



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:37 PM UTC

PDB ID : 8S36 / pdb_00008s36
EMDB ID : EMD-19689
Title : DNA-bound Type IV-A3 CRISPR effector in complex with DinG helicase from *K. pneumoniae* (state II)
Authors : Skorupskaite, A.; Ragozius, V.; Cepaite, R.; Klein, N.; Randau, L.; Malinauskaite, L.; Pausch, P.
Deposited on : 2024-02-19
Resolution : 2.90 Å (reported)
Based on initial models : 8RC2, .

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:

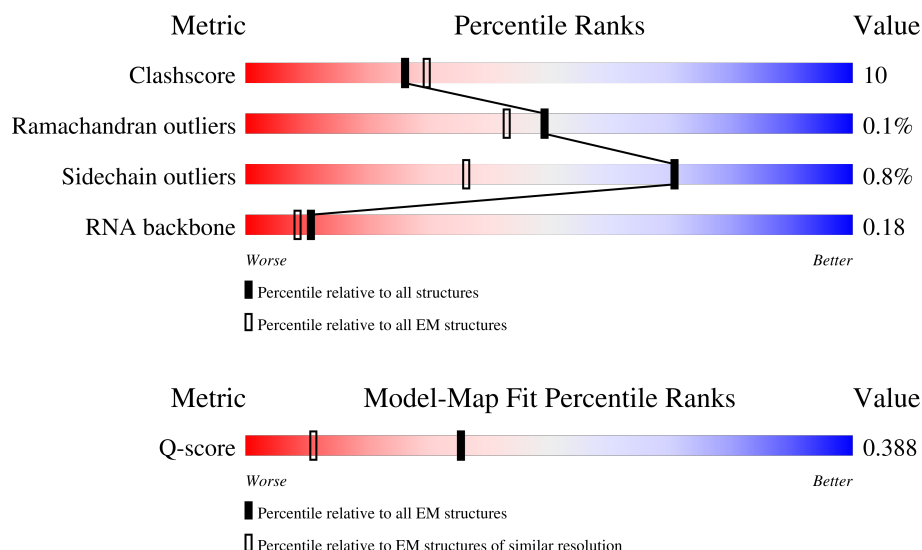
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	350	
1	B	350	
1	C	350	

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Mol	Chain	Length	Quality of chain
1	D	350	
1	E	350	
1	L	350	
2	F	235	
3	G	263	
4	H	61	
5	I	60	
6	J	60	
7	M	624	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 47348 atoms, of which 23099 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CRISPR type AFERR-associated protein Csf2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	342	Total	C	H	N	O	S	0	0
			5252	1655	2608	470	510	9		
1	B	342	Total	C	H	N	O	S	0	0
			5252	1655	2608	470	510	9		
1	C	342	Total	C	H	N	O	S	0	0
			5252	1655	2608	470	510	9		
1	D	342	Total	C	H	N	O	S	0	0
			5251	1655	2607	470	510	9		
1	E	249	Total	C	H	N	O	S	0	0
			3720	1191	1838	334	351	6		
1	L	204	Total	C	H	N	O	S	0	0
			3113	1000	1544	278	286	5		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	344	GLY	-	expression tag	UNP A0A333ESG5
A	345	HIS	-	expression tag	UNP A0A333ESG5
A	346	HIS	-	expression tag	UNP A0A333ESG5
A	347	HIS	-	expression tag	UNP A0A333ESG5
A	348	HIS	-	expression tag	UNP A0A333ESG5
A	349	HIS	-	expression tag	UNP A0A333ESG5
A	350	HIS	-	expression tag	UNP A0A333ESG5
B	344	GLY	-	expression tag	UNP A0A333ESG5
B	345	HIS	-	expression tag	UNP A0A333ESG5
B	346	HIS	-	expression tag	UNP A0A333ESG5
B	347	HIS	-	expression tag	UNP A0A333ESG5
B	348	HIS	-	expression tag	UNP A0A333ESG5
B	349	HIS	-	expression tag	UNP A0A333ESG5
B	350	HIS	-	expression tag	UNP A0A333ESG5
C	344	GLY	-	expression tag	UNP A0A333ESG5
C	345	HIS	-	expression tag	UNP A0A333ESG5
C	346	HIS	-	expression tag	UNP A0A333ESG5
C	347	HIS	-	expression tag	UNP A0A333ESG5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	348	HIS	-	expression tag	UNP A0A333ESG5
C	349	HIS	-	expression tag	UNP A0A333ESG5
C	350	HIS	-	expression tag	UNP A0A333ESG5
D	344	GLY	-	expression tag	UNP A0A333ESG5
D	345	HIS	-	expression tag	UNP A0A333ESG5
D	346	HIS	-	expression tag	UNP A0A333ESG5
D	347	HIS	-	expression tag	UNP A0A333ESG5
D	348	HIS	-	expression tag	UNP A0A333ESG5
D	349	HIS	-	expression tag	UNP A0A333ESG5
D	350	HIS	-	expression tag	UNP A0A333ESG5
E	344	GLY	-	expression tag	UNP A0A333ESG5
E	345	HIS	-	expression tag	UNP A0A333ESG5
E	346	HIS	-	expression tag	UNP A0A333ESG5
E	347	HIS	-	expression tag	UNP A0A333ESG5
E	348	HIS	-	expression tag	UNP A0A333ESG5
E	349	HIS	-	expression tag	UNP A0A333ESG5
E	350	HIS	-	expression tag	UNP A0A333ESG5
L	344	GLY	-	expression tag	UNP A0A333ESG5
L	345	HIS	-	expression tag	UNP A0A333ESG5
L	346	HIS	-	expression tag	UNP A0A333ESG5
L	347	HIS	-	expression tag	UNP A0A333ESG5
L	348	HIS	-	expression tag	UNP A0A333ESG5
L	349	HIS	-	expression tag	UNP A0A333ESG5
L	350	HIS	-	expression tag	UNP A0A333ESG5

- Molecule 2 is a protein called CRISPR type AFERR-associated protein Csf3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	F	235	Total	C	H	N	O	S	0	0
			3625	1150	1833	305	330	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	84	MET	VAL	conflict	UNP A0A8G1XN67
F	103	THR	ILE	conflict	UNP A0A8G1XN67

- Molecule 3 is a protein called CRISPR type AFERR-associated protein Csf1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	263	Total	C	H	N	O	S	0	0
			4209	1343	2119	353	382	12		

- Molecule 4 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	H	37	Total	C	H	N	O	P	0	0
			1187	352	400	142	257	36		

- Molecule 5 is a DNA chain called TS-DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	I	39	Total	C	H	N	O	P	0	0
			1230	375	438	138	240	39		

- Molecule 6 is a DNA chain called NTS-NDA.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	J	32	Total	C	H	N	O	P	0	0
			1019	314	359	127	187	32		

- Molecule 7 is a protein called DEAD/DEAH box helicase.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	M	519	Total	C	H	N	O	S	0	0
			8237	2614	4137	693	770	23		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	292	GLU	LYS	conflict	UNP A0A422ZM74
M	412	ASN	ASP	conflict	UNP A0A422ZM74
M	421	GLY	ASP	conflict	UNP A0A422ZM74
M	435	GLN	HIS	conflict	UNP A0A422ZM74
M	618	PHE	CYS	conflict	UNP A0A422ZM74

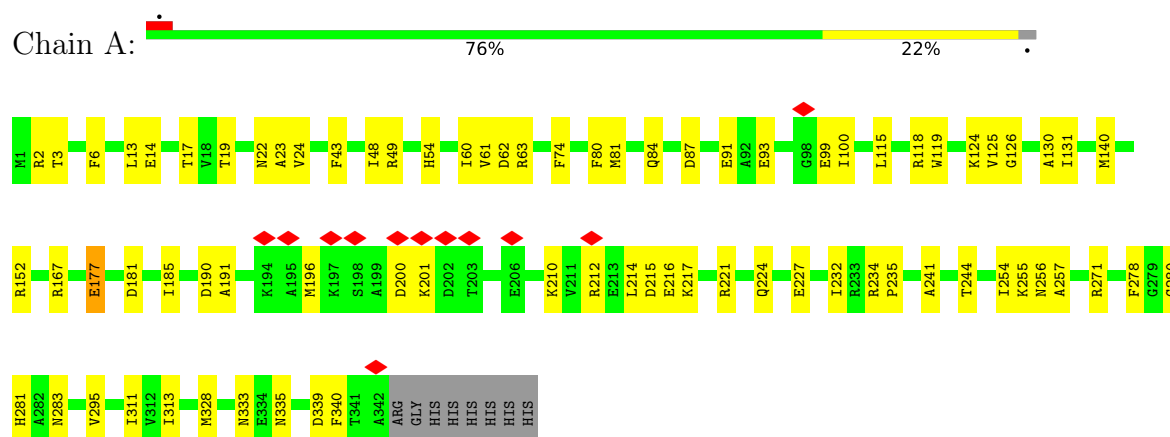
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
8	G	1	Total	Zn	0
			1	1	

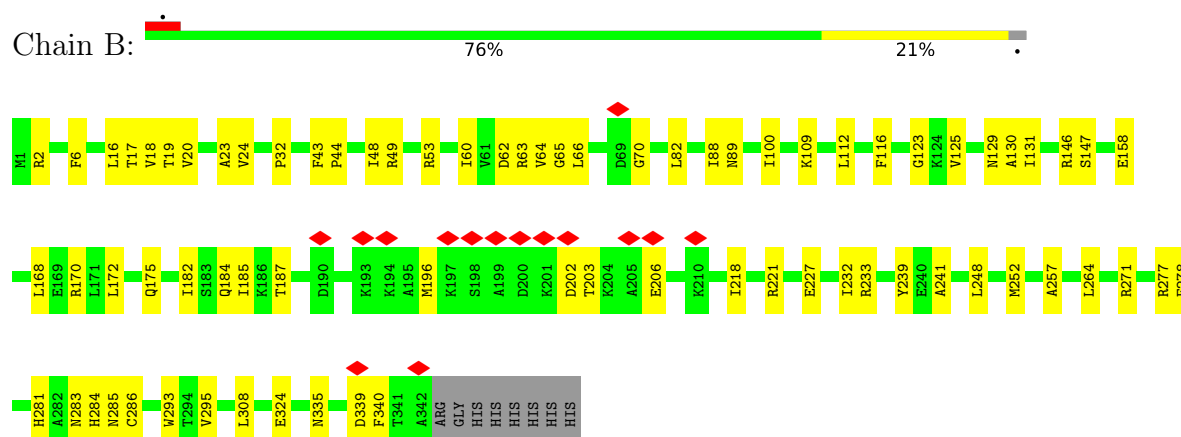
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

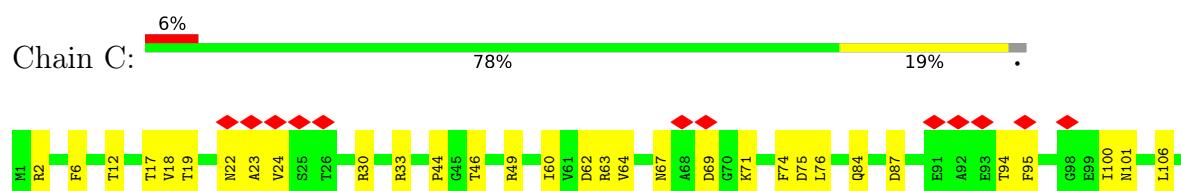
• Molecule 1: CRISPR type AFERR-associated protein Csf2

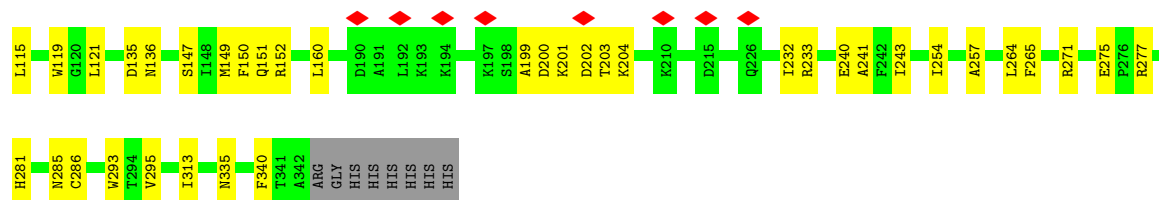


• Molecule 1: CRISPR type AFERR-associated protein Csf2

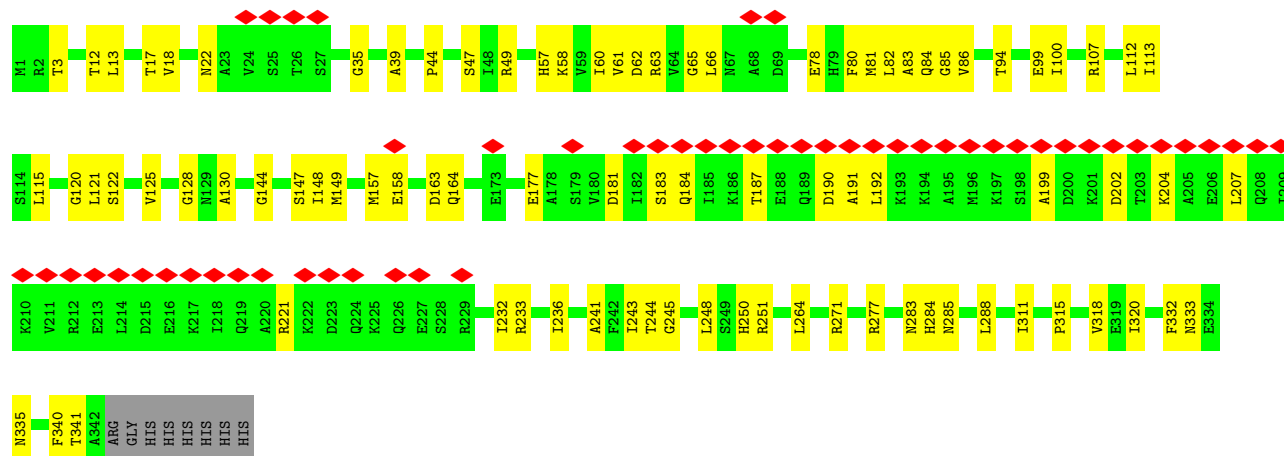
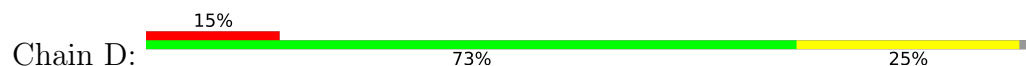


