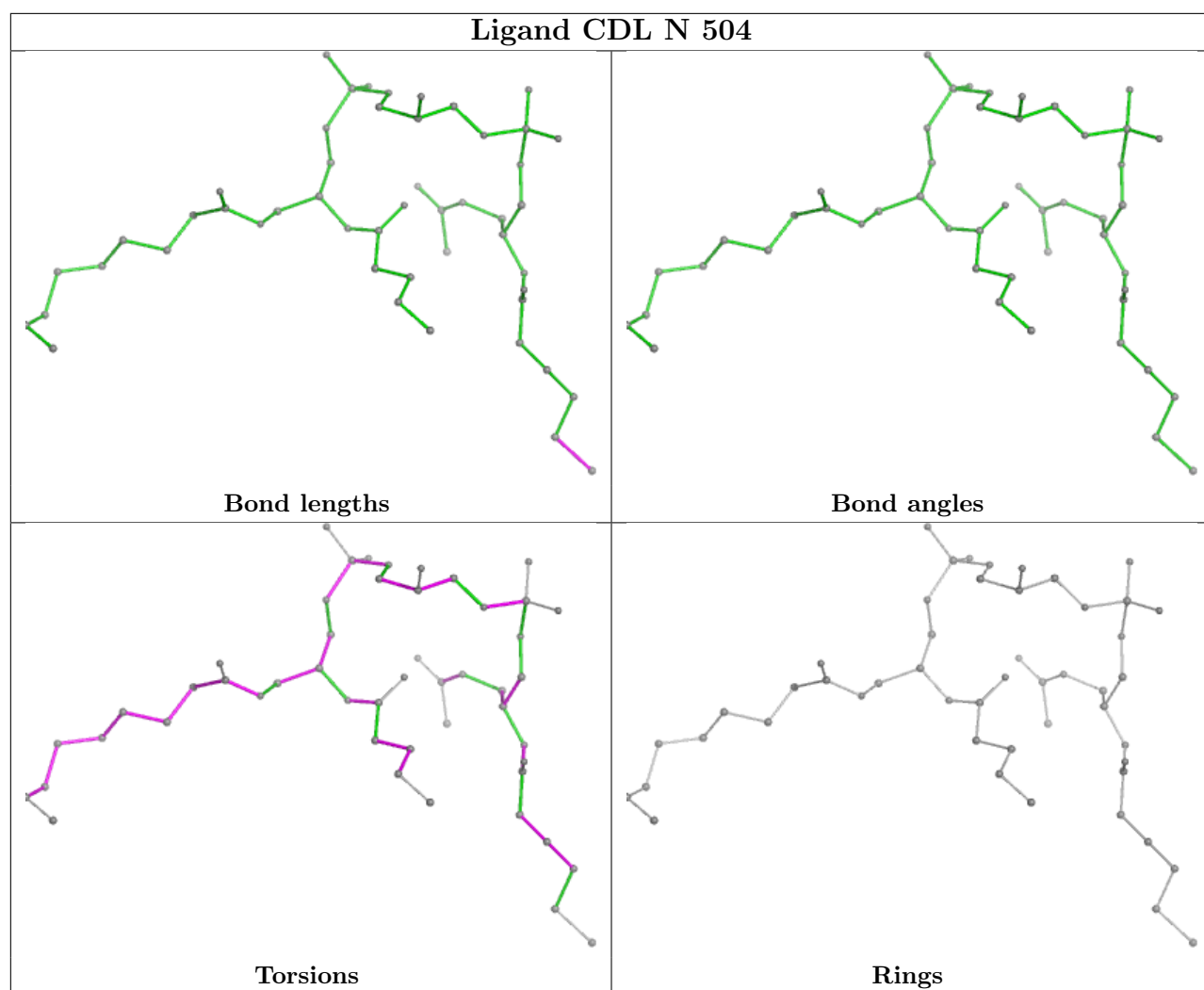


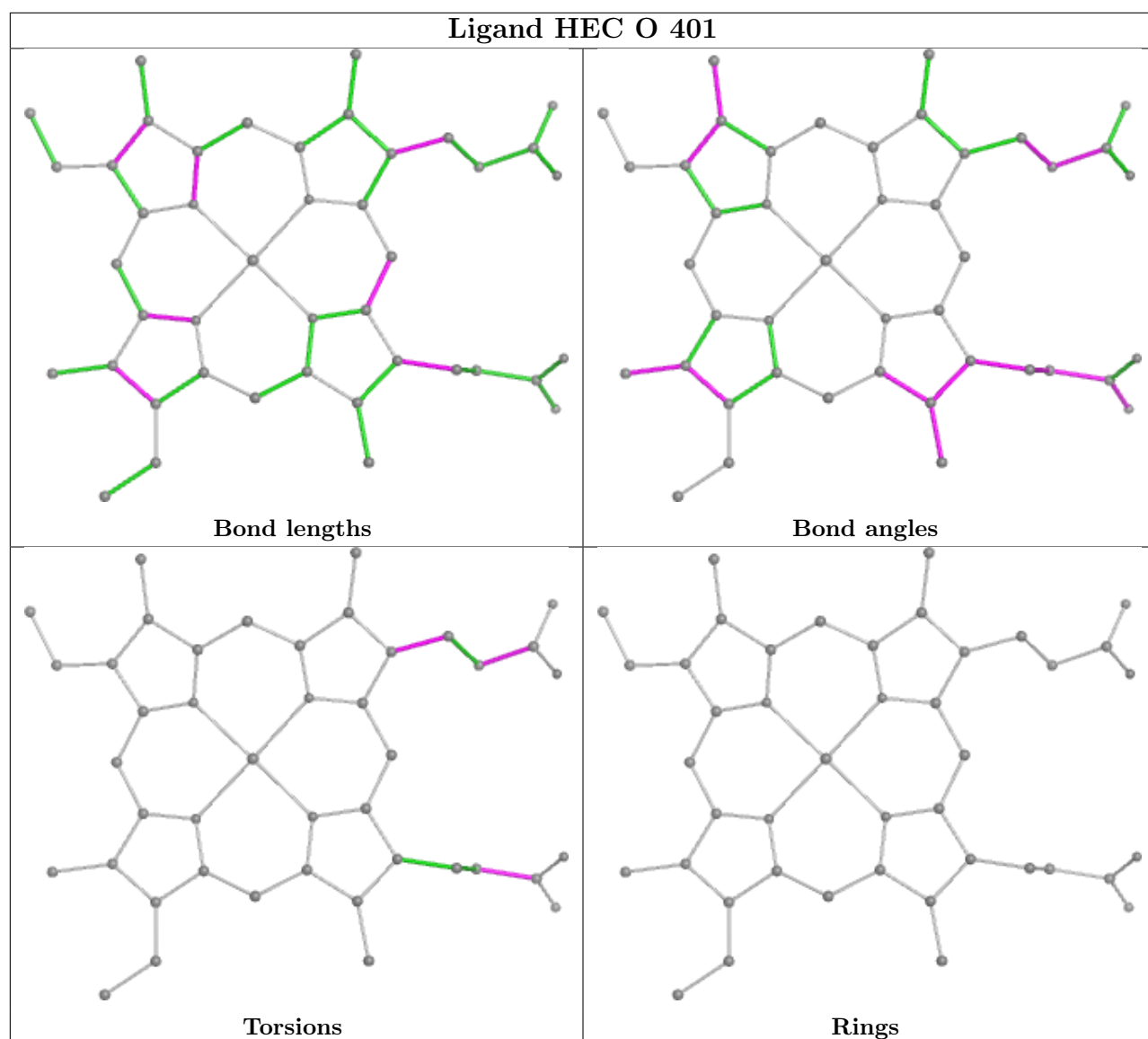


