



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 12:40 PM UTC

PDB ID : 6XAS / pdb_00006xas
EMDB ID : EMD-22114
Title : CryoEM Structure of E. coli Rho-dependent Transcription Pre-termination Complex
Authors : Hao, Z.T.; Kim, H.K.; Walz, T.; Nudler, E.
Deposited on : 2020-06-04
Resolution : 3.80 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.dev132
MolProbity : 4-5-2 with Phenix2.0
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

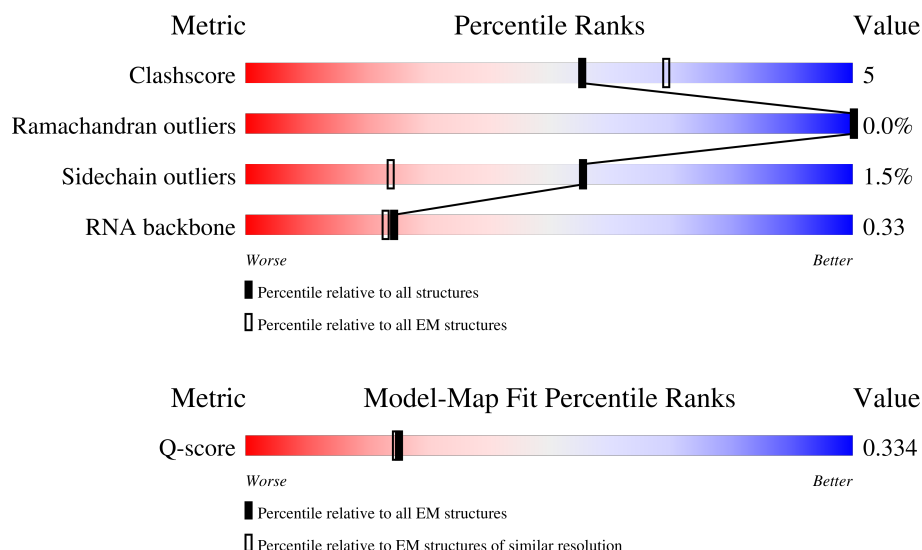
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.



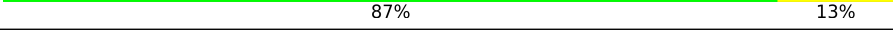
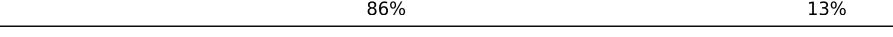
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	495	
2	W	91	
3	N	29	

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Mol	Chain	Length	Quality of chain
4	T	29	 66%34%
5	R	60	 17%8%5%70%
6	H	329	 54%12%34%
6	K	329	 74%11%15%
7	I	1342	 84%14%..
8	J	1416	 79%14%6%
9	A	419	 81%12%7%
9	B	419	 91%9%
9	C	419	 87%13%
9	D	419	 87%13%
9	E	419	 86%13%
9	F	419	 72%11%18%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 46887 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 Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	200	Total	C	N	O	S	0	0
			1611	1002	289	317	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	W	55	Total	C	N	O	S	0	0
			430	265	81	83	1		

- Molecule 3 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	26	Total	C	N	O	P	0	0
			527	251	97	154	25		

- Molecule 4 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	29	Total	C	N	O	P	0	0
			583	279	99	177	28		

- Molecule 5 is a RNA chain called RNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	18	Total	C	N	O	P	0	0
			386	172	72	124	18		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	280	Total	C	N	O	S	0	0
			2024	1254	364	400	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	218	Total	C	N	O	S	0	0
			1683	1051	297	329	6		

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	1323	Total	C	N	O	S	0	0
			10429	6542	1815	2028	44		

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	1327	Total	C	N	O	S	0	0
			10336	6493	1846	1948	49		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	VAL	-	expression tag	UNP P0A8T7
J	1408	LEU	-	expression tag	UNP P0A8T7
J	1409	GLU	-	expression tag	UNP P0A8T7
J	1410	VAL	-	expression tag	UNP P0A8T7
J	1411	HIS	-	expression tag	UNP P0A8T7
J	1412	HIS	-	expression tag	UNP P0A8T7
J	1413	HIS	-	expression tag	UNP P0A8T7
J	1414	HIS	-	expression tag	UNP P0A8T7
J	1415	HIS	-	expression tag	UNP P0A8T7
J	1416	HIS	-	expression tag	UNP P0A8T7

- Molecule 9 is a protein called Transcription termination factor Rho.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		
9	A	388	Total	C	N	O	S	0	0
			3058	1928	544	572	14		
9	B	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		
9	D	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		
9	E	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	345	Total	C	N	O	S	0	0
			2697	1697	482	507	11		

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

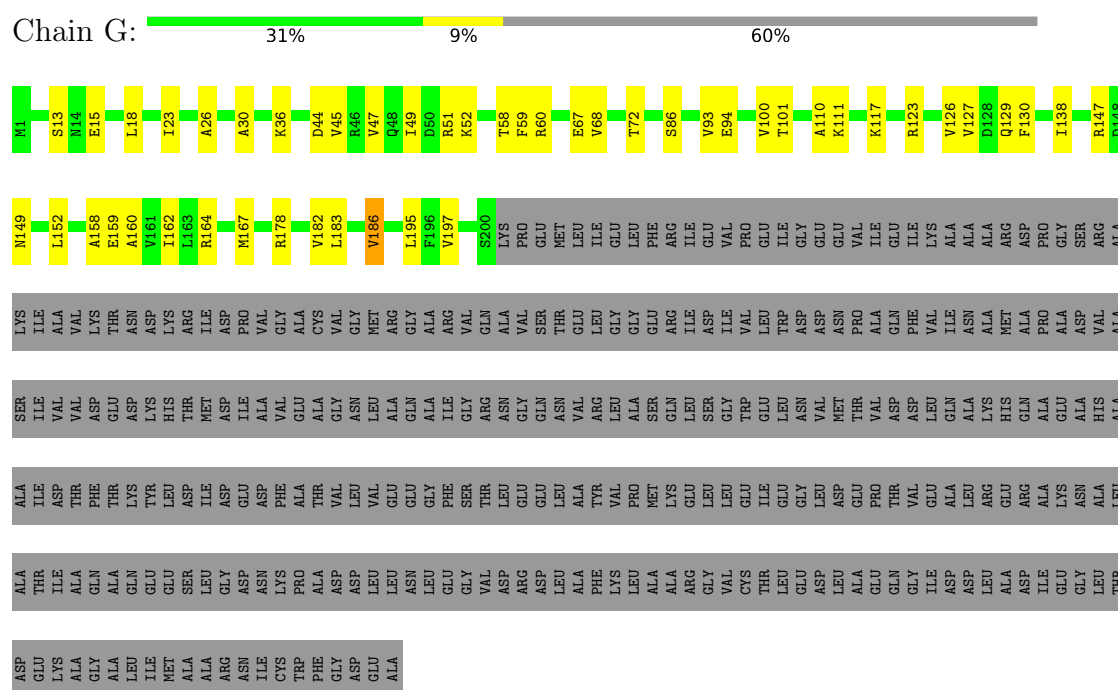
- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

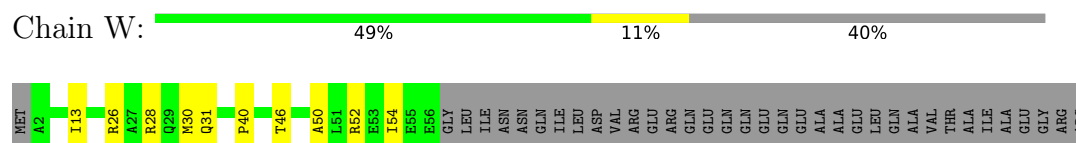
3 Residue-property plots

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.

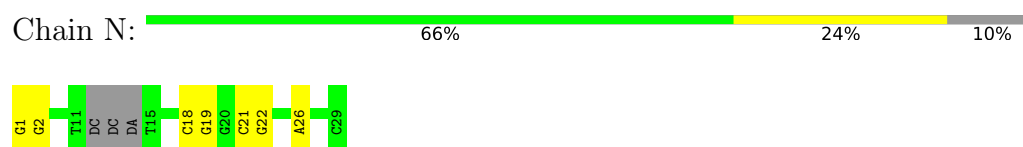
- Molecule 1: Transcription termination/antitermination protein Nusa



- Molecule 2: DNA-directed RNA polymerase subunit omega



- Molecule 3: DNA (29-MER)



- Molecule 4: DNA (29-MER)

Chain T:  66% 34%



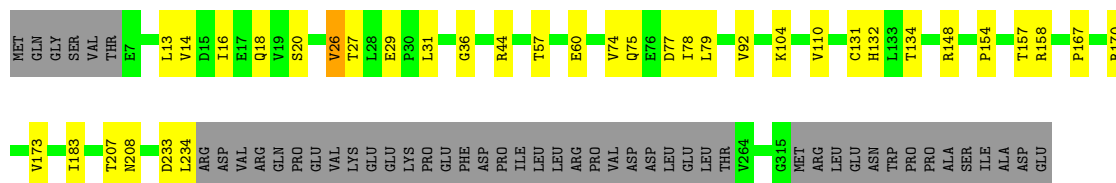
• Molecule 5: RNA (60-MER)

Chain R:  17% 8% 5% 70%



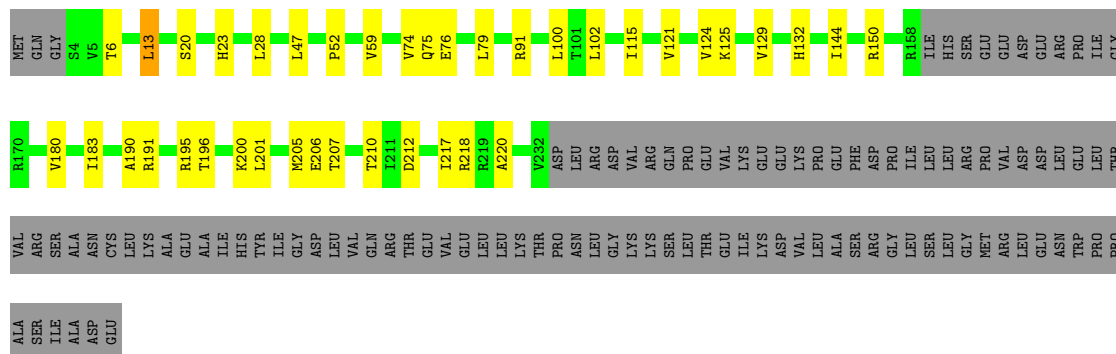
• Molecule 6: DNA-directed RNA polymerase subunit alpha

Chain K:  74% 11% 15%



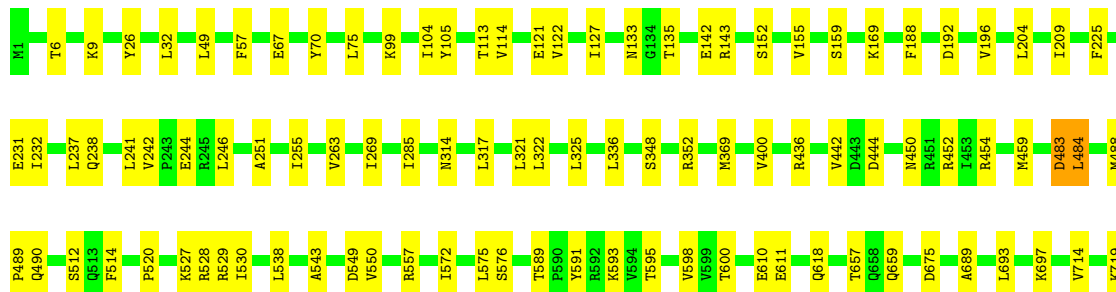
• Molecule 6: DNA-directed RNA polymerase subunit alpha

Chain H:  54% 12% 34%



• Molecule 7: DNA-directed RNA polymerase subunit beta

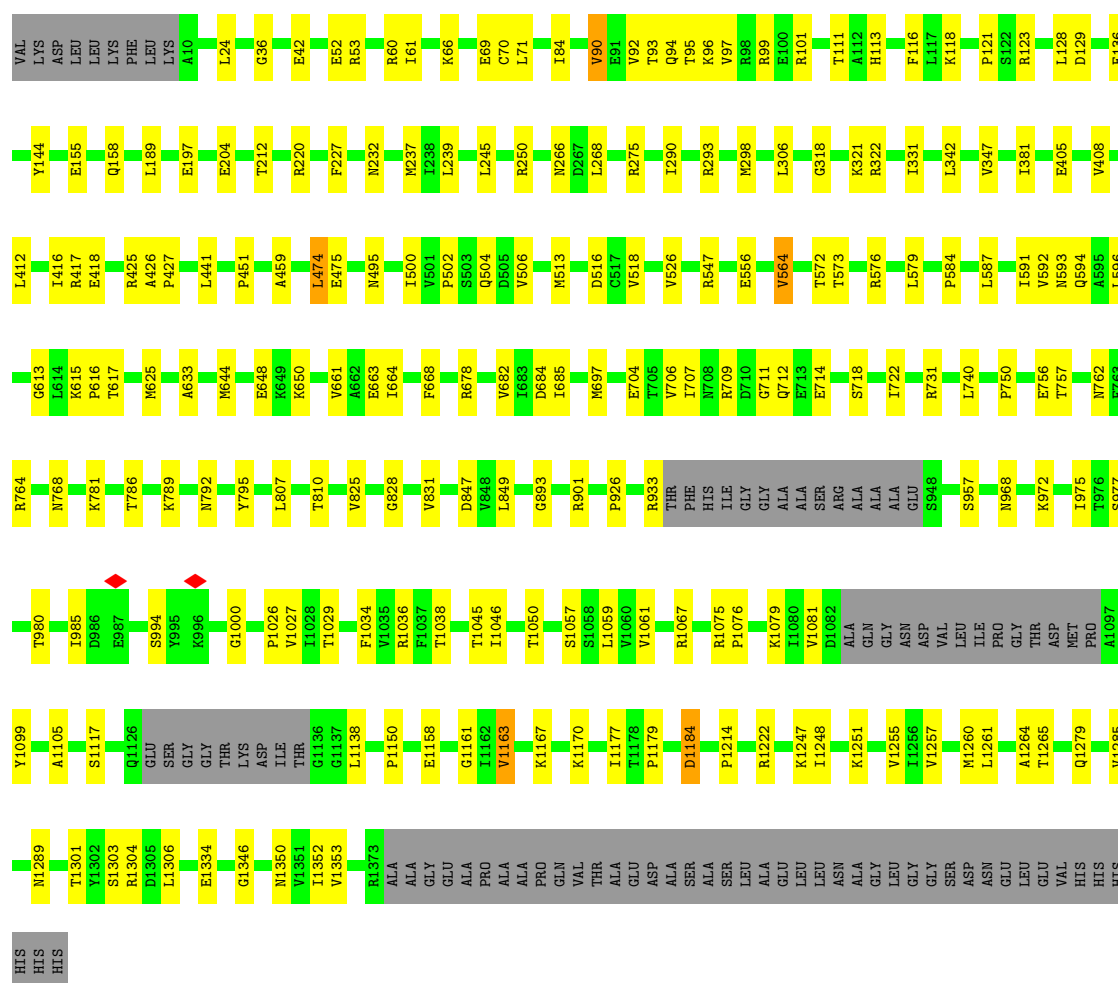
Chain I:  84% 14% ..





