



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:11 AM UTC

PDB ID : 8Z99 / pdb_00008z99
EMDB ID : EMD-39857
Title : Cryo-EM structure of NTR-bound type VII CRISPR-Cas complex at substrate-engaged state +I
Authors : Zhang, H.; Deng, Z.; Li, X.
Deposited on : 2024-04-22
Resolution : 3.20 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:

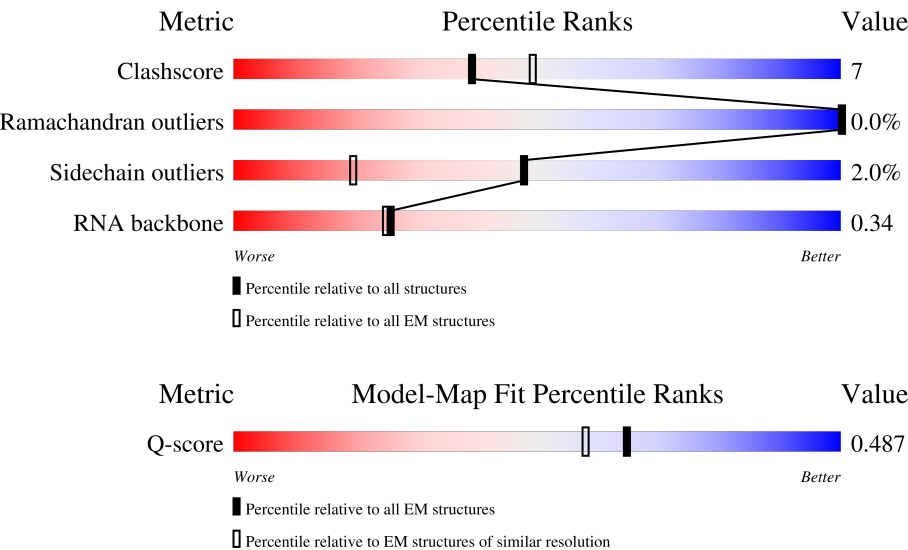
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	200	
1	B	200	
1	C	200	

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Mol	Chain	Length	Quality of chain
1	D	200	
1	E	200	
1	F	200	
1	J	200	
1	P	200	
2	G	240	
3	H	609	
3	I	609	
3	K	609	
3	L	609	
4	M	60	
5	N	60	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 25517 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 a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	163	Total	C	N	O	S	0	0
			1232	774	219	231	8		
1	B	199	Total	C	N	O	S	0	0
			1539	959	276	296	8		
1	C	199	Total	C	N	O	S	0	0
			1539	960	277	294	8		
1	D	199	Total	C	N	O	S	0	0
			1547	965	278	296	8		
1	E	199	Total	C	N	O	S	0	0
			1537	960	277	292	8		
1	F	194	Total	C	N	O	S	0	0
			1492	929	267	288	8		
1	J	199	Total	C	N	O	S	0	0
			1541	962	275	296	8		
1	P	194	Total	C	N	O	S	0	0
			1437	896	256	277	8		

- Molecule 2 is a protein called a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	210	Total	C	N	O	S	0	0
			1364	852	243	264	5		

- Molecule 3 is a protein called a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	582	Total	C	N	O	S	0	0
			4649	2962	784	886	17		
3	I	160	Total	C	N	O	S	0	0
			1341	859	225	250	7		
3	K	372	Total	C	N	O	S	0	0
			2859	1838	476	535	10		
3	L	160	Total	C	N	O	S	0	0
			1315	847	228	234	6		

- Molecule 4 is a RNA chain called RNA (54-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	54	Total	C	N	O	P	0	0
			1130	505	187	384	54		

- Molecule 5 is a RNA chain called RNA (49-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	46	Total	C	N	O	P	0	0
			986	442	188	310	46		

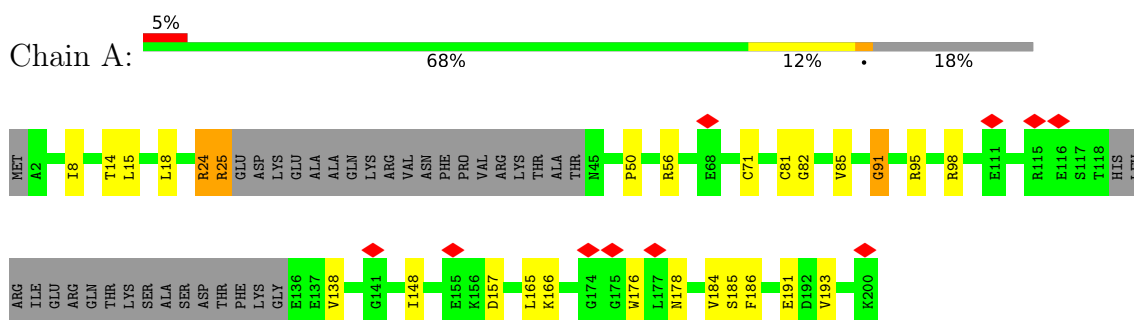
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Zn	0
			1	1	
6	B	1	Total	Zn	0
			1	1	
6	C	1	Total	Zn	0
			1	1	
6	D	1	Total	Zn	0
			1	1	
6	E	1	Total	Zn	0
			1	1	
6	F	1	Total	Zn	0
			1	1	
6	H	1	Total	Zn	0
			1	1	
6	J	1	Total	Zn	0
			1	1	
6	P	1	Total	Zn	0
			1	1	

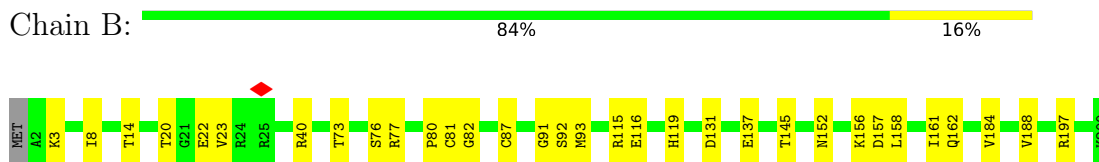
3 Residue-property plots [i](#)

