



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 04:48 PM UTC

PDB ID : 6YRK / pdb_00006yrk
EMDB ID : EMD-10890
Title : P140-P110 complex fitted into the cryo-electron density map of the heterodimer
Authors : Scheffer, M.P.; Aparicio, D.
Deposited on : 2020-04-20
Resolution : 4.10 Å (reported)
Based on initial models : 6RUT, 6R3T

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

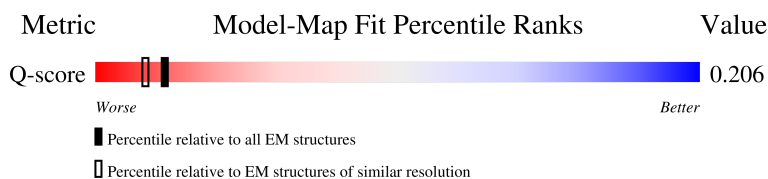
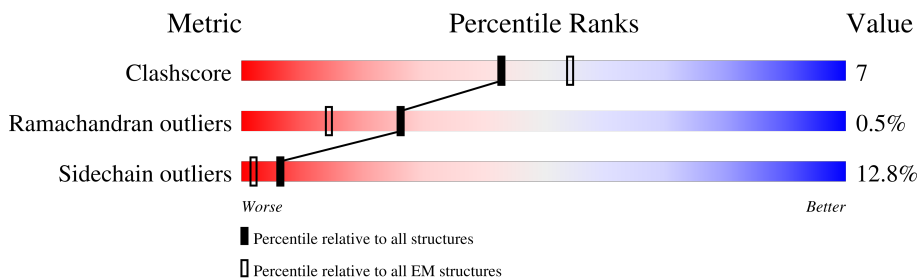
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	777	15% 79% 18% .
2	B	1160	17% 70% 25% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15058 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 Mgp-operon protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	777	Total	C	N	O	S	0	0
			5982	3740	1003	1233	6		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP P22747
A	?	-	ILE	deletion	UNP P22747
A	?	-	GLY	deletion	UNP P22747
A	?	-	GLY	deletion	UNP P22747
A	?	-	GLY	deletion	UNP P22747
A	?	-	SER	deletion	UNP P22747
A	?	-	SER	deletion	UNP P22747
A	?	-	SER	deletion	UNP P22747
A	?	-	SER	deletion	UNP P22747
A	?	-	SER	deletion	UNP P22747
A	?	-	SER	deletion	UNP P22747

- Molecule 2 is a protein called Adhesin P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1160	Total	C	N	O	S	0	0
			9076	5750	1541	1772	13		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASN	deletion	UNP P20796
B	?	-	SER	deletion	UNP P20796
B	?	-	SER	deletion	UNP P20796
B	?	-	ASP	deletion	UNP P20796
B	?	-	LYS	deletion	UNP P20796
B	?	-	ALA	deletion	UNP P20796

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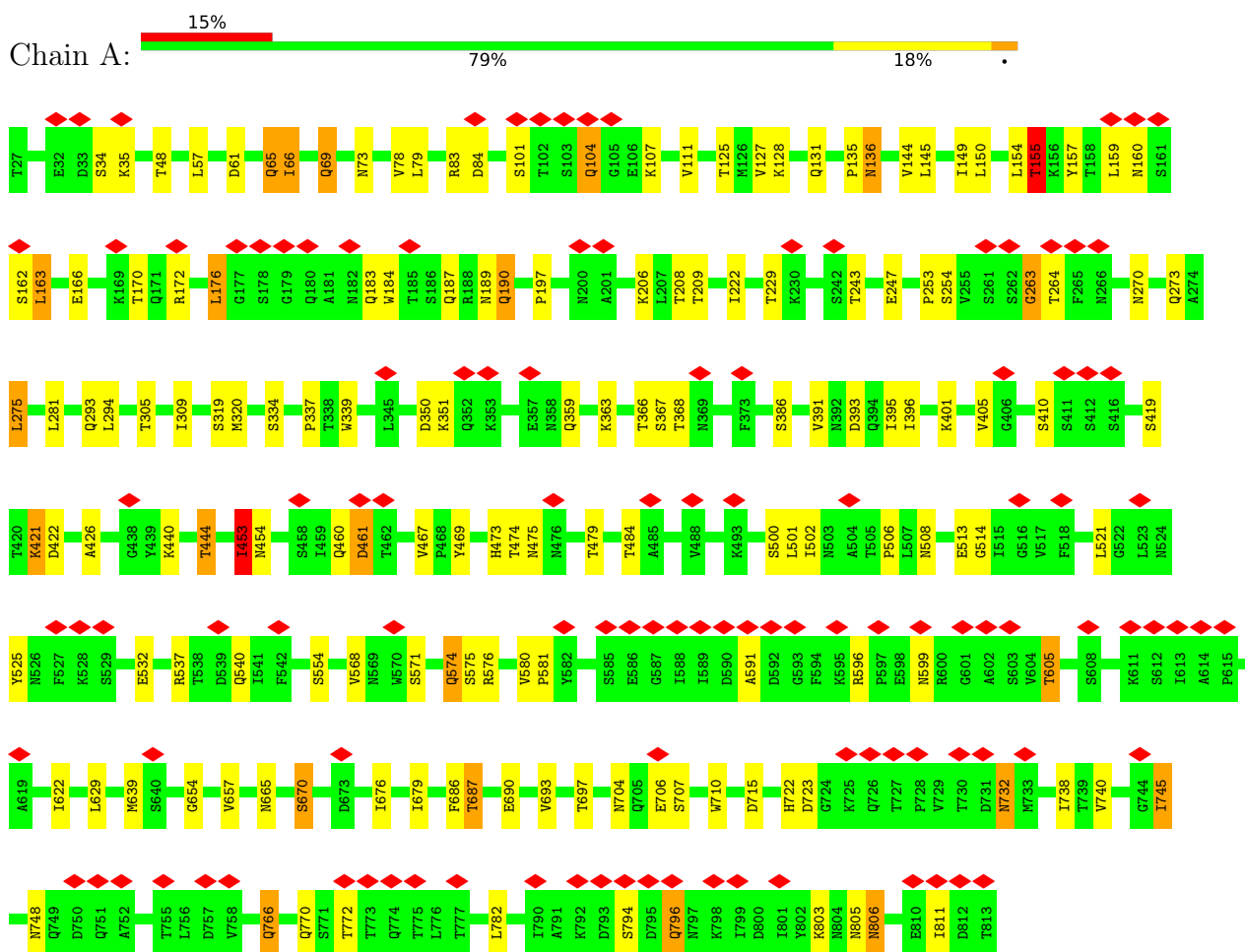
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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP P20796
B	?	-	GLN	deletion	UNP P20796
B	?	-	SER	deletion	UNP P20796
B	?	-	PRO	deletion	UNP P20796
B	?	-	SER	deletion	UNP P20796
B	?	-	THR	deletion	UNP P20796
B	?	-	SER	deletion	UNP P20796
B	?	-	ALA	deletion	UNP P20796
B	789	ALA	SER	conflict	UNP P20796
B	?	-	SER	deletion	UNP P20796
B	?	-	SER	deletion	UNP P20796
B	?	-	THR	deletion	UNP P20796
B	?	-	THR	deletion	UNP P20796
B	?	-	TYR	deletion	UNP P20796
B	?	-	ASP	deletion	UNP P20796
B	?	-	THR	deletion	UNP P20796
B	?	-	SER	deletion	UNP P20796
B	?	-	GLN	deletion	UNP P20796
B	?	-	GLY	deletion	UNP P20796
B	?	-	ASN	deletion	UNP P20796

