



Full wwPDB EM Validation Report ⓘ

Nov 27, 2022 – 10:25 PM EST

PDB ID : 7LUV
EMDB ID : EMD-23527
Title : Cryo-EM structure of the yeast THO-Sub2 complex
Authors : Xie, Y.; Ren, Y.
Deposited on : 2021-02-23
Resolution : 3.70 Å(reported)

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A user guide is available at

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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) : 2.31.2

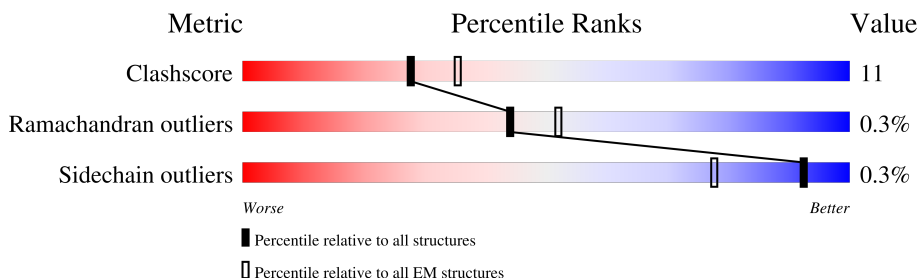
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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 $\leq 5\%$. 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	603	
2	B	261	
3	C	1262	
4	D	256	
5	E	385	
6	M	446	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18773 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 THO complex subunit HPR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	483	Total	C	N	O	S	0	0
			4026	2599	657	751	19		

- Molecule 2 is a protein called THO complex subunit THP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	189	Total	C	N	O	S	0	0
			1576	998	266	306	6		

- Molecule 3 is a protein called THO complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	911	Total	C	N	O	S	0	0
			6828	4404	1142	1260	22		

There are 229 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	expression tag	UNP P53552
C	-3	ALA	-	expression tag	UNP P53552
C	-2	MET	-	expression tag	UNP P53552
C	-1	GLY	-	expression tag	UNP P53552
C	0	SER	-	expression tag	UNP P53552
C	37	UNK	TRP	conflict	UNP P53552
C	38	UNK	PRO	conflict	UNP P53552
C	39	UNK	GLU	conflict	UNP P53552
C	40	UNK	ARG	conflict	UNP P53552
C	41	UNK	SER	conflict	UNP P53552
C	42	UNK	LYS	conflict	UNP P53552
C	43	UNK	THR	conflict	UNP P53552
C	44	UNK	LEU	conflict	UNP P53552
C	45	UNK	CYS	conflict	UNP P53552
C	46	UNK	SER	conflict	UNP P53552

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Chain	Residue	Modelled	Actual	Comment	Reference
C	47	UNK	ASP	conflict	UNP P53552
C	48	UNK	PHE	conflict	UNP P53552
C	49	UNK	THR	conflict	UNP P53552
C	50	UNK	ALA	conflict	UNP P53552
C	51	UNK	LEU	conflict	UNP P53552
C	75	UNK	ASN	conflict	UNP P53552
C	76	UNK	ASP	conflict	UNP P53552
C	77	UNK	GLU	conflict	UNP P53552
C	78	UNK	ASN	conflict	UNP P53552
C	79	UNK	SER	conflict	UNP P53552
C	80	UNK	PRO	conflict	UNP P53552
C	81	UNK	LEU	conflict	UNP P53552
C	82	UNK	LYS	conflict	UNP P53552
C	83	UNK	LEU	conflict	UNP P53552
C	84	UNK	SER	conflict	UNP P53552
C	85	UNK	ASP	conflict	UNP P53552
C	86	UNK	VAL	conflict	UNP P53552
C	87	UNK	ALA	conflict	UNP P53552
C	88	UNK	SER	conflict	UNP P53552
C	89	UNK	PHE	conflict	UNP P53552
C	90	UNK	THR	conflict	UNP P53552
C	91	UNK	ASN	conflict	UNP P53552
C	92	UNK	GLU	conflict	UNP P53552
C	93	UNK	LEU	conflict	UNP P53552
C	94	UNK	VAL	conflict	UNP P53552
C	95	UNK	ASN	conflict	UNP P53552
C	96	UNK	HIS	conflict	UNP P53552
C	97	UNK	GLU	conflict	UNP P53552
C	98	UNK	ARG	conflict	UNP P53552
C	99	UNK	GLN	conflict	UNP P53552
C	100	UNK	VAL	conflict	UNP P53552
C	101	UNK	SER	conflict	UNP P53552
C	102	UNK	GLN	conflict	UNP P53552
C	103	UNK	ALA	conflict	UNP P53552
C	104	UNK	SER	conflict	UNP P53552
C	105	UNK	ILE	conflict	UNP P53552
C	106	UNK	VAL	conflict	UNP P53552
C	107	UNK	GLY	conflict	UNP P53552
C	108	UNK	LYS	conflict	UNP P53552
C	109	UNK	MET	conflict	UNP P53552
C	110	UNK	PHE	conflict	UNP P53552
C	111	UNK	ILE	conflict	UNP P53552

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Chain	Residue	Modelled	Actual	Comment	Reference
C	112	UNK	ALA	conflict	UNP P53552
C	113	UNK	VAL	conflict	UNP P53552
C	114	UNK	SER	conflict	UNP P53552
C	115	UNK	SER	conflict	UNP P53552
C	116	UNK	THR	conflict	UNP P53552
C	117	UNK	VAL	conflict	UNP P53552
C	118	UNK	PRO	conflict	UNP P53552
C	119	UNK	ASN	conflict	UNP P53552
C	120	UNK	ILE	conflict	UNP P53552
C	121	UNK	ASN	conflict	UNP P53552
C	122	UNK	ASP	conflict	UNP P53552
C	6941	UNK	GLN	conflict	UNP P53552
C	6942	UNK	LEU	conflict	UNP P53552
C	6943	UNK	ASN	conflict	UNP P53552
C	6944	UNK	SER	conflict	UNP P53552
C	6945	UNK	ASN	conflict	UNP P53552
C	6946	UNK	GLU	conflict	UNP P53552
C	6947	UNK	ASN	conflict	UNP P53552
C	6948	UNK	PHE	conflict	UNP P53552
C	6949	UNK	SER	conflict	UNP P53552
C	6950	UNK	ILE	conflict	UNP P53552
C	6951	UNK	ASP	conflict	UNP P53552
C	6991	UNK	GLU	conflict	UNP P53552
C	6992	UNK	LEU	conflict	UNP P53552
C	6993	UNK	ILE	conflict	UNP P53552
C	6994	UNK	GLU	conflict	UNP P53552
C	6995	UNK	GLY	conflict	UNP P53552
C	6996	UNK	ALA	conflict	UNP P53552
C	6997	UNK	GLU	conflict	UNP P53552
C	6998	UNK	PHE	conflict	UNP P53552
C	6999	UNK	SER	conflict	UNP P53552
C	7000	UNK	ASP	conflict	UNP P53552
C	7001	UNK	VAL	conflict	UNP P53552
C	7002	UNK	ASP	conflict	UNP P53552
C	7003	UNK	LEU	conflict	UNP P53552
C	7004	UNK	THR	conflict	UNP P53552
C	7005	UNK	LYS	conflict	UNP P53552
C	7006	UNK	ILE	conflict	UNP P53552
C	7007	UNK	SER	conflict	UNP P53552
C	7008	UNK	LYS	conflict	UNP P53552
C	7009	UNK	ASP	conflict	UNP P53552
C	7010	UNK	LEU	conflict	UNP P53552

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Chain	Residue	Modelled	Actual	Comment	Reference
C	7011	UNK	PHE	conflict	UNP P53552
C	7012	UNK	THR	conflict	UNP P53552
C	7028	UNK	THR	conflict	UNP P53552
C	7029	UNK	PHE	conflict	UNP P53552
C	7030	UNK	TRP	conflict	UNP P53552
C	7031	UNK	ARG	conflict	UNP P53552
C	7032	UNK	LEU	conflict	UNP P53552
C	7033	UNK	SER	conflict	UNP P53552
C	7034	UNK	LEU	conflict	UNP P53552
C	7035	UNK	TYR	conflict	UNP P53552
C	7036	UNK	ASP	conflict	UNP P53552
C	7037	UNK	ILE	conflict	UNP P53552
C	7038	UNK	HIS	conflict	UNP P53552
C	7039	UNK	PHE	conflict	UNP P53552
C	7040	UNK	ASP	conflict	UNP P53552
C	7047	UNK	LYS	conflict	UNP P53552
C	7048	UNK	SER	conflict	UNP P53552
C	7049	UNK	LEU	conflict	UNP P53552
C	7050	UNK	TYR	conflict	UNP P53552
C	7051	UNK	ASP	conflict	UNP P53552
C	7052	UNK	GLU	conflict	UNP P53552
C	7053	UNK	ARG	conflict	UNP P53552
C	7054	UNK	LYS	conflict	UNP P53552
C	7055	UNK	ASN	conflict	UNP P53552
C	7056	UNK	ALA	conflict	UNP P53552
C	7057	UNK	LEU	conflict	UNP P53552
C	7058	UNK	SER	conflict	UNP P53552
C	7059	UNK	GLY	conflict	UNP P53552
C	7060	UNK	GLU	conflict	UNP P53552
C	7131	UNK	ASN	conflict	UNP P53552
C	7132	UNK	THR	conflict	UNP P53552
C	7133	UNK	GLY	conflict	UNP P53552
C	7134	UNK	HIS	conflict	UNP P53552
C	7135	UNK	MET	conflict	UNP P53552
C	7136	UNK	SER	conflict	UNP P53552
C	7137	UNK	ASN	conflict	UNP P53552
C	7138	UNK	ARG	conflict	UNP P53552
C	7139	UNK	LYS	conflict	UNP P53552
C	7140	UNK	LYS	conflict	UNP P53552
C	7141	UNK	HIS	conflict	UNP P53552
C	7142	UNK	LEU	conflict	UNP P53552
C	7143	UNK	ILE	conflict	UNP P53552

