



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:51 PM UTC

PDB ID : 8YHE / pdb_00008yhe
EMDB ID : EMD-39288
Title : Cryo-EM structure of CTR-bound type VII CRISPR-Cas complex at post-state II
Authors : Zhang, H.; Deng, Z.; Li, X.
Deposited on : 2024-02-28
Resolution : 3.07 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:

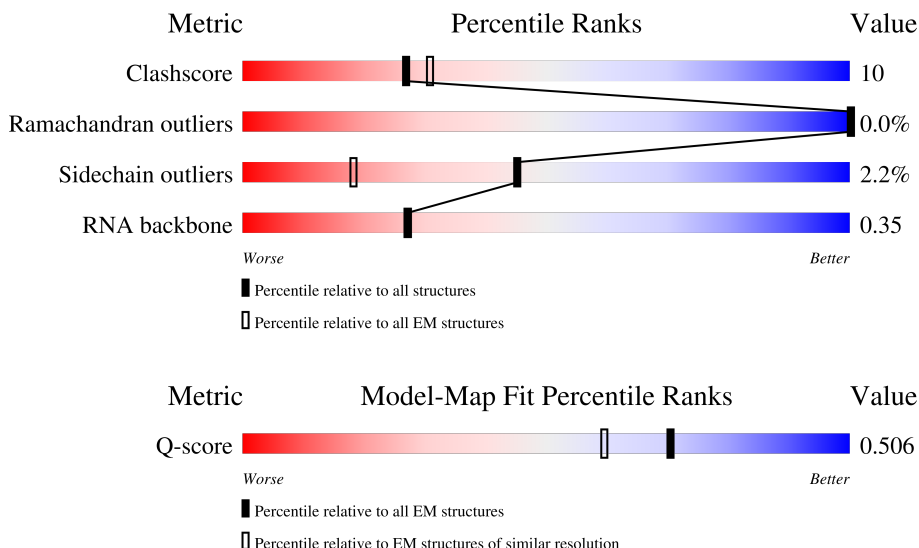
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.07 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.



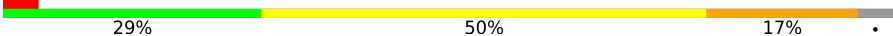
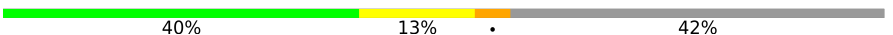
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13977 (2.57 - 3.57)

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	
2	G	240	
3	H	608	
3	I	608	
3	K	608	
3	L	608	
4	M	48	
5	N	52	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 21183 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 protein structure.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	115	Total	C	N	O	S	0	0
			675	412	123	135	5		
1	B	189	Total	C	N	O	S	0	0
			1415	885	245	277	8		
1	C	199	Total	C	N	O	S	0	0
			1508	942	266	292	8		
1	D	199	Total	C	N	O	S	0	0
			1529	954	273	294	8		
1	E	198	Total	C	N	O	S	0	0
			1518	948	269	293	8		
1	F	189	Total	C	N	O	S	0	0
			1428	893	249	278	8		
1	J	197	Total	C	N	O	S	0	0
			1529	953	274	294	8		

- Molecule 2 is a protein called protein structure.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	213	Total	C	N	O	S	0	0
			1515	980	246	286	3		

- Molecule 3 is a protein called protein structure.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	524	Total	C	N	O	S	0	0
			4127	2642	692	779	14		
3	I	157	Total	C	N	O	S	0	0
			1310	843	219	242	6		
3	K	237	Total	C	N	O	S	0	0
			1931	1241	322	361	7		
3	L	144	Total	C	N	O	S	0	0
			1091	697	181	210	3		

- Molecule 4 is a RNA chain called RNA (46-MER).

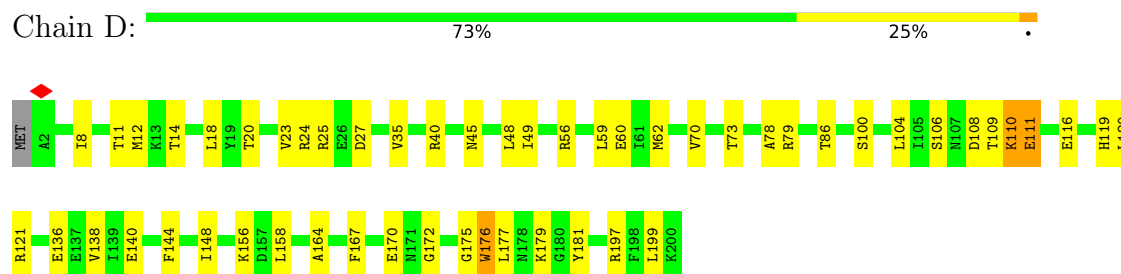
Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	46	Total	C	N	O	P	0	0
			963	430	161	326	46		

- Molecule 5 is a RNA chain called RNA (29-MER).

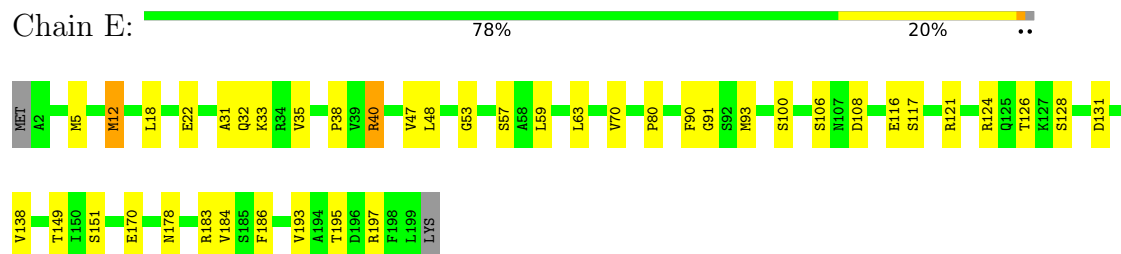
Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	30	Total	C	N	O	P	0	0
			635	285	113	207	30		

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

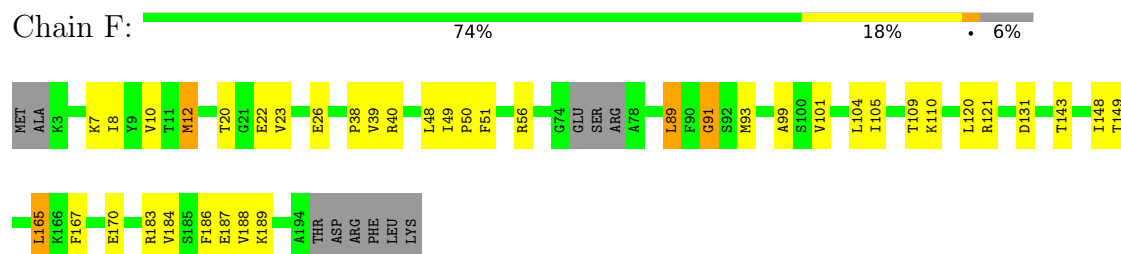
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Zn	0
			1	1	
6	B	1	Total	Zn	0
			1	1	
6	C	1	Total	Zn	0
			1	1	
6	D	1	Total	Zn	0
			1	1	
6	E	1	Total	Zn	0
			1	1	
6	F	1	Total	Zn	0
			1	1	
6	H	2	Total	Zn	0
			2	2	
6	J	1	Total	Zn	0
			1	1	



