



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:13 PM UTC

PDB ID : 9JPU / pdb_00009jpu
EMDB ID : EMD-61715
Title : CryoEM structure of mouse RAG SEC-PHD
Authors : Chen, X.; Yao, L.; Yang, W.; Gellert, M.
Deposited on : 2024-09-26
Resolution : 3.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

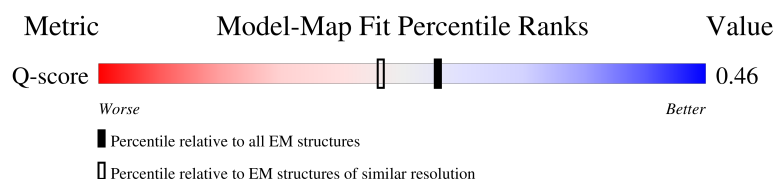
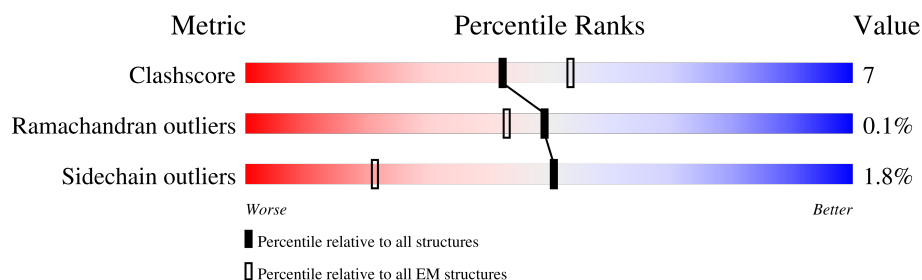
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.25 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.



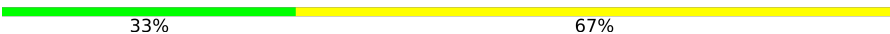
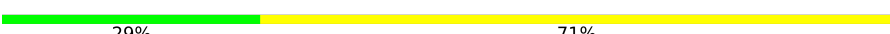
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14599 (2.75 - 3.75)

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	1040	 44% 9% 47%
1	C	1040	 45% 8% 47%
2	B	527	 53% 13% 35%
2	D	527	 51% 14% 35%

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Mol	Chain	Length	Quality of chain
2	E	527	 9% 87%
3	F	15	 33% 67%
4	G	14	 64% 36%
5	L	15	 60% 40%
6	M	14	 29% 71%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 15963 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 V(D)J recombination-activating protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	548	Total	C	N	O	S	1	0
			4411	2782	773	823	33		
1	C	547	Total	C	N	O	S	0	0
			4397	2775	770	820	32		

- Molecule 2 is a protein called V(D)J recombination-activating protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	344	Total	C	N	O	S	3	0
			2716	1733	465	499	19		
2	D	345	Total	C	N	O	S	1	0
			2694	1720	458	497	19		
2	E	69	Total	C	N	O	S	0	1
			554	351	90	105	8		

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*GP*CP*TP*GP*TP*AP*TP*CP*AP*CP*TP*GP*TP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	15	Total	C	N	O	P	0	0
			309	147	54	93	15		

- Molecule 4 is a DNA chain called DNA (5'-D(P*TP*TP*TP*GP*CP*AP*TP*CP*AP*CP*TP*GP*TP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	14	Total	C	N	O	P	0	0
			285	137	46	88	14		

- Molecule 5 is a DNA chain called DNA (5'-D(*CP*AP*CP*AP*GP*TP*GP*AP*TP*AP*CP*AP*GP*CP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	15	Total	C	N	O	P	0	0
			303	145	59	85	14		

- Molecule 6 is a DNA chain called DNA (5'-D(*CP*AP*CP*AP*GP*TP*GP*AP*TP*GP*CP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	14	Total	C	N	O	P	0	0
			286	137	58	78	13		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Ca	0
			1	1	
7	C	1	Total	Ca	0
			1	1	

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

Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	Zn	0
			1	1	
8	C	1	Total	Zn	0
			1	1	
8	E	2	Total	Zn	0
			2	2	

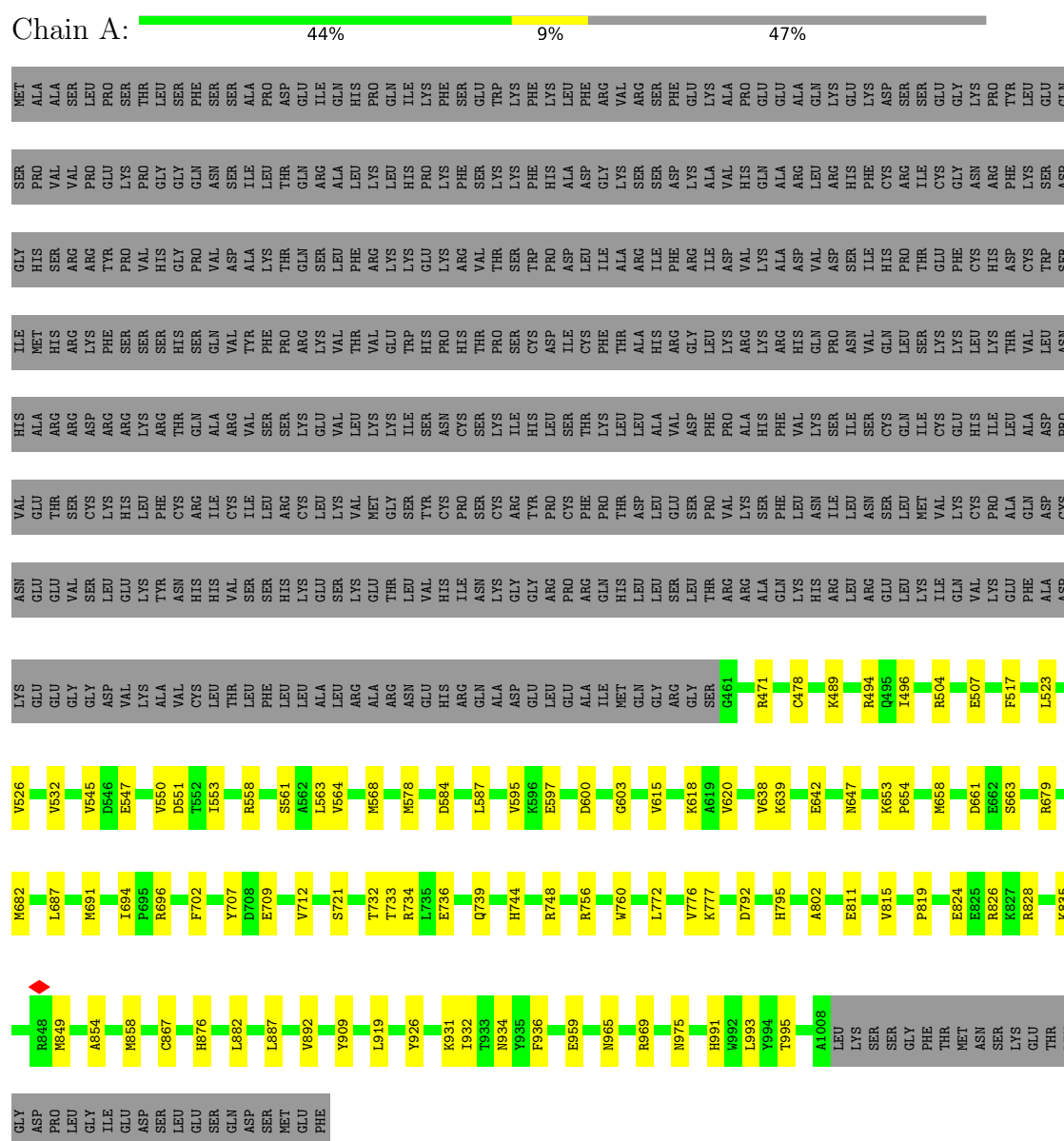
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	A	2	Total	O	0
			2	2	

3 Residue-property plots

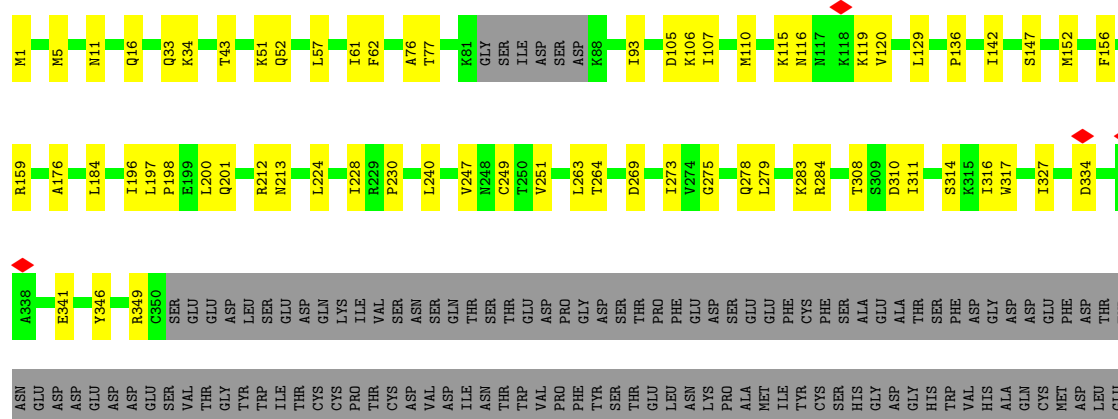
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: V(D)J recombination-activating protein 1