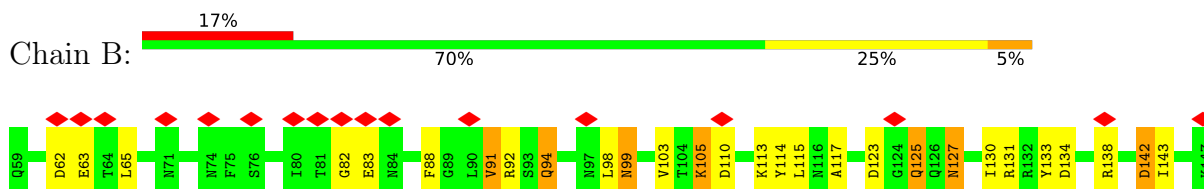
3 Residue-property plots

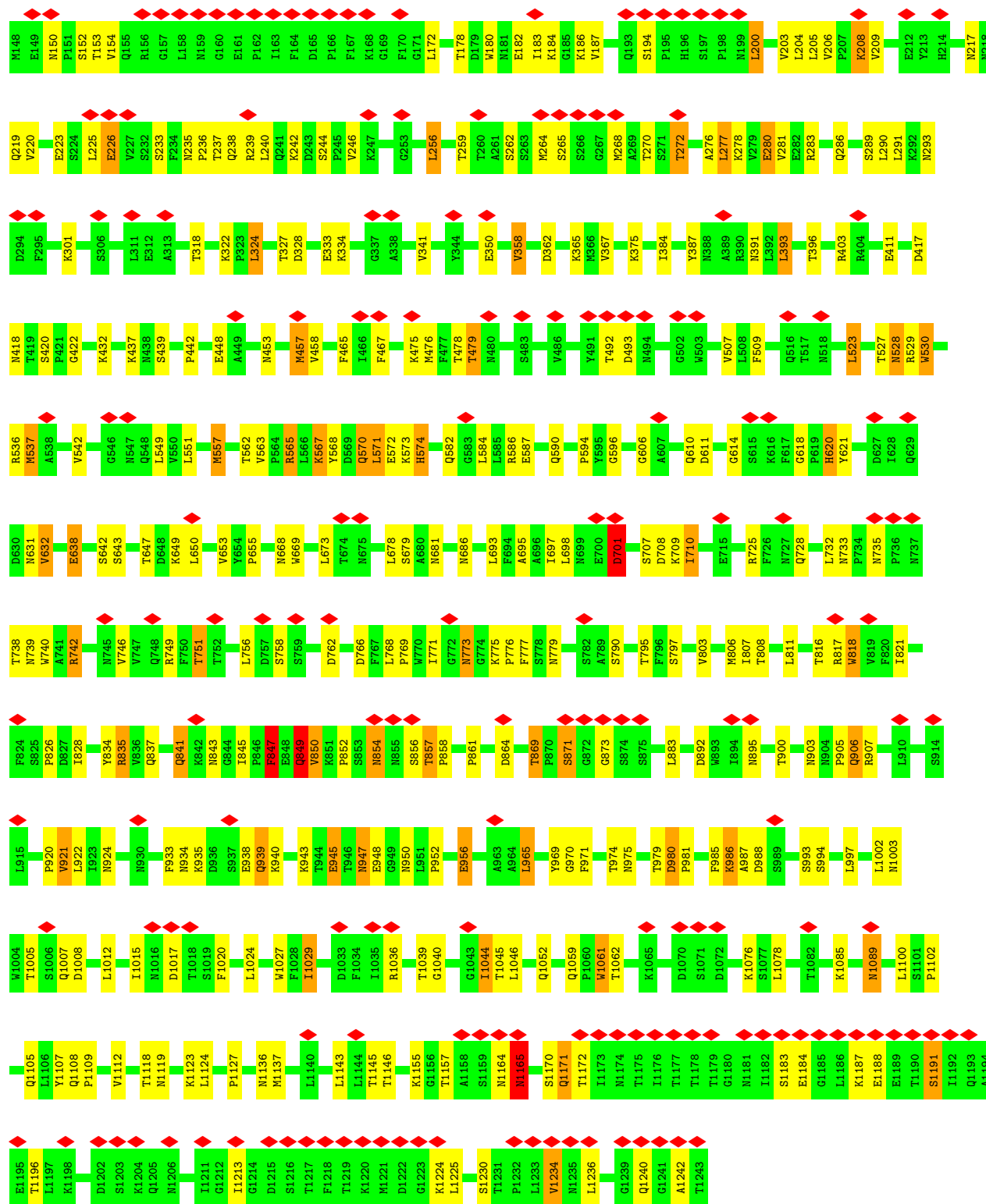
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Mgp-operon protein 3



• Molecule 2: Adhesin P1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37009	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 ($e^-/\text{\AA}^2$)	7.5	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	0.034	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	283.5, 283.5, 283.5	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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	0.83	1/6105 (0.0%)	1.33	33/8298 (0.4%)
2	B	0.87	5/9303 (0.1%)	1.38	67/12656 (0.5%)
All	All	0.85	6/15408 (0.0%)	1.36	100/20954 (0.5%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	537	MET	SD-CE	-6.27	1.63	1.79
2	B	557	MET	SD-CE	-5.96	1.64	1.79
2	B	1020	PHE	CA-C	5.80	1.59	1.52
2	B	457	MET	SD-CE	-5.30	1.66	1.79
1	A	502	ILE	CA-C	5.23	1.59	1.52
2	B	206	VAL	CA-C	5.09	1.56	1.52

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	99	ASN	CA-CB-CG	9.30	121.90	112.60
2	B	701	ASP	CA-CB-CG	8.53	121.13	112.60
2	B	987	ALA	CA-C-N	8.37	133.40	121.02
2	B	987	ALA	C-N-CA	8.37	133.40	121.02
2	B	849	GLN	CA-C-N	7.33	131.47	120.77
2	B	849	GLN	C-N-CA	7.33	131.47	120.77
2	B	849	GLN	N-CA-C	-7.26	101.53	111.56
2	B	225	LEU	CA-C-N	7.00	131.31	120.75
2	B	225	LEU	C-N-CA	7.00	131.31	120.75
2	B	647	THR	CA-C-N	6.79	129.68	120.38
2	B	647	THR	C-N-CA	6.79	129.68	120.38
2	B	134	ASP	CA-CB-CG	6.71	119.31	112.60
2	B	530	TRP	N-CA-C	-6.70	97.81	108.73
2	B	217	ASN	CA-CB-CG	6.62	119.22	112.60
2	B	632	VAL	N-CA-C	-6.60	106.09	112.29
2	B	856	SER	N-CA-C	-6.59	102.58	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	SER	CA-C-N	6.50	128.98	120.28
1	A	162	SER	C-N-CA	6.50	128.98	120.28
2	B	563	VAL	N-CA-CB	6.37	115.42	110.45
1	A	160	ASN	CA-CB-CG	6.26	118.86	112.60
1	A	155	THR	CA-C-N	6.24	129.27	120.28
1	A	155	THR	C-N-CA	6.24	129.27	120.28
2	B	970	GLY	CA-C-N	6.14	129.12	120.28
2	B	970	GLY	C-N-CA	6.14	129.12	120.28
2	B	762	ASP	CA-C-N	6.11	128.47	120.28
2	B	762	ASP	C-N-CA	6.11	128.47	120.28
2	B	1165	ASN	N-CA-C	6.07	116.25	108.24
1	A	183	GLN	CA-C-N	5.92	128.14	120.44
1	A	183	GLN	C-N-CA	5.92	128.14	120.44
2	B	574	HIS	CA-C-N	5.80	128.32	120.38
2	B	574	HIS	C-N-CA	5.80	128.32	120.38
2	B	818	TRP	CA-C-N	5.79	127.97	120.56
2	B	818	TRP	C-N-CA	5.79	127.97	120.56
1	A	805	ASN	CA-C-N	5.73	130.55	122.46
1	A	805	ASN	C-N-CA	5.73	130.55	122.46
1	A	144	VAL	N-CA-C	-5.70	106.14	111.45
2	B	246	VAL	CA-C-N	5.67	128.82	120.82
2	B	246	VAL	C-N-CA	5.67	128.82	120.82
2	B	847	PHE	CA-C-N	5.65	131.60	121.15
2	B	847	PHE	C-N-CA	5.65	131.60	121.15
2	B	509	PHE	CA-CB-CG	5.54	119.34	113.80
2	B	947	ASN	CA-C-N	5.53	128.24	120.28
2	B	947	ASN	C-N-CA	5.53	128.24	120.28
1	A	461	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	513	GLU	CA-C-N	5.51	126.22	119.99
1	A	513	GLU	C-N-CA	5.51	126.22	119.99
2	B	631	ASN	CA-CB-CG	5.51	118.11	112.60
2	B	183	ILE	CA-C-N	5.50	129.08	120.82
2	B	183	ILE	C-N-CA	5.50	129.08	120.82
1	A	422	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	184	TRP	CA-C-N	5.48	127.89	120.38
1	A	184	TRP	C-N-CA	5.48	127.89	120.38
2	B	856	SER	CA-C-N	5.48	135.17	121.80
2	B	856	SER	C-N-CA	5.48	135.17	121.80
1	A	732	ASN	CA-CB-CG	5.44	118.04	112.60
2	B	507	VAL	CA-C-N	5.43	128.10	120.28
2	B	507	VAL	C-N-CA	5.43	128.10	120.28
1	A	263	GLY	N-CA-C	5.43	118.30	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1119	ASN	CA-C-N	5.41	127.47	120.44
2	B	1119	ASN	C-N-CA	5.41	127.47	120.44
1	A	473	HIS	N-CA-C	5.39	118.12	110.10
2	B	62	ASP	CA-CB-CG	5.37	117.97	112.60
2	B	217	ASN	CA-C-N	5.36	128.21	120.38
2	B	217	ASN	C-N-CA	5.36	128.21	120.38
1	A	723	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	101	SER	CA-C-N	5.33	128.82	120.82
1	A	101	SER	C-N-CA	5.33	128.82	120.82
2	B	208	LYS	CA-C-N	5.33	127.28	120.56
2	B	208	LYS	C-N-CA	5.33	127.28	120.56
1	A	772	THR	N-CA-C	-5.32	106.67	114.39
2	B	142	ASP	N-CA-C	5.31	119.45	111.96
2	B	417	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	554	SER	CA-C-N	5.31	127.39	120.28
1	A	554	SER	C-N-CA	5.31	127.39	120.28
1	A	61	ASP	CA-C-N	5.30	128.12	120.38
1	A	61	ASP	C-N-CA	5.30	128.12	120.38
2	B	854	ASN	CA-CB-CG	5.26	117.86	112.60
1	A	745	ILE	N-CA-CB	5.25	116.84	110.95
2	B	980	ASP	CA-CB-CG	5.25	117.84	112.60
2	B	1089	ASN	CA-CB-CG	5.23	117.83	112.60
1	A	686	PHE	CA-CB-CG	5.22	119.03	113.80
2	B	847	PHE	CA-CB-CG	5.22	119.02	113.80
2	B	1155	LYS	CA-C-N	5.21	125.87	119.99
2	B	1155	LYS	C-N-CA	5.21	125.87	119.99
2	B	571	LEU	CA-C-N	5.18	127.48	120.38
2	B	571	LEU	C-N-CA	5.18	127.48	120.38
1	A	145	LEU	CA-C-N	5.16	127.50	120.54
1	A	145	LEU	C-N-CA	5.16	127.50	120.54
2	B	1145	THR	CA-C-N	5.14	127.48	120.54
2	B	1145	THR	C-N-CA	5.14	127.48	120.54
2	B	861	PRO	N-CA-C	-5.08	103.30	111.38
1	A	766	GLN	CA-C-N	5.08	127.40	120.54
1	A	766	GLN	C-N-CA	5.08	127.40	120.54
2	B	779	ASN	CA-C-N	5.07	127.05	120.26
2	B	779	ASN	C-N-CA	5.07	127.05	120.26
2	B	82	GLY	CA-C-N	5.03	129.19	121.19
2	B	82	GLY	C-N-CA	5.03	129.19	121.19
2	B	103	VAL	CA-C-N	5.03	128.01	120.87
2	B	103	VAL	C-N-CA	5.03	128.01	120.87
2	B	858	PRO	N-CA-C	5.01	119.07	111.15

There are no chirality outliers.