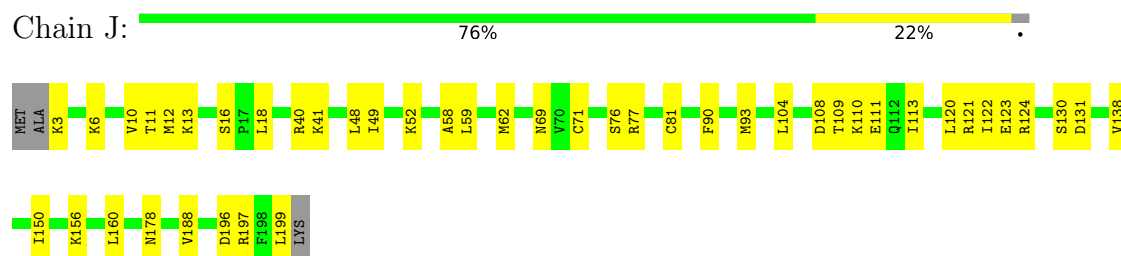
- Molecule 1: protein structure



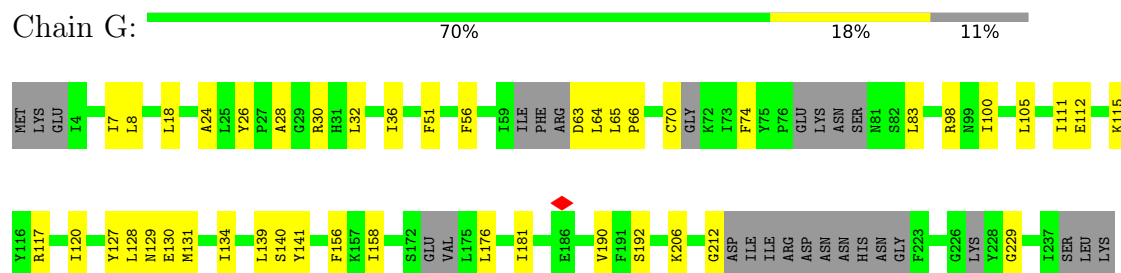
- Molecule 1: protein structure



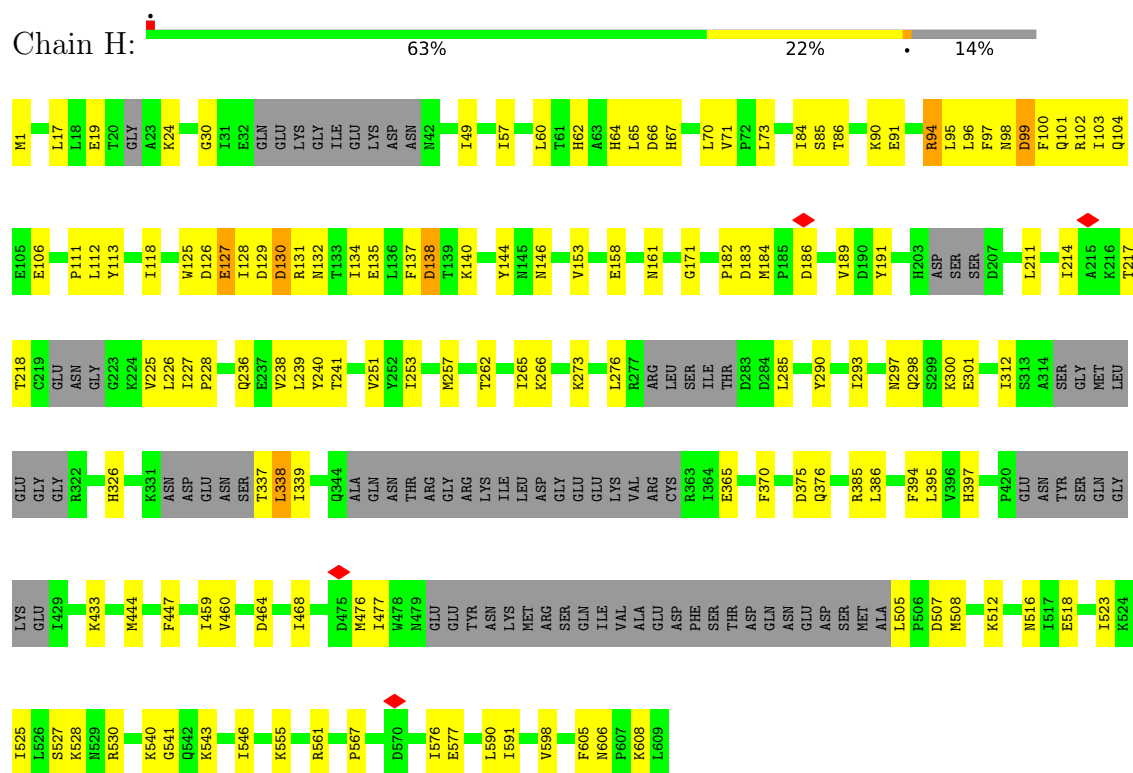
- Molecule 1: protein structure



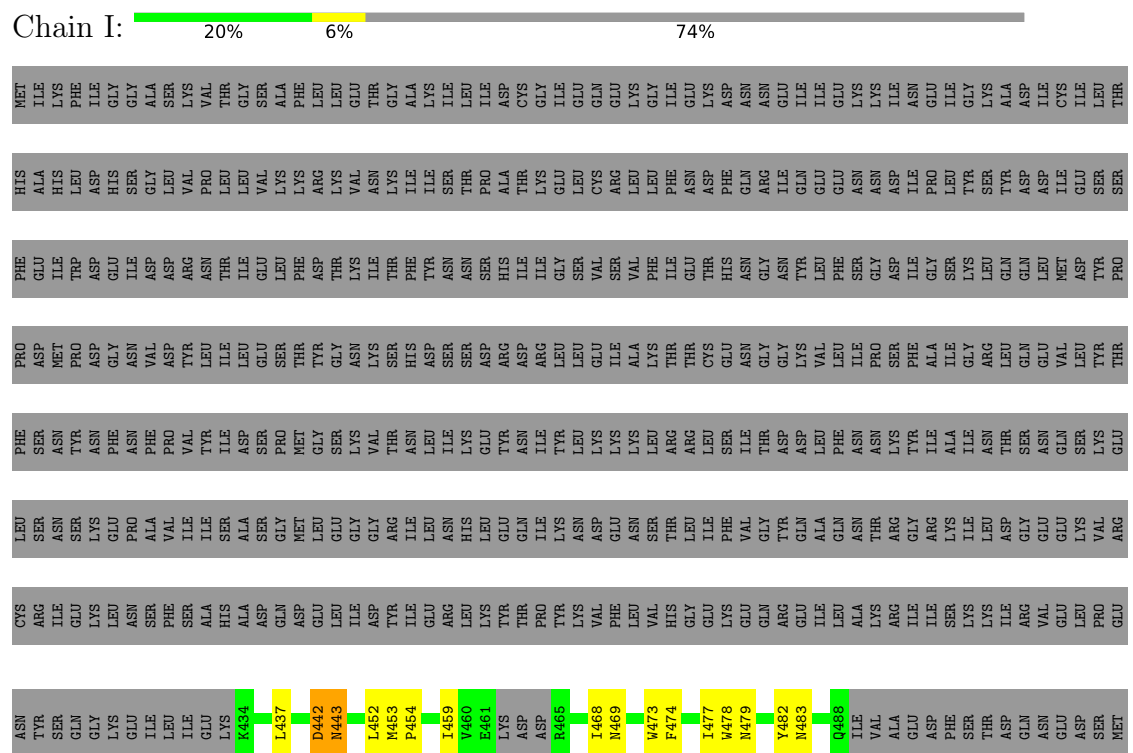
- Molecule 2: protein structure



- Molecule 3: protein structure

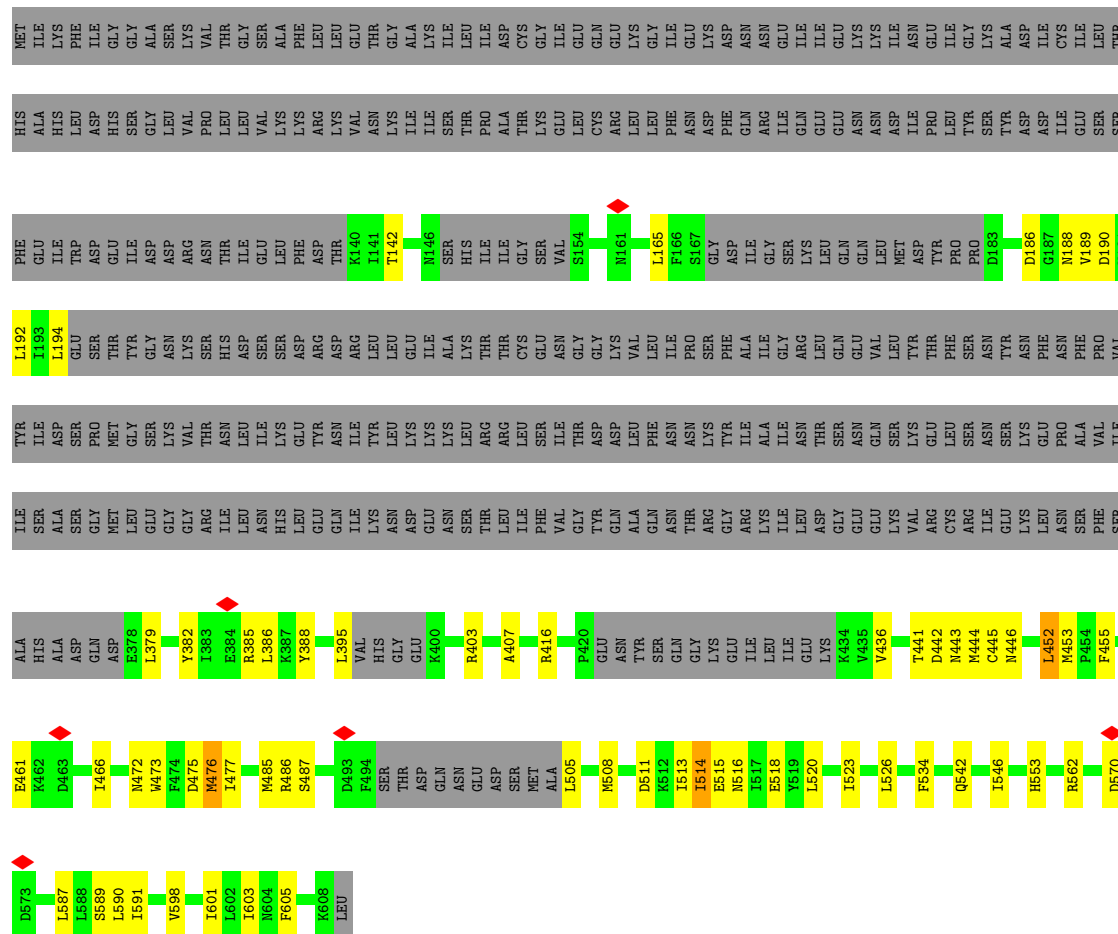


- Molecule 3: protein structure





• Molecule 3: protein structure



• Molecule 3: protein structure





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100000	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	1.615	Depositor
Minimum map value	-0.851	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.134	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	0.52	0/677	0.71	1/923 (0.1%)
1	B	0.45	2/1433 (0.1%)	0.68	0/1932
1	C	0.32	1/1527 (0.1%)	0.56	1/2055 (0.0%)
1	D	0.62	5/1548 (0.3%)	0.67	4/2079 (0.2%)
1	E	0.48	2/1537 (0.1%)	0.62	1/2065 (0.0%)
1	F	0.42	0/1445	0.67	1/1944 (0.1%)
1	J	0.57	4/1548 (0.3%)	0.69	6/2077 (0.3%)
2	G	0.40	1/1540 (0.1%)	0.77	0/2081
3	H	0.45	4/4198 (0.1%)	0.72	8/5675 (0.1%)
3	I	0.39	1/1340 (0.1%)	0.70	0/1811
3	K	0.45	3/1969 (0.2%)	0.76	6/2662 (0.2%)
3	L	0.52	1/1114 (0.1%)	0.89	2/1523 (0.1%)
4	M	0.25	0/1073	0.44	0/1668
5	N	0.24	0/709	0.42	0/1101
All	All	0.45	24/21658 (0.1%)	0.68	30/29596 (0.1%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	76	SER	C-N	9.92	1.46	1.33
3	H	98	ASN	C-N	-9.25	1.21	1.33
1	D	110	LYS	C-N	8.57	1.45	1.33
1	J	11	THR	C-N	8.43	1.45	1.33
1	D	111	GLU	C-N	-8.28	1.22	1.33
1	D	70	VAL	C-N	8.26	1.44	1.33
1	B	143	THR	C-N	-8.09	1.23	1.33
1	J	77	ARG	C-N	-7.96	1.22	1.33
1	D	79	ARG	C-N	-7.91	1.23	1.33
1	B	142	ALA	C-N	-7.75	1.22	1.33
1	E	31	ALA	C-N	-7.72	1.22	1.33
3	K	475	ASP	C-N	7.53	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	443	ASN	C-N	-7.02	1.21	1.33
3	K	476	MET	C-N	-6.78	1.25	1.33
3	H	99	ASP	C-N	6.39	1.42	1.33
3	H	338	LEU	C-N	-6.13	1.25	1.33
2	G	139	LEU	C-N	-6.09	1.24	1.33
1	D	176	TRP	CA-C	-5.87	1.46	1.53
1	J	12	MET	C-N	5.54	1.41	1.33
1	E	40	ARG	CA-C	-5.48	1.45	1.52
3	K	142	THR	C-N	5.34	1.41	1.33
3	L	477	ILE	CG1-CD1	-5.26	1.31	1.51
1	C	107	ASN	C-N	5.20	1.40	1.33
3	H	182	PRO	C-N	-5.04	1.26	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	91	GLY	N-CA-C	8.81	123.15	112.48
1	D	70	VAL	O-C-N	6.92	130.68	123.20
3	L	525	ILE	N-CA-C	-6.69	106.27	112.96
1	J	16	SER	CA-C-N	-6.68	112.77	119.92
1	J	16	SER	C-N-CA	-6.68	112.77	119.92
1	J	69	ASN	CB-CA-C	6.51	120.02	110.26
3	K	452	LEU	N-CA-C	6.22	118.64	109.69
3	L	603	ILE	N-CA-C	6.02	116.20	110.42
3	H	130	ASP	N-CA-C	5.87	118.78	110.50
1	J	12	MET	N-CA-C	5.73	118.07	108.73
3	K	475	ASP	O-C-N	5.73	129.32	122.27
1	J	76	SER	O-C-N	5.58	129.80	122.93
3	H	98	ASN	O-C-N	-5.56	115.81	122.15
1	C	91	GLY	N-CA-C	5.56	117.23	111.95
1	E	31	ALA	O-C-N	-5.53	114.83	122.46
1	D	78	ALA	O-C-N	-5.48	116.55	123.01
1	D	110	LYS	CA-C-N	-5.43	114.31	122.07
1	D	110	LYS	C-N-CA	-5.43	114.31	122.07
3	K	476	MET	CA-C-N	5.39	128.08	120.42
3	K	476	MET	C-N-CA	5.39	128.08	120.42
3	K	190	ASP	N-CA-C	5.36	117.12	111.28
3	H	138	ASP	O-C-N	-5.35	115.48	122.59
3	H	395	LEU	N-CA-C	5.31	117.34	110.65
3	H	94	ARG	N-CA-C	-5.30	105.19	110.97
3	H	397	HIS	N-CA-C	5.17	116.96	110.91
1	A	188	VAL	CA-C-O	-5.15	118.15	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	69	ASN	CA-CB-CG	5.13	117.73	112.60
3	H	99	ASP	CA-C-N	-5.11	113.38	120.38
3	H	99	ASP	C-N-CA	-5.11	113.38	120.38
3	K	142	THR	O-C-N	5.00	128.40	122.20

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	675	0	487	9	0
1	B	1415	0	1383	32	0
1	C	1508	0	1506	26	0
1	D	1529	0	1549	37	0
1	E	1518	0	1536	28	0
1	F	1428	0	1429	27	0
1	J	1529	0	1557	24	0
2	G	1515	0	1358	28	0
3	H	4127	0	4004	95	0
3	I	1310	0	1260	28	0
3	K	1931	0	1824	45	0
3	L	1091	0	922	41	0
4	M	963	0	488	31	0
5	N	635	0	324	7	0
6	A	1	0	0	0	0
6	B	1	0	0	1	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	2	0	0	0	0
6	J	1	0	0	0	0
All	All	21183	0	19627	402	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 10.

