Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 12:05 AM JST

PDB ID	:	7F4U
EMDB ID	:	EMD-31454
Title	:	Cryo-EM structure of TELO2-TTI1-TTI2 complex
Authors	:	Cho, Y.; Kim, Y.
Deposited on	:	2021-06-21
Resolution	:	4.20 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:

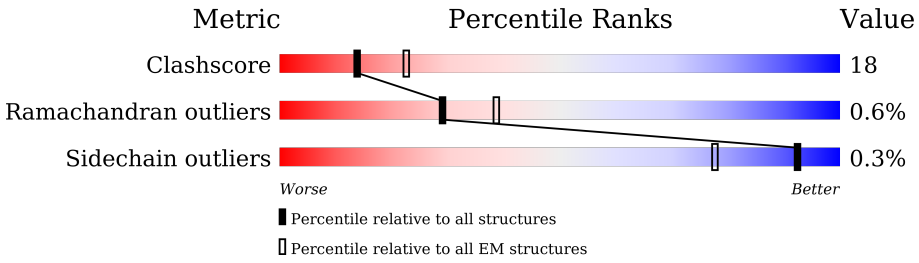
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	837	11% 29% 23% 47%
2	B	1095	7% 49% 14% 37%
3	C	508	18% 81%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8079 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 Telomere length regulation protein TEL2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	440	Total	C	N	O	S	0	0
			3416	2174	609	615	18		

- Molecule 2 is a protein called TELO2-interacting protein 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	690	Total	C	N	O	S	0	0
			4178	2594	770	798	16		

There are 232 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	MET	-	initiating methionine	UNP O43156
B	-4	HIS	-	expression tag	UNP O43156
B	-3	HIS	-	expression tag	UNP O43156
B	-2	HIS	-	expression tag	UNP O43156
B	-1	HIS	-	expression tag	UNP O43156
B	0	HIS	-	expression tag	UNP O43156
B	166	UNK	LYS	conflict	UNP O43156
B	167	UNK	SER	conflict	UNP O43156
B	168	UNK	LYS	conflict	UNP O43156
B	169	UNK	GLN	conflict	UNP O43156
B	170	UNK	ILE	conflict	UNP O43156
B	171	UNK	LYS	conflict	UNP O43156
B	172	UNK	ILE	conflict	UNP O43156
B	173	UNK	ALA	conflict	UNP O43156
B	174	UNK	ALA	conflict	UNP O43156
B	175	UNK	LEU	conflict	UNP O43156
B	176	UNK	LYS	conflict	UNP O43156
B	177	UNK	CYS	conflict	UNP O43156
B	178	UNK	LEU	conflict	UNP O43156
B	179	UNK	GLN	conflict	UNP O43156
B	180	UNK	VAL	conflict	UNP O43156

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Chain	Residue	Modelled	Actual	Comment	Reference
B	181	UNK	LEU	conflict	UNP O43156
B	182	UNK	LEU	conflict	UNP O43156
B	183	UNK	LEU	conflict	UNP O43156
B	184	UNK	GLN	conflict	UNP O43156
B	185	UNK	CYS	conflict	UNP O43156
B	193	UNK	SER	conflict	UNP O43156
B	194	UNK	LEU	conflict	UNP O43156
B	195	UNK	ASP	conflict	UNP O43156
B	196	UNK	GLU	conflict	UNP O43156
B	197	UNK	LEU	conflict	UNP O43156
B	198	UNK	GLU	conflict	UNP O43156
B	199	UNK	GLN	conflict	UNP O43156
B	200	UNK	LYS	conflict	UNP O43156
B	201	UNK	GLN	conflict	UNP O43156
B	202	UNK	LEU	conflict	UNP O43156
B	203	UNK	GLY	conflict	UNP O43156
B	204	UNK	ASP	conflict	UNP O43156
B	205	UNK	LEU	conflict	UNP O43156
B	206	UNK	PHE	conflict	UNP O43156
B	207	UNK	ALA	conflict	UNP O43156
B	208	UNK	SER	conflict	UNP O43156
B	209	UNK	PHE	conflict	UNP O43156
B	210	UNK	LEU	conflict	UNP O43156
B	211	UNK	PRO	conflict	UNP O43156
B	212	UNK	GLY	conflict	UNP O43156
B	213	UNK	ILE	conflict	UNP O43156
B	214	UNK	SER	conflict	UNP O43156
B	215	UNK	THR	conflict	UNP O43156
B	216	UNK	ALA	conflict	UNP O43156
B	217	UNK	LEU	conflict	UNP O43156
B	218	UNK	THR	conflict	UNP O43156
B	219	UNK	ARG	conflict	UNP O43156
B	220	UNK	LEU	conflict	UNP O43156
B	221	UNK	ILE	conflict	UNP O43156
B	222	UNK	THR	conflict	UNP O43156
B	857	UNK	PRO	conflict	UNP O43156
B	858	UNK	LEU	conflict	UNP O43156
B	859	UNK	GLN	conflict	UNP O43156
B	860	UNK	ILE	conflict	UNP O43156
B	861	UNK	GLN	conflict	UNP O43156
B	862	UNK	ILE	conflict	UNP O43156
B	863	UNK	ALA	conflict	UNP O43156

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Chain	Residue	Modelled	Actual	Comment	Reference
B	864	UNK	MET	conflict	UNP O43156
B	865	UNK	ASP	conflict	UNP O43156
B	866	UNK	VAL	conflict	UNP O43156
B	867	UNK	MET	conflict	UNP O43156
B	868	UNK	GLU	conflict	UNP O43156
B	869	UNK	ARG	conflict	UNP O43156
B	870	UNK	CYS	conflict	UNP O43156
B	871	UNK	ILE	conflict	UNP O43156
B	872	UNK	HIS	conflict	UNP O43156
B	873	UNK	LEU	conflict	UNP O43156
B	874	UNK	LEU	conflict	UNP O43156
B	875	UNK	SER	conflict	UNP O43156
B	876	UNK	ASP	conflict	UNP O43156
B	877	UNK	LYS	conflict	UNP O43156
B	878	UNK	ASN	conflict	UNP O43156
B	879	UNK	LEU	conflict	UNP O43156
B	880	UNK	GLN	conflict	UNP O43156
B	881	UNK	ILE	conflict	UNP O43156
B	882	UNK	ARG	conflict	UNP O43156
B	883	UNK	LEU	conflict	UNP O43156
B	884	UNK	LYS	conflict	UNP O43156
B	885	UNK	VAL	conflict	UNP O43156
B	886	UNK	LEU	conflict	UNP O43156
B	887	UNK	ASP	conflict	UNP O43156
B	888	UNK	VAL	conflict	UNP O43156
B	889	UNK	LEU	conflict	UNP O43156
B	890	UNK	ASP	conflict	UNP O43156
B	891	UNK	LEU	conflict	UNP O43156
B	892	UNK	CYS	conflict	UNP O43156
B	893	UNK	VAL	conflict	UNP O43156
B	894	UNK	VAL	conflict	UNP O43156
B	895	UNK	VAL	conflict	UNP O43156
B	896	UNK	LEU	conflict	UNP O43156
B	897	UNK	GLN	conflict	UNP O43156
B	898	UNK	SER	conflict	UNP O43156
B	899	UNK	HIS	conflict	UNP O43156
B	900	UNK	LYS	conflict	UNP O43156
B	901	UNK	ASN	conflict	UNP O43156
B	902	UNK	GLN	conflict	UNP O43156
B	903	UNK	LEU	conflict	UNP O43156
B	904	UNK	LEU	conflict	UNP O43156
B	905	UNK	PRO	conflict	UNP O43156

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Chain	Residue	Modelled	Actual	Comment	Reference
B	906	UNK	LEU	conflict	UNP O43156
B	907	UNK	ALA	conflict	UNP O43156
B	908	UNK	HIS	conflict	UNP O43156
B	909	UNK	GLN	conflict	UNP O43156
B	910	UNK	ALA	conflict	UNP O43156
B	911	UNK	TRP	conflict	UNP O43156
B	912	UNK	PRO	conflict	UNP O43156
B	913	UNK	SER	conflict	UNP O43156
B	914	UNK	LEU	conflict	UNP O43156
B	915	UNK	VAL	conflict	UNP O43156
B	916	UNK	HIS	conflict	UNP O43156
B	922	UNK	ALA	conflict	UNP O43156
B	923	UNK	PRO	conflict	UNP O43156
B	924	UNK	LEU	conflict	UNP O43156
B	925	UNK	ALA	conflict	UNP O43156
B	926	UNK	VAL	conflict	UNP O43156
B	927	UNK	LEU	conflict	UNP O43156
B	928	UNK	ARG	conflict	UNP O43156
B	929	UNK	ALA	conflict	UNP O43156
B	930	UNK	PHE	conflict	UNP O43156
B	931	UNK	LYS	conflict	UNP O43156
B	932	UNK	VAL	conflict	UNP O43156
B	933	UNK	LEU	conflict	UNP O43156
B	934	UNK	ARG	conflict	UNP O43156
B	935	UNK	THR	conflict	UNP O43156
B	936	UNK	LEU	conflict	UNP O43156
B	937	UNK	GLY	conflict	UNP O43156
B	938	UNK	SER	conflict	UNP O43156
B	939	UNK	LYS	conflict	UNP O43156
B	940	UNK	CYS	conflict	UNP O43156
B	941	UNK	GLY	conflict	UNP O43156
B	942	UNK	ASP	conflict	UNP O43156
B	943	UNK	PHE	conflict	UNP O43156
B	944	UNK	LEU	conflict	UNP O43156
B	945	UNK	ARG	conflict	UNP O43156
B	946	UNK	SER	conflict	UNP O43156
B	947	UNK	ARG	conflict	UNP O43156
B	948	UNK	PHE	conflict	UNP O43156
B	949	UNK	CYS	conflict	UNP O43156
B	950	UNK	LYS	conflict	UNP O43156
B	951	UNK	ASP	conflict	UNP O43156
B	952	UNK	VAL	conflict	UNP O43156

