



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 03:31 AM UTC

PDB ID : 9VTR / pdb_00009vtr
EMDB ID : EMD-65340
Title : Target DNA-bound type I-F3 TniQ-Cascade of *Vibrio parahaemolyticus* in full R-loop state 2
Authors : Ishihara, K.; Numata, T.
Deposited on : 2025-07-11
Resolution : 2.89 Å(reported)
Based on initial model : .

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:

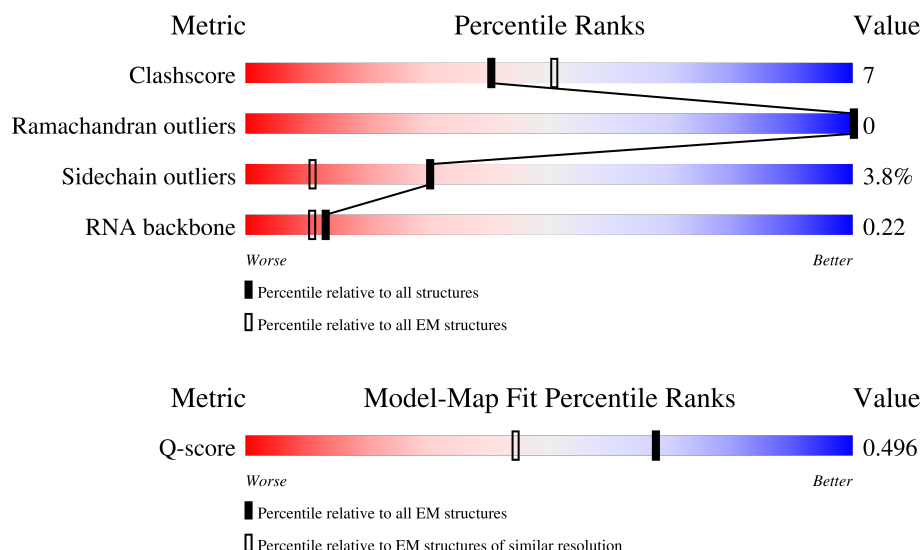
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.89 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	12148 (2.39 - 3.39)

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	1	60	
2	2	75	
3	3	75	

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Mol	Chain	Length	Quality of chain
4	A	347	 89% 10% .
4	B	347	 85% 14% ..
4	C	347	 82% 17% .
4	D	347	 84% 15%
4	E	347	 83% 14% ..
4	F	347	 66% 18% . 14%
5	G	640	 7% 75% 14% 11%
6	H	198	 77% 13% . 9%
7	I	406	 23% 67% 25% . 6%
7	J	406	 11% 60% 24% . 15%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 29332 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 RNA chain called crRNA from *Vibrio parahaemolyticus*.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	57	Total	C	N	O	P	0	0
			1221	548	231	386	56		

- Molecule 2 is a DNA chain called Target strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	37	Total	C	N	O	P	0	0
			759	362	130	230	37		

- Molecule 3 is a DNA chain called Non-target strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	6	Total	C	N	O	P	0	0
			123	58	23	36	6		

- Molecule 4 is a protein called Type I-F CRISPR-associated protein Csy3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	345	Total	C	N	O	S	0	0
			2725	1739	461	512	13		
4	B	345	Total	C	N	O	S	0	0
			2745	1752	463	517	13		
4	C	345	Total	C	N	O	S	0	0
			2752	1756	463	520	13		
4	D	346	Total	C	N	O	S	0	0
			2756	1758	464	521	13		
4	E	340	Total	C	N	O	S	0	0
			2727	1741	458	515	13		
4	F	297	Total	C	N	O	S	0	0
			2392	1537	401	442	12		

- Molecule 5 is a protein called CRISPR-associated protein Csy2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	568	Total	C	N	O	S	0	0
			4231	2671	766	773	21		

There are 97 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	293	UNK	THR	conflict	UNP Q87GC9
G	294	UNK	GLU	conflict	UNP Q87GC9
G	295	UNK	SER	conflict	UNP Q87GC9
G	296	UNK	SER	conflict	UNP Q87GC9
G	297	UNK	VAL	conflict	UNP Q87GC9
G	298	UNK	TRP	conflict	UNP Q87GC9
G	299	UNK	VAL	conflict	UNP Q87GC9
G	300	UNK	ILE	conflict	UNP Q87GC9
G	301	UNK	SER	conflict	UNP Q87GC9
G	302	UNK	PRO	conflict	UNP Q87GC9
G	303	UNK	ASN	conflict	UNP Q87GC9
G	304	UNK	LYS	conflict	UNP Q87GC9
G	305	UNK	LEU	conflict	UNP Q87GC9
G	306	UNK	ALA	conflict	UNP Q87GC9
G	307	UNK	LEU	conflict	UNP Q87GC9
G	308	UNK	ARG	conflict	UNP Q87GC9
G	309	UNK	LYS	conflict	UNP Q87GC9
G	310	UNK	LYS	conflict	UNP Q87GC9
G	311	UNK	SER	conflict	UNP Q87GC9
G	312	UNK	ILE	conflict	UNP Q87GC9
G	313	UNK	ILE	conflict	UNP Q87GC9
G	314	UNK	GLY	conflict	UNP Q87GC9
G	315	UNK	ASP	conflict	UNP Q87GC9
G	316	UNK	ILE	conflict	UNP Q87GC9
G	317	UNK	LYS	conflict	UNP Q87GC9
G	318	UNK	MET	conflict	UNP Q87GC9
G	319	UNK	MET	conflict	UNP Q87GC9
G	320	UNK	LEU	conflict	UNP Q87GC9
G	321	UNK	SER	conflict	UNP Q87GC9
G	322	UNK	GLN	conflict	UNP Q87GC9
G	323	UNK	TRP	conflict	UNP Q87GC9
G	324	UNK	LEU	conflict	UNP Q87GC9
G	325	UNK	ARG	conflict	UNP Q87GC9
G	326	UNK	THR	conflict	UNP Q87GC9
G	327	UNK	THR	conflict	UNP Q87GC9
G	328	UNK	PRO	conflict	UNP Q87GC9
G	329	UNK	THR	conflict	UNP Q87GC9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	330	UNK	HIS	conflict	UNP Q87GC9
G	331	UNK	GLU	conflict	UNP Q87GC9
G	332	UNK	GLU	conflict	UNP Q87GC9
G	333	UNK	LYS	conflict	UNP Q87GC9
G	334	UNK	LEU	conflict	UNP Q87GC9
G	335	UNK	ASP	conflict	UNP Q87GC9
G	336	UNK	ILE	conflict	UNP Q87GC9
G	337	UNK	ARG	conflict	UNP Q87GC9
G	338	UNK	LYS	conflict	UNP Q87GC9
G	339	UNK	LEU	conflict	UNP Q87GC9
G	340	UNK	THR	conflict	UNP Q87GC9
G	341	UNK	GLU	conflict	UNP Q87GC9
G	342	UNK	ARG	conflict	UNP Q87GC9
G	343	UNK	PHE	conflict	UNP Q87GC9
G	344	UNK	ASN	conflict	UNP Q87GC9
G	345	UNK	VAL	conflict	UNP Q87GC9
G	346	UNK	ASP	conflict	UNP Q87GC9
G	347	UNK	LEU	conflict	UNP Q87GC9
G	348	UNK	ALA	conflict	UNP Q87GC9
G	349	UNK	LYS	conflict	UNP Q87GC9
G	350	UNK	THR	conflict	UNP Q87GC9
G	351	UNK	LYS	conflict	UNP Q87GC9
G	352	UNK	PHE	conflict	UNP Q87GC9
G	353	UNK	ALA	conflict	UNP Q87GC9
G	354	UNK	ASN	conflict	UNP Q87GC9
G	355	UNK	ARG	conflict	UNP Q87GC9
G	356	UNK	TYR	conflict	UNP Q87GC9
G	357	UNK	ALA	conflict	UNP Q87GC9
G	358	UNK	TYR	conflict	UNP Q87GC9
G	359	UNK	ASP	conflict	UNP Q87GC9
G	360	UNK	PRO	conflict	UNP Q87GC9
G	361	UNK	LEU	conflict	UNP Q87GC9
G	362	UNK	LEU	conflict	UNP Q87GC9
G	363	UNK	THR	conflict	UNP Q87GC9
G	364	UNK	GLN	conflict	UNP Q87GC9
G	365	UNK	LEU	conflict	UNP Q87GC9
G	366	UNK	ILE	conflict	UNP Q87GC9
G	367	UNK	TYR	conflict	UNP Q87GC9
G	?	UNK	ASN	conflict	UNP Q87GC9
G	?	UNK	CYS	conflict	UNP Q87GC9
G	?	UNK	ILE	conflict	UNP Q87GC9
G	?	UNK	GLY	conflict	UNP Q87GC9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	?	UNK	SER	conflict	UNP Q87GC9
G	?	UNK	ILE	conflict	UNP Q87GC9
G	?	UNK	ILE	conflict	UNP Q87GC9
G	?	UNK	HIS	conflict	UNP Q87GC9
G	?	UNK	SER	conflict	UNP Q87GC9
G	?	UNK	PRO	conflict	UNP Q87GC9
G	?	UNK	PRO	conflict	UNP Q87GC9
G	?	UNK	GLN	conflict	UNP Q87GC9
G	?	UNK	TYR	conflict	UNP Q87GC9
G	?	UNK	ALA	conflict	UNP Q87GC9
G	?	UNK	PRO	conflict	UNP Q87GC9
G	?	UNK	LYS	conflict	UNP Q87GC9
G	?	UNK	CYS	conflict	UNP Q87GC9
G	?	UNK	GLU	conflict	UNP Q87GC9
G	?	UNK	GLY	conflict	UNP Q87GC9
G	?	UNK	ASN	conflict	UNP Q87GC9
G	?	UNK	ASP	conflict	UNP Q87GC9
G	?	UNK	ASP	conflict	UNP Q87GC9

- Molecule 6 is a protein called CRISPR-associated protein, Csy4 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	181	Total	C	N	O	S	0	0
			1452	926	258	265	3		

- Molecule 7 is a protein called TniQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	381	Total	C	N	O	S	0	0
			2798	1788	491	504	15		
7	J	347	Total	C	N	O	S	0	0
			2650	1684	466	483	17		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-6	GLY	-	expression tag	UNP Q87GD0
I	-5	PRO	-	expression tag	UNP Q87GD0
I	-4	ARG	-	expression tag	UNP Q87GD0
I	-3	ILE	-	expression tag	UNP Q87GD0
I	-2	SER	-	expression tag	UNP Q87GD0
I	-1	GLU	-	expression tag	UNP Q87GD0

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Chain	Residue	Modelled	Actual	Comment	Reference
I	0	PHE	-	expression tag	UNP Q87GD0
J	-6	GLY	-	expression tag	UNP Q87GD0
J	-5	PRO	-	expression tag	UNP Q87GD0
J	-4	ARG	-	expression tag	UNP Q87GD0
J	-3	ILE	-	expression tag	UNP Q87GD0
J	-2	SER	-	expression tag	UNP Q87GD0
J	-1	GLU	-	expression tag	UNP Q87GD0
J	0	PHE	-	expression tag	UNP Q87GD0

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	1	1	Total 1	Mg 1	0

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.

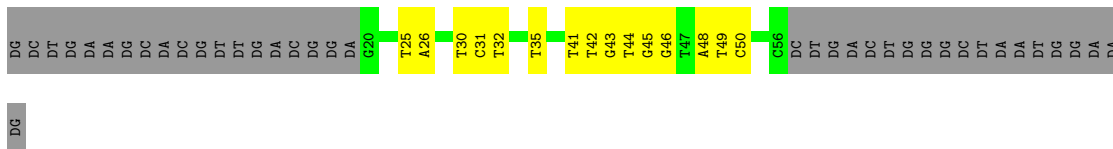
- Molecule 1: crRNA from *Vibrio parahaemolyticus*

Chain 1: 



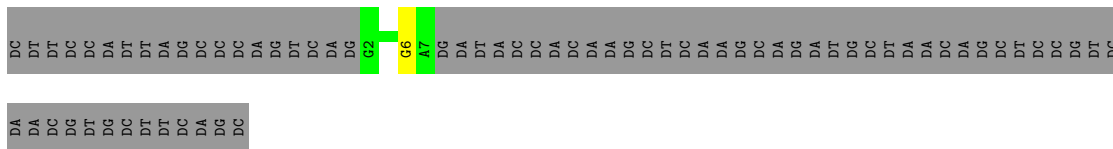
- Molecule 2: Target strand DNA

Chain 2: 




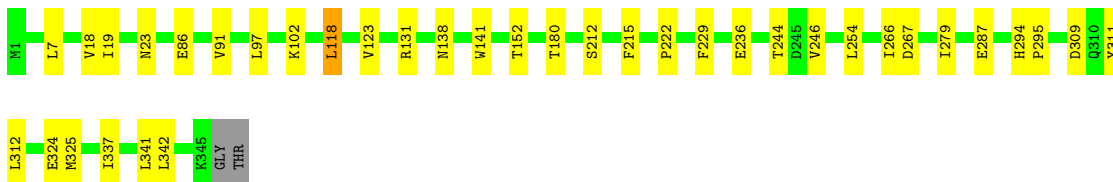
- Molecule 3: Non-target strand DNA

Chain 3: 




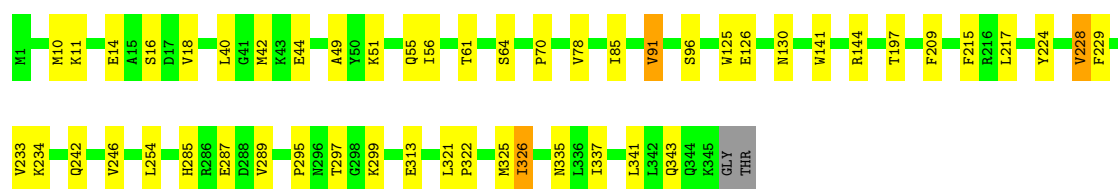
- Molecule 4: Type I-F CRISPR-associated protein Csy3

Chain A: 




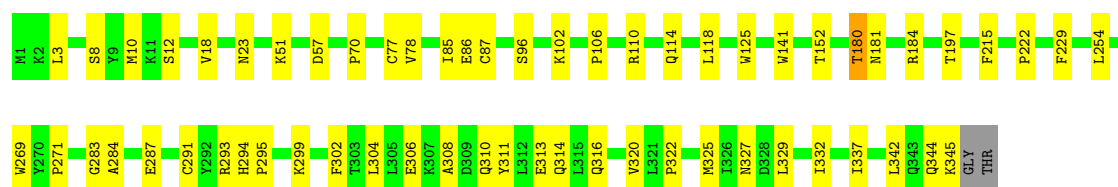
- Molecule 4: Type I-F CRISPR-associated protein Csy3

Chain B:  85% 14% ..