All (402) 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:B:84:CYS:HG	6:B:301:ZN:ZN	0.67	0.91
3:K:189:VAL:HG11	3:K:386:LEU:HD21	1.53	0.90
3:H:227:ILE:HG22	3:H:339:ILE:HB	1.53	0.88
3:I:452:LEU:HD23	3:L:460:VAL:HG13	1.58	0.86
3:K:485:MET:HE1	3:L:471:LYS:HZ3	1.42	0.83
1:D:176:TRP:HB3	1:D:179:LYS:HD3	1.61	0.82
3:I:443:ASN:HD21	3:K:486:ARG:HH22	1.27	0.81
3:L:526:LEU:HD21	3:L:587:LEU:HD21	1.61	0.81
3:H:95:LEU:HB3	3:H:257:MET:HE1	1.64	0.80
2:G:192:SER:OG	4:M:-6:U:H5''	1.83	0.79
3:H:239:LEU:HD11	3:H:253:ILE:HD11	1.68	0.76
2:G:192:SER:CB	4:M:-6:U:H5''	2.18	0.74
1:B:84:CYS:SG	1:B:87:CYS:HB2	2.28	0.73
3:L:588:LEU:O	3:L:591:ILE:HG12	1.88	0.72
3:K:485:MET:HE2	3:K:485:MET:HA	1.72	0.70
3:H:85:SER:HB3	3:H:125:TRP:HE1	1.56	0.70
3:I:542:GLN:HG3	3:I:591:ILE:HG22	1.72	0.70
3:K:444:MET:HE3	3:K:452:LEU:O	1.92	0.69
1:B:49:ILE:HB	1:B:104:LEU:HB2	1.73	0.69
3:H:144:TYR:O	3:H:153:VAL:HA	1.93	0.69
3:I:443:ASN:HD22	3:I:596:ASN:HB3	1.58	0.68
3:H:85:SER:O	3:H:127:GLU:HA	1.94	0.68
1:E:32:GLN:HA	1:E:35:VAL:O	1.94	0.68
1:J:156:LYS:O	1:J:160:LEU:HD12	1.93	0.67
3:H:66:ASP:HB2	3:H:67:HIS:HD2	1.59	0.66
5:N:37:C:H3'	5:N:38:U:O4'	1.95	0.66
1:J:41:LYS:HZ2	1:J:110:LYS:HD3	1.60	0.66
3:I:542:GLN:HG3	3:I:591:ILE:CG2	2.26	0.66
3:K:508:MET:HG3	3:K:513:ILE:HG13	1.78	0.66
3:H:227:ILE:HD11	3:H:312:ILE:HG12	1.77	0.65
1:B:88:SER:HA	1:B:95:ARG:NH2	2.12	0.65
3:H:57:ILE:HD11	3:H:137:PHE:HD1	1.60	0.65
3:H:65:LEU:O	3:H:66:ASP:C	2.38	0.65
2:G:192:SER:HB3	4:M:-6:U:H5''	1.79	0.65
3:H:73:LEU:HD13	3:H:112:LEU:HB3	1.78	0.64
1:B:12:MET:O	1:B:143:THR:HA	1.97	0.63
1:J:121:ARG:HB3	1:J:131:ASP:HB2	1.80	0.63
2:G:65:LEU:HB2	2:G:117:ARG:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:91:GLU:HG3	3:H:94:ARG:HH21	1.63	0.63
1:D:111:GLU:O	1:D:111:GLU:HG2	1.98	0.63
3:L:598:VAL:HA	3:L:601:ILE:HD12	1.79	0.62
3:H:236:GLN:HG2	3:H:265:ILE:HG13	1.81	0.62
3:I:526:LEU:HD21	3:I:587:LEU:HD11	1.81	0.61
3:H:226:LEU:HD12	3:H:326:HIS:HB3	1.82	0.61
3:H:1:MET:HE1	3:H:161:ASN:HB2	1.83	0.61
1:J:93:MET:HE1	4:M:14:A:H2	1.65	0.61
3:K:526:LEU:HD21	3:K:587:LEU:HD11	1.83	0.60
3:L:530:ARG:NH2	3:L:563:ASN:O	2.35	0.60
3:H:84:ILE:HG13	3:H:126:ASP:O	2.02	0.60
3:L:526:LEU:HD11	3:L:587:LEU:CD2	2.31	0.60
1:F:7:LYS:NZ	1:F:149:THR:OG1	2.34	0.60
1:A:13:LYS:H	1:A:185:SER:HB3	1.67	0.60
1:B:59:LEU:HG	1:B:164:ALA:HB2	1.84	0.59
1:F:49:ILE:HB	1:F:104:LEU:HB2	1.84	0.59
4:M:12:G:H1'	4:M:13:G:C8	2.37	0.59
3:H:127:GLU:HG3	3:H:540:LYS:HD3	1.85	0.59
1:C:98:ARG:NH1	1:C:152:ASN:O	2.36	0.59
3:H:104:GLN:OE1	3:H:111:PRO:HA	2.02	0.58
3:I:468:ILE:HD11	3:L:437:LEU:HD21	1.84	0.58
3:K:485:MET:HE1	3:L:471:LYS:NZ	2.16	0.58
3:L:564:TRP:HB2	3:L:580:TYR:CE1	2.40	0.57
1:D:172:GLY:HA3	1:D:177:LEU:HD22	1.87	0.57
2:G:30:ARG:NH1	2:G:190:VAL:O	2.37	0.57
3:L:530:ARG:HH22	5:N:34:A:H5''	1.70	0.57
3:K:436:VAL:HA	3:K:466:ILE:O	2.05	0.57
1:B:5:MET:HG2	1:B:151:SER:HA	1.87	0.57
1:C:59:LEU:HG	1:C:164:ALA:HB2	1.87	0.57
3:H:60:LEU:HD21	3:H:71:VAL:HG21	1.87	0.57
3:I:567:PRO:HG2	3:I:576:ILE:HG12	1.87	0.56
1:E:40:ARG:HD3	1:E:48:LEU:HB3	1.86	0.56
1:D:62:MET:HE3	1:D:167:PHE:HB2	1.86	0.56
1:B:12:MET:HE3	1:B:184:VAL:HG21	1.87	0.56
3:H:90:LYS:HD3	3:H:127:GLU:OE2	2.06	0.56
3:K:542:GLN:NE2	3:K:591:ILE:O	2.39	0.56
4:M:19:A:HO2'	4:M:20:A:H8	1.52	0.55
1:F:188:VAL:HG12	1:F:189:LYS:H	1.71	0.55
1:E:124:ARG:NH1	4:M:11:U:OP1	2.39	0.55
3:H:525:ILE:HD11	3:H:567:PRO:HG3	1.87	0.55
3:H:189:VAL:O	3:K:416:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:65:LEU:HG	3:H:96:LEU:HD12	1.88	0.55
3:I:505:LEU:HD21	3:I:546:ILE:HD11	1.88	0.55
1:J:49:ILE:HB	1:J:104:LEU:HB2	1.88	0.55
1:B:177:LEU:O	1:B:183:ARG:NH2	2.40	0.55
2:G:36:ILE:HG22	2:G:51:PHE:CZ	2.43	0.54
1:E:80:PRO:HD2	1:E:93:MET:HE2	1.87	0.54
3:H:228:PRO:HD2	3:H:339:ILE:O	2.07	0.54
3:I:478:TRP:O	3:I:482:TYR:HB3	2.07	0.54
3:K:511:ASP:OD2	3:K:511:ASP:N	2.41	0.54
3:H:85:SER:HB3	3:H:125:TRP:NE1	2.22	0.54
3:L:587:LEU:O	3:L:591:ILE:HG23	2.07	0.54
1:A:8:ILE:HA	1:A:190:SER:HA	1.88	0.54
1:F:167:PHE:O	1:F:170:GLU:HG3	2.07	0.54
1:B:100:SER:OG	1:C:183:ARG:NH2	2.41	0.54
1:D:25:ARG:NH1	1:E:116:GLU:OE1	2.41	0.54
2:G:128:LEU:O	2:G:129:ASN:C	2.51	0.54
1:B:120:LEU:HA	1:B:132:THR:HG22	1.90	0.54
2:G:26:TYR:CE2	2:G:83:LEU:HD11	2.43	0.54
1:D:23:VAL:HB	1:E:117:SER:HB2	1.90	0.54
1:E:100:SER:HB3	1:F:183:ARG:HH22	1.73	0.54
3:I:531:ILE:HG23	3:I:602:LEU:HD22	1.90	0.53
1:D:60:GLU:HG2	1:D:86:THR:HG21	1.89	0.53
2:G:32:LEU:HD12	2:G:64:LEU:HD11	1.90	0.53
3:K:186:ASP:OD1	3:K:186:ASP:N	2.41	0.53
3:K:534:PHE:HE2	3:K:590:LEU:HD23	1.73	0.53
3:K:436:VAL:HG22	3:K:466:ILE:HB	1.90	0.53
1:D:109:THR:OG1	1:D:110:LYS:N	2.42	0.53
3:K:445:CYS:SG	3:K:446:ASN:N	2.82	0.53
3:H:276:LEU:HD22	3:H:285:LEU:HD11	1.91	0.53
3:I:437:LEU:HD21	3:L:435:VAL:HG11	1.90	0.52
1:E:12:MET:HB2	1:E:186:PHE:CD1	2.45	0.52
1:J:6:LYS:HB3	1:J:150:ILE:HB	1.90	0.52
3:K:473:TRP:HA	3:K:476:MET:SD	2.50	0.52
3:K:165:LEU:HD12	3:K:192:LEU:HD12	1.92	0.52
1:B:107:ASN:HD21	1:B:145:THR:HG23	1.74	0.52
3:H:129:ASP:CG	3:H:541:GLY:HA3	2.35	0.52
1:D:49:ILE:HB	1:D:104:LEU:HB2	1.92	0.52
1:F:188:VAL:HG12	1:F:189:LYS:N	2.25	0.52
2:G:36:ILE:HD13	2:G:134:ILE:HD13	1.90	0.52
3:H:444:MET:HE3	3:K:461:GLU:HB2	1.90	0.52
1:B:12:MET:SD	1:B:104:LEU:HD13	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:PHE:HZ	1:F:165:LEU:HD11	1.75	0.51
1:A:163:SER:O	1:A:166:LYS:N	2.44	0.51
1:C:108:ASP:HB2	1:C:113:ILE:HG21	1.92	0.51
1:E:33:LYS:HE3	3:K:487:SER:HB2	1.92	0.51
3:H:62:HIS:HE2	3:H:67:HIS:CE1	2.28	0.51
1:F:23:VAL:HB	2:G:100:ILE:HG23	1.90	0.51
3:H:184:MET:HE3	3:H:385:ARG:HB3	1.91	0.51
1:A:84:CYS:HB2	1:A:87:CYS:SG	2.49	0.51
3:H:523:ILE:HD12	3:H:567:PRO:HB3	1.93	0.51
3:H:211:LEU:HD21	3:H:238:VAL:HG13	1.92	0.51
2:G:128:LEU:O	2:G:131:MET:N	2.44	0.51
3:H:19:GLU:HG2	3:H:24:LYS:HG2	1.92	0.51
1:J:52:LYS:NZ	4:M:16:U:OP1	2.43	0.51
1:C:77:ARG:HH21	3:H:561:ARG:HH21	1.59	0.51
1:B:101:VAL:HG22	1:B:148:ILE:HG12	1.93	0.51
1:D:18:LEU:HB3	1:D:138:VAL:HB	1.92	0.51
1:F:20:THR:HG21	1:F:50:PRO:HD2	1.93	0.51
1:C:12:MET:HB3	1:C:144:PHE:HB2	1.92	0.51
1:E:18:LEU:HB3	1:E:138:VAL:HB	1.93	0.51
1:A:7:LYS:O	1:A:191:GLU:N	2.41	0.50
1:C:16:SER:OG	1:C:180:GLY:O	2.29	0.50
1:E:178:ASN:ND2	4:M:9:G:OP1	2.40	0.50
3:H:528:LYS:O	3:H:606:ASN:ND2	2.44	0.50
3:K:189:VAL:CG1	3:K:386:LEU:HD11	2.41	0.50
3:L:595:LYS:HG2	3:L:596:ASN:N	2.26	0.50
1:A:156:LYS:O	1:A:160:LEU:HG	2.12	0.50
1:C:51:PHE:HZ	1:C:165:LEU:HD21	1.76	0.50
1:E:121:ARG:HB3	1:E:131:ASP:HB2	1.94	0.50
3:H:262:THR:HG22	3:H:266:LYS:HZ3	1.76	0.50
1:B:102:ASP:OD1	1:B:146:ALA:HB1	2.11	0.50
1:E:59:LEU:HD12	1:E:90:PHE:HE2	1.76	0.50
3:H:101:GLN:NE2	3:H:113:TYR:O	2.42	0.50
2:G:8:LEU:HD22	2:G:156:PHE:HB3	1.93	0.50
3:I:530:ARG:NH2	3:I:563:ASN:O	2.44	0.49
3:H:30:GLY:HA2	3:H:70:LEU:H	1.77	0.49
1:J:93:MET:HE1	4:M:14:A:C2	2.47	0.49
2:G:51:PHE:HB3	4:M:-8:G:N9	2.28	0.49
2:G:140:SER:O	2:G:141:TYR:CD2	2.64	0.49
3:H:102:ARG:NH2	3:H:106:GLU:OE1	2.45	0.49
3:K:189:VAL:HG11	3:K:386:LEU:HD11	1.94	0.49
3:L:470:ASP:HB2	3:L:472:ASN:OD1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LYS:HE3	1:C:178:ASN:HB3	1.93	0.49
2:G:181:ILE:HD12	2:G:229:GLY:HA3	1.95	0.49
3:H:293:ILE:HG23	3:H:298:GLN:HB2	1.93	0.49
1:J:122:ILE:O	1:J:124:ARG:NH1	2.43	0.49
1:F:12:MET:SD	1:F:186:PHE:CE1	3.05	0.49
3:H:459:ILE:HB	3:K:453:MET:HB3	1.93	0.49
3:H:49:ILE:HG13	3:H:73:LEU:HD23	1.95	0.49
3:H:530:ARG:HH22	5:N:16:U:H5''	1.77	0.49
3:K:508:MET:SD	3:K:589:SER:OG	2.69	0.49
3:L:530:ARG:HH12	5:N:34:A:H5''	1.77	0.49
1:D:120:LEU:O	4:M:16:U:O2'	2.30	0.49
3:I:584:TYR:O	3:I:588:LEU:HB2	2.13	0.49
3:H:57:ILE:HD11	3:H:137:PHE:CD1	2.46	0.48
3:L:472:ASN:OD1	3:L:473:TRP:N	2.46	0.48
1:C:14:THR:HA	1:C:184:VAL:HG12	1.94	0.48
3:H:91:GLU:HG3	3:H:94:ARG:NH2	2.26	0.48
3:H:227:ILE:O	3:H:227:ILE:HG13	2.13	0.48
3:H:227:ILE:CG2	3:H:339:ILE:HB	2.36	0.48
3:H:476:MET:SD	3:H:476:MET:N	2.86	0.48
1:F:12:MET:HE3	1:F:184:VAL:HG11	1.96	0.48
3:H:590:LEU:HG	3:H:598:VAL:HG22	1.94	0.48
2:G:18:LEU:HD21	2:G:24:ALA:HB2	1.96	0.48
3:L:525:ILE:HA	3:L:565:ASN:HB2	1.96	0.48
3:L:535:TRP:C	3:L:537:GLU:N	2.67	0.48
3:L:596:ASN:HA	3:L:599:TYR:HB3	1.96	0.48
1:D:197:ARG:NH2	1:E:170:GLU:OE1	2.47	0.48
1:F:56:ARG:NH2	1:F:91:GLY:O	2.46	0.48
1:C:77:ARG:NH2	3:H:561:ARG:HH21	2.11	0.48
1:D:14:THR:HG22	1:D:140:GLU:HA	1.96	0.47
3:H:91:GLU:O	3:H:95:LEU:HD13	2.14	0.47
3:H:214:ILE:HA	3:H:217:THR:HG22	1.94	0.47
3:K:508:MET:HE1	3:K:516:ASN:ND2	2.28	0.47
3:L:526:LEU:HD11	3:L:587:LEU:HD22	1.96	0.47
1:D:106:SER:OG	1:D:108:ASP:O	2.31	0.47
1:D:73:THR:HG23	1:E:124:ARG:HH21	1.79	0.47
3:L:526:LEU:HD11	3:L:587:LEU:HD21	1.96	0.47
1:B:10:VAL:HG12	1:B:188:VAL:HG22	1.97	0.47
1:F:26:GLU:HB2	2:G:98:ARG:HD2	1.95	0.47
1:J:58:ALA:O	1:J:62:MET:HG3	2.14	0.47
1:E:47:VAL:HG11	1:E:138:VAL:HG21	1.96	0.47
3:K:441:THR:OG1	3:K:442:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:GLN:N	1:B:154:GLN:OE1	2.48	0.47
2:G:181:ILE:HD13	2:G:206:LYS:HD3	1.96	0.47
3:L:597:LYS:HA	3:L:600:ASN:HD21	1.79	0.47
5:N:37:C:H2'	5:N:37:C:O2	2.14	0.47
1:D:8:ILE:HB	1:D:148:ILE:HB	1.97	0.47
