



Full wwPDB EM Validation Report ⓘ

Sep 21, 2026 – 11:12 AM EDT

PDB ID : 9Y78 / pdb_00009y78
EMDB ID : EMD-72645
Title : Cryo-EM structure of Mycobacterium tuberculosis transcription initiation complex containing 2nt RNA in complex with UMN141
Authors : You, L.L.; Ebright, R.H.
Deposited on : 2025-09-09
Resolution : 2.54 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

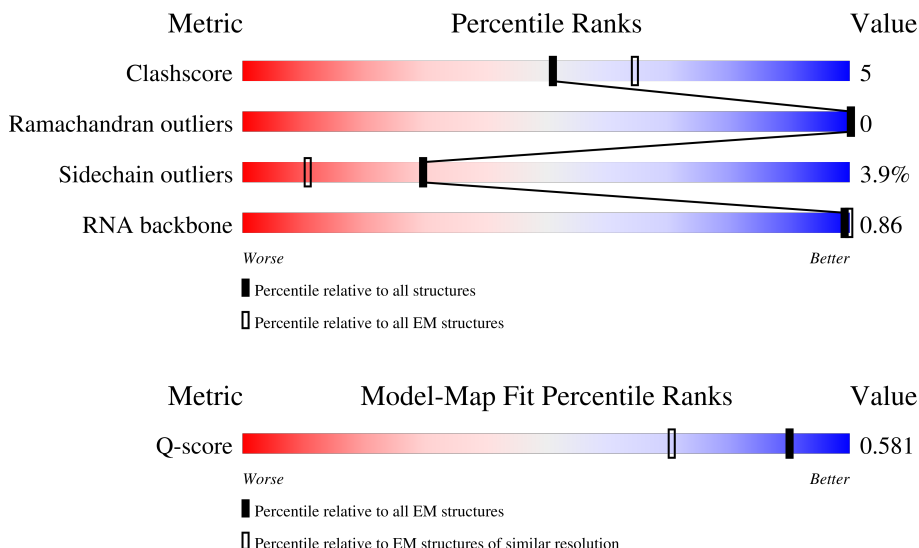
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.54 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.



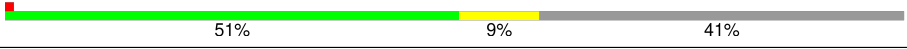
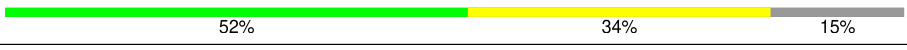
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7403 (2.04 - 3.04)

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

Mol	Chain	Length	Quality of chain
1	A	368	
1	B	368	
2	C	1174	

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Mol	Chain	Length	Quality of chain
3	D	1317	
4	E	110	
5	F	537	
6	G	62	
7	H	62	
8	J	2	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 27472 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	A	224	Total	C	N	O	S	0	0
			1708	1076	294	336	2		
1	B	237	Total	C	N	O	S	0	0
			1775	1120	304	348	3		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP P9WGZ1
A	-19	GLY	-	expression tag	UNP P9WGZ1
A	-18	HIS	-	expression tag	UNP P9WGZ1
A	-17	HIS	-	expression tag	UNP P9WGZ1
A	-16	HIS	-	expression tag	UNP P9WGZ1
A	-15	HIS	-	expression tag	UNP P9WGZ1
A	-14	HIS	-	expression tag	UNP P9WGZ1
A	-13	HIS	-	expression tag	UNP P9WGZ1
A	-12	HIS	-	expression tag	UNP P9WGZ1
A	-11	HIS	-	expression tag	UNP P9WGZ1
A	-10	HIS	-	expression tag	UNP P9WGZ1
A	-9	HIS	-	expression tag	UNP P9WGZ1
A	-8	SER	-	expression tag	UNP P9WGZ1
A	-7	SER	-	expression tag	UNP P9WGZ1
A	-6	GLY	-	expression tag	UNP P9WGZ1
A	-5	HIS	-	expression tag	UNP P9WGZ1
A	-4	ILE	-	expression tag	UNP P9WGZ1
A	-3	GLU	-	expression tag	UNP P9WGZ1
A	-2	GLY	-	expression tag	UNP P9WGZ1
A	-1	ARG	-	expression tag	UNP P9WGZ1
A	0	HIS	-	expression tag	UNP P9WGZ1
B	-20	MET	-	expression tag	UNP P9WGZ1
B	-19	GLY	-	expression tag	UNP P9WGZ1
B	-18	HIS	-	expression tag	UNP P9WGZ1
B	-17	HIS	-	expression tag	UNP P9WGZ1
B	-16	HIS	-	expression tag	UNP P9WGZ1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP P9WGZ1
B	-14	HIS	-	expression tag	UNP P9WGZ1
B	-13	HIS	-	expression tag	UNP P9WGZ1
B	-12	HIS	-	expression tag	UNP P9WGZ1
B	-11	HIS	-	expression tag	UNP P9WGZ1
B	-10	HIS	-	expression tag	UNP P9WGZ1
B	-9	HIS	-	expression tag	UNP P9WGZ1
B	-8	SER	-	expression tag	UNP P9WGZ1
B	-7	SER	-	expression tag	UNP P9WGZ1
B	-6	GLY	-	expression tag	UNP P9WGZ1
B	-5	HIS	-	expression tag	UNP P9WGZ1
B	-4	ILE	-	expression tag	UNP P9WGZ1
B	-3	GLU	-	expression tag	UNP P9WGZ1
B	-2	GLY	-	expression tag	UNP P9WGZ1
B	-1	ARG	-	expression tag	UNP P9WGZ1
B	0	HIS	-	expression tag	UNP P9WGZ1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1118	Total	C	N	O	S	0	0
			8660	5424	1519	1678	39		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	5	MET	-	initiating methionine	UNP P9WGY9
C	1147	GLU	LEU	conflict	UNP P9WGY9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1262	Total	C	N	O	S	0	0
			9855	6173	1791	1851	40		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	VAL	-	insertion	UNP P9WGY7

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	82	Total	C	N	O	0	0
			645	412	107	126		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	319	Total	C	N	O	S	0	0
			2526	1576	458	483	9		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-8	MET	-	initiating methionine	UNP P9WGI1
F	-7	ALA	-	expression tag	UNP P9WGI1
F	-6	ASP	-	expression tag	UNP P9WGI1
F	-5	LEU	-	expression tag	UNP P9WGI1
F	-4	ASN	-	expression tag	UNP P9WGI1
F	-3	TRP	-	expression tag	UNP P9WGI1
F	-2	MET	-	expression tag	UNP P9WGI1
F	-1	ILE	-	expression tag	UNP P9WGI1
F	0	SER	-	expression tag	UNP P9WGI1
F	1	VAL	MET	conflict	UNP P9WGI1
F	137	GLY	ASP	conflict	UNP P9WGI1
F	170	GLY	ASP	conflict	UNP P9WGI1

- Molecule 6 is a DNA chain called DNA (53-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	53	Total	C	N	O	P	0	0
			1094	517	206	318	53		

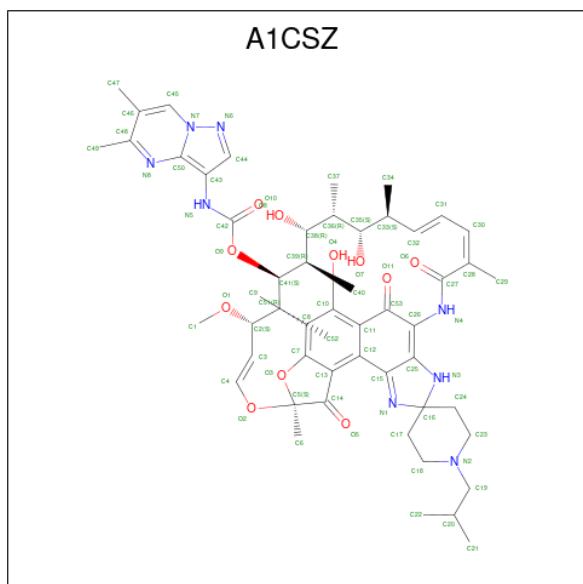
- Molecule 7 is a DNA chain called DNA (53-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	53	Total	C	N	O	P	0	0
			1092	516	207	316	53		

- Molecule 8 is a RNA chain called RNA (5'-R(*GP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	2	Total	C	N	O	P	0	0
			42	20	10	11	1		

- Molecule 9 is (9S,12E,14S,15R,16S,17R,18R,19R,20S,21S,22E,24Z)-6,18,20-trihydroxy-14-methoxy-7,9,15,17,19,21,25-heptamethyl-1'-(2-methylpropyl)-5,10,26-trioxo-3,5,9,10-tetrahydrospiro[9,4-(epoxypentadeca[1,11,13]trienoimino)furo[2',3':7,8]naphtho[1,2-d]imidazole-2,4'-piperidin]-16-yl [(8R)-5,6-dimethylpyrazolo[1,5-a]pyrimidin-3-yl]carbamate (CCD ID: A1CSZ) (formula: C₅₃H₆₈N₈O₁₁).



Mol	Chain	Residues	Atoms				AltConf
9	C	1	Total	C	N	O	0
			72	53	8	11	

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

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

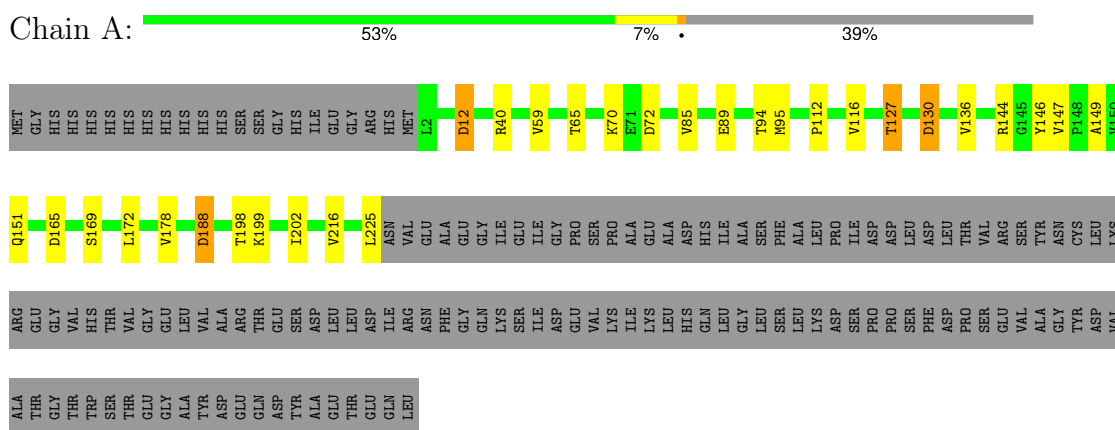
- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
11	D	1	Total	Mg	0
			1	1	

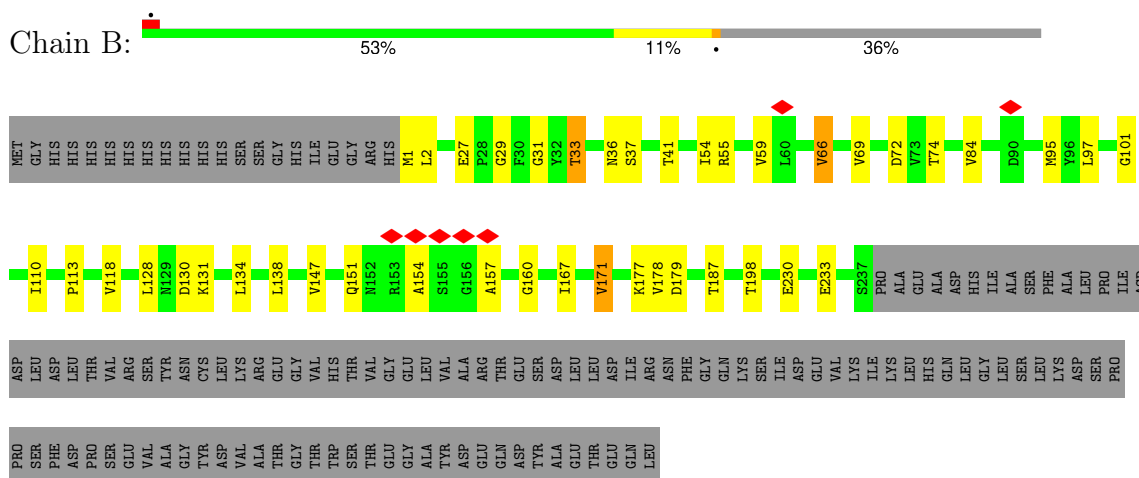
3 Residue-property plots

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.

