



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:24 AM UTC

PDB ID : 9UG3 / pdb_00009ug3
EMDB ID : EMD-64131
Title : Structure of SARS-CoV-2 spike-CD147 complex at 3.75 Angstroms resolution
Authors : Zhang, S.J.; Yang, Z.W.; Lin, P.; Bian, H.J.; Zhu, P.; Zhang, L.; Chen, Z.N.
Deposited on : 2025-04-11
Resolution : 3.75 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:

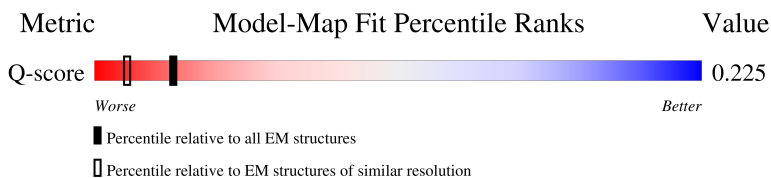
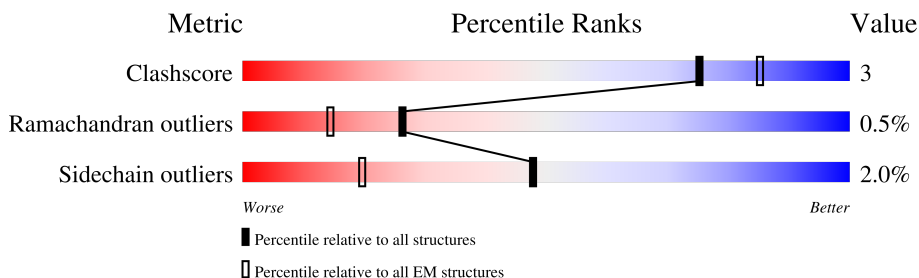
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.75 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	10301 (3.25 - 4.25)

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	1120	
1	B	1120	
1	C	1120	
2	D	181	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 54386 atoms, of which 26833 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1120	Total	C	H	N	O	S	0	0
			17217	5554	8496	1457	1671	39		
1	B	1120	Total	C	H	N	O	S	0	0
			17217	5554	8496	1457	1671	39		
1	C	1120	Total	C	H	N	O	S	0	0
			17216	5554	8495	1457	1671	39		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called Basigin.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	181	Total	C	H	N	O	S	0	0
			2736	862	1346	238	282	8		

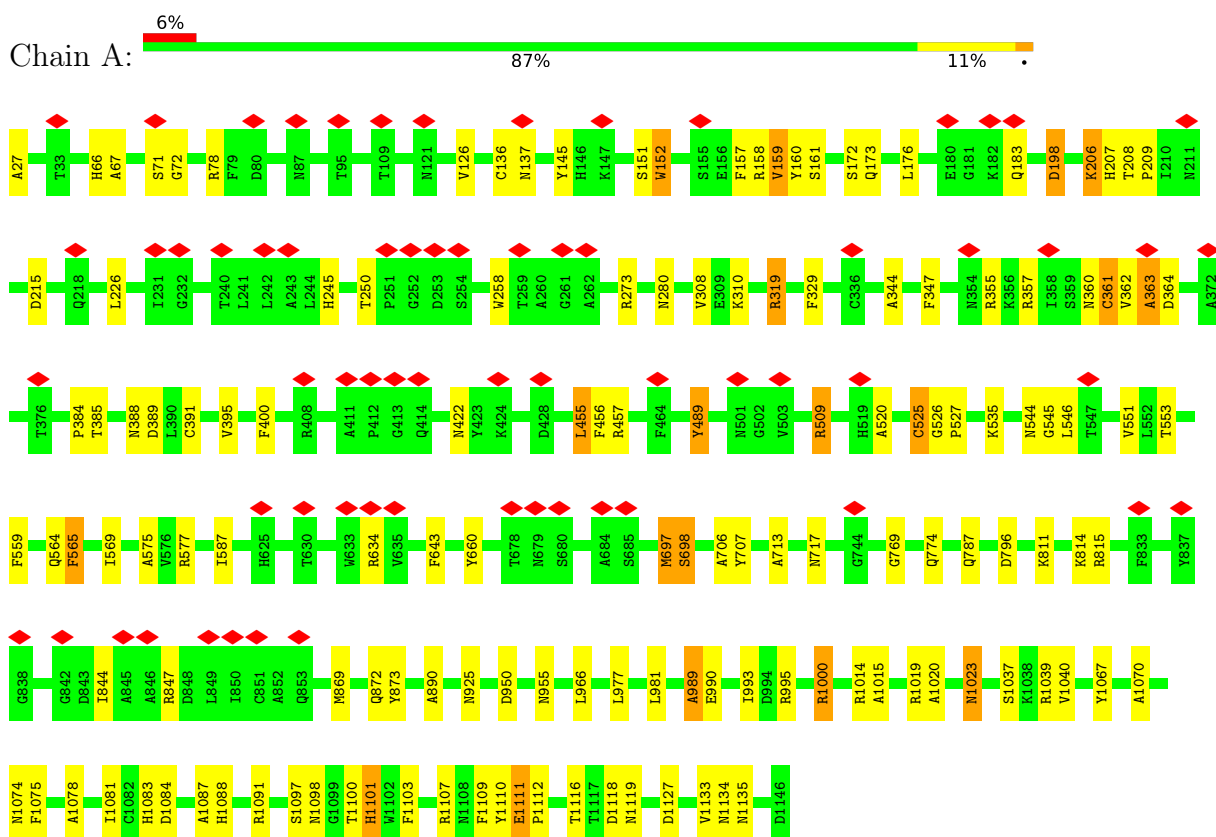
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	23	ALA	-	expression tag	UNP P35613

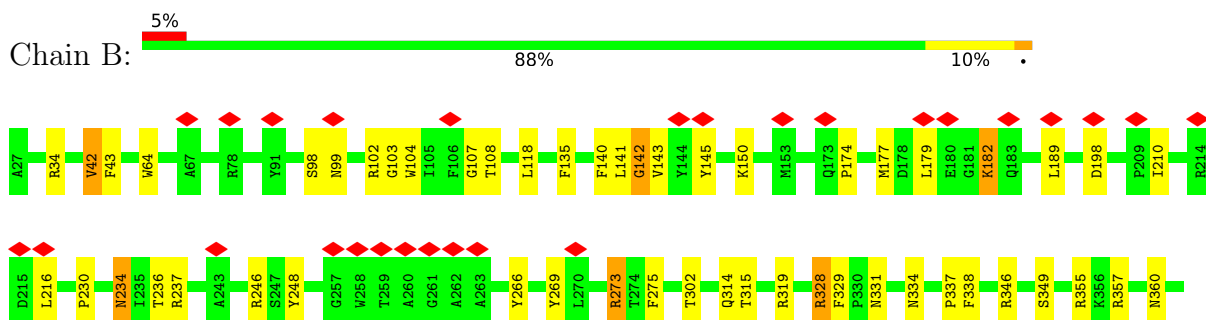
3 Residue-property plots

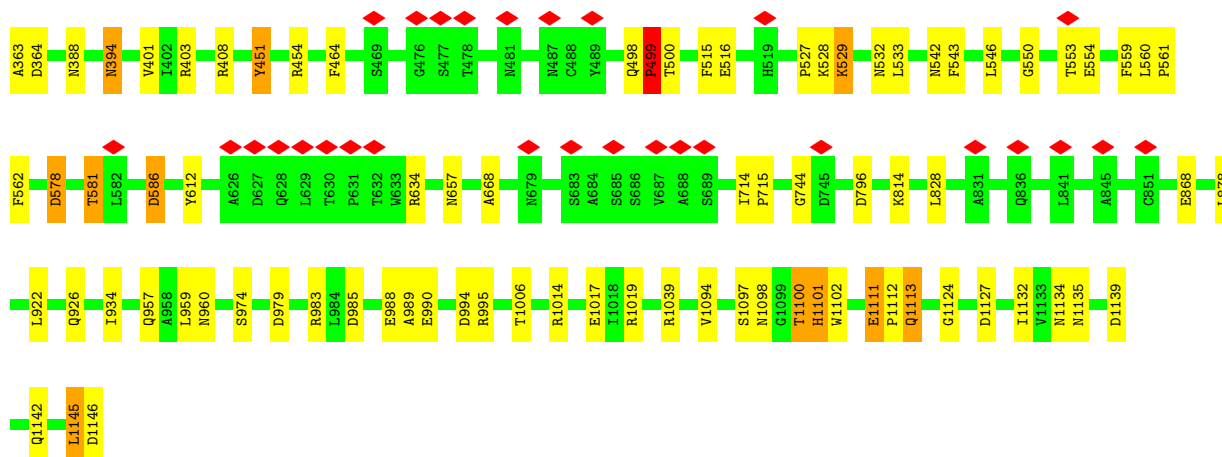
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Spike glycoprotein

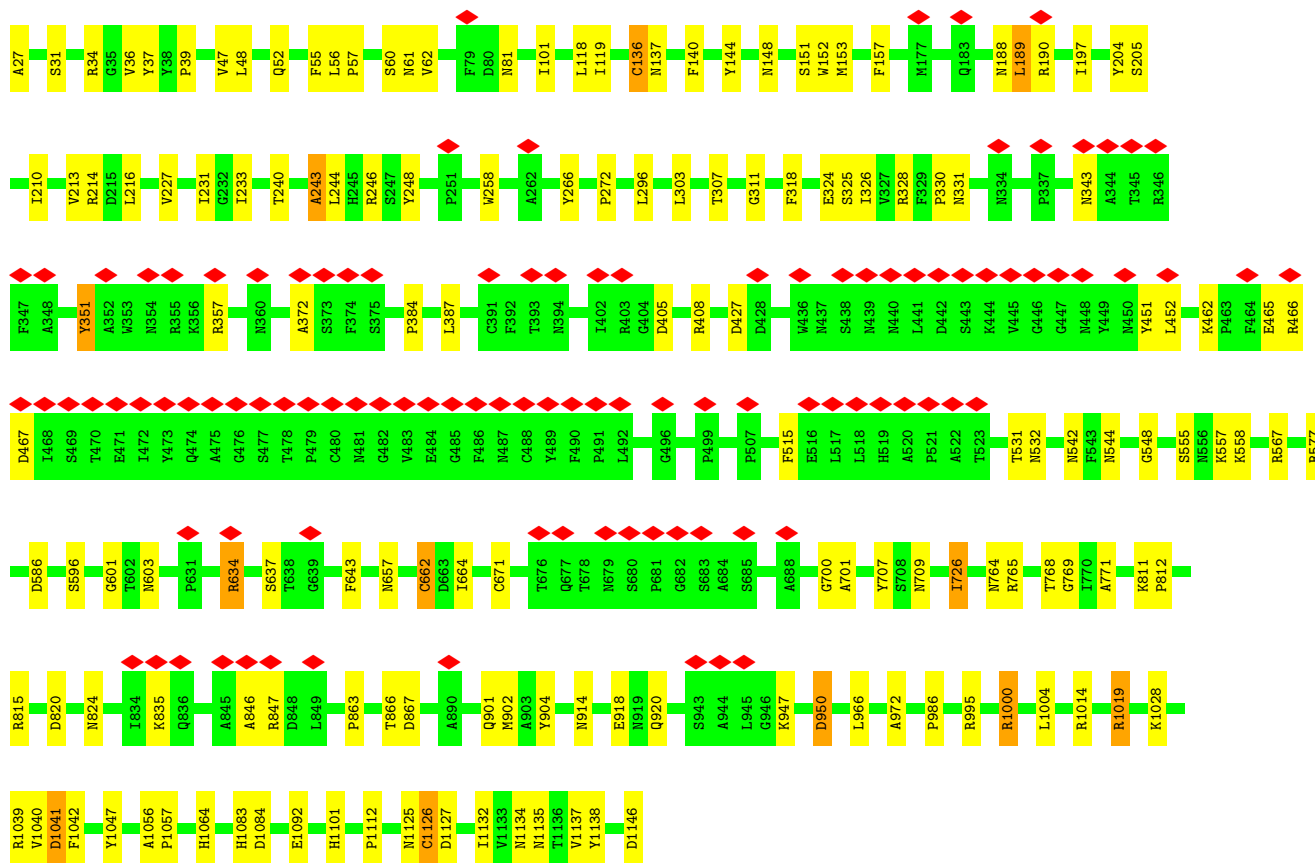
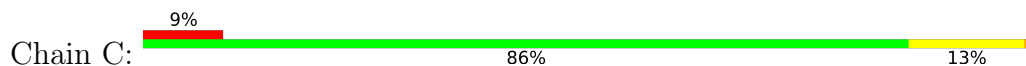


