



Full wwPDB EM Validation Report ⓘ

Apr 18, 2026 – 07:43 am BST

PDB ID : 9RWZ / pdb_00009rwz
EMDB ID : EMD-54352
Title : ZSWIM8-CUL3 complex bound to AGO2-miR-7-CYRANO
Authors : Farnung, J.; Slobodyanyuk, E.; Bartel, D.P.; Schulman, B.A.
Deposited on : 2025-07-10
Resolution : 3.10 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:

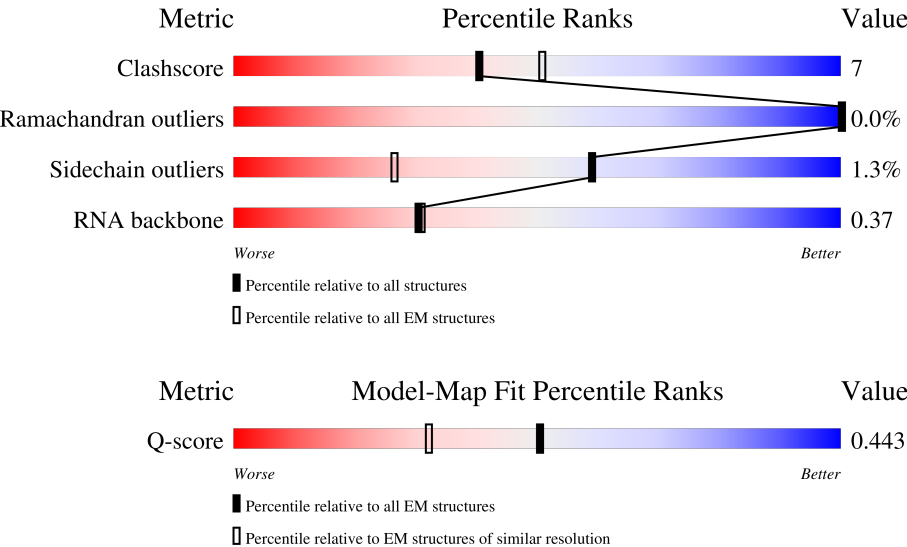
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.10 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	14724 (2.60 - 3.60)

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	870	
2	B	118	
2	C	118	

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Mol	Chain	Length	Quality of chain
3	D	112	
3	E	112	
4	G	24	
5	H	396	
5	I	396	
6	T	120	
7	M	1866	
7	N	1866	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 28601 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 argonaute-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	823	Total	C	N	O	S	0	0
			6579	4180	1186	1171	42		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP Q9UKV8
A	-9	GLY	-	expression tag	UNP Q9UKV8
A	-8	SER	-	expression tag	UNP Q9UKV8
A	-7	SER	-	expression tag	UNP Q9UKV8
A	-6	HIS	-	expression tag	UNP Q9UKV8
A	-5	HIS	-	expression tag	UNP Q9UKV8
A	-4	HIS	-	expression tag	UNP Q9UKV8
A	-3	HIS	-	expression tag	UNP Q9UKV8
A	-2	HIS	-	expression tag	UNP Q9UKV8
A	-1	HIS	-	expression tag	UNP Q9UKV8
A	0	GLY	-	expression tag	UNP Q9UKV8
A	1	SER	-	expression tag	UNP Q9UKV8

- Molecule 2 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	97	Total	C	N	O	S	0	0
			763	482	130	148	3		
2	C	97	Total	C	N	O	S	0	0
			763	482	130	148	3		

- Molecule 3 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	100	Total	C	N	O	S	0	0
			783	501	126	150	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	99	Total	C	N	O	S	0	0
			779	499	125	149	6		

- Molecule 4 is a RNA chain called miR-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	24	Total	C	N	O	P	0	0
			512	228	85	175	24		

- Molecule 5 is a protein called Cullin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	174	Total	C	N	O	S	0	0
			1447	905	268	262	12		
5	I	175	Total	C	N	O	S	0	0
			1452	908	269	263	12		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	342	ARG	ILE	engineered mutation	UNP Q13618
H	346	ASP	LEU	engineered mutation	UNP Q13618
H	391	GLU	-	expression tag	UNP Q13618
H	392	ASN	-	expression tag	UNP Q13618
H	393	LEU	-	expression tag	UNP Q13618
H	394	TYR	-	expression tag	UNP Q13618
H	395	PHE	-	expression tag	UNP Q13618
H	396	GLN	-	expression tag	UNP Q13618
I	342	ARG	ILE	engineered mutation	UNP Q13618
I	346	ASP	LEU	engineered mutation	UNP Q13618
I	391	GLU	-	expression tag	UNP Q13618
I	392	ASN	-	expression tag	UNP Q13618
I	393	LEU	-	expression tag	UNP Q13618
I	394	TYR	-	expression tag	UNP Q13618
I	395	PHE	-	expression tag	UNP Q13618
I	396	GLN	-	expression tag	UNP Q13618

- Molecule 6 is a RNA chain called CYRANO trigger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	26	Total	C	N	O	P	0	0
			547	247	99	175	26		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	G	-	expression tag	GB 2994212338
T	117	A	-	expression tag	GB 2994212338
T	118	A	-	expression tag	GB 2994212338
T	119	A	-	expression tag	GB 2994212338
T	120	A	-	expression tag	GB 2994212338

- Molecule 7 is a protein called Zinc finger SWIM domain-containing protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	1013	Total	C	N	O	S	0	0
			7499	4726	1337	1393	43		
7	M	1031	Total	C	N	O	S	0	0
			7475	4707	1325	1400	43		

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	1838	GLY	-	expression tag	UNP A7E2V4
N	1839	TRP	-	expression tag	UNP A7E2V4
N	1840	SER	-	expression tag	UNP A7E2V4
N	1841	HIS	-	expression tag	UNP A7E2V4
N	1842	PRO	-	expression tag	UNP A7E2V4
N	1843	GLN	-	expression tag	UNP A7E2V4
N	1844	PHE	-	expression tag	UNP A7E2V4
N	1845	GLU	-	expression tag	UNP A7E2V4
N	1846	LYS	-	expression tag	UNP A7E2V4
N	1847	GLY	-	expression tag	UNP A7E2V4
N	1848	GLY	-	expression tag	UNP A7E2V4
N	1849	GLY	-	expression tag	UNP A7E2V4
N	1850	SER	-	expression tag	UNP A7E2V4
N	1851	GLY	-	expression tag	UNP A7E2V4
N	1852	GLY	-	expression tag	UNP A7E2V4
N	1853	GLY	-	expression tag	UNP A7E2V4
N	1854	SER	-	expression tag	UNP A7E2V4
N	1855	GLY	-	expression tag	UNP A7E2V4
N	1856	GLY	-	expression tag	UNP A7E2V4
N	1857	SER	-	expression tag	UNP A7E2V4
N	1858	ALA	-	expression tag	UNP A7E2V4
N	1859	TRP	-	expression tag	UNP A7E2V4
N	1860	SER	-	expression tag	UNP A7E2V4
N	1861	HIS	-	expression tag	UNP A7E2V4

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Chain	Residue	Modelled	Actual	Comment	Reference
N	1862	PRO	-	expression tag	UNP A7E2V4
N	1863	GLN	-	expression tag	UNP A7E2V4
N	1864	PHE	-	expression tag	UNP A7E2V4
N	1865	GLU	-	expression tag	UNP A7E2V4
N	1866	LYS	-	expression tag	UNP A7E2V4
M	1838	GLY	-	expression tag	UNP A7E2V4
M	1839	TRP	-	expression tag	UNP A7E2V4
M	1840	SER	-	expression tag	UNP A7E2V4
M	1841	HIS	-	expression tag	UNP A7E2V4
M	1842	PRO	-	expression tag	UNP A7E2V4
M	1843	GLN	-	expression tag	UNP A7E2V4
M	1844	PHE	-	expression tag	UNP A7E2V4
M	1845	GLU	-	expression tag	UNP A7E2V4
M	1846	LYS	-	expression tag	UNP A7E2V4
M	1847	GLY	-	expression tag	UNP A7E2V4
M	1848	GLY	-	expression tag	UNP A7E2V4
M	1849	GLY	-	expression tag	UNP A7E2V4
M	1850	SER	-	expression tag	UNP A7E2V4
M	1851	GLY	-	expression tag	UNP A7E2V4
M	1852	GLY	-	expression tag	UNP A7E2V4
M	1853	GLY	-	expression tag	UNP A7E2V4
M	1854	SER	-	expression tag	UNP A7E2V4
M	1855	GLY	-	expression tag	UNP A7E2V4
M	1856	GLY	-	expression tag	UNP A7E2V4
M	1857	SER	-	expression tag	UNP A7E2V4
M	1858	ALA	-	expression tag	UNP A7E2V4
M	1859	TRP	-	expression tag	UNP A7E2V4
M	1860	SER	-	expression tag	UNP A7E2V4
M	1861	HIS	-	expression tag	UNP A7E2V4
M	1862	PRO	-	expression tag	UNP A7E2V4
M	1863	GLN	-	expression tag	UNP A7E2V4
M	1864	PHE	-	expression tag	UNP A7E2V4
M	1865	GLU	-	expression tag	UNP A7E2V4
M	1866	LYS	-	expression tag	UNP A7E2V4

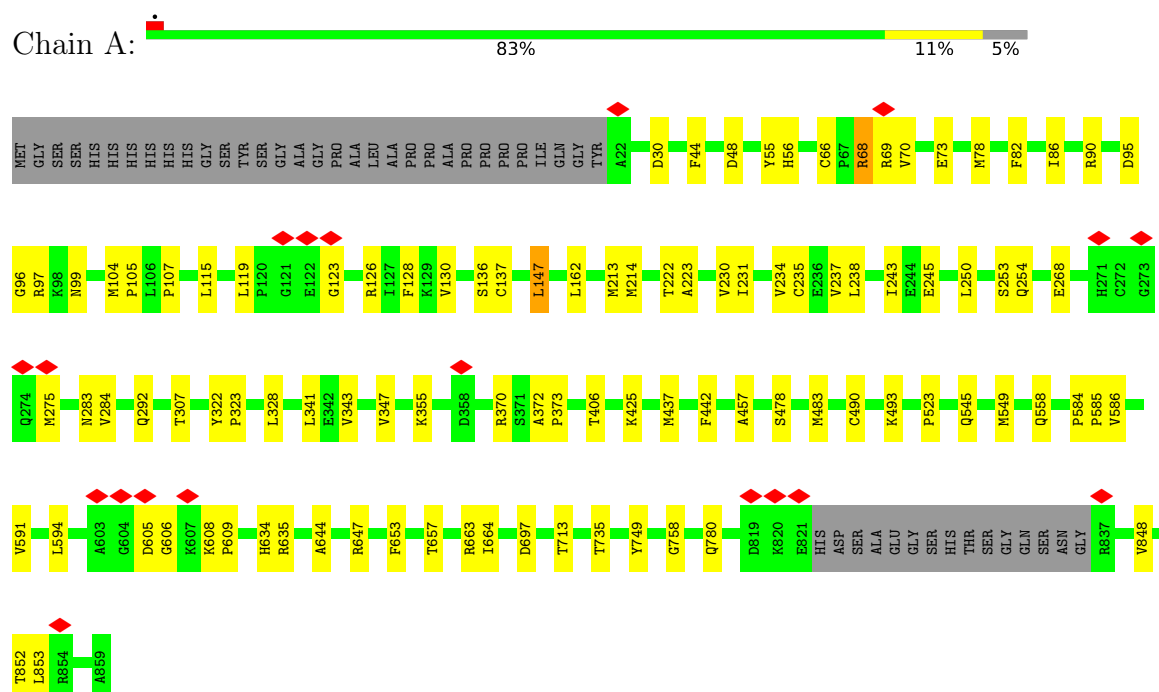
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
8	N	1	Total Zn 1 1	0
8	M	1	Total Zn 1 1	0