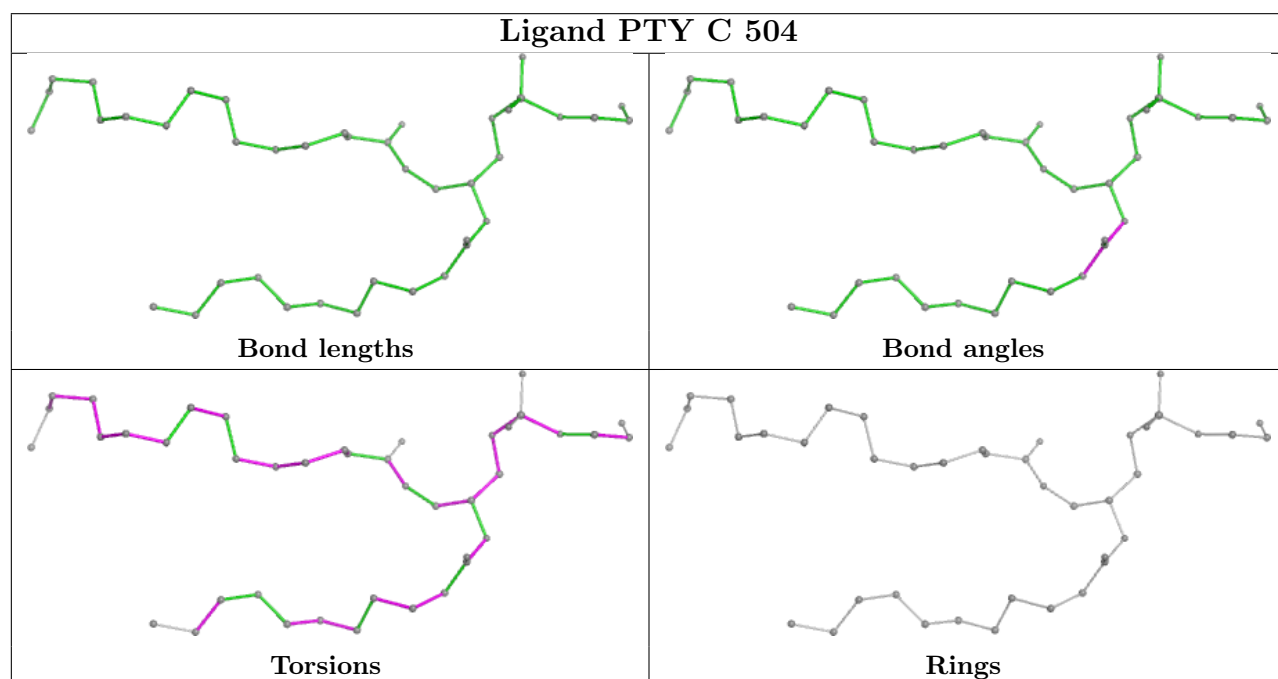
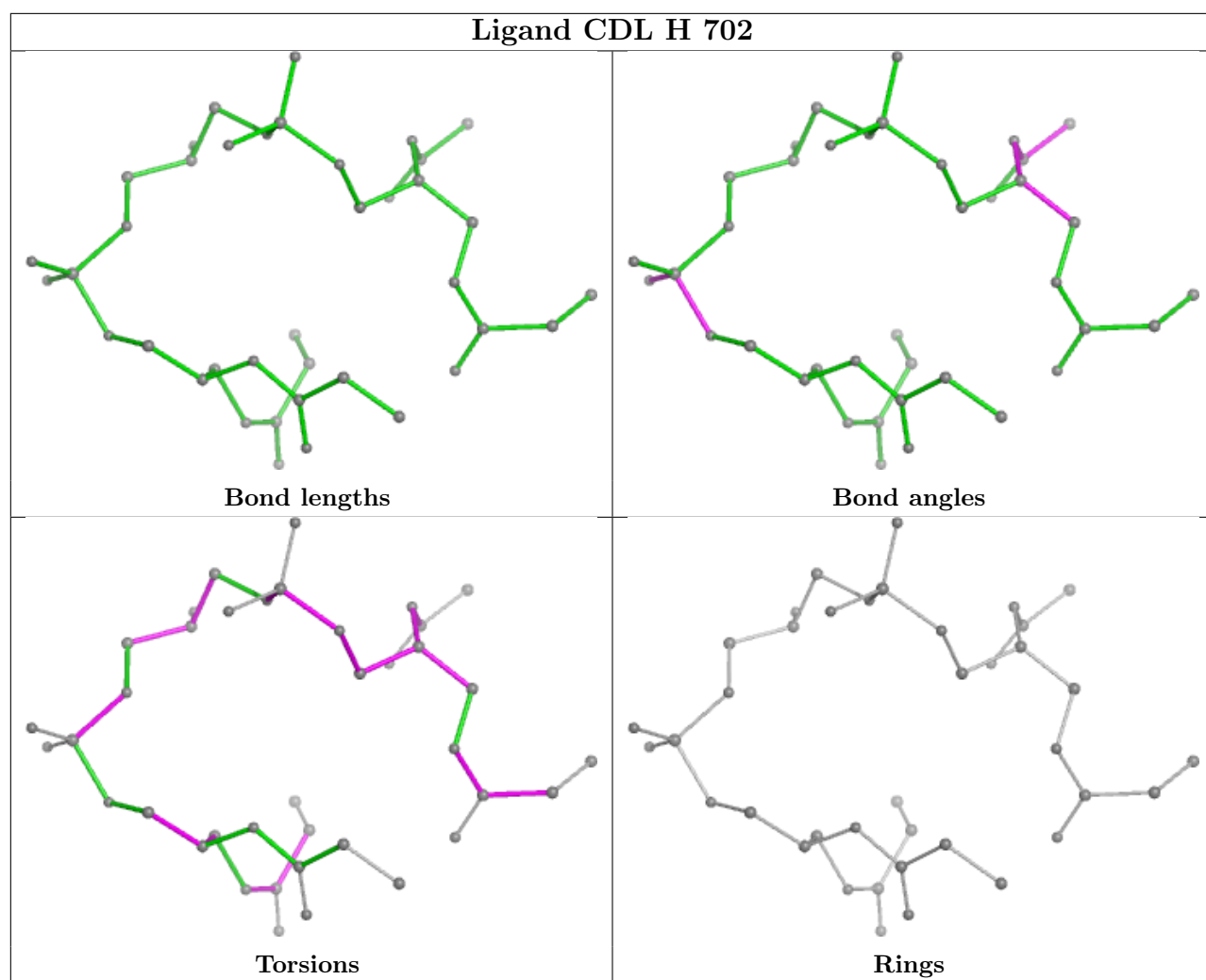


