



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 06:34 AM EDT

PDB ID : 6WTI / pdb_00006wti
EMDB ID : EMD-21897
Title : The Cryo-EM structure of the ubiquinol oxidase from Escherichia coli
Authors : Su, C.-C.
Deposited on : 2020-05-02
Resolution : 2.38 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:

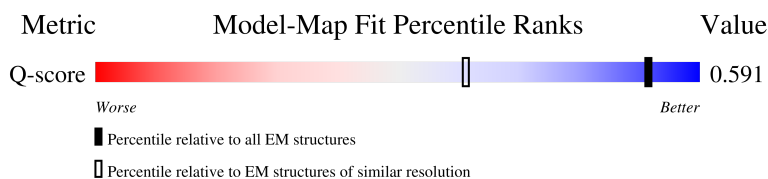
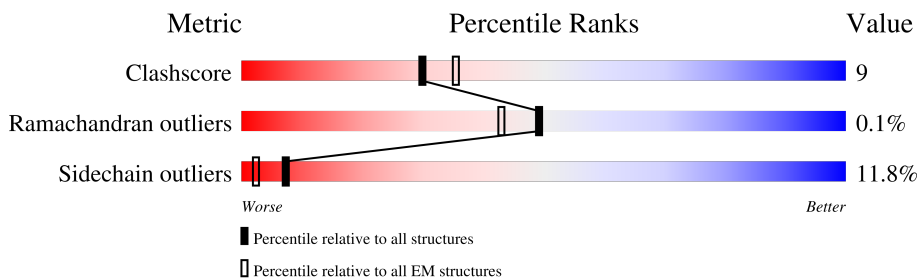
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 2.38 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	4811 (1.88 - 2.88)

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	663	
2	B	315	
3	C	204	
4	D	109	

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	HEO	A	1002	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9980 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome o ubiquinol oxidase, subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	660	Total	C	N	O	S	0	0
			5240	3516	829	858	37		

- Molecule 2 is a protein called Ubiquinol oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	262	Total	C	N	O	S	0	0
			2047	1337	332	367	11		

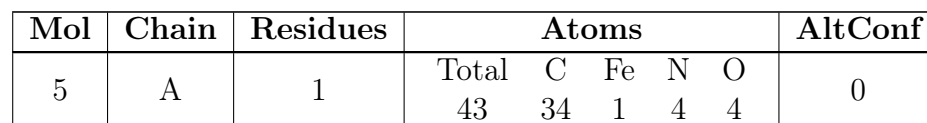
- Molecule 3 is a protein called Cytochrome o ubiquinol oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	186	Total	C	N	O	S	0	0
			1459	975	230	241	13		

- Molecule 4 is a protein called Cytochrome o ubiquinol oxidase, subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	99	Total	C	N	O	S	0	0
			769	514	119	125	11		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



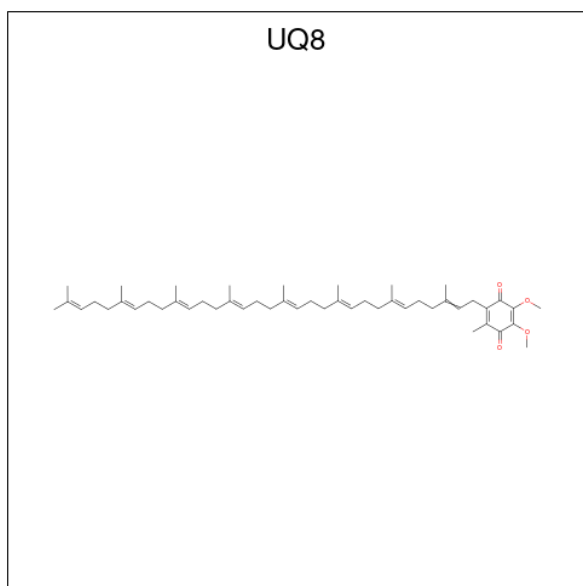
- # HEO

Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	Fe	N	O	0
			59	49	1	4	5	

- 

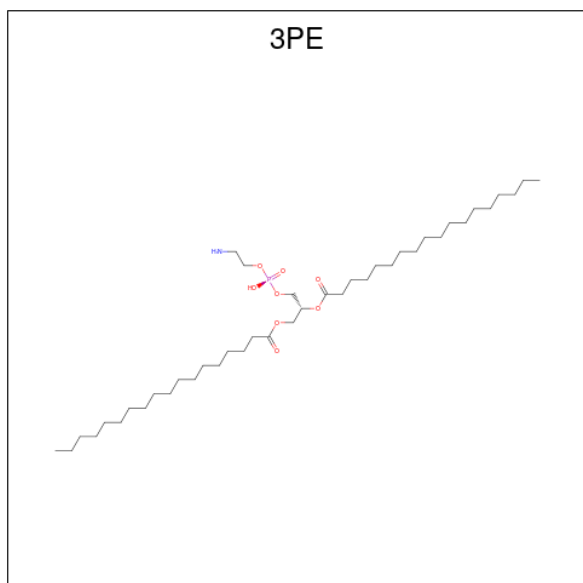
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Cu	0
			1	1	

- Molecule 8 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$).



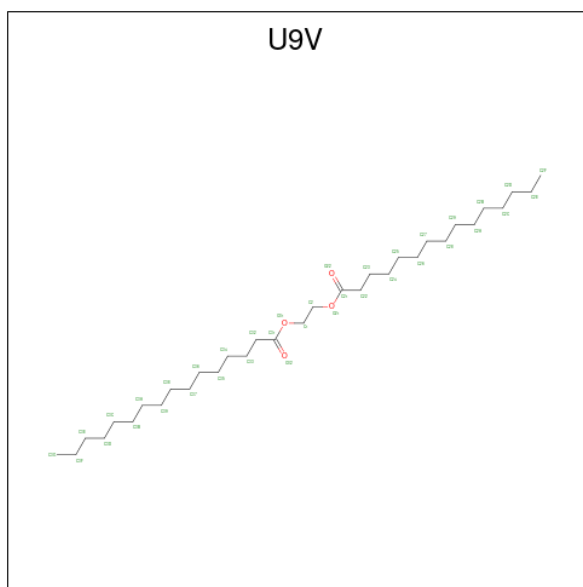
Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			53	49	4	

- Molecule 9 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total C N O P 47 37 1 8 1	0
9	A	1	Total C O 28 24 4	0
9	A	1	Total C 10 10	0
9	A	1	Total C O P 26 18 7 1	0
9	B	1	Total C O 14 12 2	0
9	C	1	Total C N O P 47 37 1 8 1	0
9	C	1	Total C N O P 40 30 1 8 1	0
9	D	1	Total C N O P 45 35 1 8 1	0
9	D	1	Total C 17 17	0

- Molecule 10 is pentadecyl(tetradecyl)peroxyanhydride (CCD ID: U9V) (formula: $C_{33}H_{64}O_4$).

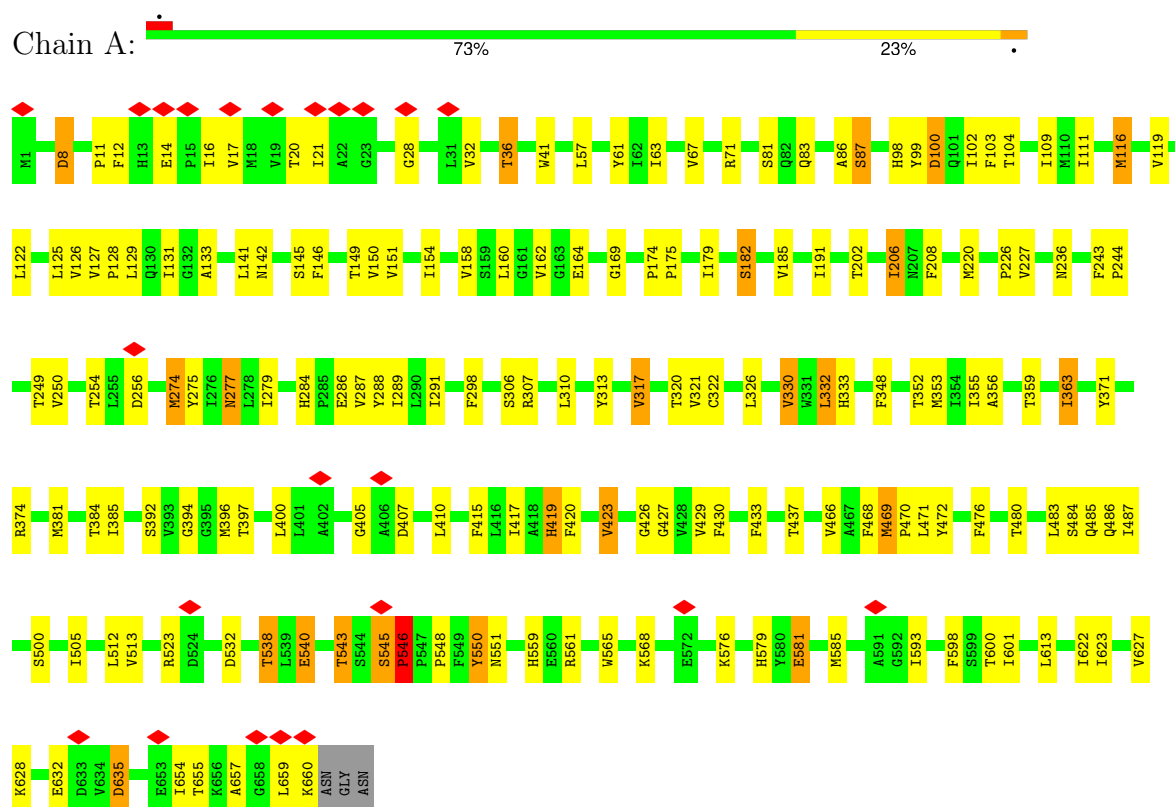


Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C O 35 31 4	0

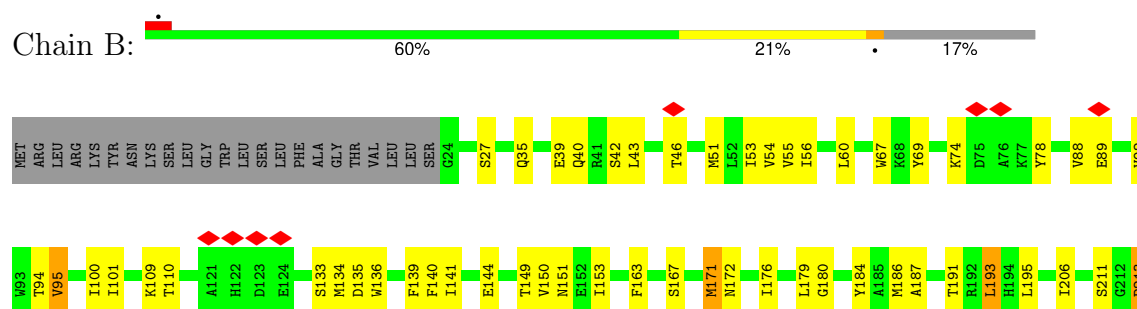
3 Residue-property plots

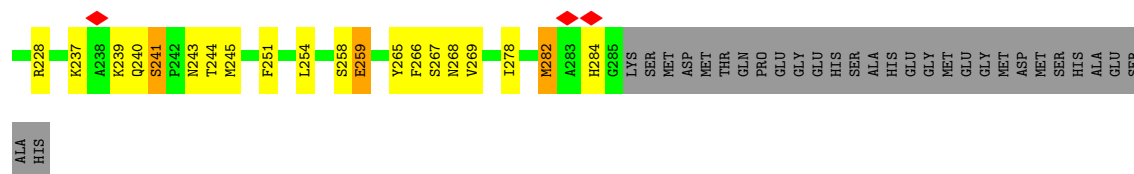
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

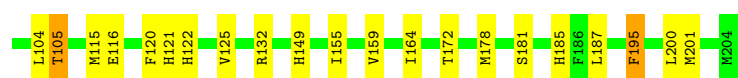


- Molecule 2: Ubiquinol oxidase subunit 2

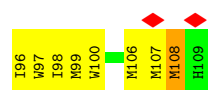
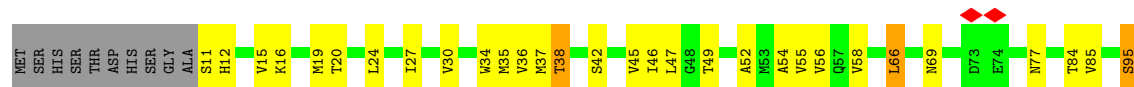




• Molecule 3: Cytochrome o ubiquinol oxidase



• Molecule 4: Cytochrome o ubiquinol oxidase, subunit IV



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	334222	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	6.271	Depositor
Minimum map value	-3.624	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.410	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	114.48, 91.8, 104.76	wwPDB
Map dimensions	97, 85, 106	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UQ8, HEM, 3PE, U9V, HEO, CU

