



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 09:11 AM UTC

PDB ID : 8FVU / pdb_00008fvu
EMDB ID : EMD-29493
Title : Cryo-EM structure of human Needle/NAIP/NLRC4 (R288A)
Authors : Matico, R.E.; Yu, X.; Miller, R.; Somani, S.; Ricketts, M.D.; Kumar, N.;
Steele, R.A.; Medley, Q.; Berger, S.; Faustin, B.; Sharma, S.
Deposited on : 2023-01-19
Resolution : 3.60 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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

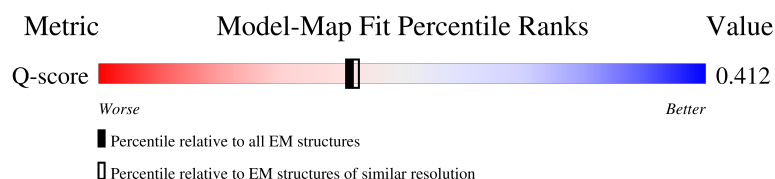
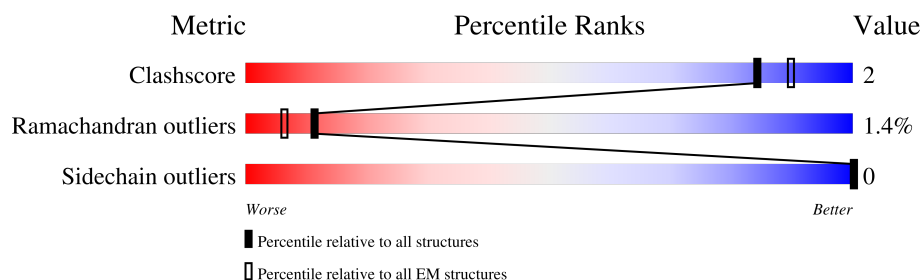
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	1409	
2	B	1030	
3	U	374	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18758 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 Baculoviral IAP repeat-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1361	Total	C	N	O	S	0	0
			10905	6978	1830	2025	72		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	expression tag	UNP Q13075
A	-4	GLU	-	expression tag	UNP Q13075
A	-3	TYR	-	expression tag	UNP Q13075
A	-2	CYS	-	expression tag	UNP Q13075
A	-1	PHE	-	expression tag	UNP Q13075
A	0	ASN	-	expression tag	UNP Q13075

- Molecule 2 is a protein called NLR family CARD domain-containing protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	904	Total	C	N	O	S	0	0
			7198	4605	1217	1339	37		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	ALA	-	expression tag	UNP Q9NPP4
B	-4	GLU	-	expression tag	UNP Q9NPP4
B	-3	TYR	-	expression tag	UNP Q9NPP4
B	-2	CYS	-	expression tag	UNP Q9NPP4
B	-1	PHE	-	expression tag	UNP Q9NPP4
B	0	ASN	-	expression tag	UNP Q9NPP4
B	288	ALA	ARG	engineered mutation	UNP Q9NPP4

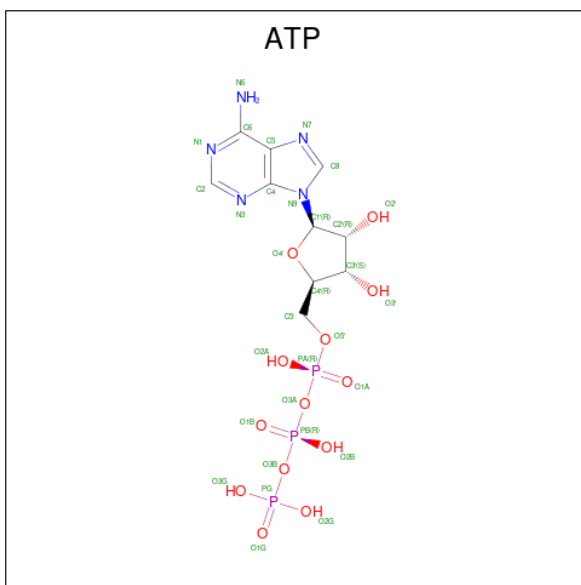
- Molecule 3 is a protein called Lethal factor, Type III secretion system protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	U	79	Total	C	N	O	S	0	0
			621	384	106	128	3		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	-303	GLY	-	expression tag	UNP P15917
U	-302	SER	-	expression tag	UNP P15917
U	-301	SER	-	expression tag	UNP P15917
U	-300	HIS	-	expression tag	UNP P15917
U	-299	HIS	-	expression tag	UNP P15917
U	-298	HIS	-	expression tag	UNP P15917
U	-297	HIS	-	expression tag	UNP P15917
U	-296	HIS	-	expression tag	UNP P15917
U	-295	HIS	-	expression tag	UNP P15917
U	-294	SER	-	expression tag	UNP P15917
U	-293	SER	-	expression tag	UNP P15917
U	-292	GLY	-	expression tag	UNP P15917
U	-291	LEU	-	expression tag	UNP P15917
U	-290	VAL	-	expression tag	UNP P15917
U	-289	PRO	-	expression tag	UNP P15917
U	-288	ARG	-	expression tag	UNP P15917
U	-287	GLY	-	expression tag	UNP P15917
U	-286	SER	-	expression tag	UNP P15917
U	-285	HIS	-	expression tag	UNP P15917
U	-284	MET	-	expression tag	UNP P15917
U	-20	SER	-	linker	UNP P15917
U	-19	THR	-	linker	UNP P15917
U	-18	ARG	-	linker	UNP P15917
U	-9	THR	ALA	conflict	UNP Q63K18
U	8	THR	ASP	conflict	UNP Q63K18
U	15	GLN	LYS	conflict	UNP Q63K18

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

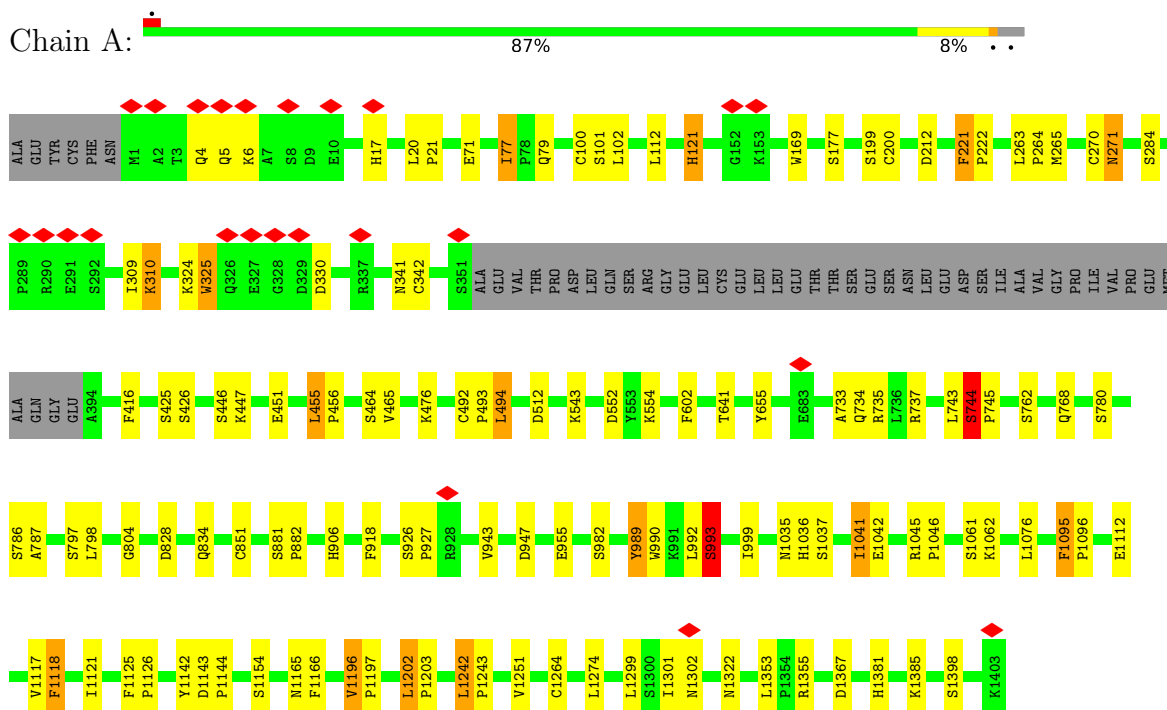
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
5	A	3	Total Zn 3 3	0

