



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 01:01 AM UTC

PDB ID : 8TOE / pdb_00008toe
EMDB ID : EMD-41448
Title : Escherichia coli RNA polymerase unwinding intermediate (I1c) at the lambda PR promoter
Authors : Darst, S.A.; Saecker, R.M.; Mueller, A.U.
Deposited on : 2023-08-03
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:

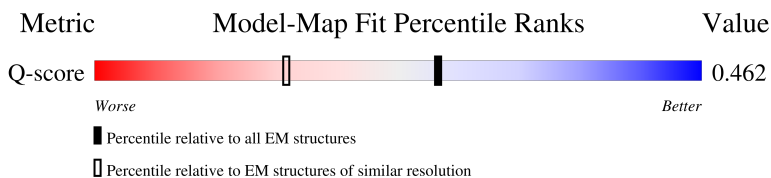
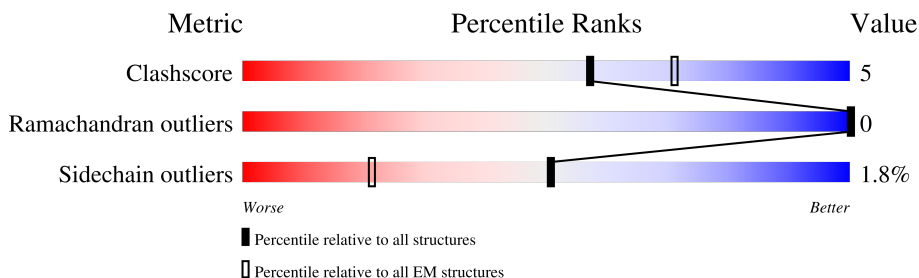
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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.



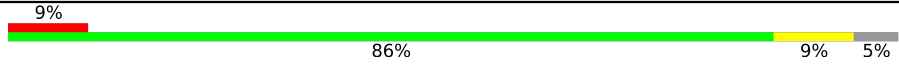
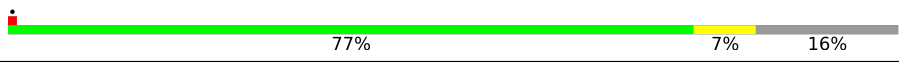
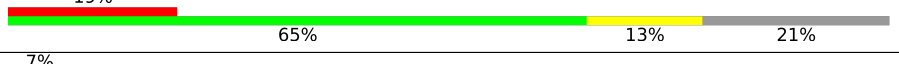


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	G	329	62% (Green), 8% (Yellow), 29% (Grey)
1	H	329	55% (Green), 12% (Yellow), 33% (Grey)
1	M	329	18% (Red), 19% (Orange), 78% (Green)
2	I	1342	88% (Green), 11% (Yellow)

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Mol	Chain	Length	Quality of chain
3	J	1407	
4	K	91	
5	L	613	
6	O	105	
7	P	105	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 30996 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	G	232	Total 1773	C 1108	N 315	O 344	S 6	0	0
1	H	219	Total 1685	C 1054	N 295	O 330	S 6	0	0
1	M	73	Total 572	C 362	N 100	O 108	S 2	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	I	1336	Total 10518	C 6604	N 1833	O 2038	S 43	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	1335	Total 10381	C 6522	N 1851	O 1959	S 49	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	K	76	Total 605	C 368	N 115	O 121	S 1	0	0

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L	482	Total 3858	C 2416	N 691	O 728	S 23	0	0

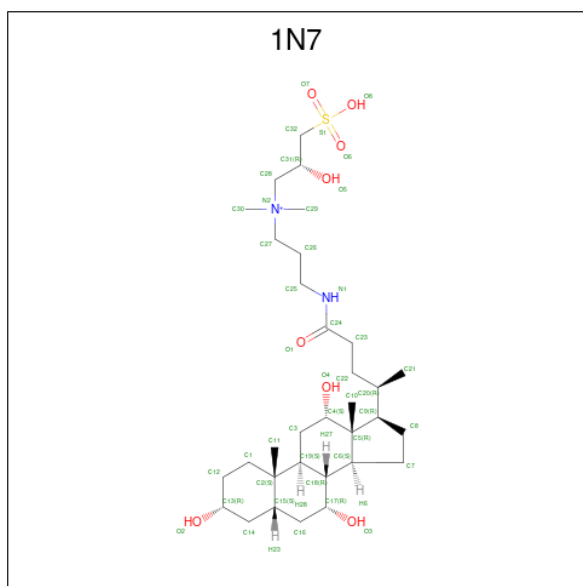
- Molecule 6 is a DNA chain called Nontemplate strand of lambda PR promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	O	40	820	391	140	249	40	0	0

- Molecule 7 is a DNA chain called Template strand of lambda PR promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	P	34	701	331	140	196	34	0	0

- Molecule 8 is CHAPSO (CCD ID: 1N7) (formula: C₃₂H₅₉N₂O₈S).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
8	I	1	26	23	3	0
8	J	1	27	24	3	0
8	L	1	27	24	3	0

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
9	J	1	1	1	0

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
10	J	2	Total 2	Zn 2	0

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	137962	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.477	Depositor
Minimum map value	-2.707	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	324.096, 324.096, 324.096	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84400004, 0.84400004, 0.84400004	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: ZN, 1N7, MG

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	G	0.15	0/1795	0.29	0/2436
1	H	0.13	0/1704	0.30	0/2310
1	M	0.08	0/579	0.22	0/784
2	I	0.16	0/10684	0.30	0/14415
3	J	0.13	0/10538	0.29	2/14229 (0.0%)
4	K	0.11	0/607	0.28	0/817
5	L	0.17	0/3906	0.32	0/5252
6	O	0.18	0/915	0.51	2/1409 (0.1%)
7	P	0.17	0/789	0.37	0/1215
All	All	0.15	0/31517	0.31	4/42867 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	O	74	DG	OP2-P-O3'	6.56	127.68	108.00
6	O	74	DG	O3'-P-O5'	-6.25	94.62	104.00
3	J	707	ILE	CA-C-N	5.91	132.33	121.70
3	J	707	ILE	C-N-CA	5.91	132.33	121.70

