



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 12:06 AM EDT

PDB ID : 9N3Z / pdb_00009n3z
EMDB ID : EMD-48863
Title : Type IV-A1 CRISPR effector complex bound to dsDNA and CasDinG - locked state
Authors : Kiernan, K.A.; Taylor, D.W.
Deposited on : 2025-02-01
Resolution : 3.04 Å(reported)
Based on initial model : 7XG3

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.dev133
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) : 2.50

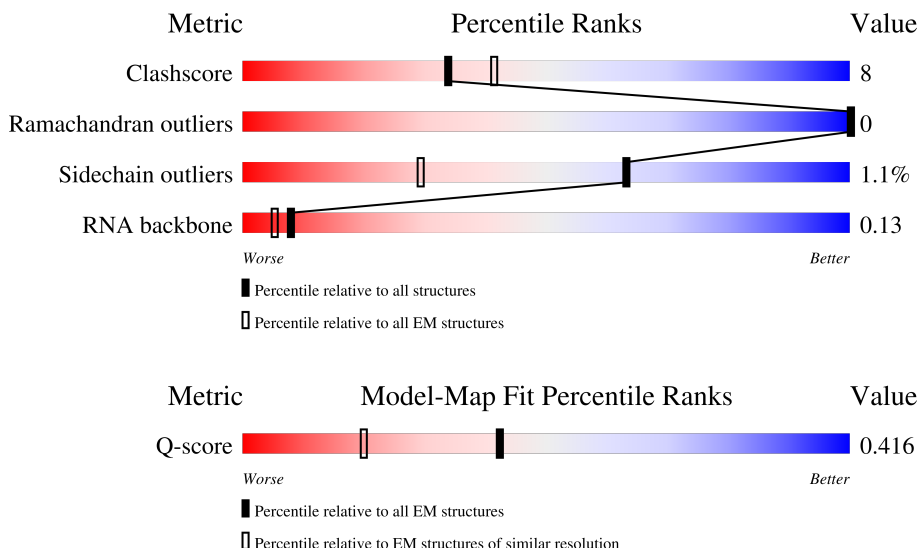
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.04 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.



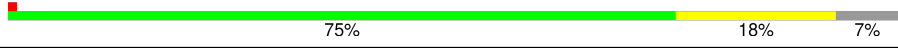
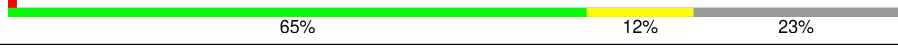
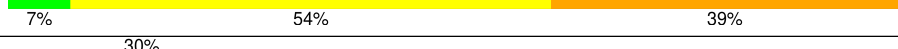
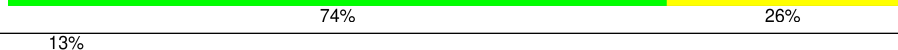
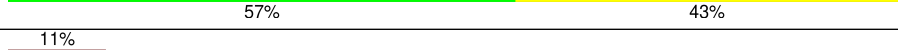
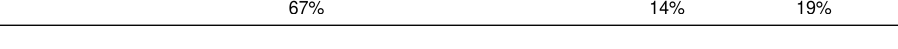
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13952 (2.54 - 3.54)

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	241	
2	B	220	
3	C	359	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	359	
3	E	359	
3	F	359	
3	G	359	
4	H	232	
5	I	61	
6	J	47	
7	K	47	
8	L	748	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 25215 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CRISPR type AFERR-associated protein Csf1 (Cas8).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	241	Total	C	N	O	S	0	0
			1890	1198	335	345	12		

- Molecule 2 is a protein called CCRISPR type AFERR-associated protein Csf3 (Cas5).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	220	Total	C	N	O	S	0	0
			1715	1084	317	305	9		

- Molecule 3 is a protein called CRISPR type AFERR-associated protein Csf2 (Cas7).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	329	Total	C	N	O	S	0	0
			2488	1570	439	467	12		
3	D	334	Total	C	N	O	S	0	0
			2513	1585	443	473	12		
3	E	331	Total	C	N	O	S	0	0
			2485	1566	438	469	12		
3	F	333	Total	C	N	O	S	0	0
			2489	1569	437	471	12		
3	G	276	Total	C	N	O	S	0	0
			2089	1323	364	391	11		

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	MET	-	initiating methionine	UNP A0AAB0B1V3
C	-9	TRP	-	expression tag	UNP A0AAB0B1V3
C	-8	SER	-	expression tag	UNP A0AAB0B1V3
C	-7	HIS	-	expression tag	UNP A0AAB0B1V3
C	-6	PRO	-	expression tag	UNP A0AAB0B1V3
C	-5	GLN	-	expression tag	UNP A0AAB0B1V3
C	-4	PHE	-	expression tag	UNP A0AAB0B1V3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLU	-	expression tag	UNP A0AAB0B1V3
C	-2	LYS	-	expression tag	UNP A0AAB0B1V3
C	-1	GLY	-	expression tag	UNP A0AAB0B1V3
C	0	ALA	-	expression tag	UNP A0AAB0B1V3
D	-10	MET	-	initiating methionine	UNP A0AAB0B1V3
D	-9	TRP	-	expression tag	UNP A0AAB0B1V3
D	-8	SER	-	expression tag	UNP A0AAB0B1V3
D	-7	HIS	-	expression tag	UNP A0AAB0B1V3
D	-6	PRO	-	expression tag	UNP A0AAB0B1V3
D	-5	GLN	-	expression tag	UNP A0AAB0B1V3
D	-4	PHE	-	expression tag	UNP A0AAB0B1V3
D	-3	GLU	-	expression tag	UNP A0AAB0B1V3
D	-2	LYS	-	expression tag	UNP A0AAB0B1V3
D	-1	GLY	-	expression tag	UNP A0AAB0B1V3
D	0	ALA	-	expression tag	UNP A0AAB0B1V3
E	-10	MET	-	initiating methionine	UNP A0AAB0B1V3
E	-9	TRP	-	expression tag	UNP A0AAB0B1V3
E	-8	SER	-	expression tag	UNP A0AAB0B1V3
E	-7	HIS	-	expression tag	UNP A0AAB0B1V3
E	-6	PRO	-	expression tag	UNP A0AAB0B1V3
E	-5	GLN	-	expression tag	UNP A0AAB0B1V3
E	-4	PHE	-	expression tag	UNP A0AAB0B1V3
E	-3	GLU	-	expression tag	UNP A0AAB0B1V3
E	-2	LYS	-	expression tag	UNP A0AAB0B1V3
E	-1	GLY	-	expression tag	UNP A0AAB0B1V3
E	0	ALA	-	expression tag	UNP A0AAB0B1V3
F	-10	MET	-	initiating methionine	UNP A0AAB0B1V3
F	-9	TRP	-	expression tag	UNP A0AAB0B1V3
F	-8	SER	-	expression tag	UNP A0AAB0B1V3
F	-7	HIS	-	expression tag	UNP A0AAB0B1V3
F	-6	PRO	-	expression tag	UNP A0AAB0B1V3
F	-5	GLN	-	expression tag	UNP A0AAB0B1V3
F	-4	PHE	-	expression tag	UNP A0AAB0B1V3
F	-3	GLU	-	expression tag	UNP A0AAB0B1V3
F	-2	LYS	-	expression tag	UNP A0AAB0B1V3
F	-1	GLY	-	expression tag	UNP A0AAB0B1V3
F	0	ALA	-	expression tag	UNP A0AAB0B1V3
G	-10	MET	-	initiating methionine	UNP A0AAB0B1V3
G	-9	TRP	-	expression tag	UNP A0AAB0B1V3
G	-8	SER	-	expression tag	UNP A0AAB0B1V3
G	-7	HIS	-	expression tag	UNP A0AAB0B1V3
G	-6	PRO	-	expression tag	UNP A0AAB0B1V3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	-5	GLN	-	expression tag	UNP A0AAB0B1V3
G	-4	PHE	-	expression tag	UNP A0AAB0B1V3
G	-3	GLU	-	expression tag	UNP A0AAB0B1V3
G	-2	LYS	-	expression tag	UNP A0AAB0B1V3
G	-1	GLY	-	expression tag	UNP A0AAB0B1V3
G	0	ALA	-	expression tag	UNP A0AAB0B1V3

- Molecule 4 is a protein called CRISPR type AFERR-associated protein Csf5 (Cas5).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	232	Total	C	N	O	S	0	0
			1783	1139	318	319	7		

- Molecule 5 is a RNA chain called crRNA (61-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	61	Total	C	N	O	P	0	0
			1314	586	247	421	60		

- Molecule 6 is a DNA chain called DNA, non-target strand (47-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	47	Total	C	N	O	P	0	0
			974	460	191	276	47		

- Molecule 7 is a DNA chain called DNA, target strand (47-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	47	Total	C	N	O	P	0	0
			953	455	163	288	47		

- Molecule 8 is a protein called CRISPR-associated DEAD/DEAH-box helicase CasDinG.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	604	Total	C	N	O	S	0	0
			4521	2863	810	830	18		

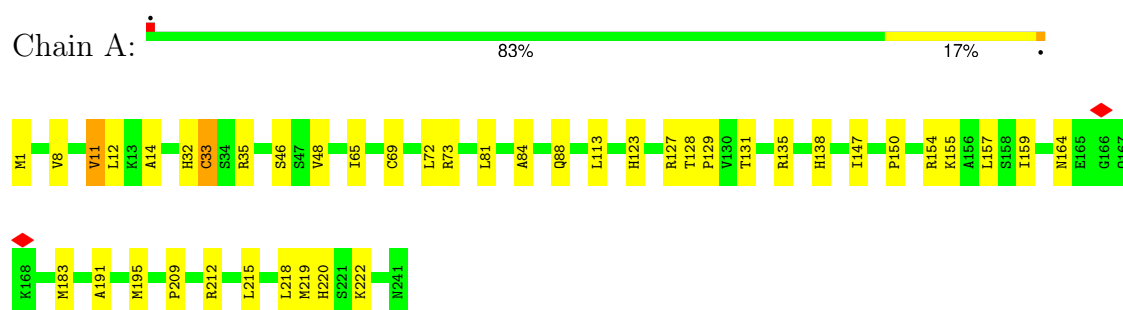
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total 1	Zn 1	0

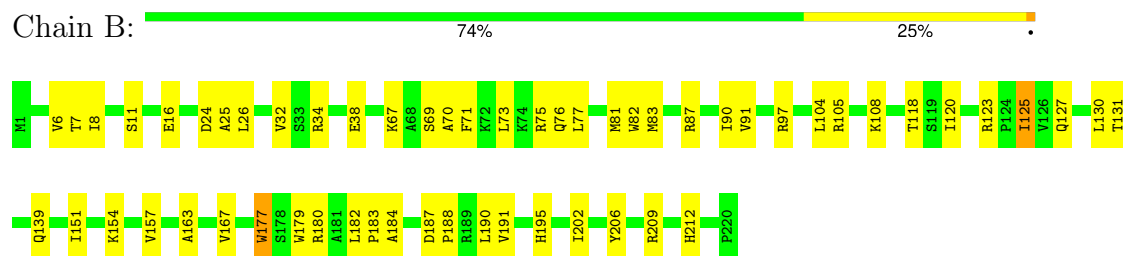
3 Residue-property plots

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.

