



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:12 AM UTC

PDB ID : 9G9D / pdb_00009g9d
EMDB ID : EMD-51148
Title : CryoEM structure of Enterococcus italicus Csm-crRNA-CTR (4.3) complex
Authors : Jungfer, K.; Jinek, M.
Deposited on : 2024-07-25
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

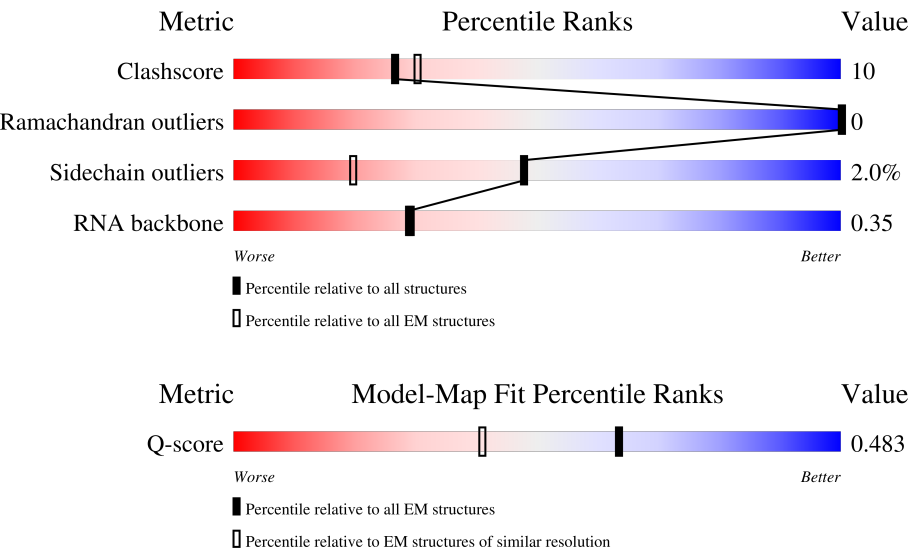
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	B	140	68%23%9% 14%
1	C	140	61%32%6% 23%
1	J	140	74%21% 23%

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Mol	Chain	Length	Quality of chain
2	D	214	
2	E	214	
2	F	214	
2	I	214	
3	G	307	
4	R	45	
5	T	47	
6	H	379	
7	A	774	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 21333 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 CRISPR system Cms protein Csm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	132	Total	C	N	O	S	0	0
			1102	708	186	206	2		
1	B	128	Total	C	N	O	S	0	0
			1065	690	175	198	2		
1	J	135	Total	C	N	O	S	0	0
			1124	723	190	209	2		

- Molecule 2 is a protein called CRISPR system Cms endoribonuclease Csm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	210	Total	C	N	O	S	0	0
			1620	1019	288	309	4		
2	E	210	Total	C	N	O	S	0	0
			1620	1019	288	309	4		
2	D	200	Total	C	N	O	S	0	0
			1548	976	274	295	3		
2	I	210	Total	C	N	O	S	0	0
			1620	1019	288	309	4		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	32	ALA	ASP	engineered mutation	UNP E6LHV5
E	32	ALA	ASP	engineered mutation	UNP E6LHV5
D	32	ALA	ASP	engineered mutation	UNP E6LHV5
I	32	ALA	ASP	engineered mutation	UNP E6LHV5

- Molecule 3 is a protein called CRISPR system Cms protein Csm4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	296	Total	C	N	O	S	0	0
			2341	1509	384	443	5		

- Molecule 4 is a RNA chain called RNA (35-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	38	Total	C	N	O	P	0	0
			816	366	158	255	37		

- Molecule 5 is a RNA chain called RNA (35-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	T	35	Total	C	N	O	P	0	0
			740	330	125	250	35		

- Molecule 6 is a protein called CRISPR system Cms protein Csm5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	310	Total	C	N	O	S	0	0
			2510	1625	430	447	8		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	350	LEU	-	expression tag	UNP E6LHV3
H	351	GLU	-	expression tag	UNP E6LHV3
H	352	VAL	-	expression tag	UNP E6LHV3
H	353	LEU	-	expression tag	UNP E6LHV3
H	354	PHE	-	expression tag	UNP E6LHV3
H	355	GLN	-	expression tag	UNP E6LHV3
H	356	GLY	-	expression tag	UNP E6LHV3
H	357	PRO	-	expression tag	UNP E6LHV3
H	358	GLY	-	expression tag	UNP E6LHV3
H	359	GLY	-	expression tag	UNP E6LHV3
H	360	GLY	-	expression tag	UNP E6LHV3
H	361	TRP	-	expression tag	UNP E6LHV3
H	362	SER	-	expression tag	UNP E6LHV3
H	363	HIS	-	expression tag	UNP E6LHV3
H	364	PRO	-	expression tag	UNP E6LHV3
H	365	GLN	-	expression tag	UNP E6LHV3
H	366	PHE	-	expression tag	UNP E6LHV3
H	367	GLU	-	expression tag	UNP E6LHV3
H	368	LYS	-	expression tag	UNP E6LHV3
H	369	GLY	-	expression tag	UNP E6LHV3
H	370	GLY	-	expression tag	UNP E6LHV3
H	371	GLY	-	expression tag	UNP E6LHV3
H	372	TRP	-	expression tag	UNP E6LHV3

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Chain	Residue	Modelled	Actual	Comment	Reference
H	373	SER	-	expression tag	UNP E6LHV3
H	374	HIS	-	expression tag	UNP E6LHV3
H	375	PRO	-	expression tag	UNP E6LHV3
H	376	GLN	-	expression tag	UNP E6LHV3
H	377	PHE	-	expression tag	UNP E6LHV3
H	378	GLU	-	expression tag	UNP E6LHV3
H	379	LYS	-	expression tag	UNP E6LHV3

- Molecule 7 is a protein called CRISPR system single-strand-specific deoxyribonuclease Cas10/Csm1 (subtype III-A).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	653	Total	C	N	O	S	0	0
			5227	3338	866	1000	23		

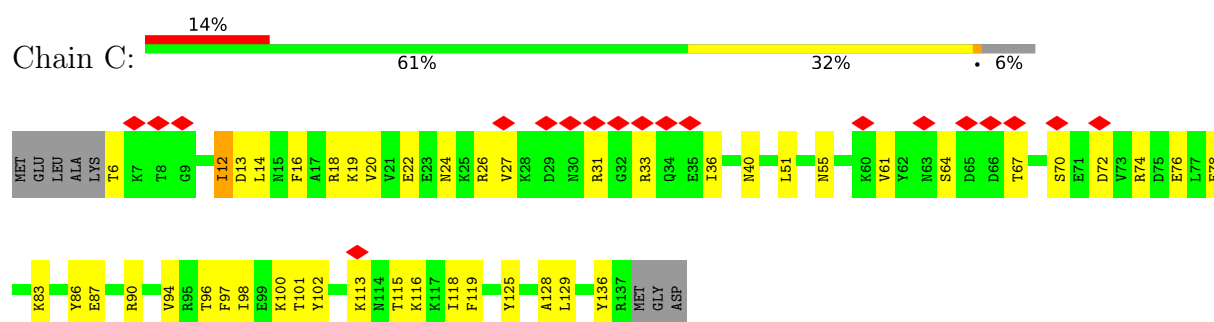
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP E6LHV7
A	-17	HIS	-	expression tag	UNP E6LHV7
A	-16	HIS	-	expression tag	UNP E6LHV7
A	-15	HIS	-	expression tag	UNP E6LHV7
A	-14	HIS	-	expression tag	UNP E6LHV7
A	-13	HIS	-	expression tag	UNP E6LHV7
A	-12	HIS	-	expression tag	UNP E6LHV7
A	-11	HIS	-	expression tag	UNP E6LHV7
A	-10	HIS	-	expression tag	UNP E6LHV7
A	-9	HIS	-	expression tag	UNP E6LHV7
A	-8	HIS	-	expression tag	UNP E6LHV7
A	-7	LEU	-	expression tag	UNP E6LHV7
A	-6	GLU	-	expression tag	UNP E6LHV7
A	-5	VAL	-	expression tag	UNP E6LHV7
A	-4	LEU	-	expression tag	UNP E6LHV7
A	-3	PHE	-	expression tag	UNP E6LHV7
A	-2	GLN	-	expression tag	UNP E6LHV7
A	-1	GLY	-	expression tag	UNP E6LHV7
A	0	PRO	-	expression tag	UNP E6LHV7
A	1	SER	-	expression tag	UNP E6LHV7

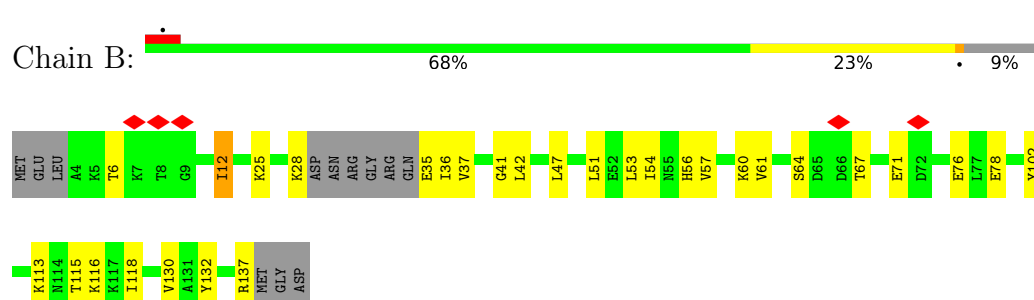
3 Residue-property plots [i](#)

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.

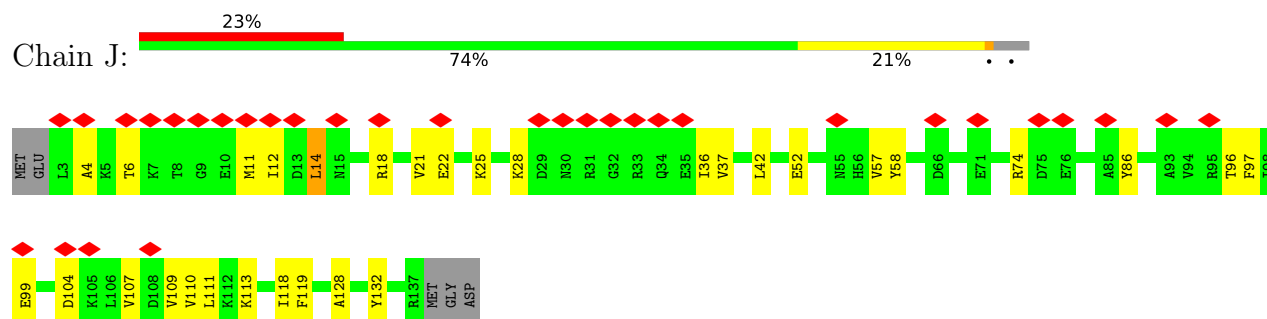
- Molecule 1: CRISPR system Cms protein Csm2



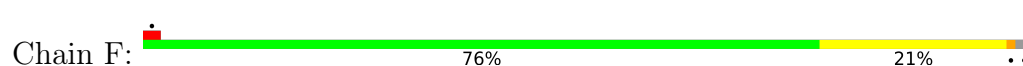
- Molecule 1: CRISPR system Cms protein Csm2

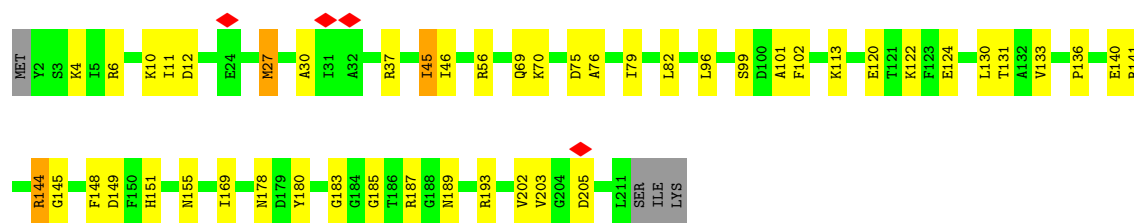


- Molecule 1: CRISPR system Cms protein Csm2

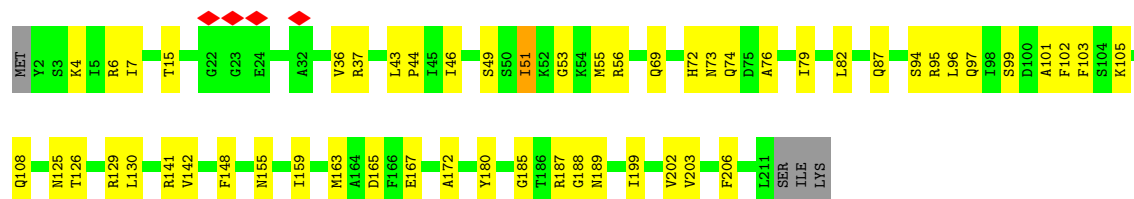


- Molecule 2: CRISPR system Cms endoribonuclease Csm3

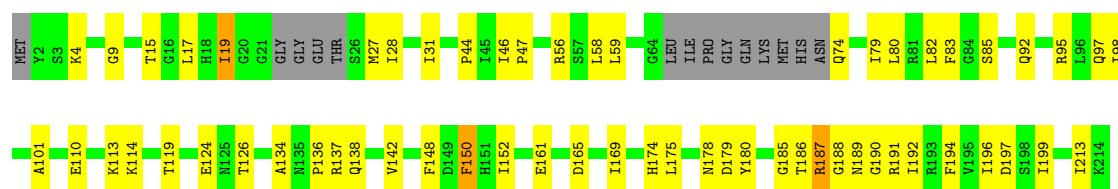




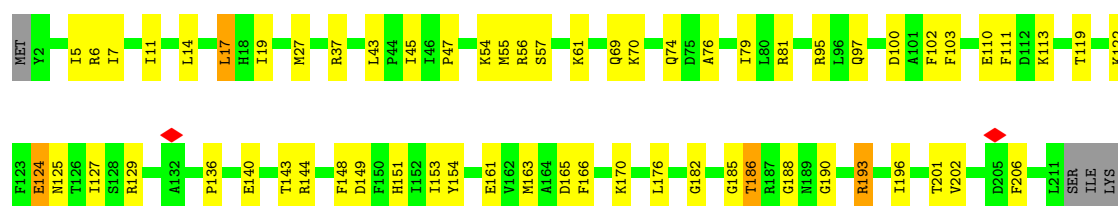
• Molecule 2: CRISPR system Cms endoribonuclease Csm3



