Full wwPDB EM Validation Report (i)

Aug 27, 2026 – 02:31 am BST

PDB ID	:	7OY2 / pdb_00007oy2
EMDB ID	:	EMD-13108
Title	:	High resolution structure of cytochrome bd-II oxidase from E. coli
Authors	:	Grund, T.N.; Wu, D.; Bald, D.; Michel, H.; Safarian, S.
Deposited on	:	2021-06-23
Resolution	:	2.06 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 (i) 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 (i)) were used in the production of this report:

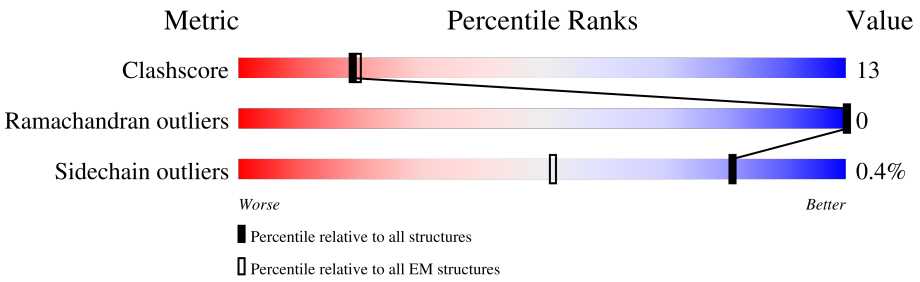
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

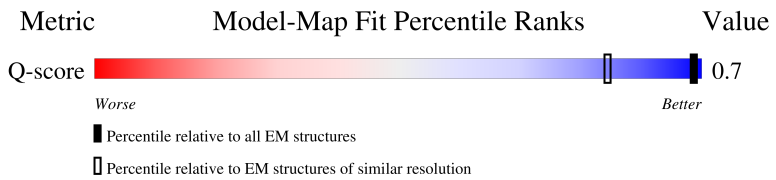
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.06 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	1895 (1.56 - 2.56)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	378	73% 27%
2	C	514	66% 22% 12%
3	X	61	31% 15% 54%

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
7	HEB	C	602	X	-	-	-
7	HEB	C	603	X	-	-	-
8	HDD	C	604	X	-	-	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 7166 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 bd-II ubiquinol oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	376	2980	2006	473	481	20	0	0

- Molecule 2 is a protein called Cytochrome bd-II ubiquinol oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	454	3620	2392	591	611	26	0	0

- Molecule 3 is a protein called Putative cytochrome bd-II ubiquinol oxidase subunit AppX.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	X	28	237	166	34	34	3	0	0

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	31	ILE	-	expression tag	UNP P24244
X	32	GLU	-	expression tag	UNP P24244
X	33	GLY	-	expression tag	UNP P24244
X	34	ARG	-	expression tag	UNP P24244
X	35	GLY	-	expression tag	UNP P24244
X	36	THR	-	expression tag	UNP P24244
X	37	SER	-	expression tag	UNP P24244
X	38	GLY	-	expression tag	UNP P24244
X	39	SER	-	expression tag	UNP P24244
X	40	SER	-	expression tag	UNP P24244
X	41	GLY	-	expression tag	UNP P24244
X	42	SER	-	expression tag	UNP P24244
X	43	GLY	-	expression tag	UNP P24244
X	44	SER	-	expression tag	UNP P24244
X	45	GLY	-	expression tag	UNP P24244

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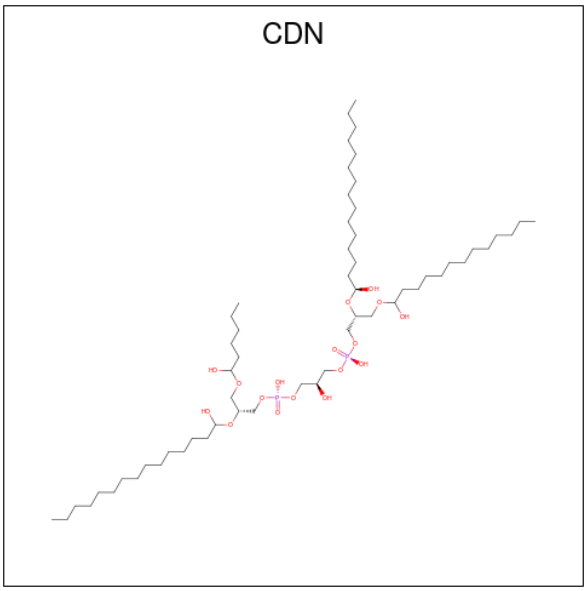
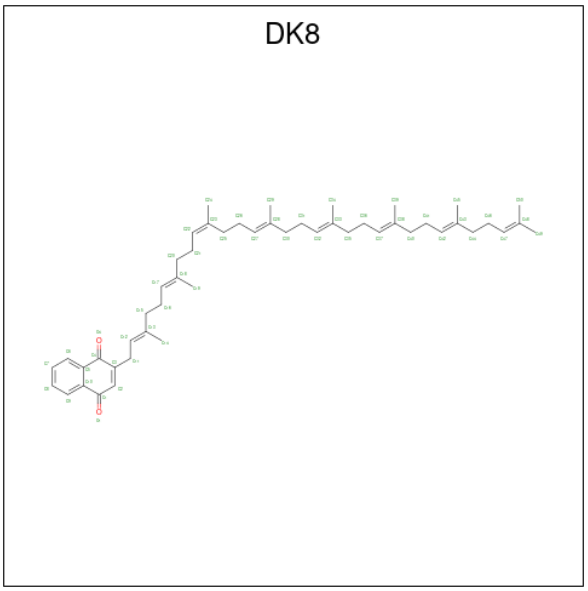
Chain	Residue	Modelled	Actual	Comment	Reference
X	46	GLY	-	expression tag	UNP P24244
X	47	SER	-	expression tag	UNP P24244
X	48	GLY	-	expression tag	UNP P24244
X	49	SER	-	expression tag	UNP P24244
X	50	GLY	-	expression tag	UNP P24244
X	51	GLY	-	expression tag	UNP P24244
X	52	GLY	-	expression tag	UNP P24244
X	53	GLY	-	expression tag	UNP P24244
X	54	TRP	-	expression tag	UNP P24244
X	55	SER	-	expression tag	UNP P24244
X	56	HIS	-	expression tag	UNP P24244
X	57	PRO	-	expression tag	UNP P24244
X	58	GLN	-	expression tag	UNP P24244
X	59	PHE	-	expression tag	UNP P24244
X	60	GLU	-	expression tag	UNP P24244
X	61	LYS	-	expression tag	UNP P24244

- Molecule 4 is CARDIOLIPIN (CCD ID: CDN) (formula: $C_{58}H_{120}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



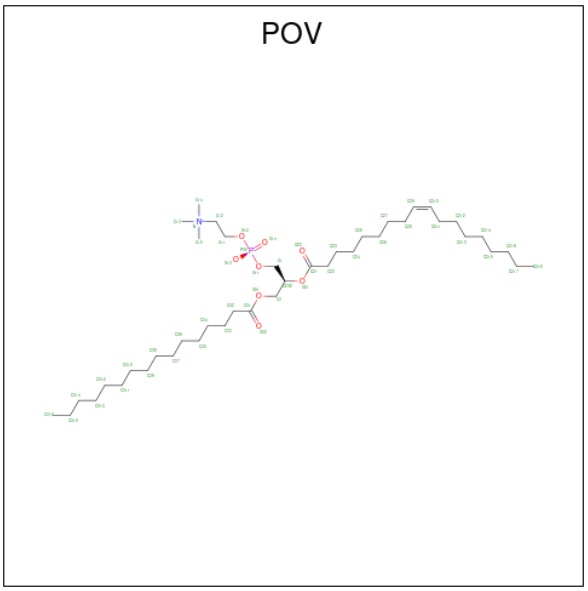
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
4	B	1	69	50	17	2	0

- Molecule 5 is 2-[(2 {E},6 {E},10 {Z},14 {E},18 {E},22 {E},26 {E})-3,7,11,15,19,23,27,31-octamethyldotriaconta-2,6,10,14,18,22,26,30-octaenyl]naphthalene-1,4-dione (CCD ID: DK8) (formula: $C_{50}H_{70}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
5	B	1	52	50	2	0

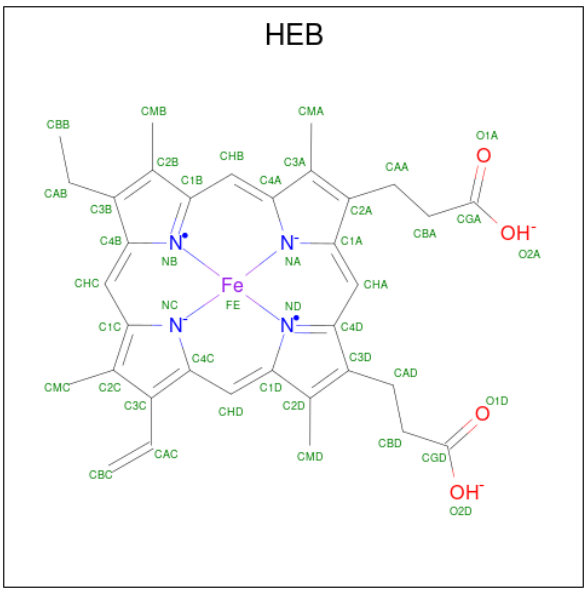
- Molecule 6 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: $C_{42}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	C	1	52	42	1	8	1	0

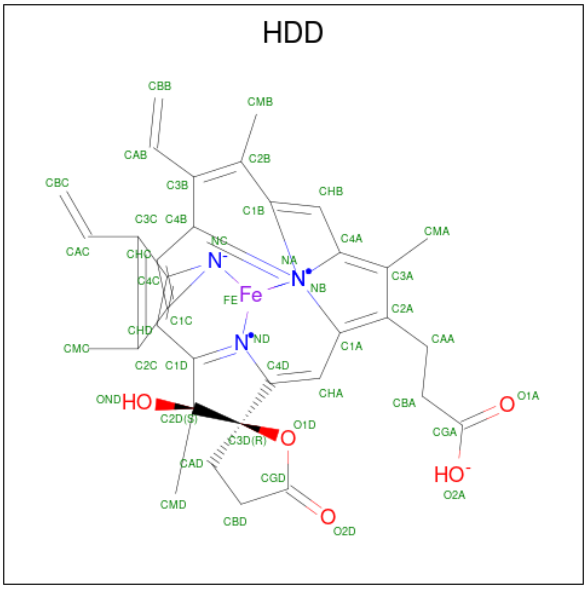
- Molecule 7 is HEME B/C (CCD ID: HEB) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of

Interest" by depositor).



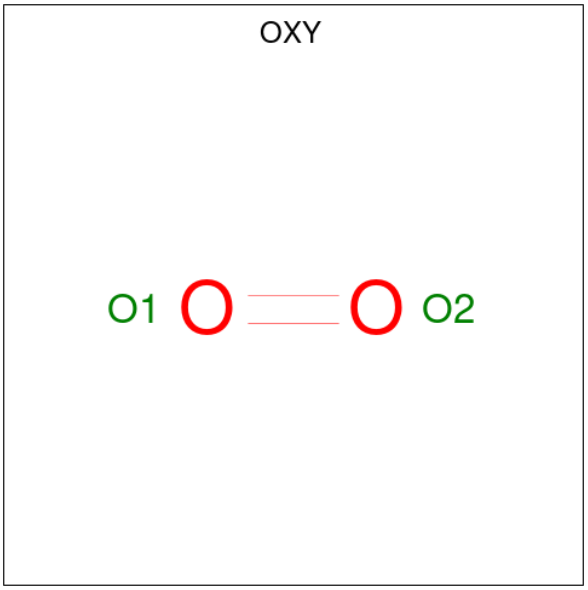
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
7	C	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
7	C	1	43	34	1	4	4	0

- Molecule 8 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: HDD) (formula: $C_{34}H_{32}FeN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
8	C	1	44	34	1	4	5	0

- Molecule 9 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
			Total	O	
9	C	1	2	2	0

- Molecule 10 is water.

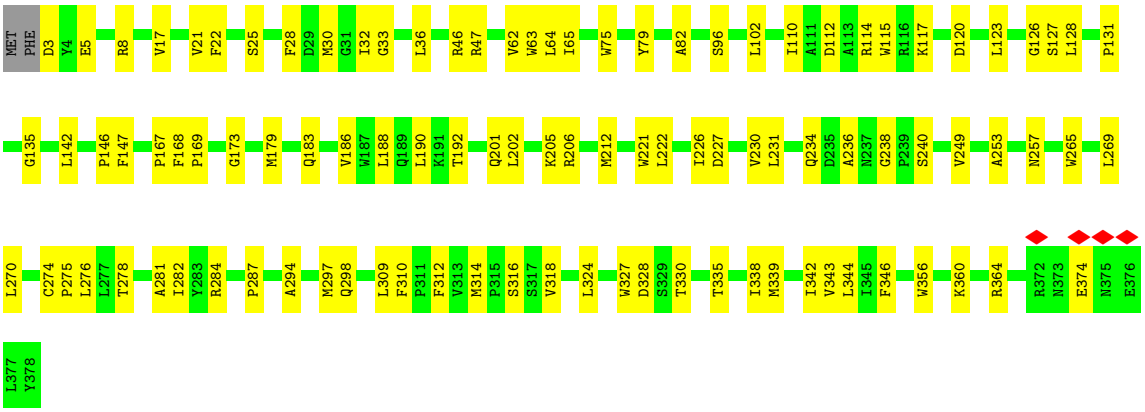
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
10	B	10	10	10	0
			Total	O	
10	C	14	14	14	0

3 Residue-property plots (i)

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

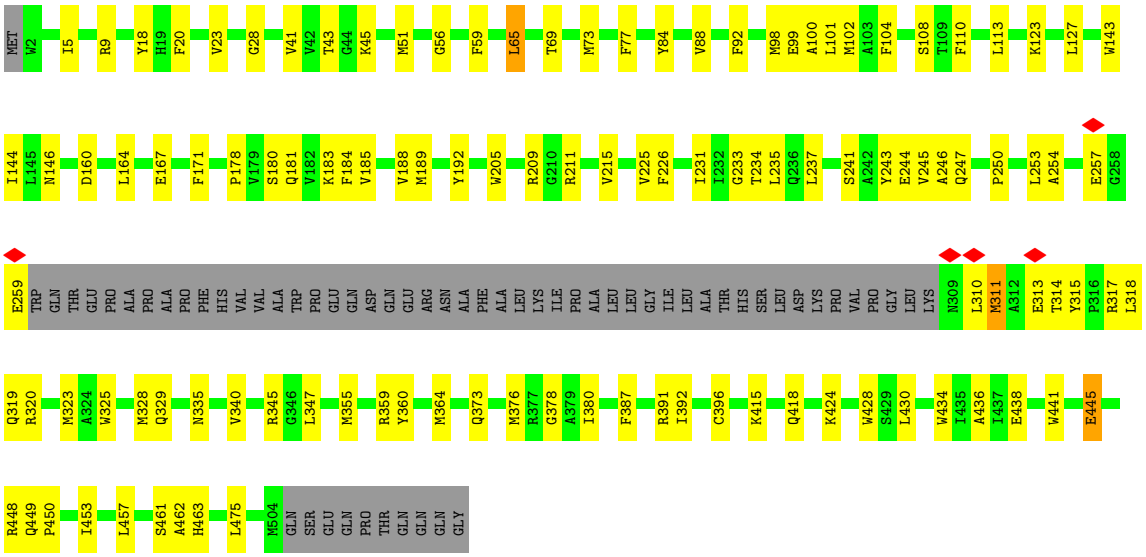
• Molecule 1: Cytochrome bd-II ubiquinol oxidase subunit 2