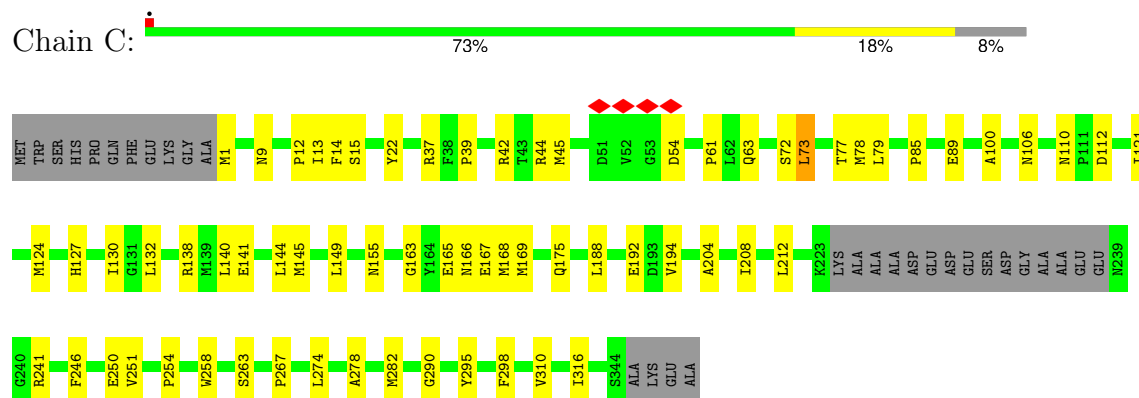
- Molecule 1: CRISPR type AFERR-associated protein Csf1 (Cas8)



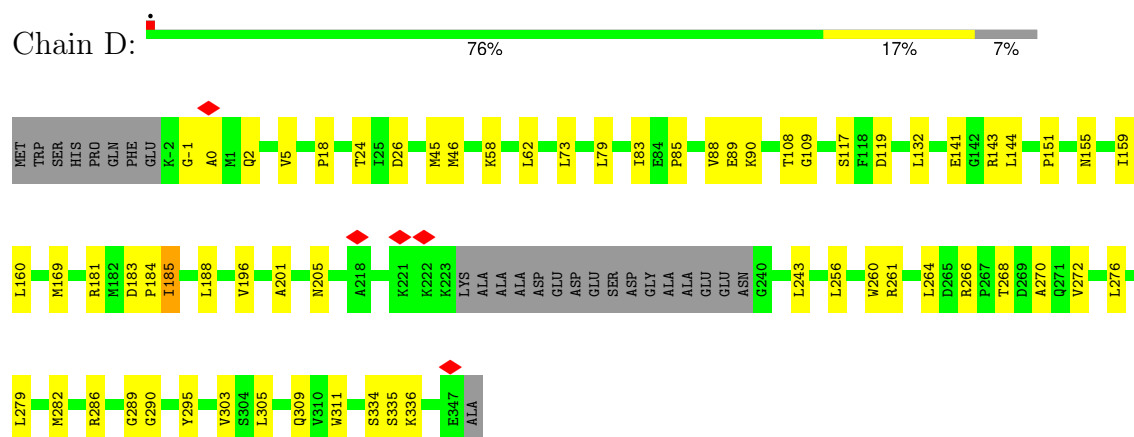
- Molecule 2: CCRISPR type AFERR-associated protein Csf3 (Cas5)



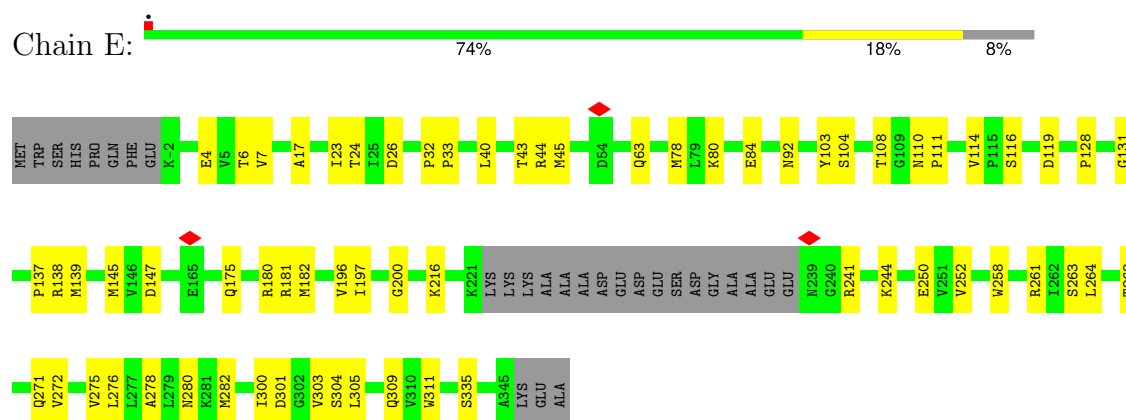
- Molecule 3: CRISPR type AFERR-associated protein Csf2 (Cas7)



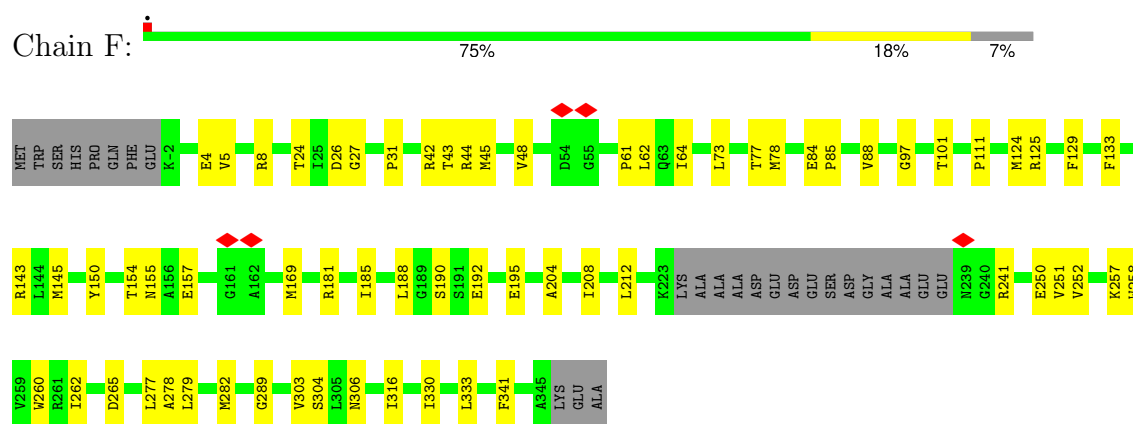
- Molecule 3: CRISPR type AFERR-associated protein Csf2 (Cas7)



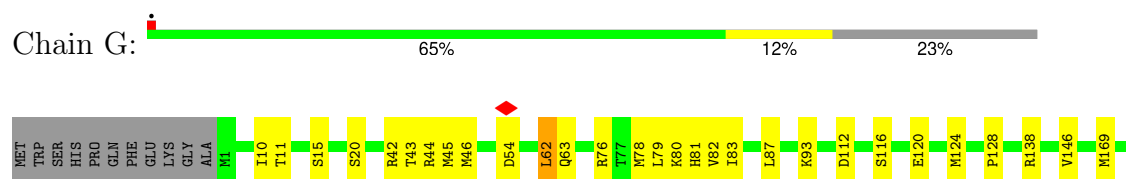
- Molecule 3: CRISPR type AFERR-associated protein Csf2 (Cas7)

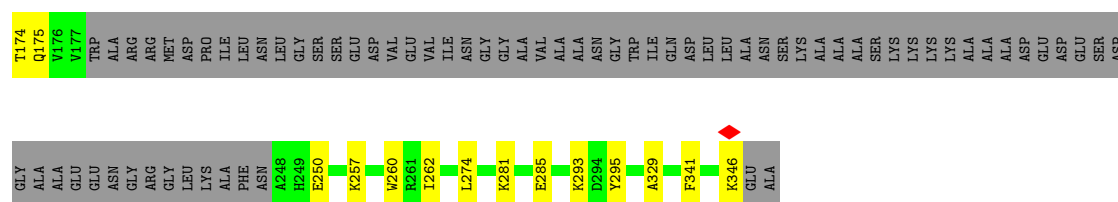


- Molecule 3: CRISPR type AFERR-associated protein Csf2 (Cas7)

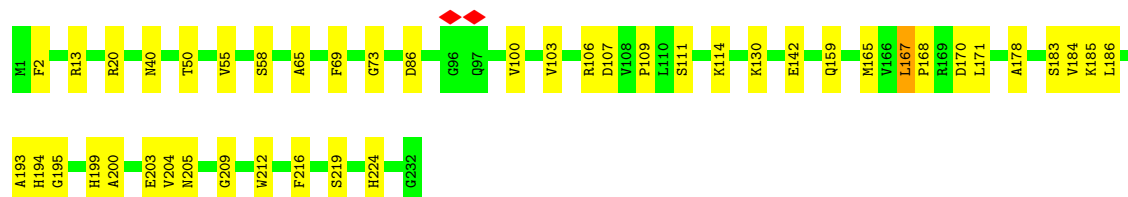
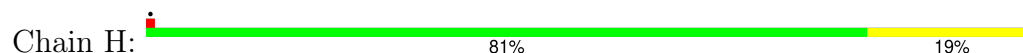


- Molecule 3: CRISPR type AFERR-associated protein Csf2 (Cas7)

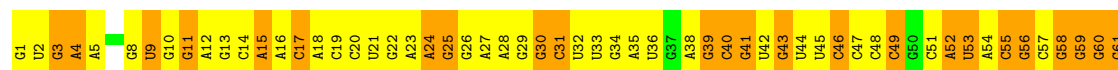




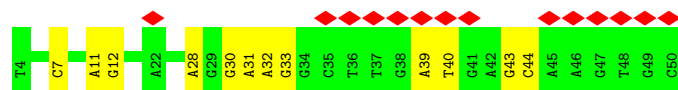
- Molecule 4: CRISPR type AFERR-associated protein Csf5 (Cas6)



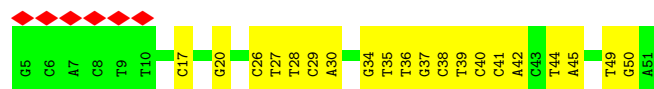
- Molecule 5: crRNA (61-MER)



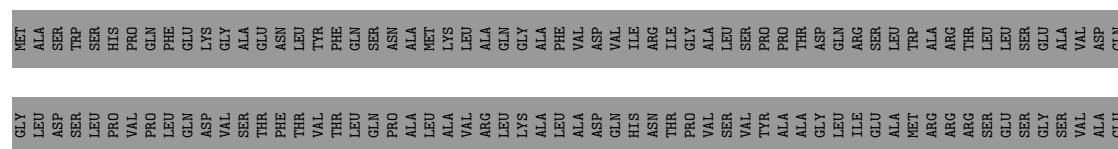
- Molecule 6: DNA, non-target strand (47-MER)