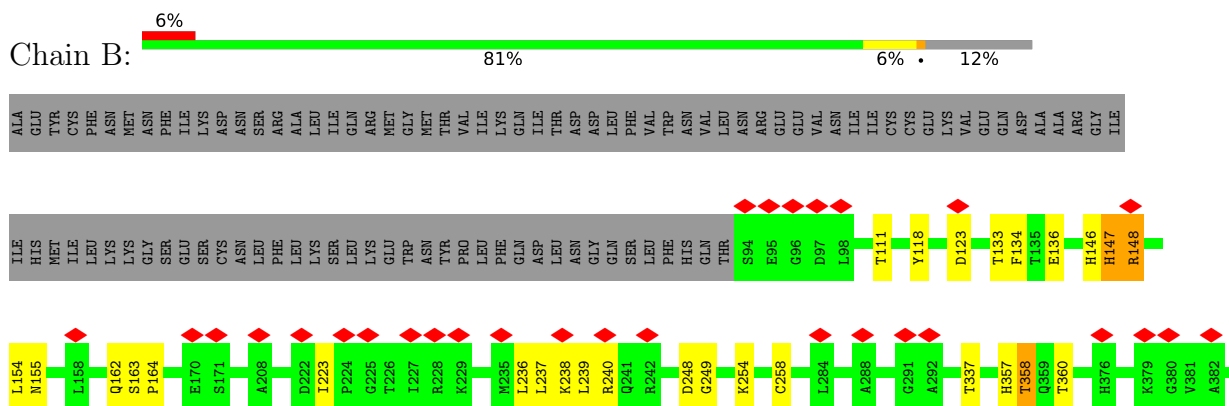
3 Residue-property plots

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: Baculoviral IAP repeat-containing protein 1



• Molecule 2: NLR family CARD domain-containing protein 4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	106381	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.015	Depositor
Minimum map value	-0.619	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	398.16, 398.16, 398.16	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.948, 0.948, 0.948	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: ATP, 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	0.64	0/11143	0.91	86/15055 (0.6%)
2	B	0.64	0/7331	0.86	35/9890 (0.4%)
3	U	0.66	0/631	0.77	2/853 (0.2%)
All	All	0.64	0/19105	0.89	123/25798 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	360	THR	N-CA-C	-8.52	104.91	114.62
1	A	221	PHE	CA-C-N	7.89	127.53	119.56
1	A	221	PHE	C-N-CA	7.89	127.53	119.56
1	A	737	ARG	CA-C-N	7.65	127.60	120.03
1	A	737	ARG	C-N-CA	7.65	127.60	120.03
1	A	993	SER	CA-C-N	7.49	127.94	119.93
1	A	993	SER	C-N-CA	7.49	127.94	119.93
1	A	906	HIS	CA-C-N	7.43	127.07	119.56
1	A	906	HIS	C-N-CA	7.43	127.07	119.56
1	A	1076	LEU	CA-C-N	7.40	127.04	119.56
1	A	1076	LEU	C-N-CA	7.40	127.04	119.56
1	A	943	VAL	CA-C-N	7.40	127.35	120.03
1	A	943	VAL	C-N-CA	7.40	127.35	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1353	LEU	CA-C-N	7.39	127.56	119.87
1	A	1353	LEU	C-N-CA	7.39	127.56	119.87
2	B	906	VAL	CA-C-N	7.35	127.06	119.56
2	B	906	VAL	C-N-CA	7.35	127.06	119.56
2	B	223	ILE	CA-C-N	7.22	127.14	120.21
2	B	223	ILE	C-N-CA	7.22	127.14	120.21
1	A	982	SER	CA-C-N	7.19	127.63	119.93
1	A	982	SER	C-N-CA	7.19	127.63	119.93
1	A	851	CYS	CA-C-N	7.16	127.48	119.32
1	A	851	CYS	C-N-CA	7.16	127.48	119.32
1	A	744	SER	CA-C-N	7.09	128.70	119.84
1	A	744	SER	C-N-CA	7.09	128.70	119.84
2	B	644	ILE	CA-C-N	7.03	127.00	119.76
2	B	644	ILE	C-N-CA	7.03	127.00	119.76
1	A	71	GLU	CA-C-N	6.92	126.55	119.56
1	A	71	GLU	C-N-CA	6.92	126.55	119.56
1	A	1242	LEU	CA-C-N	6.91	126.84	120.21
1	A	1242	LEU	C-N-CA	6.91	126.84	120.21
1	A	451	GLU	CA-C-N	6.86	126.77	119.85
1	A	451	GLU	C-N-CA	6.86	126.77	119.85
1	A	655	TYR	CA-C-N	6.83	126.45	119.56
1	A	655	TYR	C-N-CA	6.83	126.45	119.56
2	B	118	TYR	CA-C-N	6.80	126.43	119.56
2	B	118	TYR	C-N-CA	6.80	126.43	119.56
1	A	121	HIS	CA-C-N	6.72	126.86	119.87
1	A	121	HIS	C-N-CA	6.72	126.86	119.87
1	A	1154	SER	CA-C-N	6.71	126.34	119.56
1	A	1154	SER	C-N-CA	6.71	126.34	119.56
1	A	330	ASP	CA-C-N	6.69	126.38	119.56
1	A	330	ASP	C-N-CA	6.69	126.38	119.56
1	A	169	TRP	CA-C-N	6.66	126.64	119.78
1	A	169	TRP	C-N-CA	6.66	126.64	119.78
1	A	955	GLU	CA-C-N	6.55	126.31	119.76
1	A	955	GLU	C-N-CA	6.55	126.31	119.76
2	B	258	CYS	CA-C-N	6.49	127.00	119.47
2	B	258	CYS	C-N-CA	6.49	127.00	119.47
1	A	263	LEU	CA-C-N	6.48	127.94	119.84
1	A	263	LEU	C-N-CA	6.48	127.94	119.84
1	A	780	SER	CA-C-N	6.48	126.10	119.56
1	A	780	SER	C-N-CA	6.48	126.10	119.56
2	B	254	LYS	CA-C-N	6.46	126.38	119.28
2	B	254	LYS	C-N-CA	6.46	126.38	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	834	GLN	CA-C-N	6.46	126.96	119.47
1	A	834	GLN	C-N-CA	6.46	126.96	119.47
1	A	342	CYS	CA-C-N	6.45	126.67	119.32
1	A	342	CYS	C-N-CA	6.45	126.67	119.32
1	A	177	SER	CA-C-N	6.40	126.02	119.56
1	A	177	SER	C-N-CA	6.40	126.02	119.56
2	B	978	LEU	CA-C-N	6.36	126.12	119.76
2	B	978	LEU	C-N-CA	6.36	126.12	119.76
1	A	804	GLY	CA-C-N	6.28	126.48	119.32
1	A	804	GLY	C-N-CA	6.28	126.48	119.32
2	B	463	GLU	CA-C-N	6.26	125.95	119.56
2	B	463	GLU	C-N-CA	6.26	125.95	119.56
2	B	591	ILE	CA-C-N	6.26	126.28	119.90
2	B	591	ILE	C-N-CA	6.26	126.28	119.90
2	B	602	LEU	CA-C-N	6.25	126.22	120.03
2	B	602	LEU	C-N-CA	6.25	126.22	120.03
1	A	212	ASP	CA-C-N	6.22	126.69	119.47
1	A	212	ASP	C-N-CA	6.22	126.69	119.47
3	U	30	ASP	CA-C-N	6.20	125.82	119.56
3	U	30	ASP	C-N-CA	6.20	125.82	119.56
1	A	798	LEU	CA-C-N	6.19	126.10	119.85
1	A	798	LEU	C-N-CA	6.19	126.10	119.85
2	B	886	LEU	CA-C-N	6.15	126.47	119.83
2	B	886	LEU	C-N-CA	6.15	126.47	119.83
1	A	1398	SER	CA-C-N	6.13	126.10	120.03
1	A	1398	SER	C-N-CA	6.13	126.10	120.03
1	A	602	PHE	CA-C-N	6.08	125.84	119.76
1	A	602	PHE	C-N-CA	6.08	125.84	119.76
2	B	934	ASN	CA-C-N	6.01	125.95	119.76
2	B	934	ASN	C-N-CA	6.01	125.95	119.76
1	A	77	ILE	CA-C-N	5.95	126.10	119.32
1	A	77	ILE	C-N-CA	5.95	126.10	119.32
1	A	926	SER	CA-C-N	5.94	127.27	119.84
1	A	926	SER	C-N-CA	5.94	127.27	119.84
1	A	999	ILE	CA-C-N	5.90	125.45	119.19
1	A	999	ILE	C-N-CA	5.90	125.45	119.19
1	A	492	CYS	CA-C-N	5.84	125.79	119.78
1	A	492	CYS	C-N-CA	5.84	125.79	119.78
1	A	1202	LEU	CA-C-N	5.83	125.53	119.82
1	A	1202	LEU	C-N-CA	5.83	125.53	119.82
1	A	641	THR	CA-C-N	5.80	126.20	119.47
1	A	641	THR	C-N-CA	5.80	126.20	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	136	GLU	CA-C-N	5.80	125.71	119.85
2	B	136	GLU	C-N-CA	5.80	125.71	119.85
2	B	337	THR	CA-C-N	5.79	127.07	119.84
2	B	337	THR	C-N-CA	5.79	127.07	119.84
2	B	111	THR	CA-C-N	5.78	125.63	119.28
2	B	111	THR	C-N-CA	5.78	125.63	119.28
1	A	112	LEU	CA-C-N	5.73	125.85	119.32
1	A	112	LEU	C-N-CA	5.73	125.85	119.32
1	A	1042	GLU	N-CA-C	-5.73	108.09	114.62
1	A	918	PHE	CA-C-N	5.58	126.06	120.14
1	A	918	PHE	C-N-CA	5.58	126.06	120.14
1	A	1121	ILE	CA-C-N	5.57	125.58	119.90
1	A	1121	ILE	C-N-CA	5.57	125.58	119.90
1	A	416	PHE	N-CA-C	-5.55	107.05	113.88
1	A	1095	PHE	CA-C-N	5.46	125.81	119.47
1	A	1095	PHE	C-N-CA	5.46	125.81	119.47
1	A	1196	VAL	CA-C-N	5.29	124.96	119.56
1	A	1196	VAL	C-N-CA	5.29	124.96	119.56
1	A	1381	HIS	CA-C-N	5.22	125.27	119.32
1	A	1381	HIS	C-N-CA	5.22	125.27	119.32
2	B	751	LEU	CA-C-N	5.20	126.33	119.84
2	B	751	LEU	C-N-CA	5.20	126.33	119.84
2	B	980	ASP	CA-C-N	5.18	125.48	119.47
2	B	980	ASP	C-N-CA	5.18	125.48	119.47
1	A	455	LEU	CA-C-N	5.09	124.75	119.56
1	A	455	LEU	C-N-CA	5.09	124.75	119.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	993	SER	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	A	10905	0	10876	51	0
2	B	7198	0	7299	33	0
3	U	621	0	594	2	0
4	A	31	0	12	1	0
5	A	3	0	0	0	0
All	All	18758	0	18781	86	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 2.

