



Full wwPDB EM Validation Report ⓘ

Jun 4, 2026 – 12:24 pm BST

PDB ID : 9SEJ / pdb_00009sej
EMDB ID : EMD-54812
Title : E.coli cytochrome bd-I dimer bound to Aurachin D
Authors : van der Velden, T.T.; Kayastha, K.; Bruenle, S.; Jeuken, L.J.C.
Deposited on : 2025-08-19
Resolution : 2.47 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

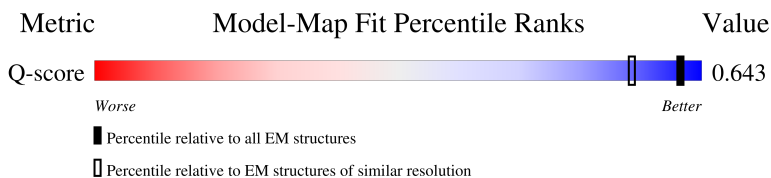
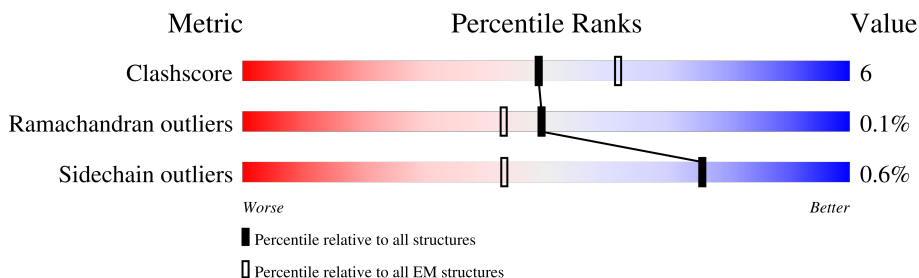
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.47 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.



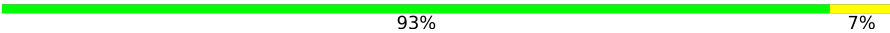
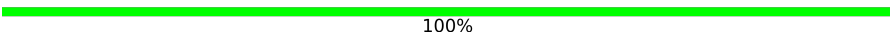
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6086 (1.98 - 2.97)

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	
1	a	522	
2	B	379	
2	b	379	

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Mol	Chain	Length	Quality of chain
3	H	29	 93% 7%
3	h	29	 100%
4	X	37	 73% 8% 19%
4	x	37	 78% 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
10	A1JN4	A	607	X	-	-	-
10	A1JN4	a	607	X	-	-	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 32006 atoms, of which 16031 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	513	Total	C	H	N	O	S	0	0
			8108	2663	4068	648	705	24		
1	a	513	Total	C	H	N	O	S	0	0
			8103	2663	4063	648	705	24		

- 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		

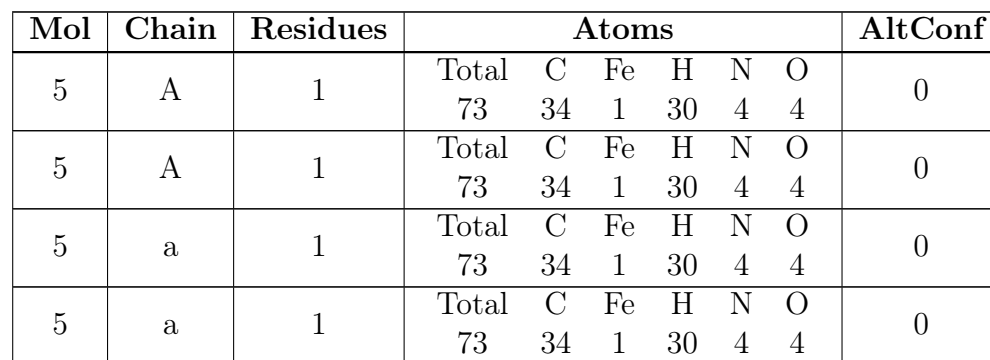
- Molecule 3 is a protein called Cytochrome bd-I ubiquinol oxidase CydH (Uncharacterized protein YnhF).

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

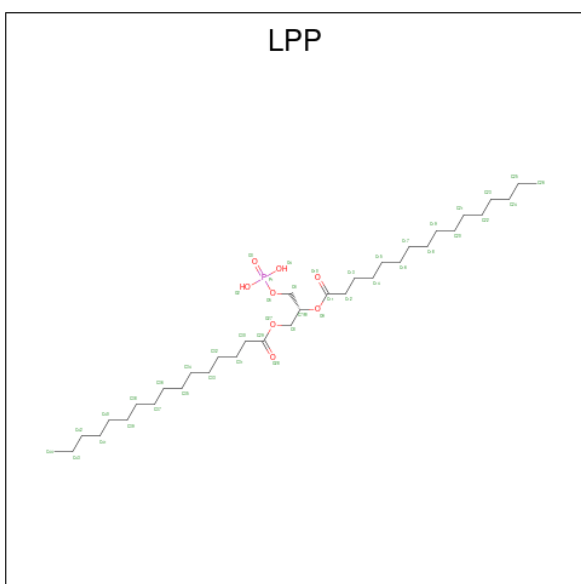
- Molecule 4 is a protein called Cytochrome bd-I ubiquinol oxidase subunit X.

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: $C_{34}H_{32}FeN_4O_4$).

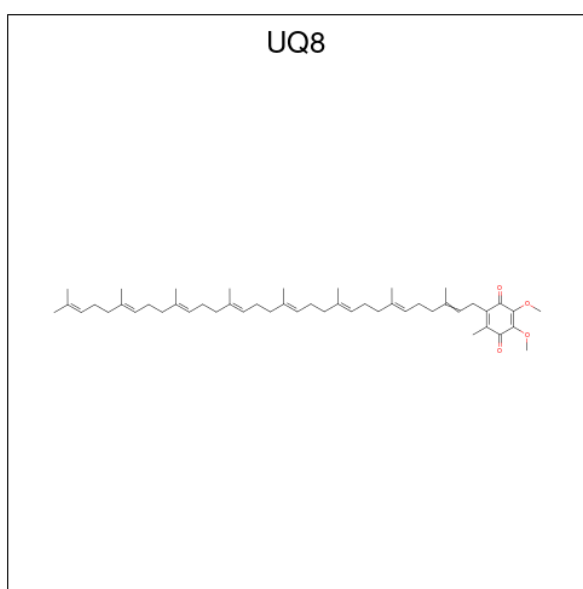


- Molecule 6 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: $C_{35}H_{69}O_8P$).



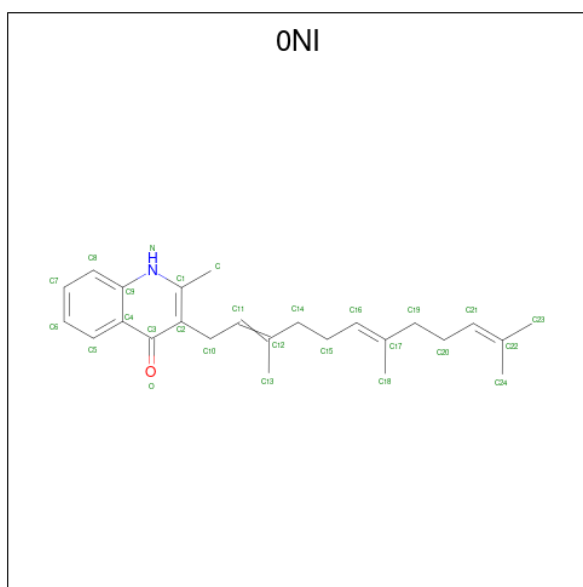
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	H	O	P	0
			111	35	67	8	1	
6	B	1	Total	C	H	O	P	0
			111	35	67	8	1	
6	a	1	Total	C	H	O	P	0
			111	35	67	8	1	
6	b	1	Total	C	H	O	P	0
			111	35	67	8	1	

- Molecule 7 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$) (labeled as "Ligand of Interest" by depositor).



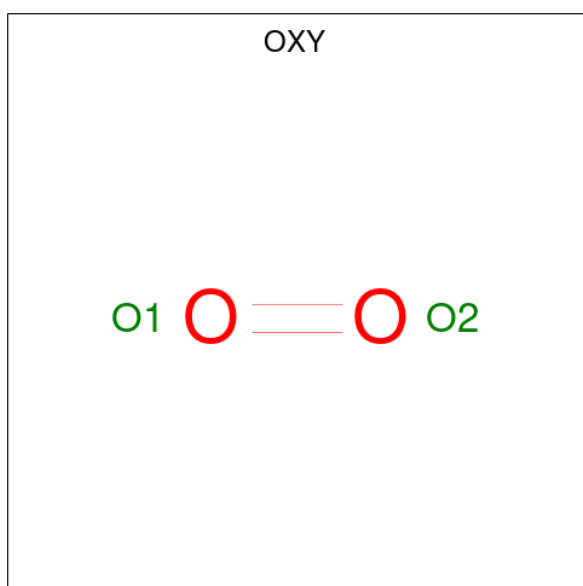
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	H	O	0
			127	49	74	4	
7	B	1	Total	C	H	O	0
			127	49	74	4	
7	a	1	Total	C	H	O	0
			127	49	74	4	
7	b	1	Total	C	H	O	0
			127	49	74	4	

- Molecule 8 is Aurachin D (CCD ID: 0NI) (formula: $C_{25}H_{33}NO$) (labeled as "Ligand of Interest" by depositor).



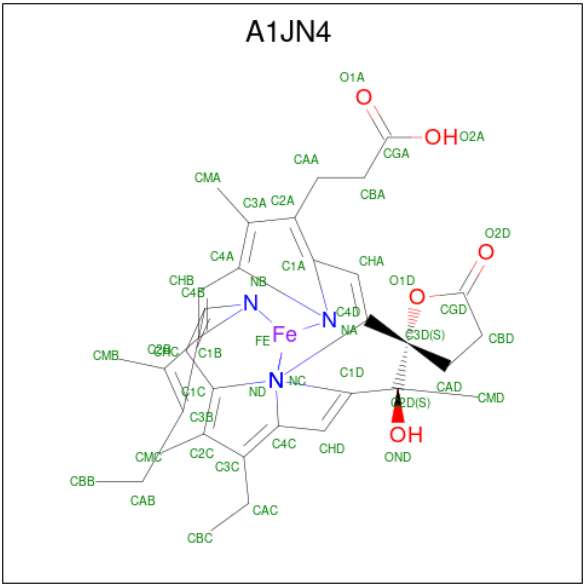
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	H	N	O	0
			60	25	33	1	1	
8	a	1	Total	C	H	N	O	0
			60	25	33	1	1	

- Molecule 9 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



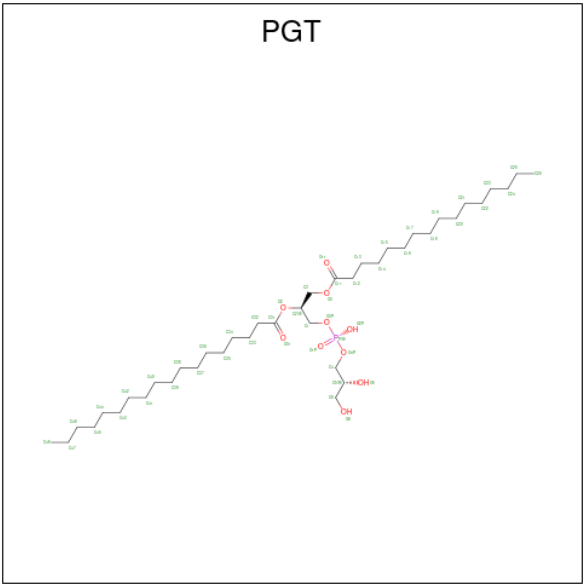
Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	O	0
			2	2	
9	a	1	Total	O	0
			2	2	

- Molecule 10 is TRANS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: A1JN4) (formula: C₃₄H₃₆FeN₄O₅).



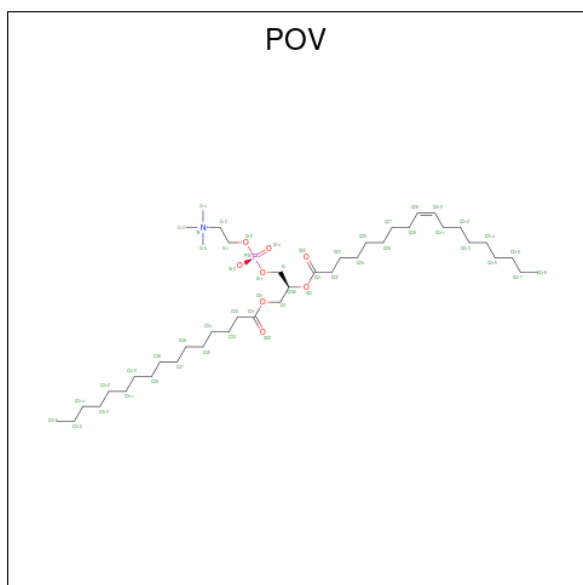
Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
10	A	1	75	34	1	31	4	5	0
10	a	1	Total	C	Fe	H	N	O	0
			75	34	1	31	4	5	

- Molecule 11 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	H	O	P	0
			129	40	78	10	1	
11	a	1	Total	C	H	O	P	0
			129	40	78	10	1	

- Molecule 12 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
12	b	1	Total	C	N	O	P	0
			52	42	1	8	1	

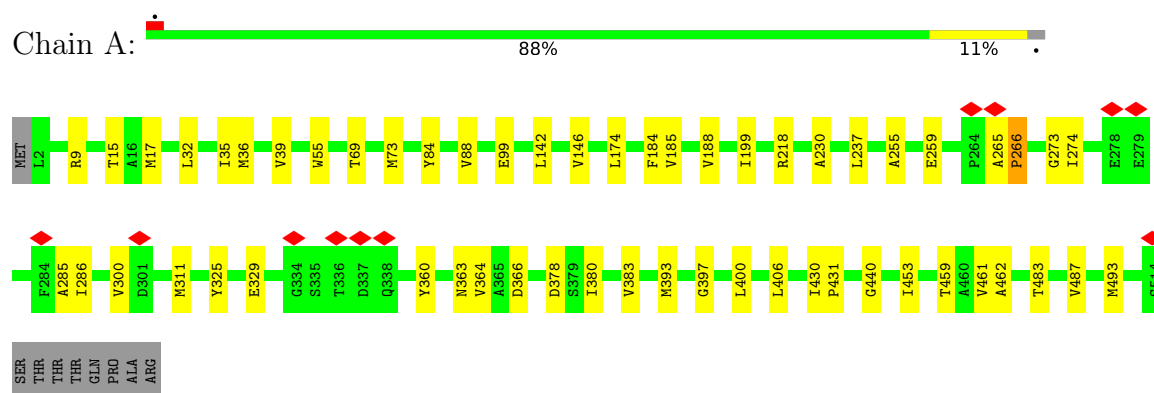
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf
13	A	31	Total	O	0
			31	31	
13	B	28	Total	O	0
			28	28	
13	a	22	Total	O	0
			22	22	
13	b	26	Total	O	0
			26	26	

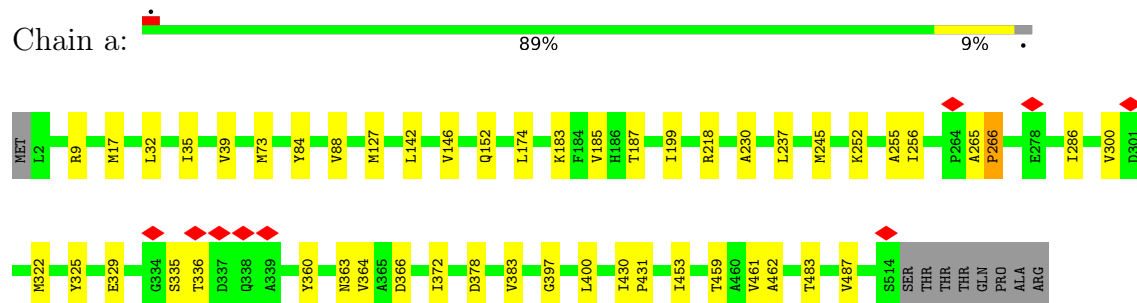
3 Residue-property plots

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.

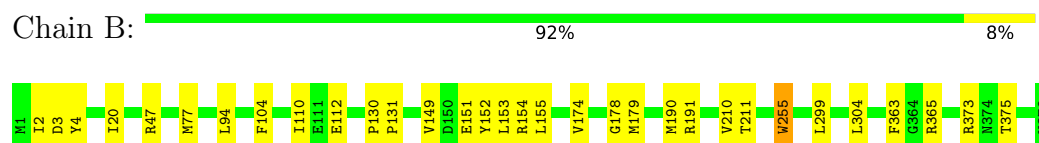
- Molecule 1: Cytochrome bd-I ubiquinol oxidase subunit 1



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



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

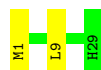


- Molecule 2: Cytochrome bd-I ubiquinol oxidase subunit 2





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

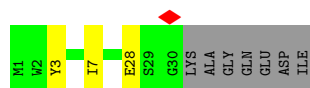


- Molecule 3: Cytochrome bd-I ubiquinol oxidase CydH (Uncharacterized protein YnhF)

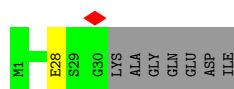
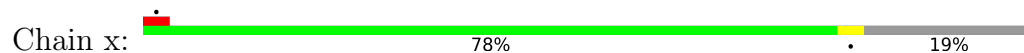


There are no outlier residues recorded for this chain.

- 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	255127	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	0.515	Depositor
Minimum map value	-0.275	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0547	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, OXY, POV, HEM, LPP, PGT, A1JN4, 0NI

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	0.26	0/4146	0.35	0/5624
1	a	0.24	0/4146	0.32	0/5624
2	B	0.28	0/3083	0.37	2/4212 (0.0%)
2	b	0.28	0/3083	0.38	2/4212 (0.0%)
3	H	0.11	0/211	0.20	0/286
3	h	0.10	0/211	0.18	0/286
4	X	0.14	0/239	0.24	0/326
4	x	0.12	0/239	0.18	0/326
All	All	0.26	0/15358	0.35	4/20896 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	174	VAL	CA-C-N	9.29	132.27	120.56
2	b	174	VAL	C-N-CA	9.29	132.27	120.56
2	B	174	VAL	CA-C-N	7.77	130.36	120.56
2	B	174	VAL	C-N-CA	7.77	130.36	120.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4040	4068	4066	44	0
1	a	4040	4063	4066	42	0
2	B	2996	3025	3025	31	0
2	b	2996	3025	3025	24	0
3	H	210	222	238	1	0
3	h	210	222	238	0	0
4	X	232	219	230	2	0
4	x	232	219	230	1	0
5	A	86	60	60	13	0
5	a	86	60	60	13	0
6	A	44	67	67	3	0
6	B	44	67	67	1	0
6	a	44	67	67	2	0
6	b	44	67	67	1	0
7	A	53	74	74	9	0
7	B	53	74	74	2	0
7	a	53	74	74	6	0
7	b	53	74	74	2	0
8	A	27	33	0	1	0
8	a	27	33	0	1	0
9	A	2	0	0	1	0
9	a	2	0	0	0	0
10	A	44	31	0	1	0
10	a	44	31	0	0	0
11	A	51	78	78	2	0
11	a	51	78	78	1	0
12	B	52	0	82	11	0
12	b	52	0	82	12	0
13	A	31	0	0	5	0
13	B	28	0	0	3	0
13	a	22	0	0	2	0
13	b	26	0	0	0	0
All	All	15975	16031	16122	184	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 6.