There are no planarity outliers.

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	5982	0	5775	62	0
2	B	9076	0	8814	144	0
All	All	15058	0	14589	196	0

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

All (196) 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:440:LYS:O	1:A:444:THR:HG23	1.63	0.97
2:B:527:THR:HG23	2:B:678:LEU:HD23	1.46	0.94
1:A:66:ILE:HD11	1:A:69:GLN:HG3	1.54	0.90
2:B:280:GLU:HG3	2:B:650:LEU:HD12	1.59	0.85
2:B:766:ASP:OD2	2:B:797:SER:HB3	1.84	0.78
2:B:924:ASN:HB2	2:B:985:PHE:HA	1.67	0.77
1:A:596:ARG:HB2	1:A:599:ASN:ND2	2.00	0.76
2:B:988:ASP:OD1	2:B:993:SER:HB2	1.86	0.75
1:A:66:ILE:HD12	1:A:78:VAL:HG13	1.67	0.75
1:A:474:THR:HG21	1:A:479:THR:CG2	2.18	0.74
2:B:65:LEU:HB3	2:B:91:VAL:HG13	1.70	0.73
1:A:474:THR:HG21	1:A:479:THR:HG21	1.70	0.73
1:A:65:GLN:HE22	1:A:83:ARG:HG3	1.55	0.72
1:A:136:ASN:HD22	1:A:136:ASN:H	1.37	0.71
1:A:687:THR:HG23	1:A:690:GLU:OE1	1.90	0.70
1:A:104:GLN:HA	1:A:104:GLN:OE1	1.91	0.70
2:B:773:ASN:HD22	2:B:775:LYS:HB2	1.55	0.70
1:A:596:ARG:HB2	1:A:599:ASN:HD22	1.54	0.69
1:A:155:THR:HG22	1:A:157:TYR:H	1.58	0.69
2:B:835:ARG:HD3	2:B:845:ILE:HG21	1.76	0.68
2:B:537:MET:HE1	2:B:551:LEU:HD21	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:262:SER:HB2	2:B:643:SER:HB3	1.76	0.67
2:B:286:GLN:OE1	2:B:289:SER:HB3	1.97	0.65
2:B:994:SER:HB2	2:B:1137:MET:HE2	1.78	0.65
2:B:1005:THR:HG22	2:B:1007:GLN:H	1.63	0.64
1:A:794:SER:H	1:A:796:GLN:HE22	1.45	0.63
1:A:187:GLN:O	1:A:190:GLN:HG2	1.99	0.62
2:B:226:GLU:HB2	2:B:239:ARG:CZ	2.29	0.62
1:A:460:GLN:HG3	2:B:895:ASN:HB2	1.82	0.62
2:B:278:LYS:HB2	2:B:650:LEU:HD11	1.82	0.62
2:B:527:THR:HG23	2:B:678:LEU:CD2	2.25	0.61
2:B:590:GLN:CD	2:B:906:GLN:HG2	2.26	0.61
2:B:921:VAL:HG13	2:B:965:LEU:HD13	1.83	0.61
2:B:341:VAL:HG22	2:B:358:VAL:HB	1.83	0.60
1:A:475:ASN:O	2:B:817:ARG:HD2	2.01	0.60
1:A:166:GLU:HG3	1:A:206:LYS:HB2	1.83	0.60
2:B:110:ASP:HA	2:B:220:VAL:HG13	1.83	0.59
1:A:475:ASN:ND2	2:B:817:ARG:H	2.00	0.59
2:B:934:ASN:O	2:B:938:GLU:HB2	2.01	0.59
1:A:135:PRO:HB3	1:A:337:PRO:HG2	1.85	0.59
2:B:268:MET:HB2	2:B:871:SER:OG	2.02	0.58
1:A:670:SER:HA	1:A:679:ILE:HG22	1.85	0.58
2:B:611:ASP:OD1	2:B:614:GLY:HA2	2.03	0.57
2:B:237:THR:HG22	2:B:1108:GLN:HG3	1.87	0.57
2:B:240:LEU:HB2	2:B:584:LEU:HD22	1.86	0.57
2:B:115:LEU:HD11	2:B:324:LEU:HD22	1.87	0.57
2:B:807:ILE:HG21	2:B:828:ILE:HD12	1.86	0.57
1:A:475:ASN:HD22	2:B:817:ARG:H	1.51	0.57
2:B:849:GLN:HE22	2:B:883:LEU:HD12	1.69	0.57
1:A:66:ILE:HD12	1:A:78:VAL:CG1	2.35	0.56
1:A:197:PRO:HD2	1:A:453:ILE:HD11	1.88	0.55
2:B:590:GLN:OE1	2:B:906:GLN:HG2	2.06	0.55
1:A:66:ILE:HD11	1:A:69:GLN:CG	2.31	0.55
2:B:695:ALA:HB3	2:B:751:THR:HG22	1.88	0.55
2:B:1046:LEU:HD12	2:B:1213:ILE:HD12	1.87	0.55
2:B:773:ASN:HB3	2:B:775:LYS:H	1.72	0.55
2:B:773:ASN:HD21	2:B:975:ASN:HB3	1.72	0.54
2:B:777:PHE:O	2:B:795:THR:HG22	2.07	0.54
2:B:391:ASN:HD22	2:B:418:ASN:HD22	1.56	0.53
1:A:766:GLN:O	2:B:742:ARG:HD2	2.07	0.53
2:B:1234:VAL:HG13	2:B:1236:LEU:HG	1.89	0.53
2:B:194:SER:HB2	2:B:200:LEU:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:ASN:HD22	2:B:236:PRO:HD2	1.73	0.53
2:B:1003:ASN:HB3	2:B:1102:PRO:HG2	1.91	0.53
2:B:98:LEU:HD12	2:B:125:GLN:HG2	1.90	0.52
1:A:111:VAL:HG11	1:A:309:ILE:HG21	1.91	0.52
1:A:514:GLY:HA2	1:A:605:THR:HG23	1.92	0.52
2:B:852:PRO:HB2	2:B:857:THR:HG22	1.89	0.52
2:B:476:MET:H	2:B:479:THR:HG22	1.74	0.51
2:B:1008:ASP:HB3	2:B:1061:TRP:CD1	2.45	0.51
2:B:283:ARG:HD2	2:B:290:LEU:HD23	1.91	0.51
2:B:528:ASN:ND2	2:B:530:TRP:HE3	2.09	0.51
2:B:769:PRO:HA	2:B:776:PRO:HA	1.93	0.50
1:A:281:LEU:H	1:A:293:GLN:HE22	1.59	0.50
2:B:693:LEU:HD21	2:B:1024:LEU:HD22	1.94	0.50
2:B:244:SER:HB2	2:B:568:TYR:O	2.12	0.50
1:A:693:VAL:HG21	1:A:738:ILE:HD11	1.93	0.49
2:B:952:PRO:HG2	2:B:956:GLU:HG2	1.93	0.49
2:B:362:ASP:HB3	2:B:365:LYS:HG2	1.93	0.49
2:B:268:MET:HG3	2:B:638:GLU:OE1	2.13	0.49
2:B:277:LEU:HB2	2:B:653:VAL:HB	1.94	0.49
2:B:920:PRO:HB2	2:B:997:LEU:HG	1.94	0.49
2:B:1029:ILE:HD11	2:B:1044:ILE:HG12	1.95	0.49
1:A:521:LEU:HD23	1:A:580:VAL:HG23	1.95	0.49
2:B:903:ASN:O	2:B:907:ARG:HG3	2.12	0.49
2:B:969:TYR:HB3	2:B:971:PHE:CD1	2.47	0.49
2:B:492:THR:HG22	2:B:493:ASP:N	2.28	0.49
2:B:742:ARG:HG2	2:B:742:ARG:HH11	1.78	0.48
2:B:892:ASP:HA	2:B:900:THR:HG23	1.96	0.48
2:B:138:ARG:HG2	2:B:1242:ALA:HB1	1.94	0.48
1:A:710:TRP:HB2	1:A:740:VAL:HB	1.96	0.48
2:B:1165:ASN:C	2:B:1165:ASN:HD22	2.21	0.48
1:A:704:ASN:HB3	1:A:707:SER:HB2	1.95	0.48
1:A:273:GLN:HG2	1:A:722:HIS:HD2	1.79	0.47
2:B:939:GLN:HE21	2:B:950:ASN:HB2	1.80	0.47
1:A:806:ASN:ND2	2:B:701:ASP:O	2.48	0.47
2:B:180:TRP:O	2:B:184:LYS:HB2	2.15	0.47
2:B:570:GLN:HG3	2:B:573:LYS:HE3	1.96	0.47
2:B:549:LEU:HD23	2:B:698:LEU:HB2	1.97	0.47
2:B:92:ARG:HD3	2:B:94:GLN:NE2	2.30	0.46
1:A:475:ASN:ND2	2:B:816:THR:H	2.13	0.46
2:B:1078:LEU:HD22	2:B:1225:LEU:HD23	1.97	0.46
2:B:1027:TRP:CE3	2:B:1046:LEU:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:LEU:HD23	2:B:565:ARG:HD2	1.97	0.46
2:B:837:GLN:HB3	2:B:841:GLN:HB3	1.98	0.46
2:B:1109:PRO:HB3	2:B:1137:MET:HE1	1.98	0.46
1:A:127:VAL:HG12	1:A:128:LYS:HG3	1.97	0.46
2:B:808:THR:HG23	2:B:826:PRO:CG	2.46	0.46
2:B:259:THR:HG22	2:B:278:LYS:HD3	1.96	0.46
1:A:222:ILE:HD12	1:A:270:ASN:HD21	1.81	0.46
2:B:668:ASN:HB2	2:B:669:TRP:CE3	2.50	0.46
2:B:924:ASN:ND2	2:B:986:LYS:H	2.14	0.46
2:B:223:GLU:HG3	2:B:478:THR:OG1	2.16	0.46
2:B:945:GLU:H	2:B:945:GLU:HG3	1.38	0.46
1:A:454:ASN:ND2	1:A:467:VAL:H	2.14	0.45
1:A:525:TYR:CE1	1:A:591:ALA:HB1	2.50	0.45
2:B:697:ILE:HD12	2:B:749:ARG:HB2	1.98	0.45
2:B:841:GLN:HE21	2:B:841:GLN:HA	1.81	0.45
2:B:988:ASP:CG	2:B:993:SER:HB2	2.41	0.45
1:A:461:ASP:HB3	2:B:811:LEU:HD13	1.99	0.45
1:A:506:PRO:HB2	1:A:540:GLN:HA	1.99	0.45
2:B:735:ASN:HB2	2:B:738:THR:HG23	1.98	0.45
2:B:1112:VAL:HA	2:B:1127:PRO:HA	1.98	0.45
2:B:1191:SER:HB3	2:B:1196:THR:HG23	1.97	0.45
1:A:135:PRO:HA	1:A:337:PRO:HD2	1.98	0.45
2:B:65:LEU:HD21	2:B:127:ASN:HB3	1.99	0.45
2:B:272:THR:HG21	2:B:864:ASP:HB3	1.99	0.45
2:B:777:PHE:HB3	2:B:795:THR:CG2	2.46	0.45
1:A:574:GLN:HE21	1:A:575:SER:H	1.64	0.45
2:B:105:LYS:H	2:B:105:LYS:HD2	1.81	0.45
2:B:114:TYR:O	2:B:117:ALA:HB3	2.17	0.45
1:A:405:VAL:HG11	1:A:426:ALA:HB2	1.98	0.45
1:A:410:SER:HB2	1:A:421:LYS:HG3	1.97	0.44
2:B:834:TYR:CZ	2:B:945:GLU:HG2	2.53	0.44
2:B:933:PHE:HZ	2:B:939:GLN:HG2	1.82	0.44
2:B:457:MET:HA	2:B:465:PHE:O	2.17	0.44
2:B:276:ALA:HB2	2:B:655:PRO:HD3	1.99	0.44
1:A:275:LEU:HD12	1:A:275:LEU:HA	1.88	0.44
1:A:320:MET:HE3	1:A:339:TRP:HZ3	1.82	0.44
2:B:523:LEU:HG	2:B:557:MET:HE1	1.98	0.44
2:B:186:LYS:HB3	2:B:205:LEU:HB3	2.00	0.44
2:B:422:GLY:HA2	2:B:439:SER:HB2	2.00	0.44
2:B:387:TYR:O	2:B:391:ASN:HB2	2.18	0.43
2:B:1040:GLY:HA3	2:B:1183:SER:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:467:PHE:CG	2:B:542:VAL:HG21	2.53	0.43
2:B:574:HIS:CE1	2:B:596:GLY:HA3	2.53	0.43
2:B:492:THR:CG2	2:B:493:ASP:N	2.81	0.43
2:B:1062:THR:HG21	2:B:1085:LYS:HB2	2.01	0.43
1:A:155:THR:CG2	1:A:157:TYR:H	2.27	0.43
2:B:620:HIS:CD2	2:B:620:HIS:H	2.36	0.43
2:B:847:PHE:CE1	2:B:850:VAL:HB	2.54	0.43
1:A:172:ARG:O	1:A:176:LEU:HB2	2.19	0.43
2:B:152:SER:HB2	2:B:172:LEU:HD22	2.00	0.43
2:B:131:ARG:HD2	2:B:133:TYR:CE1	2.53	0.43
1:A:253:PRO:HD2	1:A:263:GLY:HA3	2.01	0.43
2:B:758:SER:HA	2:B:907:ARG:NH1	2.33	0.43
2:B:92:ARG:HD3	2:B:94:GLN:HE22	1.83	0.42
2:B:742:ARG:HG2	2:B:742:ARG:NH1	2.35	0.42
1:A:460:GLN:NE2	2:B:816:THR:OG1	2.51	0.42
2:B:567:LYS:HD3	2:B:621:TYR:CE2	2.53	0.42
2:B:834:TYR:OH	2:B:945:GLU:HG2	2.18	0.42
2:B:1234:VAL:CG1	2:B:1236:LEU:HG	2.50	0.42
1:A:396:ILE:HG22	1:A:629:LEU:HD21	2.00	0.42
2:B:375:LYS:HA	2:B:442:PRO:HB3	2.02	0.42
2:B:536:ARG:NH1	2:B:686:ASN:HB3	2.34	0.42
1:A:474:THR:CG2	1:A:479:THR:CG2	2.94	0.42
2:B:256:LEU:HD13	2:B:606:GLY:HA3	2.02	0.42
2:B:327:THR:HG21	2:B:367:VAL:HG21	2.01	0.42
2:B:1003:ASN:ND2	2:B:1146:THR:HG21	2.34	0.42
1:A:163:LEU:HD23	1:A:622:ILE:HD11	2.01	0.41
1:A:34:SER:HB2	1:A:65:GLN:HB2	2.01	0.41
1:A:359:GLN:HG2	1:A:405:VAL:HG12	2.02	0.41
1:A:469:TYR:CE1	2:B:818:TRP:HD1	2.38	0.41
2:B:475:LYS:HD2	2:B:479:THR:O	2.19	0.41
2:B:739:ASN:O	2:B:742:ARG:HB2	2.21	0.41
2:B:1076:LYS:HE3	2:B:1171:GLN:HG3	2.03	0.41
2:B:821:ILE:HD11	2:B:828:ILE:HD11	2.02	0.41
2:B:943:LYS:HB3	2:B:948:GLU:HB2	2.03	0.41
1:A:697:THR:HB	1:A:715:ASP:O	2.21	0.41
1:A:293:GLN:NE2	1:A:293:GLN:HA	2.36	0.41
1:A:639:MET:HB2	1:A:748:ASN:O	2.21	0.41
2:B:115:LEU:HD22	2:B:209:VAL:HG11	2.01	0.41
2:B:123:ASP:OD1	2:B:208:LYS:HE2	2.21	0.41
2:B:223:GLU:HG2	2:B:1100:LEU:HD23	2.03	0.41
2:B:1105:GLN:HB2	2:B:1107:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:PRO:HG3	1:A:654:GLY:HA3	2.03	0.41
2:B:594:PRO:HG2	2:B:1124:LEU:HD22	2.03	0.41
2:B:869:THR:HG22	2:B:873:GLY:HA2	2.02	0.41
2:B:244:SER:HB3	2:B:571:LEU:HB2	2.02	0.40
2:B:281:VAL:HG22	2:B:293:ASN:HA	2.03	0.40
2:B:710:ILE:HD12	2:B:740:TRP:HA	2.03	0.40
1:A:405:VAL:HG22	1:A:501:LEU:HD11	2.04	0.40
2:B:467:PHE:CD1	2:B:542:VAL:HG21	2.56	0.40
2:B:980:ASP:HA	2:B:981:PRO:HD3	1.98	0.40
2:B:903:ASN:HB2	2:B:905:PRO:HD2	2.03	0.40
2:B:940:LYS:HB2	2:B:948:GLU:HB3	2.03	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	769/777 (99%)	715 (93%)	51 (7%)	3 (0%)	30 65
2	B	1148/1160 (99%)	1071 (93%)	71 (6%)	6 (0%)	24 61
All	All	1917/1937 (99%)	1786 (93%)	122 (6%)	9 (0%)	26 61