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Chain	Residue	Modelled	Actual	Comment	Reference
B	953	UNK	LEU	conflict	UNP O43156
B	954	UNK	PRO	conflict	UNP O43156
B	955	UNK	LYS	conflict	UNP O43156
B	956	UNK	LEU	conflict	UNP O43156
B	957	UNK	ALA	conflict	UNP O43156
B	958	UNK	GLY	conflict	UNP O43156
B	959	UNK	SER	conflict	UNP O43156
B	977	UNK	THR	conflict	UNP O43156
B	978	UNK	LEU	conflict	UNP O43156
B	979	UNK	ALA	conflict	UNP O43156
B	980	UNK	PHE	conflict	UNP O43156
B	981	UNK	LYS	conflict	UNP O43156
B	982	UNK	LEU	conflict	UNP O43156
B	983	UNK	GLN	conflict	UNP O43156
B	984	UNK	LEU	conflict	UNP O43156
B	985	UNK	ALA	conflict	UNP O43156
B	986	UNK	VAL	conflict	UNP O43156
B	987	UNK	LEU	conflict	UNP O43156
B	988	UNK	GLN	conflict	UNP O43156
B	989	UNK	GLY	conflict	UNP O43156
B	990	UNK	LEU	conflict	UNP O43156
B	991	UNK	GLY	conflict	UNP O43156
B	992	UNK	PRO	conflict	UNP O43156
B	993	UNK	LEU	conflict	UNP O43156
B	994	UNK	CYS	conflict	UNP O43156
B	995	UNK	GLU	conflict	UNP O43156
B	996	UNK	ARG	conflict	UNP O43156
B	997	UNK	LEU	conflict	UNP O43156
B	998	UNK	ASP	conflict	UNP O43156
B	999	UNK	LEU	conflict	UNP O43156
B	1000	UNK	GLY	conflict	UNP O43156
B	1001	UNK	GLU	conflict	UNP O43156
B	1002	UNK	GLY	conflict	UNP O43156
B	1003	UNK	ASP	conflict	UNP O43156
B	1021	UNK	VAL	conflict	UNP O43156
B	1022	UNK	LYS	conflict	UNP O43156
B	1023	UNK	LEU	conflict	UNP O43156
B	1024	UNK	GLN	conflict	UNP O43156
B	1025	UNK	GLU	conflict	UNP O43156
B	1026	UNK	ALA	conflict	UNP O43156
B	1027	UNK	ALA	conflict	UNP O43156
B	1028	UNK	ARG	conflict	UNP O43156

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1029	UNK	SER	conflict	UNP O43156
B	1030	UNK	VAL	conflict	UNP O43156
B	1031	UNK	PHE	conflict	UNP O43156
B	1032	UNK	LEU	conflict	UNP O43156
B	1033	UNK	HIS	conflict	UNP O43156
B	1034	UNK	LEU	conflict	UNP O43156
B	1035	UNK	MET	conflict	UNP O43156
B	1036	UNK	LYS	conflict	UNP O43156
B	1037	UNK	VAL	conflict	UNP O43156
B	1038	UNK	ASP	conflict	UNP O43156
B	1039	UNK	PRO	conflict	UNP O43156
B	1040	UNK	ASP	conflict	UNP O43156
B	1041	UNK	SER	conflict	UNP O43156
B	1042	UNK	THR	conflict	UNP O43156
B	1043	UNK	TRP	conflict	UNP O43156
B	1044	UNK	PHE	conflict	UNP O43156
B	1045	UNK	LEU	conflict	UNP O43156
B	1046	UNK	LEU	conflict	UNP O43156
B	1047	UNK	ASN	conflict	UNP O43156
B	1048	UNK	GLU	conflict	UNP O43156
B	1049	UNK	LEU	conflict	UNP O43156
B	1050	UNK	TYR	conflict	UNP O43156
B	1051	UNK	CYS	conflict	UNP O43156
B	1052	UNK	PRO	conflict	UNP O43156
B	1053	UNK	VAL	conflict	UNP O43156
B	1054	UNK	GLN	conflict	UNP O43156
B	1055	UNK	PHE	conflict	UNP O43156
B	1056	UNK	THR	conflict	UNP O43156
B	1057	UNK	PRO	conflict	UNP O43156
B	1058	UNK	PRO	conflict	UNP O43156
B	1059	UNK	HIS	conflict	UNP O43156
B	1060	UNK	PRO	conflict	UNP O43156
B	1061	UNK	SER	conflict	UNP O43156
B	1062	UNK	LEU	conflict	UNP O43156
B	1063	UNK	HIS	conflict	UNP O43156
B	1064	UNK	PRO	conflict	UNP O43156
B	1065	UNK	VAL	conflict	UNP O43156
B	1066	UNK	GLN	conflict	UNP O43156
B	1067	UNK	LEU	conflict	UNP O43156
B	1068	UNK	HIS	conflict	UNP O43156
B	1069	UNK	GLY	conflict	UNP O43156
B	1070	UNK	ALA	conflict	UNP O43156

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1071	UNK	SER	conflict	UNP O43156

- Molecule 3 is a protein called TELO2-interacting protein 2.

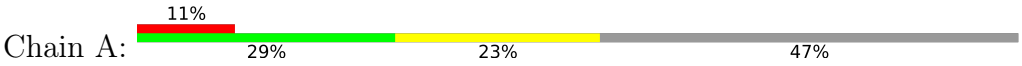
Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	97	Total	C	N	O	0	0
			485	291	97	97		

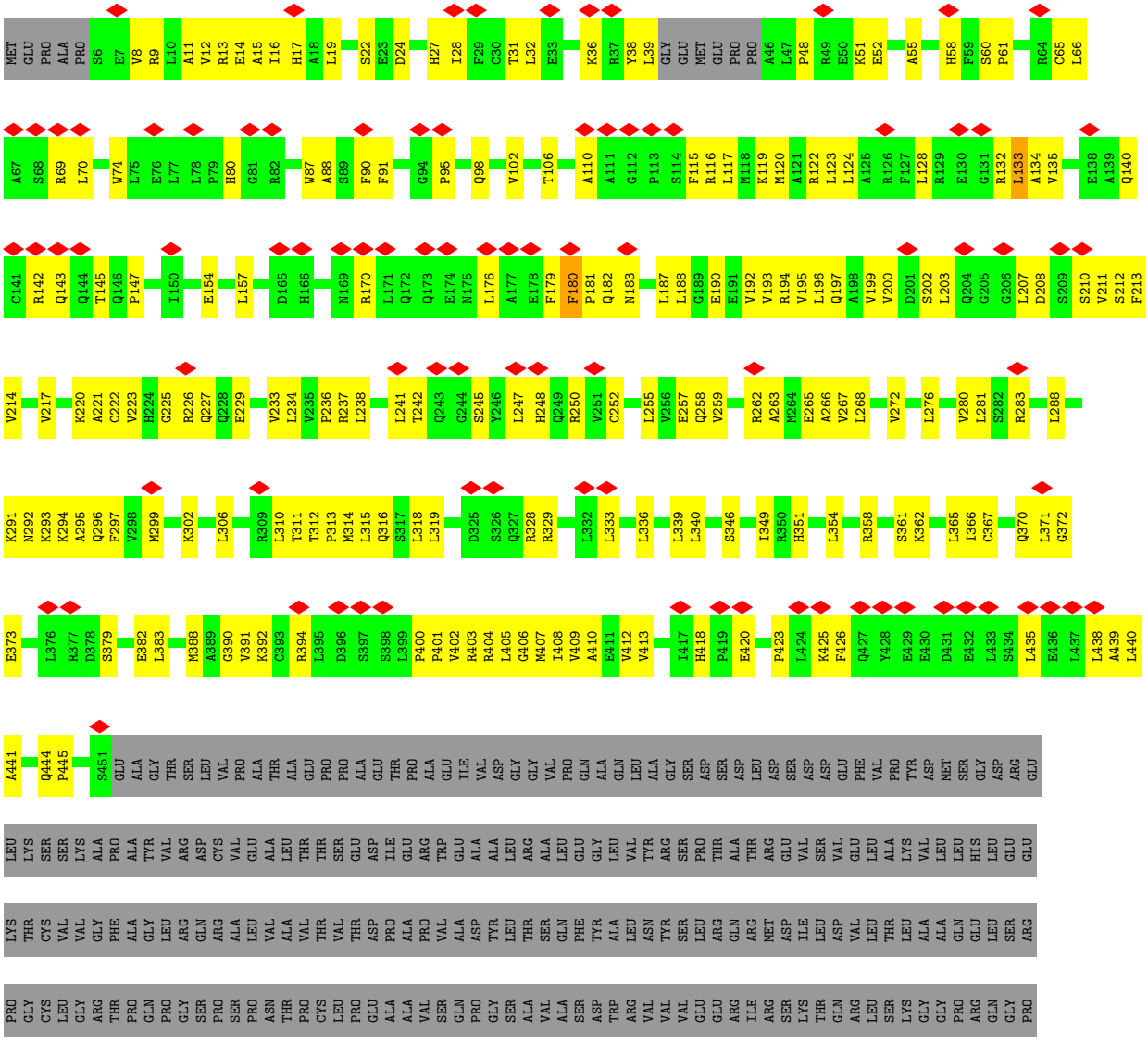
3 Residue-property plots (i)