All (184) 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:69:THR:O	13:A:701:HOH:O	1.86	0.92
5:A:603:HEM:HHC	5:A:603:HEM:HBB2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:O	13:A:702:HOH:O	1.99	0.81
1:a:174:LEU:O	13:a:701:HOH:O	1.98	0.81
5:a:603:HEM:HBB2	5:a:603:HEM:HHC	1.63	0.80
5:A:601:HEM:HBB2	5:A:601:HEM:HMB2	1.63	0.79
5:a:601:HEM:HMB2	5:a:601:HEM:HBB2	1.64	0.79
2:B:4:TYR:OH	13:B:501:HOH:O	2.01	0.78
1:a:146:VAL:O	13:a:702:HOH:O	2.02	0.78
5:a:603:HEM:HBC2	5:a:603:HEM:HHD	1.64	0.78
1:A:218:ARG:NH2	4:X:28:GLU:OE1	2.17	0.77
5:A:603:HEM:HBC2	5:A:603:HEM:HHD	1.63	0.77
1:A:146:VAL:O	13:A:703:HOH:O	2.02	0.76
5:A:601:HEM:HHD	5:A:601:HEM:HBC2	1.69	0.74
1:a:360:TYR:OH	1:a:378:ASP:OD2	2.05	0.74
5:a:601:HEM:HBC2	5:a:601:HEM:HHD	1.68	0.74
1:A:329:GLU:OE2	2:B:152:TYR:OH	2.06	0.73
1:A:15:THR:O	13:A:704:HOH:O	2.06	0.73
1:A:286:ILE:HG22	1:A:286:ILE:O	1.89	0.70
1:a:230:ALA:HA	7:a:604:UQ8:H4MA	1.75	0.68
5:A:603:HEM:HBA1	5:A:603:HEM:HHA	1.76	0.67
5:a:603:HEM:HHA	5:a:603:HEM:HBA1	1.76	0.67
1:A:285:ALA:C	1:A:286:ILE:HD12	2.21	0.66
7:A:604:UQ8:H20A	7:A:604:UQ8:H23	1.77	0.65
1:a:286:ILE:O	1:a:286:ILE:HG22	1.95	0.65
1:A:230:ALA:HA	7:A:604:UQ8:H4MA	1.79	0.64
1:A:360:TYR:OH	1:A:378:ASP:OD2	2.15	0.64
5:A:601:HEM:HHA	5:A:601:HEM:HBA1	1.80	0.63
1:a:185:VAL:HB	1:a:237:LEU:HD22	1.80	0.63
2:B:104:PHE:O	13:B:502:HOH:O	2.16	0.63
2:B:191:ARG:HH11	12:B:402:POV:H24	1.64	0.63
5:a:601:HEM:HBA1	5:a:601:HEM:HHA	1.82	0.62
1:A:73:MET:HE3	1:A:73:MET:HA	1.82	0.62
1:A:185:VAL:HB	1:A:237:LEU:HD22	1.82	0.62
2:b:191:ARG:HH11	12:b:402:POV:H24	1.64	0.61
1:A:400:LEU:HD12	5:A:601:HEM:HBB1	1.83	0.61
1:a:400:LEU:HD12	5:a:601:HEM:HBB1	1.83	0.60
2:B:363:PHE:CE2	12:B:402:POV:H3A	2.37	0.60
1:A:265:ALA:HB1	1:A:266:PRO:CD	2.33	0.59
2:B:365:ARG:H	12:B:402:POV:H12A	1.66	0.58
1:a:265:ALA:HB1	1:a:266:PRO:CD	2.34	0.58
6:a:602:LPP:H261	6:a:602:LPP:H443	1.85	0.58
1:A:493:MET:HE3	6:A:602:LPP:H432	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:365:ARG:CD	12:b:402:POV:H15B	2.34	0.58
1:A:17:MET:HG2	5:A:603:HEM:HBC1	1.86	0.58
2:B:365:ARG:CG	12:B:402:POV:H15B	2.34	0.57
1:a:218:ARG:NH2	4:x:28:GLU:OE1	2.37	0.57
1:a:73:MET:HE3	1:a:73:MET:HA	1.86	0.57
2:b:365:ARG:H	12:b:402:POV:H12A	1.68	0.57
6:A:602:LPP:H261	6:A:602:LPP:H443	1.87	0.57
1:a:35:ILE:O	1:a:39:VAL:HG23	2.05	0.56
1:A:35:ILE:O	1:A:39:VAL:HG23	2.06	0.55
1:A:266:PRO:HG3	1:A:300:VAL:HG23	1.88	0.55
2:b:365:ARG:CG	12:b:402:POV:H15B	2.37	0.55
1:A:406:LEU:HD11	7:A:604:UQ8:H37A	1.89	0.55
1:a:461:VAL:O	2:b:154:ARG:NH2	2.40	0.54
5:A:601:HEM:O2A	13:A:705:HOH:O	2.18	0.54
1:a:335:SER:O	1:a:336:THR:HG23	2.08	0.54
5:a:601:HEM:HBB2	5:a:601:HEM:CMB	2.37	0.54
1:a:17:MET:HG2	5:a:603:HEM:HBC1	1.89	0.53
1:a:9:ARG:HD3	1:a:459:THR:HG21	1.90	0.53
7:b:403:UQ8:O4	7:b:403:UQ8:H3MB	2.08	0.53
1:a:266:PRO:HG3	1:a:300:VAL:HG23	1.89	0.53
2:B:365:ARG:HG3	12:B:402:POV:H15B	1.89	0.53
2:b:363:PHE:CE2	12:b:402:POV:H3A	2.44	0.52
3:H:1:MET:HE1	3:H:9:LEU:HD12	1.91	0.52
7:a:604:UQ8:H38	7:a:604:UQ8:H35A	1.92	0.52
2:B:365:ARG:CD	12:B:402:POV:H15B	2.39	0.52
7:B:403:UQ8:O4	7:B:403:UQ8:H3MB	2.09	0.52
2:b:20:ILE:HD11	2:b:304:LEU:CD1	2.40	0.51
2:b:151:GLU:H	2:b:151:GLU:CD	2.17	0.51
1:a:286:ILE:O	1:a:286:ILE:CG2	2.59	0.51
2:B:151:GLU:H	2:B:151:GLU:CD	2.18	0.51
2:B:179:MET:HA	2:B:211:THR:HG21	1.93	0.51
5:A:601:HEM:HBB2	5:A:601:HEM:CMB	2.37	0.51
1:a:265:ALA:HB1	1:a:266:PRO:HD3	1.93	0.51
1:A:285:ALA:O	1:A:286:ILE:HD12	2.11	0.51
1:a:255:ALA:O	1:a:383:VAL:HG13	2.12	0.50
1:a:88:VAL:HG11	1:a:453:ILE:HG13	1.94	0.50
1:a:461:VAL:O	1:a:461:VAL:HG12	2.12	0.50
1:A:461:VAL:HG12	1:A:461:VAL:O	2.12	0.50
1:a:265:ALA:O	1:a:266:PRO:C	2.54	0.50
1:a:329:GLU:OE1	2:b:152:TYR:OH	2.30	0.50
2:b:365:ARG:HG3	12:b:402:POV:H15B	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ALA:O	1:A:266:PRO:C	2.55	0.49
1:A:286:ILE:O	1:A:286:ILE:CG2	2.56	0.49
1:A:9:ARG:HD3	1:A:459:THR:HG21	1.93	0.49
1:A:255:ALA:O	1:A:383:VAL:HG13	2.12	0.49
2:B:149:VAL:HG13	2:B:153:LEU:HA	1.95	0.49
2:B:179:MET:HG3	2:B:299:LEU:HD23	1.95	0.49
4:X:3:TYR:O	4:X:7:ILE:HG13	2.13	0.48
1:a:245:MET:HE1	1:a:256:ILE:CD1	2.43	0.48
2:B:20:ILE:HD11	2:B:304:LEU:CD1	2.43	0.48
1:A:88:VAL:HG11	1:A:453:ILE:HG13	1.94	0.48
1:A:184:PHE:O	1:A:188:VAL:HG22	2.13	0.48
2:b:149:VAL:HG13	2:b:153:LEU:HA	1.94	0.48
1:A:311:MET:HG3	1:A:380:ILE:HD13	1.96	0.48
2:B:191:ARG:NH2	13:B:505:HOH:O	2.38	0.48
7:A:604:UQ8:H10B	7:A:604:UQ8:C13	2.44	0.48
2:b:262:THR:HG22	2:b:264:ILE:HD12	1.94	0.48
7:A:604:UQ8:H4MB	7:A:604:UQ8:O5	2.14	0.47
7:B:403:UQ8:O5	7:B:403:UQ8:H4MA	2.14	0.47
1:A:461:VAL:O	2:B:154:ARG:NH2	2.47	0.47
1:A:366:ASP:O	1:A:366:ASP:OD1	2.32	0.47
8:A:605:ONI:C11	8:A:605:ONI:C	2.93	0.47
7:a:604:UQ8:H8	7:a:604:UQ8:C1M	2.45	0.47
2:B:47:ARG:HH12	2:B:375:THR:HG23	1.80	0.47
8:a:605:ONI:C11	8:a:605:ONI:C	2.93	0.47
7:b:403:UQ8:H4MA	7:b:403:UQ8:O5	2.14	0.47
1:a:245:MET:HE1	1:a:256:ILE:HD13	1.96	0.46
1:A:266:PRO:CG	1:A:300:VAL:HG23	2.45	0.46
2:b:20:ILE:HD11	2:b:304:LEU:HD13	1.97	0.46
2:b:2:ILE:HG22	2:b:3:ASP:N	2.30	0.46
2:B:373:ARG:CZ	2:B:373:ARG:HB2	2.45	0.46
1:a:230:ALA:HA	7:a:604:UQ8:C4M	2.46	0.46
1:a:325:TYR:CD2	1:a:364:VAL:HG22	2.50	0.46
1:a:483:THR:O	1:a:487:VAL:HG23	2.16	0.46
1:a:335:SER:O	1:a:336:THR:CG2	2.64	0.45
1:A:325:TYR:CD2	1:A:364:VAL:HG22	2.51	0.45
1:a:265:ALA:CB	1:a:266:PRO:CD	2.94	0.45
2:b:365:ARG:HB2	12:b:402:POV:H14A	1.97	0.45
11:A:608:PGT:H482	11:A:608:PGT:C44	2.46	0.45
1:a:266:PRO:CG	1:a:300:VAL:HG23	2.46	0.45
2:B:2:ILE:HG22	2:B:3:ASP:N	2.31	0.45
7:A:604:UQ8:C13	7:A:604:UQ8:C10	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:607:A1JN4:CBA	10:A:607:A1JN4:CHA	2.94	0.45
2:B:20:ILE:HD11	2:B:304:LEU:HD13	1.98	0.45
7:A:604:UQ8:H27	7:A:604:UQ8:H30	1.69	0.45
2:b:110:ILE:HG22	2:b:112:GLU:H	1.82	0.45
2:B:178:GLY:C	2:B:211:THR:CG2	2.90	0.44
11:a:608:PGT:H482	11:a:608:PGT:C44	2.47	0.44
1:A:84:TYR:HB2	1:A:462:ALA:HB1	1.99	0.44
1:A:393:MET:HE2	1:A:440:GLY:HA2	2.00	0.44
2:B:110:ILE:HG22	2:B:112:GLU:H	1.82	0.44
6:a:602:LPP:H443	6:a:602:LPP:C26	2.48	0.44
1:a:366:ASP:O	1:a:366:ASP:OD1	2.36	0.44
2:b:25:THR:HG22	12:b:402:POV:H21A	1.99	0.44
1:A:265:ALA:HB1	1:A:266:PRO:HD2	2.00	0.44
2:B:190:MET:O	12:B:402:POV:H2	2.17	0.44
2:B:365:ARG:HB2	12:B:402:POV:H14A	1.99	0.44
1:a:397:GLY:HA2	5:a:601:HEM:HBB1	2.00	0.43
2:B:210:VAL:HG11	6:B:401:LPP:C22	2.48	0.43
1:A:483:THR:O	1:A:487:VAL:HG23	2.18	0.43
5:A:603:HEM:HHA	5:A:603:HEM:CBA	2.47	0.43
7:A:604:UQ8:H37	7:A:604:UQ8:H40	1.73	0.43
1:A:397:GLY:HA2	5:A:601:HEM:HBB1	2.00	0.43
1:a:152:GLN:OE1	1:a:252:LYS:NZ	2.52	0.43
5:A:603:HEM:HBC2	5:A:603:HEM:CHD	2.39	0.43
5:a:603:HEM:HHA	5:a:603:HEM:CBA	2.47	0.43
12:b:402:POV:O22	12:b:402:POV:H24A	2.19	0.43
5:a:601:HEM:HBC2	5:a:601:HEM:CHD	2.40	0.42
2:b:179:MET:HG3	2:b:299:LEU:HD23	2.00	0.42
7:A:604:UQ8:O5	7:A:604:UQ8:C8	2.67	0.42
2:B:365:ARG:NH1	12:B:402:POV:H1	2.34	0.42
1:a:187:THR:OG1	5:a:601:HEM:O1A	2.37	0.42
2:B:363:PHE:CD2	12:B:402:POV:H22	2.55	0.42
1:a:32:LEU:HD13	1:a:199:ILE:HD12	2.01	0.42
1:A:36:MET:HE1	1:A:55:TRP:CD1	2.55	0.42
1:A:142:LEU:O	1:A:146:VAL:HG23	2.20	0.42
6:A:602:LPP:H443	6:A:602:LPP:C26	2.49	0.42
2:B:365:ARG:HH11	12:B:402:POV:H1	1.85	0.42
1:a:127:MET:HE2	1:a:127:MET:HB3	1.96	0.42
1:A:273:GLY:O	1:A:274:ILE:HD13	2.20	0.41
1:A:430:ILE:N	1:A:431:PRO:CD	2.83	0.41
2:B:130:PRO:HB2	2:B:131:PRO:HD3	2.02	0.41
2:b:207:ALA:O	2:b:211:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:430:ILE:N	1:a:431:PRO:CD	2.84	0.41
1:A:99:GLU:OE1	9:A:606:OXY:O2	2.38	0.41
2:b:25:THR:CG2	12:b:402:POV:H21C	2.51	0.41
1:A:32:LEU:HD13	1:A:199:ILE:HD12	2.01	0.41
2:b:130:PRO:HB2	2:b:131:PRO:HD3	2.01	0.41
2:b:190:MET:O	12:b:402:POV:H2	2.20	0.41
1:a:183:LYS:O	1:a:187:THR:OG1	2.39	0.41
2:b:210:VAL:HG11	6:b:401:LPP:C22	2.50	0.41
1:a:84:TYR:HB2	1:a:462:ALA:HB1	2.02	0.41
1:a:322:MET:HE1	1:a:372:ILE:HD11	2.03	0.41
2:b:365:ARG:NH1	12:b:402:POV:H1	2.36	0.41
2:B:77:MET:HE3	2:B:155:LEU:HD11	2.03	0.41
1:A:265:ALA:CB	1:A:266:PRO:CD	2.99	0.41
11:A:608:PGT:O3P	11:A:608:PGT:O6	2.39	0.40
7:a:604:UQ8:H35A	7:a:604:UQ8:C38	2.51	0.40
2:B:255:TRP:HA	2:B:255:TRP:CE3	2.56	0.40
1:a:142:LEU:O	1:a:146:VAL:HG23	2.22	0.40
7:a:604:UQ8:O5	7:a:604:UQ8:H4MB	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	511/522 (98%)	496 (97%)	14 (3%)	1 (0%)	43	61
1	a	511/522 (98%)	497 (97%)	13 (2%)	1 (0%)	43	61
2	B	377/379 (100%)	373 (99%)	4 (1%)	0	100	100
2	b	377/379 (100%)	371 (98%)	6 (2%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	X	28/37 (76%)	28 (100%)	0	0	100	100
4	x	28/37 (76%)	28 (100%)	0	0	100	100
All	All	1886/1934 (98%)	1847 (98%)	37 (2%)	2 (0%)	49	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	PRO
1	a	266	PRO

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	418/426 (98%)	416 (100%)	2 (0%)	81	91
1	a	418/426 (98%)	417 (100%)	1 (0%)	87	94
2	B	313/313 (100%)	311 (99%)	2 (1%)	78	90
2	b	313/313 (100%)	309 (99%)	4 (1%)	61	80
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%)	23 (100%)	0	100	100
All	All	1556/1582 (98%)	1547 (99%)	9 (1%)	76	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259	GLU
1	A	363	ASN
2	B	94	LEU
2	B	255	TRP
1	a	363	ASN

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Mol	Chain	Res	Type
2	b	1	MET
2	b	94	LEU
2	b	117	ASN
2	b	255	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	80	ASN
1	A	330	GLN
2	B	163	GLN
2	B	245	ASN
2	B	374	ASN
1	a	86	HIS
1	a	287	GLN
1	a	330	GLN
2	b	163	GLN
2	b	374	ASN
3	h	29	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

22 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	$\# Z > 2$
10	A1JN4	A	607	1,9	46,52,52	2.93	14 (30%)	62,89,89	4.63	37 (59%)
12	POV	B	402	-	51,51,51	0.50	0	57,59,59	0.43	0
5	HEM	a	603	1	50,50,50	1.45	7 (14%)	66,82,82	1.36	10 (15%)
12	POV	b	402	-	51,51,51	0.50	0	57,59,59	0.43	0
11	PGT	a	608	-	50,50,50	1.10	4 (8%)	53,56,56	1.04	2 (3%)
7	UQ8	a	604	-	53,53,53	1.25	2 (3%)	64,67,67	1.63	18 (28%)
6	LPP	a	602	-	43,43,43	1.08	2 (4%)	47,48,48	1.18	2 (4%)
7	UQ8	B	403	-	53,53,53	2.27	18 (33%)	64,67,67	4.21	27 (42%)
5	HEM	A	603	1	50,50,50	1.45	7 (14%)	66,82,82	1.36	11 (16%)
7	UQ8	b	403	-	53,53,53	2.27	19 (35%)	64,67,67	4.25	27 (42%)
5	HEM	a	601	1	50,50,50	1.44	7 (14%)	66,82,82	1.40	10 (15%)
8	ONI	a	605	-	28,28,28	4.34	15 (53%)	34,37,37	8.35	12 (35%)
9	OXY	a	606	10	1,1,1	0.15	0	-	-	-
6	LPP	A	602	-	43,43,43	1.08	2 (4%)	47,48,48	1.18	2 (4%)
7	UQ8	A	604	-	53,53,53	1.20	2 (3%)	64,67,67	1.55	16 (25%)
11	PGT	A	608	-	50,50,50	1.10	4 (8%)	53,56,56	1.03	2 (3%)
5	HEM	A	601	1	50,50,50	1.45	6 (12%)	66,82,82	1.44	10 (15%)
6	LPP	B	401	-	43,43,43	1.10	2 (4%)	47,48,48	1.10	2 (4%)
10	A1JN4	a	607	1,9	46,52,52	2.92	15 (32%)	62,89,89	4.61	39 (62%)
8	ONI	A	605	-	28,28,28	4.32	15 (53%)	34,37,37	8.35	12 (35%)
6	LPP	b	401	-	43,43,43	1.10	2 (4%)	47,48,48	1.11	2 (4%)
9	OXY	A	606	10	1,1,1	0.15	0	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	A1JN4	A	607	1,9	2/2/12/12	9/9/89/89	0/1/9/9
12	POV	B	402	-	-	17/55/55/55	-
5	HEM	a	603	1	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	POV	b	402	-	-	18/55/55/55	-
11	PGT	a	608	-	-	28/55/55/55	-
7	UQ8	a	604	-	-	13/51/75/75	0/1/1/1
6	LPP	a	602	-	-	25/45/45/45	-
7	UQ8	B	403	-	-	8/51/75/75	0/1/1/1
5	HEM	A	603	1	-	6/14/54/54	-
7	UQ8	b	403	-	-	8/51/75/75	0/1/1/1
5	HEM	a	601	1	-	3/14/54/54	-
8	0NI	a	605	-	-	4/17/17/17	0/2/2/2
6	LPP	A	602	-	-	24/45/45/45	-
7	UQ8	A	604	-	-	14/51/75/75	0/1/1/1
11	PGT	A	608	-	-	26/55/55/55	-
5	HEM	A	601	1	-	3/14/54/54	-
6	LPP	B	401	-	-	20/45/45/45	-
10	A1JN4	a	607	1,9	2/2/12/12	5/9/89/89	0/1/9/9
8	0NI	A	605	-	-	4/17/17/17	0/2/2/2
6	LPP	b	401	-	-	22/45/45/45	-

All (143) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	607	A1JN4	C3D-C2D	-11.78	1.25	1.55
10	a	607	A1JN4	C3D-C2D	-11.77	1.25	1.55
8	a	605	0NI	C1-C2	10.32	1.52	1.36
8	A	605	0NI	C1-C2	10.30	1.52	1.36
7	b	403	UQ8	C6-C1	9.94	1.53	1.35
7	B	403	UQ8	C6-C1	9.91	1.53	1.35
8	a	605	0NI	C10-C11	8.76	1.63	1.50
8	A	605	0NI	C10-C11	8.74	1.63	1.50
8	a	605	0NI	C1-N	8.70	1.47	1.36
8	A	605	0NI	C1-N	8.66	1.47	1.36
8	A	605	0NI	C9-N	7.92	1.53	1.39
8	a	605	0NI	C9-N	7.91	1.53	1.39
7	a	604	UQ8	C6-C1	7.88	1.49	1.35
7	A	604	UQ8	C6-C1	7.49	1.48	1.35
10	a	607	A1JN4	O1D-C3D	6.66	1.57	1.46
10	A	607	A1JN4	O1D-C3D	6.61	1.57	1.46
8	A	605	0NI	C19-C17	6.01	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	605	0NI	C19-C17	6.00	1.63	1.51
10	a	607	A1JN4	CBB-CAB	-5.79	1.25	1.51
10	A	607	A1JN4	CBB-CAB	-5.79	1.25	1.51
10	a	607	A1JN4	CBC-CAC	-5.67	1.26	1.51
10	A	607	A1JN4	CBC-CAC	-5.66	1.26	1.51
8	a	605	0NI	C10-C2	5.46	1.60	1.51
8	A	605	0NI	C10-C2	5.32	1.60	1.51
8	a	605	0NI	C14-C12	5.00	1.61	1.51
8	A	605	0NI	C14-C12	4.99	1.61	1.51
8	A	605	0NI	C11-C12	4.61	1.44	1.33
8	a	605	0NI	C11-C12	4.61	1.44	1.33
7	B	403	UQ8	C4-C3	4.34	1.53	1.36
7	b	403	UQ8	C4-C3	4.33	1.53	1.36
10	a	607	A1JN4	O1D-CGD	-4.07	1.29	1.35
10	A	607	A1JN4	O1D-CGD	-4.04	1.29	1.35
10	A	607	A1JN4	CBD-CGD	-3.98	1.42	1.50
10	a	607	A1JN4	CBD-CGD	-3.94	1.42	1.50
5	A	603	HEM	FE-NA	3.93	2.08	1.95
5	a	603	HEM	FE-NA	3.91	2.08	1.95
5	a	601	HEM	FE-NA	3.78	2.07	1.95
5	A	601	HEM	FE-NC	3.75	2.07	1.95
5	A	601	HEM	FE-NA	3.68	2.07	1.95
10	a	607	A1JN4	CAD-C3D	3.66	1.60	1.53
10	A	607	A1JN4	CAD-C3D	3.65	1.60	1.53
8	A	605	0NI	C18-C17	3.63	1.60	1.50
5	A	603	HEM	FE-NC	3.61	2.07	1.95
5	a	603	HEM	FE-NC	3.61	2.07	1.95
8	a	605	0NI	C18-C17	3.58	1.59	1.50
8	A	605	0NI	C16-C17	3.58	1.41	1.33
8	a	605	0NI	C16-C17	3.57	1.41	1.33
5	a	601	HEM	FE-NC	3.56	2.07	1.95
10	A	607	A1JN4	OND-C2D	3.52	1.49	1.42
10	a	607	A1JN4	OND-C2D	3.47	1.49	1.42
7	b	403	UQ8	C7-C8	3.47	1.55	1.50
5	A	601	HEM	FE-NB	3.46	2.05	1.94
8	A	605	0NI	C-C1	3.45	1.55	1.49
8	a	605	0NI	C-C1	3.42	1.55	1.49
5	a	601	HEM	FE-NB	3.42	2.05	1.94
7	B	403	UQ8	C7-C8	3.37	1.55	1.50
10	A	607	A1JN4	C1B-NB	-3.35	1.33	1.39
6	b	401	LPP	O27-C29	3.32	1.43	1.33
6	B	401	LPP	O27-C29	3.31	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	a	607	A1JN4	C1B-NB	-3.29	1.33	1.39
11	a	608	PGT	O3-C11	3.24	1.42	1.33
5	A	603	HEM	FE-NB	3.22	2.04	1.94
11	A	608	PGT	O3-C11	3.22	1.42	1.33
5	a	603	HEM	FE-NB	3.21	2.04	1.94
6	B	401	LPP	O9-C11	3.15	1.43	1.34
8	a	605	0NI	C4-C3	3.14	1.54	1.48
6	a	602	LPP	O9-C11	3.13	1.43	1.34
6	b	401	LPP	O9-C11	3.13	1.43	1.34
7	B	403	UQ8	C11-C9	3.12	1.57	1.51
7	b	403	UQ8	C11-C9	3.12	1.57	1.51
6	A	602	LPP	O9-C11	3.12	1.43	1.34
8	A	605	0NI	C4-C3	3.10	1.54	1.48
6	A	602	LPP	O27-C29	3.02	1.42	1.33
6	a	602	LPP	O27-C29	3.01	1.42	1.33
7	A	604	UQ8	C4-C3	3.01	1.48	1.36
8	a	605	0NI	C15-C16	3.00	1.60	1.50
10	a	607	A1JN4	C4C-NC	-2.99	1.34	1.39
8	A	605	0NI	C15-C16	2.98	1.60	1.50
10	A	607	A1JN4	C4C-NC	-2.94	1.34	1.39
5	A	601	HEM	CAC-C3C	2.86	1.55	1.47
7	a	604	UQ8	C4-C3	2.85	1.48	1.36
5	a	601	HEM	CAC-C3C	2.83	1.55	1.47
5	a	601	HEM	FE-ND	2.75	2.03	1.94
5	a	601	HEM	CAB-C3B	2.74	1.54	1.47
5	A	601	HEM	CAB-C3B	2.74	1.54	1.47
11	a	608	PGT	O2-C31	2.74	1.42	1.34
5	A	601	HEM	FE-ND	2.73	2.03	1.94
11	A	608	PGT	O2-C31	2.72	1.42	1.34
5	a	603	HEM	CAB-C3B	2.69	1.54	1.47
10	A	607	A1JN4	C2A-C3A	-2.68	1.31	1.38
5	A	603	HEM	CAB-C3B	2.67	1.54	1.47
11	a	608	PGT	O2-C2	-2.64	1.40	1.46
11	A	608	PGT	O2-C2	-2.63	1.40	1.46
5	a	603	HEM	CAC-C3C	2.62	1.54	1.47
5	A	603	HEM	CAC-C3C	2.60	1.54	1.47
10	a	607	A1JN4	C2A-C3A	-2.56	1.32	1.38
5	a	603	HEM	FE-ND	2.51	2.02	1.94
5	A	603	HEM	FE-ND	2.49	2.02	1.94
10	A	607	A1JN4	CMC-C2C	2.48	1.56	1.50
7	B	403	UQ8	C26-C24	2.47	1.56	1.51
10	a	607	A1JN4	CMC-C2C	2.46	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	b	403	UQ8	C31-C29	2.43	1.56	1.51
7	B	403	UQ8	C31-C29	2.42	1.56	1.51
7	b	403	UQ8	C26-C24	2.42	1.56	1.51
7	B	403	UQ8	C21-C19	2.38	1.56	1.51
7	B	403	UQ8	C6-C5	2.37	1.53	1.46
7	b	403	UQ8	C6-C5	2.36	1.53	1.46
7	b	403	UQ8	C21-C19	2.35	1.56	1.51
7	B	403	UQ8	C36-C34	2.35	1.56	1.51
7	b	403	UQ8	C36-C34	2.31	1.56	1.51
7	B	403	UQ8	C7-C6	2.30	1.55	1.51
7	b	403	UQ8	C7-C6	2.30	1.55	1.51
7	b	403	UQ8	C16-C14	2.24	1.56	1.51
7	B	403	UQ8	C16-C14	2.23	1.55	1.51
8	a	605	0NI	C7-C6	2.22	1.43	1.38
8	A	605	0NI	C7-C6	2.21	1.43	1.38
7	B	403	UQ8	C20-C19	2.21	1.56	1.50
11	a	608	PGT	P-O3P	2.20	1.68	1.59
11	A	608	PGT	P-O3P	2.19	1.68	1.59
7	b	403	UQ8	C20-C19	2.14	1.56	1.50
10	a	607	A1JN4	C4A-C3A	2.09	1.48	1.43
7	b	403	UQ8	C40-C39	2.08	1.56	1.50
7	b	403	UQ8	C15-C14	2.08	1.56	1.50
7	b	403	UQ8	O4-C4	2.08	1.42	1.36
7	B	403	UQ8	O4-C4	2.08	1.41	1.36
10	A	607	A1JN4	O2A-CGA	-2.08	1.23	1.30
7	B	403	UQ8	C40-C39	2.07	1.56	1.50
8	a	605	0NI	C24-C22	2.07	1.55	1.50
7	B	403	UQ8	C15-C14	2.07	1.56	1.50
10	a	607	A1JN4	CHA-C1A	-2.06	1.34	1.39
7	b	403	UQ8	C41-C39	2.06	1.55	1.51
7	b	403	UQ8	O5-C5	-2.06	1.18	1.23
7	B	403	UQ8	C35-C34	2.04	1.55	1.50
7	b	403	UQ8	O2-C2	-2.04	1.18	1.23
5	A	603	HEM	C2A-C3A	-2.04	1.33	1.38
7	B	403	UQ8	C41-C39	2.04	1.55	1.51
10	A	607	A1JN4	CBA-CAA	2.04	1.58	1.52
8	A	605	0NI	C24-C22	2.04	1.55	1.50
7	B	403	UQ8	O5-C5	-2.03	1.19	1.23
5	a	601	HEM	CMC-C2C	2.03	1.55	1.50
5	a	603	HEM	C2A-C3A	-2.02	1.33	1.38
10	a	607	A1JN4	CBA-CAA	2.02	1.58	1.52
7	b	403	UQ8	C35-C34	2.02	1.55	1.50