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	G	1773	0	1793	14	0
1	H	1685	0	1719	23	0
1	M	572	0	602	6	0
2	I	10518	0	10537	94	0
3	J	10381	0	10600	78	0
4	K	605	0	612	5	0
5	L	3858	0	3895	50	0
6	O	820	0	456	8	0
7	P	701	0	379	2	0
8	I	26	0	35	11	0
8	J	27	0	38	13	0
8	L	27	0	37	14	0
9	J	1	0	0	0	0
10	J	2	0	0	0	0
All	All	30996	0	30703	297	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (297) 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)
8:J:1504:1N7:C3	8:J:1504:1N7:C19	1.83	1.55
8:L:701:1N7:C3	8:L:701:1N7:C19	1.83	1.53
8:I:1401:1N7:C3	8:I:1401:1N7:C19	1.82	1.53
2:I:201:ARG:NH2	2:I:370:MET:SD	2.47	0.88
5:L:602:SER:N	5:L:605:GLU:OE2	2.15	0.79
5:L:552:THR:N	5:L:555:GLU:OE2	2.17	0.77
1:H:15:ASP:OD1	1:H:27:THR:OG1	2.00	0.76
2:I:749:ASP:N	2:I:749:ASP:OD1	2.15	0.76
2:I:624:ASP:OD1	2:I:625:GLU:N	2.19	0.76
3:J:665:GLN:OE1	3:J:678:ARG:NH1	2.21	0.74
8:I:1401:1N7:C3	8:I:1401:1N7:C2	2.65	0.73
1:G:45:ARG:NH2	2:I:1084:ASP:OD1	2.22	0.73
5:L:167:ASP:OD1	5:L:258:GLN:NE2	2.20	0.73
8:L:701:1N7:C3	8:L:701:1N7:C2	2.66	0.72
5:L:381:GLU:OE1	5:L:381:GLU:N	2.22	0.72
2:I:91:THR:OG1	2:I:138:ILE:O	2.04	0.72
2:I:987:GLU:O	2:I:991:LYS:NZ	2.23	0.72
3:J:1057:SER:OG	3:J:1110:GLU:OE2	2.08	0.70
8:J:1504:1N7:C3	8:J:1504:1N7:C2	2.67	0.69
2:I:444:ASP:O	2:I:450:ASN:ND2	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:557:LYS:NZ	5:L:561:MET:SD	2.63	0.68
2:I:197:ARG:NH1	2:I:201:ARG:O	2.27	0.68
2:I:573:ASN:N	2:I:573:ASN:OD1	2.27	0.68
4:K:42:GLU:N	4:K:42:GLU:OE1	2.27	0.68
3:J:1158:GLU:N	3:J:1158:GLU:OE1	2.27	0.67
2:I:148:GLN:OE1	2:I:454:ARG:NH1	2.28	0.67
5:L:513:ASP:OD1	5:L:514:ASP:N	2.29	0.66
1:G:13:LEU:HD12	1:G:13:LEU:O	1.95	0.65
5:L:234:THR:OG1	5:L:248:GLU:OE1	2.12	0.64
5:L:575:GLU:N	5:L:575:GLU:OE1	2.28	0.64
2:I:185:ASP:N	2:I:185:ASP:OD1	2.29	0.64
2:I:406:ASN:ND2	2:I:413:GLU:O	2.30	0.64
3:J:1048:ARG:NH2	3:J:1058:SER:O	2.31	0.64
5:L:505:ILE:CD1	8:L:701:1N7:H25	2.28	0.64
2:I:728:ASP:OD1	2:I:729:ALA:N	2.31	0.63
5:L:116:GLU:N	5:L:116:GLU:OE1	2.31	0.63
3:J:1173:ARG:NH2	3:J:1200:GLU:OE2	2.31	0.62
5:L:247:GLU:OE1	5:L:247:GLU:N	2.31	0.62
3:J:1205:GLU:OE1	3:J:1205:GLU:N	2.32	0.62
2:I:189:ASP:OD1	2:I:191:LYS:N	2.30	0.61
3:J:70:CYS:SG	3:J:71:LEU:N	2.73	0.61
8:J:1504:1N7:H24	8:L:701:1N7:H2	1.83	0.60
3:J:140:TYR:OH	3:J:312:ARG:NH2	2.34	0.60
3:J:388:ARG:NH2	3:J:414:GLU:OE2	2.34	0.60
2:I:714:VAL:O	2:I:767:GLN:NE2	2.35	0.60
2:I:631:GLU:OE1	2:I:631:GLU:N	2.35	0.60
2:I:651:ASP:OD1	2:I:651:ASP:N	2.35	0.59
5:L:505:ILE:HD13	8:L:701:1N7:H25	1.84	0.59
5:L:490:PRO:O	5:L:492:ASP:N	2.36	0.59
2:I:1061:GLN:NE2	2:I:1240:ASP:OD1	2.35	0.59
1:G:233:ASP:N	1:G:233:ASP:OD1	2.35	0.59
5:L:489:MET:HE3	5:L:494:ILE:HG12	1.83	0.59
2:I:318:SER:OG	2:I:320:ASP:OD1	2.18	0.58
5:L:271:ASN:OD1	5:L:274:ARG:NH2	2.35	0.58
2:I:626:GLU:OE2	2:I:628:HIS:ND1	2.36	0.58
5:L:358:VAL:O	5:L:362:ASN:ND2	2.36	0.58
2:I:1271:GLY:N	2:I:1274:GLU:OE1	2.36	0.58
1:H:16:ILE:HG22	1:H:26:VAL:HG22	1.86	0.57
3:J:568:SER:OG	3:J:570:LYS:NZ	2.37	0.57
8:J:1504:1N7:C3	8:J:1504:1N7:C18	2.72	0.57
1:H:77:ASP:OD1	1:H:78:ILE:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:712:GLN:OE1	3:J:712:GLN:N	2.37	0.57
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.37	0.57
8:L:701:1N7:H31	8:L:701:1N7:H5	1.84	0.57
1:G:102:LEU:HD23	1:G:142:MET:CE	2.35	0.57
2:I:374:GLU:OE2	5:L:99:ARG:NH1	2.38	0.57
3:J:1210:ILE:HG22	3:J:1211:SER:H	1.69	0.57
5:L:292:VAL:O	5:L:296:LYS:N	2.37	0.57
5:L:430:TYR:HA	6:O:75:DA:H4'	1.87	0.57
2:I:65:ASN:ND2	2:I:483:ASP:OD2	2.38	0.56
3:J:963:VAL:HG23	3:J:975:ILE:HG23	1.86	0.56
3:J:510:LEU:HD11	3:J:624:ILE:HG23	1.87	0.56
1:G:102:LEU:HD23	1:G:142:MET:HE2	1.88	0.56
2:I:620:ASN:ND2	2:I:620:ASN:O	2.39	0.56
5:L:568:ASN:OD1	5:L:569:THR:N	2.38	0.55
1:H:131:CYS:SG	1:H:132:HIS:N	2.79	0.55
2:I:742:TYR:O	2:I:744:GLY:N	2.39	0.55
3:J:1174:ARG:NH2	3:J:1187:GLU:OE1	2.37	0.55
5:L:280:VAL:HG22	5:L:347:ILE:HD12	1.88	0.55
1:M:290:LEU:O	1:M:290:LEU:HD23	2.07	0.55
3:J:707:ILE:HG22	3:J:713:GLU:HA	1.89	0.54
1:H:207:THR:HG22	1:H:208:ASN:H	1.72	0.54
8:J:1504:1N7:C16	8:L:701:1N7:H2	2.37	0.54
5:L:293:GLU:OE1	5:L:293:GLU:N	2.40	0.54
1:M:270:LEU:O	1:M:274:ALA:N	2.41	0.54
2:I:895:LEU:HD12	2:I:895:LEU:H	1.74	0.53
5:L:552:THR:OG1	5:L:555:GLU:OE1	2.26	0.53
2:I:353:VAL:HG12	2:I:353:VAL:O	2.07	0.53
3:J:1208:ASP:OD1	3:J:1209:VAL:N	2.37	0.53
5:L:601:PRO:O	5:L:602:SER:OG	2.20	0.53
2:I:196:VAL:HG21	2:I:209:ILE:HD12	1.91	0.53
8:J:1504:1N7:C17	8:L:701:1N7:H2	2.39	0.53
2:I:903:ARG:O	2:I:907:GLY:N	2.40	0.53
3:J:386:GLU:OE2	3:J:394:ILE:N	2.42	0.53
5:L:428:SER:OG	6:O:79:DT:O4	2.27	0.53
5:L:577:GLY:O	5:L:581:ASP:N	2.40	0.52
1:H:29:GLU:HB3	1:H:30:PRO:HD3	1.92	0.52
3:J:416:ILE:HG22	3:J:416:ILE:O	2.09	0.52
2:I:65:ASN:OD1	2:I:66:SER:N	2.42	0.52
3:J:475:GLU:OE2	4:K:28:ARG:NH1	2.38	0.52
2:I:1010:GLN:O	2:I:1014:LEU:HD23	2.09	0.52
3:J:964:LYS:N	3:J:977:SER:OG	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:80:HIS:O	3:J:83:VAL:HG12	2.09	0.52
3:J:195:GLU:OE1	3:J:195:GLU:N	2.39	0.52
1:G:50:SER:O	1:G:51:MET:HE2	2.09	0.51
1:H:172:LEU:HD23	1:H:172:LEU:H	1.74	0.51
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.92	0.51
3:J:799:ARG:NH1	3:J:1146:GLU:OE2	2.44	0.51
1:H:181:GLU:O	3:J:535:ARG:NH1	2.43	0.51
8:I:1401:1N7:H24	8:I:1401:1N7:O2	2.10	0.51
3:J:572:THR:HG21	3:J:589:TYR:CE2	2.46	0.51
4:K:3:ARG:NH2	4:K:55:GLU:OE1	2.43	0.51
5:L:138:PRO:HD3	5:L:353:LEU:HD12	1.91	0.51
5:L:309:ASN:OD1	5:L:311:THR:OG1	2.28	0.51
1:G:162:GLU:OE2	1:G:165:GLU:N	2.44	0.51
3:J:857:LEU:HD11	3:J:871:LEU:HD21	1.93	0.51
2:I:489:PRO:HA	2:I:492:MET:HE2	1.92	0.50
3:J:572:THR:HG21	3:J:589:TYR:OH	2.11	0.50
2:I:254:ASP:OD1	2:I:255:ILE:N	2.45	0.50
3:J:1164:SER:N	3:J:1176:VAL:O	2.45	0.50
3:J:75:TYR:CD2	3:J:83:VAL:HG11	2.47	0.50
2:I:808:ASN:H	3:J:633:ALA:HB2	1.77	0.50
2:I:989:LEU:HD12	2:I:992:LEU:HD21	1.93	0.50
1:H:192:VAL:O	1:H:194:GLN:N	2.45	0.50
1:H:212:ASP:OD1	1:H:212:ASP:N	2.44	0.50
2:I:748:ILE:HD11	2:I:966:ILE:HD12	1.94	0.50
5:L:94:THR:OG1	5:L:95:THR:N	2.45	0.50
2:I:811:ASN:O	2:I:811:ASN:ND2	2.44	0.49
3:J:29:MET:HE3	3:J:29:MET:HA	1.93	0.49
2:I:314:ASN:O	2:I:314:ASN:ND2	2.46	0.49
5:L:163:THR:O	5:L:260:ARG:NH2	2.45	0.49
8:L:701:1N7:C3	8:L:701:1N7:C18	2.72	0.49
5:L:426:LYS:O	5:L:427:PHE:C	2.55	0.49
3:J:349:TYR:HB3	3:J:470:VAL:HG13	1.95	0.49
3:J:1072:LYS:O	3:J:1075:ARG:NH1	2.45	0.49
2:I:582:ASN:OD1	2:I:583:GLU:N	2.42	0.48
3:J:1051:ASP:O	3:J:1055:GLY:N	2.45	0.48
3:J:707:ILE:HA	3:J:708:ASN:HB2	1.95	0.48
2:I:1333:LEU:HD13	3:J:115:TRP:CH2	2.48	0.48
5:L:305:LEU:HD11	5:L:322:MET:HE1	1.94	0.48
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.95	0.48
2:I:738:GLU:OE1	2:I:738:GLU:N	2.41	0.48
1:H:33:ARG:NH1	2:I:820:GLU:OE2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:4:SER:OG	1:H:5:VAL:N	2.47	0.48
3:J:1356:LEU:O	3:J:1366:HIS:NE2	2.41	0.48
3:J:1210:ILE:O	3:J:1211:SER:C	2.57	0.48
1:H:197:ASP:N	1:H:197:ASP:OD1	2.48	0.47
8:L:701:1N7:H36	8:L:701:1N7:H30	1.64	0.47
2:I:205:PRO:O	2:I:208:ILE:HG22	2.14	0.47
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.97	0.47
2:I:317:LEU:HD21	2:I:322:LEU:HD21	1.96	0.47
2:I:577:VAL:HG23	2:I:661:VAL:O	2.14	0.47
8:I:1401:1N7:C3	8:I:1401:1N7:C1	2.93	0.47
8:I:1401:1N7:H7	8:I:1401:1N7:O3	2.15	0.47
2:I:320:ASP:OD1	2:I:321:LEU:N	2.47	0.47
4:K:15:ASN:OD1	4:K:16:ARG:N	2.48	0.47
2:I:1070:HIS:NE2	2:I:1114:GLU:OE1	2.43	0.47
3:J:661:VAL:HG23	3:J:682:VAL:HG22	1.96	0.47
1:H:202:VAL:HG12	1:H:202:VAL:O	2.15	0.46
2:I:408:SER:O	2:I:431:LYS:NZ	2.46	0.46
2:I:525:THR:HG21	2:I:687:ARG:CD	2.45	0.46
2:I:1240:ASP:OD1	2:I:1240:ASP:N	2.49	0.46
3:J:342:LEU:HD13	3:J:1352:ILE:HG23	1.98	0.46
7:P:43:DG:H2'	7:P:44:DT:H72	1.97	0.46
2:I:675:ASP:OD2	2:I:677:ASN:ND2	2.44	0.46
2:I:967:LEU:HD13	2:I:1021:LEU:HD11	1.97	0.46
8:I:1401:1N7:H5	8:I:1401:1N7:H31	1.98	0.46
3:J:960:LEU:HD13	3:J:963:VAL:CG1	2.45	0.46
2:I:303:ASP:O	2:I:307:GLY:N	2.48	0.46
2:I:876:GLU:OE1	2:I:927:THR:HG22	2.15	0.46
8:L:701:1N7:H15	8:L:701:1N7:H27	1.72	0.46
3:J:111:THR:O	3:J:239:LEU:N	2.46	0.46
3:J:194:LEU:HD22	3:J:224:LEU:HD13	1.97	0.46
5:L:555:GLU:OE1	5:L:555:GLU:N	2.35	0.46
3:J:871:LEU:C	3:J:871:LEU:HD23	2.41	0.46
2:I:273:HIS:O	2:I:277:LEU:HD13	2.17	0.45
2:I:452:ARG:NH2	2:I:458:GLU:OE2	2.49	0.45
1:M:250:ASP:OD2	1:M:252:ILE:HG22	2.17	0.45
1:G:74:VAL:HG12	1:G:133:LEU:HD23	1.98	0.45
5:L:227:GLN:HG3	5:L:252:LEU:HD13	1.99	0.45
3:J:1098:GLN:OE1	3:J:1098:GLN:N	2.50	0.45
6:O:59:DT:H4'	6:O:60:DT:OP1	2.16	0.45
1:G:28:LEU:HD12	1:G:28:LEU:N	2.32	0.45
2:I:411:ARG:NH2	2:I:427:ASP:OD2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:598:VAL:HG22	2:I:628:HIS:CD2	2.51	0.45
2:I:1255:THR:HG23	2:I:1255:THR:O	2.16	0.45
3:J:572:THR:HG22	3:J:593:ASN:OD1	2.16	0.45
2:I:1103:VAL:HG11	2:I:1112:ILE:HD11	1.97	0.45
3:J:736:GLN:N	3:J:736:GLN:OE1	2.50	0.45
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.17	0.45
1:M:292:THR:OG1	1:M:295:LEU:HD13	2.16	0.45
1:H:83:LEU:HD11	3:J:526:VAL:HG12	1.98	0.45
1:G:155:ALA:O	1:G:159:ILE:HG22	2.18	0.44
2:I:28:LEU:O	2:I:28:LEU:HD12	2.16	0.44
2:I:521:LEU:O	2:I:525:THR:HG22	2.17	0.44
2:I:739:ASP:OD1	2:I:739:ASP:N	2.49	0.44
2:I:453:ILE:HD11	2:I:587:LEU:HD21	1.99	0.44
2:I:897:PRO:O	2:I:898:GLU:HB2	2.18	0.44
3:J:951:GLN:NE2	3:J:1014:GLY:O	2.51	0.44
3:J:1275:LEU:N	3:J:1275:LEU:HD12	2.32	0.44
5:L:565:ILE:HG22	5:L:566:ASP:OD1	2.17	0.44
8:I:1401:1N7:C3	8:I:1401:1N7:C18	2.73	0.44
3:J:848:VAL:HB	3:J:858:VAL:HG22	2.00	0.44
1:G:98:VAL:HG22	1:G:99:ILE:N	2.33	0.44
2:I:851:THR:OG1	2:I:853:ASP:OD2	2.34	0.44
8:J:1504:1N7:C3	8:J:1504:1N7:C1	2.96	0.44
8:J:1504:1N7:C3	8:J:1504:1N7:H1	2.48	0.44
1:H:78:ILE:O	1:H:79:LEU:HB3	2.18	0.43
3:J:151:MET:SD	3:J:151:MET:N	2.80	0.43
3:J:952:VAL:HG13	3:J:1014:GLY:H	1.82	0.43
5:L:290:LEU:HB3	5:L:333:VAL:HG21	1.99	0.43
2:I:802:VAL:HG21	2:I:1098:LEU:HD22	2.00	0.43
5:L:426:LYS:O	5:L:428:SER:N	2.51	0.43
1:G:224:LEU:HD23	1:H:228:LEU:HD11	2.01	0.43
2:I:967:LEU:HD12	2:I:1025:PHE:CE1	2.53	0.43
5:L:514:ASP:OD1	5:L:515:GLU:N	2.51	0.43
3:J:964:LYS:O	3:J:976:THR:N	2.39	0.43
5:L:119:ILE:HD13	5:L:122:ARG:HH21	1.83	0.43
2:I:131:THR:HG22	2:I:132:ASP:N	2.33	0.43
3:J:801:VAL:HG12	3:J:920:ALA:HB3	2.00	0.43
5:L:484:ALA:HB2	5:L:491:GLU:HA	1.99	0.43
3:J:1349:GLU:OE1	3:J:1349:GLU:N	2.52	0.43
2:I:1037:THR:HG22	2:I:1037:THR:O	2.18	0.43
8:J:1504:1N7:H26	8:L:701:1N7:H2	2.00	0.43
1:M:260:LEU:HD23	1:M:262:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:20:SER:OG	1:H:21:SER:N	2.50	0.43
3:J:354:VAL:HG12	3:J:355:ILE:N	2.34	0.43
2:I:350:THR:O	2:I:354:ASP:N	2.52	0.43
3:J:948:SER:OG	3:J:949:SER:N	2.51	0.43
3:J:858:VAL:O	3:J:858:VAL:HG23	2.18	0.43
2:I:485:ASP:OD1	2:I:486:THR:N	2.44	0.42
2:I:131:THR:HG22	2:I:132:ASP:OD1	2.19	0.42
8:J:1504:1N7:O3	8:J:1504:1N7:H21	2.18	0.42
6:O:69:DG:H4'	6:O:70:DC:OP1	2.19	0.42
1:G:104:LYS:HG2	1:G:110:VAL:HG22	2.01	0.42
3:J:516:ASP:OD1	3:J:516:ASP:N	2.52	0.42
3:J:1289:ASN:OD1	3:J:1290:ARG:N	2.52	0.42
8:J:1504:1N7:H14	8:J:1504:1N7:H29	1.73	0.42
8:L:701:1N7:C3	8:L:701:1N7:C1	2.96	0.42
2:I:542:ARG:HE	2:I:542:ARG:HB2	1.71	0.42
5:L:479:THR:HG23	5:L:482:GLU:H	1.83	0.42
2:I:1256:GLN:NE2	5:L:525:ASP:OD2	2.53	0.42
8:I:1401:1N7:H14	8:I:1401:1N7:H29	1.83	0.42
4:K:3:ARG:NH1	4:K:55:GLU:OE1	2.50	0.42
2:I:179:TYR:CZ	8:I:1401:1N7:H21	2.55	0.42
2:I:595:THR:O	2:I:596:ASP:C	2.62	0.42
5:L:562:ARG:NH2	7:P:51:DG:OP1	2.53	0.42
1:H:28:LEU:N	1:H:28:LEU:HD12	2.35	0.42
5:L:511:ILE:HG22	5:L:517:SER:O	2.19	0.42
6:O:60:DT:H2'	6:O:61:DT:H71	2.02	0.42
6:O:69:DG:H2'	6:O:70:DC:O5'	2.20	0.42
3:J:644:MET:O	3:J:764:ARG:NE	2.53	0.42
3:J:1183:SER:OG	3:J:1184:ASP:N	2.53	0.42
5:L:487:MET:CE	5:L:489:MET:HE2	2.50	0.42
2:I:748:ILE:HD11	2:I:966:ILE:CD1	2.50	0.41
2:I:1046:VAL:O	2:I:1046:VAL:HG23	2.21	0.41
3:J:122:SER:O	3:J:125:GLY:N	2.53	0.41
1:M:316:MET:SD	1:M:316:MET:N	2.91	0.41
2:I:549:ASP:OD1	2:I:550:VAL:N	2.51	0.41
3:J:894:VAL:HG12	3:J:895:CYS:N	2.35	0.41
5:L:136:GLU:OE1	5:L:364:ARG:NH2	2.53	0.41
2:I:132:ASP:N	2:I:132:ASP:OD1	2.53	0.41
3:J:213:LYS:O	3:J:217:LEU:HG	2.21	0.41
3:J:528:THR:O	3:J:528:THR:HG22	2.21	0.41
5:L:509:THR:O	5:L:509:THR:HG23	2.19	0.41
1:H:61:ILE:O	1:H:64:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:638:SER:OG	2:I:639:LYS:N	2.53	0.41
3:J:388:ARG:NH1	3:J:414:GLU:OE1	2.53	0.41
3:J:162:GLU:O	3:J:166:LEU:HD23	2.21	0.41
1:H:76:GLU:OE1	1:H:84:ASN:ND2	2.51	0.41
5:L:99:ARG:NH2	6:O:81:DG:O6	2.53	0.41
1:H:118:ASP:HB2	1:H:121:VAL:HG22	2.03	0.41
3:J:975:ILE:HD12	3:J:997:VAL:HG11	2.02	0.41
5:L:558:VAL:HG22	5:L:591:GLU:OE2	2.21	0.41
2:I:672:GLU:OE1	2:I:1186:VAL:O	2.39	0.41
2:I:685:MET:HE2	2:I:1071:GLY:HA2	2.03	0.41
2:I:978:VAL:HG13	2:I:979:LEU:CD1	2.51	0.41
2:I:1106:ARG:O	2:I:1108:ASN:N	2.46	0.41
8:I:1401:1N7:C3	8:I:1401:1N7:H1	2.51	0.41
8:I:1401:1N7:O3	8:I:1401:1N7:C7	2.65	0.41
8:L:701:1N7:H17	8:L:701:1N7:H4	2.01	0.41
1:H:89:ALA:HB3	1:H:124:VAL:CG1	2.51	0.41
2:I:30:ILE:HG23	2:I:31:GLN:N	2.36	0.41
2:I:638:SER:O	2:I:639:LYS:C	2.64	0.41
2:I:179:TYR:OH	2:I:458:GLU:OE2	2.36	0.40
6:O:65:DT:H2"	6:O:66:DC:C6	2.56	0.40
2:I:845:LEU:H	2:I:845:LEU:HD12	1.87	0.40
2:I:967:LEU:HD12	2:I:1025:PHE:CZ	2.56	0.40
3:J:304:ASP:OD1	3:J:305:ALA:N	2.54	0.40
3:J:382:TYR:HE1	3:J:401:VAL:HG21	1.86	0.40
5:L:421:TYR:H	5:L:421:TYR:HD1	1.69	0.40
2:I:221:LEU:HD12	2:I:336:LEU:HD13	2.04	0.40
3:J:975:ILE:CD1	3:J:997:VAL:HG11	2.51	0.40
8:J:1504:1N7:H13	8:J:1504:1N7:H27	1.68	0.40
8:J:1504:1N7:H27	8:J:1504:1N7:H15	1.66	0.40
3:J:416:ILE:O	3:J:416:ILE:CG2	2.68	0.40
3:J:120:LEU:HB3	3:J:121:PRO:HD3	2.03	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	G	230/329 (70%)	219 (95%)	11 (5%)	0	100	100
1	H	215/329 (65%)	198 (92%)	17 (8%)	0	100	100
1	M	71/329 (22%)	70 (99%)	1 (1%)	0	100	100
2	I	1330/1342 (99%)	1255 (94%)	75 (6%)	0	100	100
3	J	1329/1407 (94%)	1264 (95%)	65 (5%)	0	100	100
4	K	74/91 (81%)	71 (96%)	3 (4%)	0	100	100
5	L	472/613 (77%)	454 (96%)	18 (4%)	0	100	100
All	All	3721/4440 (84%)	3531 (95%)	190 (5%)	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	G	193/286 (68%)	185 (96%)	8 (4%)	27	61
1	H	187/286 (65%)	184 (98%)	3 (2%)	55	83
1	M	65/286 (23%)	65 (100%)	0	100	100
2	I	1147/1157 (99%)	1122 (98%)	25 (2%)	45	77
3	J	1119/1168 (96%)	1107 (99%)	12 (1%)	65	88
4	K	65/75 (87%)	65 (100%)	0	100	100
5	L	411/540 (76%)	401 (98%)	10 (2%)	43	75
All	All	3187/3798 (84%)	3129 (98%)	58 (2%)	51	80

