



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:56 PM UTC

PDB ID : 9VTP / pdb_00009vtp
EMDB ID : EMD-65338
Title : Target DNA-bound type I-F3 TniQ-Cascade of *Vibrio parahaemolyticus* in partial R-loop state
Authors : Ishihara, K.; Numata, T.
Deposited on : 2025-07-11
Resolution : 2.68 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:

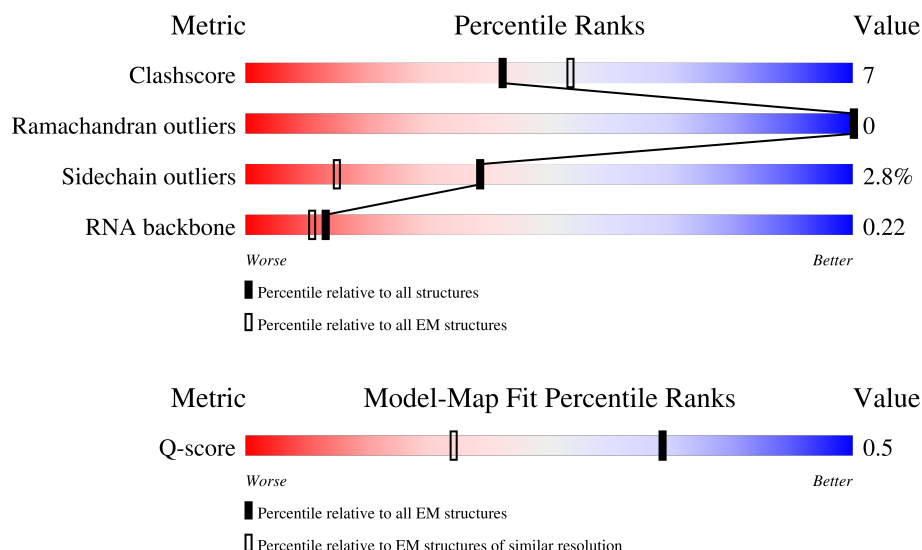
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.68 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	9255 (2.18 - 3.18)

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	 87% 12% .
4	B	347	 89% 10% .
4	C	347	 90% 10% .
4	D	347	 85% 14% .
4	E	347	 86% 13% .
4	F	347	 69% 16% . 13%
5	G	640	 9% 80% 12% 8%
6	H	198	 7% 71% 24% . .
7	I	406	 25% 69% 25% . 6%
7	J	406	 11% 66% 21% . 12%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 29818 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 from *Vibrio alginolyticus* K08M03 plasmid pL300.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	35	Total	C	N	O	P	0	0
			721	343	125	218	35		

- Molecule 3 is a DNA chain called Non-target strand DNA from *Vibrio alginolyticus* strain K08M3 plasmid pL300.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	6	Total	C	N	O	P	0	0
			119	56	22	35	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
			2752	1756	463	520	13		
4	C	345	Total	C	N	O	S	0	0
			2767	1764	464	526	13		
4	D	346	Total	C	N	O	S	0	0
			2771	1766	465	527	13		
4	E	345	Total	C	N	O	S	0	0
			2767	1764	464	526	13		
4	F	301	Total	C	N	O	S	0	0
			2418	1552	405	449	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	588	Total	C	N	O	S	0	0
			4425	2793	798	812	22		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	358	UNK	THR	conflict	UNP Q87GC9
G	359	UNK	THR	conflict	UNP Q87GC9
G	360	UNK	PRO	conflict	UNP Q87GC9
G	361	UNK	THR	conflict	UNP Q87GC9
G	362	UNK	HIS	conflict	UNP Q87GC9
G	363	UNK	GLU	conflict	UNP Q87GC9
G	364	UNK	GLU	conflict	UNP Q87GC9
G	365	UNK	LYS	conflict	UNP Q87GC9
G	366	UNK	LEU	conflict	UNP Q87GC9
G	367	UNK	ASP	conflict	UNP Q87GC9
G	368	UNK	ILE	conflict	UNP Q87GC9
G	369	UNK	ARG	conflict	UNP Q87GC9
G	370	UNK	LYS	conflict	UNP Q87GC9
G	371	UNK	LEU	conflict	UNP Q87GC9
G	372	UNK	THR	conflict	UNP Q87GC9
G	373	UNK	GLU	conflict	UNP Q87GC9
G	374	UNK	ARG	conflict	UNP Q87GC9
G	375	UNK	PHE	conflict	UNP Q87GC9
G	376	UNK	ASN	conflict	UNP Q87GC9
G	377	UNK	VAL	conflict	UNP Q87GC9
G	378	UNK	ASP	conflict	UNP Q87GC9
G	379	UNK	LEU	conflict	UNP Q87GC9
G	380	UNK	ALA	conflict	UNP Q87GC9
G	381	UNK	LYS	conflict	UNP Q87GC9
G	381A	UNK	THR	conflict	UNP Q87GC9
G	381B	UNK	LYS	conflict	UNP Q87GC9
G	381C	UNK	PHE	conflict	UNP Q87GC9
G	381D	UNK	ALA	conflict	UNP Q87GC9
G	381E	UNK	ASN	conflict	UNP Q87GC9
G	381F	UNK	ARG	conflict	UNP Q87GC9
G	381G	UNK	TYR	conflict	UNP Q87GC9
G	381H	UNK	ALA	conflict	UNP Q87GC9
G	381I	UNK	TYR	conflict	UNP Q87GC9
G	381J	UNK	ASP	conflict	UNP Q87GC9
G	382	UNK	PRO	conflict	UNP Q87GC9
G	383	UNK	LEU	conflict	UNP Q87GC9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	384	UNK	LEU	conflict	UNP Q87GC9
G	385	UNK	THR	conflict	UNP Q87GC9
G	386	UNK	GLN	conflict	UNP Q87GC9
G	387	UNK	LEU	conflict	UNP Q87GC9
G	388	UNK	ILE	conflict	UNP Q87GC9
G	389	UNK	TYR	conflict	UNP Q87GC9
G	389A	UNK	ASN	conflict	UNP Q87GC9
G	389B	UNK	CYS	conflict	UNP Q87GC9
G	389C	UNK	ILE	conflict	UNP Q87GC9
G	389D	UNK	GLY	conflict	UNP Q87GC9
G	389E	UNK	SER	conflict	UNP Q87GC9
G	389F	UNK	ILE	conflict	UNP Q87GC9
G	389G	UNK	ILE	conflict	UNP Q87GC9
G	389H	UNK	HIS	conflict	UNP Q87GC9
G	389I	UNK	SER	conflict	UNP Q87GC9
G	389J	UNK	PRO	conflict	UNP Q87GC9
G	389K	UNK	PRO	conflict	UNP Q87GC9
G	389L	UNK	GLN	conflict	UNP Q87GC9
G	389M	UNK	TYR	conflict	UNP Q87GC9
G	389N	UNK	ALA	conflict	UNP Q87GC9
G	389O	UNK	PRO	conflict	UNP Q87GC9
G	389P	UNK	LYS	conflict	UNP Q87GC9
G	389Q	UNK	CYS	conflict	UNP Q87GC9
G	389R	UNK	GLU	conflict	UNP Q87GC9
G	389S	UNK	GLY	conflict	UNP Q87GC9
G	389T	UNK	ASN	conflict	UNP Q87GC9
G	389U	UNK	ASP	conflict	UNP Q87GC9
G	389V	UNK	ASP	conflict	UNP Q87GC9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	193	Total	C	N	O	S	0	0
			1550	982	275	288	5		

- Molecule 7 is a protein called TniQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	383	Total	C	N	O	S	0	0
			2911	1858	507	527	19		
7	J	358	Total	C	N	O	S	0	0
			2670	1698	470	483	19		

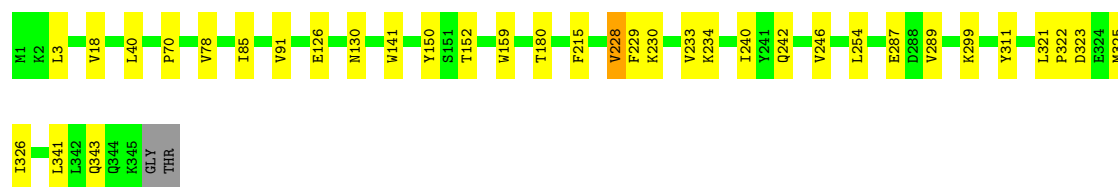
There are 14 discrepancies between the modelled and reference sequences:

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
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).

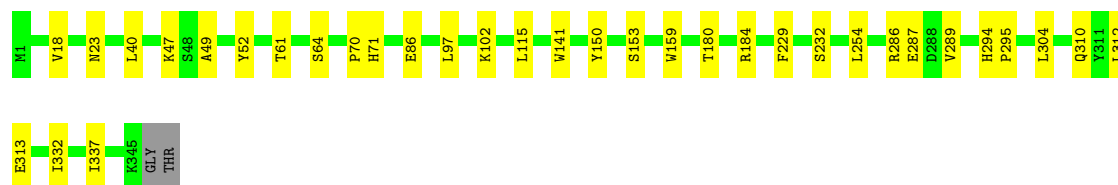
Mol	Chain	Residues	Atoms	AltConf
8	1	1	Total Mg 1 1	0

Chain B:  89% 10%



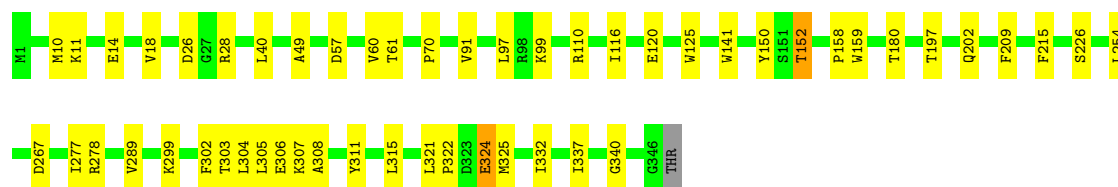
- Molecule 4: Type I-F CRISPR-associated protein Csy3

Chain C:  90% 10%



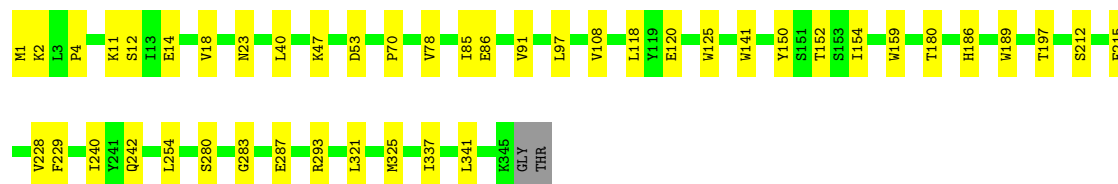
- Molecule 4: Type I-F CRISPR-associated protein Csy3

Chain D:  85% 14%



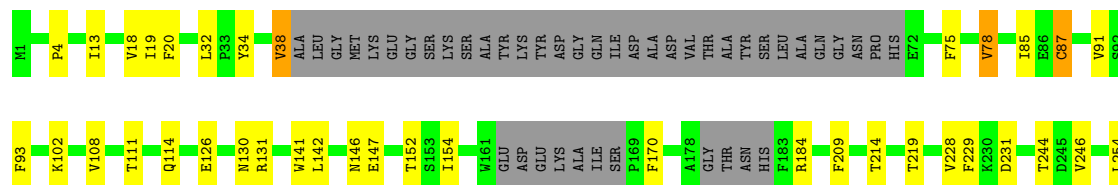
- Molecule 4: Type I-F CRISPR-associated protein Csy3