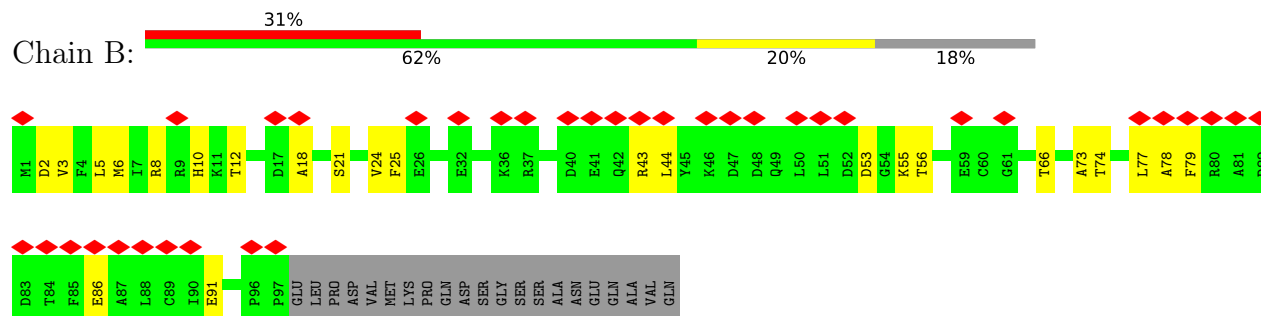
3 Residue-property plots

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

• Molecule 1: Protein argonaute-2

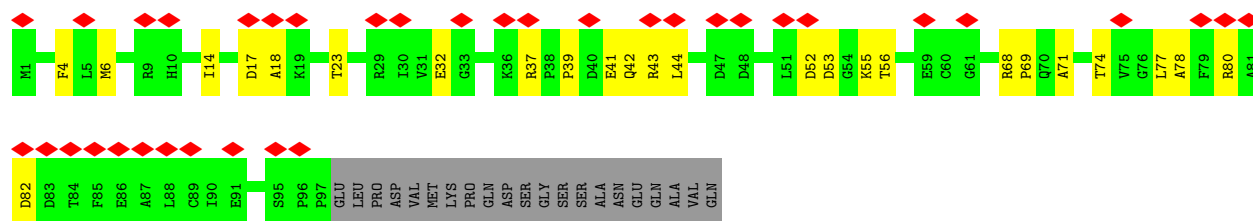


• Molecule 2: Elongin-B



• Molecule 2: Elongin-B

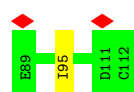
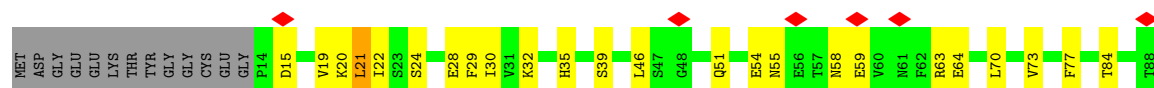




• Molecule 3: Elongin-C



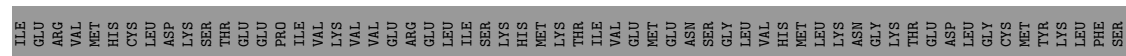
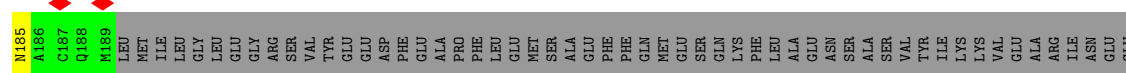
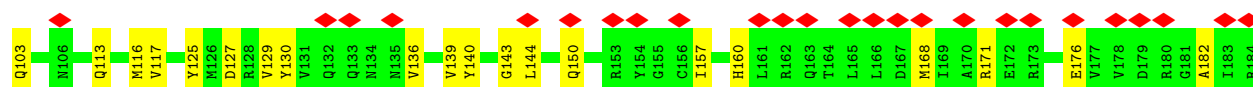
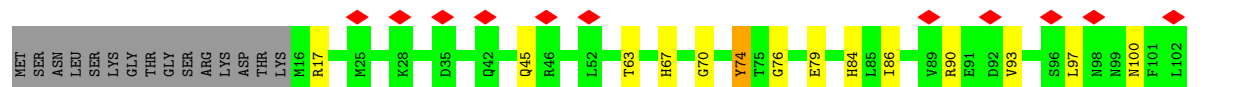
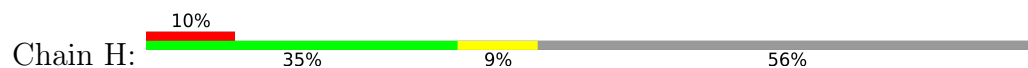
• Molecule 3: Elongin-C



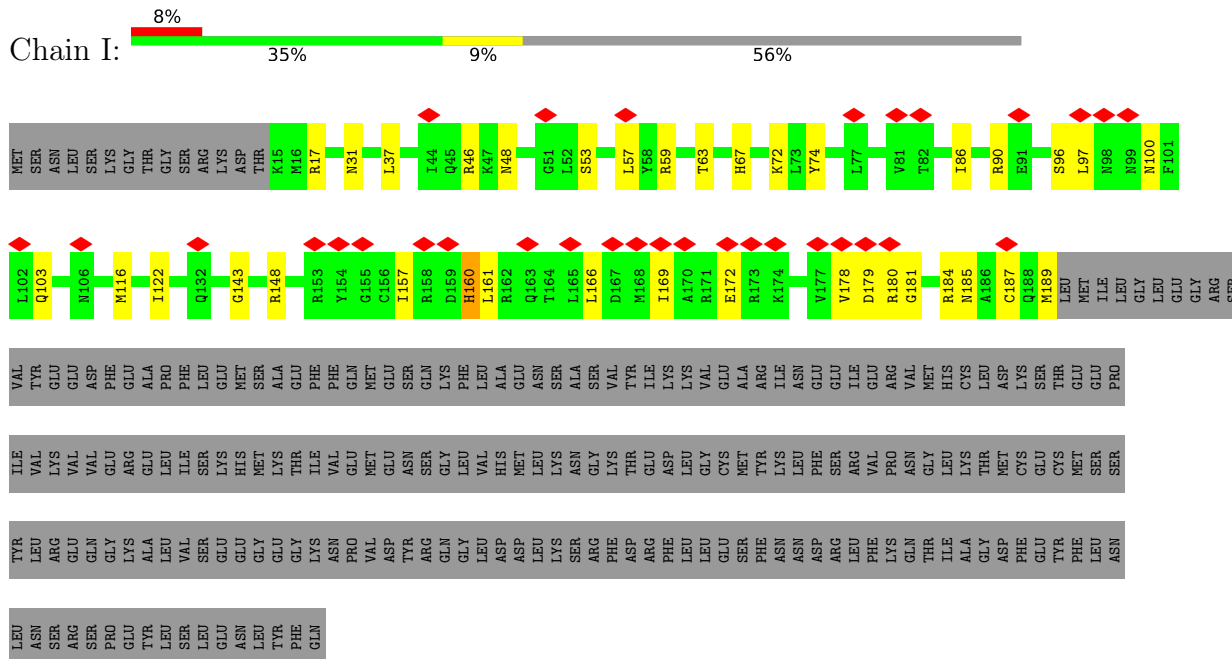
• Molecule 4: miR-7



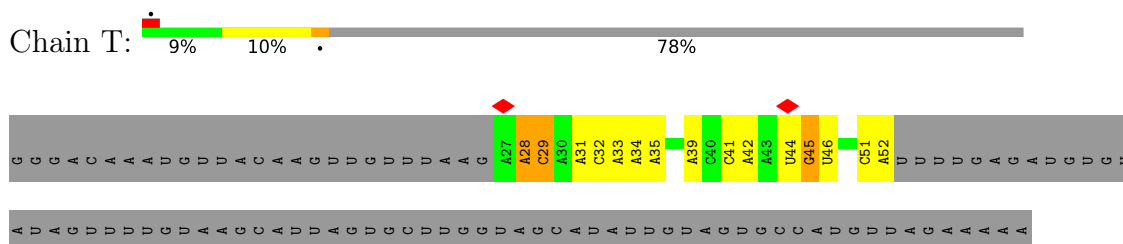
• Molecule 5: Cullin-3



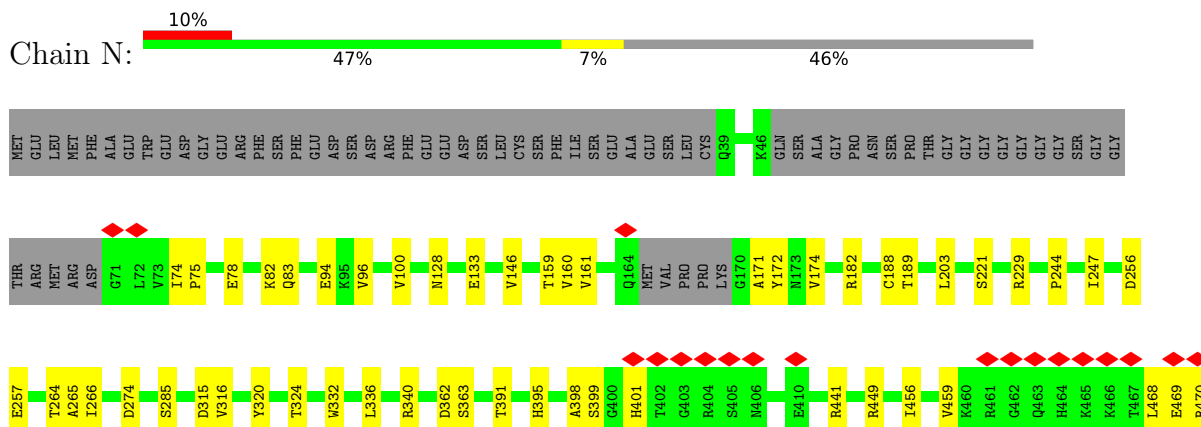
- Molecule 5: Cullin-3



- Molecule 6: CYRANO trigger RNA



- Molecule 7: Zinc finger SWIM domain-containing protein 8







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	230859	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	188.067	Depositor
Minimum map value	-6.312	Depositor
Average map value	0.013	Depositor
Map value standard deviation	1.145	Depositor
Recommended contour level	7	Depositor
Map size (Å)	524.3392, 524.3392, 524.3392	wwPDB
Map dimensions	616, 616, 616	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8512, 0.8512, 0.8512	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/6735	0.38	0/9117
2	B	0.12	0/778	0.28	0/1052
2	C	0.12	0/778	0.26	0/1052
3	D	0.25	0/801	0.36	0/1085
3	E	0.20	0/797	0.31	0/1079
4	G	0.34	0/571	0.41	0/886
5	H	0.18	0/1468	0.30	0/1977
5	I	0.17	0/1473	0.30	0/1984
6	T	0.29	0/611	0.35	0/947
7	M	0.38	0/7627	0.43	0/10403
7	N	0.37	0/7657	0.41	0/10423
All	All	0.33	0/29296	0.39	0/40005