- Molecule 1: V(D)J recombination-activating protein 1

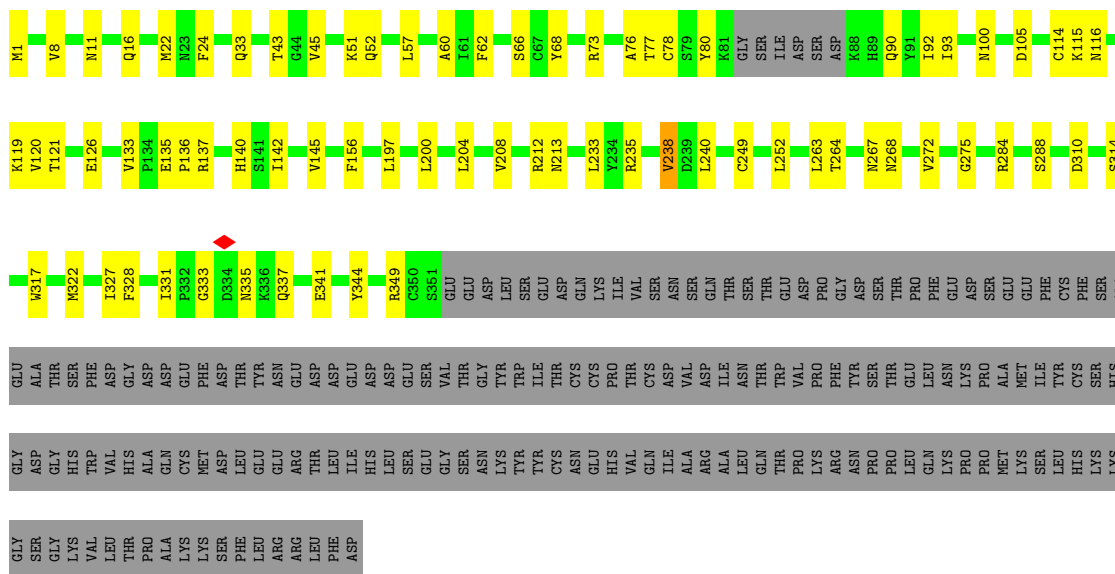
E959	R761	D551	LYS	ASN	VAL	HIS	ILE	GLY	SER	MET
G960		T552	GLU	GLU	THR	ALA	ARG	HIS	SER	ALA
N961	E767	I553	GLY	VAL	SER	THR	ARG	HIS	VAL	ALA
N965	E771	B568	GLY	SER	CYS	ASP	ARG	LYS	ARG	VAL
R969	L772	V569	ASP	LEU	LYS	ARG	PHE	TYR	GLU	PRO
R969	L772	D560	VAL	GLU	HIS	ARG	SER	PRO	LYS	SER
L988	D774	L563	LYS	TYR	PHE	LYS	SER	VAL	GLY	LEU
R775	V776	V563	ALA	ASN	CYS	THR	HIS	GLY	GLY	SER
V776		V564	VAL	ASN	PHE	THR	HIS	CYS	GLN	PHE
T995		D585	CYS	HIS	ARG	GLN	SER	PRO	VAL	ASN
V779	V779		LEU	HIS	ILE	ALA	GLN	VAL	ASN	SER
S780		V593	THR	VAL	CYS	ARG	VAL	ASP	SER	SER
A781	A781	V593	ALA	LEU	SER	VAL	TYR	ALA	ILE	SER
LEU		V594	PHE	SER	LEU	SER	PHE	LYS	LEU	PRO
LYS	I785	V595	LEU	HIS	ARG	SER	PRO	THR	THR	GLY
SER		V596	LEU	LYS	CYS	GLY	ARG	GLN	GLN	GLU
SER	I791	B597	ALA	GLU	LEU	GLY	LYS	ARG	ARG	ILE
GLY		G603	ARG	SER	LYS	LEU	VAL	PHE	ALA	GLN
THR	Y805		ALA	GLU	VAL	LEU	VAL	THR	LEU	HIS
THR	L810	V615	ARG	THR	GLY	GLY	ILE	LYS	LEU	PRO
MET	E811		ASN	LEU	SER	SER	TRP	HIS	PRO	LYS
ASN		R621	GLY	VAL	TYR	SER	ILE	LYS	ARG	ILE
SER	N820		HIS	HIS	CYS	ASN	PRO	HIS	LYS	PHI
LYS	A821	M627	ARG	ILE	PRO	CYS	THR	ARG	PHI	SER
THR		D834	GLN	ASN	SER	SER	VAL	SER	GLY	TRP
LEU	X835	N647	ALA	GLY	CYS	LYS	PRO	THR	LYS	LYS
GLY		X653	ASP	GLY	ARG	ILE	SER	SER	LYS	PHI
ASP	X856	L666	GLN	LEU	ASP	LEU	ALA	ALA	LYS	VAL
SER		T669	GLY	LEU	LEU	LEU	ILE	ILE	SER	ARG
LEU	C867	L676	ARG	SER	GLU	VAL	ARG	PHE	ASP	PHE
GLU			GLY	LEU	SER	ASP	GLY	LYS	LYS	GLY
SER	R875		SER	THR	PRO	PHE	ILE	ILE	ALA	LYS
GLN	H876	R679	SER	ARG	VAL	PRO	LYS	ASP	VAL	PRO
ASP			D461	ARG	LYS	ALA	ARG	VAL	HIS	PRO
SER	S895	M682	C467	ALA	SER	HIS	LYS	GLN	GLN	GLU
MET				GLA	PHE	PHE	ARG	ALA	ALA	GLU
GLU	E901	L687	H482	LYS	LEU	VAL	HIS	ASP	LEU	ALA
PHE				HIS	ASN	GLN	GLN	VAL	ARG	ALA
	Q914	B696	K489	ARG	ILE	SER	PRO	ASP	ARG	LYS
				LEU	LEU	ILE	ASN	SER	HIS	GLY
	L920	T705	R494	ARG	ASN	SER	VAL	ILE	PHE	LYS
			Q495	GLU	SER	CYS	GLN	ILE	PHE	LYS
	R927	G717	L496	LEU	LEU	GLN	LEU	PRO	ARG	ASP
	Y928			LYS	MET	ILE	SER	THR	ILE	SER
		C730	L500	ILE	VAL	CYS	LYS	GLY	CYS	GLY
	T932			GLN	LYS	GLU	LYS	PHE	GLY	GLY
			L503	VAL	CYS	HIS	LEU	CYS	ASN	LYS
	K938	R734	R504	LYS	PRO	ILE	LYS	ARG	PHI	PRO
				GLU	ALA	LEU	THR	ASP	PHE	TYR
	H942	V742	E507	PHE	GLN	ALA	VAL	CYS	LYS	LYS
	Y943			ASP	ASP	LEU	TRP	ASN	SER	GLN
		V769	V560	CYS	PRO	ARG	ASN	STR	ASN	GLY



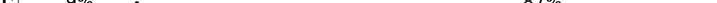
[illegible]

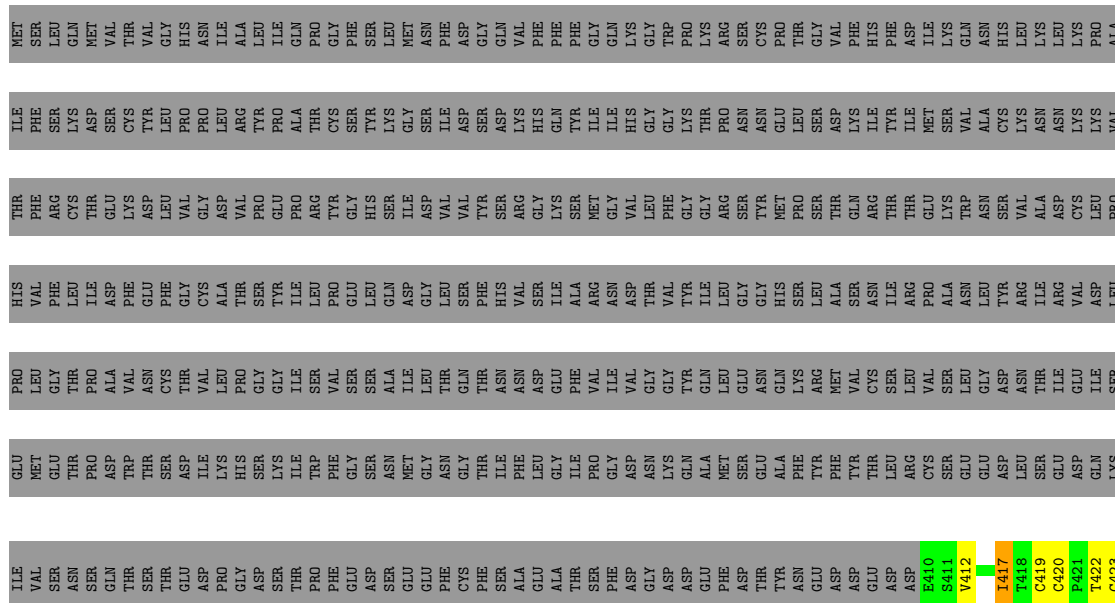
- Molecule 2: V(D)J recombination-activating protein 2

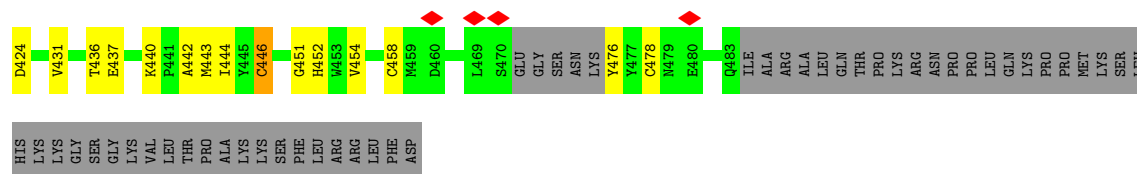
Chain D:  51% 14% 35%



- Molecule 2: V(D)J recombination-activating protein 2

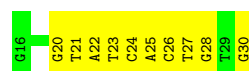
Chain E:  9% . 87%





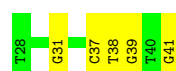
- Molecule 3: DNA (5'-D(P*GP*GP*CP*TP*GP*TP*AP*TP*CP*AP*CP*TP*GP*TP*G)-3')

Chain F: 33% 67%



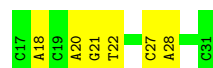
- Molecule 4: DNA (5'-D(P*TP*TP*TP*GP*CP*AP*TP*CP*AP*CP*TP*GP*TP*G)-3')

Chain G: 64% 36%



- Molecule 5: DNA (5'-D(*CP*AP*CP*AP*GP*TP*GP*AP*TP*AP*CP*AP*GP*CP*C)-3')