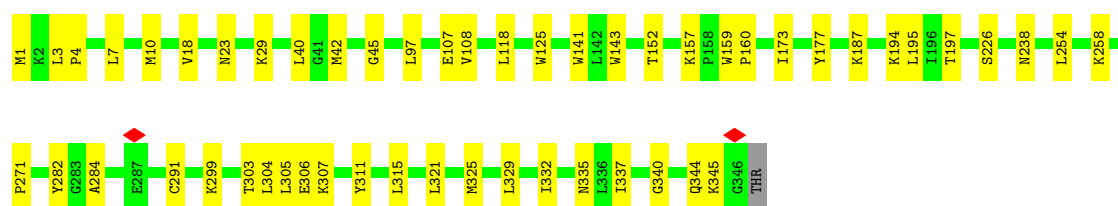
• Molecule 4: Type I-F CRISPR-associated protein Csy3

Chain C:  82% 17% .




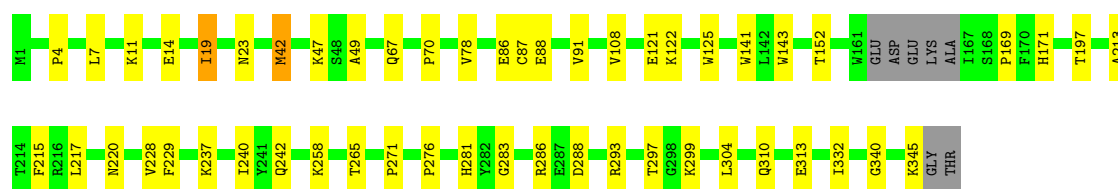
• Molecule 4: Type I-F CRISPR-associated protein Csy3

Chain D:  84% 15%



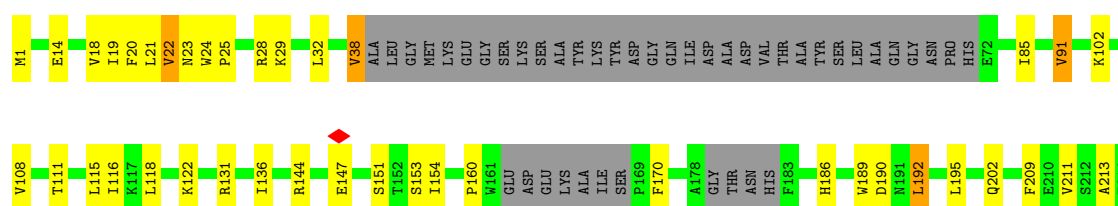
• Molecule 4: Type I-F CRISPR-associated protein Csy3

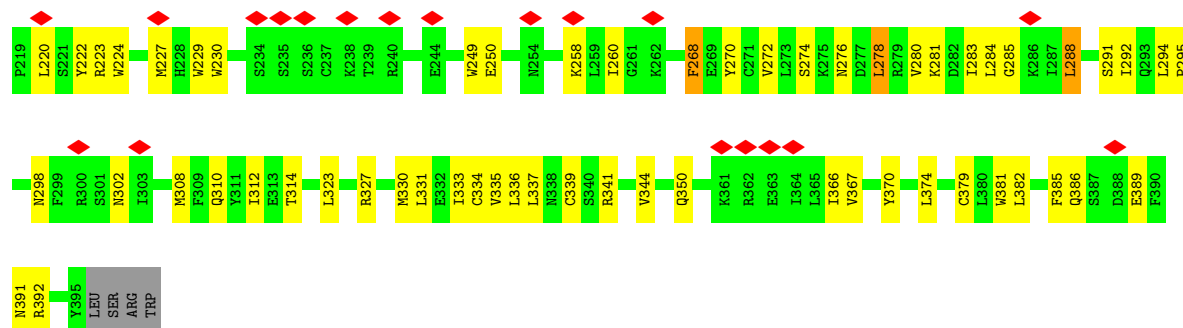
Chain E:  83% 14% ..



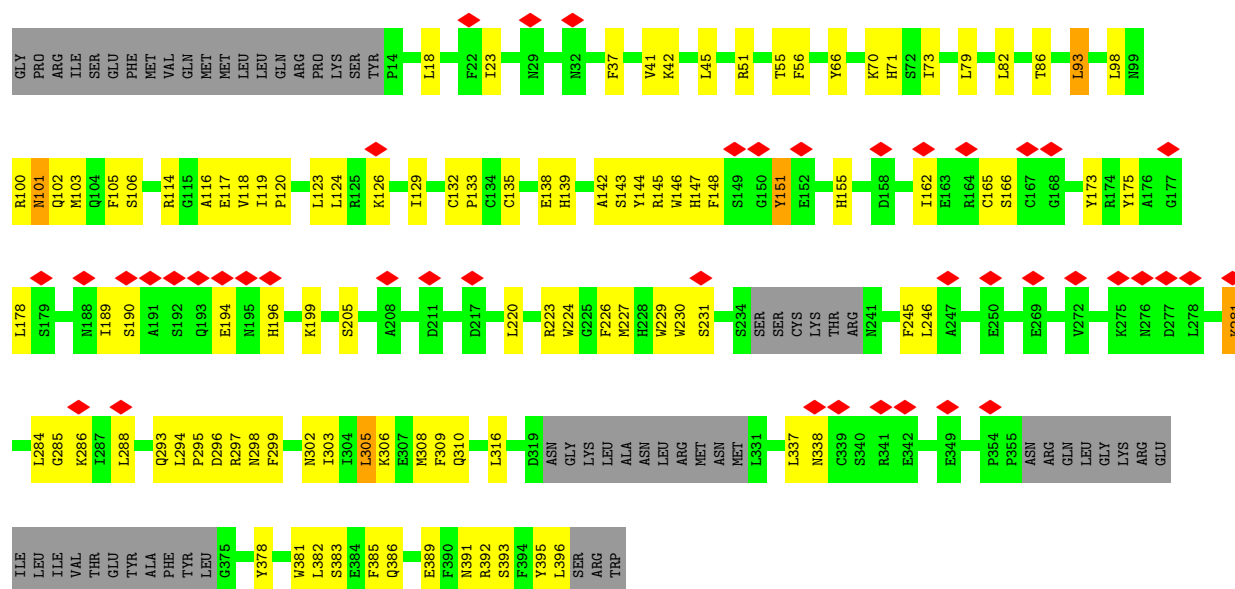
• Molecule 4: Type I-F CRISPR-associated protein Csy3

Chain F:  66% 18% 14%





• Molecule 7: ThiQ



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12291	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.92	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.545	Depositor
Minimum map value	-0.659	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	345.91998, 345.91998, 345.91998	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.752, 0.752, 0.752	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1	0.12	0/1368	0.30	0/2129
2	2	0.20	0/848	0.42	0/1308
3	3	0.14	0/137	0.30	0/209
4	A	0.12	0/2797	0.30	0/3800
4	B	0.10	0/2818	0.25	0/3826
4	C	0.12	0/2825	0.29	0/3836
4	D	0.10	0/2829	0.25	0/3841
4	E	0.10	0/2799	0.26	0/3798
4	F	0.12	0/2455	0.32	0/3330
5	G	0.11	0/4090	0.30	0/5564
6	H	0.12	0/1483	0.35	0/1995
7	I	0.14	0/2867	0.41	0/3910
7	J	0.15	0/2717	0.43	1/3689 (0.0%)
All	All	0.12	0/30033	0.32	1/41235 (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
7	J	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	308	MET	CA-CB-CG	5.94	125.97	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	J	106	SER	Peptide

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	1	1221	0	620	5	0
2	2	759	0	421	15	0
3	3	123	0	68	1	0
4	A	2725	0	2625	20	0
4	B	2745	0	2650	30	0
4	C	2752	0	2664	36	0
4	D	2756	0	2667	35	0
4	E	2727	0	2650	37	0
4	F	2392	0	2312	37	0
5	G	4231	0	3915	54	0
6	H	1452	0	1408	17	0
7	I	2798	0	2427	76	0
7	J	2650	0	2373	74	0
8	1	1	0	0	0	0
All	All	29332	0	26800	394	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 7.

