



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 10:06 AM UTC

PDB ID : 8ABL / pdb_00008abl
EMDB ID : EMD-15325
Title : Complex III2 from *Yarrowia lipolytica*, with decylubiquinol and antimycin A, consensus refinement
Authors : Wieferig, J.P.; Kuhlbrandt, W.
Deposited on : 2022-07-04
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

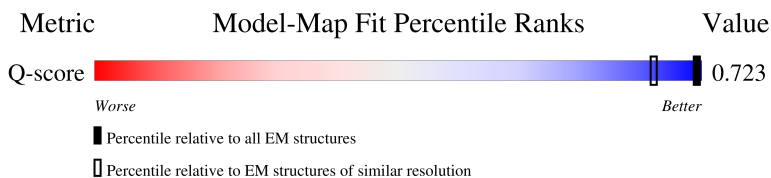
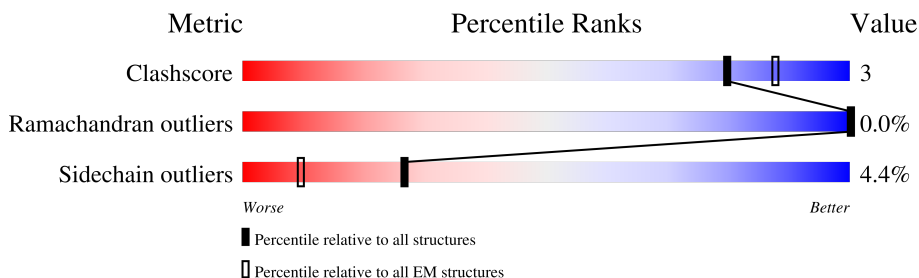
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.10 Å.

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

















Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2317 (1.60 - 2.60)

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	94% (green), 5% (yellow), 1% (orange), 0% (red), 0% (grey)
1	N	385	94% (green), 5% (yellow), 1% (orange), 0% (red), 0% (grey)
2	E	225	26% (green), 1% (yellow), 72% (grey)
2	P	225	27% (green), 72% (grey)

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Mol	Chain	Length	Quality of chain
3	G	128	 87% 9% ..
3	R	128	 88% 9% ..
4	F	137	 7% 48% . 48%
4	Q	137	 7% 48% . 48%
5	A	474	 87% 5% 8%
5	L	474	 83% 8% . 8%
6	B	417	 83% 12% ..
6	M	417	 82% 14% .
7	D	330	 69% 5% 26%
7	O	330	 70% . 26%
8	H	93	 87% .. 9%
8	S	93	 88% .. 9%
9	I	69	 77% . 22%
9	T	69	 77% . 22%
10	J	82	 87% .. 9%
10	U	82	 83% 9% 9%

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 31660 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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
2	P	63	Total	C	N	O	S	0	0
			478	305	78	91	4		
2	E	63	Total	C	N	O	S	0	0
			478	305	78	91	4		

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

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

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

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

- Molecule 7 is a protein called YALI0A17468p.

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

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

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

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

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

- Molecule 10 is a protein called YALI0C12210p.

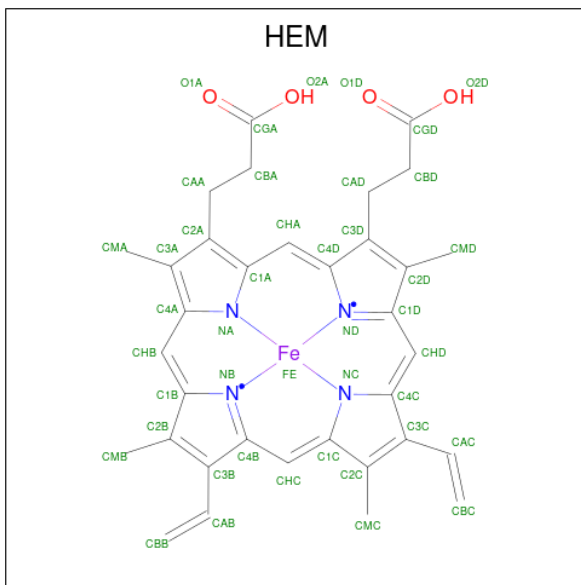
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	J	75	Total 598	C 403	N 99	O 96	0	0

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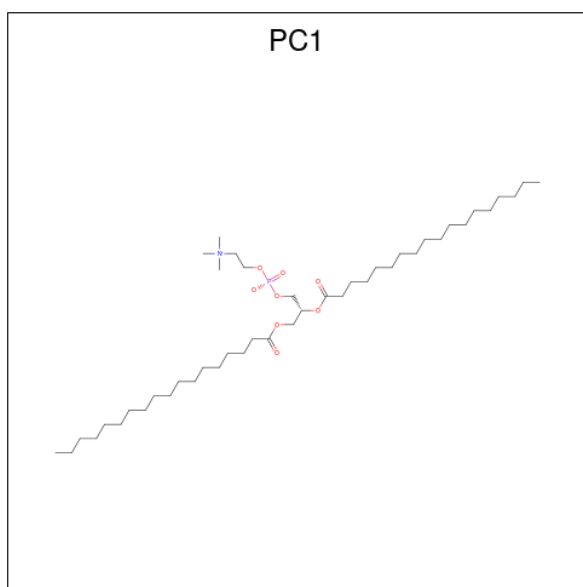
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	U	75	598	403	99	96	0	0

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



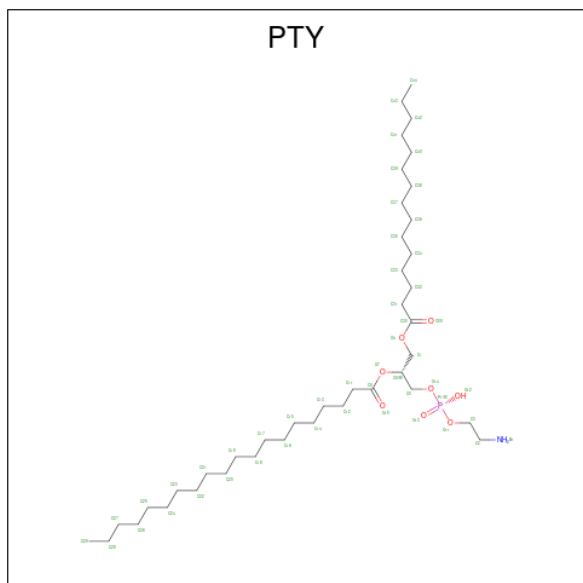
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
11	C	1	43	34	1	4	4	0
11	C	1	43	34	1	4	4	0
11	N	1	43	34	1	4	4	0
11	N	1	43	34	1	4	4	0

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



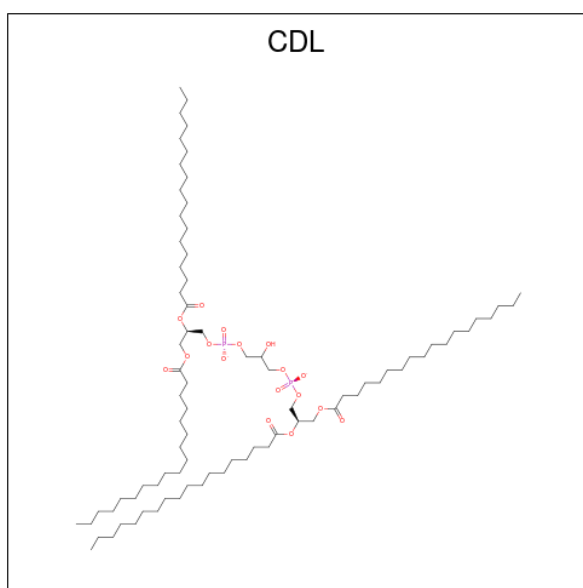
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	C	1	Total 38	28	1	8	1	0
12	I	1	Total 32	22	1	8	1	0
12	N	1	Total 38	28	1	8	1	0
12	T	1	Total 32	22	1	8	1	0

- Molecule 13 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



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

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



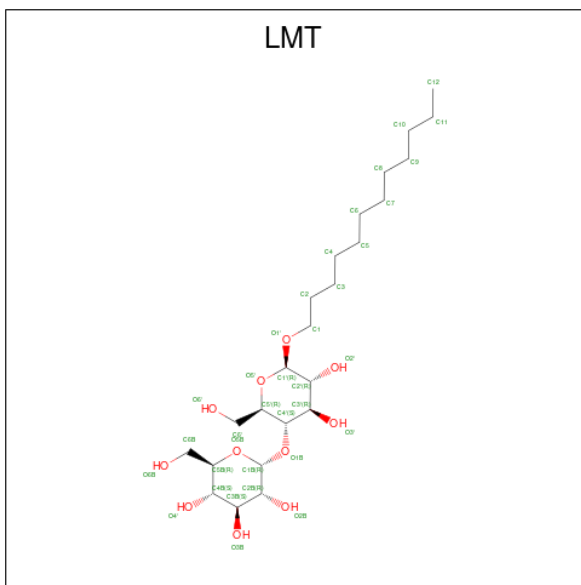
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
14	C	1	Total 48	C 29	O 17	P 2	0
14	A	1	Total 42	C 25	O 15	P 2	0
14	A	1	Total 47	C 30	O 15	P 2	0
14	H	1	Total 50	C 31	O 17	P 2	0
14	H	1	Total 39	C 20	O 17	P 2	0
14	N	1	Total 48	C 29	O 17	P 2	0
14	L	1	Total 42	C 25	O 15	P 2	0
14	L	1	Total 47	C 30	O 15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

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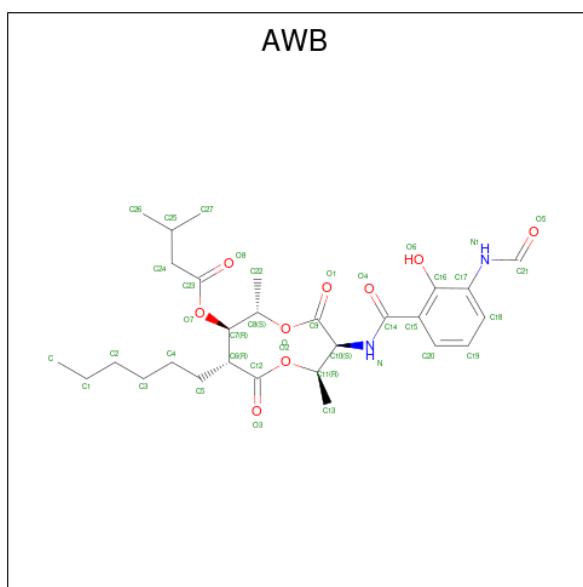
Mol	Chain	Residues	Atoms				AltConf
14	S	1	Total	C	O	P	0
			50	31	17	2	
14	S	1	Total	C	O	P	0
			39	20	17	2	

- Molecule 15 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



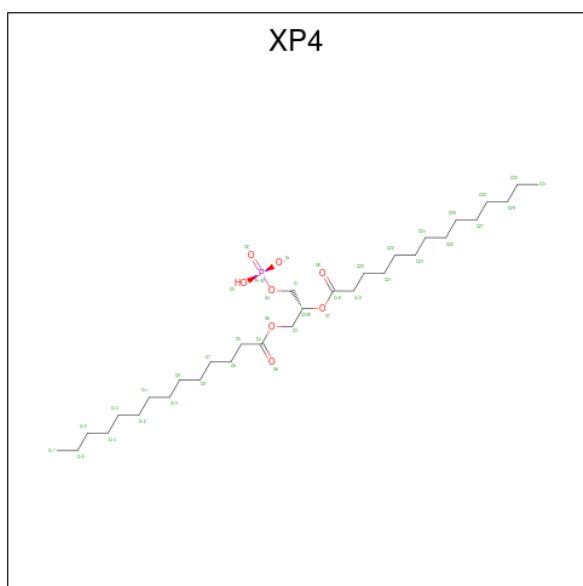
Mol	Chain	Residues	Atoms			AltConf
15	C	1	Total	C	O	0
			35	24	11	
15	J	1	Total	C	O	0
			35	24	11	
15	N	1	Total	C	O	0
			35	24	11	
15	U	1	Total	C	O	0
			35	24	11	

- 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 (CCD ID: AWB) (formula: C₂₈H₄₀N₂O₉) (labeled as "Ligand of Interest" by depositor).



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

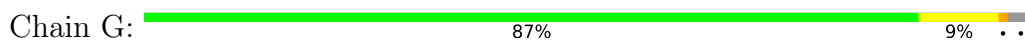
- Molecule 17 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: XP4) (formula: $C_{31}H_{60}O_8P$).



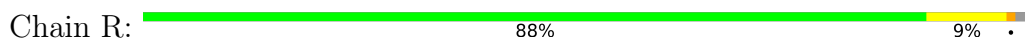
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
17	A	1	24	15	8	1	0

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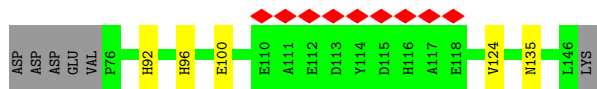
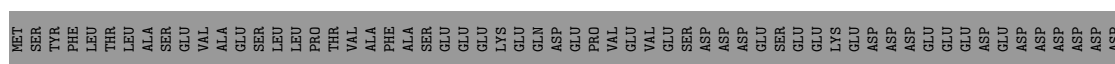
• Molecule 3: Cytochrome b-c1 complex subunit 7



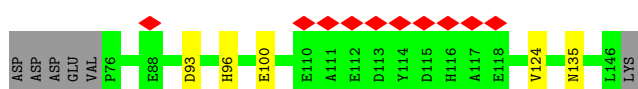
• Molecule 3: Cytochrome b-c1 complex subunit 7



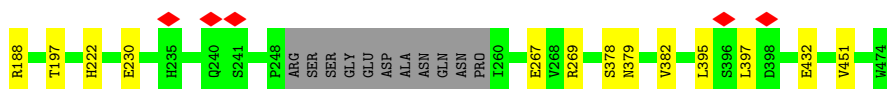
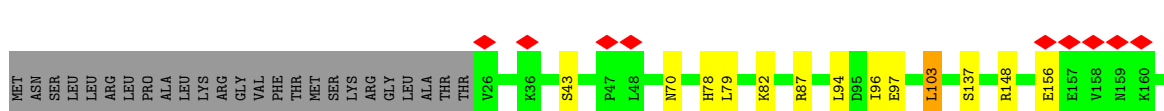
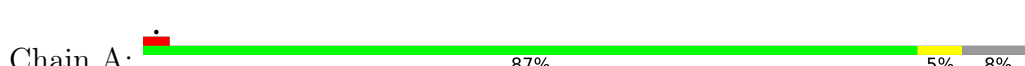
• Molecule 4: YALI0F24673p



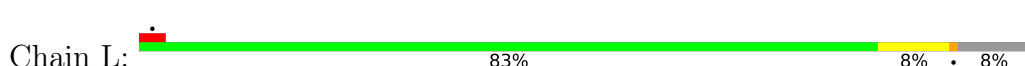
• Molecule 4: YALI0F24673p

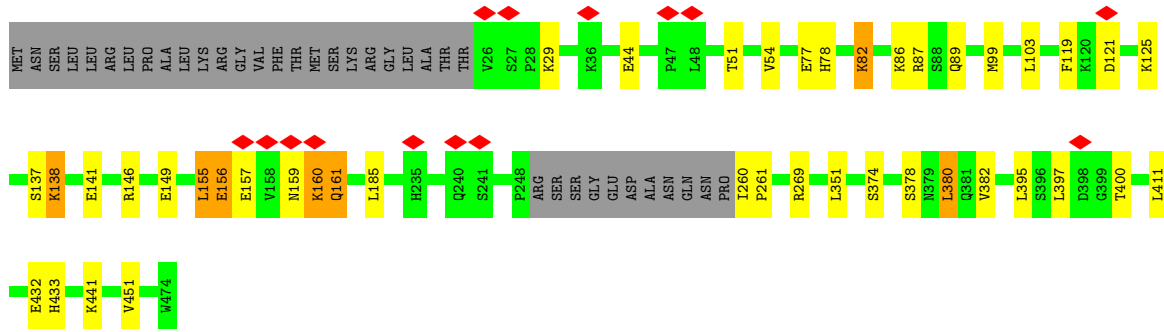


• Molecule 5: YALI0A14806p

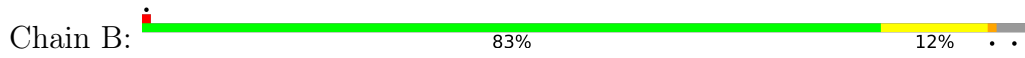


• Molecule 5: YALI0A14806p

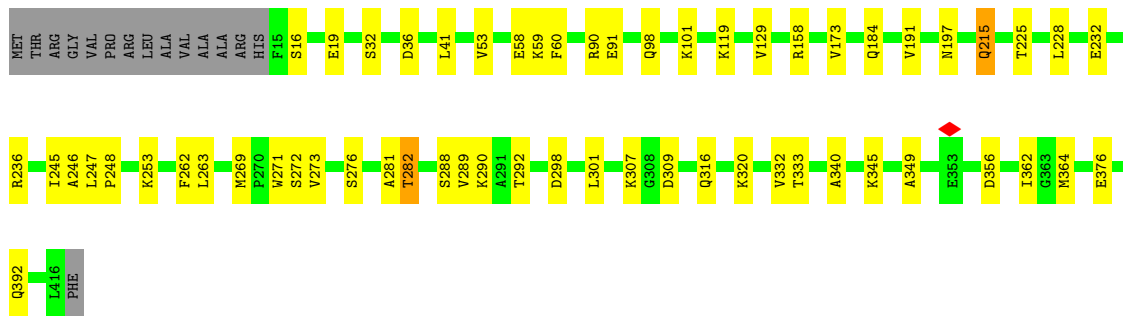
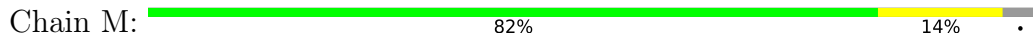




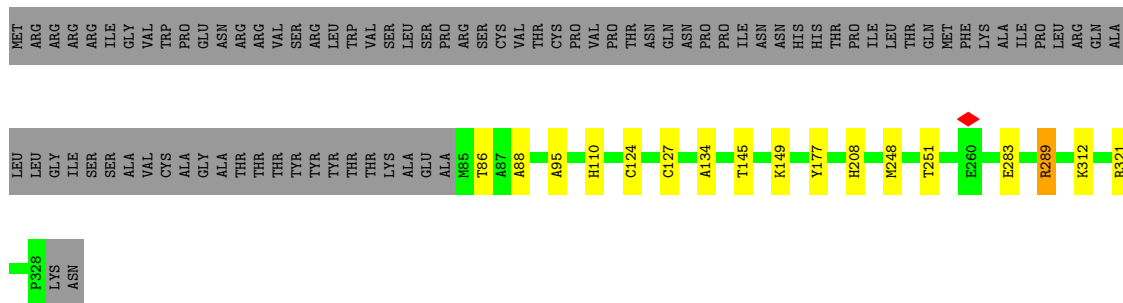
• Molecule 6: Cytochrome b-c1 complex subunit 2, mitochondrial



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



• Molecule 7: YALI0A17468p





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	225162	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	0.223	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.021	Depositor
Map size (\AA)	301.32, 301.32, 301.32	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.837, 0.837, 0.837	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.60	0/3153	1.02	4/4305 (0.1%)
1	N	0.59	0/3153	1.02	3/4305 (0.1%)
2	E	0.57	0/487	1.10	1/654 (0.2%)
2	P	0.60	0/487	1.09	1/654 (0.2%)
3	G	0.56	0/1012	1.04	1/1373 (0.1%)
3	R	0.55	0/1012	1.05	3/1373 (0.2%)
4	F	0.49	0/595	1.06	0/805
4	Q	0.48	0/595	1.13	2/805 (0.2%)
5	A	0.56	0/3510	1.09	7/4768 (0.1%)
5	L	0.55	0/3510	1.07	3/4768 (0.1%)
6	B	0.56	0/3069	1.09	8/4178 (0.2%)
6	M	0.56	0/3069	1.08	9/4178 (0.2%)
7	D	0.57	0/1950	1.13	9/2656 (0.3%)
7	O	0.57	0/1950	1.11	8/2656 (0.3%)
8	H	0.57	0/717	1.08	1/975 (0.1%)
8	S	0.57	0/717	1.08	1/975 (0.1%)
9	I	0.50	0/465	1.04	0/629
9	T	0.50	0/465	1.04	0/629
10	J	0.53	0/620	1.05	1/846 (0.1%)
10	U	0.54	0/620	1.04	1/846 (0.1%)
All	All	0.56	0/31156	1.07	63/42378 (0.1%)

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	283	GLU	CB-CA-C	-10.59	95.71	111.27
7	O	283	GLU	CB-CA-C	-10.43	95.94	111.27
6	B	90	ARG	CG-CD-NE	-9.32	91.48	112.00
7	O	289	ARG	CG-CD-NE	-9.16	91.85	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	289	ARG	CG-CD-NE	-9.16	91.86	112.00
7	D	283	GLU	CB-CG-CD	-8.67	97.86	112.60
2	P	62	ARG	CB-CG-CD	-8.64	91.43	111.30
2	E	62	ARG	CB-CG-CD	-8.59	91.55	111.30
6	M	90	ARG	CG-CD-NE	-8.36	93.61	112.00
1	N	16	TYR	CA-C-N	-7.41	113.92	122.14
1	N	16	TYR	C-N-CA	-7.41	113.92	122.14
1	C	16	TYR	CA-C-N	-7.29	114.05	122.14
1	C	16	TYR	C-N-CA	-7.29	114.05	122.14
4	Q	96	HIS	CB-CA-C	-7.22	98.81	110.79
6	B	158	ARG	CG-CD-NE	-7.00	96.61	112.00
6	M	158	ARG	CG-CD-NE	-6.90	96.83	112.00
4	Q	93	ASP	CA-CB-CG	6.71	119.31	112.60
5	A	148	ARG	CB-CA-C	6.50	122.65	110.63
5	A	379	ASN	CA-CB-CG	-6.34	106.26	112.60
7	O	289	ARG	NE-CZ-NH1	-6.32	115.19	121.50
3	G	76	ARG	CD-NE-CZ	6.28	133.19	124.40
3	R	76	ARG	CD-NE-CZ	6.28	133.19	124.40
5	L	269	ARG	CG-CD-NE	-6.26	98.23	112.00
7	D	289	ARG	NE-CZ-NH1	-6.26	115.24	121.50
6	B	197	ASN	CB-CA-C	6.15	119.99	111.63
6	M	197	ASN	CB-CA-C	6.08	119.90	111.63
5	A	269	ARG	CG-CD-NE	-5.98	98.84	112.00
5	L	451	VAL	CA-C-N	-5.85	118.06	122.33
5	L	451	VAL	C-N-CA	-5.85	118.06	122.33
3	R	65	THR	CA-CB-OG1	-5.77	100.94	109.60
7	O	208	HIS	CA-C-N	-5.75	116.60	123.44
7	O	208	HIS	C-N-CA	-5.75	116.60	123.44
7	D	208	HIS	CA-C-N	-5.72	116.63	123.44
7	D	208	HIS	C-N-CA	-5.72	116.63	123.44
5	A	451	VAL	CA-C-N	-5.69	118.18	122.33
5	A	451	VAL	C-N-CA	-5.69	118.18	122.33
6	M	392	GLN	CB-CG-CD	-5.62	103.05	112.60
8	H	86	ARG	CB-CA-C	-5.61	101.83	110.81
6	B	215	GLN	CB-CA-C	-5.58	98.10	109.65
1	N	74	PHE	CA-CB-CG	-5.55	108.25	113.80
8	S	86	ARG	CB-CA-C	-5.55	101.93	110.81
6	M	215	GLN	CB-CA-C	-5.54	98.17	109.65
3	R	112	GLU	CB-CG-CD	5.53	122.00	112.60
1	C	74	PHE	CA-CB-CG	-5.52	108.28	113.80
7	D	110	HIS	CA-CB-CG	-5.50	108.30	113.80
1	C	283	ARG	CG-CD-NE	5.49	124.09	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	110	HIS	CA-CB-CG	-5.46	108.34	113.80
5	A	70	ASN	CB-CA-C	5.38	117.92	110.16
7	D	86	THR	CA-CB-OG1	-5.32	101.62	109.60
10	J	18	PRO	CB-CA-C	-5.22	104.73	111.46
6	B	119	LYS	CA-C-N	-5.21	114.75	122.41
6	B	119	LYS	C-N-CA	-5.21	114.75	122.41
10	U	18	PRO	CB-CA-C	-5.20	104.75	111.46
6	M	119	LYS	CA-C-N	-5.20	114.77	122.41
6	M	119	LYS	C-N-CA	-5.20	114.77	122.41
7	D	321	ARG	CB-CG-CD	-5.18	99.38	111.30
7	O	321	ARG	CB-CG-CD	-5.18	99.38	111.30
6	M	184	GLN	CB-CG-CD	-5.15	103.84	112.60
6	B	411	PRO	CB-CA-C	-5.14	104.49	111.12
5	A	148	ARG	CG-CD-NE	5.11	123.25	112.00
7	O	289	ARG	NE-CZ-NH2	5.03	123.73	119.20
6	M	119	LYS	CB-CA-C	-5.02	102.39	110.77
6	B	119	LYS	CB-CA-C	-5.02	102.39	110.77

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3052	0	3113	15	0
1	N	3052	0	3113	12	0
2	E	478	0	473	2	0
2	P	478	0	473	9	0
3	G	994	0	1022	2	0
3	R	994	0	1022	3	0
4	F	579	0	511	2	0
4	Q	579	0	511	2	0
5	A	3446	0	3369	12	0
5	L	3446	0	3369	12	0
6	B	3008	0	2991	16	0
6	M	3008	0	2991	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	1893	0	1834	16	0
7	O	1893	0	1834	15	0
8	H	690	0	673	3	0
8	S	690	0	673	2	0
9	I	452	0	435	1	0
9	T	452	0	435	1	0
10	J	598	0	615	2	0
10	U	598	0	615	4	0
11	C	86	0	60	7	0
11	N	86	0	60	5	0
12	C	38	0	50	2	0
12	I	32	0	38	2	0
12	N	38	0	50	1	0
12	T	32	0	38	2	0
13	C	41	0	58	6	0
13	D	41	0	58	2	0
13	N	41	0	58	7	0
13	P	41	0	58	12	0
14	A	89	0	85	3	0
14	C	48	0	40	1	0
14	H	89	0	66	7	0
14	L	89	0	85	1	0
14	N	48	0	40	1	0
14	S	89	0	66	6	0
15	C	35	0	46	4	0
15	J	35	0	46	0	0
15	N	35	0	46	1	0
15	U	35	0	46	0	0
16	C	39	0	40	2	0
16	N	39	0	40	4	0
17	A	24	0	22	1	0
17	L	24	0	22	1	0
18	D	43	0	32	11	0
18	O	43	0	32	11	0
All	All	31660	0	31354	172	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 3.