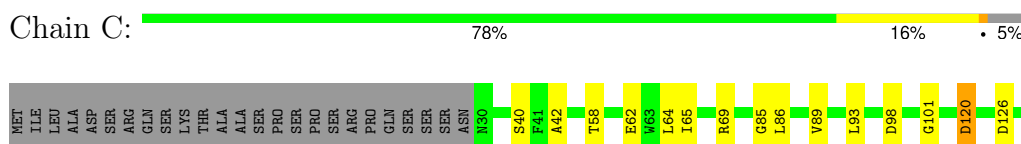
• Molecule 1: DNA-directed RNA polymerase subunit alpha

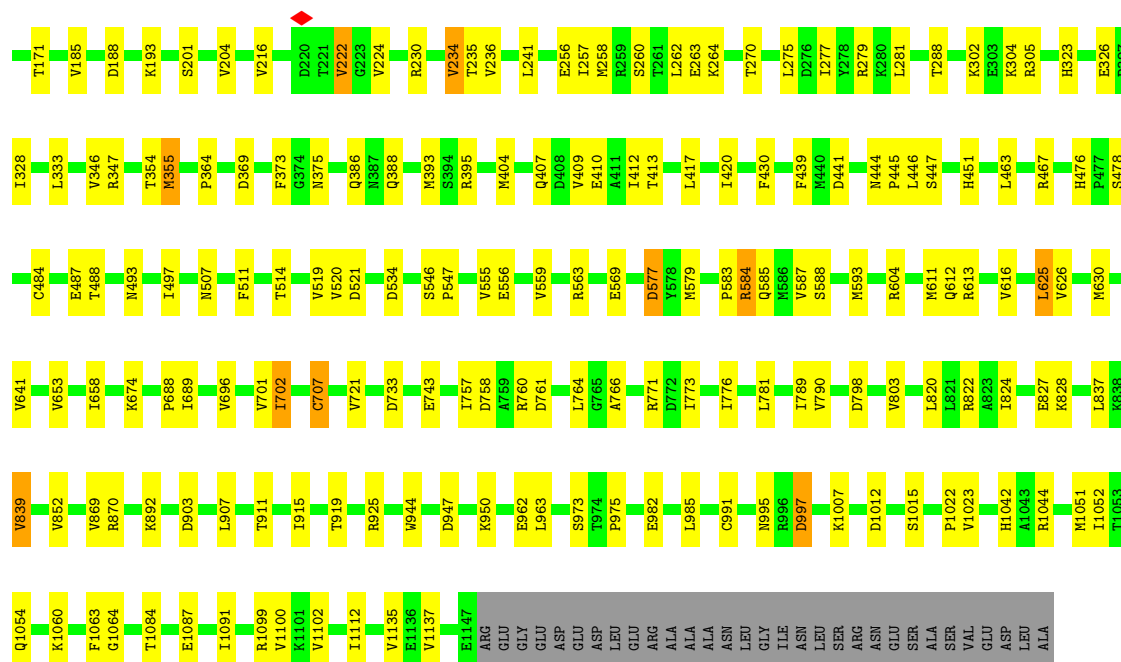


• Molecule 1: DNA-directed RNA polymerase subunit alpha

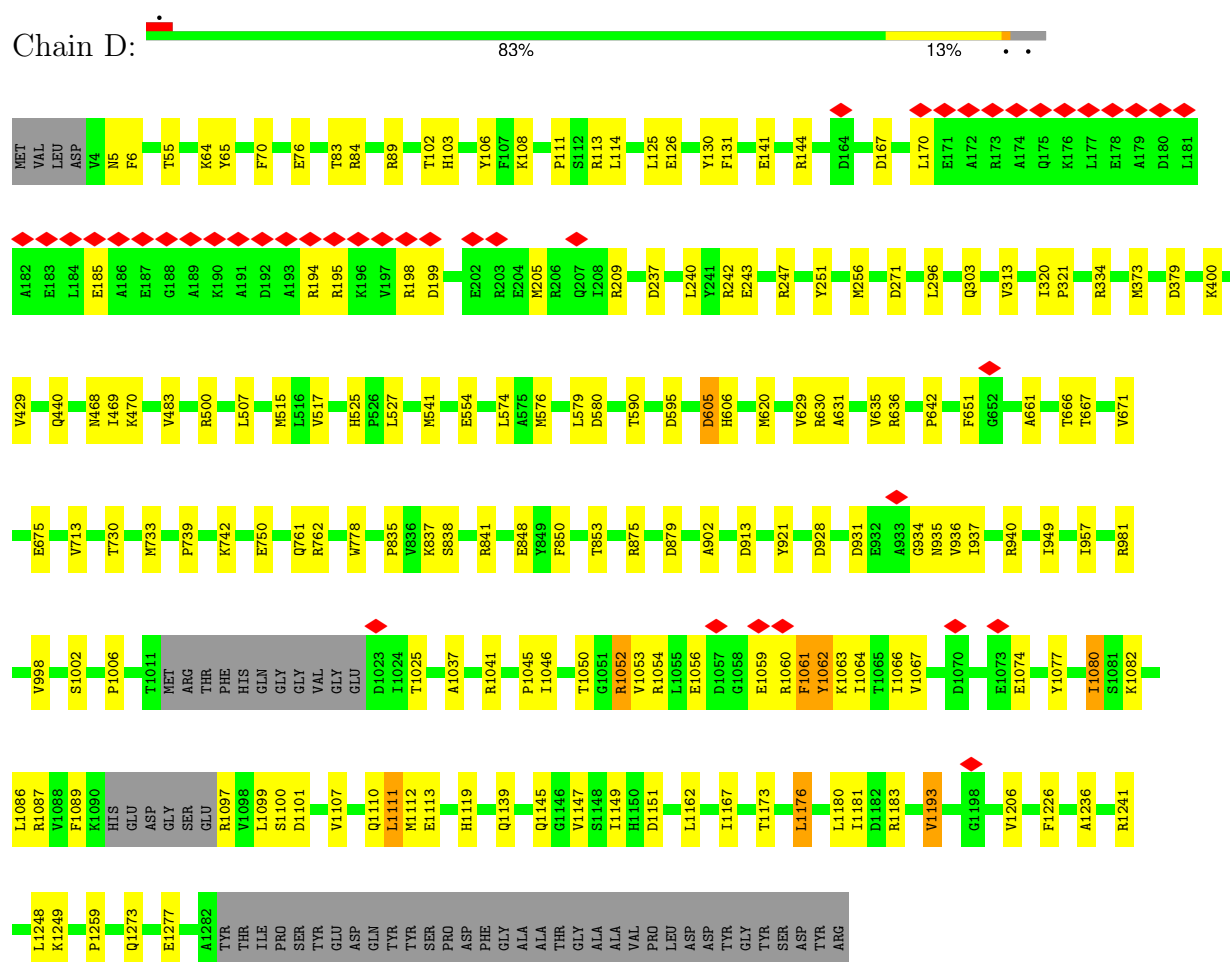


• Molecule 2: DNA-directed RNA polymerase subunit beta





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



- Molecule 4: DNA-directed RNA polymerase subunit omega

Frequency	Percentage
Daily	63%
Weekly	12%
Monthly	25%



Frequency	Percentage
Daily	51%
Weekly	9%
Monthly	41%



Category	Percentage
Very good	52%
Good	34%
Not good	15%



Response	Percentage
Yes, the U.S. is a democracy	61%
No, the U.S. is not a democracy	24%
Don't know	15%



Category	Percentage
Green	50%
Yellow	50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94463	Depositor
Resolution determination method	Not provided	
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57.35	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.223	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.036	Depositor
Map size ($\text{\AA}$)	285.04, 285.04, 285.04	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.509, 0.509, 0.509	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, A1CSZ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.14	0/1734	0.25	0/2359
1	B	0.12	0/1802	0.24	0/2454
2	C	0.15	0/8819	0.26	0/11957
3	D	0.14	0/10019	0.24	0/13546
4	E	0.14	0/658	0.23	0/896
5	F	0.10	0/2557	0.20	0/3447
6	G	0.18	0/1228	0.30	0/1895
7	H	0.17	0/1226	0.28	0/1891
8	J	0.09	0/47	0.09	0/72
All	All	0.14	0/28090	0.25	0/38517

