



Full wwPDB EM Validation Report ⓘ

Apr 29, 2025 – 01:40 pm BST

PDB ID : 9GOS / pdb_00009gos
EMDB ID : EMD-51499
Title : CryoEM structure of the native Chlamydomonas reinhardtii Flagella Membrane Glycoprotein 1B.
Authors : Nievergelt, A.P.; Hoepfner, L.M.; Matrino, F.; Scholz, M.; Foster, H.E.; Rodenfels, J.; von Appen, A.; Hippler, M.; Pigino, G.
Deposited on : 2024-09-06
Resolution : 3.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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<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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

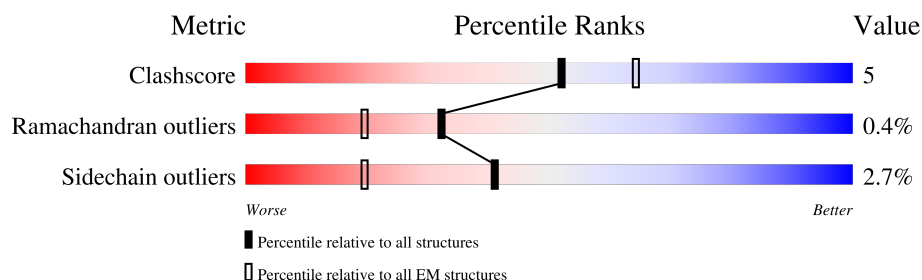
1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	4545	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 54175 atoms, of which 27330 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.

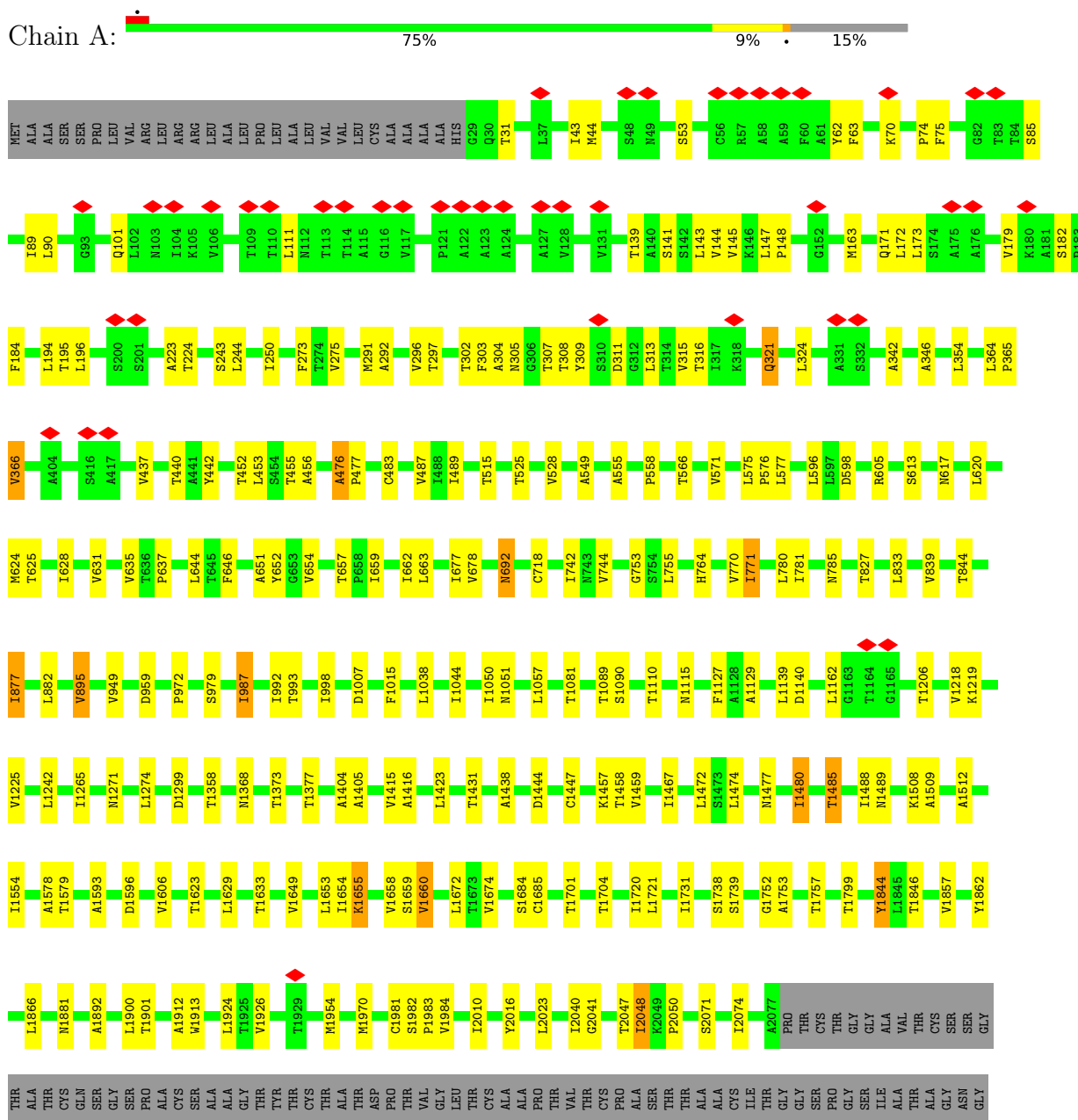
- Molecule 1 is a protein called Flagella Membrane Glycoprotein 1B.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	3878	Total	C	H	N	O	S	0	0
			54175	16804	27330	4408	5538	95		

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: Flagella Membrane Glycoprotein 1B