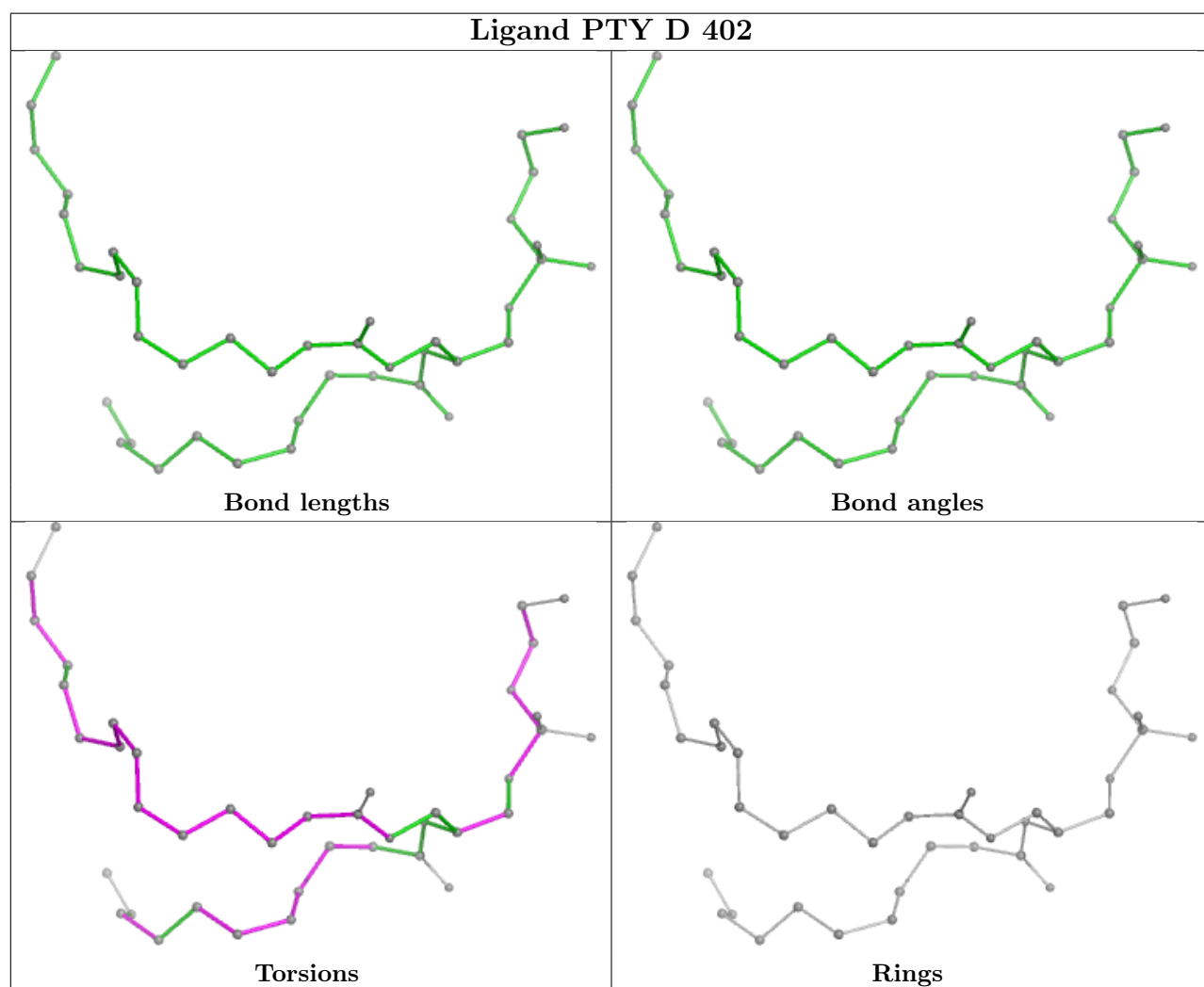
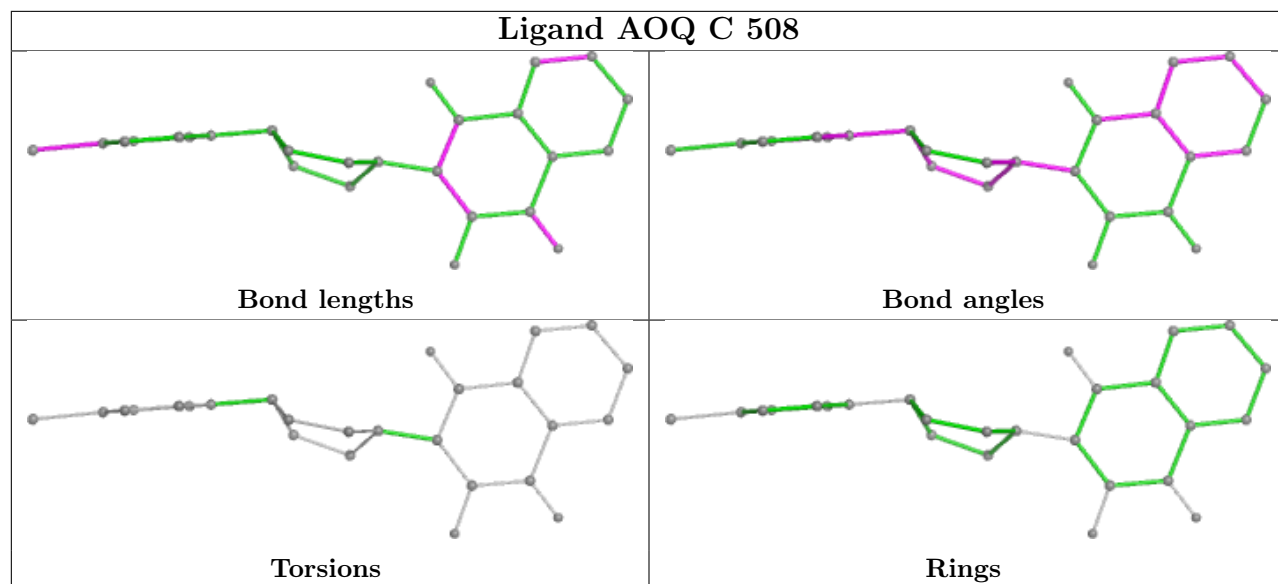


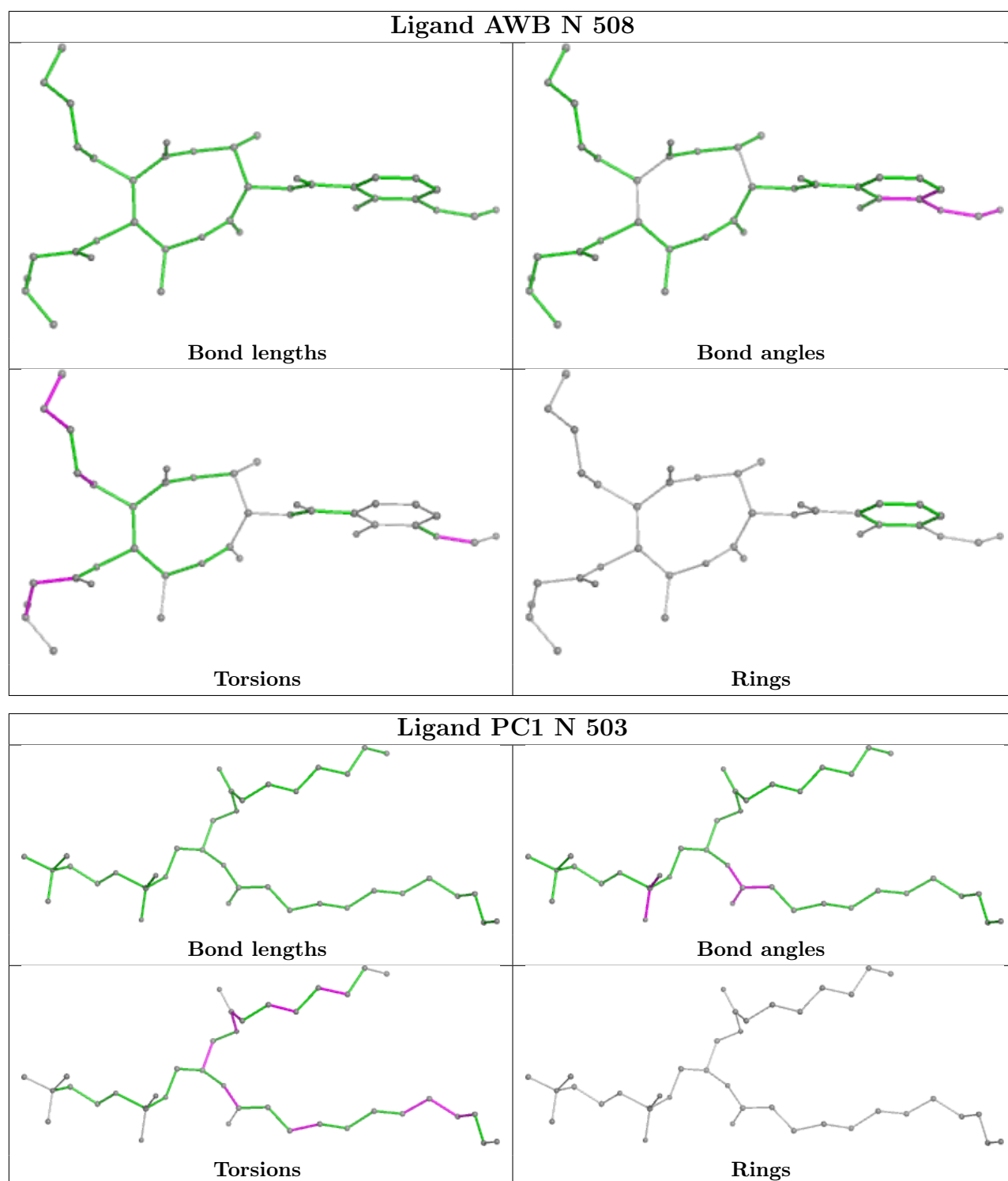












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

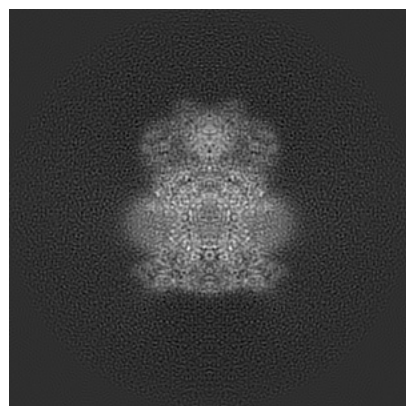
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15313. These allow visual inspection of the internal detail of the map and identification of artifacts.

