



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:37 PM UTC

PDB ID : 7YIU / pdb_00007yiu
EMDB ID : EMD-33864
Title : Cryo-EM structure of the C6-ceramide-bound SPT-ORMDL3 complex
Authors : Xie, T.; Liu, P.; Gong, X.
Deposited on : 2022-07-18
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

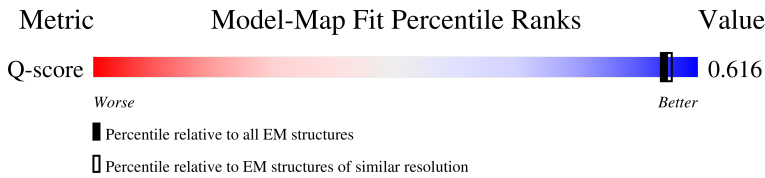
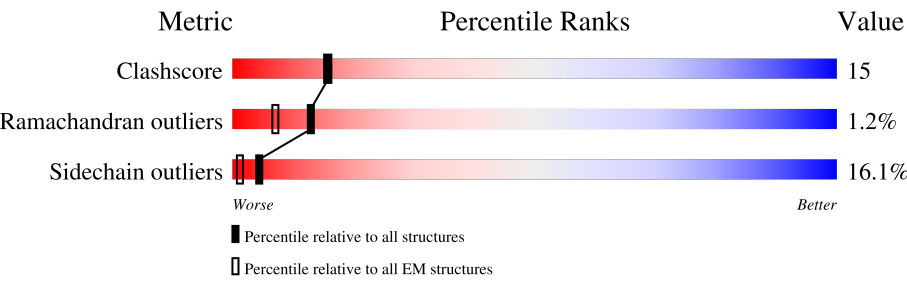
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	562	12% 61% 23% 5% 11%
2	E	50	46% 20% 20% 14%
3	D	153	71% 23% 6%
4	C	92	33% 17% 48%

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Mol	Chain	Length	Quality of chain
5	A	423	 A horizontal bar chart showing the quality of chain 5. The bar is divided into three segments: green (69%), yellow (25%), and orange (7%). The segments are labeled with their respective percentages: 69%, 25%, and 7%.

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
8	R16	D	803	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9285 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 Serine palmitoyltransferase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	499	Total	C	N	O	S	0	0
			3940	2515	682	719	24		

- Molecule 2 is a protein called Serine palmitoyltransferase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	43	Total	C	N	O	S	0	0
			341	233	52	55	1		

- Molecule 3 is a protein called ORM1-like protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	153	Total	C	N	O	S	0	0
			1236	818	204	208	6		

- Molecule 4 is a protein called Serine palmitoyltransferase small subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	48	Total	C	N	O	S	0	0
			411	281	58	67	5		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	MET	-	initiating methionine	UNP Q969W0
C	-19	ALA	-	expression tag	UNP Q969W0
C	-18	ASP	-	expression tag	UNP Q969W0
C	-17	TYR	-	expression tag	UNP Q969W0
C	-16	LYS	-	expression tag	UNP Q969W0
C	-15	ASP	-	expression tag	UNP Q969W0
C	-14	ASP	-	expression tag	UNP Q969W0
C	-13	ASP	-	expression tag	UNP Q969W0
C	-12	ASP	-	expression tag	UNP Q969W0

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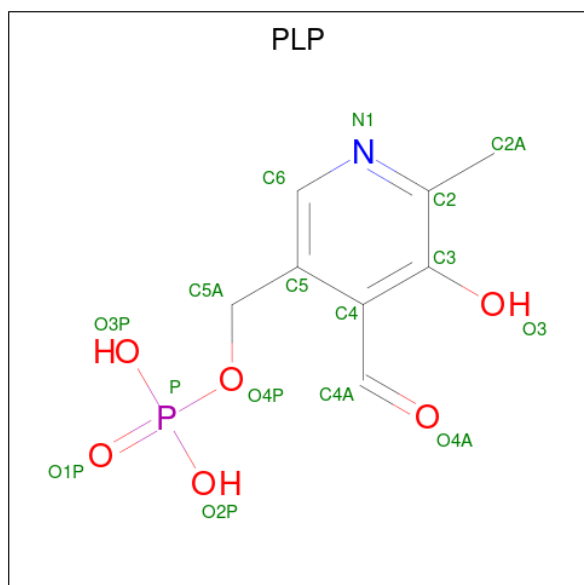
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	LYS	-	expression tag	UNP Q969W0
C	-10	SER	-	expression tag	UNP Q969W0
C	-9	GLY	-	expression tag	UNP Q969W0
C	-8	PRO	-	expression tag	UNP Q969W0
C	-7	ASP	-	expression tag	UNP Q969W0
C	-6	GLU	-	expression tag	UNP Q969W0
C	-5	VAL	-	expression tag	UNP Q969W0
C	-4	ASP	-	expression tag	UNP Q969W0
C	-3	ALA	-	expression tag	UNP Q969W0
C	-2	SER	-	expression tag	UNP Q969W0
C	-1	GLY	-	expression tag	UNP Q969W0
C	0	ARG	-	expression tag	UNP Q969W0

- Molecule 5 is a protein called Serine palmitoyltransferase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	423	Total	C	N	O	S	0	0
			3285	2086	563	620	16		

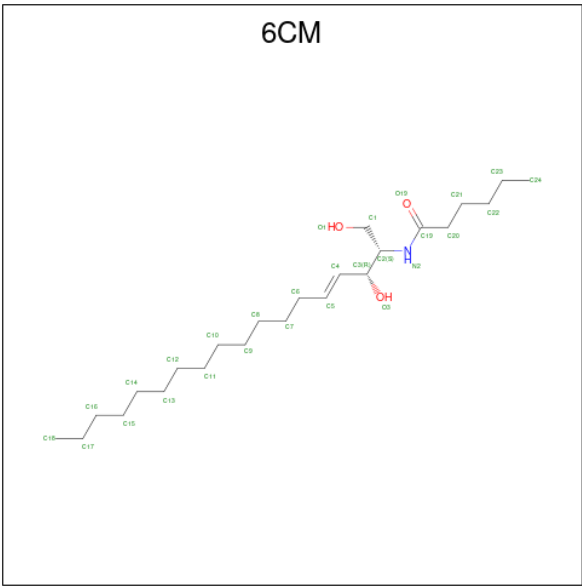
- Molecule 6 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	P	0
			15	8	1	5	1	

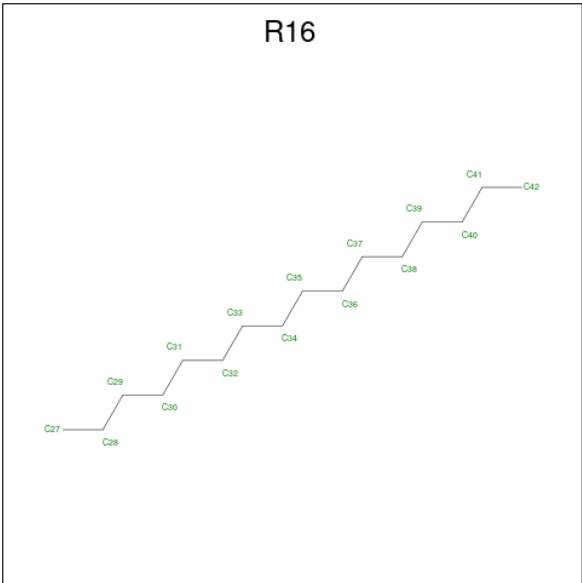
- Molecule 7 is N-((E,2S,3R)-1,3-DIHYDROXYOCTADEC-4-EN-2-YL)HEXANAMIDE

(CCD ID: 6CM) (formula: C₂₄H₄₇NO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
7	D	1	Total	C	N	O	0
			28	24	1	3	

- Molecule 8 is HEXADECANE (CCD ID: R16) (formula: C₁₆H₃₄).

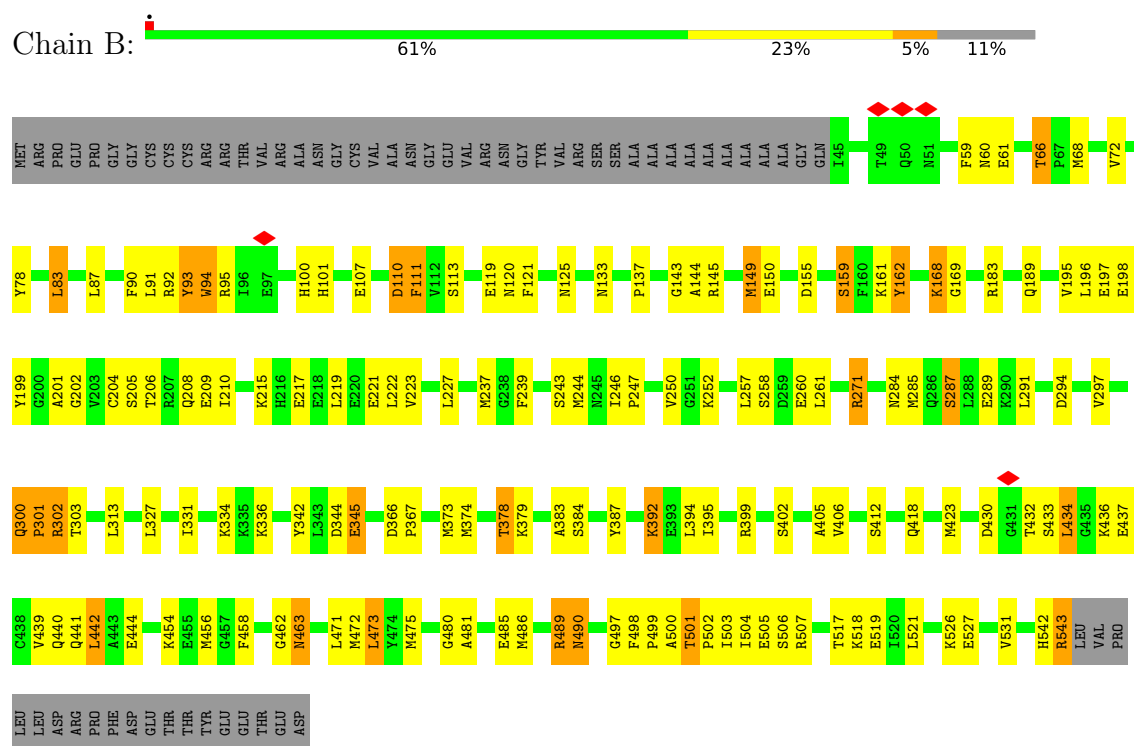


Mol	Chain	Residues	Atoms		AltConf
8	D	1	Total	C	0
			16	16	
8	D	1	Total	C	0
			13	13	

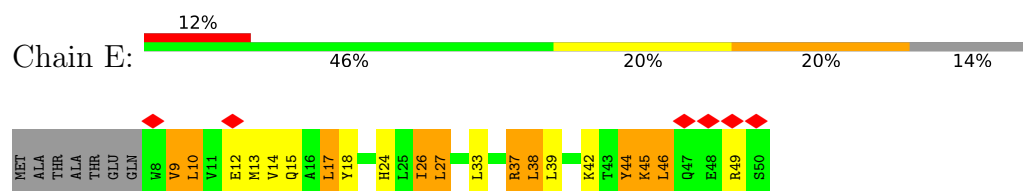
3 Residue-property plots

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: Serine palmitoyltransferase 2

