



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 09:02 AM UTC

PDB ID : 7FJQ / pdb_00007fjq
EMDB ID : EMD-31627
Title : Cryo EM structure of lysosomal ATPase
Authors : Zhang, S.S.
Deposited on : 2021-08-04
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
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

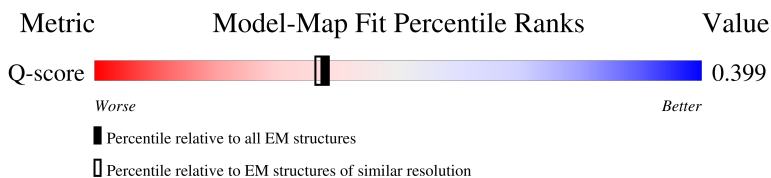
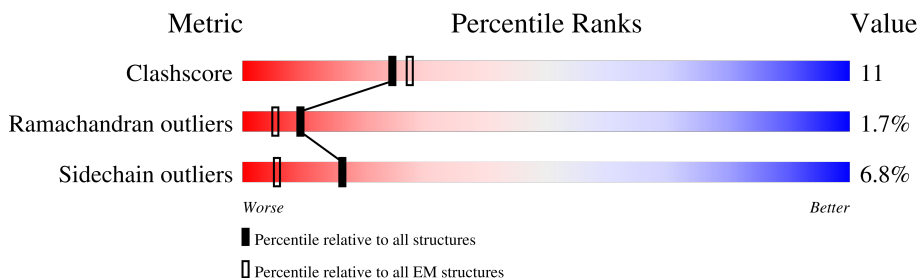
1 Overall quality at a glance

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	1153	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7086 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.

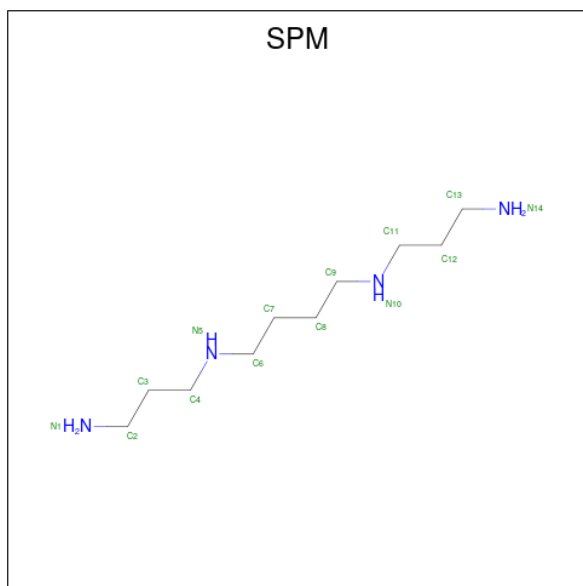
- Molecule 1 is a protein called Polyamine-transporting ATPase 13A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	973	7072	4560	1199	1269	44	0	0

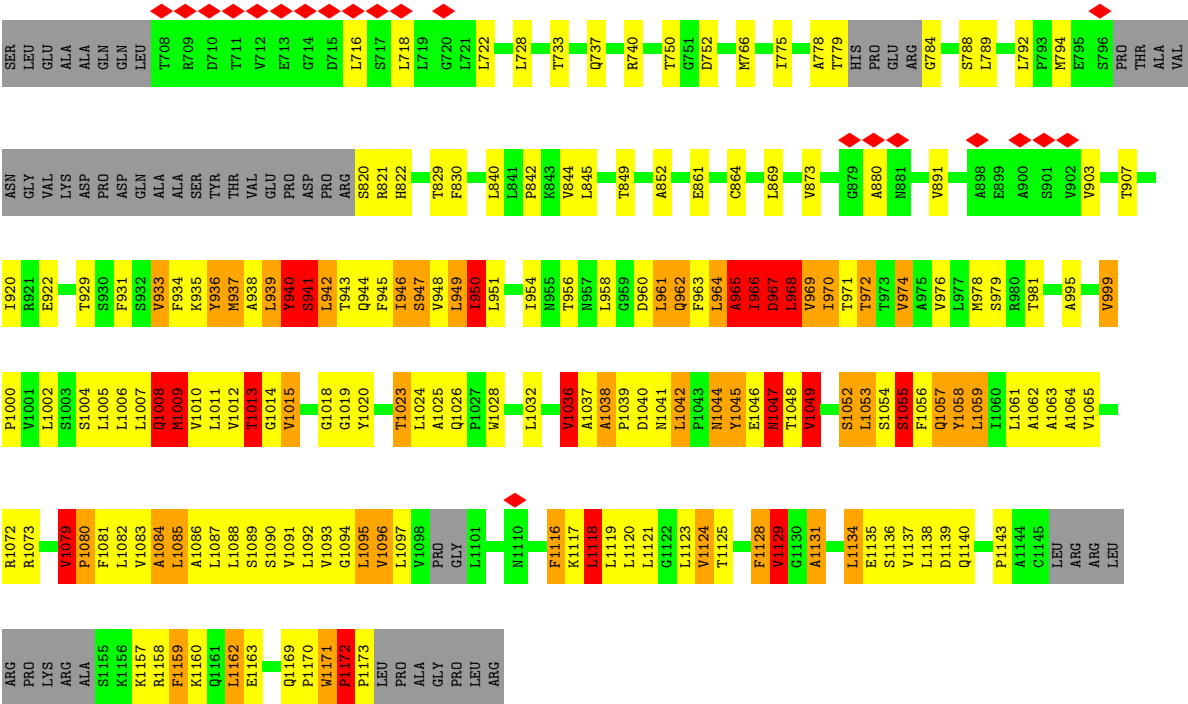
There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TRP	deletion	UNP Q9NQ11
A	?	-	VAL	deletion	UNP Q9NQ11
A	?	-	LEU	deletion	UNP Q9NQ11
A	?	-	GLU	deletion	UNP Q9NQ11
A	?	-	GLU	deletion	UNP Q9NQ11
A	?	-	GLU	deletion	UNP Q9NQ11
A	?	-	PRO	deletion	UNP Q9NQ11
A	?	-	ALA	deletion	UNP Q9NQ11
A	?	-	ALA	deletion	UNP Q9NQ11
A	?	-	ASP	deletion	UNP Q9NQ11
A	?	-	SER	deletion	UNP Q9NQ11
A	?	-	ALA	deletion	UNP Q9NQ11
A	?	-	PHE	deletion	UNP Q9NQ11
A	?	-	GLY	deletion	UNP Q9NQ11
A	?	-	THR	deletion	UNP Q9NQ11
A	?	-	GLN	deletion	UNP Q9NQ11
A	?	-	VAL	deletion	UNP Q9NQ11
A	?	-	LEU	deletion	UNP Q9NQ11
A	?	-	ALA	deletion	UNP Q9NQ11
A	?	-	VAL	deletion	UNP Q9NQ11
A	?	-	MET	deletion	UNP Q9NQ11
A	?	-	ARG	deletion	UNP Q9NQ11
A	?	-	PRO	deletion	UNP Q9NQ11
A	?	-	PRO	deletion	UNP Q9NQ11
A	?	-	LEU	deletion	UNP Q9NQ11
A	?	-	TRP	deletion	UNP Q9NQ11
A	?	-	GLU	deletion	UNP Q9NQ11

- Molecule 2 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	N	0
			14	10	4	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	256000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.722	Depositor
Minimum map value	-2.106	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	263.496, 263.496, 263.496	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	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: SPM

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	1.37	128/7210 (1.8%)	1.36	135/9858 (1.4%)