All (394) 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:J:101:ASN:HD21	7:J:103:MET:HG2	1.20	1.04
2:2:48:DA:H62	4:D:238:ASN:HD21	1.25	0.82
4:F:118:LEU:HD11	4:F:316:GLN:HB3	1.61	0.82
7:I:294:LEU:HB2	7:I:295:PRO:HD3	1.63	0.80
7:I:381:TRP:HA	7:I:385:PHE:HB2	1.63	0.79
7:J:101:ASN:ND2	7:J:103:MET:HG2	1.97	0.78
7:J:294:LEU:HB2	7:J:295:PRO:HD3	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:31:DC:H2'	2:2:32:DT:H72	1.65	0.77
4:B:322:PRO:HG2	4:B:325:MET:HG2	1.67	0.77
7:I:212:VAL:HG12	7:I:214:PRO:HD2	1.67	0.76
7:I:350:GLN:HE22	7:J:70:LYS:HE2	1.53	0.73
7:J:55:THR:HG21	7:J:71:HIS:HB2	1.70	0.73
4:F:85:ILE:HD11	4:F:215:PHE:HD2	1.52	0.73
4:D:45:GLY:H	4:E:281:HIS:HD2	1.40	0.70
5:G:558:VAL:HG23	5:G:602:ILE:HD11	1.73	0.69
7:I:79:LEU:HB3	7:I:93:LEU:HD22	1.74	0.68
5:G:26:LEU:HD13	5:G:250:LEU:HD11	1.74	0.68
4:D:125:TRP:HB2	4:D:197:THR:HG22	1.74	0.68
4:D:304:LEU:HB3	4:D:332:ILE:HD11	1.75	0.68
5:G:127:SER:HB2	5:G:245:THR:HG22	1.75	0.67
7:I:220:LEU:HA	7:I:223:ARG:HG3	1.77	0.67
4:E:152:THR:HG23	4:E:215:PHE:HB3	1.77	0.67
4:B:56:ILE:HG12	4:C:295:PRO:HB2	1.76	0.67
4:D:18:VAL:HB	4:D:254:LEU:HB2	1.77	0.67
7:I:298:ASN:HD22	7:I:389:GLU:HG3	1.60	0.66
4:F:122:LYS:HE2	4:F:316:GLN:HA	1.77	0.66
5:G:239:THR:O	5:G:257:LYS:HA	1.97	0.65
4:A:18:VAL:HB	4:A:254:LEU:HB2	1.78	0.64
7:I:100:ARG:HA	7:I:112:LEU:HG	1.79	0.64
5:G:37:ILE:HD12	5:G:38:GLU:H	1.60	0.64
4:F:18:VAL:HB	4:F:254:LEU:HB2	1.78	0.64
5:G:581:PRO:HB2	5:G:592:LYS:HE2	1.80	0.64
4:E:297:THR:HG23	4:E:299:LYS:H	1.63	0.63
4:F:301:LEU:HD13	4:F:335:ASN:HD22	1.62	0.63
7:J:126:LYS:H	7:J:126:LYS:HD3	1.62	0.63
7:I:123:LEU:HD12	7:I:149:SER:HB2	1.79	0.63
5:G:407:THR:HG22	5:G:572:CYS:HB2	1.80	0.63
7:J:220:LEU:HA	7:J:223:ARG:HD2	1.79	0.62
4:E:283:GLY:H	4:E:293:ARG:HB2	1.64	0.62
4:C:12:SER:HB2	4:C:337:ILE:HG23	1.81	0.62
6:H:46:LEU:HD21	6:H:55:LYS:H	1.65	0.62
7:J:42:LYS:HD2	7:J:56:PHE:HB3	1.81	0.62
7:J:133:PRO:HG2	7:J:162:ILE:HD12	1.82	0.62
7:J:284:LEU:HG	7:J:288:LEU:HB2	1.82	0.61
4:C:23:ASN:HD21	4:C:86:GLU:HB2	1.65	0.61
4:B:49:ALA:HB1	4:C:295:PRO:HG3	1.83	0.61
4:E:11:LYS:HD2	4:E:14:GLU:HG2	1.81	0.61
4:F:116:ILE:HD11	4:F:336:LEU:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:226:SER:HB2	4:D:254:LEU:HA	1.82	0.61
6:H:77:GLN:O	6:H:81:LEU:HD12	2.01	0.60
7:J:98:LEU:HD13	7:J:114:ARG:HB2	1.83	0.60
5:G:567:LEU:HD11	5:G:605:PHE:HB2	1.83	0.60
4:A:325:MET:HA	4:A:325:MET:HE2	1.84	0.59
7:I:121:ARG:HG2	7:I:124:LEU:HD23	1.83	0.59
7:I:133:PRO:HD2	7:I:159:VAL:HG21	1.84	0.59
7:I:212:VAL:HB	7:I:215:LEU:HB2	1.83	0.59
7:I:229:TRP:CD1	7:I:291:SER:HG	2.20	0.59
7:I:25:VAL:HA	7:I:28:LYS:HD3	1.84	0.59
7:I:222:TYR:HA	7:I:295:PRO:HG2	1.85	0.59
5:G:577:ARG:HH21	5:G:580:THR:HA	1.68	0.59
1:I:30:G:C2	4:A:341:LEU:HD13	2.38	0.59
7:I:327:ARG:HB3	7:I:370:TYR:HB3	1.85	0.58
4:C:308:ALA:HA	4:C:311:TYR:HD1	1.68	0.58
4:F:23:ASN:HB3	4:F:29:LYS:HZ3	1.67	0.58
4:E:121:GLU:HG3	4:E:122:LYS:HD3	1.85	0.58
7:J:18:LEU:H	7:J:142:ALA:HB3	1.68	0.58
4:C:10:MET:HB3	4:C:96:SER:HB3	1.83	0.58
7:J:299:PHE:HE1	7:J:305:LEU:HB3	1.67	0.58
5:G:89:PHE:HA	5:G:247:MET:HE3	1.85	0.57
7:J:381:TRP:HA	7:J:385:PHE:HB2	1.86	0.57
4:C:18:VAL:HB	4:C:254:LEU:HB2	1.86	0.57
4:F:24:TRP:HB2	4:F:28:ARG:HB2	1.86	0.57
7:I:331:LEU:O	7:I:335:VAL:HG12	2.04	0.57
4:B:341:LEU:HD23	4:B:343:GLN:HE22	1.69	0.57
4:E:141:TRP:H	4:E:141:TRP:CD1	2.23	0.57
4:A:23:ASN:HD21	4:A:86:GLU:HB2	1.70	0.57
7:I:258:LYS:N	7:I:258:LYS:HE2	2.20	0.56
5:G:37:ILE:HD12	5:G:38:GLU:N	2.19	0.56
7:I:18:LEU:HD11	7:I:63:ILE:HG12	1.87	0.56
7:I:180:GLY:HA3	7:I:188:ASN:HA	1.86	0.56
5:G:272:HIS:HA	5:G:607:THR:HG23	1.87	0.56
5:G:416:MET:HE1	5:G:444:VAL:HG21	1.88	0.56
7:I:391:ASN:ND2	7:J:116:ALA:HA	2.21	0.56
4:B:228:VAL:HG12	4:B:242:GLN:HG2	1.87	0.55
4:C:304:LEU:HB3	4:C:332:ILE:HD11	1.87	0.55
7:J:299:PHE:CE2	7:J:396:LEU:HD22	2.42	0.55
5:G:547:ASN:HB2	5:G:604:LYS:HD2	1.89	0.55
4:B:10:MET:HB3	4:B:96:SER:HB3	1.88	0.55
4:E:228:VAL:HG12	4:E:242:GLN:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:66:TYR:HA	7:J:100:ARG:HG2	1.88	0.55
7:J:138:GLU:HG2	7:J:139:HIS:CE1	2.42	0.55
2:2:50:DC:H5'	2:2:50:DC:C6	2.42	0.54
5:G:429:ASN:HB3	5:G:503:LEU:HD22	1.89	0.54
7:I:268:PHE:CE1	7:I:283:ILE:HG12	2.42	0.54
4:C:314:GLN:HG2	4:C:325:MET:HE1	1.89	0.54
5:G:522:HIS:HB2	5:G:525:ARG:HH12	1.72	0.54
7:J:165:CYS:HB2	7:J:189:ILE:HD13	1.88	0.54
7:I:103:MET:HE1	7:I:105:PHE:HA	1.89	0.54
4:F:20:PHE:O	4:F:32:LEU:HB2	2.08	0.54
4:D:1:MET:HE3	4:D:108:VAL:HG13	1.89	0.53
1:1:29:A:C4	4:A:341:LEU:HD11	2.44	0.53
7:I:284:LEU:HD12	7:I:288:LEU:HB2	1.90	0.53
2:2:26:DA:H5'	2:2:26:DA:C8	2.43	0.53
4:F:115:LEU:HD23	4:F:312:LEU:HB2	1.90	0.53
7:I:294:LEU:HB2	7:I:295:PRO:CD	2.38	0.53
4:D:321:LEU:HD12	4:D:325:MET:HG2	1.90	0.53
4:C:271:PRO:HD3	4:C:299:LYS:HG3	1.89	0.53
4:D:141:TRP:CD1	4:D:141:TRP:H	2.25	0.53
7:I:330:MET:C	7:I:330:MET:HE3	2.34	0.53
7:J:129:ILE:HD13	7:J:147:HIS:CE1	2.44	0.52
7:J:281:LYS:HA	7:J:285:GLY:HA3	1.92	0.52
4:D:271:PRO:HD3	4:D:299:LYS:HG3	1.91	0.52
4:F:271:PRO:HD3	4:F:299:LYS:HE3	1.91	0.52
7:J:337:LEU:HD13	7:J:338:ASN:N	2.24	0.52
7:J:224:TRP:HA	7:J:227:MET:HE1	1.90	0.52
4:A:141:TRP:H	4:A:141:TRP:CD1	2.28	0.51
4:A:229:PHE:CZ	4:C:70:PRO:HG3	2.45	0.51
4:B:125:TRP:HB2	4:B:197:THR:HG22	1.93	0.51
4:E:23:ASN:HD21	4:E:86:GLU:HB2	1.75	0.51
4:F:304:LEU:HB3	4:F:332:ILE:HD11	1.91	0.51
5:G:584:LYS:HG3	5:G:593:HIS:HB3	1.92	0.51
4:B:229:PHE:CZ	4:E:70:PRO:HG3	2.45	0.51
6:H:103:ARG:HA	6:H:165:ASN:O	2.10	0.51
7:J:392:ARG:HD2	7:J:396:LEU:HG	1.90	0.51
7:J:117:GLU:HG3	7:J:119:ILE:HD11	1.92	0.51
4:D:173:ILE:HA	4:D:177:TYR:HD1	1.76	0.51
4:B:61:THR:HG23	4:B:64:SER:H	1.75	0.51
4:F:160:PRO:HG2	4:F:195:LEU:HD22	1.92	0.51
5:G:116:LEU:HD22	5:G:117:PRO:HD2	1.92	0.51
7:J:138:GLU:HG2	7:J:139:HIS:ND1	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:416:MET:HE3	5:G:416:MET:HA	1.94	0.50
7:J:119:ILE:HB	7:J:148:PHE:HE2	1.77	0.50
7:J:155:HIS:HB2	7:J:205:SER:HA	1.94	0.50
7:J:23:ILE:HD13	7:J:178:LEU:H	1.77	0.50
4:B:11:LYS:HD2	4:B:14:GLU:HG3	1.92	0.50
7:J:126:LYS:H	7:J:126:LYS:CD	2.25	0.50
4:D:159:TRP:CD1	5:G:520:ILE:HD11	2.46	0.50
7:J:37:PHE:O	7:J:41:VAL:HG12	2.12	0.50
3:3:6:DG:N2	5:G:244:ALA:HB3	2.27	0.49
7:I:203:ILE:HD12	7:I:204:ALA:N	2.27	0.49
7:I:113:ILE:HG21	7:J:386:GLN:HB3	1.94	0.49
4:B:144:ARG:HG2	4:B:224:TYR:CD2	2.47	0.49
6:H:100:LEU:HD22	6:H:192:LEU:HD21	1.94	0.49
7:I:250:GLU:OE1	7:I:250:GLU:HA	2.12	0.49
7:J:391:ASN:C	7:J:396:LEU:HD23	2.38	0.49
4:B:126:GLU:O	4:B:130:ASN:HB2	2.12	0.49
4:D:143:TRP:CD1	4:D:258:LYS:HE3	2.47	0.49
4:B:18:VAL:HB	4:B:254:LEU:HB2	1.95	0.49
4:C:51:LYS:HZ2	4:C:57:ASP:HA	1.78	0.49
4:F:118:LEU:HD21	4:F:315:LEU:HB3	1.94	0.49
4:E:4:PRO:HD3	4:E:108:VAL:HG21	1.94	0.49
4:A:222:PRO:HG3	4:F:14:GLU:OE1	2.13	0.49
4:D:311:TYR:O	4:D:315:LEU:HD12	2.12	0.49
7:I:222:TYR:CD1	7:I:295:PRO:HG2	2.48	0.49
4:A:267:ASP:HB2	4:A:279:ILE:HD13	1.95	0.49
4:B:287:GLU:O	4:C:102:LYS:HA	2.13	0.49
4:C:269:TRP:HB3	4:C:327:ASN:HB3	1.94	0.49
4:C:284:ALA:HA	4:C:291:CYS:HA	1.95	0.49
7:I:75:ARG:O	7:I:79:LEU:HG	2.13	0.49
7:I:308:MET:O	7:I:312:ILE:HG13	2.12	0.49
7:J:299:PHE:CE1	7:J:305:LEU:HB3	2.46	0.49
4:C:152:THR:HG23	4:C:215:PHE:HB3	1.93	0.48
7:I:391:ASN:HD21	7:J:116:ALA:HA	1.77	0.48
4:E:4:PRO:HG2	4:E:7:LEU:HB2	1.93	0.48
5:G:399:ILE:HD13	5:G:508:ILE:HG21	1.95	0.48
4:C:125:TRP:HB2	4:C:197:THR:HG22	1.94	0.48
4:E:87:CYS:SG	4:E:215:PHE:HE1	2.36	0.48
6:H:73:ARG:HH22	7:I:270:TYR:HE2	1.62	0.48
7:I:129:ILE:HG22	7:I:147:HIS:HB3	1.93	0.48
4:B:299:LYS:HA	4:B:299:LYS:HD3	1.68	0.48
5:G:96:GLY:HA3	5:G:191:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:4:PRO:HD3	4:D:108:VAL:HG21	1.96	0.48
4:E:19:ILE:HD11	4:E:88:GLU:HB2	1.96	0.48
7:I:382:LEU:HD21	7:I:392:ARG:HD2	1.95	0.48
7:I:99:ASN:HD21	7:J:383:SER:HA	1.77	0.48
7:J:293:GLN:HB2	7:J:296:ASP:C	2.39	0.48
7:I:260:ILE:HD11	7:I:308:MET:HE1	1.96	0.47
2:2:43:DG:H4'	4:E:47:LYS:HD3	1.95	0.47
5:G:542:ARG:HB3	5:G:605:PHE:HB3	1.96	0.47
4:C:3:LEU:HB2	4:C:344:GLN:HE21	1.78	0.47
5:G:135:PHE:HB3	5:G:136:LEU:HD12	1.96	0.47
7:J:303:ILE:O	7:J:306:LYS:HG3	2.14	0.47
1:1:6:A:O4'	4:D:340:GLY:HA2	2.15	0.47
4:C:302:PHE:O	4:C:306:GLU:HG2	2.15	0.47
2:2:44:DT:H2''	2:2:45:DG:C8	2.50	0.47
4:C:77:CYS:HA	4:C:222:PRO:HA	1.96	0.47
4:D:23:ASN:ND2	4:D:29:LYS:HG3	2.30	0.47
5:G:430:VAL:HA	5:G:503:LEU:HD13	1.96	0.47
4:D:194:LYS:HB2	4:D:194:LYS:HE2	1.61	0.47
4:E:42:MET:HE3	4:E:42:MET:HB2	1.75	0.47
4:F:38:VAL:HG21	6:H:145:ALA:HA	1.96	0.47
4:F:136:ILE:HG13	4:F:263:ILE:HD12	1.97	0.47
7:J:123:LEU:HD12	7:J:148:PHE:HB3	1.97	0.47
4:B:16:SER:HB2	4:E:220:ASN:HB2	1.96	0.47
6:H:185:LEU:HD12	6:H:186:GLY:N	2.30	0.47
7:I:222:TYR:HE2	7:I:302:ASN:HB2	1.80	0.47
4:F:85:ILE:HD12	4:F:85:ILE:C	2.39	0.47
7:J:199:LYS:HE2	7:J:246:LEU:HD13	1.97	0.47
7:J:381:TRP:CH2	7:J:396:LEU:HD11	2.49	0.47
4:C:180:THR:O	4:C:184:ARG:HG2	2.14	0.47
7:J:298:ASN:HB2	7:J:389:GLU:HG3	1.95	0.47
4:E:215:PHE:CE2	4:E:217:LEU:HD11	2.50	0.47
7:I:65:PRO:HG3	7:I:79:LEU:HD11	1.96	0.46
4:D:23:ASN:HD22	4:D:29:LYS:HG3	1.80	0.46
4:C:114:GLN:HA	4:C:114:GLN:OE1	2.16	0.46
5:G:260:MET:HB3	5:G:260:MET:HE2	1.77	0.46
7:I:206:TRP:CG	7:I:215:LEU:HG	2.51	0.46
7:I:268:PHE:HE1	7:I:283:ILE:HG12	1.80	0.46
7:J:132:CYS:HB3	7:J:135:CYS:HB2	1.97	0.46
