



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:10 AM UTC

PDB ID : 8X31 / pdb_00008x31
EMDB ID : EMD-38025
Title : The piccolo NuA4 bound to the H2A.Z nucleosome complex with Ac-CoA at resetting state
Authors : Wang, L.; Zhang, H.; Zhu, H.; Zhu, P.
Deposited on : 2023-11-10
Resolution : 6.20 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:

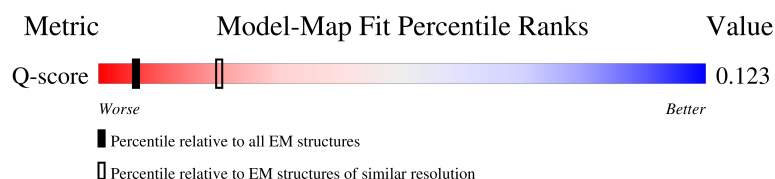
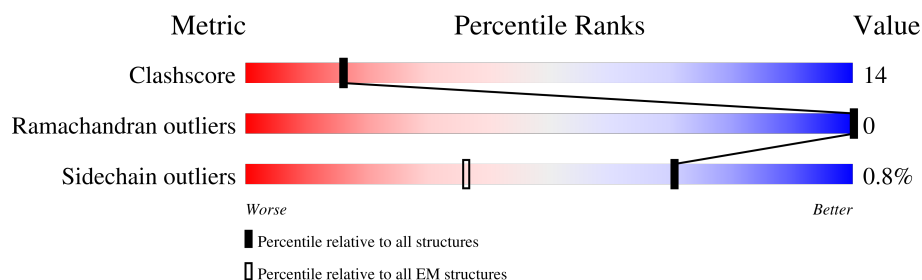
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 6.20 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	-
Q-score	-	25397	537 (5.70 - 6.70)

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	L	537	 96%
2	N	120	 41% 19% 38%
3	K	469	 32% 26% 42%
4	M	586	 25% 14% 61%

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Mol	Chain	Length	Quality of chain
5	I	146	
5	J	146	
6	A	136	
6	E	136	
7	B	102	
7	F	102	
8	C	134	
8	G	134	
9	D	131	
9	H	131	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16944 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 Maltose/maltodextrin-binding periplasmic protein,Chromatin modification-related protein EAF6.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	L	23	Total	C	N	O	0	0
			205	127	30	48		

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-86	VAL	ALA	conflict	UNP P0AEX9
L	-31	ASN	-	linker	UNP P0AEX9
L	-30	SER	-	linker	UNP P0AEX9
L	-29	SER	-	linker	UNP P0AEX9
L	-28	SER	-	linker	UNP P0AEX9
L	-27	ASN	-	linker	UNP P0AEX9
L	-26	ASN	-	linker	UNP P0AEX9
L	-25	ASN	-	linker	UNP P0AEX9
L	-24	ASN	-	linker	UNP P0AEX9
L	-23	ASN	-	linker	UNP P0AEX9
L	-22	ASN	-	linker	UNP P0AEX9
L	-21	ASN	-	linker	UNP P0AEX9
L	-20	ASN	-	linker	UNP P0AEX9
L	-19	ASN	-	linker	UNP P0AEX9
L	-18	ASN	-	linker	UNP P0AEX9
L	-17	LEU	-	linker	UNP P0AEX9
L	-16	GLY	-	linker	UNP P0AEX9
L	-15	ILE	-	linker	UNP P0AEX9
L	-14	GLU	-	linker	UNP P0AEX9
L	-13	GLY	-	linker	UNP P0AEX9
L	-12	ARG	-	linker	UNP P0AEX9
L	-11	ILE	-	linker	UNP P0AEX9
L	-10	SER	-	linker	UNP P0AEX9
L	-9	GLU	-	linker	UNP P0AEX9
L	-8	PHE	-	linker	UNP P0AEX9
L	-7	GLU	-	linker	UNP P0AEX9
L	-6	ASN	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-5	LEU	-	linker	UNP P0AEX9
L	-4	TYR	-	linker	UNP P0AEX9
L	-3	PHE	-	linker	UNP P0AEX9
L	-2	GLN	-	linker	UNP P0AEX9
L	-1	GLY	-	linker	UNP P0AEX9
L	0	HIS	-	linker	UNP P0AEX9

- Molecule 2 is a protein called Chromatin modification-related protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	75	Total	C	N	O	S	0	0
			604	382	101	118	3		

- Molecule 3 is a protein called Histone acetyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	274	Total	C	N	O	S	0	0
			2309	1495	385	419	10		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-23	MET	-	initiating methionine	UNP A0A6A5Q414
K	-22	GLY	-	expression tag	UNP A0A6A5Q414
K	-21	SER	-	expression tag	UNP A0A6A5Q414
K	-20	SER	-	expression tag	UNP A0A6A5Q414
K	-19	HIS	-	expression tag	UNP A0A6A5Q414
K	-18	HIS	-	expression tag	UNP A0A6A5Q414
K	-17	HIS	-	expression tag	UNP A0A6A5Q414
K	-16	HIS	-	expression tag	UNP A0A6A5Q414
K	-15	HIS	-	expression tag	UNP A0A6A5Q414
K	-14	HIS	-	expression tag	UNP A0A6A5Q414
K	-13	SER	-	expression tag	UNP A0A6A5Q414
K	-12	GLN	-	expression tag	UNP A0A6A5Q414
K	-11	ASP	-	expression tag	UNP A0A6A5Q414
K	-10	HIS	-	expression tag	UNP A0A6A5Q414
K	-9	GLU	-	expression tag	UNP A0A6A5Q414
K	-8	ASN	-	expression tag	UNP A0A6A5Q414
K	-7	LEU	-	expression tag	UNP A0A6A5Q414
K	-6	TYR	-	expression tag	UNP A0A6A5Q414
K	-5	PHE	-	expression tag	UNP A0A6A5Q414
K	-4	GLN	-	expression tag	UNP A0A6A5Q414

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-3	GLY	-	expression tag	UNP A0A6A5Q414
K	-2	ALA	-	expression tag	UNP A0A6A5Q414
K	-1	GLY	-	expression tag	UNP A0A6A5Q414
K	0	SER	-	expression tag	UNP A0A6A5Q414

- Molecule 4 is a protein called glutathione transferase, Enhancer of polycomb-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	230	Total	C	N	O	S	0	0
			1919	1217	325	369	8		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	33	SER	-	linker	UNP Q540A3
M	34	ASP	-	linker	UNP Q540A3
M	35	LEU	-	linker	UNP Q540A3
M	36	VAL	-	linker	UNP Q540A3
M	37	PRO	-	linker	UNP Q540A3
M	38	ARG	-	linker	UNP Q540A3
M	39	GLY	-	linker	UNP Q540A3
M	40	SER	-	linker	UNP Q540A3
M	41	GLU	-	linker	UNP Q540A3
M	42	ASN	-	linker	UNP Q540A3
M	43	LEU	-	linker	UNP Q540A3
M	44	TYR	-	linker	UNP Q540A3
M	45	PHE	-	linker	UNP Q540A3
M	46	GLN	-	linker	UNP Q540A3
M	47	GLY	-	linker	UNP Q540A3
M	48	HIS	-	linker	UNP Q540A3
M	49	MET	-	linker	UNP Q540A3

- Molecule 5 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	146	Total	C	N	O	P	0	0
			2990	1430	541	874	145		
5	J	146	Total	C	N	O	P	0	0
			2990	1430	541	874	145		

- Molecule 6 is a protein called Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	A	97	Total	C	N	O	0	0
			801	508	155	138		
6	E	97	Total	C	N	O	0	0
			801	508	155	138		

- Molecule 7 is a protein called Histone H4.

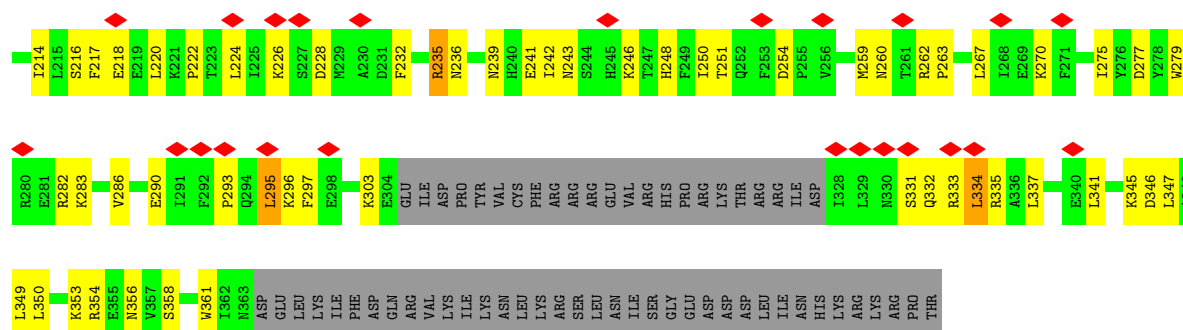
Mol	Chain	Residues	Atoms				AltConf	Trace
7	B	79	Total	C	N	O	0	0
			633	399	123	111		
7	F	80	Total	C	N	O	0	0
			641	405	124	112		

- Molecule 8 is a protein called Histone H2A.

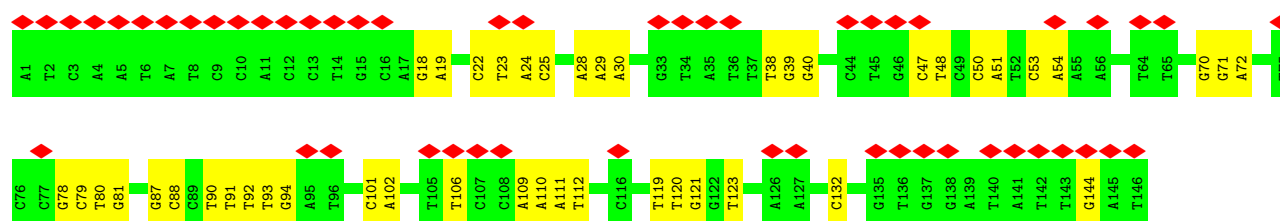
Mol	Chain	Residues	Atoms				AltConf	Trace
8	C	98	Total	C	N	O	0	0
			750	471	145	134		
8	G	108	Total	C	N	O	0	0
			829	524	160	145		

- Molecule 9 is a protein called Histone H2B.

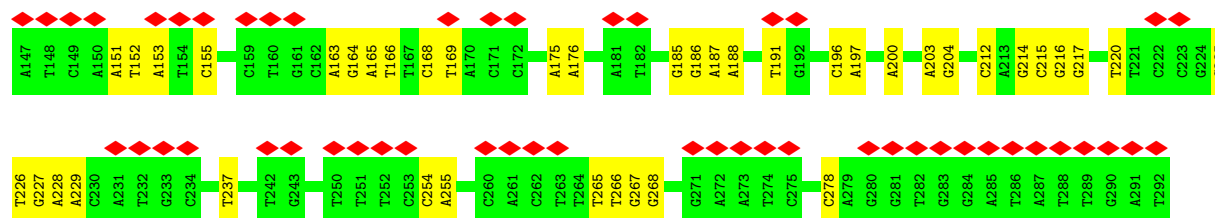
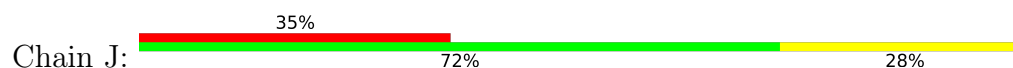
Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	93	Total	C	N	O	S	0	0
			726	456	127	142	1		
9	H	96	Total	C	N	O	S	0	0
			746	467	131	147	1		



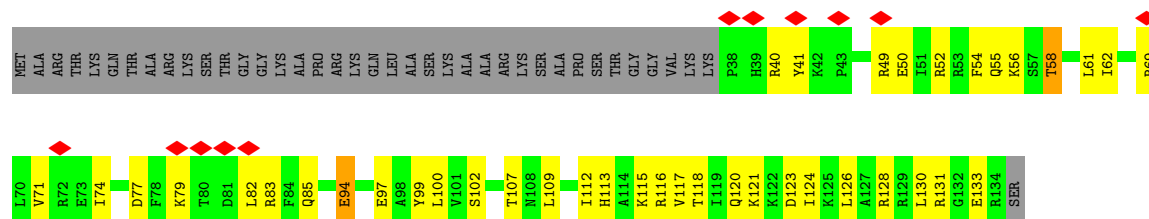
• Molecule 5: DNA (146-MER)



• Molecule 5: DNA (146-MER)