• Molecule 1: Spike glycoprotein

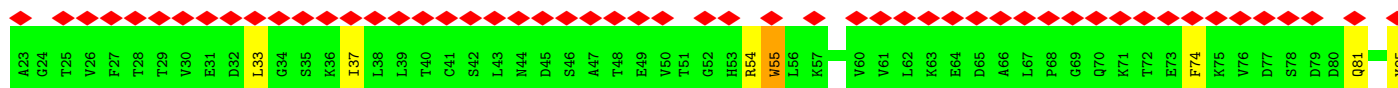
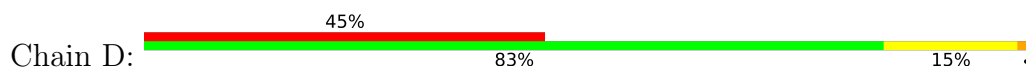


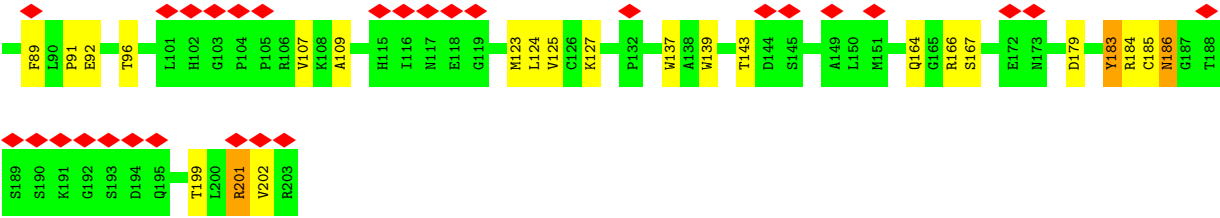


• Molecule 1: Spike glycoprotein



• Molecule 2: Basigin





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	62906	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 ($e^-/\text{\AA}^2$)	53.55	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	34.950	Depositor
Minimum map value	-18.260	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.79	Depositor
Map size (Å)	279.18, 279.18, 279.18	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84599996, 0.84599996, 0.84599996	Depositor

5 Model quality

5.1 Standard geometry

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	1.29	25/8927 (0.3%)	1.50	95/12156 (0.8%)
1	B	1.18	11/8927 (0.1%)	1.45	78/12156 (0.6%)
1	C	1.21	21/8927 (0.2%)	1.47	86/12156 (0.7%)
2	D	1.06	0/1417	1.52	7/1918 (0.4%)
All	All	1.22	57/28198 (0.2%)	1.48	266/38386 (0.7%)

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	6
1	B	0	4
1	C	0	6
2	D	0	2
All	All	0	18

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1101	HIS	ND1-CE1	-8.70	1.23	1.32
1	C	328	ARG	CZ-NH2	-8.33	1.22	1.33
1	B	668	ALA	CA-CB	-7.43	1.42	1.53
1	C	1101	HIS	ND1-CE1	-7.36	1.25	1.32
1	A	1087	ALA	CA-CB	-7.31	1.42	1.53
1	A	1020	ALA	CA-CB	-7.30	1.42	1.53
1	A	1083	HIS	ND1-CE1	-7.17	1.25	1.32
1	C	548	GLY	N-CA	-7.14	1.38	1.45
1	A	1015	ALA	CA-CB	-7.11	1.42	1.53
1	A	989	ALA	CA-CB	-7.09	1.42	1.53
1	C	1064	HIS	ND1-CE1	-7.08	1.25	1.32
1	A	1088	HIS	ND1-CE1	-7.07	1.25	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	363	ALA	CA-CB	-7.05	1.43	1.53
1	A	890	ALA	CA-CB	-6.90	1.42	1.53
1	A	363	ALA	CA-CB	-6.88	1.42	1.53
1	A	520	ALA	CA-CB	-6.86	1.42	1.53
1	C	771	ALA	CA-CB	-6.82	1.42	1.53
1	C	328	ARG	CZ-NH1	-6.80	1.23	1.32
1	C	1083	HIS	ND1-CE1	-6.77	1.25	1.32
1	C	972	ALA	CA-CB	-6.74	1.42	1.53
1	A	706	ALA	CA-CB	-6.67	1.42	1.53
1	A	575	ALA	CA-CB	-6.56	1.42	1.53
1	C	311	GLY	N-CA	-6.55	1.39	1.45
1	C	701	ALA	CA-CB	-6.45	1.42	1.53
1	C	769	GLY	N-CA	-6.41	1.38	1.45
1	A	1078	ALA	CA-CB	-6.37	1.43	1.53
1	B	230	PRO	CA-CB	-6.37	1.47	1.53
1	A	344	ALA	CA-CB	-6.37	1.42	1.53
1	A	713	ALA	CA-CB	-6.30	1.42	1.53
1	C	542	ASN	CA-CB	-5.97	1.46	1.53
1	B	337	PRO	CA-CB	-5.97	1.46	1.53
1	B	328	ARG	CZ-NH2	-5.60	1.26	1.33
1	A	526	GLY	N-CA	-5.59	1.37	1.44
1	A	1101	HIS	ND1-CE1	-5.59	1.26	1.32
1	B	107	GLY	N-CA	-5.52	1.39	1.45
1	C	601	GLY	N-CA	-5.50	1.37	1.45
1	C	1039	ARG	CZ-NH2	-5.40	1.26	1.33
1	A	1112	PRO	CA-CB	-5.38	1.46	1.53
1	A	1014	ARG	CZ-NH2	-5.37	1.26	1.33
1	C	27	ALA	N-CA	-5.29	1.38	1.49
1	B	550	GLY	N-CA	-5.27	1.39	1.45
1	A	577	ARG	CZ-NH2	-5.25	1.26	1.33
1	C	700	GLY	N-CA	-5.23	1.37	1.45
1	A	27	ALA	N-CA	-5.22	1.38	1.49
1	B	1112	PRO	CA-CB	-5.22	1.46	1.53
1	C	408	ARG	CZ-NH2	-5.21	1.26	1.33
1	A	1097	SER	CA-CB	-5.21	1.46	1.53
1	A	769	GLY	N-CA	-5.20	1.39	1.45
1	C	603	ASN	CA-CB	-5.17	1.47	1.54
1	A	1037	SER	CA-CB	-5.17	1.46	1.53
1	A	545	GLY	N-CA	-5.16	1.37	1.45
1	B	331	ASN	CA-CB	-5.16	1.46	1.52
1	C	328	ARG	CD-NE	-5.16	1.39	1.46
1	C	863	PRO	CA-CB	-5.08	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1112	PRO	CA-CB	-5.04	1.47	1.53
1	B	983	ARG	CZ-NH2	-5.04	1.26	1.33
1	A	1098	ASN	CG-ND2	-5.01	1.22	1.33