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6579	0	6632	65	0
2	B	763	0	758	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	763	0	758	37	0
3	D	783	0	768	14	0
3	E	779	0	766	20	0
4	G	512	0	254	4	0
5	H	1447	0	1451	25	0
5	I	1452	0	1453	23	0
6	T	547	0	282	8	0
7	M	7475	0	6870	91	0
7	N	7499	0	7058	93	0
8	M	1	0	0	0	0
8	N	1	0	0	0	0
All	All	28601	0	27050	391	0

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

All (391) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:42:GLN:HG3	2:C:77:LEU:HD11	1.42	1.00
2:C:42:GLN:HG3	2:C:77:LEU:CD1	1.94	0.98
5:H:140:TYR:CE2	5:H:144:LEU:HD11	2.07	0.90
2:C:42:GLN:HE21	2:C:44:LEU:HD21	1.37	0.88
5:H:140:TYR:CZ	5:H:144:LEU:HD11	2.10	0.87
7:M:1396:CYS:SG	7:M:1397:MET:N	2.55	0.80
5:I:148:ARG:NH2	5:I:189:MET:SD	2.55	0.79
2:B:77:LEU:HD11	2:B:79:PHE:CE1	2.18	0.78
2:B:66:THR:O	2:B:66:THR:HG22	1.83	0.78
2:C:42:GLN:HE21	2:C:44:LEU:CD2	1.97	0.77
7:M:389:VAL:HG21	7:M:417:ALA:HB2	1.66	0.75
7:M:74:ILE:CG2	7:M:78:GLU:HB2	2.18	0.73
7:N:398:ALA:O	7:N:976:PRO:HD2	1.87	0.73
2:C:44:LEU:CD2	2:C:77:LEU:HD13	2.18	0.73
5:H:17:ARG:NH2	7:M:94:GLU:OE2	2.21	0.71
7:N:1367:PRO:HG3	7:N:1398:ALA:HB1	1.72	0.70
7:N:1337:PRO:O	7:N:1340:ALA:HB3	1.91	0.69
3:E:46:LEU:HD12	3:E:46:LEU:O	1.93	0.69
5:H:171:ARG:HB3	5:H:176:GLU:HB3	1.75	0.68
3:D:32:LYS:HB2	3:D:35:HIS:HB2	1.75	0.68
1:A:283:ASN:OD1	1:A:284:VAL:N	2.25	0.68
5:I:86:ILE:HG23	5:I:90:ARG:HE	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:151:GLN:HE21	7:M:178:PHE:HZ	1.39	0.68
5:H:86:ILE:HG13	5:H:90:ARG:HE	1.59	0.68
7:N:852:ASN:OD1	7:N:898:GLU:OE2	2.12	0.67
5:H:168:MET:SD	5:H:171:ARG:NH1	2.62	0.67
7:N:74:ILE:HG23	7:N:75:PRO:HD2	1.76	0.67
2:B:77:LEU:CD1	2:B:79:PHE:CE1	2.77	0.66
7:M:74:ILE:HG22	7:M:78:GLU:HB2	1.75	0.66
7:N:994:MET:HG3	7:N:1007:ILE:HD11	1.77	0.66
2:C:23:THR:HA	2:C:56:THR:HA	1.77	0.66
3:E:54:GLU:OE2	5:I:53:SER:OG	2.13	0.65
5:H:140:TYR:CE2	5:H:144:LEU:CD1	2.78	0.65
7:N:1388:ASP:OD1	7:N:1389:ASN:N	2.30	0.65
7:N:441:ARG:NH1	7:N:484:PHE:O	2.30	0.65
7:N:913:THR:HG22	7:N:913:THR:O	1.95	0.65
7:N:182:ARG:NH1	7:N:285:SER:OG	2.29	0.65
1:A:343:VAL:HG23	1:A:343:VAL:O	1.97	0.64
7:N:1351:ASP:CG	7:N:1354:MET:H	2.06	0.64
3:D:48:GLY:O	3:D:55:ASN:ND2	2.31	0.64
7:M:1385:LYS:C	7:M:1387:GLN:H	2.06	0.63
2:B:8:ARG:NH2	2:B:91:GLU:O	2.31	0.63
5:I:57:LEU:HD23	5:I:122:ILE:HD13	1.80	0.63
7:N:128:ASN:ND2	7:N:133:GLU:CD	2.57	0.63
7:M:1393:GLU:O	7:M:1396:CYS:SG	2.48	0.63
1:A:162:LEU:CD1	1:A:213:MET:HE2	2.29	0.63
7:N:1331:ASP:C	7:N:1333:HIS:H	2.06	0.63
3:E:84:THR:HG23	3:E:84:THR:O	1.97	0.63
2:C:42:GLN:CG	2:C:77:LEU:CD1	2.75	0.62
5:H:90:ARG:NH2	5:H:150:GLN:OE1	2.31	0.62
7:N:1389:ASN:HB3	7:N:1423:LEU:CD1	2.29	0.62
1:A:328:LEU:HD13	1:A:341:LEU:HD21	1.80	0.62
7:M:894:LEU:HD13	7:M:902:MET:HE1	1.82	0.62
1:A:231:ILE:HB	1:A:243:ILE:HD13	1.81	0.62
5:I:181:GLY:O	5:I:185:ASN:ND2	2.32	0.62
7:N:469:GLU:HG3	7:N:470:ARG:HG3	1.83	0.61
1:A:478:SER:OG	1:A:483:MET:O	2.17	0.61
2:C:44:LEU:HD23	2:C:77:LEU:HD13	1.82	0.61
5:I:17:ARG:NH1	7:N:94:GLU:OE2	2.34	0.61
1:A:586:VAL:HG12	1:A:591:VAL:HG21	1.83	0.61
2:C:44:LEU:CD2	2:C:77:LEU:HB2	2.31	0.61
7:M:1001:GLN:C	7:M:1003:LYS:H	2.08	0.61
7:N:1389:ASN:HB3	7:N:1423:LEU:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:44:LEU:HD23	2:C:77:LEU:CD1	2.31	0.60
1:A:605:ASP:OD1	1:A:606:GLY:N	2.34	0.60
2:C:42:GLN:NE2	2:C:44:LEU:HD21	2.11	0.60
2:C:32:GLU:HG3	2:C:39:PRO:HG3	1.83	0.60
7:M:299:LYS:HZ3	7:M:371:ILE:HG22	1.67	0.60
7:M:290:ASP:HB2	7:M:293:THR:HB	1.84	0.60
7:N:146:VAL:HG12	7:N:160:VAL:HG22	1.83	0.59
7:M:970:VAL:HG21	7:M:978:LEU:HD23	1.84	0.59
7:M:136:ARG:HE	7:M:198:THR:HG21	1.67	0.59
7:M:1705:GLY:O	7:M:1708:ALA:HB3	2.03	0.58
2:C:44:LEU:HD23	2:C:77:LEU:CB	2.34	0.58
7:N:1274:HIS:HD2	7:N:1276:ASN:HB2	1.69	0.58
7:N:1662:HIS:HA	7:N:1665:HIS:HB2	1.85	0.58
7:N:961:VAL:HG13	7:N:1010:LYS:HG3	1.85	0.58
7:N:1377:ILE:HD12	7:N:1412:VAL:HG21	1.86	0.57
1:A:78:MET:HE1	1:A:130:VAL:HG11	1.86	0.57
2:C:44:LEU:HA	2:C:77:LEU:HA	1.84	0.57
7:N:1229:VAL:HB	7:N:1232:GLN:HG3	1.86	0.57
1:A:234:VAL:HA	1:A:237:VAL:HG12	1.87	0.57
1:A:634:HIS:ND1	1:A:635:ARG:HG2	2.19	0.57
7:N:1410:PRO:HA	7:N:1413:LEU:HD12	1.86	0.57
2:C:42:GLN:HE21	2:C:44:LEU:CG	2.18	0.57
1:A:123:GLY:HA2	7:N:320:TYR:HE1	1.70	0.56
1:A:44:PHE:HB3	1:A:214:MET:HE3	1.86	0.56
2:C:44:LEU:HD23	2:C:77:LEU:HA	1.87	0.56
3:D:14:PRO:O	3:D:33:ARG:NH1	2.38	0.56
7:M:293:THR:O	7:M:297:ASN:ND2	2.38	0.56
2:C:42:GLN:HE21	2:C:77:LEU:HD13	1.69	0.56
3:E:15:ASP:O	3:E:58:ASN:ND2	2.38	0.56
3:E:95:ILE:HB	7:N:83:GLN:HG3	1.87	0.56
2:B:21:SER:O	2:B:56:THR:OG1	2.17	0.56
7:N:917:TYR:HD1	7:N:967:LYS:HB2	1.71	0.56
3:E:20:LYS:HE2	3:E:22:ILE:HD11	1.87	0.56
7:N:1299:TRP:CH2	7:N:1332:GLY:O	2.58	0.56
7:M:293:THR:HG22	7:M:294:LEU:HG	1.87	0.56
7:N:96:VAL:HG21	7:N:100:VAL:HG13	1.88	0.55
6:T:32:C:H2'	6:T:33:A:H8	1.71	0.55
7:M:1693:SER:O	7:M:1697:THR:N	2.34	0.55
1:A:457:ALA:HB1	1:A:549:MET:HE2	1.89	0.55
3:D:68:HIS:HD2	3:D:69:VAL:HG13	1.72	0.55
7:M:130:SER:OG	7:M:133:GLU:OE1	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:122:LEU:HD11	7:M:353:ILE:HG23	1.89	0.55
3:E:24:SER:HA	3:E:63:ARG:HH21	1.71	0.55
2:B:66:THR:O	2:B:66:THR:CG2	2.54	0.54
1:A:848:VAL:HB	1:A:853:LEU:HD13	1.89	0.54
1:A:493:LYS:NZ	7:M:1258:THR:O	2.39	0.54
2:C:44:LEU:HD23	2:C:77:LEU:HB2	1.87	0.54
5:I:172:GLU:HB2	5:I:178:VAL:HG22	1.88	0.54
7:M:401:HIS:CD2	7:M:402:THR:H	2.26	0.54
7:M:401:HIS:CG	7:M:402:THR:N	2.76	0.54
7:M:1396:CYS:SG	7:M:1420:TRP:CZ2	3.01	0.54
5:I:116:MET:HE2	5:I:143:GLY:HA3	1.90	0.54
7:N:332:TRP:HE3	7:N:977:LEU:HD22	1.73	0.54
2:C:44:LEU:HD21	2:C:77:LEU:HD13	1.91	0.53
7:N:1338:GLU:O	7:N:1339:VAL:C	2.52	0.53
7:M:889:LEU:HD12	7:M:892:ILE:HD12	1.90	0.53
1:A:86:ILE:O	1:A:107:PRO:HD2	2.08	0.53
3:D:39:SER:OG	3:D:42:ILE:HG12	2.08	0.53
7:N:1388:ASP:OD1	7:N:1390:LEU:N	2.42	0.53
7:M:1385:LYS:C	7:M:1387:GLN:N	2.67	0.53
7:M:1388:ASP:O	7:M:1390:LEU:N	2.41	0.53
1:A:90:ARG:HH11	1:A:104:MET:HE3	1.72	0.53
7:M:401:HIS:CG	7:M:402:THR:H	2.24	0.53