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	19	VAL
1	G	56	VAL

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Mol	Chain	Res	Type
1	G	74	VAL
1	G	97	GLU
1	G	100	LEU
1	G	173	VAL
1	G	233	ASP
1	G	235	ARG
1	H	13	LEU
1	H	14	VAL
1	H	66	HIS
2	I	185	ASP
2	I	189	ASP
2	I	513	GLN
2	I	516	ASP
2	I	542	ARG
2	I	550	VAL
2	I	573	ASN
2	I	651	ASP
2	I	657	THR
2	I	697	LYS
2	I	699	LEU
2	I	739	ASP
2	I	748	ILE
2	I	749	ASP
2	I	811	ASN
2	I	912	ASP
2	I	1000	LEU
2	I	1003	THR
2	I	1109	ILE
2	I	1225	VAL
2	I	1227	VAL
2	I	1233	LEU
2	I	1240	ASP
2	I	1256	GLN
2	I	1269	ARG
3	J	76	LYS
3	J	304	ASP
3	J	387	LEU
3	J	413	ASP
3	J	430	HIS
3	J	470	VAL
3	J	473	THR
3	J	489	ASN

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Mol	Chain	Res	Type
3	J	800	LEU
3	J	807	LEU
3	J	925	GLU
3	J	1367	GLN
5	L	124	GLU
5	L	145	LEU
5	L	353	LEU
5	L	381	GLU
5	L	384	LEU
5	L	388	ILE
5	L	394	TYR
5	L	402	LEU
5	L	488	LEU
5	L	494	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	41	ASN
2	I	46	GLN
2	I	150	HIS
2	I	314	ASN
2	I	725	GLN
2	I	737	ASN
2	I	767	GLN
2	I	894	GLN
2	I	955	GLN
2	I	1256	GLN
3	J	364	HIS
3	J	651	HIS
3	J	720	ASN
3	J	739	GLN
3	J	921	GLN
3	J	1197	ASN
3	J	1326	GLN
4	K	43	ASN
4	K	62	GLN
5	L	129	GLN
5	L	345	GLN

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](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	1N7	L	701	-	30,30,46	5.27	15 (50%)	47,48,72	2.46	15 (31%)
8	1N7	J	1504	-	30,30,46	5.32	16 (53%)	47,48,72	2.62	16 (34%)
8	1N7	I	1401	-	29,29,46	5.30	15 (51%)	47,47,72	2.60	14 (29%)