• Molecule 1: CRISPR type AFERR-associated protein Csf2

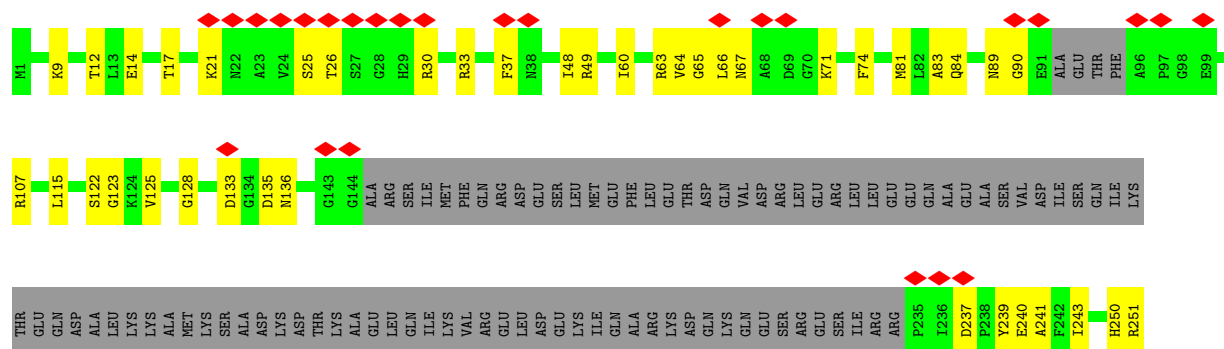




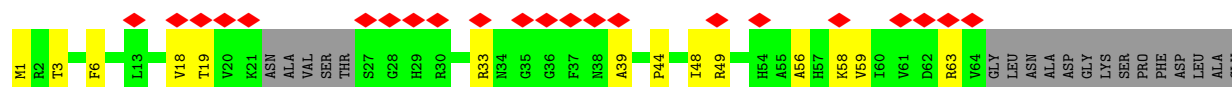
• Molecule 1: CRISPR type AFERR-associated protein Csf2

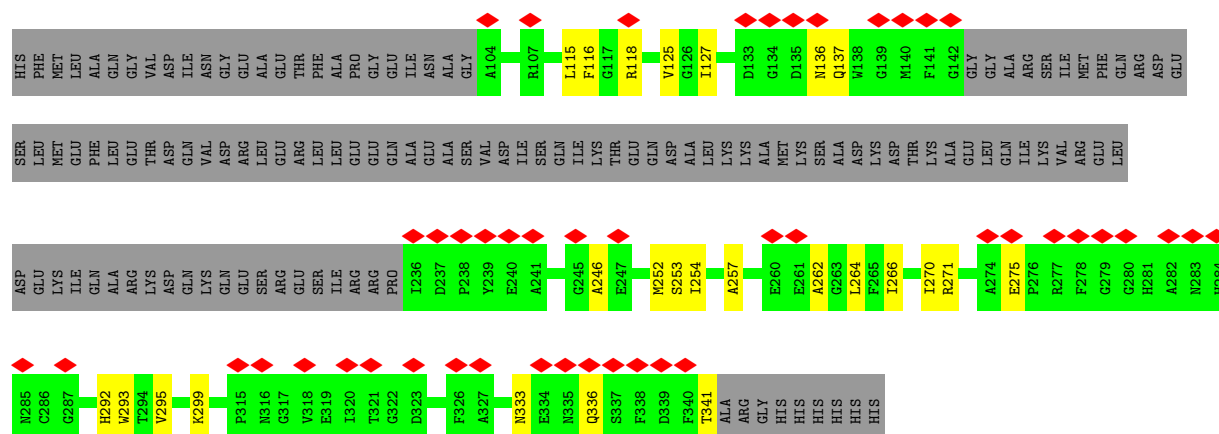


• Molecule 1: CRISPR type AFERR-associated protein Csf2

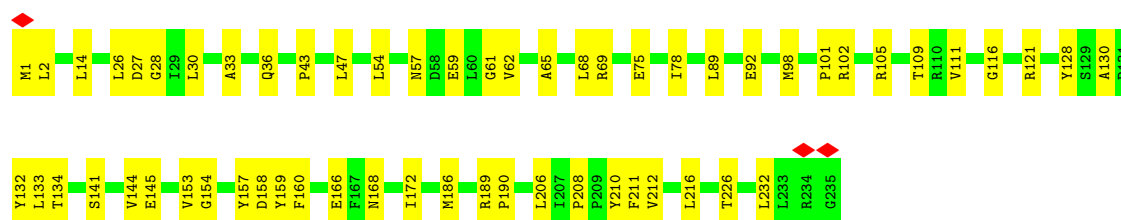
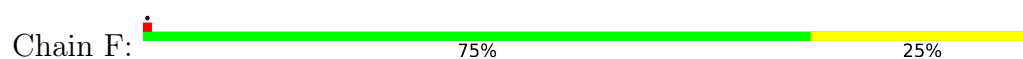


• Molecule 1: CRISPR type AFERR-associated protein Csf2

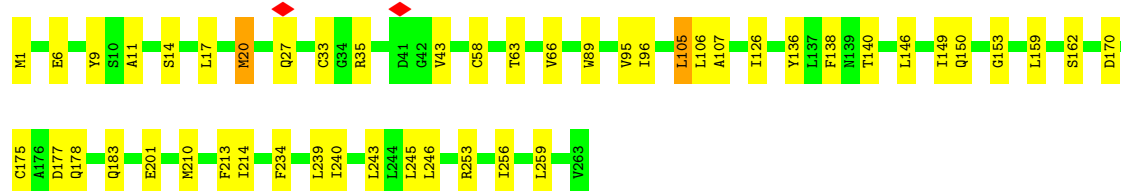
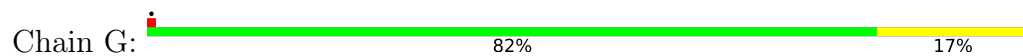




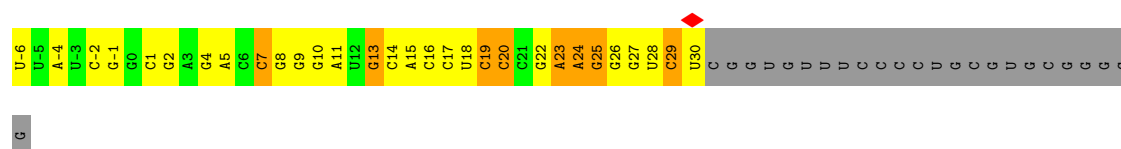
• Molecule 2: CRISPR type AFERR-associated protein Csf3



• Molecule 3: CRISPR type AFERR-associated protein Csf1



• Molecule 4: crRNA



• Molecule 5: TS-DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48197	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.31	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	92000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.533	Depositor
Minimum map value	-0.177	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	396.0, 396.0, 396.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.15	0/2693	0.40	0/3635
1	B	0.13	0/2693	0.32	0/3635
1	C	0.15	0/2693	0.36	0/3635
1	D	0.14	0/2693	0.38	0/3635
1	E	0.15	0/1926	0.40	0/2610
1	L	0.16	0/1606	0.42	0/2175
2	F	0.15	0/1833	0.39	0/2496
3	G	0.14	0/2137	0.35	0/2901
4	H	0.15	0/879	0.37	0/1369
5	I	0.24	0/884	0.49	0/1361
6	J	0.21	0/742	0.48	0/1143
7	M	0.17	0/4178	0.46	0/5659
All	All	0.16	0/24957	0.40	0/34254

