



Full wwPDB EM Validation Report ⓘ

Apr 14, 2026 – 10:26 am BST

PDB ID : 9SFJ / pdb_00009sfj
EMDB ID : EMD-54826
Title : E.coli cytochrome bd-I dimer in the MK bound open and closed state
Authors : van der Velden, T.T.; Kaystha, K.; Bruenle, S.; Jeuken, L.J.C.
Deposited on : 2025-08-19
Resolution : 2.52 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 : 1.8.4, CSD as541be (2020)
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

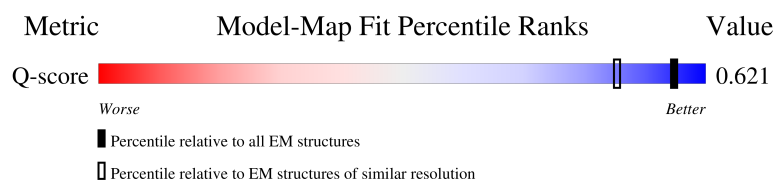
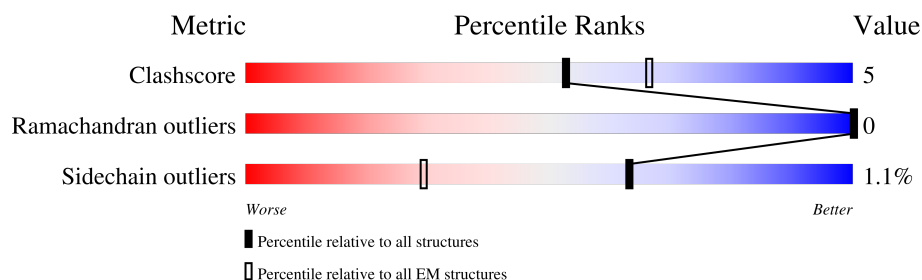
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.52 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	7226 (2.02 - 3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	522	 82% 7% 10%
1	a	522	 88% 11% .
2	B	379	 92% 8%
2	b	379	 91% 9%

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Mol	Chain	Length	Quality of chain
3	H	29	 93% 7%
3	h	29	 86% 14%
4	X	37	 68% 14% 19%
4	x	37	 65% 16% 19%

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
6	A1JN4	A	602	X	-	-	-
6	A1JN4	a	607	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 31200 atoms, of which 15734 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 bd-I ubiquinol oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	468	Total	C	H	N	O	S	0	0
			7407	2434	3717	594	637	25		
1	a	514	Total	C	H	N	O	S	0	0
			8116	2668	4068	649	706	25		

- Molecule 2 is a protein called Cytochrome bd-I ubiquinol oxidase subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	379	Total	C	H	N	O	S	0	0
			6021	1986	3025	483	505	22		
2	b	379	Total	C	H	N	O	S	0	0
			6021	1986	3025	483	505	22		

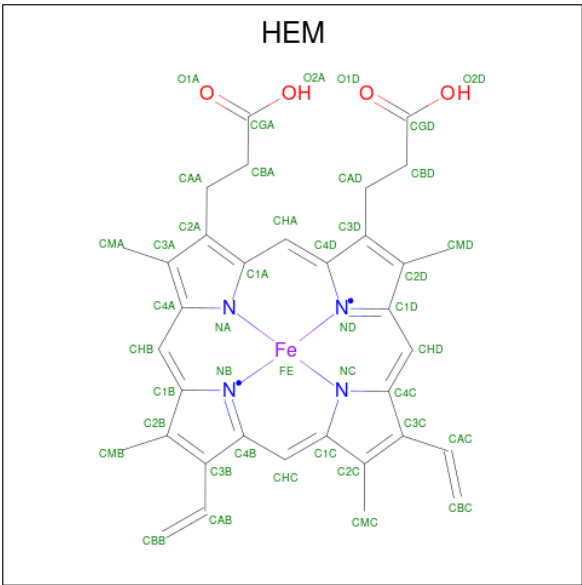
- Molecule 3 is a protein called Cytochrome bd-I ubiquinol oxidase CydH (Uncharacterized protein YnhF).

Mol	Chain	Residues	Atoms						AltConf	Trace
3	H	29	Total	C	H	N	O	S	0	0
			424	139	215	32	37	1		
3	h	29	Total	C	H	N	O	S	0	0
			432	139	222	32	38	1		

- Molecule 4 is a protein called Cytochrome bd-I ubiquinol oxidase subunit X.

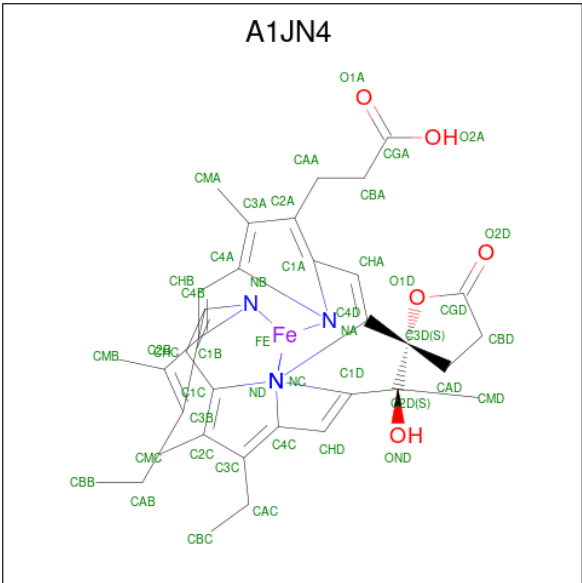
Mol	Chain	Residues	Atoms						AltConf	Trace
4	X	30	Total	C	H	N	O	S	0	0
			451	157	219	34	39	2		
4	x	30	Total	C	H	N	O	S	0	0
			451	157	219	34	39	2		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



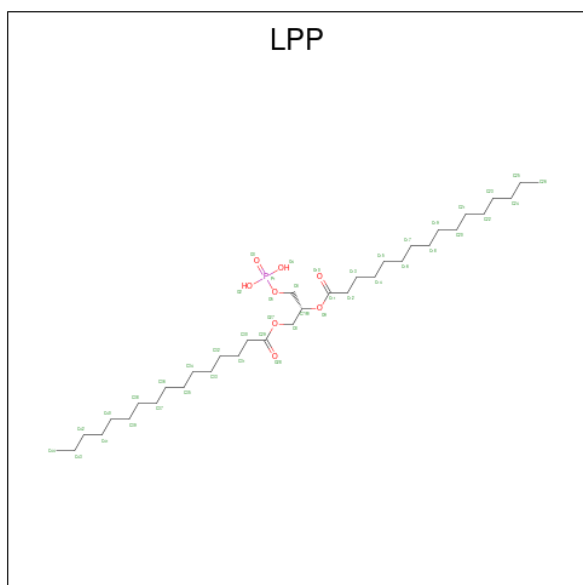
Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
5	A	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
5	a	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
5	a	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 6 is TRANS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: A1JN4) (formula: $C_{34}H_{36}FeN_4O_5$).



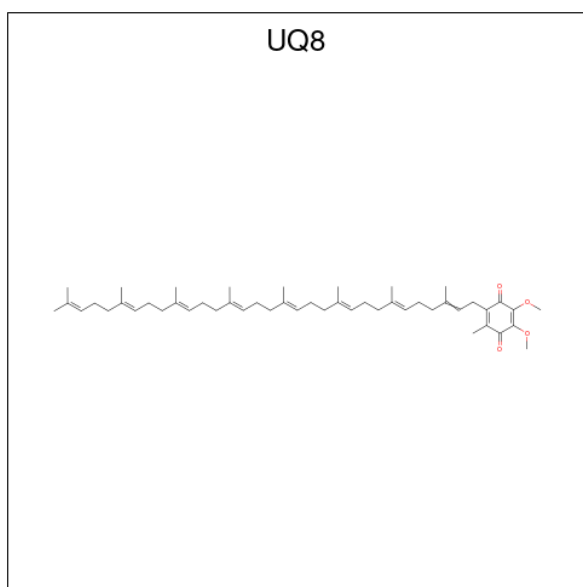
Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	Fe	H	N	O	0
			75	34	1	31	4	5	
6	a	1	Total	C	Fe	H	N	O	0
			75	34	1	31	4	5	

- Molecule 7 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: $C_{35}H_{69}O_8P$).



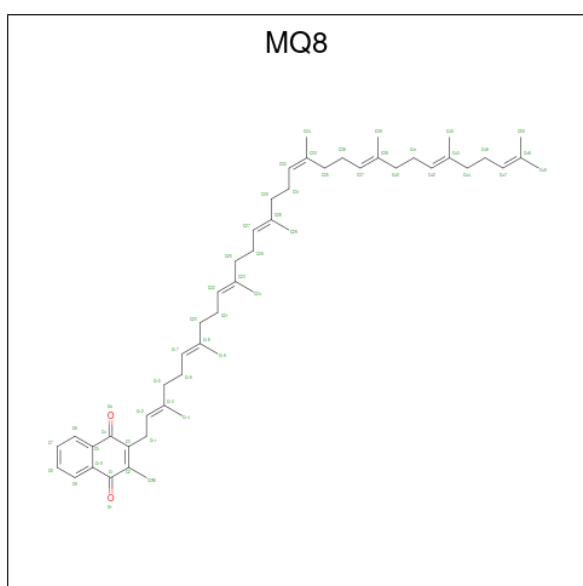
Mol	Chain	Residues	Atoms						AltConf
7	A	1	Total	C	H	O	P		0
			111	35	67	8	1		
7	B	1	Total	C	H	O	P		0
			111	35	67	8	1		
7	a	1	Total	C	H	O	P		0
			111	35	67	8	1		
7	a	1	Total	C	H	O	P		0
			111	35	67	8	1		
7	b	1	Total	C	H	O	P		0
			111	35	67	8	1		
7	x	1	Total	C	H	O	P		0
			111	35	67	8	1		

- Molecule 8 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$) (labeled as "Ligand of Interest" by depositor).



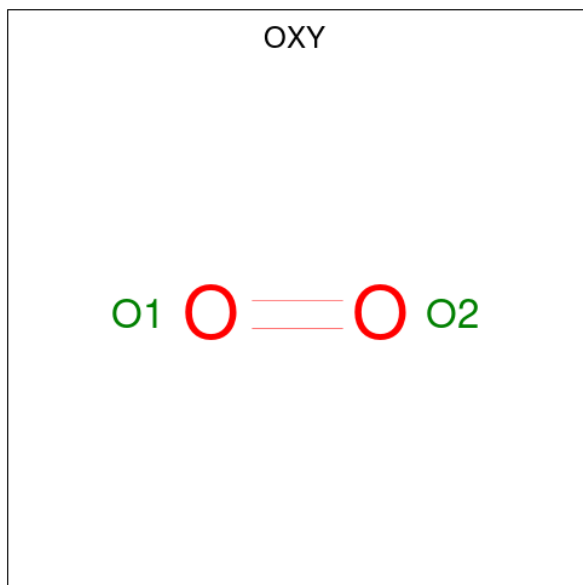
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	H	O	0
			127	49	74	4	
8	B	1	Total	C	H	O	0
			127	49	74	4	
8	a	1	Total	C	H	O	0
			127	49	74	4	
8	b	1	Total	C	H	O	0
			127	49	74	4	

- Molecule 9 is MENAQUINONE 8 (CCD ID: MQ8) (formula: $C_{51}H_{72}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	H	O	0
			125	51	72	2	
9	a	1	Total	C	H	O	0
			125	51	72	2	

- Molecule 10 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms		AltConf
10	a	1	Total	O	0
			2	2	

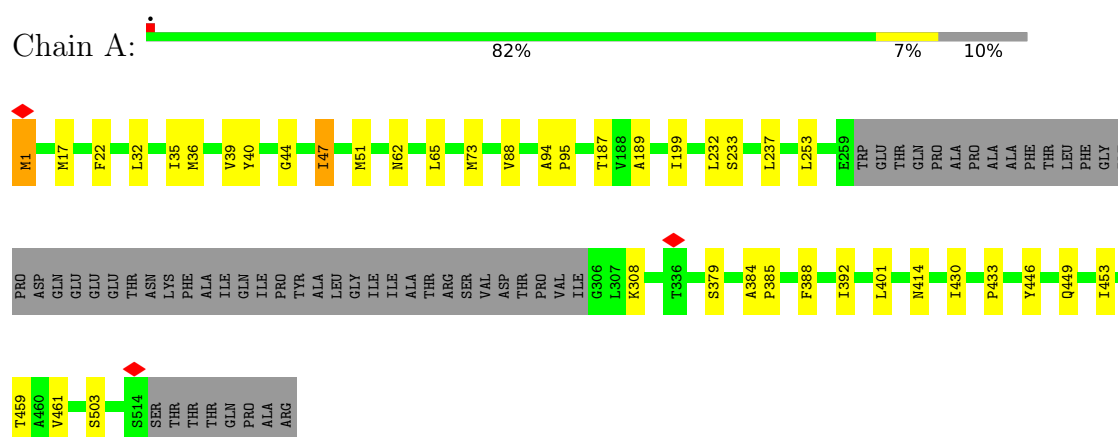
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	O	0
			1	1	
11	B	1	Total	O	0
			1	1	
11	a	3	Total	O	0
			3	3	
11	b	4	Total	O	0
			4	4	

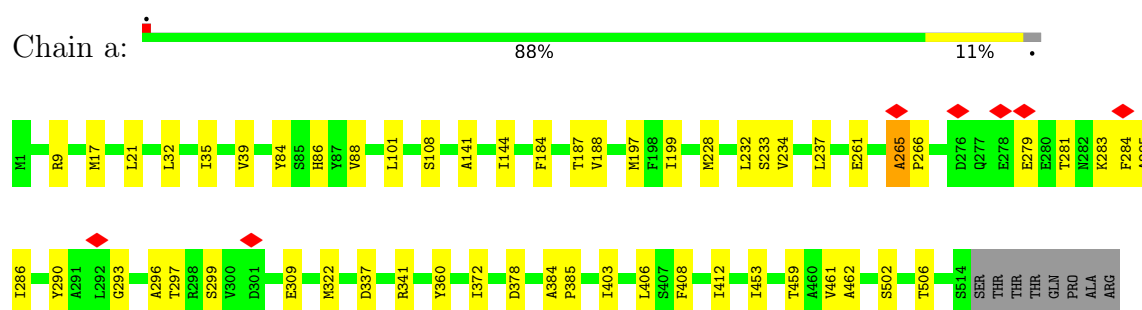
3 Residue-property plots

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.

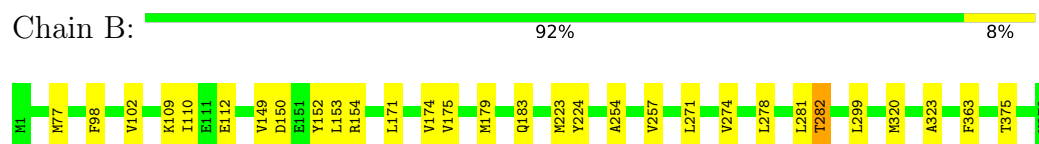
- Molecule 1: Cytochrome bd-I ubiquinol oxidase subunit 1



- Molecule 1: Cytochrome bd-I ubiquinol oxidase subunit 1

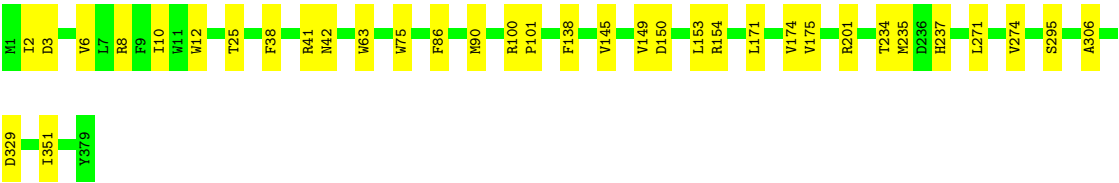


- Molecule 2: Cytochrome bd-I ubiquinol oxidase subunit 2



- Molecule 2: Cytochrome bd-I ubiquinol oxidase subunit 2

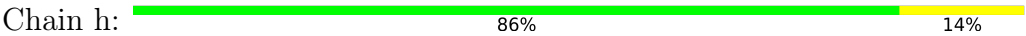




● Molecule 3: Cytochrome bd-I ubiquinol oxidase CydH (Uncharacterized protein YnhF)



● Molecule 3: Cytochrome bd-I ubiquinol oxidase CydH (Uncharacterized protein YnhF)



● Molecule 4: Cytochrome bd-I ubiquinol oxidase subunit X



● Molecule 4: Cytochrome bd-I ubiquinol oxidase subunit X



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	224083	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	2.005	Depositor
Minimum map value	-1.153	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.125	Depositor
Map size (Å)	316.8, 316.8, 316.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UQ8, LPP, OXY, A1JN4, HEM, MQ8

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/3784	0.42	6/5122 (0.1%)
1	a	0.16	0/4154	0.27	0/5634
2	B	0.14	0/3083	0.32	2/4212 (0.0%)
2	b	0.15	0/3083	0.31	2/4212 (0.0%)
3	H	0.12	0/210	0.19	0/286
3	h	0.15	0/211	0.32	0/286
4	X	0.15	0/239	0.25	0/326
4	x	0.14	0/239	0.20	0/326
All	All	0.15	0/15003	0.33	10/20404 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	MET	CA-C-N	10.32	141.25	121.54
1	A	1	MET	C-N-CA	10.32	141.25	121.54
1	A	47	ILE	CA-C-N	9.27	134.39	120.31
1	A	47	ILE	C-N-CA	9.27	134.39	120.31
1	A	503	SER	CA-C-N	8.19	132.08	120.28
1	A	503	SER	C-N-CA	8.19	132.08	120.28
2	B	174	VAL	CA-C-N	8.05	131.50	120.46
2	B	174	VAL	C-N-CA	8.05	131.50	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	174	VAL	CA-C-N	8.05	131.48	120.46
2	b	174	VAL	C-N-CA	8.05	131.48	120.46

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	265	ALA	Peptide

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	A	3690	3717	3726	30	0
1	a	4048	4068	4078	36	0
2	B	2996	3025	3025	21	0
2	b	2996	3025	3025	22	0
3	H	209	215	238	2	0
3	h	210	222	238	3	0
4	X	232	219	230	3	0
4	x	232	219	230	3	0
5	A	86	60	60	13	0
5	a	86	60	60	14	0
6	A	44	31	0	0	0
6	a	44	31	0	1	0
7	A	44	67	67	4	0
7	B	44	67	67	0	0
7	a	88	134	134	3	0
7	b	44	67	67	0	0
7	x	44	67	67	0	0
8	A	53	74	74	10	0
8	B	53	74	74	5	0
8	a	53	74	74	12	0
8	b	53	74	74	8	0
9	A	53	72	72	7	0
9	a	53	72	72	6	0
10	a	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	a	3	0	0	1	0
11	b	4	0	0	0	0
All	All	15466	15734	15752	165	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 5.

