



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:37 AM UTC

PDB ID : 6WTD / pdb_00006wtd
EMDB ID : EMD-21894
Title : Monomer yeast ATP synthase Fo reconstituted in nanodisc with inhibitor of Bedaquiline bound
Authors : Mueller, D.M.; Srivastava, A.P.; Symersky, J.; Luo, M.; Liao, M.F.
Deposited on : 2020-05-02
Resolution : 4.20 Å(reported)
Based on initial model : 6CP7

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

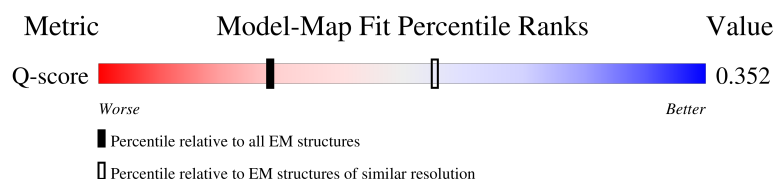
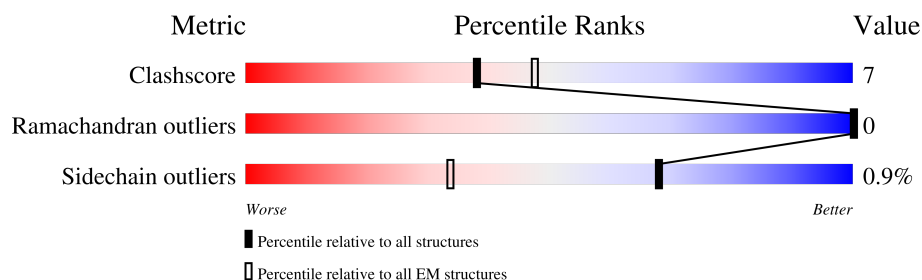
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	K	76	16% 70% 26% ..
1	L	76	13% 74% 24% .
1	M	76	12% 87% 12% .
1	N	76	8% 72% 24% ..

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Mol	Chain	Length	Quality of chain
1	O	76	
1	P	76	
1	Q	76	
1	R	76	
1	S	76	
1	T	76	
2	8	48	
3	X	249	
4	Z	209	
5	7	173	
6	U	95	
7	J	37	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9139 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 ATP synthase subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	74	Total	C	N	O	S	0	0
			534	358	82	90	4		
1	L	74	Total	C	N	O	S	0	0
			529	353	82	91	3		
1	M	75	Total	C	N	O	S	0	0
			535	358	83	91	3		
1	N	74	Total	C	N	O	S	0	0
			532	356	82	91	3		
1	O	74	Total	C	N	O	S	0	0
			533	357	82	91	3		
1	P	74	Total	C	N	O	S	0	0
			529	352	82	91	4		
1	Q	74	Total	C	N	O	S	0	0
			526	350	82	91	3		
1	R	75	Total	C	N	O	S	0	0
			522	345	83	92	2		
1	S	74	Total	C	N	O	S	0	0
			529	353	82	91	3		
1	T	74	Total	C	N	O	S	0	0
			529	355	81	90	3		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	FME	-	initiating methionine	UNP P61829
L	1	FME	-	initiating methionine	UNP P61829
M	1	FME	-	initiating methionine	UNP P61829
N	1	FME	-	initiating methionine	UNP P61829
O	1	FME	-	initiating methionine	UNP P61829
P	1	FME	-	initiating methionine	UNP P61829
Q	1	FME	-	initiating methionine	UNP P61829
R	1	FME	-	initiating methionine	UNP P61829
S	1	FME	-	initiating methionine	UNP P61829
T	1	FME	-	initiating methionine	UNP P61829

- Molecule 2 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	8	42	Total	C	N	O	S	0	0
			364	256	52	53	3		

- Molecule 3 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	X	223	Total	C	N	O	S	0	0
			1750	1192	262	286	10		

- Molecule 4 is a protein called ATP synthase subunit 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Z	54	Total	C	N	O	S	0	0
			393	253	64	75	1		

- Molecule 5 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	67	Total	C	N	O	S	0	0
			520	329	86	103	2		

- Molecule 6 is a protein called ATP synthase subunit f, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	68	Total	C	N	O	S	0	0
			522	346	89	86	1		

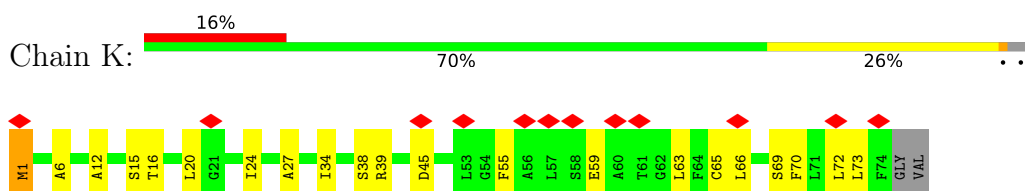
- Molecule 7 is a protein called ATP synthase subunit J, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	37	Total	C	N	O	S	0	0
			292	197	45	48	2		

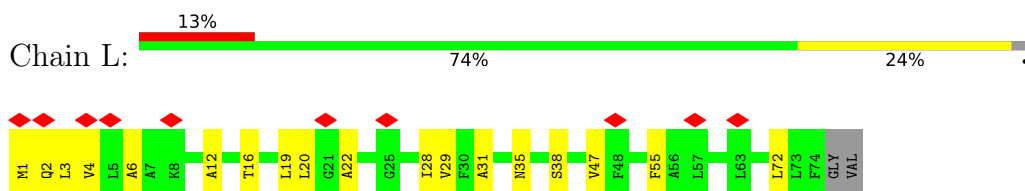
3 Residue-property plots [i](#)

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.

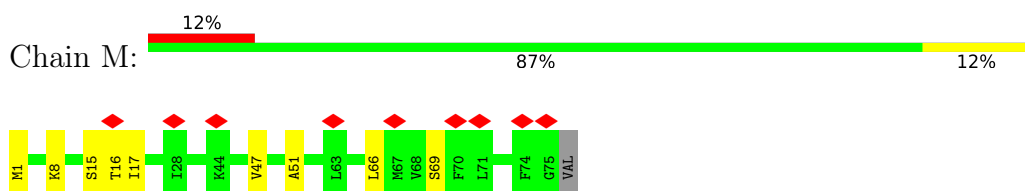
- Molecule 1: ATP synthase subunit 9, mitochondrial



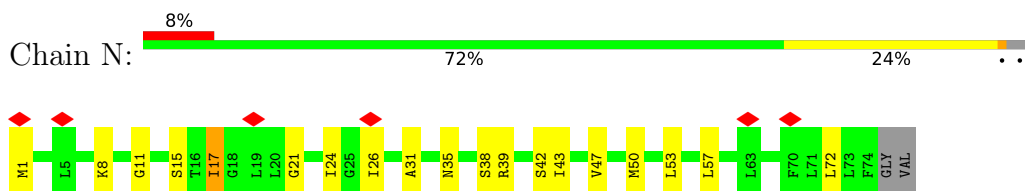
- Molecule 1: ATP synthase subunit 9, mitochondrial



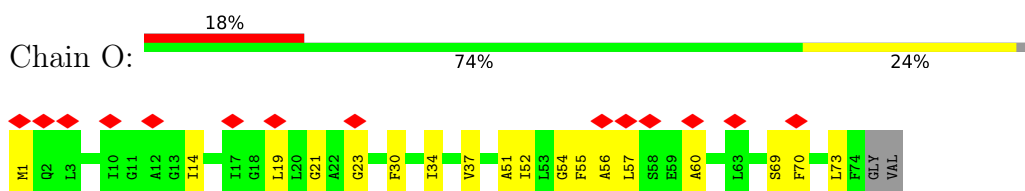
- Molecule 1: ATP synthase subunit 9, mitochondrial