7:M:1001:GLN:NE2	7:M:1276:ASN:OD1	2.41	0.53
2:B:91:GLU:N	2:B:91:GLU:OE1	2.41	0.53
6:T:32:C:H2'	6:T:33:A:C8	2.44	0.53
7:N:229:ARG:NH2	7:M:227:LEU:O	2.42	0.53
7:M:965:GLY:HA3	7:M:1010:LYS:HE3	1.90	0.53
1:A:545:GLN:NE2	4:G:1:U:OP3	2.42	0.52
7:M:380:GLU:OE1	7:M:458:ASN:ND2	2.35	0.52
2:C:17:ASP:OD1	2:C:18:ALA:N	2.43	0.52
7:M:91:GLU:HG2	7:M:95:LYS:HD2	1.92	0.52
7:M:793:THR:HG23	7:M:840:LEU:HD22	1.91	0.52
7:N:1388:ASP:HB3	7:N:1391:MET:HB2	1.91	0.52
7:M:492:LEU:HD22	7:M:495:VAL:HG22	1.90	0.52
2:B:43:ARG:NH1	2:B:86:GLU:O	2.42	0.51
7:M:91:GLU:O	7:M:95:LYS:HG3	2.11	0.51
7:M:1392:LEU:HD23	7:M:1422:TRP:CZ3	2.45	0.51
2:C:23:THR:HG22	2:C:56:THR:HB	1.92	0.51
7:N:1411:GLU:OE1	7:N:1411:GLU:N	2.39	0.51
7:M:863:GLU:OE1	7:M:905:ARG:NH1	2.44	0.51
1:A:437:MET:HE1	1:A:442:PHE:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:1316:MET:SD	7:N:1345:ARG:NH2	2.77	0.51
7:N:1331:ASP:C	7:N:1333:HIS:N	2.68	0.51
1:A:68:ARG:HH21	1:A:97:ARG:HG2	1.76	0.51
7:M:164:GLN:HG2	7:M:166:VAL:HG23	1.92	0.51
7:N:1330:TRP:CZ2	7:N:1368:HIS:NE2	2.78	0.51
5:I:179:ASP:OD1	5:I:180:ARG:N	2.41	0.51
7:M:74:ILE:HG23	7:M:75:PRO:HD2	1.92	0.51
7:M:997:TYR:O	7:M:1004:LEU:HD11	2.11	0.51
3:D:40:GLY:HA2	3:D:43:LYS:HE3	1.92	0.50
5:H:45:GLN:HB3	5:H:84:HIS:CE1	2.46	0.50
7:N:391:THR:HG22	7:N:471:LEU:HB2	1.92	0.50
2:C:6:MET:HE3	2:C:74:THR:HB	1.93	0.50
7:M:299:LYS:NZ	7:M:371:ILE:HG22	2.25	0.50
5:I:166:LEU:HA	5:I:169:ILE:HG22	1.94	0.50
7:M:952:ASP:OD1	7:M:953:GLU:N	2.44	0.50
7:N:970:VAL:HG11	7:N:978:LEU:HD23	1.93	0.50
1:A:848:VAL:HG12	1:A:852:THR:HG23	1.93	0.49
2:C:52:ASP:HB3	2:C:55:LYS:HG3	1.93	0.49
7:N:171:ALA:HB1	7:N:189:THR:HG23	1.94	0.49
5:H:93:VAL:HG12	5:H:157:ILE:HD12	1.93	0.49
7:N:1330:TRP:CH2	7:N:1336:PRO:HA	2.46	0.49
1:A:30:ASP:OD1	1:A:30:ASP:N	2.44	0.49
5:I:157:ILE:O	5:I:161:LEU:N	2.37	0.49
2:B:43:ARG:HB2	2:B:78:ALA:HB3	1.95	0.49
7:N:336:LEU:HG	7:N:340:ARG:HD3	1.94	0.49
7:N:1274:HIS:C	7:N:1276:ASN:H	2.21	0.49
1:A:697:ASP:OD1	1:A:697:ASP:N	2.46	0.49
5:H:63:THR:O	5:H:67:HIS:ND1	2.44	0.49
5:H:171:ARG:NE	5:H:176:GLU:OE1	2.44	0.49
1:A:136:SER:OG	1:A:137:CYS:N	2.45	0.48
5:I:37:LEU:HG	5:I:57:LEU:HD11	1.94	0.48
2:B:5:LEU:HA	2:B:73:ALA:O	2.13	0.48
3:D:25:ASP:O	3:D:27:HIS:ND1	2.37	0.48
7:M:1690:PHE:C	7:M:1692:ARG:H	2.21	0.48
2:B:77:LEU:HD11	2:B:79:PHE:CZ	2.47	0.48
7:N:932:VAL:HG12	7:N:932:VAL:O	2.11	0.48
7:N:859:MET:O	7:N:863:GLU:HG2	2.13	0.48
7:N:1306:SER:C	7:N:1308:VAL:H	2.22	0.48
2:C:42:GLN:NE2	2:C:44:LEU:HD11	2.29	0.48
7:M:159:THR:HG23	7:M:172:TYR:HB3	1.95	0.48
7:N:221:SER:OG	7:N:274:ASP:OD2	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:492:LEU:HD11	7:M:788:GLU:HG2	1.95	0.48
7:M:149:PRO:HB2	7:M:214:VAL:HG12	1.96	0.48
7:M:1385:LYS:O	7:M:1387:GLN:N	2.40	0.47
3:E:46:LEU:O	3:E:46:LEU:CD1	2.62	0.47
7:M:1385:LYS:HB2	7:M:1392:LEU:HD22	1.96	0.47
7:N:1364:SER:O	7:N:1367:PRO:HD2	2.14	0.47
7:M:1001:GLN:C	7:M:1003:LYS:N	2.73	0.47
2:B:44:LEU:HG	2:B:77:LEU:HB3	1.97	0.47
1:A:44:PHE:O	1:A:406:THR:OG1	2.20	0.47
2:C:56:THR:O	2:C:56:THR:OG1	2.32	0.47
7:N:1338:GLU:O	7:N:1341:SER:N	2.48	0.47
7:M:1659:HIS:O	7:M:1664:LEU:N	2.33	0.47
1:A:523:PRO:HA	1:A:549:MET:HE3	1.97	0.47
5:H:125:TYR:O	5:H:129:VAL:HG22	2.15	0.47
5:I:189:MET:HE2	5:I:189:MET:HA	1.97	0.47
1:A:162:LEU:HD12	1:A:213:MET:HE2	1.97	0.47
1:A:222:THR:HG22	1:A:223:ALA:H	1.80	0.47
7:M:1384:CYS:O	7:M:1387:GLN:HB2	2.15	0.47
5:H:116:MET:HE2	5:H:143:GLY:HA3	1.96	0.47
7:N:1389:ASN:HA	7:N:1392:LEU:HB3	1.97	0.47
3:D:21:LEU:HA	3:D:60:VAL:O	2.15	0.46
3:E:46:LEU:HD12	3:E:46:LEU:C	2.40	0.46
7:N:398:ALA:HA	7:N:872:LYS:HG3	1.97	0.46
1:A:69:ARG:O	1:A:73:GLU:HG3	2.16	0.46
4:G:6:G:O2'	4:G:7:A:H8	1.98	0.46
5:H:97:LEU:HB3	5:H:160:HIS:CD2	2.51	0.46
7:N:244:PRO:O	7:N:247:ILE:HG13	2.15	0.46
5:H:171:ARG:O	5:H:176:GLU:N	2.35	0.46
7:M:103:GLN:CD	7:M:103:GLN:H	2.23	0.46
7:M:490:TYR:OH	7:M:791:ARG:NH1	2.48	0.46
7:N:456:ILE:O	7:N:459:VAL:HG12	2.15	0.46
2:B:2:ASP:OD1	2:B:3:VAL:N	2.48	0.46
7:N:1000:ASP:OD1	7:N:1001:GLN:N	2.48	0.46
2:C:42:GLN:NE2	2:C:77:LEU:HD13	2.30	0.46
5:H:100:ASN:OD1	5:H:103:GLN:HB2	2.16	0.46
7:N:362:ASP:OD1	7:N:363:SER:N	2.49	0.46
2:B:12:THR:HA	3:E:28:GLU:HG2	1.98	0.46
5:I:31:ASN:OD1	5:I:72:LYS:NZ	2.48	0.46
1:A:119:LEU:HD13	1:A:126:ARG:HH21	1.81	0.46
7:N:449:ARG:NH2	7:N:483:TYR:OH	2.49	0.46
6:T:34:A:H2'	6:T:35:A:C8	2.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:MET:HG3	2:B:74:THR:HA	1.98	0.45
3:D:19:VAL:HG12	3:D:58:ASN:HD21	1.82	0.45
1:A:95:ASP:CG	1:A:96:GLY:H	2.23	0.45
5:I:97:LEU:HB3	5:I:160:HIS:CE1	2.51	0.45
1:A:237:VAL:HG13	1:A:238:LEU:HG	1.98	0.45
5:H:76:GLY:O	5:H:79:GLU:HG3	2.16	0.45
7:N:1337:PRO:HA	7:N:1372:LEU:HD13	1.98	0.45
1:A:147:LEU:HD21	1:A:213:MET:HG2	1.98	0.45
3:E:21:LEU:HD12	3:E:70:LEU:HD21	1.98	0.45
7:N:161:VAL:HG12	7:N:172:TYR:CE2	2.52	0.45
2:B:24:VAL:HG23	2:B:55:LYS:O	2.16	0.45
1:A:322:TYR:N	1:A:323:PRO:HD3	2.31	0.45
1:A:370:ARG:O	1:A:758:GLY:HA2	2.17	0.45
7:M:177:MET:HE2	7:M:177:MET:HB3	1.71	0.45
7:M:804:PRO:HB3	7:M:860:PHE:HE2	1.82	0.45
1:A:56:HIS:NE2	1:A:99:ASN:OD1	2.35	0.45
7:N:814:ALA:O	7:N:819:ASN:ND2	2.45	0.45
7:N:391:THR:HB	7:N:468:LEU:HD12	1.99	0.45
7:M:452:GLN:O	7:M:455:VAL:HG12	2.16	0.45
7:M:769:ARG:O	7:M:772:VAL:HG22	2.17	0.45
7:M:1395:ALA:O	7:M:1396:CYS:C	2.60	0.45
3:E:84:THR:O	3:E:84:THR:CG2	2.63	0.44
4:G:20:U:N3	4:G:21:U:C5	2.84	0.44
7:N:74:ILE:CG2	7:N:75:PRO:HD2	2.44	0.44
7:M:1321:ALA:HA	7:M:1324:THR:HG22	1.98	0.44
1:A:292:GLN:O	1:A:307:THR:HA	2.17	0.44
7:N:315:ASP:OD1	7:N:316:VAL:N	2.50	0.44
7:N:809:VAL:HG22	7:N:826:GLN:HG2	1.98	0.44
7:M:1327:VAL:HG23	7:M:1328:GLU:HG3	1.98	0.44
1:A:608:LYS:HA	1:A:609:PRO:HD3	1.86	0.44
3:E:39:SER:HB3	3:E:77:PHE:CZ	2.52	0.44
7:M:1255:ASN:ND2	7:M:1257:SER:O	2.51	0.44
7:M:1286:LEU:HD12	7:M:1311:ILE:HD12	1.99	0.44
7:M:1366:LEU:HD22	7:M:1399:VAL:HG22	1.99	0.44
3:E:64:GLU:OE2	5:I:59:ARG:NH2	2.47	0.44
1:A:90:ARG:HD3	1:A:104:MET:HB2	1.99	0.44
1:A:713:THR:HG21	1:A:749:TYR:OH	2.18	0.44
7:N:1326:LEU:HD12	7:N:1326:LEU:HA	1.83	0.44