Chain B: 73% 27%



• Molecule 2: Cytochrome bd-II ubiquinol oxidase subunit 1

Chain C: 66% 22% 12%



• Molecule 3: Putative cytochrome bd-II ubiquinol oxidase subunit AppX

Chain X: 31% 15% 54%

M1 W2 Y3 V8 L12 M13 T18 L19 V20 L21 V22 L28 LYS SER ILE GLU GLY ARG GLY THR SER GLY SER SER GLY SER GLY SER GLY GLY SER GLY SER GLY GLY GLY GLY TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	533309	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	108	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	0.166	Depositor
Minimum map value	-0.062	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	214.272, 214.272, 214.272	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	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: OXY, CDN, DK8, HEB, POV, HDD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	B	0.25	0/3073	0.46	0/4197
2	C	0.32	0/3723	0.52	2/5060 (0.0%)
3	X	0.21	0/245	0.37	0/336
All	All	0.29	0/7041	0.49	2/9593 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	392	ILE	N-CA-C	-6.37	104.31	110.42
2	C	445	GLU	CB-CA-C	6.06	121.85	109.67

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2980	0	3066	69	0
2	C	3620	0	3630	112	0
3	X	237	0	254	8	0
4	B	69	0	96	3	0
5	B	52	0	0	0	0
6	C	52	0	82	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	86	0	64	21	0
8	C	44	0	31	7	0
9	C	2	0	0	1	0
10	B	10	0	0	0	0
10	C	14	0	0	1	0
All	All	7166	0	7223	185	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 13.

All (185) 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)
2:C:185:VAL:CG1	2:C:237:LEU:HD21	1.49	1.39
2:C:185:VAL:HG12	2:C:237:LEU:CD2	1.51	1.36
2:C:185:VAL:CG1	2:C:237:LEU:CD2	2.05	1.32
2:C:185:VAL:HG11	2:C:237:LEU:HD21	1.26	1.10
2:C:185:VAL:HG12	2:C:237:LEU:HD22	1.27	1.08
2:C:185:VAL:HB	2:C:237:LEU:HD23	1.48	0.95
2:C:185:VAL:CB	2:C:237:LEU:CD2	2.48	0.90
2:C:185:VAL:CB	2:C:237:LEU:HD23	2.04	0.87
2:C:253:LEU:O	2:C:257:GLU:HG2	1.74	0.87
2:C:84:TYR:HB2	2:C:462:ALA:HB1	1.58	0.86
2:C:246:ALA:HA	2:C:253:LEU:HD12	1.59	0.82
2:C:441:TRP:CE2	7:C:602:HEB:HAB2	2.15	0.81
2:C:99:GLU:OE1	2:C:144:ILE:HB	1.82	0.79
2:C:246:ALA:CA	2:C:253:LEU:HD12	2.15	0.76
1:B:212:MET:HE1	1:B:276:LEU:HD12	1.67	0.76
2:C:449:GLN:NE2	7:C:602:HEB:O1D	2.14	0.75
2:C:185:VAL:HB	2:C:237:LEU:CD2	2.13	0.73
1:B:202:LEU:HD21	1:B:206:ARG:HH11	1.53	0.73
2:C:250:PRO:HB2	2:C:310:LEU:HD22	1.73	0.71
3:X:1:MET:HE1	3:X:3:TYR:HB2	1.70	0.71
1:B:142:LEU:HD13	1:B:222:LEU:HD11	1.73	0.70
1:B:190:LEU:HG	1:B:287:PRO:HB2	1.75	0.69
1:B:147:PHE:O	1:B:316:SER:OG	2.11	0.68
2:C:88:VAL:HG11	2:C:453:ILE:HG13	1.75	0.68
1:B:356:TRP:O	1:B:360:LYS:HG2	1.94	0.68
4:B:401:CDN:H332	4:B:401:CDN:H111	1.75	0.67
2:C:108:SER:O	10:C:701:HOH:O	2.12	0.67
2:C:181:GLN:HB3	3:X:2:TRP:HB2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ILE:HG12	1:B:188:LEU:HG	1.76	0.66
2:C:99:GLU:OE1	9:C:605:OXY:O1	2.15	0.65
1:B:25:SER:HG	1:B:63:TRP:CD1	2.16	0.64
1:B:30:MET:O	1:B:127:SER:HB3	1.97	0.64
2:C:430:LEU:HD23	6:C:601:POV:H28A	1.79	0.64
1:B:343:VAL:HA	2:C:101:LEU:HD21	1.79	0.64
2:C:448:ARG:HH22	7:C:602:HEB:C4D	2.11	0.64
1:B:281:ALA:HA	1:B:284:ARG:HE	1.62	0.62
7:C:602:HEB:HBC1	7:C:602:HEB:HMC3	1.81	0.62
2:C:160:ASP:HB2	2:C:167:GLU:HG3	1.81	0.62
2:C:110:PHE:HD1	2:C:113:LEU:HD12	1.66	0.60
1:B:294:ALA:O	1:B:298:GLN:HG2	2.01	0.60
1:B:167:PRO:HB2	1:B:221:TRP:HH2	1.65	0.60
2:C:323:MET:HB3	2:C:347:LEU:HD13	1.83	0.60
1:B:22:PHE:CE1	1:B:64:LEU:HB2	2.38	0.59
2:C:41:VAL:HG22	2:C:123:LYS:HG3	1.84	0.59
2:C:20:PHE:CD1	7:C:602:HEB:HBB1	2.38	0.58
2:C:235:LEU:HA	7:C:603:HEB:HBB3	1.84	0.58
2:C:108:SER:OG	8:C:604:HDD:O2A	2.20	0.58
2:C:311:MET:HG2	2:C:380:ILE:HG13	1.86	0.58
1:B:102:LEU:HD21	2:C:65:LEU:HD13	1.86	0.57
1:B:281:ALA:HB2	1:B:284:ARG:HH11	1.70	0.57
2:C:146:ASN:HA	2:C:180:SER:HB3	1.87	0.56
2:C:254:ALA:HB1	2:C:259:GLU:OE1	2.05	0.56
1:B:342:ILE:HD13	2:C:98:MET:SD	2.45	0.56
1:B:96:SER:HB2	1:B:126:GLY:HA2	1.88	0.56
2:C:310:LEU:O	2:C:314:THR:HG23	2.06	0.56
2:C:144:ILE:HG13	7:C:602:HEB:HMC3	1.87	0.55
2:C:23:VAL:HG22	8:C:604:HDD:HAD1	1.89	0.54
1:B:28:PHE:HB3	1:B:183:GLN:HG3	1.90	0.54
2:C:448:ARG:HH12	7:C:602:HEB:HBD2	1.72	0.53
1:B:110:ILE:HB	1:B:115:TRP:CD1	2.43	0.53
1:B:338:ILE:HD13	2:C:171:PHE:HB2	1.89	0.53
2:C:234:THR:HG21	7:C:603:HEB:HBC1	1.89	0.53
2:C:246:ALA:CB	2:C:253:LEU:HD12	2.38	0.53
2:C:387:PHE:O	2:C:391:ARG:HG2	2.07	0.53
2:C:205:TRP:CE2	6:C:601:POV:H33A	2.44	0.52
2:C:189:MET:HE2	2:C:192:TYR:HD2	1.73	0.52
1:B:201:GLN:O	1:B:205:LYS:HG2	2.10	0.52
2:C:192:TYR:HB3	2:C:226:PHE:CE2	2.45	0.52
2:C:315:TYR:CZ	2:C:319:GLN:NE2	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:MET:HG2	1:B:297:MET:HE3	1.92	0.51
1:B:65:ILE:HD13	8:C:604:HDD:HBA2	1.93	0.51
2:C:441:TRP:CD2	7:C:602:HEB:HAB2	2.46	0.51
1:B:167:PRO:HB2	1:B:221:TRP:CH2	2.46	0.51
2:C:69:THR:O	2:C:73:MET:HG2	2.11	0.51
2:C:164:LEU:HD22	2:C:328:MET:HE2	1.93	0.50
1:B:231:LEU:HD21	1:B:234:GLN:HB3	1.93	0.50
2:C:396:CYS:HB2	2:C:436:ALA:HB2	1.92	0.50
1:B:275:PRO:HG3	1:B:297:MET:SD	2.51	0.50
2:C:23:VAL:HG22	8:C:604:HDD:CAD	2.40	0.50
2:C:189:MET:HE2	2:C:192:TYR:CD2	2.46	0.50
1:B:339:MET:HE1	2:C:98:MET:HG3	1.93	0.50
1:B:79:TYR:OH	2:C:77:PHE:HB2	2.13	0.49
2:C:441:TRP:HB3	7:C:602:HEB:CMB	2.42	0.49
1:B:346:PHE:CE1	2:C:102:MET:HG2	2.47	0.49
2:C:225:VAL:HG21	3:X:20:VAL:HG11	1.94	0.49
1:B:47:ARG:HH12	1:B:374:GLU:HG3	1.77	0.49
2:C:189:MET:HE1	3:X:13:MET:SD	2.53	0.49
8:C:604:HDD:HMC3	8:C:604:HDD:HBC1	1.95	0.49
1:B:5:GLU:HG3	1:B:236:ALA:HB1	1.95	0.49
1:B:186:VAL:HG13	1:B:282:ILE:HD11	1.94	0.49
2:C:355:MET:HE2	2:C:461:SER:HB3	1.95	0.48
2:C:244:GLU:OE2	2:C:244:GLU:HA	2.12	0.48
2:C:181:GLN:HG2	3:X:3:TYR:CZ	2.48	0.48
2:C:9:ARG:HD2	7:C:602:HEB:O2A	2.14	0.47
2:C:378:GLY:O	2:C:450:PRO:HG3	2.14	0.47
2:C:359:ARG:HD3	2:C:360:TYR:CZ	2.48	0.47
2:C:359:ARG:HD3	2:C:360:TYR:CE1	2.50	0.47
2:C:441:TRP:CD1	7:C:603:HEB:HAD2	2.49	0.46
2:C:441:TRP:CG	7:C:603:HEB:HAD2	2.51	0.46
1:B:147:PHE:CE1	1:B:314:MET:HG2	2.50	0.46
2:C:434:TRP:HB3	6:C:601:POV:H21E	1.97	0.46
1:B:240:SER:HA	1:B:328:ASP:HA	1.98	0.46
1:B:36:LEU:HD11	1:B:46:ARG:HD3	1.97	0.46
2:C:51:MET:HG2	2:C:215:VAL:HG13	1.98	0.46
2:C:110:PHE:CD1	2:C:113:LEU:HD12	2.48	0.46
2:C:185:VAL:CB	2:C:237:LEU:HD21	2.21	0.46
1:B:46:ARG:HD2	1:B:120:ASP:OD2	2.16	0.45
1:B:314:MET:HB3	1:B:324:LEU:HB2	1.97	0.45
1:B:112:ASP:OD1	1:B:114:ARG:NH1	2.45	0.45
1:B:135:GLY:HA3	1:B:173:GLY:HA2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:243:TYR:O	2:C:247:GLN:HG2	2.15	0.45
1:B:287:PRO:HD2	4:B:401:CDN:HA22	1.99	0.45
1:B:222:LEU:HA	1:B:226:ILE:HD12	1.99	0.45
1:B:168:PHE:HB3	1:B:169:PRO:HD3	1.97	0.45
2:C:43:THR:HB	2:C:45:LYS:HE3	1.98	0.45
2:C:434:TRP:O	2:C:438:GLU:HG2	2.16	0.45
2:C:246:ALA:HB1	2:C:253:LEU:HD12	1.98	0.45
2:C:335:ASN:ND2	2:C:340:VAL:HG21	2.31	0.45
1:B:230:VAL:HG23	1:B:253:ALA:HB1	1.99	0.45
1:B:8:ARG:HD3	1:B:327:TRP:HA	1.98	0.45
1:B:360:LYS:HB3	1:B:360:LYS:HE3	1.66	0.44
2:C:41:VAL:HG21	2:C:127:LEU:HD22	1.99	0.44
2:C:315:TYR:HB2	2:C:376:MET:HE3	1.99	0.44
1:B:8:ARG:HG2	1:B:330:THR:HG21	1.98	0.44
1:B:192:THR:O	1:B:364:ARG:NH2	2.49	0.44
2:C:84:TYR:HA	2:C:457:LEU:HD21	1.99	0.44
2:C:445:GLU:CD	2:C:448:ARG:HH21	2.26	0.44
2:C:184:PHE:O	2:C:188:VAL:HG22	2.18	0.44
2:C:415:LYS:HB3	2:C:418:GLN:HB2	1.98	0.44
1:B:309:LEU:O	1:B:312:PHE:N	2.51	0.43
2:C:5:ILE:HG12	2:C:463:HIS:CG	2.53	0.43
3:X:18:THR:O	3:X:22:VAL:HG23	2.18	0.43
1:B:146:PRO:HA	1:B:318:VAL:HG13	1.99	0.43
2:C:183:LYS:NZ	7:C:603:HEB:O2D	2.49	0.43
2:C:314:THR:O	2:C:318:LEU:HG	2.18	0.43
8:C:604:HDD:HMD2	8:C:604:HDD:HAD2	1.77	0.43
1:B:3:ASP:N	1:B:3:ASP:OD1	2.51	0.43
2:C:424:LYS:O	2:C:428:TRP:HD1	2.02	0.43
2:C:241:SER:O	2:C:245:VAL:HG13	2.18	0.43
2:C:18:TYR:HD2	2:C:69:THR:HG21	1.84	0.43
2:C:23:VAL:HG13	8:C:604:HDD:HMD2	2.00	0.43
2:C:84:TYR:O	2:C:88:VAL:HG22	2.19	0.43
1:B:257:ASN:ND2	1:B:310:PHE:O	2.43	0.43
1:B:62:VAL:HA	1:B:65:ILE:HD12	2.01	0.43
2:C:28:GLY:HA2	2:C:192:TYR:HD1	1.83	0.43
2:C:231:ILE:O	2:C:235:LEU:HG	2.19	0.43
2:C:144:ILE:HD12	2:C:144:ILE:HA	1.95	0.42
4:B:401:CDN:H532	4:B:401:CDN:H561	1.76	0.42
1:B:270:LEU:O	1:B:274:CYS:HB2	2.20	0.42
1:B:278:THR:O	1:B:282:ILE:HG12	2.20	0.42
1:B:17:VAL:O	1:B:21:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ALA:HA	1:B:314:MET:HE1	2.02	0.42
2:C:100:ALA:HA	2:C:104:PHE:HB2	2.01	0.42
2:C:102:MET:CE	2:C:143:TRP:HE1	2.33	0.42
1:B:33:GLY:HA3	1:B:127:SER:OG	2.20	0.42
1:B:22:PHE:CD1	1:B:64:LEU:HB2	2.55	0.41
1:B:117:LYS:HB3	1:B:117:LYS:HE3	1.51	0.41
1:B:335:THR:O	1:B:339:MET:HG2	2.20	0.41
1:B:342:ILE:HG21	2:C:98:MET:HG2	2.02	0.41
1:B:128:LEU:O	1:B:131:PRO:HD2	2.21	0.41
1:B:8:ARG:NH1	1:B:238:GLY:O	2.48	0.41
1:B:75:TRP:CD1	1:B:330:THR:HG22	2.55	0.41
3:X:1:MET:HE1	3:X:3:TYR:CB	2.47	0.41
2:C:209:ARG:HB2	2:C:211:ARG:HG2	2.03	0.41
2:C:183:LYS:HE2	2:C:183:LYS:HB2	1.90	0.41
2:C:441:TRP:CZ2	7:C:603:HEB:HBD1	2.55	0.41
3:X:8:VAL:O	3:X:12:LEU:HG	2.21	0.41
1:B:265:TRP:O	1:B:269:LEU:HG	2.21	0.41
2:C:441:TRP:HB3	7:C:602:HEB:HMB1	2.03	0.41
2:C:325:TRP:O	2:C:329:GLN:HG2	2.20	0.41
2:C:189:MET:SD	2:C:233:GLY:HA3	2.61	0.40
2:C:325:TRP:CZ3	2:C:364:MET:HG3	2.56	0.40
2:C:475:LEU:HD23	2:C:475:LEU:HA	1.93	0.40
1:B:33:GLY:HA2	1:B:123:LEU:CD2	2.51	0.40
1:B:227:ASP:HB3	1:B:249:VAL:HG12	2.03	0.40
2:C:178:PRO:HB2	2:C:244:GLU:OE1	2.20	0.40
2:C:345:ARG:HD3	2:C:345:ARG:HA	1.86	0.40
2:C:92:PHE:HZ	7:C:602:HEB:HAC	1.86	0.40
2:C:373:GLN:HA	2:C:376:MET:HB2	2.03	0.40
7:C:602:HEB:HMB1	7:C:602:HEB:HAB	1.89	0.40
7:C:602:HEB:HHC	7:C:602:HEB:HBB2	2.03	0.40
7:C:602:HEB:O2D	7:C:602:HEB:HHA	2.22	0.40
1:B:344:LEU:HD23	1:B:344:LEU:HA	1.77	0.40
2:C:56:GLY:HA2	2:C:59:PHE:HB3	2.03	0.40
2:C:317:ARG:HG2	2:C:320:ARG:NH1	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	374/378 (99%)	370 (99%)	4 (1%)	0	100	100
2	C	450/514 (88%)	447 (99%)	3 (1%)	0	100	100
3	X	26/61 (43%)	26 (100%)	0	0	100	100
All	All	850/953 (89%)	843 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	B	316/318 (99%)	316 (100%)	0	100	100
2	C	372/422 (88%)	369 (99%)	3 (1%)	73	77
3	X	27/48 (56%)	27 (100%)	0	100	100
All	All	715/788 (91%)	712 (100%)	3 (0%)	81	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	65	LEU
2	C	311	MET
2	C	313	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
2	C	76	GLN
2	C	319	GLN
2	C	329	GLN
2	C	339	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	CDN	B	401	-	68,68,76	0.91	2 (2%)	70,80,88	0.84	2 (2%)
7	HEB	C	603	2	50,50,50	4.54	28 (56%)	65,82,82	5.56	40 (61%)
9	OXY	C	605	8	1,1,1	0.13	0	-		
7	HEB	C	602	2	50,50,50	4.55	28 (56%)	65,82,82	5.51	42 (64%)
5	DK8	B	402	-	53,53,53	2.10	18 (33%)	65,67,67	1.94	19 (29%)
6	POV	C	601	-	51,51,51	1.08	6 (11%)	57,59,59	1.01	2 (3%)
8	HDD	C	604	9,2	50,52,52	2.61	24 (48%)	56,89,89	2.52	20 (35%)