All (172) 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)
2:P:84:VAL:CG2	13:P:301:PTY:H441	1.46	1.45
7:O:124:CYS:SG	18:O:401:HEC:HBB3	1.61	1.41
7:D:124:CYS:SG	18:D:401:HEC:HBB3	1.62	1.36
7:O:124:CYS:SG	18:O:401:HEC:CBB	2.28	1.21
7:D:124:CYS:SG	18:D:401:HEC:CBB	2.29	1.19
7:D:127:CYS:SG	18:D:401:HEC:HBC3	1.84	1.17
2:P:84:VAL:HG23	13:P:301:PTY:C44	1.77	1.14
7:O:127:CYS:SG	18:O:401:HEC:HBC3	1.87	1.14
2:P:84:VAL:CG2	13:P:301:PTY:C44	2.31	1.08
2:P:84:VAL:HG22	13:P:301:PTY:H441	1.24	1.08
7:D:127:CYS:SG	18:D:401:HEC:CAC	2.41	1.08
7:D:127:CYS:SG	18:D:401:HEC:CBC	2.40	1.08
2:P:84:VAL:HG23	13:P:301:PTY:H441	1.16	1.08
7:O:127:CYS:SG	18:O:401:HEC:CAC	2.41	1.07
7:O:127:CYS:SG	18:O:401:HEC:CBC	2.42	1.07
5:A:395:LEU:HD23	6:B:34:ILE:HD12	1.34	1.06
7:D:124:CYS:SG	18:D:401:HEC:CAB	2.45	1.05
7:O:124:CYS:SG	18:O:401:HEC:CAB	2.46	1.04
10:U:11:LYS:HG2	10:U:12:PRO:HD2	1.53	0.90
5:A:156:GLU:OE2	5:A:188:ARG:NH1	2.06	0.89
6:M:91:GLU:HG2	6:M:364:MET:HE1	1.54	0.88
14:A:3001:CDL:OB9	14:A:3001:CDL:HB4	1.77	0.84
1:C:58:ALA:H	1:C:173:ASN:HD22	1.26	0.83
5:A:395:LEU:CD2	6:B:34:ILE:HD12	2.13	0.77
3:R:17:SER:HB2	3:R:20:LEU:HB2	1.66	0.77
5:A:395:LEU:HD23	6:B:34:ILE:CD1	2.13	0.75
3:G:17:SER:HB2	3:G:20:LEU:HB2	1.66	0.75
1:C:180:PHE:HE2	1:N:180:PHE:HE2	1.36	0.73
2:P:84:VAL:HG23	13:P:301:PTY:C43	2.18	0.72
2:P:84:VAL:HG22	13:P:301:PTY:C44	2.09	0.72
1:C:195:LEU:HD22	15:C:506:LMT:H102	1.73	0.69
11:C:501:HEM:HBC2	11:C:501:HEM:HHD	1.74	0.69
11:N:501:HEM:HBC2	11:N:501:HEM:HHD	1.75	0.68
2:P:84:VAL:CG2	13:P:301:PTY:C43	2.72	0.67
14:H:702:CDL:C72	14:H:702:CDL:HB61	2.26	0.66
14:H:702:CDL:C72	14:H:702:CDL:CB6	2.75	0.65
15:N:506:LMT:H62	16:N:507:AWB:H3	1.78	0.65
14:S:702:CDL:C72	14:S:702:CDL:CB6	2.75	0.64
5:A:96:ILE:HD13	6:B:269:MET:HG2	1.80	0.64
14:S:702:CDL:C72	14:S:702:CDL:HB61	2.28	0.63
1:C:58:ALA:H	1:C:173:ASN:ND2	1.95	0.63
11:C:501:HEM:HBC2	11:C:501:HEM:CHD	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:262:PHE:HB2	6:B:340:ALA:HB2	1.82	0.60
4:F:135:ASN:HB3	7:D:95:ALA:HB2	1.83	0.60
3:G:55:MET:HE1	3:G:102:LEU:HD21	1.82	0.60
1:C:3:LEU:HD11	14:N:505:CDL:HB32	1.83	0.60
1:C:226:SER:HB3	13:C:504:PTY:H331	1.83	0.60
14:C:505:CDL:HB32	1:N:3:LEU:HD11	1.84	0.59
13:C:504:PTY:HC12	13:C:504:PTY:H112	1.86	0.58
1:N:330:ILE:HD12	12:N:503:PC1:H2A1	1.85	0.57
4:Q:135:ASN:HB3	7:O:95:ALA:HB2	1.85	0.57
7:D:127:CYS:SG	18:D:401:HEC:C3C	2.93	0.57
7:O:127:CYS:SG	18:O:401:HEC:C3C	2.91	0.57
6:M:316:GLN:HE21	6:M:320:LYS:HE2	1.70	0.57
11:N:501:HEM:HBC2	11:N:501:HEM:CHD	2.30	0.56
1:C:330:ILE:HD12	12:C:503:PC1:H2A1	1.87	0.56
6:M:36:ASP:OD1	6:M:98:GLN:HG3	2.03	0.56
8:S:51:ARG:HH21	14:S:701:CDL:HA21	1.70	0.56
5:A:378:SER:HA	5:A:432:GLU:OE1	2.07	0.55
1:C:230:LEU:HD11	13:C:504:PTY:H332	1.89	0.55
3:R:55:MET:HE1	3:R:102:LEU:HD21	1.89	0.54
7:D:124:CYS:SG	18:D:401:HEC:C3B	2.95	0.54
16:N:507:AWB:O3	16:N:507:AWB:H4A	2.07	0.54
1:N:139:MET:HE1	1:N:269:ILE:HA	1.90	0.53
6:M:41:LEU:CD2	6:M:191:VAL:HG22	2.38	0.53
6:B:41:LEU:CD2	6:B:191:VAL:HG22	2.38	0.53
15:C:506:LMT:H72	16:C:507:AWB:H2A	1.91	0.52
5:A:43:SER:CB	5:A:222:HIS:HD2	2.22	0.52
6:M:262:PHE:HB2	6:M:340:ALA:HB2	1.90	0.52
9:T:19:VAL:HG22	12:T:201:PC1:H332	1.91	0.52
13:C:504:PTY:H132	2:E:72:PHE:CE2	2.44	0.52
14:A:3001:CDL:H1	14:A:3002:CDL:HA4	1.91	0.51
1:N:229:ASP:HB2	13:N:504:PTY:H382	1.92	0.51
5:A:43:SER:HB3	5:A:222:HIS:HD2	1.75	0.50
1:N:226:SER:HB3	13:N:504:PTY:H331	1.92	0.50
8:H:51:ARG:HH21	14:H:701:CDL:HA22	1.76	0.50
7:O:124:CYS:SG	18:O:401:HEC:C3B	2.98	0.50
5:L:78:HIS:HA	6:M:271:TRP:CD1	2.47	0.50
2:P:84:VAL:HG23	13:P:301:PTY:H431	1.94	0.50
11:C:501:HEM:HHD	11:C:501:HEM:CBC	2.42	0.49
6:B:102:GLN:H	6:B:102:GLN:HG3	1.38	0.48
4:Q:124:VAL:HG11	7:O:88:ALA:HB2	1.94	0.48
5:A:382:VAL:HG21	5:A:432:GLU:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:402:PTY:H132	13:D:402:PTY:H161	1.50	0.48
13:P:301:PTY:H311	13:P:301:PTY:H141	1.96	0.48
5:A:395:LEU:HD22	6:B:98:GLN:HG2	1.95	0.48
17:L:3003:XP4:H8	10:U:35:PHE:HE1	1.78	0.48
13:N:504:PTY:H111	12:T:201:PC1:O31	2.14	0.48
4:F:124:VAL:HG11	7:D:88:ALA:HB2	1.95	0.48
6:M:59:LYS:HB3	6:M:129:VAL:HG13	1.94	0.47
6:M:345:LYS:HE2	6:M:345:LYS:HB3	1.56	0.47
1:N:184:TYR:CD2	11:N:501:HEM:HBC1	2.50	0.47
11:N:501:HEM:HHD	11:N:501:HEM:CBC	2.42	0.47
9:I:22:ILE:HG21	12:I:201:PC1:H331	1.95	0.47
11:C:502:HEM:HMC2	11:C:502:HEM:HBC2	1.97	0.47
8:H:56:ALA:HA	14:H:701:CDL:H132	1.96	0.47
5:L:382:VAL:HG21	5:L:432:GLU:HA	1.96	0.47
6:B:41:LEU:HD23	6:B:191:VAL:HG22	1.97	0.47
6:B:84:LEU:HD12	6:B:97:THR:HG22	1.97	0.46
11:N:502:HEM:HBC2	11:N:502:HEM:HMC2	1.98	0.46
13:C:504:PTY:H132	2:E:72:PHE:HE2	1.80	0.46
15:C:506:LMT:H31	15:C:506:LMT:H61	1.39	0.46
13:D:402:PTY:H352	13:D:402:PTY:H381	1.34	0.46
6:B:24:LYS:HB3	6:B:366:LEU:HD22	1.96	0.46
10:J:11:LYS:HD2	10:J:12:PRO:HD2	1.98	0.46
5:L:119:PHE:HE1	6:M:349:ALA:HB2	1.81	0.46
1:C:190:LEU:HD21	11:C:502:HEM:HBB1	1.98	0.46
12:I:201:PC1:H322	12:I:201:PC1:H351	1.57	0.46
6:M:282:THR:HG22	6:M:289:VAL:HG23	1.98	0.46
13:N:504:PTY:H372	13:N:504:PTY:H402	1.70	0.46
6:M:41:LEU:HD23	6:M:191:VAL:HG22	1.97	0.45
13:N:504:PTY:H342	13:N:504:PTY:H311	1.34	0.45
6:M:281:ALA:HB1	6:M:320:LYS:HB2	1.98	0.45
13:N:504:PTY:H331	13:N:504:PTY:H362	1.42	0.45
5:L:155:LEU:HD23	5:L:155:LEU:HA	1.81	0.45
6:M:53:VAL:HG12	6:M:173:VAL:HG13	1.98	0.45
13:P:301:PTY:H132	13:P:301:PTY:H161	1.68	0.45
5:A:78:HIS:HA	6:B:271:TRP:CD1	2.52	0.45
17:A:3003:XP4:H8	10:J:35:PHE:HE1	1.82	0.45
1:C:184:TYR:CD2	11:C:501:HEM:HBC1	2.52	0.45
5:L:156:GLU:H	5:L:156:GLU:HG3	1.62	0.45
14:S:701:CDL:OB3	14:S:702:CDL:O1	2.34	0.45
7:O:248:MET:HB2	18:O:401:HEC:C1D	2.47	0.45
8:S:56:ALA:HA	14:S:701:CDL:H132	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:TRP:CZ3	7:D:289:ARG:HG3	2.51	0.44
14:A:3002:CDL:H132	14:A:3002:CDL:H522	1.98	0.44
1:N:76:TRP:CZ3	7:O:289:ARG:HG3	2.52	0.44
5:L:160:LYS:HA	5:L:160:LYS:HD2	1.53	0.44
5:L:161:GLN:H	5:L:161:GLN:HG2	1.53	0.44
18:D:401:HEC:HAB	18:D:401:HEC:HHC	1.78	0.44
7:D:248:MET:HB2	18:D:401:HEC:C1D	2.47	0.44
6:M:246:ALA:HB1	6:M:301:LEU:HD11	2.00	0.44
10:U:29:SER:HA	10:U:32:ILE:HG12	2.00	0.44
16:N:507:AWB:H18	16:N:507:AWB:H21	1.78	0.44
1:N:27:ASN:HB2	14:S:701:CDL:OB4	2.18	0.43
14:H:702:CDL:H311	14:H:702:CDL:HA62	1.55	0.43
5:L:380:LEU:H	5:L:380:LEU:HG	1.62	0.43
7:O:251:THR:HG21	18:O:401:HEC:HMC1	2.00	0.43
1:N:178:ARG:HE	1:N:178:ARG:HB3	1.70	0.43
5:L:138:LYS:HB2	5:L:138:LYS:HE2	1.65	0.43
7:D:145:THR:O	7:D:149:LYS:HG3	2.19	0.42
3:R:52:THR:HG22	3:R:54:ASN:H	1.84	0.42
14:L:3001:CDL:H1	14:L:3002:CDL:HA4	2.01	0.42
16:N:507:AWB:O6	16:N:507:AWB:N	2.52	0.42
5:A:96:ILE:HG12	5:A:103:LEU:HD13	2.01	0.42
1:N:156:TRP:CE3	1:N:157:LEU:HG	2.53	0.42
7:O:251:THR:HG21	18:O:401:HEC:CMC	2.50	0.42
1:C:227:PHE:CZ	13:C:504:PTY:H322	2.55	0.42
6:B:247:LEU:HD13	6:B:393:LEU:HB3	2.00	0.42
1:C:178:ARG:HE	1:C:178:ARG:HB3	1.63	0.42
1:N:227:PHE:HZ	13:N:504:PTY:HC6	1.85	0.42
11:C:501:HEM:CHD	11:C:501:HEM:CBC	2.98	0.42
7:O:134:ALA:HA	7:O:177:TYR:HA	2.02	0.42
7:D:134:ALA:HA	7:D:177:TYR:HA	2.02	0.41
6:M:316:GLN:HE21	6:M:320:LYS:CE	2.30	0.41
7:D:312:LYS:HE3	14:H:702:CDL:H112	2.01	0.41
13:P:301:PTY:H352	13:P:301:PTY:H381	1.75	0.41
5:L:82:LYS:HA	5:L:89:GLN:HG3	2.02	0.41
6:B:263:LEU:HA	6:B:277:PRO:HG2	2.01	0.41
1:C:27:ASN:HB2	14:H:701:CDL:HB22	2.02	0.41
5:L:260:ILE:HA	5:L:261:PRO:HD3	1.96	0.41
6:M:263:LEU:HD23	6:M:263:LEU:HA	1.91	0.41
15:C:506:LMT:H52	15:C:506:LMT:H81	1.80	0.41
6:M:228:LEU:HG	6:M:248:PRO:HB2	2.03	0.41
12:C:503:PC1:O32	8:H:55:GLN:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:HIS:HA	1:C:173:ASN:HD21	1.87	0.40
6:B:47:TYR:HB3	6:B:220:VAL:CG1	2.50	0.40
6:B:249:ILE:HD11	6:B:302:PHE:HB2	2.04	0.40
5:L:99:MET:HE2	5:L:99:MET:HB2	1.76	0.40
10:U:30:LYS:HA	10:U:30:LYS:HD3	1.94	0.40
16:C:507:AWB:O6	16:C:507:AWB:N	2.51	0.40
7:D:251:THR:HG21	18:D:401:HEC:CMC	2.52	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%)	373 (98%)	8 (2%)	0	100	100
1	N	381/385 (99%)	373 (98%)	8 (2%)	0	100	100
2	E	61/225 (27%)	59 (97%)	2 (3%)	0	100	100
2	P	61/225 (27%)	59 (97%)	2 (3%)	0	100	100
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%)	425 (98%)	9 (2%)	0	100	100
5	L	434/474 (92%)	423 (98%)	11 (2%)	0	100	100
6	B	400/417 (96%)	388 (97%)	11 (3%)	1 (0%)	36	36
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	83/93 (89%)	82 (99%)	1 (1%)	0	100	100
8	S	83/93 (89%)	82 (99%)	1 (1%)	0	100	100
9	I	52/69 (75%)	51 (98%)	1 (2%)	0	100	100
9	T	52/69 (75%)	51 (98%)	1 (2%)	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	3834/4680 (82%)	3748 (98%)	85 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	368	SER

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	331/333 (99%)	326 (98%)	5 (2%)	57	65
1	N	331/333 (99%)	325 (98%)	6 (2%)	51	60
2	E	50/182 (28%)	47 (94%)	3 (6%)	17	15
2	P	50/182 (28%)	49 (98%)	1 (2%)	48	56
3	G	113/117 (97%)	104 (92%)	9 (8%)	11	8
3	R	113/117 (97%)	109 (96%)	4 (4%)	32	35
4	F	61/123 (50%)	58 (95%)	3 (5%)	22	22
4	Q	61/123 (50%)	60 (98%)	1 (2%)	55	64
5	A	377/407 (93%)	366 (97%)	11 (3%)	37	42
5	L	377/407 (93%)	344 (91%)	33 (9%)	9	7
6	B	311/322 (97%)	277 (89%)	34 (11%)	6	4
6	M	311/322 (97%)	282 (91%)	29 (9%)	8	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	D	192/268 (72%)	192 (100%)	0	100	100
7	O	192/268 (72%)	192 (100%)	0	100	100
8	H	67/71 (94%)	66 (98%)	1 (2%)	57	65
8	S	67/71 (94%)	66 (98%)	1 (2%)	57	65
9	I	46/57 (81%)	46 (100%)	0	100	100
9	T	46/57 (81%)	46 (100%)	0	100	100
10	J	63/68 (93%)	62 (98%)	1 (2%)	55	64
10	U	63/68 (93%)	63 (100%)	0	100	100
All	All	3222/3896 (83%)	3080 (96%)	142 (4%)	27	26

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	157	LEU
1	C	178	ARG
1	C	197	HIS
1	C	288	LYS
1	C	324	LEU
2	P	62	ARG
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	50	GLU
3	G	112	GLU
3	G	123	GLU
4	F	92	HIS
4	F	96	HIS
4	F	100	GLU
5	A	79	LEU
5	A	82	LYS
5	A	87	ARG
5	A	94	LEU
5	A	97	GLU
5	A	103	LEU
5	A	137	SER
5	A	197	THR

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Mol	Chain	Res	Type
5	A	230	GLU
5	A	267	GLU
5	A	397	LEU
6	B	19	GLU
6	B	45	SER
6	B	58	GLU
6	B	60	PHE
6	B	79	LEU
6	B	102	GLN
6	B	168	GLN
6	B	180	GLU
6	B	215	GLN
6	B	225	THR
6	B	226	THR
6	B	228	LEU
6	B	232	GLU
6	B	236	ARG
6	B	238	SER
6	B	239	THR
6	B	247	LEU
6	B	249	ILE
6	B	269	MET
6	B	273	VAL
6	B	276	SER
6	B	282	THR
6	B	288	SER
6	B	292	THR
6	B	307	LYS
6	B	309	ASP
6	B	332	VAL
6	B	345	LYS
6	B	376	GLU
6	B	387	SER
6	B	388	GLU
6	B	396	SER
6	B	401	VAL
6	B	414	ASP
8	H	51	ARG
10	J	11	LYS
1	N	178	ARG
1	N	197	HIS
1	N	255	ASP

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Mol	Chain	Res	Type
1	N	270	VAL
1	N	288	LYS
1	N	324	LEU
2	E	54	LYS
2	E	55	ASP
2	E	65	SER
3	R	17	SER
3	R	19	LEU
3	R	22	LYS
3	R	23	ILE
4	Q	100	GLU
5	L	29	LYS
5	L	44	GLU
5	L	51	THR
5	L	54	VAL
5	L	77	GLU
5	L	82	LYS
5	L	86	LYS
5	L	87	ARG
5	L	103	LEU
5	L	121	ASP
5	L	125	LYS
5	L	137	SER
5	L	138	LYS
5	L	141	GLU
5	L	146	ARG
5	L	149	GLU
5	L	155	LEU
5	L	156	GLU
5	L	157	GLU
5	L	159	ASN
5	L	160	LYS
5	L	161	GLN
5	L	185	LEU
5	L	351	LEU
5	L	374	SER
5	L	378	SER
5	L	380	LEU
5	L	395	LEU
5	L	397	LEU
5	L	400	THR
5	L	411	LEU

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Mol	Chain	Res	Type
5	L	433	HIS
5	L	441	LYS
6	M	16	SER
6	M	19	GLU
6	M	32	SER
6	M	58	GLU
6	M	60	PHE
6	M	101	LYS
6	M	215	GLN
6	M	225	THR
6	M	232	GLU
6	M	236	ARG
6	M	245	ILE
6	M	247	LEU
6	M	253	LYS
6	M	269	MET
6	M	272	SER
6	M	273	VAL
6	M	276	SER
6	M	282	THR
6	M	288	SER
6	M	290	LYS
6	M	292	THR
6	M	298	ASP
6	M	307	LYS
6	M	309	ASP
6	M	332	VAL
6	M	333	THR
6	M	356	ASP
6	M	362	ILE
6	M	376	GLU
8	S	51	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	173	ASN
1	C	202	HIS
2	P	90	ASN
3	G	84	HIS
4	F	92	HIS
4	F	109	GLN

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Mol	Chain	Res	Type
4	F	132	HIS
5	A	74	HIS
5	A	159	ASN
5	A	222	HIS
5	A	410	GLN
6	B	63	GLN
6	B	87	HIS
6	B	122	GLN
6	B	184	GLN
6	B	189	GLN
6	B	215	GLN
6	B	229	HIS
6	B	257	HIS
6	B	408	HIS
7	D	193	GLN
7	D	208	HIS
9	I	49	GLN
10	J	70	HIS
1	N	202	HIS
2	E	90	ASN
3	R	84	HIS
4	Q	96	HIS
4	Q	109	GLN
5	L	50	GLN
5	L	410	GLN
6	M	63	GLN
6	M	122	GLN
6	M	184	GLN
6	M	215	GLN
6	M	229	HIS
6	M	316	GLN
6	M	408	HIS
7	O	193	GLN
7	O	208	HIS
9	T	49	GLN
10	U	70	HIS

5.3.3 RNA

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](#)

32 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
11	HEM	N	501	1	50,50,50	1.53	8 (16%)	67,82,82	1.96	17 (25%)
11	HEM	C	501	1	50,50,50	1.54	7 (14%)	67,82,82	1.93	18 (26%)
14	CDL	S	702	-	38,38,99	0.42	0	44,50,111	1.16	3 (6%)
15	LMT	C	506	-	36,36,36	0.49	0	47,47,47	1.03	5 (10%)
14	CDL	L	3002	-	46,46,99	0.34	0	51,56,111	0.84	3 (5%)
14	CDL	H	702	-	38,38,99	0.41	0	44,50,111	1.17	5 (11%)
15	LMT	J	101	-	36,36,36	0.51	0	47,47,47	1.48	5 (10%)
16	AWB	N	507	-	40,40,40	2.20	14 (35%)	34,54,54	3.13	13 (38%)
18	HEC	O	401	7	46,50,50	2.46	22 (47%)	58,82,82	2.37	25 (43%)
12	PC1	N	503	-	37,37,53	0.72	1 (2%)	43,45,61	1.01	4 (9%)
15	LMT	U	101	-	36,36,36	0.44	0	47,47,47	1.11	5 (10%)
14	CDL	C	505	-	47,47,99	0.41	0	53,59,111	0.81	2 (3%)
13	PTY	N	504	-	40,40,49	0.34	0	43,45,54	0.72	1 (2%)
12	PC1	I	201	-	31,31,53	0.38	0	37,39,61	0.73	0
14	CDL	H	701	-	49,49,99	0.36	0	55,61,111	0.81	1 (1%)
14	CDL	N	505	-	47,47,99	0.41	0	53,59,111	0.79	2 (3%)
11	HEM	N	502	1	50,50,50	1.62	8 (16%)	67,82,82	2.19	20 (29%)
14	CDL	S	701	-	49,49,99	0.37	0	55,61,111	0.80	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	XP4	L	3003	-	23,23,39	1.39	2 (8%)	26,28,44	1.98	6 (23%)
12	PC1	T	201	-	31,31,53	0.35	0	37,39,61	0.59	0
18	HEC	D	401	7	46,50,50	2.49	22 (47%)	58,82,82	2.43	27 (46%)
12	PC1	C	503	-	37,37,53	0.72	1 (2%)	43,45,61	1.11	4 (9%)
17	XP4	A	3003	-	23,23,39	1.34	2 (8%)	26,28,44	2.17	6 (23%)
14	CDL	A	3001	-	41,41,99	0.44	0	45,51,111	0.70	1 (2%)
11	HEM	C	502	1	50,50,50	1.59	7 (14%)	67,82,82	2.15	18 (26%)
15	LMT	N	506	-	36,36,36	0.55	0	47,47,47	0.91	2 (4%)
13	PTY	C	504	-	40,40,49	0.36	0	43,45,54	0.81	2 (4%)
13	PTY	P	301	-	40,40,49	0.45	0	43,45,54	0.61	0
14	CDL	A	3002	-	46,46,99	0.35	0	51,56,111	0.81	3 (5%)
14	CDL	L	3001	-	41,41,99	0.42	0	45,51,111	1.02	3 (6%)
13	PTY	D	402	-	40,40,49	0.45	0	43,45,54	0.48	0
16	AWB	C	507	-	40,40,40	2.26	12 (30%)	34,54,54	2.66	9 (26%)

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
11	HEM	N	501	1	-	4/14/54/54	-
11	HEM	C	501	1	-	4/14/54/54	-
14	CDL	S	702	-	-	25/48/48/110	-
15	LMT	C	506	-	-	14/21/61/61	0/2/2/2
14	CDL	L	3002	-	-	28/54/54/110	-
14	CDL	H	702	-	-	26/48/48/110	-
15	LMT	J	101	-	-	10/21/61/61	0/2/2/2
16	AWB	N	507	-	-	11/38/53/53	0/1/2/2
18	HEC	O	401	7	-	4/14/54/54	-
12	PC1	N	503	-	-	10/41/41/57	-
15	LMT	U	101	-	-	7/21/61/61	0/2/2/2
14	CDL	C	505	-	-	28/57/57/110	-
13	PTY	N	504	-	-	30/44/44/53	-
12	PC1	I	201	-	-	16/35/35/57	-
14	CDL	H	701	-	-	28/59/59/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CDL	N	505	-	-	29/57/57/110	-
11	HEM	N	502	1	-	4/14/54/54	-
14	CDL	S	701	-	-	33/59/59/110	-
17	XP4	L	3003	-	-	0/24/24/41	-
12	PC1	T	201	-	-	10/35/35/57	-
18	HEC	D	401	7	-	3/14/54/54	-
12	PC1	C	503	-	-	10/41/41/57	-
17	XP4	A	3003	-	-	1/24/24/41	-
14	CDL	A	3001	-	-	13/48/48/110	-
11	HEM	C	502	1	-	4/14/54/54	-
15	LMT	N	506	-	-	17/21/61/61	0/2/2/2
13	PTY	C	504	-	-	31/44/44/53	-
13	PTY	P	301	-	-	22/44/44/53	-
14	CDL	A	3002	-	-	26/54/54/110	-
14	CDL	L	3001	-	-	21/48/48/110	-
13	PTY	D	402	-	-	24/44/44/53	-
16	AWB	C	507	-	-	6/38/53/53	0/1/2/2