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	7

All (128) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	TYR	CA-C	-16.04	1.31	1.52
1	A	255	HIS	CA-C	-13.16	1.35	1.52
1	A	965	ALA	CA-C	-12.64	1.36	1.52
1	A	964	LEU	C-O	-11.20	1.11	1.24
1	A	941	SER	CA-C	-10.84	1.39	1.52
1	A	936	TYR	CA-C	-10.64	1.39	1.52
1	A	1055	SER	CA-CB	-9.94	1.37	1.53
1	A	257	TYR	N-CA	-9.71	1.33	1.46
1	A	941	SER	CA-CB	-9.51	1.38	1.53
1	A	1171	TRP	CA-C	-9.42	1.42	1.53
1	A	483	TYR	CA-C	-9.27	1.40	1.52
1	A	454	LEU	N-CA	8.95	1.57	1.46
1	A	1055	SER	C-O	8.80	1.34	1.24
1	A	999	VAL	CA-C	-8.69	1.44	1.52
1	A	961	LEU	C-O	-8.40	1.13	1.24
1	A	999	VAL	C-O	-8.22	1.14	1.24
1	A	232	LEU	CA-C	-8.20	1.42	1.52
1	A	1137	VAL	C-O	-8.14	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1052	SER	C-O	8.02	1.33	1.24
1	A	940	TYR	CA-C	-7.96	1.42	1.52
1	A	963	PHE	CA-CB	-7.85	1.40	1.53
1	A	443	SER	C-O	-7.85	1.15	1.24
1	A	476	ALA	CA-CB	-7.84	1.41	1.53
1	A	1057	GLN	CA-C	-7.81	1.42	1.52
1	A	1081	PHE	C-O	-7.73	1.15	1.24
1	A	1079	VAL	CA-CB	-7.50	1.48	1.53
1	A	965	ALA	C-O	-7.50	1.15	1.24
1	A	454	LEU	C-O	7.47	1.33	1.24
1	A	1081	PHE	CA-C	-7.43	1.43	1.52
1	A	947	SER	CA-C	-7.32	1.43	1.52
1	A	936	TYR	C-O	-7.29	1.15	1.24
1	A	1169	GLN	CA-C	-7.28	1.46	1.52
1	A	963	PHE	CA-C	-7.27	1.43	1.52
1	A	467	VAL	CA-C	-7.23	1.43	1.52
1	A	1013	THR	CA-C	-7.22	1.43	1.52
1	A	948	VAL	CA-CB	-7.15	1.45	1.54
1	A	459	ILE	CA-CB	-7.05	1.45	1.54
1	A	947	SER	CA-CB	-7.04	1.42	1.53
1	A	1159	PHE	CA-C	-7.03	1.43	1.52
1	A	1062	ALA	CA-C	-7.00	1.44	1.52
1	A	464	LEU	CA-C	-6.99	1.43	1.52
1	A	256	TYR	N-CA	-6.89	1.37	1.46
1	A	1091	VAL	CA-CB	-6.88	1.45	1.54
1	A	467	VAL	C-O	-6.86	1.16	1.24
1	A	1124	VAL	CA-CB	-6.80	1.46	1.54
1	A	1084	ALA	C-O	-6.78	1.16	1.24
1	A	442	TYR	CA-C	-6.77	1.44	1.52
1	A	1049	VAL	CA-CB	-6.72	1.46	1.54
1	A	1014	GLY	C-O	-6.40	1.16	1.23
1	A	964	LEU	CA-C	-6.33	1.44	1.52
1	A	1047	ASN	C-O	-6.30	1.16	1.24
1	A	444	ILE	CA-C	-6.26	1.45	1.52
1	A	947	SER	C-O	-6.23	1.16	1.24
1	A	936	TYR	CA-CB	-6.21	1.43	1.53
1	A	1023	THR	CA-C	-6.20	1.44	1.52
1	A	969	VAL	CA-CB	-6.18	1.47	1.54
1	A	456	GLU	C-O	-6.17	1.17	1.24
1	A	464	LEU	C-O	-6.15	1.17	1.24
1	A	443	SER	CA-CB	-6.12	1.43	1.53
1	A	1055	SER	N-CA	-6.11	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	461	ALA	CA-CB	-6.08	1.43	1.53
1	A	463	ASP	CA-C	-6.08	1.44	1.52
1	A	944	GLN	C-O	-6.06	1.17	1.24
1	A	933	VAL	CA-CB	-6.03	1.47	1.54
1	A	1063	ALA	CA-CB	-6.02	1.44	1.53
1	A	1062	ALA	CA-CB	-5.97	1.44	1.53
1	A	1131	ALA	CA-C	-5.96	1.45	1.52
1	A	1063	ALA	C-O	-5.94	1.17	1.24
1	A	962	GLN	CA-C	-5.93	1.45	1.52
1	A	965	ALA	CA-CB	-5.90	1.44	1.53
1	A	1057	GLN	CA-CB	-5.89	1.44	1.53
1	A	1134	LEU	CA-C	-5.88	1.45	1.52
1	A	253	ALA	N-CA	-5.87	1.38	1.46
1	A	1093	VAL	CA-C	-5.84	1.45	1.52
1	A	961	LEU	CA-C	-5.82	1.44	1.52
1	A	965	ALA	N-CA	-5.82	1.39	1.46
1	A	942	LEU	C-O	-5.80	1.16	1.24
1	A	253	ALA	CA-CB	-5.79	1.44	1.53
1	A	1015	VAL	CA-CB	-5.78	1.47	1.54
1	A	465	VAL	C-O	-5.75	1.17	1.24
1	A	967	ASP	CA-CB	-5.74	1.44	1.53
1	A	474	PRO	CA-CB	-5.72	1.45	1.53
1	A	938	ALA	CA-CB	-5.69	1.44	1.53
1	A	966	ILE	CA-C	-5.67	1.46	1.52
1	A	461	ALA	N-CA	-5.66	1.39	1.46
1	A	1131	ALA	CA-CB	-5.66	1.44	1.53
1	A	261	LEU	CA-C	-5.63	1.45	1.52
1	A	963	PHE	C-O	-5.57	1.17	1.24
1	A	934	PHE	CA-C	-5.56	1.45	1.52
1	A	950	ILE	CA-C	-5.56	1.45	1.52
1	A	1137	VAL	CA-C	-5.55	1.45	1.52
1	A	945	PHE	CA-C	-5.54	1.45	1.52
1	A	260	ALA	CA-CB	-5.52	1.44	1.53
1	A	946	ILE	C-O	-5.49	1.17	1.24
1	A	962	GLN	N-CA	-5.49	1.39	1.46
1	A	1085	LEU	N-CA	-5.47	1.39	1.46
1	A	1008	GLN	N-CA	-5.46	1.39	1.46
1	A	1065	VAL	CA-CB	-5.46	1.47	1.54
1	A	941	SER	C-O	-5.46	1.17	1.24
1	A	968	LEU	CA-C	-5.45	1.45	1.52
1	A	463	ASP	CA-CB	-5.43	1.44	1.53
1	A	969	VAL	C-N	-5.42	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	960	ASP	CA-CB	-5.41	1.44	1.53
1	A	1140	GLN	N-CA	5.39	1.53	1.46
1	A	1084	ALA	CA-C	-5.37	1.45	1.52
1	A	260	ALA	CA-C	-5.37	1.45	1.52
1	A	1018	GLY	CA-C	-5.36	1.46	1.52
1	A	1064	ALA	CA-CB	-5.35	1.45	1.53
1	A	962	GLN	C-O	-5.35	1.17	1.24
1	A	1081	PHE	CA-CB	-5.33	1.44	1.53
1	A	1093	VAL	C-O	-5.30	1.17	1.24
1	A	1079	VAL	CA-C	-5.30	1.47	1.52
1	A	1089	SER	CA-C	-5.29	1.46	1.52
1	A	937	MET	CA-C	-5.20	1.46	1.52
1	A	972	THR	CA-CB	-5.18	1.46	1.53
1	A	233	VAL	CA-C	-5.18	1.46	1.52
1	A	941	SER	N-CA	-5.15	1.40	1.46
1	A	482	LEU	CA-C	-5.12	1.45	1.52
1	A	974	VAL	N-CA	-5.10	1.40	1.46
1	A	255	HIS	N-CA	5.09	1.52	1.46
1	A	971	THR	CA-CB	-5.09	1.46	1.54
1	A	979	SER	CA-CB	-5.07	1.46	1.52
1	A	1053	LEU	CA-CB	-5.06	1.45	1.53
1	A	933	VAL	C-O	-5.03	1.18	1.23
1	A	1162	LEU	CA-C	-5.03	1.46	1.52
1	A	939	LEU	C-O	-5.01	1.18	1.24
1	A	478	THR	C-O	-5.01	1.18	1.24
1	A	976	VAL	CA-CB	-5.01	1.48	1.54

