



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 10:45 PM UTC

PDB ID : 8BGW / pdb_00008bgw
EMDB ID : EMD-16041
Title : CryoEM structure of quinol-dependent Nitric Oxide Reductase (qNOR) from *Alcaligenes xylosoxidans* at 2.2 Å resolution
Authors : Flynn, A.; Antonyuk, S.V.; Eady, R.R.; Muench, S.P.; Hasnain, S.S.
Deposited on : 2022-10-28
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

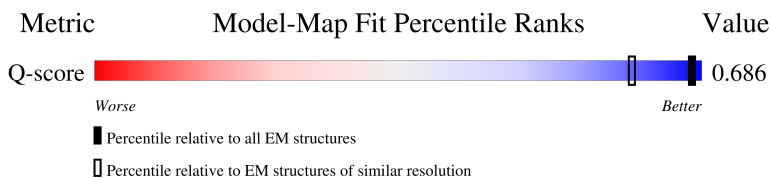
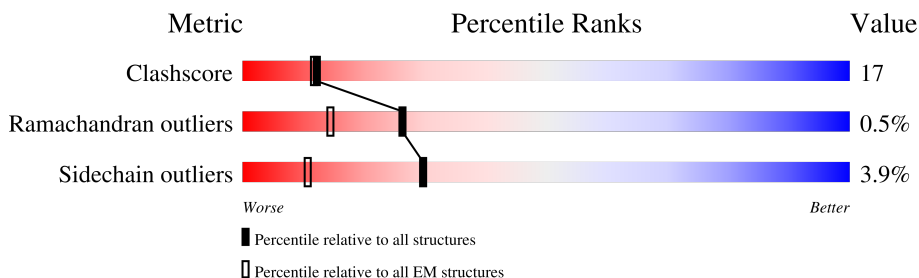
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 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	3184 (1.71 - 2.70)

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	761	
1	B	761	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	UQ1	A	806	-	-	X	-

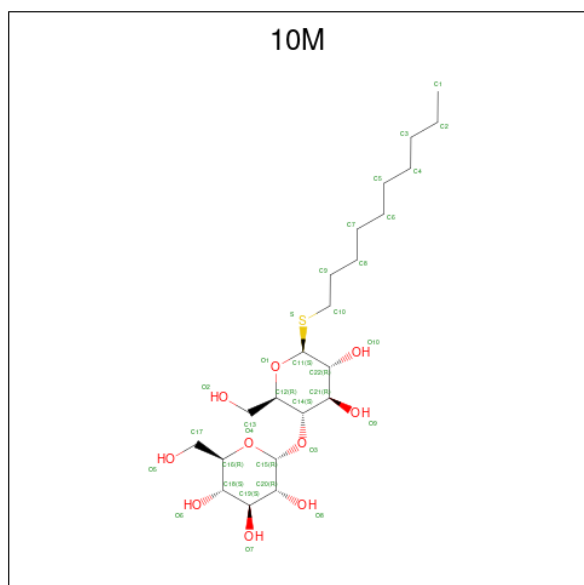
- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Fe	0
			1	1	
3	B	1	Total	Fe	0
			1	1	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

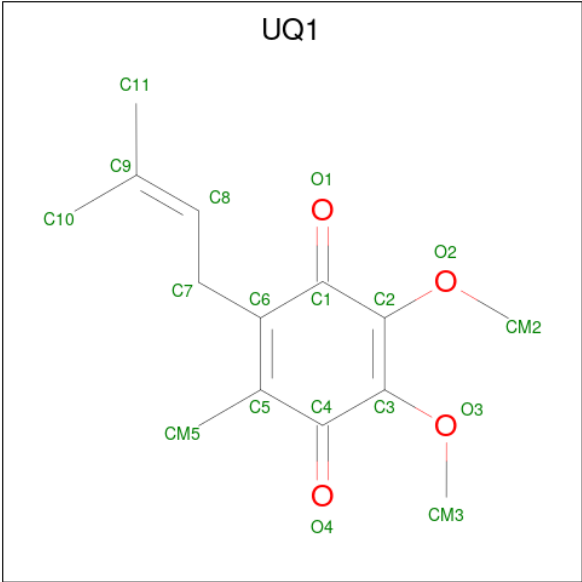
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	
4	B	1	Total	Ca	0
			1	1	

- Molecule 5 is decyl 4-O-alpha-D-glucopyranosyl-1-thio-beta-D-glucopyranoside (CCD ID: 10M) (formula: C₂₂H₄₂O₁₀S).



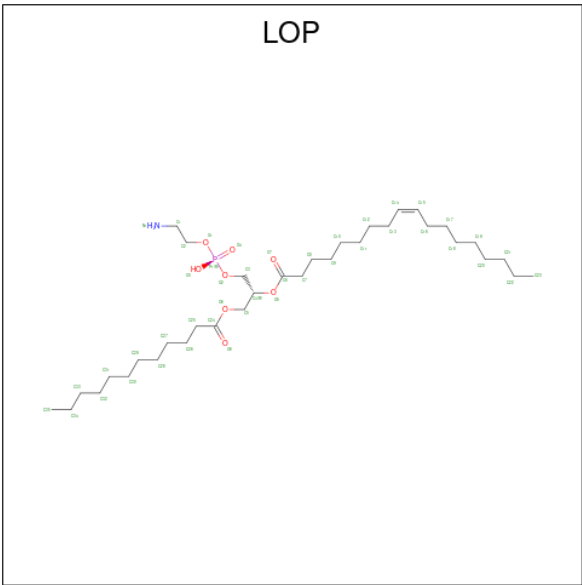
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	S	0
			33	22	10	1	
5	B	1	Total	C	O	S	0
			33	22	10	1	

- Molecule 6 is UBIQUINONE-1 (CCD ID: UQ1) (formula: C₁₄H₁₈O₄).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			18	14	4	
6	B	1	Total	C	O	0
			18	14	4	

- Molecule 7 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (CCD ID: LOP) (formula: C₃₅H₆₈NO₈P).



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Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	O			0
			36	32	4			
7	A	1	Total	C	O			0
			37	33	4			
7	A	1	Total	C	O			0
			25	23	2			
7	A	1	Total	C	O			0
			19	18	1			
7	A	1	Total	C				0
			25	25				
7	A	1	Total	C				0
			9	9				
7	B	1	Total	C	N	O	P	0
			42	32	1	8	1	
7	B	1	Total	C	O			0
			28	24	4			
7	B	1	Total	C	O			0
			37	33	4			
7	B	1	Total	C	O			0
			28	27	1			
7	B	1	Total	C	O			0
			14	12	2			
7	B	1	Total	C	O			0
			29	28	1			

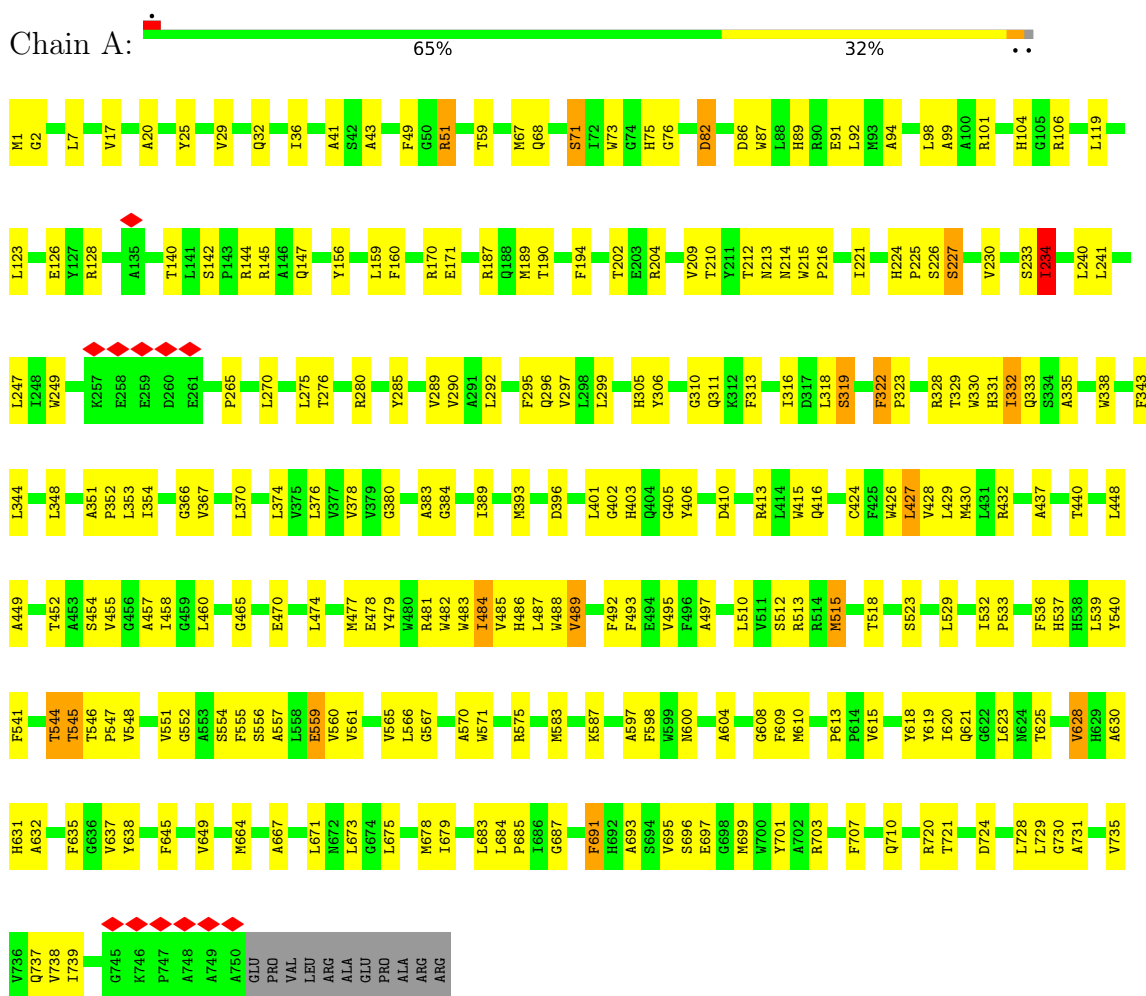
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	A	230	Total	O	0
			230	230	
8	B	219	Total	O	0
			219	219	

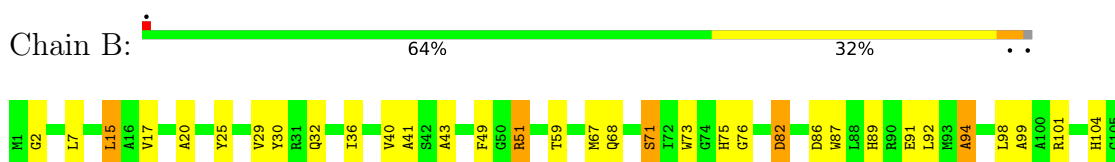
3 Residue-property plots

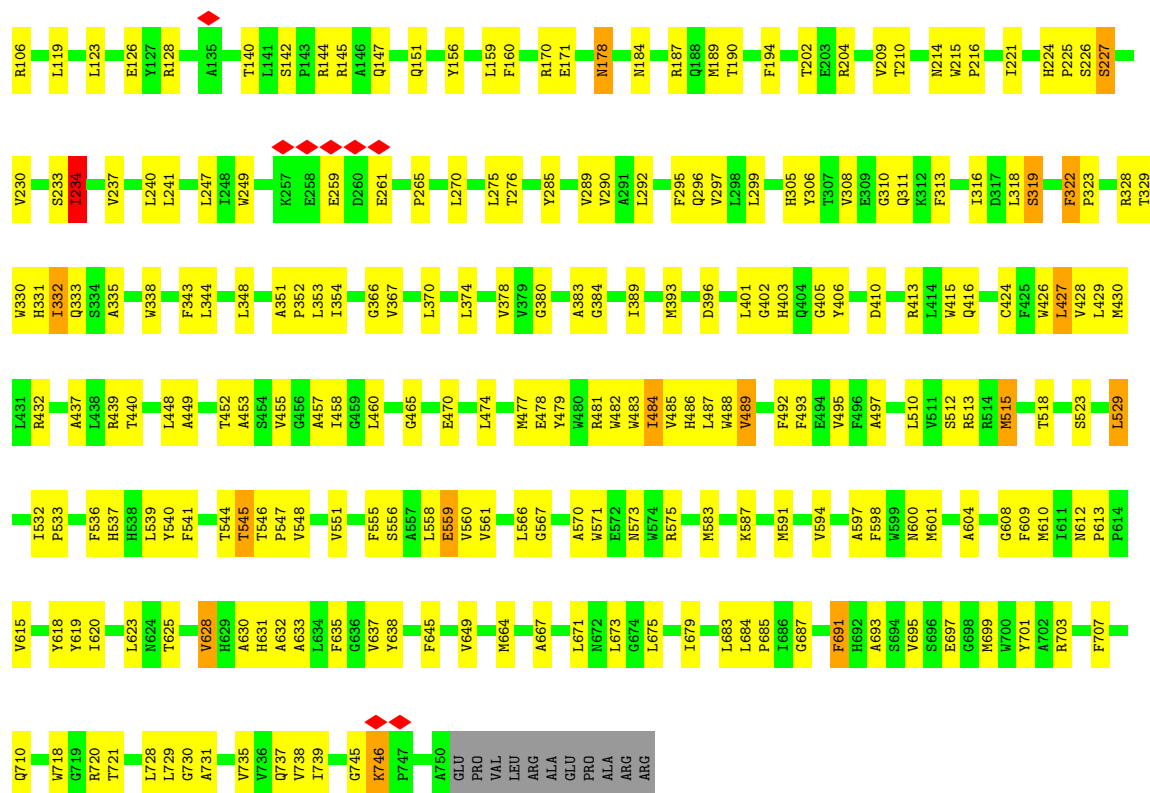
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Nitric oxide reductase subunit B



• Molecule 1: Nitric oxide reductase subunit B





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	404950	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	34.9	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.180	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	364.0, 364.0, 364.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.91, 0.91, 0.91	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, 10M, FE, CA, UQ1, LOP

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	0.92	1/6122 (0.0%)	1.55	14/8357 (0.2%)
1	B	0.91	1/6121 (0.0%)	1.54	14/8355 (0.2%)
All	All	0.91	2/12243 (0.0%)	1.55	28/16712 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	331	HIS	CD2-NE2	-5.07	1.32	1.37
1	B	331	HIS	CD2-NE2	-5.07	1.32	1.37

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ASP	CA-CB-CG	-8.00	104.60	112.60
1	B	82	ASP	CA-CB-CG	-7.91	104.69	112.60
1	B	635	PHE	CA-CB-CG	-7.03	106.77	113.80
1	A	635	PHE	CA-CB-CG	-7.02	106.78	113.80
1	A	598	PHE	CA-CB-CG	-6.24	107.56	113.80
1	B	598	PHE	CA-CB-CG	-6.21	107.59	113.80
1	A	628	VAL	N-CA-C	-5.83	104.64	110.30
1	B	628	VAL	N-CA-C	-5.83	104.64	110.30
1	A	545	THR	CA-C-N	5.80	128.24	120.58
1	A	545	THR	C-N-CA	5.80	128.24	120.58
1	A	89	HIS	CA-CB-CG	-5.77	108.03	113.80
1	B	89	HIS	CA-CB-CG	-5.76	108.03	113.80
1	B	545	THR	CA-C-N	5.75	128.16	120.58
1	B	545	THR	C-N-CA	5.75	128.16	120.58
1	A	631	HIS	CA-CB-CG	-5.67	108.14	113.80
1	B	631	HIS	CA-CB-CG	-5.62	108.18	113.80
1	A	322	PHE	CA-CB-CG	-5.50	108.30	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	PHE	CA-CB-CG	-5.45	108.35	113.80
1	A	691	PHE	N-CA-C	-5.40	105.40	111.28
1	B	94	ALA	N-CA-C	-5.38	105.33	111.14
1	A	94	ALA	N-CA-C	-5.37	105.34	111.14
1	A	234	ILE	N-CA-C	-5.36	105.50	110.53
1	B	691	PHE	N-CA-C	-5.36	105.44	111.28
1	B	234	ILE	N-CA-C	-5.34	105.51	110.53
1	B	383	ALA	N-CA-C	-5.33	105.39	111.14
1	A	383	ALA	N-CA-C	-5.23	105.47	111.07
1	B	329	THR	CA-CB-OG1	-5.08	101.98	109.60
1	A	329	THR	CA-CB-OG1	-5.08	101.99	109.60

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	5921	0	5855	213	0
1	B	5920	0	5851	212	0
2	A	86	0	60	10	0
2	B	86	0	60	11	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	33	0	42	7	0
5	B	33	0	42	16	0
6	A	18	0	18	7	0
6	B	18	0	18	6	0
7	A	181	0	286	7	0
7	B	178	0	274	3	0
8	A	230	0	0	16	0
8	B	219	0	0	12	0
All	All	12927	0	12506	426	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 17.