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
4	CDN	B	401	-	-	35/79/79/87	-
7	HEB	C	603	2	1/1/3/8	8/14/54/54	-
7	HEB	C	602	2	1/1/3/8	7/14/54/54	-
5	DK8	B	402	-	-	10/47/63/63	0/2/2/2
8	HDD	C	604	9,2	1/1/8/14	2/9/89/89	0/1/9/9
6	POV	C	601	-	-	22/55/55/55	-

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	602	HEB	FE-ND	12.80	2.34	1.94
7	C	603	HEB	FE-ND	12.53	2.33	1.94
7	C	603	HEB	C1C-C2C	-8.64	1.22	1.43
7	C	602	HEB	C1B-C2B	-8.50	1.28	1.44
7	C	602	HEB	C1C-C2C	-8.41	1.23	1.43
7	C	603	HEB	C1A-C2A	-7.97	1.31	1.45
7	C	603	HEB	C4A-NA	7.84	1.54	1.39
7	C	603	HEB	C1B-C2B	-7.52	1.30	1.44
7	C	602	HEB	C4A-NA	7.51	1.54	1.39
7	C	602	HEB	C1A-C2A	-7.34	1.32	1.45
7	C	602	HEB	C4D-ND	6.96	1.53	1.38
7	C	603	HEB	FE-NB	6.87	2.16	1.94
7	C	602	HEB	CHA-C4D	6.87	1.54	1.39
7	C	603	HEB	C4D-ND	6.41	1.52	1.38
7	C	603	HEB	CHA-C4D	6.41	1.53	1.39
7	C	603	HEB	FE-NC	6.33	2.16	1.95
7	C	602	HEB	FE-NB	6.31	2.14	1.94
7	C	602	HEB	FE-NC	6.28	2.16	1.95
7	C	602	HEB	C3B-C2B	-6.07	1.23	1.36
7	C	602	HEB	C1C-NC	5.91	1.51	1.39
7	C	603	HEB	C1C-NC	5.90	1.51	1.39
7	C	603	HEB	C2A-C3A	-5.89	1.24	1.36
7	C	603	HEB	C1D-C2D	-5.86	1.33	1.44
7	C	602	HEB	C1D-C2D	-5.61	1.33	1.44
7	C	602	HEB	C2A-C3A	-5.54	1.24	1.36
5	B	402	DK8	C10-C1	5.53	1.57	1.48
5	B	402	DK8	C2-C3	5.51	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	603	HEB	CHC-C1C	5.43	1.51	1.39
7	C	603	HEB	CHD-C1D	5.39	1.49	1.38
7	C	603	HEB	CHB-C4A	5.32	1.48	1.38
7	C	602	HEB	CHD-C1D	5.32	1.49	1.38
7	C	603	HEB	C3B-C2B	-5.28	1.25	1.36
7	C	603	HEB	C3C-C2C	-5.16	1.23	1.41
7	C	602	HEB	C4A-C3A	-5.13	1.35	1.45
7	C	603	HEB	C4B-NB	5.03	1.49	1.40
7	C	602	HEB	CHC-C1C	4.98	1.50	1.39
7	C	603	HEB	FE-NA	4.92	2.11	1.95
7	C	602	HEB	FE-NA	4.89	2.11	1.95
5	B	402	DK8	C5-C4	4.81	1.57	1.48
7	C	602	HEB	C4B-NB	4.79	1.48	1.40
7	C	602	HEB	C3C-C2C	-4.59	1.25	1.41
7	C	602	HEB	C4B-C3B	-4.57	1.37	1.45
7	C	602	HEB	CHB-C4A	4.45	1.47	1.38
7	C	603	HEB	C4A-C3A	-4.43	1.36	1.45
7	C	602	HEB	CHA-C1A	4.42	1.47	1.38
8	C	604	HDD	O1D-CGD	4.38	1.42	1.35
8	C	604	HDD	C3C-C2C	4.37	1.46	1.37
8	C	604	HDD	C4C-NC	-4.32	1.31	1.39
7	C	602	HEB	CBC-CAC	4.32	1.51	1.30
7	C	603	HEB	CBC-CAC	4.31	1.51	1.30
8	C	604	HDD	O1D-C3D	-4.30	1.39	1.46
7	C	603	HEB	C4B-C3B	-4.27	1.37	1.45
8	C	604	HDD	CHD-C4C	4.27	1.46	1.38
8	C	604	HDD	FE-NB	4.22	2.07	1.94
7	C	603	HEB	C1B-NB	4.22	1.47	1.38
7	C	602	HEB	CHC-C4B	4.15	1.47	1.38
8	C	604	HDD	CHC-C1C	4.13	1.46	1.38
7	C	603	HEB	CHC-C4B	4.12	1.46	1.38
8	C	604	HDD	C1C-NC	-4.05	1.31	1.39
8	C	604	HDD	C1A-NA	-4.02	1.32	1.39
7	C	603	HEB	CHB-C1B	3.94	1.48	1.39
8	C	604	HDD	C1B-NB	-3.88	1.33	1.40
7	C	602	HEB	C1B-NB	3.86	1.46	1.38
8	C	604	HDD	C3B-C2B	3.74	1.44	1.37
4	B	401	CDN	OA6-CA4	-3.71	1.39	1.44
8	C	604	HDD	C4A-NA	-3.65	1.32	1.39
7	C	602	HEB	CHB-C1B	3.62	1.47	1.39
8	C	604	HDD	C1D-ND	-3.57	1.33	1.35
8	C	604	HDD	CHC-C4B	3.56	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	604	HDD	CHA-C1A	3.52	1.47	1.39
7	C	603	HEB	CHA-C1A	3.51	1.45	1.38
8	C	604	HDD	CHB-C1B	3.41	1.45	1.38
8	C	604	HDD	FE-NC	3.38	2.06	1.95
5	B	402	DK8	C39-C38	3.35	1.59	1.50
5	B	402	DK8	C15-C13	3.34	1.58	1.51
8	C	604	HDD	FE-NA	3.25	2.06	1.95
8	C	604	HDD	CHD-C1D	-3.19	1.32	1.41
7	C	603	HEB	C4C-NC	3.12	1.45	1.39
8	C	604	HDD	FE-ND	-3.05	1.85	1.94
5	B	402	DK8	O1-C1	-2.98	1.17	1.24
4	B	401	CDN	OB6-CB4	-2.94	1.40	1.44
5	B	402	DK8	C45-C43	2.91	1.58	1.50
7	C	602	HEB	C4C-NC	2.87	1.45	1.39
8	C	604	HDD	CHB-C4A	2.83	1.45	1.39
5	B	402	DK8	C36-C37	2.79	1.59	1.50
5	B	402	DK8	C2-C1	2.75	1.50	1.44
5	B	402	DK8	O4-C4	-2.67	1.17	1.23
6	C	601	POV	O21-C21	2.61	1.41	1.34
5	B	402	DK8	C11-C12	2.61	1.54	1.50
5	B	402	DK8	C40-C38	2.56	1.56	1.51
5	B	402	DK8	C11-C3	2.52	1.53	1.51
5	B	402	DK8	C19-C18	2.51	1.57	1.50
6	C	601	POV	O31-C31	2.43	1.40	1.33
8	C	604	HDD	C4B-NB	-2.42	1.33	1.38
5	B	402	DK8	C27-C28	2.38	1.38	1.33
7	C	603	HEB	C1A-NA	2.31	1.44	1.39
7	C	602	HEB	C1A-NA	2.24	1.44	1.39
6	C	601	POV	P-O11	2.24	1.68	1.59
6	C	601	POV	O31-C3	-2.22	1.40	1.45
6	C	601	POV	O21-C2	-2.22	1.41	1.46
8	C	604	HDD	C2A-C3A	2.21	1.44	1.38
5	B	402	DK8	C14-C13	2.10	1.56	1.50
5	B	402	DK8	C31-C32	2.09	1.57	1.50
6	C	601	POV	C15-N	-2.07	1.44	1.50
5	B	402	DK8	C35-C33	2.07	1.55	1.51
8	C	604	HDD	C4A-C3A	2.06	1.48	1.43