LYS	GLN	PRO	ILE	ASN	LYS	SER	R4059	A3924	L3605	P3336	T3006	T2773	S2420	ASN	CYS	PRO
LYS	SER	ALA	THR	ALA	ASP	PRO	N4060	N3925	V3606	N3337	S3007	T2773	T2439	CYS	THR	GLY
ASN	THR	PHE	ALA	VAL	THR	PRO	G4061	L3926	V3625	A3340	T3016	L2787	T2439	ILE	THR	CYS
THR	ILE	THR	GLN	GLY	PRO	SER	S4062	L3932	V3653	V3350	L3017	V2789	K2457	PHE	THR	ALA
ALA	THR	GLN	LEU	ALA	PRO	PRO	A4063	G3945	K3673	L3354	K3022	T2811	L2482	SER	THR	ALA
ALA	THR	GLN	ALA	VAL	THR	SER	A4064	A3946	D3674	V3377	M3023	L2812	S2496	GLY	THR	ALA
ALA	THR	GLN	GLN	THR	THR	THR	A4065	D3947	Q3675	V3378	Y3024	K2849	A2497	THR	GLY	ALA
ALA	THR	GLN	ALA	ASP	ALA	ALA	A4070	G3950	V3680	V3378	P3030	V2855	N2501	GLY	THR	THR
ALA	THR	GLN	THR	ASP	ASN	THR	C4071	A3951	S3698	L3381	L3033	V2855	R2502	LEU	SER	ALA
ALA	THR	GLN	LEU	THR	SER	SER	A4072	V3951	S3698	V3380	L3034	V2889	T2524	VAL	ASP	ALA
ALA	THR	GLN	ALA	VAL	ALA	ALA	V4073	L3952	T3707	V3390	L3034	V2889	T2524	VAL	ALA	GLY
ALA	THR	GLN	ALA	THR	THR	THR	S4074	A3953	L3708	C3420	A3035	V2874	N2541	THR	ALA	ALA
ALA	THR	GLN	VAL	THR	GLY	LEU	A4075	G3970	C3733	S3424	T3040	V2880	T2560	CYS	GLY	GLY
ALA	THR	GLN	LEU	THR	ALA	ALA	D4076	A3971	C3733	S3424	P3041	V2881	D2561	THR	THR	ILE
ALA	THR	GLN	ALA	THR	GLY	THR	G4077	D3972	V3749	L3430	V3049	T2882	S2601	GLY	GLY	SER
ALA	THR	GLN	ALA	THR	GLY	THR	L4078	D3972	C3754	N3452	V3052	G2893	T2607	THR	GLY	TYR
ALA	THR	GLN	ALA	THR	GLY	THR	L4082	T3975	L3765	V3461	L3075	T2904	T2607	CYS	GLY	SER
ALA	THR	GLN	ALA	THR	GLY	THR	A4086	A3977	L3765	V3461	L3075	T2904	T2607	CYS	GLY	SER
ALA	THR	GLN	ALA	THR	GLY	THR	A4087	V3978	V3777	A3464	S3092	Q2906	L2617	SER	PRO	THR
ALA	THR	GLN	ALA	THR	GLY	THR	Y4088	A3983	V3777	A3464	S3092	Q2906	L2617	SER	PRO	THR
ALA	THR	GLN	ALA	THR	GLY	THR	K4089	S3984	Y3799	T3465	L3099	L2907	T2624	GLY	CYS	THR
ALA	THR	GLN	ALA	THR	GLY	THR	P4090	F3985	Y3799	T3465	L3099	L2907	T2624	GLY	CYS	THR
ALA	THR	GLN	ALA	THR	GLY	THR	M4091	V3986	D3604	N3488	L3109	D2909	L2627	THR	THR	THR
ALA	THR	GLN	ALA	THR	GLY	THR	A4092	G3987	D3604	N3488	L3109	D2909	L2627	THR	THR	THR
ALA	THR	GLN	ALA	THR	GLY	THR	A4096	V4016	V3811	V3493	S3136	T2919	V2639	ALA	ALA	ALA
ALA	THR	GLN	ALA	THR	GLY	THR	D4097	L4017	A3812	T3497	S3136	T2919	V2639	ALA	ALA	ALA
ALA	THR	GLN	ALA	THR	GLY	THR	V4098	V4018	T3813	T3497	I3145	P2930	T2666	ALA	ALA	ALA
ALA	THR	GLN	ALA	THR	GLY	THR	A4099	V4019	S3620	L3498	V3147	P2930	T2666	ALA	ALA	ALA
ALA	THR	GLN	ALA	THR	GLY	THR	V4100	P4020	P3827	A3501	L3226	V2935	F2678	VAL	GLY	GLY
ALA	THR	GLN	ALA	THR	GLY	THR	S4101	A4029	I3832	V3504	A3227	A2936	V2696	SER	SER	SER
ALA	THR	GLN	ALA	THR	GLY	THR	L4105	A4030	I3832	V3505	A3228	A2936	V2696	ALA	ALA	ALA
ALA	THR	GLN	ALA	THR	GLY	THR	R4106	T4031	I3845	V3505	A3228	A2936	V2696	ALA	ALA	ALA
ALA	THR	GLN	ALA	THR	GLY	THR	A4107	T4032	C3862	T3525	R3294	L2949	L2717	ASN	ASN	ASN
ALA	THR	GLN	ALA	THR	GLY	THR	A4114	A4033	M3863	P3526	T3295	L2949	L2717	ASN	ASN	ASN
ALA	THR	GLN	ALA	THR	GLY	THR	Y4115	V4041	L3864	T3527	I3296	T2960	K2719	THR	THR	THR
ALA	THR	GLN	ALA	THR	GLY	THR	V4116	V4042	T3528	T3528	S3297	V2973	A2723	ALA	ASP	ASP
ALA	THR	GLN	ALA	THR	GLY	THR	P4117	L4043	S3559	S3559	S3298	K2974	T2726	THR	SER	SER
ALA	THR	GLN	ALA	THR	GLY	THR	T4124	T4046	T3886	T3587	D3307	V2977	T2726	THR	SER	SER
ALA	THR	GLN	ALA	THR	GLY	THR	V4126	A4047	V3887	T3587	D3307	V2977	T2726	THR	SER	SER
ALA	THR	GLN	ALA	THR	GLY	THR	A4127	A4048	V3887	T3587	D3307	V2977	T2726	THR	SER	SER
ALA	THR	GLN	ALA	THR	GLY	THR	S4128	A4049	R3897	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	P4129	D4050	R3897	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	P4129	C4051	R3897	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4052	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4053	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4054	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4055	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4056	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4057	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4058	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4059	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4060	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4061	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4062	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4063	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4064	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4065	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4066	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4067	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4068	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4069	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4070	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4071	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4072	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4073	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4074	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4075	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4076	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4077	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4078	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4079	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4080	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4081	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4082	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4083	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4084	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4085	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4086	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4087	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4088	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4089	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4090	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4091	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4092	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4093	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4094	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4095	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4096	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4097	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4098	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4099	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4100	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4101	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY	THR	PRO	A4102	V3887	A3600	L3317	Y2981	P2741	LYS	LYS	LYS
ALA	THR	GLN	ALA	THR	GLY											

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	583765	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 ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.208	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	488.96, 488.96, 488.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.955, 0.955, 0.955	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.15	0/27240	0.35	0/37509

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2640	THR	Peptide
1	A	2893	GLY	Peptide

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	26845	27330	27329	283	0
All	All	26845	27330	27329	283	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 5.