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	1N7	L	701	-	-	7/7/72/92	0/4/4/4
8	1N7	J	1504	-	-	5/7/72/92	0/4/4/4
8	1N7	I	1401	-	-	6/6/71/92	0/4/4/4

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1504	1N7	C3-C19	18.26	1.83	1.53
8	L	701	1N7	C3-C19	18.10	1.83	1.53
8	I	1401	1N7	C3-C19	17.95	1.82	1.53
8	J	1504	1N7	C3-C4	12.68	1.73	1.53
8	L	701	1N7	C3-C4	12.32	1.73	1.53
8	I	1401	1N7	C3-C4	12.08	1.73	1.53
8	L	701	1N7	C5-C4	-9.54	1.39	1.54
8	I	1401	1N7	C5-C4	-9.54	1.39	1.54
8	J	1504	1N7	C5-C4	-9.32	1.40	1.54
8	J	1504	1N7	C2-C19	-9.16	1.40	1.56
8	L	701	1N7	C2-C19	-9.13	1.40	1.56
8	I	1401	1N7	C2-C19	-9.11	1.40	1.56
8	L	701	1N7	C8-C7	6.30	1.71	1.54
8	I	1401	1N7	C8-C7	6.27	1.71	1.54
8	J	1504	1N7	C8-C7	6.25	1.71	1.54
8	J	1504	1N7	C5-C6	-5.03	1.47	1.55
8	L	701	1N7	C5-C6	-4.91	1.47	1.55
8	J	1504	1N7	C18-C6	-4.79	1.44	1.53
8	I	1401	1N7	C5-C6	-4.76	1.47	1.55
8	L	701	1N7	C18-C6	-4.55	1.45	1.53
8	I	1401	1N7	O4-C4	-4.13	1.36	1.43
8	L	701	1N7	O4-C4	-4.12	1.36	1.43
8	I	1401	1N7	C18-C6	-4.11	1.46	1.53
8	J	1504	1N7	O4-C4	-4.07	1.36	1.43
8	I	1401	1N7	C7-C6	3.43	1.61	1.54
8	L	701	1N7	C7-C6	3.42	1.61	1.54
8	J	1504	1N7	C7-C6	3.30	1.61	1.54
8	L	701	1N7	C14-C15	-3.29	1.48	1.53
8	J	1504	1N7	C14-C15	-3.06	1.48	1.53
8	J	1504	1N7	C2-C15	3.04	1.60	1.55
8	I	1401	1N7	C20-C9	-2.94	1.49	1.54
8	L	701	1N7	C2-C15	2.90	1.59	1.55
8	J	1504	1N7	C20-C9	-2.88	1.49	1.54
8	I	1401	1N7	C14-C15	-2.88	1.49	1.53
8	L	701	1N7	C20-C9	-2.81	1.49	1.54
8	I	1401	1N7	C14-C13	2.78	1.56	1.52
8	I	1401	1N7	C2-C15	2.77	1.59	1.55
8	J	1504	1N7	C5-C9	2.50	1.59	1.55
8	J	1504	1N7	C14-C13	2.48	1.56	1.52
8	L	701	1N7	C14-C13	2.45	1.56	1.52
8	L	701	1N7	C5-C9	2.42	1.59	1.55
8	I	1401	1N7	C5-C9	2.38	1.59	1.55
8	J	1504	1N7	O2-C13	-2.26	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	701	1N7	O2-C13	-2.26	1.36	1.43
8	I	1401	1N7	O2-C13	-2.25	1.36	1.43
8	J	1504	1N7	C16-C15	2.14	1.57	1.53

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1401	1N7	C9-C5-C4	-8.88	109.68	117.67
8	J	1504	1N7	C9-C5-C4	-8.33	110.17	117.67
8	L	701	1N7	C9-C5-C4	-8.15	110.33	117.67
8	I	1401	1N7	C6-C5-C4	6.96	113.78	107.42
8	J	1504	1N7	C5-C9-C20	-6.90	111.12	119.48
8	I	1401	1N7	C5-C9-C20	-5.89	112.34	119.48
8	L	701	1N7	C5-C9-C20	-5.75	112.52	119.48
8	L	701	1N7	C7-C6-C18	-5.64	110.62	118.36
8	J	1504	1N7	C7-C6-C18	-5.37	110.99	118.36
8	J	1504	1N7	C9-C5-C6	5.35	105.48	100.11
8	I	1401	1N7	C7-C6-C18	-5.17	111.26	118.36
8	I	1401	1N7	C19-C3-C4	-5.14	107.57	114.29
8	L	701	1N7	C6-C5-C4	4.48	111.51	107.42
8	J	1504	1N7	C6-C5-C4	4.09	111.16	107.42
8	L	701	1N7	C19-C3-C4	-4.08	108.95	114.29
8	J	1504	1N7	C7-C6-C5	4.03	107.45	103.54
8	L	701	1N7	C9-C5-C6	4.01	104.13	100.11
8	J	1504	1N7	C5-C6-C18	-3.88	109.80	114.72
8	I	1401	1N7	C3-C19-C2	-3.77	109.88	113.70
8	J	1504	1N7	C8-C9-C5	3.69	107.12	103.54
8	L	701	1N7	C14-C15-C2	-3.46	108.98	112.66
8	I	1401	1N7	C16-C15-C2	-3.36	109.08	112.66
8	I	1401	1N7	C9-C5-C6	3.25	103.38	100.11
8	L	701	1N7	C3-C19-C2	-3.25	110.41	113.70
8	I	1401	1N7	C19-C18-C17	-3.06	108.01	111.86
8	I	1401	1N7	C15-C16-C17	-2.98	110.85	114.40
8	I	1401	1N7	C21-C20-C9	-2.95	108.46	112.88
8	L	701	1N7	C19-C18-C17	-2.92	108.18	111.86
8	J	1504	1N7	C2-C19-C18	-2.92	108.58	111.84
8	J	1504	1N7	C21-C20-C9	-2.80	108.68	112.88
8	L	701	1N7	C7-C6-C5	2.74	106.20	103.54
8	J	1504	1N7	C3-C19-C2	-2.67	111.00	113.70
8	L	701	1N7	C21-C20-C9	-2.63	108.93	112.88
8	J	1504	1N7	C16-C15-C2	-2.61	109.89	112.66
8	J	1504	1N7	C15-C16-C17	-2.56	111.35	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	701	1N7	C8-C9-C5	2.43	105.90	103.54
8	J	1504	1N7	C14-C15-C2	-2.40	110.11	112.66
8	J	1504	1N7	C19-C18-C17	-2.35	108.90	111.86
8	I	1401	1N7	C12-C1-C2	-2.21	109.00	112.74
8	L	701	1N7	C2-C19-C18	-2.21	109.38	111.84
8	I	1401	1N7	C3-C4-C5	-2.20	109.03	111.26
8	L	701	1N7	C6-C18-C17	-2.16	108.98	111.85
8	I	1401	1N7	C8-C9-C5	2.14	105.61	103.54
8	J	1504	1N7	C19-C3-C4	-2.08	111.57	114.29
8	L	701	1N7	C5-C6-C18	-2.02	112.16	114.72

There are no chirality outliers.

All (18) torsion outliers are listed below:

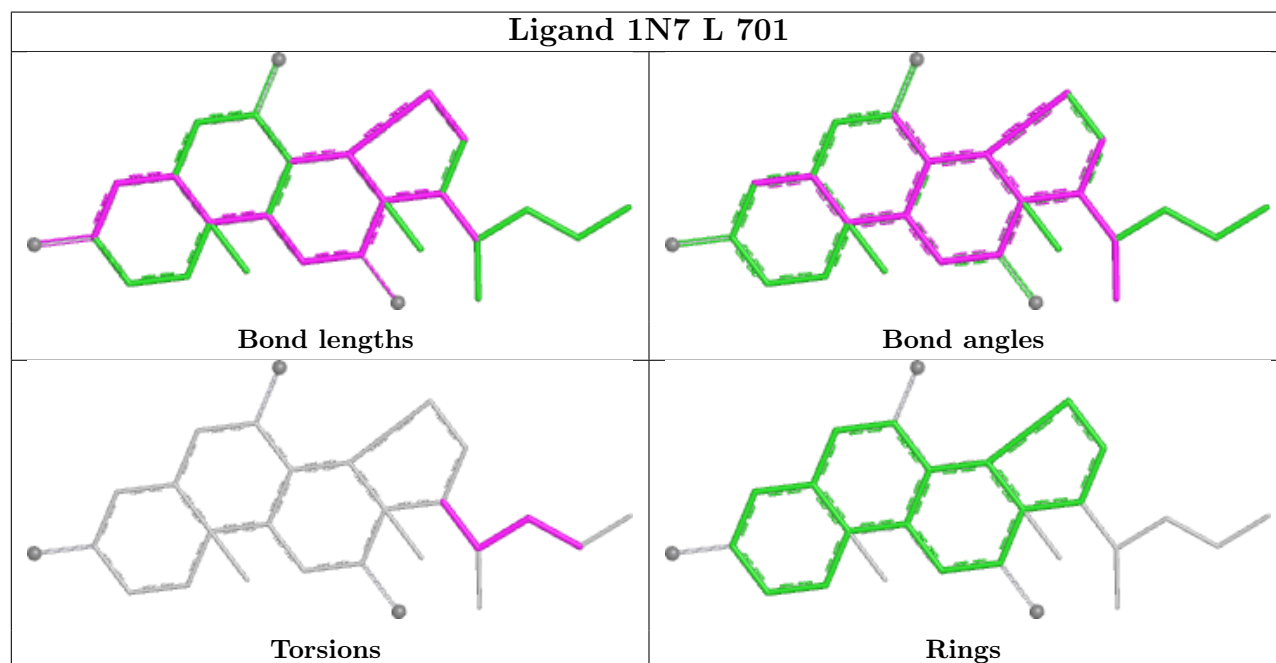
Mol	Chain	Res	Type	Atoms
8	L	701	1N7	C21-C20-C22-C23
8	I	1401	1N7	C21-C20-C9-C5
8	J	1504	1N7	C21-C20-C9-C5
8	L	701	1N7	C9-C20-C22-C23
8	I	1401	1N7	C21-C20-C9-C8
8	J	1504	1N7	C21-C20-C9-C8
8	I	1401	1N7	C22-C20-C9-C5
8	I	1401	1N7	C21-C20-C22-C23
8	J	1504	1N7	C22-C20-C9-C5
8	L	701	1N7	C21-C20-C9-C5
8	L	701	1N7	C20-C22-C23-C24
8	L	701	1N7	C21-C20-C9-C8
8	I	1401	1N7	C22-C20-C9-C8
8	J	1504	1N7	C22-C20-C9-C8
8	L	701	1N7	C22-C20-C9-C5
8	J	1504	1N7	C21-C20-C22-C23
8	L	701	1N7	C22-C20-C9-C8
8	I	1401	1N7	C9-C20-C22-C23