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	1052	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1708	0	1750	18	0
1	B	1775	0	1809	22	0
2	C	8660	0	8600	112	0
3	D	9855	0	9922	99	0
4	E	645	0	642	8	0
5	F	2526	0	2557	34	0
6	G	1094	0	595	15	0
7	H	1092	0	594	12	0
8	J	42	0	23	1	0
9	C	72	0	0	0	0
10	D	2	0	0	0	0
11	D	1	0	0	0	0
All	All	27472	0	26492	288	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 (288) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ARG:HH12	2:C:903:ASP:HB3	1.47	0.79
5:F:516:HIS:HD2	5:F:518:SER:H	1.30	0.76
3:D:1052:ARG:NH2	3:D:1067:VAL:HG23	2.05	0.72
3:D:739:PRO:HG2	3:D:742:LYS:HB2	1.73	0.71
2:C:101:GLY:O	2:C:142:ASN:ND2	2.24	0.70
2:C:997:ASP:N	2:C:997:ASP:OD1	2.25	0.69
3:D:167:ASP:HA	3:D:170:LEU:HD12	1.75	0.69
1:B:97:LEU:HB2	1:B:110:ILE:HG22	1.75	0.68
3:D:1277:GLU:N	3:D:1277:GLU:OE2	2.26	0.67
3:D:605:ASP:OD1	3:D:605:ASP:N	2.29	0.65
3:D:875:ARG:NH2	3:D:1226:PHE:O	2.30	0.64
2:C:593:MET:HB2	2:C:612:GLN:HE22	1.62	0.64
2:C:563:ARG:NH1	2:C:569:GLU:OE2	2.32	0.62
3:D:1006:PRO:HG2	3:D:1149:ILE:HD11	1.80	0.62
2:C:42:ALA:HB2	2:C:975:PRO:HG2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:263:GLU:HB2	2:C:264:LYS:HE2	1.81	0.61
2:C:577:ASP:OD1	2:C:577:ASP:N	2.32	0.61
2:C:150:GLN:NE2	2:C:413:THR:OG1	2.34	0.60
3:D:1052:ARG:O	3:D:1052:ARG:NH1	2.34	0.60
7:H:29:DG:H2''	7:H:30:DG:H5''	1.83	0.60
2:C:467:ARG:NH2	6:G:63:DT:OP2	2.33	0.60
3:D:195:ARG:HH12	3:D:199:ASP:HB2	1.66	0.60
3:D:194:ARG:O	3:D:198:ARG:NH1	2.33	0.60
1:A:172:LEU:HD13	1:A:199:LYS:HG3	1.83	0.60
3:D:1053:VAL:HG21	3:D:1099:LEU:HD21	1.84	0.60
2:C:761:ASP:HA	2:C:766:ALA:HA	1.84	0.59
5:F:282:MET:HE2	5:F:282:MET:HA	1.85	0.59
3:D:525:HIS:HE1	3:D:527:LEU:HD12	1.68	0.59
5:F:430:GLU:OE2	7:H:19:DG:N2	2.35	0.59
2:C:630:MET:O	2:C:630:MET:HG3	2.03	0.59
2:C:388:GLN:HG3	2:C:430:PHE:HB2	1.85	0.58
3:D:500:ARG:HB2	3:D:541:MET:HE2	1.85	0.58
1:B:1:MET:N	1:B:230:GLU:OE2	2.32	0.58
2:C:323:HIS:HB3	2:C:326:GLU:HB2	1.86	0.58
3:D:879:ASP:OD2	3:D:1249:LYS:NZ	2.37	0.58
3:D:937:ILE:HD13	3:D:957:ILE:HD11	1.86	0.58
3:D:1052:ARG:HH21	3:D:1067:VAL:HG23	1.69	0.58
3:D:1087:ARG:HA	3:D:1113:GLU:HG2	1.85	0.58
3:D:1180:LEU:HD22	3:D:1206:VAL:HG11	1.85	0.58
3:D:1063:LYS:NZ	3:D:1064:ILE:O	2.37	0.58
2:C:696:VAL:HG11	2:C:702:ILE:HD11	1.84	0.57
3:D:1086:LEU:HD12	3:D:1099:LEU:HB3	1.86	0.57
3:D:1162:LEU:O	3:D:1183:ARG:NH2	2.37	0.57
2:C:1054:GLN:HB3	2:C:1099:ARG:HH12	1.69	0.57
2:C:305:ARG:NH2	6:G:59:DG:O6	2.36	0.56
7:H:18:DA:H2''	7:H:19:DG:H5'	1.86	0.56
1:B:151:GLN:OE1	1:B:151:GLN:N	2.35	0.56
3:D:334:ARG:NH1	5:F:419:GLU:O	2.39	0.56
1:B:167:ILE:HG23	3:D:620:MET:HE1	1.86	0.56
2:C:62:GLU:OE2	2:C:69:ARG:NH1	2.38	0.56
3:D:1064:ILE:HG23	3:D:1077:TYR:HB2	1.87	0.56
3:D:750:GLU:OE1	3:D:837:LYS:NZ	2.39	0.56
2:C:771:ARG:NH2	2:C:781:LEU:O	2.39	0.56
2:C:1012:ASP:OD2	2:C:1015:SER:OG	2.22	0.56
2:C:1084:THR:OG1	3:D:554:GLU:OE1	2.22	0.55
3:D:1167:ILE:HD11	3:D:1181:ILE:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:52:DA:H2''	6:G:53:DA:H5''	1.87	0.55
5:F:252:ARG:NH2	5:F:287:ASP:OD1	2.38	0.55
3:D:1059:GLU:HG2	3:D:1060:ARG:HG3	1.88	0.55
5:F:274:PRO:HG2	5:F:277:GLN:HB3	1.88	0.55
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	1.88	0.55
5:F:386:LEU:HD23	5:F:394:PRO:HB3	1.88	0.55
2:C:369:ASP:O	2:C:375:ASN:ND2	2.30	0.55
2:C:409:VAL:O	2:C:410:GLU:HG3	2.07	0.54
2:C:441:ASP:H	2:C:451:HIS:HD2	1.56	0.54
2:C:733:ASP:OD1	2:C:925:ARG:NH2	2.41	0.54
3:D:205:MET:HG3	3:D:209:ARG:HH21	1.72	0.54
2:C:154:MET:HE3	2:C:393:MET:HE1	1.90	0.53
2:C:1052:ILE:O	3:D:89:ARG:NH2	2.42	0.53
3:D:636:ARG:HD2	3:D:661:ALA:HB1	1.91	0.53
3:D:1100:SER:OG	3:D:1101:ASP:N	2.41	0.53
5:F:488:THR:HG23	5:F:491:GLU:H	1.74	0.53
1:B:171:VAL:HA	1:B:198:THR:HA	1.90	0.53
5:F:301:ARG:HD3	6:G:55:DG:C8	2.43	0.53
2:C:789:ILE:HG23	2:C:803:VAL:HG22	1.89	0.53
3:D:64:LYS:NZ	3:D:76:GLU:OE2	2.37	0.53
5:F:500:ARG:NH1	7:H:47:DT:O4	2.42	0.53
3:D:1173:THR:HB	3:D:1193:VAL:HG21	1.89	0.53
1:A:12:ASP:N	1:A:12:ASP:OD1	2.41	0.53
6:G:42:DG:H2''	6:G:43:DT:H5''	1.91	0.53
2:C:658:ILE:HD11	2:C:688:PRO:HB3	1.91	0.53
3:D:114:LEU:HB3	3:D:125:LEU:HD21	1.90	0.53
3:D:1045:PRO:HB2	3:D:1111:LEU:HD23	1.91	0.52
3:D:1056:GLU:HG2	3:D:1063:LYS:HB3	1.91	0.52
2:C:758:ASP:OD2	2:C:760:ARG:NH2	2.42	0.52
2:C:445:PRO:HD2	2:C:707:CYS:HB2	1.90	0.52
3:D:400:LYS:HE3	5:F:434:GLN:HE22	1.74	0.52
3:D:271:ASP:OD1	3:D:303:GLN:NE2	2.37	0.51
6:G:32:DA:H61	7:H:44:DT:H3	1.59	0.51
2:C:476:HIS:HD2	2:C:478:SER:H	1.56	0.51
3:D:243:GLU:OE1	3:D:247:ARG:NH1	2.43	0.51
6:G:33:DG:H2''	6:G:34:DG:H5''	1.92	0.51
2:C:773:ILE:HB	2:C:776:ILE:HG12	1.91	0.50
3:D:838:SER:OG	3:D:848:GLU:OE1	2.27	0.50
3:D:850:PHE:O	3:D:853:THR:OG1	2.29	0.50
5:F:501:GLU:OE1	7:H:48:DC:N4	2.36	0.50
6:G:37:DC:H2'	6:G:38:DG:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:778:TRP:CD2	3:D:835:PRO:HG3	2.47	0.50
1:A:95:MET:HB3	1:A:112:PRO:HA	1.93	0.50
1:A:169:SER:O	1:A:199:LYS:NZ	2.38	0.49
5:F:295:LEU:O	5:F:299:ASN:ND2	2.44	0.49
3:D:761:GLN:HB3	3:D:762:ARG:HH22	1.76	0.49
3:D:1236:ALA:HA	3:D:1241:ARG:HG3	1.93	0.49
3:D:935:ASN:OD1	3:D:935:ASN:N	2.44	0.49
2:C:982:GLU:OE1	3:D:841:ARG:NH1	2.38	0.49
3:D:928:ASP:OD1	3:D:940:ARG:N	2.46	0.49
4:E:81:PRO:HB3	4:E:94:ILE:HG21	1.95	0.49
1:B:55:ARG:HH22	1:B:160:GLY:H	1.60	0.48
2:C:354:THR:HG22	2:C:364:PRO:HA	1.95	0.48
2:C:40:SER:HA	2:C:973:SER:HB3	1.94	0.48
3:D:1041:ARG:HG2	3:D:1041:ARG:HH11	1.78	0.48
4:E:47:VAL:HG21	4:E:53:LEU:HB2	1.94	0.48
5:F:330:ARG:NH1	5:F:333:GLU:OE1	2.46	0.48
2:C:892:LYS:NZ	8:J:2:A:OP1	2.40	0.48
3:D:554:GLU:HG3	4:E:54:VAL:HG11	1.94	0.48
2:C:126:ASP:OD2	2:C:870:ARG:NH2	2.45	0.48
2:C:546:SER:HB2	2:C:579:MET:HE3	1.94	0.48
1:B:37:SER:O	1:B:41:THR:OG1	2.29	0.48
1:B:128:LEU:HD11	1:B:134:LEU:HD22	1.95	0.48
2:C:555:VAL:HG23	2:C:556:GLU:HG3	1.96	0.48
1:A:188:ASP:OD1	1:A:188:ASP:N	2.45	0.48
2:C:514:THR:OG1	2:C:585:GLN:NE2	2.37	0.48
1:A:40:ARG:HE	1:B:33:THR:HG22	1.78	0.48
2:C:420:ILE:HG12	5:F:388:GLN:HE22	1.78	0.48
2:C:757:ILE:HD12	2:C:837:LEU:HB2	1.95	0.48
2:C:822:ARG:HH11	2:C:827:GLU:HB3	1.78	0.48
5:F:266:LEU:HD21	5:F:272:LYS:HD3	1.96	0.48
6:G:34:DG:N2	7:H:43:DC:O2	2.47	0.48
3:D:998:VAL:O	3:D:1002:SER:OG	2.27	0.47
2:C:1042:HIS:HB2	2:C:1060:LYS:HG3	1.96	0.47
2:C:493:ASN:HB3	2:C:497:ILE:HD12	1.97	0.47
2:C:583:PRO:O	2:C:584:ARG:HG2	2.14	0.47
3:D:440:GLN:HG2	3:D:515:MET:HE3	1.95	0.47
3:D:1089:PHE:O	3:D:1097:ARG:N	2.48	0.47
1:B:95:MET:HG2	1:B:113:PRO:HD2	1.97	0.47
2:C:487:GLU:OE1	2:C:588:SER:OG	2.31	0.47
3:D:185:GLU:OE2	3:D:194:ARG:NH1	2.48	0.47
1:B:177:LYS:NZ	1:B:179:ASP:OD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ASP:OD1	1:B:72:ASP:N	2.36	0.47
1:A:85:VAL:HG11	1:A:95:MET:HE1	1.95	0.46
3:D:144:ARG:HB2	3:D:251:TYR:HD2	1.80	0.46
2:C:758:ASP:N	2:C:758:ASP:OD1	2.47	0.46
1:A:144:ARG:NH2	1:B:27:GLU:OE2	2.48	0.46
1:B:36:ASN:ND2	2:C:1015:SER:O	2.48	0.46
2:C:304:LYS:HD3	2:C:304:LYS:HA	1.61	0.46
5:F:301:ARG:HB3	6:G:54:DT:H1'	1.97	0.46
7:H:38:DC:H2''	7:H:39:DG:C8	2.50	0.46
2:C:514:THR:HG1	2:C:585:GLN:HE21	1.61	0.46
2:C:1100:VAL:HG12	5:F:447:ALA:HB2	1.98	0.46
3:D:1046:ILE:HG22	3:D:1110:GLN:HB3	1.98	0.46
7:H:11:DT:H2'	7:H:12:DG:C8	2.51	0.46
1:B:130:ASP:O	1:B:131:LYS:HG2	2.16	0.46
2:C:407:GLN:HE21	2:C:412:ILE:HG22	1.80	0.46
2:C:563:ARG:HD2	2:C:563:ARG:HA	1.62	0.46
2:C:630:MET:HE2	2:C:630:MET:HB2	1.71	0.46
3:D:1052:ARG:HH11	3:D:1053:VAL:CA	2.28	0.46
5:F:217:LYS:HD2	5:F:217:LYS:HA	1.73	0.46
3:D:296:LEU:HD23	3:D:1176:LEU:HD11	1.98	0.45
3:D:373:MET:HE1	5:F:322:GLN:HG3	1.98	0.45
2:C:275:LEU:O	2:C:279:ARG:HG3	2.16	0.45
3:D:103:HIS:HB3	3:D:106:TYR:HD2	1.81	0.45
1:A:151:GLN:HA	1:A:151:GLN:OE1	2.16	0.45
2:C:1102:VAL:HG23	2:C:1112:ILE:HG23	1.99	0.45
7:H:30:DG:H2''	7:H:31:DC:H5''	1.98	0.45
2:C:444:ASN:HD22	2:C:446:LEU:H	1.63	0.45
3:D:64:LYS:NZ	3:D:65:TYR:OH	2.48	0.45
3:D:468:ASN:ND2	3:D:470:LYS:HB2	2.32	0.45
6:G:60:DC:H2''	6:G:61:DT:C5	2.51	0.45
2:C:547:PRO:HB2	2:C:555:VAL:HG22	1.99	0.45
3:D:102:THR:HG22	3:D:313:VAL:HG22	1.98	0.45
3:D:1006:PRO:HB3	3:D:1147:VAL:HG11	1.99	0.45
3:D:1054:ARG:HH12	3:D:1056:GLU:HB3	1.82	0.45
3:D:666:THR:OG1	3:D:667:THR:N	2.49	0.45
3:D:1037:ALA:O	3:D:1119:HIS:NE2	2.43	0.45
2:C:277:ILE:HG23	2:C:281:LEU:HD12	2.00	0.45
2:C:625:LEU:HD12	2:C:625:LEU:HA	1.84	0.45
2:C:98:ASP:OD1	2:C:98:ASP:N	2.47	0.44
3:D:1067:VAL:HG22	3:D:1074:GLU:OE2	2.17	0.44
1:A:65:THR:HG21	2:C:674:LYS:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:58:DA:H2''	6:G:59:DG:H5'	1.98	0.44
2:C:689:ILE:HD11	2:C:701:VAL:HG12	1.97	0.44
3:D:131:PHE:HD2	3:D:256:MET:HE3	1.83	0.44
3:D:580:ASP:OD1	3:D:580:ASP:N	2.51	0.44
2:C:995:ASN:OD1	2:C:995:ASN:N	2.44	0.44
2:C:1023:VAL:HA	3:D:730:THR:HG21	1.98	0.44
2:C:1054:GLN:O	2:C:1099:ARG:NH1	2.50	0.44
3:D:1062:TYR:OH	3:D:1082:LYS:O	2.23	0.44
2:C:69:ARG:HH11	2:C:69:ARG:HB3	1.83	0.44
2:C:347:ARG:HD2	2:C:355:MET:HB2	1.99	0.44
3:D:108:LYS:HD2	3:D:108:LYS:HA	1.78	0.44
3:D:595:ASP:HB3	3:D:631:ALA:HB2	1.98	0.44
2:C:120:ASP:OD1	2:C:120:ASP:N	2.37	0.44
2:C:950:LYS:HA	2:C:950:LYS:HD3	1.79	0.44
2:C:721:VAL:HG23	2:C:915:ILE:HG23	1.98	0.44
2:C:764:LEU:HD12	2:C:764:LEU:H	1.82	0.44
2:C:820:LEU:HD23	5:F:460:LEU:HD21	2.00	0.44
2:C:907:LEU:HD12	2:C:911:THR:HB	1.99	0.44
2:C:947:ASP:OD1	2:C:947:ASP:N	2.44	0.44
3:D:83:THR:OG1	3:D:84:ARG:N	2.51	0.44
2:C:241:LEU:HD23	2:C:241:LEU:HA	1.88	0.43
2:C:507:ASN:HB2	2:C:511:PHE:O	2.17	0.43
2:C:824:ILE:O	5:F:515:ARG:NE	2.48	0.43
5:F:405:ILE:HD12	5:F:409:LYS:HB3	2.00	0.43
3:D:576:MET:HB2	3:D:576:MET:HE3	1.75	0.43
3:D:1059:GLU:C	3:D:1060:ARG:HG3	2.43	0.43
4:E:38:PRO:HG2	4:E:43:LEU:HD11	2.01	0.43
4:E:39:PRO:HG2	4:E:42:GLU:HG3	2.00	0.43
1:A:70:LYS:HB3	1:A:127:THR:HG23	1.99	0.43
1:A:198:THR:HG21	1:A:202:ILE:HG13	2.00	0.43
2:C:484:CYS:HB2	2:C:588:SER:HB3	2.01	0.43
5:F:242:ASN:ND2	5:F:245:GLU:OE2	2.51	0.43
6:G:51:DT:H2''	6:G:52:DA:H5''	2.01	0.43
2:C:386:GLN:HE21	2:C:386:GLN:HB3	1.73	0.43
3:D:507:LEU:HD12	3:D:574:LEU:HD12	2.00	0.43
1:A:149:ALA:N	1:A:165:ASP:OD1	2.51	0.42
5:F:263:MET:HE1	5:F:281:MET:HG2	2.01	0.42
2:C:476:HIS:CD2	2:C:478:SER:H	2.36	0.42
2:C:944:TRP:HB2	2:C:991:CYS:O	2.19	0.42
3:D:1273:GLN:NE2	4:E:105:GLU:OE2	2.46	0.42
1:A:130:ASP:OD1	1:A:130:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:VAL:HG13	1:B:69:VAL:HB	2.01	0.42
2:C:828:LYS:HD3	2:C:828:LYS:HA	1.87	0.42
3:D:111:PRO:O	3:D:113:ARG:NH1	2.53	0.42
1:A:72:ASP:OD1	1:A:72:ASP:N	2.41	0.42
1:B:154:ALA:HB1	1:B:157:ALA:HB3	2.00	0.42
2:C:193:LYS:HA	2:C:193:LYS:HD3	1.75	0.42
2:C:64:LEU:HA	2:C:85:GLY:HA3	2.02	0.42
3:D:902:ALA:H	3:D:913:ASP:HB2	1.84	0.42
3:D:931:ASP:O	3:D:934:GLY:N	2.48	0.42
2:C:230:ARG:HB3	2:C:230:ARG:HH11	1.84	0.42
3:D:590:THR:O	3:D:630:ARG:HB3	2.19	0.42
4:E:33:LEU:O	4:E:36:THR:OG1	2.36	0.42
3:D:1052:ARG:NH1	3:D:1054:ARG:N	2.68	0.42
2:C:798:ASP:HA	2:C:839:VAL:HG22	2.01	0.41
3:D:1248:LEU:HD23	3:D:1259:PRO:HD2	2.01	0.41
2:C:216:VAL:HG22	2:C:222:VAL:HB	2.02	0.41
2:C:1044:ARG:NH1	2:C:1064:GLY:O	2.53	0.41
5:F:263:MET:HE1	5:F:281:MET:CG	2.49	0.41
5:F:334:LYS:HB3	5:F:334:LYS:HE3	1.84	0.41
3:D:1139:GLN:NE2	3:D:1151:ASP:OD1	2.39	0.41
5:F:277:GLN:O	5:F:281:MET:HB3	2.21	0.41
5:F:397:GLU:OE1	5:F:397:GLU:N	2.51	0.41
2:C:333:LEU:HD12	2:C:333:LEU:HA	1.88	0.41
2:C:604:ARG:CZ	2:C:925:ARG:HD3	2.51	0.41
2:C:58:THR:O	2:C:62:GLU:HG2	2.21	0.41
2:C:188:ASP:OD1	2:C:201:SER:OG	2.33	0.41
2:C:420:ILE:HD11	5:F:387:LEU:HD21	2.03	0.41
2:C:520:VAL:HG22	2:C:521:ASP:OD1	2.21	0.41
2:C:604:ARG:HA	2:C:604:ARG:HD3	1.85	0.41
2:C:822:ARG:HD3	2:C:827:GLU:HB3	2.01	0.41
3:D:1061:PHE:HB2	3:D:1080:ILE:O	2.21	0.41
4:E:84:GLU:HA	4:E:84:GLU:OE2	2.20	0.41
5:F:513:LYS:HB2	5:F:513:LYS:HE3	1.84	0.41
1:B:101:GLY:HA2	1:B:131:LYS:HA	2.03	0.41
2:C:171:THR:HB	2:C:439:PHE:HE1	1.86	0.41
2:C:395:ARG:HD3	7:H:24:DA:C5	2.56	0.41
3:D:373:MET:HE2	3:D:373:MET:HB2	1.93	0.41
3:D:579:LEU:HB3	3:D:580:ASP:H	1.67	0.41
3:D:1086:LEU:HD22	3:D:1112:MET:HE3	2.03	0.41
1:A:146:TYR:CG	2:C:743:GLU:HG2	2.55	0.41
1:A:172:LEU:HD12	1:A:172:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:MET:HE3	1:B:138:LEU:HD12	2.03	0.41
2:C:224:VAL:HG12	2:C:234:VAL:HA	2.02	0.41
2:C:302:LYS:HD3	2:C:302:LYS:HA	1.86	0.41
2:C:444:ASN:O	2:C:447:SER:OG	2.35	0.41
1:B:110:ILE:HD11	1:B:118:VAL:HG21	2.03	0.40
2:C:93:LEU:HD13	2:C:393:MET:HB3	2.02	0.40
3:D:1053:VAL:HG23	3:D:1064:ILE:HD11	2.03	0.40
6:G:25:DC:H2'	6:G:26:DT:H71	2.02	0.40
1:B:177:LYS:HB2	1:B:177:LYS:HE2	1.69	0.40
3:D:130:TYR:OH	3:D:379:ASP:OD2	2.34	0.40
1:B:29:GLY:C	1:B:31:GLY:H	2.29	0.40
2:C:86:LEU:HD23	2:C:86:LEU:HA	1.91	0.40
2:C:417:LEU:HD23	2:C:417:LEU:HA	1.96	0.40
2:C:584:ARG:O	2:C:587:VAL:HG22	2.22	0.40
2:C:1007:LYS:HB3	2:C:1022:PRO:HB2	2.02	0.40
3:D:237:ASP:HB3	3:D:240:LEU:HB3	2.03	0.40
3:D:642:PRO:HG2	3:D:651:PHE:HE2	1.86	0.40
3:D:671:VAL:O	3:D:675:GLU:HG3	2.20	0.40
3:D:1052:ARG:O	3:D:1066:ILE:HD13	2.21	0.40
5:F:423:LEU:HD23	5:F:423:LEU:HA	1.88	0.40
6:G:35:DC:H2''	6:G:36:DC:C6	2.56	0.40
3:D:141:GLU:OE1	3:D:144:ARG:NH2	2.54	0.40
5:F:382:ILE:HD13	5:F:402:GLU:HG3	2.03	0.40
2:C:1102:VAL:HG23	2:C:1112:ILE:HD12	2.03	0.40
3:D:320:ILE:HG12	3:D:321:PRO:HD2	2.04	0.40
3:D:921:TYR:CE1	3:D:949:ILE:HG13	2.57	0.40
5:F:313:ARG:NH2	7:H:26:DA:O4'	2.55	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	A	222/368 (60%)	217 (98%)	5 (2%)	0	100	100
1	B	235/368 (64%)	226 (96%)	9 (4%)	0	100	100
2	C	1116/1174 (95%)	1084 (97%)	32 (3%)	0	100	100
3	D	1256/1317 (95%)	1235 (98%)	21 (2%)	0	100	100
4	E	80/110 (73%)	79 (99%)	1 (1%)	0	100	100
5	F	317/537 (59%)	312 (98%)	5 (2%)	0	100	100
All	All	3226/3874 (83%)	3153 (98%)	73 (2%)	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	A	193/315 (61%)	180 (93%)	13 (7%)	15	21
1	B	197/315 (62%)	185 (94%)	12 (6%)	17	25
2	C	943/995 (95%)	893 (95%)	50 (5%)	20	31
3	D	1042/1096 (95%)	1014 (97%)	28 (3%)	39	58
4	E	69/90 (77%)	69 (100%)	0	100	100
5	F	266/433 (61%)	262 (98%)	4 (2%)	57	74
All	All	2710/3244 (84%)	2603 (96%)	107 (4%)	30	43