All (283) 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:987:ILE:HD12	1:A:1050:ILE:HD12	1.59	0.84
1:A:839:VAL:HG13	1:A:844:THR:HG21	1.61	0.82
1:A:1984:VAL:HG21	1:A:2010:ILE:HD13	1.68	0.76
1:A:3294:ARG:NH2	1:A:3317:LEU:HD13	2.01	0.75
1:A:2935:VAL:HG11	1:A:2949:LEU:HD22	1.67	0.75
1:A:525:THR:HG22	1:A:555:ALA:HA	1.69	0.73
1:A:3022:LYS:NZ	1:A:3033:ILE:HD12	2.05	0.71
1:A:1926:VAL:O	1:A:1926:VAL:HG13	1.92	0.70
1:A:2415:ALA:HB1	1:A:2457:LYS:HD3	1.75	0.69
1:A:3034:LEU:HD11	1:A:3075:LEU:HD12	1.74	0.68
1:A:1720:ILE:HB	1:A:1731:ILE:HD12	1.76	0.68
1:A:1127:PHE:CD1	1:A:1139:LEU:HD11	2.29	0.67
1:A:2373:LEU:HD22	1:A:2383:TYR:CE1	2.31	0.66
1:A:3390:VAL:HG11	1:A:3424:SER:HA	1.77	0.65
1:A:1377:THR:OG1	1:A:1404:ALA:HB1	1.96	0.65
1:A:1225:VAL:CG1	1:A:1274:LEU:HD11	2.27	0.64
1:A:3708:LEU:HD21	1:A:3827:PRO:HB2	1.78	0.64
1:A:1225:VAL:HG13	1:A:1274:LEU:HD11	1.81	0.62
1:A:617:ASN:OD1	1:A:617:ASN:O	2.17	0.62
1:A:2881:VAL:O	1:A:2881:VAL:HG13	2.00	0.62
1:A:959:ASP:O	1:A:959:ASP:OD2	2.17	0.61
1:A:163:MET:HE2	1:A:182:SER:OG	2.01	0.61
1:A:780:LEU:HD12	1:A:785:ASN:O	2.01	0.61
1:A:184:PHE:CD2	1:A:196:LEU:HD23	2.35	0.61
1:A:2339:ALA:HB1	1:A:2340:PRO:HD3	1.83	0.61
1:A:483:CYS:O	1:A:487:VAL:HG22	2.00	0.61
1:A:476:ALA:HB3	1:A:477:PRO:CD	2.31	0.60
1:A:3294:ARG:HH21	1:A:3317:LEU:HD13	1.66	0.60
1:A:637:PRO:O	1:A:654:VAL:HG22	2.02	0.60
1:A:987:ILE:CD1	1:A:1050:ILE:HD12	2.31	0.60
1:A:3022:LYS:HZ2	1:A:3033:ILE:HD12	1.65	0.60
1:A:987:ILE:HD12	1:A:1050:ILE:CD1	2.32	0.60
1:A:163:MET:HE1	1:A:184:PHE:HB2	1.83	0.58
1:A:755:LEU:O	1:A:755:LEU:HD23	2.03	0.58
1:A:476:ALA:HB3	1:A:477:PRO:HD2	1.86	0.58
1:A:3464:ALA:O	1:A:3465:THR:HG22	2.04	0.58
1:A:365:PRO:O	1:A:366:VAL:HG22	2.05	0.57
1:A:2373:LEU:HD23	1:A:2374:LYS:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1954:MET:HE1	1:A:2023:LEU:CB	2.35	0.57
1:A:644:LEU:HD22	1:A:652:TYR:CE1	2.39	0.56
1:A:2541:ASN:O	1:A:2617:LEU:HD12	2.05	0.56
1:A:3527:THR:HG22	1:A:3528:THR:H	1.71	0.56
1:A:173:LEU:HG	1:A:179:VAL:HG22	1.86	0.56
1:A:195:THR:C	1:A:196:LEU:HD12	2.31	0.56
1:A:2865:VAL:HG13	1:A:2865:VAL:O	2.05	0.56
1:A:987:ILE:HD13	1:A:987:ILE:H	1.71	0.56
1:A:172:LEU:C	1:A:173:LEU:HD12	2.31	0.55
1:A:302:THR:HG22	1:A:303:PHE:H	1.70	0.55
1:A:1862:TYR:HB2	1:A:1926:VAL:HG21	1.87	0.55
1:A:1431:THR:HG21	1:A:1438:ALA:HB1	1.87	0.55
1:A:2339:ALA:CB	1:A:2340:PRO:CD	2.85	0.55
1:A:476:ALA:CB	1:A:477:PRO:CD	2.85	0.54
1:A:625:THR:O	1:A:628:ILE:HG22	2.07	0.54
1:A:437:VAL:HG21	1:A:442:TYR:OH	2.07	0.54
1:A:4126:VAL:HB	1:A:4127:PRO:HD3	1.88	0.54
1:A:1926:VAL:O	1:A:1926:VAL:CG1	2.54	0.54
1:A:3862:CYS:SG	1:A:3873:VAL:HG22	2.47	0.54
1:A:1857:VAL:HG22	1:A:1901:THR:HG22	1.89	0.53
1:A:2339:ALA:HB1	1:A:2340:PRO:CD	2.38	0.53
1:A:1857:VAL:HG11	1:A:1970:MET:HE1	1.90	0.53
1:A:194:LEU:HD21	1:A:196:LEU:HD13	1.89	0.53
1:A:598:ASP:OD1	1:A:598:ASP:C	2.52	0.53
1:A:2880:VAL:HG12	1:A:2881:VAL:H	1.74	0.52
1:A:1044:ILE:HD11	1:A:1162:LEU:HG	1.90	0.52
1:A:1115:ASN:OD1	1:A:1127:PHE:HB2	2.09	0.52
1:A:3832:ILE:HG12	1:A:3864:LEU:HD22	1.91	0.52
1:A:2881:VAL:O	1:A:2882:ILE:C	2.53	0.52
1:A:173:LEU:HD12	1:A:173:LEU:N	2.25	0.52
1:A:307:THR:HG21	1:A:437:VAL:CG1	2.40	0.52
1:A:1485:THR:HG23	1:A:1512:ALA:HB1	1.92	0.52
1:A:184:PHE:HD2	1:A:196:LEU:HB3	1.75	0.52
1:A:1862:TYR:CB	1:A:1926:VAL:HG21	2.40	0.52
1:A:1127:PHE:CE1	1:A:1139:LEU:HD11	2.45	0.52
1:A:1225:VAL:HG13	1:A:1274:LEU:CD1	2.38	0.52
1:A:2050:PRO:O	1:A:2384:THR:HG22	2.10	0.51
1:A:4091:MET:HG3	1:A:4091:MET:O	2.09	0.51
1:A:1508:LYS:HG2	1:A:1509:ALA:H	1.75	0.51
1:A:1654:ILE:HG22	1:A:1655:LYS:H	1.76	0.51
1:A:1954:MET:HE1	1:A:2023:LEU:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3673:LYS:HD2	1:A:3674:ASP:OD2	2.11	0.50
1:A:833:LEU:HD21	1:A:839:VAL:HG23	1.94	0.50
1:A:1474:LEU:C	1:A:1474:LEU:HD12	2.37	0.50
1:A:1050:ILE:HG22	1:A:1051:ASN:N	2.27	0.50
1:A:143:LEU:HD22	1:A:145:VAL:HG23	1.93	0.49
1:A:3707:THR:HG22	1:A:3708:LEU:H	1.77	0.49
1:A:250:ILE:HG23	1:A:304:ALA:HA	1.94	0.49
1:A:827:THR:HG22	1:A:827:THR:O	2.12	0.49
1:A:2935:VAL:HG11	1:A:2949:LEU:CD2	2.40	0.49
1:A:839:VAL:CG1	1:A:844:THR:HG21	2.38	0.49
1:A:1629:LEU:HB3	1:A:1731:ILE:HG23	1.93	0.49
1:A:3329:LEU:O	1:A:3350:VAL:HG22	2.13	0.49
1:A:147:LEU:HD12	1:A:148:PRO:HD2	1.93	0.49
1:A:3251:PRO:HG2	1:A:3340:ALA:HB2	1.95	0.49
1:A:1658:VAL:HG23	1:A:1659:SER:N	2.28	0.49
1:A:2982:GLU:O	1:A:2983:LEU:C	2.56	0.49
1:A:1089:THR:HG22	1:A:1090:SER:N	2.27	0.48
1:A:3052:VAL:HG22	1:A:3099:ILE:HD12	1.95	0.48
1:A:3307:ASP:OD2	1:A:3307:ASP:C	2.55	0.48
1:A:3024:TYR:HB3	1:A:3030:PRO:HB3	1.96	0.48
1:A:3708:LEU:HD23	1:A:3708:LEU:O	2.13	0.48
1:A:596:LEU:HD23	1:A:605:ARG:HG3	1.94	0.48
1:A:1485:THR:CG2	1:A:1512:ALA:HB1	2.44	0.48
1:A:307:THR:HG21	1:A:437:VAL:HG12	1.95	0.48
1:A:646:PHE:C	1:A:646:PHE:CD1	2.91	0.48
1:A:3597:ILE:HG23	1:A:3698:SER:O	2.14	0.48
1:A:2373:LEU:HD22	1:A:2383:TYR:CD1	2.49	0.48
1:A:195:THR:O	1:A:196:LEU:HD12	2.14	0.48
1:A:993:THR:HG22	1:A:1081:THR:CG2	2.43	0.48
1:A:624:MET:HE3	1:A:628:ILE:HG23	1.96	0.48
1:A:2326:THR:OG1	1:A:2348:ALA:HB3	2.14	0.48
1:A:2338:THR:HA	1:A:2341:TYR:CE2	2.49	0.48
1:A:2908:ILE:HD11	1:A:2973:TRP:CD2	2.48	0.48
1:A:3296:ILE:HG22	1:A:3297:SER:N	2.29	0.48
1:A:3708:LEU:HD21	1:A:3827:PRO:CB	2.44	0.48
1:A:1457:LYS:O	1:A:1458:THR:HB	2.14	0.47
1:A:663:LEU:HD13	1:A:744:VAL:CG2	2.45	0.47
1:A:3497:THR:C	1:A:3498:LEU:HD12	2.39	0.47
1:A:576:PRO:O	1:A:577:LEU:HD23	2.14	0.47
1:A:3335:THR:HB	1:A:3336:PRO:HD3	1.95	0.47
1:A:437:VAL:HG21	1:A:442:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:VAL:O	1:A:549:ALA:HB2	2.15	0.47
1:A:4096:VAL:HG21	1:A:4124:ILE:HD12	1.96	0.47
1:A:2624:THR:O	1:A:2624:THR:HG22	2.15	0.47
1:A:1954:MET:HE1	1:A:2023:LEU:HB3	1.96	0.47
1:A:2496:SER:O	1:A:2497:ALA:HB3	2.14	0.47
1:A:3381:ILE:O	1:A:3390:VAL:HA	2.15	0.47
1:A:2418:VAL:HB	1:A:2419:PRO:HD2	1.97	0.46
1:A:2880:VAL:HG12	1:A:2881:VAL:N	2.29	0.46
1:A:992:ILE:HG23	1:A:992:ILE:O	2.16	0.46
1:A:1218:VAL:HG12	1:A:1219:LYS:H	1.80	0.46
1:A:3326:THR:HG22	1:A:3354:LEU:O	2.15	0.46
1:A:3862:CYS:SG	1:A:3873:VAL:HG13	2.55	0.46
1:A:3559:SER:HB2	1:A:3680:VAL:HG12	1.97	0.46
1:A:273:PHE:O	1:A:275:VAL:HG23	2.16	0.46
1:A:305:ASN:O	1:A:308:THR:N	2.48	0.46
1:A:882:LEU:CD2	1:A:895:VAL:HG12	2.46	0.46
1:A:3952:LEU:HD13	1:A:3978:VAL:HG22	1.98	0.46
1:A:307:THR:O	1:A:311:ASP:HA	2.15	0.46
1:A:2337:PHE:CE1	1:A:2340:PRO:O	2.69	0.46
1:A:992:ILE:HD12	1:A:998:ILE:CG1	2.45	0.45
1:A:3452:ASN:OD1	1:A:3461:TYR:HB2	2.16	0.45