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	507	AWB	C21-N1	7.76	1.44	1.34
16	N	507	AWB	C21-N1	5.76	1.42	1.34
11	C	502	HEM	FE-NB	5.67	2.12	1.94
11	C	501	HEM	FE-NB	5.64	2.12	1.94
11	N	501	HEM	FE-NB	5.53	2.11	1.94
18	D	401	HEC	C4B-NB	-5.23	1.29	1.39
18	O	401	HEC	C4B-NB	-5.18	1.29	1.39
17	L	3003	XP4	O7-C18	5.06	1.46	1.35
16	N	507	AWB	O7-C23	4.90	1.48	1.34
11	N	502	HEM	FE-NB	4.85	2.09	1.94
17	A	3003	XP4	O7-C18	4.81	1.45	1.35
18	D	401	HEC	CHD-C4C	4.59	1.47	1.38
16	N	507	AWB	O-C8	-4.52	1.39	1.46
16	C	507	AWB	O7-C23	4.46	1.46	1.34
16	C	507	AWB	C14-N	4.44	1.44	1.34
18	D	401	HEC	C1B-NB	-4.32	1.31	1.39
16	C	507	AWB	O-C8	-4.31	1.40	1.46
18	O	401	HEC	CHD-C4C	4.28	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	401	HEC	CHA-C1A	4.27	1.46	1.38
18	O	401	HEC	CHA-C1A	4.17	1.46	1.38
18	O	401	HEC	C1B-NB	-4.16	1.31	1.39
18	D	401	HEC	C1A-NA	-4.12	1.31	1.39
18	D	401	HEC	C2A-C3A	4.11	1.45	1.36
18	O	401	HEC	C2A-C3A	4.11	1.45	1.36
16	C	507	AWB	O2-C11	-4.07	1.40	1.46
18	O	401	HEC	C4D-ND	-4.03	1.32	1.39
11	C	501	HEM	FE-NC	4.01	2.08	1.95
18	D	401	HEC	C4A-NA	-4.01	1.32	1.39
11	N	501	HEM	FE-NC	4.01	2.08	1.95
16	N	507	AWB	C14-N	4.00	1.43	1.34
11	N	502	HEM	C1B-NB	-3.97	1.33	1.40
11	C	502	HEM	C1B-NB	-3.95	1.33	1.40
16	N	507	AWB	O2-C11	-3.94	1.40	1.46
18	O	401	HEC	C4A-NA	-3.88	1.32	1.39
16	C	507	AWB	C17-N1	3.84	1.47	1.41
18	O	401	HEC	C1A-NA	-3.79	1.32	1.39
18	D	401	HEC	C4D-ND	-3.74	1.32	1.39
18	O	401	HEC	CHB-C4A	3.71	1.45	1.38
11	C	502	HEM	FE-NC	3.61	2.07	1.95
18	D	401	HEC	C4C-NC	-3.60	1.32	1.39
18	O	401	HEC	C4C-NC	-3.59	1.32	1.39
18	D	401	HEC	CAC-C3C	3.56	1.46	1.35
18	O	401	HEC	CAC-C3C	3.54	1.46	1.35
16	N	507	AWB	C20-C15	-3.53	1.34	1.39
16	N	507	AWB	C15-C16	-3.48	1.35	1.41
18	D	401	HEC	CHB-C4A	3.42	1.45	1.38
18	D	401	HEC	CHA-C4D	3.36	1.47	1.39
18	O	401	HEC	CHA-C4D	3.26	1.46	1.39
16	C	507	AWB	C24-C23	3.09	1.56	1.50
17	A	3003	XP4	O5-C4	3.09	1.42	1.33
17	L	3003	XP4	O5-C4	3.07	1.42	1.33
16	N	507	AWB	C17-C16	-3.07	1.35	1.40
11	N	502	HEM	FE-NC	3.07	2.05	1.95
16	N	507	AWB	O5-C21	-2.98	1.10	1.22
11	C	501	HEM	C1B-NB	-2.97	1.35	1.40
18	D	401	HEC	CAB-C3B	2.96	1.44	1.35
18	O	401	HEC	CHC-C4B	2.95	1.44	1.38
11	N	502	HEM	C4B-NB	-2.94	1.33	1.38
18	O	401	HEC	CAB-C3B	2.88	1.44	1.35
11	N	502	HEM	C4D-ND	-2.87	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	N	501	HEM	C1B-NB	-2.87	1.35	1.40
11	C	502	HEM	C4B-NB	-2.78	1.33	1.38
11	C	502	HEM	C4D-ND	-2.73	1.35	1.40
18	O	401	HEC	CHC-C1C	2.72	1.45	1.39
18	D	401	HEC	C3B-C4B	-2.71	1.41	1.46
18	D	401	HEC	CHC-C4B	2.71	1.43	1.38
18	O	401	HEC	C1D-ND	-2.62	1.34	1.39
18	D	401	HEC	C1D-ND	-2.61	1.34	1.39
11	C	502	HEM	C3C-C4C	-2.59	1.41	1.46
18	O	401	HEC	C3B-C4B	-2.59	1.41	1.46
18	D	401	HEC	C1C-NC	-2.58	1.34	1.39
18	O	401	HEC	C1C-NC	-2.58	1.34	1.39
11	N	501	HEM	O2D-CGD	-2.54	1.22	1.30
18	O	401	HEC	C3D-C2D	2.53	1.45	1.38
18	D	401	HEC	C3D-C2D	2.51	1.45	1.38
18	D	401	HEC	CHC-C1C	2.50	1.45	1.39
11	N	502	HEM	C3C-C4C	-2.50	1.41	1.46
16	C	507	AWB	O7-C7	-2.45	1.41	1.44
11	C	501	HEM	C4B-NB	-2.43	1.34	1.38
16	N	507	AWB	C24-C23	2.37	1.55	1.50
18	D	401	HEC	CHD-C1D	2.34	1.44	1.39
11	C	501	HEM	O2D-CGD	-2.33	1.23	1.30
11	N	501	HEM	C4D-ND	-2.32	1.36	1.40
11	N	501	HEM	C4B-NB	-2.31	1.34	1.38
18	O	401	HEC	CHB-C1B	2.28	1.44	1.39
11	N	502	HEM	C1C-C2C	-2.25	1.40	1.45
16	C	507	AWB	C17-C16	-2.25	1.36	1.40
11	N	501	HEM	C1C-C2C	-2.23	1.40	1.45
11	C	501	HEM	C1C-C2C	-2.23	1.40	1.45
11	C	501	HEM	C4D-ND	-2.16	1.36	1.40
16	C	507	AWB	O5-C21	-2.16	1.13	1.22
16	C	507	AWB	O-C9	2.14	1.39	1.34
12	C	503	PC1	C22-C21	2.12	1.56	1.50
18	O	401	HEC	O2A-CGA	-2.11	1.23	1.30
16	N	507	AWB	O4-C14	-2.11	1.18	1.23
16	C	507	AWB	O4-C14	-2.11	1.18	1.23
12	N	503	PC1	C22-C21	2.11	1.56	1.50
11	N	501	HEM	C1C-NC	-2.10	1.35	1.39
11	C	502	HEM	C1C-C2C	-2.10	1.41	1.45
16	N	507	AWB	C19-C18	2.09	1.42	1.38
18	D	401	HEC	CHB-C1B	2.08	1.44	1.39
11	N	502	HEM	FE-ND	-2.08	1.88	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	401	HEC	O2A-CGA	-2.07	1.24	1.30
18	O	401	HEC	CHD-C1D	2.05	1.44	1.39
16	N	507	AWB	O7-C7	-2.04	1.41	1.44
16	N	507	AWB	O-C9	2.03	1.38	1.34

All (211) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	N	507	AWB	C17-N1-C21	-8.84	109.17	126.87
16	N	507	AWB	O-C9-O1	-8.30	113.80	124.10
16	C	507	AWB	O5-C21-N1	-8.05	114.68	125.72
17	A	3003	XP4	O7-C18-C19	7.41	124.31	111.09
11	C	502	HEM	CHD-C4C-NC	7.03	132.11	124.45
11	N	502	HEM	CHD-C4C-NC	6.89	131.95	124.45
17	L	3003	XP4	O7-C18-C19	6.78	123.17	111.09
16	N	507	AWB	O2-C12-O3	-6.56	115.96	124.10
16	N	507	AWB	O5-C21-N1	-6.49	116.82	125.72
15	J	101	LMT	C1-O1'-C1'	-6.32	102.89	113.68
16	C	507	AWB	C17-N1-C21	-6.10	114.65	126.87
16	C	507	AWB	O-C9-O1	-5.92	116.76	124.10
18	D	401	HEC	C2A-C1A-NA	5.54	115.67	110.32
11	N	502	HEM	CHA-C4D-ND	5.29	130.91	124.37
11	N	501	HEM	CHC-C4B-NB	5.11	129.92	124.42
11	C	502	HEM	CHA-C4D-ND	5.07	130.64	124.37
18	O	401	HEC	CAA-CBA-CGA	-5.06	100.25	113.67
11	C	502	HEM	CHC-C4B-NB	5.04	129.85	124.42
18	D	401	HEC	C2B-C1B-NB	5.03	118.21	110.14
16	C	507	AWB	O2-C12-O3	-4.98	117.93	124.10
16	N	507	AWB	C10-N-C14	-4.95	111.53	121.53
17	A	3003	XP4	O7-C18-O8	-4.95	113.44	122.99
11	N	502	HEM	CHC-C4B-NB	4.94	129.74	124.42
18	D	401	HEC	CAA-CBA-CGA	-4.86	100.77	113.67
18	O	401	HEC	C1D-C2D-C3D	-4.82	101.29	106.82
11	N	502	HEM	CHD-C1D-ND	4.74	129.53	124.42
11	C	501	HEM	CHC-C4B-NB	4.72	129.50	124.42
16	N	507	AWB	O-C9-C10	4.66	117.61	110.28
18	O	401	HEC	C2B-C1B-NB	4.61	117.54	110.14
11	C	502	HEM	CHD-C1D-ND	4.61	129.38	124.42
14	L	3001	CDL	OB6-CB4-CB3	-4.58	93.87	109.70
18	O	401	HEC	C2A-C1A-NA	4.55	114.72	110.32
11	N	501	HEM	C1B-NB-C4B	4.46	110.49	105.21
11	C	501	HEM	CHD-C1D-ND	4.46	129.22	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	J	101	LMT	O5'-C1'-O1'	-4.43	99.56	110.04
18	D	401	HEC	CBC-CAC-C3C	-4.40	118.65	127.43
18	D	401	HEC	C1D-C2D-C3D	-4.38	101.80	106.82
17	L	3003	XP4	O7-C18-O8	-4.37	114.55	122.99
11	N	502	HEM	C4C-CHD-C1D	-4.33	116.81	126.02
11	N	501	HEM	CHD-C1D-ND	4.25	129.00	124.42
11	C	502	HEM	O2A-CGA-O1A	-4.20	112.52	123.33
11	N	502	HEM	O2A-CGA-O1A	-4.18	112.59	123.33
18	O	401	HEC	CBC-CAC-C3C	-4.15	119.15	127.43
16	C	507	AWB	C10-N-C14	-4.09	113.26	121.53
18	D	401	HEC	CHD-C4C-NC	4.04	128.85	124.45
11	C	502	HEM	C4C-CHD-C1D	-4.00	117.51	126.02
11	C	501	HEM	C1B-NB-C4B	3.97	109.90	105.21
11	C	502	HEM	C1B-NB-C4B	3.95	109.88	105.21
18	O	401	HEC	C2D-C1D-ND	3.91	116.41	110.14
11	N	501	HEM	CBA-CAA-C2A	-3.89	101.77	112.53
16	C	507	AWB	C18-C17-C16	-3.86	117.25	119.75
11	C	501	HEM	CBA-CAA-C2A	-3.81	102.01	112.53
18	O	401	HEC	C3D-C4D-ND	3.76	114.33	110.15
16	N	507	AWB	C18-C17-C16	3.75	122.17	119.75
12	C	503	PC1	O21-C21-C22	-3.70	103.47	111.48
11	C	501	HEM	CBC-CAC-C3C	-3.69	109.07	127.53
11	N	501	HEM	CBC-CAC-C3C	-3.66	109.23	127.53
12	C	503	PC1	O22-C21-C22	3.59	137.82	123.78
18	D	401	HEC	C1A-C2A-C3A	-3.58	102.40	107.11
16	C	507	AWB	C20-C15-C16	3.53	122.18	118.76
18	O	401	HEC	CMD-C2D-C1D	3.52	130.79	125.42
18	D	401	HEC	CMD-C2D-C1D	3.52	130.78	125.42
18	D	401	HEC	CMB-C2B-C3B	3.47	134.71	126.55
11	N	502	HEM	C1B-NB-C4B	3.44	109.28	105.21
11	N	502	HEM	CHD-C1D-C2D	-3.40	119.66	125.03
11	C	502	HEM	C4C-NC-C1C	3.39	111.35	105.82
11	C	501	HEM	CHA-C1A-NA	3.38	130.00	123.86
18	O	401	HEC	C1A-C2A-C3A	-3.34	102.71	107.11
11	C	501	HEM	CHD-C1D-C2D	-3.33	119.76	125.03
18	D	401	HEC	CHD-C4C-C3C	-3.33	119.60	125.21
18	D	401	HEC	C2D-C1D-ND	3.33	115.48	110.14
18	O	401	HEC	CMB-C2B-C3B	3.33	134.38	126.55
11	C	502	HEM	C4C-C3C-C2C	3.33	109.70	106.81
11	N	501	HEM	CHD-C1D-C2D	-3.30	119.81	125.03
16	C	507	AWB	O7-C23-C24	3.30	117.35	111.43
18	O	401	HEC	CBD-CAD-C3D	-3.29	103.44	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	702	CDL	OA5-PA1-OA3	-3.29	95.90	108.94
11	C	502	HEM	CHD-C1D-C2D	-3.24	119.92	125.03
12	N	503	PC1	O22-C21-C22	3.21	136.34	123.78
11	N	502	HEM	C1A-CHA-C4D	-3.21	118.70	126.25
14	H	702	CDL	CB4-OB6-CB5	3.19	123.49	117.85
11	N	501	HEM	C3B-C4B-NB	-3.19	107.18	109.47
18	D	401	HEC	CMC-C2C-C1C	3.17	130.25	125.42
18	D	401	HEC	CHC-C4B-C3B	-3.17	119.87	125.21
11	C	501	HEM	CHA-C4D-ND	3.16	128.27	124.37
11	N	501	HEM	CHA-C1A-NA	3.15	129.57	123.86
18	O	401	HEC	CHB-C1B-C2B	-3.15	118.29	127.43
18	D	401	HEC	C4A-C3A-C2A	-3.14	102.31	106.97
18	O	401	HEC	CHD-C4C-NC	3.14	127.87	124.45
14	S	702	CDL	CB4-OB6-CB5	3.12	123.36	117.85
18	D	401	HEC	CHB-C1B-C2B	-3.10	118.44	127.43
11	N	501	HEM	O2D-CGD-O1D	-3.09	115.38	123.33
11	C	501	HEM	O2D-CGD-O1D	-3.09	115.38	123.33
11	N	501	HEM	CHA-C4D-ND	3.09	128.19	124.37
18	D	401	HEC	CBD-CAD-C3D	-3.06	104.07	112.53
14	S	702	CDL	OA5-PA1-OA3	-3.02	96.97	108.94
11	N	501	HEM	C2A-C1A-NA	-3.00	106.82	110.15
14	L	3002	CDL	OA5-PA1-OA3	-2.99	97.09	108.94
11	C	501	HEM	CAC-C3C-C4C	2.98	131.94	124.82
11	C	501	HEM	C1A-CHA-C4D	-2.98	119.25	126.25
11	C	502	HEM	O2A-CGA-CBA	2.97	123.39	114.00
11	N	501	HEM	CAC-C3C-C4C	2.97	131.91	124.82
11	C	502	HEM	O2D-CGD-CBD	2.96	123.35	114.00
11	C	502	HEM	CBD-CAD-C3D	-2.95	104.37	112.53
11	N	502	HEM	CBD-CAD-C3D	-2.95	104.38	112.53
11	N	502	HEM	O2D-CGD-CBD	2.94	123.27	114.00
17	L	3003	XP4	O5-C4-O6	-2.92	116.32	123.63
11	C	501	HEM	CHC-C1C-NC	2.92	127.63	124.45
11	C	501	HEM	C2A-C1A-NA	-2.92	106.91	110.15
18	D	401	HEC	C3A-C4A-NA	2.91	115.01	109.64
18	O	401	HEC	C4A-C3A-C2A	-2.87	102.72	106.97
15	U	101	LMT	C1-O1'-C1'	-2.86	108.79	113.68
11	N	502	HEM	O2A-CGA-CBA	2.85	123.01	114.00
11	N	501	HEM	C1A-CHA-C4D	-2.83	119.59	126.25
11	C	502	HEM	C1A-CHA-C4D	-2.83	119.59	126.25
17	A	3003	XP4	O4-P1-O2	-2.81	98.84	106.44
11	N	502	HEM	CHA-C4D-C3D	-2.81	120.05	125.23
12	N	503	PC1	O21-C21-C22	-2.79	105.44	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	O	401	HEC	C2C-C1C-NC	2.78	114.60	110.14
11	N	502	HEM	C4C-NC-C1C	2.77	110.34	105.82
16	C	507	AWB	O-C9-C10	2.76	114.63	110.28
14	S	702	CDL	OB6-CB4-CB6	2.74	118.19	108.34
18	D	401	HEC	C3D-C4D-ND	2.70	113.15	110.15
18	O	401	HEC	CHC-C4B-C3B	-2.70	120.66	125.21
18	O	401	HEC	CHD-C4C-C3C	-2.70	120.66	125.21
11	N	501	HEM	CHA-C4D-C3D	-2.69	120.27	125.23
14	H	702	CDL	OB6-CB4-CB6	2.67	117.92	108.34
13	N	504	PTY	O14-P1-O13	-2.67	98.36	108.94
11	C	502	HEM	CHA-C4D-C3D	-2.66	120.32	125.23
18	O	401	HEC	C3A-C4A-NA	2.65	114.54	109.64
11	N	502	HEM	O2D-CGD-O1D	-2.65	116.52	123.33
15	C	506	LMT	C2'-C3'-C4'	2.65	115.69	109.68
14	S	701	CDL	OA6-CA4-CA3	2.64	117.80	108.34
18	O	401	HEC	CHD-C1D-C2D	-2.64	119.78	127.43
11	N	502	HEM	C4C-C3C-C2C	2.63	109.09	106.81
15	U	101	LMT	O5'-C1'-O1'	-2.62	103.85	110.04
11	N	502	HEM	CHB-C1B-NB	2.62	127.61	124.37
14	L	3001	CDL	OB2-PB2-OB3	2.59	119.19	108.94
17	A	3003	XP4	O5-C4-O6	-2.59	117.16	123.63
15	J	101	LMT	C3-C2-C1	-2.57	102.28	113.47
11	C	501	HEM	CHA-C4D-C3D	-2.57	120.49	125.23
15	U	101	LMT	C4-C3-C2	-2.56	101.44	114.37
11	N	501	HEM	CHB-C1B-NB	2.56	127.53	124.37
11	N	501	HEM	CHC-C1C-NC	2.55	127.23	124.45
14	N	505	CDL	OB6-CB4-CB3	2.55	117.50	108.34
14	H	701	CDL	OB6-CB4-CB6	2.55	117.49	108.34
18	D	401	HEC	CHD-C1D-C2D	-2.54	120.06	127.43
18	O	401	HEC	CMC-C2C-C1C	2.53	129.27	125.42
14	C	505	CDL	OB6-CB4-CB3	2.53	117.40	108.34
15	N	506	LMT	C1B-O1B-C4'	-2.52	112.00	117.98
18	O	401	HEC	CHC-C1C-C2C	-2.51	120.14	127.43
14	A	3001	CDL	OB8-CB6-CB4	2.49	117.58	105.85
15	J	101	LMT	C3'-C4'-C5'	2.49	116.45	110.93
15	U	101	LMT	O6'-C6'-C5'	-2.47	102.93	111.33
15	C	506	LMT	C1-O1'-C1'	-2.44	109.51	113.68
18	D	401	HEC	CHA-C1A-C2A	-2.44	121.01	124.86
15	N	506	LMT	C2'-C3'-C4'	2.41	115.15	109.68
18	D	401	HEC	CMA-C3A-C4A	2.41	128.97	124.73
17	A	3003	XP4	O7-C2-C3	-2.41	99.71	108.34
13	C	504	PTY	O11-P1-O13	-2.40	99.42	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	501	HEM	CAC-C3C-C2C	-2.38	120.70	128.43
15	J	101	LMT	O5'-C1'-C2'	2.37	115.24	110.37
14	L	3002	CDL	OA6-CA4-CA6	2.35	116.78	108.34
12	N	503	PC1	O21-C21-O22	-2.35	118.21	123.70
18	D	401	HEC	CHB-C4A-NA	-2.35	121.89	124.45
12	C	503	PC1	C23-C22-C21	2.34	122.28	113.69
11	C	501	HEM	CHB-C1B-NB	2.34	127.26	124.37
18	D	401	HEC	CAD-C3D-C4D	2.34	129.51	124.94
15	U	101	LMT	C4B-C3B-C2B	2.34	114.94	110.83
14	A	3002	CDL	OA2-PA1-OA3	2.33	118.19	108.94
18	D	401	HEC	C2C-C1C-NC	2.33	113.87	110.14
14	L	3002	CDL	OA2-PA1-OA3	2.32	118.12	108.94
17	A	3003	XP4	O5-C3-C2	-2.31	101.73	108.40
15	C	506	LMT	C1'-C2'-C3'	2.28	114.81	110.01
12	N	503	PC1	C23-C22-C21	2.28	122.06	113.69
14	A	3002	CDL	OA5-PA1-OA3	-2.28	99.91	108.94
14	A	3002	CDL	OA6-CA4-CA6	2.28	116.51	108.34
16	N	507	AWB	C20-C15-C16	2.27	120.96	118.76
18	O	401	HEC	CAA-C2A-C1A	2.26	129.44	124.85
14	N	505	CDL	CB4-OB6-CB5	2.25	123.17	117.80
14	C	505	CDL	CB4-OB6-CB5	2.23	123.14	117.80
11	N	502	HEM	CHA-C1A-NA	2.22	127.89	123.86
11	C	501	HEM	C3B-C4B-NB	-2.22	107.87	109.47
16	N	507	AWB	O8-C23-C24	-2.21	119.52	124.65
18	O	401	HEC	CAD-C3D-C4D	2.20	129.25	124.94
11	C	502	HEM	CBA-CAA-C2A	-2.20	106.44	112.53
16	N	507	AWB	C20-C19-C18	-2.19	117.42	120.24
13	C	504	PTY	O12-P1-O11	2.19	117.47	107.57
11	N	502	HEM	CHD-C4C-C3C	-2.18	121.53	125.21
11	C	502	HEM	O1D-CGD-CBD	-2.18	116.19	123.09
11	N	501	HEM	CAC-C3C-C2C	-2.17	121.36	128.43
17	L	3003	XP4	O5-C3-C2	-2.17	102.14	108.40
12	C	503	PC1	O21-C21-O22	-2.14	118.70	123.70
18	O	401	HEC	O2D-CGD-CBD	2.13	120.74	114.00
16	N	507	AWB	O4-C14-N	2.13	126.52	122.47
15	C	506	LMT	O5'-C1'-C2'	2.12	114.72	110.37
18	D	401	HEC	O2D-CGD-CBD	2.11	120.67	114.00
11	C	501	HEM	C4C-NC-C1C	2.11	109.26	105.82
17	L	3003	XP4	O5-C4-C5	2.11	118.26	111.83
17	L	3003	XP4	O7-C2-C3	-2.10	100.80	108.34
18	D	401	HEC	CHC-C1C-C2C	-2.07	121.41	127.43
14	H	702	CDL	OB6-CB5-C51	2.07	114.78	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	502	HEM	CHB-C1B-NB	2.05	126.90	124.37
16	N	507	AWB	O4-C14-C15	-2.04	117.29	121.03
14	L	3001	CDL	OB8-CB6-CB4	2.04	115.45	105.85
18	O	401	HEC	CAD-CBD-CGD	-2.04	108.27	113.67
11	N	502	HEM	CMD-C2D-C1D	2.02	128.20	125.03
14	H	702	CDL	OA2-PA1-OA3	2.02	116.94	108.94
18	D	401	HEC	CBB-CAB-C3B	-2.02	123.40	127.43
15	C	506	LMT	C1B-O1B-C4'	-2.02	113.20	117.98
16	N	507	AWB	O7-C23-C24	2.01	115.03	111.43

There are no chirality outliers.