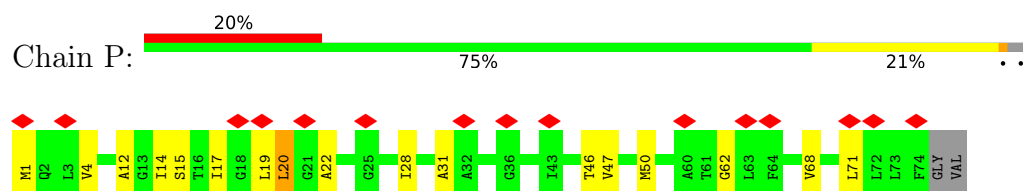
- Molecule 1: ATP synthase subunit 9, mitochondrial



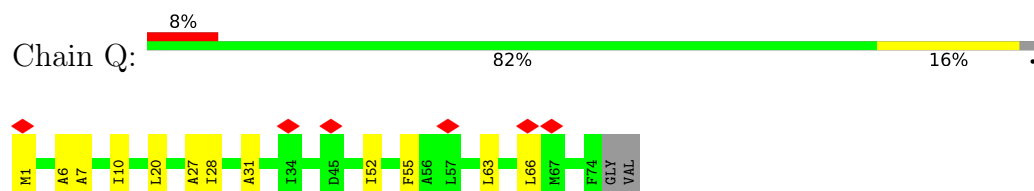
- Molecule 1: ATP synthase subunit 9, mitochondrial



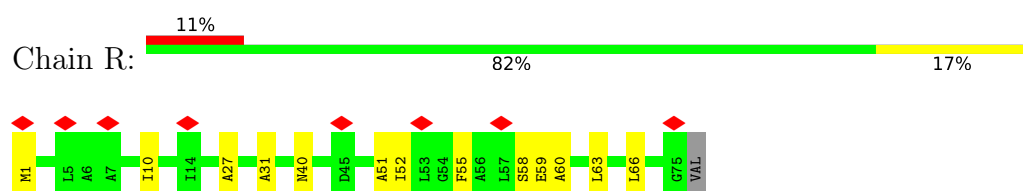
- Molecule 1: ATP synthase subunit 9, mitochondrial



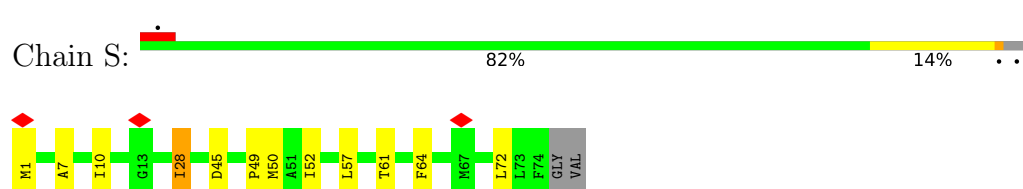
- Molecule 1: ATP synthase subunit 9, mitochondrial



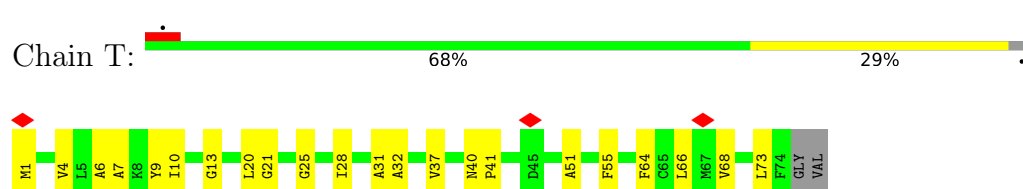
- Molecule 1: ATP synthase subunit 9, mitochondrial



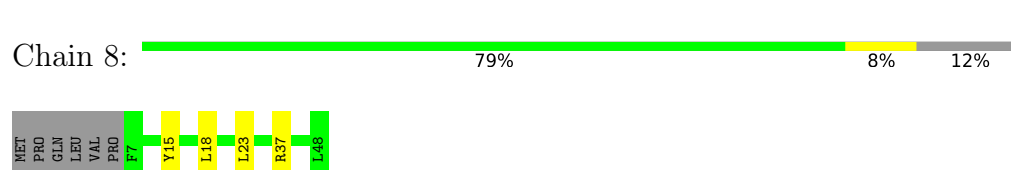
- Molecule 1: ATP synthase subunit 9, mitochondrial