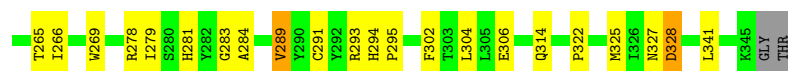
Chain E:  86% 13%



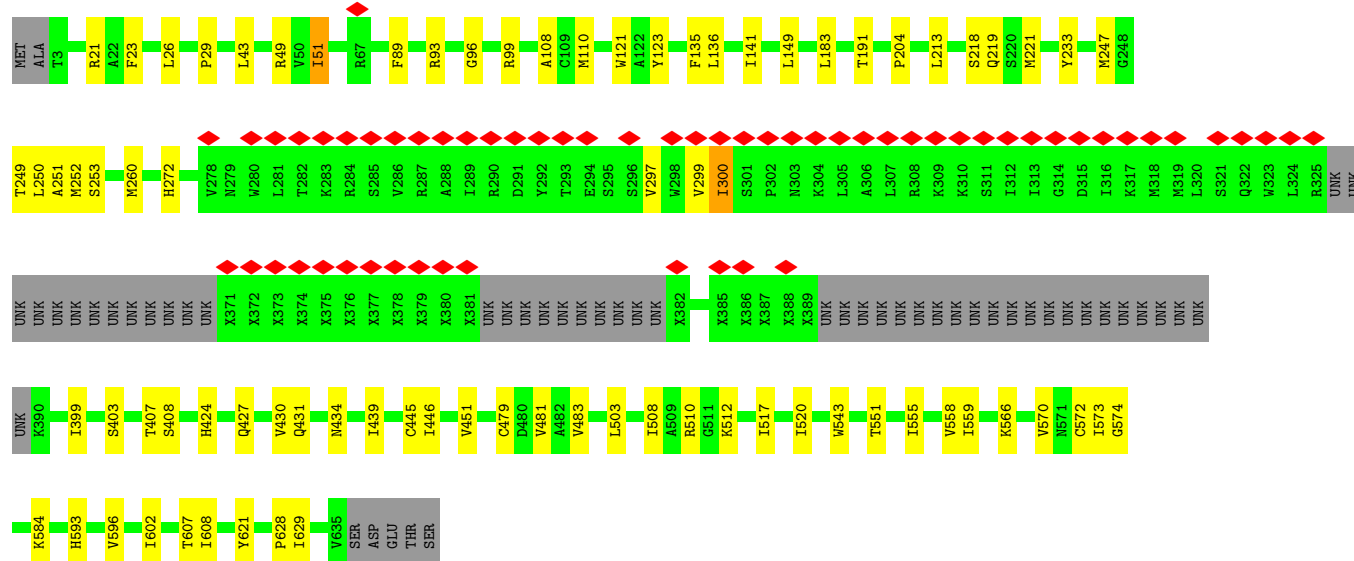
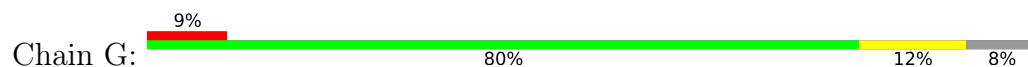
- Molecule 4: Type I-F CRISPR-associated protein Csy3

Chain F:  69% 16% 13%

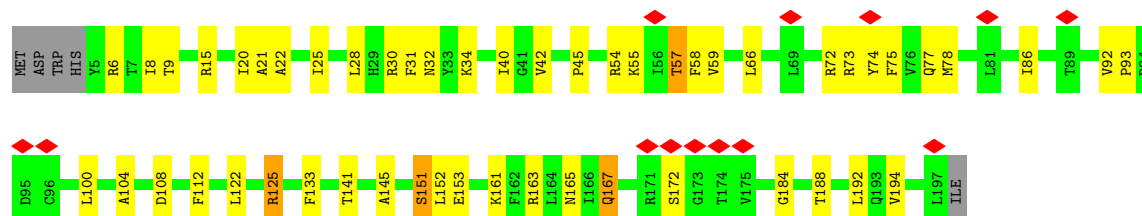




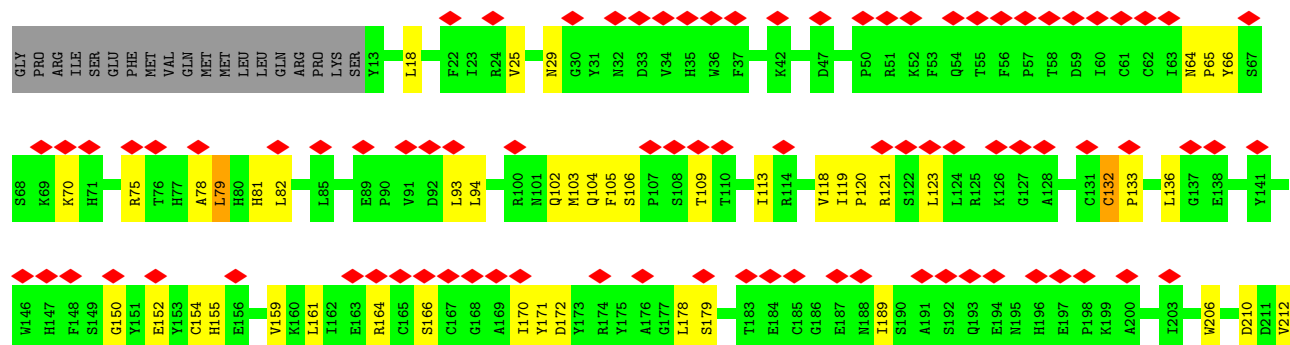
• Molecule 5: CRISPR-associated protein Csy2

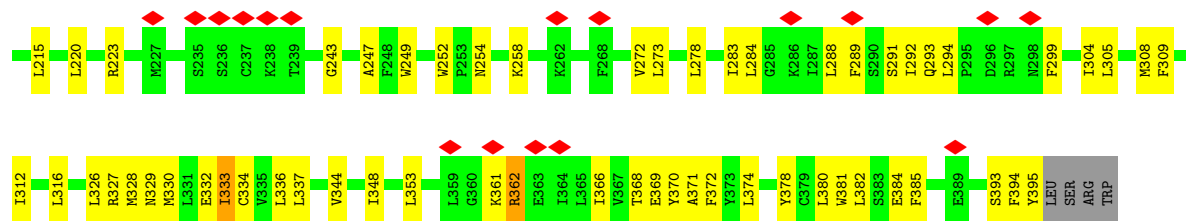


• Molecule 6: CRISPR-associated protein, Csy4 family

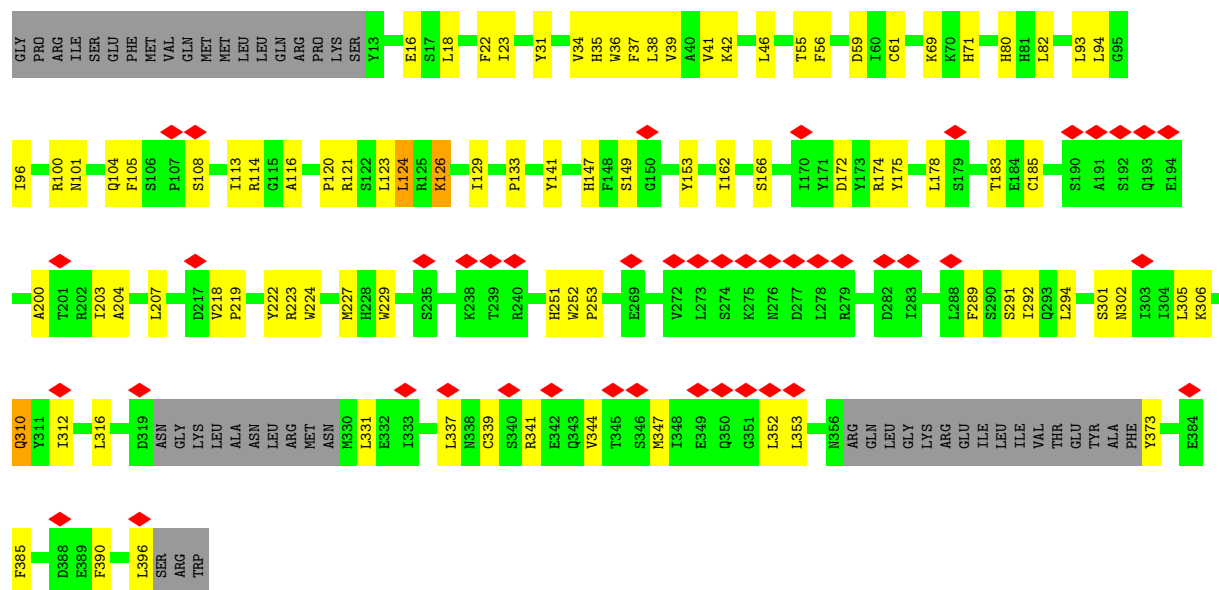


• Molecule 7: TniQ





• Molecule 7: ThiQ



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	31509	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 ($e^-/\text{\AA}^2$)	50.31	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	1.925	Depositor
Minimum map value	-0.691	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.16	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 [i](#)

5.1 Standard geometry [i](#)

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	0.14	0/1368	0.33	0/2129
2	2	0.20	0/806	0.46	0/1244
3	3	0.15	0/132	0.27	0/200
4	A	0.12	0/2797	0.27	0/3800
4	B	0.12	0/2825	0.27	0/3836
4	C	0.12	0/2840	0.26	0/3854
4	D	0.12	0/2844	0.27	0/3859
4	E	0.12	0/2840	0.28	0/3854
4	F	0.12	0/2482	0.29	0/3369
5	G	0.11	0/4421	0.28	0/6014
6	H	0.12	0/1583	0.38	0/2130
7	I	0.13	0/2985	0.38	0/4061
7	J	0.14	0/2736	0.39	0/3724
All	All	0.13	0/30659	0.31	0/42074

