



Full wwPDB EM Validation Report ⓘ

Jun 4, 2026 – 12:24 pm BST

PDB ID : 9SFV / pdb_00009sfv
EMDB ID : EMD-54866
Title : E.coli cytochrome bd-I dimer in the apo and MK bound closed state
Authors : van der Velden, T.T.; Kayastha, K.; Bruenle, S.; Jeuken, L.J.C.
Deposited on : 2025-08-21
Resolution : 2.61 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:

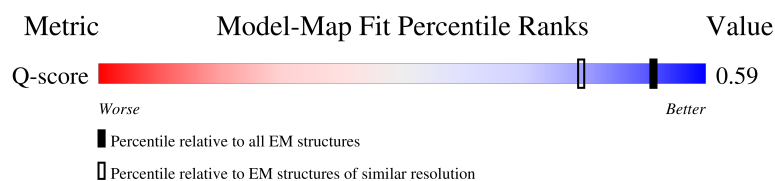
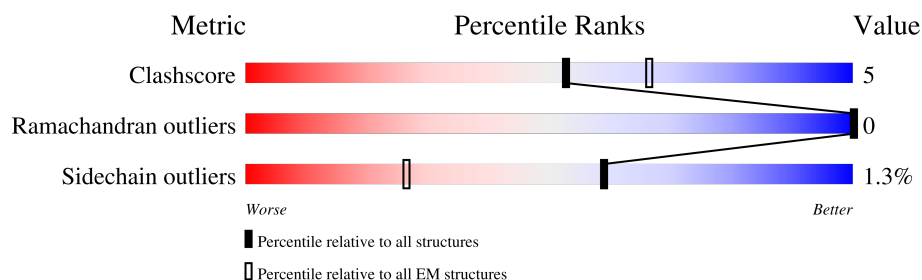
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

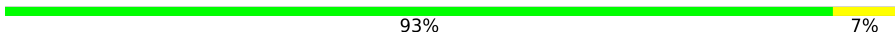
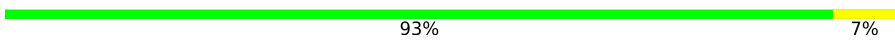
The reported resolution of this entry is 2.61 Å.

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	8735 (2.11 - 3.11)

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	B	379	
1	b	379	
2	H	29	
2	h	29	

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Mol	Chain	Length	Quality of chain
3	X	37	 73%8%19%
3	x	37	 70%11%19%
4	A	522	 80%9%11%
4	a	522	 88%10% ..

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
9	A1JN4	A	605	X	-	-	-
9	A1JN4	a	606	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 31070 atoms, of which 15662 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 2.

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

- Molecule 2 is a protein called Cytochrome bd-I ubiquinol oxidase CydH (Uncharacterized protein YnhF).

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

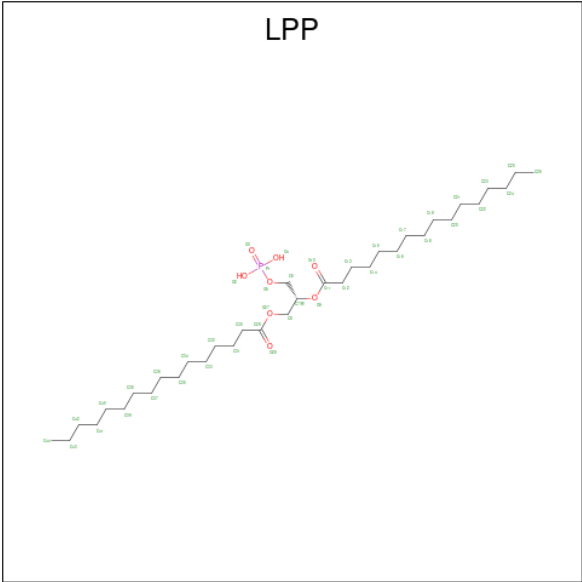
- Molecule 3 is a protein called Cytochrome bd-I ubiquinol oxidase subunit X.

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

- Molecule 4 is a protein called Cytochrome bd-I ubiquinol oxidase subunit 1.

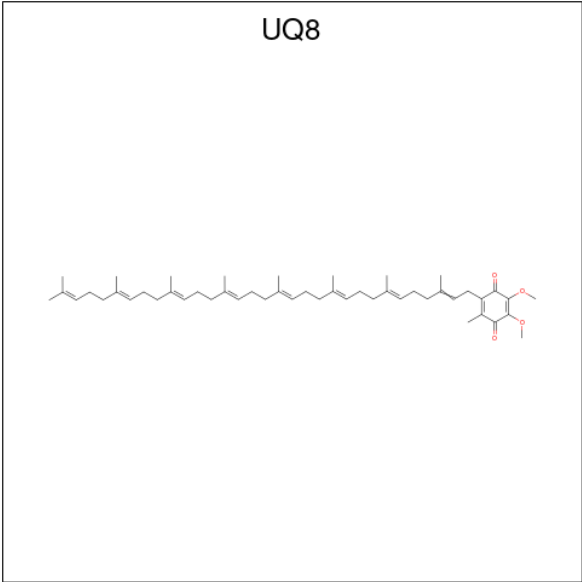
Mol	Chain	Residues	Atoms						AltConf	Trace
4	a	514	Total	C	H	N	O	S	0	0
			8116	2668	4068	649	706	25		
4	A	467	Total	C	H	N	O	S	0	0
			7399	2429	3717	593	636	24		

- Molecule 5 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: C₃₅H₆₉O₈P).



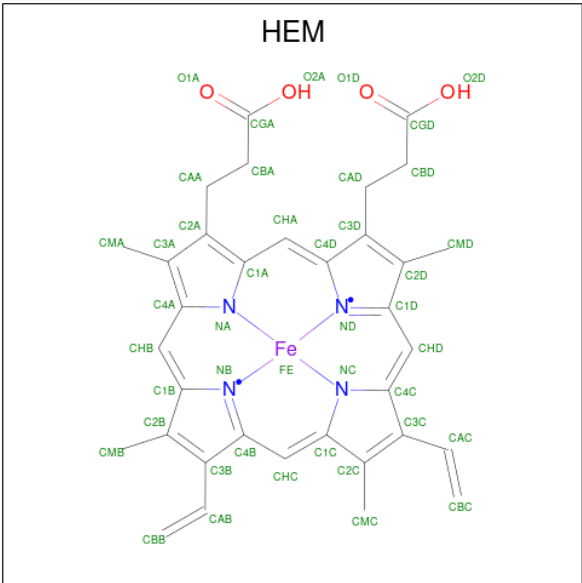
Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	H	O	P	0
			111	35	67	8	1	
5	X	1	Total	C	H	O	P	0
			111	35	67	8	1	
5	a	1	Total	C	H	O	P	0
			111	35	67	8	1	
5	b	1	Total	C	H	O	P	0
			111	35	67	8	1	
5	x	1	Total	C	H	O	P	0
			111	35	67	8	1	
5	A	1	Total	C	H	O	P	0
			111	35	67	8	1	

- Molecule 6 is Ubiquinone-8 (CCD ID: UQ8) (formula: C₄₉H₇₄O₄).



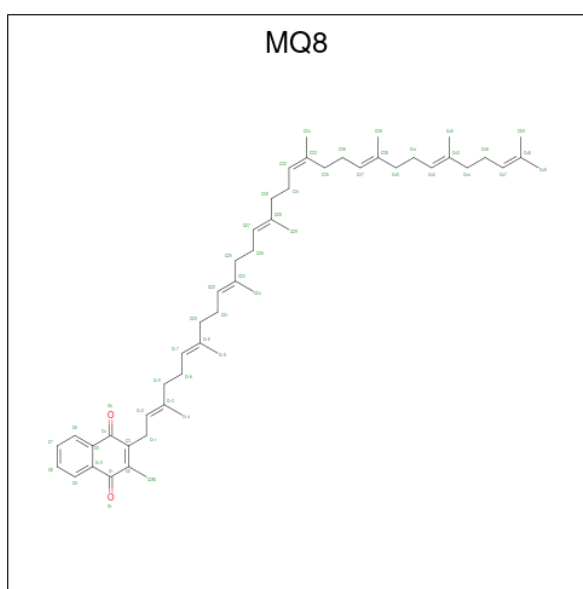
Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	H	O	0
			127	49	74	4	
6	a	1	Total	C	H	O	0
			127	49	74	4	
6	b	1	Total	C	H	O	0
			127	49	74	4	
6	A	1	Total	C	H	O	0
			127	49	74	4	

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



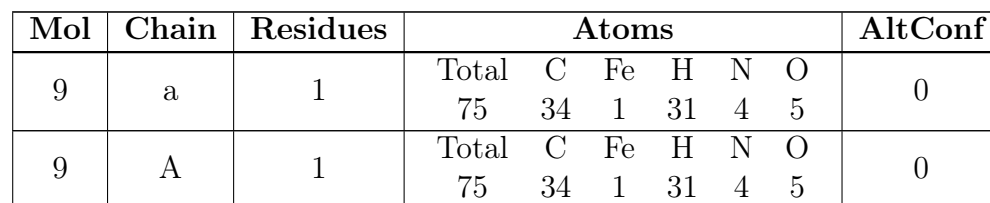
Mol	Chain	Residues	Atoms						AltConf
7	a	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
7	a	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
7	A	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
7	A	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 8 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
8	a	1	Total	C	H	O	0
			125	51	72	2	

- Molecule 9 is TRANS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: A1JN4) (formula: $C_{34}H_{36}FeN_4O_5$).



- OXY
- O1 O2

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

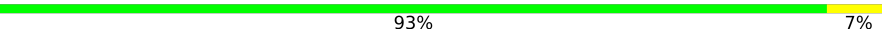
- Molecule 11 is water.

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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Cytochrome bd-I ubiquinol oxidase subunit 2

Chain B: 



- Molecule 1: Cytochrome bd-I ubiquinol oxidase subunit 2

Chain b: 



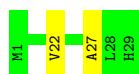
- Molecule 2: Cytochrome bd-I ubiquinol oxidase CydH (Uncharacterized protein YnhF)

Chain H: 



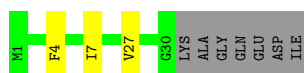
- Molecule 2: Cytochrome bd-I ubiquinol oxidase CydH (Uncharacterized protein YnhF)

Chain h: 



- Molecule 3: Cytochrome bd-I ubiquinol oxidase subunit X

Chain X: 



- Molecule 3: Cytochrome bd-I ubiquinol oxidase subunit X

Chain x:  70% 11% 19%



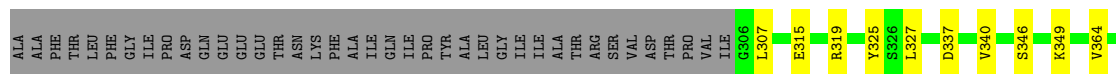
- Molecule 4: Cytochrome bd-I ubiquinol oxidase subunit 1

Chain a:  88% 10% ..



- Molecule 4: Cytochrome bd-I ubiquinol oxidase subunit 1

Chain A:  80% 9% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	152474	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	1.561	Depositor
Minimum map value	-0.985	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.0938	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LPP, UQ8, A1JN4, OXY, 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	B	0.17	0/3083	0.31	2/4212 (0.0%)
1	b	0.19	0/3083	0.33	2/4212 (0.0%)
2	H	0.13	0/210	0.22	0/286
2	h	0.14	0/211	0.22	0/286
3	X	0.17	0/239	0.24	0/326
3	x	0.17	0/239	0.18	0/326
4	A	0.19	0/3776	0.40	4/5112 (0.1%)
4	a	0.20	0/4154	0.27	0/5634
All	All	0.19	0/14995	0.33	8/20394 (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
4	A	0	1
4	a	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	47	ILE	CA-C-N	10.63	136.47	120.31
4	A	47	ILE	C-N-CA	10.63	136.47	120.31
4	A	503	SER	CA-C-N	10.49	136.26	120.31
4	A	503	SER	C-N-CA	10.49	136.26	120.31
1	b	174	VAL	CA-C-N	7.92	131.31	120.46
1	b	174	VAL	C-N-CA	7.92	131.31	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	VAL	CA-C-N	7.46	129.96	120.56
1	B	174	VAL	C-N-CA	7.46	129.96	120.56