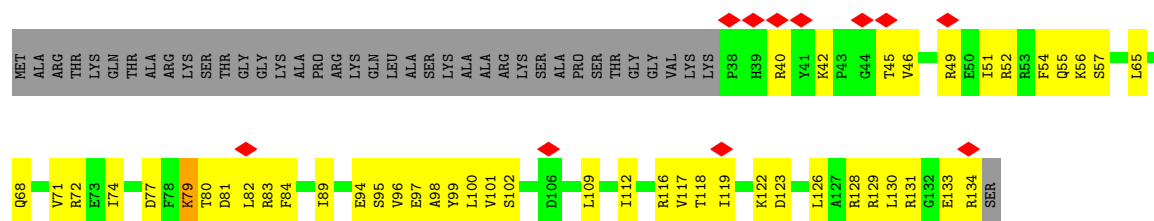


• Molecule 6: Histone H3

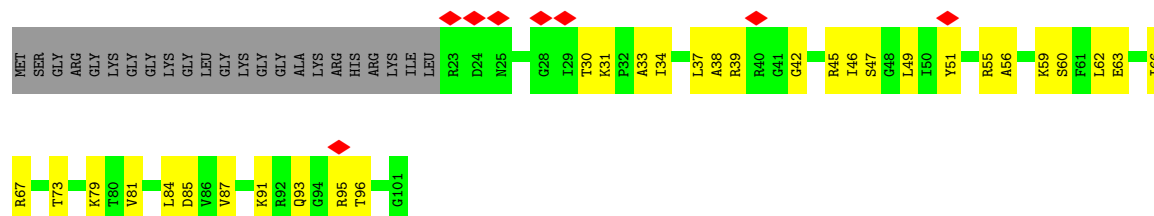


• Molecule 6: Histone H3

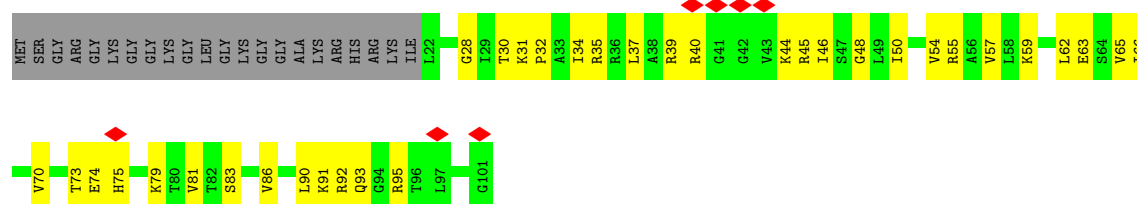




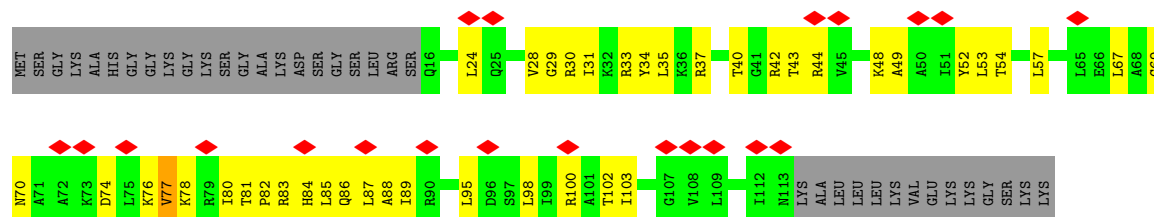
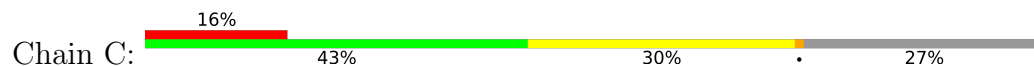
• Molecule 7: Histone H4



• Molecule 7: Histone H4

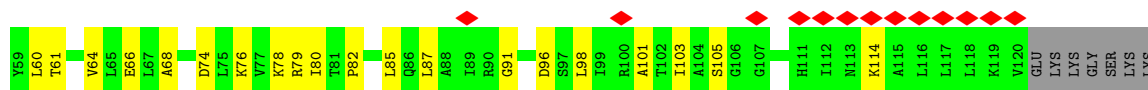


• Molecule 8: Histone H2A

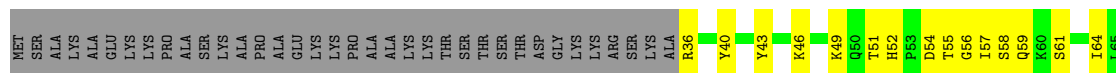
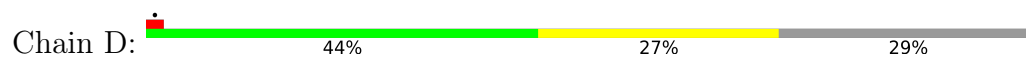


• Molecule 8: Histone H2A

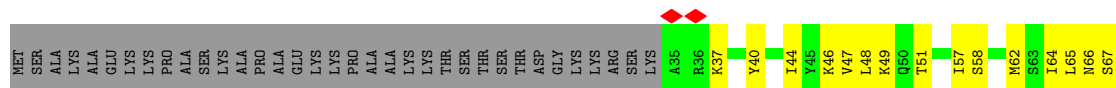




• Molecule 9: Histone H2B



• Molecule 9: Histone H2B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15537	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	14.887	Depositor
Minimum map value	-2.275	Depositor
Average map value	0.030	Depositor
Map value standard deviation	0.400	Depositor
Recommended contour level	1.39	Depositor
Map size (Å)	312.0, 312.0, 312.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	L	0.33	0/209	0.70	0/281
2	N	0.43	0/608	1.00	3/816 (0.4%)
3	K	0.46	0/2370	0.91	2/3203 (0.1%)
4	M	0.45	0/1959	0.88	2/2639 (0.1%)
5	I	0.52	0/3354	0.65	0/5175
5	J	0.51	0/3354	0.59	0/5175
6	A	0.41	0/812	0.80	0/1086
6	E	0.44	0/812	0.89	2/1086 (0.2%)
7	B	0.47	0/640	0.87	0/857
7	F	0.43	0/648	0.95	0/868
8	C	0.38	0/759	0.81	0/1023
8	G	0.48	0/838	0.90	0/1128
9	D	0.45	0/736	0.82	0/991
9	H	0.42	0/756	0.79	0/1017
All	All	0.47	0/17855	0.78	9/25345 (0.0%)

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
2	N	0	2
3	K	0	6
4	M	0	5
7	F	0	1
8	G	0	2
9	H	0	1
All	All	0	17

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	11	ILE	N-CA-C	-10.09	103.64	113.53
3	K	268	VAL	CA-C-N	7.56	130.39	120.26
3	K	268	VAL	C-N-CA	7.56	130.39	120.26
4	M	286	VAL	N-CA-CB	-6.71	103.36	112.28
2	N	14	VAL	CB-CA-C	5.69	120.62	111.29
2	N	14	VAL	N-CA-CB	-5.43	102.27	111.23
4	M	286	VAL	CB-CA-C	5.43	118.74	111.85
6	E	79	LYS	CA-C-N	5.24	129.11	121.31
6	E	79	LYS	C-N-CA	5.24	129.11	121.31

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	F	44	LYS	Peptide
8	G	18	SER	Peptide
8	G	38	HIS	Peptide
9	H	40	TYR	Peptide
3	K	181	TYR	Peptide
3	K	226	ASN	Peptide
3	K	305	ILE	Peptide
3	K	313	ARG	Peptide
3	K	400	GLN	Peptide
3	K	436	PHE	Peptide
4	M	176	VAL	Peptide
4	M	181	SER	Peptide
4	M	295	LEU	Peptide
4	M	334	LEU	Peptide
4	M	70	LEU	Peptide
2	N	80	GLN	Peptide
2	N	92	THR	Peptide

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	L	205	0	168	4	0
2	N	604	0	628	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	2309	0	2291	97	0
4	M	1919	0	1865	69	0
5	I	2990	0	1651	41	0
5	J	2990	0	1651	43	0
6	A	801	0	851	37	0
6	E	801	0	851	46	0
7	B	633	0	674	24	0
7	F	641	0	685	31	0
8	C	750	0	796	38	0
8	G	829	0	898	38	0
9	D	726	0	748	28	0
9	H	746	0	766	38	0
All	All	16944	0	14523	449	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 14.