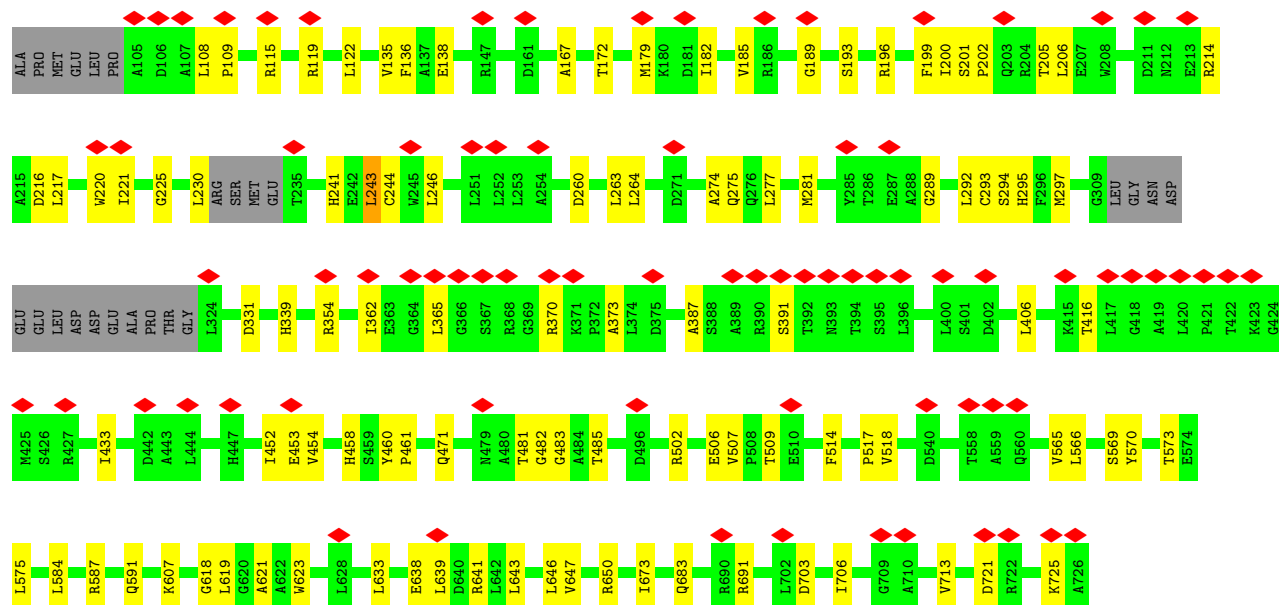


- Molecule 7: DNA, target strand (47-MER)



- Molecule 8: CRISPR-associated DEAD/DEAH-box helicase CasDinG





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38045	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.279	Depositor
Minimum map value	-0.327	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	426.5984, 426.5984, 426.5984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8332, 0.8332, 0.8332	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: 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	0.26	0/1938	0.53	0/2635
2	B	0.27	0/1760	0.49	1/2390 (0.0%)
3	C	0.20	0/2537	0.46	0/3439
3	D	0.19	0/2562	0.46	0/3473
3	E	0.19	0/2534	0.45	0/3439
3	F	0.19	0/2538	0.44	0/3446
3	G	0.25	0/2132	0.52	0/2893
4	H	0.21	0/1818	0.54	2/2454 (0.1%)
5	I	0.73	0/1472	0.94	0/2297
6	J	0.41	0/1096	0.63	0/1691
7	K	0.53	0/1064	0.81	0/1638
8	L	0.24	0/4612	0.54	2/6287 (0.0%)
All	All	0.30	0/26063	0.56	5/36082 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	142	GLU	N-CA-C	-6.50	107.22	114.62
4	H	86	ASP	CA-CB-CG	5.70	118.30	112.60
8	L	454	VAL	N-CA-C	-5.67	101.61	108.53
8	L	570	TYR	CB-CA-C	-5.51	110.21	116.54
2	B	177	TRP	N-CA-C	-5.02	107.16	113.28

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	1890	0	1878	25	0
2	B	1715	0	1704	51	0
3	C	2488	0	2495	48	0
3	D	2513	0	2512	41	0
3	E	2485	0	2473	45	0
3	F	2489	0	2466	42	0
3	G	2089	0	2094	26	0
4	H	1783	0	1816	30	0
5	I	1314	0	663	51	0
6	J	974	0	526	9	0
7	K	953	0	532	25	0
8	L	4521	0	4547	67	0
9	A	1	0	0	0	0
All	All	25215	0	23706	399	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 8.