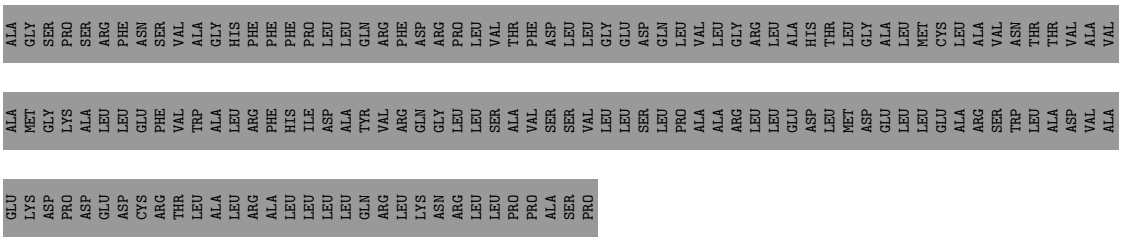
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Telomere length regulation protein TEL2 homolog

Chain A:

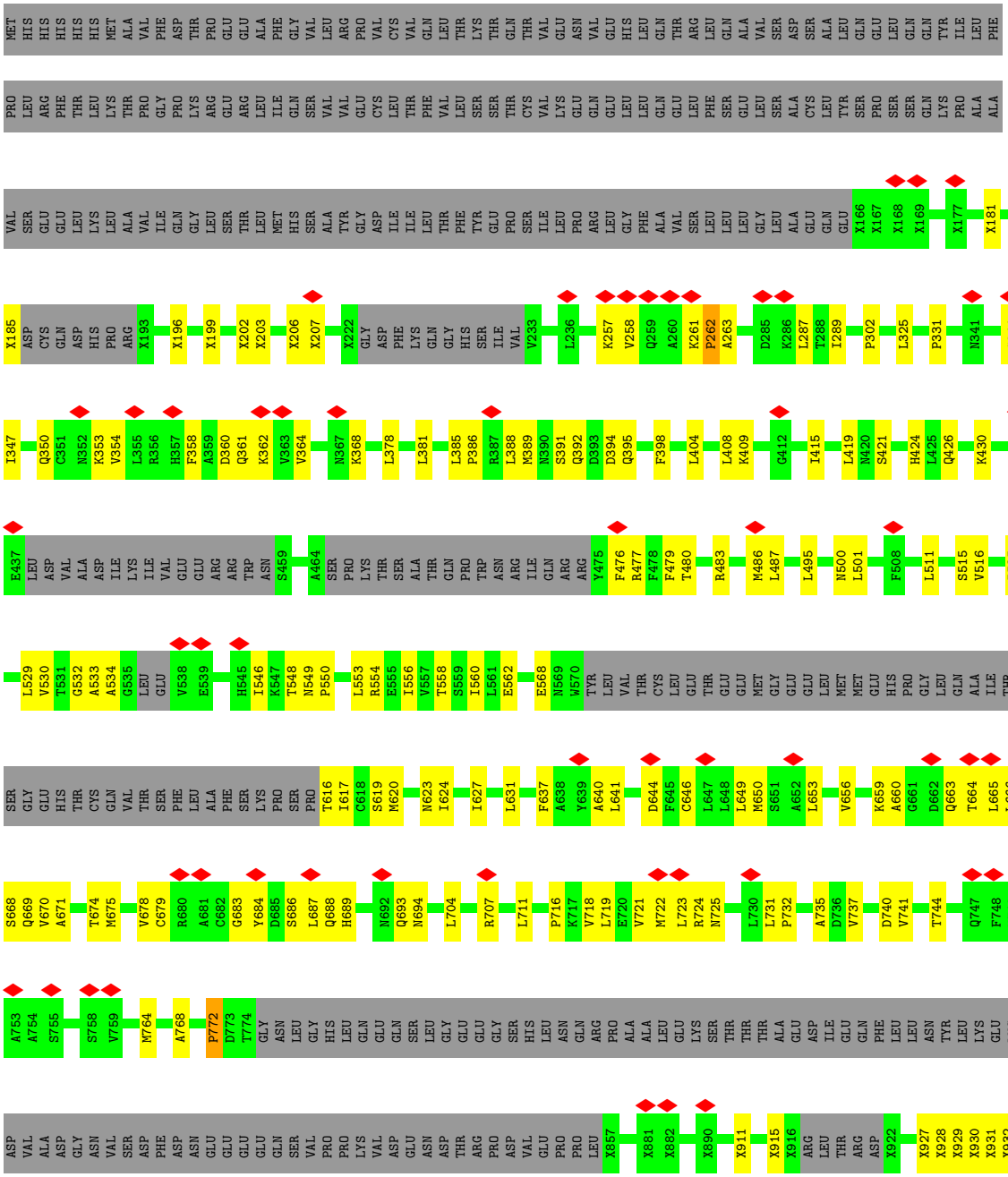


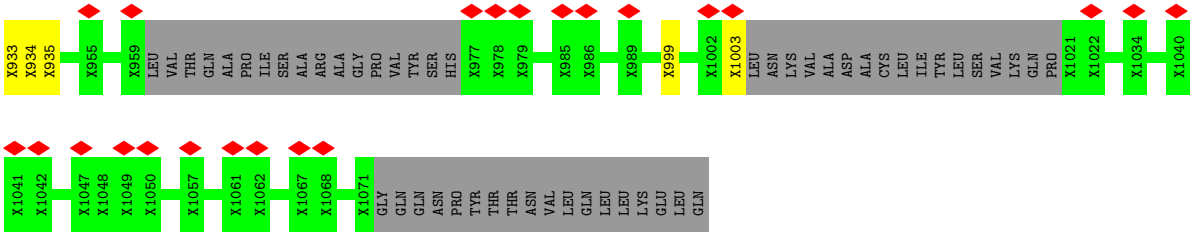




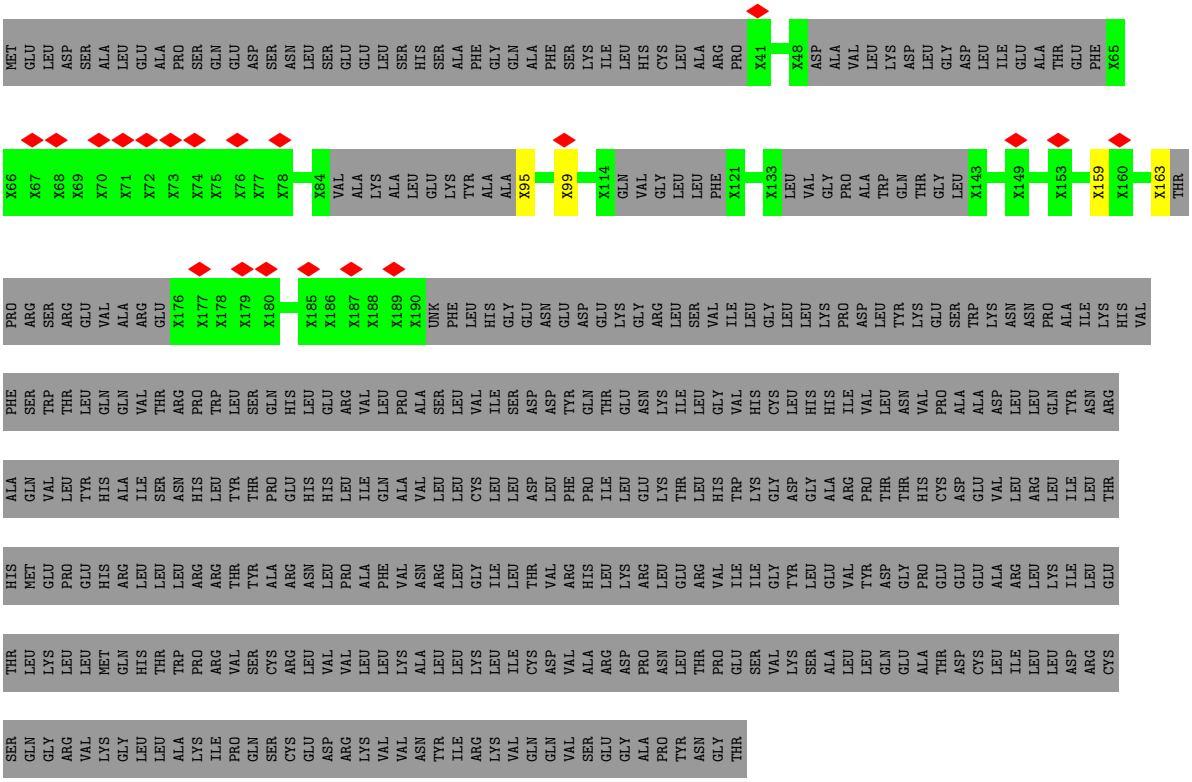
• Molecule 2: TELO2-interacting protein 1 homolog

Chain B:





• Molecule 3: TELO2-interacting protein 2



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	323679	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.950	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	374.50003, 374.50003, 374.50003	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	0.27	0/3477	0.50	0/4706
2	B	0.28	0/3079	0.51	6/4215 (0.1%)
All	All	0.27	0/6556	0.50	6/8921 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	345	PRO	N-CA-CB	5.99	110.49	103.30
2	B	331	PRO	N-CA-CB	5.81	110.27	103.30
2	B	302	PRO	N-CA-CB	5.78	110.24	103.30
2	B	262	PRO	N-CA-CB	5.78	110.23	103.30
2	B	732	PRO	N-CA-CB	5.73	110.17	103.30
2	B	772	PRO	N-CA-CB	5.51	109.92	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	PHE	Peptide
2	B	364	VAL	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	3416	0	3521	156	0
2	B	4178	0	2791	99	0
3	C	485	0	109	2	0
All	All	8079	0	6421	256	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 18.