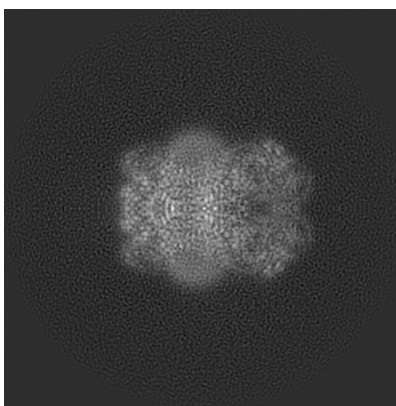
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

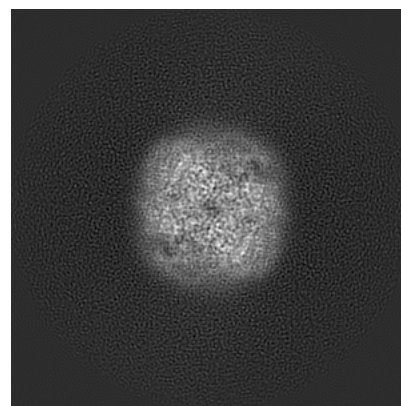
6.1.1 Primary map



X

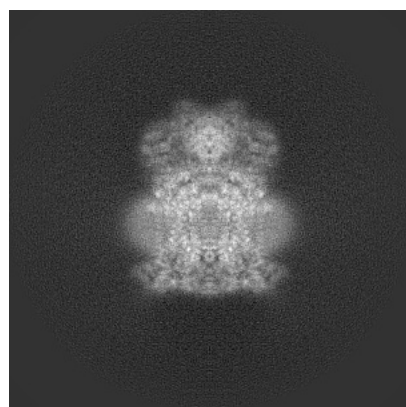


Y

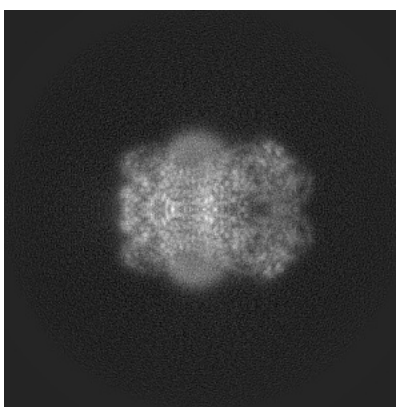


Z

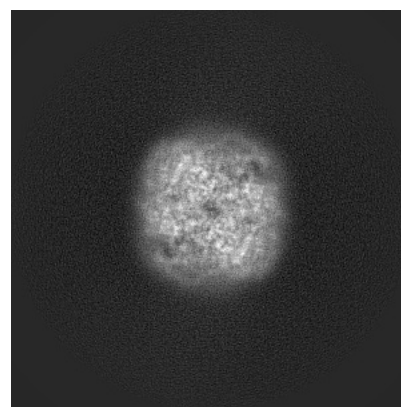
6.1.2 Raw map



X



Y

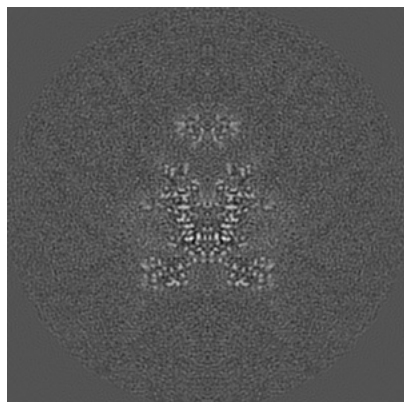


Z

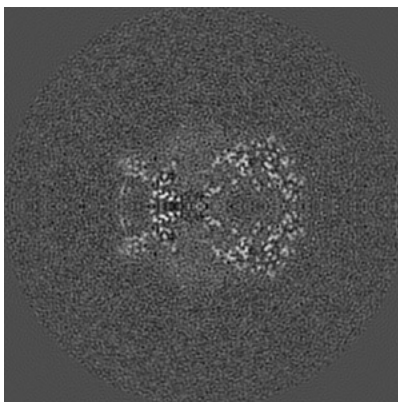
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

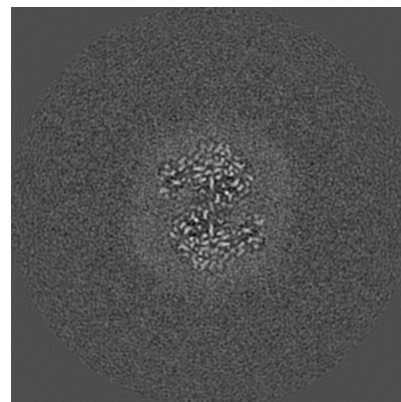
6.2.1 Primary map



X Index: 180

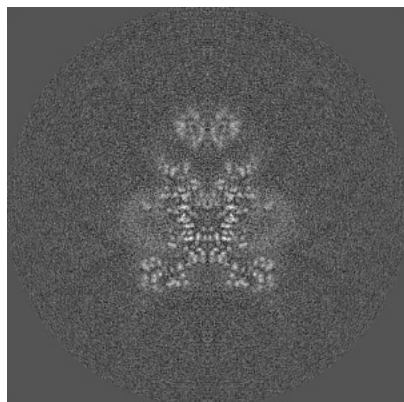


Y Index: 180

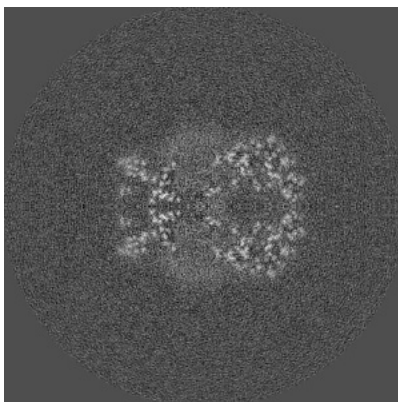


Z Index: 180

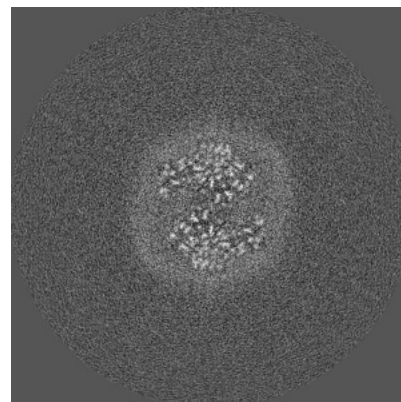
6.2.2 Raw map



X Index: 180



Y Index: 180

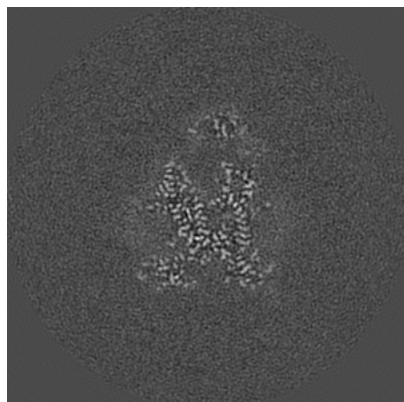


Z Index: 180

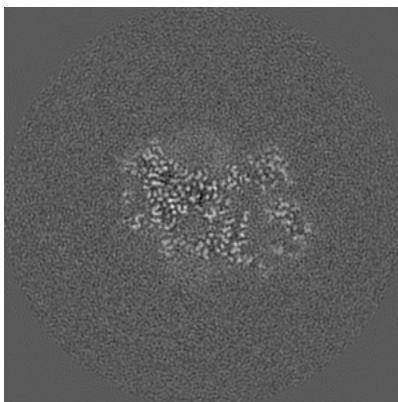
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