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Chain	Residue	Modelled	Actual	Comment	Reference
C	7144	UNK	GLN	conflict	UNP P53552
C	7145	UNK	ASN	conflict	UNP P53552
C	7146	UNK	GLN	conflict	UNP P53552
C	7147	UNK	ILE	conflict	UNP P53552
C	7148	UNK	LYS	conflict	UNP P53552
C	7149	UNK	ASP	conflict	UNP P53552
C	7150	UNK	ILE	conflict	UNP P53552
C	7159	UNK	LEU	conflict	UNP P53552
C	7160	UNK	VAL	conflict	UNP P53552
C	7161	UNK	THR	conflict	UNP P53552
C	7162	UNK	GLY	conflict	UNP P53552
C	7163	UNK	ILE	conflict	UNP P53552
C	7164	UNK	SER	conflict	UNP P53552
C	7165	UNK	HIS	conflict	UNP P53552
C	7166	UNK	GLN	conflict	UNP P53552
C	7167	UNK	ARG	conflict	UNP P53552
C	7168	UNK	ALA	conflict	UNP P53552
C	7169	UNK	PHE	conflict	UNP P53552
C	7170	UNK	LYS	conflict	UNP P53552
C	7171	UNK	LYS	conflict	UNP P53552
C	7172	UNK	THR	conflict	UNP P53552
C	7173	UNK	SER	conflict	UNP P53552
C	7174	UNK	GLU	conflict	UNP P53552
C	7175	UNK	PHE	conflict	UNP P53552
C	7176	UNK	ILE	conflict	UNP P53552
C	7180	UNK	SER	conflict	UNP P53552
C	7181	UNK	GLU	conflict	UNP P53552
C	7182	UNK	LYS	conflict	UNP P53552
C	7183	UNK	SER	conflict	UNP P53552
C	7184	UNK	ASN	conflict	UNP P53552
C	7185	UNK	VAL	conflict	UNP P53552
C	7186	UNK	TRP	conflict	UNP P53552
C	7187	UNK	ASN	conflict	UNP P53552
C	7188	UNK	LYS	conflict	UNP P53552
C	7189	UNK	ASP	conflict	UNP P53552
C	7190	UNK	CYS	conflict	UNP P53552
C	7191	UNK	GLY	conflict	UNP P53552
C	7192	UNK	GLU	conflict	UNP P53552
C	7193	UNK	ASP	conflict	UNP P53552
C	7194	UNK	GLN	conflict	UNP P53552
C	7195	UNK	ILE	conflict	UNP P53552
C	7196	UNK	LYS	conflict	UNP P53552

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Chain	Residue	Modelled	Actual	Comment	Reference
C	7197	UNK	ILE	conflict	UNP P53552
C	7198	UNK	PHE	conflict	UNP P53552
C	7199	UNK	LEU	conflict	UNP P53552
C	7200	UNK	GLN	conflict	UNP P53552
C	7201	UNK	ASN	conflict	UNP P53552
C	7211	UNK	CYS	conflict	UNP P53552
C	7212	UNK	VAL	conflict	UNP P53552
C	7213	UNK	VAL	conflict	UNP P53552
C	7214	UNK	PRO	conflict	UNP P53552
C	7215	UNK	ARG	conflict	UNP P53552
C	7216	UNK	VAL	conflict	UNP P53552
C	7217	UNK	LEU	conflict	UNP P53552
C	7218	UNK	PHE	conflict	UNP P53552
C	7219	UNK	SER	conflict	UNP P53552
C	7220	UNK	PRO	conflict	UNP P53552
C	7221	UNK	SER	conflict	UNP P53552
C	7222	UNK	ASP	conflict	UNP P53552
C	7223	UNK	ALA	conflict	UNP P53552
C	7224	UNK	LEU	conflict	UNP P53552
C	7225	UNK	PHE	conflict	UNP P53552
C	7234	UNK	SER	conflict	UNP P53552
C	7235	UNK	SER	conflict	UNP P53552
C	7236	UNK	PHE	conflict	UNP P53552
C	7237	UNK	PHE	conflict	UNP P53552
C	7238	UNK	ILE	conflict	UNP P53552
C	7239	UNK	PHE	conflict	UNP P53552
C	7240	UNK	MET	conflict	UNP P53552
C	7241	UNK	ALA	conflict	UNP P53552
C	7242	UNK	PHE	conflict	UNP P53552
C	7243	UNK	ARG	conflict	UNP P53552
C	7244	UNK	THR	conflict	UNP P53552
C	7245	UNK	GLU	conflict	UNP P53552
C	7246	UNK	ASN	conflict	UNP P53552
C	7247	UNK	LEU	conflict	UNP P53552
C	7248	UNK	MET	conflict	UNP P53552
C	7256	UNK	SER	conflict	UNP P53552
C	7257	UNK	ILE	conflict	UNP P53552
C	7258	UNK	LEU	conflict	UNP P53552
C	7259	UNK	ASN	conflict	UNP P53552
C	7260	UNK	THR	conflict	UNP P53552
C	7261	UNK	CYS	conflict	UNP P53552
C	7262	UNK	ILE	conflict	UNP P53552

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Chain	Residue	Modelled	Actual	Comment	Reference
C	7263	UNK	THR	conflict	UNP P53552
C	7264	UNK	SER	conflict	UNP P53552
C	7265	UNK	ASN	conflict	UNP P53552
C	7266	UNK	ILE	conflict	UNP P53552

- Molecule 4 is a protein called THO complex subunit MFT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	150	Total	C	N	O	S	0	0
			1212	761	210	239	2		

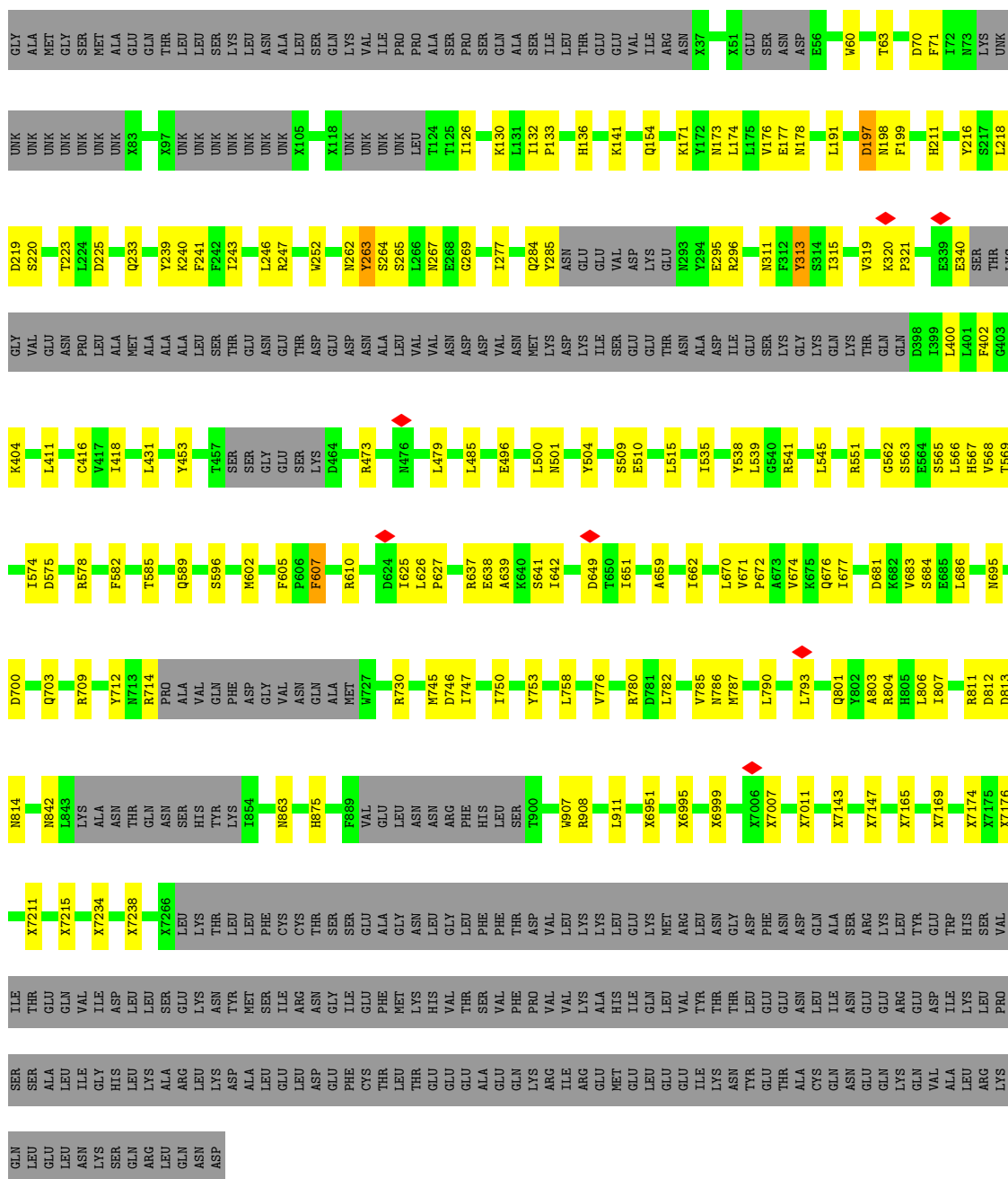
- Molecule 5 is a protein called Tex1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	271	Total	C	N	O	S	0	0
			2121	1362	348	400	11		

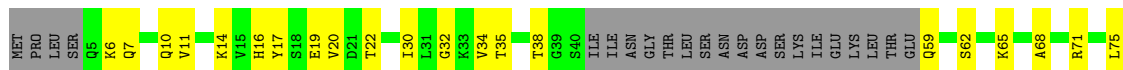
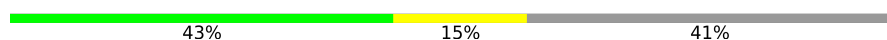
- Molecule 6 is a protein called ATP-dependent RNA helicase SUB2.

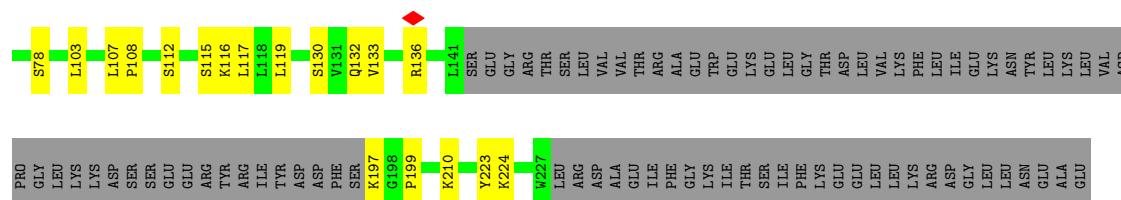
Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	374	Total	C	N	O	S	0	0
			3010	1916	523	560	11		

Chain C:

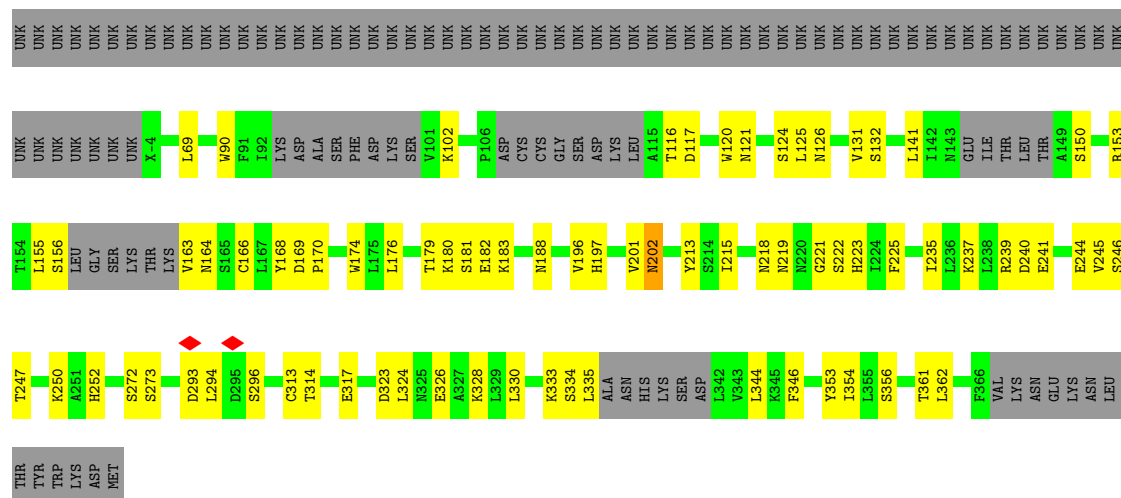


Chain D:

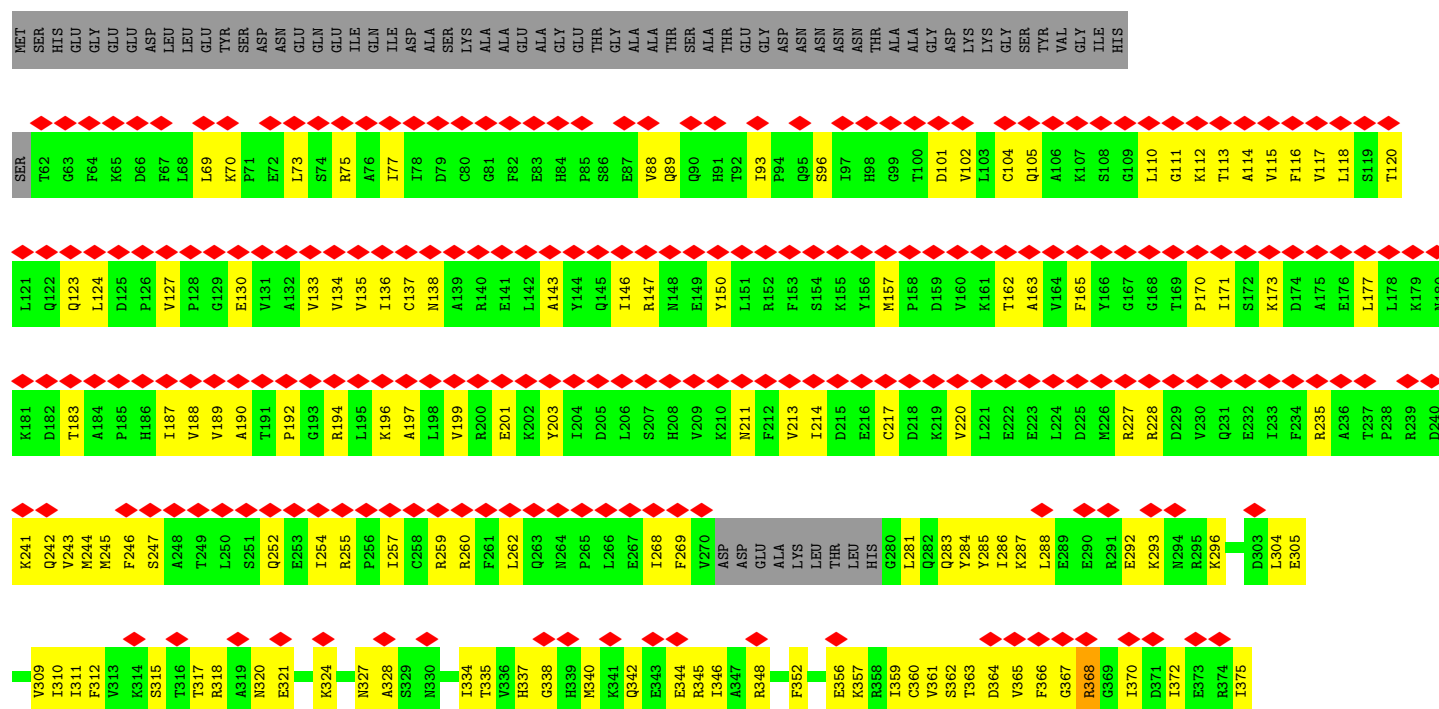




• Molecule 5: Tex1



• Molecule 6: ATP-dependent RNA helicase SUB2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30066	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	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.036	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	340.55002, 340.55002, 340.55002	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.6811, 0.6811, 0.6811	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	0.42	0/4121	0.49	0/5566
2	B	0.36	0/1601	0.47	0/2154
3	C	0.43	0/5932	0.50	0/8028
4	D	0.37	0/1225	0.46	0/1642
5	E	0.42	0/2138	0.53	1/2895 (0.0%)
6	M	0.30	0/3063	0.46	0/4131
All	All	0.40	0/18080	0.49	1/24416 (0.0%)

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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	E	120	TRP	C-N-CA	-5.60	107.69	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	LEU	Peptide
2	B	149	PRO	Peptide