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2644	2608	2608	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2644	2608	2608	55	0
1	C	2644	2608	2608	50	0
1	D	2644	2607	2608	63	0
1	E	1882	1838	1838	43	0
1	L	1569	1544	1544	31	0
2	F	1792	1833	1833	50	0
3	G	2090	2119	2119	37	0
4	H	787	400	402	33	0
5	I	792	438	439	4	0
6	J	660	359	360	2	0
7	M	4100	4137	4153	114	0
8	G	1	0	0	0	0
All	All	24249	23099	23120	478	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (478) 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)
3:G:246:LEU:HD13	3:G:256:ILE:HD11	1.57	0.86
4:H:13:G:O2'	4:H:14:C:O4'	1.96	0.84
1:B:49:ARG:NH1	4:H:5:A:OP1	2.14	0.79
4:H:1:C:O2'	4:H:2:G:O4'	1.99	0.79
7:M:361:SER:OG	7:M:363:THR:O	2.01	0.79
1:B:283:ASN:O	1:C:49:ARG:NH1	2.15	0.79
7:M:448:THR:HG23	7:M:486:ILE:HG22	1.65	0.79
1:D:49:ARG:NH1	4:H:17:C:OP1	2.16	0.78
1:L:63:ARG:NH2	1:L:333:ASN:O	2.16	0.78
3:G:95:VAL:HG13	3:G:146:LEU:HD12	1.65	0.78
7:M:380:THR:OG1	7:M:382:ASP:OD1	2.01	0.77
7:M:365:THR:OG1	7:M:368:THR:OG1	2.03	0.77
3:G:136:TYR:O	3:G:140:THR:OG1	2.01	0.77
4:H:10:G:O2'	4:H:11:A:O4'	2.02	0.76
1:D:107:ARG:NH2	1:D:122:SER:O	2.19	0.75
2:F:121:ARG:NH1	4:H:-2:C:O2	2.20	0.75
7:M:218:ASP:OD2	7:M:359:THR:OG1	2.04	0.75
7:M:202:ARG:NH1	7:M:206:ASP:OD1	2.20	0.74
7:M:374:CYS:SG	7:M:387:ARG:NH2	2.59	0.74
1:A:167:ARG:NH2	1:B:89:ASN:OD1	2.20	0.74
1:E:135:ASP:OD1	1:E:136:ASN:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:GLU:N	1:C:275:GLU:OE1	2.22	0.73
7:M:120:LEU:HD22	7:M:133:LEU:HD22	1.71	0.72
1:A:49:ARG:NH1	4:H:-1:G:OP1	2.23	0.72
7:M:503:GLN:NE2	7:M:505:PHE:O	2.23	0.72
1:A:62:ASP:OD2	1:A:271:ARG:NH1	2.23	0.72
1:B:239:TYR:OH	1:B:286:CYS:SG	2.48	0.71
1:C:46:THR:OG1	4:H:13:G:OP1	2.05	0.71
1:D:277:ARG:NH2	1:D:285:ASN:OD1	2.24	0.71
1:D:157:MET:HE3	1:D:157:MET:HA	1.74	0.70
1:D:63:ARG:NH2	1:D:335:ASN:O	2.24	0.70
3:G:89:TRP:O	3:G:153:GLY:N	2.24	0.70
1:A:280:GLY:N	4:H:2:G:OP1	2.25	0.69
3:G:35:ARG:NH2	3:G:58:CYS:SG	2.65	0.69
1:E:259:ASP:OD1	1:E:260:GLU:N	2.26	0.69
1:C:62:ASP:OD2	1:C:271:ARG:NH1	2.25	0.69
1:C:147:SER:O	1:D:84:GLN:NE2	2.26	0.68
1:D:285:ASN:ND2	1:E:251:ARG:O	2.26	0.68
1:D:63:ARG:NH1	1:D:332:PHE:O	2.27	0.68
1:L:118:ARG:NH2	1:L:341:THR:OG1	2.26	0.68
1:B:63:ARG:NH2	1:B:335:ASN:O	2.26	0.68
7:M:521:MET:HE3	7:M:522:LYS:N	2.09	0.68
1:L:18:VAL:HG13	1:L:19:THR:HG23	1.76	0.67
7:M:27:GLY:O	7:M:30:THR:OG1	2.12	0.67
2:F:30:LEU:HD21	2:F:144:VAL:HG22	1.76	0.67
1:C:63:ARG:NH2	1:C:335:ASN:O	2.27	0.67
1:A:185:ILE:HG23	1:A:214:LEU:HD12	1.77	0.67
1:L:49:ARG:NH1	1:L:125:VAL:O	2.28	0.67
7:M:371:GLU:OE2	7:M:552:ARG:NH1	2.28	0.67
1:D:177:GLU:OE1	1:D:221:ARG:NH2	2.28	0.67
1:E:64:VAL:HG21	1:E:74:PHE:CZ	2.30	0.66
1:A:152:ARG:NH2	4:H:7:C:O2'	2.29	0.66
1:A:93:GLU:O	1:A:118:ARG:NH2	2.28	0.66
1:B:49:ARG:NH2	1:B:125:VAL:O	2.28	0.66
7:M:398:MET:O	7:M:398:MET:HE3	1.94	0.66
1:A:131:ILE:HG13	2:F:14:LEU:HD13	1.78	0.66
2:F:189:ARG:NH1	2:F:190:PRO:O	2.29	0.66
3:G:234:PHE:CD2	3:G:243:LEU:HD11	2.31	0.66
1:L:58:LYS:NZ	1:L:275:GLU:OE2	2.27	0.65
1:E:254:ILE:HD11	1:E:265:PHE:CD2	2.32	0.65
1:E:63:ARG:NH2	1:E:335:ASN:O	2.30	0.65
1:A:14:GLU:OE2	1:B:129:ASN:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ILE:HD11	2:F:212:VAL:HG11	1.79	0.64
2:F:75:GLU:N	2:F:75:GLU:OE1	2.28	0.64
1:E:64:VAL:HG21	1:E:74:PHE:HZ	1.62	0.64
3:G:6:GLU:OE1	3:G:6:GLU:N	2.30	0.64
4:H:25:G:O2'	4:H:26:G:O4'	2.15	0.64
7:M:9:SER:OG	7:M:93:GLN:NE2	2.31	0.64
1:A:81:MET:HE2	1:A:81:MET:HA	1.79	0.64
1:A:63:ARG:NH2	1:A:335:ASN:O	2.31	0.64
1:E:14:GLU:OE2	1:E:285:ASN:ND2	2.30	0.64
3:G:246:LEU:HD12	3:G:253:ARG:HG2	1.80	0.63
1:D:94:THR:HG22	1:D:120:GLY:HA2	1.79	0.63
1:L:257:ALA:HB1	1:L:262:ALA:HB2	1.81	0.63
4:H:16:C:O2'	4:H:17:C:O4'	2.11	0.63
3:G:149:ILE:HG23	3:G:159:LEU:HD11	1.80	0.62
1:D:149:MET:SD	1:E:83:ALA:HB3	2.39	0.62
1:B:100:ILE:HG21	2:F:101:PRO:HG3	1.79	0.62
1:C:277:ARG:NH2	1:C:285:ASN:OD1	2.32	0.62
7:M:502:GLU:OE1	7:M:502:GLU:N	2.32	0.62
1:C:232:ILE:HG23	1:D:86:VAL:HG11	1.80	0.62
1:A:140:MET:HE3	1:A:140:MET:HA	1.80	0.62
1:A:118:ARG:NH1	1:A:119:TRP:O	2.33	0.62
1:C:285:ASN:ND2	1:D:251:ARG:O	2.32	0.61
3:G:27:GLN:N	3:G:27:GLN:OE1	2.33	0.61
7:M:71:ASN:N	7:M:216:GLU:OE2	2.33	0.61
1:A:60:ILE:HD12	1:A:340:PHE:CZ	2.35	0.61
3:G:136:TYR:CE1	3:G:140:THR:HG21	2.36	0.61
7:M:568:SER:OG	7:M:571:ASP:OD1	2.19	0.61
1:D:49:ARG:NH2	1:D:125:VAL:O	2.33	0.61
7:M:35:VAL:O	7:M:385:SER:N	2.34	0.61
7:M:400:LEU:HD11	7:M:402:ILE:HG23	1.82	0.61
1:A:61:VAL:HG12	1:A:74:PHE:CE2	2.35	0.61
1:L:1:MET:HE2	1:L:1:MET:HA	1.83	0.61
1:B:48:ILE:HG23	1:B:278:PHE:CZ	2.35	0.61
7:M:76:MET:HE3	7:M:104:MET:SD	2.39	0.61
1:A:167:ARG:NE	1:A:227:GLU:OE2	2.32	0.60
1:B:146:ARG:NE	1:B:232:ILE:O	2.34	0.60
7:M:115:VAL:HG11	7:M:137:ALA:HA	1.83	0.60
7:M:191:ALA:O	7:M:195:VAL:HG12	2.02	0.60
2:F:1:MET:HE3	2:F:2:LEU:N	2.17	0.60
7:M:70:THR:O	7:M:190:HIS:N	2.35	0.60
1:A:3:THR:HG21	2:F:36:GLN:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ILE:HD12	1:C:340:PHE:CZ	2.37	0.60
1:B:175:GLN:OE1	1:B:232:ILE:N	2.35	0.59
4:H:4:G:O2'	4:H:5:A:O4'	2.14	0.59
1:D:144:GLY:O	1:E:21:LYS:NZ	2.34	0.59
7:M:79:ILE:HD11	7:M:187:VAL:HG11	1.84	0.59
1:L:266:ILE:O	1:L:270:ILE:HG23	2.02	0.59
7:M:103:LEU:HD22	7:M:180:ALA:CB	2.32	0.59
7:M:103:LEU:HD22	7:M:180:ALA:HB1	1.84	0.59
1:B:60:ILE:HD12	1:B:340:PHE:CZ	2.38	0.59
1:C:49:ARG:NE	4:H:11:A:OP1	2.33	0.59
3:G:210:MET:SD	3:G:214:ILE:HD12	2.43	0.59
1:C:151:GLN:OE1	1:C:233:ARG:NH1	2.35	0.58
2:F:109:THR:HG21	6:J:-5:DG:OP1	2.02	0.58
7:M:596:GLU:OE1	7:M:596:GLU:N	2.36	0.58
3:G:33:CYS:SG	3:G:35:ARG:NE	2.77	0.58
1:L:136:ASN:OD1	1:L:137:GLN:N	2.35	0.58
1:E:48:ILE:HG23	1:E:278:PHE:CZ	2.37	0.58
1:E:33:ARG:NH2	1:E:240:GLU:OE2	2.37	0.58
1:D:18:VAL:HG11	1:D:44:PRO:CD	2.33	0.58
1:D:243:ILE:HD12	1:D:244:THR:O	2.04	0.58
1:D:233:ARG:NH1	5:I:-26:DC:O2	2.36	0.58
1:A:3:THR:HG23	1:A:255:LYS:HA	1.86	0.57
1:B:18:VAL:HG11	1:B:44:PRO:CD	2.33	0.57
1:B:60:ILE:HD11	1:B:264:LEU:HD11	1.85	0.57
3:G:201:GLU:OE1	3:G:245:LEU:HD11	2.03	0.57
1:D:63:ARG:NH2	1:D:333:ASN:O	2.37	0.57
4:H:7:C:O2'	4:H:8:G:O4'	2.16	0.57
1:B:281:HIS:N	4:H:9:G:OP2	2.32	0.56
1:E:81:MET:HE2	1:E:81:MET:HA	1.86	0.56
1:C:152:ARG:NH2	4:H:19:C:O2'	2.38	0.56
2:F:78:ILE:HD12	2:F:130:ALA:HB2	1.86	0.56
2:F:145:GLU:HB2	2:F:172:ILE:HD12	1.86	0.56
7:M:223:MET:HE2	7:M:223:MET:O	2.06	0.56
1:C:18:VAL:HG11	1:C:44:PRO:CD	2.35	0.56
1:B:182:ILE:HG23	1:B:218:ILE:HD12	1.88	0.56
2:F:134:THR:HG21	2:F:232:LEU:HD13	1.87	0.56
7:M:569:GLU:OE1	7:M:569:GLU:N	2.38	0.56
1:B:158:GLU:OE1	1:B:158:GLU:N	2.39	0.56
7:M:90:ILE:HD12	7:M:91:ALA:N	2.21	0.56
1:D:80:PHE:O	1:D:85:GLY:N	2.39	0.56
7:M:148:GLU:OE1	7:M:148:GLU:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:601:VAL:HG12	7:M:604:ARG:HH21	1.71	0.56
1:L:18:VAL:HG22	1:L:19:THR:H	1.71	0.55
1:D:81:MET:HE2	1:D:81:MET:HA	1.88	0.55
1:D:113:ILE:HG22	1:D:121:LEU:HD23	1.89	0.55
1:E:49:ARG:NE	4:H:23:A:OP1	2.29	0.55
1:E:254:ILE:HG22	1:E:257:ALA:HB2	1.87	0.55
1:D:192:LEU:HB3	1:D:207:LEU:HD21	1.89	0.55
2:F:59:GLU:N	2:F:59:GLU:OE1	2.40	0.55
1:L:48:ILE:HG22	1:L:127:ILE:HG21	1.87	0.55
1:B:184:GLN:O	1:B:187:THR:OG1	2.24	0.55
1:C:277:ARG:NH1	1:C:286:CYS:O	2.40	0.55
1:D:183:SER:O	1:D:187:THR:HG23	2.07	0.55
3:G:240:ILE:HG23	7:M:622:ILE:HG12	1.89	0.55
1:C:135:ASP:OD1	1:C:136:ASN:N	2.40	0.55
1:B:206:GLU:OE1	1:B:206:GLU:N	2.38	0.54
3:G:170:ASP:OD2	3:G:170:ASP:N	2.37	0.54