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	449	GLN	Peptide
4	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	B	2996	3025	3025	19	0
1	b	2996	3025	3025	18	0
2	H	209	215	238	3	0
2	h	210	222	238	2	0
3	X	232	219	230	4	0
3	x	232	219	230	3	0
4	A	3682	3717	3714	35	0
4	a	4048	4068	4078	45	0
5	A	44	67	67	3	0
5	B	44	67	67	1	0
5	X	44	67	67	3	0
5	a	44	67	67	2	0
5	b	44	67	67	0	0
5	x	44	67	67	0	0
6	A	53	74	74	11	0
6	B	53	74	74	5	0
6	a	53	74	74	9	0
6	b	53	74	74	5	0
7	A	86	60	60	12	0
7	a	86	60	60	15	0
8	a	53	72	72	14	0
9	A	44	31	0	1	0
9	a	44	31	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	2	0	0	0	0
10	a	2	0	0	0	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	a	4	0	0	1	0
11	b	4	0	0	1	0
All	All	15408	15662	15668	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)
5:A:602:LPP:H442	5:A:602:LPP:H261	1.54	0.89
7:A:603:HEM:HBC2	7:A:603:HEM:HHD	1.60	0.82
1:b:45:GLU:OE2	1:b:199:ARG:NH2	2.12	0.82
7:a:603:HEM:HBC2	7:a:603:HEM:HHD	1.60	0.82
4:a:32:LEU:HD13	4:a:199:ILE:HD12	1.62	0.79
4:a:329:GLU:OE1	1:b:152:TYR:OH	1.99	0.79
7:A:601:HEM:HHD	7:A:601:HEM:HBC2	1.64	0.79
7:A:603:HEM:HHC	7:A:603:HEM:HBB2	1.65	0.76
4:A:187:THR:OG1	7:A:601:HEM:O1A	2.05	0.75
7:a:601:HEM:HBC2	7:a:601:HEM:HHD	1.69	0.74
4:a:296:ALA:HA	8:a:605:MQ8:H2M1	1.70	0.74
4:a:187:THR:OG1	7:a:601:HEM:O2A	2.06	0.73
7:a:603:HEM:HBB2	7:a:603:HEM:HHC	1.69	0.73
4:A:405:ALA:HB1	6:A:604:UQ8:H30A	1.71	0.73
7:a:601:HEM:O1A	11:a:701:HOH:O	2.09	0.70
6:A:604:UQ8:H20A	6:A:604:UQ8:H23	1.73	0.69
4:a:400:LEU:HD12	7:a:601:HEM:HBB1	1.74	0.69
4:A:5:VAL:HG22	4:A:463:ASN:HD21	1.59	0.67
4:A:17:MET:HG2	7:A:603:HEM:HBC1	1.76	0.67
7:A:603:HEM:HBA1	7:A:603:HEM:HHA	1.78	0.66
7:a:603:HEM:HHA	7:a:603:HEM:HBA1	1.77	0.66
7:a:601:HEM:HMB2	7:a:601:HEM:HBB2	1.80	0.64
4:a:29:MET:HE3	4:a:199:ILE:HD11	1.80	0.64
1:b:219:GLY:HA3	6:b:402:UQ8:H4MB	1.81	0.63
4:a:272:PHE:CE1	8:a:605:MQ8:H452	2.33	0.62
1:b:264:ILE:HD12	1:b:264:ILE:H	1.66	0.61
7:A:601:HEM:HBB2	7:A:601:HEM:HMB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:a:602:LPP:H261	5:a:602:LPP:H443	1.82	0.61
1:b:90:MET:CE	6:b:402:UQ8:H30B	2.31	0.60
4:a:48:TYR:OH	3:x:25:GLU:OE2	2.16	0.59
4:a:9:ARG:NH2	2:h:27:ALA:O	2.35	0.59
4:A:32:LEU:HD13	4:A:199:ILE:HD12	1.84	0.58
5:A:602:LPP:H442	5:A:602:LPP:C26	2.31	0.58
7:a:601:HEM:HBA1	7:a:601:HEM:HHA	1.84	0.58
4:A:108:SER:OG	9:A:605:A1JN4:O2A	2.22	0.57
4:a:35:ILE:O	4:a:39:VAL:HG23	2.04	0.57
4:A:197:MET:HE1	4:A:403:ILE:HG21	1.86	0.57
1:B:282:THR:HG21	1:B:294:PHE:HE2	1.69	0.57
4:a:265:ALA:HB1	4:a:266:PRO:HD2	1.87	0.56
1:b:84:SER:OG	11:b:501:HOH:O	2.18	0.54
4:a:197:MET:HE1	4:a:403:ILE:HG21	1.89	0.54
1:b:148:ASN:HB2	1:b:320:MET:HE3	1.90	0.54
7:A:601:HEM:HBB2	7:A:601:HEM:CMB	2.37	0.53
4:A:184:PHE:O	4:A:188:VAL:HG22	2.08	0.53
4:A:307:LEU:HD11	4:A:383:VAL:HG21	1.90	0.53
4:A:405:ALA:CB	6:A:604:UQ8:H30A	2.39	0.53
4:a:296:ALA:HA	8:a:605:MQ8:C2M	2.38	0.52
4:A:212:ASP:N	4:A:212:ASP:OD1	2.41	0.52
7:a:601:HEM:HBB2	7:a:601:HEM:CMB	2.39	0.52
1:B:231:VAL:HG11	1:B:235:MET:HE2	1.91	0.52
4:a:273:GLY:C	4:a:274:ILE:HD12	2.35	0.52
6:b:402:UQ8:O4	6:b:402:UQ8:H3MB	2.10	0.51
1:B:372:GLU:HA	1:B:372:GLU:OE1	2.11	0.51
6:b:402:UQ8:H3MB	6:b:402:UQ8:C4M	2.41	0.51
4:a:391:ARG:HA	8:a:605:MQ8:H293	1.92	0.51
4:A:62:ASN:OD1	5:A:602:LPP:H441	2.11	0.51
1:B:351:ILE:HD11	4:A:101:LEU:O	2.12	0.50
6:A:604:UQ8:H10B	6:A:604:UQ8:C13	2.41	0.50
4:a:272:PHE:HE1	8:a:605:MQ8:H452	1.75	0.50
6:a:604:UQ8:H10A	6:a:604:UQ8:C13	2.42	0.50
4:a:247:ASP:OD2	4:a:317:ARG:NH1	2.44	0.50
4:a:271:LEU:HD12	8:a:605:MQ8:C26	2.42	0.50
2:H:8:SER:OG	4:A:491:PHE:N	2.43	0.49
6:A:604:UQ8:C13	6:A:604:UQ8:C10	2.90	0.49
4:a:233:SER:HB2	4:a:237:LEU:HD12	1.95	0.49
4:a:309:GLU:O	4:a:309:GLU:OE1	2.31	0.48
7:a:603:HEM:HHA	7:a:603:HEM:CBA	2.43	0.48
1:B:320:MET:O	1:B:320:MET:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:38:PHE:CD1	1:b:38:PHE:N	2.78	0.48
3:x:4:PHE:O	3:x:7:ILE:HG22	2.13	0.48
4:a:265:ALA:HB1	4:a:266:PRO:CD	2.43	0.48
4:A:94:ALA:HB3	4:A:95:PRO:HD3	1.95	0.48
4:a:257:GLU:OE2	4:a:270:THR:OG1	2.31	0.48
6:a:604:UQ8:H15A	6:a:604:UQ8:C18	2.44	0.48
4:A:9:ARG:CD	4:A:459:THR:HG21	2.44	0.48
4:A:307:LEU:CD1	4:A:383:VAL:HG21	2.44	0.48
4:A:448:ARG:O	4:A:448:ARG:CG	2.63	0.47
4:a:17:MET:HE1	2:h:22:VAL:CG1	2.45	0.47
7:A:603:HEM:HHA	7:A:603:HEM:CBA	2.43	0.47
3:X:7:ILE:HD11	5:X:101:LPP:C26	2.45	0.47
4:A:84:TYR:HB2	4:A:462:ALA:HB1	1.97	0.46
7:A:601:HEM:HHA	7:A:601:HEM:HBA1	1.97	0.46
4:a:273:GLY:N	4:a:387:TYR:OH	2.49	0.46
1:B:149:VAL:HG13	1:B:153:LEU:HA	1.97	0.46
1:b:149:VAL:HG13	1:b:153:LEU:HA	1.98	0.46
4:a:84:TYR:HB2	4:a:462:ALA:HB1	1.98	0.46
4:a:288:ILE:N	4:a:288:ILE:HD12	2.30	0.46
4:a:394:VAL:HB	8:a:605:MQ8:H292	1.97	0.46
1:B:24:VAL:HG21	5:B:401:LPP:H263	1.98	0.46
1:b:90:MET:HE1	6:b:402:UQ8:H30B	1.98	0.45
1:b:110:ILE:HG22	1:b:112:GLU:H	1.81	0.45
1:B:362:MET:HE1	4:A:117:GLY:HA2	1.98	0.45
4:A:142:LEU:O	4:A:146:VAL:HG23	2.17	0.45
3:X:4:PHE:O	3:X:7:ILE:HG22	2.17	0.45
4:a:400:LEU:HD12	7:a:601:HEM:CBB	2.45	0.45
4:a:158:ASP:C	4:a:158:ASP:OD1	2.60	0.45
1:B:29:ASP:OD2	1:B:57:TRP:HA	2.17	0.45
1:B:219:GLY:HA3	6:B:402:UQ8:H4MB	1.97	0.45
3:X:7:ILE:HD11	5:X:101:LPP:H263	1.99	0.44
4:a:287:GLN:C	4:a:288:ILE:HD12	2.42	0.44
7:A:601:HEM:HBC2	7:A:601:HEM:CHD	2.40	0.44
4:A:197:MET:HE1	4:A:403:ILE:CG2	2.46	0.44
6:a:604:UQ8:C13	6:a:604:UQ8:C10	2.96	0.44
4:a:82:SER:OG	4:a:464:SER:OG	2.14	0.44
4:a:269:PHE:CE2	8:a:605:MQ8:H251	2.53	0.44
6:a:604:UQ8:C23	6:a:604:UQ8:H20B	2.48	0.44
1:b:212:LEU:HD13	1:b:273:VAL:O	2.18	0.44
1:B:134:ILE:HG21	6:B:402:UQ8:H21	2.00	0.44
6:a:604:UQ8:O5	6:a:604:UQ8:H4MA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:346:SER:O	4:A:349:LYS:NZ	2.48	0.44
6:A:604:UQ8:H12	6:A:604:UQ8:H15	1.75	0.44
1:B:150:ASP:OD1	1:B:150:ASP:C	2.60	0.44
6:a:604:UQ8:H35	6:a:604:UQ8:H32	1.80	0.43
2:H:18:LEU:O	2:H:22:VAL:HG23	2.18	0.43
1:b:37:ARG:CZ	1:b:37:ARG:HB3	2.48	0.43
4:a:274:ILE:HD13	4:a:284:PHE:CZ	2.53	0.43
8:a:605:MQ8:H493	8:a:605:MQ8:H441	2.01	0.43
4:a:189:ALA:O	4:a:193:VAL:HG23	2.18	0.43
1:b:231:VAL:HG11	1:b:235:MET:HG3	2.00	0.43
1:B:361:LYS:HE3	4:A:121:LEU:HD23	2.01	0.43
4:a:265:ALA:O	4:a:266:PRO:C	2.61	0.43
4:A:315:GLU:CD	4:A:319:ARG:HE	2.27	0.43
2:H:16:LEU:O	2:H:20:VAL:HG23	2.18	0.43
1:b:255:TRP:HA	1:b:255:TRP:CE3	2.54	0.43
4:a:296:ALA:HB2	8:a:605:MQ8:H142	1.99	0.43
6:A:604:UQ8:H15A	6:A:604:UQ8:H18	2.00	0.43
4:A:325:TYR:CE2	4:A:364:VAL:HG21	2.53	0.43
4:a:272:PHE:CZ	8:a:605:MQ8:H452	2.53	0.43
4:a:13:ALA:O	4:a:17:MET:HG3	2.19	0.42
4:A:337:ASP:O	4:A:340:VAL:HG22	2.19	0.42
4:a:187:THR:O	4:a:190:SER:OG	2.32	0.42
4:a:430:ILE:O	4:a:433:PRO:HD2	2.20	0.42
4:A:315:GLU:OE1	4:A:315:GLU:C	2.63	0.42
1:B:23:ALA:HB2	6:B:402:UQ8:C20	2.50	0.42
6:A:604:UQ8:O5	6:A:604:UQ8:H4MA	2.19	0.42
1:B:2:ILE:HG22	1:B:3:ASP:N	2.34	0.42
1:B:166:ASN:O	1:B:167:PRO:C	2.63	0.42
7:a:603:HEM:HBA1	7:a:603:HEM:CHA	2.47	0.42
6:a:604:UQ8:H30	6:a:604:UQ8:H27	1.81	0.41
4:a:158:ASP:OD1	4:a:158:ASP:O	2.38	0.41
1:b:275:LEU:N	1:b:276:PRO:HD2	2.35	0.41
4:a:240:GLU:OE2	4:a:240:GLU:N	2.53	0.41
4:a:81:TRP:CZ2	7:a:603:HEM:HBA2	2.55	0.41
1:B:232:LYS:HD3	1:B:249:VAL:HG22	2.01	0.41
3:X:27:VAL:HG11	4:A:414:ASN:ND2	2.36	0.41
7:a:603:HEM:HHC	7:a:603:HEM:CBB	2.44	0.41
8:a:605:MQ8:H262	8:a:605:MQ8:H241	1.87	0.41
4:a:398:PHE:CE2	8:a:605:MQ8:H243	2.55	0.41
1:b:188:LEU:O	1:b:192:THR:OG1	2.32	0.41
1:B:282:THR:HG21	1:B:294:PHE:CE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:402:UQ8:H42A	6:B:402:UQ8:H40B	1.80	0.41
7:A:603:HEM:HHC	7:A:603:HEM:CBB	2.43	0.41
1:B:16:GLY:HA3	6:B:402:UQ8:H46B	2.02	0.41
4:A:51:MET:HG3	4:A:215:PHE:CE2	2.56	0.41
4:A:188:VAL:HG23	6:A:604:UQ8:H3M	2.03	0.41
4:A:315:GLU:OE1	4:A:315:GLU:O	2.39	0.41
4:A:189:ALA:HB2	6:A:604:UQ8:C3M	2.52	0.40
6:a:604:UQ8:H8	6:a:604:UQ8:C1M	2.51	0.40
8:a:605:MQ8:O4	8:a:605:MQ8:C12	2.69	0.40
5:X:101:LPP:H381	6:a:604:UQ8:H15B	2.04	0.40
4:a:218:ARG:NH2	3:x:28:GLU:OE1	2.54	0.40
5:a:602:LPP:H261	5:a:602:LPP:C44	2.50	0.40
1:b:255:TRP:HA	1:b:255:TRP:HE3	1.86	0.40
4:A:5:VAL:HG22	4:A:463:ASN:ND2	2.32	0.40
4:A:405:ALA:HB1	6:A:604:UQ8:C30	2.47	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	B	377/379 (100%)	368 (98%)	9 (2%)	0	100	100
1	b	377/379 (100%)	371 (98%)	6 (2%)	0	100	100
2	H	27/29 (93%)	27 (100%)	0	0	100	100
2	h	27/29 (93%)	27 (100%)	0	0	100	100
3	X	28/37 (76%)	28 (100%)	0	0	100	100
3	x	28/37 (76%)	28 (100%)	0	0	100	100
4	A	463/522 (89%)	452 (98%)	11 (2%)	0	100	100
4	a	512/522 (98%)	498 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1839/1934 (95%)	1799 (98%)	40 (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	B	313/313 (100%)	312 (100%)	1 (0%)	86	94
1	b	313/313 (100%)	309 (99%)	4 (1%)	61	81
2	H	24/24 (100%)	23 (96%)	1 (4%)	26	50
2	h	24/24 (100%)	24 (100%)	0	100	100
3	X	23/28 (82%)	23 (100%)	0	100	100
3	x	23/28 (82%)	23 (100%)	0	100	100
4	A	380/426 (89%)	375 (99%)	5 (1%)	61	81
4	a	419/426 (98%)	410 (98%)	9 (2%)	47	72
All	All	1519/1582 (96%)	1499 (99%)	20 (1%)	59	81

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	241	SER
2	H	4	ASP
4	a	82	SER
4	a	86	HIS
4	a	234	VAL
4	a	270	THR
4	a	271	LEU
4	a	326	SER
4	a	346	SER
4	a	361	THR
4	a	502	SER
1	b	17	VAL

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Mol	Chain	Res	Type
1	b	45	GLU
1	b	211	THR
1	b	255	TRP
4	A	172	SER
4	A	212	ASP
4	A	253	LEU
4	A	327	LEU
4	A	502	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	143	GLN
3	X	26	HIS
4	a	11	GLN
4	a	76	GLN
4	a	330	GLN
4	a	510	HIS
1	b	143	GLN
1	b	197	HIS
1	b	242	ASN
1	b	258	ASN
1	b	261	ASN
1	b	376	HIS
4	A	86	HIS
4	A	314	HIS
4	A	463	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

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$
9	A1JN4	a	606	4	46,52,52	2.90	16 (34%)	62,89,89	4.63	38 (61%)
5	LPP	b	401	-	43,43,43	1.08	2 (4%)	47,48,48	1.10	2 (4%)
5	LPP	x	101	-	43,43,43	1.09	2 (4%)	47,48,48	1.12	2 (4%)
7	HEM	A	601	4	50,50,50	1.36	6 (12%)	66,82,82	1.27	6 (9%)
7	HEM	a	601	4	50,50,50	1.36	6 (12%)	66,82,82	1.31	7 (10%)
10	OXY	A	606	9	1,1,1	0.15	0	-		
5	LPP	A	602	-	43,43,43	1.08	2 (4%)	47,48,48	1.12	2 (4%)
6	UQ8	B	402	-	53,53,53	2.27	18 (33%)	64,67,67	4.12	26 (40%)
7	HEM	A	603	4	50,50,50	1.39	8 (16%)	66,82,82	1.27	7 (10%)
5	LPP	X	101	-	43,43,43	1.10	2 (4%)	47,48,48	1.04	2 (4%)
10	OXY	a	607	-	1,1,1	0.16	0	-		
6	UQ8	A	604	-	53,53,53	1.18	2 (3%)	64,67,67	1.58	13 (20%)
6	UQ8	b	402	-	53,53,53	2.25	15 (28%)	64,67,67	4.13	25 (39%)
6	UQ8	a	604	-	53,53,53	1.20	2 (3%)	64,67,67	1.50	15 (23%)
5	LPP	B	401	-	43,43,43	1.11	2 (4%)	47,48,48	1.15	2 (4%)
8	MQ8	a	605	-	54,54,54	1.24	2 (3%)	66,69,69	1.53	16 (24%)
9	A1JN4	A	605	10,4	46,52,52	2.90	16 (34%)	62,89,89	4.61	37 (59%)
7	HEM	a	603	4	50,50,50	1.40	7 (14%)	66,82,82	1.28	8 (12%)
5	LPP	a	602	-	43,43,43	1.06	2 (4%)	47,48,48	1.19	2 (4%)

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	A1JN4	a	606	4	1/1/12/12	3/9/89/89	0/1/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	UQ8	A	604	-	-	13/51/75/75	0/1/1/1
6	UQ8	b	402	-	-	12/51/75/75	0/1/1/1
5	LPP	b	401	-	-	13/45/45/45	-
5	LPP	B	401	-	-	18/45/45/45	-
6	UQ8	a	604	-	-	14/51/75/75	0/1/1/1
7	HEM	a	603	4	-	4/14/54/54	-
5	LPP	A	602	-	-	18/45/45/45	-
6	UQ8	B	402	-	-	6/51/75/75	0/1/1/1
7	HEM	A	603	4	-	6/14/54/54	-
5	LPP	x	101	-	-	17/45/45/45	-
7	HEM	A	601	4	-	5/14/54/54	-
5	LPP	a	602	-	-	19/45/45/45	-
5	LPP	X	101	-	-	17/45/45/45	-
8	MQ8	a	605	-	-	10/47/67/67	0/2/2/2
9	A1JN4	A	605	10,4	1/1/12/12	3/9/89/89	0/1/9/9
7	HEM	a	601	4	-	7/14/54/54	-

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	606	A1JN4	C3D-C2D	-11.79	1.25	1.55
9	A	605	A1JN4	C3D-C2D	-11.79	1.25	1.55
6	b	402	UQ8	C6-C1	10.09	1.53	1.35
6	B	402	UQ8	C6-C1	10.00	1.53	1.35
6	a	604	UQ8	C6-C1	7.57	1.49	1.35
6	A	604	UQ8	C6-C1	7.45	1.48	1.35
8	a	605	MQ8	C3-C2	7.41	1.48	1.35
9	A	605	A1JN4	O1D-C3D	6.79	1.57	1.46
9	a	606	A1JN4	O1D-C3D	6.72	1.57	1.46
9	a	606	A1JN4	CBB-CAB	-5.69	1.26	1.51
9	A	605	A1JN4	CBB-CAB	-5.68	1.26	1.51
9	a	606	A1JN4	CBC-CAC	-5.51	1.26	1.51
9	A	605	A1JN4	CBC-CAC	-5.51	1.26	1.51
9	A	605	A1JN4	OND-C2D	4.39	1.51	1.42
6	B	402	UQ8	C4-C3	4.32	1.53	1.36
9	a	606	A1JN4	OND-C2D	4.31	1.51	1.42
8	a	605	MQ8	C10-C5	4.27	1.47	1.40
6	b	402	UQ8	C4-C3	4.26	1.53	1.36
9	a	606	A1JN4	CBD-CGD	-3.70	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	605	A1JN4	CBD-CGD	-3.62	1.42	1.50
9	A	605	A1JN4	O1D-CGD	-3.48	1.30	1.35
9	a	606	A1JN4	O1D-CGD	-3.48	1.30	1.35
6	B	402	UQ8	C7-C8	3.45	1.55	1.50
7	A	601	HEM	FE-NC	3.39	2.06	1.95
7	a	601	HEM	FE-NA	3.36	2.06	1.95
5	B	401	LPP	O27-C29	3.32	1.43	1.33
7	a	601	HEM	FE-NC	3.29	2.06	1.95
7	a	603	HEM	FE-NC	3.27	2.06	1.95
5	X	101	LPP	O27-C29	3.25	1.42	1.33
7	A	603	HEM	FE-NA	3.22	2.06	1.95
7	a	603	HEM	FE-NA	3.22	2.06	1.95
6	b	402	UQ8	C7-C8	3.19	1.55	1.50
5	x	101	LPP	O27-C29	3.18	1.42	1.33
5	B	401	LPP	O9-C11	3.18	1.43	1.34
9	a	606	A1JN4	C1B-NB	-3.17	1.33	1.39
7	A	603	HEM	FE-NC	3.12	2.05	1.95
5	b	401	LPP	O9-C11	3.12	1.43	1.34
9	A	605	A1JN4	CAD-C3D	3.11	1.59	1.53
9	a	606	A1JN4	CAD-C3D	3.10	1.59	1.53
5	b	401	LPP	O27-C29	3.10	1.42	1.33
5	a	602	LPP	O27-C29	3.09	1.42	1.33
5	A	602	LPP	O9-C11	3.05	1.42	1.34
5	A	602	LPP	O27-C29	3.05	1.42	1.33
7	A	601	HEM	FE-NA	3.05	2.05	1.95
9	A	605	A1JN4	C1B-NB	-3.04	1.33	1.39
5	a	602	LPP	O9-C11	3.04	1.42	1.34
5	X	101	LPP	O9-C11	3.04	1.42	1.34
6	A	604	UQ8	C4-C3	3.01	1.48	1.36
5	x	101	LPP	O9-C11	3.00	1.42	1.34
7	a	603	HEM	FE-NB	2.89	2.03	1.94
6	a	604	UQ8	C4-C3	2.83	1.47	1.36
7	A	601	HEM	CAC-C3C	2.80	1.55	1.47
6	B	402	UQ8	C11-C9	2.79	1.57	1.51
6	b	402	UQ8	C11-C9	2.78	1.57	1.51
6	b	402	UQ8	C21-C19	2.73	1.57	1.51
7	a	601	HEM	CAC-C3C	2.70	1.54	1.47
7	A	601	HEM	FE-ND	2.70	2.03	1.94
7	a	601	HEM	FE-NB	2.68	2.03	1.94
7	A	603	HEM	FE-NB	2.64	2.03	1.94
7	a	603	HEM	CAB-C3B	2.64	1.54	1.47
6	B	402	UQ8	C16-C14	2.63	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	601	HEM	FE-NB	2.62	2.02	1.94
7	A	603	HEM	FE-ND	2.62	2.02	1.94
6	B	402	UQ8	C31-C29	2.61	1.56	1.51
7	a	603	HEM	CAC-C3C	2.56	1.54	1.47
7	a	601	HEM	CAB-C3B	2.55	1.54	1.47
7	A	603	HEM	CAB-C3B	2.54	1.54	1.47
7	A	601	HEM	CAB-C3B	2.53	1.54	1.47
7	A	603	HEM	CAC-C3C	2.53	1.54	1.47
7	a	603	HEM	FE-ND	2.53	2.02	1.94
6	B	402	UQ8	C26-C24	2.51	1.56	1.51
6	b	402	UQ8	C26-C24	2.50	1.56	1.51
6	B	402	UQ8	C7-C6	2.47	1.55	1.51
7	a	601	HEM	FE-ND	2.44	2.02	1.94
6	B	402	UQ8	C6-C5	2.42	1.53	1.46
6	b	402	UQ8	C6-C5	2.42	1.53	1.46
9	A	605	A1JN4	CBA-CAA	2.41	1.59	1.52
9	a	606	A1JN4	C4C-NC	-2.40	1.35	1.39
9	A	605	A1JN4	CMC-C2C	2.39	1.55	1.50
6	b	402	UQ8	C31-C29	2.38	1.56	1.51
6	b	402	UQ8	C7-C6	2.37	1.55	1.51
9	a	606	A1JN4	CBA-CAA	2.36	1.59	1.52
6	b	402	UQ8	C16-C14	2.35	1.56	1.51
6	B	402	UQ8	C21-C19	2.30	1.56	1.51
9	A	605	A1JN4	C4C-NC	-2.30	1.35	1.39
9	a	606	A1JN4	CMC-C2C	2.30	1.55	1.50
9	A	605	A1JN4	C2A-C3A	-2.30	1.32	1.38
9	a	606	A1JN4	C4A-C3A	2.29	1.48	1.43
6	b	402	UQ8	C36-C34	2.24	1.55	1.51
9	A	605	A1JN4	CMB-C2B	2.22	1.55	1.50
9	a	606	A1JN4	CMB-C2B	2.19	1.55	1.50
7	A	603	HEM	C2A-C3A	-2.14	1.33	1.38
9	A	605	A1JN4	C4A-C3A	2.11	1.48	1.43
7	a	603	HEM	C2A-C3A	-2.11	1.33	1.38
6	b	402	UQ8	C30-C29	2.11	1.56	1.50
6	b	402	UQ8	C40-C39	2.10	1.56	1.50
6	B	402	UQ8	C30-C29	2.10	1.56	1.50
6	B	402	UQ8	C25-C24	2.09	1.56	1.50
6	b	402	UQ8	O5-C5	-2.07	1.18	1.23
7	A	603	HEM	C3B-C2B	-2.07	1.33	1.37
9	a	606	A1JN4	C1A-NA	-2.07	1.35	1.39
9	A	605	A1JN4	C1A-NA	-2.07	1.35	1.39
6	B	402	UQ8	C15-C14	2.06	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	402	UQ8	C36-C34	2.05	1.55	1.51
6	b	402	UQ8	O2-C2	-2.04	1.18	1.23
9	a	606	A1JN4	C2A-C3A	-2.03	1.33	1.38
6	B	402	UQ8	O5-C5	-2.02	1.19	1.23
6	B	402	UQ8	O4-C4	2.02	1.41	1.36
6	B	402	UQ8	O2-C2	-2.01	1.19	1.23
6	B	402	UQ8	C41-C39	2.01	1.55	1.51