All (165) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:309:GLU:N	1:a:309:GLU:OE1	2.09	0.85
7:A:603:LPP:H442	7:A:603:LPP:H261	1.58	0.84
1:A:187:THR:OG1	5:A:601:HEM:O1A	1.96	0.82
5:A:604:HEM:HBC2	5:A:604:HEM:HHD	1.62	0.82
8:a:604:UQ8:H10A	8:a:604:UQ8:C15	2.10	0.81
5:a:603:HEM:HBC2	5:a:603:HEM:HHD	1.63	0.81
5:a:601:HEM:HBC2	5:a:601:HEM:HHD	1.64	0.80
5:A:604:HEM:HHC	5:A:604:HEM:HBB2	1.67	0.77
5:a:603:HEM:HBB2	5:a:603:HEM:HHC	1.66	0.77
1:a:187:THR:OG1	5:a:601:HEM:O1A	2.01	0.77
8:a:604:UQ8:H10A	8:a:604:UQ8:H15B	1.73	0.70
9:A:606:MQ8:H241	9:A:606:MQ8:C27	2.23	0.69
2:B:183:GLN:HG3	2:B:299:LEU:HD11	1.74	0.69
5:a:603:HEM:HHA	5:a:603:HEM:HBA1	1.76	0.68
5:A:604:HEM:HBA1	5:A:604:HEM:HHA	1.77	0.66
1:a:322:MET:HE1	1:a:372:ILE:HD11	1.79	0.64
7:A:603:LPP:H442	7:A:603:LPP:C26	2.27	0.64
9:a:605:MQ8:H191	9:a:605:MQ8:C22	2.28	0.63
5:A:601:HEM:HHD	5:A:601:HEM:HBC2	1.79	0.63
8:A:605:UQ8:C13	8:A:605:UQ8:H10A	2.28	0.63
1:a:184:PHE:O	1:a:188:VAL:HG22	1.97	0.63
2:B:320:MET:HE2	2:B:323:ALA:HB2	1.81	0.62
2:B:179:MET:HE3	2:B:299:LEU:CD2	2.30	0.61
1:A:232:LEU:HD22	8:A:605:UQ8:H17A	1.82	0.61
1:a:237:LEU:HD11	8:a:604:UQ8:H10	1.83	0.60
5:A:601:HEM:HHD	9:A:606:MQ8:H61	1.82	0.60
1:A:392:ILE:HD11	9:A:606:MQ8:H452	1.84	0.60
5:A:601:HEM:HHA	5:A:601:HEM:HBA1	1.84	0.59
1:A:32:LEU:HD13	1:A:199:ILE:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:17:MET:HG2	5:a:603:HEM:HBC1	1.84	0.58
2:b:8:ARG:NH1	2:b:237:HIS:O	2.37	0.58
2:b:235:MET:HE1	2:b:329:ASP:HB2	1.86	0.58
8:A:605:UQ8:H1MB	8:A:605:UQ8:H8	1.85	0.58
5:a:601:HEM:O2A	11:a:701:HOH:O	2.17	0.57
8:A:605:UQ8:C13	8:A:605:UQ8:C10	2.82	0.57
1:A:88:VAL:HG11	1:A:453:ILE:HG13	1.86	0.57
1:a:237:LEU:CD1	8:a:604:UQ8:H10	2.36	0.56
2:B:223:MET:HE3	8:B:402:UQ8:H4MB	1.87	0.56
8:b:402:UQ8:O3	8:b:402:UQ8:H4MB	2.07	0.55
5:A:601:HEM:HBB2	5:A:601:HEM:HMB2	1.89	0.55
9:a:605:MQ8:H341	9:a:605:MQ8:C37	2.36	0.55
3:h:6:LYS:HB3	3:h:6:LYS:NZ	2.21	0.55
7:a:602:LPP:H261	7:a:602:LPP:H443	1.89	0.55
2:b:25:THR:HG1	2:b:63:TRP:CD1	2.25	0.55
1:a:265:ALA:HB1	1:a:266:PRO:HD2	1.89	0.55
1:A:253:LEU:HD23	9:A:606:MQ8:H143	1.89	0.55
2:B:278:LEU:O	2:B:282:THR:OG1	2.22	0.55
2:b:306:ALA:HB2	8:b:402:UQ8:C10	2.37	0.54
1:A:17:MET:HG2	5:A:604:HEM:HBC1	1.88	0.54
2:B:179:MET:HE3	2:B:299:LEU:HD22	1.87	0.54
8:a:604:UQ8:C25	8:a:604:UQ8:C28	2.86	0.54
9:a:605:MQ8:H191	9:a:605:MQ8:H221	1.89	0.54
5:a:601:HEM:HMB2	5:a:601:HEM:HBB2	1.90	0.54
1:A:237:LEU:HD21	8:A:605:UQ8:H10	1.89	0.54
5:a:601:HEM:HBA1	5:a:601:HEM:HHA	1.89	0.53
1:a:9:ARG:HD3	1:a:459:THR:HG21	1.91	0.53
2:B:150:ASP:C	2:B:150:ASP:OD2	2.52	0.53
2:b:306:ALA:HB2	8:b:402:UQ8:H10B	1.90	0.53
1:A:446:TYR:OH	3:H:29:HIS:HB3	2.08	0.53
4:X:4:PHE:O	4:X:7:ILE:HG22	2.09	0.52
2:b:149:VAL:HG13	2:b:153:LEU:HA	1.91	0.52
8:B:402:UQ8:H4MA	8:B:402:UQ8:O3	2.10	0.52
1:A:384:ALA:HB3	1:A:385:PRO:HD3	1.91	0.52
1:a:285:ALA:C	1:a:286:ILE:HD12	2.35	0.52
1:a:293:GLY:O	1:a:297:THR:OG1	2.28	0.51
1:a:296:ALA:HB2	9:a:605:MQ8:H142	1.92	0.51
5:a:603:HEM:HBC2	5:a:603:HEM:CHD	2.38	0.51
1:A:1:MET:SD	1:A:1:MET:N	2.79	0.51
1:a:9:ARG:NH2	3:h:27:ALA:O	2.44	0.51
1:a:35:ILE:O	1:a:39:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:VAL:O	2:B:320:MET:HE1	2.12	0.50
1:a:233:SER:HB3	1:a:237:LEU:HD22	1.94	0.50
1:a:461:VAL:HG12	1:a:461:VAL:O	2.12	0.50
5:a:601:HEM:HBC2	5:a:601:HEM:CHD	2.39	0.49
5:a:601:HEM:HBB2	5:a:601:HEM:CMB	2.42	0.49
1:a:337:ASP:O	1:a:341:ARG:NH1	2.45	0.49
8:a:604:UQ8:H10A	8:a:604:UQ8:C14	2.42	0.49
2:B:254:ALA:O	2:B:257:VAL:HG22	2.13	0.49
2:B:179:MET:HE3	2:B:299:LEU:HD23	1.95	0.49
2:B:223:MET:CE	8:B:402:UQ8:H4MB	2.43	0.49
1:a:265:ALA:HB1	1:a:266:PRO:CD	2.43	0.48
1:a:32:LEU:HD13	1:a:199:ILE:HD12	1.94	0.48
1:A:388:PHE:HB3	9:A:606:MQ8:H453	1.94	0.48
1:A:449:GLN:OE1	1:A:459:THR:HG21	2.13	0.48
1:a:232:LEU:HD13	8:a:604:UQ8:H13	1.96	0.48
5:a:603:HEM:HHA	5:a:603:HEM:CBA	2.43	0.47
4:X:17:GLY:O	4:X:20:THR:HG22	2.14	0.47
2:b:12:TRP:NE1	8:b:402:UQ8:H40A	2.29	0.47
2:b:38:PHE:O	2:b:41:ARG:NH1	2.48	0.47
9:A:606:MQ8:H162	9:A:606:MQ8:H141	1.67	0.47
4:x:14:CYS:O	4:x:18:VAL:HG23	2.15	0.47
1:A:62:ASN:OD1	7:A:603:LPP:H441	2.15	0.46
2:B:271:LEU:HA	2:B:274:VAL:HG22	1.97	0.46
4:x:4:PHE:O	4:x:7:ILE:HG22	2.15	0.46
2:b:138:PHE:CZ	8:b:402:UQ8:H35B	2.50	0.46
2:B:98:PHE:O	2:B:102:VAL:HG22	2.16	0.46
1:A:35:ILE:O	1:A:39:VAL:HG23	2.16	0.46
2:b:171:LEU:O	2:b:175:VAL:HG23	2.15	0.46
2:B:171:LEU:O	2:B:175:VAL:HG23	2.16	0.46
2:B:363:PHE:C	2:B:363:PHE:CD1	2.94	0.46
5:A:601:HEM:HBB2	5:A:601:HEM:CMB	2.45	0.45
1:a:108:SER:OG	6:a:607:A1JN4:O2A	2.33	0.45
1:A:73:MET:HA	1:A:73:MET:HE2	1.99	0.45
2:B:223:MET:HB3	2:B:224:TYR:HD1	1.82	0.45
1:A:308:LYS:HE2	1:A:308:LYS:H	1.82	0.45
1:a:384:ALA:HB3	1:a:385:PRO:HD3	1.99	0.45
1:A:36:MET:HG2	1:A:51:MET:HE3	1.98	0.44
5:A:604:HEM:HHA	5:A:604:HEM:CBA	2.45	0.44
2:b:100:ARG:HB2	2:b:101:PRO:HD3	2.00	0.44
1:A:47:ILE:O	1:A:51:MET:HG3	2.18	0.44
2:b:75:TRP:HH2	8:b:402:UQ8:H40	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:606:MQ8:C12	9:A:606:MQ8:O4	2.66	0.44
1:A:189:ALA:HB2	8:A:605:UQ8:H3MB	1.99	0.44
1:A:232:LEU:HD22	8:A:605:UQ8:C17	2.47	0.44
2:b:150:ASP:OD1	2:b:150:ASP:C	2.60	0.44
7:A:603:LPP:H241	3:H:15:VAL:HG21	2.00	0.44
1:a:101:LEU:O	2:b:351:ILE:HD11	2.17	0.44
8:A:605:UQ8:H27	8:A:605:UQ8:H30	1.86	0.44
7:a:602:LPP:H443	7:a:602:LPP:C26	2.47	0.44
8:a:604:UQ8:C28	8:a:604:UQ8:H25B	2.48	0.43
1:A:401:LEU:HG	8:A:605:UQ8:H30	2.00	0.43
1:A:461:VAL:O	2:B:154:ARG:NH2	2.51	0.43
2:B:150:ASP:OD2	2:B:152:TYR:N	2.50	0.43
2:B:149:VAL:HG13	2:B:153:LEU:HA	2.00	0.43
2:b:271:LEU:HA	2:b:274:VAL:HG22	2.00	0.43
1:a:461:VAL:O	2:b:154:ARG:NH2	2.52	0.43
1:a:406:LEU:HD21	8:a:604:UQ8:H36	2.01	0.43
2:b:6:VAL:HG12	2:b:10:ILE:HD12	2.01	0.43
5:A:601:HEM:HBC2	5:A:601:HEM:CHD	2.48	0.43
1:A:22:PHE:CZ	1:A:65:LEU:HD13	2.53	0.43
3:h:18:LEU:O	3:h:22:VAL:HG23	2.18	0.43
2:B:109:LYS:C	2:B:110:ILE:HD12	2.43	0.43
9:a:605:MQ8:H141	9:a:605:MQ8:H162	1.54	0.43
1:a:408:PHE:CZ	1:a:412:ILE:HD11	2.53	0.42
8:a:604:UQ8:H4MA	4:x:13:ALA:HB2	2.01	0.42
1:a:360:TYR:OH	1:a:378:ASP:OD2	2.35	0.42
1:a:84:TYR:HB2	1:a:462:ALA:HB1	2.00	0.42
1:a:265:ALA:O	1:a:266:PRO:C	2.62	0.42
1:a:283:LYS:O	1:a:284:PHE:C	2.62	0.42
1:A:233:SER:HB3	1:A:237:LEU:HD12	2.01	0.42
8:a:604:UQ8:H27	8:a:604:UQ8:H30	1.82	0.42
1:A:237:LEU:HD11	8:A:605:UQ8:C1	2.50	0.42
2:b:86:PHE:O	2:b:90:MET:HG2	2.19	0.42
8:B:402:UQ8:H30B	8:B:402:UQ8:H32A	1.87	0.42
1:a:279:GLU:O	1:a:281:THR:HG23	2.20	0.42
2:b:75:TRP:CH2	8:b:402:UQ8:H40	2.55	0.42
8:b:402:UQ8:H22A	8:b:402:UQ8:H20B	1.80	0.42
2:b:2:ILE:HG22	2:b:3:ASP:N	2.35	0.42
1:a:21:LEU:HB3	7:a:602:LPP:H263	2.02	0.41
1:a:88:VAL:HG11	1:a:453:ILE:HG13	2.01	0.41
2:b:234:THR:HG23	2:b:234:THR:O	2.20	0.41
1:A:308:LYS:N	1:A:308:LYS:HD3	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:604:HEM:HBC2	5:A:604:HEM:CHD	2.38	0.41
2:B:110:ILE:HG22	2:B:112:GLU:H	1.84	0.41
4:X:25:GLU:CD	4:X:25:GLU:C	2.89	0.41
1:a:228:MET:HE1	8:a:604:UQ8:H25A	2.02	0.41
1:A:94:ALA:HB3	1:A:95:PRO:HD3	2.02	0.41
1:A:430:ILE:O	1:A:433:PRO:HD2	2.21	0.41
5:a:603:HEM:HHC	5:a:603:HEM:CBB	2.45	0.41
1:a:141:ALA:HA	1:a:144:ILE:HG22	2.03	0.41
1:a:197:MET:HE1	1:a:403:ILE:HG21	2.02	0.41
1:A:40:TYR:O	1:A:44:GLY:N	2.53	0.40
9:a:605:MQ8:H341	9:a:605:MQ8:H371	2.03	0.40
8:B:402:UQ8:H22A	8:B:402:UQ8:H20B	1.86	0.40
2:b:201:ARG:HH11	2:b:201:ARG:HG2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	464/522 (89%)	457 (98%)	7 (2%)	0	100	100
1	a	512/522 (98%)	502 (98%)	10 (2%)	0	100	100
2	B	377/379 (100%)	372 (99%)	5 (1%)	0	100	100
2	b	377/379 (100%)	372 (99%)	5 (1%)	0	100	100
3	H	27/29 (93%)	27 (100%)	0	0	100	100
3	h	27/29 (93%)	27 (100%)	0	0	100	100
4	X	28/37 (76%)	28 (100%)	0	0	100	100
4	x	28/37 (76%)	28 (100%)	0	0	100	100
All	All	1840/1934 (95%)	1813 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	381/426 (89%)	379 (100%)	2 (0%)	81	91
1	a	419/426 (98%)	412 (98%)	7 (2%)	53	77
2	B	313/313 (100%)	309 (99%)	4 (1%)	61	81
2	b	313/313 (100%)	310 (99%)	3 (1%)	68	85
3	H	24/24 (100%)	24 (100%)	0	100	100
3	h	24/24 (100%)	24 (100%)	0	100	100
4	X	23/28 (82%)	23 (100%)	0	100	100
4	x	23/28 (82%)	22 (96%)	1 (4%)	26	49
All	All	1520/1582 (96%)	1503 (99%)	17 (1%)	63	83

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	379	SER
1	A	414	ASN
2	B	77	MET
2	B	281	LEU
2	B	282	THR
2	B	375	THR
1	a	86	HIS
1	a	234	VAL
1	a	261	GLU
1	a	290	TYR
1	a	299	SER
1	a	502	SER
1	a	506	THR
2	b	42	ASN
2	b	145	VAL
2	b	295	SER
4	x	15	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	374	GLN
1	A	513	GLN
2	B	56	HIS
4	X	26	HIS
1	a	152	GLN
1	a	263	GLN
2	b	374	ASN

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](#)

19 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	$\# Z > 2$
5	HEM	a	603	1	50,50,50	1.44	7 (14%)	66,82,82	1.32	9 (13%)
5	HEM	A	601	1	50,50,50	1.43	6 (12%)	66,82,82	1.32	7 (10%)
10	OXY	a	608	6	1,1,1	0.15	0	-		
8	UQ8	B	402	-	53,53,53	2.27	15 (28%)	64,67,67	4.11	26 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MQ8	a	605	-	54,54,54	2.74	24 (44%)	66,69,69	7.78	27 (40%)
7	LPP	a	606	-	43,43,43	1.11	2 (4%)	47,48,48	1.18	3 (6%)
6	A1JN4	a	607	1,10	46,52,52	2.90	16 (34%)	62,89,89	4.61	39 (62%)
8	UQ8	A	605	-	53,53,53	1.21	2 (3%)	64,67,67	1.51	14 (21%)
7	LPP	B	401	-	43,43,43	1.09	2 (4%)	47,48,48	1.16	2 (4%)
6	A1JN4	A	602	1	46,52,52	2.91	14 (30%)	62,89,89	4.63	38 (61%)
7	LPP	a	602	-	43,43,43	1.08	2 (4%)	47,48,48	1.16	2 (4%)
7	LPP	A	603	-	43,43,43	1.07	2 (4%)	47,48,48	1.08	2 (4%)
9	MQ8	A	606	-	54,54,54	2.76	24 (44%)	66,69,69	7.87	28 (42%)
7	LPP	x	101	-	43,43,43	1.10	2 (4%)	47,48,48	1.11	2 (4%)
8	UQ8	a	604	-	53,53,53	1.18	2 (3%)	64,67,67	1.49	13 (20%)
5	HEM	a	601	1	50,50,50	1.38	6 (12%)	66,82,82	1.30	6 (9%)
7	LPP	b	401	-	43,43,43	1.10	2 (4%)	47,48,48	1.14	2 (4%)
5	HEM	A	604	1	50,50,50	1.44	7 (14%)	66,82,82	1.31	8 (12%)
8	UQ8	b	402	-	53,53,53	2.31	15 (28%)	64,67,67	4.01	26 (40%)

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
9	MQ8	a	605	-	-	11/47/67/67	0/2/2/2
5	HEM	a	603	1	-	6/14/54/54	-
7	LPP	x	101	-	-	21/45/45/45	-
6	A1JN4	A	602	1	1/1/12/12	6/9/89/89	0/1/9/9
7	LPP	a	606	-	-	24/45/45/45	-
6	A1JN4	a	607	1,10	1/1/12/12	5/9/89/89	0/1/9/9
5	HEM	A	601	1	-	3/14/54/54	-
8	UQ8	a	604	-	-	12/51/75/75	0/1/1/1
7	LPP	a	602	-	-	20/45/45/45	-
7	LPP	A	603	-	-	14/45/45/45	-
5	HEM	a	601	1	-	5/14/54/54	-
9	MQ8	A	606	-	-	11/47/67/67	0/2/2/2
8	UQ8	A	605	-	-	8/51/75/75	0/1/1/1
7	LPP	b	401	-	-	23/45/45/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	LPP	B	401	-	-	21/45/45/45	-
8	UQ8	B	402	-	-	7/51/75/75	0/1/1/1
5	HEM	A	604	1	-	6/14/54/54	-
8	UQ8	b	402	-	-	9/51/75/75	0/1/1/1

All (150) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	602	A1JN4	C3D-C2D	-11.70	1.26	1.55
6	a	607	A1JN4	C3D-C2D	-11.64	1.26	1.55
8	b	402	UQ8	C6-C1	10.23	1.53	1.35
8	B	402	UQ8	C6-C1	10.05	1.53	1.35
9	a	605	MQ8	C3-C2	8.00	1.49	1.35
9	A	606	MQ8	C3-C2	7.87	1.49	1.35
8	A	605	UQ8	C6-C1	7.56	1.49	1.35
8	a	604	UQ8	C6-C1	7.46	1.48	1.35
6	A	602	A1JN4	O1D-C3D	6.73	1.57	1.46
6	a	607	A1JN4	O1D-C3D	6.68	1.57	1.46
6	A	602	A1JN4	CBB-CAB	-5.68	1.26	1.51
6	a	607	A1JN4	CBB-CAB	-5.66	1.26	1.51
6	A	602	A1JN4	CBC-CAC	-5.50	1.27	1.51
6	a	607	A1JN4	CBC-CAC	-5.48	1.27	1.51
9	A	606	MQ8	C40-C38	5.09	1.61	1.51
9	A	606	MQ8	C5-C4	5.04	1.57	1.48
9	a	605	MQ8	C10-C1	5.03	1.57	1.48
9	a	605	MQ8	C5-C4	4.97	1.57	1.48
9	A	606	MQ8	C10-C1	4.96	1.57	1.48
9	a	605	MQ8	C30-C28	4.81	1.61	1.51
9	a	605	MQ8	C40-C38	4.80	1.61	1.51
9	A	606	MQ8	C25-C23	4.78	1.61	1.51
9	a	605	MQ8	C35-C33	4.66	1.61	1.51
9	A	606	MQ8	C35-C33	4.62	1.60	1.51
9	A	606	MQ8	C15-C13	4.58	1.60	1.51
9	a	605	MQ8	C15-C13	4.48	1.60	1.51
6	a	607	A1JN4	OND-C2D	4.45	1.51	1.42
6	A	602	A1JN4	OND-C2D	4.43	1.51	1.42
9	a	605	MQ8	C25-C23	4.38	1.60	1.51
8	B	402	UQ8	C4-C3	4.37	1.54	1.36
8	b	402	UQ8	C4-C3	4.34	1.53	1.36
9	A	606	MQ8	C30-C28	4.29	1.60	1.51
9	a	605	MQ8	C20-C18	4.28	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	606	MQ8	C11-C12	4.17	1.56	1.50
5	A	601	HEM	FE-NC	3.81	2.08	1.95
5	a	603	HEM	FE-NC	3.80	2.08	1.95
5	a	603	HEM	FE-NA	3.79	2.08	1.95
9	A	606	MQ8	C20-C18	3.74	1.59	1.51
9	a	605	MQ8	C11-C12	3.72	1.56	1.50
6	a	607	A1JN4	CBD-CGD	-3.62	1.42	1.50
5	A	604	HEM	FE-NA	3.61	2.07	1.95
6	A	602	A1JN4	O1D-CGD	-3.61	1.29	1.35
6	A	602	A1JN4	CBD-CGD	-3.58	1.42	1.50
6	a	607	A1JN4	O1D-CGD	-3.56	1.29	1.35
9	a	605	MQ8	C44-C43	3.50	1.58	1.51
5	a	601	HEM	FE-NC	3.42	2.06	1.95
6	A	602	A1JN4	CAD-C3D	3.39	1.59	1.53
9	A	606	MQ8	C44-C43	3.38	1.58	1.51
8	b	402	UQ8	C7-C8	3.37	1.55	1.50
5	a	601	HEM	FE-NA	3.37	2.06	1.95
5	A	604	HEM	FE-NC	3.34	2.06	1.95
8	B	402	UQ8	C7-C8	3.32	1.55	1.50
6	a	607	A1JN4	CAD-C3D	3.29	1.59	1.53
5	A	601	HEM	FE-NA	3.28	2.06	1.95
9	A	606	MQ8	C11-C3	3.27	1.56	1.51
7	x	101	LPP	O27-C29	3.27	1.42	1.33
7	b	401	LPP	O27-C29	3.25	1.42	1.33
7	B	401	LPP	O27-C29	3.23	1.42	1.33
7	a	606	LPP	O27-C29	3.21	1.42	1.33
7	a	606	LPP	O9-C11	3.18	1.43	1.34
5	A	604	HEM	FE-ND	3.16	2.04	1.94
7	a	602	LPP	O9-C11	3.14	1.43	1.34
7	a	602	LPP	O27-C29	3.11	1.42	1.33
7	A	603	LPP	O9-C11	3.09	1.43	1.34
5	A	604	HEM	FE-NB	3.09	2.04	1.94
5	A	601	HEM	FE-ND	3.09	2.04	1.94
5	A	601	HEM	FE-NB	3.08	2.04	1.94
6	a	607	A1JN4	C1B-NB	-3.07	1.33	1.39
7	B	401	LPP	O9-C11	3.05	1.42	1.34
7	A	603	LPP	O27-C29	3.05	1.42	1.33
7	b	401	LPP	O9-C11	3.03	1.42	1.34
6	A	602	A1JN4	C1B-NB	-3.03	1.33	1.39
8	A	605	UQ8	C4-C3	3.00	1.48	1.36
7	x	101	LPP	O9-C11	2.99	1.42	1.34
8	a	604	UQ8	C4-C3	2.94	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	a	601	HEM	FE-NB	2.94	2.03	1.94
9	a	605	MQ8	C45-C43	2.88	1.58	1.50
8	b	402	UQ8	C26-C24	2.87	1.57	1.51
9	a	605	MQ8	C11-C3	2.86	1.56	1.51
8	b	402	UQ8	C11-C9	2.86	1.57	1.51
8	B	402	UQ8	C11-C9	2.84	1.57	1.51
5	a	603	HEM	FE-ND	2.83	2.03	1.94
9	A	606	MQ8	C45-C43	2.82	1.57	1.50
5	a	601	HEM	FE-ND	2.78	2.03	1.94
5	A	601	HEM	CAB-C3B	2.77	1.55	1.47
5	A	601	HEM	CAC-C3C	2.76	1.55	1.47
5	a	601	HEM	CAC-C3C	2.76	1.54	1.47
8	b	402	UQ8	C21-C19	2.70	1.56	1.51
5	A	604	HEM	CAB-C3B	2.70	1.54	1.47
5	a	603	HEM	CAC-C3C	2.68	1.54	1.47
5	a	603	HEM	CAB-C3B	2.68	1.54	1.47
5	a	603	HEM	FE-NB	2.68	2.03	1.94
9	A	606	MQ8	C41-C42	2.66	1.59	1.50
8	B	402	UQ8	C21-C19	2.66	1.56	1.51
5	A	604	HEM	CAC-C3C	2.65	1.54	1.47
5	a	601	HEM	CAB-C3B	2.64	1.54	1.47
9	a	605	MQ8	C41-C42	2.64	1.59	1.50
8	b	402	UQ8	C7-C6	2.61	1.55	1.51
9	A	606	MQ8	C29-C28	2.61	1.57	1.50
8	B	402	UQ8	C31-C29	2.59	1.56	1.51
9	A	606	MQ8	C14-C13	2.55	1.57	1.50
8	B	402	UQ8	C26-C24	2.49	1.56	1.51
6	a	607	A1JN4	CBA-CAA	2.46	1.59	1.52
8	b	402	UQ8	C16-C14	2.44	1.56	1.51
8	b	402	UQ8	C6-C5	2.43	1.53	1.46
9	a	605	MQ8	C21-C22	2.42	1.58	1.50
9	a	605	MQ8	C36-C37	2.42	1.58	1.50
6	A	602	A1JN4	CMC-C2C	2.42	1.55	1.50
6	a	607	A1JN4	CMC-C2C	2.41	1.55	1.50
6	A	602	A1JN4	C4C-NC	-2.41	1.35	1.39
6	a	607	A1JN4	CMB-C2B	2.41	1.55	1.50
9	A	606	MQ8	C21-C22	2.40	1.58	1.50
8	B	402	UQ8	C16-C14	2.40	1.56	1.51
8	b	402	UQ8	C36-C34	2.39	1.56	1.51
6	A	602	A1JN4	CBA-CAA	2.39	1.59	1.52
8	B	402	UQ8	C6-C5	2.37	1.53	1.46
6	A	602	A1JN4	CMB-C2B	2.37	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	605	MQ8	C29-C28	2.36	1.56	1.50
8	b	402	UQ8	C31-C29	2.35	1.56	1.51
6	A	602	A1JN4	C4A-C3A	2.33	1.48	1.43
9	a	605	MQ8	C14-C13	2.31	1.56	1.50
6	a	607	A1JN4	C4A-C3A	2.30	1.48	1.43
9	A	606	MQ8	C24-C23	2.30	1.56	1.50
9	A	606	MQ8	C36-C37	2.27	1.57	1.50
8	B	402	UQ8	C36-C34	2.24	1.55	1.51
9	A	606	MQ8	C31-C32	2.23	1.57	1.50
9	a	605	MQ8	C31-C32	2.19	1.57	1.50
8	B	402	UQ8	C7-C6	2.18	1.55	1.51
6	a	607	A1JN4	C4C-NC	-2.17	1.35	1.39
9	A	606	MQ8	C26-C27	2.16	1.57	1.50
9	a	605	MQ8	C24-C23	2.16	1.56	1.50
9	a	605	MQ8	C19-C18	2.14	1.56	1.50
9	a	605	MQ8	O4-C4	-2.14	1.18	1.23
8	B	402	UQ8	C30-C29	2.13	1.56	1.50
9	A	606	MQ8	C27-C28	2.11	1.38	1.33
8	b	402	UQ8	C40-C39	2.11	1.56	1.50
8	b	402	UQ8	C35-C34	2.10	1.56	1.50
9	a	605	MQ8	C42-C43	2.10	1.38	1.33
9	A	606	MQ8	O4-C4	-2.09	1.18	1.23
8	b	402	UQ8	O4-C4	2.09	1.42	1.36
8	b	402	UQ8	C30-C29	2.06	1.56	1.50
8	B	402	UQ8	C40-C39	2.06	1.56	1.50
8	B	402	UQ8	O5-C5	-2.04	1.18	1.23
6	a	607	A1JN4	C2A-C3A	-2.04	1.33	1.38
5	a	603	HEM	C2A-C3A	-2.03	1.33	1.38
8	B	402	UQ8	O2-C2	-2.03	1.19	1.23
9	A	606	MQ8	C19-C18	2.02	1.55	1.50
9	a	605	MQ8	C27-C28	2.01	1.37	1.33
6	a	607	A1JN4	C1A-NA	-2.01	1.35	1.39
5	A	604	HEM	C2A-C3A	-2.01	1.33	1.38