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	603	HEB	C3C-C4C-NC	-17.52	99.47	110.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	602	HEB	C1D-C2D-C3D	15.95	123.72	106.96
7	C	603	HEB	C1D-C2D-C3D	15.83	123.60	106.96
7	C	602	HEB	C3C-C4C-NC	-15.00	101.02	110.25
7	C	602	HEB	C1B-C2B-C3B	13.14	120.77	106.96
7	C	603	HEB	C1B-C2B-C3B	12.85	120.47	106.96
7	C	602	HEB	C2A-C1A-NA	-11.40	99.23	110.32
7	C	603	HEB	C2D-C1D-ND	-11.03	96.77	109.84
7	C	603	HEB	C3C-C2C-C1C	11.00	120.44	107.16
7	C	603	HEB	C3D-C4D-ND	-10.65	100.03	110.36
7	C	602	HEB	C1A-C2A-C3A	10.60	120.95	107.13
7	C	603	HEB	C2A-C1A-NA	-10.48	100.12	110.32
7	C	602	HEB	C3D-C4D-ND	-10.40	100.28	110.36
7	C	602	HEB	C3B-C4B-NB	-10.38	98.61	110.17
7	C	603	HEB	C1A-C2A-C3A	10.33	120.59	107.13
7	C	602	HEB	C2D-C1D-ND	-10.28	97.66	109.84
7	C	603	HEB	C1D-ND-C4D	9.74	115.14	105.07
7	C	602	HEB	C3C-C2C-C1C	9.55	118.69	107.16
7	C	602	HEB	C2B-C1B-NB	-9.44	98.57	109.88
7	C	602	HEB	C1D-ND-C4D	9.20	114.58	105.07
7	C	603	HEB	C2B-C1B-NB	-8.75	99.41	109.88
7	C	603	HEB	C3B-C4B-NB	-8.49	100.72	110.17
8	C	604	HDD	C3C-C2C-C1C	-7.06	100.34	107.08
7	C	602	HEB	CMC-C2C-C1C	-6.86	114.92	125.37
8	C	604	HDD	C3B-C2B-C1B	-6.27	101.83	106.49
7	C	603	HEB	CMB-C2B-C1B	-6.19	115.61	125.04
5	B	402	DK8	C11-C12-C13	-6.18	116.50	126.79
7	C	603	HEB	C3A-C4A-NA	-5.68	99.20	109.69
7	C	603	HEB	CMC-C2C-C1C	-5.63	116.79	125.37
7	C	602	HEB	CHA-C4D-C3D	5.63	133.11	124.84
7	C	603	HEB	C2C-C1C-NC	-5.32	101.98	110.08
7	C	602	HEB	CMB-C2B-C1B	-5.23	117.07	125.04
7	C	602	HEB	C3A-C4A-NA	-5.21	100.06	109.69
7	C	603	HEB	CHB-C1B-C2B	5.16	133.04	124.98
7	C	602	HEB	CHB-C1B-C2B	5.09	132.94	124.98
8	C	604	HDD	C2B-C1B-NB	5.01	115.78	109.84
7	C	602	HEB	CHA-C1A-NA	5.01	129.85	124.44
7	C	603	HEB	CHA-C1A-NA	4.73	129.55	124.44
8	C	604	HDD	CMA-C3A-C4A	4.66	132.47	125.37
8	C	604	HDD	C4A-C3A-C2A	-4.62	101.42	106.83
7	C	602	HEB	C4B-NB-C1B	4.59	109.81	105.07
7	C	603	HEB	CMD-C2D-C1D	-4.57	118.07	125.04
7	C	602	HEB	CMD-C2D-C1D	-4.50	118.19	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	604	HDD	CBA-CAA-C2A	-4.48	100.18	112.63
5	B	402	DK8	C11-C3-C4	4.39	120.45	116.88
7	C	603	HEB	CAA-C2A-C3A	-4.25	119.96	127.88
7	C	602	HEB	CHC-C4B-C3B	4.24	133.28	125.33
7	C	603	HEB	CHA-C4D-C3D	4.19	131.00	124.84
7	C	603	HEB	CHA-C4D-ND	4.18	128.97	124.42
7	C	602	HEB	C2C-C1C-NC	-4.06	103.90	110.08
7	C	603	HEB	CHC-C4B-C3B	3.96	132.77	125.33
6	C	601	POV	O21-C21-C22	3.96	120.03	111.50
7	C	602	HEB	CAA-C2A-C1A	-3.95	117.45	124.89
7	C	602	HEB	CAD-CBD-CGD	-3.92	105.17	113.60
7	C	603	HEB	CHB-C4A-C3A	3.91	133.68	125.48
8	C	604	HDD	CHC-C1C-NC	-3.82	120.31	124.44
8	C	604	HDD	C2A-C1A-NA	3.77	114.36	110.15
5	B	402	DK8	C26-C27-C28	-3.74	118.65	127.66
7	C	602	HEB	CHB-C1B-NB	3.74	128.48	124.42
7	C	602	HEB	CHA-C1A-C2A	3.69	130.92	124.94
7	C	602	HEB	C4B-C3B-C2B	3.65	112.21	106.90
5	B	402	DK8	C41-C42-C43	-3.63	118.92	127.66
5	B	402	DK8	C31-C32-C33	-3.54	119.13	127.66
5	B	402	DK8	C11-C3-C2	-3.50	118.70	123.30
8	C	604	HDD	C3A-C4A-NA	3.48	115.39	110.08
7	C	603	HEB	CAA-CBA-CGA	-3.48	106.11	113.60
7	C	603	HEB	C4A-C3A-C2A	3.45	111.98	106.94
7	C	603	HEB	C4B-NB-C1B	3.40	108.59	105.07
7	C	602	HEB	CAA-C2A-C3A	-3.38	121.58	127.88
7	C	603	HEB	CHA-C1A-C2A	3.32	130.31	124.94
7	C	603	HEB	CHD-C4C-NC	3.24	129.80	123.85
5	B	402	DK8	C21-C22-C23	-3.21	119.94	127.66
7	C	602	HEB	CHB-C4A-C3A	3.21	132.21	125.48
7	C	602	HEB	C4A-NA-C1A	3.17	108.45	105.35
7	C	603	HEB	CHD-C1D-C2D	3.14	135.46	126.73
8	C	604	HDD	CAD-CBD-CGD	-3.12	99.74	104.56
8	C	604	HDD	CHB-C1B-C2B	-3.11	118.09	126.73
7	C	602	HEB	CHB-C4A-NA	3.04	127.73	124.44
8	C	604	HDD	C2C-C1C-NC	3.04	115.29	109.69
7	C	602	HEB	CAD-C3D-C4D	3.03	129.96	124.66
7	C	602	HEB	CHC-C4B-NB	3.03	128.10	124.37
7	C	602	HEB	CHD-C4C-NC	3.01	129.39	123.85
7	C	602	HEB	C4A-C3A-C2A	2.99	111.31	106.94
8	C	604	HDD	C4D-ND-C1D	2.97	108.25	105.16
5	B	402	DK8	C50-C48-C49	2.96	121.14	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	602	HEB	CMD-C2D-C3D	-2.96	118.09	126.12
7	C	603	HEB	CAA-C2A-C1A	-2.93	119.37	124.89
5	B	402	DK8	C16-C17-C18	-2.89	120.70	127.66
7	C	603	HEB	CHB-C1B-NB	2.89	127.55	124.42
7	C	603	HEB	CMD-C2D-C3D	-2.87	118.32	126.12
8	C	604	HDD	C4B-C3B-C2B	-2.85	104.85	107.11
7	C	603	HEB	CAB-C3B-C4B	-2.85	121.11	124.81
8	C	604	HDD	CMC-C2C-C1C	2.83	129.71	124.71
7	C	602	HEB	CHD-C1D-C2D	2.81	134.52	126.73
7	C	602	HEB	CHD-C1D-ND	2.79	127.81	124.37
7	C	603	HEB	C4A-NA-C1A	2.79	108.08	105.35
7	C	603	HEB	CHD-C1D-ND	2.75	127.76	124.37
7	C	603	HEB	CHC-C1C-NC	2.74	128.88	123.85
8	C	604	HDD	C2D-C1D-CHD	-2.73	119.01	123.33
7	C	603	HEB	C4B-C3B-C2B	2.69	110.81	106.90
5	B	402	DK8	C19-C18-C20	2.66	119.74	115.27
5	B	402	DK8	C34-C33-C35	2.65	119.73	115.27
8	C	604	HDD	C4C-C3C-C2C	-2.64	104.58	106.75
7	C	602	HEB	CBA-CAA-C2A	-2.61	105.36	112.63
8	C	604	HDD	O1D-C3D-CAD	2.60	107.90	103.01
5	B	402	DK8	C29-C28-C30	2.57	119.59	115.27
6	C	601	POV	O31-C31-C32	2.54	119.87	111.91
5	B	402	DK8	C14-C13-C15	2.49	119.47	115.27
7	C	603	HEB	CHB-C4A-NA	2.48	127.12	124.44
7	C	602	HEB	CMA-C3A-C4A	-2.42	120.44	124.71
5	B	402	DK8	C46-C47-C48	-2.41	119.51	127.75
5	B	402	DK8	C36-C37-C38	-2.38	121.94	127.66
5	B	402	DK8	C39-C38-C40	2.34	119.20	115.27
8	C	604	HDD	CHC-C4B-NB	-2.33	121.89	124.42
5	B	402	DK8	C45-C43-C44	2.25	119.05	115.27
4	B	401	CDN	C12-C11-CA5	-2.20	108.29	113.38
4	B	401	CDN	C72-C71-CB7	-2.19	108.32	113.38
5	B	402	DK8	C24-C23-C25	2.18	118.94	115.27
7	C	602	HEB	C4D-C3D-C2D	-2.16	103.76	106.90
7	C	603	HEB	CBD-CAD-C3D	-2.15	106.66	112.63
5	B	402	DK8	C5-C4-C3	2.11	119.48	116.62
7	C	602	HEB	CBB-CAB-C3B	-2.09	106.67	112.43
7	C	603	HEB	CAD-CBD-CGD	-2.06	109.18	113.60
8	C	604	HDD	CAA-CBA-CGA	-2.04	109.22	113.60
7	C	602	HEB	CHA-C4D-ND	2.01	126.60	124.42

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	C	602	HEB	NA
7	C	603	HEB	NA
8	C	604	HDD	NC

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	401	CDN	CB2-OB2-PB2-OB5
4	B	401	CDN	CB2-OB2-PB2-OB3
4	B	401	CDN	CB2-OB2-PB2-OB4
4	B	401	CDN	C71-CB7-OB8-CB6
4	B	401	CDN	C72-C71-CB7-OB9
4	B	401	CDN	CA3-OA5-PA1-OA2
4	B	401	CDN	C31-CA7-OA8-CA6
4	B	401	CDN	OA7-CA5-OA6-CA4
5	B	402	DK8	C18-C20-C21-C22
5	B	402	DK8	C23-C25-C26-C27
6	C	601	POV	C11-O12-P-O13
6	C	601	POV	C22-C21-O21-C2
8	C	604	HDD	C2B-C3B-CAB-CBB
8	C	604	HDD	C4B-C3B-CAB-CBB
6	C	601	POV	C32-C31-O31-C3
6	C	601	POV	O22-C21-O21-C2
6	C	601	POV	O32-C31-O31-C3
5	B	402	DK8	C28-C30-C31-C32
4	B	401	CDN	OB6-CB4-CB6-OB8
6	C	601	POV	C31-C32-C33-C34
6	C	601	POV	C11-O12-P-O11
6	C	601	POV	C24-C25-C26-C27
6	C	601	POV	C23-C24-C25-C26
5	B	402	DK8	C45-C43-C44-C46
6	C	601	POV	C214-C215-C216-C217
6	C	601	POV	C33-C34-C35-C36
4	B	401	CDN	C51-C52-C53-C54
4	B	401	CDN	C34-C35-C36-C37
5	B	402	DK8	C32-C33-C35-C36
5	B	402	DK8	C42-C43-C44-C46
4	B	401	CDN	C57-C58-C59-C60
4	B	401	CDN	C58-C59-C60-C61
6	C	601	POV	C35-C36-C37-C38
5	B	402	DK8	C24-C23-C25-C26
5	B	402	DK8	C34-C33-C35-C36
6	C	601	POV	C310-C311-C312-C313

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Mol	Chain	Res	Type	Atoms
6	C	601	POV	C34-C35-C36-C37
4	B	401	CDN	CB3-CB4-CB6-OB8
4	B	401	CDN	C59-C60-C61-C62
4	B	401	CDN	C52-C51-CB5-OB6
7	C	603	HEB	C4C-C3C-CAC-CBC
4	B	401	CDN	C54-C55-C56-C57
4	B	401	CDN	CB3-CB4-OB6-CB5
4	B	401	CDN	CB6-CB4-OB6-CB5
4	B	401	CDN	C14-C15-C16-C17
7	C	603	HEB	C2C-C3C-CAC-CBC
4	B	401	CDN	C15-C16-C17-C18
4	B	401	CDN	C32-C33-C34-C35
7	C	603	HEB	C2B-C3B-CAB-CBB
4	B	401	CDN	C60-C61-C62-C63
4	B	401	CDN	CA5-C11-C12-C13
6	C	601	POV	C313-C314-C315-C316
4	B	401	CDN	CB3-OB5-PB2-OB2
4	B	401	CDN	CA3-OA5-PA1-OA3
4	B	401	CDN	CA2-OA2-PA1-OA3
6	C	601	POV	C36-C37-C38-C39
7	C	603	HEB	C4B-C3B-CAB-CBB
4	B	401	CDN	OA5-CA3-CA4-OA6
6	C	601	POV	C11-C12-N-C14
4	B	401	CDN	C72-C71-CB7-OB8
4	B	401	CDN	OA5-CA3-CA4-CA6
5	B	402	DK8	C22-C23-C25-C26
7	C	602	HEB	C2B-C3B-CAB-CBB
7	C	602	HEB	CAA-CBA-CGA-O1A
7	C	603	HEB	CAD-CBD-CGD-O1D
4	B	401	CDN	CA7-C31-C32-C33
7	C	602	HEB	CAD-CBD-CGD-O1D
6	C	601	POV	C11-C12-N-C13
7	C	603	HEB	CAD-CBD-CGD-O2D
7	C	602	HEB	CAA-CBA-CGA-O2A
4	B	401	CDN	CA4-CA3-OA5-PA1
6	C	601	POV	O21-C2-C3-O31
7	C	602	HEB	C4B-C3B-CAB-CBB
6	C	601	POV	C11-C12-N-C15
7	C	602	HEB	CAD-CBD-CGD-O2D
4	B	401	CDN	C32-C31-CA7-OA9
7	C	602	HEB	C2C-C3C-CAC-CBC
5	B	402	DK8	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
4	B	401	CDN	C36-C37-C38-C39
4	B	401	CDN	CA2-OA2-PA1-OA5
7	C	603	HEB	CAA-CBA-CGA-O2A
7	C	603	HEB	CAA-CBA-CGA-O1A
6	C	601	POV	O31-C31-C32-C33
6	C	601	POV	O32-C31-C32-C33

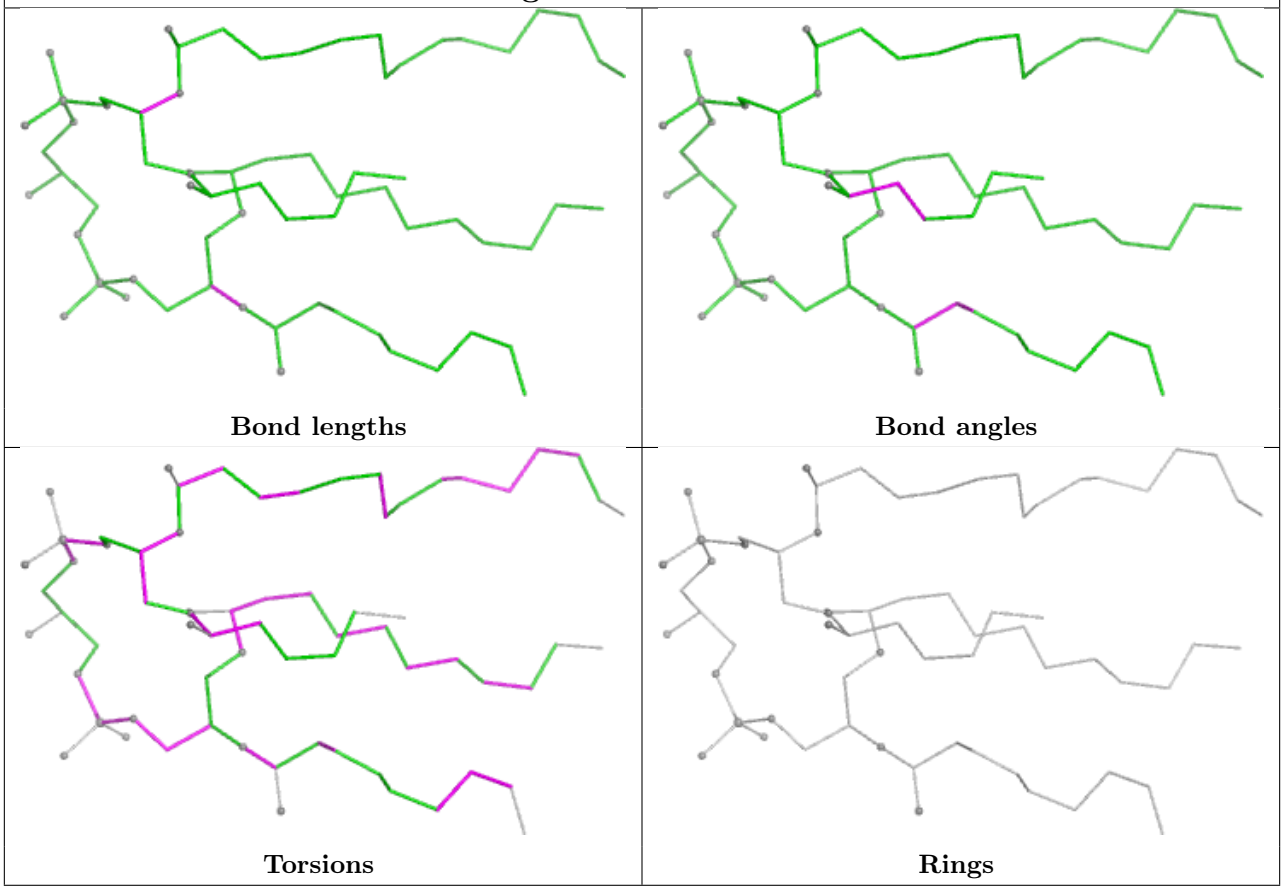
There are no ring outliers.