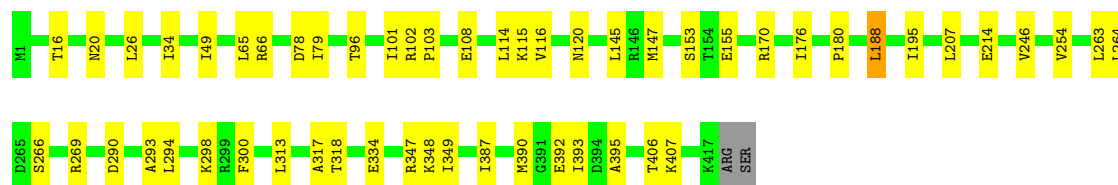
• Molecule 8: DNA-directed RNA polymerase subunit beta'

Chain J: 79% 14% 6%



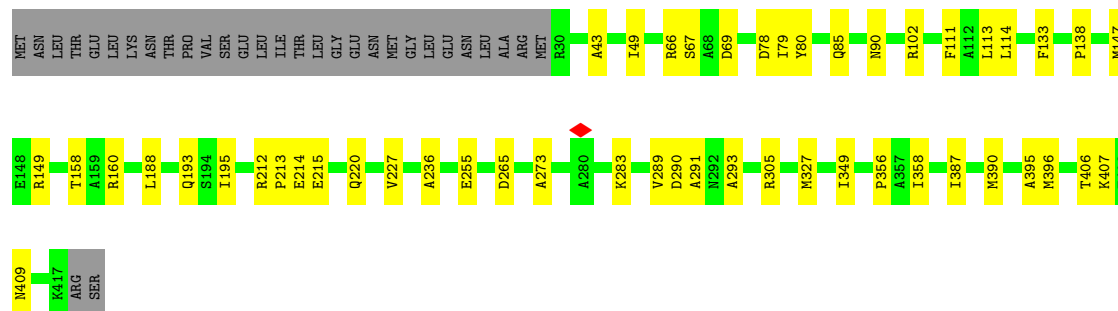
• Molecule 9: Transcription termination factor Rho

Chain C: 87% 13%



• Molecule 9: Transcription termination factor Rho

Chain A: 81% 12% 7%



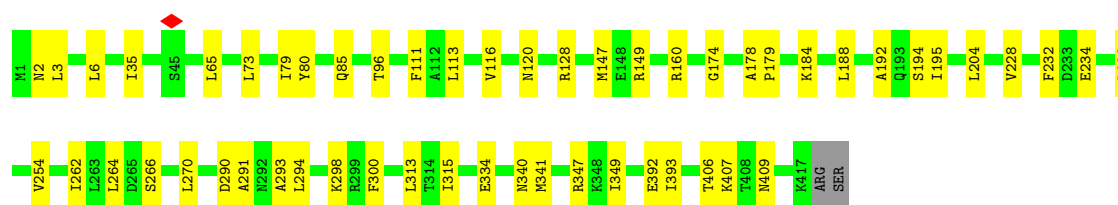
• Molecule 9: Transcription termination factor Rho

Chain B: 91% 9%



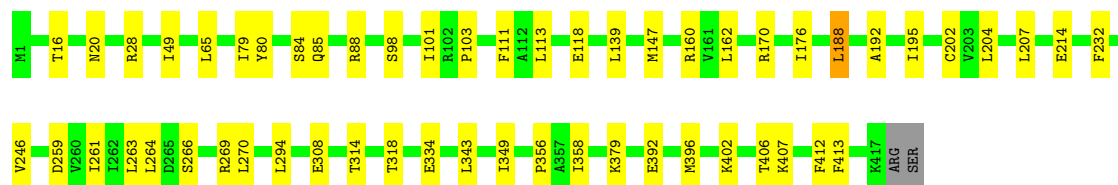
• Molecule 9: Transcription termination factor Rho

Chain D: 87% 13%

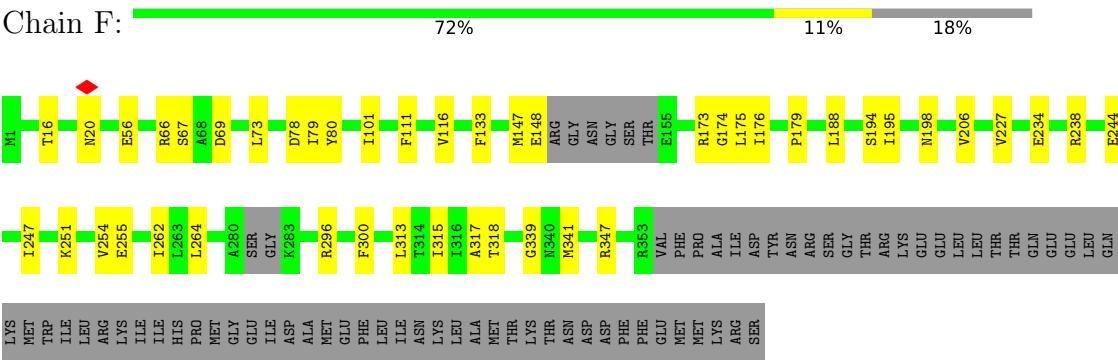


• Molecule 9: Transcription termination factor Rho

Chain E: 86% 13%



● Molecule 9: Transcription termination factor Rho



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	82394	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.413	Depositor
Minimum map value	-0.247	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0045	Depositor
Map size ($\text{\AA}$)	388.08, 388.08, 388.08	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.078, 1.078, 1.078	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.13	0/1629	0.37	0/2197
2	W	0.13	0/432	0.35	0/582
3	N	0.19	0/589	0.36	0/904
4	T	0.23	0/650	0.38	0/1000
5	R	0.10	0/430	0.29	0/666
6	H	0.11	0/1702	0.32	0/2306
6	K	0.12	0/2045	0.34	0/2779
7	I	0.14	0/10594	0.36	0/14292
8	J	0.12	0/10490	0.34	0/14157
9	A	0.09	0/3106	0.27	0/4182
9	B	0.11	0/3329	0.27	0/4483
9	C	0.11	0/3329	0.29	0/4483
9	D	0.10	0/3329	0.28	0/4483
9	E	0.09	0/3329	0.27	0/4483
9	F	0.10	0/2734	0.27	0/3683
All	All	0.12	0/47717	0.32	0/64680