All (449) 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)
5:I:106:DT:H3	5:J:187:DA:H61	0.98	0.97
5:I:106:DT:H3	5:J:187:DA:N6	1.68	0.90
9:H:94:ALA:O	9:H:98:GLN:HB2	1.72	0.90
3:K:230:ARG:HH21	3:K:279:ARG:HE	1.33	0.76
6:A:126:LEU:O	6:A:130:LEU:HB2	1.89	0.73
7:F:92:ARG:HH22	9:H:104:ILE:HG13	1.54	0.73
3:K:209:LYS:HB3	4:M:165:ASP:HA	1.71	0.72
8:G:22:ALA:HB3	8:G:24:LEU:HB3	1.73	0.71
5:I:106:DT:O2	5:J:187:DA:N1	2.24	0.70
5:I:30:DA:H3'	8:C:29:GLY:HA3	1.72	0.70
3:K:312:GLN:HG2	3:K:313:ARG:HG2	1.74	0.69
6:E:133:GLU:HG2	6:E:134:ARG:HG3	1.73	0.69
4:M:296:LYS:HG3	4:M:303:LYS:HA	1.75	0.69
3:K:386:HIS:HA	3:K:389:LYS:HG2	1.77	0.67
8:G:79:ARG:NH1	8:G:80:ILE:O	2.28	0.67
9:D:57:ILE:O	9:D:59:GLN:NE2	2.30	0.65
4:M:239:ASN:HA	4:M:242:ILE:HG22	1.78	0.65
5:I:90:DT:H3'	6:E:65:LEU:HB2	1.78	0.65
9:D:106:PRO:HB2	9:D:109:LEU:HD21	1.79	0.65
3:K:230:ARG:NH1	3:K:234:VAL:O	2.30	0.64
8:C:43:THR:HG23	9:D:91:THR:HA	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:72:ARG:NH2	6:E:82:LEU:O	2.30	0.64
8:G:35:LEU:O	8:G:38:HIS:ND1	2.30	0.64
4:M:173:ASN:HA	4:M:177:ASN:HD22	1.63	0.64
6:E:77:ASP:OD1	6:E:77:ASP:N	2.30	0.64
2:N:28:ILE:HD11	2:N:89:LEU:HD21	1.80	0.64
5:I:28:DA:OP1	9:D:36:ARG:NH2	2.31	0.64
3:K:407:GLU:HA	3:K:410:LEU:HD23	1.80	0.63
6:E:79:LYS:HG3	6:E:80:THR:HG22	1.81	0.63
5:J:217:DG:H3'	6:E:116:ARG:HG2	1.80	0.62
8:C:95:LEU:HA	8:C:98:LEU:HB2	1.81	0.62
7:B:93:GLN:HE22	7:B:95:ARG:HB2	1.63	0.62
6:E:80:THR:OG1	7:F:79:LYS:NZ	2.32	0.62
9:D:40:TYR:HB3	9:D:43:TYR:HB2	1.82	0.61
6:E:51:ILE:HD13	7:F:39:ARG:HA	1.83	0.61
7:B:47:SER:HB2	7:B:49:LEU:HD23	1.82	0.61
3:K:203:GLN:OE1	3:K:250:ASN:ND2	2.32	0.61
6:A:116:ARG:HE	6:A:118:THR:HB	1.64	0.61
6:E:71:VAL:HA	6:E:74:ILE:HG12	1.82	0.61
3:K:411:ASP:O	3:K:415:ARG:N	2.31	0.61
2:N:32:ASP:HB2	4:M:354:ARG:HH21	1.66	0.60
3:K:259:LEU:O	3:K:262:LYS:NZ	2.27	0.60
7:F:70:VAL:HA	7:F:73:THR:HG22	1.83	0.60
2:N:89:LEU:O	2:N:93:ALA:N	2.34	0.60
3:K:425:ASP:OD1	3:K:428:ARG:NH1	2.34	0.60
2:N:9:GLN:OE1	3:K:242:ARG:NH2	2.34	0.60
3:K:166:ASN:ND2	3:K:178:GLU:OE2	2.32	0.60
6:A:131:ARG:O	6:E:131:ARG:NH2	2.35	0.60
5:J:196:DC:H4'	6:E:83:ARG:HE	1.66	0.59
3:K:172:MET:O	3:K:310:GLN:NE2	2.36	0.59
3:K:205:PHE:HB2	3:K:211:TYR:HB2	1.84	0.59
7:F:31:LYS:H	7:F:55:ARG:HH22	1.49	0.59
4:M:262:ARG:NH1	4:M:263:PRO:O	2.34	0.59
4:M:283:LYS:HZ2	4:M:290:GLU:HG2	1.68	0.59
3:K:271:PHE:HB2	3:K:293:GLU:HA	1.83	0.59
5:J:163:DA:H2''	5:J:164:DG:H2'	1.84	0.59
5:I:25:DC:N4	5:J:267:DG:O6	2.36	0.59
7:B:38:ALA:O	7:B:42:GLY:N	2.36	0.59
3:K:259:LEU:HD22	3:K:306:LEU:HB2	1.85	0.59
3:K:408:ASP:HB2	3:K:412:ARG:HH21	1.68	0.59
6:A:117:VAL:HB	7:B:45:ARG:HD2	1.85	0.59
6:A:131:ARG:NH1	6:E:130:LEU:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:14:VAL:HG22	2:N:17:LEU:HD22	1.86	0.58
7:B:39:ARG:NH1	7:B:42:GLY:O	2.36	0.58
4:M:235:ARG:O	4:M:239:ASN:N	2.36	0.58
6:A:113:HIS:O	6:A:115:LYS:NZ	2.37	0.58
8:C:34:TYR:O	8:C:37:ARG:NH1	2.37	0.58
8:C:85:LEU:HD12	8:C:88:ALA:HB3	1.84	0.58
9:H:107:GLY:HA2	9:H:110:ALA:HB3	1.85	0.58
6:A:99:TYR:O	6:A:102:SER:OG	2.21	0.57
2:N:16:ASN:HD22	4:M:151:SER:HB3	1.69	0.57
5:I:111:DA:H5'	8:G:46:GLY:H	1.69	0.57
7:F:74:GLU:OE2	9:H:102:ARG:NH1	2.36	0.57
7:F:28:GLY:O	7:F:55:ARG:NH1	2.37	0.57
8:G:87:LEU:O	8:G:91:GLY:N	2.36	0.57
8:C:85:LEU:HB2	8:C:103:ILE:HD13	1.86	0.57
3:K:425:ASP:OD1	3:K:425:ASP:N	2.36	0.57
6:E:55:GLN:NE2	7:F:40:ARG:O	2.38	0.57
3:K:240:ASP:N	3:K:240:ASP:OD1	2.36	0.57
4:M:132:GLU:OE1	4:M:135:LYS:NZ	2.33	0.57
9:H:116:GLU:OE1	9:H:119:ARG:NE	2.37	0.56
3:K:198:ASP:H	3:K:204:TYR:HD1	1.51	0.56
3:K:221:ARG:NH2	3:K:281:GLU:O	2.39	0.56
9:H:107:GLY:O	9:H:111:LYS:HB2	2.05	0.56
3:K:385:LEU:O	3:K:389:LYS:N	2.39	0.56
5:I:38:DT:H4'	5:I:39:DG:H5'	1.88	0.56
9:H:72:ILE:HA	9:H:75:ARG:HG2	1.87	0.56
7:F:74:GLU:O	9:H:95:ARG:NH2	2.39	0.56
6:A:128:ARG:HE	6:A:133:GLU:H	1.54	0.56
3:K:372:GLU:O	3:K:376:MET:N	2.40	0.55
4:M:192:LEU:HD13	4:M:275:ILE:HG12	1.88	0.55
5:I:29:DA:O3'	8:C:33:ARG:NH1	2.38	0.55
8:G:33:ARG:HA	8:G:36:LYS:HB2	1.88	0.55
7:F:46:ILE:HG22	7:F:48:GLY:H	1.70	0.55
3:K:388:ALA:HB1	3:K:393:ILE:HG22	1.89	0.55
9:H:62:MET:HE3	9:H:66:ASN:HB2	1.89	0.55
4:M:61:SER:OG	4:M:62:VAL:N	2.38	0.55
3:K:370:ILE:HG12	4:M:63:LYS:HA	1.88	0.55
4:M:358:SER:HA	4:M:361:TRP:HD1	1.71	0.55
5:J:176:DA:H3'	8:G:29:GLY:H	1.72	0.55
3:K:379:MET:HG2	3:K:384:ILE:HD13	1.88	0.55
5:I:123:DT:OP1	9:H:37:LYS:N	2.39	0.55
5:J:278:DC:OP1	8:C:78:LYS:N	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:30:THR:H	7:B:33:ALA:HB3	1.72	0.54
4:M:341:LEU:HB2	4:M:345:LYS:HE2	1.89	0.54
8:G:80:ILE:HG23	8:G:82:PRO:HD2	1.89	0.54
8:G:98:LEU:HD21	9:H:72:ILE:HD12	1.90	0.54
5:J:166:DT:OP1	9:H:57:ILE:N	2.34	0.54
6:E:68:GLN:HA	6:E:71:VAL:HG12	1.89	0.54
8:C:74:ASP:OD2	8:C:83:ARG:NH1	2.31	0.54
8:G:76:LYS:NZ	8:G:78:LYS:O	2.40	0.54
8:C:77:VAL:O	9:D:56:GLY:N	2.32	0.54
7:F:59:LYS:HA	7:F:62:LEU:HG	1.90	0.54
3:K:366:LYS:HE3	8:G:114:LYS:HG2	1.90	0.54
6:A:107:THR:HG21	6:A:124:ILE:HG22	1.90	0.53
6:E:116:ARG:NH2	6:E:123:ASP:OD2	2.41	0.53
5:I:87:DG:H2''	5:I:88:DC:H2'	1.90	0.53
7:B:31:LYS:HA	7:B:34:ILE:HG12	1.89	0.53
4:M:217:PHE:HA	4:M:220:LEU:HB2	1.90	0.53
6:E:82:LEU:HD23	7:F:79:LYS:HD2	1.90	0.53
6:E:99:TYR:O	6:E:102:SER:OG	2.25	0.53
3:K:358:ILE:HA	3:K:361:LEU:HB3	1.90	0.53
3:K:357:LEU:O	3:K:361:LEU:N	2.42	0.52
4:M:242:ILE:HD13	4:M:349:LEU:HD12	1.91	0.52
9:D:58:SER:O	9:D:61:SER:OG	2.25	0.52
6:A:120:GLN:N	6:A:123:ASP:OD2	2.42	0.52
6:E:117:VAL:HG13	7:F:45:ARG:HG2	1.90	0.52
6:E:133:GLU:OE2	6:E:134:ARG:NH1	2.42	0.52
8:G:21:ARG:NH2	9:H:126:SER:OG	2.41	0.52
3:K:227:GLU:HB2	4:M:147:TYR:HB3	1.90	0.52
9:D:71:ASP:HA	9:D:74:GLU:HG3	1.91	0.52
6:E:65:LEU:HA	6:E:68:GLN:HG3	1.91	0.52
1:L:30:ASP:OD1	1:L:30:ASP:N	2.38	0.52
2:N:16:ASN:ND2	2:N:20:GLU:OE2	2.43	0.52
2:N:97:ILE:O	4:M:345:LYS:NZ	2.35	0.52
3:K:308:LEU:HG	3:K:310:GLN:H	1.74	0.52
6:E:54:PHE:HA	6:E:57:SER:HB3	1.91	0.52
7:F:63:GLU:HA	7:F:66:ILE:HG12	1.92	0.52
8:G:51:ILE:HD11	9:H:97:ILE:HG23	1.91	0.52
9:H:76:ILE:HG22	9:H:104:ILE:HD13	1.92	0.52
2:N:16:ASN:O	2:N:20:GLU:N	2.42	0.52
4:M:209:MET:SD	4:M:209:MET:N	2.75	0.52
4:M:349:LEU:O	4:M:353:LYS:N	2.43	0.52
5:J:151:DA:N3	6:A:41:TYR:OH	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:8:GLU:O	2:N:12:GLN:N	2.42	0.51
4:M:332:GLN:HG2	4:M:333:ARG:HG3	1.91	0.51
9:H:97:ILE:HA	9:H:100:ALA:HB3	1.91	0.51
3:K:188:GLU:HB2	3:K:189:LEU:HD12	1.92	0.51
6:A:58:THR:OG1	8:G:105:SER:O	2.28	0.51
3:K:408:ASP:N	3:K:408:ASP:OD1	2.42	0.51
8:C:85:LEU:O	8:C:88:ALA:N	2.42	0.51
4:M:59:LYS:HZ1	9:H:112:HIS:HB2	1.75	0.51
8:C:40:THR:O	8:C:42:ARG:NH1	2.43	0.51
8:C:89:ILE:HA	8:C:95:LEU:HD21	1.92	0.51
3:K:223:PRO:HD2	3:K:277:THR:HG21	1.93	0.51
3:K:230:ARG:NH1	3:K:231:ASP:OD1	2.44	0.51
4:M:167:ARG:NE	4:M:168:ASP:OD1	2.44	0.51
5:J:203:DA:H2"	5:J:204:DG:C8	2.45	0.51
4:M:210:ASP:OD1	4:M:210:ASP:N	2.43	0.51
8:C:82:PRO:O	8:C:86:GLN:N	2.42	0.51
8:C:48:LYS:HE3	9:D:97:ILE:HB	1.93	0.51
8:G:64:VAL:O	8:G:68:ALA:N	2.43	0.51
3:K:169:ARG:HA	3:K:179:PRO:HD3	1.94	0.50
5:I:72:DA:N6	5:J:220:DT:O4	2.44	0.50
6:A:71:VAL:HA	6:A:74:ILE:HG22	1.94	0.50
6:A:100:LEU:HD13	7:B:37:LEU:HD13	1.92	0.50
8:C:80:ILE:O	8:C:84:HIS:N	2.35	0.50
7:F:54:VAL:HA	7:F:57:VAL:HG12	1.92	0.50
9:H:46:LYS:HG2	9:H:49:LYS:HE3	1.92	0.50
4:M:332:GLN:O	4:M:335:ARG:NH1	2.42	0.50
5:J:228:DA:OP1	7:B:46:ILE:N	2.40	0.50
5:I:18:DG:H2"	5:I:19:DA:C8	2.47	0.50
3:K:235:SER:OG	3:K:277:THR:O	2.20	0.50
8:C:30:ARG:O	8:C:34:TYR:N	2.44	0.50
6:E:71:VAL:HG11	6:E:89:ILE:HD12	1.94	0.50
8:G:66:GLU:HG3	8:G:87:LEU:HD22	1.93	0.50
2:N:92:THR:HA	2:N:95:PHE:H	1.76	0.50
6:E:42:LYS:HB3	6:E:45:THR:HG22	1.94	0.50
3:K:409:ILE:HA	3:K:412:ARG:HG2	1.94	0.49
7:B:91:LYS:HA	7:B:96:THR:HB	1.94	0.49
8:C:77:VAL:HG22	9:D:55:THR:HA	1.94	0.49
3:K:245:ARG:NH2	3:K:269:ASP:OD1	2.45	0.49
3:K:301:ASN:ND2	3:K:349:TYR:OH	2.44	0.49
6:E:119:ILE:HD11	7:F:46:ILE:HG23	1.94	0.49
2:N:91:ASN:ND2	4:M:250:ILE:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:172:MET:HG3	3:K:197:ILE:HB	1.94	0.49
5:I:92:DT:H2'	5:I:93:DT:C6	2.47	0.49
8:G:24:LEU:H	8:G:24:LEU:HD23	1.77	0.49
5:J:151:DA:H2''	5:J:152:DT:H5''	1.94	0.49
5:J:226:DT:H2''	5:J:227:DG:H5''	1.93	0.49
7:F:30:THR:H	7:F:55:ARG:NH1	2.10	0.49
4:M:214:ILE:HG12	4:M:279:TRP:HZ3	1.78	0.49
3:K:228:ILE:HB	3:K:429:LEU:HA	1.94	0.49
5:I:120:DT:H1'	5:I:121:DG:C5	2.47	0.49
9:D:54:ASP:N	9:D:54:ASP:OD1	2.42	0.49
8:G:53:LEU:HA	8:G:56:VAL:HG12	1.95	0.49
5:I:81:DG:H21	6:E:40:ARG:HH22	1.59	0.49
3:K:222:HIS:HB3	3:K:284:HIS:CD2	2.47	0.49
9:D:109:LEU:O	9:D:113:ALA:CB	2.61	0.49
2:N:3:PRO:HA	2:N:6:VAL:HG12	1.95	0.48
3:K:259:LEU:HB2	3:K:306:LEU:HD13	1.94	0.48
4:M:295:LEU:HB2	4:M:297:PHE:HB2	1.95	0.48
5:J:186:DG:H2''	5:J:187:DA:C8	2.48	0.48
7:B:63:GLU:HG3	7:B:67:ARG:HH21	1.78	0.48
5:I:40:DG:OP1	9:D:91:THR:N	2.33	0.48
9:D:122:THR:O	9:D:126:SER:CB	2.61	0.48
4:M:334:LEU:HB2	4:M:337:LEU:HG	1.93	0.48
3:K:371:ASP:OD1	3:K:371:ASP:N	2.44	0.48
9:D:108:GLU:O	9:D:112:HIS:ND1	2.46	0.48
8:G:54:THR:HG21	9:H:117:GLY:HA2	1.95	0.48
7:B:63:GLU:HA	7:B:66:ILE:HG12	1.95	0.48
9:D:122:THR:O	9:D:126:SER:OG	2.32	0.48
7:B:30:THR:OG1	7:B:31:LYS:N	2.47	0.48
9:D:109:LEU:HA	9:D:112:HIS:CE1	2.49	0.48
6:E:52:ARG:O	6:E:56:LYS:CB	2.62	0.48
8:G:61:THR:HA	8:G:64:VAL:HG22	1.94	0.48
3:K:170:ILE:HB	3:K:177:ILE:HB	1.94	0.48
4:M:251:THR:OG1	4:M:254:ASP:N	2.47	0.48
8:C:31:ILE:O	8:C:35:LEU:N	2.43	0.48
8:G:41:GLY:O	8:G:42:ARG:NE	2.46	0.48
3:K:259:LEU:HD12	3:K:261:HIS:HD2	1.79	0.48
5:I:132:DC:OP1	8:G:78:LYS:N	2.31	0.47
6:E:98:ALA:HA	6:E:101:VAL:HG22	1.96	0.47
3:K:353:TRP:HB3	3:K:384:ILE:HD11	1.96	0.47
6:A:79:LYS:HB3	6:A:82:LEU:HD11	1.96	0.47
2:N:93:ALA:HA	2:N:96:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:347:LEU:HD13	4:M:350:LEU:HD13	1.97	0.47
5:J:229:DA:H4'	6:A:40:ARG:HE	1.79	0.47
3:K:356:THR:O	3:K:359:THR:OG1	2.21	0.47
8:G:58:GLU:OE1	9:H:112:HIS:ND1	2.46	0.47
1:L:39:LYS:HG2	4:M:347:LEU:HG	1.97	0.47
8:C:102:THR:HG21	7:F:95:ARG:HD3	1.95	0.47
2:N:91:ASN:O	2:N:95:PHE:N	2.47	0.47
3:K:180:TRP:HB2	3:K:258:PHE:HA	1.97	0.47
3:K:358:ILE:HD11	3:K:416:LEU:HD21	1.96	0.47
3:K:381:THR:O	3:K:385:LEU:N	2.42	0.47
4:M:353:LYS:HD2	4:M:356:ASN:HB3	1.96	0.47
8:C:42:ARG:NE	8:G:42:ARG:HH12	2.12	0.47