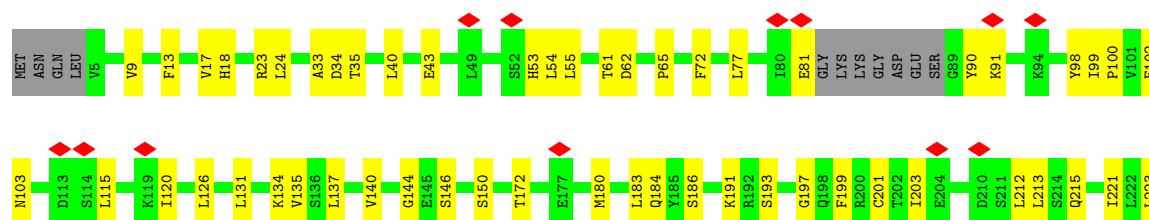
• Molecule 2: CRISPR system Cms endoribonuclease Csm3



• Molecule 2: CRISPR system Cms endoribonuclease Csm3



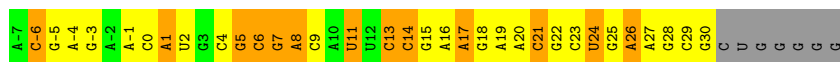
• Molecule 3: CRISPR system Cms protein Csm4





• Molecule 4: RNA (35-MER)

Chain R: 11% 44% 29% 16%



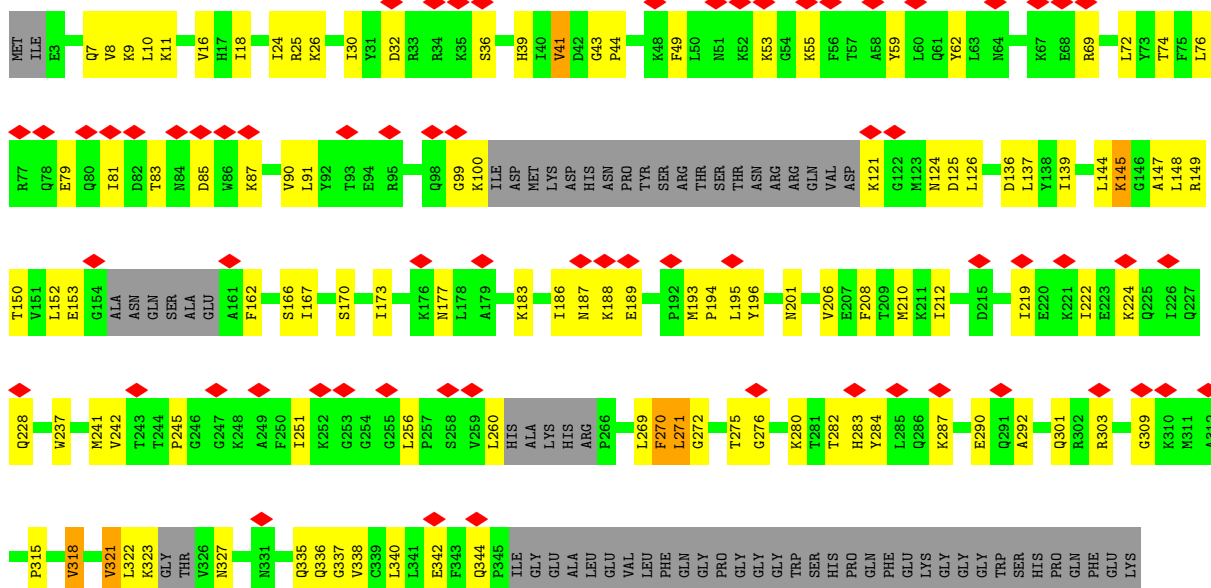
• Molecule 5: RNA (35-MER)

Chain T: 43% 30% 26%



• Molecule 6: CRISPR system Cms protein Csm5

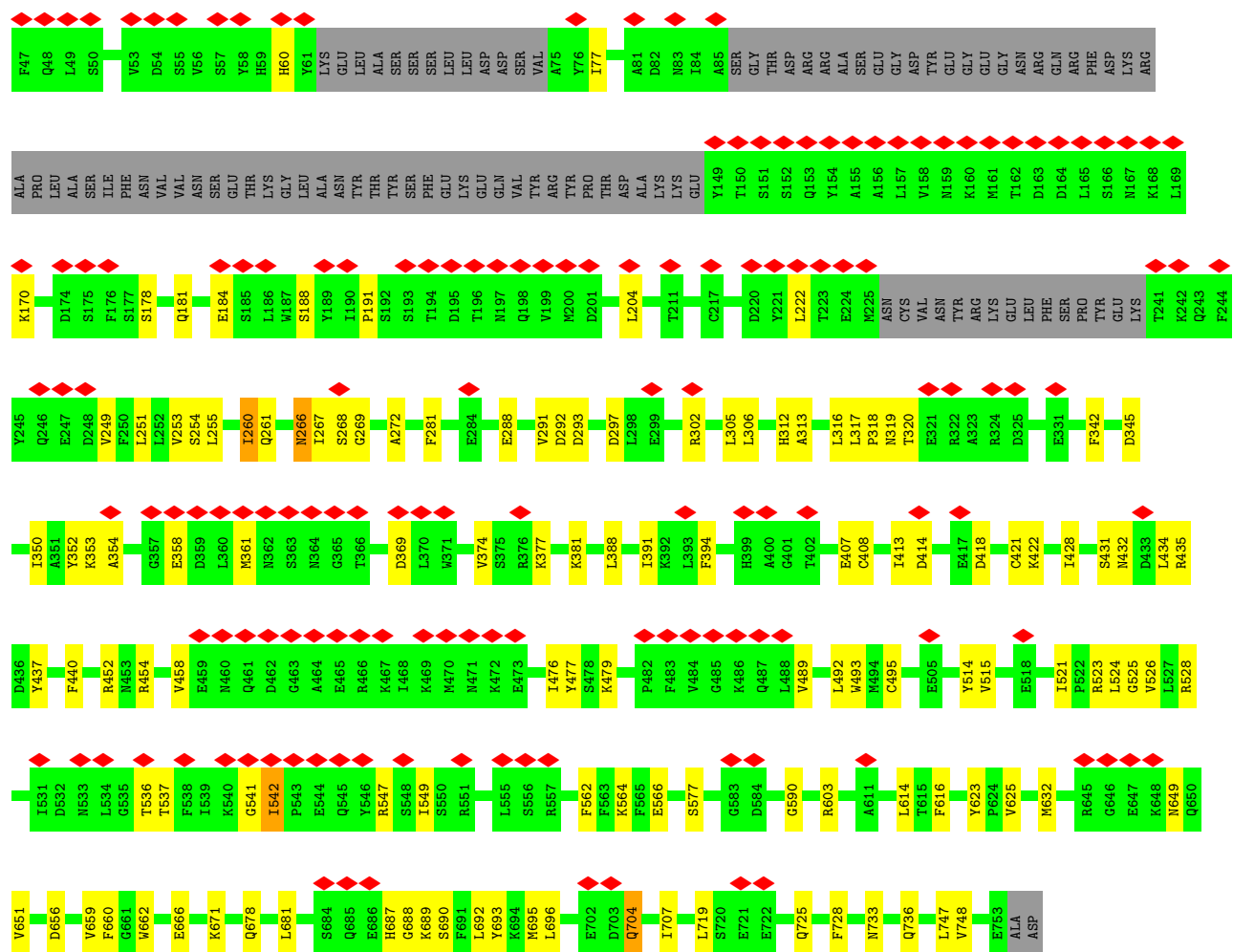
Chain H: 17% 53% 27% 18%



• Molecule 7: CRISPR system single-strand-specific deoxyribonuclease Cas10/Csm1 (subtype III-A)

Chain A: 23% 67% 17% 16%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78260	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66.51	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.774	Depositor
Minimum map value	-0.454	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.07	Depositor
Map size ($\text{\AA}$)	312.0, 312.0, 312.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.65, 0.65, 0.65	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.35	0/1081	0.51	0/1452
1	C	0.64	0/1119	0.90	0/1504
1	J	0.35	0/1141	0.51	0/1533
2	D	0.61	0/1570	0.86	1/2110 (0.0%)
2	E	0.42	0/1646	0.64	0/2216
2	F	0.29	0/1646	0.44	0/2216
2	I	0.55	0/1646	0.75	1/2216 (0.0%)
3	G	0.39	0/2389	0.56	0/3219
4	R	0.65	0/915	1.03	0/1426
5	T	0.68	0/824	0.90	0/1281
6	H	0.40	0/2565	0.59	1/3456 (0.0%)
7	A	0.37	0/5323	0.58	2/7178 (0.0%)
All	All	0.45	0/21865	0.67	5/29807 (0.0%)

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
2	D	0	1
2	F	0	1
2	I	0	1
All	All	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	186	THR	N-CA-C	-6.03	104.71	111.28
7	A	266	ASN	N-CA-C	-5.89	105.28	112.88
7	A	268	SER	N-CA-C	-5.67	105.10	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	270	PHE	N-CA-CB	-5.42	102.78	110.58
2	D	150	PHE	CA-CB-CG	5.37	119.17	113.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	187	ARG	Sidechain
2	F	144	ARG	Sidechain
2	I	193	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1065	0	1097	22	0
1	C	1102	0	1127	34	0
1	J	1124	0	1156	20	0
2	D	1548	0	1567	44	0
2	E	1620	0	1634	40	0
2	F	1620	0	1634	34	0
2	I	1620	0	1634	42	0
3	G	2341	0	2340	51	0
4	R	816	0	416	28	0
5	T	740	0	376	7	0
6	H	2510	0	2566	76	0
7	A	5227	0	5237	84	0
All	All	21333	0	20784	423	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 10.