4:D:195:LEU:HD23	4:D:195:LEU:HA	1.82	0.46
4:E:271:PRO:HD3	4:E:299:LYS:HG3	1.97	0.46
6:H:46:LEU:HD22	6:H:55:LYS:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:78:VAL:HG21	4:E:217:LEU:HD13	1.97	0.46
7:I:76:THR:HA	7:I:79:LEU:HG	1.98	0.46
5:G:450:HIS:O	5:G:479:CYS:HA	2.16	0.46
6:H:103:ARG:H	6:H:187:ASN:ND2	2.14	0.46
7:J:391:ASN:O	7:J:396:LEU:HD23	2.15	0.46
5:G:72:TRP:CD1	5:G:177:ILE:HG12	2.51	0.46
6:H:20:ILE:HD11	7:I:272:VAL:HA	1.97	0.46
7:I:66:TYR:HB3	7:I:100:ARG:HB2	1.98	0.46
2:2:30:DT:H2''	2:2:31:DC:O4'	2.16	0.46
7:J:70:LYS:HB3	7:J:71:HIS:CD2	2.51	0.46
4:B:234:LYS:HA	4:B:234:LYS:HD3	1.81	0.45
7:J:119:ILE:HG23	7:J:224:TRP:HB3	1.98	0.45
7:I:116:ALA:HB2	7:J:393:SER:OG	2.17	0.45
4:E:125:TRP:HB2	4:E:197:THR:HG22	1.98	0.45
7:I:278:LEU:HG	7:I:283:ILE:HD11	1.98	0.45
7:I:292:ILE:HD11	7:I:336:LEU:HA	1.98	0.45
4:F:294:HIS:CG	4:F:295:PRO:HD2	2.52	0.45
7:I:227:MET:HE3	7:I:230:TRP:HB3	1.97	0.45
5:G:111:LEU:HD12	5:G:112:SER:N	2.32	0.45
4:F:228:VAL:HG12	4:F:242:GLN:HG2	1.98	0.45
5:G:26:LEU:HD11	5:G:226:TYR:HB3	1.98	0.45
6:H:46:LEU:HD11	6:H:54:ARG:H	1.81	0.45
1:1:38:C:OP2	4:F:261:ALA:HB2	2.17	0.45
2:2:42:DT:H2''	2:2:43:DG:O4'	2.17	0.45
4:F:22:VAL:HB	4:F:85:ILE:HG22	1.98	0.45
5:G:136:LEU:HA	5:G:149:LEU:HB2	1.99	0.45
7:I:65:PRO:HA	7:I:75:ARG:HD2	1.99	0.45
7:I:341:ARG:NH1	7:I:341:ARG:HB2	2.32	0.45
7:J:102:GLN:N	7:J:102:GLN:OE1	2.50	0.45
7:J:166:SER:HB3	7:J:189:ILE:HD11	1.99	0.45
4:A:19:ILE:HD13	4:A:19:ILE:HA	1.87	0.45
4:C:78:VAL:HG22	4:C:85:ILE:HD11	1.99	0.45
5:G:451:VAL:HG22	5:G:479:CYS:HB3	1.98	0.45
7:J:143:SER:HB3	7:J:146:TRP:CE2	2.52	0.45
7:I:143:SER:HG	7:I:146:TRP:CD1	2.35	0.45
7:J:309:PHE:CE2	7:J:396:LEU:HD12	2.52	0.45
4:C:106:PRO:O	4:C:110:ARG:HG3	2.17	0.45
4:E:310:GLN:O	4:E:313:GLU:HG3	2.17	0.45
4:D:284:ALA:HA	4:D:291:CYS:HA	1.99	0.44
7:I:120:PRO:HD2	7:I:224:TRP:HB3	1.98	0.44
7:J:310:GLN:HG3	7:J:395:TYR:CZ	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:287:GLU:O	4:F:102:LYS:HA	2.17	0.44
5:G:54:LYS:H	5:G:54:LYS:HG2	1.59	0.44
5:G:228:VAL:HG11	5:G:559:ILE:HG13	1.99	0.44
4:E:265:THR:HG22	4:E:276:PRO:HB2	1.98	0.44
4:E:299:LYS:HD3	4:E:299:LYS:HA	1.77	0.44
5:G:244:ALA:HB1	5:G:251:ALA:HB1	1.99	0.44
4:B:40:LEU:HD13	4:C:229:PHE:HE2	1.82	0.44
6:H:121:ARG:O	6:H:124:ARG:HG3	2.17	0.44
7:J:297:ARG:HD2	7:J:338:ASN:OD1	2.17	0.44
4:C:310:GLN:O	4:C:313:GLU:HG3	2.18	0.44
6:H:15:ARG:HB2	7:I:272:VAL:O	2.18	0.44
4:E:304:LEU:HB3	4:E:332:ILE:HD11	2.00	0.44
7:I:114:ARG:HB3	7:I:117:GLU:OE1	2.17	0.44
7:J:178:LEU:HD12	7:J:178:LEU:O	2.18	0.44
2:2:35:DT:C2	4:B:70:PRO:HG2	2.53	0.44
4:B:51:LYS:HE3	4:B:51:LYS:HB3	1.83	0.44
4:B:141:TRP:CD1	4:B:141:TRP:H	2.34	0.44
4:F:19:ILE:HD13	4:F:19:ILE:HA	1.85	0.44
5:G:130:MET:HB3	5:G:252:MET:HE3	2.00	0.44
4:A:152:THR:HG23	4:A:215:PHE:HB3	1.99	0.43
5:G:608:ILE:HD11	5:G:617:TYR:CZ	2.53	0.43
4:A:97:LEU:HD13	4:A:337:ILE:HG13	2.00	0.43
7:I:334:CYS:HA	7:I:339:CYS:HB2	2.00	0.43
4:D:159:TRP:CZ2	5:G:498:ARG:HG2	2.54	0.43
4:D:303:THR:O	4:D:307:LYS:HG2	2.18	0.43
7:J:145:ARG:HD2	7:J:151:TYR:CE1	2.54	0.43
4:B:78:VAL:HG13	4:B:85:ILE:HD11	1.99	0.43
4:B:215:PHE:HE2	4:B:217:LEU:HD11	1.83	0.43
5:G:393:LEU:HD23	5:G:486:ILE:HD11	2.00	0.43
2:2:41:DT:O4'	4:E:70:PRO:HD2	2.18	0.43
4:D:299:LYS:HA	4:D:299:LYS:HD3	1.84	0.43
4:F:108:VAL:HA	4:F:111:THR:HG22	2.00	0.43
7:J:79:LEU:HD12	7:J:93:LEU:HG	2.01	0.43
2:2:26:DA:H5''	4:F:343:GLN:HG3	2.00	0.43
4:B:40:LEU:HD13	4:C:229:PHE:CE2	2.54	0.43
4:F:153:SER:O	4:F:213:ALA:HA	2.18	0.43
7:J:18:LEU:HG	7:J:144:TYR:HA	2.01	0.43
4:C:294:HIS:CG	4:C:295:PRO:HD2	2.53	0.43
4:D:3:LEU:HD21	4:D:305:LEU:HB3	2.01	0.43
7:I:103:MET:HE3	7:I:295:PRO:O	2.19	0.43
4:A:118:LEU:HD12	4:A:312:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:226:PHE:HA	7:J:229:TRP:CD1	2.53	0.43
7:J:305:LEU:HD22	7:J:305:LEU:HA	1.85	0.43
4:A:311:TYR:CE1	4:A:325:MET:HE1	2.54	0.43
4:B:51:LYS:HD3	4:B:55:GLN:HE21	1.82	0.43
4:E:345:LYS:HD2	4:E:345:LYS:HA	1.73	0.43
7:I:132:CYS:HB3	7:I:135:CYS:HB2	2.01	0.43
7:I:206:TRP:CE2	7:I:223:ARG:HD3	2.54	0.43
4:A:324:GLU:HG2	4:A:325:MET:N	2.34	0.43
7:I:337:LEU:HB2	7:I:339:CYS:SG	2.58	0.43
5:G:140:PHE:HZ	5:G:149:LEU:HD12	1.83	0.42
4:F:144:ARG:HD2	7:J:51:ARG:HH22	1.84	0.42
5:G:35:THR:HA	5:G:36:PRO:HD3	1.86	0.42
7:I:386:GLN:OE1	7:I:391:ASN:HA	2.19	0.42
7:J:226:PHE:HA	7:J:229:TRP:NE1	2.33	0.42
7:I:115:GLY:O	7:J:391:ASN:HB2	2.19	0.42
7:J:316:LEU:HD22	7:J:378:TYR:CD1	2.54	0.42
4:C:322:PRO:HD2	4:C:325:MET:HE3	1.99	0.42
4:F:131:ARG:HD3	4:F:266:ILE:HB	2.01	0.42
4:C:118:LEU:HD11	4:C:316:GLN:HG2	2.01	0.42
4:E:19:ILE:H	4:E:19:ILE:HG13	1.75	0.42
4:E:169:PRO:HG2	4:E:171:HIS:NE2	2.35	0.42
7:I:101:ASN:HB2	7:I:113:ILE:HG22	2.00	0.42
4:A:102:LYS:HA	4:C:287:GLU:O	2.19	0.42
5:G:116:LEU:HD23	5:G:116:LEU:HA	1.91	0.42
5:G:588:LEU:HD23	5:G:588:LEU:HA	1.83	0.42
7:J:302:ASN:C	7:J:302:ASN:OD1	2.63	0.42
5:G:26:LEU:HD12	5:G:26:LEU:HA	1.85	0.42
7:I:22:PHE:HD2	7:I:63:ILE:HD11	1.85	0.42
7:I:203:ILE:HD12	7:I:204:ALA:H	1.84	0.42
4:C:141:TRP:CD1	4:C:141:TRP:H	2.36	0.42
4:F:274:ASP:OD1	7:J:55:THR:HG23	2.20	0.42
6:H:34:LYS:HG3	6:H:35:TYR:CD1	2.54	0.42
6:H:111:THR:HG22	6:H:113:ALA:H	1.84	0.42
7:J:124:LEU:HD23	7:J:148:PHE:HE1	1.84	0.42
4:F:24:TRP:HB3	4:F:25:PRO:HD2	2.02	0.42
7:J:299:PHE:HE2	7:J:396:LEU:HD22	1.83	0.42
4:A:7:LEU:HA	4:A:102:LYS:O	2.20	0.42
4:B:321:LEU:HD12	4:B:326:ILE:HD11	2.02	0.42
7:J:41:VAL:HG21	7:J:82:LEU:HD11	2.01	0.42
7:J:286:LYS:HD2	7:J:286:LYS:HA	1.74	0.42
2:2:25:DT:H2'	2:2:26:DA:N7	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:157:LYS:HB3	4:D:157:LYS:HE2	1.87	0.41
5:G:110:MET:HB3	5:G:110:MET:HE2	1.71	0.41
1:1:12:A:O4'	4:E:340:GLY:HA2	2.20	0.41
4:B:91:VAL:HG13	4:B:209:PHE:HB2	2.02	0.41
7:I:337:LEU:HD21	7:I:381:TRP:HB2	2.02	0.41
2:2:35:DT:O4'	4:B:70:PRO:HD2	2.19	0.41
4:D:118:LEU:HD23	4:D:118:LEU:HA	1.87	0.41
4:D:160:PRO:HB2	4:D:195:LEU:HD21	2.02	0.41
5:G:221:MET:HG3	5:G:409:VAL:HG11	2.03	0.41
6:H:23:LYS:HD2	6:H:23:LYS:HA	1.60	0.41
6:H:72:ARG:NH1	6:H:72:ARG:HA	2.36	0.41
5:G:504:LEU:HD12	5:G:504:LEU:HA	1.90	0.41
4:D:345:LYS:HB2	5:G:197:TYR:CZ	2.55	0.41
4:E:283:GLY:N	4:E:293:ARG:HB2	2.32	0.41
4:F:186:HIS:HB3	4:F:189:TRP:HB2	2.02	0.41
5:G:631:LEU:HD23	5:G:631:LEU:HA	1.89	0.41
4:A:131:ARG:HD3	4:A:266:ILE:HB	2.03	0.41
4:D:40:LEU:HD13	4:E:229:PHE:CE2	2.56	0.41
7:J:194:GLU:H	7:J:196:HIS:CE1	2.39	0.41
4:A:294:HIS:CG	4:A:295:PRO:HD2	2.55	0.41
4:D:1:MET:HB3	4:D:306:GLU:O	2.20	0.41
4:C:299:LYS:HD3	4:C:299:LYS:HA	1.67	0.41
4:E:143:TRP:CD1	4:E:258:LYS:HE3	2.56	0.41
4:F:14:GLU:HA	4:F:14:GLU:OE2	2.20	0.41
4:F:154:ILE:O	4:F:170:PHE:HB2	2.21	0.41
5:G:536:ILE:O	5:G:536:ILE:HD12	2.21	0.41
5:G:571:ASN:HD22	5:G:603:ILE:HD12	1.86	0.41
7:I:20:SER:HB3	7:I:142:ALA:H	1.85	0.41
7:I:22:PHE:O	7:I:25:VAL:HG12	2.21	0.41
7:I:112:LEU:HD13	7:I:121:ARG:HG3	2.03	0.41
7:I:382:LEU:HD23	7:I:382:LEU:HA	1.91	0.41
2:2:49:DT:C4	2:2:50:DC:N4	2.89	0.41
4:C:283:GLY:H	4:C:293:ARG:HB2	1.86	0.41
4:E:237:LYS:HG2	4:E:240:ILE:HG12	2.03	0.41
4:F:192:LEU:HD12	4:F:192:LEU:HA	1.80	0.41
7:I:119:ILE:HD12	7:I:224:TRP:CD2	2.56	0.41
7:I:281:LYS:HA	7:I:285:GLY:HA3	2.03	0.41
7:I:379:CYS:HB3	7:J:73:ILE:HG23	2.03	0.41
4:B:42:MET:O	4:B:44:GLU:HG2	2.20	0.40
4:C:87:CYS:SG	4:C:215:PHE:HE1	2.44	0.40
4:F:91:VAL:HG13	4:F:209:PHE:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:45:LEU:HD22	7:J:56:PHE:CE2	2.56	0.40
2:2:45:DG:H2''	2:2:46:DG:O4'	2.20	0.40
4:D:4:PRO:HG2	4:D:7:LEU:HB2	2.03	0.40
4:D:329:LEU:HD12	4:D:329:LEU:HA	1.92	0.40
4:F:144:ARG:O	4:F:147:GLU:HG3	2.22	0.40
5:G:210:TYR:HB2	5:G:591:TYR:CE2	2.56	0.40
7:I:216:PRO:HG3	7:I:249:TRP:CH2	2.57	0.40
4:C:329:LEU:HD23	4:C:329:LEU:HA	1.92	0.40
4:E:86:GLU:HA	4:E:213:ALA:O	2.21	0.40
4:B:295:PRO:HG2	4:E:49:ALA:HB1	2.03	0.40
4:D:42:MET:HE3	4:D:42:MET:HB2	1.75	0.40
4:D:97:LEU:HD13	4:D:337:ILE:HG12	2.04	0.40
5:G:47:THR:HG23	5:G:131:ASN:O	2.21	0.40
7:I:310:GLN:O	7:I:314:THR:HG23	2.21	0.40
4:E:143:TRP:NE1	4:E:258:LYS:HG2	2.36	0.40
7:I:207:LEU:HA	7:I:223:ARG:HD2	2.04	0.40
7:J:105:PHE:CZ	7:J:120:PRO:HD3	2.57	0.40
7:J:309:PHE:CZ	7:J:396:LEU:HD12	2.57	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	
4	A	343/347 (99%)	335 (98%)	8 (2%)	0	100	100
4	B	343/347 (99%)	333 (97%)	10 (3%)	0	100	100
4	C	343/347 (99%)	330 (96%)	13 (4%)	0	100	100
4	D	344/347 (99%)	335 (97%)	9 (3%)	0	100	100
4	E	336/347 (97%)	323 (96%)	13 (4%)	0	100	100
4	F	287/347 (83%)	274 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	G	518/640 (81%)	490 (95%)	28 (5%)	0	100	100
6	H	177/198 (89%)	166 (94%)	11 (6%)	0	100	100
7	I	377/406 (93%)	336 (89%)	41 (11%)	0	100	100
7	J	339/406 (84%)	301 (89%)	38 (11%)	0	100	100
All	All	3407/3732 (91%)	3223 (95%)	184 (5%)	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	
4	A	291/303 (96%)	280 (96%)	11 (4%)	29	64
4	B	295/303 (97%)	284 (96%)	11 (4%)	30	64
4	C	298/303 (98%)	292 (98%)	6 (2%)	48	78
4	D	298/303 (98%)	291 (98%)	7 (2%)	44	76
4	E	298/303 (98%)	292 (98%)	6 (2%)	48	78
4	F	259/303 (86%)	242 (93%)	17 (7%)	15	43
5	G	419/488 (86%)	407 (97%)	12 (3%)	37	71
6	H	151/176 (86%)	145 (96%)	6 (4%)	28	62
7	I	247/368 (67%)	229 (93%)	18 (7%)	13	38
7	J	258/368 (70%)	244 (95%)	14 (5%)	20	51
All	All	2814/3218 (87%)	2706 (96%)	108 (4%)	30	64