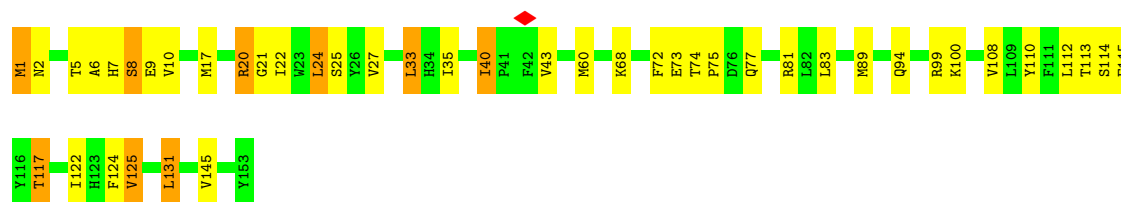


• Molecule 2: Serine palmitoyltransferase 1

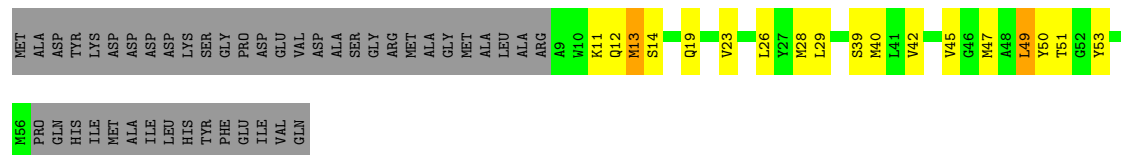
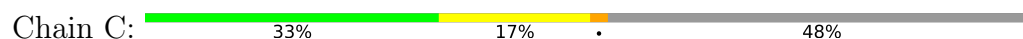


• Molecule 3: ORM1-like protein 3

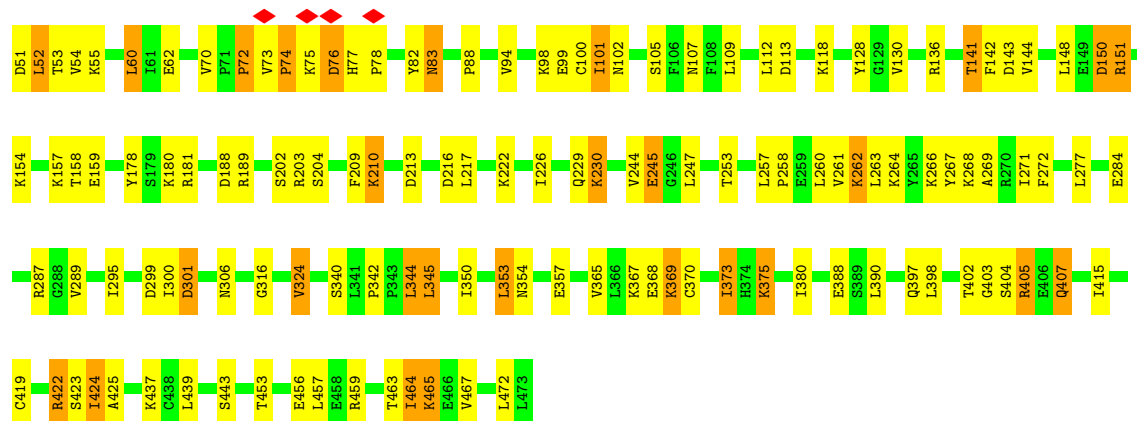




• Molecule 4: Serine palmitoyltransferase small subunit A



• Molecule 5: Serine palmitoyltransferase 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	337730	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.214	Depositor
Minimum map value	-0.124	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.028	Depositor
Map size ($\text{\AA}$)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	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: 6CM, R16, PLP

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	0.41	0/4024	0.74	7/5432 (0.1%)
2	E	0.38	0/348	0.76	0/474
3	D	0.41	0/1272	0.71	0/1736
4	C	0.37	0/426	0.74	0/580
5	A	0.36	0/3345	0.68	3/4521 (0.1%)
All	All	0.39	0/9415	0.72	10/12743 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	LYS	N-CA-C	7.10	119.69	111.02
1	B	497	GLY	N-CA-C	6.31	121.63	112.60
5	A	78	PRO	N-CA-CB	6.24	110.19	103.33
1	B	300	GLN	CA-C-N	6.10	127.47	119.84
1	B	300	GLN	C-N-CA	6.10	127.47	119.84
1	B	456	MET	N-CA-C	-6.01	106.08	113.41
1	B	462	GLY	N-CA-C	5.46	122.82	112.62
5	A	342	PRO	CA-C-N	5.16	125.46	119.47
5	A	342	PRO	C-N-CA	5.16	125.46	119.47
1	B	472	MET	N-CA-C	5.13	117.08	108.73

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	3940	0	3927	120	0
2	E	341	0	354	22	0
3	D	1236	0	1271	43	0
4	C	411	0	401	10	0
5	A	3285	0	3305	90	0
6	B	15	0	6	3	0
7	D	28	0	47	3	0
8	D	29	0	56	10	0
All	All	9285	0	9367	271	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 15.