All (499) 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	C11-O13-P-O14
12	T	201	PC1	C11-O13-P-O11
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	C	504	PTY	C5-O14-P1-O11
13	C	504	PTY	C5-O14-P1-O12
13	P	301	PTY	C5-O14-P1-O11
13	D	402	PTY	N1-C2-C3-O11
13	D	402	PTY	C3-O11-P1-O13
13	D	402	PTY	C5-O14-P1-O11
13	D	402	PTY	C5-O14-P1-O12
13	N	504	PTY	C11-C8-O7-C6
13	N	504	PTY	C3-O11-P1-O12
13	N	504	PTY	C3-O11-P1-O13
13	N	504	PTY	C5-O14-P1-O11
13	N	504	PTY	C5-O14-P1-O13
14	C	505	CDL	O1-C1-CA2-OA2
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

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Mol	Chain	Res	Type	Atoms
14	C	505	CDL	CB2-OB2-PB2-OB4
14	C	505	CDL	CB2-OB2-PB2-OB5
14	C	505	CDL	CB3-OB5-PB2-OB2
14	C	505	CDL	CB3-OB5-PB2-OB3
14	A	3001	CDL	CB3-CB4-CB6-OB8
14	A	3001	CDL	CB4-CB6-OB8-CB7
14	A	3002	CDL	CA2-C1-CB2-OB2
14	A	3002	CDL	CA2-OA2-PA1-OA4
14	A	3002	CDL	CA2-OA2-PA1-OA5
14	A	3002	CDL	CB2-OB2-PB2-OB3
14	A	3002	CDL	CB3-OB5-PB2-OB2
14	A	3002	CDL	CB3-OB5-PB2-OB3
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	CA2-OA2-PA1-OA5
14	H	702	CDL	C31-CA7-OA8-CA6
14	H	702	CDL	CB3-OB5-PB2-OB4
14	H	702	CDL	OB9-CB7-OB8-CB6
14	N	505	CDL	O1-C1-CA2-OA2
14	N	505	CDL	CB2-C1-CA2-OA2
14	N	505	CDL	CA3-OA5-PA1-OA3
14	N	505	CDL	C11-CA5-OA6-CA4
14	N	505	CDL	CB2-OB2-PB2-OB3
14	N	505	CDL	CB2-OB2-PB2-OB4
14	N	505	CDL	CB2-OB2-PB2-OB5
14	N	505	CDL	CB3-OB5-PB2-OB2
14	N	505	CDL	CB3-OB5-PB2-OB3
14	L	3001	CDL	CB2-C1-CA2-OA2
14	L	3001	CDL	CA2-C1-CB2-OB2
14	L	3001	CDL	CB2-OB2-PB2-OB4
14	L	3001	CDL	CB2-OB2-PB2-OB5
14	L	3001	CDL	OB5-CB3-CB4-CB6
14	L	3001	CDL	CB3-CB4-CB6-OB8
14	L	3002	CDL	CA2-C1-CB2-OB2
14	L	3002	CDL	CA2-OA2-PA1-OA4
14	L	3002	CDL	CA2-OA2-PA1-OA5
14	L	3002	CDL	CB2-OB2-PB2-OB3
14	L	3002	CDL	CB3-OB5-PB2-OB3
14	L	3002	CDL	OB5-CB3-CB4-OB6
14	S	701	CDL	CA2-OA2-PA1-OA4
14	S	701	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
14	S	702	CDL	CA2-OA2-PA1-OA4
14	S	702	CDL	CA2-OA2-PA1-OA5
14	S	702	CDL	CB3-OB5-PB2-OB4
15	C	506	LMT	O5'-C1'-O1'-C1
15	N	506	LMT	O5'-C1'-O1'-C1
16	C	507	AWB	C10-C11-O2-C12
16	N	507	AWB	C10-C11-O2-C12
14	H	702	CDL	C51-CB5-OB6-CB4
14	S	702	CDL	C51-CB5-OB6-CB4
14	H	702	CDL	OB7-CB5-OB6-CB4
14	H	702	CDL	OA9-CA7-OA8-CA6
14	S	702	CDL	OA9-CA7-OA8-CA6
14	S	702	CDL	C31-CA7-OA8-CA6
14	S	702	CDL	OB7-CB5-OB6-CB4
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	S	701	CDL	OB9-CB7-OB8-CB6
14	S	702	CDL	OB9-CB7-OB8-CB6
14	L	3001	CDL	OA9-CA7-OA8-CA6
13	C	504	PTY	O10-C8-O7-C6
13	N	504	PTY	O10-C8-O7-C6
14	C	505	CDL	OA7-CA5-OA6-CA4
14	N	505	CDL	OA7-CA5-OA6-CA4
14	S	701	CDL	OB7-CB5-OB6-CB4
12	T	201	PC1	C32-C31-O31-C3
14	H	701	CDL	C71-CB7-OB8-CB6
14	S	701	CDL	C71-CB7-OB8-CB6
14	S	701	CDL	C51-CB5-OB6-CB4
15	C	506	LMT	O5B-C5B-C6B-O6B
14	H	701	CDL	OA9-CA7-OA8-CA6
14	A	3001	CDL	C31-CA7-OA8-CA6
14	H	702	CDL	C71-CB7-OB8-CB6
14	S	702	CDL	C71-CB7-OB8-CB6
15	C	506	LMT	C3-C4-C5-C6
14	H	701	CDL	C31-CA7-OA8-CA6
14	A	3001	CDL	OA5-CA3-CA4-OA6
14	A	3002	CDL	O1-C1-CB2-OB2
14	L	3001	CDL	OA5-CA3-CA4-OA6
14	L	3001	CDL	OB5-CB3-CB4-OB6
14	L	3002	CDL	O1-C1-CB2-OB2
14	S	702	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
14	L	3001	CDL	C31-CA7-OA8-CA6
14	A	3001	CDL	OB6-CB4-CB6-OB8
15	N	506	LMT	O5B-C5B-C6B-O6B
15	C	506	LMT	C4B-C5B-C6B-O6B
15	N	506	LMT	C4'-C5'-C6'-O6'
13	N	504	PTY	C31-C32-C33-C34
13	N	504	PTY	C33-C34-C35-C36
13	D	402	PTY	C13-C14-C15-C16
13	P	301	PTY	C37-C38-C39-C40
12	I	201	PC1	C32-C33-C34-C35
15	U	101	LMT	C11-C10-C9-C8
14	L	3002	CDL	C11-CA5-OA6-CA4
14	C	505	CDL	CA2-C1-CB2-OB2
14	H	702	CDL	CB2-C1-CA2-OA2
14	H	702	CDL	CA2-C1-CB2-OB2
14	S	701	CDL	CA2-C1-CB2-OB2
14	S	702	CDL	CA2-C1-CB2-OB2
12	C	503	PC1	C32-C31-O31-C3
13	P	301	PTY	C31-C30-O4-C1
13	D	402	PTY	C35-C36-C37-C38
15	J	101	LMT	C4-C5-C6-C7
15	N	506	LMT	C4B-C5B-C6B-O6B
15	J	101	LMT	C2-C3-C4-C5
13	P	301	PTY	C13-C14-C15-C16
13	C	504	PTY	C31-C32-C33-C34
14	S	701	CDL	OA9-CA7-OA8-CA6
15	N	506	LMT	C2'-C1'-O1'-C1
14	H	702	CDL	O1-C1-CA2-OA2
13	P	301	PTY	C35-C36-C37-C38
13	N	504	PTY	C37-C38-C39-C40
13	C	504	PTY	C35-C36-C37-C38
14	A	3002	CDL	C11-CA5-OA6-CA4
15	J	101	LMT	O5B-C5B-C6B-O6B
12	I	201	PC1	C32-C31-O31-C3
13	N	504	PTY	C8-C11-C12-C13
14	H	701	CDL	CA5-C11-C12-C13
13	P	301	PTY	C33-C34-C35-C36
14	L	3001	CDL	OB9-CB7-OB8-CB6
14	A	3001	CDL	CB7-C71-C72-C73
13	D	402	PTY	C40-C41-C42-C43
13	D	402	PTY	C30-C31-C32-C33
14	C	505	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
14	N	505	CDL	CA7-C31-C32-C33
14	L	3002	CDL	CA7-C31-C32-C33
13	P	301	PTY	O30-C30-O4-C1
14	S	701	CDL	C31-CA7-OA8-CA6
12	T	201	PC1	C21-C22-C23-C24
13	P	301	PTY	C30-C31-C32-C33
14	S	701	CDL	CA5-C11-C12-C13
12	I	201	PC1	O32-C31-O31-C3
14	C	505	CDL	O1-C1-CB2-OB2
14	H	702	CDL	O1-C1-CB2-OB2
14	L	3001	CDL	O1-C1-CB2-OB2
14	S	701	CDL	O1-C1-CB2-OB2
14	S	702	CDL	O1-C1-CB2-OB2
12	T	201	PC1	C31-C32-C33-C34
14	H	701	CDL	CB7-C71-C72-C73
14	L	3001	CDL	OB6-CB4-CB6-OB8
14	H	701	CDL	CB5-C51-C52-C53
15	J	101	LMT	O5'-C5'-C6'-O6'
14	L	3001	CDL	C71-CB7-OB8-CB6
15	N	506	LMT	O5'-C5'-C6'-O6'
12	I	201	PC1	C21-C22-C23-C24
14	L	3001	CDL	CB7-C71-C72-C73
14	S	701	CDL	CB7-C71-C72-C73
14	A	3002	CDL	OA7-CA5-OA6-CA4
14	L	3002	CDL	OA7-CA5-OA6-CA4
14	A	3001	CDL	OA5-CA3-CA4-CA6
14	L	3001	CDL	OA5-CA3-CA4-CA6
14	S	702	CDL	CB2-C1-CA2-OA2
12	N	503	PC1	C32-C31-O31-C3
15	C	506	LMT	C5-C6-C7-C8
15	C	506	LMT	C2'-C1'-O1'-C1
13	N	504	PTY	C11-C12-C13-C14
14	N	505	CDL	O1-C1-CB2-OB2
12	C	503	PC1	O32-C31-O31-C3
16	N	507	AWB	C2-C3-C4-C5
12	N	503	PC1	O32-C31-O31-C3
14	S	701	CDL	C74-C75-C76-C77
14	A	3001	CDL	C71-C72-C73-C74
12	I	201	PC1	C31-C32-C33-C34
13	D	402	PTY	C8-C11-C12-C13
13	C	504	PTY	C37-C38-C39-C40
15	C	506	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
14	N	505	CDL	CA2-C1-CB2-OB2
13	P	301	PTY	C41-C42-C43-C44
13	N	504	PTY	C15-C16-C17-C18
14	S	701	CDL	C11-C12-C13-C14
15	U	101	LMT	C4-C5-C6-C7
13	C	504	PTY	C8-C11-C12-C13
14	A	3002	CDL	CA7-C31-C32-C33
13	C	504	PTY	C13-C14-C15-C16
14	H	701	CDL	C11-C12-C13-C14
15	N	506	LMT	C2-C3-C4-C5
12	C	503	PC1	C28-C29-C2A-C2B
15	U	101	LMT	C3-C4-C5-C6
13	P	301	PTY	C34-C35-C36-C37
13	D	402	PTY	C31-C30-O4-C1
14	H	701	CDL	C74-C75-C76-C77
14	L	3002	CDL	C12-C13-C14-C15
13	N	504	PTY	C32-C33-C34-C35
14	C	505	CDL	OB7-CB5-OB6-CB4
14	N	505	CDL	OB7-CB5-OB6-CB4
13	C	504	PTY	C14-C15-C16-C17
12	N	503	PC1	C28-C29-C2A-C2B
13	P	301	PTY	C40-C41-C42-C43
13	D	402	PTY	C38-C39-C40-C41
13	D	402	PTY	C11-C12-C13-C14
15	C	506	LMT	C4-C5-C6-C7
13	C	504	PTY	C15-C16-C17-C18
13	P	301	PTY	C31-C32-C33-C34
14	C	505	CDL	C51-CB5-OB6-CB4
14	H	701	CDL	C51-CB5-OB6-CB4
14	N	505	CDL	C51-CB5-OB6-CB4
13	D	402	PTY	C16-C17-C18-C19
16	N	507	AWB	C3-C4-C5-C6
13	D	402	PTY	C32-C33-C34-C35
13	D	402	PTY	C12-C13-C14-C15
15	J	101	LMT	C6-C7-C8-C9
16	C	507	AWB	C3-C4-C5-C6
14	H	701	CDL	C71-C72-C73-C74
16	N	507	AWB	C23-C24-C25-C27
13	D	402	PTY	O14-C5-C6-O7
16	C	507	AWB	C1-C2-C3-C4
14	H	701	CDL	C73-C74-C75-C76
12	C	503	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
12	N	503	PC1	O21-C2-C3-O31
14	A	3002	CDL	C51-CB5-OB6-CB4
14	L	3002	CDL	C51-CB5-OB6-CB4
13	N	504	PTY	C14-C15-C16-C17
13	C	504	PTY	C38-C39-C40-C41
14	H	701	CDL	OB7-CB5-OB6-CB4
14	S	701	CDL	CB2-C1-CA2-OA2
12	N	503	PC1	C26-C27-C28-C29
14	L	3001	CDL	CB4-CB6-OB8-CB7
15	N	506	LMT	C3'-C4'-O1B-C1B
13	D	402	PTY	O30-C30-O4-C1
13	P	301	PTY	C11-C12-C13-C14
13	D	402	PTY	O14-C5-C6-C1
14	A	3002	CDL	OA5-CA3-CA4-CA6
14	H	702	CDL	OB5-CB3-CB4-CB6
14	S	702	CDL	OB5-CB3-CB4-CB6
14	S	701	CDL	C71-C72-C73-C74
13	P	301	PTY	C16-C17-C18-C19
13	N	504	PTY	C16-C17-C18-C19
12	C	503	PC1	C26-C27-C28-C29
13	C	504	PTY	C33-C34-C35-C36
15	J	101	LMT	C7-C8-C9-C10
13	C	504	PTY	O4-C1-C6-C5
13	N	504	PTY	O4-C1-C6-C5
14	S	702	CDL	CB3-CB4-CB6-OB8
13	C	504	PTY	C12-C13-C14-C15
12	T	201	PC1	C33-C34-C35-C36
15	N	506	LMT	C7-C8-C9-C10
15	C	506	LMT	O1'-C1-C2-C3
13	D	402	PTY	C14-C15-C16-C17
14	A	3002	CDL	CA6-CA4-OA6-CA5
14	H	702	CDL	CB6-CB4-OB6-CB5
14	L	3002	CDL	CA6-CA4-OA6-CA5
14	S	702	CDL	CB6-CB4-OB6-CB5
15	U	101	LMT	C7-C8-C9-C10
14	L	3001	CDL	C71-C72-C73-C74
12	C	503	PC1	C22-C23-C24-C25
14	H	702	CDL	OA5-CA3-CA4-OA6
14	S	701	CDL	OA5-CA3-CA4-OA6
13	N	504	PTY	C34-C35-C36-C37
14	A	3002	CDL	C12-C13-C14-C15
13	C	504	PTY	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
13	N	504	PTY	C41-C42-C43-C44
13	D	402	PTY	C41-C42-C43-C44
15	J	101	LMT	C9-C10-C11-C12
13	C	504	PTY	C11-C12-C13-C14
15	C	506	LMT	C6-C7-C8-C9
15	N	506	LMT	C9-C10-C11-C12
13	P	301	PTY	C38-C39-C40-C41
15	C	506	LMT	C9-C10-C11-C12
15	N	506	LMT	C5'-C4'-O1B-C1B
12	N	503	PC1	C22-C23-C24-C25
14	L	3001	CDL	C32-C33-C34-C35
14	S	701	CDL	C75-C76-C77-C78
15	J	101	LMT	O1'-C1-C2-C3
14	H	701	CDL	C75-C76-C77-C78
12	I	201	PC1	C34-C35-C36-C37
15	C	506	LMT	C2-C1-O1'-C1'
15	N	506	LMT	C2-C1-O1'-C1'
16	N	507	AWB	C1-C2-C3-C4
15	N	506	LMT	C1-C2-C3-C4
14	H	701	CDL	OB5-CB3-CB4-CB6
14	L	3002	CDL	OA5-CA3-CA4-CA6
14	L	3001	CDL	O1-C1-CA2-OA2
14	L	3002	CDL	CA5-C11-C12-C13
16	C	507	AWB	C-C1-C2-C3
14	L	3002	CDL	C11-C12-C13-C14
14	N	505	CDL	C11-C12-C13-C14
15	C	506	LMT	C1-C2-C3-C4
14	L	3002	CDL	OB7-CB5-OB6-CB4
13	N	504	PTY	C36-C37-C38-C39
15	J	101	LMT	C4B-C5B-C6B-O6B
14	A	3002	CDL	OB7-CB5-OB6-CB4
14	A	3002	CDL	C33-C34-C35-C36
13	C	504	PTY	C17-C18-C19-C20
14	L	3002	CDL	C13-C14-C15-C16
14	H	701	CDL	CA3-CA4-CA6-OA8
14	H	702	CDL	CB3-CB4-CB6-OB8
14	S	701	CDL	CA3-CA4-CA6-OA8
14	N	505	CDL	C13-C14-C15-C16
14	L	3002	CDL	C34-C35-C36-C37
13	N	504	PTY	C12-C13-C14-C15
14	A	3002	CDL	C34-C35-C36-C37
14	L	3002	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
13	C	504	PTY	C40-C41-C42-C43
13	D	402	PTY	C31-C32-C33-C34
13	N	504	PTY	O4-C1-C6-O7
14	H	702	CDL	OB6-CB4-CB6-OB8
14	N	505	CDL	OB6-CB4-CB6-OB8
14	S	701	CDL	OA6-CA4-CA6-OA8
14	S	702	CDL	OB6-CB4-CB6-OB8
14	C	505	CDL	C13-C14-C15-C16
13	C	504	PTY	C39-C40-C41-C42
13	P	301	PTY	C14-C15-C16-C17
13	P	301	PTY	C12-C13-C14-C15
13	N	504	PTY	C38-C39-C40-C41
13	N	504	PTY	O14-C5-C6-C1
14	H	702	CDL	OA5-CA3-CA4-CA6
14	S	701	CDL	OA5-CA3-CA4-CA6
14	A	3002	CDL	CA5-C11-C12-C13
14	S	701	CDL	C73-C74-C75-C76
15	U	101	LMT	C5-C6-C7-C8
14	L	3002	CDL	O1-C1-CA2-OA2
16	N	507	AWB	C23-C24-C25-C26
16	N	507	AWB	O8-C23-O7-C7
13	P	301	PTY	O14-C5-C6-O7
14	S	701	CDL	OB5-CB3-CB4-OB6
13	D	402	PTY	C36-C37-C38-C39
14	H	701	CDL	CB3-CB4-CB6-OB8
13	P	301	PTY	C8-C11-C12-C13
15	J	101	LMT	C4'-C5'-C6'-O6'
14	C	505	CDL	OB6-CB4-CB6-OB8
14	H	701	CDL	OA6-CA4-CA6-OA8
12	I	201	PC1	C33-C34-C35-C36
14	N	505	CDL	CA4-CA3-OA5-PA1
14	S	701	CDL	O1-C1-CA2-OA2
14	S	701	CDL	C51-C52-C53-C54
14	A	3001	CDL	C72-C73-C74-C75
14	N	505	CDL	C31-C32-C33-C34
15	N	506	LMT	C6-C7-C8-C9
12	C	503	PC1	C27-C28-C29-C2A
14	C	505	CDL	C31-C32-C33-C34
14	S	702	CDL	OA5-CA3-CA4-CA6
16	N	507	AWB	C24-C23-O7-C7
14	A	3001	CDL	OB5-CB3-CB4-OB6
14	H	701	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
14	C	505	CDL	CA4-CA3-OA5-PA1
14	S	702	CDL	OA5-CA3-CA4-OA6
12	N	503	PC1	C27-C28-C29-C2A
13	C	504	PTY	O4-C1-C6-O7
12	C	503	PC1	C1-C2-C3-O31
12	N	503	PC1	C1-C2-C3-O31
12	T	201	PC1	C1-C2-C3-O31
14	S	701	CDL	CB3-CB4-CB6-OB8
14	H	701	CDL	C51-C52-C53-C54
12	I	201	PC1	C1-O11-P-O14
13	C	504	PTY	C3-O11-P1-O12
13	C	504	PTY	C5-O14-P1-O13
13	P	301	PTY	C5-O14-P1-O13
13	N	504	PTY	C3-O11-P1-O14
13	N	504	PTY	C5-O14-P1-O12
14	C	505	CDL	CA2-OA2-PA1-OA3
14	C	505	CDL	CA3-OA5-PA1-OA2
14	C	505	CDL	CA3-OA5-PA1-OA4
14	C	505	CDL	CB3-OB5-PB2-OB4
14	A	3002	CDL	CB3-OB5-PB2-OB4
14	H	702	CDL	CB2-OB2-PB2-OB3
14	H	702	CDL	CB3-OB5-PB2-OB2
14	H	702	CDL	CB3-OB5-PB2-OB3
14	N	505	CDL	CA2-OA2-PA1-OA3
14	N	505	CDL	CA3-OA5-PA1-OA2
14	N	505	CDL	CA3-OA5-PA1-OA4
14	N	505	CDL	CB3-OB5-PB2-OB4
14	L	3002	CDL	CB3-OB5-PB2-OB2
14	L	3002	CDL	CB3-OB5-PB2-OB4
14	S	701	CDL	CA2-OA2-PA1-OA3
14	S	702	CDL	CB2-OB2-PB2-OB3
14	S	702	CDL	CB3-OB5-PB2-OB2
14	S	702	CDL	CB3-OB5-PB2-OB3
14	A	3002	CDL	C13-C14-C15-C16
16	N	507	AWB	C-C1-C2-C3
15	C	506	LMT	C2-C3-C4-C5
14	S	701	CDL	OB5-CB3-CB4-CB6
13	N	504	PTY	O14-C5-C6-O7
14	H	701	CDL	OB5-CB3-CB4-OB6
14	S	701	CDL	CB5-C51-C52-C53
13	C	504	PTY	O30-C30-O4-C1
12	I	201	PC1	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
16	C	507	AWB	O8-C23-C24-C25
15	N	506	LMT	C5-C6-C7-C8
16	C	507	AWB	O7-C23-C24-C25
14	H	702	CDL	C32-C31-CA7-OA8
13	C	504	PTY	C31-C30-O4-C1
14	N	505	CDL	OA5-CA3-CA4-OA6
14	A	3001	CDL	C72-C71-CB7-OB8
12	I	201	PC1	O21-C2-C3-O31
11	C	502	HEM	CAD-CBD-CGD-O2D
14	C	505	CDL	C11-C12-C13-C14
14	L	3002	CDL	C52-C53-C54-C55
11	C	502	HEM	CAA-CBA-CGA-O1A
11	N	502	HEM	CAA-CBA-CGA-O1A
14	A	3001	CDL	OB5-CB3-CB4-CB6
14	L	3002	CDL	CB2-C1-CA2-OA2
11	C	501	HEM	CAA-CBA-CGA-O1A
11	N	501	HEM	CAA-CBA-CGA-O1A
14	H	701	CDL	CA3-CA4-OA6-CA5
11	C	501	HEM	CAA-CBA-CGA-O2A
11	N	501	HEM	CAA-CBA-CGA-O2A
11	N	502	HEM	CAD-CBD-CGD-O2D
15	N	506	LMT	O1'-C1-C2-C3
14	L	3002	CDL	CB5-C51-C52-C53
14	C	505	CDL	OA5-CA3-CA4-OA6
11	N	502	HEM	CAD-CBD-CGD-O1D
14	H	701	CDL	OA5-CA3-CA4-CA6
15	N	506	LMT	C4-C5-C6-C7
18	D	401	HEC	CAA-CBA-CGA-O2A
15	U	101	LMT	C6-C7-C8-C9
14	H	701	CDL	OB6-CB4-CB6-OB8
18	O	401	HEC	CAA-CBA-CGA-O2A
13	N	504	PTY	C17-C18-C19-C20
11	C	502	HEM	CAD-CBD-CGD-O1D
14	S	702	CDL	C32-C31-CA7-OA9
11	C	501	HEM	CAD-CBD-CGD-O2D
11	N	501	HEM	CAD-CBD-CGD-O2D
13	C	504	PTY	O14-C5-C6-C1
14	A	3002	CDL	OA6-CA4-CA6-OA8
14	A	3002	CDL	CB5-C51-C52-C53
11	N	502	HEM	CAA-CBA-CGA-O2A
18	O	401	HEC	CAA-CBA-CGA-O1A
18	D	401	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
14	L	3001	CDL	C72-C71-CB7-OB8
14	A	3002	CDL	O1-C1-CA2-OA2
14	A	3002	CDL	C31-CA7-OA8-CA6
11	C	502	HEM	CAA-CBA-CGA-O2A
13	N	504	PTY	O30-C30-O4-C1
13	N	504	PTY	C30-C31-C32-C33
14	C	505	CDL	CB6-CB4-OB6-CB5
14	N	505	CDL	CB6-CB4-OB6-CB5
14	S	701	CDL	CA3-CA4-OA6-CA5
13	D	402	PTY	C34-C35-C36-C37
11	C	501	HEM	CAD-CBD-CGD-O1D
11	N	501	HEM	CAD-CBD-CGD-O1D
14	H	701	CDL	CA2-C1-CB2-OB2
14	A	3002	CDL	OA9-CA7-OA8-CA6
14	L	3002	CDL	C31-C32-C33-C34
14	H	702	CDL	C32-C31-CA7-OA9
13	N	504	PTY	C31-C30-O4-C1
14	C	505	CDL	OA5-CA3-CA4-CA6
14	N	505	CDL	OA5-CA3-CA4-CA6
14	H	701	CDL	C72-C71-CB7-OB8
14	S	702	CDL	C32-C31-CA7-OA8
16	N	507	AWB	O8-C23-C24-C25
14	S	701	CDL	C72-C71-CB7-OB8
12	I	201	PC1	C22-C21-O21-C2
12	I	201	PC1	O21-C21-C22-C23
15	U	101	LMT	O5'-C5'-C6'-O6'
13	P	301	PTY	O4-C30-C31-C32
12	C	503	PC1	O31-C31-C32-C33
12	N	503	PC1	O31-C31-C32-C33
18	O	401	HEC	CAD-CBD-CGD-O2D
14	H	702	CDL	C72-C71-CB7-OB8
13	C	504	PTY	C6-C5-O14-P1
14	H	702	CDL	CB4-CB3-OB5-PB2
14	S	702	CDL	CB4-CB3-OB5-PB2
18	O	401	HEC	CAD-CBD-CGD-O1D
13	C	504	PTY	O14-C5-C6-O7
14	L	3002	CDL	OA5-CA3-CA4-OA6
17	A	3003	XP4	O4-C1-C2-O7
14	N	505	CDL	C71-CB7-OB8-CB6
14	H	701	CDL	C72-C71-CB7-OB9
12	I	201	PC1	O22-C21-C22-C23
12	N	503	PC1	O32-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
14	S	701	CDL	OA7-CA5-OA6-CA4
18	D	401	HEC	CAD-CBD-CGD-O1D
12	C	503	PC1	O32-C31-C32-C33
13	P	301	PTY	O30-C30-C31-C32
14	S	701	CDL	C72-C71-CB7-OB9
14	C	505	CDL	C32-C31-CA7-OA8
14	N	505	CDL	C32-C31-CA7-OA8
16	N	507	AWB	O7-C23-C24-C25
13	D	402	PTY	O4-C30-C31-C32

There are no ring outliers.