All (426) 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:B:305:HIS:ND1	6:B:806:UQ1:HM21	1.72	1.03
1:B:305:HIS:ND1	6:B:806:UQ1:CM2	2.32	0.92
1:A:230:VAL:HG13	5:A:805:10M:H6	1.50	0.91
1:B:529:LEU:HD11	1:B:558:LEU:HD13	1.59	0.81
1:B:233:SER:OG	1:B:615:VAL:HG12	1.80	0.81
1:B:305:HIS:CE1	6:B:806:UQ1:HM21	2.16	0.81
1:A:270:LEU:HD22	1:A:353:LEU:HD11	1.64	0.80
1:A:233:SER:OG	1:A:615:VAL:HG12	1.80	0.80
1:A:454:SER:OG	1:A:495:VAL:HG12	1.82	0.80
6:A:806:UQ1:C8	6:A:806:UQ1:HM51	2.11	0.79
1:B:270:LEU:HD22	1:B:353:LEU:HD11	1.64	0.78
1:A:615:VAL:HG21	5:A:805:10M:H7A	1.66	0.77
1:A:214:ASN:ND2	8:A:901:HOH:O	2.19	0.76
1:B:86:ASP:OD2	1:B:156:TYR:OH	2.04	0.75
1:B:529:LEU:CD1	1:B:558:LEU:HD13	2.16	0.75
1:A:86:ASP:OD2	1:A:156:TYR:OH	2.04	0.75
2:A:801:HEM:HBC2	2:A:801:HEM:HMC2	1.69	0.75
2:B:802:HEM:HBC2	2:B:802:HEM:HMC2	1.69	0.74
1:B:75:HIS:HD2	1:B:478:GLU:OE2	1.73	0.71
1:B:311:GLN:HA	1:B:319:SER:OG	1.91	0.70
1:A:311:GLN:HA	1:A:319:SER:OG	1.91	0.70
1:B:59:THR:HG22	1:B:470:GLU:HG2	1.74	0.70
1:A:59:THR:HG22	1:A:470:GLU:HG2	1.75	0.69
1:A:483:TRP:O	1:A:487:LEU:HB3	1.93	0.68
1:B:483:TRP:O	1:B:487:LEU:HB3	1.93	0.68
1:B:30:TYR:HB3	7:B:811:LOP:H321	1.76	0.68
1:A:25:TYR:O	1:A:29:VAL:HG23	1.94	0.68
1:B:628:VAL:HG13	1:B:679:ILE:HG23	1.76	0.68
1:A:544:THR:HG21	1:A:548:VAL:HG11	1.75	0.67
1:A:628:VAL:HG13	1:A:679:ILE:HG23	1.76	0.67
1:B:25:TYR:O	1:B:29:VAL:HG23	1.95	0.67
1:A:249:TRP:CE3	1:B:567:GLY:HA2	2.31	0.65
1:A:567:GLY:HA2	1:B:249:TRP:CE3	2.31	0.65
1:A:224:HIS:HB2	8:A:929:HOH:O	1.96	0.64
1:A:495:VAL:HG11	7:A:807:LOP:C21	2.27	0.64
1:B:187:ARG:O	1:B:190:THR:OG1	2.14	0.64
1:B:234:ILE:HG12	5:B:801:10M:H4	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:MET:SD	1:B:737:GLN:HG2	2.39	0.63
1:B:465:GLY:N	1:B:484:ILE:HD11	2.14	0.63
1:B:75:HIS:HD2	1:B:478:GLU:CD	2.07	0.62
1:A:664:MET:SD	1:A:737:GLN:HG2	2.39	0.62
1:A:465:GLY:N	1:A:484:ILE:HD11	2.14	0.62
1:A:537:HIS:HA	1:A:540:TYR:CE1	2.34	0.62
1:B:537:HIS:HA	1:B:540:TYR:CE1	2.34	0.62
1:A:619:TYR:CE2	5:B:801:10M:H10A	2.34	0.62
1:B:99:ALA:HB1	1:B:119:LEU:HD22	1.82	0.62
1:B:224:HIS:HB2	8:B:941:HOH:O	2.00	0.62
1:B:684:LEU:HA	8:B:977:HOH:O	2.00	0.61
1:B:731:ALA:O	1:B:735:VAL:HG23	2.00	0.61
5:B:801:10M:O9	5:B:801:10M:O1	2.11	0.61
1:A:695:VAL:HG21	1:B:230:VAL:HG11	1.82	0.61
1:A:99:ALA:HB1	1:A:119:LEU:HD22	1.82	0.61
1:A:230:VAL:HG11	1:B:695:VAL:HG21	1.81	0.61
1:A:632:ALA:HB2	1:A:679:ILE:HD11	1.83	0.61
1:A:731:ALA:O	1:A:735:VAL:HG23	2.01	0.61
1:B:632:ALA:HB2	1:B:679:ILE:HD11	1.83	0.61
1:A:187:ARG:O	1:A:190:THR:OG1	2.14	0.61
1:A:684:LEU:HA	8:A:985:HOH:O	2.00	0.60
1:B:15:LEU:HD21	7:B:809:LOP:H352	1.83	0.60
1:A:75:HIS:HD1	1:A:478:GLU:CD	2.09	0.59
1:A:213:ASN:HB3	8:A:947:HOH:O	2.02	0.59
1:A:29:VAL:HG22	1:A:544:THR:CG2	2.33	0.59
1:B:230:VAL:HG13	5:B:801:10M:C8	2.33	0.58
1:B:87:TRP:CD1	1:B:87:TRP:C	2.82	0.58
1:B:510:LEU:HD11	1:B:583:MET:SD	2.44	0.58
1:B:308:VAL:CG2	6:B:806:UQ1:HM23	2.34	0.58
1:A:230:VAL:HG13	5:A:805:10M:C6	2.28	0.58
5:A:805:10M:H1A	5:B:801:10M:H2A	1.86	0.58
1:B:214:ASN:O	1:B:618:TYR:OH	2.17	0.58
1:B:316:ILE:HG23	1:B:318:LEU:CD2	2.34	0.58
1:B:126:GLU:OE2	1:B:142:SER:OG	2.20	0.58
1:A:316:ILE:HG23	1:A:318:LEU:CD2	2.34	0.57
1:A:512:SER:HG	1:A:515:MET:H	1.52	0.57
1:B:270:LEU:CD2	1:B:353:LEU:HD21	2.34	0.57
1:A:270:LEU:CD2	1:A:353:LEU:HD21	2.34	0.57
1:A:510:LEU:HD11	1:A:583:MET:SD	2.44	0.57
1:A:354:ILE:HG21	1:A:448:LEU:HD11	1.86	0.57
1:B:71:SER:OG	1:B:703:ARG:NH1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:TRP:CH2	1:B:575:ARG:HD2	2.39	0.57
1:A:571:TRP:CH2	1:A:575:ARG:HD2	2.39	0.57
1:B:354:ILE:HG21	1:B:448:LEU:HD11	1.87	0.57
1:A:87:TRP:C	1:A:87:TRP:CD1	2.82	0.56
1:A:126:GLU:OE2	1:A:142:SER:OG	2.20	0.56
1:A:233:SER:HG	1:A:615:VAL:HG12	1.70	0.56
1:B:295:PHE:CE2	1:B:299:LEU:HD11	2.41	0.56
1:B:539:LEU:HB3	1:B:544:THR:HG21	1.87	0.56
1:B:512:SER:HG	1:B:515:MET:H	1.52	0.56
1:A:214:ASN:CG	8:A:901:HOH:O	2.48	0.56
1:A:71:SER:OG	1:A:703:ARG:NH1	2.38	0.55
1:A:721:THR:HA	6:A:806:UQ1:HM53	1.88	0.55
1:A:667:ALA:O	1:A:671:LEU:HG	2.07	0.55
1:A:424:CYS:O	1:A:427:LEU:HB3	2.07	0.55
1:B:305:HIS:ND1	6:B:806:UQ1:O2	2.39	0.54
1:A:68:GLN:NE2	1:A:410:ASP:OD2	2.31	0.54
1:B:424:CYS:O	1:B:427:LEU:HB3	2.07	0.54
1:A:566:LEU:HD12	1:A:600:ASN:HB3	1.90	0.54
1:A:212:THR:OG1	1:A:215:TRP:O	2.22	0.54
1:A:230:VAL:HG22	5:A:805:10M:H7A	1.88	0.54
1:A:295:PHE:CE2	1:A:299:LEU:HD11	2.41	0.54
1:B:230:VAL:HG13	5:B:801:10M:H8	1.88	0.54
1:B:573:ASN:HB2	8:B:961:HOH:O	2.06	0.54
1:B:667:ALA:O	1:B:671:LEU:HG	2.07	0.54
1:A:495:VAL:HG11	7:A:807:LOP:H211	1.90	0.54
1:B:566:LEU:HD12	1:B:600:ASN:HB3	1.90	0.54
1:B:403:HIS:CE1	1:B:410:ASP:HB3	2.43	0.53
1:A:403:HIS:CE1	1:A:410:ASP:HB3	2.43	0.53
1:A:36:ILE:HG22	1:A:51:ARG:HA	1.91	0.53
1:A:615:VAL:HG22	5:B:801:10M:H7A	1.91	0.53
1:B:237:VAL:HG21	5:B:801:10M:H2	1.89	0.53
5:B:801:10M:O9	5:B:801:10M:S	2.65	0.53
1:A:544:THR:CG2	1:A:548:VAL:HG21	2.39	0.53
1:A:214:ASN:O	1:A:618:TYR:OH	2.17	0.53
1:A:413:ARG:NE	1:A:416:GLN:OE1	2.40	0.53
1:B:68:GLN:NE2	1:B:410:ASP:OD2	2.31	0.53
1:B:36:ILE:HG22	1:B:51:ARG:HA	1.90	0.52
1:B:474:LEU:O	1:B:478:GLU:HG2	2.10	0.52
1:A:479:TYR:HA	1:A:539:LEU:HD11	1.92	0.52
2:A:801:HEM:HMB1	2:A:801:HEM:HBB2	1.92	0.52
1:B:128:ARG:HD2	1:B:221:ILE:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:TYR:CZ	5:B:801:10M:H10A	2.44	0.52
1:B:171:GLU:O	1:B:310:GLY:HA3	2.10	0.52
1:A:305:HIS:ND1	6:A:806:UQ1:HM21	2.25	0.52
1:B:707:PHE:CE1	1:B:710:GLN:NE2	2.77	0.52
1:B:683:LEU:HD21	1:B:720:ARG:NH1	2.25	0.51
2:B:803:HEM:HMB1	2:B:803:HEM:HBB2	1.92	0.51
1:A:351:ALA:HB3	1:A:352:PRO:HD3	1.92	0.51
1:B:230:VAL:HG21	5:B:801:10M:H10	1.91	0.51
1:A:171:GLU:O	1:A:310:GLY:HA3	2.10	0.51
1:A:299:LEU:HD13	1:A:330:TRP:HB3	1.93	0.51
1:A:683:LEU:HD21	1:A:720:ARG:NH1	2.25	0.51
1:B:71:SER:HG	1:B:703:ARG:HH12	1.55	0.51
1:B:479:TYR:HA	1:B:539:LEU:HD11	1.91	0.51
1:A:128:ARG:HD2	1:A:221:ILE:O	2.10	0.51
1:A:474:LEU:O	1:A:478:GLU:HG2	2.11	0.51
1:B:299:LEU:HD13	1:B:330:TRP:HB3	1.93	0.51
1:B:348:LEU:HD11	1:B:370:LEU:HD23	1.93	0.51
1:A:495:VAL:HG11	7:A:807:LOP:H212	1.92	0.51
1:B:210:THR:OG1	1:B:214:ASN:N	2.42	0.51
1:B:560:VAL:HG21	1:B:609:PHE:HB2	1.93	0.51
1:A:565:VAL:HB	7:A:813:LOP:H312	1.92	0.50
1:A:428:VAL:O	1:A:432:ARG:HG2	2.11	0.50
1:A:270:LEU:HD22	1:A:353:LEU:CD1	2.38	0.50
1:A:533:PRO:HB2	1:A:555:PHE:CB	2.42	0.50
1:A:615:VAL:HG13	5:B:801:10M:C5	2.41	0.50
1:B:428:VAL:O	1:B:432:ARG:HG2	2.11	0.50
1:A:348:LEU:HD11	1:A:370:LEU:HD23	1.93	0.50
1:A:560:VAL:HG21	1:A:609:PHE:HB2	1.93	0.50
1:A:632:ALA:HA	1:A:675:LEU:HD21	1.93	0.50
1:B:7:LEU:HD11	1:B:518:THR:HG23	1.93	0.50
1:A:7:LEU:HD11	1:A:518:THR:HG23	1.93	0.50
1:A:210:THR:OG1	1:A:214:ASN:N	2.42	0.50
1:A:615:VAL:HG13	5:B:801:10M:H5	1.94	0.50
1:B:151:GLN:NE2	8:B:918:HOH:O	2.44	0.50
1:A:73:TRP:HA	1:A:215:TRP:CZ3	2.47	0.50
1:A:98:LEU:HB3	1:A:144:ARG:HD3	1.93	0.49
1:A:559:GLU:HA	8:A:911:HOH:O	2.11	0.49
1:B:735:VAL:O	1:B:739:ILE:HG12	2.12	0.49
1:B:351:ALA:HB3	1:B:352:PRO:HD3	1.92	0.49
1:A:344:LEU:HD22	1:A:426:TRP:CD2	2.48	0.49
5:A:805:10M:H8A	1:B:619:TYR:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:GLN:HG3	8:B:1005:HOH:O	2.13	0.49
1:B:406:TYR:CE1	1:B:477:MET:HE2	2.47	0.49
1:B:413:ARG:NE	1:B:416:GLN:OE1	2.41	0.49
1:B:632:ALA:HA	1:B:675:LEU:HD21	1.93	0.49
1:A:406:TYR:CE1	1:A:477:MET:HE2	2.48	0.49
1:B:73:TRP:HA	1:B:215:TRP:CZ3	2.47	0.49
1:B:344:LEU:HD22	1:B:426:TRP:CD2	2.48	0.49
1:B:98:LEU:HB3	1:B:144:ARG:HD3	1.93	0.49
1:A:707:PHE:CE1	1:A:710:GLN:NE2	2.77	0.49
2:A:802:HEM:HMB1	2:A:802:HEM:HBB2	1.93	0.49
1:B:276:THR:HG21	1:B:352:PRO:HB2	1.94	0.49
2:B:802:HEM:HMB1	2:B:802:HEM:HBB2	1.93	0.49
1:A:735:VAL:O	1:A:739:ILE:HG12	2.12	0.49
1:B:344:LEU:HD22	1:B:426:TRP:CG	2.48	0.49
1:B:533:PRO:HB2	1:B:555:PHE:CB	2.42	0.49
1:A:240:LEU:HD22	1:A:609:PHE:CD1	2.48	0.49
1:A:276:THR:HG21	1:A:352:PRO:HB2	1.94	0.49
1:A:537:HIS:HD1	1:A:556:SER:CB	2.25	0.48
1:A:615:VAL:HG21	5:A:805:10M:C7	2.40	0.48
1:A:227:SER:HB2	8:A:1002:HOH:O	2.13	0.48
1:A:487:LEU:HD11	1:A:532:ILE:HG12	1.96	0.48
1:B:240:LEU:HD22	1:B:609:PHE:CD1	2.48	0.48
1:B:537:HIS:HD1	1:B:556:SER:CB	2.25	0.48
1:B:610:MET:HE2	8:B:944:HOH:O	2.13	0.48
1:A:1:MET:HE2	7:A:807:LOP:H91	1.94	0.48
1:A:570:ALA:HB2	1:A:597:ALA:CB	2.44	0.48
1:A:566:LEU:CD1	1:A:600:ASN:HB3	2.44	0.48
1:B:270:LEU:HD22	1:B:353:LEU:CD1	2.38	0.48
1:B:457:ALA:HB1	1:B:492:PHE:CG	2.49	0.48
1:A:489:VAL:O	1:A:493:PHE:HB2	2.14	0.48
1:B:489:VAL:O	1:B:493:PHE:HB2	2.13	0.48
1:B:620:ILE:HA	1:B:623:LEU:HD12	1.96	0.48
1:A:610:MET:HE2	8:A:952:HOH:O	2.13	0.48
1:B:570:ALA:HB2	1:B:597:ALA:CB	2.44	0.48
1:A:92:LEU:HB3	1:A:123:LEU:HD21	1.95	0.48
1:A:620:ILE:HA	1:A:623:LEU:HD12	1.96	0.48
6:A:806:UQ1:HM51	6:A:806:UQ1:H8	1.93	0.47
1:B:366:GLY:HA3	1:B:429:LEU:HD21	1.96	0.47
1:B:693:ALA:HB2	1:B:707:PHE:CZ	2.49	0.47
1:B:746:LYS:HG3	1:B:746:LYS:O	2.14	0.47
1:A:344:LEU:HD22	1:A:426:TRP:CG	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:ALA:HB2	1:A:707:PHE:CZ	2.49	0.47
1:B:92:LEU:HB3	1:B:123:LEU:HD21	1.95	0.47
1:B:94:ALA:HB1	1:B:151:GLN:HE21	1.79	0.47
1:B:184:ASN:OD1	1:B:187:ARG:NH2	2.48	0.47
1:B:209:VAL:HG22	1:B:226:SER:OG	2.15	0.47
1:B:487:LEU:HD11	1:B:532:ILE:HG12	1.96	0.47
1:A:233:SER:HG	1:A:615:VAL:CG1	2.28	0.47
1:A:541:PHE:CZ	1:A:618:TYR:HA	2.50	0.47
1:A:544:THR:HG22	1:A:548:VAL:HG21	1.96	0.47
1:B:306:TYR:OH	1:B:322:PHE:O	2.30	0.47
1:B:541:PHE:CZ	1:B:618:TYR:HA	2.50	0.47
1:B:532:ILE:HB	1:B:533:PRO:HD3	1.97	0.47
1:B:393:MET:HE3	1:B:402:GLY:HA2	1.96	0.47
1:B:566:LEU:CD1	1:B:600:ASN:HB3	2.44	0.47
1:A:393:MET:HE3	1:A:402:GLY:HA2	1.96	0.47
1:A:449:ALA:O	1:A:452:THR:HG22	2.14	0.47
1:A:561:VAL:HG11	7:A:809:LOP:H201	1.96	0.47
1:B:32:GLN:O	1:B:204:ARG:NH1	2.43	0.47
1:B:625:THR:OG1	8:B:901:HOH:O	2.21	0.47
1:A:91:GLU:OE2	1:A:145:ARG:NE	2.46	0.46
1:A:457:ALA:HB1	1:A:492:PHE:CG	2.49	0.46
1:B:638:TYR:HE1	2:B:803:HEM:CBB	2.28	0.46
1:A:437:ALA:HB3	1:A:448:LEU:HD21	1.98	0.46
1:B:449:ALA:O	1:B:452:THR:HG22	2.14	0.46
1:A:366:GLY:HA3	1:A:429:LEU:HD21	1.96	0.46
1:B:374:LEU:O	1:B:378:VAL:HG23	2.15	0.46
1:A:234:ILE:HD11	1:B:610:MET:O	2.15	0.46
1:A:638:TYR:CE2	2:A:802:HEM:CBB	2.99	0.46
1:A:687:GLY:HA3	8:A:985:HOH:O	2.16	0.46
1:B:91:GLU:OE2	1:B:145:ARG:NE	2.46	0.46
1:B:539:LEU:O	1:B:544:THR:OG1	2.23	0.46
6:A:806:UQ1:C8	6:A:806:UQ1:CM5	2.85	0.46
1:A:374:LEU:O	1:A:378:VAL:HG23	2.15	0.46
1:A:637:VAL:HG11	2:A:802:HEM:HBB1	1.98	0.46
1:B:638:TYR:CE1	2:B:803:HEM:CBB	2.99	0.46
1:A:285:TYR:OH	1:A:367:VAL:O	2.31	0.46
1:A:292:LEU:CB	1:A:338:TRP:HB3	2.46	0.46
1:A:620:ILE:CG2	1:A:691:PHE:CD1	2.99	0.46
1:B:285:TYR:O	1:B:289:VAL:HG23	2.16	0.46
1:B:292:LEU:CB	1:B:338:TRP:HB3	2.46	0.46
1:B:615:VAL:HG21	5:B:801:10M:H9A	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:LEU:HD23	1:A:455:VAL:HG12	1.98	0.46
1:A:610:MET:O	1:B:234:ILE:HD11	2.16	0.46
1:A:638:TYR:HE2	2:A:802:HEM:CBB	2.29	0.46
1:A:532:ILE:HB	1:A:533:PRO:HD3	1.97	0.45
1:A:285:TYR:O	1:A:289:VAL:HG23	2.16	0.45
1:A:290:VAL:HG11	1:A:738:VAL:HB	1.98	0.45
1:A:98:LEU:HD11	1:A:147:GLN:HG3	1.98	0.45
1:A:209:VAL:HG22	1:A:226:SER:OG	2.16	0.45
1:B:290:VAL:HG11	1:B:738:VAL:HB	1.98	0.45
1:B:311:GLN:HA	1:B:319:SER:HG	1.81	0.45
1:B:486:HIS:CD2	1:B:486:HIS:C	2.95	0.45
1:A:406:TYR:HB3	1:A:481:ARG:HD3	1.98	0.45
1:B:718[B]:TRP:CZ3	6:B:806:UQ1:O3	2.69	0.45
1:B:160:PHE:CD1	1:B:189:MET:HE1	2.52	0.45
1:B:406:TYR:HB3	1:B:481:ARG:HD3	1.99	0.45
1:B:482:TRP:CE3	1:B:485:VAL:HB	2.52	0.45
1:B:620:ILE:CG2	1:B:691:PHE:CD2	2.99	0.45
1:A:625:THR:OG1	8:A:902:HOH:O	2.20	0.45
1:B:216:PRO:HB2	1:B:699:MET:HB3	1.99	0.45
1:A:216:PRO:HB2	1:A:699:MET:HB3	1.99	0.45
1:A:691:PHE:CZ	1:B:230:VAL:HG12	2.52	0.45
1:B:247:LEU:HD22	1:B:561:VAL:HG12	1.99	0.45
1:B:437:ALA:HB3	1:B:448:LEU:HD21	1.97	0.45
1:B:637:VAL:HG11	2:B:803:HEM:HBB1	1.98	0.45
1:B:691:PHE:O	1:B:695:VAL:HG23	2.17	0.45
1:A:328:ARG:O	1:A:332:ILE:HD13	2.17	0.45
1:A:610:MET:CG	1:B:234:ILE:HD12	2.47	0.45
1:A:621:GLN:NE2	8:A:948:HOH:O	2.50	0.45
1:A:684:LEU:HB3	1:A:685:PRO:HD3	1.98	0.45
1:B:234:ILE:HG12	5:B:801:10M:C4	2.46	0.45
1:B:71:SER:HG	1:B:703:ARG:NH1	2.13	0.44
1:B:427:LEU:HD23	1:B:455:VAL:HG12	1.98	0.44
1:B:687:GLY:HA3	8:B:977:HOH:O	2.17	0.44
1:A:159:LEU:O	1:A:170:ARG:HD3	2.18	0.44
1:A:230:VAL:HG12	1:B:691:PHE:CZ	2.52	0.44
1:A:482:TRP:CE3	1:A:485:VAL:HB	2.52	0.44
1:A:724:ASP:CB	6:A:806:UQ1:HM52	2.46	0.44
1:B:529:LEU:HD13	1:B:558:LEU:HD13	1.99	0.44
2:B:802:HEM:HMC2	2:B:802:HEM:CBC	2.44	0.44
1:A:67:MET:HB3	1:A:76:GLY:HA2	2.00	0.44
1:A:160:PHE:CD1	1:A:189:MET:HE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:VAL:HG12	1:A:728:LEU:HD23	1.99	0.44
1:A:486:HIS:CD2	1:A:486:HIS:C	2.95	0.44
1:A:275:LEU:O	1:A:280:ARG:NH1	2.49	0.44
1:A:296:GLN:NE2	1:A:335:ALA:HB2	2.32	0.44
1:A:691:PHE:O	1:A:695:VAL:HG23	2.17	0.44
1:B:178:ASN:HD22	1:B:178:ASN:HA	1.50	0.44
1:B:492:PHE:HA	1:B:495:VAL:HG22	1.98	0.44
1:A:247:LEU:HD22	1:A:561:VAL:HG12	1.99	0.44
1:B:227:SER:HB2	8:B:990:HOH:O	2.16	0.44
1:B:296:GLN:NE2	1:B:335:ALA:HB2	2.32	0.44
1:B:297:VAL:HG12	1:B:728:LEU:HD23	1.99	0.44
1:B:328:ARG:O	1:B:332:ILE:HD13	2.17	0.44
1:B:537:HIS:HD1	1:B:556:SER:HB3	1.83	0.44
1:B:546:THR:HG23	1:B:547:PRO:HD3	2.00	0.44
1:B:292:LEU:O	1:B:296:GLN:HB2	2.18	0.44
1:B:405:GLY:C	8:B:992:HOH:O	2.61	0.44
1:B:546:THR:N	1:B:547:PRO:HD2	2.33	0.44
1:B:684:LEU:HB3	1:B:685:PRO:HD3	1.98	0.44
1:A:2:GLY:N	8:A:950:HOH:O	2.51	0.44
1:B:98:LEU:HD11	1:B:147:GLN:HG3	2.00	0.44
1:A:604:ALA:O	1:A:608:GLY:HA3	2.17	0.43
1:B:67:MET:HB3	1:B:76:GLY:HA2	2.00	0.43
1:B:159:LEU:O	1:B:170:ARG:HD3	2.18	0.43
1:B:292:LEU:HB3	1:B:338:TRP:HB3	2.00	0.43
1:A:292:LEU:O	1:A:296:GLN:HB2	2.18	0.43
1:A:484:ILE:O	1:A:488:TRP:HB3	2.19	0.43
1:A:537:HIS:HD1	1:A:556:SER:HB3	1.83	0.43
1:A:546:THR:N	1:A:547:PRO:HD2	2.33	0.43
1:B:313:PHE:HB3	1:B:318:LEU:HD23	2.00	0.43
1:A:306:TYR:OH	1:A:322:PHE:O	2.30	0.43
1:A:405:GLY:C	8:A:1000:HOH:O	2.61	0.43
1:B:426:TRP:O	1:B:430:MET:HG2	2.18	0.43
1:A:458:ILE:HD12	1:A:493:PHE:CD2	2.53	0.43
1:B:453:ALA:HB1	7:B:809:LOP:H353	2.00	0.43
1:B:604:ALA:O	1:B:608:GLY:HA3	2.17	0.43
1:A:234:ILE:HD12	1:B:610:MET:CG	2.48	0.43
1:A:426:TRP:O	1:A:430:MET:HG2	2.19	0.43
1:A:484:ILE:N	1:A:484:ILE:CD1	2.82	0.43
1:A:313:PHE:HB3	1:A:318:LEU:HD23	2.00	0.43
1:A:552:GLY:O	1:A:556:SER:OG	2.32	0.43
1:A:609:PHE:O	1:A:610:MET:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:TYR:CD2	1:B:551:VAL:HG21	2.54	0.43
1:A:560:VAL:HG23	2:A:802:HEM:CBC	2.49	0.43
1:B:270:LEU:HD22	1:B:353:LEU:HD21	2.01	0.43
1:B:458:ILE:HD12	1:B:493:PHE:CD1	2.53	0.43
1:B:484:ILE:O	1:B:488:TRP:HB3	2.19	0.43
1:A:32:GLN:O	1:A:204:ARG:NH1	2.43	0.43
1:A:225:PRO:HD3	1:A:618:TYR:CE2	2.54	0.43
1:A:529:LEU:HD23	7:A:809:LOP:H232	2.01	0.43
2:A:801:HEM:HBB2	2:A:801:HEM:CMB	2.49	0.43
1:B:202:THR:O	1:B:210:THR:HA	2.19	0.43
1:B:318:LEU:HD13	1:B:318:LEU:HA	1.93	0.43
1:B:559:GLU:OE2	2:B:803:HEM:CBC	2.67	0.43
1:B:2:GLY:N	8:B:940:HOH:O	2.51	0.43
1:B:632:ALA:HB2	1:B:679:ILE:CD1	2.49	0.43
1:B:697:GLU:HB2	1:B:701:TYR:CD2	2.54	0.43
1:A:25:TYR:CD2	1:A:551:VAL:HG21	2.54	0.42
1:A:559:GLU:OE2	2:A:802:HEM:CBC	2.67	0.42
1:A:227:SER:CB	8:A:1002:HOH:O	2.67	0.42
1:A:323:PRO:HG2	1:A:389:ILE:HG21	2.01	0.42
1:A:202:THR:O	1:A:210:THR:HA	2.19	0.42
1:A:333:GLN:HG3	8:A:1035:HOH:O	2.19	0.42
1:A:546:THR:HG23	1:A:547:PRO:HD3	2.00	0.42
1:B:384:GLY:HA3	1:B:401:LEU:O	2.19	0.42
1:B:545:THR:C	1:B:547:PRO:HD2	2.44	0.42
1:B:560:VAL:HG23	2:B:803:HEM:CBC	2.49	0.42
1:A:380:GLY:HA3	1:A:415:TRP:CH2	2.55	0.42
1:A:610:MET:HG3	1:B:234:ILE:HD12	2.01	0.42
1:B:25:TYR:CE1	1:B:547:PRO:HB2	2.54	0.42
1:B:225:PRO:HD3	1:B:618:TYR:CE2	2.54	0.42
1:B:609:PHE:O	1:B:610:MET:C	2.62	0.42
1:A:384:GLY:HA3	1:A:401:LEU:O	2.19	0.42
1:B:230:VAL:HG13	5:B:801:10M:H8A	1.99	0.42
1:B:630:ALA:HB1	2:B:803:HEM:HMA3	2.02	0.42
1:A:449:ALA:HA	1:A:452:THR:HG22	2.01	0.42
1:A:545:THR:C	1:A:547:PRO:HD2	2.44	0.42
1:B:380:GLY:HA3	1:B:415:TRP:CH2	2.55	0.42
1:B:449:ALA:HA	1:B:452:THR:HG22	2.01	0.42
2:B:802:HEM:HBB2	2:B:802:HEM:CMB	2.50	0.42
1:A:630:ALA:HB1	2:A:802:HEM:HMA3	2.02	0.42
1:B:17:VAL:O	1:B:20:ALA:HB3	2.20	0.42
1:A:17:VAL:O	1:A:20:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:HB3	1:A:338:TRP:HB3	2.01	0.42
1:A:59:THR:HG22	1:A:470:GLU:CG	2.48	0.42
1:A:482:TRP:CZ3	1:A:485:VAL:HB	2.55	0.42
1:B:295:PHE:CZ	1:B:299:LEU:HD11	2.55	0.42
1:B:323:PRO:HG2	1:B:389:ILE:HG21	2.01	0.42
1:A:25:TYR:CE1	1:A:547:PRO:HB2	2.54	0.42
1:A:270:LEU:HD22	1:A:353:LEU:HD21	2.01	0.42
1:A:697:GLU:HB2	1:A:701:TYR:CD2	2.54	0.42
1:B:482:TRP:CZ3	1:B:485:VAL:HB	2.55	0.42
1:A:71:SER:HB2	1:A:82:ASP:OD1	2.20	0.41
1:B:71:SER:HB2	1:B:82:ASP:OD1	2.20	0.41
1:B:484:ILE:N	1:B:484:ILE:CD1	2.82	0.41
1:A:533:PRO:HB2	1:A:555:PHE:CG	2.56	0.41
1:B:285:TYR:OH	1:B:367:VAL:O	2.31	0.41
1:A:536:PHE:CD1	1:A:548:VAL:HG13	2.55	0.41
1:A:609:PHE:HB3	1:B:241:LEU:CD1	2.50	0.41
1:B:533:PRO:HB2	1:B:555:PHE:CG	2.56	0.41
1:A:104:HIS:C	1:A:106:ARG:H	2.29	0.41
1:A:241:LEU:CD1	1:B:609:PHE:HB3	2.50	0.41
1:A:554:SER:O	1:A:557:ALA:HB3	2.21	0.41
1:A:667:ALA:HA	1:A:730:GLY:O	2.20	0.41
1:B:536:PHE:CD1	1:B:548:VAL:HG13	2.55	0.41
1:A:41:ALA:O	1:A:140:THR:HA	2.21	0.41
1:A:234:ILE:HD12	1:B:610:MET:HG3	2.02	0.41
1:A:343:PHE:CE2	1:A:497:ALA:HB2	2.56	0.41
1:A:406:TYR:CE2	1:A:477:MET:HG3	2.56	0.41
1:B:43:ALA:HA	1:B:140:THR:CG2	2.51	0.41
1:B:427:LEU:CD2	1:B:455:VAL:HG12	2.51	0.41
1:B:667:ALA:HA	1:B:730:GLY:O	2.21	0.41
1:A:632:ALA:HB2	1:A:679:ILE:CD1	2.49	0.41
1:B:41:ALA:O	1:B:140:THR:HA	2.21	0.41
1:A:43:ALA:HA	1:A:140:THR:CG2	2.51	0.41
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.91	0.41
1:A:609:PHE:O	1:A:613:PRO:HD3	2.21	0.41
1:B:49:PHE:HZ	1:B:194:PHE:CD2	2.39	0.41
1:B:343:PHE:CE2	1:B:497:ALA:HB2	2.56	0.41
1:B:645:PHE:O	1:B:649:VAL:HG23	2.21	0.41
1:A:305:HIS:ND1	6:A:806:UQ1:CM2	2.84	0.41
1:A:696:SER:OG	1:A:697:GLU:OE1	2.33	0.41
1:B:59:THR:HG22	1:B:470:GLU:CG	2.48	0.41
1:B:104:HIS:C	1:B:106:ARG:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:PHE:O	1:B:613:PRO:HD3	2.21	0.41
1:B:633:ALA:O	1:B:637:VAL:HB	2.21	0.41
1:A:71:SER:HG	1:A:703:ARG:HH12	1.65	0.40
1:A:295:PHE:CZ	1:A:299:LEU:HD11	2.55	0.40
1:A:645:PHE:O	1:A:649:VAL:HG23	2.21	0.40
1:B:601:MET:HE3	1:B:601:MET:HB3	1.98	0.40
1:A:427:LEU:CD2	1:A:455:VAL:HG12	2.50	0.40
1:B:406:TYR:CE2	1:B:477:MET:HG3	2.56	0.40
1:A:699:MET:SD	8:A:960:HOH:O	2.63	0.40
1:B:594:VAL:HG22	8:B:961:HOH:O	2.20	0.40
1:A:49:PHE:HZ	1:A:194:PHE:CD2	2.39	0.40
1:A:678:MET:HG2	1:A:724:ASP:OD1	2.21	0.40
1:B:439:ARG:HA	1:B:439:ARG:HD3	1.97	0.40
1:A:292:LEU:HD23	1:A:292:LEU:HA	1.93	0.40
1:B:40:VAL:HG21	1:B:49:PHE:CE2	2.56	0.40
1:B:612:ASN:N	1:B:613:PRO:CD	2.84	0.40
1:B:628:VAL:HG23	1:B:683:LEU:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	750/761 (99%)	701 (94%)	46 (6%)	3 (0%)	30	34
1	B	750/761 (99%)	700 (93%)	45 (6%)	5 (1%)	18	19
All	All	1500/1522 (99%)	1401 (93%)	91 (6%)	8 (0%)	26	27