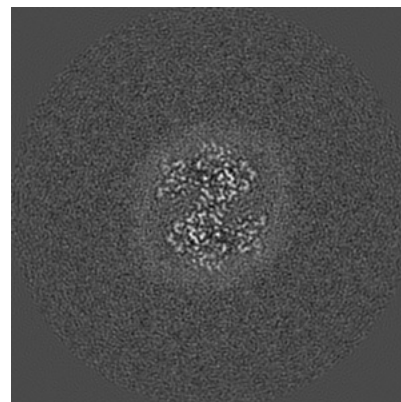
6.3.1 Primary map



X Index: 174

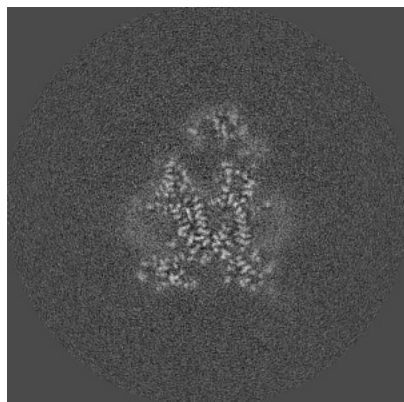


Y Index: 195

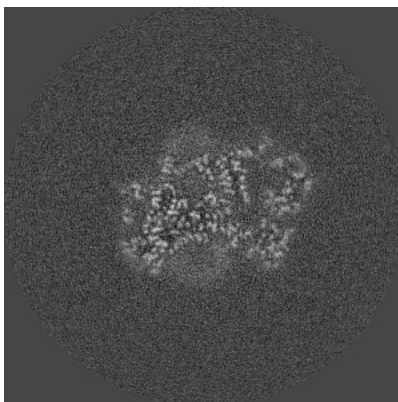


Z Index: 182

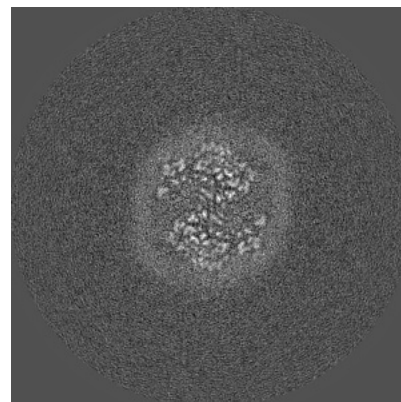
6.3.2 Raw map



X Index: 174



Y Index: 165

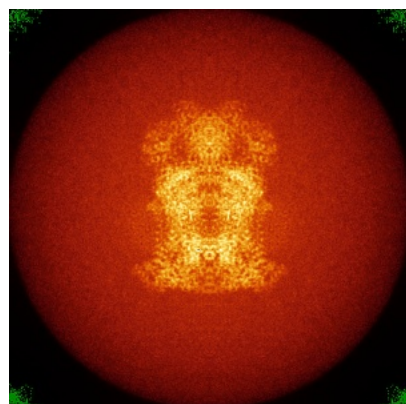


Z Index: 181

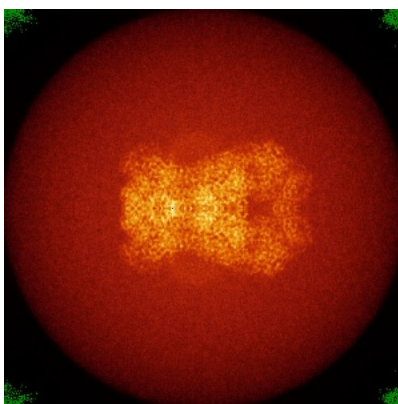
The images above show the largest variance slices of the map in three orthogonal directions.

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

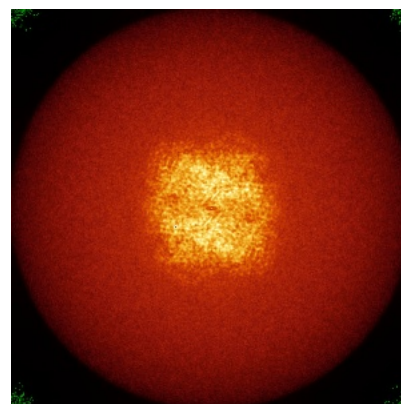
6.4.1 Primary map



X

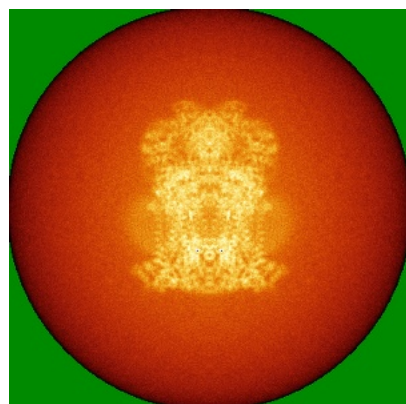


Y

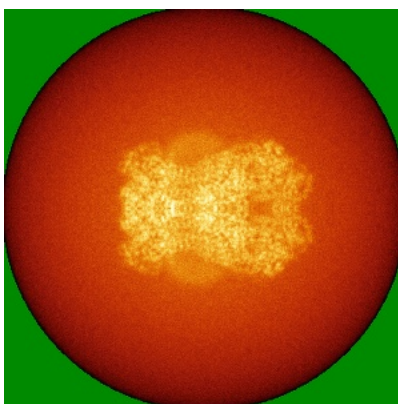


Z

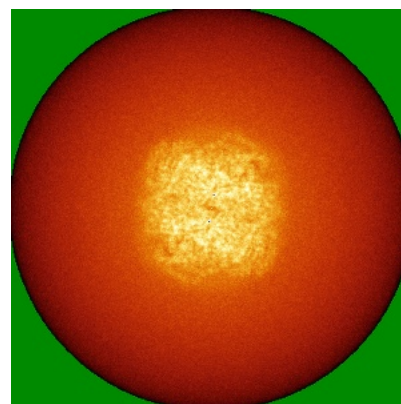
6.4.2 Raw map



X



Y

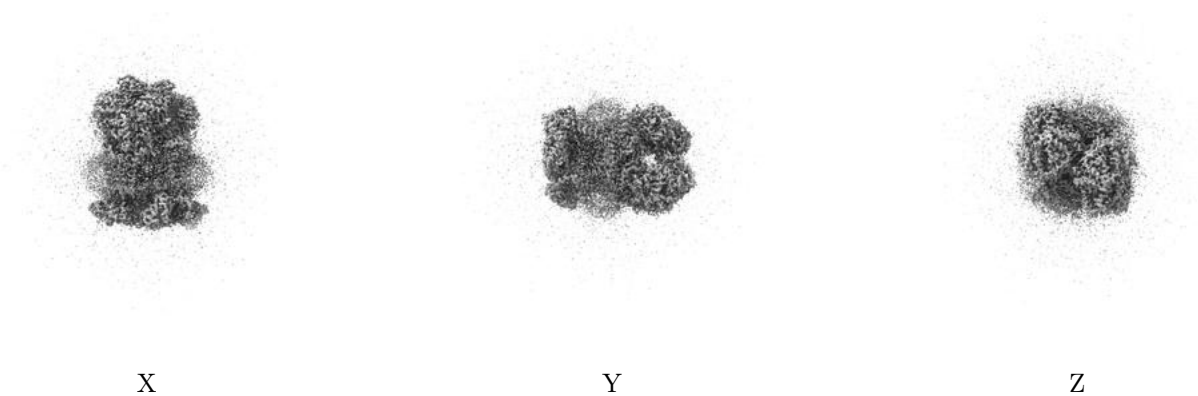


Z

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.

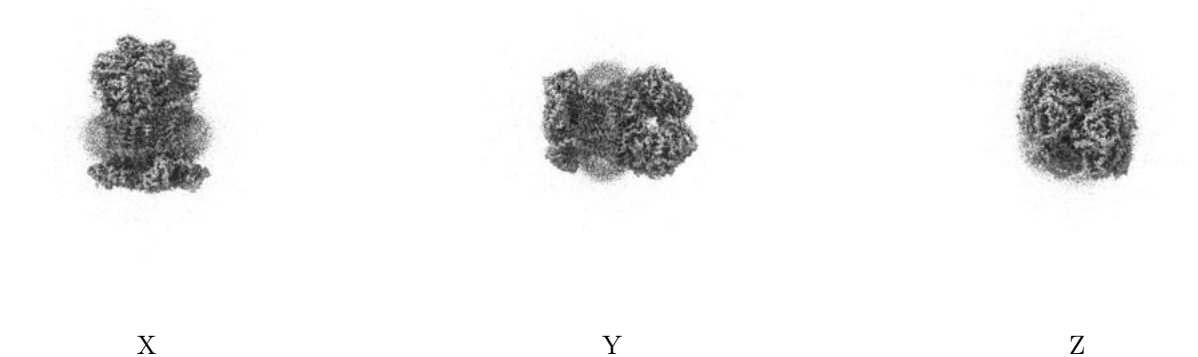
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. 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.

