



Full wwPDB EM Validation Report ⓘ

Aug 6, 2025 – 11:14 AM EDT

PDB ID : 9MSH / pdb_00009msh
EMDB ID : EMD-48589
Title : de novo SigN RNA polymerase open complex (RPo)
Authors : Mueller, A.U.; Darst, S.A.
Deposited on : 2025-01-09
Resolution : 2.80 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.dev126
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

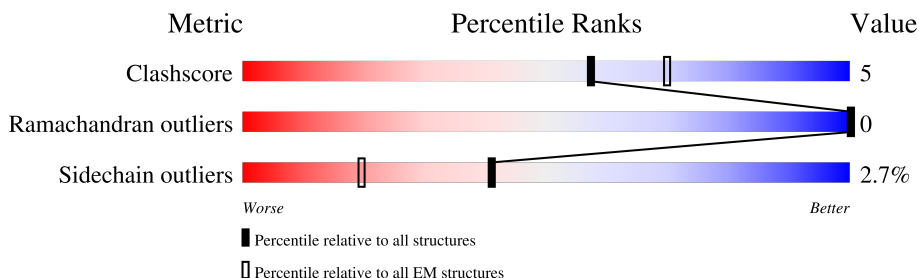
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	84% 9% 7%
1	H	329	56% 11% 32%
2	I	1342	88% 12%
3	J	1415	82% 12% 5%
4	K	91	80% 18%
5	M	477	64% 13% 23%
6	U	90	28% 27% 46%
7	V	90	28% 27% 46%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 31061 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
1	G	307	Total	C	N	O	S	0	0
			2382	1491	419	464	8		
1	H	223	Total	C	N	O	S	0	0
			1718	1074	302	336	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	1340	Total	C	N	O	S	0	0
			10567	6631	1841	2052	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	1350	Total	C	N	O	S	0	0
			10508	6606	1871	1981	50		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1408	LEU	-	expression tag	UNP P0A8T7
J	1409	GLU	-	expression tag	UNP P0A8T7
J	1410	LEU	-	expression tag	UNP P0A8T7
J	1411	GLU	-	expression tag	UNP P0A8T7
J	1412	VAL	-	expression tag	UNP P0A8T7
J	1413	LEU	-	expression tag	UNP P0A8T7
J	1414	PHE	-	expression tag	UNP P0A8T7
J	1415	GLN	-	expression tag	UNP P0A8T7

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	75	Total	C	N	O	S	0	0
			600	365	114	120	1		

- Molecule 5 is a protein called RNA polymerase sigma-54 factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	369	Total	C	N	O	S	0	0
			2917	1834	496	579	8		

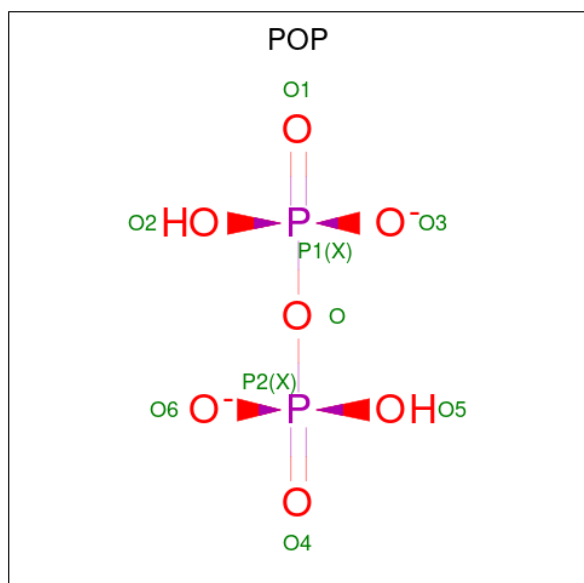
- Molecule 6 is a DNA chain called dhsU (-60 to +30) non-template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	49	Total	C	N	O	P	0	0
			1018	483	210	276	49		

- Molecule 7 is a DNA chain called dhsU (-60 to +30) template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	V	49	Total	C	N	O	P	0	0
			991	480	150	312	49		

- Molecule 8 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			AltConf
8	I	1	Total	O	P	0
			9	7	2	

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

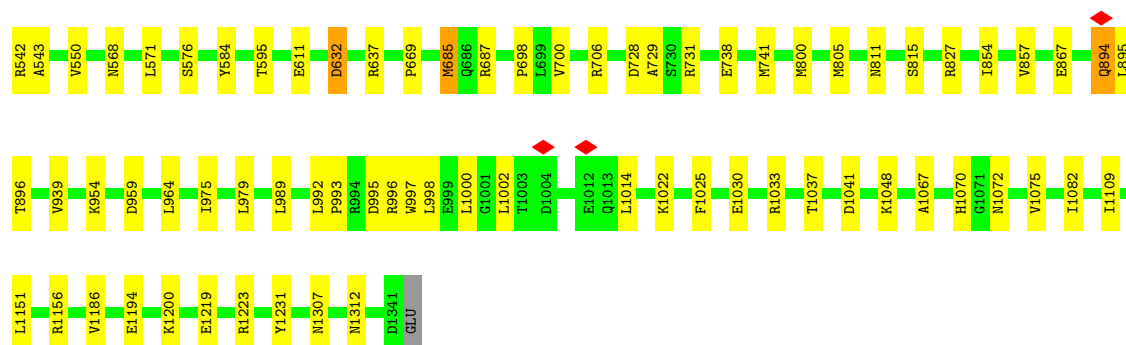
Mol	Chain	Residues	Atoms		AltConf
9	J	1	Total 1	Mg 1	0

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

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

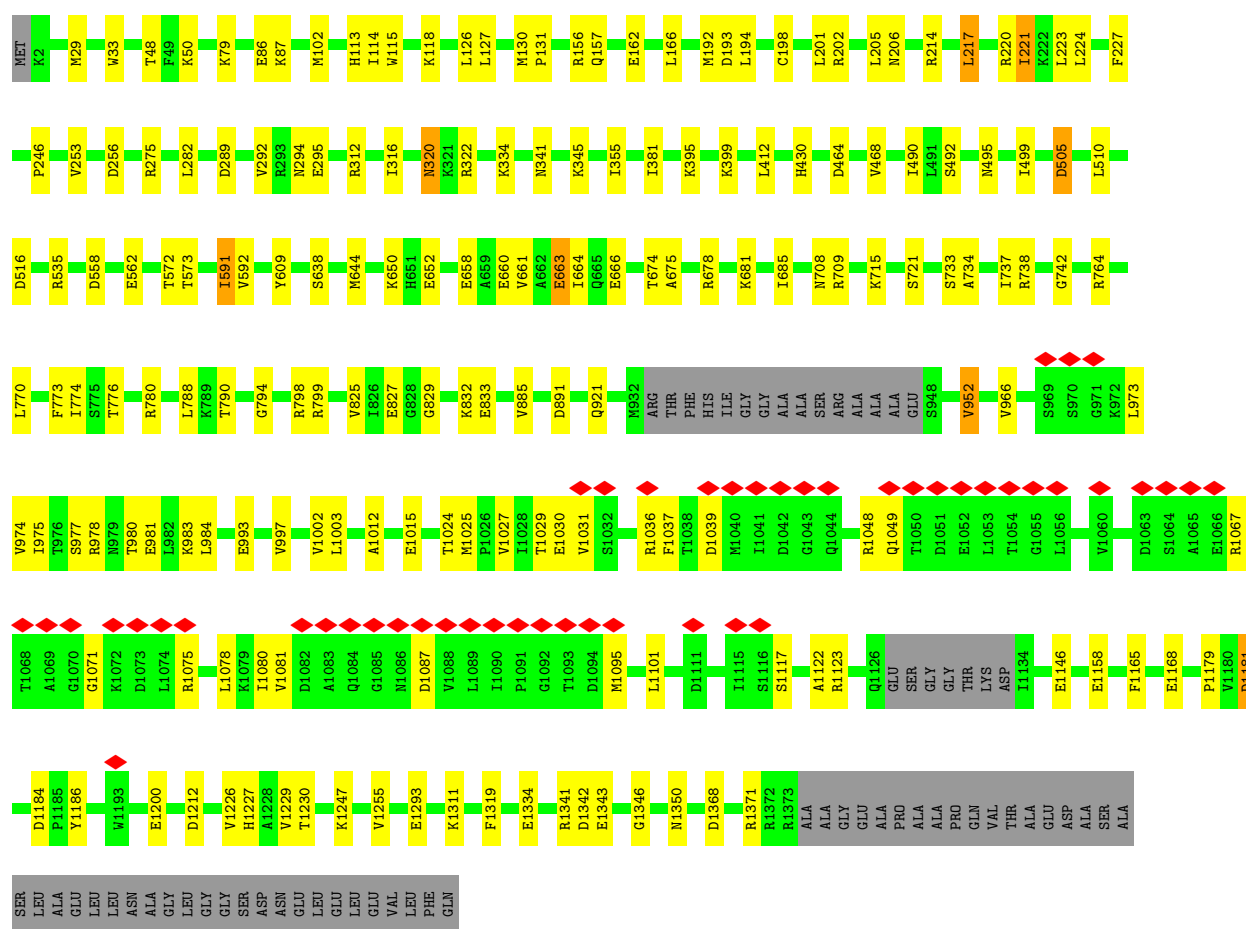
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		AltConf
11	G	24	Total 24	O 24	0
11	H	10	Total 10	O 10	0
11	I	151	Total 151	O 151	0
11	J	117	Total 117	O 117	0
11	K	10	Total 10	O 10	0
11	M	30	Total 30	O 30	0
11	U	3	Total 3	O 3	0
11	V	3	Total 3	O 3	0



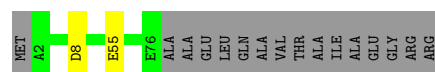
- Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain J: 82% 12% • 5%

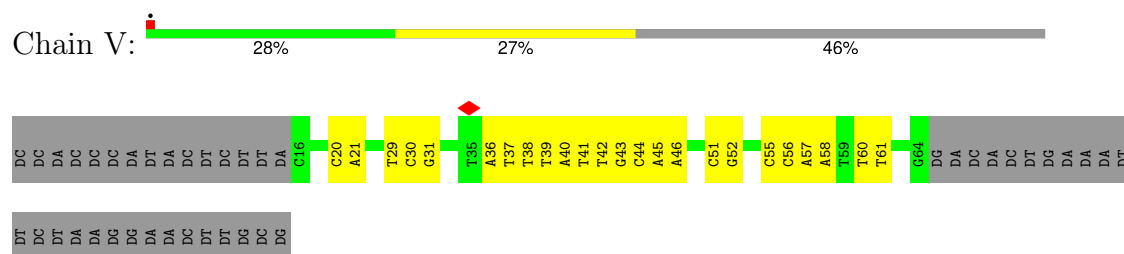
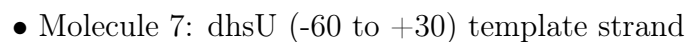
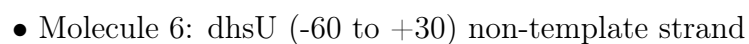


- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K: 80% 18%



- Molecule 5: RNA polymerase sigma-54 factor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45631	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 ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.791	Depositor
Minimum map value	-0.315	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	385.28, 385.28, 385.28	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	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: MG, ZN, POP

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	0.14	0/2411	0.29	0/3267
1	H	0.13	0/1738	0.30	0/2355
2	I	0.15	0/10736	0.28	0/14487
3	J	0.14	0/10666	0.28	0/14398
4	K	0.12	0/602	0.21	0/810
5	M	0.12	0/2970	0.25	0/4035
6	U	0.19	0/1150	0.39	0/1773
7	V	0.20	0/1102	0.47	0/1698
All	All	0.14	0/31375	0.29	0/42823

There are no bond length outliers.