All (266) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	182	LYS	CA-CB-CG	23.76	161.61	114.10
1	B	500	THR	N-CA-C	13.07	127.14	111.33
1	B	329	PHE	CA-CB-CG	7.90	121.70	113.80
1	C	405	ASP	CA-CB-CG	7.85	120.45	112.60
1	C	846	ALA	N-CA-C	7.75	119.80	111.36
1	C	1127	ASP	CA-CB-CG	7.73	120.33	112.60
1	C	384	PRO	CA-C-N	7.68	130.57	120.28
1	C	384	PRO	C-N-CA	7.68	130.57	120.28
1	A	559	PHE	CA-CB-CG	7.65	121.45	113.80
1	B	960	ASN	CA-CB-CG	7.64	120.24	112.60
1	C	1125	ASN	CA-CB-CG	7.62	120.22	112.60
1	A	361	CYS	CA-C-N	7.59	131.31	120.98
1	A	361	CYS	C-N-CA	7.59	131.31	120.98
1	B	198	ASP	CA-CB-CG	7.50	120.10	112.60
1	C	532	ASN	CA-CB-CG	7.50	120.09	112.60
1	C	324	GLU	CA-C-N	7.45	133.48	123.05
1	C	324	GLU	C-N-CA	7.45	133.48	123.05
1	B	42	VAL	O-C-N	-7.43	115.03	122.99
1	A	544	ASN	CA-CB-CG	7.36	119.96	112.60
1	C	427	ASP	CA-CB-CG	7.35	119.95	112.60
1	B	388	ASN	CA-CB-CG	7.35	119.95	112.60
1	C	343	ASN	CA-CB-CG	7.28	119.88	112.60
1	C	1135	ASN	CA-CB-CG	7.27	119.87	112.60
1	A	1098	ASN	CA-CB-CG	7.22	119.83	112.60
1	A	158	ARG	NE-CZ-NH2	7.18	125.66	119.20
1	A	1135	ASN	CA-CB-CG	7.16	119.75	112.60
1	A	1075	PHE	CA-CB-CG	7.08	120.89	113.80
1	C	1084	ASP	CA-CB-CG	7.08	119.69	112.60
1	B	234	ASN	CA-CB-CG	7.04	119.64	112.60
1	C	603	ASN	CA-CB-CG	7.03	119.63	112.60
1	C	467	ASP	CA-CB-CG	6.98	119.58	112.60
1	A	950	ASP	CA-CB-CG	6.97	119.58	112.60
1	A	955	ASN	CA-CB-CG	6.97	119.57	112.60
1	A	1103	PHE	CA-CB-CG	6.96	120.76	113.80
1	C	542	ASN	CA-CB-CG	6.96	119.56	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1134	ASN	CA-CB-CG	6.94	119.54	112.60
1	A	1134	ASN	CA-CB-CG	6.94	119.54	112.60
1	A	364	ASP	CA-CB-CG	6.93	119.53	112.60
1	B	331	ASN	CA-CB-CG	6.93	119.53	112.60
1	C	643	PHE	CA-CB-CG	6.93	120.73	113.80
1	B	657	ASN	CA-CB-CG	6.89	119.49	112.60
1	C	1042	PHE	CA-CB-CG	6.87	120.67	113.80
1	A	509	ARG	NE-CZ-NH2	6.87	125.38	119.20
1	A	360	ASN	CA-CB-CG	6.84	119.44	112.60
1	C	544	ASN	CA-CB-CG	6.84	119.44	112.60
1	A	1083	HIS	CA-CB-CG	6.83	120.63	113.80
1	A	1119	ASN	CA-CB-CG	6.83	119.43	112.60
1	C	157	PHE	CA-CB-CG	6.81	120.61	113.80
1	B	1139	ASP	CA-CB-CG	6.79	119.39	112.60
2	D	184	ARG	NE-CZ-NH2	6.79	125.31	119.20
1	B	1135	ASN	CA-CB-CG	6.78	119.38	112.60
1	B	364	ASP	CA-CB-CG	6.78	119.38	112.60
1	B	107	GLY	N-CA-C	6.75	119.66	110.69
1	B	543	PHE	CA-CB-CG	6.72	120.53	113.80
1	B	532	ASN	CA-CB-CG	6.72	119.32	112.60
1	A	1107	ARG	NE-CZ-NH2	6.72	125.25	119.20
1	A	1084	ASP	CA-CB-CG	6.69	119.29	112.60
1	B	586	ASP	CA-CB-CG	6.69	119.29	112.60
1	C	1083	HIS	CA-CB-CG	6.69	120.49	113.80
1	B	1134	ASN	CA-CB-CG	6.68	119.28	112.60
1	B	979	ASP	CA-CB-CG	6.67	119.27	112.60
1	C	1041	ASP	CA-CB-CG	6.64	119.25	112.60
1	B	542	ASN	CA-CB-CG	6.61	119.21	112.60
1	C	657	ASN	CA-CB-CG	6.58	119.19	112.60
1	C	1101	HIS	CA-CB-CG	6.57	120.37	113.80
1	B	499	PRO	N-CA-C	6.57	125.99	112.47
2	D	91	PRO	CA-C-N	6.54	129.38	123.10
2	D	91	PRO	C-N-CA	6.54	129.38	123.10
1	A	1074	ASN	CA-CB-CG	6.53	119.13	112.60
1	B	140	PHE	CA-CB-CG	6.49	120.29	113.80
1	B	1127	ASP	CA-CB-CG	6.49	119.09	112.60
1	A	925	ASN	CA-CB-CG	6.49	119.08	112.60
1	C	61	ASN	CA-CB-CG	6.47	119.07	112.60
1	C	331	ASN	CA-CB-CG	6.44	119.04	112.60
1	C	205	SER	N-CA-C	6.37	117.90	108.60
1	A	815	ARG	NE-CZ-NH2	6.37	124.94	119.20
1	C	1064	HIS	CA-CB-CG	6.36	120.16	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	988	GLU	O-C-N	-6.36	113.75	122.46
1	A	995	ARG	NE-CZ-NH2	6.35	124.92	119.20
1	B	102	ARG	NE-CZ-NH2	6.35	124.91	119.20
1	A	1088	HIS	CA-CB-CG	6.33	120.13	113.80
1	A	273	ARG	NE-CZ-NH2	6.32	124.89	119.20
1	B	334	ASN	CA-CB-CG	6.30	118.90	112.60
1	A	389	ASP	CA-CB-CG	6.29	118.89	112.60
1	B	1014	ARG	NE-CZ-NH2	6.28	124.85	119.20
2	D	54	ARG	NE-CZ-NH2	6.28	124.85	119.20
1	A	385	THR	O-C-N	-6.26	115.52	122.03
1	B	1101	HIS	CA-CB-CG	6.22	120.02	113.80
1	B	550	GLY	N-CA-C	6.19	119.79	110.75
1	A	157	PHE	N-CA-C	6.15	117.74	108.46
1	B	182	LYS	CB-CG-CD	-6.11	97.24	111.30
1	A	565	PHE	CA-CB-CG	6.11	119.91	113.80
1	C	986	PRO	N-CA-C	6.11	118.15	110.70
1	A	400	PHE	CA-CB-CG	6.08	119.88	113.80
1	B	360	ASN	CA-CB-CG	6.07	118.67	112.60
1	C	307	THR	CA-C-N	6.07	130.71	123.19
1	C	307	THR	C-N-CA	6.07	130.71	123.19
1	B	355	ARG	NE-CZ-NH2	6.06	124.66	119.20
1	B	338	PHE	CA-CB-CG	6.06	119.86	113.80
1	A	1109	PHE	CA-C-N	6.06	129.43	120.95
1	A	1109	PHE	C-N-CA	6.06	129.43	120.95
1	B	273	ARG	NE-CZ-NH2	6.04	124.63	119.20
1	C	567	ARG	NE-CZ-NH2	6.02	124.62	119.20
1	C	577	ARG	NE-CZ-NH2	5.97	124.58	119.20
1	A	1127	ASP	CA-CB-CG	5.97	118.57	112.60
1	A	1070	ALA	N-CA-C	5.96	117.37	108.31
1	A	697	MET	CA-C-N	5.95	129.94	121.42
1	A	697	MET	C-N-CA	5.95	129.94	121.42
1	B	346	ARG	NE-CZ-NH2	5.94	124.55	119.20
1	B	528	LYS	CA-C-N	5.90	131.48	122.93
1	B	528	LYS	C-N-CA	5.90	131.48	122.93
1	B	357	ARG	NE-CZ-NH2	5.89	124.50	119.20
1	A	577	ARG	N-CA-CB	5.88	118.81	110.46
1	C	157	PHE	N-CA-C	5.88	119.76	112.47
1	A	388	ASN	CA-CB-CG	5.87	118.47	112.60
1	C	136	CYS	N-CA-C	5.86	123.28	110.80
1	B	578	ASP	CA-CB-CG	5.81	118.41	112.60
1	C	515	PHE	CA-CB-CG	5.81	119.61	113.80
1	C	330	PRO	CA-C-N	5.80	130.72	122.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	330	PRO	C-N-CA	5.80	130.72	122.24
1	A	1081	ILE	CA-C-N	5.80	131.64	122.94
1	A	1081	ILE	C-N-CA	5.80	131.64	122.94
1	A	151	SER	N-CA-C	5.80	119.04	107.62
1	A	564	GLN	CA-CB-CG	5.75	125.60	114.10
1	C	325	SER	CA-C-N	5.75	130.67	123.14
1	C	325	SER	C-N-CA	5.75	130.67	123.14
1	C	1014	ARG	NE-CZ-NH2	5.75	124.37	119.20
1	B	796	ASP	CA-CB-CG	5.73	118.33	112.60
1	C	328	ARG	CD-NE-CZ	5.72	132.41	124.40
2	D	92	GLU	CB-CA-C	5.72	116.09	110.71
1	A	634	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	C	244	LEU	N-CA-C	5.71	118.30	110.24
1	B	1113	GLN	CA-C-N	5.71	128.15	120.50
1	B	1113	GLN	C-N-CA	5.71	128.15	120.50
1	B	529	LYS	CA-C-N	5.69	128.95	120.87
1	B	529	LYS	C-N-CA	5.69	128.95	120.87
1	C	357	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	C	246	ARG	NE-CZ-NH2	5.67	124.31	119.20
1	A	546	LEU	CA-C-N	5.67	130.82	123.00
1	A	546	LEU	C-N-CA	5.67	130.82	123.00
1	A	136	CYS	N-CA-C	5.66	119.24	111.54
1	C	1146	ASP	CA-CB-CG	5.66	118.26	112.60
1	B	634	ARG	NE-CZ-NH2	5.64	124.28	119.20
1	A	457	ARG	NE-CZ-NH2	5.64	124.28	119.20
2	D	109	ALA	N-CA-CB	-5.64	102.58	110.25
1	C	60	SER	CA-C-N	5.62	130.12	122.19
1	C	60	SER	C-N-CA	5.62	130.12	122.19
1	C	1135	ASN	N-CA-C	5.60	115.64	108.24
1	A	787	GLN	CA-C-N	5.58	127.98	120.50
1	A	787	GLN	C-N-CA	5.58	127.98	120.50
1	B	1019	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	B	408	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	A	347	PHE	CA-CB-CG	5.56	119.36	113.80
1	B	559	PHE	CA-CB-CG	5.55	119.35	113.80
1	B	331	ASN	CA-C-N	5.55	129.92	122.93
1	B	331	ASN	C-N-CA	5.55	129.92	122.93
1	B	1039	ARG	NE-CZ-NH2	5.54	124.19	119.20
1	A	160	TYR	N-CA-C	5.53	117.68	108.99
1	C	214	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	C	1000	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	C	326	ILE	CA-C-N	5.51	130.65	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	326	ILE	C-N-CA	5.51	130.65	122.99
1	C	213	VAL	N-CA-C	5.50	115.75	110.74
1	A	422	ASN	N-CA-C	5.49	117.12	111.03
1	C	815	ARG	NE-CZ-NH2	5.47	124.13	119.20
1	A	388	ASN	CA-C-N	5.47	130.71	121.14
1	A	388	ASN	C-N-CA	5.47	130.71	121.14
1	A	362	VAL	N-CA-CB	5.46	117.03	110.31
1	A	152	TRP	N-CA-C	5.46	119.18	112.03
1	A	395	VAL	N-CA-C	-5.45	100.51	109.12
1	C	151	SER	CA-C-N	5.45	128.45	120.71
1	C	151	SER	C-N-CA	5.45	128.45	120.71
1	A	159	VAL	N-CA-C	5.44	120.66	109.34
1	B	532	ASN	N-CA-CB	5.44	118.00	110.17
1	A	1088	HIS	CE1-NE2-CD2	-5.43	103.57	109.00
1	A	525	CYS	N-CA-C	5.42	115.28	108.45
1	C	1083	HIS	CE1-NE2-CD2	-5.42	103.58	109.00
1	A	1110	TYR	O-C-N	-5.41	116.28	122.93
1	B	1112	PRO	CA-C-N	5.41	131.05	122.94
1	B	1112	PRO	C-N-CA	5.41	131.05	122.94
1	A	1091	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	B	1146	ASP	CA-CB-CG	5.39	117.99	112.60
1	C	1064	HIS	CE1-NE2-CD2	-5.39	103.61	109.00
1	B	1101	HIS	CE1-NE2-CD2	-5.37	103.63	109.00
1	C	1101	HIS	CE1-NE2-CD2	-5.37	103.63	109.00
1	B	498	GLN	CA-C-N	5.36	126.54	119.84
1	B	498	GLN	C-N-CA	5.36	126.54	119.84
1	C	1083	HIS	CG-CD2-NE2	5.36	112.56	107.20
1	A	78	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	B	142	GLY	N-CA-C	5.33	120.08	111.38
1	A	319	ARG	NE-CZ-NH2	5.33	123.99	119.20
1	A	1083	HIS	CE1-NE2-CD2	-5.32	103.68	109.00
1	A	384	PRO	CA-C-N	5.31	127.66	120.65
1	A	384	PRO	C-N-CA	5.31	127.66	120.65
1	C	532	ASN	N-CA-C	5.30	116.90	108.79
1	A	280	ASN	CA-C-N	5.30	127.64	120.38
1	A	280	ASN	C-N-CA	5.30	127.64	120.38
1	B	1100	THR	CA-C-N	5.30	131.22	121.85
1	B	1100	THR	C-N-CA	5.30	131.22	121.85
1	A	811	LYS	CB-CG-CD	5.26	123.40	111.30
1	C	1019	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	C	1101	HIS	CG-CD2-NE2	5.26	112.46	107.20
1	A	355	ARG	NE-CZ-NH2	5.24	123.92	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1064	HIS	CG-CD2-NE2	5.23	112.43	107.20
1	C	847	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	C	995	ARG	NE-CZ-NH2	5.23	123.90	119.20
1	A	161	SER	N-CA-C	5.23	119.41	113.19
1	A	1133	VAL	CA-C-N	5.22	130.50	122.93
1	A	1133	VAL	C-N-CA	5.22	130.50	122.93
1	A	698	SER	N-CA-CB	5.22	117.94	110.06
1	B	1101	HIS	ND1-CG-CD2	-5.22	100.88	106.10
1	C	920	GLN	N-CA-C	5.21	116.65	111.07
1	B	1124	GLY	CA-C-N	5.21	131.50	122.64
1	B	1124	GLY	C-N-CA	5.21	131.50	122.64
1	B	1101	HIS	CG-CD2-NE2	5.20	112.40	107.20
1	A	1083	HIS	CG-CD2-NE2	5.20	112.40	107.20
1	C	34	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	A	329	PHE	CA-C-N	5.20	126.33	119.84
1	A	329	PHE	C-N-CA	5.20	126.33	119.84
1	C	152	TRP	N-CA-C	5.20	117.77	110.23
1	A	357	ARG	NE-CZ-NH2	5.19	123.88	119.20
1	B	403	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	C	296	LEU	N-CA-CB	5.19	117.67	109.94
1	A	310	LYS	CA-CB-CG	5.18	124.47	114.10
1	A	455	LEU	CB-CA-C	5.18	118.37	109.15
1	B	1113	GLN	CA-CB-CG	5.18	124.46	114.10
1	A	814	LYS	CB-CG-CD	5.18	123.21	111.30
1	B	532	ASN	CA-C-N	5.18	128.20	120.95
1	B	532	ASN	C-N-CA	5.18	128.20	120.95
1	A	1088	HIS	CG-CD2-NE2	5.17	112.37	107.20
1	B	319	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	A	1039	ARG	NE-CZ-NH2	5.16	123.84	119.20
2	D	201	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	A	1111	GLU	CA-C-N	5.16	125.06	119.85
1	A	1111	GLU	C-N-CA	5.16	125.06	119.85
1	B	237	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	C	1126	CYS	CA-C-N	5.16	128.15	120.31
1	C	1126	CYS	C-N-CA	5.16	128.15	120.31
1	C	1127	ASP	CA-C-N	5.15	128.28	123.08
1	C	1127	ASP	C-N-CA	5.15	128.28	123.08
1	C	548	GLY	N-CA-C	5.15	118.50	110.88
1	C	531	THR	N-CA-C	5.14	120.02	113.18
1	C	137	ASN	CA-CB-CG	5.14	117.74	112.60
1	C	1028	LYS	CB-CG-CD	5.13	123.11	111.30
1	A	137	ASN	N-CA-C	5.13	121.73	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	A	990	GLU	CB-CG-CD	5.12	121.31	112.60
1	B	515	PHE	CA-CB-CG	5.12	118.92	113.80
1	A	717	ASN	O-C-N	-5.11	116.92	123.26
1	A	1014	ARG	CA-CB-CG	5.11	124.33	114.10
1	A	847	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	C	311	GLY	N-CA-C	5.10	118.43	110.88
1	B	364	ASP	N-CA-CB	5.10	117.99	110.49
1	A	1000	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	C	765	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	C	243	ALA	CA-C-N	5.07	128.05	120.90
1	C	243	ALA	C-N-CA	5.07	128.05	120.90
1	B	814	LYS	CG-CD-CE	5.07	122.95	111.30
1	A	872	GLN	CB-CG-CD	5.05	121.19	112.60
1	B	533	LEU	N-CA-CB	5.04	117.36	109.85
1	C	634	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	B	995	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	C	466	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	A	643	PHE	CA-CB-CG	5.03	118.83	113.80
1	A	215	ASP	CA-CB-CG	5.02	117.62	112.60
1	B	334	ASN	N-CA-CB	5.00	117.40	110.04