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	THR
2	B	618	GLY
2	B	847	PHE
2	B	1188	GLU
2	B	854	ASN
1	A	367	SER
2	B	586	ARG

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Mol	Chain	Res	Type
1	A	453	ILE
2	B	143	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	681/681 (100%)	608 (89%)	73 (11%)	6	23
2	B	1011/1011 (100%)	868 (86%)	143 (14%)	3	17
All	All	1692/1692 (100%)	1476 (87%)	216 (13%)	6	19

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	48	THR
1	A	57	LEU
1	A	65	GLN
1	A	66	ILE
1	A	69	GLN
1	A	73	ASN
1	A	79	LEU
1	A	84	ASP
1	A	104	GLN
1	A	107	LYS
1	A	125	THR
1	A	131	GLN
1	A	136	ASN
1	A	149	ILE
1	A	150	LEU
1	A	154	LEU
1	A	155	THR
1	A	159	LEU
1	A	163	LEU
1	A	170	THR

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Mol	Chain	Res	Type
1	A	176	LEU
1	A	189	ASN
1	A	190	GLN
1	A	208	THR
1	A	209	THR
1	A	229	THR
1	A	243	THR
1	A	247	GLU
1	A	254	SER
1	A	264	THR
1	A	275	LEU
1	A	294	LEU
1	A	305	THR
1	A	319	SER
1	A	334	SER
1	A	350	ASP
1	A	351	LYS
1	A	363	LYS
1	A	366	THR
1	A	386	SER
1	A	391	VAL
1	A	393	ASP
1	A	395	ILE
1	A	401	LYS
1	A	419	SER
1	A	421	LYS
1	A	444	THR
1	A	453	ILE
1	A	484	THR
1	A	500	SER
1	A	508	ASN
1	A	532	GLU
1	A	537	ARG
1	A	568	VAL
1	A	571	SER
1	A	574	GLN
1	A	576	ARG
1	A	605	THR
1	A	657	VAL
1	A	665	ASN
1	A	670	SER
1	A	676	ILE