All (423) 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:A:413:ILE:HG21	7:A:421:CYS:SG	1.63	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:413:ILE:CG2	7:A:421:CYS:SG	2.40	1.09
1:C:113:LYS:HG2	1:C:118:ILE:HG13	1.51	0.91
7:A:413:ILE:HG21	7:A:421:CYS:HG	1.12	0.86
3:G:281:GLY:HA3	3:G:299:LYS:HA	1.57	0.85
1:J:21:VAL:HG11	1:J:132:TYR:HB3	1.65	0.79
2:I:186:THR:HA	6:H:166:SER:HA	1.65	0.78
6:H:287:LYS:HB2	6:H:292:ALA:HB2	1.66	0.77
7:A:681:LEU:HD11	7:A:692:LEU:HD11	1.66	0.75
3:G:237:LEU:HD11	7:A:391:ILE:HD12	1.68	0.74
2:D:80:LEU:HG	2:D:85:SER:HB2	1.69	0.73
3:G:72:PHE:HB3	3:G:98:TYR:HB3	1.71	0.72
6:H:187:ASN:HB3	6:H:321:VAL:HG12	1.72	0.70
2:F:130:LEU:HD22	2:I:70:LYS:HA	1.73	0.70
3:G:134:LYS:HA	4:R:1:A:H5'	1.74	0.69
7:A:678:GLN:HG2	7:A:747:LEU:HD13	1.73	0.69
7:A:537:THR:O	7:A:541:GLY:N	2.25	0.69
6:H:99:GLY:HA2	6:H:327:ASN:HD21	1.59	0.68
1:C:61:VAL:HG11	1:C:119:PHE:HD2	1.59	0.68
2:F:46:ILE:HB	2:F:101:ALA:HB3	1.76	0.68
7:A:495:CYS:HB2	7:A:564:LYS:HA	1.74	0.68
1:J:74:ARG:NH1	1:J:111:LEU:O	2.27	0.67
6:H:30:ILE:HB	6:H:39:HIS:HB2	1.76	0.67
6:H:100:LYS:NZ	6:H:196:TYR:OH	2.27	0.67
3:G:287:SER:HB2	3:G:294:VAL:H	1.59	0.66
6:H:145:LYS:HE2	6:H:162:PHE:HB3	1.75	0.66
2:F:4:LYS:NZ	2:F:155:ASN:OD1	2.26	0.66
6:H:193:MET:HE3	6:H:195:LEU:HD13	1.76	0.66
2:F:4:LYS:HB2	2:F:203:VAL:HB	1.76	0.66
2:D:180:TYR:CG	2:D:185:GLY:HA3	2.31	0.66
5:T:41:C:H2'	5:T:42:A:C8	2.31	0.65
2:E:43:LEU:HD23	2:E:103:PHE:HB3	1.79	0.65
7:A:353:LYS:HB2	7:A:377:LYS:HE3	1.79	0.65
6:H:148:LEU:O	6:H:152:LEU:HB2	1.96	0.64
6:H:8:VAL:HB	6:H:208:PHE:HB2	1.78	0.64
7:A:269:GLY:HA2	7:A:272:ALA:HB2	1.78	0.64
6:H:186:ILE:HD12	6:H:322:LEU:HD23	1.79	0.64
2:I:69:GLN:NE2	2:I:74:GLN:O	2.30	0.64
7:A:452:ARG:HD2	7:A:454:ARG:HH12	1.63	0.64
2:E:49:SER:HB3	2:D:187:ARG:HB3	1.80	0.64
2:I:45:ILE:HD11	2:I:100:ASP:HB3	1.78	0.63
2:D:19:ILE:HG21	2:D:47:PRO:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:THR:O	1:B:116:LYS:N	2.31	0.62
1:B:28:LYS:O	1:B:35:GLU:N	2.32	0.62
7:A:18:LYS:HG2	7:A:22:ARG:HE	1.62	0.62
2:E:82:LEU:HD22	2:E:96:LEU:HG	1.82	0.62
2:E:99:SER:HA	2:D:188:GLY:HA2	1.82	0.62
2:I:129:ARG:HH12	6:H:149:ARG:HD3	1.63	0.62
2:D:74:GLN:HB2	2:D:79:ILE:HD11	1.80	0.62
6:H:260:LEU:HD21	6:H:340:LEU:HD12	1.80	0.61
6:H:147:ALA:HB1	6:H:269:LEU:HD11	1.82	0.61
1:C:51:LEU:O	1:C:55:ASN:ND2	2.33	0.61
6:H:270:PHE:HB3	6:H:275:THR:HG21	1.82	0.61
2:F:69:GLN:NE2	2:F:75:ASP:OD1	2.27	0.61
2:D:46:ILE:HB	2:D:101:ALA:HB3	1.83	0.61
2:I:129:ARG:HB3	6:H:282:THR:HG22	1.83	0.61
2:D:28:ILE:HG12	7:A:748:VAL:HG11	1.82	0.61
7:A:350:ILE:O	7:A:381:LYS:NZ	2.30	0.61
7:A:687:HIS:CD2	7:A:719:LEU:HD13	2.35	0.61
2:D:110:GLU:O	2:D:114:LYS:NZ	2.34	0.61
1:J:25:LYS:HZ2	1:J:36:ILE:HD12	1.66	0.61
7:A:306:LEU:HD11	7:A:316:LEU:HB2	1.83	0.61
7:A:434:LEU:O	7:A:479:LYS:NZ	2.31	0.61
2:D:4:LYS:NZ	3:G:186:SER:OG	2.26	0.60
2:I:5:ILE:HG12	2:I:201:THR:HG22	1.83	0.60
2:D:101:ALA:HB1	2:D:148:PHE:HB3	1.83	0.60
5:T:14:A:H1'	2:I:136:PRO:HG2	1.83	0.60
2:I:37:ARG:NH2	2:I:140:GLU:OE2	2.34	0.59
2:E:125:ASN:HD22	4:R:13:C:H4'	1.66	0.59
1:C:6:THR:HG23	1:C:102:TYR:CE2	2.36	0.59
6:H:24:ILE:HD11	6:H:126:LEU:HD23	1.84	0.59
2:F:70:LYS:HG2	2:E:130:LEU:HD22	1.85	0.59
2:E:102:PHE:HZ	2:D:15:THR:HG22	1.68	0.59
1:C:97:PHE:CE1	1:C:101:THR:HG21	2.38	0.58
2:D:98:ILE:HG23	2:D:152:ILE:HG12	1.86	0.58
6:H:62:TYR:OH	6:H:74:THR:OG1	2.18	0.58
7:A:515:VAL:HG11	7:A:625:VAL:HB	1.84	0.58
2:I:57:SER:O	2:I:61:LYS:HG2	2.03	0.58
7:A:358:GLU:HA	7:A:361:MET:HE2	1.85	0.58
7:A:437:TYR:HB2	7:A:458:VAL:HG12	1.86	0.58
3:G:137:LEU:HD23	3:G:146:SER:HB3	1.85	0.58
6:H:137:LEU:HB2	6:H:173:ILE:HB	1.84	0.58
7:A:525:GLY:N	7:A:590:GLY:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ARG:NH1	1:C:136:TYR:OH	2.37	0.58
6:H:30:ILE:HD11	6:H:76:LEU:HD12	1.86	0.57
6:H:276:GLY:HA2	6:H:323:LYS:HG3	1.86	0.57
1:C:86:TYR:CE2	1:C:90:ARG:HD2	2.39	0.57
7:A:537:THR:HG21	7:A:614:LEU:HD21	1.86	0.57
2:D:17:LEU:HD12	2:D:190:GLY:HA2	1.87	0.57
1:C:27:VAL:HA	1:C:36:ILE:HD13	1.87	0.57
3:G:17:VAL:HG12	3:G:197:GLY:HA2	1.84	0.57
6:H:9:LYS:HB2	6:H:342:GLU:HB3	1.87	0.57
2:E:46:ILE:HB	2:E:101:ALA:HB3	1.87	0.57
7:A:689:LYS:HE2	7:A:693:TYR:HE1	1.69	0.56
3:G:184:GLN:NE2	3:G:201:CYS:SG	2.71	0.56
4:R:-4:A:H2'	4:R:-3:G:C8	2.40	0.56
6:H:210:MET:HE1	6:H:219:ILE:HD13	1.87	0.56
2:F:27:MET:HG2	2:F:30:ALA:HB2	1.86	0.56
1:J:110:VAL:HG22	1:J:118:ILE:HG22	1.88	0.56
2:E:180:TYR:CG	2:E:185:GLY:HA3	2.41	0.56
3:G:65:PRO:HB3	3:G:126:LEU:HD13	1.88	0.56
2:I:37:ARG:NH2	2:I:119:THR:OG1	2.39	0.56
7:A:293:ASP:HB3	7:A:452:ARG:HE	1.71	0.56
2:E:56:ARG:NH2	2:E:72:HIS:O	2.39	0.55
4:R:21:C:H2'	4:R:22:G:C8	2.41	0.55
6:H:242:VAL:HG22	6:H:251:ILE:HD11	1.89	0.55
7:A:255:LEU:HG	7:A:313:ALA:HB3	1.88	0.55
2:D:185:GLY:HA2	2:D:189:ASN:O	2.05	0.55
1:J:28:LYS:HD3	1:J:37:VAL:HG21	1.87	0.55
1:C:20:VAL:O	1:C:24:ASN:ND2	2.28	0.55
1:J:113:LYS:HG2	1:J:118:ILE:HG13	1.89	0.55
3:G:9:VAL:HG13	3:G:203:ILE:HG12	1.89	0.55
2:F:99:SER:HA	2:E:188:GLY:HA2	1.88	0.55
2:I:11:ILE:N	2:I:148:PHE:O	2.30	0.55
2:I:14:LEU:HD21	2:I:193:ARG:HB2	1.89	0.55
2:E:69:GLN:HG3	2:E:74:GLN:HB2	1.89	0.55
1:C:14:LEU:HD12	1:B:78:GLU:HB3	1.88	0.54
1:B:47:LEU:HD22	1:B:130:VAL:HG22	1.89	0.54
2:F:82:LEU:HD22	2:F:96:LEU:HG	1.89	0.54
7:A:526:VAL:HG21	7:A:632:MET:HB3	1.89	0.54
7:A:342:PHE:HB3	7:A:345:ASP:HB2	1.90	0.54
2:E:141:ARG:NH1	2:E:189:ASN:OD1	2.37	0.54
6:H:7:GLN:N	6:H:344:GLN:O	2.37	0.54
7:A:603:ARG:HA	7:A:616:PHE:HE1	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:247:ARG:O	3:G:296:ARG:NH1	2.41	0.53
2:F:102:PHE:HZ	2:E:15:THR:HG22	1.73	0.53
3:G:135:VAL:HG22	4:R:1:A:H5''	1.90	0.53
7:A:413:ILE:HG23	7:A:421:CYS:SG	2.43	0.53
1:B:51:LEU:HA	1:B:54:ILE:HG22	1.89	0.53
7:A:666:GLU:HG2	7:A:671:LYS:HE2	1.90	0.53
2:I:122:LYS:NZ	2:I:124:GLU:OE1	2.41	0.53
7:A:178:SER:HA	7:A:181:GLN:HE21	1.74	0.53
7:A:414:ASP:HB3	7:A:422:LYS:HD2	1.90	0.53
1:B:113:LYS:HB3	1:B:118:ILE:HG21	1.90	0.53
2:E:180:TYR:CD1	2:E:185:GLY:HA3	2.44	0.53
3:G:228:ALA:HB1	3:G:232:GLU:HB2	1.91	0.53
6:H:283:HIS:HB2	6:H:287:LYS:HE3	1.90	0.52
2:D:27:MET:HE3	2:D:27:MET:HA	1.92	0.52
3:G:33:ALA:N	3:G:62:ASP:OD1	2.42	0.52
7:A:255:LEU:HB3	7:A:350:ILE:HG12	1.90	0.52
3:G:91:LYS:NZ	7:A:536:THR:OG1	2.41	0.52
2:F:124:GLU:HB3	4:R:19:A:OP2	2.10	0.52
2:D:44:PRO:HG3	2:D:119:THR:HG23	1.92	0.52
6:H:32:ASP:O	6:H:36:SER:N	2.43	0.52
6:H:41:VAL:HG12	6:H:90:VAL:HG22	1.91	0.52
1:C:61:VAL:HG11	1:C:119:PHE:CD2	2.41	0.52
2:E:4:LYS:NZ	2:E:155:ASN:OD1	2.42	0.52
2:D:124:GLU:HB2	2:D:137:ARG:HG3	1.91	0.52
5:T:8:C:N3	6:H:194:PRO:HD3	2.24	0.52
7:A:253:VAL:HG21	7:A:317:LEU:HD12	1.91	0.52
2:D:175:LEU:O	2:D:179:ASP:N	2.43	0.52
4:R:-4:A:H2'	4:R:-3:G:H8	1.74	0.52
7:A:267:ILE:HD12	7:A:272:ALA:HB1	1.92	0.51
3:G:61:THR:HG23	3:G:223:LEU:HB3	1.91	0.51
2:D:97:GLN:HB3	3:G:193:SER:HA	1.92	0.51
2:E:187:ARG:HD3	4:R:11:U:H5'	1.91	0.51
1:J:6:THR:HB	1:J:12:ILE:HD11	1.91	0.51
7:A:562:PHE:HA	7:A:566:GLU:HB3	1.93	0.51
1:B:28:LYS:HD3	1:B:37:VAL:HG21	1.93	0.51
1:B:115:THR:HG23	1:B:118:ILE:H	1.74	0.51
3:G:9:VAL:HG22	3:G:203:ILE:HG23	1.93	0.51
1:C:67:THR:O	1:C:116:LYS:N	2.43	0.51
6:H:315:PRO:HG2	6:H:318:VAL:HG22	1.92	0.51
3:G:100:PRO:HD2	3:G:103:ASN:HB2	1.92	0.51
2:I:127:ILE:HD13	6:H:280:LYS:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:35:THR:HG23	4:R:-6:C:H1'	1.92	0.51
2:I:144:ARG:HH12	6:H:136:ASP:HB2	1.76	0.51
2:F:131:THR:HB	2:F:133:VAL:HG12	1.93	0.50
6:H:11:LYS:HD3	6:H:340:LEU:HD22	1.93	0.50
6:H:139:ILE:HD12	6:H:206:VAL:HG11	1.92	0.50
1:J:58:TYR:HA	1:J:119:PHE:HE2	1.76	0.50
2:E:55:MET:HG2	2:E:172:ALA:HB1	1.93	0.50
2:E:76:ALA:H	2:E:79:ILE:HD12	1.75	0.50
2:D:113:LYS:O	2:D:114:LYS:HG2	2.11	0.50
6:H:188:LYS:HB3	6:H:245:PRO:HD2	1.94	0.50
4:R:4:C:H2'	4:R:5:G:H1'	1.94	0.50
6:H:144:LEU:HB3	6:H:167:ILE:HG21	1.94	0.50
1:C:67:THR:OG1	1:C:115:THR:OG1	2.30	0.50
1:J:42:LEU:HD22	1:J:97:PHE:HB2	1.94	0.50
6:H:301:GLN:HG3	6:H:309:GLY:HA2	1.94	0.50
3:G:131:LEU:HD11	3:G:150:SER:HB3	1.92	0.49
7:A:476:ILE:HB	7:A:489:VAL:HG12	1.92	0.49
7:A:521:ILE:HG12	7:A:523:ARG:HG2	1.95	0.49
7:A:623:TYR:HB2	7:A:632:MET:HE2	1.94	0.49
2:F:205:ASP:OD1	2:F:205:ASP:N	2.45	0.49
6:H:152:LEU:HD11	6:H:222:ILE:HA	1.94	0.49
7:A:514:TYR:OH	7:A:577:SER:OG	2.12	0.49
6:H:270:PHE:CE2	6:H:338:VAL:HG22	2.47	0.49
1:C:19:LYS:HA	1:C:22:GLU:HG2	1.95	0.49
2:I:81:ARG:NH1	2:I:165:ASP:OD1	2.37	0.49
7:A:651:VAL:HG12	7:A:660:PHE:O	2.12	0.49
3:G:226:ALA:O	3:G:269:PHE:N	2.44	0.49
2:F:11:ILE:N	2:F:148:PHE:O	2.37	0.49
1:C:78:GLU:HB3	1:J:14:LEU:HD23	1.94	0.49
2:F:180:TYR:CD1	2:F:185:GLY:HA3	2.48	0.48
2:E:6:ARG:HB2	2:E:202:VAL:HG23	1.95	0.48
1:J:86:TYR:HE2	6:H:25:ARG:HD2	1.78	0.48
2:D:169:ILE:HG21	2:D:213:ILE:HD12	1.95	0.48
3:G:228:ALA:HB2	3:G:279:PHE:CD1	2.48	0.48
2:I:97:GLN:HB2	2:I:153:ILE:HB	1.96	0.48
6:H:224:LYS:O	6:H:228:GLN:HG2	2.13	0.48
7:A:318:PRO:HB2	7:A:320:THR:HG22	1.95	0.48
3:G:34:ASP:HA	3:G:297:TYR:HB3	1.95	0.48
2:I:43:LEU:HD23	2:I:103:PHE:HB3	1.95	0.48
2:I:110:GLU:HA	2:I:113:LYS:HE2	1.95	0.48
6:H:275:THR:HG22	6:H:336:GLN:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:275:THR:HG22	6:H:337:GLY:HA3	1.96	0.48
1:C:94:VAL:O	1:C:98:ILE:HG12	2.14	0.48
4:R:24:U:H5'	2:I:125:ASN:O	2.14	0.48
2:D:9:GLY:HA3	2:D:150:PHE:CE2	2.48	0.48
6:H:275:THR:CG2	6:H:337:GLY:HA3	2.43	0.48
2:D:136:PRO:HB3	4:R:7:G:N1	2.28	0.47
6:H:26:LYS:HE2	6:H:69:ARG:HA	1.95	0.47
2:E:53:GLY:HA3	4:R:6:C:O4'	2.13	0.47
2:D:56:ARG:HH11	2:D:83:PHE:HB2	1.78	0.47
7:A:431:SER:HA	7:A:434:LEU:HD23	1.95	0.47
1:C:61:VAL:O	1:C:64:SER:OG	2.23	0.47
2:E:99:SER:OG	2:D:191:ARG:NH1	2.46	0.47
7:A:254:SER:HB2	7:A:312:HIS:HE1	1.80	0.47
6:H:49:PHE:CZ	6:H:85:ASP:HB3	2.49	0.47
7:A:524:LEU:HD23	7:A:632:MET:HE1	1.96	0.47
2:E:187:ARG:NH1	4:R:11:U:OP2	2.48	0.47