6 monomers are involved in 35 short contacts:

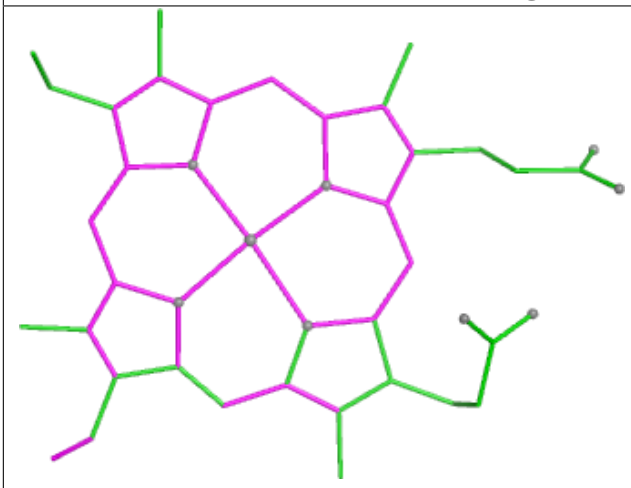
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	CDN	3	0
7	C	603	HEB	6	0
9	C	605	OXY	1	0
7	C	602	HEB	15	0
6	C	601	POV	3	0
8	C	604	HDD	7	0

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 then 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.

