Full wwPDB EM Validation Report

Nov 19, 2024 – 06:13 pm GMT

PDB ID	:	9GCK
EMDB ID	:	EMD-51231
Title	:	yeast TFIIIC TauA subcomplex bound to a tRNA gene
Authors	:	Seifert-Davila, W.; Girbig, M.; Hauptmann, L.; Hoffmann, T.; Eustermann, S.; Mueller, C.; Chaban, A.; Duss, O.; Baudin, F.
Deposited on	:	2024-08-02
Resolution	:	3.70 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:

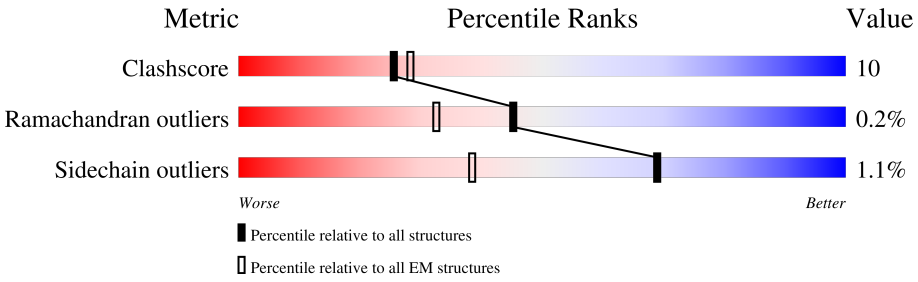
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1201	8% 31% 5% 64%
2	B	1029	20% 8% 71%
3	C	606	29% 8% 62%
4	D	435	43% 71% 5% 23%
5	E	45	42% 91% 9%
6	F	45	42% 87% 11%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12298 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 Transcription factor tau 138 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	429	3491	2222	610	645	14	0	0

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1161	GLU	-	expression tag	UNP P34111
A	1162	ASN	-	expression tag	UNP P34111
A	1163	LEU	-	expression tag	UNP P34111
A	1164	TYR	-	expression tag	UNP P34111
A	1165	PHE	-	expression tag	UNP P34111
A	1166	GLN	-	expression tag	UNP P34111
A	1167	SER	-	expression tag	UNP P34111
A	1168	MET	-	expression tag	UNP P34111
A	1169	SER	-	expression tag	UNP P34111
A	1170	ALA	-	expression tag	UNP P34111
A	1171	SER	-	expression tag	UNP P34111
A	1172	ALA	-	expression tag	UNP P34111
A	1173	TRP	-	expression tag	UNP P34111
A	1174	SER	-	expression tag	UNP P34111
A	1175	HIS	-	expression tag	UNP P34111
A	1176	PRO	-	expression tag	UNP P34111
A	1177	GLN	-	expression tag	UNP P34111
A	1178	PHE	-	expression tag	UNP P34111
A	1179	GLU	-	expression tag	UNP P34111
A	1180	LYS	-	expression tag	UNP P34111
A	1181	GLY	-	expression tag	UNP P34111
A	1182	GLY	-	expression tag	UNP P34111
A	1183	GLY	-	expression tag	UNP P34111
A	1184	SER	-	expression tag	UNP P34111
A	1185	GLY	-	expression tag	UNP P34111
A	1186	GLY	-	expression tag	UNP P34111
A	1187	GLY	-	expression tag	UNP P34111
A	1188	SER	-	expression tag	UNP P34111

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1189	GLY	-	expression tag	UNP P34111
A	1190	GLY	-	expression tag	UNP P34111
A	1191	SER	-	expression tag	UNP P34111
A	1192	ALA	-	expression tag	UNP P34111
A	1193	TRP	-	expression tag	UNP P34111
A	1194	SER	-	expression tag	UNP P34111
A	1195	HIS	-	expression tag	UNP P34111
A	1196	PRO	-	expression tag	UNP P34111
A	1197	GLN	-	expression tag	UNP P34111
A	1198	PHE	-	expression tag	UNP P34111
A	1199	GLU	-	expression tag	UNP P34111
A	1200	LYS	-	expression tag	UNP P34111
A	1201	SER	-	expression tag	UNP P34111

- Molecule 2 is a protein called Transcription factor tau 131 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	294	Total	C	N	O	S	0	0
			2443	1574	411	447	11		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1026	ARG	-	expression tag	UNP P33339
B	1027	SER	-	expression tag	UNP P33339
B	1028	GLY	-	expression tag	UNP P33339
B	1029	GLY	-	expression tag	UNP P33339

- Molecule 3 is a protein called Transcription factor tau 95 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	231	Total	C	N	O	S	0	0
			1823	1162	308	348	5		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	expression tag	UNP P32367
C	-11	HIS	-	expression tag	UNP P32367
C	-10	HIS	-	expression tag	UNP P32367
C	-9	HIS	-	expression tag	UNP P32367
C	-8	HIS	-	expression tag	UNP P32367

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	HIS	-	expression tag	UNP P32367
C	-6	GLU	-	expression tag	UNP P32367
C	-5	ASN	-	expression tag	UNP P32367
C	-4	LEU	-	expression tag	UNP P32367
C	-3	TYR	-	expression tag	UNP P32367
C	-2	PHE	-	expression tag	UNP P32367
C	-1	GLN	-	expression tag	UNP P32367
C	0	SER	-	expression tag	UNP P32367

- Molecule 4 is a protein called Transcription factor tau 55 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	333	Total	C	N	O	S	0	0
			2696	1732	448	505	11		

- Molecule 5 is a DNA chain called DNA (45-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	45	Total	C	N	O	P	0	0
			900	450	90	315	45		

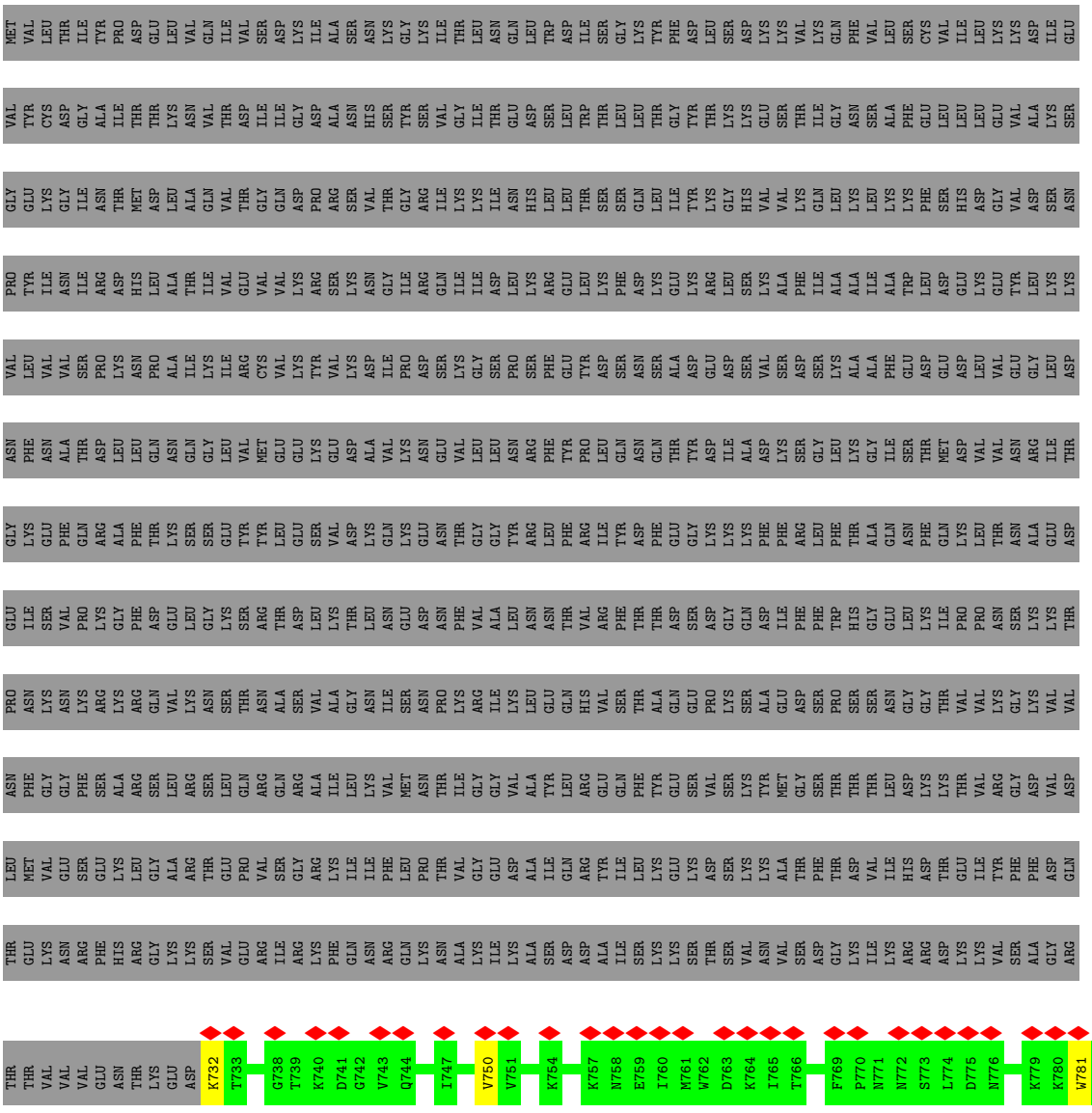
- Molecule 6 is a DNA chain called DNA (45-MER).

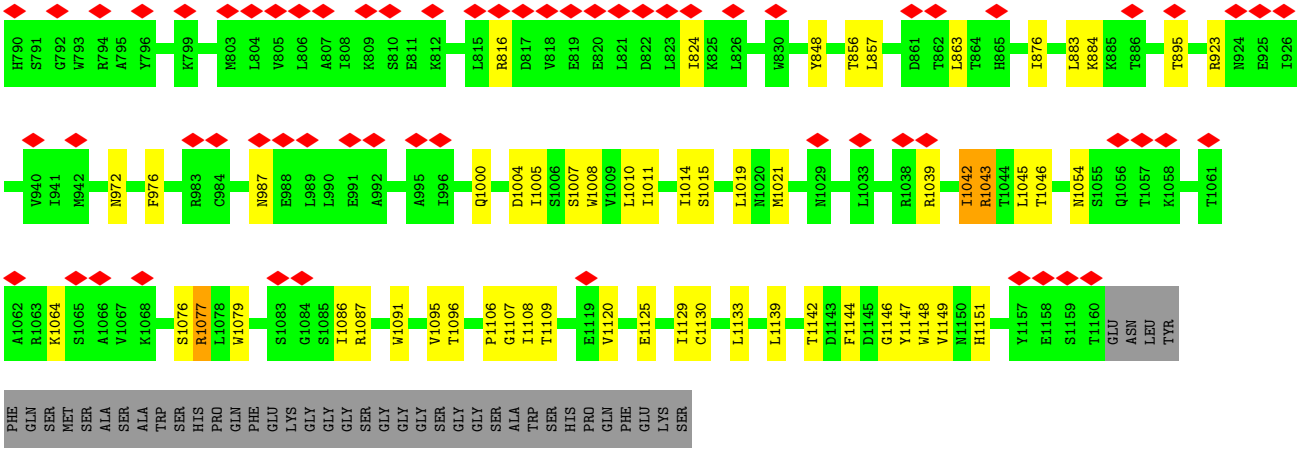
Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	45	Total	C	N	O	P	0	0
			945	450	225	225	45		

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.