1:E:53:GLY:O	1:E:57:SER:OG	2.31	0.47
1:E:100:SER:HB2	1:E:149:THR:OG1	2.14	0.47
1:E:193:VAL:HB	1:E:197:ARG:HD3	1.96	0.47
3:H:140:LYS:HB2	3:H:158:GLU:HB2	1.96	0.47
1:D:40:ARG:HG2	1:D:48:LEU:HB3	1.97	0.47
3:H:508:MET:HE1	3:H:516:ASN:HD22	1.80	0.47
1:C:196:ASP:OD1	1:C:196:ASP:N	2.36	0.46
3:H:130:ASP:OD1	3:H:543:LYS:NZ	2.44	0.46
3:H:134:ILE:O	3:H:140:LYS:HA	2.14	0.46
3:I:530:ARG:HH22	5:N:22:A:H5''	1.79	0.46
1:D:140:GLU:OE1	1:D:140:GLU:N	2.43	0.46
1:E:22:GLU:HB2	1:E:38:PRO:HG2	1.97	0.46
2:G:65:LEU:H	2:G:117:ARG:HG2	1.79	0.46
1:J:59:LEU:HD12	1:J:90:PHE:HE2	1.80	0.46
3:H:546:ILE:HG12	3:H:591:ILE:HG21	1.96	0.46
1:B:84:CYS:SG	1:B:87:CYS:CB	3.01	0.46
1:D:24:ARG:HB2	1:D:27:ASP:HB2	1.96	0.46
3:H:144:TYR:HB3	3:H:183:ASP:HB3	1.96	0.46
1:J:71:CYS:HB3	1:J:81:CYS:SG	2.54	0.46
3:K:194:LEU:HD22	3:K:379:LEU:HD12	1.97	0.46
3:K:553:HIS:O	3:K:562:ARG:NH1	2.48	0.46
1:C:49:ILE:HB	1:C:104:LEU:HB2	1.98	0.46
1:D:100:SER:OG	1:E:183:ARG:NH2	2.48	0.46
3:H:433:LYS:HD3	3:H:464:ASP:HA	1.97	0.46
3:I:578:LYS:HE3	3:I:578:LYS:HB3	1.77	0.46
3:I:459:ILE:HG13	3:L:455:PHE:CD1	2.50	0.46
3:K:189:VAL:HG13	3:K:189:VAL:O	2.16	0.46
4:M:19:A:O2'	4:M:20:A:H8	1.98	0.46
1:A:52:LYS:HB2	1:A:101:VAL:HB	1.98	0.46
3:K:485:MET:SD	3:L:458:PHE:HE1	2.39	0.46
1:B:6:LYS:HB3	1:B:150:ILE:HB	1.99	0.45
1:F:20:THR:O	1:F:40:ARG:N	2.48	0.45
1:J:108:ASP:HB2	1:J:113:ILE:HG12	1.97	0.45
1:E:12:MET:HE3	1:E:184:VAL:HG11	1.98	0.45
3:H:90:LYS:HD3	3:H:127:GLU:CD	2.40	0.45
1:D:59:LEU:HG	1:D:164:ALA:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:36:ILE:HG22	2:G:51:PHE:HZ	1.82	0.45
3:H:99:ASP:O	3:H:100:PHE:C	2.59	0.45
3:L:455:PHE:HD2	3:L:457:GLY:H	1.65	0.45
1:C:18:LEU:HB3	1:C:138:VAL:HB	1.97	0.45
3:H:375:ASP:OD1	3:H:376:GLN:N	2.50	0.45
1:J:41:LYS:HB3	1:J:41:LYS:HE3	1.76	0.45
3:K:505:LEU:HD11	3:K:546:ILE:HD11	1.99	0.45
3:K:514:ILE:O	3:K:518:GLU:HG3	2.17	0.45
1:B:95:ARG:HB3	1:B:95:ARG:NH1	2.32	0.45
3:K:513:ILE:HG21	3:K:590:LEU:HD13	1.98	0.45
1:F:8:ILE:HB	1:F:148:ILE:HG12	1.99	0.45
1:F:40:ARG:HG2	1:F:48:LEU:HB2	1.97	0.45
3:K:518:GLU:HG2	3:K:605:PHE:HZ	1.82	0.45
1:A:7:LYS:O	1:A:190:SER:HA	2.16	0.45
3:H:146:ASN:O	3:H:171:GLY:N	2.44	0.45
3:I:442:ASP:OD1	3:I:442:ASP:N	2.49	0.45
1:D:35:VAL:HG11	1:D:136:GLU:HB2	1.98	0.45
3:H:460:VAL:HG22	3:K:452:LEU:CD2	2.46	0.45
3:L:471:LYS:HE3	3:L:471:LYS:HB3	1.81	0.45
1:D:20:THR:O	1:D:40:ARG:N	2.47	0.44
1:B:7:LYS:HD2	1:B:149:THR:HG23	1.99	0.44
1:C:104:LEU:HB3	1:C:144:PHE:HB3	2.00	0.44
1:D:20:THR:HG21	1:D:49:ILE:HG12	1.99	0.44
1:D:45:ASN:O	1:D:110:LYS:N	2.45	0.44
1:F:120:LEU:HB2	4:M:5:U:H3'	1.99	0.44
3:L:535:TRP:C	3:L:537:GLU:H	2.25	0.44
1:B:12:MET:HB2	1:B:144:PHE:HB2	1.99	0.44
1:B:58:ALA:O	1:B:62:MET:HG3	2.17	0.44
1:C:92:SER:O	4:M:21:A:H5'	2.16	0.44
3:H:555:LYS:HE3	3:H:555:LYS:HB2	1.84	0.44
1:J:123:GLU:HG2	1:J:130:SER:HB2	2.00	0.44
4:M:9:G:C6	4:M:10:C:N4	2.85	0.44
1:E:63:LEU:HB3	1:E:70:VAL:HG21	1.98	0.44
3:H:17:LEU:HD21	3:H:24:LYS:HE3	1.99	0.44
1:J:18:LEU:HB3	1:J:138:VAL:HB	1.99	0.44
1:B:178:ASN:ND2	4:M:33:U:OP1	2.51	0.44
1:J:40:ARG:HG2	1:J:48:LEU:HB3	1.99	0.44
3:K:520:LEU:HD23	3:K:523:ILE:HD11	1.99	0.44
1:D:110:LYS:HE2	1:D:110:LYS:HB3	1.81	0.44
1:J:120:LEU:O	4:M:22:U:O2'	2.35	0.44
1:B:16:SER:OG	1:B:183:ARG:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:12:MET:O	1:F:143:THR:HA	2.17	0.44
3:H:225:VAL:HG22	3:H:227:ILE:HG23	1.99	0.44
3:L:599:TYR:CZ	3:L:603:ILE:HD11	2.53	0.44
1:C:178:ASN:ND2	4:M:27:U:OP1	2.40	0.44
2:G:111:ILE:HD12	2:G:112:GLU:O	2.17	0.44
3:H:94:ARG:O	3:H:95:LEU:C	2.60	0.44
3:I:443:ASN:O	3:I:453:MET:HG3	2.17	0.44
1:C:12:MET:HE3	1:C:104:LEU:HD22	2.00	0.43
1:C:177:LEU:O	1:C:183:ARG:NH2	2.42	0.43
1:C:101:VAL:HG22	1:C:148:ILE:HG12	1.99	0.43
1:F:101:VAL:HA	1:F:148:ILE:HG22	1.99	0.43
2:G:127:TYR:O	2:G:130:GLU:HB3	2.18	0.43
3:L:469:ASN:HD22	3:L:473:TRP:NE1	2.16	0.43
1:D:120:LEU:HD12	1:D:120:LEU:HA	1.83	0.43
1:D:156:LYS:HE3	1:D:156:LYS:HB3	1.78	0.43
1:F:121:ARG:HB3	1:F:131:ASP:HB2	2.01	0.43
3:H:608:LYS:HD2	3:H:608:LYS:N	2.34	0.43
3:H:189:VAL:HG21	3:H:386:LEU:HD22	2.00	0.43
4:M:3:U:O4	4:M:4:C:N4	2.51	0.43
3:L:525:ILE:HD11	3:L:580:TYR:CD1	2.54	0.43
1:F:22:GLU:HB3	1:F:38:PRO:HG2	2.00	0.43
3:H:97:PHE:HB3	3:H:118:ILE:HD12	1.99	0.43
3:H:527:SER:OG	5:N:17:U:OP1	2.35	0.43
3:L:549:ILE:HG22	3:L:584:TYR:CE1	2.54	0.43
1:C:13:LYS:HG2	1:C:141:GLY:HA2	2.01	0.43
3:H:191:TYR:HB3	3:H:394:PHE:HE1	1.84	0.43
3:H:240:TYR:CZ	3:H:276:LEU:HD21	2.54	0.43
3:K:403:ARG:O	3:K:407:ALA:N	2.44	0.43
1:B:36:ASN:N	1:B:134:LYS:O	2.48	0.43
1:E:59:LEU:HD23	1:E:59:LEU:HA	1.87	0.43
3:H:137:PHE:O	3:H:138:ASP:C	2.62	0.43
1:C:108:ASP:HB2	1:C:113:ILE:CG2	2.48	0.42
1:J:3:LYS:HE3	1:J:3:LYS:HB3	1.91	0.42
1:D:119:HIS:NE2	1:D:181:TYR:OH	2.41	0.42
1:D:170:GLU:OE2	1:J:197:ARG:NH2	2.42	0.42
1:E:106:SER:OG	1:E:108:ASP:O	2.34	0.42
1:F:89:LEU:HD23	1:F:99:ALA:HB2	2.02	0.42
3:I:546:ILE:HD13	3:I:546:ILE:HA	1.92	0.42
3:L:470:ASP:OD1	3:L:470:ASP:N	2.52	0.42
4:M:13:G:H2'	4:M:14:A:H8	1.84	0.42
3:H:507:ASP:OD2	3:H:507:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:18:G:C2	4:M:19:A:C6	3.07	0.42
1:B:91:GLY:HA3	4:M:27:U:H5''	2.02	0.42
1:D:110:LYS:HG2	1:D:111:GLU:H	1.83	0.42
3:H:64:HIS:O	3:H:65:LEU:C	2.59	0.42
3:H:86:THR:HA	3:H:128:ILE:O	2.20	0.42
3:H:447:PHE:HB2	3:L:454:PRO:HB2	2.01	0.42
3:H:186:ASP:OD1	3:H:186:ASP:N	2.49	0.42
3:H:241:THR:HG21	3:H:370:PHE:HE1	1.85	0.42
3:K:189:VAL:HG11	3:K:386:LEU:CD2	2.35	0.42
1:A:157:ASP:HA	1:A:160:LEU:HD12	2.02	0.42
1:C:121:ARG:NH1	4:M:28:G:N3	2.68	0.42
1:F:110:LYS:HE2	1:F:110:LYS:HB3	1.81	0.42
1:F:187:GLU:HG3	1:F:188:VAL:N	2.35	0.42
3:H:273:LYS:HB2	3:H:276:LEU:HD12	2.01	0.42
3:I:479:ASN:O	3:I:483:ASN:ND2	2.53	0.42
3:K:395:LEU:HD23	3:K:395:LEU:HA	1.93	0.42
1:B:98:ARG:NH2	1:B:154:GLN:OE1	2.52	0.42
1:F:91:GLY:HA3	4:M:-3:A:H5''	2.02	0.42
3:H:505:LEU:HD12	3:H:505:LEU:HA	1.85	0.42
1:E:126:THR:OG1	1:E:128:SER:OG	2.31	0.42
3:H:128:ILE:HD11	3:H:132:ASN:CG	2.45	0.42
3:H:512:LYS:HA	3:H:512:LYS:HD2	1.87	0.42
2:G:28:ALA:HA	2:G:63:ASP:HB3	2.02	0.41
3:H:218:THR:HG21	3:H:337:THR:HG23	2.00	0.41
1:J:109:THR:HG23	1:J:111:GLU:H	1.85	0.41
3:K:188:ASN:HB3	3:K:388:TYR:HD2	1.84	0.41
1:C:40:ARG:HG2	1:C:48:LEU:HB3	2.01	0.41
1:C:92:SER:OG	1:C:93:MET:N	2.53	0.41
3:H:251:VAL:O	3:H:290:TYR:HA	2.19	0.41
3:H:518:GLU:HG3	3:H:605:PHE:HE1	1.84	0.41
3:K:508:MET:HE1	3:K:516:ASN:HD22	1.85	0.41
1:D:121:ARG:HB2	4:M:16:U:H1'	2.01	0.41
3:H:131:ARG:HH11	3:H:183:ASP:CG	2.28	0.41
3:H:298:GLN:HA	3:H:301:GLU:HG2	2.02	0.41
3:I:525:ILE:HD11	3:I:567:PRO:HG3	2.02	0.41
3:L:530:ARG:HH21	3:L:564:TRP:HA	1.86	0.41
1:C:79:ARG:O	1:C:79:ARG:HG3	2.21	0.41
3:H:129:ASP:OD2	3:H:541:GLY:HA3	2.19	0.41
3:H:226:LEU:HD23	3:H:228:PRO:HD3	2.03	0.41
3:I:474:PHE:HA	3:I:477:ILE:HG22	2.02	0.41
3:K:570:ASP:OD1	3:K:570:ASP:N	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:MET:HE2	1:D:144:PHE:HB2	2.02	0.41
1:E:91:GLY:HA3	4:M:3:U:H5''	2.02	0.41
1:F:109:THR:OG1	1:F:110:LYS:N	2.53	0.41
3:I:474:PHE:O	3:I:478:TRP:HB2	2.20	0.41
1:J:178:ASN:ND2	4:M:21:A:OP1	2.54	0.41
1:B:104:LEU:HD23	1:B:146:ALA:HB2	2.02	0.41
3:L:469:ASN:HD22	3:L:473:TRP:CD1	2.38	0.41
3:L:518:GLU:O	3:L:522:ASN:HB2	2.21	0.41
1:D:56:ARG:O	1:D:60:GLU:HG3	2.20	0.41
1:D:176:TRP:O	1:D:181:TYR:HB2	2.21	0.41
1:F:189:LYS:HE2	1:F:189:LYS:HB2	1.84	0.41
3:I:599:TYR:O	3:I:603:ILE:HB	2.21	0.41
1:J:196:ASP:HB2	1:J:199:LEU:HD12	2.02	0.41
1:B:96:ALA:HB2	4:M:26:G:H4'	2.02	0.41
3:K:382:TYR:HA	3:K:385:ARG:HG2	2.02	0.41
3:L:531:ILE:HG12	3:L:602:LEU:HD22	2.03	0.41
2:G:7:ILE:HG21	2:G:115:LYS:HE3	2.02	0.41
3:I:454:PRO:HA	3:L:458:PHE:CD1	2.56	0.41
3:I:469:ASN:ND2	3:I:473:TRP:HB2	2.35	0.41
1:D:175:GLY:O	1:D:177:LEU:HG	2.20	0.41
3:H:127:GLU:H	3:H:127:GLU:HG2	1.43	0.41
3:K:590:LEU:HG	3:K:598:VAL:HG22	2.02	0.41
4:M:0:U:H1'	4:M:1:C:C5	2.56	0.41
1:B:16:SER:HB3	1:B:183:ARG:HB2	2.03	0.40
3:H:297:ASN:HA	3:H:300:LYS:HD2	2.03	0.40
3:K:472:ASN:O	3:K:476:MET:HG3	2.21	0.40
1:E:5:MET:HG3	1:E:195:THR:HG22	2.02	0.40
3:L:597:LYS:HA	3:L:600:ASN:ND2	2.36	0.40
3:I:564:TRP:HH2	3:I:587:LEU:HD12	1.86	0.40
1:J:10:VAL:HG12	1:J:188:VAL:HG12	2.02	0.40
1:D:199:LEU:HD23	1:D:199:LEU:HA	1.90	0.40
2:G:66:PRO:HB2	2:G:74:PHE:HD2	1.86	0.40
2:G:176:LEU:O	2:G:212:GLY:N	2.54	0.40
2:G:105:LEU:HD21	4:M:-2:A:C5	2.57	0.40
3:H:567:PRO:HG2	3:H:576:ILE:HG12	2.03	0.40
3:L:587:LEU:HD13	3:L:587:LEU:HA	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/200 (52%)	97 (92%)	8 (8%)	0	100	100
1	B	185/200 (92%)	178 (96%)	7 (4%)	0	100	100
1	C	197/200 (98%)	194 (98%)	3 (2%)	0	100	100
1	D	197/200 (98%)	191 (97%)	6 (3%)	0	100	100
1	E	196/200 (98%)	191 (97%)	5 (3%)	0	100	100
1	F	185/200 (92%)	181 (98%)	4 (2%)	0	100	100
1	J	195/200 (98%)	190 (97%)	5 (3%)	0	100	100
2	G	199/240 (83%)	181 (91%)	18 (9%)	0	100	100
3	H	502/608 (83%)	467 (93%)	35 (7%)	0	100	100
3	I	151/608 (25%)	142 (94%)	9 (6%)	0	100	100
3	K	223/608 (37%)	206 (92%)	16 (7%)	1 (0%)	30	58
3	L	136/608 (22%)	128 (94%)	8 (6%)	0	100	100
All	All	2471/4072 (61%)	2346 (95%)	124 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	443	ASN