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	605	A1JN4	O1D-C3D-C4D	-13.11	81.60	108.25
9	a	606	A1JN4	O1D-C3D-C4D	-12.86	82.12	108.25
6	b	402	UQ8	C40-C39-C41	-11.51	95.91	115.27
6	B	402	UQ8	C20-C19-C21	-11.42	96.06	115.27
6	b	402	UQ8	C25-C24-C26	-11.06	96.66	115.27
6	B	402	UQ8	C35-C34-C36	-10.92	96.89	115.27
9	a	606	A1JN4	C3B-C4B-NB	-10.71	99.91	110.32
6	b	402	UQ8	C15-C14-C16	-10.69	97.28	115.27
9	A	605	A1JN4	C3B-C4B-NB	-10.63	99.98	110.32
6	B	402	UQ8	C10-C9-C11	-10.54	97.54	115.27
9	A	605	A1JN4	CHD-C1D-ND	10.17	139.11	124.20
9	a	606	A1JN4	CHD-C1D-ND	10.03	138.90	124.20
6	B	402	UQ8	C25-C24-C26	-9.99	98.46	115.27
6	b	402	UQ8	C10-C9-C11	-9.88	98.65	115.27
6	b	402	UQ8	C35-C34-C36	-9.67	99.00	115.27
6	B	402	UQ8	C40-C39-C41	-9.47	99.34	115.27
9	a	606	A1JN4	C4B-NB-C1B	9.47	114.62	105.35
6	b	402	UQ8	C20-C19-C21	-9.46	99.36	115.27
6	B	402	UQ8	C15-C14-C16	-9.44	99.40	115.27
6	B	402	UQ8	C30-C29-C31	-9.19	99.81	115.27
6	b	402	UQ8	C30-C29-C31	-9.16	99.85	115.27
9	A	605	A1JN4	C4B-NB-C1B	9.03	114.19	105.35
9	a	606	A1JN4	C4C-NC-C1C	8.94	114.11	105.35
9	A	605	A1JN4	O1D-C3D-CAD	-8.69	86.67	103.01
9	a	606	A1JN4	O1D-C3D-CAD	-8.65	86.75	103.01
9	A	605	A1JN4	C4C-NC-C1C	8.50	113.67	105.35
6	B	402	UQ8	C46-C44-C45	-8.44	95.96	114.60
6	b	402	UQ8	C46-C44-C45	-8.02	96.89	114.60
9	A	605	A1JN4	CHC-C4B-NB	7.18	132.20	124.44
9	a	606	A1JN4	CAC-C3C-C4C	-7.10	115.07	124.92
9	A	605	A1JN4	C4B-C3B-C2B	7.07	116.33	107.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	606	A1JN4	C4B-C3B-C2B	6.67	115.82	107.13
9	a	606	A1JN4	O1D-CGD-CBD	-6.63	103.50	110.19
9	A	605	A1JN4	CAC-C3C-C4C	-6.62	115.73	124.92
9	a	606	A1JN4	C3C-C4C-NC	-6.59	102.78	110.15
9	a	606	A1JN4	CHC-C4B-NB	6.57	131.54	124.44
9	A	605	A1JN4	C2A-C1A-NA	-6.46	102.92	110.15
9	a	606	A1JN4	C2A-C1A-NA	-6.39	103.00	110.15
9	A	605	A1JN4	C3C-C4C-NC	-6.28	103.12	110.15
9	A	605	A1JN4	O1D-CGD-CBD	-6.14	104.00	110.19
9	a	606	A1JN4	OND-C2D-CMD	-6.12	98.31	109.59
9	a	606	A1JN4	C4A-NA-C1A	6.07	111.29	105.35
9	A	605	A1JN4	CAB-C3B-C4B	-6.03	115.19	124.68
9	A	605	A1JN4	OND-C2D-CMD	-5.96	98.62	109.59
9	A	605	A1JN4	C4A-NA-C1A	5.78	111.01	105.35
9	A	605	A1JN4	CHB-C1B-NB	5.77	130.68	124.44
6	B	402	UQ8	C21-C19-C18	5.73	132.72	121.12
9	a	606	A1JN4	CHB-C1B-NB	5.71	130.62	124.44
9	a	606	A1JN4	CAB-C3B-C4B	-5.71	115.69	124.68
6	b	402	UQ8	C41-C39-C38	5.28	131.81	121.12
6	B	402	UQ8	C36-C34-C33	5.22	131.69	121.12
6	b	402	UQ8	C16-C14-C13	5.15	131.54	121.12
6	b	402	UQ8	C36-C34-C33	5.14	131.52	121.12
9	a	606	A1JN4	O1A-CGA-CBA	-5.12	106.62	123.08
9	A	605	A1JN4	O1A-CGA-CBA	-5.08	106.78	123.08
9	A	605	A1JN4	C1A-C2A-C3A	5.06	114.85	106.89
6	B	402	UQ8	C11-C9-C8	5.04	131.31	121.12
9	A	605	A1JN4	C2D-C1D-CHD	-5.00	116.03	124.28
6	B	402	UQ8	C26-C24-C23	4.98	131.20	121.12
9	a	606	A1JN4	C1A-C2A-C3A	4.98	114.73	106.89
6	B	402	UQ8	C41-C39-C38	4.91	131.05	121.12
6	b	402	UQ8	C26-C24-C23	4.87	130.96	121.12
9	a	606	A1JN4	C2D-C1D-CHD	-4.81	116.34	124.28
6	b	402	UQ8	C21-C19-C18	4.77	130.77	121.12
6	B	402	UQ8	C16-C14-C13	4.64	130.50	121.12
9	A	605	A1JN4	O2A-CGA-O1A	4.46	134.41	123.30
5	a	602	LPP	O9-C11-C12	4.38	120.94	111.50
9	a	606	A1JN4	O2A-CGA-O1A	4.33	134.09	123.30
6	b	402	UQ8	C31-C29-C28	4.28	129.78	121.12
6	b	402	UQ8	C11-C9-C8	4.28	129.77	121.12
9	A	605	A1JN4	CHD-C4C-NC	4.26	131.68	123.85
5	A	602	LPP	O9-C11-C12	4.24	120.64	111.50
9	a	606	A1JN4	CHD-C4C-NC	4.17	131.53	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	606	A1JN4	CHA-C4D-ND	-4.08	118.22	124.20
5	B	401	LPP	O9-C11-C12	4.07	120.27	111.50
6	B	402	UQ8	C31-C29-C28	4.03	129.28	121.12
9	A	605	A1JN4	CHA-C4D-ND	-4.03	118.30	124.20
5	x	101	LPP	O9-C11-C12	4.01	120.15	111.50
9	a	606	A1JN4	CAC-C3C-C2C	3.97	133.22	126.86
6	A	604	UQ8	C27-C28-C29	-3.96	118.12	127.66
9	a	606	A1JN4	C4A-C3A-C2A	-3.80	102.38	106.83
9	A	605	A1JN4	C4A-C3A-C2A	-3.75	102.44	106.83
6	A	604	UQ8	C15-C14-C16	3.74	121.56	115.27
9	A	605	A1JN4	CAC-C3C-C2C	3.66	132.72	126.86
6	a	604	UQ8	C20-C19-C21	3.66	121.42	115.27
5	b	401	LPP	O9-C11-C12	3.65	119.38	111.50
9	A	605	A1JN4	C1B-C2B-C3B	-3.65	101.61	106.94
9	a	606	A1JN4	C3D-C4D-CHA	3.57	134.93	124.34
5	X	101	LPP	O9-C11-C12	3.56	119.16	111.50
6	b	402	UQ8	C7-C8-C9	3.50	132.62	126.79
6	B	402	UQ8	C45-C44-C43	3.41	132.50	122.65
9	A	605	A1JN4	CAA-CBA-CGA	-3.40	106.28	113.60
6	b	402	UQ8	C25-C24-C23	3.39	132.36	123.68
9	A	605	A1JN4	C3D-C4D-CHA	3.38	134.36	124.34
6	b	402	UQ8	C40-C39-C38	3.33	132.22	123.68
9	a	606	A1JN4	C1B-C2B-C3B	-3.27	102.16	106.94
6	b	402	UQ8	C45-C44-C43	3.27	132.10	122.65
6	a	604	UQ8	C25-C24-C26	3.27	120.77	115.27
8	a	605	MQ8	C16-C17-C18	-3.26	119.81	127.66
9	a	606	A1JN4	CAA-CBA-CGA	-3.23	106.66	113.60
9	a	606	A1JN4	C1C-CHC-C4B	-3.16	114.98	124.74
6	b	402	UQ8	C10-C9-C8	3.08	131.57	123.68
6	B	402	UQ8	C46-C44-C43	3.07	131.51	122.65
9	a	606	A1JN4	C4C-C3C-C2C	3.06	111.71	106.89
6	B	402	UQ8	C35-C34-C33	3.01	131.41	123.68
9	A	605	A1JN4	C1C-CHC-C4B	-3.00	115.48	124.74
6	a	604	UQ8	C35-C34-C36	2.99	120.30	115.27
7	A	601	HEM	C4D-ND-C1D	2.98	108.15	105.07
7	a	601	HEM	C4D-ND-C1D	2.97	108.14	105.07
9	A	605	A1JN4	C4C-C3C-C2C	2.96	111.55	106.89
7	a	603	HEM	CAA-C2A-C1A	2.96	130.71	124.89
7	A	603	HEM	CAA-C2A-C1A	2.95	130.69	124.89
6	B	402	UQ8	C20-C19-C18	2.92	131.18	123.68
6	b	402	UQ8	C15-C14-C13	2.92	131.18	123.68
7	a	601	HEM	C4A-NA-C1A	2.92	108.20	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	402	UQ8	C10-C9-C8	2.91	131.15	123.68
6	a	604	UQ8	C10-C9-C8	-2.91	116.22	123.68
9	a	606	A1JN4	CAA-C2A-C1A	-2.90	119.19	124.89
6	b	402	UQ8	C46-C44-C43	2.89	131.00	122.65
7	A	601	HEM	C4C-NC-C1C	2.89	108.17	105.35
7	A	601	HEM	C4A-NA-C1A	2.88	108.17	105.35
8	a	605	MQ8	C11-C12-C13	-2.86	122.03	126.79
6	A	604	UQ8	C32-C33-C34	-2.85	120.79	127.66
6	B	402	UQ8	C30-C29-C28	2.81	130.90	123.68
8	a	605	MQ8	C26-C27-C28	-2.80	120.93	127.66
6	A	604	UQ8	C37-C38-C39	-2.79	120.94	127.66
8	a	605	MQ8	C24-C23-C25	2.77	119.93	115.27
7	a	601	HEM	C4C-NC-C1C	2.76	108.05	105.35
5	a	602	LPP	O27-C29-C30	2.73	120.49	111.91
6	B	402	UQ8	C7-C8-C9	2.71	131.30	126.79
9	a	606	A1JN4	CHA-C1A-C2A	2.70	131.26	125.36
9	A	605	A1JN4	CHA-C1A-C2A	2.70	131.26	125.36
5	B	401	LPP	O27-C29-C30	2.70	120.38	111.91
6	A	604	UQ8	C25-C24-C26	2.64	119.71	115.27
8	a	605	MQ8	C45-C43-C44	2.64	119.71	115.27
5	X	101	LPP	O27-C29-C30	2.63	120.16	111.91
9	A	605	A1JN4	OND-C2D-C3D	-2.62	103.94	110.45
9	a	606	A1JN4	CBB-CAB-C3B	2.62	119.65	112.43
8	a	605	MQ8	C34-C33-C32	-2.61	116.97	123.68
6	A	604	UQ8	C25-C24-C23	-2.61	116.98	123.68
7	a	601	HEM	C1B-NB-C4B	2.60	107.76	105.07
6	b	402	UQ8	C30-C29-C28	2.60	130.35	123.68
9	A	605	A1JN4	CAA-C2A-C1A	-2.60	119.78	124.89
7	A	601	HEM	C1B-NB-C4B	2.59	107.75	105.07
6	a	604	UQ8	C20-C19-C18	-2.58	117.06	123.68
6	B	402	UQ8	C25-C24-C23	2.58	130.30	123.68
5	x	101	LPP	O27-C29-C30	2.56	119.94	111.91
6	A	604	UQ8	C12-C13-C14	-2.55	121.51	127.66
5	b	401	LPP	O27-C29-C30	2.55	119.92	111.91
9	a	606	A1JN4	C2C-C1C-NC	-2.53	106.22	110.08
7	a	603	HEM	C1B-NB-C4B	2.53	107.68	105.07
6	a	604	UQ8	C12-C13-C14	-2.52	121.59	127.66
6	B	402	UQ8	C15-C14-C13	2.50	130.09	123.68
8	a	605	MQ8	C34-C33-C35	2.46	119.41	115.27
6	A	604	UQ8	C10-C9-C8	-2.46	117.37	123.68
5	A	602	LPP	O27-C29-C30	2.45	119.59	111.91
9	A	605	A1JN4	C2C-C1C-NC	-2.45	106.36	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	604	UQ8	C20-C19-C18	-2.44	117.42	123.68
9	a	606	A1JN4	OND-C2D-C3D	-2.43	104.41	110.45
7	A	603	HEM	C1B-NB-C4B	2.42	107.57	105.07
6	b	402	UQ8	C20-C19-C18	2.41	129.86	123.68
8	a	605	MQ8	C30-C31-C32	-2.41	103.97	111.88
6	B	402	UQ8	C1M-C1-C6	-2.40	120.48	124.40
6	a	604	UQ8	C30-C29-C31	2.40	119.30	115.27
7	A	603	HEM	C4D-ND-C1D	2.38	107.53	105.07
8	a	605	MQ8	O4-C4-C3	-2.38	116.73	120.56
7	a	603	HEM	C4D-ND-C1D	2.37	107.52	105.07
9	a	606	A1JN4	CMA-C3A-C2A	2.37	130.73	125.61
7	a	603	HEM	C4A-NA-C1A	2.36	107.66	105.35
6	a	604	UQ8	C25-C24-C23	-2.35	117.64	123.68
7	A	603	HEM	C4A-NA-C1A	2.34	107.64	105.35
7	a	603	HEM	CAA-C2A-C3A	-2.34	121.71	127.07
9	A	605	A1JN4	CHC-C1C-NC	2.34	128.15	123.85
6	A	604	UQ8	C30-C29-C31	2.32	119.18	115.27
6	A	604	UQ8	C1M-C1-C6	-2.32	120.62	124.40
6	A	604	UQ8	C10-C9-C11	2.31	119.15	115.27
7	A	603	HEM	CAA-C2A-C3A	-2.30	121.80	127.07
9	A	605	A1JN4	CMA-C3A-C2A	2.28	130.55	125.61
7	A	603	HEM	C4C-NC-C1C	2.28	107.58	105.35
9	a	606	A1JN4	CHC-C1C-NC	2.28	128.04	123.85
8	a	605	MQ8	C50-C48-C49	2.28	119.64	114.60
9	A	605	A1JN4	CBB-CAB-C3B	2.28	118.71	112.43
7	a	603	HEM	C4C-NC-C1C	2.28	107.58	105.35
6	a	604	UQ8	C46-C44-C45	2.27	119.62	114.60
6	B	402	UQ8	C40-C39-C38	2.26	129.48	123.68
6	A	604	UQ8	C46-C44-C45	2.25	119.58	114.60
8	a	605	MQ8	C14-C13-C15	2.24	119.04	115.27
9	a	606	A1JN4	CHC-C4B-C3B	2.23	128.55	124.94
6	b	402	UQ8	C35-C34-C33	2.23	129.40	123.68
6	a	604	UQ8	C32-C33-C34	-2.22	122.32	127.66
6	a	604	UQ8	C15-C14-C16	2.21	118.99	115.27
7	a	601	HEM	C2A-C1A-NA	-2.20	107.68	110.15
9	A	605	A1JN4	CBA-CAA-C2A	-2.19	106.53	112.63
7	a	601	HEM	C3D-C4D-ND	-2.18	107.74	110.17
7	a	603	HEM	CHA-C4D-ND	2.17	127.05	124.37
6	a	604	UQ8	C11-C9-C8	2.16	125.50	121.12
7	A	601	HEM	C3D-C4D-ND	-2.16	107.76	110.17
6	a	604	UQ8	C40-C39-C41	2.16	118.90	115.27
7	A	601	HEM	C2A-C1A-NA	-2.16	107.74	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	603	HEM	CHA-C4D-ND	2.15	127.03	124.37
7	a	601	HEM	CHD-C1D-ND	2.14	126.74	124.42
8	a	605	MQ8	C19-C18-C20	2.13	118.85	115.27
6	a	604	UQ8	C42-C43-C44	-2.12	120.50	127.75
8	a	605	MQ8	C5-C4-C3	2.09	122.25	118.42
6	a	604	UQ8	C37-C38-C39	-2.09	122.64	127.66
9	a	606	A1JN4	O1D-CGD-O2D	2.07	122.65	120.80
7	a	603	HEM	CAD-CBD-CGD	-2.07	109.16	113.60
8	a	605	MQ8	C21-C22-C23	-2.05	122.72	127.66
8	a	605	MQ8	C41-C42-C43	-2.04	122.74	127.66
8	a	605	MQ8	C10-C5-C4	-2.04	118.47	120.68

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	a	606	A1JN4	NB
9	A	605	A1JN4	NB