Chain L: 60% 40%



- Molecule 6: DNA (5'-D(*CP*AP*CP*AP*GP*TP*GP*AP*TP*GP*CP*AP*AP*A)-3')

Chain M: 29% 71%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57418	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; cryoSPARC	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.628	Depositor
Minimum map value	-0.325	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	279.84, 279.84, 279.84	wwPDB
Map dimensions	264, 264, 264	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.11	0/4508	0.27	0/6080
1	C	0.11	0/4494	0.30	3/6061 (0.0%)
2	B	0.10	0/2785	0.25	0/3774
2	D	0.10	0/2763	0.27	0/3748
2	E	0.09	0/572	0.24	0/783
3	F	0.21	0/345	0.40	0/531
4	G	0.20	0/317	0.44	0/487
5	L	0.19	0/340	0.32	0/522
6	M	0.18	0/322	0.33	0/495
All	All	0.11	0/16446	0.28	3/22481 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	943	VAL	CA-C-N	-6.12	113.44	120.04
1	C	943	VAL	C-N-CA	-6.12	113.44	120.04
1	C	943	VAL	N-CA-C	5.32	120.38	108.88

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	4411	0	4363	56	0
1	C	4397	0	4350	48	0
2	B	2716	0	2666	36	0
2	D	2694	0	2629	43	0
2	E	554	0	493	16	0
3	F	309	0	170	10	0
4	G	285	0	160	6	0
5	L	303	0	169	5	0
6	M	286	0	158	8	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
8	E	2	0	0	0	0
9	A	2	0	0	0	0
All	All	15963	0	15158	209	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (209) 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:D:1:MET:HA	2:D:349:ARG:O	1.66	0.96
1:C:730:CYS:SG	1:C:942:HIS:CE1	2.72	0.82
2:B:1:MET:HA	2:B:349:ARG:O	1.83	0.78
1:A:721:SER:HB3	2:E:431:VAL:HG11	1.69	0.74
2:E:452:HIS:CE1	2:E:478:CYS:SG	2.79	0.74
1:A:756:ARG:HB3	1:A:776:VAL:HG23	1.70	0.73
2:D:105:ASP:HB3	2:D:136:PRO:HG3	1.75	0.69
2:E:446:CYS:SG	2:E:452:HIS:CD2	2.84	0.69
1:A:639:LYS:HD3	1:A:642:GLU:HB2	1.75	0.69
1:C:552:THR:HG21	1:C:667:THR:HG21	1.78	0.66
1:A:547:GLU:OE2	2:B:159:ARG:NH1	2.29	0.65
5:L:21:DG:H2'	5:L:22:DT:H71	1.79	0.65
1:C:666:GLU:OE1	2:D:73:ARG:NH1	2.30	0.64
1:C:959:GLU:OE1	4:G:41:DG:N2	2.30	0.64
1:C:653:LYS:NZ	1:C:995:THR:O	2.29	0.62
1:A:959:GLU:OE1	3:F:30:DG:N2	2.33	0.62
2:E:446:CYS:O	2:E:451:GLY:HA2	1.99	0.61
2:D:284:ARG:NH2	2:D:288:SER:OG	2.33	0.61
2:B:116:ASN:HB2	2:B:119:LYS:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:594:VAL:HG13	1:C:627:MET:HB3	1.82	0.61
3:F:27:DT:H2'	3:F:28:DG:C8	2.35	0.60
2:D:264:THR:HB	2:D:327:ILE:HD11	1.82	0.60
1:A:545:VAL:HG23	2:B:316:ILE:HG22	1.83	0.60
2:B:264:THR:HB	2:B:327:ILE:HD11	1.84	0.60
4:G:38:DT:H2'	4:G:39:DG:C8	2.38	0.58
2:B:51:LYS:HE2	2:B:52:GLN:HE22	1.69	0.58
2:B:212:ARG:NH1	2:B:269:ASP:OD1	2.33	0.58
1:C:811:GLU:OE2	1:C:875:ARG:NE	2.33	0.57
1:A:647:ASN:HB3	1:A:959:GLU:HB2	1.85	0.57
2:D:77:THR:HG22	2:D:93:ILE:HG12	1.85	0.57
1:A:931:LYS:NZ	2:E:422:THR:O	2.38	0.57
1:C:805:TYR:OH	1:C:834:ASP:OD1	2.22	0.57
2:B:5:MET:SD	2:B:5:MET:N	2.76	0.56
1:A:760:TRP:HB2	1:A:776:VAL:HG11	1.86	0.56
1:A:882:LEU:HD13	1:A:919:LEU:HD22	1.87	0.56
2:B:147:SER:HB3	2:B:240:LEU:HD12	1.88	0.56
2:B:198:PRO:O	2:B:201:GLN:NE2	2.39	0.56
1:C:482:HIS:HB2	1:C:500:LEU:HD11	1.87	0.56
1:A:471:ARG:NH2	1:A:478:CYS:SG	2.79	0.56
1:A:587:LEU:O	1:A:696:ARG:NH1	2.39	0.56
1:A:600:ASP:OD2	1:A:965:ASN:ND2	2.38	0.56
2:D:45:VAL:HG23	2:D:60:ALA:HB3	1.87	0.55
1:C:791:ILE:HG22	1:C:938:LYS:HD3	1.87	0.55
5:L:18:DA:C8	5:L:18:DA:H5'	2.41	0.55
2:B:197:LEU:HD13	2:B:249:CYS:HB2	1.88	0.55
2:D:267:ASN:OD1	2:D:268:ASN:N	2.38	0.55
2:D:322:MET:HE3	2:D:328:PHE:HB2	1.88	0.55
1:C:597:GLU:OE1	1:C:679:ARG:NH1	2.39	0.55
2:D:11:ASN:HD21	2:D:57:LEU:HB2	1.72	0.54
6:M:22:DT:H2''	6:M:23:DG:C8	2.42	0.54
1:A:969:ARG:NH2	3:F:30:DG:OP2	2.40	0.53
2:D:208:VAL:HG13	2:D:263:LEU:HD12	1.89	0.53
1:A:553:ILE:HG12	1:A:615:VAL:HG11	1.91	0.53
1:A:748:ARG:NH2	1:A:777:LYS:O	2.41	0.53
2:D:335:ASN:HD22	2:D:337:GLN:HG2	1.74	0.53
1:A:532:VAL:HG21	1:A:558:ARG:HD3	1.90	0.53
1:A:709:GLU:OE2	1:A:934:ASN:ND2	2.42	0.53
1:C:761:ARG:NH1	2:D:126:GLU:OE1	2.42	0.52
1:C:553:ILE:HG12	1:C:615:VAL:HG11	1.92	0.52
2:D:16:GLN:NE2	2:D:33:GLN:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:115:LYS:HG3	2:D:120:VAL:HG22	1.92	0.51
1:A:682:MET:HE3	1:A:702:PHE:CZ	2.46	0.51
1:A:691:MET:HE2	1:A:696:ARG:HD2	1.93	0.51
1:A:584:ASP:N	1:A:584:ASP:OD1	2.44	0.51
2:B:77:THR:HG22	2:B:93:ILE:HG22	1.93	0.51
2:B:278:GLN:HG3	2:B:284:ARG:HB2	1.93	0.50
1:C:773:ARG:HA	1:C:776:VAL:HG12	1.93	0.50
2:E:452:HIS:HE1	2:E:478:CYS:SG	2.27	0.50
1:A:824:GLU:O	1:A:828:ARG:HG2	2.12	0.50
1:C:938:LYS:O	1:C:943:VAL:HG23	2.12	0.50
2:D:197:LEU:HD13	2:D:200:LEU:HD12	1.93	0.50
1:A:620:VAL:HB	1:A:658:MET:HG2	1.93	0.50
1:A:661:ASP:OD2	1:A:663:SER:OG	2.20	0.50
1:C:564:VAL:HG22	1:C:687:LEU:HD21	1.94	0.49
2:B:107:ILE:HD12	2:B:129:LEU:HD21	1.94	0.49
3:F:21:DT:H2'	3:F:22:DA:C8	2.47	0.49
1:A:991:HIS:O	1:A:995:THR:HG22	2.12	0.49
2:B:156:PHE:HE1	2:B:200:LEU:HD13	1.78	0.49
2:E:417:ILE:HD11	2:E:443:MET:HE1	1.94	0.49
2:D:156:PHE:HE1	2:D:200:LEU:HD13	1.77	0.49
1:A:835:LYS:HD2	2:D:333:GLY:HA2	1.95	0.49
2:B:152:MET:HG2	2:B:184:LEU:HD21	1.95	0.49
2:B:308:THR:OG1	2:B:310:ASP:OD1	2.28	0.49
1:A:597:GLU:OE1	1:A:679:ARG:NH2	2.46	0.49
1:A:682:MET:HE3	1:A:702:PHE:HZ	1.78	0.49
1:A:707:TYR:HB2	1:A:712:VAL:HG23	1.95	0.49
1:C:943:VAL:HG12	1:C:943:VAL:O	2.12	0.49
2:B:105:ASP:HB3	2:B:136:PRO:HG3	1.95	0.48
1:C:742:VAL:HG11	1:C:914:GLN:HG2	1.96	0.48
1:A:826:ARG:HH22	2:E:420:CYS:C	2.21	0.48
1:A:523:LEU:HB3	1:A:526:VAL:HB	1.95	0.48
2:B:16:GLN:HB3	2:B:34:LYS:HB2	1.96	0.48
2:B:228:ILE:HG13	2:B:230:PRO:HD3	1.96	0.48
1:A:578:MET:HE1	1:A:587:LEU:HB2	1.95	0.48
1:C:559:TYR:OH	1:C:597:GLU:OE2	2.30	0.48
1:A:653:LYS:HA	1:A:995:THR:HG21	1.96	0.48
2:E:419:CYS:SG	2:E:458:CYS:CB	2.98	0.48
1:A:654:PRO:HG3	1:A:991:HIS:HB3	1.95	0.47
2:D:264:THR:HG23	2:D:272:VAL:HB	1.95	0.47
1:C:776:VAL:HG22	1:C:779:VAL:HB	1.95	0.47
3:F:26:DC:H2'	3:F:27:DT:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:THR:HG21	1:A:744:HIS:CD2	2.50	0.47
1:C:647:ASN:HB3	1:C:959:GLU:HB2	1.97	0.47
1:C:820:ASN:OD1	1:C:821:ALA:N	2.48	0.47
1:C:494:ARG:HE	1:C:496:ILE:HD11	1.80	0.47