All (241) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	605	0NI	C10-C11-C12	-23.33	87.95	126.79
8	a	605	0NI	C10-C11-C12	-23.15	88.25	126.79
8	A	605	0NI	C14-C12-C11	21.09	163.79	121.12
8	a	605	0NI	C14-C12-C11	21.05	163.72	121.12
8	A	605	0NI	C13-C12-C14	-20.34	81.06	115.27
8	a	605	0NI	C13-C12-C14	-20.28	81.16	115.27
8	a	605	0NI	C13-C12-C11	-16.03	82.56	123.68
8	A	605	0NI	C13-C12-C11	-15.96	82.74	123.68
8	a	605	0NI	C18-C17-C19	-14.46	90.94	115.27
8	A	605	0NI	C18-C17-C19	-14.32	91.18	115.27
8	a	605	0NI	C18-C17-C16	14.15	159.97	123.68
8	A	605	0NI	C18-C17-C16	14.14	159.94	123.68
8	a	605	0NI	C15-C16-C17	12.93	158.79	127.66
8	A	605	0NI	C15-C16-C17	12.75	158.36	127.66
10	a	607	A1JN4	O1D-C3D-C4D	-12.36	83.13	108.25
10	A	607	A1JN4	O1D-C3D-C4D	-12.22	83.43	108.25
7	b	403	UQ8	C15-C14-C16	-11.30	96.26	115.27
7	B	403	UQ8	C15-C14-C16	-11.28	96.30	115.27
7	B	403	UQ8	C25-C24-C26	-10.94	96.86	115.27
7	b	403	UQ8	C25-C24-C26	-10.92	96.90	115.27
7	B	403	UQ8	C30-C29-C31	-10.91	96.92	115.27
7	b	403	UQ8	C30-C29-C31	-10.87	96.98	115.27
7	b	403	UQ8	C35-C34-C36	-10.50	97.60	115.27
7	b	403	UQ8	C40-C39-C41	-10.41	97.76	115.27
7	B	403	UQ8	C40-C39-C41	-10.38	97.80	115.27
10	a	607	A1JN4	CHD-C1D-ND	10.05	138.94	124.20
10	A	607	A1JN4	CHD-C1D-ND	10.03	138.91	124.20
7	B	403	UQ8	C35-C34-C36	-10.03	98.40	115.27
7	B	403	UQ8	C10-C9-C11	-9.86	98.68	115.27
10	a	607	A1JN4	C3B-C4B-NB	-9.86	100.73	110.32
10	A	607	A1JN4	C4C-NC-C1C	9.84	114.99	105.35
10	A	607	A1JN4	C3B-C4B-NB	-9.84	100.75	110.32
7	b	403	UQ8	C10-C9-C11	-9.83	98.73	115.27
10	a	607	A1JN4	C4C-NC-C1C	9.78	114.93	105.35
7	b	403	UQ8	C20-C19-C21	-9.70	98.95	115.27
10	A	607	A1JN4	O1D-C3D-CAD	-9.61	84.93	103.01
10	a	607	A1JN4	O1D-C3D-CAD	-9.48	85.19	103.01
7	B	403	UQ8	C20-C19-C21	-9.24	99.72	115.27
10	a	607	A1JN4	C4B-NB-C1B	8.50	113.67	105.35
7	B	403	UQ8	C46-C44-C45	-8.49	95.85	114.60
7	b	403	UQ8	C46-C44-C45	-8.49	95.86	114.60
8	a	605	0NI	C24-C22-C23	-8.43	95.99	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	605	0NI	C24-C22-C23	-8.41	96.03	114.60
10	A	607	A1JN4	C4B-NB-C1B	8.22	113.40	105.35
10	A	607	A1JN4	C3C-C4C-NC	-7.75	101.48	110.15
10	a	607	A1JN4	C3C-C4C-NC	-7.68	101.56	110.15
10	A	607	A1JN4	CAC-C3C-C4C	-7.43	114.61	124.92
10	a	607	A1JN4	CAC-C3C-C4C	-7.36	114.70	124.92
10	A	607	A1JN4	OND-C2D-CMD	-6.71	97.25	109.59
10	A	607	A1JN4	CHC-C4B-NB	6.69	131.68	124.44
10	a	607	A1JN4	CHC-C4B-NB	6.64	131.62	124.44
10	a	607	A1JN4	OND-C2D-CMD	-6.59	97.47	109.59
10	a	607	A1JN4	CAB-C3B-C4B	-6.42	114.57	124.68
10	A	607	A1JN4	CAB-C3B-C4B	-6.40	114.61	124.68
10	A	607	A1JN4	C4B-C3B-C2B	6.32	115.36	107.13
10	A	607	A1JN4	C2A-C1A-NA	-6.30	103.10	110.15
10	a	607	A1JN4	C4B-C3B-C2B	6.27	115.30	107.13
8	A	605	0NI	C19-C17-C16	-6.05	108.86	121.12
8	a	605	0NI	C19-C17-C16	-5.95	109.07	121.12
10	A	607	A1JN4	O1A-CGA-CBA	-5.88	104.19	123.08
10	a	607	A1JN4	C2A-C1A-NA	-5.85	103.61	110.15
10	a	607	A1JN4	O1A-CGA-CBA	-5.79	104.48	123.08
7	b	403	UQ8	C11-C9-C8	5.65	132.56	121.12
10	A	607	A1JN4	CHB-C1B-NB	5.64	130.54	124.44
7	B	403	UQ8	C11-C9-C8	5.64	132.53	121.12
10	a	607	A1JN4	CHB-C1B-NB	5.60	130.50	124.44
7	b	403	UQ8	C26-C24-C23	5.47	132.19	121.12
7	B	403	UQ8	C26-C24-C23	5.45	132.15	121.12
7	B	403	UQ8	C31-C29-C28	5.34	131.93	121.12
10	A	607	A1JN4	C1A-C2A-C3A	5.28	115.21	106.89
7	b	403	UQ8	C31-C29-C28	5.27	131.78	121.12
10	A	607	A1JN4	O1D-CGD-CBD	-5.22	104.92	110.19
10	a	607	A1JN4	C1A-C2A-C3A	5.18	115.05	106.89
7	B	403	UQ8	C41-C39-C38	4.99	131.22	121.12
7	b	403	UQ8	C41-C39-C38	4.97	131.18	121.12
7	b	403	UQ8	C36-C34-C33	4.84	130.92	121.12
10	a	607	A1JN4	O1D-CGD-CBD	-4.76	105.39	110.19
7	B	403	UQ8	C16-C14-C13	4.73	130.68	121.12
10	A	607	A1JN4	CHA-C4D-ND	-4.70	117.31	124.20
7	b	403	UQ8	C16-C14-C13	4.68	130.59	121.12
10	A	607	A1JN4	C4A-NA-C1A	4.68	109.93	105.35
7	b	403	UQ8	C21-C19-C18	4.65	130.53	121.12
7	B	403	UQ8	C36-C34-C33	4.57	130.37	121.12
10	a	607	A1JN4	CHA-C4D-ND	-4.53	117.56	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	a	602	LPP	O9-C11-C12	4.46	121.11	111.50
10	a	607	A1JN4	C4A-NA-C1A	4.46	109.71	105.35
7	B	403	UQ8	C21-C19-C18	4.44	130.11	121.12
6	A	602	LPP	O9-C11-C12	4.42	121.03	111.50
10	A	607	A1JN4	CHD-C4C-NC	4.38	131.90	123.85
10	a	607	A1JN4	CHD-C4C-NC	4.36	131.87	123.85
6	b	401	LPP	O9-C11-C12	4.35	120.88	111.50
10	A	607	A1JN4	C3D-C4D-CHA	4.33	137.20	124.34
10	a	607	A1JN4	O2A-CGA-O1A	4.28	133.97	123.30
6	B	401	LPP	O9-C11-C12	4.27	120.70	111.50
7	A	604	UQ8	C15-C14-C16	4.20	122.33	115.27
10	a	607	A1JN4	C2D-C1D-CHD	-4.19	117.36	124.28
10	A	607	A1JN4	C2D-C1D-CHD	-4.18	117.38	124.28
11	a	608	PGT	O2-C31-C32	4.09	120.31	111.50
10	a	607	A1JN4	C3D-C4D-CHA	4.08	136.45	124.34
11	A	608	PGT	O2-C31-C32	4.03	120.18	111.50
10	A	607	A1JN4	C4A-C3A-C2A	-4.00	102.15	106.83
10	a	607	A1JN4	C4A-C3A-C2A	-3.98	102.17	106.83
10	A	607	A1JN4	C4C-C3C-C2C	3.83	112.92	106.89
10	a	607	A1JN4	C4C-C3C-C2C	3.80	112.88	106.89
7	b	403	UQ8	C15-C14-C13	3.69	133.14	123.68
7	B	403	UQ8	C15-C14-C13	3.64	133.00	123.68
7	a	604	UQ8	C10-C9-C8	-3.61	114.42	123.68
10	A	607	A1JN4	CAC-C3C-C2C	3.50	132.47	126.86
10	a	607	A1JN4	CAC-C3C-C2C	3.47	132.42	126.86
5	A	601	HEM	C4D-ND-C1D	3.43	108.62	105.07
10	A	607	A1JN4	O2A-CGA-O1A	3.40	131.77	123.30
10	a	607	A1JN4	CBB-CAB-C3B	3.34	121.63	112.43
5	a	601	HEM	C4D-ND-C1D	3.34	108.52	105.07
7	a	604	UQ8	C15-C14-C16	3.33	120.88	115.27
8	A	605	0NI	C24-C22-C21	3.30	132.17	122.65
5	A	601	HEM	C4A-NA-C1A	3.29	108.57	105.35
8	a	605	0NI	C24-C22-C21	3.29	132.17	122.65
7	b	403	UQ8	C45-C44-C43	3.28	132.12	122.65
7	B	403	UQ8	C45-C44-C43	3.26	132.08	122.65
7	B	403	UQ8	C46-C44-C43	3.26	132.07	122.65
7	b	403	UQ8	C46-C44-C43	3.24	132.02	122.65
10	A	607	A1JN4	CBB-CAB-C3B	3.23	121.33	112.43
5	a	601	HEM	C4A-NA-C1A	3.17	108.45	105.35
8	a	605	0NI	C23-C22-C21	3.17	131.80	122.65
10	A	607	A1JN4	C1B-C2B-C3B	-3.16	102.33	106.94
8	A	605	0NI	C23-C22-C21	3.15	131.76	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	b	403	UQ8	C35-C34-C33	3.04	131.48	123.68
10	A	607	A1JN4	C1C-CHC-C4B	-3.04	115.34	124.74
5	A	601	HEM	C4C-NC-C1C	3.03	108.31	105.35
10	a	607	A1JN4	C1B-C2B-C3B	-2.99	102.57	106.94
5	a	601	HEM	C4C-NC-C1C	2.97	108.26	105.35
7	a	604	UQ8	C32-C33-C34	-2.96	120.54	127.66
5	A	603	HEM	C1B-NB-C4B	2.96	108.13	105.07
7	a	604	UQ8	C8-C7-C6	-2.95	104.08	112.05
5	A	601	HEM	CAA-C2A-C1A	2.94	130.68	124.89
7	B	403	UQ8	C35-C34-C33	2.94	131.22	123.68
5	a	601	HEM	C1B-NB-C4B	2.93	108.10	105.07
10	a	607	A1JN4	C1C-CHC-C4B	-2.92	115.70	124.74
5	a	603	HEM	C1B-NB-C4B	2.92	108.09	105.07
7	b	403	UQ8	C30-C29-C28	2.92	131.16	123.68
8	A	605	0NI	C10-C2-C3	-2.88	115.42	118.50
7	B	403	UQ8	C30-C29-C28	2.88	131.07	123.68
5	A	601	HEM	C1B-NB-C4B	2.88	108.04	105.07
7	A	604	UQ8	C30-C29-C31	2.87	120.10	115.27
7	b	403	UQ8	C40-C39-C38	2.87	131.04	123.68
5	a	603	HEM	CAA-C2A-C1A	2.87	130.54	124.89
5	A	603	HEM	CAA-C2A-C1A	2.86	130.52	124.89
7	a	604	UQ8	C25-C24-C26	2.86	120.07	115.27
7	A	604	UQ8	C10-C9-C11	2.85	120.07	115.27
7	B	403	UQ8	C40-C39-C38	2.84	130.97	123.68
10	a	607	A1JN4	CAA-C2A-C1A	-2.81	119.35	124.89
8	a	605	0NI	C10-C2-C3	-2.80	115.50	118.50
7	B	403	UQ8	C25-C24-C23	2.78	130.82	123.68
10	a	607	A1JN4	CBA-CAA-C2A	-2.78	104.91	112.63
10	A	607	A1JN4	CHA-C1A-C2A	2.78	131.42	125.36
5	A	603	HEM	C4A-NA-C1A	2.77	108.06	105.35
7	b	403	UQ8	C25-C24-C23	2.76	130.76	123.68
5	A	603	HEM	C4D-ND-C1D	2.74	107.91	105.07
7	A	604	UQ8	C10-C9-C8	-2.74	116.64	123.68
10	a	607	A1JN4	OND-C2D-C3D	-2.73	103.66	110.45
5	a	603	HEM	C4D-ND-C1D	2.73	107.89	105.07
5	a	603	HEM	C4A-NA-C1A	2.71	108.00	105.35
10	a	607	A1JN4	CAA-CBA-CGA	-2.71	107.78	113.60
7	a	604	UQ8	C35-C34-C36	2.69	119.80	115.27
7	a	604	UQ8	C11-C9-C8	2.68	126.54	121.12
10	A	607	A1JN4	OND-C2D-C3D	-2.67	103.81	110.45
7	b	403	UQ8	C20-C19-C18	2.66	130.51	123.68
10	A	607	A1JN4	CHC-C1C-NC	2.65	128.73	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	b	403	UQ8	C1M-C1-C6	-2.63	120.11	124.40
5	A	603	HEM	C4C-NC-C1C	2.60	107.89	105.35
10	A	607	A1JN4	C2C-C1C-NC	-2.59	106.14	110.08
5	a	601	HEM	CAA-C2A-C1A	2.59	129.98	124.89
7	B	403	UQ8	C1M-C1-C6	-2.58	120.20	124.40
7	A	604	UQ8	C32-C33-C34	-2.57	121.47	127.66
10	A	607	A1JN4	CAA-CBA-CGA	-2.57	108.07	113.60
6	A	602	LPP	O27-C29-C30	2.56	119.95	111.91
6	a	602	LPP	O27-C29-C30	2.56	119.95	111.91
7	a	604	UQ8	C25-C24-C23	-2.56	117.11	123.68
5	A	601	HEM	C3D-C4D-ND	-2.55	107.33	110.17
5	a	603	HEM	C4C-NC-C1C	2.55	107.84	105.35
7	a	604	UQ8	C37-C38-C39	-2.54	121.54	127.66
10	a	607	A1JN4	C2C-C1C-NC	-2.53	106.23	110.08
7	B	403	UQ8	C20-C19-C18	2.53	130.17	123.68
7	a	604	UQ8	C46-C44-C45	2.52	120.17	114.60
7	a	604	UQ8	C40-C39-C41	2.52	119.51	115.27
11	a	608	PGT	O3-C11-C12	2.52	119.81	111.91
10	a	607	A1JN4	CHC-C1C-NC	2.50	128.45	123.85
7	a	604	UQ8	C42-C43-C44	-2.48	119.28	127.75
7	A	604	UQ8	C27-C28-C29	-2.48	121.70	127.66
5	A	601	HEM	C2A-C1A-NA	-2.47	107.38	110.15
7	a	604	UQ8	C22-C23-C24	-2.46	121.73	127.66
5	a	601	HEM	C3D-C4D-ND	-2.46	107.43	110.17
11	A	608	PGT	O3-C11-C12	2.45	119.61	111.91
7	A	604	UQ8	C20-C19-C18	-2.40	117.53	123.68
7	a	604	UQ8	C12-C13-C14	-2.39	121.90	127.66
7	A	604	UQ8	C25-C24-C23	-2.39	117.56	123.68
5	A	601	HEM	CAA-C2A-C3A	-2.37	121.64	127.07
10	a	607	A1JN4	OND-C2D-C1D	-2.36	107.14	111.92
5	a	603	HEM	CHA-C4D-ND	2.36	127.28	124.37
5	A	603	HEM	CHA-C4D-ND	2.35	127.27	124.37
7	a	604	UQ8	C20-C19-C18	-2.31	117.76	123.68
5	a	601	HEM	C2A-C1A-NA	-2.30	107.57	110.15
7	a	604	UQ8	C27-C28-C29	-2.30	122.12	127.66
5	a	603	HEM	C3B-C2B-C1B	2.30	108.19	106.49
5	A	603	HEM	C3B-C2B-C1B	2.29	108.19	106.49
7	A	604	UQ8	C1M-C1-C6	-2.29	120.66	124.40
7	b	403	UQ8	C12-C13-C14	2.29	133.17	127.66
10	A	607	A1JN4	OND-C2D-C1D	-2.27	107.32	111.92
7	A	604	UQ8	C46-C44-C45	2.25	119.57	114.60
6	B	401	LPP	O27-C29-C30	2.25	118.96	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	604	UQ8	C35-C34-C36	2.24	119.04	115.27
7	a	604	UQ8	C10-C9-C11	2.24	119.03	115.27
7	B	403	UQ8	C12-C13-C14	2.23	133.03	127.66
7	A	604	UQ8	C40-C39-C41	2.23	119.02	115.27
6	b	401	LPP	O27-C29-C30	2.23	118.89	111.91
5	a	603	HEM	CAA-C2A-C3A	-2.22	121.99	127.07
5	A	603	HEM	CAA-C2A-C3A	-2.22	121.99	127.07
7	A	604	UQ8	C37-C38-C39	-2.19	122.39	127.66
10	a	607	A1JN4	CHA-C1A-C2A	2.19	130.14	125.36
5	A	601	HEM	CAD-CBD-CGD	-2.16	108.96	113.60
10	A	607	A1JN4	CMA-C3A-C4A	2.15	128.65	125.37
5	a	601	HEM	CAD-CBD-CGD	-2.14	108.99	113.60
7	B	403	UQ8	C32-C33-C34	2.13	132.80	127.66
7	b	403	UQ8	C32-C33-C34	2.11	132.74	127.66
7	B	403	UQ8	C27-C28-C29	2.10	132.71	127.66
7	A	604	UQ8	C42-C43-C44	-2.09	120.61	127.75
7	b	403	UQ8	C27-C28-C29	2.09	132.69	127.66
5	A	601	HEM	C2D-C1D-ND	-2.08	107.39	109.88
5	a	603	HEM	C3D-C4D-ND	-2.08	107.85	110.17
5	a	603	HEM	CAD-CBD-CGD	-2.08	109.13	113.60
10	a	607	A1JN4	C1C-C2C-C3C	-2.08	104.40	106.83
5	A	603	HEM	C3D-C4D-ND	-2.07	107.86	110.17
5	A	603	HEM	CAD-CBD-CGD	-2.06	109.16	113.60
7	a	604	UQ8	C20-C19-C21	2.05	118.71	115.27
5	A	603	HEM	C2A-C1A-NA	-2.04	107.87	110.15
5	a	601	HEM	CAA-C2A-C3A	-2.03	122.42	127.07
10	a	607	A1JN4	CMA-C3A-C4A	2.03	128.46	125.37
7	A	604	UQ8	C20-C19-C21	2.03	118.68	115.27
10	A	607	A1JN4	C1C-C2C-C3C	-2.02	104.47	106.83
5	a	601	HEM	C2D-C1D-ND	-2.01	107.47	109.88
7	A	604	UQ8	C12-C13-C14	-2.01	122.83	127.66