All (256) 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:245:SER:HB2	1:A:248:HIS:HB2	1.52	0.91
1:A:346:SER:O	1:A:351:HIS:ND1	2.09	0.85
1:A:157:LEU:HD13	1:A:220:LYS:HB3	1.60	0.82
2:B:568:GLU:O	2:B:659:LYS:NZ	2.13	0.81
1:A:407:MET:O	1:A:410:ALA:HB3	1.81	0.80
1:A:11:ALA:O	1:A:15:ALA:N	2.16	0.76
1:A:9:ARG:O	1:A:12:VAL:HB	1.87	0.74
2:B:665:LEU:O	2:B:669:GLN:CB	2.36	0.74
1:A:311:THR:H	1:A:314:MET:HB3	1.51	0.74
2:B:663:GLN:HG3	2:B:667:ILE:H	1.52	0.73
2:B:421:SER:HB2	2:B:424:HIS:HD2	1.51	0.73
2:B:930:UNK:O	2:B:934:UNK:N	2.22	0.72
2:B:257:LYS:O	2:B:261:LYS:N	2.22	0.72
1:A:133:LEU:O	1:A:135:VAL:N	2.20	0.71
1:A:19:LEU:O	1:A:69:ARG:NH2	2.22	0.71
1:A:142:ARG:HH21	1:A:143:GLN:HG3	1.56	0.70
2:B:415:ILE:HG22	2:B:419:LEU:HG	1.73	0.70
2:B:325:LEU:O	2:B:362:LYS:NZ	2.26	0.69
2:B:679:CYS:HA	2:B:684:TYR:HB2	1.74	0.69
2:B:641:LEU:HD11	2:B:644:ASP:HB3	1.75	0.69
2:B:693:GLN:HG3	2:B:694:ASN:H	1.59	0.68
1:A:145:THR:HG22	1:A:147:PRO:HD2	1.77	0.67
1:A:91:PHE:HB2	1:A:123:LEU:HD11	1.77	0.67
1:A:319:LEU:HD22	1:A:366:ILE:HG22	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LEU:H	1:A:314:MET:HE2	1.60	0.67
1:A:312:THR:HB	1:A:313:PRO:HD3	1.77	0.66
1:A:391:VAL:O	1:A:403:ARG:NH2	2.28	0.66
1:A:106:THR:O	1:A:110:ALA:N	2.24	0.66
3:C:159:UNK:O	3:C:163:UNK:N	2.28	0.66
2:B:911:UNK:O	2:B:915:UNK:N	2.28	0.66
1:A:38:TYR:O	1:A:51:LYS:NZ	2.27	0.65
1:A:268:LEU:HD11	1:A:296:GLN:HG3	1.78	0.64
2:B:386:PRO:HA	2:B:389:MET:HG3	1.80	0.64
3:C:95:UNK:O	3:C:99:UNK:N	2.32	0.63
1:A:295:ALA:O	1:A:299:MET:HG2	1.98	0.63
2:B:679:CYS:O	2:B:683:GLY:N	2.32	0.63
2:B:716:PRO:HA	2:B:719:LEU:HD13	1.80	0.63
2:B:927:UNK:O	2:B:931:UNK:N	2.31	0.63
1:A:220:LYS:HA	1:A:223:VAL:HG22	1.81	0.62
2:B:723:LEU:HD12	2:B:764:MET:HA	1.79	0.62
1:A:140:GLN:HE21	1:A:207:LEU:HD13	1.63	0.62
2:B:202:UNK:O	2:B:206:UNK:N	2.33	0.61
2:B:999:UNK:O	2:B:1003:UNK:N	2.33	0.61
1:A:199:VAL:O	1:A:202:SER:OG	2.17	0.61
2:B:501:LEU:HD11	2:B:533:ALA:HB2	1.83	0.61
1:A:288:LEU:O	1:A:292:ASN:N	2.34	0.61
1:A:190:GLU:O	1:A:194:ARG:HG2	2.01	0.61
2:B:929:UNK:O	2:B:933:UNK:N	2.34	0.60
1:A:116:ARG:O	1:A:120:MET:N	2.28	0.60
2:B:388:LEU:O	2:B:392:GLN:NE2	2.31	0.59
1:A:358:ARG:NH1	1:A:441:ALA:O	2.23	0.59
1:A:229:GLU:O	1:A:233:VAL:HB	2.02	0.59
1:A:238:LEU:HA	1:A:283:ARG:HH12	1.67	0.59
1:A:365:LEU:HD22	1:A:412:VAL:HG11	1.84	0.59
1:A:157:LEU:HD11	1:A:217:VAL:HA	1.84	0.59
2:B:688:GLN:NE2	2:B:725:ASN:O	2.35	0.59
1:A:404:ARG:NH1	1:A:435:LEU:O	2.36	0.59
1:A:234:LEU:O	1:A:238:LEU:N	2.22	0.58
1:A:133:LEU:C	1:A:135:VAL:H	2.07	0.58
2:B:616:THR:HG1	2:B:619:SER:HG	1.42	0.58
1:A:391:VAL:HA	1:A:394:ARG:HD3	1.86	0.58
1:A:349:ILE:HG12	2:B:424:HIS:NE2	2.19	0.57
2:B:928:UNK:O	2:B:932:UNK:N	2.37	0.57
1:A:55:ALA:HB1	1:A:95:PRO:HB3	1.86	0.57
2:B:619:SER:O	2:B:623:ASN:ND2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:394:ASP:O	2:B:395:GLN:HG3	2.04	0.57
1:A:115:PHE:H	1:A:117:LEU:HD23	1.68	0.57
2:B:181:UNK:O	2:B:185:UNK:N	2.32	0.56
1:A:48:PRO:O	1:A:52:GLU:N	2.38	0.56
1:A:288:LEU:HD22	1:A:292:ASN:HB2	1.86	0.56
2:B:388:LEU:O	2:B:391:SER:OG	2.24	0.56
2:B:515:SER:OG	2:B:516:VAL:N	2.39	0.56
1:A:213:PHE:O	1:A:217:VAL:HG23	2.06	0.56
1:A:409:VAL:HG22	1:A:413:VAL:HG13	1.88	0.56
2:B:723:LEU:HD22	2:B:724:ARG:HH11	1.71	0.55
1:A:194:ARG:O	1:A:197:GLN:HG3	2.07	0.55
2:B:656:VAL:HA	2:B:659:LYS:HB2	1.88	0.55
1:A:401:PRO:O	1:A:404:ARG:HB2	2.06	0.55
2:B:737:VAL:O	2:B:741:VAL:N	2.25	0.55
1:A:193:VAL:HG13	1:A:237:ARG:HH12	1.71	0.55
2:B:550:PRO:O	2:B:554:ARG:HG3	2.08	0.54
1:A:358:ARG:NH1	1:A:445:PRO:HG2	2.23	0.54
1:A:392:LYS:O	1:A:403:ARG:NH2	2.40	0.54
2:B:500:ASN:OD1	2:B:501:LEU:N	2.41	0.54
2:B:731:LEU:O	2:B:735:ALA:N	2.41	0.54
1:A:200:VAL:HG11	1:A:248:HIS:CD2	2.43	0.54
2:B:650:MET:SD	2:B:650:MET:N	2.81	0.54
1:A:193:VAL:HG22	1:A:237:ARG:HH22	1.74	0.53
1:A:259:VAL:HG11	1:A:267:VAL:HG21	1.90	0.53
2:B:556:ILE:O	2:B:560:ILE:HG12	2.09	0.53
1:A:310:LEU:HG	1:A:313:PRO:HD2	1.91	0.53
1:A:405:LEU:O	1:A:408:ILE:HG12	2.08	0.53
2:B:663:GLN:HB3	2:B:667:ILE:HB	1.91	0.53
1:A:291:LYS:HD2	1:A:329:ARG:HD3	1.91	0.52
1:A:196:LEU:HD12	1:A:255:LEU:HD13	1.90	0.52
1:A:349:ILE:O	1:A:351:HIS:ND1	2.42	0.52
2:B:385:LEU:O	2:B:388:LEU:HG	2.10	0.52
1:A:222:CYS:O	1:A:226:ARG:NH1	2.42	0.52
1:A:311:THR:HA	1:A:315:LEU:H	1.73	0.52
2:B:663:GLN:HE21	2:B:666:LEU:H	1.57	0.52
1:A:362:LYS:O	1:A:366:ILE:HG13	2.09	0.52
2:B:525:ILE:O	2:B:529:LEU:HG	2.10	0.52
1:A:14:GLU:HA	1:A:17:HIS:HB2	1.92	0.51
1:A:24:ASP:HB2	1:A:27:HIS:ND1	2.26	0.51
2:B:534:ALA:HB2	2:B:640:ALA:HB1	1.92	0.51
2:B:718:VAL:HA	2:B:721:VAL:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:HD11	1:A:367:CYS:HB3	1.92	0.51
1:A:423:PRO:O	1:A:426:PHE:HB2	2.11	0.51
1:A:358:ARG:HH11	1:A:445:PRO:HG2	1.76	0.51
2:B:476:PHE:HA	2:B:487:LEU:HB3	1.92	0.51
1:A:48:PRO:HA	1:A:51:LYS:HB2	1.92	0.50
1:A:340:LEU:HB3	1:A:383:LEU:HD13	1.94	0.50
1:A:203:LEU:HD22	1:A:247:LEU:HD11	1.93	0.50
2:B:196:UNK:O	2:B:199:UNK:CB	2.59	0.50
1:A:9:ARG:O	1:A:13:ARG:HG2	2.11	0.50
2:B:495:LEU:HG	2:B:532:GLY:HA2	1.93	0.50
1:A:272:VAL:HG12	1:A:281:LEU:HD21	1.94	0.49
1:A:276:LEU:HB2	1:A:280:VAL:HG21	1.93	0.49
1:A:65:CYS:O	1:A:69:ARG:HB3	2.12	0.49
1:A:247:LEU:HA	1:A:250:ARG:HG2	1.94	0.49
2:B:663:GLN:NE2	2:B:666:LEU:H	2.10	0.49
1:A:58:HIS:C	1:A:61:PRO:HD2	2.33	0.49
2:B:664:THR:O	2:B:668:SER:HB3	2.12	0.49
2:B:718:VAL:HG23	2:B:719:LEU:HD12	1.94	0.49
1:A:192:VAL:HA	1:A:195:VAL:HG12	1.94	0.49
1:A:233:VAL:O	1:A:237:ARG:HG2	2.12	0.49
2:B:688:GLN:HE21	2:B:725:ASN:C	2.15	0.49
2:B:931:UNK:O	2:B:935:UNK:N	2.44	0.49
1:A:12:VAL:HG13	1:A:58:HIS:ND1	2.27	0.49
1:A:390:GLY:O	1:A:394:ARG:HG3	2.13	0.49
1:A:268:LEU:O	1:A:272:VAL:HG22	2.13	0.49