7:F:31:LYS:NZ	7:F:32:PRO:O	2.44	0.47
2:N:3:PRO:HG3	2:N:111:LEU:HD13	1.96	0.47
3:K:191:ASP:OD1	3:K:191:ASP:N	2.46	0.47
5:I:70:DG:H2''	5:I:71:DG:H2'	1.95	0.47
8:G:45:VAL:N	9:H:92:ILE:O	2.47	0.47
1:L:39:LYS:HD2	1:L:42:GLU:HB3	1.97	0.47
9:H:80:ALA:HB2	9:H:97:ILE:HD13	1.96	0.47
3:K:256:LYS:HD3	3:K:260:ASP:HA	1.97	0.47
3:K:290:PHE:HB3	3:K:305:ILE:HD13	1.97	0.46
3:K:396:TYR:HA	3:K:401:HIS:HA	1.96	0.46
9:H:44:ILE:HA	9:H:47:VAL:HG12	1.97	0.46
6:A:85:GLN:N	7:B:81:VAL:O	2.48	0.46
3:K:385:LEU:HA	3:K:388:ALA:HB3	1.95	0.46
4:M:262:ARG:NH1	4:M:267:LEU:HB2	2.31	0.46
5:I:28:DA:H1'	5:I:29:DA:C5	2.50	0.46
8:C:49:ALA:HA	8:C:52:TYR:HB3	1.96	0.46
3:K:233:TYR:HE2	3:K:314:MET:HE1	1.80	0.46
4:M:243:ASN:O	4:M:246:LYS:NZ	2.36	0.46
9:D:51:THR:OG1	9:D:52:HIS:N	2.43	0.46
6:E:118:THR:HA	7:F:45:ARG:O	2.16	0.46
4:M:267:LEU:HD12	4:M:270:LYS:HB2	1.97	0.46
5:I:132:DC:H3'	8:G:76:LYS:HE2	1.98	0.46
8:G:57:LEU:HD23	8:G:60:LEU:HD11	1.96	0.46
5:I:80:DT:O4	5:J:212:DC:N4	2.49	0.46
9:D:66:ASN:HA	9:D:69:VAL:HG12	1.98	0.46
7:F:75:HIS:O	9:H:95:ARG:NH1	2.38	0.46
6:E:100:LEU:HD11	7:F:37:LEU:HD22	1.98	0.46
7:F:34:ILE:HA	7:F:37:LEU:HB2	1.98	0.46
9:H:107:GLY:O	9:H:111:LYS:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:236:ASN:HA	4:M:239:ASN:HB3	1.98	0.46
7:F:62:LEU:HA	7:F:65:VAL:HG12	1.97	0.46
8:G:98:LEU:HB3	8:G:101:ALA:HB3	1.98	0.46
9:H:48:LEU:O	9:H:51:THR:OG1	2.32	0.45
5:J:165:DA:H5''	9:H:58:SER:HA	1.99	0.45
6:E:94:GLU:HA	6:E:97:GLU:HG2	1.97	0.45
4:M:216:SER:OG	4:M:218:GLU:OE1	2.27	0.45
8:G:44:ARG:HG3	9:H:92:ILE:HB	1.97	0.45
3:K:189:LEU:HD11	4:M:293:PRO:HD2	1.98	0.45
5:I:144:DG:H4'	6:A:41:TYR:HA	1.98	0.45
8:G:18:SER:H	8:G:20:ALA:HB2	1.81	0.45
8:G:48:LYS:HB3	9:H:94:ALA:HB2	1.98	0.45
8:G:96:ASP:OD1	8:G:96:ASP:N	2.48	0.45
9:H:105:LEU:HD12	9:H:106:PRO:HD2	1.98	0.45
3:K:220:LEU:HD21	3:K:224:PRO:HD3	1.99	0.45
5:I:47:DC:H1'	5:I:48:DT:C5	2.52	0.45
5:J:153:DA:H3'	6:A:49:ARG:HH21	1.82	0.45
6:A:113:HIS:NE2	6:E:122:LYS:HG3	2.31	0.45
3:K:174:LYS:HE2	4:M:129:THR:HA	1.99	0.45
5:J:163:DA:H1'	5:J:164:DG:H5'	1.98	0.45
9:D:79:GLU:HA	9:D:82:LYS:HG2	1.99	0.45
2:N:16:ASN:ND2	4:M:150:PHE:O	2.50	0.45
6:A:83:ARG:O	7:B:81:VAL:N	2.49	0.45
7:B:84:LEU:HA	7:B:87:VAL:HG12	1.98	0.45
8:C:54:THR:HA	8:C:57:LEU:HD12	1.99	0.45
3:K:180:TRP:H	3:K:258:PHE:HD1	1.65	0.45
5:J:217:DG:H5''	6:E:116:ARG:HB3	1.98	0.45
6:A:55:GLN:NE2	7:B:39:ARG:O	2.47	0.45
6:A:109:LEU:HA	6:A:112:ILE:HG22	1.99	0.45
2:N:97:ILE:HD12	4:M:345:LYS:HA	1.99	0.45
8:G:74:ASP:OD1	8:G:74:ASP:N	2.40	0.45
4:M:260:ASN:OD1	4:M:260:ASN:N	2.46	0.44
5:I:18:DG:H2''	5:I:19:DA:H8	1.81	0.44
7:B:85:ASP:N	7:B:85:ASP:OD1	2.47	0.44
3:K:172:MET:SD	3:K:285:HIS:NE2	2.88	0.44
3:K:198:ASP:HB2	3:K:211:TYR:HE1	1.82	0.44
6:A:77:ASP:OD1	6:A:77:ASP:N	2.48	0.44
5:I:22:DC:C6	5:I:23:DT:H72	2.51	0.44
5:J:225:DC:H2''	5:J:226:DT:C4	2.52	0.44
6:A:109:LEU:HD21	6:E:129:ARG:CZ	2.47	0.44
6:E:84:PHE:HA	7:F:81:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:90:LEU:HA	7:F:93:GLN:HG3	2.00	0.44
5:I:50:DC:OP2	6:A:85:GLN:NE2	2.42	0.44
5:I:93:DT:H2''	5:I:94:DG:H5''	1.99	0.44
5:J:217:DG:P	6:E:117:VAL:H	2.40	0.44
7:B:59:LYS:HA	7:B:62:LEU:HG	1.99	0.44
3:K:231:ASP:OD1	3:K:234:VAL:N	2.36	0.44
5:I:53:DC:H2''	5:I:54:DA:C8	2.53	0.44
5:I:78:DG:H1'	5:I:79:DC:C2	2.53	0.44
6:A:83:ARG:HG2	7:B:79:LYS:HD2	2.00	0.44
7:B:51:TYR:O	7:B:55:ARG:HD3	2.18	0.44
9:H:115:SER:O	9:H:118:THR:OG1	2.26	0.44
6:E:95:SER:OG	6:E:96:VAL:N	2.51	0.44
7:F:83:SER:HA	7:F:86:VAL:HG12	2.00	0.44
4:M:72:ASN:HA	4:M:74:LEU:HD23	1.99	0.44
7:B:56:ALA:O	7:B:60:SER:OG	2.27	0.44
9:D:118:THR:HA	9:D:121:VAL:HG12	2.00	0.44
2:N:9:GLN:O	2:N:13:ASP:N	2.34	0.43
3:K:433:PRO:HA	3:K:434:PRO:HD3	1.84	0.43
6:E:81:ASP:OD1	6:E:81:ASP:N	2.51	0.43
3:K:223:PRO:O	3:K:225:GLY:N	2.48	0.43
6:A:79:LYS:HD3	6:A:82:LEU:HD21	2.00	0.43
7:B:73:THR:HG21	7:B:81:VAL:HG22	2.00	0.43
6:E:97:GLU:HA	6:E:100:LEU:HG	2.00	0.43
9:H:94:ALA:O	9:H:98:GLN:CB	2.57	0.43
3:K:175:TYR:N	3:K:310:GLN:OE1	2.48	0.43
8:C:85:LEU:HD12	8:C:85:LEU:HA	1.86	0.43
3:K:406:ASN:OD1	3:K:406:ASN:N	2.46	0.43
4:M:222:PRO:O	4:M:226:LYS:NZ	2.50	0.43
8:C:100:ARG:NH2	7:F:91:LYS:O	2.44	0.43
2:N:101:LEU:HD21	4:M:345:LYS:HE3	2.00	0.43
4:M:279:TRP:O	4:M:282:ARG:NH1	2.52	0.43
8:C:69:GLY:H	8:C:87:LEU:HD11	1.83	0.43
1:L:33:GLN:OE1	1:L:33:GLN:N	2.51	0.43
2:N:9:GLN:HA	2:N:12:GLN:HB2	1.99	0.43
3:K:346:LEU:HD23	3:K:350:ARG:HE	1.84	0.43
4:M:331:SER:OG	4:M:332:GLN:OE1	2.25	0.43
5:I:112:DT:OP1	8:G:44:ARG:N	2.32	0.43
6:E:46:VAL:HA	6:E:49:ARG:HE	1.83	0.43
8:G:85:LEU:HD23	8:G:103:ILE:HB	2.01	0.43
2:N:7:LEU:HB2	4:M:337:LEU:HD21	2.01	0.43
3:K:179:PRO:HA	3:K:258:PHE:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:228:ILE:HB	3:K:430:ILE:H	1.84	0.43
3:K:361:LEU:HG	4:M:67:LYS:HE2	2.01	0.43
4:M:228:ASP:OD1	4:M:232:PHE:N	2.49	0.43
4:M:347:LEU:HA	4:M:350:LEU:HD13	2.00	0.43
5:J:187:DA:H1'	5:J:188:DA:H5'	2.00	0.43
6:E:128:ARG:HG3	6:E:133:GLU:HB3	2.00	0.43
3:K:281:GLU:HB3	4:M:140:SER:HA	2.00	0.43
3:K:249:ARG:HE	3:K:267:ASP:HB3	1.83	0.42
8:G:25:GLN:HB2	8:G:57:LEU:HD21	2.01	0.42
3:K:381:THR:HA	3:K:384:ILE:HG22	2.01	0.42
5:I:92:DT:O4	5:J:200:DA:N6	2.51	0.42
5:J:216:DG:O3'	7:F:45:ARG:NE	2.34	0.42
8:C:81:THR:HA	8:C:84:HIS:HB3	2.01	0.42
8:C:85:LEU:HD13	8:C:103:ILE:HG21	2.01	0.42
3:K:355:ASP:OD1	3:K:355:ASP:N	2.52	0.42
4:M:346:ASP:OD1	4:M:346:ASP:N	2.50	0.42
9:D:46:LYS:HA	9:D:49:LYS:HG2	2.01	0.42
5:I:101:DC:N4	5:J:191:DT:O4	2.53	0.42
5:J:185:DG:H3'	9:H:90:SER:HB3	2.01	0.42
6:A:131:ARG:C	6:E:131:ARG:HH22	2.26	0.42
7:B:30:THR:O	7:B:34:ILE:N	2.37	0.42
7:F:32:PRO:HB2	7:F:35:ARG:HG3	2.02	0.42
8:G:52:TYR:CE1	9:H:97:ILE:HG12	2.54	0.42
3:K:209:LYS:HE3	4:M:166:GLU:HB2	2.02	0.42
8:C:54:THR:HA	8:C:57:LEU:HB2	2.01	0.42
2:N:9:GLN:HE21	2:N:13:ASP:HB3	1.85	0.42
3:K:413:TYR:HA	3:K:416:LEU:HG	2.00	0.42
4:M:346:ASP:OD1	4:M:347:LEU:N	2.51	0.42
5:J:175:DA:H2'	5:J:176:DA:C5	2.55	0.42
5:J:227:DG:H2''	5:J:228:DA:C8	2.54	0.42
2:N:80:GLN:HG2	2:N:81:SER:HB3	2.01	0.42
9:D:120:ALA:HA	9:D:123:LYS:HG2	2.00	0.42
9:H:118:THR:HA	9:H:121:VAL:HG22	2.01	0.42
5:I:91:DT:OP2	6:E:65:LEU:N	2.44	0.42
6:A:50:GLU:O	6:A:54:PHE:HB2	2.20	0.42
8:G:32:LYS:HD3	8:G:32:LYS:HA	1.85	0.42
4:M:241:GLU:N	4:M:241:GLU:OE1	2.53	0.42
5:I:109:DA:H1'	5:I:110:DA:H5'	2.02	0.42
3:K:427:ASN:OD1	3:K:428:ARG:N	2.53	0.41
5:I:39:DG:O3'	9:D:91:THR:OG1	2.36	0.41
5:J:254:DC:H2''	5:J:255:DA:N7	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:58:THR:OG1	6:A:58:THR:O	2.33	0.41
9:D:51:THR:OG1	9:D:52:HIS:ND1	2.53	0.41
9:H:98:GLN:HE21	9:H:114:VAL:HG22	1.85	0.41
3:K:351:ALA:O	3:K:354:SER:OG	2.28	0.41
3:K:410:LEU:HA	3:K:413:TYR:HE1	1.85	0.41
5:J:186:DG:H2''	5:J:187:DA:N7	2.35	0.41
5:J:237:DT:OP1	6:A:69:ARG:NH2	2.52	0.41
9:H:64:ILE:O	9:H:67:SER:OG	2.35	0.41
2:N:94:LEU:HA	2:N:94:LEU:HD23	1.82	0.41
5:I:24:DA:N6	5:J:268:DG:O6	2.53	0.41
5:J:265:DT:H2''	5:J:266:DT:C6	2.55	0.41
3:K:186:PRO:HA	3:K:189:LEU:HB2	2.02	0.41
3:K:232:ASP:OD1	3:K:232:ASP:N	2.53	0.41
3:K:313:ARG:N	3:K:316:TYR:OH	2.53	0.41
5:I:101:DC:H2'	5:I:102:DA:C8	2.55	0.41
5:J:278:DC:P	8:C:77:VAL:H	2.43	0.41
3:K:214:TYR:HA	3:K:217:LYS:HB3	2.01	0.41
3:K:230:ARG:NH2	3:K:279:ARG:HE	2.10	0.41
6:E:126:LEU:HG	6:E:129:ARG:HH21	1.84	0.41
3:K:179:PRO:HA	3:K:258:PHE:CE1	2.55	0.41
3:K:369:THR:HA	4:M:64:GLN:HA	2.03	0.41
4:M:220:LEU:HB3	4:M:224:LEU:HD23	2.02	0.41
4:M:248:HIS:CE1	4:M:259:MET:HG2	2.55	0.41
7:F:39:ARG:HH22	7:F:46:ILE:HD11	1.85	0.41
5:I:119:DT:H2''	5:I:120:DT:H5'	2.02	0.41
5:J:278:DC:H3'	8:C:76:LYS:HE2	2.02	0.41
6:A:61:LEU:HD22	6:A:62:ILE:HD13	2.03	0.41
5:J:168:DC:H2'	5:J:169:DT:H71	2.02	0.41
8:C:49:ALA:O	8:C:53:LEU:N	2.32	0.41
6:E:109:LEU:HD12	6:E:112:ILE:HD11	2.03	0.41
3:K:186:PRO:HB2	3:K:190:THR:HG23	2.02	0.41
3:K:195:ILE:HD13	3:K:195:ILE:HA	1.93	0.41
3:K:226:ASN:OD1	4:M:150:PHE:N	2.53	0.41
4:M:277:ASP:OD1	4:M:277:ASP:N	2.53	0.41
5:J:214:DG:H2''	5:J:215:DC:C2	2.56	0.41
8:C:24:LEU:HD11	8:C:53:LEU:HD12	2.02	0.41
9:D:109:LEU:O	9:D:113:ALA:HB3	2.20	0.41
4:M:167:ARG:NH2	4:M:168:ASP:OD2	2.54	0.40
4:M:173:ASN:HA	4:M:177:ASN:ND2	2.33	0.40
5:I:51:DA:P	6:A:83:ARG:HD3	2.61	0.40
6:A:52:ARG:HH12	6:A:56:LYS:HZ2	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:94:GLU:HA	6:A:97:GLU:HB2	2.03	0.40
8:C:67:LEU:HA	8:C:87:LEU:HG	2.02	0.40
3:K:276:MET:HE3	3:K:320:LEU:HG	2.03	0.40
8:C:28:VAL:HA	8:C:53:LEU:HD11	2.03	0.40
6:E:52:ARG:O	6:E:56:LYS:HB2	2.20	0.40
3:K:393:ILE:HA	3:K:393:ILE:HD12	1.77	0.40
3:K:414:ASN:HA	3:K:417:LYS:HB2	2.03	0.40
4:M:262:ARG:HH12	4:M:267:LEU:HB2	1.86	0.40
8:C:44:ARG:HB3	9:D:92:ILE:HB	2.04	0.40
9:H:121:VAL:HA	9:H:124:TYR:HD2	1.86	0.40
4:M:67:LYS:NZ	4:M:68:ILE:O	2.54	0.40
5:J:155:DC:OP2	6:A:52:ARG:NH2	2.51	0.40
5:J:197:DA:OP1	6:E:72:ARG:NH1	2.55	0.40
8:C:77:VAL:O	9:D:55:THR:OG1	2.28	0.40
3:K:213:ARG:NH2	4:M:187:ASP:HB3	2.36	0.40
3:K:250:ASN:O	3:K:254:LEU:N	2.46	0.40
4:M:177:ASN:HD21	4:M:189:PHE:HZ	1.69	0.40
8:C:70:ASN:HB3	8:C:83:ARG:CZ	2.52	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	L	21/537 (4%)	19 (90%)	2 (10%)	0	100	100
2	N	71/120 (59%)	67 (94%)	4 (6%)	0	100	100
3	K	272/469 (58%)	221 (81%)	51 (19%)	0	100	100
4	M	224/586 (38%)	181 (81%)	43 (19%)	0	100	100
6	A	95/136 (70%)	87 (92%)	8 (8%)	0	100	100
6	E	95/136 (70%)	84 (88%)	11 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	B	77/102 (76%)	72 (94%)	5 (6%)	0	100	100
7	F	78/102 (76%)	66 (85%)	12 (15%)	0	100	100
8	C	96/134 (72%)	89 (93%)	7 (7%)	0	100	100
8	G	106/134 (79%)	98 (92%)	8 (8%)	0	100	100
9	D	91/131 (70%)	81 (89%)	10 (11%)	0	100	100
9	H	94/131 (72%)	93 (99%)	1 (1%)	0	100	100
All	All	1320/2718 (49%)	1158 (88%)	162 (12%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	23/442 (5%)	23 (100%)	0	100	100
2	N	70/111 (63%)	70 (100%)	0	100	100
3	K	255/434 (59%)	254 (100%)	1 (0%)	84	84
4	M	217/542 (40%)	216 (100%)	1 (0%)	81	83
6	A	85/113 (75%)	82 (96%)	3 (4%)	32	53
6	E	85/113 (75%)	85 (100%)	0	100	100
7	B	67/81 (83%)	67 (100%)	0	100	100
7	F	68/81 (84%)	67 (98%)	1 (2%)	57	72
8	C	77/103 (75%)	76 (99%)	1 (1%)	61	74
8	G	86/103 (84%)	85 (99%)	1 (1%)	63	75
9	D	81/109 (74%)	80 (99%)	1 (1%)	63	75
9	H	82/109 (75%)	81 (99%)	1 (1%)	63	75
All	All	1196/2341 (51%)	1186 (99%)	10 (1%)	70	80