3:D:66:PRO:HG2	3:D:69:VAL:HG22	2.00	0.44
3:E:51:GLN:HA	3:E:55:ASN:ND2	2.33	0.44
4:G:21:U:C2	4:G:22:G:N7	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:826:GLN:OE1	7:N:826:GLN:N	2.47	0.44
7:M:784:GLY:O	7:M:786:SER:N	2.51	0.44
7:N:1323:LEU:HD21	7:N:1354:MET:HE3	1.99	0.44
7:N:1374:PRO:O	7:N:1378:GLN:NE2	2.51	0.44
3:E:19:VAL:O	3:E:30:ILE:HA	2.18	0.43
6:T:33:A:H2'	6:T:34:A:H8	1.83	0.43
7:N:264:THR:HG22	7:N:265:ALA:N	2.32	0.43
3:E:21:LEU:HG	3:E:29:PHE:HB2	1.99	0.43
5:H:127:ASP:OD2	5:H:139:VAL:HG22	2.18	0.43
1:A:230:VAL:O	1:A:234:VAL:HG23	2.18	0.43
1:A:584:PRO:HA	1:A:585:PRO:HD3	1.89	0.43
2:B:56:THR:OG1	2:B:56:THR:O	2.35	0.43
3:D:32:LYS:HD2	3:D:35:HIS:CE1	2.54	0.43
7:M:173:ASN:HB2	7:M:189:THR:HG21	2.01	0.43
3:E:70:LEU:HA	3:E:73:VAL:HG12	2.01	0.43
6:T:34:A:H2'	6:T:35:A:H8	1.84	0.43
7:N:256:ASP:OD1	7:N:256:ASP:N	2.52	0.43
1:A:48:ASP:OD1	1:A:48:ASP:N	2.42	0.43
2:B:25:PHE:HD1	2:B:53:ASP:HB3	1.84	0.43
6:T:45:G:H2'	6:T:46:U:C6	2.54	0.43
7:N:473:PRO:HA	7:N:476:ARG:NH1	2.34	0.43
1:A:275:MET:HE3	1:A:275:MET:HB3	1.92	0.43
3:E:32:LYS:HB3	3:E:35:HIS:CG	2.53	0.43
7:N:174:VAL:HG23	7:N:203:LEU:HD22	2.00	0.43
1:A:372:ALA:HB3	1:A:373:PRO:HD3	2.01	0.43
1:A:653:PHE:O	1:A:657:THR:HG22	2.18	0.43
7:N:1331:ASP:O	7:N:1333:HIS:N	2.39	0.43
7:M:295:THR:O	7:M:299:LYS:HG3	2.19	0.43
7:M:826:GLN:H	7:M:826:GLN:HG2	1.64	0.43
1:A:355:LYS:HD3	1:A:355:LYS:HA	1.80	0.43
5:H:74:TYR:HE2	5:H:136:VAL:HG11	1.83	0.43
5:I:97:LEU:HB3	5:I:160:HIS:NE2	2.33	0.43
7:N:264:THR:HG22	7:N:266:ILE:HG22	2.01	0.43
7:M:866:ARG:HD3	7:M:878:LEU:HD13	2.00	0.43
5:H:97:LEU:HD22	5:H:160:HIS:CG	2.54	0.42
7:M:964:LEU:HD21	7:M:1011:LEU:HB2	2.01	0.42
1:A:222:THR:HG22	1:A:223:ALA:N	2.33	0.42
2:B:10:HIS:HA	2:B:91:GLU:CD	2.45	0.42
3:D:50:GLY:H	3:D:55:ASN:ND2	2.16	0.42
5:H:113:GLN:O	5:H:117:VAL:HG22	2.20	0.42
5:I:184:ARG:HA	5:I:187:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLU:N	1:A:245:GLU:OE1	2.51	0.42
3:E:20:LYS:HD3	3:E:59:GLU:HG2	2.01	0.42
7:M:74:ILE:CG2	7:M:78:GLU:CB	2.94	0.42
7:M:1000:ASP:O	7:M:1004:LEU:HD13	2.19	0.42
1:A:594:LEU:HD13	1:A:664:ILE:HG23	2.02	0.42
5:I:100:ASN:OD1	5:I:103:GLN:HB2	2.19	0.42
7:N:1707:ALA:O	7:N:1711:GLY:N	2.52	0.42
7:M:290:ASP:OD1	7:M:290:ASP:N	2.51	0.42
5:I:46:ARG:O	5:I:48:ASN:N	2.50	0.42
7:N:889:LEU:HD21	7:N:928:PHE:CE2	2.55	0.42
3:D:22:ILE:HG12	3:D:28:GLU:HG2	2.01	0.42
1:A:268:GLU:HG3	1:A:347:VAL:HG22	2.01	0.42
2:B:77:LEU:HD13	2:B:79:PHE:CE1	2.55	0.42
2:C:42:GLN:CG	2:C:77:LEU:HD13	2.49	0.42
7:M:1299:TRP:CD1	7:M:1299:TRP:H	2.37	0.42
1:A:55:TYR:CZ	1:A:105:PRO:HG3	2.55	0.42
7:M:143:MET:O	7:M:144:ARG:HD2	2.20	0.42
2:B:3:VAL:HG22	2:B:18:ALA:O	2.20	0.42
7:M:909:LEU:HD21	7:M:963:ALA:HB2	2.02	0.42
7:M:1397:MET:HE2	7:M:1397:MET:HB3	1.93	0.42
1:A:119:LEU:HD12	1:A:128:PHE:HE2	1.85	0.42
7:N:78:GLU:O	7:N:82:LYS:HG3	2.20	0.42
1:A:70:VAL:O	1:A:73:GLU:N	2.53	0.41
2:B:77:LEU:C	2:B:77:LEU:HD12	2.45	0.41
2:C:44:LEU:HD23	2:C:77:LEU:CA	2.47	0.41
5:H:182:ALA:HA	5:H:185:ASN:ND2	2.34	0.41
1:A:735:THR:HG21	1:A:780:GLN:OE1	2.20	0.41
1:A:82:PHE:CE2	1:A:115:LEU:HD22	2.55	0.41
2:C:53:ASP:OD1	2:C:53:ASP:N	2.52	0.41
5:I:63:THR:O	5:I:67:HIS:HD2	2.04	0.41
7:N:324:THR:O	7:N:324:THR:OG1	2.38	0.41
7:M:142:ARG:HD3	7:M:142:ARG:HA	1.81	0.41
7:M:902:MET:SD	7:M:932:VAL:HG11	2.61	0.41
1:A:558:GLN:HE21	6:T:52:A:H2'	1.84	0.41
7:N:1330:TRP:O	7:N:1330:TRP:CE3	2.73	0.41
2:C:14:ILE:HG12	3:D:30:ILE:HB	2.01	0.41
7:N:188:CYS:SG	7:N:189:THR:N	2.94	0.41
7:M:199:HIS:CD2	7:M:199:HIS:N	2.87	0.41
7:M:1389:ASN:O	7:M:1392:LEU:N	2.50	0.41
7:M:1391:MET:HE3	7:M:1391:MET:HB3	1.68	0.41
1:A:425:LYS:HE2	1:A:425:LYS:HB3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4:PHE:CE2	2:C:69:PRO:HG3	2.56	0.41
7:N:811:PRO:O	7:N:813:PRO:HD3	2.20	0.41
7:M:112:SER:O	7:M:112:SER:OG	2.35	0.41
7:M:1390:LEU:O	7:M:1393:GLU:N	2.54	0.41
2:C:80:ARG:HG2	2:C:82:ASP:H	1.85	0.41
7:N:1329:CYS:C	7:N:1331:ASP:N	2.76	0.41
7:M:299:LYS:HE3	7:M:299:LYS:HB2	1.73	0.41
7:M:914:LEU:HB3	7:M:918:ARG:NH1	2.35	0.41
7:M:998:LYS:HE2	7:M:998:LYS:HB3	1.90	0.41
1:A:68:ARG:O	1:A:69:ARG:C	2.64	0.41
1:A:558:GLN:HE21	1:A:558:GLN:HB2	1.72	0.41
1:A:644:ALA:O	1:A:647:ARG:HG2	2.19	0.41
2:C:43:ARG:HB2	2:C:78:ALA:HB3	2.02	0.41
2:C:68:ARG:HG3	2:C:71:ALA:HB3	2.02	0.41
5:I:180:ARG:HH21	5:I:184:ARG:HH22	1.68	0.41
7:N:395:HIS:C	7:N:871:THR:HG21	2.46	0.41
7:N:1338:GLU:C	7:N:1340:ALA:N	2.79	0.41
7:N:1662:HIS:O	7:N:1666:ALA:HB2	2.21	0.41
5:H:86:ILE:HG13	5:H:90:ARG:NE	2.31	0.41
7:N:1335:THR:HB	7:N:1337:PRO:HD2	2.02	0.41
7:M:445:CYS:HB2	7:M:482:CYS:SG	2.61	0.41
1:A:250:LEU:HD22	1:A:253:SER:HB3	2.02	0.40
1:A:250:LEU:HB2	1:A:254:GLN:H	1.86	0.40
2:B:77:LEU:CD1	2:B:79:PHE:CD1	3.05	0.40
2:C:42:GLN:NE2	2:C:44:LEU:CG	2.82	0.40
5:H:70:GLY:HA3	5:H:130:TYR:CE2	2.56	0.40
6:T:28:A:O2'	6:T:29:C:O5'	2.37	0.40
7:N:913:THR:O	7:N:913:THR:CG2	2.65	0.40
7:N:1314:GLN:O	7:N:1318:ILE:HG12	2.21	0.40
7:M:1232:GLN:HG2	7:M:1233:PRO:HD2	2.02	0.40
2:C:42:GLN:HG2	2:C:44:LEU:HG	2.03	0.40
7:N:161:VAL:HG12	7:N:172:TYR:HE2	1.86	0.40
7:N:1395:ALA:O	7:N:1399:VAL:HG23	2.22	0.40
5:I:96:SER:OG	5:I:100:ASN:O	2.39	0.40
7:N:159:THR:HA	7:N:172:TYR:O	2.21	0.40
7:N:1329:CYS:C	7:N:1331:ASP:H	2.30	0.40
7:M:115:GLU:N	7:M:115:GLU:OE1	2.54	0.40
1:A:591:VAL:HG22	1:A:663:ARG:HB2	2.03	0.40
2:C:37:ARG:NH2	2:C:41:GLU:OE2	2.55	0.40
7:N:257:GLU:HB3	7:N:266:ILE:HG21	2.03	0.40
7:M:914:LEU:HB3	7:M:918:ARG:HH12	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	819/870 (94%)	752 (92%)	67 (8%)	0	100	100
2	B	95/118 (80%)	93 (98%)	2 (2%)	0	100	100
2	C	95/118 (80%)	86 (90%)	9 (10%)	0	100	100
3	D	98/112 (88%)	93 (95%)	5 (5%)	0	100	100
3	E	97/112 (87%)	88 (91%)	9 (9%)	0	100	100
5	H	172/396 (43%)	158 (92%)	14 (8%)	0	100	100
5	I	173/396 (44%)	165 (95%)	8 (5%)	0	100	100
7	M	1013/1866 (54%)	927 (92%)	85 (8%)	1 (0%)	48	78
7	N	993/1866 (53%)	924 (93%)	69 (7%)	0	100	100
All	All	3555/5854 (61%)	3286 (92%)	268 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	M	1386	GLU