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	513	ARG

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Mol	Chain	Res	Type
1	B	513	ARG
1	A	489	VAL
1	B	489	VAL
1	B	745	GLY
1	A	265	PRO
1	B	265	PRO
1	B	746	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	586/596 (98%)	566 (97%)	20 (3%)	32	44
1	B	586/596 (98%)	561 (96%)	25 (4%)	26	35
All	All	1172/1192 (98%)	1127 (96%)	45 (4%)	30	40

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ARG
1	A	71	SER
1	A	101	ARG
1	A	227	SER
1	A	234	ILE
1	A	319	SER
1	A	332	ILE
1	A	376	LEU
1	A	396	ASP
1	A	427	LEU
1	A	440	THR
1	A	460	LEU
1	A	484	ILE
1	A	515	MET
1	A	523	SER
1	A	544	THR

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Mol	Chain	Res	Type
1	A	559	GLU
1	A	587	LYS
1	A	673	LEU
1	A	729	LEU
1	B	15	LEU
1	B	51	ARG
1	B	71	SER
1	B	101	ARG
1	B	178	ASN
1	B	227	SER
1	B	234	ILE
1	B	259	GLU
1	B	261	GLU
1	B	275	LEU
1	B	319	SER
1	B	332	ILE
1	B	396	ASP
1	B	427	LEU
1	B	440	THR
1	B	460	LEU
1	B	484	ILE
1	B	515	MET
1	B	523	SER
1	B	529	LEU
1	B	559	GLU
1	B	587	LYS
1	B	591	MET
1	B	673	LEU
1	B	729	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	GLN
1	A	333	GLN
1	A	612	ASN
1	A	621	GLN
1	B	75	HIS
1	B	178	ASN
1	B	224	HIS
1	B	333	GLN
1	B	612	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 4 are monoatomic - leaving 21 for Mogul analysis.

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	$\# Z > 2$
2	HEM	A	802	1,4,8	50,50,50	2.17	14 (28%)	67,82,82	1.73	17 (25%)
5	10M	A	805	-	34,34,34	1.08	2 (5%)	44,45,45	1.20	3 (6%)
2	HEM	A	801	1,4	50,50,50	2.11	14 (28%)	67,82,82	1.81	15 (22%)
2	HEM	B	802	1,4	50,50,50	2.11	14 (28%)	67,82,82	1.81	15 (22%)
7	LOP	B	812	-	27,27,44	1.40	3 (11%)	25,25,49	0.92	3 (12%)
7	LOP	B	811	-	13,13,44	1.15	1 (7%)	13,13,49	0.80	1 (7%)
6	UQ1	A	806	-	18,18,18	1.04	2 (11%)	24,25,25	0.89	1 (4%)
6	UQ1	B	806	-	18,18,18	1.05	3 (16%)	24,25,25	1.31	3 (12%)
7	LOP	A	808	-	35,35,44	0.25	0	36,36,49	0.27	0
7	LOP	A	813	-	8,8,44	0.25	0	7,7,49	0.27	0
7	LOP	A	807	-	28,28,44	1.20	3 (10%)	26,26,49	0.70	2 (7%)
7	LOP	A	811	-	18,18,44	0.98	1 (5%)	17,17,49	0.59	1 (5%)
7	LOP	B	808	-	27,27,44	0.33	0	28,28,49	0.28	0
7	LOP	A	812	-	23,23,44	1.14	2 (8%)	21,21,49	0.84	2 (9%)
7	LOP	A	809	-	36,36,44	0.30	0	38,38,49	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	LOP	A	810	-	23,23,44	0.28	0	22,22,49	0.29	0
7	LOP	B	809	-	36,36,44	0.28	0	38,38,49	0.30	0
2	HEM	B	803	1,4,8	50,50,50	2.17	14 (28%)	67,82,82	1.73	17 (25%)
7	LOP	B	810	-	26,26,44	1.37	3 (11%)	24,24,49	0.96	3 (12%)
5	10M	B	801	-	34,34,34	1.00	2 (5%)	44,45,45	1.57	7 (15%)
7	LOP	B	807	-	41,41,44	0.33	0	44,46,49	0.42	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
2	HEM	A	802	1,4,8	-	2/14/54/54	-
5	10M	A	805	-	-	11/19/59/59	0/2/2/2
2	HEM	A	801	1,4	-	2/14/54/54	-
2	HEM	B	802	1,4	-	2/14/54/54	-
7	LOP	B	812	-	-	13/23/23/48	-
7	LOP	B	811	-	-	8/11/11/48	-
6	UQ1	A	806	-	-	6/9/33/33	0/1/1/1
6	UQ1	B	806	-	-	3/9/33/33	0/1/1/1
7	LOP	A	808	-	-	19/35/35/48	-
7	LOP	A	813	-	-	2/6/6/48	-
7	LOP	A	807	-	-	16/24/24/48	-
7	LOP	A	811	-	-	12/16/16/48	-
7	LOP	B	808	-	-	12/27/27/48	-
7	LOP	A	812	-	-	10/19/19/48	-
7	LOP	A	809	-	-	18/37/37/48	-
7	LOP	A	810	-	-	5/20/20/48	-
7	LOP	B	809	-	-	12/37/37/48	-
2	HEM	B	803	1,4,8	-	2/14/54/54	-
7	LOP	B	810	-	-	11/22/22/48	-
5	10M	B	801	-	-	9/19/59/59	0/2/2/2
7	LOP	B	807	-	-	23/45/45/48	-

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	HEM	C1B-NB	-5.03	1.31	1.40
2	B	803	HEM	FE-NB	5.02	2.10	1.94
7	B	812	LOP	C12-C13	-5.02	1.31	1.52
2	A	802	HEM	FE-NB	5.01	2.10	1.94
2	B	803	HEM	C1B-NB	-4.99	1.31	1.40
2	B	803	HEM	C4D-ND	-4.87	1.31	1.40
2	A	802	HEM	C4D-ND	-4.86	1.31	1.40
2	A	802	HEM	C4C-NC	-4.82	1.30	1.39
2	A	801	HEM	C1B-NB	-4.82	1.31	1.40
2	B	803	HEM	C4C-NC	-4.81	1.30	1.39
2	B	802	HEM	C1B-NB	-4.73	1.32	1.40
2	A	801	HEM	C1D-ND	-4.68	1.29	1.38
2	B	802	HEM	C1D-ND	-4.65	1.29	1.38
2	B	802	HEM	FE-NB	4.57	2.09	1.94
2	A	801	HEM	FE-NB	4.54	2.08	1.94
5	B	801	10M	C10-S	-4.47	1.75	1.81
2	A	801	HEM	C4C-NC	-4.27	1.31	1.39
2	B	802	HEM	C4C-NC	-4.27	1.31	1.39
2	A	802	HEM	C1D-ND	-4.15	1.30	1.38
2	B	803	HEM	C1D-ND	-4.13	1.30	1.38
7	A	807	LOP	O6-C24	-4.13	1.21	1.42
5	A	805	10M	C10-S	-4.13	1.75	1.81
7	B	810	LOP	O6-C24	-4.12	1.21	1.42
7	B	810	LOP	C12-C11	-4.11	1.31	1.51
7	A	811	LOP	O5-C6	-4.10	1.21	1.42
2	B	803	HEM	C4B-NB	-4.06	1.30	1.38
7	B	812	LOP	O6-C24	-4.04	1.21	1.42
2	A	802	HEM	C4B-NB	-4.04	1.30	1.38
7	A	812	LOP	C11-C10	-3.98	1.32	1.51
2	B	802	HEM	C4D-ND	-3.93	1.33	1.40
2	A	801	HEM	C4D-ND	-3.89	1.33	1.40
7	B	811	LOP	C33-C32	-3.88	1.32	1.51
5	A	805	10M	C11-S	-3.84	1.74	1.80
2	A	801	HEM	C1C-NC	-3.75	1.32	1.39
2	B	802	HEM	C1C-NC	-3.71	1.32	1.39
7	B	810	LOP	C15-C14	3.69	1.52	1.31
2	A	801	HEM	C4A-NA	-3.68	1.32	1.39
2	A	801	HEM	FE-NC	3.67	2.07	1.95
2	B	802	HEM	FE-NC	3.66	2.07	1.95
7	A	812	LOP	C15-C14	3.62	1.52	1.31
2	B	802	HEM	C4A-NA	-3.61	1.32	1.39
7	A	807	LOP	C13-C14	-3.56	1.30	1.50
2	B	802	HEM	C4B-NB	-3.30	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C4B-NB	-3.30	1.32	1.38
2	A	801	HEM	FE-ND	-3.29	1.84	1.94
2	B	802	HEM	FE-ND	-3.29	1.84	1.94
2	B	803	HEM	C4A-NA	-3.25	1.33	1.39
2	A	802	HEM	C4A-NA	-3.24	1.33	1.39
7	B	812	LOP	C15-C14	3.22	1.50	1.31
2	A	802	HEM	C1C-NC	-3.21	1.33	1.39
2	B	803	HEM	C1C-NC	-3.18	1.33	1.39
7	A	807	LOP	C15-C14	3.16	1.49	1.31
2	A	802	HEM	FE-NC	3.09	2.05	1.95
2	B	802	HEM	C1C-C2C	-3.08	1.39	1.45
2	B	803	HEM	FE-NC	3.06	2.05	1.95
2	A	801	HEM	C1C-C2C	-3.05	1.39	1.45
6	A	806	UQ1	C3-C4	-2.69	1.41	1.48
2	A	802	HEM	CHD-C1D	-2.66	1.33	1.39
2	B	803	HEM	CHD-C1D	-2.64	1.33	1.39
6	B	806	UQ1	C3-C4	-2.61	1.41	1.48
2	B	803	HEM	C3C-C4C	-2.61	1.41	1.46
2	A	801	HEM	C1A-C2A	-2.50	1.39	1.44
2	A	802	HEM	C3C-C4C	-2.48	1.41	1.46
2	B	802	HEM	C1A-C2A	-2.46	1.39	1.44
2	B	803	HEM	C1C-C2C	-2.41	1.40	1.45
2	A	802	HEM	C1C-C2C	-2.37	1.40	1.45
6	B	806	UQ1	C2-C1	-2.35	1.42	1.48
2	A	801	HEM	C1B-C2B	-2.27	1.39	1.44
2	B	802	HEM	C1B-C2B	-2.25	1.40	1.44
6	A	806	UQ1	C6-C5	2.17	1.39	1.35
2	A	802	HEM	C1A-NA	-2.12	1.35	1.39
2	B	803	HEM	C1A-NA	-2.11	1.35	1.39
2	A	801	HEM	C3C-C4C	-2.11	1.42	1.46
2	B	802	HEM	C3C-C4C	-2.10	1.42	1.46
2	B	803	HEM	O2A-CGA	-2.10	1.23	1.30
6	B	806	UQ1	C6-C5	2.06	1.38	1.35
5	B	801	10M	O1-C11	2.03	1.45	1.42
2	A	802	HEM	O2A-CGA	-2.02	1.24	1.30

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	801	10M	C11-C22-C21	-5.58	99.63	110.55
2	B	802	HEM	CBD-CAD-C3D	-5.01	98.68	112.53
2	A	801	HEM	CBD-CAD-C3D	-5.00	98.71	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	802	HEM	CHC-C4B-NB	4.66	129.44	124.42
2	A	801	HEM	CHC-C4B-NB	4.65	129.43	124.42
2	B	803	HEM	CAD-CBD-CGD	-4.22	102.48	113.67
2	A	802	HEM	CAD-CBD-CGD	-4.17	102.61	113.67
2	B	802	HEM	CAA-CBA-CGA	-4.14	102.67	113.67
2	B	803	HEM	CHC-C4B-NB	4.13	128.87	124.42
2	A	801	HEM	CAA-CBA-CGA	-4.10	102.79	113.67
2	A	802	HEM	CHC-C4B-NB	4.07	128.81	124.42
2	A	801	HEM	CHD-C1D-ND	3.99	128.72	124.42
2	B	802	HEM	CHD-C1D-ND	3.97	128.70	124.42
2	A	801	HEM	CHA-C4D-ND	3.97	129.28	124.37
2	B	802	HEM	CHA-C4D-ND	3.94	129.24	124.37
2	B	803	HEM	C1B-NB-C4B	3.85	109.77	105.21
6	B	806	UQ1	C3-C2-C1	-3.82	113.67	120.69
2	A	802	HEM	C1B-NB-C4B	3.80	109.71	105.21
2	B	803	HEM	CBA-CAA-C2A	-3.73	102.22	112.53
2	A	802	HEM	C4B-C3B-C2B	-3.70	103.88	107.28
2	A	802	HEM	CBA-CAA-C2A	-3.68	102.37	112.53
2	B	803	HEM	C4B-C3B-C2B	-3.45	104.11	107.28
2	B	802	HEM	C1B-NB-C4B	3.45	109.29	105.21
2	A	801	HEM	C1B-NB-C4B	3.45	109.29	105.21
2	A	801	HEM	CHA-C4D-C3D	-3.30	119.14	125.23
2	B	802	HEM	CHA-C4D-C3D	-3.27	119.20	125.23
5	B	801	10M	O9-C21-C22	-3.23	102.77	110.38
2	A	802	HEM	C1D-C2D-C3D	-3.09	103.73	106.98
2	B	803	HEM	C1D-C2D-C3D	-3.02	103.81	106.98
6	B	806	UQ1	C6-C5-C4	-2.91	116.87	119.17
2	A	802	HEM	CMD-C2D-C1D	2.88	129.53	125.03
2	B	803	HEM	CMD-C2D-C1D	2.80	129.41	125.03
5	A	805	10M	O9-C21-C14	2.76	117.02	109.94
5	B	801	10M	O10-C22-C21	2.65	116.62	110.38
7	B	812	LOP	C11-C12-C13	2.64	126.53	113.86
2	A	801	HEM	CAD-C3D-C4D	2.62	129.27	124.70
2	B	802	HEM	CAD-C3D-C4D	2.60	129.24	124.70
7	B	810	LOP	C11-C12-C13	2.60	126.36	113.86
5	B	801	10M	C15-O4-C16	2.58	118.77	113.72
5	A	805	10M	C22-C21-C14	-2.57	103.86	109.68
2	A	801	HEM	CHB-C1B-NB	2.56	127.53	124.37
2	B	802	HEM	CHB-C1B-NB	2.53	127.50	124.37
2	B	803	HEM	C4C-NC-C1C	2.47	109.86	105.82
2	A	802	HEM	C4C-NC-C1C	2.43	109.79	105.82
7	B	810	LOP	C12-C11-C10	2.43	126.66	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	801	10M	C21-C14-C12	-2.43	105.55	110.93
2	B	803	HEM	O2D-CGD-CBD	2.42	121.64	114.00
2	B	803	HEM	CHD-C4C-NC	2.41	127.08	124.45
2	A	802	HEM	O2D-CGD-CBD	2.41	121.61	114.00
2	A	802	HEM	C2D-C1D-ND	2.41	112.69	109.90
2	B	803	HEM	CHD-C1D-C2D	-2.40	121.24	125.03
2	A	801	HEM	C4B-C3B-C2B	-2.38	105.09	107.28
2	B	803	HEM	C2D-C1D-ND	2.37	112.64	109.90
7	A	812	LOP	C11-C10-C9	2.36	126.31	114.37
2	B	802	HEM	C4B-C3B-C2B	-2.35	105.12	107.28
2	A	801	HEM	O2A-CGA-CBA	2.35	121.43	114.00
2	A	802	HEM	CAA-CBA-CGA	-2.34	107.45	113.67
2	A	802	HEM	CHD-C4C-NC	2.34	127.00	124.45
6	A	806	UQ1	C7-C6-C5	-2.34	120.88	124.89
2	B	803	HEM	CAA-CBA-CGA	-2.33	107.48	113.67
2	A	802	HEM	CHD-C1D-C2D	-2.32	121.37	125.03
2	B	802	HEM	O2A-CGA-CBA	2.30	121.26	114.00
7	B	811	LOP	C33-C32-C31	2.29	125.93	114.37
2	B	803	HEM	CHA-C4D-ND	2.27	127.17	124.37
7	B	812	LOP	O6-C24-C25	2.26	125.82	111.44
2	A	802	HEM	CHA-C4D-ND	2.25	127.15	124.37
2	A	801	HEM	C1A-CHA-C4D	-2.25	120.96	126.25
7	A	812	LOP	C12-C11-C10	2.25	125.72	114.37
2	B	802	HEM	C1A-CHA-C4D	-2.24	120.99	126.25
5	A	805	10M	O10-C22-C11	2.23	114.27	110.30
5	B	801	10M	C15-C20-C19	2.20	114.65	110.01
7	A	811	LOP	O5-C6-C7	2.20	125.43	111.44
2	B	803	HEM	O2A-CGA-O1A	-2.17	117.75	123.33
2	A	802	HEM	O2A-CGA-O1A	-2.17	117.75	123.33
7	B	812	LOP	C12-C13-C14	2.15	124.62	112.60
2	A	801	HEM	CHD-C1D-C2D	-2.14	121.64	125.03
7	A	807	LOP	C12-C13-C14	2.14	124.60	112.60
7	A	807	LOP	O6-C24-C25	2.14	125.00	111.44
2	B	802	HEM	C4D-C3D-C2D	-2.13	103.79	106.89
2	A	801	HEM	C4D-C3D-C2D	-2.13	103.79	106.89
6	B	806	UQ1	C2-C3-C4	-2.13	116.78	120.69
2	B	802	HEM	CHD-C1D-C2D	-2.12	121.67	125.03
2	A	802	HEM	CHA-C1A-NA	2.10	127.67	123.86
2	B	803	HEM	CHA-C1A-NA	2.08	127.64	123.86
7	B	810	LOP	O6-C24-C25	2.08	124.64	111.44
2	B	803	HEM	CHB-C1B-NB	2.06	126.91	124.37
2	A	801	HEM	O2A-CGA-O1A	-2.03	118.12	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	802	HEM	O2A-CGA-O1A	-2.03	118.12	123.33
5	B	801	10M	O10-C22-C11	2.02	113.89	110.30
2	A	802	HEM	CHB-C1B-NB	2.02	126.86	124.37

There are no chirality outliers.