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	41/170 (24%)	39 (95%)	2 (5%)	22	51
1	B	148/170 (87%)	146 (99%)	2 (1%)	59	73
1	C	160/170 (94%)	156 (98%)	4 (2%)	42	66
1	D	165/170 (97%)	162 (98%)	3 (2%)	51	70
1	E	164/170 (96%)	162 (99%)	2 (1%)	63	75
1	F	153/170 (90%)	146 (95%)	7 (5%)	24	53
1	J	167/170 (98%)	166 (99%)	1 (1%)	78	81
2	G	136/209 (65%)	132 (97%)	4 (3%)	37	63
3	H	443/557 (80%)	435 (98%)	8 (2%)	51	70
3	I	143/557 (26%)	141 (99%)	2 (1%)	59	73
3	K	204/557 (37%)	198 (97%)	6 (3%)	37	63
3	L	102/557 (18%)	98 (96%)	4 (4%)	28	57
All	All	2026/3627 (56%)	1981 (98%)	45 (2%)	45	68

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	SER
1	A	100	SER
1	B	70	VAL
1	B	143	THR
1	C	36	ASN
1	C	123	GLU
1	C	152	ASN
1	C	189	LYS
1	D	11	THR
1	D	116	GLU
1	D	158	LEU
1	E	12	MET
1	E	151	SER
1	F	10	VAL
1	F	12	MET
1	F	39	VAL
1	F	89	LEU
1	F	93	MET
1	F	105	ILE
1	F	165	LEU
2	G	56	PHE
2	G	70	CYS

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Mol	Chain	Res	Type
2	G	120	ILE
2	G	158	ILE
3	H	103	ILE
3	H	127	GLU
3	H	135	GLU
3	H	338	LEU
3	H	365	GLU
3	H	468	ILE
3	H	477	ILE
3	H	577	GLU
3	I	442	ASP
3	I	589	SER
1	J	13	LYS
3	K	455	PHE
3	K	477	ILE
3	K	514	ILE
3	K	515	GLU
3	K	601	ILE
3	K	603	ILE
3	L	437	LEU
3	L	441	THR
3	L	587	LEU
3	L	591	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	107	ASN
1	B	152	ASN
1	C	171	ASN
1	D	36	ASN
1	D	152	ASN
1	D	178	ASN
1	F	112	GLN
1	F	125	GLN
3	H	67	HIS
3	H	297	ASN
3	I	443	ASN
3	I	556	ASN
3	I	558	ASN
1	J	36	ASN
3	K	469	ASN

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Mol	Chain	Res	Type
3	K	529	ASN
3	K	558	ASN
3	L	522	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	M	45/48 (93%)	15 (33%)	0
5	N	29/52 (55%)	5 (17%)	0
All	All	74/100 (74%)	20 (27%)	0

All (20) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	M	-7	U
4	M	-6	U
4	M	-2	A
4	M	0	U
4	M	4	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	31	C
4	M	36	C
4	M	37	G
5	N	10	A
5	N	33	G
5	N	36	G
5	N	37	C
5	N	38	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [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.

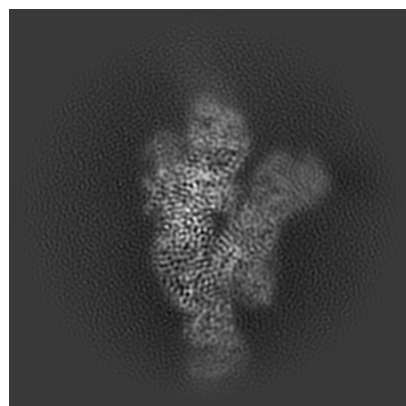
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39288. These allow visual inspection of the internal detail of the map and identification of artifacts.