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1172	PRO	N-CA-C	-20.17	86.09	110.70
1	A	1117	LYS	N-CA-C	-11.35	98.66	111.71
1	A	441	ILE	N-CA-C	-11.25	101.88	111.56
1	A	258	TRP	N-CA-C	10.72	123.97	111.11
1	A	1042	LEU	N-CA-C	10.69	133.44	109.81
1	A	960	ASP	N-CA-C	10.29	122.25	111.14
1	A	972	THR	N-CA-C	-10.26	101.26	113.88
1	A	1096	VAL	N-CA-C	10.18	120.20	110.42
1	A	1054	SER	N-CA-C	10.04	122.22	111.28
1	A	999	VAL	CA-C-N	-10.00	108.57	118.97
1	A	999	VAL	C-N-CA	-10.00	108.57	118.97
1	A	236	ALA	N-CA-C	9.85	122.10	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	LEU	N-CA-C	8.83	129.61	110.80
1	A	1042	LEU	CA-C-N	-8.56	113.00	121.65
1	A	1042	LEU	C-N-CA	-8.56	113.00	121.65
1	A	228	TYR	CA-C-N	-8.40	109.74	119.32
1	A	228	TYR	C-N-CA	-8.40	109.74	119.32
1	A	1013	THR	N-CA-C	-8.29	102.25	111.28
1	A	1157	LYS	N-CA-C	-8.13	98.24	110.28
1	A	61	PRO	N-CA-CB	8.10	111.76	103.25
1	A	1055	SER	CA-C-N	-8.09	109.44	120.28
1	A	1055	SER	C-N-CA	-8.09	109.44	120.28
1	A	933	VAL	N-CA-C	-8.06	104.88	111.81
1	A	936	TYR	N-CA-C	-8.04	102.52	111.28
1	A	255	HIS	CB-CA-C	-8.03	94.43	110.42
1	A	999	VAL	N-CA-CB	8.02	115.55	110.50
1	A	965	ALA	N-CA-C	-7.96	102.55	111.07
1	A	253	ALA	N-CA-C	-7.87	102.32	112.23
1	A	1091	VAL	CB-CA-C	-7.86	101.53	112.14
1	A	1079	VAL	N-CA-CB	7.81	115.42	110.50
1	A	457	ILE	CA-C-N	-7.80	110.73	120.56
1	A	457	ILE	C-N-CA	-7.80	110.73	120.56
1	A	1008	GLN	N-CA-C	-7.79	102.79	111.28
1	A	1095	LEU	N-CA-C	-7.77	102.75	111.07
1	A	257	TYR	CB-CA-C	7.76	125.87	110.42
1	A	944	GLN	N-CA-CB	7.73	121.48	110.12
1	A	256	TYR	CB-CA-C	-7.72	95.06	110.42
1	A	69	PRO	N-CA-CB	7.62	110.17	102.17
1	A	1045	TYR	N-CA-C	7.47	122.96	113.55
1	A	460	ARG	N-CA-C	7.46	119.49	111.36
1	A	458	VAL	N-CA-C	7.46	117.58	110.42
1	A	978	MET	CA-C-N	-7.42	111.23	122.21
1	A	978	MET	C-N-CA	-7.42	111.23	122.21
1	A	979	SER	N-CA-C	7.35	122.10	110.70
1	A	1058	TYR	CA-C-N	-7.35	110.43	120.28
1	A	1058	TYR	C-N-CA	-7.35	110.43	120.28
1	A	1079	VAL	CA-C-N	-7.28	110.97	119.05
1	A	1079	VAL	C-N-CA	-7.28	110.97	119.05
1	A	1143	PRO	N-CA-CB	7.24	110.85	103.25
1	A	1119	LEU	N-CA-C	-7.10	103.54	111.28
1	A	1085	LEU	N-CA-C	-7.08	103.49	111.07
1	A	1057	GLN	N-CA-C	7.02	118.93	111.28
1	A	1097	LEU	N-CA-C	7.00	120.48	112.57
1	A	261	LEU	N-CA-C	-6.99	103.66	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1009	MET	CB-CG-SD	-6.96	91.80	112.70
1	A	949	LEU	N-CA-C	6.96	118.95	111.36
1	A	121	PRO	N-CA-CB	6.96	110.19	103.51
1	A	1009	MET	N-CA-C	6.91	118.81	111.28
1	A	257	TYR	N-CA-C	-6.89	96.11	110.80
1	A	1088	LEU	N-CA-C	-6.85	103.89	111.36
1	A	965	ALA	CA-C-O	-6.83	113.65	120.82
1	A	457	ILE	CB-CA-C	-6.68	103.42	111.97
1	A	1064	ALA	N-CA-C	6.67	118.55	111.28
1	A	943	THR	N-CA-CB	6.63	119.86	110.12
1	A	119	PRO	N-CA-CB	6.58	110.16	103.25
1	A	473	LEU	CA-C-N	-6.57	111.75	119.05
1	A	473	LEU	C-N-CA	-6.57	111.75	119.05
1	A	967	ASP	O-C-N	-6.48	115.29	122.03
1	A	1038	ALA	N-CA-C	6.46	124.08	109.81
1	A	1082	LEU	N-CA-C	-6.37	104.33	111.28
1	A	963	PHE	CB-CA-C	-6.35	100.05	110.85
1	A	1171	TRP	N-CA-C	6.32	120.47	108.97
1	A	966	ILE	N-CA-CB	6.30	117.48	110.62
1	A	1041	ASN	N-CA-C	-6.25	105.59	112.72
1	A	1128	PHE	CB-CA-C	-6.24	101.08	110.88
1	A	300	PRO	N-CA-CB	6.22	110.17	103.33
1	A	258	TRP	N-CA-CB	-6.21	100.69	109.94
1	A	1040	ASP	N-CA-C	-6.15	104.41	112.41
1	A	963	PHE	N-CA-C	-6.15	104.66	111.36
1	A	964	LEU	CA-C-O	-6.10	114.09	120.55
1	A	1125	THR	CB-CA-C	-6.04	100.77	110.79
1	A	1120	LEU	N-CA-CB	5.99	118.92	110.12
1	A	1086	ALA	N-CA-C	5.96	117.86	111.36
1	A	958	LEU	O-C-N	-5.93	116.03	122.79
1	A	1013	THR	N-CA-CB	5.87	118.74	110.12
1	A	1018	GLY	N-CA-C	-5.85	105.71	112.73
1	A	966	ILE	CB-CA-C	-5.73	104.65	111.81
1	A	937	MET	N-CA-C	5.72	117.52	111.28
1	A	968	LEU	CA-C-N	-5.72	113.24	120.56
1	A	968	LEU	C-N-CA	-5.72	113.24	120.56
1	A	1081	PHE	CB-CA-C	-5.72	101.12	110.85
1	A	941	SER	CB-CA-C	-5.70	101.93	110.88
1	A	1129	VAL	N-CA-C	-5.69	104.82	110.62
1	A	1169	GLN	CA-C-N	-5.68	114.41	120.03
1	A	1169	GLN	C-N-CA	-5.68	114.41	120.03
1	A	1055	SER	N-CA-CB	-5.62	101.86	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	LEU	CA-C-N	-5.61	112.76	120.28
1	A	261	LEU	C-N-CA	-5.61	112.76	120.28
1	A	1095	LEU	CA-C-N	-5.60	113.50	120.56
1	A	1095	LEU	C-N-CA	-5.60	113.50	120.56
1	A	255	HIS	N-CA-CB	5.60	119.95	110.49
1	A	1038	ALA	CA-C-N	-5.59	112.85	119.84
1	A	1038	ALA	C-N-CA	-5.59	112.85	119.84
1	A	254	ASP	CA-C-O	-5.55	113.21	119.98
1	A	255	HIS	N-CA-C	-5.54	99.00	110.80
1	A	974	VAL	CB-CA-C	5.51	119.83	112.22
1	A	1170	PRO	CA-C-N	-5.48	116.27	123.34
1	A	1170	PRO	C-N-CA	-5.48	116.27	123.34
1	A	1159	PHE	N-CA-C	-5.46	105.32	111.28
1	A	943	THR	N-CA-C	-5.46	105.33	111.28
1	A	464	LEU	N-CA-CB	5.42	118.09	110.12
1	A	458	VAL	N-CA-CB	5.41	116.88	110.55
1	A	268	SER	CA-C-N	-5.35	111.86	120.64
1	A	268	SER	C-N-CA	-5.35	111.86	120.64
1	A	1053	LEU	N-CA-C	-5.35	105.44	111.28
1	A	966	ILE	CA-C-O	-5.32	115.60	121.29
1	A	1010	VAL	N-CA-C	-5.26	105.25	110.62
1	A	444	ILE	CA-C-N	-5.26	113.61	120.44
1	A	444	ILE	C-N-CA	-5.26	113.61	120.44
1	A	480	CYS	CA-C-N	-5.24	112.34	120.31
1	A	480	CYS	C-N-CA	-5.24	112.34	120.31
1	A	262	CYS	N-CA-C	5.23	116.98	111.28
1	A	1139	ASP	N-CA-C	-5.22	105.59	111.28
1	A	966	ILE	O-C-N	-5.21	116.57	121.94
1	A	840	LEU	CA-C-N	5.15	126.53	120.09
1	A	840	LEU	C-N-CA	5.15	126.53	120.09
1	A	233	VAL	CB-CA-C	-5.09	105.45	111.97
1	A	1036	VAL	CB-CA-C	-5.08	102.95	111.29
1	A	1118	LEU	N-CA-C	5.07	116.88	111.36
1	A	948	VAL	N-CA-C	-5.06	105.45	110.62
1	A	969	VAL	N-CA-C	5.06	115.28	110.53
1	A	964	LEU	CA-CB-CG	5.05	133.97	116.30
1	A	481	THR	N-CA-C	5.01	117.63	111.82
1	A	461	ALA	CA-C-N	-5.00	112.70	120.31
1	A	461	ALA	C-N-CA	-5.00	112.70	120.31

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1044	ASN	Mainchain
1	A	289	VAL	Peptide
1	A	965	ALA	Mainchain
1	A	966	ILE	Mainchain
1	A	967	ASP	Mainchain
1	A	968	LEU	Mainchain
1	A	969	VAL	Mainchain

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	7072	0	6988	149	0
2	A	14	0	26	1	0
All	All	7086	0	7014	149	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 11.