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	4026	0	3972	78	0
2	B	1576	0	1565	33	0
3	C	6828	0	6118	116	0
4	D	1212	0	1242	33	0
5	E	2121	0	2100	47	0
6	M	3010	0	3049	121	0
All	All	18773	0	18046	393	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 (393) 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:215:PRO:O	1:A:221:ASN:ND2	2.09	0.86
1:A:278:LEU:HD21	1:A:444:ASN:HA	1.59	0.84
6:M:138:ASN:HB2	6:M:220:VAL:HG22	1.60	0.82
6:M:70:LYS:HE2	6:M:73:LEU:HG	1.61	0.82
1:A:196:THR:H	1:A:199:HIS:HD2	1.26	0.81
6:M:214:ILE:O	6:M:245:MET:HA	1.81	0.80
3:C:807:ILE:O	6:M:75:ARG:NH2	2.13	0.79
3:C:703:GLN:NE2	3:C:746:ASP:O	2.17	0.78
6:M:386:GLU:OE2	6:M:425:ARG:NH1	2.18	0.77
1:A:472:TYR:OH	1:A:476:ARG:NH2	2.17	0.77
5:E:317:GLU:HB3	5:E:335:LEU:HB2	1.67	0.76
6:M:89:GLN:NE2	6:M:111:GLY:O	2.18	0.76
6:M:241:LYS:HE2	6:M:243:VAL:HB	1.69	0.75
2:B:121:LEU:O	2:B:125:SER:OG	2.05	0.74
6:M:372:ILE:HG21	6:M:375:ILE:HD12	1.69	0.74
6:M:135:VAL:HB	6:M:189:VAL:HG22	1.70	0.73
5:E:163:VAL:HA	5:E:179:THR:HG22	1.68	0.73
1:A:454:TYR:HA	1:A:458:ASN:HD22	1.55	0.72
1:A:385:GLN:NE2	2:B:108:GLU:OE2	2.23	0.72
6:M:380:ASN:ND2	6:M:408:SER:OG	2.19	0.72
3:C:539:LEU:HD11	3:C:545:LEU:HD22	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:333:LYS:HG2	5:E:334:SER:H	1.55	0.71
6:M:286:ILE:HD11	6:M:433:PHE:HB3	1.72	0.71
3:C:538:TYR:HD1	3:C:541:ARG:HE	1.39	0.70
3:C:7007:UNK:O	3:C:7011:UNK:CB	2.39	0.70
6:M:147:ARG:HA	6:M:150:TYR:HD2	1.58	0.69
2:B:76:ARG:HH12	2:B:80:LEU:HB2	1.57	0.69
1:A:504:GLU:O	3:C:267:ASN:ND2	2.26	0.69
6:M:337:HIS:ND1	6:M:338:GLY:O	2.21	0.69
4:D:6:LYS:O	4:D:10:GLN:HB2	1.93	0.68
6:M:364:ASP:O	6:M:368:ARG:NH1	2.25	0.68
6:M:163:ALA:O	6:M:189:VAL:HB	1.93	0.68
1:A:44:LEU:O	1:A:109:ASN:ND2	2.26	0.68
6:M:284:TYR:HB2	6:M:407:ILE:HG12	1.75	0.68
2:B:142:TYR:O	2:B:143:GLU:HG2	1.93	0.67
3:C:7211:UNK:O	3:C:7215:UNK:N	2.28	0.67
3:C:607:PHE:HB3	3:C:610:ARG:HH11	1.60	0.67
1:A:388:GLN:O	1:A:395:ARG:NH2	2.28	0.66
6:M:124:LEU:HD22	6:M:187:ILE:HD11	1.77	0.66
6:M:389:GLN:HA	6:M:392:HIS:HD2	1.61	0.65
6:M:309:VAL:HG12	6:M:377:LEU:HB3	1.78	0.65
3:C:269:GLY:HA3	3:C:311:ASN:HB2	1.79	0.65
6:M:102:VAL:HB	6:M:244:MET:HG2	1.77	0.65
6:M:133:VAL:HB	6:M:187:ILE:HD12	1.79	0.65
5:E:218:ASN:OD1	5:E:219:ASN:N	2.30	0.64
5:E:296:SER:OG	5:E:314:THR:OG1	2.15	0.64
6:M:196:LYS:HA	6:M:199:VAL:HG12	1.79	0.64
1:A:60:ASP:OD1	1:A:61:ARG:N	2.31	0.64
2:B:100:ILE:HG12	4:D:103:LEU:HD12	1.80	0.63
6:M:392:HIS:O	6:M:396:ARG:HG2	1.98	0.63
1:A:469:PRO:HA	1:A:472:TYR:HB3	1.80	0.63
1:A:378:ASN:ND2	1:A:381:CYS:SG	2.72	0.63
3:C:473:ARG:O	3:C:479:LEU:HA	1.98	0.63
6:M:96:SER:O	6:M:123:GLN:NE2	2.32	0.63
6:M:211:ASN:HA	6:M:242:GLN:O	1.99	0.62
2:B:34:LEU:HD23	2:B:37:LEU:HD12	1.81	0.62
2:B:147:TRP:CZ3	2:B:149:PRO:HB3	2.34	0.62
6:M:317:THR:O	6:M:321:GLU:HB2	1.99	0.62
2:B:72:LYS:O	2:B:75:THR:HG22	2.00	0.62
1:A:410:ARG:HB2	1:A:452:CYS:SG	2.39	0.62
3:C:677:ILE:HD11	3:C:684:SER:HA	1.81	0.62
3:C:216:TYR:O	3:C:218:LEU:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:7143:UNK:O	3:C:7147:UNK:CB	2.48	0.62
6:M:380:ASN:HB2	6:M:408:SER:HA	1.81	0.61
1:A:372:MET:HB3	1:A:397:GLN:HE22	1.66	0.61
4:D:59:GLN:NE2	4:D:62:SER:OG	2.33	0.61
6:M:228:ARG:HH12	6:M:235:ARG:HH21	1.48	0.61
5:E:196:VAL:HG12	5:E:197:HIS:H	1.66	0.61
5:E:215:ILE:HA	5:E:225:PHE:O	2.01	0.61
6:M:105:GLN:HB3	6:M:269:PHE:HA	1.83	0.60
2:B:142:TYR:HB3	3:C:485:LEU:HD23	1.82	0.60
2:B:185:ARG:HH21	4:D:199:PRO:HD3	1.67	0.60
3:C:178:ASN:HD21	3:C:216:TYR:HB3	1.66	0.60
3:C:262:ASN:OD1	3:C:265:SER:OG	2.19	0.60
1:A:370:THR:HG22	3:C:211:HIS:CE1	2.37	0.60
1:A:470:ASP:OD1	1:A:473:ARG:NH2	2.32	0.59
1:A:352:PHE:HZ	4:D:117:LEU:HD12	1.68	0.59
1:A:318:GLU:OE2	1:A:326:ALA:N	2.35	0.59
2:B:76:ARG:NH1	2:B:80:LEU:HB2	2.18	0.58
6:M:104:CYS:HB3	6:M:246:PHE:HD1	1.67	0.58
3:C:267:ASN:HB3	3:C:313:TYR:HD2	1.68	0.58
3:C:7234:UNK:O	3:C:7238:UNK:N	2.36	0.58
3:C:262:ASN:O	3:C:264:SER:N	2.37	0.58
4:D:34:VAL:O	4:D:38:THR:OG1	2.15	0.58
2:B:103:TYR:HA	4:D:107:LEU:HD21	1.86	0.58
3:C:674:VAL:HG11	3:C:709:ARG:HG3	1.85	0.58
3:C:219:ASP:OD1	3:C:220:SER:N	2.37	0.57
1:A:372:MET:HB3	1:A:397:GLN:NE2	2.19	0.57
3:C:582:PHE:O	3:C:585:THR:HG22	2.04	0.57
6:M:201:GLU:N	6:M:201:GLU:OE1	2.38	0.57
3:C:154:GLN:HE21	4:D:7:GLN:HB3	1.69	0.57
1:A:6:GLU:OE2	1:A:10:ASN:ND2	2.33	0.57
1:A:516:LYS:HB2	3:C:578:ARG:HH22	1.69	0.57
6:M:317:THR:O	6:M:321:GLU:CB	2.52	0.56
1:A:491:ASP:OD1	1:A:492:GLY:N	2.36	0.56
5:E:235:ILE:O	5:E:246:SER:OG	2.20	0.56
6:M:170:PRO:HG2	6:M:173:LYS:HB3	1.86	0.56
2:B:58:HIS:CE1	2:B:62:ILE:HD11	2.41	0.56
4:D:65:LYS:O	4:D:68:ALA:HB3	2.06	0.56
1:A:193:ILE:HG23	1:A:194:LEU:HD12	1.88	0.56
6:M:113:THR:HA	6:M:116:PHE:CE1	2.41	0.56
3:C:596:SER:HB2	3:C:695:ASN:HD21	1.71	0.56
6:M:423:GLN:HE21	6:M:430:ILE:HB	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:110:LEU:HB2	6:M:112:LYS:NZ	2.21	0.55
5:E:235:ILE:HB	5:E:247:THR:HG22	1.87	0.55
6:M:366:PHE:HA	6:M:370:ILE:HG13	1.88	0.55
5:E:174:TRP:CZ3	5:E:188:ASN:HB3	2.41	0.55
6:M:320:ASN:O	6:M:324:LYS:HG3	2.06	0.55
1:A:176:GLU:N	1:A:176:GLU:OE1	2.40	0.55
5:E:252:HIS:CD2	5:E:272:SER:HB2	2.42	0.55
3:C:263:TYR:CE1	3:C:418:ILE:HG23	2.43	0.54
1:A:185:LEU:HD22	1:A:203:LYS:HG3	1.88	0.54
1:A:411:ASN:ND2	1:A:483:GLU:OE1	2.41	0.54
6:M:70:LYS:NZ	6:M:157:MET:SD	2.75	0.54
5:E:272:SER:OG	5:E:273:SER:N	2.40	0.54
3:C:340:GLU:OE2	3:C:637:ARG:NH1	2.41	0.54
3:C:400:LEU:HD23	3:C:400:LEU:H	1.71	0.54
3:C:671:VAL:HG13	3:C:672:PRO:HD3	1.90	0.54
6:M:327:ASN:OD1	6:M:328:ALA:N	2.41	0.54
6:M:387:ALA:HB3	6:M:425:ARG:NH1	2.23	0.54
3:C:141:LYS:HD2	4:D:17:TYR:HE2	1.71	0.53
3:C:610:ARG:NH2	3:C:700:ASP:OD2	2.41	0.53
6:M:69:LEU:HD11	6:M:118:LEU:HD21	1.89	0.53
6:M:335:THR:O	6:M:348:ARG:NH1	2.40	0.53
1:A:62:ASP:OD1	1:A:110:ARG:NH2	2.41	0.53
3:C:908:ARG:NH1	3:C:6951:UNK:O	2.40	0.53
5:E:121:ASN:HB3	5:E:168:TYR:CZ	2.43	0.53
2:B:160:TYR:OH	2:B:171:ASP:OD1	2.25	0.53
3:C:70:ASP:OD1	3:C:71:PHE:N	2.41	0.53
6:M:415:ASP:O	6:M:419:LEU:HB2	2.07	0.53
2:B:150:SER:O	2:B:153:LEU:N	2.40	0.53
3:C:812:ASP:OD1	3:C:813:ASP:N	2.42	0.52
5:E:237:LYS:HE3	5:E:239:ARG:HD3	1.90	0.52
6:M:344:GLU:OE2	6:M:348:ARG:NE	2.42	0.52
3:C:602:MET:HA	3:C:605:PHE:CE2	2.44	0.52
3:C:565:SER:O	3:C:568:VAL:N	2.43	0.52
1:A:473:ARG:NH2	3:C:233:GLN:OE1	2.39	0.52
3:C:295:GLU:OE1	3:C:295:GLU:N	2.30	0.52
3:C:225:ASP:HB3	3:C:277:ILE:HG21	1.90	0.52
6:M:340:MET:O	6:M:345:ARG:NH2	2.43	0.52
1:A:30:ARG:HG3	1:A:31:HIS:N	2.25	0.51
1:A:349:ARG:NH1	3:C:197:ASP:OD2	2.43	0.51
4:D:75:LEU:O	4:D:78:SER:OG	2.15	0.51
6:M:257:ILE:HA	6:M:260:ARG:HE	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:TYR:CE2	3:C:191:LEU:HD13	2.46	0.51
3:C:908:ARG:HH11	3:C:6951:UNK:C	2.23	0.51
3:C:173:ASN:O	3:C:174:LEU:HD12	2.10	0.51
6:M:245:MET:SD	6:M:245:MET:N	2.84	0.51
2:B:32:ASP:O	2:B:35:SER:OG	2.14	0.51
3:C:320:LYS:HB3	3:C:321:PRO:HD3	1.92	0.51
6:M:287:LYS:HA	6:M:410:VAL:HB	1.93	0.51
3:C:453:TYR:OH	3:C:551:ARG:NH1	2.41	0.51
3:C:662:ILE:HD11	3:C:670:LEU:HG	1.92	0.51
6:M:89:GLN:HB3	6:M:93:ILE:HD12	1.93	0.51
3:C:132:ILE:O	3:C:136:HIS:NE2	2.43	0.50
5:E:181:SER:HA	5:E:201:VAL:HG11	1.92	0.50
6:M:288:LEU:HB2	6:M:292:GLU:OE1	2.10	0.50
6:M:320:ASN:OD1	6:M:321:GLU:N	2.45	0.50
6:M:415:ASP:O	6:M:419:LEU:CB	2.60	0.50
1:A:33:PRO:O	1:A:147:ARG:NH2	2.44	0.50
3:C:60:TRP:O	3:C:63:THR:OG1	2.28	0.50
3:C:574:ILE:HG13	3:C:575:ASP:N	2.25	0.50
6:M:114:ALA:O	6:M:118:LEU:HB2	2.12	0.50
5:E:164:ASN:HD22	5:E:180:LYS:HG3	1.77	0.50
6:M:162:THR:HG22	6:M:187:ILE:HB	1.93	0.50
3:C:649:ASP:HB3	6:M:356:GLU:OE2	2.12	0.50
6:M:337:HIS:CE1	6:M:340:MET:HB2	2.47	0.50
1:A:484:LYS:HG2	3:C:284:GLN:HE22	1.76	0.49
5:E:202:ASN:O	5:E:202:ASN:ND2	2.46	0.49
6:M:127:VAL:HG13	6:M:130:GLU:HB2	1.94	0.49
6:M:389:GLN:HA	6:M:392:HIS:CD2	2.46	0.49
4:D:32:GLY:O	4:D:35:THR:OG1	2.23	0.49
6:M:146:ILE:HG22	6:M:150:TYR:CE2	2.48	0.49
1:A:133:SER:HG	1:A:136:THR:H	1.59	0.49
1:A:465:LYS:HB2	1:A:472:TYR:CE1	2.48	0.49
3:C:807:ILE:C	6:M:75:ARG:HH22	2.12	0.49
4:D:112:SER:O	4:D:115:SER:OG	2.18	0.49
3:C:126:ILE:HG22	3:C:130:LYS:HE2	1.94	0.49
4:D:30:ILE:HB	4:D:71:ARG:HH11	1.78	0.49
4:D:116:LYS:O	4:D:119:LEU:HG	2.13	0.49
6:M:117:VAL:HG23	6:M:150:TYR:CE1	2.48	0.49
1:A:352:PHE:CZ	4:D:117:LEU:HD12	2.47	0.49
3:C:315:ILE:O	3:C:319:VAL:HG23	2.13	0.49
3:C:602:MET:HA	3:C:605:PHE:CD2	2.47	0.49
6:M:399:ARG:HE	6:M:400:PHE:H	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:VAL:HG11	1:A:29:ILE:HD13	1.94	0.48
1:A:230:ALA:O	1:A:268:ILE:HD11	2.13	0.48
3:C:745:MET:HG3	3:C:747:ILE:HG23	1.94	0.48
1:A:252:ASP:OD1	1:A:253:VAL:N	2.46	0.48
6:M:113:THR:O	6:M:117:VAL:HG12	2.12	0.48
1:A:40:HIS:CE1	1:A:42:SER:HB3	2.48	0.48
3:C:589:GLN:O	3:C:589:GLN:HG2	2.13	0.48
6:M:367:GLY:O	6:M:392:HIS:HB3	2.14	0.48
6:M:101:ASP:HB3	6:M:262:LEU:HD23	1.95	0.48
3:C:496:GLU:HG2	3:C:504:TYR:O	2.13	0.48
1:A:8:ILE:O	1:A:12:ILE:HG12	2.14	0.48
5:E:141:LEU:O	5:E:150:SER:OG	2.24	0.48