There are no bond angle outliers.

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	2382	0	2438	15	0
1	H	1718	0	1756	22	0
2	I	10567	0	10585	87	0
3	J	10508	0	10746	100	0
4	K	600	0	607	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	2917	0	2869	34	0
6	U	1018	0	547	20	0
7	V	991	0	565	19	0
8	I	9	0	0	0	0
9	J	1	0	0	0	0
10	J	2	0	0	0	0
11	G	24	0	0	0	0
11	H	10	0	0	0	0
11	I	151	0	0	2	0
11	J	117	0	0	2	0
11	K	10	0	0	0	0
11	M	30	0	0	0	0
11	U	3	0	0	0	0
11	V	3	0	0	0	0
All	All	31061	0	30113	281	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 (281) 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:I:302:ILE:HG22	2:I:309:LEU:HA	1.72	0.71
5:M:379:SER:OG	5:M:383:ARG:NH1	2.23	0.71
2:I:232:ILE:HA	2:I:237:LEU:HA	1.76	0.68
3:J:1311:LYS:NZ	6:U:66:DA:OP1	2.28	0.67
5:M:437:LEU:O	5:M:473:ARG:NH2	2.28	0.67
7:V:51:DC:H2'	7:V:52:DG:C8	2.31	0.66
1:H:58:GLU:OE2	1:H:170:ARG:NH2	2.29	0.65
5:M:407:VAL:HG11	5:M:453:VAL:HG12	1.79	0.65
3:J:322:ARG:NH2	5:M:107:ASP:O	2.31	0.63
3:J:650:LYS:NZ	3:J:742:GLY:O	2.32	0.63
3:J:975:ILE:HD12	3:J:997:VAL:HG11	1.80	0.63
5:M:365:MET:HE2	5:M:370:ILE:HD11	1.82	0.62
5:M:134:SER:H	5:M:137:ASP:HB2	1.65	0.62
2:I:867:GLU:N	2:I:867:GLU:OE1	2.33	0.61
3:J:977:SER:OG	3:J:980:THR:OG1	2.18	0.61
6:U:31:DA:H2''	6:U:32:DA:C8	2.36	0.61
2:I:322:LEU:HD23	2:I:325:LEU:HD21	1.83	0.61
2:I:528:ARG:NH2	2:I:576:SER:O	2.34	0.60
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:468:PRO:O	5:M:473:ARG:NH1	2.33	0.60
7:V:44:DC:H2''	7:V:45:DA:C8	2.37	0.60
2:I:452:ARG:NH1	2:I:584:TYR:O	2.31	0.60
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.35	0.60
2:I:214:ASN:HA	2:I:359:ARG:HD3	1.84	0.60
2:I:232:ILE:HG12	2:I:237:LEU:HB3	1.84	0.60
7:V:29:DT:H2'	7:V:30:DC:C6	2.36	0.59
3:J:320:ASN:HB2	3:J:322:ARG:HG2	1.83	0.59
3:J:102:MET:HG2	3:J:246:PRO:HD3	1.85	0.59
2:I:60:GLN:HB3	2:I:67:GLU:HG3	1.84	0.58
1:H:71:LYS:NZ	1:H:139:SER:O	2.35	0.58
3:J:1181:ASP:OD1	3:J:1181:ASP:N	2.35	0.58
6:U:39:DC:H2'	6:U:40:DG:C8	2.38	0.58
5:M:285:TRP:NE1	5:M:356:GLU:OE1	2.29	0.58
5:M:333:LEU:O	5:M:337:ASN:ND2	2.36	0.58
3:J:973:LEU:HD23	3:J:1003:LEU:HD12	1.86	0.57
2:I:17:LYS:NZ	2:I:1194:GLU:OE2	2.28	0.57
7:V:41:DT:H2'	7:V:42:DT:H71	1.87	0.57
2:I:451:ARG:NH1	11:I:1518:HOH:O	2.37	0.57
5:M:359:GLU:OE2	5:M:401:TYR:OH	2.23	0.56
1:H:181:GLU:O	3:J:535:ARG:NH1	2.37	0.56
2:I:324:LYS:O	2:I:327:GLN:NE2	2.38	0.56
1:H:61:ILE:HB	1:H:64:VAL:HB	1.88	0.56
3:J:708:ASN:OD1	3:J:709:ARG:N	2.37	0.56
5:M:431:GLU:HB2	5:M:437:LEU:HD13	1.87	0.56
5:M:327:LYS:O	5:M:331:LYS:NZ	2.39	0.56
2:I:466:VAL:O	2:I:470:ARG:NH1	2.39	0.55
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.88	0.55
2:I:989:LEU:O	2:I:997:TRP:NE1	2.37	0.55
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.40	0.55
5:M:207:ASP:N	5:M:207:ASP:OD1	2.40	0.55
2:I:992:LEU:HD22	2:I:996:ARG:HG2	1.89	0.55
5:M:231:ASP:OD1	5:M:234:THR:N	2.39	0.55
3:J:127:LEU:O	3:J:220:ARG:NH2	2.41	0.54
3:J:1200:GLU:CD	3:J:1200:GLU:H	2.15	0.54
6:U:72:DG:H2''	6:U:73:DA:C8	2.43	0.54
2:I:256:GLU:HB3	2:I:261:VAL:HG22	1.89	0.54
2:I:540:ARG:NH1	2:I:568:ASN:OD1	2.35	0.54
3:J:1341:ARG:NH1	3:J:1343:GLU:OE2	2.40	0.54
1:G:62:ASP:OD1	1:G:63:GLY:N	2.41	0.54
2:I:728:ASP:OD1	2:I:729:ALA:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.90	0.53
6:U:27:DC:H2"	6:U:28:DA:C8	2.43	0.53
1:G:25:LYS:HG2	1:G:204:GLU:HG3	1.89	0.53
6:U:30:DA:H2"	6:U:31:DA:C8	2.42	0.53
7:V:36:DA:H1'	7:V:37:DT:C4	2.43	0.53
3:J:156:ARG:HG3	3:J:157:GLN:HG3	1.91	0.53
5:M:234:THR:HG22	5:M:237:ARG:HH12	1.73	0.53
3:J:921:GLN:NE2	11:J:1611:HOH:O	2.37	0.53
3:J:1039:ASP:OD2	3:J:1075:ARG:N	2.42	0.53
5:M:144:ILE:HG12	5:M:161:ILE:HD13	1.91	0.53
3:J:1027:VAL:HB	3:J:1122:ALA:HB3	1.91	0.52
2:I:316:GLU:OE1	2:I:316:GLU:N	2.38	0.52
1:G:8:PHE:HD2	1:G:32:GLU:HG3	1.74	0.52
3:J:1024:THR:HG21	3:J:1123:ARG:HB3	1.91	0.52
2:I:687:ARG:NH1	11:I:1526:HOH:O	2.42	0.52
5:M:469:PRO:HB3	6:U:34:DT:H5"	1.90	0.52
2:I:18:ARG:O	2:I:1156:ARG:NH1	2.39	0.52
2:I:196:VAL:HG23	2:I:206:ALA:HA	1.90	0.51
3:J:652:GLU:OE1	3:J:652:GLU:N	2.43	0.51
1:G:20:SER:OG	1:G:21:SER:N	2.41	0.51
2:I:466:VAL:O	2:I:469:VAL:HG22	2.10	0.51
3:J:644:MET:O	3:J:764:ARG:NH1	2.36	0.51
1:G:60:GLU:HG2	1:G:143:ARG:HH21	1.76	0.51
1:H:46:ILE:HD11	1:H:224:LEU:HD13	1.92	0.50
3:J:773:PHE:O	3:J:776:THR:OG1	2.29	0.50
6:U:65:DA:H2"	6:U:66:DA:C8	2.46	0.50
3:J:201:LEU:HD11	3:J:220:ARG:HH11	1.76	0.50
1:G:212:ASP:HB3	1:G:215:GLU:HG2	1.93	0.50
3:J:794:GLY:HA3	7:V:31:DG:H1	1.75	0.50
1:H:29:GLU:HB3	1:H:200:LYS:HG3	1.93	0.50
3:J:289:ASP:HA	3:J:292:VAL:HG22	1.92	0.50
3:J:495:ASN:HD22	3:J:1247:LYS:HB3	1.77	0.50
3:J:130:MET:HG2	3:J:131:PRO:HD2	1.94	0.50
2:I:241:LEU:HD11	2:I:246:LEU:HD11	1.93	0.50
3:J:29:MET:HE3	3:J:33:TRP:HE1	1.77	0.50
3:J:381:ILE:HD11	3:J:412:LEU:HD13	1.92	0.50
2:I:611:GLU:OE2	2:I:637:ARG:NH2	2.44	0.49
2:I:685:MET:HE3	2:I:1067:ALA:HB1	1.94	0.49
1:H:104:LYS:NZ	1:H:114:ASP:OD2	2.37	0.49
2:I:550:VAL:HG23	3:J:780:ARG:HD2	1.94	0.49
3:J:1158:GLU:HB3	3:J:1186:TYR:HE2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:798:ARG:NH1	11:J:1616:HOH:O	2.44	0.49
2:I:342:ASP:OD1	2:I:343:HIS:N	2.45	0.49
5:M:158:LEU:HD21	5:M:179:LEU:HD22	1.95	0.49
6:U:32:DA:H1'	6:U:33:DT:H5'	1.95	0.49
1:G:85:LEU:HD11	1:G:142:MET:HE1	1.93	0.49
3:J:1165:PHE:HE1	3:J:1200:GLU:HB3	1.78	0.49
2:I:103:VAL:HG12	2:I:117:ILE:HG22	1.94	0.48
7:V:57:DA:H2''	7:V:58:DA:C8	2.48	0.48
2:I:484:LEU:HD23	2:I:487:LEU:HD12	1.94	0.48
5:M:451:ILE:HG22	5:M:453:VAL:HG13	1.95	0.48
5:M:436:PRO:HD3	5:M:474:LYS:HB3	1.95	0.48
2:I:314:ASN:OD1	2:I:352:ARG:NH2	2.46	0.48
3:J:794:GLY:HA3	7:V:31:DG:N1	2.29	0.48
3:J:572:THR:OG1	3:J:573:THR:N	2.46	0.48
5:M:379:SER:HG	5:M:383:ARG:HH12	1.61	0.48
1:G:97:GLU:OE2	1:G:145:LYS:NZ	2.34	0.48
3:J:114:ILE:HD11	3:J:312:ARG:HB2	1.96	0.48
1:H:167:PRO:HD2	1:H:170:ARG:HH11	1.79	0.48
2:I:213:LEU:HD13	2:I:422:LYS:HG2	1.95	0.48
2:I:317:LEU:HD13	2:I:322:LEU:HD21	1.95	0.48
3:J:505:ASP:N	3:J:505:ASP:OD1	2.45	0.48
6:U:31:DA:H2''	6:U:32:DA:H8	1.79	0.48
1:H:101:THR:HG22	1:H:143:ARG:HG2	1.94	0.48
2:I:7:GLU:OE1	2:I:706:ARG:NH1	2.47	0.48
6:U:43:DA:H2''	6:U:44:DA:C8	2.48	0.48
7:V:60:DT:H4'	7:V:61:DT:OP1	2.14	0.48
2:I:444:ASP:O	2:I:450:ASN:ND2	2.44	0.48
2:I:471:VAL:HG23	2:I:497:PRO:HB2	1.96	0.48
3:J:829:GLY:HA2	3:J:993:GLU:HG3	1.97	0.47
5:M:188:VAL:HG11	5:M:205:GLN:HG3	1.97	0.47
1:H:118:ASP:OD1	1:H:119:GLY:N	2.48	0.47
2:I:698:PRO:HA	2:I:1231:TYR:CE1	2.50	0.47
3:J:205:LEU:HD11	3:J:214:ARG:HG3	1.95	0.47
1:H:52:PRO:HG3	1:H:150:ARG:HH12	1.79	0.47
1:H:195:ARG:H	1:H:195:ARG:HG2	1.53	0.47
3:J:1067:ARG:HD3	3:J:1071:GLY:HA3	1.97	0.47
6:U:49:DA:H2''	6:U:50:DA:O5'	2.15	0.47
3:J:126:LEU:HD23	3:J:223:LEU:HD22	1.97	0.46
3:J:952:VAL:HG13	3:J:984:LEU:HD11	1.96	0.46
2:I:55:SER:OG	2:I:465:ARG:NH1	2.43	0.46
3:J:974:VAL:HG12	3:J:1002:VAL:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:349:GLU:O	2:I:353:VAL:HG23	2.15	0.46