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	59	VAL
1	A	89	GLU
1	A	94	THR
1	A	116	VAL
1	A	127	THR
1	A	130	ASP

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Mol	Chain	Res	Type
1	A	136	VAL
1	A	147	VAL
1	A	178	VAL
1	A	188	ASP
1	A	216	VAL
1	A	225	LEU
1	B	2	LEU
1	B	33	THR
1	B	54	ILE
1	B	59	VAL
1	B	66	VAL
1	B	74	THR
1	B	84	VAL
1	B	147	VAL
1	B	171	VAL
1	B	178	VAL
1	B	187	THR
1	B	233	GLU
2	C	65	ILE
2	C	89	VAL
2	C	120	ASP
2	C	185	VAL
2	C	204	VAL
2	C	222	VAL
2	C	234	VAL
2	C	235	THR
2	C	236	VAL
2	C	256	GLU
2	C	257	ILE
2	C	258	MET
2	C	260	SER
2	C	262	LEU
2	C	270	THR
2	C	288	THR
2	C	328	ILE
2	C	346	VAL
2	C	355	MET
2	C	373	PHE
2	C	404	MET
2	C	463	LEU
2	C	488	THR
2	C	519	VAL

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Mol	Chain	Res	Type
2	C	534	ASP
2	C	559	VAL
2	C	577	ASP
2	C	584	ARG
2	C	611	MET
2	C	613	ARG
2	C	616	VAL
2	C	625	LEU
2	C	626	VAL
2	C	641	VAL
2	C	653	VAL
2	C	702	ILE
2	C	707	CYS
2	C	790	VAL
2	C	839	VAL
2	C	852	VAL
2	C	869	VAL
2	C	919	THR
2	C	962	GLU
2	C	963	LEU
2	C	985	LEU
2	C	997	ASP
2	C	1051	MET
2	C	1063	PHE
2	C	1135	VAL
2	C	1137	VAL
3	D	5	ASN
3	D	6	PHE
3	D	55	THR
3	D	70	PHE
3	D	126	GLU
3	D	242	ARG
3	D	429	VAL
3	D	469	ILE
3	D	483	VAL
3	D	517	VAL
3	D	605	ASP
3	D	606	HIS
3	D	629	VAL
3	D	635	VAL
3	D	713	VAL
3	D	733	MET