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

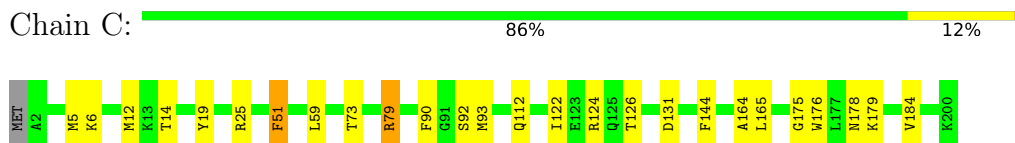
- Molecule 1: a protein



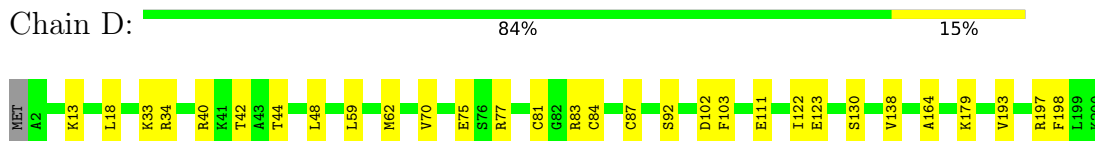
- Molecule 1: a protein



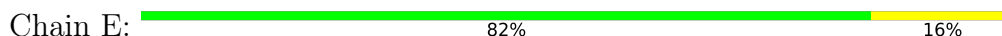
- Molecule 1: a protein



- Molecule 1: a protein



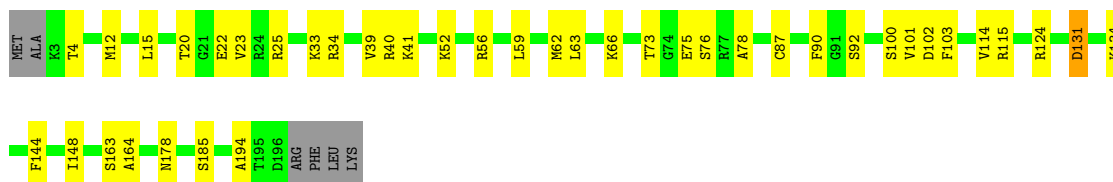
- Molecule 1: a protein





- Molecule 1: a protein

Chain F: 76% 20%



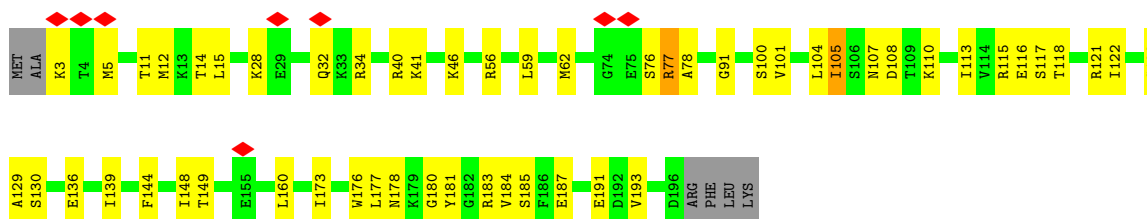
- Molecule 1: a protein

Chain J: 90% 10%



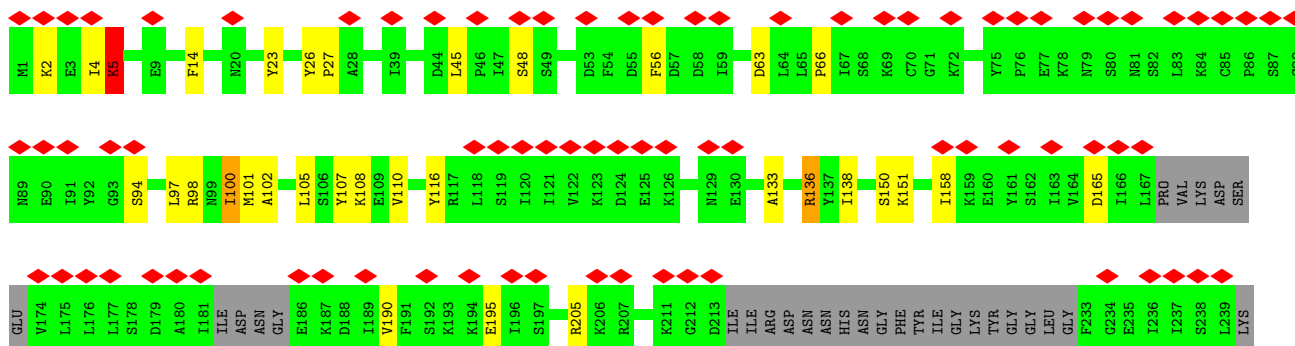
- Molecule 1: a protein

Chain P: 70% 26%



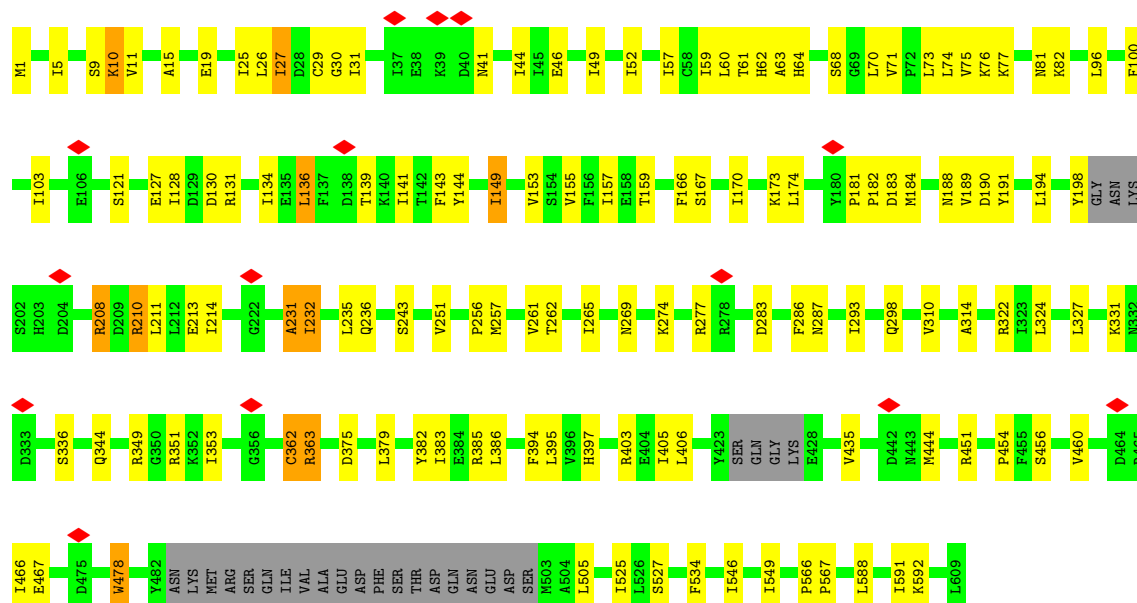
- Molecule 2: a protein

Chain G: 34% 74% 12% 12%

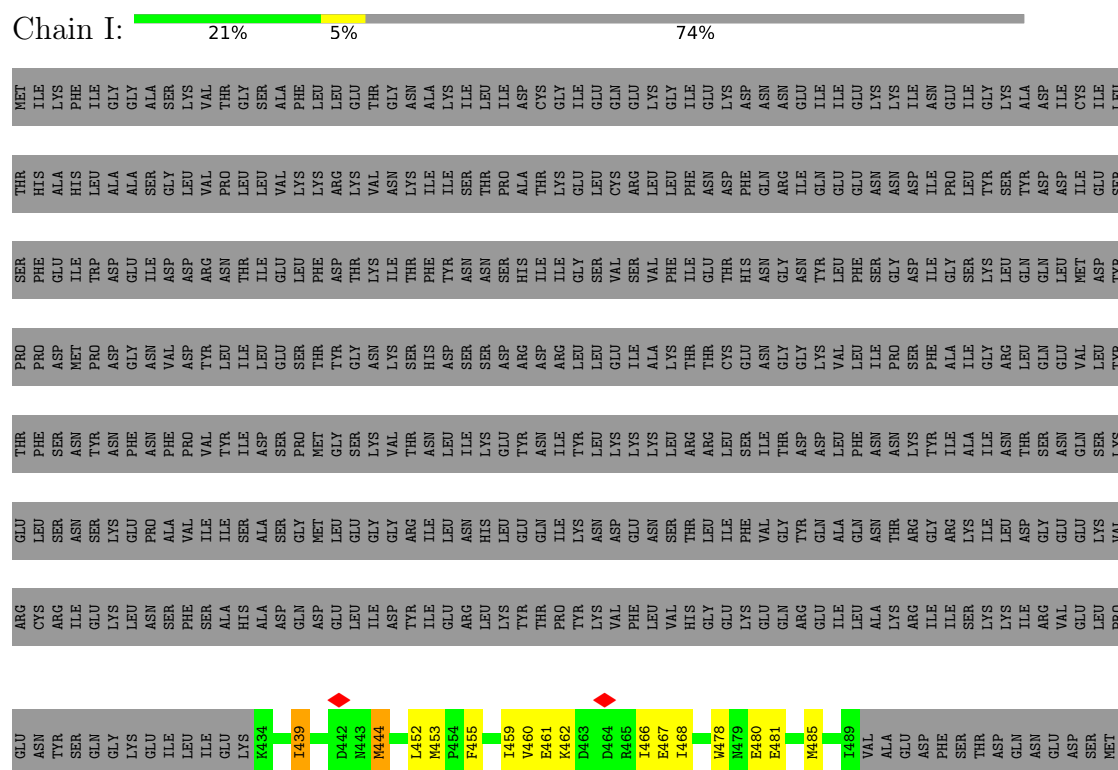


- Molecule 3: a protein

Chain H: 73% 21%

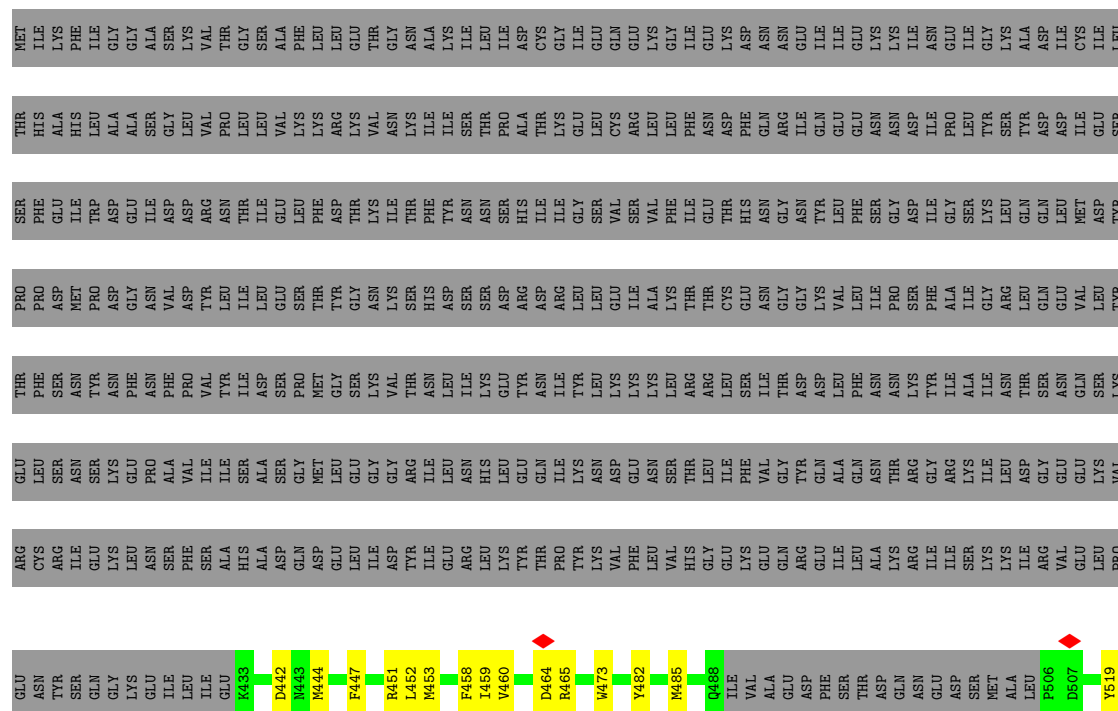


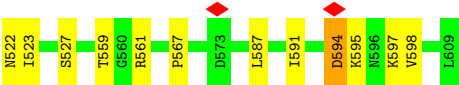
- Molecule 3: a protein



- Molecule 3: a protein



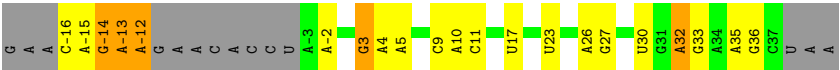




• Molecule 4: RNA (54-MER)



• Molecule 5: RNA (49-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.282	Depositor
Minimum map value	-0.653	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.14	Depositor
Map size ($\text{\AA}$)	285.0, 285.0, 285.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.95, 0.95, 0.95	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	0.57	0/1245	0.87	1/1669 (0.1%)
1	B	0.47	2/1558 (0.1%)	0.70	1/2091 (0.0%)
1	C	0.47	0/1558	0.74	0/2090
1	D	0.49	3/1566 (0.2%)	0.76	0/2099
1	E	0.40	0/1556	0.71	1/2087 (0.0%)
1	F	0.54	3/1510 (0.2%)	0.81	0/2027
1	J	0.44	0/1560	0.70	0/2092
1	P	0.62	3/1455 (0.2%)	0.90	3/1962 (0.2%)
2	G	0.65	4/1383 (0.3%)	0.88	7/1876 (0.4%)
3	H	0.55	2/4732 (0.0%)	0.82	1/6389 (0.0%)
3	I	0.60	4/1372 (0.3%)	0.84	2/1852 (0.1%)
3	K	0.51	1/2907 (0.0%)	0.81	0/3937
3	L	0.68	4/1346 (0.3%)	0.96	3/1818 (0.2%)
4	M	0.44	0/1259	0.61	0/1957
5	N	0.34	0/1104	0.49	0/1716
All	All	0.53	26/26111 (0.1%)	0.79	19/35662 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
1	D	0	1
1	F	0	1
1	P	0	3
3	H	0	3
All	All	0	12

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	550	THR	C-N	9.00	1.45	1.33
3	L	465	ARG	C-N	8.74	1.43	1.33
3	L	464	ASP	C-N	8.56	1.45	1.33
1	P	76	SER	C-N	-8.33	1.23	1.33
3	L	594	ASP	C-N	7.64	1.43	1.33
2	G	4	ILE	C-N	7.34	1.43	1.33
2	G	101	MET	C-N	-7.12	1.24	1.33
1	B	161	ILE	C-N	-6.96	1.24	1.33
1	P	3	LYS	C-N	6.96	1.42	1.33
2	G	100	ILE	C-N	-6.88	1.23	1.33
3	I	480	GLU	C-N	-6.79	1.24	1.33
1	B	162	GLN	C-N	6.57	1.42	1.33
1	F	25	ARG	C-N	-6.51	1.25	1.33
1	P	107	ASN	C-N	6.45	1.42	1.33
3	I	551	GLN	C-N	-6.44	1.26	1.33
3	I	481	GLU	C-N	6.43	1.42	1.33
3	H	183	ASP	C-N	-6.09	1.26	1.33
1	F	33	LYS	C-N	5.74	1.41	1.33
3	H	231	ALA	C-N	-5.74	1.27	1.33
2	G	98	ARG	C-N	5.69	1.41	1.33
1	F	34	ARG	C-N	-5.58	1.25	1.33
1	D	75	GLU	C-N	-5.49	1.26	1.33
3	L	595	LYS	C-N	-5.37	1.26	1.34
1	D	33	LYS	C-N	5.31	1.41	1.33
1	D	34	ARG	C-N	-5.22	1.26	1.33
3	K	75	VAL	C-N	-5.09	1.27	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	550	THR	O-C-N	6.96	129.50	122.12
1	A	91	GLY	N-CA-C	6.89	120.26	111.37
2	G	56	PHE	O-C-N	-5.77	117.74	123.62
2	G	136	ARG	N-CA-C	-5.74	105.17	111.82
3	L	464	ASP	O-C-N	5.57	129.48	122.23
1	P	77	ARG	CA-C-N	5.53	131.11	123.04
1	P	77	ARG	C-N-CA	5.53	131.11	123.04
1	B	161	ILE	O-C-N	-5.47	116.22	121.90
3	L	442	ASP	N-CA-C	-5.45	103.50	110.53
2	G	4	ILE	O-C-N	5.31	128.50	123.03
1	P	78	ALA	CB-CA-C	-5.29	110.04	117.23
2	G	101	MET	CA-C-N	5.25	131.31	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	101	MET	C-N-CA	5.25	131.31	123.23
3	L	594	ASP	O-C-N	5.24	129.39	122.36
2	G	5	LYS	CA-C-N	-5.23	115.93	121.48
2	G	5	LYS	C-N-CA	-5.23	115.93	121.48
3	I	480	GLU	O-C-N	-5.13	116.78	122.07
3	H	269	ASN	CA-CB-CG	5.08	117.68	112.60
1	E	149	THR	CA-CB-CG2	5.07	119.13	110.50