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	268	VAL
4	M	235	ARG
6	A	58	THR
6	A	94	GLU
6	A	121	LYS
8	C	77	VAL
9	D	64	ILE
7	F	50	ILE
8	G	33	ARG
9	H	65	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	34	GLN
2	N	16	ASN
2	N	107	ASN
3	K	261	HIS
3	K	392	ASN
4	M	245	HIS
4	M	287	ASN
6	A	39	HIS
6	A	93	GLN
7	B	93	GLN
8	C	111	HIS
6	E	85	GLN
8	G	111	HIS
9	H	98	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

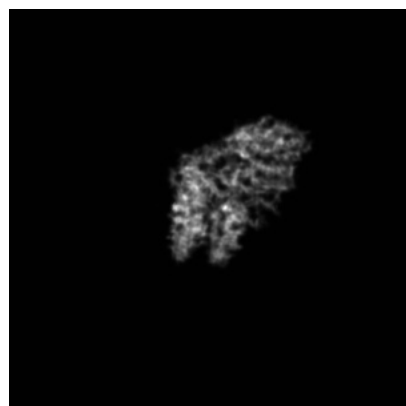
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38025. These allow visual inspection of the internal detail of the map and identification of artifacts.

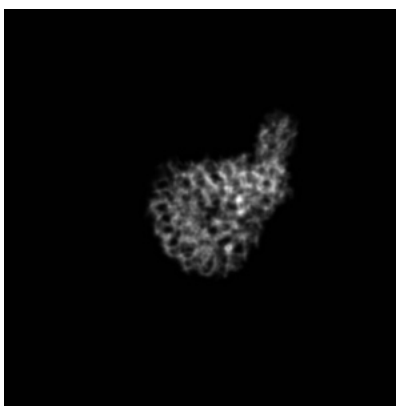
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

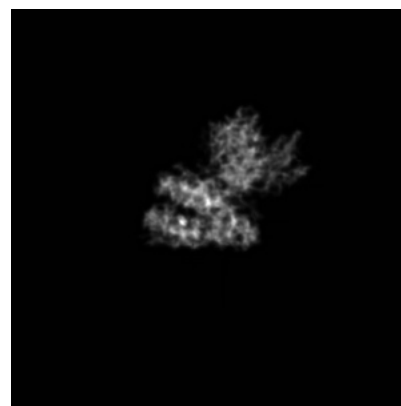
6.1.1 Primary map



X

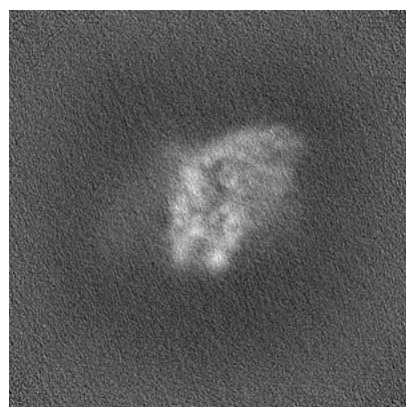


Y

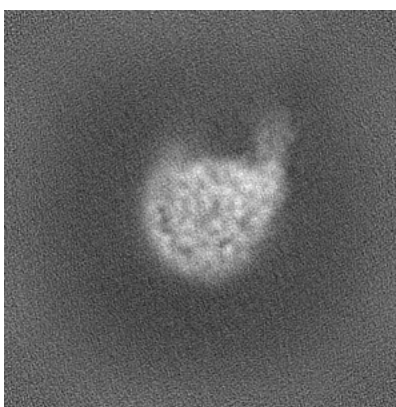


Z

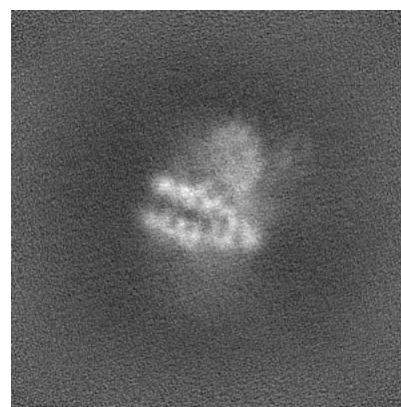
6.1.2 Raw map



X



Y

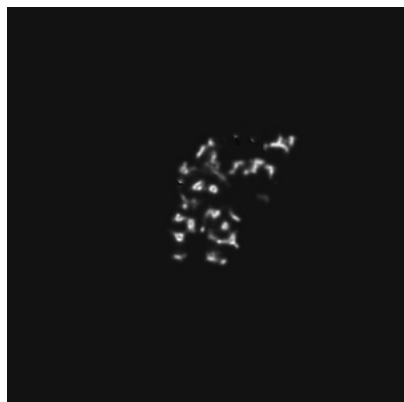


Z

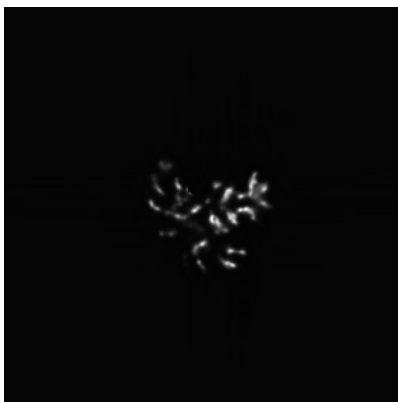
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