1:A:223:ALA:O	1:A:224:THR:HG23	2.16	0.45
1:A:453:LEU:HD11	1:A:528:VAL:HG23	1.98	0.45
1:A:3504:VAL:HG23	1:A:3505:VAL:O	2.17	0.45
1:A:275:VAL:HG12	1:A:313:LEU:CD2	2.47	0.45
1:A:302:THR:HG22	1:A:303:PHE:N	2.31	0.45
1:A:1299:ASP:OD2	1:A:1508:LYS:NZ	2.50	0.45
1:A:1982:SER:N	1:A:1983:PRO:CD	2.79	0.45
1:A:3377:VAL:HG22	1:A:3378:THR:N	2.31	0.45
1:A:677:ILE:HG22	1:A:678:VAL:N	2.32	0.45
1:A:2326:THR:O	1:A:2347:LEU:HA	2.16	0.45
1:A:2811:THR:HG22	1:A:2812:LEU:H	1.81	0.45
1:A:3016:THR:C	1:A:3017:LEU:HD12	2.41	0.45
1:A:3897:ARG:HA	1:A:3906:SER:HA	1.98	0.45
1:A:143:LEU:HD23	1:A:144:VAL:N	2.32	0.45
1:A:2936:ALA:O	1:A:2937:SER:CB	2.65	0.45
1:A:3845:ILE:HG22	1:A:3887:VAL:HG13	1.99	0.45
1:A:3033:ILE:HG12	1:A:3034:LEU:H	1.82	0.45
1:A:307:THR:O	1:A:366:VAL:HG21	2.17	0.44
1:A:3820:SER:HA	1:A:3875:LEU:HD12	2.00	0.44
1:A:184:PHE:CE2	1:A:196:LEU:HD23	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1377:THR:HA	1:A:1405:ALA:O	2.17	0.44
1:A:3625:VAL:HG22	1:A:3675:GLN:OE1	2.18	0.44
1:A:571:VAL:HG21	1:A:659:ILE:HD12	1.98	0.44
1:A:489:ILE:HA	1:A:525:THR:O	2.18	0.44
1:A:558:PRO:CB	1:A:577:LEU:HD21	2.48	0.44
1:A:1654:ILE:HD11	1:A:1721:LEU:HG	1.99	0.44
1:A:1274:LEU:N	1:A:1274:LEU:HD12	2.33	0.44
1:A:2071:SER:HB3	1:A:2373:LEU:HD21	2.00	0.44
1:A:2074:ILE:HG23	1:A:2305:ASP:O	2.18	0.44
1:A:3023:MET:HE1	1:A:3041:PRO:HB3	2.00	0.44
1:A:3708:LEU:HD23	1:A:3708:LEU:C	2.43	0.44
1:A:53:SER:OG	1:A:111:LEU:HD12	2.17	0.44
1:A:1480:ILE:HD13	1:A:1480:ILE:H	1.83	0.44
1:A:1593:ALA:O	1:A:1596:ASP:OD2	2.36	0.44
1:A:2560:THR:HG22	1:A:2561:ASP:N	2.33	0.44
1:A:291:MET:HE3	1:A:292:ALA:O	2.18	0.43
1:A:3493:VAL:O	1:A:3493:VAL:CG1	2.66	0.43
1:A:3680:VAL:HG12	1:A:3680:VAL:O	2.16	0.43
1:A:882:LEU:HD22	1:A:895:VAL:HG12	1.99	0.43
1:A:2752:THR:O	1:A:2752:THR:CG2	2.66	0.43
1:A:770:VAL:O	1:A:771:ILE:HB	2.18	0.43
1:A:2997:VAL:HG23	1:A:2997:VAL:O	2.18	0.43
1:A:3487:ILE:HD11	1:A:3585:ALA:O	2.18	0.43
1:A:4096:VAL:CG2	1:A:4124:ILE:HD12	2.49	0.43
1:A:43:ILE:HG22	1:A:44:MET:N	2.32	0.43
1:A:1015:PHE:CE2	1:A:1057:LEU:HD22	2.53	0.43
1:A:1467:ILE:CG1	1:A:1472:LEU:HD13	2.48	0.43
1:A:1488:ILE:HG22	1:A:1489:ASN:N	2.34	0.43
1:A:2337:PHE:O	1:A:2338:THR:OG1	2.33	0.43
1:A:2723:ALA:HB3	1:A:2726:THR:HB	2.00	0.43
1:A:244:LEU:HG	1:A:304:ALA:HB1	2.01	0.43
1:A:781:ILE:HD12	1:A:972:PRO:HG2	1.99	0.43
1:A:1457:LYS:O	1:A:1477:ASN:CG	2.62	0.43
1:A:2678:PHE:CE1	1:A:2709:VAL:HG22	2.54	0.43
1:A:2930:PRO:HD3	1:A:2960:THR:O	2.17	0.43
1:A:4126:VAL:HB	1:A:4127:PRO:CD	2.49	0.43
1:A:1127:PHE:CE1	1:A:1139:LEU:CD1	3.02	0.43
1:A:1274:LEU:HD12	1:A:1274:LEU:H	1.84	0.43
1:A:1912:ALA:O	1:A:1913:TRP:HB2	2.19	0.43
1:A:2909:ASP:CG	1:A:2910:SER:N	2.77	0.43
1:A:1129:ALA:O	1:A:1139:LEU:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2408:LEU:HD23	1:A:2409:GLN:H	1.84	0.43
1:A:2908:ILE:HD11	1:A:2973:TRP:CE3	2.54	0.43
1:A:3006:THR:HG22	1:A:3007:SER:N	2.34	0.43
1:A:2040:ILE:HG22	1:A:2041:GLY:N	2.33	0.43
1:A:2747:TYR:CE1	1:A:2755:ALA:HB3	2.54	0.43
1:A:3049:VAL:CG1	1:A:3109:LEU:HD13	2.49	0.43
1:A:3146:ILE:CG2	1:A:3147:VAL:N	2.82	0.42
1:A:184:PHE:CD1	1:A:184:PHE:N	2.87	0.42
1:A:662:ILE:HG22	1:A:764:HIS:HB2	2.01	0.42
1:A:1415:VAL:HG12	1:A:1415:VAL:O	2.19	0.42
1:A:1416:ALA:HB3	1:A:1423:LEU:O	2.18	0.42
1:A:1892:ALA:O	1:A:1900:LEU:HD12	2.19	0.42
1:A:354:LEU:O	1:A:452:THR:HG22	2.19	0.42
1:A:839:VAL:HG11	1:A:877:ILE:HG21	2.01	0.42
1:A:1458:THR:HG22	1:A:1459:VAL:N	2.34	0.42
1:A:1866:LEU:HD13	1:A:1924:LEU:HD23	2.00	0.42
1:A:184:PHE:CD2	1:A:196:LEU:HB3	2.54	0.42
1:A:2908:ILE:CG2	1:A:2982:GLU:HB3	2.50	0.42
1:A:3033:ILE:HG12	1:A:3034:LEU:N	2.35	0.42
1:A:307:THR:HG22	1:A:311:ASP:O	2.20	0.42
1:A:1139:LEU:HG	1:A:1140:ASP:N	2.35	0.42
1:A:3600:ALA:HB3	1:A:3603:THR:HB	2.00	0.42
1:A:455:THR:HG22	1:A:456:ALA:H	1.85	0.42
1:A:644:LEU:C	1:A:644:LEU:HD23	2.45	0.42
1:A:2047:THR:HG22	1:A:2048:ILE:N	2.34	0.42
1:A:74:PRO:O	1:A:90:LEU:HD23	2.19	0.42
1:A:742:ILE:O	1:A:742:ILE:HG23	2.20	0.42
1:A:1752:GLY:O	1:A:1753:ALA:HB3	2.19	0.42
1:A:3924:ALA:HB3	1:A:4016:VAL:HG11	2.02	0.42
1:A:316:THR:HB	1:A:342:ALA:HA	2.02	0.42
1:A:1444:ASP:OD2	1:A:1444:ASP:C	2.63	0.42
1:A:2607:THR:HG23	1:A:2627:LEU:HD21	2.01	0.42
1:A:3377:VAL:HG22	1:A:3378:THR:H	1.84	0.42
1:A:3733:CYS:SG	1:A:3765:LEU:HD23	2.60	0.42
1:A:1578:ALA:C	1:A:1579:THR:HG1	2.26	0.41
1:A:2719:LYS:HB3	1:A:2727:LEU:HB3	2.02	0.41
1:A:2983:LEU:O	1:A:2984:SER:HB3	2.19	0.41
1:A:2906:GLN:HA	1:A:2940:ILE:HD12	2.02	0.41
1:A:3777:VAL:HG11	1:A:3804:ASP:OD1	2.20	0.41
1:A:3926:LEU:HB2	1:A:4018:VAL:HG12	2.02	0.41
1:A:780:LEU:HB2	1:A:877:ILE:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:SER:O	1:A:620:LEU:HD12	2.20	0.41
1:A:3606:VAL:HG22	1:A:3653:VAL:O	2.20	0.41
1:A:171:GLN:CG	1:A:173:LEU:HD11	2.50	0.41
1:A:3226:LEU:C	1:A:3226:LEU:HD12	2.46	0.41
1:A:3597:ILE:O	1:A:3604:VAL:HA	2.21	0.41
1:A:31:THR:HG23	1:A:31:THR:O	2.21	0.41
1:A:44:MET:SD	1:A:85:SER:HB3	2.61	0.41
1:A:75:PHE:HA	1:A:89:ILE:O	2.21	0.41
1:A:631:VAL:HG22	1:A:753:GLY:O	2.21	0.41
1:A:1467:ILE:HG13	1:A:1472:LEU:HD13	2.02	0.41
1:A:2974:LYS:HD3	1:A:2977:VAL:HG23	2.01	0.41
1:A:2714:ALA:HB3	1:A:2717:LEU:HD11	2.02	0.41
1:A:2849:LYS:O	1:A:2849:LYS:HG3	2.19	0.41
1:A:308:THR:O	1:A:309:TYR:HB2	2.19	0.41
1:A:321:GLN:OE1	1:A:324:LEU:HB3	2.21	0.41
1:A:566:THR:O	1:A:566:THR:HG22	2.21	0.41
1:A:2909:ASP:O	1:A:2982:GLU:HG2	2.21	0.41
1:A:3600:ALA:HB1	1:A:3601:PRO:HD2	2.03	0.41
1:A:4020:PRO:HG3	1:A:4107:ALA:HB2	2.02	0.41
1:A:243:SER:HG	1:A:346:ALA:HB3	1.86	0.41
1:A:644:LEU:O	1:A:651:ALA:HB2	2.21	0.41
1:A:2372:TYR:N	1:A:2372:TYR:CD1	2.89	0.41
1:A:62:TYR:HB3	1:A:70:LYS:HB2	2.04	0.40
1:A:992:ILE:HD12	1:A:998:ILE:HG12	2.03	0.40
1:A:2420:SER:HB3	1:A:2985:GLY:HA3	2.02	0.40
1:A:2741:PRO:O	1:A:2874:VAL:HG22	2.21	0.40
1:A:139:THR:HG22	1:A:141:SER:H	1.87	0.40
1:A:1757:THR:HG23	1:A:1799:THR:HG23	2.03	0.40
1:A:2904:THR:CG2	1:A:2944:PHE:HB2	2.51	0.40
1:A:2908:ILE:HG22	1:A:2982:GLU:HB3	2.03	0.40
1:A:3488:ASN:HB2	1:A:3501:ALA:HB3	2.03	0.40
1:A:315:VAL:HG22	1:A:316:THR:N	2.37	0.40
1:A:692:ASN:OD1	1:A:718:CYS:O	2.39	0.40
1:A:1653:LEU:O	1:A:1660:VAL:HB	2.21	0.40
1:A:296:VAL:HG23	1:A:297:THR:HG23	2.02	0.40
1:A:663:LEU:HD13	1:A:744:VAL:HG21	2.04	0.40
1:A:1554:ILE:HD11	1:A:1606:VAL:CG1	2.52	0.40
1:A:2419:PRO:CB	1:A:2984:SER:OG	2.69	0.40
1:A:2639:VAL:HG13	1:A:2640:THR:N	2.36	0.40
1:A:3040:THR:HB	1:A:3041:PRO:CD	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	3874/4545 (85%)	3543 (92%)	316 (8%)	15 (0%)	30 63