All (254) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	606	MQ8	C30-C28-C27	21.03	163.67	121.12
9	A	606	MQ8	C44-C43-C42	20.90	163.41	121.12
9	a	605	MQ8	C30-C28-C27	20.57	162.73	121.12
9	a	605	MQ8	C44-C43-C42	20.24	162.07	121.12
9	A	606	MQ8	C19-C18-C17	17.02	167.33	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	605	MQ8	C34-C33-C35	-16.80	87.01	115.27
9	A	606	MQ8	C34-C33-C35	-16.17	88.06	115.27
9	A	606	MQ8	C39-C38-C37	15.82	164.26	123.68
9	a	605	MQ8	C34-C33-C32	15.74	164.05	123.68
9	A	606	MQ8	C34-C33-C32	15.73	164.03	123.68
9	a	605	MQ8	C24-C23-C25	-15.72	88.83	115.27
9	a	605	MQ8	C19-C18-C17	15.68	163.91	123.68
9	a	605	MQ8	C24-C23-C22	15.68	163.91	123.68
9	a	605	MQ8	C14-C13-C12	15.56	163.59	123.68
9	a	605	MQ8	C39-C38-C37	15.38	163.12	123.68
9	a	605	MQ8	C39-C38-C40	-15.23	89.66	115.27
9	a	605	MQ8	C45-C43-C44	-14.95	90.13	115.27
9	A	606	MQ8	C24-C23-C25	-14.88	90.24	115.27
9	A	606	MQ8	C14-C13-C15	-14.77	90.43	115.27
9	A	606	MQ8	C19-C18-C20	-14.76	90.44	115.27
9	A	606	MQ8	C45-C43-C44	-14.66	90.60	115.27
9	A	606	MQ8	C29-C28-C30	-14.46	90.94	115.27
9	A	606	MQ8	C14-C13-C12	14.31	160.38	123.68
9	A	606	MQ8	C24-C23-C22	14.27	160.28	123.68
9	a	605	MQ8	C19-C18-C20	-13.83	92.00	115.27
9	A	606	MQ8	C39-C38-C40	-13.80	92.06	115.27
6	a	607	A1JN4	O1D-C3D-C4D	-13.26	81.30	108.25
6	A	602	A1JN4	O1D-C3D-C4D	-13.04	81.76	108.25
9	a	605	MQ8	C29-C28-C30	-12.19	94.77	115.27
9	a	605	MQ8	C14-C13-C15	-10.98	96.80	115.27
8	b	402	UQ8	C15-C14-C16	-10.91	96.92	115.27
9	a	605	MQ8	C15-C13-C12	-10.79	99.28	121.12
8	B	402	UQ8	C25-C24-C26	-10.77	97.16	115.27
8	B	402	UQ8	C15-C14-C16	-10.65	97.36	115.27
8	B	402	UQ8	C35-C34-C36	-10.56	97.51	115.27
6	a	607	A1JN4	C3B-C4B-NB	-10.51	100.10	110.32
8	B	402	UQ8	C40-C39-C41	-10.47	97.66	115.27
6	A	602	A1JN4	C3B-C4B-NB	-10.40	100.20	110.32
8	b	402	UQ8	C30-C29-C31	-10.17	98.16	115.27
6	A	602	A1JN4	CHD-C1D-ND	10.16	139.10	124.20
8	b	402	UQ8	C10-C9-C11	-9.99	98.47	115.27
8	B	402	UQ8	C10-C9-C11	-9.95	98.52	115.27
6	a	607	A1JN4	CHD-C1D-ND	9.89	138.70	124.20
8	b	402	UQ8	C40-C39-C41	-9.59	99.13	115.27
6	A	602	A1JN4	C4B-NB-C1B	9.43	114.58	105.35
8	b	402	UQ8	C25-C24-C26	-9.39	99.48	115.27
8	b	402	UQ8	C35-C34-C36	-9.37	99.52	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	a	607	A1JN4	C4B-NB-C1B	9.34	114.50	105.35
9	A	606	MQ8	C20-C18-C17	-9.34	102.21	121.12
8	B	402	UQ8	C20-C19-C21	-9.34	99.56	115.27
8	B	402	UQ8	C30-C29-C31	-9.32	99.59	115.27
8	b	402	UQ8	C20-C19-C21	-9.30	99.62	115.27
6	A	602	A1JN4	C4C-NC-C1C	9.04	114.20	105.35
6	a	607	A1JN4	C4C-NC-C1C	8.98	114.14	105.35
6	A	602	A1JN4	O1D-C3D-CAD	-8.79	86.48	103.01
6	a	607	A1JN4	O1D-C3D-CAD	-8.67	86.70	103.01
9	A	606	MQ8	C40-C38-C37	-8.64	103.64	121.12
8	b	402	UQ8	C46-C44-C45	-8.51	95.81	114.60
9	a	605	MQ8	C20-C18-C17	-8.45	104.02	121.12
9	a	605	MQ8	C29-C28-C27	-8.27	102.47	123.68
8	B	402	UQ8	C46-C44-C45	-8.17	96.56	114.60
9	A	606	MQ8	C29-C28-C27	-7.17	105.28	123.68
6	A	602	A1JN4	CHC-C4B-NB	7.15	132.18	124.44
9	A	606	MQ8	C45-C43-C42	-6.90	105.97	123.68
9	a	605	MQ8	C40-C38-C37	-6.88	107.19	121.12
6	A	602	A1JN4	O1D-CGD-CBD	-6.87	103.26	110.19
9	a	605	MQ8	C25-C23-C22	-6.87	107.22	121.12
6	A	602	A1JN4	CAB-C3B-C4B	-6.70	114.13	124.68
6	a	607	A1JN4	C3C-C4C-NC	-6.70	102.66	110.15
6	a	607	A1JN4	C4B-C3B-C2B	6.66	115.80	107.13
6	A	602	A1JN4	C4B-C3B-C2B	6.66	115.80	107.13
6	a	607	A1JN4	CHC-C4B-NB	6.63	131.61	124.44
6	A	602	A1JN4	C3C-C4C-NC	-6.55	102.83	110.15
6	a	607	A1JN4	CAC-C3C-C4C	-6.55	115.83	124.92
9	A	606	MQ8	C35-C33-C32	-6.54	107.89	121.12
6	A	602	A1JN4	C2A-C1A-NA	-6.49	102.90	110.15
6	a	607	A1JN4	C2A-C1A-NA	-6.46	102.92	110.15
6	A	602	A1JN4	CAC-C3C-C4C	-6.30	116.17	124.92
6	a	607	A1JN4	CAB-C3B-C4B	-6.27	114.80	124.68
9	a	605	MQ8	C45-C43-C42	-6.20	107.76	123.68
6	a	607	A1JN4	OND-C2D-CMD	-6.17	98.23	109.59
6	A	602	A1JN4	OND-C2D-CMD	-6.06	98.43	109.59
6	A	602	A1JN4	C4A-NA-C1A	6.05	111.27	105.35
9	a	605	MQ8	C35-C33-C32	-6.04	108.90	121.12
6	a	607	A1JN4	O1D-CGD-CBD	-5.98	104.16	110.19
6	a	607	A1JN4	C4A-NA-C1A	5.92	111.14	105.35
9	A	606	MQ8	C15-C13-C12	-5.90	109.17	121.12
9	A	606	MQ8	C25-C23-C22	-5.75	109.47	121.12
6	a	607	A1JN4	CHB-C1B-NB	5.69	130.59	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	602	A1JN4	CHB-C1B-NB	5.55	130.44	124.44
8	b	402	UQ8	C16-C14-C13	5.40	132.05	121.12
8	B	402	UQ8	C16-C14-C13	5.20	131.63	121.12
6	a	607	A1JN4	C1A-C2A-C3A	5.13	114.97	106.89
6	A	602	A1JN4	O1A-CGA-CBA	-5.13	106.61	123.08
8	b	402	UQ8	C11-C9-C8	5.12	131.48	121.12
8	B	402	UQ8	C36-C34-C33	5.11	131.46	121.12
6	a	607	A1JN4	O1A-CGA-CBA	-5.05	106.86	123.08
6	A	602	A1JN4	C1A-C2A-C3A	5.02	114.78	106.89
6	A	602	A1JN4	C2D-C1D-CHD	-4.98	116.05	124.28
9	A	606	MQ8	C11-C12-C13	4.98	135.09	126.79
8	B	402	UQ8	C11-C9-C8	4.92	131.08	121.12
8	b	402	UQ8	C21-C19-C18	4.89	131.02	121.12
8	B	402	UQ8	C26-C24-C23	4.88	131.00	121.12
8	b	402	UQ8	C31-C29-C28	4.88	130.99	121.12
8	B	402	UQ8	C41-C39-C38	4.86	130.95	121.12
8	B	402	UQ8	C21-C19-C18	4.73	130.68	121.12
7	a	606	LPP	O9-C11-C12	4.69	121.61	111.50
6	a	607	A1JN4	C2D-C1D-CHD	-4.69	116.54	124.28
8	b	402	UQ8	C41-C39-C38	4.59	130.40	121.12
8	b	402	UQ8	C26-C24-C23	4.57	130.36	121.12
8	B	402	UQ8	C31-C29-C28	4.55	130.33	121.12
8	b	402	UQ8	C36-C34-C33	4.52	130.26	121.12
7	B	401	LPP	O9-C11-C12	4.29	120.76	111.50
6	a	607	A1JN4	O2A-CGA-O1A	4.27	133.95	123.30
9	A	606	MQ8	C11-C3-C4	4.26	123.06	118.50
6	A	602	A1JN4	O2A-CGA-O1A	4.25	133.89	123.30
7	a	602	LPP	O9-C11-C12	4.23	120.62	111.50
6	a	607	A1JN4	CHD-C4C-NC	4.19	131.56	123.85
7	A	603	LPP	O9-C11-C12	4.15	120.45	111.50
7	b	401	LPP	O9-C11-C12	4.07	120.28	111.50
6	a	607	A1JN4	C4A-C3A-C2A	-4.00	102.15	106.83
6	a	607	A1JN4	CHA-C4D-ND	-3.96	118.39	124.20
6	A	602	A1JN4	C4A-C3A-C2A	-3.88	102.29	106.83
7	x	101	LPP	O9-C11-C12	3.86	119.82	111.50
6	A	602	A1JN4	CHD-C4C-NC	3.72	130.70	123.85
6	a	607	A1JN4	C3D-C4D-CHA	3.64	135.13	124.34
8	A	605	UQ8	C40-C39-C41	3.63	121.38	115.27
6	A	602	A1JN4	CHA-C4D-ND	-3.60	118.93	124.20
8	b	402	UQ8	C45-C44-C43	3.56	132.93	122.65
6	A	602	A1JN4	C3D-C4D-CHA	3.53	134.81	124.34
6	a	607	A1JN4	CAC-C3C-C2C	3.47	132.42	126.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	602	A1JN4	C1B-C2B-C3B	-3.46	101.89	106.94
6	a	607	A1JN4	C1B-C2B-C3B	-3.42	101.95	106.94
8	a	604	UQ8	C30-C29-C31	3.37	120.94	115.27
6	A	602	A1JN4	CAC-C3C-C2C	3.36	132.25	126.86
9	A	606	MQ8	C21-C22-C23	3.36	135.75	127.66
8	B	402	UQ8	C45-C44-C43	3.23	131.98	122.65
9	a	605	MQ8	C31-C30-C28	3.23	123.59	112.98
8	A	605	UQ8	C25-C24-C26	3.19	120.64	115.27
8	B	402	UQ8	C25-C24-C23	3.15	131.76	123.68
8	A	605	UQ8	C37-C38-C39	-3.15	120.08	127.66
5	A	601	HEM	C4A-NA-C1A	3.15	108.43	105.35
6	A	602	A1JN4	CAA-CBA-CGA	-3.14	106.85	113.60
9	a	605	MQ8	C16-C15-C13	3.10	123.16	112.98
6	a	607	A1JN4	CAA-CBA-CGA	-3.09	106.95	113.60
6	a	607	A1JN4	C4C-C3C-C2C	3.09	111.75	106.89
6	a	607	A1JN4	CAA-C2A-C1A	-3.07	118.85	124.89
8	a	604	UQ8	C40-C39-C41	3.05	120.41	115.27
6	a	607	A1JN4	C1C-CHC-C4B	-3.05	115.31	124.74
8	B	402	UQ8	C46-C44-C43	3.05	131.45	122.65
5	A	601	HEM	C4D-ND-C1D	3.02	108.19	105.07
5	a	601	HEM	C4A-NA-C1A	3.02	108.30	105.35
8	b	402	UQ8	C7-C8-C9	3.01	131.81	126.79
8	B	402	UQ8	C40-C39-C38	3.00	131.38	123.68
5	a	601	HEM	C4D-ND-C1D	3.00	108.17	105.07
8	a	604	UQ8	C25-C24-C26	3.00	120.32	115.27
9	A	606	MQ8	C2M-C2-C3	-2.99	119.53	124.40
8	b	402	UQ8	C46-C44-C43	2.98	131.26	122.65
6	A	602	A1JN4	C4C-C3C-C2C	2.98	111.58	106.89
7	b	401	LPP	O27-C29-C30	2.97	121.22	111.91
8	a	604	UQ8	C27-C28-C29	-2.95	120.55	127.66
8	A	605	UQ8	C10-C9-C8	-2.92	116.19	123.68
6	A	602	A1JN4	C1C-CHC-C4B	-2.91	115.73	124.74
5	a	603	HEM	C1B-NB-C4B	2.91	108.08	105.07
7	a	602	LPP	O27-C29-C30	2.87	120.92	111.91
8	b	402	UQ8	C15-C14-C13	2.87	131.03	123.68
8	B	402	UQ8	C35-C34-C33	2.86	131.01	123.68
8	B	402	UQ8	C15-C14-C13	2.85	131.00	123.68
5	a	601	HEM	C1B-NB-C4B	2.83	108.00	105.07
5	a	603	HEM	CAA-C2A-C1A	2.80	130.40	124.89
6	a	607	A1JN4	CBB-CAB-C3B	2.80	120.14	112.43
8	b	402	UQ8	C30-C29-C28	2.79	130.84	123.68
5	A	601	HEM	C4C-NC-C1C	2.78	108.07	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	602	A1JN4	CAA-C2A-C1A	-2.78	119.42	124.89
5	A	604	HEM	C1B-NB-C4B	2.77	107.94	105.07
9	a	605	MQ8	C41-C42-C43	2.75	134.29	127.66
5	A	601	HEM	C1B-NB-C4B	2.74	107.91	105.07
5	a	601	HEM	C4C-NC-C1C	2.74	108.03	105.35
5	A	604	HEM	CAA-C2A-C1A	2.71	130.23	124.89
5	A	604	HEM	C4D-ND-C1D	2.68	107.84	105.07
5	a	603	HEM	C4D-ND-C1D	2.67	107.83	105.07
7	x	101	LPP	O27-C29-C30	2.66	120.25	111.91
5	a	603	HEM	C4A-NA-C1A	2.64	107.94	105.35
6	A	602	A1JN4	CHA-C1A-C2A	2.64	131.12	125.36
6	A	602	A1JN4	C2C-C1C-NC	-2.63	106.08	110.08
8	b	402	UQ8	C40-C39-C38	2.62	130.41	123.68
8	B	402	UQ8	C10-C9-C8	2.62	130.39	123.68
6	a	607	A1JN4	C2C-C1C-NC	-2.59	106.14	110.08
6	a	607	A1JN4	CHA-C1A-C2A	2.57	130.98	125.36
5	A	604	HEM	C4A-NA-C1A	2.56	107.85	105.35
8	A	605	UQ8	C32-C33-C34	-2.55	121.52	127.66
8	a	604	UQ8	C35-C34-C36	2.55	119.56	115.27
6	A	602	A1JN4	CBB-CAB-C3B	2.54	119.44	112.43
7	a	606	LPP	O27-C29-C30	2.53	119.86	111.91
8	b	402	UQ8	C35-C34-C33	2.51	130.12	123.68
8	a	604	UQ8	C37-C38-C39	-2.50	121.64	127.66
7	B	401	LPP	O27-C29-C30	2.50	119.75	111.91
8	B	402	UQ8	C30-C29-C28	2.49	130.08	123.68
6	A	602	A1JN4	CHC-C1C-NC	2.48	128.41	123.85
8	b	402	UQ8	C10-C9-C8	2.47	130.02	123.68
8	b	402	UQ8	C25-C24-C23	2.47	130.00	123.68
8	a	604	UQ8	C8-C7-C6	-2.46	105.41	112.05
6	a	607	A1JN4	OND-C2D-C3D	-2.46	104.34	110.45
8	a	604	UQ8	C46-C44-C45	2.43	119.97	114.60
5	a	603	HEM	C3B-C2B-C1B	2.40	108.27	106.49
8	a	604	UQ8	C36-C34-C33	-2.40	116.26	121.12
6	a	607	A1JN4	CMA-C3A-C2A	2.39	130.77	125.61
8	A	605	UQ8	C46-C44-C45	2.38	119.86	114.60
5	A	604	HEM	C4C-NC-C1C	2.38	107.68	105.35
6	A	602	A1JN4	CMA-C3A-C2A	2.38	130.75	125.61
8	A	605	UQ8	C12-C13-C14	-2.38	121.94	127.66
5	a	603	HEM	C4C-NC-C1C	2.37	107.67	105.35
6	a	607	A1JN4	CHC-C1C-NC	2.37	128.21	123.85
8	B	402	UQ8	C20-C19-C18	2.36	129.74	123.68
5	a	603	HEM	CHA-C4D-ND	2.36	127.28	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	a	604	UQ8	C20-C19-C18	-2.31	117.74	123.68
8	a	604	UQ8	C25-C24-C23	-2.31	117.74	123.68
8	B	402	UQ8	C1M-C1-C6	-2.31	120.63	124.40
9	a	605	MQ8	C36-C37-C38	2.31	133.22	127.66
8	B	402	UQ8	C7-C8-C9	2.29	130.60	126.79
6	A	602	A1JN4	OND-C2D-C3D	-2.29	104.76	110.45
9	a	605	MQ8	C2M-C2-C3	-2.29	120.67	124.40
9	A	606	MQ8	C2M-C2-C1	2.28	120.04	116.27
8	A	605	UQ8	C1M-C1-C6	-2.27	120.69	124.40
8	A	605	UQ8	C22-C23-C24	-2.27	122.20	127.66
6	a	607	A1JN4	CBA-CAA-C2A	-2.25	106.36	112.63
5	A	604	HEM	CAD-CBD-CGD	-2.24	108.79	113.60
8	a	604	UQ8	C22-C23-C24	-2.23	122.29	127.66
5	a	601	HEM	C3D-C4D-ND	-2.22	107.70	110.17
5	A	604	HEM	C3B-C2B-C1B	2.21	108.13	106.49
8	b	402	UQ8	C20-C19-C18	2.20	129.33	123.68
8	A	605	UQ8	C11-C9-C8	2.19	125.55	121.12
9	A	606	MQ8	O4-C4-C5	-2.18	118.03	121.56
5	A	601	HEM	C3D-C4D-ND	-2.16	107.76	110.17
8	A	605	UQ8	C25-C24-C23	-2.16	118.15	123.68
7	A	603	LPP	O27-C29-C30	2.15	118.67	111.91
5	a	603	HEM	CAA-C2A-C3A	-2.15	122.14	127.07
5	a	601	HEM	C2A-C1A-NA	-2.15	107.74	110.15
8	A	605	UQ8	C42-C43-C44	-2.15	120.42	127.75
7	a	606	LPP	O9-C11-O10	-2.14	118.52	123.70
8	A	605	UQ8	C8-C7-C6	-2.13	106.29	112.05
5	A	601	HEM	C2A-C1A-NA	-2.08	107.82	110.15
5	a	603	HEM	CAD-CBD-CGD	-2.08	109.13	113.60
8	a	604	UQ8	C20-C19-C21	2.08	118.77	115.27
6	a	607	A1JN4	CHC-C4B-C3B	2.07	128.29	124.94
8	A	605	UQ8	C20-C19-C18	-2.07	118.37	123.68
5	A	604	HEM	CAA-C2A-C3A	-2.05	122.36	127.07
8	b	402	UQ8	C27-C28-C29	2.05	132.60	127.66
6	a	607	A1JN4	CMB-C2B-C3B	2.05	131.68	126.12
9	a	605	MQ8	C2M-C2-C1	2.03	119.64	116.27
9	A	606	MQ8	C31-C32-C33	2.03	132.54	127.66
6	A	602	A1JN4	CBA-CAA-C2A	-2.03	107.00	112.63
5	A	601	HEM	CAA-C2A-C1A	2.02	128.87	124.89
6	A	602	A1JN4	CMB-C2B-C3B	2.01	131.59	126.12