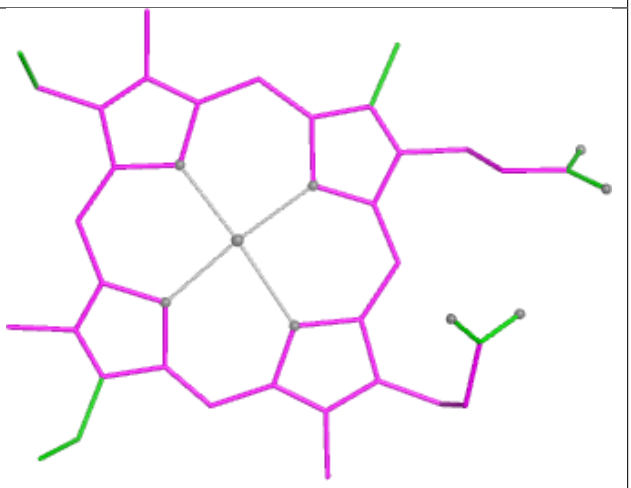
Ligand CDN B 401



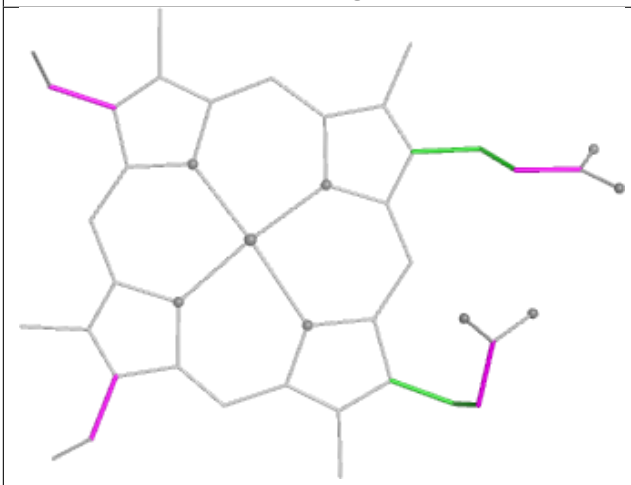
Ligand HEB C 603



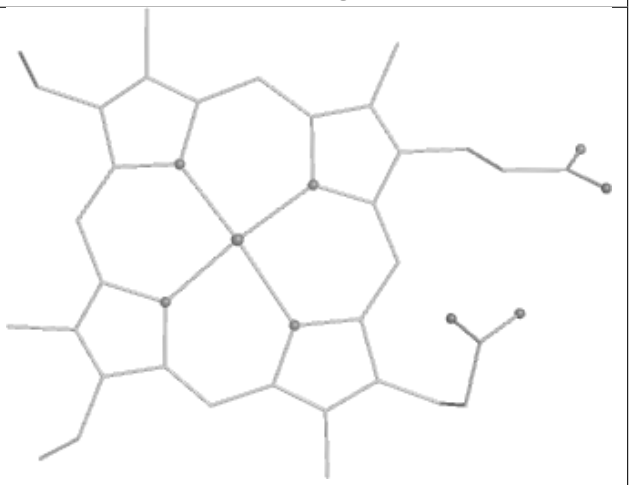
Bond lengths



Bond angles



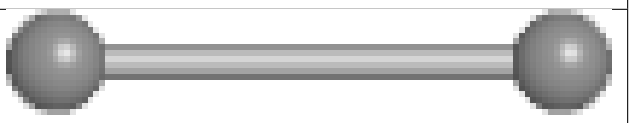
Torsions



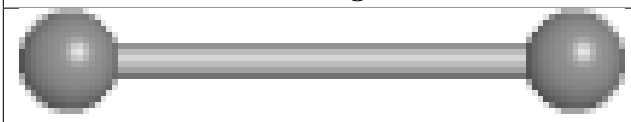
Rings

Ligand OXY C 605

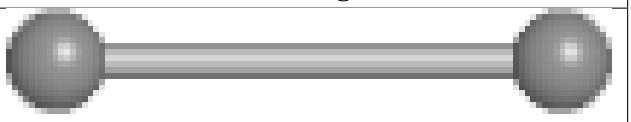
Bond lengths



Bond angles

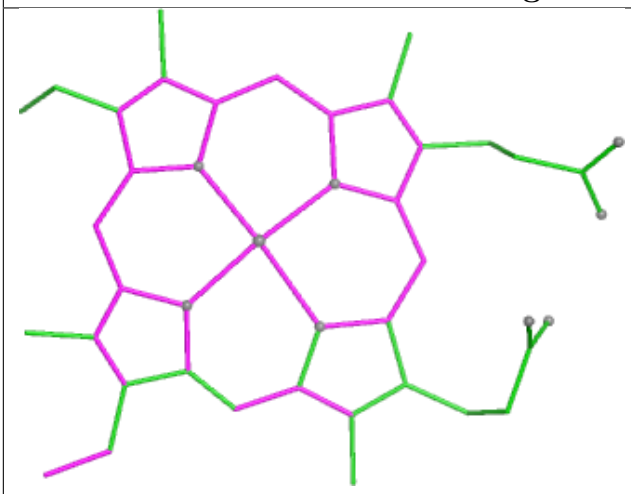


Torsions

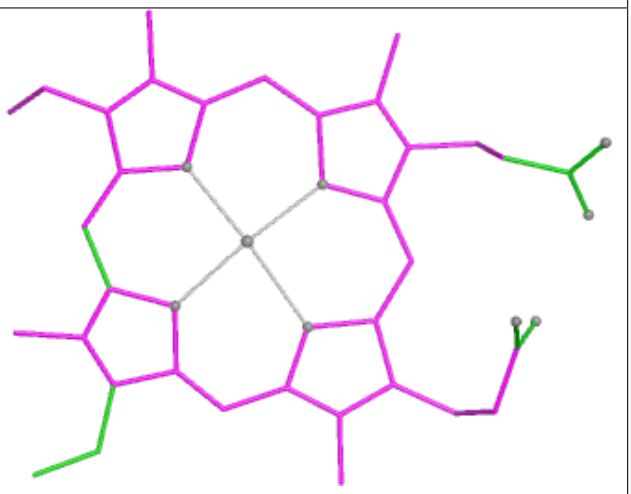


Rings

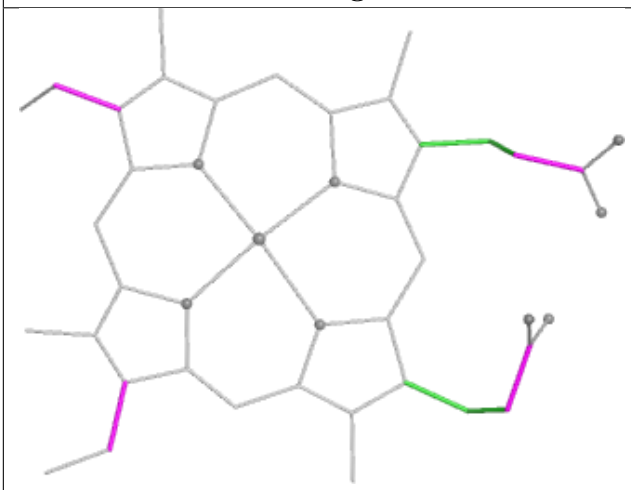
Ligand HEB C 602



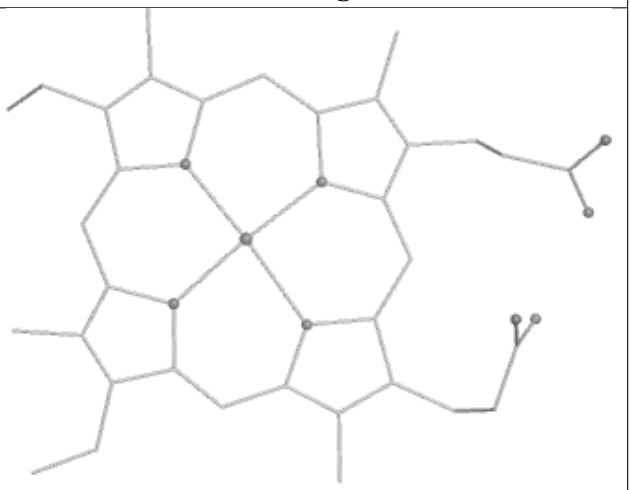
Bond lengths



Bond angles

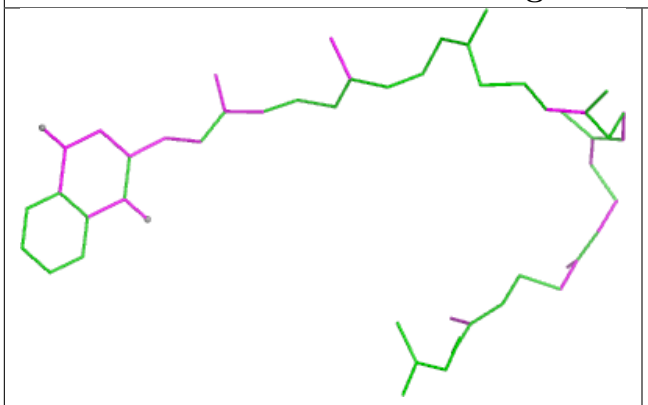


Torsions

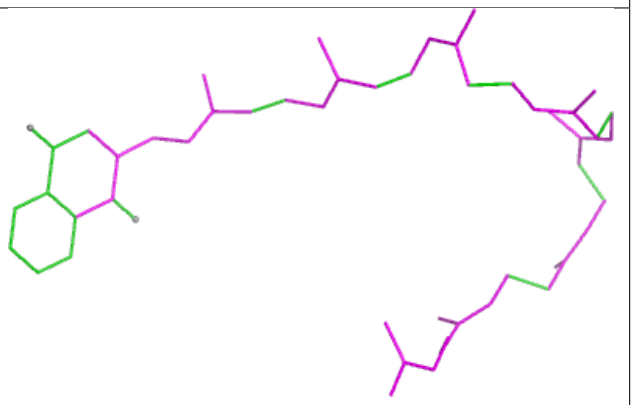


Rings

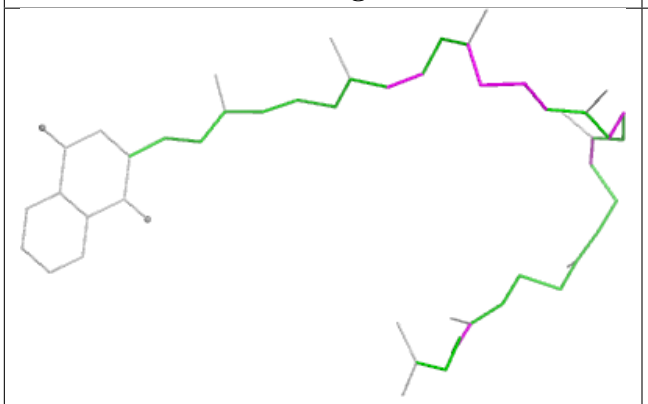
Ligand DK8 B 402



Bond lengths



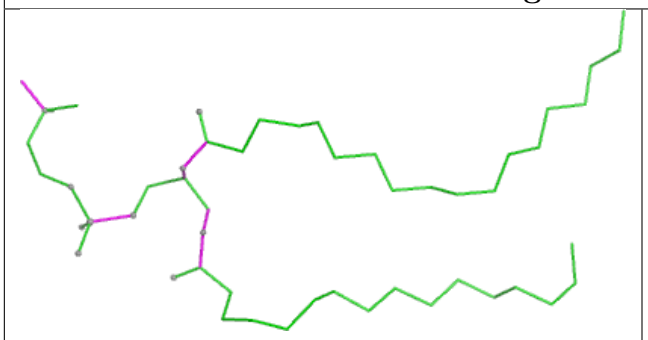
Bond angles



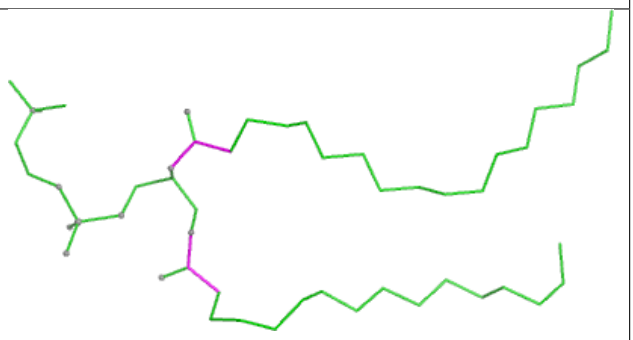
Torsions

Rings

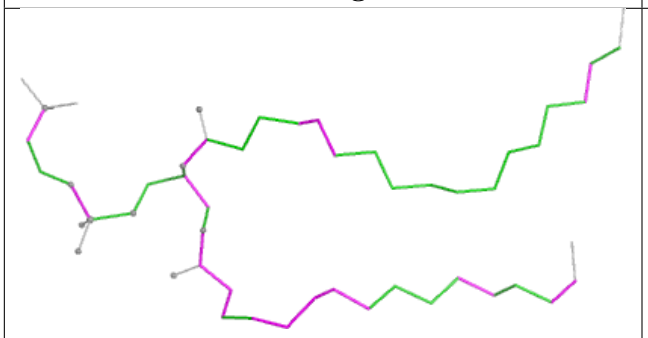
Ligand POV C 601



Bond lengths

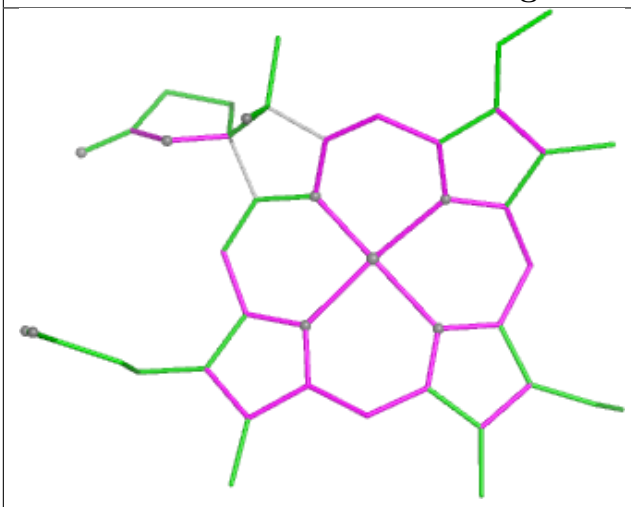
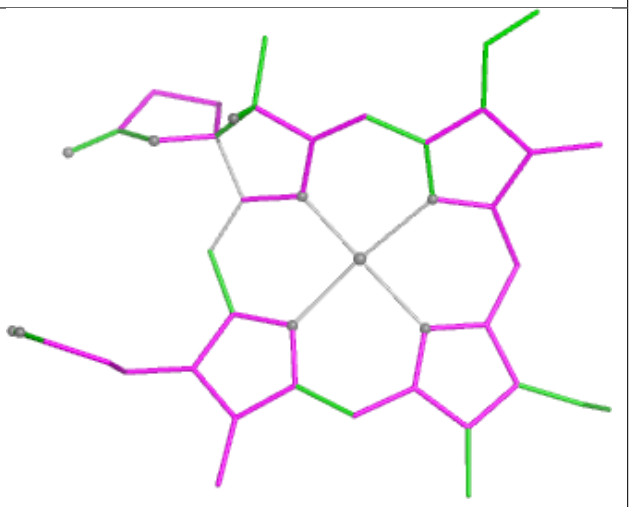
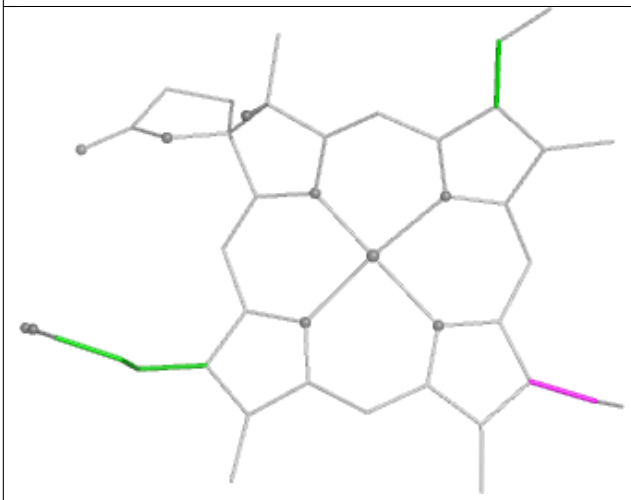
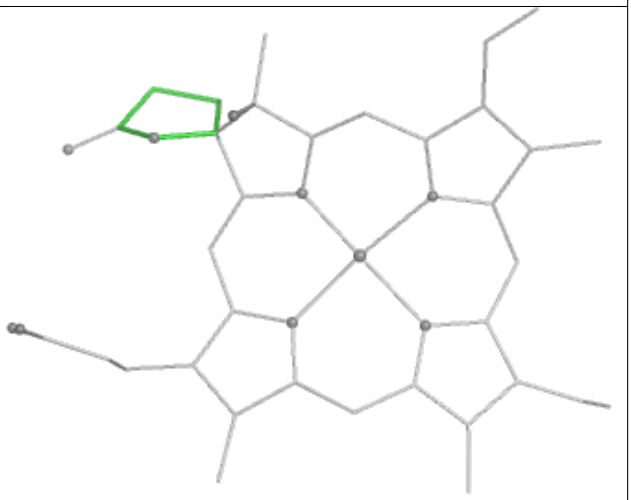


Bond angles



Torsions

Rings

Ligand HDD C 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

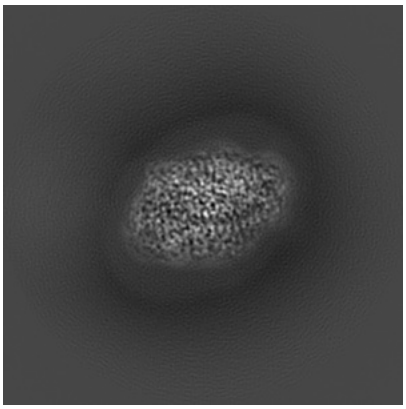
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13108. These allow visual inspection of the internal detail of the map and identification of artifacts.

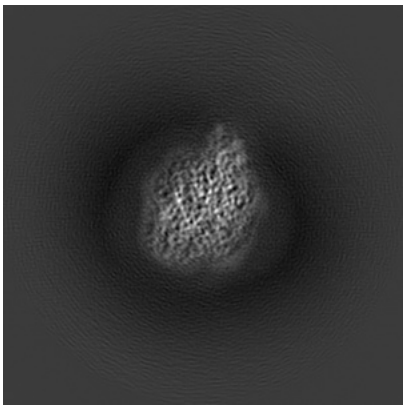
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

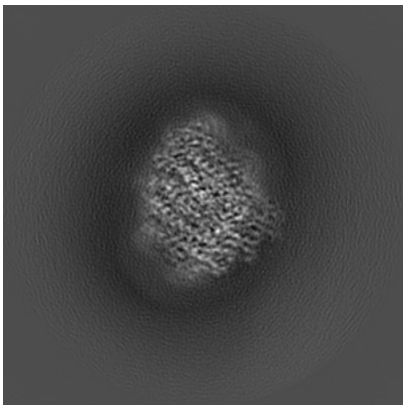
6.1.1 Primary map



X

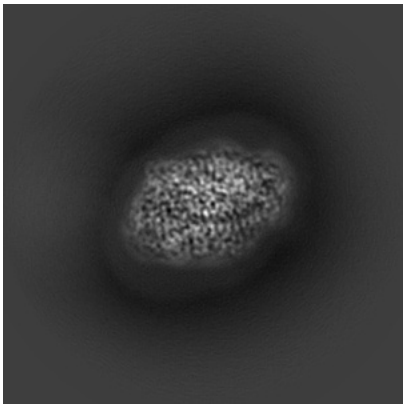


Y

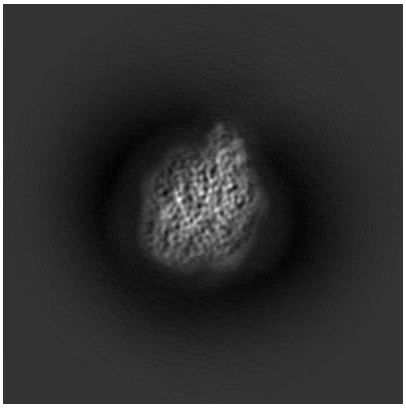


Z

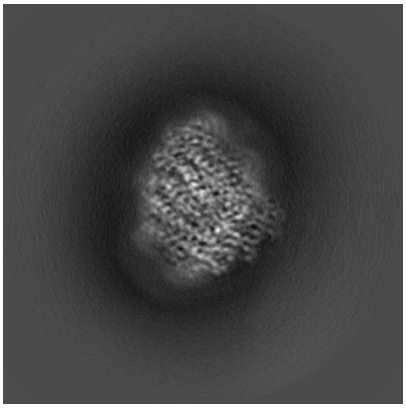
6.1.2 Raw map



X



Y

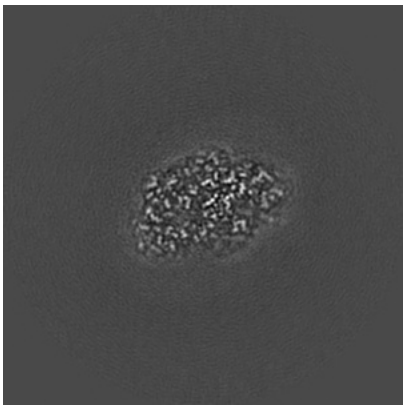


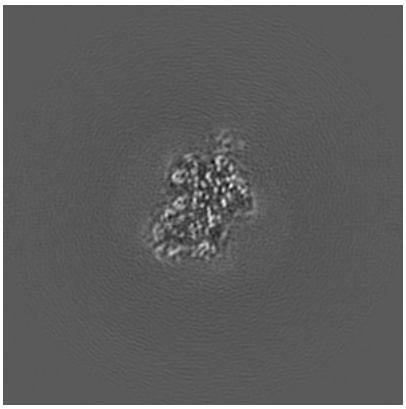
Z

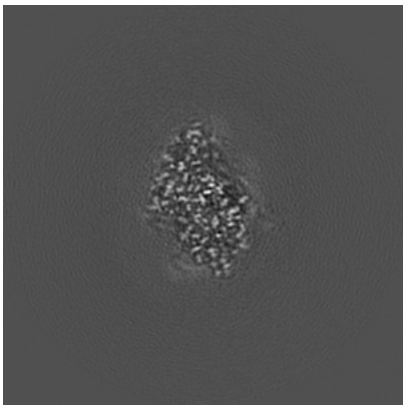
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

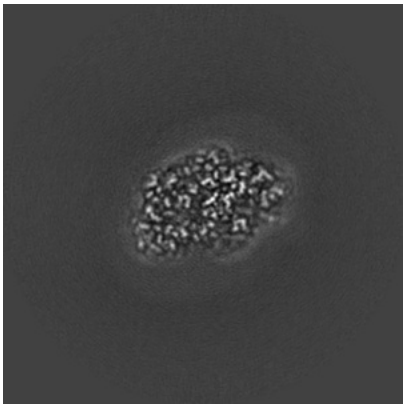
6.2.1 Primary map

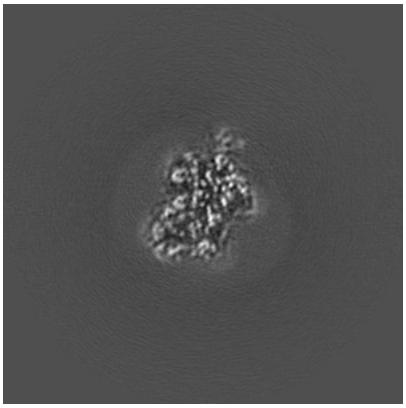

X Index: 128

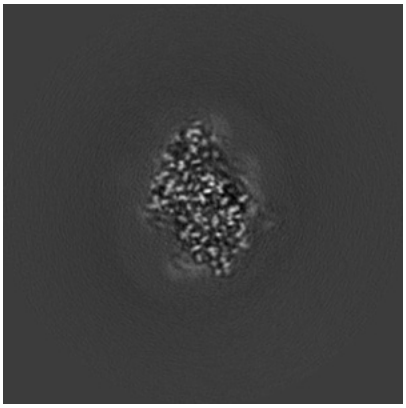

Y Index: 128


Z Index: 128

6.2.2 Raw map


X Index: 128

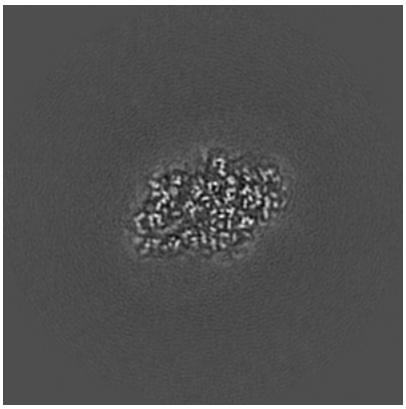

Y Index: 128

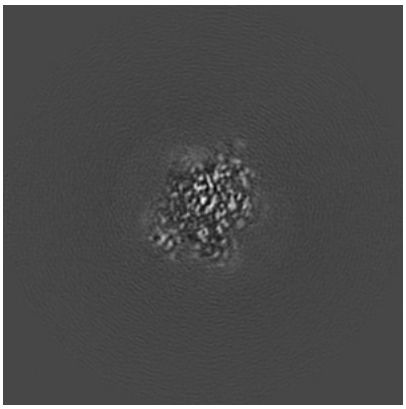

Z Index: 128

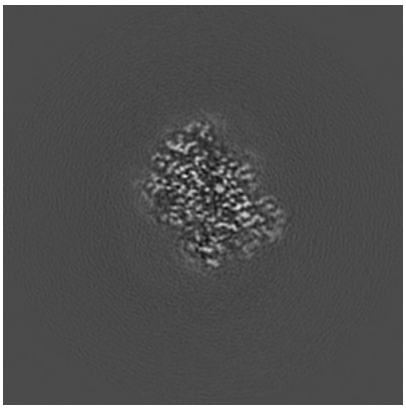
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