3:J:674:THR:OG1	3:J:675:ALA:N	2.42	0.46
3:J:827:GLU:HB3	3:J:832:LYS:HE2	1.98	0.46
7:V:29:DT:H2''	7:V:30:DC:O5'	2.14	0.46
2:I:731:ARG:NH2	2:I:959:ASP:OD1	2.49	0.46
7:V:56:DC:H2''	7:V:57:DA:C8	2.51	0.46
2:I:205:PRO:HB2	2:I:208:ILE:HG12	1.98	0.46
2:I:228:VAL:HG22	2:I:245:ARG:HH12	1.81	0.46
2:I:185:ASP:OD1	2:I:185:ASP:N	2.49	0.46
2:I:894:GLN:HG3	2:I:896:THR:HG23	1.98	0.46
3:J:825:VAL:HB	3:J:833:GLU:HB3	1.97	0.46
1:H:127:GLN:N	1:H:127:GLN:OE1	2.49	0.46
2:I:738:GLU:HA	2:I:741:MET:HG3	1.98	0.46
2:I:1307:ASN:HB3	2:I:1312:ASN:O	2.16	0.46
1:H:57:THR:HG23	1:H:158:ARG:NH1	2.32	0.45
2:I:465:ARG:O	2:I:469:VAL:HG13	2.16	0.45
3:J:516:ASP:OD1	3:J:516:ASP:N	2.47	0.45
7:V:36:DA:H1'	7:V:37:DT:C5	2.51	0.45
3:J:193:ASP:OD1	3:J:194:LEU:N	2.47	0.45
1:H:192:VAL:HG12	1:H:193:GLU:H	1.81	0.45
1:G:154:PRO:HG2	1:G:157:THR:HG23	1.98	0.45
2:I:368:ARG:HE	2:I:376:PRO:HD3	1.81	0.45
2:I:800:MET:HE1	2:I:827:ARG:HD3	1.98	0.45
3:J:975:ILE:HD11	3:J:1003:LEU:HD11	1.98	0.45
2:I:975:ILE:HG12	2:I:1014:LEU:HD23	1.98	0.45
3:J:113:HIS:CE1	3:J:115:TRP:HB2	2.51	0.45
7:V:55:DC:H2''	7:V:56:DC:C6	2.52	0.45
4:K:8:ASP:HB2	4:K:55:GLU:HG2	1.98	0.45
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.50	0.44
3:J:282:LEU:HD22	3:J:295:GLU:HG3	1.98	0.44
3:J:1048:ARG:NH2	3:J:1049:GLN:O	2.49	0.44
1:G:282:VAL:HG13	1:G:316:MET:HB2	2.00	0.44
2:I:504:GLU:OE2	2:I:508:SER:OG	2.35	0.44
5:M:329:LEU:O	5:M:333:LEU:HG	2.17	0.44
7:V:39:DT:H2''	7:V:40:DA:H5'	2.00	0.44
2:I:669:PRO:O	2:I:1070:HIS:HE1	2.00	0.44
2:I:448:LEU:HD23	2:I:448:LEU:HA	1.87	0.44
3:J:1078:LEU:HG	3:J:1101:LEU:HD21	1.98	0.44
7:V:20:DC:H2''	7:V:21:DA:C8	2.53	0.44
7:V:38:DT:H2''	7:V:39:DT:H5''	2.00	0.43
2:I:230:PHE:HB2	2:I:333:ILE:HB	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:339:ASN:HB2	2:I:342:ASP:O	2.19	0.43
2:I:404:LYS:HD2	2:I:407:ARG:HH21	1.83	0.43
3:J:591:ILE:HG22	3:J:592:VAL:HG13	1.99	0.43
1:G:5:VAL:O	1:H:150:ARG:NH2	2.49	0.43
2:I:371:ARG:NH2	6:U:55:DT:O4	2.50	0.43
3:J:1012:ALA:N	3:J:1015:GLU:OE2	2.46	0.43
3:J:733:SER:O	3:J:737:ILE:HG12	2.18	0.43
5:M:382:SER:OG	6:U:45:DT:OP2	2.18	0.43
1:H:114:ASP:OD1	1:H:114:ASP:N	2.51	0.43
2:I:854:ILE:HB	2:I:857:VAL:HG22	2.01	0.43
3:J:1346:GLY:O	3:J:1350:ASN:ND2	2.48	0.43
5:M:199:LEU:HB3	5:M:220:ILE:HD13	2.01	0.43
7:V:45:DA:H1'	7:V:46:DA:H5'	2.00	0.43
3:J:48:THR:HG23	3:J:50:LYS:HG2	2.00	0.43
3:J:162:GLU:O	3:J:166:LEU:HG	2.18	0.43
3:J:256:ASP:OD1	3:J:256:ASP:N	2.48	0.43
3:J:664:ILE:HG22	3:J:678:ARG:HG2	2.00	0.43
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	2.00	0.43
2:I:954:LYS:HB3	2:I:954:LYS:HE2	1.77	0.43
1:H:66:HIS:CD2	1:H:68:TYR:H	2.37	0.43
2:I:995:ASP:HA	2:I:998:LEU:HD12	2.01	0.43
3:J:558:ASP:N	3:J:562:GLU:O	2.52	0.43
3:J:1168:GLU:OE1	3:J:1168:GLU:N	2.52	0.43
7:V:42:DT:H2''	7:V:43:DG:C8	2.54	0.42
2:I:178:PRO:HA	2:I:397:LEU:HD12	2.01	0.42
3:J:660:GLU:HB3	3:J:685:ILE:HD13	2.01	0.42
5:M:119:THR:HG22	5:M:266:THR:HG21	2.00	0.42
2:I:106:GLU:HG3	2:I:115:LYS:HB2	2.00	0.42
2:I:271:ALA:O	2:I:275:ARG:HG3	2.19	0.42
2:I:979:LEU:HD12	2:I:1002:LEU:HD11	2.01	0.42
3:J:202:ARG:HG3	3:J:221:ILE:HD12	2.01	0.42
3:J:658:GLU:HA	3:J:661:VAL:HG22	2.00	0.42
6:U:65:DA:H2''	6:U:66:DA:H8	1.84	0.42
2:I:473:ARG:HH21	6:U:55:DT:H4'	1.84	0.42
3:J:341:ASN:O	3:J:345:LYS:HE2	2.19	0.42
3:J:1031:VAL:HG23	3:J:1080:ILE:HG21	2.02	0.42
1:H:120:ASP:OD1	1:H:120:ASP:N	2.50	0.42
2:I:632:ASP:OD1	2:I:632:ASP:N	2.51	0.42
3:J:978:ARG:HH22	3:J:1025:MET:HE3	1.84	0.42
3:J:981:GLU:OE1	3:J:983:LYS:HG3	2.20	0.42
3:J:355:ILE:HD11	3:J:464:ASP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1048:LYS:HE3	2:I:1048:LYS:HB2	1.85	0.42
3:J:1037:PHE:CD1	3:J:1078:LEU:HD22	2.55	0.42
7:V:31:DG:H5"	7:V:31:DG:N3	2.34	0.42
2:I:698:PRO:C	2:I:700:VAL:H	2.28	0.42
3:J:198:CYS:SG	3:J:224:LEU:HB3	2.60	0.42
3:J:734:ALA:O	3:J:738:ARG:HG3	2.20	0.42
3:J:770:LEU:O	3:J:774:ILE:HG12	2.19	0.42
5:M:243:GLU:O	5:M:247:LYS:HG2	2.19	0.42
1:G:13:LEU:HG	1:H:231:PHE:HE1	1.84	0.42
2:I:533:LEU:HD21	2:I:571:LEU:HD13	2.02	0.42
2:I:539:THR:O	2:I:543:ALA:HB2	2.20	0.42
3:J:205:LEU:HD13	3:J:217:LEU:HB2	2.02	0.42
3:J:1036:ARG:NH2	3:J:1081:VAL:HG11	2.35	0.42
2:I:992:LEU:HD23	2:I:992:LEU:HA	1.86	0.41
5:M:323:LEU:O	5:M:327:LYS:HG2	2.20	0.41
3:J:118:LYS:HE3	3:J:312:ARG:HG2	2.01	0.41
3:J:664:ILE:HD13	3:J:681:LYS:HD3	2.02	0.41
5:M:302:HIS:HA	6:U:57:DC:O2	2.20	0.41
1:G:135:ASP:HB3	1:G:138:ALA:HB2	2.00	0.41
2:I:811:ASN:HA	2:I:815:SER:HB2	2.01	0.41
2:I:993:PRO:HG2	2:I:996:ARG:HB2	2.03	0.41
2:I:1223:ARG:NH2	3:J:721:SER:OG	2.50	0.41
3:J:1095:MET:SD	3:J:1095:MET:N	2.94	0.41
3:J:1226:VAL:O	3:J:1229:VAL:HG12	2.20	0.41
5:M:125:MET:O	5:M:129:GLU:HG2	2.21	0.41
2:I:106:GLU:HB2	2:I:113:THR:HB	2.03	0.41
2:I:1109:ILE:HD12	3:J:644:MET:HE1	2.03	0.41
2:I:65:ASN:OD1	2:I:65:ASN:N	2.44	0.41
3:J:275:ARG:HD3	3:J:275:ARG:HA	1.88	0.41
3:J:492:SER:HB2	3:J:499:ILE:HG23	2.03	0.41
3:J:663:GLU:O	3:J:666:GLU:HG3	2.20	0.41
3:J:495:ASN:ND2	3:J:1247:LYS:HB3	2.36	0.41
6:U:42:DA:H2"	6:U:43:DA:H8	1.86	0.41
2:I:318:SER:OG	2:I:320:ASP:OD1	2.33	0.41
2:I:989:LEU:HD12	2:I:989:LEU:HA	1.83	0.41
2:I:96:LEU:HD22	2:I:127:ILE:HD11	2.03	0.41
2:I:542:ARG:NH2	6:U:61:DG:OP2	2.53	0.41
3:J:715:LYS:HE2	3:J:715:LYS:HB2	1.95	0.41
3:J:799:ARG:NH1	3:J:1146:GLU:OE2	2.52	0.41
3:J:1319:PHE:CE1	3:J:1342:ASP:HB2	2.55	0.41
5:M:469:PRO:O	5:M:473:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:297:LYS:HB3	1:G:297:LYS:HE2	1.82	0.41
2:I:964:LEU:HD23	2:I:1025:PHE:CD1	2.56	0.41
2:I:995:ASP:OD1	2:I:995:ASP:N	2.52	0.41
3:J:79:LYS:HB3	5:M:164:SER:HB3	2.03	0.41
3:J:490:ILE:HD11	3:J:609:TYR:CE1	2.56	0.41
3:J:1227:HIS:HA	3:J:1230:THR:HG22	2.03	0.41
1:H:83:LEU:HD23	1:H:83:LEU:HA	1.92	0.40
3:J:127:LEU:HG	3:J:192:MET:HE1	2.02	0.40
3:J:395:LYS:O	3:J:399:LYS:HD3	2.21	0.40
3:J:1030:GLU:O	3:J:1117:SER:OG	2.31	0.40
3:J:86:GLU:CD	3:J:86:GLU:H	2.29	0.40
6:U:47:DG:H2''	6:U:48:DC:O5'	2.21	0.40
2:I:468:LEU:HD23	2:I:468:LEU:HA	1.90	0.40
2:I:805:MET:HE3	2:I:805:MET:HB2	1.92	0.40
5:M:214:GLU:H	5:M:214:GLU:HG2	1.63	0.40
5:M:445:LEU:O	5:M:448:GLU:HG2	2.21	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	301/329 (92%)	295 (98%)	6 (2%)	0	100	100
1	H	219/329 (67%)	215 (98%)	4 (2%)	0	100	100
2	I	1338/1342 (100%)	1300 (97%)	38 (3%)	0	100	100
3	J	1344/1415 (95%)	1306 (97%)	38 (3%)	0	100	100
4	K	73/91 (80%)	73 (100%)	0	0	100	100
5	M	365/477 (76%)	349 (96%)	16 (4%)	0	100	100
All	All	3640/3983 (91%)	3538 (97%)	102 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	G	266/286 (93%)	262 (98%)	4 (2%)	60	86
1	H	191/286 (67%)	183 (96%)	8 (4%)	25	58
2	I	1155/1157 (100%)	1125 (97%)	30 (3%)	41	75
3	J	1134/1176 (96%)	1104 (97%)	30 (3%)	41	75
4	K	65/75 (87%)	65 (100%)	0	100	100
5	M	324/428 (76%)	310 (96%)	14 (4%)	25	57
All	All	3135/3408 (92%)	3049 (97%)	86 (3%)	41	74