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	602	A1JN4	NB
6	a	607	A1JN4	NB

All (212) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	HEM	C1A-C2A-CAA-CBA
5	A	601	HEM	C3A-C2A-CAA-CBA
5	a	601	HEM	C1A-C2A-CAA-CBA
7	A	603	LPP	C12-C11-O9-C7
7	B	401	LPP	C6-O5-P1-O2
7	B	401	LPP	C6-O5-P1-O4
7	B	401	LPP	O5-C6-C7-O9
7	a	602	LPP	C6-O5-P1-O2
7	a	602	LPP	C6-O5-P1-O3
7	a	602	LPP	C6-O5-P1-O4
7	a	602	LPP	C12-C11-O9-C7
7	a	606	LPP	C6-O5-P1-O2
7	a	606	LPP	C6-O5-P1-O3
7	a	606	LPP	O10-C11-O9-C7
7	a	606	LPP	C12-C11-O9-C7
7	b	401	LPP	C6-O5-P1-O2
7	b	401	LPP	C6-O5-P1-O3
7	b	401	LPP	C6-O5-P1-O4
7	b	401	LPP	C12-C11-O9-C7
8	A	605	UQ8	C34-C36-C37-C38
8	A	605	UQ8	C25-C24-C26-C27
8	A	605	UQ8	C23-C24-C26-C27
8	b	402	UQ8	C34-C36-C37-C38
8	b	402	UQ8	C9-C11-C12-C13
8	b	402	UQ8	C1-C6-C7-C8
8	b	402	UQ8	C5-C6-C7-C8
9	A	606	MQ8	C12-C11-C3-C2
9	A	606	MQ8	C12-C11-C3-C4
9	A	606	MQ8	C23-C25-C26-C27
9	A	606	MQ8	C28-C30-C31-C32
9	a	605	MQ8	C12-C11-C3-C4
9	a	605	MQ8	C12-C13-C15-C16
9	a	605	MQ8	C14-C13-C15-C16
9	a	605	MQ8	C18-C20-C21-C22
9	a	605	MQ8	C29-C28-C30-C31
6	a	607	A1JN4	C4C-C3C-CAC-CBC
7	a	602	LPP	O28-C29-O27-C8

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Mol	Chain	Res	Type	Atoms
7	b	401	LPP	O28-C29-O27-C8
6	a	607	A1JN4	C2C-C3C-CAC-CBC
6	A	602	A1JN4	C4B-C3B-CAB-CBB
7	a	602	LPP	C30-C29-O27-C8
7	b	401	LPP	C30-C29-O27-C8
6	A	602	A1JN4	C2B-C3B-CAB-CBB
6	A	602	A1JN4	C4C-C3C-CAC-CBC
6	A	602	A1JN4	C2C-C3C-CAC-CBC
7	A	603	LPP	O10-C11-O9-C7
7	b	401	LPP	O10-C11-O9-C7
7	x	101	LPP	C30-C29-O27-C8
9	a	605	MQ8	C27-C28-C30-C31
7	a	602	LPP	O10-C11-O9-C7
7	x	101	LPP	O28-C29-O27-C8
6	a	607	A1JN4	C2B-C3B-CAB-CBB
5	A	604	HEM	C1A-C2A-CAA-CBA
5	a	603	HEM	C1A-C2A-CAA-CBA
8	A	605	UQ8	C40-C39-C41-C42
8	B	402	UQ8	C9-C11-C12-C13
9	A	606	MQ8	C18-C20-C21-C22
9	A	606	MQ8	C38-C40-C41-C42
9	A	606	MQ8	C43-C44-C46-C47
7	a	606	LPP	C30-C29-O27-C8
7	x	101	LPP	O5-C6-C7-O9
5	A	604	HEM	C3A-C2A-CAA-CBA
5	a	601	HEM	C3A-C2A-CAA-CBA
5	a	603	HEM	C3A-C2A-CAA-CBA
7	A	603	LPP	C30-C31-C32-C33
7	B	401	LPP	C29-C30-C31-C32
7	x	101	LPP	C11-C12-C13-C14
7	a	606	LPP	O28-C29-O27-C8
9	A	606	MQ8	C33-C35-C36-C37
9	a	605	MQ8	C38-C40-C41-C42
7	A	603	LPP	C21-C22-C23-C24
7	a	602	LPP	C17-C18-C19-C20
7	a	602	LPP	C39-C40-C41-C42
7	a	606	LPP	C37-C38-C39-C40
7	b	401	LPP	C18-C19-C20-C21
7	x	101	LPP	C31-C32-C33-C34
6	a	607	A1JN4	C4B-C3B-CAB-CBB
7	a	606	LPP	C15-C16-C17-C18
7	b	401	LPP	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
8	A	605	UQ8	C38-C39-C41-C42
7	a	602	LPP	C20-C21-C22-C23
7	a	602	LPP	C31-C32-C33-C34
7	b	401	LPP	C12-C13-C14-C15
9	a	605	MQ8	C43-C44-C46-C47
7	a	606	LPP	C30-C31-C32-C33
7	b	401	LPP	C40-C41-C42-C43
7	a	602	LPP	C37-C38-C39-C40
7	a	602	LPP	C34-C35-C36-C37
7	b	401	LPP	C22-C23-C24-C25
7	a	606	LPP	C11-C12-C13-C14
7	a	606	LPP	C20-C21-C22-C23
7	b	401	LPP	C21-C22-C23-C24
7	a	602	LPP	C29-C30-C31-C32
7	B	401	LPP	C39-C40-C41-C42
7	b	401	LPP	C34-C35-C36-C37
7	B	401	LPP	C35-C36-C37-C38
7	b	401	LPP	C20-C21-C22-C23
7	a	606	LPP	C17-C18-C19-C20
7	x	101	LPP	C35-C36-C37-C38
7	B	401	LPP	C21-C22-C23-C24
7	x	101	LPP	O5-C6-C7-C8
7	x	101	LPP	C20-C21-C22-C23
7	x	101	LPP	C37-C38-C39-C40
7	x	101	LPP	C34-C35-C36-C37
7	a	606	LPP	C6-C7-C8-O27
9	a	605	MQ8	C12-C11-C3-C2
7	B	401	LPP	C32-C33-C34-C35
8	a	604	UQ8	C29-C31-C32-C33
7	b	401	LPP	C16-C17-C18-C19
8	A	605	UQ8	C35-C34-C36-C37
8	B	402	UQ8	C5-C6-C7-C8
7	A	603	LPP	C12-C13-C14-C15
7	B	401	LPP	C6-O5-P1-O3
7	B	401	LPP	C41-C42-C43-C44
8	A	605	UQ8	C33-C34-C36-C37
7	b	401	LPP	C7-C8-O27-C29
7	B	401	LPP	C33-C34-C35-C36
7	B	401	LPP	O5-C6-C7-C8
9	a	605	MQ8	C33-C35-C36-C37
7	B	401	LPP	C11-C12-C13-C14
7	b	401	LPP	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
7	B	401	LPP	C19-C20-C21-C22
7	b	401	LPP	O5-C6-C7-O9
7	a	606	LPP	C29-C30-C31-C32
7	x	101	LPP	C29-C30-C31-C32
7	a	606	LPP	C12-C13-C14-C15
7	B	401	LPP	C31-C32-C33-C34
7	a	606	LPP	C35-C36-C37-C38
7	b	401	LPP	O5-C6-C7-C8
7	A	603	LPP	C32-C33-C34-C35
7	A	603	LPP	C33-C34-C35-C36
7	A	603	LPP	C8-C7-O9-C11
7	a	602	LPP	C8-C7-O9-C11
7	B	401	LPP	C12-C11-O9-C7
5	A	601	HEM	C4C-C3C-CAC-CBC
5	A	604	HEM	C4B-C3B-CAB-CBB
5	A	604	HEM	C4C-C3C-CAC-CBC
5	a	601	HEM	C4C-C3C-CAC-CBC
5	a	603	HEM	C4B-C3B-CAB-CBB
5	a	603	HEM	C4C-C3C-CAC-CBC
7	a	602	LPP	C12-C13-C14-C15
7	a	602	LPP	C16-C17-C18-C19
7	B	401	LPP	O10-C11-O9-C7
7	A	603	LPP	C37-C38-C39-C40
8	b	402	UQ8	C6-C7-C8-C9
7	x	101	LPP	C39-C40-C41-C42
7	A	603	LPP	C40-C41-C42-C43
7	x	101	LPP	C18-C19-C20-C21
7	a	606	LPP	O9-C7-C8-O27
8	B	402	UQ8	C1-C6-C7-C8
7	x	101	LPP	C17-C18-C19-C20
8	b	402	UQ8	C39-C41-C42-C43
7	B	401	LPP	C37-C38-C39-C40
8	a	604	UQ8	C35-C34-C36-C37
8	a	604	UQ8	C15-C14-C16-C17
8	A	605	UQ8	C24-C26-C27-C28
8	a	604	UQ8	C9-C11-C12-C13
8	a	604	UQ8	C19-C21-C22-C23
7	b	401	LPP	C38-C39-C40-C41
6	A	602	A1JN4	CAA-CBA-CGA-O2A
8	a	604	UQ8	C20-C19-C21-C22
7	b	401	LPP	C30-C31-C32-C33
7	a	606	LPP	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
6	A	602	A1JN4	CAA-CBA-CGA-O1A
7	A	603	LPP	C17-C18-C19-C20
8	b	402	UQ8	C5-C4-O4-C4M
7	B	401	LPP	C13-C14-C15-C16
7	a	602	LPP	C41-C42-C43-C44
7	A	603	LPP	C6-C7-C8-O27
7	a	602	LPP	C38-C39-C40-C41
7	a	606	LPP	C33-C34-C35-C36
7	a	606	LPP	C6-C7-O9-C11
7	a	606	LPP	C8-C7-O9-C11
8	B	402	UQ8	C40-C39-C41-C42
7	B	401	LPP	O9-C11-C12-C13
9	A	606	MQ8	C3-C11-C12-C13
8	a	604	UQ8	C13-C14-C16-C17
7	x	101	LPP	C38-C39-C40-C41
8	b	402	UQ8	C14-C16-C17-C18
5	A	604	HEM	CAD-CBD-CGD-O1D
7	x	101	LPP	C40-C41-C42-C43
8	B	402	UQ8	C5-C4-O4-C4M
6	a	607	A1JN4	CAA-CBA-CGA-O1A
8	a	604	UQ8	C25-C24-C26-C27
9	A	606	MQ8	C19-C18-C20-C21
8	a	604	UQ8	C34-C36-C37-C38
8	B	402	UQ8	C38-C39-C41-C42
7	a	602	LPP	O9-C7-C8-O27
7	b	401	LPP	C19-C20-C21-C22
7	x	101	LPP	C21-C22-C23-C24
7	a	606	LPP	C6-O5-P1-O4
7	x	101	LPP	C6-O5-P1-O2
8	a	604	UQ8	C33-C34-C36-C37
8	a	604	UQ8	C18-C19-C21-C22
7	a	606	LPP	O27-C29-C30-C31
7	B	401	LPP	C23-C24-C25-C26
9	a	605	MQ8	C39-C38-C40-C41
7	x	101	LPP	C16-C17-C18-C19
7	x	101	LPP	C6-O5-P1-O3
7	A	603	LPP	O5-C6-C7-O9
9	A	606	MQ8	C35-C36-C37-C38
7	A	603	LPP	O5-C6-C7-C8
5	a	603	HEM	CAD-CBD-CGD-O1D
5	a	601	HEM	CAD-CBD-CGD-O2D
8	B	402	UQ8	C15-C14-C16-C17

Continued on next page...

Continued from previous page...

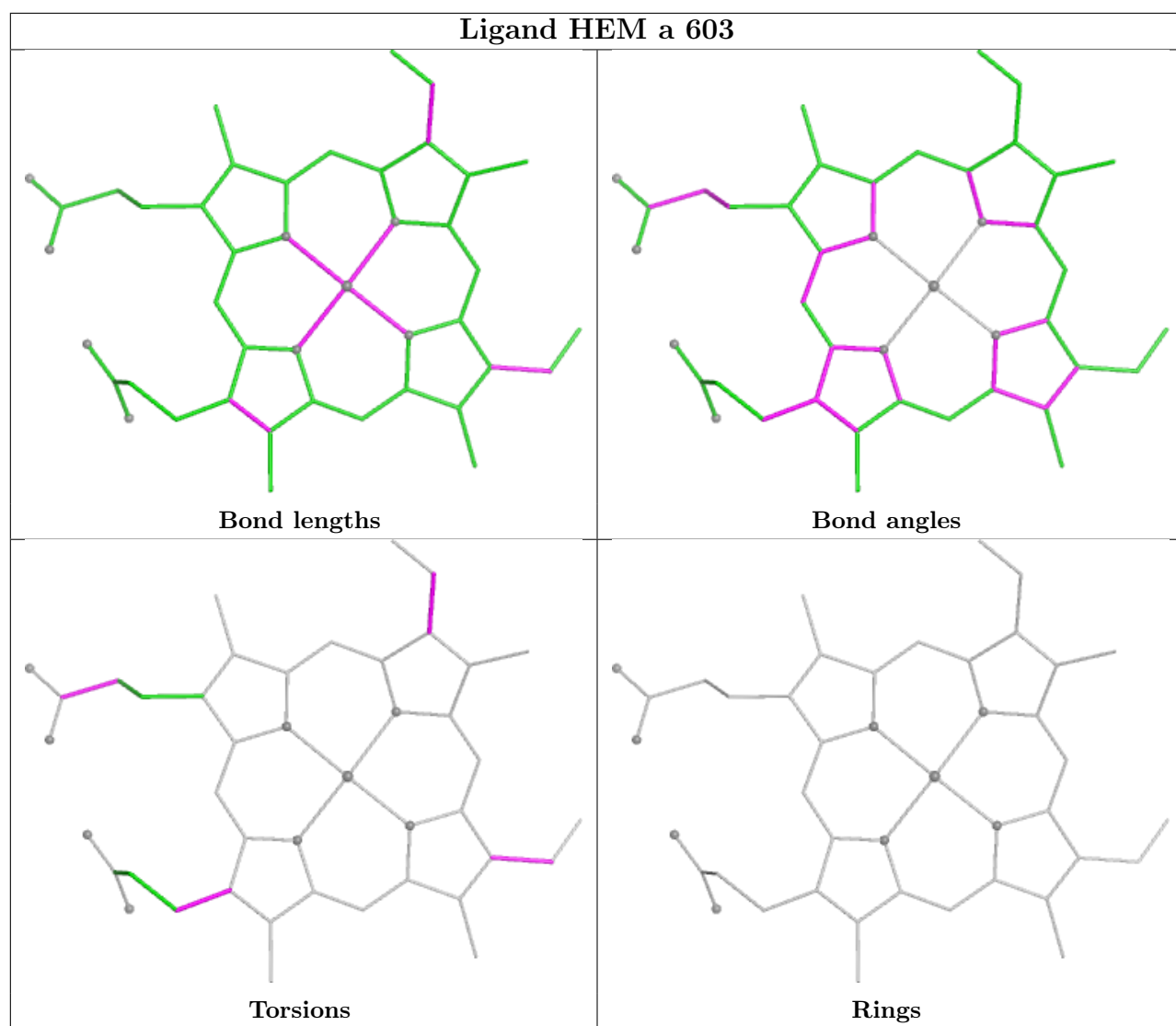
Mol	Chain	Res	Type	Atoms
5	A	604	HEM	CAD-CBD-CGD-O2D
7	a	606	LPP	O28-C29-C30-C31
8	b	402	UQ8	C36-C37-C38-C39
5	a	601	HEM	CAD-CBD-CGD-O1D
5	a	603	HEM	CAD-CBD-CGD-O2D
7	x	101	LPP	C22-C23-C24-C25
8	a	604	UQ8	C14-C16-C17-C18

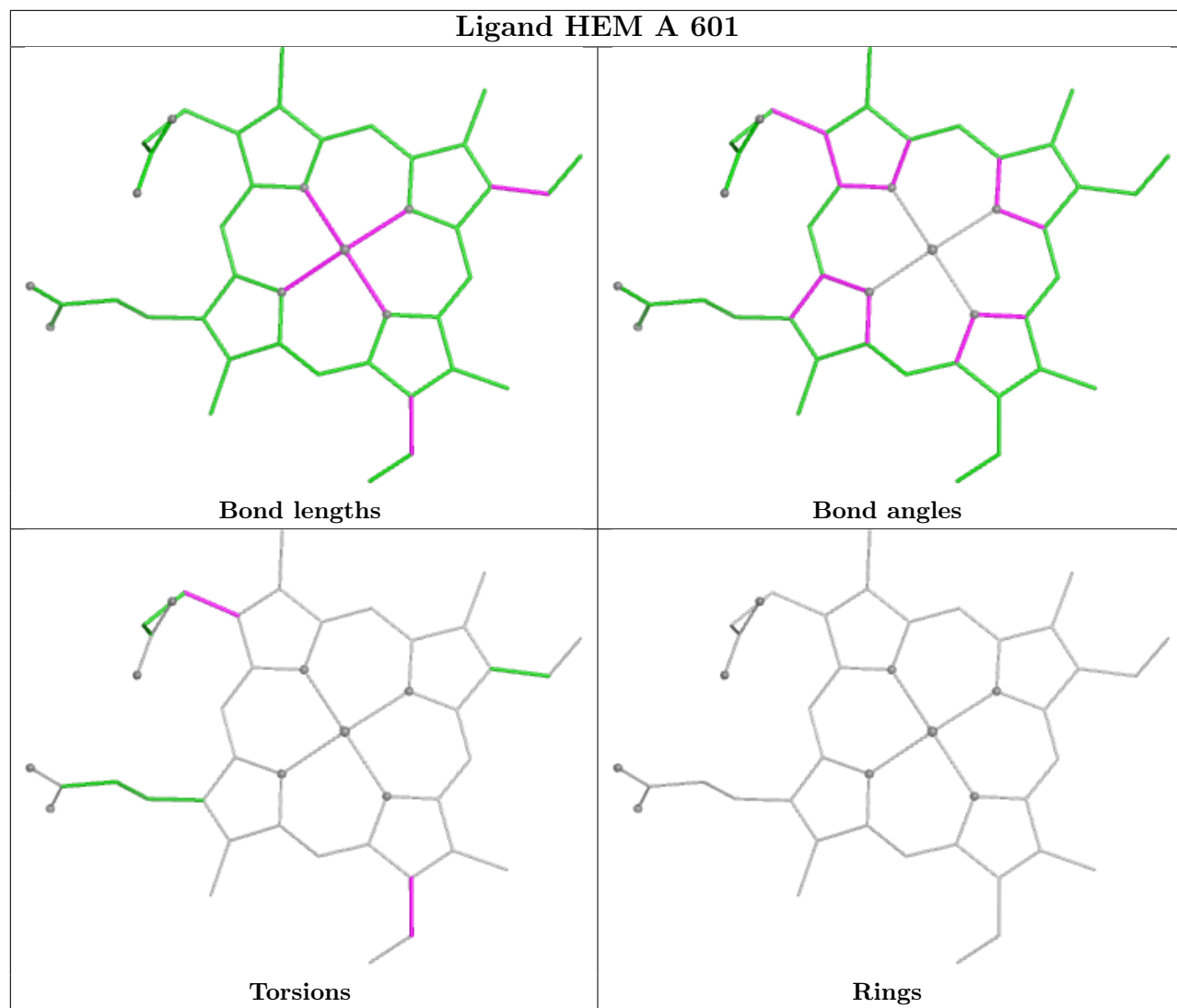
There are no ring outliers.