- Molecule 1: ATP synthase subunit 9, mitochondrial

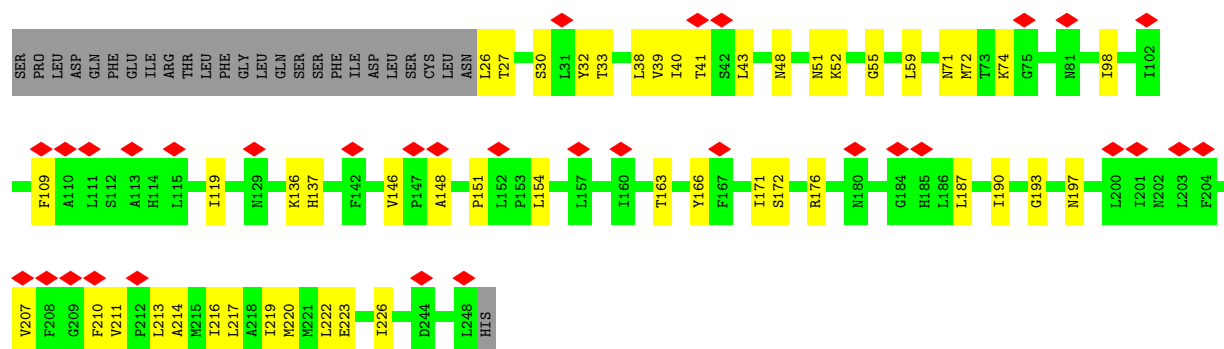


- Molecule 2: ATP synthase protein 8

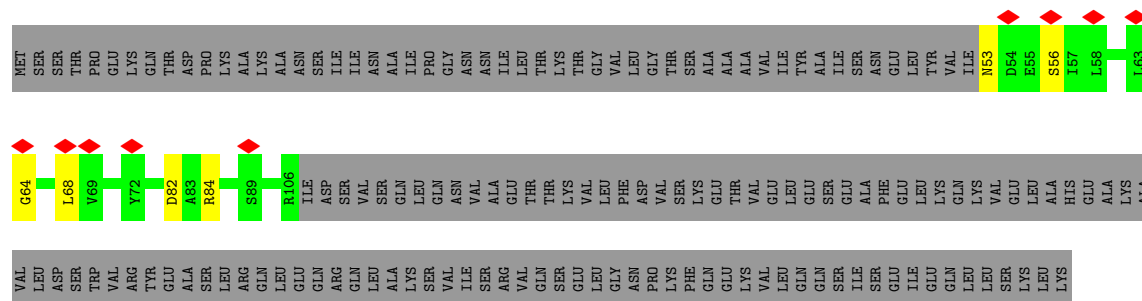


- Molecule 3: ATP synthase subunit a

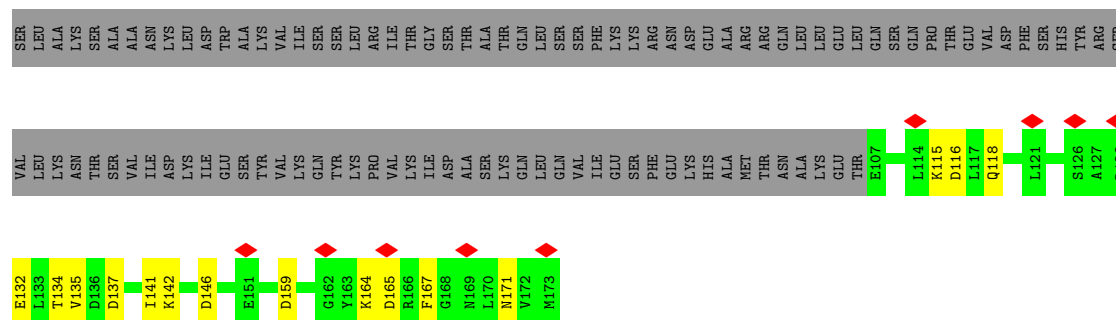




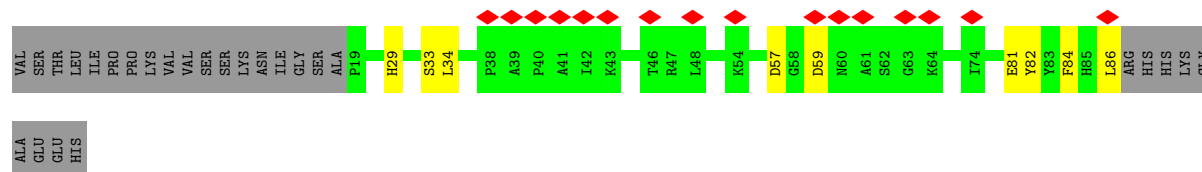
- Molecule 4: ATP synthase subunit 4, mitochondrial



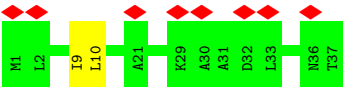
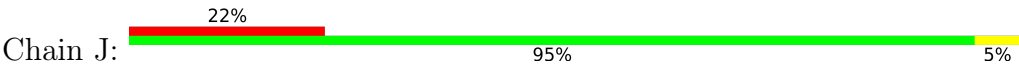
- Molecule 5: ATP synthase subunit d, mitochondrial



- Molecule 6: ATP synthase subunit f, mitochondrial



- Molecule 7: ATP synthase subunit J, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	47169	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 ($e^-/\text{\AA}^2$)	8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.234	Depositor
Minimum map value	-0.182	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.043	Depositor
Map size (Å)	238.08, 238.08, 238.08	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FME

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	K	0.34	0/532	0.68	0/721
1	L	0.33	0/530	0.70	2/718 (0.3%)
1	M	0.31	0/535	0.64	0/724
1	N	0.34	0/533	0.72	2/722 (0.3%)
1	O	0.32	0/533	0.64	0/722
1	P	0.31	0/527	0.63	0/714
1	Q	0.34	0/527	0.69	0/714
1	R	0.39	0/521	0.65	0/707
1	S	0.37	0/530	0.64	0/718
1	T	0.39	0/529	0.64	0/717
2	8	0.32	0/374	0.69	0/503
3	X	0.34	0/1796	0.74	3/2451 (0.1%)
4	Z	0.27	0/398	0.54	0/538
5	7	0.27	0/527	0.51	0/709
6	U	0.25	0/540	0.60	0/731
7	J	0.25	0/302	0.60	0/410
All	All	0.33	0/9234	0.66	7/12519 (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	T	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	211	VAL	CA-C-N	-7.63	113.94	121.65
3	X	211	VAL	C-N-CA	-7.63	113.94	121.65
1	N	17	ILE	N-CA-C	-6.96	106.44	113.47
1	N	26	ILE	N-CA-C	-6.25	106.42	112.29
3	X	98	ILE	N-CA-C	-5.80	106.75	111.91
1	L	47	VAL	CA-C-N	5.16	126.20	120.06
1	L	47	VAL	C-N-CA	5.16	126.20	120.06

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	T	64	PHE	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	K	534	0	575	18	0
1	L	529	0	562	10	0
1	M	535	0	571	5	0
1	N	532	0	571	13	0
1	O	533	0	573	13	0
1	P	529	0	560	11	0
1	Q	526	0	553	5	0
1	R	522	0	544	9	0
1	S	529	0	562	10	0
1	T	529	0	567	19	0
2	8	364	0	390	3	0
3	X	1750	0	1841	29	0
4	Z	393	0	377	5	0
5	7	520	0	511	11	0
6	U	522	0	483	5	0
7	J	292	0	298	1	0
All	All	9139	0	9538	139	0