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	91	VAL
4	A	118	LEU
4	A	123	VAL
4	A	138	ASN

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Mol	Chain	Res	Type
4	A	180	THR
4	A	212	SER
4	A	236	GLU
4	A	244	THR
4	A	246	VAL
4	A	309	ASP
4	A	342	LEU
4	B	91	VAL
4	B	228	VAL
4	B	233	VAL
4	B	246	VAL
4	B	285	HIS
4	B	289	VAL
4	B	297	THR
4	B	313	GLU
4	B	326	ILE
4	B	335	ASN
4	B	337	ILE
4	C	8	SER
4	C	180	THR
4	C	181	ASN
4	C	320	VAL
4	C	342	LEU
4	C	345	LYS
4	D	10	MET
4	D	107	GLU
4	D	152	THR
4	D	187	LYS
4	D	282	TYR
4	D	335	ASN
4	D	344	GLN
4	E	19	ILE
4	E	42	MET
4	E	67	GLN
4	E	91	VAL
4	E	286	ARG
4	E	288	ASP
4	F	1	MET
4	F	21	LEU
4	F	22	VAL
4	F	38	VAL
4	F	91	VAL

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Mol	Chain	Res	Type
4	F	151	SER
4	F	190	ASP
4	F	192	LEU
4	F	202	GLN
4	F	211	VAL
4	F	215	PHE
4	F	228	VAL
4	F	230	LYS
4	F	246	VAL
4	F	285	HIS
4	F	289	VAL
4	F	297	THR
5	G	76	PHE
5	G	97	VAL
5	G	98	ILE
5	G	146	VAL
5	G	177	ILE
5	G	183	LEU
5	G	225	CYS
5	G	449	ILE
5	G	481	VAL
5	G	559	ILE
5	G	606	LEU
5	G	608	ILE
6	H	20	ILE
6	H	23	LYS
6	H	42	VAL
6	H	89	THR
6	H	99	VAL
6	H	132	ILE
7	I	124	LEU
7	I	147	HIS
7	I	153	TYR
7	I	156	GLU
7	I	159	VAL
7	I	203	ILE
7	I	268	PHE
7	I	274	SER
7	I	276	ASN
7	I	278	LEU
7	I	280	VAL
7	I	288	LEU

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Mol	Chain	Res	Type
7	I	323	LEU
7	I	333	ILE
7	I	344	VAL
7	I	366	ILE
7	I	367	VAL
7	I	374	LEU
7	J	86	THR
7	J	93	LEU
7	J	101	ASN
7	J	118	VAL
7	J	151	TYR
7	J	173	TYR
7	J	175	TYR
7	J	190	SER
7	J	230	TRP
7	J	231	SER
7	J	245	PHE
7	J	281	LYS
7	J	305	LEU
7	J	382	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	171	HIS
4	A	227	GLN
4	B	69	ASN
4	B	220	ASN
4	B	343	GLN
4	C	23	ASN
4	C	55	GLN
4	C	171	HIS
4	C	191	ASN
4	C	344	GLN
4	D	204	ASN
4	D	238	ASN
4	E	5	ASN
4	E	23	ASN
4	E	138	ASN
4	F	146	ASN
4	F	171	HIS
4	F	186	HIS

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Mol	Chain	Res	Type
4	F	202	GLN
4	F	296	ASN
4	F	335	ASN
5	G	396	ASN
5	G	556	GLN
6	H	187	ASN
7	I	29	ASN
7	I	64	ASN
7	I	350	GLN
7	J	35	HIS
7	J	101	ASN
7	J	139	HIS
7	J	147	HIS
7	J	228	HIS
7	J	386	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	55/60 (91%)	24 (43%)	0

All (24) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	3	G
1	1	9	G
1	1	10	A
1	1	14	A
1	1	15	C
1	1	20	A
1	1	21	G
1	1	22	C
1	1	26	A
1	1	27	G
1	1	32	U
1	1	33	G
1	1	34	C
1	1	35	U
1	1	36	A
1	1	39	A
1	1	40	G

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Mol	Chain	Res	Type
1	1	41	G
1	1	48	G
1	1	53	A
1	1	54	U
1	1	55	A
1	1	56	G
1	1	60	G

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

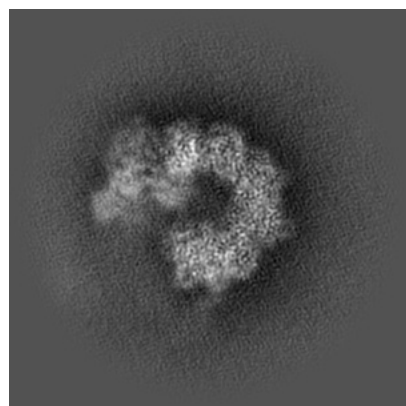
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65340. These allow visual inspection of the internal detail of the map and identification of artifacts.

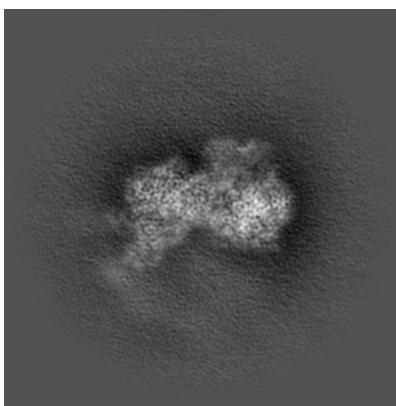
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

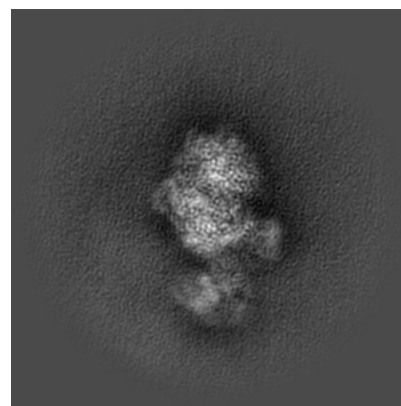
6.1.1 Primary map



X

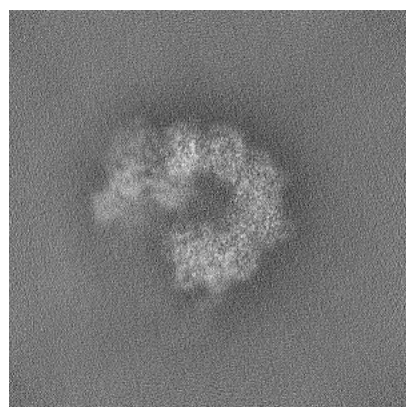


Y

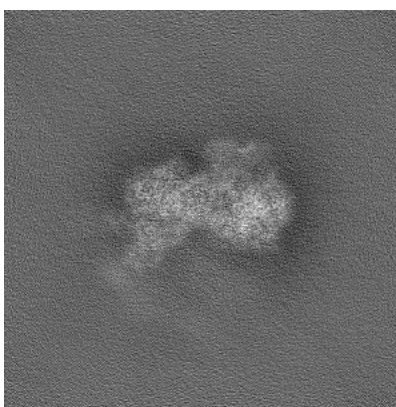


Z

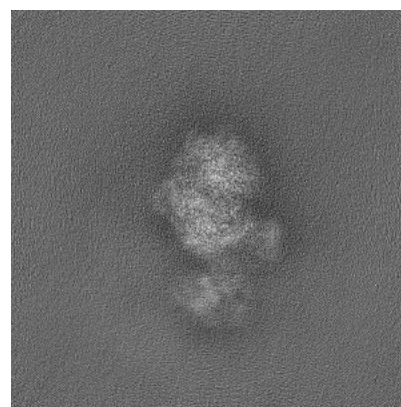
6.1.2 Raw map



X



Y

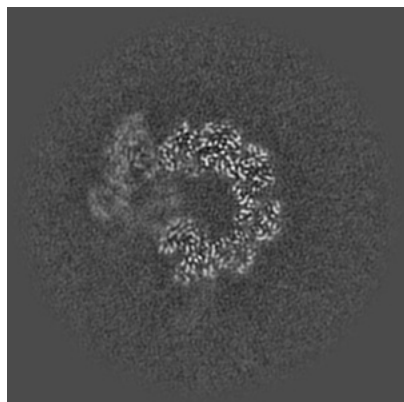


Z

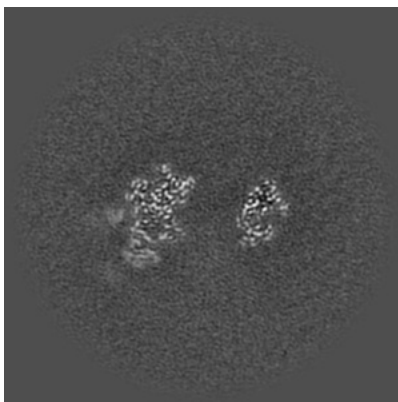
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