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	0.43	0/5417	0.65	16/7385 (0.2%)
2	B	0.49	0/2107	0.75	8/2869 (0.3%)
3	C	0.34	0/1502	0.49	0/2040
4	D	0.36	0/789	0.44	0/1077
All	All	0.43	0/9815	0.63	24/13371 (0.2%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	546	PRO	N-CA-C	-10.94	97.36	110.70
1	A	356	ALA	N-CA-C	10.30	122.50	111.28
2	B	282	MET	N-CA-C	9.45	124.28	111.24
1	A	16	ILE	N-CA-C	9.00	118.99	110.53
2	B	94	THR	N-CA-C	7.96	119.95	111.28
1	A	561	ARG	N-CA-C	6.75	118.29	111.07
2	B	151	ASN	N-CA-C	6.67	120.78	112.24
1	A	559	HIS	O-C-N	-6.50	115.50	122.19
2	B	213	PRO	N-CA-C	6.08	121.99	113.53
1	A	550	TYR	N-CA-C	-6.07	99.29	109.07
1	A	185	VAL	N-CA-C	6.04	120.85	113.00
2	B	135	ASP	CA-C-O	-5.92	114.29	120.92
1	A	545	SER	CA-C-N	5.74	126.29	120.38
1	A	545	SER	C-N-CA	5.74	126.29	120.38
1	A	185	VAL	CA-C-N	5.72	126.33	119.98
1	A	185	VAL	C-N-CA	5.72	126.33	119.98
1	A	191	ILE	N-CA-C	5.61	115.80	110.42
2	B	95	VAL	CA-C-N	-5.58	113.14	119.28
2	B	95	VAL	C-N-CA	-5.58	113.14	119.28
1	A	100	ASP	CB-CA-C	5.53	120.25	110.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	GLU	N-CA-C	5.40	120.45	109.60
1	A	206	ILE	CB-CA-C	-5.35	104.92	112.14
1	A	427	GLY	N-CA-C	5.28	119.52	112.77
2	B	259	GLU	N-CA-C	5.02	117.01	109.23

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	5240	0	5247	110	0
2	B	2047	0	2040	44	0
3	C	1459	0	1467	17	0
4	D	769	0	800	18	0
5	A	43	0	30	9	0
6	A	59	0	56	5	0
7	A	1	0	0	0	0
8	A	53	0	74	8	0
9	A	111	0	148	1	0
9	B	14	0	18	0	0
9	C	87	0	122	1	0
9	D	62	0	94	0	0
10	A	35	0	0	0	0
All	All	9980	0	10096	182	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 9.

All (182) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:SER:HB2	1:A:546:PRO:CD	1.57	1.33
1:A:545:SER:CB	1:A:546:PRO:HD3	1.65	1.26
1:A:208:PHE:HB2	1:A:236:ASN:OD1	1.51	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:HIS:HD2	1:A:330:VAL:HG23	1.27	0.97
1:A:284:HIS:CD2	1:A:330:VAL:HG23	2.00	0.96
1:A:208:PHE:CB	1:A:236:ASN:OD1	2.27	0.83
1:A:426:GLY:O	1:A:430:PHE:HB2	1.80	0.81
5:A:1001:HEM:HHD	5:A:1001:HEM:HBC2	1.62	0.79
1:A:545:SER:HB2	1:A:546:PRO:HD3	0.81	0.76
1:A:396:MET:HG3	2:B:51:MET:SD	2.25	0.76
6:A:1002:HEO:H272	2:B:55:VAL:HG22	1.67	0.75
1:A:11:PRO:HG2	1:A:17:VAL:HG11	1.66	0.75
1:A:284:HIS:CD2	1:A:330:VAL:CG2	2.69	0.75
2:B:254:LEU:HD12	2:B:254:LEU:O	1.86	0.74
1:A:660:LYS:HD2	1:A:660:LYS:C	2.14	0.73
2:B:186:MET:HE1	4:D:106:MET:HE1	1.69	0.72
2:B:150:VAL:HG23	2:B:266:PHE:HE1	1.54	0.72
1:A:131:ILE:HA	1:A:220:MET:HE1	1.77	0.66
1:A:523:ARG:HH12	9:A:1009:3PE:C31	2.08	0.66
1:A:71:ARG:NH1	8:A:1004:UQ8:H1M	2.11	0.65
8:A:1004:UQ8:H4MB	8:A:1004:UQ8:H3MA	1.79	0.64
1:A:613:LEU:HD12	1:A:613:LEU:O	1.98	0.63
8:A:1004:UQ8:H1MA	8:A:1004:UQ8:C8	2.29	0.62
1:A:274:MET:HE2	3:C:49:VAL:HG21	1.79	0.62
1:A:601:ILE:CG2	1:A:613:LEU:HD11	2.29	0.62
3:C:86:ALA:HB2	3:C:101:TRP:HB3	1.82	0.61
1:A:284:HIS:HD2	1:A:330:VAL:CG2	2.07	0.61
4:D:107:MET:HE3	4:D:108:MET:H	1.65	0.61
1:A:545:SER:CB	1:A:546:PRO:CD	2.41	0.60
1:A:111:ILE:HG12	5:A:1001:HEM:CBC	2.32	0.59
1:A:146:PHE:O	1:A:150:VAL:HG23	2.02	0.59
2:B:43:LEU:HD13	2:B:110:THR:HG21	1.84	0.59
1:A:71:ARG:HD3	1:A:109:ILE:HD13	1.84	0.59
1:A:288:TYR:HA	1:A:291:ILE:HG22	1.85	0.59
1:A:111:ILE:CD1	5:A:1001:HEM:HBC1	2.33	0.59
1:A:182:SER:O	1:A:182:SER:OG	2.14	0.59
1:A:313:TYR:O	1:A:317:VAL:HG13	2.03	0.58
1:A:111:ILE:HD13	5:A:1001:HEM:HBC1	1.85	0.57
3:C:86:ALA:HB2	3:C:101:TRP:CB	2.34	0.57
1:A:36:THR:OG1	1:A:41:TRP:NE1	2.37	0.56
1:A:635:ASP:N	1:A:635:ASP:OD1	2.38	0.56
2:B:134:MET:HE2	2:B:139:PHE:HB2	1.87	0.56
1:A:601:ILE:HG21	1:A:613:LEU:HD11	1.87	0.56
2:B:171:MET:HE1	2:B:184:TYR:CD2	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1002:HEO:C18	6:A:1002:HEO:H261	2.35	0.55
3:C:25:LYS:NZ	9:C:401:3PE:O12	2.40	0.55
1:A:160:LEU:HD23	1:A:160:LEU:O	2.07	0.54
2:B:245:MET:HE1	2:B:251:PHE:HA	1.89	0.54
1:A:298:PHE:CD1	1:A:384:THR:HG23	2.42	0.54
4:D:45:VAL:O	4:D:49:THR:HG23	2.08	0.53
1:A:317:VAL:O	1:A:320:THR:HG22	2.09	0.52
1:A:476:PHE:O	2:B:27:SER:OG	2.27	0.52
1:A:162:VAL:HG13	1:A:162:VAL:O	2.09	0.52
1:A:532:ASP:OD2	1:A:568:LYS:NZ	2.39	0.52
3:C:75:LEU:HD12	3:C:115:MET:CE	2.40	0.52
1:A:540:GLU:O	1:A:543:THR:OG1	2.28	0.51
1:A:102:ILE:HG13	8:A:1004:UQ8:H3MB	1.93	0.51
1:A:400:LEU:HB2	2:B:51:MET:HE1	1.92	0.51
1:A:63:ILE:O	1:A:67:VAL:HG13	2.11	0.51
4:D:99:MET:H	4:D:99:MET:HE2	1.76	0.51
1:A:104:THR:HG23	1:A:169:GLY:C	2.36	0.50
1:A:8:ASP:OD1	1:A:8:ASP:N	2.40	0.50
4:D:34:TRP:O	4:D:38:THR:OG1	2.28	0.50
1:A:206:ILE:CD1	3:C:31:ILE:HG22	2.42	0.50
3:C:75:LEU:HD12	3:C:115:MET:HE2	1.93	0.50
2:B:133:SER:OG	2:B:172:ASN:ND2	2.45	0.50
2:B:244:THR:HG22	2:B:268:ASN:HB2	1.93	0.50
1:A:330:VAL:HG11	1:A:352:THR:HA	1.94	0.49
2:B:180:GLY:HA3	2:B:195:LEU:HD21	1.94	0.49
1:A:374:ARG:NH1	2:B:78:TYR:HB2	2.28	0.49
1:A:407:ASP:OD1	6:A:1002:HEO:O2A	2.31	0.49
2:B:176:ILE:HG21	2:B:179:LEU:HD12	1.93	0.49
2:B:241:SER:O	2:B:267:SER:OG	2.29	0.49
1:A:353:MET:O	2:B:100:ILE:HD12	2.13	0.49
5:A:1001:HEM:HHD	5:A:1001:HEM:CBC	2.38	0.49
2:B:150:VAL:HG23	2:B:266:PHE:CE1	2.40	0.49
3:C:125:VAL:O	3:C:125:VAL:HG12	2.12	0.49
3:C:195:PHE:C	3:C:195:PHE:CD1	2.90	0.49
1:A:657:ALA:O	1:A:660:LYS:O	2.29	0.49
3:C:185:HIS:NE2	4:D:11:SER:OG	2.40	0.49
2:B:136:TRP:CZ2	2:B:213:PRO:HD2	2.48	0.49
3:C:155:ILE:O	3:C:159:VAL:HG13	2.12	0.48
1:A:20:THR:HG21	8:A:1004:UQ8:H10A	1.95	0.48
1:A:330:VAL:O	1:A:333:HIS:ND1	2.45	0.48
1:A:317:VAL:O	1:A:321:VAL:HG23	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:TYR:CD2	1:A:484:SER:OG	2.62	0.48
4:D:107:MET:HE3	4:D:107:MET:HA	1.94	0.48
1:A:468:PHE:HD1	1:A:471:LEU:HD12	1.79	0.48
2:B:42:SER:O	2:B:46:THR:HG23	2.13	0.48
1:A:485:GLN:O	1:A:486:GLN:C	2.56	0.48
1:A:122:LEU:O	1:A:126:VAL:HG12	2.14	0.47
6:A:1002:HEO:HBD1	6:A:1002:HEO:HMD3	1.94	0.47
2:B:136:TRP:HZ2	2:B:213:PRO:HD2	1.79	0.47
2:B:163:PHE:CD1	2:B:193:LEU:HD23	2.49	0.47
1:A:655:THR:O	1:A:659:LEU:HB2	2.14	0.47
3:C:79:SER:O	3:C:105:THR:HG23	2.13	0.47
1:A:298:PHE:HD1	1:A:384:THR:HG23	1.79	0.47
2:B:35:GLN:O	2:B:39:GLU:OE2	2.32	0.47
1:A:277:ASN:CG	4:D:99:MET:HE1	2.40	0.47
5:A:1001:HEM:HBC2	5:A:1001:HEM:CHD	2.33	0.46
1:A:322:CYS:O	1:A:326:LEU:HD12	2.15	0.46
1:A:419:HIS:O	1:A:423:VAL:HG22	2.15	0.46
1:A:20:THR:CG2	8:A:1004:UQ8:H10A	2.46	0.46
1:A:243:PHE:N	1:A:244:PRO:CD	2.78	0.46
1:A:21:ILE:HD11	1:A:160:LEU:HD22	1.98	0.46
1:A:359:THR:O	1:A:363:ILE:HG23	2.16	0.46
1:A:417:ILE:HD12	5:A:1001:HEM:HBA2	1.98	0.46
1:A:417:ILE:HA	1:A:420:PHE:CE2	2.51	0.46
2:B:88:VAL:O	2:B:92:VAL:HG23	2.15	0.46
2:B:282:MET:O	2:B:282:MET:HG3	2.16	0.46
1:A:226:PRO:HB3	1:A:538:THR:HG21	1.98	0.45
1:A:174:PRO:HG3	1:A:275:TYR:HB3	1.97	0.45
4:D:52:ALA:O	4:D:56:VAL:HG23	2.17	0.45
1:A:151:VAL:HG22	1:A:600:THR:OG1	2.16	0.45
2:B:149:THR:HG22	2:B:265:TYR:CD1	2.52	0.45
3:C:51:VAL:HG13	3:C:52:ASN:N	2.32	0.45
1:A:480:THR:HG22	1:A:483:LEU:HD11	1.99	0.45
1:A:601:ILE:HG22	1:A:613:LEU:HD11	1.97	0.45
2:B:243:ASN:O	2:B:244:THR:HG23	2.17	0.45
1:A:381:MET:O	1:A:385:ILE:HD12	2.16	0.45
1:A:396:MET:CG	2:B:51:MET:SD	3.01	0.45
2:B:254:LEU:HD12	2:B:254:LEU:C	2.42	0.45
1:A:286:GLU:HA	1:A:289:ILE:HD12	1.98	0.45
1:A:550:TYR:CD1	1:A:550:TYR:O	2.70	0.44
2:B:140:PHE:CG	2:B:153:ILE:CG2	3.00	0.44
1:A:154:ILE:O	1:A:158:VAL:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:ILE:HD12	2:B:206:ILE:C	2.42	0.44
1:A:111:ILE:CD1	5:A:1001:HEM:CBC	2.96	0.44
8:A:1004:UQ8:C8	8:A:1004:UQ8:C1M	2.96	0.44
2:B:245:MET:O	2:B:269:VAL:HA	2.18	0.44
1:A:548:PRO:HG2	1:A:550:TYR:O	2.18	0.43
4:D:95:SER:O	4:D:99:MET:HE2	2.18	0.43
1:A:129:LEU:HD23	1:A:551:ASN:HB3	2.00	0.43
2:B:180:GLY:HA3	2:B:195:LEU:CD2	2.47	0.43
3:C:149:HIS:HB3	3:C:187:LEU:HD21	1.99	0.43
1:A:284:HIS:O	1:A:287:VAL:HG22	2.18	0.43
1:A:579:HIS:NE2	1:A:581:GLU:OE1	2.51	0.43
1:A:394:GLY:O	1:A:397:THR:OG1	2.35	0.43
2:B:139:PHE:CZ	2:B:245:MET:HE2	2.54	0.43
1:A:98:HIS:O	8:A:1004:UQ8:H3MB	2.19	0.43
1:A:174:PRO:HG2	1:A:175:PRO:HD3	1.99	0.43
1:A:100:ASP:HA	1:A:103:PHE:CE2	2.54	0.42
1:A:397:THR:HG21	1:A:472:TYR:CZ	2.53	0.42
1:A:469:MET:N	1:A:470:PRO:CD	2.82	0.42
1:A:598:PHE:HA	1:A:601:ILE:HD12	2.01	0.42
4:D:99:MET:O	4:D:100:TRP:C	2.61	0.42
4:D:27:ILE:HA	4:D:30:VAL:HG12	2.02	0.42
1:A:466:VAL:O	1:A:466:VAL:HG12	2.18	0.42
3:C:101:TRP:O	3:C:105:THR:OG1	2.37	0.42
1:A:433:PHE:O	1:A:437:THR:HG22	2.20	0.42
1:A:410:LEU:HD22	1:A:415:PHE:CG	2.54	0.42
1:A:660:LYS:C	1:A:660:LYS:CD	2.88	0.42
4:D:84:THR:O	4:D:85:VAL:C	2.62	0.42
4:D:97:TRP:O	4:D:98:ILE:C	2.63	0.42
1:A:332:LEU:HB3	1:A:348:PHE:CD2	2.55	0.41
1:A:127:VAL:HB	1:A:128:PRO:HD3	2.02	0.41
1:A:371:TYR:O	2:B:69:TYR:CG	2.73	0.41
3:C:30:TRP:CZ3	4:D:66:LEU:HD21	2.55	0.41
1:A:623:ILE:O	1:A:627:VAL:HG23	2.21	0.41
2:B:245:MET:HE1	2:B:251:PHE:HD1	1.85	0.41
3:C:27:PHE:O	3:C:31:ILE:HG12	2.19	0.41
1:A:227:VAL:HG21	1:A:310:LEU:CD2	2.50	0.41
2:B:167:SER:O	2:B:187:ALA:HA	2.21	0.41
1:A:28:GLY:O	1:A:32:VAL:HG23	2.21	0.41
1:A:126:VAL:HG22	1:A:126:VAL:O	2.20	0.41
1:A:160:LEU:HD23	1:A:160:LEU:C	2.46	0.41
1:A:83:GLN:O	1:A:87:SER:OG	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ALA:HB3	1:A:487:ILE:HD12	2.02	0.41
1:A:250:VAL:O	1:A:254:THR:HG22	2.20	0.41
2:B:150:VAL:CG2	2:B:266:PHE:HE1	2.27	0.41
2:B:171:MET:HE2	2:B:171:MET:HB3	1.88	0.41
4:D:107:MET:HE3	4:D:107:MET:CA	2.51	0.41
1:A:116:MET:HE1	1:A:289:ILE:HG21	2.03	0.40
1:A:417:ILE:CD1	5:A:1001:HEM:HBA2	2.51	0.40
1:A:371:TYR:O	2:B:69:TYR:CD2	2.74	0.40
1:A:405:GLY:O	2:B:40:GLN:OE1	2.40	0.40
1:A:133:ALA:O	1:A:551:ASN:ND2	2.54	0.40
4:D:54:ALA:O	4:D:58:VAL:HG23	2.21	0.40
2:B:149:THR:HG22	2:B:265:TYR:HD1	1.87	0.40
1:A:57:LEU:HD13	1:A:142:ASN:HB3	2.03	0.40
6:A:1002:H2O:H212	2:B:54:VAL:HB	2.03	0.40
4:D:95:SER:O	4:D:96:ILE:C	2.65	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	658/663 (99%)	630 (96%)	27 (4%)	1 (0%)	43	56
2	B	260/315 (82%)	246 (95%)	14 (5%)	0	100	100
3	C	184/204 (90%)	179 (97%)	5 (3%)	0	100	100
4	D	97/109 (89%)	88 (91%)	9 (9%)	0	100	100
All	All	1199/1291 (93%)	1143 (95%)	55 (5%)	1 (0%)	49	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	546	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	544/547 (100%)	494 (91%)	50 (9%)	8	12
2	B	218/262 (83%)	194 (89%)	24 (11%)	6	8
3	C	153/166 (92%)	128 (84%)	25 (16%)	2	2
4	D	86/94 (92%)	67 (78%)	19 (22%)	1	1
All	All	1001/1069 (94%)	883 (88%)	118 (12%)	7	6