All (86) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LEU:N	1:A:21:PRO:CD	2.63	0.62
1:A:493:PRO:O	1:A:494:LEU:CB	2.49	0.61
3:U:69:PHE:O	3:U:70:ARG:C	2.43	0.61
1:A:828:ASP:OD2	1:A:1385:LYS:NZ	2.34	0.59
1:A:552:ASP:OD1	1:A:554:LYS:NZ	2.35	0.59
1:A:989:TYR:O	1:A:990:TRP:C	2.46	0.58
2:B:146:HIS:O	2:B:147:HIS:C	2.46	0.58
1:A:992:LEU:O	1:A:993:SER:C	2.49	0.54
2:B:797:HIS:O	2:B:798:LEU:C	2.51	0.54
1:A:4:GLN:NE2	1:A:121:HIS:NE2	2.56	0.53
1:A:743:LEU:O	1:A:744:SER:C	2.51	0.53
1:A:1299:LEU:O	1:A:1302:ASN:ND2	2.42	0.53
1:A:1035:ASN:O	1:A:1037:SER:N	2.42	0.52
1:A:1117:VAL:O	1:A:1118:PHE:HB2	2.10	0.52
1:A:476:LYS:NZ	4:A:1501:ATP:O1G	2.39	0.52
2:B:933:LYS:O	2:B:934:ASN:C	2.52	0.51
2:B:236:LEU:O	2:B:238:LYS:N	2.44	0.51
2:B:357:HIS:O	2:B:358:THR:CB	2.58	0.51
2:B:932:GLY:N	2:B:933:LYS:HB2	2.25	0.51
1:A:309:ILE:O	1:A:310:LYS:C	2.54	0.50
1:A:270:CYS:O	1:A:271:ASN:C	2.55	0.50
2:B:147:HIS:O	2:B:148:ARG:HB3	2.11	0.50
2:B:133:THR:O	2:B:134:PHE:C	2.53	0.49
1:A:221:PHE:N	1:A:222:PRO:CD	2.75	0.49
1:A:199:SER:OG	1:A:200:CYS:N	2.45	0.48
1:A:1202:LEU:N	1:A:1203:PRO:CD	2.77	0.48
1:A:100:CYS:SG	1:A:101:SER:N	2.87	0.48
2:B:147:HIS:O	2:B:148:ARG:CB	2.60	0.48
1:A:464:SER:OG	1:A:465:VAL:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:954:TRP:CZ2	2:B:1005:TRP:CZ2	3.03	0.47
1:A:1095:PHE:HB2	1:A:1096:PRO:HD3	1.96	0.47
1:A:1165:ASN:O	1:A:1166:PHE:C	2.57	0.47
1:A:1125:PHE:N	1:A:1126:PRO:CD	2.77	0.47
1:A:493:PRO:O	1:A:494:LEU:HB3	2.14	0.47
2:B:413:VAL:O	2:B:414:SER:C	2.58	0.47
2:B:615:ASP:OD1	2:B:615:ASP:C	2.58	0.46
1:A:446:SER:OG	1:A:447:LYS:N	2.49	0.46
1:A:101:SER:OG	1:A:102:LEU:N	2.44	0.46
1:A:733:ALA:O	1:A:735:ARG:N	2.49	0.46
2:B:971:ASP:O	2:B:972:PHE:C	2.58	0.46
1:A:1274:LEU:HB2	1:A:1301:ILE:HD12	1.98	0.46
2:B:248:ASP:OD1	2:B:249:GLY:N	2.50	0.45
1:A:425:SER:OG	1:A:426:SER:N	2.49	0.45
2:B:123:ASP:N	2:B:123:ASP:OD1	2.49	0.45
1:A:324:LYS:O	1:A:325:TRP:C	2.59	0.45
1:A:455:LEU:N	1:A:456:PRO:CD	2.80	0.45
1:A:1062:LYS:NZ	1:A:1112:GLU:OE2	2.49	0.44
2:B:162:GLN:C	2:B:163:SER:O	2.58	0.44
2:B:817:SER:O	2:B:818:GLU:HB2	2.17	0.44
1:A:1061:SER:OG	1:A:1062:LYS:N	2.47	0.44
2:B:239:LEU:O	2:B:240:ARG:C	2.61	0.44
2:B:931:PHE:O	2:B:932:GLY:C	2.60	0.44
1:A:1041:ILE:HG22	1:A:1041:ILE:O	2.18	0.44
1:A:881:SER:N	1:A:882:PRO:CD	2.80	0.44
1:A:1045:ARG:N	1:A:1046:PRO:CD	2.80	0.44
3:U:65:ILE:HG22	3:U:69:PHE:CZ	2.52	0.44
2:B:163:SER:HB2	2:B:164:PRO:CD	2.48	0.44
2:B:758:SER:OG	2:B:759:LEU:N	2.48	0.44
1:A:17:HIS:ND1	1:A:17:HIS:O	2.51	0.44
1:A:786:SER:OG	1:A:787:ALA:N	2.48	0.44
2:B:534:LEU:O	2:B:535:GLN:HB2	2.18	0.44
1:A:1045:ARG:HB3	1:A:1046:PRO:HD3	1.99	0.43
1:A:1367:ASP:OD1	1:A:1367:ASP:C	2.60	0.43
1:A:947:ASP:OD1	1:A:947:ASP:C	2.61	0.43
1:A:1196:VAL:N	1:A:1197:PRO:CD	2.81	0.43
1:A:1322:ASN:OD1	1:A:1355:ARG:NH1	2.51	0.43
1:A:1242:LEU:HA	1:A:1243:PRO:HD3	1.89	0.43
2:B:436:LYS:O	2:B:437:PRO:C	2.62	0.43
1:A:20:LEU:N	1:A:21:PRO:HD3	2.35	0.42
2:B:776:ASN:C	2:B:776:ASN:OD1	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1143:ASP:N	1:A:1144:PRO:HD3	2.35	0.42
1:A:1251:VAL:O	1:A:1251:VAL:HG12	2.20	0.41
2:B:846:ASN:OD1	2:B:847:LEU:N	2.53	0.41
2:B:748:ASN:C	2:B:750:ARG:H	2.28	0.41
2:B:933:LYS:HG3	2:B:934:ASN:N	2.36	0.41
1:A:4:GLN:O	1:A:5:GLN:HB2	2.21	0.41
1:A:744:SER:HA	1:A:745:PRO:HD3	1.87	0.41
2:B:154:LEU:O	2:B:155:ASN:HB2	2.21	0.41
2:B:725:THR:OG1	2:B:726:ILE:N	2.53	0.41
2:B:848:VAL:O	2:B:849:LYS:HB2	2.20	0.41
1:A:77:ILE:HG22	1:A:79:GLN:H	1.86	0.40
1:A:762:SER:O	1:A:768:GLN:NE2	2.54	0.40
1:A:1142:TYR:O	1:A:1143:ASP:C	2.65	0.40
2:B:163:SER:O	2:B:164:PRO:C	2.65	0.40
2:B:409:GLU:OE1	2:B:436:LYS:NZ	2.50	0.40
2:B:776:ASN:O	2:B:777:GLU:HB2	2.21	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	1357/1409 (96%)	1245 (92%)	92 (7%)	20 (2%)	8	37
2	B	900/1030 (87%)	822 (91%)	66 (7%)	12 (1%)	9	39
3	U	77/374 (21%)	74 (96%)	2 (3%)	1 (1%)	9	39
All	All	2334/2813 (83%)	2141 (92%)	160 (7%)	33 (1%)	11	38