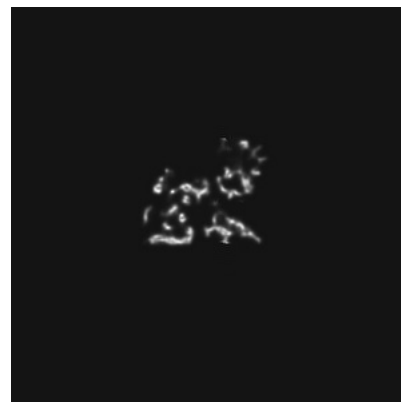
6.2.1 Primary map



X Index: 150

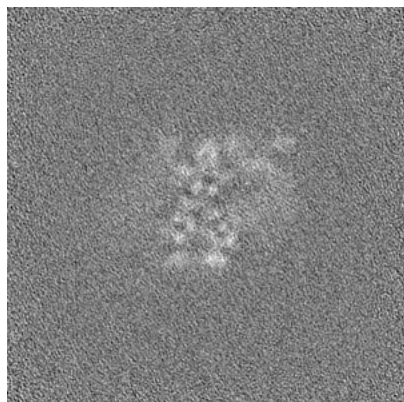


Y Index: 150

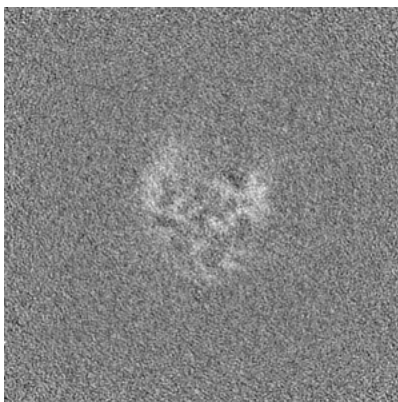


Z Index: 150

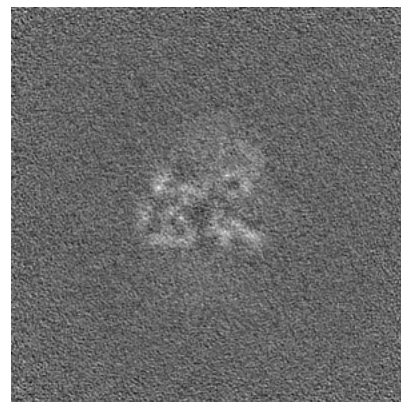
6.2.2 Raw map



X Index: 150



Y Index: 150

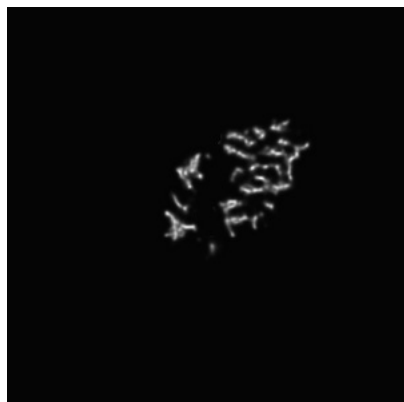


Z Index: 150

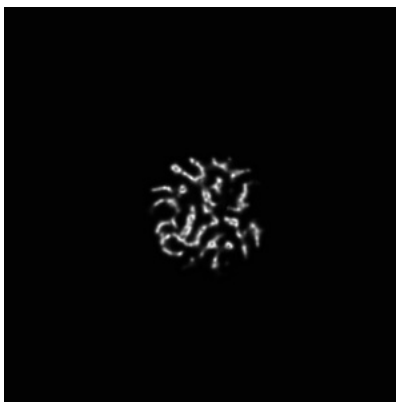
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 175

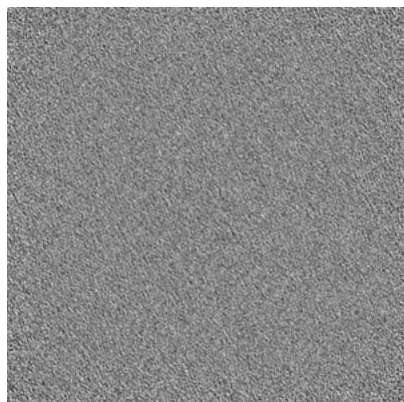


Y Index: 132

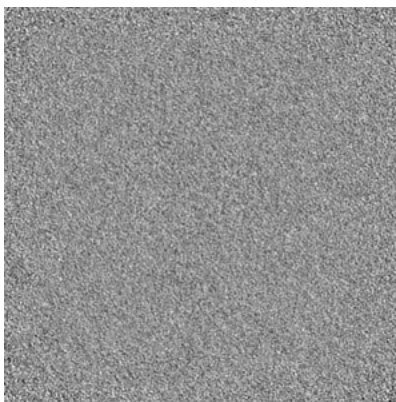


Z Index: 166

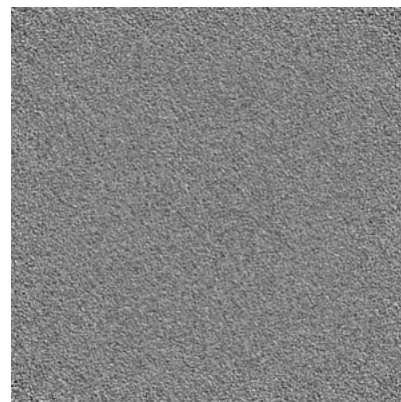
6.3.2 Raw map



X Index: 0



Y Index: 0

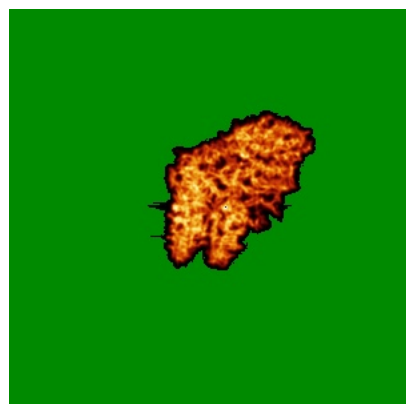


Z Index: 0

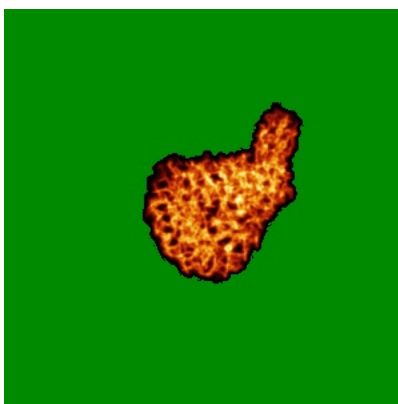
The images above show the largest variance slices of the map in three orthogonal directions.

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

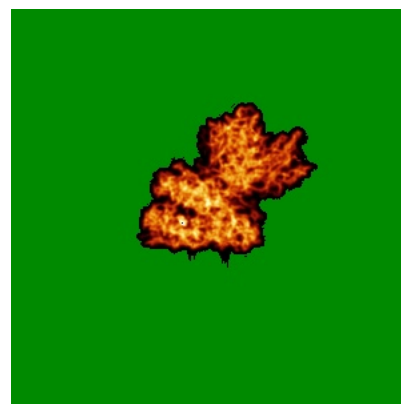
6.4.1 Primary map



X

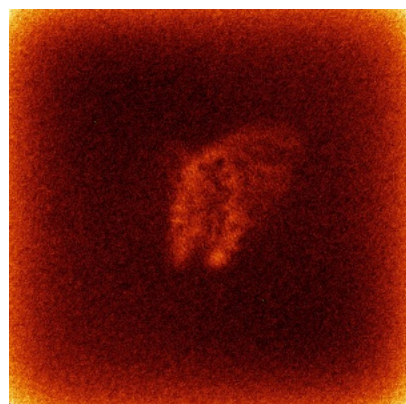


Y

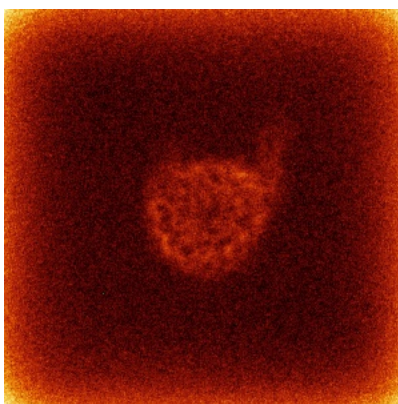


Z

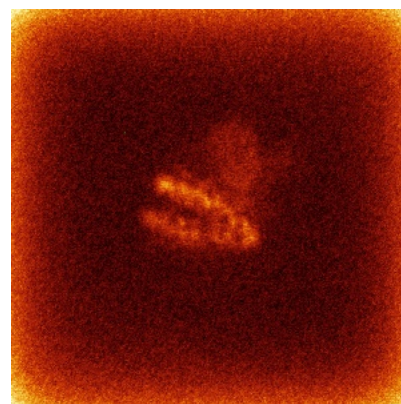
6.4.2 Raw map



X



Y

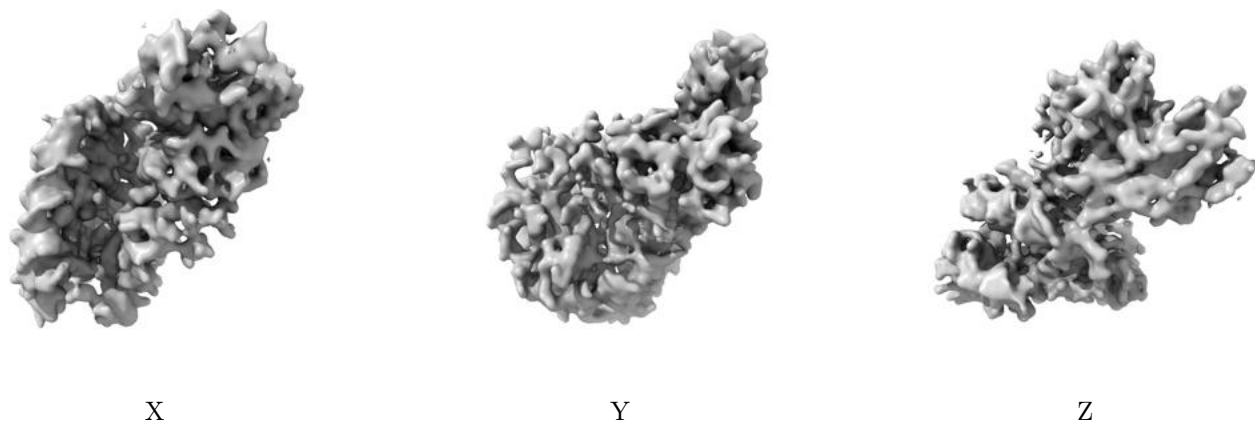


Z

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.

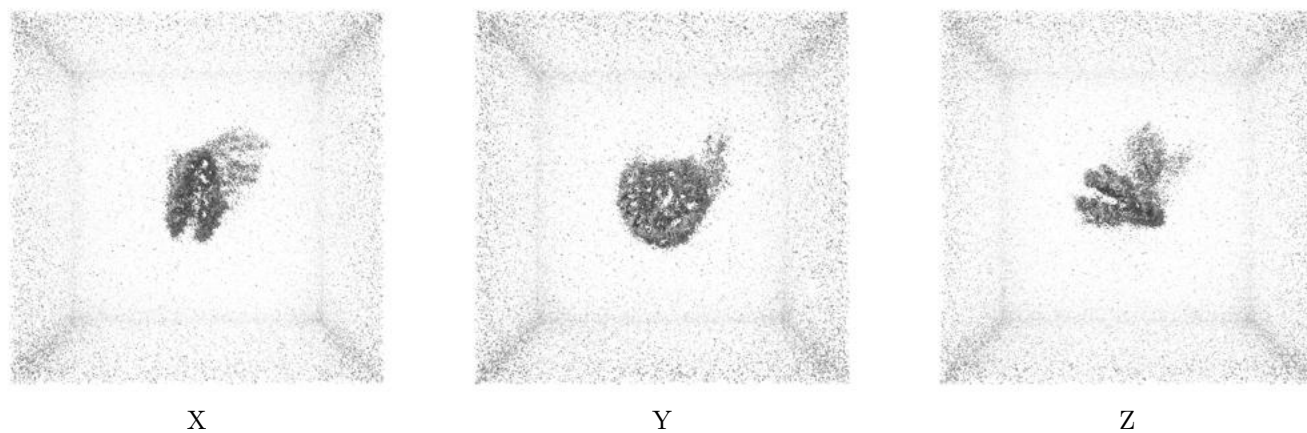
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.39. 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.