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Mol	Chain	Res	Type
3	D	936	VAL
3	D	981	ARG
3	D	1025	THR
3	D	1050	THR
3	D	1061	PHE
3	D	1062	TYR
3	D	1080	ILE
3	D	1107	VAL
3	D	1111	LEU
3	D	1145	GLN
3	D	1176	LEU
3	D	1193	VAL
5	F	258	TYR
5	F	261	GLN
5	F	345	THR
5	F	392	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	B	17	ASN
1	B	185	GLN
2	C	150	GLN
2	C	293	GLN
2	C	386	GLN
2	C	407	GLN
2	C	442	GLN
2	C	444	ASN
2	C	451	HIS
2	C	476	HIS
2	C	612	GLN
2	C	662	HIS
2	C	680	HIS
2	C	986	GLN
3	D	267	ASN
3	D	304	GLN
3	D	329	GLN
3	D	369	ASN
3	D	416	ASN
3	D	468	ASN
3	D	540	GLN

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Mol	Chain	Res	Type
3	D	639	GLN
3	D	693	GLN
3	D	748	HIS
3	D	759	GLN
3	D	787	GLN
3	D	810	ASN
3	D	852	ASN
3	D	1110	GLN
3	D	1153	HIS
4	E	70	GLN
4	E	100	HIS
5	F	242	ASN
5	F	261	GLN
5	F	322	GLN
5	F	362	GLN
5	F	388	GLN
5	F	425	GLN
5	F	434	GLN
5	F	516	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	J	1/2 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 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	$\# Z > 2$
9	A1CSZ	C	1201	-	72,79,79	0.72	2 (2%)	102,121,121	1.39	15 (14%)

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
9	A1CSZ	C	1201	-	-	7/63/120/120	0/7/8/8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1201	A1CSZ	C46-C48	-3.53	1.43	1.47
9	C	1201	A1CSZ	C45-C46	2.48	1.38	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1201	A1CSZ	C51-C2-C3	4.06	120.90	112.11
9	C	1201	A1CSZ	O2-C5-C14	3.78	122.38	111.99
9	C	1201	A1CSZ	C7-C13-C14	-3.67	104.08	107.16
9	C	1201	A1CSZ	C43-C50-N8	3.27	133.64	123.42
9	C	1201	A1CSZ	C6-C5-C14	-2.99	106.54	113.90
9	C	1201	A1CSZ	C47-C46-C48	2.99	121.56	118.22
9	C	1201	A1CSZ	C53-C26-N4	2.95	121.67	115.21
9	C	1201	A1CSZ	C31-C30-C28	2.65	134.13	126.64
9	C	1201	A1CSZ	C17-C16-N1	-2.61	109.17	111.44
9	C	1201	A1CSZ	C13-C12-C11	-2.51	116.62	119.91
9	C	1201	A1CSZ	C25-C26-C53	-2.17	118.56	121.19
9	C	1201	A1CSZ	C12-C15-C25	-2.13	121.36	123.42
9	C	1201	A1CSZ	C24-C16-C17	-2.10	109.70	111.79
9	C	1201	A1CSZ	C24-C16-N1	-2.04	109.66	111.44
9	C	1201	A1CSZ	C46-C45-N7	-2.02	118.23	121.32

There are no chirality outliers.

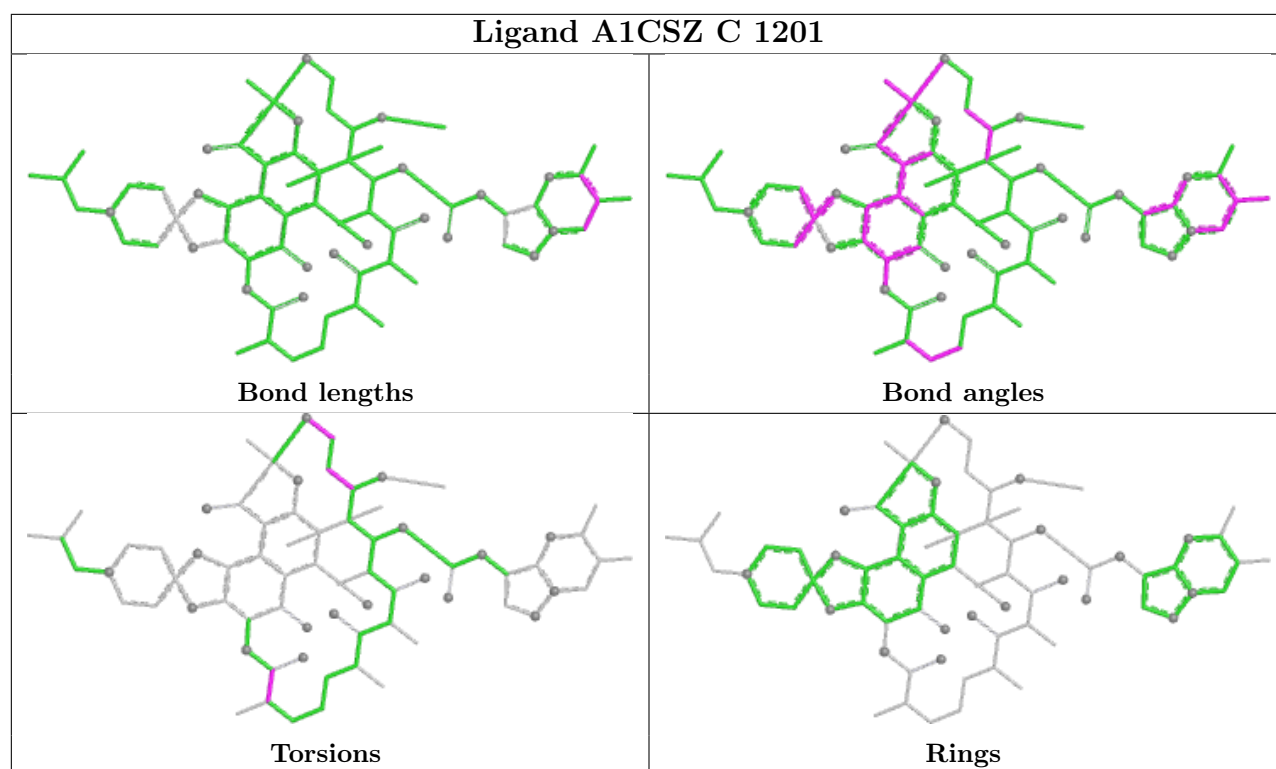
All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	1201	A1CSZ	C51-C2-C3-C4
9	C	1201	A1CSZ	N4-C27-C28-C30
9	C	1201	A1CSZ	O6-C27-C28-C30
9	C	1201	A1CSZ	C3-C4-O2-C5
9	C	1201	A1CSZ	N4-C27-C28-C29
9	C	1201	A1CSZ	O6-C27-C28-C29
9	C	1201	A1CSZ	O1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

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.

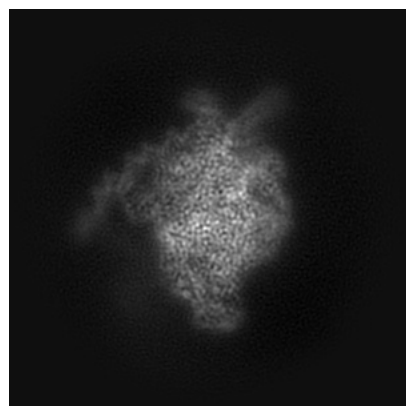
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72645. These allow visual inspection of the internal detail of the map and identification of artifacts.

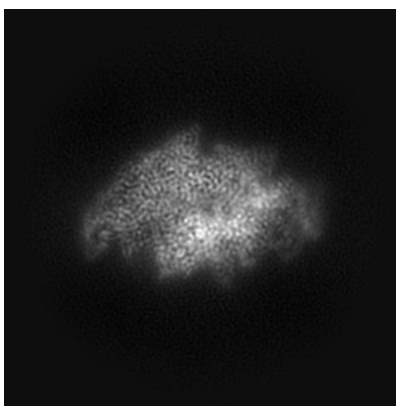
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

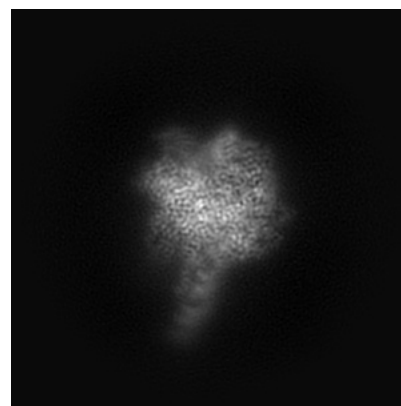
6.1.1 Primary map



X

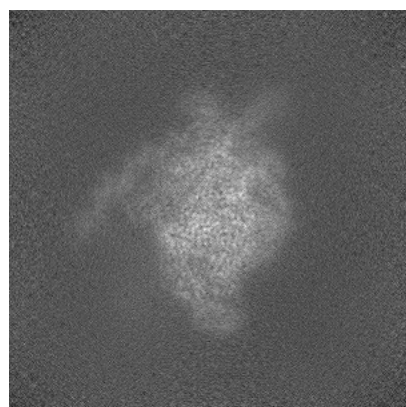


Y

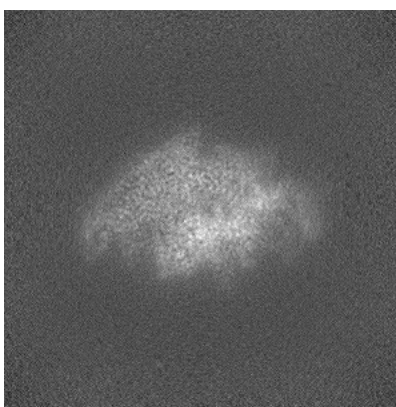


Z

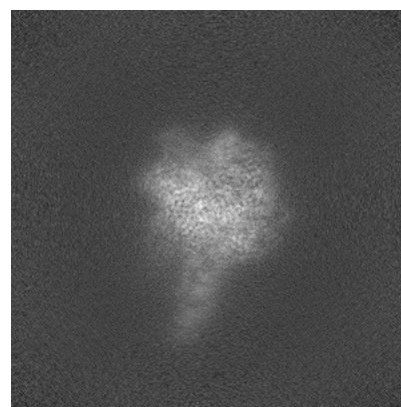
6.1.2 Raw map



X



Y

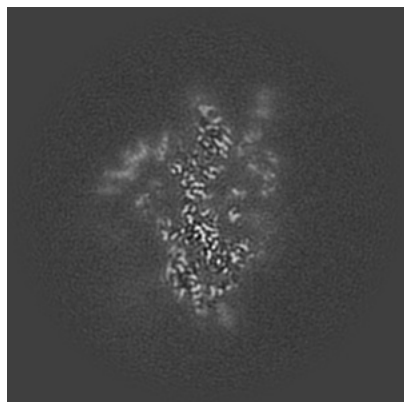


Z

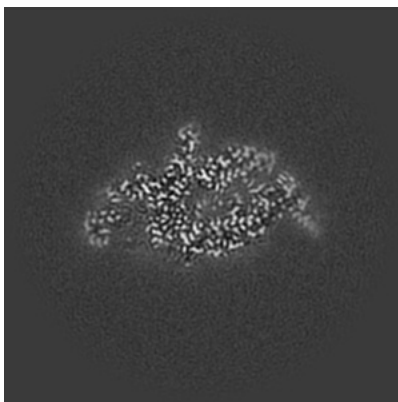
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