All (149) 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:844:VAL:HG22	1:A:1171:TRP:HZ3	1.26	0.98
1:A:1023:THR:HG21	1:A:1049:VAL:HG11	1.52	0.92
1:A:448:TYR:HB2	1:A:457:ILE:HD11	1.57	0.87
1:A:949:LEU:C	1:A:951:LEU:H	1.79	0.86
1:A:844:VAL:HG22	1:A:1171:TRP:CZ3	2.12	0.84
1:A:256:TYR:O	1:A:258:TRP:N	2.20	0.74
1:A:256:TYR:O	1:A:257:TYR:C	2.29	0.72
1:A:949:LEU:C	1:A:951:LEU:N	2.48	0.72
1:A:250:LEU:HD11	1:A:462:LEU:CB	2.21	0.70
1:A:452:VAL:HG21	1:A:457:ILE:HG13	1.77	0.66
1:A:844:VAL:CG2	1:A:1171:TRP:CZ3	2.79	0.66
1:A:250:LEU:HD11	1:A:462:LEU:HB3	1.79	0.64
1:A:1055:SER:HB2	1:A:1092:LEU:HD13	1.80	0.64
1:A:463:ASP:CG	2:A:1201:SPM:H91	2.25	0.62
1:A:750:THR:HG22	1:A:752:ASP:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LEU:HD11	1:A:462:LEU:HB2	1.84	0.60
1:A:970:ILE:O	1:A:974:VAL:HG22	2.00	0.60
1:A:240:TYR:CE2	1:A:474:PRO:HG2	2.37	0.59
1:A:317:CYS:HA	1:A:394:VAL:HA	1.85	0.59
1:A:464:LEU:HD21	1:A:949:LEU:HD11	1.82	0.59
1:A:452:VAL:CG2	1:A:457:ILE:HG13	2.33	0.58
1:A:1172:PRO:O	1:A:1173:PRO:C	2.46	0.58
1:A:524:ASP:HA	1:A:576:LYS:HG2	1.84	0.58
1:A:779:THR:HG1	1:A:784:GLY:N	2.01	0.58
1:A:733:THR:O	1:A:737:GLN:NE2	2.37	0.58
1:A:369:HIS:HB3	1:A:372:HIS:HB2	1.86	0.58
1:A:1008:GLN:HE21	1:A:1131:ALA:HB1	1.69	0.58
1:A:440:THR:OG1	1:A:461:ALA:HB1	2.04	0.57
1:A:581:THR:HG23	1:A:610:PRO:HD3	1.85	0.57
1:A:1171:TRP:N	1:A:1172:PRO:HD3	2.18	0.56
1:A:258:TRP:H	1:A:258:TRP:CD1	2.22	0.56
1:A:543:PRO:HB2	1:A:581:THR:HB	1.87	0.56
1:A:821:ARG:NH1	1:A:1172:PRO:HG2	2.21	0.55
1:A:1007:LEU:HD12	1:A:1138:LEU:HD11	1.87	0.55
1:A:560:ALA:HB2	1:A:637:MET:HE1	1.89	0.55
1:A:931:PHE:O	1:A:935:LYS:HG2	2.06	0.55
1:A:347:GLY:HA3	1:A:880:ALA:HA	1.88	0.54
1:A:228:TYR:O	1:A:229:PRO:C	2.43	0.53
1:A:339:MET:HG2	1:A:353:LEU:HA	1.88	0.53
1:A:750:THR:HB	1:A:852:ALA:HA	1.90	0.53
1:A:339:MET:SD	1:A:382:GLN:NE2	2.82	0.53
1:A:460:ARG:HH22	1:A:1038:ALA:HB3	1.72	0.53
1:A:263:ILE:HD11	1:A:472:ALA:HB2	1.91	0.53
1:A:903:VAL:HG21	1:A:907:THR:HB	1.89	0.53
1:A:822:HIS:ND1	1:A:849:THR:OG1	2.41	0.53
1:A:775:ILE:HB	1:A:792:LEU:HB2	1.90	0.52
1:A:740:ARG:NH1	1:A:766:MET:O	2.42	0.52
1:A:778:ALA:HB2	1:A:789:LEU:HD13	1.90	0.51
1:A:1007:LEU:HB3	1:A:1134:LEU:HD21	1.92	0.51
1:A:175:TRP:HA	1:A:181:ALA:HB1	1.91	0.51
1:A:258:TRP:N	1:A:258:TRP:CD1	2.79	0.51
1:A:642:ALA:HB2	1:A:649:PRO:HB3	1.91	0.51
1:A:1019:GLY:O	1:A:1023:THR:HG23	2.11	0.51
1:A:1024:LEU:C	1:A:1026:GLN:H	2.19	0.51
1:A:477:MET:HE1	1:A:933:VAL:HG23	1.92	0.51
1:A:1158:ARG:O	1:A:1159:PHE:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:CYS:SG	1:A:330:ASP:N	2.85	0.50
1:A:967:ASP:O	1:A:968:LEU:C	2.51	0.50
1:A:1079:VAL:O	1:A:1080:PRO:C	2.50	0.50
1:A:448:TYR:O	1:A:449:ARG:C	2.48	0.49
1:A:966:ILE:O	1:A:967:ASP:C	2.52	0.49
1:A:244:GLN:NE2	1:A:471:PRO:O	2.41	0.48
1:A:940:TYR:O	1:A:941:SER:C	2.51	0.48
1:A:473:LEU:H	1:A:474:PRO:CD	2.25	0.48
1:A:318:LEU:N	1:A:393:ALA:O	2.47	0.48
1:A:254:ASP:O	1:A:255:HIS:HB2	2.13	0.48
1:A:949:LEU:O	1:A:951:LEU:N	2.45	0.48
1:A:519:THR:HA	1:A:728:LEU:HA	1.96	0.48
1:A:164:ARG:HB2	1:A:174:ILE:HG13	1.94	0.48
1:A:327:MET:SD	1:A:378:THR:OG1	2.70	0.48
1:A:295:VAL:HG21	1:A:328:PRO:HG3	1.96	0.47
1:A:488:LEU:HD21	1:A:922:GLU:HG3	1.96	0.47
1:A:1036:VAL:HB	1:A:1037:ALA:H	1.42	0.47
1:A:1159:PHE:CE2	1:A:1160:LYS:HG3	2.49	0.47
1:A:269:ILE:HG22	1:A:273:LEU:HD23	1.97	0.47
1:A:775:ILE:HD11	1:A:794:MET:HG3	1.95	0.47
1:A:1094:GLY:O	1:A:1095:LEU:C	2.57	0.47
1:A:444:ILE:O	1:A:445:PHE:C	2.54	0.47
1:A:1008:GLN:NE2	1:A:1131:ALA:HB1	2.30	0.47
1:A:473:LEU:H	1:A:474:PRO:HD2	1.80	0.47
1:A:1047:ASN:O	1:A:1048:THR:C	2.56	0.47
1:A:448:TYR:HB2	1:A:457:ILE:CD1	2.38	0.47
1:A:1072:ARG:HG3	1:A:1073:ARG:H	1.80	0.47
1:A:1012:VAL:O	1:A:1013:THR:C	2.56	0.46
1:A:335:ALA:HB3	1:A:392:LEU:HB2	1.96	0.46
1:A:574:ASP:HB2	1:A:577:MET:HE2	1.97	0.46
1:A:820:SER:OG	1:A:821:ARG:N	2.46	0.46
1:A:999:VAL:O	1:A:1000:PRO:C	2.53	0.46
1:A:1055:SER:O	1:A:1056:PHE:C	2.53	0.46
1:A:233:VAL:O	1:A:234:ASP:C	2.53	0.46
1:A:1058:TYR:O	1:A:1059:LEU:C	2.56	0.46
1:A:172:ARG:NH1	1:A:215:ILE:O	2.49	0.46
1:A:929:THR:O	1:A:933:VAL:HG22	2.16	0.46
1:A:508:GLN:OE1	1:A:1159:PHE:CZ	2.69	0.45
1:A:678:GLN:HA	1:A:681:THR:HG22	1.98	0.45
1:A:788:SER:OG	1:A:789:LEU:N	2.49	0.45
1:A:1024:LEU:O	1:A:1026:GLN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:ALA:O	1:A:485:GLN:C	2.59	0.45
1:A:935:LYS:O	1:A:936:TYR:C	2.55	0.45
1:A:1009:MET:O	1:A:1013:THR:HG23	2.16	0.45
1:A:1028:TRP:HZ3	1:A:1045:TYR:CZ	2.35	0.45
1:A:248:ILE:HD11	1:A:263:ILE:HG22	1.99	0.45
1:A:775:ILE:N	1:A:792:LEU:O	2.49	0.45
1:A:437:LEU:HA	1:A:440:THR:HG22	1.98	0.45
1:A:473:LEU:HB3	1:A:474:PRO:HD3	1.98	0.45
1:A:1128:PHE:O	1:A:1129:VAL:C	2.56	0.45
1:A:1045:TYR:O	1:A:1049:VAL:HG12	2.17	0.44
1:A:981:THR:HG22	1:A:1073:ARG:HB3	1.98	0.44
1:A:236:ALA:C	1:A:238:ASN:H	2.25	0.44
1:A:463:ASP:O	1:A:467:VAL:HG13	2.17	0.44
1:A:509:LEU:HD12	1:A:873:VAL:HG12	1.99	0.44
1:A:939:LEU:HG	1:A:1005:LEU:HD22	2.00	0.44
1:A:965:ALA:O	1:A:966:ILE:O	2.36	0.44
1:A:964:LEU:O	1:A:965:ALA:C	2.58	0.43
1:A:504:GLY:HA2	1:A:891:VAL:HG21	1.99	0.43
1:A:260:ALA:O	1:A:261:LEU:C	2.58	0.43
1:A:507:LEU:HD12	1:A:920:ILE:HG22	2.00	0.43
1:A:689:ALA:HB1	1:A:718:LEU:HD21	2.00	0.43
1:A:965:ALA:O	1:A:966:ILE:C	2.59	0.43
1:A:254:ASP:N	1:A:254:ASP:OD1	2.51	0.43
1:A:1084:ALA:O	1:A:1085:LEU:C	2.55	0.43
1:A:540:VAL:HG21	1:A:546:LEU:HD22	1.99	0.43
1:A:946:ILE:HD12	1:A:946:ILE:HG23	1.76	0.43
1:A:1116:PHE:C	1:A:1118:LEU:N	2.70	0.43
1:A:947:SER:HA	1:A:950:ILE:HG22	2.00	0.43
1:A:1052:SER:O	1:A:1053:LEU:C	2.60	0.43
1:A:497:HIS:HD2	1:A:500:ARG:HB2	1.83	0.43
1:A:956:THR:HG21	1:A:1044:ASN:HD21	1.83	0.42
1:A:255:HIS:CG	1:A:256:TYR:N	2.67	0.42
1:A:1009:MET:HB2	1:A:1009:MET:HE2	1.15	0.42
1:A:1019:GLY:O	1:A:1020:TYR:C	2.58	0.42
1:A:842:PRO:HB3	1:A:869:LEU:HD21	2.00	0.42
1:A:255:HIS:O	1:A:256:TYR:C	2.61	0.42
1:A:664:CYS:HA	1:A:716:LEU:H	1.85	0.42
1:A:548:VAL:HG23	1:A:552:LEU:HD11	2.02	0.41
1:A:226:LYS:O	1:A:279:ARG:NH2	2.52	0.41
1:A:240:TYR:OH	1:A:474:PRO:HD2	2.20	0.41
1:A:441:ILE:HG13	1:A:442:TYR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:PHE:HE1	1:A:845:LEU:HD11	1.86	0.41
1:A:528:VAL:HG22	1:A:722:LEU:HD23	2.03	0.41
1:A:420:LYS:HE2	1:A:995:ALA:HB2	2.03	0.41
1:A:460:ARG:O	1:A:461:ALA:C	2.59	0.41
1:A:778:ALA:H	1:A:829:THR:HG23	1.85	0.41
1:A:205:SER:O	1:A:209:GLN:N	2.49	0.41
1:A:1004:SER:O	1:A:1005:LEU:C	2.61	0.40
1:A:1007:LEU:O	1:A:1008:GLN:C	2.57	0.40
1:A:861:GLU:HA	1:A:864:CYS:HB3	2.03	0.40
1:A:775:ILE:HD11	1:A:794:MET:HE3	2.03	0.40
1:A:338:CYS:SG	1:A:339:MET:N	2.95	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	953/1153 (83%)	840 (88%)	97 (10%)	16 (2%)	7 35