All (399) 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)
2:B:73:LEU:HD13	2:B:130:LEU:HD13	1.32	1.11
2:B:71:PHE:HB3	2:B:130:LEU:CD1	2.04	0.88
2:B:71:PHE:HB3	2:B:130:LEU:HD11	1.54	0.87
1:A:215:LEU:O	1:A:219:MET:HB2	1.85	0.76
6:J:43:DG:H2''	6:J:44:DC:H5'	1.70	0.71
6:J:39:DA:H1'	6:J:40:DT:C6	2.27	0.70
3:D:290:GLY:HA3	3:D:295:TYR:HB2	1.73	0.70
3:D:309:GLN:HE22	3:D:311:TRP:HB3	1.58	0.69
7:K:29:DC:H2''	7:K:30:DA:C8	2.28	0.67
8:L:200:ILE:HG12	8:L:246:LEU:H	1.58	0.67
6:J:32:DA:H2''	8:L:196:ARG:HE	1.57	0.67
4:H:216:PHE:CE1	5:I:59:G:H5'	2.29	0.67
8:L:365:LEU:HD11	8:L:433:ILE:HD11	1.76	0.67
3:D:5:VAL:HG23	3:D:260:TRP:HB3	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:619:LEU:HD12	8:L:621:ALA:H	1.60	0.66
5:I:11:G:H2'	5:I:12:A:H8	1.59	0.65
8:L:274:ALA:HA	8:L:277:LEU:HB2	1.78	0.65
2:B:71:PHE:CB	2:B:130:LEU:HD11	2.27	0.65
2:B:188:PRO:HA	2:B:191:VAL:HG22	1.77	0.65
7:K:36:DT:H2''	7:K:37:DG:H5''	1.78	0.65
2:B:69:SER:HB2	2:B:177:TRP:HA	1.79	0.64
2:B:73:LEU:CD1	2:B:130:LEU:HD13	2.19	0.64
1:A:131:THR:HG22	1:A:138:HIS:H	1.63	0.63
5:I:57:C:H3'	5:I:58:G:H8	1.64	0.63
7:K:49:DT:H2''	7:K:50:DG:C8	2.33	0.62
3:C:132:LEU:HD22	3:C:144:LEU:HG	1.81	0.62
2:B:69:SER:OG	2:B:179:TRP:HB3	2.00	0.62
7:K:36:DT:H2''	7:K:37:DG:C5'	2.30	0.62
3:C:246:PHE:HB2	7:K:36:DT:H1'	1.82	0.61
8:L:189:GLY:HA3	8:L:289:GLY:HA3	1.80	0.61
8:L:362:ILE:HA	8:L:365:LEU:HB2	1.82	0.61
3:C:212:LEU:HD11	3:E:114:VAL:HG13	1.81	0.61
6:J:33:DG:H2'	8:L:196:ARG:HD3	1.81	0.61
8:L:241:HIS:HE1	8:L:244:CYS:HB3	1.64	0.61
2:B:71:PHE:HB3	2:B:130:LEU:CG	2.29	0.60
3:E:196:VAL:HG21	3:F:84:GLU:HG2	1.82	0.60
8:L:200:ILE:HG22	8:L:202:PRO:HD3	1.82	0.59
8:L:200:ILE:HG23	8:L:246:LEU:HD22	1.84	0.59
3:C:121:ILE:HG12	3:C:140:LEU:HD11	1.82	0.59
3:F:154:THR:HA	3:F:157:GLU:HG3	1.85	0.59
4:H:69:PHE:H	4:H:73:GLY:HA3	1.68	0.59
3:D:201:ALA:O	3:D:205:ASN:ND2	2.35	0.59
5:I:46:C:H2'	5:I:47:C:C6	2.37	0.59
2:B:32:VAL:HG21	5:I:1:G:H1'	1.84	0.59
3:C:39:PRO:HG3	7:K:38:DC:H5'	1.83	0.59
3:C:72:SER:HB3	5:I:8:G:H5'	1.85	0.59
3:C:9:ASN:HD22	3:C:13:ILE:HG12	1.69	0.58
2:B:26:LEU:HD21	2:B:151:ILE:HD12	1.85	0.58
2:B:91:VAL:HG21	3:D:141:GLU:HB3	1.85	0.58
3:F:78:MET:HB3	3:F:129:PHE:HE1	1.69	0.58
2:B:70:ALA:HB3	2:B:179:TRP:HD1	1.68	0.58
3:G:116:SER:HB3	3:G:138:ARG:HD2	1.85	0.58
2:B:71:PHE:HB3	2:B:130:LEU:HG	1.85	0.58
3:E:137:PRO:HD2	3:E:138:ARG:HH21	1.68	0.57
7:K:39:DT:H2''	7:K:40:DC:H5'	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:200:ILE:HA	8:L:246:LEU:HB2	1.84	0.57
3:D:185:ILE:HA	3:D:188:LEU:HD23	1.85	0.57
8:L:633:LEU:O	8:L:691:ARG:NH2	2.38	0.57
3:E:116:SER:HB3	3:E:138:ARG:HD2	1.86	0.57
2:B:70:ALA:HB3	2:B:179:TRP:CD1	2.40	0.57
3:C:14:PHE:HB2	3:C:251:VAL:HG12	1.86	0.57
6:J:11:DA:H2''	6:J:12:DG:C8	2.40	0.57
5:I:8:G:O3'	5:I:9:U:H4'	2.06	0.56
3:E:309:GLN:HE22	3:E:311:TRP:HB3	1.69	0.56
3:C:149:LEU:HD22	3:C:258:TRP:HB3	1.87	0.56
3:F:111:PRO:HD2	7:K:28:DT:H5''	1.88	0.56
8:L:214:ARG:HD2	8:L:217:LEU:HD12	1.87	0.56
3:D:132:LEU:HB3	3:D:144:LEU:HB2	1.88	0.56
3:D:196:VAL:HG21	3:E:84:GLU:HB3	1.88	0.55
8:L:638:GLU:HG2	8:L:639:LEU:HD12	1.88	0.55
8:L:502:ARG:HD2	8:L:514:PHE:HZ	1.71	0.55
1:A:123:HIS:O	1:A:127:ARG:NE	2.32	0.55
3:C:290:GLY:HA3	3:C:295:TYR:HB2	1.88	0.55
1:A:69:CYS:HA	1:A:72:LEU:HB2	1.87	0.55
3:F:78:MET:HG3	3:F:278:ALA:HB2	1.88	0.55
3:G:128:PRO:HG3	3:G:329:ALA:HB1	1.89	0.55
8:L:179:MET:HB3	8:L:185:VAL:HG11	1.87	0.55
3:C:165:GLU:HA	3:C:168:MET:HE3	1.88	0.55
3:E:7:VAL:HG12	3:E:300:ILE:HA	1.89	0.54
5:I:41:G:H2'	5:I:42:U:C6	2.41	0.54
1:A:1:MET:HG3	1:A:88:GLN:HG2	1.88	0.54
3:F:133:PHE:O	5:I:24:A:H5'	2.08	0.54
8:L:225:GLY:HA2	8:L:244:CYS:HA	1.88	0.54
3:D:-1:GLY:HA2	3:D:266:ARG:H	1.71	0.54
3:E:45:MET:HA	3:E:63:GLN:HA	1.89	0.54
7:K:41:DC:H2''	7:K:42:DA:C8	2.42	0.54
3:G:81:HIS:HB3	3:G:281:LYS:HD2	1.88	0.54
7:K:37:DG:H2'	7:K:37:DG:N3	2.21	0.54
8:L:587:ARG:HA	8:L:607:LYS:HE2	1.90	0.54
3:C:282:MET:HG2	3:C:298:PHE:HZ	1.71	0.54
3:F:279:LEU:HD21	3:F:303:VAL:HG21	1.89	0.54
4:H:185:LYS:HA	4:H:193:ALA:HA	1.89	0.54
5:I:24:A:H2'	5:I:25:G:C8	2.43	0.54
3:D:184:PRO:HG3	3:E:104:SER:HB2	1.89	0.54
4:H:167:LEU:HD11	4:H:171:LEU:HD11	1.90	0.54
3:G:43:THR:HG22	3:G:250:GLU:HG2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:124:MET:HE2	3:F:341:PHE:HB2	1.90	0.53
3:F:5:VAL:HB	3:F:260:TRP:HB3	1.89	0.53
3:F:24:THR:OG1	3:F:27:GLY:O	2.24	0.53
4:H:185:LYS:N	5:I:42:U:O2'	2.41	0.53
8:L:650:ARG:HA	8:L:703:ASP:HB2	1.90	0.53
3:C:1:MET:HG2	3:C:267:PRO:HG3	1.89	0.53
2:B:83:MET:O	3:C:44:ARG:NH2	2.42	0.53
3:F:61:PRO:O	3:F:155:ASN:ND2	2.41	0.53
2:B:90:ILE:HD12	2:B:90:ILE:H	1.74	0.53
3:D:268:THR:HG22	3:D:270:ALA:H	1.74	0.53
3:E:128:PRO:HA	3:E:271:GLN:HG2	1.89	0.53
3:F:85:PRO:HA	3:F:88:VAL:HG12	1.91	0.52
5:I:60:G:H2'	5:I:61:G:C8	2.44	0.52
8:L:706:ILE:HD13	8:L:713:VAL:HB	1.90	0.52
1:A:32:HIS:O	2:B:209:ARG:NH2	2.39	0.52
3:C:63:GLN:OE1	3:C:63:GLN:N	2.43	0.52
2:B:83:MET:HE1	5:I:9:U:C4	2.45	0.52
3:F:185:ILE:HA	3:F:188:LEU:HD23	1.90	0.52
3:E:7:VAL:HG23	3:E:258:TRP:HB2	1.92	0.52
3:G:120:GLU:O	3:G:124:MET:HG2	2.09	0.52
3:F:181:ARG:HB2	5:I:31:C:O2'	2.10	0.52
3:F:212:LEU:HD11	4:H:103:VAL:HG21	1.92	0.52
5:I:11:G:H2'	5:I:12:A:C8	2.43	0.52
1:A:113:LEU:HD11	1:A:128:THR:HG23	1.91	0.51
3:C:61:PRO:O	3:C:155:ASN:ND2	2.42	0.51
3:E:241:ARG:CD	7:K:27:DT:H5'	2.40	0.51
3:G:42:ARG:HA	3:G:250:GLU:HB3	1.91	0.51
8:L:199:PHE:HD2	8:L:274:ALA:HB1	1.75	0.51
2:B:83:MET:HE2	2:B:120:ILE:HD11	1.91	0.51
3:D:289:GLY:HA3	5:I:16:A:H5'	1.93	0.51
3:E:145:MET:HB2	3:E:263:SER:HB2	1.92	0.51
3:F:24:THR:HG23	3:F:31:PRO:HG3	1.92	0.51
5:I:43:G:N3	5:I:43:G:H2'	2.25	0.51
1:A:135:ARG:NH2	2:B:195:HIS:O	2.43	0.51
3:G:78:MET:HE2	3:G:274:LEU:HG	1.92	0.51
4:H:159:GLN:HE22	4:H:212:TRP:HA	1.75	0.51
8:L:354:ARG:HB3	8:L:460:TYR:HH	1.75	0.51
3:E:23:ILE:HB	3:E:40:LEU:HD22	1.92	0.51
5:I:29:G:H2'	5:I:30:G:C8	2.46	0.51
2:B:97:ARG:HD2	2:B:104:LEU:HD23	1.93	0.51
3:C:165:GLU:OE2	8:L:502:ARG:NH1	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:1:G:N3	5:I:1:G:H2'	2.26	0.51
3:D:151:PRO:HB3	3:D:256:LEU:HD21	1.92	0.50
2:B:118:THR:O	7:K:42:DA:H4'	2.11	0.50
3:D:62:LEU:HD13	3:D:155:ASN:HB2	1.93	0.50
3:E:147:ASP:HB3	3:E:261:ARG:HB2	1.93	0.50
8:L:108:LEU:HD12	8:L:122:LEU:HD21	1.93	0.50
7:K:35:DT:H2''	7:K:36:DT:O5'	2.12	0.50
8:L:406:LEU:HD11	8:L:452:ILE:HD11	1.93	0.50
2:B:8:ILE:CD1	2:B:151:ILE:HG13	2.41	0.50
3:D:279:LEU:HA	3:D:282:MET:HG2	1.92	0.50
3:C:246:PHE:CB	7:K:36:DT:H1'	2.42	0.50
3:E:175:GLN:NE2	3:F:45:MET:O	2.37	0.50
4:H:178:ALA:HA	4:H:200:ALA:HA	1.92	0.50
3:C:310:VAL:HG13	3:C:316:ILE:HD12	1.94	0.49
8:L:241:HIS:CE1	8:L:244:CYS:HB3	2.46	0.49
2:B:25:ALA:HB2	2:B:206:TYR:HE2	1.76	0.49
8:L:200:ILE:HB	8:L:274:ALA:HB3	1.95	0.49
3:C:127:HIS:HB3	3:C:130:ILE:HB	1.95	0.49
3:C:163:GLY:HA2	8:L:502:ARG:HH12	1.77	0.49
5:I:54:A:H4'	5:I:55:C:C6	2.47	0.49
7:K:44:DT:H2'	7:K:45:DA:C8	2.48	0.49
3:E:139:MET:O	5:I:17:C:O2'	2.29	0.49
3:F:62:LEU:HD13	3:F:155:ASN:HB2	1.93	0.49
2:B:8:ILE:HD13	2:B:151:ILE:HG13	1.94	0.49
1:A:11:VAL:HG12	1:A:88:GLN:HA	1.94	0.49
3:F:330:ILE:HA	3:F:333:LEU:HD23	1.94	0.49
4:H:107:ASP:N	7:K:17:DC:OP1	2.40	0.49
3:E:111:PRO:HG2	7:K:34:DG:H5''	1.95	0.49
5:I:18:A:H2'	5:I:19:C:C6	2.48	0.49
1:A:215:LEU:O	1:A:219:MET:CB	2.58	0.49
3:D:181:ARG:HB2	5:I:19:C:H1'	1.95	0.49
3:E:180:ARG:HH12	5:I:28:A:H1'	1.78	0.49
2:B:154:LYS:HD3	5:I:5:A:OP2	2.13	0.48
3:C:254:PRO:HB2	3:D:159:ILE:HD11	1.94	0.48
3:C:141:GLU:HG3	5:I:5:A:H4'	1.95	0.48
3:C:241:ARG:NH2	7:K:37:DG:OP1	2.46	0.48
3:F:181:ARG:HB2	5:I:31:C:HO2'	1.79	0.48
5:I:53:U:H2'	5:I:54:A:N3	2.29	0.48
4:H:199:HIS:HE2	5:I:39:G:H8	1.62	0.48
3:D:108:THR:OG1	3:D:109:GLY:N	2.46	0.48
3:C:22:TYR:HB3	3:C:37:ARG:HB2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:108:THR:HG22	3:E:110:ASN:H	1.77	0.48
3:G:83:ILE:O	3:G:87:LEU:HB2	2.14	0.48
3:D:18:PRO:HB3	5:I:15:A:N7	2.29	0.48
3:F:195:GLU:O	3:G:93:LYS:NZ	2.47	0.48
4:H:186:LEU:HD21	5:I:61:G:H2'	1.95	0.48
3:G:146:VAL:HG22	3:G:262:ILE:HD12	1.96	0.47
3:E:24:THR:OG1	3:E:26:ASP:OD1	2.30	0.47
3:G:45:MET:HA	3:G:63:GLN:HA	1.94	0.47
1:A:191:ALA:O	1:A:195:MET:HG3	2.15	0.47
3:D:89:GLU:OE2	3:D:90:LYS:NZ	2.46	0.47
3:C:54:ASP:OD1	3:C:54:ASP:N	2.45	0.47
3:E:92:ASN:HB3	3:E:335:SER:HB3	1.96	0.47
3:C:77:THR:HG21	3:C:282:MET:HE2	1.97	0.47
3:C:145:MET:HB3	3:C:263:SER:HB2	1.97	0.47
3:F:190:SER:HB3	3:F:192:GLU:HG3	1.96	0.47
3:D:303:VAL:HB	3:D:311:TRP:HB2	1.97	0.47
8:L:481:THR:HG22	8:L:483:GLY:H	1.79	0.47
8:L:721:ASP:OD1	8:L:725:LYS:NZ	2.39	0.47
8:L:471:GLN:HA	8:L:506:GLU:HG3	1.96	0.46
8:L:502:ARG:NH2	8:L:509:THR:OG1	2.48	0.46
2:B:73:LEU:HD13	2:B:130:LEU:CD1	2.23	0.46
3:D:117:SER:OG	3:D:119:ASP:OD1	2.31	0.46
3:E:119:ASP:OD1	3:E:119:ASP:N	2.48	0.46
3:F:8:ARG:HG3	3:F:257:LYS:HG2	1.98	0.46
4:H:106:ARG:NH2	5:I:36:U:H1'	2.30	0.46
3:E:303:VAL:HB	3:E:311:TRP:HB2	1.97	0.46
5:I:56:G:H2'	5:I:57:C:H6	1.81	0.46
8:L:136:PHE:HZ	8:L:507:VAL:HG21	1.81	0.46
2:B:177:TRP:CH2	2:B:190:LEU:HD11	2.50	0.46
3:E:282:MET:HB3	3:E:300:ILE:HD11	1.98	0.46
3:F:64:ILE:HG22	3:F:150:TYR:HA	1.97	0.46
2:B:108:LYS:HB2	2:B:108:LYS:HE3	1.75	0.46
3:E:305:LEU:HD12	3:E:305:LEU:HA	1.86	0.46