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	ASN

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Mol	Chain	Res	Type
1	A	1036	HIS
2	B	147	HIS
2	B	148	ARG
2	B	237	LEU
2	B	358	THR
1	A	310	LYS
1	A	325	TRP
1	A	494	LEU
1	A	734	GLN
1	A	1264	CYS
2	B	932	GLY
1	A	264	PRO
1	A	744	SER
1	A	797	SER
1	A	989	TYR
1	A	1118	PHE
2	B	414	SER
3	U	29	SER
1	A	6	LYS
1	A	265	MET
1	A	284	SER
1	A	512	ASP
2	B	818	GLU
2	B	999	GLU
1	A	341	ASN
1	A	543	LYS
2	B	437	PRO
2	B	535	GLN
2	B	799	THR
1	A	927	PRO
2	B	612	ILE
1	A	1041	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1192/1262 (94%)	1192 (100%)	0	100	100
2	B	807/916 (88%)	807 (100%)	0	100	100
3	U	68/333 (20%)	68 (100%)	0	100	100
All	All	2067/2511 (82%)	2067 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	444	HIS
1	A	639	GLN
1	A	862	HIS
1	A	1089	GLN
1	A	1116	ASN
1	A	1130	HIS
1	A	1258	GLN
1	A	1263	HIS
1	A	1331	HIS
2	B	180	GLN
2	B	348	GLN
2	B	800	HIS
3	U	21	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ATP	A	1501	-	32,33,33	1.72	5 (15%)	48,52,52	2.08	12 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	1501	-	-	0/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1501	ATP	C5-C4	5.46	1.48	1.39
4	A	1501	ATP	C5-N7	-4.70	1.30	1.39
4	A	1501	ATP	C5-C6	3.03	1.49	1.41
4	A	1501	ATP	C2-N3	2.32	1.38	1.33
4	A	1501	ATP	C8-N9	-2.09	1.34	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1501	ATP	C5-C4-N3	-6.17	118.22	126.72
4	A	1501	ATP	N3-C4-N9	5.91	137.23	127.17
4	A	1501	ATP	N3-C2-N1	-4.50	121.76	128.58
4	A	1501	ATP	C2-N3-C4	4.26	122.24	111.83
4	A	1501	ATP	C3'-C2'-C1'	2.84	106.83	101.46
4	A	1501	ATP	C5-N7-C8	2.51	107.39	103.45
4	A	1501	ATP	O4'-C1'-C2'	-2.47	101.34	106.62
4	A	1501	ATP	C1'-N9-C8	-2.42	121.73	127.09
4	A	1501	ATP	C6-C5-N7	2.34	136.61	132.09
4	A	1501	ATP	C4-C5-N7	-2.29	107.96	110.58
4	A	1501	ATP	C5-C6-N6	-2.10	118.09	123.29
4	A	1501	ATP	C4-N9-C8	2.08	107.93	105.74

There are no chirality outliers.

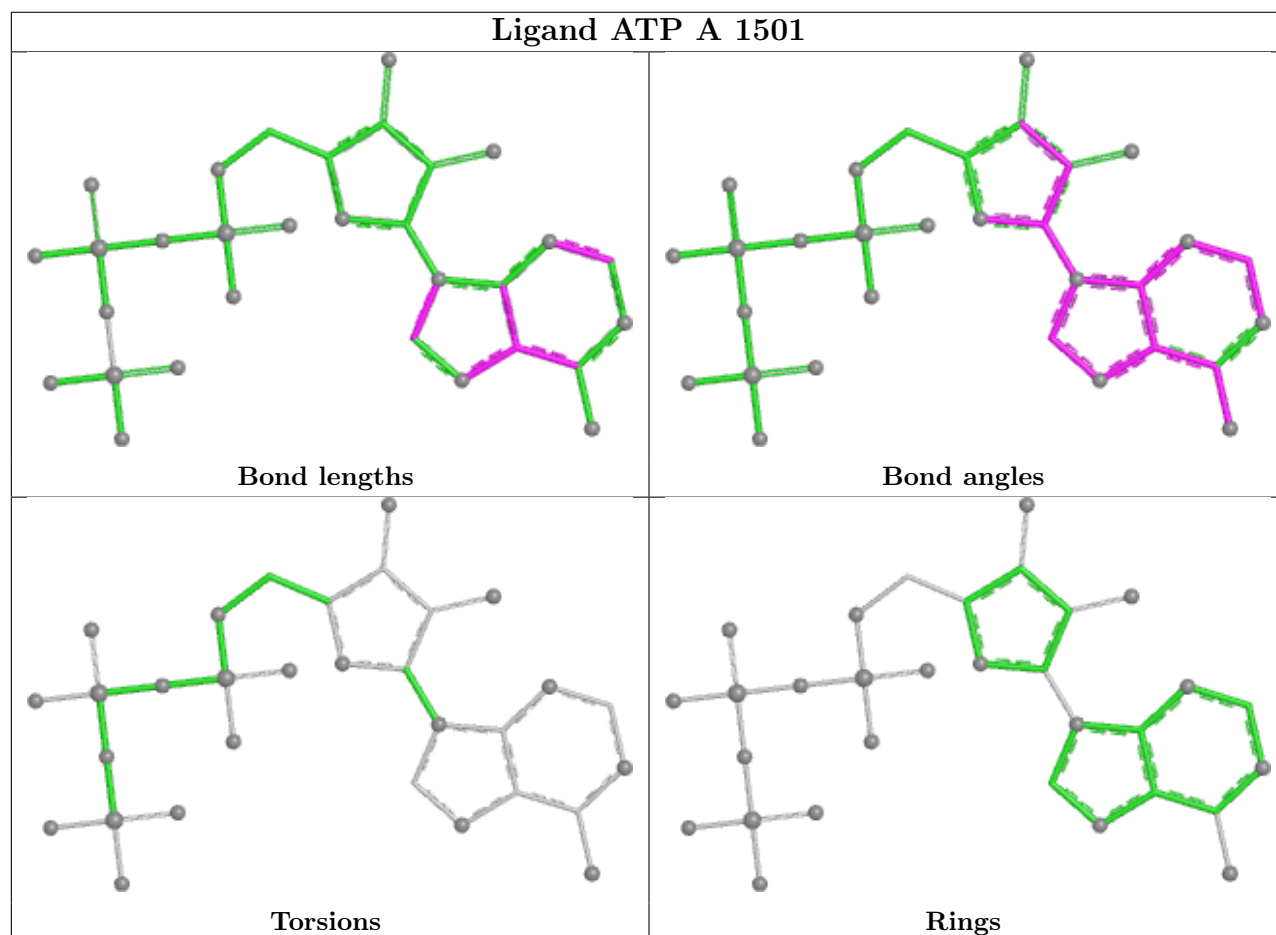
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1501	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

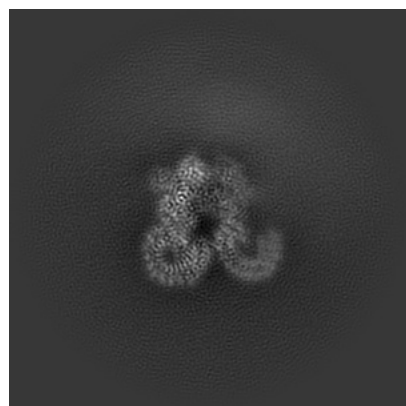
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29493. These allow visual inspection of the internal detail of the map and identification of artifacts.

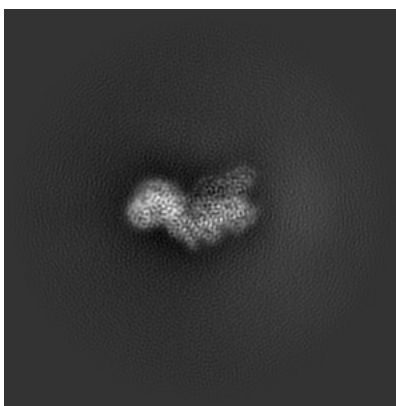
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