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	PRO
1	A	255	HIS
1	A	454	LEU
1	A	1172	PRO
1	A	119	PRO
1	A	1025	ALA
1	A	484	ALA
1	A	954	ILE
1	A	1036	VAL
1	A	188	LEU

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Mol	Chain	Res	Type
1	A	485	GLN
1	A	299	ARG
1	A	1039	PRO
1	A	118	GLU
1	A	1042	LEU
1	A	473	LEU

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	724/980 (74%)	675 (93%)	49 (7%)	14	42

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	LEU
1	A	262	CYS
1	A	263	ILE
1	A	264	PHE
1	A	265	LEU
1	A	474	PRO
1	A	479	VAL
1	A	480	CYS
1	A	482	LEU
1	A	937	MET
1	A	940	TYR
1	A	941	SER
1	A	942	LEU
1	A	950	ILE
1	A	961	LEU
1	A	962	GLN
1	A	970	ILE
1	A	972	THR
1	A	1002	LEU
1	A	1006	LEU

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Mol	Chain	Res	Type
1	A	1008	GLN
1	A	1009	MET
1	A	1011	LEU
1	A	1013	THR
1	A	1015	VAL
1	A	1032	LEU
1	A	1046	GLU
1	A	1047	ASN
1	A	1049	VAL
1	A	1055	SER
1	A	1057	GLN
1	A	1059	LEU
1	A	1061	LEU
1	A	1079	VAL
1	A	1080	PRO
1	A	1083	VAL
1	A	1087	LEU
1	A	1090	SER
1	A	1096	VAL
1	A	1116	PHE
1	A	1118	LEU
1	A	1121	LEU
1	A	1123	LEU
1	A	1124	VAL
1	A	1129	VAL
1	A	1135	GLU
1	A	1136	SER
1	A	1162	LEU
1	A	1163	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	GLN
1	A	219	ASN
1	A	341	ASN
1	A	390	HIS
1	A	497	HIS
1	A	726	ASN
1	A	836	HIS

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](#)

1 ligand is modelled in this entry.

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	$\# Z > 2$
2	SPM	A	1201	-	13,13,13	0.28	0	12,12,12	1.58	3 (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
2	SPM	A	1201	-	-	3/11/11/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	SPM	C7-C6-N5	-3.06	103.87	112.07
2	A	1201	SPM	C11-N10-C9	-2.29	102.59	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	SPM	C3-C4-N5	-2.09	106.47	112.07

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	SPM	C8-C9-N10-C11
2	A	1201	SPM	C3-C4-N5-C6
2	A	1201	SPM	C2-C3-C4-N5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	SPM	1	0

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.

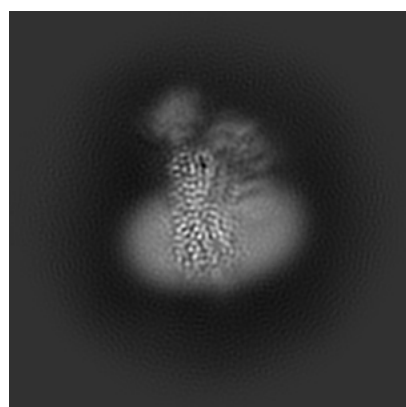
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31627. These allow visual inspection of the internal detail of the map and identification of artifacts.