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

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	1611	0	1624	28	0
2	W	430	0	445	5	0
3	N	527	0	294	8	0
4	T	583	0	329	9	0
5	R	386	0	197	3	0
6	H	1683	0	1719	24	0
6	K	2024	0	1911	21	0
7	I	10429	0	10443	111	0
8	J	10336	0	10564	122	0
9	A	3058	0	3125	28	0
9	B	3280	0	3359	19	0
9	C	3280	0	3359	33	0
9	D	3280	0	3359	29	0
9	E	3280	0	3359	34	0
9	F	2697	0	2771	25	0
10	J	1	0	0	0	0
11	J	2	0	0	0	0
All	All	46887	0	46858	470	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 (470) 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)
7:I:104:ILE:HG21	7:I:484:LEU:HB2	1.52	0.89
7:I:104:ILE:HG21	7:I:484:LEU:CB	2.08	0.83
8:J:1167:LYS:HD3	8:J:1170:LYS:HD2	1.70	0.74
3:N:19:DG:OP2	3:N:19:DG:H3'	1.87	0.74
8:J:155:GLU:HB3	8:J:158:GLN:HB2	1.70	0.73
8:J:1346:GLY:O	8:J:1350:ASN:ND2	2.24	0.70
7:I:528:ARG:NH2	7:I:576:SER:O	2.26	0.69
1:G:162:ILE:HG12	1:G:197:VAL:HB	1.73	0.69
9:F:73:LEU:HD13	9:F:238:ARG:HE	1.58	0.68
6:K:167:PRO:HD2	6:K:170:ARG:HE	1.58	0.68
9:C:102:ARG:HG3	9:C:114:LEU:HB2	1.76	0.67
6:H:20:SER:HB3	6:H:23:HIS:HB3	1.75	0.67
7:I:720:ARG:HE	7:I:736:VAL:HG11	1.61	0.65
7:I:1010:GLN:HA	7:I:1013:GLN:HB3	1.79	0.65
6:K:131:CYS:SG	6:K:132:HIS:N	2.69	0.65
8:J:644:MET:O	8:J:764:ARG:NH1	2.30	0.65
9:F:262:ILE:HB	9:F:315:ILE:HG12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:268:LEU:HB3	8:J:306:LEU:HD23	1.78	0.64
9:D:149:ARG:HE	9:D:194:SER:HA	1.62	0.64
7:I:57:PHE:HD2	7:I:70:TYR:HB2	1.62	0.64
8:J:318:GLY:N	8:J:322:ARG:O	2.31	0.64
8:J:121:PRO:HG2	8:J:123:ARG:HH12	1.63	0.64
8:J:268:LEU:HD23	8:J:306:LEU:HA	1.80	0.64
7:I:192:ASP:OD2	7:I:436:ARG:NH2	2.32	0.63
6:K:60:GLU:HG2	6:K:170:ARG:HA	1.81	0.63
9:E:349:ILE:HD11	9:E:392:GLU:HB3	1.81	0.63
9:A:66:ARG:NH1	9:A:78:ASP:OD2	2.32	0.62
6:K:16:ILE:HG12	6:K:26:VAL:HG13	1.81	0.62
8:J:417:ARG:HG2	8:J:418:GLU:HG3	1.82	0.62
8:J:807:LEU:HD13	8:J:1255:VAL:HG13	1.81	0.62
9:E:170:ARG:NH1	9:E:202:CYS:SG	2.72	0.62
9:B:234:GLU:OE2	9:B:238:ARG:NH1	2.32	0.62
2:W:40:PRO:O	2:W:52:ARG:NH2	2.33	0.62
7:I:808:ASN:N	7:I:808:ASN:HD22	1.98	0.61
7:I:657:THR:HB	7:I:1187:PHE:HB2	1.81	0.61
9:C:66:ARG:NH1	9:C:78:ASP:OD2	2.33	0.61
8:J:968:ASN:HD21	8:J:972:LYS:HB2	1.66	0.61
7:I:1254:VAL:O	8:J:99:ARG:NH2	2.32	0.61
8:J:60:ARG:HG2	8:J:90:VAL:HG12	1.81	0.61
8:J:121:PRO:O	8:J:123:ARG:NH1	2.33	0.61
9:F:66:ARG:NH1	9:F:78:ASP:OD2	2.34	0.61
7:I:204:LEU:HD11	7:I:369:MET:HG2	1.83	0.60
9:D:6:LEU:HD23	9:D:35:ILE:HG23	1.82	0.60
1:G:164:ARG:HA	1:G:167:MET:HE2	1.82	0.60
7:I:1142:ARG:NH2	7:I:1166:ASP:OD1	2.34	0.60
1:G:60:ARG:NH1	1:G:72:THR:O	2.34	0.60
7:I:400:VAL:HG21	7:I:452:ARG:HD2	1.84	0.59
9:F:73:LEU:HB2	9:F:238:ARG:HH21	1.67	0.59
9:D:85:GLN:NE2	9:D:113:LEU:O	2.35	0.59
9:D:128:ARG:HB2	9:E:28:ARG:HD3	1.84	0.59
6:H:91:ARG:NH2	6:H:210:THR:O	2.35	0.59
9:C:114:LEU:HG	9:C:115:LYS:HD3	1.82	0.59
9:E:85:GLN:NE2	9:E:113:LEU:O	2.35	0.59
9:E:207:LEU:HD13	9:E:246:VAL:HG21	1.85	0.59
8:J:1045:THR:O	8:J:1067:ARG:NH2	2.36	0.59
8:J:1163:VAL:HG13	8:J:1177:ILE:HG12	1.85	0.59
1:G:186:VAL:HB	1:G:195:LEU:HD23	1.83	0.58
6:K:44:ARG:HG3	6:K:183:ILE:HB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:28:LEU:HD12	6:H:201:LEU:HD23	1.84	0.58
8:J:1161:GLY:HA3	8:J:1179:PRO:HA	1.85	0.58
8:J:968:ASN:HA	8:J:1117:SER:HB2	1.86	0.58
9:A:80:TYR:N	9:A:111:PHE:O	2.36	0.58
9:F:254:VAL:HG21	9:F:313:LEU:HB2	1.85	0.58
6:H:47:LEU:HD13	6:H:220:ALA:HB2	1.85	0.58
9:F:16:THR:O	9:F:20:ASN:ND2	2.31	0.58
8:J:275:ARG:HH11	8:J:298:MET:HB3	1.69	0.58
7:I:488:MET:HE3	7:I:489:PRO:HD2	1.86	0.57
7:I:811:ASN:O	7:I:1099:ASN:ND2	2.36	0.57
9:E:80:TYR:N	9:E:111:PHE:O	2.35	0.57
9:A:149:ARG:HH21	9:A:193:GLN:HB3	1.70	0.57
7:I:444:ASP:O	7:I:450:ASN:ND2	2.37	0.57
8:J:495:ASN:ND2	8:J:1247:LYS:O	2.37	0.57
7:I:841:ARG:HD3	7:I:1046:VAL:HG12	1.87	0.57
8:J:1179:PRO:HD2	8:J:1184:ASP:HB3	1.87	0.57
7:I:317:LEU:HA	7:I:321:LEU:HD12	1.86	0.57
8:J:381:ILE:HD11	8:J:412:LEU:HD13	1.84	0.57
9:A:90:ASN:ND2	9:B:28:ARG:O	2.37	0.57
8:J:1285:VAL:O	8:J:1289:ASN:ND2	2.36	0.56
8:J:1150:PRO:HG3	8:J:1214:PRO:HB2	1.87	0.56
8:J:1158:GLU:OE2	8:J:1222:ARG:NH2	2.38	0.56
9:D:179:PRO:HB2	9:D:347:ARG:HH11	1.70	0.56
6:K:92:VAL:O	6:K:148:ARG:NH2	2.39	0.56
3:N:22:DG:H22	4:T:8:DC:H42	1.54	0.56
7:I:67:GLU:OE1	7:I:105:TYR:OH	2.22	0.56
8:J:584:PRO:HG2	8:J:587:LEU:HD13	1.87	0.56
7:I:1313:HIS:HB2	8:J:474:LEU:HD13	1.87	0.56
7:I:589:THR:OG1	7:I:659:GLN:NE2	2.39	0.56
9:C:349:ILE:HD11	9:C:392:GLU:HB3	1.88	0.56
6:H:59:VAL:HG22	6:H:144:ILE:HA	1.88	0.55
7:I:6:THR:HG21	7:I:782:VAL:H	1.71	0.55
7:I:595:THR:OG1	7:I:598:VAL:O	2.24	0.55
7:I:1153:ALA:O	7:I:1155:VAL:N	2.39	0.55
6:K:14:VAL:HG21	6:K:29:GLU:HB2	1.88	0.55
8:J:828:GLY:HA2	8:J:994:SER:HB2	1.88	0.55
9:C:79:ILE:HD13	9:C:101:ILE:HG21	1.86	0.55
9:E:98:SER:HB2	9:E:118:GLU:HB3	1.88	0.55
7:I:231:GLU:N	7:I:238:GLN:O	2.38	0.55
8:J:1036:ARG:HE	8:J:1081:VAL:HG21	1.71	0.55
7:I:143:ARG:NH2	7:I:512:SER:O	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:28:ARG:NH2	8:J:475:GLU:OE2	2.40	0.54
8:J:1264:ALA:HA	8:J:1304:ARG:HA	1.89	0.54
9:B:266:SER:HB2	9:B:269:ARG:HB2	1.88	0.54
7:I:152:SER:HB3	7:I:452:ARG:HG3	1.89	0.54
1:G:51:ARG:HH12	1:G:52:LYS:HE2	1.71	0.54
9:A:158:THR:HA	9:A:356:PRO:HG3	1.88	0.54
9:A:212:ARG:NH1	9:A:215:GLU:OE2	2.40	0.54
7:I:530:ILE:HD11	7:I:575:LEU:HD13	1.90	0.54
7:I:719:LYS:O	7:I:779:ARG:NH1	2.40	0.54
8:J:36:GLY:HA3	8:J:61:ILE:HD12	1.89	0.54
9:A:283:LYS:HE2	9:B:279:PRO:HA	1.90	0.54
1:G:130:PHE:HZ	1:G:138:ILE:HG21	1.73	0.54
7:I:159:SER:HB3	7:I:442:VAL:HG11	1.89	0.54
7:I:122:VAL:HG23	7:I:490:GLN:HG3	1.88	0.54
9:E:49:ILE:HD12	9:E:103:PRO:HD3	1.90	0.54
9:E:188:LEU:HD21	9:E:263:LEU:HB3	1.90	0.54
4:T:2:DG:OP1	8:J:212:THR:OG1	2.26	0.54
7:I:839:VAL:HG12	7:I:1049:ILE:HD12	1.90	0.54
9:C:348:LYS:HG2	9:C:393:ILE:HD11	1.90	0.53
1:G:178:ARG:HH22	9:A:213:PRO:HG2	1.74	0.53
9:E:261:ILE:HG12	9:E:314:THR:HB	1.91	0.53
8:J:416:ILE:HG21	8:J:441:LEU:HD13	1.89	0.53
8:J:709:ARG:HB2	8:J:714:GLU:HB2	1.91	0.53
4:T:15:DT:H2'	4:T:16:DA:H8	1.74	0.53
9:F:173:ARG:HE	9:F:339:GLY:HA2	1.74	0.53
9:B:16:THR:O	9:B:20:ASN:ND2	2.33	0.53
9:F:80:TYR:N	9:F:111:PHE:O	2.41	0.53
7:I:689:ALA:HB2	7:I:1233:LEU:HD23	1.91	0.53
1:G:18:LEU:HG	1:G:23:ILE:HD12	1.91	0.53
1:G:152:LEU:N	1:G:160:ALA:O	2.42	0.53
9:D:234:GLU:OE2	9:D:238:ARG:NH1	2.41	0.52
6:H:74:VAL:HG12	6:H:76:GLU:H	1.73	0.52
7:I:870:ILE:HG13	7:I:884:VAL:HG12	1.91	0.52
9:B:379:LYS:HD3	9:B:413:PHE:HB3	1.92	0.52
1:G:123:ARG:NH2	1:G:159:GLU:O	2.40	0.52
7:I:104:ILE:H	7:I:114:VAL:HG13	1.75	0.52
7:I:255:ILE:HB	7:I:263:VAL:HB	1.90	0.52
8:J:118:LYS:NZ	8:J:136:GLU:OE2	2.32	0.52
8:J:227:PHE:HZ	8:J:237:MET:HE3	1.74	0.52
9:C:16:THR:O	9:C:20:ASN:ND2	2.34	0.52
9:F:67:SER:OG	9:F:69:ASP:OD1	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:139:LEU:HD12	9:E:308:GLU:HB2	1.92	0.52
7:I:483:ASP:OD2	7:I:483:ASP:N	2.43	0.52
9:A:67:SER:OG	9:A:69:ASP:OD1	2.27	0.52
9:C:96:THR:HB	9:C:120:ASN:HA	1.92	0.51
1:G:86:SER:HB2	9:E:88:ARG:NH1	2.25	0.51
4:T:21:DT:H2'	4:T:22:DC:C6	2.46	0.51
5:R:60:A:OP1	7:I:1073:LYS:NZ	2.31	0.51
6:H:100:LEU:HD11	6:H:121:VAL:HG21	1.92	0.51
8:J:678:ARG:NH2	8:J:756:GLU:OE2	2.44	0.51
9:B:290:ASP:HB3	9:B:293:ALA:HB2	1.93	0.51
3:N:1:DG:H2''	3:N:2:DG:C8	2.46	0.51
8:J:786:THR:HA	8:J:789:LYS:HE2	1.94	0.51
9:D:340:ASN:ND2	9:E:214:GLU:OE2	2.43	0.51
6:H:47:LEU:HG	6:H:180:VAL:HG11	1.93	0.50
7:I:538:LEU:HD13	7:I:543:ALA:HB2	1.93	0.50
7:I:618:GLN:OE1	8:J:768:ASN:ND2	2.44	0.50
8:J:129:ASP:OD2	8:J:220:ARG:NH1	2.41	0.50
9:C:153:SER:OG	9:C:155:GLU:OE1	2.26	0.50
7:I:748:ILE:HD13	7:I:966:ILE:HG21	1.92	0.50
4:T:15:DT:H2'	4:T:16:DA:C8	2.47	0.50
6:H:13:LEU:HD23	6:H:13:LEU:H	1.77	0.50
7:I:104:ILE:HG21	7:I:484:LEU:HB3	1.90	0.50
7:I:1010:GLN:O	7:I:1014:LEU:N	2.44	0.50
7:I:802:VAL:HG12	7:I:1096:ILE:HB	1.93	0.50
8:J:712:GLN:OE1	8:J:712:GLN:N	2.45	0.50
7:I:850:ILE:HG12	7:I:1048:LYS:HD3	1.93	0.50
8:J:901:ARG:O	8:J:1251:LYS:NZ	2.44	0.50
9:D:290:ASP:OD1	9:D:291:ALA:N	2.44	0.50
9:E:349:ILE:HG21	9:E:396:MET:HG3	1.93	0.50
9:F:56:GLU:OE1	9:F:66:ARG:NE	2.45	0.50
8:J:70:CYS:SG	8:J:71:LEU:N	2.83	0.50
9:A:236:ALA:HB1	9:A:273:ALA:HB1	1.93	0.50
7:I:75:LEU:HD21	7:I:127:ILE:HD11	1.92	0.50
6:K:77:ASP:OD1	6:K:78:ILE:N	2.45	0.49
8:J:648:GLU:N	8:J:648:GLU:OE1	2.44	0.49
8:J:661:VAL:HA	8:J:664:ILE:HG22	1.93	0.49
6:H:79:LEU:HD21	8:J:526:VAL:HG21	1.93	0.49
7:I:808:ASN:H	8:J:633:ALA:HB2	1.77	0.49
7:I:1127:LYS:HE3	7:I:1131:MET:HE3	1.93	0.49
9:C:96:THR:N	9:C:120:ASN:OD1	2.41	0.49
9:E:16:THR:O	9:E:20:ASN:ND2	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:529:ARG:HD2	7:I:572:ILE:HG22	1.94	0.49
8:J:1050:THR:HG23	8:J:1057:SER:HB3	1.94	0.49
8:J:1350:ASN:HA	8:J:1353:VAL:HG12	1.93	0.49
9:C:294:LEU:HD13	9:C:334:GLU:HG2	1.94	0.49
6:H:124:VAL:HG13	6:H:125:LYS:HG3	1.93	0.49
7:I:593:LYS:O	7:I:600:THR:OG1	2.26	0.49
9:B:289:VAL:HG22	9:B:327:MET:HG3	1.93	0.49
9:C:298:LYS:HD3	9:D:232:PHE:HB2	1.95	0.49
9:D:2:ASN:OD1	9:D:3:LEU:N	2.46	0.49
9:D:65:LEU:HB2	9:D:79:ILE:HB	1.95	0.49
6:H:102:LEU:HD13	6:H:115:ILE:HG12	1.93	0.49
7:I:520:PRO:HG3	7:I:714:VAL:HG11	1.95	0.49
4:T:26:DG:H2"	4:T:27:DC:C5	2.48	0.48
7:I:1120:ALA:HB1	7:I:1198:LEU:HG	1.94	0.48
9:E:147:MET:HE1	9:E:195:ILE:HG13	1.95	0.48
9:E:176:ILE:HA	9:E:343:LEU:HB3	1.95	0.48
8:J:113:HIS:HB3	8:J:116:PHE:HD1	1.78	0.48
9:C:145:LEU:HD21	9:C:170:ARG:HE	1.78	0.48
9:E:379:LYS:HD3	9:E:413:PHE:HB3	1.95	0.48
9:D:80:TYR:N	9:D:111:PHE:O	2.41	0.48
9:A:147:MET:HE1	9:A:195:ILE:HG13	1.94	0.48
9:A:220:GLN:HA	9:A:227:VAL:HG21	1.96	0.48
7:I:99:LYS:HG2	7:I:121:GLU:HB3	1.96	0.48
7:I:1109:ILE:HD11	8:J:740:LEU:HD22	1.95	0.48
9:C:264:LEU:HD22	9:C:300:PHE:HE1	1.79	0.48
9:D:174:GLY:HA2	9:D:341:MET:HB3	1.96	0.48
9:F:244:GLU:OE2	9:F:296:ARG:NH2	2.42	0.48
8:J:592:VAL:HA	8:J:596:LEU:HD11	1.96	0.48
7:I:1200:LYS:HE3	7:I:1206:THR:HG21	1.95	0.48
8:J:94:GLN:HG3	8:J:96:LYS:HE2	1.96	0.48
9:F:147:MET:HE1	9:F:195:ILE:HG13	1.96	0.48
7:I:1123:GLY:HA3	7:I:1204:LEU:HD11	1.95	0.48
8:J:957:SER:HB3	8:J:985:ILE:HB	1.94	0.48
9:C:65:LEU:HB2	9:C:79:ILE:HB	1.96	0.48
9:E:160:ARG:NH1	9:E:407:LYS:O	2.47	0.48
6:K:57:THR:HA	6:K:173:VAL:HB	1.96	0.47
6:H:47:LEU:HD23	6:H:183:ILE:HD12	1.96	0.47
7:I:232:ILE:HG12	7:I:237:LEU:HG	1.96	0.47
8:J:504:GLN:HG3	8:J:731:ARG:HB2	1.95	0.47
9:A:290:ASP:HB3	9:A:293:ALA:HB2	1.94	0.47
8:J:1046:ILE:HD12	8:J:1059:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:86:SER:HB3	9:E:84:SER:HB2	1.96	0.47
8:J:24:LEU:HD12	8:J:232:ASN:HB3	1.96	0.47
8:J:111:THR:O	8:J:239:LEU:N	2.47	0.47
9:A:290:ASP:OD1	9:A:291:ALA:N	2.47	0.47
9:C:290:ASP:HB3	9:C:293:ALA:HB2	1.95	0.47
1:G:127:VAL:HG13	1:G:195:LEU:HD21	1.97	0.47
7:I:823:VAL:HG22	7:I:1060:ILE:HG21	1.96	0.47
8:J:704:GLU:H	8:J:718:SER:HB2	1.79	0.47
7:I:1117:LEU:HD13	7:I:1195:ILE:HG12	1.97	0.47
8:J:513:MET:HE1	8:J:579:LEU:HD13	1.97	0.47
9:A:138:PRO:HG3	9:A:305:ARG:HD3	1.96	0.47
9:F:179:PRO:HB2	9:F:347:ARG:HH11	1.80	0.47
6:H:191:ARG:HA	6:H:195:ARG:O	2.15	0.47
9:C:49:ILE:HD12	9:C:103:PRO:HG3	1.95	0.47
7:I:1326:LEU:HD12	8:J:331:ILE:HD12	1.97	0.47