1:A:238:LEU:O	1:A:242:THR:OG1	2.27	0.48
1:A:227:GLN:N	1:A:227:GLN:OE1	2.46	0.48
2:B:398:PHE:HB2	2:B:486:MET:SD	2.53	0.48
1:A:418:HIS:O	1:A:420:GLU:N	2.47	0.48
2:B:704:LEU:HD23	2:B:707:ARG:HE	1.79	0.48
1:A:176:LEU:HD13	1:A:180:PHE:CD2	2.49	0.48
1:A:229:GLU:OE2	1:A:229:GLU:N	2.40	0.48
2:B:430:LYS:HA	2:B:433:ILE:HD12	1.95	0.48
2:B:477:ARG:H	2:B:487:LEU:HD13	1.78	0.48
2:B:740:ASP:O	2:B:744:THR:N	2.47	0.48
1:A:183:ASN:O	1:A:187:LEU:HG	2.14	0.48
1:A:16:ILE:HA	1:A:19:LEU:HB3	1.96	0.48
2:B:627:ILE:HG23	2:B:667:ILE:HD11	1.96	0.47
1:A:22:SER:OG	1:A:69:ARG:NH2	2.45	0.47
1:A:291:LYS:HA	1:A:297:PHE:CE2	2.50	0.47
2:B:671:ALA:O	2:B:675:MET:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ARG:HB3	1:A:329:ARG:NH2	2.30	0.47
2:B:404:LEU:O	2:B:408:LEU:HG	2.15	0.47
1:A:80:HIS:ND1	1:A:80:HIS:O	2.48	0.47
2:B:385:LEU:N	2:B:386:PRO:HD3	2.30	0.47
2:B:479:PHE:O	2:B:480:THR:OG1	2.25	0.47
2:B:666:LEU:O	2:B:670:VAL:HG23	2.14	0.47
1:A:180:PHE:CG	1:A:181:PRO:HD3	2.50	0.47
2:B:378:LEU:O	2:B:381:LEU:HG	2.15	0.47
1:A:188:LEU:O	1:A:192:VAL:HG13	2.15	0.46
2:B:686:SER:O	2:B:689:HIS:N	2.39	0.46
1:A:32:LEU:HD23	1:A:32:LEU:HA	1.81	0.46
1:A:88:ALA:O	1:A:91:PHE:N	2.47	0.46
1:A:388:MET:HA	1:A:391:VAL:HG12	1.97	0.46
1:A:406:GLY:O	1:A:409:VAL:HG12	2.15	0.46
1:A:241:LEU:HD11	1:A:252:CYS:SG	2.56	0.46
2:B:287:LEU:O	2:B:289:ILE:N	2.48	0.46
2:B:671:ALA:O	2:B:674:THR:OG1	2.25	0.46
2:B:649:LEU:O	2:B:653:LEU:HG	2.15	0.45
1:A:199:VAL:HB	1:A:207:LEU:HD21	1.99	0.45
1:A:87:TRP:HZ3	1:A:122:ARG:HH12	1.64	0.45
1:A:210:SER:O	1:A:214:VAL:HG22	2.17	0.45
1:A:263:ALA:C	1:A:265:GLU:H	2.20	0.45
2:B:430:LYS:NZ	2:B:511:LEU:HD11	2.32	0.45
2:B:646:CYS:HA	2:B:649:LEU:HD21	1.98	0.45
2:B:203:UNK:O	2:B:207:UNK:N	2.49	0.45
2:B:409:LYS:HB2	2:B:409:LYS:HE3	1.82	0.45
2:B:620:MET:HA	2:B:623:ASN:HD22	1.82	0.45
1:A:11:ALA:HA	1:A:14:GLU:HB2	1.98	0.45
2:B:347:ILE:O	2:B:350:GLN:NE2	2.49	0.45
1:A:195:VAL:O	1:A:199:VAL:HG22	2.16	0.45
1:A:444:GLN:HB2	1:A:445:PRO:HD3	1.99	0.44
1:A:70:LEU:HD13	1:A:74:TRP:CG	2.52	0.44
1:A:354:LEU:HD12	1:A:354:LEU:H	1.81	0.44
2:B:620:MET:O	2:B:624:ILE:HG12	2.18	0.44
1:A:36:LYS:HB2	1:A:90:PHE:HE1	1.81	0.44
1:A:116:ARG:HA	1:A:119:LYS:HE2	1.99	0.44
1:A:208:ASP:HA	1:A:211:VAL:HB	1.99	0.44
1:A:372:GLY:N	1:A:373:GLU:OE1	2.51	0.44
1:A:379:SER:O	1:A:382:GLU:HG3	2.18	0.44
1:A:333:LEU:HA	1:A:336:LEU:HD12	1.99	0.44
2:B:617:ILE:HD12	2:B:620:MET:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ALA:O	1:A:265:GLU:N	2.51	0.44
1:A:394:ARG:HE	1:A:402:VAL:HG12	1.83	0.44
1:A:176:LEU:O	1:A:180:PHE:HB2	2.18	0.44
1:A:98:GLN:O	1:A:102:VAL:HG12	2.18	0.43
1:A:257:GLU:O	1:A:293:LYS:HE3	2.18	0.43
1:A:60:SER:OG	1:A:61:PRO:HD3	2.17	0.43
2:B:360:ASP:OD1	2:B:361:GLN:HG3	2.18	0.43
1:A:19:LEU:HD21	1:A:65:CYS:HB2	1.99	0.43
1:A:313:PRO:O	1:A:316:GLN:HB3	2.18	0.43
1:A:358:ARG:O	1:A:361:SER:OG	2.21	0.43
1:A:438:LEU:HG	1:A:440:LEU:H	1.83	0.43
2:B:548:THR:OG1	2:B:549:ASN:N	2.51	0.43
2:B:718:VAL:O	2:B:722:MET:HG2	2.19	0.43
1:A:200:VAL:HG11	1:A:248:HIS:CG	2.53	0.43
1:A:294:LYS:HA	1:A:297:PHE:HD2	1.83	0.43
2:B:558:THR:O	2:B:562:GLU:HG2	2.18	0.43
2:B:656:VAL:O	2:B:660:ALA:N	2.52	0.43
1:A:28:ILE:HA	1:A:31:THR:HG22	2.00	0.43
1:A:241:LEU:O	1:A:245:SER:OG	2.36	0.43
1:A:212:SER:HA	1:A:258:GLN:HE22	1.83	0.43
1:A:221:ALA:O	1:A:225:GLY:N	2.52	0.43
2:B:381:LEU:O	2:B:385:LEU:HG	2.19	0.42
1:A:13:ARG:O	1:A:17:HIS:N	2.38	0.42
1:A:328:ARG:HD2	1:A:329:ARG:HH12	1.84	0.42
2:B:354:VAL:HG22	2:B:358:PHE:CZ	2.55	0.42
2:B:711:LEU:HD23	2:B:711:LEU:HA	1.88	0.42
1:A:404:ARG:NH2	1:A:435:LEU:HB3	2.34	0.42
2:B:483:ARG:HB3	2:B:486:MET:HG2	2.01	0.42
2:B:550:PRO:HA	2:B:553:LEU:HD12	2.02	0.42
2:B:693:GLN:OE1	2:B:693:GLN:HA	2.19	0.42
1:A:268:LEU:HD23	1:A:268:LEU:HA	1.84	0.42
2:B:353:LYS:HD3	2:B:353:LYS:HA	1.74	0.42
2:B:694:ASN:OD1	2:B:694:ASN:N	2.52	0.42
1:A:288:LEU:O	1:A:291:LYS:N	2.53	0.42
2:B:684:TYR:CE1	2:B:693:GLN:HG2	2.55	0.42
1:A:438:LEU:HD12	1:A:439:ALA:H	1.84	0.42
1:A:124:LEU:O	1:A:128:LEU:HG	2.20	0.42
1:A:233:VAL:C	1:A:236:PRO:HD2	2.41	0.42
1:A:394:ARG:NH1	1:A:402:VAL:O	2.53	0.42
1:A:400:PRO:N	1:A:401:PRO:HD2	2.35	0.41
1:A:302:LYS:HB2	1:A:306:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:GLN:NE2	1:A:371:LEU:O	2.53	0.41
1:A:36:LYS:HA	1:A:39:LEU:HB2	2.01	0.41
1:A:181:PRO:HB2	1:A:182:GLN:NE2	2.36	0.41
2:B:258:VAL:HA	2:B:263:ALA:HB3	2.02	0.41
1:A:238:LEU:HD12	1:A:283:ARG:HH22	1.85	0.41
1:A:154:GLU:OE2	1:A:220:LYS:HE3	2.21	0.41
1:A:265:GLU:OE1	1:A:266:ALA:N	2.53	0.41
2:B:368:LYS:HA	2:B:368:LYS:HD2	1.69	0.41
1:A:66:LEU:HG	1:A:87:TRP:CD1	2.56	0.41
1:A:128:LEU:O	1:A:132:ARG:HB2	2.21	0.41
1:A:142:ARG:NH2	1:A:143:GLN:HG3	2.29	0.41
1:A:179:PHE:HA	1:A:183:ASN:HB2	2.03	0.41
1:A:315:LEU:HA	1:A:318:LEU:HB3	2.03	0.41
1:A:402:VAL:O	1:A:405:LEU:HB2	2.21	0.41
2:B:426:GLN:O	2:B:430:LYS:HG2	2.21	0.41
2:B:530:VAL:HG11	2:B:637:PHE:CE1	2.55	0.41
2:B:627:ILE:O	2:B:631:LEU:HG	2.20	0.41
2:B:675:MET:O	2:B:678:VAL:HG22	2.21	0.40
1:A:8:VAL:O	1:A:12:VAL:N	2.41	0.40
1:A:170:ARG:HA	1:A:170:ARG:NH2	2.37	0.40
1:A:188:LEU:HD23	1:A:188:LEU:HA	1.93	0.40
1:A:410:ALA:HA	1:A:413:VAL:HG22	2.02	0.40
2:B:546:ILE:HD12	2:B:546:ILE:HA	1.97	0.40
2:B:768:ALA:O	2:B:772:PRO:N	2.54	0.40
1:A:234:LEU:HA	1:A:237:ARG:HB2	2.03	0.40
1:A:339:LEU:HD13	1:A:367:CYS:SG	2.61	0.40
1:A:408:ILE:O	1:A:412:VAL:HG23	2.22	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	436/837 (52%)	371 (85%)	63 (14%)	2 (0%)	29 68
2	B	454/1095 (42%)	386 (85%)	65 (14%)	3 (1%)	22 62
All	All	890/1932 (46%)	757 (85%)	128 (14%)	5 (1%)	29 64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	ALA
2	B	687	LEU
2	B	262	PRO
2	B	344	SER
1	A	133	LEU