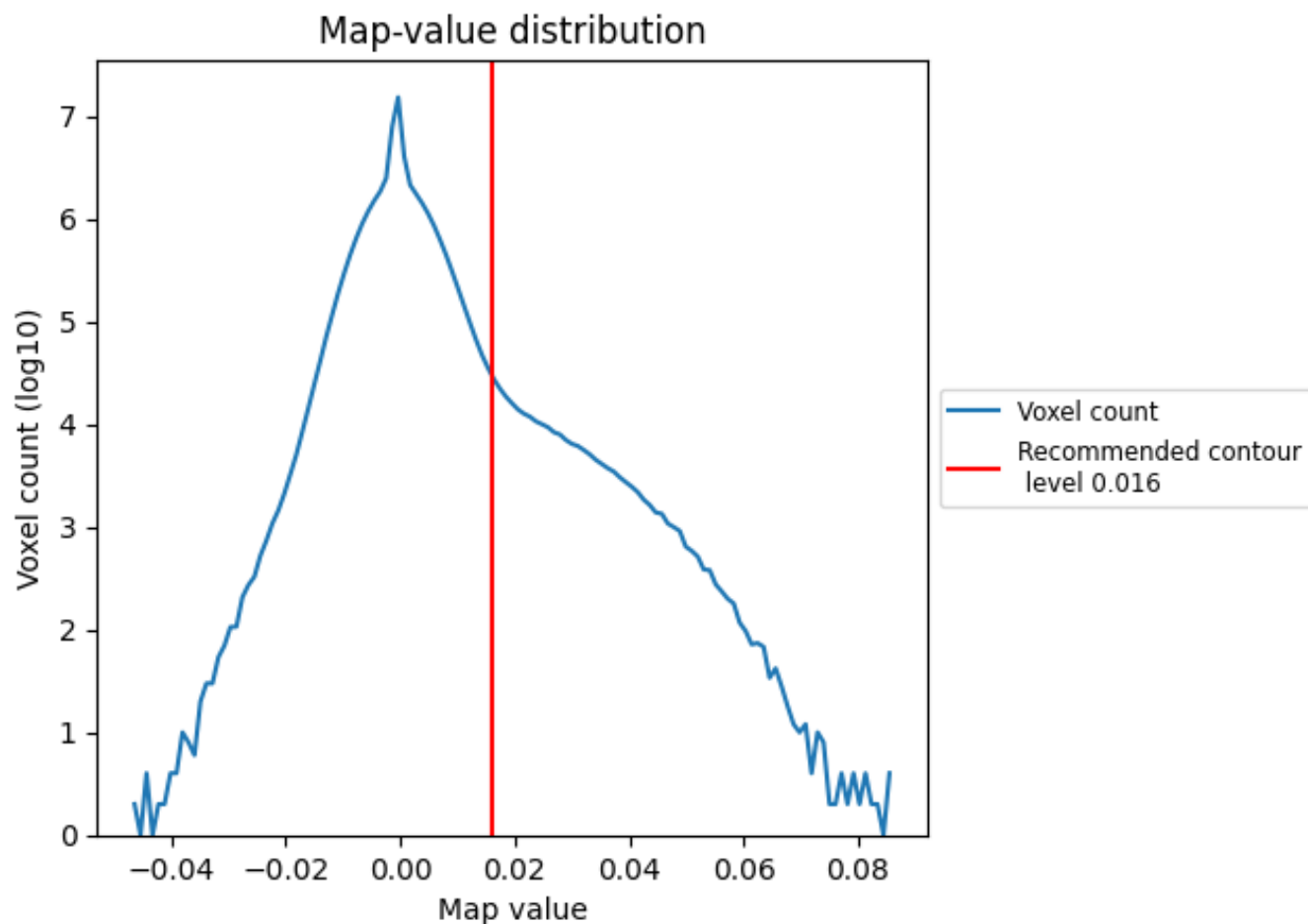
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

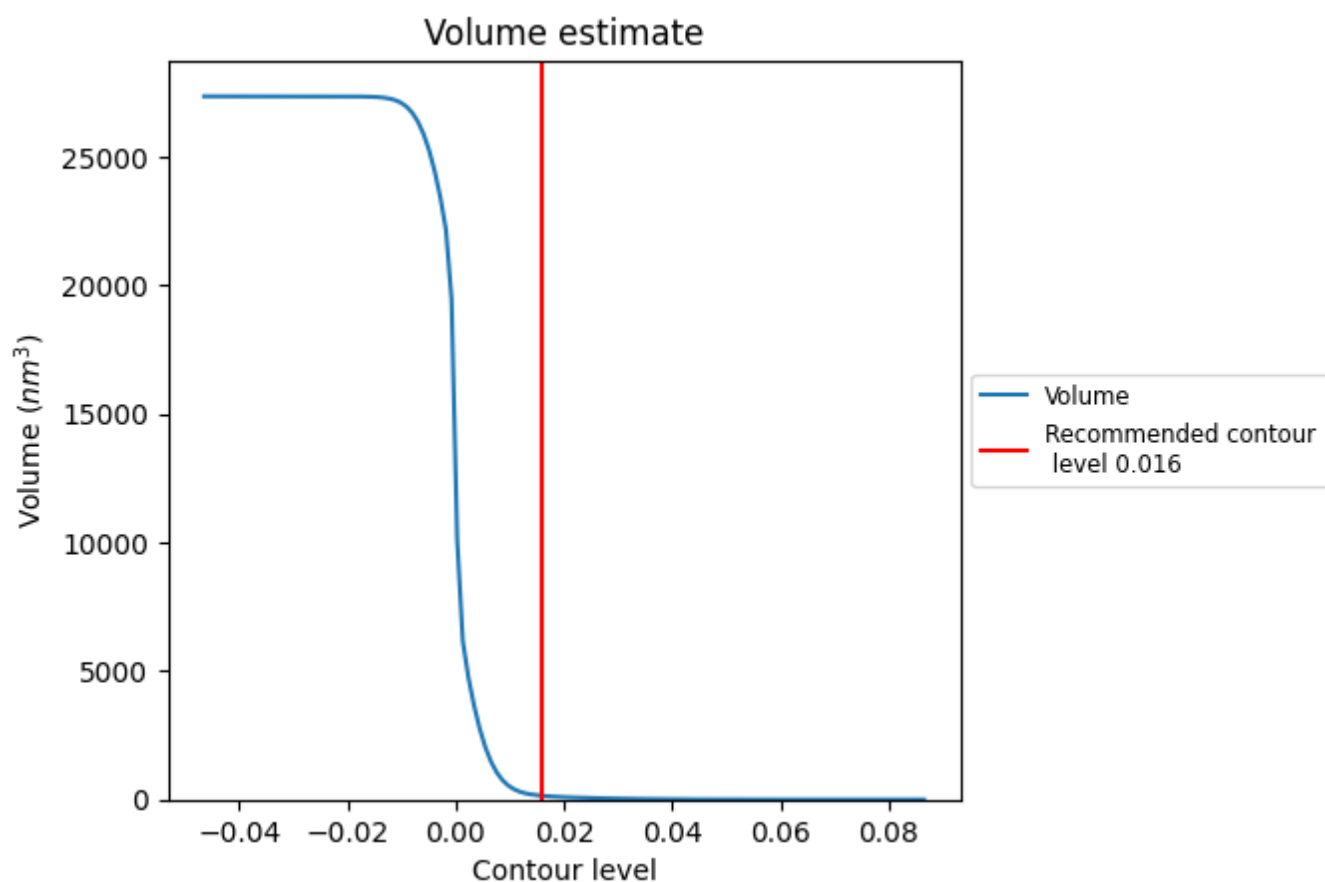
This section contains the results of statistical analysis of the map.

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.