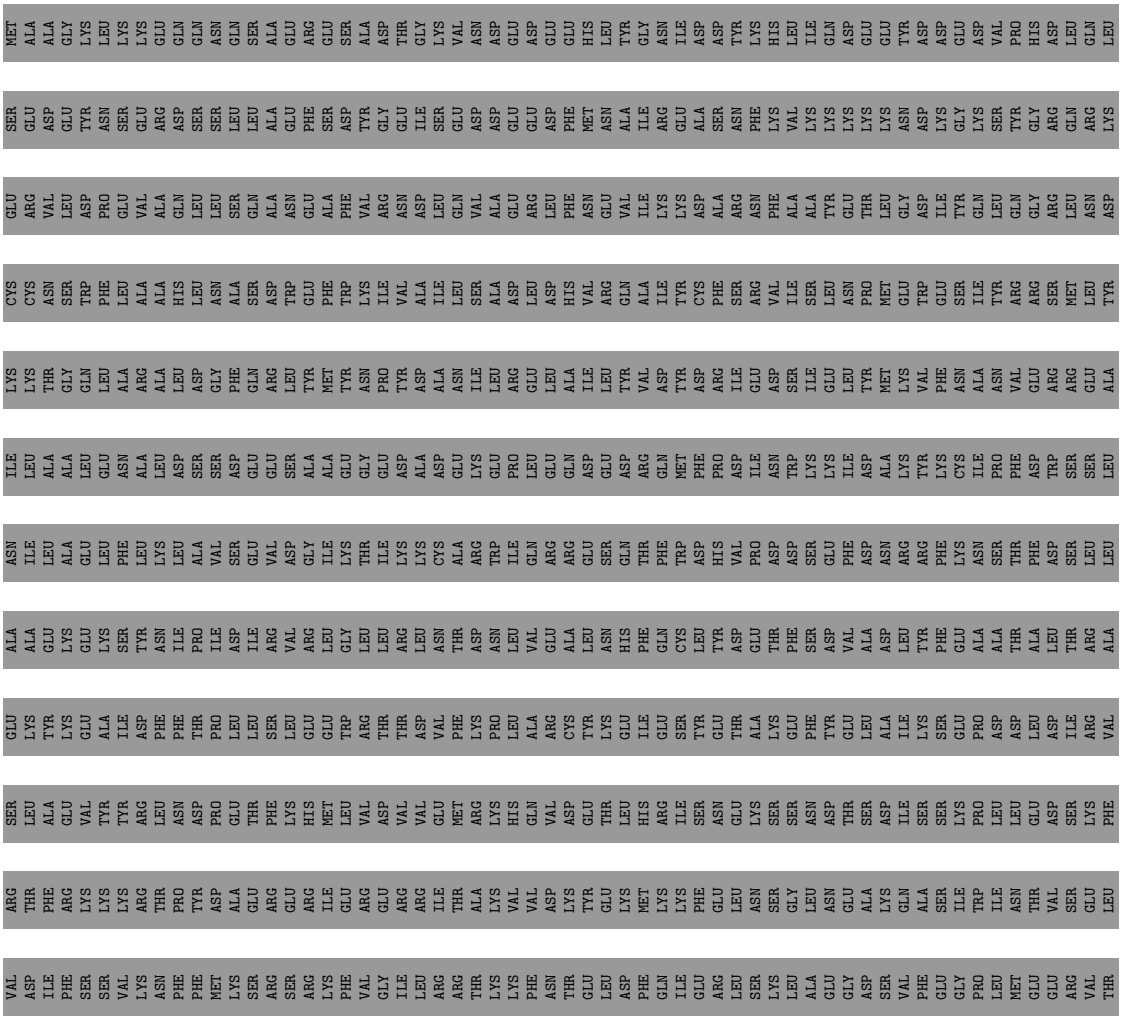
- Molecule 1: Transcription factor tau 138 kDa subunit

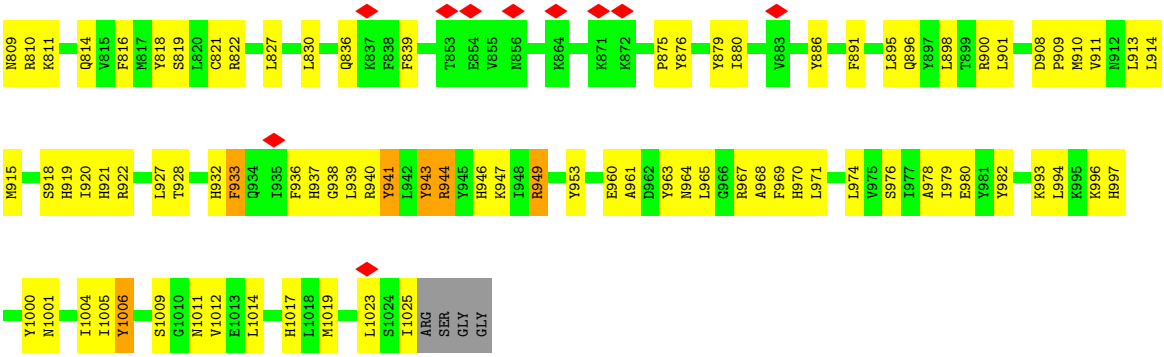




• Molecule 2: Transcription factor tau 131 kDa subunit

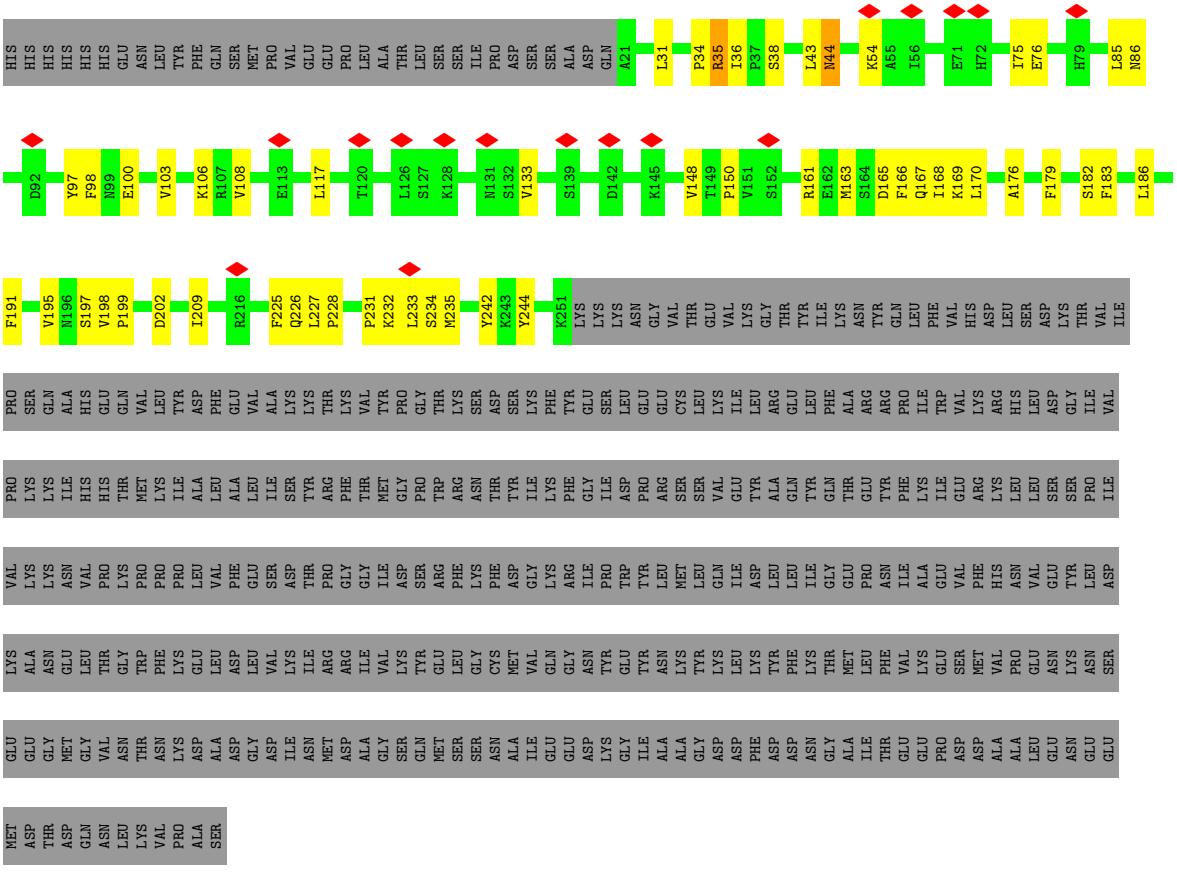
Chain B:





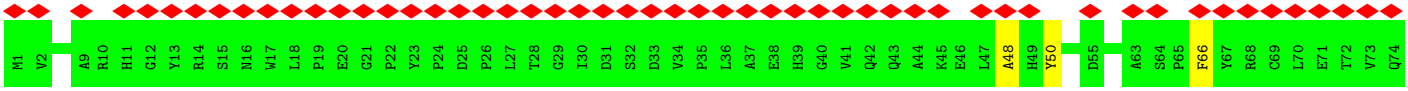
• Molecule 3: Transcription factor tau 95 kDa subunit

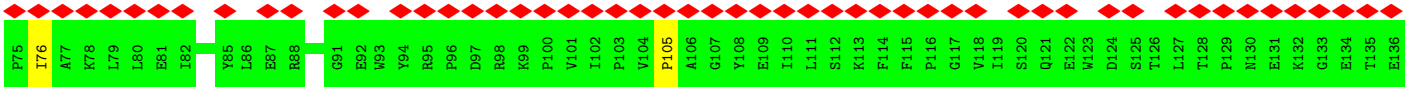
Chain C:

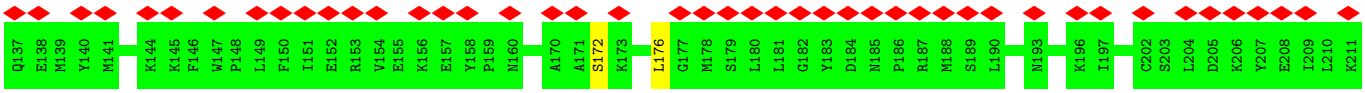


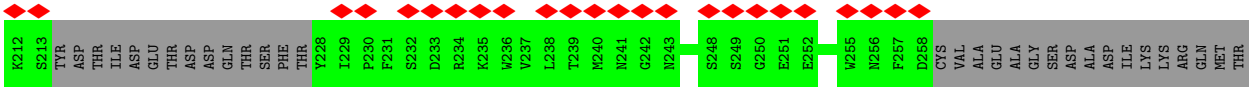
• Molecule 4: Transcription factor tau 55 kDa subunit

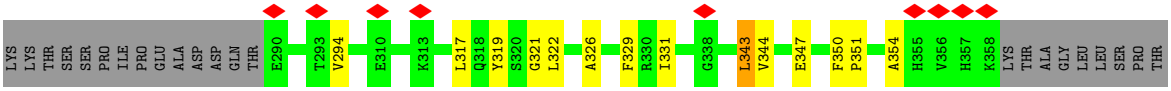
Chain D:

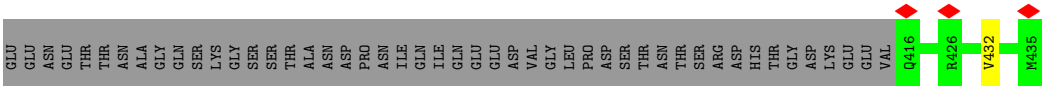




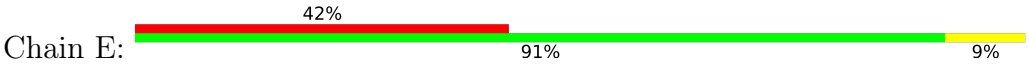


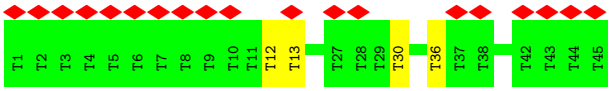




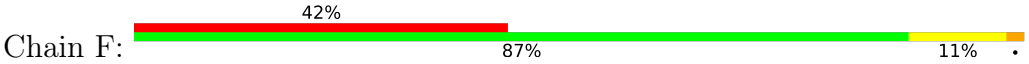


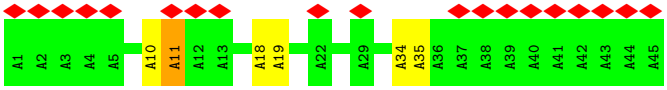
• Molecule 5: DNA (45-MER)





• Molecule 6: DNA (45-MER)





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114621	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 ($e^-/Å^2$)	39.6	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.026	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	263.04, 263.04, 263.04	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	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	0.74	1/3556 (0.0%)	0.95	5/4807 (0.1%)
2	B	0.77	0/2495	1.00	5/3365 (0.1%)
3	C	0.72	0/1865	0.90	1/2523 (0.0%)
4	D	0.71	0/2765	0.77	0/3748
5	E	0.96	0/989	1.30	0/1526
6	F	0.83	0/1079	1.31	2/1661 (0.1%)
All	All	0.76	1/12749 (0.0%)	0.99	13/17630 (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	2
2	B	0	3
3	C	0	2
4	D	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1076	SER	CA-CB	-5.45	1.44	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	949	ARG	NE-CZ-NH1	-7.57	116.52	120.30
1	A	1087	ARG	NE-CZ-NH2	7.53	124.07	120.30
1	A	1087	ARG	NE-CZ-NH1	-7.41	116.59	120.30
2	B	1006	TYR	CB-CG-CD1	7.07	125.24	121.00
6	F	11	DA	C3'-C2'-C1'	-6.80	94.34	102.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1077	ARG	NE-CZ-NH1	-6.47	117.07	120.30
2	B	933	PHE	CB-CG-CD1	5.95	124.96	120.80
3	C	44	ASN	CB-CA-C	5.43	121.26	110.40
2	B	941	TYR	CB-CA-C	5.41	121.22	110.40
1	A	1077	ARG	NE-CZ-NH2	5.10	122.85	120.30
2	B	944	ARG	NE-CZ-NH2	5.07	122.84	120.30
1	A	923	ARG	NE-CZ-NH1	-5.06	117.77	120.30
6	F	11	DA	C8-N9-C1'	-5.02	118.66	127.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1086	ILE	Peptide
1	A	856	THR	Peptide
2	B	808	PHE	Peptide
2	B	943	TYR	Sidechain
2	B	944	ARG	Sidechain
3	C	242	TYR	Peptide
3	C	35	ARG	Peptide
4	D	343	LEU	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	3491	0	3589	59	0
2	B	2443	0	2431	170	0
3	C	1823	0	1844	117	0
4	D	2696	0	2650	28	0
5	E	900	0	541	8	0
6	F	945	0	496	9	0
All	All	12298	0	11551	235	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 10.