5.3.2 Protein sidechains [i](#)

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	725/761 (95%)	720 (99%)	5 (1%)	76	82
2	B	84/103 (82%)	84 (100%)	0	100	100
2	C	84/103 (82%)	84 (100%)	0	100	100
3	D	87/96 (91%)	86 (99%)	1 (1%)	65	78
3	E	87/96 (91%)	86 (99%)	1 (1%)	65	78
5	H	159/361 (44%)	158 (99%)	1 (1%)	78	83
5	I	159/361 (44%)	157 (99%)	2 (1%)	61	77
7	M	699/1507 (46%)	684 (98%)	15 (2%)	47	71
7	N	730/1507 (48%)	719 (98%)	11 (2%)	57	75
All	All	2814/4895 (58%)	2778 (99%)	36 (1%)	59	77

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	CYS
1	A	68	ARG
1	A	147	LEU
1	A	235	CYS
1	A	490	CYS
3	D	70	LEU
3	E	21	LEU
5	H	74	TYR
5	I	74	TYR
5	I	160	HIS
7	N	399	SER
7	N	401	HIS
7	N	764	LEU
7	N	1007	ILE
7	N	1278	HIS
7	N	1326	LEU
7	N	1327	VAL
7	N	1330	TRP
7	N	1331	ASP
7	N	1334	LEU
7	N	1335	THR
7	M	188	CYS
7	M	247	ILE

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Mol	Chain	Res	Type
7	M	303	HIS
7	M	451	TRP
7	M	894	LEU
7	M	1307	HIS
7	M	1379	ARG
7	M	1385	LYS
7	M	1386	GLU
7	M	1387	GLN
7	M	1388	ASP
7	M	1391	MET
7	M	1392	LEU
7	M	1393	GLU
7	M	1424	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	GLN
1	A	247	GLN
1	A	432	GLN
1	A	558	GLN
1	A	568	ASN
1	A	581	GLN
1	A	621	HIS
1	A	681	HIS
1	A	772	ASN
1	A	840	GLN
2	C	42	GLN
3	D	58	ASN
5	H	69	HIS
5	H	185	ASN
5	I	67	HIS
7	N	228	GLN
7	N	463	GLN
7	N	1278	HIS
7	N	1378	GLN
7	N	1657	ASN
7	N	1663	HIS
7	M	199	HIS
7	M	231	GLN
7	M	237	GLN
7	M	401	HIS

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Mol	Chain	Res	Type
7	M	850	HIS
7	M	881	GLN
7	M	1298	ASN
7	M	1333	HIS
7	M	1383	GLN
7	M	1389	ASN
7	M	1426	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	G	23/24 (95%)	5 (21%)	0
6	T	25/120 (20%)	9 (36%)	0
All	All	48/144 (33%)	14 (29%)	0

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	G	7	A
4	G	11	G
4	G	16	U
4	G	23	U
4	G	24	U
6	T	28	A
6	T	29	C
6	T	31	A
6	T	39	A
6	T	41	C
6	T	42	A
6	T	44	U
6	T	45	G
6	T	51	C

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 2 ligands modelled in this entry, 2 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.

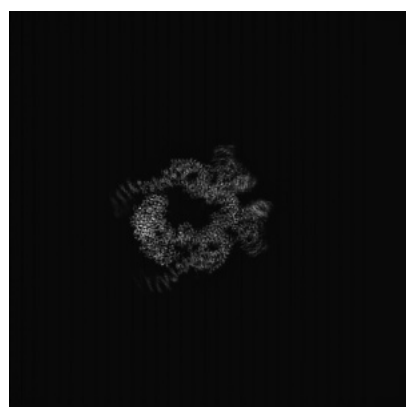
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54352. These allow visual inspection of the internal detail of the map and identification of artifacts.

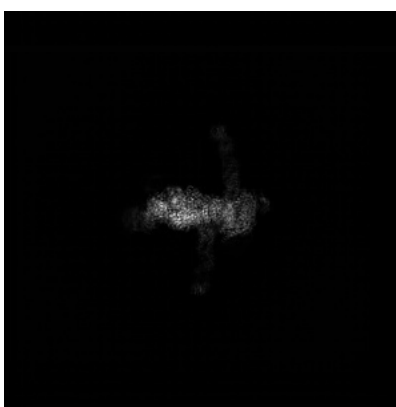
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

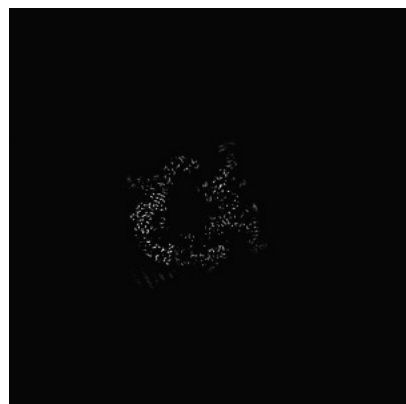


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 308



Y Index: 308

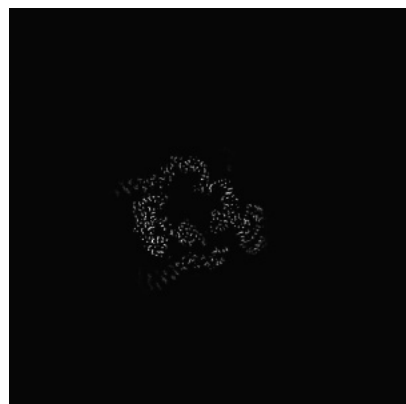


Z Index: 308

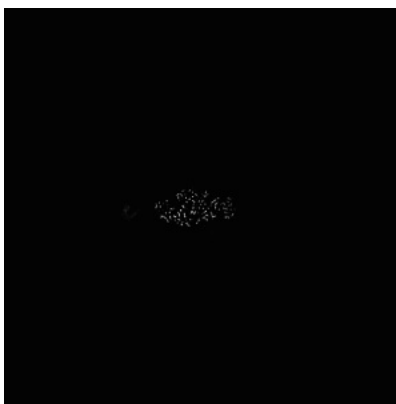
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

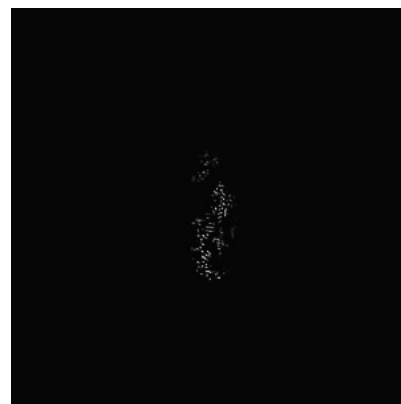
6.3.1 Primary map



X Index: 299



Y Index: 218

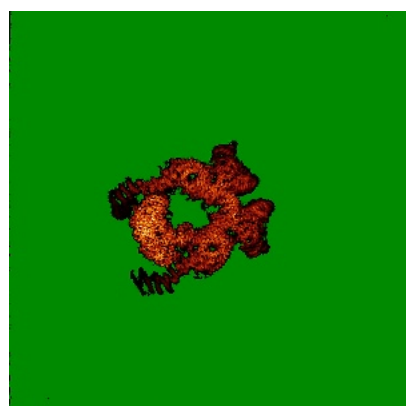


Z Index: 262

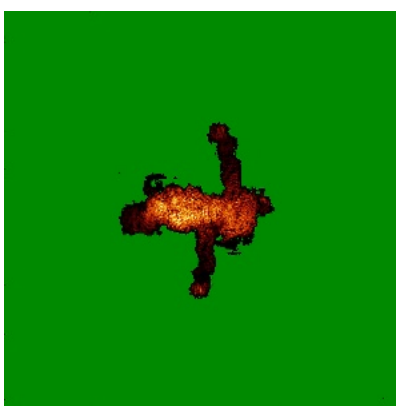
The images above show the largest variance slices of the map in three orthogonal directions.