1:C:558:ARG:NH2	1:C:560:ASP:OD2	2.41	0.47
2:D:145:VAL:HG21	2:D:238:VAL:HG11	1.95	0.47
2:D:317:TRP:HB3	2:D:331:ILE:HD13	1.97	0.47
1:A:736:GLU:HA	1:A:739:GLN:HG2	1.96	0.47
3:F:30:DG:O6	5:L:18:DA:N6	2.48	0.47
2:D:135:GLU:HG2	2:D:137:ARG:HH21	1.80	0.47
2:D:212:ARG:HG3	2:D:213:ASN:H	1.79	0.47
1:A:824:GLU:HG3	1:A:828:ARG:HE	1.80	0.46
1:A:828:ARG:HH12	2:D:344:TYR:HB3	1.79	0.46
1:C:585:ASP:O	1:C:696:ARG:NH2	2.47	0.46
6:M:20:DA:C4	6:M:21:DG:C8	3.04	0.46
2:D:197:LEU:HD22	2:D:249:CYS:HB2	1.97	0.46
1:A:811:GLU:OE2	1:A:926:TYR:OH	2.31	0.46
3:F:24:DC:H2'	3:F:25:DA:C8	2.51	0.46
5:L:27:DC:H2''	5:L:28:DA:C8	2.51	0.46
1:A:494:ARG:HE	1:A:496:ILE:HD11	1.81	0.46
1:A:489:LYS:NZ	4:G:31:DG:OP1	2.42	0.46
2:D:156:PHE:HE2	2:D:204:LEU:HB2	1.80	0.46
4:G:37:DC:H2'	4:G:38:DT:C6	2.51	0.46
1:A:694:ILE:H	1:A:694:ILE:HD12	1.81	0.46
1:C:767:GLU:OE2	1:C:775:ARG:NH2	2.42	0.45
1:C:843:LEU:HD21	1:C:856:LYS:HD2	1.99	0.45
2:D:76:ALA:HB1	2:D:142:ILE:HG22	1.97	0.45
1:A:551:ASP:OD1	1:A:551:ASP:N	2.48	0.45
6:M:26:DG:H2''	6:M:27:DC:C6	2.51	0.45
2:B:283:LYS:NZ	2:B:314:SER:OG	2.44	0.45
1:C:733:THR:OG1	1:C:734:ARG:N	2.50	0.45
1:A:504:ARG:O	1:A:507:GLU:HG2	2.16	0.45
1:C:760:TRP:HB2	1:C:776:VAL:HG21	1.97	0.45
4:G:41:DG:O6	6:M:18:DA:N6	2.49	0.45
1:C:467:CYS:HB2	1:C:503:LEU:HD21	2.00	0.44
1:C:657:LEU:HG	1:C:988:LEU:HD13	2.00	0.44
1:C:767:GLU:HB3	1:C:771:GLU:HB2	2.00	0.44
1:C:850:ASN:N	1:C:850:ASN:OD1	2.48	0.44
2:E:437:GLU:HG2	2:E:442:ALA:H	1.81	0.44
1:A:517:PHE:HB2	1:A:687:LEU:HD11	2.00	0.44
2:D:275:GLY:HA2	2:D:317:TRP:CZ2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:116:ASN:HB2	2:D:119:LYS:HG3	2.00	0.44
2:B:76:ALA:HB1	2:B:142:ILE:HG22	1.99	0.44
1:C:895:SER:OG	1:C:901:GLU:OE1	2.27	0.44
2:B:116:ASN:N	2:B:119:LYS:O	2.49	0.44
2:B:283:LYS:NZ	2:B:311:ILE:O	2.51	0.43
2:E:420:CYS:H	2:E:423:CYS:HB2	1.83	0.43
1:A:867:CYS:O	1:A:876:HIS:NE2	2.51	0.43
2:D:310:ASP:O	2:D:314:SER:OG	2.27	0.43
2:E:446:CYS:HA	2:E:476:TYR:HB3	2.00	0.43
1:A:568:MET:HA	1:A:568:MET:HE2	1.99	0.43
1:A:734:ARG:NH1	2:E:424:ASP:OD2	2.50	0.43
2:B:43:THR:HG21	2:B:61:ILE:HA	1.99	0.43
3:F:22:DA:H2'	3:F:23:DT:H71	2.00	0.43
2:E:444:ILE:HG23	2:E:454:VAL:HG23	2.00	0.43
1:C:717:GLY:HA2	1:C:781:ALA:HB3	2.00	0.43
2:D:43:THR:HG22	2:D:68:TYR:HE2	1.84	0.43
2:E:446:CYS:SG	2:E:452:HIS:HD2	2.34	0.43
2:B:11:ASN:HB2	2:B:57:LEU:HD13	1.99	0.43
1:C:920:LEU:HD22	1:C:928:TYR:HD2	1.84	0.43
1:C:504:ARG:O	1:C:507:GLU:HG2	2.18	0.43
2:D:114:CYS:SG	2:D:121:THR:OG1	2.72	0.43
1:A:792:ASP:OD2	1:A:795:HIS:ND1	2.49	0.42
1:A:854:ALA:O	1:A:858:MET:HG2	2.20	0.42
5:L:20:DA:C4	5:L:21:DG:C8	3.06	0.42
1:A:802:ALA:HA	1:A:849:MET:HE3	2.01	0.42
2:B:212:ARG:HG3	2:B:213:ASN:H	1.84	0.42
2:B:263:LEU:HD12	2:B:273:ILE:HD11	2.01	0.42
1:C:621:ARG:NH1	1:C:961:ASN:OD1	2.52	0.42
2:D:22:MET:HE2	2:D:24:PHE:HE2	1.83	0.42
2:D:78:CYS:SG	2:D:92:ILE:HB	2.59	0.42
2:D:235:ARG:HH11	2:D:252:LEU:HD11	1.83	0.42
2:B:176:ALA:HA	2:B:224:LEU:HD23	2.00	0.42
1:C:621:ARG:HD3	1:C:965:ASN:ND2	2.34	0.42
2:E:440:LYS:HE2	2:E:440:LYS:HB2	1.93	0.42
2:D:51:LYS:HE2	2:D:52:GLN:HE22	1.85	0.42
1:A:772:LEU:O	1:A:776:VAL:HG12	2.19	0.42
1:C:810:LEU:HD22	1:C:927:ARG:HD2	2.01	0.42
2:D:233:LEU:HD22	2:D:252:LEU:HB2	2.02	0.42
3:F:26:DC:H2'	3:F:27:DT:H6	1.85	0.42
2:B:275:GLY:HA2	2:B:317:TRP:CZ2	2.55	0.42
1:C:867:CYS:O	1:C:876:HIS:NE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:ASN:ND2	2:D:57:LEU:HB2	2.33	0.42
6:M:23:DG:H2''	6:M:24:DA:C8	2.55	0.42
2:B:16:GLN:NE2	2:B:33:GLN:O	2.50	0.42
1:C:563:LEU:HD22	1:C:682:MET:HE1	2.02	0.42
2:B:43:THR:HB	2:B:62:PHE:CD2	2.55	0.41
1:A:892:VAL:HG21	1:A:909:TYR:HD2	1.85	0.41
2:B:334:ASP:HB2	1:C:835:LYS:HG3	2.02	0.41
1:C:849:MET:HE3	1:C:849:MET:HB2	1.98	0.41
2:D:62:PHE:HB3	2:D:66:SER:OG	2.20	0.41
2:D:137:ARG:HG3	2:D:140:HIS:CE1	2.55	0.41
2:D:80:TYR:HB3	2:D:90:GLN:HG3	2.01	0.41
1:A:603:GLY:HA2	1:A:618:LYS:HG2	2.02	0.41
2:B:110:MET:HE3	2:B:110:MET:HB2	1.99	0.41
2:B:115:LYS:HG3	2:B:120:VAL:HG22	2.02	0.41
1:C:489:LYS:NZ	3:F:20:DG:OP1	2.40	0.41
2:B:310:ASP:OD2	2:B:346:TYR:OH	2.36	0.41
1:C:669:THR:HG21	2:D:100:ASN:HA	2.03	0.41
1:C:676:ILE:HG13	1:C:785:ILE:HG12	2.03	0.41
2:D:235:ARG:NH1	2:D:252:LEU:HD11	2.36	0.41
6:M:27:DC:H2''	6:M:28:DA:H8	1.86	0.40
6:M:19:DC:H2''	6:M:20:DA:C8	2.56	0.40
1:C:603:GLY:O	1:C:969:ARG:NH2	2.50	0.40
1:A:561:SER:O	1:A:564:VAL:HG12	2.22	0.40
4:G:37:DC:H2'	4:G:38:DT:H6	1.87	0.40
1:A:815:VAL:O	1:A:819:PRO:HB3	2.21	0.40
6:M:21:DG:H2'	6:M:22:DT:H71	2.02	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	547/1040 (53%)	529 (97%)	18 (3%)	0	100	100
1	C	545/1040 (52%)	530 (97%)	15 (3%)	0	100	100
2	B	343/527 (65%)	334 (97%)	9 (3%)	0	100	100
2	D	342/527 (65%)	325 (95%)	16 (5%)	1 (0%)	36	66
2	E	65/527 (12%)	61 (94%)	4 (6%)	0	100	100
All	All	1842/3661 (50%)	1779 (97%)	62 (3%)	1 (0%)	49	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	341	GLU

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	486/933 (52%)	476 (98%)	10 (2%)	47	66
1	C	484/933 (52%)	478 (99%)	6 (1%)	63	74
2	B	302/469 (64%)	296 (98%)	6 (2%)	48	66
2	D	298/469 (64%)	294 (99%)	4 (1%)	61	73
2	E	63/469 (13%)	59 (94%)	4 (6%)	16	43
All	All	1633/3273 (50%)	1603 (98%)	30 (2%)	51	69

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	550	VAL
1	A	563	LEU
1	A	595	VAL
1	A	638	VAL
1	A	733	THR
1	A	887	LEU
1	A	932	ILE

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Mol	Chain	Res	Type
1	A	936	PHE
1	A	975	ASN
1	A	993	LEU
2	B	106	LYS
2	B	196	ILE
2	B	247	VAL
2	B	251	VAL
2	B	279	LEU
2	B	341	GLU
1	C	550	VAL
1	C	593	VAL
1	C	595	VAL
1	C	705	THR
1	C	733	THR
1	C	932	ILE
2	D	8	VAL
2	D	133	VAL
2	D	238	VAL
2	D	240	LEU
2	E	412	VAL
2	E	417	ILE
2	E	436	THR
2	E	446	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	515	HIS
1	A	978	GLN
2	B	10	HIS
2	B	11	ASN
2	B	52	GLN
1	C	975	ASN
1	C	990	HIS
2	D	4	GLN
2	D	23	ASN
2	D	278	GLN
2	E	448	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 6 ligands modelled in this entry, 6 are 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.