3:C:175:GLN:NE2	3:D:45:MET:O	2.49	0.46
4:H:130:LYS:HE2	4:H:130:LYS:HB3	1.83	0.46
3:G:10:ILE:HG13	3:G:11:THR:HG23	1.98	0.45
1:A:209:PRO:HA	1:A:212:ARG:HG3	1.98	0.45
3:F:26:ASP:OD2	3:G:20:SER:N	2.41	0.45
3:F:204:ALA:O	3:F:208:ILE:HG12	2.16	0.45
8:L:172:THR:HG23	8:L:292:LEU:HD13	1.97	0.45
4:H:183:SER:HA	4:H:195:GLY:HA2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:44:DT:H2'	7:K:45:DA:H8	1.81	0.45
3:C:144:LEU:HD23	3:C:144:LEU:HA	1.83	0.45
3:E:241:ARG:HD2	7:K:27:DT:H5'	1.99	0.45
4:H:203:GLU:OE2	4:H:204:VAL:N	2.50	0.45
2:B:11:SER:HB3	2:B:163:ALA:HB2	1.99	0.45
3:C:110:ASN:HB2	3:C:112:ASP:OD1	2.16	0.45
3:D:184:PRO:HD3	3:D:243:LEU:HD23	1.98	0.45
5:I:39:G:N3	5:I:39:G:H2'	2.31	0.45
8:L:230:LEU:HB2	8:L:243:LEU:HD13	1.97	0.45
8:L:569:SER:HB3	8:L:619:LEU:HB3	1.98	0.45
3:F:145:MET:HE2	3:F:145:MET:HB3	1.83	0.45
4:H:114:LYS:HE2	4:H:205:ASN:HD22	1.82	0.45
8:L:201:SER:HB3	8:L:263:LEU:HD23	1.98	0.45
8:L:115:ARG:HA	8:L:119:ARG:HG3	1.99	0.45
8:L:331:ASP:HA	8:L:482:GLY:H	1.82	0.45
3:F:4:GLU:HB2	3:F:304:SER:HB3	1.99	0.45
3:F:289:GLY:HA3	5:I:28:A:H5'	1.98	0.45
3:G:76:ARG:O	3:G:80:LYS:HG2	2.16	0.45
3:G:174:THR:OG1	3:G:175:GLN:N	2.49	0.45
5:I:3:G:H4'	5:I:4:A:C8	2.52	0.45
8:L:275:GLN:HE21	8:L:275:GLN:HB3	1.56	0.45
2:B:105:ARG:HH21	6:J:7:DC:H5'	1.81	0.45
3:G:112:ASP:HB3	3:G:346:LYS:HE2	1.98	0.45
4:H:167:LEU:HD12	4:H:168:PRO:HD2	1.99	0.45
5:I:2:U:C6	5:I:4:A:H4'	2.52	0.45
8:L:135:VAL:HB	8:L:485:THR:HA	1.99	0.45
4:H:58:SER:N	4:H:65:ALA:O	2.46	0.44
4:H:111:SER:O	4:H:209:GLY:N	2.50	0.44
2:B:187:ASP:N	2:B:187:ASP:OD1	2.50	0.44
3:C:12:PRO:HG3	3:C:254:PRO:HD3	1.99	0.44
3:D:24:THR:HG23	3:D:26:ASP:H	1.81	0.44
3:F:241:ARG:HH12	7:K:20:DG:H1'	1.81	0.44
3:E:43:THR:OG1	3:E:250:GLU:O	2.35	0.44
8:L:453:GLU:O	8:L:461:PRO:HA	2.17	0.44
1:A:48:VAL:HG12	1:A:73:ARG:NH2	2.32	0.44
1:A:220:HIS:HD2	1:A:222:LYS:HG3	1.82	0.44
3:G:46:MET:N	3:G:62:LEU:O	2.43	0.44
7:K:35:DT:H4'	7:K:36:DT:OP1	2.17	0.44
8:L:387:ALA:O	8:L:391:SER:N	2.48	0.44
1:A:183:MET:HA	2:B:81:MET:HB2	1.99	0.44
2:B:123:ARG:HD3	2:B:123:ARG:HA	1.78	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:58:LYS:HA	3:D:58:LYS:HD2	1.77	0.44
8:L:206:LEU:HB2	8:L:221:ILE:HG21	1.99	0.44
1:A:81:LEU:HD12	1:A:84:ALA:HB3	1.99	0.44
5:I:56:G:H2'	5:I:57:C:C6	2.53	0.44
8:L:641:ARG:HA	8:L:641:ARG:HD3	1.81	0.44
4:H:20:ARG:NH1	4:H:219:SER:OG	2.51	0.44
6:J:33:DG:H2'	8:L:196:ARG:CD	2.46	0.44
1:A:33:CYS:HB2	1:A:35:ARG:HG2	1.99	0.44
3:D:5:VAL:HG12	3:D:303:VAL:HG22	1.99	0.44
3:E:276:LEU:O	3:E:280:ASN:HB2	2.17	0.44
8:L:167:ALA:HB3	8:L:292:LEU:HD21	2.00	0.44
6:J:28:DA:O3'	8:L:458:HIS:NE2	2.51	0.43
8:L:294:SER:HB3	8:L:297:MET:SD	2.58	0.43
2:B:16:GLU:OE2	2:B:75:ARG:NH2	2.50	0.43
3:C:15:SER:O	3:C:44:ARG:N	2.51	0.43
8:L:138:GLU:HB3	8:L:517:PRO:HB3	2.00	0.43
3:E:197:ILE:HG23	3:E:200:GLY:HA2	2.01	0.43
3:E:264:LEU:HD13	3:E:272:VAL:HG12	2.01	0.43
1:A:46:SER:HA	1:A:65:ILE:HD13	2.00	0.43
3:D:286:ARG:HG3	3:E:145:MET:HE1	2.01	0.43
3:E:131:GLY:HA3	3:E:271:GLN:HE22	1.83	0.43
3:E:271:GLN:O	3:E:275:VAL:HG23	2.18	0.43
8:L:109:PRO:HB2	8:L:182:ILE:HG23	1.99	0.43
8:L:373:ALA:HA	8:L:416:THR:HB	2.00	0.43
3:C:169:MET:HE2	3:C:169:MET:HB3	1.85	0.43
3:E:6:THR:HG22	3:E:301:ASP:HB3	2.00	0.43
3:F:279:LEU:HD22	3:F:316:ILE:HD11	2.01	0.43
3:F:260:TRP:CE2	3:F:262:ILE:HD11	2.53	0.43
3:D:0:ALA:HA	3:D:2:GLN:HE21	1.84	0.43
3:F:125:ARG:HH21	3:F:143:ARG:HG2	1.83	0.43
1:A:138:HIS:CE1	1:A:147:ILE:HD11	2.54	0.43
3:E:80:LYS:HG2	3:E:103:TYR:OH	2.19	0.43
3:C:79:LEU:HA	3:C:79:LEU:HD23	1.81	0.42
1:A:33:CYS:HB2	1:A:35:ARG:H	1.84	0.42
2:B:76:GLN:HE21	2:B:127:GLN:HG3	1.84	0.42
3:D:334:SER:OG	3:D:335:SER:N	2.52	0.42
8:L:566:LEU:HB3	8:L:623:TRP:CE2	2.54	0.42
1:A:8:VAL:HG13	1:A:14:ALA:HB3	2.02	0.42
2:B:7:THR:HG23	2:B:131:THR:HG22	2.01	0.42
2:B:25:ALA:HB2	2:B:206:TYR:CE2	2.55	0.42
4:H:184:VAL:O	4:H:194:HIS:N	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:VAL:HG13	2:B:167:VAL:HG22	2.00	0.42
2:B:154:LYS:HB2	2:B:157:VAL:HG12	2.00	0.42
2:B:209:ARG:HA	2:B:212:HIS:CE1	2.55	0.42
3:E:182:MET:HA	3:E:244:LYS:HA	2.02	0.42
3:G:257:LYS:HE3	3:G:257:LYS:HB3	1.84	0.42
3:G:260:TRP:CE2	3:G:262:ILE:HD11	2.54	0.42
5:I:4:A:H2'	5:I:5:A:C8	2.54	0.42
2:B:82:TRP:HB2	2:B:125:ILE:HD12	2.00	0.42
3:C:188:LEU:HD13	3:C:194:VAL:HG12	2.01	0.42
3:D:79:LEU:HD12	3:D:83:ILE:HB	2.02	0.42
4:H:50:THR:HG23	5:I:59:G:H21	1.85	0.42
7:K:26:DC:H2''	7:K:27:DT:O5'	2.19	0.42
3:C:42:ARG:NH1	3:C:250:GLU:OE1	2.53	0.42
5:I:38:A:H1'	5:I:39:G:O6	2.19	0.42
8:L:339:HIS:NE2	8:L:683:GLN:OE1	2.53	0.42
8:L:365:LEU:O	8:L:370:ARG:NH2	2.42	0.42
2:B:77:LEU:HD12	2:B:127:GLN:HB3	2.01	0.42
4:H:2:PHE:HA	4:H:109:PRO:HA	2.01	0.42
6:J:30:DG:H2'	6:J:31:DA:N3	2.35	0.42
8:L:281:MET:HE2	8:L:281:MET:HB3	1.94	0.42
3:E:78:MET:HG3	3:E:278:ALA:HB2	2.02	0.42
3:G:293:LYS:HD2	3:G:295:TYR:CE2	2.55	0.42
3:E:216:LYS:HA	3:E:216:LYS:HD2	1.97	0.41
3:G:15:SER:O	3:G:44:ARG:N	2.52	0.41
3:G:45:MET:HE3	3:G:45:MET:HB2	1.87	0.41
1:A:155:LYS:O	1:A:159:ILE:HG23	2.20	0.41
4:H:40:ASN:ND2	4:H:55:VAL:O	2.48	0.41
5:I:51:C:H2'	5:I:52:A:C1'	2.50	0.41
8:L:294:SER:OG	8:L:295:HIS:N	2.53	0.41
8:L:591:GLN:NE2	8:L:618:GLY:HA2	2.34	0.41
3:C:141:GLU:HA	5:I:5:A:O3'	2.19	0.41
3:C:204:ALA:O	3:C:208:ILE:HG13	2.19	0.41
3:E:4:GLU:HB2	3:E:304:SER:HB2	2.02	0.41
3:G:81:HIS:NE2	3:G:285:GLU:OE2	2.53	0.41
4:H:170:ASP:OD1	4:H:170:ASP:N	2.40	0.41
3:F:42:ARG:HA	3:F:250:GLU:HB3	2.02	0.41
1:A:128:THR:HA	1:A:129:PRO:HD3	1.89	0.41
3:C:166:ASN:OD1	3:C:167:GLU:HG3	2.21	0.41
3:D:143:ARG:NH1	3:D:266:ARG:O	2.54	0.41
3:E:241:ARG:HD3	7:K:27:DT:H5'	2.01	0.41
4:H:111:SER:HA	4:H:165:MET:HE1	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:196:ARG:NH1	8:L:264:LEU:HD22	2.35	0.41
8:L:565:VAL:HA	8:L:647:VAL:HB	2.03	0.41
3:D:160:LEU:HA	3:D:261:ARG:HH22	1.86	0.41
3:E:17:ALA:HB2	3:E:44:ARG:HA	2.02	0.41
3:G:169:MET:H	3:G:169:MET:HG3	1.63	0.41
8:L:217:LEU:HA	8:L:220:TRP:HB3	2.01	0.41
1:A:157:LEU:HD21	1:A:218:LEU:HD13	2.02	0.41
2:B:67:LYS:HE2	2:B:177:TRP:CZ2	2.55	0.41
3:F:145:MET:HE1	3:F:265:ASP:HB2	2.03	0.41
4:H:167:LEU:HA	4:H:168:PRO:HD3	1.94	0.41
3:C:73:LEU:O	3:C:77:THR:HG22	2.21	0.41
3:C:78:MET:HG2	3:C:278:ALA:HB2	2.02	0.41
3:C:241:ARG:HD2	7:K:39:DT:H5'	2.03	0.41
3:D:336:LYS:H	3:D:336:LYS:HG2	1.59	0.41
3:F:97:GLY:O	3:F:101:THR:OG1	2.36	0.41
3:G:79:LEU:HD23	3:G:79:LEU:HA	1.91	0.41
4:H:13:ARG:NH2	5:I:40:C:O2'	2.53	0.41
8:L:643:LEU:HD21	8:L:646:LEU:HD13	2.03	0.41
2:B:180:ARG:HH12	2:B:182:LEU:HD23	1.86	0.41
3:D:46:MET:HE3	3:D:46:MET:HB3	1.97	0.41
3:D:183:ASP:HA	3:D:184:PRO:HD3	1.95	0.41
3:D:264:LEU:HA	3:D:264:LEU:HD12	1.85	0.41
3:G:124:MET:HE2	3:G:341:PHE:HB2	2.03	0.41
5:I:38:A:H1'	5:I:39:G:C6	2.56	0.41
5:I:55:C:H6	5:I:56:G:H1'	1.85	0.41
5:I:57:C:H3'	5:I:58:G:C8	2.51	0.41
3:C:124:MET:HE1	3:C:138:ARG:HD2	2.03	0.41
3:D:272:VAL:O	3:D:276:LEU:HG	2.21	0.41
3:F:277:LEU:HD23	3:F:277:LEU:HA	1.90	0.41
5:I:49:C:H42	5:I:58:G:H1	1.69	0.41
8:L:205:THR:HG23	8:L:260:ASP:HB3	2.03	0.41
8:L:216:ASP:OD1	8:L:216:ASP:N	2.53	0.41
2:B:24:ASP:OD1	2:B:24:ASP:N	2.47	0.40
2:B:34:ARG:O	2:B:38:GLU:HG3	2.21	0.40
3:C:100:ALA:HB1	3:C:106:ASN:HB2	2.03	0.40
3:C:192:GLU:OE1	3:C:192:GLU:N	2.47	0.40
3:E:43:THR:HG21	3:E:252:VAL:HG23	2.03	0.40
3:F:279:LEU:HA	3:F:282:MET:HG2	2.03	0.40
3:F:169:MET:HB3	3:F:169:MET:HE3	1.75	0.40
8:L:673:ILE:H	8:L:673:ILE:HG13	1.68	0.40
1:A:150:PRO:O	1:A:154:ARG:HG2	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:PRO:O	2:B:184:ALA:C	2.64	0.40
3:C:85:PRO:O	3:C:89:GLU:HG2	2.22	0.40
3:D:169:MET:HE3	3:D:169:MET:HB3	1.90	0.40
3:E:32:PRO:HA	3:E:33:PRO:HD3	1.97	0.40
8:L:193:SER:HB3	8:L:293:CYS:HA	2.03	0.40
2:B:139:GLN:OE1	2:B:139:GLN:N	2.49	0.40
4:H:167:LEU:HD11	4:H:171:LEU:CD1	2.51	0.40
4:H:186:LEU:HD11	5:I:61:G:C2	2.56	0.40
2:B:87:ARG:NH1	5:I:8:G:O2'	2.54	0.40
3:C:78:MET:HE3	3:C:274:LEU:HG	2.04	0.40
3:D:85:PRO:HA	3:D:88:VAL:HG22	2.03	0.40
3:D:305:LEU:HD12	3:D:305:LEU:HA	1.93	0.40
3:E:181:ARG:HB2	5:I:25:G:H1'	2.03	0.40
3:F:43:THR:OG1	3:F:44:ARG:N	2.55	0.40
3:F:73:LEU:O	3:F:77:THR:HG23	2.21	0.40
3:F:252:VAL:HG11	3:F:258:TRP:HZ2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	239/241 (99%)	233 (98%)	6 (2%)	0	100	100
2	B	218/220 (99%)	209 (96%)	9 (4%)	0	100	100
3	C	325/359 (90%)	310 (95%)	15 (5%)	0	100	100
3	D	330/359 (92%)	315 (96%)	15 (4%)	0	100	100
3	E	327/359 (91%)	316 (97%)	11 (3%)	0	100	100
3	F	329/359 (92%)	315 (96%)	14 (4%)	0	100	100
3	G	272/359 (76%)	260 (96%)	12 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	230/232 (99%)	225 (98%)	5 (2%)	0	100	100
8	L	598/748 (80%)	570 (95%)	28 (5%)	0	100	100
All	All	2868/3236 (89%)	2753 (96%)	115 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/210 (99%)	204 (98%)	4 (2%)	50	73
2	B	176/177 (99%)	174 (99%)	2 (1%)	65	80
3	C	263/283 (93%)	261 (99%)	2 (1%)	73	83
3	D	263/283 (93%)	261 (99%)	2 (1%)	73	83
3	E	260/283 (92%)	259 (100%)	1 (0%)	84	87
3	F	259/283 (92%)	256 (99%)	3 (1%)	63	79
3	G	223/283 (79%)	220 (99%)	3 (1%)	61	79
4	H	189/190 (100%)	186 (98%)	3 (2%)	55	76
8	L	464/602 (77%)	459 (99%)	5 (1%)	65	80
All	All	2305/2594 (89%)	2280 (99%)	25 (1%)	63	80