3:G:180:MET:O	3:G:184:GLN:HG3	2.13	0.47
1:J:57:VAL:HG13	1:J:119:PHE:HZ	1.79	0.47
6:H:270:PHE:HB3	6:H:275:THR:CG2	2.44	0.47
7:A:260:ILE:H	7:A:260:ILE:HG13	1.46	0.47
3:G:115:LEU:HD23	3:G:115:LEU:H	1.78	0.47
2:D:126:THR:OG1	4:R:5:G:H2'	2.14	0.47
1:C:16:PHE:HA	1:C:19:LYS:HG2	1.97	0.47
1:B:25:LYS:HZ3	1:B:36:ILE:HG23	1.79	0.47
2:F:141:ARG:NH1	2:F:189:ASN:OD1	2.37	0.47
2:E:105:LYS:HA	2:E:108:GLN:HB2	1.97	0.46
7:A:353:LYS:HB3	7:A:374:VAL:HG22	1.97	0.46
1:B:12:ILE:HD12	1:B:106:LEU:HD11	1.96	0.46
5:T:9:G:H5''	6:H:125:ASP:CG	2.40	0.46
7:A:413:ILE:CG2	7:A:421:CYS:HG	2.02	0.46
1:J:11:MET:SD	1:J:11:MET:N	2.76	0.46
1:C:87:GLU:HB3	1:C:94:VAL:HG11	1.97	0.46
2:F:136:PRO:HB3	4:R:19:A:C6	2.51	0.46
7:A:22:ARG:HH12	7:A:191:PRO:HG2	1.79	0.46
7:A:432:ASN:OD1	7:A:435:ARG:NH2	2.48	0.46
1:J:58:TYR:HA	1:J:119:PHE:CE2	2.51	0.46
7:A:251:LEU:HG	7:A:319:ASN:HA	1.97	0.46
1:B:61:VAL:O	1:B:64:SER:OG	2.30	0.46
3:G:183:LEU:HA	3:G:186:SER:HB2	1.98	0.46
2:I:55:MET:HG3	2:I:176:LEU:HD22	1.98	0.46
2:F:76:ALA:HB3	2:F:79:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:55:LEU:HD22	3:G:283:ILE:HG21	1.98	0.46
4:R:8:A:H2'	4:R:9:C:C6	2.51	0.46
2:E:203:VAL:HG22	2:D:174:HIS:CE1	2.51	0.46
3:G:43:GLU:OE2	3:G:186:SER:OG	2.33	0.46
6:H:41:VAL:HA	6:H:91:LEU:H	1.81	0.46
3:G:77:LEU:HD12	3:G:273:SER:HA	1.97	0.45
2:I:76:ALA:HB3	2:I:79:ILE:HD13	1.97	0.45
6:H:335:GLN:HG3	6:H:338:VAL:HG21	1.97	0.45
7:A:418:ASP:OD1	7:A:418:ASP:N	2.44	0.45
7:A:15:ASP:HB3	7:A:204:LEU:HD11	1.99	0.45
1:C:6:THR:HG23	1:C:102:TYR:HE2	1.79	0.45
3:G:223:LEU:HB2	3:G:301:PHE:HB3	1.99	0.45
1:J:104:ASP:HA	1:J:107:VAL:HG12	1.98	0.45
7:A:493:TRP:O	7:A:564:LYS:HD2	2.17	0.45
2:D:59:LEU:HD12	2:D:83:PHE:HE2	1.81	0.45
2:D:85:SER:HB3	2:D:92:GLN:HB2	1.99	0.45
2:F:12:ASP:OD2	2:F:193:ARG:NH1	2.50	0.45
7:A:733:ASN:HB3	7:A:736:GLN:HB2	1.98	0.45
7:A:434:LEU:HA	7:A:458:VAL:HG11	1.98	0.45
2:I:95:ARG:O	2:I:154:TYR:HA	2.16	0.45
2:I:111:PHE:HE2	2:I:143:THR:HB	1.82	0.45
6:H:18:ILE:HD11	6:H:271:LEU:HD13	1.97	0.45
2:F:102:PHE:CZ	2:E:15:THR:HG22	2.52	0.45
3:G:23:ARG:NH2	7:A:266:ASN:O	2.50	0.45
2:I:17:LEU:HD12	2:I:190:GLY:HA2	1.97	0.45
7:A:542:ILE:O	7:A:547:ARG:NH2	2.50	0.45
2:F:144:ARG:HG2	2:F:145:GLY:N	2.32	0.45
7:A:421:CYS:SG	7:A:422:LYS:N	2.89	0.45
7:A:695:MET:HE2	7:A:695:MET:HB3	1.62	0.45
1:C:26:ARG:NH2	1:C:40:ASN:H	2.15	0.45
1:B:6:THR:HG22	1:B:102:TYR:CD2	2.52	0.45
1:B:104:ASP:OD1	1:B:104:ASP:N	2.49	0.45
2:E:95:ARG:NH1	2:E:165:ASP:OD2	2.49	0.45
6:H:53:LYS:HB3	6:H:55:LYS:HD3	1.98	0.45
6:H:290:GLU:CD	6:H:290:GLU:H	2.24	0.45
6:H:24:ILE:HG13	6:H:126:LEU:HB3	1.98	0.44
7:A:656:ASP:O	7:A:659:VAL:HG23	2.18	0.44
2:D:82:LEU:HD21	2:D:165:ASP:HB3	1.98	0.44
2:F:180:TYR:CG	2:F:185:GLY:HA3	2.51	0.44
7:A:34:SER:HB3	7:A:60:HIS:HB2	1.99	0.44
2:D:98:ILE:HG12	2:D:152:ILE:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:77:ILE:HD11	7:A:222:LEU:HD12	1.99	0.44
2:F:70:LYS:HA	2:E:130:LEU:HB2	1.99	0.44
2:E:142:VAL:HG11	2:E:148:PHE:CZ	2.52	0.44
4:R:26:A:H2'	4:R:27:A:C8	2.52	0.44
6:H:241:MET:HE2	6:H:322:LEU:HB2	1.99	0.44
7:A:291:VAL:HG11	7:A:305:LEU:HD22	1.99	0.44
3:G:267:TYR:CD1	7:A:394:PHE:HB3	2.53	0.44
7:A:253:VAL:HG22	7:A:352:TYR:HB3	2.00	0.44
7:A:260:ILE:HD12	7:A:261:GLN:H	1.82	0.44
2:E:202:VAL:HG11	2:D:178:ASN:HD21	1.82	0.44
7:A:288:GLU:HG3	7:A:492:LEU:HD21	2.00	0.44
2:E:126:THR:HG23	4:R:11:U:H1'	2.00	0.44
3:G:13:PHE:CD2	3:G:199:PHE:HB3	2.53	0.44
2:I:6:ARG:HE	2:I:202:VAL:HG21	1.83	0.44
2:I:201:THR:HG21	2:I:206:PHE:HB3	1.99	0.44
1:J:4:ALA:HB2	1:J:109:VAL:HG11	1.99	0.44
6:H:183:LYS:HB3	6:H:195:LEU:HD22	1.98	0.44
7:A:688:GLY:O	7:A:689:LYS:C	2.61	0.44
1:B:71:GLU:H	1:B:71:GLU:CD	2.26	0.44
3:G:81:GLU:O	3:G:90:TYR:OH	2.36	0.44
4:R:27:A:H1'	6:H:303:ARG:HH22	1.83	0.44
7:A:688:GLY:C	7:A:690:SER:N	2.75	0.44
2:E:94:SER:HB3	2:D:186:THR:HG21	1.99	0.43
1:B:53:LEU:O	1:B:57:VAL:HG23	2.18	0.43
3:G:191:LYS:HA	3:G:191:LYS:HD3	1.67	0.43
2:E:37:ARG:HA	2:E:44:PRO:HA	2.01	0.43
4:R:24:U:C4	6:H:280:LYS:HD3	2.52	0.43
2:E:51:ILE:H	2:E:51:ILE:HG13	1.61	0.43
3:G:18:HIS:CE1	3:G:24:LEU:HD12	2.53	0.43
3:G:134:LYS:HB3	4:R:1:A:OP2	2.19	0.43
1:C:125:TYR:CE2	1:C:129:LEU:HD11	2.54	0.43
2:F:37:ARG:NH1	2:F:140:GLU:OE2	2.51	0.43
2:I:129:ARG:NE	6:H:150:THR:OG1	2.51	0.43
6:H:10:LEU:HB3	6:H:206:VAL:HB	2.01	0.43
1:B:56:HIS:O	1:B:60:LYS:HG2	2.18	0.43
1:B:102:TYR:O	1:B:106:LEU:HG	2.17	0.43
2:F:149:ASP:OD1	2:F:149:ASP:N	2.51	0.43
3:G:18:HIS:NE2	3:G:24:LEU:O	2.52	0.43
7:A:440:PHE:HB2	7:A:477:TYR:HB2	2.01	0.43
1:B:37:VAL:HG13	1:B:41:GLY:H	1.83	0.43
2:E:97:GLN:HA	2:D:186:THR:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:277:GLN:NE2	3:G:278:LYS:O	2.51	0.43
6:H:43:GLY:N	6:H:44:PRO:HD2	2.34	0.43
7:A:297:ASP:OD2	7:A:452:ARG:NH2	2.52	0.43
7:A:407:GLU:H	7:A:407:GLU:HG2	1.58	0.43
2:I:149:ASP:OD1	2:I:149:ASP:N	2.46	0.43
6:H:16:VAL:HG13	6:H:272:GLY:HA3	2.01	0.43
6:H:177:ASN:C	6:H:201:ASN:HD22	2.27	0.43
2:F:96:LEU:HD11	2:F:169:ILE:HG12	2.01	0.43
2:I:27:MET:HE2	2:I:27:MET:HB3	1.88	0.43
1:J:14:LEU:HD12	1:J:128:ALA:HB2	2.01	0.42
1:C:96:THR:O	1:C:100:LYS:HG2	2.19	0.42
3:G:53:HIS:NE2	3:G:172:THR:OG1	2.40	0.42
6:H:16:VAL:HG13	6:H:272:GLY:CA	2.49	0.42
6:H:83:THR:O	6:H:87:LYS:HG2	2.19	0.42
2:I:185:GLY:C	2:I:188:GLY:H	2.28	0.42
6:H:139:ILE:N	6:H:170:SER:OG	2.47	0.42
7:A:170:LYS:HE2	7:A:170:LYS:HB2	1.87	0.42
4:R:4:C:H2'	4:R:5:G:C1'	2.50	0.42
5:T:14:A:H8	5:T:14:A:H5''	1.83	0.42
3:G:255:THR:O	3:G:291:ARG:NE	2.53	0.42
3:G:100:PRO:HD3	3:G:120:ILE:HG23	2.00	0.42
1:C:70:SER:O	1:C:74:ARG:HG3	2.20	0.42
1:C:115:THR:HG23	1:C:118:ILE:H	1.85	0.42
2:E:7:ILE:HG23	2:E:199:ILE:HG12	2.02	0.42
3:G:140:VAL:HA	3:G:144:GLY:O	2.20	0.42
2:I:196:ILE:H	2:I:196:ILE:HG13	1.73	0.42
6:H:59:TYR:CZ	6:H:72:LEU:HD13	2.55	0.42
2:E:159:ILE:HG23	2:E:206:PHE:HE1	1.85	0.42
3:G:234:VAL:HG22	7:A:388:LEU:HD21	2.02	0.42
1:J:96:THR:O	1:J:99:GLU:HG3	2.19	0.42
1:B:42:LEU:O	1:B:137:ARG:NH2	2.52	0.41
2:F:122:LYS:HZ1	2:I:47:PRO:HB3	1.84	0.41
2:D:126:THR:O	2:D:134:ALA:HA	2.20	0.41
3:G:40:LEU:HB3	3:G:54:LEU:HD21	2.02	0.41
1:C:31:ARG:HH11	1:C:33:ARG:HH22	1.68	0.41
1:J:22:GLU:HA	1:J:25:LYS:HB3	2.02	0.41
7:A:32:THR:HA	7:A:60:HIS:CD2	2.55	0.41
7:A:292:ASP:OD1	7:A:302:ARG:NH1	2.53	0.41
6:H:275:THR:O	6:H:323:LYS:HB2	2.20	0.41
2:I:163:MET:SD	2:I:163:MET:N	2.93	0.41
2:F:187:ARG:NH1	4:R:17:A:OP2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:237:TRP:HB2	6:H:284:TYR:CE2	2.54	0.41
1:C:13:ASP:N	1:C:16:PHE:HB3	2.35	0.41
1:C:26:ARG:HH22	1:C:40:ASN:H	1.67	0.41
2:F:144:ARG:HD3	2:I:102:PHE:CE1	2.55	0.41
2:E:163:MET:O	2:E:167:GLU:HG2	2.21	0.41
2:I:5:ILE:HA	2:I:201:THR:HA	2.02	0.41
2:I:7:ILE:HD11	2:I:166:PHE:CE2	2.55	0.41
1:B:110:VAL:HG13	1:B:118:ILE:HG23	2.03	0.41
2:F:99:SER:HB3	2:F:151:HIS:O	2.21	0.41
1:C:14:LEU:HD22	1:C:128:ALA:HB2	2.03	0.41
4:R:16:A:O3'	2:I:56:ARG:NH1	2.54	0.41
1:J:18:ARG:O	1:J:21:VAL:HG12	2.21	0.41
6:H:100:LYS:HB3	6:H:121:LYS:HD2	2.02	0.41
6:H:187:ASN:ND2	6:H:189:GLU:OE1	2.54	0.41
7:A:184:GLU:O	7:A:188:SER:OG	2.33	0.41
1:C:72:ASP:O	1:C:76:GLU:HG2	2.21	0.41
1:B:113:LYS:HE2	1:B:113:LYS:HB2	1.93	0.41
2:F:56:ARG:HG2	2:E:129:ARG:HH22	1.86	0.41
2:D:31:ILE:HA	2:D:138:GLN:HB2	2.03	0.41
3:G:288:ASP:N	3:G:288:ASP:OD1	2.54	0.41
6:H:186:ILE:HB	6:H:322:LEU:HB3	2.03	0.41
7:A:649:ASN:ND2	7:A:662:TRP:HD1	2.19	0.41
2:D:142:VAL:HG11	2:D:148:PHE:CZ	2.55	0.41
2:D:196:ILE:HG21	2:D:199:ILE:HD11	2.01	0.41
3:G:297:TYR:CZ	3:G:299:LYS:HB2	2.56	0.41
4:R:14:C:H2'	4:R:15:G:C8	2.56	0.41
5:T:9:G:O5'	6:H:124:ASN:HB3	2.21	0.41
2:I:19:ILE:HG12	2:I:182:GLY:HA3	2.03	0.41
7:A:251:LEU:HD23	7:A:354:ALA:HA	2.03	0.41
7:A:696:LEU:HD12	7:A:696:LEU:HA	1.88	0.41
2:D:58:LEU:HD21	2:D:179:ASP:OD2	2.21	0.40
5:T:38:U:H3'	5:T:39:G:H8	1.86	0.40
6:H:193:MET:HE3	6:H:193:MET:HB2	1.79	0.40
2:F:45:ILE:HD11	2:F:102:PHE:CE1	2.57	0.40
2:F:183:GLY:HA2	4:R:14:C:H5'	2.03	0.40
2:E:73:ASN:HB3	2:E:87:GLN:HG2	2.03	0.40
2:D:142:VAL:HG11	2:D:148:PHE:CE1	2.56	0.40
3:G:13:PHE:CD2	3:G:17:VAL:HG11	2.56	0.40
4:R:28:G:OP2	6:H:323:LYS:HE3	2.22	0.40
2:I:170:LYS:HD3	2:I:170:LYS:HA	1.86	0.40
6:H:79:GLU:HB3	6:H:81:ILE:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ASP:H	1:C:16:PHE:HB3	1.85	0.40
1:C:61:VAL:HG22	1:C:116:LYS:HG3	2.03	0.40
1:B:132:TYR:HE1	7:A:728:PHE:HZ	1.70	0.40
2:F:6:ARG:HE	2:F:202:VAL:HG21	1.87	0.40
2:D:74:GLN:HB2	2:D:79:ILE:CD1	2.49	0.40
2:D:95:ARG:NH2	2:D:161:GLU:OE1	2.43	0.40
7:A:704:GLN:HG2	7:A:707:ILE:HD12	2.03	0.40
1:C:12:ILE:HD13	1:C:16:PHE:CE2	2.57	0.40
2:D:150:PHE:CE2	2:D:194:PHE:HD1	2.38	0.40
3:G:221:ILE:HG13	3:G:274:THR:HG22	2.03	0.40
1:C:83:LYS:HD3	1:C:83:LYS:HA	1.99	0.40
2:I:6:ARG:HG3	2:I:151:HIS:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	124/140 (89%)	123 (99%)	1 (1%)	0	100	100
1	C	130/140 (93%)	129 (99%)	1 (1%)	0	100	100
1	J	133/140 (95%)	129 (97%)	4 (3%)	0	100	100
2	D	194/214 (91%)	189 (97%)	5 (3%)	0	100	100
2	E	208/214 (97%)	204 (98%)	4 (2%)	0	100	100
2	F	208/214 (97%)	204 (98%)	4 (2%)	0	100	100
2	I	208/214 (97%)	201 (97%)	7 (3%)	0	100	100
3	G	292/307 (95%)	289 (99%)	3 (1%)	0	100	100
6	H	300/379 (79%)	294 (98%)	6 (2%)	0	100	100
7	A	643/774 (83%)	632 (98%)	11 (2%)	0	100	100
All	All	2440/2736 (89%)	2394 (98%)	46 (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	B	118/128 (92%)	116 (98%)	2 (2%)	53	82
1	C	122/128 (95%)	121 (99%)	1 (1%)	73	90
1	J	124/128 (97%)	122 (98%)	2 (2%)	55	83
2	D	169/180 (94%)	166 (98%)	3 (2%)	51	80
2	E	176/180 (98%)	174 (99%)	2 (1%)	65	88
2	F	176/180 (98%)	170 (97%)	6 (3%)	32	66
2	I	176/180 (98%)	172 (98%)	4 (2%)	44	76
3	G	253/262 (97%)	248 (98%)	5 (2%)	48	78
6	H	274/330 (83%)	266 (97%)	8 (3%)	37	71
7	A	582/688 (85%)	571 (98%)	11 (2%)	50	79
All	All	2170/2384 (91%)	2126 (98%)	44 (2%)	48	78