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

All (139) 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:N:21:GLY:HA3	1:O:21:GLY:HA2	1.75	0.68
1:O:54:GLY:HA2	1:O:57:LEU:HD12	1.76	0.67
3:X:71:ASN:HD22	5:7:171:ASN:HD22	1.41	0.66
1:K:59:GLU:HB3	1:K:63:LEU:HD23	1.78	0.66
3:X:40:ILE:HA	3:X:43:LEU:HB2	1.77	0.66
1:K:20:LEU:HD11	1:T:20:LEU:HB2	1.77	0.65
3:X:146:VAL:HG22	3:X:148:ALA:H	1.63	0.64
1:O:14:ILE:HD13	1:P:14:ILE:HG12	1.80	0.63
1:P:46:THR:HG23	1:P:47:VAL:HG13	1.81	0.63
1:K:66:LEU:HD12	1:K:69:SER:HB2	1.82	0.60
3:X:216:ILE:HA	3:X:219:ILE:HD12	1.82	0.60
3:X:32:TYR:OH	3:X:109:PHE:O	2.21	0.58
3:X:55:GLY:HA2	3:X:59:LEU:HD23	1.85	0.58
1:N:31:ALA:O	1:N:35:ASN:ND2	2.37	0.58
1:T:9:TYR:O	1:T:13:GLY:N	2.37	0.57
5:7:115:LYS:HA	5:7:118:GLN:HB2	1.86	0.56
3:X:151:PRO:HD2	3:X:154:LEU:HD22	1.88	0.56
3:X:52:LYS:NZ	5:7:132:GLU:O	2.33	0.56
5:7:159:ASP:OD1	5:7:164:LYS:NZ	2.39	0.56
1:K:72:LEU:HD22	1:L:72:LEU:HD13	1.88	0.55
3:X:119:ILE:HD11	3:X:171:ILE:HG13	1.89	0.54
1:L:2:GLN:HG2	1:L:3:LEU:HD12	1.90	0.54
1:K:16:THR:HG21	1:T:68:VAL:HG21	1.90	0.54
1:L:12:ALA:O	1:L:16:THR:OG1	2.25	0.54
1:O:34:ILE:HA	1:O:37:VAL:HG22	1.90	0.54
3:X:193:GLY:O	3:X:197:ASN:ND2	2.40	0.54
1:N:35:ASN:O	1:N:39:ARG:NH2	2.41	0.53
3:X:48:ASN:ND2	3:X:51:ASN:OD1	2.40	0.53
3:X:172:SER:O	3:X:176:ARG:NH1	2.42	0.53
1:L:3:LEU:HA	1:L:6:ALA:HB2	1.90	0.53
1:Q:52:ILE:HA	1:Q:55:PHE:HB3	1.91	0.53
1:K:6:ALA:HB2	1:T:4:VAL:HB	1.92	0.52
1:L:19:LEU:HA	1:L:22:ALA:HB3	1.90	0.52
1:M:17:ILE:HG23	1:N:17:ILE:HD13	1.90	0.52
3:X:40:ILE:HG22	3:X:43:LEU:HD22	1.92	0.52
1:R:51:ALA:O	1:R:55:PHE:N	2.42	0.52
1:S:45:ASP:N	1:S:45:ASP:OD1	2.39	0.52
2:8:37:ARG:NH2	5:7:146:ASP:OD2	2.43	0.51
1:K:24:ILE:HG23	1:T:21:GLY:HA2	1.92	0.51
4:Z:53:ASN:O	4:Z:56:SER:OG	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:82:ASP:N	4:Z:82:ASP:OD1	2.42	0.51
1:Q:27:ALA:O	1:Q:31:ALA:N	2.40	0.51
5:7:141:ILE:HG22	5:7:142:LYS:HG2	1.93	0.51
1:K:27:ALA:HB2	1:T:25:GLY:HA2	1.92	0.51
1:P:22:ALA:HB2	1:P:62:GLY:HA3	1.93	0.51
1:P:28:ILE:HA	1:P:31:ALA:HB3	1.93	0.50
1:S:57:LEU:O	1:S:61:THR:OG1	2.26	0.50
6:U:82:TYR:HA	6:U:86:LEU:HB2	1.92	0.50
1:N:38:SER:OG	1:N:39:ARG:N	2.44	0.50
5:7:116:ASP:OD1	5:7:116:ASP:N	2.43	0.50
1:O:19:LEU:HA	1:P:20:LEU:HG	1.94	0.50
1:K:45:ASP:N	1:K:45:ASP:OD1	2.43	0.49
1:O:19:LEU:HD23	1:P:19:LEU:HG	1.93	0.49
3:X:223:GLU:HA	3:X:226:ILE:HB	1.94	0.49
1:N:24:ILE:HB	1:O:23:GLY:HA3	1.95	0.49
1:L:28:ILE:HA	1:L:31:ALA:HB3	1.93	0.49
6:U:57:ASP:N	6:U:57:ASP:OD1	2.40	0.49
1:K:55:PHE:O	1:K:59:GLU:N	2.45	0.49
1:R:60:ALA:HA	1:R:63:LEU:HB2	1.95	0.49
1:S:50:MET:HE1	1:T:37:VAL:HG21	1.94	0.48
1:K:70:PHE:HA	1:K:73:LEU:HD13	1.95	0.48
3:X:187:LEU:HD12	3:X:190:ILE:HD11	1.95	0.48
4:Z:64:GLY:O	4:Z:68:LEU:N	2.46	0.48
1:R:52:ILE:HA	1:R:55:PHE:HB3	1.94	0.48
1:T:28:ILE:HA	1:T:31:ALA:HB3	1.95	0.48
1:P:4:VAL:HG23	1:Q:6:ALA:HA	1.95	0.48
3:X:30:SER:OG	3:X:33:THR:OG1	2.31	0.48
1:N:47:VAL:HA	1:N:50:MET:HG2	1.96	0.48
1:T:51:ALA:O	1:T:55:PHE:N	2.46	0.48
6:U:33:SER:OG	6:U:34:LEU:N	2.47	0.47
5:7:134:THR:OG1	5:7:135:VAL:N	2.47	0.47
1:K:12:ALA:O	1:K:15:SER:OG	2.32	0.47
1:R:27:ALA:O	1:R:31:ALA:N	2.47	0.47
1:S:28:ILE:HD12	1:T:28:ILE:HG22	1.97	0.46
2:8:15:TYR:HA	2:8:18:LEU:HB3	1.97	0.46
3:X:210:PHE:HB3	3:X:213:LEU:HD13	1.98	0.46
1:R:40:ASN:N	1:R:40:ASN:OD1	2.49	0.46
1:O:51:ALA:O	1:O:55:PHE:N	2.49	0.46
1:K:27:ALA:HB1	1:T:28:ILE:HG12	1.97	0.46
1:K:39:ARG:O	1:K:39:ARG:NE	2.49	0.46
1:R:59:GLU:O	1:R:63:LEU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:66:LEU:HA	1:M:69:SER:HB2	1.98	0.46
1:T:7:ALA:HA	1:T:10:ILE:HG22	1.98	0.46
3:X:39:VAL:HG23	3:X:40:ILE:HG23	1.98	0.45
1:M:47:VAL:O	1:M:51:ALA:N	2.43	0.45
1:O:70:PHE:HA	1:O:73:LEU:HB2	1.97	0.45
1:S:49:PRO:HA	1:S:52:ILE:HG22	1.98	0.45
1:O:14:ILE:HG12	1:P:17:ILE:HD11	1.97	0.45
1:M:15:SER:OG	1:M:16:THR:N	2.49	0.45
6:U:81:GLU:HA	6:U:84:PHE:HB3	1.99	0.45
3:X:71:ASN:OD1	3:X:72:MET:N	2.50	0.45
3:X:163:THR:HA	3:X:166:TYR:HB3	1.99	0.45
1:P:47:VAL:HA	1:P:50:MET:HG2	1.99	0.44
3:X:222:LEU:O	3:X:226:ILE:N	2.49	0.44
1:R:10:ILE:HG13	1:S:10:ILE:HD13	2.00	0.44
1:T:28:ILE:O	1:T:32:ALA:N	2.50	0.44
3:X:136:LYS:HG2	3:X:137:HIS:CD2	2.53	0.44
1:N:11:GLY:O	1:N:15:SER:OG	2.36	0.44
1:L:35:ASN:HA	1:L:38:SER:HB2	1.99	0.43
5:7:165:ASP:N	5:7:165:ASP:OD1	2.50	0.43
6:U:59:ASP:OD2	6:U:59:ASP:N	2.51	0.43
1:K:1:FME:HCN	1:L:2:GLN:HA	2.00	0.43
1:N:47:VAL:HA	1:N:50:MET:HE3	2.00	0.43
1:O:30:PHE:HZ	1:O:52:ILE:HD13	1.84	0.43
1:T:40:ASN:HA	1:T:41:PRO:HD3	1.86	0.43
1:N:53:LEU:O	1:N:57:LEU:N	2.49	0.43
1:R:59:GLU:HG2	1:R:63:LEU:HG	2.01	0.43
1:N:43:ILE:HD12	1:N:43:ILE:HA	1.85	0.42
1:T:40:ASN:N	1:T:40:ASN:OD1	2.52	0.42
2:8:23:LEU:HD11	3:X:40:ILE:HD11	2.01	0.42
3:X:213:LEU:HB3	3:X:214:ALA:H	1.64	0.42
1:S:64:PHE:HB3	1:T:66:LEU:HD21	2.02	0.42
1:T:6:ALA:HA	1:T:9:TYR:CZ	2.54	0.42
1:P:68:VAL:HA	1:P:71:LEU:HB2	2.01	0.42
1:S:72:LEU:HD21	1:T:73:LEU:HD11	2.00	0.42
3:X:74:LYS:HE2	3:X:74:LYS:HB2	1.76	0.42
1:Q:63:LEU:HA	1:Q:66:LEU:HG	2.00	0.42
4:Z:84:ARG:HH22	5:7:167:PHE:HB3	1.84	0.42
5:7:137:ASP:N	5:7:137:ASP:OD1	2.52	0.42
1:N:42:SER:O	1:N:42:SER:OG	2.33	0.42
4:Z:84:ARG:HA	4:Z:84:ARG:HD2	1.94	0.42
1:S:7:ALA:HB3	1:T:6:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:69:SER:OG	1:O:70:PHE:N	2.53	0.42
3:X:38:LEU:HA	3:X:41:THR:HG22	2.01	0.42
7:J:9:ILE:HG13	7:J:10:LEU:HD12	2.01	0.42
3:X:220:MET:HE2	3:X:220:MET:HB2	1.99	0.42
1:Q:7:ALA:HA	1:Q:10:ILE:HG22	2.02	0.41
1:L:29:VAL:HG11	1:L:55:PHE:HD1	1.86	0.41
1:P:12:ALA:O	1:P:15:SER:OG	2.37	0.41
3:X:26:LEU:HB3	3:X:27:THR:H	1.66	0.41
1:N:8:LYS:HD3	1:N:72:LEU:HB2	2.02	0.41
1:K:34:ILE:O	1:K:38:SER:OG	2.28	0.41
1:K:65:CYS:O	1:K:69:SER:OG	2.28	0.41
1:O:56:ALA:O	1:O:60:ALA:N	2.54	0.41
1:R:55:PHE:O	1:R:58:SER:OG	2.31	0.41
1:S:72:LEU:HD13	1:S:72:LEU:HA	1.96	0.40
1:M:8:LYS:HA	1:M:8:LYS:HD2	1.85	0.40
1:K:20:LEU:HD23	1:L:20:LEU:HD21	2.03	0.40
3:X:214:ALA:HA	3:X:217:LEU:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	K	72/76 (95%)	64 (89%)	8 (11%)	0	100	100
1	L	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
1	M	73/76 (96%)	69 (94%)	4 (6%)	0	100	100
1	N	72/76 (95%)	65 (90%)	7 (10%)	0	100	100
1	O	72/76 (95%)	62 (86%)	10 (14%)	0	100	100
1	P	72/76 (95%)	67 (93%)	5 (7%)	0	100	100
1	Q	72/76 (95%)	70 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
1	S	72/76 (95%)	69 (96%)	3 (4%)	0	100	100
1	T	72/76 (95%)	67 (93%)	5 (7%)	0	100	100
2	8	40/48 (83%)	38 (95%)	2 (5%)	0	100	100
3	X	221/249 (89%)	203 (92%)	18 (8%)	0	100	100
4	Z	52/209 (25%)	50 (96%)	2 (4%)	0	100	100
5	7	65/173 (38%)	57 (88%)	8 (12%)	0	100	100
6	U	66/95 (70%)	58 (88%)	8 (12%)	0	100	100
7	J	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
All	All	1201/1571 (76%)	1113 (93%)	88 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	K	53/55 (96%)	53 (100%)	0	100	100
1	L	53/55 (96%)	52 (98%)	1 (2%)	50	66
1	M	53/55 (96%)	53 (100%)	0	100	100
1	N	54/55 (98%)	54 (100%)	0	100	100
1	O	54/55 (98%)	54 (100%)	0	100	100
1	P	52/55 (94%)	51 (98%)	1 (2%)	50	66
1	Q	52/55 (94%)	50 (96%)	2 (4%)	29	51
1	R	50/55 (91%)	49 (98%)	1 (2%)	48	65
1	S	53/55 (96%)	52 (98%)	1 (2%)	50	66
1	T	53/55 (96%)	53 (100%)	0	100	100
2	8	41/47 (87%)	41 (100%)	0	100	100
3	X	189/217 (87%)	188 (100%)	1 (0%)	81	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Z	37/182 (20%)	37 (100%)	0	100	100
5	7	56/158 (35%)	56 (100%)	0	100	100
6	U	45/76 (59%)	44 (98%)	1 (2%)	45	64
7	J	30/30 (100%)	30 (100%)	0	100	100
All	All	925/1260 (73%)	917 (99%)	8 (1%)	68	75