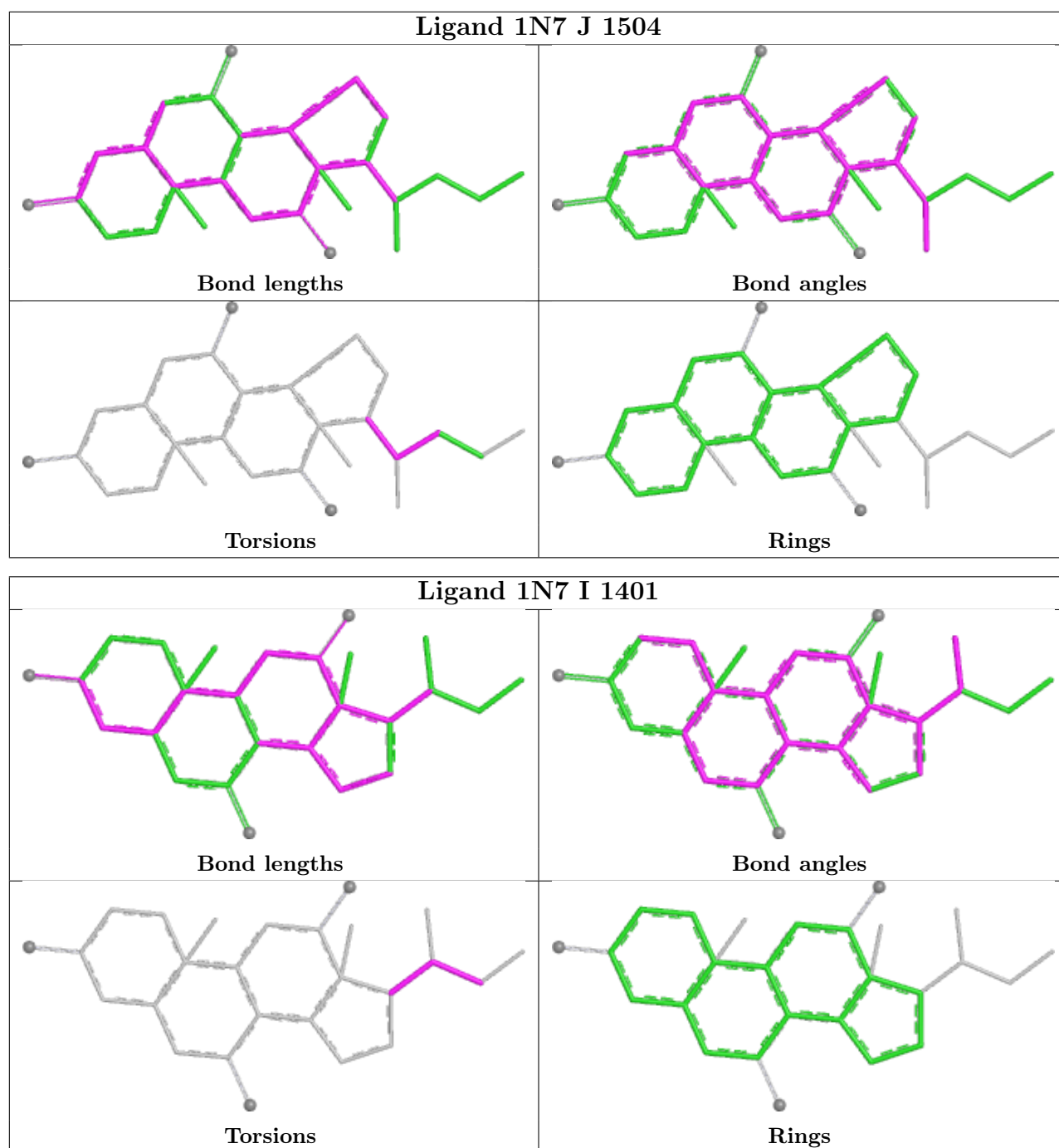
There are no ring outliers.

3 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	701	1N7	14	0
8	J	1504	1N7	13	0
8	I	1401	1N7	11	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	15:GLU	C	41:ASP	N	14.17

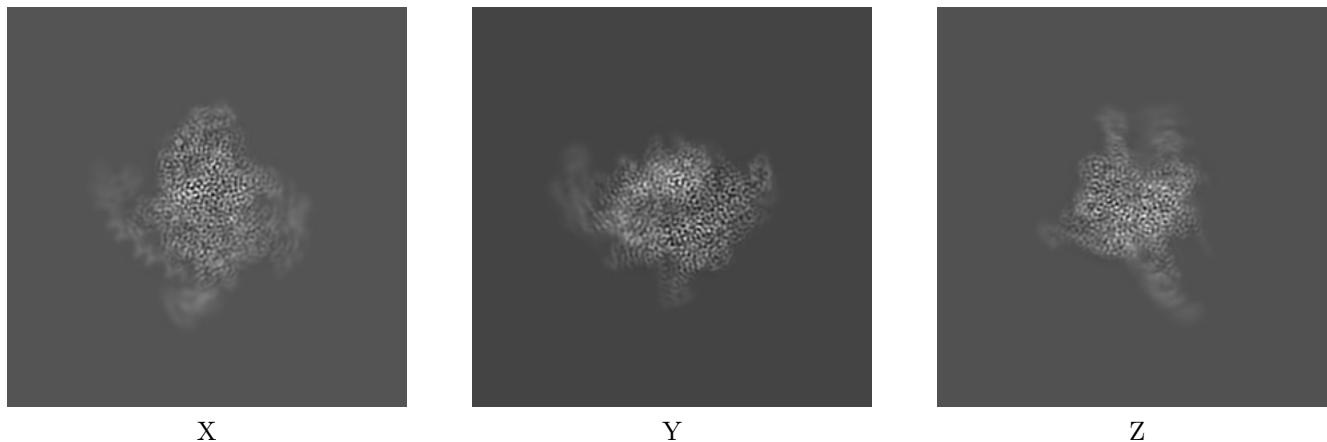
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41448. These allow visual inspection of the internal detail of the map and identification of artifacts.

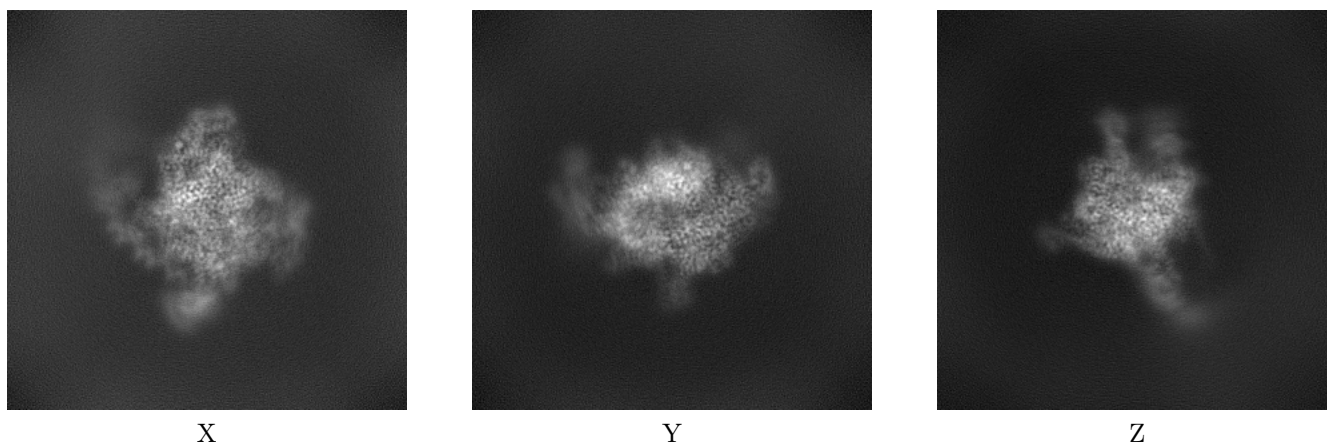
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



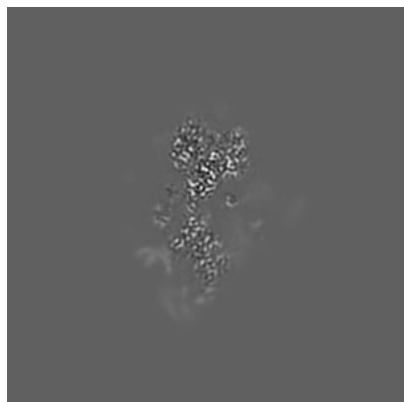
6.1.2 Raw map



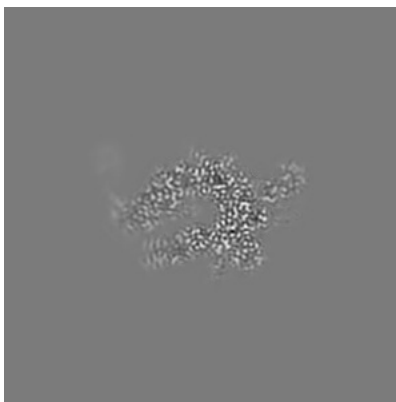
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

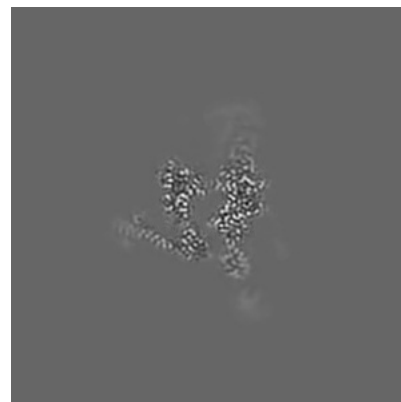
6.2.1 Primary map



X Index: 192

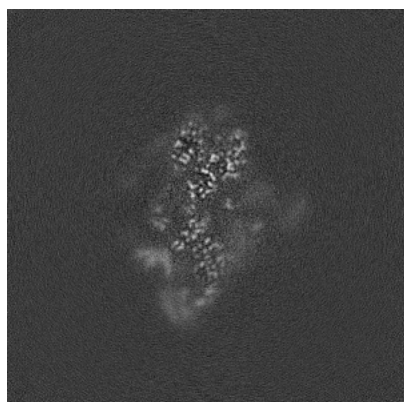


Y Index: 192

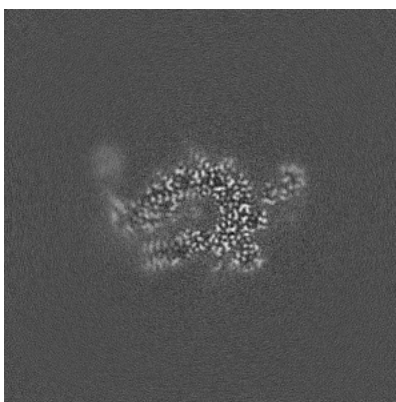


Z Index: 192

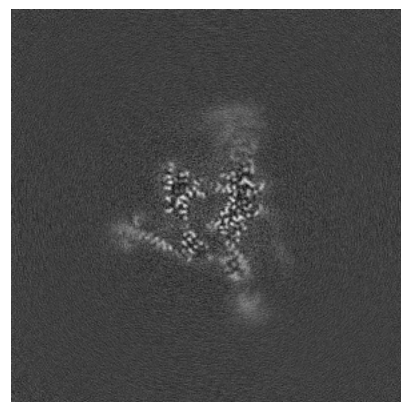
6.2.2 Raw map



X Index: 192



Y Index: 192

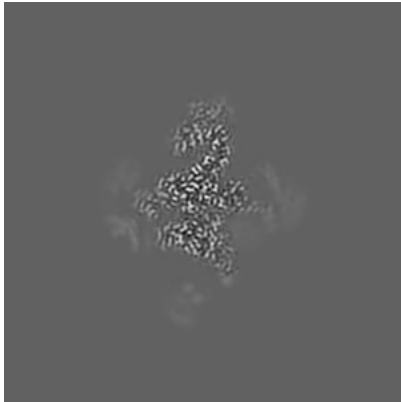


Z Index: 192

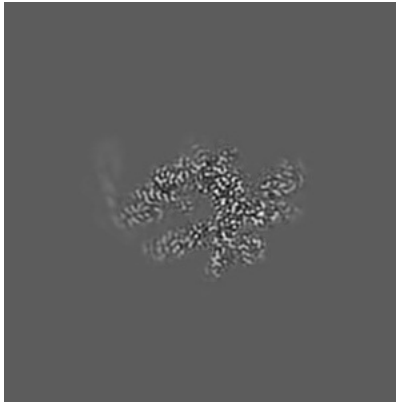
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