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	12	PHE
1	A	36	THR
1	A	61	TYR
1	A	81	SER
1	A	87	SER
1	A	116	MET
1	A	119	VAL
1	A	125	LEU
1	A	141	LEU
1	A	145	SER
1	A	149	THR
1	A	164	GLU
1	A	179	ILE
1	A	182	SER
1	A	202	THR
1	A	249	THR
1	A	256	ASP
1	A	274	MET
1	A	277	ASN
1	A	279	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	306	SER
1	A	307	ARG
1	A	317	VAL
1	A	330	VAL
1	A	332	LEU
1	A	355	ILE
1	A	363	ILE
1	A	392	SER
1	A	419	HIS
1	A	423	VAL
1	A	429	VAL
1	A	469	MET
1	A	500	SER
1	A	505	ILE
1	A	512	LEU
1	A	513	VAL
1	A	538	THR
1	A	540	GLU
1	A	543	THR
1	A	565	TRP
1	A	576	LYS
1	A	581	GLU
1	A	585	MET
1	A	593	ILE
1	A	622	ILE
1	A	628	LYS
1	A	632	GLU
1	A	635	ASP
1	A	654	ILE
2	B	53	ILE
2	B	56	ILE
2	B	60	LEU
2	B	67	TRP
2	B	74	LYS
2	B	89	GLU
2	B	95	VAL
2	B	101	ILE
2	B	109	LYS
2	B	141	ILE
2	B	144	GLU
2	B	171	MET
2	B	191	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	193	LEU
2	B	211	SER
2	B	228	ARG
2	B	237	LYS
2	B	239	LYS
2	B	240	GLN
2	B	241	SER
2	B	258	SER
2	B	259	GLU
2	B	278	ILE
2	B	284	HIS
3	C	19	HIS
3	C	33	LEU
3	C	34	MET
3	C	39	LEU
3	C	54	THR
3	C	65	GLU
3	C	80	SER
3	C	92	LYS
3	C	95	LYS
3	C	96	SER
3	C	99	ILE
3	C	104	LEU
3	C	105	THR
3	C	116	GLU
3	C	120	PHE
3	C	121	HIS
3	C	122	HIS
3	C	132	ARG
3	C	164	ILE
3	C	172	THR
3	C	178	MET
3	C	181	SER
3	C	195	PHE
3	C	200	LEU
3	C	201	MET
4	D	12	HIS
4	D	15	VAL
4	D	16	LYS
4	D	19	MET
4	D	20	THR
4	D	24	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	35	MET
4	D	36	VAL
4	D	37	MET
4	D	38	THR
4	D	42	SER
4	D	46	ILE
4	D	47	LEU
4	D	55	VAL
4	D	66	LEU
4	D	69	ASN
4	D	77	ASN
4	D	95	SER
4	D	108	MET

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	98	HIS
1	A	262	HIS
1	A	557	HIS
2	B	233	GLN
2	B	268	ASN
3	C	94	ASN
4	D	57	GLN
4	D	61	HIS
4	D	77	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

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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$
6	HEO	A	1002	1	66,66,66	4.17	15 (22%)	84,102,102	4.65	50 (59%)
9	3PE	C	402	-	39,39,50	0.98	4 (10%)	42,44,55	1.08	2 (4%)
9	3PE	A	1007	-	9,9,50	0.29	0	8,8,55	0.79	0
9	3PE	D	202	-	16,16,50	0.29	0	15,15,55	0.77	0
8	UQ8	A	1004	-	53,53,53	2.74	19 (35%)	66,67,67	2.15	19 (28%)
9	3PE	D	201	-	44,44,50	0.93	4 (9%)	47,49,55	1.16	2 (4%)
9	3PE	B	401	-	13,13,50	1.03	2 (15%)	13,13,55	1.02	1 (7%)
9	3PE	A	1009	-	22,25,50	1.15	3 (13%)	23,28,55	1.35	2 (8%)
9	3PE	C	401	-	46,46,50	0.91	4 (8%)	49,51,55	1.09	2 (4%)
10	U9V	A	1008	-	33,33,36	0.82	2 (6%)	33,33,37	1.06	0
5	HEM	A	1001	1	50,50,50	1.59	7 (14%)	67,82,82	1.68	12 (17%)
9	3PE	A	1005	-	46,46,50	0.91	4 (8%)	49,51,55	1.14	2 (4%)
9	3PE	A	1006	-	27,27,50	1.20	4 (14%)	29,29,55	1.42	4 (13%)

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
6	HEO	A	1002	1	3/3/7/15	16/34/74/74	-
9	3PE	C	402	-	-	19/43/43/54	-
9	3PE	A	1007	-	-	2/7/7/54	-
9	3PE	D	202	-	-	5/14/14/54	-
8	UQ8	A	1004	-	-	18/51/75/75	0/1/1/1
9	3PE	D	201	-	-	24/48/48/54	-
9	3PE	B	401	-	-	4/12/12/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	3PE	A	1009	-	-	12/25/27/54	-
9	3PE	C	401	-	-	15/50/50/54	-
10	U9V	A	1008	-	-	12/29/29/36	-
5	HEM	A	1001	1	-	6/14/54/54	-
9	3PE	A	1005	-	-	26/50/50/54	-
9	3PE	A	1006	-	-	10/28/28/54	-

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1002	HEO	CHC-C4B	13.19	1.64	1.38
6	A	1002	HEO	CHA-C1A	13.08	1.64	1.38
6	A	1002	HEO	CHD-C1D	12.05	1.62	1.38
6	A	1002	HEO	CHB-C4A	11.51	1.61	1.38
6	A	1002	HEO	CHD-C4C	11.01	1.64	1.39
6	A	1002	HEO	CHB-C1B	10.85	1.63	1.39
6	A	1002	HEO	CHC-C1C	10.54	1.63	1.39
8	A	1004	UQ8	C6-C1	10.26	1.53	1.35
6	A	1002	HEO	CHA-C4D	9.31	1.60	1.39
8	A	1004	UQ8	O5-C5	7.40	1.40	1.23
8	A	1004	UQ8	O2-C2	7.29	1.39	1.23
5	A	1001	HEM	FE-NB	5.47	2.11	1.94
8	A	1004	UQ8	C4-C3	4.69	1.53	1.36
5	A	1001	HEM	FE-NC	4.32	2.09	1.95
9	A	1006	3PE	O21-C2	-3.79	1.40	1.47
6	A	1002	HEO	C4A-NA	-3.41	1.33	1.39
5	A	1001	HEM	C1B-NB	-3.36	1.34	1.40
8	A	1004	UQ8	C7-C8	3.34	1.55	1.50
6	A	1002	HEO	C4D-ND	-3.28	1.32	1.38
6	A	1002	HEO	C11-C3B	3.25	1.55	1.51
5	A	1001	HEM	C4D-ND	-3.06	1.34	1.40
10	A	1008	U9V	O31-C31	2.88	1.40	1.30
8	A	1004	UQ8	C16-C14	2.87	1.57	1.51
9	C	401	3PE	O21-C2	-2.84	1.39	1.46
8	A	1004	UQ8	C36-C34	2.79	1.57	1.51
9	A	1009	3PE	O21-C2	-2.79	1.40	1.46
10	A	1008	U9V	O21-C21	2.78	1.40	1.30
9	A	1005	3PE	O21-C2	-2.76	1.40	1.46
8	A	1004	UQ8	C21-C19	2.73	1.56	1.51
5	A	1001	HEM	FE-ND	-2.71	1.86	1.94
5	A	1001	HEM	C1C-C2C	-2.70	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1004	UQ8	C41-C39	2.68	1.56	1.51
8	A	1004	UQ8	C31-C29	2.63	1.56	1.51
8	A	1004	UQ8	C7-C6	2.54	1.56	1.51
9	C	402	3PE	O21-C2	-2.53	1.40	1.46
9	A	1006	3PE	O31-C31	2.53	1.40	1.33
9	D	201	3PE	O21-C2	-2.52	1.40	1.46
9	A	1006	3PE	O31-C3	-2.46	1.39	1.45
9	C	402	3PE	O31-C31	2.45	1.40	1.33
8	A	1004	UQ8	C26-C24	2.44	1.56	1.51
8	A	1004	UQ8	C6-C5	2.43	1.53	1.46
8	A	1004	UQ8	C22-C23	2.37	1.57	1.50
8	A	1004	UQ8	C11-C9	2.37	1.56	1.51
9	D	201	3PE	O31-C31	2.36	1.40	1.33
9	A	1009	3PE	O31-C31	2.33	1.40	1.33
9	A	1005	3PE	O31-C31	2.33	1.40	1.33
9	C	401	3PE	O31-C3	-2.33	1.40	1.45
9	B	401	3PE	O31-C3	-2.32	1.40	1.45
9	B	401	3PE	O31-C31	2.32	1.40	1.33
9	A	1009	3PE	O31-C3	-2.31	1.40	1.45
6	A	1002	HEO	C1C-NC	-2.30	1.35	1.39
9	D	201	3PE	O31-C3	-2.28	1.40	1.45
6	A	1002	HEO	C1A-C2A	-2.27	1.41	1.45
6	A	1002	HEO	C3B-C2B	2.27	1.39	1.34
9	A	1005	3PE	O31-C3	-2.27	1.40	1.45
9	A	1006	3PE	O21-C21	2.25	1.40	1.34
9	D	201	3PE	O21-C21	2.23	1.40	1.34
8	A	1004	UQ8	O3-C3	2.23	1.42	1.36
8	A	1004	UQ8	C17-C18	2.21	1.57	1.50
9	A	1005	3PE	O21-C21	2.17	1.40	1.34
9	C	402	3PE	O31-C3	-2.16	1.40	1.45
9	C	401	3PE	O31-C31	2.15	1.39	1.33
8	A	1004	UQ8	C32-C33	2.14	1.56	1.50
9	C	402	3PE	O21-C21	2.14	1.40	1.34
9	C	401	3PE	O21-C21	2.13	1.40	1.34
5	A	1001	HEM	C4B-NB	-2.10	1.34	1.38
8	A	1004	UQ8	C42-C43	2.02	1.56	1.50
6	A	1002	HEO	C1D-ND	-2.01	1.36	1.40