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1067	TYR	Sidechain
1	A	319	ARG	Sidechain
1	A	489	TYR	Sidechain
1	A	660	TYR	Sidechain
1	A	707	TYR	Sidechain
1	A	873	TYR	Sidechain
1	B	248	TYR	Sidechain
1	B	34	ARG	Sidechain
1	B	451	TYR	Sidechain
1	B	612	TYR	Sidechain
1	C	1047	TYR	Sidechain
1	C	144	TYR	Sidechain
1	C	204	TYR	Sidechain
1	C	248	TYR	Sidechain
1	C	707	TYR	Sidechain
1	C	904	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	D	166	ARG	Sidechain
2	D	183	TYR	Sidechain

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	8721	8496	8492	47	0
1	B	8721	8496	8492	53	0
1	C	8721	8495	8494	63	0
2	D	1390	1346	1343	15	0
All	All	27553	26833	26821	171	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 3.

All (171) 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:258:TRP:O	1:A:258:TRP:HE3	1.25	1.17
1:A:258:TRP:O	1:A:258:TRP:CE3	1.99	1.14
1:A:774:GLN:HA	1:A:774:GLN:OE1	1.80	0.81
1:C:56:LEU:HD12	1:C:57:PRO:HD2	1.65	0.79
1:A:71:SER:O	1:A:258:TRP:CH2	2.41	0.74
1:A:989:ALA:O	1:A:993:ILE:HG13	1.90	0.72
1:A:1116:THR:HG23	1:A:1118:ASP:OD1	1.90	0.72
1:A:206:LYS:HD3	1:A:207:HIS:C	2.16	0.71
1:B:516:GLU:N	1:B:516:GLU:OE1	2.23	0.71
1:A:206:LYS:HD3	1:A:207:HIS:N	2.06	0.71
1:C:811:LYS:HG3	1:C:812:PRO:HD2	1.74	0.70
1:B:1142:GLN:NE2	1:B:1145:LEU:HD11	2.08	0.69
1:C:56:LEU:HD12	1:C:57:PRO:CD	2.23	0.68
1:B:1111:GLU:OE2	1:B:1113:GLN:HG3	1.94	0.68
1:B:302:THR:OG1	1:B:315:THR:HG22	1.94	0.68
1:C:118:LEU:C	1:C:119:ILE:HD12	2.19	0.67
1:C:303:LEU:HD23	1:C:303:LEU:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:33:LEU:HD23	2:D:33:LEU:O	1.94	0.66
1:B:108:THR:OG1	1:B:234:ASN:O	2.12	0.66
1:A:989:ALA:HB1	1:A:993:ILE:HD11	1.78	0.65
1:B:328:ARG:NH1	1:B:578:ASP:OD2	2.29	0.65
1:B:1100:THR:O	1:B:1101:HIS:ND1	2.29	0.65
1:A:1111:GLU:OE1	1:A:1111:GLU:HA	1.97	0.64
1:A:206:LYS:HG3	1:A:208:THR:OG1	1.97	0.64
1:A:1019:ARG:O	1:A:1019:ARG:HD2	1.98	0.64
1:B:990:GLU:O	1:B:994:ASP:CG	2.40	0.64
1:C:37:TYR:O	1:C:39:PRO:HD3	1.97	0.64
1:A:1019:ARG:NH1	1:A:1023:ASN:OD1	2.30	0.63
1:B:922:LEU:O	1:B:926:GLN:HG3	1.98	0.63
1:B:990:GLU:O	1:B:994:ASP:OD1	2.14	0.63
1:B:1142:GLN:OE1	1:B:1145:LEU:HD12	1.98	0.63
1:C:662:CYS:HB2	1:C:671:CYS:SG	2.38	0.63
1:B:1111:GLU:O	1:B:1111:GLU:CD	2.42	0.62
1:B:1142:GLN:HE22	1:B:1145:LEU:HD11	1.62	0.62
1:C:101:ILE:O	1:C:101:ILE:HG22	1.98	0.62
1:A:697:MET:HE2	1:A:698:SER:O	2.00	0.62
1:A:1019:ARG:NH2	1:A:1023:ASN:HB2	2.15	0.62
1:C:39:PRO:HG3	1:C:55:PHE:HZ	1.65	0.62
1:B:302:THR:HG1	1:B:315:THR:HG22	1.65	0.62
1:B:560:LEU:HD22	1:B:561:PRO:HD2	1.80	0.62
1:B:394:ASN:O	1:B:516:GLU:OE1	2.18	0.61
1:A:206:LYS:HD3	1:A:206:LYS:C	2.25	0.61
1:C:634:ARG:O	1:C:637:SER:OG	2.17	0.61
1:C:216:LEU:HD12	1:C:216:LEU:N	2.15	0.61
1:A:796:ASP:O	1:A:796:ASP:OD1	2.18	0.61
1:C:820:ASP:OD1	1:C:824:ASN:ND2	2.35	0.59
1:C:1056:ALA:HB1	1:C:1057:PRO:HD2	1.84	0.59
1:B:1017:GLU:OE1	1:C:1019:ARG:NH2	2.36	0.59
1:A:456:PHE:CE2	2:D:96:THR:HG23	2.37	0.59
1:C:39:PRO:HG3	1:C:55:PHE:CZ	2.37	0.59
1:A:966:LEU:CD2	1:A:1000:ARG:CZ	2.81	0.58
2:D:186:ASN:OD1	2:D:186:ASN:O	2.21	0.58
1:B:560:LEU:HD13	1:B:562:PHE:CE2	2.39	0.58
1:C:351:TYR:CE1	1:C:452:LEU:HB2	2.39	0.58
1:C:47:VAL:C	1:C:48:LEU:HD12	2.29	0.58
1:B:1017:GLU:OE1	1:C:1019:ARG:CZ	2.52	0.57
1:C:462:LYS:HE3	1:C:465:GLU:OE2	2.04	0.56
1:C:914:ASN:O	1:C:918:GLU:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:662:CYS:CB	1:C:671:CYS:HG	2.18	0.56
1:C:1126:CYS:SG	1:C:1132:ILE:HD13	2.46	0.56
1:C:101:ILE:HG13	1:C:240:THR:HG21	1.87	0.56
1:C:48:LEU:HD12	1:C:48:LEU:N	2.21	0.56
1:B:560:LEU:HD13	1:B:562:PHE:HE2	1.71	0.55
2:D:124:LEU:HD22	2:D:183:TYR:CB	2.37	0.54
1:B:1142:GLN:CD	1:B:1145:LEU:HD12	2.33	0.54
1:B:1142:GLN:NE2	1:B:1145:LEU:CD1	2.70	0.54
2:D:124:LEU:HD23	2:D:139:TRP:CG	2.42	0.54
1:C:555:SER:HB2	1:C:586:ASP:OD1	2.07	0.54
1:C:555:SER:CB	1:C:586:ASP:OD1	2.55	0.54
1:A:72:GLY:HA2	1:A:258:TRP:CZ2	2.44	0.54
1:C:216:LEU:H	1:C:216:LEU:CD1	2.20	0.53
2:D:124:LEU:HD22	2:D:183:TYR:HB3	1.89	0.53
1:C:966:LEU:HD23	1:C:1000:ARG:CZ	2.38	0.53
1:A:1118:ASP:OD1	1:A:1118:ASP:N	2.41	0.53
1:C:188:ASN:OD1	1:C:189:LEU:C	2.52	0.53
1:C:48:LEU:N	1:C:48:LEU:CD1	2.72	0.53
1:C:56:LEU:HD12	1:C:57:PRO:N	2.24	0.53
1:B:189:LEU:HD21	1:B:216:LEU:CD2	2.40	0.52
1:B:103:GLY:C	1:B:104:TRP:CE3	2.87	0.51
1:B:143:VAL:HG13	1:B:145:TYR:CE2	2.45	0.51
1:C:188:ASN:OD1	1:C:189:LEU:O	2.28	0.51
1:B:103:GLY:HA2	1:B:104:TRP:CE3	2.45	0.51
2:D:199:THR:HG22	2:D:201:ARG:HD2	1.93	0.51
1:B:314:GLN:O	1:B:315:THR:OG1	2.24	0.51
1:A:71:SER:O	1:A:258:TRP:CZ2	2.64	0.50
1:C:216:LEU:N	1:C:216:LEU:CD1	2.74	0.50
1:A:844:ILE:HD11	1:C:586:ASP:OD2	2.10	0.50
1:A:66:HIS:CD2	1:A:67:ALA:HB2	2.47	0.50
1:A:152:TRP:CG	1:A:245:HIS:HD1	2.30	0.49
1:C:52:GLN:NE2	1:C:272:PRO:O	2.46	0.49
2:D:186:ASN:O	2:D:186:ASN:CG	2.54	0.49
1:B:714:ILE:HG23	1:B:715:PRO:HD2	1.94	0.49
1:C:52:GLN:HE21	1:C:272:PRO:HB2	1.78	0.49
1:A:391:CYS:SG	1:A:525:CYS:HB2	2.53	0.48
1:A:206:LYS:CD	1:A:207:HIS:C	2.86	0.48
1:A:206:LYS:HD2	1:A:208:THR:HA	1.94	0.48
1:C:216:LEU:HD12	1:C:216:LEU:H	1.78	0.48
1:B:959:LEU:CD1	1:B:959:LEU:N	2.77	0.48
2:D:125:VAL:HG11	2:D:167:SER:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:SER:OG	1:A:173:GLN:N	2.47	0.47
1:A:966:LEU:CD2	1:A:1000:ARG:NH1	2.78	0.47
2:D:37:ILE:CG2	2:D:55:TRP:HE1	2.27	0.47
2:D:33:LEU:O	2:D:33:LEU:CD2	2.61	0.47
1:B:349:SER:HA	1:B:451:TYR:CE2	2.49	0.47
1:B:99:ASN:OD1	1:B:177:MET:HB2	2.15	0.47
1:C:662:CYS:CB	1:C:671:CYS:SG	3.02	0.47
1:B:189:LEU:HD12	1:B:189:LEU:HA	1.72	0.46
1:B:985:ASP:O	1:B:989:ALA:N	2.47	0.46
1:B:1142:GLN:CD	1:B:1145:LEU:CD1	2.89	0.46
1:A:569:ILE:HD12	1:A:569:ILE:H	1.80	0.46
1:B:578:ASP:OD2	1:B:581:THR:OG1	2.34	0.46
1:C:303:LEU:HD23	1:C:303:LEU:C	2.41	0.46
1:C:140:PHE:H	1:C:153:MET:HE3	1.81	0.46
1:B:560:LEU:HD23	1:B:560:LEU:HA	1.77	0.45
1:B:104:TRP:CE3	1:B:104:TRP:N	2.85	0.45
1:B:1098:ASN:OD1	1:B:1098:ASN:C	2.59	0.45
1:A:1019:ARG:HD2	1:A:1019:ARG:C	2.42	0.45
1:C:148:ASN:HD22	1:C:243:ALA:HB1	1.81	0.45
1:A:258:TRP:O	1:A:258:TRP:CD2	2.64	0.45
1:B:98:SER:HB3	1:B:145:TYR:CE2	2.52	0.44
1:C:101:ILE:O	1:C:101:ILE:CG2	2.63	0.44
1:C:31:SER:HB3	1:C:62:VAL:HG11	2.00	0.44
1:C:764:ASN:O	1:C:768:THR:OG1	2.33	0.44
1:A:535:LYS:HD2	1:A:553:THR:HA	1.99	0.44
1:A:565:PHE:O	1:B:43:PHE:N	2.50	0.44
1:C:118:LEU:O	1:C:119:ILE:HD12	2.18	0.44
1:C:726:ILE:HG12	1:C:947:LYS:H	1.83	0.44
1:A:977:LEU:HD11	1:A:981:LEU:HD11	1.99	0.43
1:C:148:ASN:ND2	1:C:243:ALA:HB1	2.33	0.43
1:C:216:LEU:CD1	1:C:266:TYR:CE2	3.01	0.43
1:C:216:LEU:HD11	1:C:266:TYR:CD1	2.54	0.43
1:A:796:ASP:O	1:A:796:ASP:CG	2.60	0.43
1:A:66:HIS:CD2	1:A:67:ALA:CB	3.02	0.43
1:C:820:ASP:OD1	1:C:820:ASP:C	2.60	0.43
1:B:401:VAL:HB	1:B:451:TYR:CE2	2.53	0.43
1:B:1111:GLU:OE2	1:B:1111:GLU:O	2.36	0.43
1:B:174:PRO:HB2	1:B:179:LEU:HD13	2.00	0.43
1:A:1100:THR:O	1:A:1101:HIS:CG	2.72	0.43
1:A:1100:THR:O	1:A:1101:HIS:ND1	2.52	0.43
1:A:183:GLN:H	1:A:209:PRO:CB	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:PHE:HB2	1:B:42:VAL:HG13	2.00	0.42
1:A:796:ASP:OD1	1:A:796:ASP:C	2.63	0.42
1:B:828:LEU:HD12	1:B:828:LEU:H	1.83	0.42
1:A:796:ASP:OD2	1:C:709:ASN:ND2	2.48	0.42
1:C:216:LEU:HD11	1:C:266:TYR:CG	2.54	0.42
1:B:64:TRP:CD1	1:B:266:TYR:CE2	3.07	0.42
1:B:553:THR:HG22	1:B:554:GLU:N	2.34	0.42
1:C:866:THR:HG22	1:C:867:ASP:N	2.35	0.42
1:C:555:SER:HB3	1:C:586:ASP:OD1	2.19	0.42
1:B:142:GLY:HA2	1:B:150:LYS:HD3	2.01	0.42
1:C:950:ASP:OD1	1:C:950:ASP:C	2.61	0.42
1:B:1132:ILE:HD12	1:B:1132:ILE:C	2.45	0.42
1:A:993:ILE:HG13	1:A:993:ILE:H	1.57	0.41
1:C:231:ILE:HG13	1:C:233:ILE:H	1.83	0.41
2:D:124:LEU:HD22	2:D:183:TYR:HB2	2.02	0.41
1:A:363:ALA:O	1:A:527:PRO:HD3	2.20	0.41
1:C:189:LEU:HD12	1:C:190:ARG:N	2.36	0.41
1:B:546:LEU:HD12	1:B:546:LEU:HA	1.96	0.41
1:A:535:LYS:CD	1:A:553:THR:HA	2.51	0.41
1:B:182:LYS:HE2	1:B:210:ILE:H	1.86	0.41
1:C:216:LEU:HD11	1:C:266:TYR:CD2	2.56	0.41
1:B:527:PRO:O	1:B:529:LYS:NZ	2.44	0.41
1:C:39:PRO:CG	1:C:55:PHE:HZ	2.30	0.41
2:D:123:MET:SD	2:D:127:LYS:HE2	2.60	0.41
1:C:119:ILE:HD12	1:C:119:ILE:N	2.35	0.41
1:C:1041:ASP:CG	1:C:1041:ASP:O	2.63	0.41
1:C:1004:LEU:HD23	1:C:1004:LEU:HA	1.83	0.40
1:C:557:LYS:C	1:C:558:LYS:HG3	2.46	0.40
1:B:1097:SER:HB2	1:B:1102:TRP:CD2	2.56	0.40
2:D:107:VAL:HG21	2:D:185:CYS:SG	2.62	0.40
2:D:55:TRP:CD1	2:D:74:PHE:CD2	3.10	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	1118/1120 (100%)	983 (88%)	131 (12%)	4 (0%)	30	61
1	B	1118/1120 (100%)	1010 (90%)	105 (9%)	3 (0%)	36	66
1	C	1118/1120 (100%)	987 (88%)	125 (11%)	6 (0%)	24	56
2	D	179/181 (99%)	143 (80%)	33 (18%)	3 (2%)	7	33
All	All	3533/3541 (100%)	3123 (88%)	394 (11%)	16 (0%)	26	56