6:M:368:ARG:HA	6:M:396:ARG:NH1	2.29	0.48
3:C:6995:UNK:O	3:C:6999:UNK:CB	2.61	0.47
6:M:311:ILE:HB	6:M:361:VAL:HG12	1.95	0.47
3:C:671:VAL:CG1	3:C:672:PRO:HD3	2.44	0.47
3:C:677:ILE:HD12	3:C:683:VAL:HG23	1.96	0.47
5:E:244:GLU:HG2	5:E:245:VAL:H	1.79	0.47
1:A:176:GLU:HB3	4:D:20:VAL:HG11	1.95	0.47
6:M:364:ASP:OD1	6:M:393:ARG:NH2	2.45	0.47
3:C:674:VAL:O	3:C:677:ILE:HG22	2.14	0.47
4:D:62:SER:O	4:D:65:LYS:HB2	2.15	0.47
6:M:194:ARG:HH21	6:M:197:ALA:HB3	1.78	0.47
6:M:342:GLN:O	6:M:345:ARG:HG2	2.15	0.47
5:E:179:THR:OG1	5:E:182:GLU:HB2	2.14	0.47
1:A:228:ILE:HD13	3:C:177:GLU:HB3	1.96	0.47
2:B:106:THR:HA	2:B:109:HIS:HD2	1.80	0.47
3:C:321:PRO:HD2	3:C:404:LYS:HB2	1.96	0.47
3:C:790:LEU:O	3:C:793:LEU:HG	2.14	0.47
5:E:221:GLY:O	5:E:222:SER:OG	2.28	0.47
6:M:177:LEU:HG	6:M:183:THR:HB	1.96	0.47
2:B:196:LEU:HD11	4:D:210:LYS:HG2	1.96	0.47
6:M:285:TYR:CZ	6:M:432:GLU:HB2	2.50	0.47
1:A:453:SER:O	1:A:458:ASN:ND2	2.48	0.47
3:C:776:VAL:O	3:C:814:ASN:ND2	2.48	0.46
5:E:218:ASN:HB2	5:E:223:HIS:HB2	1.96	0.46
3:C:7174:UNK:C	3:C:7176:UNK:H	2.28	0.46
1:A:384:LYS:O	1:A:388:GLN:HG2	2.15	0.46
3:C:565:SER:O	3:C:567:HIS:N	2.49	0.46
3:C:750:ILE:O	3:C:753:TYR:HB3	2.16	0.46
5:E:240:ASP:OD1	5:E:241:GLU:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:THR:H	1:A:199:HIS:CD2	2.18	0.46
1:A:330:VAL:O	1:A:332:THR:OG1	2.25	0.46
2:B:130:LYS:HA	2:B:147:TRP:CH2	2.51	0.46
2:B:210:TRP:CD2	4:D:224:LYS:HD3	2.50	0.46
3:C:198:ASN:OD1	3:C:199:PHE:N	2.49	0.46
3:C:780:ARG:HD3	3:C:807:ILE:HG22	1.96	0.46
1:A:473:ARG:HE	3:C:233:GLN:NE2	2.12	0.46
3:C:132:ILE:HD12	3:C:132:ILE:H	1.80	0.46
6:M:104:CYS:HA	6:M:268:ILE:O	2.15	0.46
2:B:185:ARG:NH2	4:D:199:PRO:HD3	2.30	0.46
6:M:227:ARG:NH1	6:M:257:ILE:HD11	2.31	0.46
1:A:26:PHE:CZ	1:A:30:ARG:HD3	2.51	0.46
6:M:102:VAL:O	6:M:244:MET:HA	2.15	0.46
1:A:363:ASP:OD1	1:A:364:ASP:N	2.39	0.46
1:A:28:SER:O	1:A:33:PRO:HG3	2.16	0.46
6:M:284:TYR:HA	6:M:431:ALA:O	2.16	0.45
6:M:136:ILE:HD12	6:M:190:ALA:O	2.16	0.45
6:M:352:PHE:HE2	6:M:375:ILE:HD11	1.81	0.45
1:A:289:SER:OG	1:A:290:PRO:HD3	2.16	0.45
1:A:153:MET:SD	1:A:159:PRO:HA	2.56	0.45
3:C:500:LEU:HD23	3:C:501:ASN:HB2	1.98	0.45
3:C:7165:UNK:O	3:C:7169:UNK:CB	2.64	0.45
5:E:90:TRP:CZ3	5:E:102:LYS:HB3	2.51	0.45
5:E:346:PHE:CD1	5:E:353:TYR:HB3	2.52	0.45
5:E:356:SER:HA	5:E:362:LEU:HD23	1.99	0.45
6:M:352:PHE:CE2	6:M:375:ILE:HD11	2.52	0.45
1:A:218:GLU:O	1:A:219:GLU:HB2	2.17	0.45
5:E:117:ASP:OD1	5:E:131:VAL:HB	2.17	0.45
6:M:105:GLN:HA	6:M:247:SER:O	2.16	0.45
1:A:303:TYR:CD2	1:A:467:LYS:HB3	2.52	0.45
3:C:295:GLU:HG2	3:C:296:ARG:N	2.32	0.45
2:B:143:GLU:O	2:B:145:ASP:N	2.50	0.45
6:M:217:CYS:HB3	6:M:245:MET:HB2	1.99	0.45
2:B:9:TYR:CE1	2:B:79:GLN:HB2	2.52	0.45
3:C:562:GLY:O	3:C:563:SER:OG	2.32	0.45
1:A:190:ASN:O	1:A:192:ASP:N	2.50	0.44
1:A:192:ASP:OD1	1:A:193:ILE:N	2.50	0.44
1:A:299:GLU:OE2	1:A:395:ARG:NE	2.31	0.44
3:C:141:LYS:HD2	4:D:17:TYR:CE2	2.50	0.44
3:C:239:TYR:O	3:C:240:LYS:HB2	2.16	0.44
5:E:155:LEU:O	5:E:156:SER:OG	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:HIS:O	1:A:42:SER:N	2.51	0.44
3:C:589:GLN:N	3:C:589:GLN:OE1	2.50	0.44
5:E:69:LEU:HD23	5:E:69:LEU:H	1.83	0.44
5:E:313:CYS:SG	5:E:344:LEU:HD22	2.57	0.44
1:A:127:ILE:O	1:A:131:LEU:HD23	2.17	0.44
1:A:277:ASP:OD1	1:A:280:TYR:N	2.42	0.44
1:A:455:ILE:HG13	1:A:456:CYS:N	2.31	0.44
2:B:68:LEU:O	2:B:71:ASP:N	2.50	0.44
5:E:324:LEU:C	5:E:326:GLU:H	2.21	0.44
6:M:363:THR:HG23	6:M:365:VAL:H	1.82	0.44
5:E:196:VAL:HG12	5:E:197:HIS:N	2.31	0.44
6:M:73:LEU:O	6:M:77:ILE:HG12	2.17	0.44
3:C:220:SER:O	3:C:223:THR:HG22	2.17	0.44
3:C:651:ILE:HD12	3:C:686:LEU:HD22	1.98	0.44
6:M:135:VAL:HG21	6:M:150:TYR:OH	2.16	0.44
3:C:596:SER:HB2	3:C:695:ASN:ND2	2.33	0.44
4:D:107:LEU:N	4:D:108:PRO:HD2	2.33	0.44
5:E:293:ASP:CG	5:E:294:LEU:H	2.21	0.44
6:M:368:ARG:H	6:M:368:ARG:HD3	1.82	0.44
5:E:117:ASP:OD2	5:E:166:CYS:N	2.48	0.44
6:M:114:ALA:O	6:M:118:LEU:CB	2.65	0.44
6:M:254:ILE:HA	6:M:257:ILE:HG22	1.99	0.44
2:B:211:ARG:HD3	4:D:223:TYR:HE2	1.83	0.43
6:M:309:VAL:HG22	6:M:359:ILE:HG12	1.99	0.43
3:C:676:GLN:HE22	6:M:305:GLU:CD	2.21	0.43
3:C:246:LEU:O	3:C:252:TRP:HB2	2.18	0.43
6:M:116:PHE:O	6:M:120:THR:HG23	2.18	0.43
6:M:345:ARG:HH11	6:M:365:VAL:HG11	1.83	0.43
3:C:811:ARG:O	3:C:875:HIS:NE2	2.51	0.43
6:M:342:GLN:O	6:M:346:ILE:HG12	2.18	0.43
3:C:574:ILE:HG22	3:C:605:PHE:CE1	2.53	0.43
3:C:801:GLN:HA	3:C:804:ARG:NH2	2.34	0.43
4:D:132:GLN:HE21	4:D:136:ARG:HD2	1.83	0.43
6:M:171:ILE:HG12	6:M:203:TYR:HE2	1.84	0.43
6:M:292:GLU:O	6:M:296:LYS:N	2.48	0.43
1:A:214:LEU:HB2	1:A:221:ASN:HD21	1.82	0.43
5:E:166:CYS:HA	5:E:176:LEU:O	2.19	0.43
6:M:293:LYS:HB3	6:M:381:TYR:CE1	2.53	0.43
6:M:312:PHE:HA	6:M:362:SER:O	2.19	0.43
1:A:369:PRO:HD2	2:B:107:PHE:CD2	2.53	0.43
3:C:639:ALA:HA	3:C:642:ILE:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:150:TYR:HB3	6:M:162:THR:HG21	1.99	0.43
6:M:389:GLN:O	6:M:392:HIS:HB2	2.18	0.43
1:A:372:MET:HA	1:A:394:TYR:HE1	1.84	0.43
6:M:315:SER:HB3	6:M:318:ARG:HD3	2.01	0.43
6:M:334:ILE:HB	6:M:357:LYS:HD3	2.01	0.43
3:C:785:VAL:HG22	3:C:786:ASN:O	2.19	0.42
3:C:907:TRP:HB3	3:C:911:LEU:HG	2.00	0.42
6:M:281:LEU:HB3	6:M:283:GLN:NE2	2.34	0.42
1:A:427:LEU:HD23	1:A:427:LEU:HA	1.87	0.42
3:C:842:ASN:ND2	3:C:863:ASN:OD1	2.53	0.42
6:M:89:GLN:HG2	6:M:115:VAL:CG2	2.49	0.42
3:C:625:ILE:HG22	3:C:627:PRO:HD2	2.00	0.42
6:M:192:PRO:O	6:M:196:LYS:HG2	2.19	0.42
2:B:221:MET:HG3	2:B:222:PHE:N	2.33	0.42
3:C:431:LEU:HD21	3:C:535:ILE:HG22	2.01	0.42
4:D:16:HIS:HD2	4:D:17:TYR:CE1	2.38	0.42
6:M:135:VAL:HG22	6:M:213:VAL:HB	2.01	0.42
6:M:304:LEU:HD22	6:M:443:TYR:OH	2.19	0.42
2:B:76:ARG:NE	4:D:19:GLU:OE2	2.53	0.42
3:C:659:ALA:HA	3:C:662:ILE:HG22	2.02	0.42
3:C:782:LEU:HD23	3:C:782:LEU:H	1.84	0.42
4:D:7:GLN:HA	4:D:10:GLN:HB3	2.01	0.42
1:A:384:LYS:HD2	2:B:112:ARG:HH12	1.84	0.42
3:C:712:TYR:CZ	3:C:714:ARG:HD2	2.54	0.42
4:D:7:GLN:O	4:D:10:GLN:HB3	2.20	0.42
6:M:310:ILE:HD12	6:M:360:CYS:O	2.20	0.42
4:D:11:VAL:O	4:D:14:LYS:HB3	2.19	0.42
5:E:361:THR:HG22	5:E:362:LEU:N	2.35	0.42
4:D:20:VAL:HG12	4:D:22:THR:HG23	2.02	0.42
5:E:250:LYS:O	5:E:250:LYS:HG3	2.20	0.42
5:E:333:LYS:HG2	5:E:334:SER:N	2.29	0.42
6:M:165:PHE:HE2	6:M:188:VAL:HG13	1.85	0.42
3:C:803:ALA:O	3:C:806:LEU:HB2	2.20	0.41
6:M:110:LEU:HB2	6:M:112:LYS:HZ2	1.84	0.41
6:M:134:VAL:HA	6:M:188:VAL:O	2.20	0.41
6:M:255:ARG:HB3	6:M:259:ARG:NH1	2.35	0.41
1:A:366:THR:C	1:A:367:LEU:HD12	2.40	0.41
3:C:239:TYR:C	3:C:241:PHE:H	2.24	0.41
5:E:182:GLU:O	5:E:183:LYS:HG3	2.19	0.41
6:M:368:ARG:HA	6:M:396:ARG:HH11	1.84	0.41
1:A:363:ASP:O	1:A:364:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:137:CYS:O	6:M:192:PRO:HD3	2.20	0.41
1:A:114:ALA:HB1	1:A:155:THR:OG1	2.21	0.41
1:A:368:ARG:HG2	2:B:107:PHE:CZ	2.55	0.41
6:M:165:PHE:HB2	6:M:190:ALA:HB2	2.02	0.41
1:A:141:TRP:HZ2	1:A:209:PHE:HB2	1.85	0.41
1:A:211:SER:HB2	3:C:171:LYS:NZ	2.35	0.41
3:C:243:ILE:O	3:C:247:ARG:HG2	2.21	0.41
3:C:566:LEU:HA	3:C:569:THR:HG22	2.03	0.41
3:C:575:ASP:HA	3:C:578:ARG:HG2	2.03	0.41
3:C:677:ILE:HD11	3:C:684:SER:CA	2.51	0.41
4:D:130:SER:O	4:D:133:VAL:HG12	2.21	0.41
5:E:124:SER:O	5:E:126:ASN:N	2.54	0.41
5:E:237:LYS:HE3	5:E:239:ARG:CD	2.51	0.41
6:M:252:GLN:HE22	6:M:255:ARG:NH1	2.18	0.41
2:B:185:ARG:HD3	4:D:197:LYS:N	2.36	0.41
3:C:133:PRO:O	3:C:136:HIS:HD2	2.04	0.41
3:C:411:LEU:HD22	3:C:416:CYS:SG	2.60	0.41
3:C:626:LEU:HB3	3:C:627:PRO:HD3	2.02	0.41
3:C:681:ASP:OD1	3:C:730:ARG:HG3	2.21	0.41
1:A:408:LEU:HB2	3:C:176:VAL:HG21	2.02	0.41
3:C:509:SER:OG	3:C:510:GLU:OE1	2.27	0.41
3:C:515:LEU:H	3:C:515:LEU:HG	1.59	0.41
5:E:116:THR:H	5:E:132:SER:HA	1.86	0.41
1:A:34:LEU:HA	1:A:147:ARG:HH21	1.85	0.40
2:B:169:GLY:O	2:B:173:GLN:HG3	2.21	0.40
3:C:811:ARG:HH11	3:C:875:HIS:HD2	1.68	0.40
5:E:326:GLU:HG2	5:E:328:LYS:NZ	2.36	0.40
6:M:89:GLN:HG2	6:M:115:VAL:HG22	2.02	0.40
6:M:423:GLN:NE2	6:M:430:ILE:HB	2.35	0.40
1:A:303:TYR:OH	1:A:468:ASP:OD2	2.29	0.40
1:A:471:PHE:CE2	1:A:475:ILE:HD11	2.56	0.40
3:C:285:TYR:CD1	3:C:402:PHE:HB3	2.57	0.40
5:E:169:ASP:HB2	5:E:170:PRO:HD2	2.03	0.40
2:B:130:LYS:HA	2:B:147:TRP:CZ2	2.57	0.40
5:E:225:PHE:CD1	5:E:235:ILE:HG12	2.56	0.40
5:E:344:LEU:HA	5:E:354:ILE:O	2.21	0.40
6:M:137:CYS:HB2	6:M:143:ALA:HB2	2.04	0.40
1:A:297:GLU:O	1:A:300:GLU:HG3	2.22	0.40
3:C:638:GLU:O	3:C:641:SER:OG	2.24	0.40
3:C:758:LEU:HA	3:C:758:LEU:HD23	1.91	0.40
5:E:323:ASP:HB2	5:E:330:LEU:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:88:VAL:HG21	6:M:112:LYS:HE3	2.04	0.40
6:M:410:VAL:HG21	6:M:419:LEU:HD22	2.03	0.40
6:M:424:GLU:OE1	6:M:424:GLU:N	2.48	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	473/603 (78%)	413 (87%)	58 (12%)	2 (0%)	34	69
2	B	181/261 (69%)	166 (92%)	15 (8%)	0	100	100
3	C	690/1262 (55%)	625 (91%)	62 (9%)	3 (0%)	34	69
4	D	144/256 (56%)	135 (94%)	9 (6%)	0	100	100
5	E	254/385 (66%)	214 (84%)	39 (15%)	1 (0%)	34	69
6	M	370/446 (83%)	350 (95%)	20 (5%)	0	100	100
All	All	2112/3213 (66%)	1903 (90%)	203 (10%)	6 (0%)	44	74