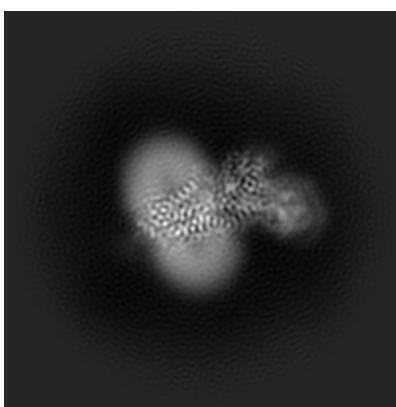
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

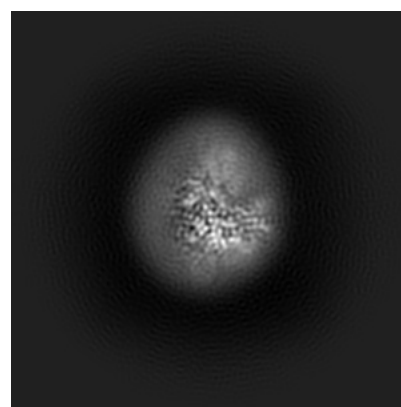
6.1.1 Primary map



X



Y

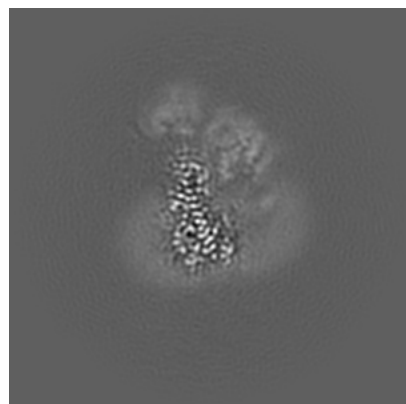


Z

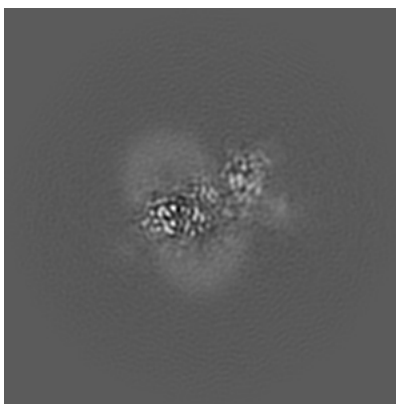
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

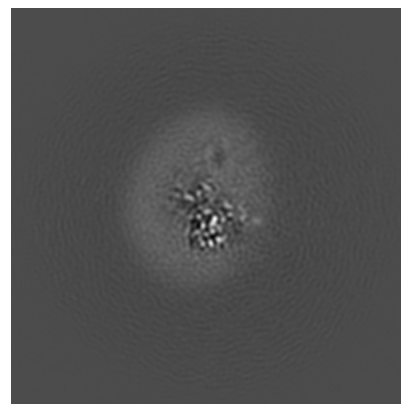
6.2.1 Primary map



X Index: 120



Y Index: 120

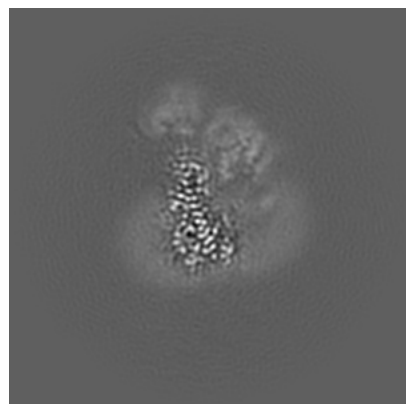


Z Index: 120

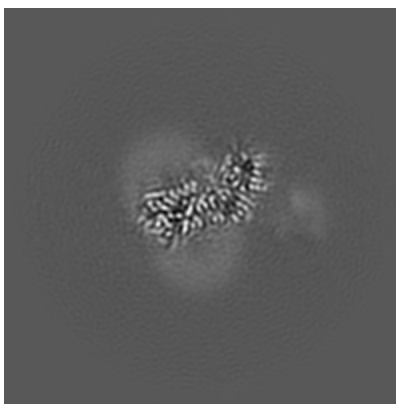
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

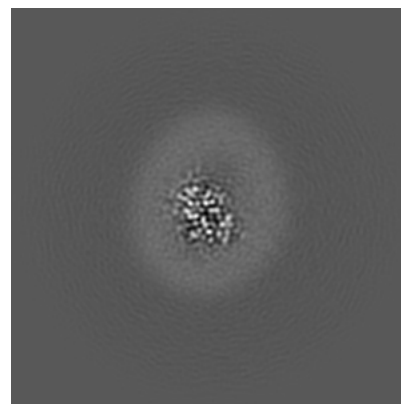
6.3.1 Primary map



X Index: 120



Y Index: 112

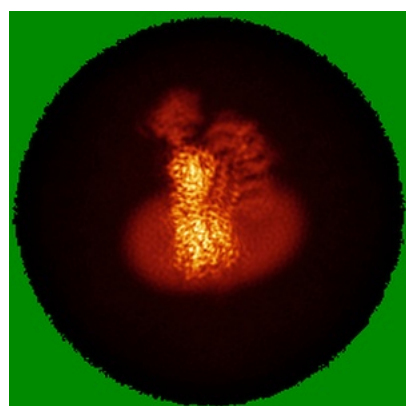


Z Index: 105

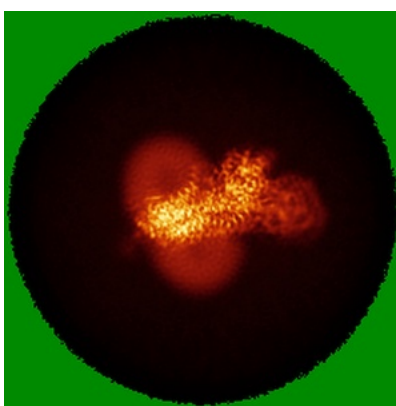
The images above show the largest variance slices of the map in three orthogonal directions.

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

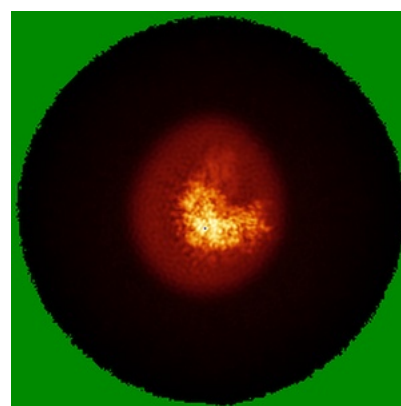
6.4.1 Primary map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

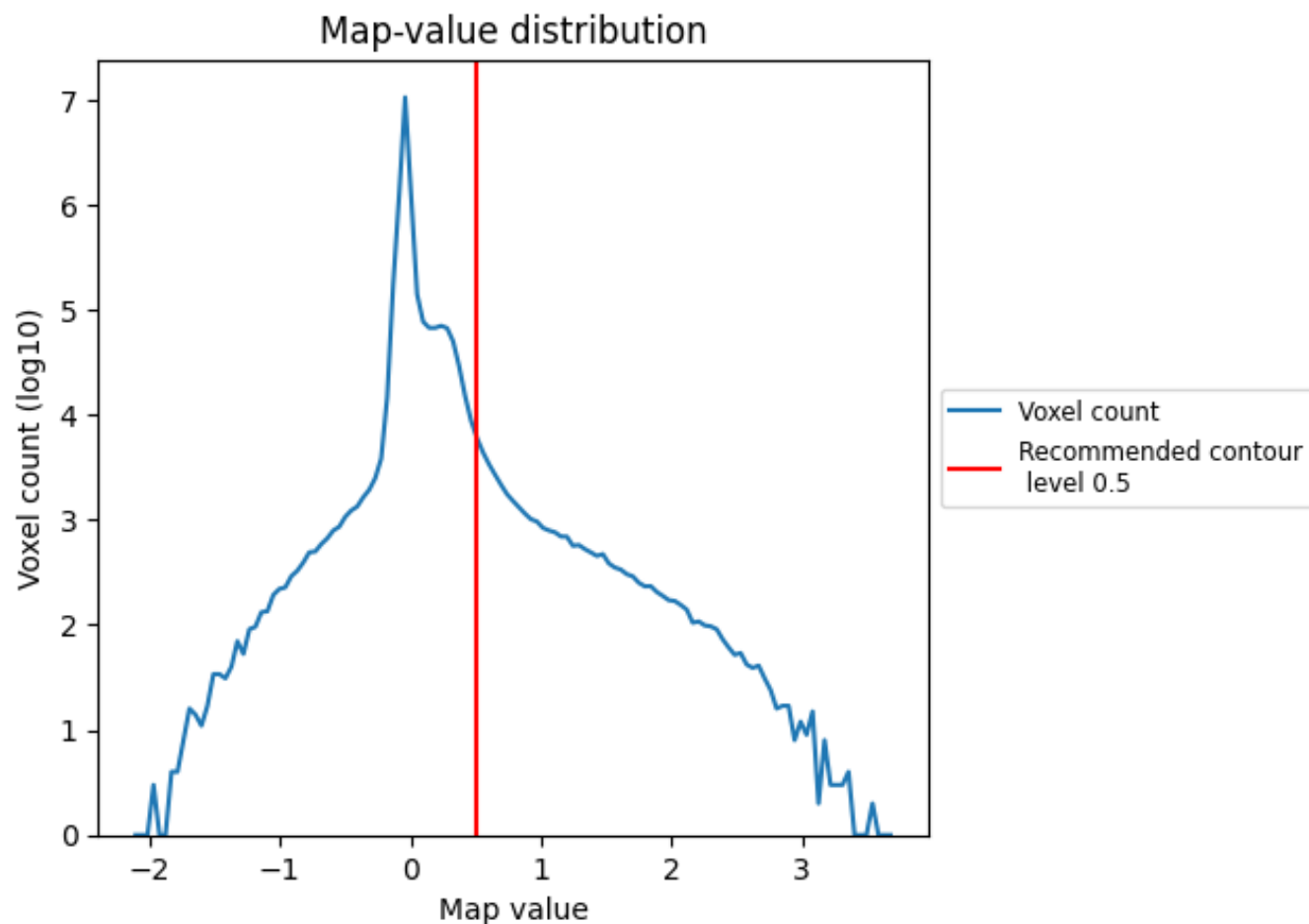
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