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	24	ARG	Sidechain
1	A	56	ARG	Sidechain
1	B	197	ARG	Sidechain
1	C	79	ARG	Sidechain
1	D	77	ARG	Sidechain
1	F	115	ARG	Sidechain
3	H	131	ARG	Sidechain
3	H	208	ARG	Sidechain
3	H	210	ARG	Sidechain
1	P	115	ARG	Sidechain
1	P	40	ARG	Sidechain
1	P	77	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1232	0	1249	19	0
1	B	1539	0	1564	17	0
1	C	1539	0	1571	20	0
1	D	1547	0	1586	15	0
1	E	1537	0	1571	25	0
1	F	1492	0	1516	33	0
1	J	1541	0	1575	15	0
1	P	1437	0	1417	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1364	0	1093	20	0
3	H	4649	0	4585	99	0
3	I	1341	0	1293	24	0
3	K	2859	0	2682	43	0
3	L	1315	0	1269	18	0
4	M	1130	0	572	27	0
5	N	986	0	502	26	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
6	J	1	0	0	0	0
6	P	1	0	0	0	0
All	All	25517	0	24045	355	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 (355) 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)
1:F:23:VAL:HG12	1:P:117:SER:HB2	1.50	0.93
3:K:61:THR:HA	3:K:67:ALA:HB3	1.60	0.82
3:K:156:PHE:HE1	3:K:163:ASN:HB3	1.46	0.80
1:A:71:CYS:SG	1:A:81:CYS:HB3	2.25	0.77
3:I:452:LEU:HD22	3:L:458:PHE:HB3	1.67	0.76
3:K:65:LEU:HD13	3:K:96:LEU:HG	1.70	0.74
3:H:29:CYS:HB3	3:H:70:LEU:HB2	1.68	0.73
3:K:75:VAL:HG21	3:K:121:SER:HA	1.69	0.73
3:H:174:LEU:HB3	3:H:208:ARG:HE	1.55	0.72
3:K:595:LYS:HE2	3:L:485:MET:HE2	1.74	0.70
3:K:60:LEU:HA	3:K:153:VAL:HG22	1.75	0.69
3:H:100:PHE:HD1	5:N:-14:G:N2	1.92	0.68
3:H:100:PHE:HD1	5:N:-14:G:H22	1.41	0.68
3:H:314:ALA:HB1	5:N:-13:A:H5'	1.76	0.68
3:H:60:LEU:HD11	3:H:71:VAL:HG21	1.74	0.68
2:G:195:GLU:HA	4:M:-9:G:H5'	1.76	0.66
3:I:526:LEU:HD21	3:I:587:LEU:HD11	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:CYS:HB2	1:D:83:ARG:HH21	1.62	0.65
1:F:56:ARG:HE	1:F:73:THR:HG21	1.62	0.65
1:A:176:TRP:HE1	4:M:45:C:H41	1.44	0.65
3:K:444:MET:HE2	3:K:451:ARG:HG3	1.79	0.65
1:A:14:THR:HA	1:A:184:VAL:HG12	1.78	0.65
1:P:12:MET:HB3	1:P:144:PHE:HB2	1.78	0.64
1:D:42:THR:HG22	1:D:44:THR:H	1.62	0.64
3:K:90:LYS:HE3	3:K:125:TRP:HB2	1.79	0.63
3:H:26:LEU:HD11	3:H:52:ILE:HG21	1.79	0.63
3:I:459:ILE:HG22	3:I:468:ILE:HG13	1.80	0.63
3:K:159:THR:HB	3:K:162:GLY:O	1.99	0.63
3:H:103:ILE:HD12	5:N:-13:A:C2	2.34	0.62
3:H:194:LEU:HD22	3:H:383:ILE:HD11	1.81	0.62
1:A:95:ARG:HG3	1:C:126:THR:HB	1.82	0.61
3:H:236:GLN:HG2	3:H:265:ILE:HG13	1.81	0.61
3:I:453:MET:HE3	3:L:459:ILE:HD12	1.82	0.61
1:C:51:PHE:HZ	1:C:165:LEU:HD21	1.65	0.61
2:G:133:ALA:O	2:G:136:ARG:HG3	2.00	0.60
3:H:96:LEU:HD23	3:H:257:MET:HE1	1.82	0.60
3:H:251:VAL:HG23	3:H:310:VAL:HB	1.82	0.60
3:H:324:LEU:HD12	5:N:-12:A:N6	2.16	0.60
1:P:41:LYS:HD2	1:P:110:LYS:HD2	1.83	0.60
1:F:56:ARG:NE	1:F:73:THR:HG21	2.17	0.60
2:G:100:ILE:HD11	2:G:107:TYR:CE1	2.37	0.60
3:H:460:VAL:HB	3:H:467:GLU:HG3	1.84	0.60
3:I:461:GLU:HA	3:I:466:ILE:HA	1.84	0.59
3:K:156:PHE:CE1	3:K:163:ASN:HB3	2.35	0.59
1:D:122:ILE:HD13	4:M:23:U:H2'	1.83	0.59
1:P:100:SER:HB3	1:P:149:THR:HB	1.83	0.59
1:P:28:LYS:O	1:P:32:GLN:HB2	2.03	0.59
1:P:14:THR:HA	1:P:184:VAL:HG12	1.85	0.59
3:H:41:ASN:HA	3:H:44:ILE:HD12	1.84	0.58
3:H:395:LEU:HD12	3:H:403:ARG:HG3	1.85	0.58
2:G:23:TYR:CE2	2:G:108:LYS:HE2	2.38	0.58
1:P:5:MET:HB2	1:P:193:VAL:HB	1.86	0.58
1:C:14:THR:HA	1:C:184:VAL:HG12	1.86	0.58
3:L:523:ILE:HG13	3:L:567:PRO:HB3	1.86	0.57
3:H:81:ASN:ND2	1:J:111:GLU:OE1	2.38	0.57
3:H:395:LEU:HD11	3:H:406:LEU:HD23	1.86	0.57
3:H:527:SER:OG	5:N:5:A:OP1	2.23	0.57
5:N:-14:G:H2'	5:N:-14:G:N3	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:10:LYS:NZ	3:H:198:TYR:OH	2.36	0.56
3:H:49:ILE:HA	3:H:52:ILE:HD12	1.88	0.56
1:P:12:MET:HE2	1:P:104:LEU:HD13	1.87	0.56
3:H:324:LEU:HD12	5:N:-12:A:H62	1.70	0.56
1:C:178:ASN:ND2	4:M:33:U:OP1	2.33	0.56
3:K:527:SER:OG	5:N:17:U:OP1	2.24	0.56
1:B:22:GLU:OE2	1:B:23:VAL:N	2.39	0.55
3:H:322:ARG:HD3	5:N:-12:A:N3	2.21	0.55
3:K:437:LEU:HD22	3:K:465:ARG:HE	1.71	0.55
3:H:9:SER:HB3	3:H:11:VAL:HG22	1.88	0.55
3:H:62:HIS:HB2	3:H:149:ILE:HD11	1.88	0.55
1:B:80:PRO:HD2	1:B:93:MET:HG2	1.88	0.55
3:I:460:VAL:HG12	3:L:452:LEU:HB3	1.87	0.55
1:J:131:ASP:OD1	4:M:28:G:N2	2.40	0.55
3:K:386:LEU:HD23	3:K:390:PRO:HD3	1.89	0.55
1:C:51:PHE:CZ	1:C:165:LEU:HD21	2.42	0.55
1:F:12:MET:HG3	1:F:144:PHE:HB2	1.88	0.55
3:I:444:MET:SD	3:I:444:MET:N	2.80	0.55
4:M:5:U:H2'	1:P:122:ILE:HD13	1.89	0.55
1:F:23:VAL:HG13	1:P:118:THR:O	2.06	0.55
1:F:59:LEU:HD12	1:F:90:PHE:HE1	1.70	0.55
3:K:503:MET:HE3	3:K:592:LYS:HE3	1.88	0.55
1:E:12:MET:HE1	1:E:49:ILE:HD12	1.89	0.54
3:H:149:ILE:HD12	3:H:232:ILE:HD11	1.89	0.54
3:H:397:HIS:O	3:H:403:ARG:NH1	2.40	0.54
1:D:198:PHE:HD1	1:E:166:LYS:HE2	1.72	0.54
3:K:90:LYS:HD2	3:K:125:TRP:HE3	1.71	0.54
3:K:484:LYS:O	3:K:488:GLN:HG2	2.08	0.54
5:N:32:A:N1	1:P:118:THR:HB	2.23	0.54
1:F:75:GLU:HB3	1:F:78:ALA:HB2	1.88	0.54
3:I:452:LEU:HD21	3:L:473:TRP:CH2	2.42	0.54
3:K:97:PHE:HB3	3:K:118:ILE:HD12	1.89	0.54
5:N:-14:G:H1'	5:N:-13:A:N7	2.23	0.54
1:P:101:VAL:HG13	1:P:148:ILE:HD12	1.88	0.54
1:E:199:LEU:HD13	1:F:62:MET:HE3	1.91	0.53
1:A:81:CYS:SG	1:A:82:GLY:N	2.82	0.53
1:F:59:LEU:HD12	1:F:90:PHE:CE1	2.43	0.53
3:H:194:LEU:HD11	3:H:379:LEU:HD22	1.90	0.53
3:H:100:PHE:HA	5:N:-14:G:H21	1.73	0.53
3:K:62:HIS:CB	3:K:146:ASN:HD21	2.22	0.53
1:B:76:SER:OG	1:B:77:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:THR:OG1	1:C:124:ARG:NH2	2.41	0.53
2:G:2:LYS:HA	2:G:165:ASP:HA	1.91	0.52
3:H:143:PHE:HB3	3:H:153:VAL:HG11	1.91	0.52
3:I:525:ILE:HD11	3:I:567:PRO:HG3	1.92	0.52
1:J:52:LYS:NZ	4:M:22:U:OP1	2.42	0.52
3:H:454:PRO:HG3	3:L:452:LEU:HD11	1.91	0.52
3:H:64:HIS:HD2	3:H:232:ILE:HD13	1.75	0.52
3:I:459:ILE:HG12	3:L:453:MET:HE2	1.92	0.52
1:P:176:TRP:HB2	1:P:181:TYR:HB2	1.90	0.52
1:F:20:THR:H	1:F:39:VAL:HG23	1.74	0.52
1:F:52:LYS:NZ	4:M:4:C:OP1	2.35	0.52
5:N:-14:G:H1'	5:N:-13:A:C8	2.45	0.52
1:D:193:VAL:HB	1:D:197:ARG:HD2	1.91	0.51
1:E:49:ILE:HB	1:E:104:LEU:HB2	1.91	0.51
3:H:63:ALA:H	3:H:149:ILE:HD11	1.75	0.51
3:H:188:ASN:ND2	3:H:190:ASP:OD1	2.43	0.51
3:H:525:ILE:HD11	3:H:567:PRO:HG3	1.93	0.51
1:P:177:LEU:O	1:P:183:ARG:NH2	2.43	0.51
1:F:23:VAL:CG1	1:P:117:SER:HB2	2.33	0.51
1:C:92:SER:OG	1:C:93:MET:N	2.44	0.51
3:H:128:ILE:HD13	3:H:134:ILE:HD13	1.93	0.51
1:P:15:LEU:HD11	1:P:185:SER:HB3	1.93	0.51
3:H:5:ILE:HB	3:H:15:ALA:HB3	1.92	0.51
4:M:9:G:O2'	4:M:10:C:H5'	2.11	0.50
3:H:100:PHE:HA	5:N:-14:G:N2	2.26	0.50
3:H:344:GLN:O	3:H:351:ARG:NH1	2.45	0.50
1:J:10:VAL:HG12	1:J:188:VAL:HG12	1.93	0.50
1:D:18:LEU:HB3	1:D:138:VAL:HB	1.93	0.50
3:H:198:TYR:HB3	5:N:-16:C:C2	2.47	0.50
1:A:50:PRO:HB2	4:M:41:A:H1'	1.92	0.50
1:C:25:ARG:NE	1:J:116:GLU:OE1	2.45	0.50
3:H:184:MET:SD	3:H:386:LEU:HD23	2.52	0.50
1:E:42:THR:HG1	1:E:46:LYS:H	1.60	0.50
1:P:11:THR:HB	1:P:187:GLU:HB2	1.93	0.50
3:H:588:LEU:HA	3:H:591:ILE:HD12	1.94	0.49
1:B:3:LYS:HD2	1:B:152:ASN:HA	1.93	0.49
3:I:460:VAL:HG23	3:I:467:GLU:HG2	1.93	0.49
3:K:94:ARG:HB3	3:K:122:PHE:CE2	2.48	0.49
1:B:87:CYS:HB3	1:B:92:SER:HB2	1.94	0.49
3:H:478:TRP:HA	3:H:478:TRP:CE3	2.47	0.49
1:B:131:ASP:OD2	1:B:131:ASP:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:139:THR:HG22	3:H:159:THR:HA	1.95	0.49
1:D:59:LEU:HG	1:D:164:ALA:HB2	1.94	0.49
3:H:59:ILE:HD13	3:H:155:VAL:HG11	1.94	0.49
1:A:91:GLY:HA3	4:M:39:U:H5''	1.94	0.49
1:A:191:GLU:HG2	1:A:193:VAL:HG23	1.95	0.49
3:H:274:LYS:HA	3:H:277:ARG:HG2	1.94	0.49
3:L:444:MET:SD	3:L:451:ARG:HB3	2.53	0.49
2:G:150:SER:OG	4:M:-4:A:OP2	2.30	0.48
3:K:505:LEU:HD13	3:K:592:LYS:HD3	1.95	0.48
3:I:439:ILE:HG12	3:I:455:PHE:CZ	2.48	0.48
1:D:123:GLU:HG3	1:D:130:SER:HB2	1.94	0.48
1:F:76:SER:HB2	1:P:130:SER:HB2	1.96	0.48
3:H:141:ILE:HG13	3:H:157:ILE:HG12	1.95	0.48
3:L:594:ASP:O	3:L:598:VAL:HG23	2.13	0.48
2:G:66:PRO:HA	2:G:116:TYR:HA	1.95	0.48
1:A:18:LEU:HB3	1:A:138:VAL:HB	1.95	0.48
2:G:26:TYR:HE2	2:G:63:ASP:HB3	1.78	0.48
3:K:145:ASN:OD1	3:K:145:ASN:N	2.46	0.48
4:M:1:C:H2'	4:M:2:U:C6	2.49	0.48
1:A:71:CYS:SG	1:A:81:CYS:CB	2.94	0.48
1:B:14:THR:HA	1:B:184:VAL:HG12	1.96	0.48
1:E:42:THR:HB	1:E:44:THR:H	1.79	0.48
1:J:20:THR:HG21	1:J:49:ILE:HG23	1.95	0.48
3:L:519:TYR:HA	3:L:522:ASN:HD21	1.77	0.48
1:A:98:ARG:NH1	1:A:157:ASP:OD2	2.36	0.48
3:H:130:ASP:OD1	3:H:144:TYR:HA	2.14	0.48
1:B:8:ILE:HG12	1:B:158:LEU:HD13	1.96	0.48
1:P:180:GLY:HA2	1:P:183:ARG:HH21	1.78	0.47
1:F:87:CYS:HB3	1:F:92:SER:HB3	1.96	0.47
3:K:379:LEU:HD23	3:K:379:LEU:HA	1.68	0.47
2:G:5:LYS:HE3	2:G:5:LYS:HB3	1.58	0.47
3:H:505:LEU:HB2	3:H:592:LYS:HE3	1.97	0.47
3:K:62:HIS:HB2	3:K:146:ASN:HD21	1.79	0.47
1:A:8:ILE:HG12	1:A:148:ILE:HB	1.97	0.47
3:H:336:SER:HB2	3:H:362:CYS:HB3	1.97	0.47
1:P:46:LYS:NZ	1:P:108:ASP:O	2.46	0.47
1:F:131:ASP:OD2	5:N:27:G:N2	2.48	0.47
4:M:-6:A:H3'	4:M:-5:A:H8	1.79	0.47
1:C:12:MET:HB3	1:C:144:PHE:HB2	1.98	0.46
3:I:478:TRP:CD1	3:K:471:LYS:HD2	2.50	0.46
3:K:65:LEU:HD12	3:K:68:SER:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:100:SER:HA	1:P:178:ASN:HA	1.98	0.46
3:H:27:ILE:HG13	3:H:166:PHE:CE2	2.50	0.46