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	A	1040	VAL
1	C	210	ILE
1	C	835	LYS
1	A	250	THR
1	B	499	PRO
2	D	81	GLN
1	A	159	VAL
1	C	258	TRP
2	D	179	ASP
1	B	464	PHE
1	C	136	CYS
1	C	372	ALA
1	C	451	TYR
2	D	164	GLN
1	B	744	GLY

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	970/970 (100%)	955 (98%)	15 (2%)	57	68
1	B	970/970 (100%)	949 (98%)	21 (2%)	45	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	970/970 (100%)	951 (98%)	19 (2%)	48	64
2	D	156/156 (100%)	149 (96%)	7 (4%)	24	48
All	All	3066/3066 (100%)	3004 (98%)	62 (2%)	48	64

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	VAL
1	A	145	TYR
1	A	176	LEU
1	A	198	ASP
1	A	206	LYS
1	A	226	LEU
1	A	308	VAL
1	A	361	CYS
1	A	455	LEU
1	A	489	TYR
1	A	509	ARG
1	A	551	VAL
1	A	587	ILE
1	A	869	MET
1	A	1023	ASN
1	B	118	LEU
1	B	135	PHE
1	B	141	LEU
1	B	236	THR
1	B	269	TYR
1	B	273	ARG
1	B	275	PHE
1	B	394	ASN
1	B	454	ARG
1	B	499	PRO
1	B	581	THR
1	B	586	ASP
1	B	868	GLU
1	B	878	LEU
1	B	934	ILE
1	B	957	GLN
1	B	974	SER
1	B	1006	THR
1	B	1094	VAL

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Mol	Chain	Res	Type
1	B	1111	GLU
1	B	1145	LEU
1	C	36	VAL
1	C	81	ASN
1	C	189	LEU
1	C	197	ILE
1	C	227	VAL
1	C	318	PHE
1	C	351	TYR
1	C	387	LEU
1	C	596	SER
1	C	662	CYS
1	C	664	ILE
1	C	726	ILE
1	C	901	GLN
1	C	902	MET
1	C	950	ASP
1	C	1040	VAL
1	C	1092	GLU
1	C	1137	VAL
1	C	1138	TYR
2	D	55	TRP
2	D	85	TYR
2	D	89	PHE
2	D	137	TRP
2	D	143	THR
2	D	186	ASN
2	D	202	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	137	ASN
1	A	188	ASN
1	A	196	ASN
1	A	370	ASN
1	A	409	GLN
1	A	414	GLN
1	A	439	ASN
1	A	536	ASN
1	A	580	GLN

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Mol	Chain	Res	Type
1	A	690	GLN
1	A	717	ASN
1	A	779	GLN
1	A	955	ASN
1	A	1058	HIS
1	A	1071	GLN
1	A	1119	ASN
1	B	122	ASN
1	B	125	ASN
1	B	146	HIS
1	B	437	ASN
1	B	498	GLN
1	B	536	ASN
1	B	544	ASN
1	B	607	GLN
1	B	710	ASN
1	B	926	GLN
1	B	949	GLN
1	B	953	ASN
1	B	954	GLN
1	B	969	ASN
1	B	1002	GLN
1	B	1005	GLN
1	B	1108	ASN
1	C	52	GLN
1	C	121	ASN
1	C	148	ASN
1	C	185	ASN
1	C	394	ASN
1	C	439	ASN
1	C	487	ASN
1	C	506	GLN
1	C	536	ASN
1	C	613	GLN
1	C	625	HIS
1	C	677	GLN
1	C	774	GLN
1	C	907	ASN
1	C	953	ASN
1	C	1083	HIS
1	C	1101	HIS
2	D	164	GLN

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Mol	Chain	Res	Type
2	D	173	ASN
2	D	175	ASN

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](#)

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.

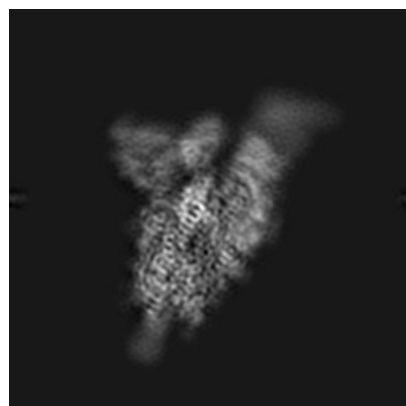
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64131. These allow visual inspection of the internal detail of the map and identification of artifacts.

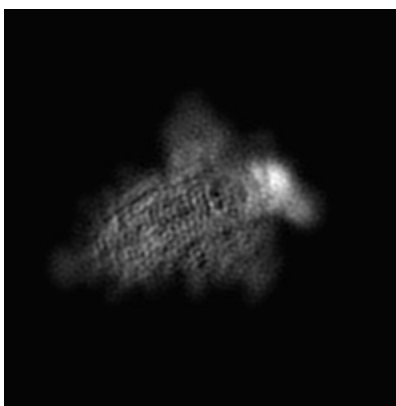
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