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	12	ILE
1	B	12	ILE
1	B	76	GLU
2	F	10	LYS
2	F	27	MET
2	F	45	ILE
2	F	113	LYS
2	F	120	GLU
2	F	178	ASN
2	E	36	VAL
2	E	51	ILE
2	D	19	ILE
2	D	192	ILE
2	D	197	ASP

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Mol	Chain	Res	Type
3	G	99	ILE
3	G	102	GLU
3	G	212	LEU
3	G	213	LEU
3	G	215	GLN
2	I	17	LEU
2	I	54	LYS
2	I	124	GLU
2	I	161	GLU
1	J	14	LEU
1	J	52	GLU
6	H	41	VAL
6	H	145	LYS
6	H	153	GLU
6	H	212	ILE
6	H	256	LEU
6	H	271	LEU
6	H	318	VAL
6	H	321	VAL
7	A	249	VAL
7	A	260	ILE
7	A	281	PHE
7	A	369	ASP
7	A	408	CYS
7	A	428	ILE
7	A	528	ARG
7	A	542	ILE
7	A	549	ILE
7	A	704	GLN
7	A	725	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	34	GLN
1	C	40	ASN
1	C	49	ASN
1	C	55	ASN
1	B	15	ASN
1	B	49	ASN
1	B	55	ASN
2	F	92	GLN

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Mol	Chain	Res	Type
2	F	160	ASN
2	E	69	GLN
2	E	97	GLN
2	E	125	ASN
2	D	62	HIS
2	D	92	GLN
2	D	97	GLN
2	D	125	ASN
2	D	155	ASN
2	D	178	ASN
3	G	57	ASN
3	G	67	ASN
3	G	184	GLN
3	G	215	GLN
3	G	289	ASN
2	I	92	GLN
2	I	178	ASN
1	J	24	ASN
1	J	49	ASN
6	H	78	GLN
6	H	80	GLN
6	H	84	ASN
6	H	124	ASN
6	H	177	ASN
6	H	187	ASN
7	A	246	GLN
7	A	304	ASN
7	A	364	ASN
7	A	399	HIS
7	A	491	ASN
7	A	678	GLN
7	A	701	ASN
7	A	706	ASN
7	A	750	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	R	37/45 (82%)	22 (59%)	8 (21%)
5	T	34/47 (72%)	8 (23%)	2 (5%)
All	All	71/92 (77%)	30 (42%)	10 (14%)

All (30) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	R	-6	C
4	R	-1	A
4	R	0	C
4	R	1	A
4	R	2	U
4	R	5	G
4	R	6	C
4	R	7	G
4	R	8	A
4	R	11	U
4	R	13	C
4	R	14	C
4	R	17	A
4	R	18	G
4	R	20	A
4	R	21	C
4	R	23	C
4	R	24	U
4	R	25	G
4	R	26	A
4	R	29	C
4	R	30	G
5	T	12	U
5	T	14	A
5	T	15	G
5	T	21	U
5	T	27	A
5	T	32	G
5	T	33	C
5	T	36	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	R	-5	G
4	R	-1	A
4	R	1	A
4	R	7	G
4	R	17	A
4	R	23	C
4	R	25	G
4	R	29	C

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Mol	Chain	Res	Type
5	T	11	U
5	T	32	G

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](#)

There are no ligands in this entry.

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.

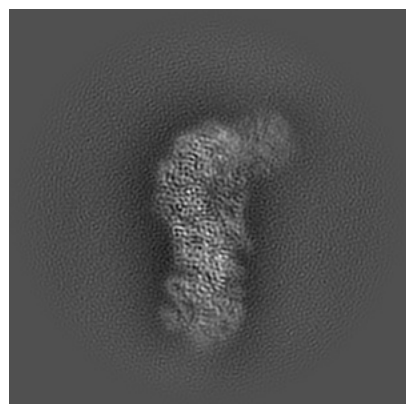
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51148. These allow visual inspection of the internal detail of the map and identification of artifacts.