30 monomers are involved in 97 short contacts:

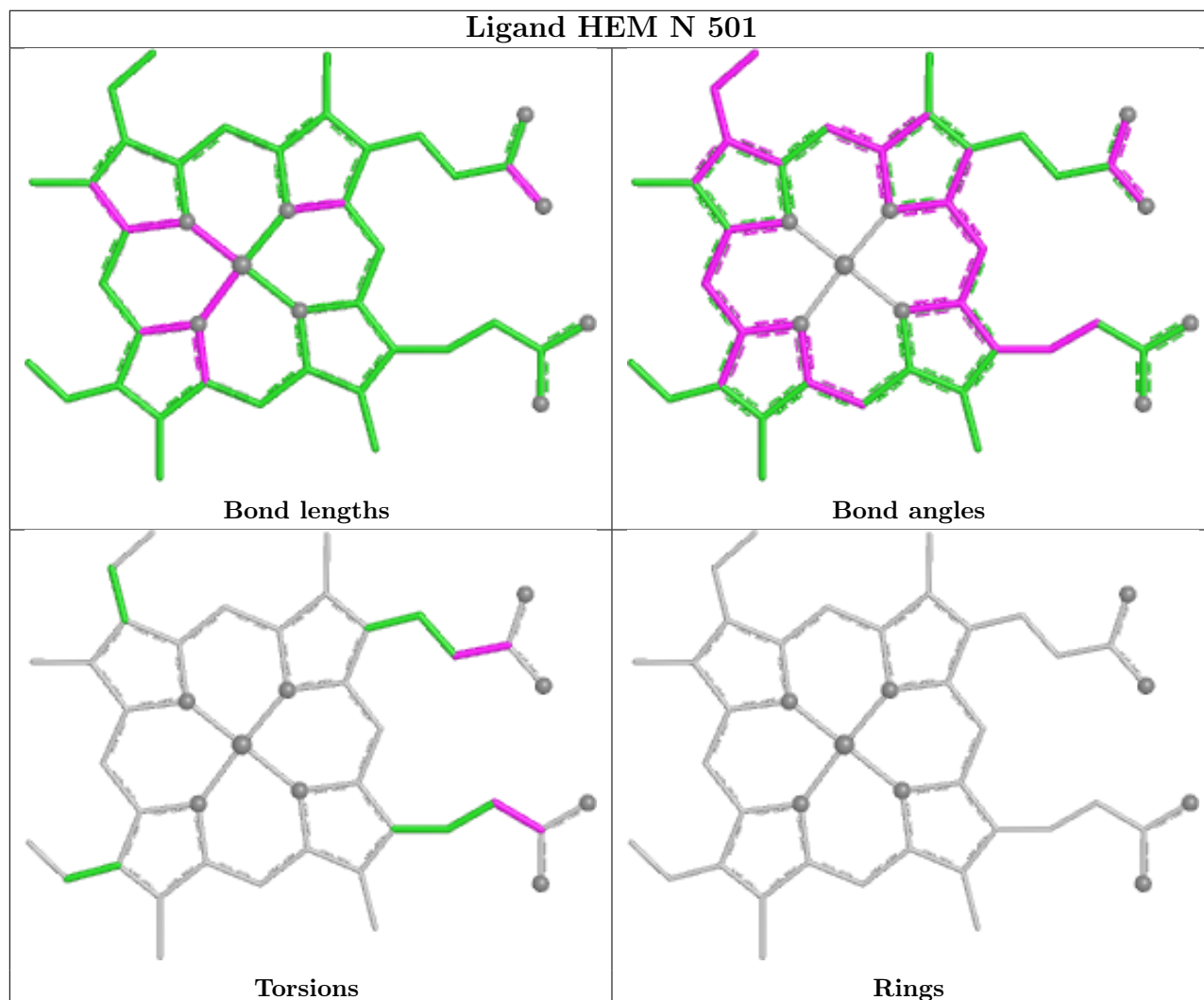
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	N	501	HEM	4	0
11	C	501	HEM	5	0
14	S	702	CDL	3	0
15	C	506	LMT	4	0
14	L	3002	CDL	1	0
14	H	702	CDL	4	0
16	N	507	AWB	4	0
18	O	401	HEC	11	0
12	N	503	PC1	1	0
14	C	505	CDL	1	0
13	N	504	PTY	7	0
12	I	201	PC1	2	0
14	H	701	CDL	3	0
14	N	505	CDL	1	0
11	N	502	HEM	1	0
14	S	701	CDL	4	0
17	L	3003	XP4	1	0
12	T	201	PC1	2	0
18	D	401	HEC	11	0
12	C	503	PC1	2	0
17	A	3003	XP4	1	0
14	A	3001	CDL	2	0
11	C	502	HEM	2	0
15	N	506	LMT	1	0
13	C	504	PTY	6	0
13	P	301	PTY	12	0
14	A	3002	CDL	2	0
14	L	3001	CDL	1	0

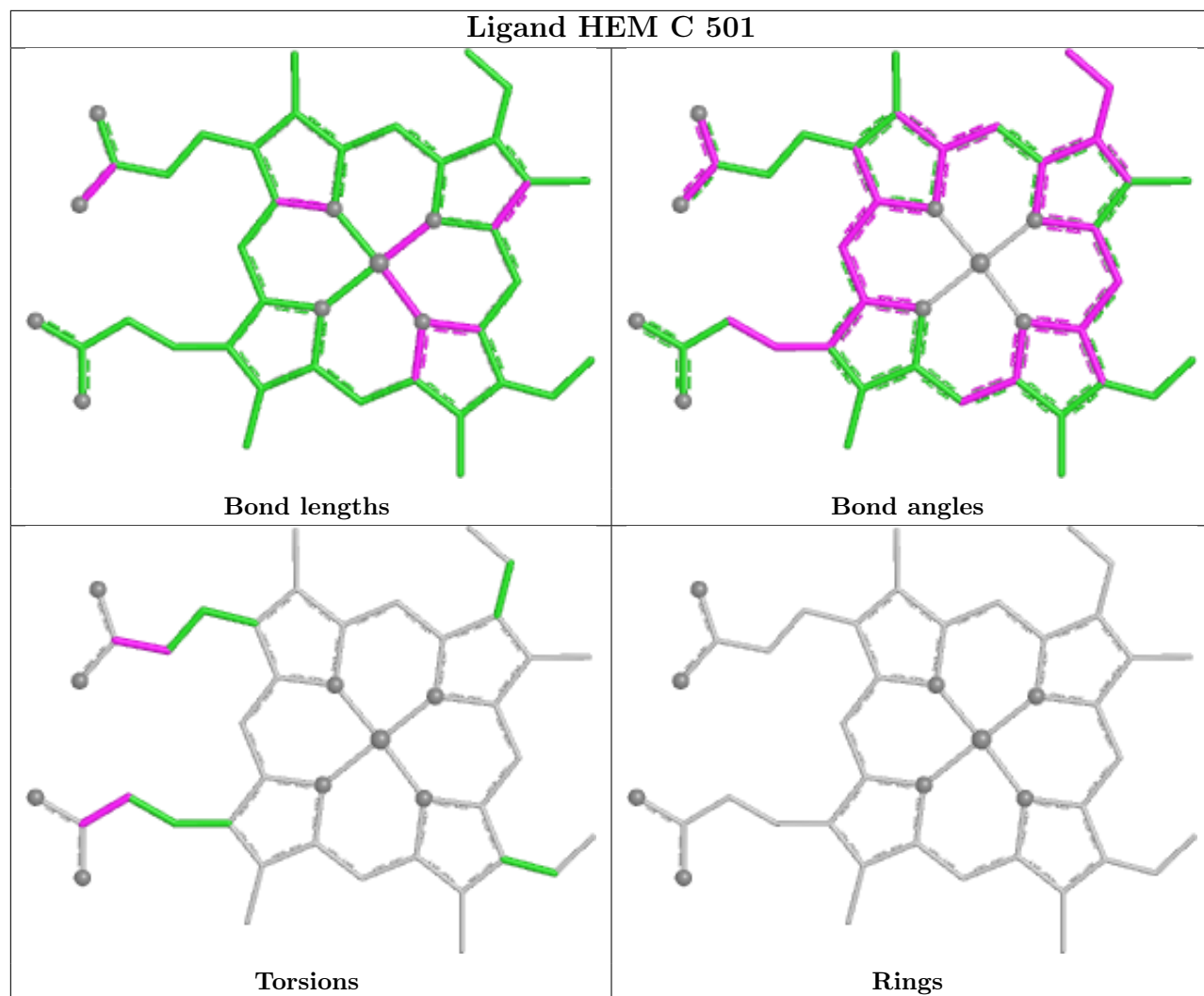
Continued on next page...

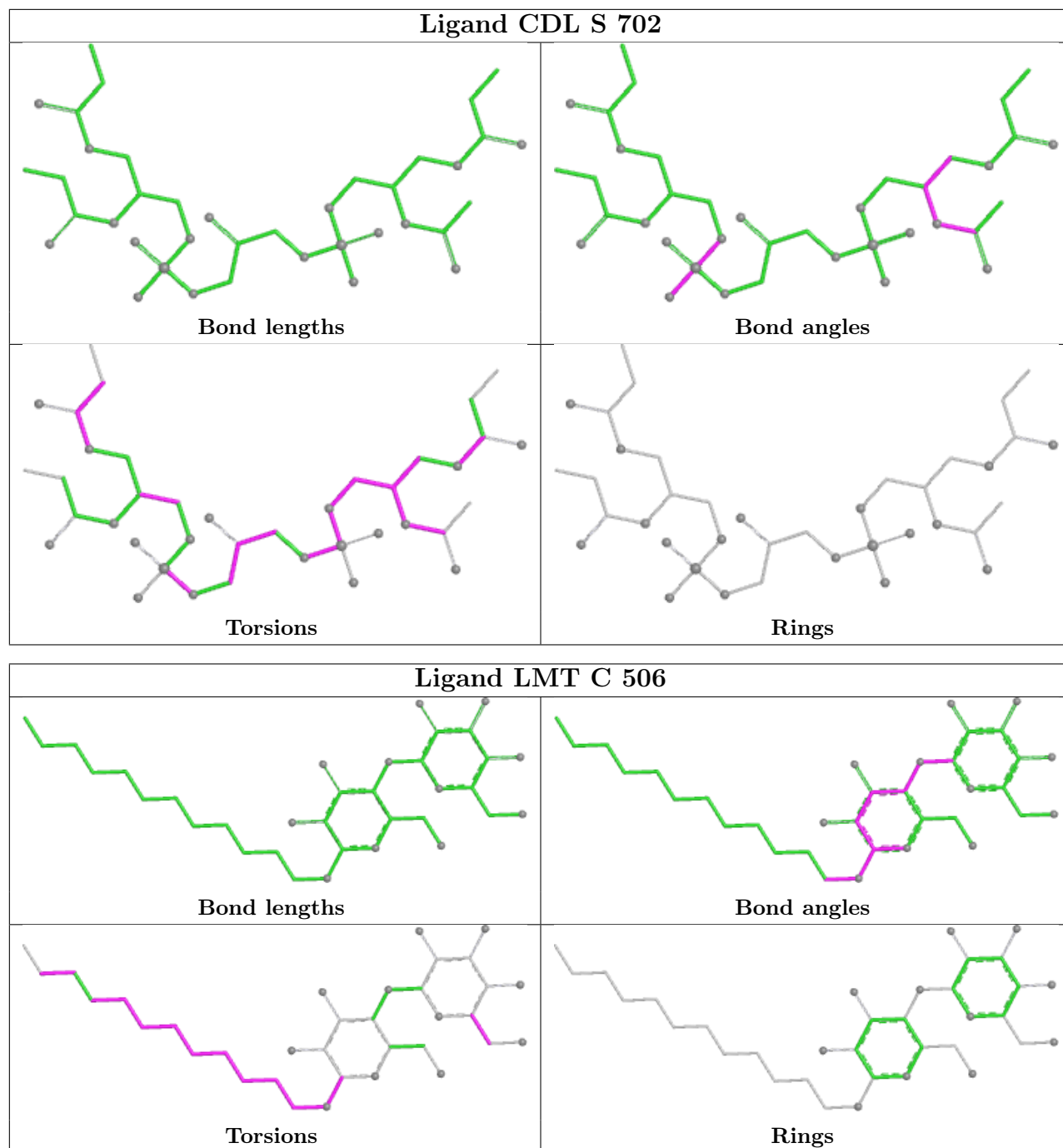
Continued from previous page...

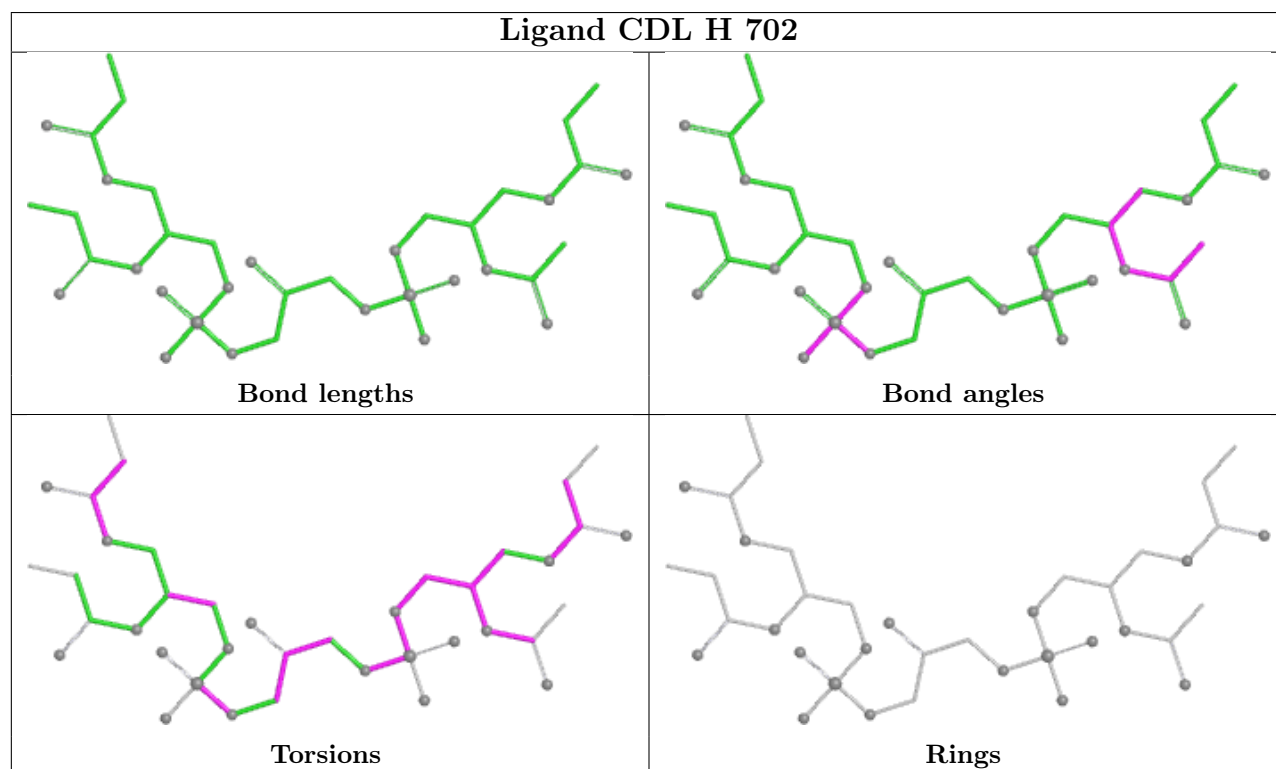
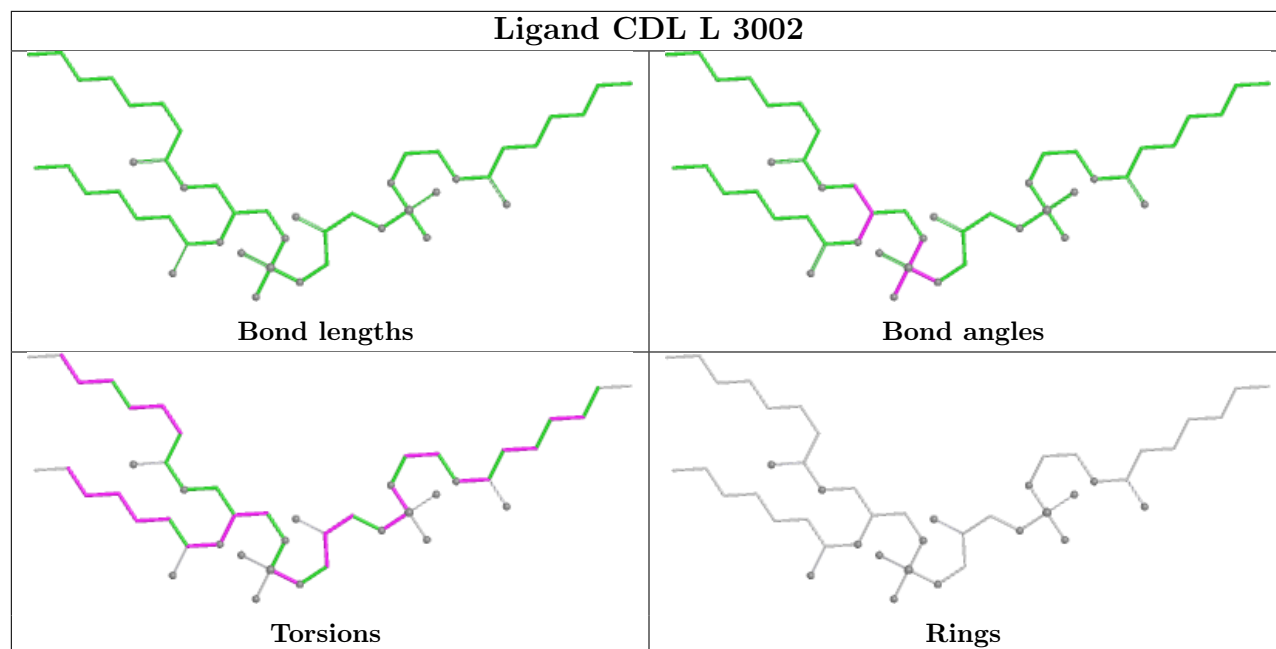
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D	402	PTY	2	0
16	C	507	AWB	2	0

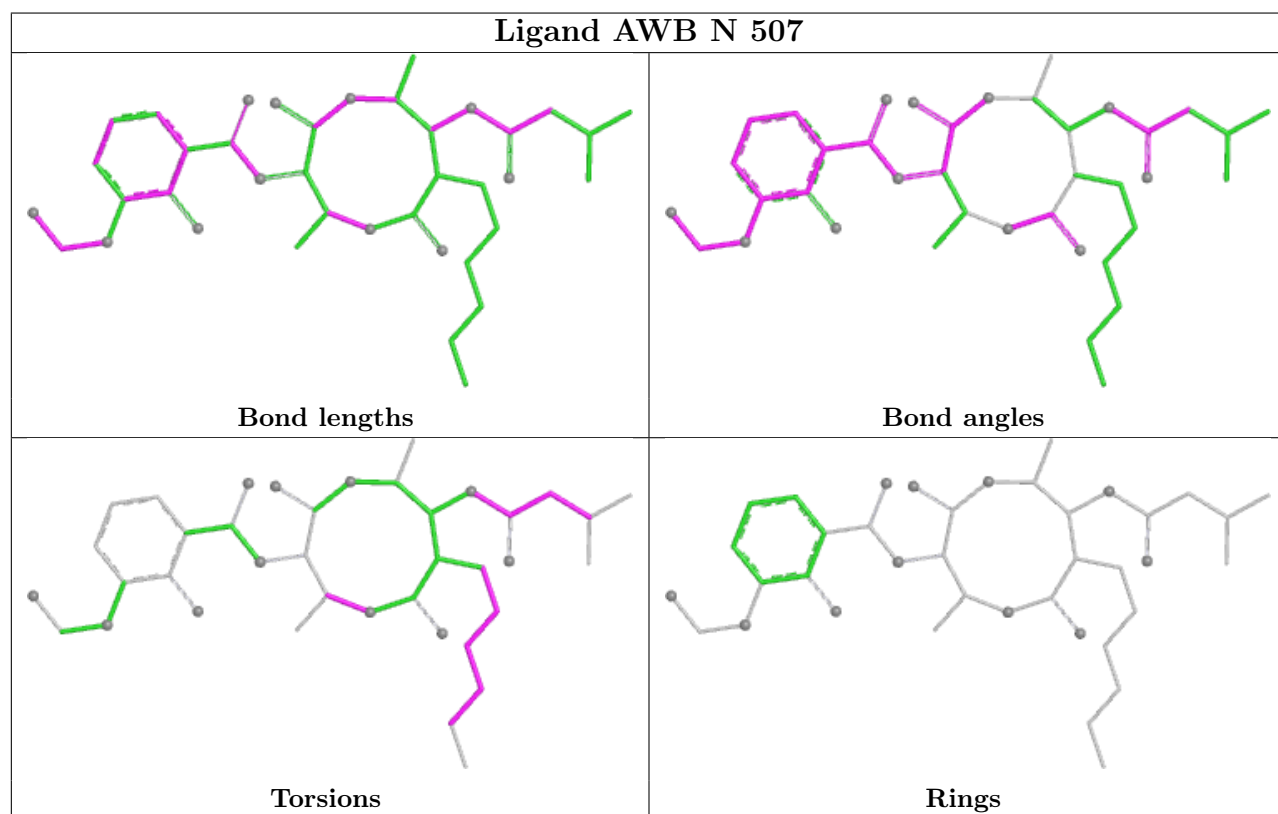
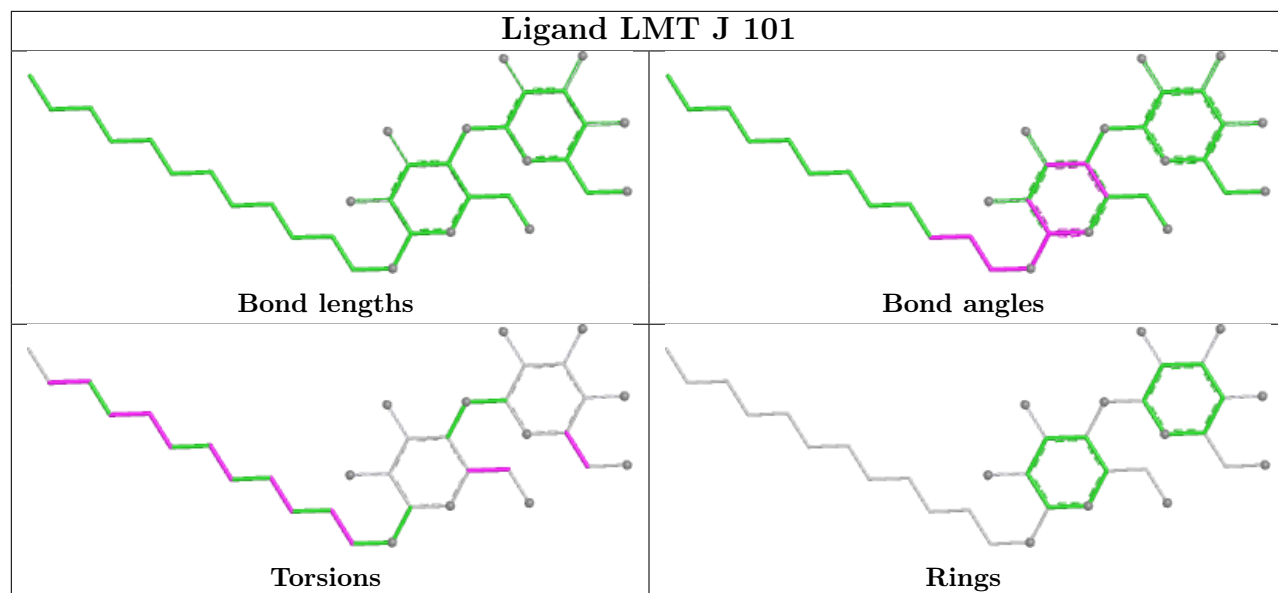
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

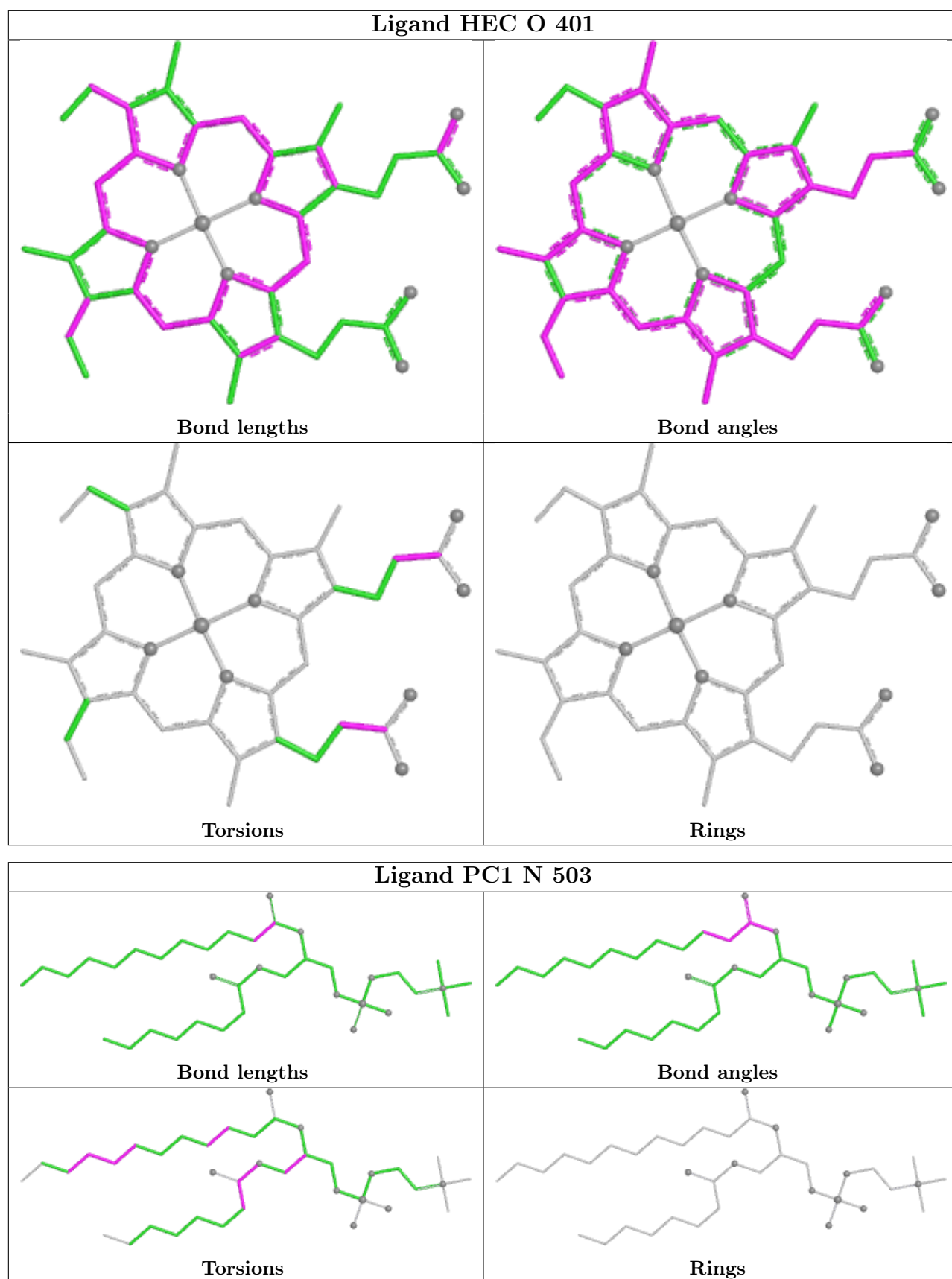


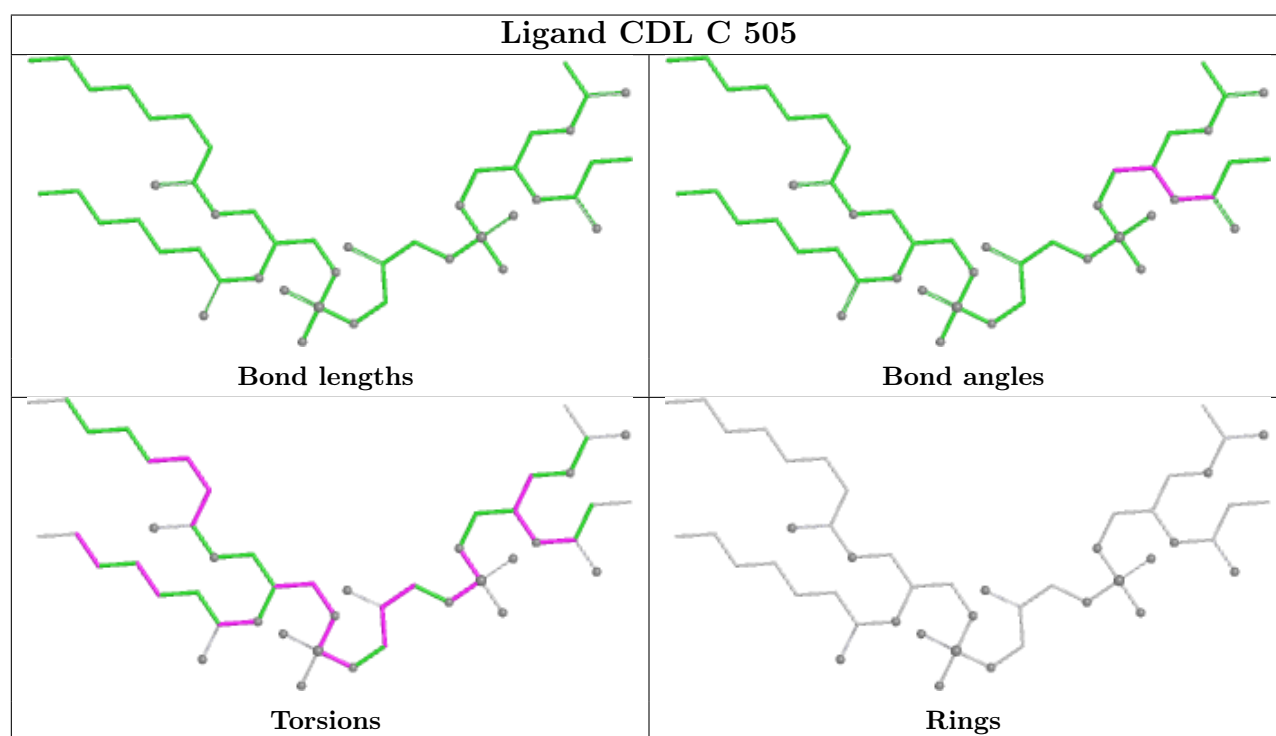
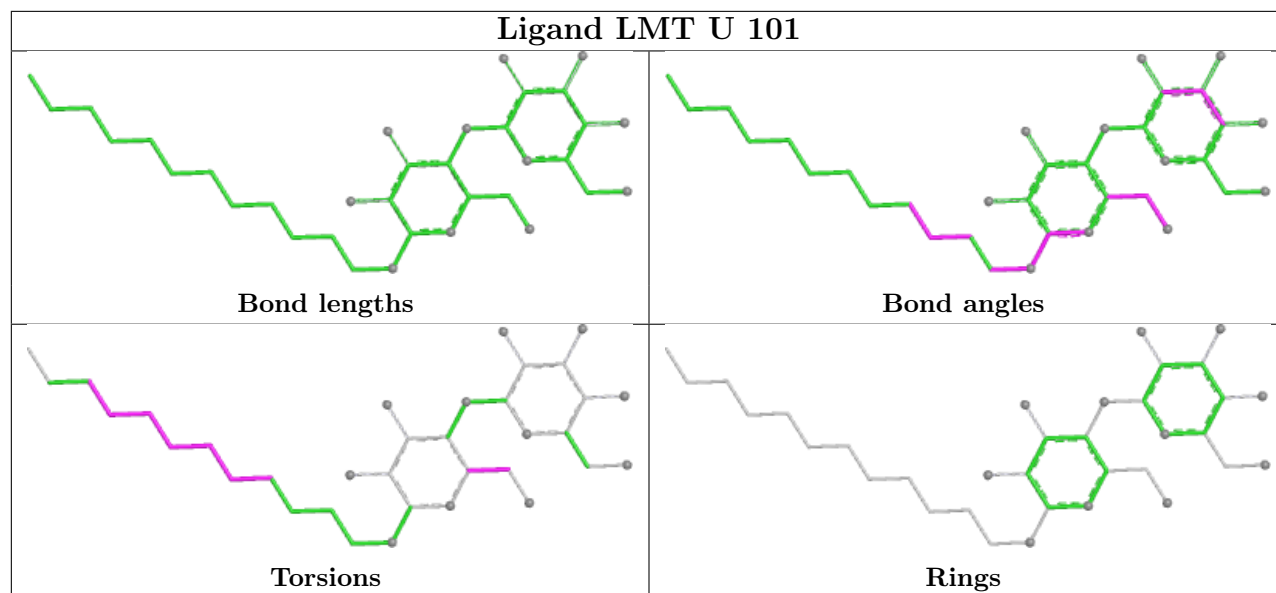