All (198) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	809	LOP	C3-C4-C5-O6
7	A	809	LOP	O5-C4-C5-O6
7	B	807	LOP	N1-C1-C2-O1
7	B	807	LOP	C2-O1-P1-O2
7	B	807	LOP	C7-C6-O5-C4
7	B	809	LOP	C7-C6-O5-C4
6	B	806	UQ1	C7-C8-C9-C10
6	B	806	UQ1	C7-C8-C9-C11
7	A	809	LOP	C25-C24-O6-C5
7	B	807	LOP	C25-C24-O6-C5
7	A	808	LOP	O8-C24-O6-C5
7	A	809	LOP	O8-C24-O6-C5
7	B	807	LOP	O8-C24-O6-C5
7	B	807	LOP	O7-C6-O5-C4
7	B	809	LOP	O7-C6-O5-C4
5	B	801	10M	O4-C15-O3-C14
7	A	808	LOP	C25-C24-O6-C5
7	B	807	LOP	C13-C14-C15-C16
5	B	801	10M	O4-C16-C17-O5
5	B	801	10M	O1-C12-C13-O2
7	A	809	LOP	C7-C6-O5-C4
6	A	806	UQ1	C7-C8-C9-C10
5	B	801	10M	C18-C16-C17-O5
5	A	805	10M	O1-C12-C13-O2
7	A	807	LOP	C13-C14-C15-C16
7	B	812	LOP	C13-C14-C15-C16
5	B	801	10M	C14-C12-C13-O2
7	A	809	LOP	O7-C6-O5-C4
7	A	808	LOP	C7-C6-O5-C4
7	B	808	LOP	C7-C6-O5-C4
7	B	808	LOP	C25-C24-O6-C5
7	B	810	LOP	C10-C11-C12-C13
7	B	810	LOP	C27-C28-C29-C30
6	A	806	UQ1	C7-C8-C9-C11

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Mol	Chain	Res	Type	Atoms
7	A	808	LOP	O7-C6-O5-C4
7	B	808	LOP	O7-C6-O5-C4
7	A	807	LOP	C16-C17-C18-C19
7	B	808	LOP	C11-C10-C9-C8
7	B	808	LOP	O8-C24-O6-C5
7	A	809	LOP	C13-C14-C15-C16
7	A	810	LOP	C7-C6-O5-C4
5	A	805	10M	C7-C8-C9-C10
7	A	808	LOP	C6-C7-C8-C9
5	A	805	10M	S-C10-C9-C8
7	A	811	LOP	C6-C7-C8-C9
7	B	812	LOP	C25-C26-C27-C28
7	B	811	LOP	C28-C29-C30-C31
7	A	812	LOP	C28-C29-C30-C31
7	A	810	LOP	O7-C6-O5-C4
7	B	809	LOP	C29-C30-C31-C32
7	B	812	LOP	C31-C32-C33-C34
5	B	801	10M	C4-C5-C6-C7
5	A	805	10M	C14-C12-C13-O2
5	B	801	10M	C6-C7-C8-C9
7	B	809	LOP	C7-C8-C9-C10
7	A	808	LOP	C27-C28-C29-C30
7	A	809	LOP	C7-C8-C9-C10
7	B	809	LOP	C19-C20-C21-C22
7	A	811	LOP	C11-C10-C9-C8
7	A	807	LOP	C10-C11-C12-C13
7	B	810	LOP	C11-C12-C13-C14
7	B	807	LOP	C17-C18-C19-C20
5	A	805	10M	C5-C6-C7-C8
7	A	811	LOP	C16-C17-C18-C19
7	B	811	LOP	C27-C28-C29-C30
7	B	808	LOP	C30-C31-C32-C33
7	B	810	LOP	C31-C32-C33-C34
7	B	807	LOP	C25-C26-C27-C28
7	A	808	LOP	C10-C11-C12-C13
7	B	811	LOP	C31-C32-C33-C34
7	B	807	LOP	C24-C25-C26-C27
6	A	806	UQ1	C5-C6-C7-C8
7	B	808	LOP	C29-C30-C31-C32
7	A	807	LOP	C9-C10-C11-C12
6	A	806	UQ1	C1-C6-C7-C8
7	B	807	LOP	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
7	A	809	LOP	C11-C12-C13-C14
7	A	811	LOP	C11-C12-C13-C14
7	A	807	LOP	C7-C8-C9-C10
7	A	809	LOP	C11-C10-C9-C8
7	B	809	LOP	C24-C25-C26-C27
7	B	811	LOP	C24-C25-C26-C27
7	A	811	LOP	C9-C10-C11-C12
7	B	807	LOP	C11-C10-C9-C8
7	B	809	LOP	C15-C16-C17-C18
7	B	812	LOP	C11-C12-C13-C14
7	B	812	LOP	C7-C8-C9-C10
7	A	808	LOP	C11-C12-C13-C14
7	A	810	LOP	C11-C12-C13-C14
7	A	807	LOP	O6-C24-C25-C26
7	A	808	LOP	C25-C26-C27-C28
7	A	809	LOP	C9-C10-C11-C12
7	A	809	LOP	C14-C15-C16-C17
7	B	808	LOP	C28-C29-C30-C31
7	B	808	LOP	C9-C10-C11-C12
5	B	801	10M	S-C10-C9-C8
7	A	807	LOP	C19-C20-C21-C22
7	B	812	LOP	C27-C28-C29-C30
7	A	812	LOP	C10-C11-C12-C13
7	A	808	LOP	C19-C20-C21-C22
7	A	811	LOP	C10-C11-C12-C13
7	B	807	LOP	C11-C12-C13-C14
7	B	812	LOP	C24-C25-C26-C27
7	A	812	LOP	C16-C17-C18-C19
7	A	808	LOP	C20-C21-C22-C23
7	A	807	LOP	C25-C26-C27-C28
5	B	801	10M	C7-C8-C9-C10
5	A	805	10M	C4-C5-C6-C7
7	A	811	LOP	C18-C19-C20-C21
7	A	807	LOP	C17-C18-C19-C20
7	B	811	LOP	C32-C33-C34-C35
7	A	809	LOP	C31-C32-C33-C34
7	A	810	LOP	C7-C8-C9-C10
7	B	810	LOP	C29-C30-C31-C32
7	B	810	LOP	C24-C25-C26-C27
7	B	809	LOP	C12-C13-C14-C15
7	A	807	LOP	C26-C27-C28-C29
7	A	811	LOP	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
7	A	808	LOP	C30-C31-C32-C33
7	A	808	LOP	C31-C32-C33-C34
7	B	809	LOP	C14-C15-C16-C17
7	B	807	LOP	C29-C30-C31-C32
7	A	809	LOP	C16-C17-C18-C19
5	A	805	10M	C3-C4-C5-C6
7	A	811	LOP	C19-C20-C21-C22
7	A	809	LOP	C19-C20-C21-C22
7	B	807	LOP	C3-C4-C5-O6
7	B	807	LOP	C7-C8-C9-C10
7	B	807	LOP	C1-C2-O1-P1
7	A	807	LOP	C15-C16-C17-C18
7	B	807	LOP	O5-C4-C5-O6
7	B	807	LOP	C10-C11-C12-C13
7	A	813	LOP	C28-C29-C30-C31
7	B	810	LOP	C17-C18-C19-C20
7	B	808	LOP	C12-C13-C14-C15
7	B	807	LOP	C9-C10-C11-C12
7	B	812	LOP	C32-C33-C34-C35
7	A	809	LOP	C30-C31-C32-C33
7	A	812	LOP	C30-C31-C32-C33
7	A	807	LOP	C18-C19-C20-C21
7	A	812	LOP	C27-C28-C29-C30
7	B	812	LOP	C17-C18-C19-C20
7	B	807	LOP	C2-O1-P1-O4
7	B	807	LOP	C3-O2-P1-O4
7	A	808	LOP	C15-C16-C17-C18
7	B	810	LOP	C15-C16-C17-C18
7	B	812	LOP	C10-C11-C12-C13
7	B	812	LOP	C6-C7-C8-C9
7	A	812	LOP	C11-C12-C13-C14
7	A	808	LOP	C26-C27-C28-C29
7	B	812	LOP	C29-C30-C31-C32
6	A	806	UQ1	C1-C2-O2-CM2
7	B	810	LOP	C28-C29-C30-C31
7	A	807	LOP	C31-C32-C33-C34
2	A	801	HEM	CAA-CBA-CGA-O1A
2	B	802	HEM	CAA-CBA-CGA-O1A
7	A	811	LOP	C14-C15-C16-C17
5	A	805	10M	C12-C14-O3-C15
5	A	805	10M	C21-C14-O3-C15
7	A	813	LOP	C24-C25-C26-C27

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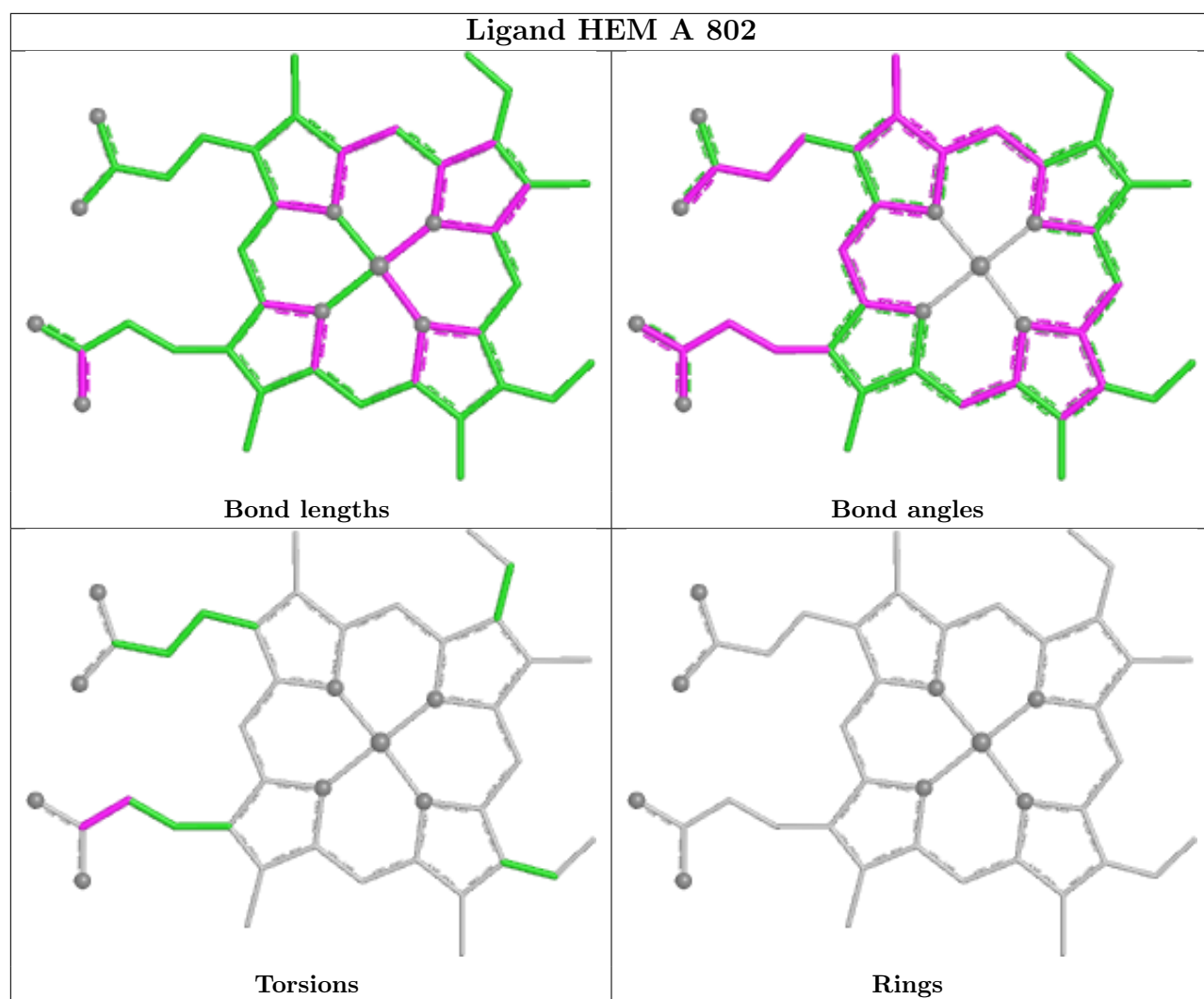
Mol	Chain	Res	Type	Atoms
6	B	806	UQ1	C1-C2-O2-CM2
2	A	801	HEM	CAA-CBA-CGA-O2A
2	B	802	HEM	CAA-CBA-CGA-O2A
7	B	811	LOP	C30-C31-C32-C33
6	A	806	UQ1	C6-C7-C8-C9
7	B	809	LOP	C20-C21-C22-C23
7	A	807	LOP	C24-C25-C26-C27
7	A	807	LOP	C12-C13-C14-C15
7	A	811	LOP	C13-C14-C15-C16
7	B	807	LOP	C16-C17-C18-C19
7	A	812	LOP	C14-C15-C16-C17
5	A	805	10M	C1-C2-C3-C4
7	B	810	LOP	C32-C33-C34-C35
7	A	809	LOP	C12-C13-C14-C15
7	B	808	LOP	O6-C24-C25-C26
7	A	808	LOP	C28-C29-C30-C31
7	A	808	LOP	C14-C15-C16-C17
7	A	809	LOP	C32-C33-C34-C35
7	A	810	LOP	C29-C30-C31-C32
7	B	809	LOP	C31-C32-C33-C34
5	A	805	10M	C9-C10-S-C11
7	A	812	LOP	C31-C32-C33-C34
7	A	808	LOP	O6-C24-C25-C26
7	B	811	LOP	O6-C24-C25-C26
7	B	811	LOP	O8-C24-C25-C26
7	B	810	LOP	C14-C15-C16-C17
7	A	812	LOP	C15-C16-C17-C18
7	A	811	LOP	O5-C6-C7-C8
7	B	812	LOP	O6-C24-C25-C26
7	A	807	LOP	C14-C15-C16-C17
7	A	812	LOP	C7-C8-C9-C10
7	B	809	LOP	C10-C11-C12-C13
2	B	803	HEM	CAA-CBA-CGA-O1A
2	A	802	HEM	CAA-CBA-CGA-O1A
2	B	803	HEM	CAA-CBA-CGA-O2A
7	A	808	LOP	O8-C24-C25-C26
2	A	802	HEM	CAA-CBA-CGA-O2A
7	B	808	LOP	O8-C24-C25-C26

There are no ring outliers.

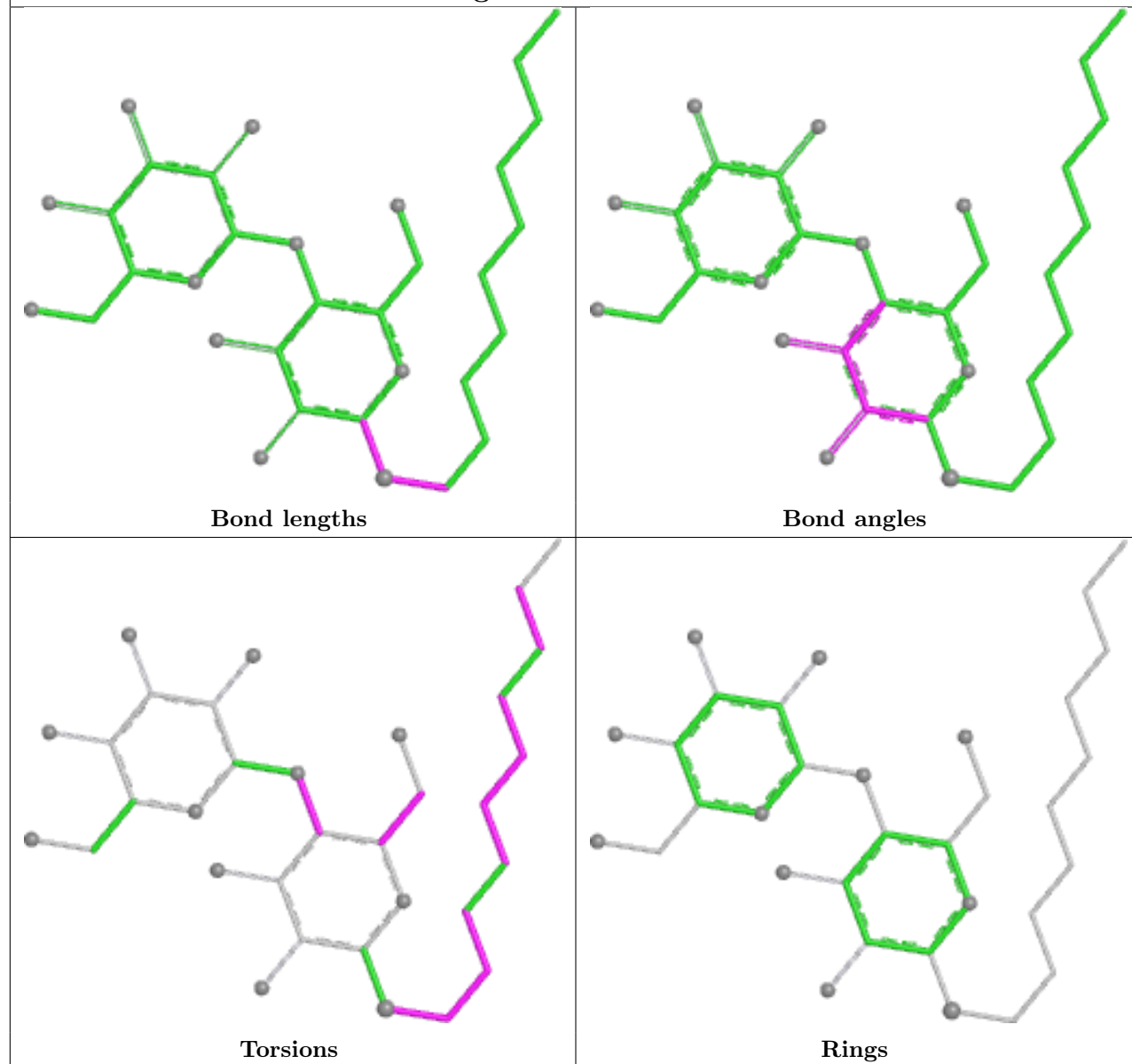
13 monomers are involved in 66 short contacts:

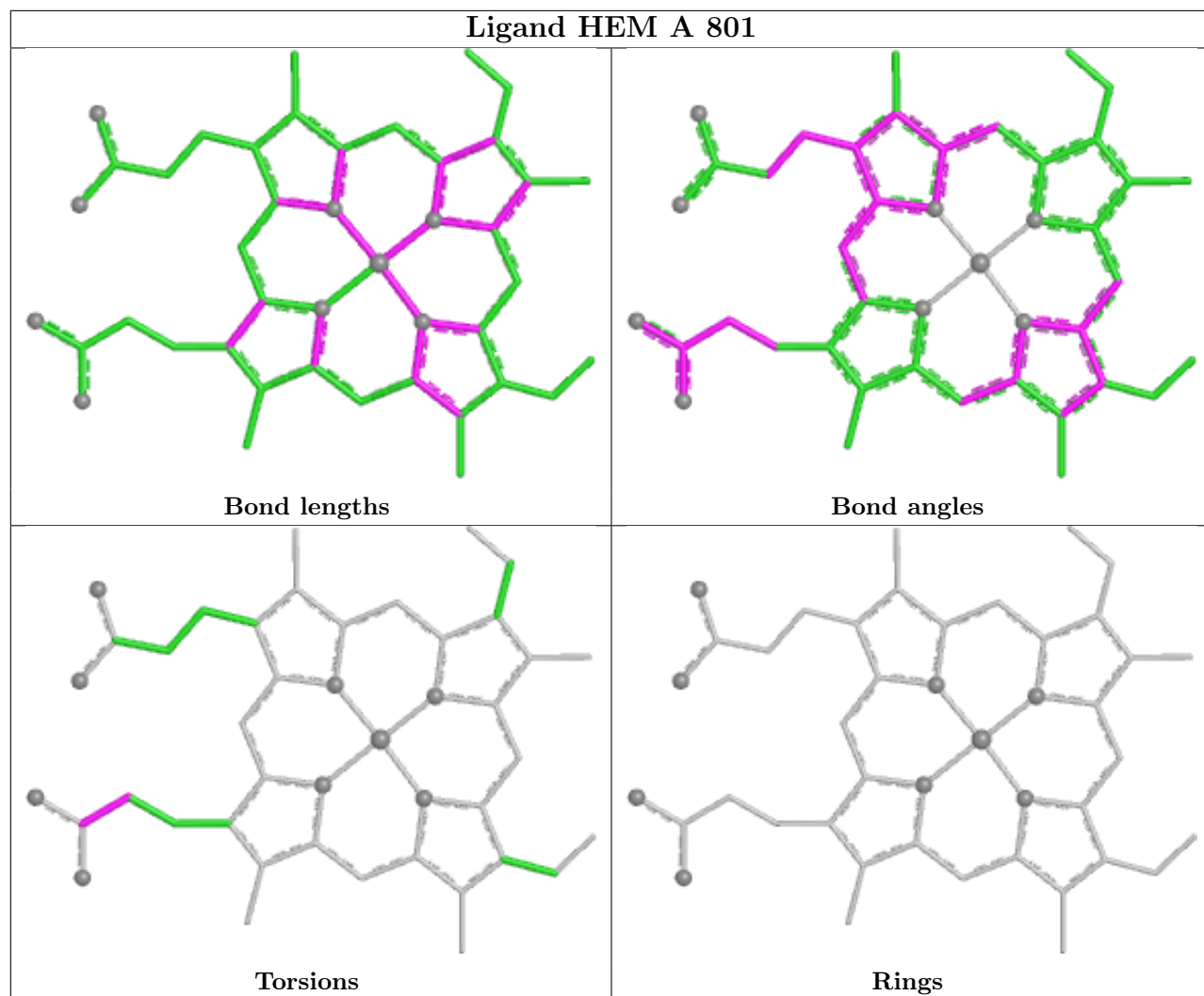
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	802	HEM	7	0
5	A	805	10M	7	0
2	A	801	HEM	3	0
2	B	802	HEM	4	0
7	B	811	LOP	1	0
6	A	806	UQ1	7	0
6	B	806	UQ1	6	0
7	A	813	LOP	1	0
7	A	807	LOP	4	0
7	A	809	LOP	2	0
7	B	809	LOP	2	0
2	B	803	HEM	7	0
5	B	801	10M	16	0