4:M:12:G:H1'	4:M:13:G:C8	2.50	0.46
3:H:1:MET:HE3	3:H:19:GLU:HB2	1.98	0.46
2:G:151:LYS:HB2	2:G:151:LYS:HE3	1.68	0.46
1:P:116:GLU:HG2	1:P:136:GLU:OE1	2.15	0.46
1:E:123:GLU:HG3	1:E:130:SER:HB3	1.97	0.46
1:F:134:LYS:HE2	5:N:26:A:H2'	1.98	0.46
3:I:439:ILE:HG21	3:I:455:PHE:CE1	2.50	0.46
3:H:214:ILE:HD11	3:H:363:ARG:HD2	1.98	0.46
3:H:231:ALA:HA	3:H:235:LEU:HD12	1.97	0.46
3:H:435:VAL:HG22	3:H:466:ILE:HB	1.98	0.46
1:D:179:LYS:HA	1:J:52:LYS:HD2	1.98	0.46
3:H:103:ILE:HB	5:N:-14:G:N2	2.30	0.46
3:K:65:LEU:CD1	3:K:68:SER:HB2	2.45	0.46
3:K:93:CYS:HB2	3:K:122:PHE:HZ	1.81	0.46
3:K:114:SER:O	3:K:118:ILE:HG12	2.15	0.46
3:L:594:ASP:OD2	3:L:597:LYS:HG3	2.16	0.46
5:N:-14:G:N3	5:N:-14:G:C2'	2.79	0.46
3:H:25:ILE:HD13	3:H:141:ILE:HD11	1.98	0.45
3:I:461:GLU:HB3	3:L:451:ARG:HB2	1.99	0.45
1:E:199:LEU:HD23	1:F:66:LYS:HD3	1.98	0.45
1:F:15:LEU:HD11	1:F:185:SER:HB2	1.98	0.45
1:F:101:VAL:HG22	1:F:148:ILE:HG23	1.98	0.45
3:L:527:SER:OG	5:N:23:U:OP1	2.34	0.45
1:C:131:ASP:OD1	5:N:3:G:N2	2.49	0.45
3:I:594:ASP:OD2	3:I:594:ASP:N	2.40	0.45
1:P:56:ARG:NH2	1:P:91:GLY:O	2.50	0.45
1:D:102:ASP:OD1	1:D:103:PHE:N	2.50	0.45
1:E:41:LYS:HD2	1:E:110:LYS:HD3	1.98	0.45
3:K:494:PHE:HZ	3:L:482:TYR:HD1	1.64	0.45
1:C:59:LEU:HG	1:C:164:ALA:HB2	1.99	0.45
3:H:274:LYS:HE2	3:H:277:ARG:HD2	1.98	0.45
3:I:462:LYS:HD2	3:I:462:LYS:HA	1.61	0.45
1:D:92:SER:O	4:M:14:A:O2'	2.35	0.45
1:F:41:LYS:HZ1	1:F:114:VAL:HG11	1.81	0.45
3:H:243:SER:OG	3:H:287:ASN:OD1	2.34	0.45
3:H:27:ILE:HG21	3:H:166:PHE:CG	2.52	0.45
3:H:184:MET:HE1	3:H:385:ARG:HB2	1.97	0.45
1:A:24:ARG:HH12	1:B:137:GLU:HG3	1.82	0.45
1:C:176:TRP:HB3	1:C:179:LYS:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:75:VAL:HG21	3:H:121:SER:HA	1.98	0.45
3:I:527:SER:OG	5:N:11:C:OP1	2.34	0.45
1:J:59:LEU:HD12	1:J:90:PHE:HE2	1.82	0.45
1:F:4:THR:HA	1:F:194:ALA:HA	1.98	0.44
1:F:22:GLU:OE1	1:F:40:ARG:HA	2.18	0.44
1:E:177:LEU:O	1:E:183:ARG:NH2	2.41	0.44
1:F:78:ALA:O	1:P:121:ARG:NH2	2.51	0.44
3:L:559:THR:HG23	3:L:561:ARG:HG2	1.99	0.44
1:A:15:LEU:HD11	1:A:185:SER:HB2	1.99	0.44
3:H:262:THR:HG23	3:H:286:PHE:HE2	1.82	0.44
3:I:524:LYS:O	3:I:565:ASN:ND2	2.46	0.44
3:H:188:ASN:OD1	3:K:416:ARG:NE	2.41	0.44
3:K:136:LEU:HD13	3:K:141:ILE:HD12	2.00	0.44
1:A:165:LEU:HD12	1:A:186:PHE:CG	2.52	0.44
1:B:8:ILE:HG23	1:B:188:VAL:HG13	1.98	0.44
3:K:60:LEU:HA	3:K:153:VAL:CG2	2.43	0.44
1:D:40:ARG:HD2	1:D:48:LEU:HB2	2.00	0.44
1:C:6:LYS:HE3	1:C:6:LYS:HB2	1.87	0.44
1:E:109:THR:HG22	1:E:111:GLU:H	1.83	0.44
2:G:102:ALA:HB3	2:G:105:LEU:HB3	1.99	0.44
3:K:71:VAL:N	3:K:72:PRO:CD	2.81	0.44
1:E:169:GLU:HG2	1:E:185:SER:HA	1.99	0.44
1:J:122:ILE:O	1:J:124:ARG:NH1	2.49	0.44
1:C:19:TYR:O	1:C:175:GLY:N	2.51	0.43
1:E:42:THR:OG1	1:E:46:LYS:N	2.49	0.43
2:G:190:VAL:HB	4:M:-7:U:C4	2.53	0.43
1:C:59:LEU:HD12	1:C:90:PHE:HE2	1.83	0.43
1:C:73:THR:O	1:J:121:ARG:NH1	2.42	0.43
3:H:256:PRO:HD2	5:N:-12:A:H4'	1.99	0.43
1:B:20:THR:O	1:B:40:ARG:N	2.51	0.43
2:G:26:TYR:HB3	2:G:66:PRO:HD3	2.01	0.43
1:C:5:MET:HE3	1:C:5:MET:HB2	1.91	0.43
3:H:191:TYR:HB3	3:H:394:PHE:HE1	1.84	0.43
1:E:59:LEU:HG	1:E:164:ALA:HB2	2.01	0.43
2:G:190:VAL:HG22	2:G:205:ARG:HA	1.99	0.43
1:J:59:LEU:HG	1:J:164:ALA:HB2	2.01	0.43
3:K:165:LEU:HD23	3:K:192:LEU:HD13	2.01	0.43
1:B:156:LYS:HA	1:B:156:LYS:HD3	1.72	0.43
3:H:546:ILE:HG23	3:H:588:LEU:HD11	2.00	0.43
1:D:40:ARG:NH2	4:M:18:G:OP1	2.46	0.43
1:F:56:ARG:HE	1:F:73:THR:CG2	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:128:ILE:HG21	3:H:134:ILE:HG21	2.00	0.43
3:H:184:MET:HE2	3:H:184:MET:HB3	1.76	0.43
3:H:184:MET:HE2	3:H:382:TYR:CE1	2.53	0.43
3:H:167:SER:HB2	3:H:170:ILE:HD11	1.99	0.43
1:E:92:SER:OG	1:E:93:MET:N	2.52	0.43
1:E:124:ARG:NH1	4:M:17:C:OP1	2.43	0.43
1:J:122:ILE:HD13	4:M:29:C:H2'	2.00	0.43
1:A:24:ARG:HH11	1:B:115:ARG:HB2	1.84	0.43
1:C:178:ASN:OD1	1:C:178:ASN:N	2.41	0.43
2:G:100:ILE:HD11	2:G:107:TYR:CZ	2.54	0.43
1:C:59:LEU:HD23	1:C:59:LEU:HA	1.85	0.42
3:H:314:ALA:CB	5:N:-13:A:H5'	2.46	0.42
1:J:81:CYS:SG	1:J:82:GLY:N	2.92	0.42
1:F:62:MET:HE1	1:F:163:SER:HB3	2.02	0.42
1:B:91:GLY:HA3	4:M:33:U:H5''	2.00	0.42
1:F:102:ASP:OD1	1:F:103:PHE:N	2.52	0.42
3:H:60:LEU:O	3:H:61:THR:C	2.62	0.42
3:I:531:ILE:HG23	3:I:602:LEU:HD22	2.02	0.42
3:K:57:ILE:O	3:K:83:ILE:HA	2.19	0.42
3:K:398:GLY:H	3:K:403:ARG:HH21	1.67	0.42
3:K:520:LEU:HA	3:K:523:ILE:HG12	2.00	0.42
2:G:102:ALA:HB1	4:M:-1:U:OP2	2.19	0.42
3:H:293:ILE:HG13	3:H:298:GLN:HB3	2.00	0.42
1:F:178:ASN:ND2	4:M:9:G:OP1	2.51	0.42
3:H:444:MET:HB3	3:H:451:ARG:HH21	1.84	0.42
3:I:549:ILE:HA	3:I:552:VAL:HG22	2.01	0.42
1:E:12:MET:HB2	1:E:186:PHE:CD1	2.55	0.42
1:E:14:THR:HA	1:E:184:VAL:HG12	2.00	0.42
3:H:46:GLU:HG2	3:H:77:LYS:HE3	2.01	0.42
1:A:18:LEU:O	1:A:138:VAL:HG23	2.20	0.42
1:E:199:LEU:HD21	1:F:63:LEU:HD23	2.01	0.42
2:G:136:ARG:C	2:G:136:ARG:HD2	2.44	0.42
3:H:456:SER:HB3	3:I:485:MET:HE3	2.01	0.42
3:I:566:PRO:HA	3:I:567:PRO:HD3	1.91	0.42
1:P:12:MET:HE3	1:P:144:PHE:HD2	1.85	0.42
3:H:274:LYS:CE	3:H:277:ARG:HD2	2.50	0.42
4:M:13:G:H2'	4:M:14:A:C8	2.55	0.42
1:E:91:GLY:HA3	4:M:9:G:H5''	2.02	0.42
1:F:59:LEU:HA	1:F:59:LEU:HD23	1.78	0.42
1:J:170:GLU:OE2	1:J:171:ASN:ND2	2.52	0.42
1:E:59:LEU:HA	1:E:59:LEU:HD23	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:105:ILE:HD13	1:P:105:ILE:HA	1.86	0.42
1:P:113:ILE:HA	1:P:139:ILE:HG12	2.01	0.42
1:C:122:ILE:HD13	4:M:35:G:H2'	2.02	0.41
1:E:16:SER:OG	1:E:17:PRO:HD2	2.20	0.41
3:H:261:VAL:O	3:H:265:ILE:HG12	2.20	0.41
1:P:128:SER:OG	1:P:129:ALA:N	2.53	0.41
1:A:166:LYS:HB2	1:A:166:LYS:HE2	1.88	0.41
3:H:73:LEU:HD12	3:H:76:LYS:HD3	2.02	0.41
1:D:13:LYS:HB3	1:D:13:LYS:HE2	1.74	0.41
3:H:49:ILE:HD11	3:H:70:LEU:HD13	2.01	0.41
3:H:327:LEU:O	3:H:331:LYS:HG3	2.20	0.41
3:H:375:ASP:OD1	3:H:375:ASP:N	2.49	0.41
3:I:587:LEU:O	3:I:591:ILE:HG13	2.20	0.41
3:K:71:VAL:CG1	3:K:72:PRO:HD3	2.50	0.41
3:H:283:ASP:OD1	3:H:283:ASP:N	2.53	0.41
1:E:73:THR:HG23	1:F:124:ARG:HH21	1.85	0.41
3:H:10:LYS:HD3	3:H:397:HIS:CE1	2.55	0.41
3:H:60:LEU:HD11	3:H:71:VAL:CG2	2.46	0.41
3:H:379:LEU:O	3:H:383:ILE:HG12	2.20	0.41
3:H:74:LEU:HD23	3:H:74:LEU:HA	1.82	0.41
3:H:363:ARG:HE	3:H:363:ARG:HB3	1.53	0.41
3:H:534:PHE:HD1	3:H:549:ILE:HD11	1.86	0.41
3:H:143:PHE:CD2	3:H:153:VAL:HG21	2.56	0.41
3:H:181:PRO:HA	3:H:182:PRO:HD2	1.96	0.41
3:L:519:TYR:HA	3:L:522:ASN:ND2	2.35	0.41
3:H:30:GLY:HA2	3:H:68:SER:O	2.20	0.41
3:H:566:PRO:HA	3:H:567:PRO:HD3	1.92	0.41
3:K:6:GLY:O	3:K:15:ALA:N	2.54	0.41
1:D:84:CYS:HB2	1:D:87:CYS:HB2	2.03	0.41
1:E:45:ASN:O	1:E:110:LYS:N	2.50	0.41
1:E:126:THR:HB	1:J:95:ARG:HG3	2.03	0.41
3:K:460:VAL:HG22	3:K:467:GLU:HB2	2.03	0.41
5:N:-14:G:H4'	5:N:-13:A:OP2	2.21	0.41
2:G:45:LEU:O	2:G:48:SER:OG	2.34	0.41
3:K:587:LEU:O	3:K:591:ILE:HG13	2.21	0.41
3:L:447:PHE:HB3	3:L:452:LEU:HD21	2.03	0.41
1:B:81:CYS:SG	1:B:82:GLY:N	2.94	0.40
1:F:92:SER:O	4:M:2:U:O2'	2.35	0.40
3:H:57:ILE:HG22	3:H:82:LYS:HB3	2.02	0.40
3:H:136:LEU:HD21	3:H:141:ILE:HD13	2.02	0.40
3:K:68:SER:O	3:K:69:GLY:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:14:PHE:CZ	2:G:27:PRO:HD3	2.57	0.40
1:P:59:LEU:HD11	1:P:160:LEU:HD13	2.03	0.40
1:F:59:LEU:HG	1:F:164:ALA:HB2	2.02	0.40
2:G:94:SER:HA	2:G:97:LEU:HD23	2.03	0.40
3:K:447:PHE:O	3:K:450:TYR:HB2	2.20	0.40
1:P:34:ARG:HA	1:P:34:ARG:HD3	1.85	0.40
1:A:25:ARG:HD2	1:B:116:GLU:HB3	2.04	0.40
3:H:173:LYS:H	3:H:173:LYS:HG2	1.69	0.40
3:H:210:ARG:HA	3:H:213:GLU:HG2	2.03	0.40
3:H:349:ARG:O	3:H:353:ILE:HG22	2.22	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	157/200 (78%)	148 (94%)	9 (6%)	0	100	100
1	B	197/200 (98%)	189 (96%)	8 (4%)	0	100	100
1	C	197/200 (98%)	191 (97%)	6 (3%)	0	100	100
1	D	197/200 (98%)	190 (96%)	7 (4%)	0	100	100
1	E	197/200 (98%)	190 (96%)	7 (4%)	0	100	100
1	F	192/200 (96%)	186 (97%)	6 (3%)	0	100	100
1	J	197/200 (98%)	192 (98%)	5 (2%)	0	100	100
1	P	192/200 (96%)	180 (94%)	12 (6%)	0	100	100
2	G	202/240 (84%)	190 (94%)	12 (6%)	0	100	100
3	H	574/609 (94%)	539 (94%)	35 (6%)	0	100	100
3	I	156/609 (26%)	146 (94%)	10 (6%)	0	100	100
3	K	350/609 (58%)	327 (93%)	22 (6%)	1 (0%)	36	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	156/609 (26%)	142 (91%)	14 (9%)	0	100	100
All	All	2964/4276 (69%)	2810 (95%)	153 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	492	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	131/170 (77%)	128 (98%)	3 (2%)	44	70
1	B	167/170 (98%)	164 (98%)	3 (2%)	51	74
1	C	167/170 (98%)	164 (98%)	3 (2%)	51	74
1	D	169/170 (99%)	166 (98%)	3 (2%)	51	74
1	E	166/170 (98%)	164 (99%)	2 (1%)	63	79
1	F	162/170 (95%)	161 (99%)	1 (1%)	78	84
1	J	168/170 (99%)	167 (99%)	1 (1%)	78	84
1	P	149/170 (88%)	145 (97%)	4 (3%)	39	68
2	G	100/209 (48%)	96 (96%)	4 (4%)	28	61
3	H	508/556 (91%)	495 (97%)	13 (3%)	40	69
3	I	147/556 (26%)	145 (99%)	2 (1%)	59	77
3	K	288/556 (52%)	281 (98%)	7 (2%)	43	70
3	L	139/556 (25%)	136 (98%)	3 (2%)	45	71
All	All	2461/3793 (65%)	2412 (98%)	49 (2%)	48	72