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ALA
3	C	263	TYR
5	E	125	LEU
3	C	197	ASP
3	C	607	PHE
1	A	228	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	458/566 (81%)	458 (100%)	0	100	100
2	B	178/242 (74%)	178 (100%)	0	100	100
3	C	657/955 (69%)	655 (100%)	2 (0%)	92	96
4	D	140/237 (59%)	140 (100%)	0	100	100
5	E	241/284 (85%)	238 (99%)	3 (1%)	71	84
6	M	331/386 (86%)	330 (100%)	1 (0%)	92	96
All	All	2005/2670 (75%)	1999 (100%)	6 (0%)	92	96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	313	TYR
3	C	787	MET
5	E	153	ARG
5	E	202	ASN
5	E	213	TYR
6	M	368	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	199	HIS
1	A	265	HIS
1	A	327	ASN
1	A	357	GLN
1	A	378	ASN
1	A	450	ASN
1	A	458	ASN
2	B	24	GLN
2	B	58	HIS
2	B	109	HIS

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Mol	Chain	Res	Type
3	C	178	ASN
3	C	211	HIS
3	C	259	ASN
3	C	281	ASN
3	C	414	HIS
3	C	487	HIS
3	C	789	GLN
4	D	59	GLN
4	D	132	GLN
5	E	72	HIS
5	E	164	ASN
5	E	305	HIS
6	M	122	GLN
6	M	252	GLN
6	M	380	ASN
6	M	392	HIS
6	M	423	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	10
5	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	913:ASN	C	6941:UNK	N	25.03
1	C	6951:UNK	C	6991:UNK	N	20.76
1	C	7225:UNK	C	7234:UNK	N	16.53
1	C	7012:UNK	C	7028:UNK	N	16.13
1	E	0:UNK	C	68:SER	N	15.50
1	C	7176:UNK	C	7180:UNK	N	14.77
1	C	7150:UNK	C	7159:UNK	N	10.40
1	C	7248:UNK	C	7256:UNK	N	9.94
1	C	7201:UNK	C	7211:UNK	N	9.34
1	C	7060:UNK	C	7131:UNK	N	8.18
1	C	7040:UNK	C	7047:UNK	N	5.52

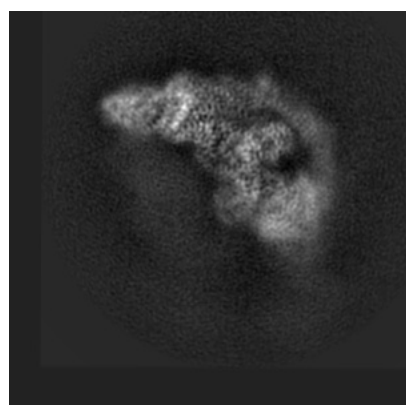
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23527. These allow visual inspection of the internal detail of the map and identification of artifacts.

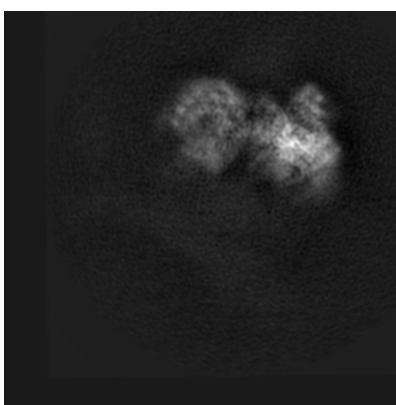
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

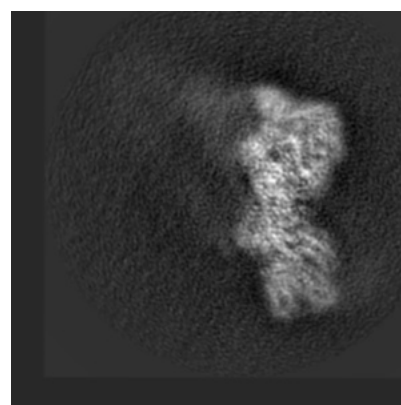
6.1.1 Primary map



X



Y

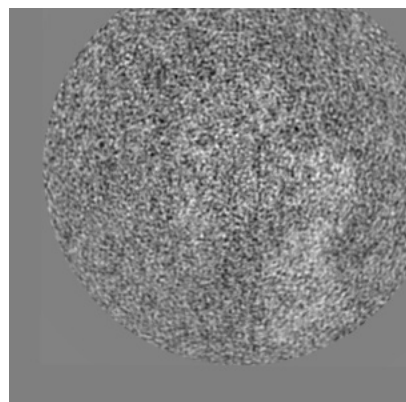


Z

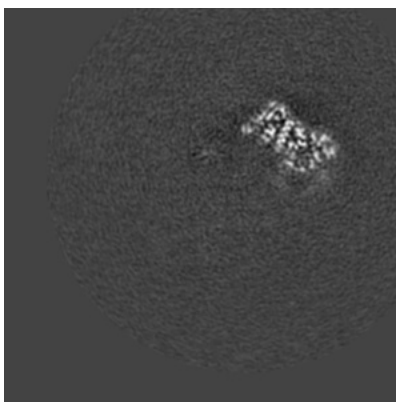
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

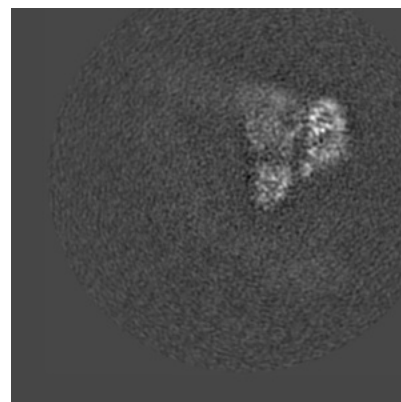
6.2.1 Primary map



X Index: 250



Y Index: 250

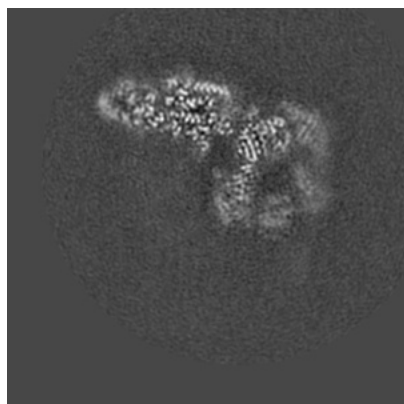


Z Index: 250

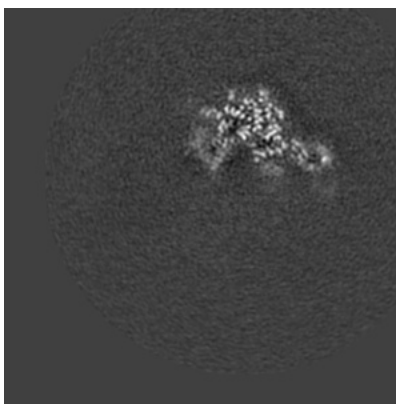
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