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1221	0	620	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2	721	0	398	18	0
3	3	119	0	67	1	0
4	A	2725	0	2625	29	0
4	B	2752	0	2664	28	0
4	C	2767	0	2685	25	0
4	D	2771	0	2688	39	0
4	E	2767	0	2685	29	0
4	F	2418	0	2336	36	0
5	G	4425	0	4175	48	0
6	H	1550	0	1520	34	0
7	I	2911	0	2641	70	0
7	J	2670	0	2345	56	0
8	1	1	0	0	0	0
All	All	29818	0	27449	383	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 (383) 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)
6:H:75:PHE:HA	6:H:78:MET:HE3	1.50	0.93
7:I:164:ARG:HG2	7:I:166:SER:H	1.41	0.83
5:G:407:THR:HG22	5:G:572:CYS:HB2	1.63	0.79
4:A:321:LEU:HD12	4:A:325:MET:HE1	1.66	0.78
7:I:178:LEU:HD23	7:I:179:SER:H	1.50	0.77
4:B:321:LEU:HD12	4:B:322:PRO:HD2	1.67	0.77
7:I:133:PRO:HB3	7:I:189:ILE:HG23	1.71	0.72
4:F:322:PRO:HD2	4:F:325:MET:HE3	1.72	0.71
5:G:446:ILE:HA	5:G:483:VAL:HG12	1.73	0.70
7:J:337:LEU:HD11	7:J:385:PHE:HB2	1.73	0.70
4:F:283:GLY:H	4:F:293:ARG:HB2	1.57	0.70
6:H:161:LYS:HZ1	6:H:163:ARG:HH21	1.38	0.69
7:I:243:GLY:HA2	7:I:247:ALA:HB3	1.75	0.69
7:J:302:ASN:C	7:J:306:LYS:HZ2	2.01	0.68
4:E:47:LYS:O	4:E:47:LYS:HD3	1.94	0.68
7:J:218:VAL:HG23	7:J:301:SER:HB3	1.76	0.67
7:I:104:GLN:HB3	7:I:293:GLN:HE22	1.60	0.67
5:G:26:LEU:HD12	5:G:253:SER:HB2	1.76	0.66
6:H:40:ILE:HD11	6:H:58:PHE:HB3	1.78	0.66
4:A:23:ASN:HD21	4:A:86:GLU:HB2	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:337:LEU:HD23	7:J:339:CYS:HB2	1.77	0.65
7:I:278:LEU:HD21	7:I:283:ILE:HG13	1.78	0.65
7:J:80:HIS:HB2	7:J:94:LEU:HD21	1.79	0.65
7:I:25:VAL:O	7:I:29:ASN:HB2	1.97	0.64
4:B:159:TRP:HB2	4:E:150:TYR:HE1	1.62	0.64
7:I:312:ILE:HD11	7:I:374:LEU:HD21	1.78	0.64
7:J:96:ILE:HG23	7:J:114:ARG:HH21	1.63	0.63
7:J:69:LYS:N	7:J:69:LYS:HE2	2.13	0.63
1:I:45:A:C4	6:H:163:ARG:HD2	2.32	0.63
4:A:66:ALA:HB2	4:F:291:CYS:HB2	1.79	0.63
7:I:220:LEU:HA	7:I:223:ARG:HB2	1.80	0.63
7:J:23:ILE:HD11	7:J:178:LEU:HD22	1.82	0.62
4:A:159:TRP:HB2	4:C:150:TYR:HE1	1.64	0.61
7:J:42:LYS:HD3	7:J:56:PHE:HB3	1.81	0.61
7:J:121:ARG:HD2	7:J:124:LEU:HD21	1.81	0.61
4:C:23:ASN:HD21	4:C:86:GLU:HB2	1.65	0.61
2:2:26:DA:H5'	2:2:26:DA:C8	2.36	0.60
4:E:125:TRP:HB2	4:E:197:THR:HG22	1.83	0.60
4:F:38:VAL:HG12	6:H:145:ALA:HA	1.83	0.60
4:D:321:LEU:HD12	4:D:325:MET:HE1	1.82	0.60
4:A:18:VAL:HB	4:A:254:LEU:HB2	1.84	0.60
1:I:30:G:C2	4:A:341:LEU:HD13	2.37	0.59
7:I:328:MET:HE1	7:I:374:LEU:HD12	1.84	0.59
7:J:123:LEU:HD12	7:J:149:SER:HB2	1.84	0.59
6:H:73:ARG:O	6:H:77:GLN:HB2	2.03	0.59
5:G:96:GLY:HA3	5:G:191:THR:HG22	1.84	0.59
4:A:63:TYR:HD1	4:F:289:VAL:HG13	1.67	0.59
5:G:558:VAL:HG23	5:G:602:ILE:HD11	1.84	0.58
7:I:79:LEU:HD11	7:I:94:LEU:HA	1.85	0.58
5:G:403:SER:HB2	5:G:510:ARG:HD3	1.85	0.58
7:J:42:LYS:O	7:J:46:LEU:HD22	2.04	0.58
4:A:10:MET:HB3	4:A:96:SER:HB3	1.85	0.58
5:G:573:ILE:HD12	5:G:573:ILE:O	2.04	0.58
7:I:292:ILE:HG12	7:I:336:LEU:HD22	1.84	0.58
6:H:6:ARG:HD2	6:H:66:LEU:HD21	1.86	0.57
7:J:104:GLN:HB3	7:J:108:SER:HA	1.86	0.57
4:E:283:GLY:H	4:E:293:ARG:HB2	1.69	0.57
4:D:302:PHE:O	4:D:306:GLU:HG2	2.05	0.57
6:H:15:ARG:HH22	6:H:54:ARG:HG2	1.69	0.57
7:I:103:MET:HE2	7:I:103:MET:N	2.19	0.57
4:D:308:ALA:HA	4:D:311:TYR:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:159:TRP:CD1	5:G:520:ILE:HD11	2.40	0.56
4:F:34:TYR:H	6:H:141:THR:HG22	1.70	0.56
7:I:330:MET:HE1	7:I:344:VAL:HB	1.87	0.56
7:I:309:PHE:HA	7:I:312:ILE:HG22	1.87	0.56
7:I:252:TRP:HH2	7:I:304:ILE:HG13	1.71	0.56
4:D:57:ASP:HB3	4:D:60:VAL:HG22	1.88	0.56
7:I:361:LYS:HE3	7:I:362:ARG:HH12	1.70	0.56
4:D:125:TRP:HB2	4:D:197:THR:HG22	1.87	0.55
4:E:1:MET:HE3	4:E:108:VAL:HG13	1.89	0.55
7:J:34:VAL:HG22	7:J:38:LEU:HD23	1.87	0.55
4:F:302:PHE:O	4:F:306:GLU:HG2	2.06	0.55
4:F:20:PHE:O	4:F:32:LEU:HB2	2.07	0.55
4:E:228:VAL:HG12	4:E:242:GLN:HG2	1.88	0.54
5:G:584:LYS:HG3	5:G:593:HIS:HB3	1.89	0.54
7:I:283:ILE:HD12	7:I:326:LEU:HD11	1.90	0.54
4:D:14:GLU:HG2	5:G:512:LYS:HG3	1.90	0.54
7:J:16:GLU:HG3	7:J:141:TYR:HB2	1.89	0.54
4:F:152:THR:HA	4:F:214:THR:O	2.08	0.54
7:I:288:LEU:HA	7:I:308:MET:HE1	1.89	0.54
4:B:228:VAL:HG12	4:B:242:GLN:HG2	1.90	0.54
2:2:37:DG:H2'	2:2:38:DA:C8	2.43	0.54
4:D:18:VAL:HB	4:D:254:LEU:HB2	1.89	0.54
4:D:322:PRO:HD2	4:D:325:MET:HE2	1.90	0.54
4:F:265:THR:HA	4:F:278:ARG:HA	1.90	0.54
5:G:543:TRP:CD1	5:G:608:ILE:HG12	2.42	0.54
4:A:61:THR:HG23	4:A:64:SER:H	1.74	0.53
1:1:12:A:C2	4:E:341:LEU:HD13	2.43	0.53
4:F:131:ARG:HB3	4:F:266:ILE:HG21	1.90	0.53
6:H:8:ILE:HG12	6:H:86:ILE:HG22	1.90	0.53
7:I:104:GLN:OE1	7:I:104:GLN:HA	2.09	0.53
7:J:218:VAL:HG13	7:J:223:ARG:HG2	1.90	0.53
7:J:344:VAL:O	7:J:347:MET:HG3	2.09	0.53
4:B:311:TYR:CE1	4:B:325:MET:HG3	2.44	0.53
7:I:278:LEU:HD22	7:I:326:LEU:HD12	1.91	0.52
4:B:78:VAL:HG13	4:B:85:ILE:HD11	1.90	0.52
7:I:65:PRO:HA	7:I:75:ARG:HD2	1.90	0.52
6:H:31:PHE:HE2	6:H:72:ARG:HB2	1.75	0.52
7:J:129:ILE:HD12	7:J:147:HIS:HA	1.91	0.52
2:2:47:DT:C2	4:D:70:PRO:HG2	2.45	0.52
4:E:12:SER:HB3	4:E:337:ILE:HG23	1.91	0.52
7:I:378:TYR:O	7:I:382:LEU:HD12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:166:SER:HB2	7:J:185:CYS:HB2	1.91	0.51
7:I:18:LEU:HD11	7:I:93:LEU:HD12	1.93	0.51
7:I:215:LEU:HD22	7:I:249:TRP:HE3	1.74	0.51
6:H:122:LEU:HB3	6:H:133:PHE:HE2	1.76	0.51
7:I:369:GLU:OE1	7:I:371:ALA:HB2	2.10	0.51
3:3:3:DA:H2''	3:3:4:DC:H5'	1.93	0.51
4:C:18:VAL:HB	4:C:254:LEU:HB2	1.92	0.51
1:1:39:A:C8	4:F:229:PHE:HA	2.45	0.51
1:1:53:A:P	6:H:125:ARG:HH21	2.33	0.51
4:A:229:PHE:CZ	4:C:70:PRO:HG3	2.45	0.51
7:I:70:LYS:HD2	7:I:70:LYS:O	2.11	0.51
4:F:19:ILE:O	4:F:87:CYS:HA	2.10	0.51
4:F:142:LEU:HB2	4:F:146:ASN:HB2	1.92	0.51
7:J:341:ARG:HH21	7:J:344:VAL:HG11	1.76	0.51
1:1:36:A:C2	4:F:341:LEU:HD13	2.46	0.50
4:B:152:THR:HG23	4:B:215:PHE:HB3	1.92	0.50
7:J:37:PHE:O	7:J:41:VAL:HG12	2.11	0.50
7:I:78:ALA:O	7:I:82:LEU:HD13	2.12	0.50
4:F:147:GLU:OE2	4:F:147:GLU:HA	2.12	0.50
7:J:153:TYR:HB3	7:J:204:ALA:HB2	1.93	0.49
4:E:141:TRP:H	4:E:141:TRP:CD1	2.29	0.49
7:I:292:ILE:HA	7:I:305:LEU:HD21	1.94	0.49
5:G:21:ARG:HB2	5:G:21:ARG:CZ	2.41	0.49
7:J:347:MET:HE2	7:J:352:LEU:HB2	1.94	0.49
4:B:341:LEU:HD23	4:B:343:GLN:HE22	1.77	0.49
5:G:29:PRO:HB2	5:G:141:ILE:HG13	1.94	0.49
5:G:399:ILE:HG12	5:G:508:ILE:HG13	1.95	0.49
6:H:45:PRO:HD3	6:H:57:THR:HG22	1.94	0.49
6:H:172:SER:HA	6:H:194:VAL:HG11	1.94	0.49
7:I:348:ILE:HD13	7:I:353:LEU:HB2	1.94	0.49
6:H:30:ARG:O	6:H:34:LYS:HG2	2.13	0.49
7:J:18:LEU:HD12	7:J:22:PHE:CE1	2.48	0.49
4:D:150:TYR:CE2	4:E:159:TRP:HB2	2.48	0.49
1:1:29:A:C4	4:A:341:LEU:HD11	2.48	0.49
7:I:119:ILE:HD12	7:I:120:PRO:HD2	1.94	0.48
4:E:18:VAL:HB	4:E:254:LEU:HB2	1.95	0.48
7:I:150:GLY:O	7:I:152:GLU:HG2	2.13	0.48
7:I:154:CYS:HB2	7:I:159:VAL:H	1.78	0.48
7:J:36:TRP:HA	7:J:39:VAL:HG22	1.95	0.48
4:E:78:VAL:HG13	4:E:85:ILE:HD11	1.95	0.48
4:D:141:TRP:CD1	4:D:141:TRP:H	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:35:DT:C2	4:B:70:PRO:HG2	2.49	0.48
6:H:21:ALA:O	6:H:25:ILE:HD13	2.14	0.48
4:A:180:THR:O	4:A:184:ARG:HD2	2.13	0.48
6:H:161:LYS:NZ	6:H:163:ARG:HH21	2.06	0.48
6:H:112:PHE:HD1	6:H:112:PHE:H	1.62	0.48
7:I:136:LEU:HD11	7:I:171:TYR:OH	2.13	0.48
2:2:33:DG:H2''	2:2:34:DC:O4'	2.13	0.48
7:I:332:GLU:O	7:I:336:LEU:HG	2.14	0.48
2:2:37:DG:H2'	2:2:38:DA:N7	2.29	0.48
2:2:50:DC:H5'	2:2:50:DC:C6	2.49	0.48
4:B:70:PRO:HG3	4:C:229:PHE:CZ	2.49	0.48
4:E:23:ASN:HD21	4:E:86:GLU:HB2	1.79	0.48
5:G:108:ALA:HB1	5:G:551:THR:HG23	1.96	0.48
2:2:30:DT:H5'	4:C:71:HIS:CE1	2.48	0.48
4:A:4:PRO:HG2	4:A:7:LEU:HB2	1.96	0.48
5:G:451:VAL:HG22	5:G:479:CYS:HB3	1.95	0.48
2:2:30:DT:H5'	4:C:71:HIS:HE1	1.79	0.47
4:B:141:TRP:CD1	4:B:141:TRP:H	2.32	0.47
5:G:213:LEU:HD22	5:G:596:VAL:HG11	1.96	0.47
5:G:249:THR:HA	5:G:252:MET:HB3	1.96	0.47
7:J:396:LEU:HD12	7:J:396:LEU:H	1.79	0.47
1:1:40:G:O2'	1:1:41:G:H5'	2.14	0.47
4:E:186:HIS:HB3	4:E:189:TRP:HB2	1.97	0.47
4:B:311:TYR:CD1	4:B:325:MET:HG3	2.50	0.47
7:I:64:ASN:HB2	7:I:66:TYR:HD1	1.80	0.47
1:1:51:G:H5'	1:1:52:A:OP2	2.15	0.47
7:J:306:LYS:O	7:J:310:GLN:HG2	2.15	0.47
4:B:150:TYR:CE2	4:C:159:TRP:HB2	2.49	0.47
4:F:4:PRO:HD3	4:F:108:VAL:HG21	1.96	0.47
5:G:247:MET:HE2	5:G:251:ALA:HB2	1.95	0.47
5:G:272:HIS:HA	5:G:607:THR:HG23	1.97	0.47
5:G:481:VAL:HG22	5:G:483:VAL:HG13	1.96	0.47
4:B:18:VAL:HB	4:B:254:LEU:HB2	1.96	0.47
4:A:12:SER:HB2	4:A:337:ILE:HG23	1.97	0.47
4:D:26:ASP:OD1	4:D:28:ARG:HG3	2.15	0.47
7:J:224:TRP:HA	7:J:227:MET:HE1	1.97	0.47
4:F:325:MET:HA	4:F:328:ASP:HB2	1.95	0.46
7:J:312:ILE:O	7:J:316:LEU:HB2	2.15	0.46
4:B:287:GLU:O	4:C:102:LYS:HA	2.16	0.46
7:J:129:ILE:HG12	7:J:174:ARG:HH21	1.79	0.46
7:I:102:GLN:C	7:I:103:MET:HE2	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:61:THR:HG23	4:C:64:SER:H	1.79	0.46
4:F:284:ALA:HA	4:F:291:CYS:HA	1.98	0.46
6:H:72:ARG:HD3	6:H:73:ARG:H	1.80	0.46
5:G:23:PHE:CD2	5:G:43:LEU:HD21	2.51	0.46
5:G:445:CYS:HB2	5:G:543:TRP:CD2	2.51	0.46
6:H:20:ILE:HD11	7:I:272:VAL:HA	1.98	0.46
4:D:10:MET:HG3	4:D:11:LYS:N	2.31	0.46
4:D:267:ASP:HB3	4:D:277:ILE:HG13	1.97	0.46
5:G:26:LEU:CD1	5:G:253:SER:HB2	2.45	0.46
7:I:329:ASN:HB3	7:I:370:TYR:CE2	2.50	0.46
4:D:159:TRP:HB2	5:G:517:ILE:HG12	1.98	0.46
4:E:4:PRO:HD3	4:E:108:VAL:HG21	1.98	0.46
2:2:42:DT:H2''	2:2:43:DG:O4'	2.15	0.45
4:D:324:GLU:HG2	4:D:325:MET:N	2.30	0.45