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG

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Mol	Chain	Res	Type
1	A	85	VAL
1	A	178	ASN
1	B	119	HIS
1	B	145	THR
1	B	157	ASP
1	C	51	PHE
1	C	79	ARG
1	C	112	GLN
1	D	62	MET
1	D	70	VAL
1	D	111	GLU
1	E	44	THR
1	E	85	VAL
1	F	131	ASP
2	G	5	LYS
2	G	110	VAL
2	G	138	ILE
2	G	158	ILE
3	H	10	LYS
3	H	27	ILE
3	H	31	ILE
3	H	127	GLU
3	H	136	LEU
3	H	149	ILE
3	H	189	VAL
3	H	211	LEU
3	H	232	ILE
3	H	362	CYS
3	H	363	ARG
3	H	405	ILE
3	H	478	TRP
3	I	439	ILE
3	I	444	MET
1	J	112	GLN
3	K	86	THR
3	K	136	LEU
3	K	440	ASN
3	K	460	VAL
3	K	473	TRP
3	K	489	ILE
3	K	492	GLU
3	L	460	VAL

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Mol	Chain	Res	Type
3	L	587	LEU
3	L	591	ILE
1	P	62	MET
1	P	105	ILE
1	P	173	ILE
1	P	191	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	32	GLN
1	C	125	GLN
1	C	162	GLN
3	H	101	GLN
3	H	161	ASN
3	H	203	HIS
3	H	522	ASN
3	H	606	ASN
3	I	606	ASN
1	J	162	GLN
3	K	132	ASN
3	K	440	ASN
3	K	469	ASN
3	K	488	GLN
3	K	558	ASN
3	K	606	ASN
3	L	522	ASN
3	L	542	GLN
3	L	556	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	M	53/60 (88%)	20 (37%)	2 (3%)
5	N	44/60 (73%)	14 (31%)	1 (2%)
All	All	97/120 (80%)	34 (35%)	3 (3%)

All (34) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	M	-8	U
4	M	-7	U
4	M	-5	A
4	M	-3	A
4	M	-2	C
4	M	-1	U
4	M	4	C
4	M	5	U
4	M	6	C
4	M	10	C
4	M	11	U
4	M	12	G
4	M	17	C
4	M	19	A
4	M	20	A
4	M	24	A
4	M	29	C
4	M	36	C
4	M	42	A
4	M	43	G
5	N	-15	A
5	N	-14	G
5	N	-13	A
5	N	-12	A
5	N	-2	A
5	N	3	G
5	N	4	A
5	N	9	C
5	N	10	A
5	N	30	U
5	N	32	A
5	N	33	G
5	N	35	A
5	N	36	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	M	10	C
4	M	30	G
5	N	-14	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 9 ligands modelled in this entry, 9 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.

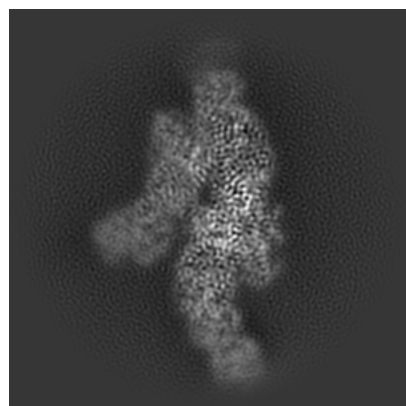
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39857. These allow visual inspection of the internal detail of the map and identification of artifacts.

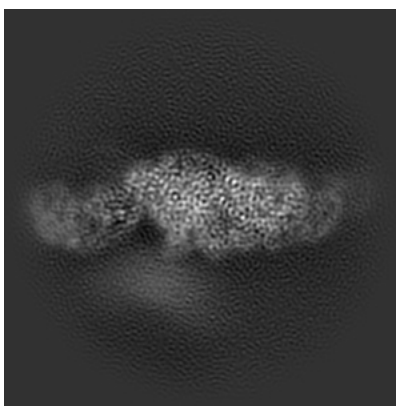
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

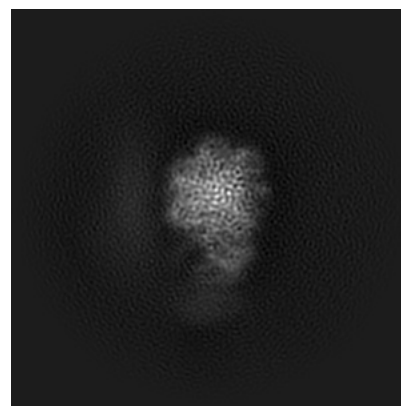
6.1.1 Primary map



X

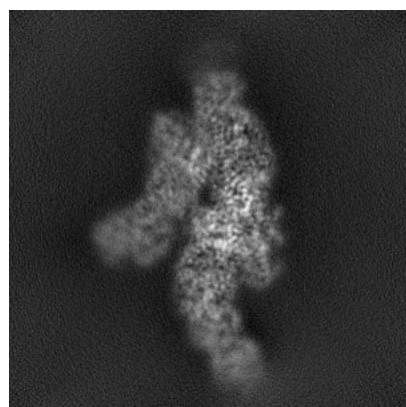


Y

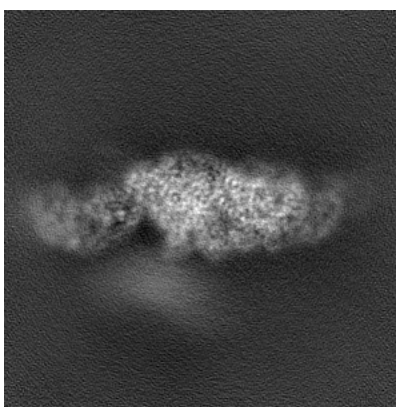


Z

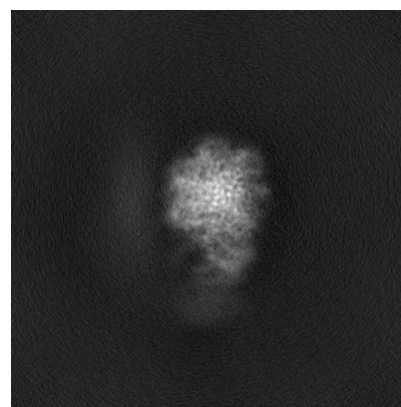
6.1.2 Raw map



X



Y

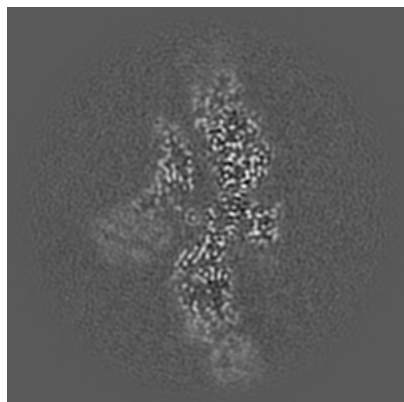


Z

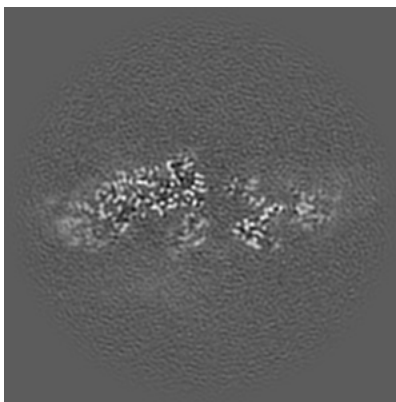
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