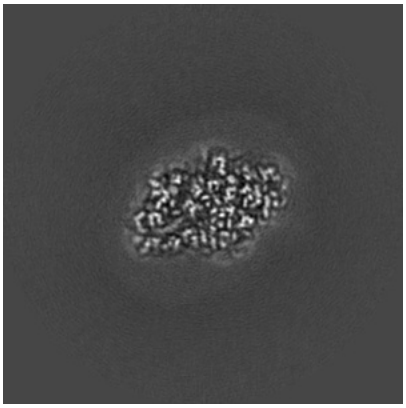
6.3.1 Primary map

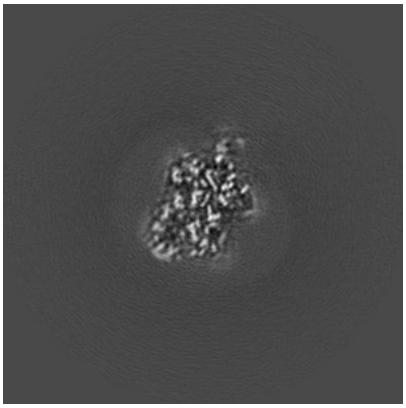

X Index: 123

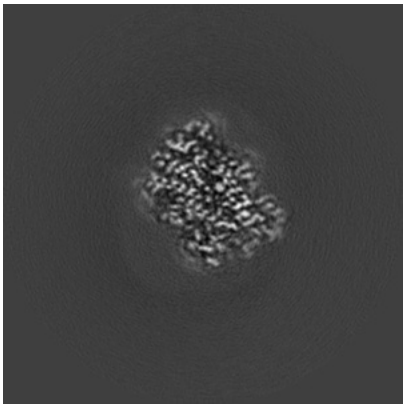

Y Index: 136


Z Index: 137

6.3.2 Raw map


X Index: 123

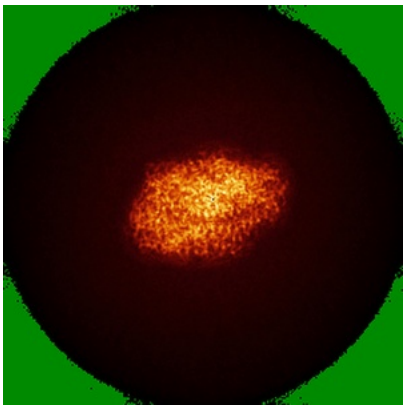

Y Index: 129

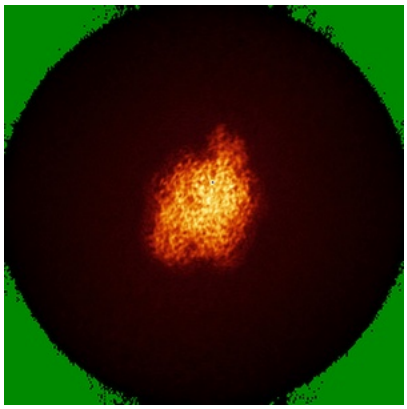

Z Index: 137

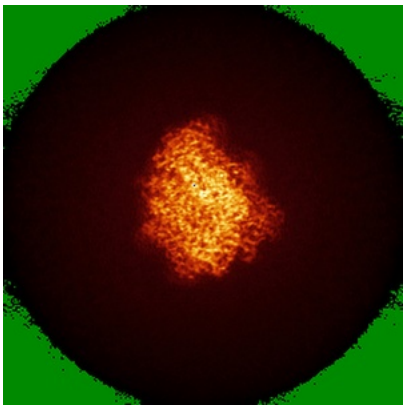
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

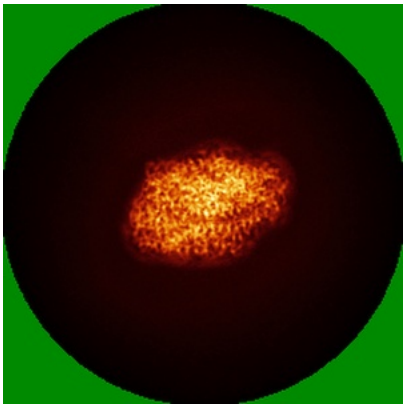
6.4.1 Primary map

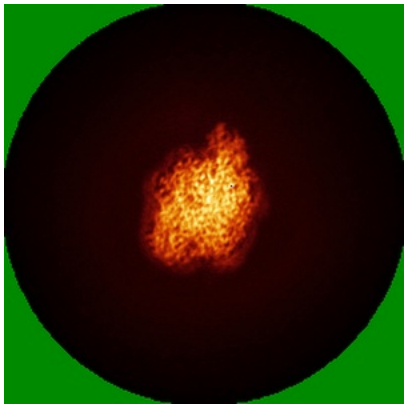

X

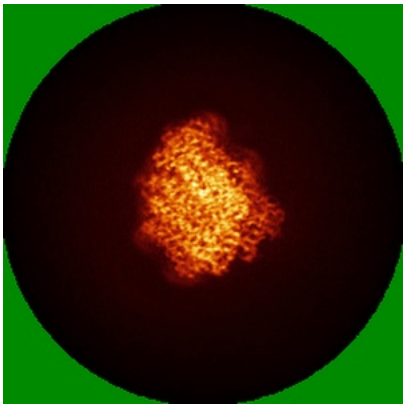

Y


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.

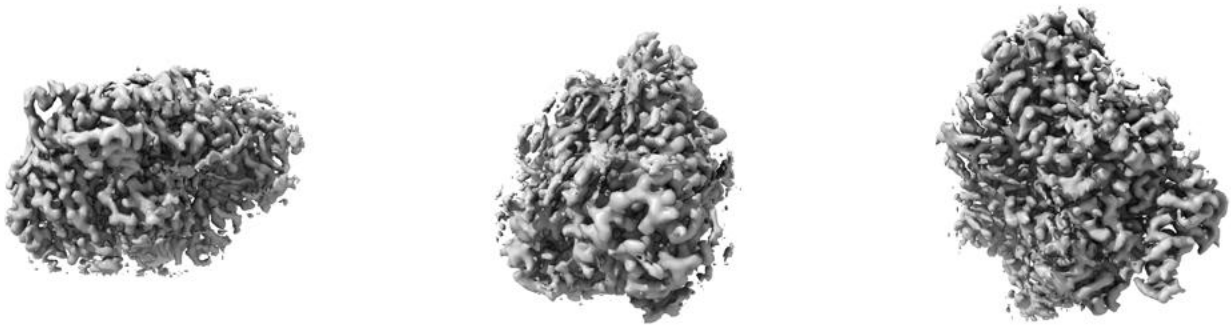
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. 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



X Y Z

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.

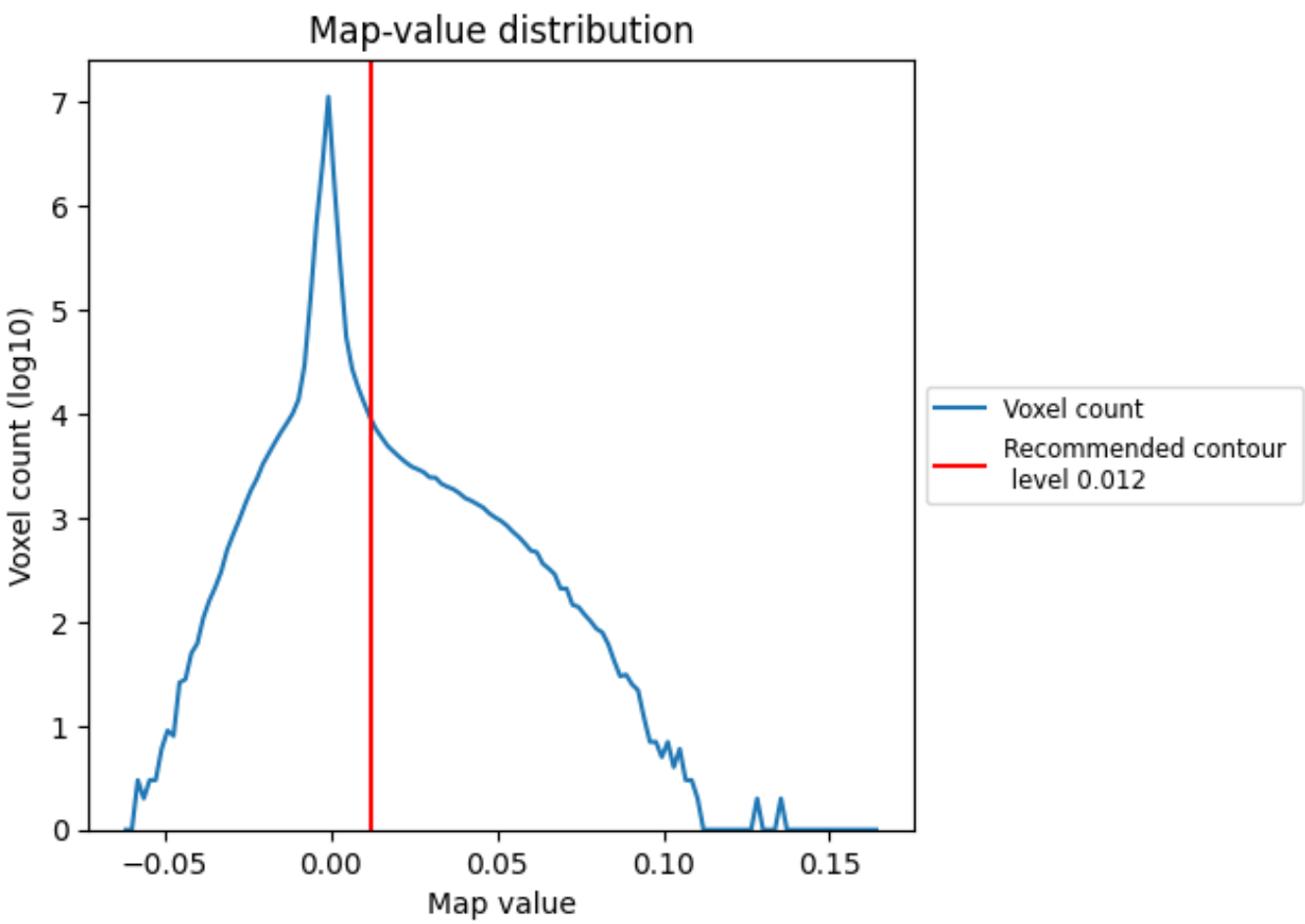
6.6 Mask visualisation (i)

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

7 Map analysis (i)

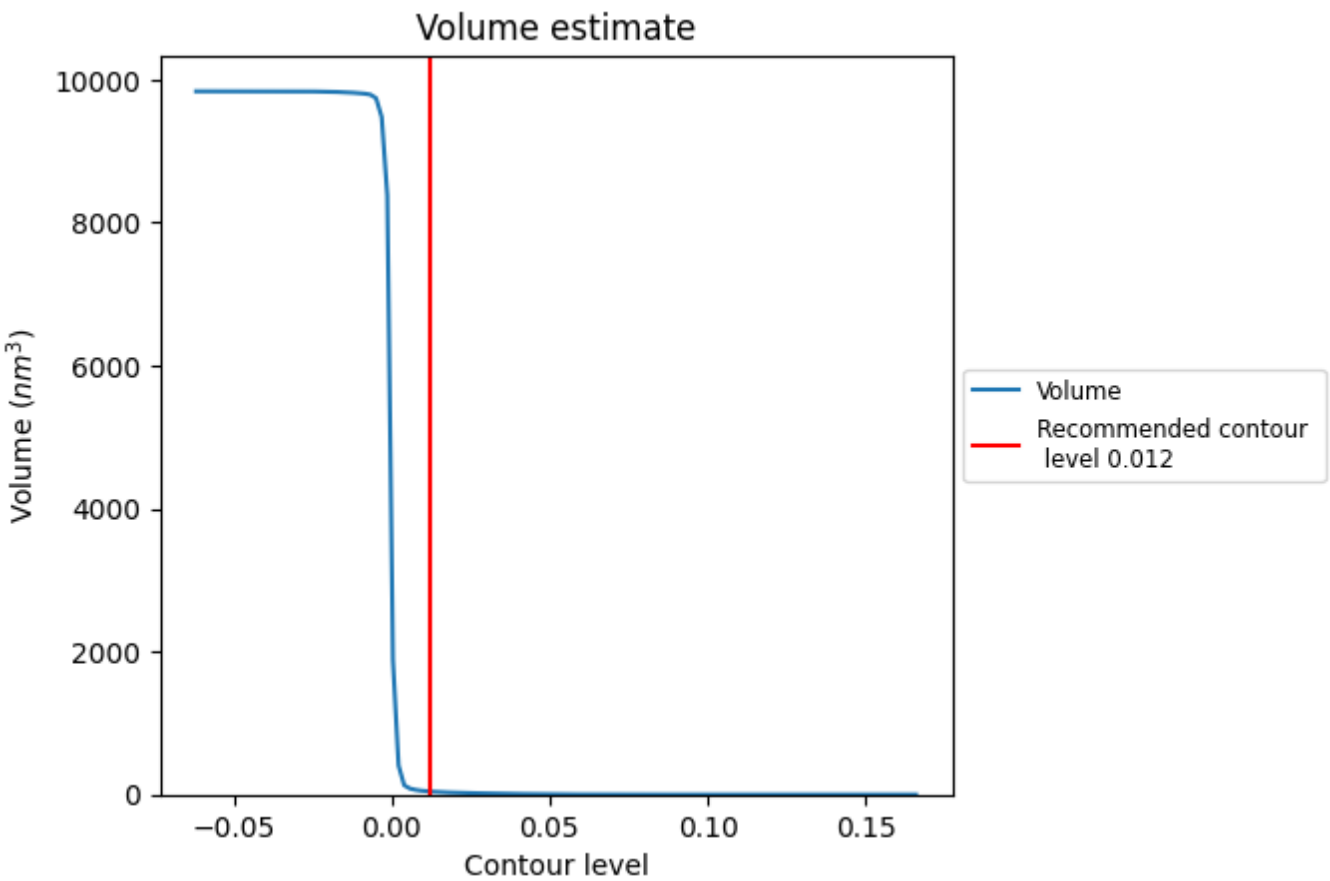
This section contains the results of statistical analysis of the map.

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.

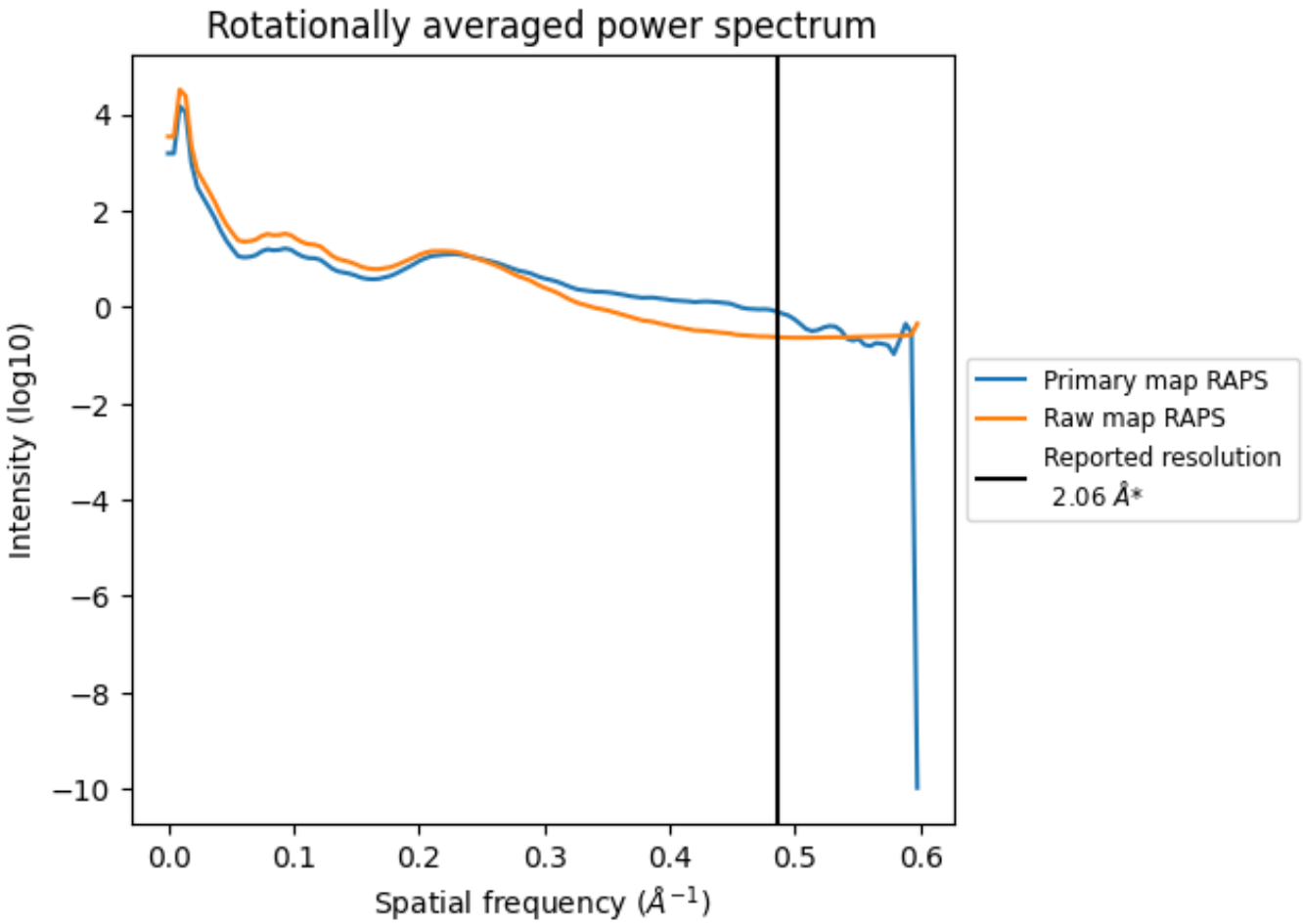
7.2 Volume estimate (i)



The volume at the recommended contour level is 43 nm^3; this corresponds to an approximate mass of 39 kDa.