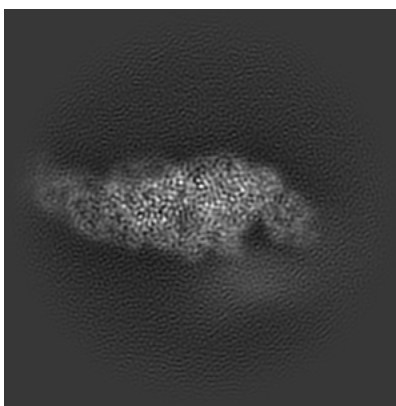
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

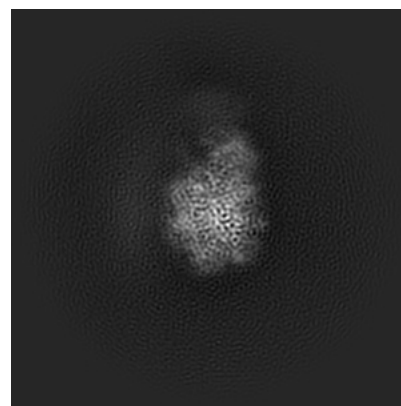
6.1.1 Primary map



X

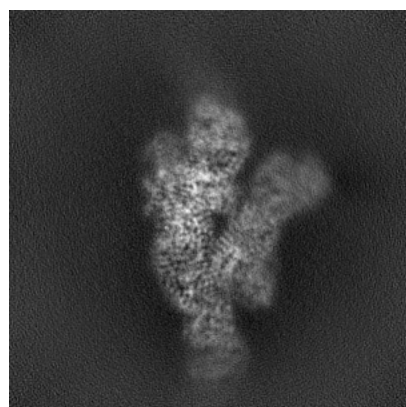


Y

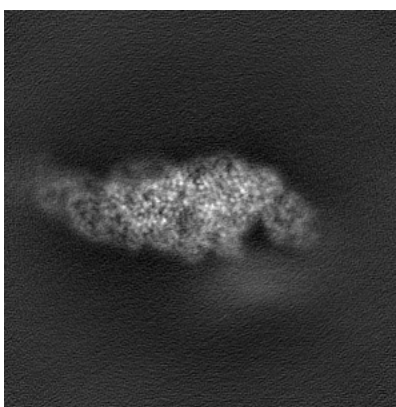


Z

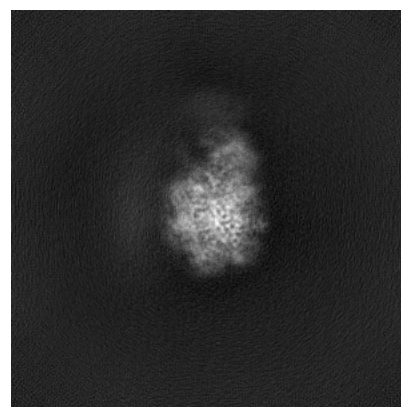
6.1.2 Raw map



X



Y

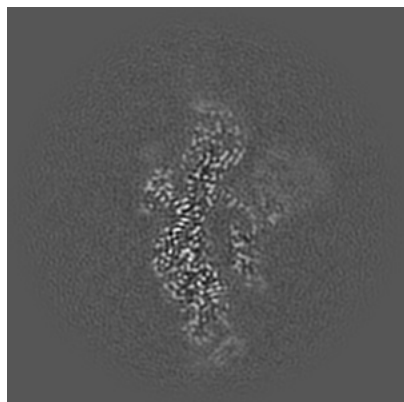


Z

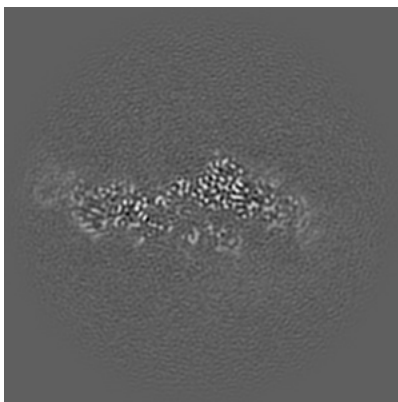
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

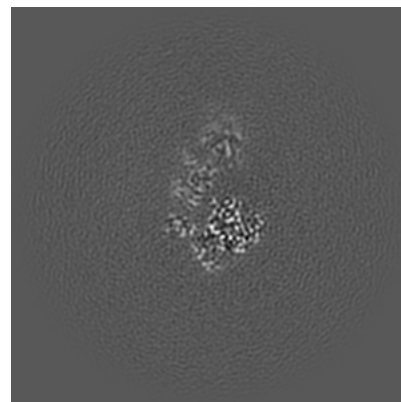
6.2.1 Primary map



X Index: 150

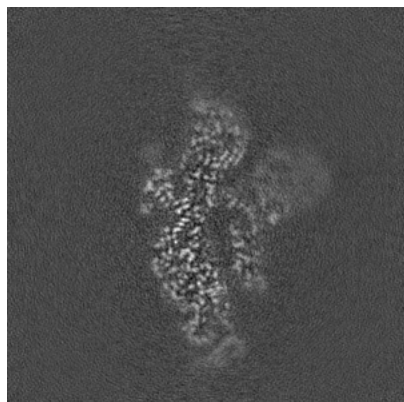


Y Index: 150

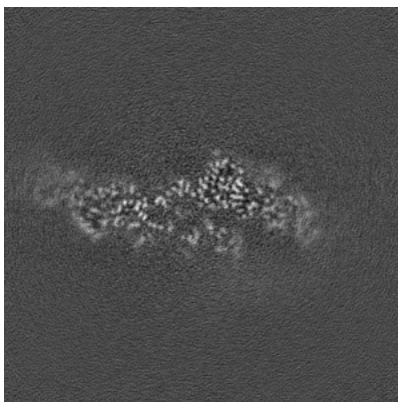


Z Index: 150

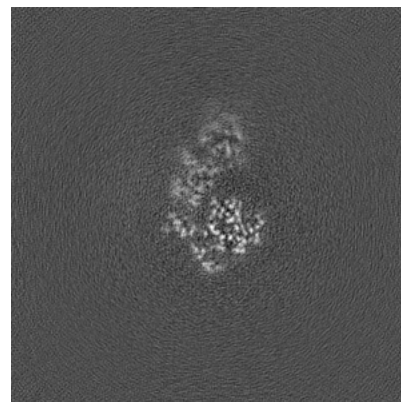
6.2.2 Raw map



X Index: 150



Y Index: 150

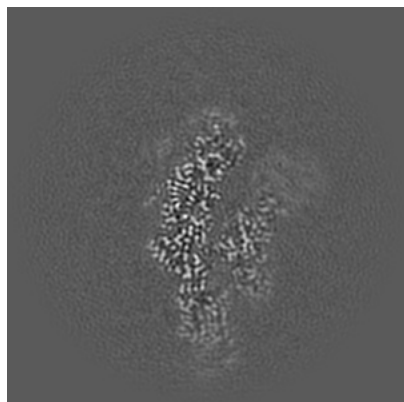


Z Index: 150

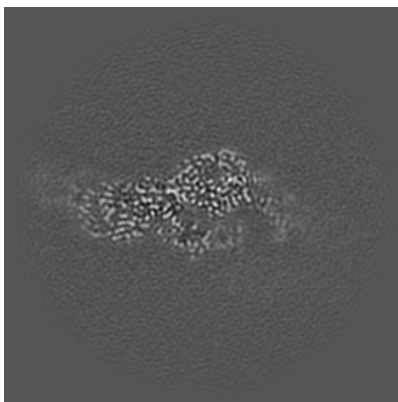
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

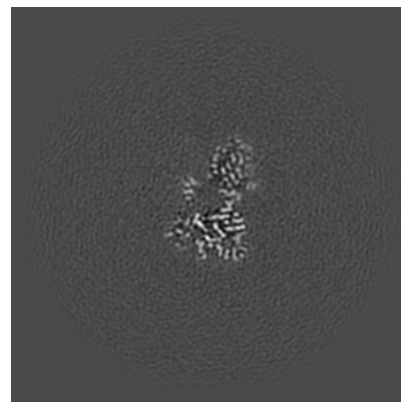
6.3.1 Primary map



X Index: 158

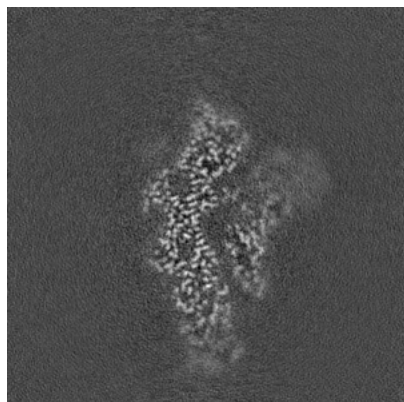


Y Index: 138

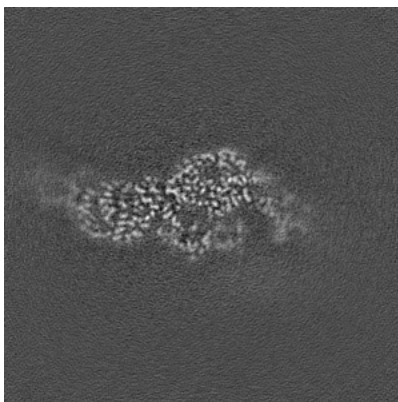


Z Index: 127

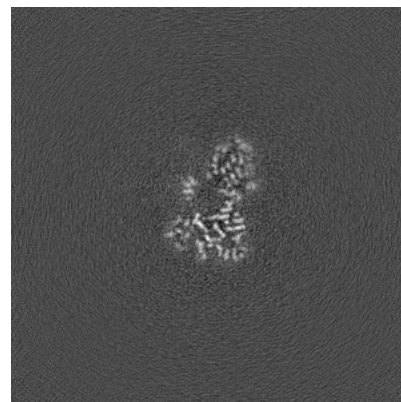
6.3.2 Raw map



X Index: 153



Y Index: 138

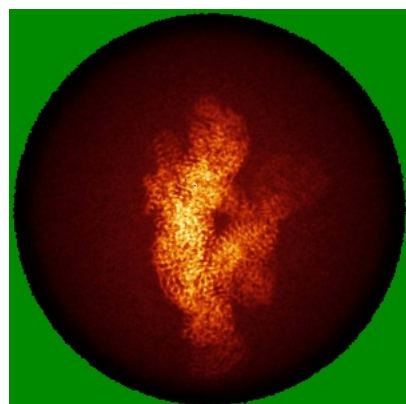


Z Index: 127

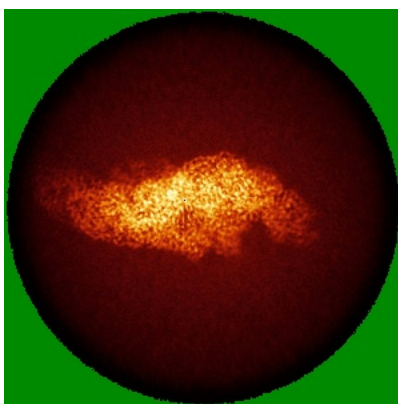
The images above show the largest variance slices of the map in three orthogonal directions.

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

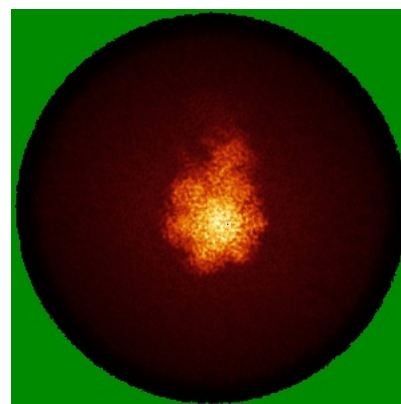
6.4.1 Primary map



X

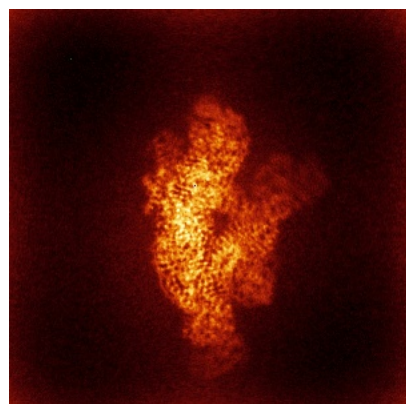


Y

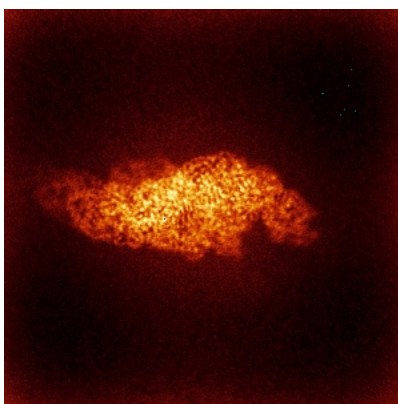


Z

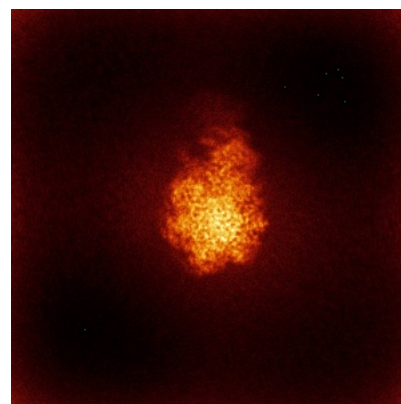
6.4.2 Raw map



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.