All (235) 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)
2:B:968:ALA:HA	3:C:166:PHE:HZ	1.10	1.17
6:F:10:DA:H2"	6:F:11:DA:C2	1.89	1.08
2:B:968:ALA:HA	3:C:166:PHE:CZ	1.90	1.07
1:A:1106:PRO:HG2	2:B:1005:ILE:HG21	1.35	1.02
2:B:910:MET:HB2	3:C:227:LEU:HB2	1.39	1.02
2:B:811:LYS:NZ	3:C:197:SER:O	1.95	0.97
3:C:133:VAL:HG22	4:D:294:VAL:HG21	1.49	0.93
2:B:911:VAL:HG23	3:C:227:LEU:HD11	1.52	0.91
2:B:911:VAL:HG23	3:C:227:LEU:CD1	2.03	0.89
2:B:932:HIS:HE1	3:C:244:TYR:O	1.55	0.88
3:C:31:LEU:HD13	4:D:331:ILE:HG23	1.57	0.87
6:F:10:DA:H2"	6:F:11:DA:N3	1.89	0.86
1:A:1106:PRO:CG	2:B:1005:ILE:HG21	2.06	0.84
2:B:891:PHE:CE2	2:B:921:HIS:HB3	2.13	0.83
1:A:732:LYS:HA	1:A:824:ILE:HD13	1.61	0.82
2:B:968:ALA:CA	3:C:166:PHE:CZ	2.63	0.81
1:A:1004:ASP:HA	2:B:932:HIS:NE2	1.96	0.81
1:A:1109:THR:HG23	2:B:1011:ASN:HA	1.60	0.80
2:B:875:PRO:CB	2:B:901:LEU:HD11	2.11	0.80
3:C:31:LEU:CD1	4:D:331:ILE:HG23	2.12	0.80
2:B:967:ARG:HE	3:C:165:ASP:HA	1.48	0.79
2:B:911:VAL:CG2	3:C:227:LEU:HD11	2.11	0.79
2:B:898:LEU:HD11	2:B:914:LEU:HD23	1.65	0.78
2:B:910:MET:CB	3:C:227:LEU:HB2	2.14	0.78
1:A:1010:LEU:HB2	2:B:936:PHE:CZ	2.19	0.78
3:C:133:VAL:CG2	4:D:294:VAL:HG21	2.13	0.77
2:B:974:LEU:HD22	3:C:244:TYR:CZ	2.21	0.75
2:B:971:LEU:HD13	3:C:234:SER:HB2	1.69	0.74
2:B:875:PRO:HB3	2:B:901:LEU:HD11	1.69	0.73
2:B:932:HIS:CE1	3:C:244:TYR:O	2.40	0.73
2:B:1000:TYR:CZ	3:C:103:VAL:HG11	2.24	0.73
3:C:170:LEU:HB3	3:C:176:ALA:HB1	1.71	0.72
2:B:921:HIS:CE1	2:B:971:LEU:HD21	2.26	0.70
6:F:10:DA:C2'	6:F:11:DA:C2	2.70	0.70
1:A:1142:THR:OG1	2:B:1014:LEU:HD22	1.91	0.69
2:B:994:LEU:HD11	3:C:97:TYR:OH	1.93	0.67
2:B:968:ALA:N	3:C:166:PHE:CE2	2.63	0.67
1:A:1004:ASP:HA	2:B:932:HIS:CE1	2.29	0.67
1:A:1015:SER:HA	2:B:943:TYR:OH	1.95	0.66
1:A:1010:LEU:CD1	2:B:936:PHE:CE2	2.78	0.66
3:C:165:ASP:O	3:C:167:GLN:NE2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:967:ARG:HG2	3:C:166:PHE:CA	2.26	0.65
2:B:911:VAL:CG2	3:C:227:LEU:CD1	2.72	0.65
2:B:875:PRO:HG3	2:B:901:LEU:HD11	1.79	0.65
1:A:1107:GLY:HA3	2:B:1006:TYR:CD1	2.32	0.64
1:A:1133:LEU:HB2	1:A:1139:LEU:HD12	1.80	0.64
1:A:1106:PRO:HD2	2:B:1005:ILE:CG2	2.28	0.64
2:B:875:PRO:CG	2:B:901:LEU:HD11	2.28	0.64
2:B:891:PHE:CZ	2:B:921:HIS:HB3	2.33	0.63
2:B:963:TYR:CE2	3:C:167:GLN:HG2	2.33	0.63
2:B:891:PHE:CD2	2:B:921:HIS:HB3	2.34	0.62
2:B:875:PRO:HA	2:B:901:LEU:HD13	1.81	0.62
1:A:848:TYR:CD1	4:D:321:GLY:HA3	2.34	0.62
1:A:1014:ILE:HG21	2:B:939:LEU:HB3	1.80	0.62
2:B:895:LEU:HD11	2:B:919:HIS:HA	1.81	0.62
2:B:967:ARG:HG2	3:C:166:PHE:CG	2.35	0.62
1:A:1010:LEU:HD12	2:B:936:PHE:CE2	2.36	0.61
2:B:814:GLN:NE2	3:C:226:GLN:O	2.28	0.61
2:B:895:LEU:HD21	2:B:919:HIS:N	2.16	0.60
2:B:997:HIS:HA	3:C:85:LEU:CD1	2.32	0.60
1:A:1004:ASP:HA	2:B:932:HIS:CD2	2.36	0.60
1:A:1106:PRO:HG2	2:B:1005:ILE:CG2	2.23	0.59
1:A:1005:ILE:HA	1:A:1008:TRP:CD1	2.37	0.59
2:B:811:LYS:CG	3:C:209:ILE:HD11	2.33	0.59
2:B:967:ARG:HG2	3:C:166:PHE:N	2.18	0.59
2:B:996:LYS:HB2	3:C:86:ASN:HD21	1.68	0.59
2:B:996:LYS:HD2	3:C:85:LEU:O	2.03	0.58
3:C:148:VAL:HB	4:D:319:TYR:CZ	2.38	0.58
2:B:895:LEU:HD22	2:B:919:HIS:CD2	2.40	0.57
2:B:911:VAL:HG23	3:C:227:LEU:HD12	1.83	0.57
3:C:148:VAL:HG21	4:D:322:LEU:CD1	2.34	0.57
1:A:1046:THR:HB	2:B:937:HIS:NE2	2.19	0.57
2:B:911:VAL:N	3:C:227:LEU:HD12	2.19	0.57
2:B:811:LYS:HG2	3:C:209:ILE:HD11	1.87	0.56
2:B:994:LEU:HD21	3:C:97:TYR:CZ	2.39	0.56
1:A:1010:LEU:HD13	2:B:936:PHE:CE2	2.39	0.56
2:B:827:LEU:HD22	3:C:232:LYS:HD2	1.88	0.56
2:B:821:CYS:HA	3:C:231:PRO:HA	1.89	0.55
3:C:182:SER:CB	3:C:191:PHE:HA	2.36	0.55
1:A:1108:ILE:HG13	2:B:1009:SER:O	2.06	0.55
2:B:908:ASP:OD2	3:C:225:PHE:N	2.38	0.55
2:B:809:ASN:ND2	3:C:199:PRO:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1005:ILE:HA	1:A:1008:TRP:HD1	1.72	0.54
2:B:875:PRO:HA	2:B:901:LEU:CD1	2.37	0.54
2:B:964:ASN:ND2	3:C:167:GLN:O	2.39	0.54
2:B:996:LYS:HB2	3:C:86:ASN:ND2	2.21	0.54
1:A:1142:THR:OG1	2:B:1014:LEU:CD2	2.54	0.54
2:B:967:ARG:HG2	3:C:166:PHE:HA	1.88	0.54
5:E:36:DT:H3	6:F:10:DA:H61	1.56	0.54
2:B:1012:VAL:HB	4:D:344:VAL:CG2	2.37	0.54
1:A:976:PHE:CE2	1:A:1096:THR:HG23	2.44	0.53
1:A:1130:CYS:HB3	1:A:1147:TYR:CD2	2.44	0.53
2:B:927:LEU:HD12	5:E:30:DT:H5'	1.91	0.53
1:A:876:ILE:N	3:C:76:GLU:OE2	2.42	0.53
1:A:1004:ASP:CA	2:B:932:HIS:NE2	2.70	0.53
2:B:968:ALA:N	3:C:166:PHE:CZ	2.77	0.53
2:B:970:HIS:CG	3:C:163:MET:SD	3.01	0.53
2:B:818:TYR:HB3	3:C:179:PHE:CE2	2.44	0.53
2:B:811:LYS:HD3	3:C:198:VAL:HG22	1.90	0.52
2:B:886:TYR:O	2:B:891:PHE:CE1	2.63	0.52
2:B:968:ALA:CA	3:C:166:PHE:CE2	2.92	0.52
2:B:1019:MET:SD	3:C:44:ASN:HB2	2.50	0.52
4:D:343:LEU:HD22	4:D:347:GLU:H	1.75	0.52
2:B:810:ARG:HG2	2:B:876:TYR:CD1	2.45	0.51
2:B:1004:ILE:HD11	3:C:161:ARG:C	2.30	0.51
1:A:1130:CYS:HB3	1:A:1147:TYR:CE2	2.46	0.51
2:B:1001:ASN:HA	2:B:1004:ILE:HG22	1.93	0.51
1:A:1015:SER:HA	2:B:943:TYR:CZ	2.45	0.51
3:C:133:VAL:HG13	4:D:294:VAL:HG21	1.93	0.51
2:B:777:MET:HA	3:C:195:VAL:HG11	1.93	0.50
2:B:967:ARG:HB3	3:C:166:PHE:CD2	2.46	0.50
2:B:1023:LEU:HB3	3:C:43:LEU:CD2	2.41	0.50
1:A:883:LEU:HD11	3:C:106:LYS:HB2	1.93	0.50
2:B:1019:MET:HG2	3:C:44:ASN:N	2.27	0.50
2:B:895:LEU:HG	2:B:918:SER:HB3	1.94	0.50
2:B:920:ILE:HG23	2:B:938:GLY:HA3	1.94	0.50
3:C:179:PHE:CE1	3:C:183:PHE:CG	3.00	0.50
2:B:967:ARG:HE	3:C:165:ASP:CA	2.22	0.49
1:A:1106:PRO:CD	2:B:1005:ILE:HG21	2.41	0.49
2:B:891:PHE:HB2	2:B:922:ARG:HA	1.94	0.49
2:B:898:LEU:HD11	2:B:914:LEU:CD2	2.39	0.49
2:B:910:MET:HG3	3:C:228:PRO:C	2.32	0.49
2:B:993:LYS:O	3:C:86:ASN:ND2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:133:VAL:HG22	4:D:294:VAL:HG11	1.93	0.49
1:A:1007:SER:HA	2:B:936:PHE:CZ	2.47	0.49
2:B:1000:TYR:HB3	3:C:85:LEU:HD11	1.93	0.49
2:B:963:TYR:HE2	3:C:167:GLN:HG2	1.74	0.49
2:B:1006:TYR:CE2	2:B:1014:LEU:HD21	2.48	0.49
2:B:949:ARG:HA	2:B:953:TYR:CD1	2.48	0.49
2:B:875:PRO:HB3	2:B:901:LEU:HD21	1.95	0.48
1:A:1010:LEU:HD12	2:B:936:PHE:HE2	1.77	0.48
1:A:1107:GLY:HA3	2:B:1006:TYR:CE1	2.48	0.48
1:A:750:VAL:HG11	1:A:781:TRP:CE2	2.49	0.48
1:A:1146:GLY:HA2	2:B:1011:ASN:HD22	1.79	0.48
2:B:974:LEU:HD22	3:C:244:TYR:OH	2.14	0.48
5:E:12:DT:O2	6:F:35:DA:C2	2.65	0.48
2:B:1000:TYR:HB3	3:C:85:LEU:CD1	2.44	0.48
2:B:901:LEU:HD23	2:B:911:VAL:HG22	1.96	0.48
2:B:967:ARG:CG	3:C:166:PHE:CG	2.97	0.48
1:A:1144:PHE:CE1	2:B:1017:HIS:CG	3.02	0.47
1:A:1106:PRO:CD	2:B:1005:ILE:CG2	2.92	0.47
2:B:830:LEU:HD12	3:C:231:PRO:HD2	1.96	0.47
2:B:927:LEU:HB2	5:E:30:DT:C5'	2.43	0.47
2:B:946:HIS:CD2	2:B:961:ALA:HB1	2.49	0.47
2:B:782:LYS:O	2:B:786:VAL:HG23	2.15	0.47
2:B:814:GLN:HG2	3:C:228:PRO:HG3	1.95	0.47
1:A:1042:ILE:HG23	1:A:1043:ARG:H	1.80	0.47
2:B:895:LEU:HD22	2:B:919:HIS:CE1	2.50	0.47
1:A:883:LEU:HD12	3:C:75:ILE:HD11	1.96	0.47
1:A:1021:MET:SD	2:B:940:ARG:HA	2.54	0.47
2:B:1004:ILE:HD11	3:C:161:ARG:HA	1.97	0.47
2:B:811:LYS:HG3	3:C:209:ILE:HD11	1.96	0.47
3:C:133:VAL:HG22	4:D:294:VAL:CG2	2.32	0.47
2:B:891:PHE:CD2	2:B:921:HIS:C	2.89	0.46
4:D:172:SER:O	4:D:176:LEU:HD12	2.16	0.46
1:A:884:LYS:HA	3:C:108:VAL:HG11	1.98	0.46
2:B:996:LYS:O	3:C:85:LEU:HD13	2.16	0.46
2:B:1000:TYR:CB	3:C:85:LEU:CD1	2.94	0.46
2:B:997:HIS:HA	3:C:85:LEU:HD13	1.97	0.46
3:C:133:VAL:CG2	4:D:294:VAL:CG2	2.91	0.46
2:B:1000:TYR:CD2	3:C:85:LEU:HD21	2.50	0.46
2:B:1000:TYR:CB	3:C:85:LEU:HD11	2.46	0.46
3:C:133:VAL:CG1	4:D:294:VAL:HG21	2.46	0.46
2:B:809:ASN:ND2	3:C:199:PRO:HG2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1000:TYR:CD1	2:B:1000:TYR:C	2.88	0.46
2:B:811:LYS:HB2	3:C:198:VAL:HG13	1.98	0.45
1:A:848:TYR:CE1	4:D:321:GLY:HA3	2.51	0.45
1:A:1077:ARG:HA	1:A:1125:GLU:HG2	1.99	0.45
1:A:1091:TRP:CZ3	1:A:1095:VAL:CG2	2.99	0.45
2:B:927:LEU:HB2	5:E:30:DT:H5"	1.97	0.45
6:F:18:DA:C6	6:F:19:DA:C6	3.05	0.45
1:A:895:THR:HG22	4:D:326:ALA:HB2	1.99	0.45
2:B:967:ARG:HG3	3:C:166:PHE:CE1	2.52	0.45
3:C:168:ILE:HG22	3:C:169:LYS:N	2.31	0.45
2:B:898:LEU:HD13	2:B:915:MET:N	2.32	0.44
2:B:811:LYS:HD2	3:C:198:VAL:HA	1.99	0.44
1:A:1149:VAL:HG23	2:B:976:SER:HB3	1.99	0.44
5:E:13:DT:O2	6:F:34:DA:C2	2.70	0.44
2:B:928:THR:N	5:E:30:DT:OP1	2.50	0.44
2:B:996:LYS:HB3	3:C:85:LEU:HB3	2.00	0.44
2:B:911:VAL:H	3:C:227:LEU:HD12	1.82	0.44
1:A:1054:ASN:OD1	2:B:947:LYS:NZ	2.29	0.44
3:C:98:PHE:CZ	3:C:170:LEU:HD12	2.53	0.44
3:C:170:LEU:CB	3:C:176:ALA:HB1	2.45	0.43
1:A:1144:PHE:HE1	2:B:1017:HIS:CG	2.36	0.43
2:B:895:LEU:CD2	2:B:918:SER:HB2	2.48	0.43
3:C:182:SER:HB3	3:C:191:PHE:HA	2.00	0.43
1:A:1014:ILE:HG13	1:A:1019:LEU:HD12	1.99	0.43
2:B:891:PHE:CB	2:B:922:ARG:HB2	2.48	0.43
4:D:66:PHE:CZ	4:D:105:PRO:HD3	2.54	0.43
1:A:1148:TRP:CE3	2:B:979:ILE:HG22	2.54	0.43
2:B:965:LEU:O	2:B:969:PHE:CD2	2.72	0.43
2:B:960:GLU:HG2	3:C:169:LYS:HB2	1.99	0.43
2:B:994:LEU:CD2	3:C:97:TYR:CZ	3.02	0.43
5:E:36:DT:H3	6:F:10:DA:N6	2.15	0.43
3:C:150:PRO:HG3	4:D:317:LEU:HD22	2.01	0.43
2:B:810:ARG:HG3	3:C:202:ASP:OD2	2.19	0.42
2:B:875:PRO:CA	2:B:901:LEU:CD1	2.97	0.42
3:C:35:ARG:O	4:D:354:ALA:HA	2.19	0.42
3:C:36:ILE:CG2	4:D:350:PHE:H	2.31	0.42
2:B:879:TYR:CE1	2:B:914:LEU:HD22	2.54	0.42
2:B:895:LEU:HD22	2:B:919:HIS:NE2	2.34	0.42
2:B:915:MET:SD	2:B:941:TYR:CG	3.12	0.42
1:A:857:LEU:HB3	4:D:432:VAL:CG1	2.50	0.42
3:C:34:PRO:HD3	4:D:50:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1011:ILE:HG23	2:B:939:LEU:HD11	2.02	0.42
1:A:1151:HIS:CE1	2:B:980:GLU:HB3	2.55	0.42
2:B:891:PHE:CZ	3:C:235:MET:HG3	2.55	0.42
2:B:1025:ILE:HG21	3:C:54:LYS:HD3	2.02	0.42
2:B:830:LEU:CD1	3:C:231:PRO:HD2	2.50	0.42
3:C:182:SER:HB2	3:C:191:PHE:HA	2.01	0.42
1:A:857:LEU:HB3	4:D:432:VAL:HG12	2.02	0.41
3:C:36:ILE:HD12	4:D:351:PRO:HA	2.03	0.41
3:C:38:SER:CB	4:D:347:GLU:OE2	2.68	0.41
2:B:822:ARG:HG2	3:C:100:GLU:O	2.21	0.41
3:C:117:LEU:HD11	4:D:329:PHE:CZ	2.56	0.41
2:B:803:LEU:HD11	2:B:816:PHE:CD2	2.55	0.41
2:B:839:PHE:CE2	2:B:880:ILE:CG2	3.03	0.41
2:B:963:TYR:CE2	3:C:167:GLN:CG	3.03	0.41
2:B:1000:TYR:OH	3:C:103:VAL:HG11	2.20	0.41
2:B:910:MET:SD	2:B:913:LEU:HD23	2.61	0.41
2:B:809:ASN:HD21	3:C:199:PRO:HG2	1.86	0.41
2:B:997:HIS:HA	3:C:85:LEU:HD12	2.01	0.41
3:C:166:PHE:HB2	3:C:233:LEU:HB2	2.02	0.41
4:D:48:ALA:HB2	4:D:76:ILE:HG12	2.02	0.41
1:A:1139:LEU:HD23	1:A:1149:VAL:HG13	2.03	0.41
2:B:744:LEU:HB3	3:C:186:LEU:O	2.21	0.41
2:B:787:LEU:HD11	2:B:819:SER:HA	2.03	0.40
2:B:1023:LEU:HB3	3:C:43:LEU:HD22	2.03	0.40
2:B:891:PHE:HB2	2:B:922:ARG:CA	2.50	0.40
1:A:1079:TRP:CZ3	1:A:1129:ILE:CD1	3.03	0.40
2:B:895:LEU:CD2	2:B:919:HIS:CD2	3.03	0.40
1:A:1079:TRP:CZ3	1:A:1129:ILE:HD11	2.56	0.40
2:B:978:ALA:HB1	2:B:982:TYR:CE2	2.56	0.40
6:F:18:DA:C6	6:F:19:DA:N6	2.89	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	427/1201 (36%)	403 (94%)	22 (5%)	2 (0%)	25 57
2	B	292/1029 (28%)	281 (96%)	10 (3%)	1 (0%)	37 67
3	C	229/606 (38%)	210 (92%)	19 (8%)	0	100 100
4	D	325/435 (75%)	312 (96%)	13 (4%)	0	100 100
All	All	1273/3271 (39%)	1206 (95%)	64 (5%)	3 (0%)	45 72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1042	ILE
2	B	909	PRO
1	A	1120	VAL