8:J:682:VAL:O	8:J:685:ILE:HG13	2.15	0.47
1:G:183:LEU:HD23	1:G:183:LEU:H	1.79	0.47
8:J:451:PRO:HG2	8:J:625:MET:SD	2.55	0.47
8:J:518:VAL:HB	8:J:707:ILE:HD11	1.97	0.47
8:J:786:THR:HA	8:J:789:LYS:HG2	1.97	0.47
6:H:212:ASP:OD1	6:H:212:ASP:N	2.46	0.46
7:I:314:ASN:O	7:I:352:ARG:NH1	2.48	0.46
8:J:245:LEU:HB3	8:J:250:ARG:HD3	1.97	0.46
7:I:99:LYS:HA	7:I:121:GLU:HA	1.97	0.46
9:E:79:ILE:HD13	9:E:101:ILE:HG21	1.96	0.46
7:I:720:ARG:HH21	7:I:736:VAL:HG21	1.81	0.46
9:C:266:SER:HB2	9:C:269:ARG:HB2	1.96	0.46
9:A:133:PHE:N	9:A:255:GLU:OE2	2.48	0.46
7:I:348:SER:O	7:I:352:ARG:HG2	2.15	0.46
7:I:1022:LYS:HA	7:I:1026:GLU:HB2	1.98	0.46
9:A:212:ARG:HB3	9:A:214:GLU:OE2	2.16	0.46
1:G:152:LEU:HB2	1:G:160:ALA:HB3	1.97	0.46
9:F:206:VAL:HB	9:F:227:VAL:HG13	1.96	0.46
9:C:254:VAL:HG21	9:C:313:LEU:HB2	1.98	0.46
9:D:262:ILE:HB	9:D:315:ILE:HG12	1.97	0.46
9:F:148:GLU:O	9:F:198:ASN:ND2	2.49	0.46
8:J:591:ILE:O	8:J:594:GLN:NE2	2.49	0.46
8:J:1034:PHE:N	8:J:1081:VAL:O	2.48	0.46
9:C:180:PRO:HD2	9:C:347:ARG:HH11	1.81	0.46
1:G:30:ALA:HB1	1:G:110:ALA:HA	1.98	0.46
8:J:781:LYS:HG3	8:J:933:ARG:HH21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:31:GLN:HB2	2:W:46:THR:HG21	1.98	0.45
3:N:21:DC:H2''	3:N:22:DG:C8	2.52	0.45
6:K:79:LEU:HD21	7:I:693:LEU:HD11	1.98	0.45
6:H:205:MET:HE1	6:H:217:ILE:HG13	1.98	0.45
7:I:882:ILE:HD13	7:I:919:ARG:HG2	1.98	0.45
8:J:644:MET:HG2	8:J:722:ILE:HD13	1.97	0.45
1:G:13:SER:HA	1:G:18:LEU:HB2	1.97	0.45
7:I:241:LEU:HD11	7:I:246:LEU:HD21	1.98	0.45
8:J:516:ASP:OD1	8:J:516:ASP:N	2.49	0.45
9:D:298:LYS:HD2	9:E:232:PHE:HB2	1.97	0.45
9:E:147:MET:HG3	9:E:162:LEU:HD22	1.97	0.45
9:F:247:ILE:HB	9:F:300:PHE:CE2	2.52	0.45
6:H:79:LEU:HD11	8:J:526:VAL:HG21	1.98	0.45
7:I:169:LYS:NZ	7:I:192:ASP:OD1	2.47	0.45
8:J:502:PRO:HB2	8:J:506:VAL:HB	1.97	0.45
9:C:349:ILE:HG12	9:C:393:ILE:HG12	1.97	0.45
9:D:73:LEU:HD13	9:D:238:ARG:NH1	2.32	0.45
7:I:1290:MET:HG3	8:J:347:VAL:HG11	1.98	0.45
8:J:426:ALA:HB3	8:J:427:PRO:HD3	1.99	0.45
9:B:147:MET:HE1	9:B:195:ILE:HG13	1.99	0.45
6:H:23:HIS:CG	6:H:206:GLU:HG2	2.51	0.45
6:H:52:PRO:HA	6:H:150:ARG:HG2	1.98	0.45
7:I:135:THR:HG21	7:I:142:GLU:HB3	1.99	0.45
7:I:591:TYR:OH	7:I:611:GLU:OE2	2.34	0.45
9:A:289:VAL:HG22	9:A:327:MET:HG3	1.99	0.45
6:K:104:LYS:HD3	6:K:110:VAL:HG22	1.99	0.45
7:I:847:PRO:HB2	7:I:1047:LEU:HD11	1.99	0.45
9:E:266:SER:O	9:E:270:LEU:N	2.37	0.45
6:K:18:GLN:NE2	6:K:20:SER:O	2.49	0.45
7:I:675:ASP:OD1	7:I:675:ASP:N	2.49	0.44
7:I:1105:SER:HB2	8:J:731:ARG:HG2	1.99	0.44
8:J:52:GLU:HG3	8:J:53:ARG:H	1.82	0.44
9:B:66:ARG:NH1	9:B:78:ASP:OD2	2.50	0.44
1:G:147:ARG:O	1:G:149:ASN:ND2	2.50	0.44
5:R:3:G:O2'	5:R:4:C:O5'	2.30	0.44
8:J:576:ARG:HD3	8:J:593:ASN:HA	1.99	0.44
9:A:85:GLN:NE2	9:A:113:LEU:O	2.46	0.44
9:E:65:LEU:HB2	9:E:79:ILE:HB	1.99	0.44
1:G:58:THR:H	1:G:100:VAL:HG22	1.82	0.44
6:K:233:ASP:HB2	6:H:218:ARG:HH21	1.82	0.44
7:I:840:SER:HG	7:I:1048:LYS:H	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:349:ILE:HD13	9:A:396:MET:HG3	1.99	0.44
9:D:147:MET:HE1	9:D:195:ILE:HG13	1.99	0.44
9:D:349:ILE:HG12	9:D:393:ILE:HG12	1.99	0.44
7:I:133:ASN:O	7:I:527:LYS:NZ	2.39	0.44
7:I:610:GLU:OE1	7:I:610:GLU:N	2.45	0.44
8:J:572:THR:OG1	8:J:573:THR:N	2.51	0.44
9:B:80:TYR:N	9:B:111:PHE:O	2.45	0.44
9:E:356:PRO:HB2	9:E:358:ILE:HG13	1.99	0.44
9:A:102:ARG:HD3	9:A:114:LEU:HD21	1.99	0.44
9:A:406:THR:OG1	9:A:407:LYS:N	2.51	0.44
9:B:79:ILE:HG12	9:B:101:ILE:HG21	2.00	0.44
8:J:128:LEU:HD21	8:J:189:LEU:HD12	1.99	0.44
8:J:1061:VAL:HB	8:J:1105:ALA:HB3	2.00	0.44
9:B:387:ILE:HG23	9:B:395:ALA:HB1	1.99	0.44
7:I:104:ILE:CG2	7:I:484:LEU:HB3	2.47	0.44
7:I:196:VAL:HG11	7:I:209:ILE:HG12	2.00	0.44
7:I:732:ILE:HD11	7:I:769:PRO:HB3	1.99	0.44
8:J:975:ILE:HG22	8:J:977:SER:H	1.83	0.44
9:D:349:ILE:HD11	9:D:392:GLU:HB3	1.99	0.44
9:F:264:LEU:HD22	9:F:300:PHE:HE1	1.83	0.44
3:N:26:DA:C8	3:N:26:DA:H5'	2.53	0.44
6:K:154:PRO:HG2	6:K:157:THR:HG23	2.00	0.44
6:H:75:GLN:HB2	6:H:132:HIS:HB2	2.00	0.44
9:C:147:MET:HE1	9:C:195:ILE:HG13	2.00	0.44
9:C:264:LEU:O	9:C:317:ALA:HA	2.18	0.44
7:I:1151:LEU:HD22	7:I:1201:LEU:HD22	1.99	0.44
8:J:1260:MET:HE2	8:J:1306:LEU:HD11	1.99	0.44
9:D:406:THR:OG1	9:D:407:LYS:N	2.50	0.44
3:N:18:DC:C2'	3:N:19:DG:H5'	2.48	0.43
7:I:838:CYS:HB3	7:I:1050:VAL:HG13	1.99	0.43
8:J:321:LYS:HD2	8:J:321:LYS:HA	1.88	0.43
8:J:975:ILE:HD13	8:J:980:THR:HG21	1.99	0.43
9:D:264:LEU:HD22	9:D:300:PHE:HE1	1.82	0.43
9:E:192:ALA:HB1	9:E:204:LEU:HD21	1.99	0.43
7:I:322:LEU:HD23	7:I:325:LEU:HD21	2.00	0.43
7:I:1154:ASP:OD1	7:I:1154:ASP:N	2.49	0.43
9:D:254:VAL:HG21	9:D:313:LEU:HB2	1.99	0.43
7:I:242:VAL:HG12	7:I:244:GLU:H	1.82	0.43
7:I:1061:GLN:HE22	7:I:1240:ASP:CG	2.25	0.43
8:J:245:LEU:O	8:J:250:ARG:NH1	2.50	0.43
8:J:250:ARG:NE	8:J:266:ASN:OD1	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:133:PHE:N	9:F:255:GLU:OE2	2.49	0.43
9:D:178:ALA:HB3	9:D:184:LYS:HD3	1.99	0.43
7:I:251:ALA:HB2	7:I:269:ILE:HD11	2.00	0.43
9:D:160:ARG:NE	9:D:409:ASN:OD1	2.48	0.43
6:K:57:THR:OG1	6:K:158:ARG:NH1	2.48	0.43
6:K:75:GLN:NE2	7:I:771:VAL:O	2.51	0.43
8:J:594:GLN:HG2	8:J:596:LEU:HD12	2.00	0.43
8:J:1265:THR:HG22	8:J:1279:GLN:HB3	2.01	0.43
4:T:27:DC:H2''	4:T:28:DC:C6	2.54	0.43
7:I:1307:ASN:HB3	7:I:1312:ASN:O	2.19	0.43
8:J:66:LYS:HB2	8:J:69:GLU:O	2.19	0.43
8:J:1000:GLY:HA3	8:J:1026:PRO:HG2	2.01	0.43
9:A:356:PRO:HB2	9:A:358:ILE:HG13	2.00	0.43
7:I:9:LYS:O	7:I:1175:ASN:ND2	2.37	0.43
9:C:188:LEU:HD21	9:C:263:LEU:HB3	2.01	0.43
9:C:26:LEU:HD23	9:C:34:ILE:HG12	2.01	0.43
6:H:13:LEU:HB3	6:H:28:LEU:HD23	2.01	0.42
8:J:847:ASP:OD1	8:J:847:ASP:N	2.51	0.42
9:C:387:ILE:HG23	9:C:395:ALA:HB1	2.01	0.42
9:A:43:ALA:HB2	9:A:49:ILE:HD11	2.01	0.42
9:B:297:PRO:HB2	9:B:335:PHE:HZ	1.84	0.42
2:W:26:ARG:HG3	2:W:30:MET:HE3	2.00	0.42
8:J:123:ARG:HH21	8:J:1334:GLU:HG2	1.83	0.42
1:G:111:LYS:HE3	7:I:899:GLU:HB3	2.01	0.42
9:E:170:ARG:NH1	9:E:259:ASP:OD2	2.53	0.42
9:E:406:THR:OG1	9:E:407:LYS:N	2.53	0.42
3:N:19:DG:H3'	3:N:19:DG:P	2.60	0.42
6:K:13:LEU:HD21	6:K:16:ILE:HD11	2.01	0.42
7:I:884:VAL:HG11	7:I:1050:VAL:HG21	2.02	0.42
9:C:207:LEU:HD13	9:C:246:VAL:HG21	2.02	0.42
1:G:26:ALA:HB2	1:G:117:LYS:HG3	2.02	0.42
9:B:176:ILE:HB	9:B:318:THR:HG22	2.01	0.42
1:G:67:GLU:HG2	1:G:68:VAL:H	1.85	0.42
6:K:27:THR:HG22	6:K:29:GLU:HG3	2.01	0.42
6:H:129:VAL:HG11	6:H:132:HIS:HE1	1.85	0.42
9:C:102:ARG:HD3	9:C:114:LEU:HD13	2.00	0.42
9:E:294:LEU:HD13	9:E:334:GLU:HG2	2.02	0.42
4:T:14:DG:H5'	8:J:795:TYR:CE1	2.55	0.42
7:I:454:ARG:HG2	7:I:459:MET:HG3	2.02	0.42
7:I:739:ASP:OD1	7:I:740:GLU:N	2.53	0.42
8:J:144:TYR:OH	8:J:293:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:79:ILE:HG13	9:A:111:PHE:HB2	2.02	0.42
9:E:176:ILE:HB	9:E:318:THR:HG22	2.02	0.42
7:I:946:LEU:O	7:I:949:GLU:HG3	2.19	0.42
8:J:810:THR:HG22	8:J:893:GLY:HA3	2.01	0.42
9:F:147:MET:HE3	9:F:194:SER:HB2	2.02	0.42
8:J:93:THR:OG1	8:J:94:GLN:N	2.53	0.42
8:J:792:ASN:HB3	8:J:1138:LEU:HD23	2.02	0.42
9:C:406:THR:OG1	9:C:407:LYS:N	2.53	0.42
9:D:266:SER:O	9:D:270:LEU:N	2.40	0.42
9:D:294:LEU:HD13	9:D:334:GLU:HG2	2.01	0.42
9:E:402:LYS:HB3	9:E:412:PHE:CE1	2.55	0.42
1:G:152:LEU:HD11	1:G:162:ILE:HD11	2.02	0.41
7:I:549:ASP:OD2	8:J:750:PRO:HB3	2.20	0.41
8:J:1029:THR:HA	8:J:1099:TYR:HE2	1.85	0.41
9:F:234:GLU:HB3	9:F:238:ARG:HD3	2.02	0.41
8:J:650:LYS:NZ	8:J:762:ASN:HD22	2.19	0.41
8:J:1265:THR:N	8:J:1303:SER:O	2.42	0.41
7:I:113:THR:OG1	7:I:114:VAL:N	2.53	0.41
7:I:1125:GLY:HA3	7:I:1179:GLY:HA2	2.01	0.41
8:J:1257:VAL:O	8:J:1261:LEU:HG	2.20	0.41
9:A:387:ILE:HA	9:A:390:MET:HE2	2.03	0.41
7:I:838:CYS:HB2	7:I:918:LEU:HD22	2.02	0.41
8:J:97:VAL:O	8:J:101:ARG:HG2	2.20	0.41
8:J:709:ARG:HD3	8:J:714:GLU:HG3	2.02	0.41
9:C:176:ILE:HB	9:C:318:THR:HG22	2.02	0.41
9:E:264:LEU:HD11	9:E:266:SER:HB3	2.01	0.41
8:J:697:MET:HE3	8:J:697:MET:HB3	2.00	0.41
8:J:926:PRO:HG3	8:J:1248:ILE:HD11	2.03	0.41
1:G:18:LEU:HD12	1:G:23:ILE:HB	2.03	0.41
1:G:45:VAL:HG13	1:G:60:ARG:HA	2.01	0.41
7:I:1041:ASP:OD1	7:I:1041:ASP:N	2.48	0.41
9:D:192:ALA:HB1	9:D:204:LEU:HD21	2.02	0.41
9:E:266:SER:OG	9:E:269:ARG:HB2	2.20	0.41
6:H:190:ALA:HB2	6:H:200:LYS:HB2	2.02	0.41
7:I:1009:ASN:O	7:I:1013:GLN:N	2.43	0.41
7:I:1297:ASP:O	7:I:1301:ARG:HG3	2.20	0.41
8:J:615:LYS:HB2	8:J:616:PRO:HD3	2.02	0.41
9:F:176:ILE:HB	9:F:318:THR:HG22	2.02	0.41
2:W:50:ALA:O	2:W:54:ILE:HG12	2.21	0.41
6:K:31:LEU:HD13	6:K:36:GLY:HA2	2.03	0.41
7:I:959:ASP:O	7:I:963:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:1082:ILE:HD12	7:I:1082:ILE:H	1.86	0.41
7:I:1304:MET:HE3	7:I:1308:ILE:HD11	2.02	0.41
9:B:296:ARG:HB2	9:B:297:PRO:HD3	2.01	0.41
9:D:96:THR:HB	9:D:120:ASN:HA	2.02	0.41
1:G:36:LYS:HE2	1:G:44:ASP:H	1.85	0.41
1:G:123:ARG:NH2	1:G:159:GLU:H	2.19	0.41
5:R:2:C:O2'	5:R:3:G:OP2	2.37	0.41
6:K:207:THR:OG1	6:K:208:ASN:N	2.52	0.41
7:I:26:TYR:HE2	7:I:32:LEU:HD12	1.86	0.41
7:I:557:ARG:HH22	7:I:611:GLU:CD	2.29	0.41
8:J:342:LEU:HD13	8:J:1352:ILE:HG23	2.03	0.41
8:J:425:ARG:HD3	8:J:459:ALA:HB2	2.02	0.41
8:J:1038:THR:HG21	8:J:1079:LYS:HE2	2.03	0.41
9:C:155:GLU:OE1	9:C:155:GLU:N	2.49	0.41
9:A:160:ARG:NE	9:A:409:ASN:OD1	2.53	0.41
9:A:387:ILE:HG23	9:A:395:ALA:HB1	2.03	0.41
9:D:290:ASP:HB3	9:D:293:ALA:HB2	2.03	0.41
9:F:79:ILE:HD13	9:F:101:ILE:HG21	2.03	0.41
6:K:134:THR:O	6:K:134:THR:OG1	2.35	0.41
8:J:786:THR:HG22	8:J:789:LYS:HE2	2.02	0.41
8:J:556:GLU:HB3	8:J:564:VAL:HG13	2.02	0.40
9:B:67:SER:OG	9:B:69:ASP:OD1	2.32	0.40
9:F:174:GLY:HA2	9:F:341:MET:HB3	2.03	0.40
8:J:42:GLU:HB2	8:J:52:GLU:HG2	2.03	0.40
8:J:668:PHE:CG	8:J:678:ARG:HD3	2.55	0.40
8:J:1075:ARG:HD3	8:J:1076:PRO:HD2	2.03	0.40
9:C:264:LEU:HG	9:C:266:SER:H	1.86	0.40
4:T:14:DG:H3'	4:T:15:DT:H71	2.04	0.40
7:I:9:LYS:HG2	7:I:1171:ARG:NH1	2.36	0.40
7:I:870:ILE:HG21	7:I:931:VAL:HG11	2.04	0.40
8:J:405:GLU:O	8:J:408:VAL:HG22	2.21	0.40
9:B:149:ARG:HH21	9:B:193:GLN:HB3	1.86	0.40
9:F:175:LEU:HD23	9:F:317:ALA:HB3	2.04	0.40
9:F:247:ILE:HG13	9:F:251:LYS:HE3	2.03	0.40
7:I:225:PHE:HB2	7:I:336:LEU:HD22	2.04	0.40
8:J:613:GLY:O	8:J:617:THR:OG1	2.39	0.40
8:J:1036:ARG:HH21	8:J:1081:VAL:HG11	1.86	0.40
9:C:387:ILE:HA	9:C:390:MET:HE2	2.01	0.40
1:G:126:VAL:HG11	1:G:158:ALA:HB2	2.03	0.40
3:N:26:DA:H5'	3:N:26:DA:H8	1.86	0.40
8:J:518:VAL:HA	8:J:547:ARG:HH12	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:709:ARG:C	8:J:711:GLY:H	2.28	0.40
9:B:264:LEU:HD22	9:B:300:PHE:HE1	1.86	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	198/495 (40%)	188 (95%)	10 (5%)	0	100	100
2	W	53/91 (58%)	52 (98%)	1 (2%)	0	100	100
6	H	214/329 (65%)	211 (99%)	3 (1%)	0	100	100
6	K	276/329 (84%)	270 (98%)	6 (2%)	0	100	100
7	I	1319/1342 (98%)	1271 (96%)	47 (4%)	1 (0%)	48	79
8	J	1319/1416 (93%)	1269 (96%)	50 (4%)	0	100	100
9	A	386/419 (92%)	385 (100%)	1 (0%)	0	100	100
9	B	415/419 (99%)	412 (99%)	3 (1%)	0	100	100
9	C	415/419 (99%)	414 (100%)	1 (0%)	0	100	100
9	D	415/419 (99%)	415 (100%)	0	0	100	100
9	E	415/419 (99%)	412 (99%)	3 (1%)	0	100	100
9	F	339/419 (81%)	338 (100%)	1 (0%)	0	100	100
All	All	5764/6516 (88%)	5637 (98%)	126 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	I	1154	ASP