5.3.2 Protein sidechains (i)

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	370/699 (53%)	368 (100%)	2 (0%)	88 93
2	B	230/775 (30%)	230 (100%)	0	100 100
All	All	600/1474 (41%)	598 (100%)	2 (0%)	92 95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	262	ARG
1	A	425	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	370	GLN
2	B	352	ASN
2	B	420	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	424	HIS
2	B	513	HIS
2	B	623	ASN
2	B	663	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

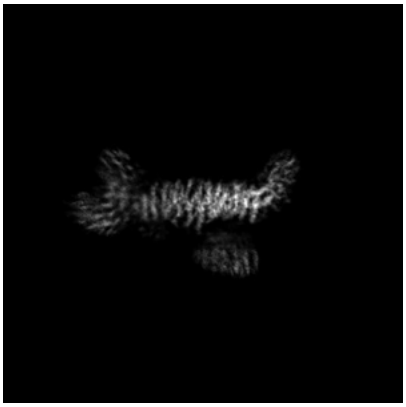
This section contains visualisations of the EMDB entry EMD-31454. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

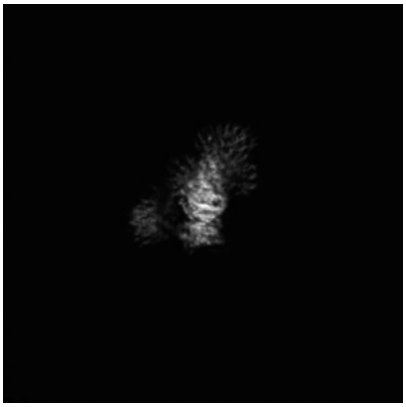
6.1 Orthogonal projections

6.1.1 Primary map

X



Y



Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 175

Y Index: 175

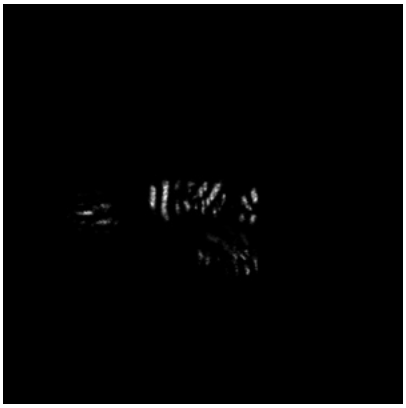
Z Index: 175

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: 176



Y Index: 170

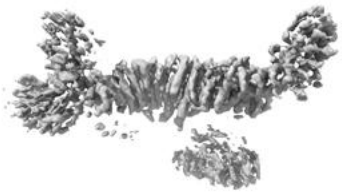
Z Index: 180

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

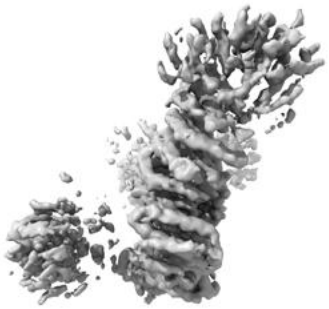
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