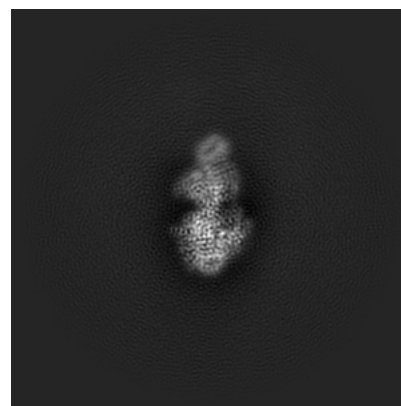
6.1.1 Primary map



X

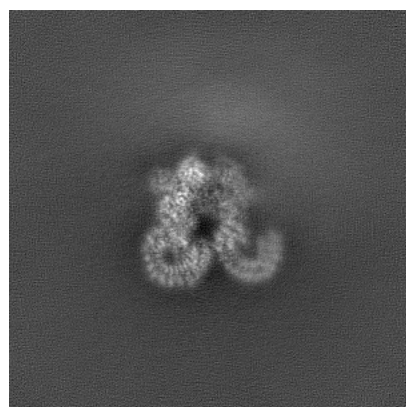


Y

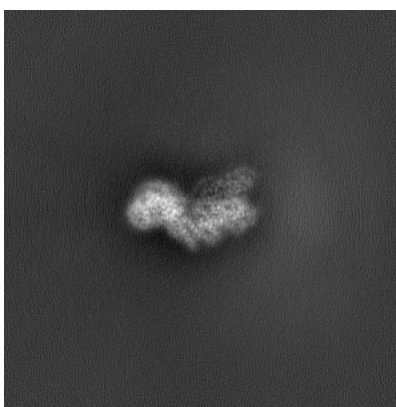


Z

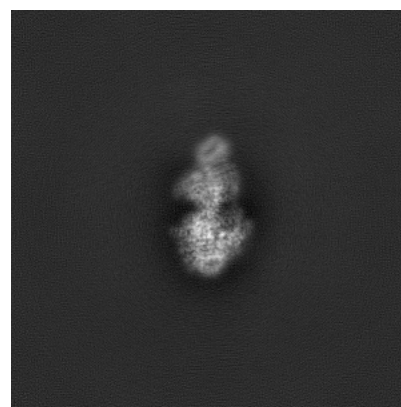
6.1.2 Raw map



X



Y

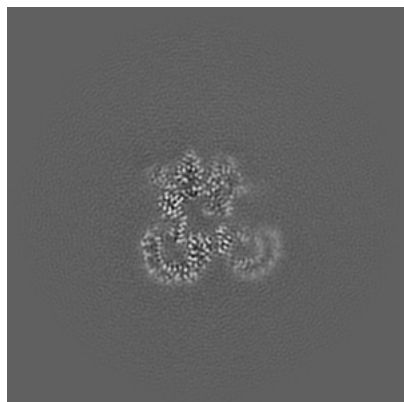


Z

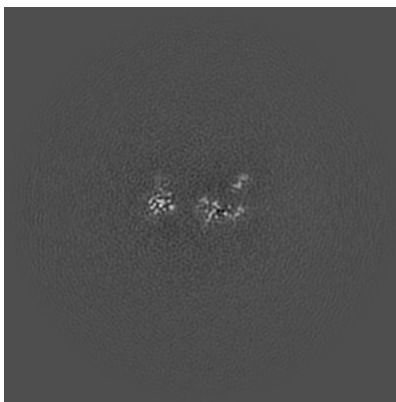
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

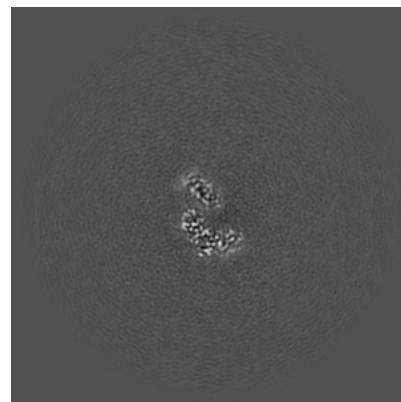
6.2.1 Primary map



X Index: 210

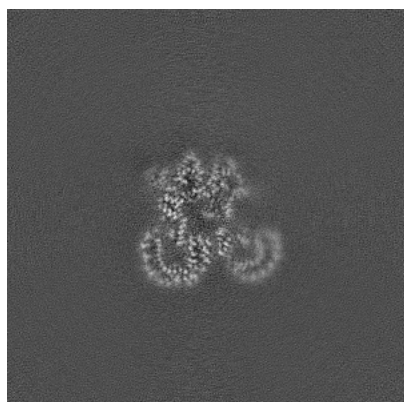


Y Index: 210

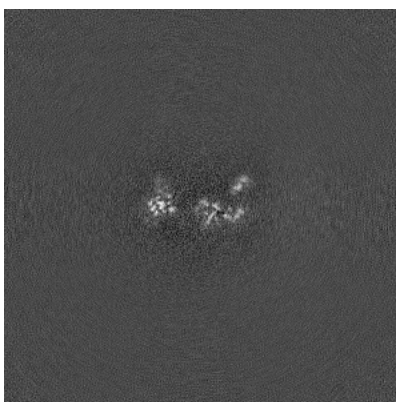


Z Index: 210

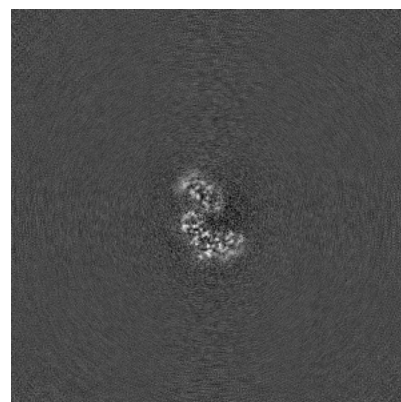
6.2.2 Raw map



X Index: 210



Y Index: 210

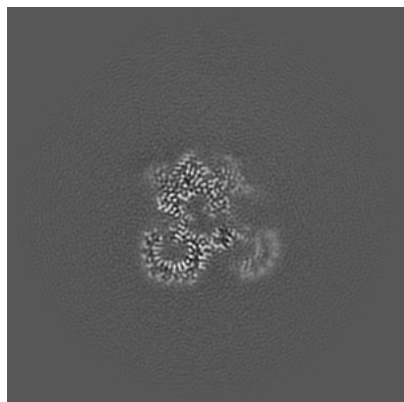


Z Index: 210

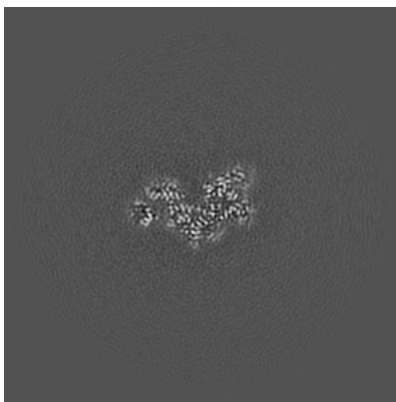
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