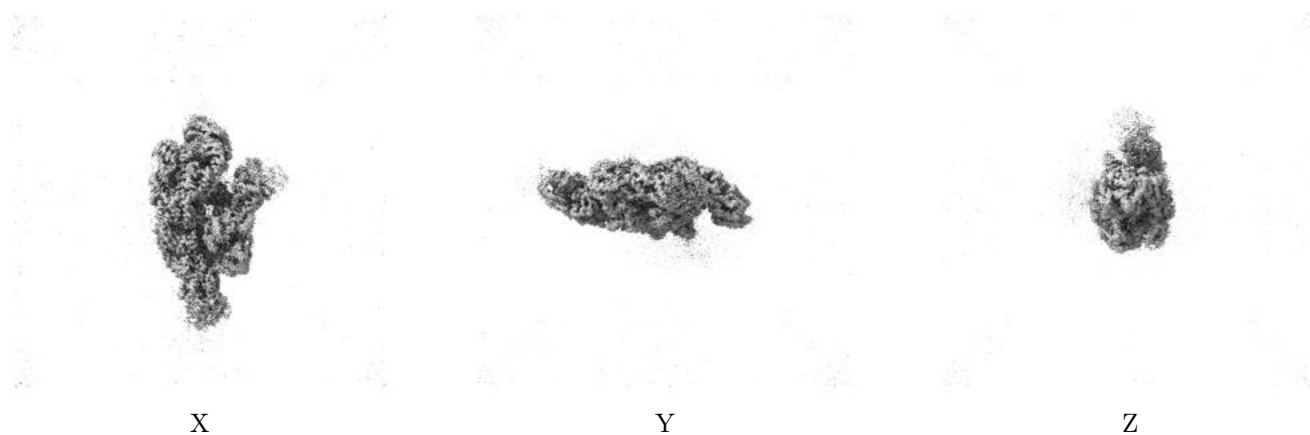
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.134. 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.

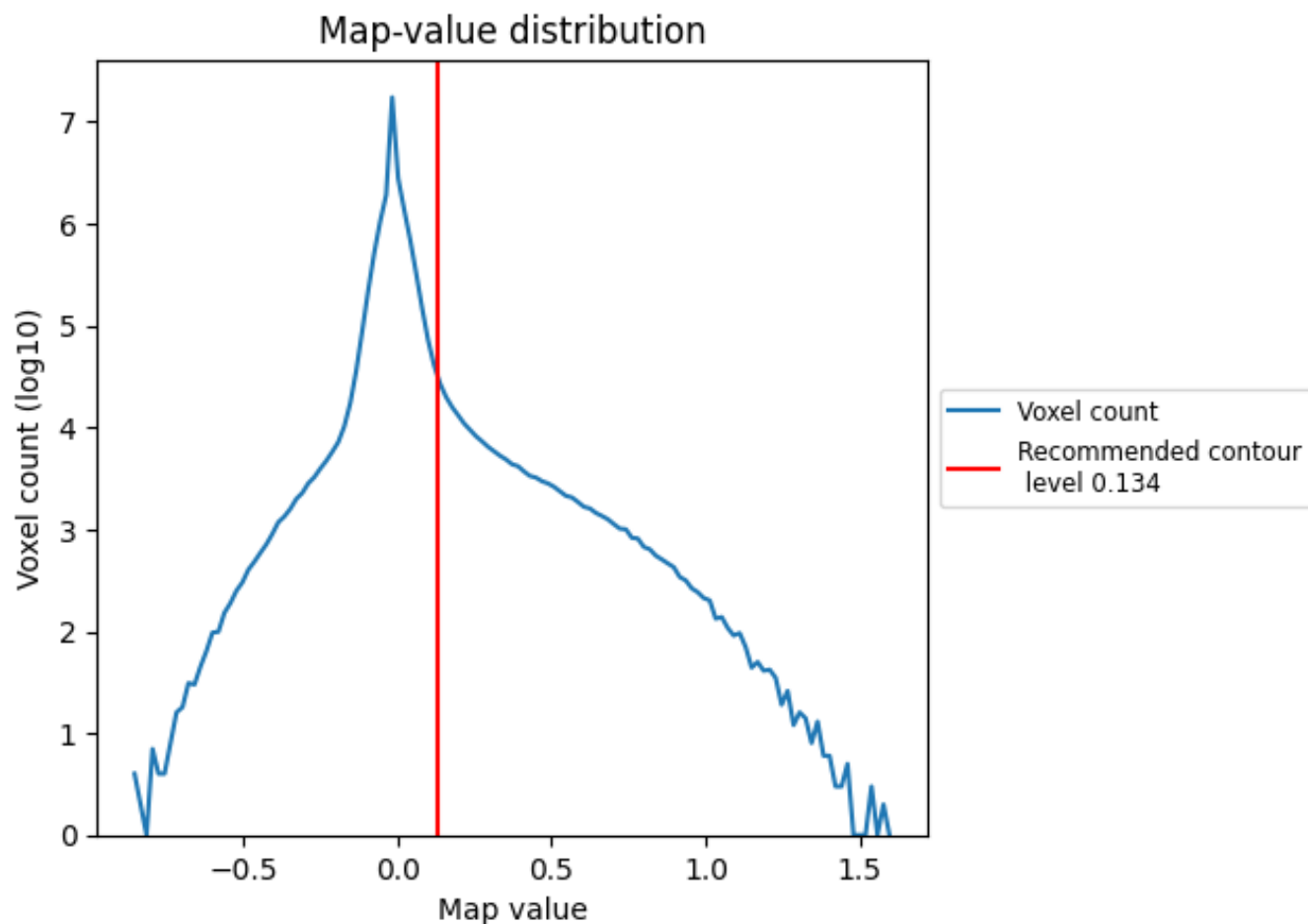
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

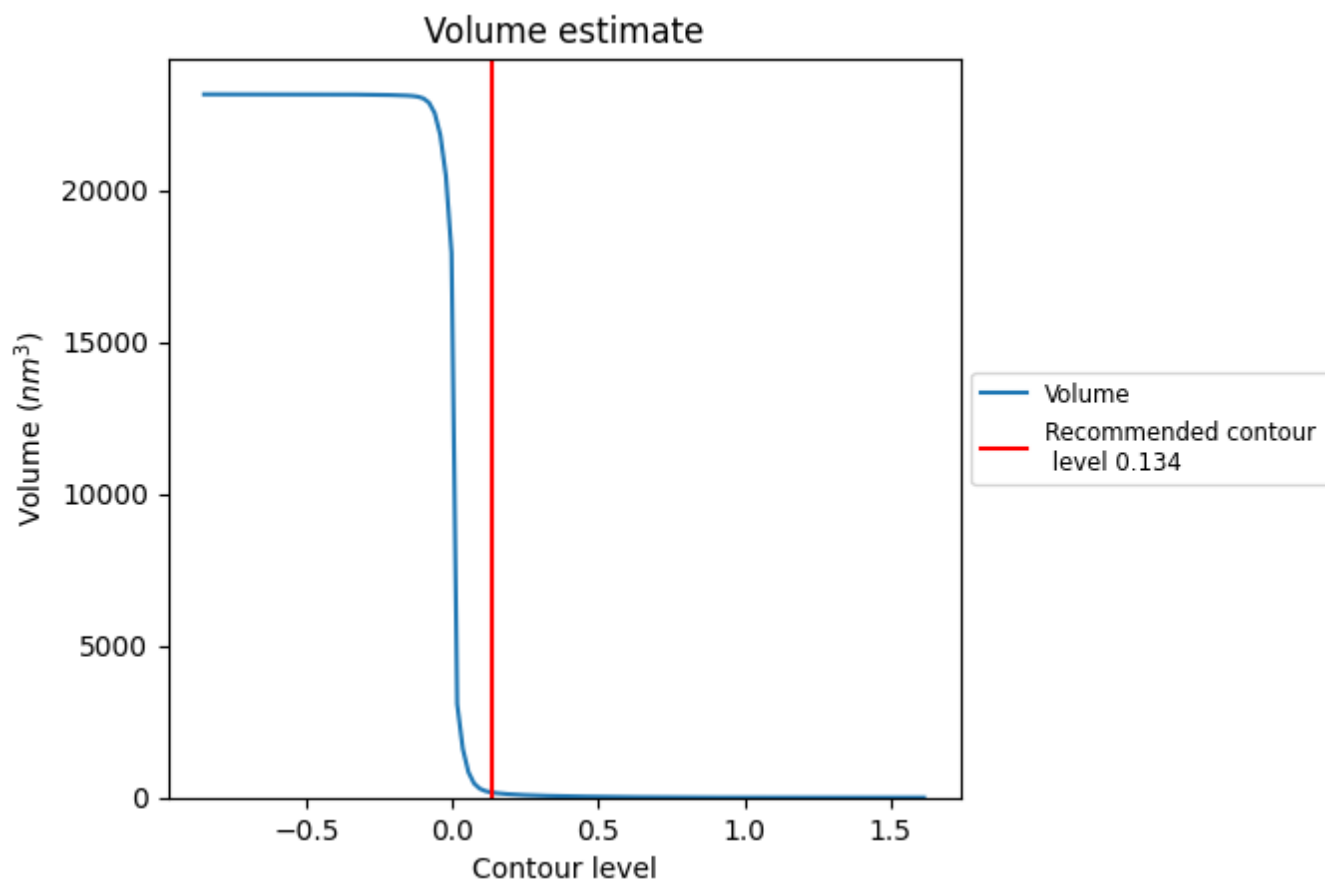
This section contains the results of statistical analysis of the map.

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.

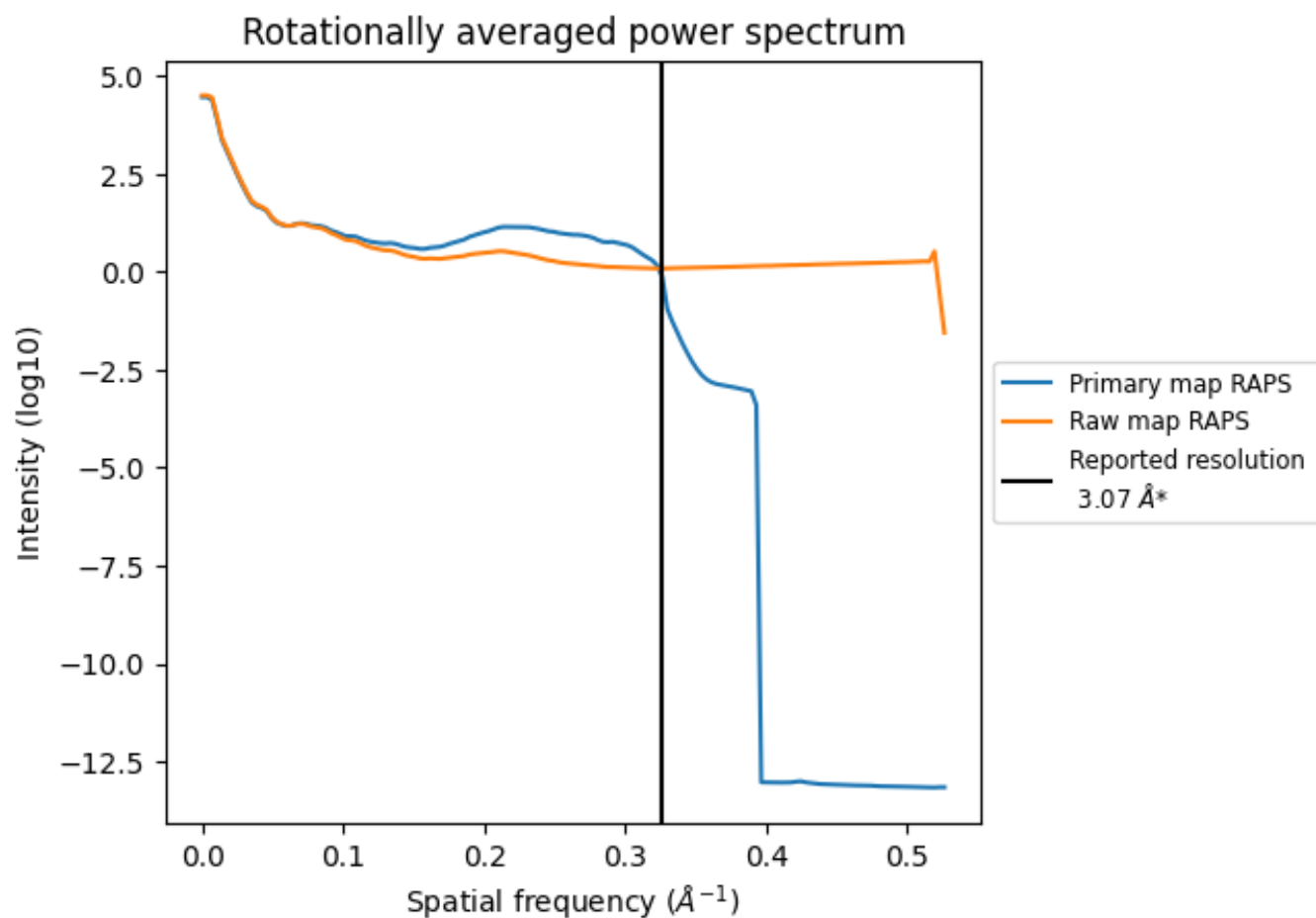
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 170 nm³; this corresponds to an approximate mass of 154 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 ⓘ