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1002	HEO	CHA-C4D-C3D	-12.31	106.82	124.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1002	HEO	C1A-CHA-C4D	-10.43	103.86	126.02
6	A	1002	HEO	C3C-C4C-NC	10.37	118.53	109.80
6	A	1002	HEO	C1C-CHC-C4B	-9.72	103.39	126.25
6	A	1002	HEO	C3D-C4D-ND	9.64	119.67	110.35
6	A	1002	HEO	C4C-CHD-C1D	-9.26	104.48	126.25
6	A	1002	HEO	C4A-CHB-C1B	-9.02	106.84	126.02
6	A	1002	HEO	CHA-C4D-ND	8.35	133.41	124.42
6	A	1002	HEO	C1D-ND-C4D	-8.05	95.67	105.21
6	A	1002	HEO	C4B-NB-C1B	-7.76	96.02	105.21
6	A	1002	HEO	C2B-C1B-NB	7.65	118.75	109.90
6	A	1002	HEO	C2D-C1D-ND	7.58	118.55	109.84
6	A	1002	HEO	C3B-C4B-NB	7.57	118.54	109.84
6	A	1002	HEO	CHB-C4A-C3A	-7.27	110.36	125.49
6	A	1002	HEO	C2A-C1A-NA	7.26	117.33	110.32
6	A	1002	HEO	O11-C11-C3B	6.76	123.66	111.26
8	A	1004	UQ8	O5-C5-C6	-6.74	108.75	121.79
6	A	1002	HEO	CHC-C1C-C2C	-6.48	108.62	127.43
6	A	1002	HEO	CHB-C1B-C2B	-6.44	114.86	125.03
8	A	1004	UQ8	O2-C2-C3	-6.33	107.62	121.03
6	A	1002	HEO	CHA-C1A-C2A	-5.99	115.40	124.86
8	A	1004	UQ8	O5-C5-C4	-5.82	108.70	121.03
6	A	1002	HEO	C4A-NA-C1A	-5.77	96.41	105.82
6	A	1002	HEO	C4C-NC-C1C	-5.61	96.68	105.82
6	A	1002	HEO	CHB-C4A-NA	5.50	130.44	124.45
6	A	1002	HEO	CHC-C1C-NC	5.30	133.48	123.86
5	A	1001	HEM	CHC-C4B-NB	5.30	130.13	124.42
6	A	1002	HEO	C12-C11-C3B	-5.28	103.87	112.12
6	A	1002	HEO	C3A-C4A-NA	5.00	118.88	109.64
6	A	1002	HEO	C2C-C1C-NC	4.75	117.76	110.14
6	A	1002	HEO	CHC-C4B-C3B	-4.65	114.07	125.80
6	A	1002	HEO	CHD-C1D-C2D	-4.62	113.81	126.95
9	D	201	3PE	O21-C21-C22	4.61	121.46	111.48
5	A	1001	HEM	CHD-C1D-ND	4.44	129.20	124.42
9	A	1005	3PE	O21-C21-C22	4.36	120.92	111.48
5	A	1001	HEM	CHA-C4D-ND	4.29	129.68	124.37
9	C	401	3PE	O21-C21-C22	4.17	120.49	111.48
6	A	1002	HEO	C4C-C3C-C2C	-4.16	102.13	107.30
8	A	1004	UQ8	O2-C2-C1	-3.98	109.61	120.73
9	A	1009	3PE	O21-C21-C22	3.87	119.85	111.48
9	C	402	3PE	O21-C21-C22	3.85	119.81	111.48
6	A	1002	HEO	C1D-C2D-C3D	-3.77	103.02	106.98
8	A	1004	UQ8	C30-C29-C31	3.63	121.52	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1002	HEO	C17-C18-C19	-3.56	119.47	127.62
6	A	1002	HEO	CHD-C4C-C3C	-3.53	112.05	127.37
9	A	1006	3PE	O21-C21-C22	3.39	118.83	111.48
6	A	1002	HEO	C4B-C3B-C2B	-3.39	101.74	107.44
8	A	1004	UQ8	C35-C34-C36	3.26	120.88	115.23
5	A	1001	HEM	CHB-C1B-NB	3.23	128.36	124.37
8	A	1004	UQ8	C10-C9-C11	3.22	120.82	115.23
5	A	1001	HEM	C1B-NB-C4B	3.12	108.91	105.21
8	A	1004	UQ8	C37-C38-C39	-3.12	120.49	127.62
8	A	1004	UQ8	C20-C19-C21	3.11	120.63	115.23
9	A	1006	3PE	O31-C31-C32	3.01	121.01	111.83
6	A	1002	HEO	CHD-C4C-NC	2.97	129.25	123.86
8	A	1004	UQ8	C40-C39-C41	2.96	120.36	115.23
6	A	1002	HEO	CMD-C2D-C1D	2.90	129.57	125.03
8	A	1004	UQ8	C22-C23-C24	-2.89	121.00	127.62
9	D	201	3PE	O31-C31-C32	2.84	120.49	111.83
8	A	1004	UQ8	C1M-C1-C6	-2.74	119.95	124.45
8	A	1004	UQ8	C3-C2-C1	-2.73	112.70	118.10
6	A	1002	HEO	C4D-C3D-C2D	-2.73	102.92	106.89
6	A	1002	HEO	C25-C23-C24	2.71	120.83	114.59
6	A	1002	HEO	C27-C19-C20	2.69	119.89	115.23
8	A	1004	UQ8	C15-C14-C16	2.67	119.86	115.23
6	A	1002	HEO	C4A-C3A-C2A	-2.64	103.05	106.97
9	A	1009	3PE	O31-C31-C32	2.60	119.78	111.83
9	C	402	3PE	O31-C31-C32	2.59	119.75	111.83
8	A	1004	UQ8	C12-C13-C14	-2.58	121.71	127.62
6	A	1002	HEO	CMA-C3A-C4A	2.57	129.25	124.73
9	C	401	3PE	O31-C31-C32	2.55	119.62	111.83
6	A	1002	HEO	CHD-C1D-ND	2.54	127.51	124.37
9	A	1005	3PE	O31-C31-C32	2.53	119.56	111.83
6	A	1002	HEO	C1A-C2A-C3A	-2.52	103.80	107.11
8	A	1004	UQ8	C25-C24-C26	2.51	119.58	115.23
6	A	1002	HEO	CHA-C1A-NA	2.50	127.17	124.45
6	A	1002	HEO	C26-C15-C16	2.46	119.50	115.23
8	A	1004	UQ8	C32-C33-C34	-2.44	122.03	127.62
5	A	1001	HEM	C1A-CHA-C4D	-2.42	120.56	126.25
5	A	1001	HEM	CHA-C4D-C3D	-2.41	120.79	125.23
5	A	1001	HEM	CHD-C1D-C2D	-2.38	121.27	125.03
6	A	1002	HEO	C13-C14-C15	-2.36	122.22	127.62
6	A	1002	HEO	CHC-C4B-NB	2.34	127.26	124.37
8	A	1004	UQ8	C7-C8-C9	-2.33	122.81	126.83
6	A	1002	HEO	CAA-C2A-C1A	2.29	129.50	124.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	HEM	C3B-C4B-NB	-2.28	107.83	109.47
6	A	1002	HEO	C3C-C2C-C1C	-2.27	104.49	107.17
6	A	1002	HEO	C21-C22-C23	-2.27	120.09	127.64
9	A	1006	3PE	O21-C2-C3	2.27	111.42	106.21
8	A	1004	UQ8	C20-C19-C18	-2.20	117.98	123.63
9	B	401	3PE	O31-C31-C32	2.20	120.45	112.14
9	A	1006	3PE	C2-O21-C21	-2.18	114.64	117.78
5	A	1001	HEM	O2D-CGD-CBD	2.13	120.72	114.00
5	A	1001	HEM	C4D-ND-C1D	2.08	107.68	105.21
6	A	1002	HEO	O2D-CGD-CBD	2.06	120.51	114.00
5	A	1001	HEM	CAD-CBD-CGD	-2.02	108.30	113.67

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1002	HEO	NB
6	A	1002	HEO	NA
6	A	1002	HEO	ND