1:A:181:ASP:OD2	1:A:221:ARG:NE	2.39	0.54
1:E:84:GLN:NE2	4:H:24:A:OP1	2.39	0.54
1:D:115:LEU:HD12	1:D:264:LEU:HD23	1.90	0.54
7:M:568:SER:OG	7:M:570:ASN:OD1	2.23	0.54
7:M:394:VAL:HG13	7:M:394:VAL:O	2.08	0.54
1:L:33:ARG:NH2	1:L:39:ALA:O	2.38	0.54
2:F:47:LEU:HD21	2:F:208:PRO:O	2.07	0.53
3:G:106:LEU:HG	3:G:126:ILE:HD11	1.89	0.53
3:G:20:MET:HG2	3:G:66:VAL:HG21	1.89	0.53
1:A:6:PHE:CD1	1:A:295:VAL:HG22	2.43	0.53
1:A:177:GLU:N	1:A:177:GLU:OE2	2.41	0.53
1:D:94:THR:HG21	4:H:15:A:C2	2.43	0.53
3:G:138:PHE:CD2	3:G:259:LEU:HD21	2.44	0.53
1:C:18:VAL:HG11	1:C:44:PRO:HD3	1.91	0.53
1:D:60:ILE:HD12	1:D:340:PHE:CZ	2.44	0.53
1:D:181:ASP:OD1	1:D:184:GLN:NE2	2.42	0.53
2:F:14:LEU:HD11	2:F:168:ASN:CG	2.35	0.52
2:F:62:VAL:HG12	2:F:206:LEU:HD12	1.91	0.52
2:F:69:ARG:O	2:F:134:THR:HG22	2.10	0.52
1:D:57:HIS:CB	1:D:83:ALA:HB2	2.40	0.52
1:A:190:ASP:OD1	1:A:191:ALA:N	2.43	0.52
3:G:9:TYR:HD1	3:G:63:THR:HG21	1.74	0.52
1:B:147:SER:O	1:C:84:GLN:NE2	2.43	0.52
1:B:233:ARG:NH1	5:I:-13:DC:OP1	2.42	0.52
1:A:54:HIS:NE2	2:F:92:GLU:OE1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:22:G:O2'	4:H:23:A:O4'	2.26	0.51
1:C:17:THR:HB	1:C:241:ALA:HB2	1.91	0.51
1:C:149:MET:CE	1:D:83:ALA:HB3	2.39	0.51
1:A:43:PHE:HB3	1:A:130:ALA:HB3	1.93	0.51
7:M:26:ALA:O	7:M:30:THR:HG23	2.10	0.51
1:B:17:THR:HB	1:B:241:ALA:HB2	1.92	0.51
1:A:63:ARG:NH1	1:A:333:ASN:O	2.43	0.51
1:A:115:LEU:O	1:A:125:VAL:HG12	2.11	0.51
1:A:48:ILE:HG23	1:A:278:PHE:CZ	2.45	0.51
1:B:16:LEU:HD11	1:B:43:PHE:CE1	2.46	0.51
7:M:472:SER:HA	7:M:475:ILE:HD12	1.93	0.51
1:E:270:ILE:HD13	1:E:318:VAL:HG11	1.92	0.51
3:G:11:ALA:CB	3:G:96:ILE:HG23	2.41	0.50
7:M:38:ILE:HD13	7:M:354:LEU:CD1	2.41	0.50
1:D:158:GLU:OE1	1:D:158:GLU:N	2.45	0.50
1:D:99:GLU:N	1:D:99:GLU:OE1	2.44	0.50
1:E:128:GLY:O	1:E:250:HIS:NE2	2.42	0.50
1:E:319:GLU:N	1:E:319:GLU:OE1	2.45	0.50
1:A:212:ARG:O	1:A:215:ASP:OD2	2.30	0.50
1:A:224:GLN:O	1:A:224:GLN:NE2	2.44	0.50
1:D:128:GLY:O	1:D:250:HIS:NE2	2.44	0.50
1:D:283:ASN:ND2	4:H:23:A:OP2	2.39	0.50
1:E:25:SER:OG	1:E:26:THR:N	2.45	0.50
1:D:288:LEU:HD23	1:E:251:ARG:HD2	1.94	0.50
1:A:244:THR:HG21	1:B:131:ILE:HG13	1.94	0.50
7:M:139:TRP:NE1	7:M:145:GLU:OE2	2.44	0.50
1:A:22:ASN:OD1	1:A:23:ALA:N	2.44	0.49
1:A:232:ILE:HD11	1:B:88:ILE:HG22	1.92	0.49
7:M:38:ILE:HD11	7:M:386:ILE:HD11	1.93	0.49
1:A:84:GLN:O	4:H:-2:C:O2'	2.29	0.49
2:F:216:LEU:HD23	2:F:216:LEU:H	1.78	0.49
7:M:54:ALA:HB1	7:M:66:PHE:CD2	2.47	0.49
7:M:524:GLU:N	7:M:524:GLU:OE1	2.45	0.49
1:C:69:ASP:OD1	1:C:69:ASP:N	2.44	0.49
4:H:19:C:O2'	4:H:20:C:O5'	2.27	0.49
1:B:64:VAL:HG23	1:B:65:GLY:H	1.77	0.49
1:C:199:ALA:HB1	1:C:203:THR:HG23	1.95	0.49
1:D:57:HIS:CG	1:D:83:ALA:HB2	2.47	0.49
1:D:147:SER:O	1:E:84:GLN:NE2	2.44	0.49
1:E:254:ILE:CG2	1:E:257:ALA:HB2	2.43	0.49
1:D:65:GLY:C	1:D:66:LEU:HD22	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:6:GLU:OE1	3:G:35:ARG:NH1	2.45	0.49
7:M:587:ASP:O	7:M:593:ARG:NH1	2.46	0.49
1:B:6:PHE:CD1	1:B:295:VAL:HG22	2.48	0.49
1:D:190:ASP:OD1	1:D:191:ALA:N	2.46	0.49
1:D:148:ILE:HD13	1:D:232:ILE:HG21	1.95	0.48
1:B:221:ARG:O	1:B:221:ARG:NH1	2.44	0.48
1:L:115:LEU:HD12	1:L:264:LEU:HD22	1.93	0.48
7:M:170:ILE:HG22	7:M:171:GLN:N	2.28	0.48
1:B:62:ASP:OD2	1:B:271:ARG:NH2	2.45	0.48
3:G:105:LEU:HD12	3:G:107:ALA:HB2	1.95	0.48
2:F:116:GLY:N	5:I:1:DT:OP2	2.44	0.48
2:F:206:LEU:HD23	2:F:216:LEU:HD21	1.95	0.48
2:F:189:ARG:NH2	2:F:210:TYR:OH	2.46	0.48
1:C:33:ARG:NH1	1:C:240:GLU:OE2	2.43	0.48
1:D:18:VAL:HG11	1:D:44:PRO:HD2	1.95	0.48
3:G:9:TYR:CD1	3:G:63:THR:HG21	2.48	0.48
7:M:111:SER:C	7:M:112:LEU:HD22	2.39	0.48
7:M:393:ASP:OD1	7:M:393:ASP:N	2.40	0.48
7:M:560:GLN:OE1	7:M:564:ARG:NH2	2.45	0.48
7:M:606:GLU:OE1	7:M:606:GLU:N	2.43	0.48
1:E:239:TYR:OH	1:E:286:CYS:SG	2.71	0.48
1:L:254:ILE:CG2	1:L:257:ALA:HB2	2.43	0.48
1:E:48:ILE:HG23	1:E:278:PHE:CE1	2.48	0.48
1:L:6:PHE:CD2	1:L:295:VAL:HG22	2.48	0.48
1:C:281:HIS:N	4:H:15:A:OP2	2.41	0.48
2:F:68:LEU:HD11	2:F:133:LEU:HG	1.95	0.48
7:M:384:ILE:HD13	7:M:387:ARG:HE	1.79	0.48
1:B:185:ILE:HB	1:B:218:ILE:HD11	1.96	0.47
1:A:283:ASN:O	1:B:49:ARG:NE	2.43	0.47
1:B:123:GLY:N	4:H:4:G:OP1	2.44	0.47
2:F:27:ASP:OD2	2:F:189:ARG:NH2	2.43	0.47
1:D:12:THR:O	1:D:245:GLY:N	2.36	0.47
2:F:105:ARG:NH1	5:I:9:DC:OP2	2.48	0.47
1:A:124:LYS:NZ	1:A:256:ASN:O	2.38	0.47
1:L:18:VAL:O	1:L:19:THR:OG1	2.25	0.47
1:E:115:LEU:O	1:E:125:VAL:HG12	2.14	0.47
4:H:19:C:O2'	4:H:20:C:O4'	2.31	0.47
3:G:240:ILE:HD12	7:M:622:ILE:HG12	1.95	0.47
7:M:100:PHE:CZ	7:M:187:VAL:HG21	2.50	0.47
1:B:252:MET:HE2	1:B:293:TRP:CE2	2.50	0.47
1:A:217:LYS:HD3	1:A:217:LYS:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:ASN:OD1	1:C:71:LYS:N	2.48	0.47
1:E:60:ILE:HD12	1:E:340:PHE:CZ	2.50	0.47
3:G:246:LEU:CD1	3:G:256:ILE:HD11	2.38	0.47
7:M:18:GLN:NE2	7:M:44:VAL:O	2.48	0.47
7:M:78:GLN:N	7:M:78:GLN:OE1	2.47	0.47
7:M:118:LEU:HD13	7:M:118:LEU:O	2.14	0.47
7:M:195:VAL:HG23	7:M:199:CYS:HB2	1.97	0.47
7:M:402:ILE:HD11	7:M:585:PRO:HD3	1.97	0.47
1:C:150:PHE:CZ	1:C:160:LEU:HD11	2.50	0.46
1:E:328:MET:SD	1:E:328:MET:N	2.87	0.46
1:B:2:ARG:O	1:B:257:ALA:N	2.42	0.46
1:B:277:ARG:NH1	1:B:285:ASN:OD1	2.47	0.46
2:F:27:ASP:OD1	2:F:28:GLY:N	2.48	0.46
2:F:132:TYR:OH	7:M:589:SER:N	2.48	0.46
3:G:1:MET:HE3	3:G:1:MET:HA	1.98	0.46
3:G:9:TYR:O	3:G:14:SER:N	2.48	0.46
1:A:215:ASP:OD2	1:A:216:GLU:N	2.48	0.46
7:M:192:MET:HA	7:M:195:VAL:HG12	1.98	0.46
2:F:154:GLY:O	4:H:-6:U:N3	2.46	0.46
7:M:83:ASP:OD2	7:M:84:ARG:NH1	2.42	0.46
1:A:2:ARG:NH2	1:A:328:MET:SD	2.88	0.46
1:A:100:ILE:CD1	2:F:212:VAL:HG11	2.43	0.46
1:A:200:ASP:O	1:A:201:LYS:HG3	2.15	0.46
1:B:100:ILE:HD11	2:F:111:VAL:HG23	1.97	0.46
7:M:487:SER:O	7:M:487:SER:OG	2.31	0.46
1:A:17:THR:HB	1:A:241:ALA:HB2	1.98	0.46
1:B:264:LEU:O	1:B:264:LEU:HD23	2.15	0.46
1:E:115:LEU:HD21	1:E:265:PHE:HB2	1.98	0.46
4:H:29:C:OP1	1:L:49:ARG:NE	2.46	0.46
1:L:59:VAL:HG23	1:L:271:ARG:HD2	1.97	0.46
7:M:448:THR:HG22	7:M:464:ILE:HG23	1.98	0.46
7:M:526:LEU:HD23	7:M:542:VAL:HG13	1.98	0.46
1:C:17:THR:HG21	1:C:281:HIS:ND1	2.31	0.46
1:C:115:LEU:HD21	1:C:265:PHE:HB2	1.98	0.46
1:L:292:HIS:O	1:L:292:HIS:ND1	2.49	0.46
7:M:33:HIS:N	7:M:351:ARG:O	2.41	0.46
1:B:168:LEU:HD22	1:D:100:ILE:HG21	1.98	0.45
1:C:254:ILE:HD11	1:C:265:PHE:CD2	2.51	0.45
1:A:311:ILE:HG22	1:A:313:ILE:CD1	2.46	0.45
1:B:168:LEU:HD23	1:B:172:LEU:HG	1.98	0.45
2:F:78:ILE:HD11	2:F:128:TYR:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:PHE:CD2	1:C:295:VAL:HG22	2.51	0.45
1:E:49:ARG:NH2	1:E:125:VAL:O	2.46	0.45
7:M:223:MET:O	7:M:226:VAL:HG22	2.16	0.45
1:A:19:THR:HG23	1:A:24:VAL:HG21	1.98	0.45
7:M:46:LYS:NZ	7:M:356:THR:OG1	2.50	0.45
1:A:87:ASP:OD2	1:A:91:GLU:N	2.49	0.45
1:C:64:VAL:HG11	1:C:74:PHE:CZ	2.52	0.45
1:C:200:ASP:OD1	1:C:201:LYS:N	2.48	0.45
3:G:105:LEU:CD1	3:G:107:ALA:HB2	2.46	0.45
1:A:339:ASP:OD1	1:A:339:ASP:N	2.49	0.45
7:M:73:HIS:HA	7:M:76:MET:SD	2.56	0.45
1:A:13:LEU:O	1:A:244:THR:HG23	2.17	0.45
1:B:283:ASN:OD1	1:B:284:HIS:N	2.49	0.45
1:C:60:ILE:HD11	1:C:264:LEU:CD1	2.47	0.45
1:D:62:ASP:OD2	1:D:271:ARG:NH2	2.50	0.45
1:D:311:ILE:HD13	1:D:320:ILE:HG12	1.98	0.45
2:F:102:ARG:NH1	6:J:-5:DG:OP2	2.50	0.45
1:C:22:ASN:OD1	1:C:23:ALA:N	2.49	0.45
2:F:62:VAL:CG1	2:F:206:LEU:HD12	2.46	0.45
2:F:157:TYR:CD2	3:G:183:GLN:HG2	2.52	0.45
1:L:3:THR:O	1:L:3:THR:HG23	2.17	0.45
1:B:19:THR:HG23	1:B:24:VAL:HG11	1.99	0.45
1:E:67:ASN:OD1	1:E:71:LYS:N	2.43	0.45
7:M:400:LEU:HD11	7:M:402:ILE:CG2	2.46	0.45