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Mol	Chain	Res	Type
1	A	687	THR
1	A	706	GLU
1	A	732	ASN
1	A	745	ILE
1	A	770	GLN
1	A	782	LEU
1	A	796	GLN
1	A	803	LYS
1	A	806	ASN
1	A	811	ILE
2	B	63	GLU
2	B	83	GLU
2	B	88	PHE
2	B	91	VAL
2	B	94	GLN
2	B	99	ASN
2	B	105	LYS
2	B	113	LYS
2	B	125	GLN
2	B	127	ASN
2	B	130	ILE
2	B	142	ASP
2	B	150	ASN
2	B	153	THR
2	B	154	VAL
2	B	178	THR
2	B	182	GLU
2	B	187	VAL
2	B	200	LEU
2	B	203	VAL
2	B	204	LEU
2	B	219	GLN
2	B	226	GLU
2	B	233	SER
2	B	238	GLN
2	B	242	LYS
2	B	256	LEU
2	B	264	MET
2	B	265	SER
2	B	270	THR
2	B	272	THR
2	B	277	LEU

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Mol	Chain	Res	Type
2	B	280	GLU
2	B	291	LEU
2	B	301	LYS
2	B	318	THR
2	B	322	LYS
2	B	324	LEU
2	B	328	ASP
2	B	333	GLU
2	B	334	LYS
2	B	350	GLU
2	B	358	VAL
2	B	384	ILE
2	B	393	LEU
2	B	396	THR
2	B	403	ARG
2	B	411	GLU
2	B	420	SER
2	B	432	LYS
2	B	437	LYS
2	B	448	GLU
2	B	453	ASN
2	B	458	VAL
2	B	479	THR
2	B	523	LEU
2	B	528	ASN
2	B	529	ARG
2	B	562	THR
2	B	565	ARG
2	B	567	LYS
2	B	570	GLN
2	B	572	GLU
2	B	582	GLN
2	B	587	GLU
2	B	610	GLN
2	B	620	HIS
2	B	632	VAL
2	B	638	GLU
2	B	642	SER
2	B	649	LYS
2	B	673	LEU
2	B	679	SER
2	B	681	ASN

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Mol	Chain	Res	Type
2	B	701	ASP
2	B	707	SER
2	B	708	ASP
2	B	709	LYS
2	B	710	ILE
2	B	725	ARG
2	B	728	GLN
2	B	732	LEU
2	B	733	ASN
2	B	742	ARG
2	B	746	VAL
2	B	751	THR
2	B	756	LEU
2	B	768	LEU
2	B	771	ILE
2	B	773	ASN
2	B	790	SER
2	B	803	VAL
2	B	806	MET
2	B	835	ARG
2	B	841	GLN
2	B	843	ASN
2	B	849	GLN
2	B	850	VAL
2	B	857	THR
2	B	869	THR
2	B	871	SER
2	B	906	GLN
2	B	921	VAL
2	B	922	LEU
2	B	935	LYS
2	B	939	GLN
2	B	945	GLU
2	B	947	ASN
2	B	956	GLU
2	B	965	LEU
2	B	974	THR
2	B	979	THR
2	B	986	LYS
2	B	1002	LEU
2	B	1012	LEU
2	B	1015	ILE

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Mol	Chain	Res	Type
2	B	1017	ASP
2	B	1029	ILE
2	B	1036	ARG
2	B	1039	THR
2	B	1044	ILE
2	B	1045	THR
2	B	1052	GLN
2	B	1059	GLN
2	B	1061	TRP
2	B	1089	ASN
2	B	1118	THR
2	B	1123	LYS
2	B	1136	ASN
2	B	1143	LEU
2	B	1157	THR
2	B	1164	ASN
2	B	1165	ASN
2	B	1170	SER
2	B	1171	GLN
2	B	1172	THR
2	B	1184	GLU
2	B	1187	LYS
2	B	1191	SER
2	B	1224	LYS
2	B	1230	SER
2	B	1234	VAL
2	B	1240	GLN

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	136	ASN
1	A	171	GLN
1	A	191	HIS
1	A	211	ASN
1	A	270	ASN
1	A	293	GLN
1	A	394	GLN
1	A	450	ASN
1	A	454	ASN
1	A	460	GLN
1	A	475	ASN

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Mol	Chain	Res	Type
1	A	530	ASN
1	A	531	GLN
1	A	574	GLN
1	A	599	ASN
1	A	645	ASN
1	A	665	ASN
1	A	722	HIS
1	A	751	GLN
1	A	796	GLN
1	A	797	ASN
2	B	95	ASN
2	B	97	ASN
2	B	99	ASN
2	B	125	GLN
2	B	127	ASN
2	B	144	ASN
2	B	218	ASN
2	B	235	ASN
2	B	302	HIS
2	B	360	HIS
2	B	381	HIS
2	B	382	HIS
2	B	391	ASN
2	B	395	GLN
2	B	528	ASN
2	B	570	GLN
2	B	582	GLN
2	B	620	HIS
2	B	733	ASN
2	B	773	ASN
2	B	841	GLN
2	B	849	GLN
2	B	854	ASN
2	B	924	ASN
2	B	939	GLN
2	B	947	ASN
2	B	1050	GLN
2	B	1052	GLN
2	B	1119	ASN
2	B	1122	ASN
2	B	1164	ASN
2	B	1165	ASN

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Mol	Chain	Res	Type
2	B	1235	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	5
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	227:VAL	C	232:SER	N	11.85
1	B	782:SER	C	789:ALA	N	11.65
1	B	1089:ASN	C	1097:ASN	N	10.05
1	B	105:LYS	C	110:ASP	N	8.60
1	A	255:VAL	C	261:SER	N	8.00

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	412:SER	C	416:SER	N	6.36
1	A	118:THR	C	121:GLY	N	6.20
1	B	1159:SER	C	1164:ASN	N	5.28

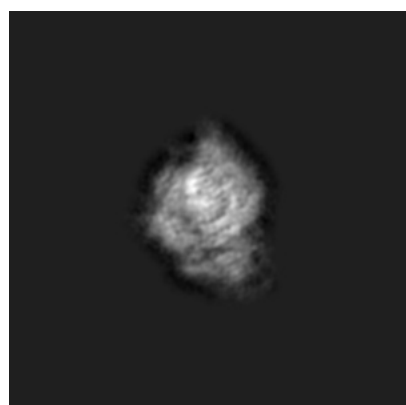
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10890. These allow visual inspection of the internal detail of the map and identification of artifacts.

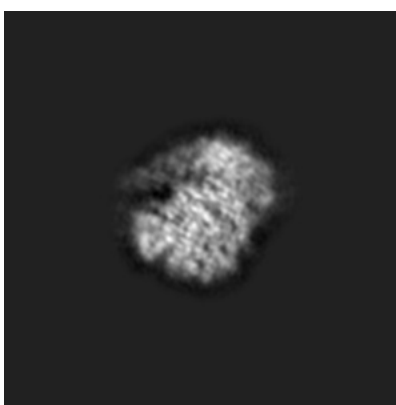
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

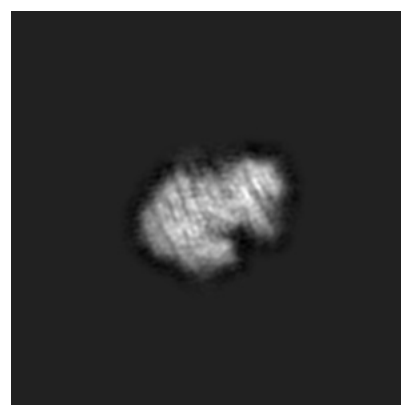
6.1.1 Primary map



X



Y

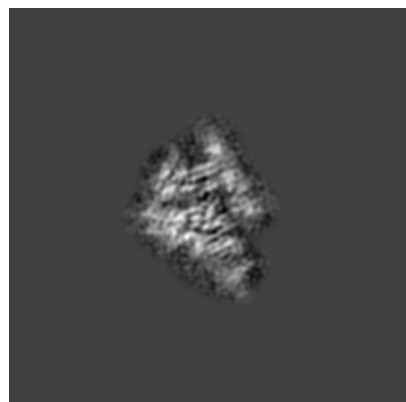


Z

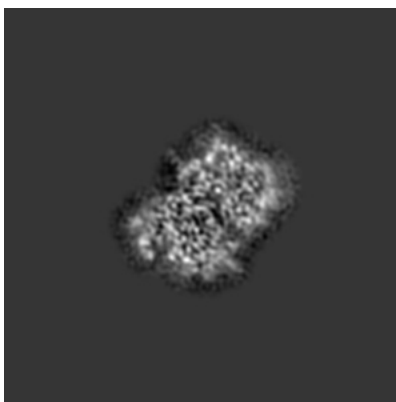
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