All (271) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:LYS:NZ	6:B:601:PLP:C4A	1.79	1.46
1:B:379:LYS:HZ1	6:B:601:PLP:C4A	1.33	1.41
1:B:501:THR:HB	1:B:502:PRO:CD	1.82	1.06
1:B:66:THR:O	3:D:20:ARG:NH1	1.93	1.02
5:A:151:ARG:NH2	5:A:354:ASN:OD1	1.97	0.98
1:B:202:GLY:O	5:A:112:LEU:HD11	1.67	0.94
1:B:379:LYS:HZ3	6:B:601:PLP:C4A	1.60	0.94
5:A:422:ARG:HG2	5:A:422:ARG:HH11	1.31	0.94
1:B:432:THR:HB	1:B:434:LEU:CD2	1.98	0.93
8:D:803:R16:H351	8:D:803:R16:H311	1.48	0.91
1:B:61:GLU:OE1	1:B:463:ASN:ND2	2.02	0.91
1:B:432:THR:HB	1:B:434:LEU:HD23	1.53	0.90
1:B:501:THR:HG22	3:D:6:ALA:HB3	1.54	0.88
5:A:300:ILE:O	5:A:301:ASP:HB2	1.73	0.88
1:B:344:ASP:OD1	1:B:374:MET:SD	2.34	0.85
1:B:501:THR:HB	1:B:502:PRO:HD3	1.59	0.84
5:A:380:ILE:HG12	5:A:465:LYS:HG3	1.59	0.84
5:A:150:ASP:OD2	5:A:154:LYS:NZ	2.11	0.84
3:D:77:GLN:O	5:A:181:ARG:HG2	1.79	0.83
2:E:27:LEU:O	2:E:27:LEU:HD12	1.77	0.83
1:B:302:ARG:HB2	1:B:302:ARG:CZ	2.07	0.83
1:B:237:MET:HE2	1:B:239:PHE:HB3	1.61	0.82
5:A:151:ARG:HH11	5:A:151:ARG:HG2	1.43	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:803:R16:H351	8:D:803:R16:C31	2.11	0.80
5:A:128:TYR:OH	5:A:143:ASP:OD1	1.99	0.79
1:B:501:THR:HG22	3:D:6:ALA:CB	2.12	0.79
1:B:66:THR:HG21	1:B:504:ILE:HD12	1.63	0.79
1:B:473:LEU:O	1:B:506:SER:O	2.00	0.79
1:B:201:ALA:O	1:B:412:SER:OG	2.01	0.79
1:B:94:TRP:H	1:B:94:TRP:CD1	1.97	0.78
1:B:378:THR:HG23	1:B:384:SER:HA	1.63	0.78
1:B:260:GLU:O	3:D:8:SER:HB2	1.84	0.78
1:B:366:ASP:OD1	1:B:367:PRO:HD2	1.84	0.77
1:B:501:THR:HB	1:B:502:PRO:HD2	1.66	0.77
1:B:399:ARG:O	5:A:82:TYR:OH	2.01	0.77
2:E:38:LEU:HD12	2:E:38:LEU:O	1.83	0.76
1:B:223:VAL:HG22	1:B:423:MET:HE1	1.67	0.75
1:B:246:ILE:N	1:B:247:PRO:HD2	2.03	0.74
1:B:418:GLN:HG3	5:A:130:VAL:HG21	1.69	0.74
1:B:392:LYS:HG3	1:B:392:LYS:O	1.86	0.74
5:A:151:ARG:HG2	5:A:151:ARG:NH1	1.99	0.73
2:E:37:ARG:HD2	2:E:37:ARG:O	1.89	0.73
5:A:257:LEU:HD23	5:A:295:ILE:HD12	1.69	0.73
2:E:17:LEU:C	2:E:17:LEU:HD23	2.14	0.72
5:A:344:LEU:C	5:A:344:LEU:HD12	2.14	0.72
1:B:433:SER:O	1:B:437:GLU:HG2	1.90	0.71
1:B:432:THR:CB	1:B:434:LEU:HD23	2.20	0.70
1:B:501:THR:CB	1:B:502:PRO:CD	2.62	0.70
5:A:158:THR:HG22	5:A:159:GLU:H	1.57	0.70
5:A:136:ARG:HE	5:A:141:THR:HB	1.55	0.69
1:B:257:LEU:CD1	1:B:291:LEU:HD23	2.21	0.69
5:A:226:ILE:O	5:A:230:LYS:HD3	1.93	0.69
5:A:375:LYS:O	5:A:375:LYS:HG2	1.92	0.69
1:B:434:LEU:N	1:B:434:LEU:HD22	2.09	0.68
1:B:93:TYR:HB3	1:B:94:TRP:CD1	2.30	0.67
3:D:60:MET:HG3	8:D:803:R16:H391	1.76	0.67
5:A:422:ARG:HG2	5:A:422:ARG:NH1	2.02	0.67
1:B:434:LEU:HD22	1:B:434:LEU:H	1.58	0.66
8:D:803:R16:H361	8:D:803:R16:H301	1.77	0.66
5:A:264:LYS:HG3	5:A:269:ALA:O	1.96	0.66
1:B:257:LEU:HD12	1:B:291:LEU:HD23	1.78	0.66
1:B:518:LYS:HE2	1:B:518:LYS:HA	1.78	0.65
3:D:81:ARG:NH2	5:A:180:LYS:HG3	2.12	0.65
1:B:378:THR:HG22	1:B:383:ALA:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:THR:CG2	1:B:504:ILE:HD12	2.27	0.64
1:B:83:LEU:HD22	7:D:801:6CM:H131	1.80	0.64
1:B:517:THR:HG22	1:B:518:LYS:H	1.63	0.64
1:B:518:LYS:HE2	1:B:518:LYS:CA	2.29	0.63
1:B:204:CYS:SG	5:A:107:ASN:HB3	2.39	0.62
1:B:434:LEU:CD2	1:B:434:LEU:H	2.12	0.62
2:E:10:LEU:HD22	2:E:10:LEU:O	1.99	0.62
5:A:253:THR:HA	5:A:388:GLU:HG2	1.82	0.61
5:A:101:ILE:N	5:A:101:ILE:HD12	2.15	0.61
1:B:208:GLN:HG3	1:B:405:ALA:O	2.01	0.61
3:D:24:LEU:HD12	3:D:24:LEU:O	2.00	0.61
4:C:13:MET:HE2	4:C:13:MET:HA	1.81	0.61
5:A:257:LEU:HD23	5:A:295:ILE:CD1	2.31	0.61
1:B:144:ALA:O	1:B:145:ARG:HG2	2.01	0.61
1:B:195:VAL:HG12	1:B:195:VAL:O	2.01	0.61
5:A:100:CYS:HB3	5:A:423:SER:HA	1.83	0.60
5:A:230:LYS:HD2	5:A:230:LYS:N	2.15	0.60
2:E:27:LEU:HD12	2:E:27:LEU:C	2.24	0.60
1:B:501:THR:CG2	3:D:6:ALA:HB3	2.31	0.60
1:B:543:ARG:CG	1:B:543:ARG:HH11	2.13	0.60
3:D:125:VAL:O	3:D:125:VAL:HG13	2.00	0.60
5:A:73:VAL:HG13	5:A:73:VAL:O	2.00	0.60
5:A:151:ARG:HH11	5:A:151:ARG:CG	2.13	0.60
5:A:306:ASN:HA	5:A:316:GLY:HA2	1.83	0.60
1:B:442:LEU:HD22	1:B:442:LEU:O	2.02	0.59
3:D:117:THR:HG23	3:D:117:THR:O	2.02	0.59
1:B:246:ILE:N	1:B:247:PRO:CD	2.65	0.59
2:E:9:VAL:HG22	2:E:9:VAL:O	2.02	0.59
3:D:108:VAL:O	3:D:112:LEU:HD12	2.02	0.59
5:A:373:ILE:O	5:A:373:ILE:HG13	2.02	0.59
1:B:300:GLN:HB3	1:B:301:PRO:HD2	1.85	0.59
1:B:543:ARG:HH11	1:B:543:ARG:CB	2.15	0.59
1:B:169:GLY:O	1:B:490:ASN:ND2	2.35	0.59
1:B:61:GLU:CD	1:B:463:ASN:HD22	2.07	0.58
1:B:302:ARG:HB2	1:B:302:ARG:NH1	2.17	0.58
1:B:223:VAL:CG2	1:B:423:MET:HE1	2.33	0.58
1:B:481:ALA:O	1:B:485:GLU:HG2	2.04	0.58
5:A:459:ARG:O	5:A:459:ARG:HG2	2.04	0.58
2:E:46:LEU:HD22	3:D:94:GLN:HE21	1.68	0.58
3:D:89:MET:O	3:D:99:ARG:NH1	2.37	0.57
1:B:458:PHE:HB3	1:B:471:LEU:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:LEU:O	1:B:91:LEU:HB2	2.03	0.57
8:D:803:R16:H301	8:D:803:R16:C36	2.34	0.57
5:A:210:LYS:HB2	5:A:213:ASP:OD1	2.05	0.57
1:B:441:GLN:O	1:B:441:GLN:HG3	2.04	0.56
1:B:500:ALA:HB1	3:D:5:THR:HB	1.87	0.56
3:D:7:HIS:HD2	3:D:9:GLU:H	1.53	0.56
1:B:119:GLU:OE1	3:D:73:GLU:CD	2.49	0.56
5:A:344:LEU:HD12	5:A:344:LEU:O	2.06	0.56
5:A:264:LYS:NZ	5:A:299:ASP:O	2.38	0.55
1:B:498:PHE:CD1	1:B:498:PHE:C	2.84	0.55
2:E:45:LYS:HG2	2:E:45:LYS:O	2.07	0.55
1:B:219:LEU:O	1:B:219:LEU:HG	2.07	0.55
1:B:162:TYR:N	1:B:162:TYR:CD2	2.73	0.55
1:B:222:LEU:HD12	1:B:222:LEU:O	2.06	0.55
5:A:398:LEU:HD11	5:A:472:LEU:HD21	1.87	0.55
1:B:395:ILE:HG22	1:B:395:ILE:O	2.07	0.54
1:B:499:PRO:HB2	3:D:1:MET:O	2.07	0.54
5:A:244:VAL:HG22	5:A:245:GLU:H	1.71	0.54
5:A:405:ARG:NH2	5:A:439:LEU:CD2	2.71	0.54
1:B:196:LEU:O	1:B:196:LEU:HG	2.08	0.54
3:D:124:PHE:C	3:D:124:PHE:CD2	2.85	0.54
5:A:257:LEU:N	5:A:258:PRO:CD	2.71	0.53
1:B:90:PHE:CD1	1:B:90:PHE:C	2.87	0.53
1:B:502:PRO:HD2	1:B:505:GLU:HB2	1.90	0.53
1:B:503:ILE:HG23	1:B:504:ILE:HG23	1.89	0.53
1:B:378:THR:CG2	1:B:383:ALA:O	2.57	0.53
1:B:271:ARG:HH12	3:D:10:VAL:CG1	2.21	0.53
3:D:10:VAL:HG12	3:D:75:PRO:HG2	1.92	0.52
3:D:10:VAL:O	3:D:74:THR:HB	2.09	0.52
3:D:74:THR:HB	3:D:75:PRO:HD2	1.90	0.52
1:B:78:TYR:OH	1:B:498:PHE:HB2	2.10	0.52
1:B:485:GLU:O	1:B:489:ARG:HG2	2.10	0.52
1:B:137:PRO:O	1:B:149:MET:HG3	2.10	0.52
1:B:313:LEU:HD23	1:B:342:TYR:HB3	1.91	0.51
1:B:505:GLU:HB3	1:B:507:ARG:HH11	1.75	0.51
5:A:101:ILE:N	5:A:101:ILE:CD1	2.73	0.51
5:A:230:LYS:N	5:A:230:LYS:CD	2.73	0.51
5:A:102:ASN:HA	5:A:425:ALA:HB3	1.93	0.51
1:B:222:LEU:HG	1:B:423:MET:HE3	1.93	0.51
8:D:803:R16:C31	8:D:803:R16:C35	2.85	0.51
1:B:542:HIS:O	1:B:543:ARG:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:38:LEU:CD1	3:D:100:LYS:HG2	2.41	0.50
5:A:405:ARG:NH2	5:A:439:LEU:HD21	2.27	0.50
1:B:302:ARG:NH1	1:B:302:ARG:CB	2.75	0.50
1:B:302:ARG:CZ	1:B:302:ARG:CB	2.88	0.50
5:A:353:LEU:O	5:A:357:GLU:HG3	2.12	0.50
1:B:155:ASP:OD1	1:B:159:SER:HB2	2.11	0.49
5:A:424:ILE:HG22	5:A:424:ILE:O	2.11	0.49
4:C:13:MET:HE2	4:C:13:MET:CA	2.42	0.49
1:B:110:ASP:OD1	1:B:110:ASP:N	2.44	0.49
3:D:115:PHE:C	3:D:115:PHE:CD2	2.90	0.49
5:A:253:THR:HA	5:A:388:GLU:CG	2.42	0.49
3:D:40:ILE:HG21	3:D:43:VAL:CG2	2.43	0.49
5:A:266:LYS:HD2	5:A:267:TYR:CE2	2.48	0.49
5:A:397:GLN:HG2	5:A:443:SER:HB3	1.95	0.49
1:B:336:LYS:O	1:B:336:LYS:HG3	2.12	0.48
1:B:543:ARG:CG	1:B:543:ARG:NH1	2.73	0.48
5:A:83:ASN:N	5:A:83:ASN:ND2	2.60	0.48
5:A:188:ASP:OD1	5:A:189:ARG:N	2.46	0.48
5:A:369:LYS:O	5:A:369:LYS:HG3	2.13	0.48
1:B:501:THR:CB	1:B:502:PRO:HD3	2.34	0.48
5:A:73:VAL:N	5:A:74:PRO:HD3	2.27	0.48
1:B:199:TYR:HA	5:A:88:PRO:HB3	1.96	0.48
8:D:803:R16:C36	8:D:803:R16:C30	2.92	0.48
5:A:101:ILE:HG12	5:A:456:GLU:OE2	2.14	0.48
1:B:111:PHE:N	1:B:111:PHE:CD1	2.82	0.48
1:B:486:MET:CE	1:B:531:VAL:HG21	2.44	0.48
1:B:430:ASP:N	1:B:430:ASP:OD1	2.44	0.47
1:B:543:ARG:NH1	1:B:543:ARG:HG3	2.28	0.47
1:B:227:LEU:HD11	1:B:387:TYR:CE2	2.49	0.47
1:B:486:MET:HE2	1:B:531:VAL:HG21	1.96	0.47
5:A:229:GLN:N	5:A:229:GLN:OE1	2.47	0.47
1:B:206:THR:HB	1:B:209:GLU:HG3	1.97	0.47
1:B:527:GLU:OE2	1:B:527:GLU:HA	2.14	0.47
5:A:62:GLU:HA	5:A:62:GLU:OE2	2.14	0.47
5:A:82:TYR:N	5:A:82:TYR:CD1	2.81	0.47
1:B:111:PHE:N	1:B:111:PHE:HD1	2.13	0.47
1:B:517:THR:HG22	1:B:518:LYS:N	2.28	0.46
4:C:12:GLN:O	4:C:12:GLN:HG2	2.12	0.46
1:B:489:ARG:O	1:B:490:ASN:CB	2.63	0.46
3:D:1:MET:HB2	3:D:2:ASN:H	1.55	0.46
3:D:73:GLU:HA	3:D:73:GLU:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:369:LYS:HB3	5:A:369:LYS:HE2	1.56	0.46
5:A:222:LYS:O	5:A:226:ILE:HG12	2.16	0.46
1:B:121:PHE:O	1:B:125:ASN:HB2	2.16	0.46
1:B:143:GLY:C	1:B:145:ARG:H	2.24	0.46
5:A:148:LEU:HD13	5:A:350:ILE:HG13	1.98	0.46
1:B:246:ILE:H	1:B:247:PRO:HD2	1.78	0.45
3:D:21:GLY:O	3:D:25:SER:HB3	2.16	0.45
1:B:83:LEU:HD12	1:B:83:LEU:HA	1.82	0.45
1:B:284:ASN:HB3	1:B:287:SER:HB3	1.97	0.45
5:A:136:ARG:NE	5:A:141:THR:HB	2.27	0.45
2:E:38:LEU:HD12	3:D:100:LYS:HG2	1.99	0.45
1:B:219:LEU:O	1:B:223:VAL:HG23	2.17	0.45
5:A:113:ASP:HA	5:A:118:LYS:HE3	1.97	0.45
1:B:498:PHE:CD1	1:B:498:PHE:O	2.70	0.45
5:A:52:LEU:HD13	5:A:52:LEU:HA	1.74	0.45
5:A:70:VAL:O	5:A:70:VAL:HG23	2.17	0.45
5:A:94:VAL:HA	5:A:98:LYS:O	2.17	0.45
2:E:44:TYR:O	2:E:44:TYR:CD1	2.70	0.45
7:D:801:6CM:H152	8:D:802:R16:H372	1.99	0.45
5:A:353:LEU:HD12	5:A:353:LEU:HA	1.75	0.45
1:B:345:GLU:H	1:B:345:GLU:HG3	1.61	0.44
2:E:37:ARG:HD2	2:E:37:ARG:C	2.42	0.44
2:E:44:TYR:O	2:E:44:TYR:CG	2.70	0.44
3:D:89:MET:HE2	3:D:89:MET:HB3	1.80	0.44
3:D:131:LEU:O	3:D:131:LEU:HG	2.17	0.44
4:C:53:TYR:CD1	4:C:53:TYR:O	2.70	0.44
3:D:108:VAL:O	3:D:112:LEU:CD1	2.66	0.44
4:C:53:TYR:O	4:C:53:TYR:CG	2.70	0.43
1:B:94:TRP:CD1	1:B:94:TRP:N	2.72	0.43
2:E:17:LEU:HD23	2:E:17:LEU:O	2.18	0.43
5:A:415:ILE:HG23	5:A:467:VAL:HG23	2.01	0.43
1:B:59:PHE:O	1:B:59:PHE:CD2	2.71	0.43
2:E:39:LEU:HD12	2:E:39:LEU:HA	1.90	0.43
4:C:28:MET:O	4:C:29:LEU:HD12	2.18	0.43
3:D:110:TYR:HA	3:D:113:THR:HG22	2.01	0.43
5:A:271:ILE:O	5:A:272:PHE:HD1	2.00	0.43
5:A:405:ARG:HH22	5:A:439:LEU:HG	1.83	0.43
5:A:437:LYS:HA	5:A:437:LYS:HD3	1.80	0.43
1:B:289:GLU:O	1:B:289:GLU:HG2	2.18	0.43
5:A:247:LEU:HD23	5:A:247:LEU:HA	1.87	0.43
5:A:344:LEU:C	5:A:344:LEU:CD1	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:262:LYS:HB2	5:A:262:LYS:HE2	1.65	0.43
4:C:13:MET:HE3	4:C:13:MET:HB2	1.84	0.43
5:A:151:ARG:CZ	5:A:354:ASN:OD1	2.64	0.43
2:E:9:VAL:HG23	2:E:12:GLU:OE1	2.19	0.43
5:A:404:SER:OG	5:A:407:GLN:NE2	2.51	0.43
1:B:119:GLU:OE1	3:D:73:GLU:OE2	2.36	0.42
5:A:158:THR:HG22	5:A:159:GLU:N	2.27	0.42
1:B:327:LEU:HD23	1:B:327:LEU:HA	1.92	0.42
5:A:178:TYR:OH	5:A:324:VAL:O	2.32	0.42
5:A:398:LEU:HD11	5:A:472:LEU:CD2	2.49	0.42
1:B:149:MET:HE3	1:B:149:MET:HB3	1.73	0.42
1:B:489:ARG:O	1:B:490:ASN:HB3	2.19	0.42
5:A:464:ILE:O	5:A:464:ILE:HG23	2.18	0.42
1:B:162:TYR:H	1:B:162:TYR:HD2	1.67	0.42
5:A:60:LEU:HD12	5:A:60:LEU:HA	1.79	0.42
4:C:19:GLN:O	4:C:23:VAL:HG22	2.19	0.42
1:B:61:GLU:HG2	1:B:463:ASN:ND2	2.34	0.42
3:D:60:MET:CG	8:D:803:R16:H391	2.47	0.42
5:A:202:SER:O	5:A:204:SER:N	2.53	0.42
3:D:7:HIS:CD2	3:D:9:GLU:HB2	2.55	0.41
3:D:77:GLN:HB2	5:A:181:ARG:HD3	2.02	0.41
5:A:72:PRO:HB2	5:A:73:VAL:H	1.58	0.41
5:A:209:PHE:CZ	5:A:217:LEU:HD12	2.55	0.41
7:D:801:6CM:H171	7:D:801:6CM:H142	1.61	0.41
8:D:803:R16:H351	8:D:803:R16:C30	2.51	0.41
3:D:33:LEU:HD12	3:D:33:LEU:O	2.20	0.41
5:A:142:PHE:CD1	5:A:142:PHE:N	2.89	0.41
5:A:390:LEU:HD23	5:A:390:LEU:H	1.85	0.41
2:E:24:HIS:CE1	3:D:124:PHE:HD1	2.38	0.41
2:E:26:ILE:N	2:E:26:ILE:HD13	2.36	0.41
2:E:37:ARG:C	2:E:37:ARG:CD	2.94	0.41
4:C:50:TYR:O	4:C:50:TYR:CD1	2.74	0.41
5:A:74:PRO:HB2	5:A:75:LYS:H	1.59	0.41
5:A:345:LEU:HD12	5:A:345:LEU:HA	1.82	0.41
2:E:38:LEU:O	3:D:100:LYS:HE2	2.20	0.41
2:E:44:TYR:CD1	2:E:44:TYR:C	2.98	0.40
5:A:82:TYR:N	5:A:82:TYR:HD1	2.19	0.40
5:A:210:LYS:HG2	5:A:216:ASP:OD2	2.21	0.40
1:B:133:ASN:HD21	1:B:480:GLY:HA2	1.87	0.40
1:B:294:ASP:HA	1:B:297:VAL:HG22	2.02	0.40
4:C:49:LEU:HD12	4:C:49:LEU:HA	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:7:HIS:HD2	3:D:9:GLU:HB2	1.86	0.40
3:D:68:LYS:HB2	3:D:83:LEU:O	2.22	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	497/562 (88%)	458 (92%)	34 (7%)	5 (1%)	12	39
2	E	41/50 (82%)	34 (83%)	5 (12%)	2 (5%)	1	6
3	D	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
4	C	46/92 (50%)	44 (96%)	2 (4%)	0	100	100
5	A	421/423 (100%)	383 (91%)	31 (7%)	7 (2%)	7	26
All	All	1156/1280 (90%)	1067 (92%)	75 (6%)	14 (1%)	13	34