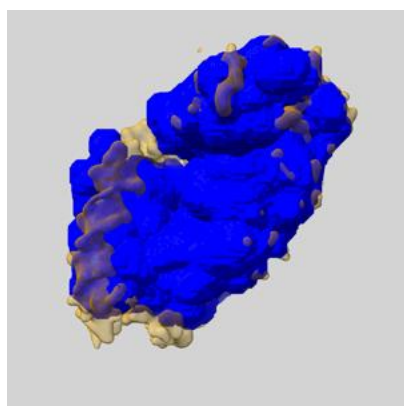
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

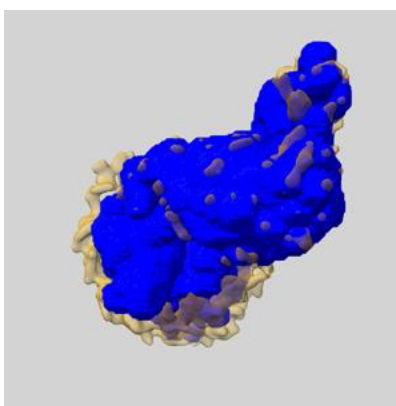
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

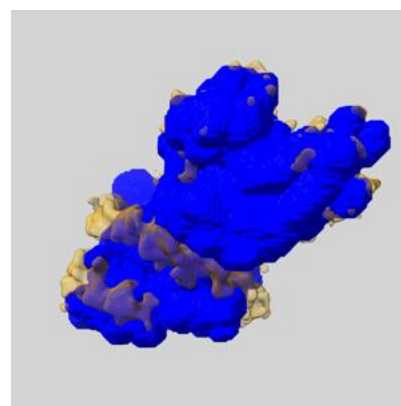
6.6.1 emd_38025_msk_1.map [i](#)



X



Y

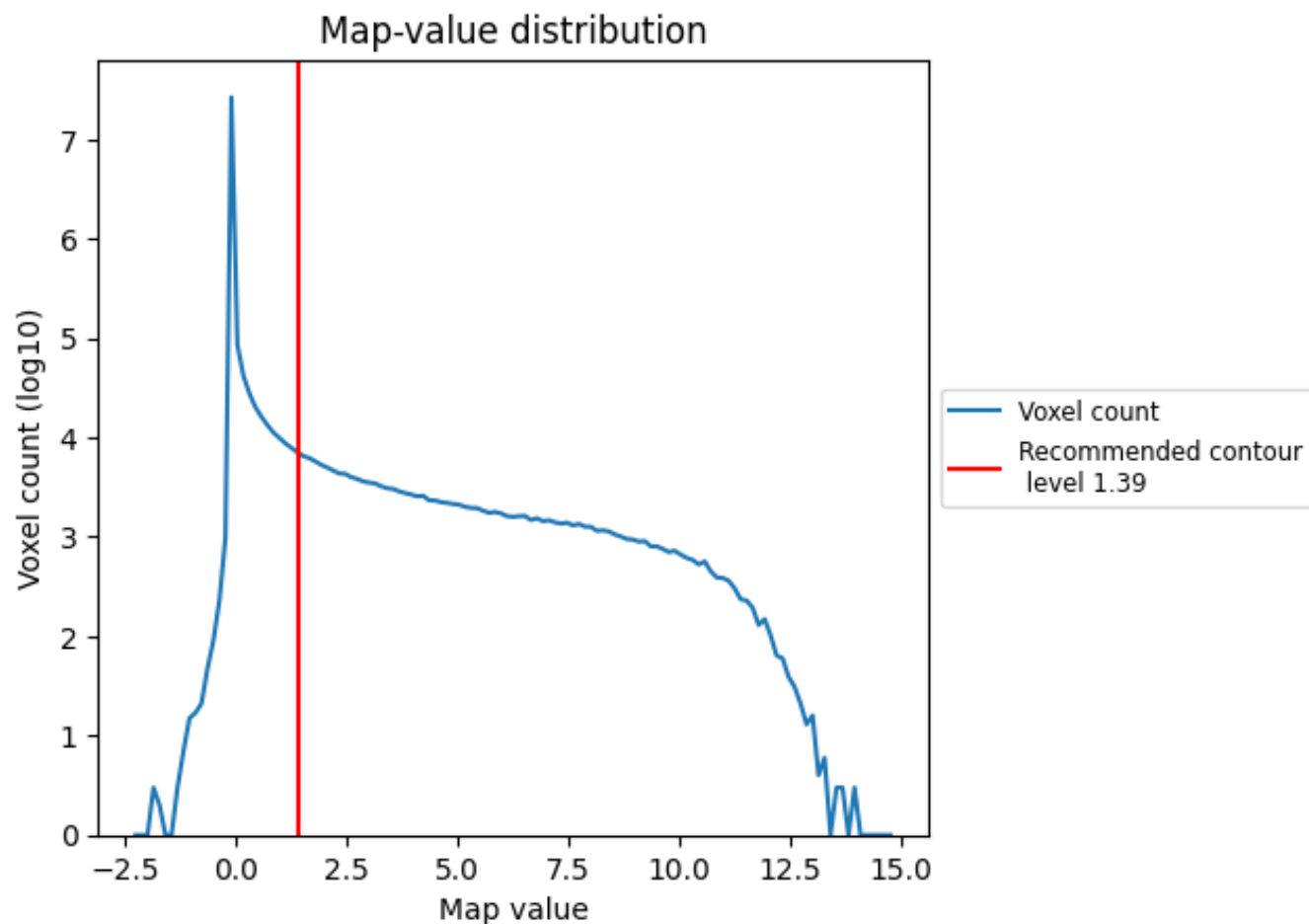


Z

7 Map analysis [i](#)

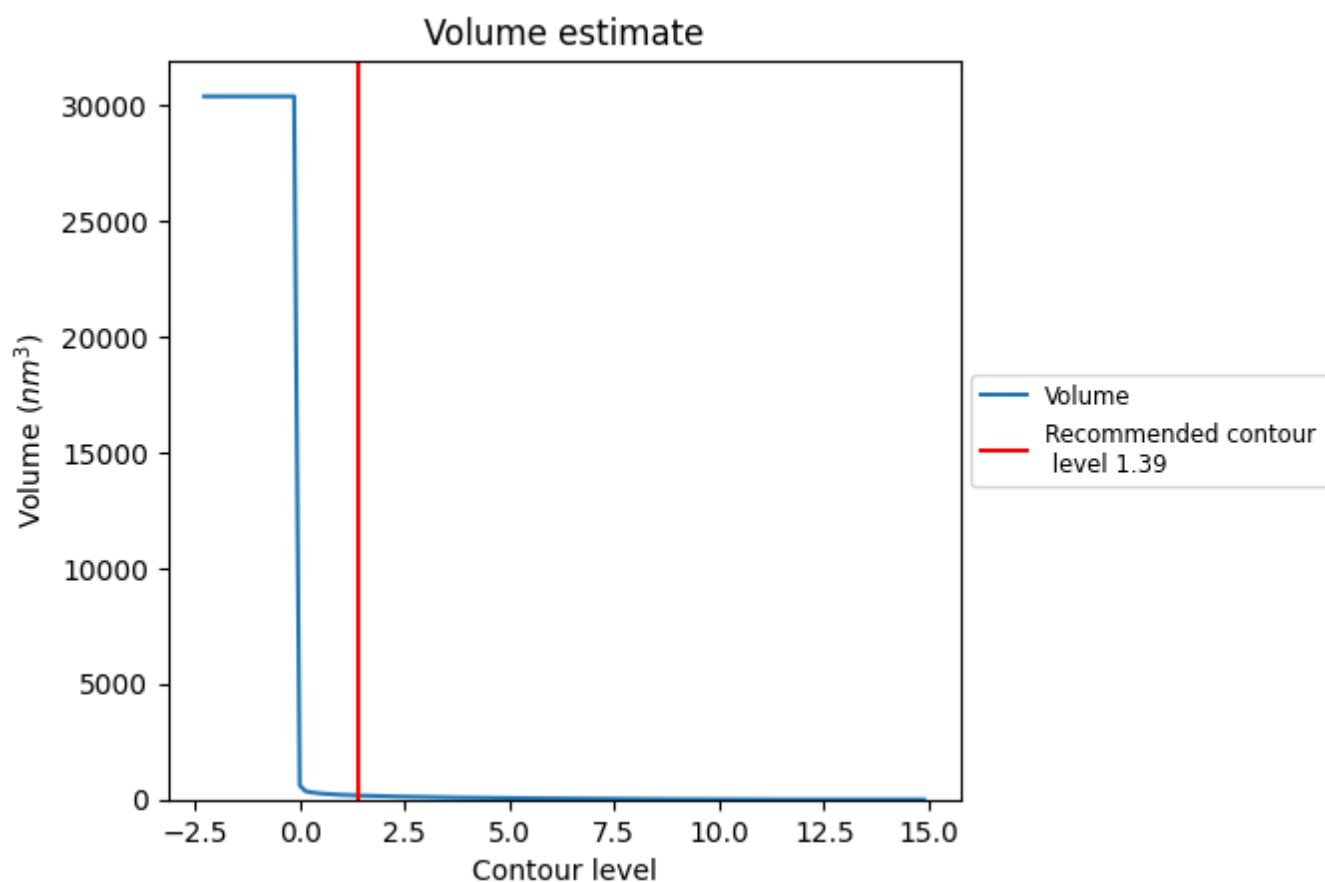
This section contains the results of statistical analysis of the map.

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.

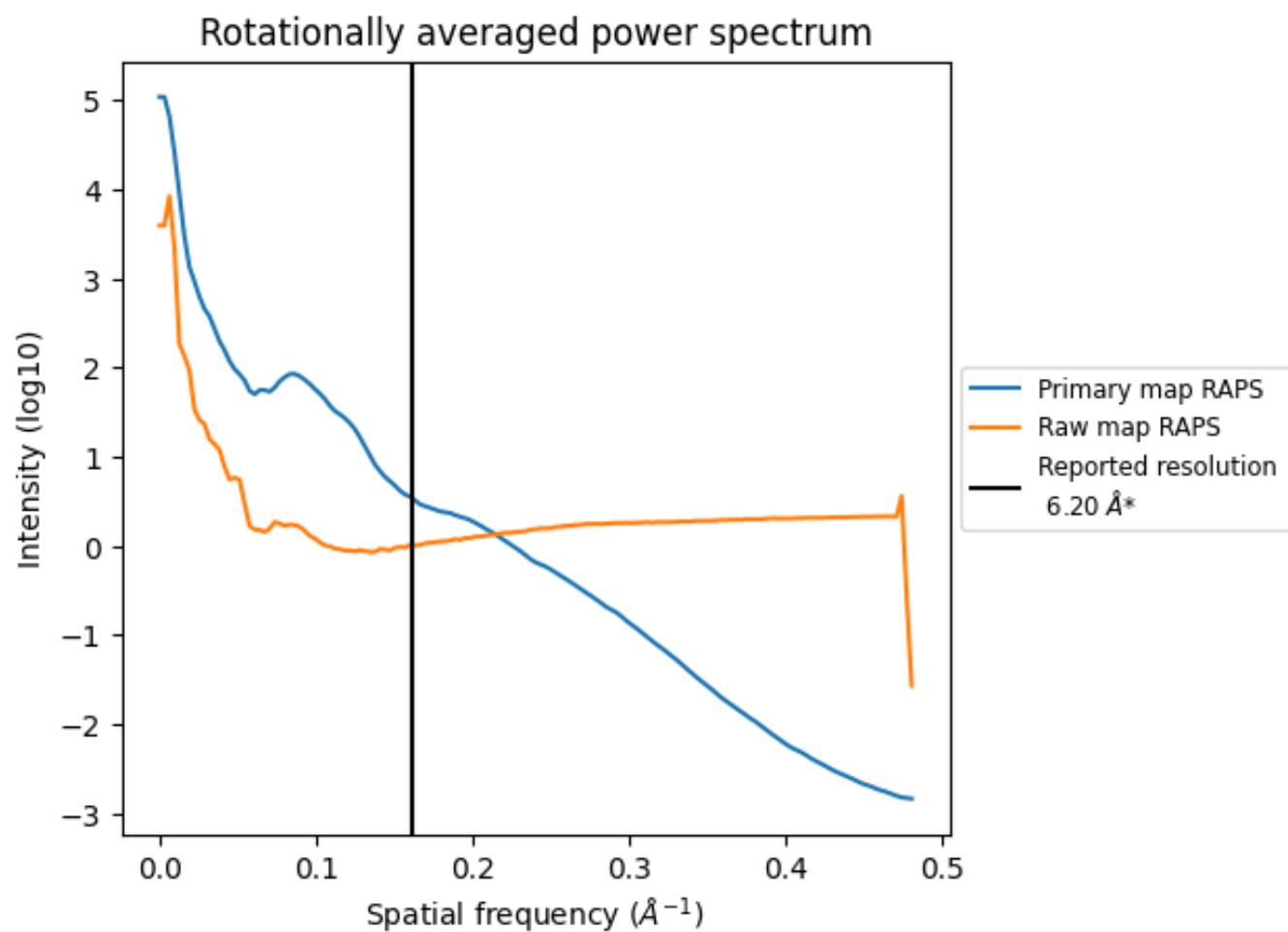
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177 nm³; this corresponds to an approximate mass of 160 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 ⓘ