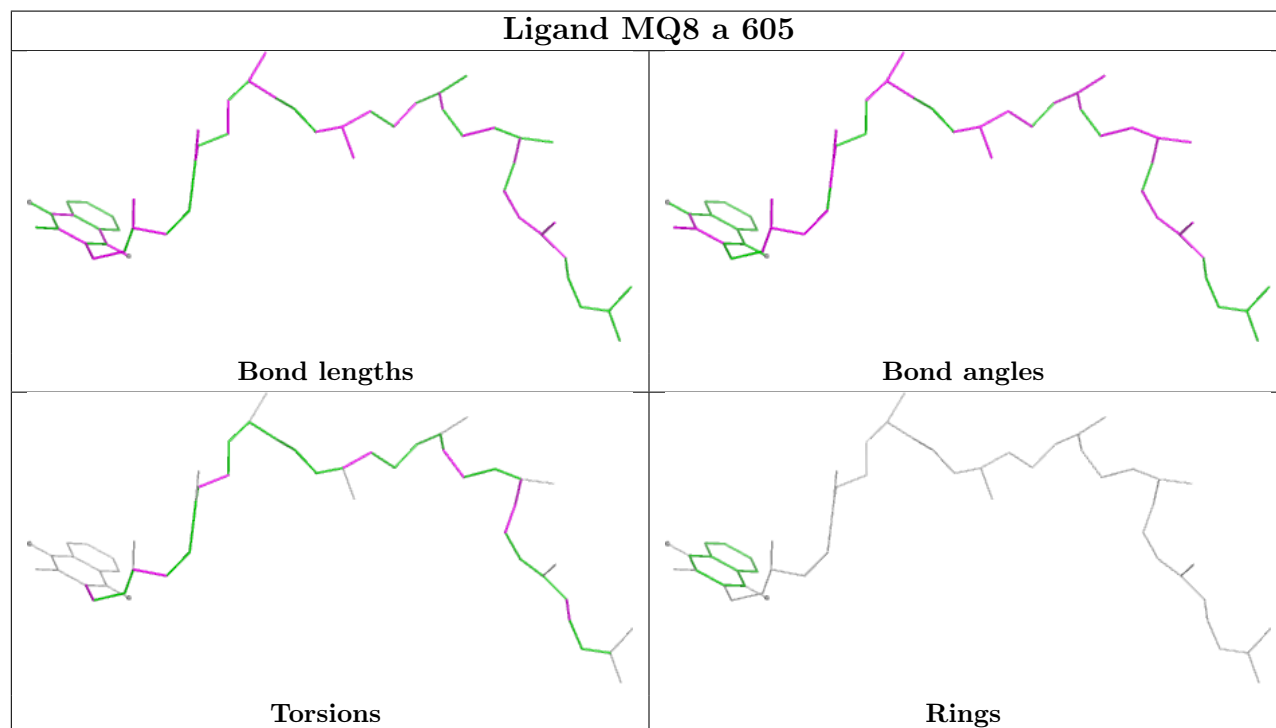
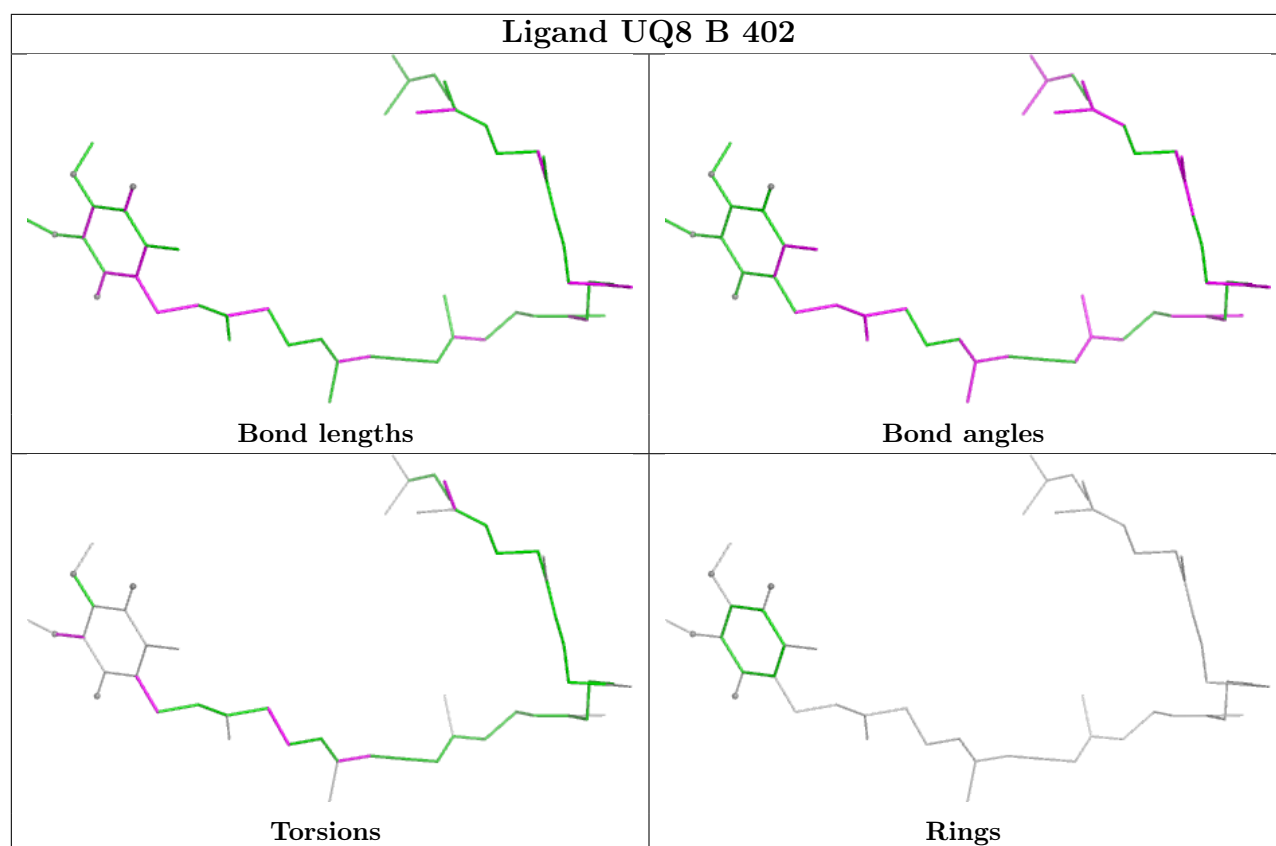
13 monomers are involved in 82 short contacts:

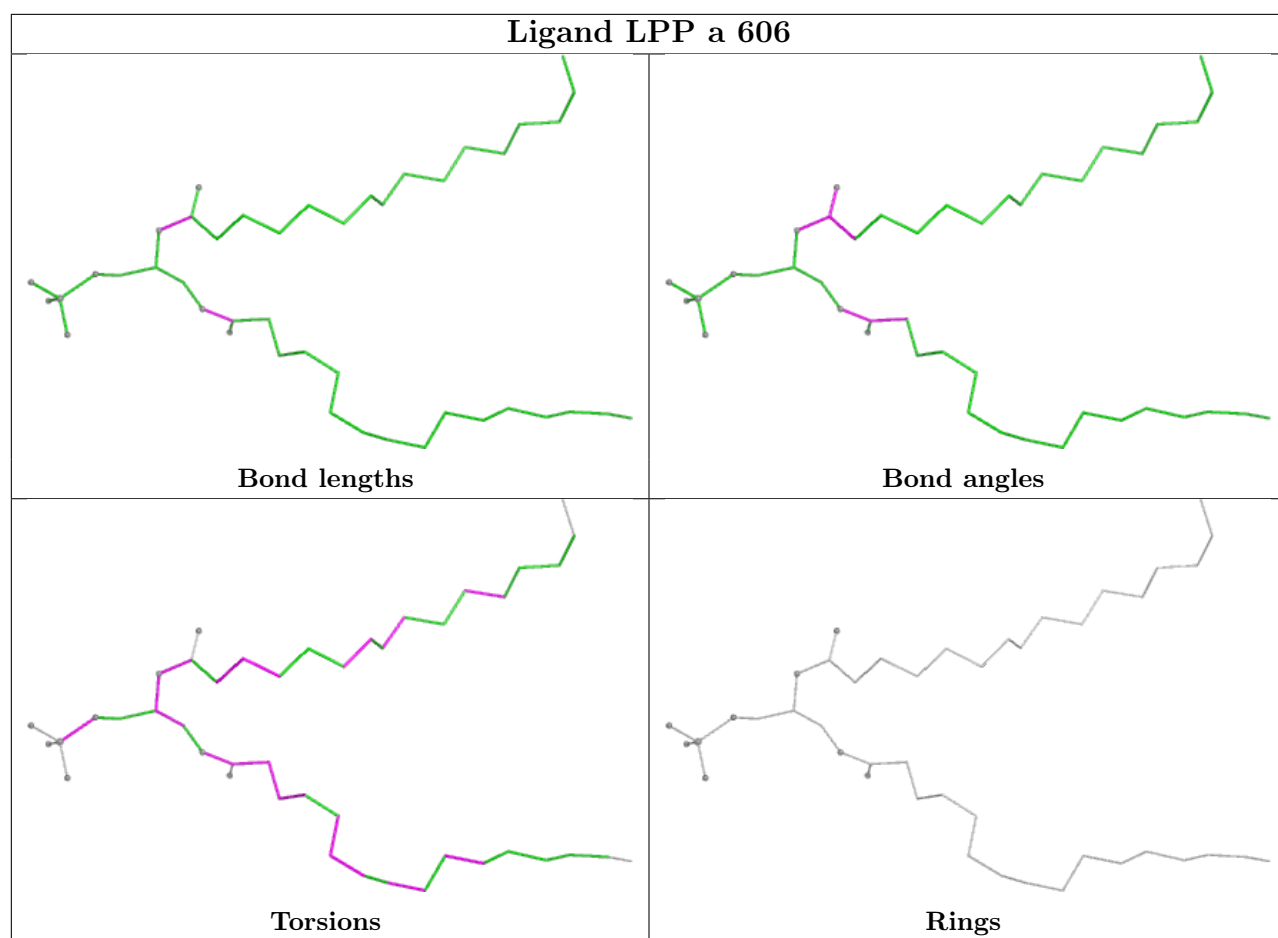
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	a	603	HEM	7	0
5	A	601	HEM	7	0
8	B	402	UQ8	5	0
9	a	605	MQ8	6	0
6	a	607	A1JN4	1	0
8	A	605	UQ8	10	0
7	a	602	LPP	3	0
7	A	603	LPP	4	0
9	A	606	MQ8	7	0
8	a	604	UQ8	12	0
5	a	601	HEM	7	0
5	A	604	HEM	6	0
8	b	402	UQ8	8	0

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.

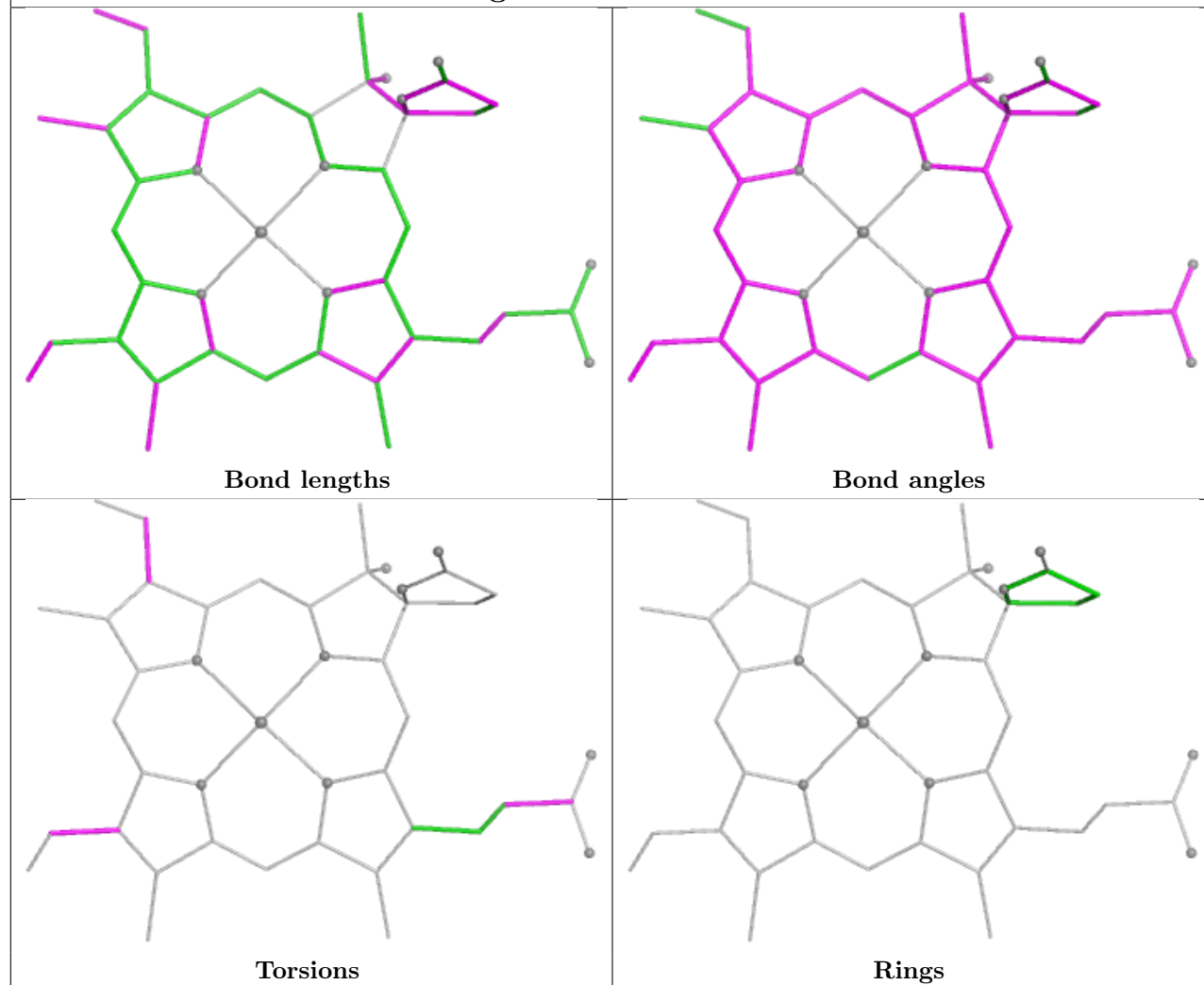




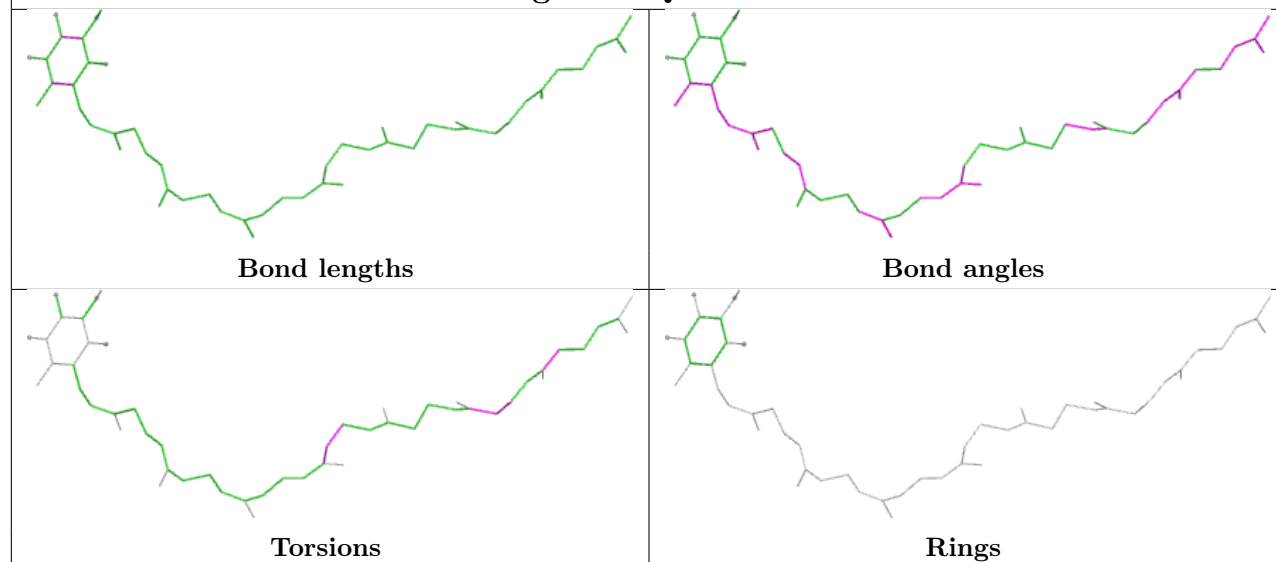


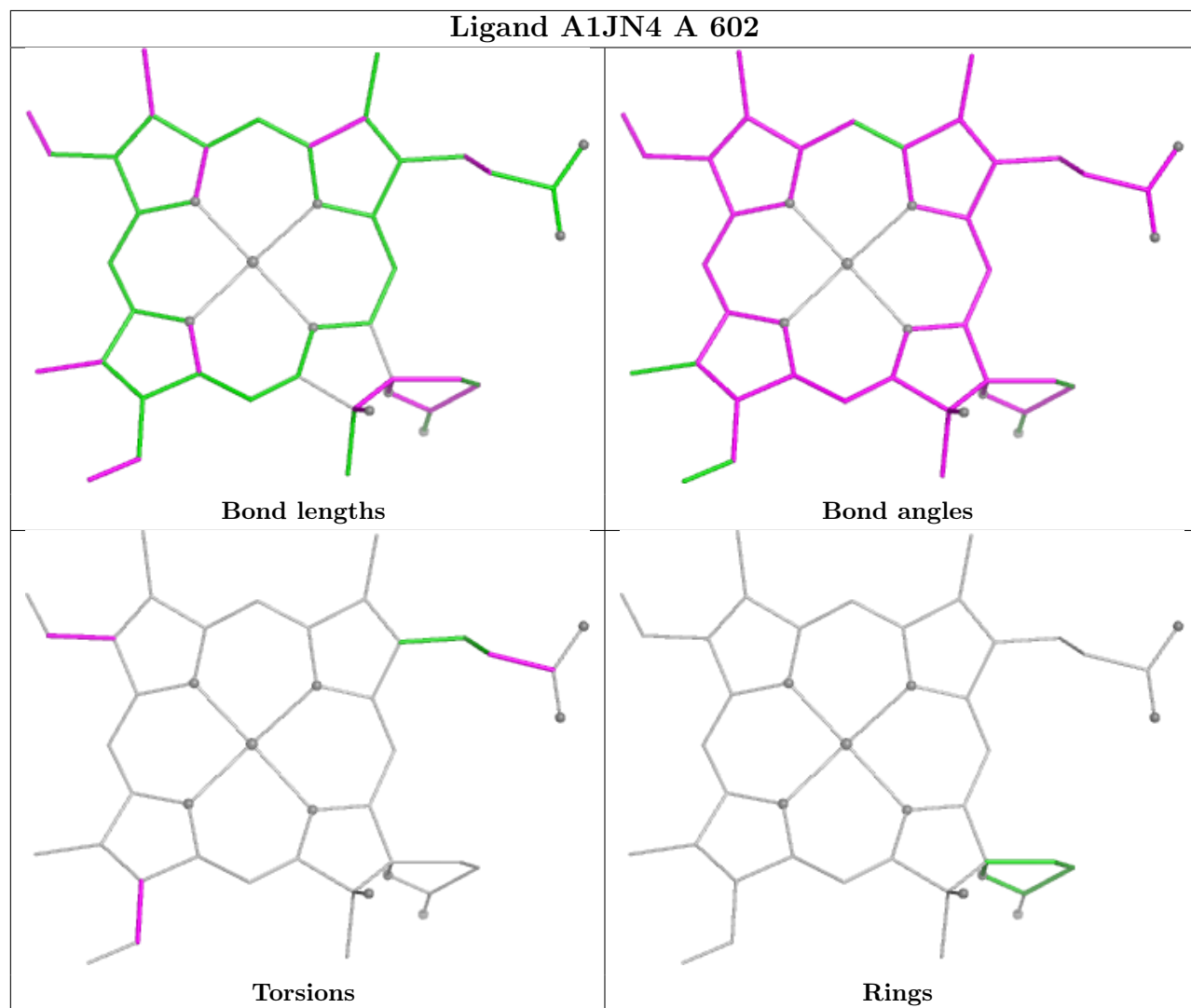
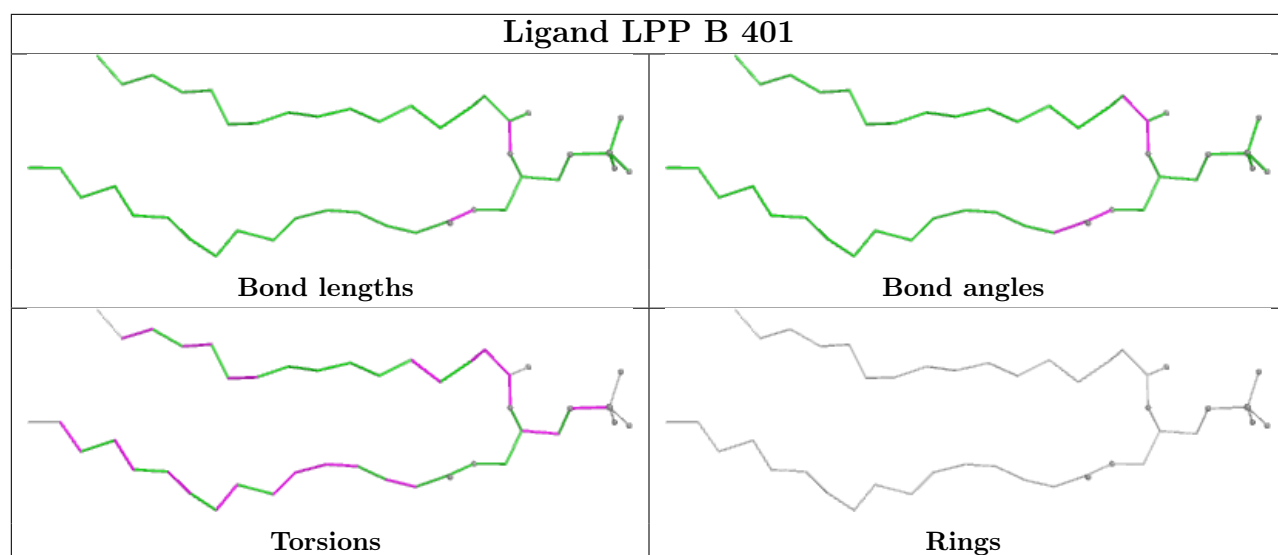