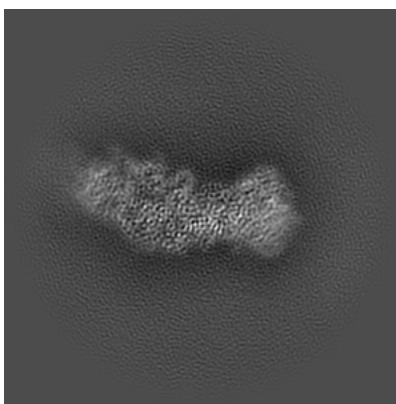
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

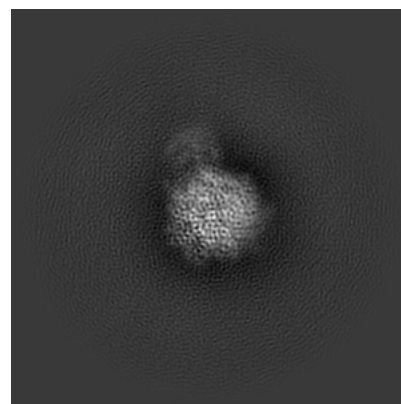
6.1.1 Primary map



X

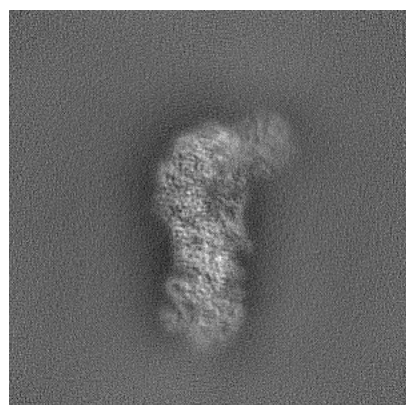


Y

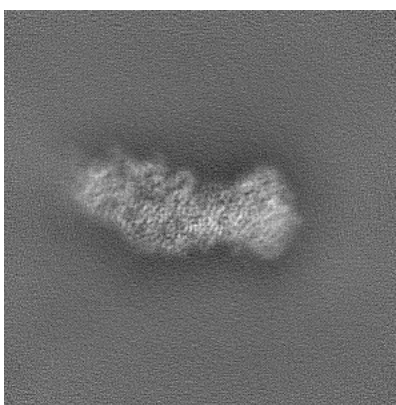


Z

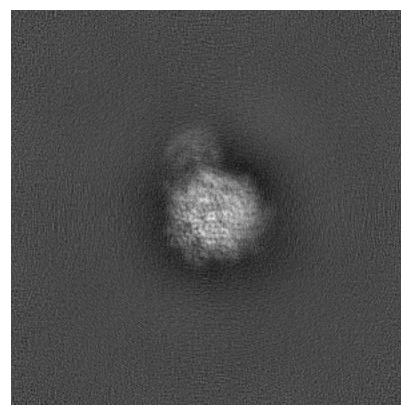
6.1.2 Raw map



X



Y

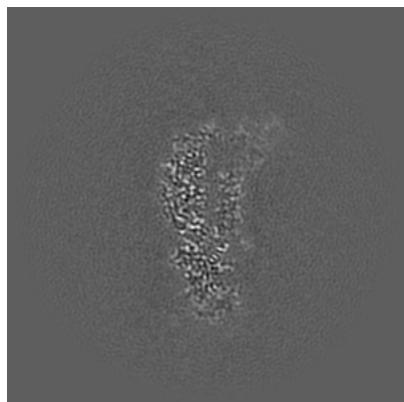


Z

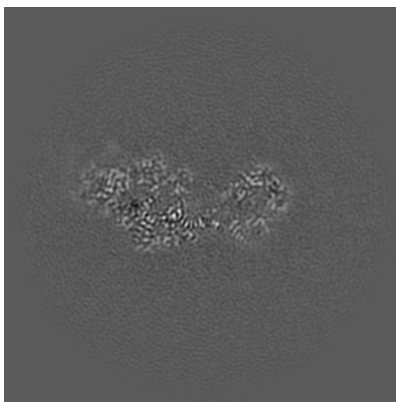
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

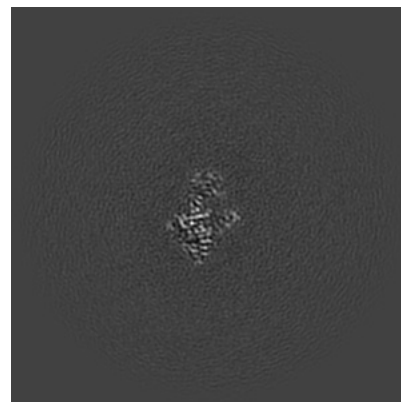
6.2.1 Primary map



X Index: 240

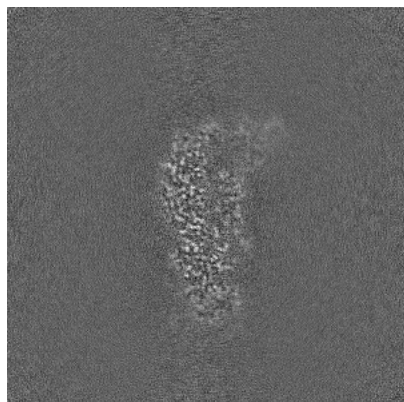


Y Index: 240

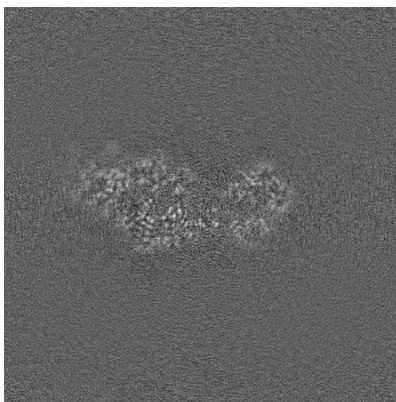


Z Index: 240

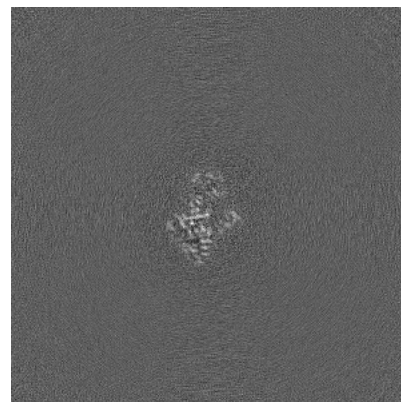
6.2.2 Raw map



X Index: 240



Y Index: 240

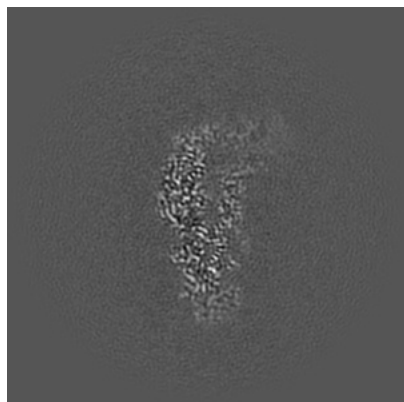


Z Index: 240

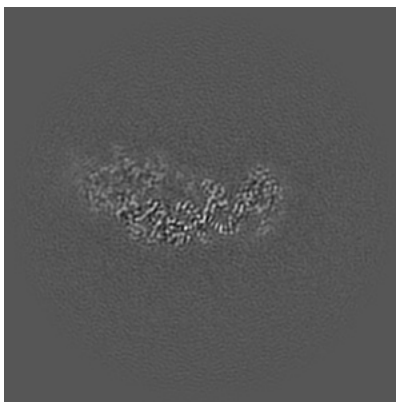
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

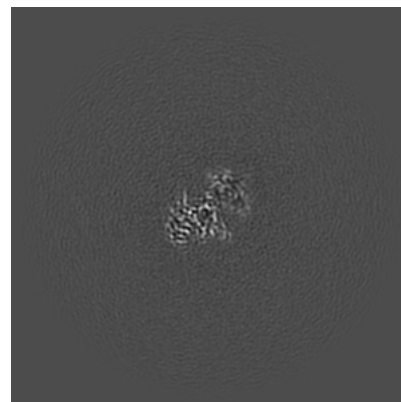
6.3.1 Primary map



X Index: 237

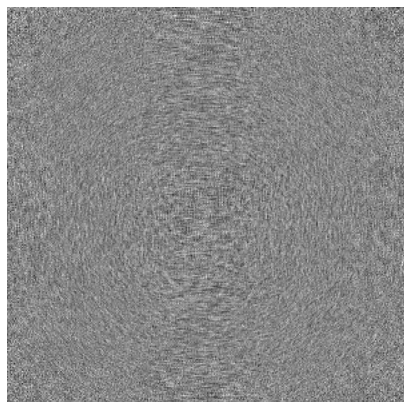


Y Index: 229

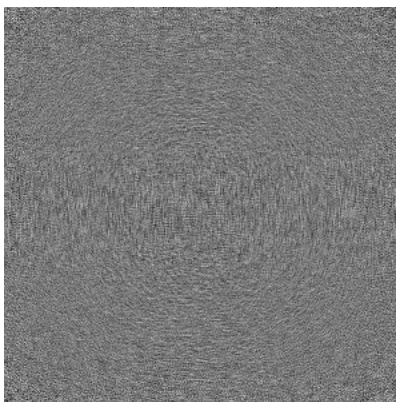


Z Index: 210

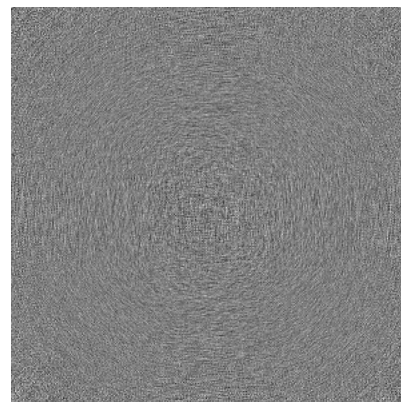
6.3.2 Raw map



X Index: 0



Y Index: 0

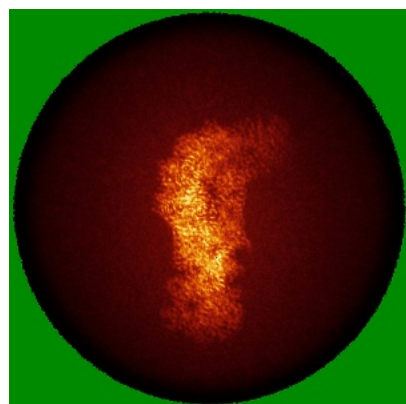


Z Index: 0

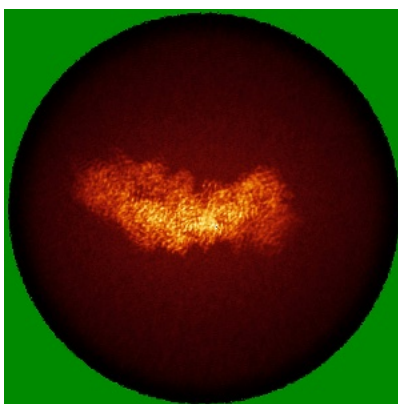
The images above show the largest variance slices of the map in three orthogonal directions.

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

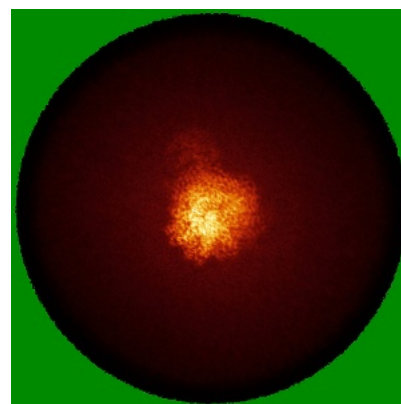
6.4.1 Primary map



X

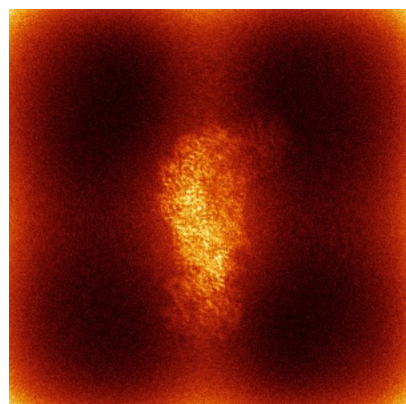


Y

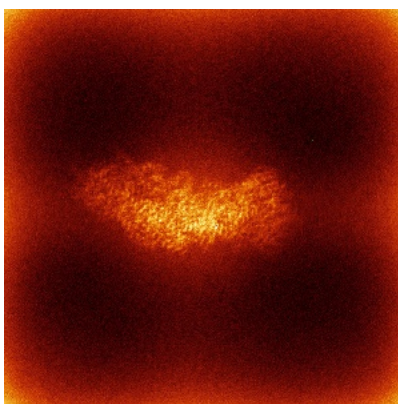


Z

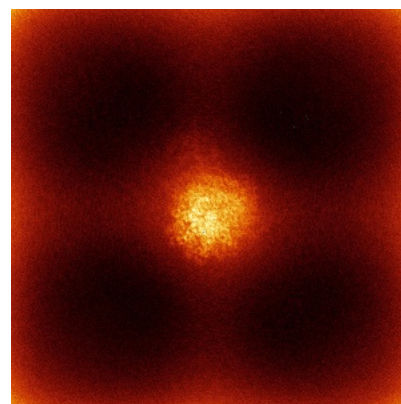
6.4.2 Raw map



X



Y

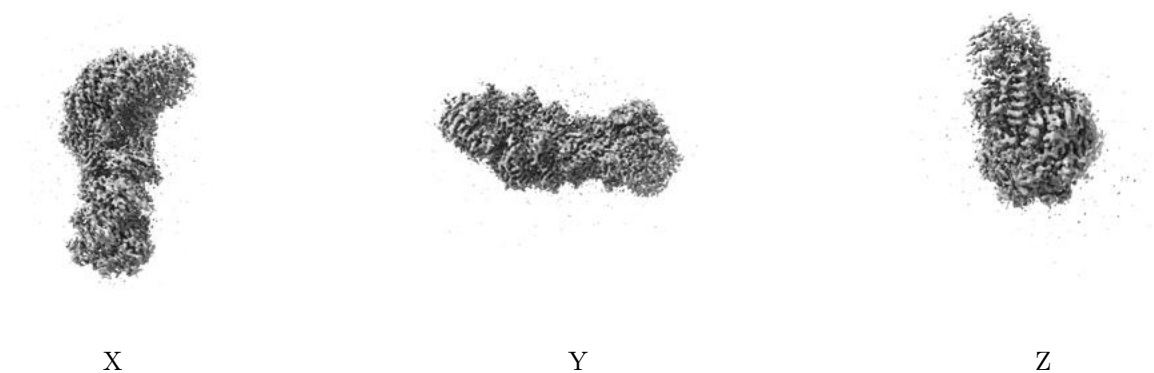


Z

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.