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	366	VAL
1	A	476	ALA
1	A	2339	ALA
1	A	3465	THR
1	A	4126	VAL
1	A	692	ASN
1	A	771	ILE
1	A	1844	TYR
1	A	3337	TRP
1	A	1368	ASN
1	A	2937	SER
1	A	2919	THR
1	A	3748	VAL
1	A	3525	THR
1	A	2882	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	2939/3422 (86%)	2861 (97%)	78 (3%)	40 67

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	PHE
1	A	101	GLN
1	A	321	GLN
1	A	364	LEU
1	A	440	THR
1	A	515	THR
1	A	575	LEU
1	A	635	VAL
1	A	657	THR
1	A	877	ILE
1	A	895	VAL
1	A	949	VAL
1	A	979	SER
1	A	987	ILE
1	A	1007	ASP
1	A	1038	LEU
1	A	1110	THR
1	A	1206	THR
1	A	1242	LEU
1	A	1265	ILE
1	A	1271	ASN
1	A	1358	THR
1	A	1373	THR
1	A	1447	CYS
1	A	1480	ILE
1	A	1485	THR
1	A	1623	THR
1	A	1633	THR
1	A	1649	VAL
1	A	1655	LYS
1	A	1660	VAL
1	A	1672	LEU
1	A	1674	VAL
1	A	1684	SER
1	A	1685	CYS
1	A	1701	THR
1	A	1704	THR
1	A	1738	SER
1	A	1739	SER
1	A	1844	TYR
1	A	1846	THR
1	A	1881	ASN

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Mol	Chain	Res	Type
1	A	1981	CYS
1	A	2016	TYR
1	A	2048	ILE
1	A	2383	TYR
1	A	2385	THR
1	A	2408	LEU
1	A	2439	THR
1	A	2482	LEU
1	A	2501	ASN
1	A	2502	ARG
1	A	2524	THR
1	A	2601	SER
1	A	2666	ILE
1	A	2696	VAL
1	A	2709	VAL
1	A	2747	TYR
1	A	2773	THR
1	A	2787	LEU
1	A	2789	VAL
1	A	2869	VAL
1	A	2904	THR
1	A	2909	ASP
1	A	2981	TYR
1	A	3092	SER
1	A	3136	SER
1	A	3295	THR
1	A	3299	THR
1	A	3420	CYS
1	A	3430	LEU
1	A	3754	CYS
1	A	3799	TYR
1	A	3811	VAL
1	A	3813	THR
1	A	3845	ILE
1	A	3872	GLN
1	A	3886	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	570	GLN
1	A	623	ASN

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Mol	Chain	Res	Type
1	A	686	ASN
1	A	805	ASN
1	A	1448	ASN
1	A	1483	GLN
1	A	2070	GLN
1	A	2458	GLN
1	A	2623	ASN
1	A	3045	ASN
1	A	3496	ASN
1	A	3914	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](#)

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.

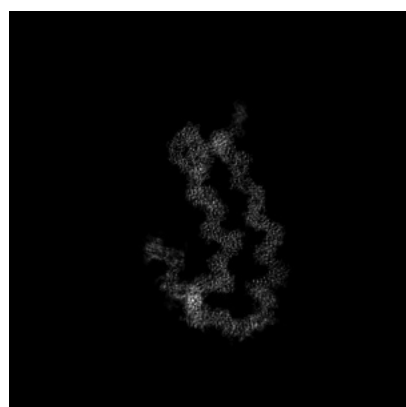
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51499. These allow visual inspection of the internal detail of the map and identification of artifacts.