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

7.3 Rotationally averaged power spectrum (i)

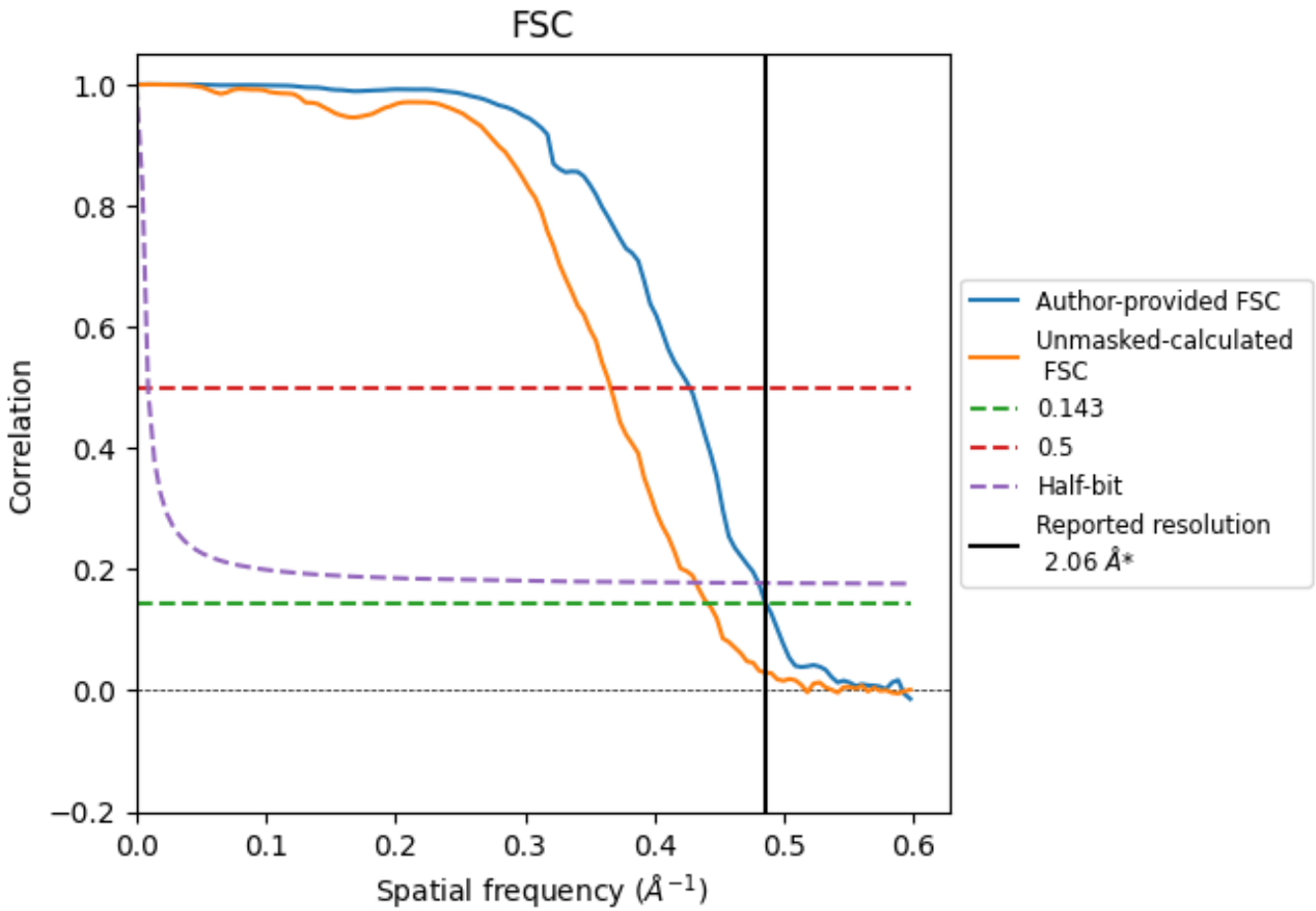


*Reported resolution corresponds to spatial frequency of 0.485 Å^{-1}

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 0.485 Å^{-1}

8.2 Resolution estimates (i)

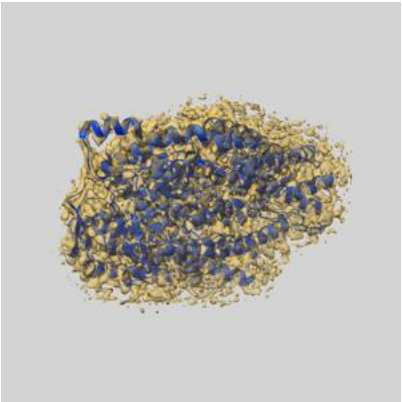
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.06	-	-
Author-provided FSC curve	2.06	2.34	2.08
Unmasked-calculated*	2.27	2.73	2.32

*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 2.27 differs from the reported value 2.06 by more than 10 %

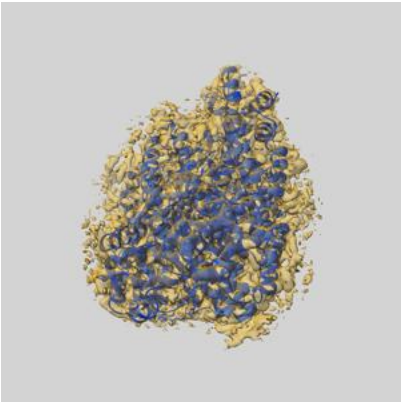
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13108 and PDB model 7OY2. Per-residue inclusion information can be found in section 3 on page 9.

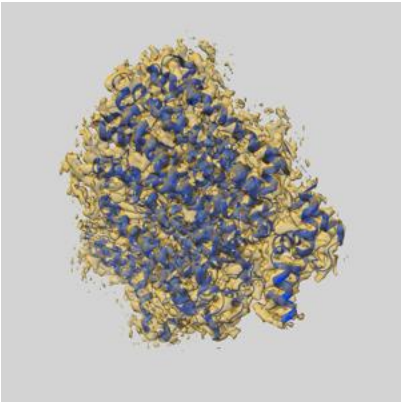
9.1 Map-model overlay (i)



X



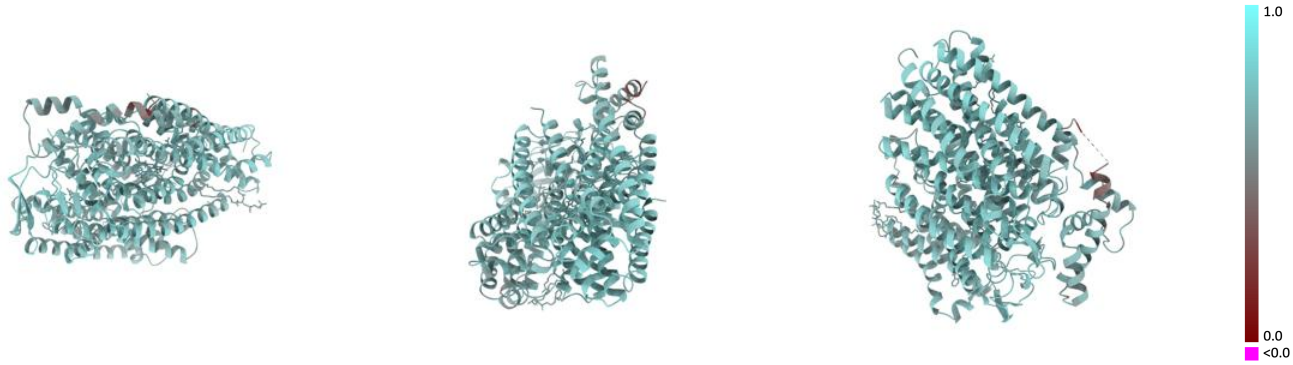
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 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.

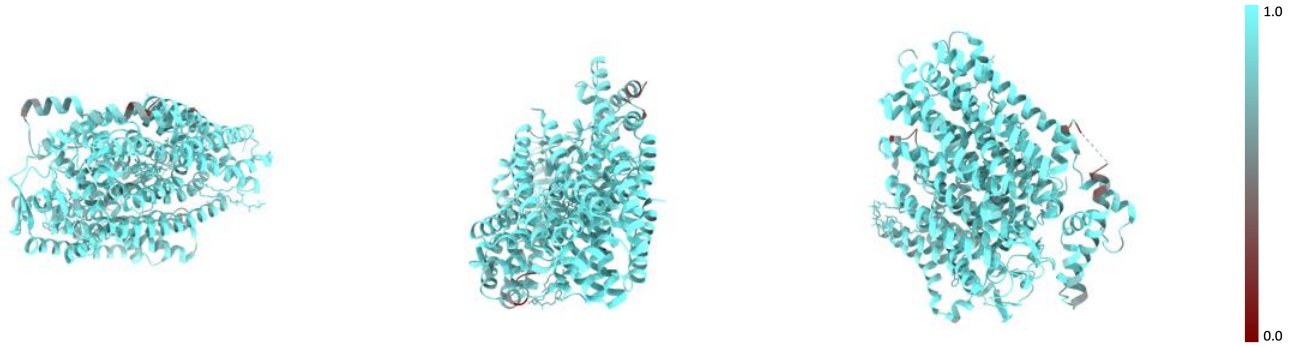
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

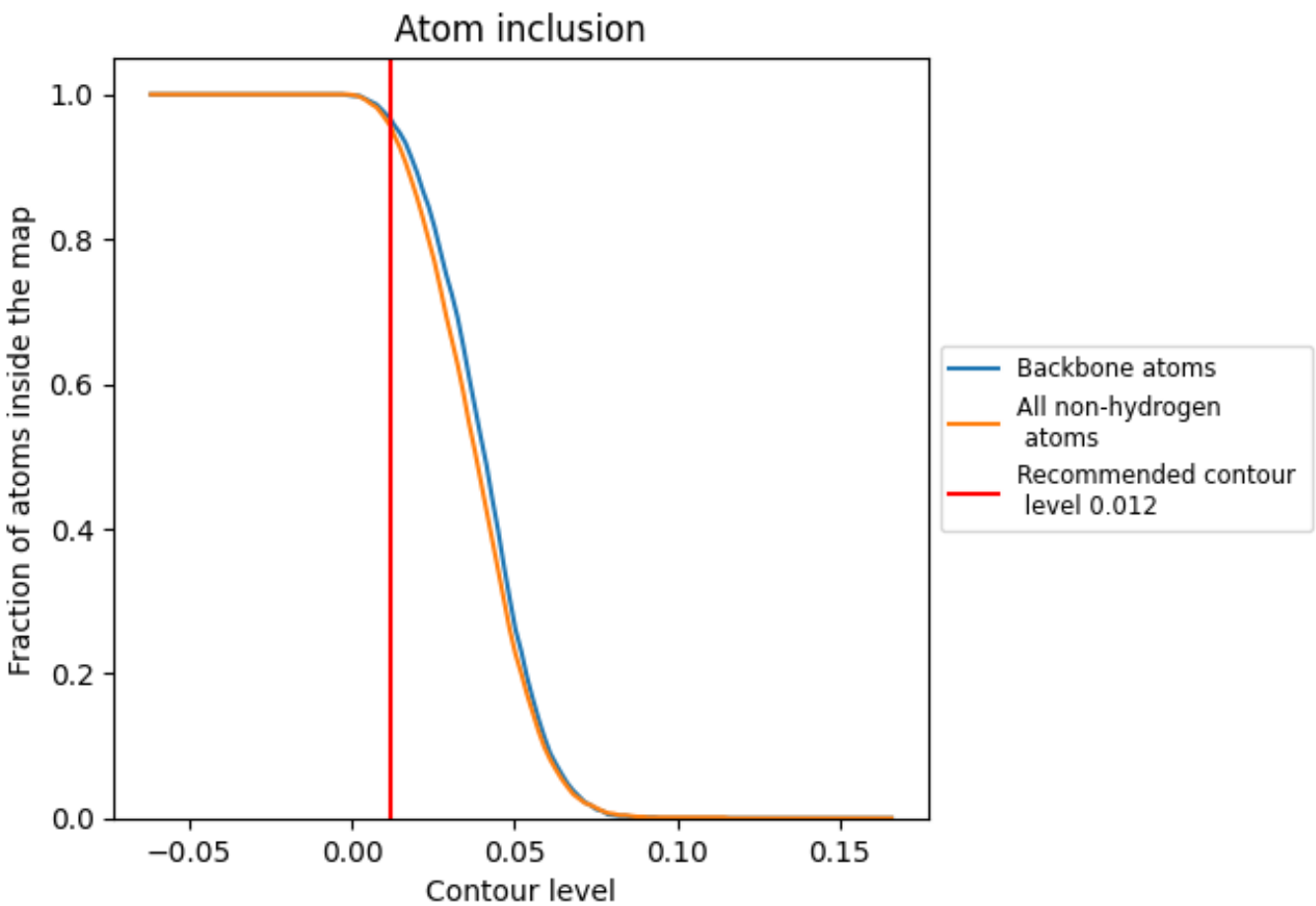
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9550	0.7000
B	0.9600	0.7030
C	0.9560	0.6990
X	0.9740	0.6960