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	124	VAL
1	G	237	VAL
1	G	282	VAL
1	G	286	GLU
1	H	19	VAL
1	H	98	VAL
1	H	100	LEU
1	H	107	ILE
1	H	120	ASP
1	H	124	VAL
1	H	159	ILE
1	H	228	LEU
2	I	39	ILE
2	I	68	LEU
2	I	141	THR
2	I	185	ASP
2	I	189	ASP
2	I	207	THR
2	I	237	LEU

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Mol	Chain	Res	Type
2	I	242	VAL
2	I	287	VAL
2	I	319	LEU
2	I	370	MET
2	I	384	LEU
2	I	419	ILE
2	I	471	VAL
2	I	595	THR
2	I	632	ASP
2	I	685	MET
2	I	894	GLN
2	I	895	LEU
2	I	939	VAL
2	I	1000	LEU
2	I	1022	LYS
2	I	1037	THR
2	I	1041	ASP
2	I	1075	VAL
2	I	1082	ILE
2	I	1151	LEU
2	I	1186	VAL
2	I	1200	LYS
2	I	1219	GLU
3	J	87	LYS
3	J	206	ASN
3	J	217	LEU
3	J	221	ILE
3	J	227	PHE
3	J	253	VAL
3	J	294	ASN
3	J	316	ILE
3	J	320	ASN
3	J	334	LYS
3	J	430	HIS
3	J	468	VAL
3	J	505	ASP
3	J	510	LEU
3	J	591	ILE
3	J	638	SER
3	J	663	GLU
3	J	788	LEU
3	J	790	THR

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Mol	Chain	Res	Type
3	J	885	VAL
3	J	891	ASP
3	J	952	VAL
3	J	966	VAL
3	J	1029	THR
3	J	1087	ASP
3	J	1181	ASP
3	J	1212	ASP
3	J	1255	VAL
3	J	1293	GLU
3	J	1334	GLU
5	M	104	TYR
5	M	109	LEU
5	M	118	GLN
5	M	214	GLU
5	M	245	VAL
5	M	275	ASP
5	M	276	VAL
5	M	286	THR
5	M	287	VAL
5	M	323	LEU
5	M	336	ARG
5	M	338	ASP
5	M	462	ARG
5	M	463	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	84	ASN
2	I	133	ASN
2	I	150	HIS
2	I	193	ASN
2	I	808	ASN
2	I	894	GLN
2	I	922	ASN
2	I	1023	HIS
2	I	1220	GLN
2	I	1237	HIS
2	I	1244	HIS
3	J	186	GLN
3	J	495	ASN

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Mol	Chain	Res	Type
3	J	519	ASN
3	J	667	GLN
3	J	720	ASN
3	J	865	HIS
3	J	1197	ASN
3	J	1218	HIS
3	J	1268	ASN
5	M	350	GLN
5	M	391	HIS
5	M	406	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	POP	I	1401	-	6,8,8	0.78	0	12,13,13	0.99	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	POP	I	1401	-	-	1/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1401	POP	P2-O-P1-O2

There are no ring outliers.

No monomer is involved in short contacts.

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.

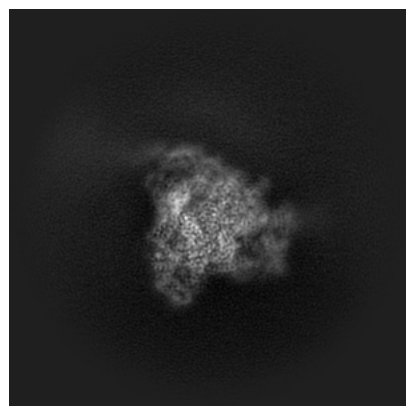
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48589. These allow visual inspection of the internal detail of the map and identification of artifacts.