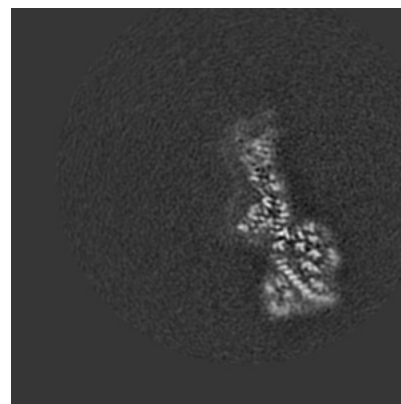
6.3.1 Primary map



X Index: 336



Y Index: 296



Z Index: 386

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

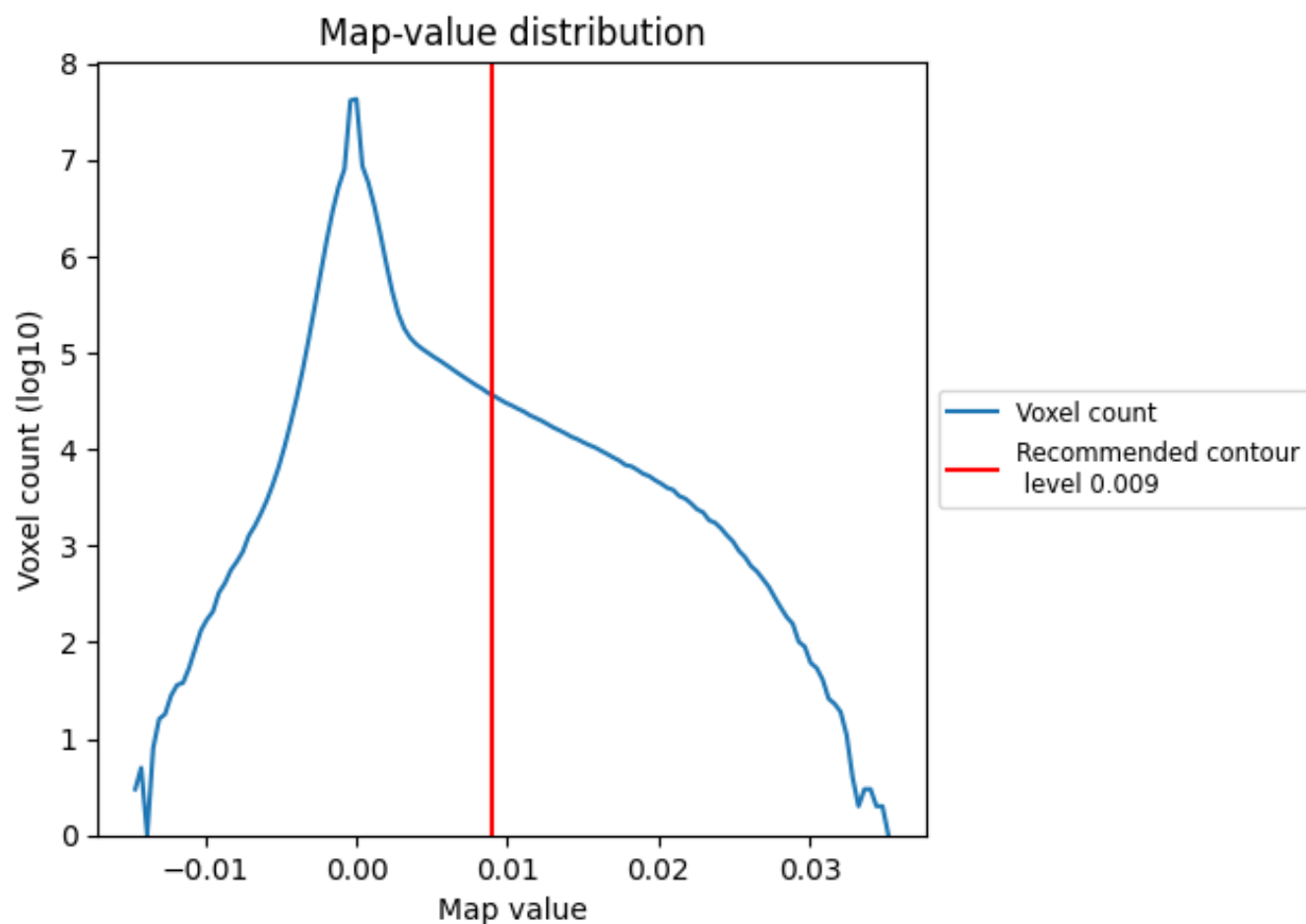
6.5 Mask visualisation

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

7 Map analysis [i](#)

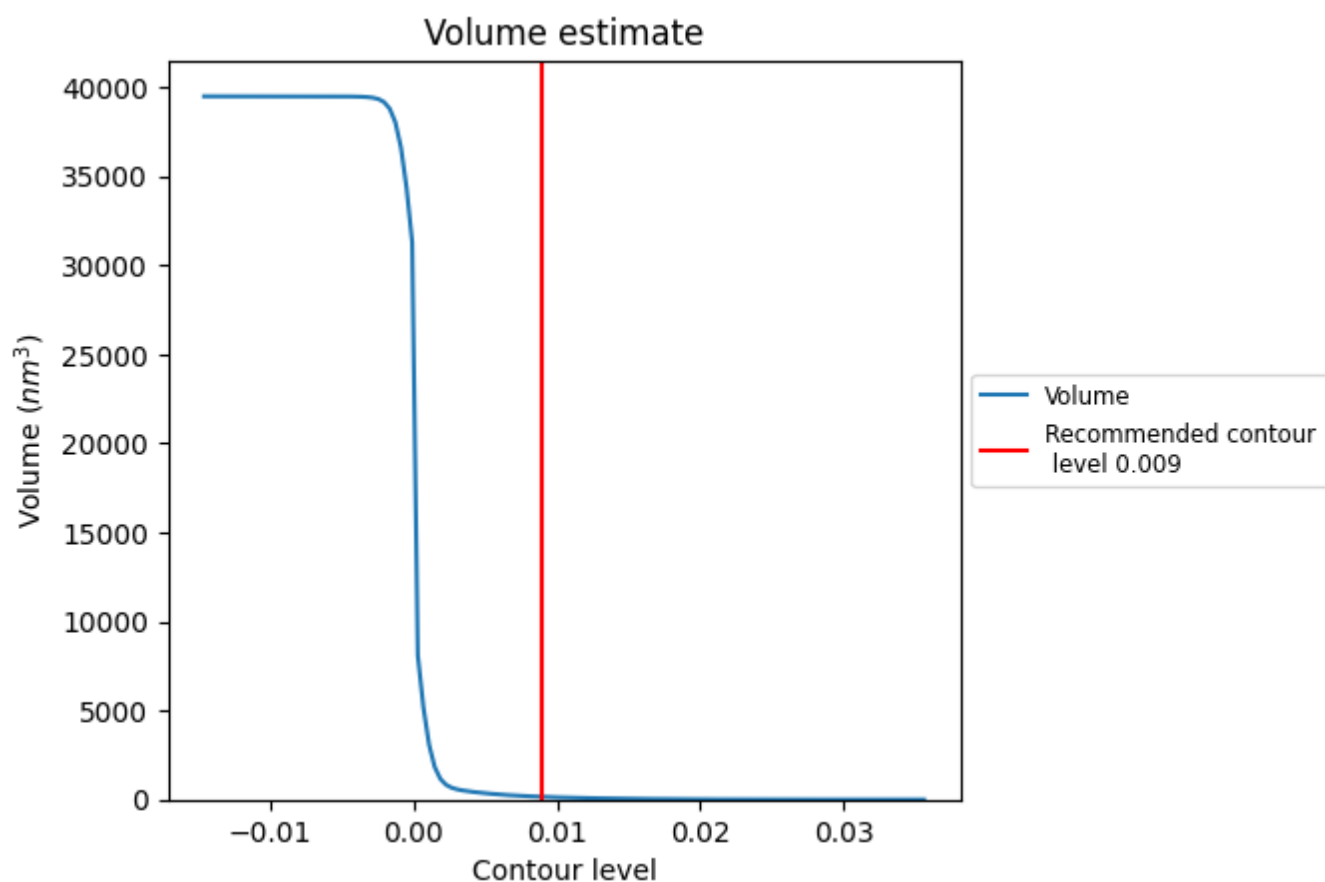
This section contains the results of statistical analysis of the map.

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.

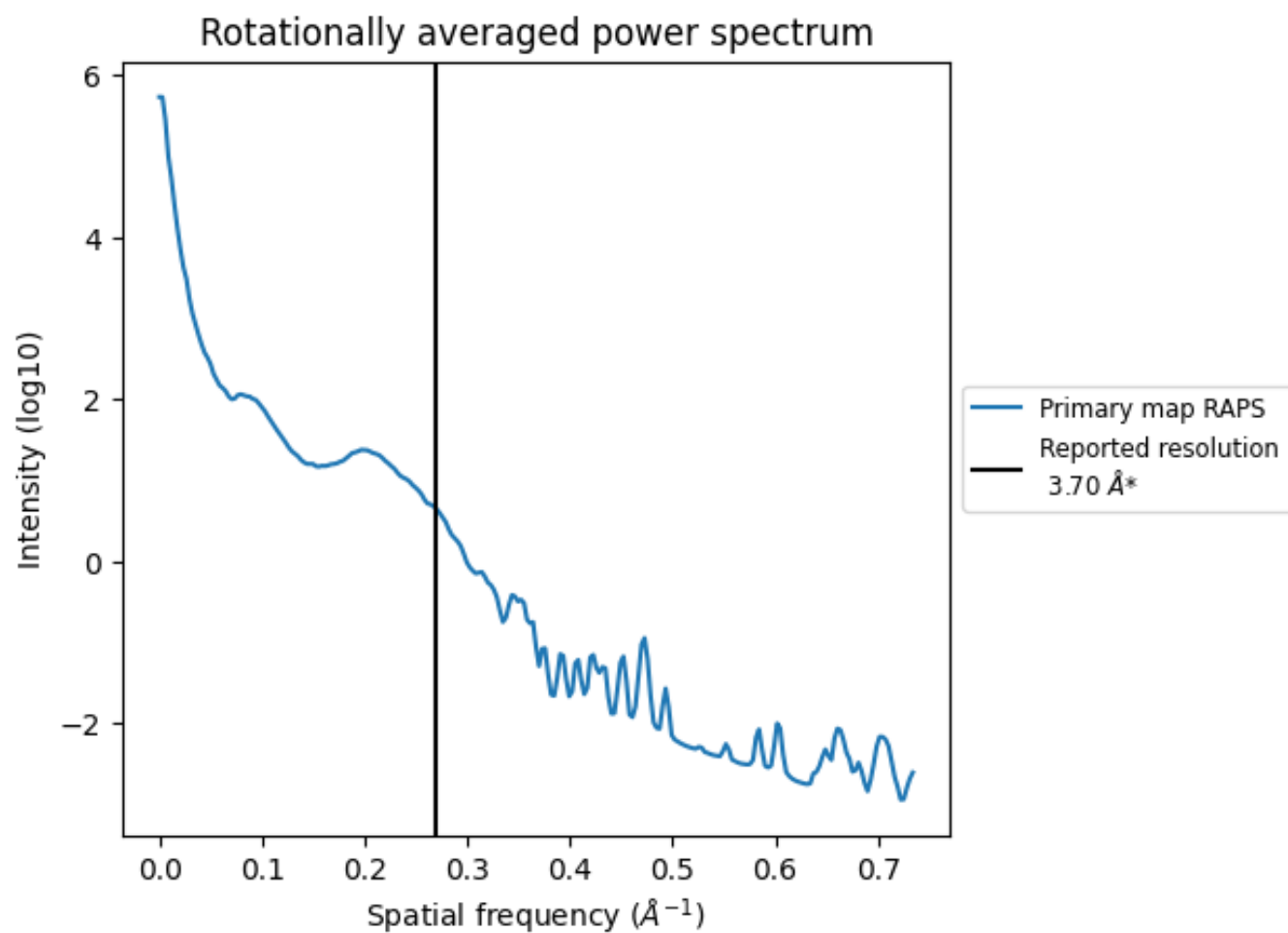
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 153 nm^3 ; this corresponds to an approximate mass of 138 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 0.270 Å⁻¹