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	4	VAL
1	P	20	LEU
1	Q	20	LEU
1	Q	28	ILE
1	R	66	LEU
1	S	28	ILE
3	X	207	VAL
6	U	29	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	2	GLN
1	N	35	ASN
3	X	180	ASN
5	7	169	ASN
5	7	171	ASN
6	U	29	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	P	1	1	8,9,10	0.92	0	8,9,11	1.58	2 (25%)
1	FME	L	1	1	5,6,10	1.37	1 (20%)	4,6,11	1.65	1 (25%)
1	FME	Q	1	1	5,6,10	1.35	1 (20%)	4,6,11	1.34	1 (25%)
1	FME	O	1	1	6,7,10	1.06	0	7,7,11	1.28	1 (14%)
1	FME	K	1	1	8,9,10	0.96	0	8,9,11	1.02	1 (12%)
1	FME	N	1	1	5,6,10	1.38	1 (20%)	4,6,11	1.61	1 (25%)
1	FME	R	1	1	6,7,10	1.08	0	7,7,11	1.33	1 (14%)
1	FME	M	1	1	6,7,10	1.03	0	7,7,11	1.28	1 (14%)
1	FME	S	1	1	5,6,10	1.30	0	4,6,11	1.59	1 (25%)
1	FME	T	1	1	6,7,10	1.04	0	7,7,11	1.32	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	P	1	1	-	2/7/9/11	-
1	FME	L	1	1	-	2/3/5/11	-
1	FME	Q	1	1	-	0/3/5/11	-
1	FME	O	1	1	-	2/5/7/11	-
1	FME	K	1	1	-	4/7/9/11	-
1	FME	N	1	1	-	0/3/5/11	-
1	FME	R	1	1	-	2/5/7/11	-
1	FME	M	1	1	-	3/5/7/11	-
1	FME	S	1	1	-	1/3/5/11	-
1	FME	T	1	1	-	2/5/7/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	1	FME	CA-N	-2.29	1.44	1.46
1	L	1	FME	CA-N	-2.27	1.44	1.46
1	Q	1	FME	CA-N	-2.13	1.44	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	1	FME	C-CA-N	3.16	115.60	109.50
1	N	1	FME	CB-CA-N	2.89	112.94	109.68
1	L	1	FME	CB-CA-N	2.80	112.84	109.68
1	S	1	FME	CB-CA-N	2.68	112.70	109.68
1	P	1	FME	CA-N-CN	2.61	126.84	122.82
1	R	1	FME	CB-CA-C	-2.33	107.00	112.62
1	Q	1	FME	CB-CA-N	2.30	112.27	109.68
1	T	1	FME	CB-CA-C	-2.26	107.16	112.62
1	M	1	FME	CB-CA-C	-2.23	107.23	112.62
1	O	1	FME	CB-CA-C	-2.15	107.42	112.62
1	K	1	FME	C-CA-N	2.13	113.62	109.50

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	K	1	FME	N-CA-CB-CG
1	K	1	FME	C-CA-CB-CG
1	L	1	FME	O-C-CA-CB
1	M	1	FME	N-CA-CB-CG
1	M	1	FME	C-CA-CB-CG
1	M	1	FME	O-C-CA-CB
1	P	1	FME	N-CA-CB-CG
1	R	1	FME	N-CA-CB-CG
1	R	1	FME	C-CA-CB-CG
1	S	1	FME	O-C-CA-CB
1	T	1	FME	N-CA-CB-CG
1	T	1	FME	C-CA-CB-CG
1	K	1	FME	CB-CG-SD-CE
1	O	1	FME	N-CA-CB-CG
1	O	1	FME	C-CA-CB-CG
1	P	1	FME	C-CA-CB-CG
1	K	1	FME	CB-CA-N-CN
1	L	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	K	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

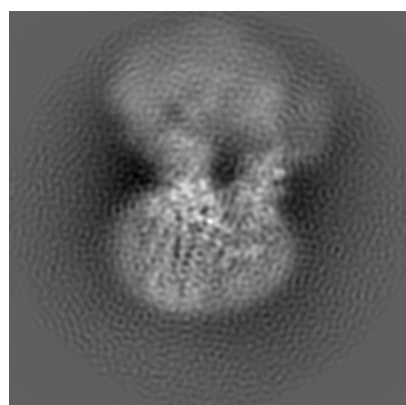
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21894. These allow visual inspection of the internal detail of the map and identification of artifacts.