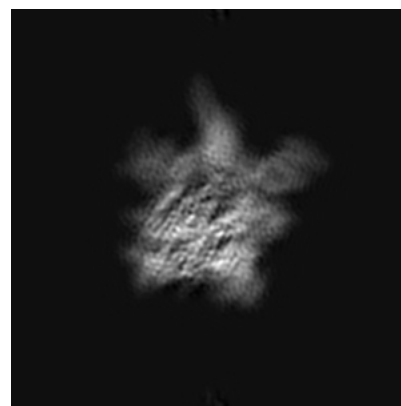
6.1.1 Primary map



X

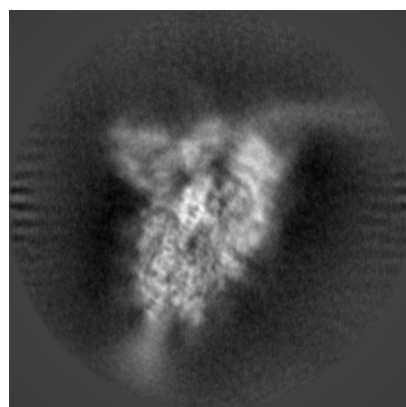


Y

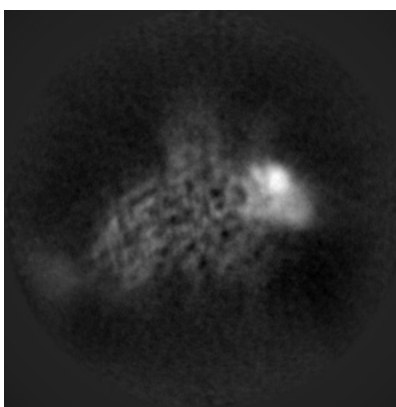


Z

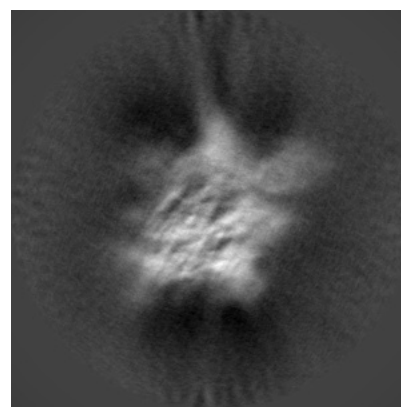
6.1.2 Raw map



X



Y

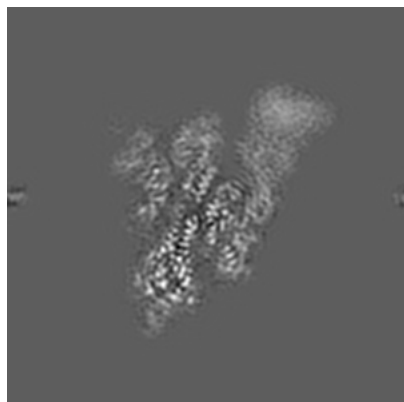


Z

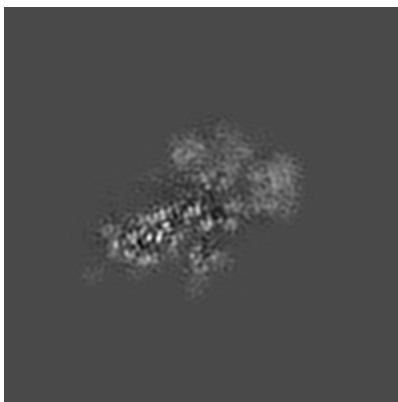
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

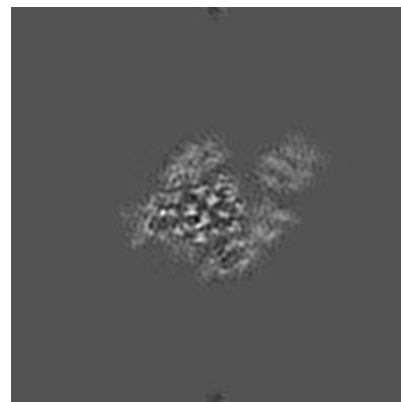
6.2.1 Primary map



X Index: 165

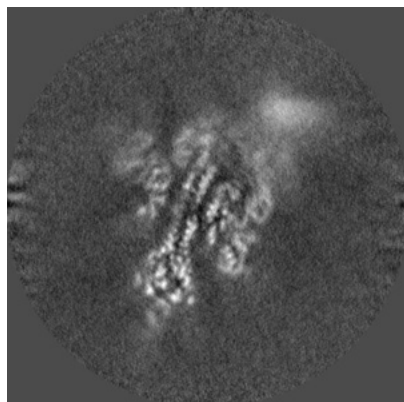


Y Index: 165

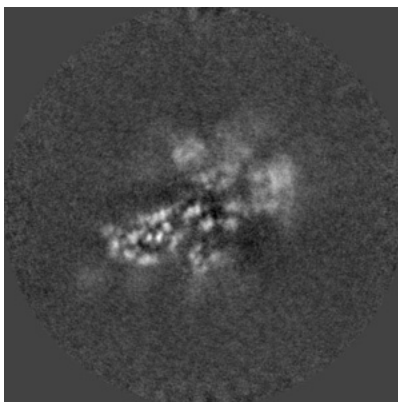


Z Index: 165

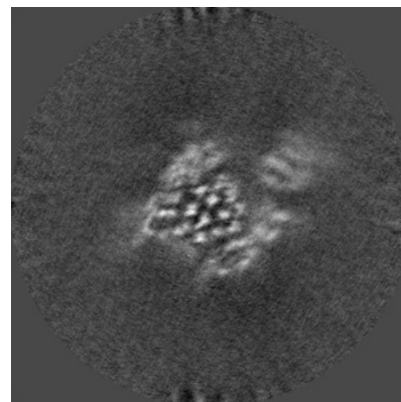
6.2.2 Raw map



X Index: 165



Y Index: 165

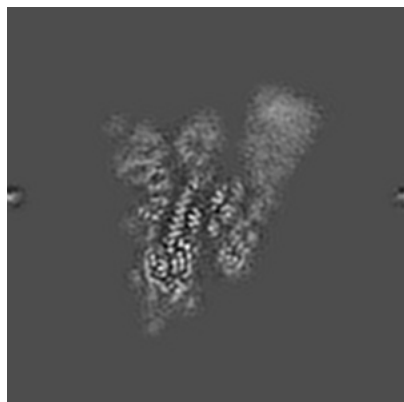


Z Index: 165

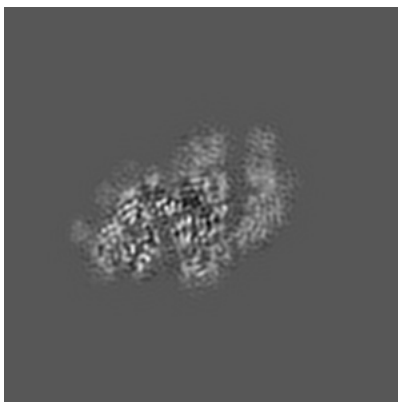
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

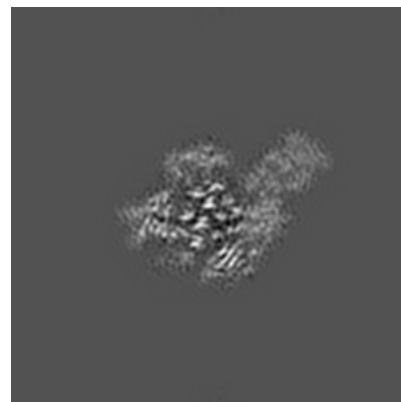
6.3.1 Primary map



X Index: 170

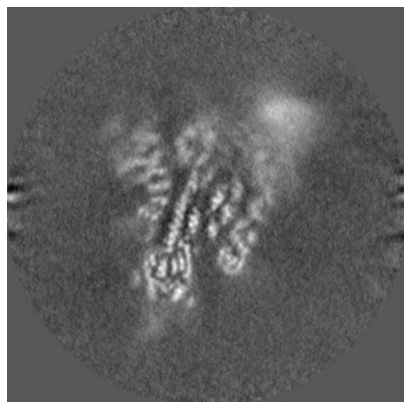


Y Index: 147

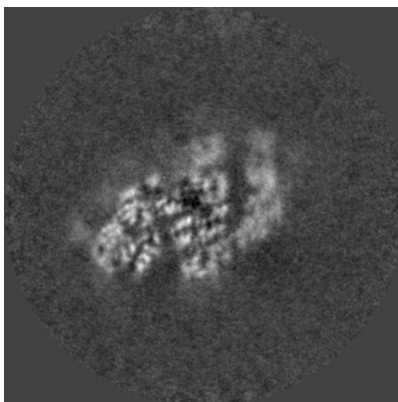


Z Index: 159

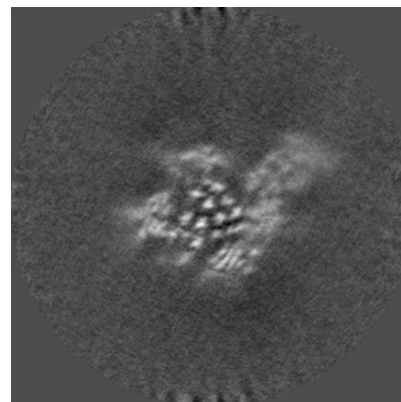
6.3.2 Raw map



X Index: 169



Y Index: 147

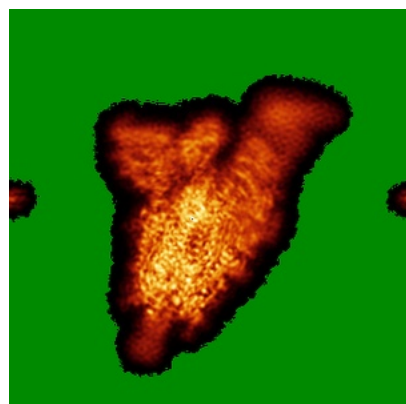


Z Index: 158

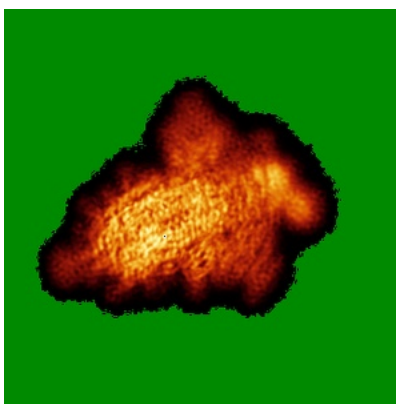
The images above show the largest variance slices of the map in three orthogonal directions.

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

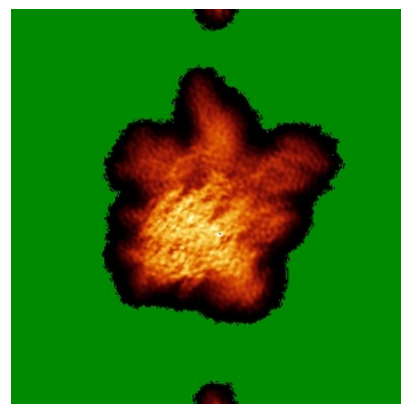
6.4.1 Primary map



X

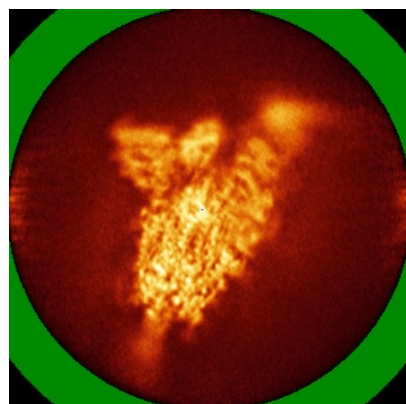


Y

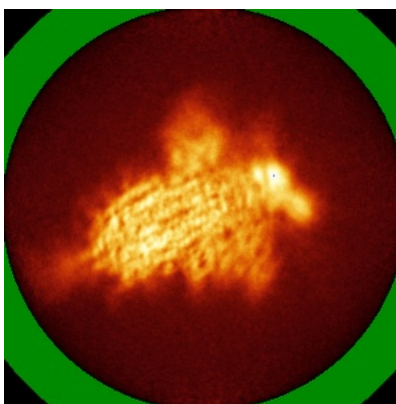


Z

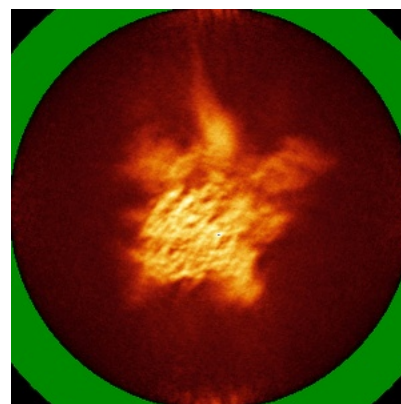
6.4.2 Raw map



X



Y

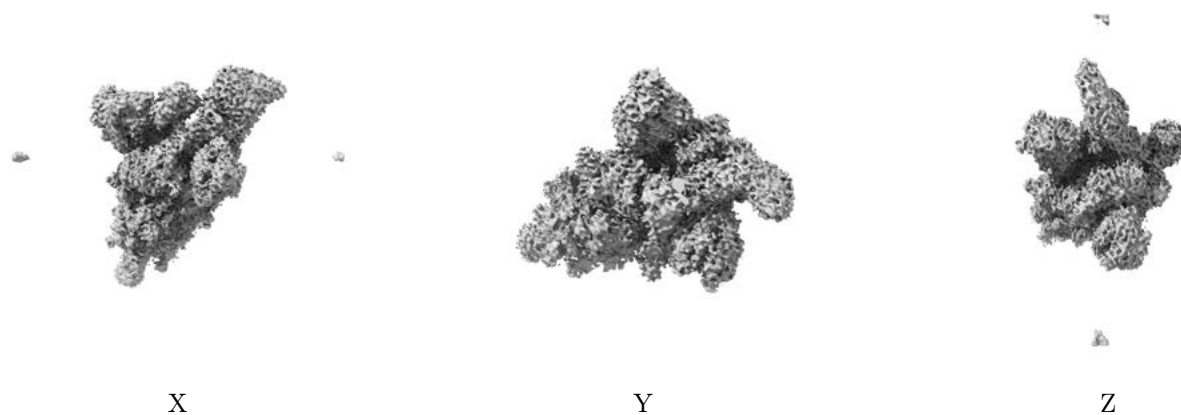


Z

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.