All (185) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	401	LPP	C12-C11-O9-C7
5	a	602	LPP	C12-C11-O9-C7
5	a	602	LPP	O28-C29-O27-C8
5	a	602	LPP	C30-C29-O27-C8
5	b	401	LPP	C6-O5-P1-O2
5	b	401	LPP	C6-O5-P1-O3
5	b	401	LPP	C6-O5-P1-O4
5	b	401	LPP	C12-C11-O9-C7
5	x	101	LPP	C6-O5-P1-O2
5	x	101	LPP	C6-O5-P1-O4
5	A	602	LPP	C12-C11-O9-C7
6	B	402	UQ8	C24-C26-C27-C28
6	a	604	UQ8	C40-C39-C41-C42
6	a	604	UQ8	C25-C24-C26-C27
6	b	402	UQ8	C41-C42-C43-C44
6	b	402	UQ8	C36-C37-C38-C39
6	b	402	UQ8	C29-C31-C32-C33
6	A	604	UQ8	C25-C24-C26-C27
6	A	604	UQ8	C23-C24-C26-C27
6	A	604	UQ8	C15-C14-C16-C17
6	A	604	UQ8	C13-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
6	A	604	UQ8	C1-C6-C7-C8
6	A	604	UQ8	C5-C6-C7-C8
7	a	601	HEM	C1A-C2A-CAA-CBA
7	a	601	HEM	C3A-C2A-CAA-CBA
7	A	601	HEM	C1A-C2A-CAA-CBA
8	a	605	MQ8	C42-C43-C44-C46
8	a	605	MQ8	C45-C43-C44-C46
5	B	401	LPP	O28-C29-O27-C8
9	a	606	A1JN4	C4C-C3C-CAC-CBC
9	A	605	A1JN4	C4C-C3C-CAC-CBC
9	a	606	A1JN4	C2C-C3C-CAC-CBC
9	A	605	A1JN4	C2C-C3C-CAC-CBC
5	B	401	LPP	O10-C11-O9-C7
5	a	602	LPP	O10-C11-O9-C7
5	A	602	LPP	O10-C11-O9-C7
5	B	401	LPP	C30-C29-O27-C8
8	a	605	MQ8	C24-C23-C25-C26
8	a	605	MQ8	C29-C28-C30-C31
6	a	604	UQ8	C23-C24-C26-C27
5	b	401	LPP	O10-C11-O9-C7
7	a	603	HEM	C1A-C2A-CAA-CBA
7	A	603	HEM	C1A-C2A-CAA-CBA
6	a	604	UQ8	C20-C19-C21-C22
6	a	604	UQ8	C38-C39-C41-C42
6	a	604	UQ8	C18-C19-C21-C22
6	B	402	UQ8	C34-C36-C37-C38
6	B	402	UQ8	C19-C21-C22-C23
6	b	402	UQ8	C39-C41-C42-C43
6	b	402	UQ8	C34-C36-C37-C38
6	A	604	UQ8	C34-C36-C37-C38
6	A	604	UQ8	C29-C31-C32-C33
8	a	605	MQ8	C18-C20-C21-C22
5	b	401	LPP	C30-C29-O27-C8
5	A	602	LPP	C30-C29-O27-C8
5	b	401	LPP	O28-C29-O27-C8
8	a	605	MQ8	C22-C23-C25-C26
8	a	605	MQ8	C27-C28-C30-C31
7	A	601	HEM	C3A-C2A-CAA-CBA
7	A	603	HEM	C3A-C2A-CAA-CBA
5	b	401	LPP	C29-C30-C31-C32
5	A	602	LPP	C30-C31-C32-C33
6	a	604	UQ8	C24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
5	A	602	LPP	O28-C29-O27-C8
5	x	101	LPP	C12-C11-O9-C7
5	x	101	LPP	O10-C11-O9-C7
6	A	604	UQ8	C40-C39-C41-C42
5	X	101	LPP	C30-C29-O27-C8
5	a	602	LPP	C29-C30-C31-C32
5	a	602	LPP	C34-C35-C36-C37
5	X	101	LPP	O5-C6-C7-O9
5	B	401	LPP	C37-C38-C39-C40
5	x	101	LPP	C19-C20-C21-C22
5	X	101	LPP	C40-C41-C42-C43
5	a	602	LPP	C20-C21-C22-C23
5	A	602	LPP	C21-C22-C23-C24
7	a	603	HEM	C3A-C2A-CAA-CBA
5	a	602	LPP	C17-C18-C19-C20
5	X	101	LPP	C38-C39-C40-C41
5	x	101	LPP	C12-C13-C14-C15
5	x	101	LPP	C32-C33-C34-C35
5	a	602	LPP	C37-C38-C39-C40
5	a	602	LPP	C39-C40-C41-C42
6	A	604	UQ8	C38-C39-C41-C42
5	X	101	LPP	O28-C29-O27-C8
5	X	101	LPP	C34-C35-C36-C37
5	x	101	LPP	C30-C29-O27-C8
5	B	401	LPP	C31-C32-C33-C34
8	a	605	MQ8	C43-C44-C46-C47
7	A	603	HEM	C4C-C3C-CAC-CBC
5	x	101	LPP	O28-C29-O27-C8
5	x	101	LPP	C15-C16-C17-C18
5	A	602	LPP	O5-C6-C7-C8
5	X	101	LPP	C6-C7-C8-O27
5	a	602	LPP	C19-C20-C21-C22
5	x	101	LPP	C30-C31-C32-C33
5	X	101	LPP	C23-C24-C25-C26
6	B	402	UQ8	C5-C6-C7-C8
6	a	604	UQ8	C5-C6-C7-C8
6	b	402	UQ8	C5-C6-C7-C8
5	a	602	LPP	C8-C7-O9-C11
5	b	401	LPP	C8-C7-O9-C11
5	B	401	LPP	C6-O5-P1-O3
5	X	101	LPP	O9-C7-C8-O27
6	a	604	UQ8	C3-C4-O4-C4M

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Mol	Chain	Res	Type	Atoms
5	A	602	LPP	C32-C33-C34-C35
5	X	101	LPP	O5-C6-C7-C8
6	A	604	UQ8	C30-C29-C31-C32
5	a	602	LPP	C32-C33-C34-C35
5	A	602	LPP	O5-C6-C7-O9
5	x	101	LPP	C36-C37-C38-C39
5	b	401	LPP	C37-C38-C39-C40
5	A	602	LPP	C16-C17-C18-C19
5	b	401	LPP	C33-C34-C35-C36
6	b	402	UQ8	C9-C11-C12-C13
5	a	602	LPP	C16-C17-C18-C19
5	A	602	LPP	C37-C38-C39-C40
5	x	101	LPP	C37-C38-C39-C40
7	a	601	HEM	C4C-C3C-CAC-CBC
7	a	603	HEM	C4C-C3C-CAC-CBC
7	A	601	HEM	C4C-C3C-CAC-CBC
7	A	603	HEM	C4B-C3B-CAB-CBB
5	A	602	LPP	C33-C34-C35-C36
5	X	101	LPP	C30-C31-C32-C33
5	x	101	LPP	C39-C40-C41-C42
5	x	101	LPP	O5-C6-C7-C8
5	B	401	LPP	C18-C19-C20-C21
5	A	602	LPP	C34-C35-C36-C37
5	B	401	LPP	O5-C6-C7-O9
6	B	402	UQ8	C1-C6-C7-C8
6	a	604	UQ8	C1-C6-C7-C8
6	b	402	UQ8	C1-C6-C7-C8
5	a	602	LPP	C38-C39-C40-C41
5	X	101	LPP	O10-C11-O9-C7
6	a	604	UQ8	C2-C3-O3-C3M
5	A	602	LPP	C12-C13-C14-C15
5	B	401	LPP	C14-C15-C16-C17
5	B	401	LPP	O5-C6-C7-C8
5	b	401	LPP	C31-C32-C33-C34
5	a	602	LPP	C6-O5-P1-O3
5	X	101	LPP	C31-C32-C33-C34
6	B	402	UQ8	C36-C37-C38-C39
5	X	101	LPP	C19-C20-C21-C22
5	B	401	LPP	C11-C12-C13-C14
6	b	402	UQ8	C23-C24-C26-C27
6	b	402	UQ8	C25-C24-C26-C27
5	X	101	LPP	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
5	b	401	LPP	C20-C21-C22-C23
7	a	601	HEM	CAA-CBA-CGA-O1A
5	B	401	LPP	C8-C7-O9-C11
9	a	606	A1JN4	CAA-CBA-CGA-O2A
5	A	602	LPP	C18-C19-C20-C21
6	a	604	UQ8	C35-C34-C36-C37
5	X	101	LPP	C12-C11-O9-C7
5	X	101	LPP	C35-C36-C37-C38
7	a	601	HEM	CAD-CBD-CGD-O2D
6	A	604	UQ8	C28-C29-C31-C32
5	B	401	LPP	C6-O5-P1-O2
5	A	602	LPP	C6-O5-P1-O2
6	a	604	UQ8	C33-C34-C36-C37
5	a	602	LPP	C12-C13-C14-C15
5	a	602	LPP	C41-C42-C43-C44
6	b	402	UQ8	C2-C3-O3-C3M
7	a	601	HEM	CAA-CBA-CGA-O2A
7	A	603	HEM	CAD-CBD-CGD-O1D
7	A	601	HEM	CAD-CBD-CGD-O2D
5	A	602	LPP	C40-C41-C42-C43
5	B	401	LPP	O9-C11-C12-C13
7	A	603	HEM	CAD-CBD-CGD-O2D
5	A	602	LPP	C14-C15-C16-C17
5	B	401	LPP	C29-C30-C31-C32
6	a	604	UQ8	C4-C3-O3-C3M
9	A	605	A1JN4	CAA-CBA-CGA-O1A
8	a	605	MQ8	C44-C46-C47-C48
5	a	602	LPP	C15-C16-C17-C18
7	a	601	HEM	CAD-CBD-CGD-O1D
6	A	604	UQ8	C6-C7-C8-C9
7	A	601	HEM	CAD-CBD-CGD-O1D
5	B	401	LPP	C6-C7-O9-C11
5	B	401	LPP	O10-C11-C12-C13
5	x	101	LPP	O27-C29-C30-C31
6	b	402	UQ8	C15-C14-C16-C17
5	x	101	LPP	C22-C23-C24-C25
8	a	605	MQ8	C28-C30-C31-C32
7	a	603	HEM	CAD-CBD-CGD-O1D

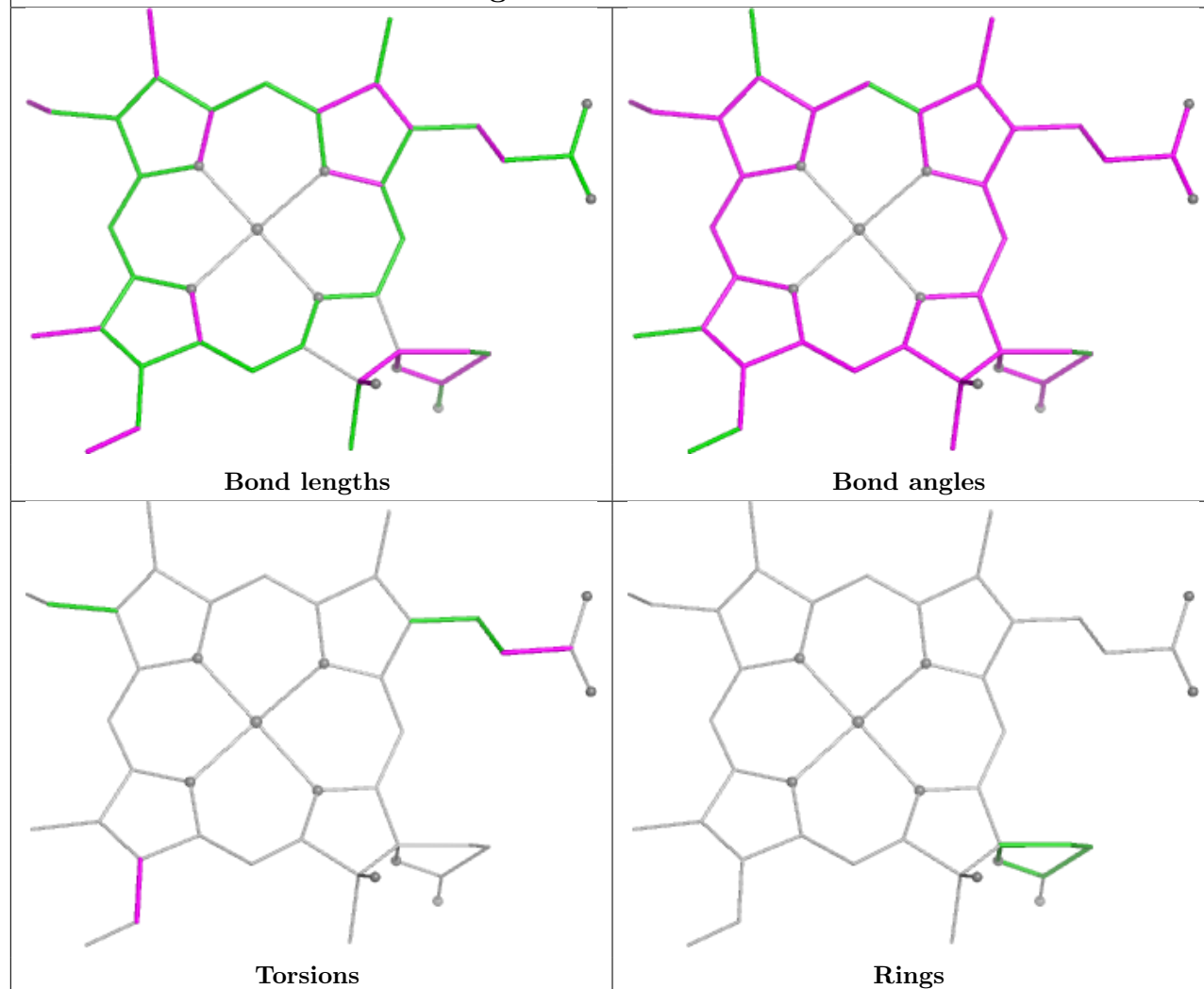
There are no ring outliers.

14 monomers are involved in 80 short contacts:

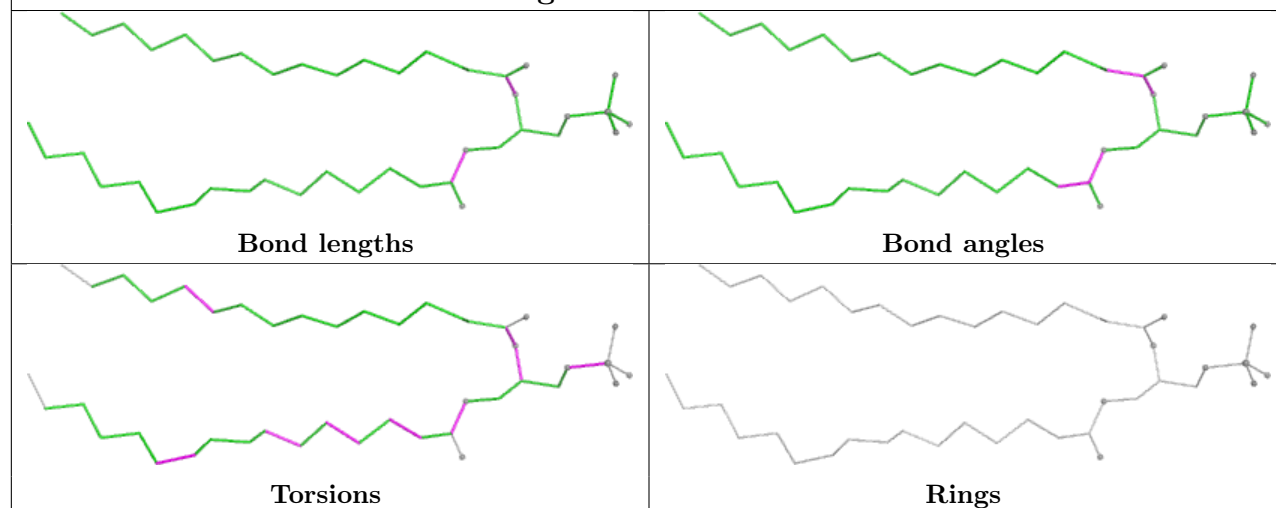
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	601	HEM	6	0
7	a	601	HEM	8	0
5	A	602	LPP	3	0
6	B	402	UQ8	5	0
7	A	603	HEM	6	0
5	X	101	LPP	3	0
6	A	604	UQ8	11	0
6	b	402	UQ8	5	0
6	a	604	UQ8	9	0
5	B	401	LPP	1	0
8	a	605	MQ8	14	0
9	A	605	A1JN4	1	0
7	a	603	HEM	7	0
5	a	602	LPP	2	0

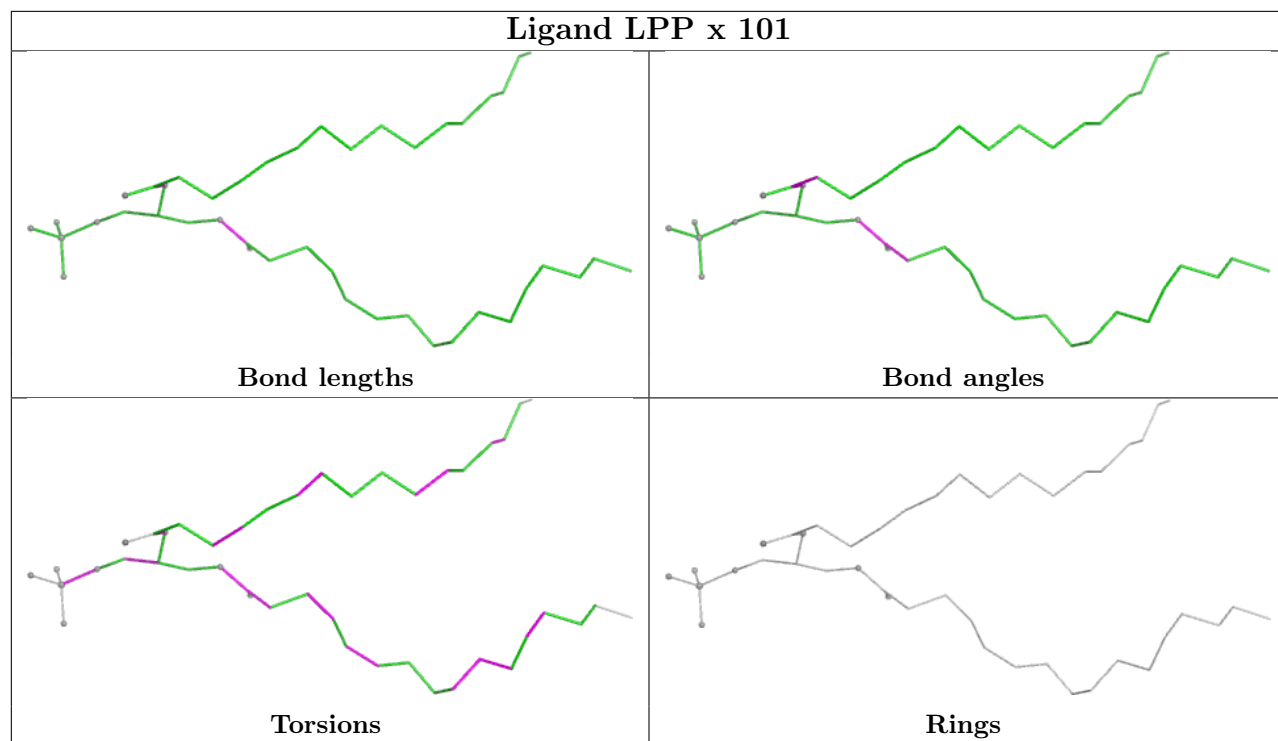
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