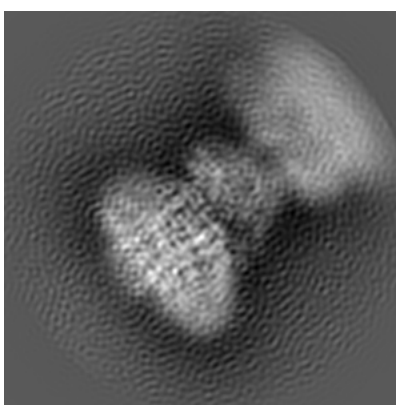
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

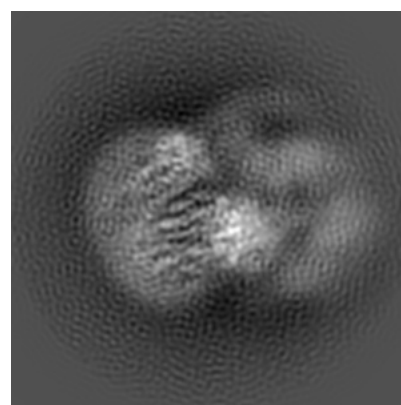
6.1.1 Primary map



X



Y

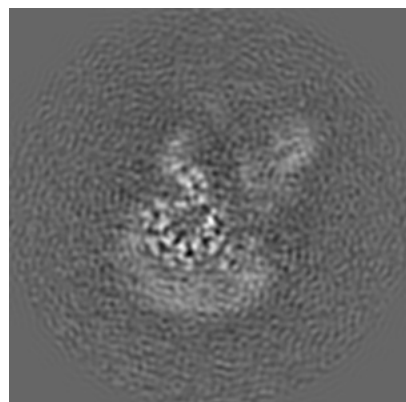


Z

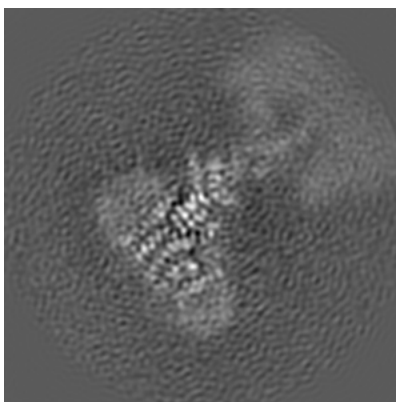
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

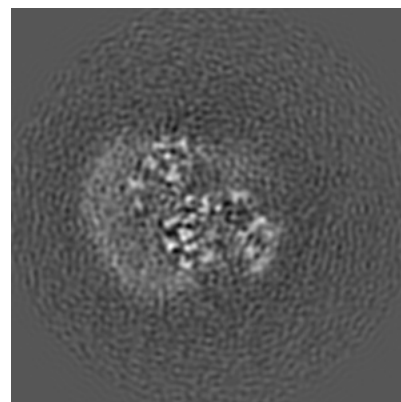
6.2.1 Primary map



X Index: 96



Y Index: 96

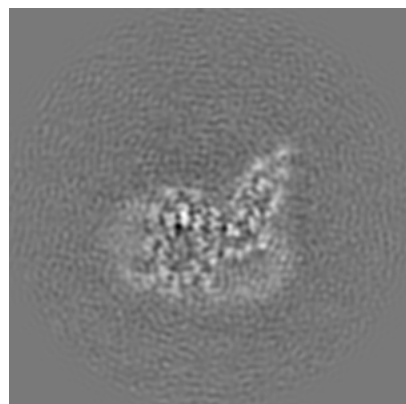


Z Index: 96

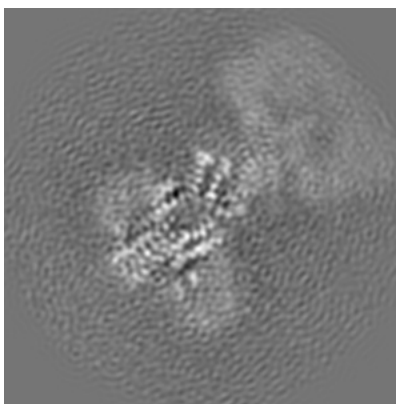
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

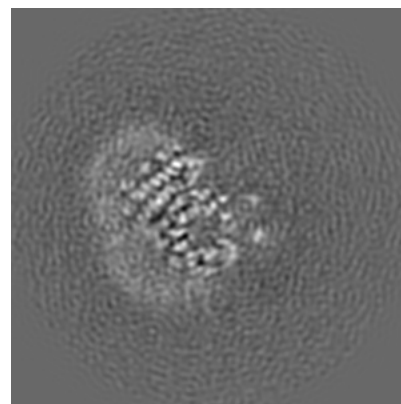
6.3.1 Primary map



X Index: 81



Y Index: 89

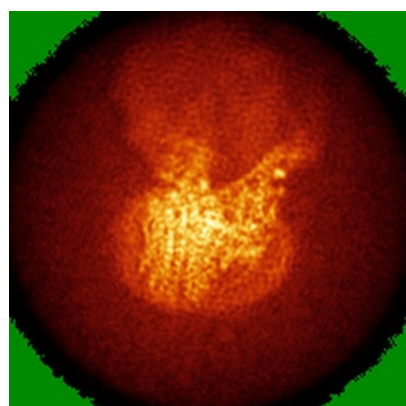


Z Index: 88

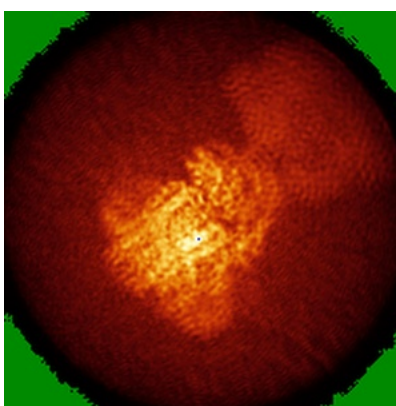
The images above show the largest variance slices of the map in three orthogonal directions.

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

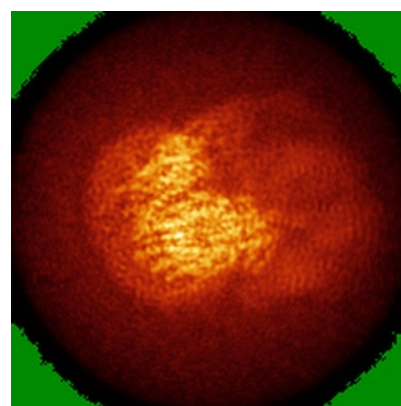
6.4.1 Primary map



X



Y

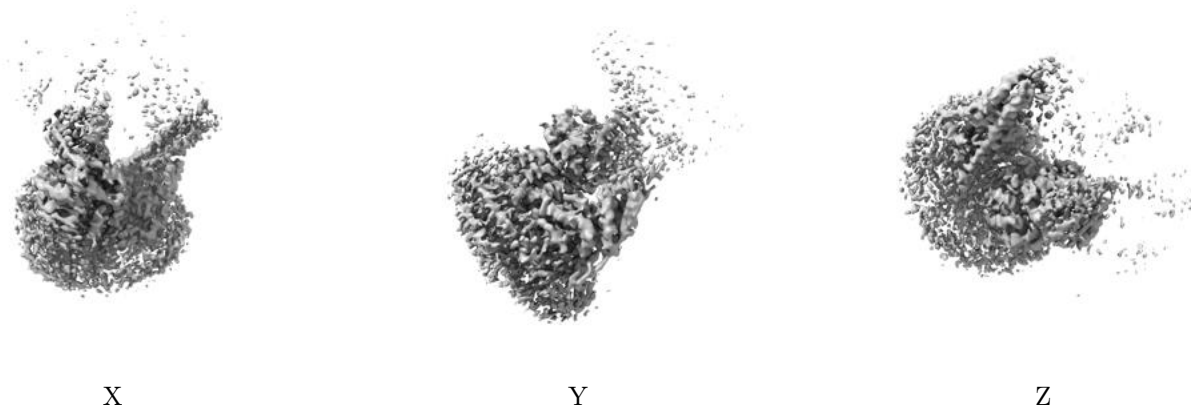


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.043. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