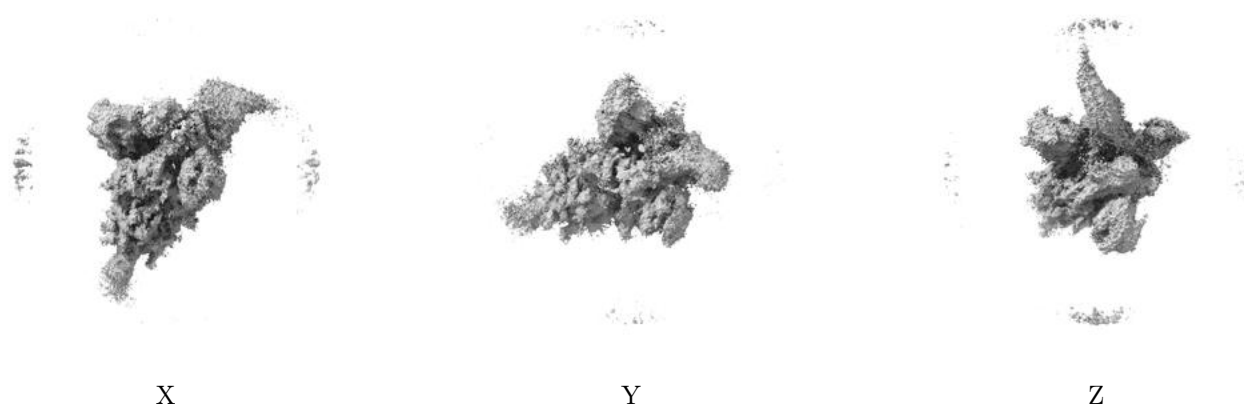
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.79. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

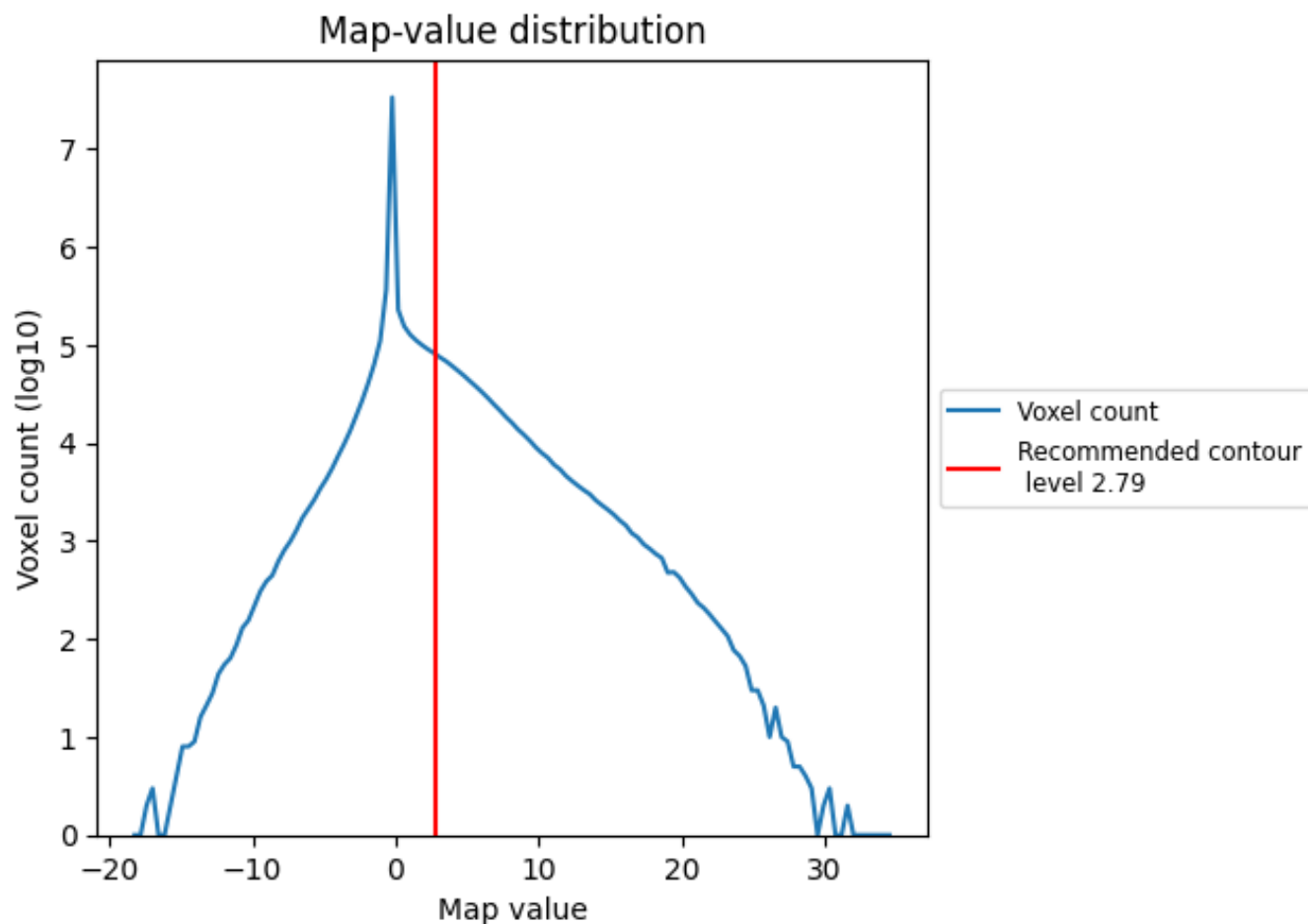
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

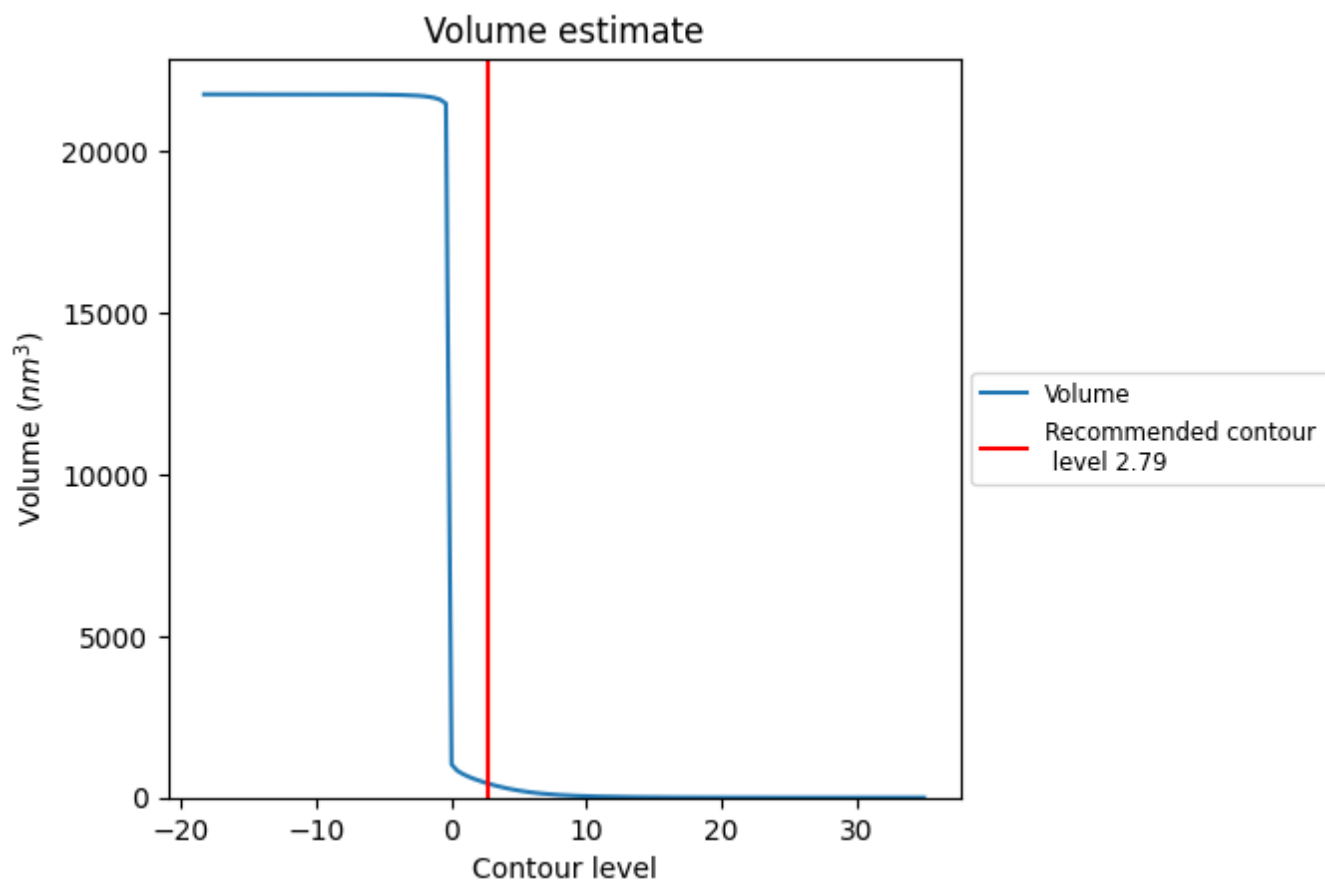
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