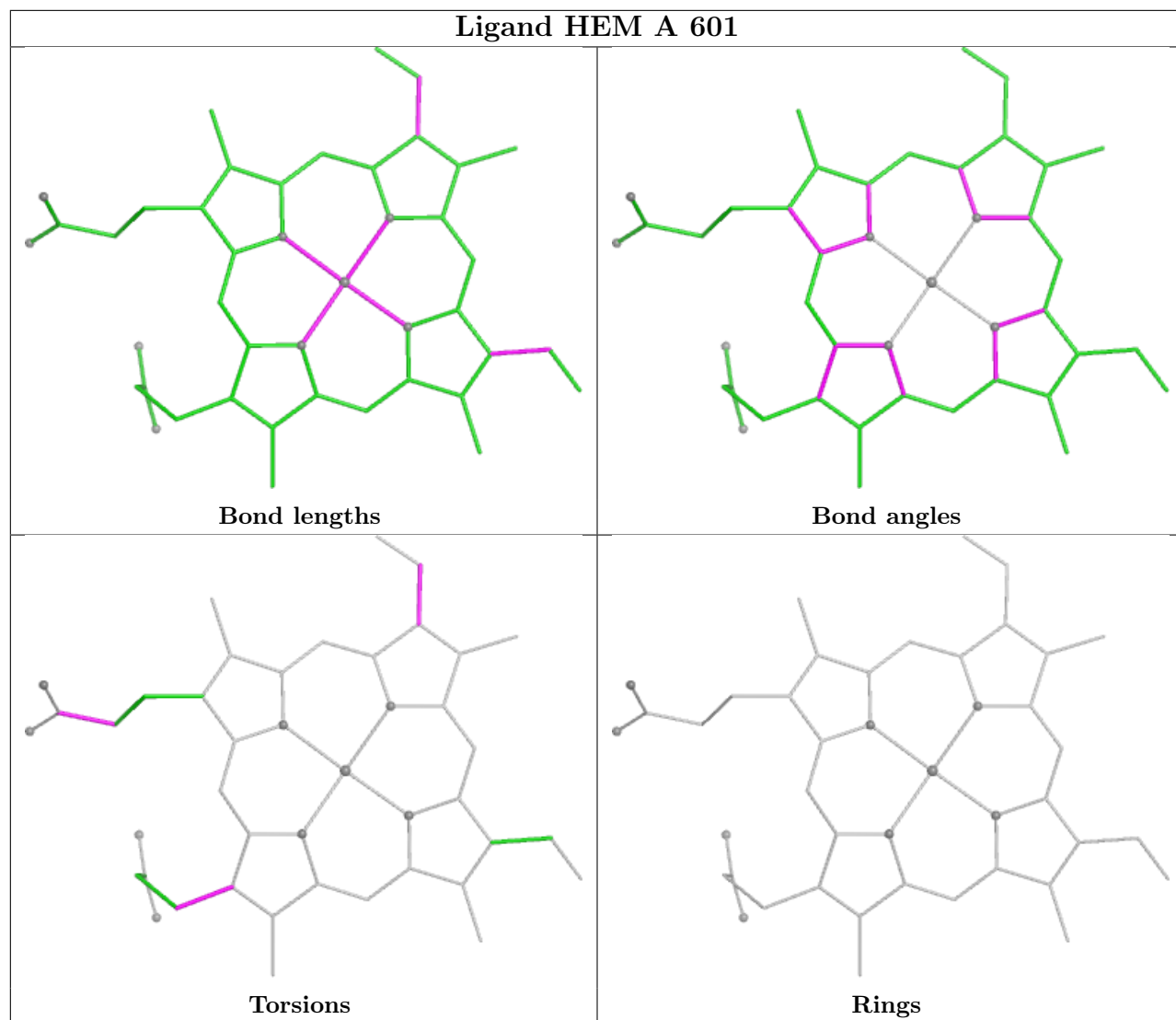
Ligand A1JN4 a 606

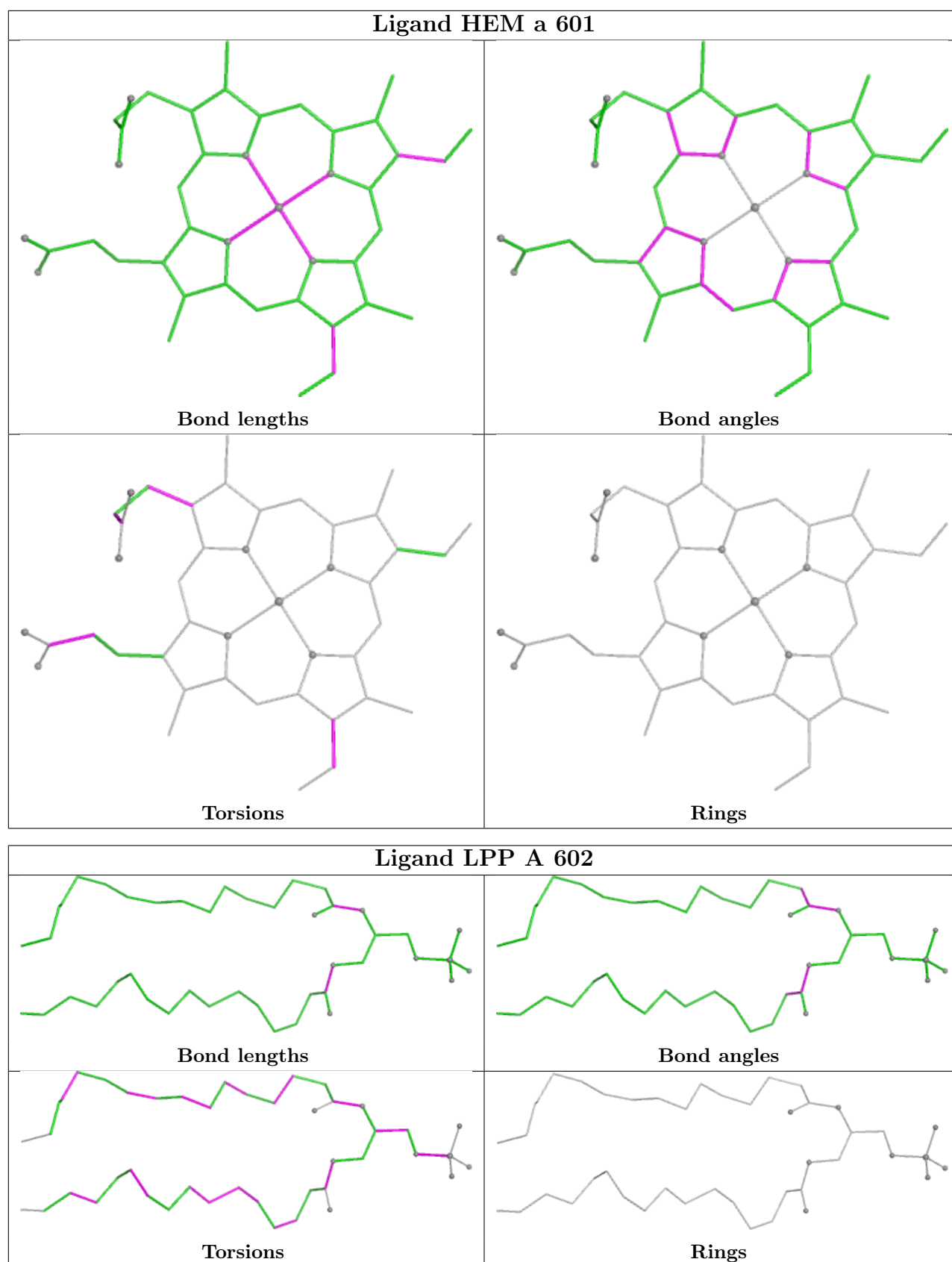


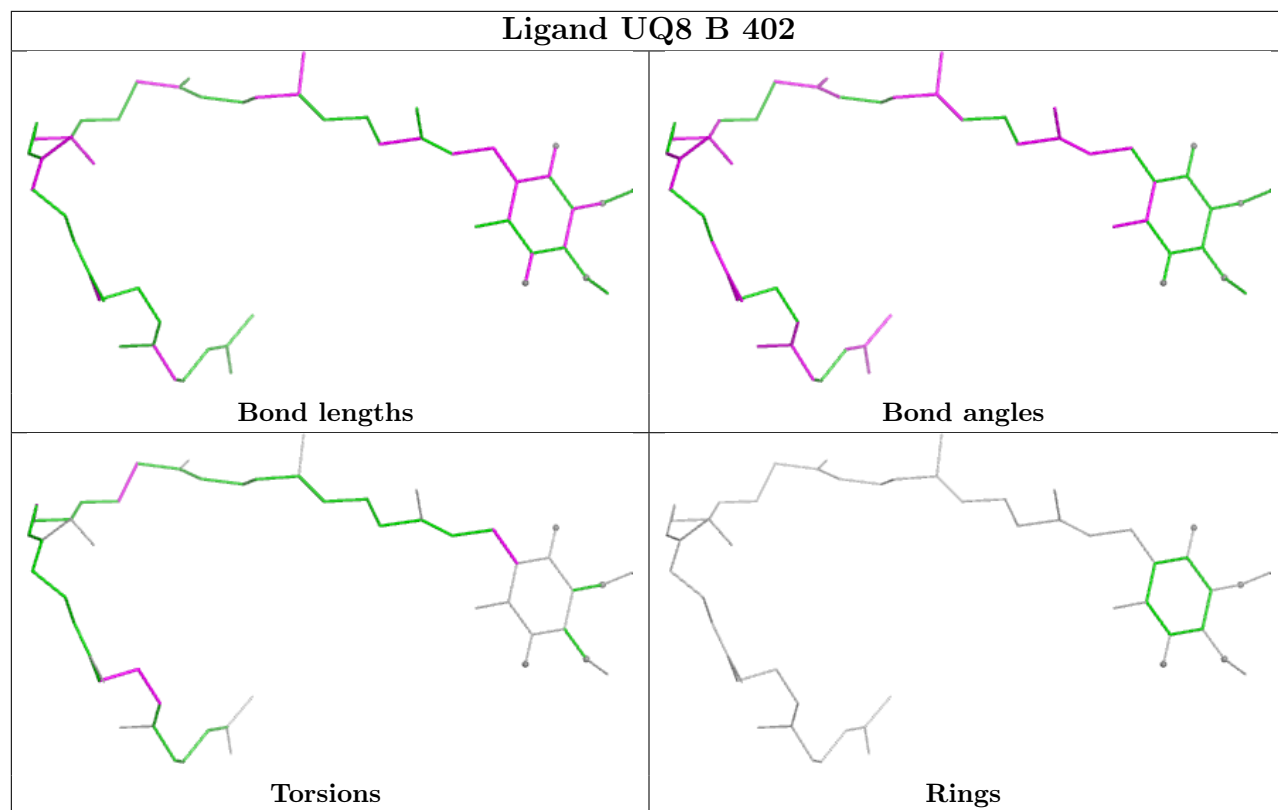
Ligand LPP b 401

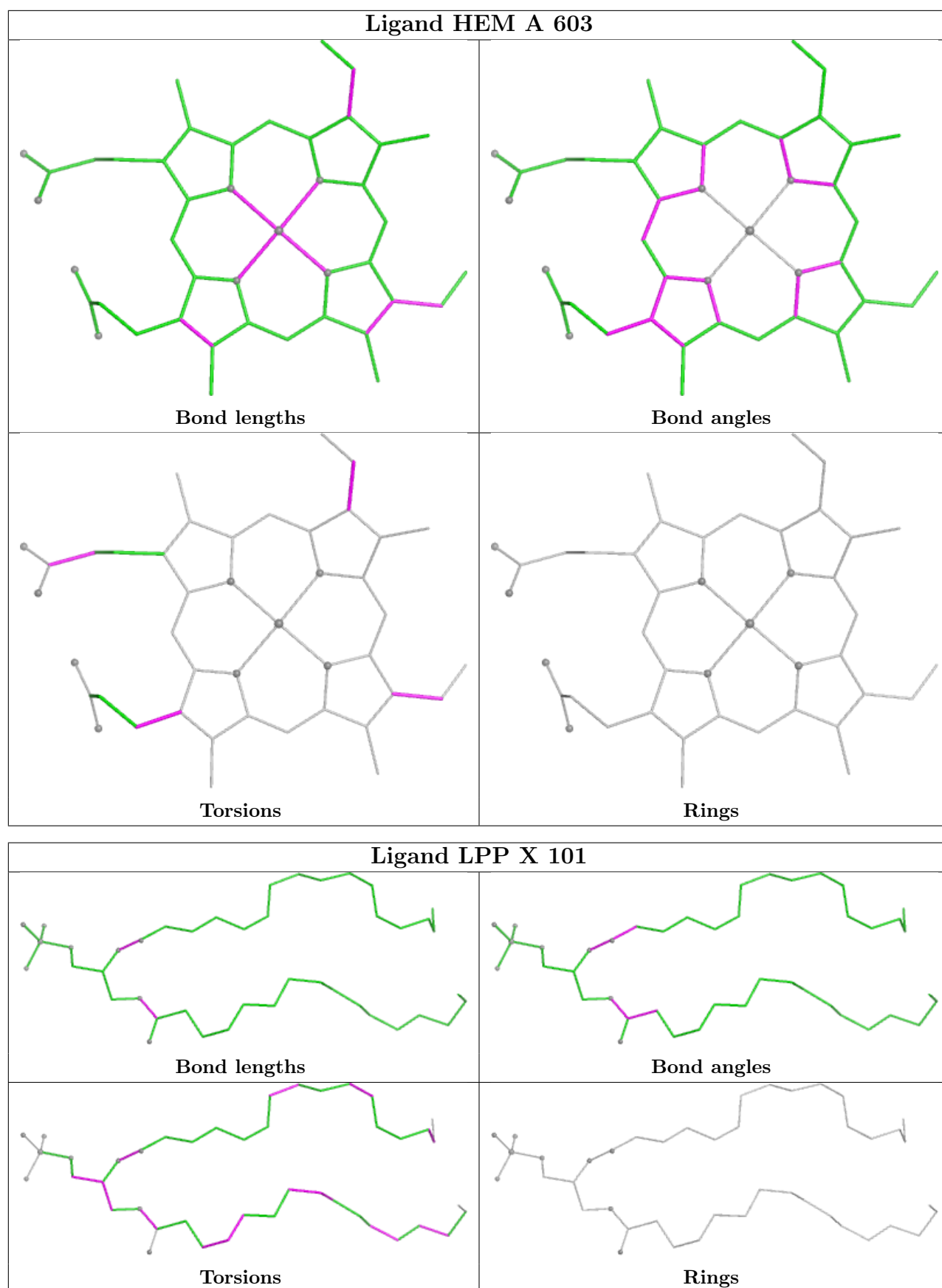


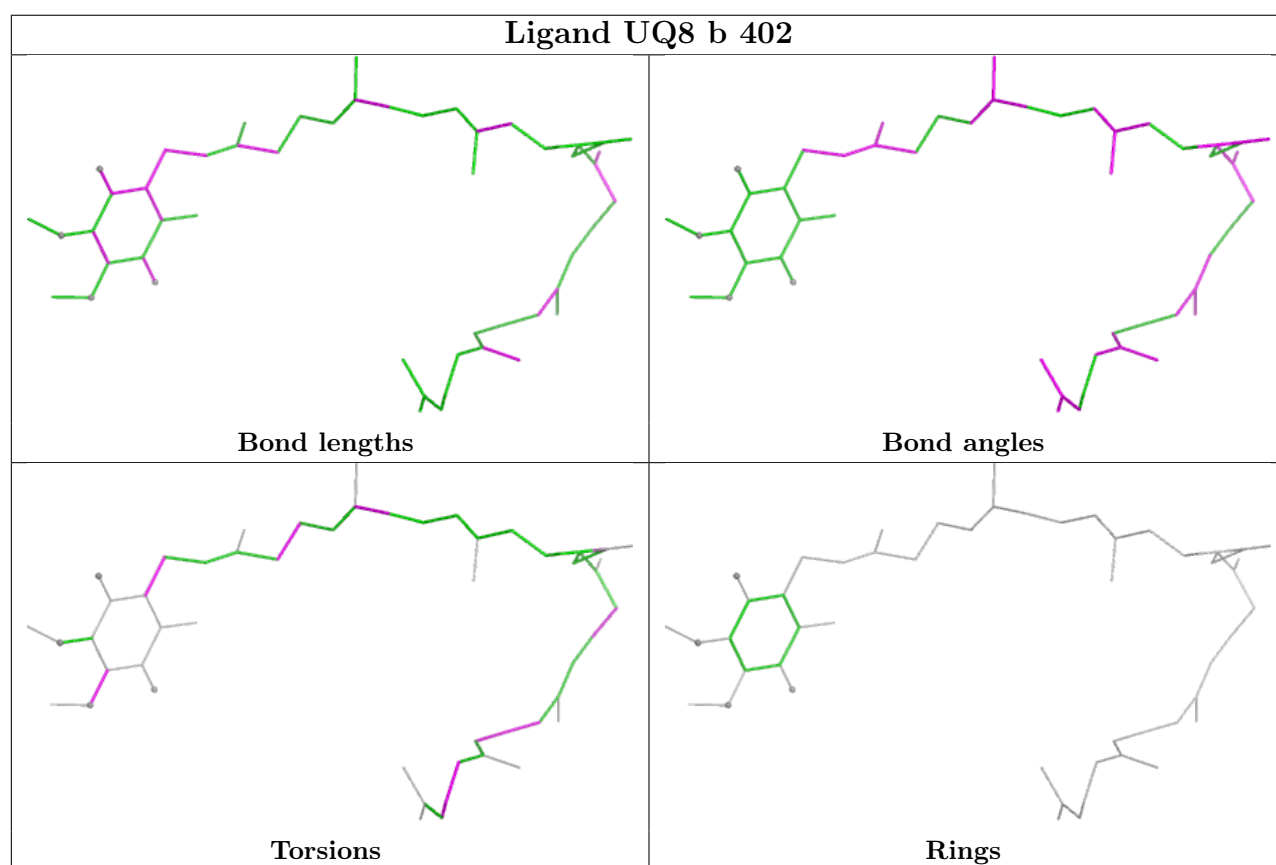
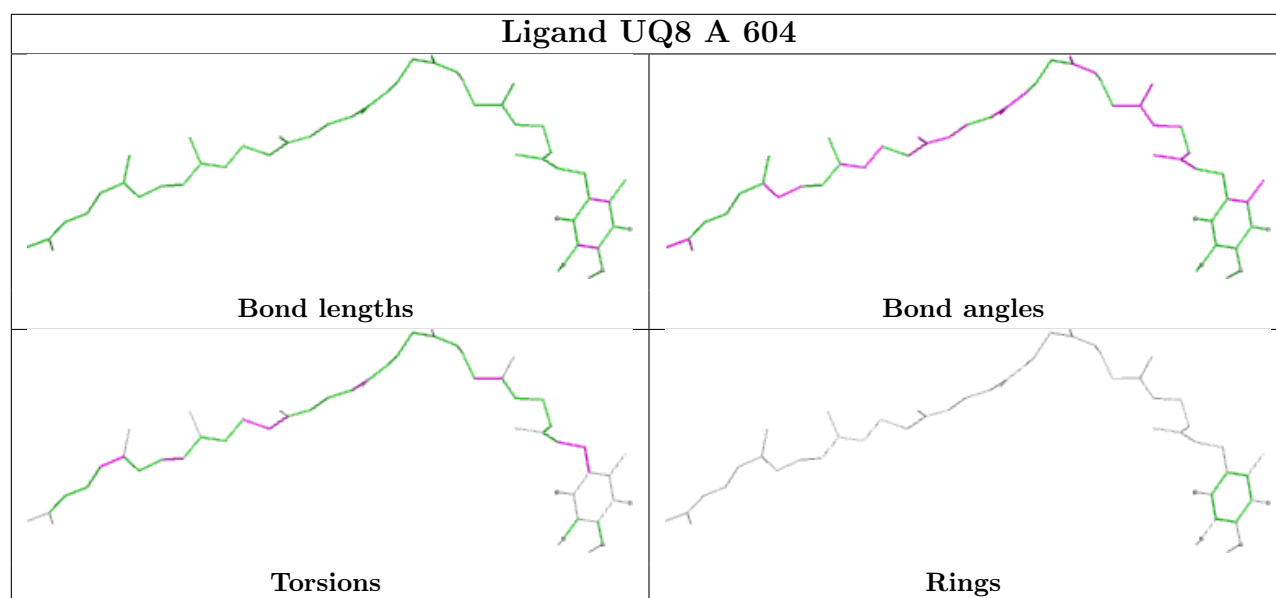