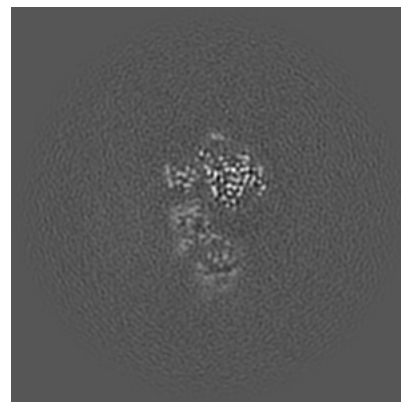
6.2.1 Primary map



X Index: 150

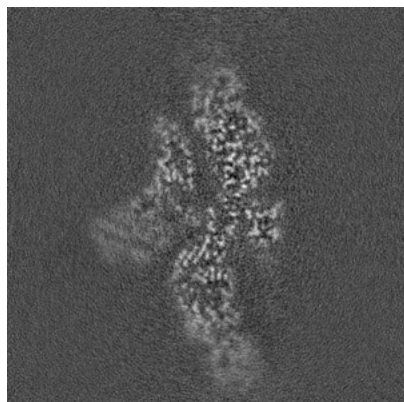


Y Index: 150

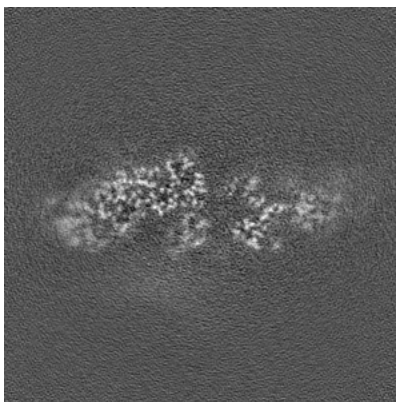


Z Index: 150

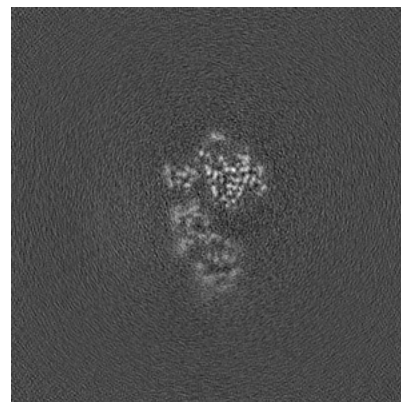
6.2.2 Raw map



X Index: 150



Y Index: 150

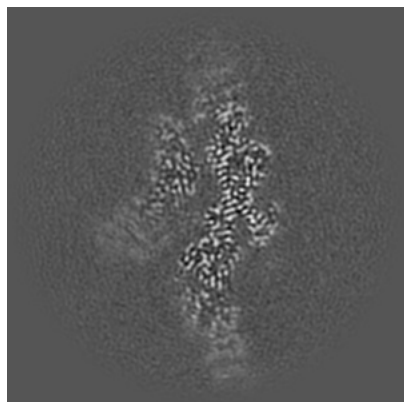


Z Index: 150

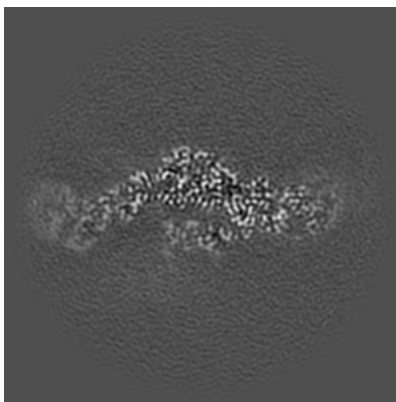
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

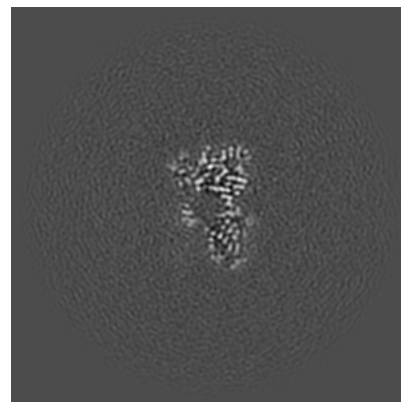
6.3.1 Primary map



X Index: 154

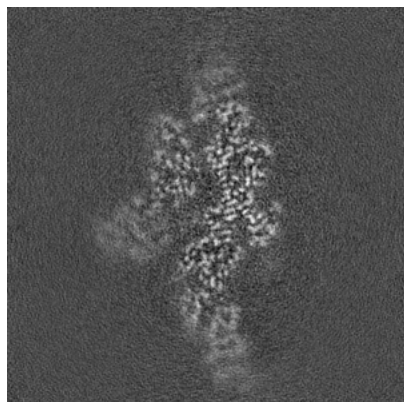


Y Index: 164

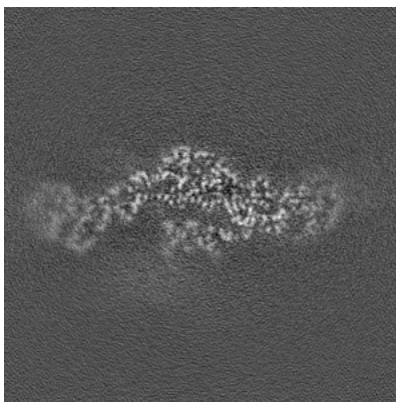


Z Index: 172

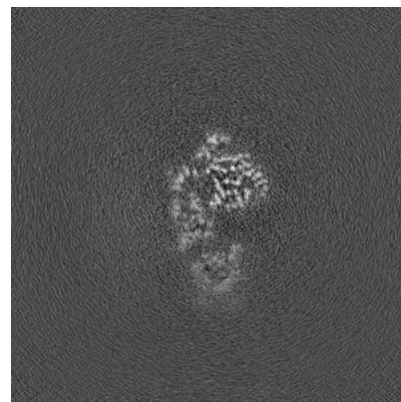
6.3.2 Raw map



X Index: 154



Y Index: 164

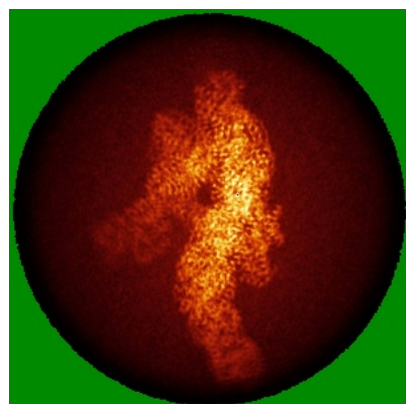


Z Index: 147

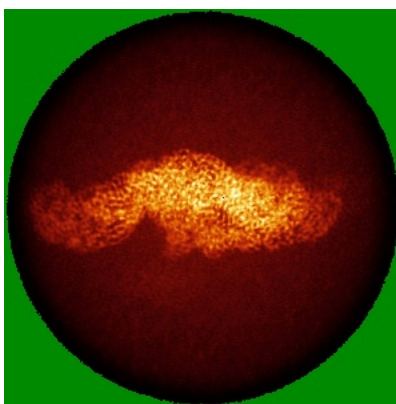
The images above show the largest variance slices of the map in three orthogonal directions.

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

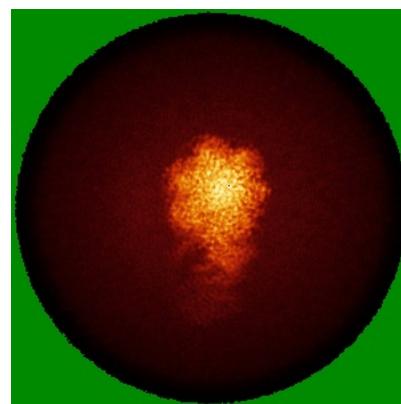
6.4.1 Primary map



X

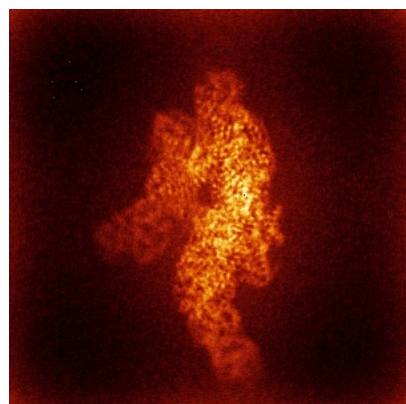


Y

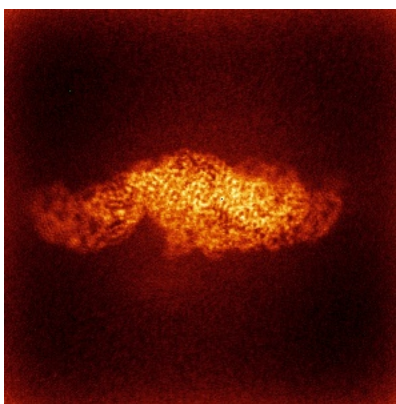


Z

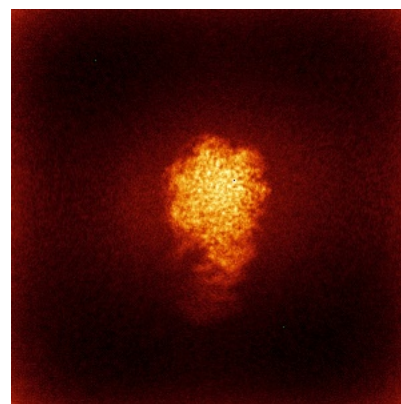
6.4.2 Raw map



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.

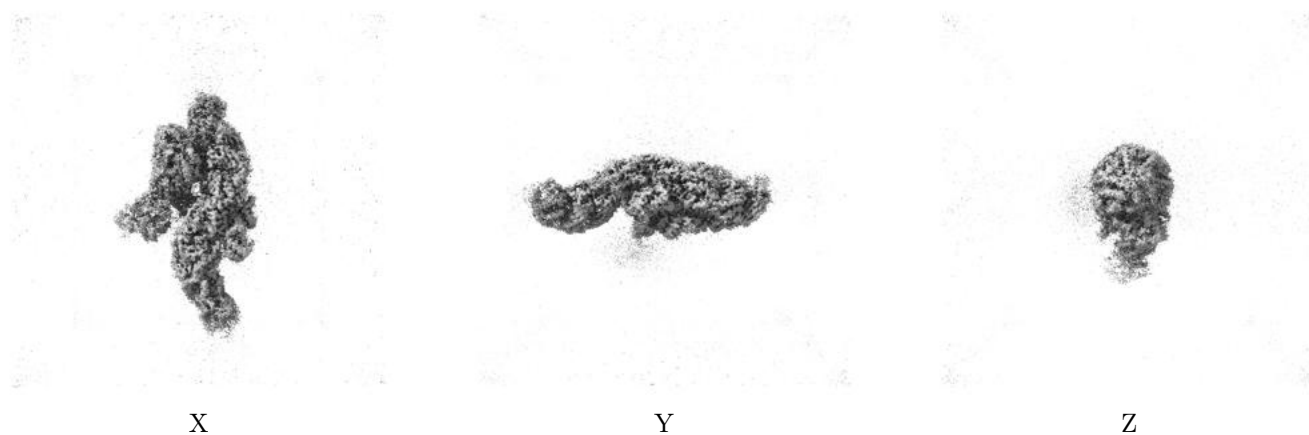
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. 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.