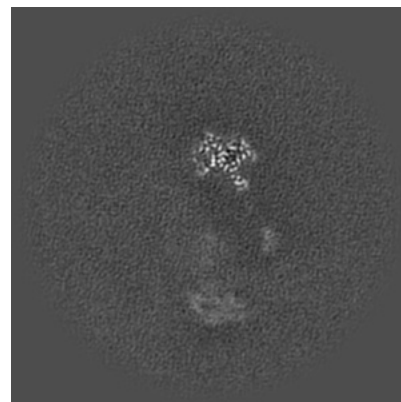
6.2.1 Primary map



X Index: 230

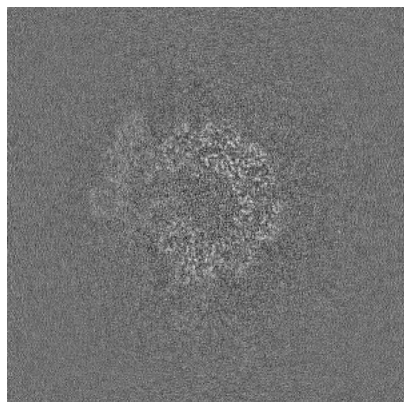


Y Index: 230

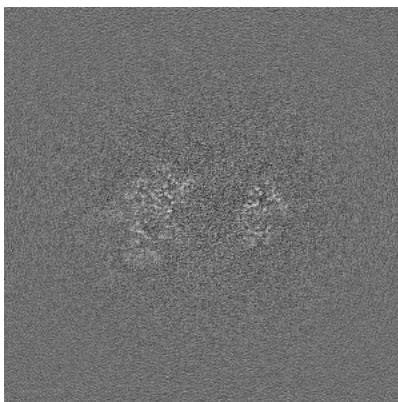


Z Index: 230

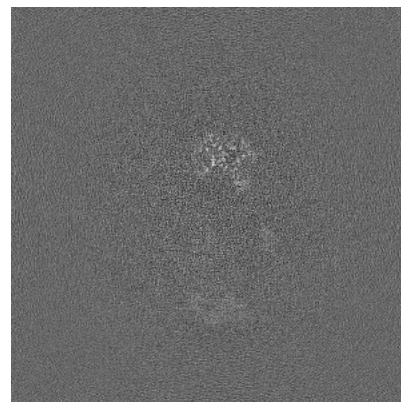
6.2.2 Raw map



X Index: 230



Y Index: 230

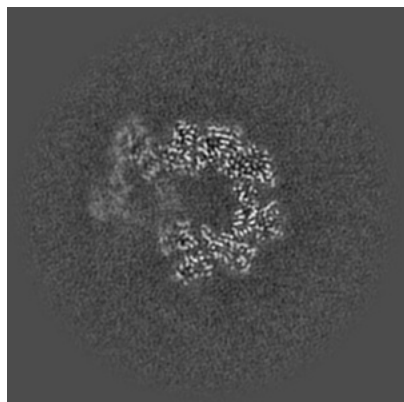


Z Index: 230

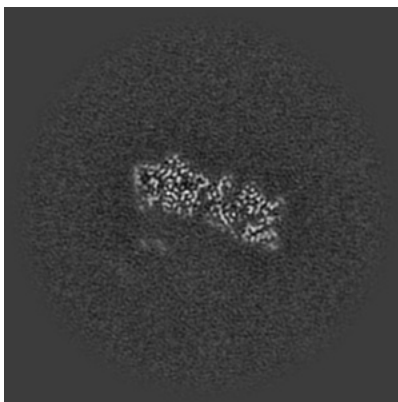
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

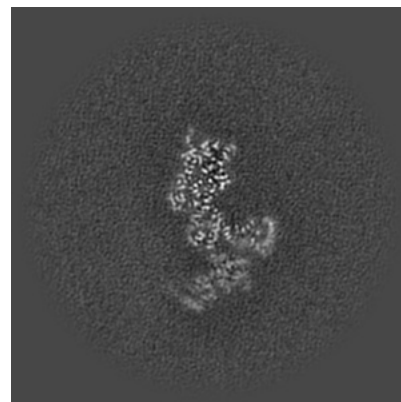
6.3.1 Primary map



X Index: 234

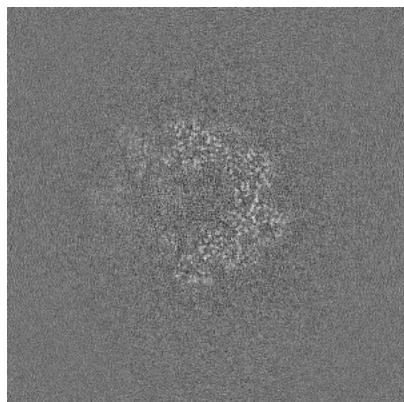


Y Index: 265

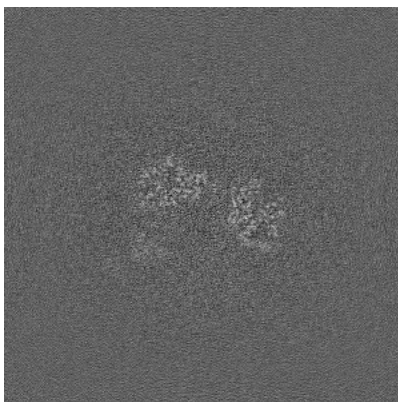


Z Index: 276

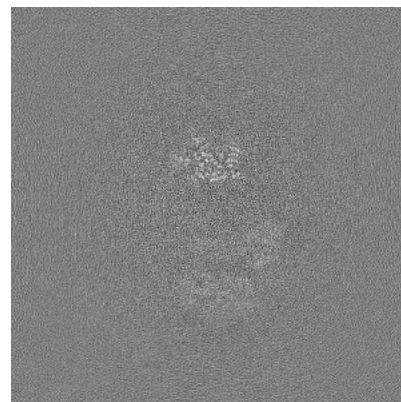
6.3.2 Raw map



X Index: 239



Y Index: 258

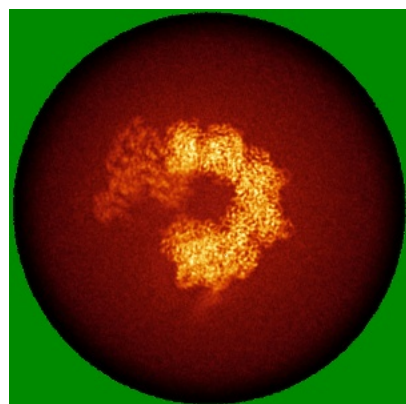


Z Index: 250

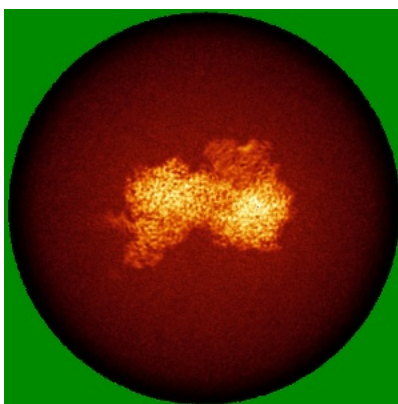
The images above show the largest variance slices of the map in three orthogonal directions.

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

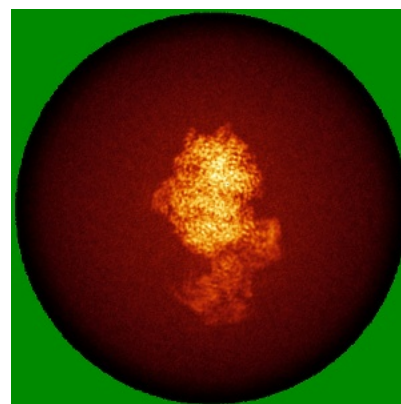
6.4.1 Primary map



X

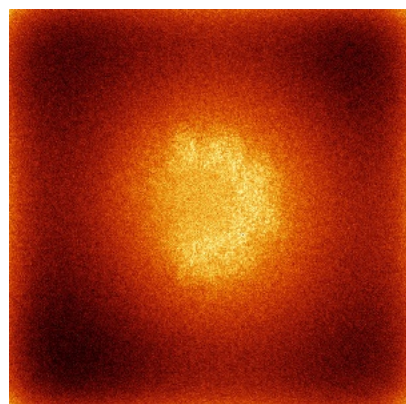


Y

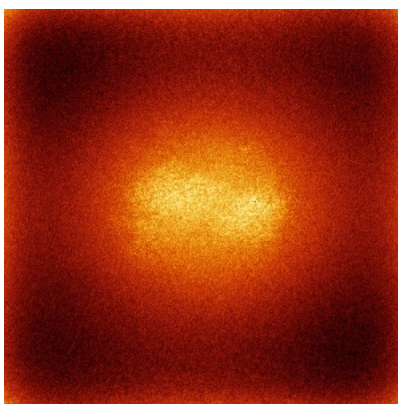


Z

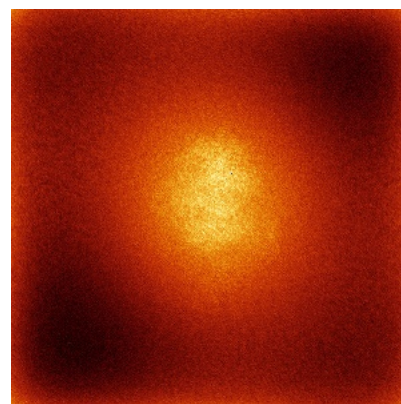
6.4.2 Raw map



X



Y

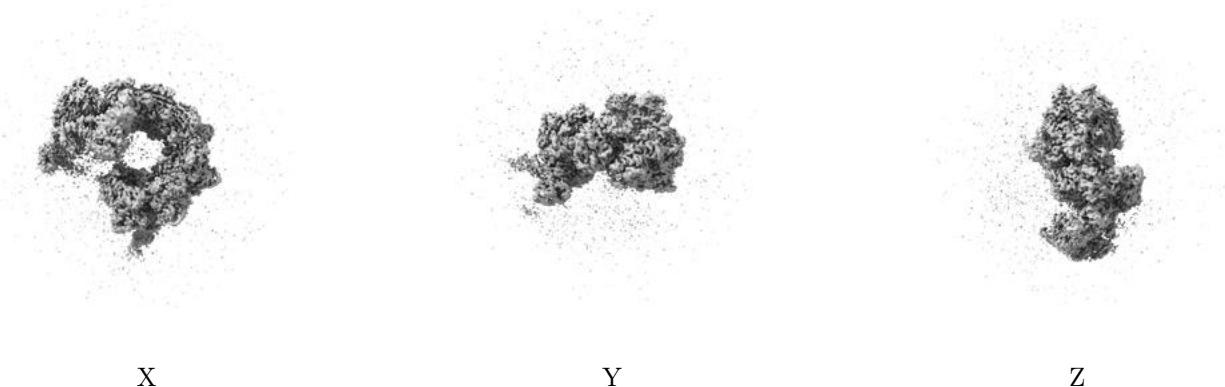


Z

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.

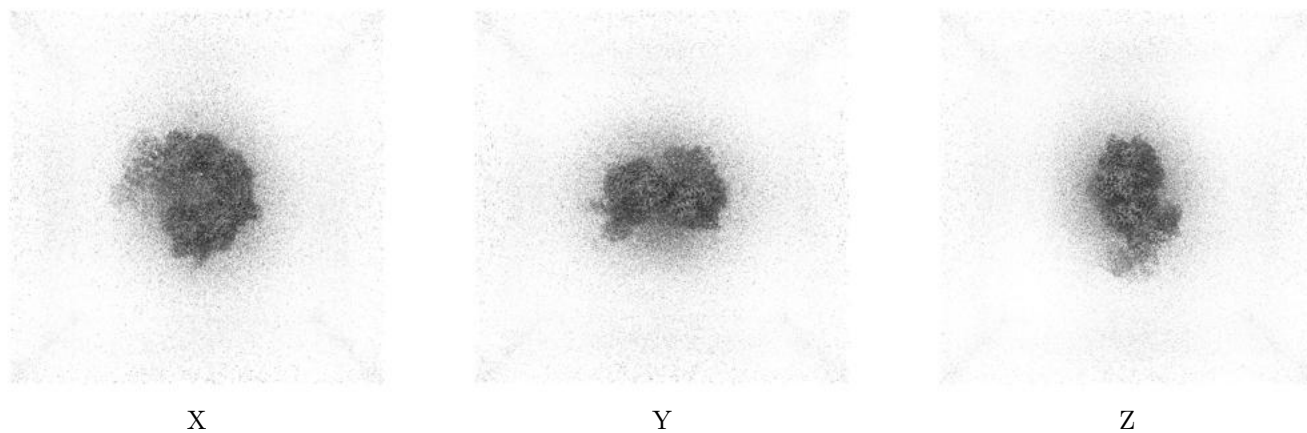
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.19. 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.