7:J:93:LEU:HD23	7:J:96:ILE:HD12	1.98	0.45
5:G:555:ILE:HA	5:G:558:VAL:HG12	1.98	0.45
4:B:325:MET:O	4:B:325:MET:HG2	2.16	0.45
7:J:200:ALA:O	7:J:203:ILE:HG13	2.17	0.45
4:D:226:SER:HB2	4:D:254:LEU:HA	1.99	0.45
4:E:120:GLU:HG3	4:E:125:TRP:HE1	1.82	0.45
6:H:74:TYR:O	6:H:78:MET:HG3	2.17	0.45
4:C:141:TRP:CD1	4:C:141:TRP:H	2.33	0.45
4:E:97:LEU:HD23	4:E:97:LEU:H	1.82	0.45
7:J:126:LYS:H	7:J:126:LYS:HD3	1.82	0.45
1:1:7:A:H5''	4:D:278:ARG:NH2	2.32	0.45
4:A:78:VAL:HG23	4:A:221:ALA:O	2.17	0.45
4:B:40:LEU:HD13	4:C:229:PHE:HE2	1.82	0.45
6:H:104:ALA:HB3	6:H:165:ASN:HB2	1.99	0.44
7:I:353:LEU:HD21	7:I:380:LEU:HD13	1.99	0.44
7:I:366:ILE:HD12	7:I:366:ILE:HA	1.80	0.44
4:D:116:ILE:HD13	4:D:116:ILE:HA	1.86	0.44
5:G:204:PRO:HG3	5:G:424:HIS:CE1	2.52	0.44
7:J:219:PRO:HD2	7:J:301:SER:HB3	1.99	0.44
7:J:229:TRP:NE1	7:J:291:SER:HB3	2.32	0.44
7:J:331:LEU:HD23	7:J:331:LEU:H	1.83	0.44
1:1:59:A:H2'	1:1:60:G:C8	2.53	0.44
4:A:78:VAL:HG13	4:A:85:ILE:HD11	1.98	0.44
4:E:321:LEU:HD13	4:E:325:MET:HE1	2.00	0.44
6:H:42:VAL:HG23	6:H:184:GLY:HA3	2.00	0.44
4:A:49:ALA:HB1	4:F:295:PRO:HG3	2.00	0.44
4:D:110:ARG:HB3	4:D:110:ARG:HH11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:28:LEU:HD12	6:H:58:PHE:CE2	2.52	0.44
7:I:164:ARG:HA	7:I:170:ILE:HA	1.99	0.44
7:I:337:LEU:HD22	7:I:385:PHE:HB3	1.99	0.44
7:I:119:ILE:HD12	7:I:119:ILE:HA	1.88	0.44
2:2:30:DT:H2''	2:2:31:DC:O4'	2.18	0.44
4:B:321:LEU:HD11	4:B:325:MET:HE1	1.99	0.44
7:I:384:GLU:OE2	7:J:100:ARG:HB2	2.18	0.44
4:A:42:MET:HG3	4:A:44:GLU:OE1	2.18	0.44
4:C:47:LYS:HD3	4:C:52:TYR:CE2	2.52	0.44
7:I:328:MET:HE3	7:I:328:MET:HB2	1.74	0.44
7:J:229:TRP:HB2	7:J:294:LEU:HD21	1.99	0.44
4:E:2:LYS:HA	4:E:2:LYS:HD2	1.81	0.43
7:I:333:ILE:HD12	7:I:334:CYS:N	2.32	0.43
4:B:228:VAL:HG22	4:B:240:ILE:HB	2.00	0.43
4:E:14:GLU:O	4:E:91:VAL:HA	2.18	0.43
4:F:126:GLU:O	4:F:130:ASN:HB2	2.19	0.43
6:H:22:ALA:HB1	6:H:153:GLU:O	2.18	0.43
7:I:105:PHE:O	7:I:106:SER:HB3	2.16	0.43
7:I:316:LEU:HD21	7:I:374:LEU:HD23	1.99	0.43
4:A:294:HIS:CG	4:A:295:PRO:HD2	2.53	0.43
4:E:86:GLU:OE2	4:E:212:SER:HB2	2.18	0.43
4:A:267:ASP:HB2	4:A:279:ILE:HD13	2.00	0.43
4:A:345:LYS:HD2	4:A:345:LYS:HA	1.73	0.43
4:C:97:LEU:HD13	4:C:337:ILE:HG13	2.00	0.43
4:D:97:LEU:HD13	4:D:337:ILE:HG13	2.01	0.43
4:E:287:GLU:OE1	4:E:287:GLU:C	2.61	0.43
7:I:178:LEU:HD23	7:I:179:SER:N	2.26	0.43
4:C:310:GLN:O	4:C:313:GLU:HG3	2.18	0.43
5:G:233:TYR:H	5:G:233:TYR:HD2	1.66	0.43
7:I:299:PHE:HB2	7:I:394:PHE:HD2	1.83	0.43
7:J:207:LEU:HD11	7:J:227:MET:HE3	2.01	0.43
1:1:6:A:O4'	4:D:340:GLY:HA2	2.19	0.43
5:G:89:PHE:HD2	5:G:247:MET:HE3	1.82	0.43
7:I:289:PHE:HZ	7:I:332:GLU:HB3	1.84	0.43
7:J:289:PHE:CD1	7:J:292:ILE:HD11	2.53	0.43
4:D:325:MET:HE2	4:D:325:MET:HB3	1.81	0.43
4:E:11:LYS:HD2	4:E:14:GLU:OE1	2.19	0.43
7:I:291:SER:HA	7:I:294:LEU:HG	1.99	0.43
7:J:302:ASN:N	7:J:306:LYS:HZ2	2.16	0.43
4:F:154:ILE:O	4:F:170:PHE:HB2	2.19	0.43
4:C:115:LEU:HA	4:C:312:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:305:LEU:HD23	4:D:305:LEU:HA	1.80	0.43
4:F:294:HIS:CG	4:F:295:PRO:HD2	2.53	0.43
5:G:431:GLN:HA	5:G:434:ASN:O	2.19	0.43
6:H:100:LEU:HB2	6:H:194:VAL:HG12	2.01	0.43
7:J:93:LEU:HD23	7:J:93:LEU:HA	1.82	0.43
2:2:54:DG:H5''	5:G:93:ARG:HA	1.99	0.42
4:A:97:LEU:HD13	4:A:337:ILE:HG12	2.01	0.42
4:E:152:THR:HG23	4:E:215:PHE:HB3	2.01	0.42
5:G:23:PHE:CE2	5:G:43:LEU:HD21	2.54	0.42
6:H:151:SER:OG	6:H:163:ARG:HD3	2.19	0.42
4:B:40:LEU:HD13	4:C:229:PHE:CE2	2.54	0.42
4:F:108:VAL:HA	4:F:111:THR:HG22	2.00	0.42
7:I:316:LEU:HD23	7:I:316:LEU:HA	1.85	0.42
1:1:55:A:H3'	1:1:56:G:H8	1.85	0.42
4:D:91:VAL:HG13	4:D:209:PHE:HB2	2.02	0.42
5:G:110:MET:HE3	5:G:110:MET:HB3	1.91	0.42
5:G:621:TYR:OH	5:G:628:PRO:HB3	2.19	0.42
6:H:152:LEU:O	6:H:163:ARG:HA	2.20	0.42
4:D:49:ALA:HA	4:D:60:VAL:HG21	2.01	0.42
5:G:149:LEU:HD12	5:G:149:LEU:HA	1.88	0.42
1:1:45:A:C5	6:H:163:ARG:HD2	2.54	0.42
2:2:25:DT:H2'	2:2:26:DA:N7	2.34	0.42
4:B:299:LYS:HD3	4:B:299:LYS:HA	1.77	0.42
4:C:304:LEU:HB3	4:C:332:ILE:HD11	2.01	0.42
4:D:303:THR:O	4:D:307:LYS:HG2	2.18	0.42
4:E:228:VAL:HG22	4:E:240:ILE:HB	2.01	0.42
4:F:278:ARG:HD3	4:F:279:ILE:O	2.18	0.42
5:G:574:GLY:HA2	5:G:628:PRO:O	2.19	0.42
4:A:102:LYS:HA	4:C:287:GLU:O	2.20	0.42
5:G:123:TYR:O	5:G:249:THR:HG23	2.19	0.42
7:I:136:LEU:HD23	7:I:136:LEU:O	2.19	0.42
7:I:258:LYS:HA	7:I:258:LYS:HD3	1.93	0.42
7:J:101:ASN:HD21	7:J:113:ILE:HB	1.84	0.42
4:B:230:LYS:NZ	4:B:233:VAL:HG22	2.34	0.42
4:C:180:THR:O	4:C:184:ARG:HG2	2.20	0.42
4:C:286:ARG:HE	4:C:286:ARG:HB3	1.66	0.42
4:D:120:GLU:HG3	4:D:125:TRP:NE1	2.35	0.42
4:F:141:TRP:CD1	4:F:141:TRP:H	2.37	0.42
5:G:221:MET:HE2	5:G:221:MET:HB2	1.71	0.42
7:J:390:PHE:HD1	7:J:390:PHE:HA	1.74	0.42
4:A:229:PHE:CE2	4:C:40:LEU:HD13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:234:LYS:HB3	4:B:234:LYS:HE3	1.65	0.42
4:D:152:THR:HB	4:D:215:PHE:HB3	2.02	0.42
7:I:132:CYS:HB3	7:I:161:LEU:HD22	2.01	0.42
7:I:309:PHE:HB3	7:I:395:TYR:OH	2.20	0.42
7:I:337:LEU:HD21	7:I:381:TRP:HB2	2.02	0.42
2:2:32:DT:H6	2:2:32:DT:H2'	1.61	0.42
4:D:158:PRO:HB3	4:D:209:PHE:HE1	1.85	0.42
4:F:18:VAL:HB	4:F:254:LEU:HB2	2.02	0.42
7:J:219:PRO:HB2	7:J:222:TYR:CE1	2.55	0.42
4:A:63:TYR:HE1	4:F:289:VAL:HG22	1.85	0.42
4:B:229:PHE:CZ	4:E:70:PRO:HG3	2.55	0.41
5:G:135:PHE:HB3	5:G:136:LEU:HD12	2.00	0.41
6:H:40:ILE:HD12	6:H:59:VAL:O	2.20	0.41
7:I:393:SER:OG	7:J:116:ALA:HB2	2.20	0.41
7:J:55:THR:HG21	7:J:71:HIS:CD2	2.55	0.41
4:D:70:PRO:HG3	4:E:229:PHE:CZ	2.55	0.41
4:D:315:LEU:HD12	4:D:315:LEU:HA	1.88	0.41
5:G:300:ILE:HD12	5:G:300:ILE:HA	1.87	0.41
5:G:427:GLN:HB2	5:G:439:ILE:HD12	2.02	0.41
7:J:133:PRO:HD2	7:J:162:ILE:HD12	2.01	0.41
4:B:321:LEU:HG	4:B:326:ILE:HD11	2.02	0.41
4:F:78:VAL:HB	4:F:85:ILE:HD11	2.01	0.41
4:F:269:TRP:HB3	4:F:327:ASN:HB3	2.02	0.41
5:G:574:GLY:HA2	5:G:629:ILE:HA	2.02	0.41
2:2:51:DC:H2''	2:2:52:DG:O4'	2.21	0.41
4:D:40:LEU:HD13	4:E:229:PHE:CE2	2.55	0.41
5:G:219:GLN:HB3	5:G:250:LEU:HD22	2.01	0.41
7:I:284:LEU:HD23	7:I:284:LEU:HA	1.88	0.41
7:I:206:TRP:NE1	7:I:223:ARG:HH11	2.18	0.41
4:F:91:VAL:HG12	4:F:209:PHE:HB2	2.02	0.41
4:F:304:LEU:HD13	4:F:328:ASP:OD1	2.21	0.41
6:H:92:VAL:HA	6:H:93:PRO:HD3	1.90	0.41
7:I:120:PRO:HG2	7:I:123:LEU:HG	2.01	0.41
2:2:48:DA:H2''	2:2:49:DT:C6	2.56	0.41
4:F:114:GLN:OE1	4:F:114:GLN:HA	2.21	0.41
5:G:49:ARG:HD2	5:G:51:ILE:HD11	2.03	0.41
6:H:104:ALA:HB2	6:H:167:GLN:HE22	1.86	0.41
2:2:44:DT:H6	2:2:44:DT:H2'	1.70	0.41
4:A:34:TYR:CD1	4:A:252:PRO:HD3	2.55	0.41
4:C:47:LYS:HE2	4:C:47:LYS:O	2.21	0.41
4:C:294:HIS:CG	4:C:295:PRO:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:99:LYS:HB3	4:D:99:LYS:HE3	1.82	0.41
4:D:158:PRO:HB3	4:D:209:PHE:CE1	2.55	0.41
7:I:254:ASN:O	7:I:258:LYS:HG2	2.21	0.41
2:2:45:DG:H2''	2:2:46:DG:O4'	2.21	0.41
4:B:126:GLU:O	4:B:130:ASN:HB2	2.20	0.41
4:B:229:PHE:CE2	4:E:40:LEU:HD13	2.56	0.41
4:F:13:ILE:HG12	4:F:93:PHE:CD2	2.56	0.41
4:F:102:LYS:HE3	4:F:102:LYS:HB2	1.81	0.41
5:G:430:VAL:HA	5:G:503:LEU:HD13	2.03	0.41
6:H:9:THR:HG23	6:H:55:LYS:NZ	2.36	0.41
7:I:327:ARG:HB3	7:I:370:TYR:HB3	2.03	0.41
7:J:105:PHE:CZ	7:J:120:PRO:HG3	2.56	0.41
7:J:105:PHE:CE2	7:J:120:PRO:HG3	2.55	0.41
7:J:337:LEU:HD21	7:J:385:PHE:CG	2.56	0.41
4:A:286:ARG:HD3	4:A:286:ARG:HA	1.79	0.41
5:G:99:ARG:HG2	5:G:121:TRP:CE3	2.55	0.41
4:A:44:GLU:HG3	4:F:281:HIS:ND1	2.36	0.40
4:D:304:LEU:HB3	4:D:332:ILE:HD11	2.03	0.40
7:I:272:VAL:HG12	7:I:273:LEU:HD22	2.03	0.40
7:I:328:MET:HB3	7:I:372:PHE:HB2	2.03	0.40
7:J:42:LYS:HB2	7:J:56:PHE:HD2	1.87	0.40
7:J:305:LEU:H	7:J:305:LEU:HD12	1.86	0.40
4:D:299:LYS:HD3	4:D:299:LYS:HA	1.77	0.40
7:I:273:LEU:HD13	7:I:273:LEU:HA	1.95	0.40
7:I:333:ILE:HD12	7:I:334:CYS:H	1.87	0.40
7:J:35:HIS:O	7:J:39:VAL:HG13	2.22	0.40
4:A:295:PRO:HG3	4:C:49:ALA:HB1	2.02	0.40
4:B:322:PRO:O	4:B:326:ILE:HG12	2.21	0.40
4:B:325:MET:HE2	4:B:326:ILE:HD13	2.03	0.40
4:D:120:GLU:HG3	4:D:125:TRP:HE1	1.85	0.40
5:G:183:LEU:HD12	5:G:183:LEU:HA	1.87	0.40
7:J:172:ASP:HB3	7:J:175:TYR:HD2	1.87	0.40
5:G:566:LYS:HD2	5:G:566:LYS:HA	1.89	0.40
7:I:210:ASP:OD1	7:I:212:VAL:HG13	2.21	0.40
7:J:252:TRP:HA	7:J:253:PRO:HA	1.89	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	
4	A	343/347 (99%)	328 (96%)	15 (4%)	0	100	100
4	B	343/347 (99%)	334 (97%)	9 (3%)	0	100	100
4	C	343/347 (99%)	331 (96%)	12 (4%)	0	100	100
4	D	344/347 (99%)	334 (97%)	10 (3%)	0	100	100
4	E	343/347 (99%)	332 (97%)	11 (3%)	0	100	100
4	F	293/347 (84%)	281 (96%)	12 (4%)	0	100	100
5	G	565/640 (88%)	542 (96%)	23 (4%)	0	100	100
6	H	191/198 (96%)	179 (94%)	12 (6%)	0	100	100
7	I	381/406 (94%)	346 (91%)	35 (9%)	0	100	100
7	J	352/406 (87%)	317 (90%)	35 (10%)	0	100	100
All	All	3498/3732 (94%)	3324 (95%)	174 (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%)	285 (98%)	6 (2%)	47	73
4	B	298/303 (98%)	291 (98%)	7 (2%)	44	71
4	C	302/303 (100%)	299 (99%)	3 (1%)	68	84
4	D	302/303 (100%)	296 (98%)	6 (2%)	48	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	302/303 (100%)	297 (98%)	5 (2%)	53	77
4	F	262/303 (86%)	249 (95%)	13 (5%)	22	45
5	G	447/519 (86%)	438 (98%)	9 (2%)	48	74
6	H	166/176 (94%)	158 (95%)	8 (5%)	23	46
7	I	282/368 (77%)	270 (96%)	12 (4%)	26	51
7	J	248/368 (67%)	237 (96%)	11 (4%)	25	50
All	All	2900/3249 (89%)	2820 (97%)	80 (3%)	38	65