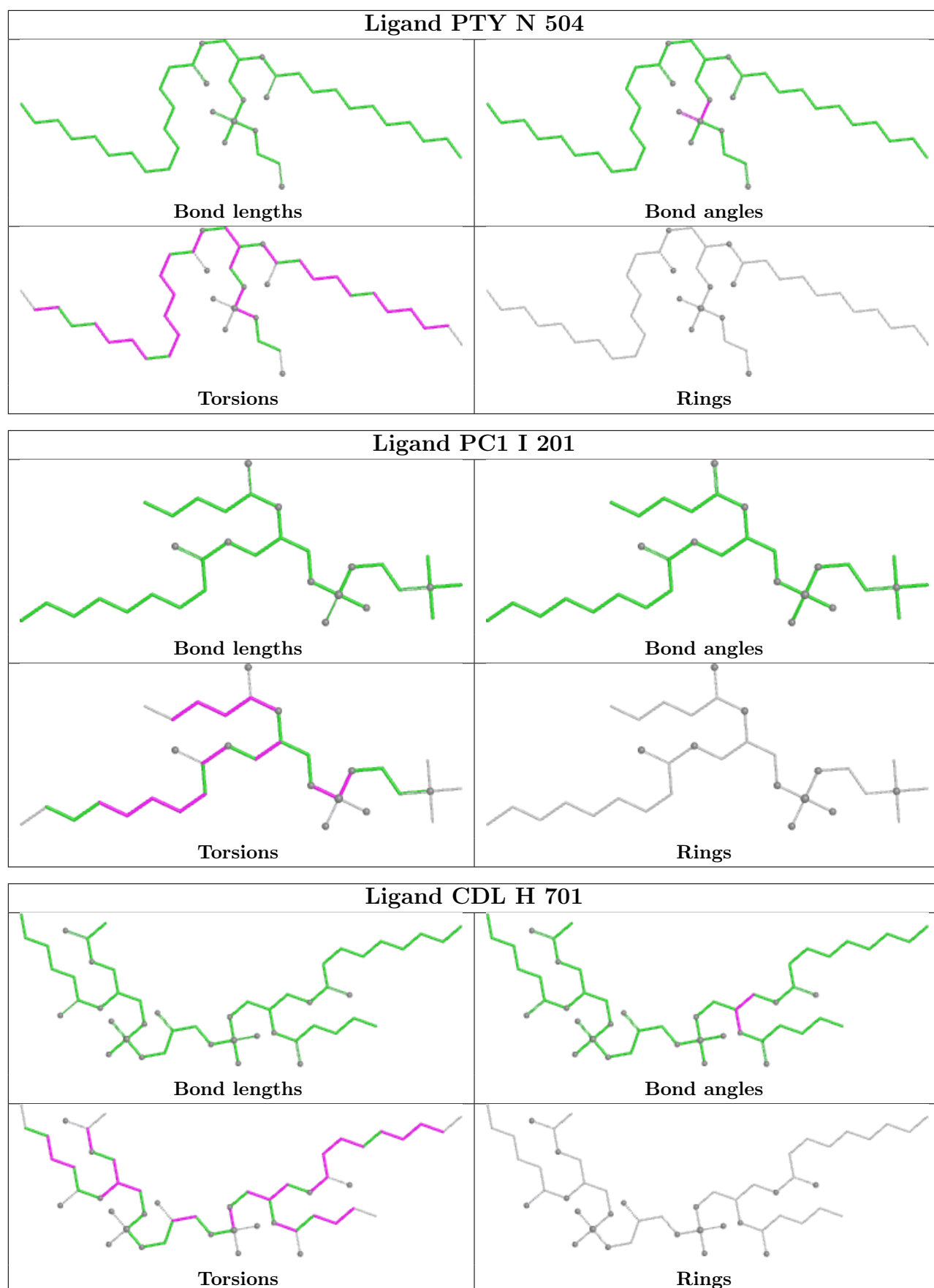


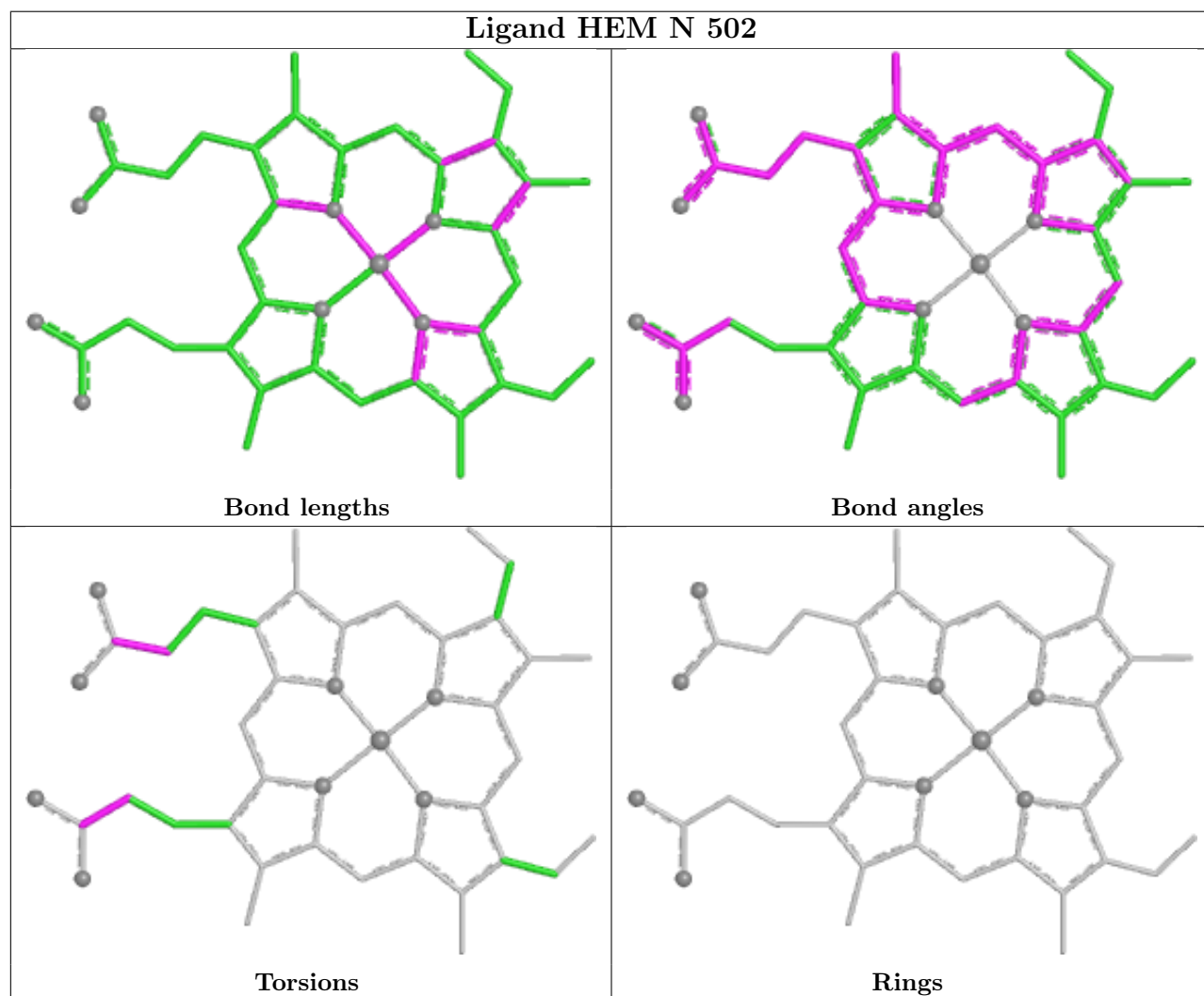
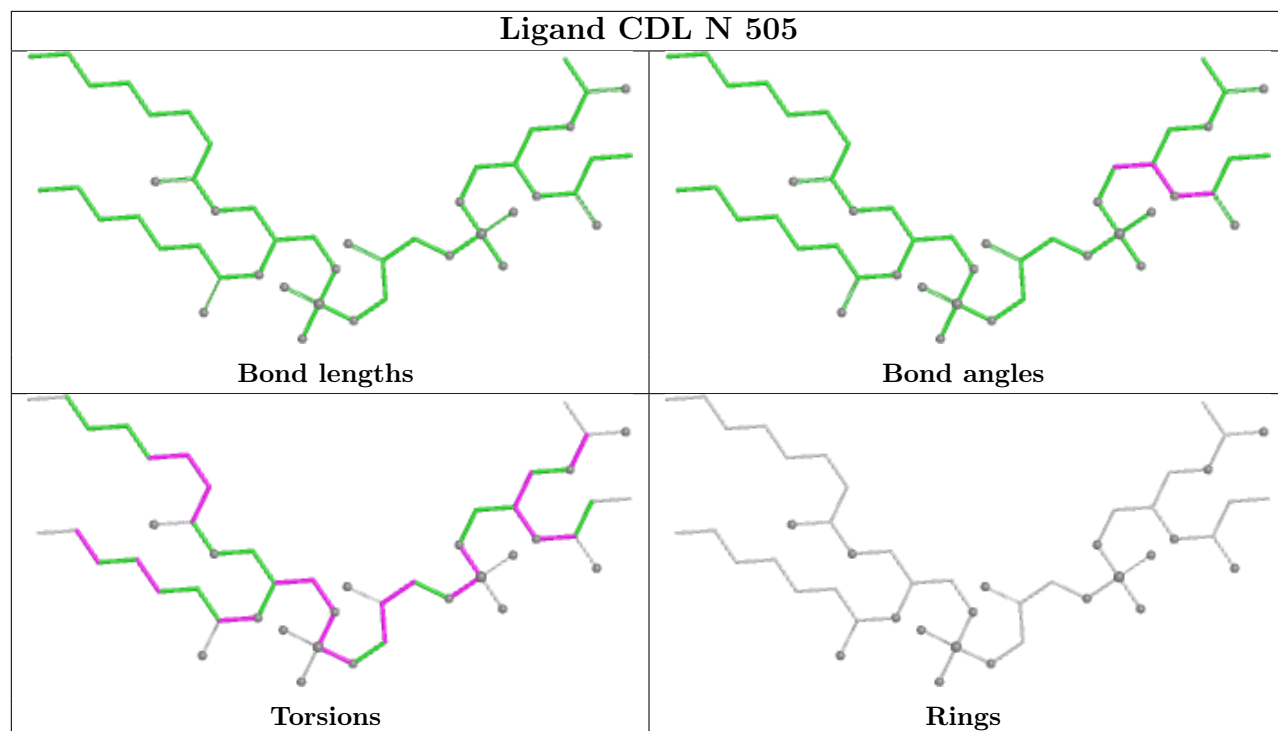


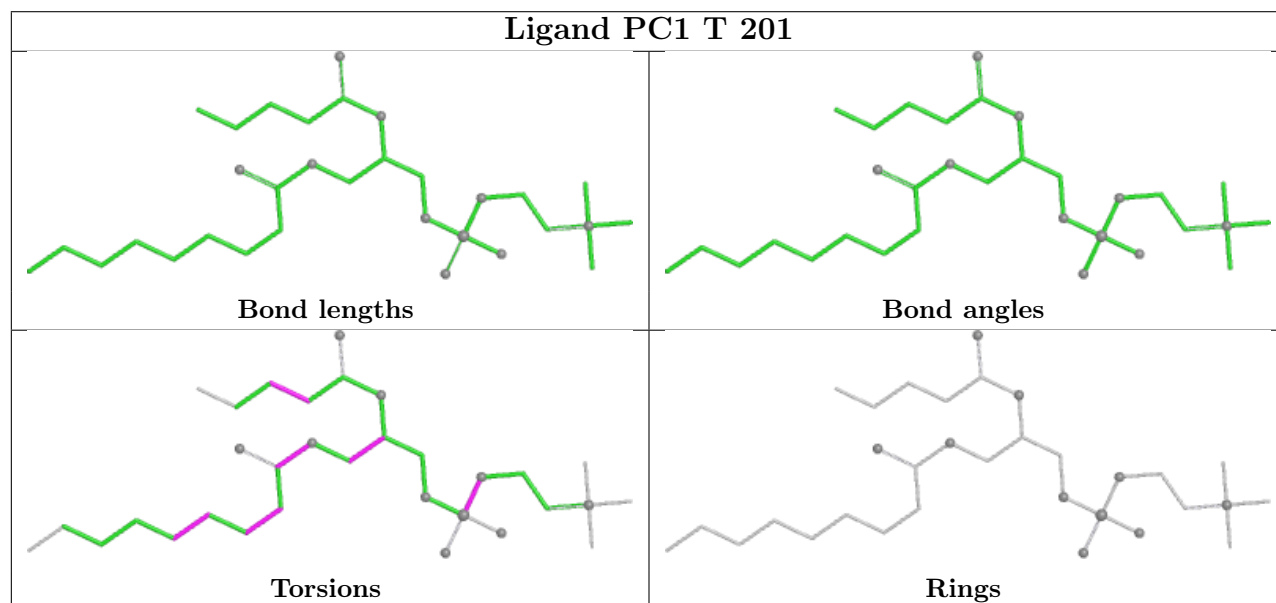
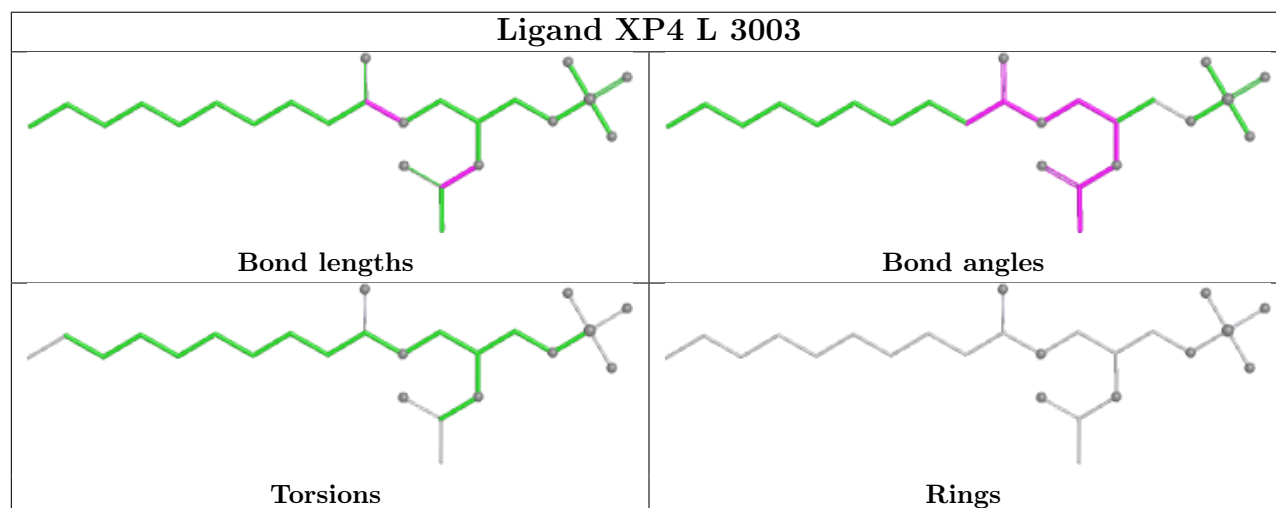
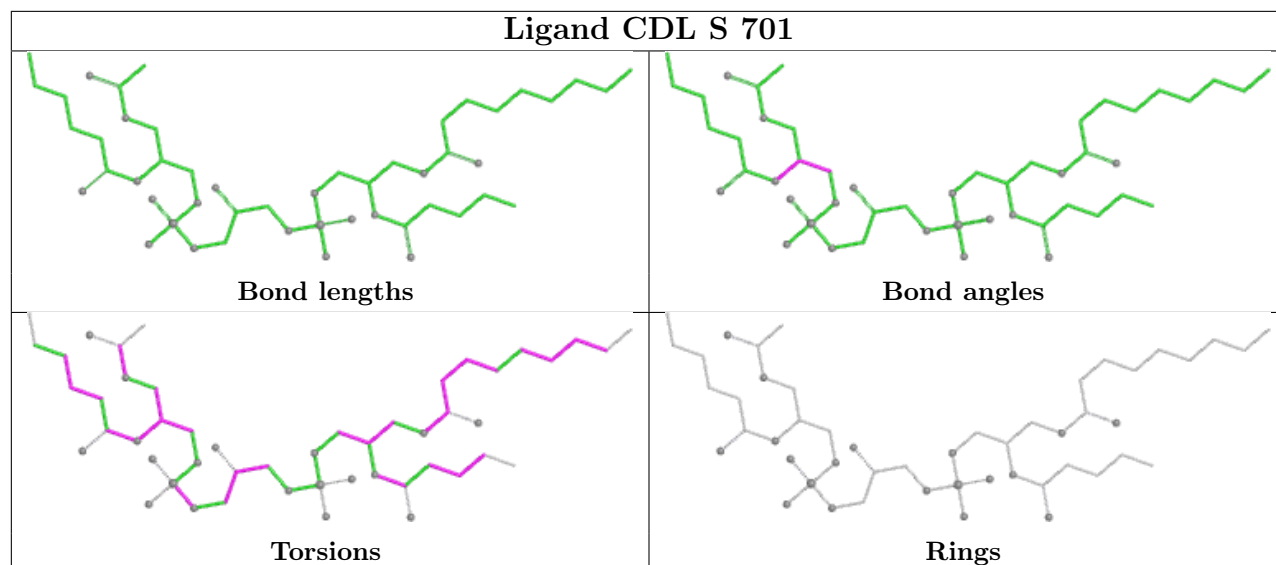


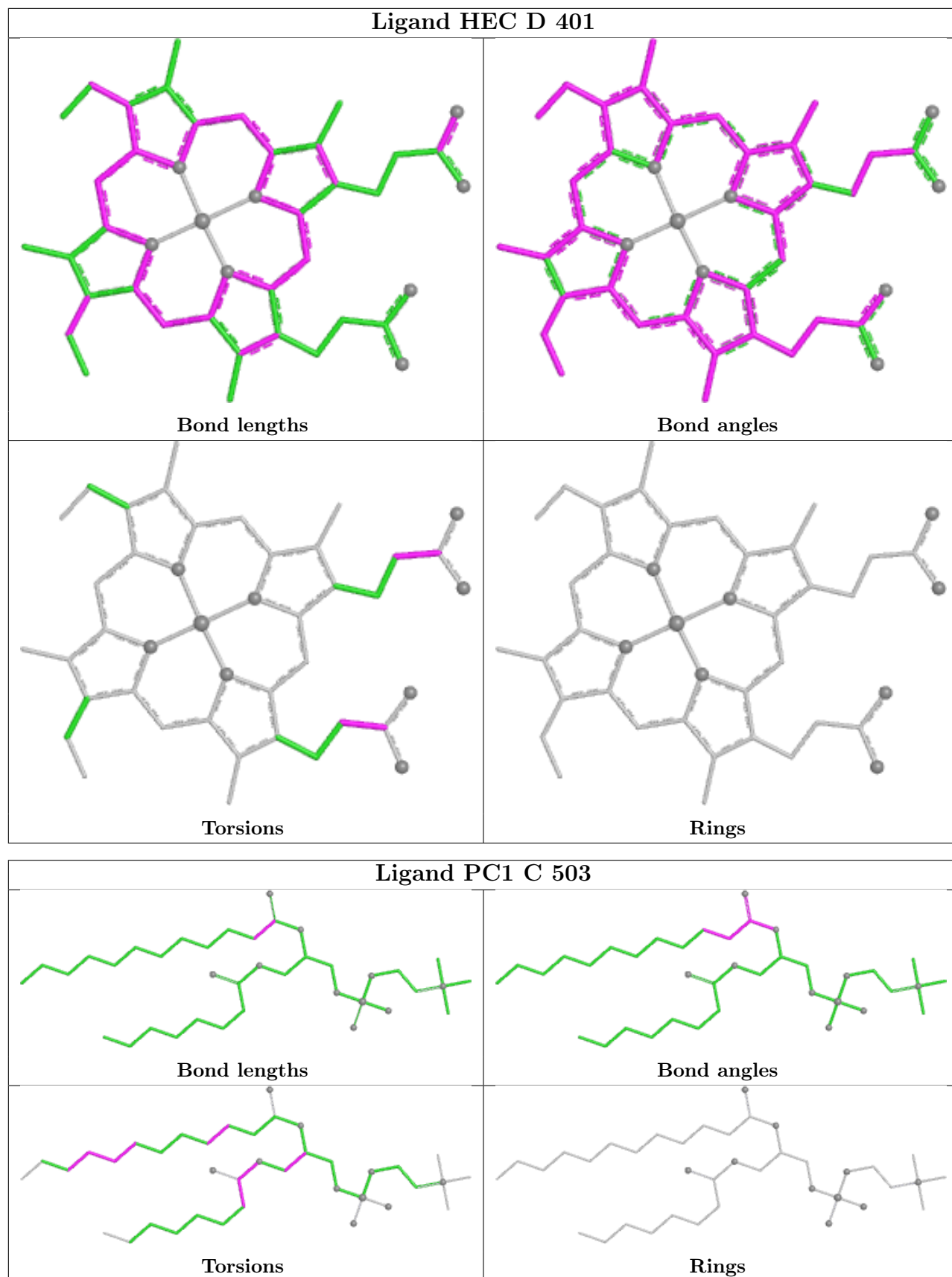


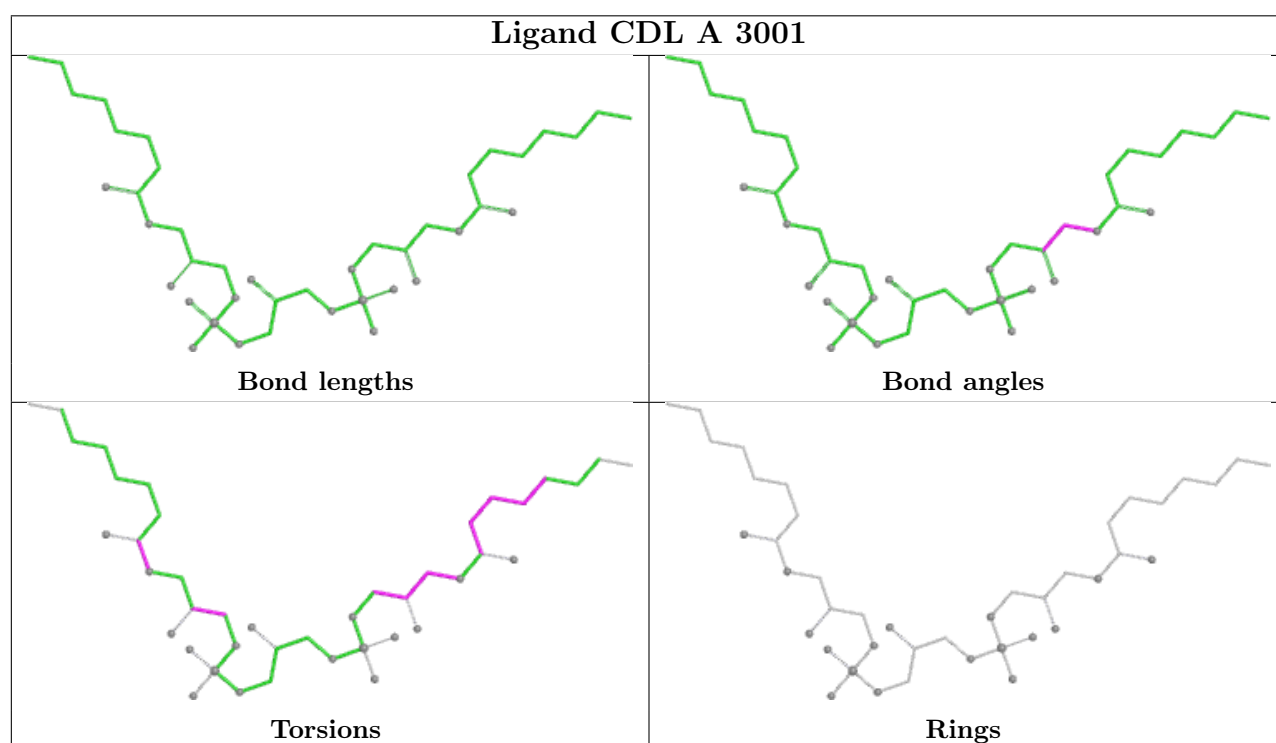
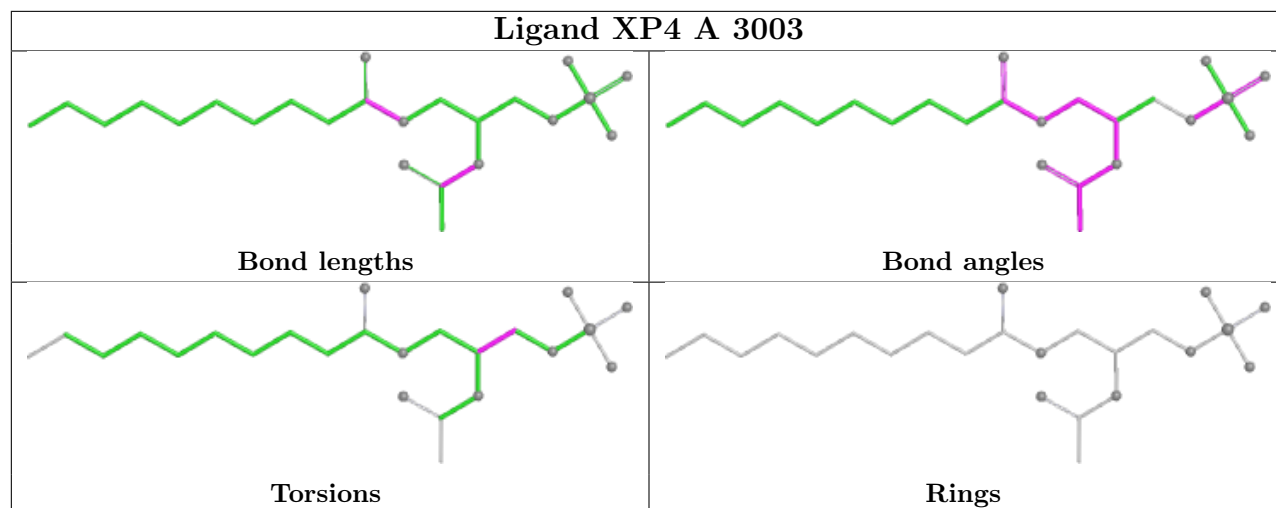