1:B:18:VAL:HG11	1:B:44:PRO:HD2	1.98	0.45
1:B:308:LEU:HD22	1:B:324:GLU:HG3	1.99	0.45
1:D:13:LEU:HD11	1:D:315:PRO:HD3	1.99	0.45
1:L:137:GLN:CD	1:L:137:GLN:O	2.60	0.45
7:M:490:ALA:O	7:M:492:VAL:HG13	2.17	0.45
1:B:20:VAL:HG21	1:B:32:PRO:HB3	1.98	0.44
3:G:95:VAL:CG1	3:G:146:LEU:HD12	2.43	0.44
3:G:150:GLN:N	3:G:175:CYS:O	2.50	0.44
7:M:18:GLN:O	7:M:22:ILE:HD13	2.17	0.44
1:C:100:ILE:HD12	1:C:101:ASN:N	2.31	0.44
7:M:373:LEU:HD13	7:M:377:LEU:CD2	2.47	0.44
1:A:221:ARG:NH1	1:A:224:GLN:OE1	2.50	0.44
1:A:254:ILE:HG22	1:A:257:ALA:HB2	1.98	0.44
1:D:130:ALA:HB1	1:D:248:LEU:HB3	1.99	0.44
1:D:199:ALA:HB3	1:D:204:LYS:NZ	2.32	0.44
1:E:107:ARG:NH2	1:E:122:SER:O	2.43	0.44
7:M:38:ILE:HD13	7:M:354:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:382:ASP:OD1	7:M:383:THR:N	2.51	0.44
1:A:6:PHE:CE1	1:A:295:VAL:HG13	2.52	0.44
1:D:35:GLY:O	1:D:39:ALA:HB2	2.18	0.44
7:M:84:ARG:HB2	7:M:85:PRO:HD3	1.99	0.44
7:M:198:MET:SD	7:M:342:ASN:ND2	2.91	0.44
1:A:54:HIS:CD2	2:F:98:MET:HE1	2.52	0.44
1:C:264:LEU:HD23	1:C:264:LEU:O	2.17	0.44
1:C:149:MET:HE1	1:D:83:ALA:HB3	1.98	0.44
7:M:175:ASP:OD1	7:M:176:ILE:N	2.50	0.44
7:M:76:MET:HE2	7:M:144:VAL:CG1	2.48	0.44
1:D:22:ASN:OD1	1:D:22:ASN:C	2.60	0.44
1:E:65:GLY:C	1:E:66:LEU:HD22	2.43	0.44
2:F:186:MET:HE3	2:F:186:MET:HA	2.00	0.44
1:E:17:THR:HB	1:E:241:ALA:HB2	2.00	0.43
2:F:211:PHE:CD1	2:F:212:VAL:HG13	2.53	0.43
2:F:226:THR:OG1	7:M:624:CYS:O	2.35	0.43
7:M:2:ASN:OD1	7:M:3:THR:N	2.50	0.43
1:A:234:ARG:NH1	1:A:235:PRO:O	2.51	0.43
1:B:18:VAL:HG11	1:B:44:PRO:HD3	2.00	0.43
1:D:17:THR:HB	1:D:241:ALA:HB2	2.00	0.43
1:A:126:GLY:HA2	2:F:160:PHE:O	2.18	0.43
1:E:12:THR:OG1	1:E:243:ILE:O	2.35	0.43
3:G:213:PHE:HB2	3:G:239:LEU:HD13	1.98	0.43
1:L:252:MET:HE1	1:L:293:TRP:CD2	2.53	0.43
1:C:202:ASP:OD1	1:C:203:THR:N	2.48	0.43
1:E:30:ARG:NH2	1:E:37:PHE:O	2.52	0.43
7:M:471:LEU:CD2	7:M:494:VAL:HG11	2.49	0.43
1:A:196:MET:HE3	1:A:196:MET:HA	1.99	0.43
2:F:157:TYR:C	2:F:158:ASP:OD2	2.62	0.43
1:L:48:ILE:CG2	1:L:127:ILE:HG21	2.49	0.43
7:M:400:LEU:CD1	7:M:402:ILE:HG23	2.47	0.43
1:D:47:SER:N	4:H:19:C:OP1	2.51	0.43
7:M:173:ILE:HD12	7:M:176:ILE:HD12	2.00	0.43
1:E:9:LYS:NZ	1:E:133:ASP:OD2	2.44	0.43
3:G:14:SER:HA	3:G:17:LEU:HD23	2.01	0.43
7:M:402:ILE:HG21	7:M:582:PHE:CE2	2.54	0.43
1:A:99:GLU:N	1:A:99:GLU:OE1	2.51	0.43
1:D:283:ASN:OD1	1:D:284:HIS:N	2.52	0.43
7:M:428:VAL:HG11	7:M:454:GLN:HG3	2.00	0.43
7:M:579:ASP:OD2	7:M:581:ARG:NH2	2.51	0.43
1:A:100:ILE:HD13	2:F:43:PRO:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:18:VAL:HG21	1:L:44:PRO:HD2	2.01	0.42
7:M:80:PHE:CE2	7:M:144:VAL:HG11	2.54	0.42
7:M:403:ALA:HB1	7:M:407:PHE:CG	2.54	0.42
7:M:16:LYS:O	7:M:16:LYS:NZ	2.48	0.42
7:M:384:ILE:HG21	7:M:387:ARG:HG3	2.02	0.42
7:M:491:SER:O	7:M:494:VAL:HG12	2.19	0.42
1:C:2:ARG:O	1:C:257:ALA:N	2.47	0.42
1:C:12:THR:OG1	1:C:243:ILE:O	2.31	0.42
1:L:49:ARG:NH2	1:L:116:PHE:O	2.51	0.42
1:C:60:ILE:HD11	1:C:264:LEU:HD11	2.00	0.42
1:C:293:TRP:CZ3	1:C:313:ILE:HD12	2.55	0.42
1:C:100:ILE:HD12	1:C:101:ASN:HB2	2.01	0.42
1:L:137:GLN:OE1	1:L:246:ALA:HB2	2.20	0.42
7:M:144:VAL:HG23	7:M:145:GLU:N	2.35	0.42
1:C:106:LEU:HD22	1:C:121:LEU:HD22	2.01	0.42
1:D:78:GLU:CD	1:D:341:THR:HG23	2.44	0.42
1:E:277:ARG:NH2	1:L:253:SER:OG	2.53	0.42
3:G:138:PHE:HD2	3:G:259:LEU:HD21	1.83	0.42
1:A:210:LYS:O	1:A:214:LEU:HD23	2.20	0.42
1:D:3:THR:HG23	1:D:3:THR:O	2.20	0.42
1:D:311:ILE:HD11	1:D:318:VAL:HG13	2.00	0.42
1:L:56:ALA:HA	1:L:59:VAL:HG12	2.01	0.42
7:M:37:LEU:C	7:M:38:ILE:HD12	2.45	0.42
7:M:224:LEU:HD11	7:M:339:ILE:HG23	2.02	0.42
7:M:513:ILE:O	7:M:515:PHE:N	2.52	0.42
1:A:80:PHE:CZ	2:F:89:LEU:HD11	2.55	0.42
1:B:6:PHE:CE1	1:B:295:VAL:HG13	2.55	0.42
1:B:170:ARG:NE	1:B:227:GLU:OE2	2.52	0.42
1:C:94:THR:OG1	1:C:95:PHE:N	2.53	0.42
1:C:264:LEU:HD23	1:C:264:LEU:C	2.45	0.42
2:F:26:LEU:HB3	2:F:65:ALA:HB1	2.00	0.42
7:M:434:ILE:HG22	7:M:436:GLY:H	1.84	0.42
7:M:509:ILE:HG23	7:M:578:LEU:CD2	2.50	0.42
1:L:252:MET:HE1	1:L:293:TRP:CG	2.54	0.42
7:M:333:ILE:N	7:M:333:ILE:HD12	2.35	0.42
7:M:416:GLU:OE1	7:M:416:GLU:N	2.53	0.42
1:C:75:ASP:OD1	1:C:76:LEU:N	2.52	0.42
1:E:89:ASN:OD1	1:E:90:GLY:N	2.53	0.42
3:G:162:SER:OG	3:G:178:GLN:O	2.38	0.42
7:M:136:LEU:HA	7:M:139:TRP:HB2	2.00	0.42
1:A:100:ILE:CG1	2:F:212:VAL:HG11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ARG:NH1	1:B:116:PHE:O	2.53	0.41
7:M:89:GLN:OE1	7:M:89:GLN:N	2.51	0.41
1:A:80:PHE:CE1	2:F:89:LEU:HD11	2.54	0.41
1:B:202:ASP:OD1	1:B:203:THR:N	2.53	0.41
3:G:9:TYR:CE1	3:G:17:LEU:HD21	2.55	0.41
7:M:84:ARG:NH2	7:M:88:GLU:OE2	2.53	0.41
7:M:521:MET:HE3	7:M:522:LYS:CA	2.49	0.41
1:B:64:VAL:HG23	1:B:65:GLY:N	2.35	0.41
1:D:202:ASP:OD1	1:D:202:ASP:O	2.39	0.41
1:D:236:ILE:HG23	4:H:23:A:N6	2.36	0.41
7:M:118:LEU:HD12	7:M:161:MET:HE3	2.02	0.41
7:M:196:ASP:OD1	7:M:346:TYR:OH	2.30	0.41
7:M:402:ILE:HG22	7:M:577:ILE:HB	2.02	0.41
1:D:18:VAL:HG11	1:D:44:PRO:HD3	2.00	0.41
1:D:58:LYS:HA	1:D:61:VAL:HG22	2.01	0.41
7:M:3:THR:HG21	7:M:56:LEU:HD12	2.01	0.41
1:B:66:LEU:HD12	1:B:70:GLY:O	2.21	0.41
7:M:123:GLU:OE1	7:M:123:GLU:N	2.54	0.41
1:A:254:ILE:N	1:A:254:ILE:HD12	2.34	0.41
1:B:130:ALA:HB1	1:B:248:LEU:HB3	2.03	0.41
2:F:159:TYR:OH	2:F:166:GLU:OE1	2.35	0.41
7:M:384:ILE:HG21	7:M:387:ARG:CG	2.51	0.41
1:B:82:LEU:O	1:B:112:LEU:HD21	2.20	0.41
1:C:94:THR:HG22	1:C:119:TRP:NE1	2.36	0.41
1:D:163:ASP:OD1	1:D:164:GLN:N	2.54	0.41
1:E:123:GLY:N	4:H:22:G:OP1	2.47	0.41
1:E:281:HIS:N	4:H:27:G:OP2	2.51	0.41
2:F:33:ALA:HB2	2:F:153:VAL:HG11	2.03	0.41
1:L:63:ARG:NH2	1:L:336:GLN:OE1	2.54	0.41
1:A:17:THR:HG21	1:A:281:HIS:ND1	2.36	0.40
1:E:237:ASP:OD2	1:E:237:ASP:C	2.64	0.40
2:F:54:LEU:HD21	2:F:65:ALA:HB2	2.02	0.40
7:M:218:ASP:HB2	7:M:556:ARG:HE	1.86	0.40
7:M:359:THR:HG22	7:M:559:LYS:HB3	2.02	0.40
1:B:20:VAL:HG23	1:B:23:ALA:HB3	2.04	0.40
1:C:24:VAL:HG12	1:C:30:ARG:H	1.86	0.40
1:D:82:LEU:HD22	1:D:112:LEU:HD23	2.04	0.40
1:E:259:ASP:HB2	1:E:328:MET:HE3	2.03	0.40
7:M:120:LEU:HD21	7:M:130:VAL:CG1	2.51	0.40
7:M:192:MET:HA	7:M:195:VAL:CG1	2.52	0.40
7:M:398:MET:HE1	7:M:400:LEU:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:57:ASN:O	2:F:61:GLY:N	2.50	0.40
1:L:18:VAL:HG21	1:L:44:PRO:CG	2.52	0.40
7:M:132:VAL:HG21	7:M:150:TYR:CZ	2.55	0.40
1:B:109:LYS:O	1:B:339:ASP:N	2.54	0.40
1:C:200:ASP:O	1:C:204:LYS:N	2.46	0.40
7:M:132:VAL:HG23	7:M:135:LYS:HE3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	340/350 (97%)	340 (100%)	0	0	100	100
1	B	340/350 (97%)	338 (99%)	2 (1%)	0	100	100
1	C	340/350 (97%)	340 (100%)	0	0	100	100
1	D	340/350 (97%)	338 (99%)	2 (1%)	0	100	100
1	E	243/350 (69%)	243 (100%)	0	0	100	100
1	L	196/350 (56%)	195 (100%)	1 (0%)	0	100	100
2	F	233/235 (99%)	233 (100%)	0	0	100	100
3	G	261/263 (99%)	261 (100%)	0	0	100	100
7	M	517/624 (83%)	506 (98%)	9 (2%)	2 (0%)	30	59
All	All	2810/3222 (87%)	2794 (99%)	14 (0%)	2 (0%)	49	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	M	333	ILE
7	M	128	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/285 (98%)	277 (100%)	1 (0%)	84	94
1	B	278/285 (98%)	277 (100%)	1 (0%)	84	94
1	C	278/285 (98%)	276 (99%)	2 (1%)	76	92
1	D	278/285 (98%)	278 (100%)	0	100	100
1	E	194/285 (68%)	194 (100%)	0	100	100
1	L	164/285 (58%)	163 (99%)	1 (1%)	78	93
2	F	200/200 (100%)	199 (100%)	1 (0%)	81	93
3	G	237/237 (100%)	233 (98%)	4 (2%)	53	82
7	M	452/539 (84%)	442 (98%)	10 (2%)	45	77
All	All	2359/2686 (88%)	2339 (99%)	20 (1%)	70	90