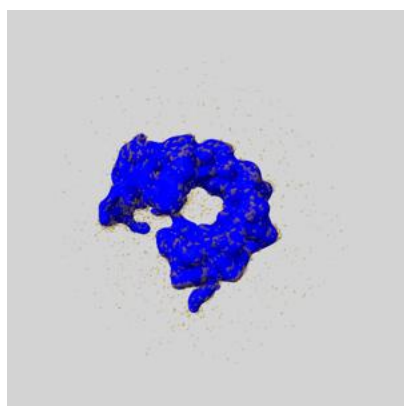
6.6 Mask visualisation [i](#)

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

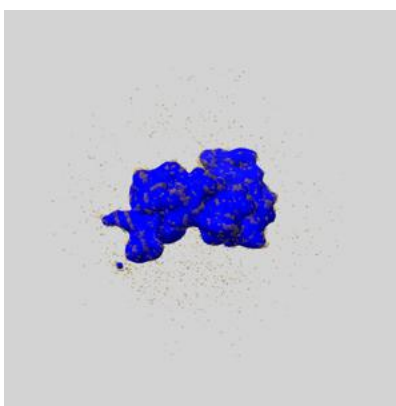
A mask typically either:

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

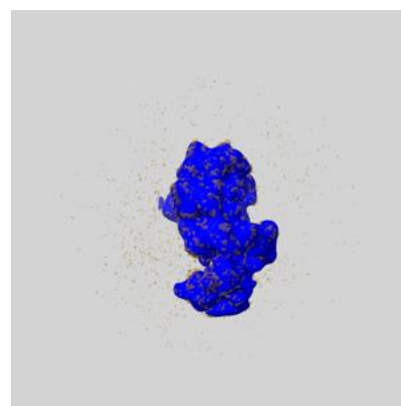
6.6.1 emd_65340_msk_1.map [i](#)



X



Y

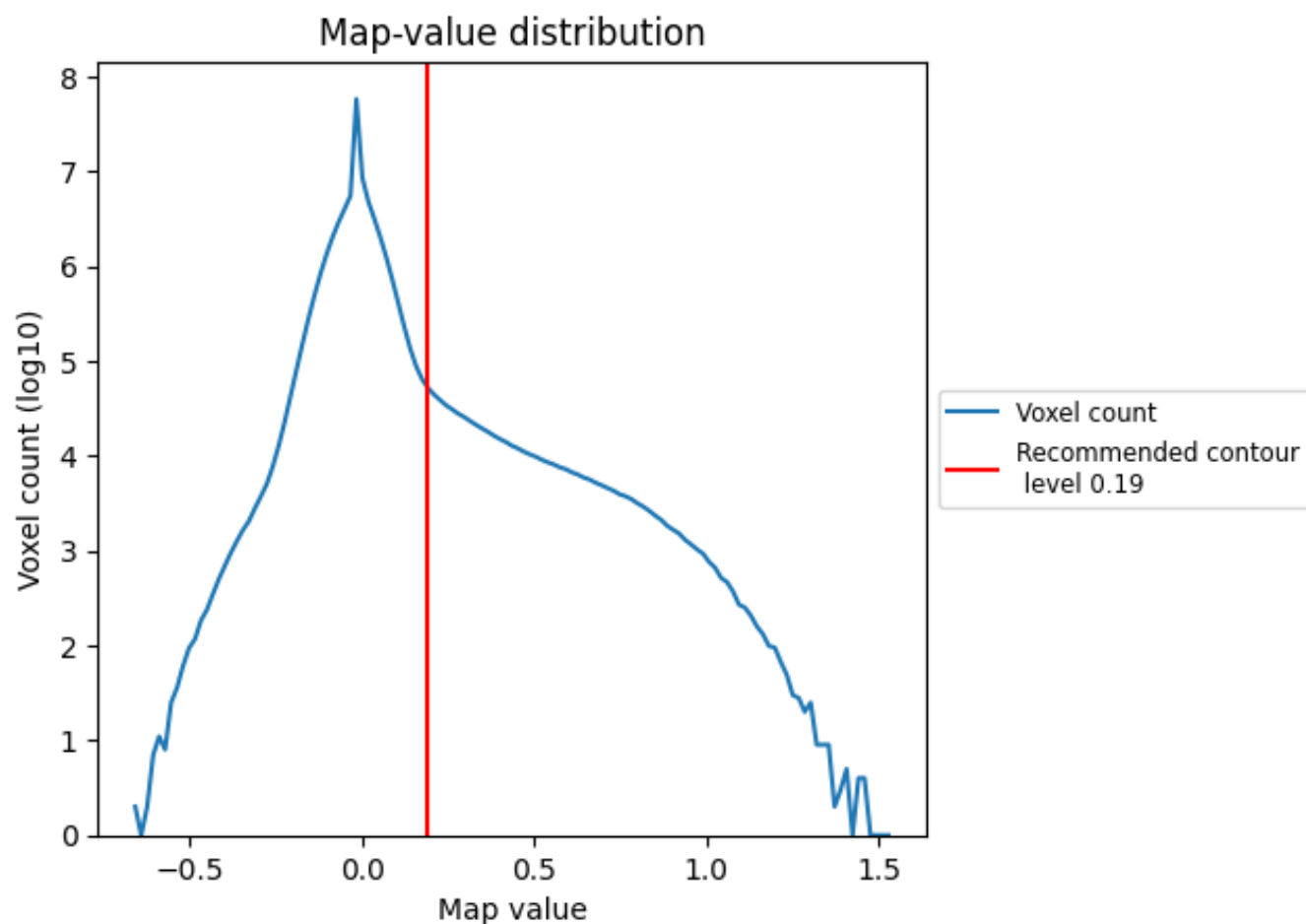


Z

7 Map analysis [i](#)

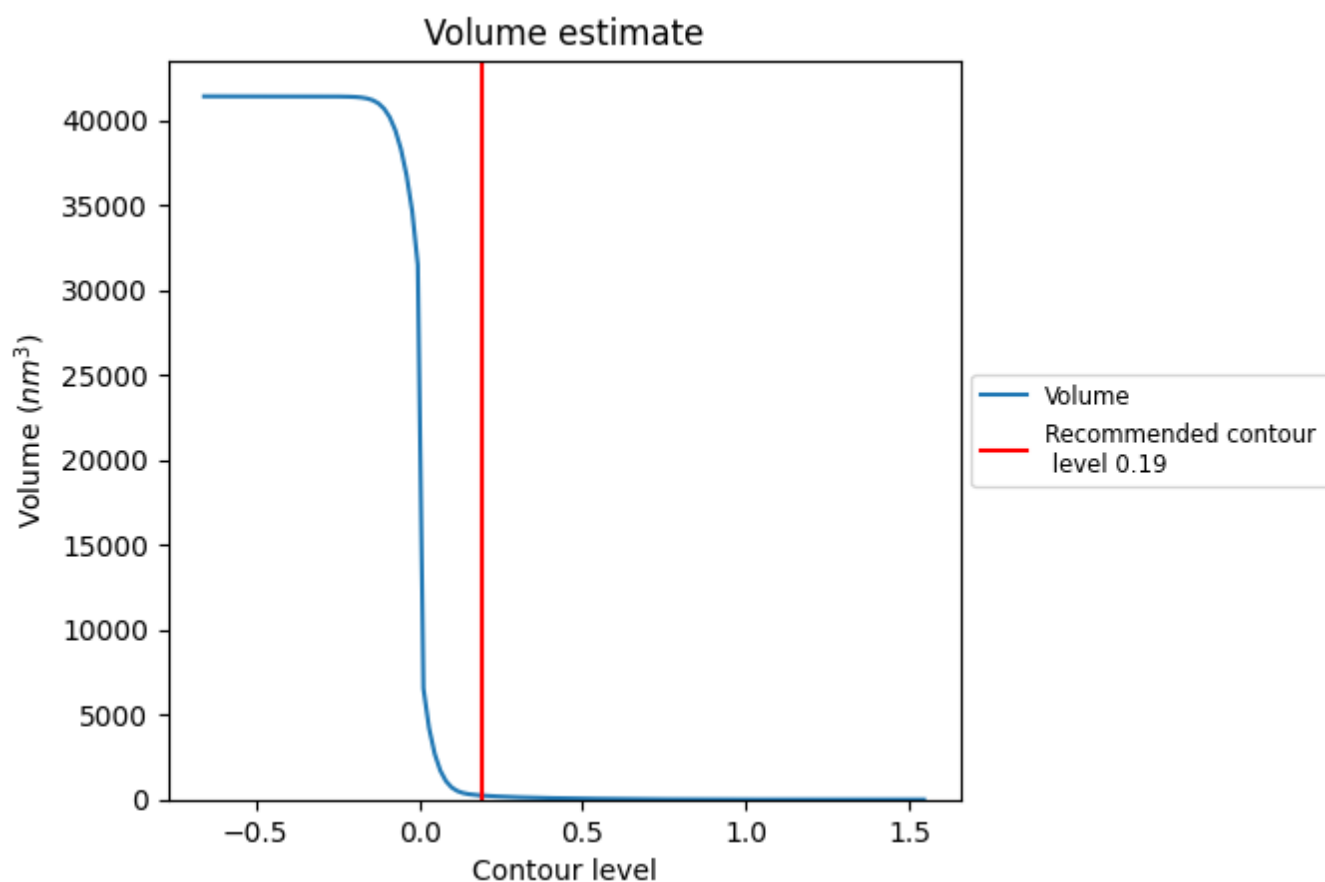
This section contains the results of statistical analysis of the map.

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.

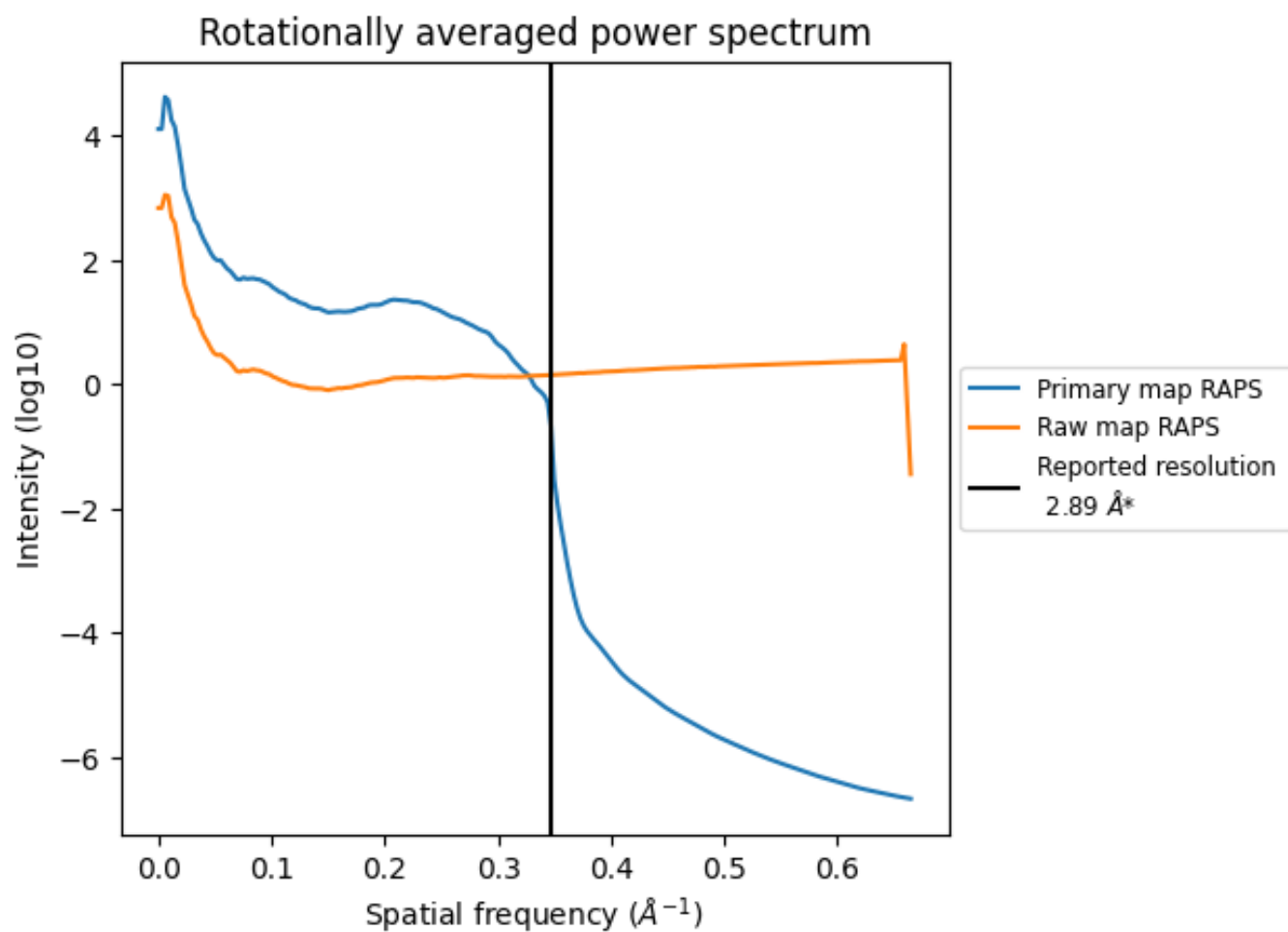
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 241 nm³; this corresponds to an approximate mass of 217 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 ⓘ