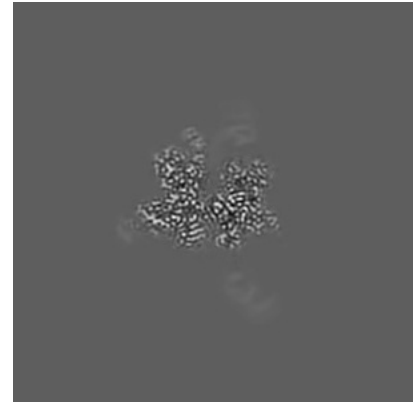
6.3.1 Primary map



X Index: 210

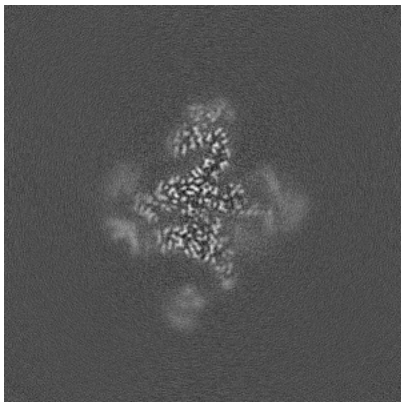


Y Index: 186

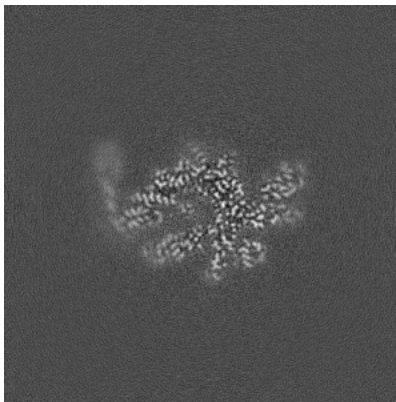


Z Index: 206

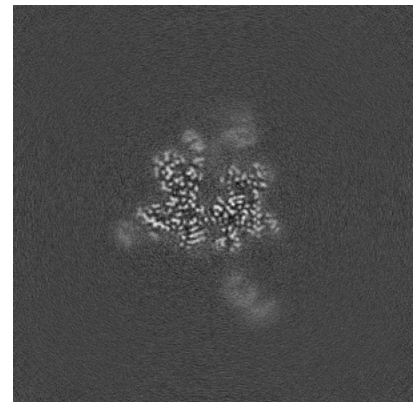
6.3.2 Raw map



X Index: 210



Y Index: 186

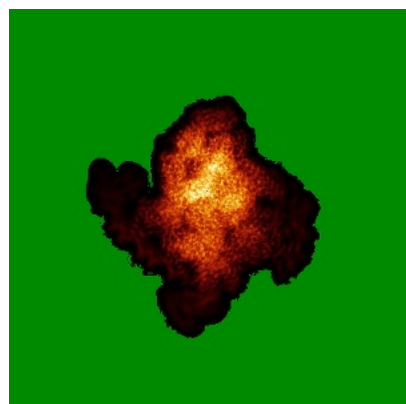


Z Index: 206

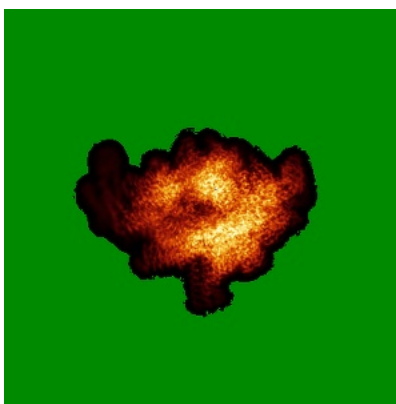
The images above show the largest variance slices of the map in three orthogonal directions.

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

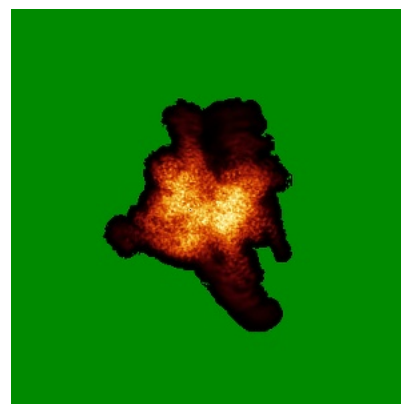
6.4.1 Primary map



X

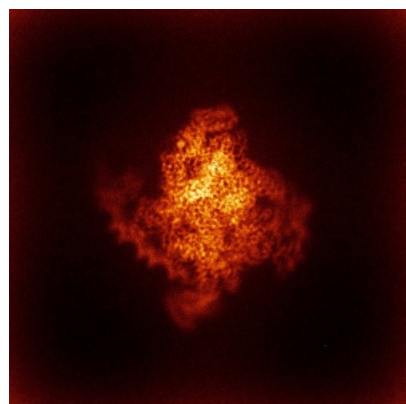


Y

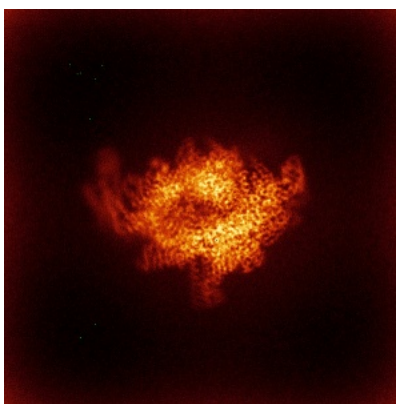


Z

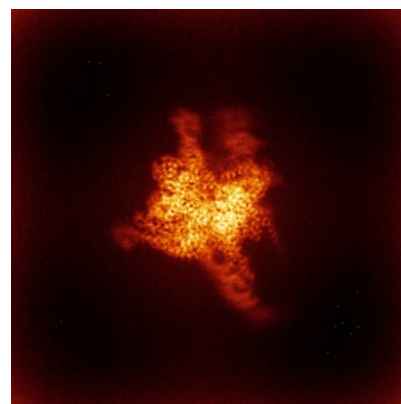
6.4.2 Raw map



X



Y

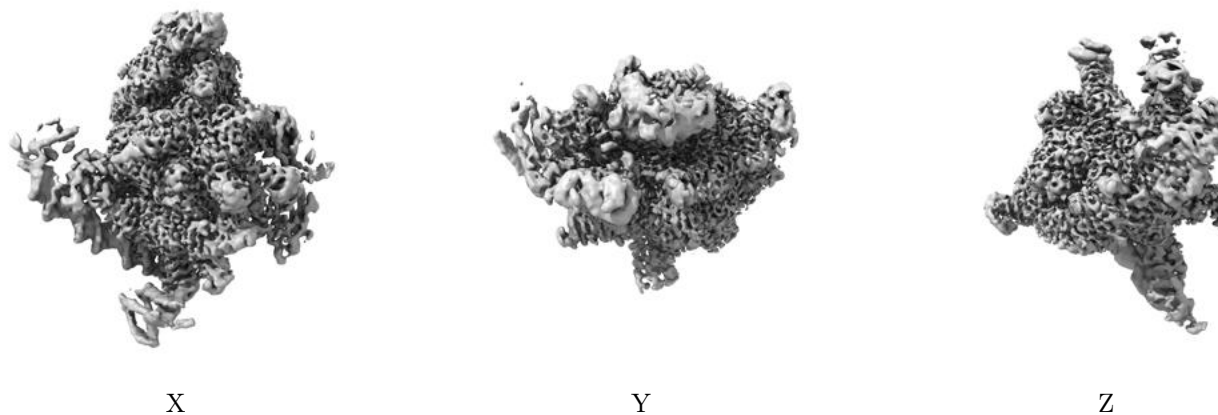


Z

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.

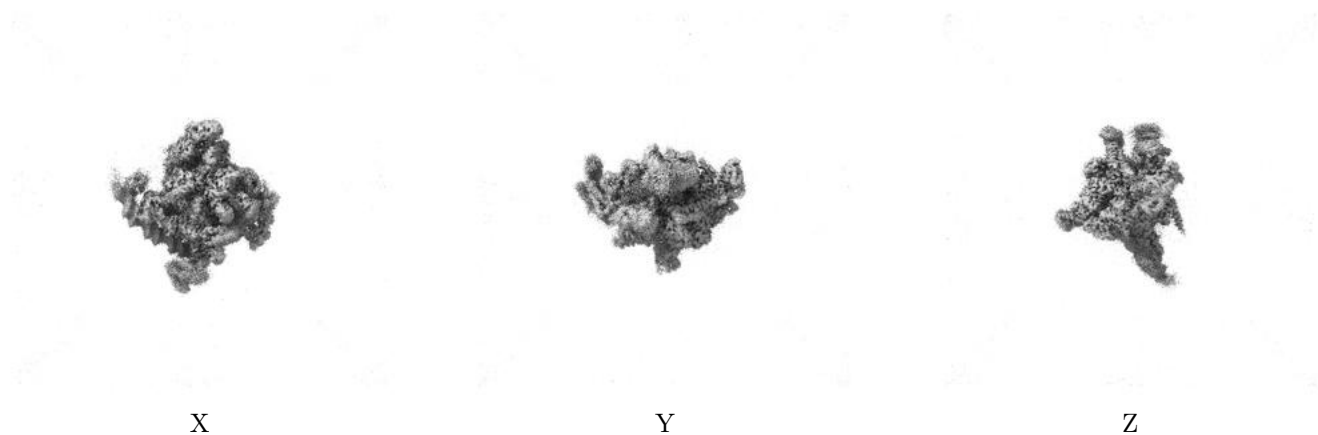
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