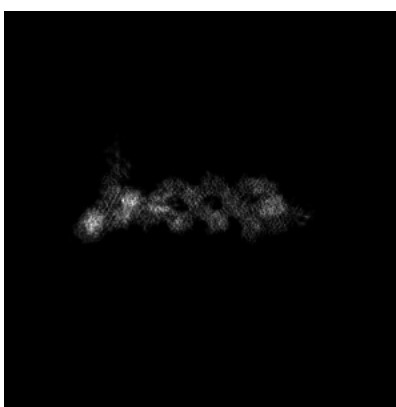
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

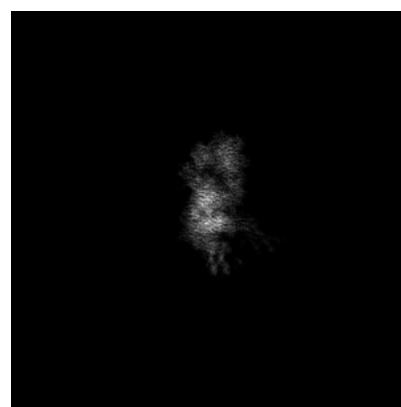
6.1.1 Primary map



X



Y

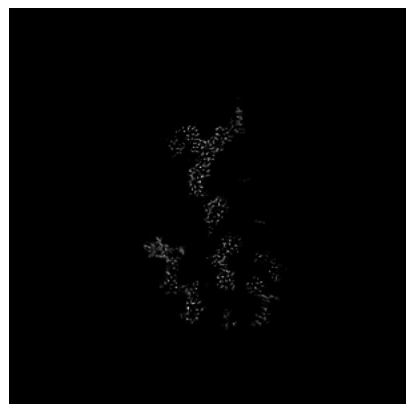


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 256



Y Index: 256

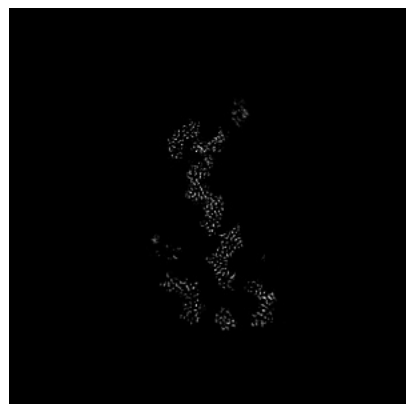


Z Index: 256

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: 251



Y Index: 244

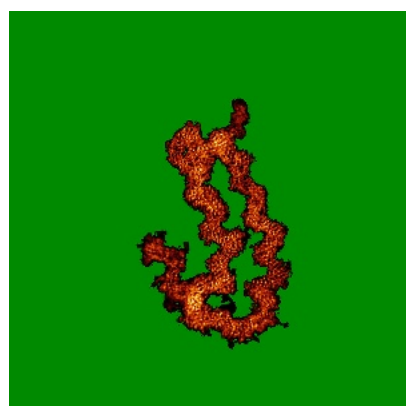


Z Index: 156

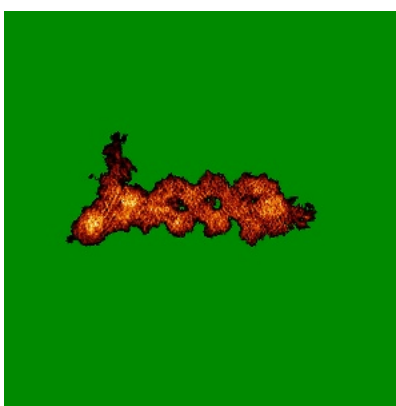
The images above show the largest variance slices of the map in three orthogonal directions.

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

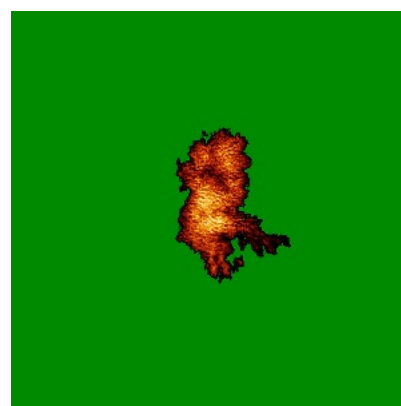
6.4.1 Primary map



X



Y

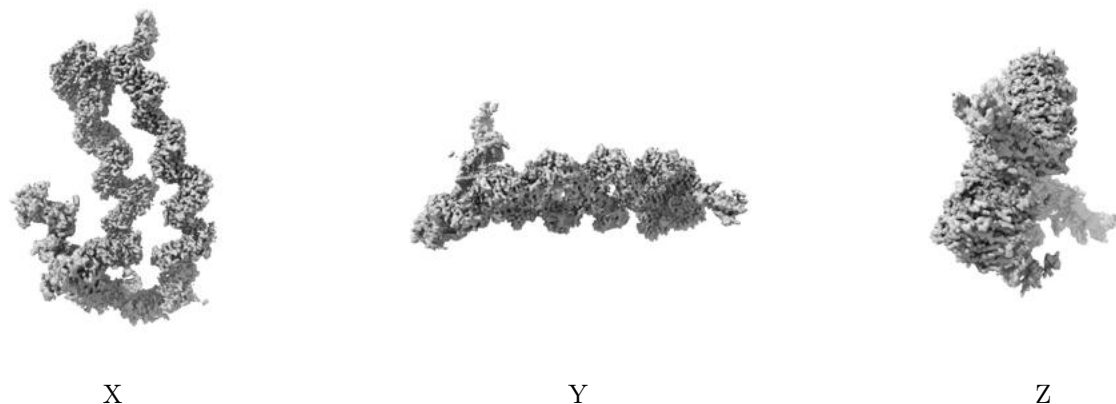


Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

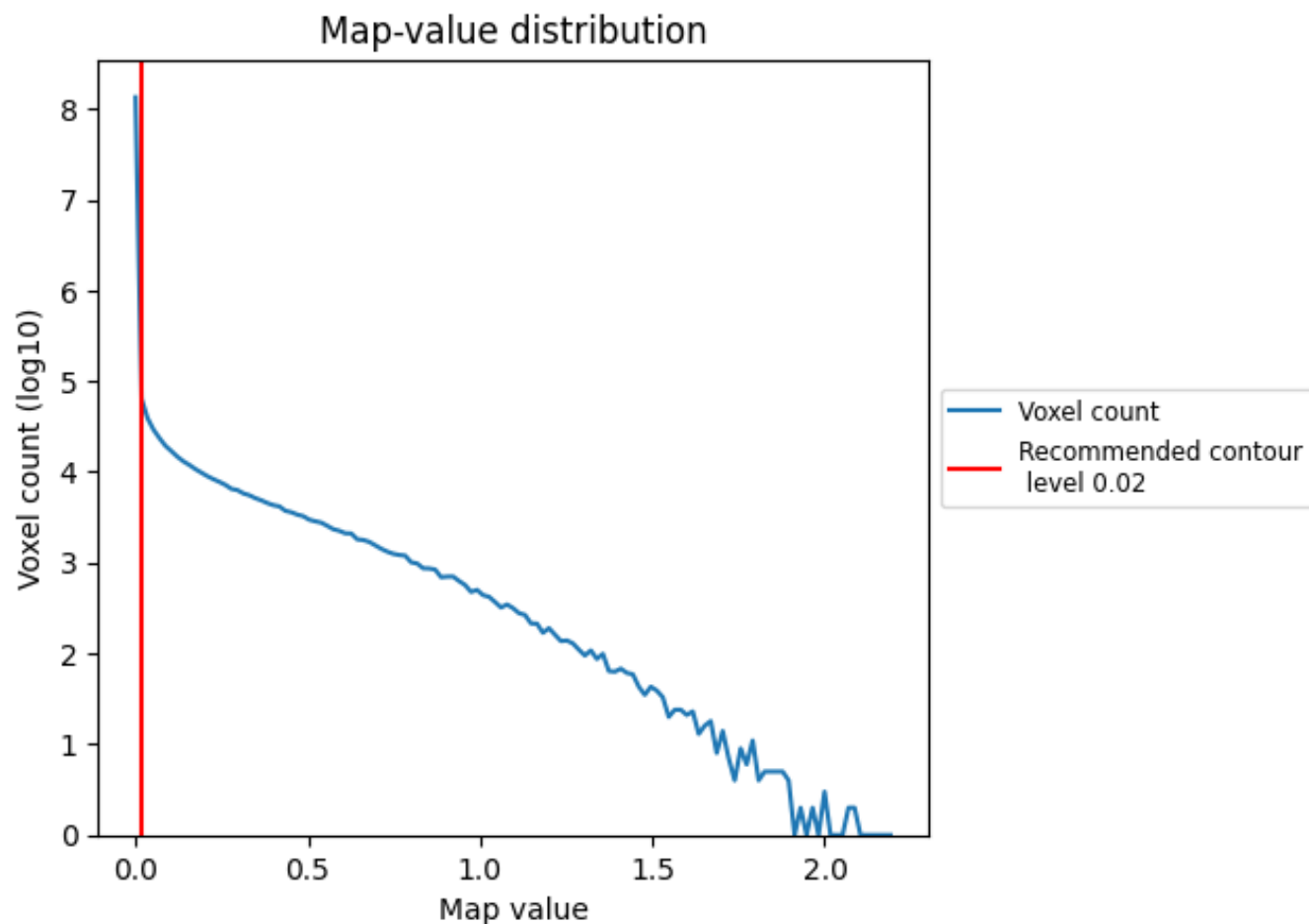
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