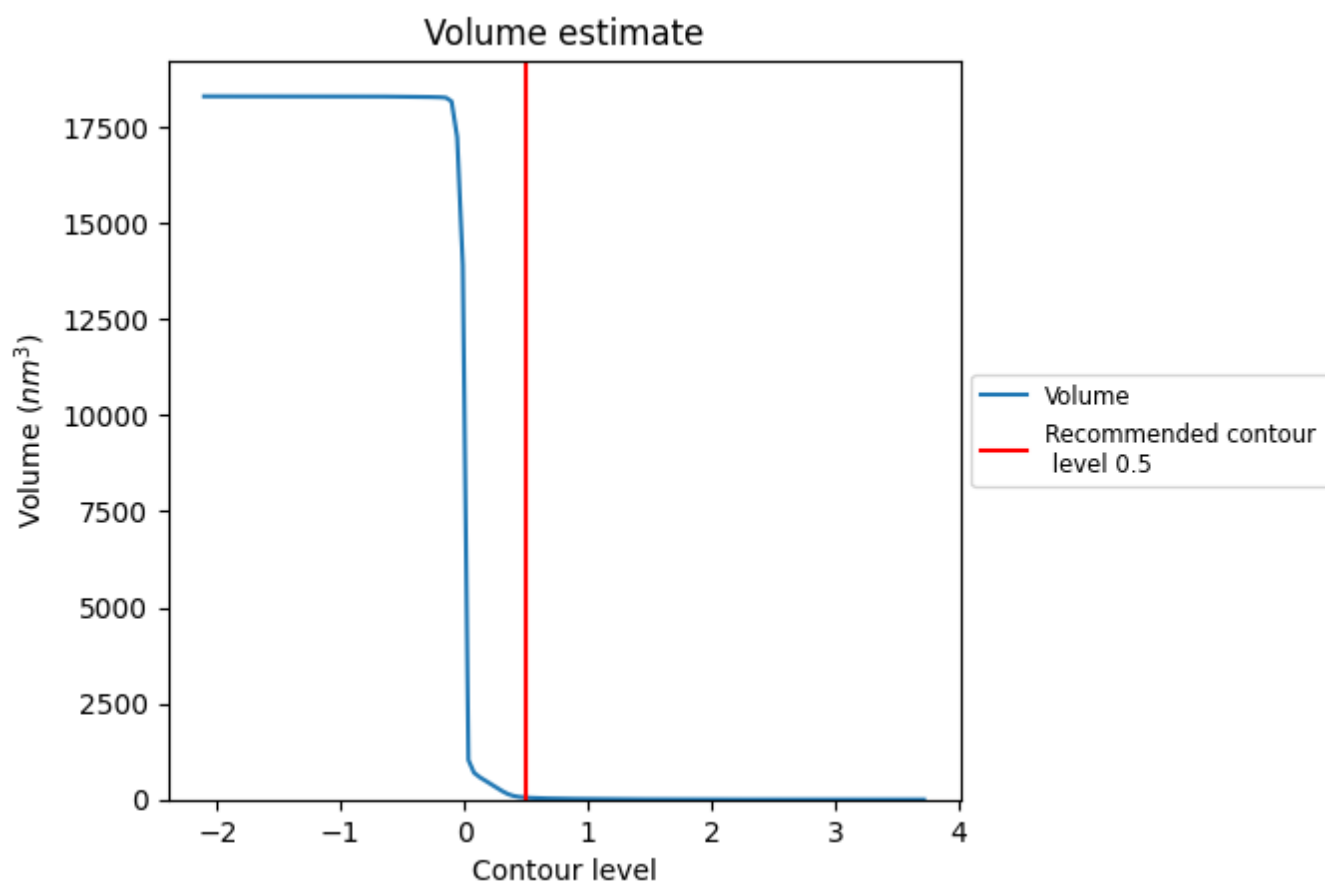
This section contains the results of statistical analysis of the map.

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.

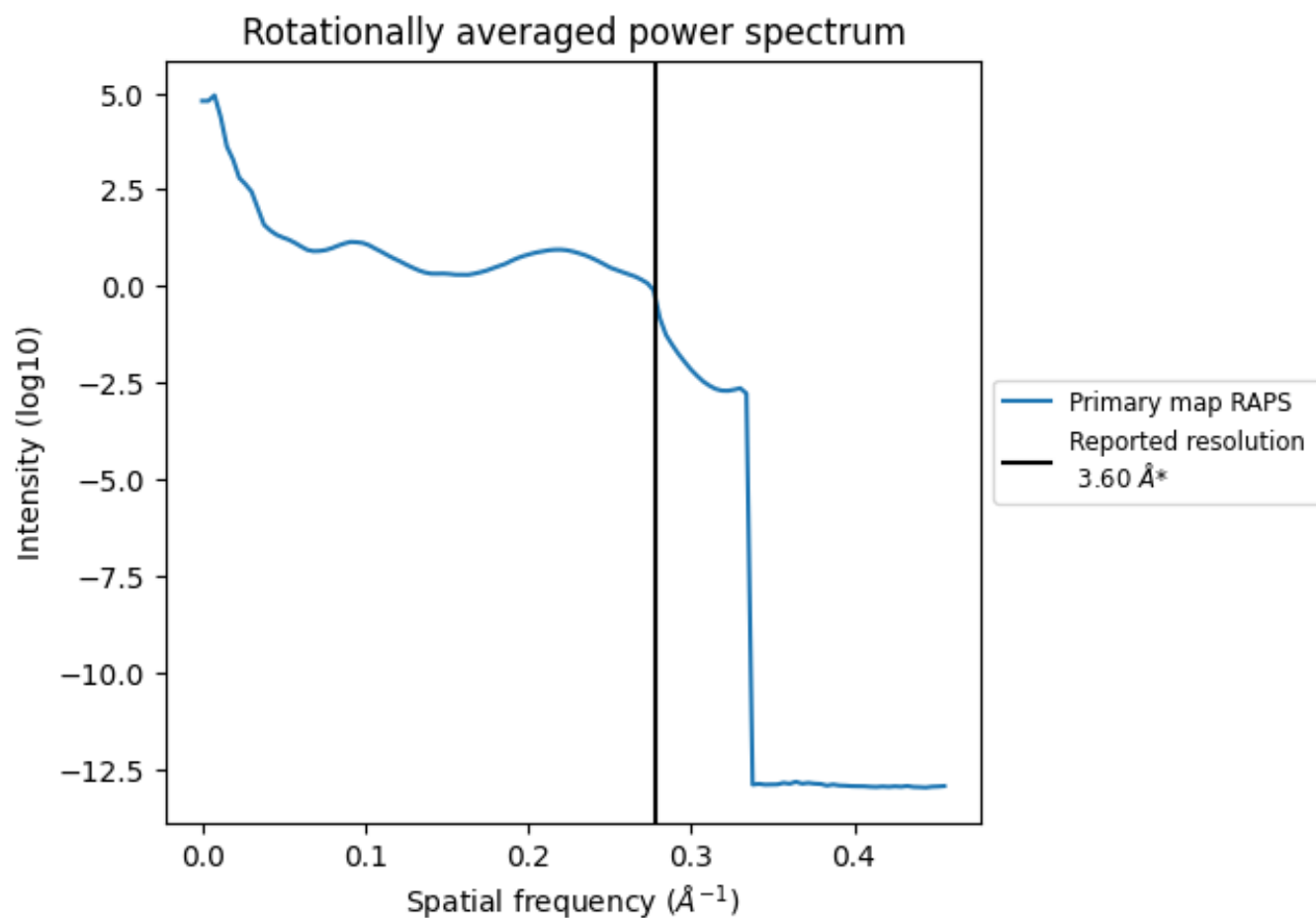
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 52 nm³; this corresponds to an approximate mass of 47 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