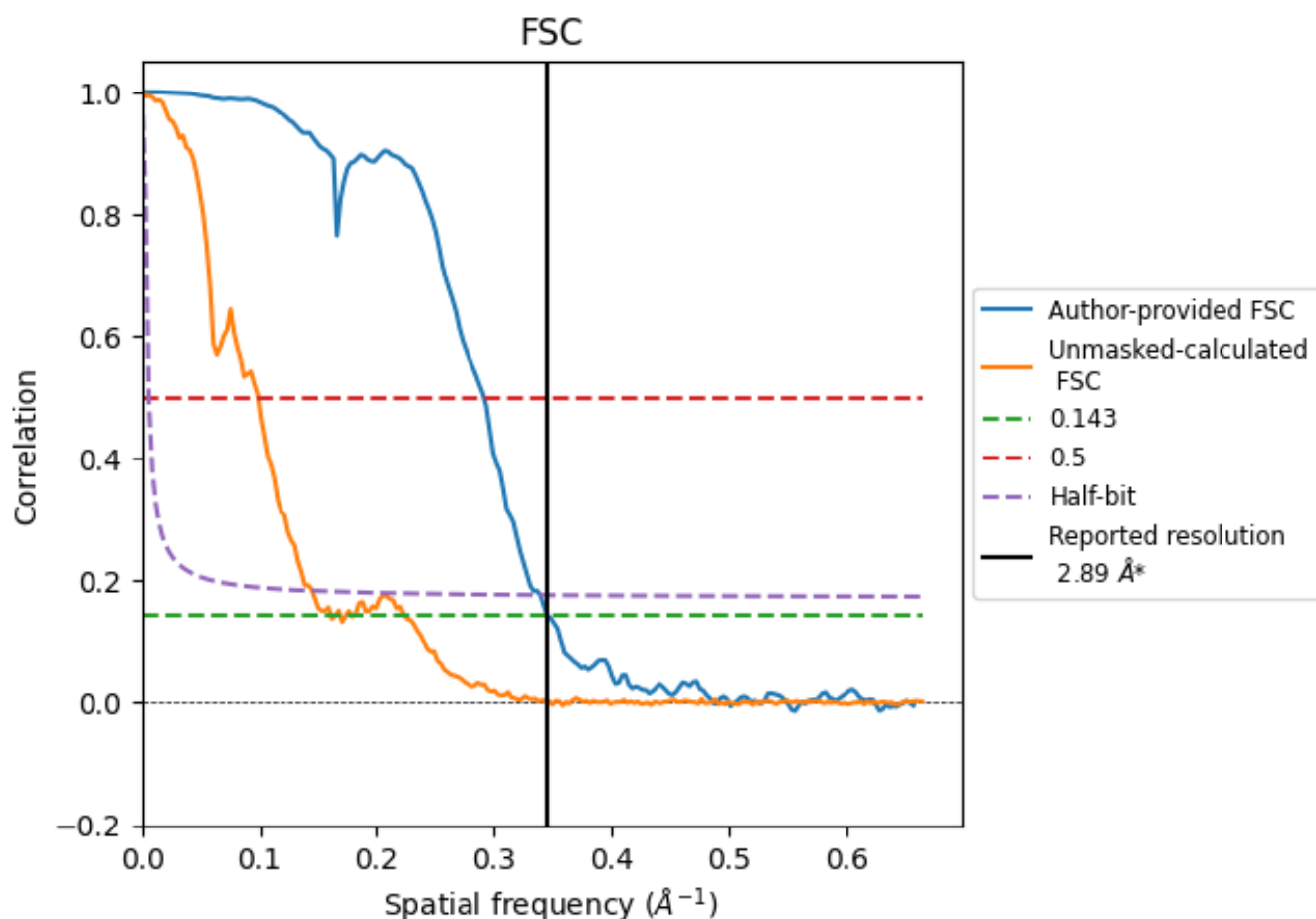


*Reported resolution corresponds to spatial frequency of 0.346 Å⁻¹

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 0.346 \AA^{-1}

8.2 Resolution estimates [i](#)

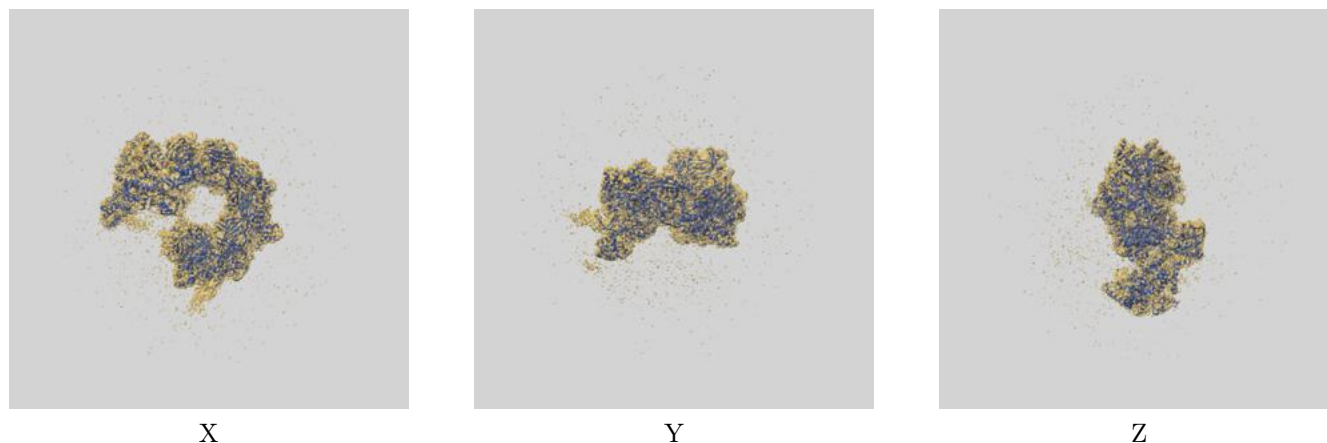
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	2.89	3.43	2.95
Unmasked-calculated*	6.21	10.13	6.89

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

9 Map-model fit [i](#)

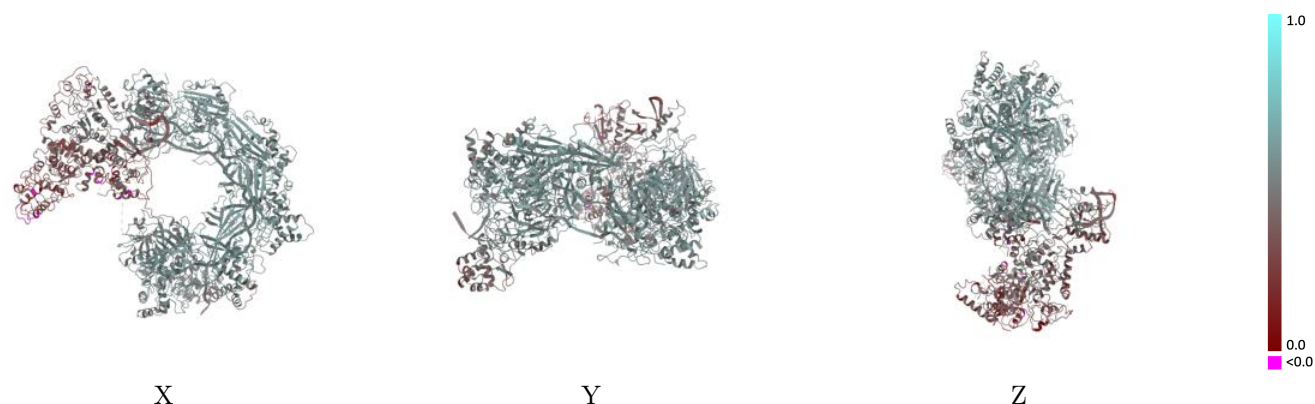
This section contains information regarding the fit between EMDB map EMD-65340 and PDB model 9VTR. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



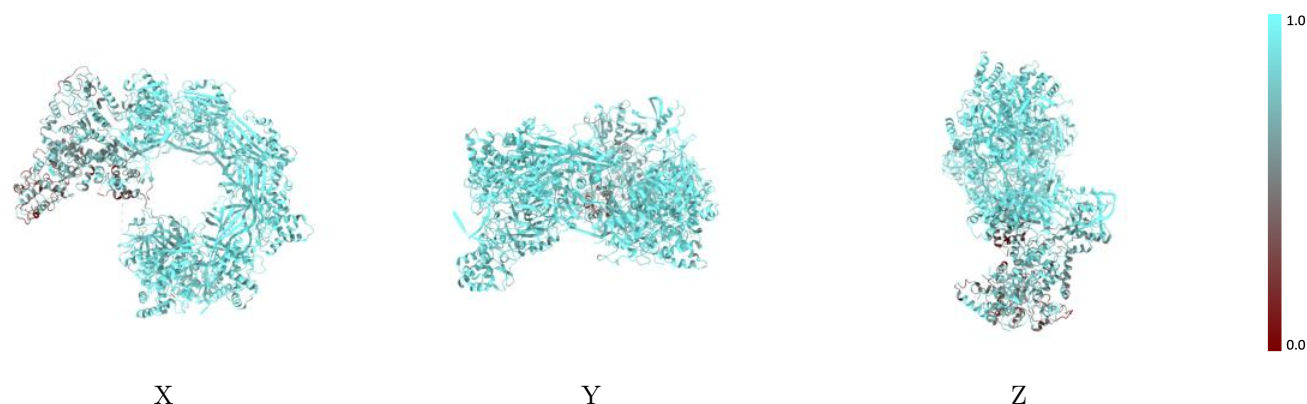
The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



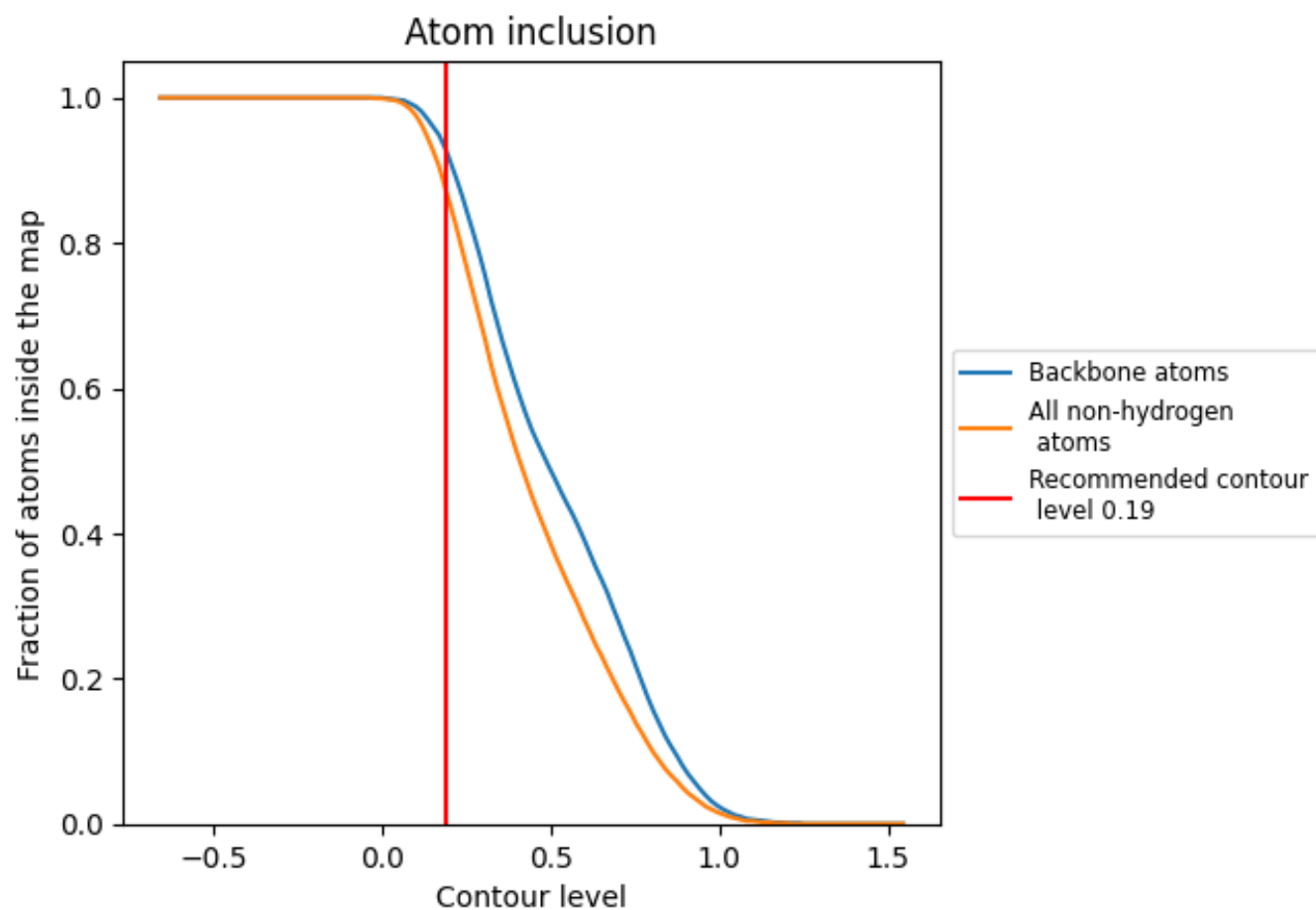
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.19).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 87% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8710	 0.4960
1	 0.9680	 0.5050
2	 0.8700	 0.5070
3	 0.9840	 0.4660
A	 0.9420	 0.5560
B	 0.9440	 0.5590
C	 0.9460	 0.5570
D	 0.9270	 0.5470
E	 0.9400	 0.5550
F	 0.9280	 0.5330
G	 0.8740	 0.4940
H	 0.8140	 0.3760
I	 0.6310	 0.3440
J	 0.6970	 0.3780