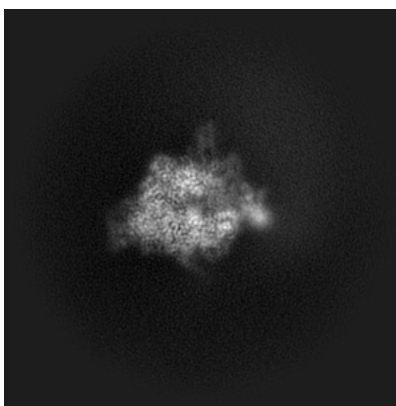
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

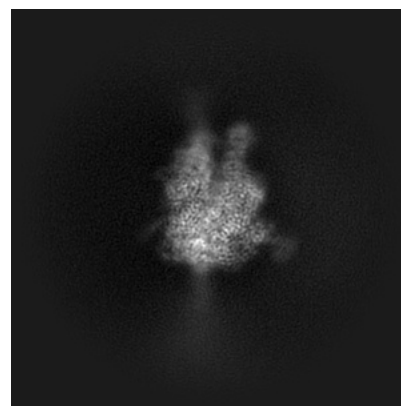
6.1.1 Primary map



X

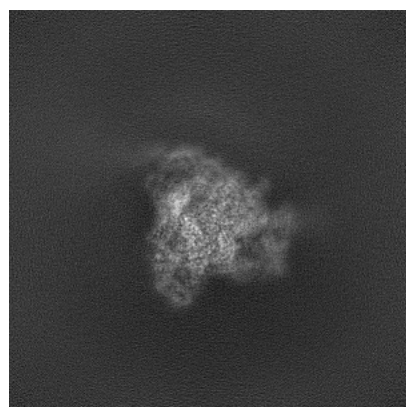


Y

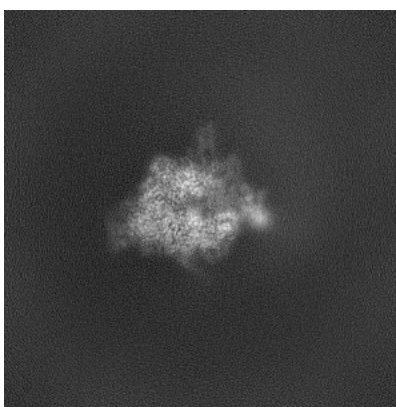


Z

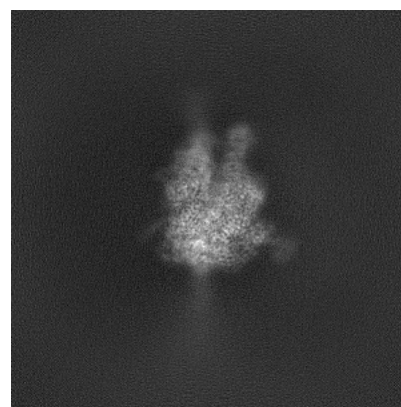
6.1.2 Raw map



X



Y

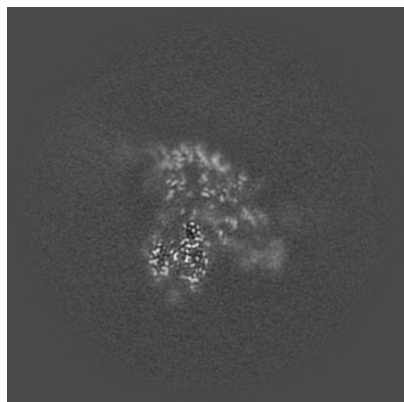


Z

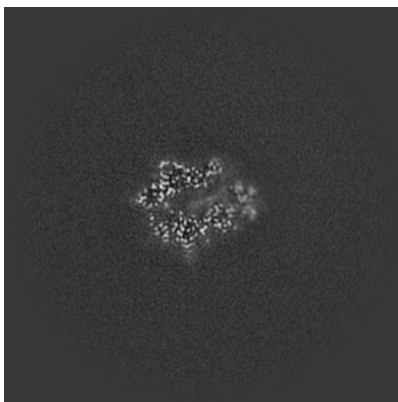
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

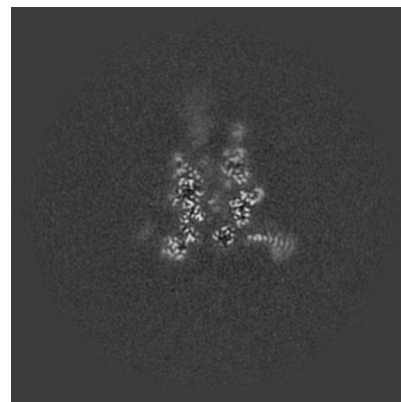
6.2.1 Primary map



X Index: 224

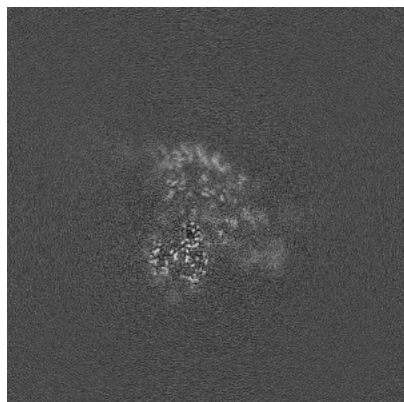


Y Index: 224

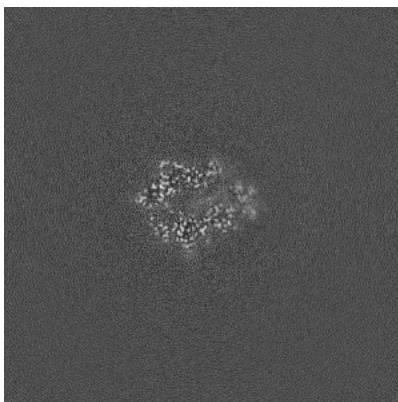


Z Index: 224

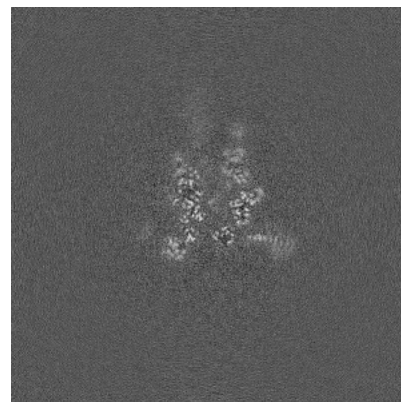
6.2.2 Raw map



X Index: 224



Y Index: 224

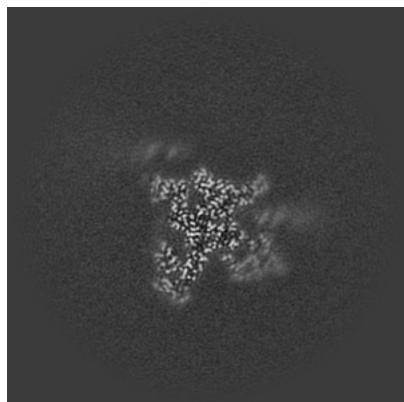


Z Index: 224

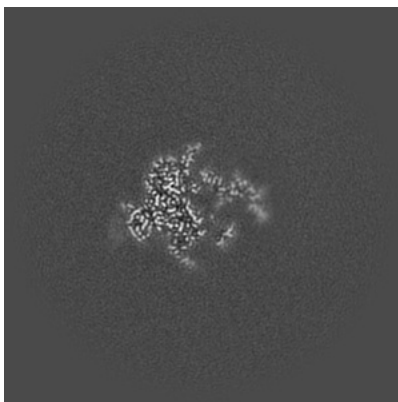
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

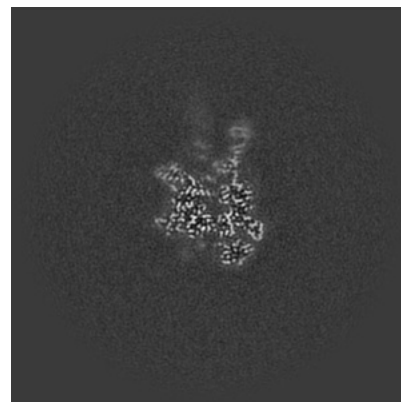
6.3.1 Primary map



X Index: 203

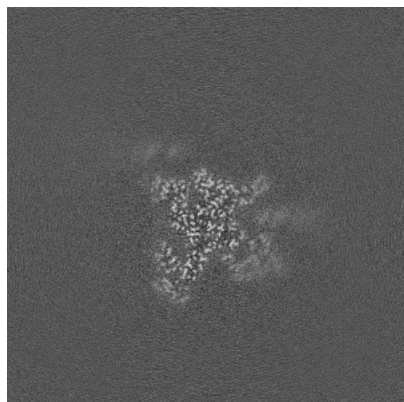


Y Index: 206

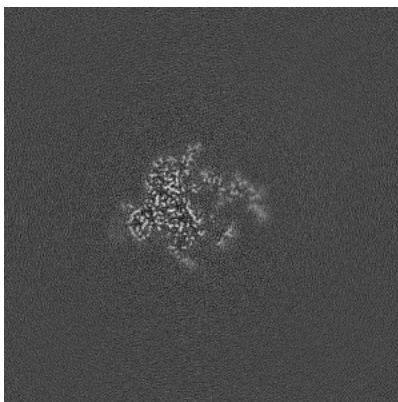


Z Index: 199

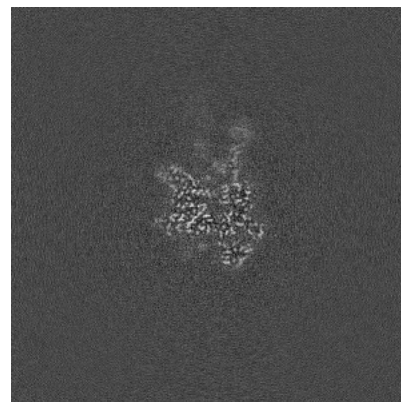
6.3.2 Raw map



X Index: 203



Y Index: 206

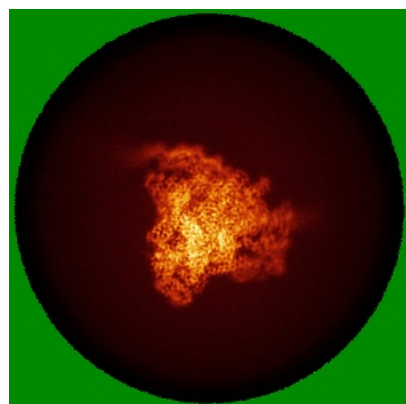


Z Index: 198

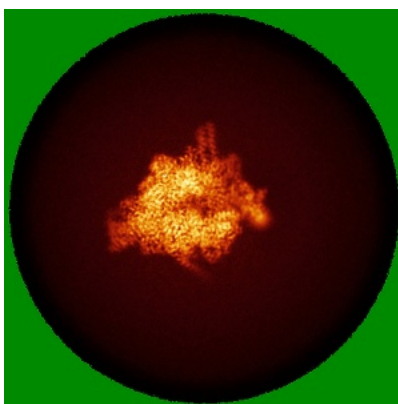
The images above show the largest variance slices of the map in three orthogonal directions.