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	176/409 (43%)	166 (94%)	10 (6%)	18	44
2	W	46/75 (61%)	45 (98%)	1 (2%)	45	63
6	H	187/286 (65%)	183 (98%)	4 (2%)	47	64
6	K	196/286 (68%)	193 (98%)	3 (2%)	57	69
7	I	1141/1157 (99%)	1121 (98%)	20 (2%)	51	67
8	J	1114/1177 (95%)	1093 (98%)	21 (2%)	50	66
9	A	331/359 (92%)	329 (99%)	2 (1%)	78	79
9	B	357/359 (99%)	355 (99%)	2 (1%)	78	79
9	C	357/359 (99%)	353 (99%)	4 (1%)	65	73
9	D	357/359 (99%)	354 (99%)	3 (1%)	73	76
9	E	357/359 (99%)	356 (100%)	1 (0%)	86	84
9	F	293/359 (82%)	291 (99%)	2 (1%)	76	77
All	All	4912/5544 (89%)	4839 (98%)	73 (2%)	55	69

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	15	GLU
1	G	47	VAL
1	G	49	ILE
1	G	59	PHE
1	G	93	VAL
1	G	94	GLU
1	G	101	THR
1	G	129	GLN
1	G	182	VAL
1	G	186	VAL
2	W	13	ILE
6	K	26	VAL
6	K	74	VAL
6	K	234	LEU

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Mol	Chain	Res	Type
6	H	6	THR
6	H	13	LEU
6	H	196	THR
6	H	207	THR
7	I	49	LEU
7	I	155	VAL
7	I	188	PHE
7	I	285	ILE
7	I	483	ASP
7	I	484	LEU
7	I	514	PHE
7	I	550	VAL
7	I	697	LYS
7	I	754	THR
7	I	808	ASN
7	I	850	ILE
7	I	887	VAL
7	I	888	THR
7	I	1018	TYR
7	I	1050	VAL
7	I	1056	VAL
7	I	1060	ILE
7	I	1132	LEU
7	I	1296	ASP
8	J	84	ILE
8	J	90	VAL
8	J	92	VAL
8	J	95	THR
8	J	197	GLU
8	J	204	GLU
8	J	290	ILE
8	J	474	LEU
8	J	500	ILE
8	J	564	VAL
8	J	663	GLU
8	J	684	ASP
8	J	706	VAL
8	J	757	THR
8	J	825	VAL
8	J	831	VAL
8	J	849	LEU
8	J	1027	VAL

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Mol	Chain	Res	Type
8	J	1163	VAL
8	J	1184	ASP
8	J	1301	THR
9	C	108	GLU
9	C	116	VAL
9	C	188	LEU
9	C	214	GLU
9	A	188	LEU
9	A	265	ASP
9	B	3	LEU
9	B	188	LEU
9	D	116	VAL
9	D	188	LEU
9	D	228	VAL
9	E	188	LEU
9	F	116	VAL
9	F	188	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	194	GLN
2	W	31	GLN
6	K	66	HIS
6	K	186	ASN
6	H	117	HIS
6	H	227	GLN
7	I	214	ASN
7	I	517	GLN
7	I	894	GLN
7	I	1061	GLN
8	J	158	GLN
8	J	186	GLN
8	J	341	ASN
8	J	465	GLN
8	J	469	HIS
8	J	720	ASN
8	J	875	ASN
9	C	8	ASN
9	C	42	HIS
9	A	42	HIS
9	A	190	ASN

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Mol	Chain	Res	Type
9	B	241	GLN
9	B	256	HIS
9	D	190	ASN
9	E	172	GLN
9	F	172	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	R	16/60 (26%)	7 (43%)	1 (6%)

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	R	2	C
5	R	3	G
5	R	4	C
5	R	5	A
5	R	6	C
5	R	52	G
5	R	54	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	R	2	C

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 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

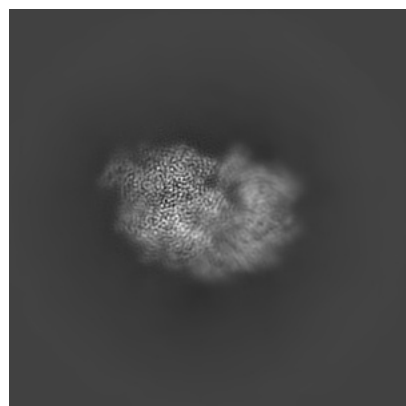
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22114. These allow visual inspection of the internal detail of the map and identification of artifacts.