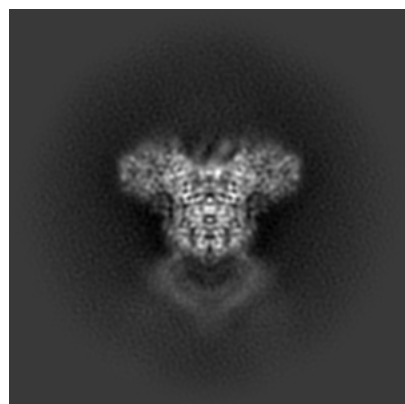
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61715. These allow visual inspection of the internal detail of the map and identification of artifacts.

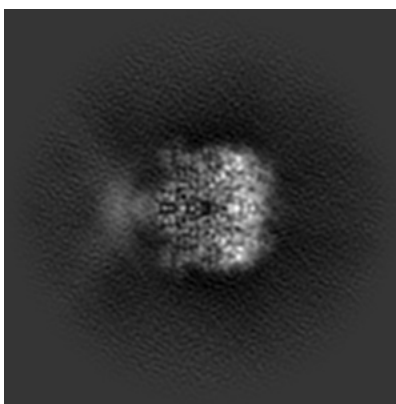
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

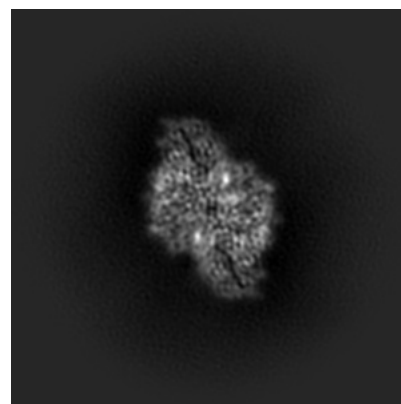
6.1.1 Primary map



X

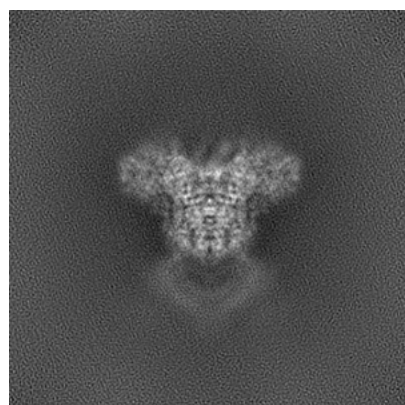


Y

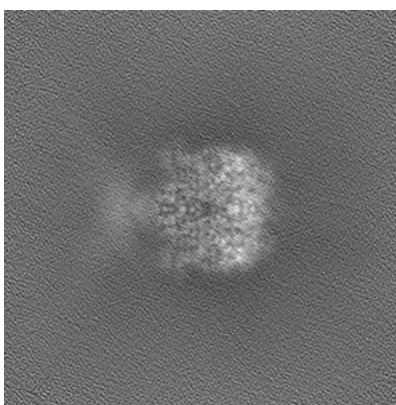


Z

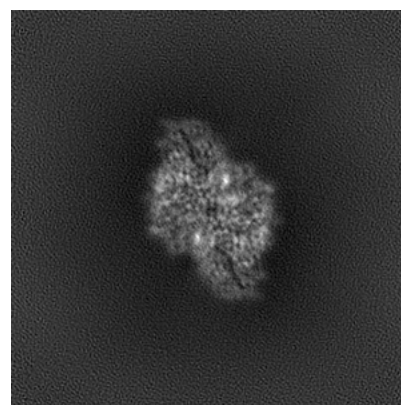
6.1.2 Raw map



X



Y

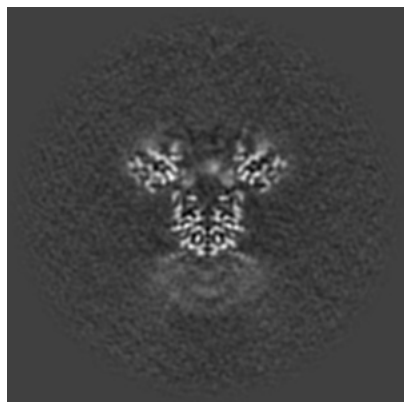


Z

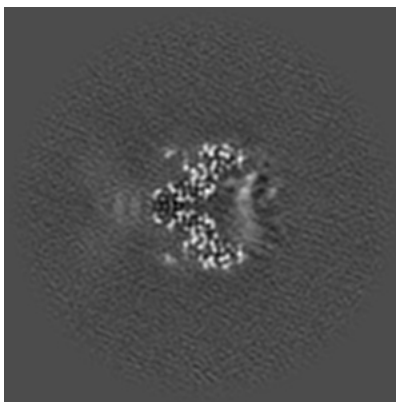
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

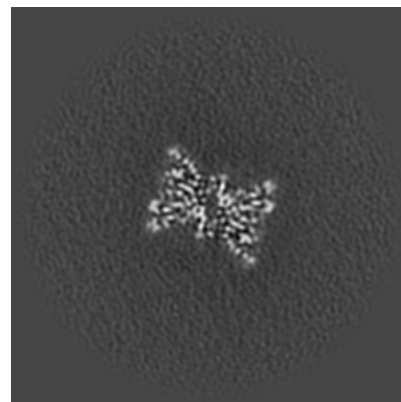
6.2.1 Primary map



X Index: 132

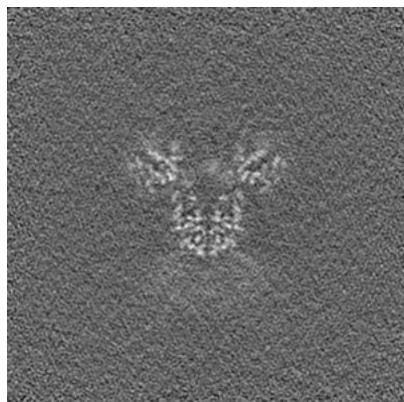


Y Index: 132

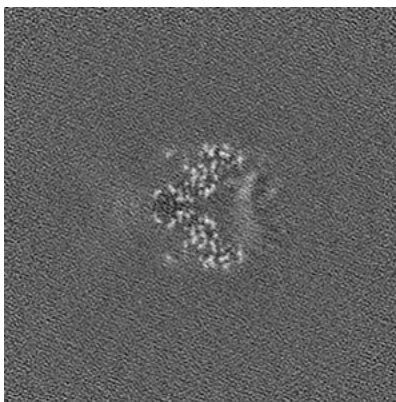


Z Index: 132

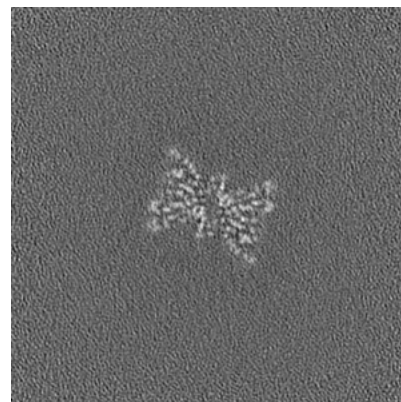
6.2.2 Raw map



X Index: 132



Y Index: 132

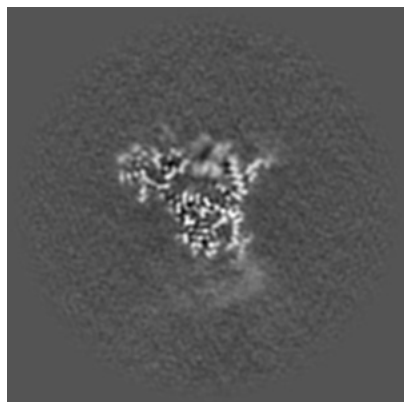


Z Index: 132

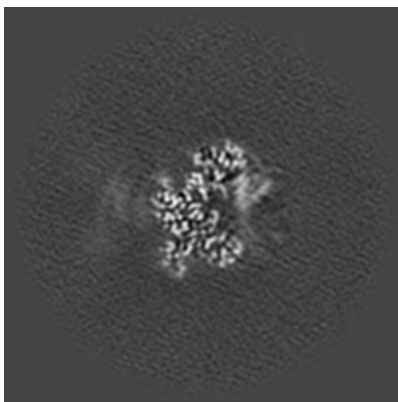
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