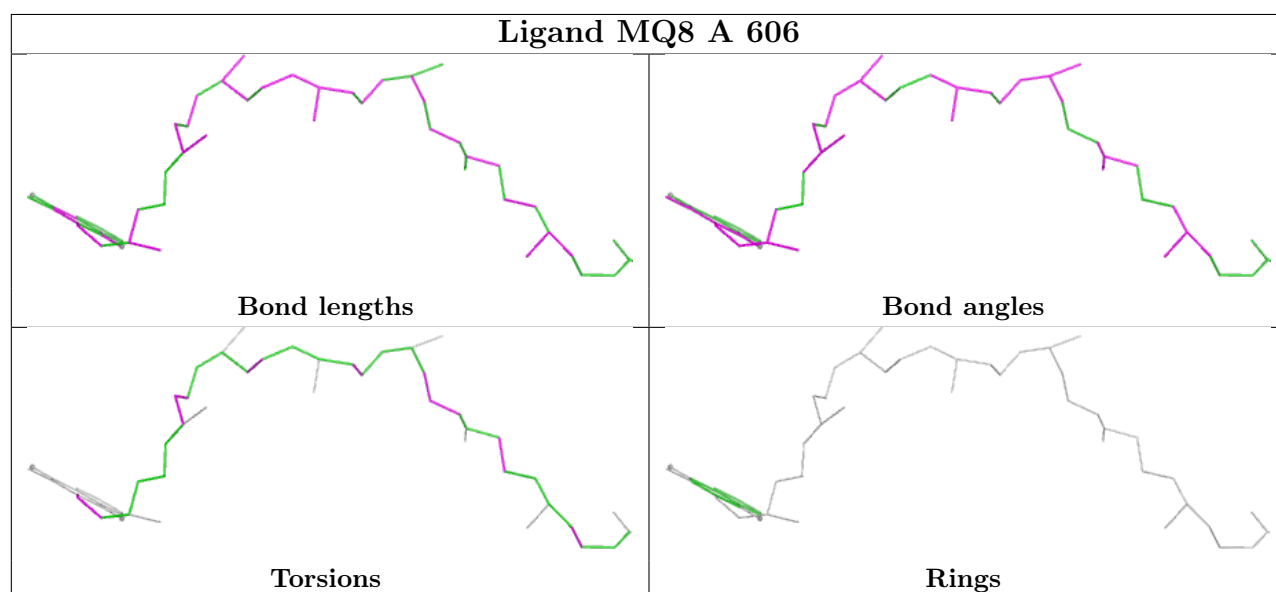
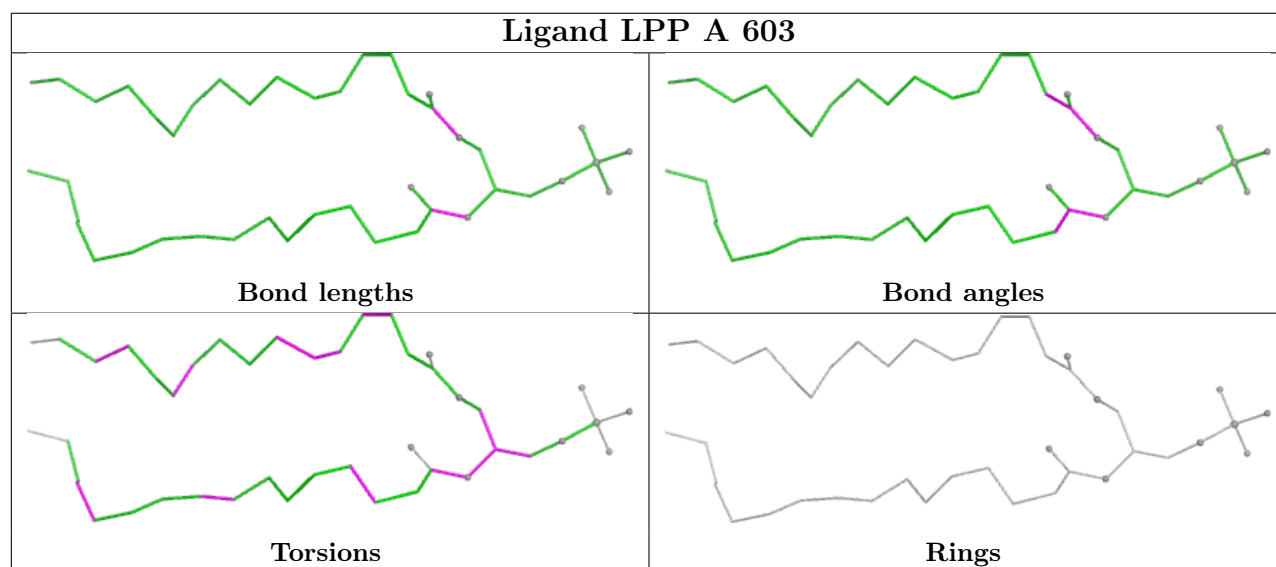
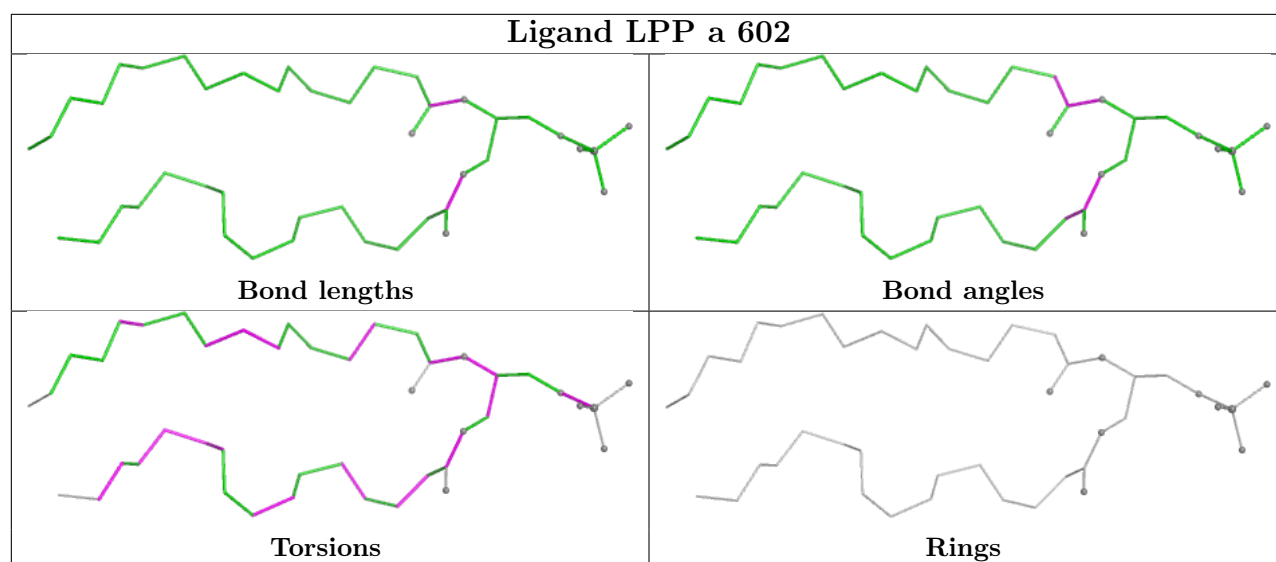
Ligand A1JN4 a 607

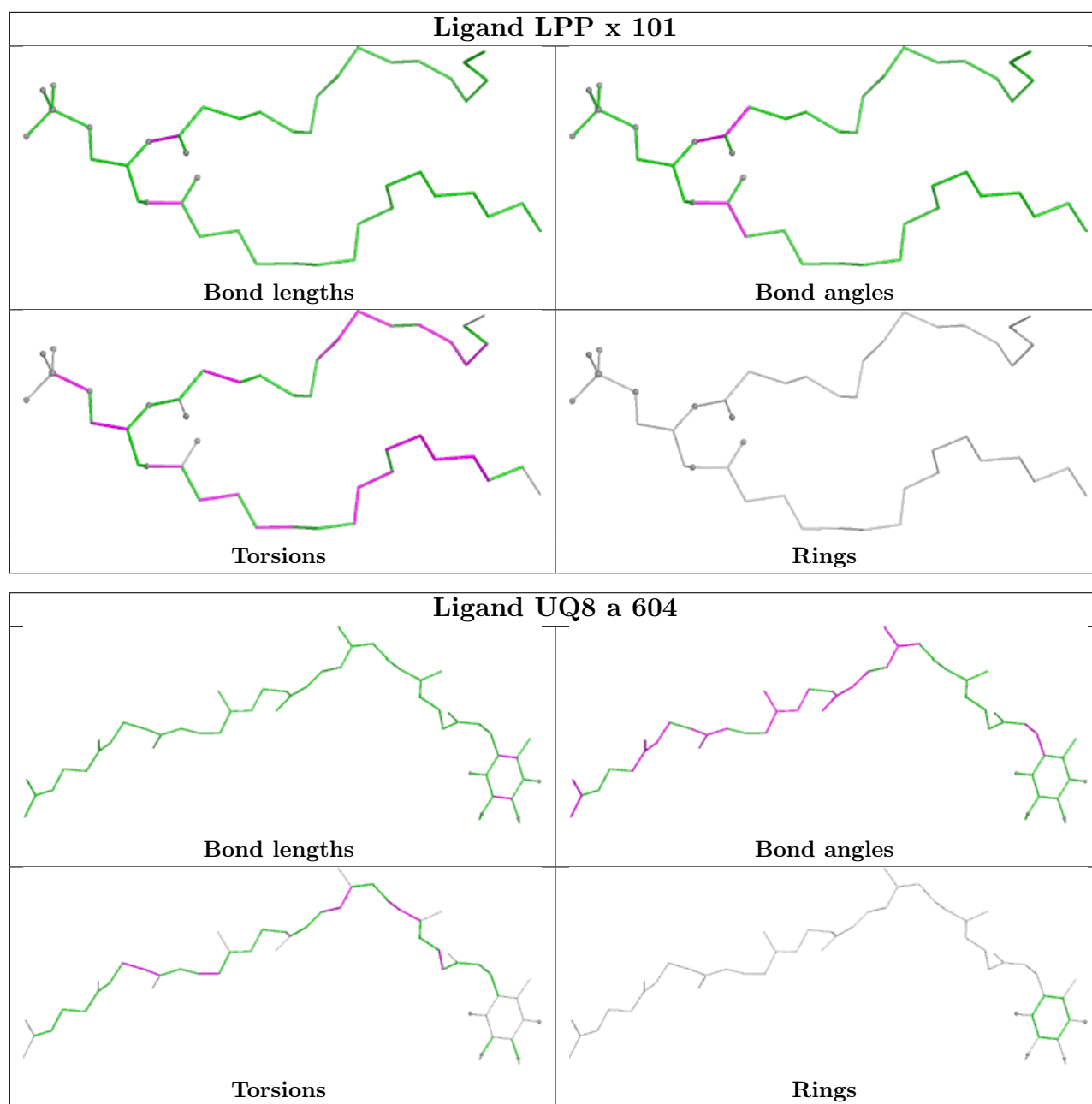


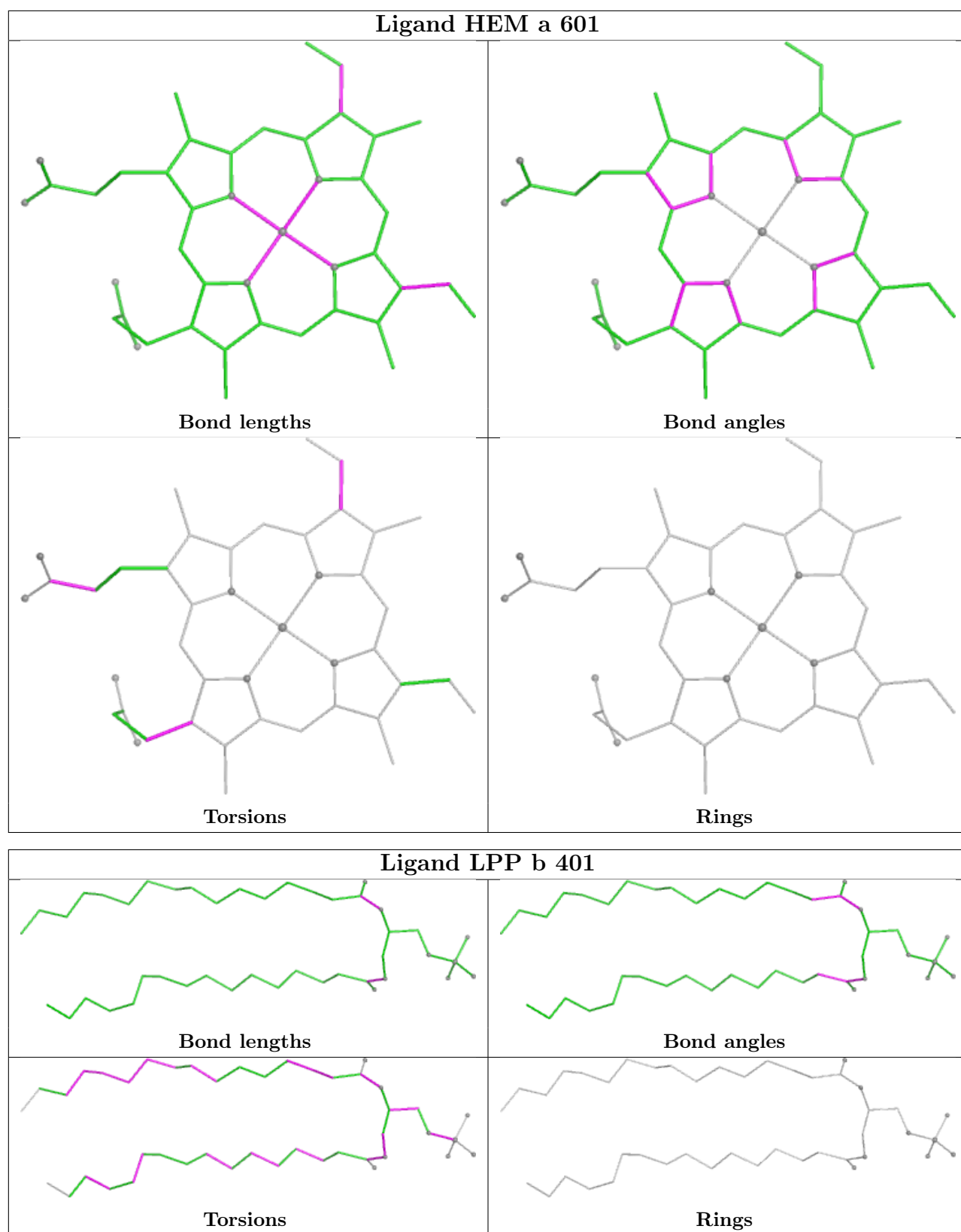
Ligand UQ8 A 605

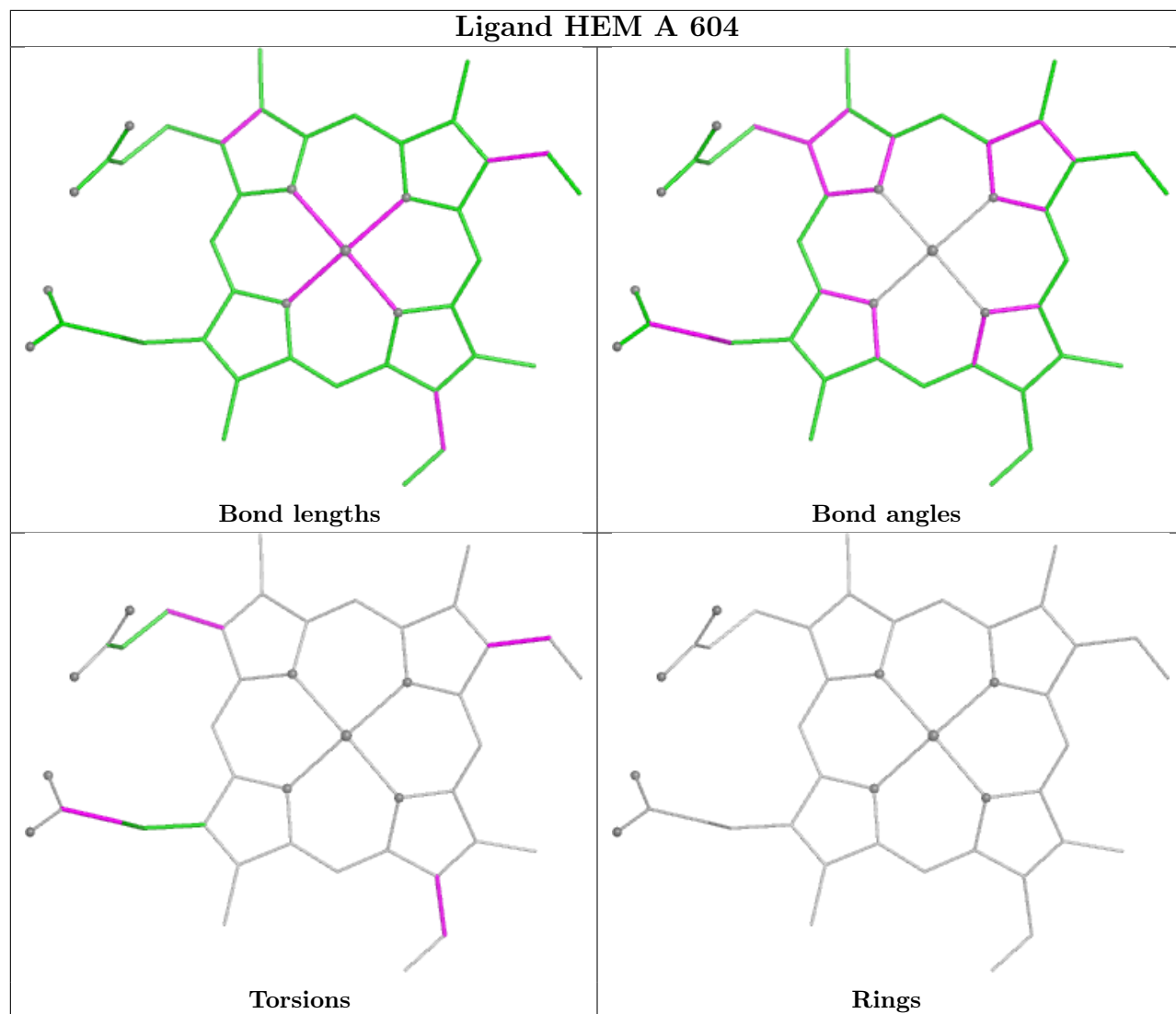


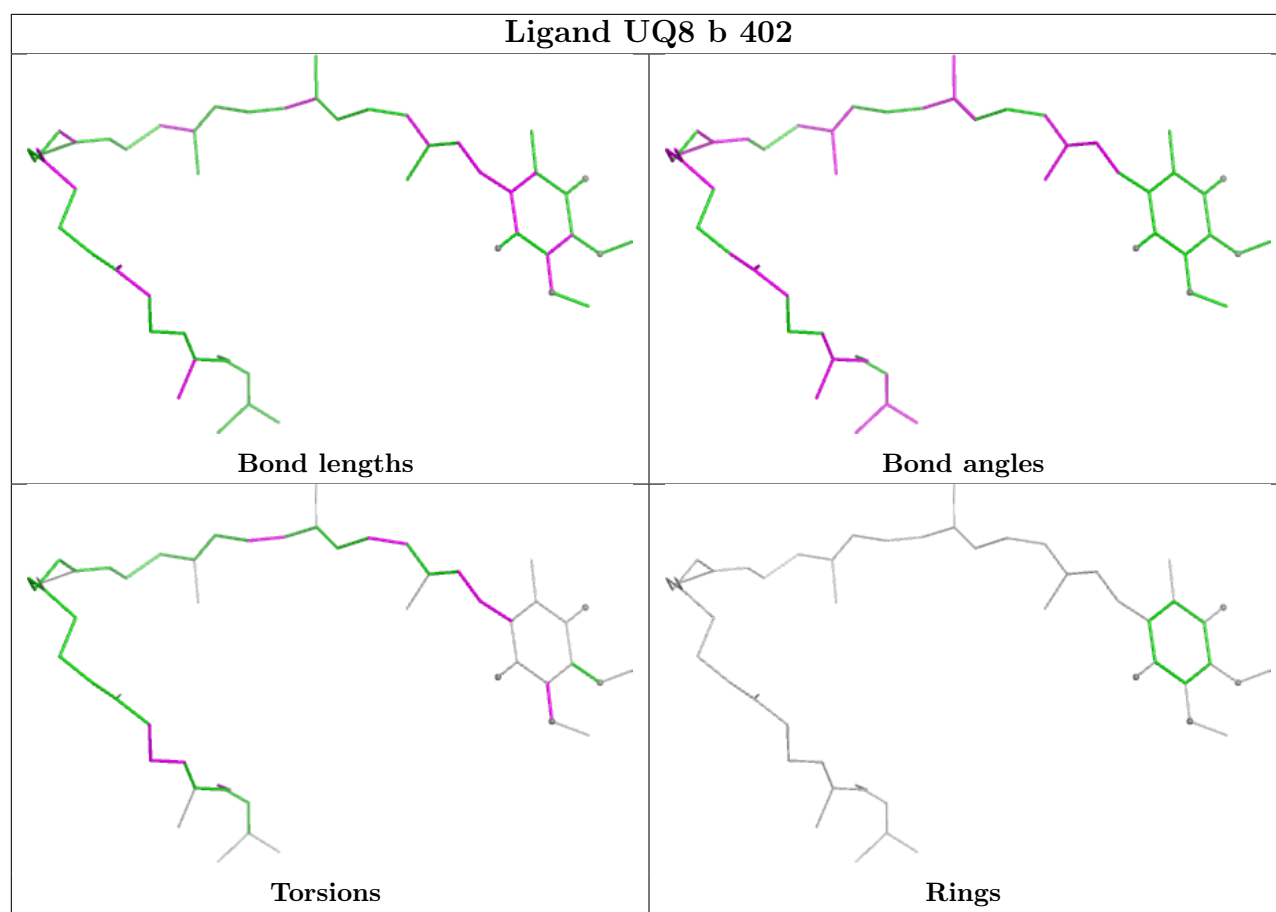












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

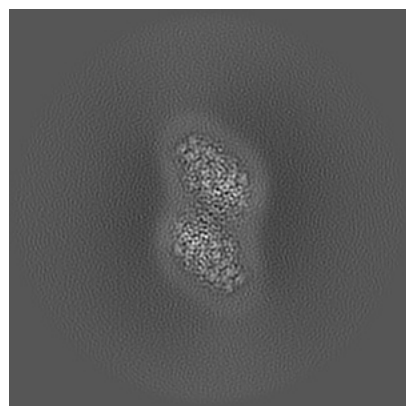
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54826. These allow visual inspection of the internal detail of the map and identification of artifacts.