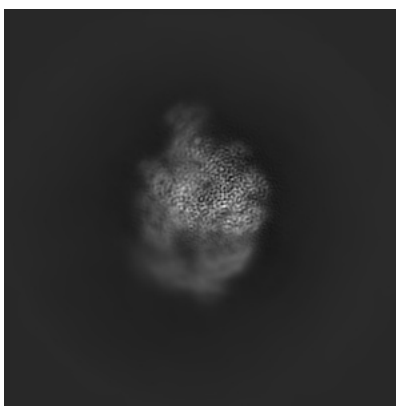
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

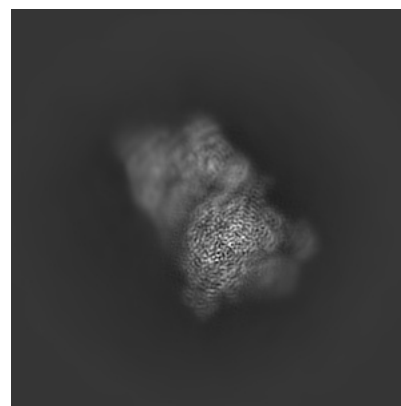
6.1.1 Primary map



X

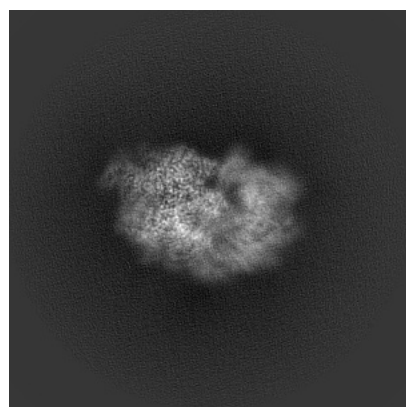


Y

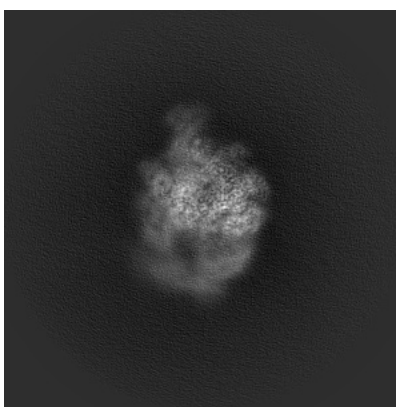


Z

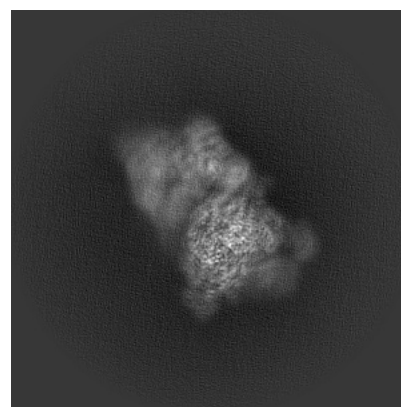
6.1.2 Raw map



X



Y

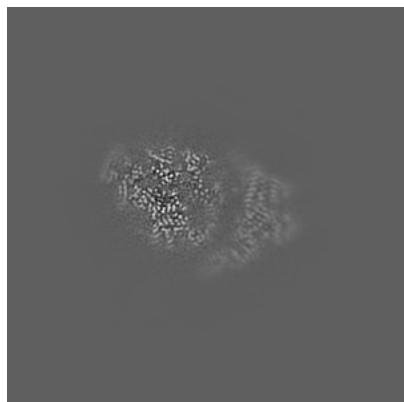


Z

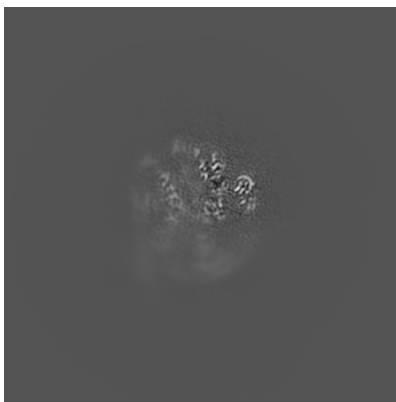
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

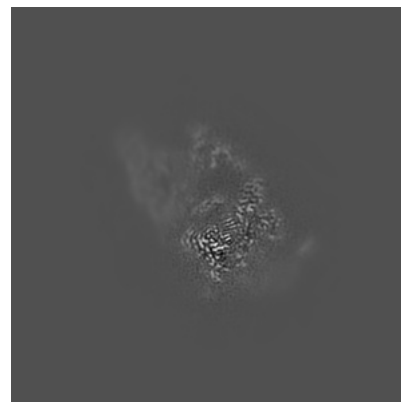
6.2.1 Primary map



X Index: 180

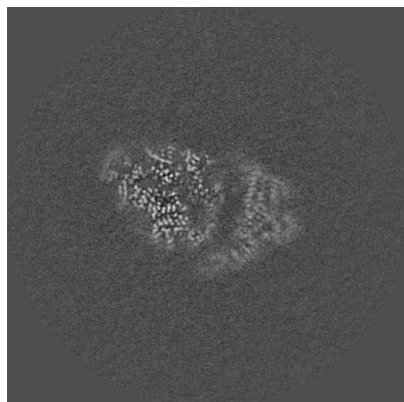


Y Index: 180

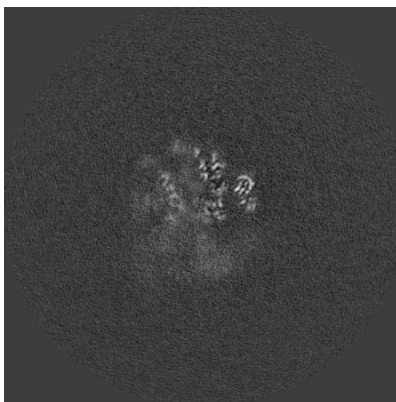


Z Index: 180

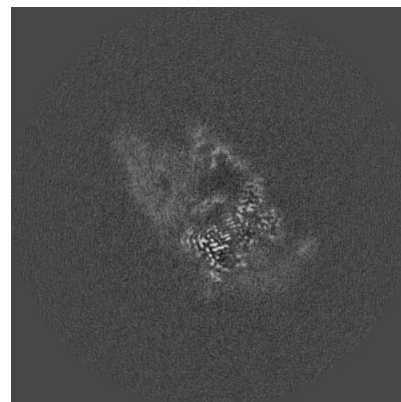
6.2.2 Raw map



X Index: 180



Y Index: 180

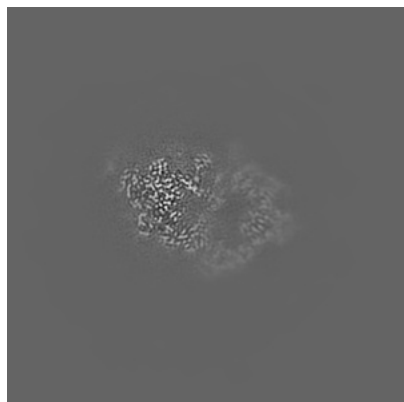


Z Index: 180

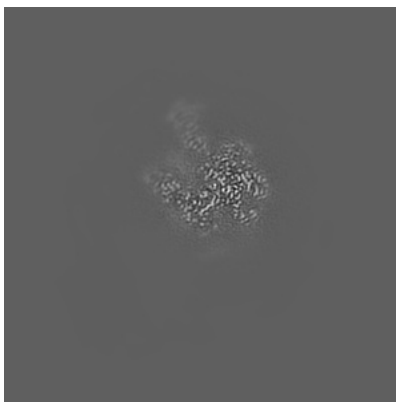
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

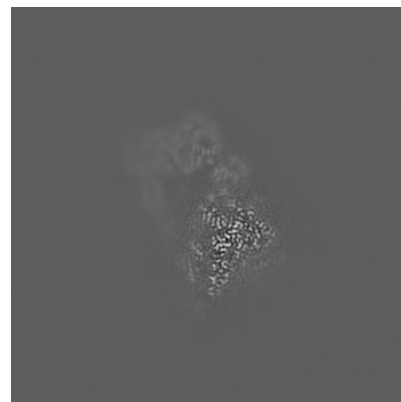
6.3.1 Primary map



X Index: 186

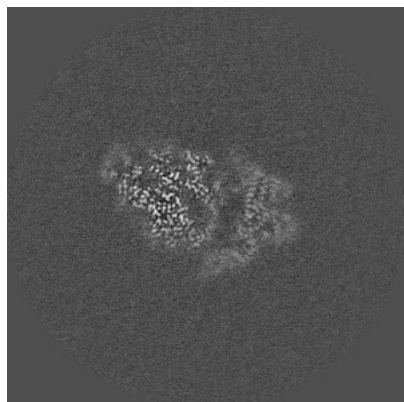


Y Index: 153

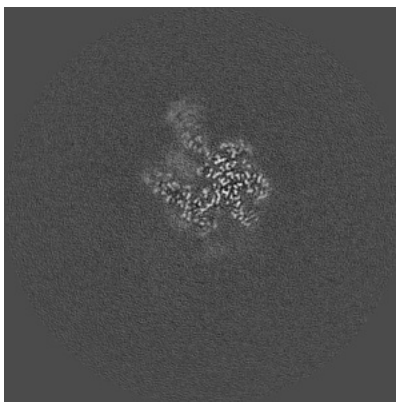


Z Index: 197

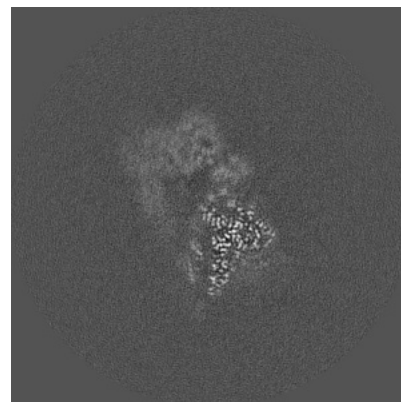
6.3.2 Raw map



X Index: 181



Y Index: 154

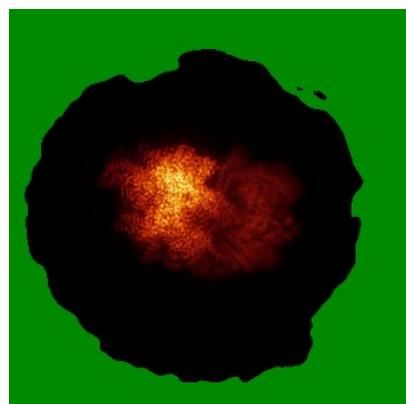


Z Index: 197

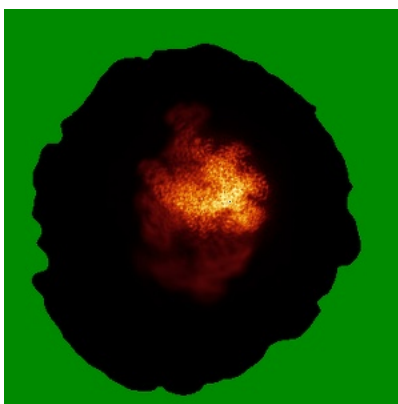
The images above show the largest variance slices of the map in three orthogonal directions.

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

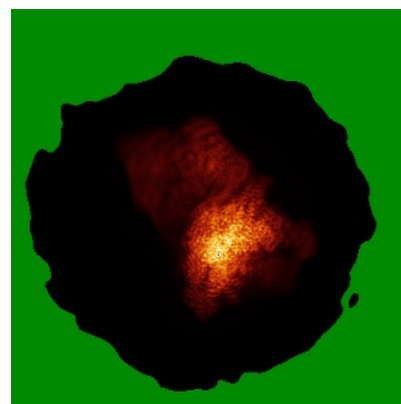
6.4.1 Primary map



X

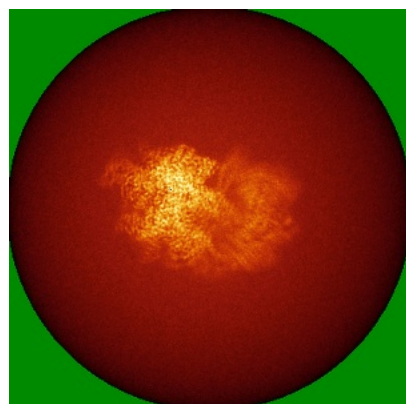


Y

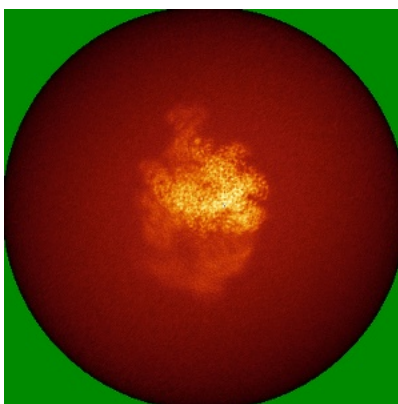


Z

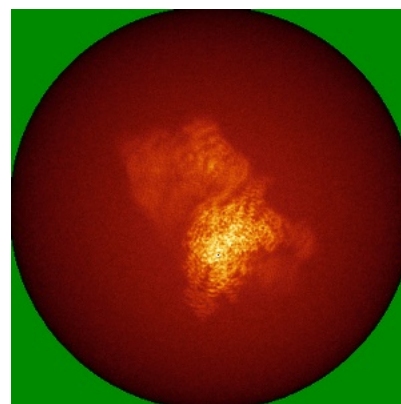
6.4.2 Raw map



X



Y

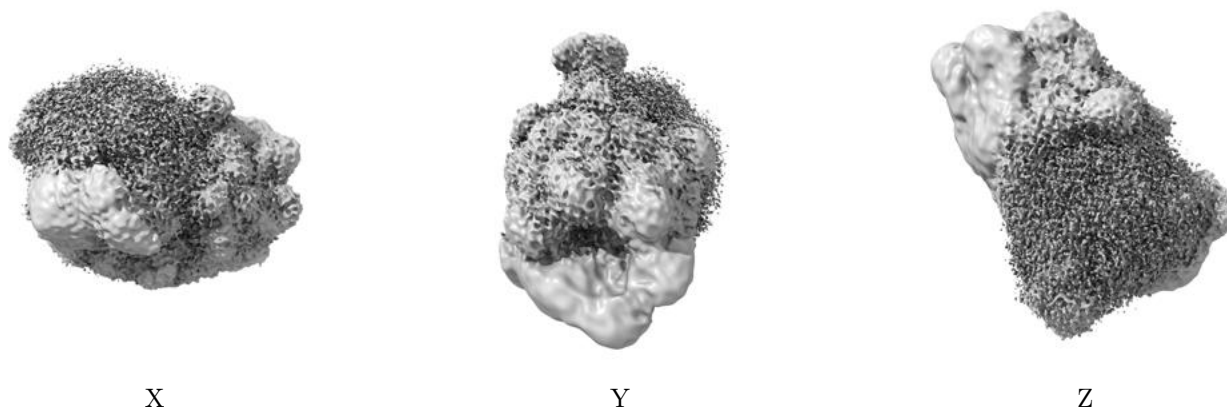


Z

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.