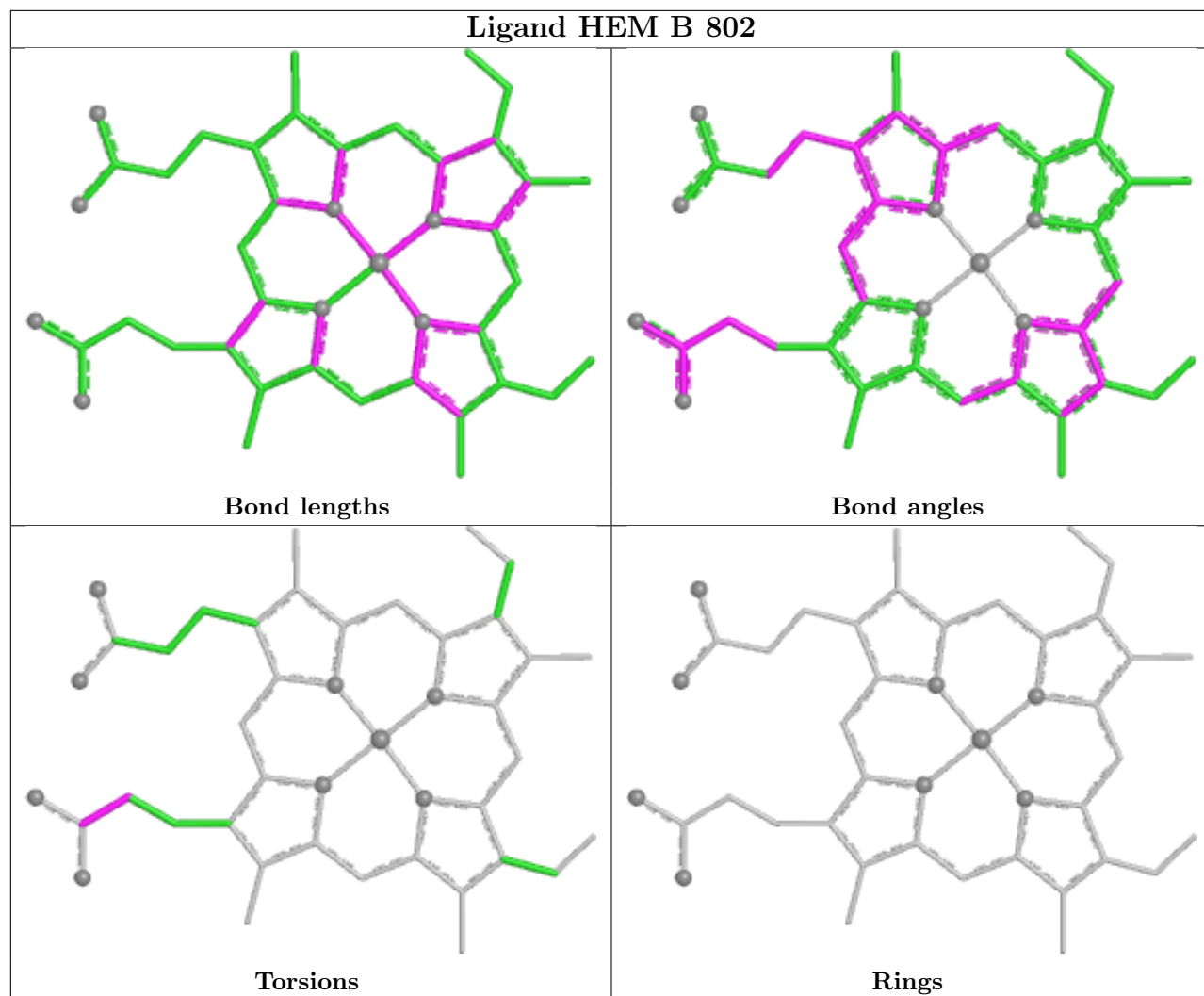
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

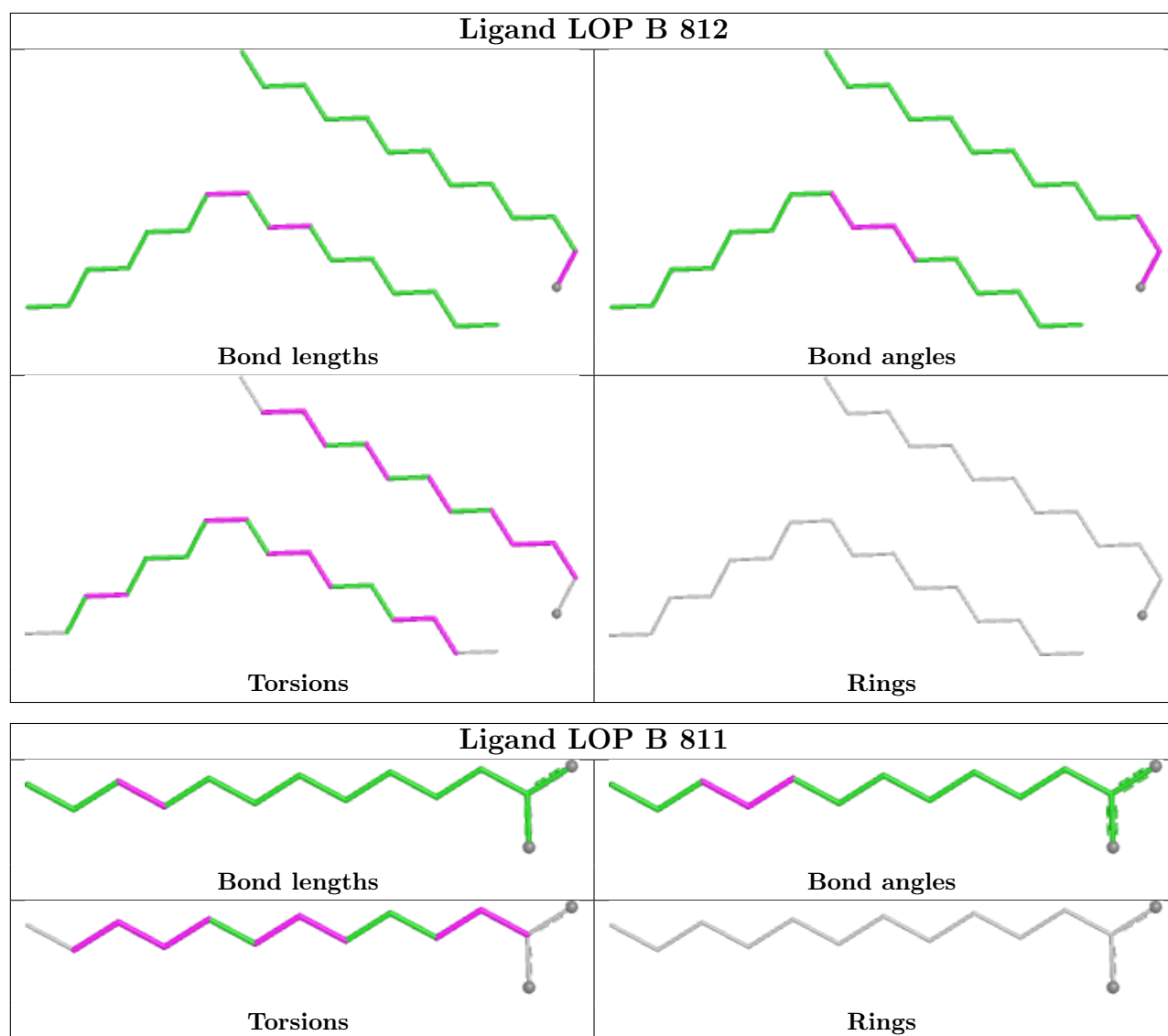


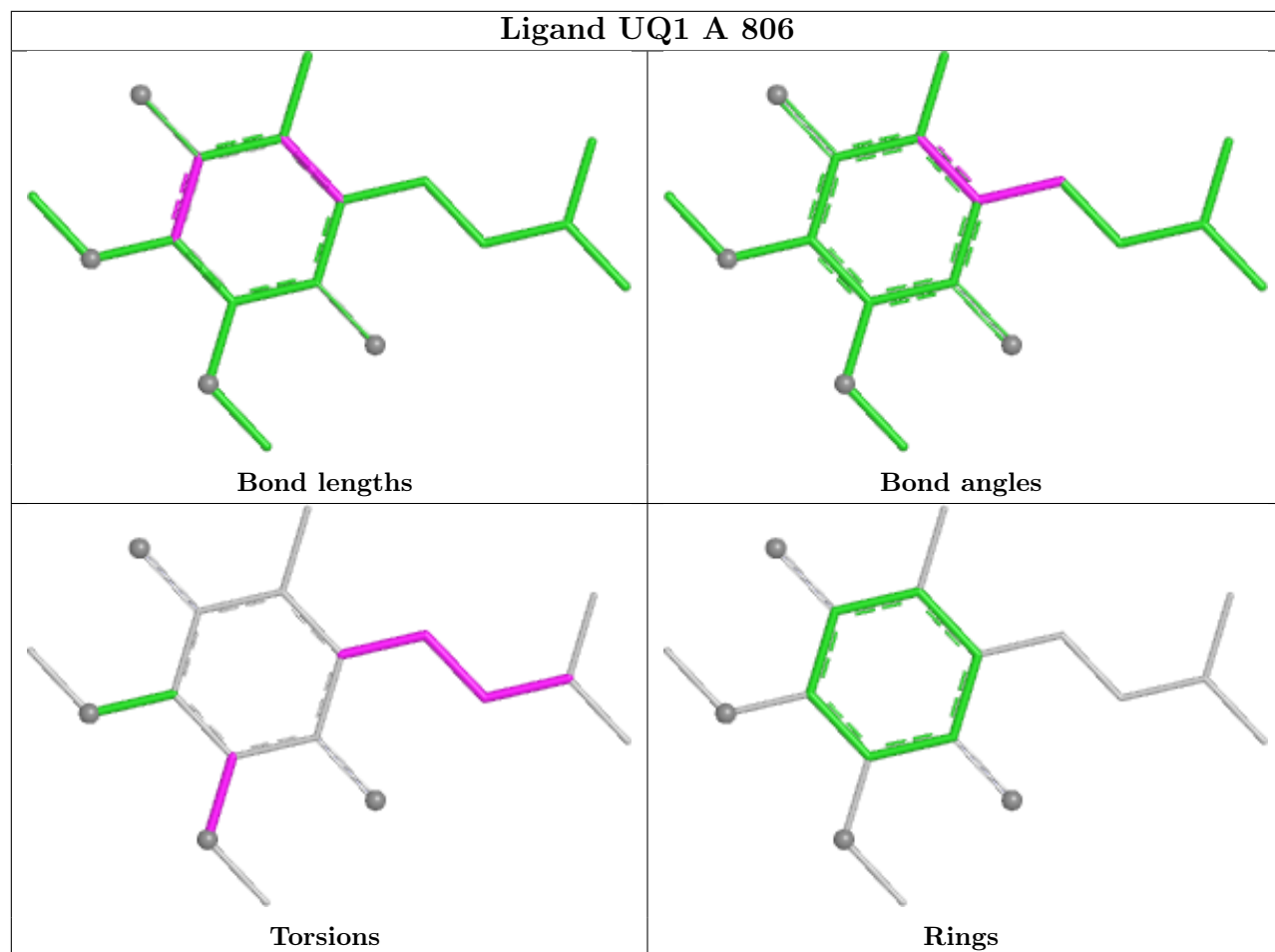
Ligand 10M A 805

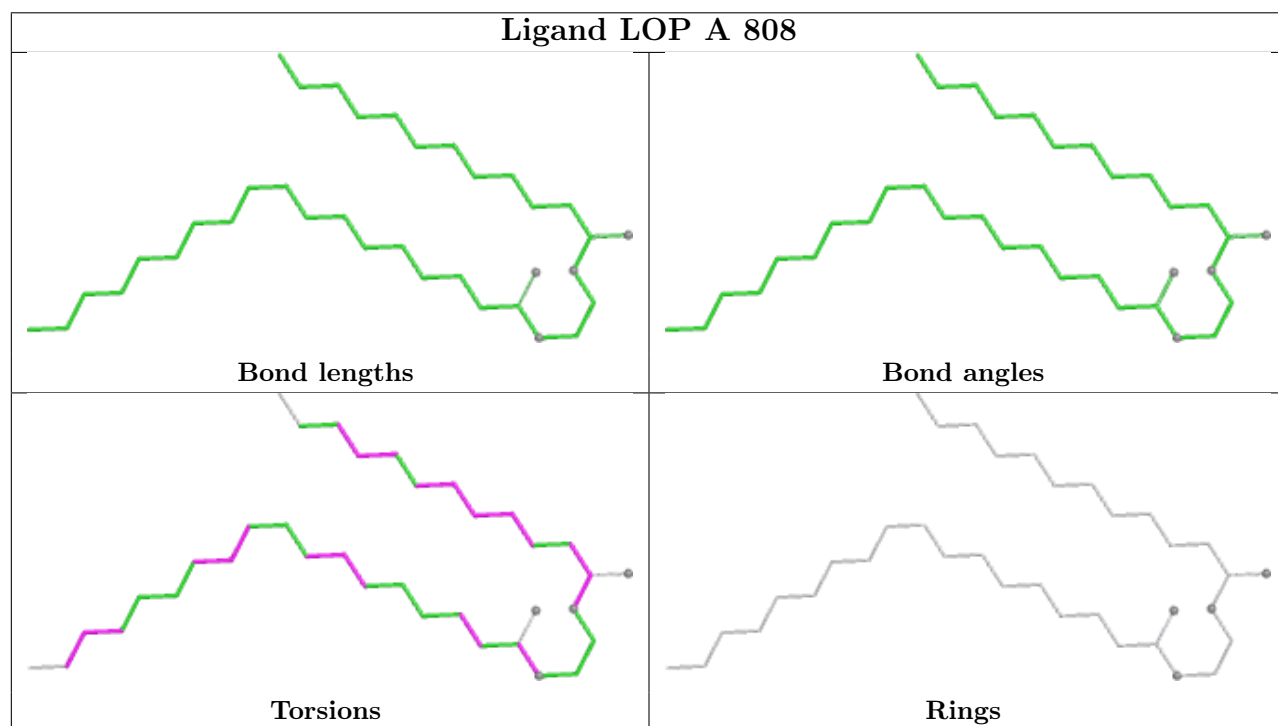
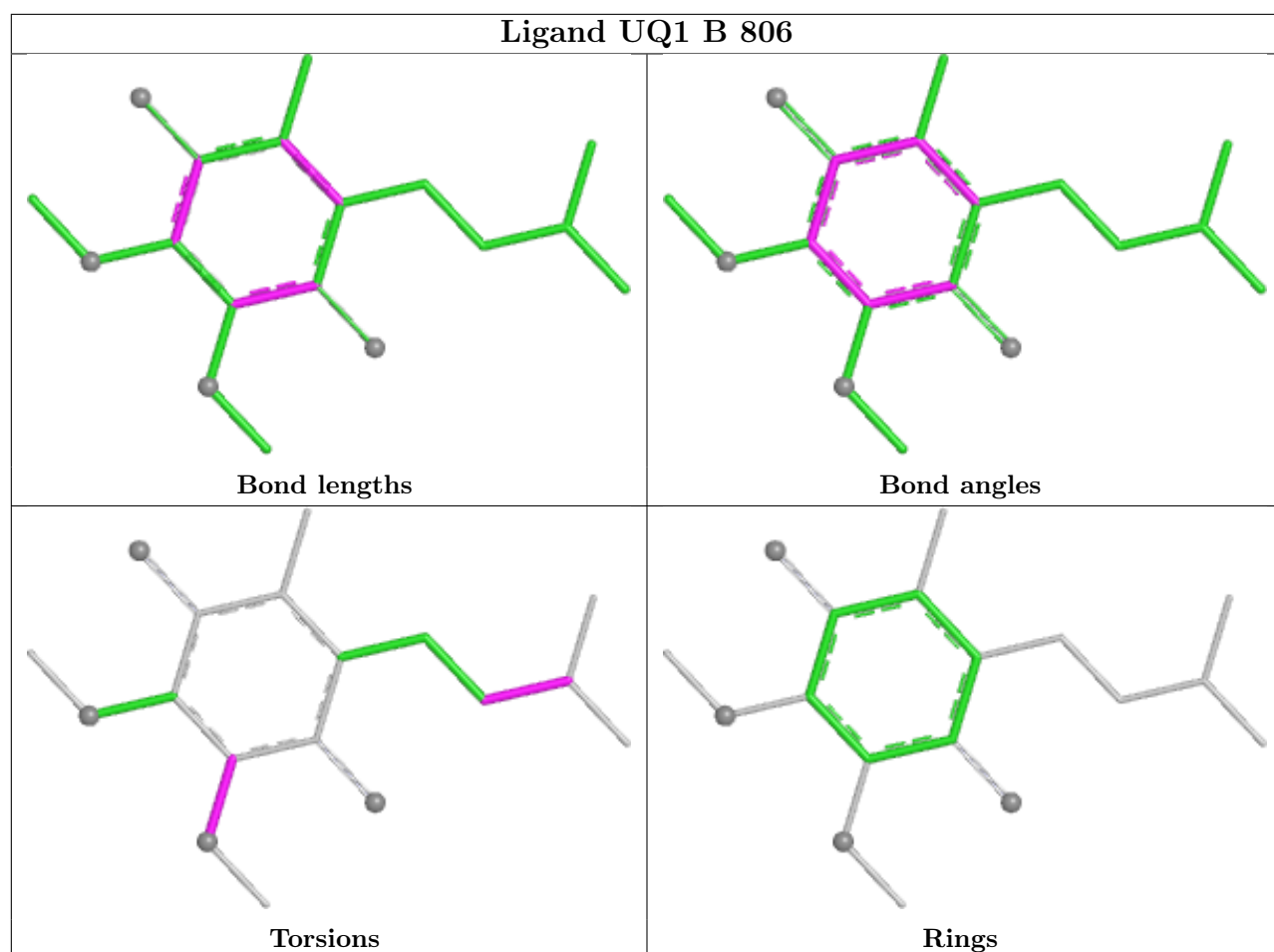


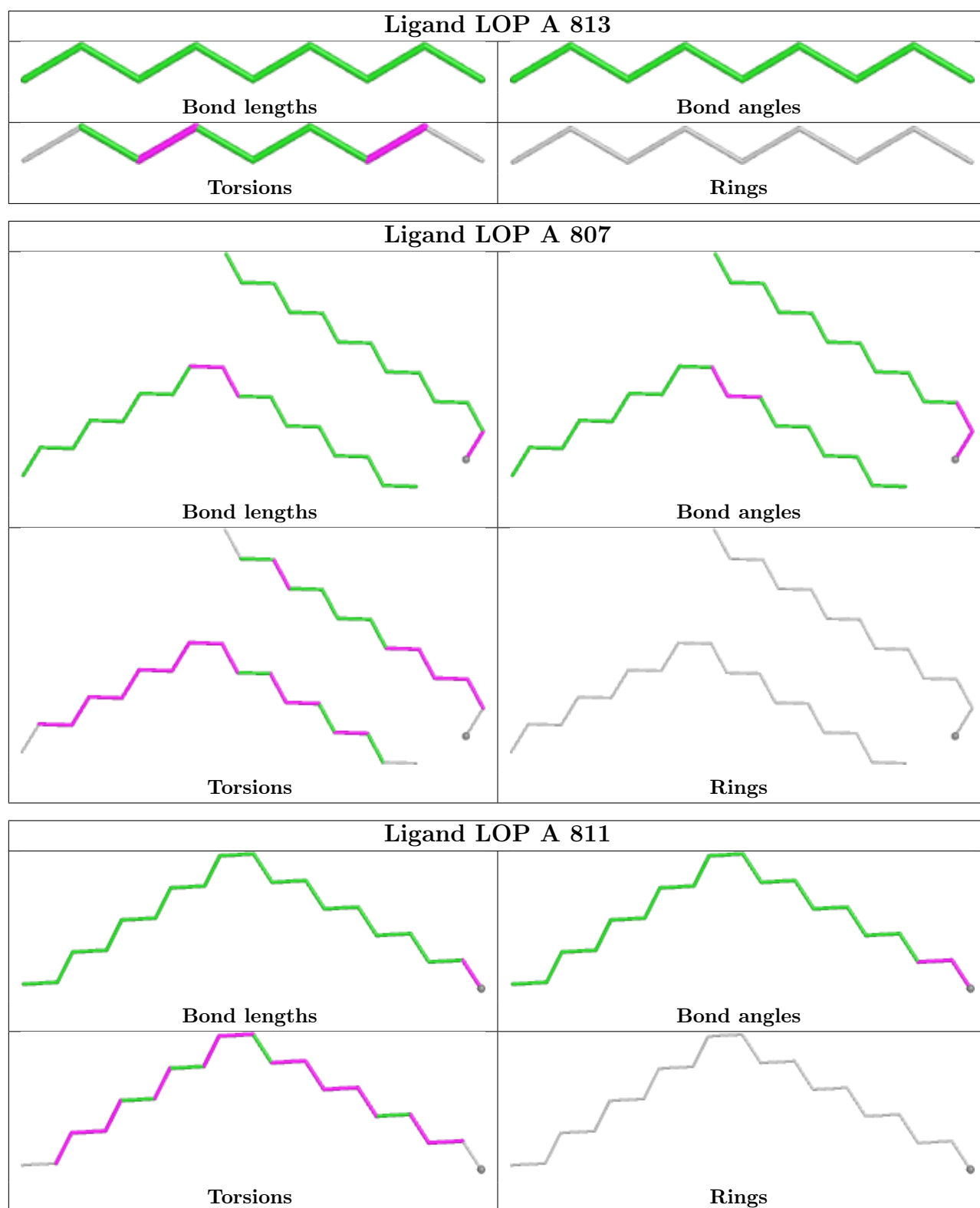


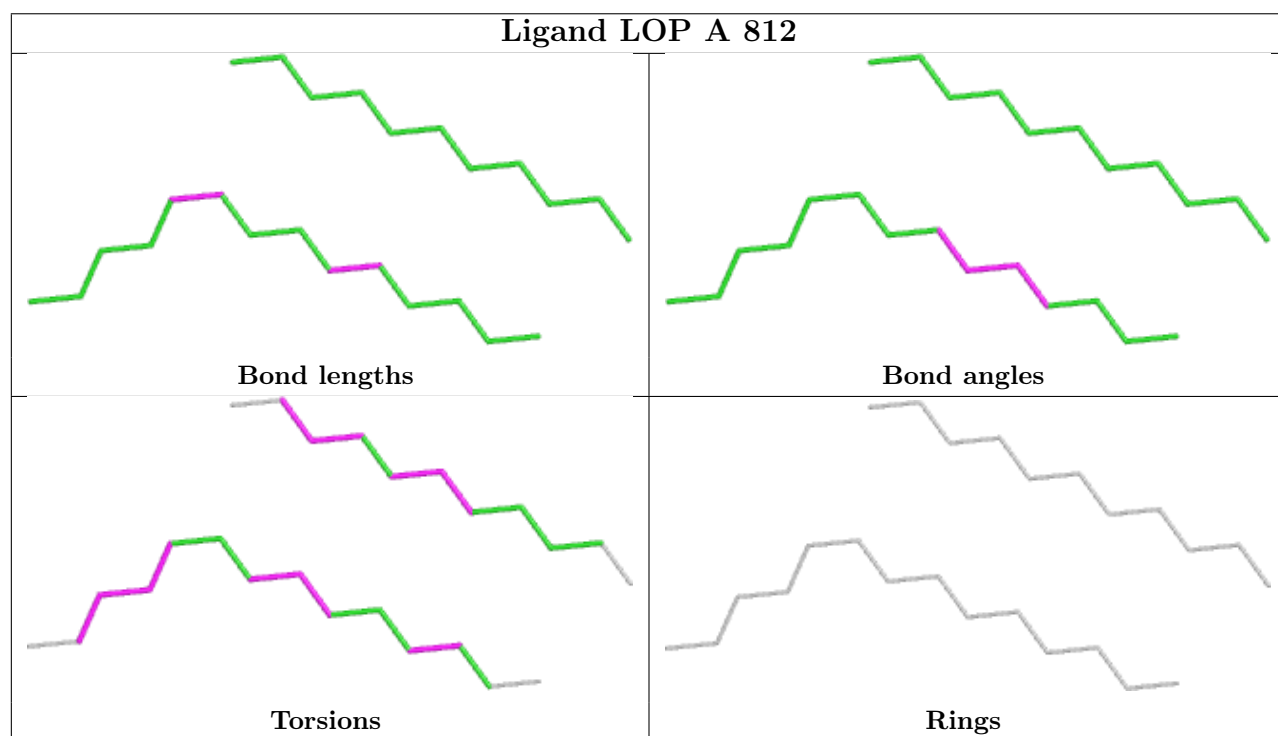
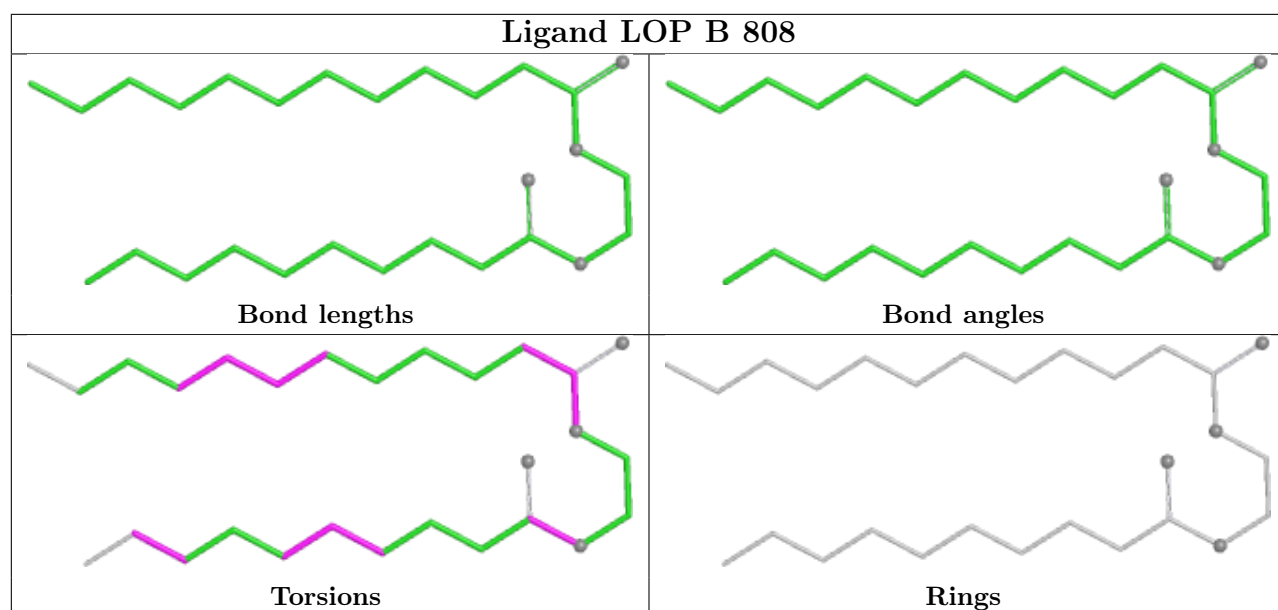