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	501	THR
5	A	72	PRO
5	A	74	PRO
1	B	490	ASN
2	E	49	ARG
1	B	95	ARG
1	B	301	PRO
5	A	76	ASP
5	A	203	ARG
5	A	210	LYS
5	A	301	ASP
1	B	100	HIS

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Mol	Chain	Res	Type
5	A	403	GLY
2	E	9	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	415/466 (89%)	351 (85%)	64 (15%)	2	9
2	E	34/44 (77%)	19 (56%)	15 (44%)	0	0
3	D	140/140 (100%)	123 (88%)	17 (12%)	5	16
4	C	43/78 (55%)	32 (74%)	11 (26%)	0	2
5	A	354/357 (99%)	302 (85%)	52 (15%)	3	10
All	All	986/1085 (91%)	827 (84%)	159 (16%)	4	8

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	60	ASN
1	B	66	THR
1	B	68	MET
1	B	72	VAL
1	B	83	LEU
1	B	92	ARG
1	B	93	TYR
1	B	94	TRP
1	B	101	HIS
1	B	107	GLU
1	B	110	ASP
1	B	111	PHE
1	B	113	SER
1	B	120	ASN
1	B	149	MET
1	B	150	GLU
1	B	159	SER

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Mol	Chain	Res	Type
1	B	161	LYS
1	B	162	TYR
1	B	168	LYS
1	B	183	ARG
1	B	189	GLN
1	B	197	GLU
1	B	198	GLU
1	B	205	SER
1	B	210	ILE
1	B	215	LYS
1	B	217	GLU
1	B	221	GLU
1	B	243	SER
1	B	244	MET
1	B	250	VAL
1	B	252	LYS
1	B	258	SER
1	B	261	LEU
1	B	271	ARG
1	B	285	MET
1	B	287	SER
1	B	302	ARG
1	B	303	THR
1	B	331	ILE
1	B	334	LYS
1	B	345	GLU
1	B	373	MET
1	B	378	THR
1	B	392	LYS
1	B	394	LEU
1	B	402	SER
1	B	406	VAL
1	B	434	LEU
1	B	436	LYS
1	B	439	VAL
1	B	440	GLN
1	B	442	LEU
1	B	444	GLU
1	B	454	LYS
1	B	463	ASN
1	B	473	LEU
1	B	475	MET

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Mol	Chain	Res	Type
1	B	489	ARG
1	B	519	GLU
1	B	521	LEU
1	B	526	LYS
1	B	543	ARG
2	E	10	LEU
2	E	13	MET
2	E	14	VAL
2	E	15	GLN
2	E	17	LEU
2	E	18	TYR
2	E	26	ILE
2	E	27	LEU
2	E	33	LEU
2	E	37	ARG
2	E	38	LEU
2	E	42	LYS
2	E	44	TYR
2	E	45	LYS
2	E	46	LEU
3	D	1	MET
3	D	8	SER
3	D	17	MET
3	D	20	ARG
3	D	22	ILE
3	D	24	LEU
3	D	27	VAL
3	D	33	LEU
3	D	35	ILE
3	D	40	ILE
3	D	72	PHE
3	D	114	SER
3	D	117	THR
3	D	122	ILE
3	D	125	VAL
3	D	131	LEU
3	D	145	VAL
4	C	11	LYS
4	C	13	MET
4	C	14	SER
4	C	26	LEU
4	C	39	SER

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Mol	Chain	Res	Type
4	C	40	MET
4	C	42	VAL
4	C	45	VAL
4	C	47	MET
4	C	49	LEU
4	C	51	THR
5	A	51	ASP
5	A	52	LEU
5	A	53	THR
5	A	54	VAL
5	A	55	LYS
5	A	60	LEU
5	A	76	ASP
5	A	77	HIS
5	A	83	ASN
5	A	99	GLU
5	A	101	ILE
5	A	105	SER
5	A	109	LEU
5	A	141	THR
5	A	144	VAL
5	A	150	ASP
5	A	151	ARG
5	A	157	LYS
5	A	230	LYS
5	A	245	GLU
5	A	260	LEU
5	A	261	VAL
5	A	262	LYS
5	A	263	LEU
5	A	268	LYS
5	A	277	LEU
5	A	284	GLU
5	A	287	ARG
5	A	289	VAL
5	A	324	VAL
5	A	340	SER
5	A	344	LEU
5	A	345	LEU
5	A	353	LEU
5	A	365	VAL
5	A	367	LYS

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Mol	Chain	Res	Type
5	A	368	GLU
5	A	369	LYS
5	A	370	CYS
5	A	373	ILE
5	A	375	LYS
5	A	402	THR
5	A	405	ARG
5	A	407	GLN
5	A	419	CYS
5	A	422	ARG
5	A	424	ILE
5	A	453	THR
5	A	457	LEU
5	A	463	THR
5	A	464	ILE
5	A	465	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	50	GLN
1	B	108	GLN
1	B	208	GLN
2	E	15	GLN
3	D	7	HIS
3	D	94	GLN
4	C	38	ASN
5	A	83	ASN
5	A	96	ASN
5	A	285	HIS
5	A	292	HIS
5	A	327	HIS
5	A	372	GLN
5	A	407	GLN
5	A	418	GLN
5	A	452	GLN