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	91	VAL
4	A	207	CYS
4	A	291	CYS
4	A	318	THR
4	A	324	GLU
4	A	342	LEU
4	B	3	LEU
4	B	91	VAL
4	B	180	THR
4	B	228	VAL
4	B	246	VAL
4	B	289	VAL
4	B	323	ASP
4	C	153	SER
4	C	232	SER
4	C	289	VAL
4	D	61	THR
4	D	152	THR
4	D	180	THR
4	D	202	GLN
4	D	289	VAL
4	D	324	GLU
4	E	53	ASP
4	E	118	LEU
4	E	154	ILE
4	E	180	THR
4	E	280	SER
4	F	38	VAL
4	F	75	PHE

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Mol	Chain	Res	Type
4	F	78	VAL
4	F	87	CYS
4	F	184	ARG
4	F	219	THR
4	F	228	VAL
4	F	231	ASP
4	F	244	THR
4	F	246	VAL
4	F	289	VAL
4	F	314	GLN
4	F	328	ASP
5	G	51	ILE
5	G	218	SER
5	G	260	MET
5	G	297	VAL
5	G	299	VAL
5	G	300	ILE
5	G	408	SER
5	G	559	ILE
5	G	570	VAL
6	H	32	ASN
6	H	57	THR
6	H	108	ASP
6	H	125	ARG
6	H	151	SER
6	H	167	GLN
6	H	188	THR
6	H	192	LEU
7	I	79	LEU
7	I	81	HIS
7	I	109	THR
7	I	113	ILE
7	I	118	VAL
7	I	121	ARG
7	I	132	CYS
7	I	155	HIS
7	I	172	ASP
7	I	333	ILE
7	I	362	ARG
7	I	368	THR
7	J	31	TYR
7	J	59	ASP

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Mol	Chain	Res	Type
7	J	61	CYS
7	J	82	LEU
7	J	124	LEU
7	J	126	LYS
7	J	183	THR
7	J	251	HIS
7	J	310	GLN
7	J	353	LEU
7	J	373	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	23	ASN
4	B	171	HIS
4	B	202	GLN
4	B	220	ASN
4	B	314	GLN
4	C	114	GLN
4	C	171	HIS
4	C	191	ASN
4	C	202	GLN
4	D	67	GLN
4	D	191	ASN
4	D	227	GLN
4	D	238	ASN
4	D	296	ASN
4	D	343	GLN
4	E	23	ASN
4	E	114	GLN
4	F	314	GLN
5	G	86	ASN
5	G	200	GLN
6	H	32	ASN
7	I	64	ASN
7	I	81	HIS
7	I	232	GLN
7	I	293	GLN
7	J	71	HIS
7	J	391	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	55/60 (91%)	20 (36%)	0

All (20) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	3	G
1	1	8	U
1	1	9	G
1	1	14	A
1	1	15	C
1	1	19	A
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	38	C
1	1	39	A
1	1	40	G
1	1	41	G
1	1	54	U
1	1	55	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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.

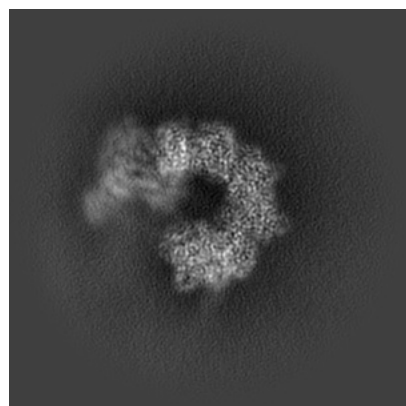
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65338. These allow visual inspection of the internal detail of the map and identification of artifacts.

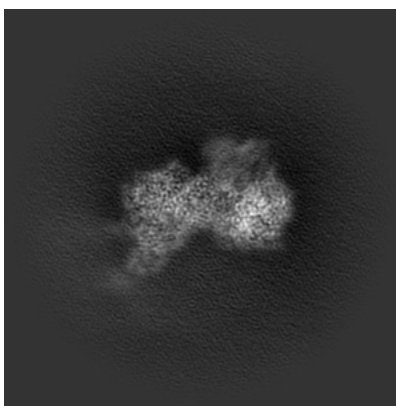
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

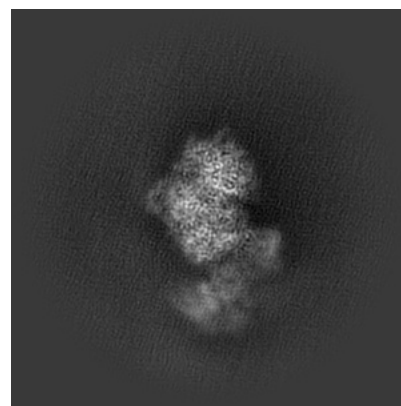
6.1.1 Primary map



X

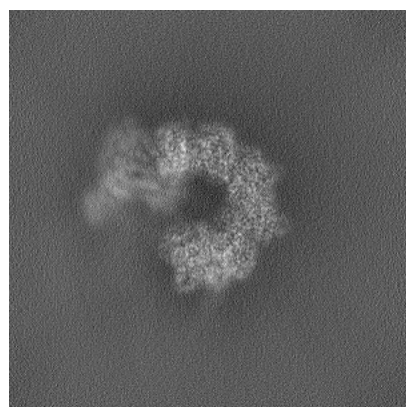


Y

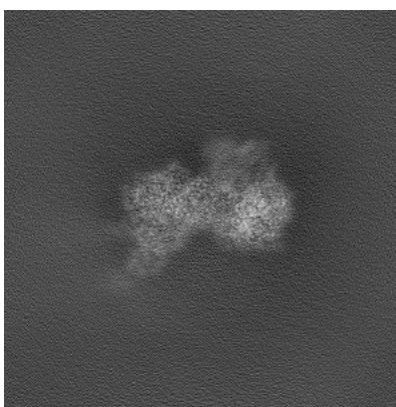


Z

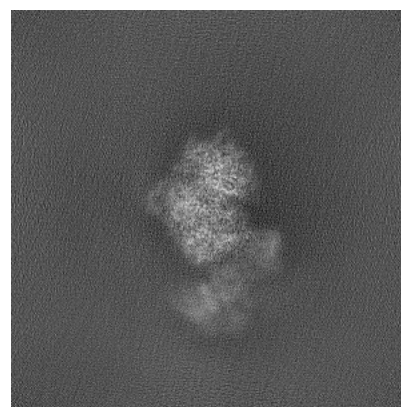
6.1.2 Raw map



X



Y

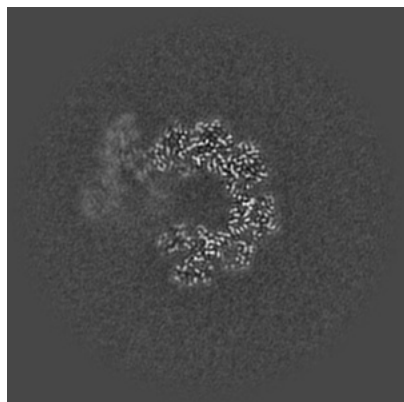


Z

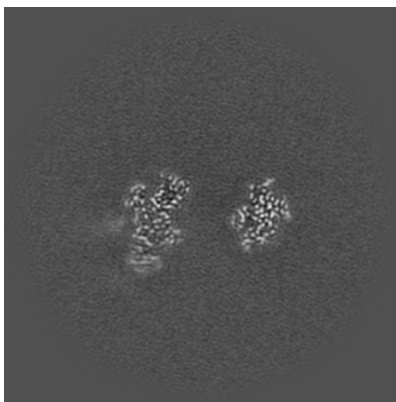
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