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	397/1079 (37%)	388 (98%)	9 (2%)	45 64
2	B	267/927 (29%)	263 (98%)	4 (2%)	60 75
3	C	214/550 (39%)	214 (100%)	0	100 100
4	D	294/384 (77%)	294 (100%)	0	100 100
All	All	1172/2940 (40%)	1159 (99%)	13 (1%)	69 80

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	816	ARG
1	A	863	LEU
1	A	972	ASN
1	A	987	ASN
1	A	1000	GLN

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Mol	Chain	Res	Type
1	A	1039	ARG
1	A	1043	ARG
1	A	1045	LEU
1	A	1064	LYS
2	B	836	GLN
2	B	896	GLN
2	B	900	ARG
2	B	933	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	836	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 oligosaccharides 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.

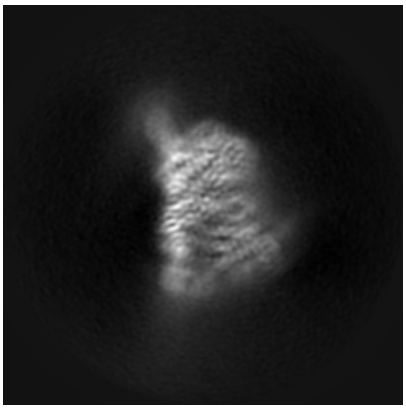
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51231. These allow visual inspection of the internal detail of the map and identification of artifacts.

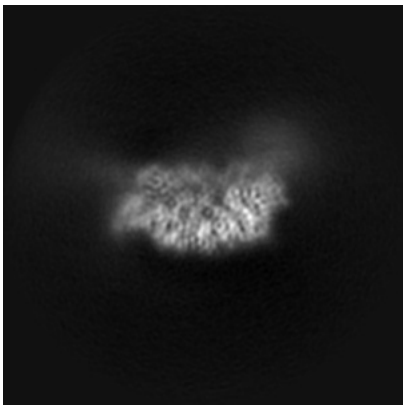
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

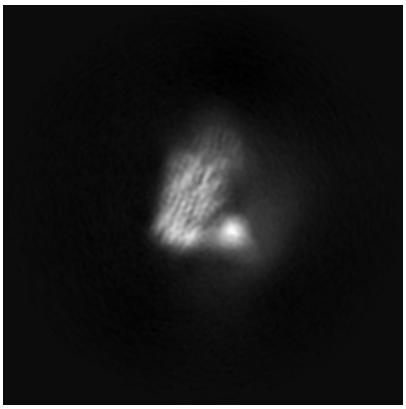
6.1.1 Primary map



X

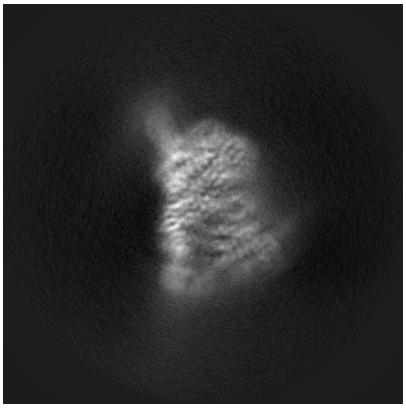


Y

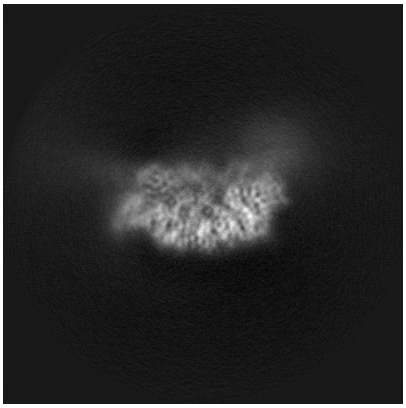


Z

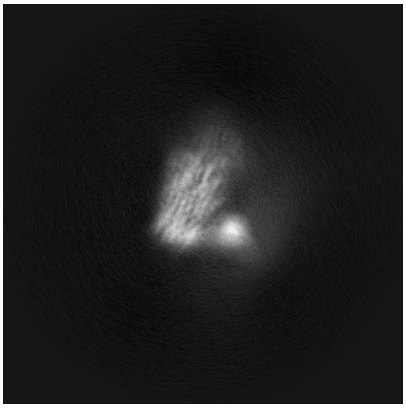
6.1.2 Raw map



X



Y

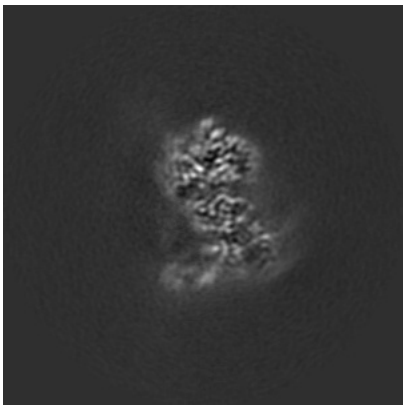


Z

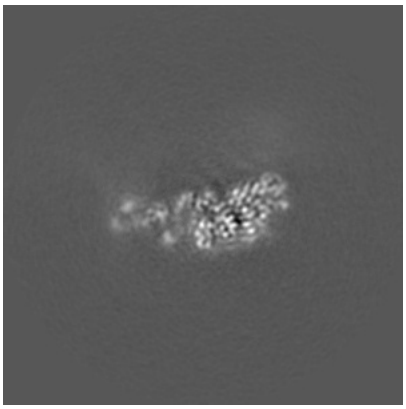
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