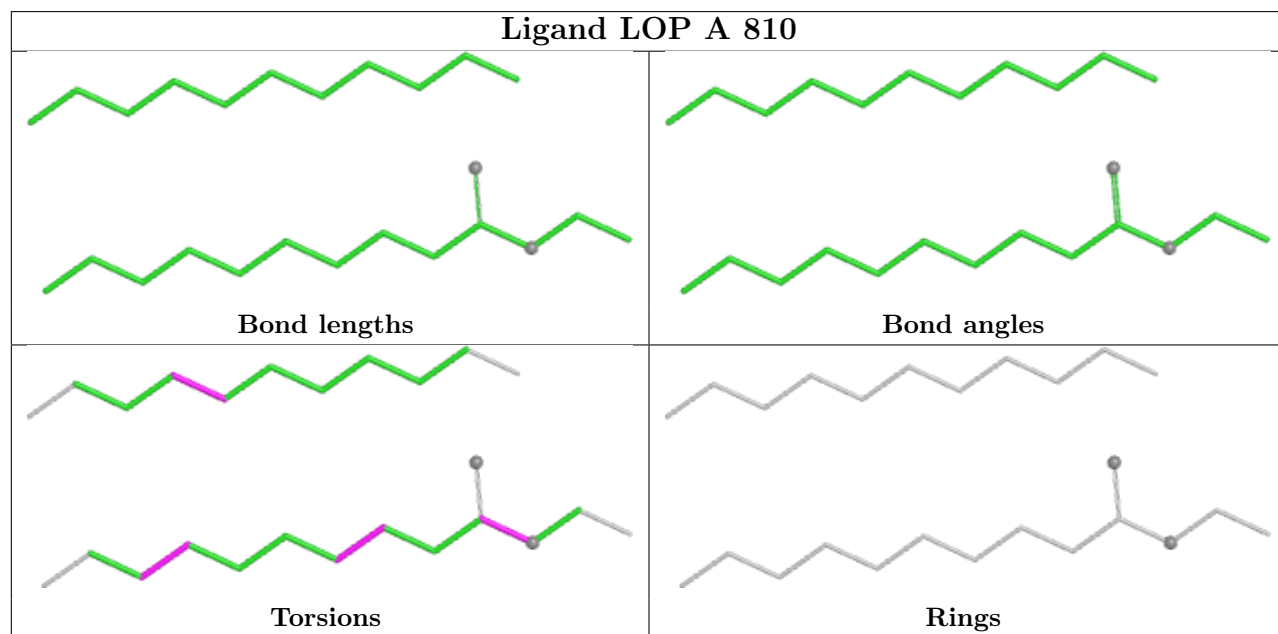
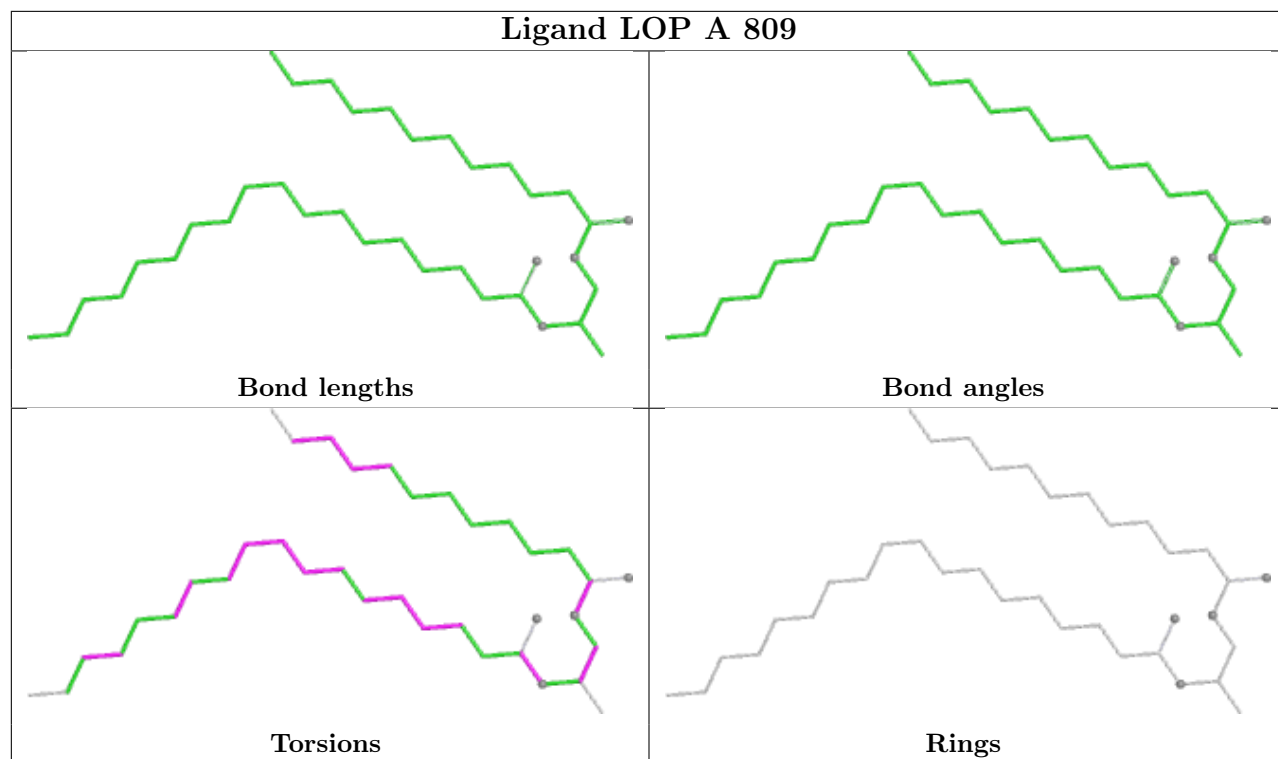