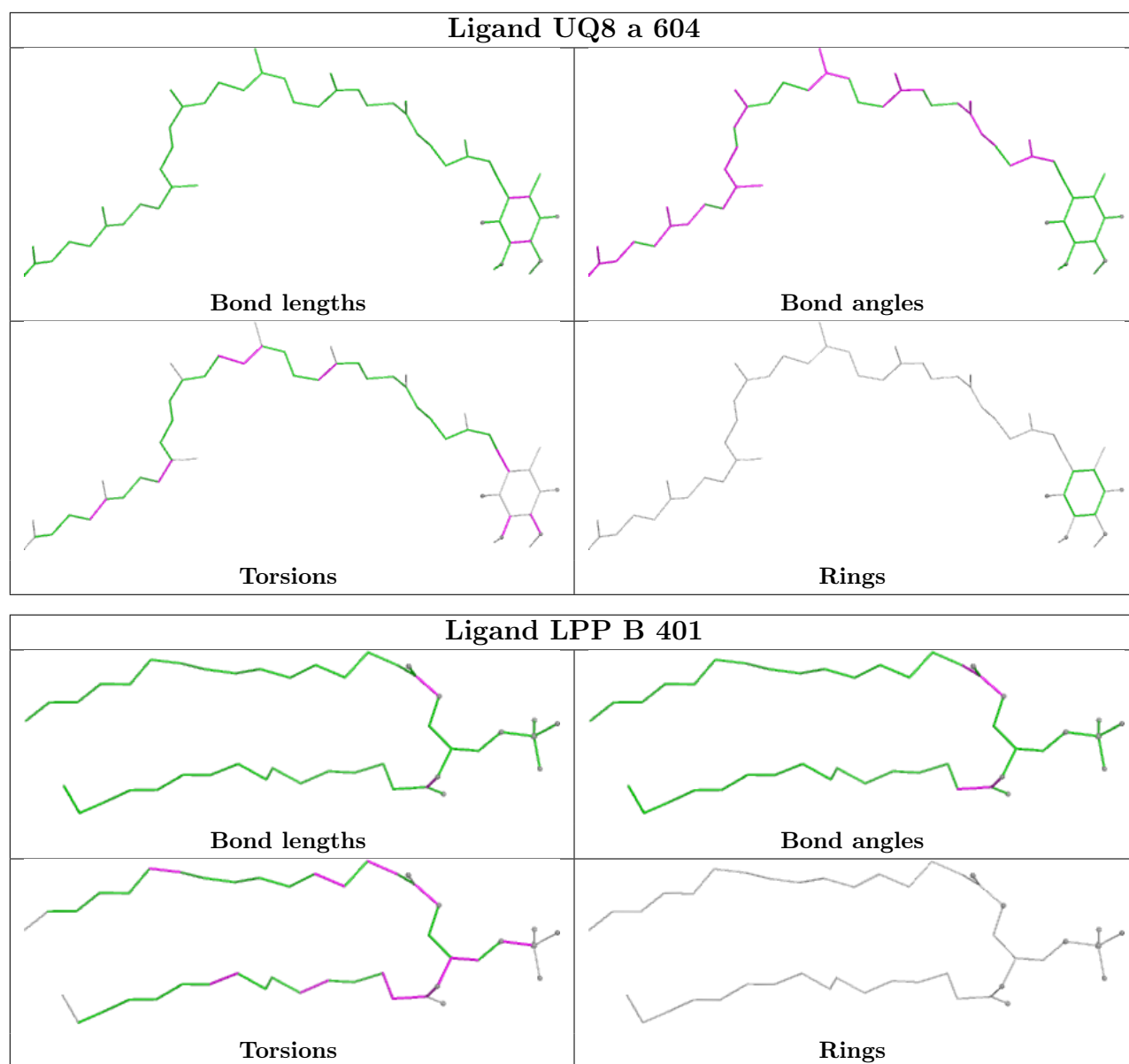


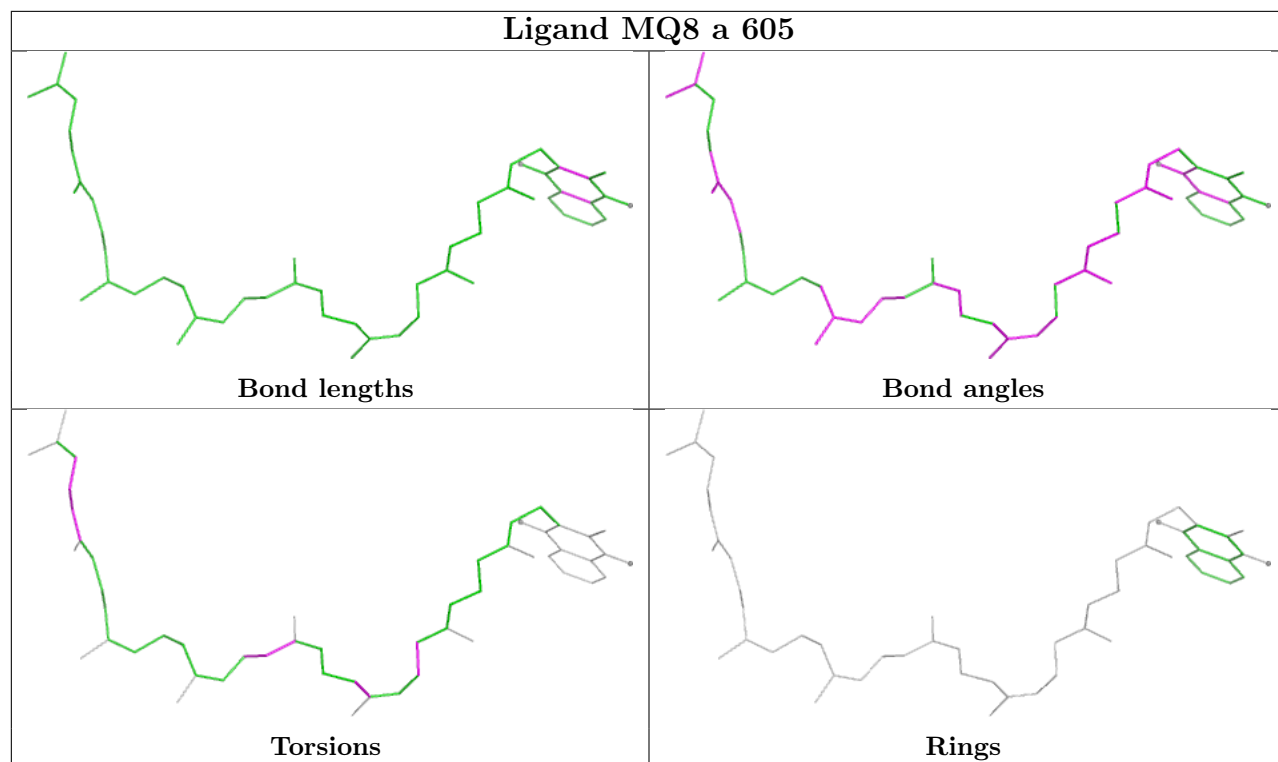




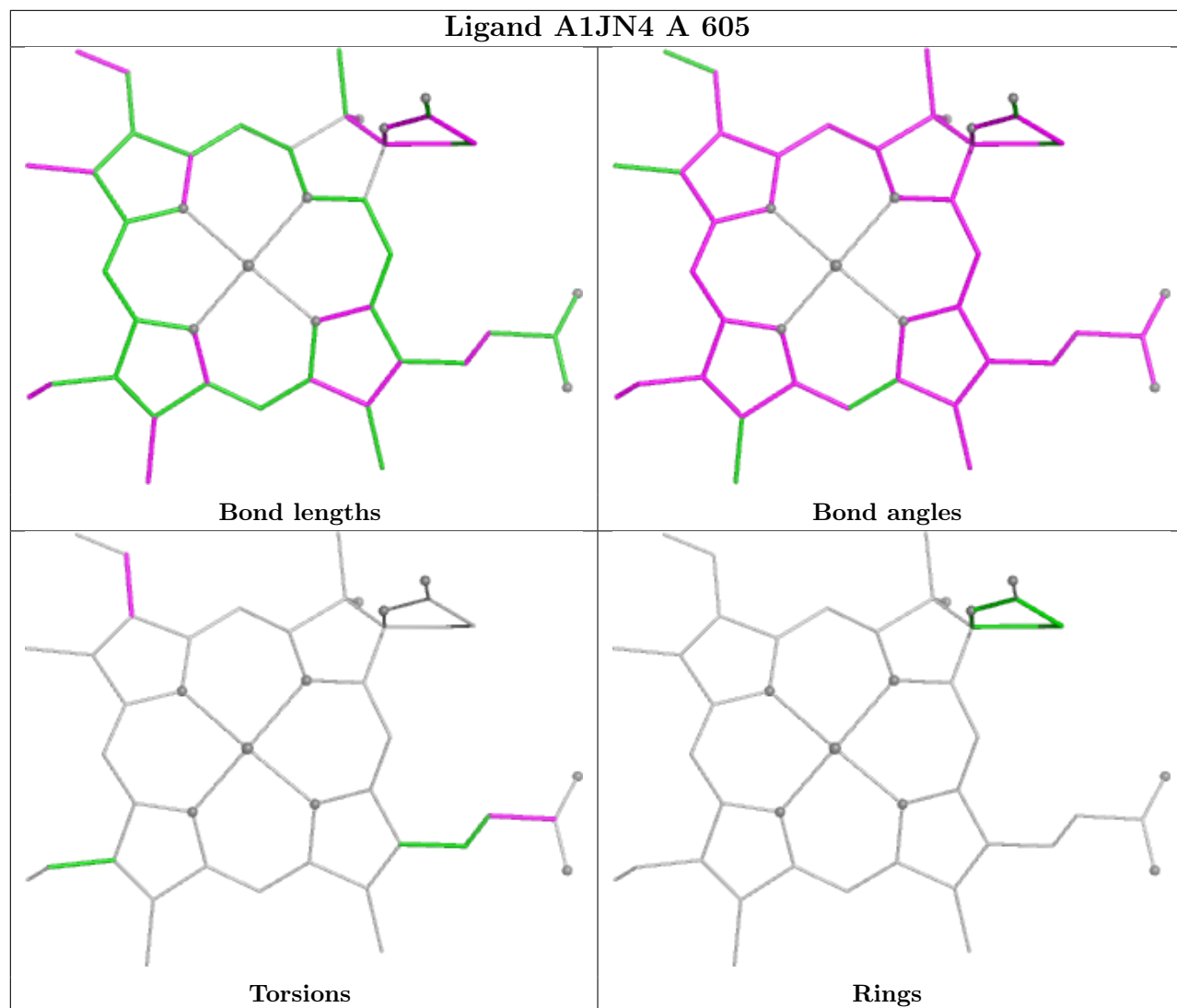


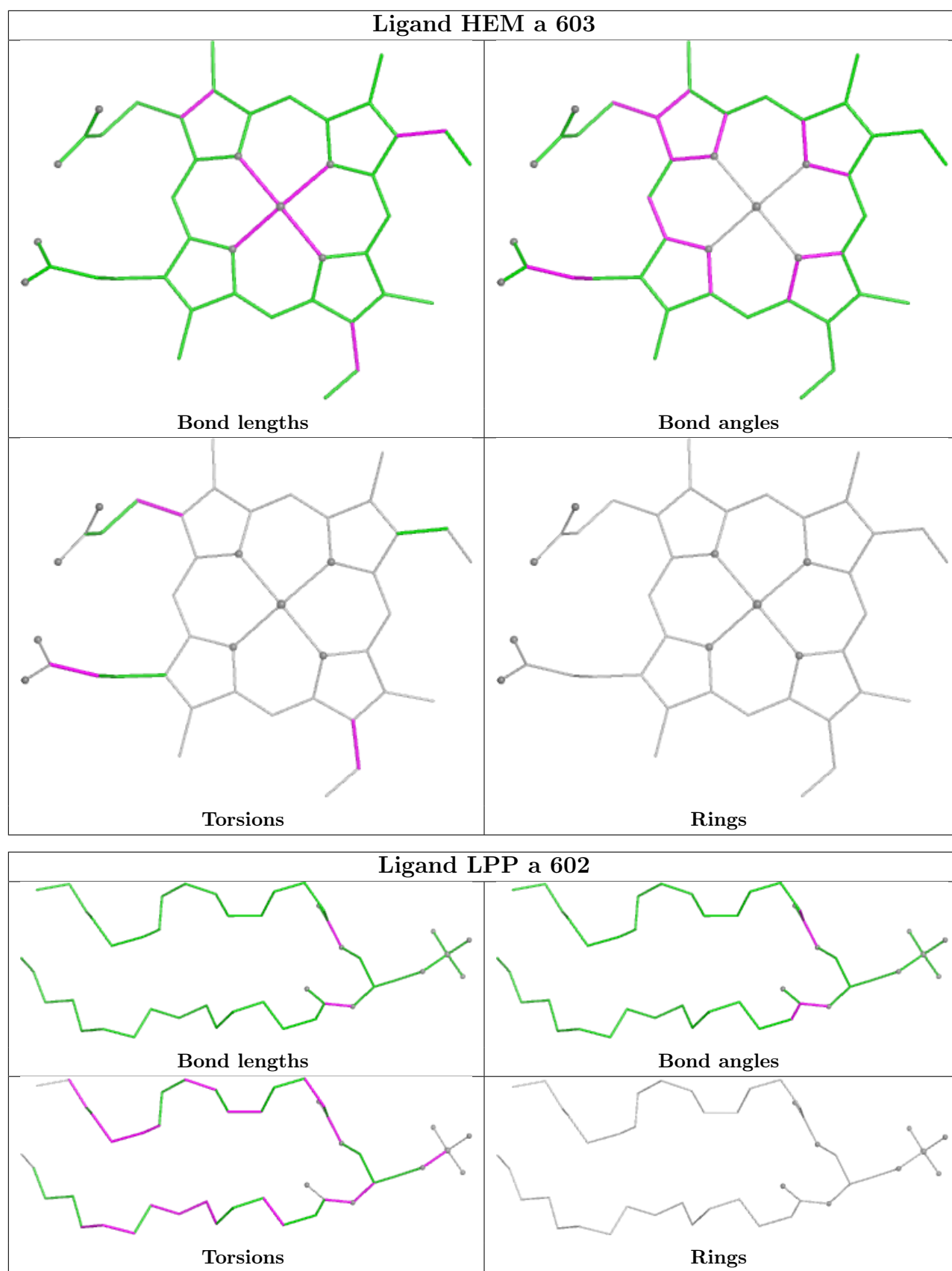






Ligand A1JN4 A 605





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.

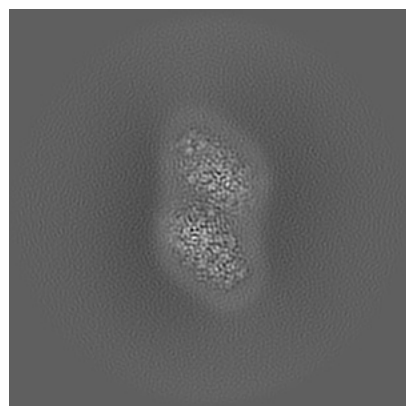
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54866. These allow visual inspection of the internal detail of the map and identification of artifacts.

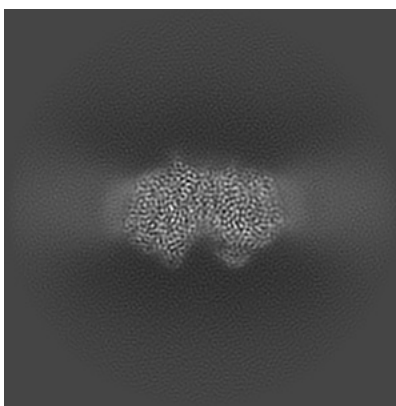
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

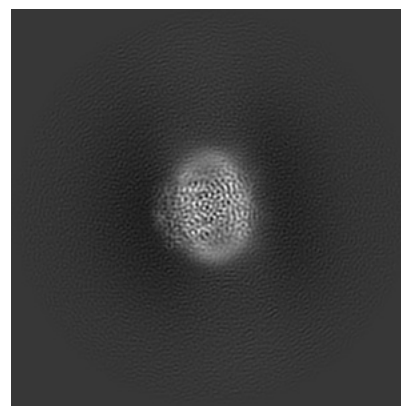
6.1.1 Primary map



X

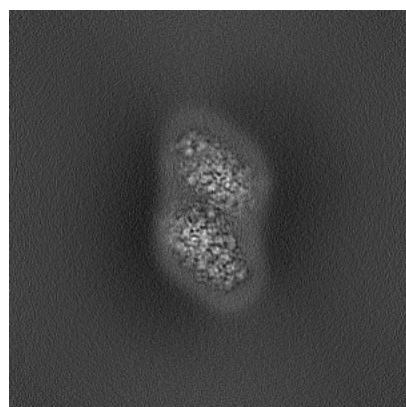


Y

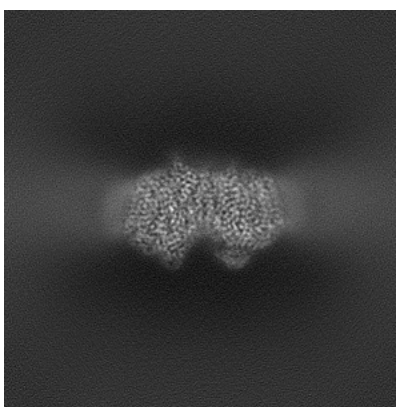


Z

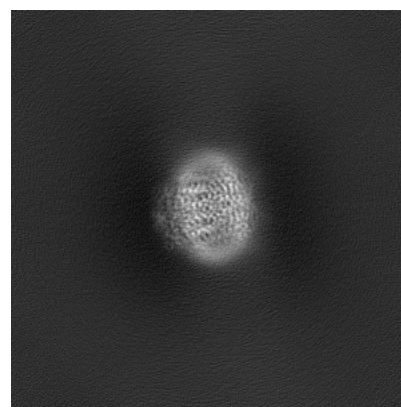
6.1.2 Raw map



X



Y

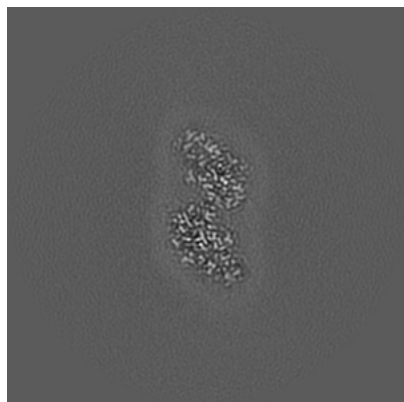


Z

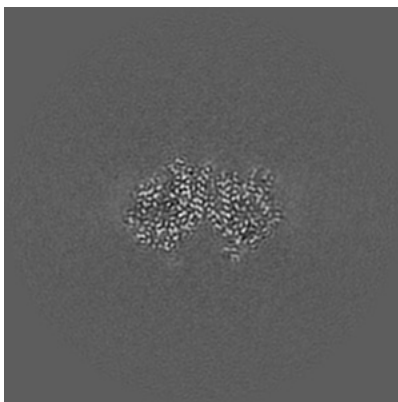
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