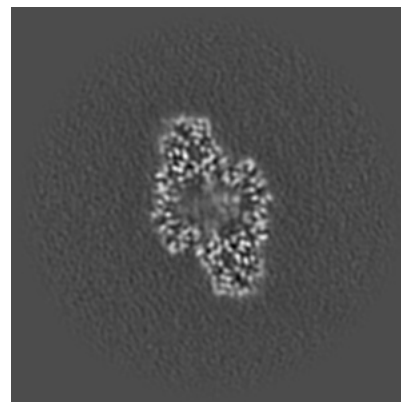
6.3.1 Primary map



X Index: 141

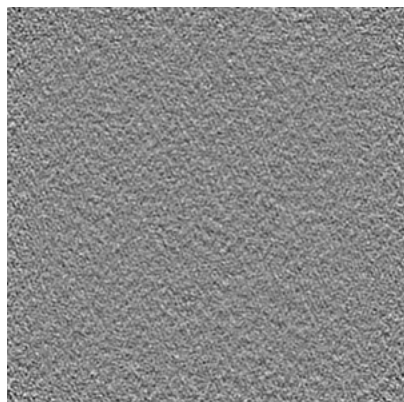


Y Index: 138

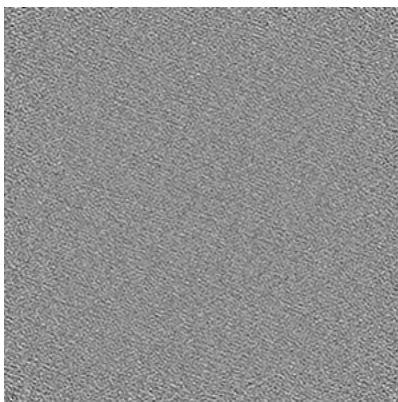


Z Index: 153

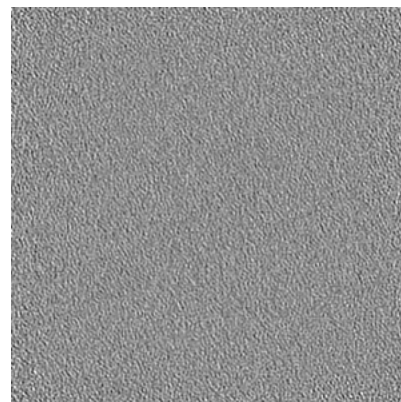
6.3.2 Raw map



X Index: 0



Y Index: 0

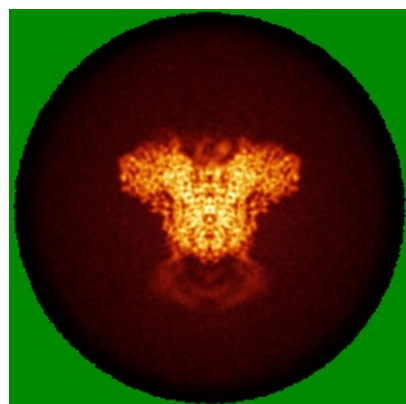


Z Index: 0

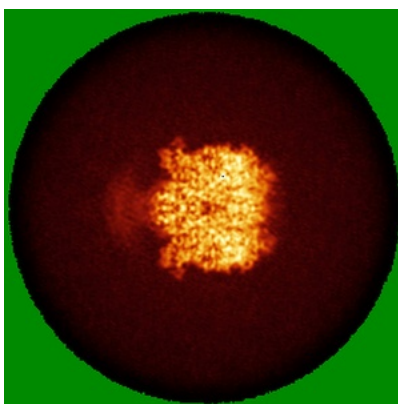
The images above show the largest variance slices of the map in three orthogonal directions.

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

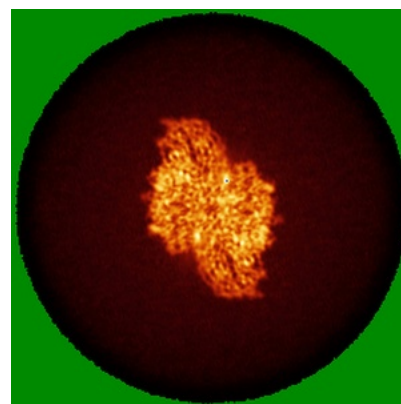
6.4.1 Primary map



X

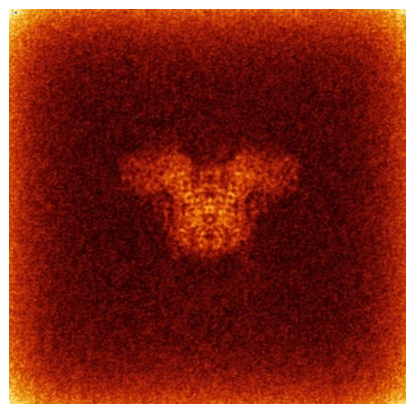


Y

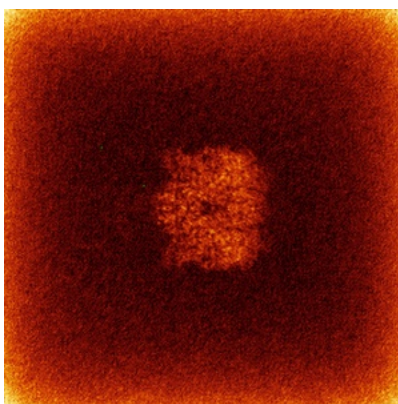


Z

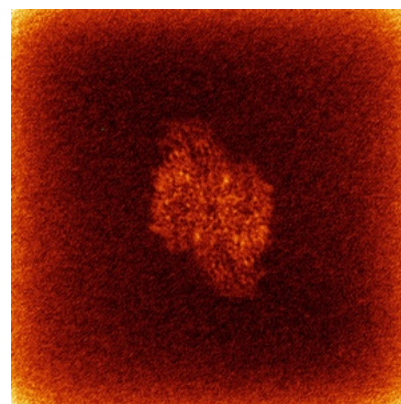
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

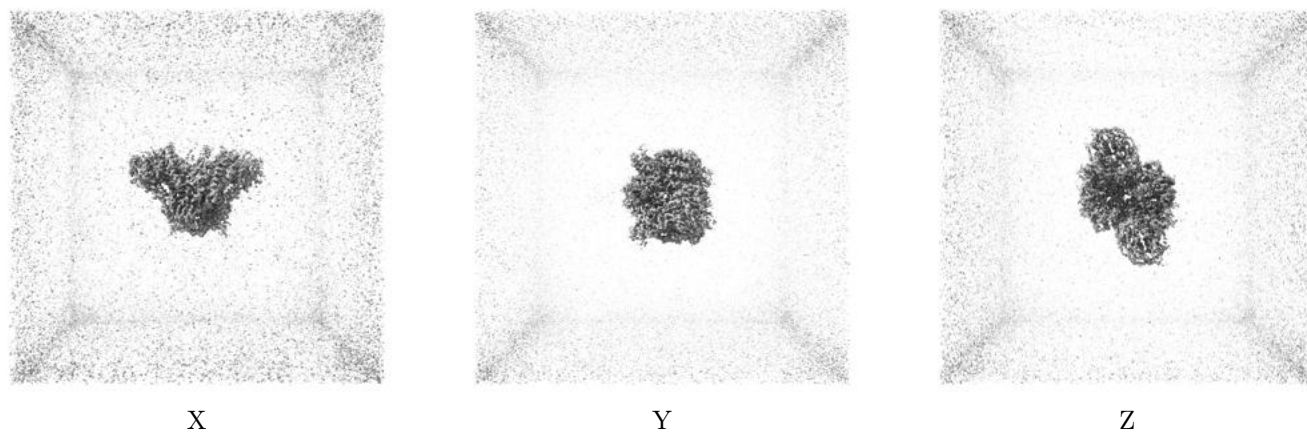
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

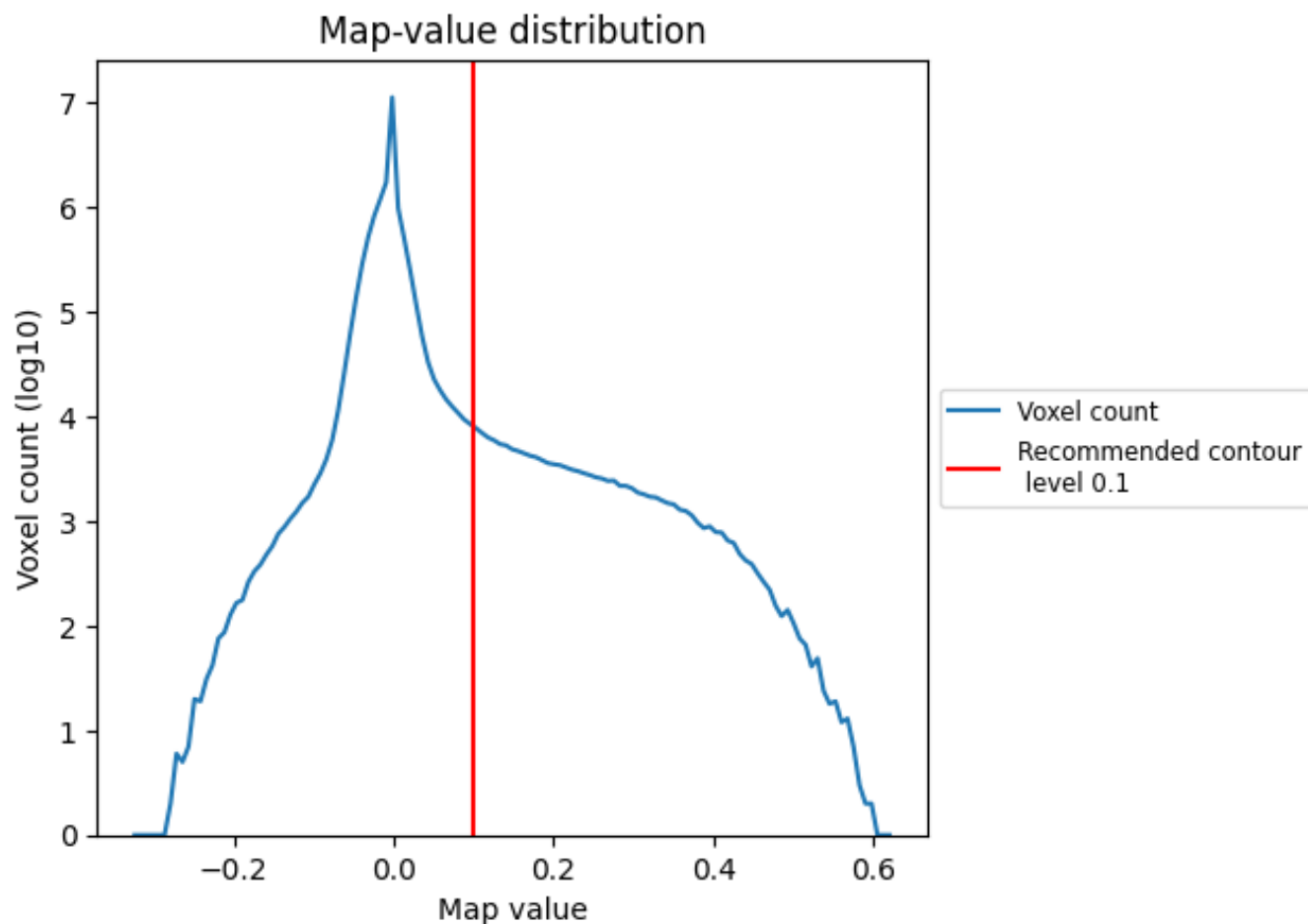
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