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	GLU
1	B	196	MET
1	C	19	THR
1	C	87	ASP
2	F	141	SER
3	G	20	MET
3	G	43	VAL
3	G	105	LEU
3	G	177	ASP
1	L	299	LYS
7	M	42	THR
7	M	48	LEU
7	M	79	ILE
7	M	101	SER
7	M	222	ASP
7	M	226	VAL
7	M	336	ASN
7	M	347	CYS

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Mol	Chain	Res	Type
7	M	370	MET
7	M	524	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	208	GLN
1	D	333	ASN
1	E	5	ASN
1	E	283	ASN
1	E	336	GLN
3	G	204	ASN
3	G	252	GLN
7	M	73	HIS
7	M	93	GLN
7	M	184	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	H	36/61 (59%)	12 (33%)	1 (2%)

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	H	-4	A
4	H	7	C
4	H	13	G
4	H	18	U
4	H	19	C
4	H	20	C
4	H	23	A
4	H	24	A
4	H	25	G
4	H	28	U
4	H	29	C
4	H	30	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	H	19	C

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.

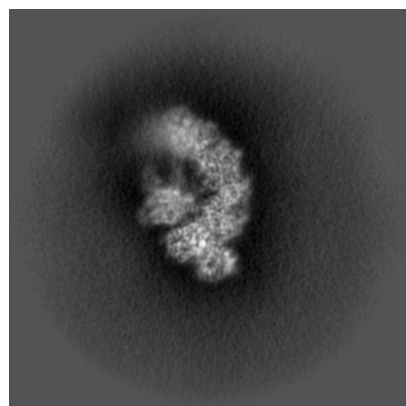
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19689. These allow visual inspection of the internal detail of the map and identification of artifacts.

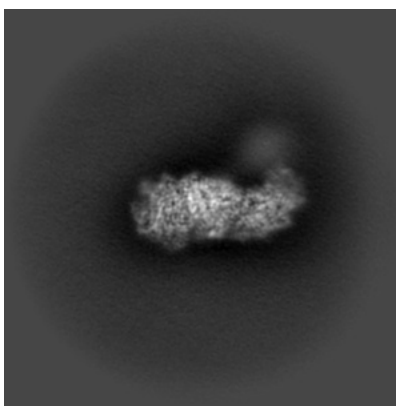
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

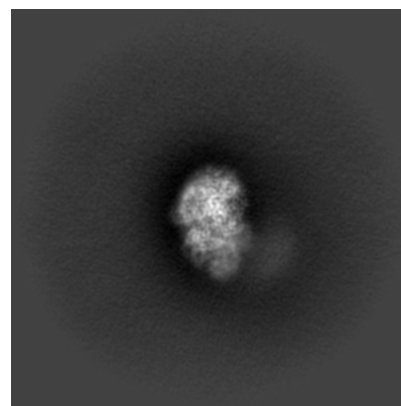
6.1.1 Primary map



X

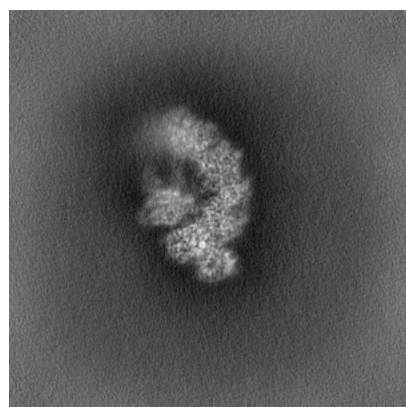


Y

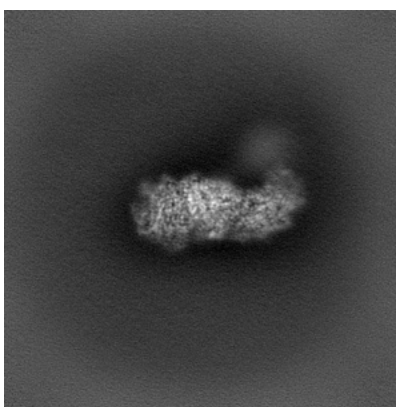


Z

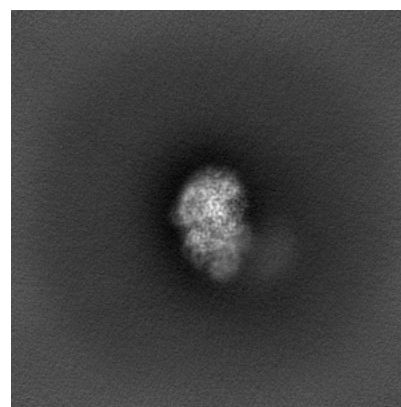
6.1.2 Raw map



X



Y

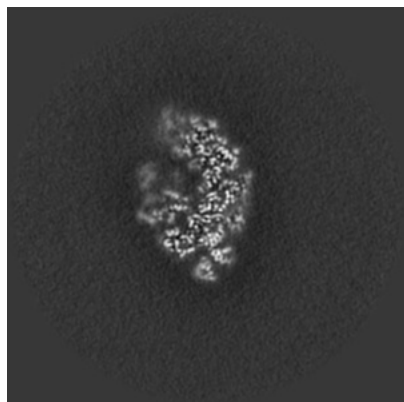


Z

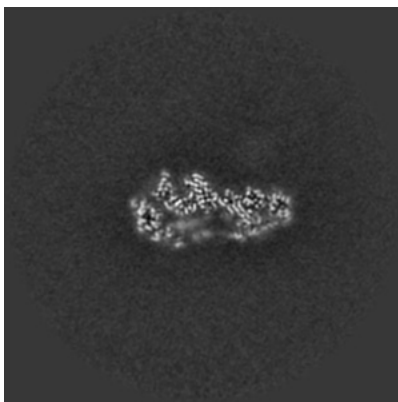
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

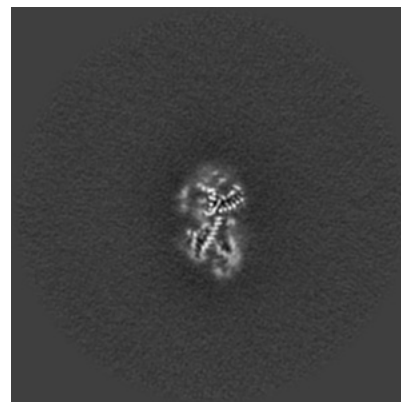
6.2.1 Primary map



X Index: 180

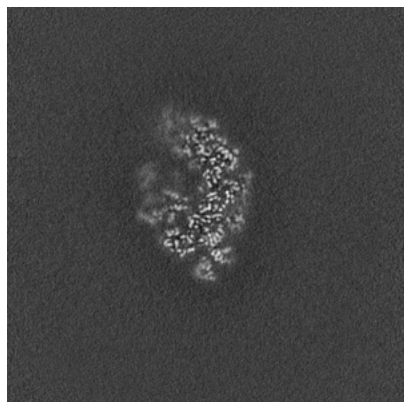


Y Index: 180

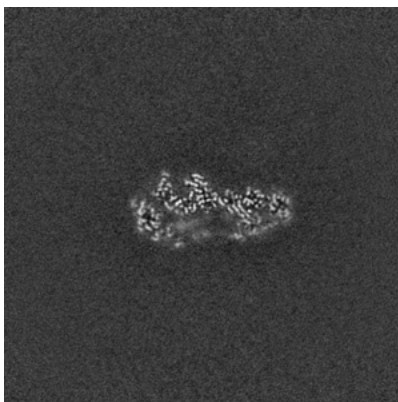


Z Index: 180

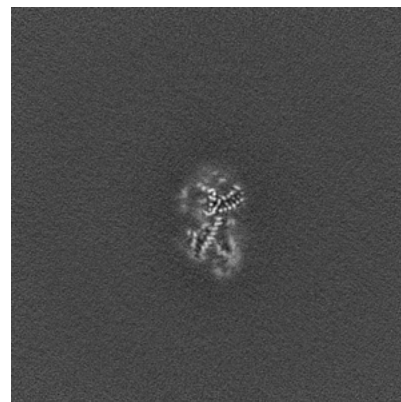
6.2.2 Raw map



X Index: 180



Y Index: 180

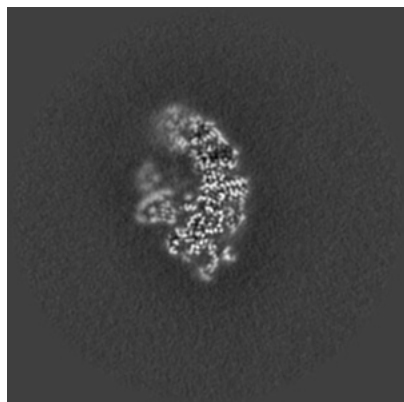


Z Index: 180

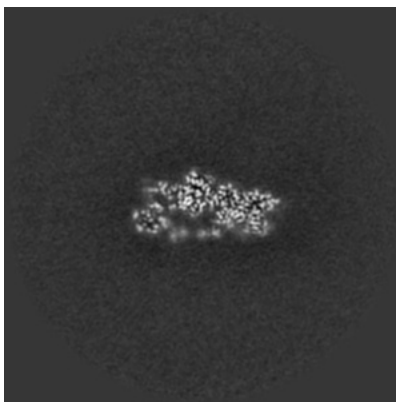
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

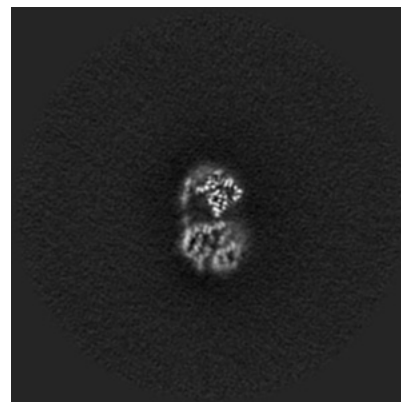
6.3.1 Primary map



X Index: 185

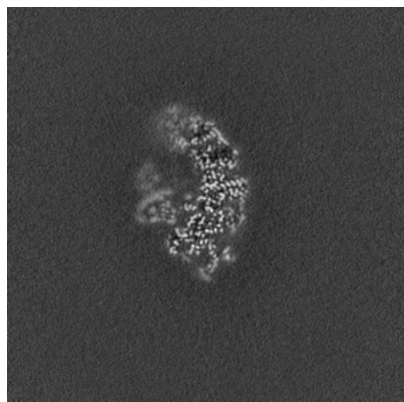


Y Index: 191

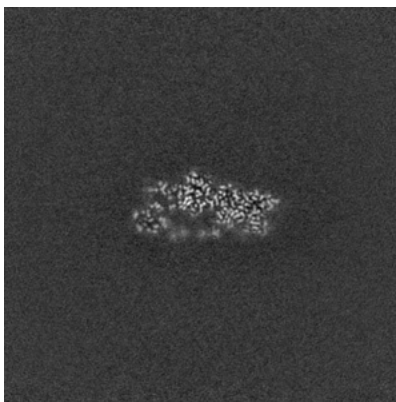


Z Index: 187

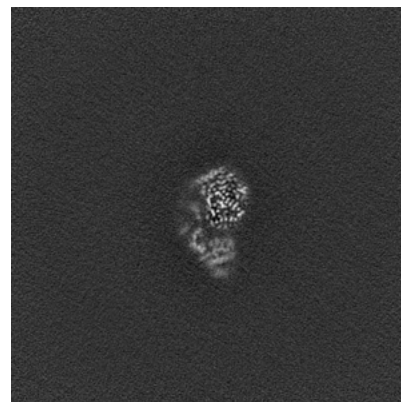
6.3.2 Raw map



X Index: 185



Y Index: 191

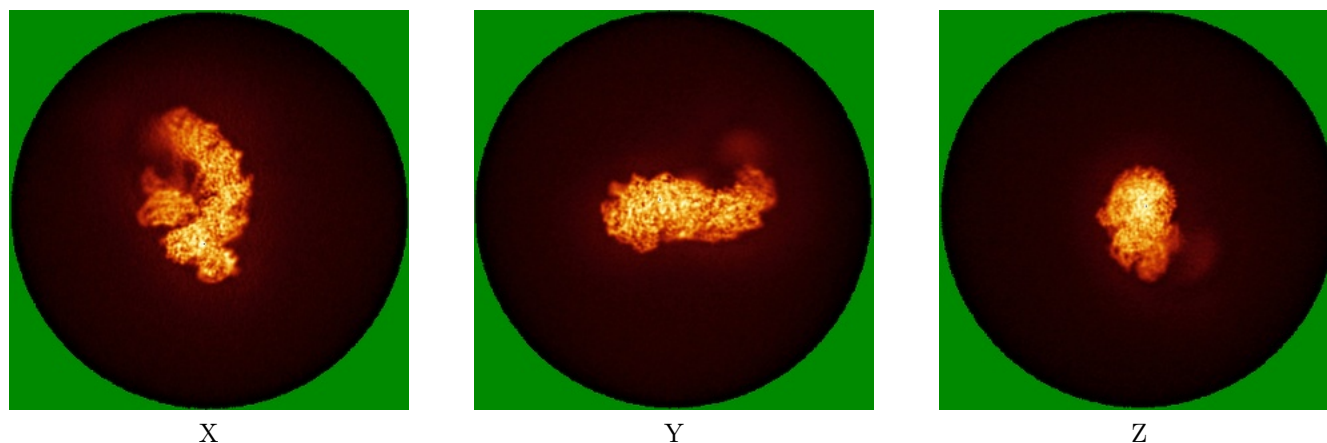


Z Index: 168

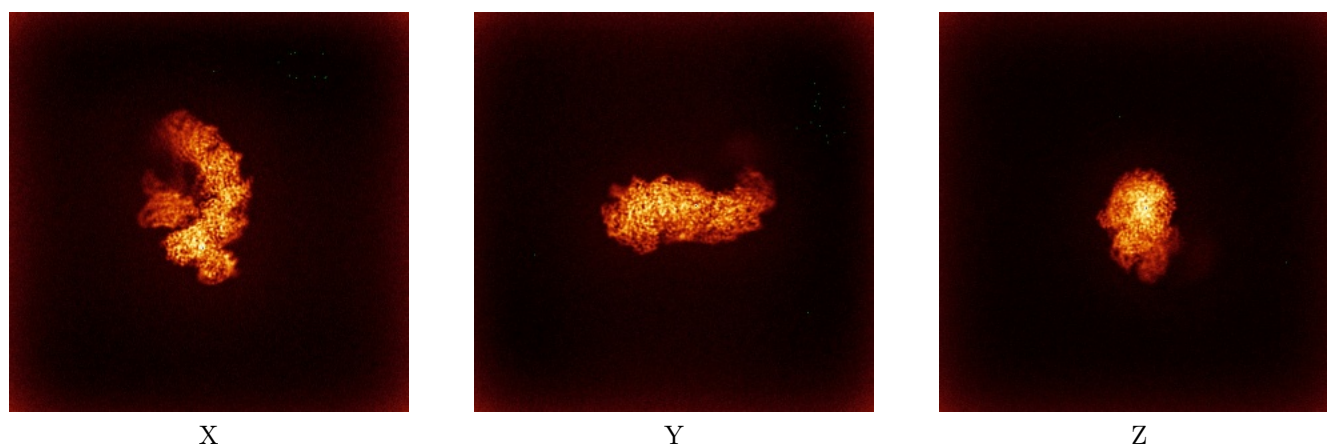
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