5.3.3 RNA ⓘ

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](#)

4 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$
8	R16	D	802	-	15,15,15	0.17	0	14,14,14	0.66	0
6	PLP	B	601	-	15,15,16	3.03	3 (20%)	21,22,23	1.18	1 (4%)
8	R16	D	803	-	12,12,15	0.20	0	11,11,14	0.63	0
7	6CM	D	801	-	26,27,27	0.31	0	27,29,29	0.76	1 (3%)

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
8	R16	D	802	-	-	8/13/13/13	-
6	PLP	B	601	-	-	3/6/6/8	0/1/1/1
8	R16	D	803	-	-	6/10/10/13	-
7	6CM	D	801	-	-	16/30/30/30	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	601	PLP	C3-C2	7.68	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	601	PLP	C5-C4	7.20	1.48	1.40
6	B	601	PLP	C3-C4	4.37	1.48	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	801	6CM	C3-C4-C5	-2.28	119.96	124.69
6	B	601	PLP	C6-N1-C2	2.20	123.19	119.20

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	601	PLP	C5A-O4P-P-O1P
6	B	601	PLP	C5A-O4P-P-O2P
7	D	801	6CM	O19-C19-N2-C2
7	D	801	6CM	C20-C19-N2-C2
7	D	801	6CM	O1-C1-C2-C3
7	D	801	6CM	N2-C2-C3-O3
7	D	801	6CM	C1-C2-C3-C4
7	D	801	6CM	C14-C15-C16-C17
8	D	803	R16	C35-C36-C37-C38
8	D	802	R16	C30-C31-C32-C33
7	D	801	6CM	C11-C10-C9-C8
8	D	803	R16	C33-C34-C35-C36
8	D	803	R16	C30-C31-C32-C33
7	D	801	6CM	C20-C21-C22-C23
8	D	803	R16	C37-C38-C39-C40
8	D	803	R16	C29-C30-C31-C32
7	D	801	6CM	O1-C1-C2-N2
8	D	802	R16	C38-C39-C40-C41
7	D	801	6CM	C12-C13-C14-C15
7	D	801	6CM	C6-C7-C8-C9
8	D	802	R16	C36-C37-C38-C39
8	D	802	R16	C39-C40-C41-C42
7	D	801	6CM	C4-C5-C6-C7
8	D	802	R16	C33-C34-C35-C36
7	D	801	6CM	C1-C2-C3-O3
8	D	802	R16	C29-C30-C31-C32
8	D	802	R16	C32-C33-C34-C35
8	D	803	R16	C28-C29-C30-C31
8	D	802	R16	C28-C29-C30-C31

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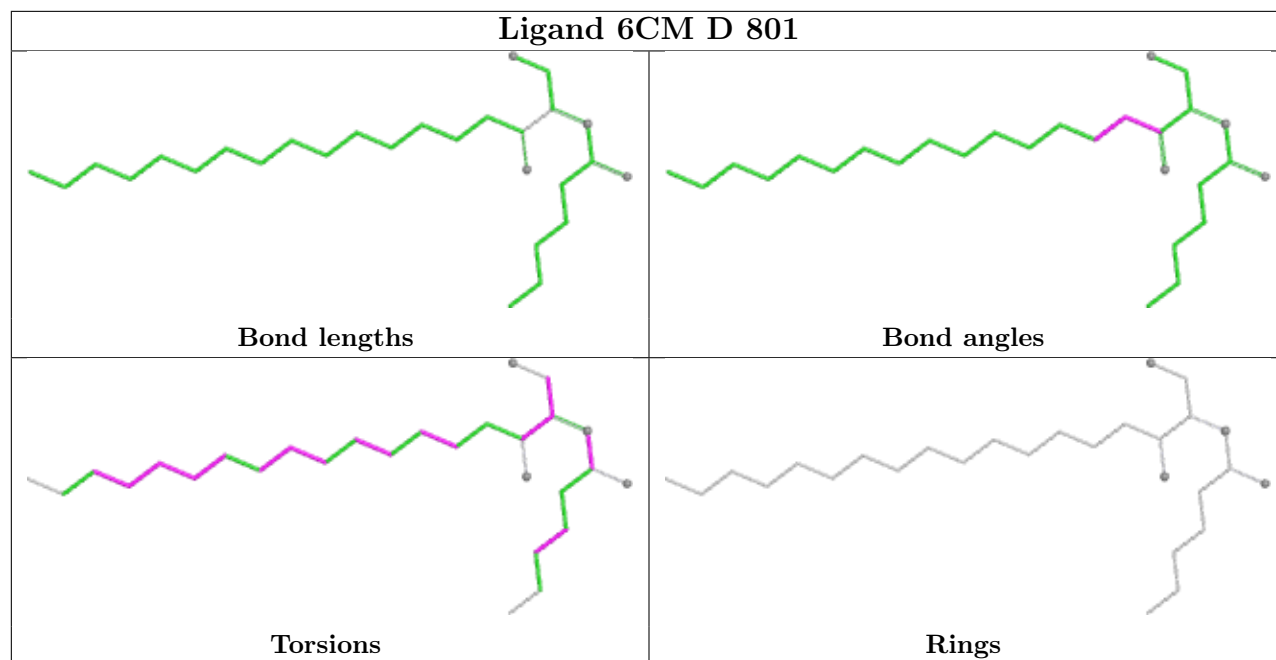
Mol	Chain	Res	Type	Atoms
6	B	601	PLP	C5A-O4P-P-O3P
7	D	801	6CM	C13-C14-C15-C16
7	D	801	6CM	C11-C12-C13-C14
7	D	801	6CM	C9-C10-C11-C12

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	802	R16	1	0
6	B	601	PLP	3	0
8	D	803	R16	9	0
7	D	801	6CM	3	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.

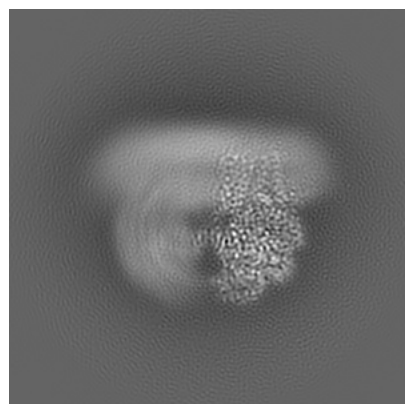
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33864. These allow visual inspection of the internal detail of the map and identification of artifacts.

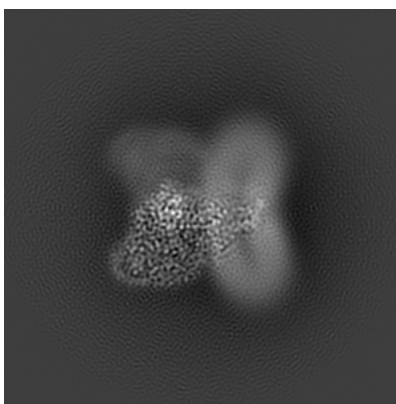
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

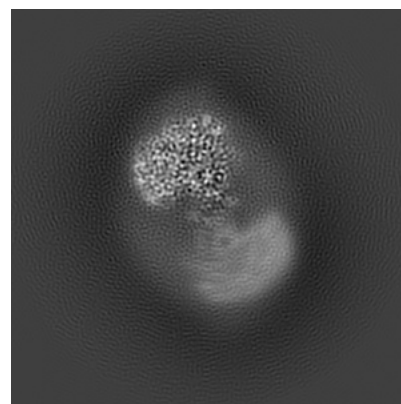
6.1.1 Primary map



X

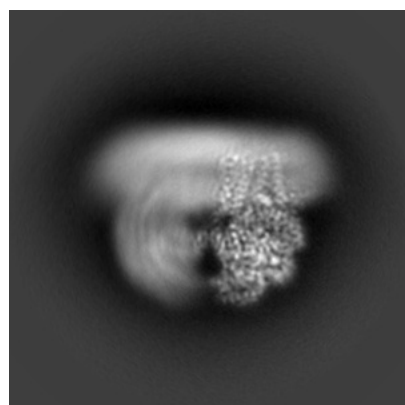


Y

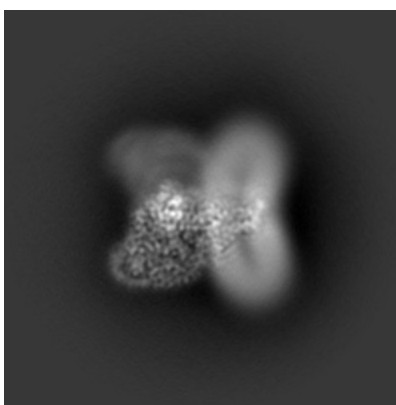


Z

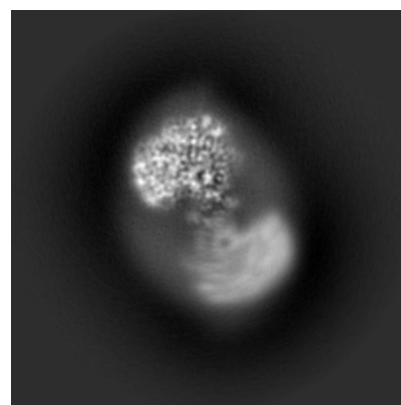
6.1.2 Raw map



X



Y

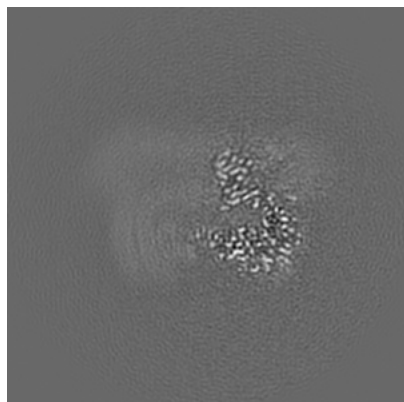


Z

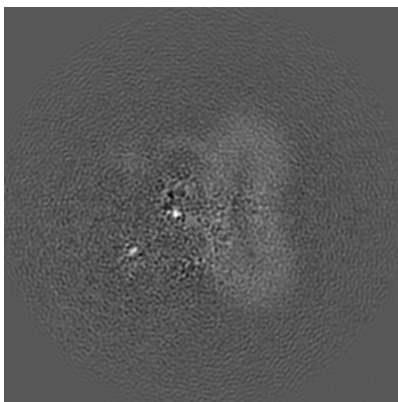
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