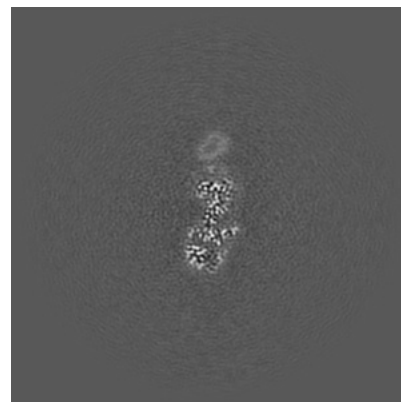
6.3.1 Primary map



X Index: 207

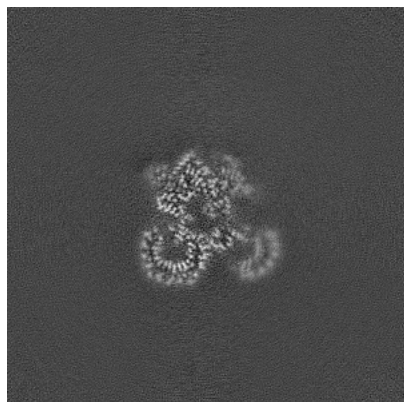


Y Index: 184

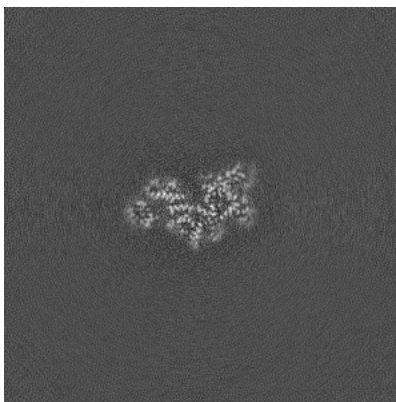


Z Index: 174

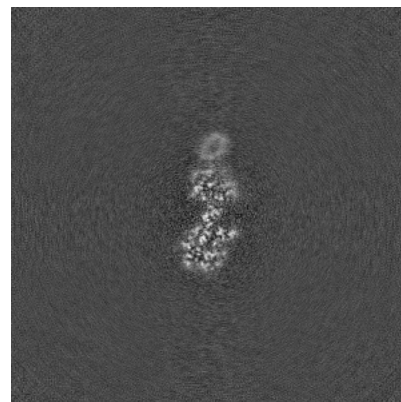
6.3.2 Raw map



X Index: 207



Y Index: 183

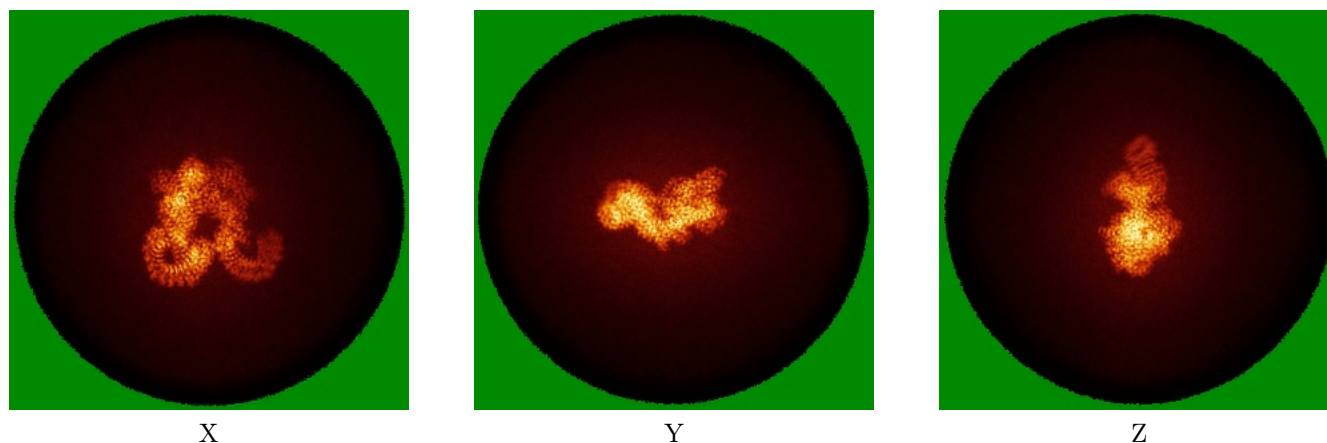


Z Index: 177

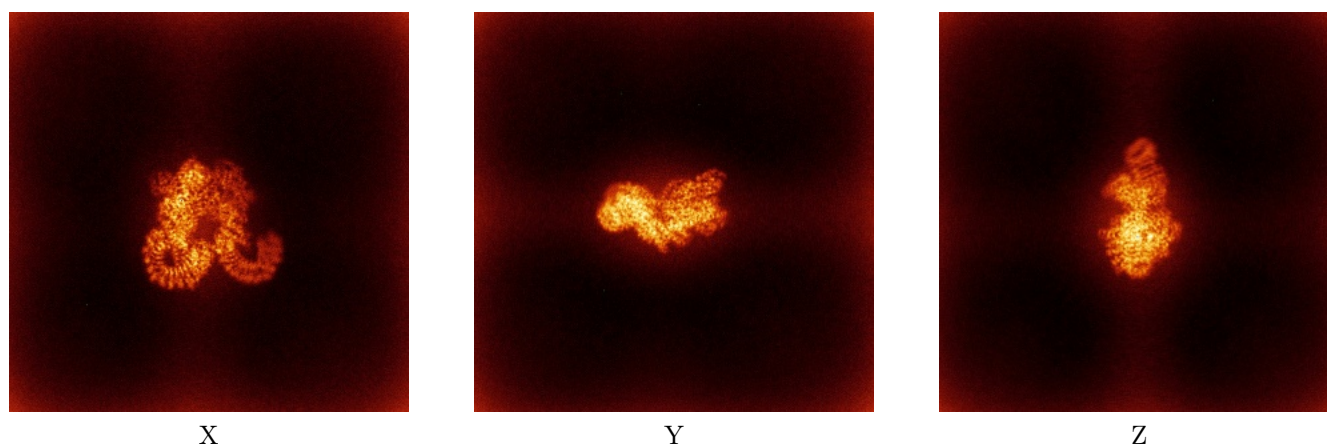
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

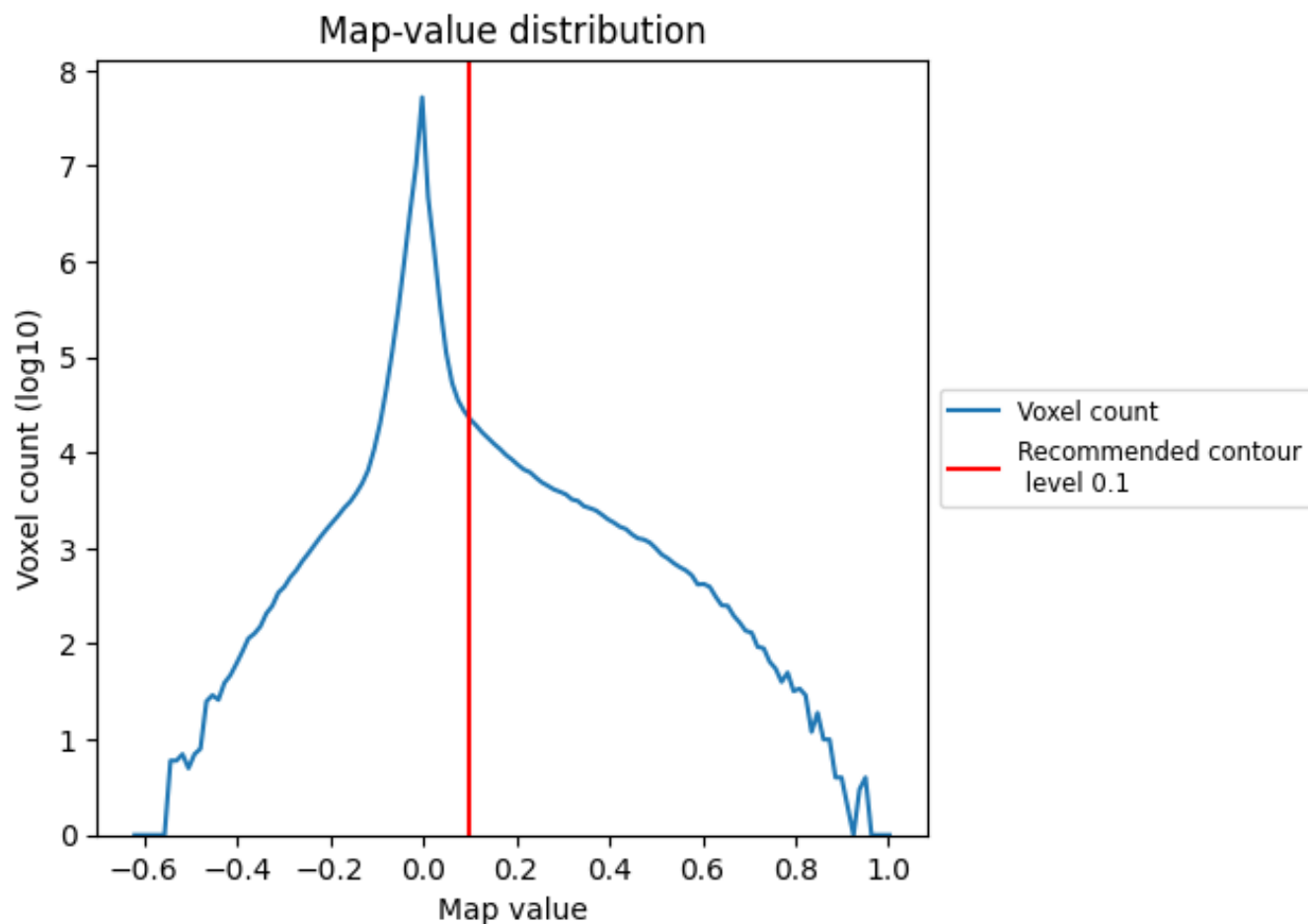
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

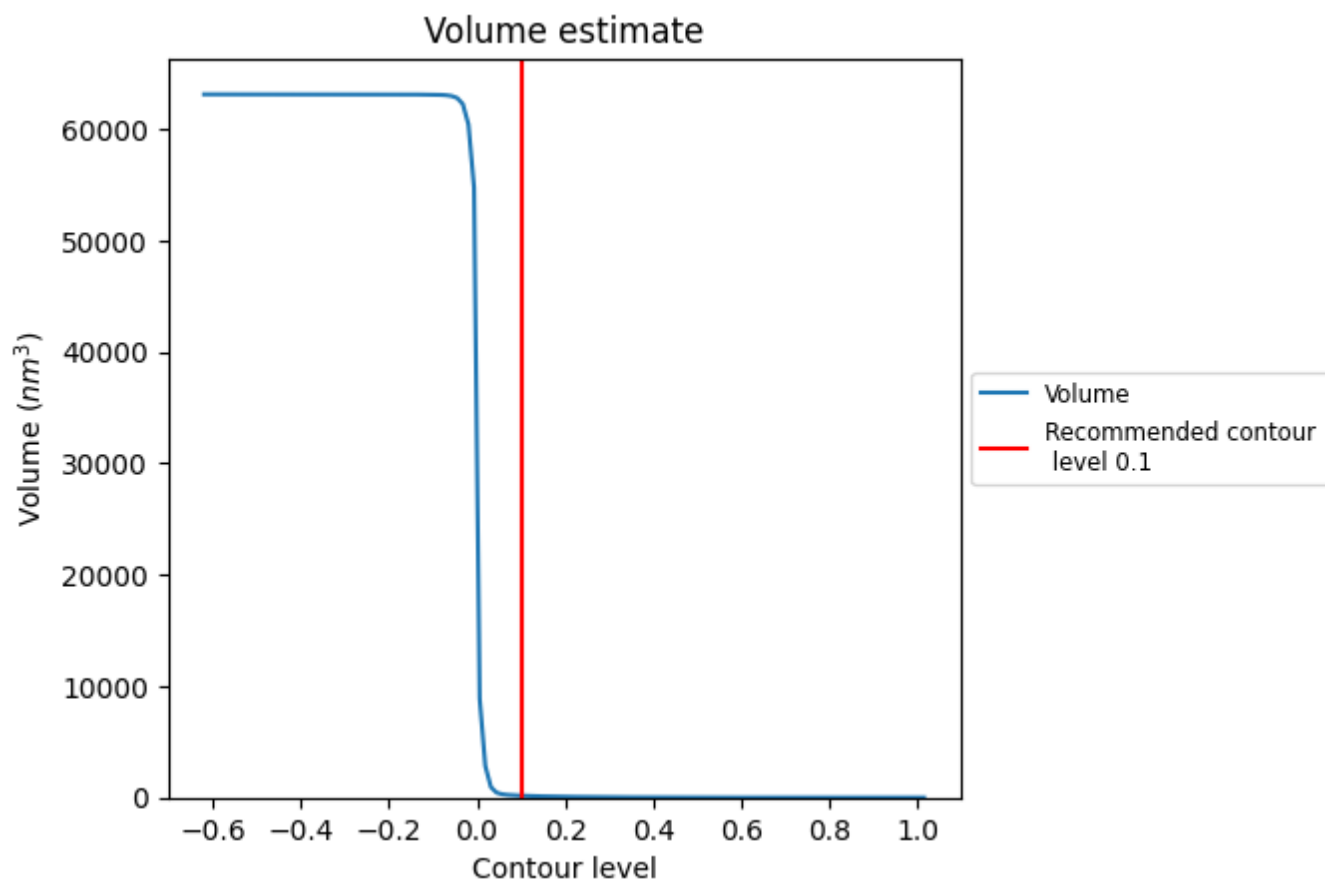
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