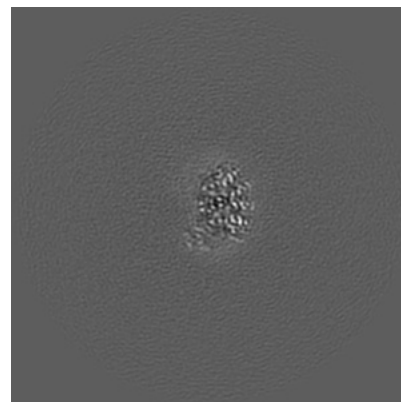
6.2.1 Primary map



X Index: 180

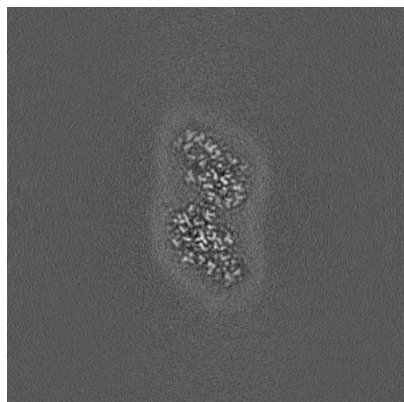


Y Index: 180

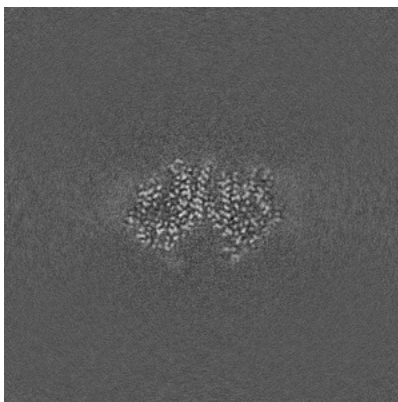


Z Index: 180

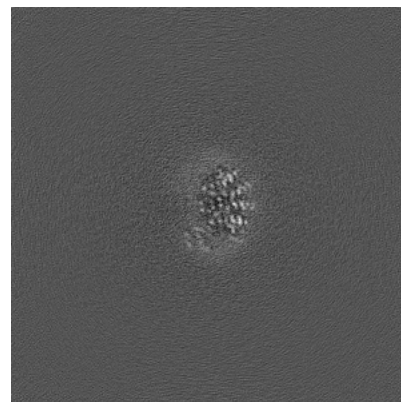
6.2.2 Raw map



X Index: 180



Y Index: 180

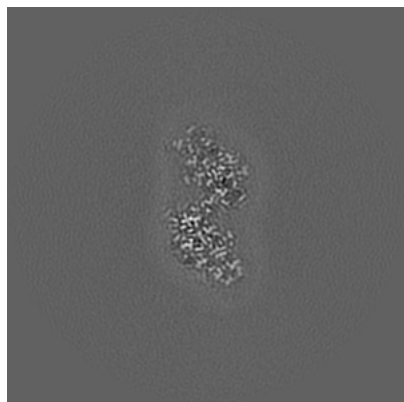


Z Index: 180

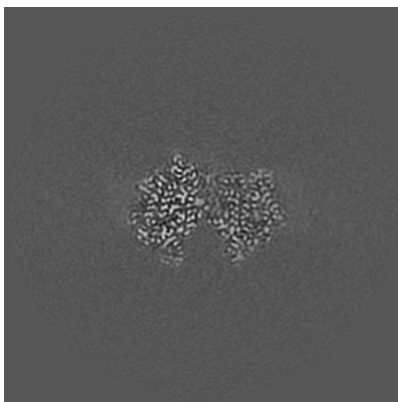
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

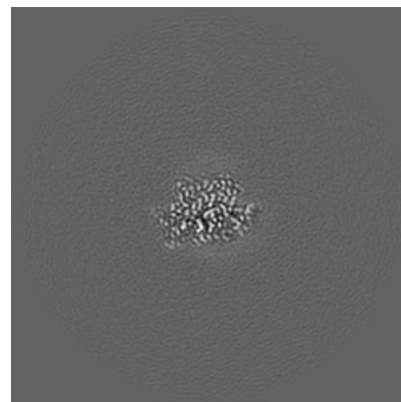
6.3.1 Primary map



X Index: 178

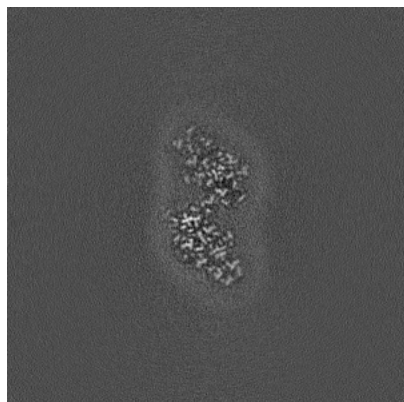


Y Index: 175

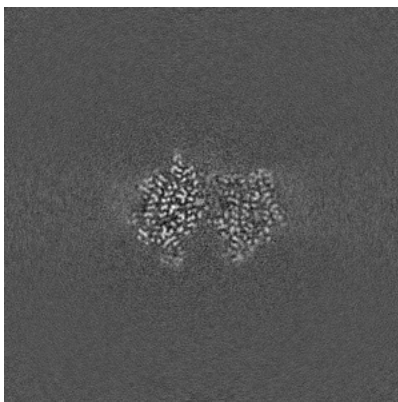


Z Index: 151

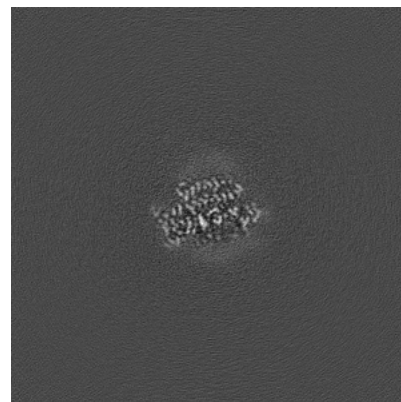
6.3.2 Raw map



X Index: 178



Y Index: 175

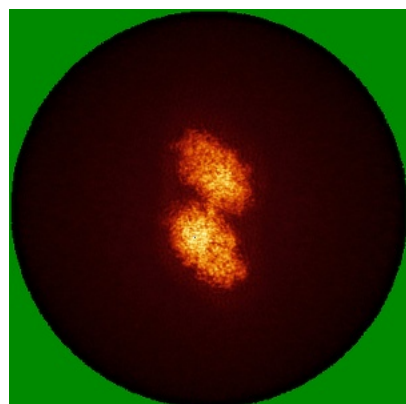


Z Index: 153

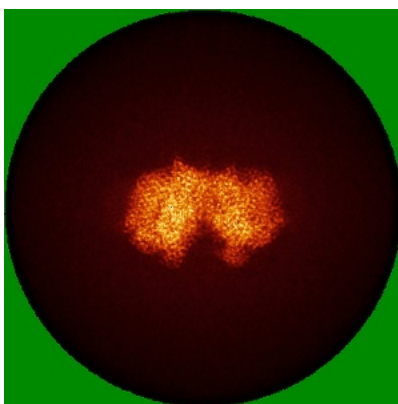
The images above show the largest variance slices of the map in three orthogonal directions.

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

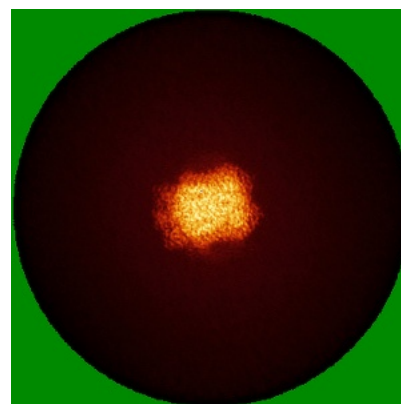
6.4.1 Primary map



X

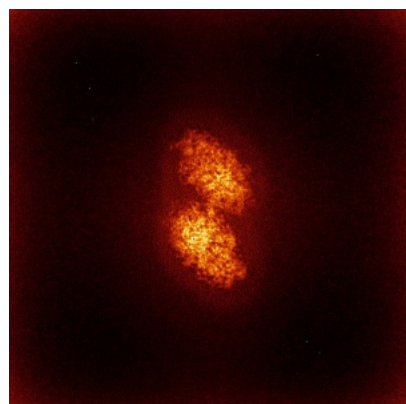


Y

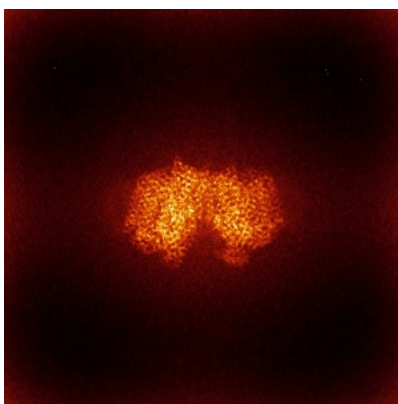


Z

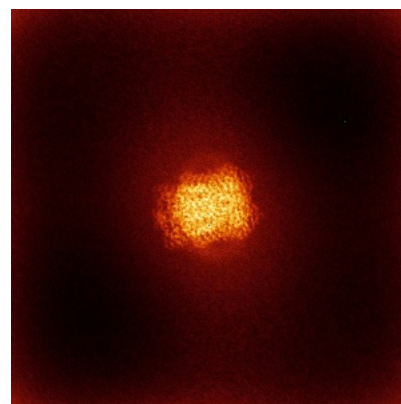
6.4.2 Raw map



X



Y

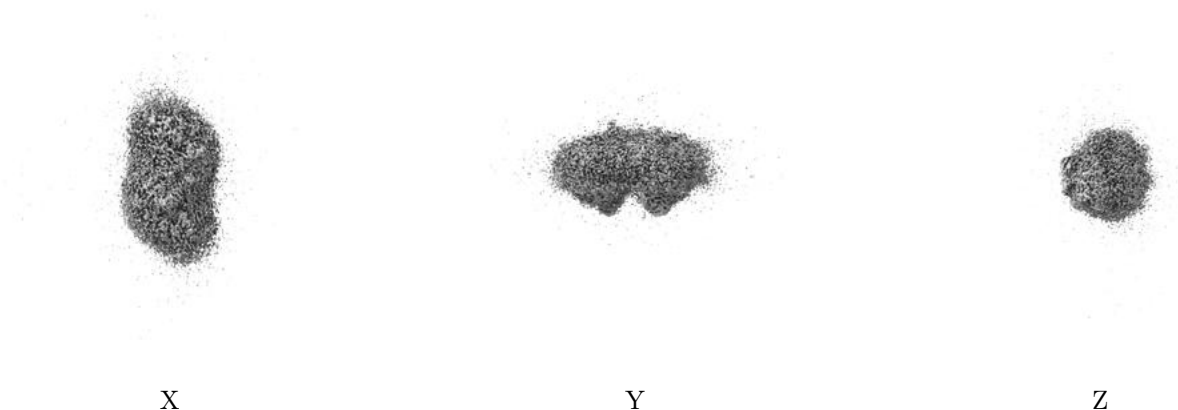


Z

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.

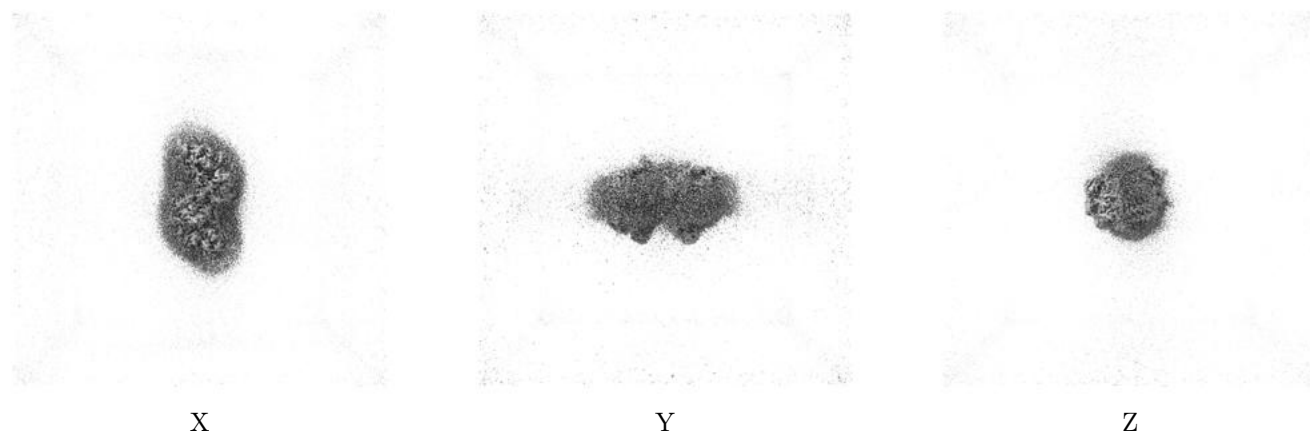
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0938. 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.

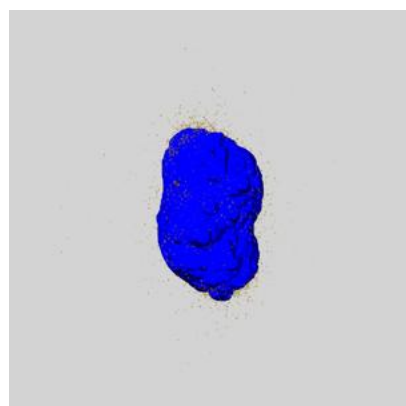
6.6 Mask visualisation [i](#)

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

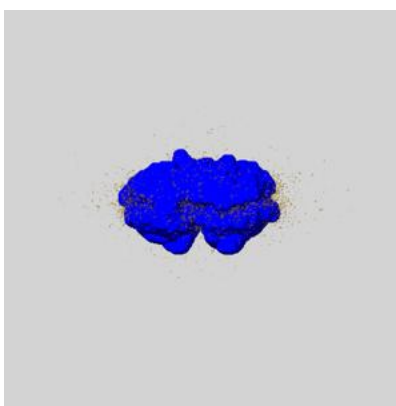
A mask typically either:

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

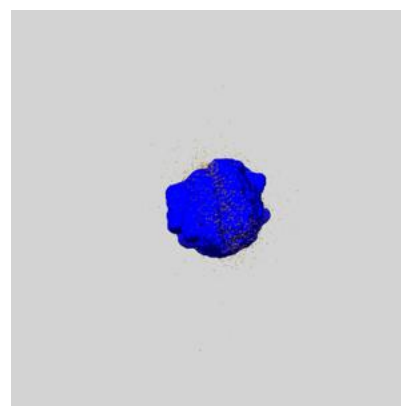
6.6.1 emd_54866_msk_1.map [i](#)



X



Y

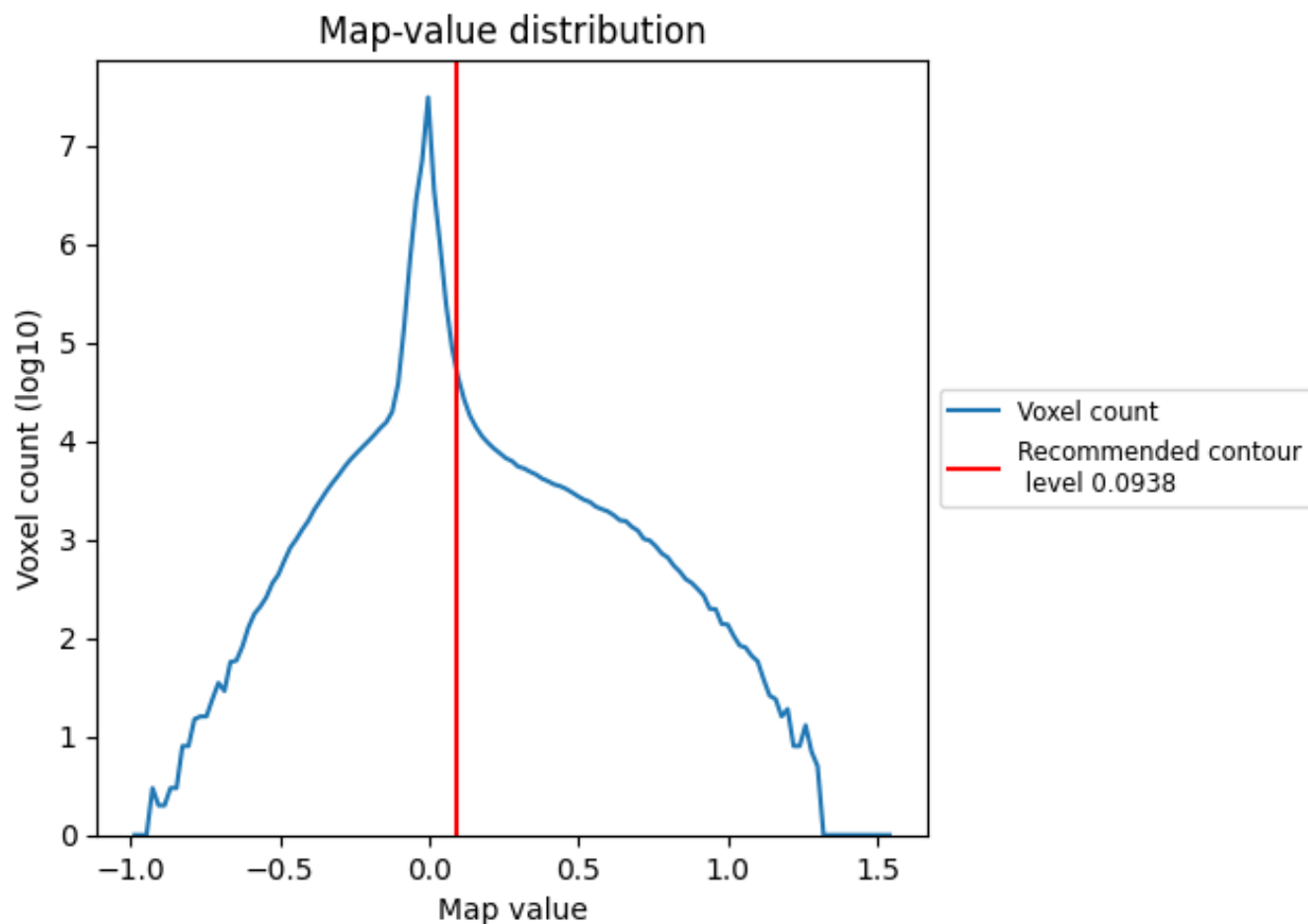


Z

7 Map analysis [i](#)

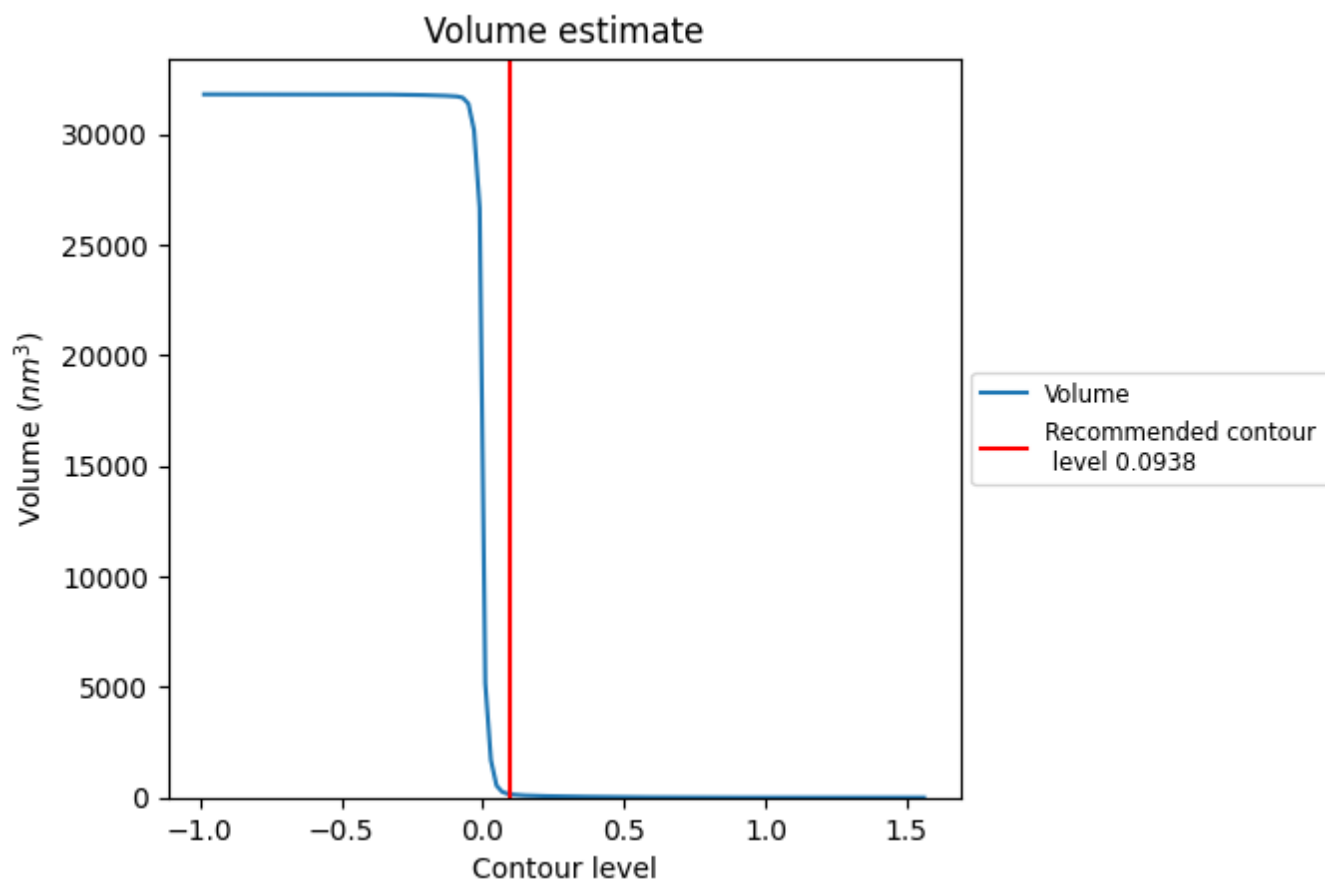
This section contains the results of statistical analysis of the map.