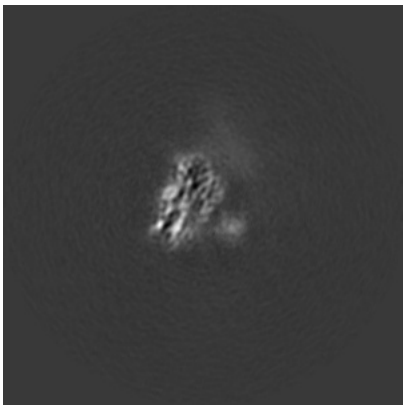
6.2.1 Primary map



X Index: 160

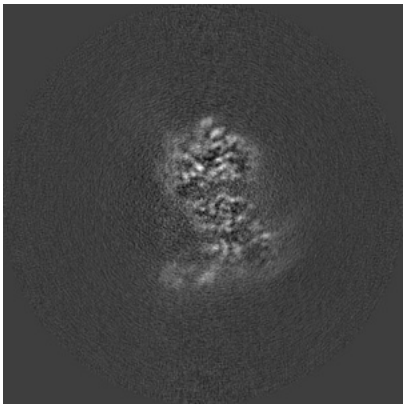


Y Index: 160

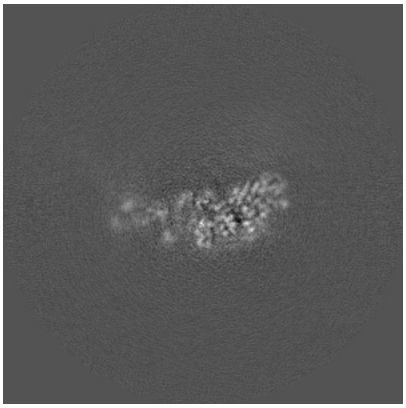


Z Index: 160

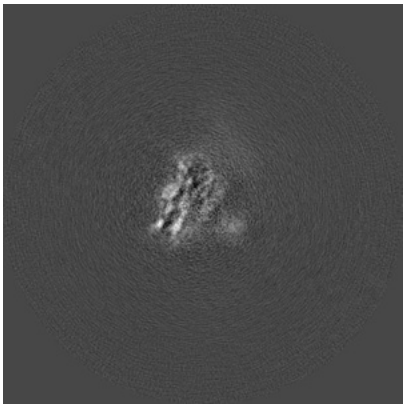
6.2.2 Raw map



X Index: 160



Y Index: 160

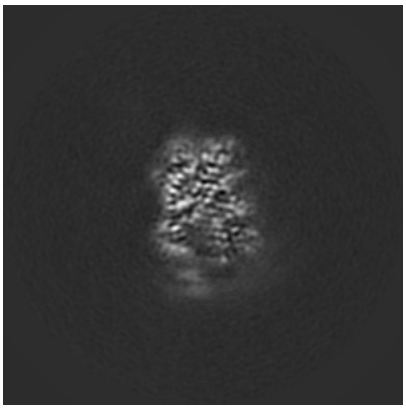


Z Index: 160

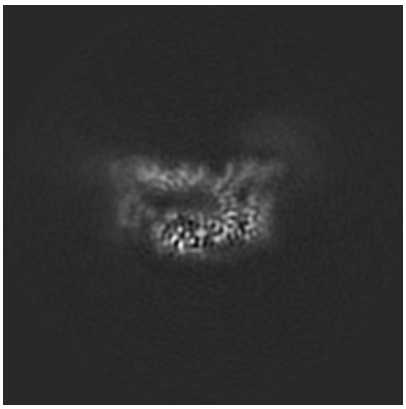
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

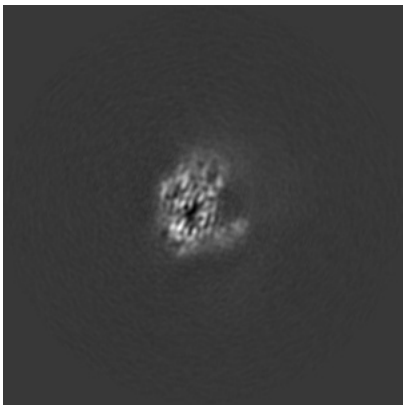
6.3.1 Primary map



X Index: 140

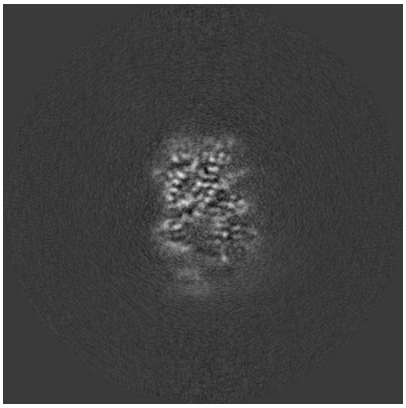


Y Index: 138

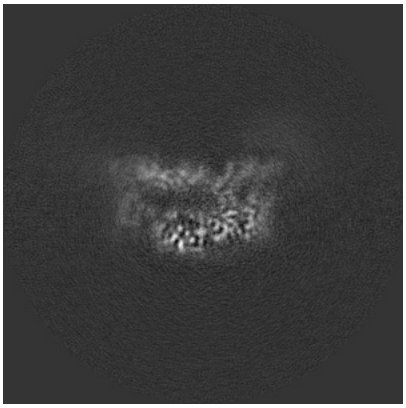


Z Index: 183

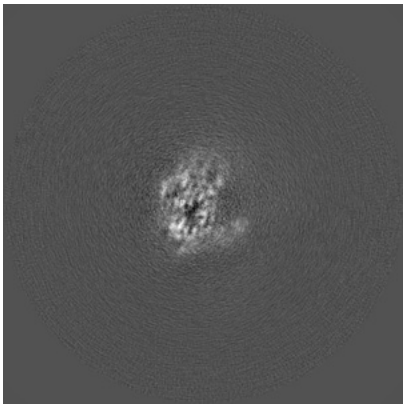
6.3.2 Raw map



X Index: 141



Y Index: 138

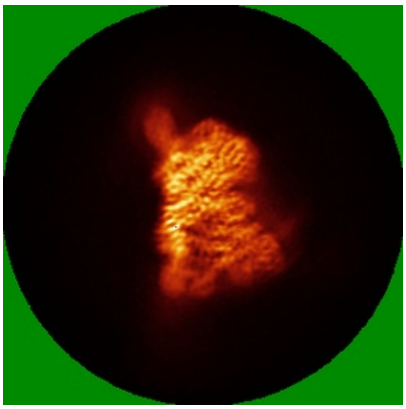


Z Index: 183

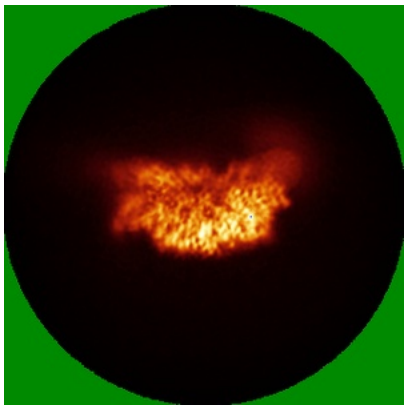
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

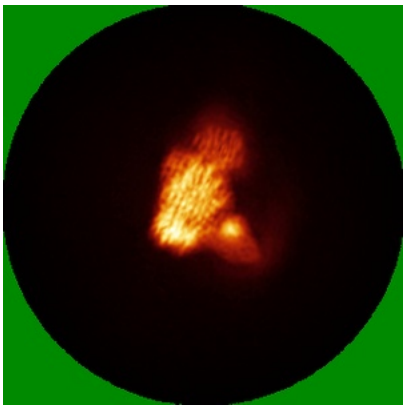
6.4.1 Primary map



X

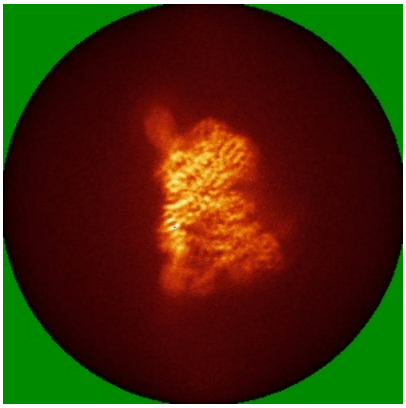


Y

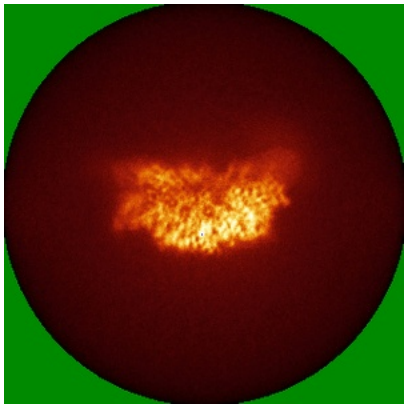


Z

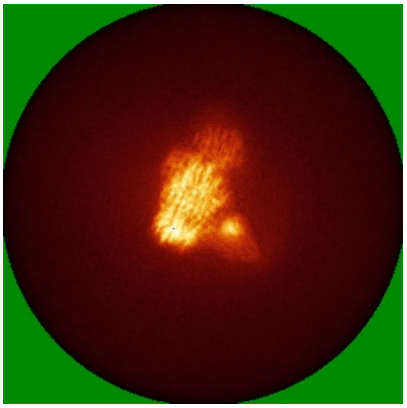
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

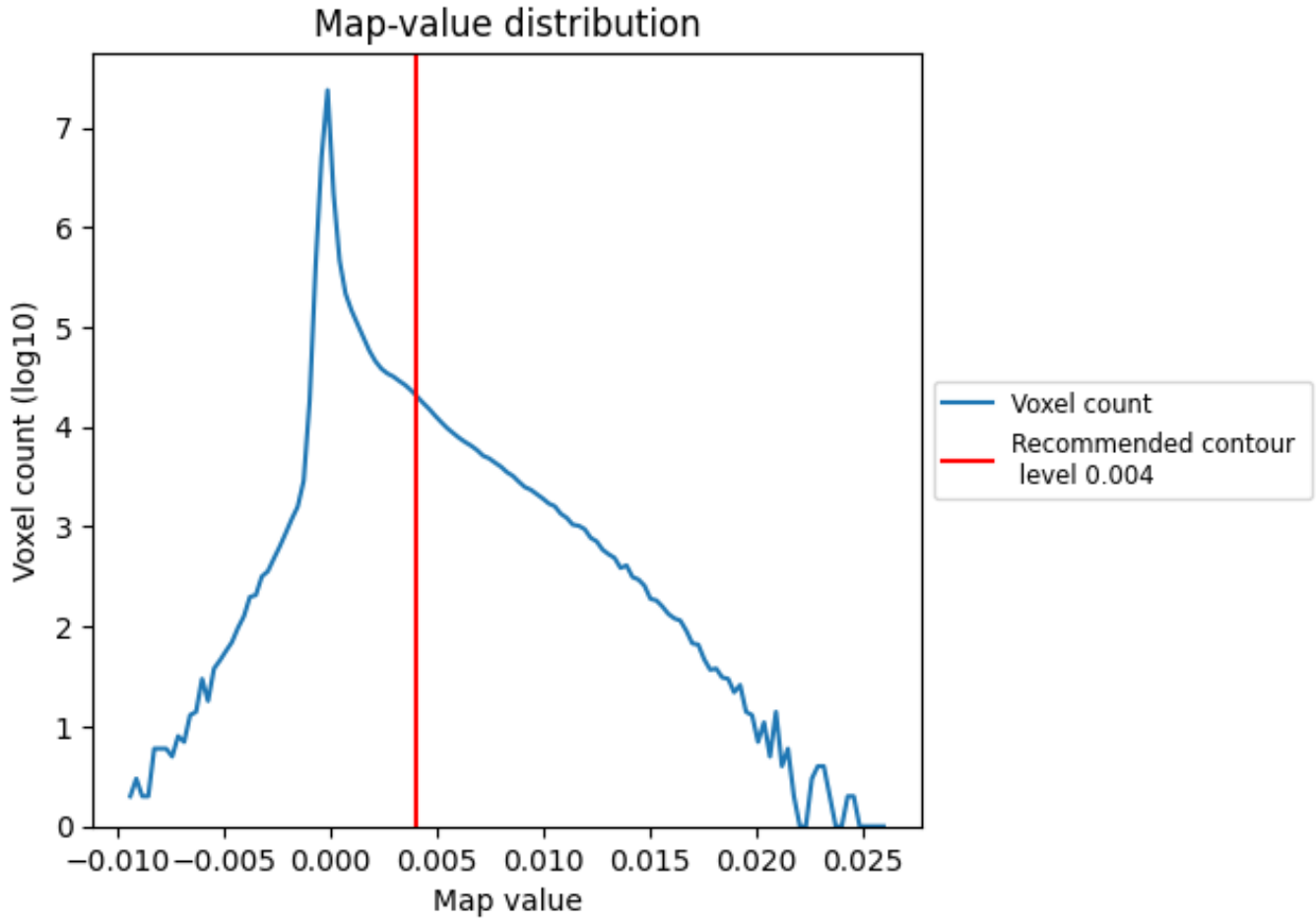
6.6 Mask visualisation (i)