All (169) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	HEM	C2B-C3B-CAB-CBB
5	A	1001	HEM	C4B-C3B-CAB-CBB
6	A	1002	HEO	C2D-C3D-CAD-CBD
6	A	1002	HEO	C4D-C3D-CAD-CBD
6	A	1002	HEO	C3B-C11-C12-C13
6	A	1002	HEO	O11-C11-C12-C13
6	A	1002	HEO	C19-C20-C21-C22
8	A	1004	UQ8	C40-C39-C41-C42
8	A	1004	UQ8	C1-C6-C7-C8
8	A	1004	UQ8	C5-C6-C7-C8
9	A	1005	3PE	C11-O13-P-O11
9	A	1005	3PE	C11-O13-P-O12
9	A	1005	3PE	O22-C21-O21-C2
9	A	1006	3PE	O21-C2-C3-O31
9	A	1006	3PE	O22-C21-O21-C2
9	A	1009	3PE	C22-C21-O21-C2
9	C	401	3PE	O13-C11-C12-N
9	C	401	3PE	C22-C21-O21-C2
9	C	402	3PE	C1-O11-P-O13
9	C	402	3PE	C1-O11-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	C	402	3PE	C11-O13-P-O11
9	C	402	3PE	C11-O13-P-O14
9	C	402	3PE	C22-C21-O21-C2
9	D	201	3PE	C1-O11-P-O12
9	D	201	3PE	C1-O11-P-O13
9	D	201	3PE	C11-O13-P-O11
9	D	201	3PE	C11-O13-P-O12
9	D	201	3PE	C11-O13-P-O14
9	D	201	3PE	O22-C21-O21-C2
9	D	201	3PE	C22-C21-O21-C2
9	A	1009	3PE	O32-C31-O31-C3
9	A	1009	3PE	C32-C31-O31-C3
9	A	1009	3PE	O22-C21-O21-C2
9	C	401	3PE	O22-C21-O21-C2
9	C	402	3PE	O22-C21-O21-C2
9	A	1006	3PE	C32-C31-O31-C3
9	A	1005	3PE	C22-C21-O21-C2
9	A	1006	3PE	C22-C21-O21-C2
8	A	1004	UQ8	C35-C34-C36-C37
8	A	1004	UQ8	C20-C19-C21-C22
8	A	1004	UQ8	C12-C11-C9-C10
8	A	1004	UQ8	C38-C39-C41-C42
8	A	1004	UQ8	C33-C34-C36-C37
8	A	1004	UQ8	C12-C11-C9-C8
9	D	201	3PE	C32-C31-O31-C3
9	A	1006	3PE	O32-C31-O31-C3
8	A	1004	UQ8	C18-C19-C21-C22
9	D	201	3PE	O32-C31-O31-C3
8	A	1004	UQ8	C19-C21-C22-C23
8	A	1004	UQ8	C14-C16-C17-C18
6	A	1002	HEO	C2A-CAA-CBA-CGA
9	A	1005	3PE	C32-C31-O31-C3
6	A	1002	HEO	C26-C15-C16-C17
8	A	1004	UQ8	C30-C29-C31-C32
6	A	1002	HEO	C14-C15-C16-C17
8	A	1004	UQ8	C28-C29-C31-C32
10	A	1008	U9V	C31-C32-C33-C34
9	A	1005	3PE	C31-C32-C33-C34
9	A	1005	3PE	O32-C31-O31-C3
9	A	1009	3PE	C31-C32-C33-C34
8	A	1004	UQ8	C9-C11-C12-C13
9	C	401	3PE	C2-C1-O11-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	C	402	3PE	C26-C27-C28-C29
9	D	202	3PE	C3C-C3D-C3E-C3F
10	A	1008	U9V	C3A-C3B-C3C-C3D
10	A	1008	U9V	C28-C29-C2A-C2B
9	C	401	3PE	C2D-C2E-C2F-C2G
9	B	401	3PE	C32-C33-C34-C35
9	C	402	3PE	C27-C28-C29-C2A
9	D	201	3PE	C37-C38-C39-C3A
9	C	402	3PE	C3A-C3B-C3C-C3D
9	A	1006	3PE	C32-C33-C34-C35
9	A	1009	3PE	O11-C1-C2-O21
5	A	1001	HEM	C4C-C3C-CAC-CBC
9	B	401	3PE	C34-C35-C36-C37
9	D	201	3PE	C36-C37-C38-C39
9	C	401	3PE	O11-C1-C2-C3
10	A	1008	U9V	C38-C39-C3A-C3B
9	C	401	3PE	C28-C29-C2A-C2B
6	A	1002	HEO	C1A-C2A-CAA-CBA
9	A	1005	3PE	C23-C24-C25-C26
10	A	1008	U9V	C35-C36-C37-C38
9	C	402	3PE	C23-C24-C25-C26
9	A	1005	3PE	C27-C28-C29-C2A
9	C	401	3PE	C33-C34-C35-C36
9	A	1005	3PE	C2E-C2F-C2G-C2H
9	C	402	3PE	C25-C26-C27-C28
9	A	1005	3PE	C36-C37-C38-C39
9	A	1009	3PE	O11-C1-C2-C3
9	A	1006	3PE	C1-C2-C3-O31
9	C	401	3PE	C2C-C2D-C2E-C2F
9	A	1006	3PE	C34-C35-C36-C37
9	D	201	3PE	C1-C2-C3-O31
9	A	1005	3PE	C2-C1-O11-P
9	D	201	3PE	C2-C1-O11-P
9	A	1005	3PE	O21-C2-C3-O31
9	C	402	3PE	O21-C2-C3-O31
9	C	401	3PE	C37-C38-C39-C3A
9	C	401	3PE	C23-C24-C25-C26
9	D	202	3PE	C33-C34-C35-C36
9	D	202	3PE	C3E-C3F-C3G-C3H
8	A	1004	UQ8	C39-C41-C42-C43
9	A	1005	3PE	C33-C34-C35-C36
9	A	1009	3PE	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	C	402	3PE	C38-C39-C3A-C3B
9	B	401	3PE	C36-C37-C38-C39
9	D	201	3PE	C23-C24-C25-C26
9	C	401	3PE	O11-C1-C2-O21
9	C	401	3PE	C35-C36-C37-C38
9	A	1005	3PE	C12-C11-O13-P
9	D	201	3PE	C12-C11-O13-P
9	D	201	3PE	C31-C32-C33-C34
9	D	201	3PE	O21-C2-C3-O31
9	A	1009	3PE	C21-C22-C23-C24
9	A	1005	3PE	C34-C35-C36-C37
6	A	1002	HEO	C3A-C2A-CAA-CBA
9	D	201	3PE	C22-C23-C24-C25
6	A	1002	HEO	C11-C12-C13-C14
9	A	1005	3PE	C1-O11-P-O14
9	A	1005	3PE	C11-O13-P-O14
9	A	1005	3PE	O13-C11-C12-N
9	C	401	3PE	C11-O13-P-O14
9	D	201	3PE	C1-O11-P-O14
9	D	202	3PE	C36-C37-C38-C39
9	D	201	3PE	C3B-C3C-C3D-C3E
9	A	1006	3PE	C26-C27-C28-C29
9	A	1007	3PE	C27-C28-C29-C2A
9	D	202	3PE	C37-C38-C39-C3A
9	D	201	3PE	C29-C2A-C2B-C2C
9	C	402	3PE	C1-C2-C3-O31
9	C	402	3PE	C1-C2-O21-C21
9	D	201	3PE	C3D-C3E-C3F-C3G
9	C	402	3PE	C32-C33-C34-C35
8	A	1004	UQ8	C25-C24-C26-C27
6	A	1002	HEO	CAA-CBA-CGA-O1A
9	D	201	3PE	C3A-C3B-C3C-C3D
9	B	401	3PE	C38-C39-C3A-C3B
10	A	1008	U9V	C3D-C3E-C3F-C3G
9	A	1009	3PE	C25-C26-C27-C28
9	A	1006	3PE	O31-C31-C32-C33
6	A	1002	HEO	CAA-CBA-CGA-O2A
9	A	1005	3PE	C38-C39-C3A-C3B
9	A	1009	3PE	C23-C24-C25-C26
9	A	1005	3PE	C39-C3A-C3B-C3C
9	C	401	3PE	C32-C33-C34-C35
9	D	201	3PE	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	A	1008	U9V	C33-C34-C35-C36
8	A	1004	UQ8	C2-C3-O3-C3M
9	A	1007	3PE	C28-C29-C2A-C2B
10	A	1008	U9V	C32-C33-C34-C35
10	A	1008	U9V	C29-C2A-C2B-C2C
5	A	1001	HEM	C3A-C2A-CAA-CBA
9	A	1009	3PE	C32-C33-C34-C35
9	A	1005	3PE	C21-C22-C23-C24
9	C	402	3PE	O21-C21-C22-C23
10	A	1008	U9V	C26-C27-C28-C29
9	A	1005	3PE	O31-C31-C32-C33
9	A	1005	3PE	C1-C2-C3-O31
6	A	1002	HEO	CAD-CBD-CGD-O1D
9	C	402	3PE	C3-C2-O21-C21
10	A	1008	U9V	C36-C37-C38-C39
6	A	1002	HEO	C12-C13-C14-C15
5	A	1001	HEM	CAA-CBA-CGA-O1A
6	A	1002	HEO	CAD-CBD-CGD-O2D
9	A	1005	3PE	O32-C31-C32-C33
9	C	402	3PE	O22-C21-C22-C23
9	A	1005	3PE	O21-C21-C22-C23
10	A	1008	U9V	C2C-C2D-C2E-C2F
5	A	1001	HEM	CAA-CBA-CGA-O2A

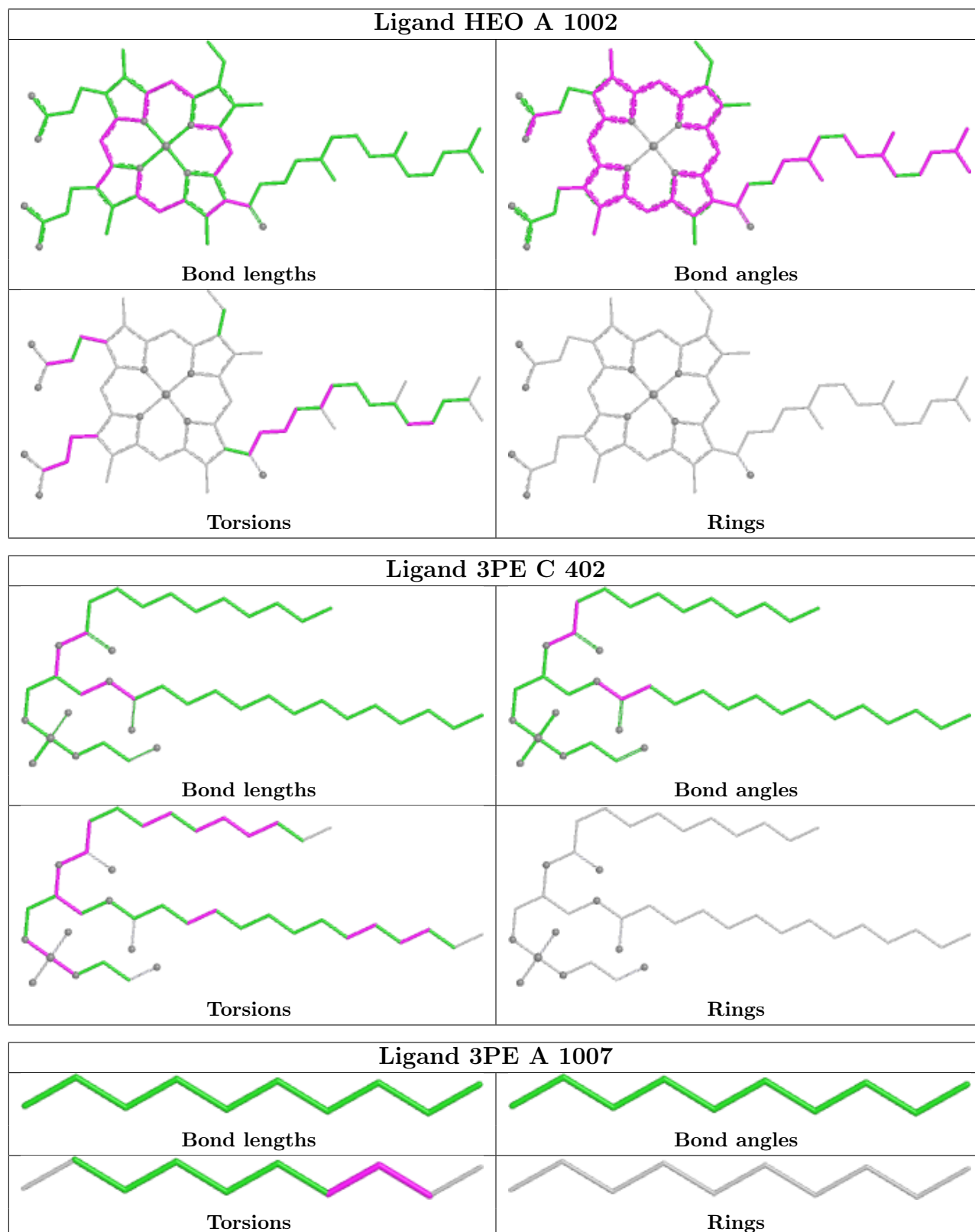
There are no ring outliers.

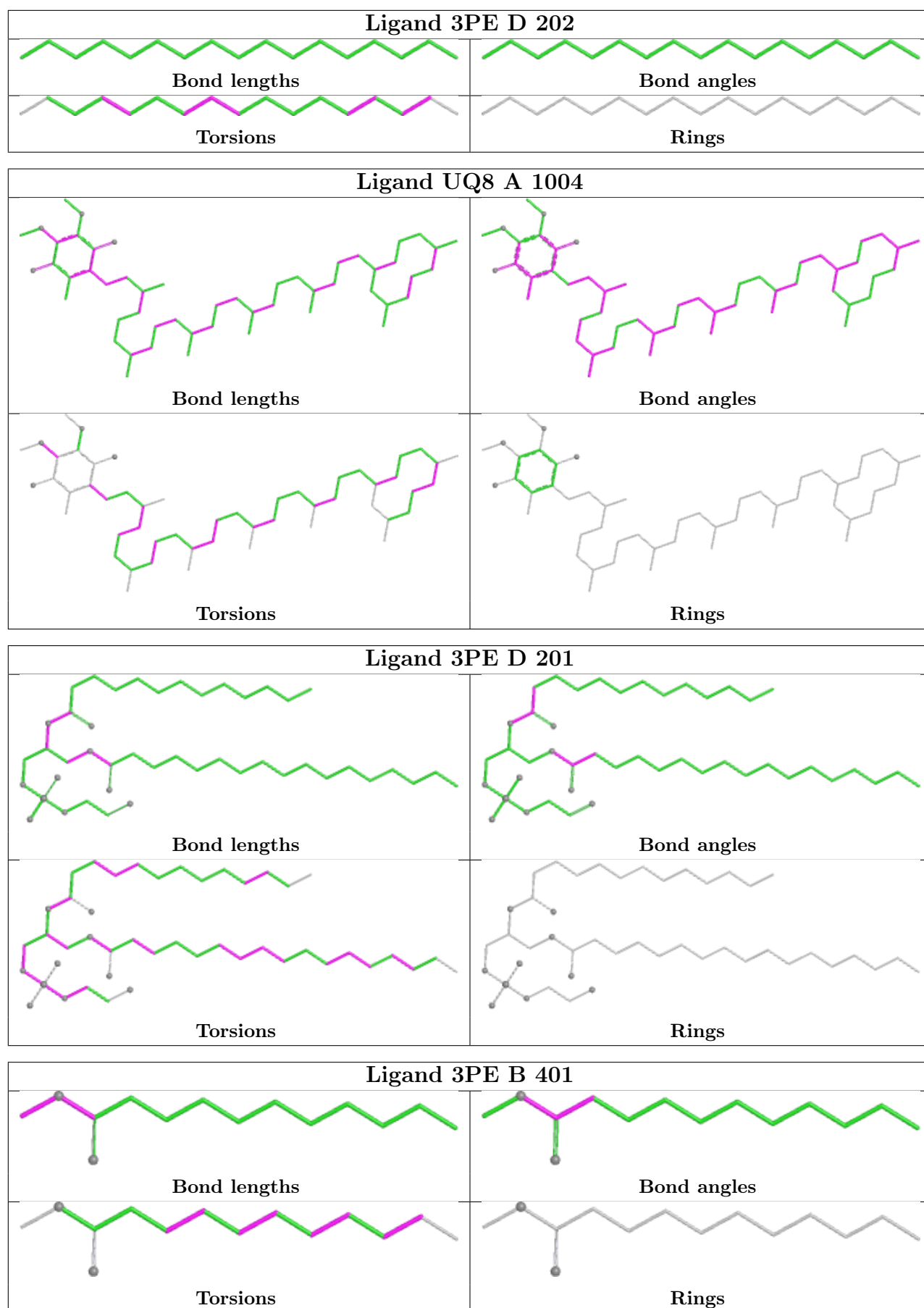
5 monomers are involved in 24 short contacts:

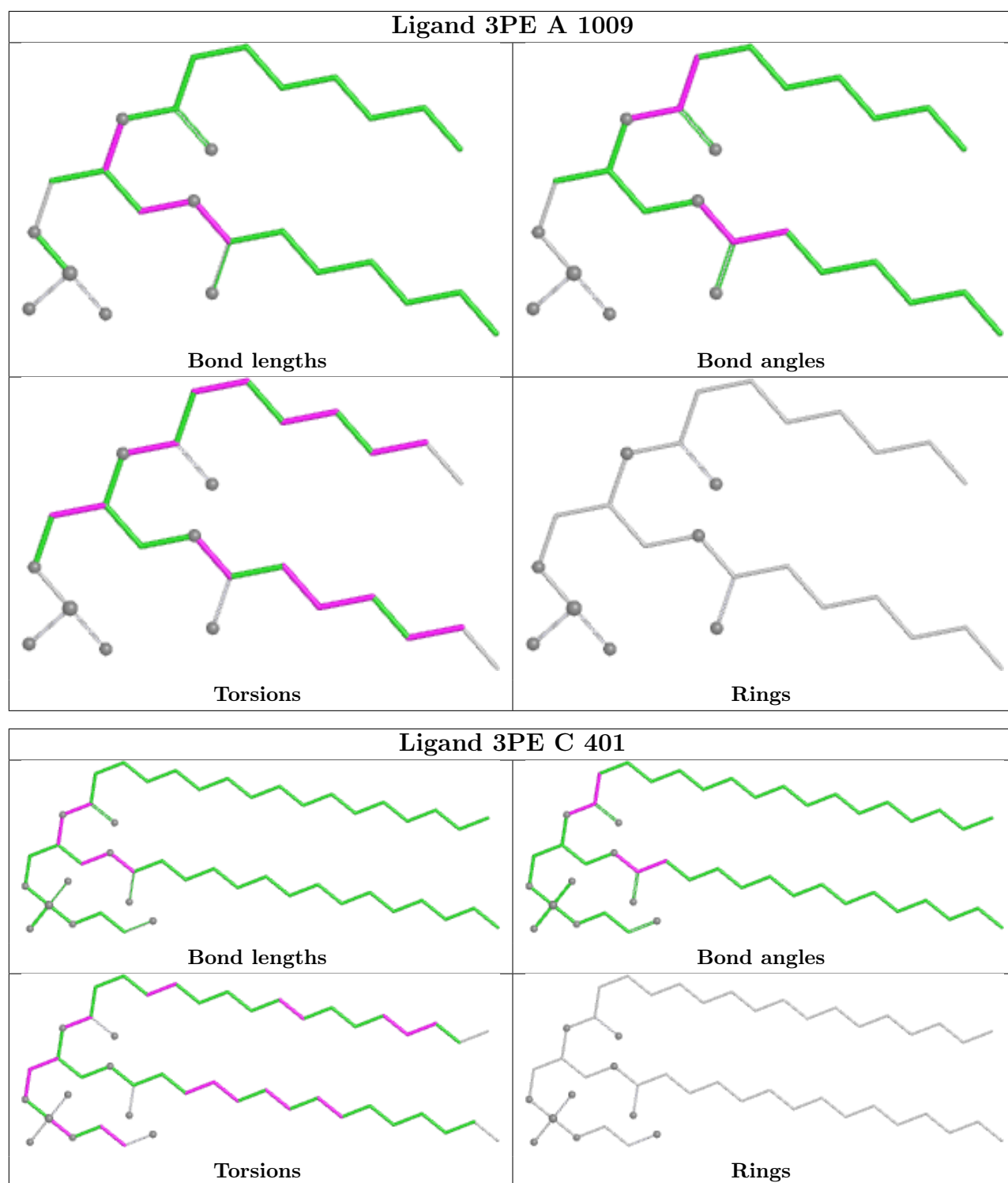
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1002	HEO	5	0
8	A	1004	UQ8	8	0
9	A	1009	3PE	1	0
9	C	401	3PE	1	0
5	A	1001	HEM	9	0

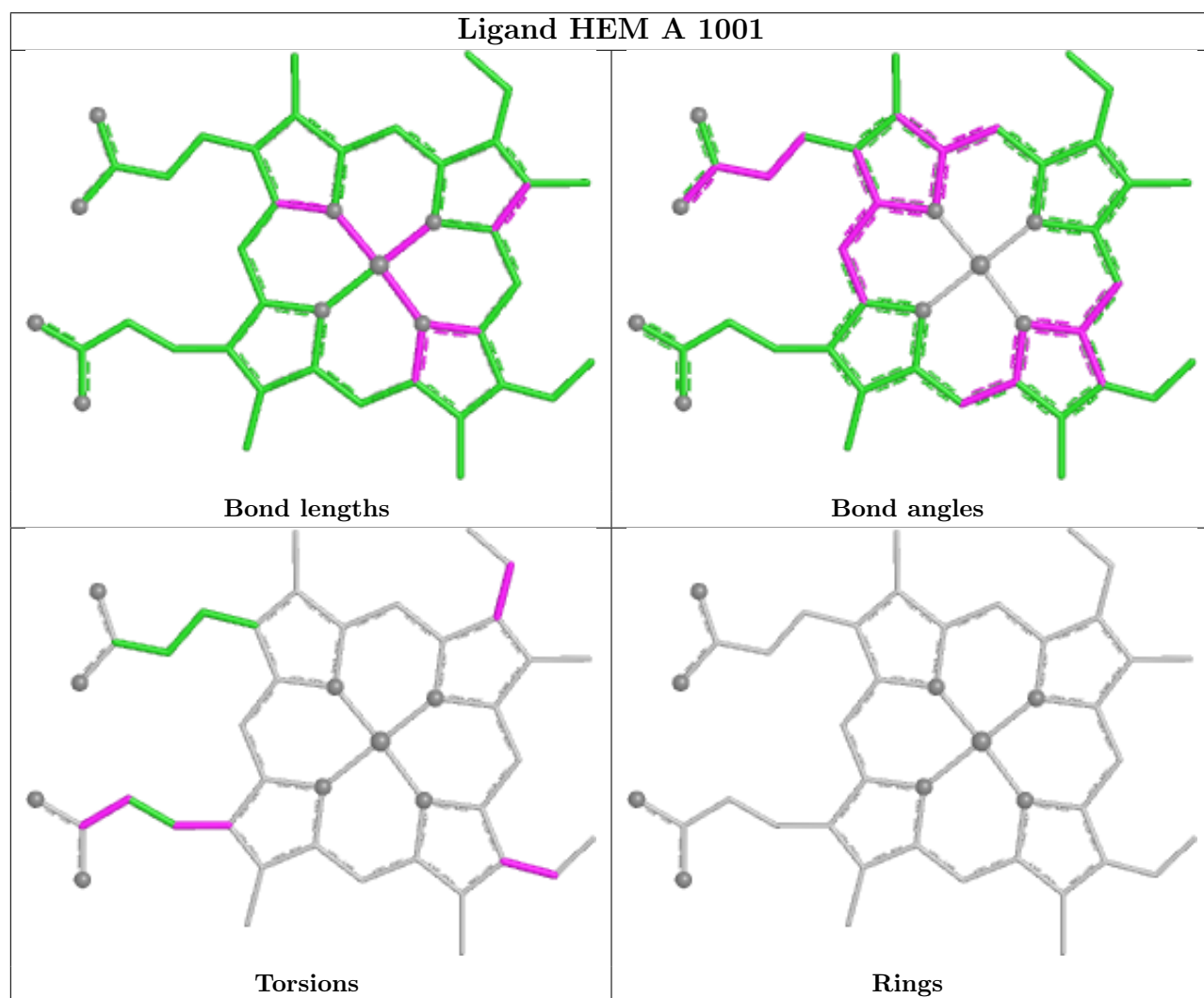
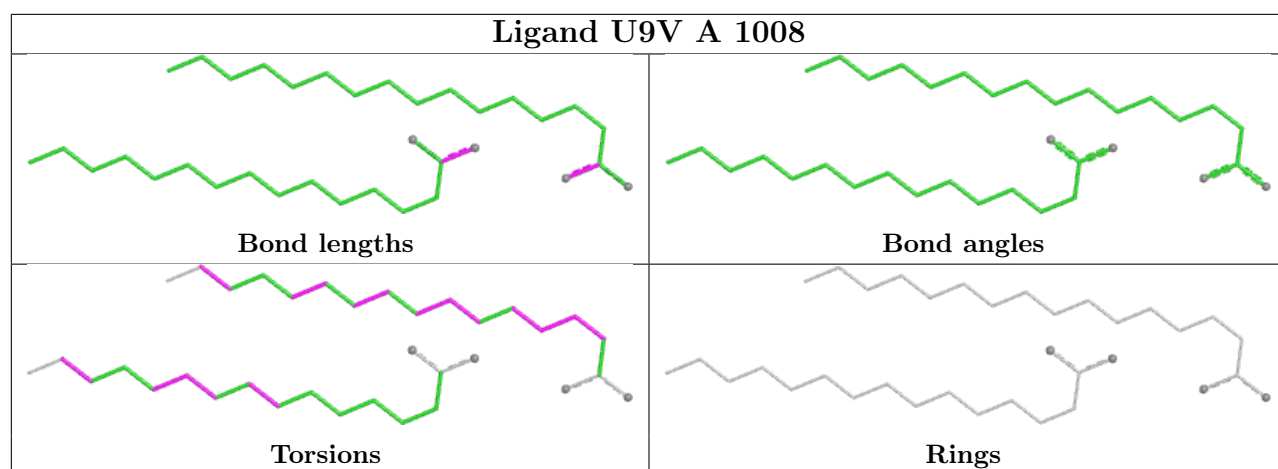
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

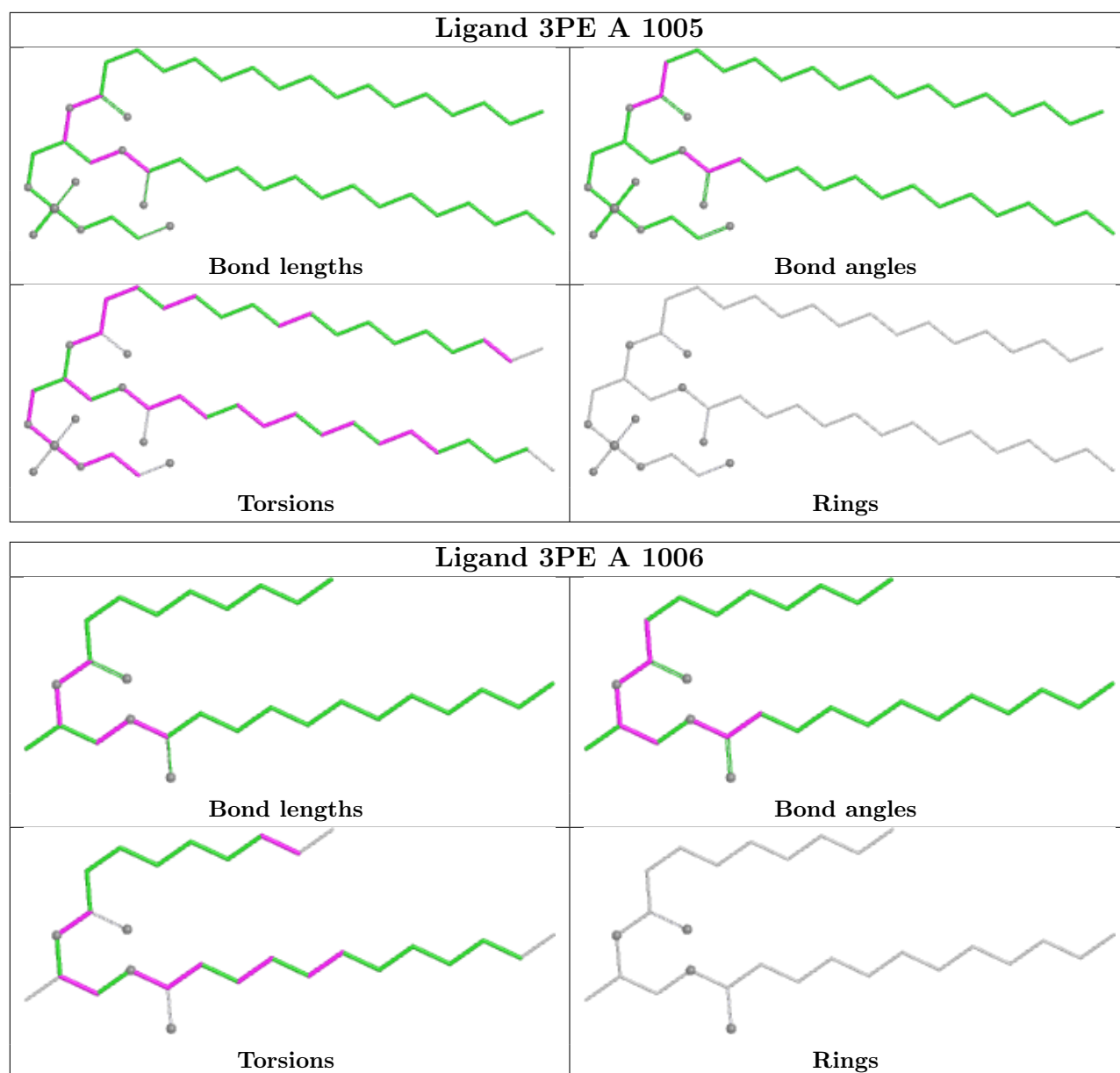
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