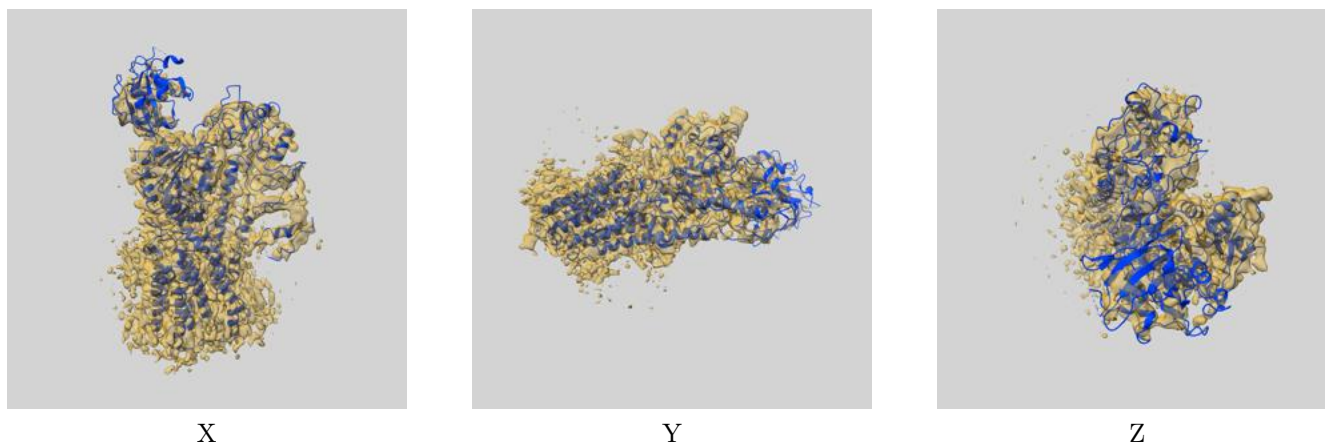
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

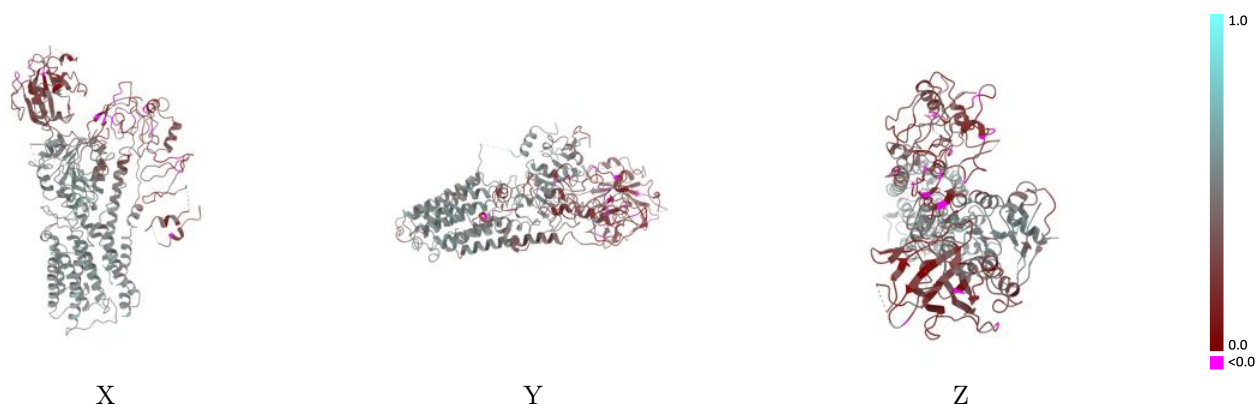
This section contains information regarding the fit between EMDB map EMD-31627 and PDB model 7FJQ. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.5 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](#)

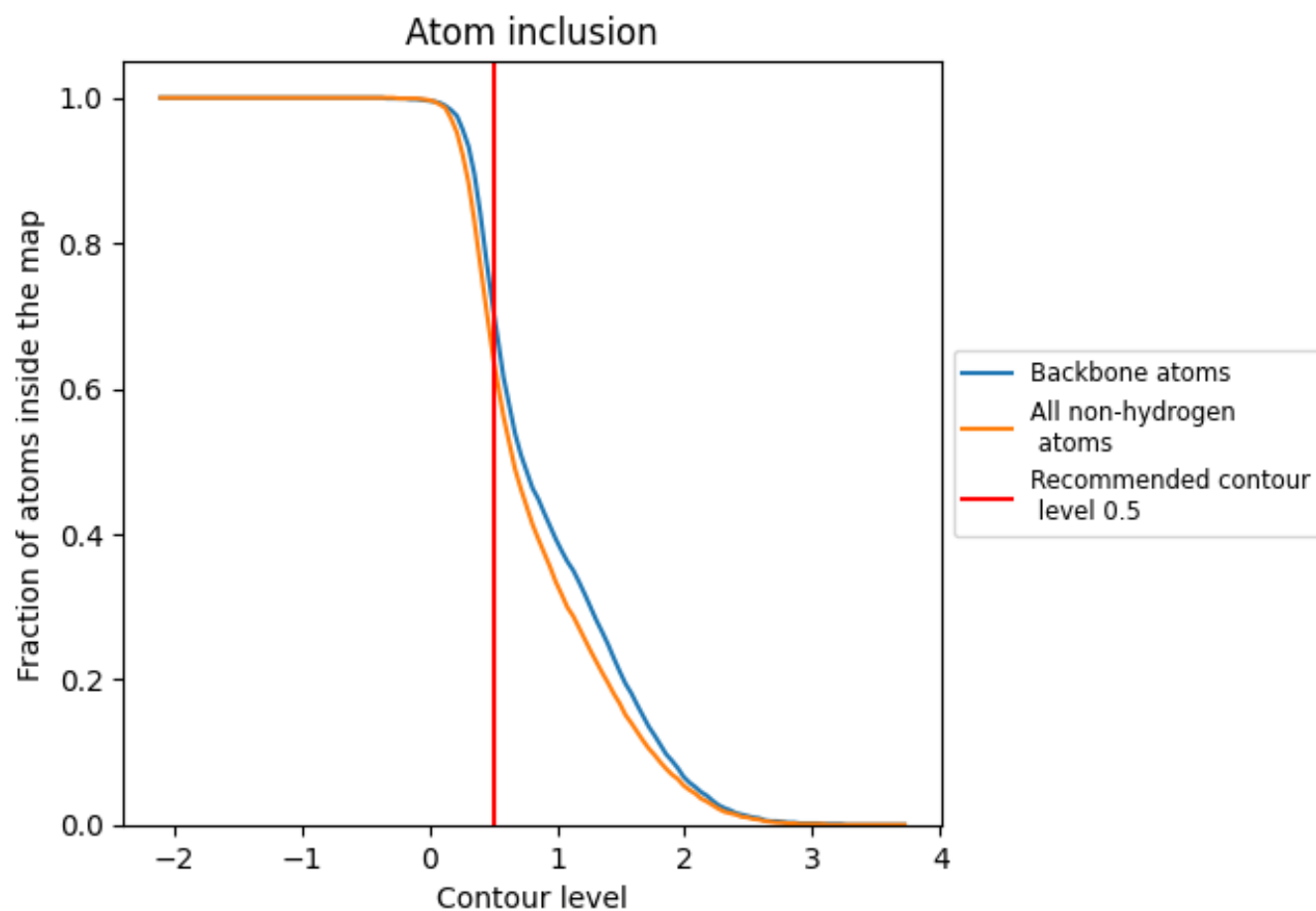


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 64% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6420	0.3990
A	0.6420	0.3990