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.

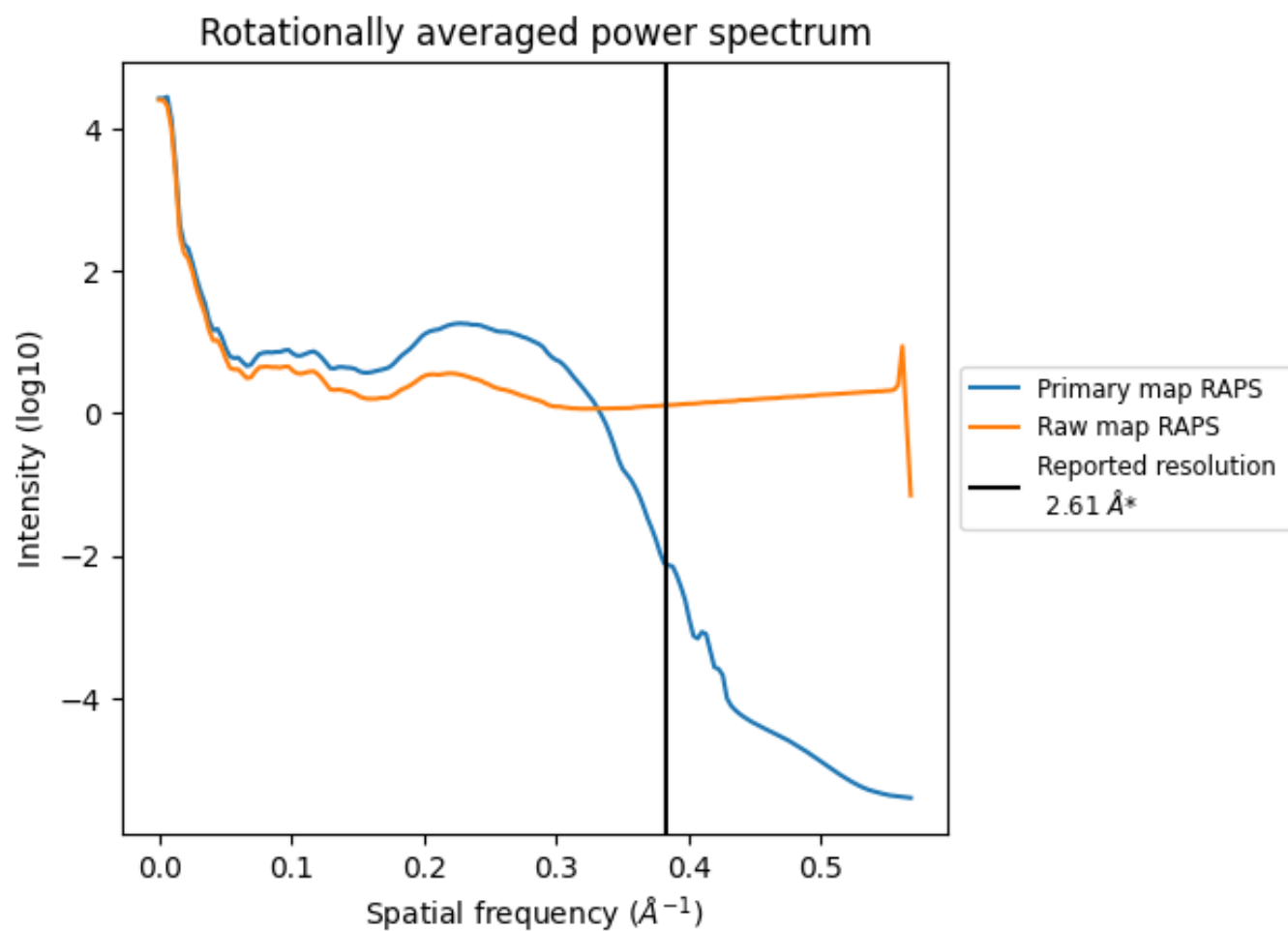
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 162 nm³; this corresponds to an approximate mass of 146 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

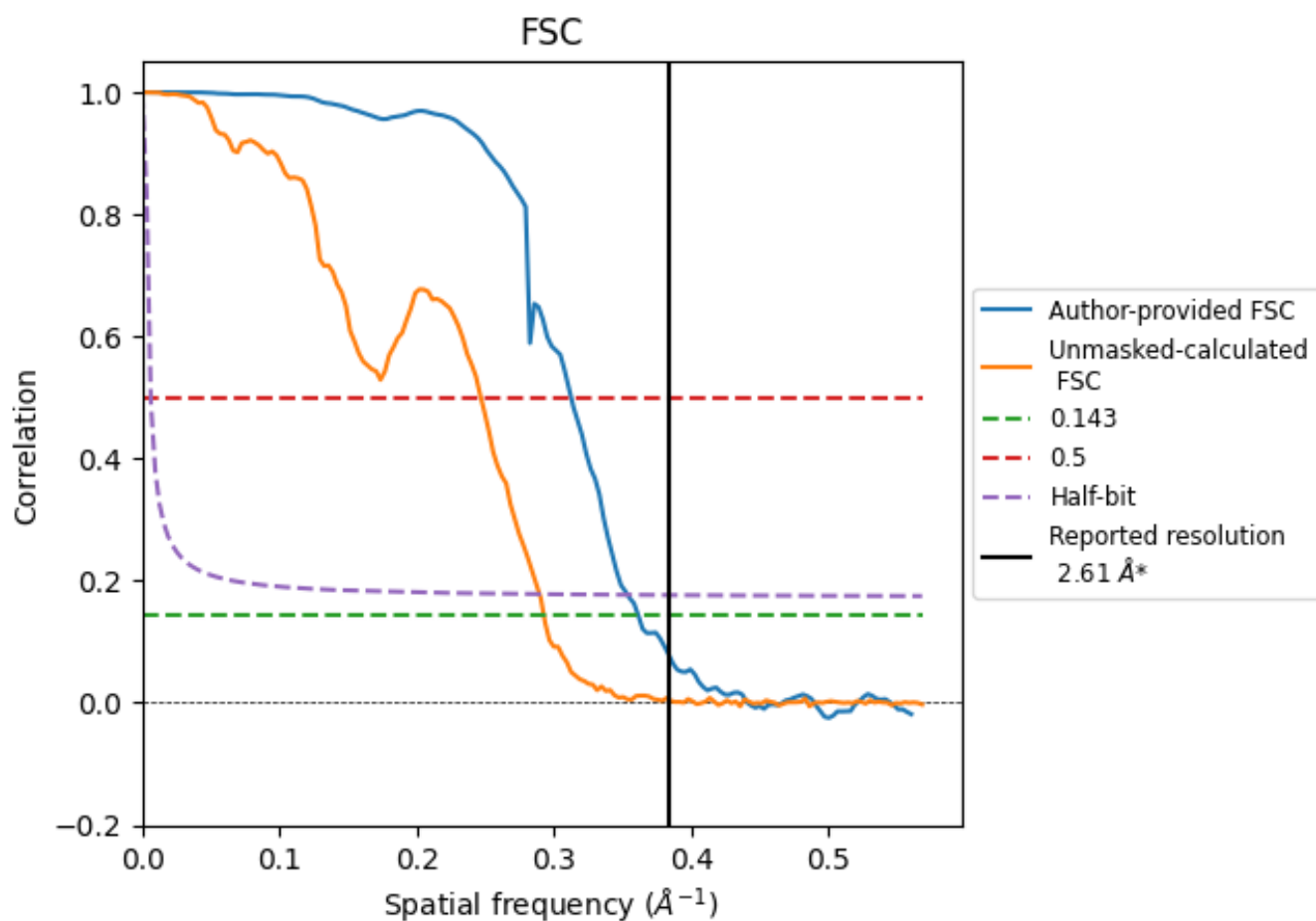


*Reported resolution corresponds to spatial frequency of 0.383 Å⁻¹

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 0.383 Å⁻¹

8.2 Resolution estimates [i](#)

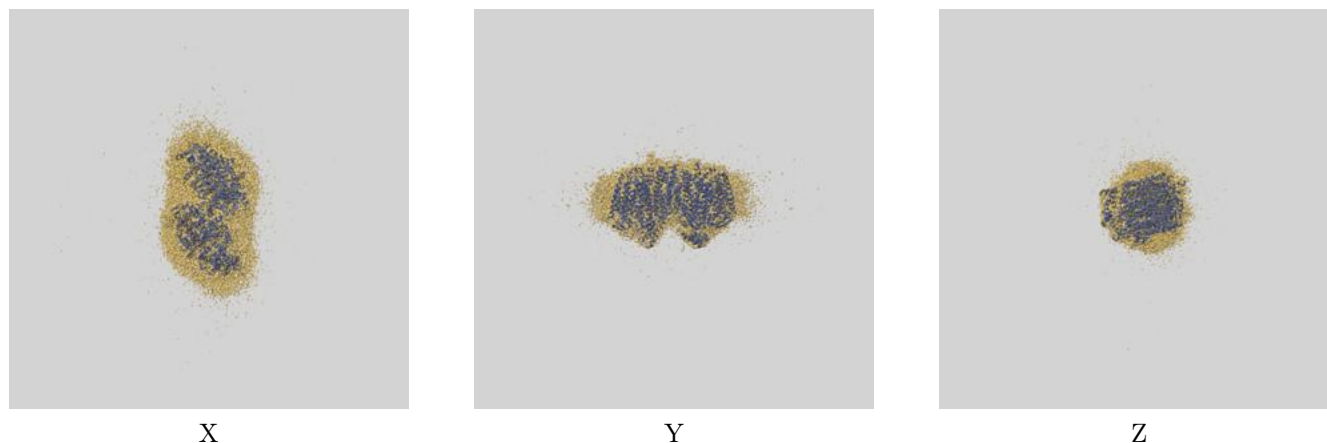
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.61	-	-
Author-provided FSC curve	2.77	3.20	2.83
Unmasked-calculated*	3.42	4.05	3.45

*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 3.42 differs from the reported value 2.61 by more than 10 %

9 Map-model fit [i](#)

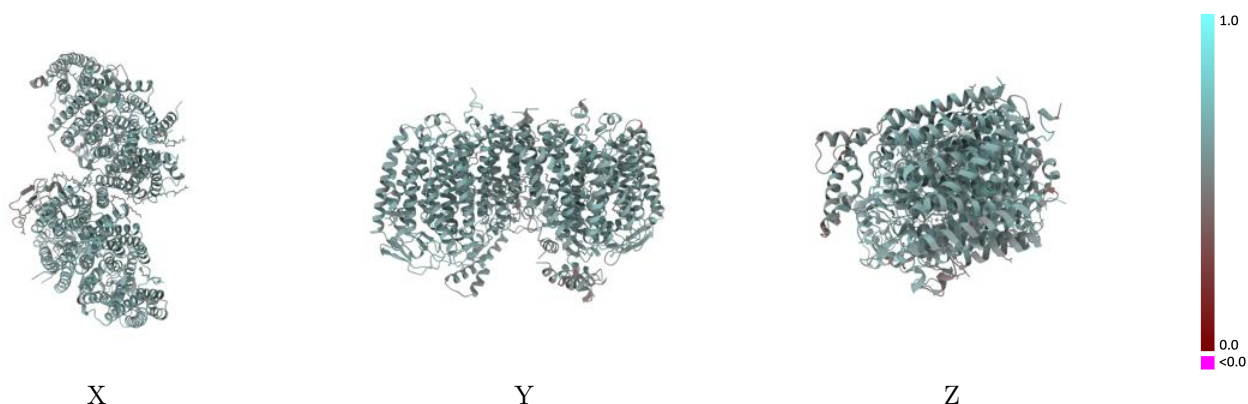
This section contains information regarding the fit between EMDB map EMD-54866 and PDB model 9SFV. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



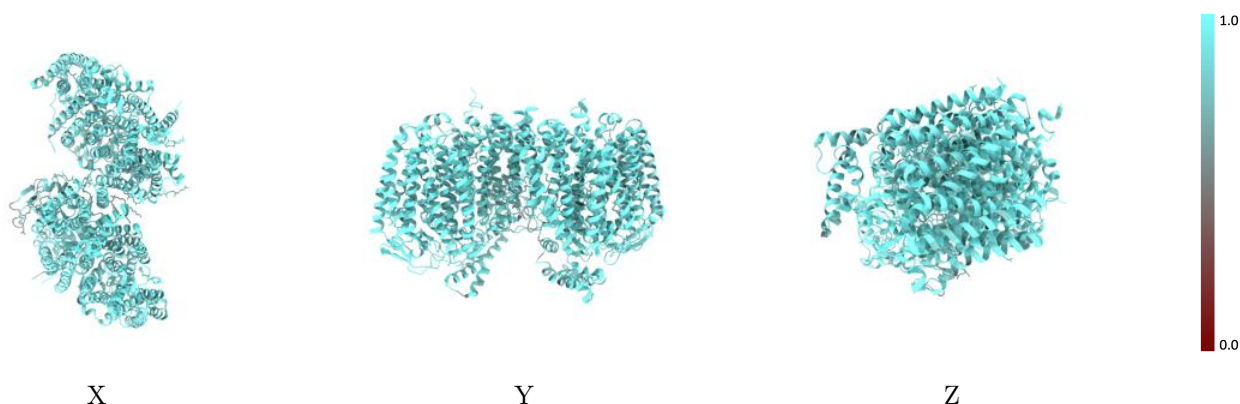
The images above show the 3D surface view of the map at the recommended contour level 0.0938 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



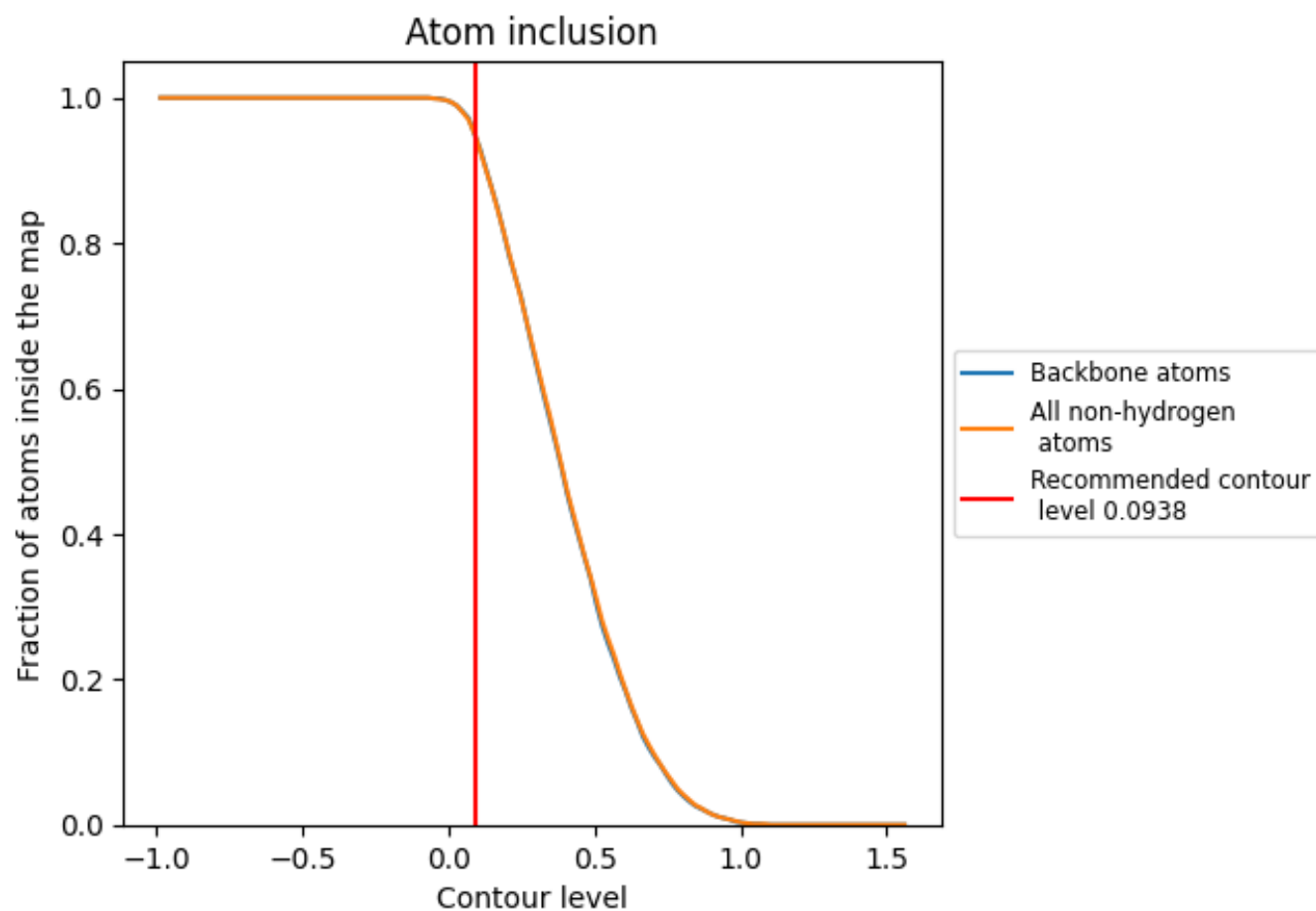
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0938).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% 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 (0.0938) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9460	0.5900
A	0.9460	0.5880
B	0.9420	0.5790
H	0.9570	0.5760
X	0.9450	0.5850
a	0.9450	0.5930
b	0.9610	0.6020
h	0.9380	0.5870
x	0.9300	0.5890

1.0

0.0

<0.0