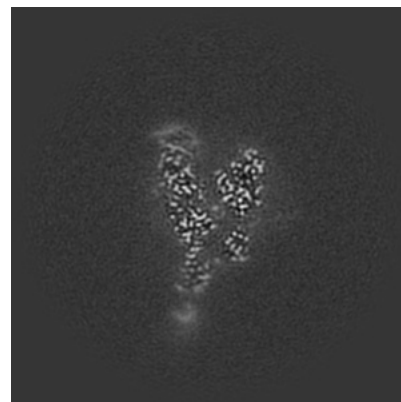
6.2.1 Primary map



X Index: 280

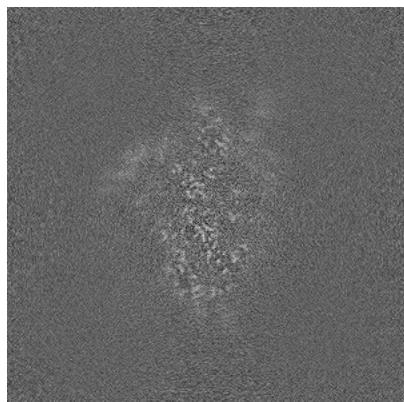


Y Index: 280

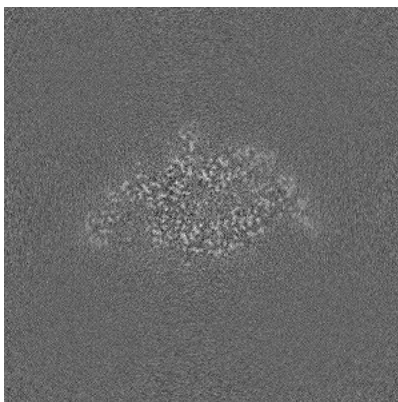


Z Index: 280

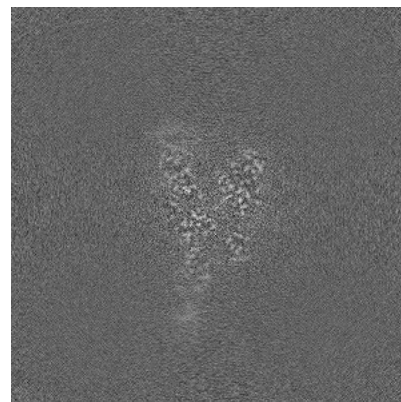
6.2.2 Raw map



X Index: 280



Y Index: 280

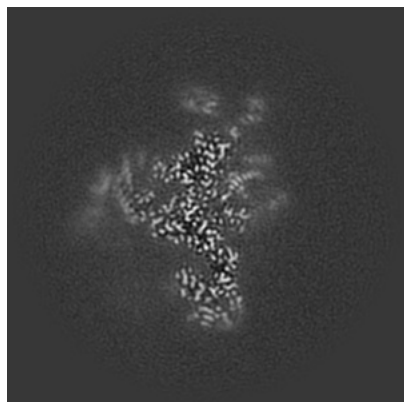


Z Index: 280

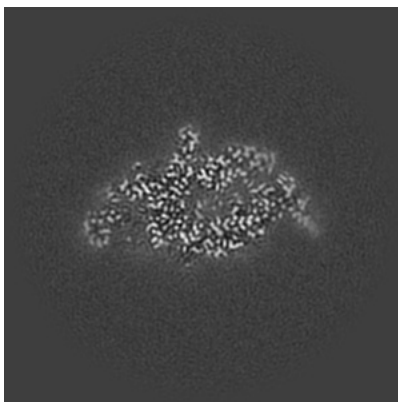
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

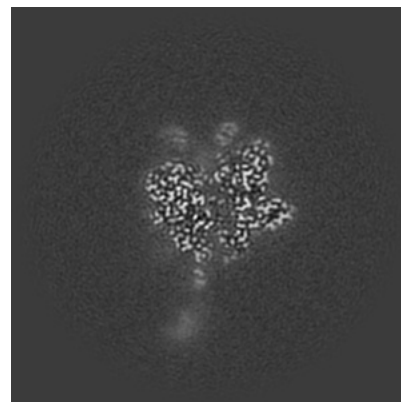
6.3.1 Primary map



X Index: 260

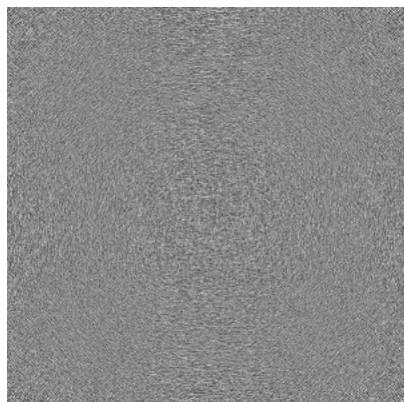


Y Index: 281

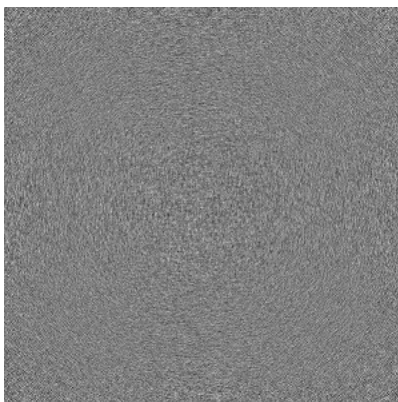


Z Index: 261

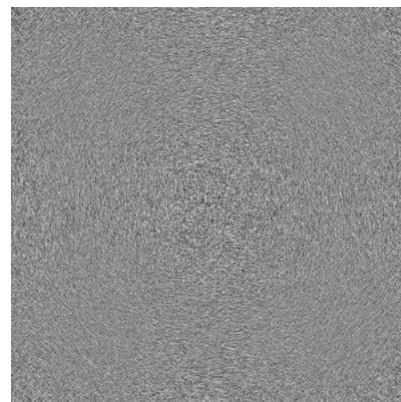
6.3.2 Raw map



X Index: 0



Y Index: 0

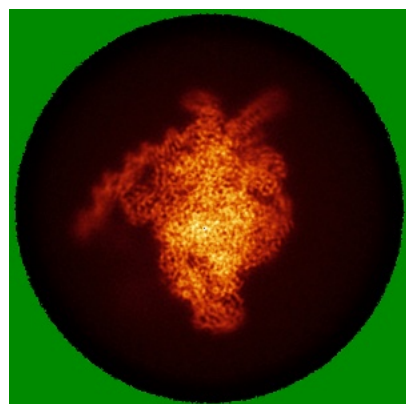


Z Index: 0

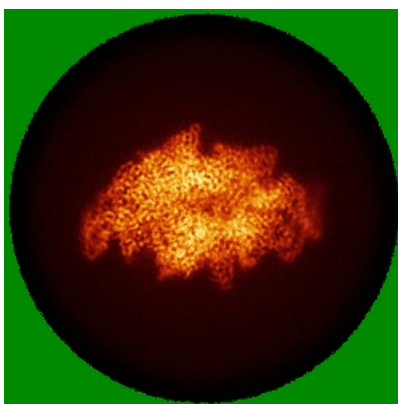
The images above show the largest variance slices of the map in three orthogonal directions.

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

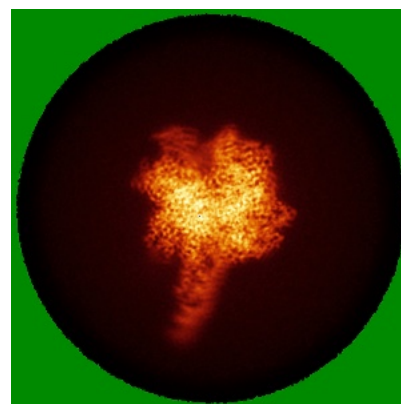
6.4.1 Primary map



X

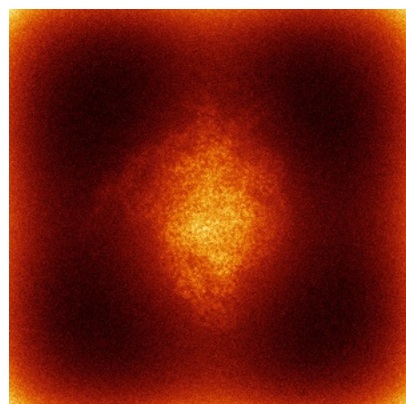


Y

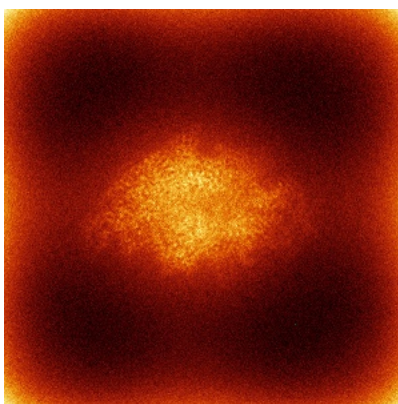


Z

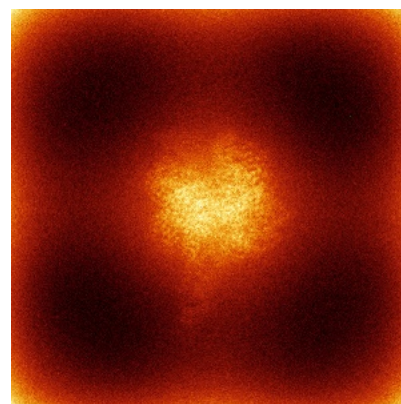
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



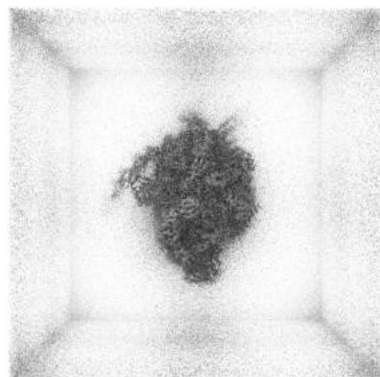
Y



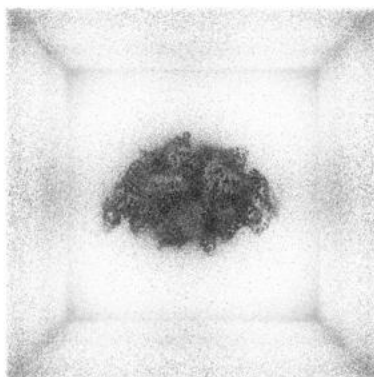
Z

The images above show the 3D surface view of the map at the recommended contour level 0.036. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

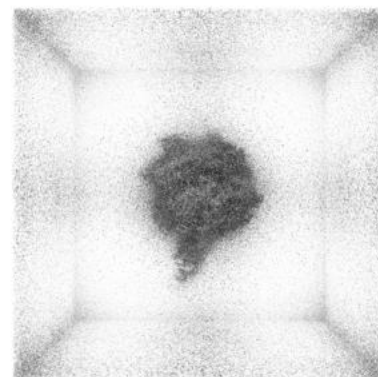
6.5.2 Raw map



X



Y



Z

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

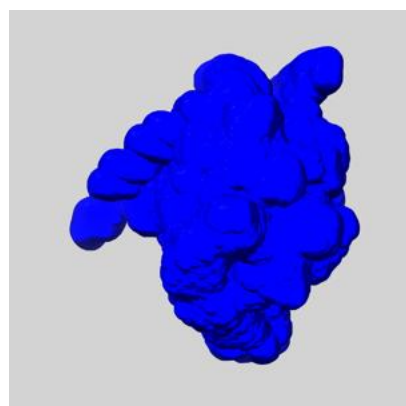
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

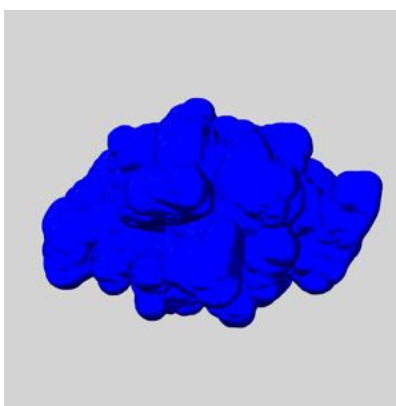
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

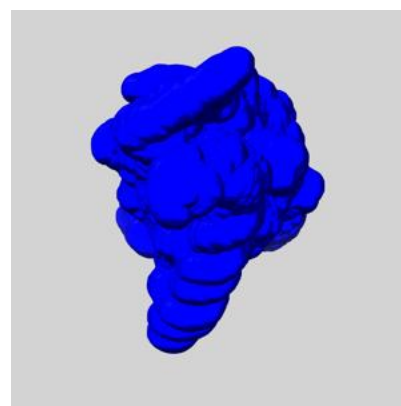
6.6.1 emd_72645_msk_1.map [i](#)