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

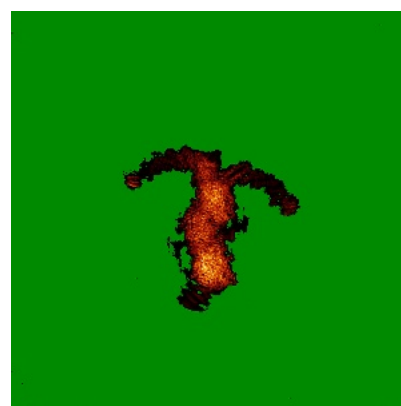
6.4.1 Primary map



X



Y

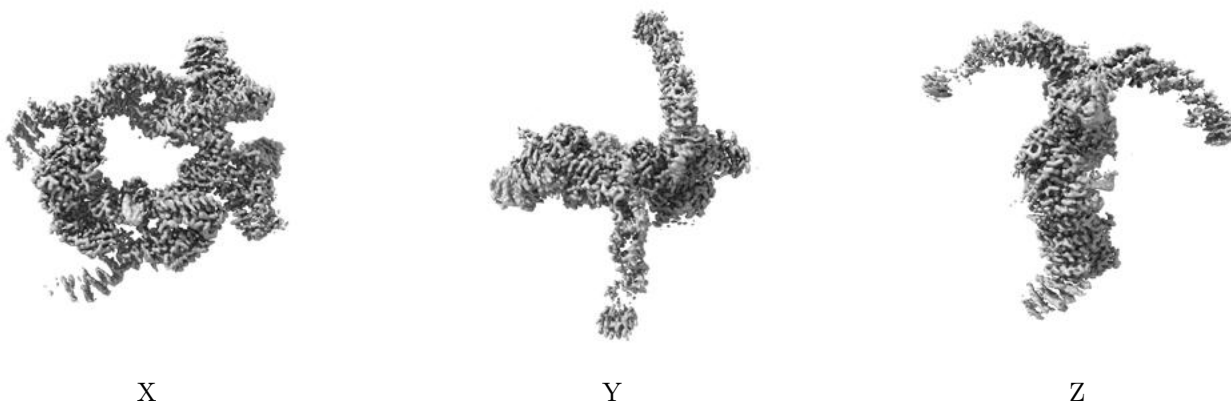


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 7.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

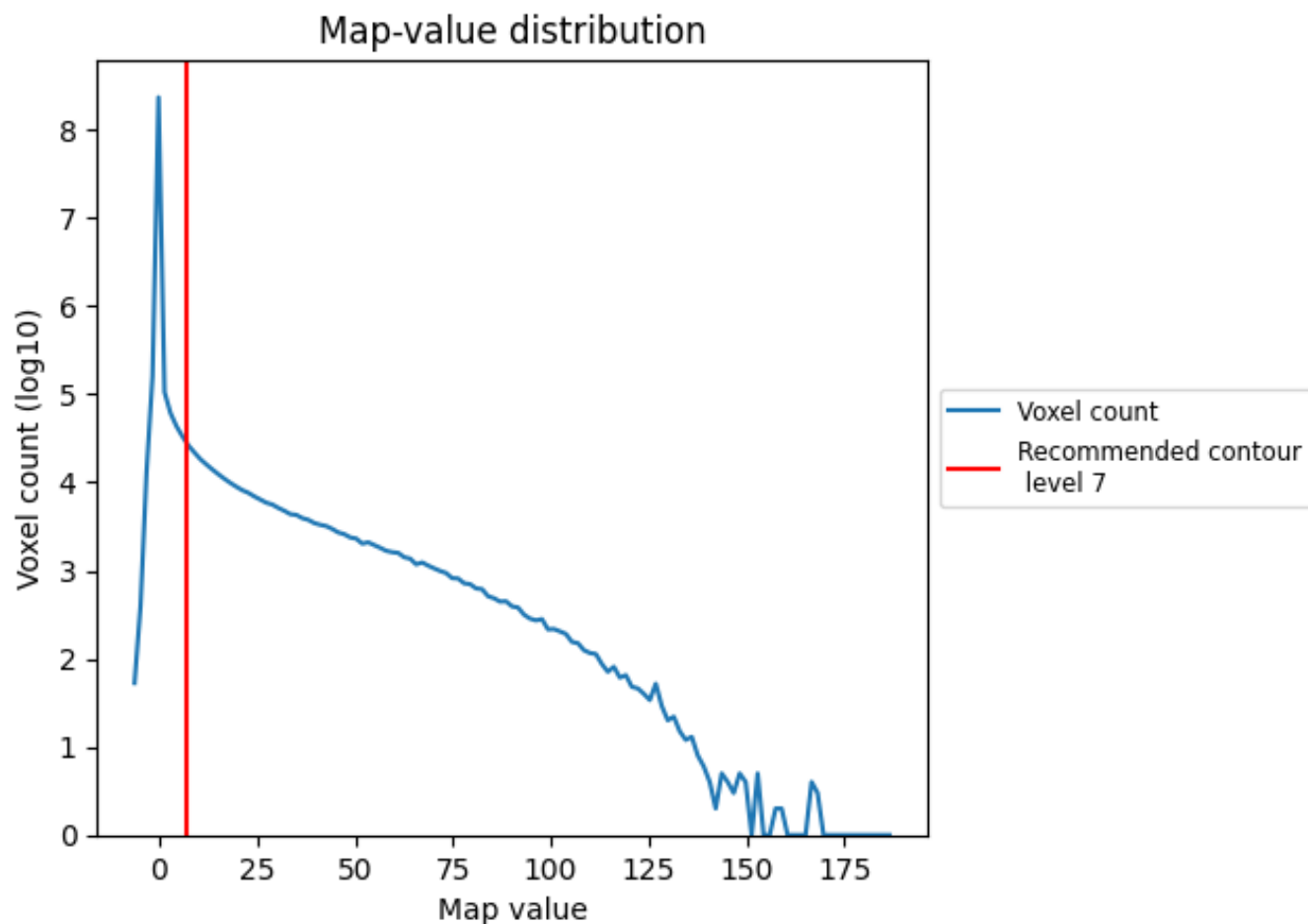
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

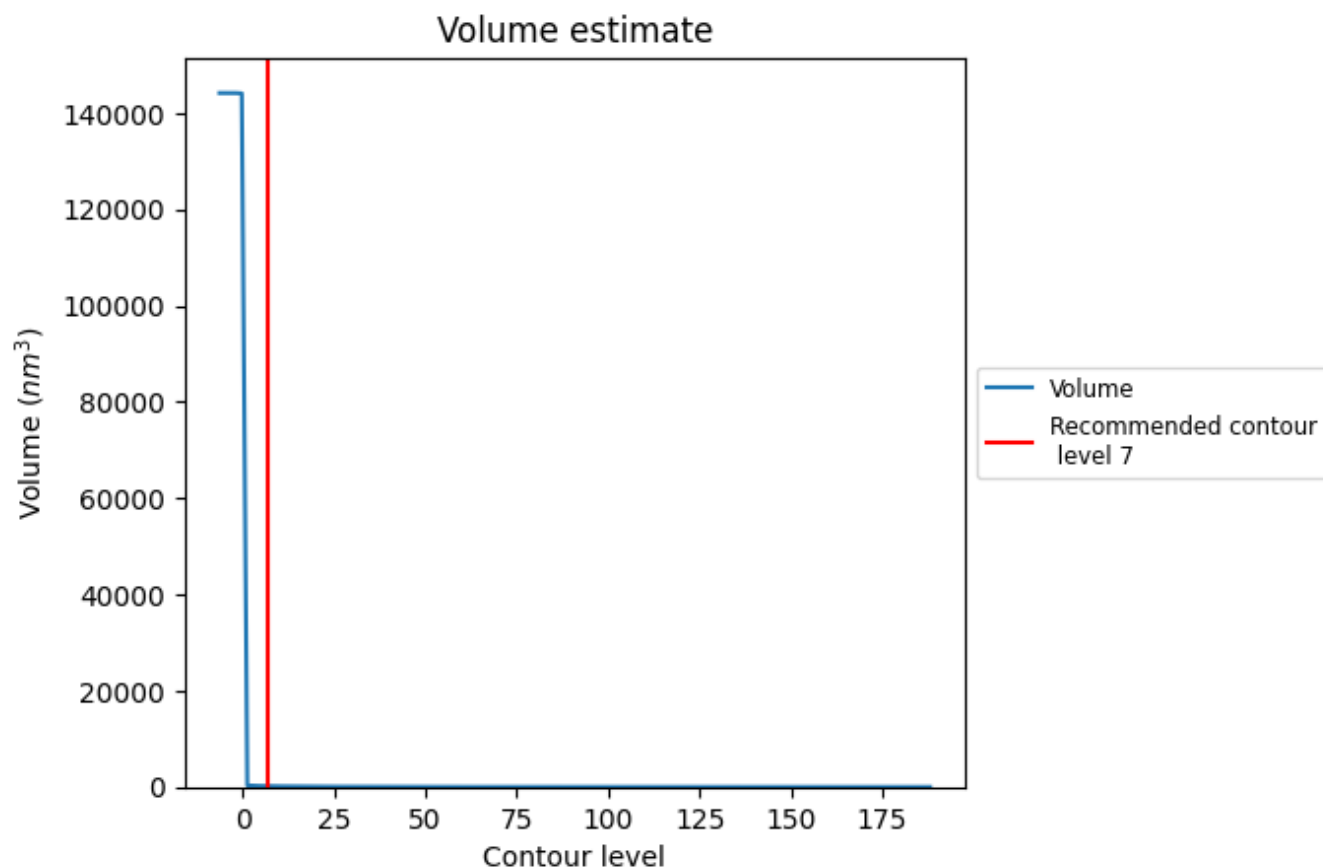
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