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

7 Map analysis

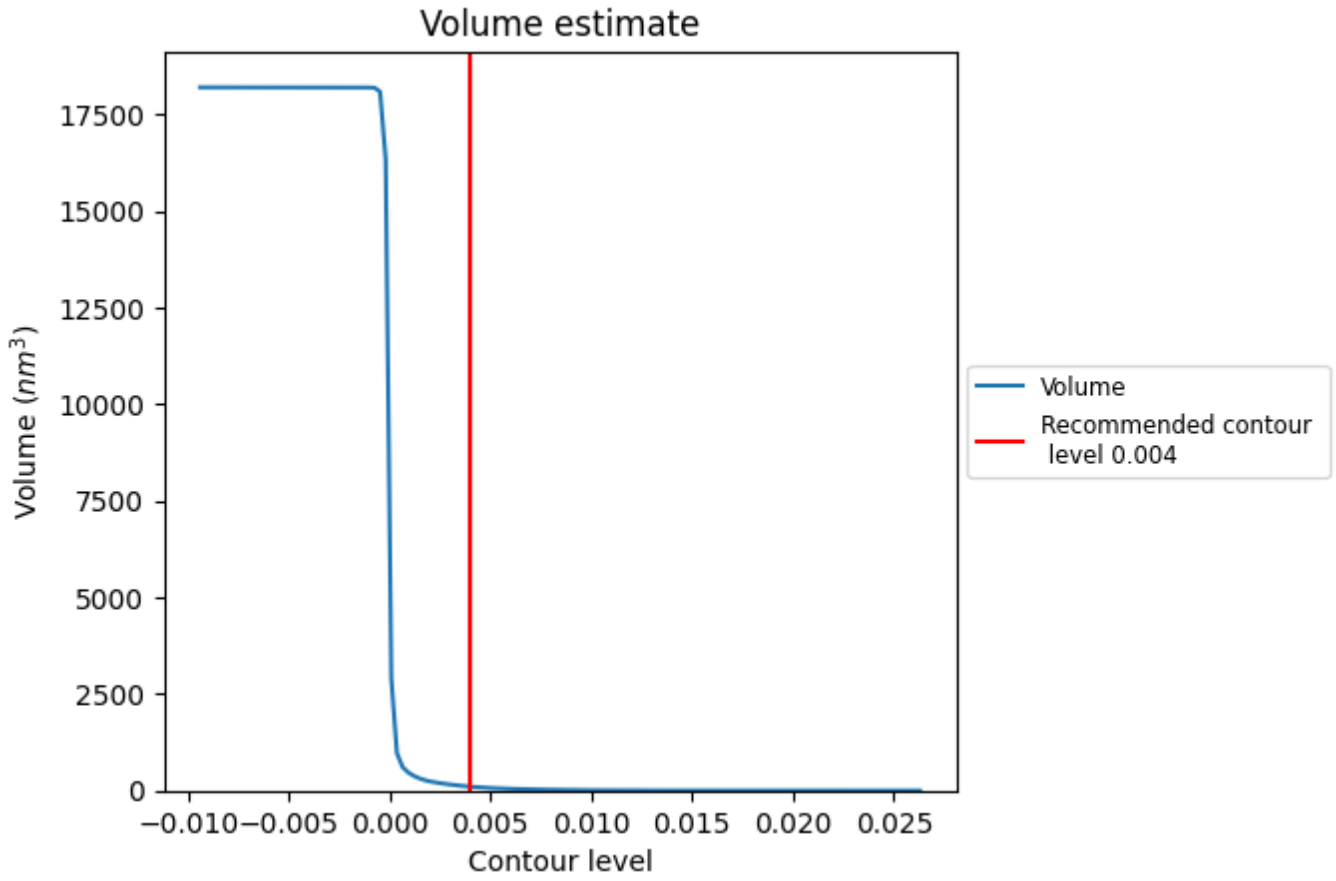
This section contains the results of statistical analysis of the map.

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.

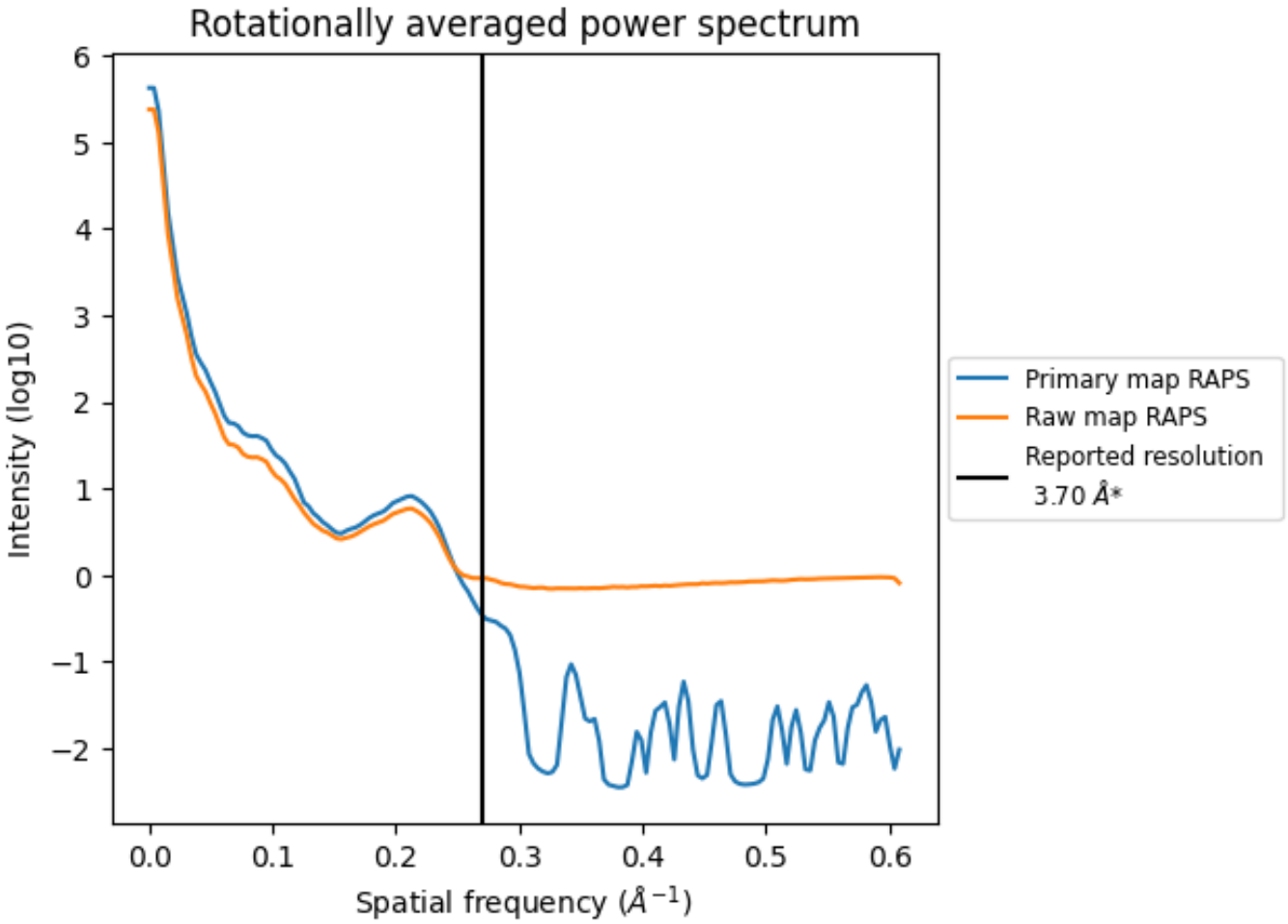
7.2 Volume estimate (i)



The volume at the recommended contour level is 101 nm^3; this corresponds to an approximate mass of 91 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)