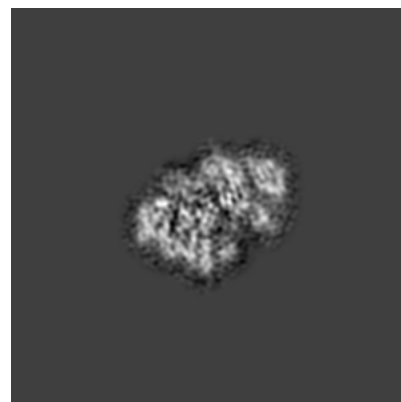
6.2.1 Primary map



X Index: 135



Y Index: 135

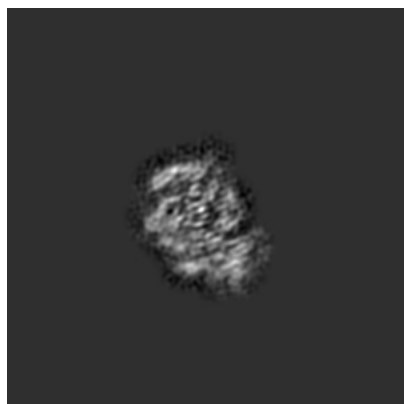


Z Index: 135

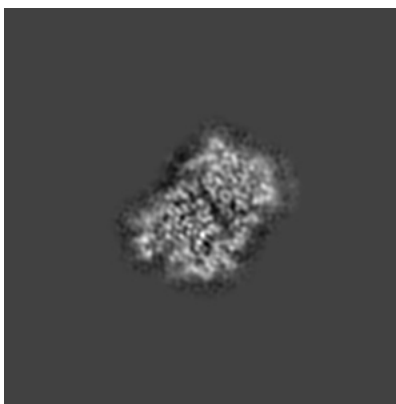
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

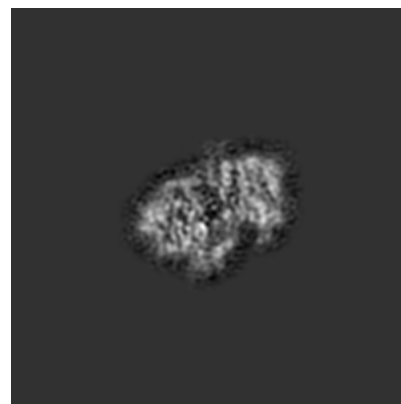
6.3.1 Primary map



X Index: 117



Y Index: 131



Z Index: 140

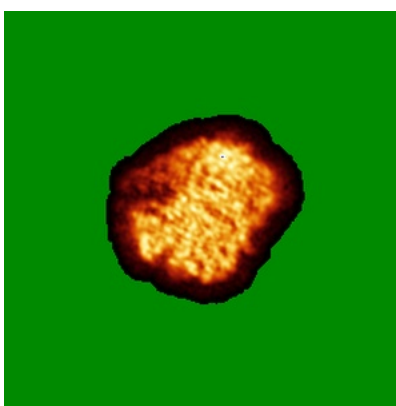
The images above show the largest variance slices of the map in three orthogonal directions.

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

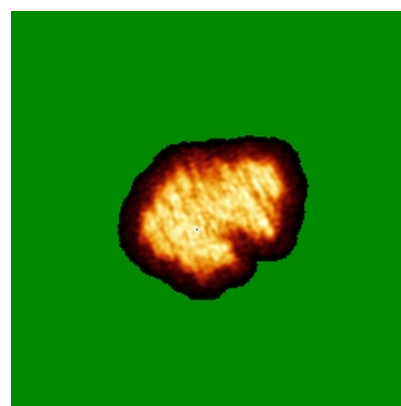
6.4.1 Primary map



X



Y

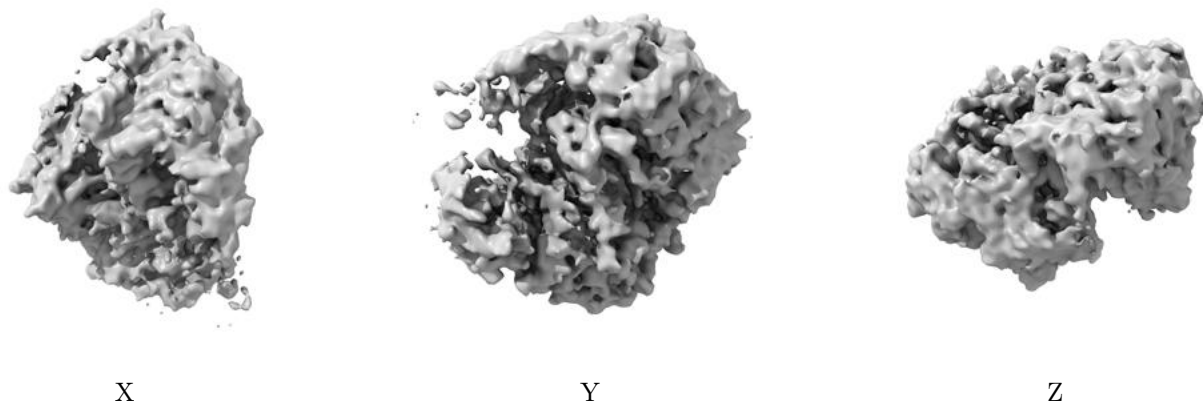


Z

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

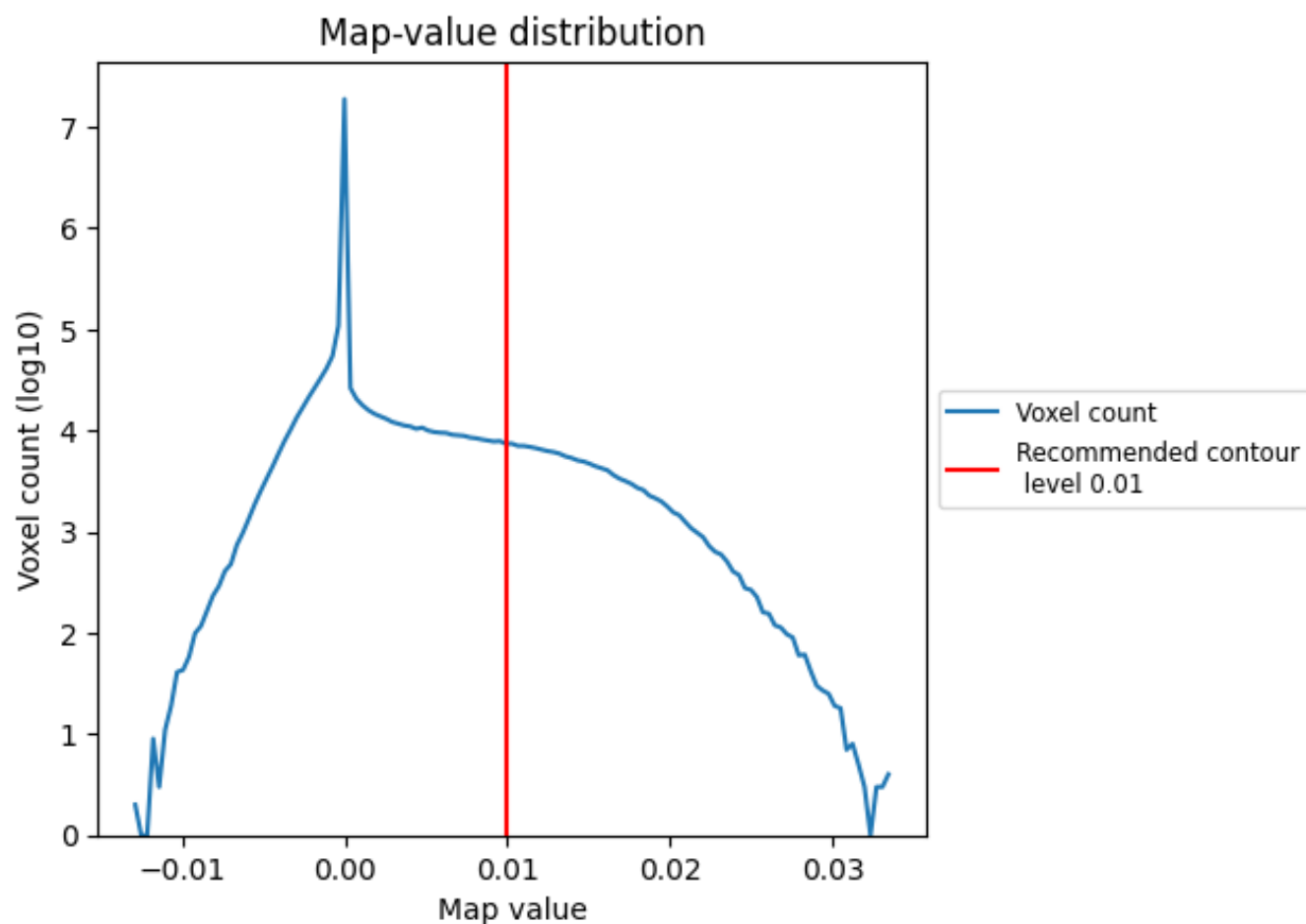
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