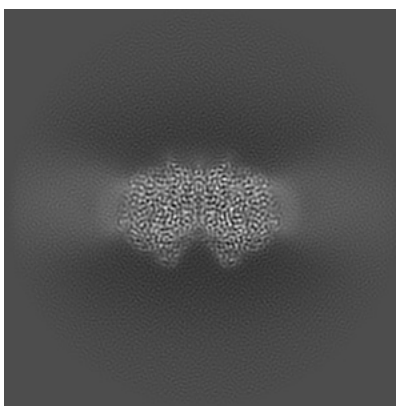
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

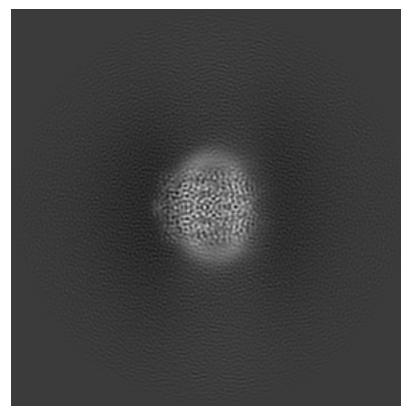
6.1.1 Primary map



X

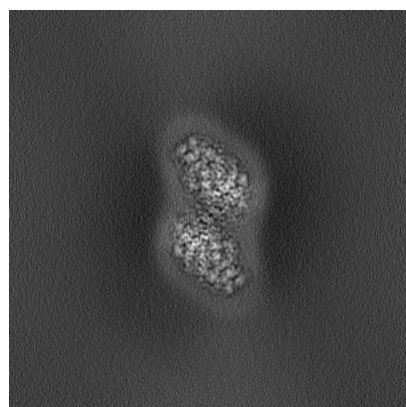


Y

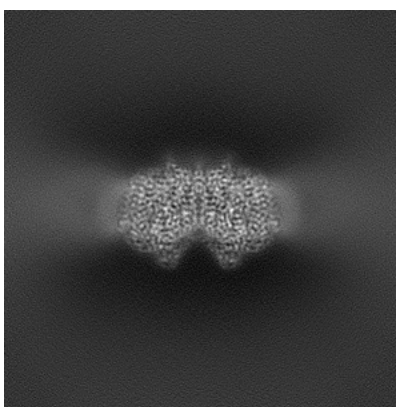


Z

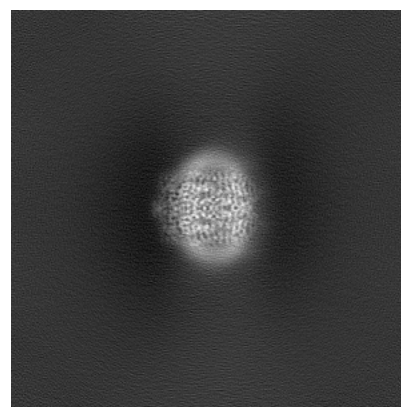
6.1.2 Raw map



X



Y

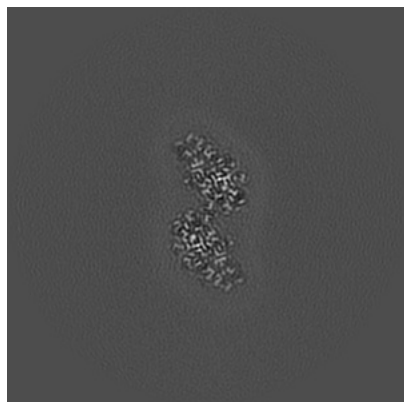


Z

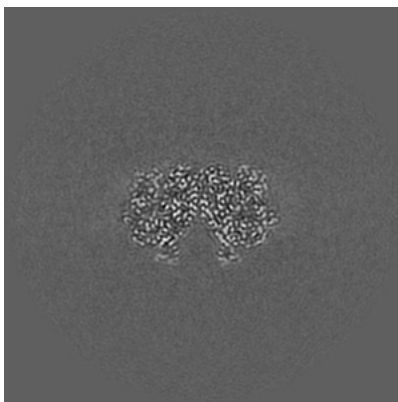
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

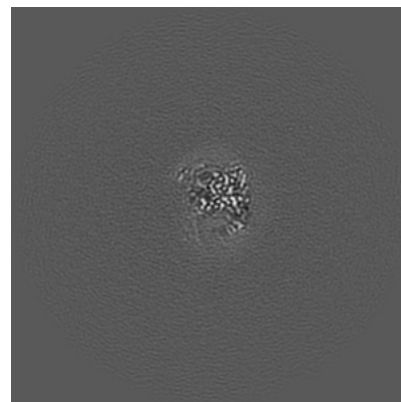
6.2.1 Primary map



X Index: 180

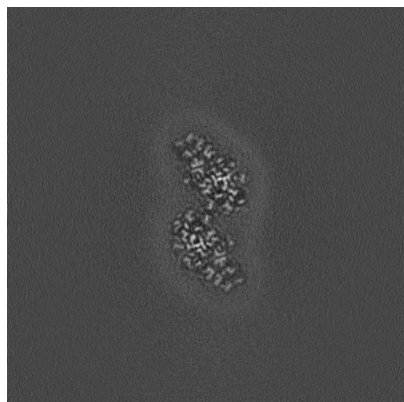


Y Index: 180

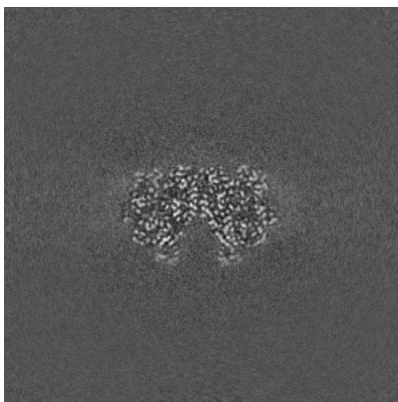


Z Index: 180

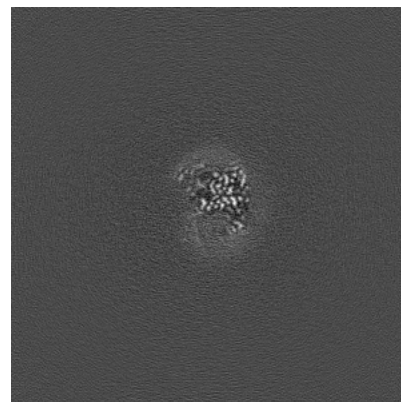
6.2.2 Raw map



X Index: 180



Y Index: 180

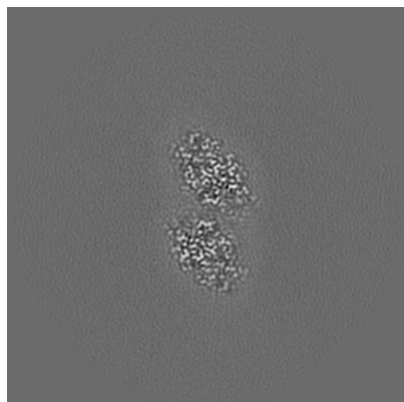


Z Index: 180

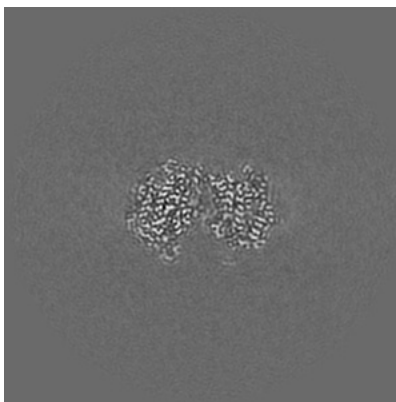
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

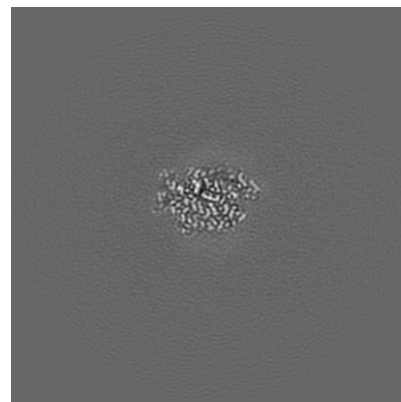
6.3.1 Primary map



X Index: 165

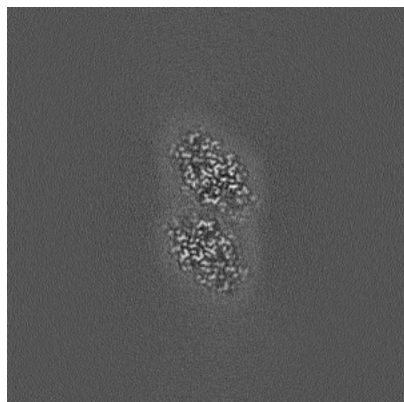


Y Index: 174

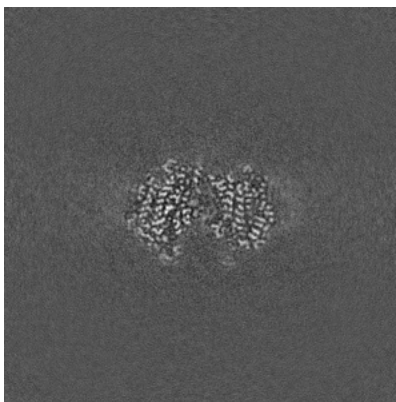


Z Index: 203

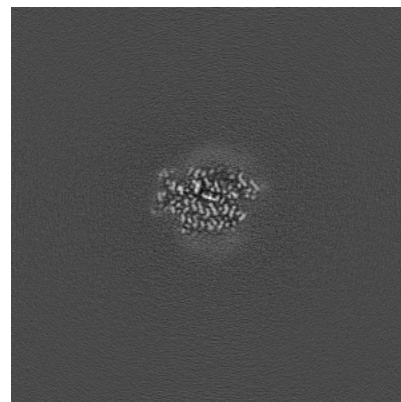
6.3.2 Raw map



X Index: 165



Y Index: 174

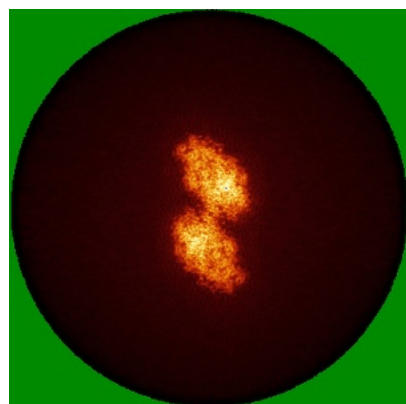


Z Index: 203

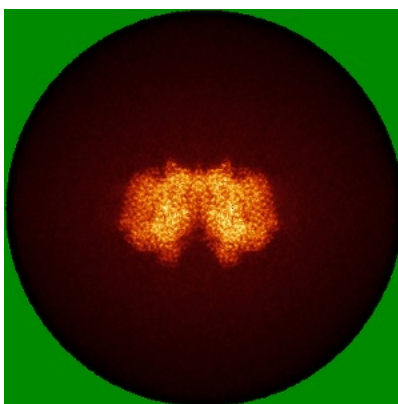
The images above show the largest variance slices of the map in three orthogonal directions.

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

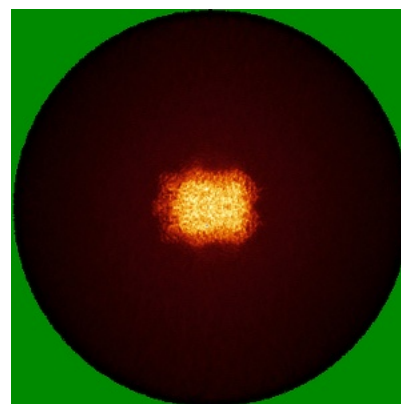
6.4.1 Primary map



X



Y

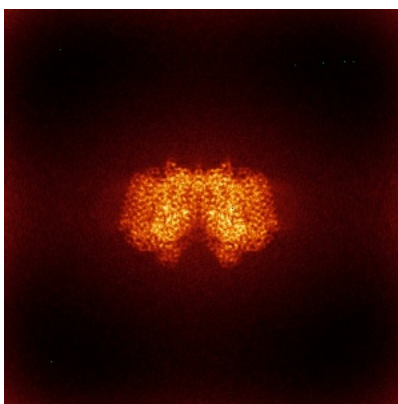


Z

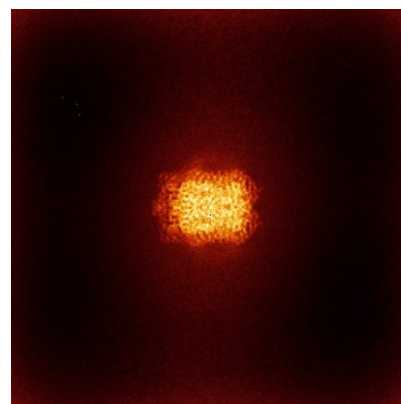
6.4.2 Raw map



X



Y

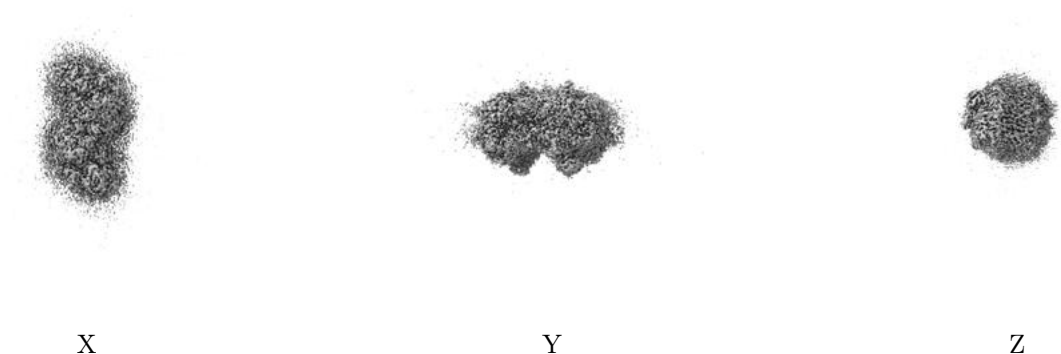


Z

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.

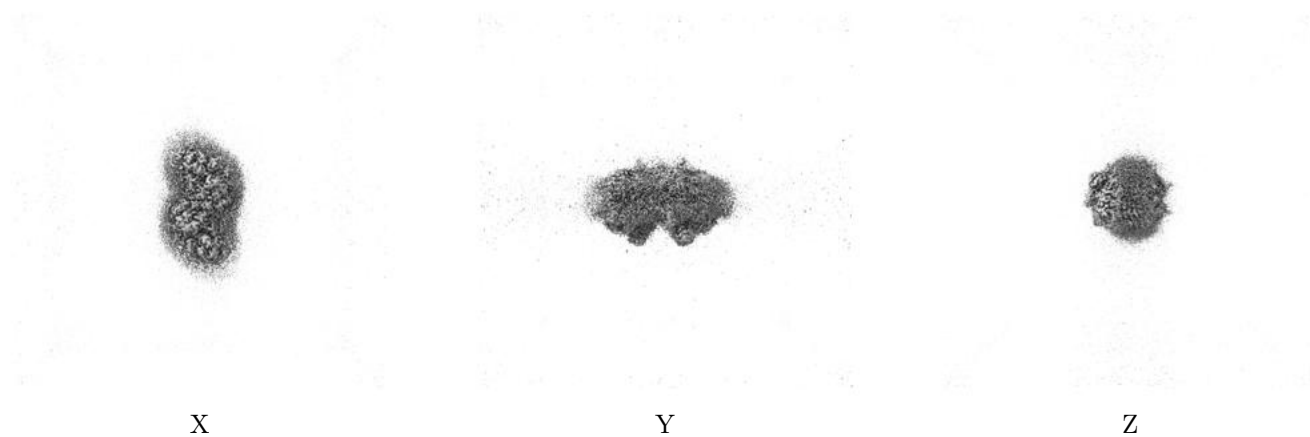
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.125. 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.

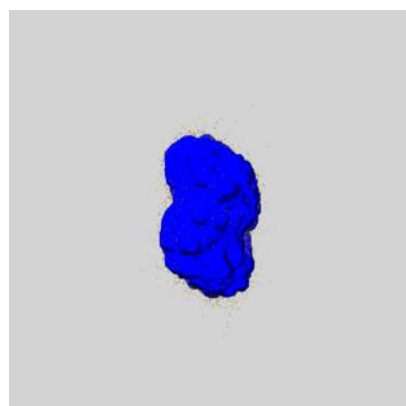
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

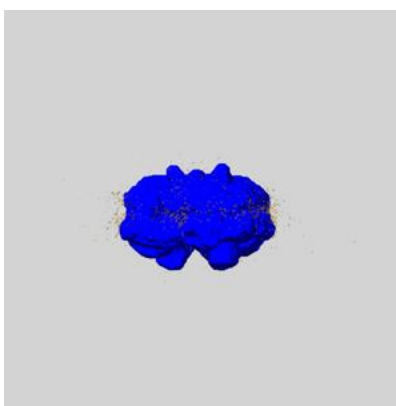
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

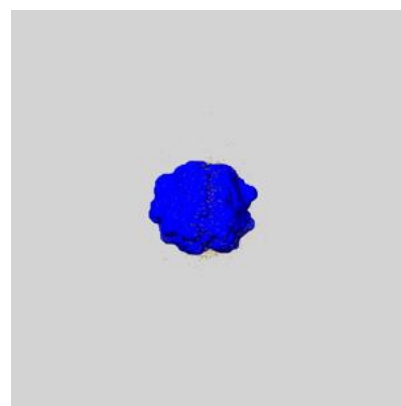
6.6.1 emd_54826_msk_1.map [i](#)