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	A	607	A1JN4	NB
10	A	607	A1JN4	ND
10	a	607	A1JN4	NB
10	a	607	A1JN4	ND

All (263) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	602	LPP	C6-O5-P1-O2
6	A	602	LPP	C6-O5-P1-O3
6	A	602	LPP	C6-O5-P1-O4
6	A	602	LPP	O9-C7-C8-O27
6	A	602	LPP	O10-C11-O9-C7
6	A	602	LPP	C12-C11-O9-C7
6	B	401	LPP	C6-O5-P1-O2
6	B	401	LPP	C6-O5-P1-O3
6	B	401	LPP	C6-O5-P1-O4
6	a	602	LPP	C6-O5-P1-O2
6	a	602	LPP	C6-O5-P1-O3
6	a	602	LPP	C6-O5-P1-O4
6	a	602	LPP	O9-C7-C8-O27
6	a	602	LPP	O10-C11-O9-C7
6	a	602	LPP	C12-C11-O9-C7
6	b	401	LPP	C6-O5-P1-O2
6	b	401	LPP	C6-O5-P1-O3
6	b	401	LPP	C6-O5-P1-O4
7	A	604	UQ8	C15-C14-C16-C17
7	A	604	UQ8	C13-C14-C16-C17
7	A	604	UQ8	C1-C6-C7-C8
7	A	604	UQ8	C5-C6-C7-C8
7	B	403	UQ8	C11-C12-C13-C14
7	a	604	UQ8	C15-C14-C16-C17
7	a	604	UQ8	C13-C14-C16-C17
7	b	403	UQ8	C11-C12-C13-C14
8	A	605	0NI	C11-C10-C2-C1
8	A	605	0NI	C11-C10-C2-C3
8	a	605	0NI	C11-C10-C2-C1
8	a	605	0NI	C11-C10-C2-C3
10	A	607	A1JN4	C1A-C2A-CAA-CBA
11	A	608	PGT	O31-C31-O2-C2
11	A	608	PGT	C4-C5-C6-O6
11	a	608	PGT	O31-C31-O2-C2
11	a	608	PGT	C1-O3P-P-O1P
11	a	608	PGT	C4-C5-C6-O6
6	A	602	LPP	O28-C29-O27-C8
6	a	602	LPP	O28-C29-O27-C8
12	b	402	POV	O32-C31-O31-C3
10	A	607	A1JN4	C4C-C3C-CAC-CBC
10	a	607	A1JN4	C4C-C3C-CAC-CBC
10	a	607	A1JN4	C2C-C3C-CAC-CBC
6	A	602	LPP	C30-C29-O27-C8

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Mol	Chain	Res	Type	Atoms
6	a	602	LPP	C30-C29-O27-C8
11	A	608	PGT	C12-C11-O3-C3
11	a	608	PGT	C12-C11-O3-C3
10	A	607	A1JN4	C2C-C3C-CAC-CBC
11	A	608	PGT	C32-C31-O2-C2
11	a	608	PGT	C32-C31-O2-C2
12	B	402	POV	O32-C31-O31-C3
7	a	604	UQ8	C20-C19-C21-C22
7	a	604	UQ8	C18-C19-C21-C22
12	b	402	POV	C32-C31-O31-C3
11	a	608	PGT	O11-C11-O3-C3
12	B	402	POV	C32-C31-O31-C3
11	A	608	PGT	O11-C11-O3-C3
5	A	601	HEM	C1A-C2A-CAA-CBA
5	A	603	HEM	C1A-C2A-CAA-CBA
5	a	601	HEM	C1A-C2A-CAA-CBA
5	a	603	HEM	C1A-C2A-CAA-CBA
7	a	604	UQ8	C12-C11-C9-C10
7	a	604	UQ8	C12-C11-C9-C8
5	a	601	HEM	C3A-C2A-CAA-CBA
7	A	604	UQ8	C24-C26-C27-C28
6	B	401	LPP	O9-C7-C8-O27
6	b	401	LPP	O9-C7-C8-O27
7	a	604	UQ8	C25-C24-C26-C27
7	a	604	UQ8	C23-C24-C26-C27
5	A	601	HEM	C3A-C2A-CAA-CBA
5	A	603	HEM	C3A-C2A-CAA-CBA
5	a	603	HEM	C3A-C2A-CAA-CBA
10	A	607	A1JN4	C3A-C2A-CAA-CBA
6	A	602	LPP	C29-C30-C31-C32
6	a	602	LPP	C29-C30-C31-C32
7	B	403	UQ8	C24-C26-C27-C28
7	B	403	UQ8	C14-C16-C17-C18
7	b	403	UQ8	C24-C26-C27-C28
7	b	403	UQ8	C14-C16-C17-C18
8	A	605	0NI	C12-C14-C15-C16
10	A	607	A1JN4	C2B-C3B-CAB-CBB
11	A	608	PGT	C31-C32-C33-C34
10	a	607	A1JN4	C2B-C3B-CAB-CBB
11	A	608	PGT	C15-C16-C17-C18
11	a	608	PGT	C15-C16-C17-C18
6	B	401	LPP	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
6	b	401	LPP	C16-C17-C18-C19
6	b	401	LPP	C36-C37-C38-C39
6	a	602	LPP	C39-C40-C41-C42
6	B	401	LPP	C36-C37-C38-C39
6	A	602	LPP	C39-C40-C41-C42
6	b	401	LPP	C30-C31-C32-C33
11	a	608	PGT	C36-C37-C38-C39
6	B	401	LPP	C30-C31-C32-C33
11	a	608	PGT	C31-C32-C33-C34
6	B	401	LPP	C34-C35-C36-C37
6	b	401	LPP	C34-C35-C36-C37
11	A	608	PGT	C36-C37-C38-C39
6	A	602	LPP	C34-C35-C36-C37
6	B	401	LPP	C20-C21-C22-C23
6	b	401	LPP	C20-C21-C22-C23
12	b	402	POV	C212-C213-C214-C215
6	a	602	LPP	C34-C35-C36-C37
11	a	608	PGT	C16-C17-C18-C19
6	A	602	LPP	C13-C14-C15-C16
6	A	602	LPP	C17-C18-C19-C20
6	a	602	LPP	C13-C14-C15-C16
6	A	602	LPP	C37-C38-C39-C40
6	a	602	LPP	C37-C38-C39-C40
11	A	608	PGT	C16-C17-C18-C19
11	A	608	PGT	O5-C5-C6-O6
11	a	608	PGT	O5-C5-C6-O6
11	A	608	PGT	C12-C13-C14-C15
6	a	602	LPP	C17-C18-C19-C20
11	a	608	PGT	C12-C13-C14-C15
7	a	604	UQ8	C30-C29-C31-C32
12	B	402	POV	C210-C211-C212-C213
7	A	604	UQ8	C3-C4-O4-C4M
7	a	604	UQ8	C3-C4-O4-C4M
11	A	608	PGT	O2-C2-C3-O3
11	a	608	PGT	O2-C2-C3-O3
11	a	608	PGT	C1-O3P-P-O4P
12	B	402	POV	C1-O11-P-O12
10	A	607	A1JN4	C4B-C3B-CAB-CBB
7	A	604	UQ8	C40-C39-C41-C42
7	A	604	UQ8	C30-C29-C31-C32
6	A	602	LPP	C6-C7-C8-O27
6	B	401	LPP	C6-C7-C8-O27

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Mol	Chain	Res	Type	Atoms
6	b	401	LPP	C6-C7-C8-O27
12	B	402	POV	C1-C2-C3-O31
12	b	402	POV	C1-C2-C3-O31
6	a	602	LPP	C20-C21-C22-C23
10	a	607	A1JN4	C4B-C3B-CAB-CBB
6	B	401	LPP	C13-C14-C15-C16
7	B	403	UQ8	C19-C21-C22-C23
7	b	403	UQ8	C19-C21-C22-C23
6	A	602	LPP	C20-C21-C22-C23
12	B	402	POV	C23-C24-C25-C26
6	b	401	LPP	C13-C14-C15-C16
11	a	608	PGT	C43-C44-C45-C46
6	A	602	LPP	C23-C24-C25-C26
6	A	602	LPP	C31-C32-C33-C34
6	a	602	LPP	C23-C24-C25-C26
6	a	602	LPP	C31-C32-C33-C34
8	a	605	0NI	C12-C14-C15-C16
11	A	608	PGT	C43-C44-C45-C46
6	a	602	LPP	C6-C7-C8-O27
11	A	608	PGT	C1-C2-C3-O3
11	a	608	PGT	C1-C2-C3-O3
7	a	604	UQ8	C28-C29-C31-C32
12	b	402	POV	C1-O11-P-O12
12	B	402	POV	O21-C2-C3-O31
7	B	403	UQ8	C9-C11-C12-C13
7	a	604	UQ8	C24-C26-C27-C28
7	b	403	UQ8	C9-C11-C12-C13
6	b	401	LPP	C31-C32-C33-C34
6	B	401	LPP	C31-C32-C33-C34
6	B	401	LPP	O5-C6-C7-C8
12	b	402	POV	O11-C1-C2-C3
11	a	608	PGT	C22-C23-C24-C25
11	A	608	PGT	C33-C34-C35-C36
11	a	608	PGT	C41-C42-C43-C44
5	A	601	HEM	C4C-C3C-CAC-CBC
5	A	603	HEM	C4B-C3B-CAB-CBB
5	A	603	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
12	b	402	POV	O21-C2-C3-O31
12	b	402	POV	C210-C211-C212-C213

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Mol	Chain	Res	Type	Atoms
6	B	401	LPP	C30-C29-O27-C8
11	A	608	PGT	C41-C42-C43-C44
6	B	401	LPP	O28-C29-O27-C8
7	A	604	UQ8	C38-C39-C41-C42
7	A	604	UQ8	C28-C29-C31-C32
7	A	604	UQ8	C6-C7-C8-C9
11	A	608	PGT	C1-O3P-P-O2P
11	a	608	PGT	C1-O3P-P-O2P
6	b	401	LPP	O5-C6-C7-C8
12	B	402	POV	O11-C1-C2-C3
11	a	608	PGT	C33-C34-C35-C36
11	A	608	PGT	C21-C22-C23-C24
12	b	402	POV	O11-C1-C2-O21
12	B	402	POV	C35-C36-C37-C38
11	a	608	PGT	C21-C22-C23-C24
12	b	402	POV	C35-C36-C37-C38
11	a	608	PGT	C35-C36-C37-C38
7	A	604	UQ8	C34-C36-C37-C38
10	A	607	A1JN4	C2A-CAA-CBA-CGA
11	A	608	PGT	C35-C36-C37-C38
12	B	402	POV	O11-C1-C2-O21
7	B	403	UQ8	C40-C39-C41-C42
7	b	403	UQ8	C40-C39-C41-C42
6	A	602	LPP	C19-C20-C21-C22
11	A	608	PGT	C1-O3P-P-O4P
12	B	402	POV	C11-O12-P-O11
12	b	402	POV	C11-O12-P-O11
12	b	402	POV	C23-C24-C25-C26
6	b	401	LPP	O28-C29-O27-C8
11	a	608	PGT	C2-C1-O3P-P
6	b	401	LPP	C30-C29-O27-C8
11	A	608	PGT	C22-C23-C24-C25
6	B	401	LPP	O5-C6-C7-O9
6	A	602	LPP	C38-C39-C40-C41
6	a	602	LPP	C38-C39-C40-C41
6	A	602	LPP	C32-C33-C34-C35
11	A	608	PGT	C2-C1-O3P-P
6	A	602	LPP	C14-C15-C16-C17
6	a	602	LPP	C19-C20-C21-C22
5	a	603	HEM	CAD-CBD-CGD-O1D
6	B	401	LPP	C22-C23-C24-C25
6	b	401	LPP	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
5	A	603	HEM	CAD-CBD-CGD-O1D
6	B	401	LPP	C15-C16-C17-C18
7	A	604	UQ8	C14-C16-C17-C18
6	a	602	LPP	C32-C33-C34-C35
6	A	602	LPP	C6-C7-O9-C11
6	a	602	LPP	C6-C7-O9-C11
12	B	402	POV	C1-C2-O21-C21
12	B	402	POV	C3-C2-O21-C21
12	b	402	POV	C3-C2-O21-C21
6	b	401	LPP	O10-C11-O9-C7
12	b	402	POV	C37-C38-C39-C310
12	B	402	POV	C37-C38-C39-C310
7	B	403	UQ8	C38-C39-C41-C42
7	b	403	UQ8	C38-C39-C41-C42
12	b	402	POV	O31-C31-C32-C33
11	a	608	PGT	C45-C46-C47-C48
12	B	402	POV	O31-C31-C32-C33
6	B	401	LPP	C12-C13-C14-C15
8	A	605	0NI	C13-C12-C14-C15
8	a	605	0NI	C13-C12-C14-C15
6	b	401	LPP	O5-C6-C7-O9
6	b	401	LPP	C15-C16-C17-C18
7	B	403	UQ8	C2-C3-O3-C3M
10	a	607	A1JN4	CAA-CBA-CGA-O1A
5	a	603	HEM	CAD-CBD-CGD-O2D
11	a	608	PGT	C20-C21-C22-C23
5	A	603	HEM	CAD-CBD-CGD-O2D
6	A	602	LPP	C8-C7-O9-C11
6	a	602	LPP	C8-C7-O9-C11
12	b	402	POV	C1-C2-O21-C21
10	A	607	A1JN4	CAA-CBA-CGA-O1A
11	A	608	PGT	O2-C31-C32-C33
6	b	401	LPP	C37-C38-C39-C40
6	b	401	LPP	C12-C13-C14-C15
11	a	608	PGT	O2-C31-C32-C33
7	b	403	UQ8	C2-C3-O3-C3M
6	b	401	LPP	C12-C11-O9-C7
11	A	608	PGT	C44-C45-C46-C47
7	a	604	UQ8	C31-C32-C33-C34
6	B	401	LPP	C37-C38-C39-C40
11	A	608	PGT	C4-O4P-P-O1P
11	a	608	PGT	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
12	B	402	POV	C1-O11-P-O14
12	b	402	POV	C1-O11-P-O14
11	A	608	PGT	O31-C31-C32-C33
12	B	402	POV	C312-C313-C314-C315
11	a	608	PGT	O31-C31-C32-C33
7	A	604	UQ8	C31-C32-C33-C34
10	A	607	A1JN4	CAA-CBA-CGA-O2A
6	a	602	LPP	C41-C42-C43-C44
6	a	602	LPP	C14-C15-C16-C17
12	b	402	POV	C312-C313-C314-C315

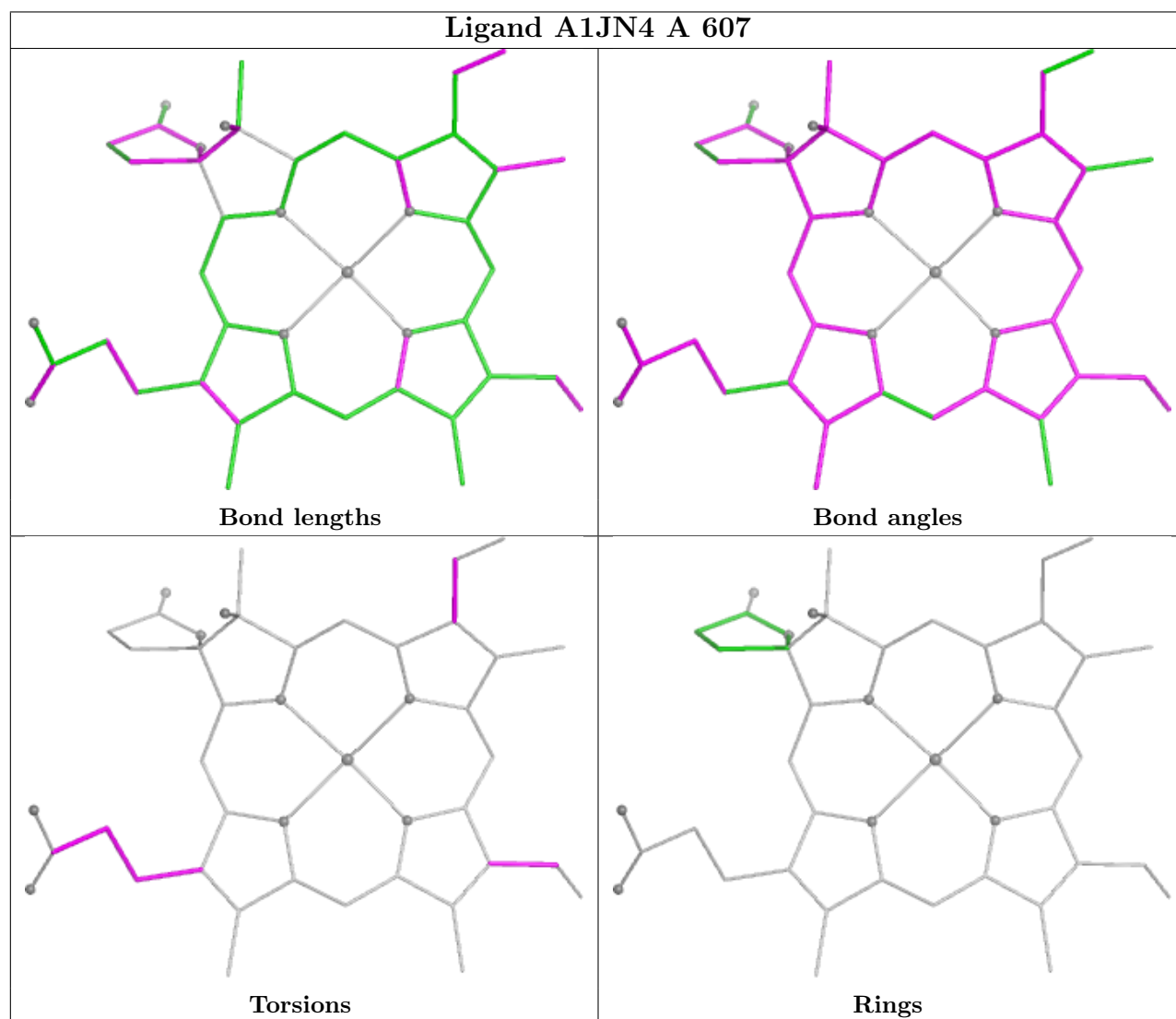
There are no ring outliers.

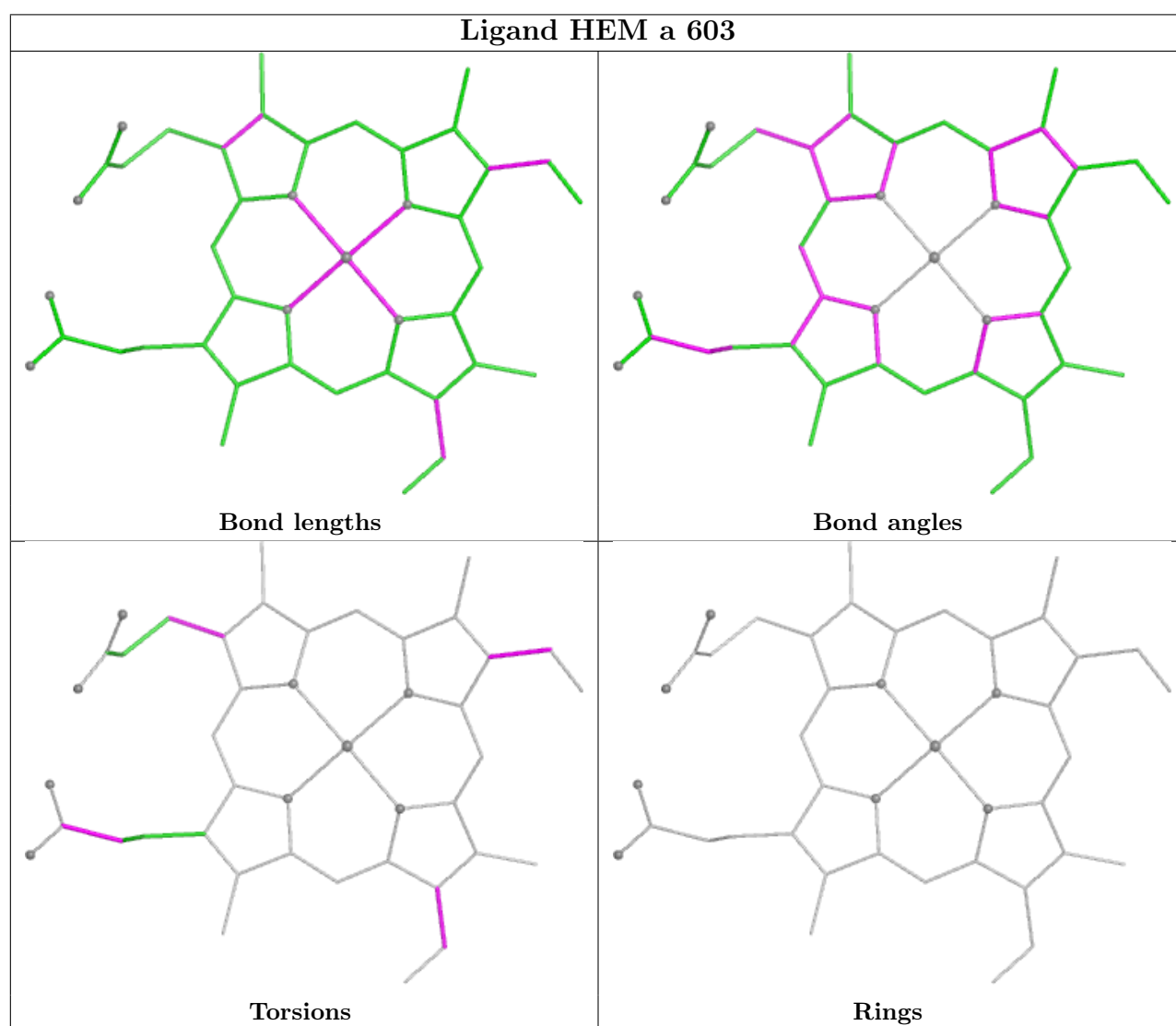
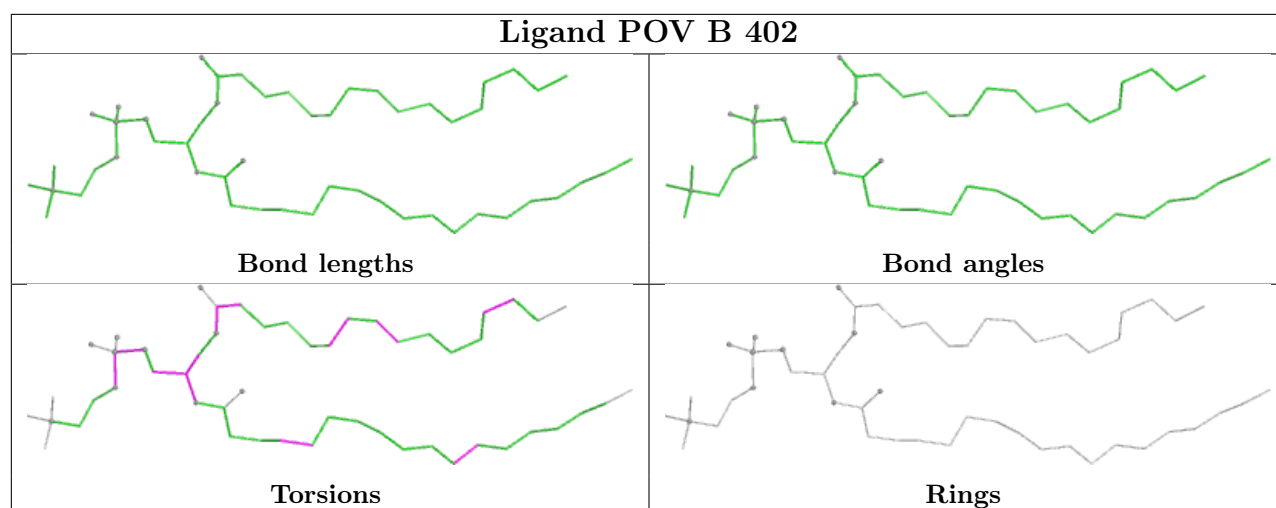
20 monomers are involved in 82 short contacts:

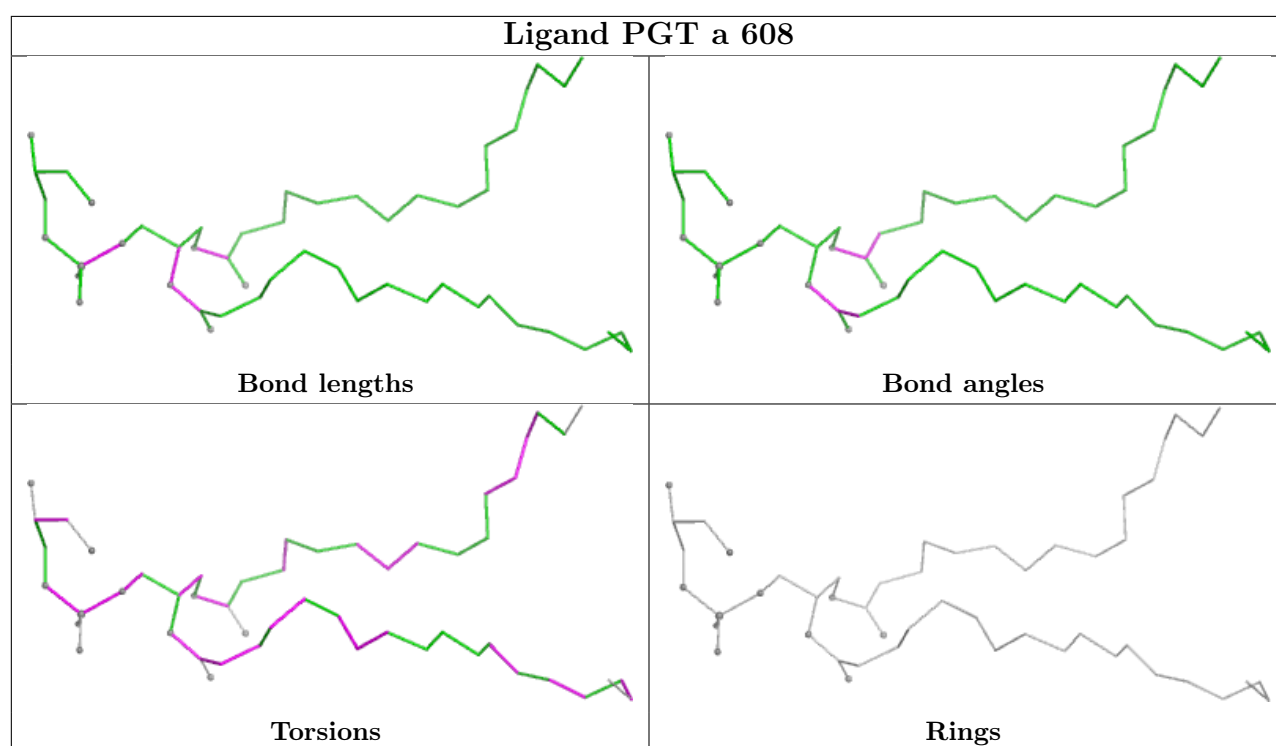
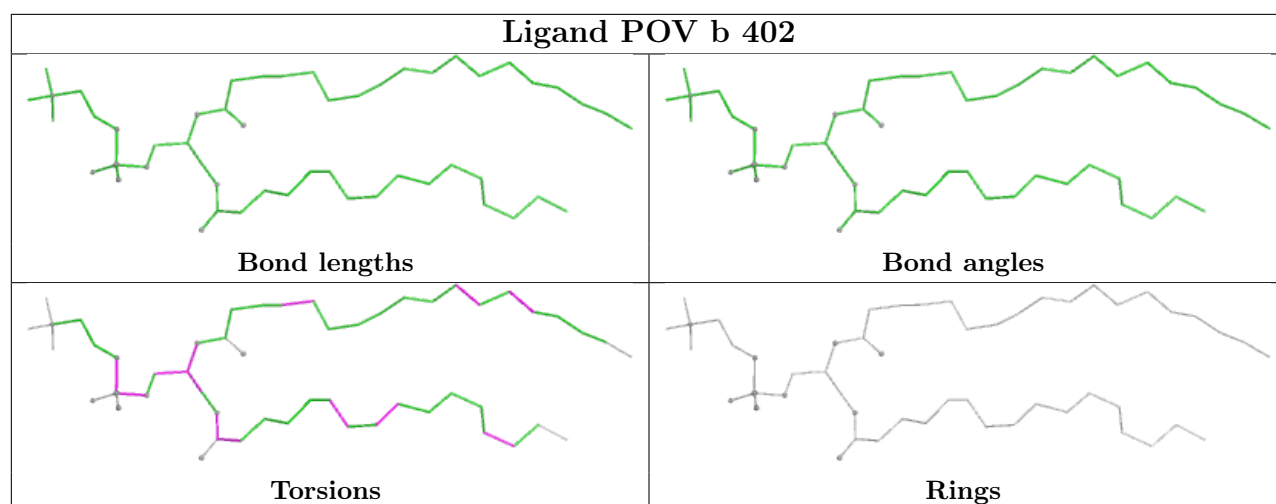
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	607	A1JN4	1	0
12	B	402	POV	11	0
5	a	603	HEM	5	0
12	b	402	POV	12	0
11	a	608	PGT	1	0
7	a	604	UQ8	6	0
6	a	602	LPP	2	0
7	B	403	UQ8	2	0
5	A	603	HEM	6	0
7	b	403	UQ8	2	0
5	a	601	HEM	8	0
8	a	605	0NI	1	0
6	A	602	LPP	3	0
7	A	604	UQ8	9	0
11	A	608	PGT	2	0
5	A	601	HEM	7	0
6	B	401	LPP	1	0
8	A	605	0NI	1	0
6	b	401	LPP	1	0
9	A	606	OXY	1	0

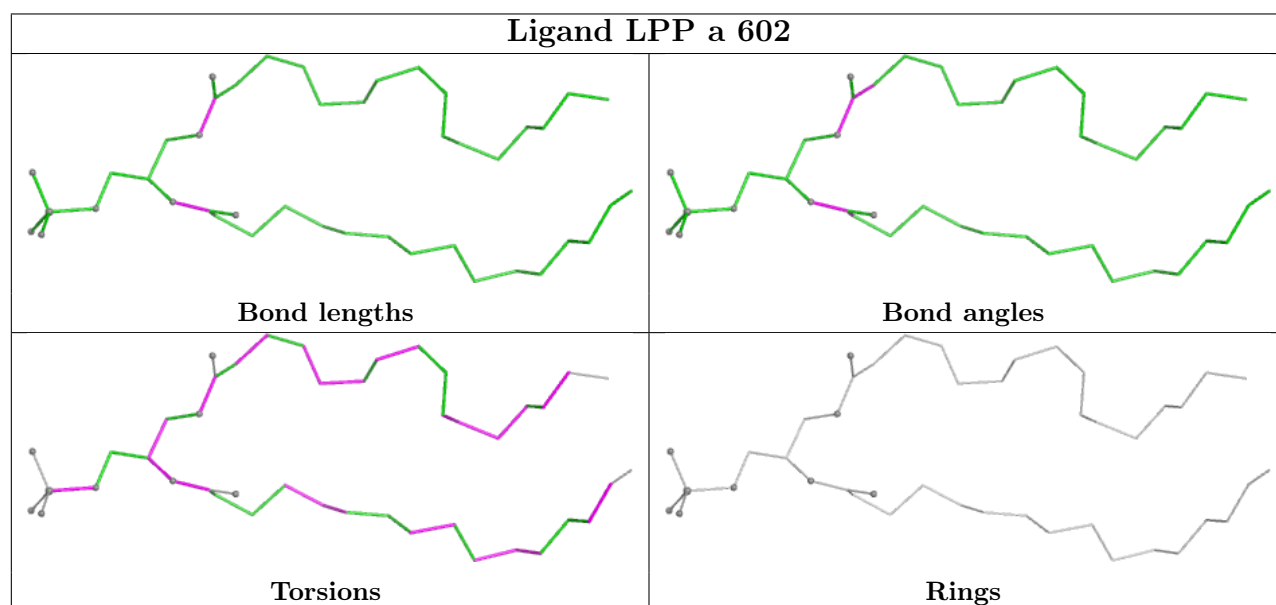
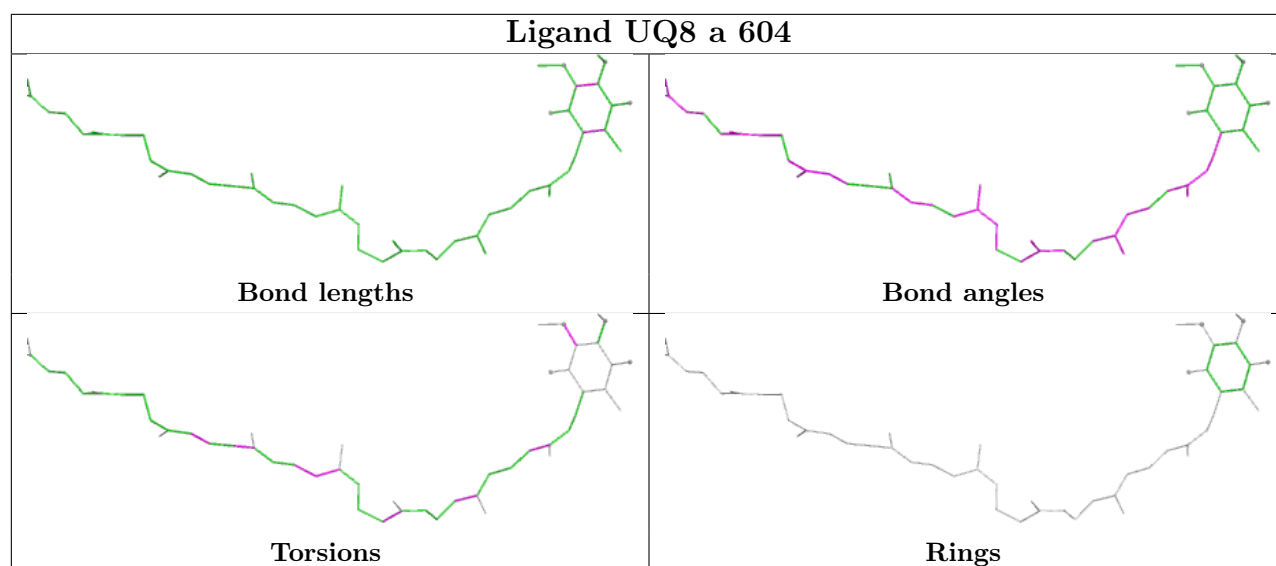
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

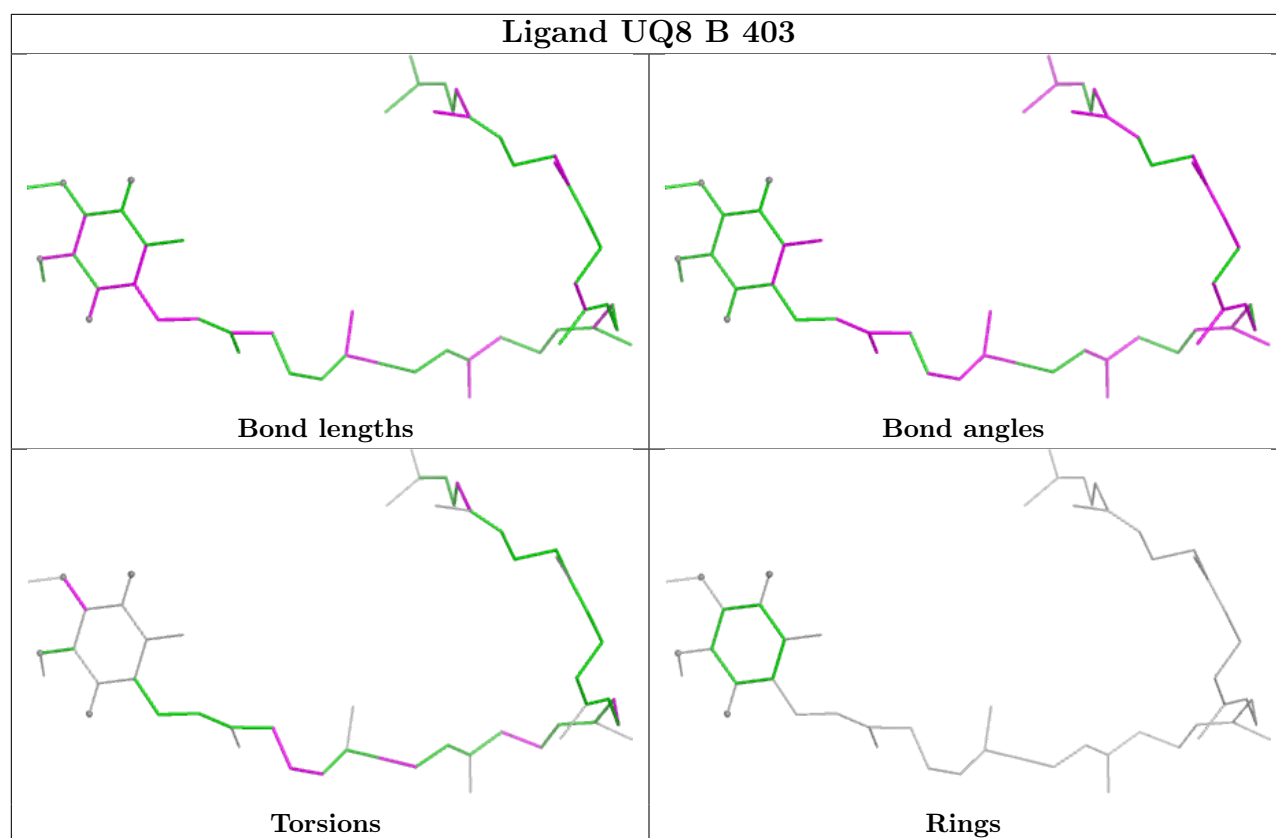
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