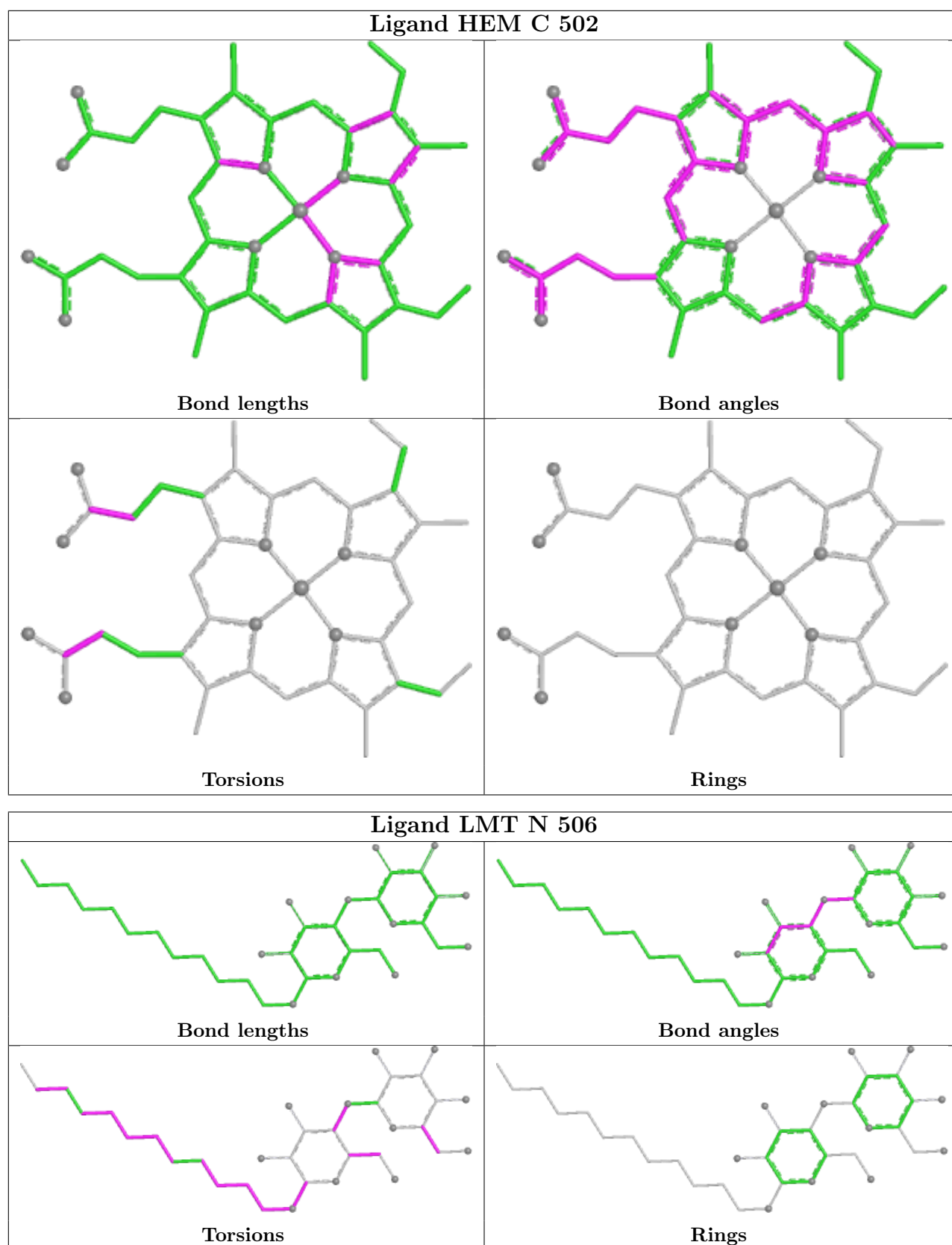


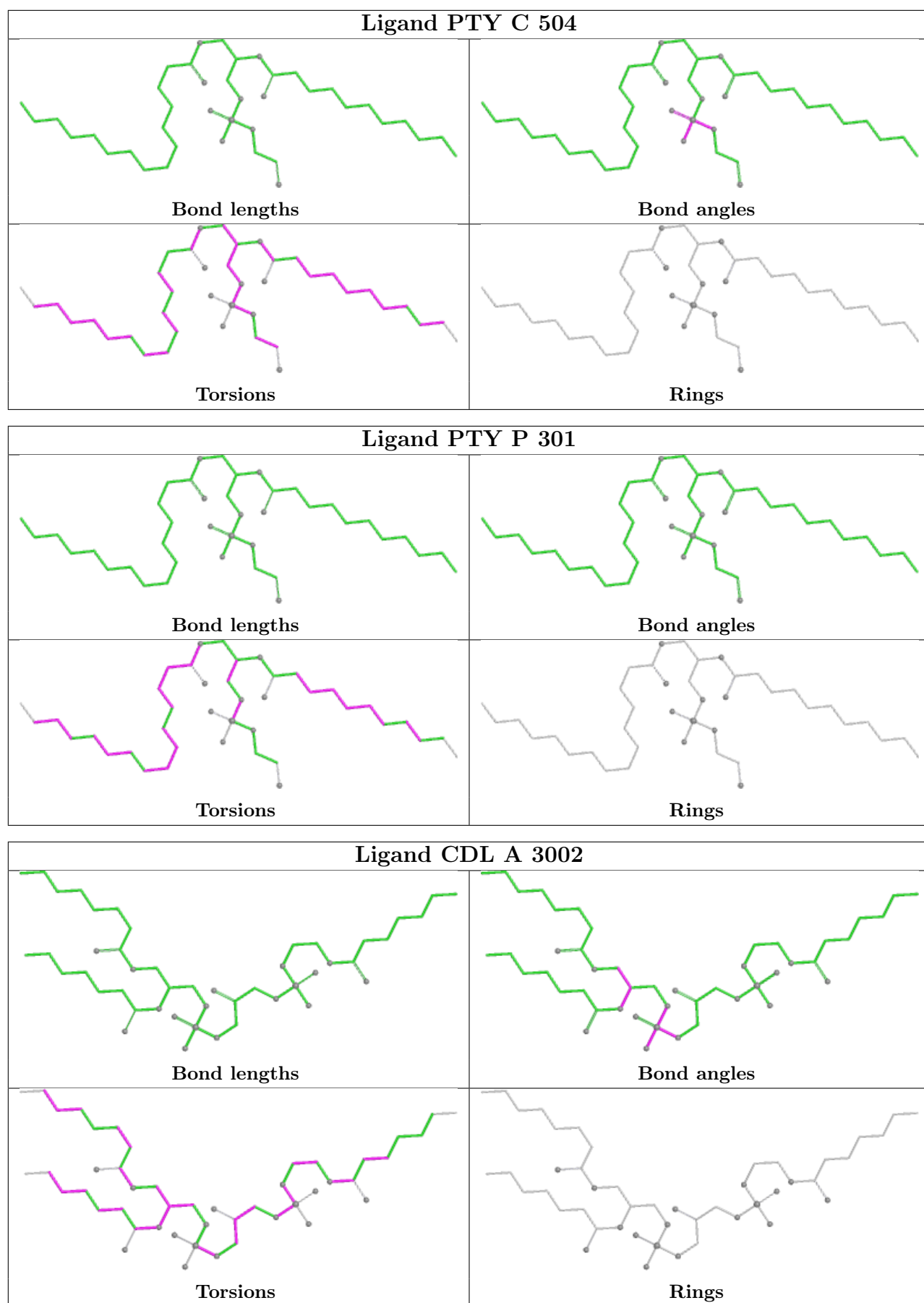


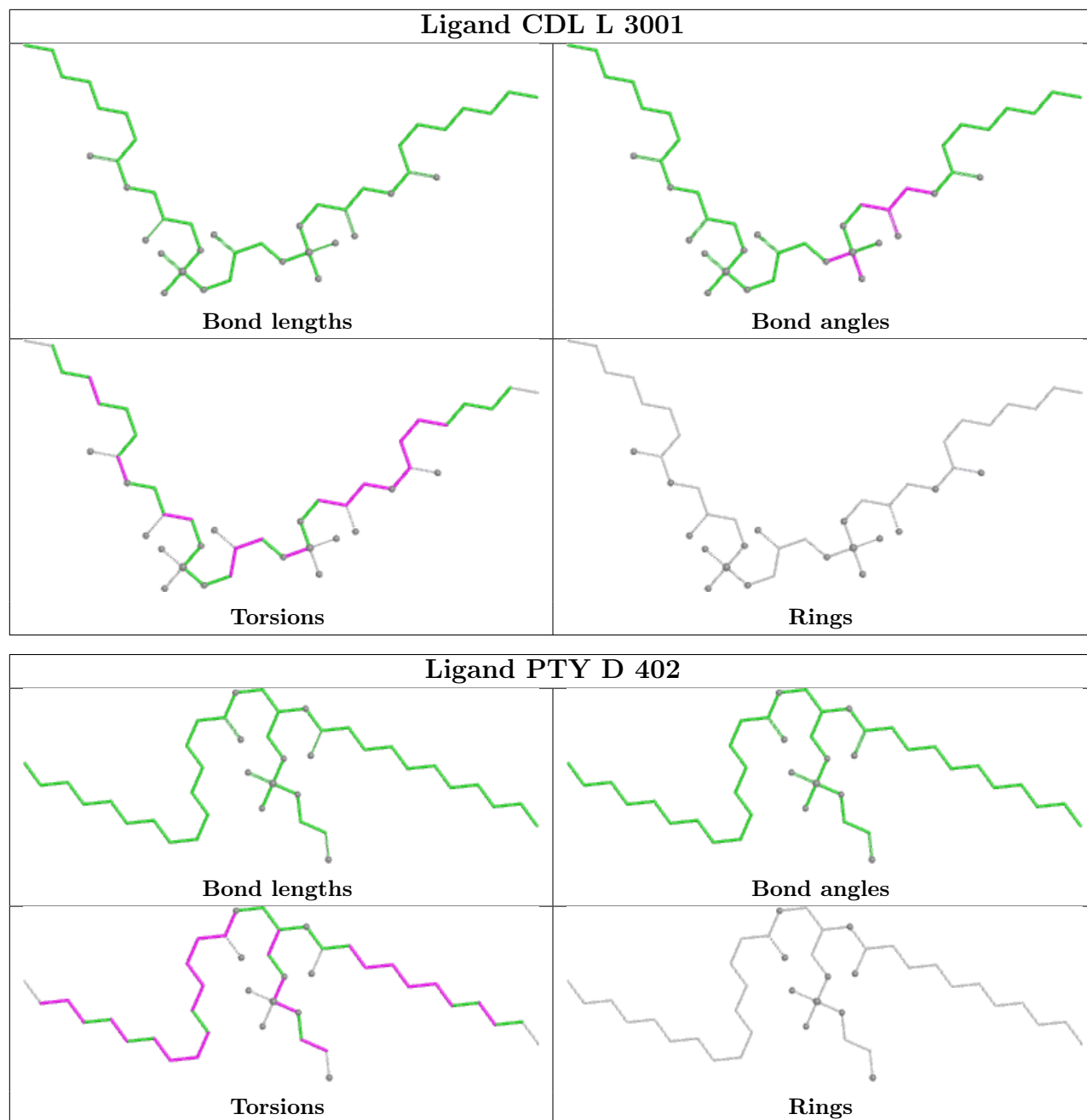


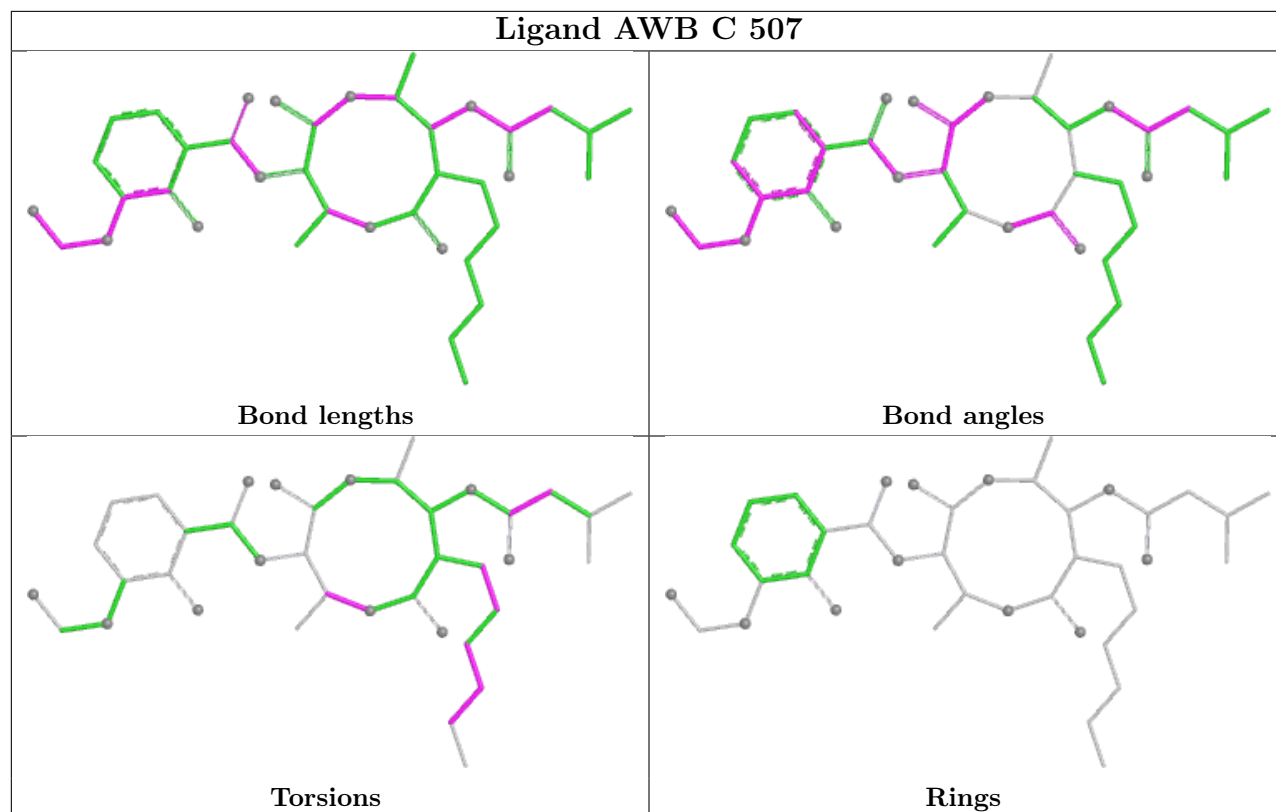












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

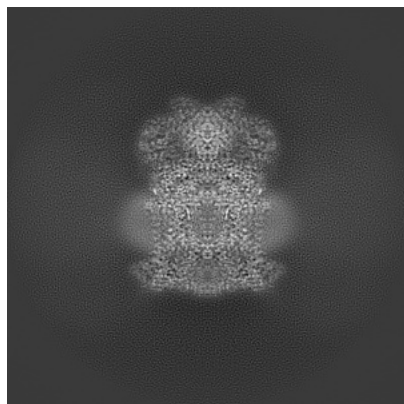
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15325. These allow visual inspection of the internal detail of the map and identification of artifacts.

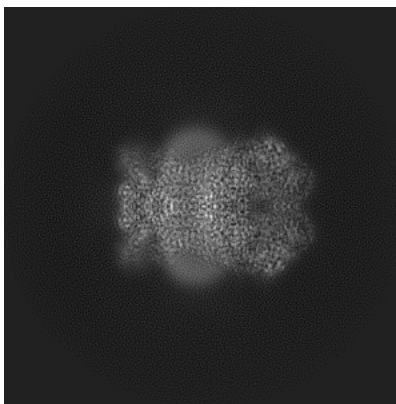
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

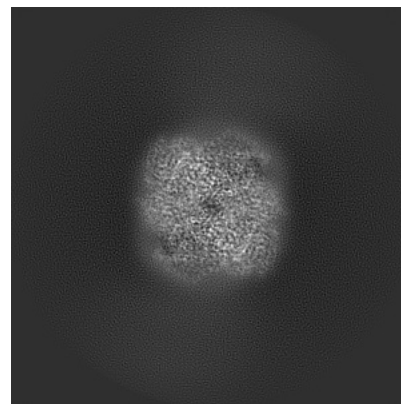
6.1.1 Primary map



X

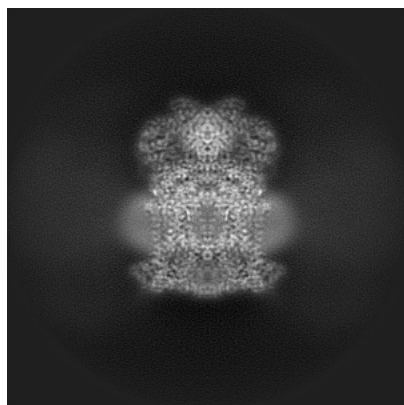


Y

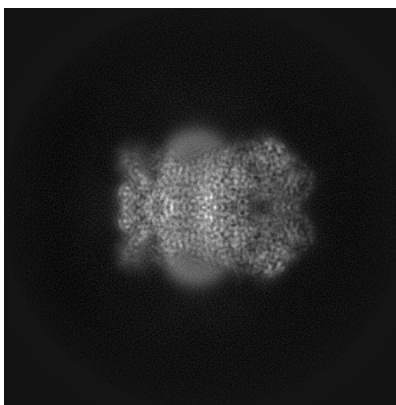


Z

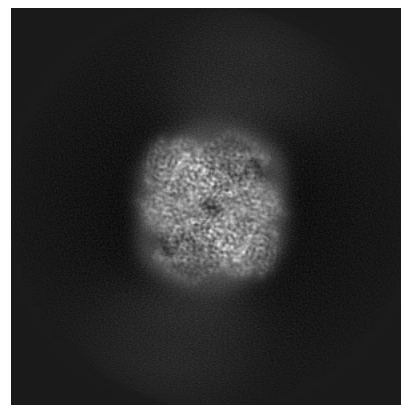
6.1.2 Raw map



X



Y

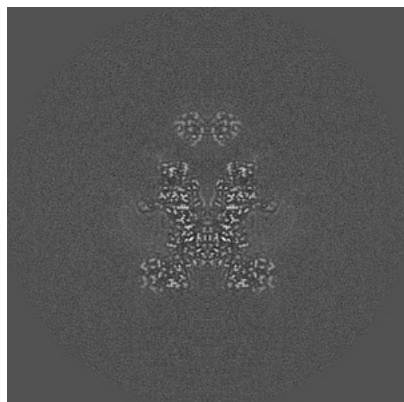


Z

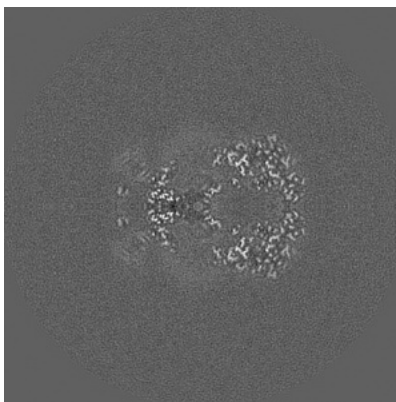
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

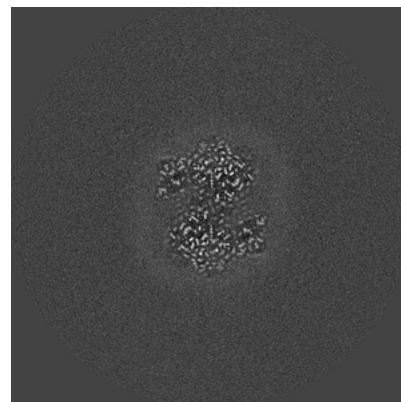
6.2.1 Primary map



X Index: 180

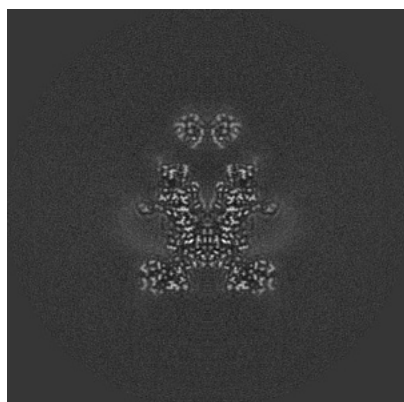


Y Index: 180

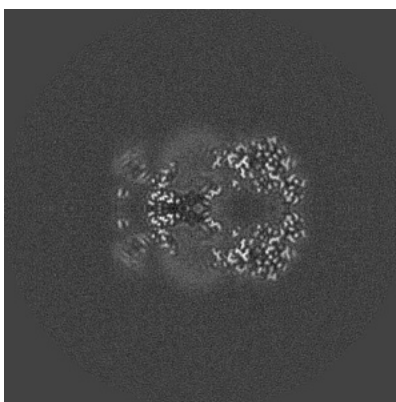


Z Index: 180

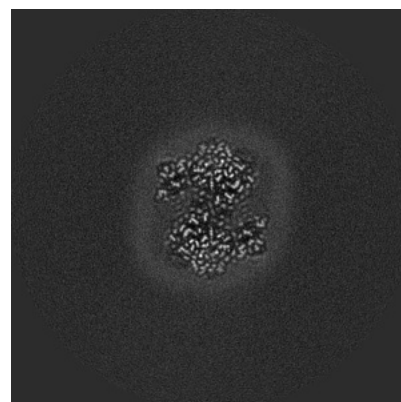
6.2.2 Raw map



X Index: 180



Y Index: 180

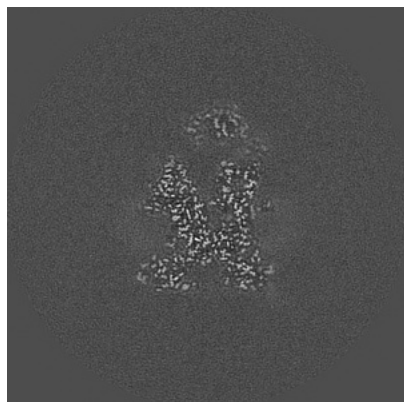


Z Index: 180

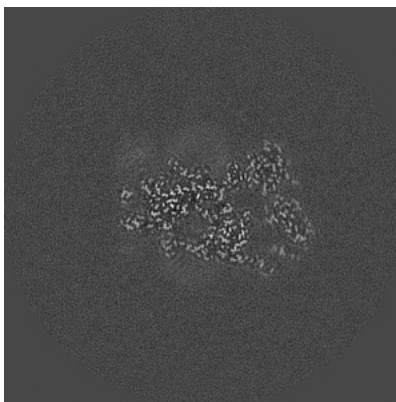
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

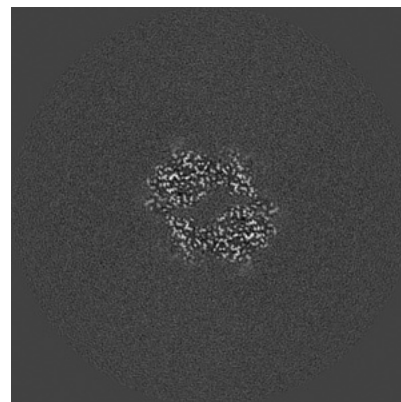
6.3.1 Primary map



X Index: 174

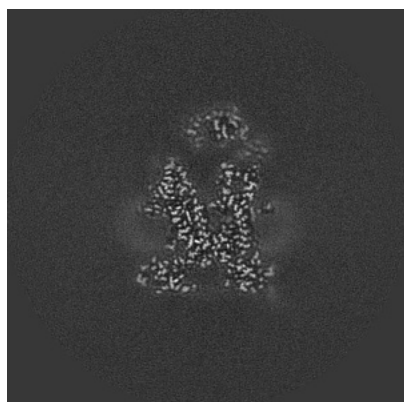


Y Index: 194

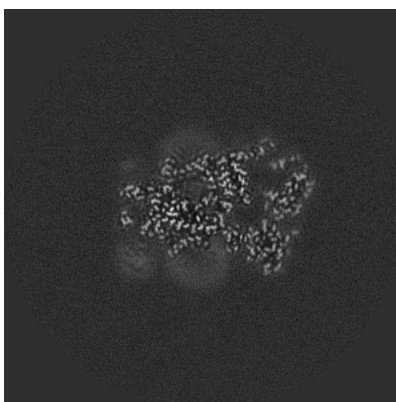


Z Index: 208

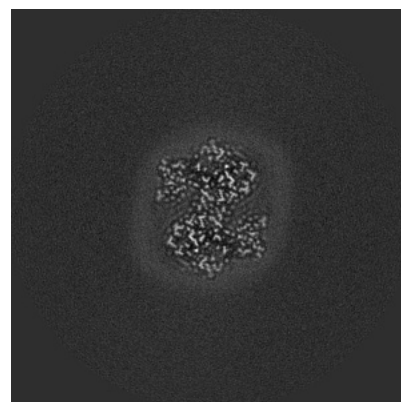
6.3.2 Raw map



X Index: 174



Y Index: 166

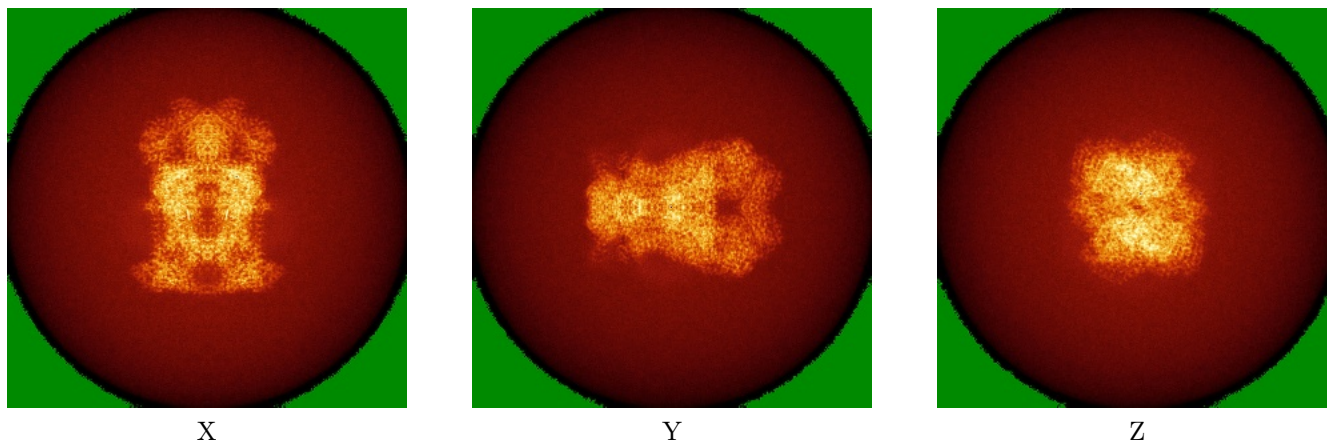


Z Index: 182

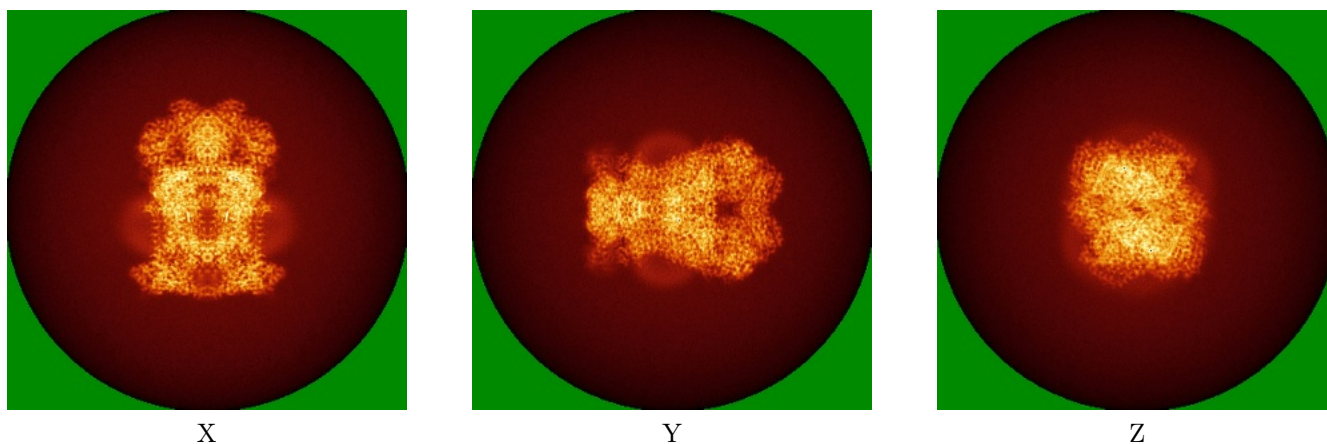
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