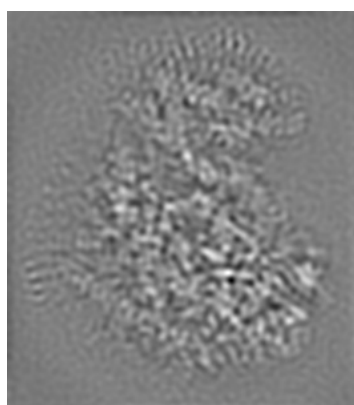
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21897. These allow visual inspection of the internal detail of the map and identification of artifacts.

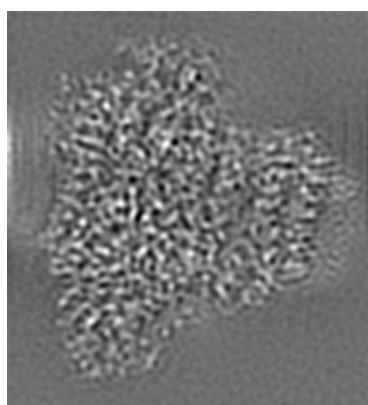
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

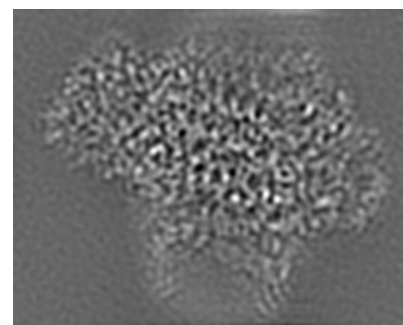
6.1.1 Primary map



X



Y

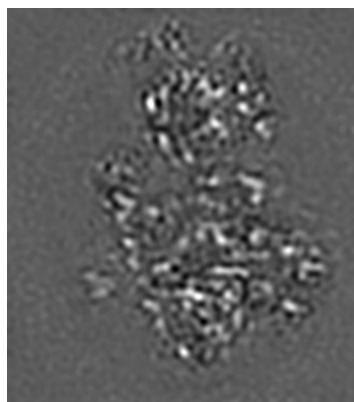


Z

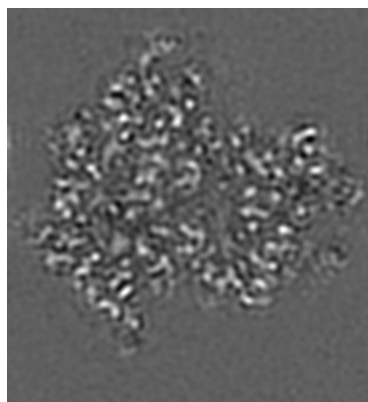
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

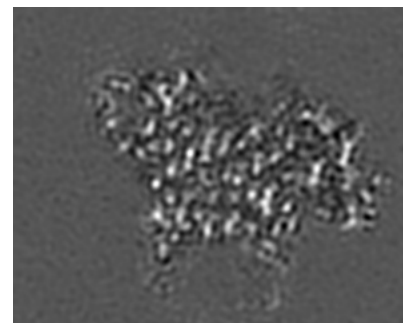
6.2.1 Primary map



X Index: 53



Y Index: 42

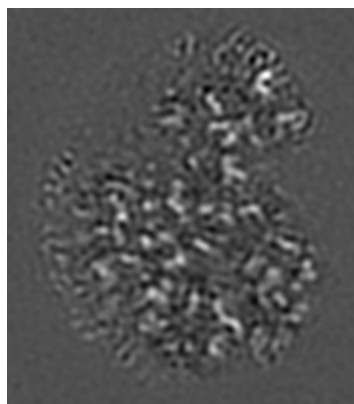


Z Index: 48

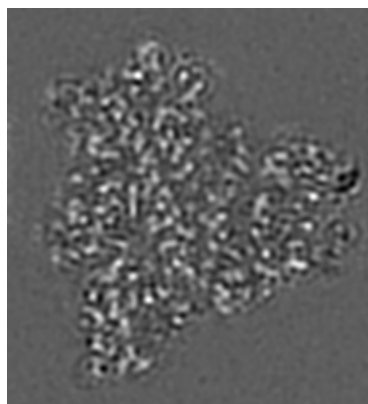
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

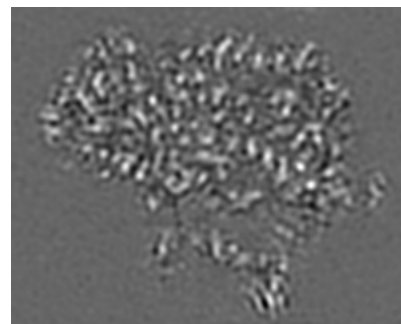
6.3.1 Primary map



X Index: 41



Y Index: 52

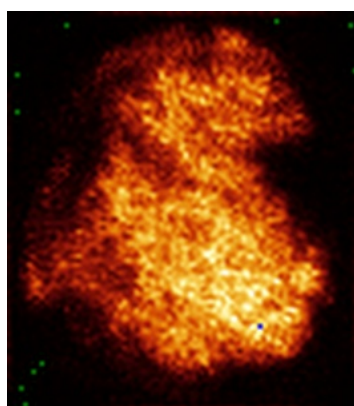


Z Index: 30

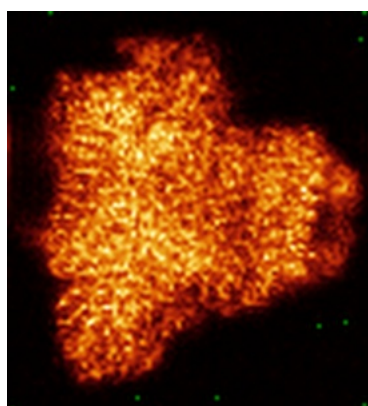
The images above show the largest variance slices of the map in three orthogonal directions.

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

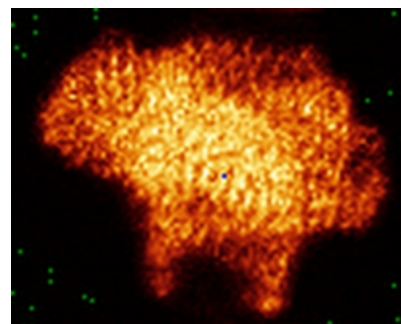
6.4.1 Primary map



X



Y

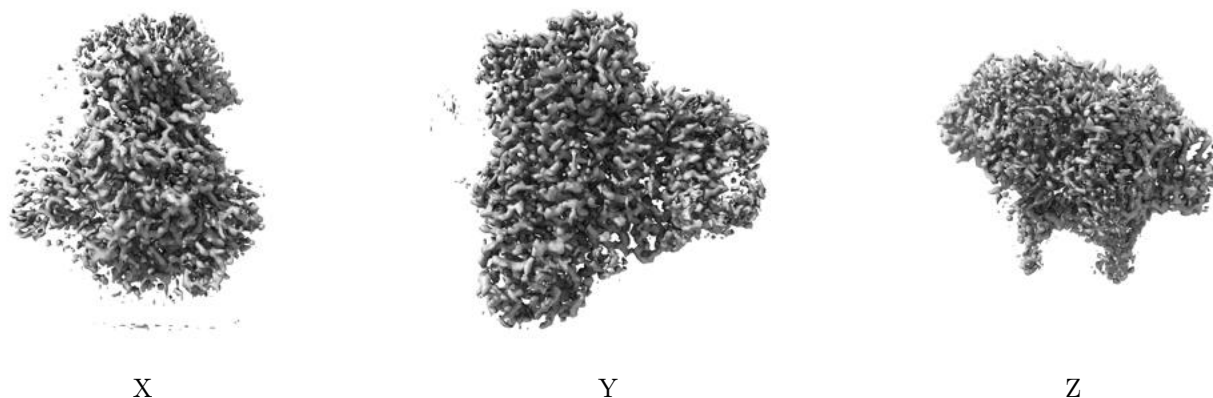


Z

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 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

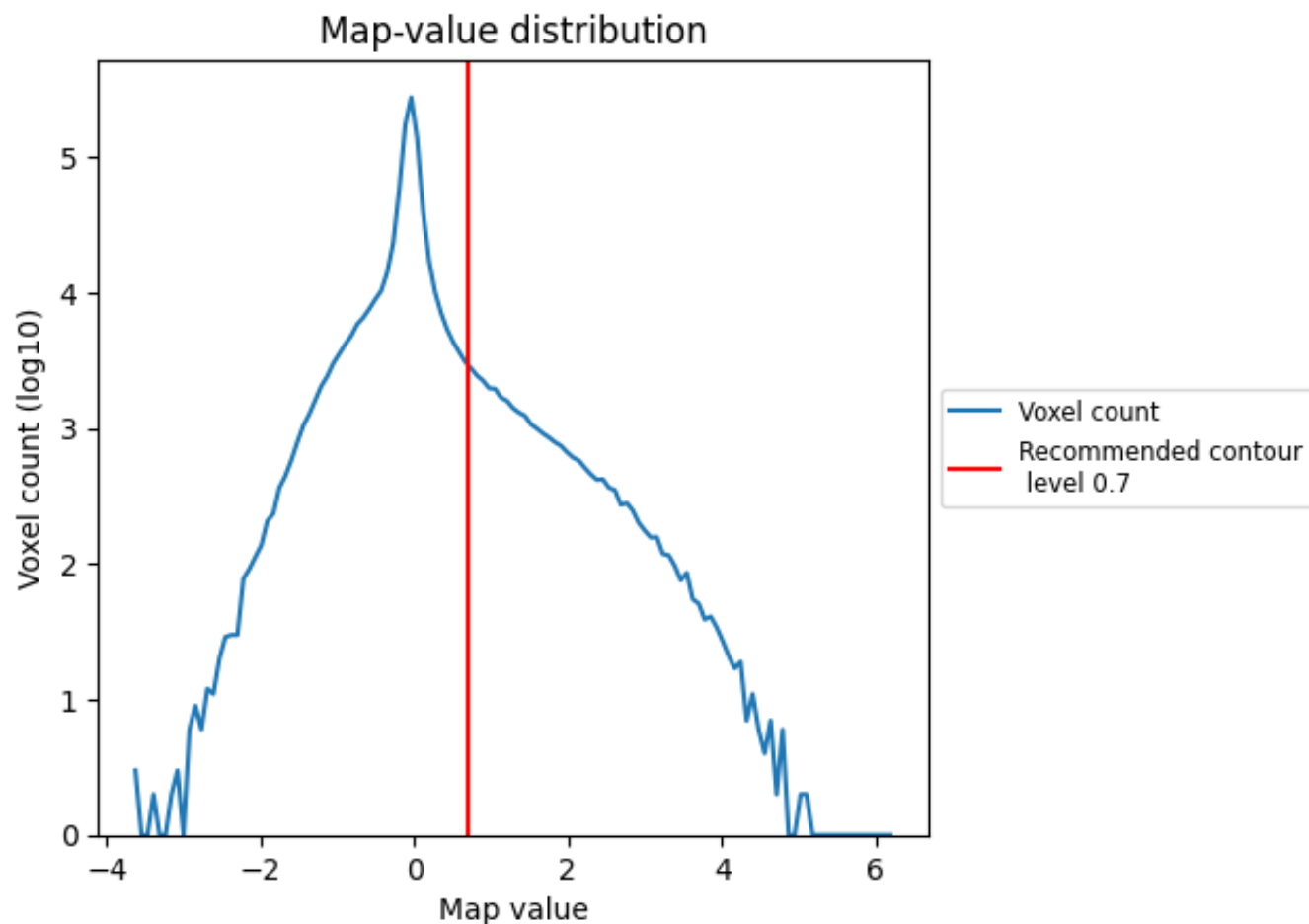
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