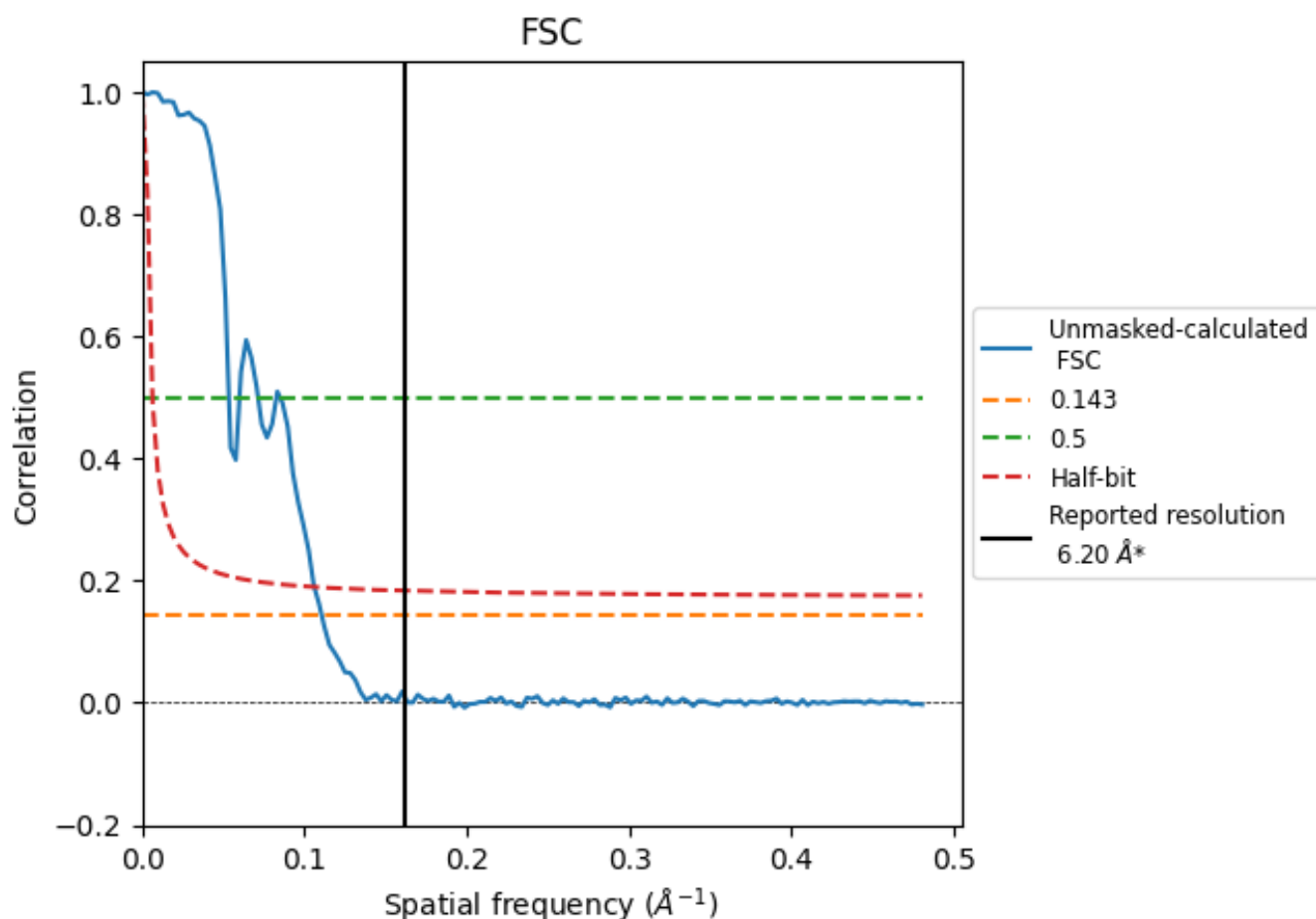


*Reported resolution corresponds to spatial frequency of $0.161 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.161 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

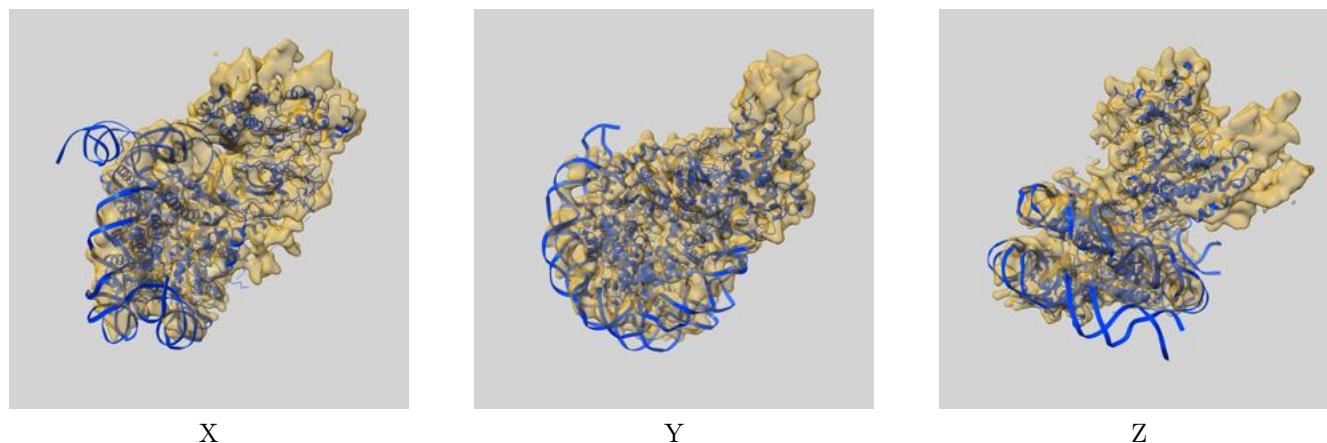
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.04	18.73	9.43

*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 9.04 differs from the reported value 6.2 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38025 and PDB model 8X31. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



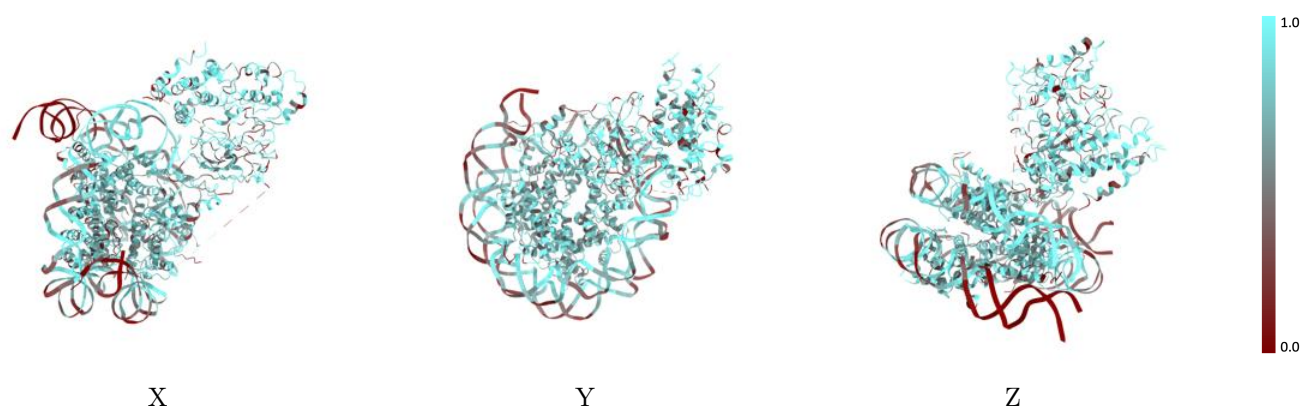
The images above show the 3D surface view of the map at the recommended contour level 1.39 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



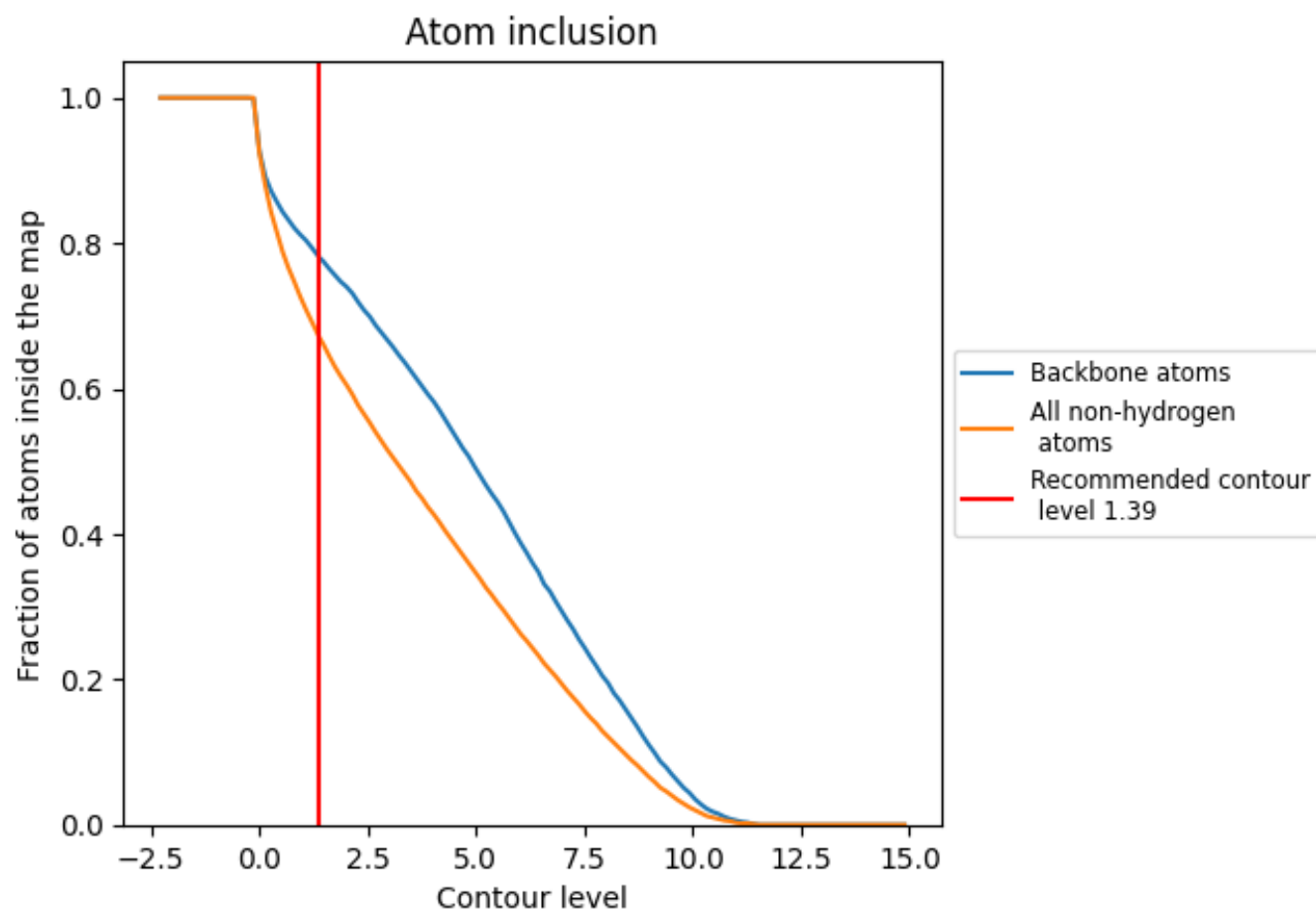
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.39).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 67% 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 (1.39) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6700	0.1230
A	0.7050	0.1180
B	0.7200	0.1280
C	0.6620	0.0930
D	0.7590	0.1610
E	0.7300	0.1160
F	0.7330	0.1390
G	0.6290	0.1080
H	0.7400	0.1540
I	0.6030	0.1340
J	0.5810	0.1250
K	0.7040	0.1000
L	0.6650	0.1280
M	0.7330	0.1150
N	0.7700	0.1330

1.0

0.0

<0.0