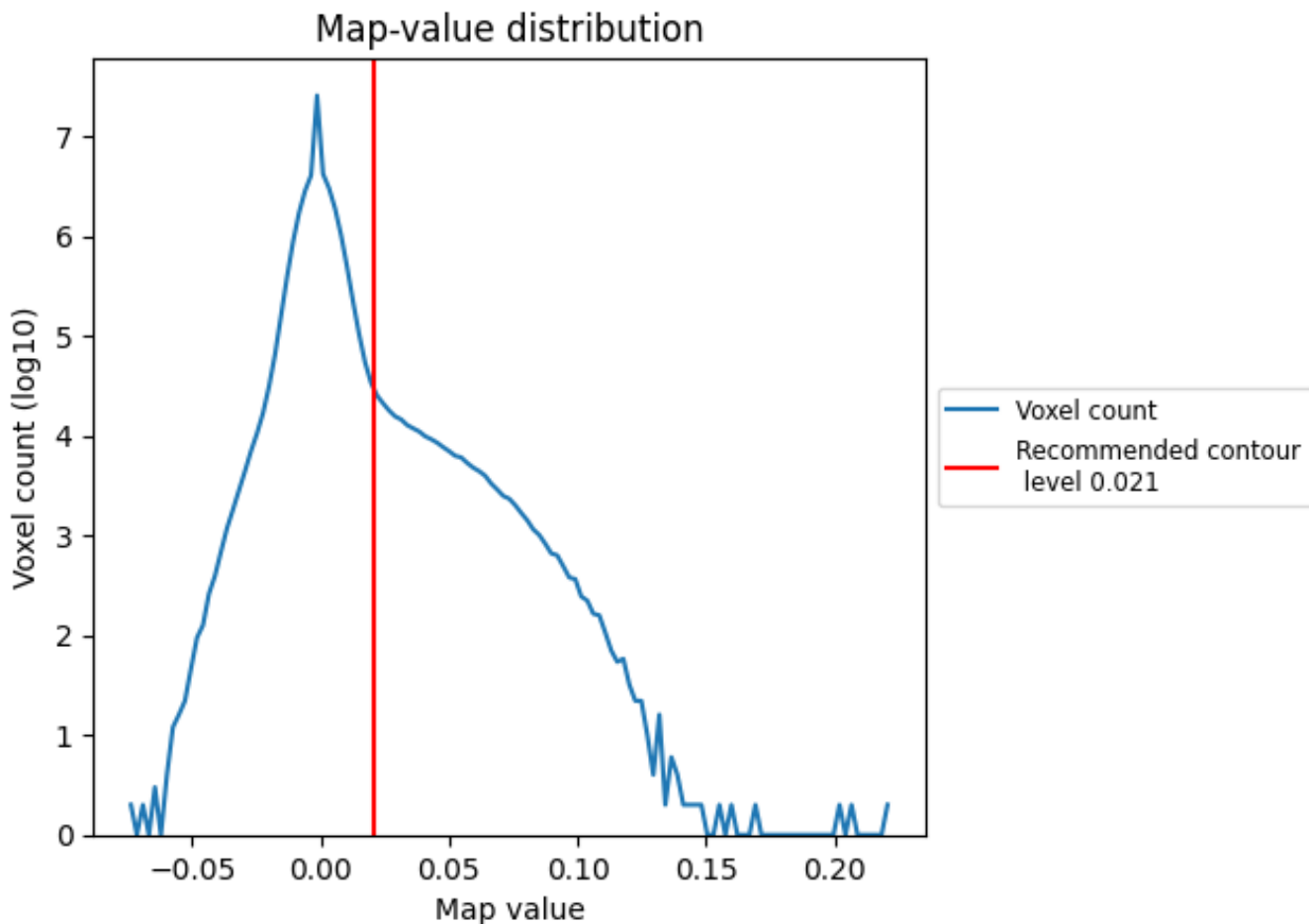
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

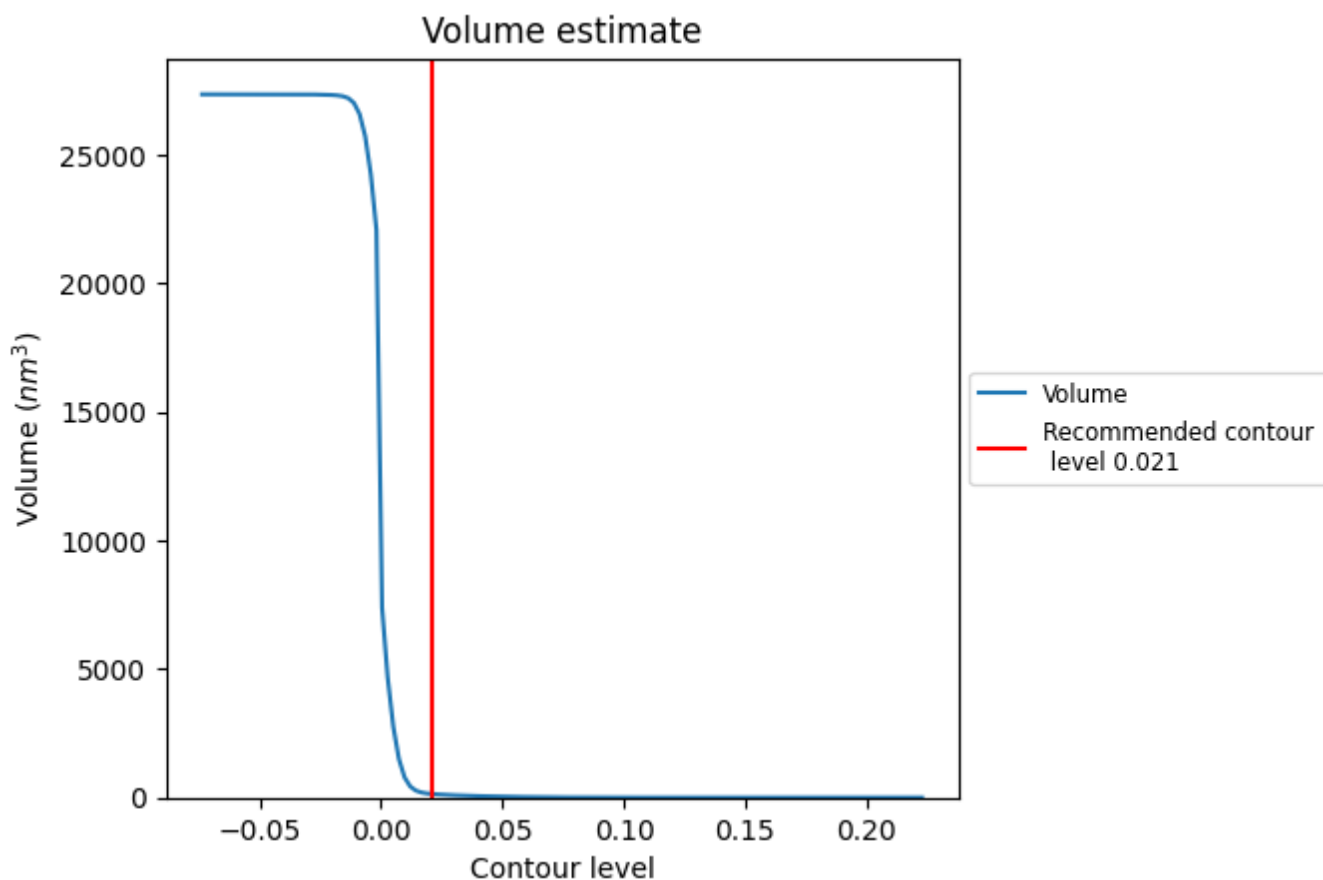
This section contains the results of statistical analysis of the map.

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.

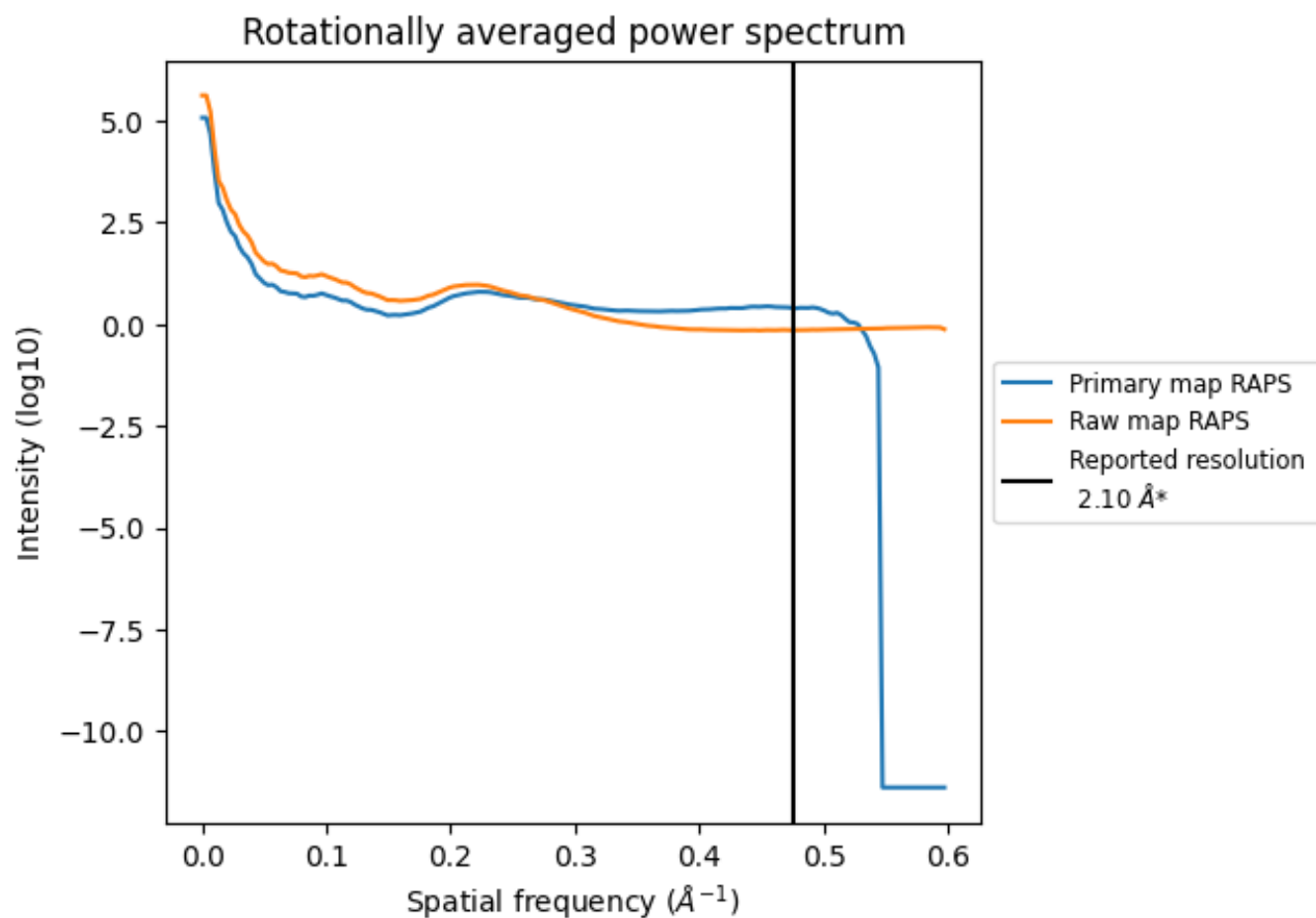
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 140 nm³; this corresponds to an approximate mass of 127 kDa.

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

7.3 Rotationally averaged power spectrum i

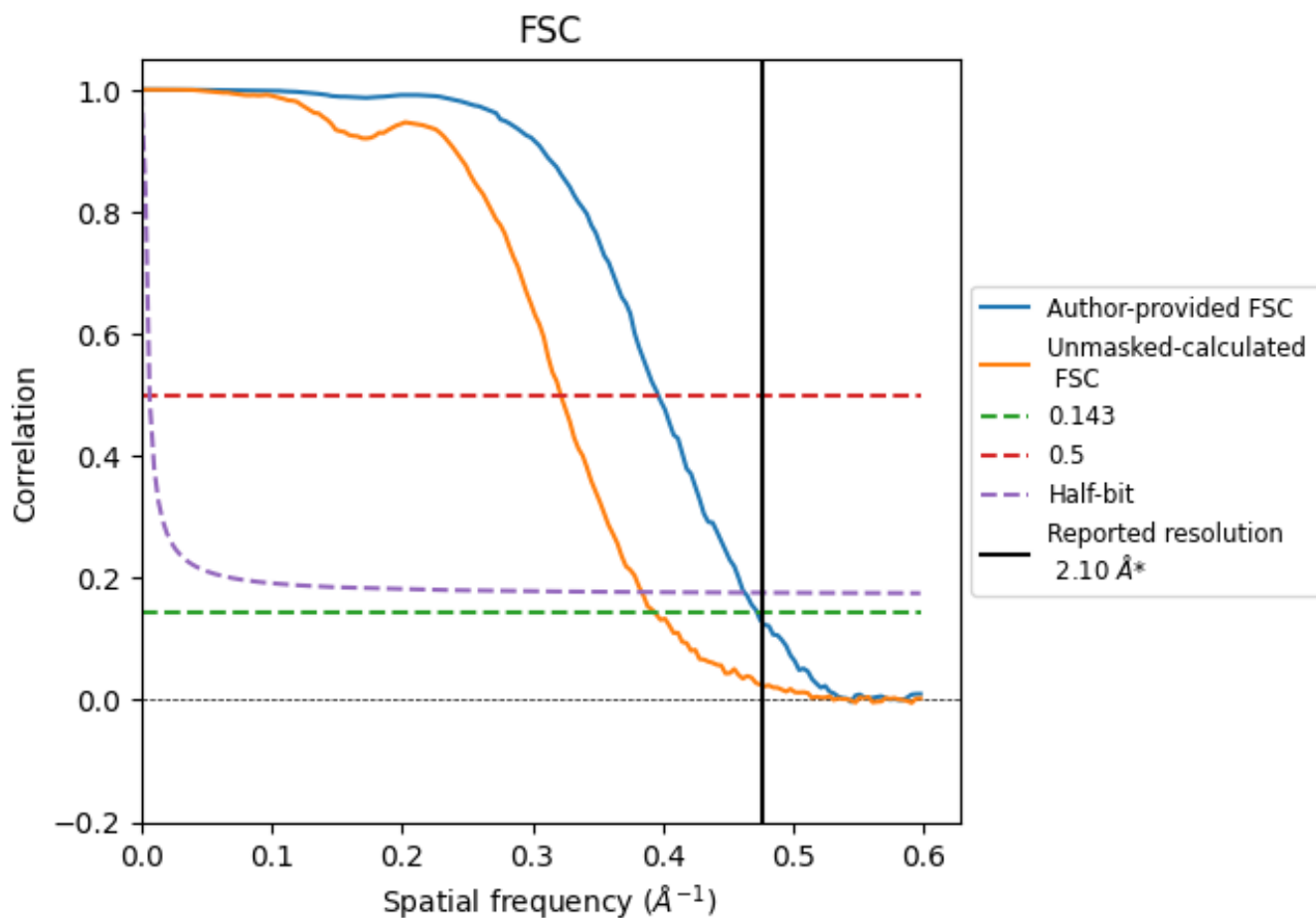


*Reported resolution corresponds to spatial frequency of 0.476 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.476 Å⁻¹

8.2 Resolution estimates [i](#)

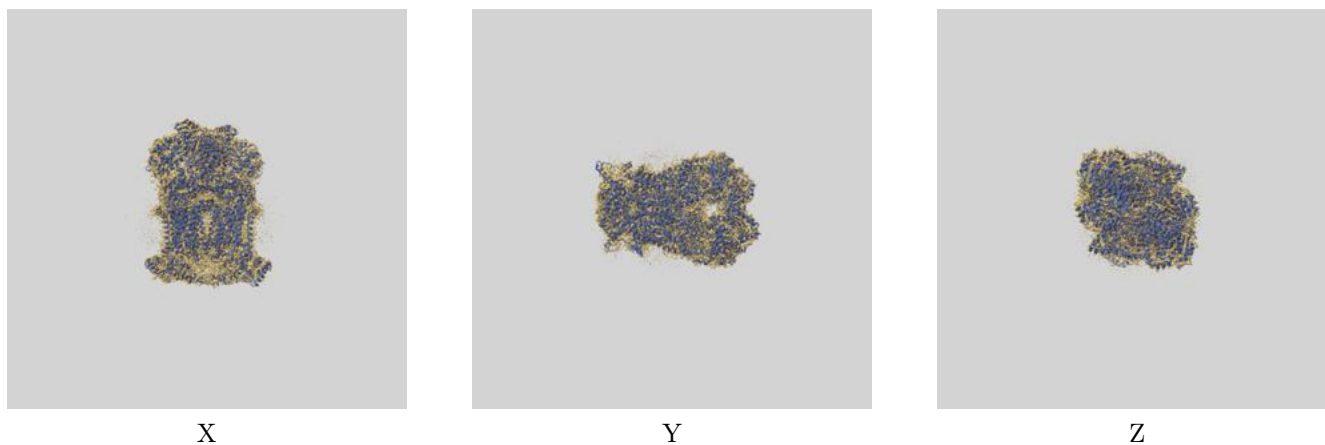
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.12	2.52	2.16
Unmasked-calculated*	2.54	3.11	2.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.54 differs from the reported value 2.1 by more than 10 %

9 Map-model fit [i](#)

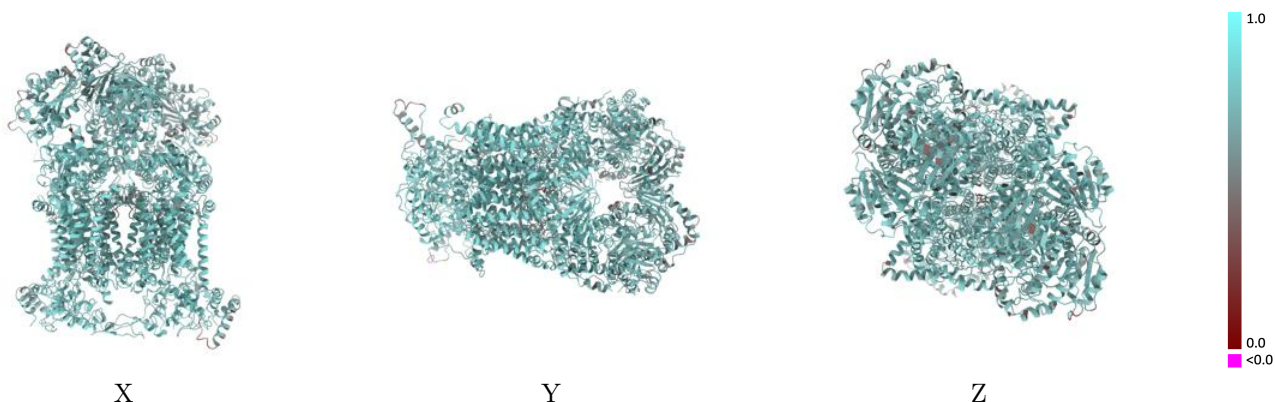
This section contains information regarding the fit between EMDB map EMD-15325 and PDB model 8ABL. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



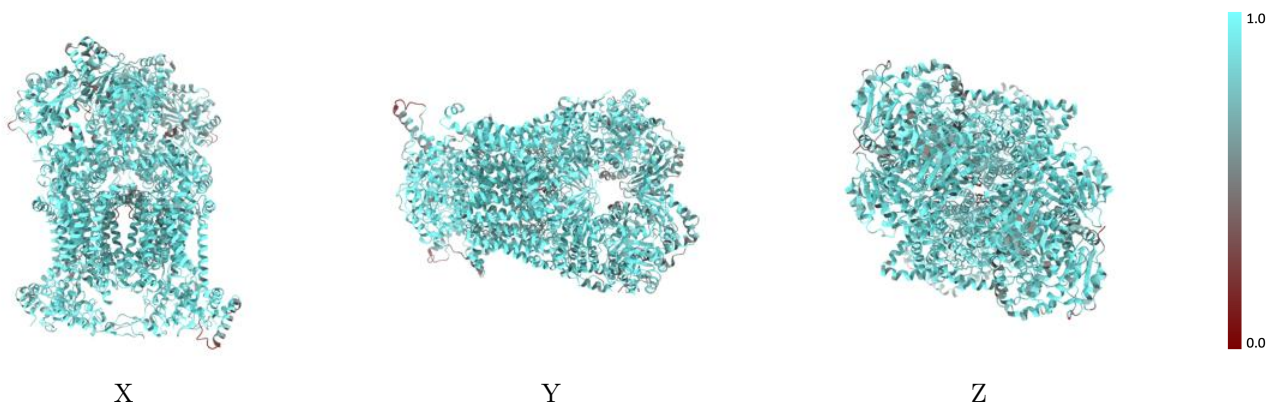
The images above show the 3D surface view of the map at the recommended contour level 0.021 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



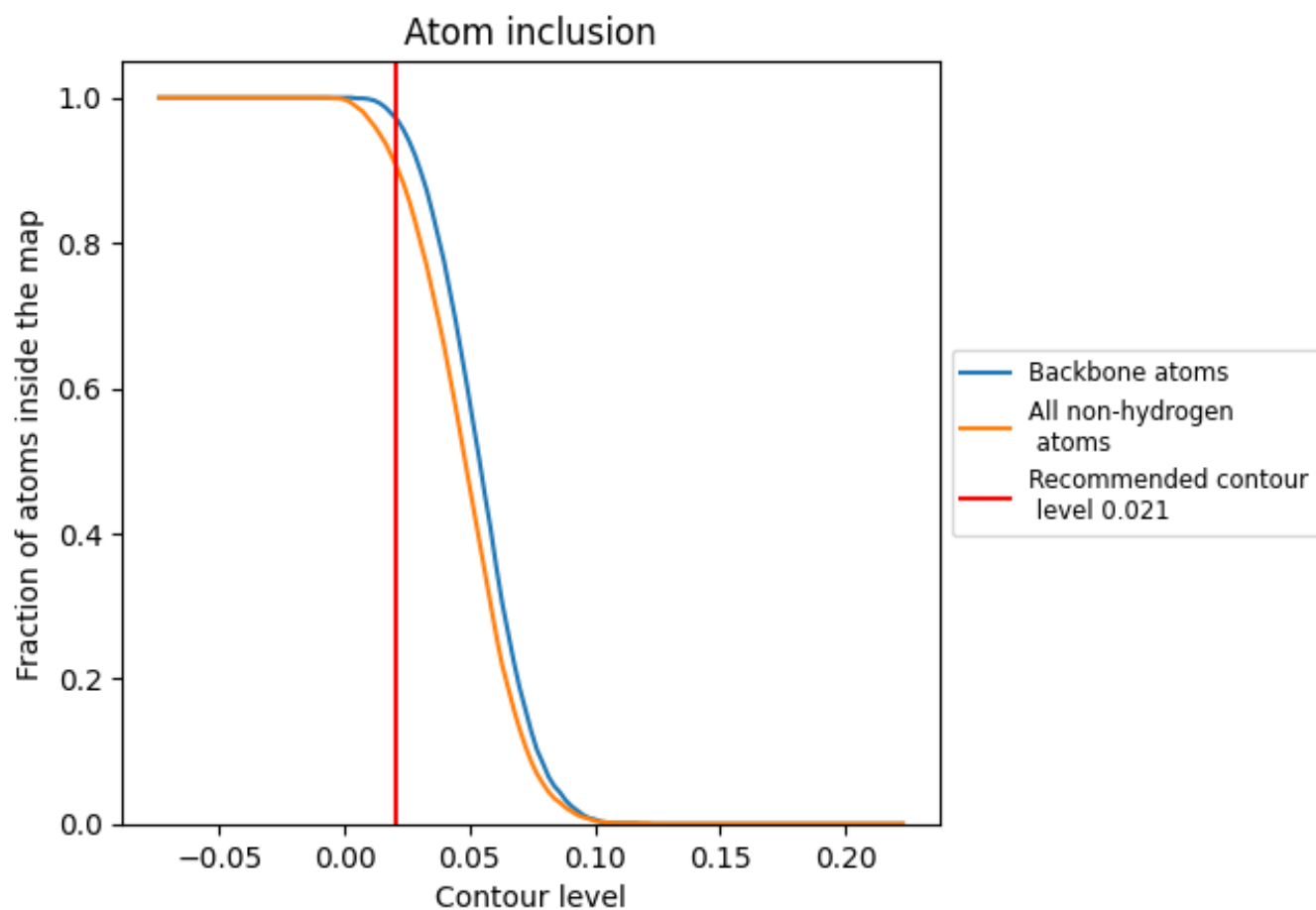
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.021).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 90% 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 (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9040	 0.7230
A	 0.8810	 0.7070
B	 0.8710	 0.6890
C	 0.9620	 0.7690
D	 0.9340	 0.7440
E	 0.9450	 0.7590
F	 0.7230	 0.6100
G	 0.9290	 0.7440
H	 0.9340	 0.7300
I	 0.9540	 0.7500
J	 0.8310	 0.6980
L	 0.8720	 0.7000
M	 0.8740	 0.6890
N	 0.9620	 0.7680
O	 0.9410	 0.7460
P	 0.9320	 0.7510
Q	 0.7230	 0.6160
R	 0.9280	 0.7460
S	 0.9330	 0.7290
T	 0.9470	 0.7480
U	 0.8380	 0.7050