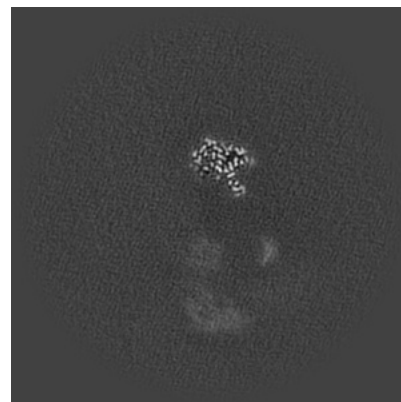
6.2.1 Primary map



X Index: 230

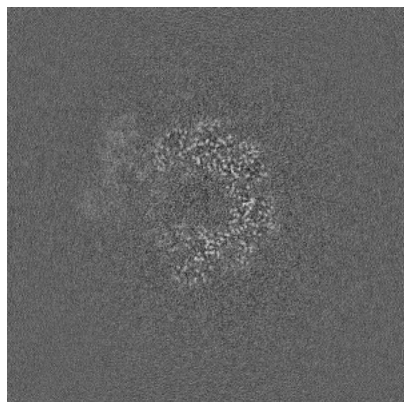


Y Index: 230

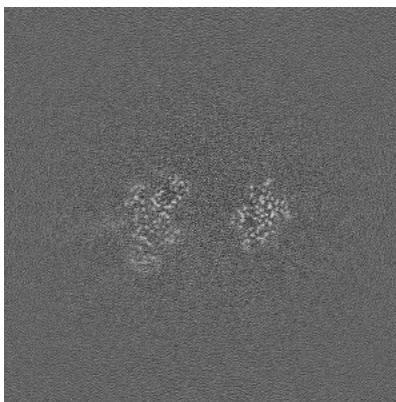


Z Index: 230

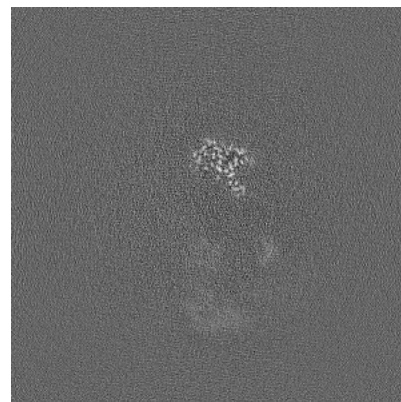
6.2.2 Raw map



X Index: 230



Y Index: 230

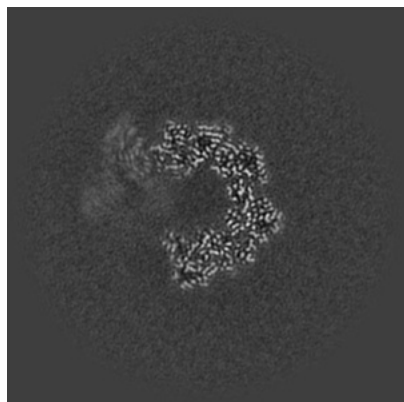


Z Index: 230

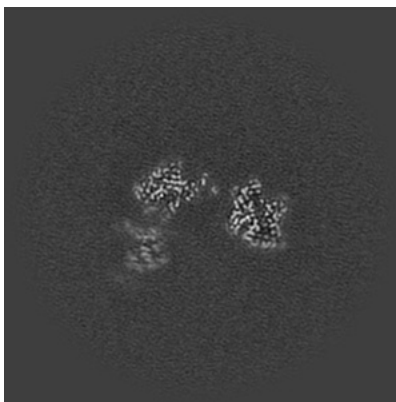
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

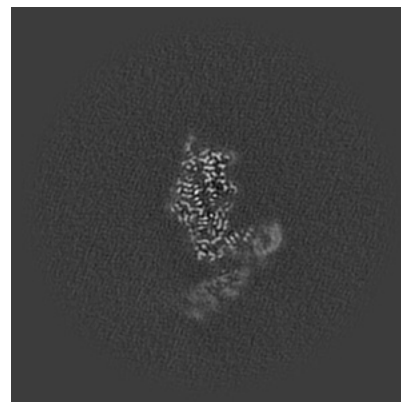
6.3.1 Primary map



X Index: 236

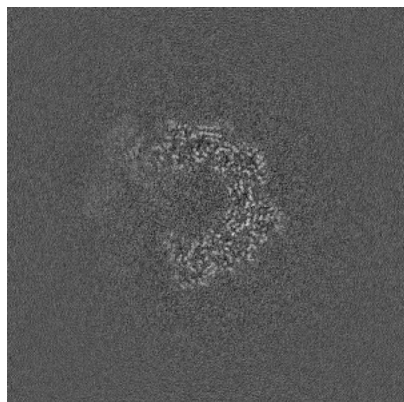


Y Index: 249

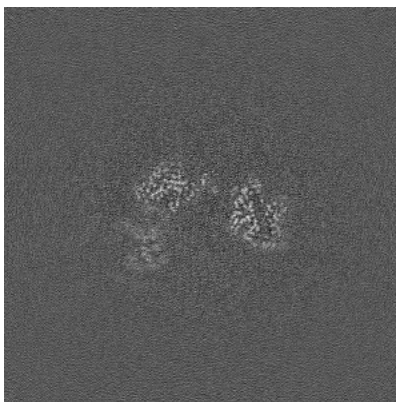


Z Index: 282

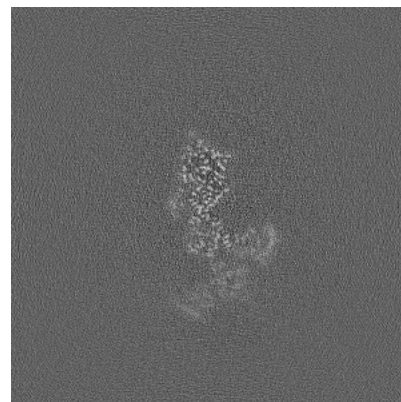
6.3.2 Raw map



X Index: 237



Y Index: 249

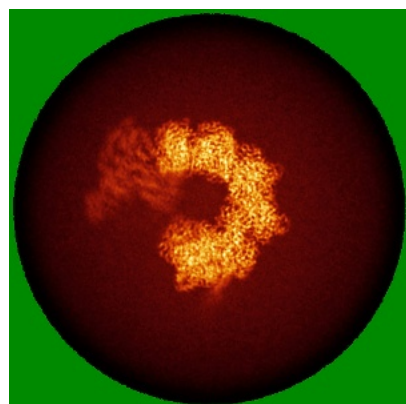


Z Index: 275

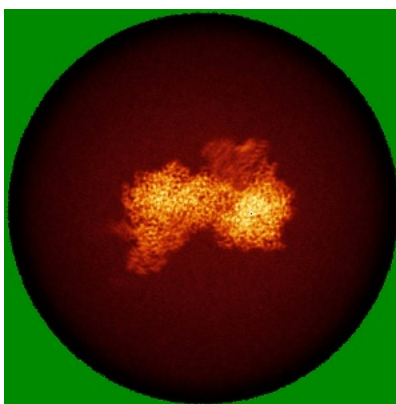
The images above show the largest variance slices of the map in three orthogonal directions.

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

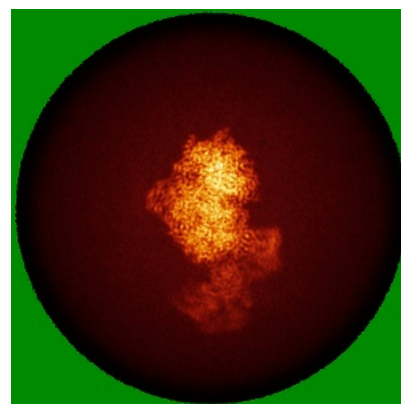
6.4.1 Primary map



X

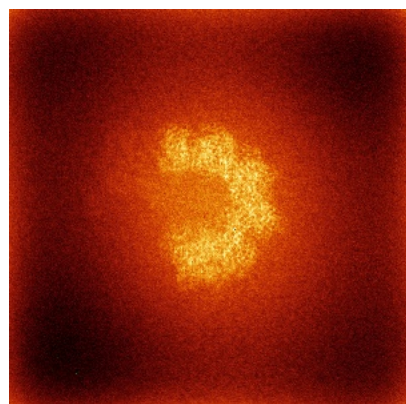


Y

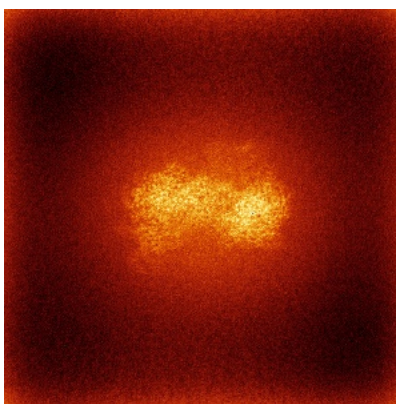


Z

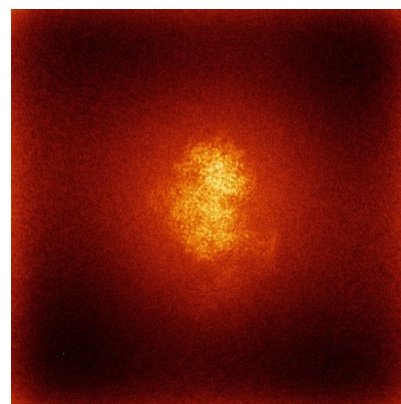
6.4.2 Raw map



X



Y

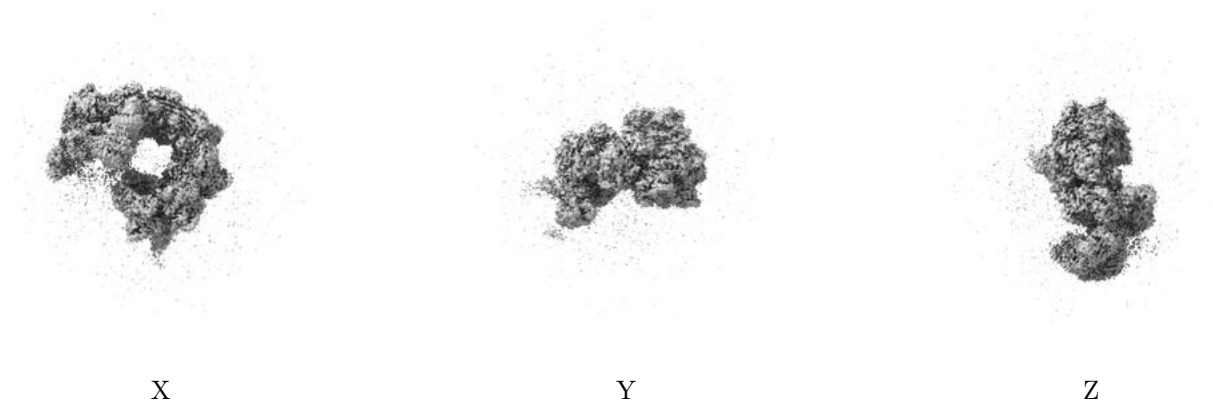


Z

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 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

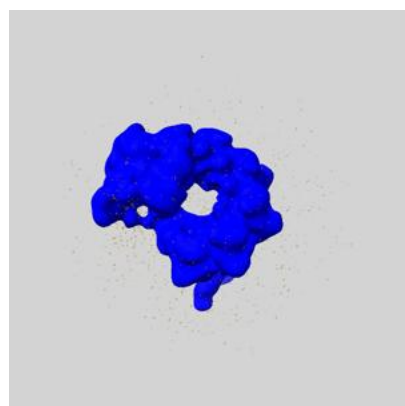
6.6 Mask visualisation [i](#)

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

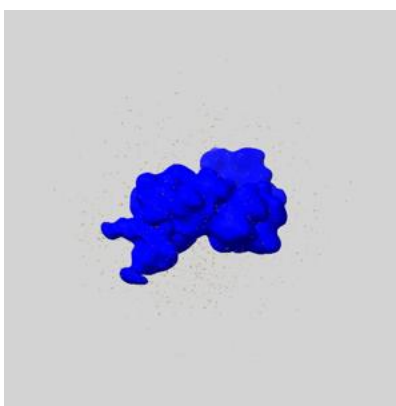
A mask typically either:

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

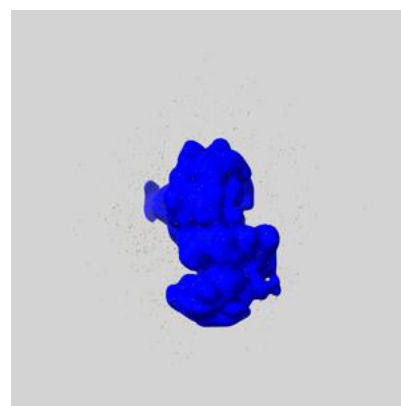
6.6.1 emd_65338_msk_1.map [i](#)