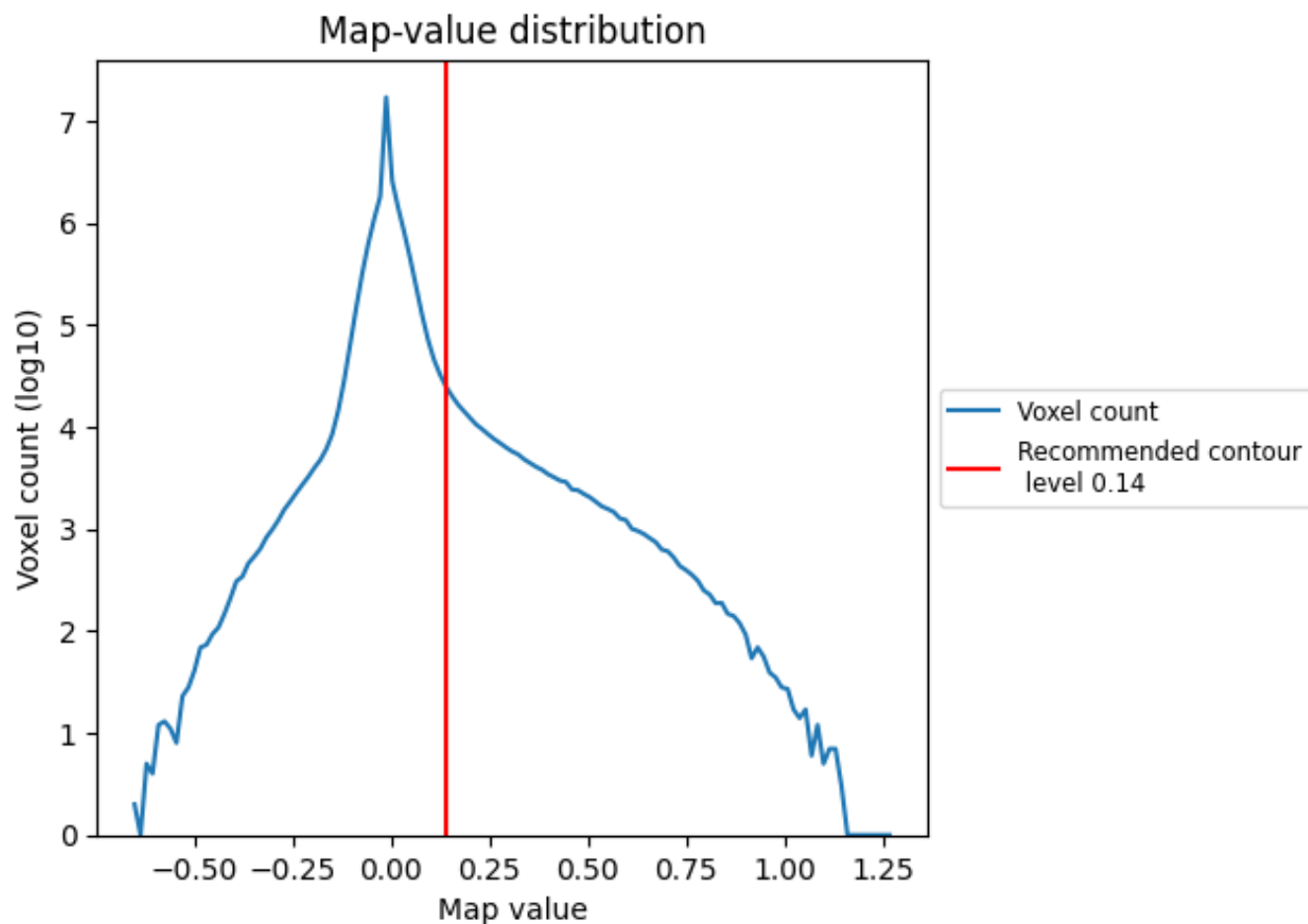
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

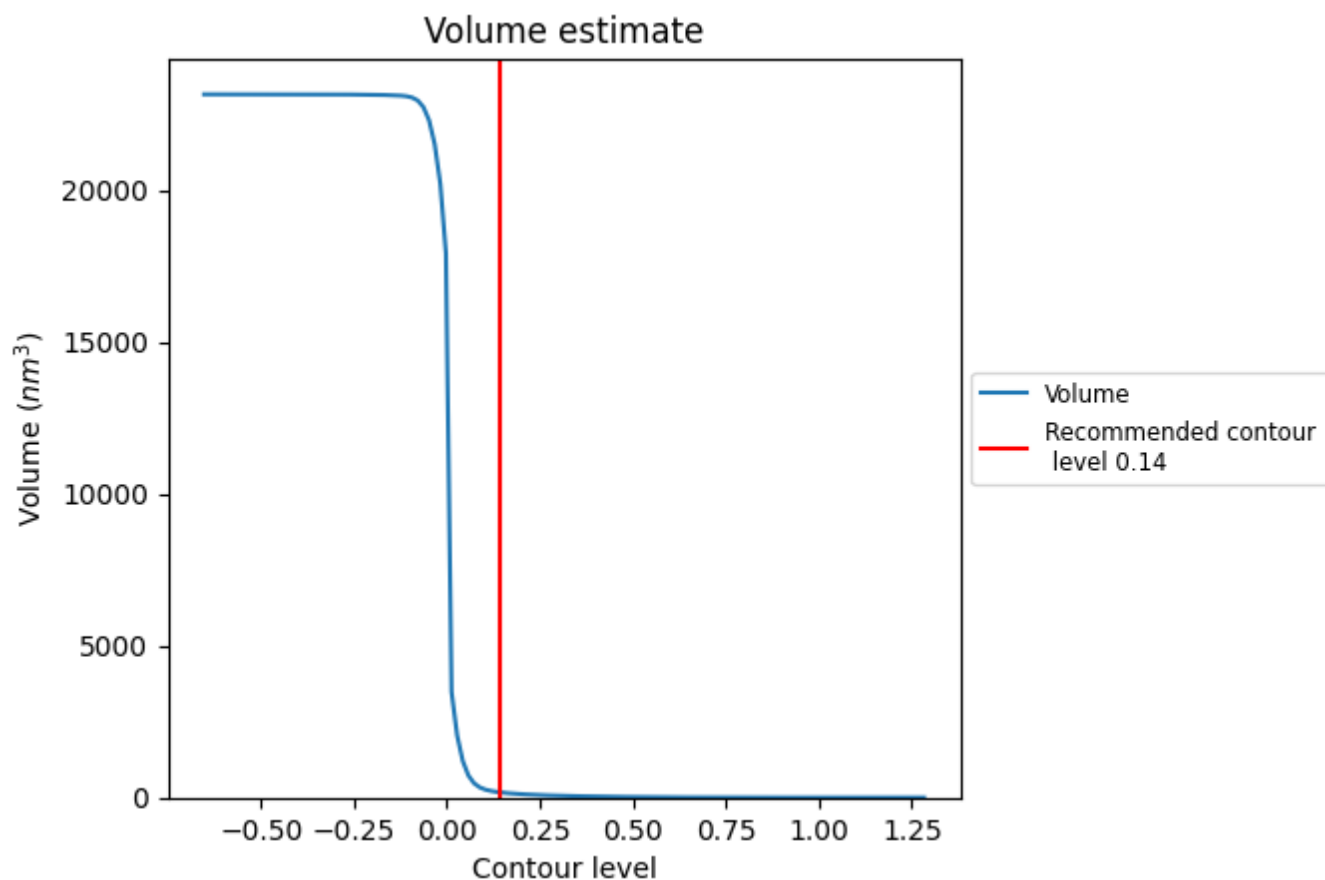
This section contains the results of statistical analysis of the map.

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.

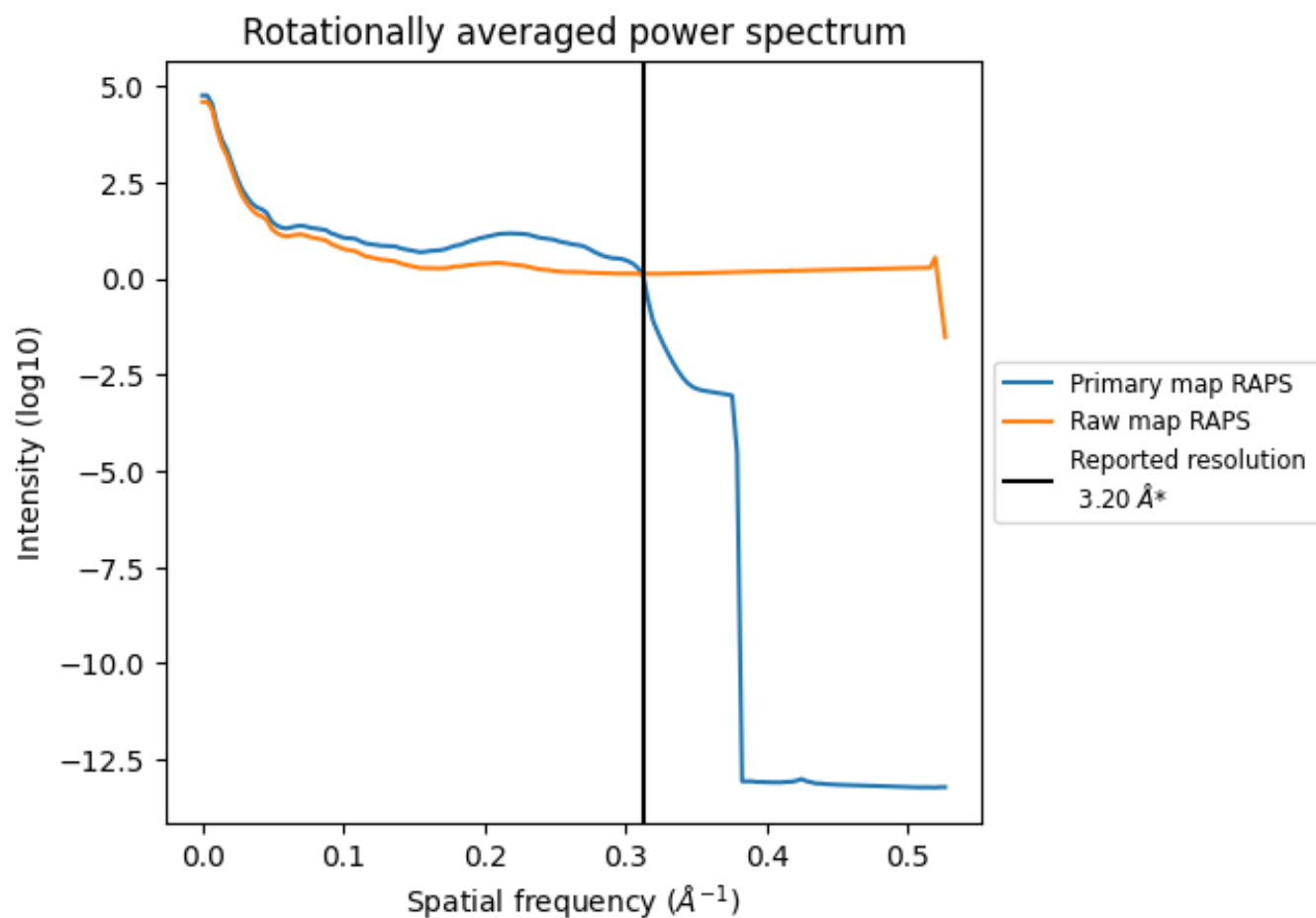
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 176 nm³; this corresponds to an approximate mass of 159 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 ⓘ