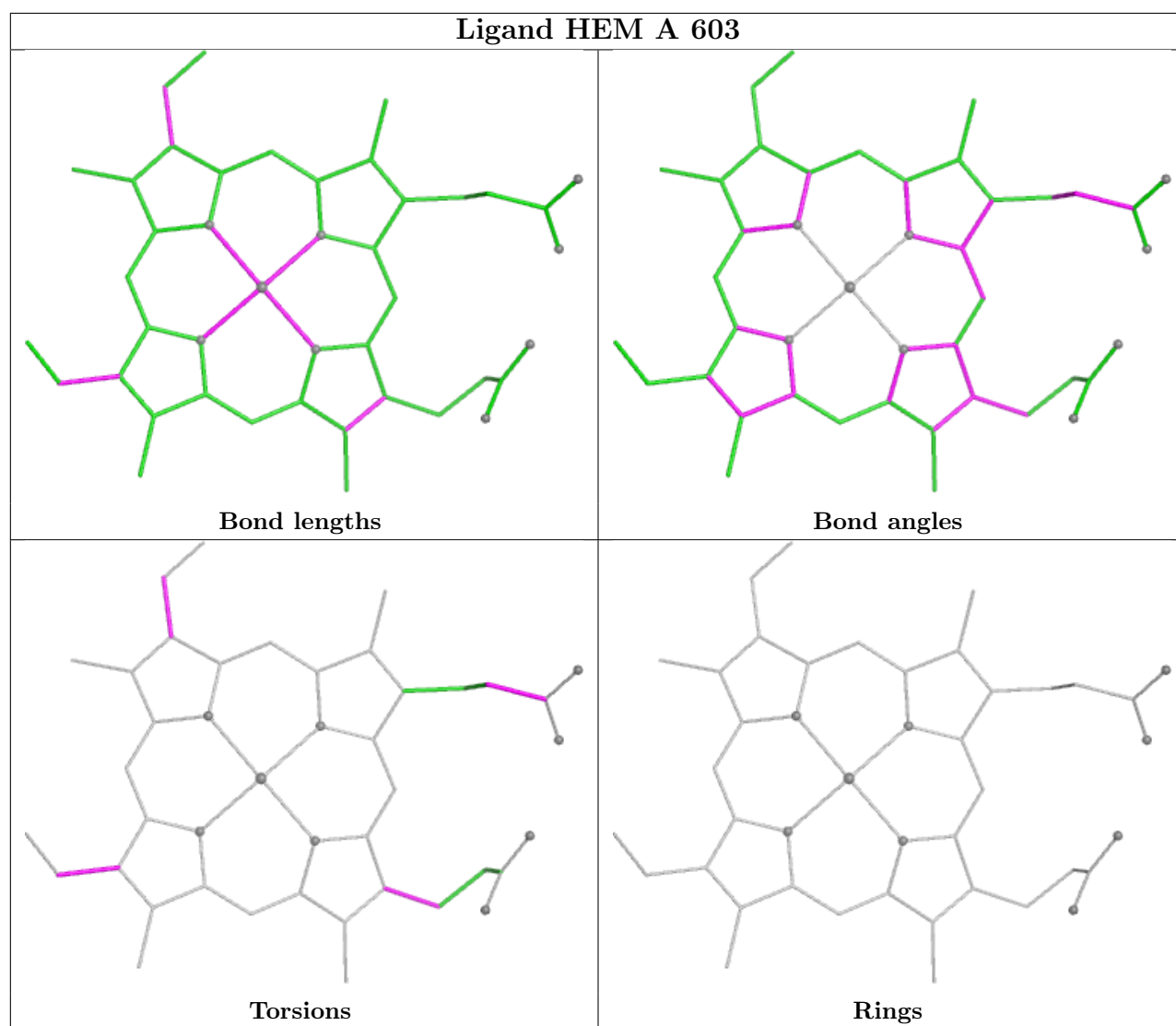


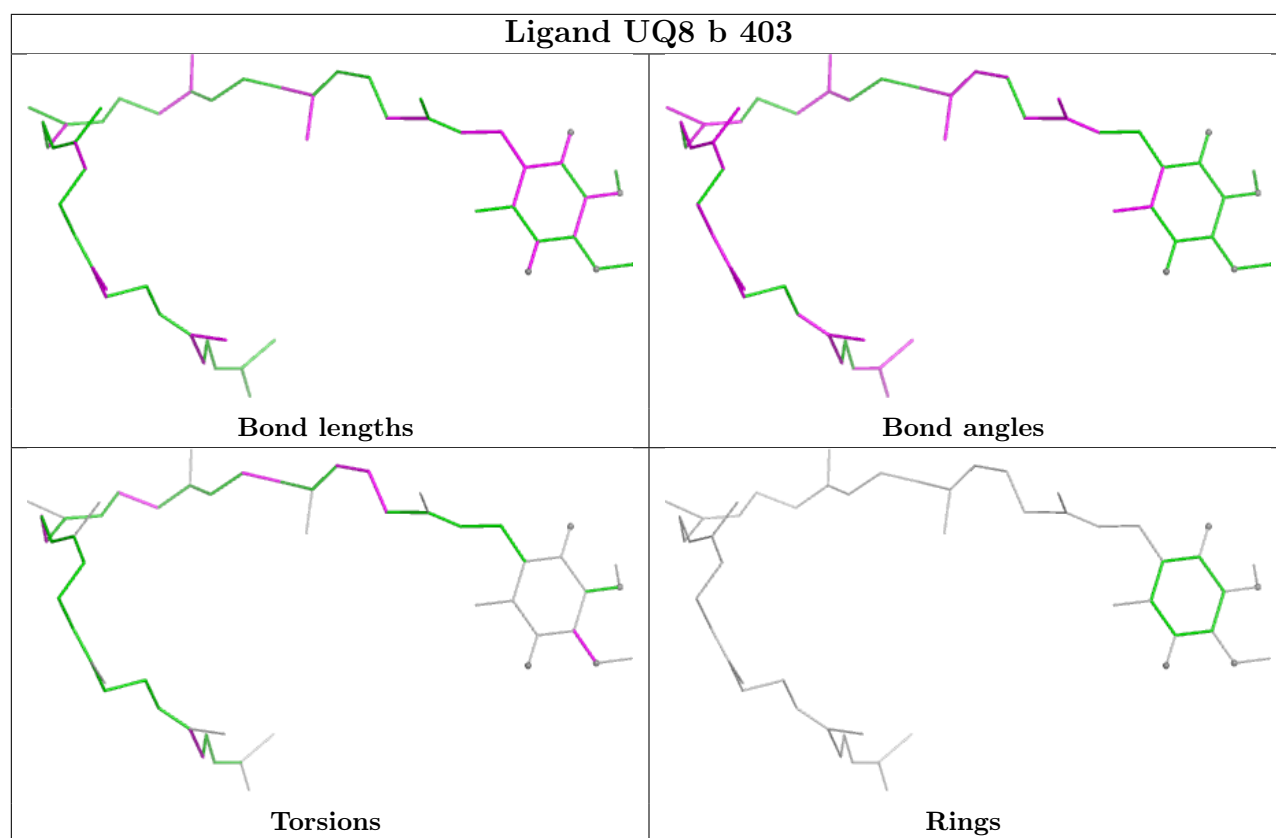


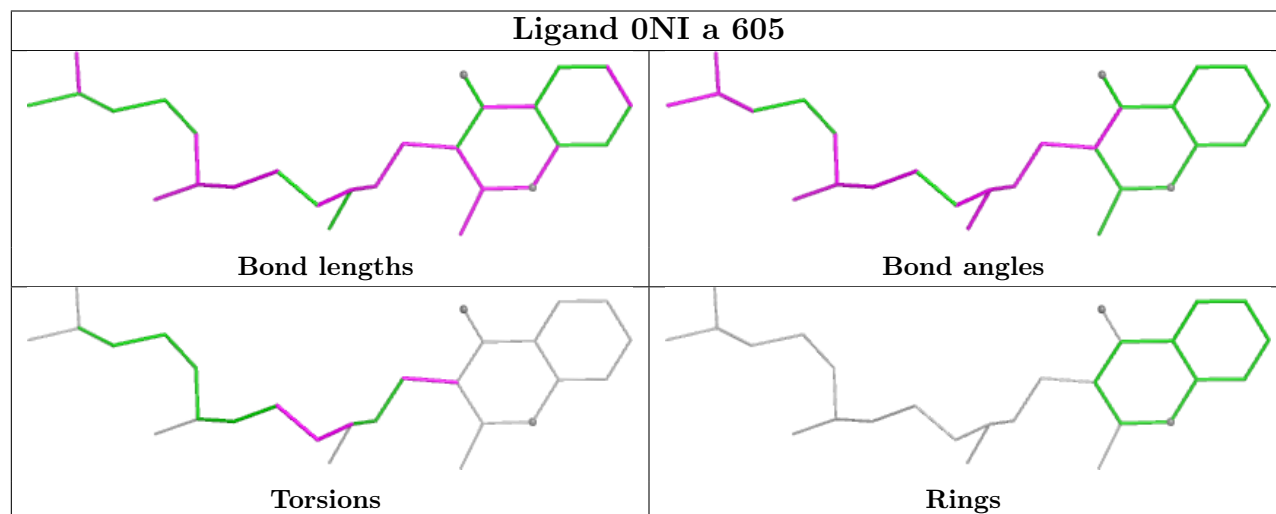
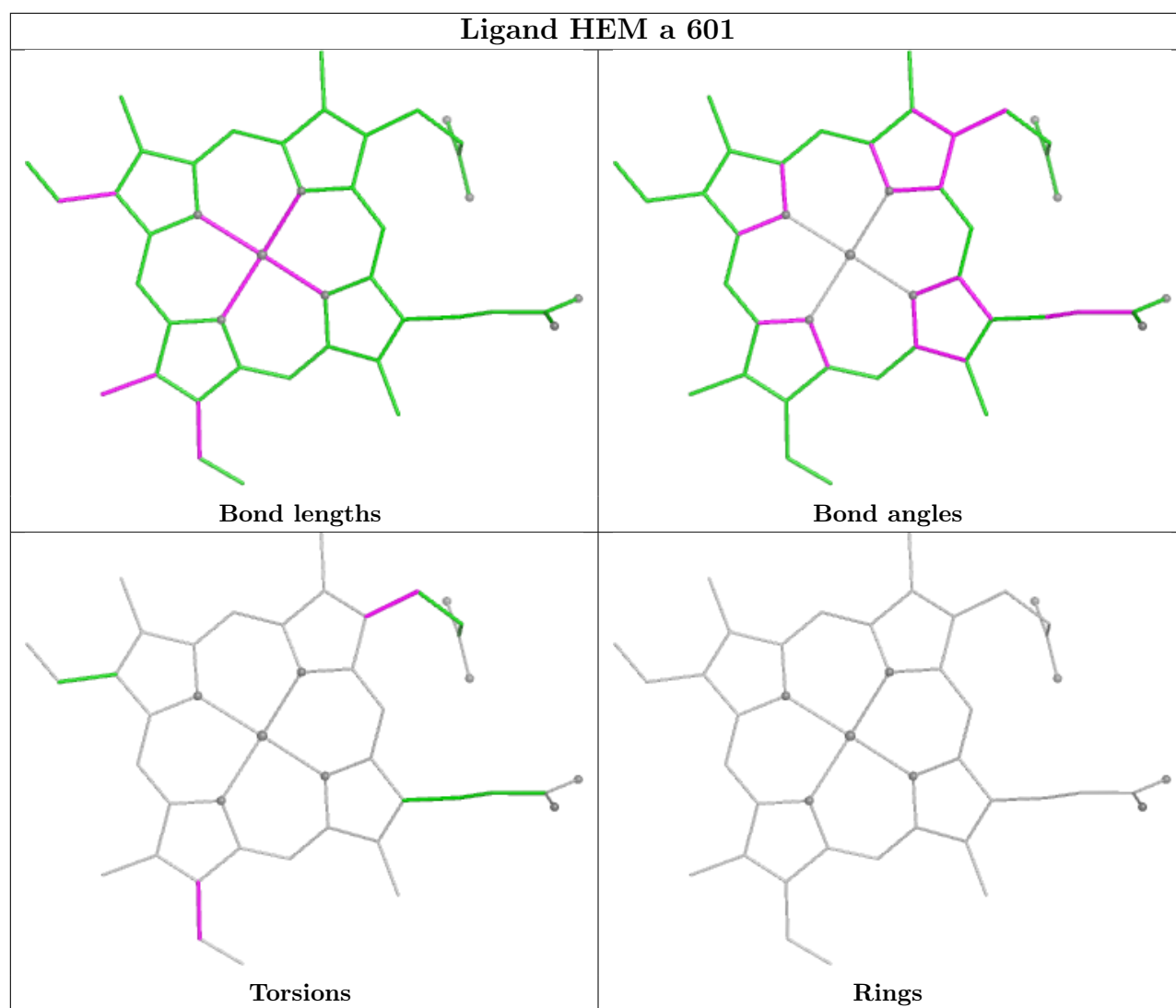


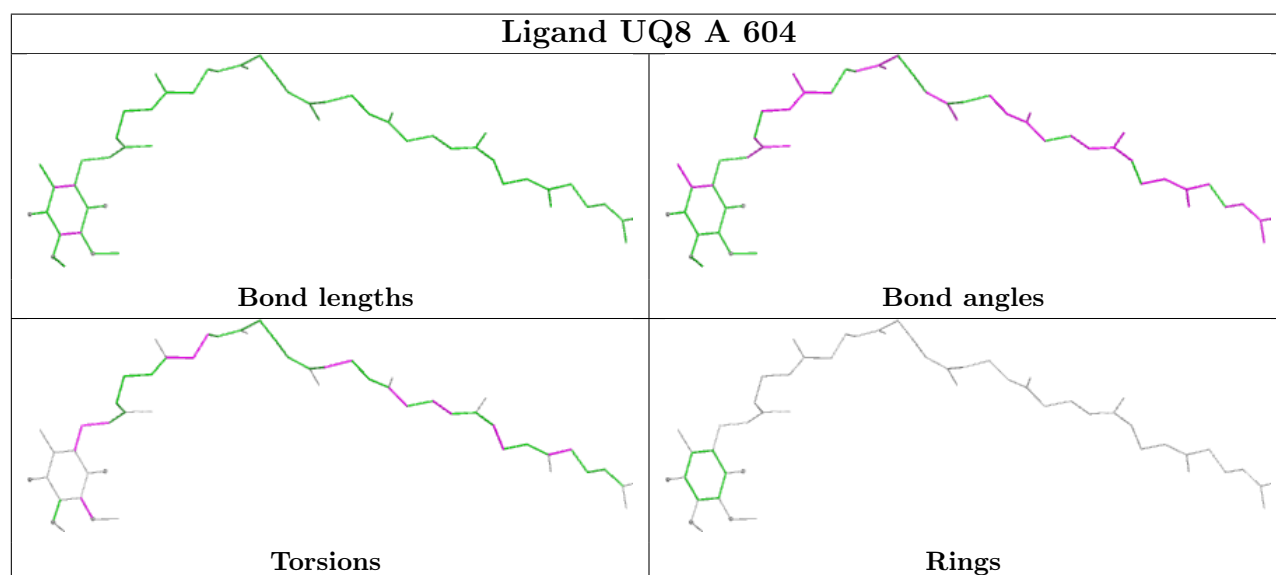
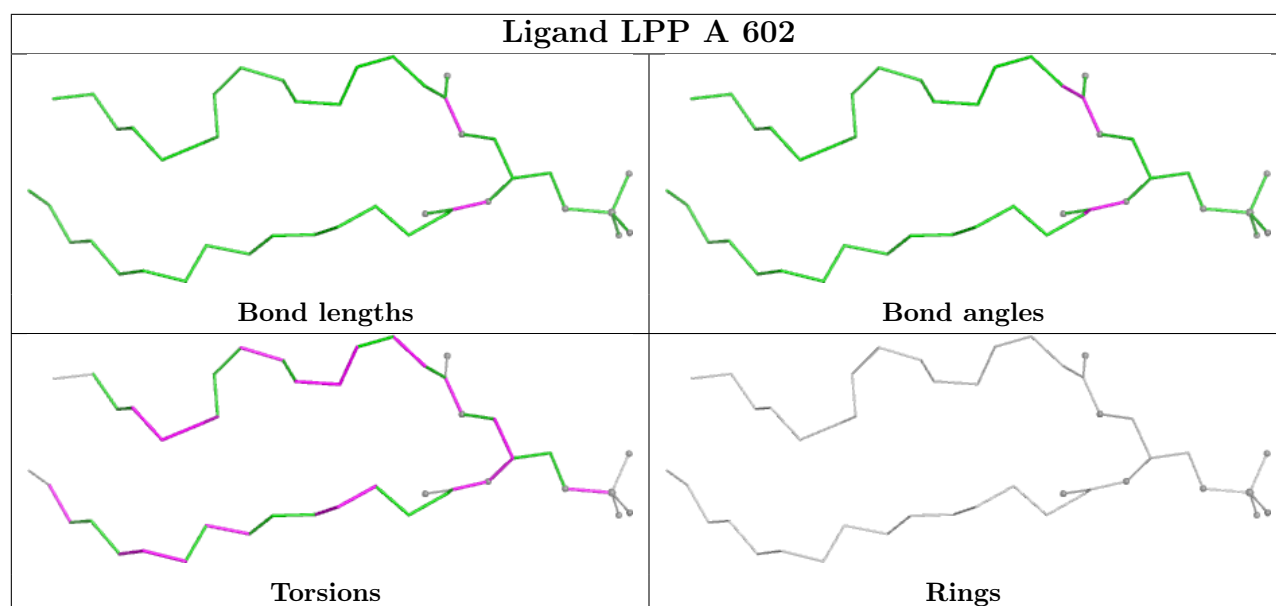


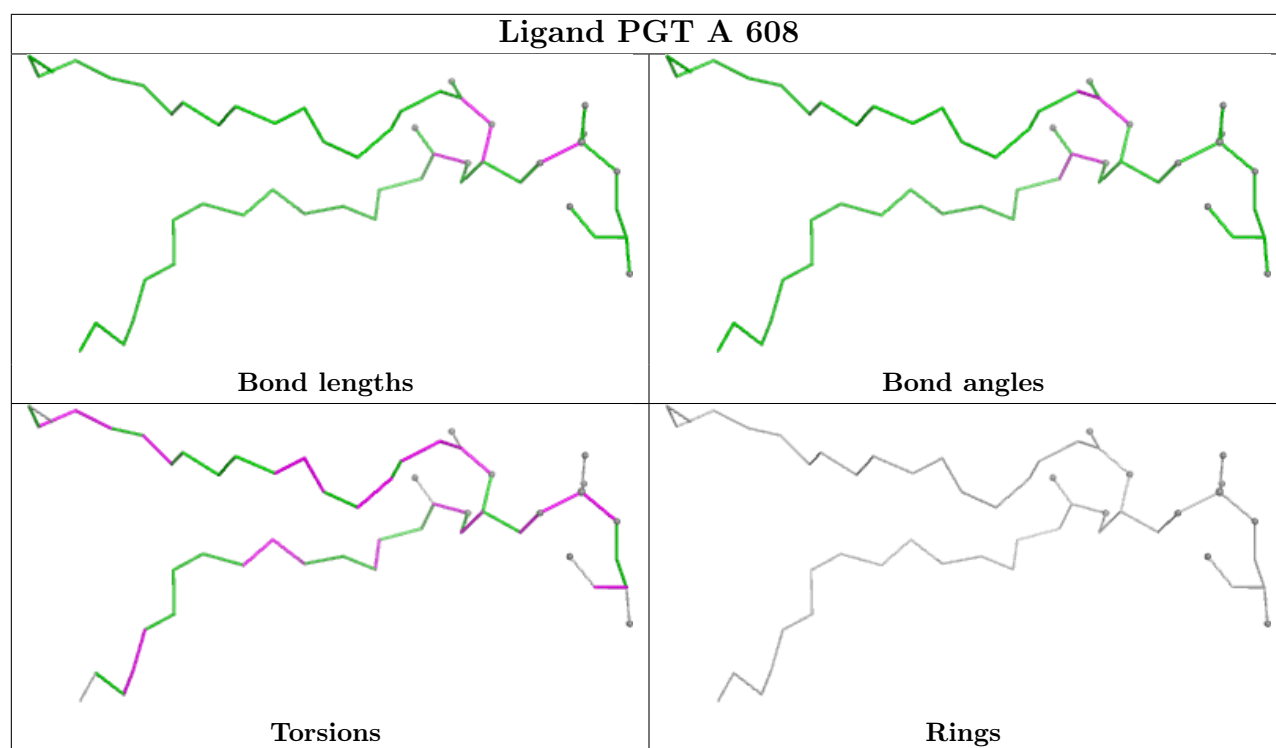


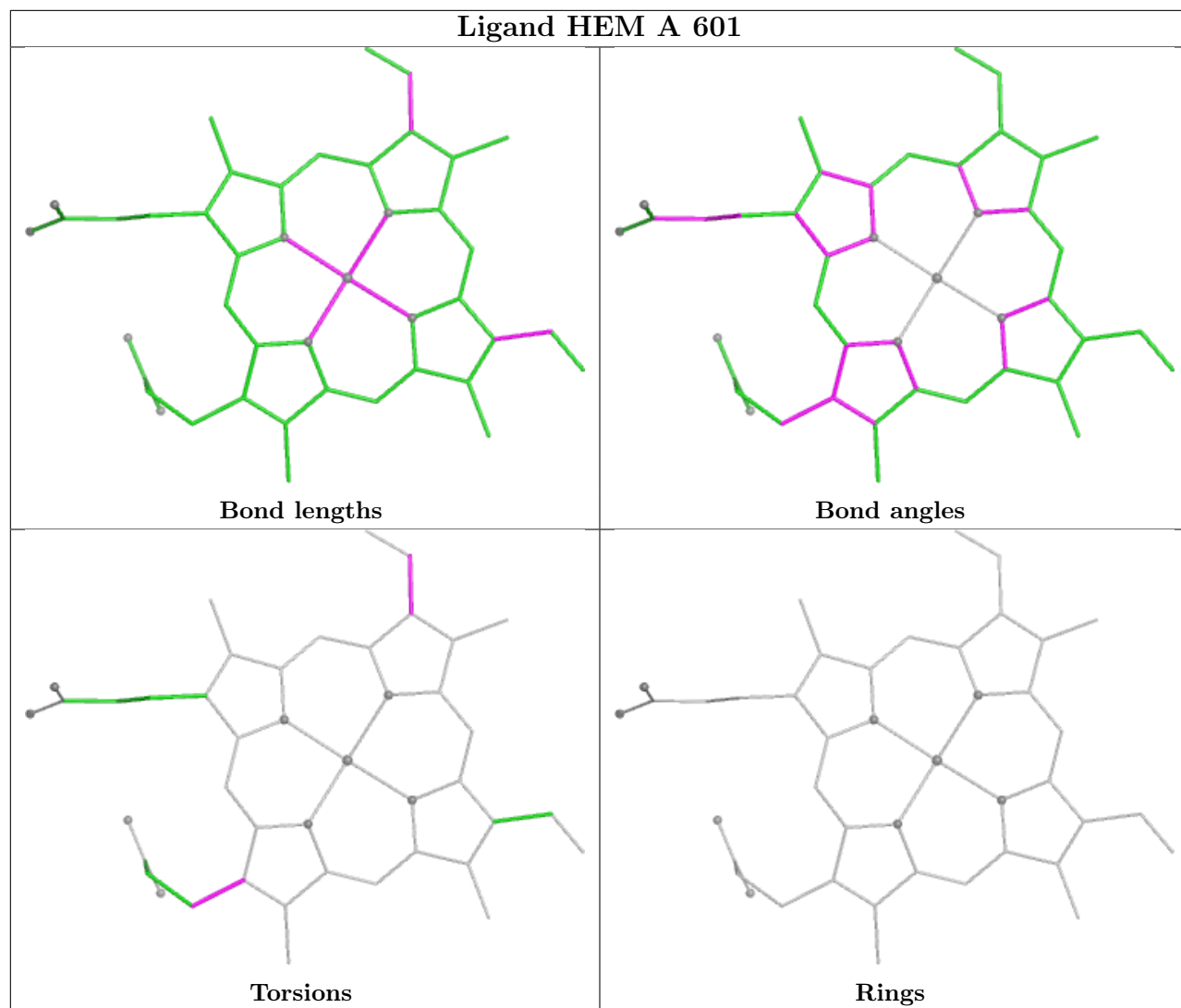


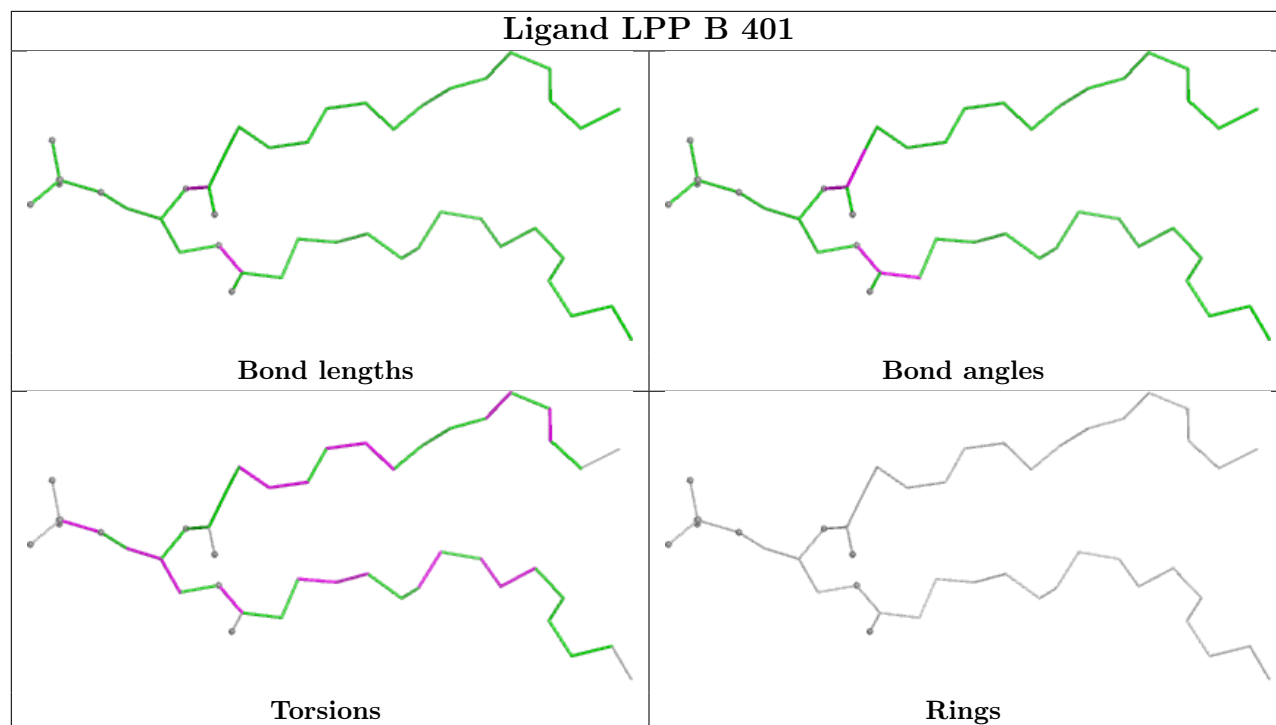


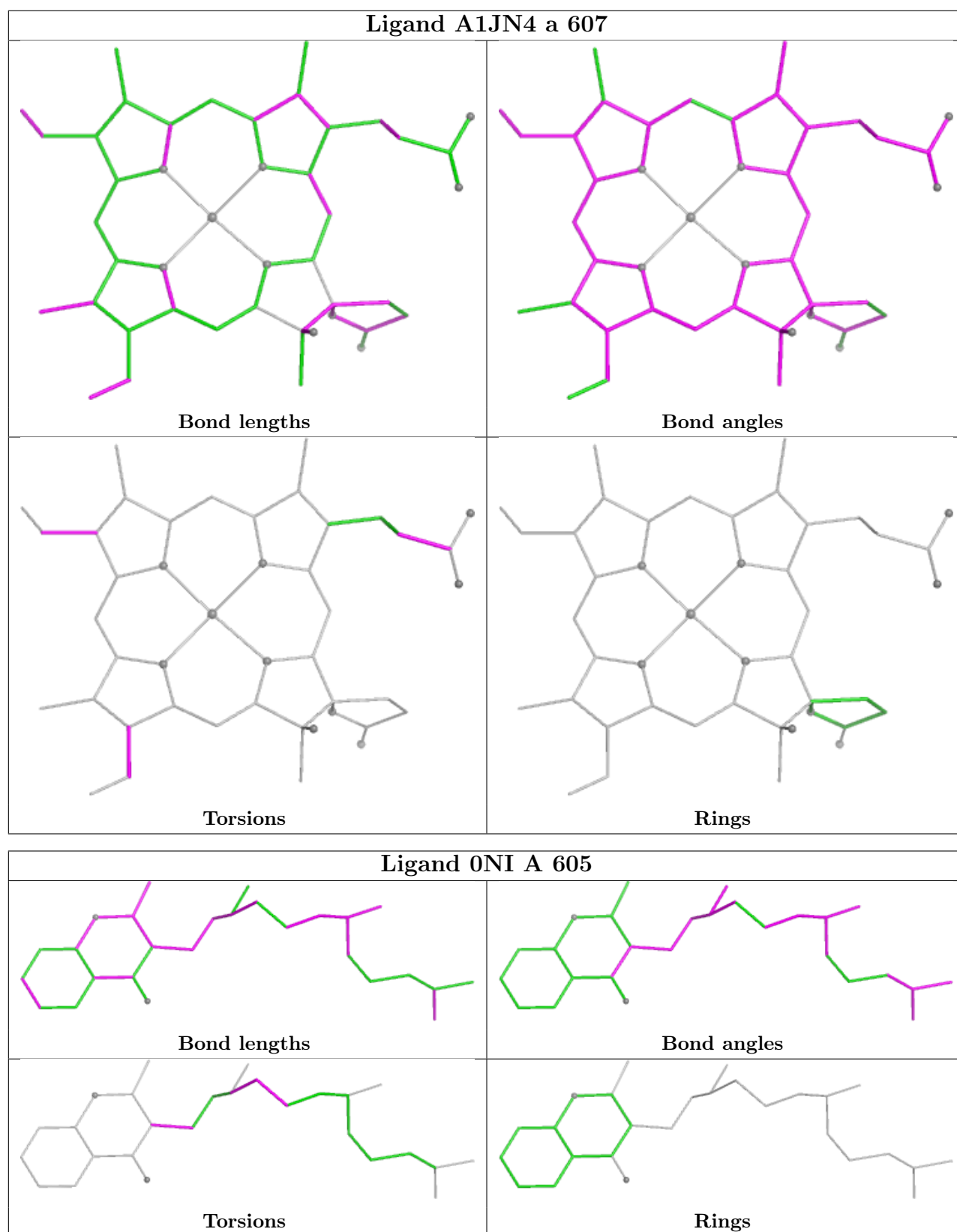


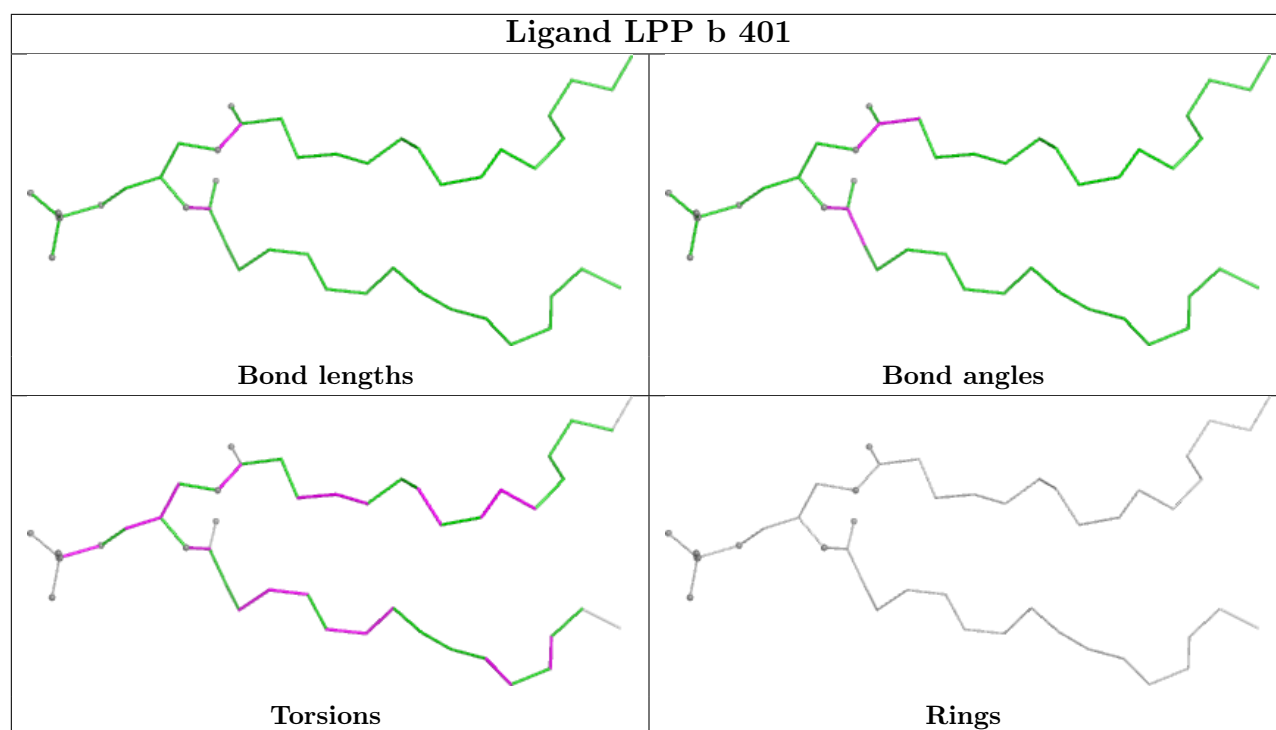












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

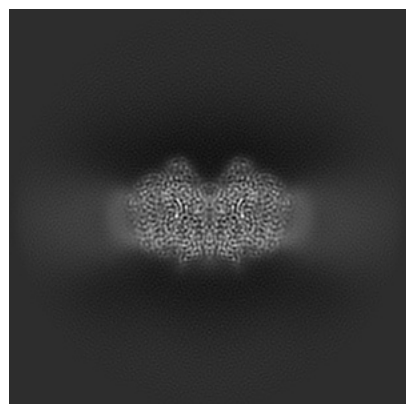
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54812. These allow visual inspection of the internal detail of the map and identification of artifacts.