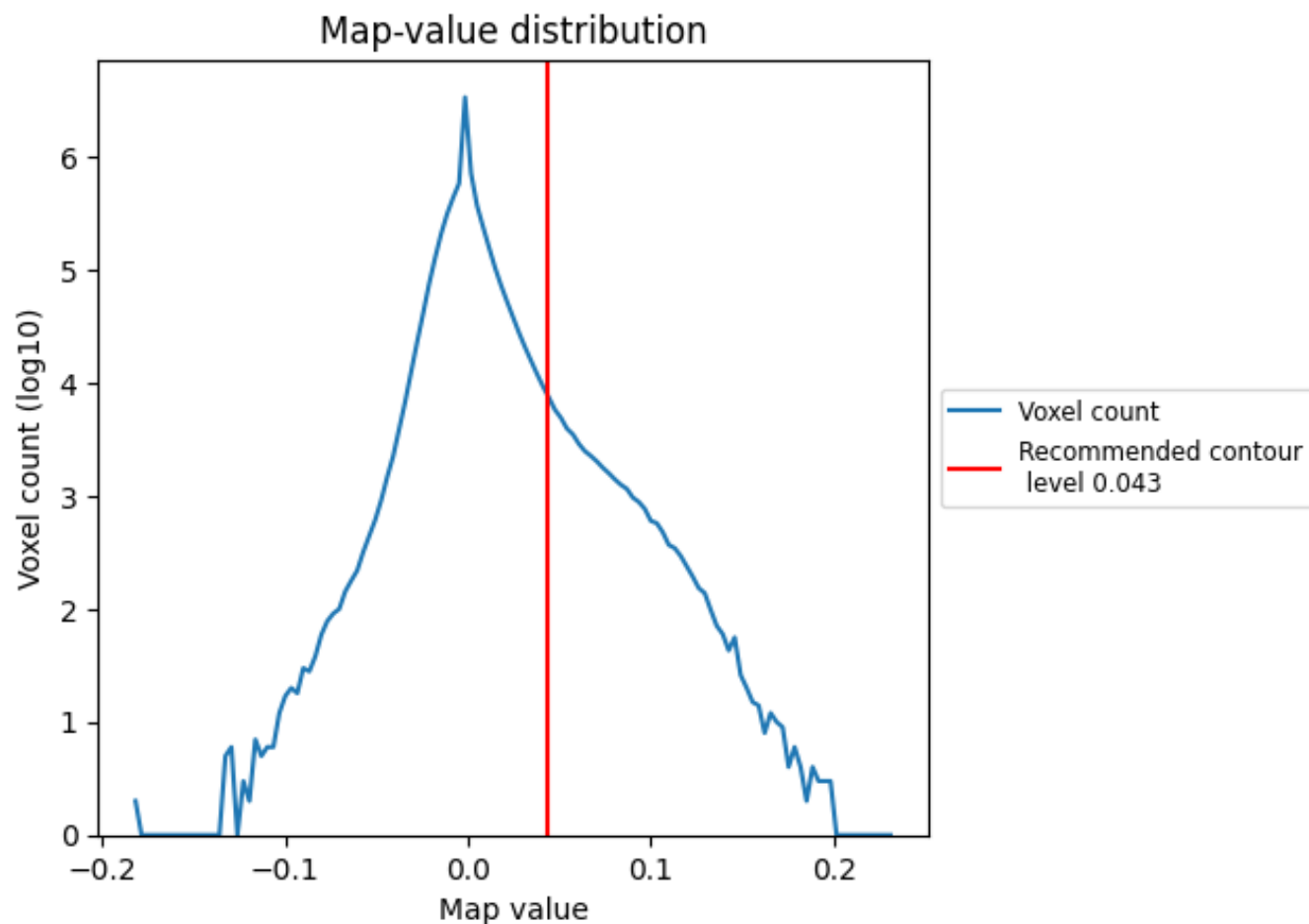
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

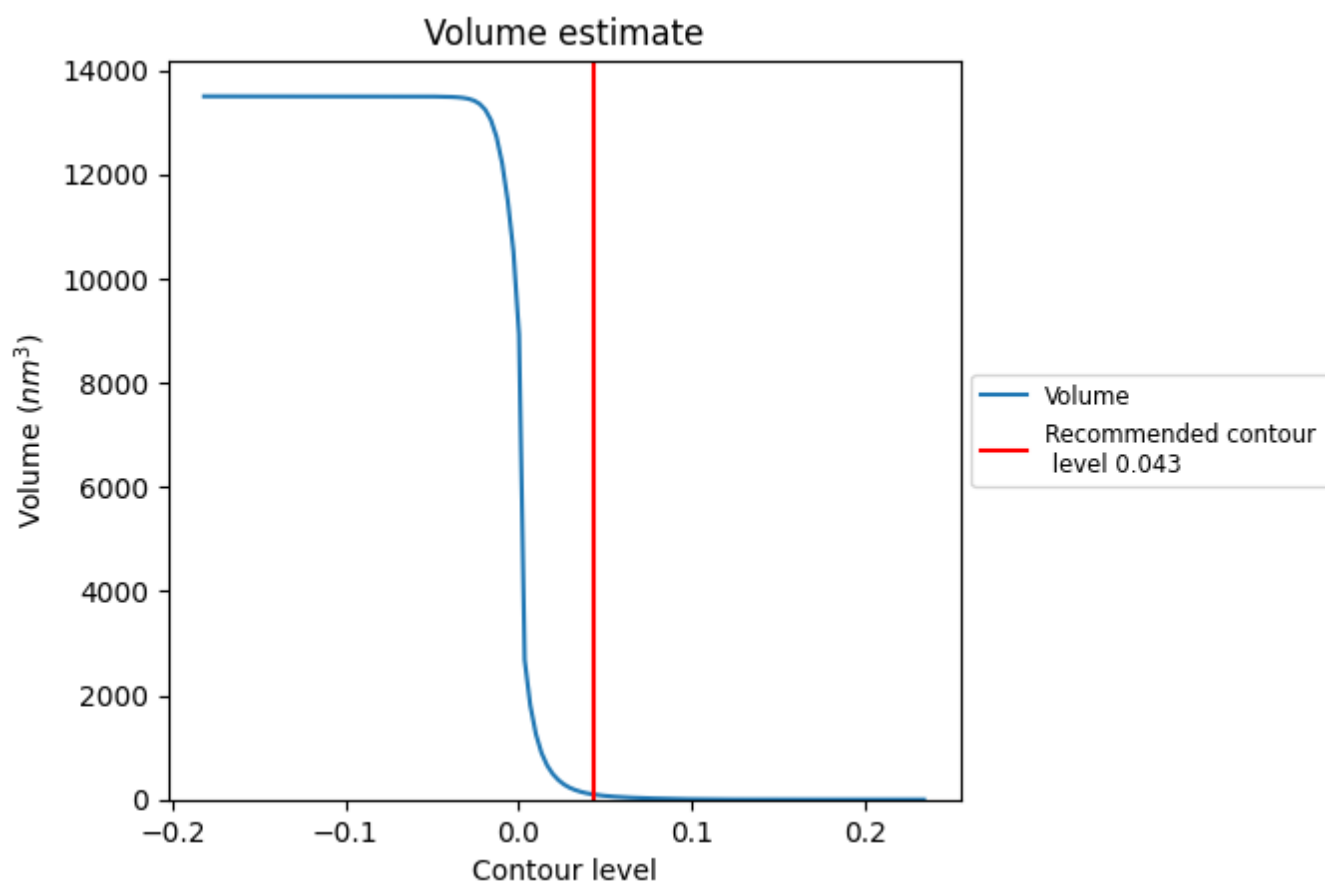
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