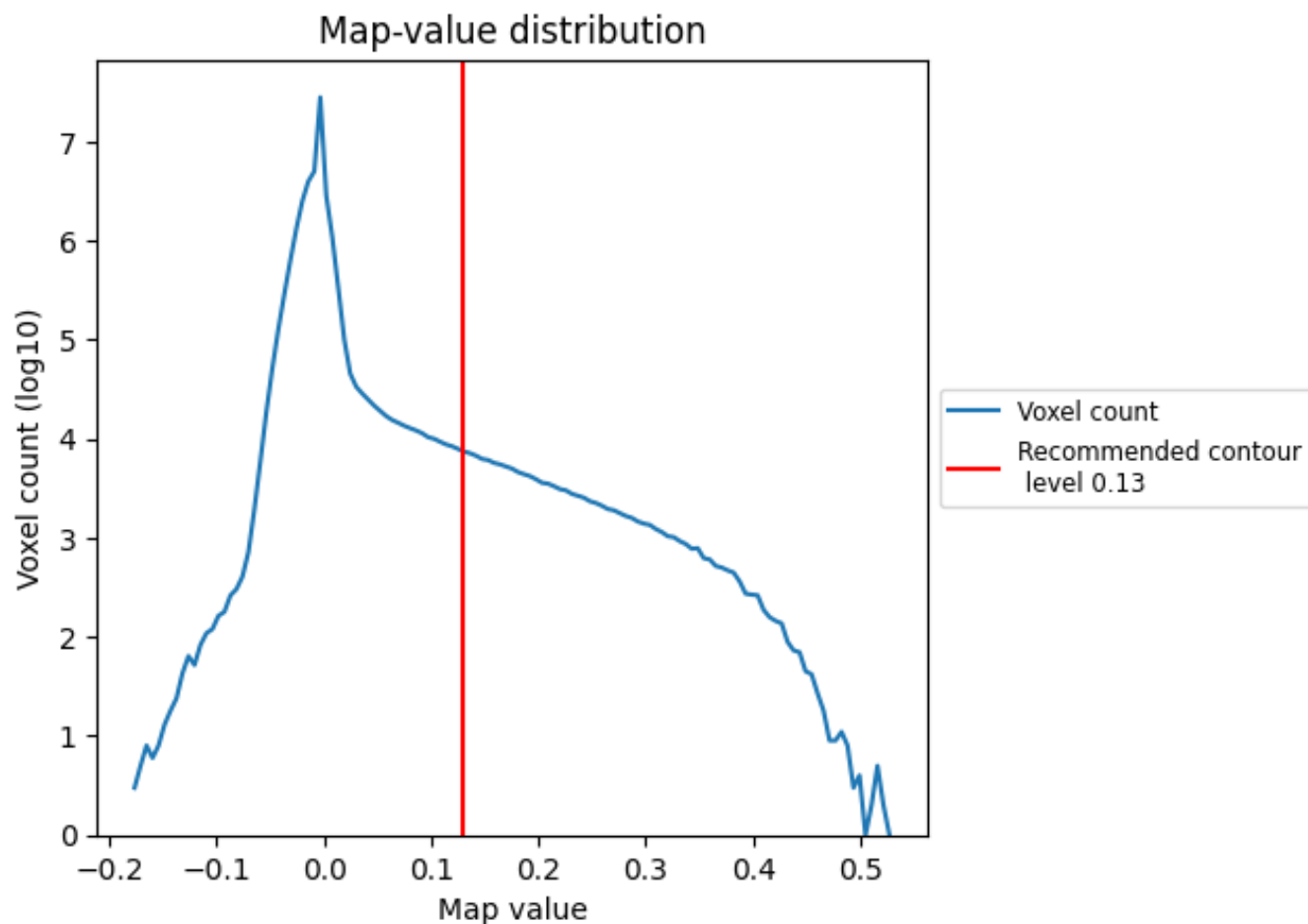
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

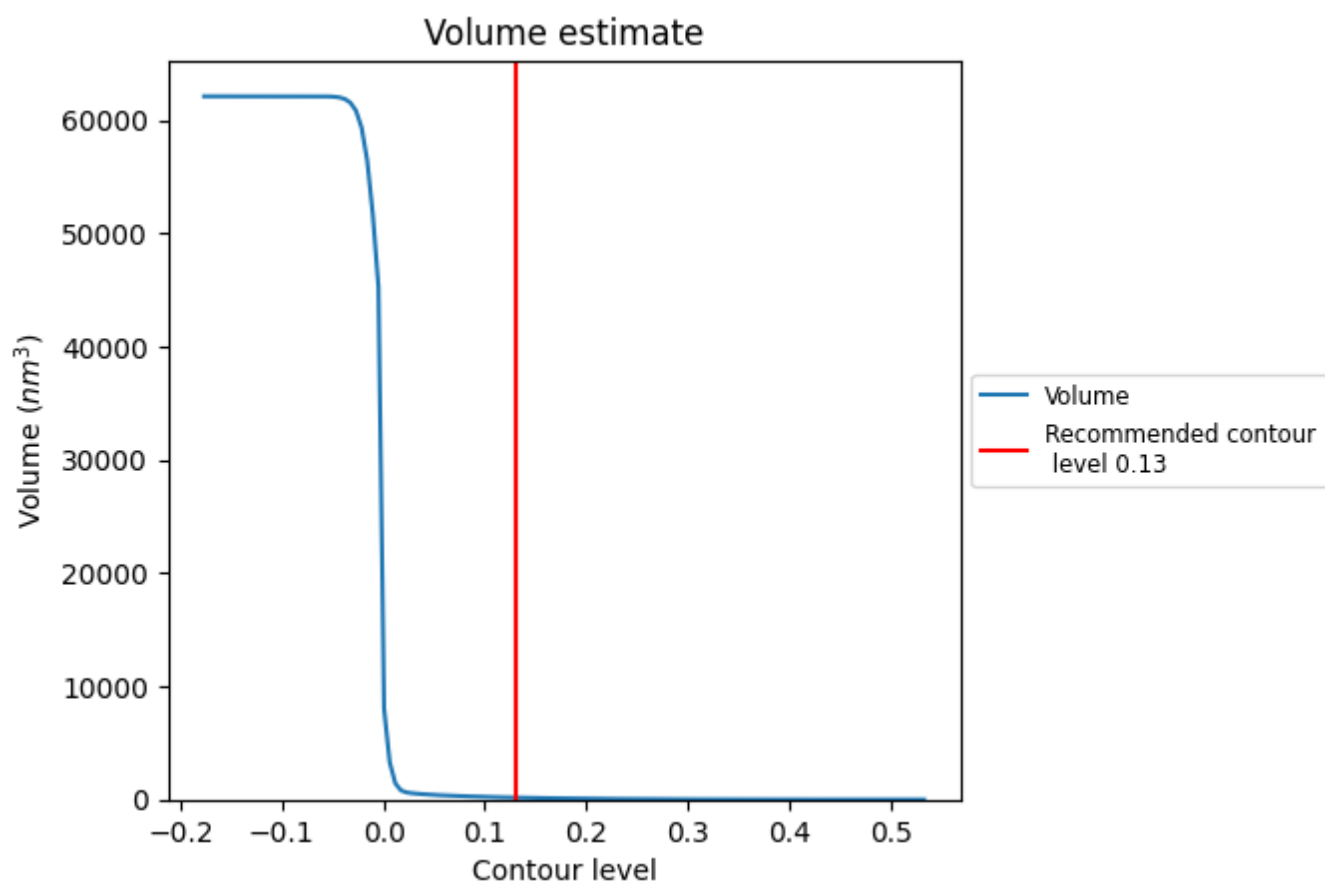
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

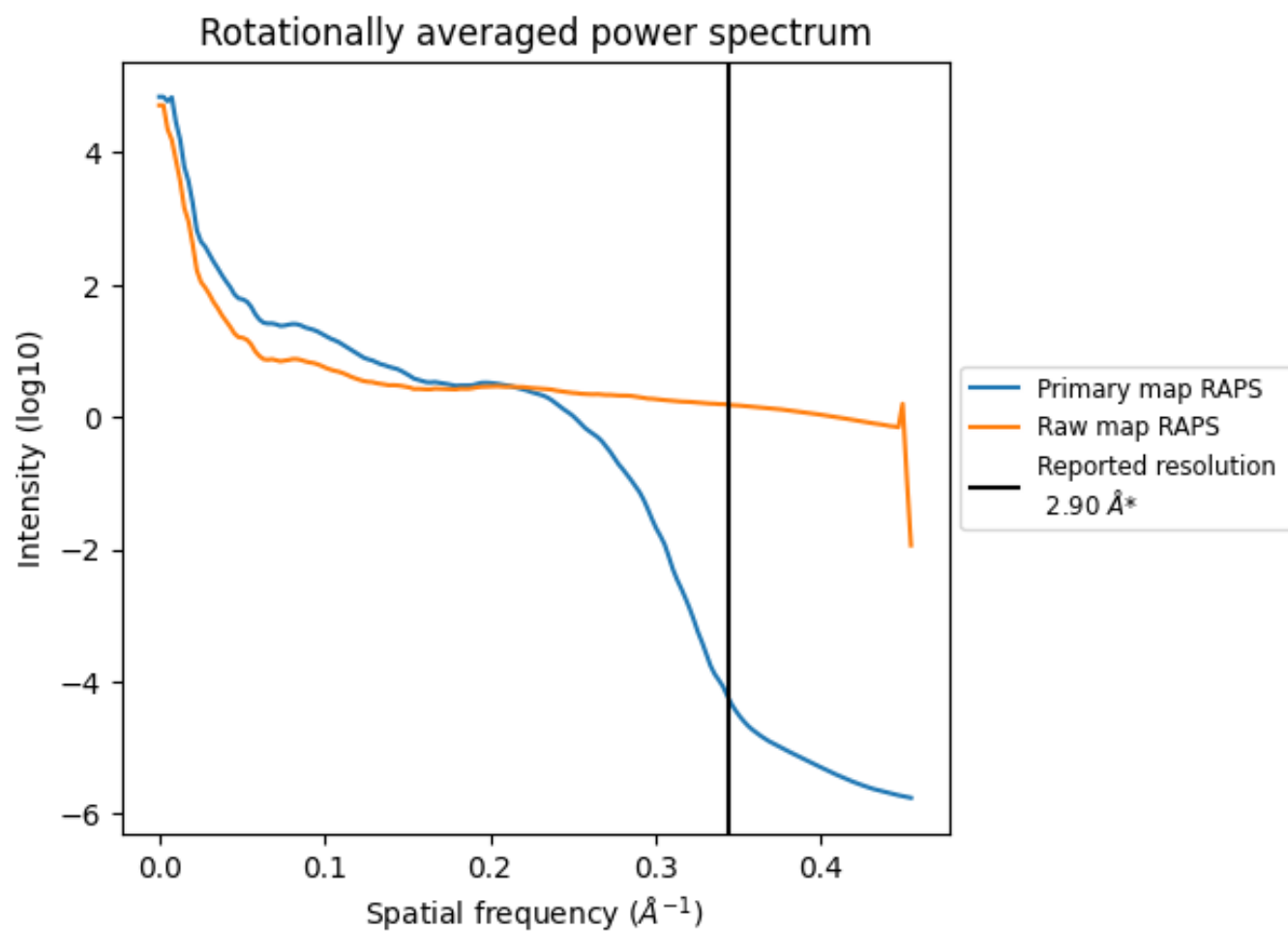
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 174 nm³; this corresponds to an approximate mass of 157 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