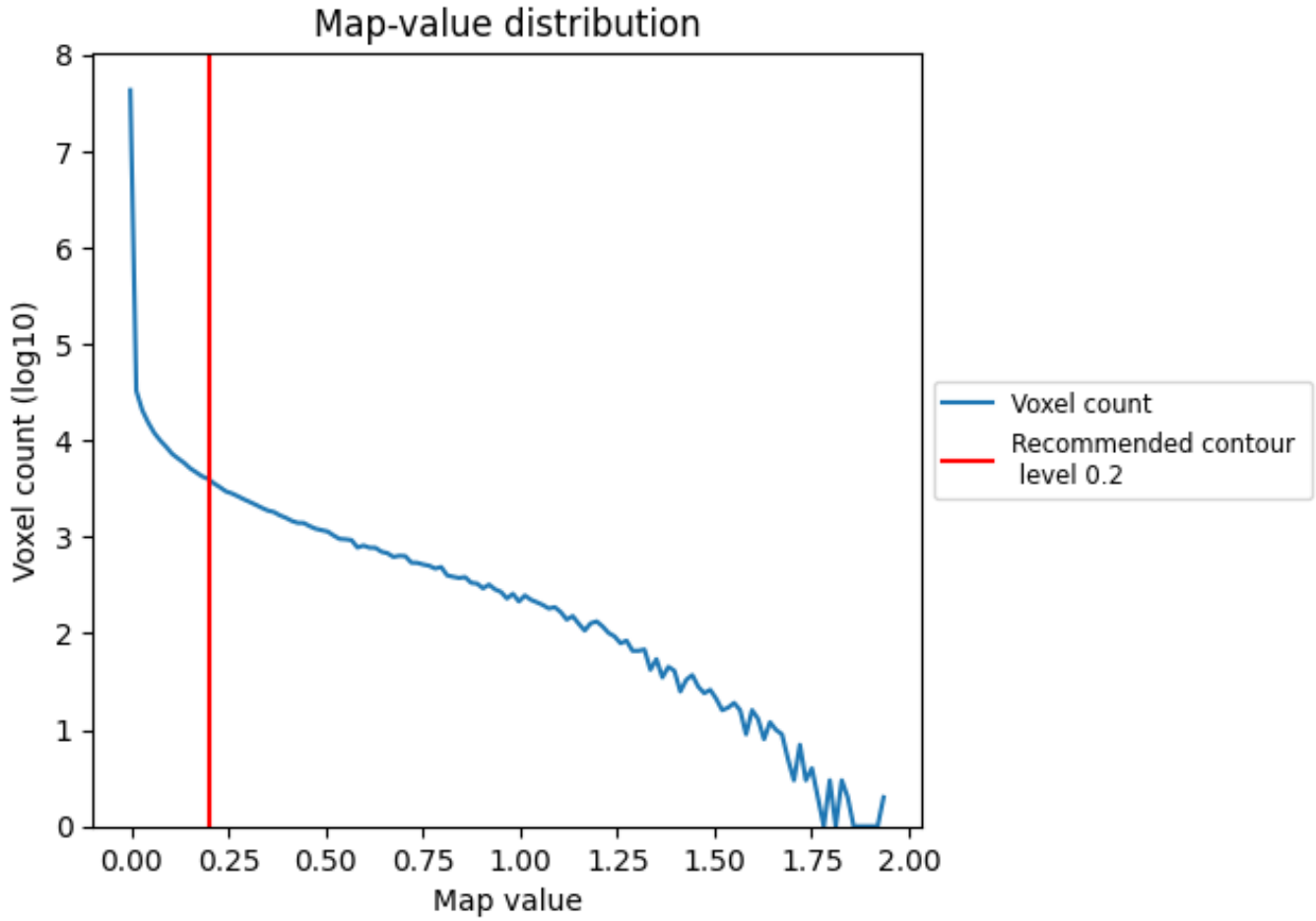
6.5 Mask visualisation (i)

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

7 Map analysis

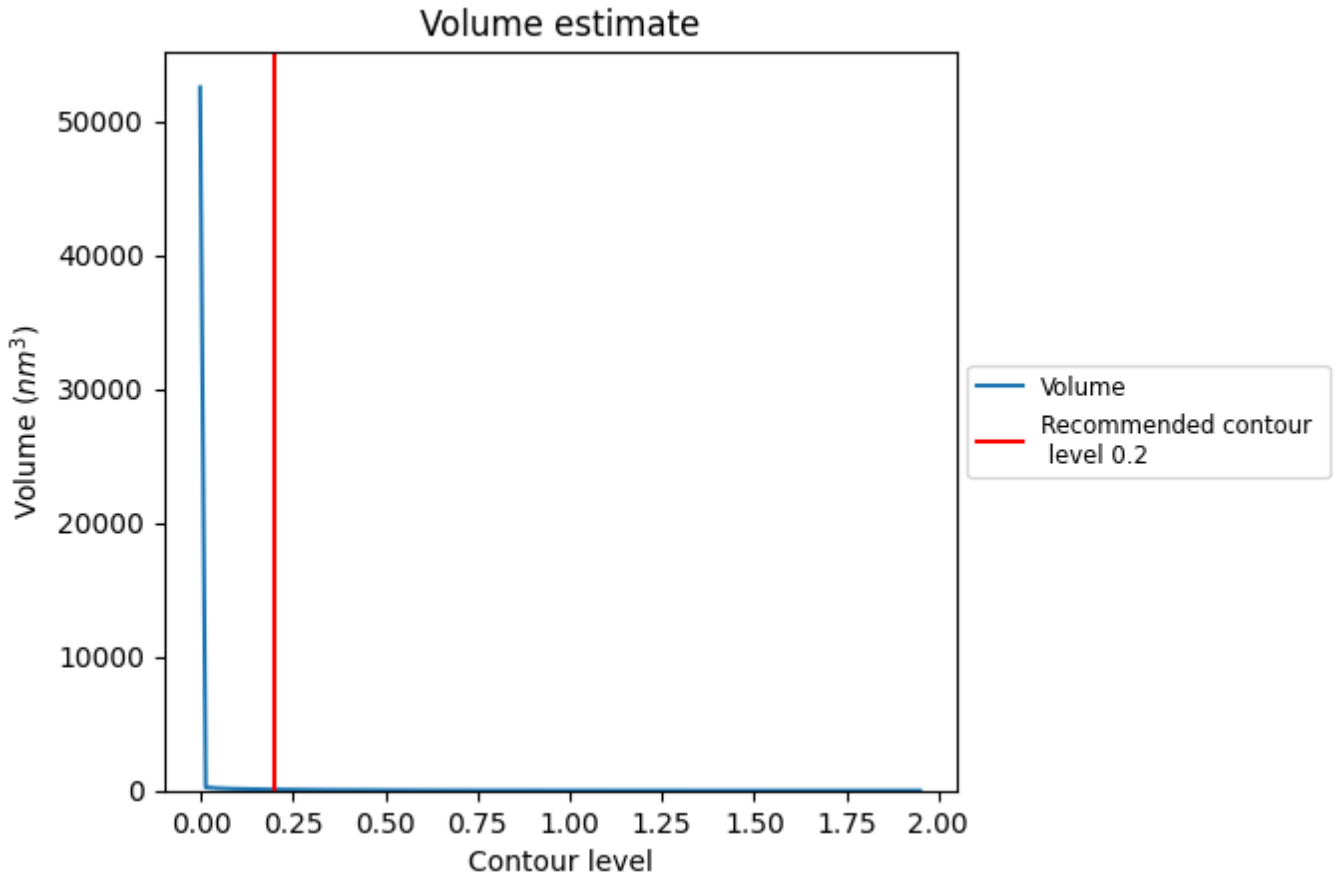
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

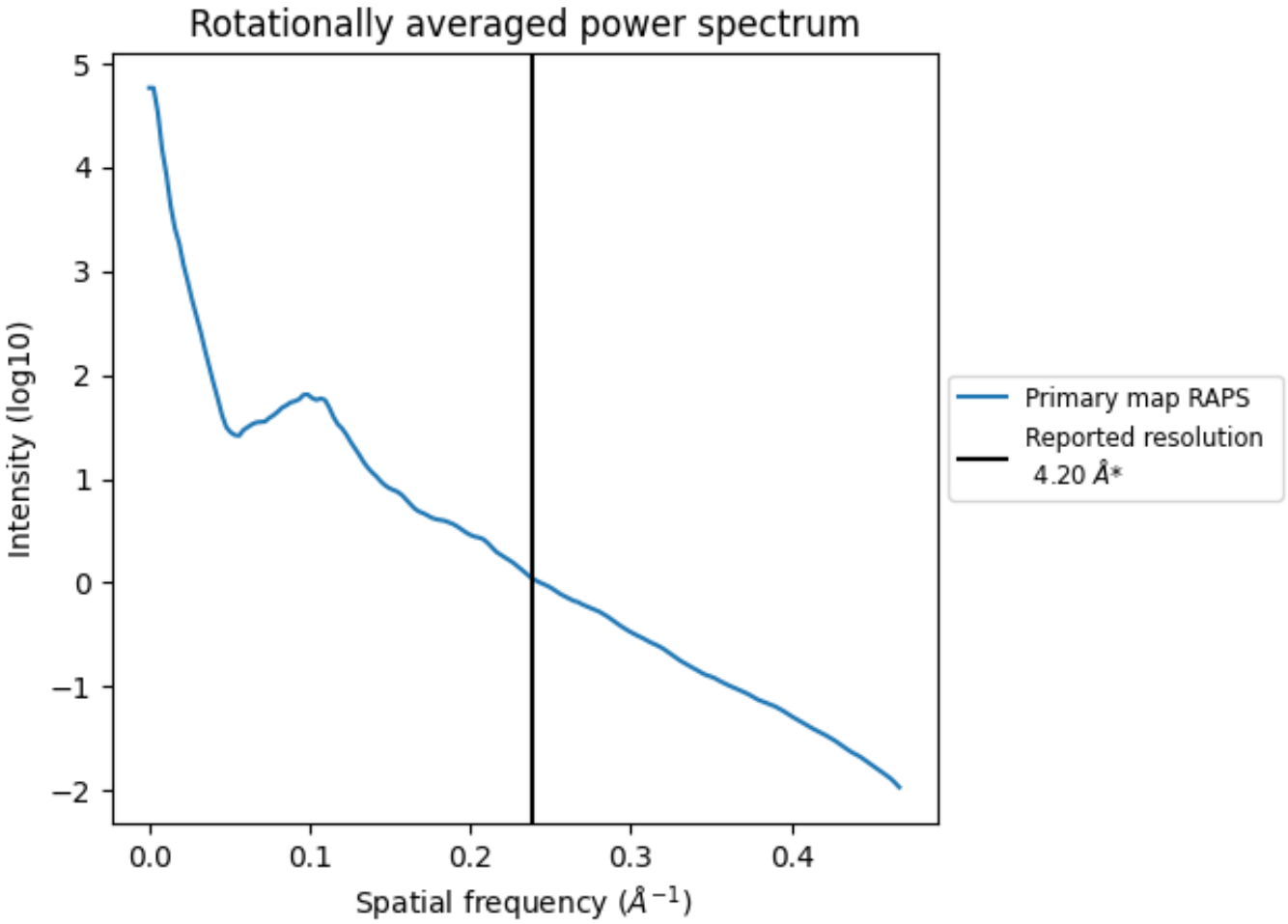
7.2 Volume estimate



The volume at the recommended contour level is 79 nm^3; this corresponds to an approximate mass of 71 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 (i)