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

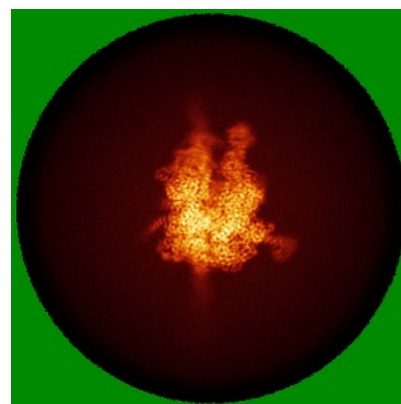
6.4.1 Primary map



X

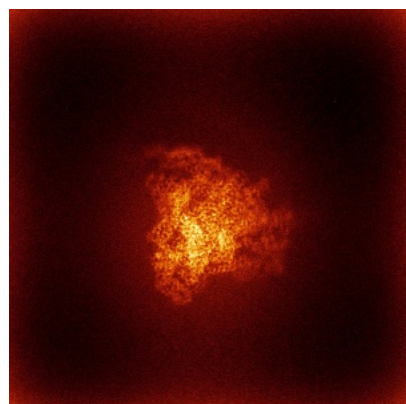


Y

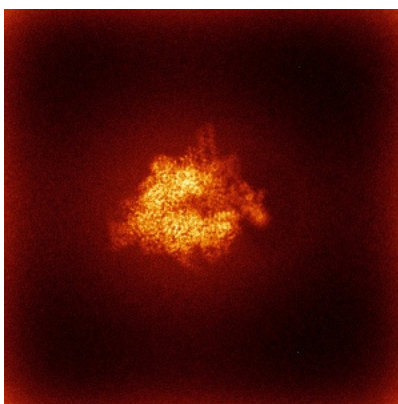


Z

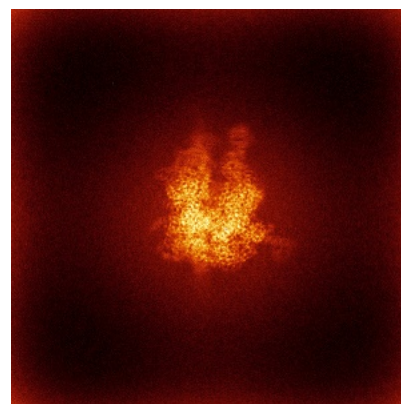
6.4.2 Raw map



X



Y

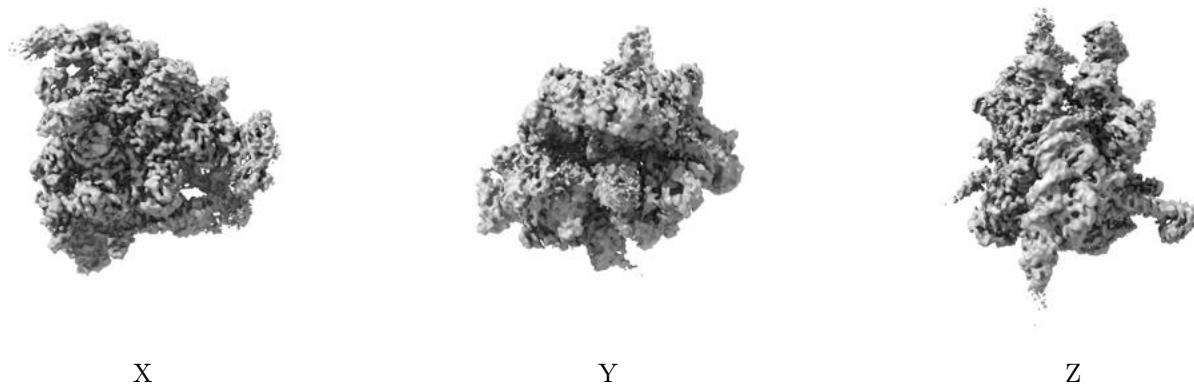


Z

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.

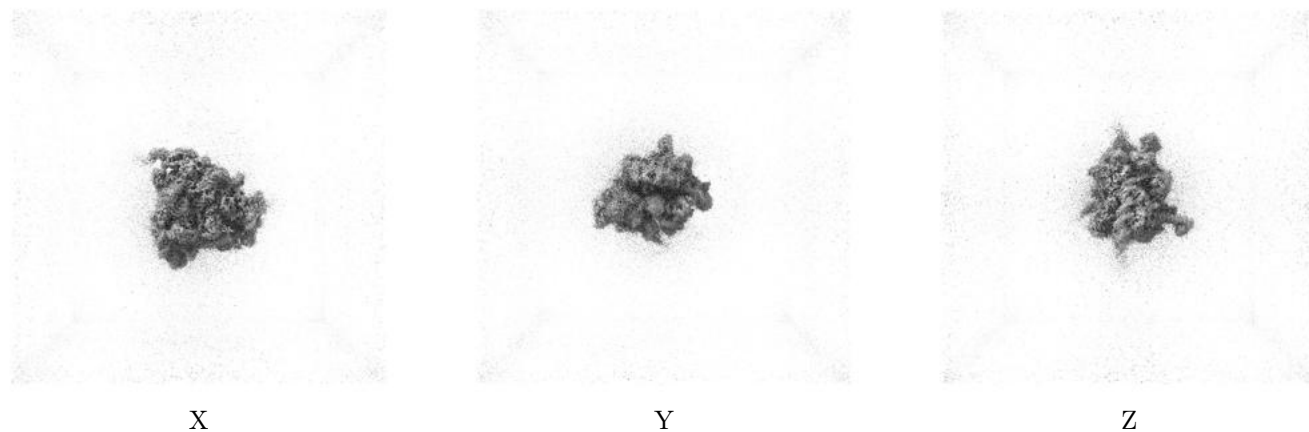
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

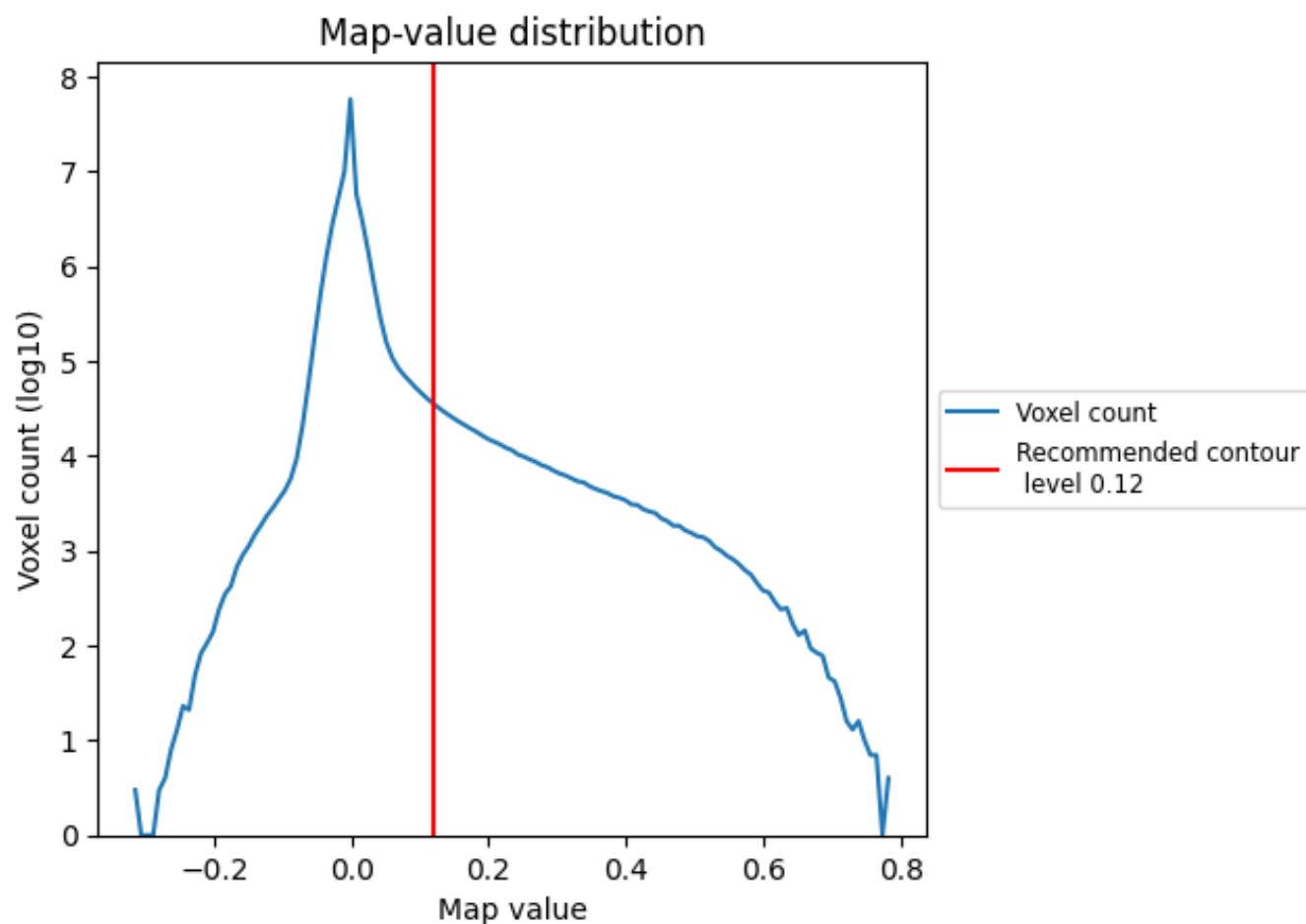
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