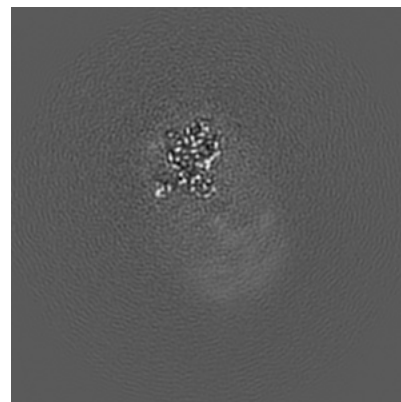
6.2.1 Primary map



X Index: 128

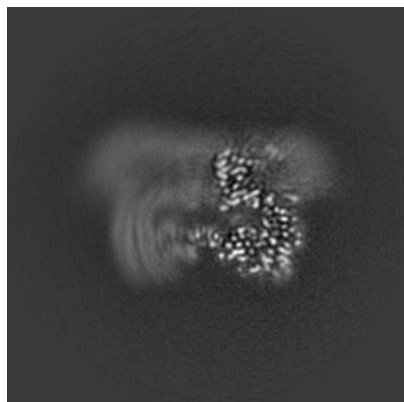


Y Index: 128

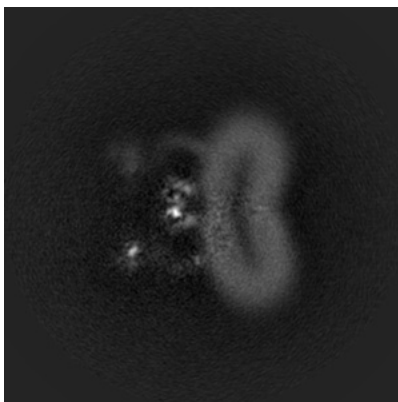


Z Index: 128

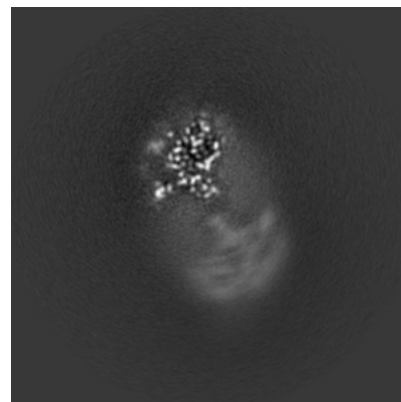
6.2.2 Raw map



X Index: 128



Y Index: 128

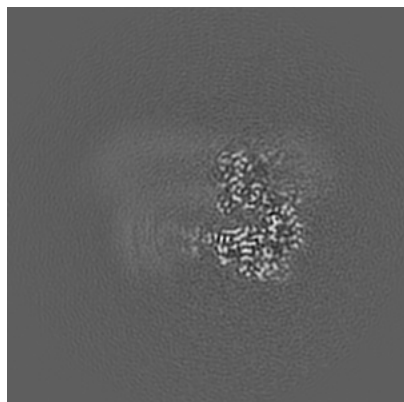


Z Index: 128

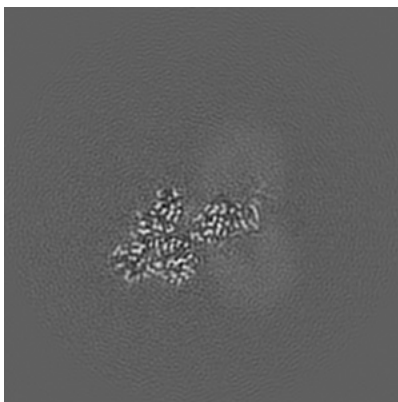
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

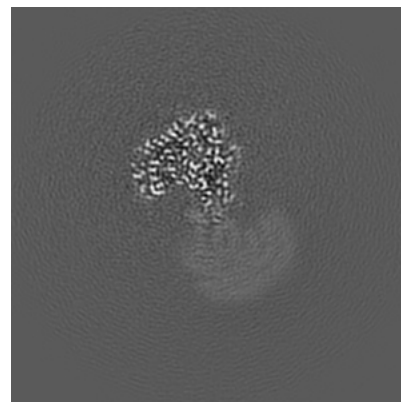
6.3.1 Primary map



X Index: 125

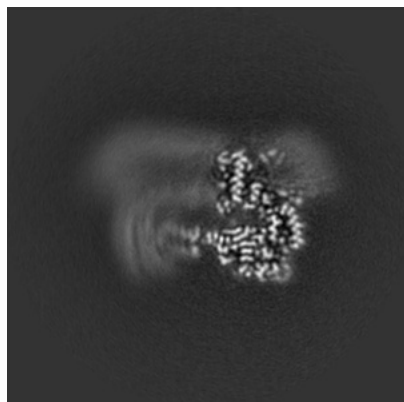


Y Index: 145

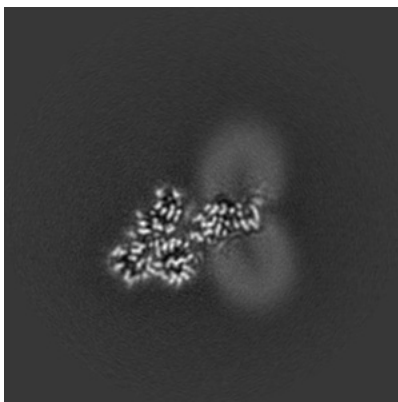


Z Index: 105

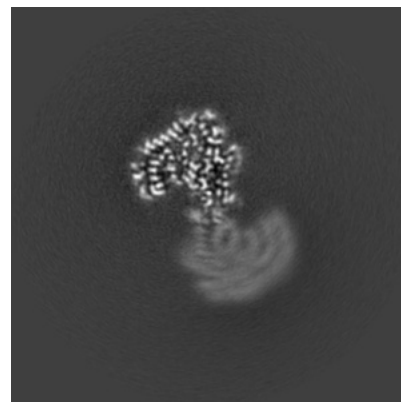
6.3.2 Raw map



X Index: 125



Y Index: 145

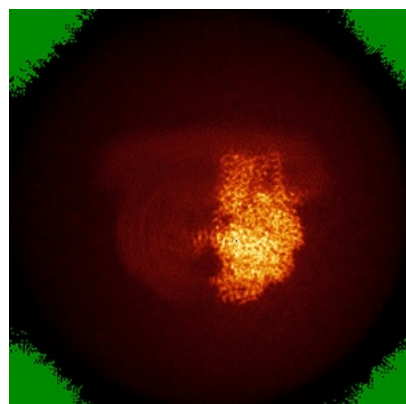


Z Index: 105

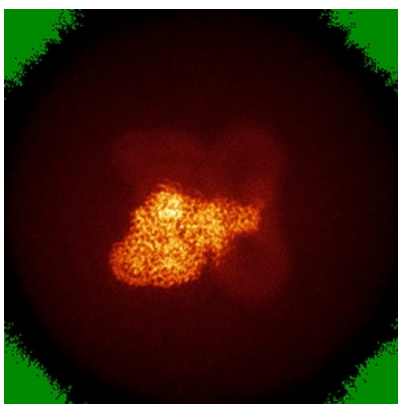
The images above show the largest variance slices of the map in three orthogonal directions.