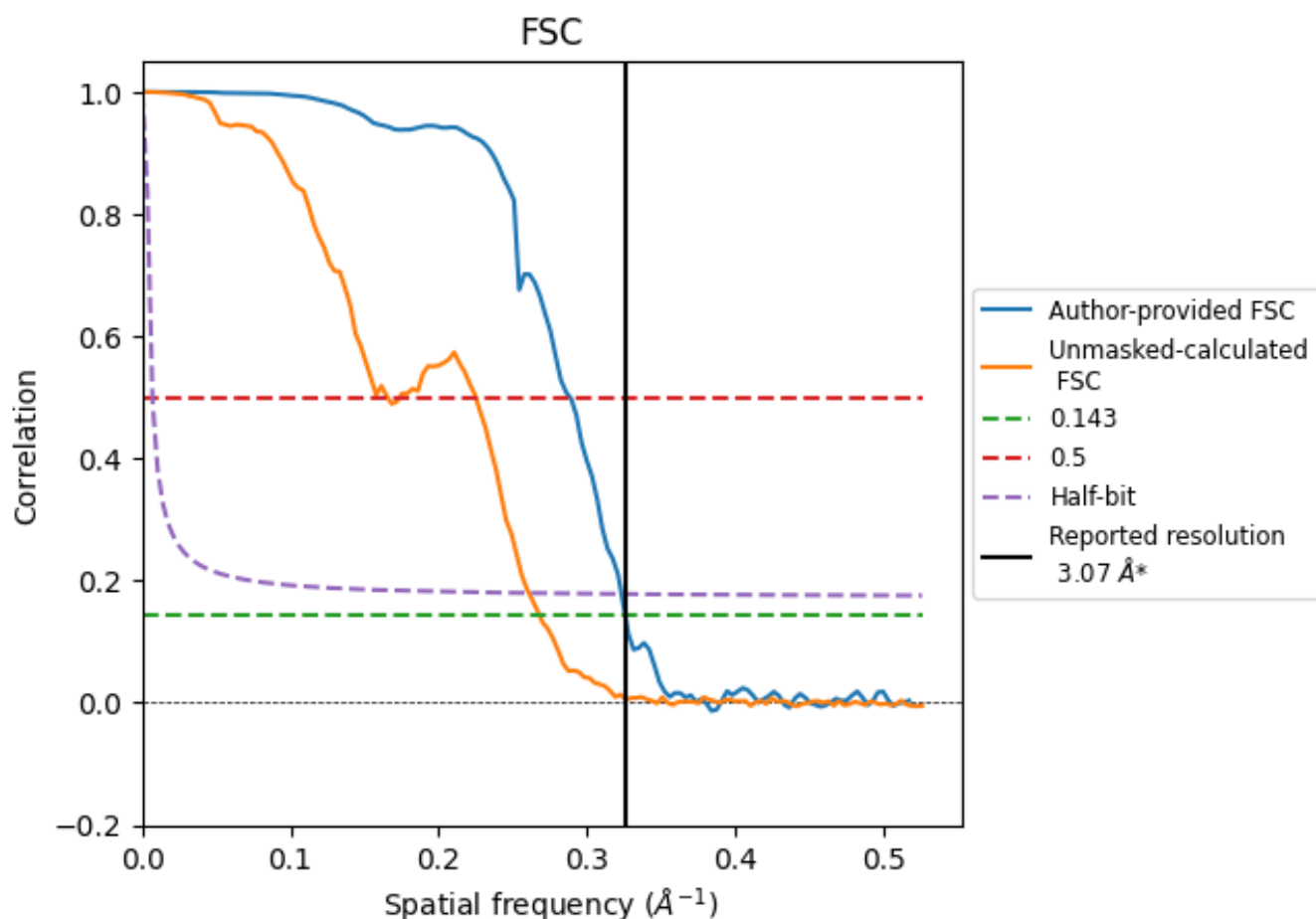


*Reported resolution corresponds to spatial frequency of 0.326 Å⁻¹

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 0.326 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.07	-	-
Author-provided FSC curve	3.07	3.47	3.09
Unmasked-calculated*	3.73	6.04	3.83

*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 3.73 differs from the reported value 3.07 by more than 10 %

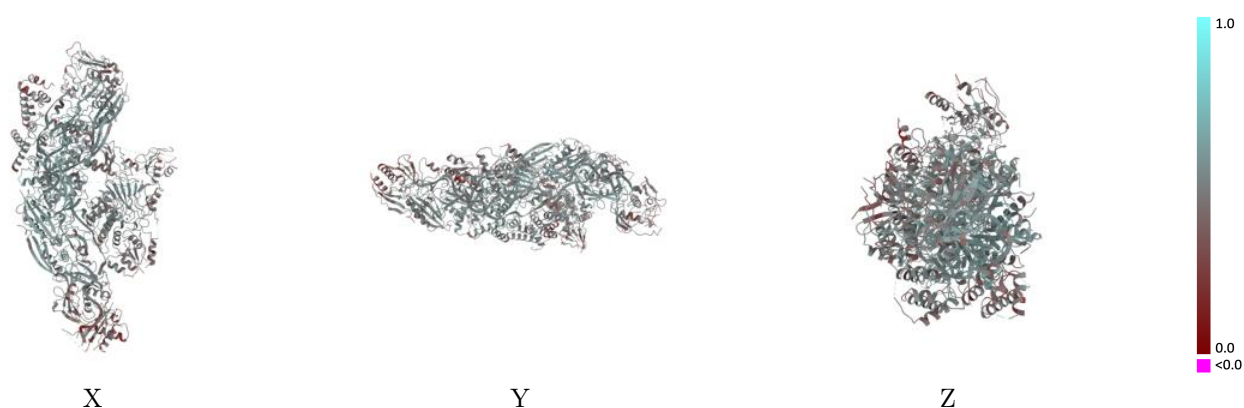
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39288 and PDB model 8YHE. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

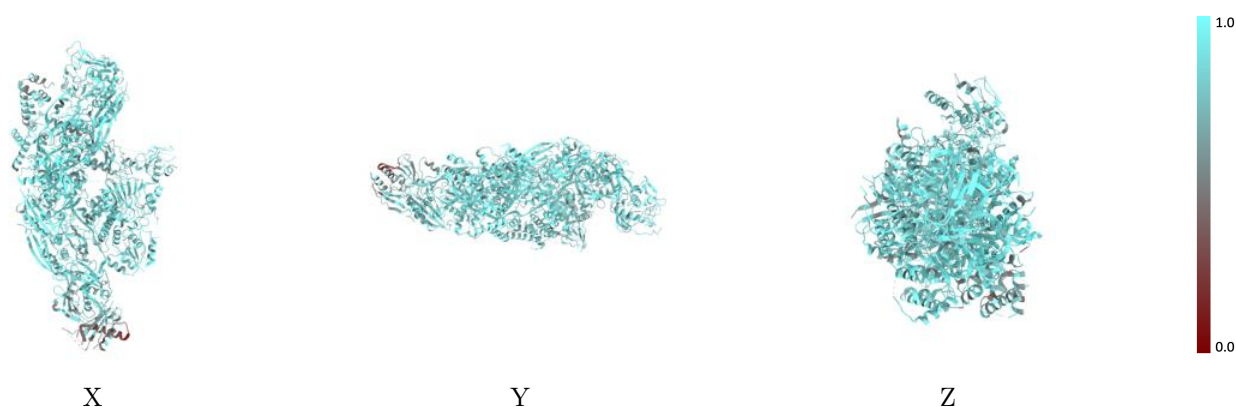
This section was not generated.

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



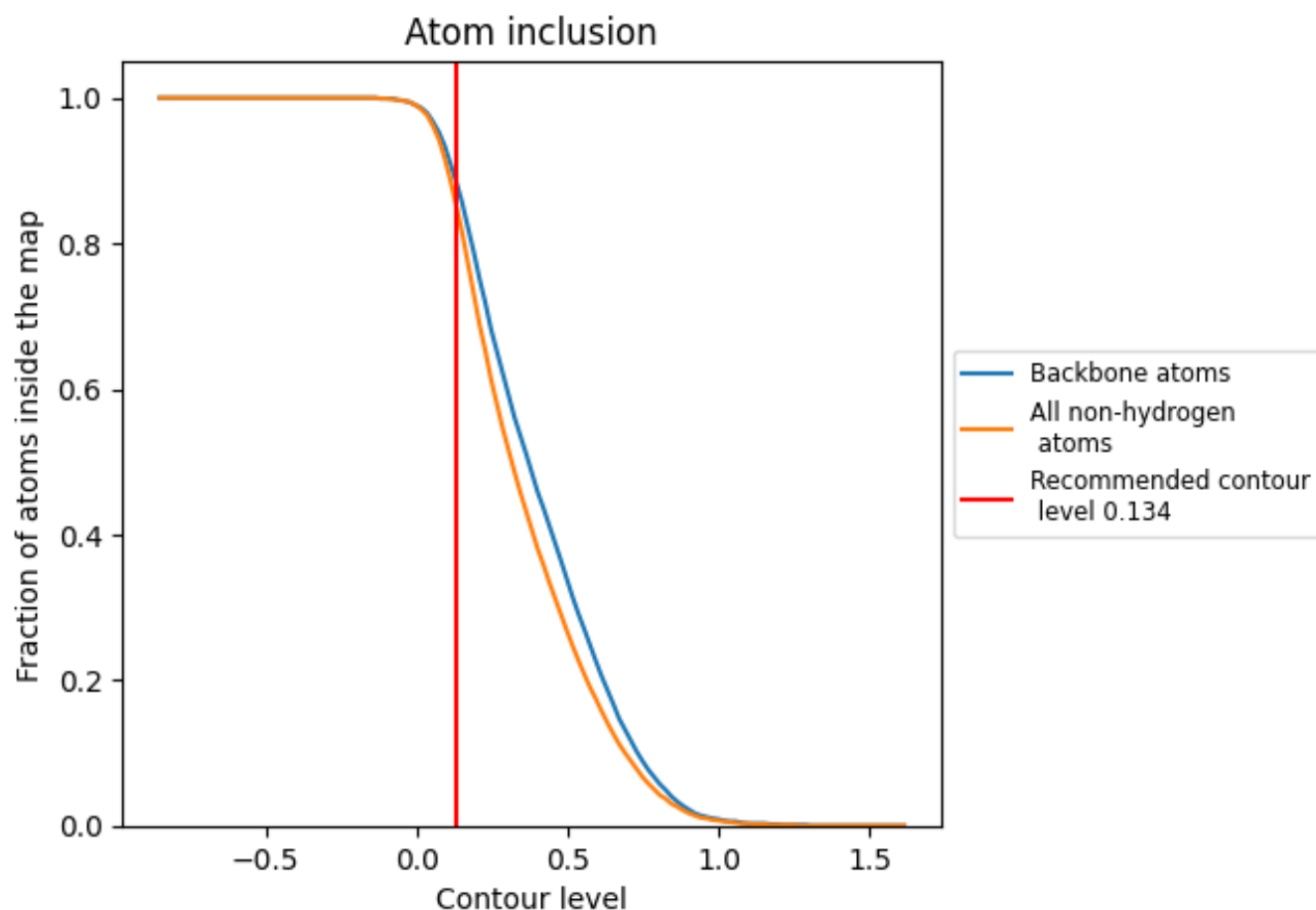
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.134).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 85% 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 (0.134) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8470	 0.5060
A	 0.5860	 0.4030
B	 0.7890	 0.4880
C	 0.8790	 0.5380
D	 0.9130	 0.5560
E	 0.9080	 0.5570
F	 0.8810	 0.5420
G	 0.8300	 0.4610
H	 0.8480	 0.4970
I	 0.8410	 0.5000
J	 0.8850	 0.5490
K	 0.8220	 0.4680
L	 0.7280	 0.4290
M	 0.9050	 0.5300
N	 0.9420	 0.5330