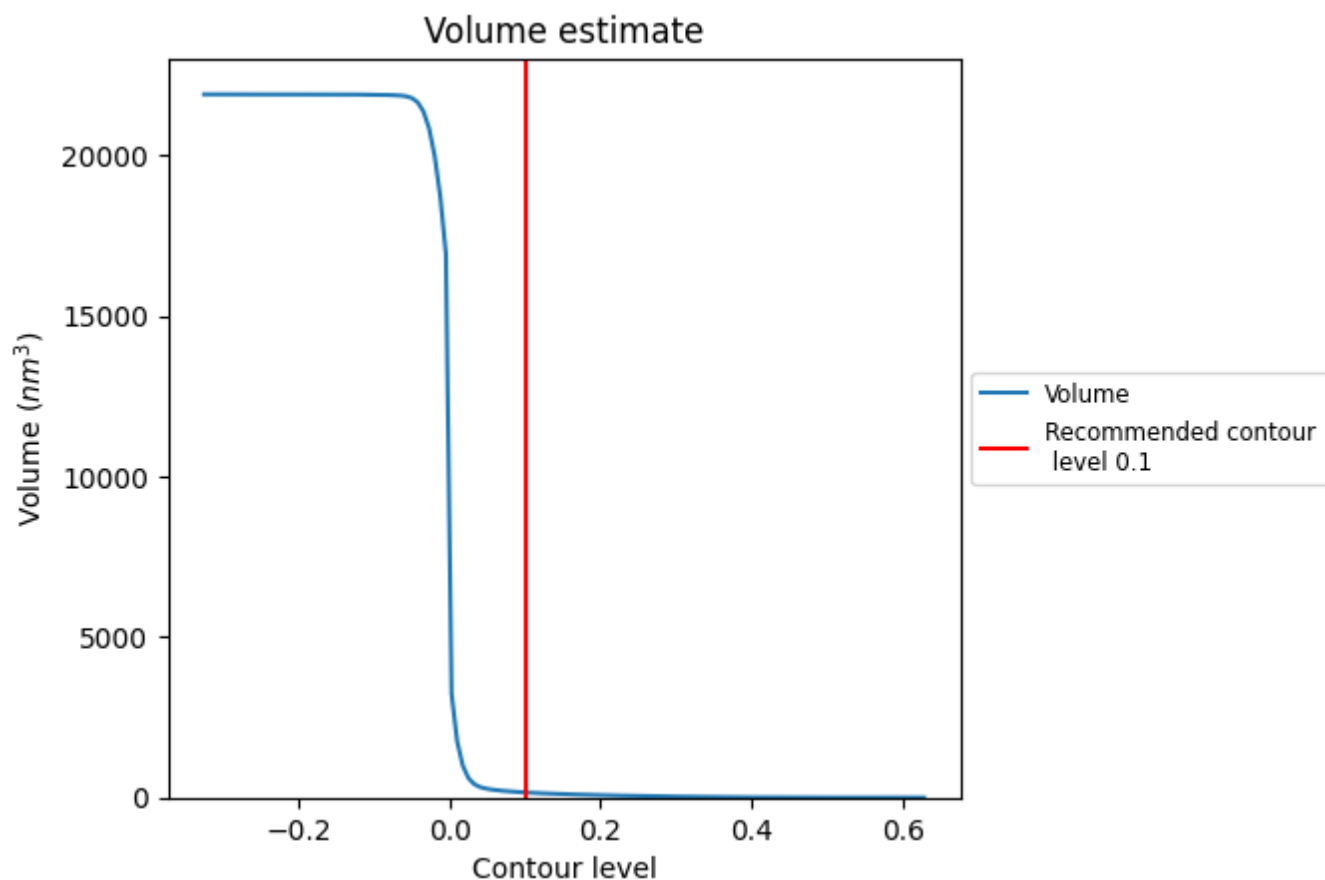
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

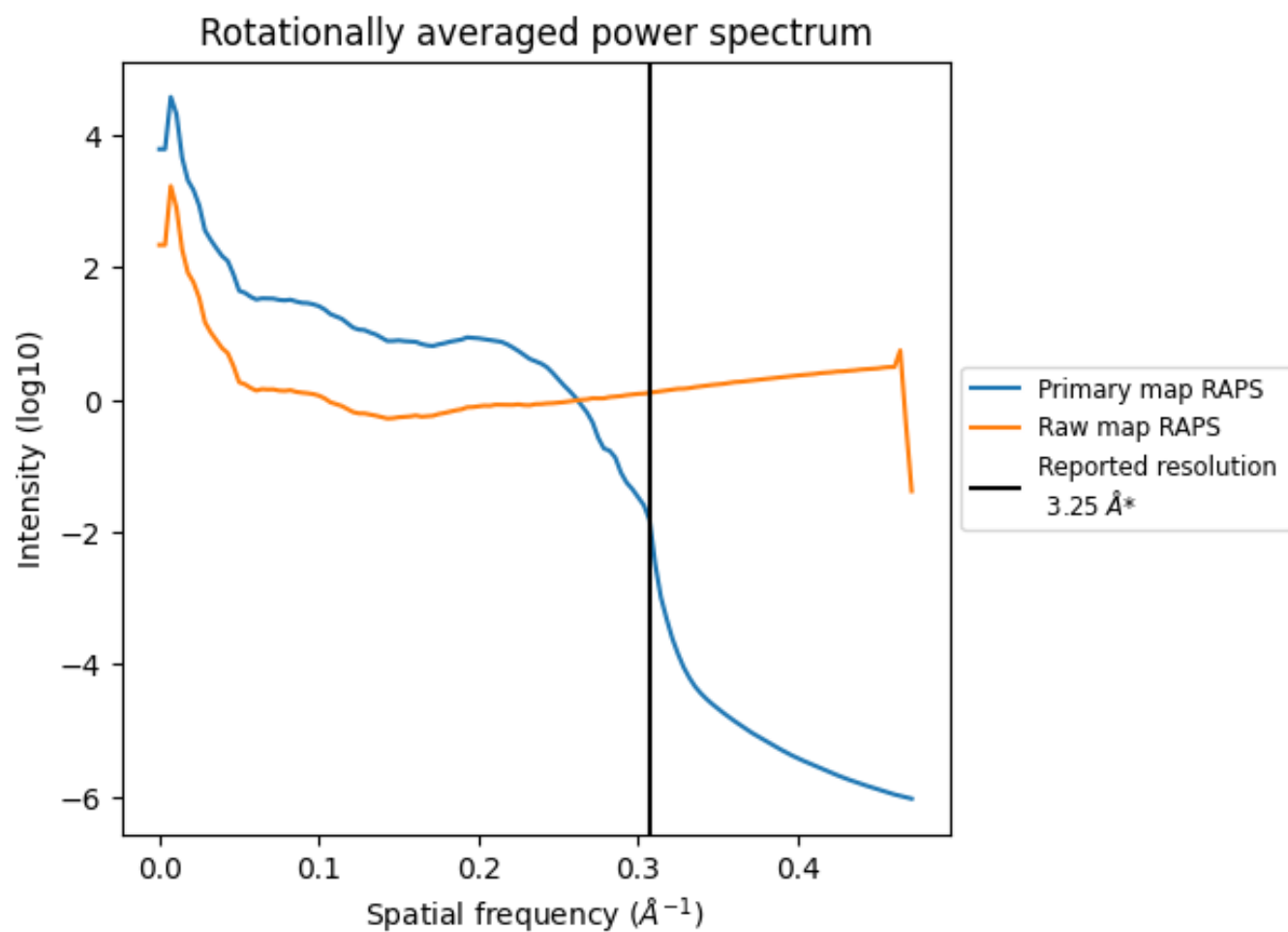
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 159 nm³; this corresponds to an approximate mass of 144 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 ⓘ