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

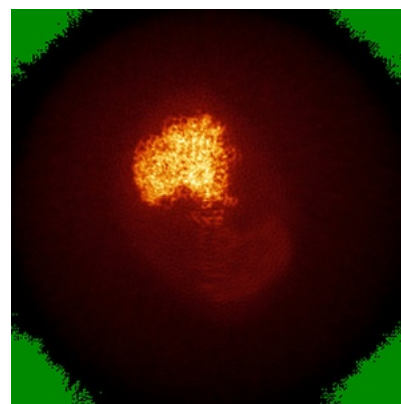
6.4.1 Primary map



X

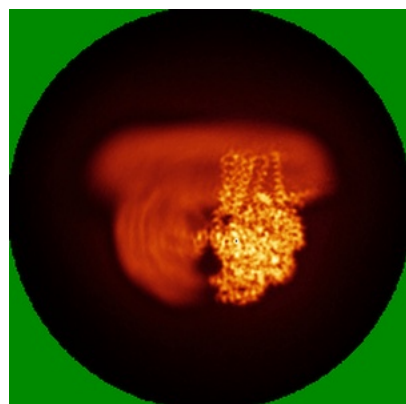


Y

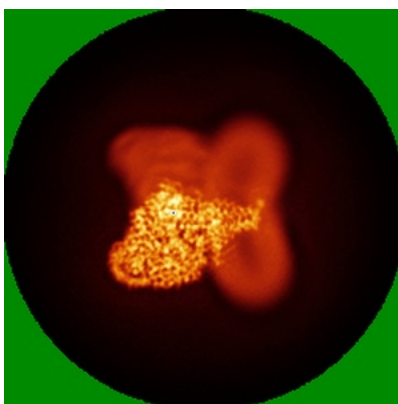


Z

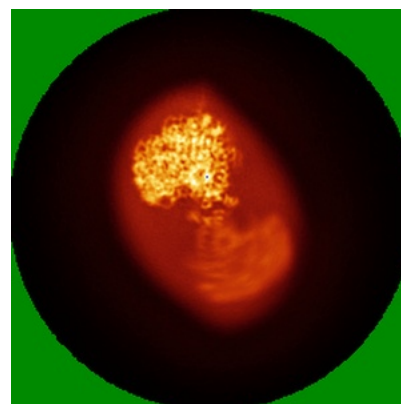
6.4.2 Raw map



X



Y

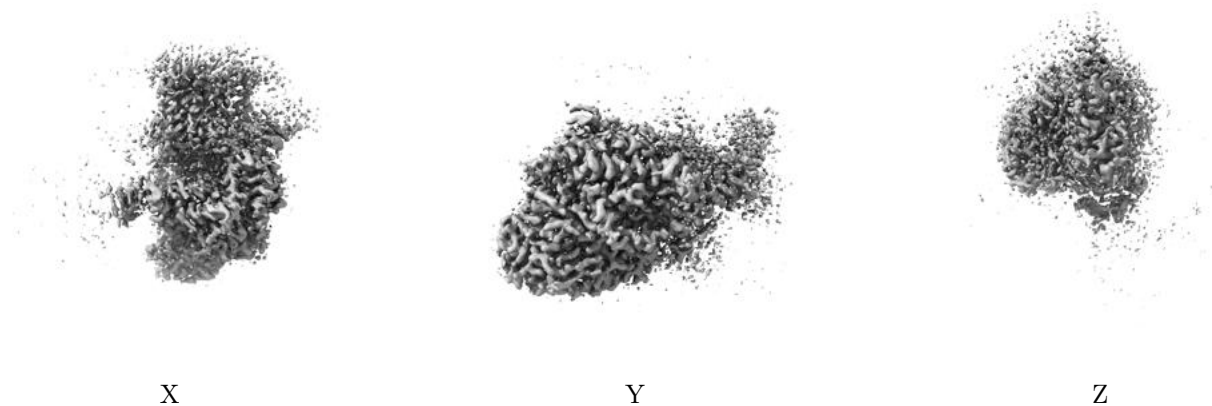


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

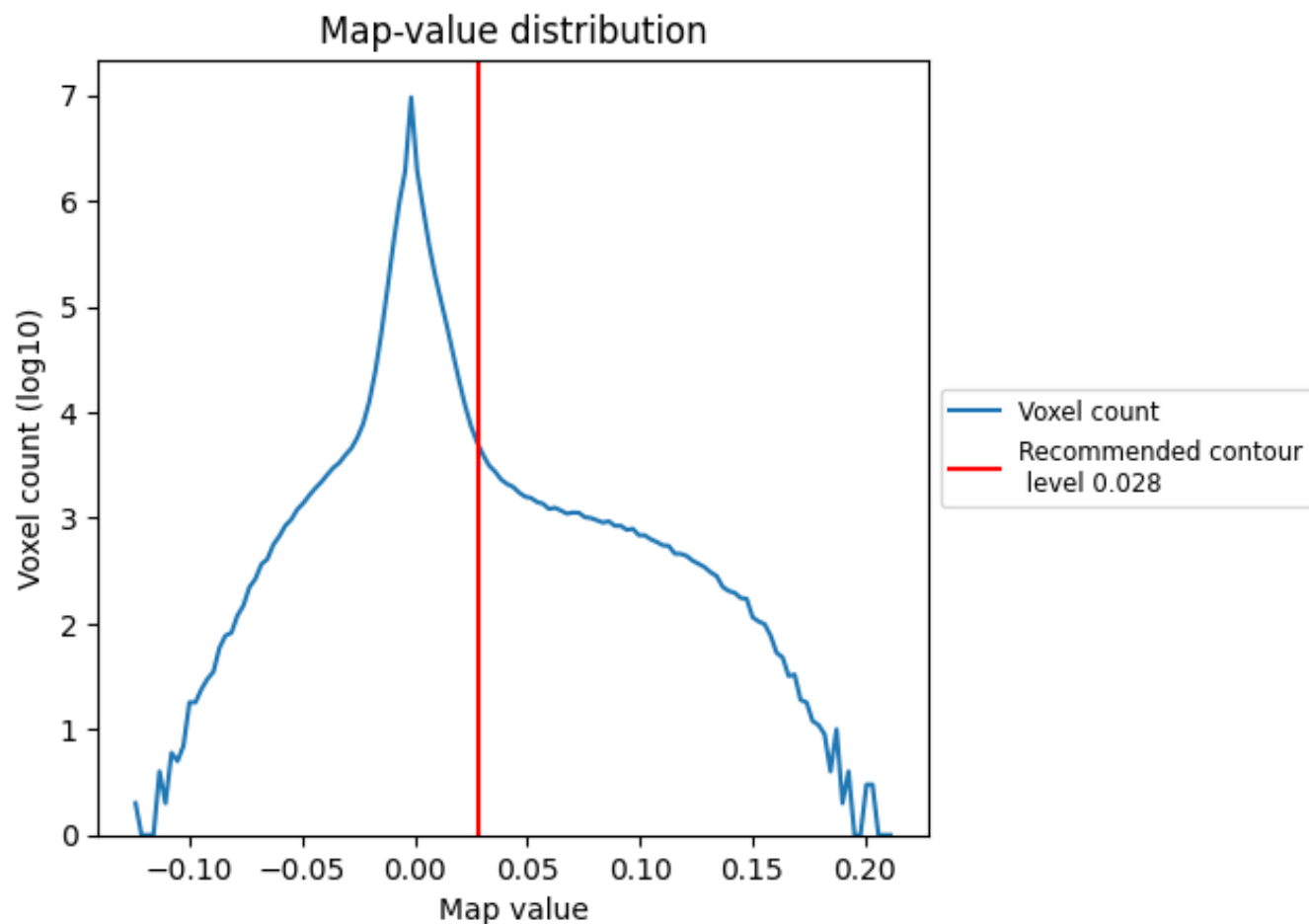
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

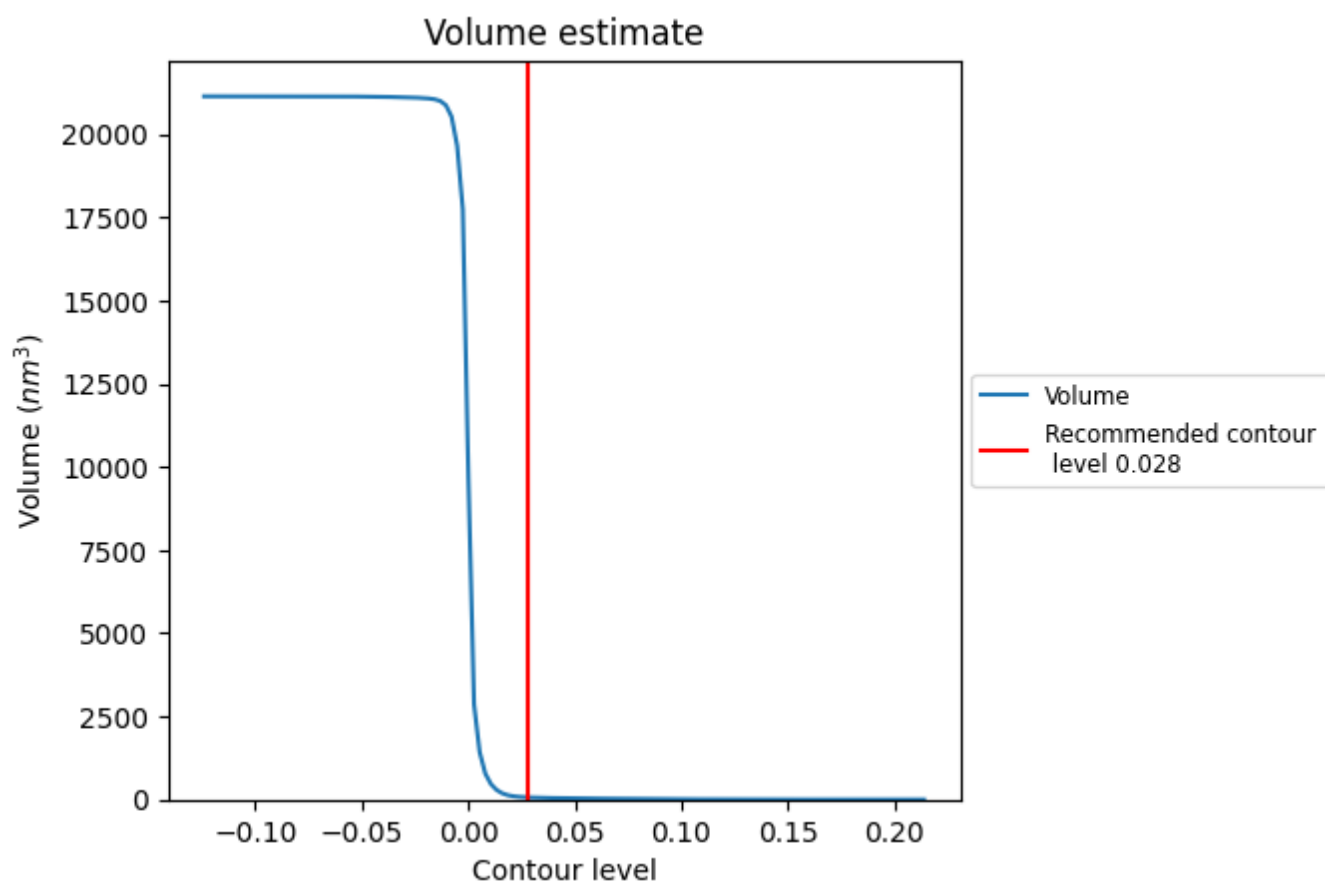
This section contains the results of statistical analysis of the map.

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.

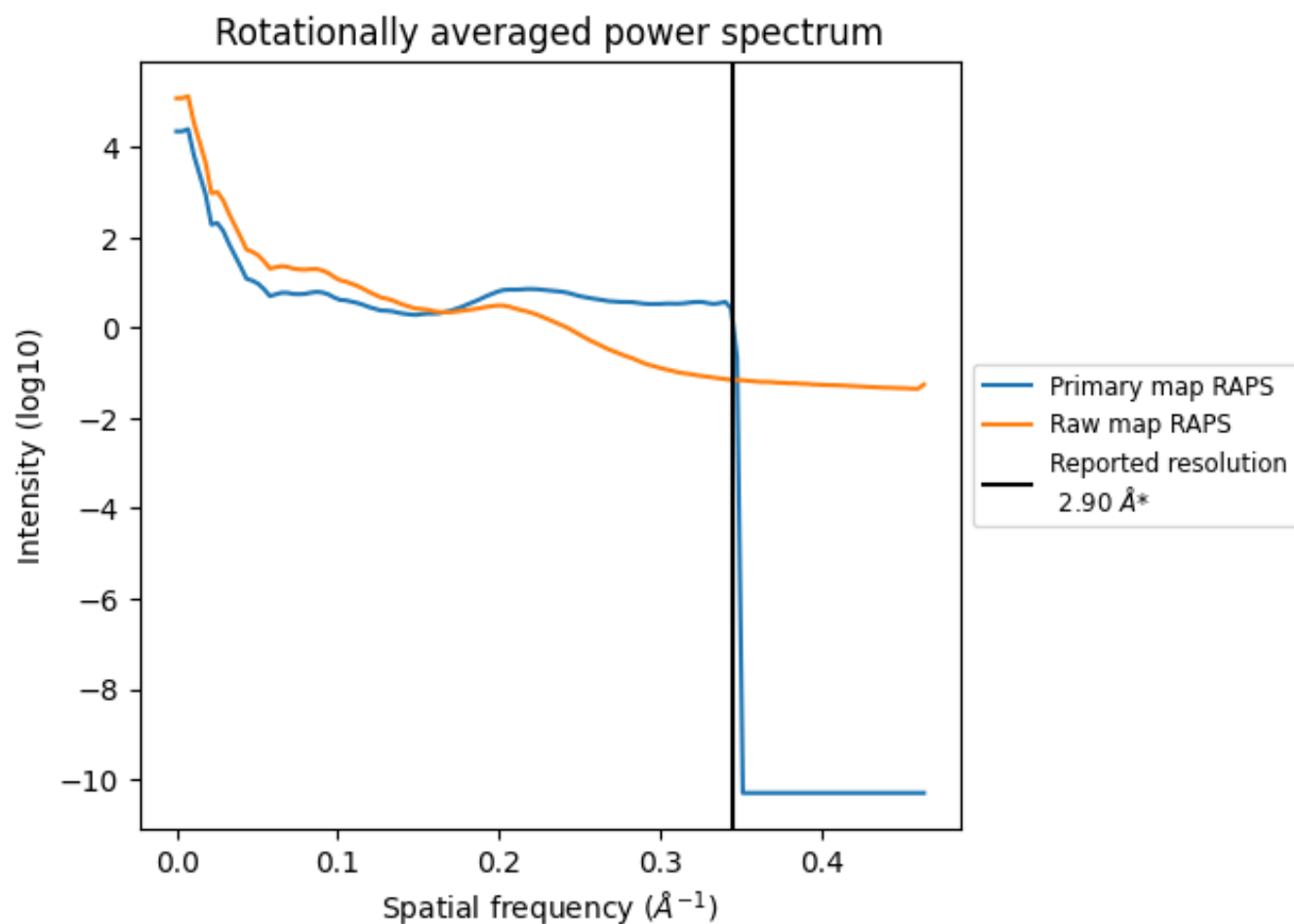
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 66 nm^3 ; this corresponds to an approximate mass of 59 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