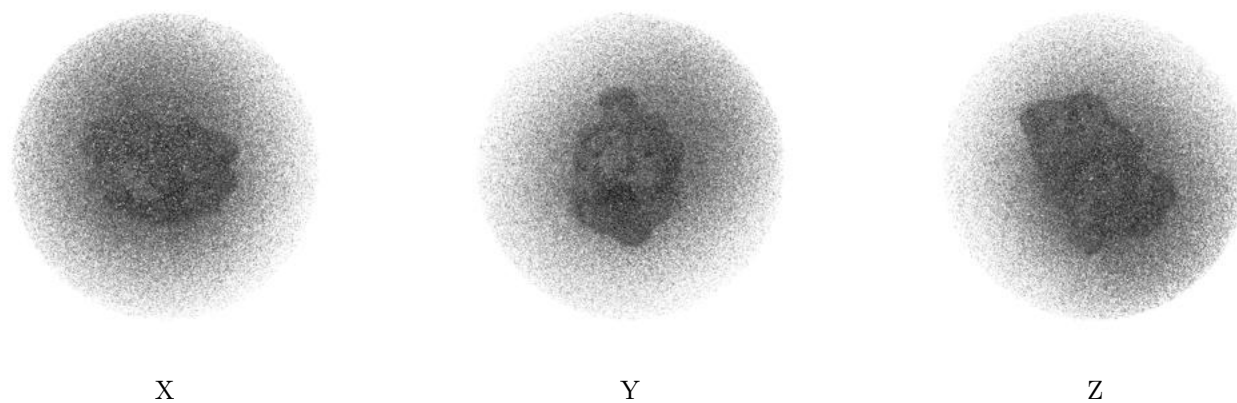
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0045. 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.

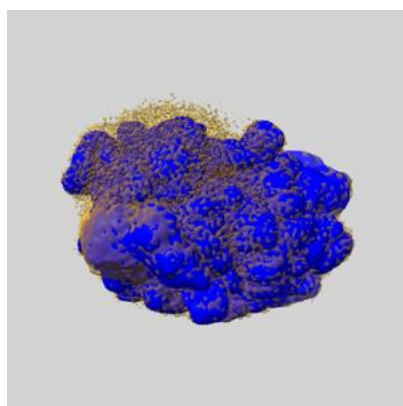
6.6 Mask visualisation [i](#)

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

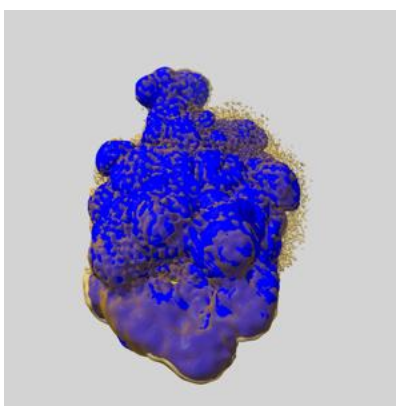
A mask typically either:

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

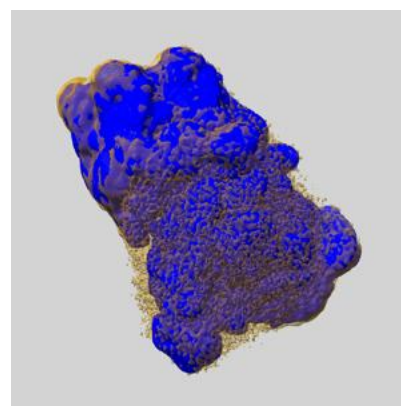
6.6.1 emd_22114_msk_1.map [i](#)



X



Y

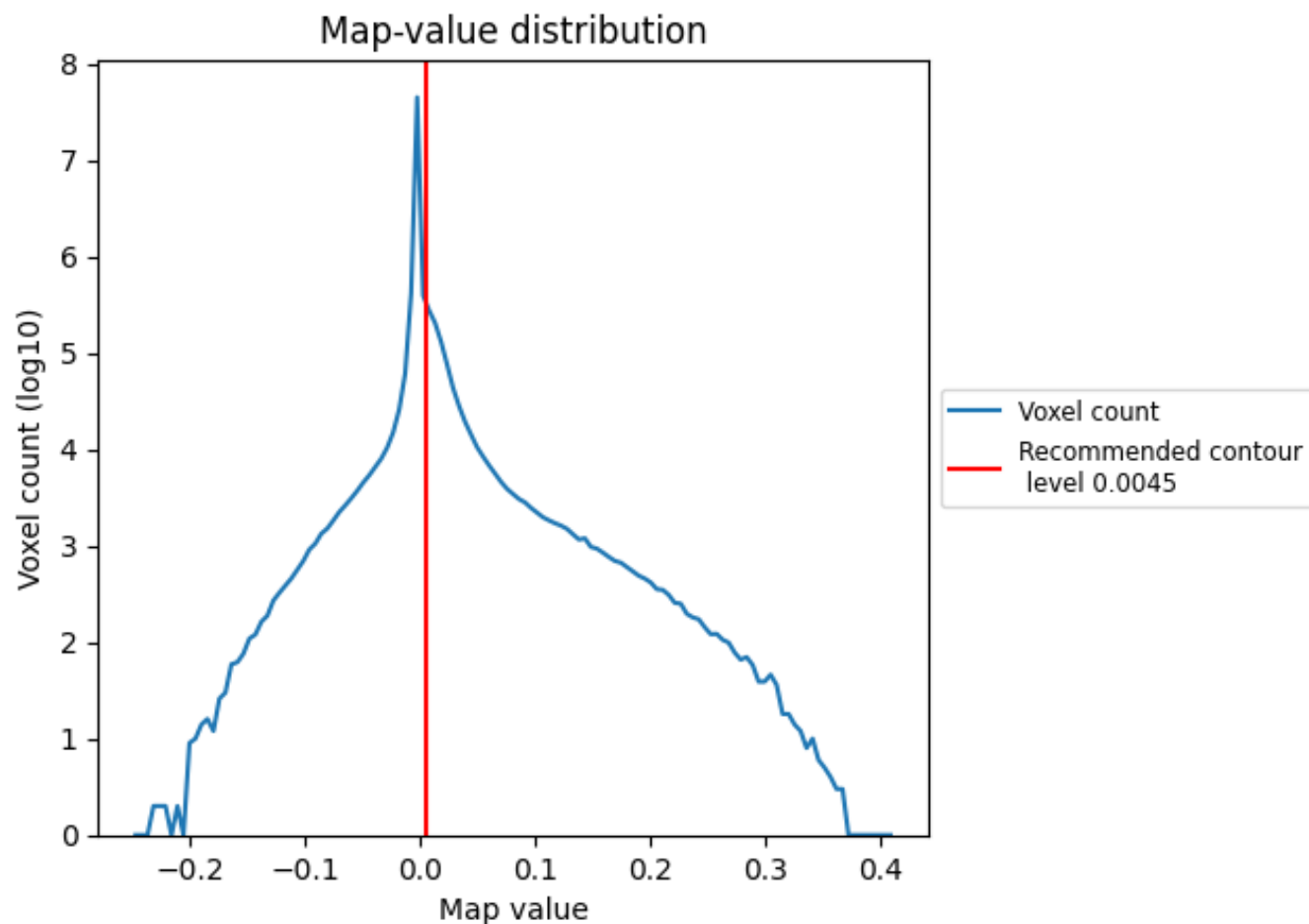


Z

7 Map analysis [i](#)

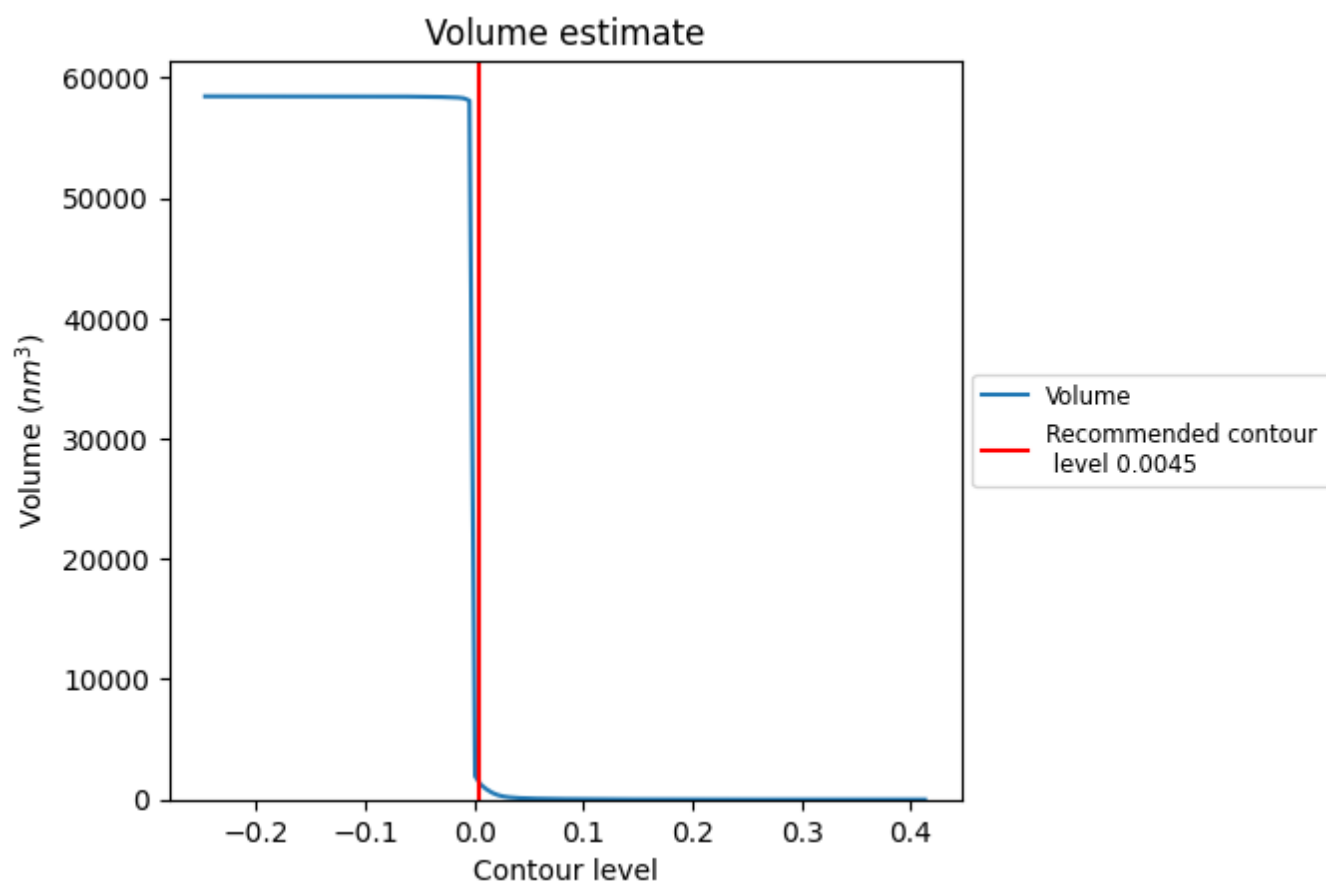
This section contains the results of statistical analysis of the map.

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.

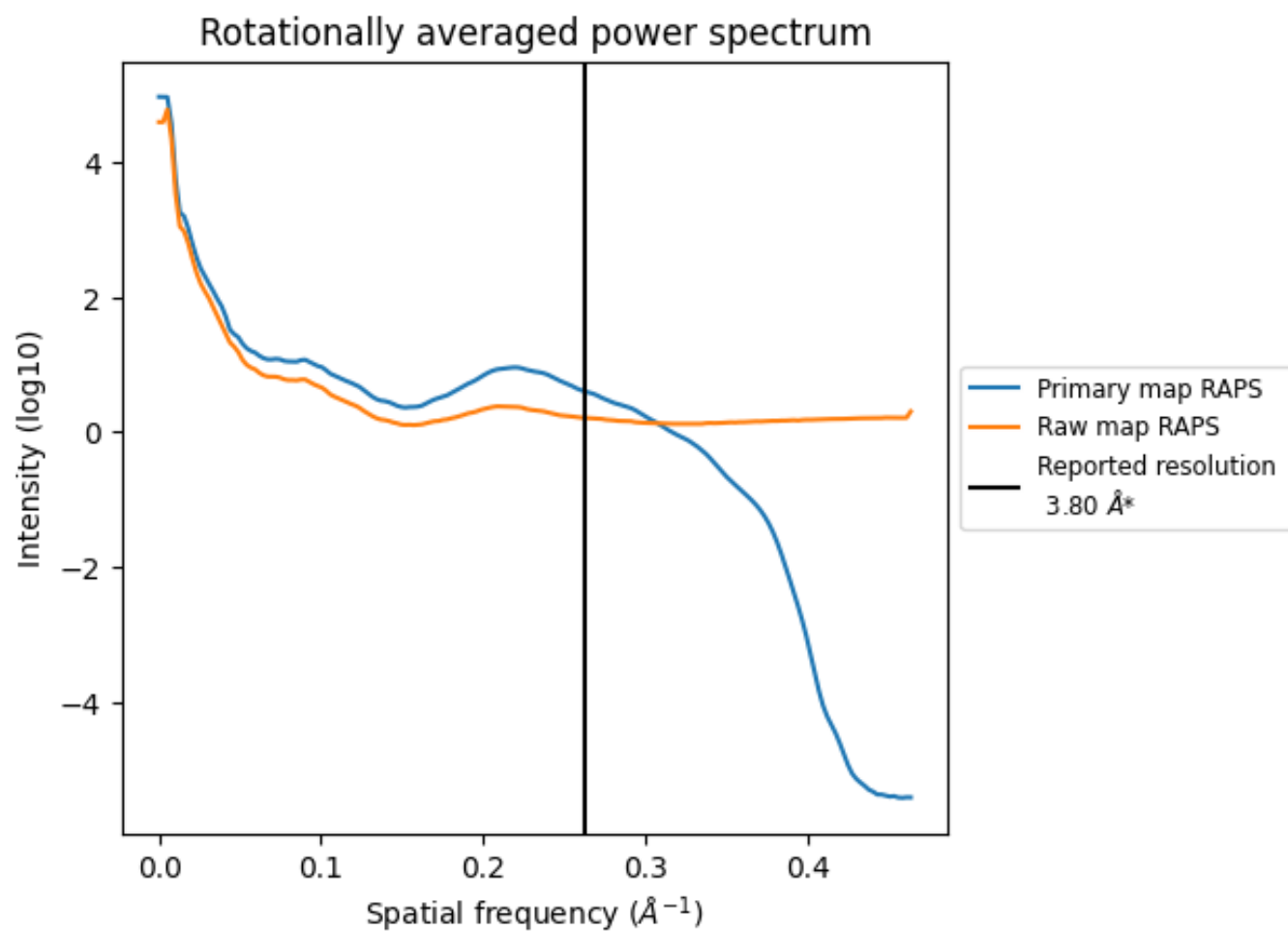
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1443 nm³; this corresponds to an approximate mass of 1304 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 ⓘ