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	12	LEU
1	A	33	CYS
1	A	164	ASN
2	B	125	ILE
2	B	202	ILE
3	C	45	MET
3	C	73	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	73	LEU
3	D	185	ILE
3	E	268	THR
3	F	48	VAL
3	F	251	VAL
3	F	306	ASN
3	G	54	ASP
3	G	62	LEU
3	G	82	VAL
4	H	100	VAL
4	H	167	LEU
4	H	224	HIS
8	L	243	LEU
8	L	518	VAL
8	L	573	THR
8	L	575	LEU
8	L	584	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	HIS
1	A	122	GLN
2	B	3	ASN
2	B	127	GLN
3	C	205	ASN
3	C	284	ASN
3	C	309	GLN
3	D	21	ASN
3	D	306	ASN
3	D	309	GLN
3	E	2	GLN
3	E	187	ASN
3	E	214	ASN
3	E	271	GLN
3	F	68	ASN
3	F	249	HIS
3	G	2	GLN
3	G	106	ASN
4	H	5	GLN
8	L	241	HIS
8	L	275	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	L	397	ASN
8	L	560	GLN
8	L	696	HIS
8	L	718	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	I	60/61 (98%)	39 (65%)	10 (16%)

All (39) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	I	3	G
5	I	4	A
5	I	9	U
5	I	10	G
5	I	11	G
5	I	13	G
5	I	14	C
5	I	15	A
5	I	17	C
5	I	20	C
5	I	21	U
5	I	22	G
5	I	23	A
5	I	24	A
5	I	25	G
5	I	26	G
5	I	27	A
5	I	30	G
5	I	31	C
5	I	32	U
5	I	33	U
5	I	34	G
5	I	35	A
5	I	39	G
5	I	40	C
5	I	41	G
5	I	43	G
5	I	44	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	I	45	U
5	I	46	C
5	I	48	C
5	I	49	C
5	I	52	A
5	I	53	U
5	I	55	C
5	I	56	G
5	I	58	G
5	I	59	G
5	I	61	G

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	I	10	G
5	I	13	G
5	I	22	G
5	I	25	G
5	I	31	C
5	I	34	G
5	I	39	G
5	I	43	G
5	I	44	U
5	I	60	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

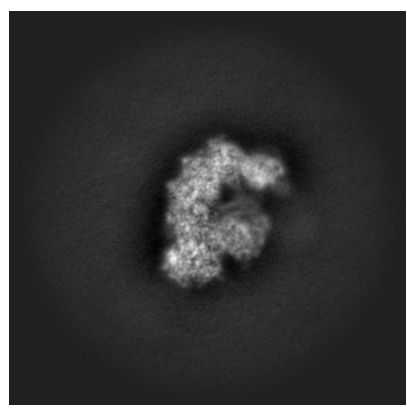
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48863. These allow visual inspection of the internal detail of the map and identification of artifacts.

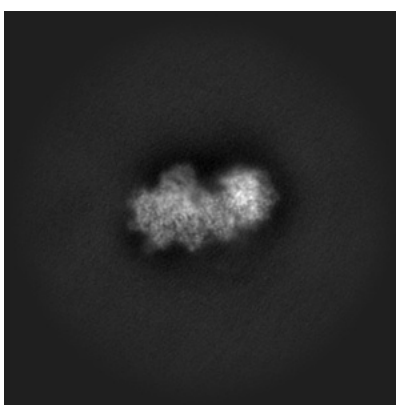
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

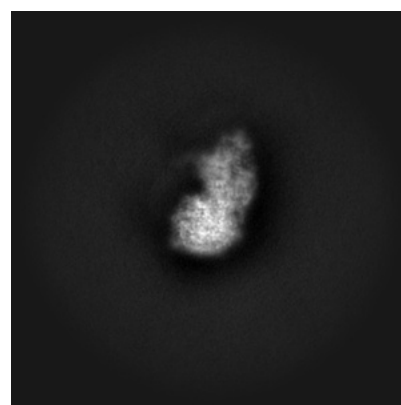
6.1.1 Primary map



X



Y

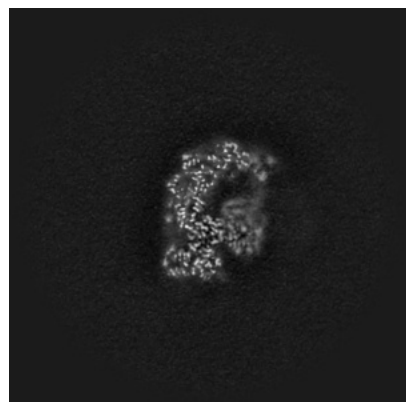


Z

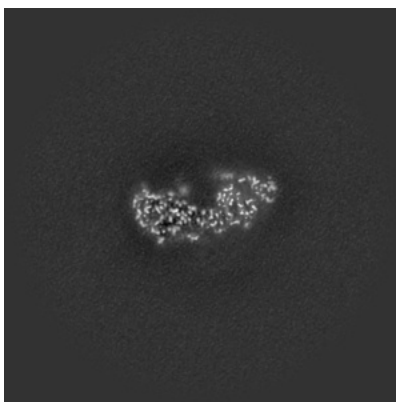
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

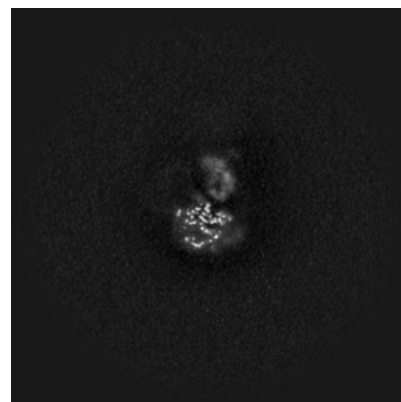
6.2.1 Primary map



X Index: 256



Y Index: 256

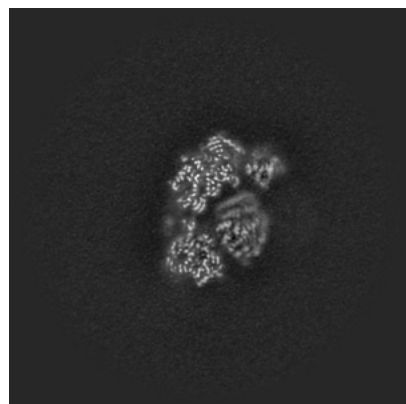


Z Index: 256

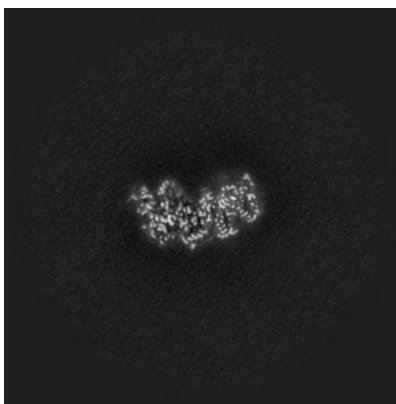
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

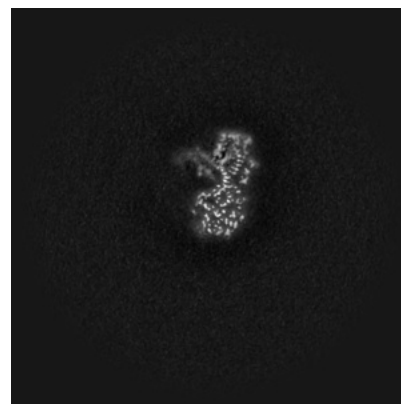
6.3.1 Primary map



X Index: 267



Y Index: 239

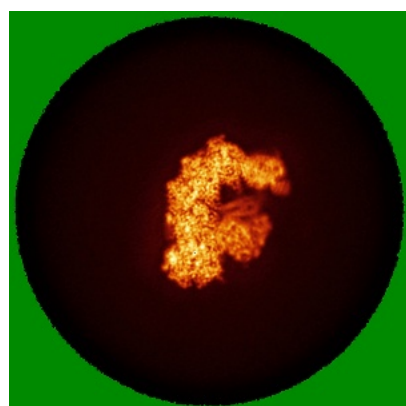


Z Index: 305

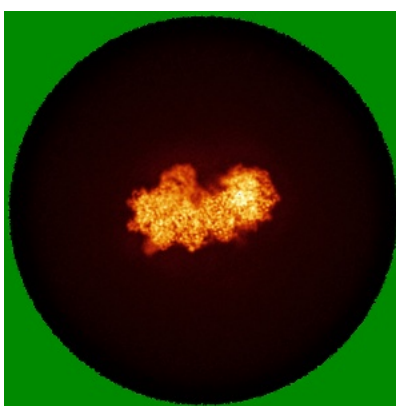
The images above show the largest variance slices of the map in three orthogonal directions.