X



Y

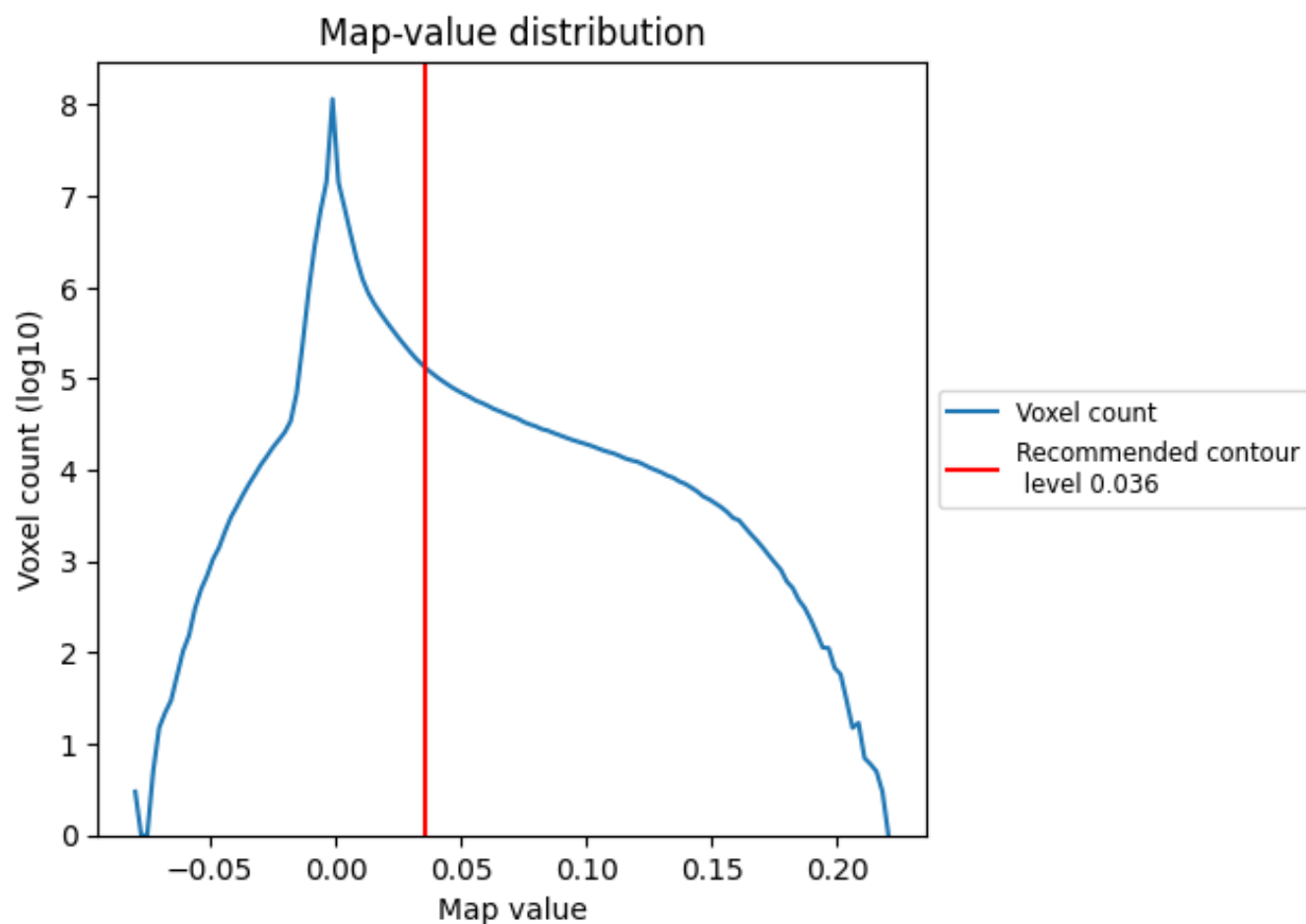


Z

7 Map analysis [i](#)

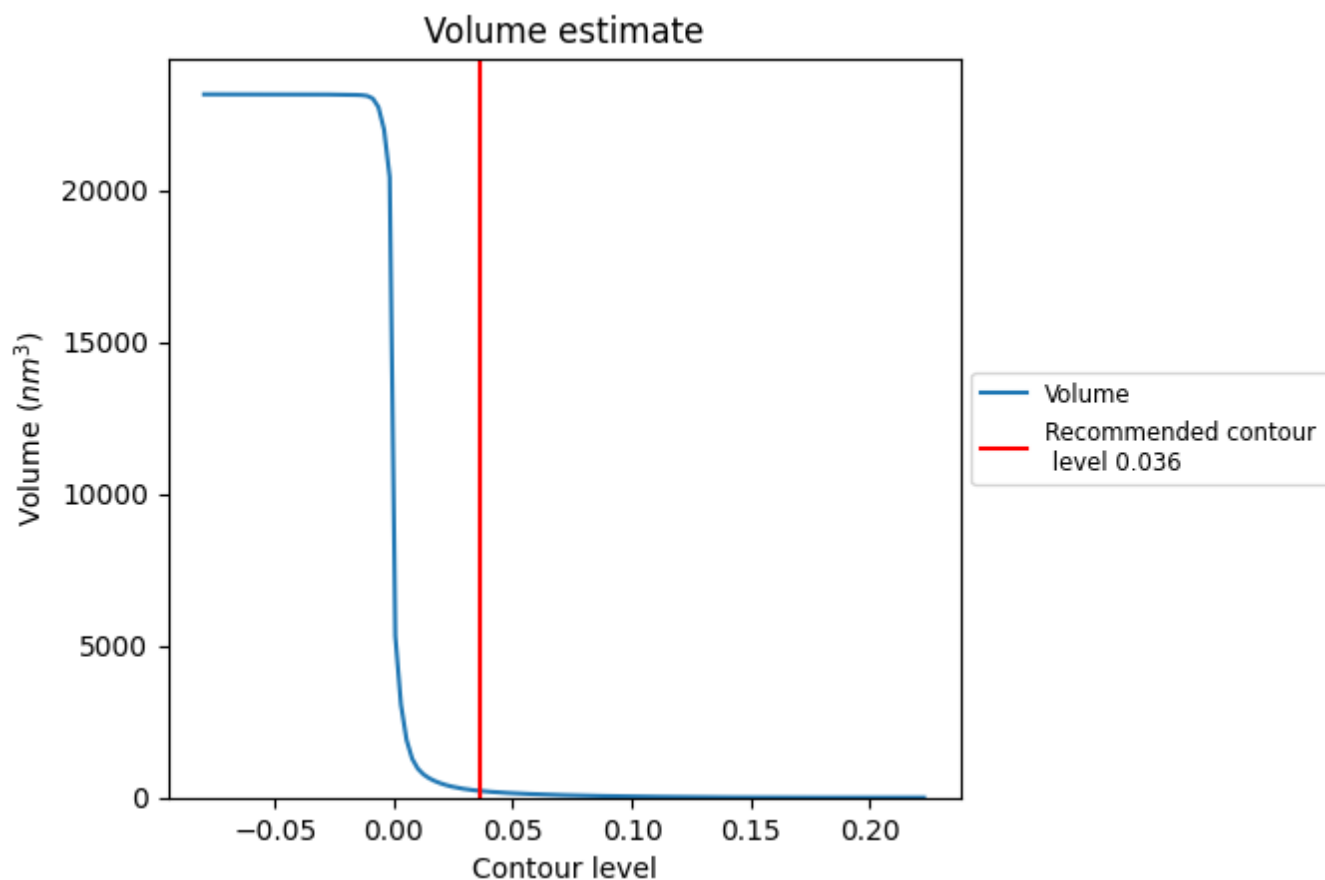
This section contains the results of statistical analysis of the map.

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.

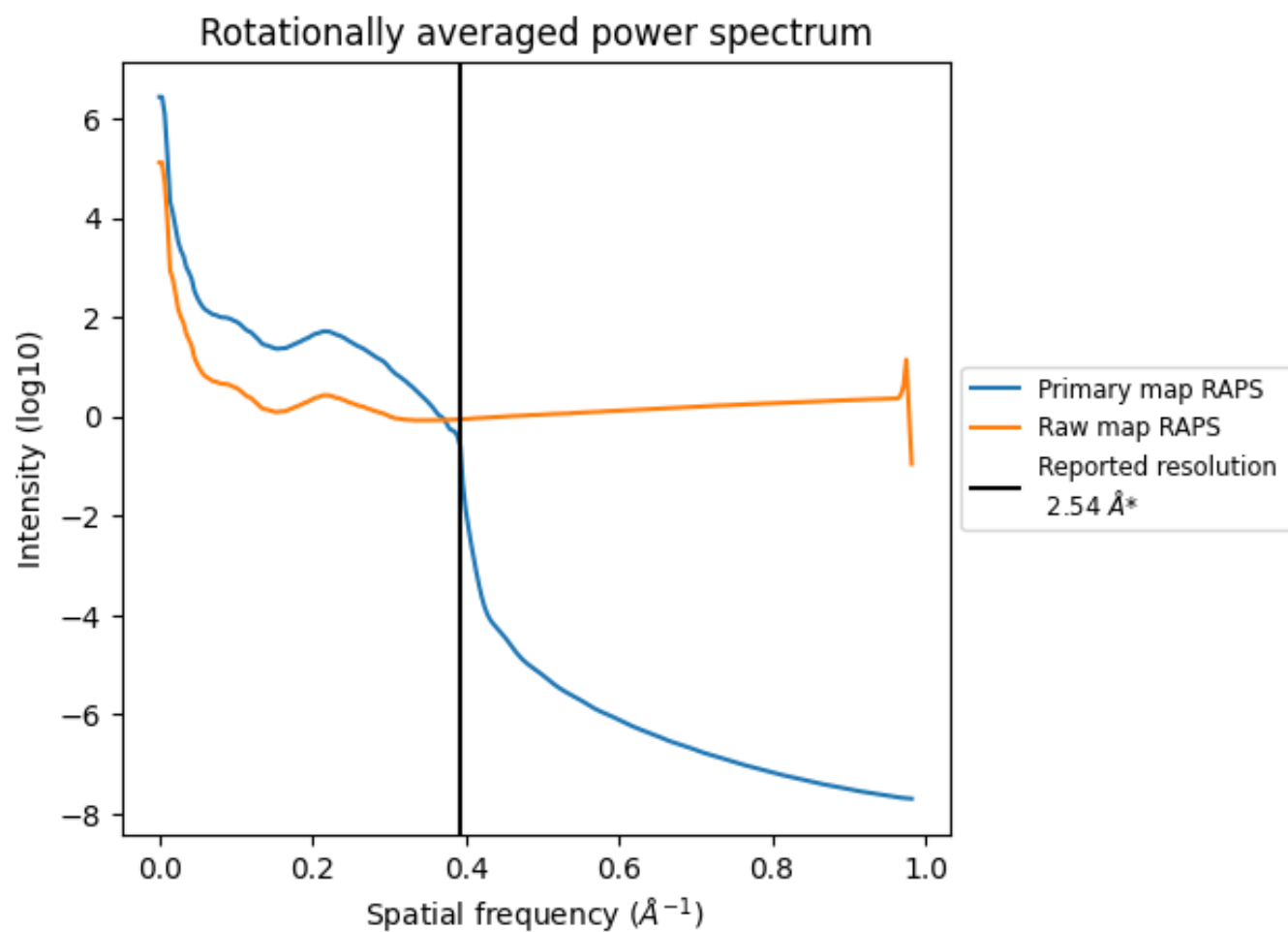
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 222 nm³; this corresponds to an approximate mass of 200 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 ⓘ