X



Y

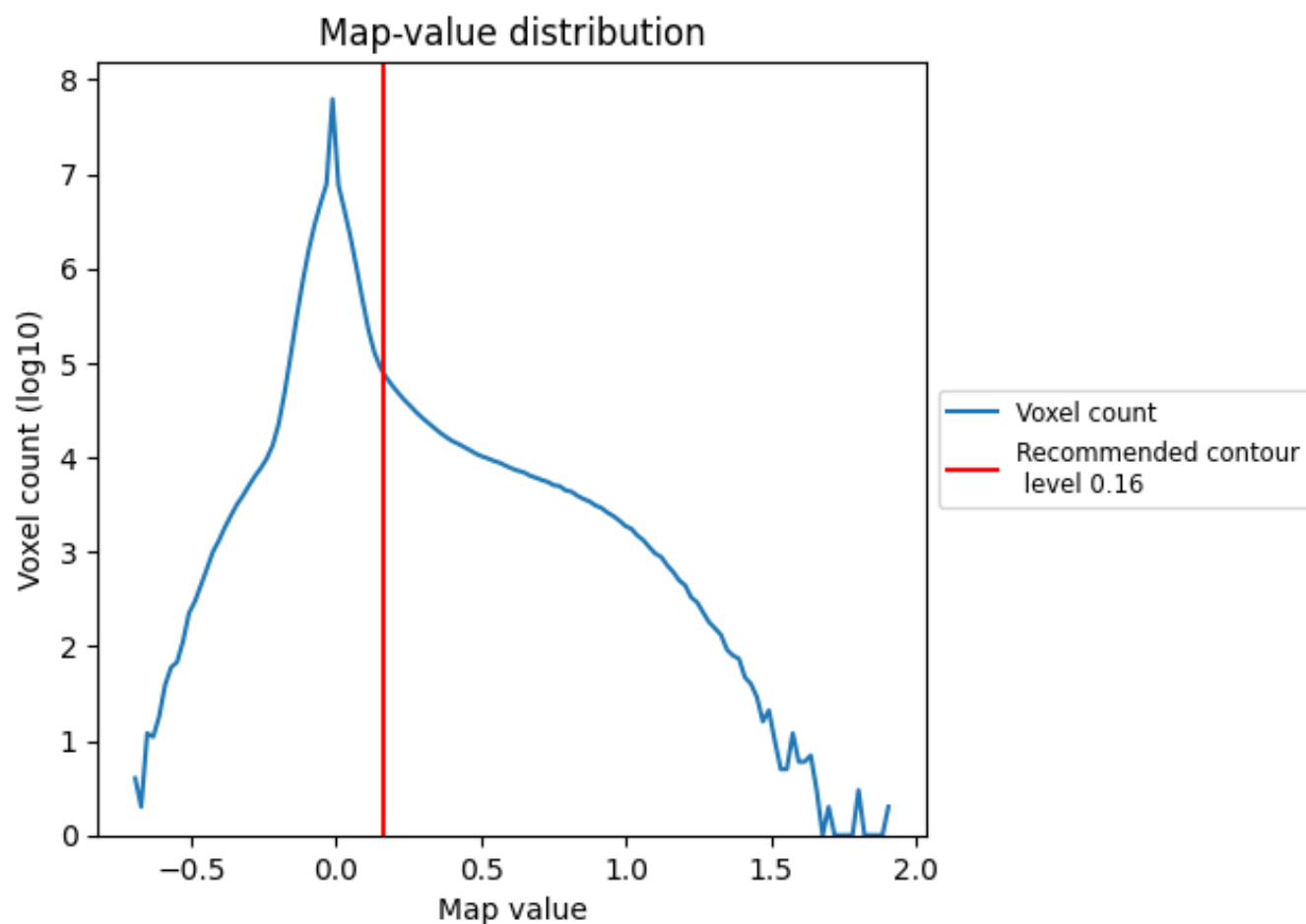


Z

7 Map analysis [i](#)

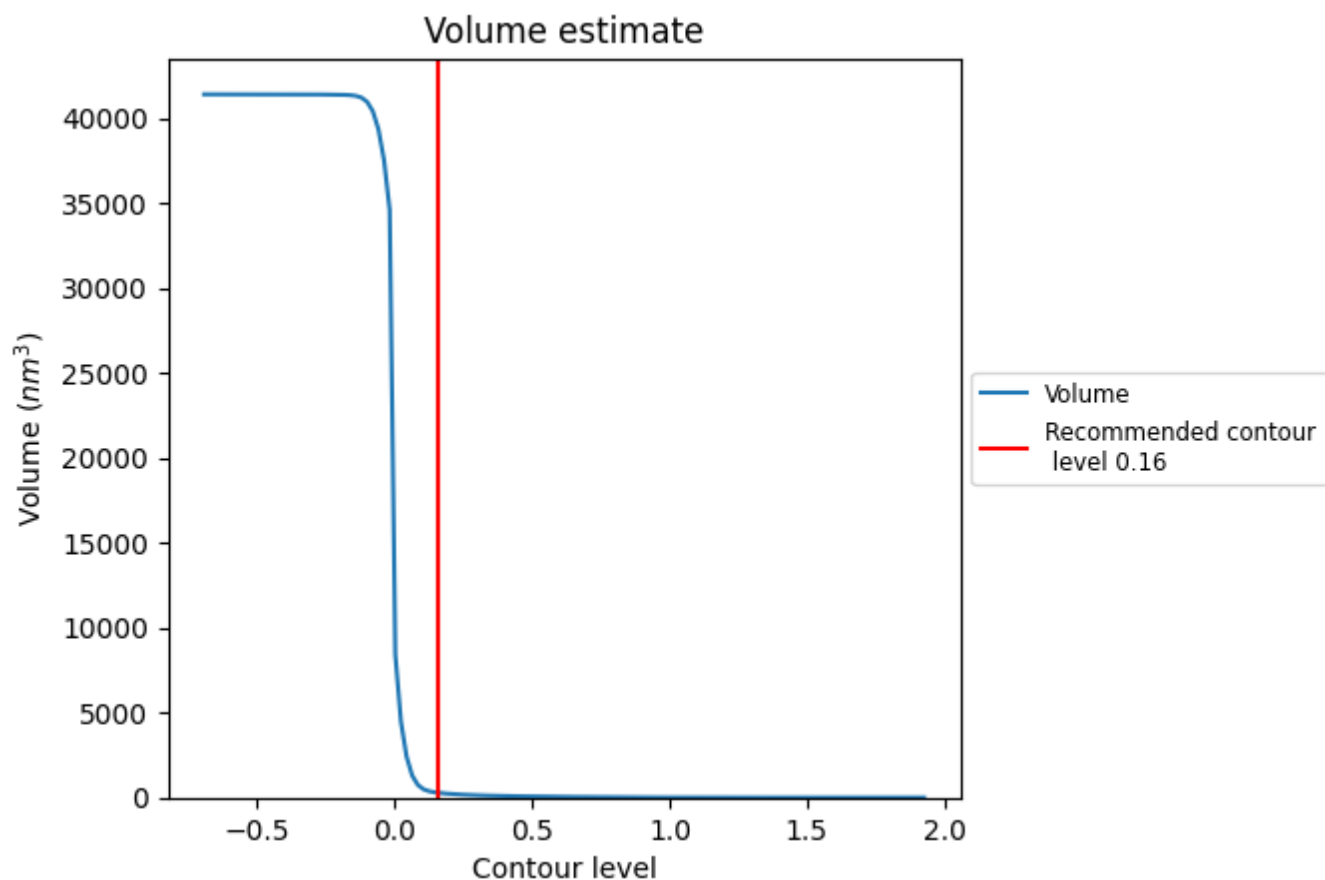
This section contains the results of statistical analysis of the map.

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.

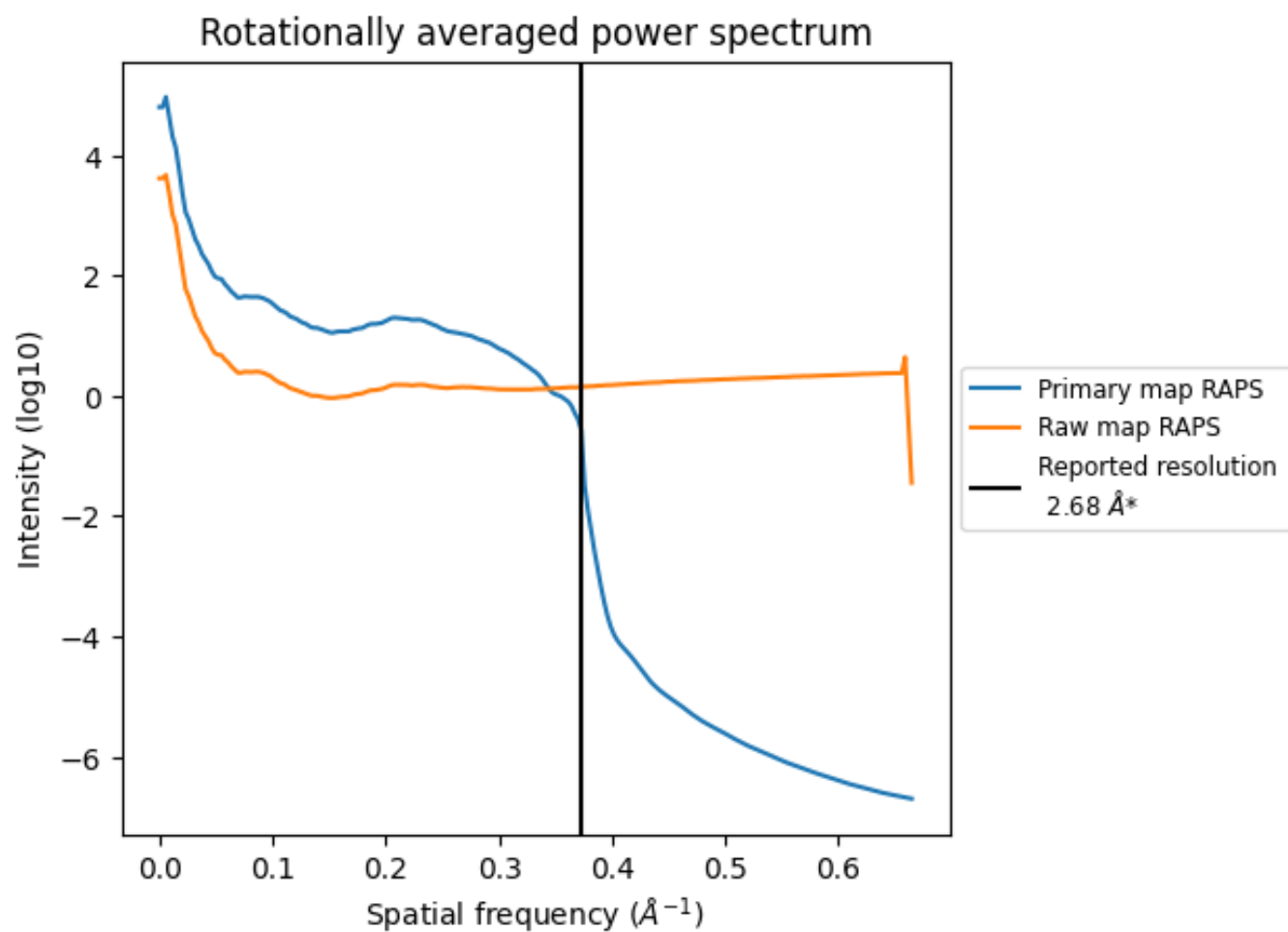
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 281 nm^3 ; this corresponds to an approximate mass of 254 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