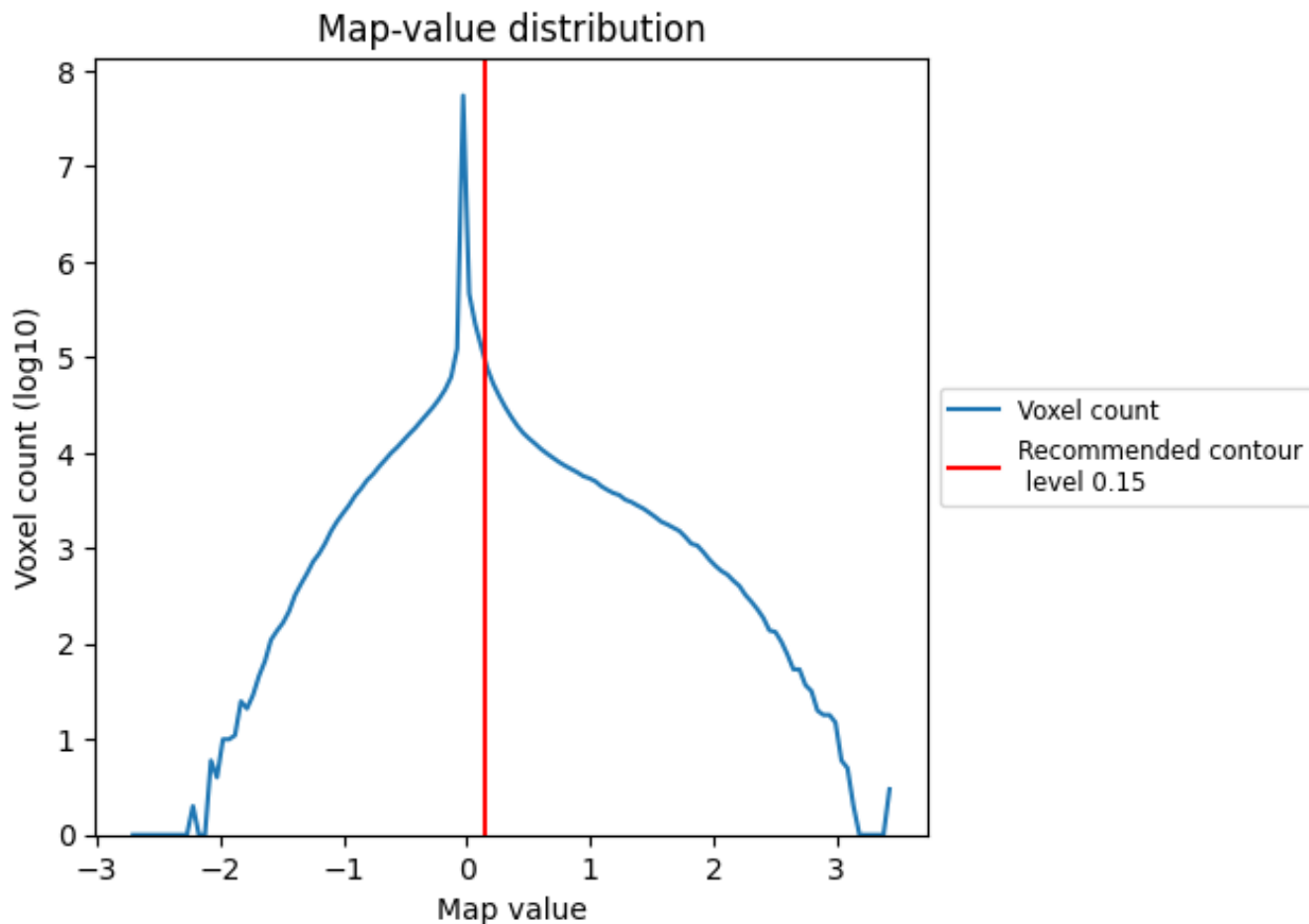
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

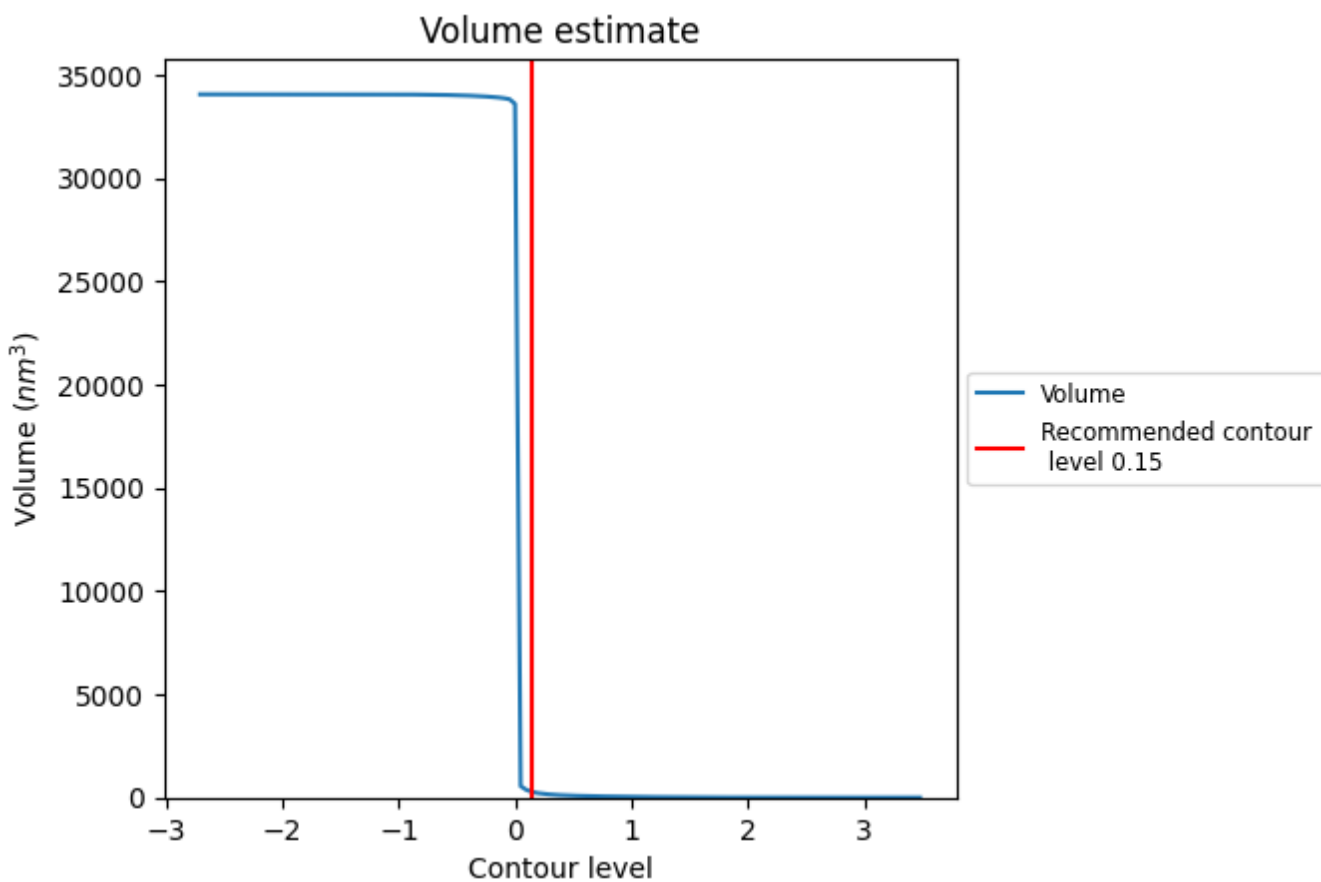
This section contains the results of statistical analysis of the map.

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.

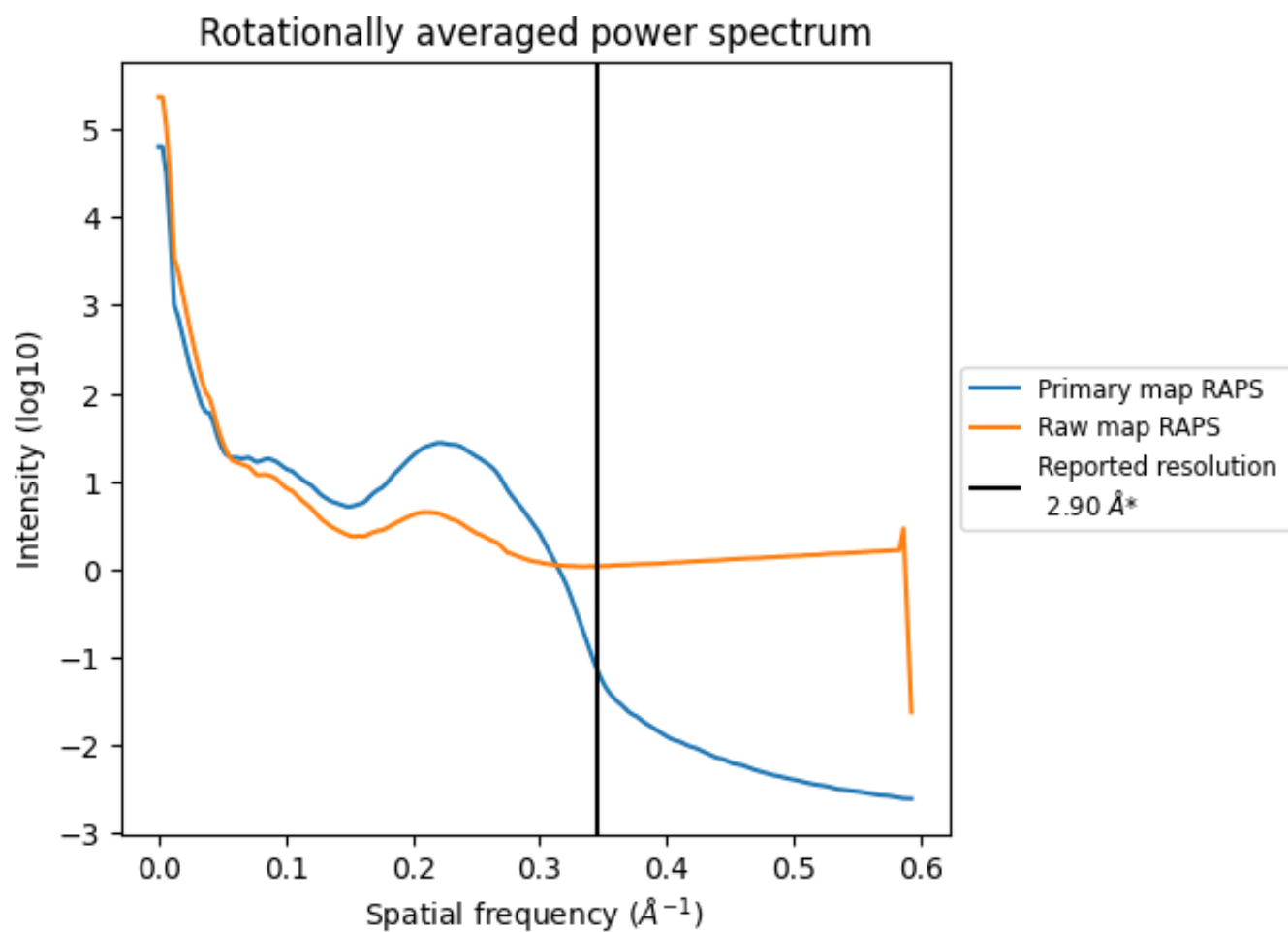
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 268 nm³; this corresponds to an approximate mass of 242 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