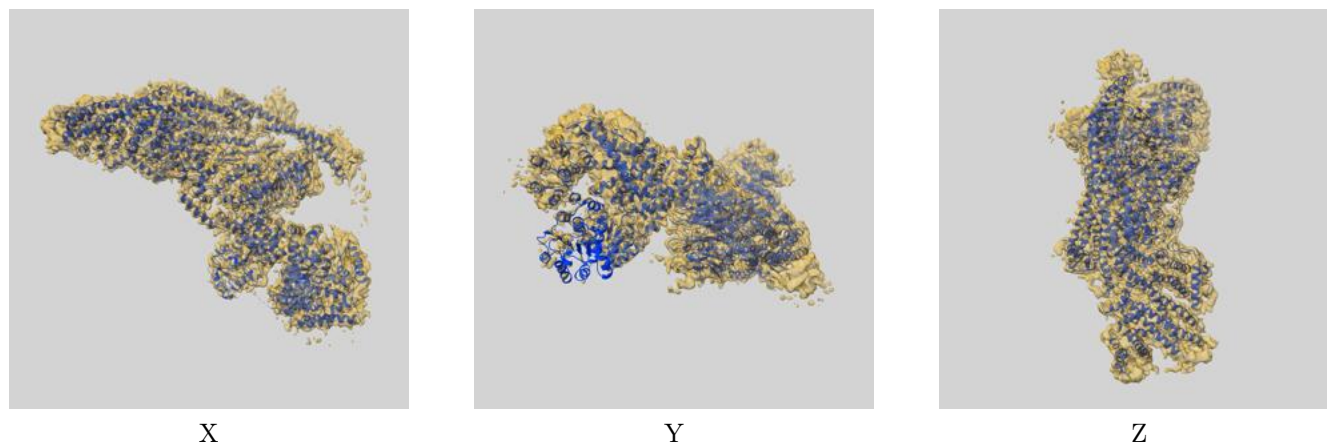
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

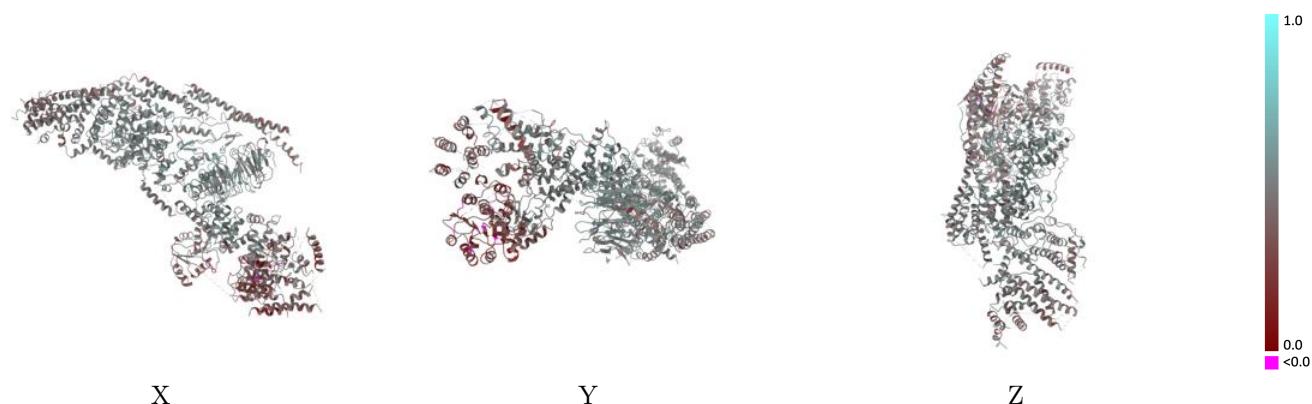
This section contains information regarding the fit between EMDB map EMD-23527 and PDB model 7LUV. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



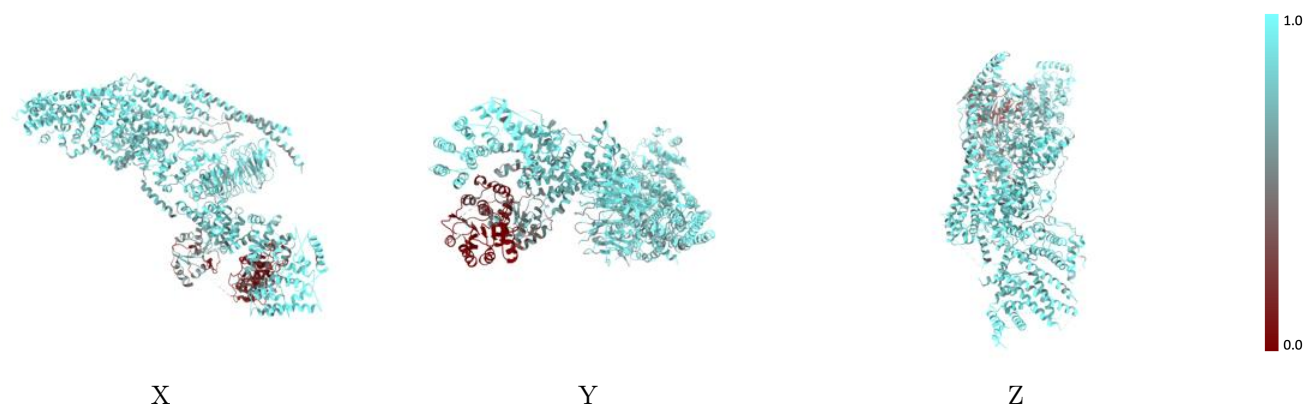
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



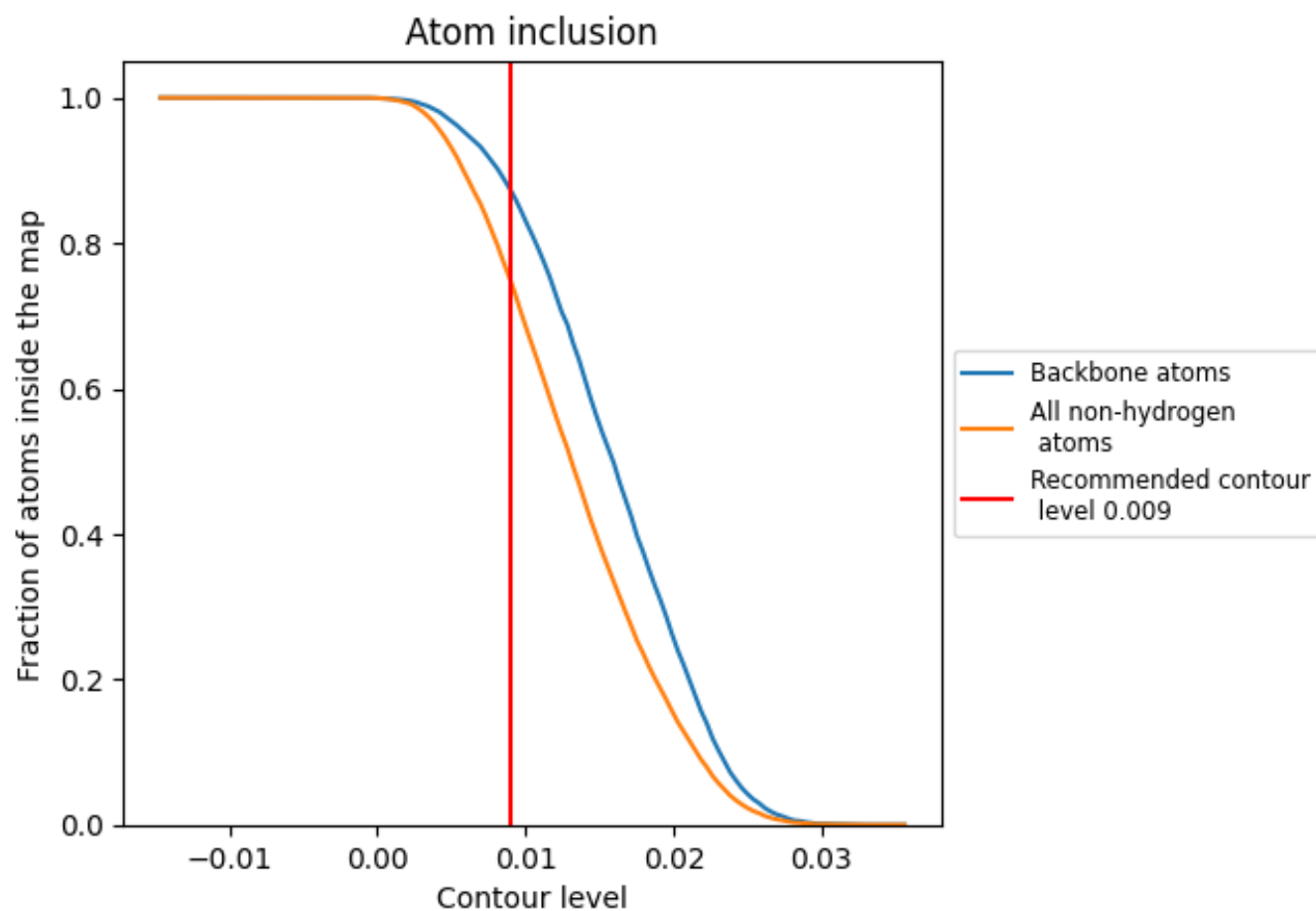
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 75% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.7486</div>	<div><div></div>0.4530</div>
A	<div><div></div>0.8309</div>	<div><div></div>0.4850</div>
B	<div><div></div>0.8177</div>	<div><div></div>0.4550</div>
C	<div><div></div>0.8552</div>	<div><div></div>0.4840</div>
D	<div><div></div>0.8253</div>	<div><div></div>0.4520</div>
E	<div><div></div>0.8290</div>	<div><div></div>0.5060</div>
M	<div><div></div>0.2709</div>	<div><div></div>0.3040</div>

1.0

0.0

<0.0