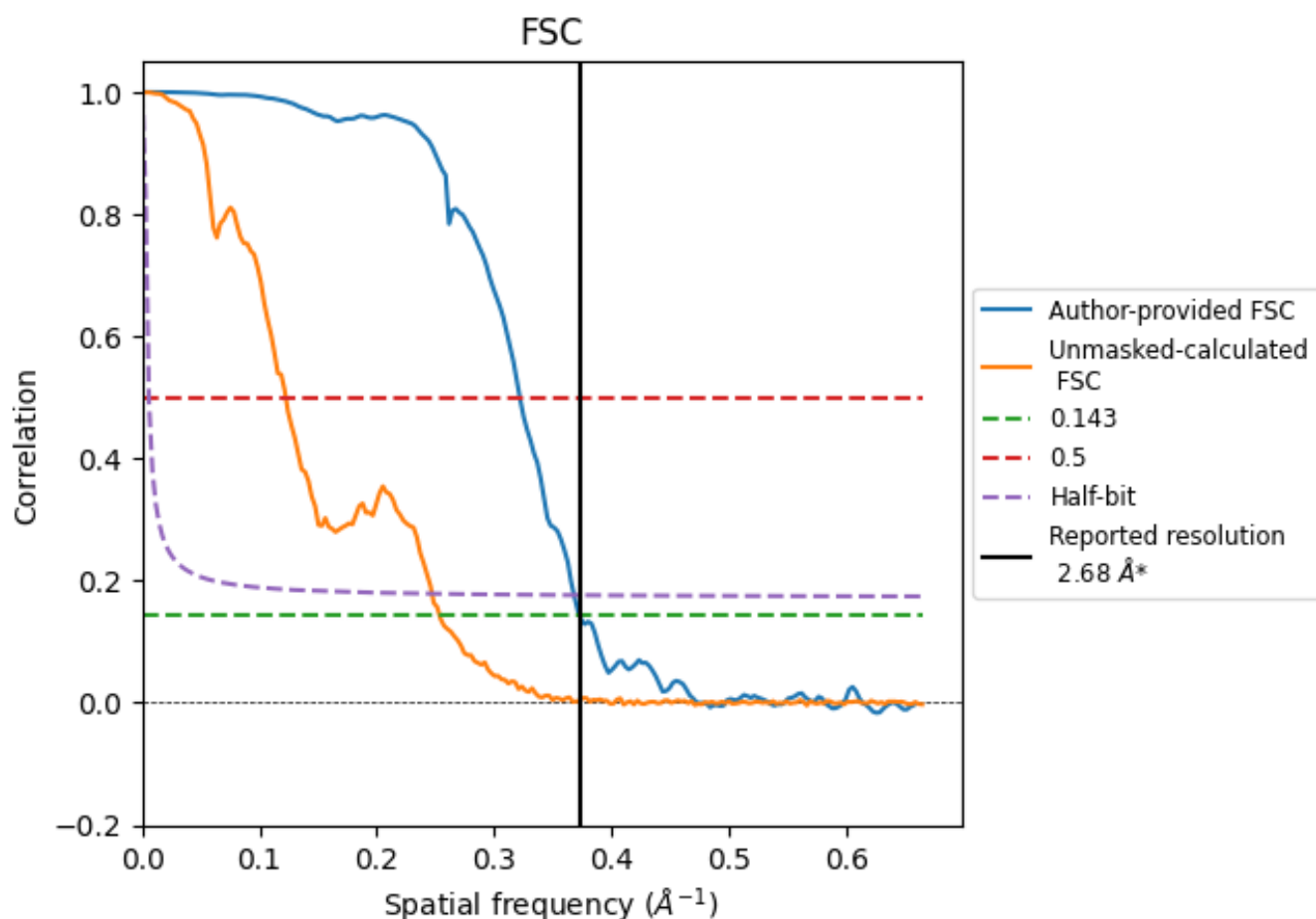


*Reported resolution corresponds to spatial frequency of 0.373 Å⁻¹

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 0.373 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

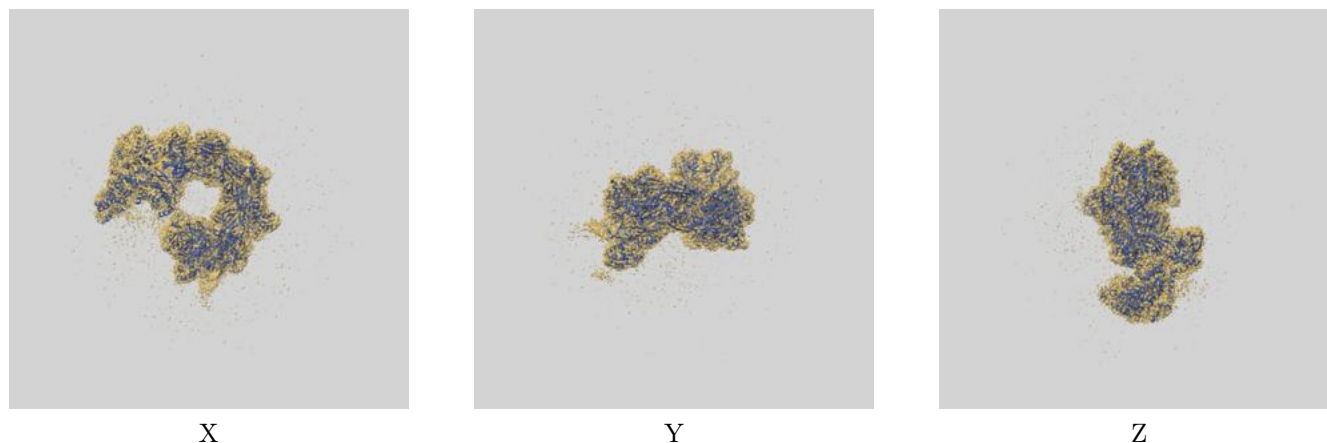
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	2.68	3.11	2.72
Unmasked-calculated*	3.94	8.17	4.05

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

9 Map-model fit [i](#)

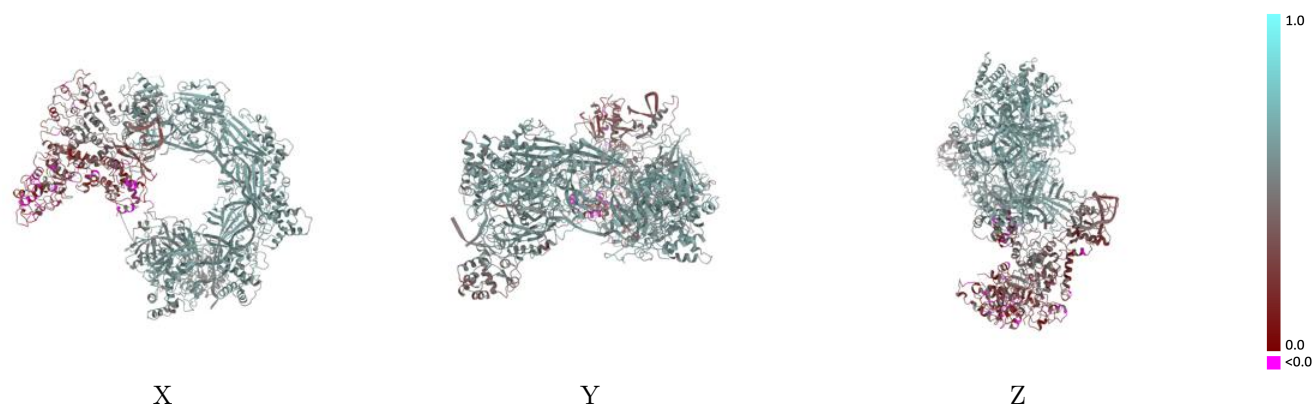
This section contains information regarding the fit between EMDB map EMD-65338 and PDB model 9VTP. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



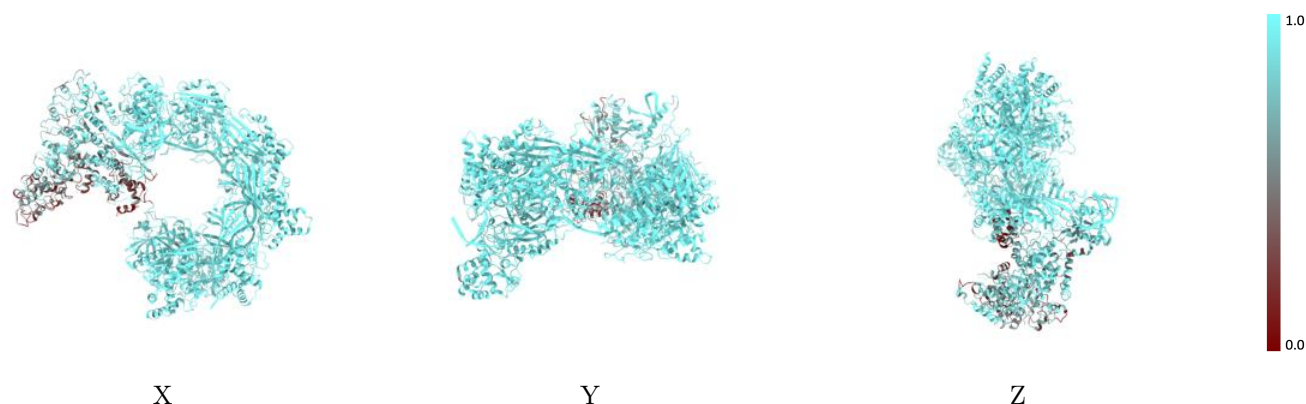
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



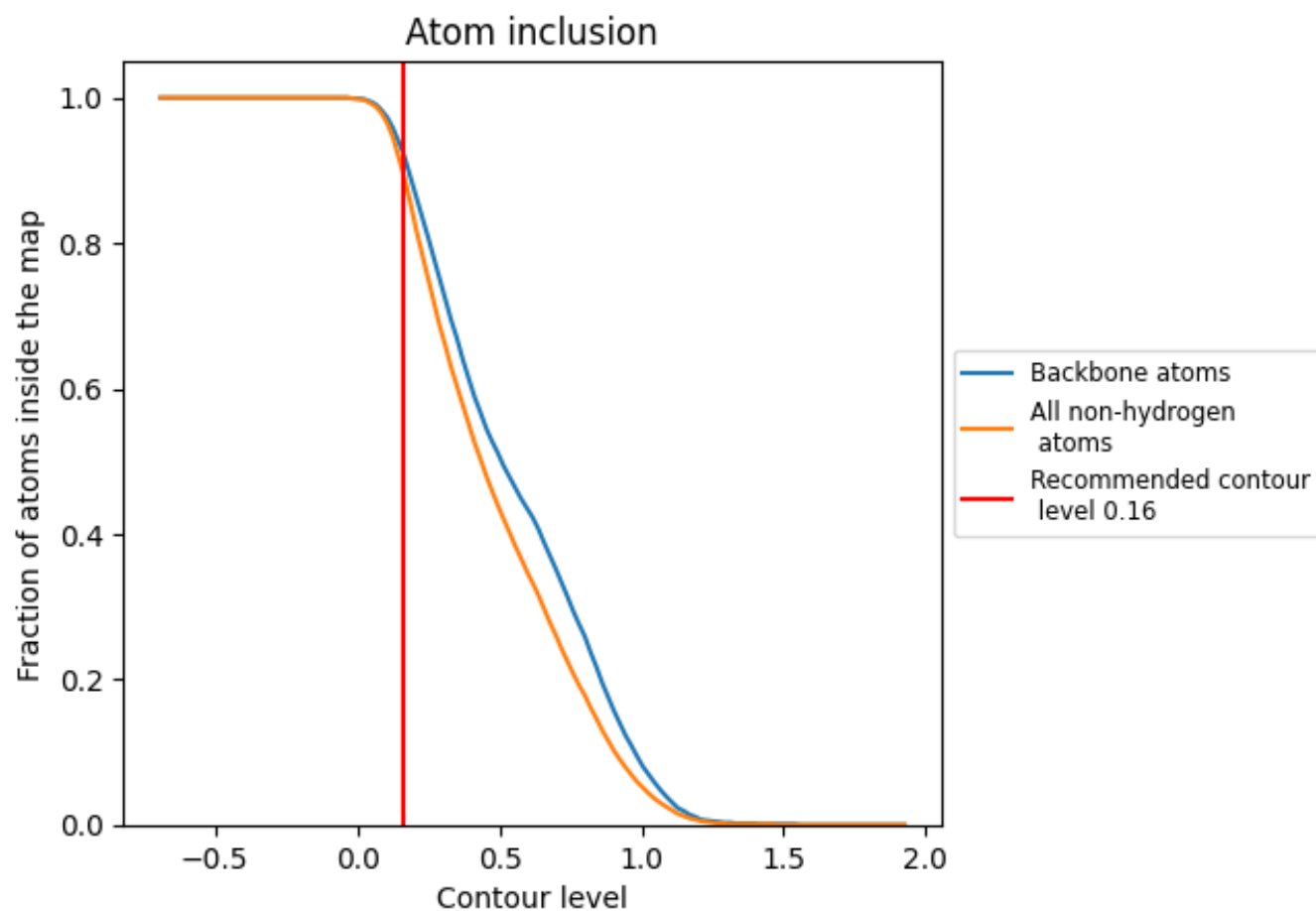
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 90% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8990	 0.5000
1	 0.9890	 0.5200
2	 0.9100	 0.5300
3	 0.9920	 0.4590
A	 0.9760	 0.5870
B	 0.9770	 0.5940
C	 0.9780	 0.5930
D	 0.9680	 0.5770
E	 0.9780	 0.5880
F	 0.9640	 0.5600
G	 0.9020	 0.5020
H	 0.7900	 0.3110
I	 0.6300	 0.2840
J	 0.7490	 0.3200