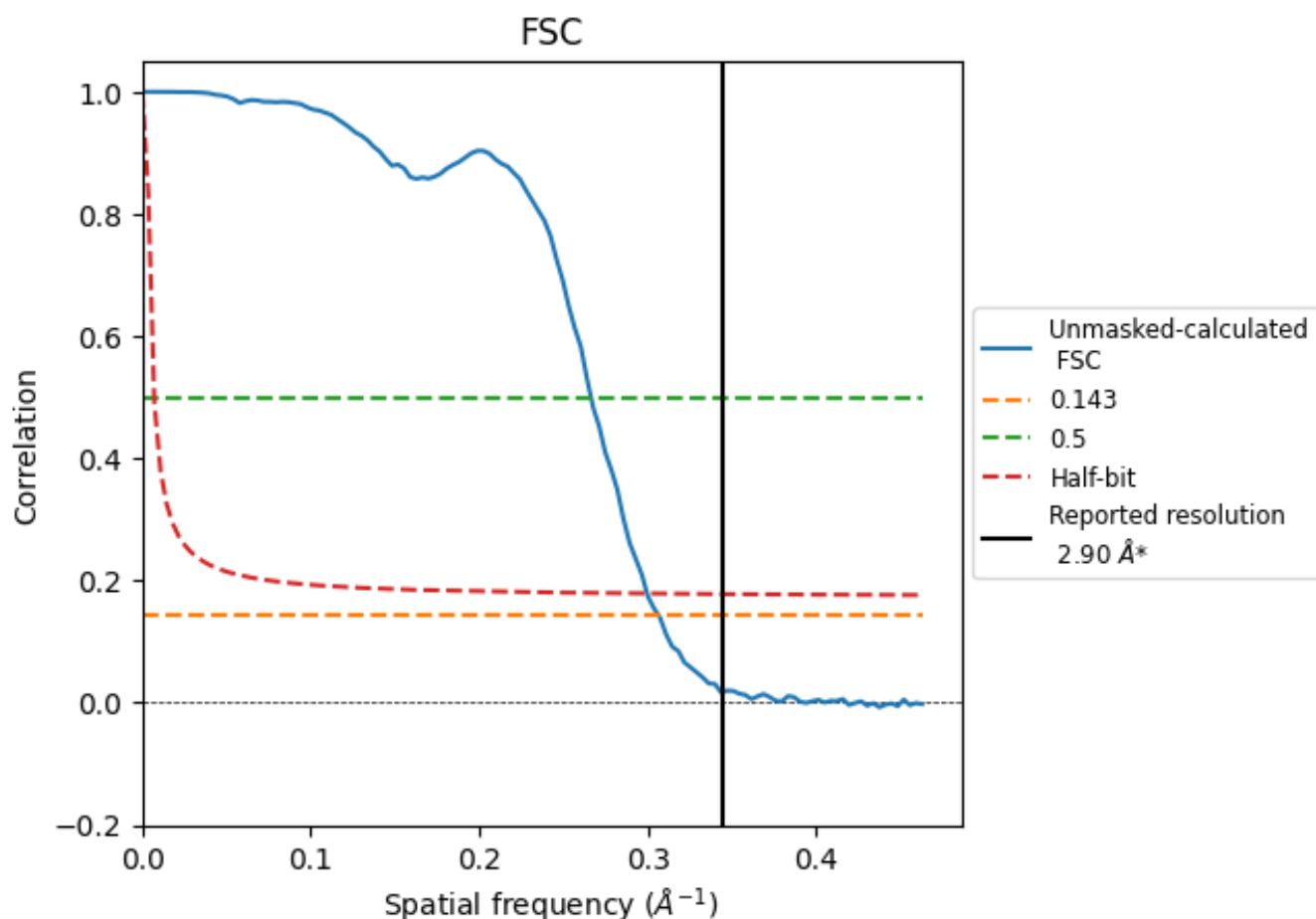


*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.26	3.75	3.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.26 differs from the reported value 2.9 by more than 10 %

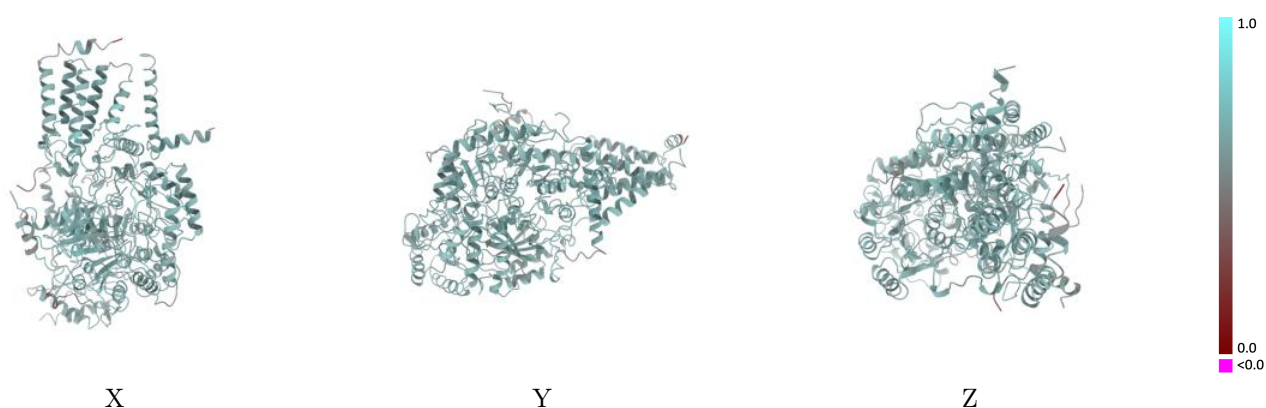
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33864 and PDB model 7YIU. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

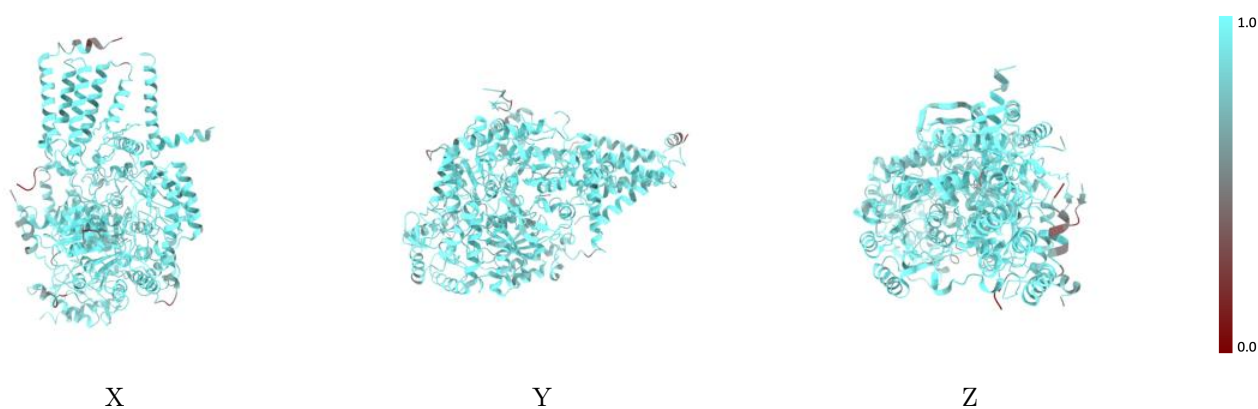
This section was not generated.

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



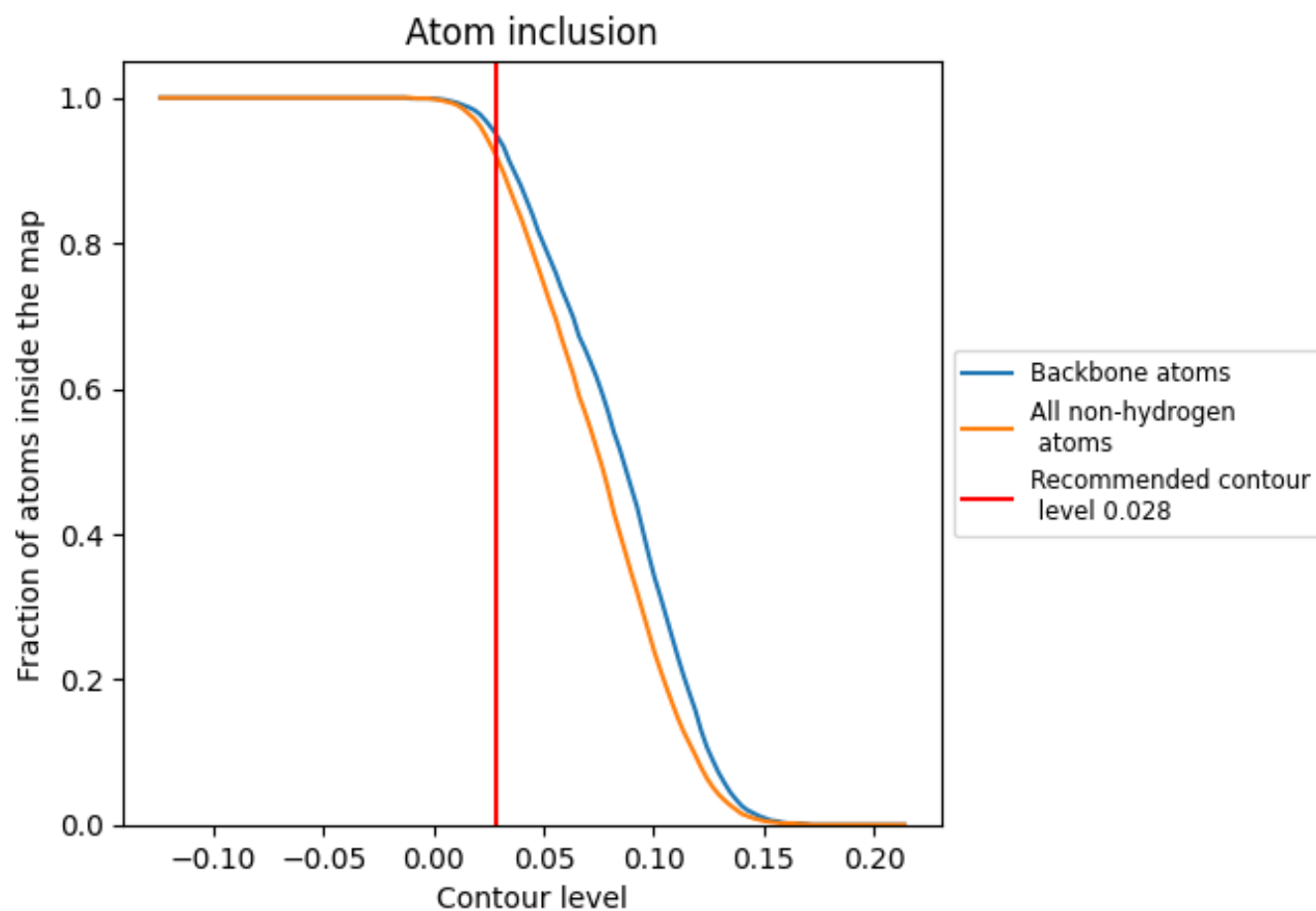
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.028).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% 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 (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9230	0.6160
A	0.9160	0.6090
B	0.9340	0.6230
C	0.9200	0.6110
D	0.9540	0.6290
E	0.7490	0.5530