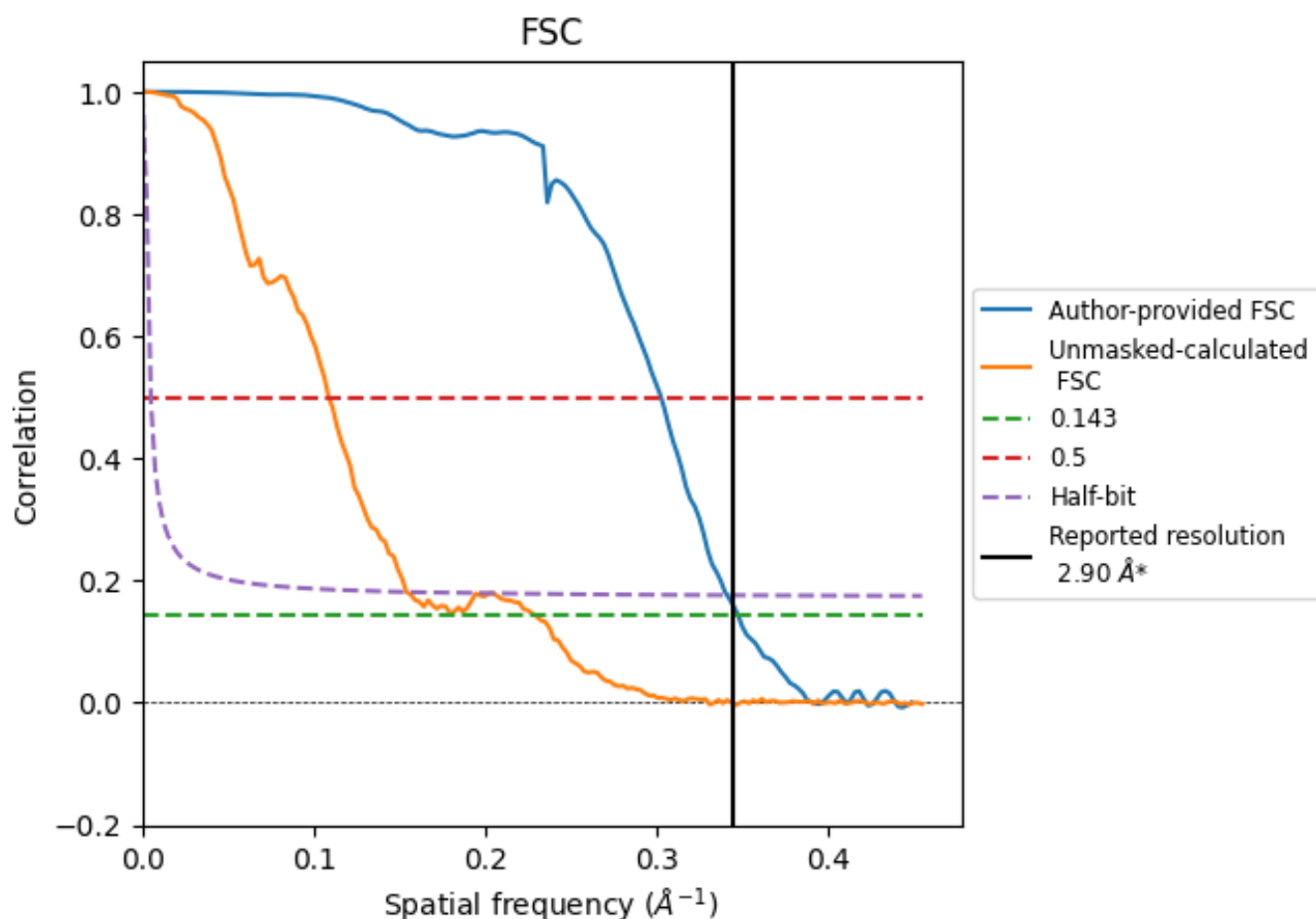


*Reported resolution corresponds to spatial frequency of $0.345 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

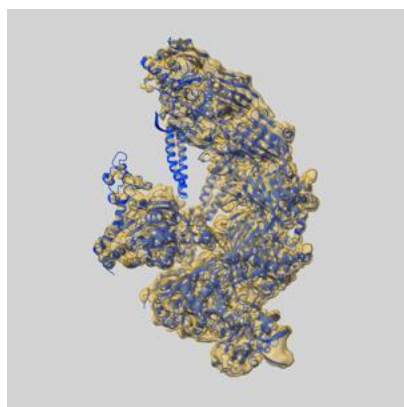
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.88	3.31	2.93
Unmasked-calculated*	4.37	9.19	6.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.37 differs from the reported value 2.9 by more than 10 %

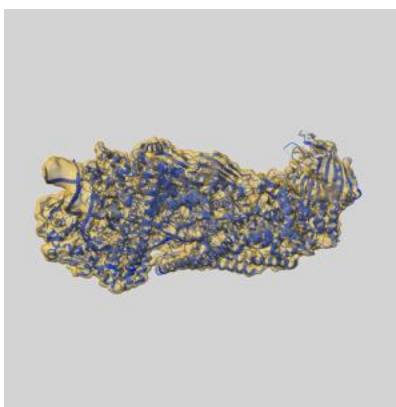
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19689 and PDB model 8S36. Per-residue inclusion information can be found in section [3](#) on page [7](#).

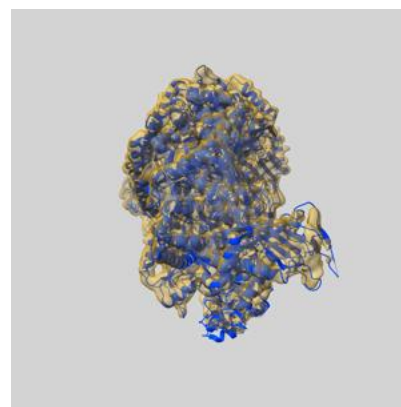
9.1 Map-model overlay [i](#)



X



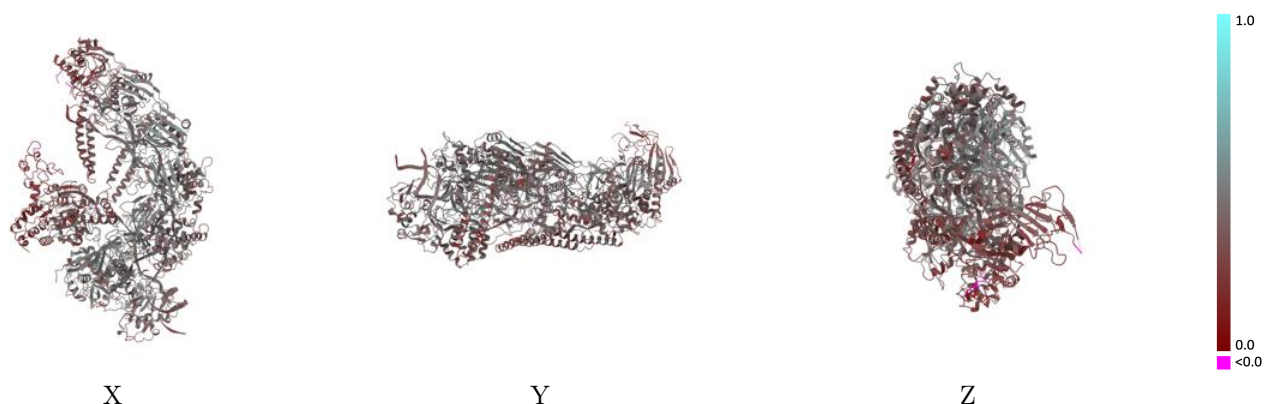
Y



Z

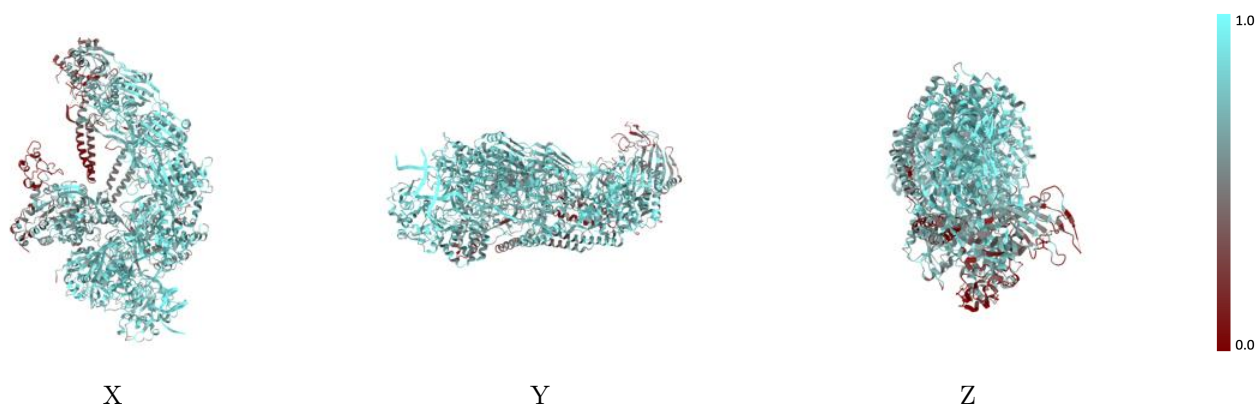
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



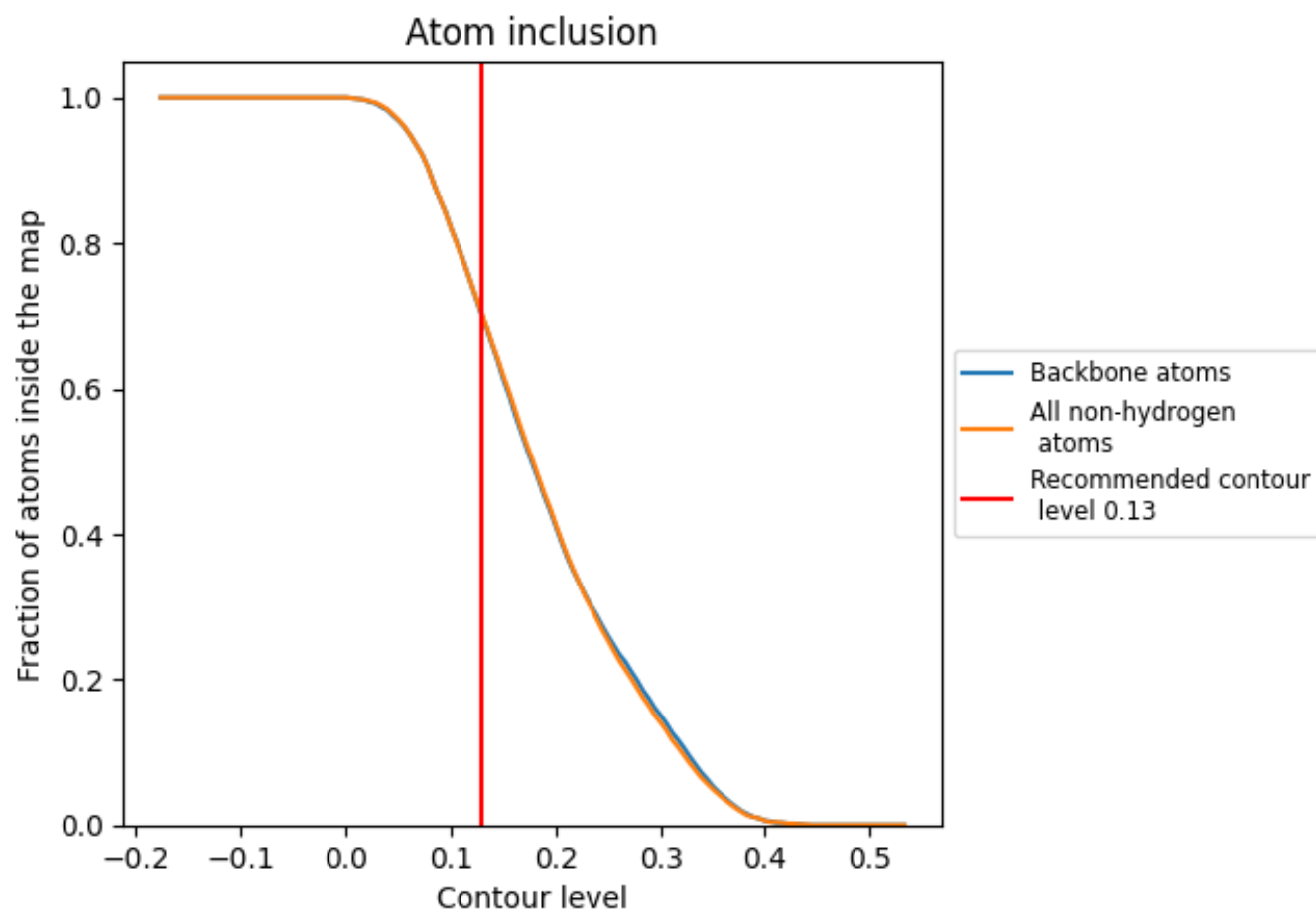
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 70% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7030	0.3880
A	0.7440	0.4160
B	0.7620	0.4270
C	0.7420	0.4140
D	0.6630	0.3990
E	0.7190	0.3970
F	0.8300	0.4530
G	0.7820	0.4030
H	0.9250	0.4440
I	0.8300	0.3930
J	0.8380	0.3600
L	0.4820	0.3020
M	0.5790	0.3060

1.0

0.0

<0.0