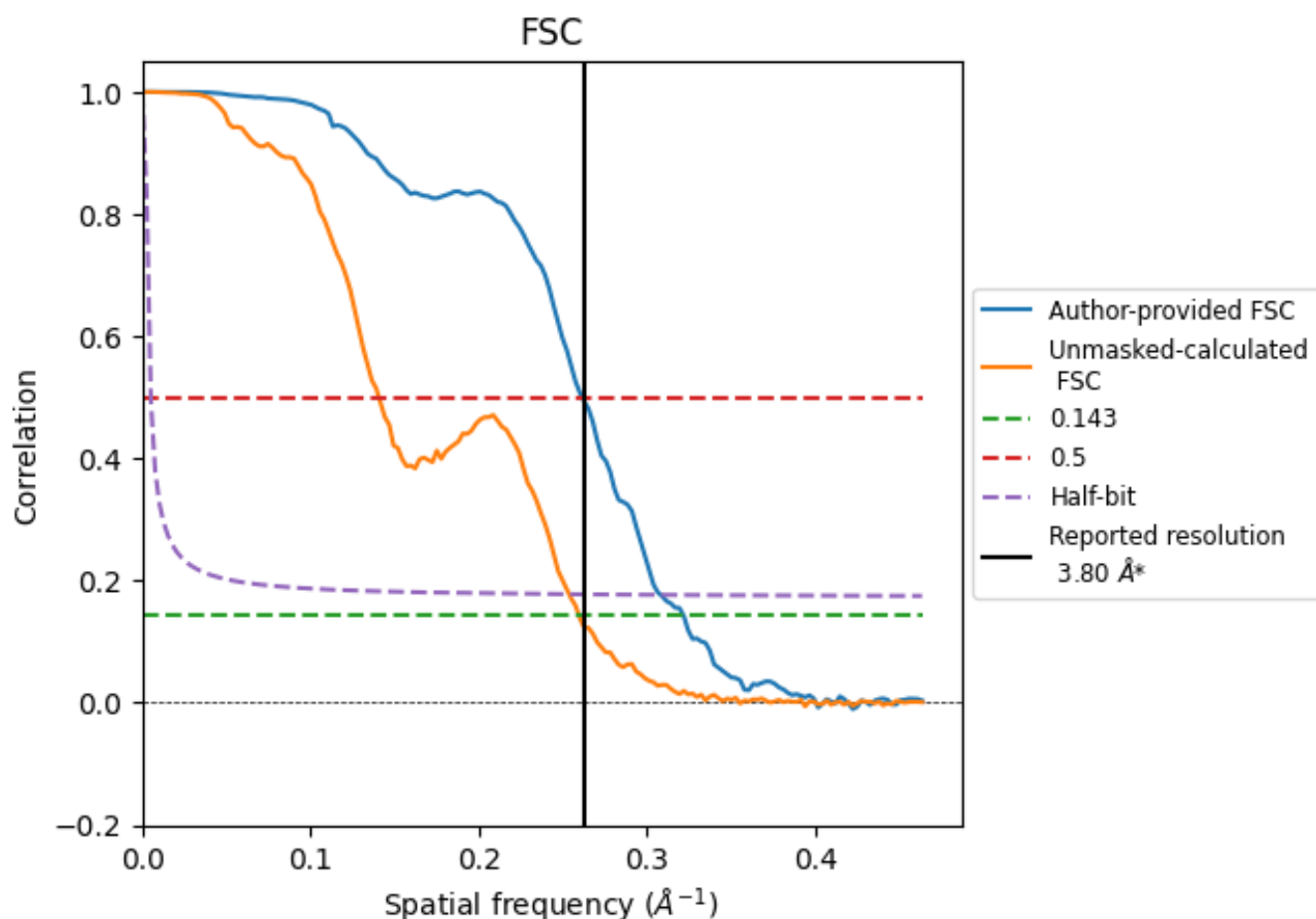


*Reported resolution corresponds to spatial frequency of $0.263 \text{ \AA}^{-1}$

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

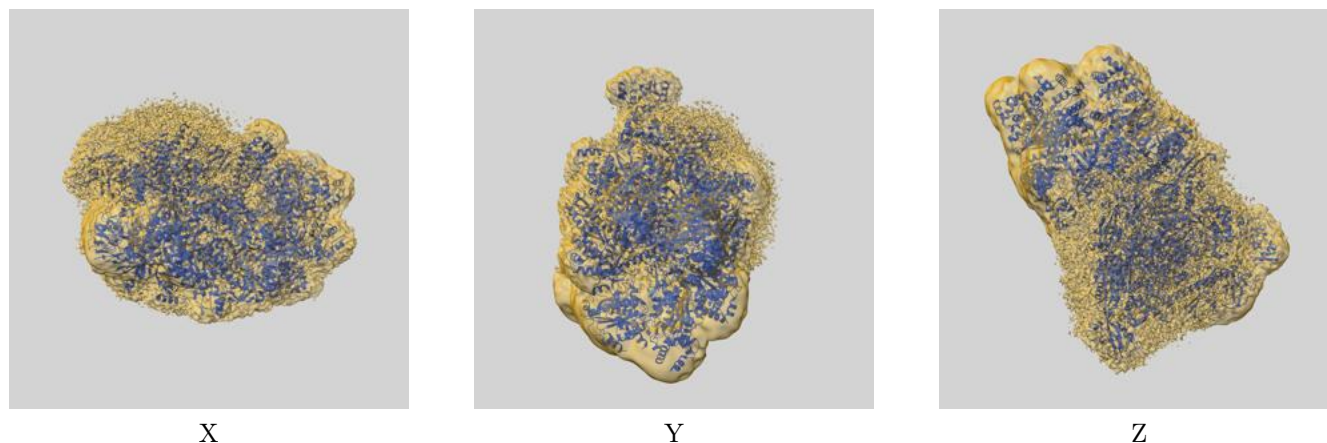
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	3.80	-
Author-provided FSC curve	3.11	3.82	3.24
Unmasked-calculated*	3.85	7.10	3.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.5 CUT-OFF 7.10 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22114 and PDB model 6XAS. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



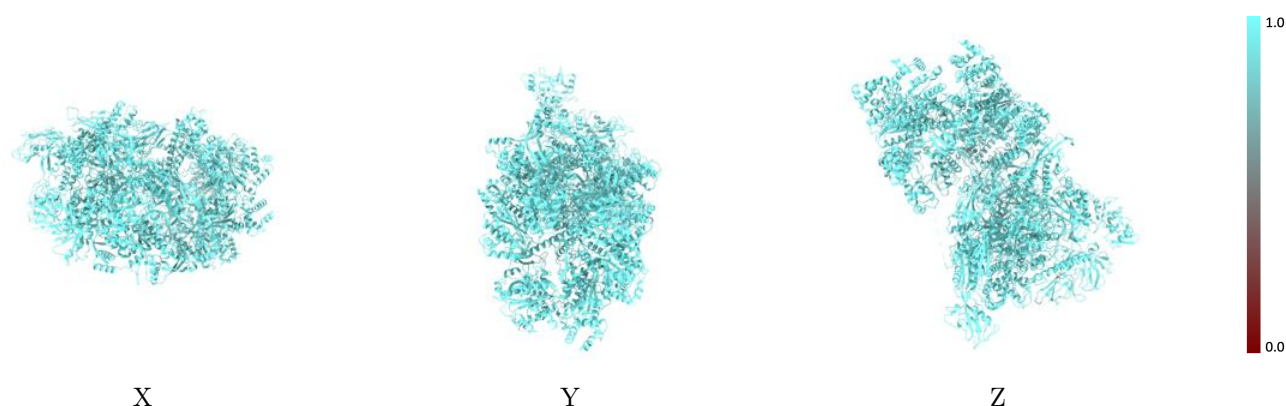
The images above show the 3D surface view of the map at the recommended contour level 0.0045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



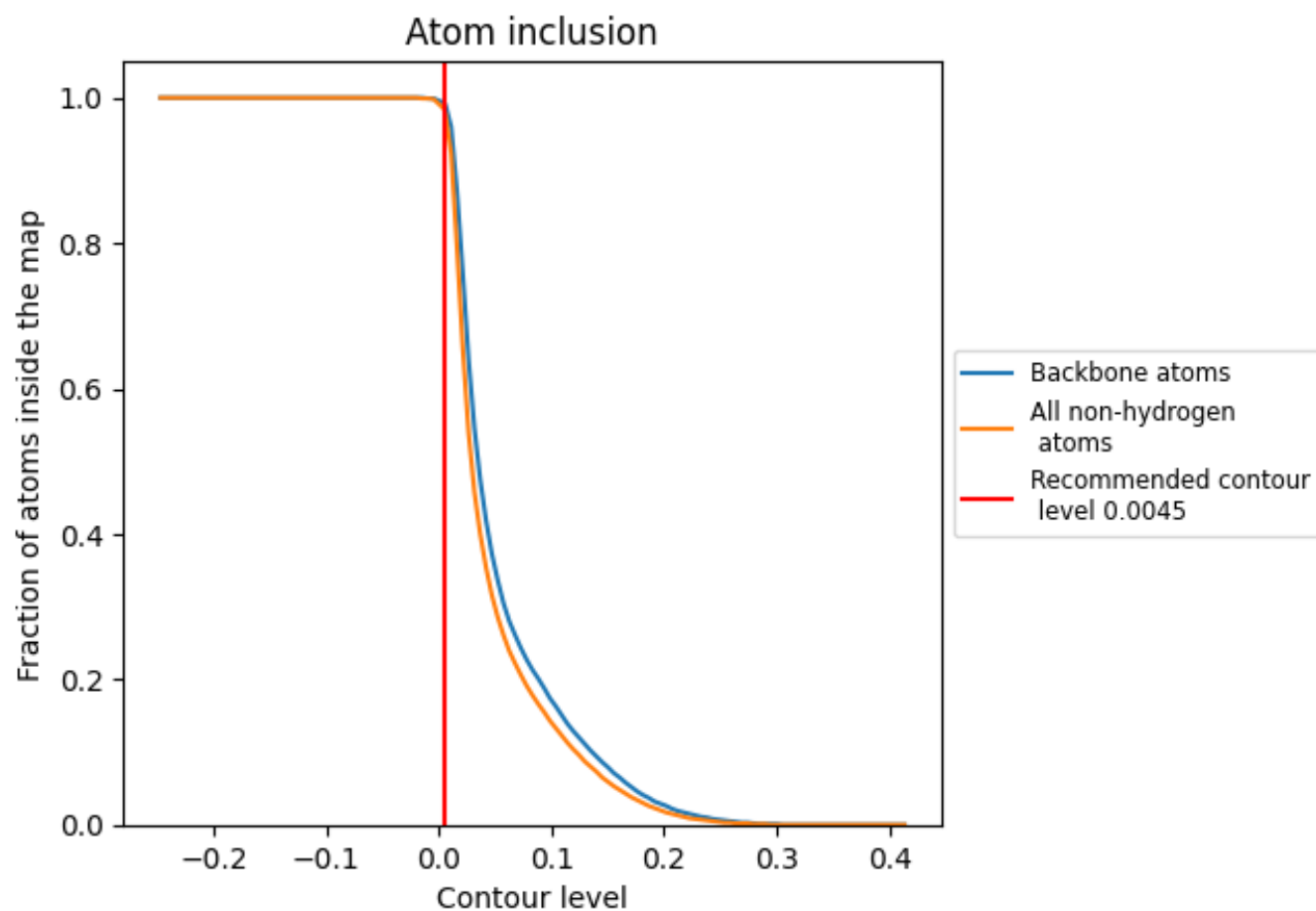
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0045).

9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.0045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9850	0.3340
A	0.9880	0.2600
B	0.9890	0.3110
C	0.9870	0.2930
D	0.9910	0.1840
E	0.9950	0.1420
F	0.9820	0.1160
G	0.9920	0.1750
H	0.9810	0.4390
I	0.9870	0.4690
J	0.9850	0.4050
K	0.9850	0.4600
N	0.9260	0.1180
R	0.9400	0.3350
T	0.9690	0.2520
W	0.8850	0.3100

1.0

0.0

<0.0