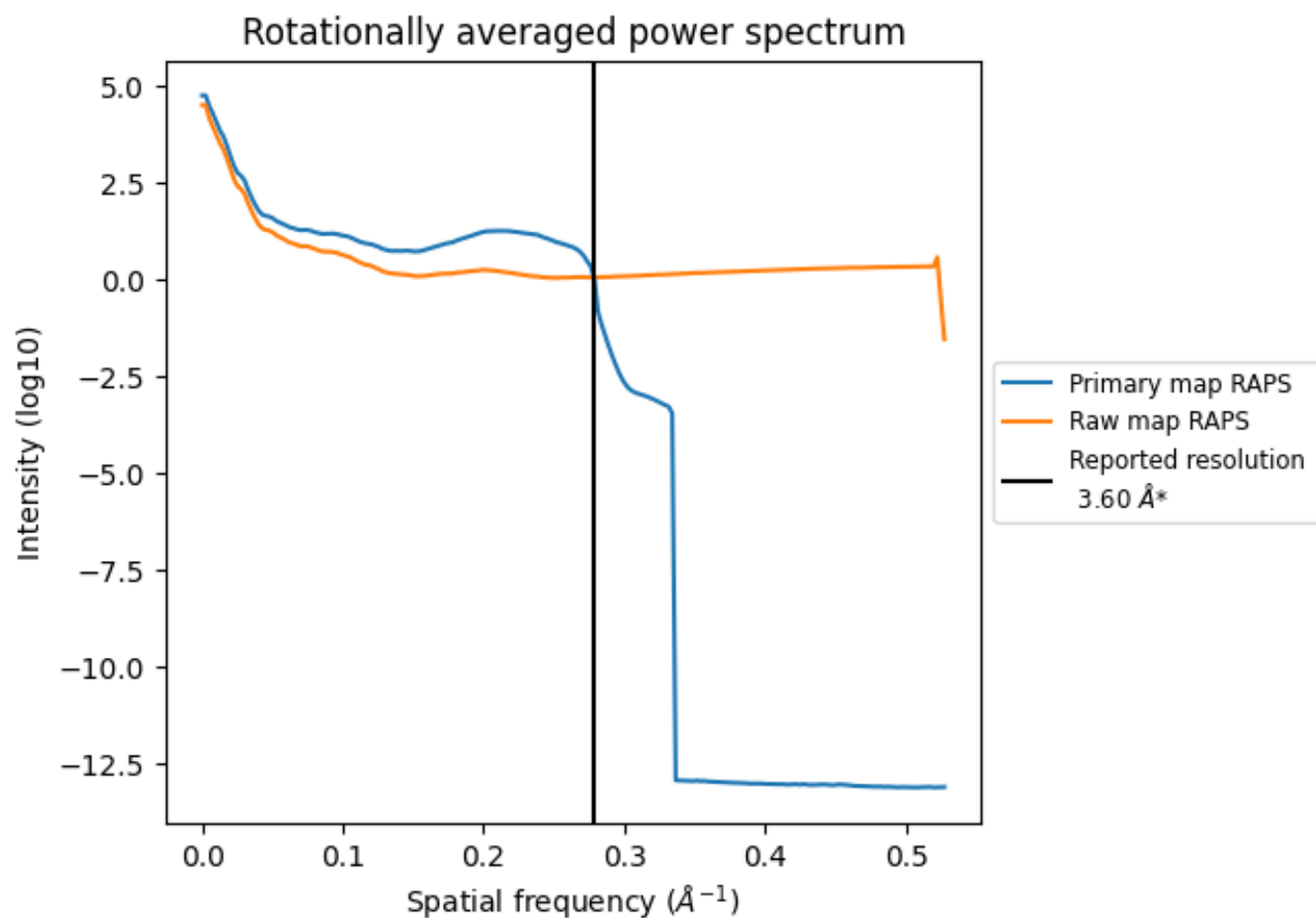
7.2 Volume estimate [i](#)



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

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

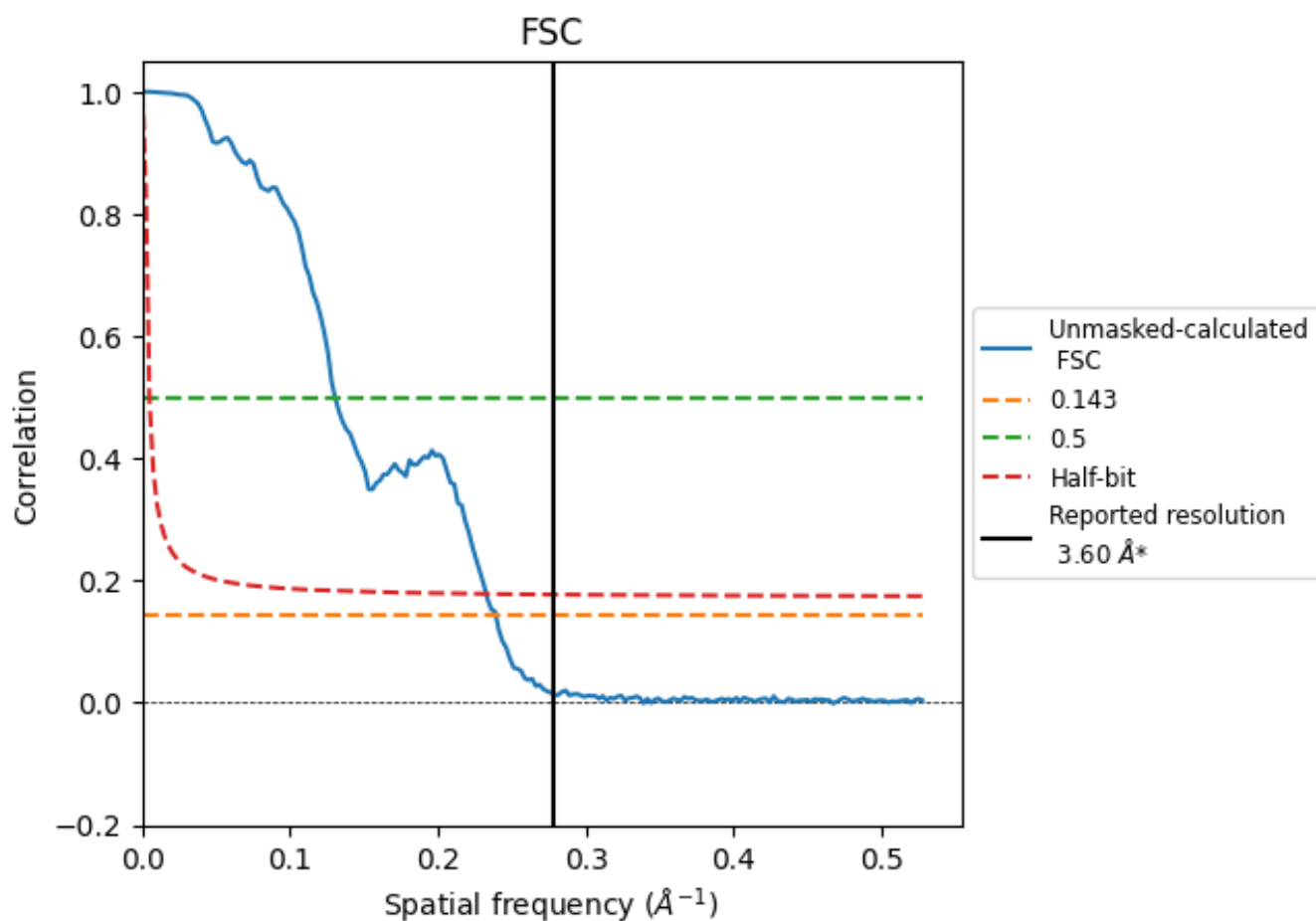


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

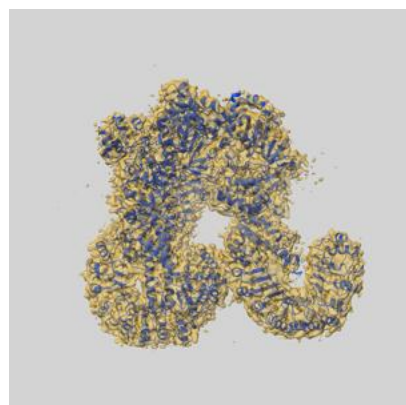
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.18	7.67	4.30

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.18 differs from the reported value 3.6 by more than 10 %

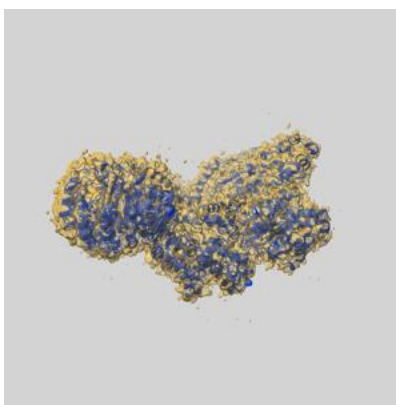
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29493 and PDB model 8FVU. Per-residue inclusion information can be found in section 3 on page 6.