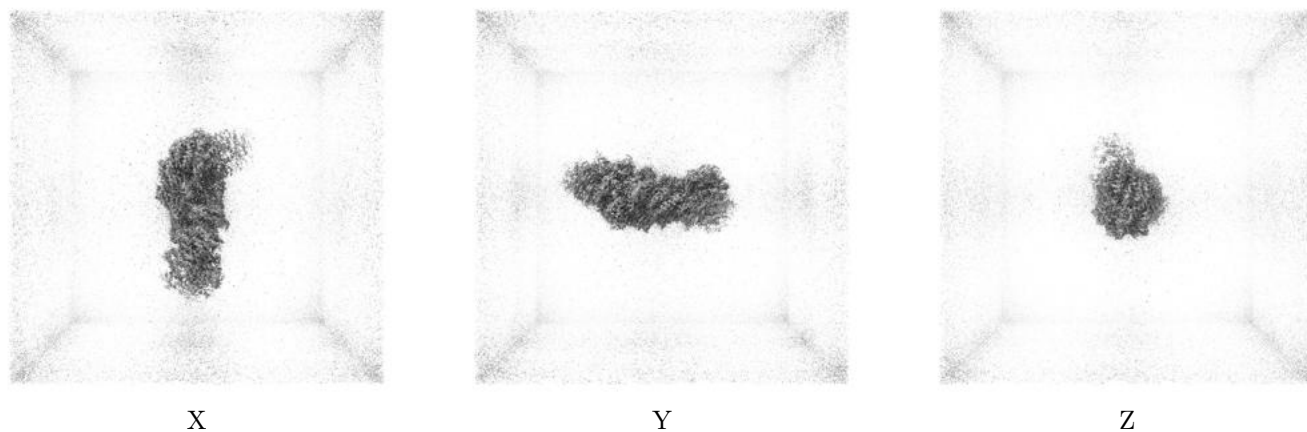
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

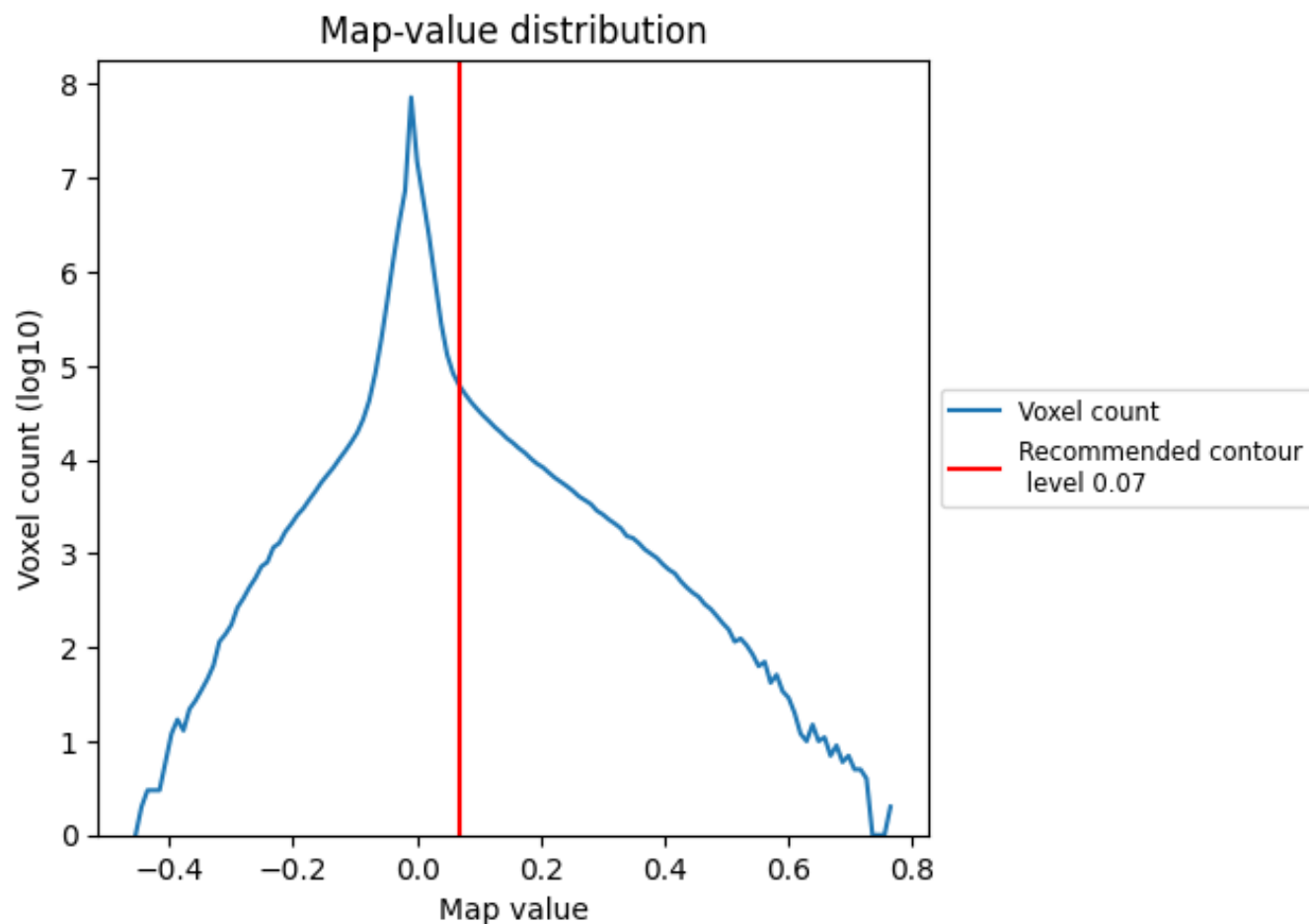
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

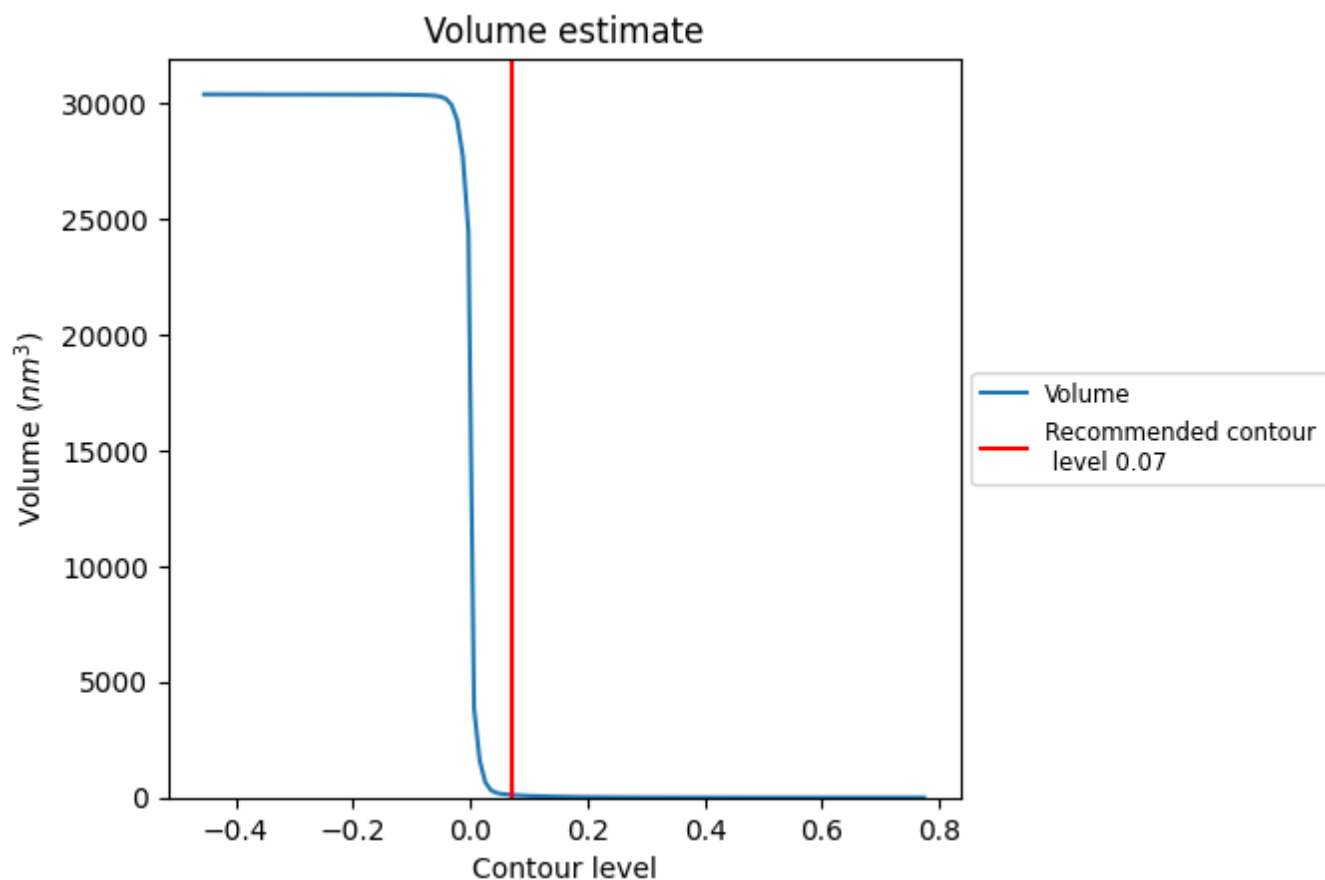
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

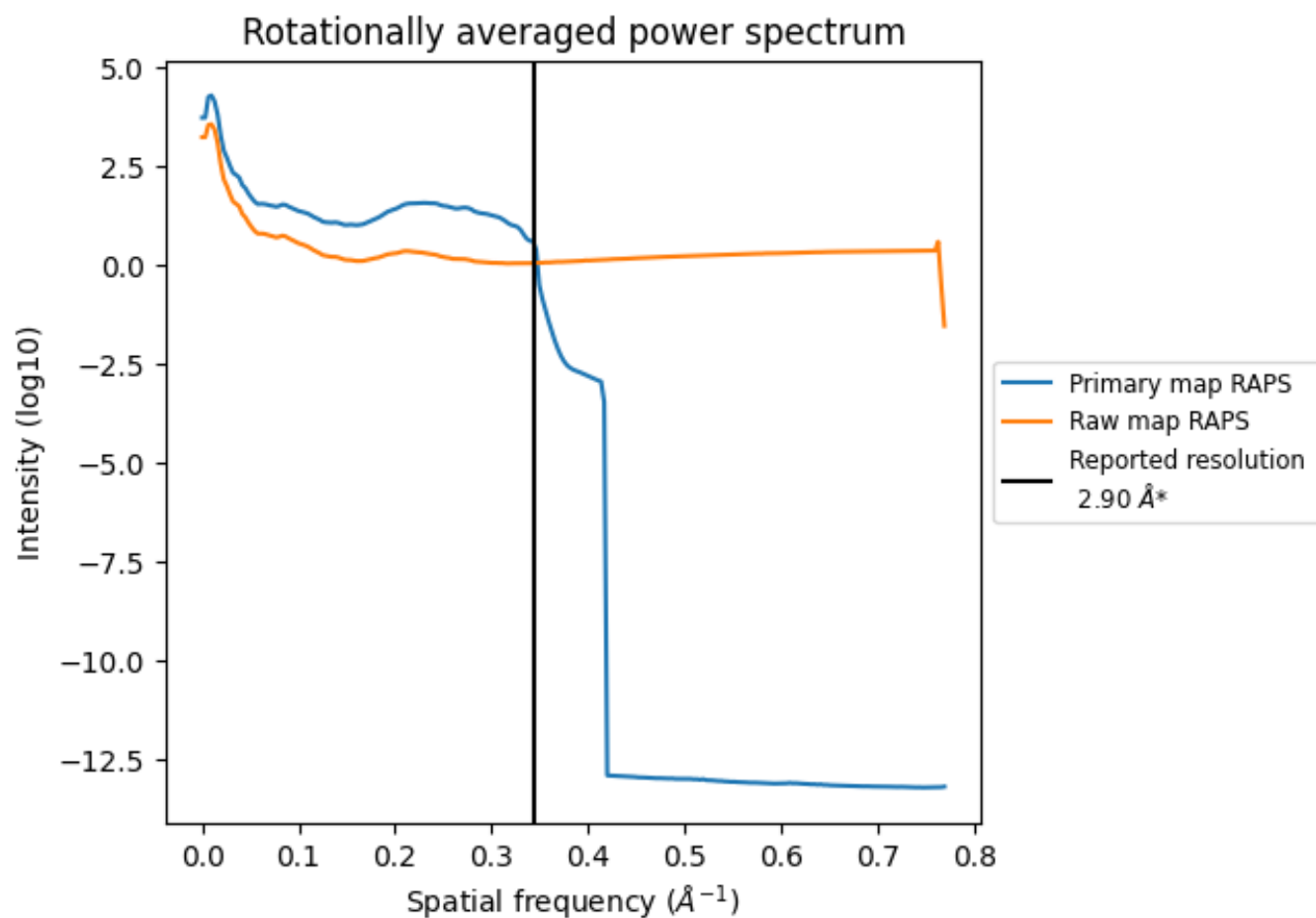
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 116 nm³; this corresponds to an approximate mass of 105 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