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

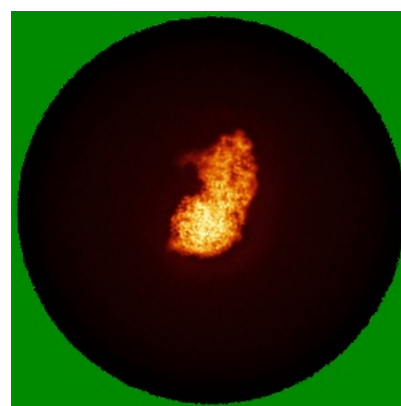
6.4.1 Primary map



X



Y



Z

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

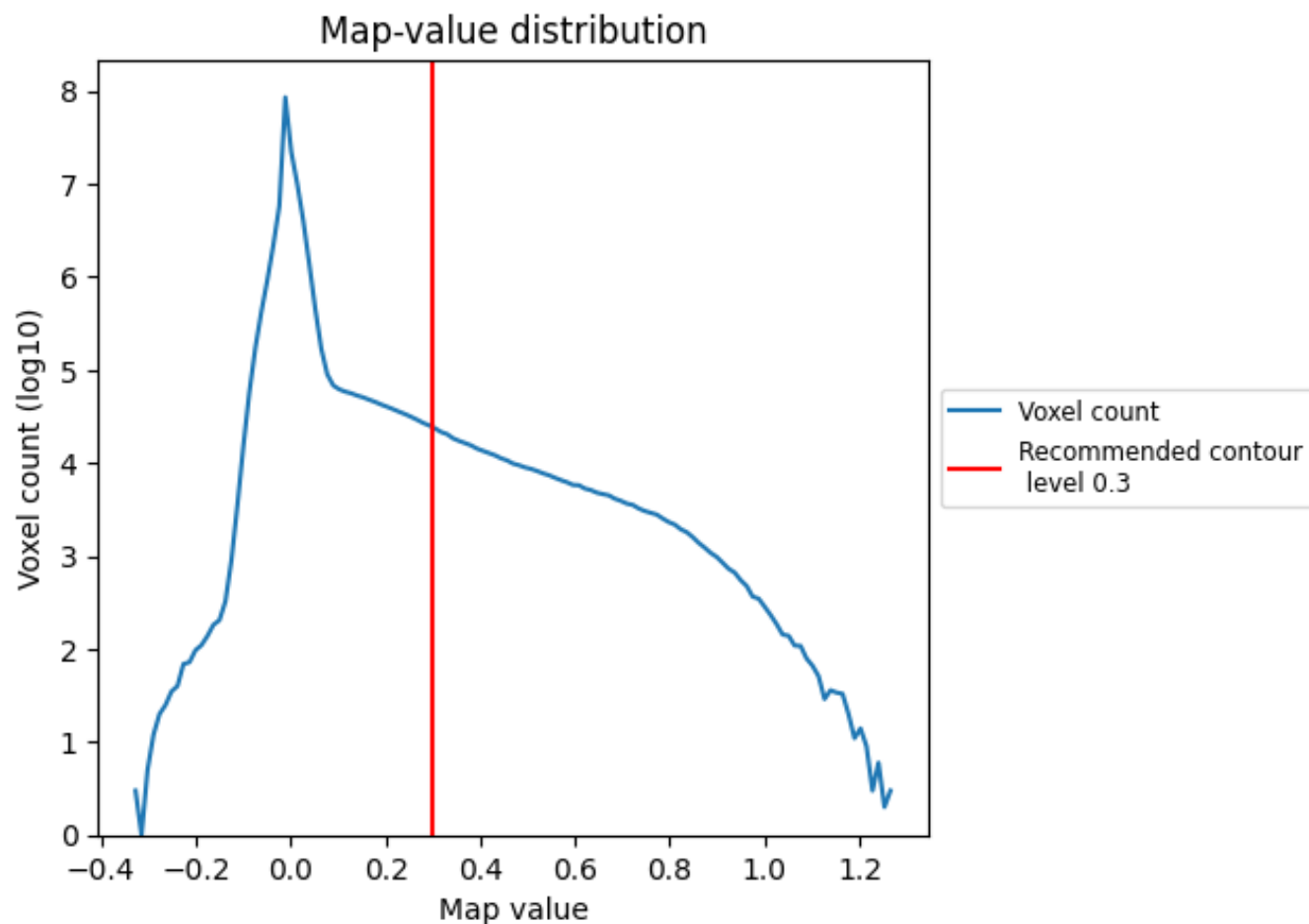
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

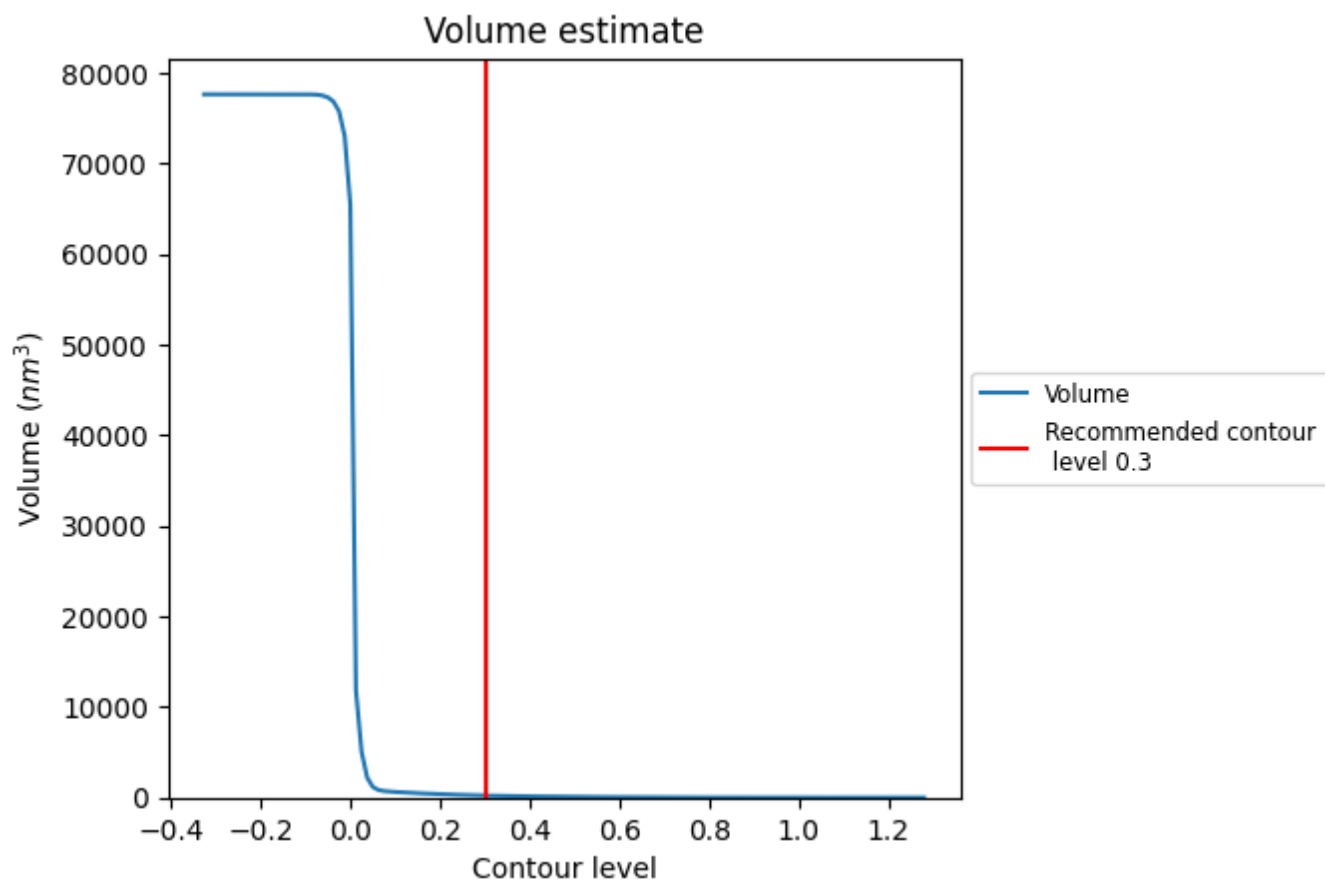
This section contains the results of statistical analysis of the map.

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.