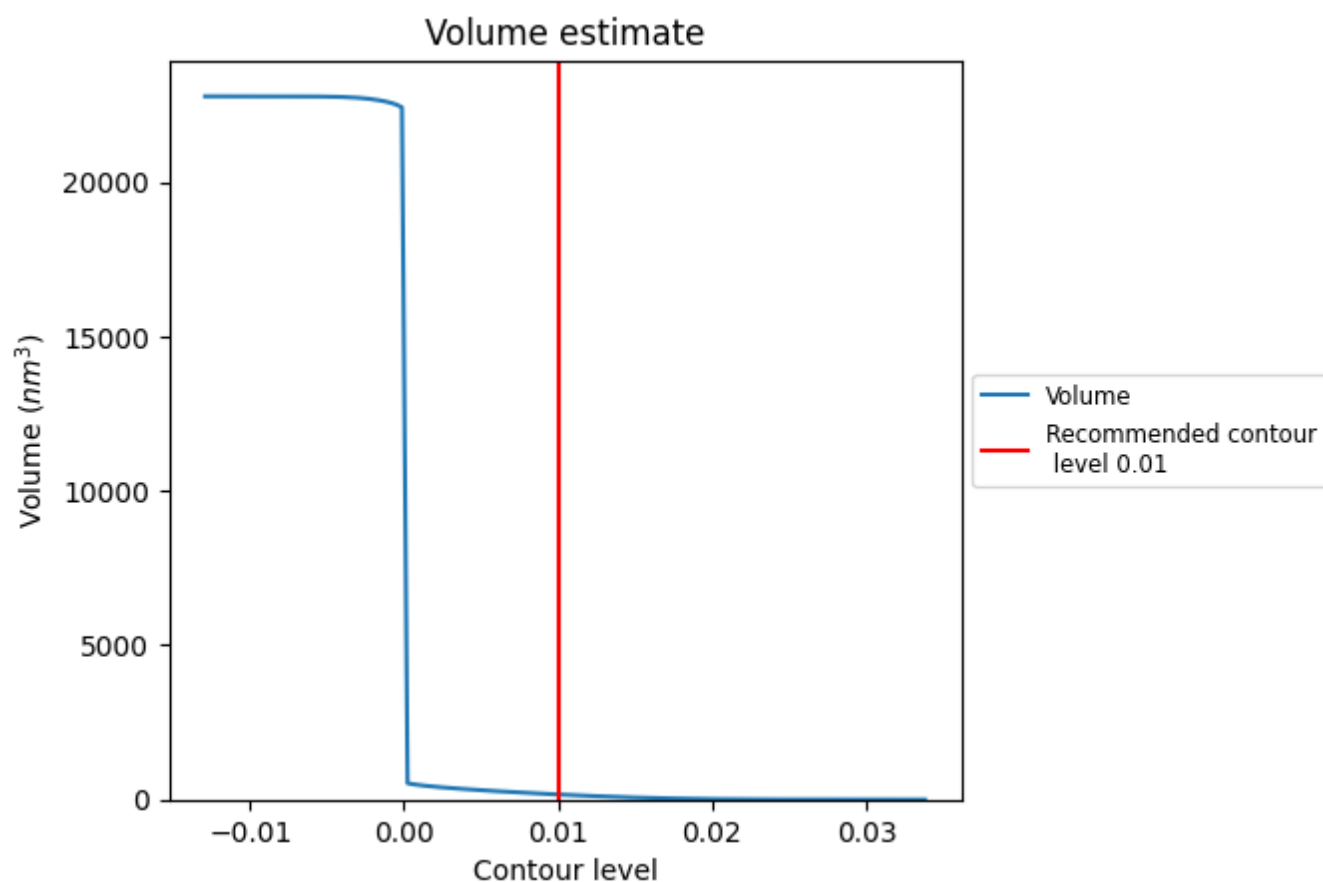
This section contains the results of statistical analysis of the map.

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.

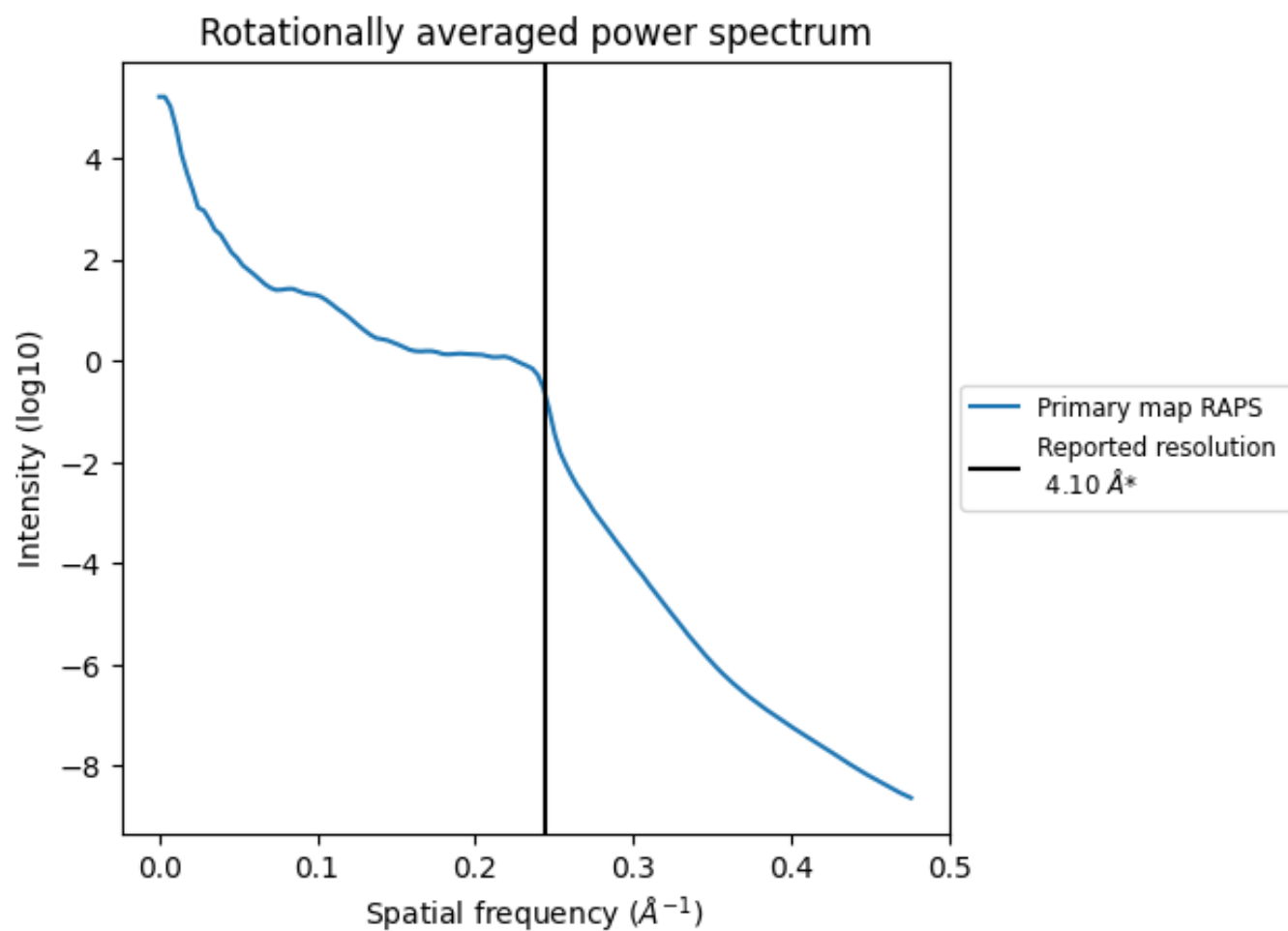
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 165 nm³; this corresponds to an approximate mass of 149 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 ⓘ