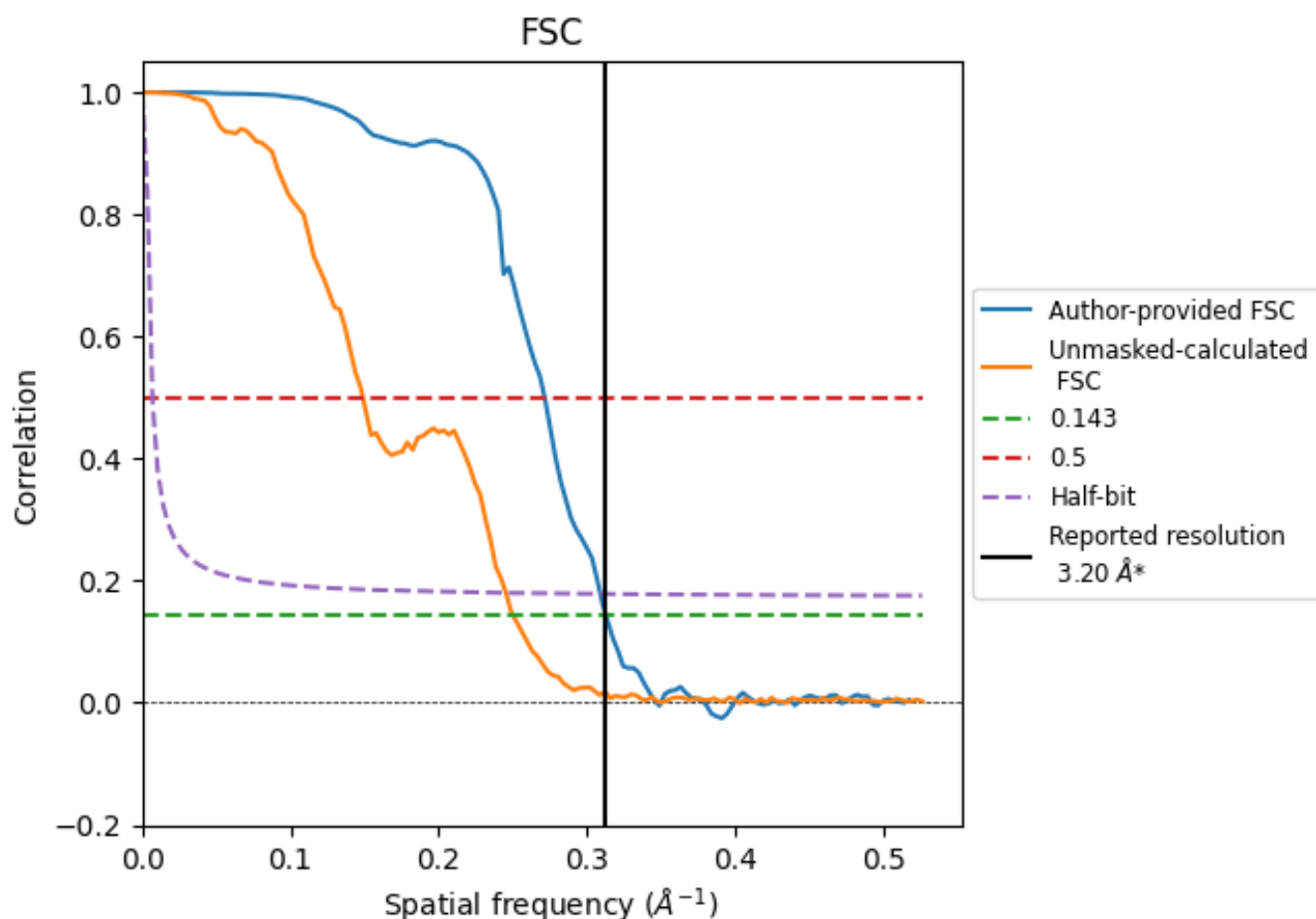


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

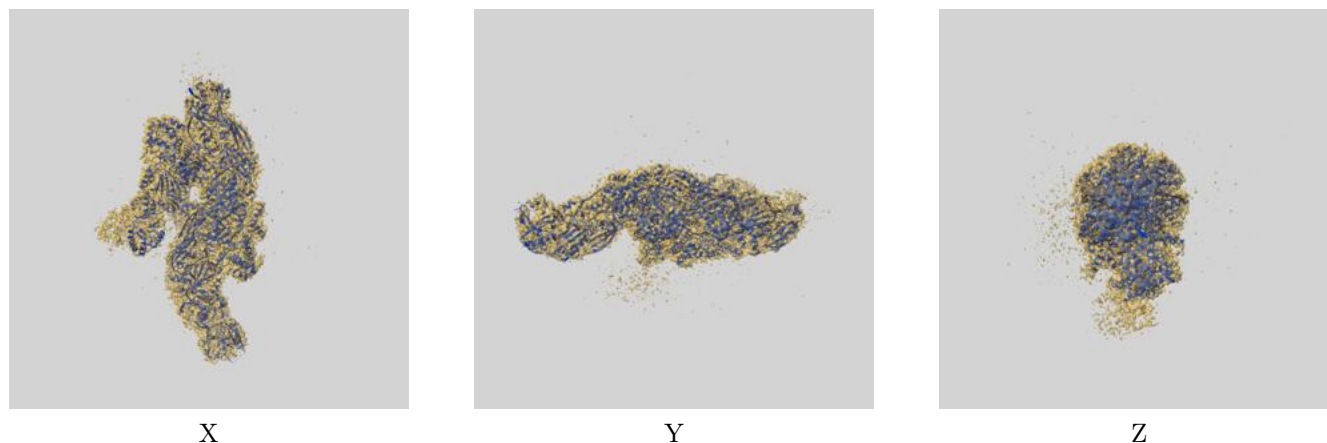
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.68	3.23
Unmasked-calculated*	4.00	6.72	4.07

*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 4.00 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

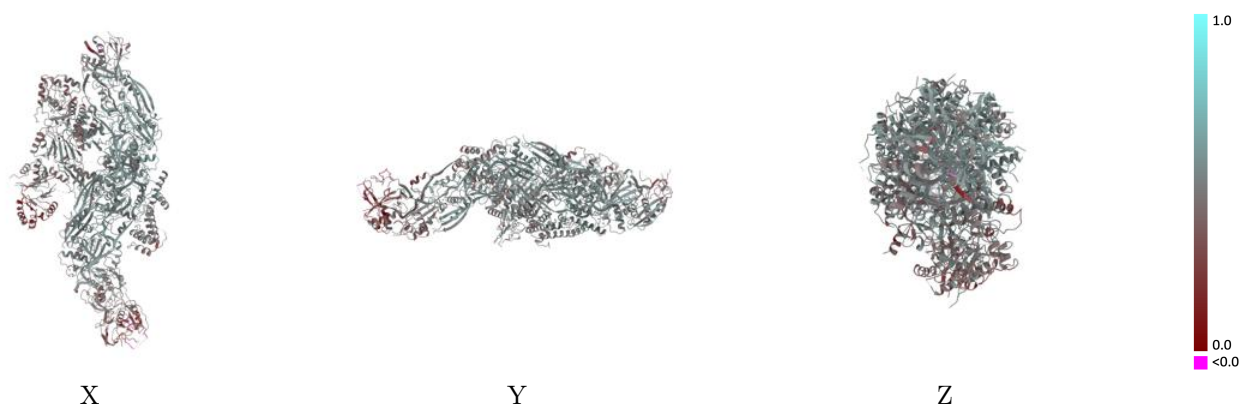
This section contains information regarding the fit between EMDB map EMD-39857 and PDB model 8Z99. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



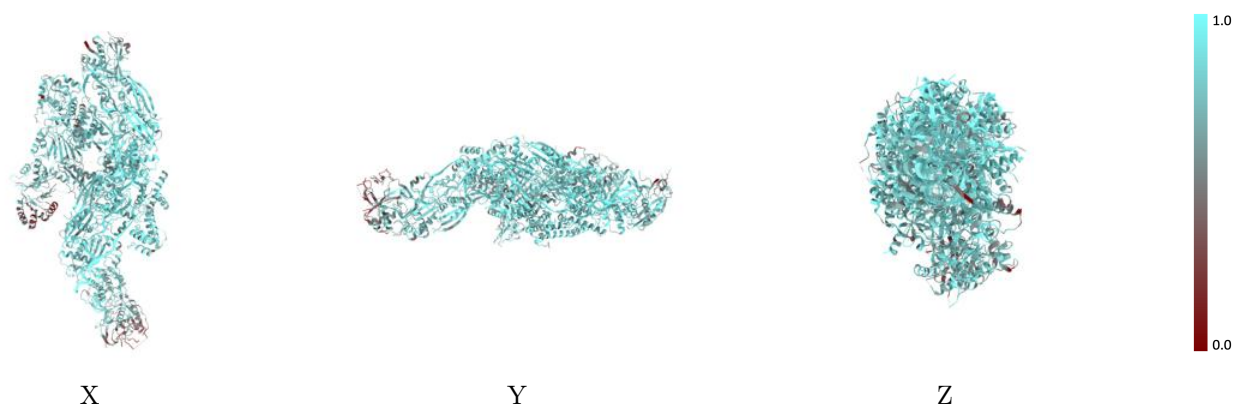
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



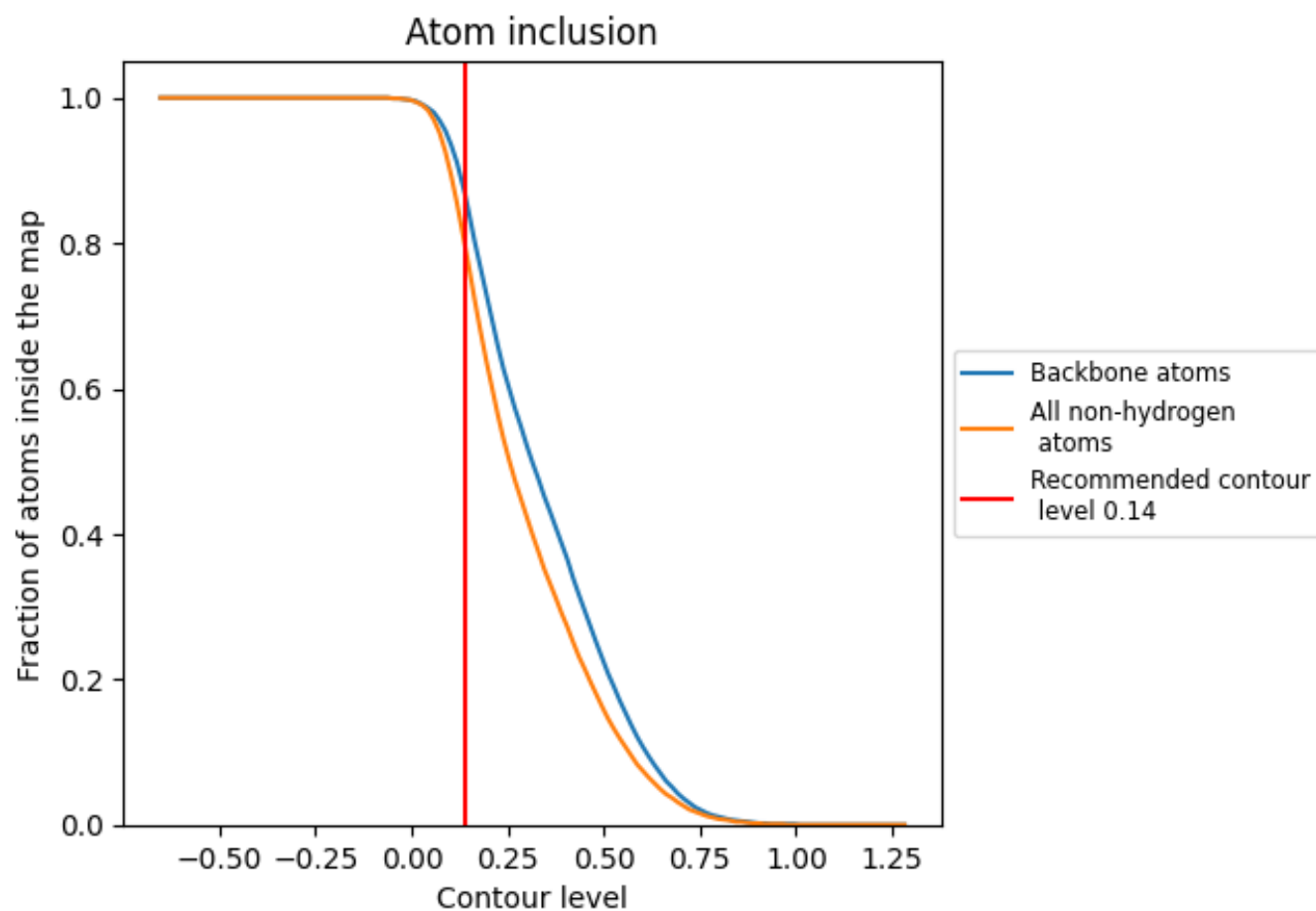
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.14).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 80% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7950	0.4870
A	0.6940	0.4590
B	0.8530	0.5240
C	0.8780	0.5450
D	0.8820	0.5510
E	0.8620	0.5400
F	0.8540	0.5250
G	0.5380	0.3410
H	0.7810	0.4760
I	0.7900	0.4880
J	0.8830	0.5470
K	0.6950	0.4350
L	0.7770	0.4560
M	0.8950	0.5060
N	0.9250	0.5100
P	0.7480	0.4530

1.0

0.0

<0.0