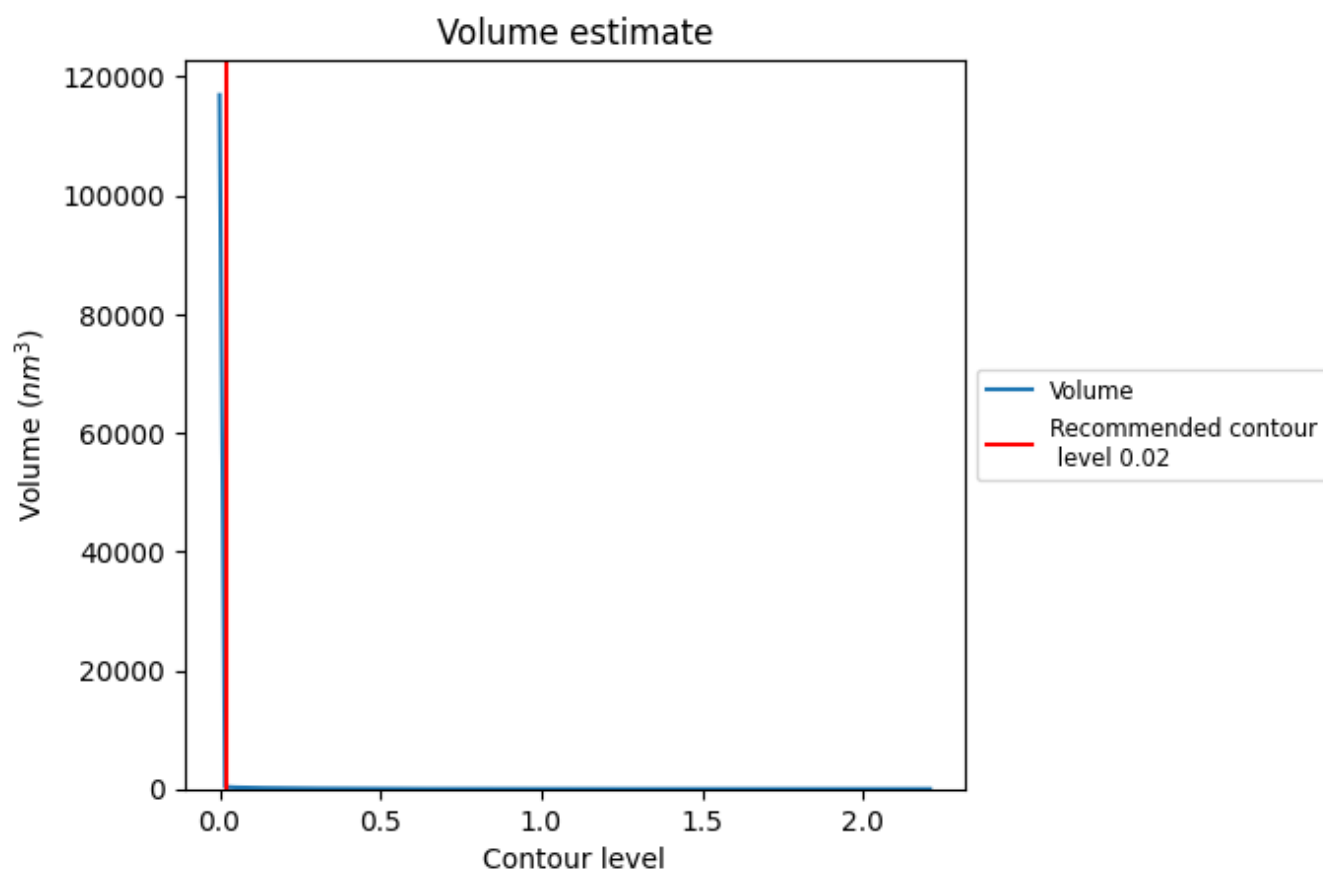
This section contains the results of statistical analysis of the map.

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.

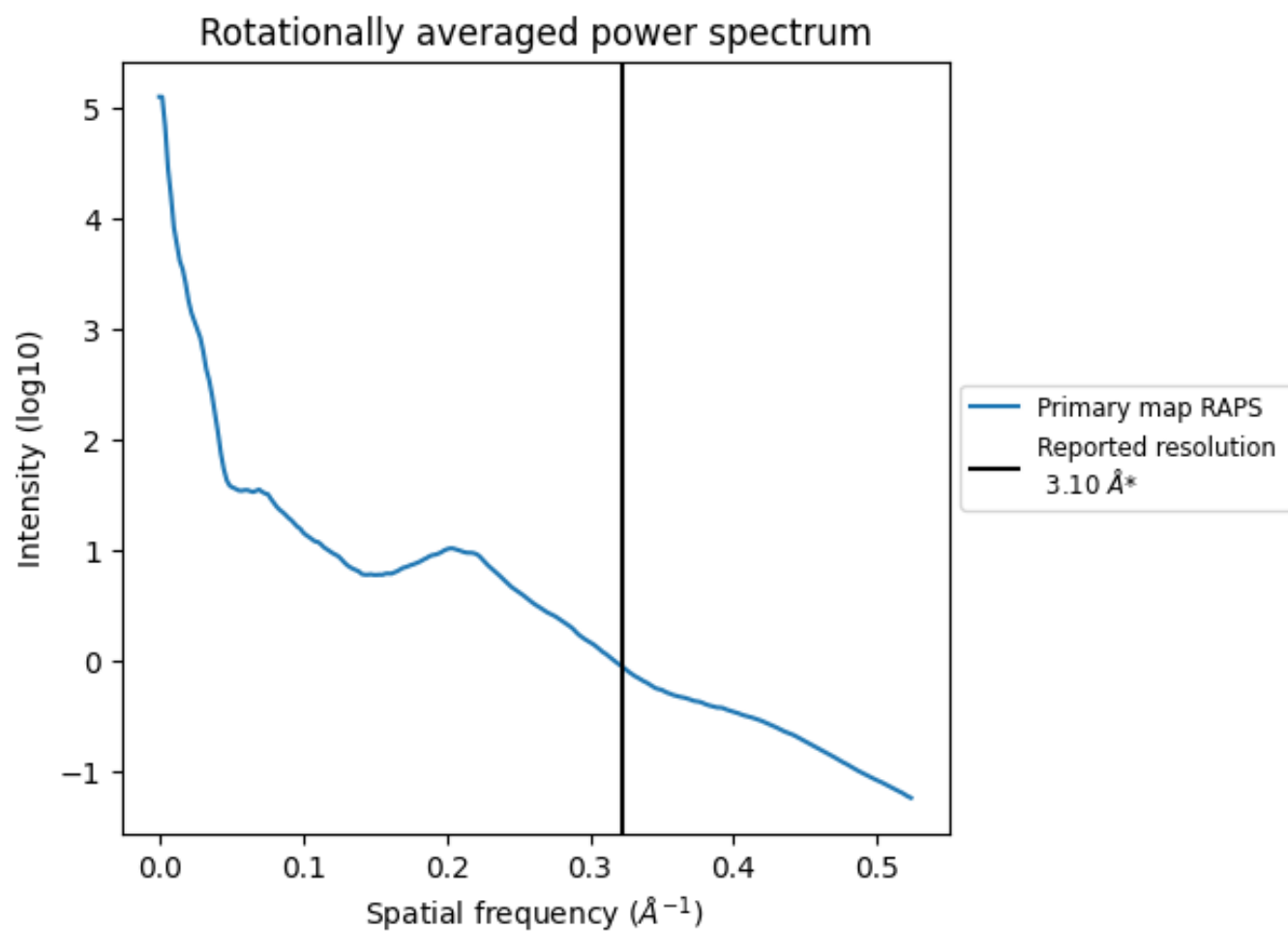
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 334 nm^3 ; this corresponds to an approximate mass of 302 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

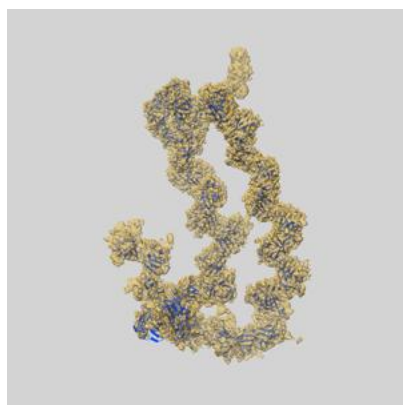
8 Fourier-Shell correlation

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

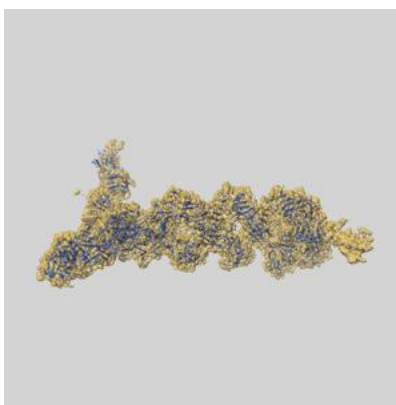
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51499 and PDB model 9GOS. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