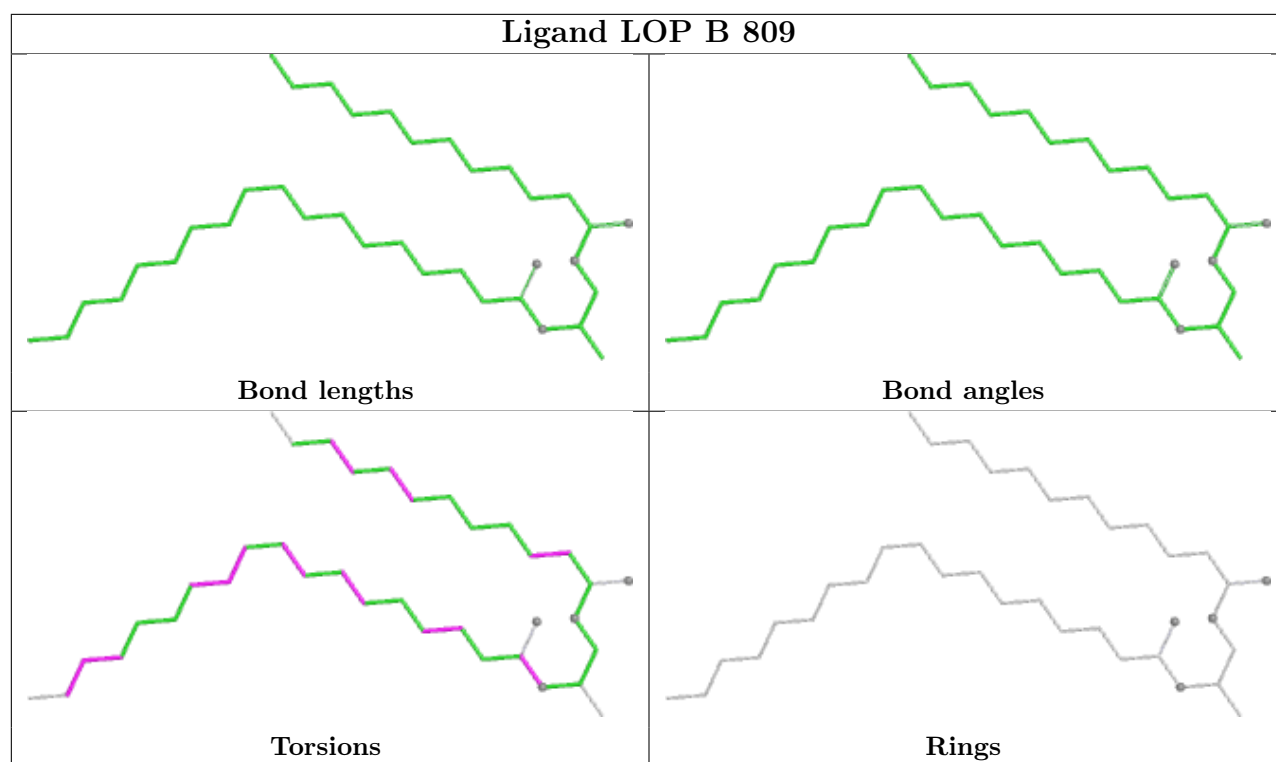


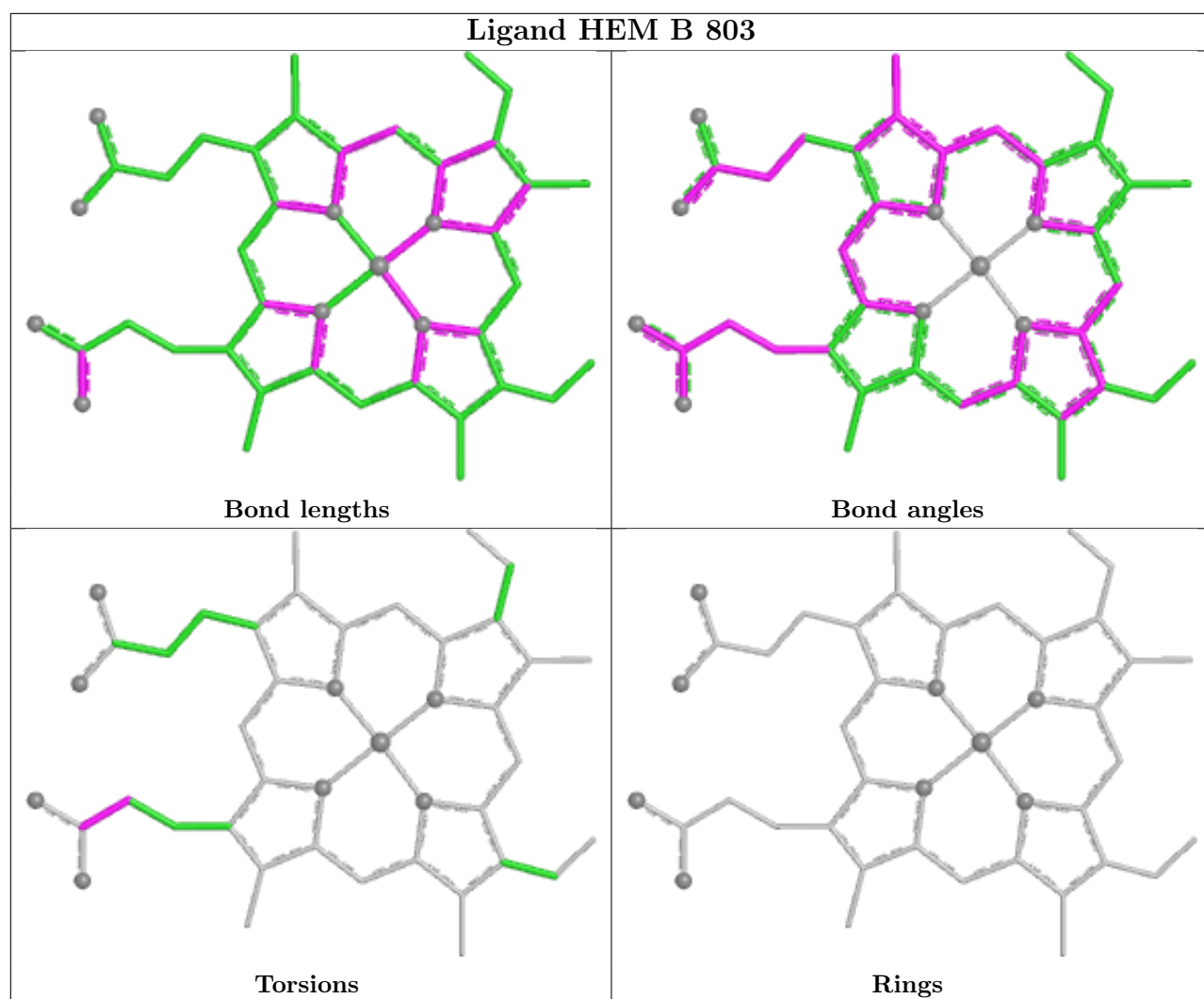


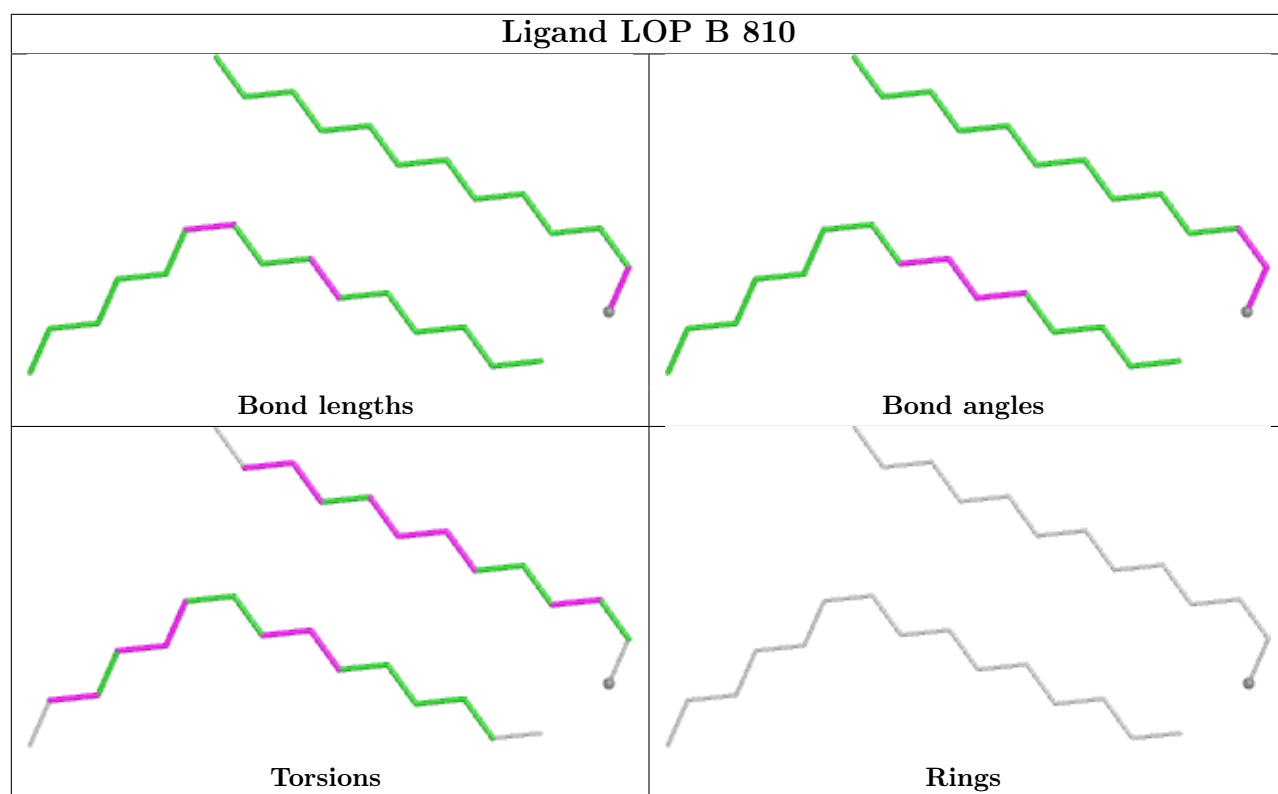


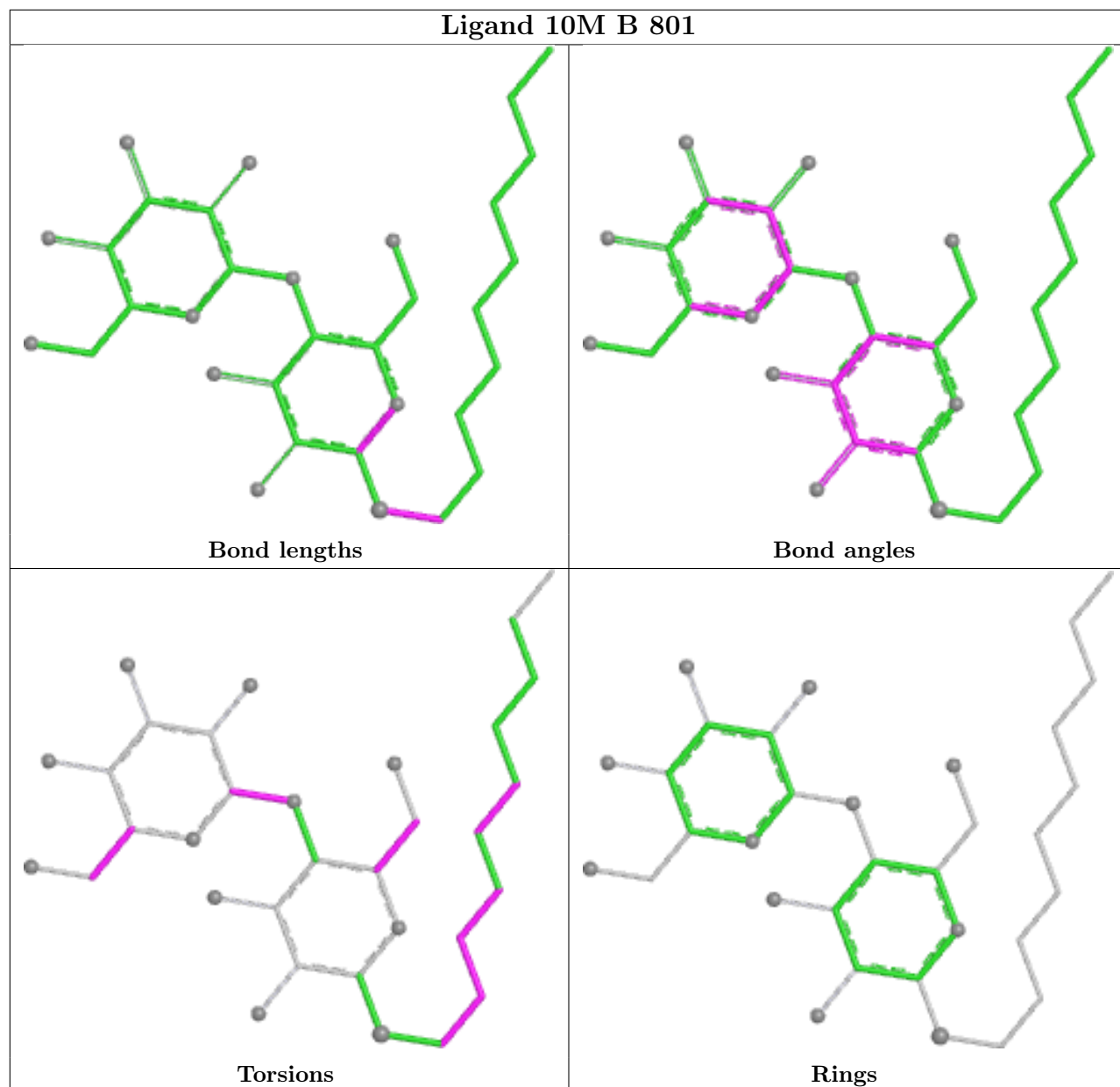


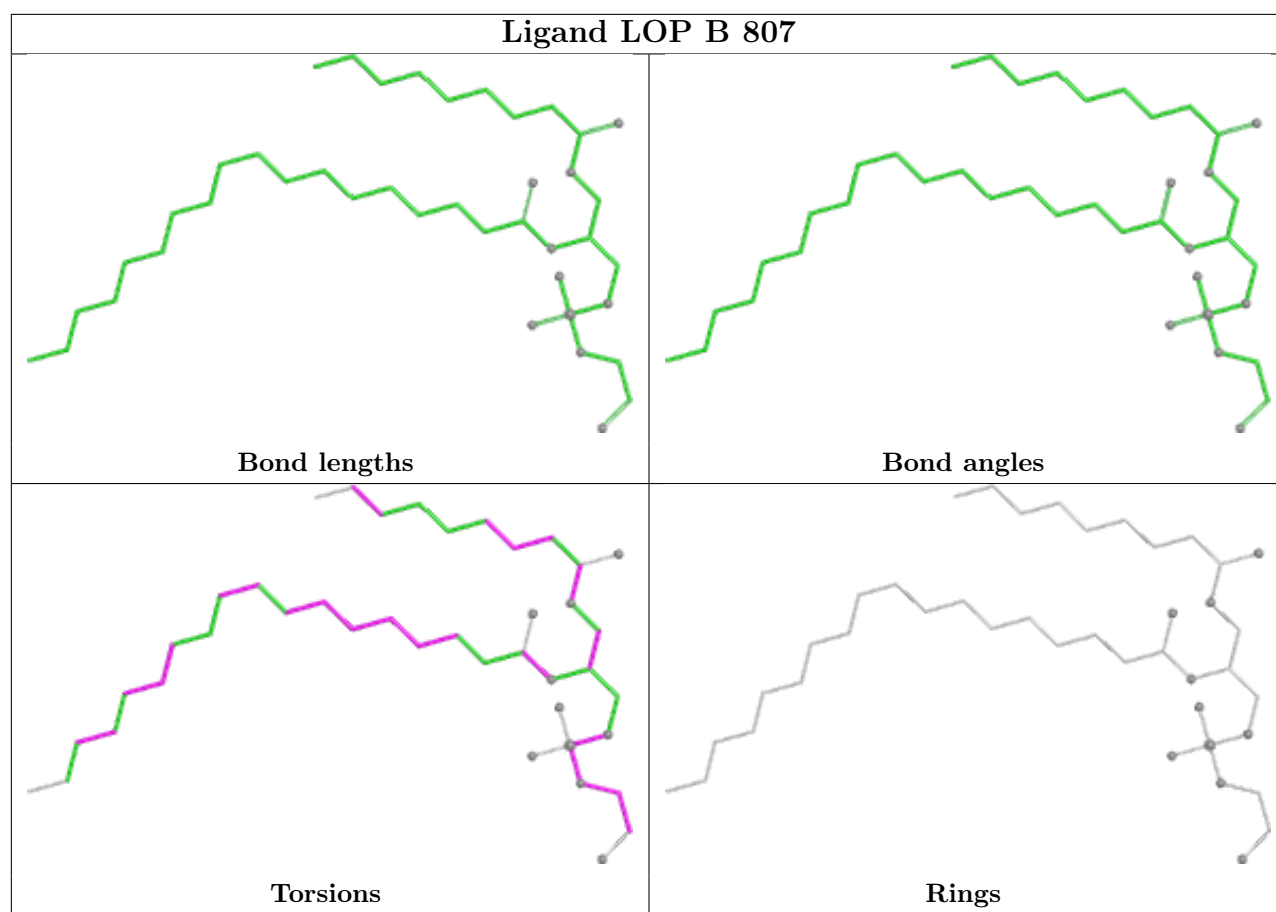












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

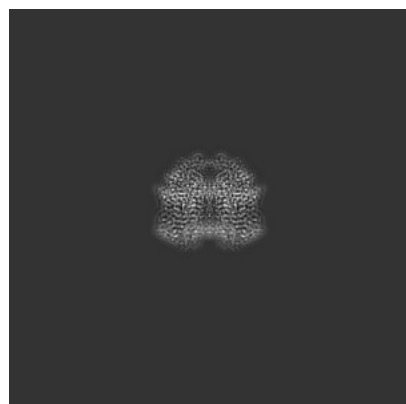
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16041. These allow visual inspection of the internal detail of the map and identification of artifacts.

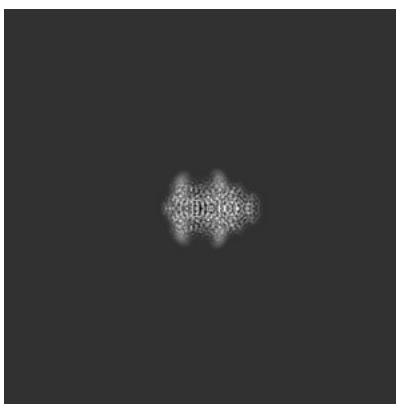
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

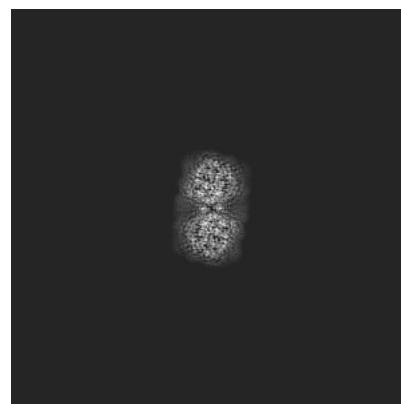
6.1.1 Primary map



X

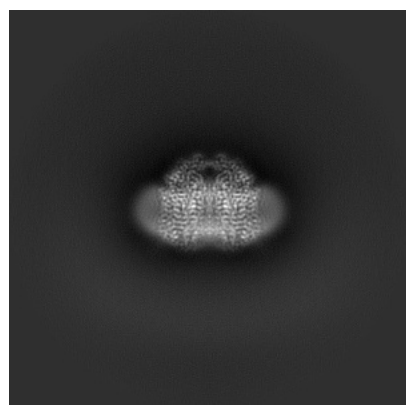


Y

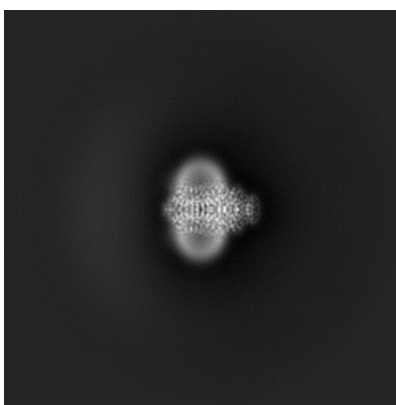


Z

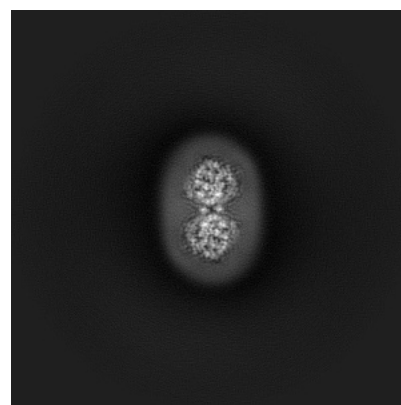
6.1.2 Raw map



X



Y

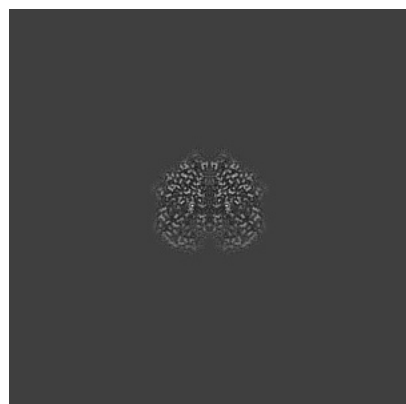


Z

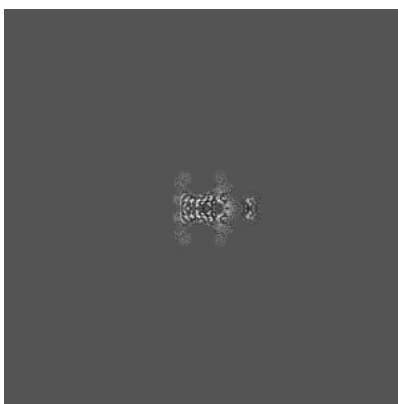
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

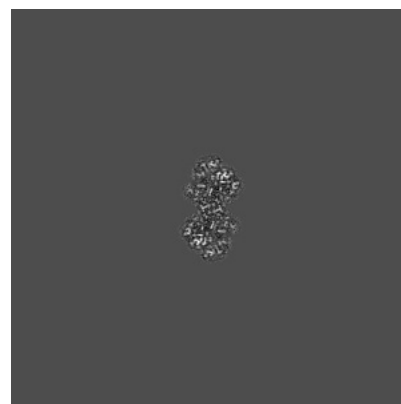
6.2.1 Primary map



X Index: 200

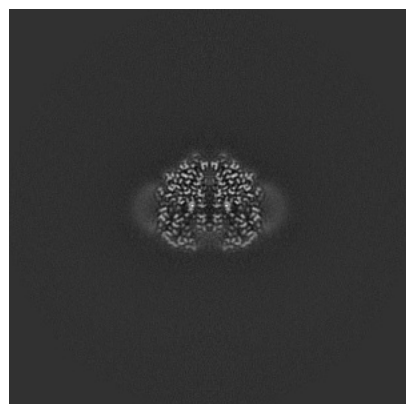


Y Index: 200

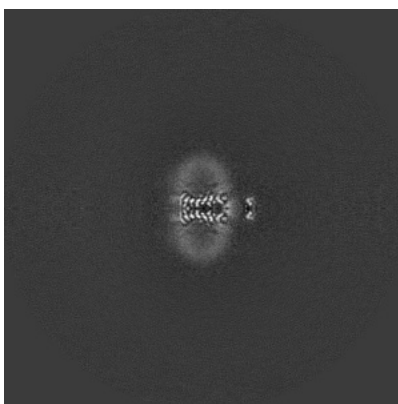


Z Index: 200

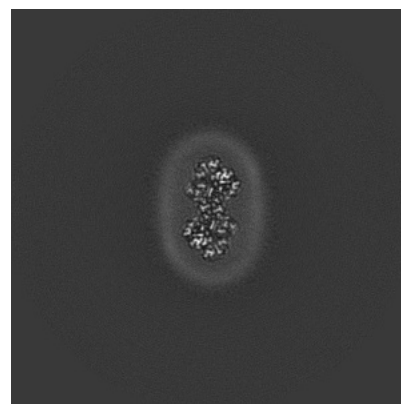
6.2.2 Raw map



X Index: 200



Y Index: 200

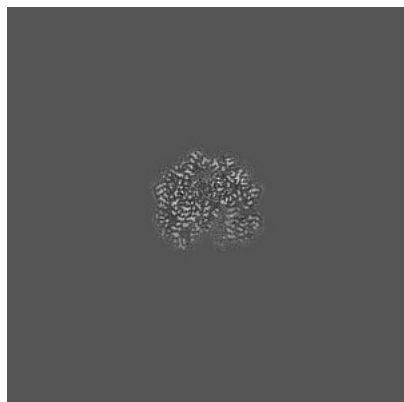


Z Index: 200

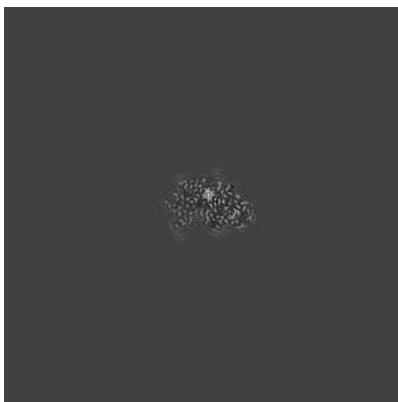
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

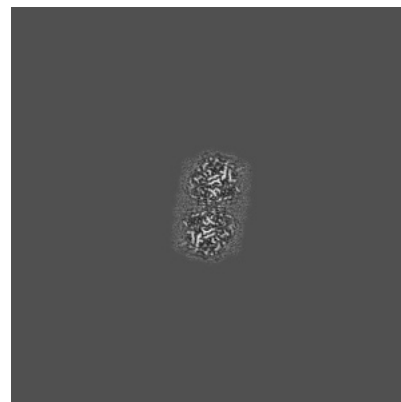
6.3.1 Primary map



X Index: 195

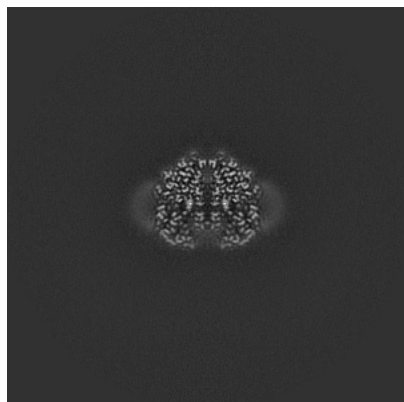


Y Index: 226

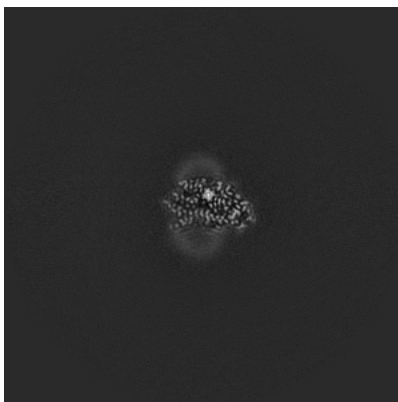


Z Index: 215

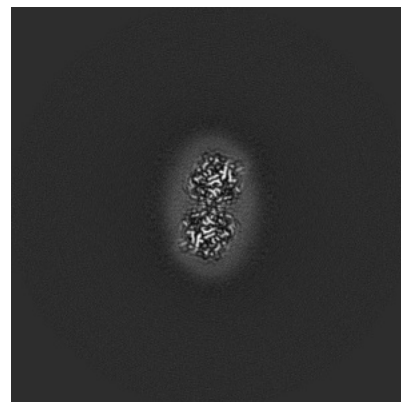
6.3.2 Raw map



X Index: 200



Y Index: 226

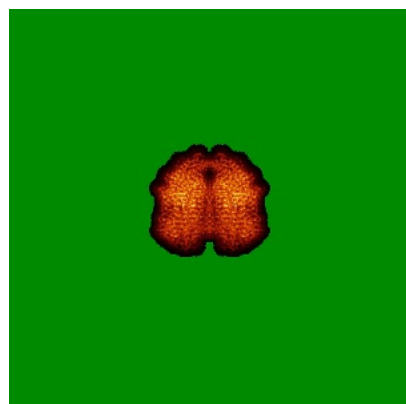


Z Index: 215

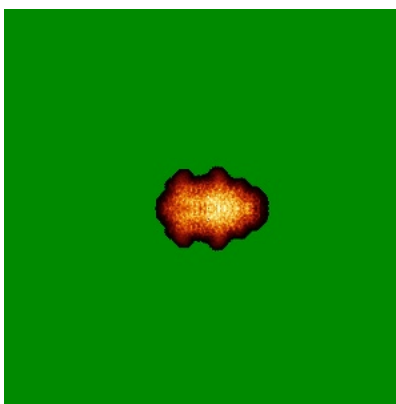
The images above show the largest variance slices of the map in three orthogonal directions.

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

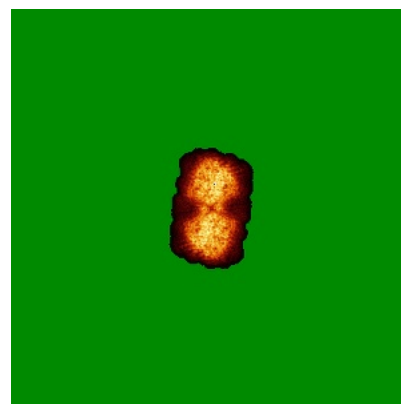
6.4.1 Primary map



X

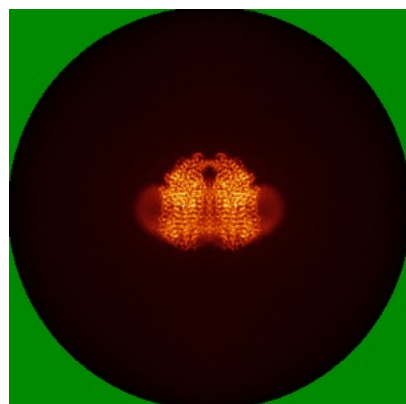


Y

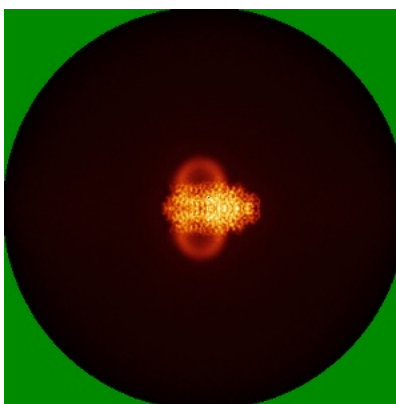


Z

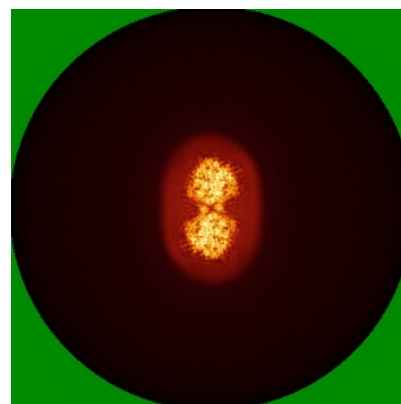
6.4.2 Raw map



X



Y

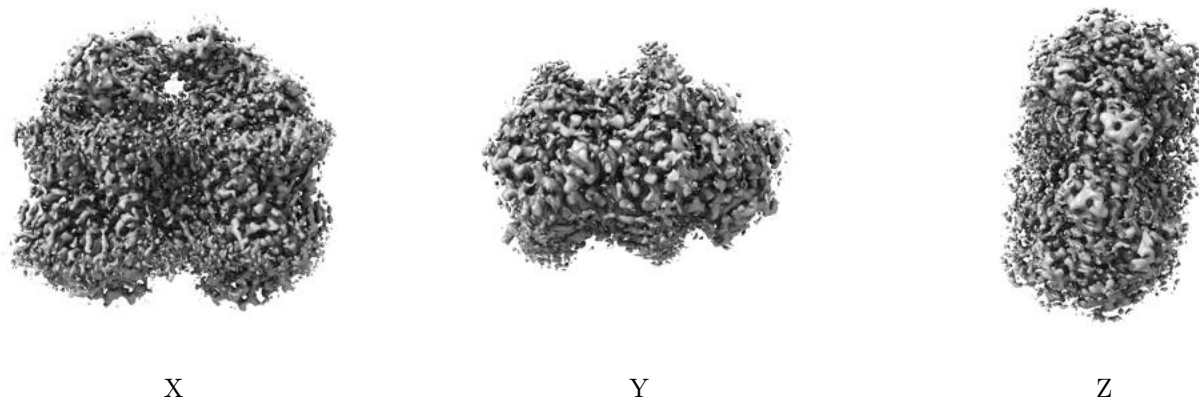


Z

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.

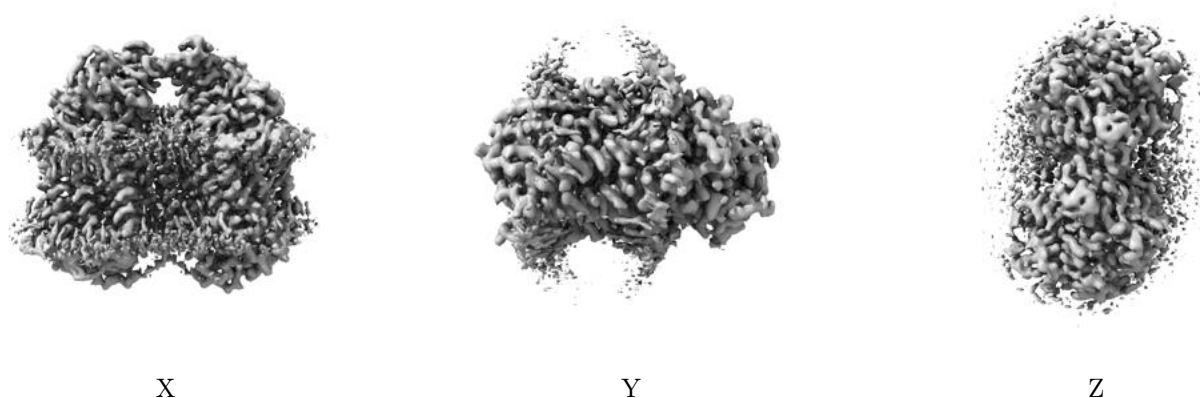
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

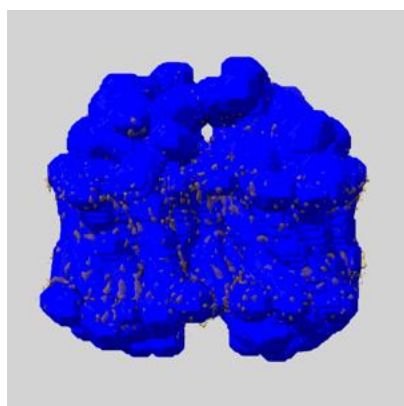
6.6 Mask visualisation [i](#)

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

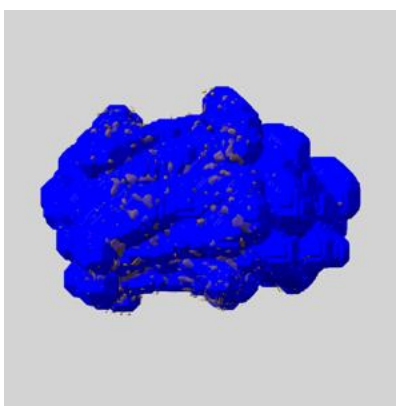
A mask typically either:

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

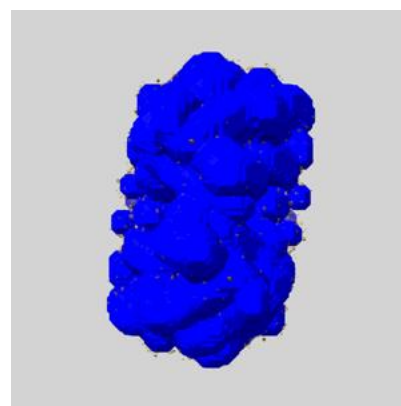
6.6.1 emd_16041_msk_1.map [i](#)