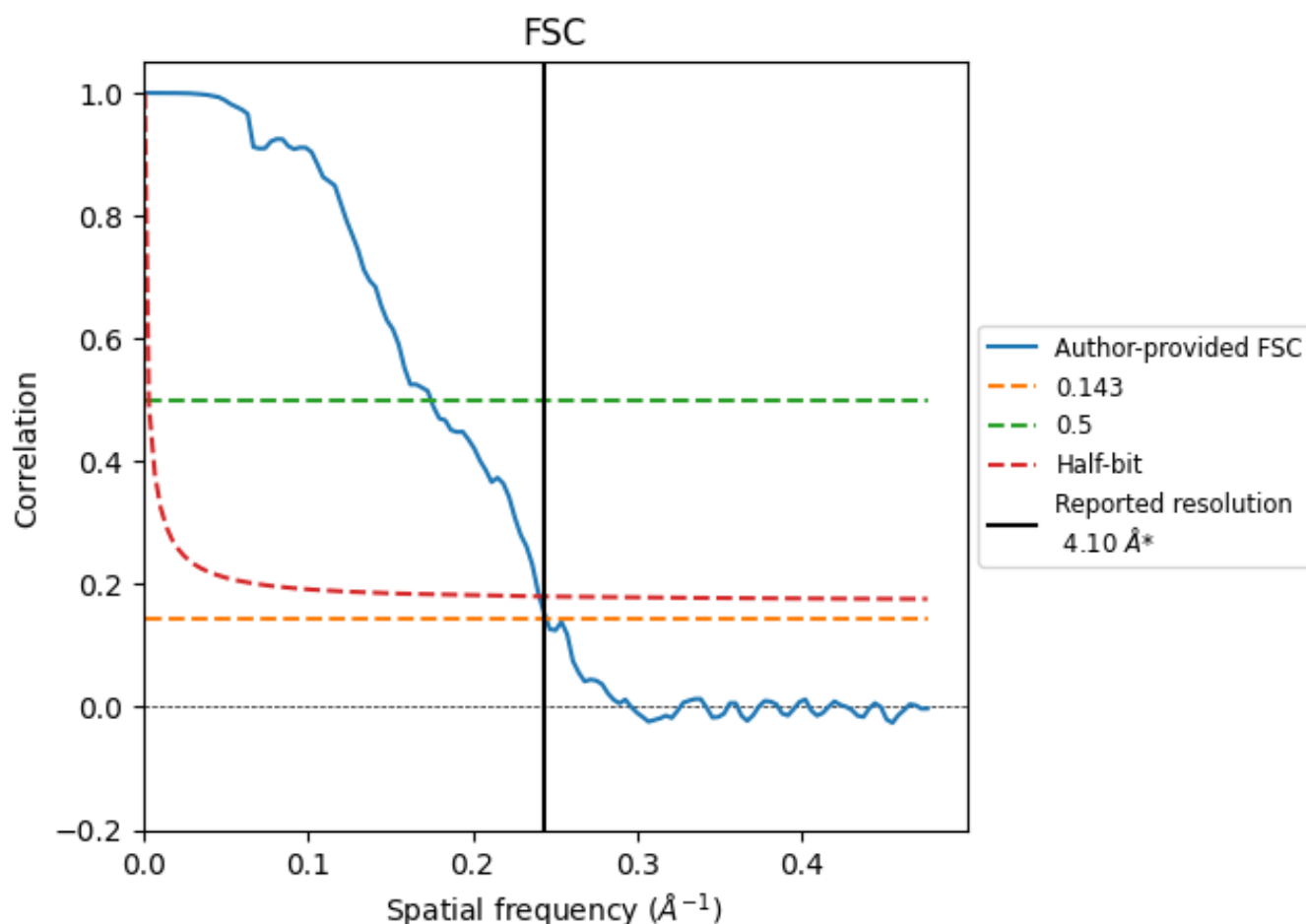


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

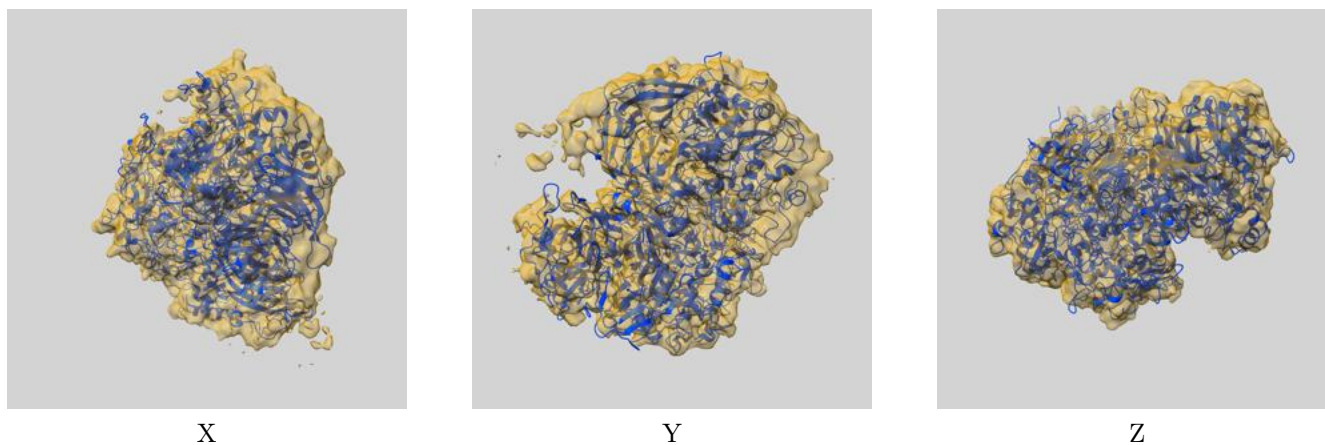
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.08	5.72	4.16
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

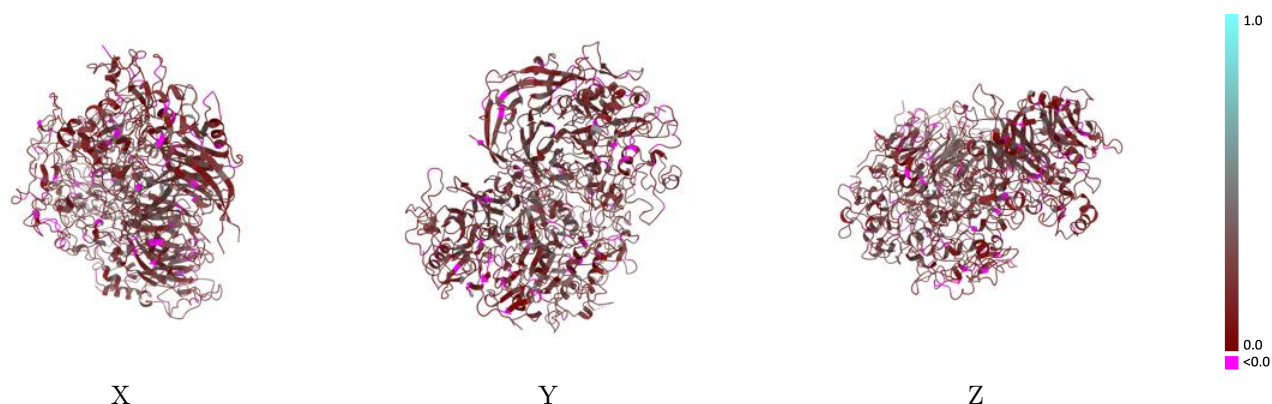
This section contains information regarding the fit between EMDB map EMD-10890 and PDB model 6YRK. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



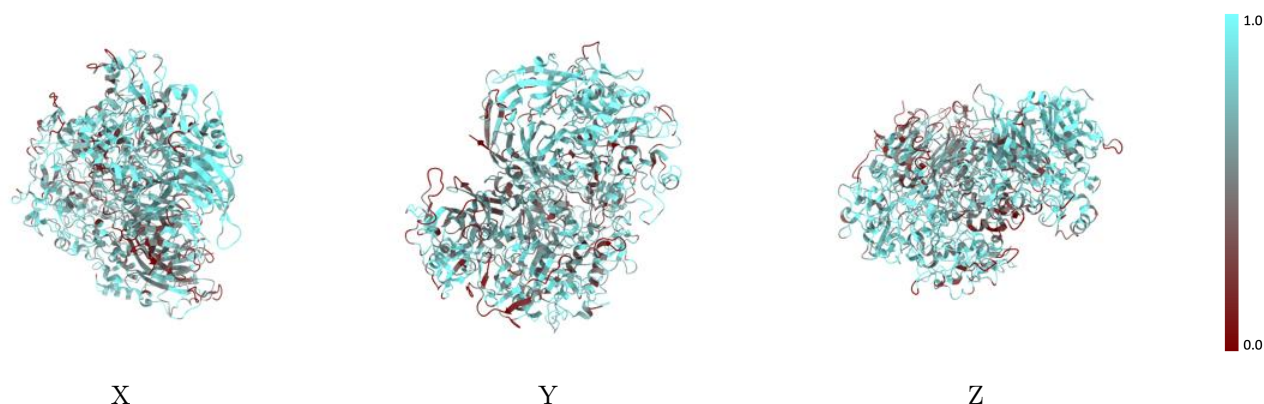
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



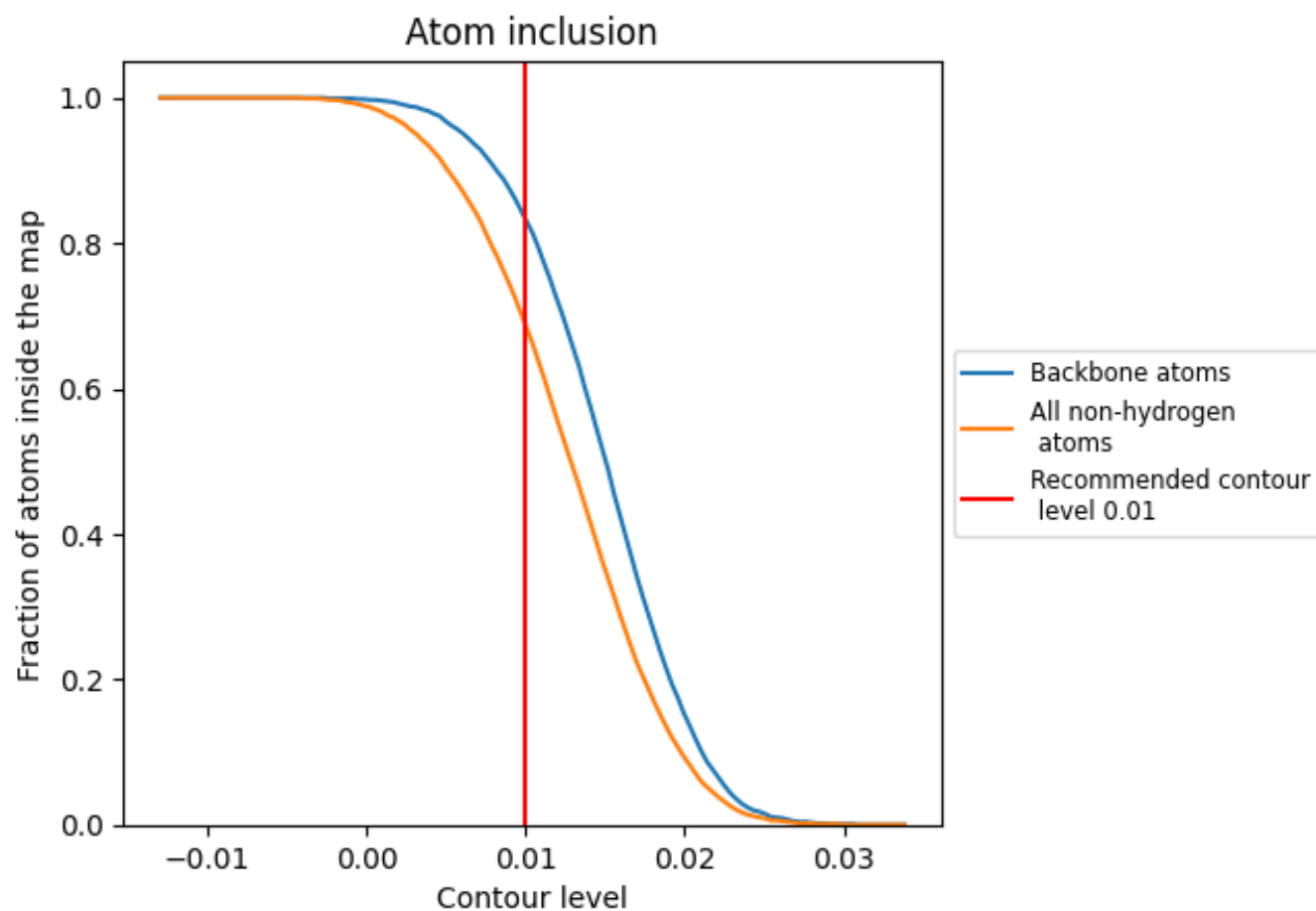
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 69% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6880	0.2060
A	0.7060	0.2030
B	0.6760	0.2090