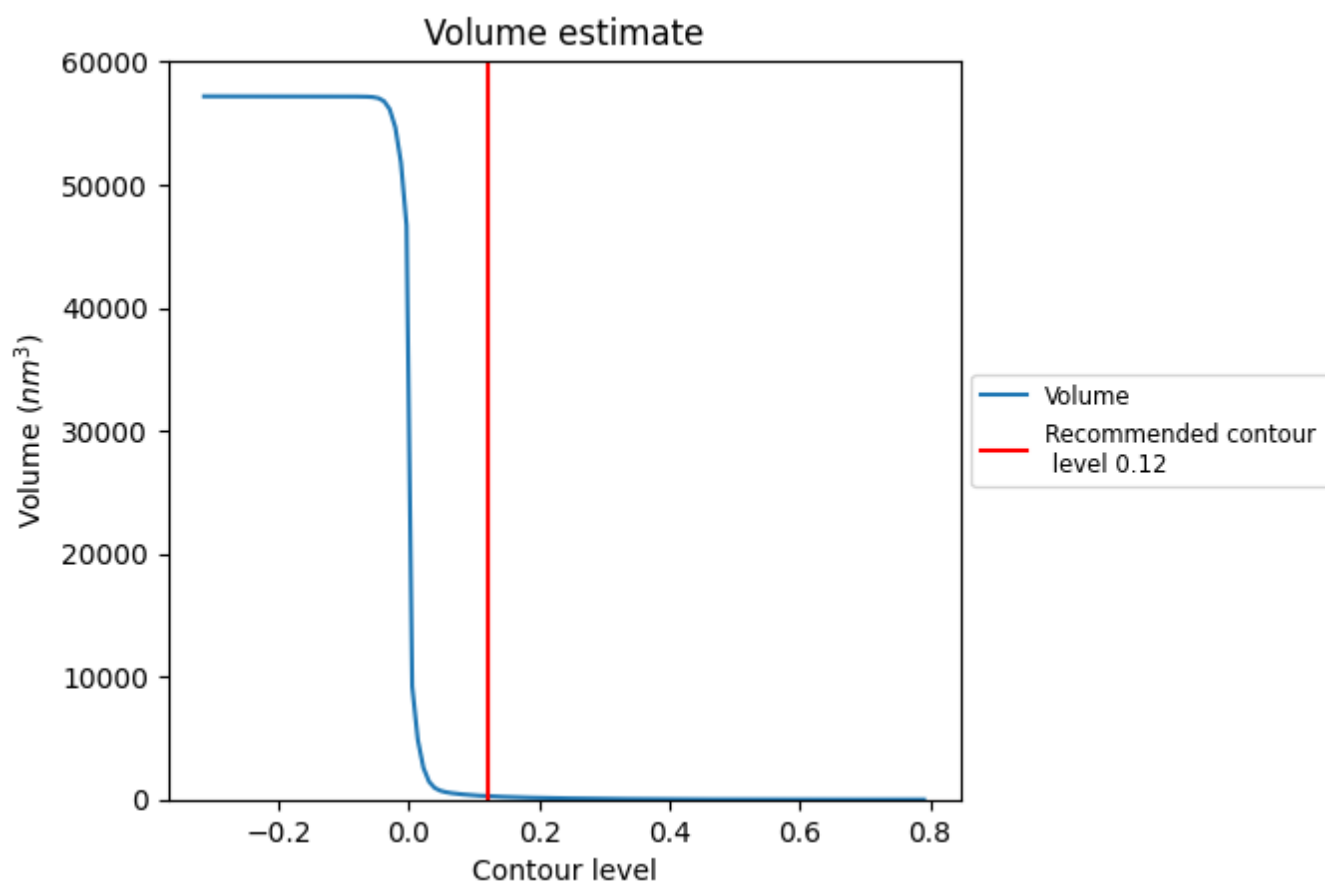
This section contains the results of statistical analysis of the map.

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.

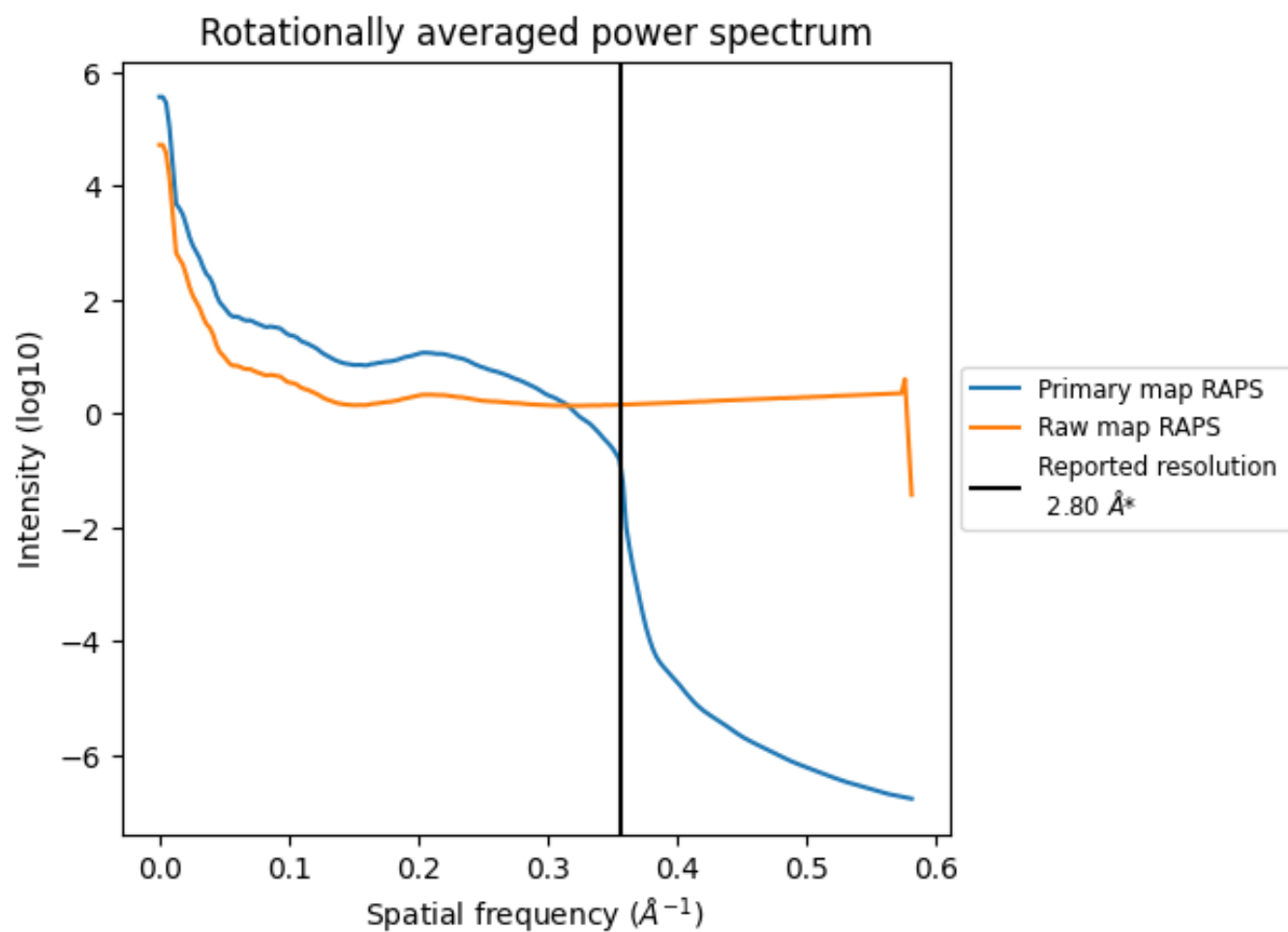
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 282 nm³; this corresponds to an approximate mass of 254 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 ⓘ

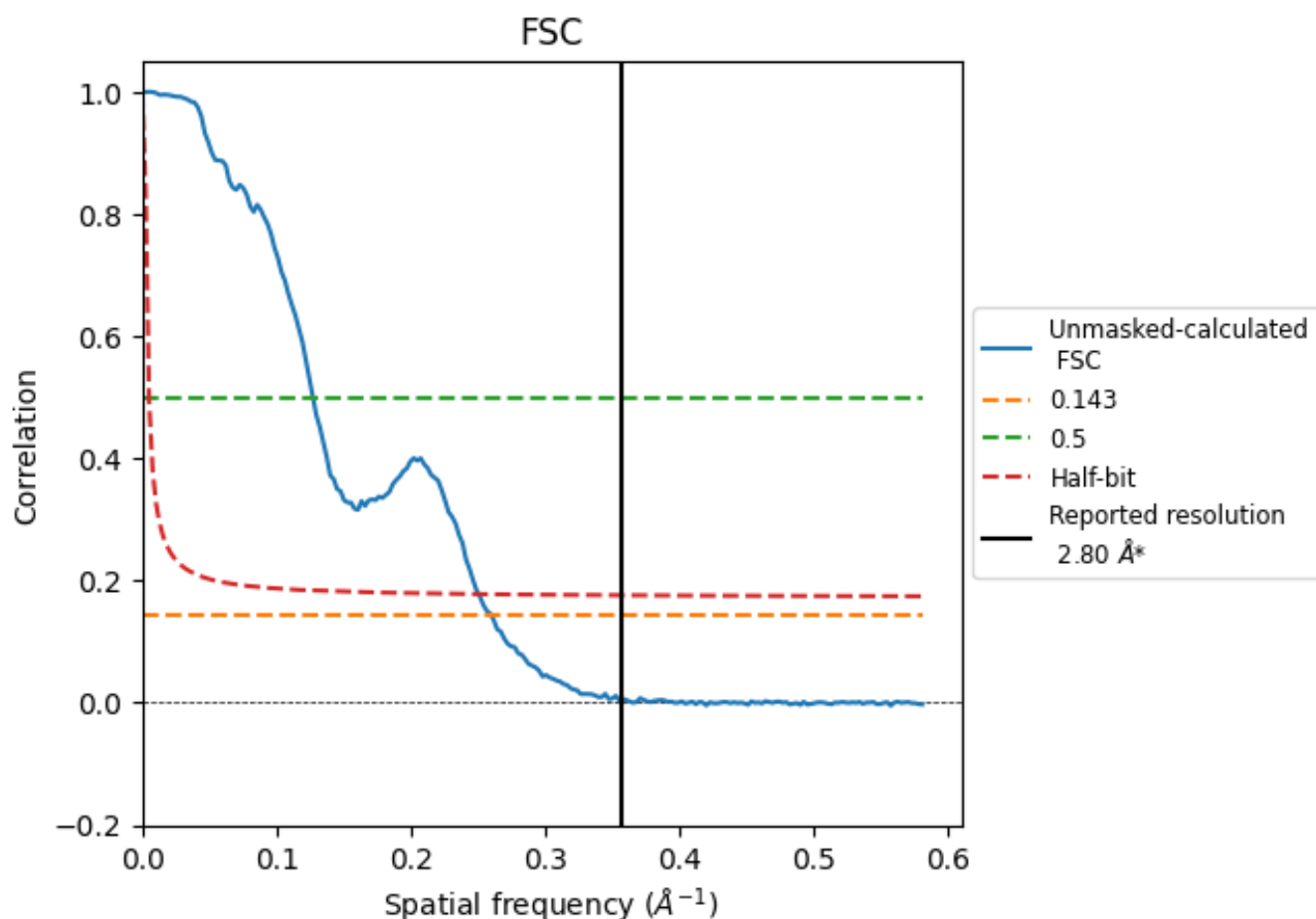


*Reported resolution corresponds to spatial frequency of 0.357 \AA^{-1}

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 0.357 \AA^{-1}

8.2 Resolution estimates [i](#)

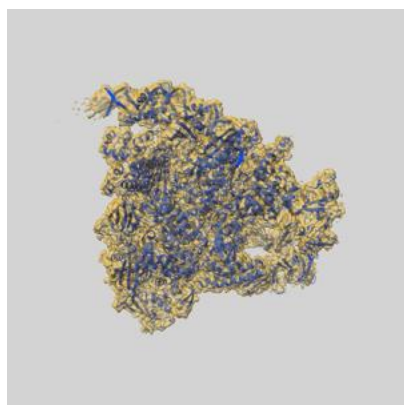
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.84	7.86	3.99