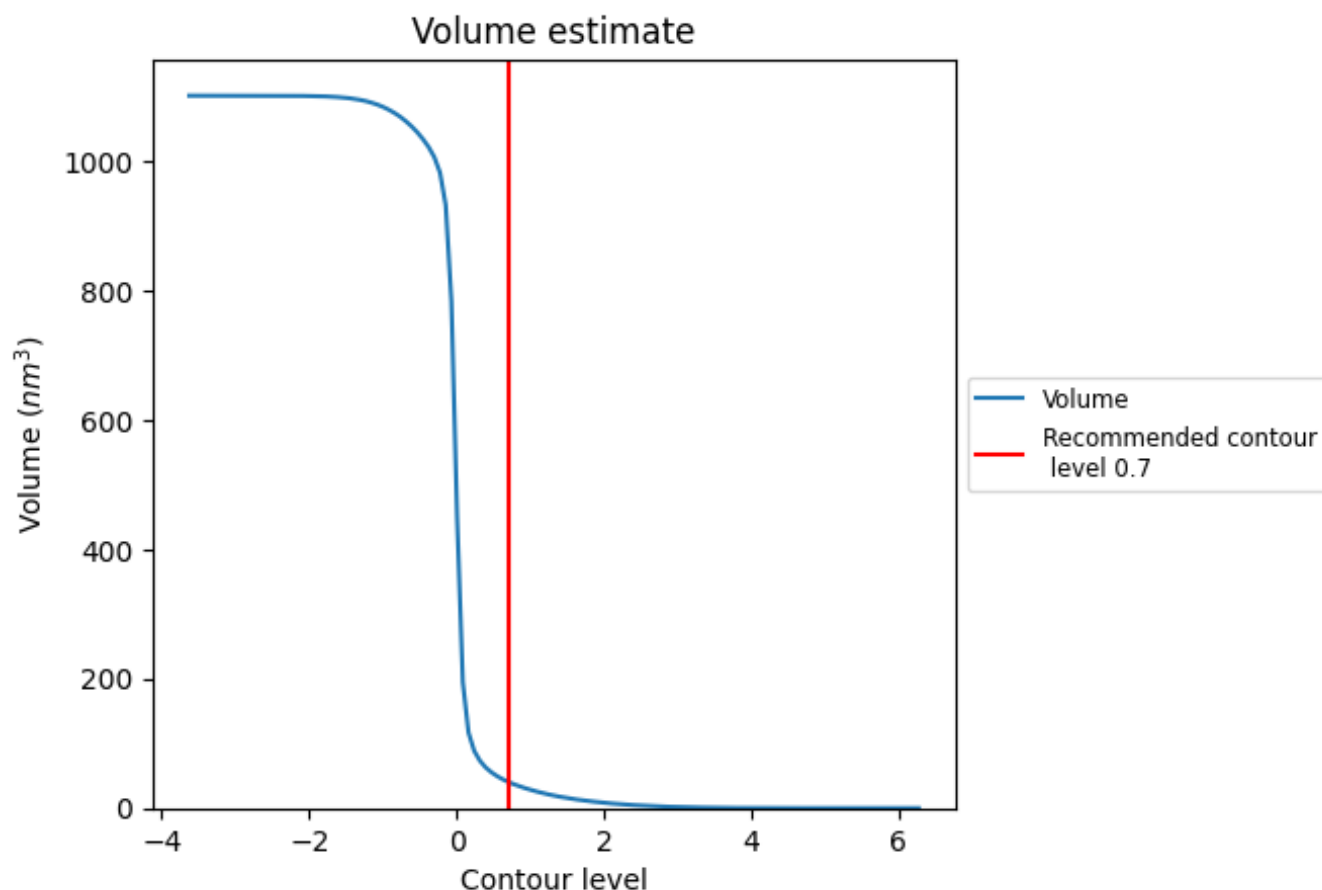
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 41 nm³; this corresponds to an approximate mass of 37 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

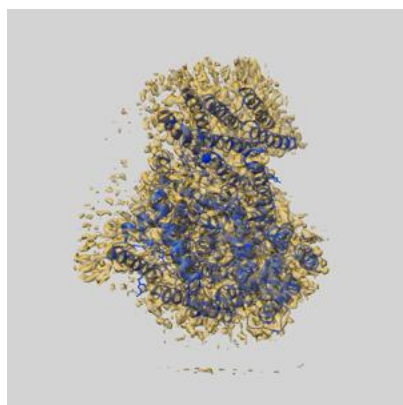
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

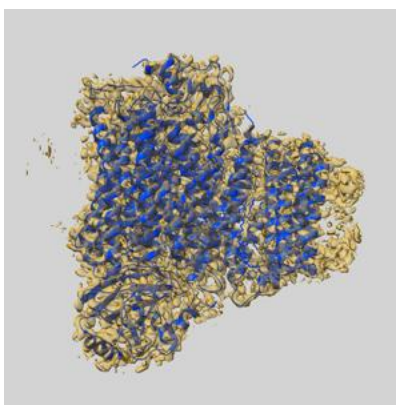
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21897 and PDB model 6WTI. Per-residue inclusion information can be found in section [3](#) on page [8](#).

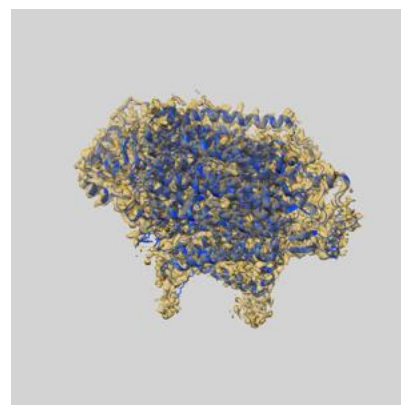
9.1 Map-model overlay [i](#)



X



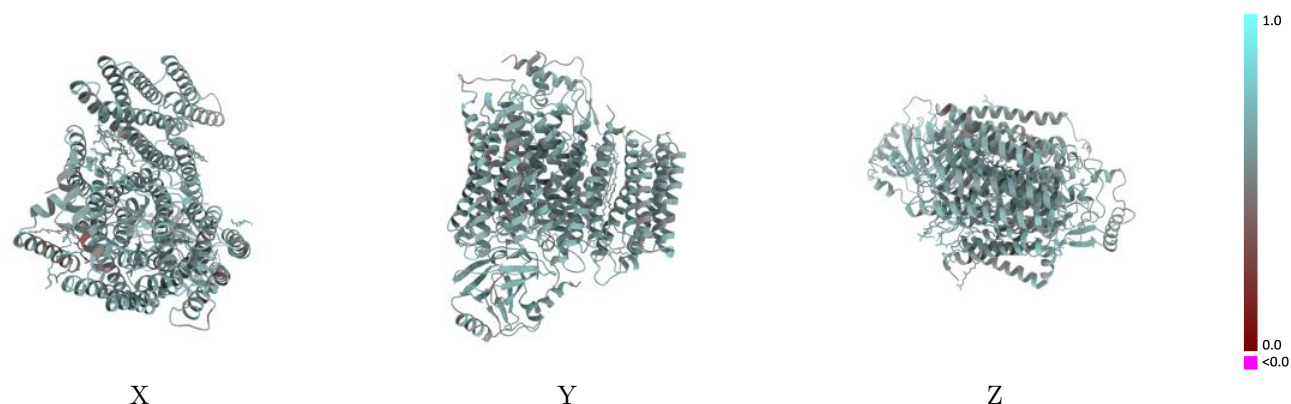
Y



Z

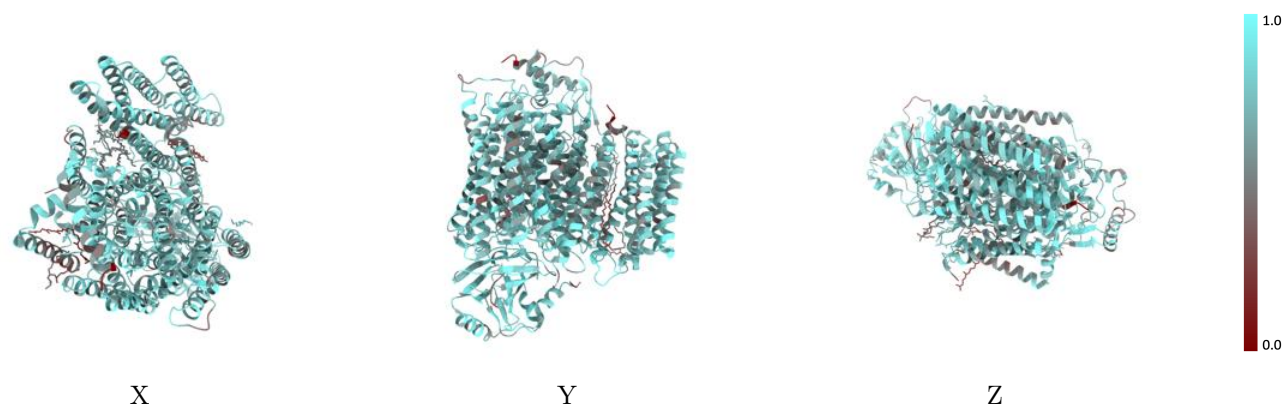
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



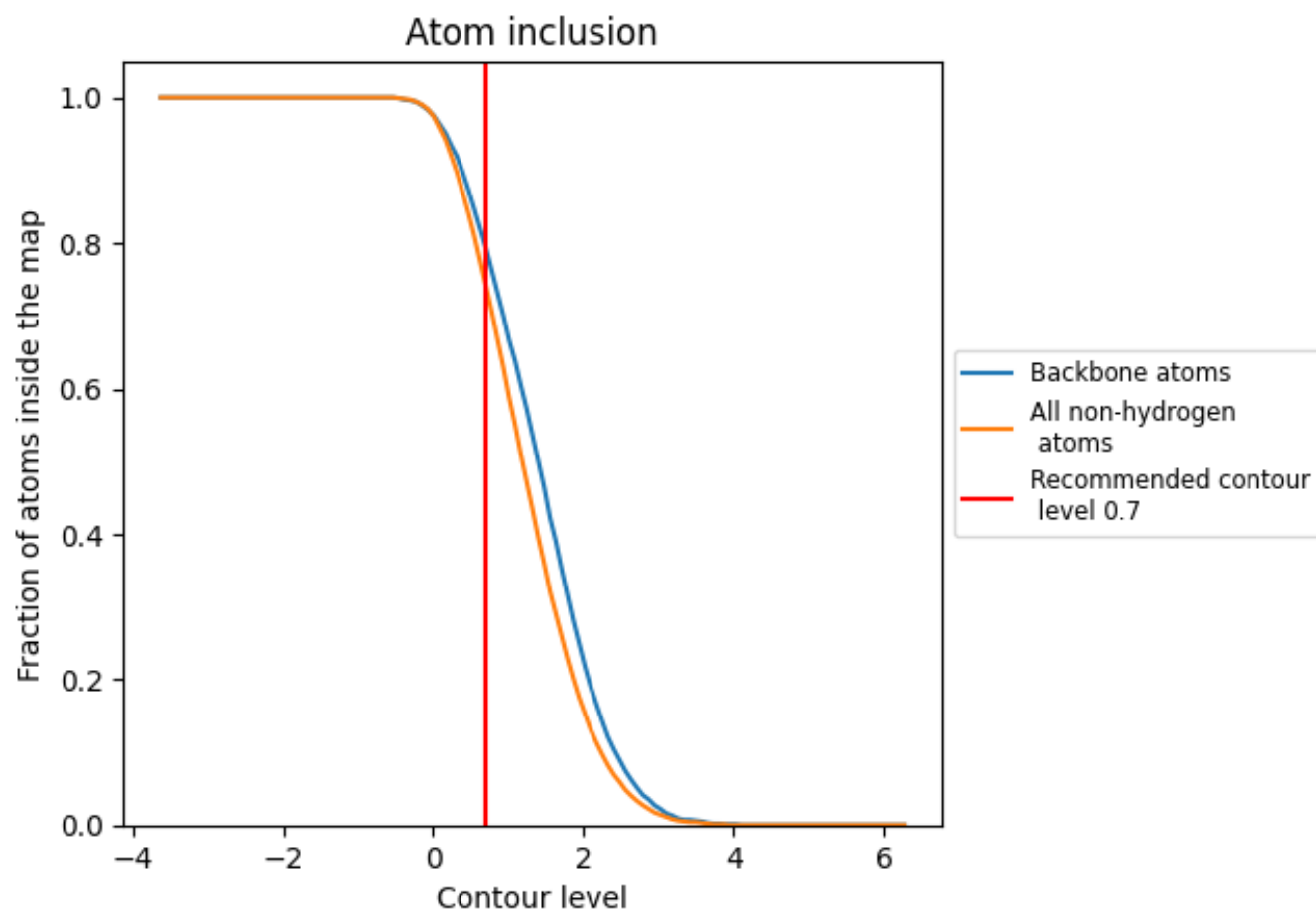
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7440	0.5910
A	0.7460	0.5930
B	0.7580	0.5900
C	0.7470	0.5940
D	0.6910	0.5790