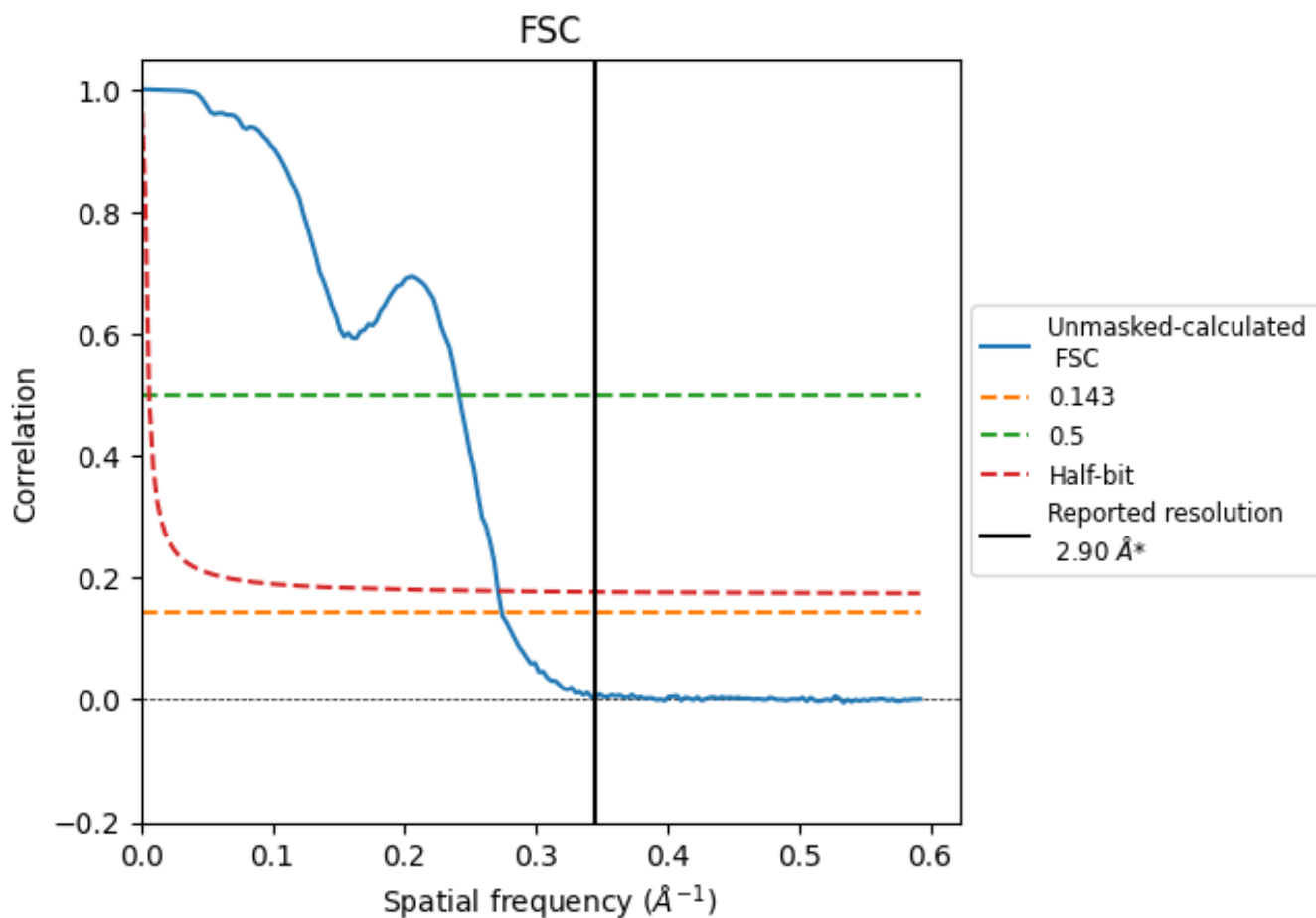


*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

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](#)

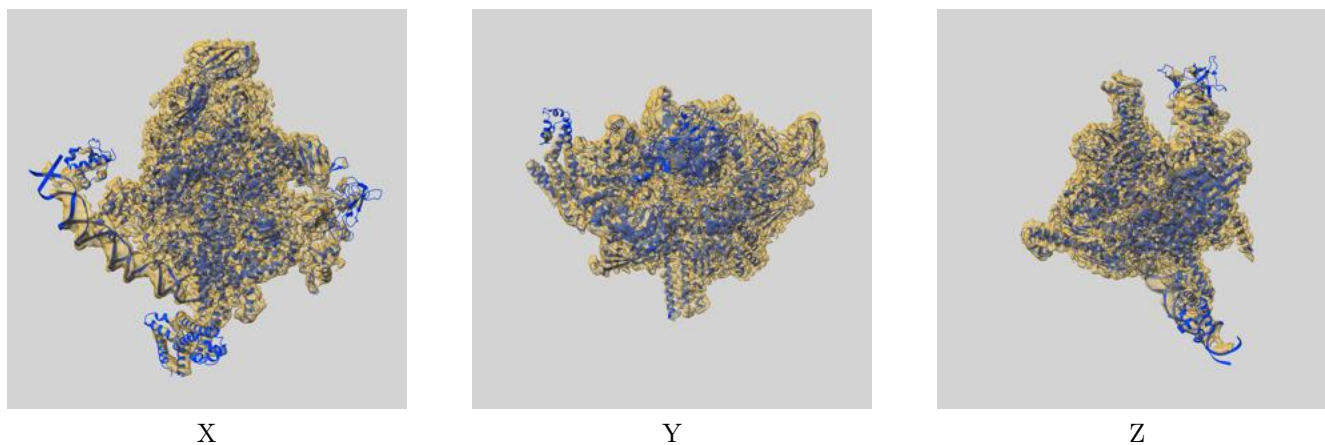
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.65	4.14	3.68

*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 3.65 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

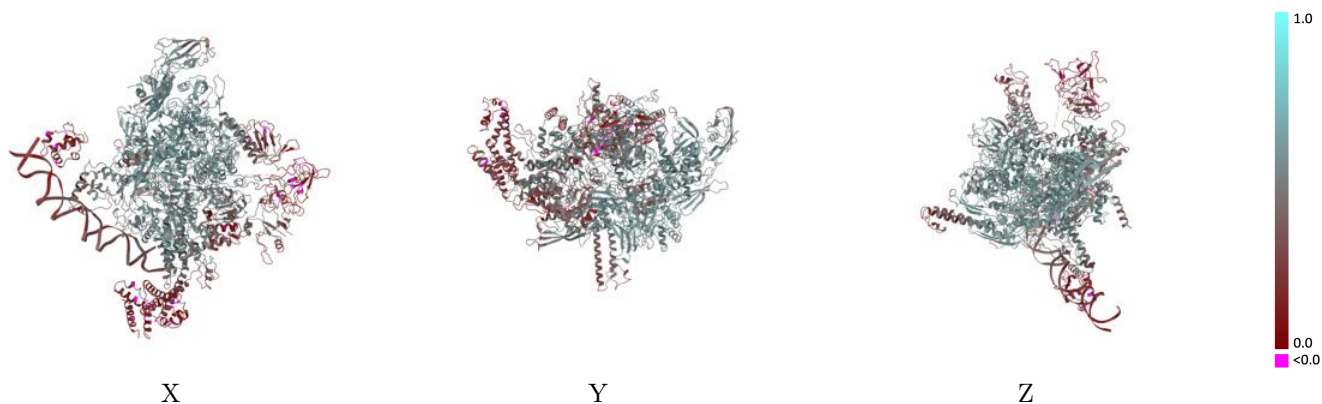
This section contains information regarding the fit between EMDB map EMD-41448 and PDB model 8TOE. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



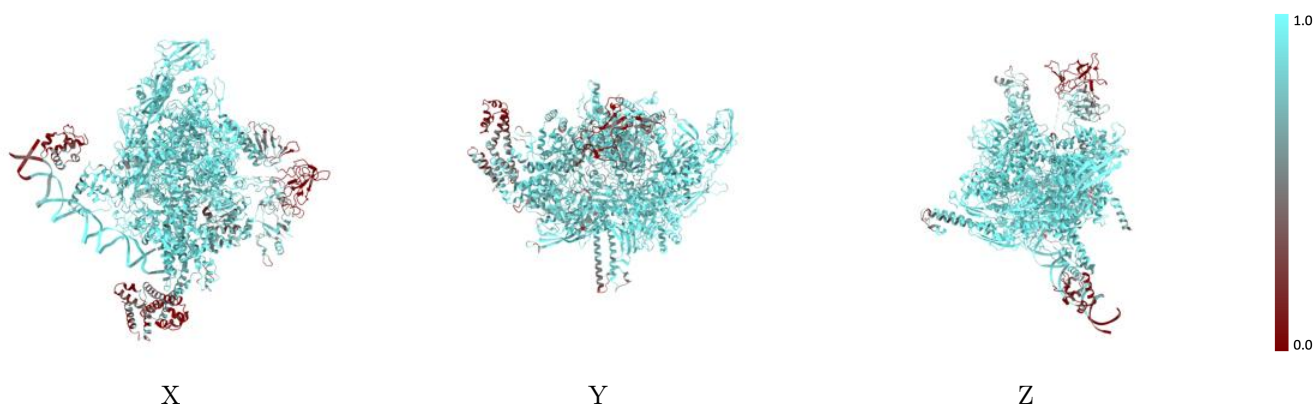
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



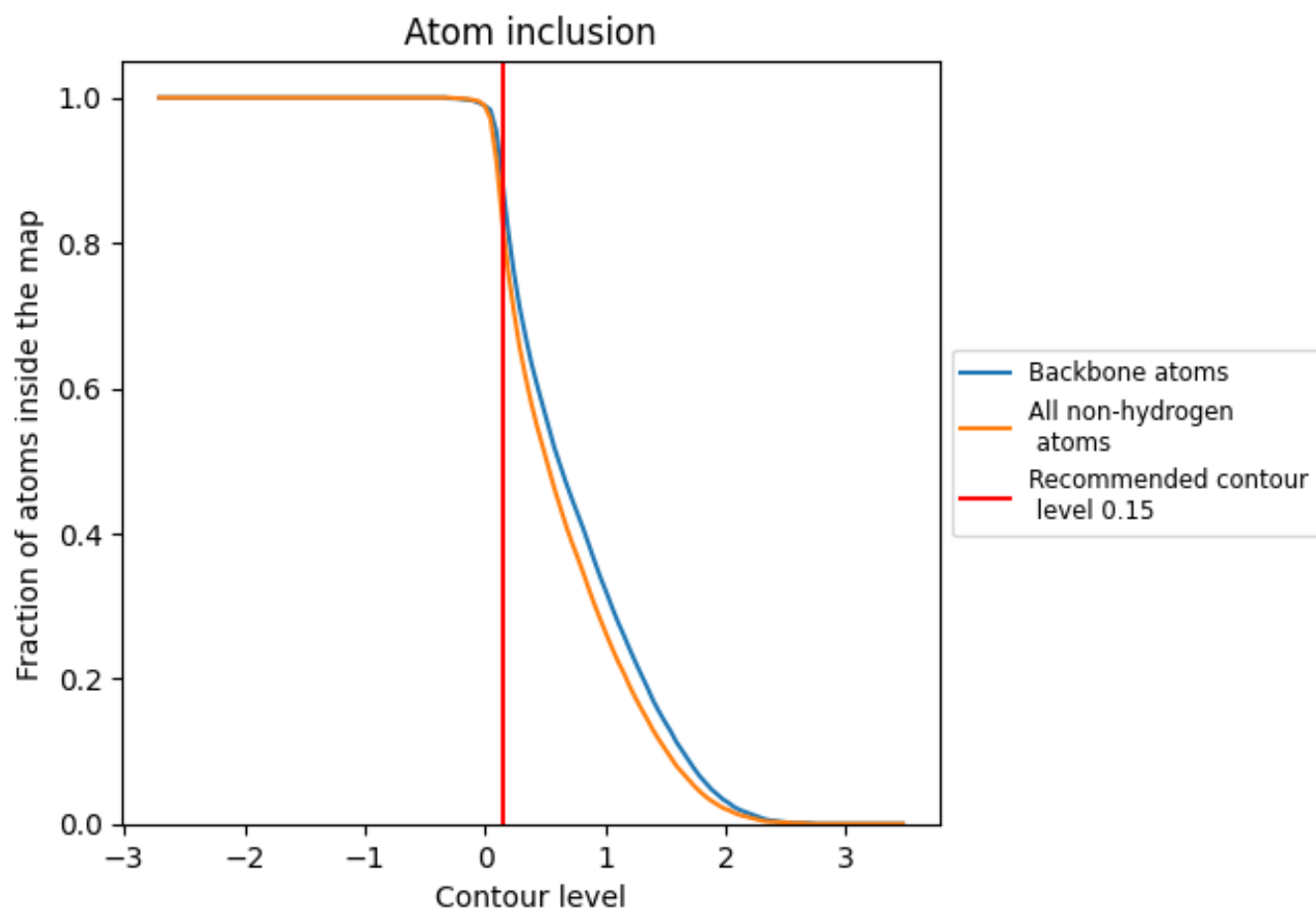
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).





















9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 82% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8240	 0.4620
G	 0.9360	 0.5550
H	 0.9180	 0.5200
I	 0.8920	 0.5110
J	 0.8280	 0.4770
K	 0.8760	 0.5190
L	 0.6470	 0.3330
M	 0.1910	 0.1610
O	 0.7550	 0.2830
P	 0.7770	 0.2600