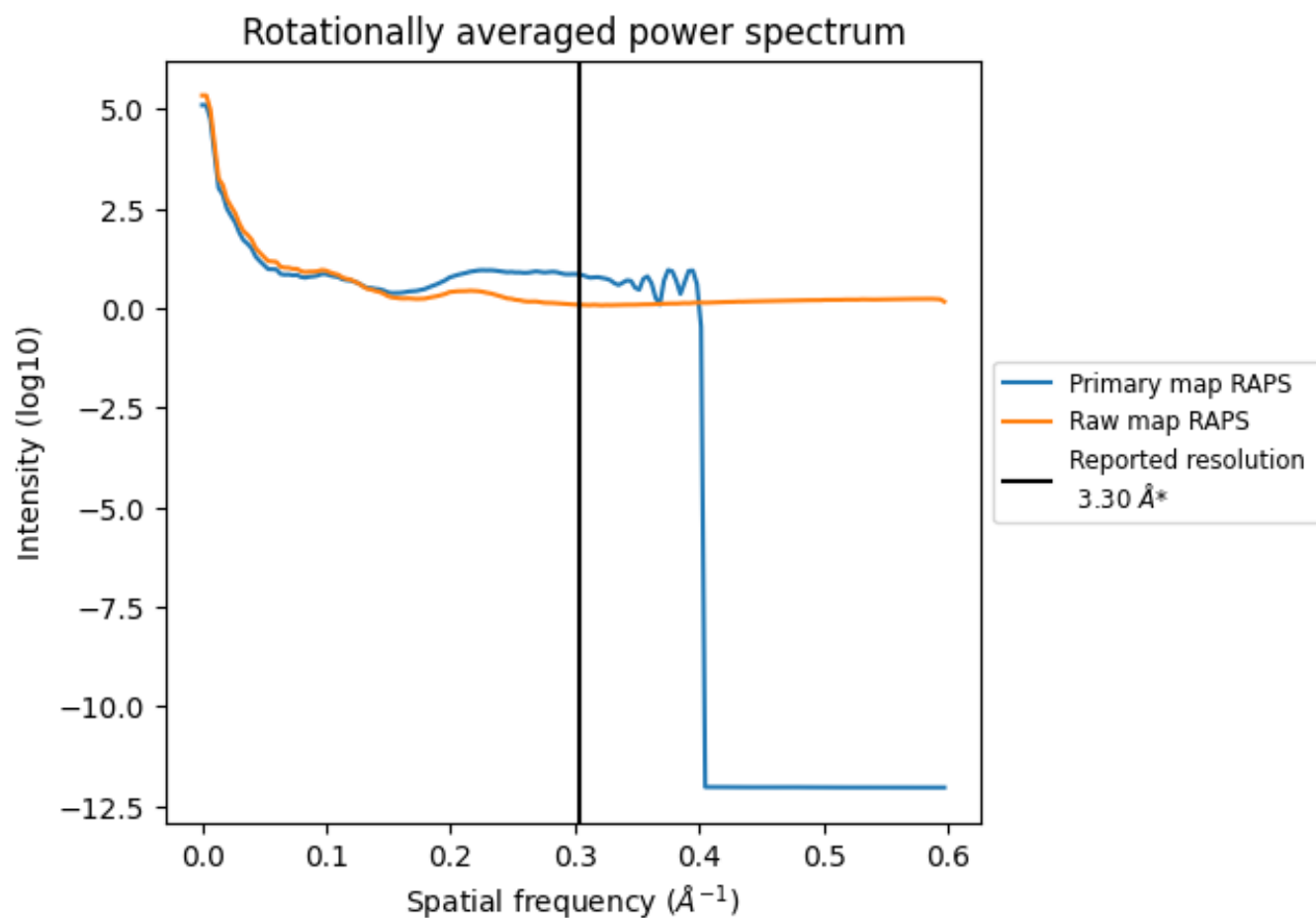
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 147 nm³; this corresponds to an approximate mass of 133 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 ⓘ

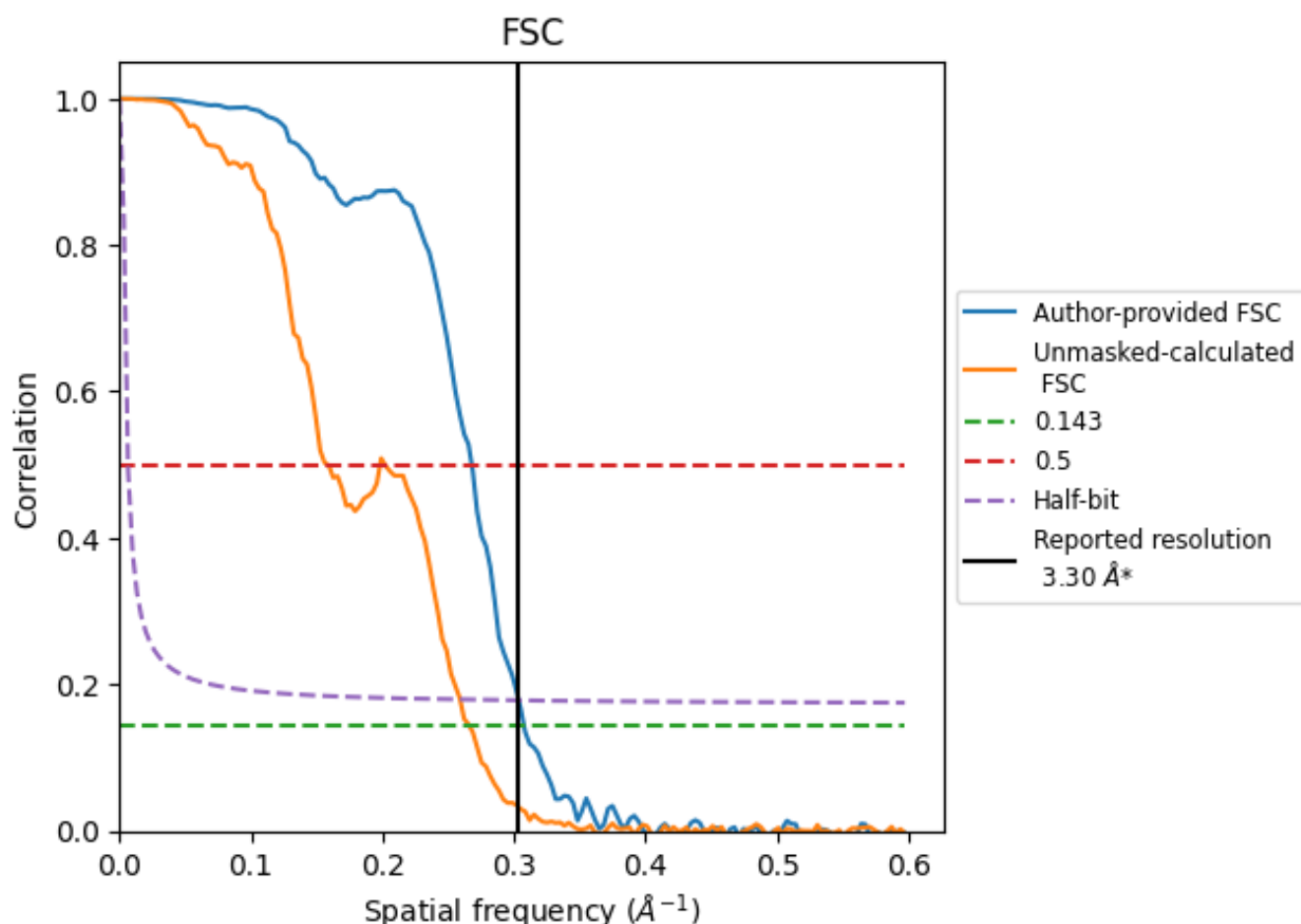


*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

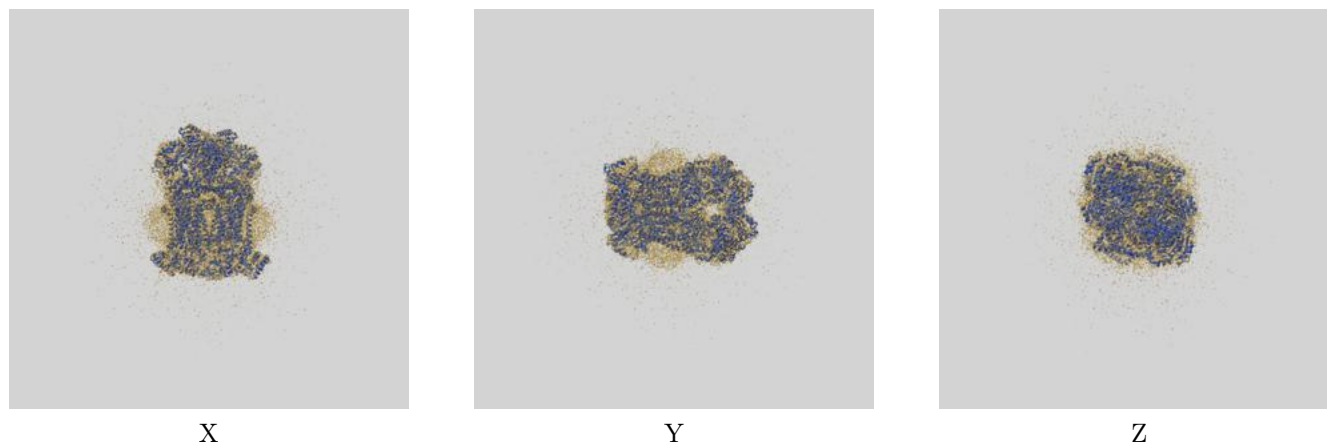
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.25	3.73	3.29
Unmasked-calculated*	3.76	6.31	3.86

*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 3.76 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