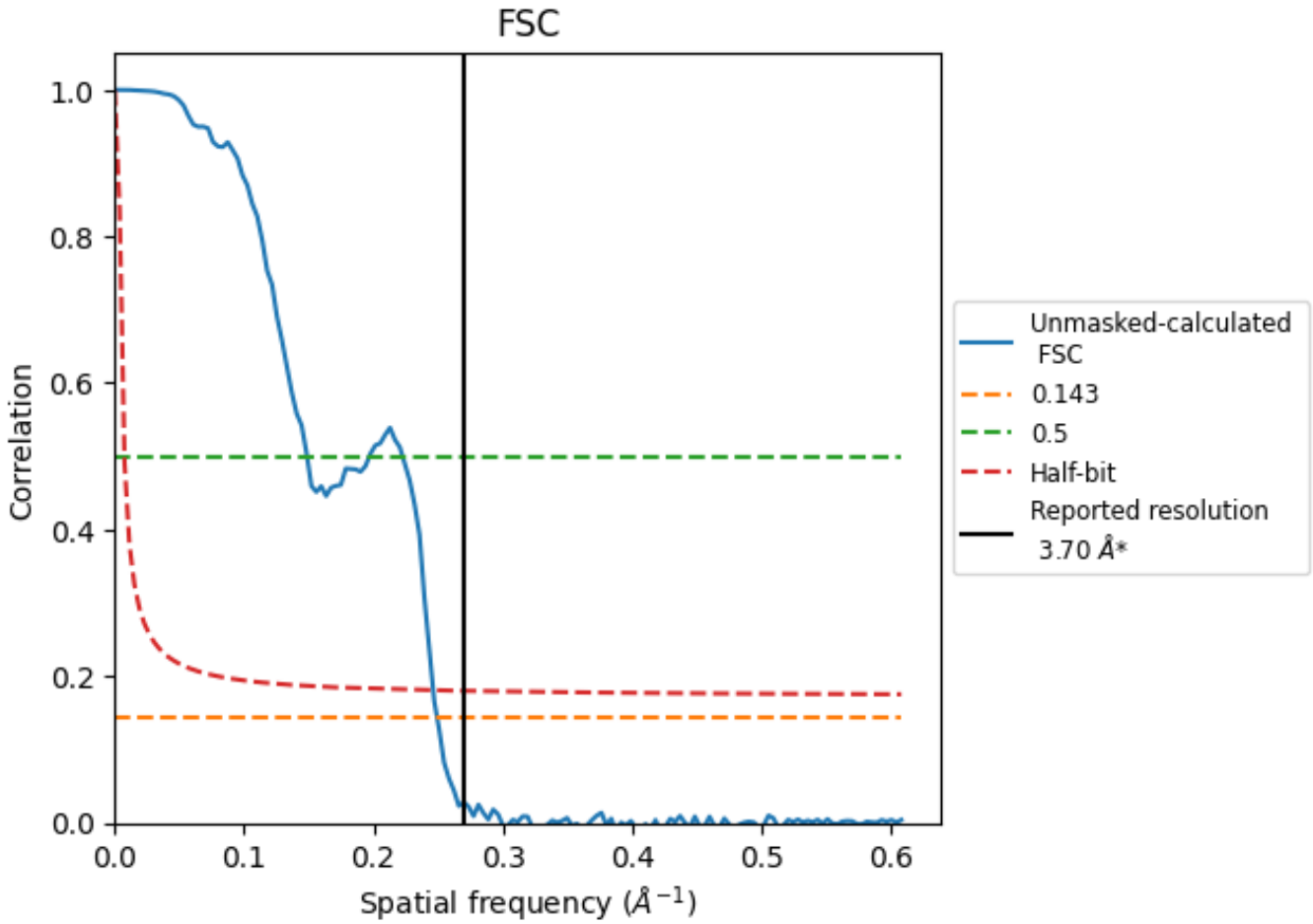


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

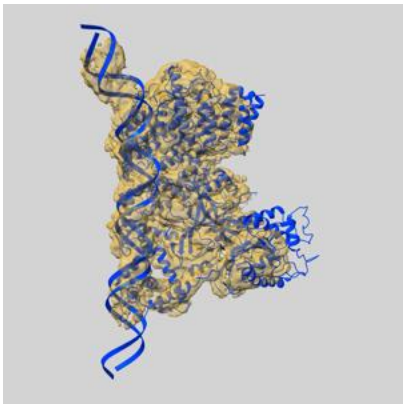
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	6.72	4.06

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

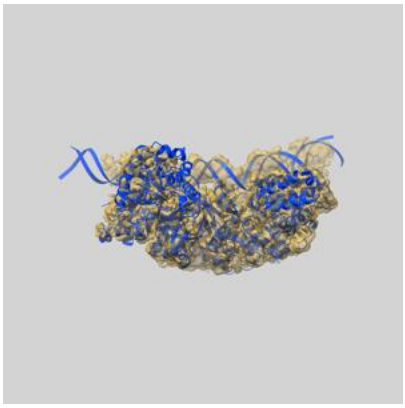
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51231 and PDB model 9GCK. Per-residue inclusion information can be found in section 3 on page 6.

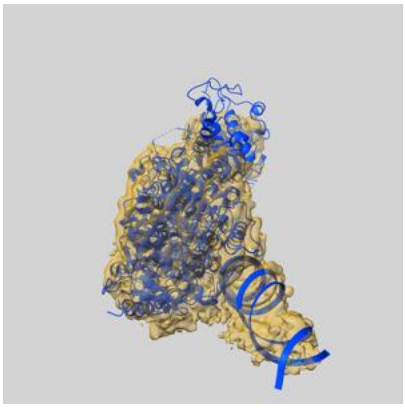
9.1 Map-model overlay



X



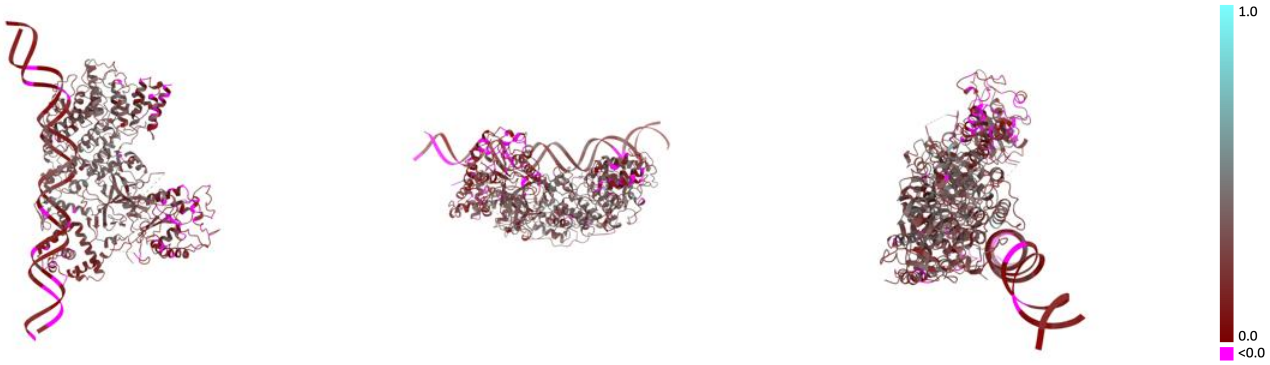
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.004 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.

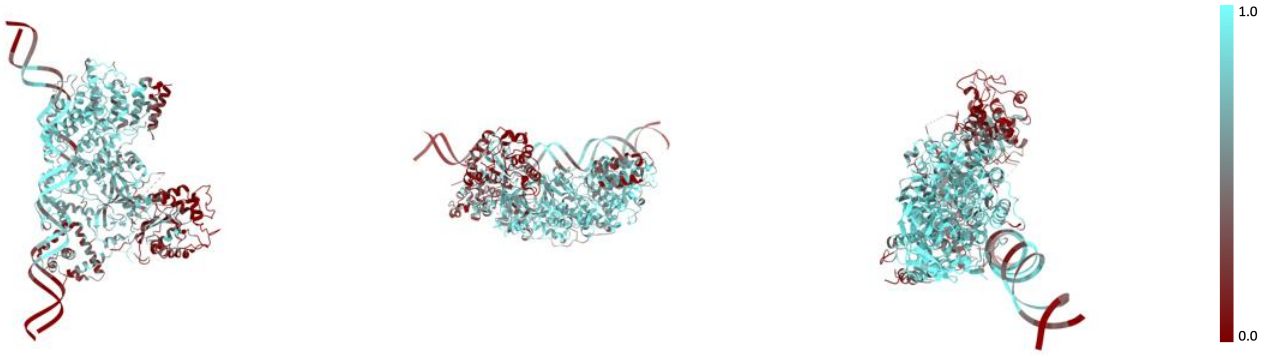
9.2 Q-score mapped to coordinate model (i)



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.

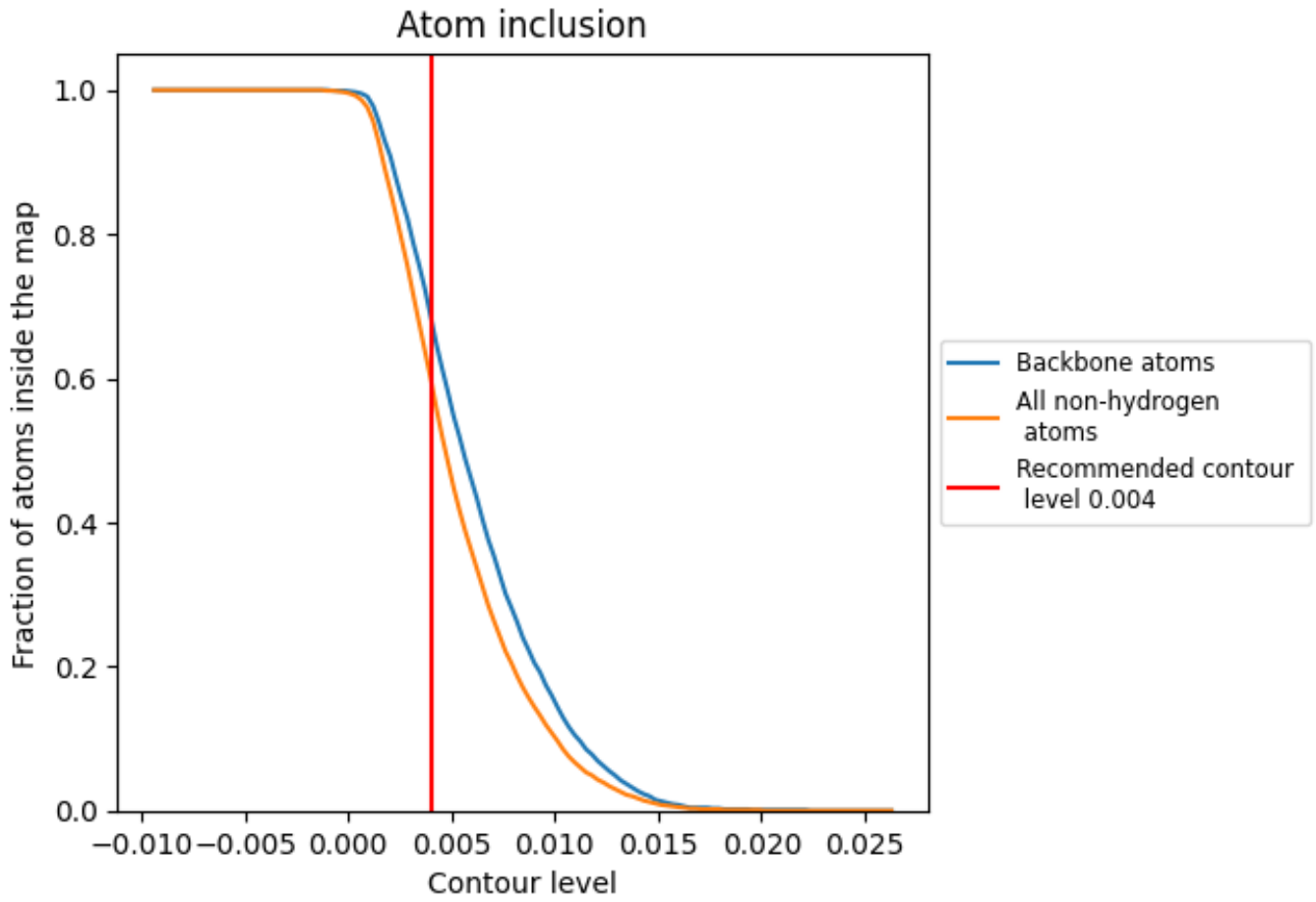
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.004).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 60% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5980	0.2360
A	0.6540	0.2500
B	0.7420	0.2940
C	0.7630	0.3270
D	0.3600	0.1870
E	0.4500	0.1220
F	0.5150	0.1030