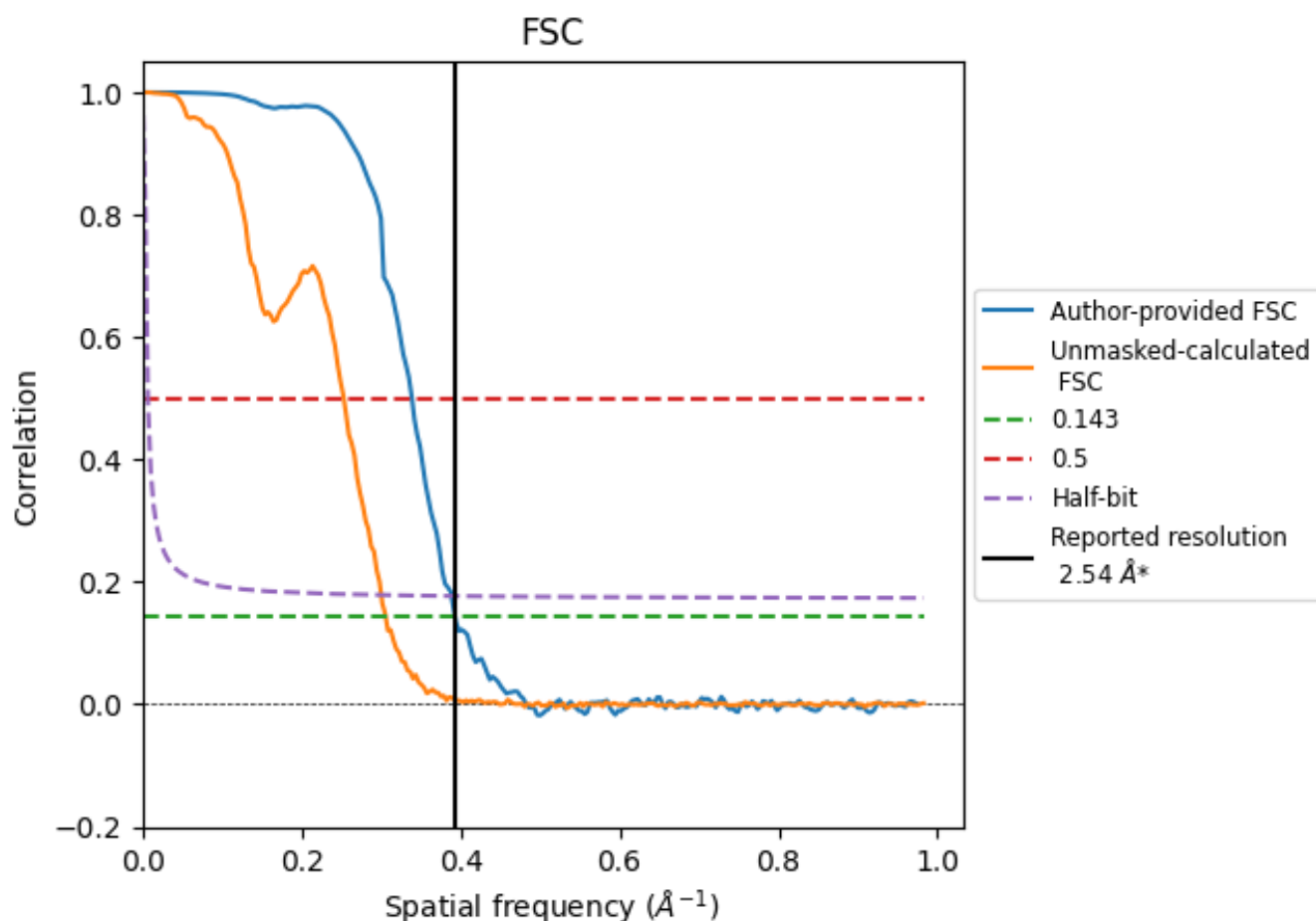


*Reported resolution corresponds to spatial frequency of $0.394 \text{ \AA}^{-1}$

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 0.394 Å⁻¹

8.2 Resolution estimates [i](#)

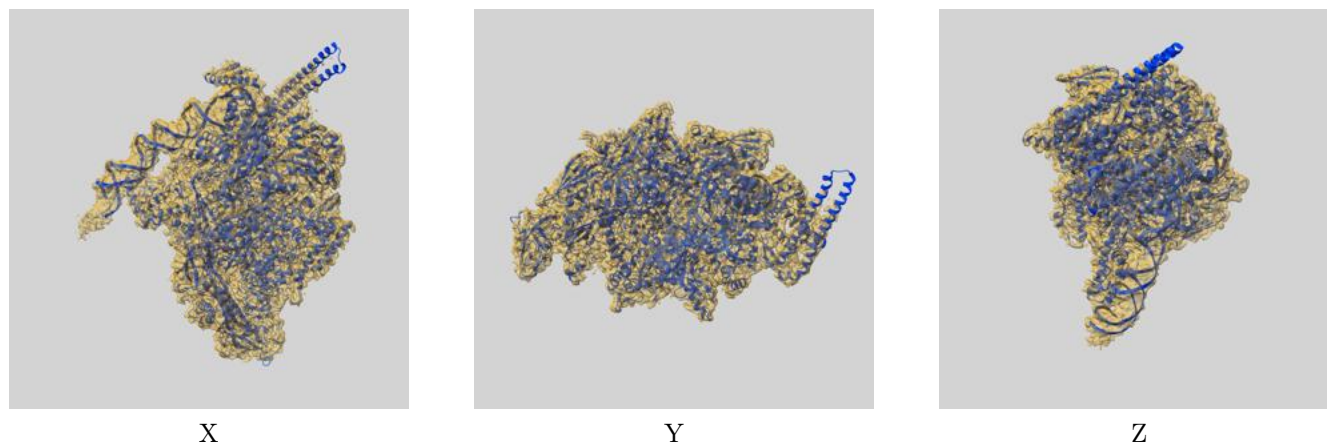
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	2.54	2.95	2.57
Unmasked-calculated*	3.27	3.95	3.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

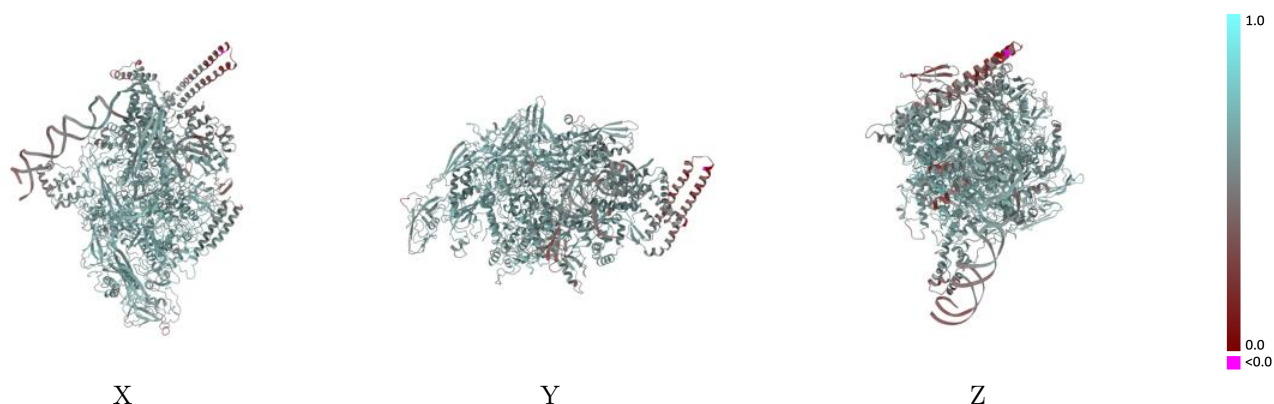
This section contains information regarding the fit between EMDB map EMD-72645 and PDB model 9Y78. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



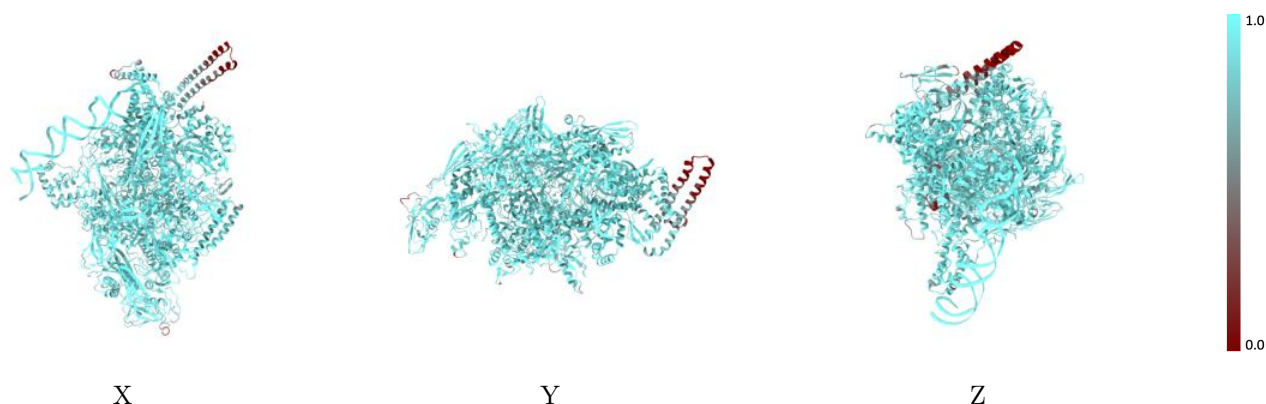
The images above show the 3D surface view of the map at the recommended contour level 0.036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



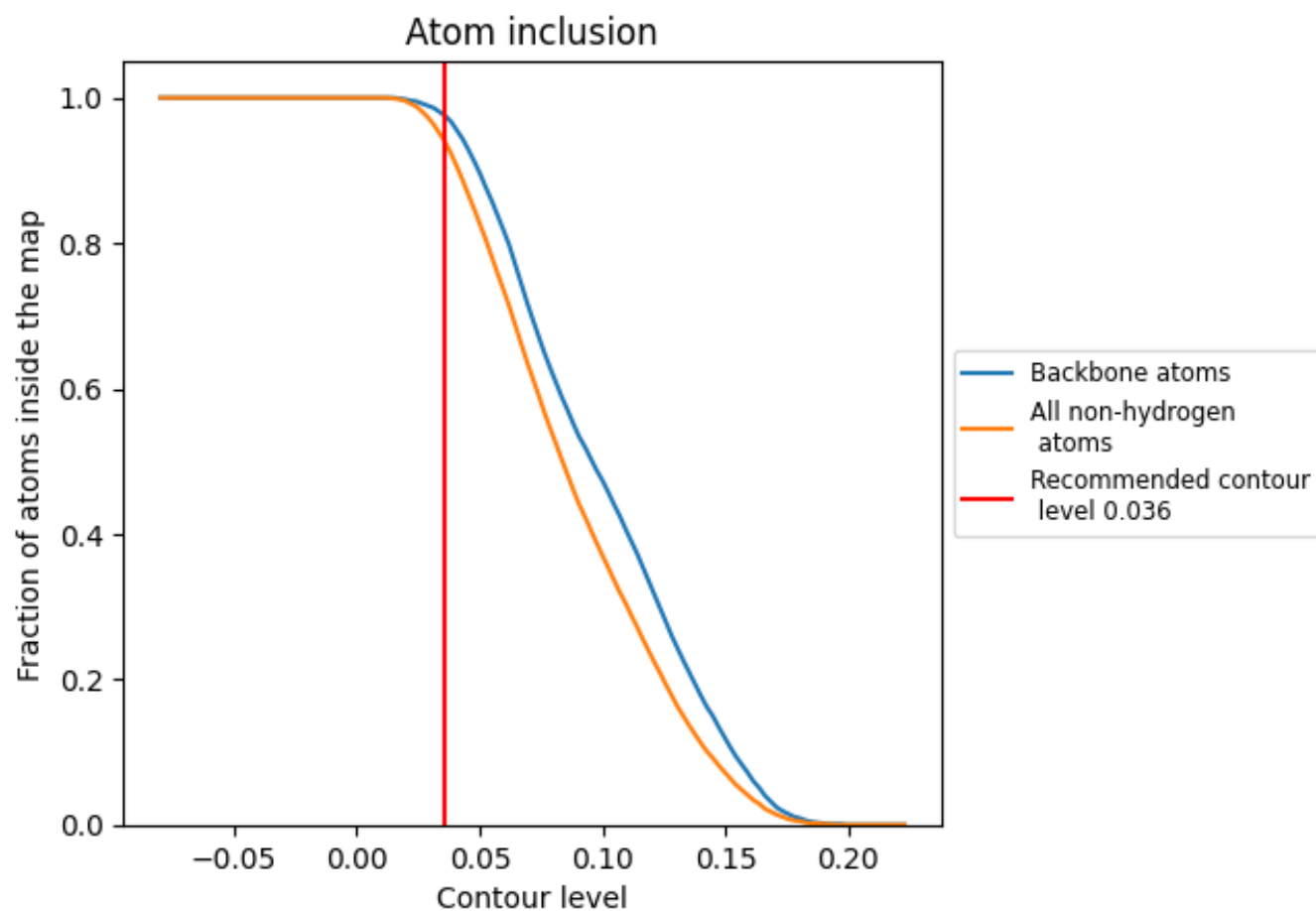
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.036).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 94% 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 (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9390	0.5810
A	0.9580	0.6060
B	0.9130	0.5700
C	0.9610	0.6050
D	0.9240	0.5840
E	0.9400	0.6020
F	0.9080	0.5380
G	0.9570	0.5040
H	0.9540	0.4950
J	1.0000	0.6490

1.0

0.0

<0.0