*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 3.84 differs from the reported value 2.8 by more than 10 %

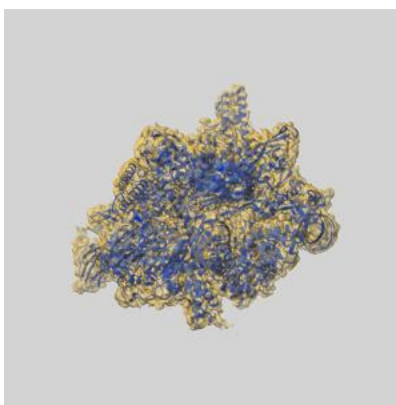
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48589 and PDB model 9MSH. Per-residue inclusion information can be found in section [3](#) on page [6](#).

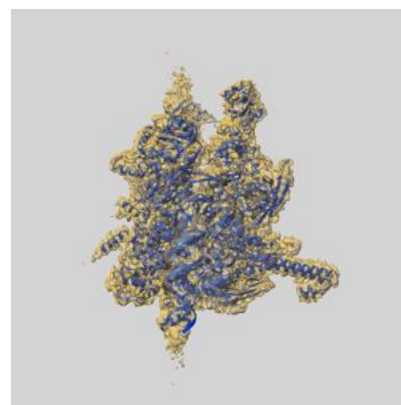
9.1 Map-model overlay [i](#)



X



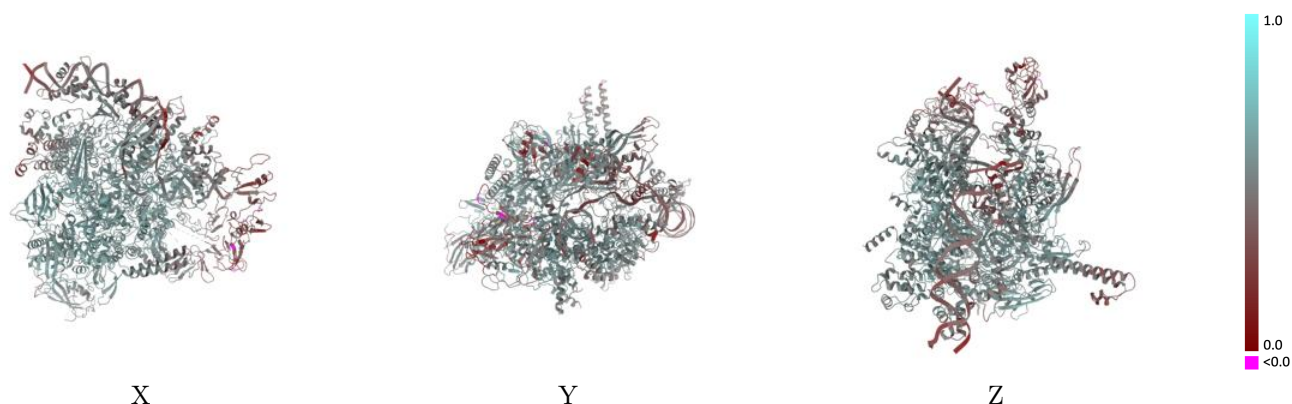
Y



Z

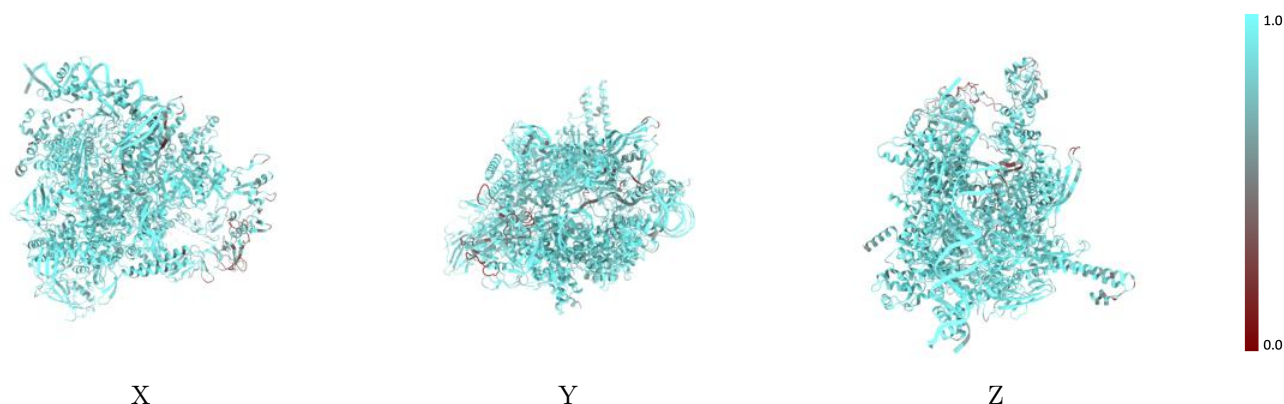
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



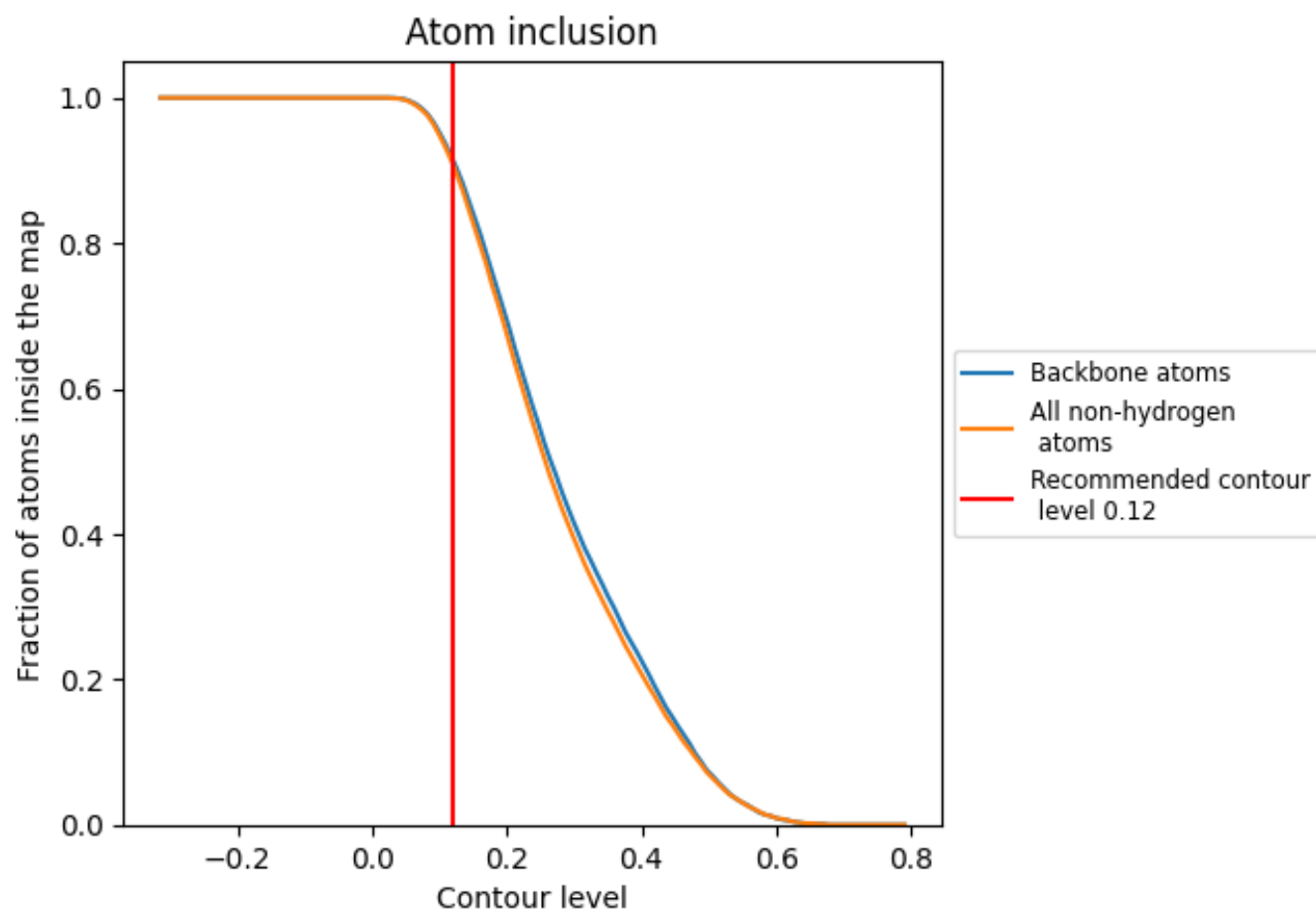
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 91% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9080	<div></div> 0.5210
G	<div></div> 0.9460	<div></div> 0.5660
H	<div></div> 0.9360	<div></div> 0.5380
I	<div></div> 0.9220	<div></div> 0.5380
J	<div></div> 0.9020	<div></div> 0.5270
K	<div></div> 0.9140	<div></div> 0.5620
M	<div></div> 0.8770	<div></div> 0.4860
U	<div></div> 0.9040	<div></div> 0.3820
V	<div></div> 0.8790	<div></div> 0.3680