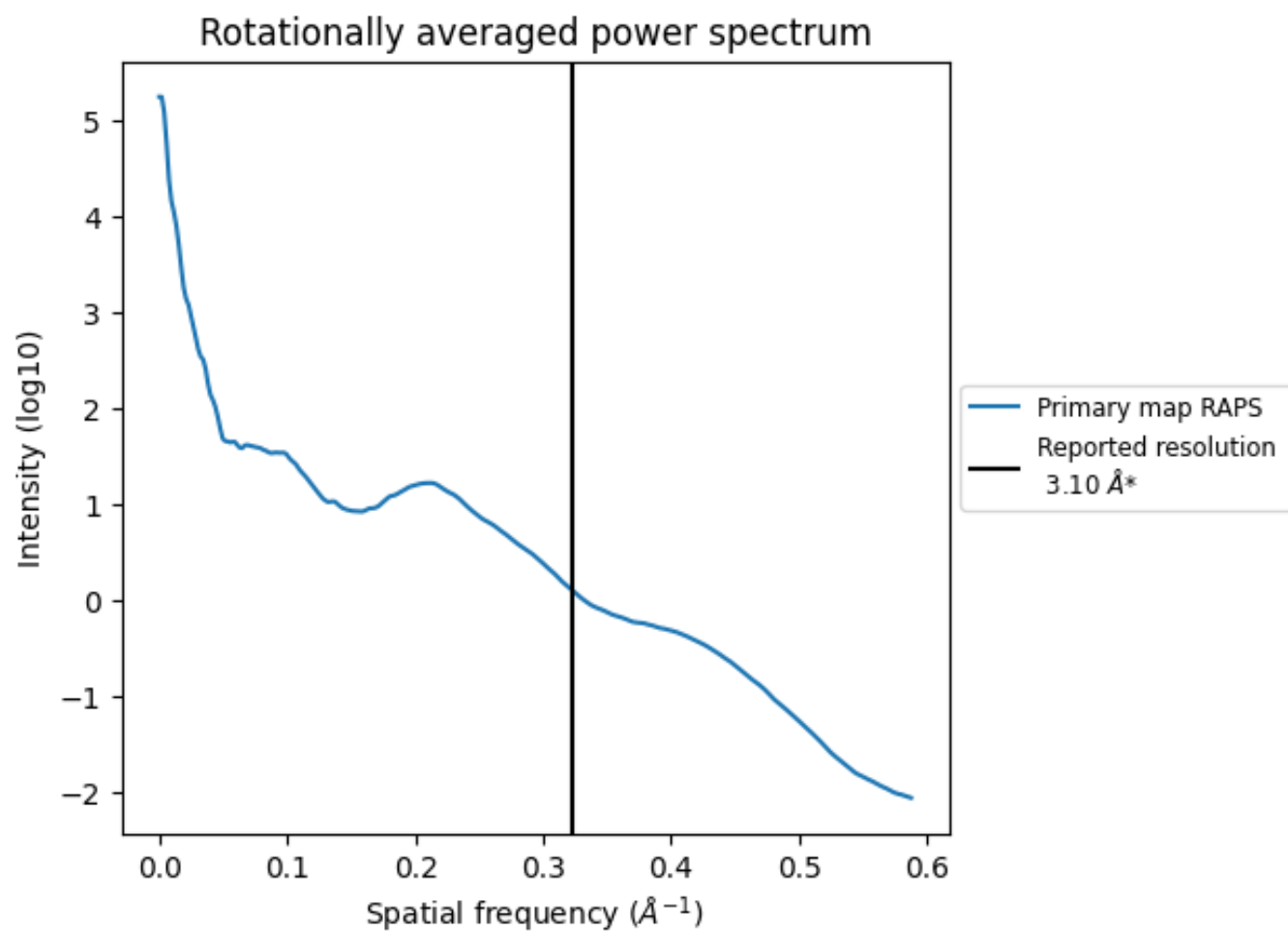
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 167 nm^3 ; this corresponds to an approximate mass of 150 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 0.323 Å⁻¹

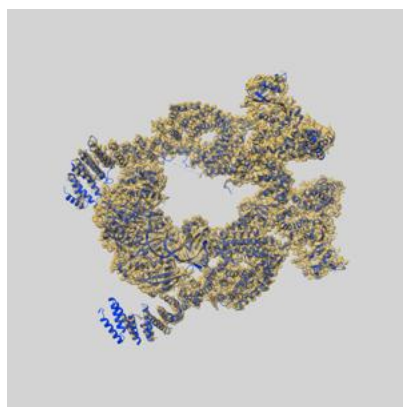
8 Fourier-Shell correlation

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

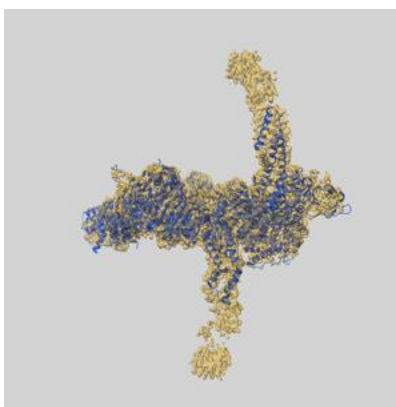
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54352 and PDB model 9RWZ. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

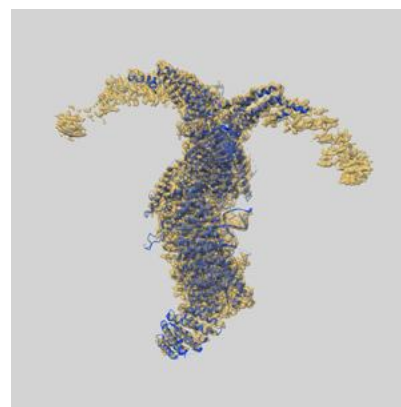
9.1 Map-model overlay [i](#)



X



Y



Z

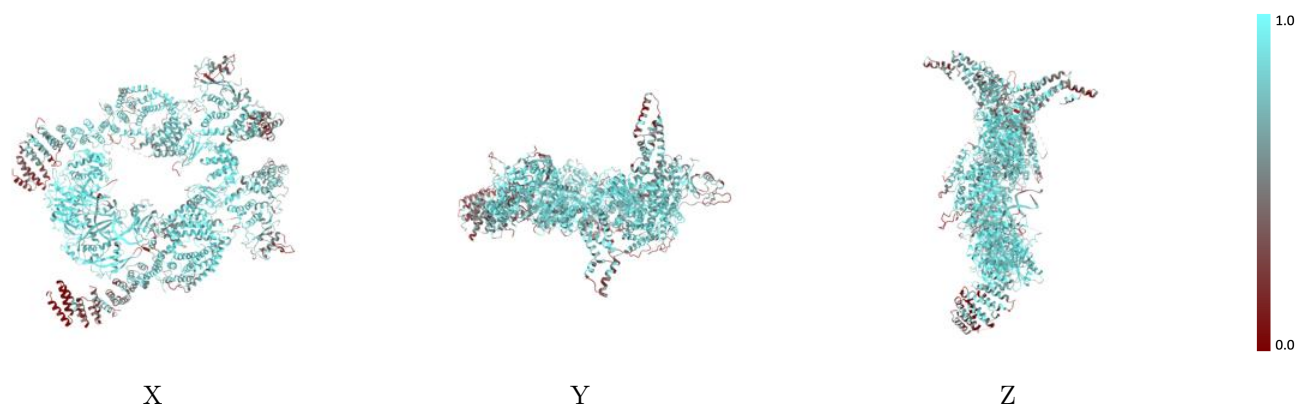
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



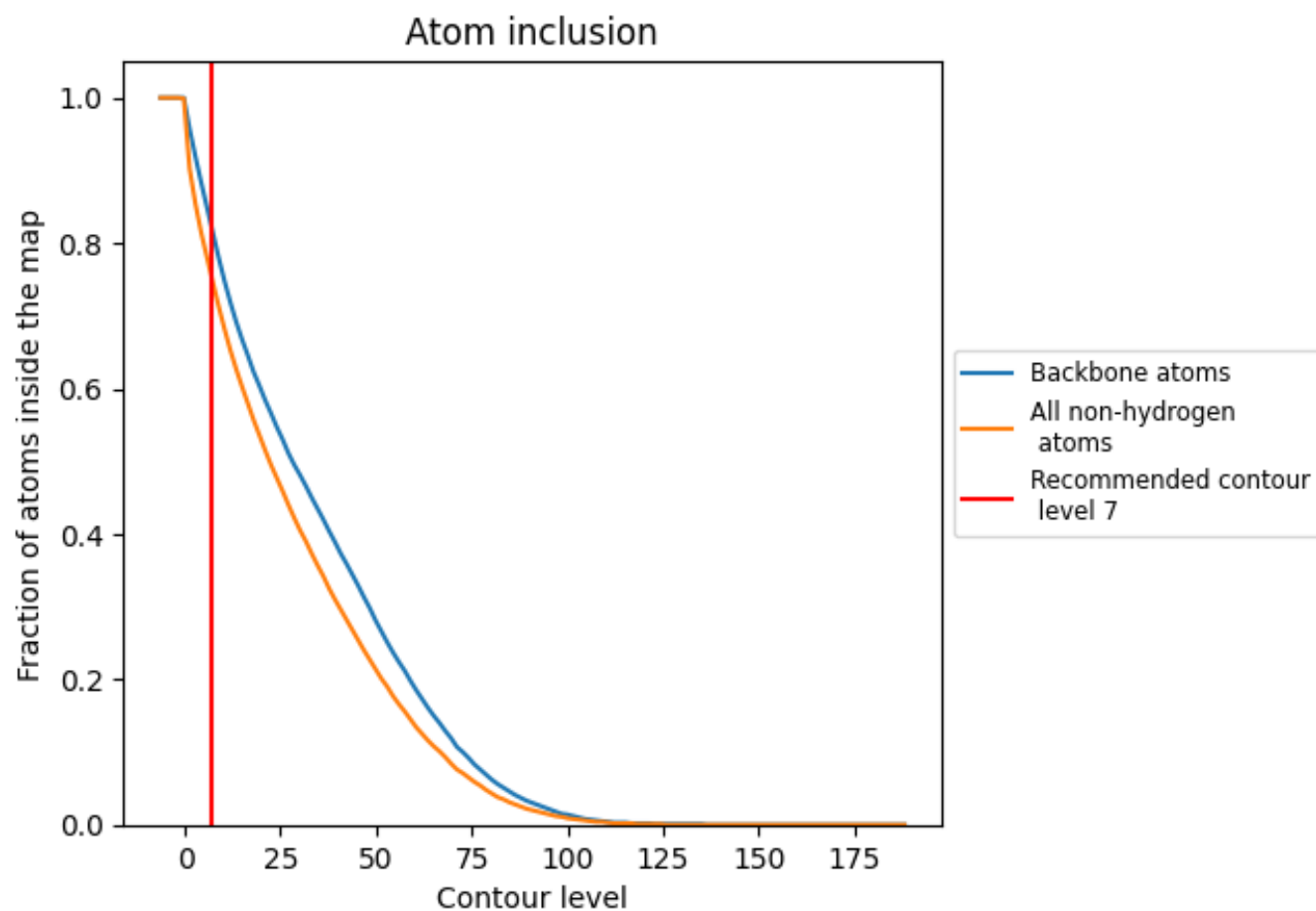
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (7).

























9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 75% 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 (7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7530	 0.4430
A	 0.8830	 0.5520
B	 0.4960	 0.1820
C	 0.4830	 0.1840
D	 0.7340	 0.4030
E	 0.7540	 0.4010
G	 0.8500	 0.5050
H	 0.6250	 0.2610
I	 0.6540	 0.2820
M	 0.7500	 0.4670
N	 0.7320	 0.4440
T	 0.8140	 0.4660