X



Y

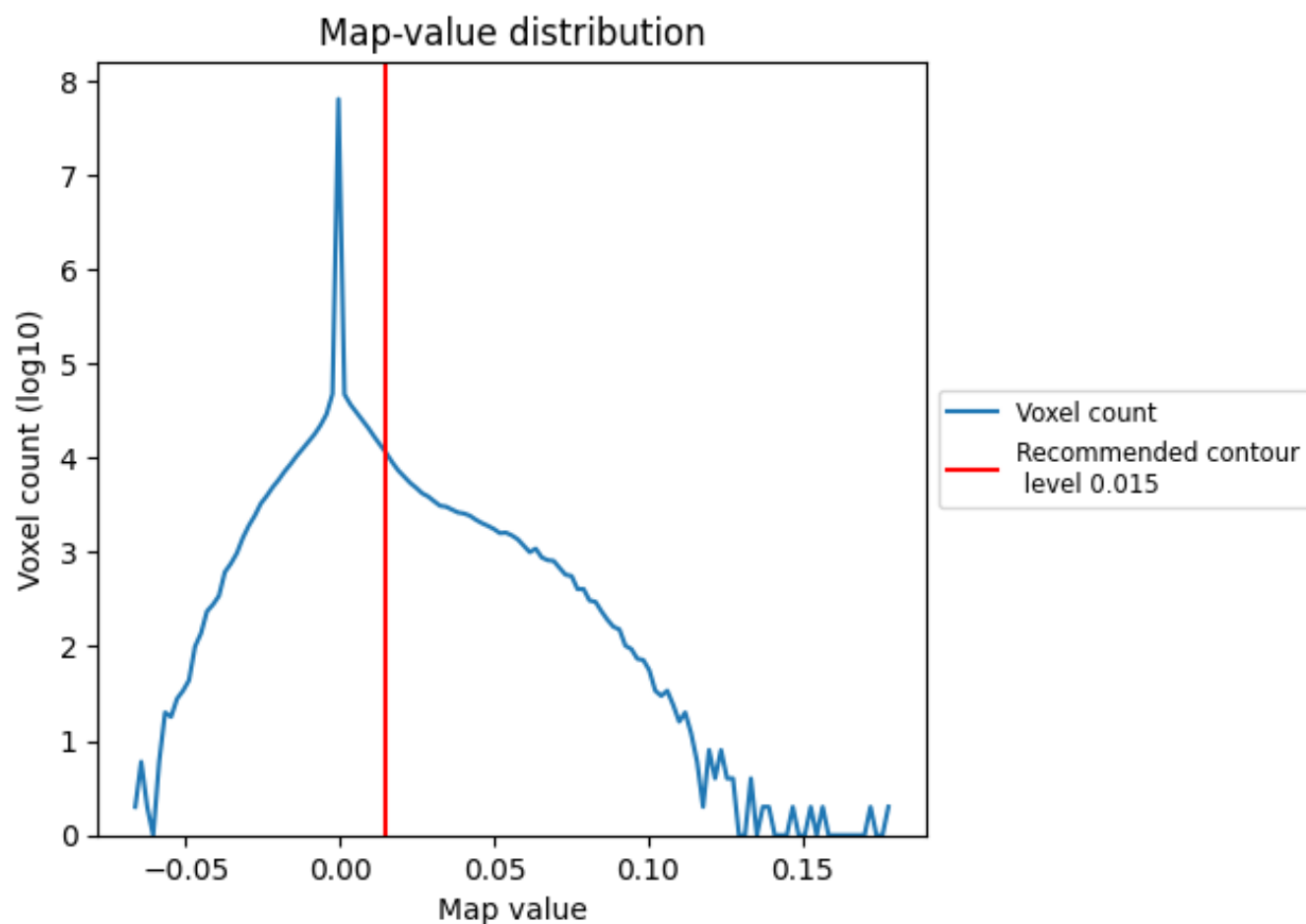


Z

7 Map analysis [i](#)

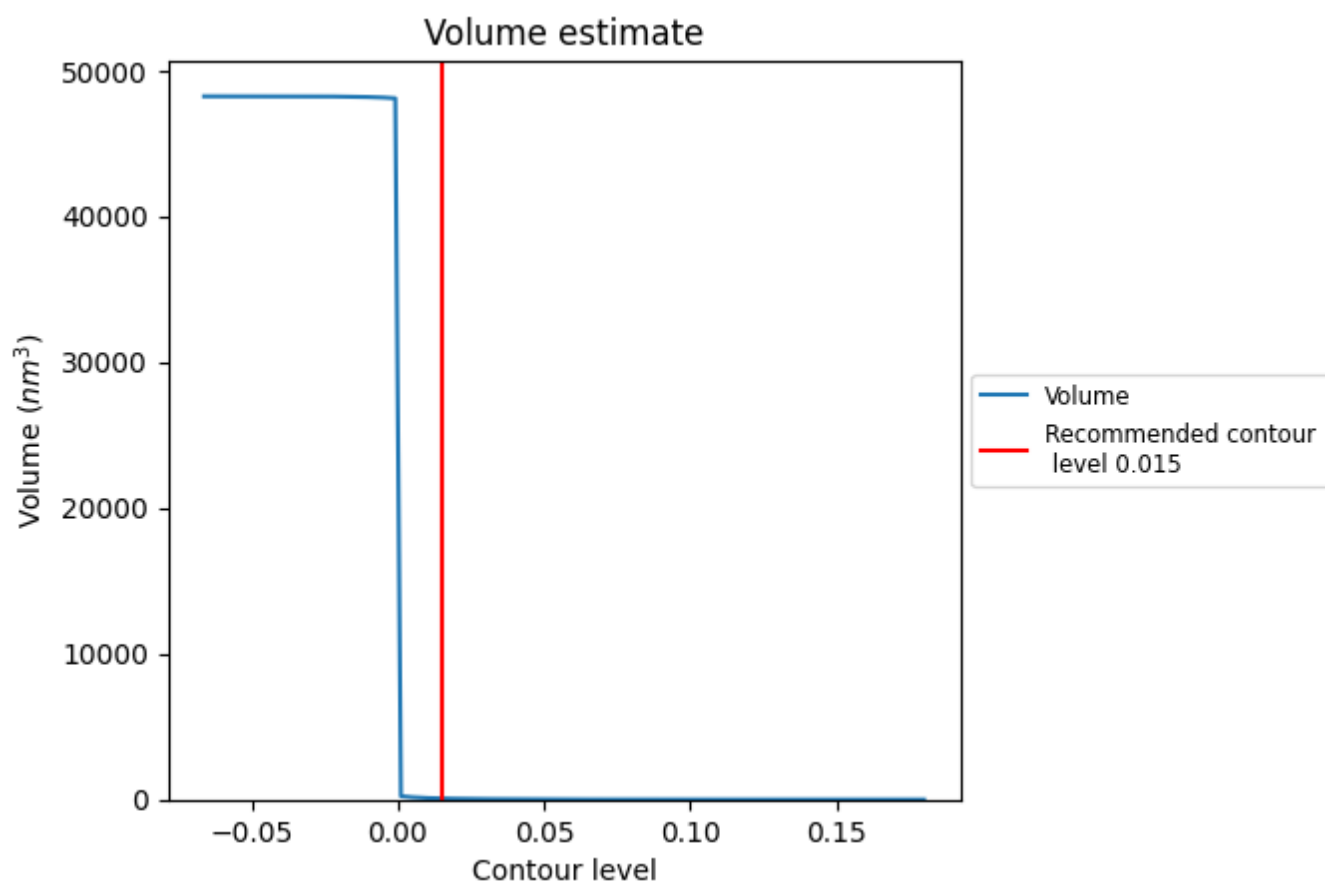
This section contains the results of statistical analysis of the map.

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.

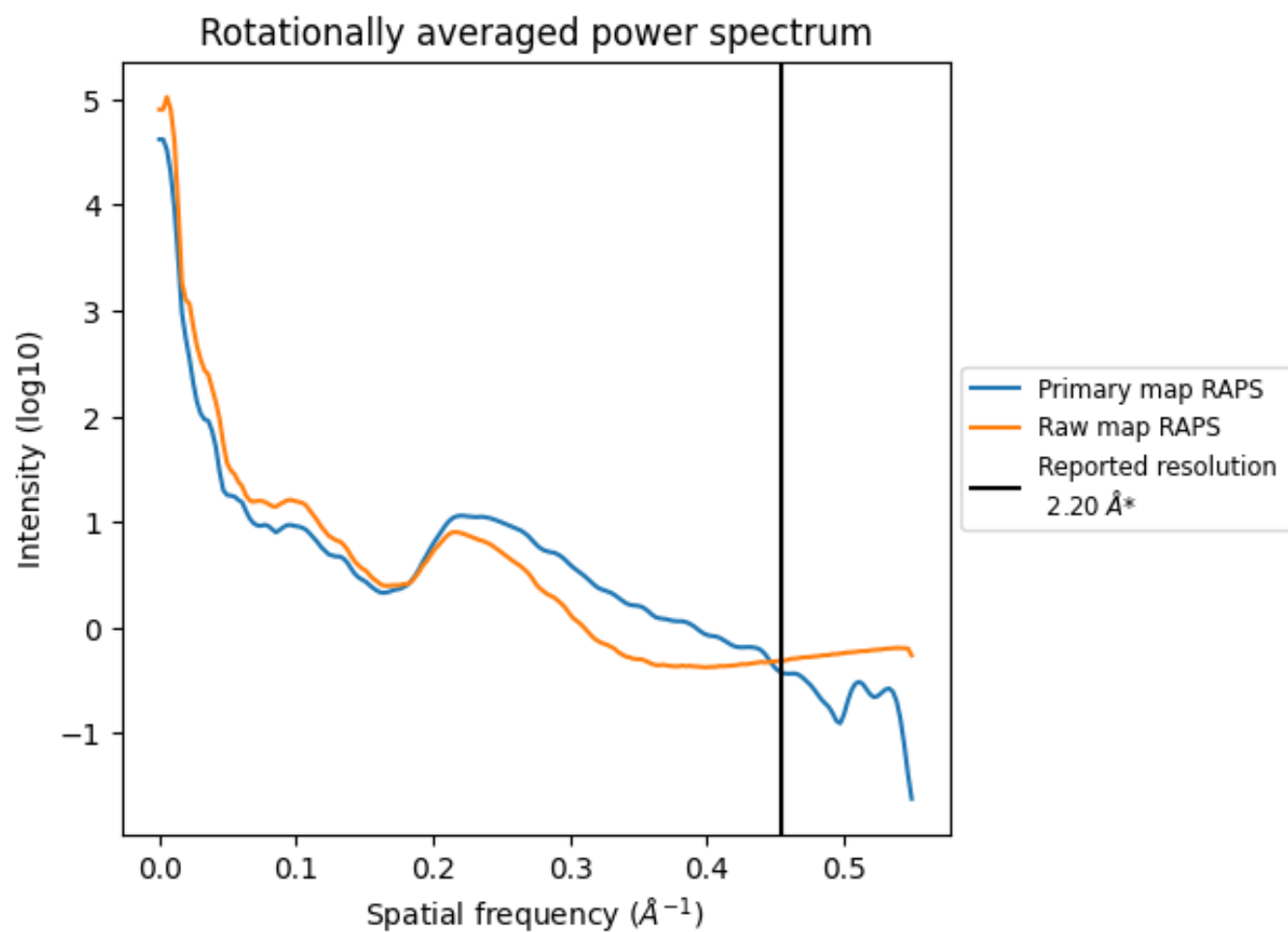
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 74 nm^3 ; this corresponds to an approximate mass of 67 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 ⓘ

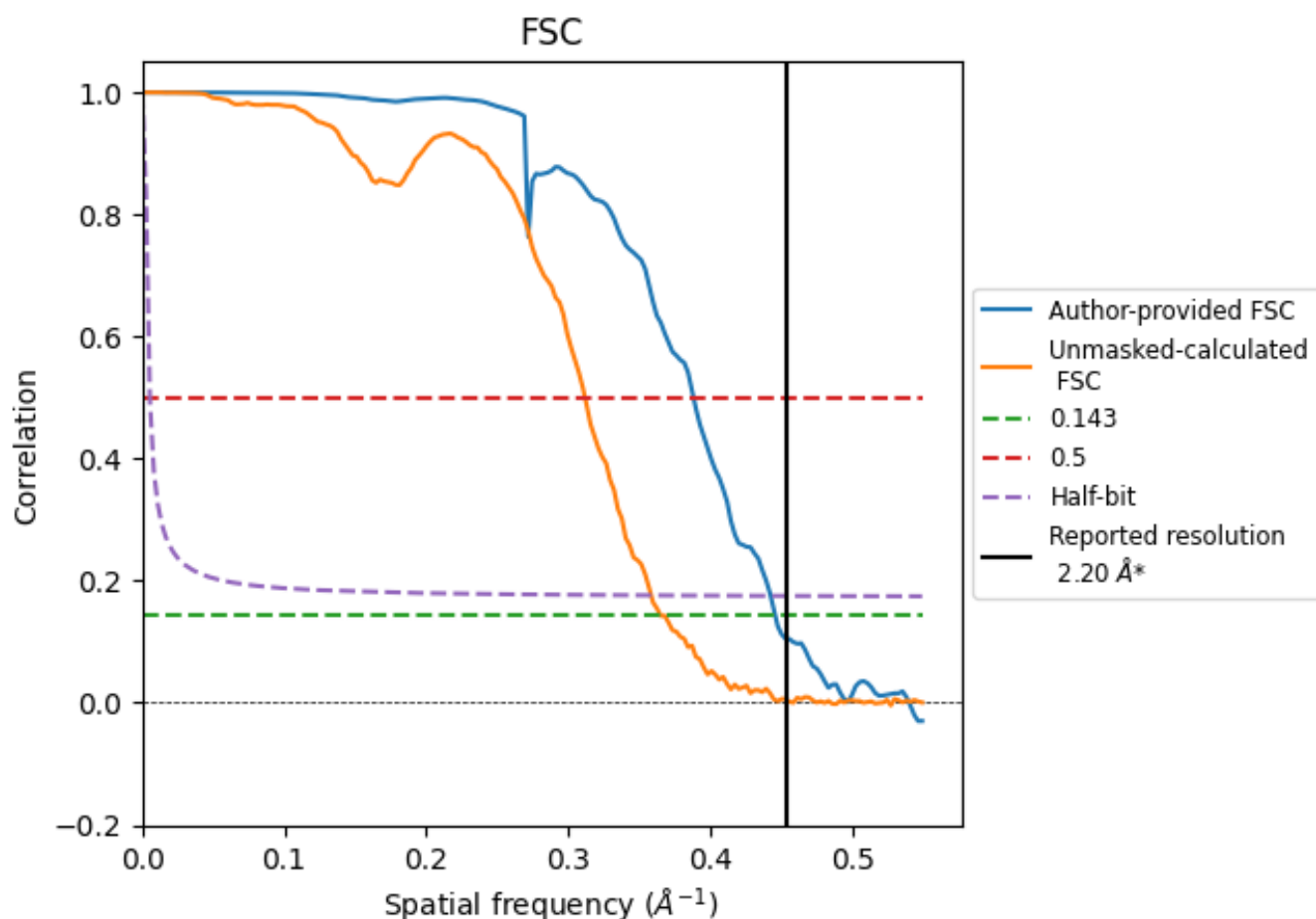


*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

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 0.455 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

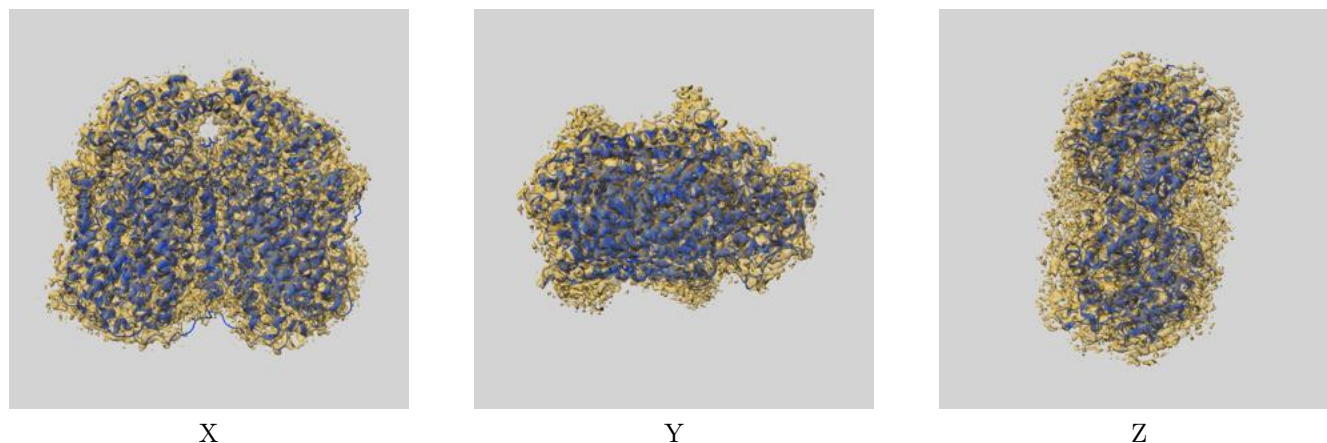
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.24	2.57	2.26
Unmasked-calculated*	2.74	3.21	2.79

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.74 differs from the reported value 2.2 by more than 10 %

9 Map-model fit [i](#)

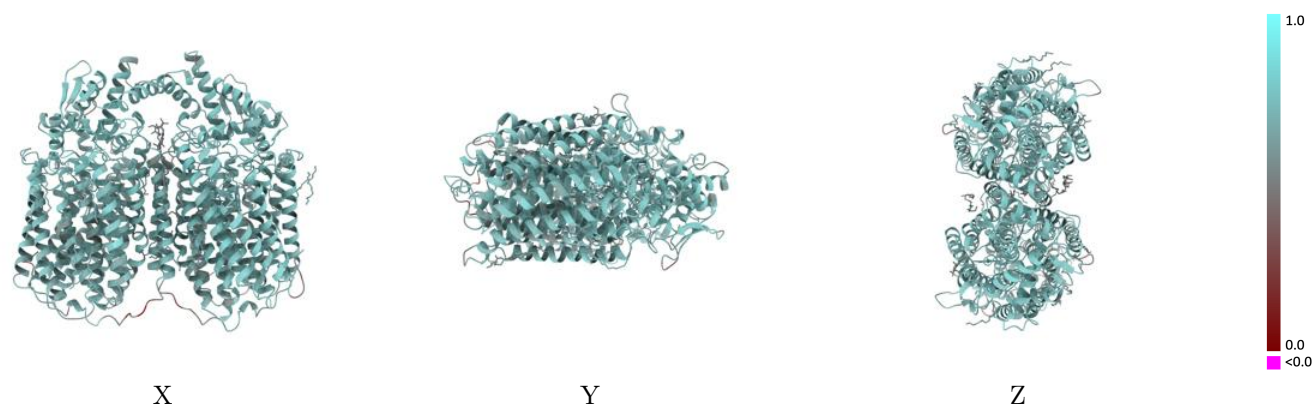
This section contains information regarding the fit between EMDB map EMD-16041 and PDB model 8BGW. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



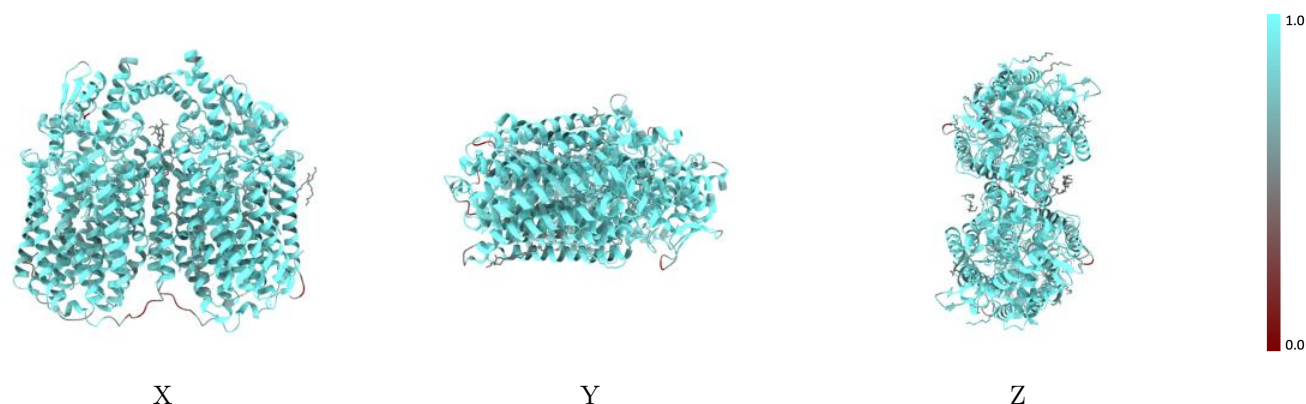
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



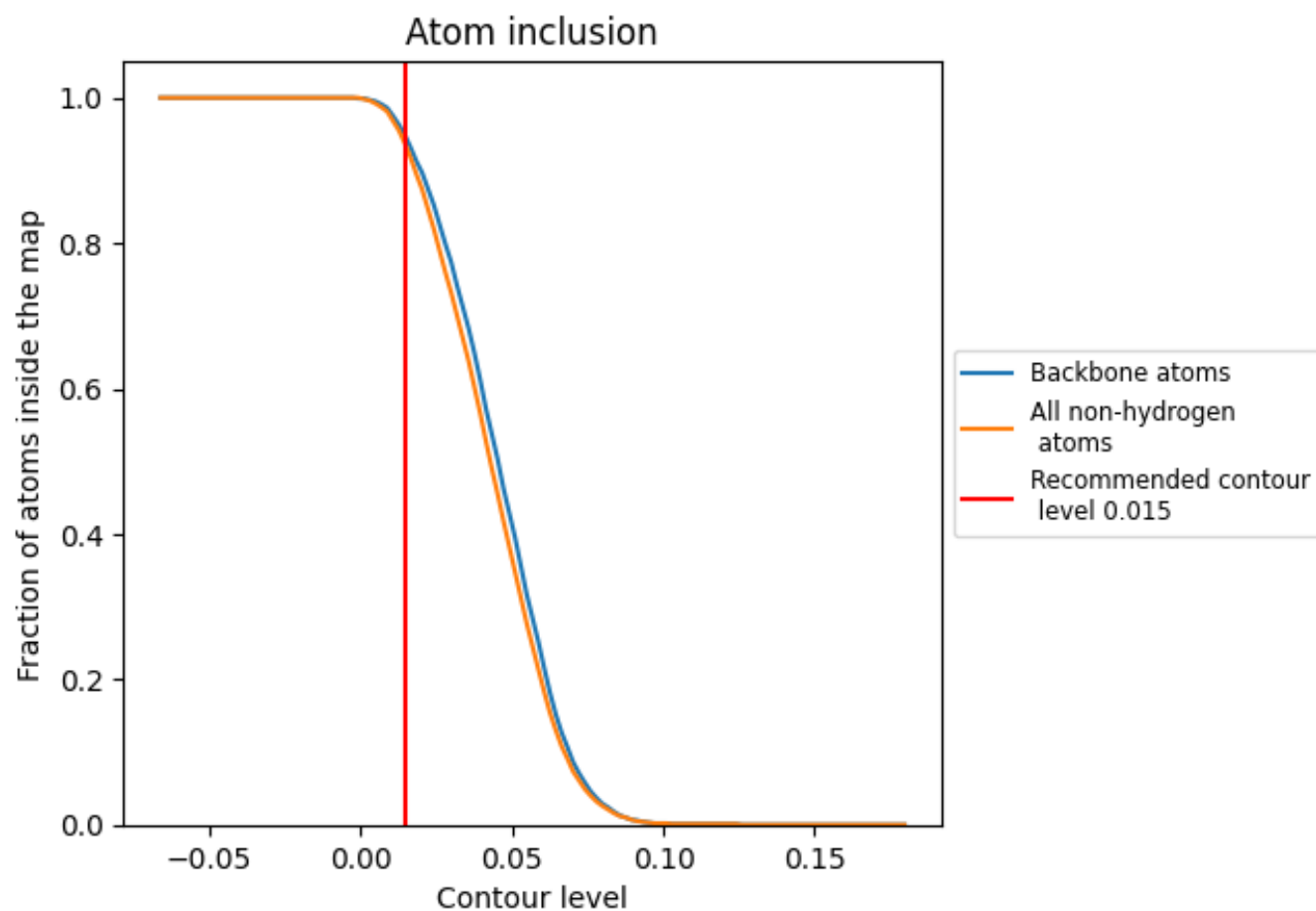
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9330	0.6860
A	0.9350	0.6850
B	0.9330	0.6860