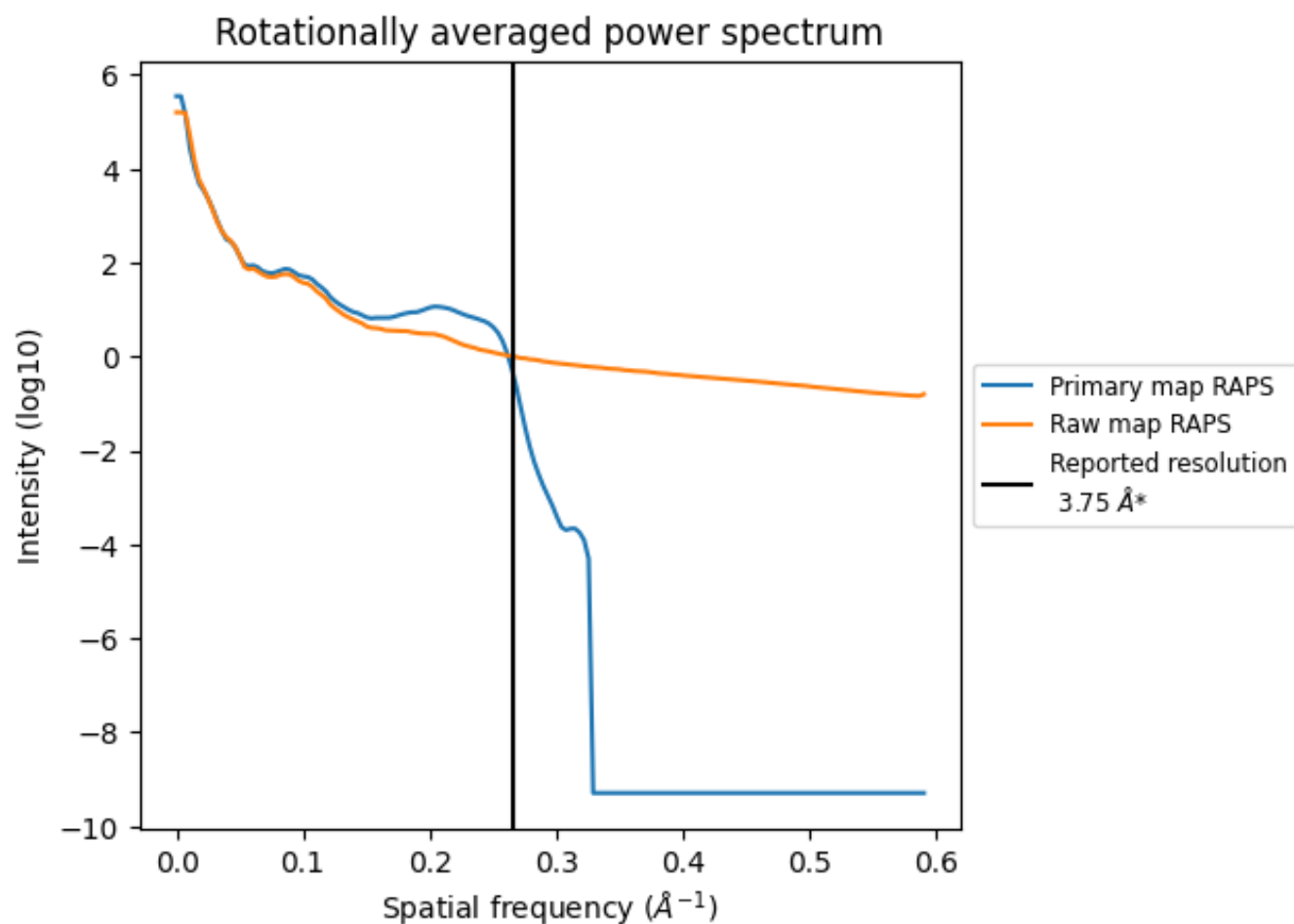
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 426 nm³; this corresponds to an approximate mass of 385 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 ⓘ

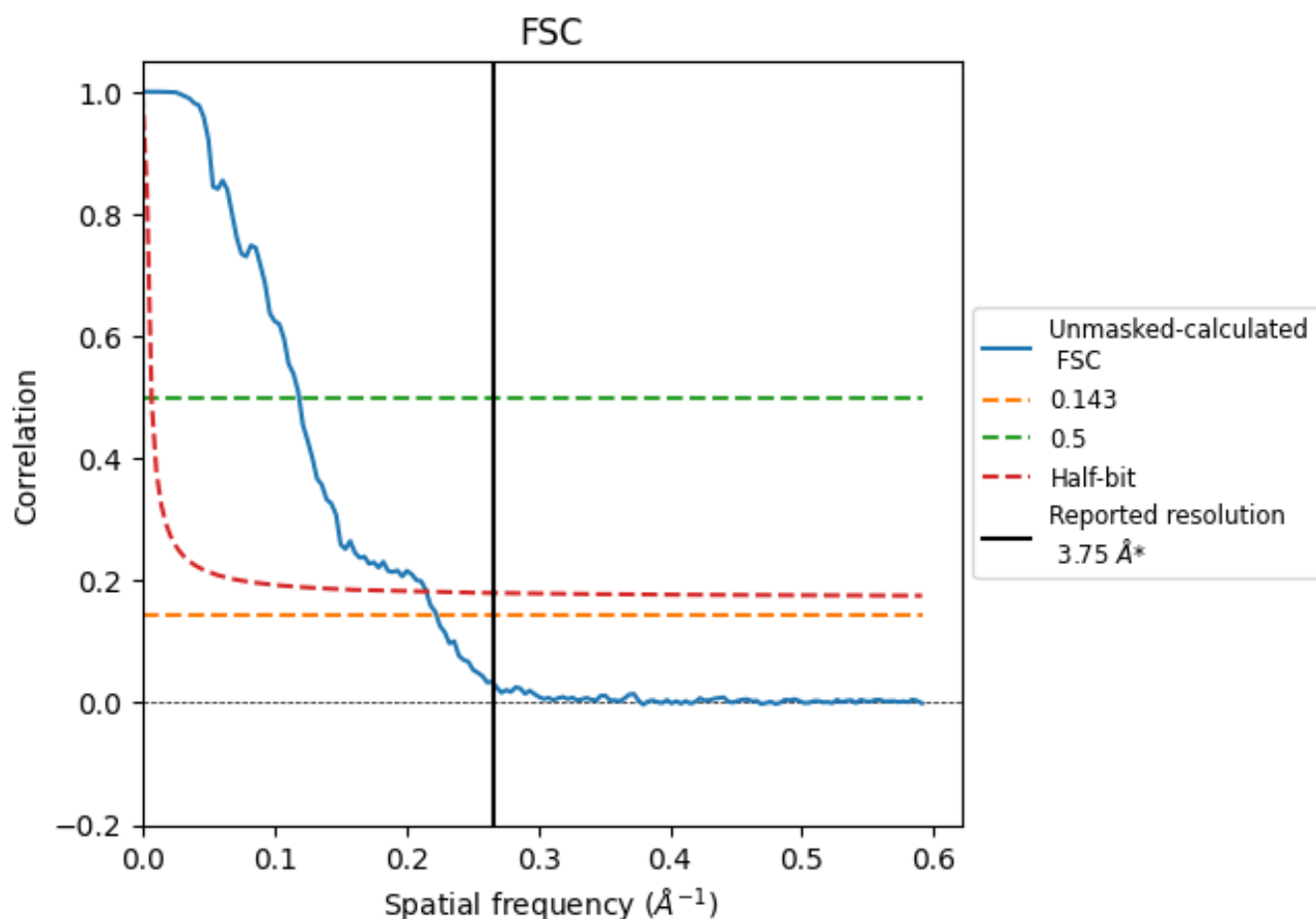


*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

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 0.267 Å⁻¹

8.2 Resolution estimates [i](#)

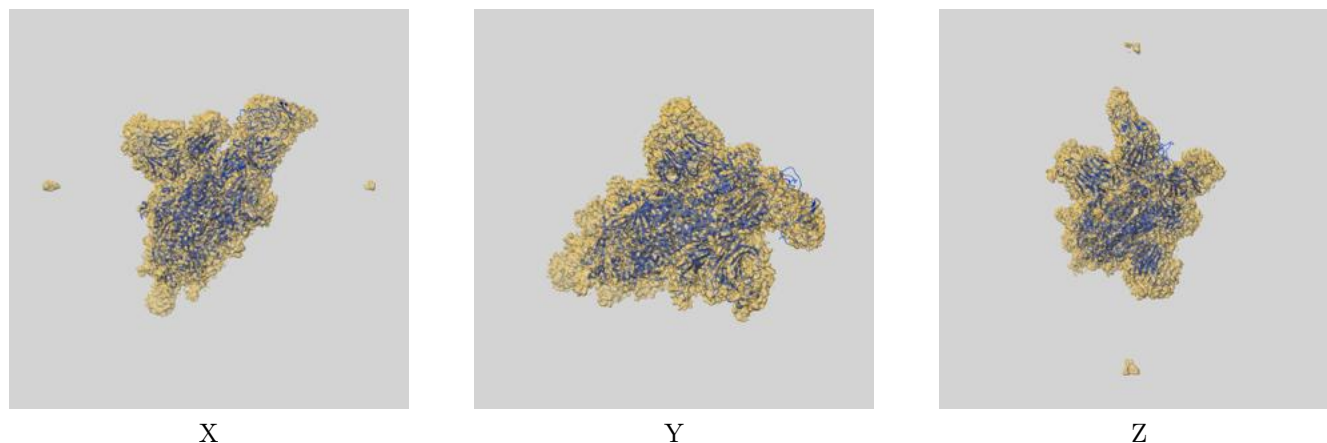
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.75	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.49	8.42	4.64

*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 4.49 differs from the reported value 3.75 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64131 and PDB model 9UG3. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 2.79 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](#)



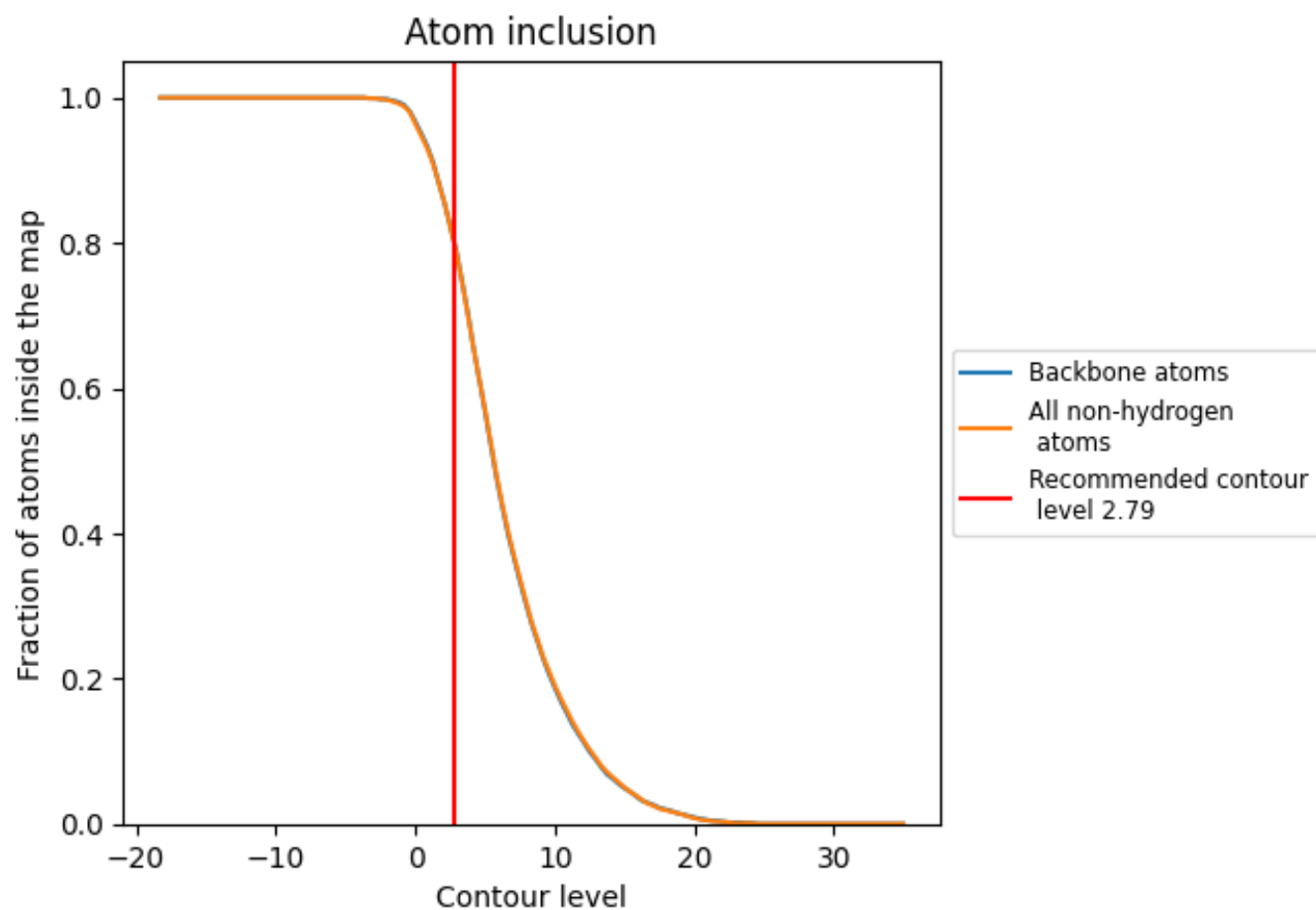
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.79).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (2.79) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8010	0.2250
A	0.8210	0.2090
B	0.8380	0.2570
C	0.8070	0.2440
D	0.5050	0.0060