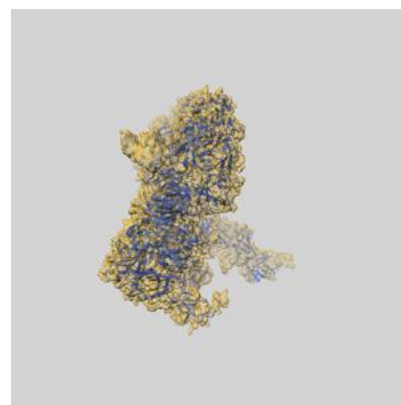
9.1 Map-model overlay [i](#)



X



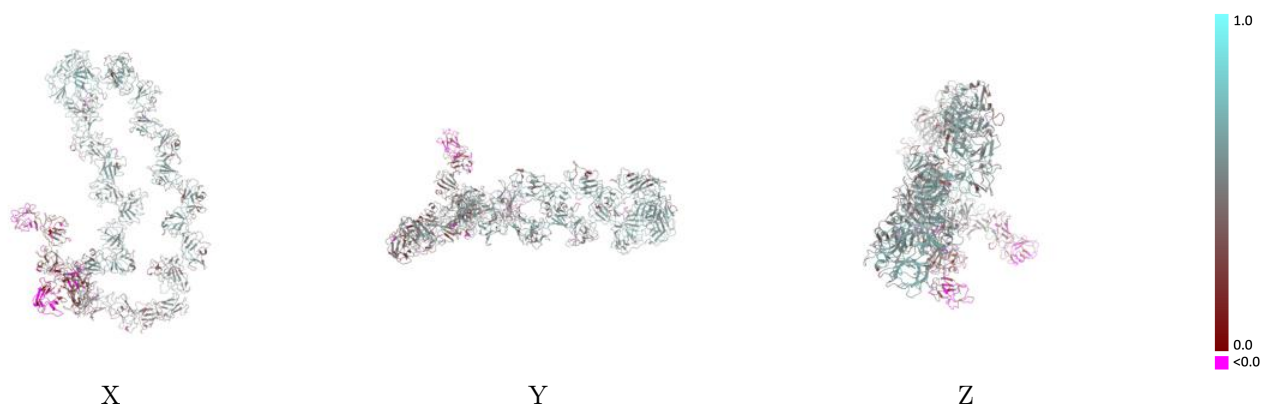
Y



Z

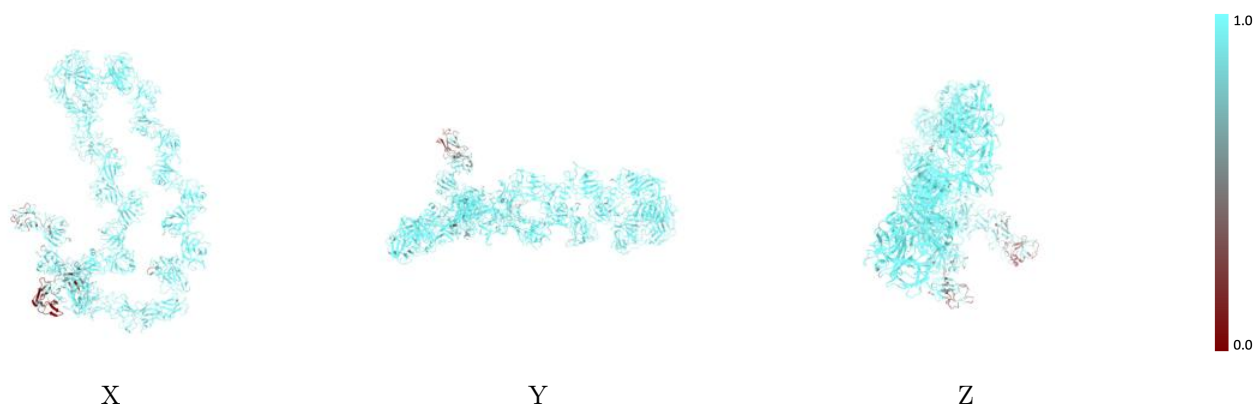
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



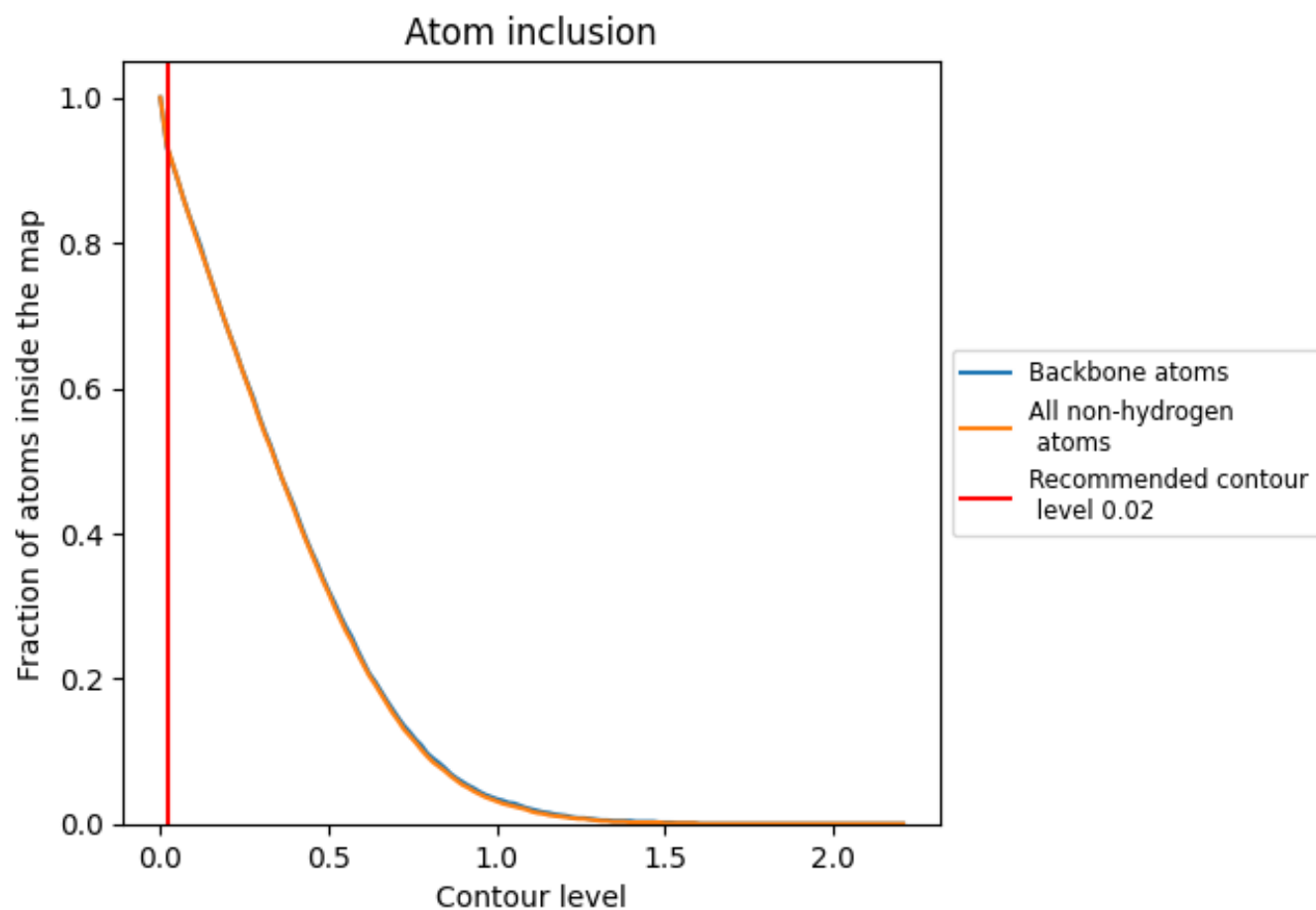
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9330	<div><div></div></div> 0.4580
A	<div><div></div></div> 0.9310	<div><div></div></div> 0.4580