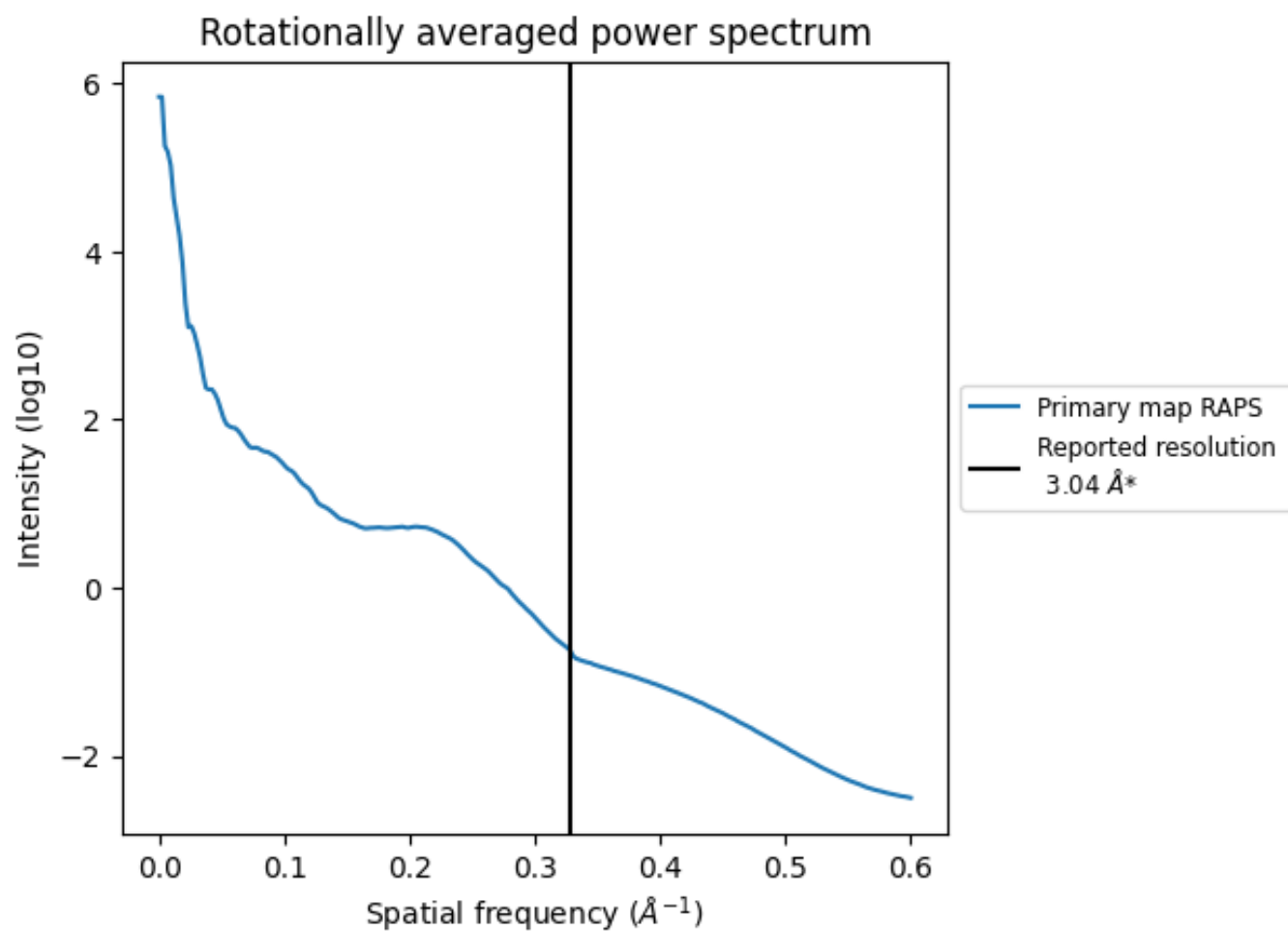
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 221 nm³; this corresponds to an approximate mass of 200 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 0.329 Å⁻¹

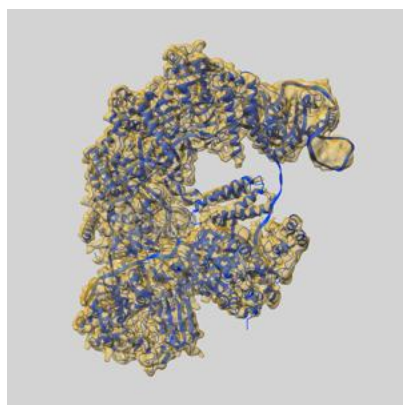
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

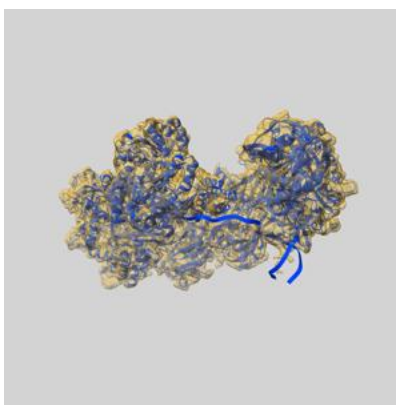
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48863 and PDB model 9N3Z. Per-residue inclusion information can be found in section [3](#) on page [8](#).

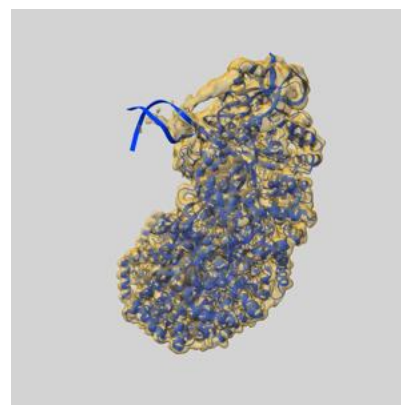
9.1 Map-model overlay [i](#)



X



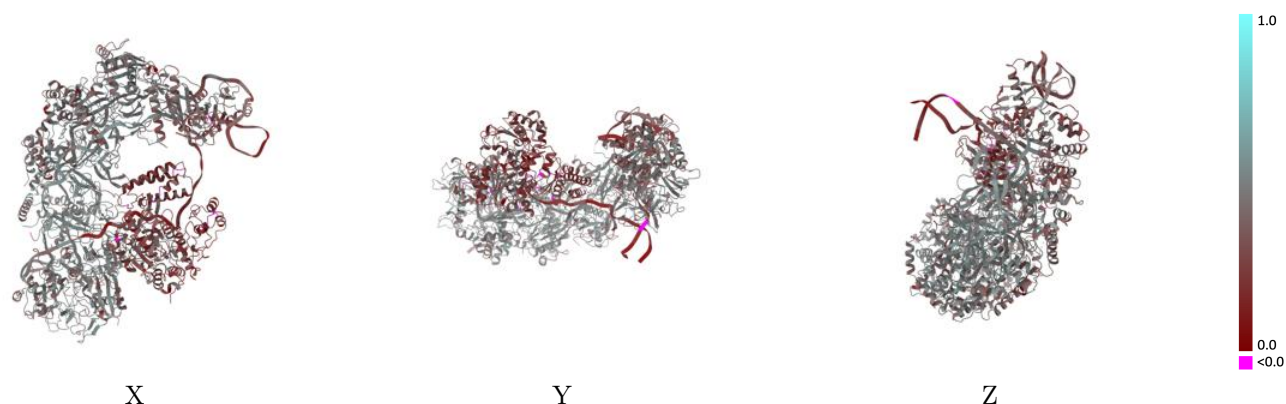
Y



Z

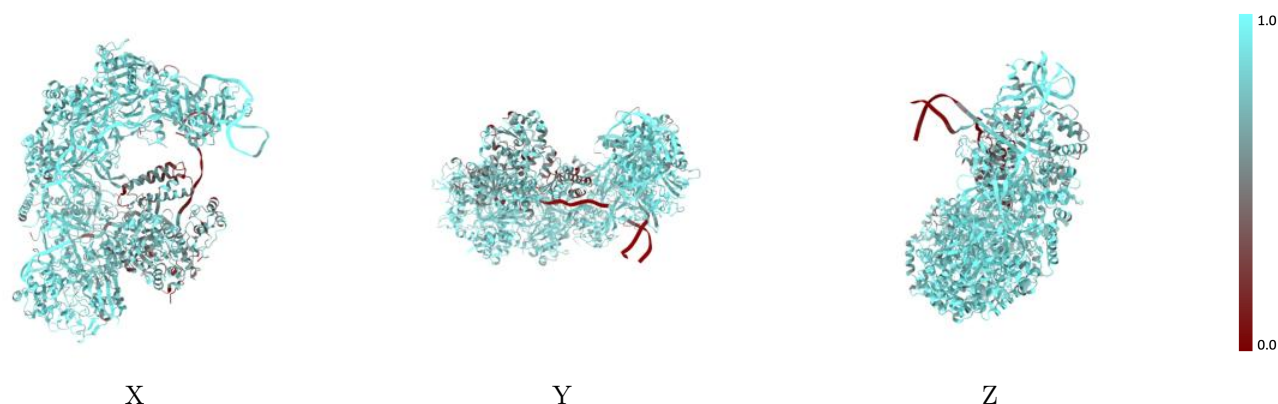
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



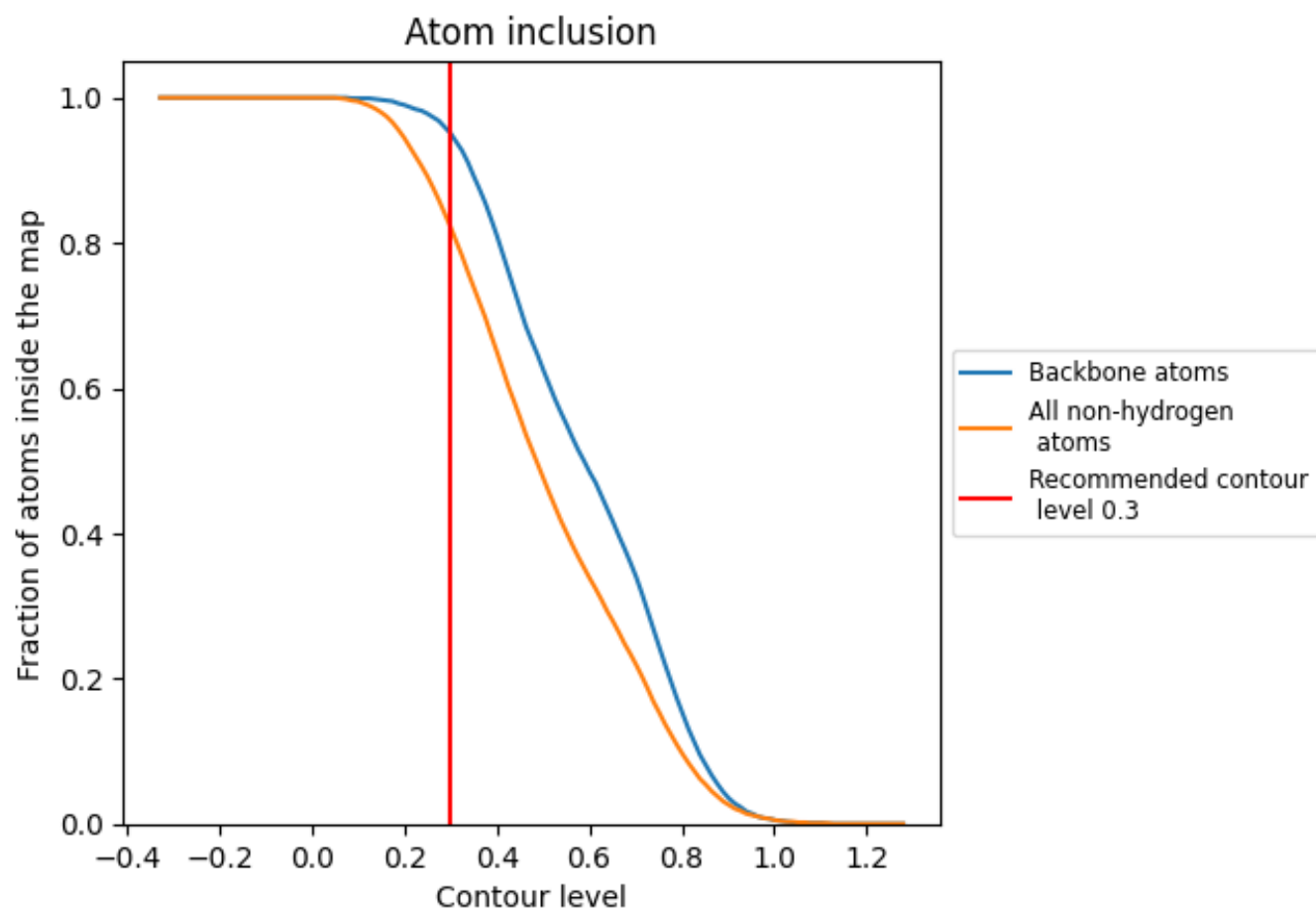
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 82% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8220	 0.4160
A	 0.8740	 0.4520
B	 0.8740	 0.4730
C	 0.8690	 0.4790
D	 0.8710	 0.4690
E	 0.8790	 0.4710
F	 0.8720	 0.4590
G	 0.8660	 0.4570
H	 0.8330	 0.3890
I	 0.9390	 0.4020
J	 0.6270	 0.2890
K	 0.8490	 0.4420
L	 0.6450	 0.2790