X



Y

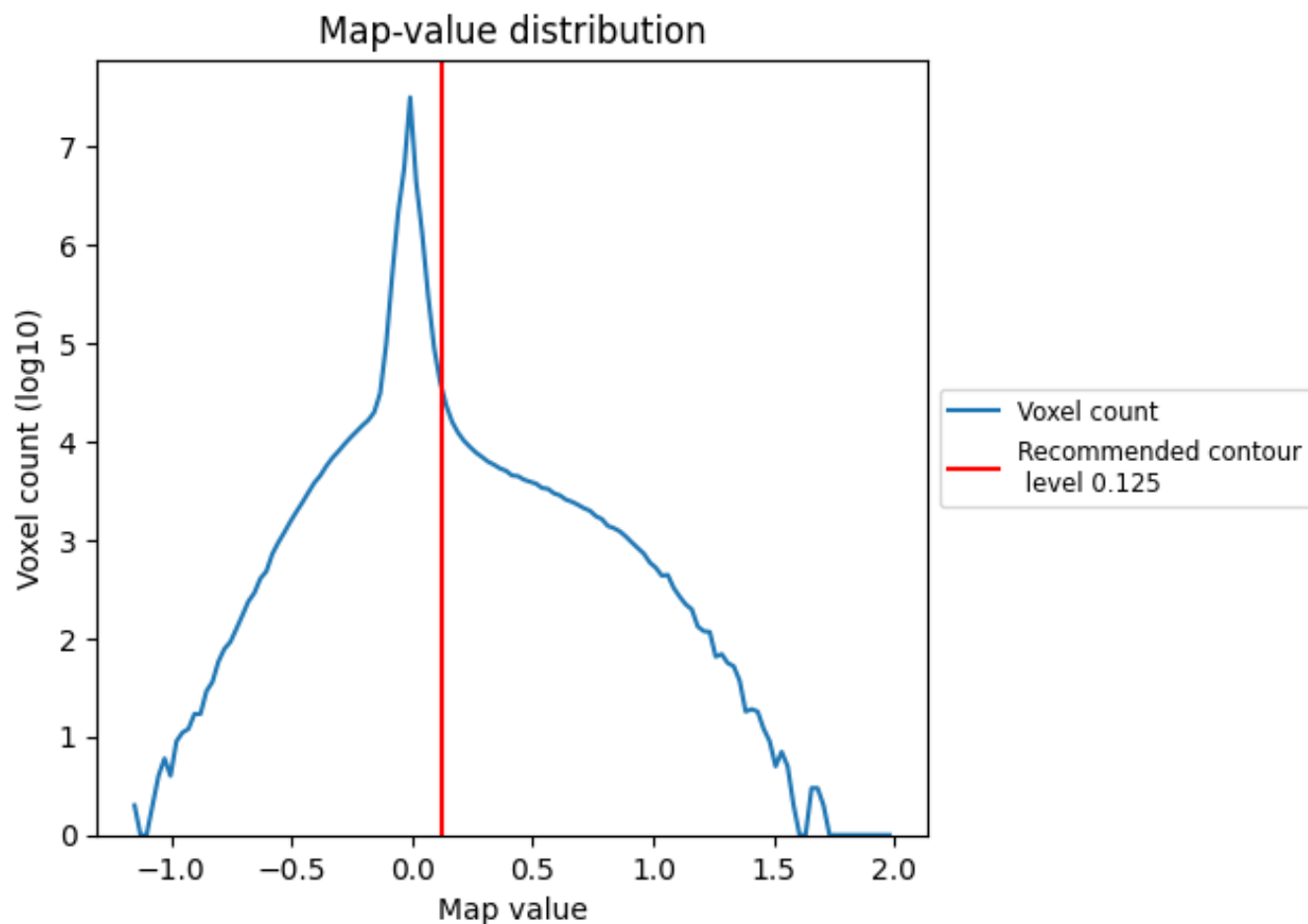


Z

7 Map analysis [i](#)

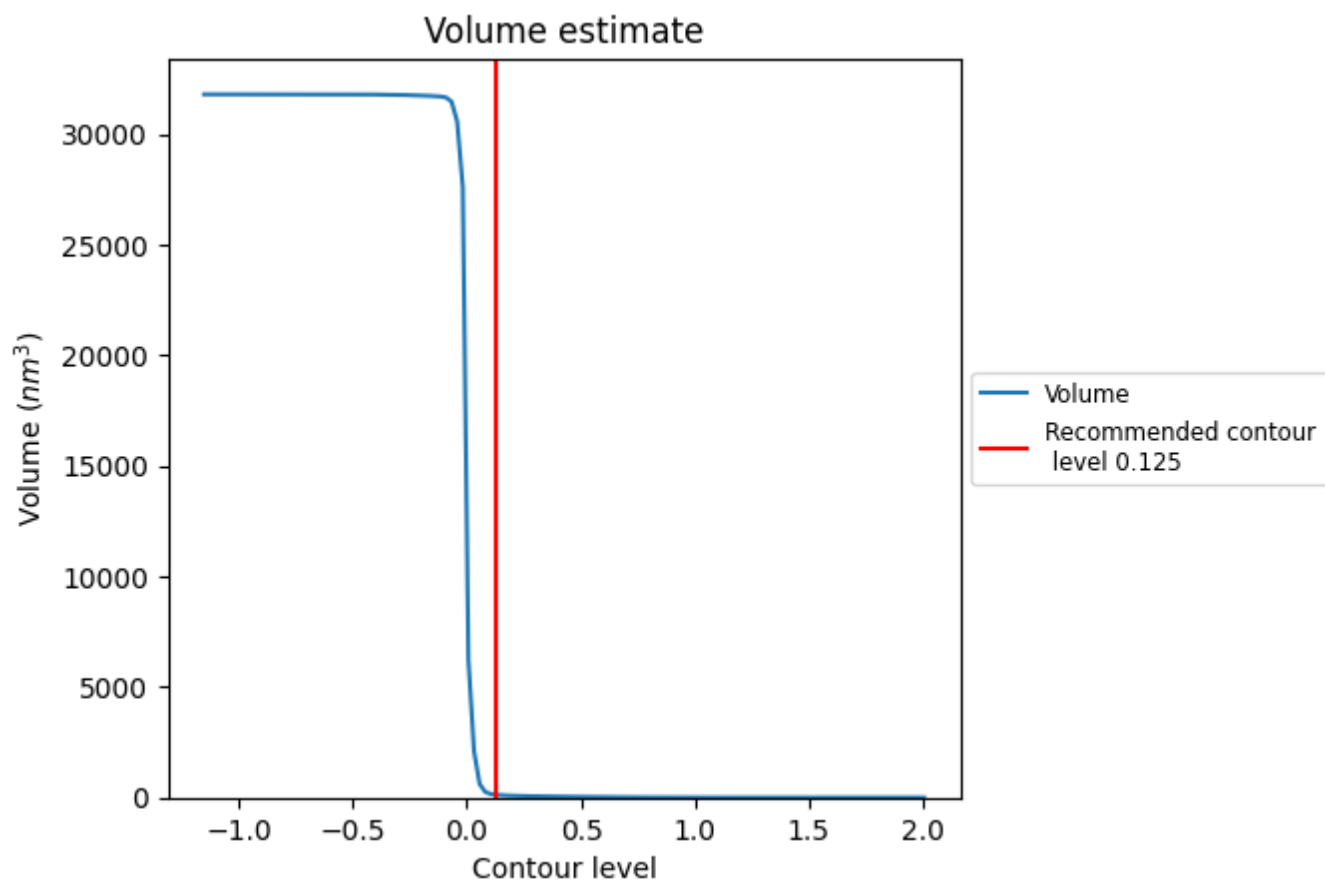
This section contains the results of statistical analysis of the map.

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.

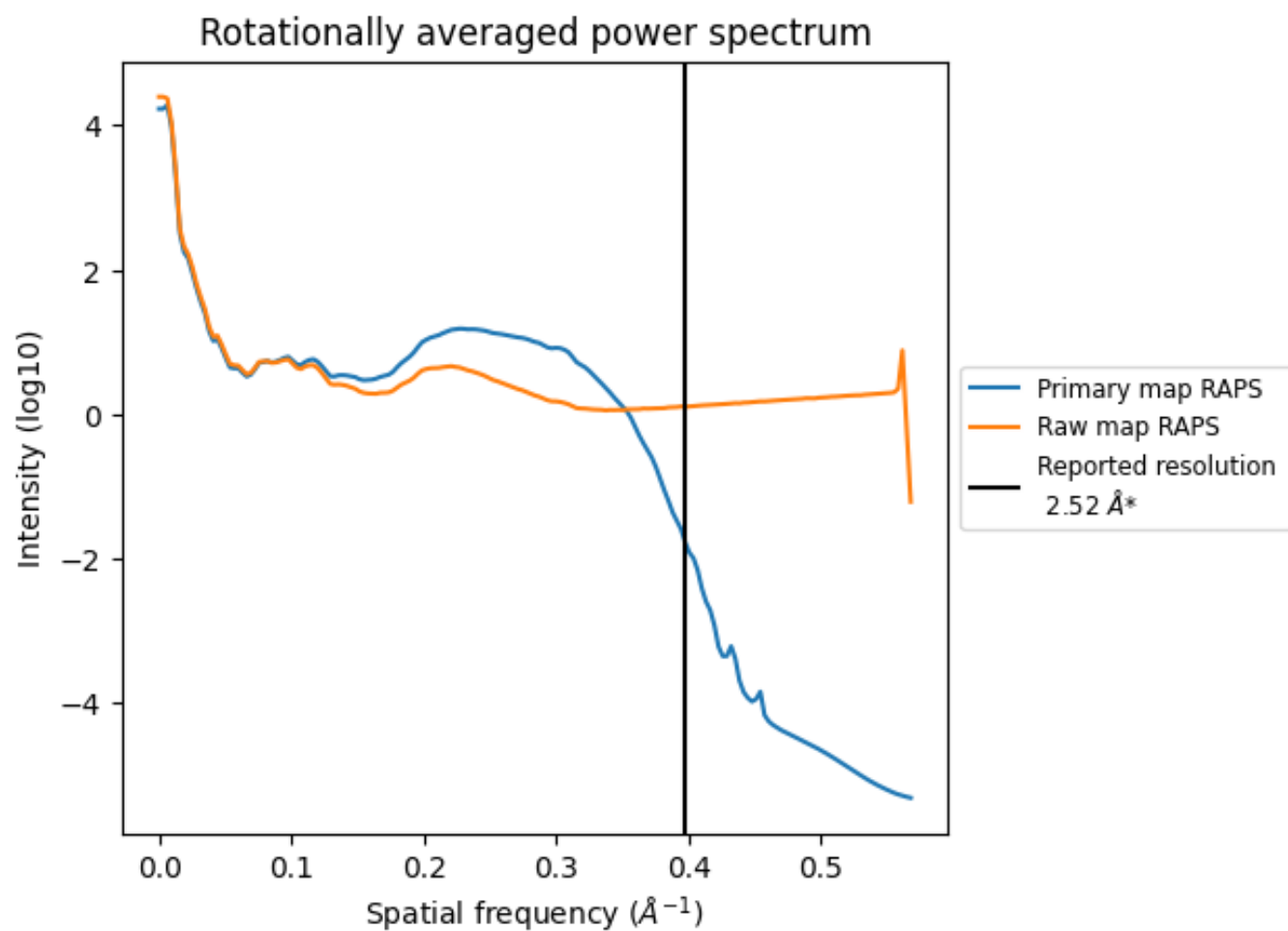
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 130 nm³; this corresponds to an approximate mass of 117 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 ⓘ

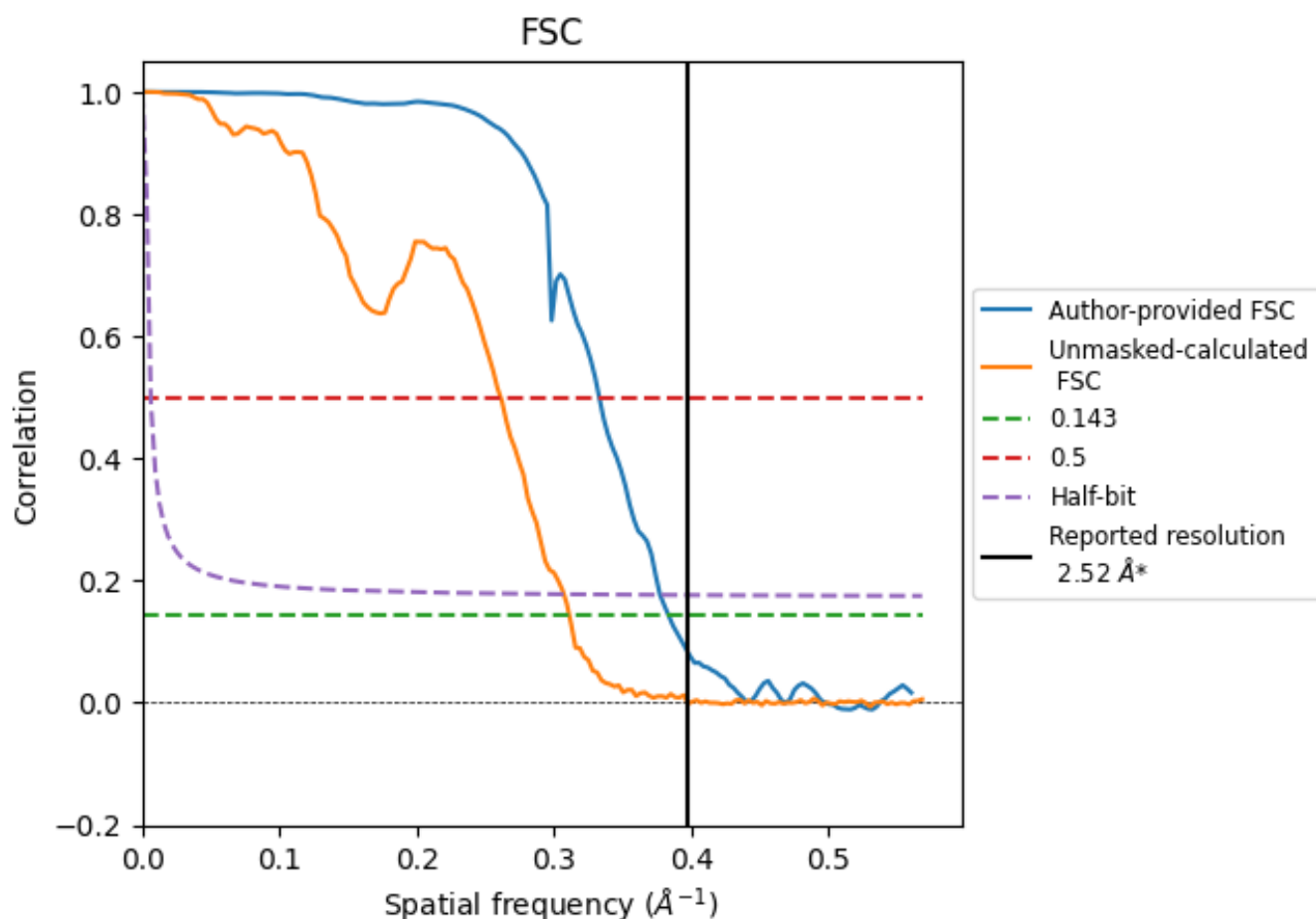


*Reported resolution corresponds to spatial frequency of 0.397 \AA^{-1}

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 0.397 \AA^{-1}

8.2 Resolution estimates [i](#)

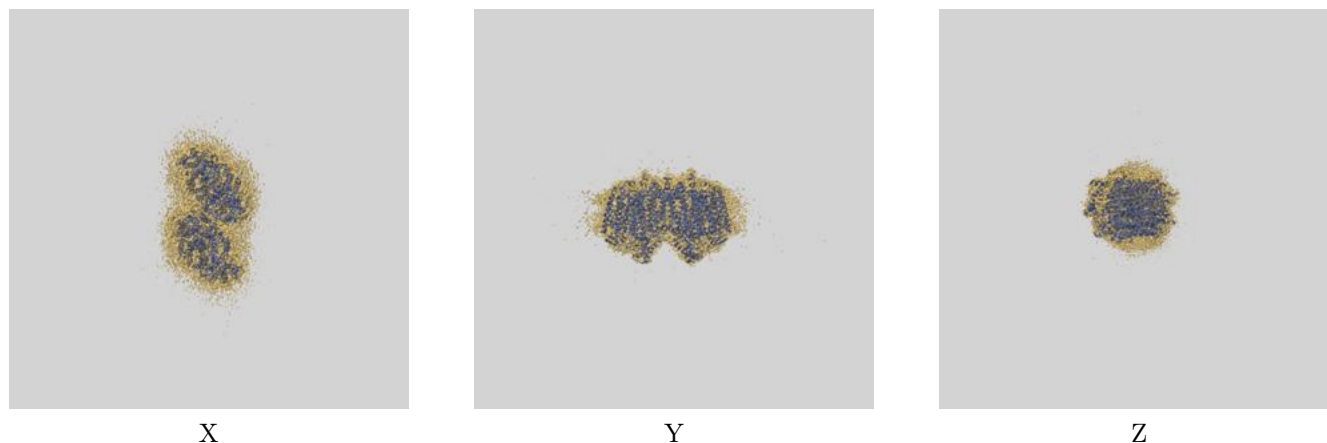
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.52	-	-
Author-provided FSC curve	2.61	3.00	2.65
Unmasked-calculated*	3.21	3.83	3.26

*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 3.21 differs from the reported value 2.52 by more than 10 %

9 Map-model fit [i](#)

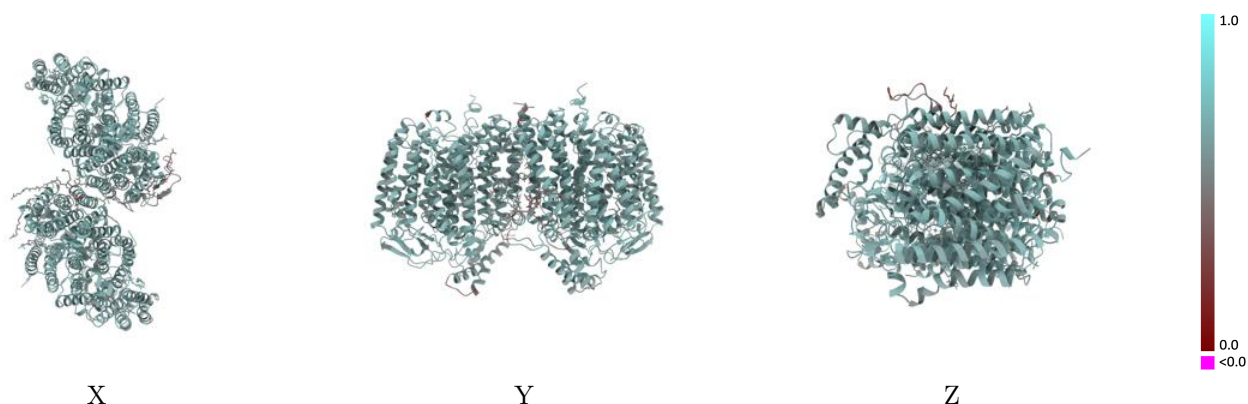
This section contains information regarding the fit between EMDB map EMD-54826 and PDB model 9SFJ. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



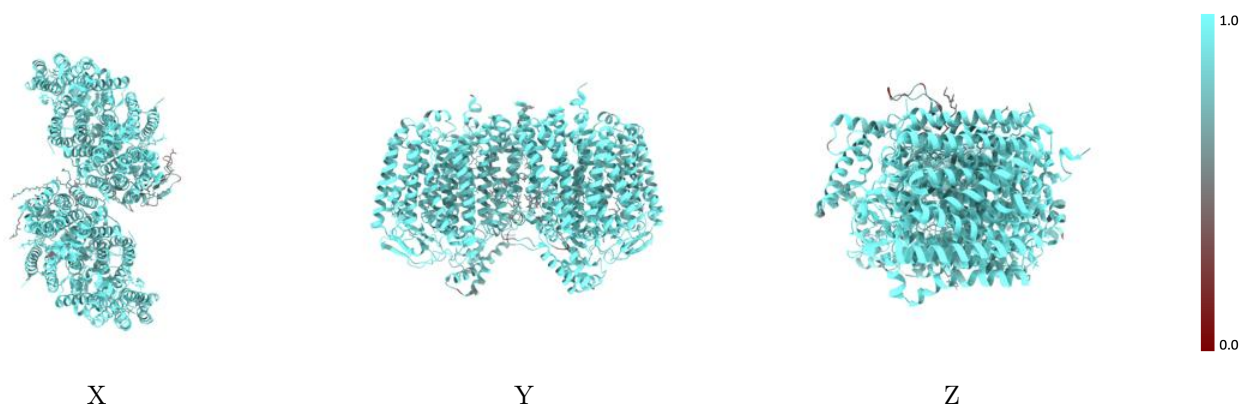
The images above show the 3D surface view of the map at the recommended contour level 0.125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



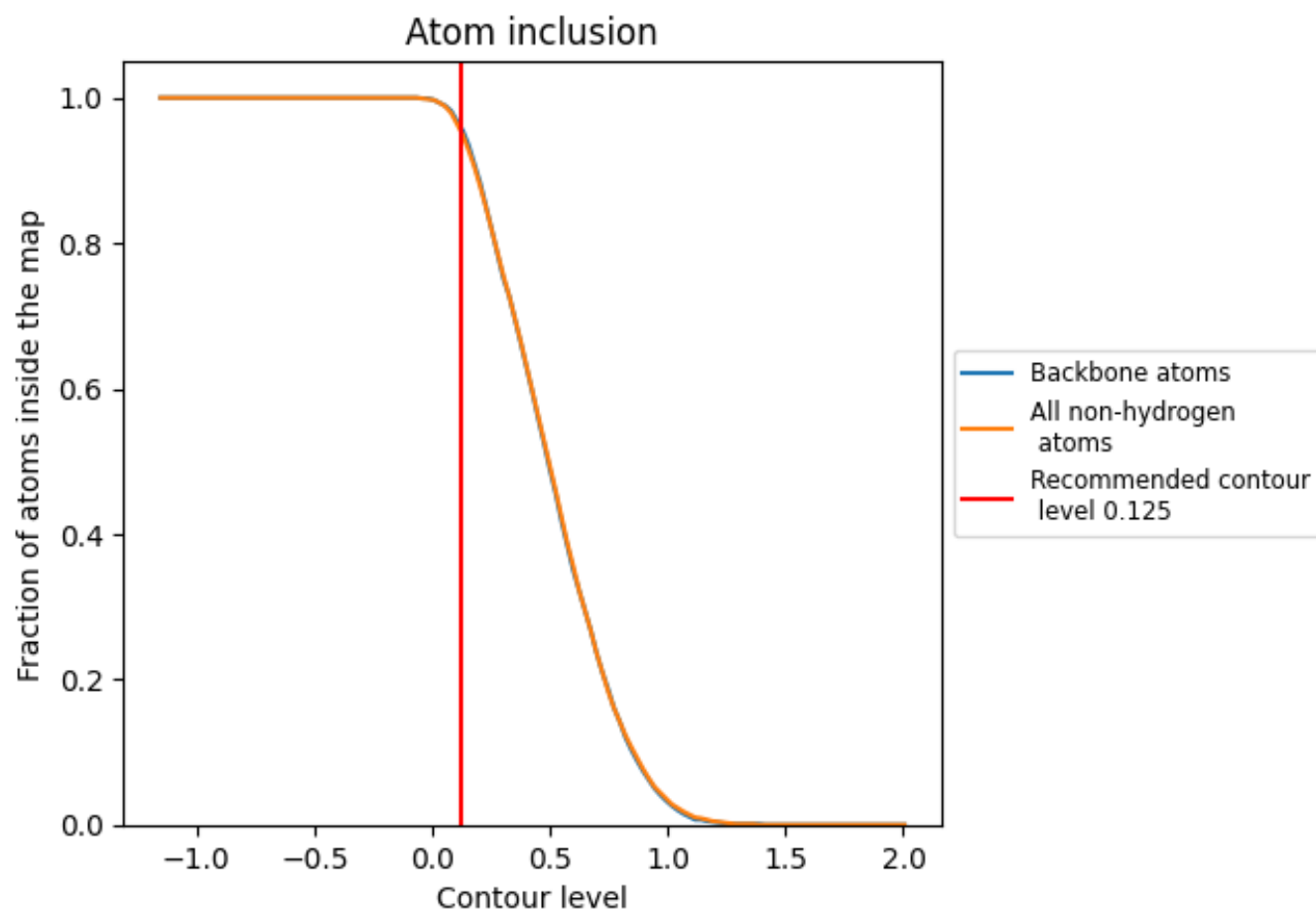
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.125).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9520	<div><div></div></div> 0.6210
A	<div><div></div></div> 0.9470	<div><div></div></div> 0.6220
B	<div><div></div></div> 0.9580	<div><div></div></div> 0.6220
H	<div><div></div></div> 0.8760	<div><div></div></div> 0.6010
X	<div><div></div></div> 0.9430	<div><div></div></div> 0.6060
a	<div><div></div></div> 0.9370	<div><div></div></div> 0.6170
b	<div><div></div></div> 0.9670	<div><div></div></div> 0.6280
h	<div><div></div></div> 0.9330	<div><div></div></div> 0.6140
x	<div><div></div></div> 0.9450	<div><div></div></div> 0.6150

1.0

0.0

<0.0