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

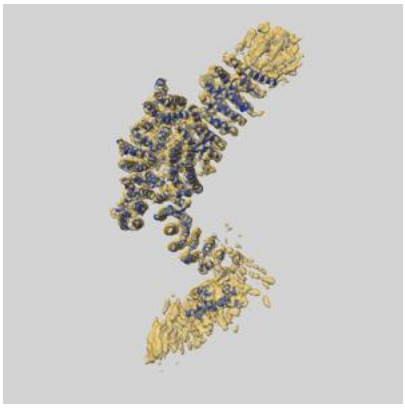
8 Fourier-Shell correlation

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

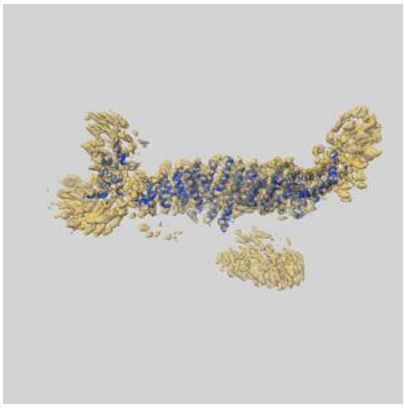
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31454 and PDB model 7F4U. Per-residue inclusion information can be found in section 3 on page 10.

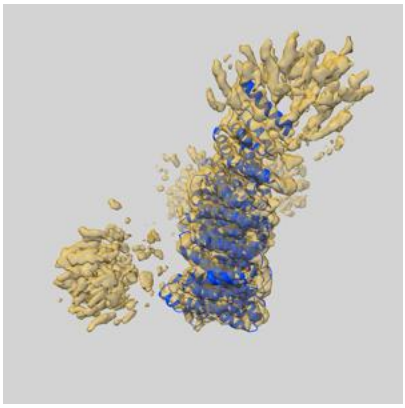
9.1 Map-model overlay



X



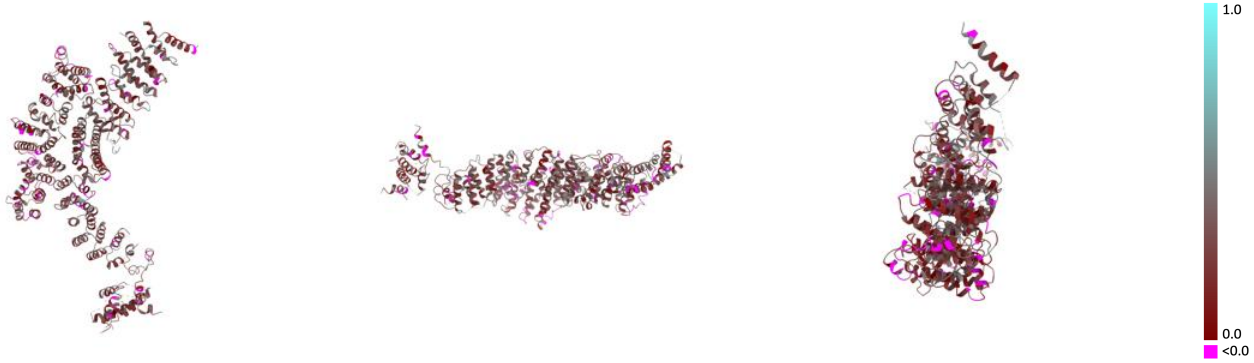
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

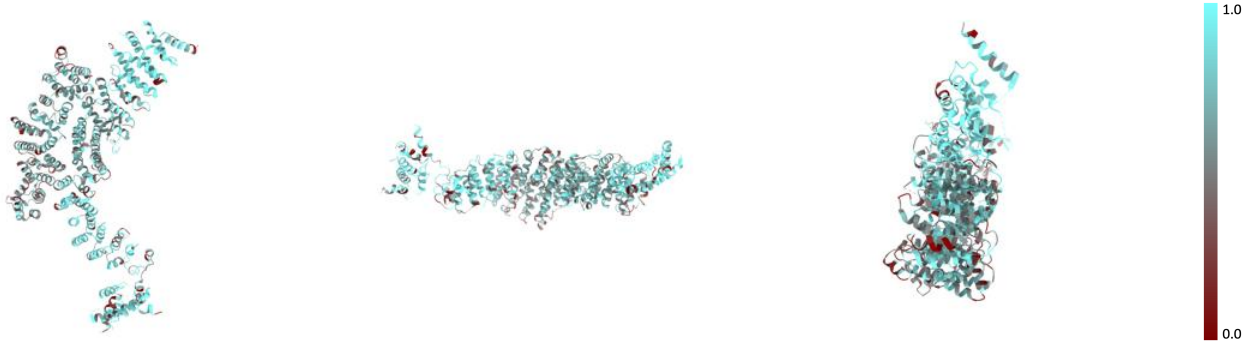
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

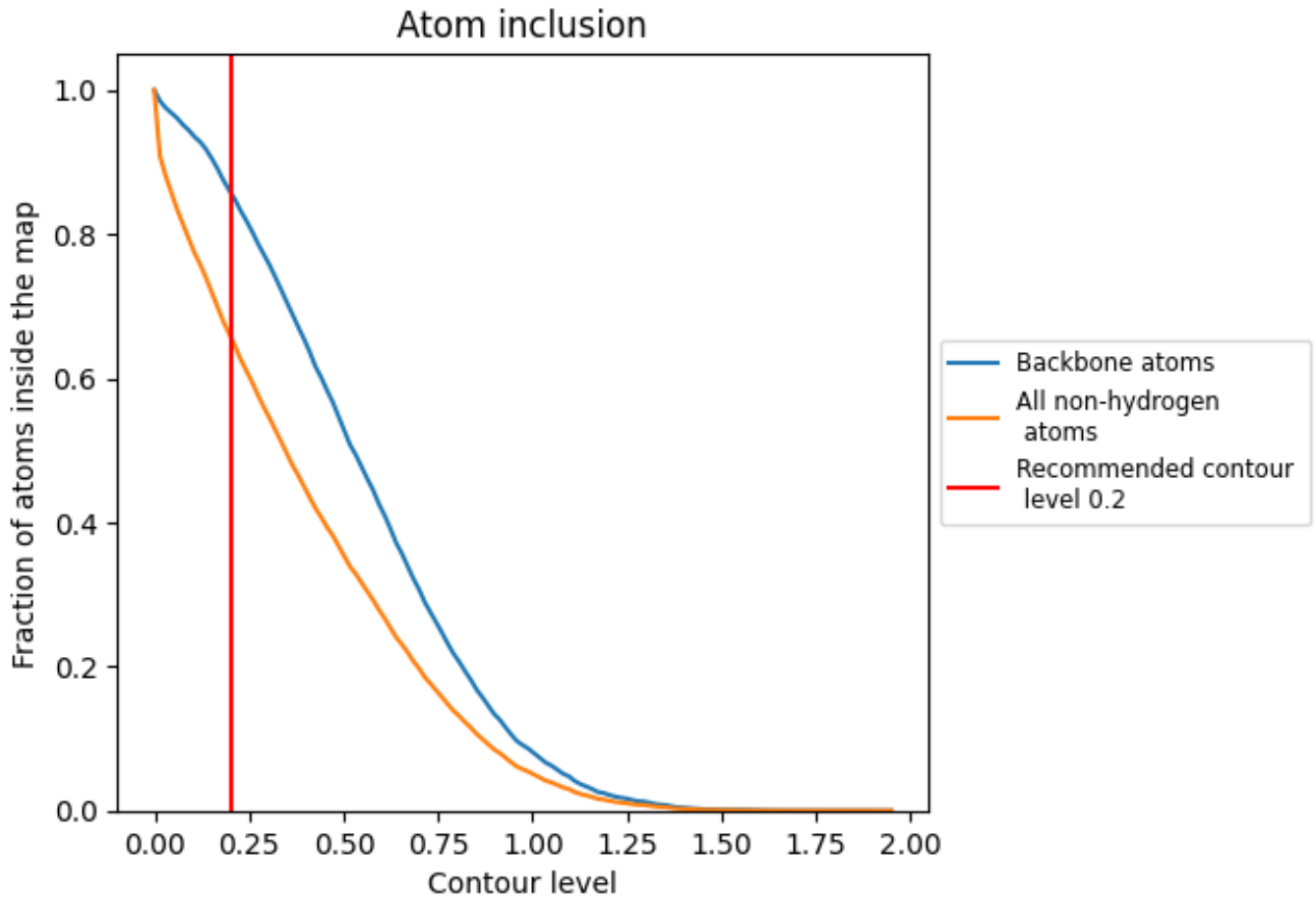
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6574	0.2560
A	0.5685	0.2120
B	0.7190	0.2900
C	0.7423	0.2690