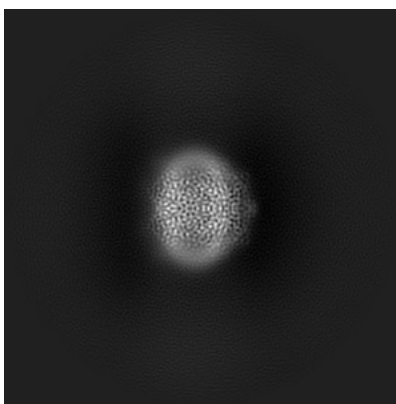
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

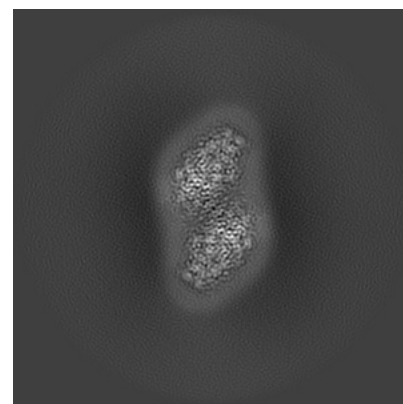
6.1.1 Primary map



X

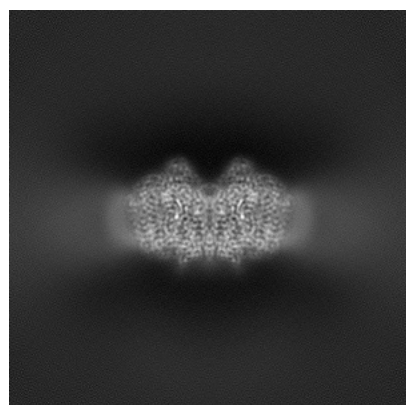


Y

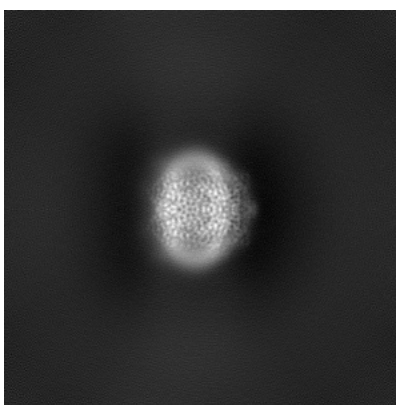


Z

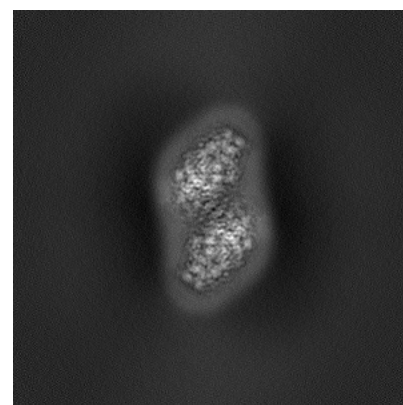
6.1.2 Raw map



X



Y

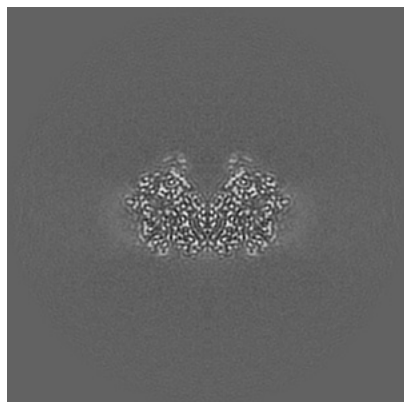


Z

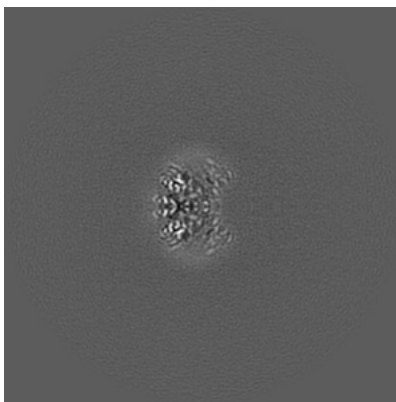
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

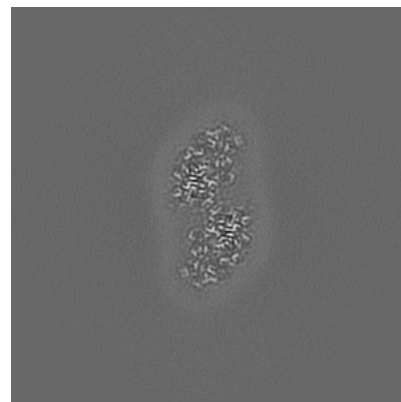
6.2.1 Primary map



X Index: 180

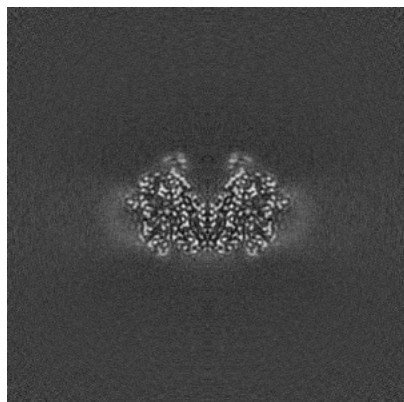


Y Index: 180

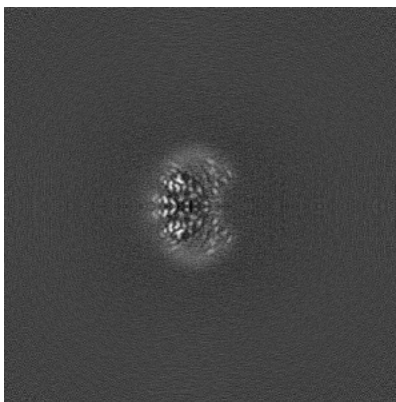


Z Index: 180

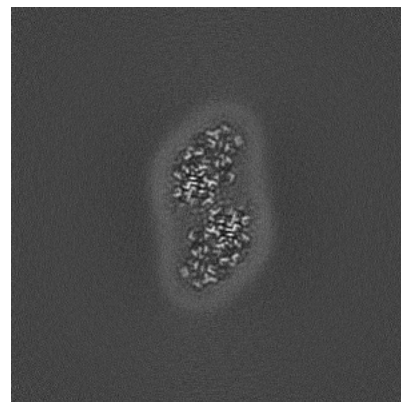
6.2.2 Raw map



X Index: 180



Y Index: 180

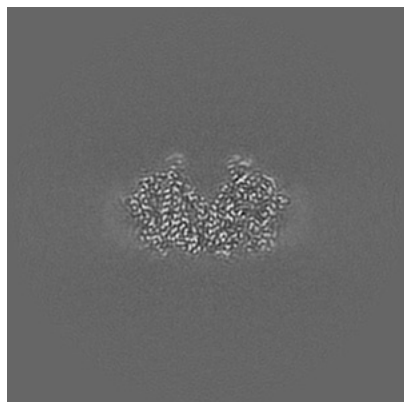


Z Index: 180

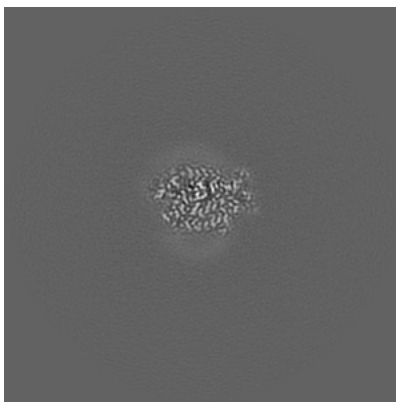
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

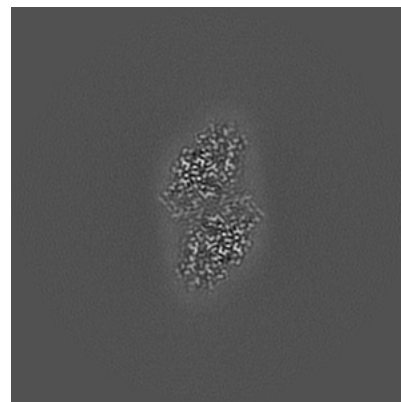
6.3.1 Primary map



X Index: 178

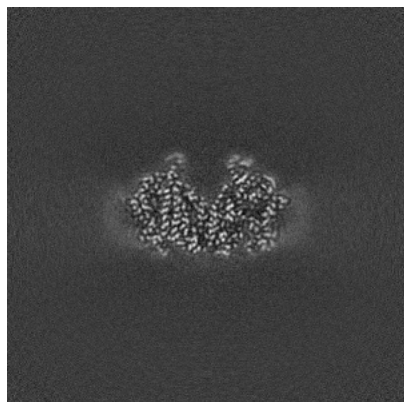


Y Index: 151

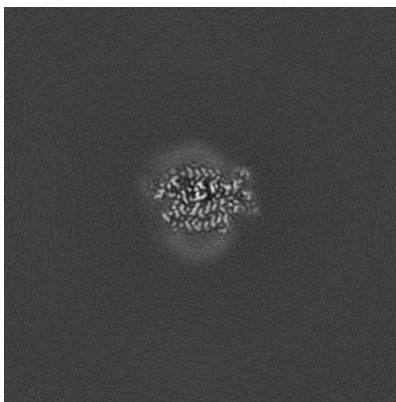


Z Index: 189

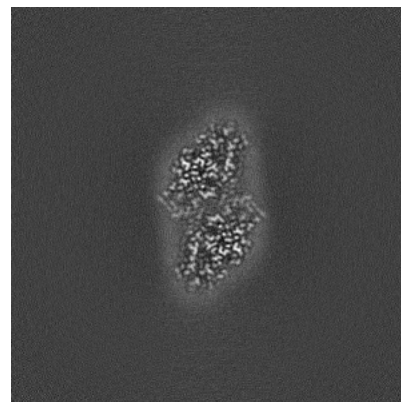
6.3.2 Raw map



X Index: 178



Y Index: 151

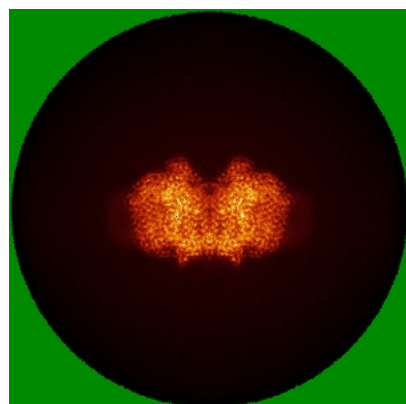


Z Index: 189

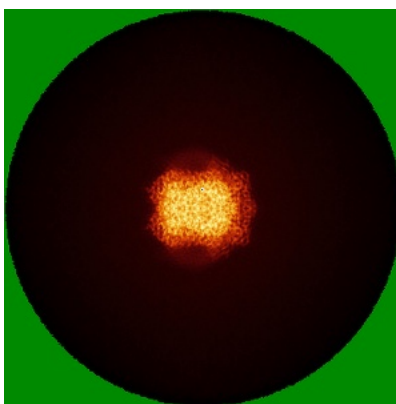
The images above show the largest variance slices of the map in three orthogonal directions.

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

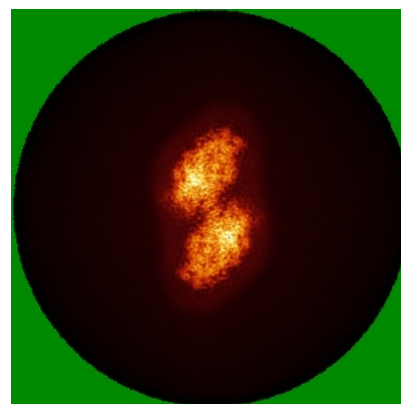
6.4.1 Primary map



X

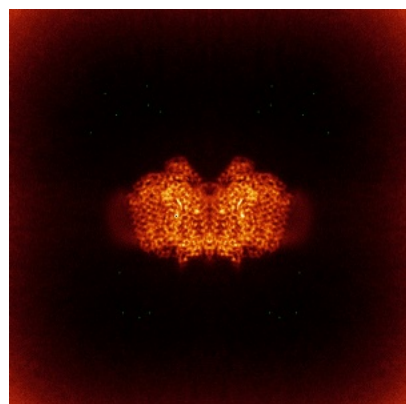


Y

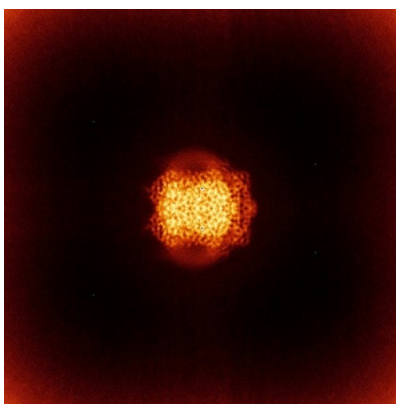


Z

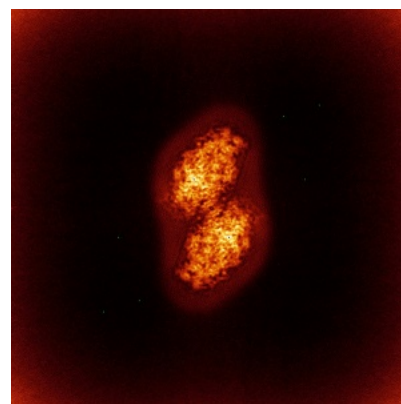
6.4.2 Raw map



X



Y

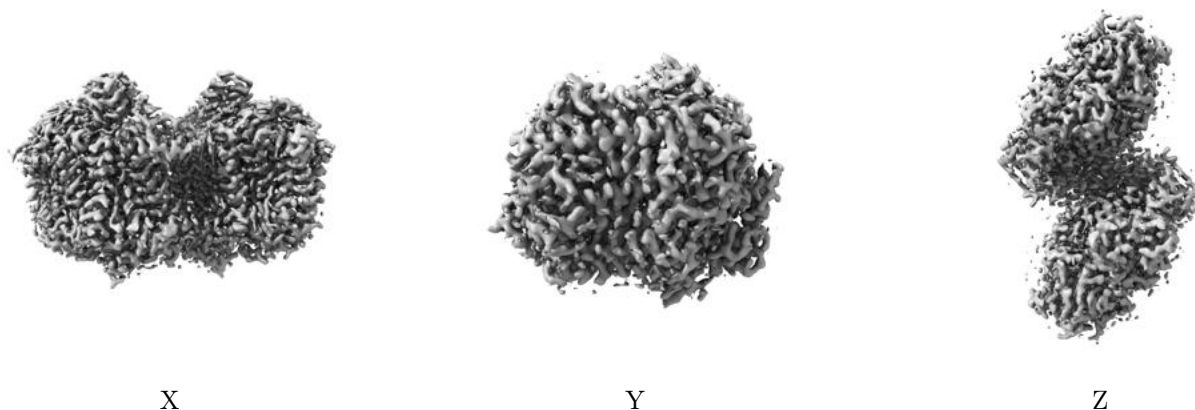


Z

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.

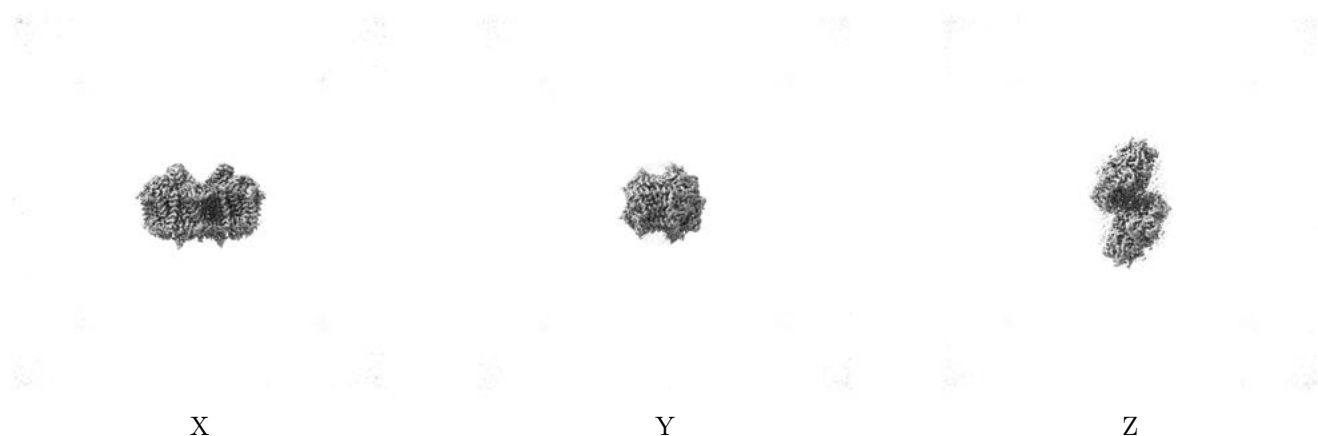
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0547. 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.