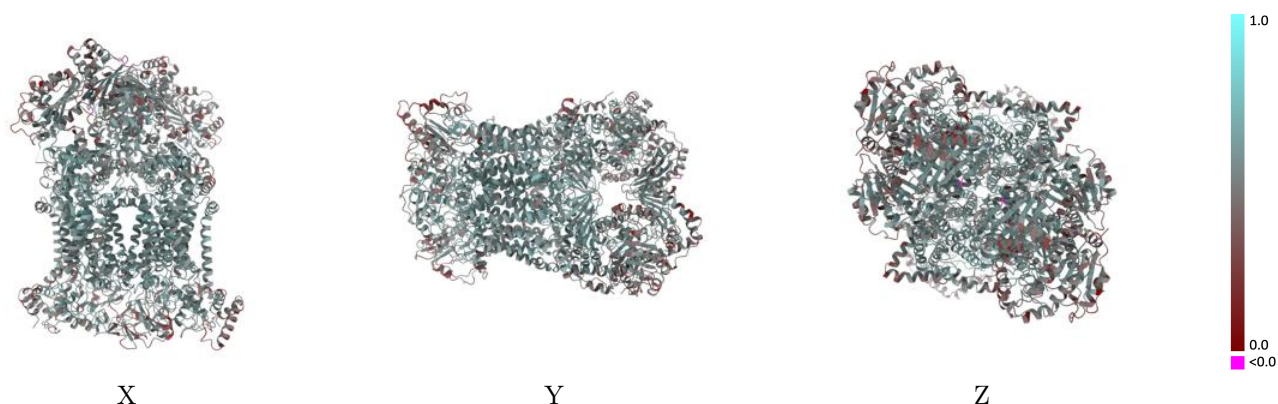
This section contains information regarding the fit between EMDB map EMD-15313 and PDB model 8AB7. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



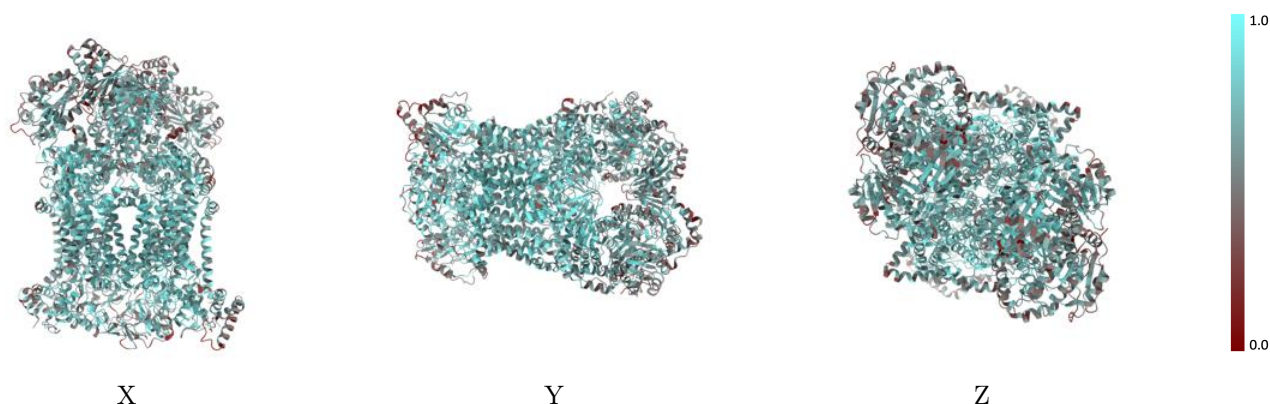
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



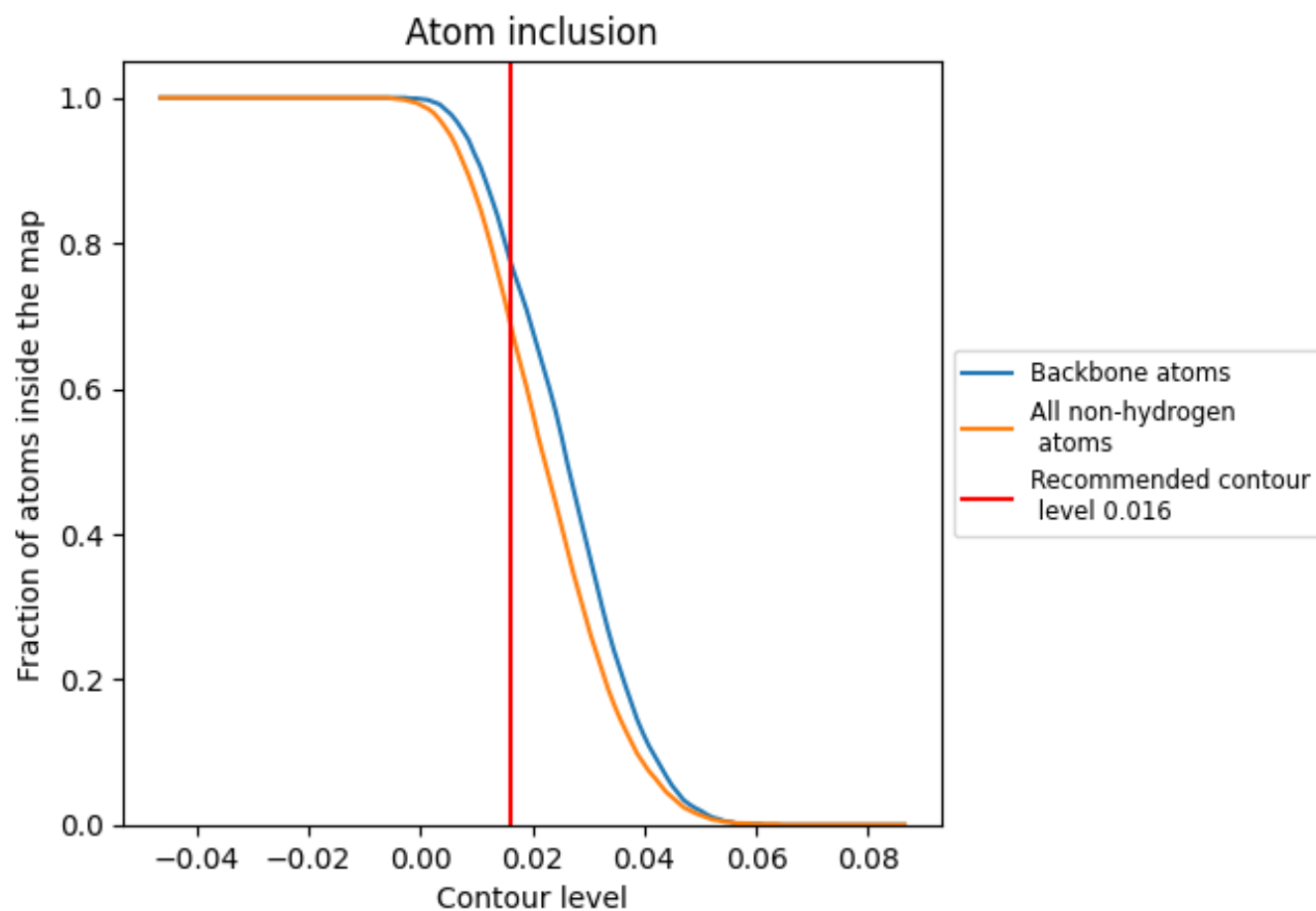
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 69% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.6920</div>	<div><div></div>0.5250</div>
A	<div><div></div>0.6560</div>	<div><div></div>0.5070</div>
B	<div><div></div>0.6300</div>	<div><div></div>0.4990</div>
C	<div><div></div>0.8040</div>	<div><div></div>0.5850</div>
D	<div><div></div>0.7470</div>	<div><div></div>0.5510</div>
E	<div><div></div>0.6830</div>	<div><div></div>0.4970</div>
F	<div><div></div>0.4820</div>	<div><div></div>0.4270</div>
G	<div><div></div>0.7040</div>	<div><div></div>0.5320</div>
H	<div><div></div>0.7210</div>	<div><div></div>0.5500</div>
I	<div><div></div>0.6860</div>	<div><div></div>0.5350</div>
J	<div><div></div>0.5850</div>	<div><div></div>0.4820</div>
L	<div><div></div>0.6580</div>	<div><div></div>0.5050</div>
M	<div><div></div>0.6270</div>	<div><div></div>0.4960</div>
N	<div><div></div>0.7990</div>	<div><div></div>0.5840</div>
O	<div><div></div>0.7530</div>	<div><div></div>0.5500</div>
P	<div><div></div>0.6750</div>	<div><div></div>0.4970</div>
Q	<div><div></div>0.4730</div>	<div><div></div>0.4230</div>
R	<div><div></div>0.7050</div>	<div><div></div>0.5300</div>
S	<div><div></div>0.7290</div>	<div><div></div>0.5520</div>
T	<div><div></div>0.6920</div>	<div><div></div>0.5360</div>
U	<div><div></div>0.5850</div>	<div><div></div>0.4910</div>

1.0

0.0

<0.0