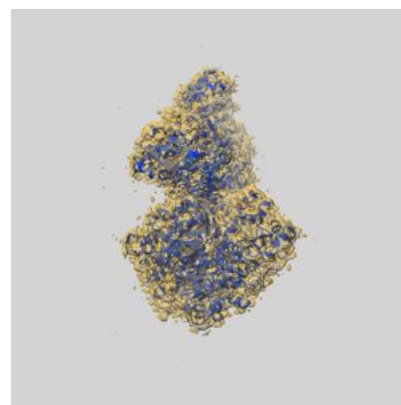
9.1 Map-model overlay [i](#)



X



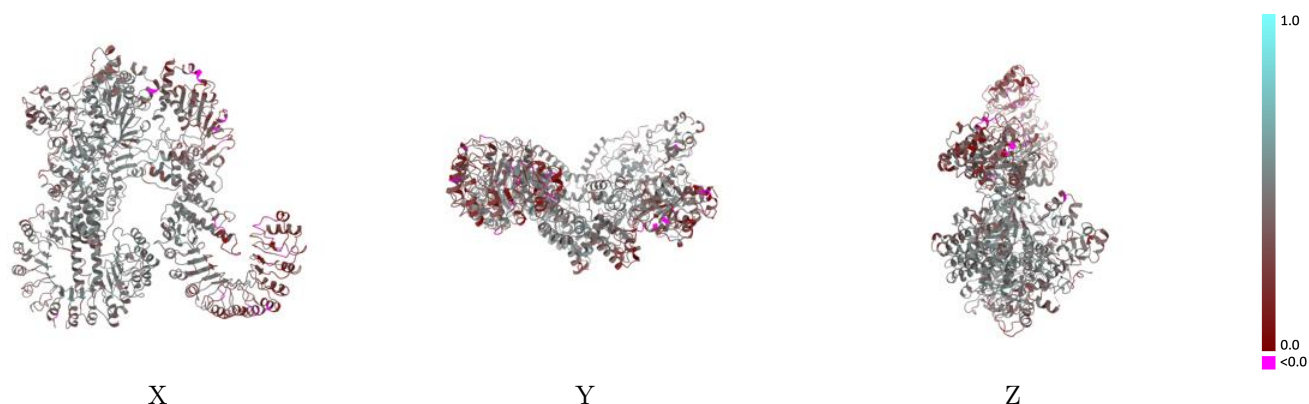
Y



Z

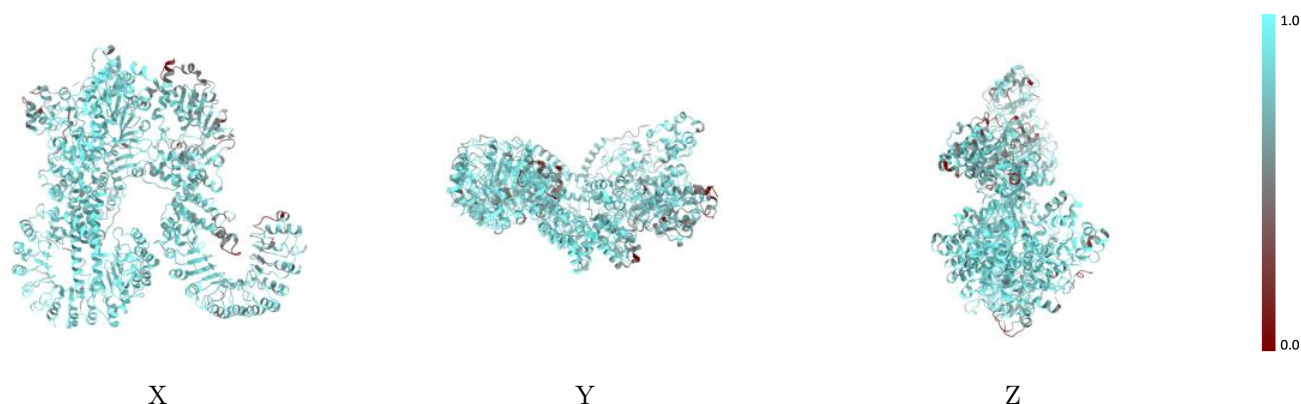
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



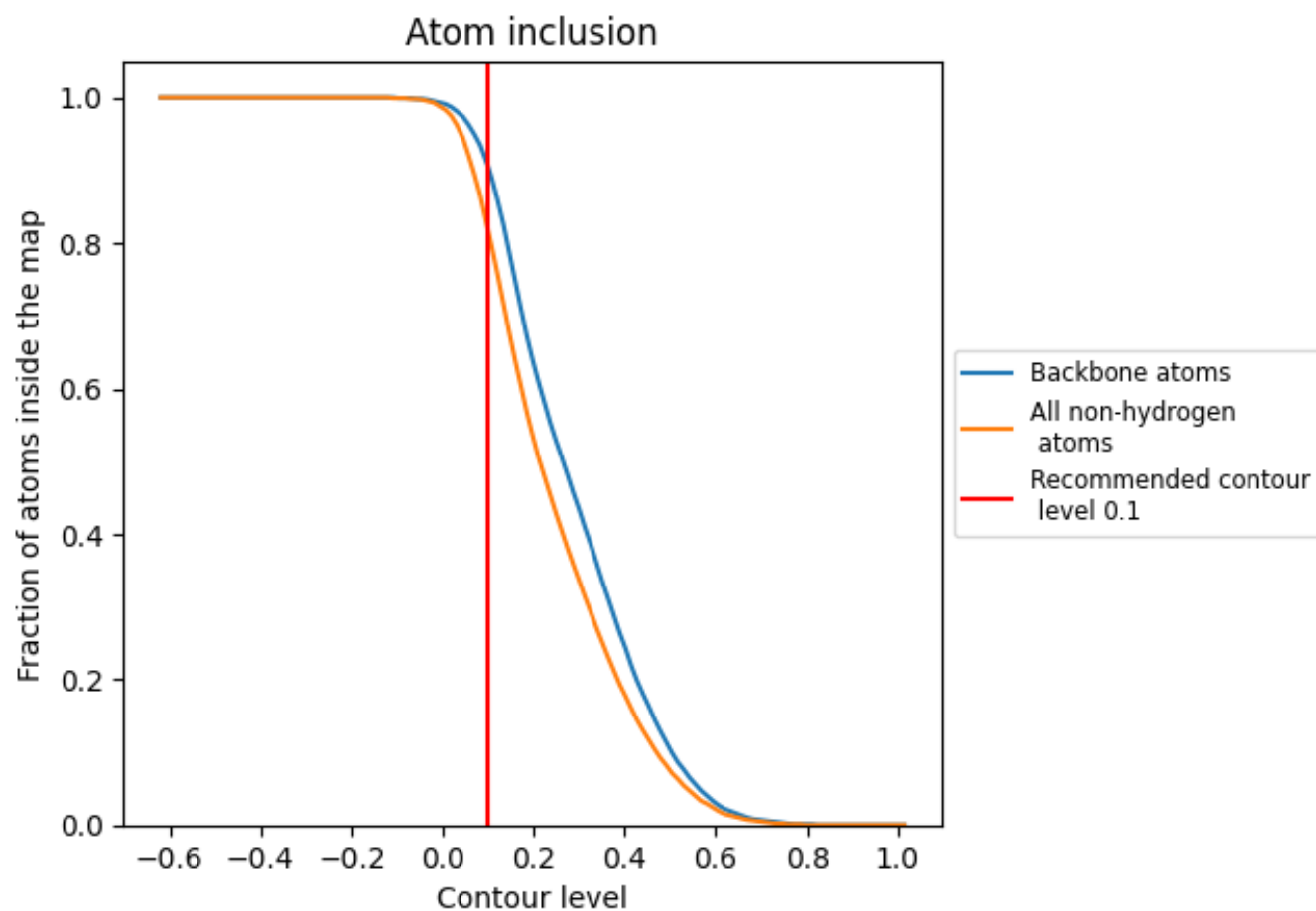
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8180	0.4120
A	0.8580	0.4550
B	0.7530	0.3420
U	0.8670	0.4610