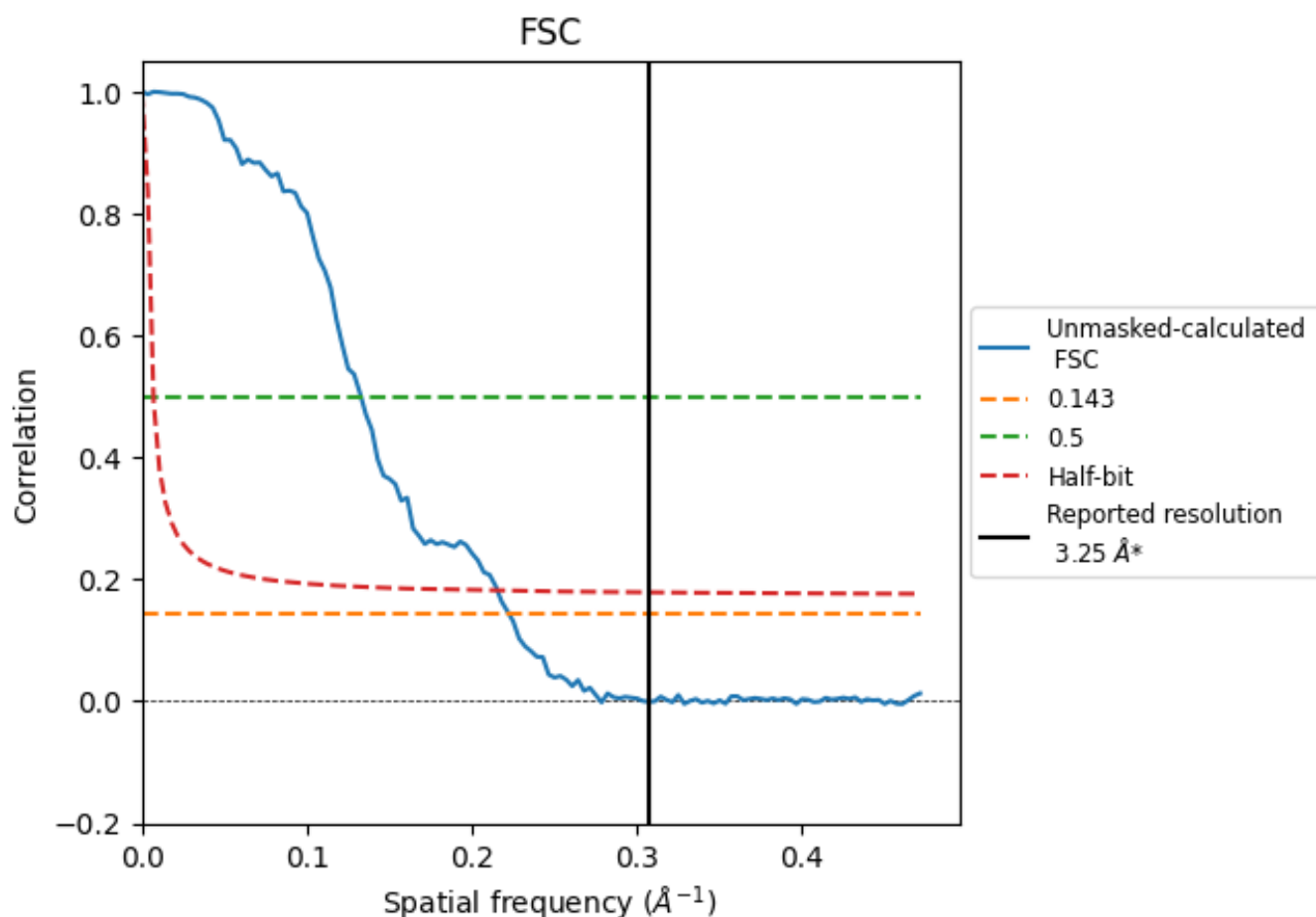


*Reported resolution corresponds to spatial frequency of 0.308 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.308 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

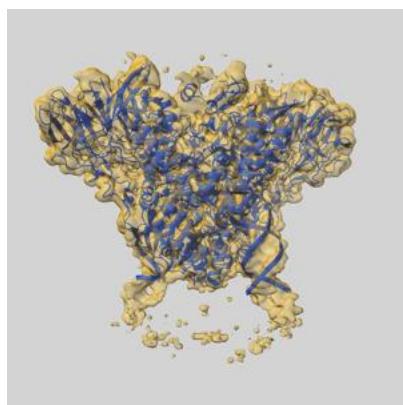
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.25	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.49	7.54	4.64

*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 4.49 differs from the reported value 3.25 by more than 10 %

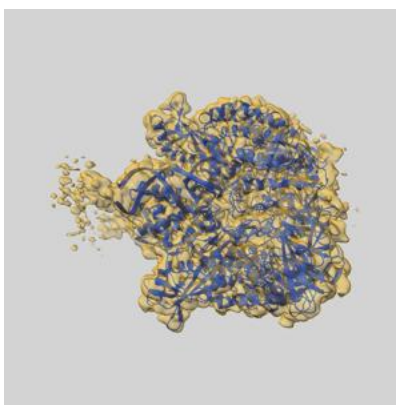
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61715 and PDB model 9JPU. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

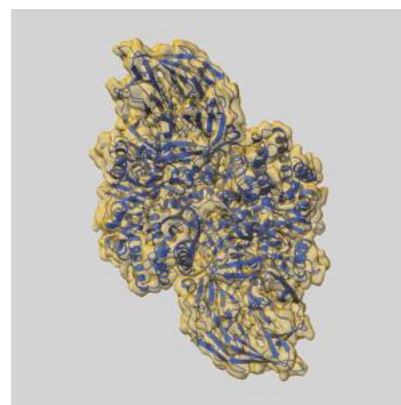
9.1 Map-model overlay [i](#)



X



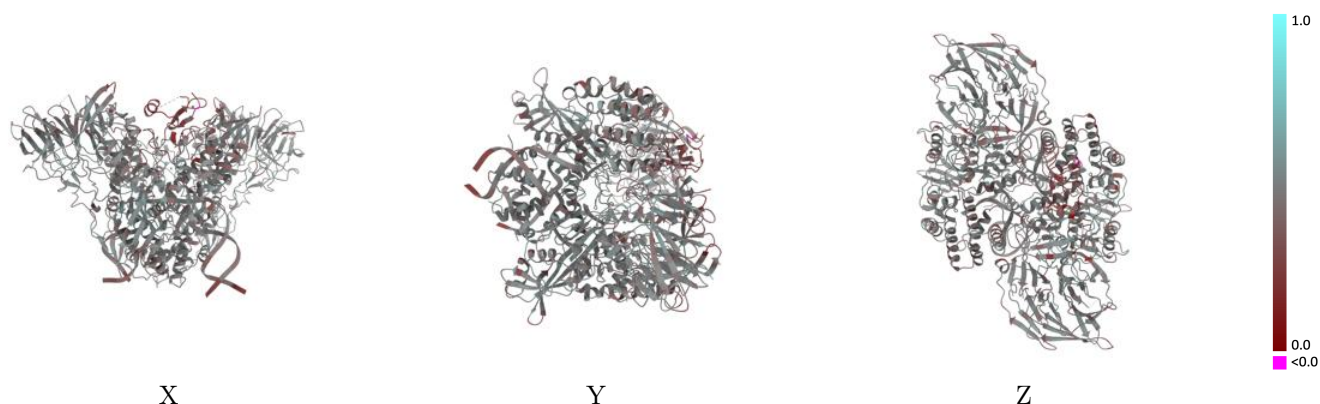
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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](#)

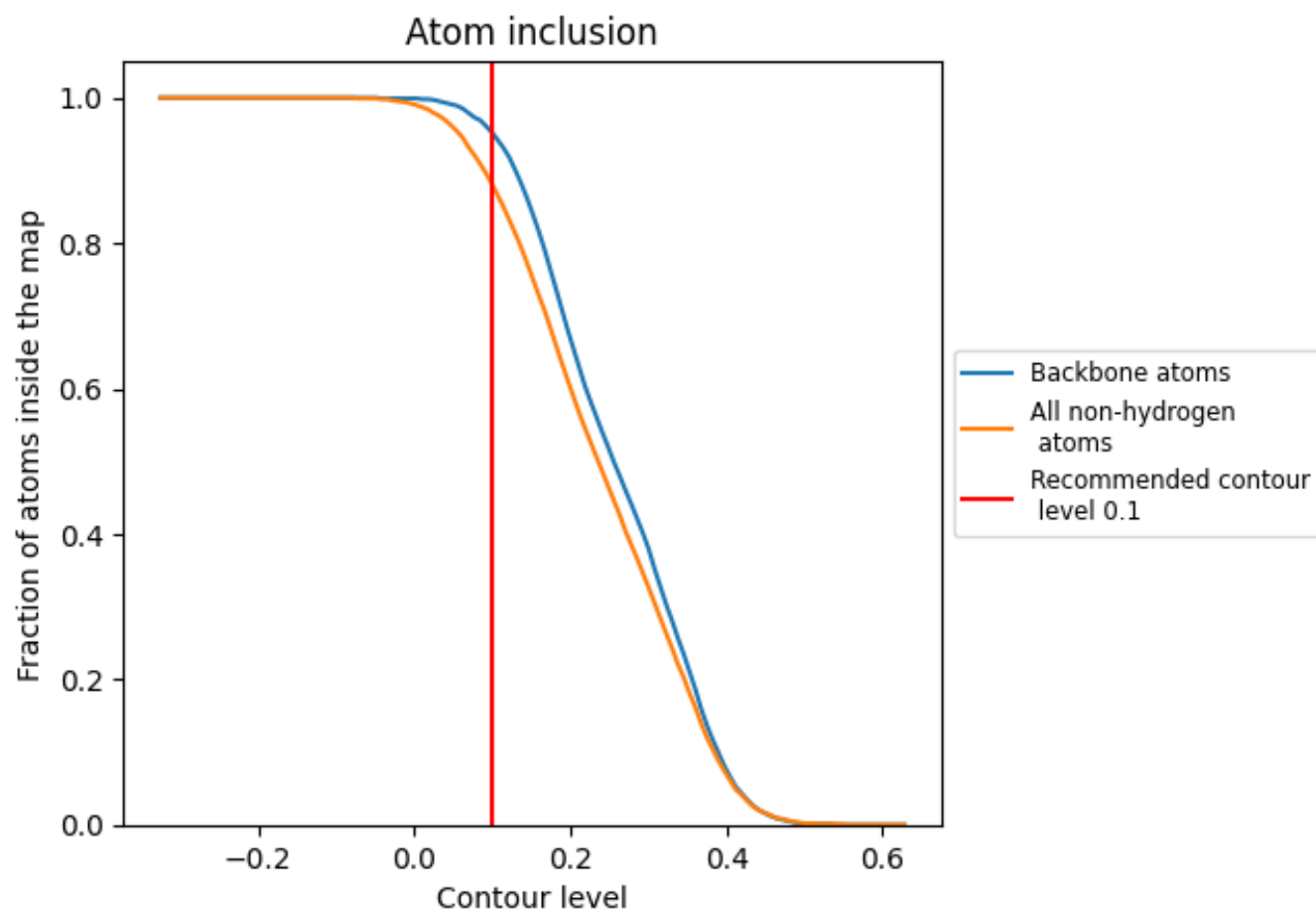


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 88% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8810	0.4600
A	0.8850	0.4700
B	0.8810	0.4660
C	0.8870	0.4720
D	0.8760	0.4670
E	0.7670	0.2810
F	0.9520	0.4300
G	0.9440	0.4480
L	0.9640	0.4290
M	0.9580	0.4210