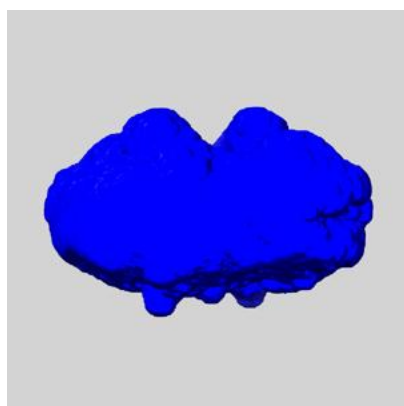
6.6 Mask visualisation [i](#)

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

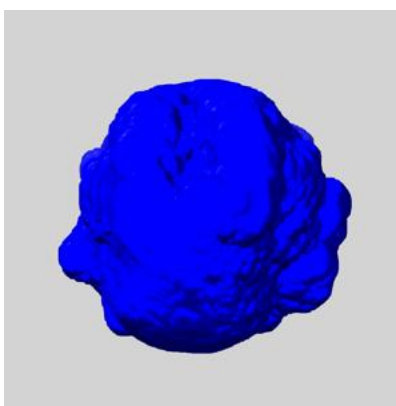
A mask typically either:

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

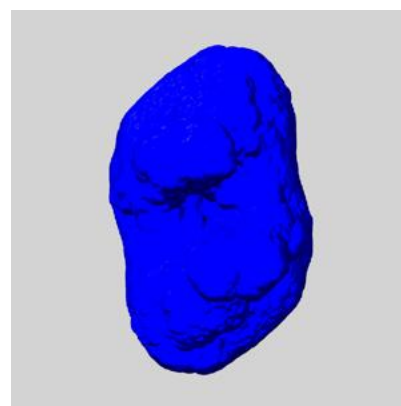
6.6.1 emd_54812_msk_1.map [i](#)



X



Y

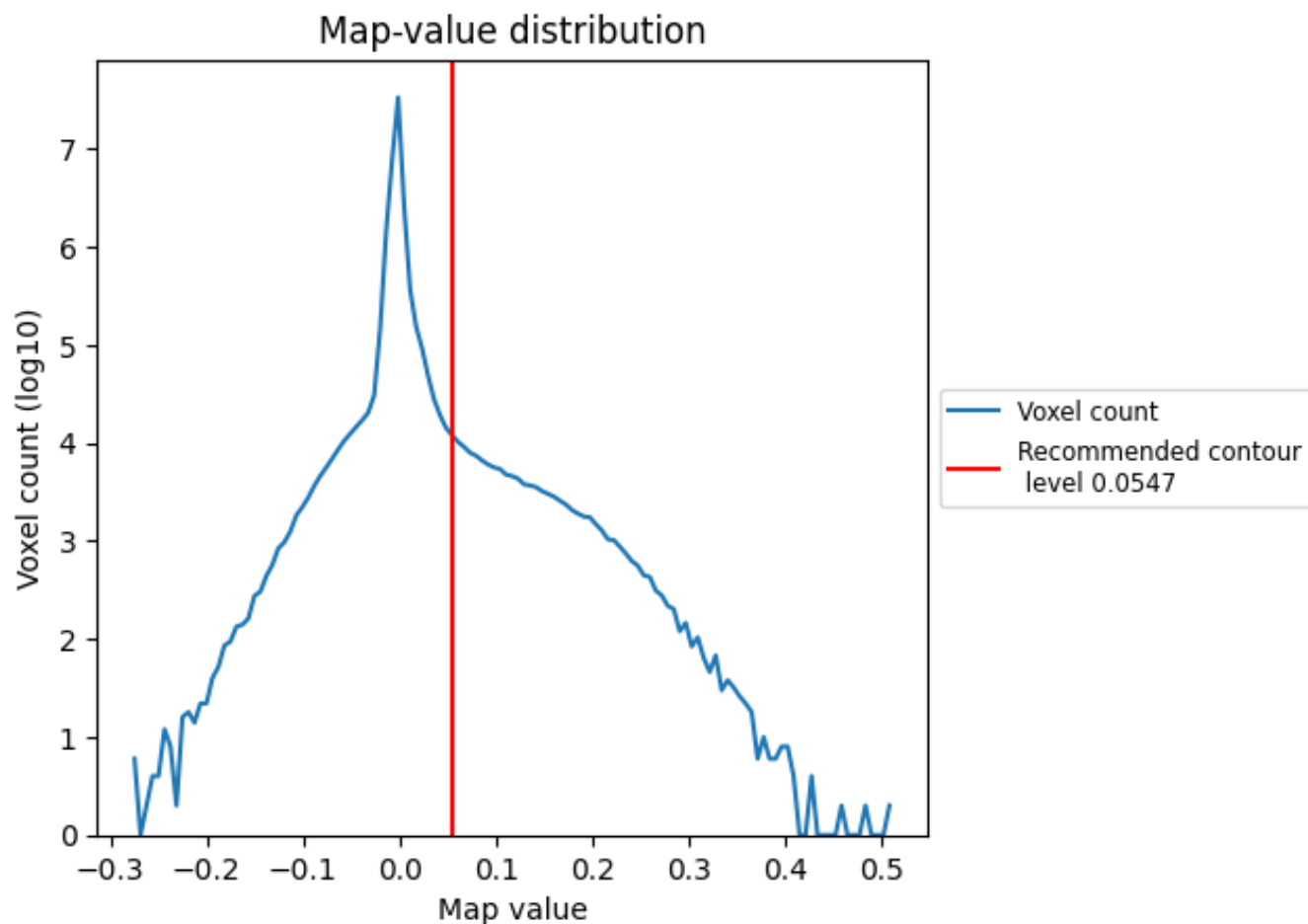


Z

7 Map analysis [i](#)

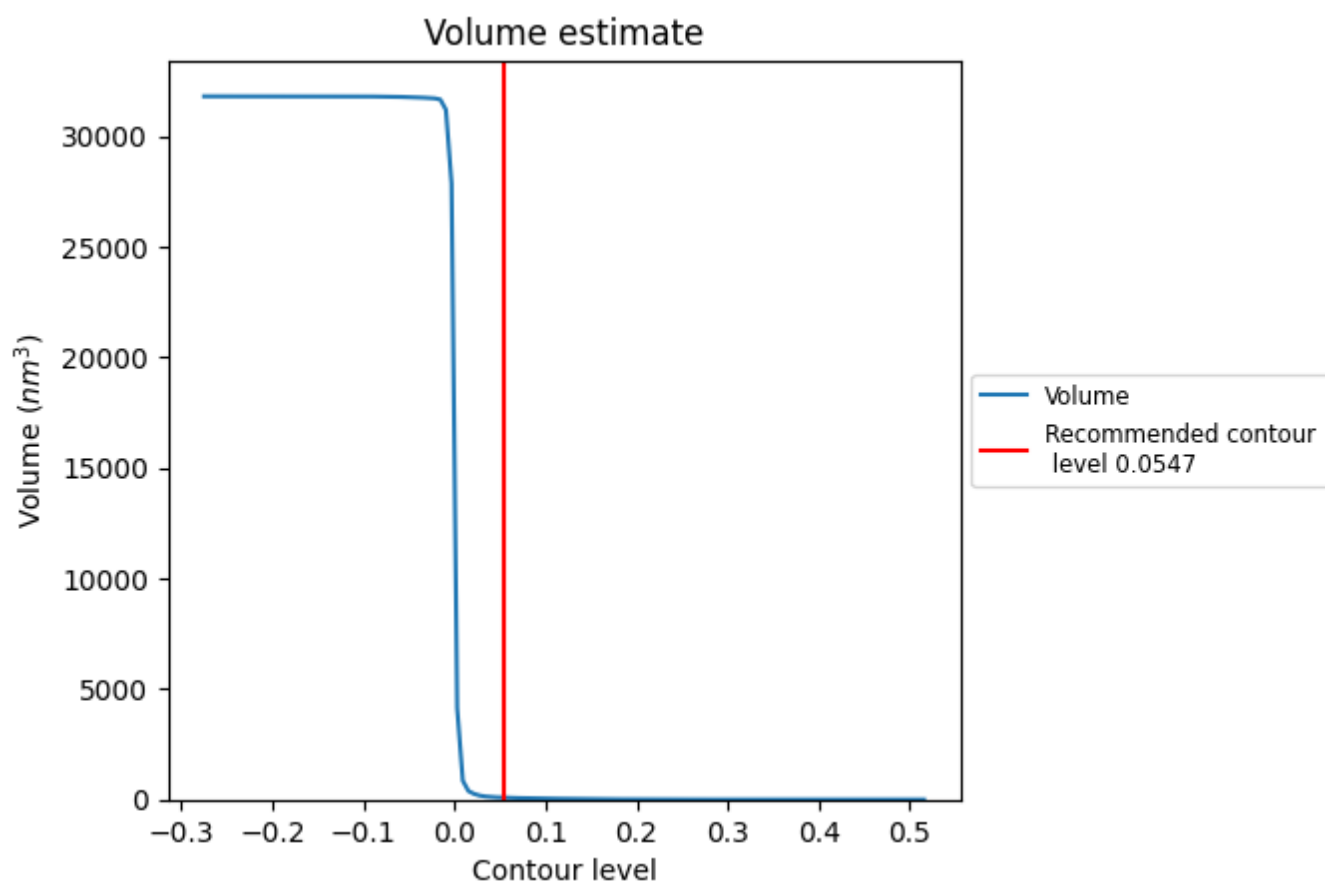
This section contains the results of statistical analysis of the map.

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.

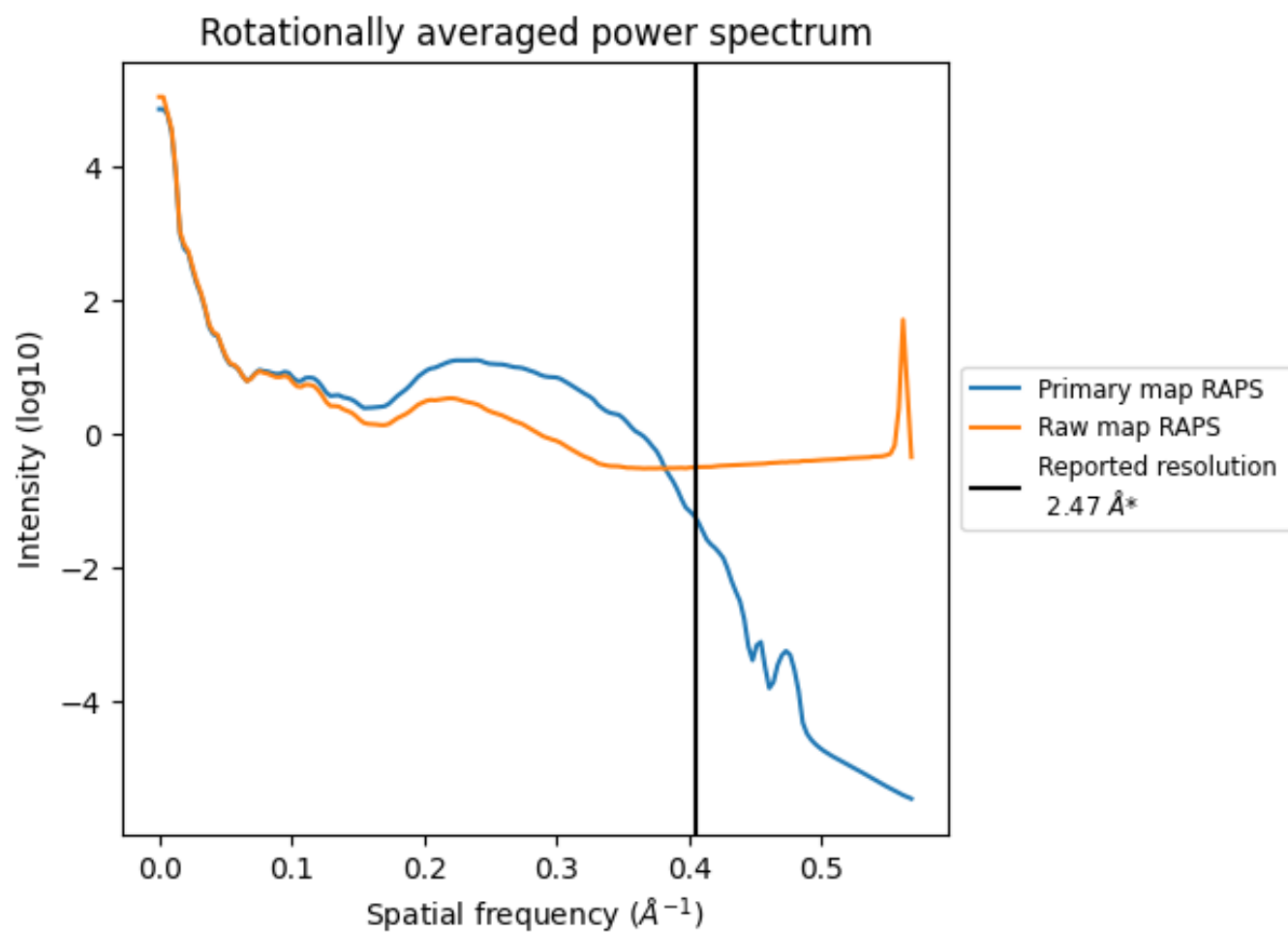
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 87 nm³; this corresponds to an approximate mass of 79 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 ⓘ

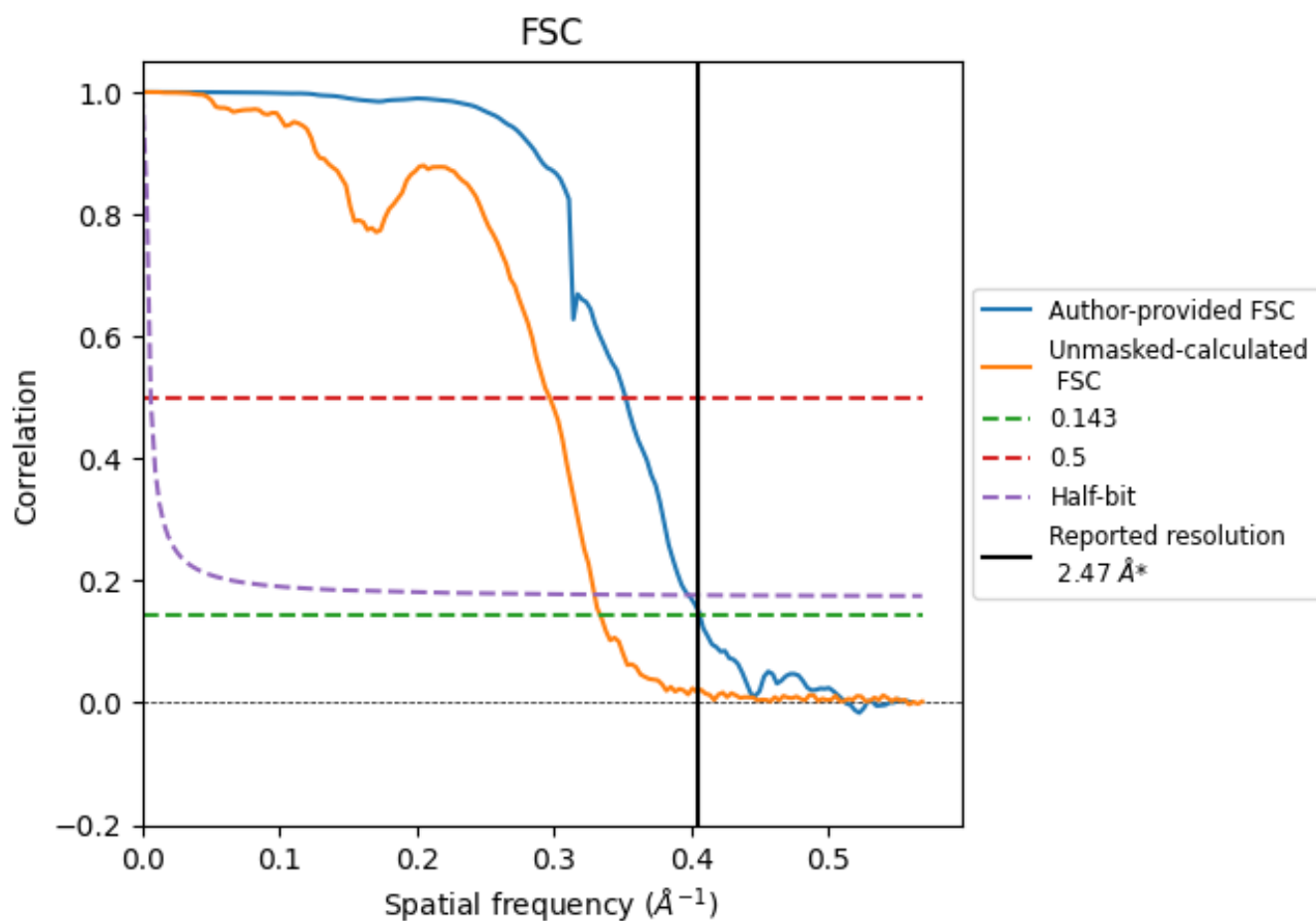


*Reported resolution corresponds to spatial frequency of 0.405 Å⁻¹

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 $0.405 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

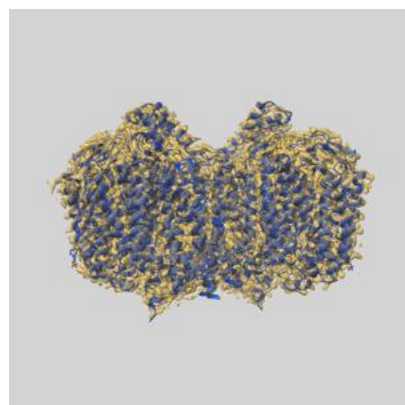
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.47	-	-
Author-provided FSC curve	2.46	2.84	2.51
Unmasked-calculated*	3.00	3.37	3.03

*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 3.00 differs from the reported value 2.47 by more than 10 %

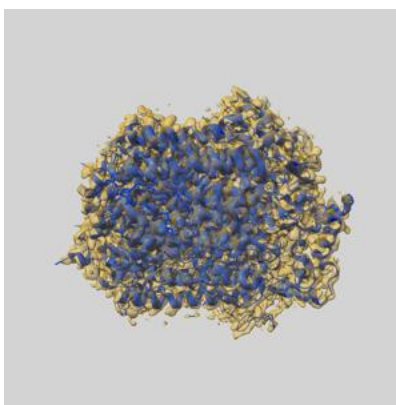
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54812 and PDB model 9SEJ. Per-residue inclusion information can be found in section [3](#) on page [10](#).

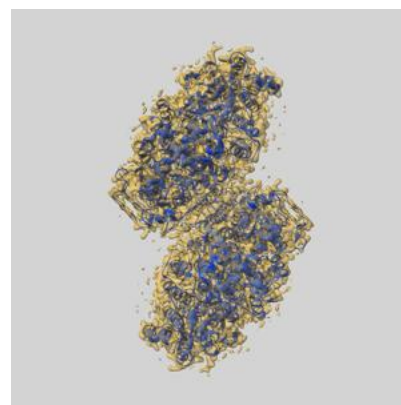
9.1 Map-model overlay [i](#)



X



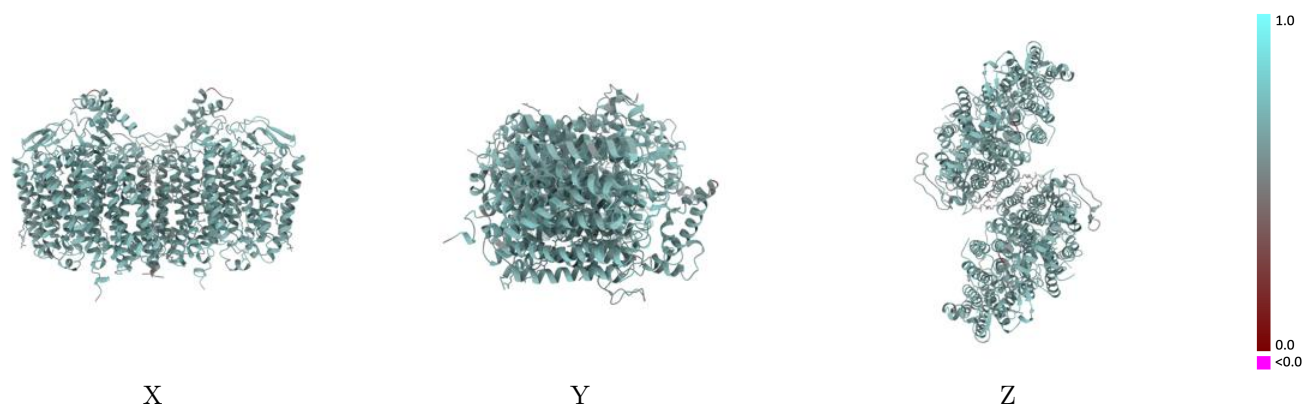
Y



Z

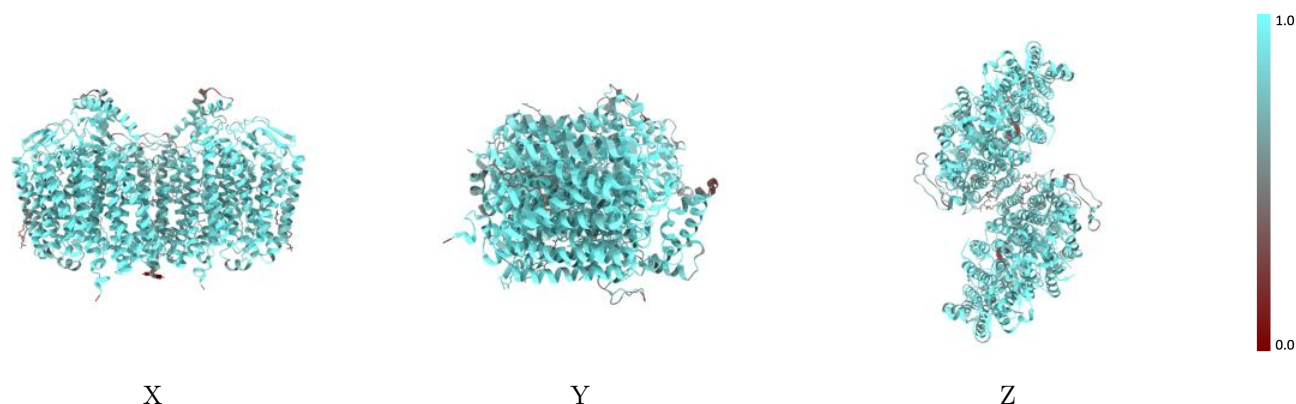
The images above show the 3D surface view of the map at the recommended contour level 0.0547 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



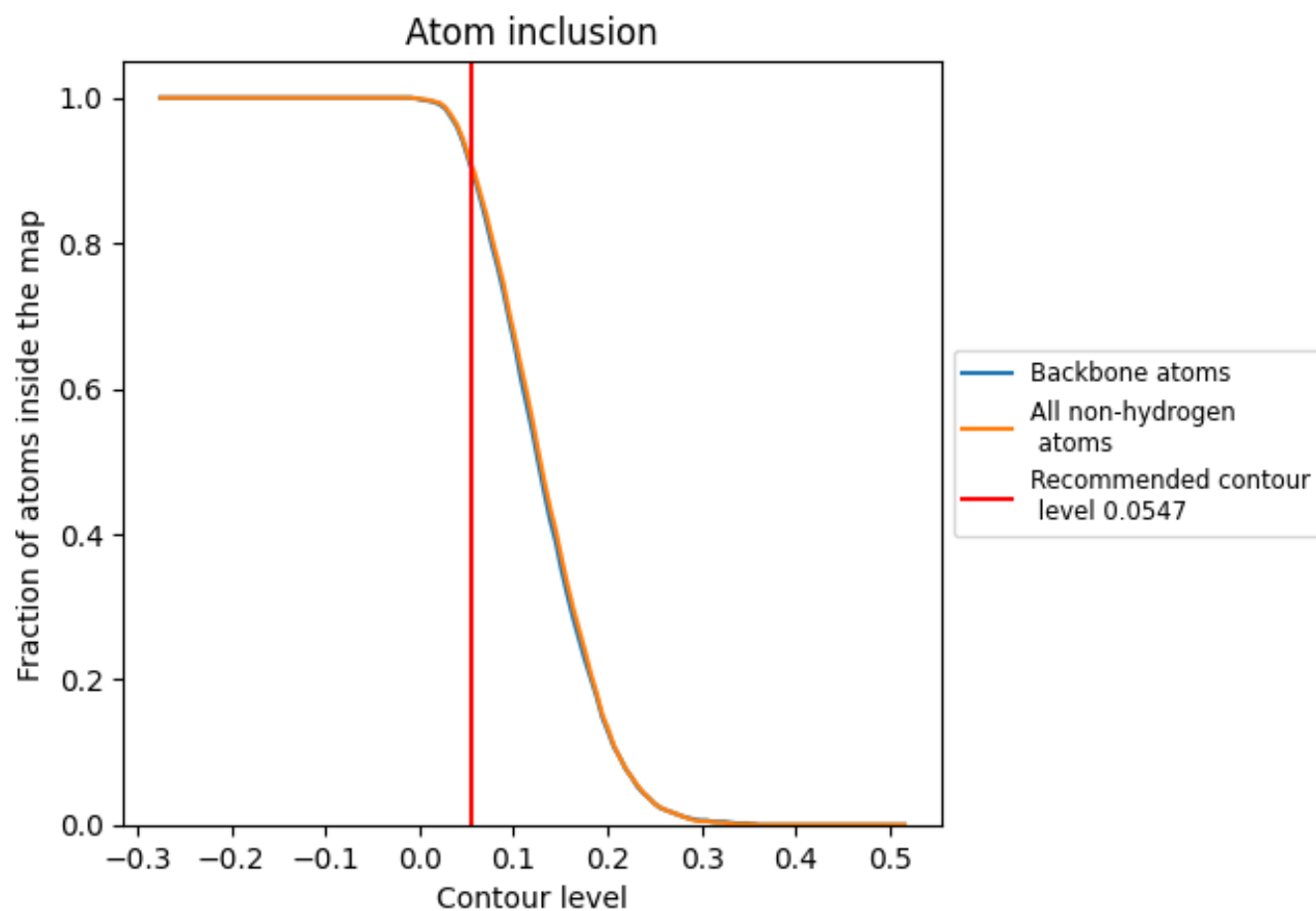
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0547).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 91% 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 (0.0547) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9100	0.6430
A	0.9070	0.6420
B	0.9170	0.6440
H	0.9240	0.6330
X	0.9260	0.6470
a	0.9090	0.6430
b	0.9180	0.6450
h	0.9190	0.6330
x	0.9300	0.6490

1.0

0.0

<0.0