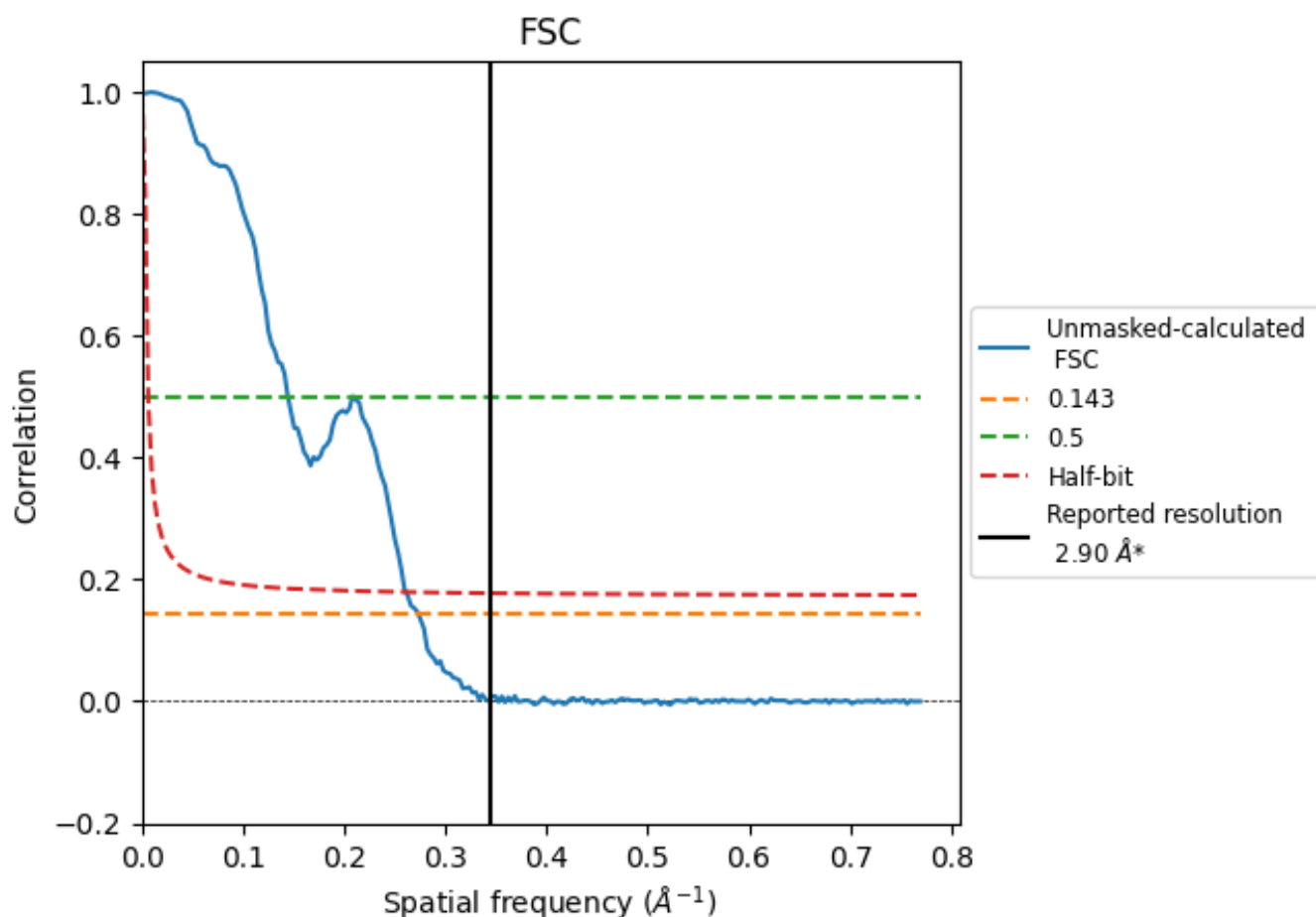


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

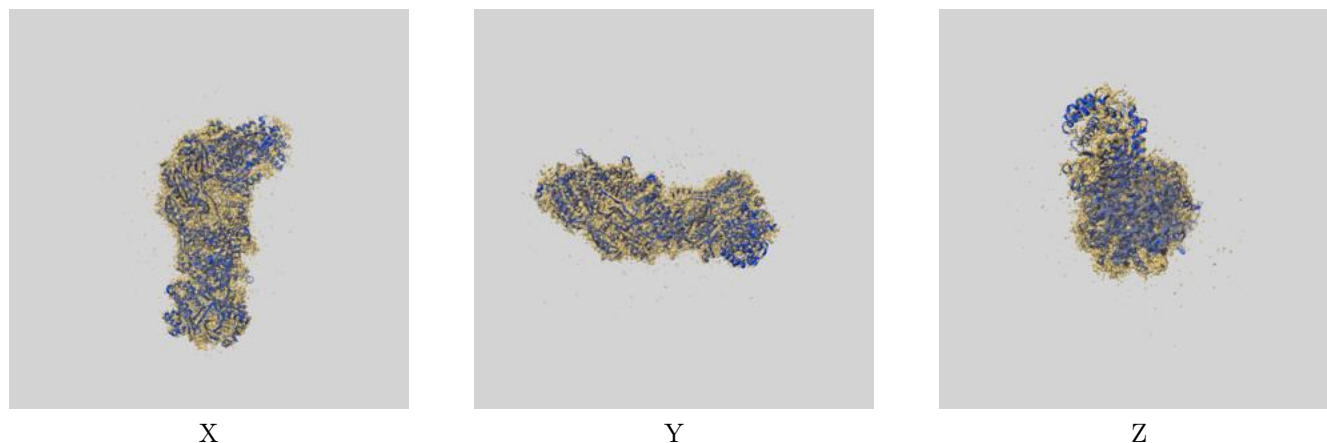
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.66	6.93	3.83

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.66 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

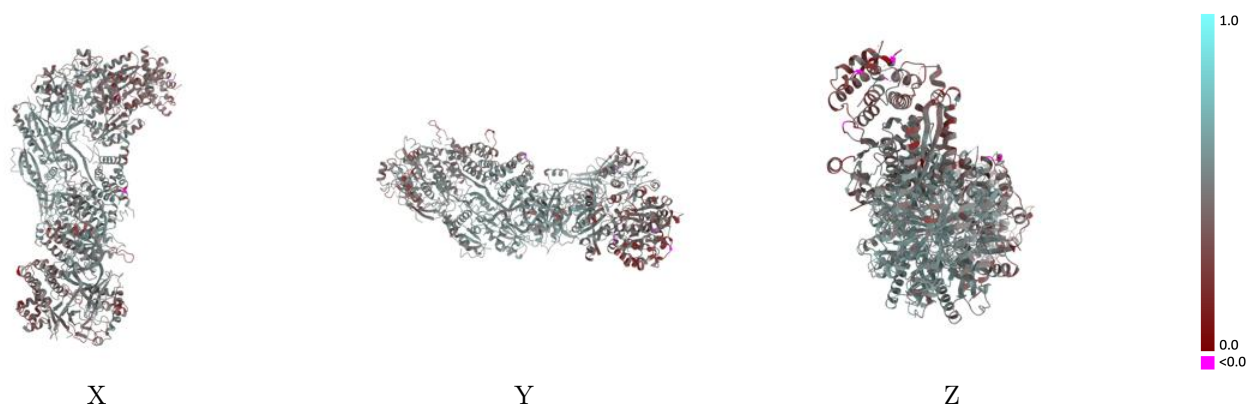
This section contains information regarding the fit between EMDB map EMD-51148 and PDB model 9G9D. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



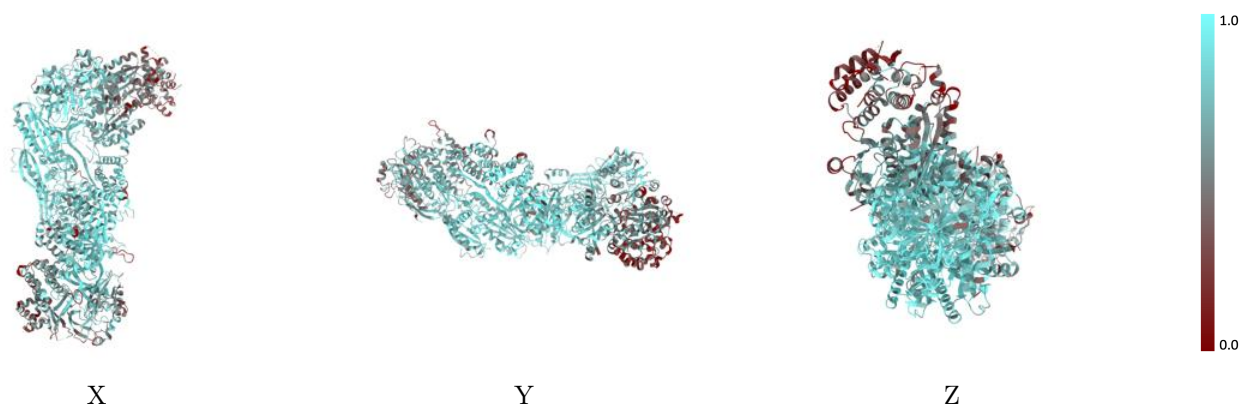
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



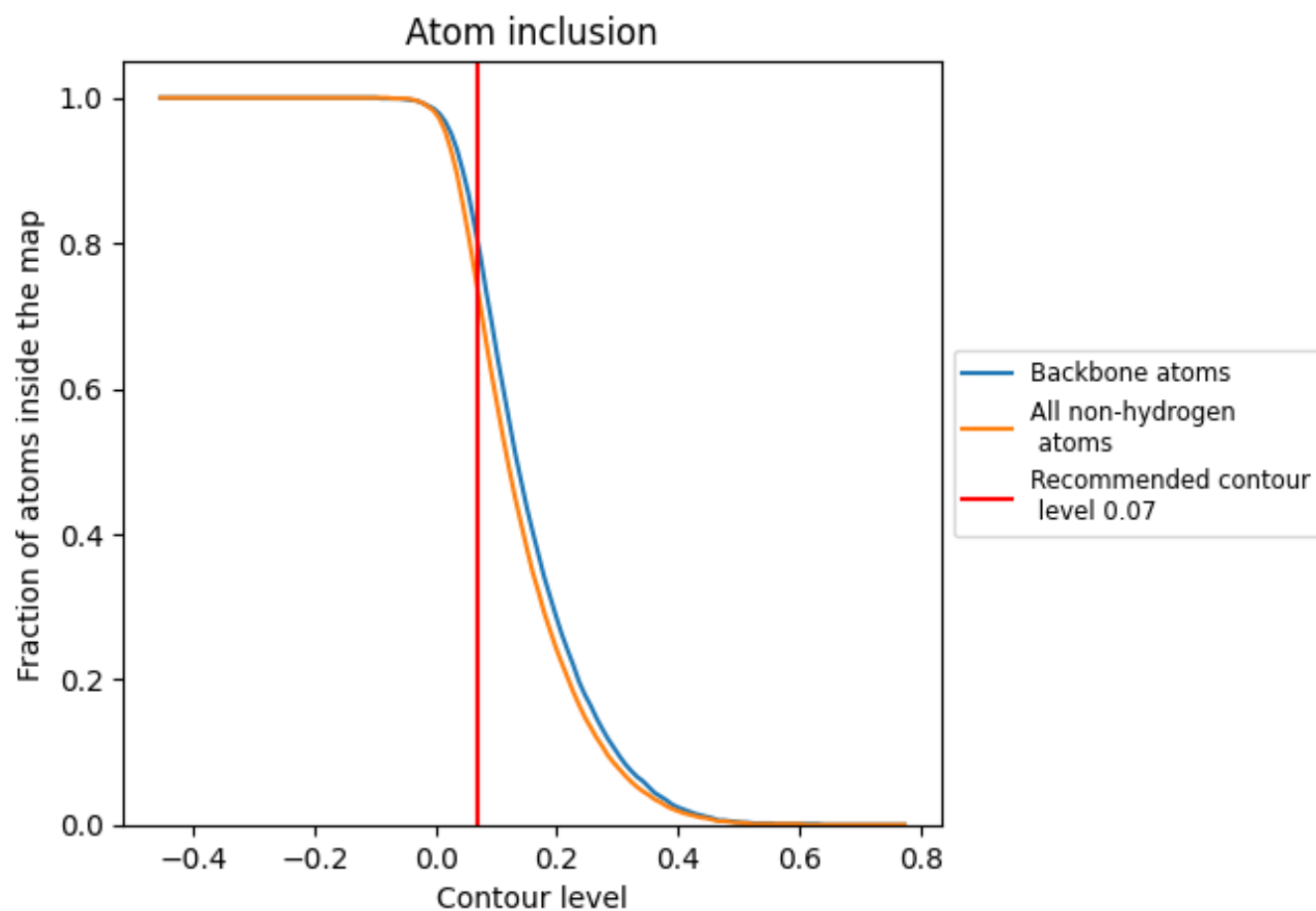
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7350	0.4830
A	0.5830	0.4240
B	0.8130	0.5040
C	0.6890	0.4370
D	0.8580	0.5340
E	0.8970	0.5630
F	0.8870	0.5640
G	0.7910	0.4970
H	0.6040	0.4340
I	0.8440	0.5360
J	0.5630	0.4050
R	0.9250	0.5440
T	0.8810	0.5230

1.0

0.0

<0.0