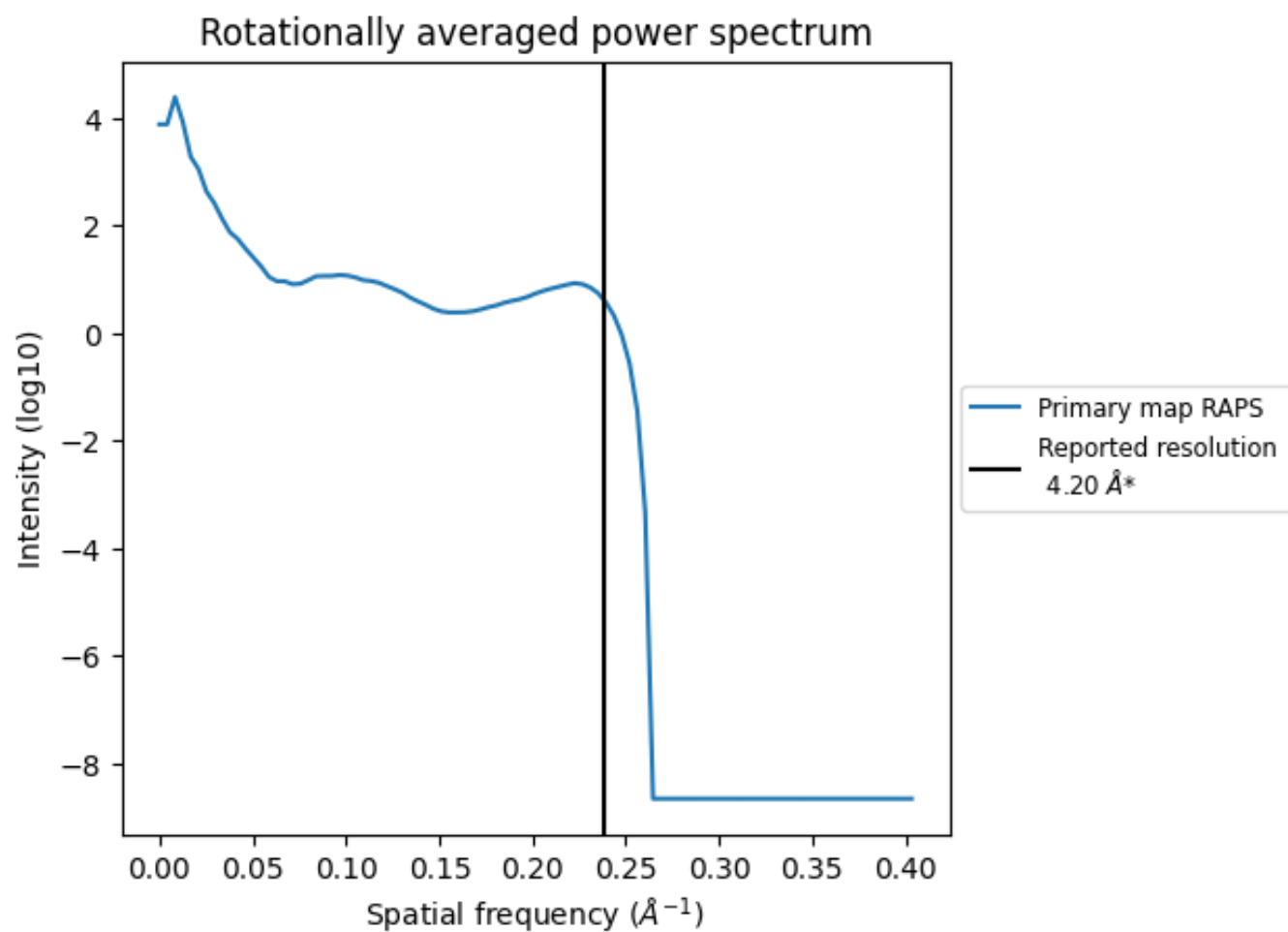
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 100 nm³; this corresponds to an approximate mass of 90 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 0.238 Å⁻¹

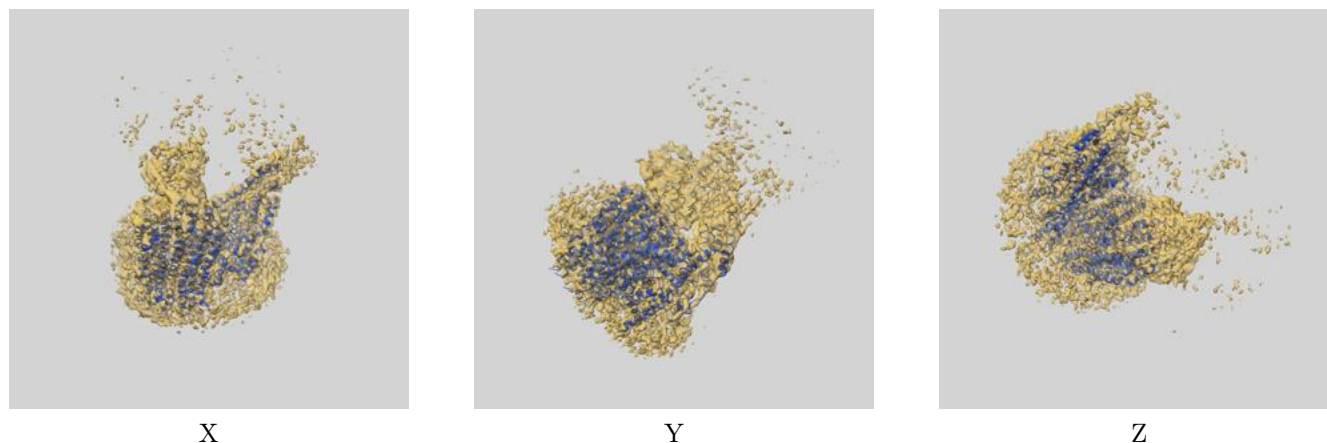
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

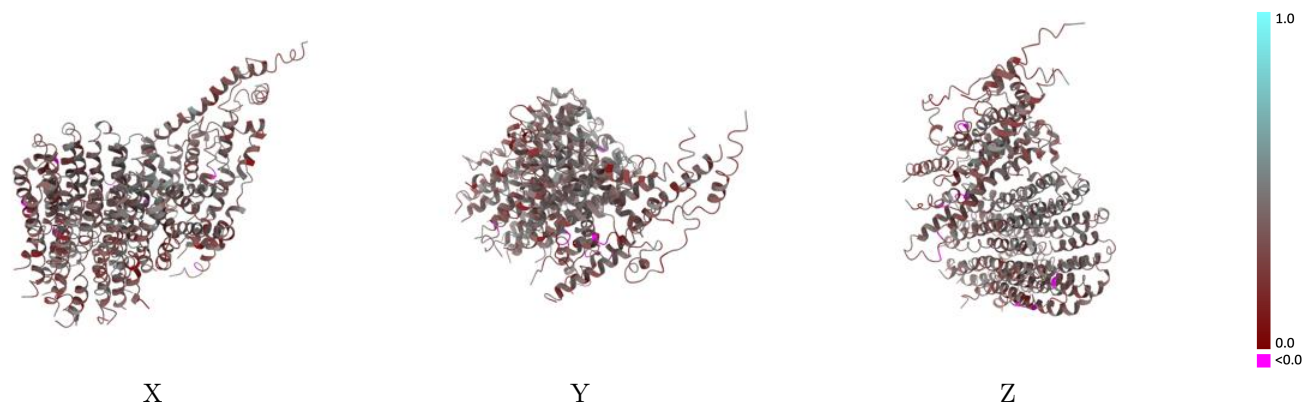
This section contains information regarding the fit between EMDB map EMD-21894 and PDB model 6WTD. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.043 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

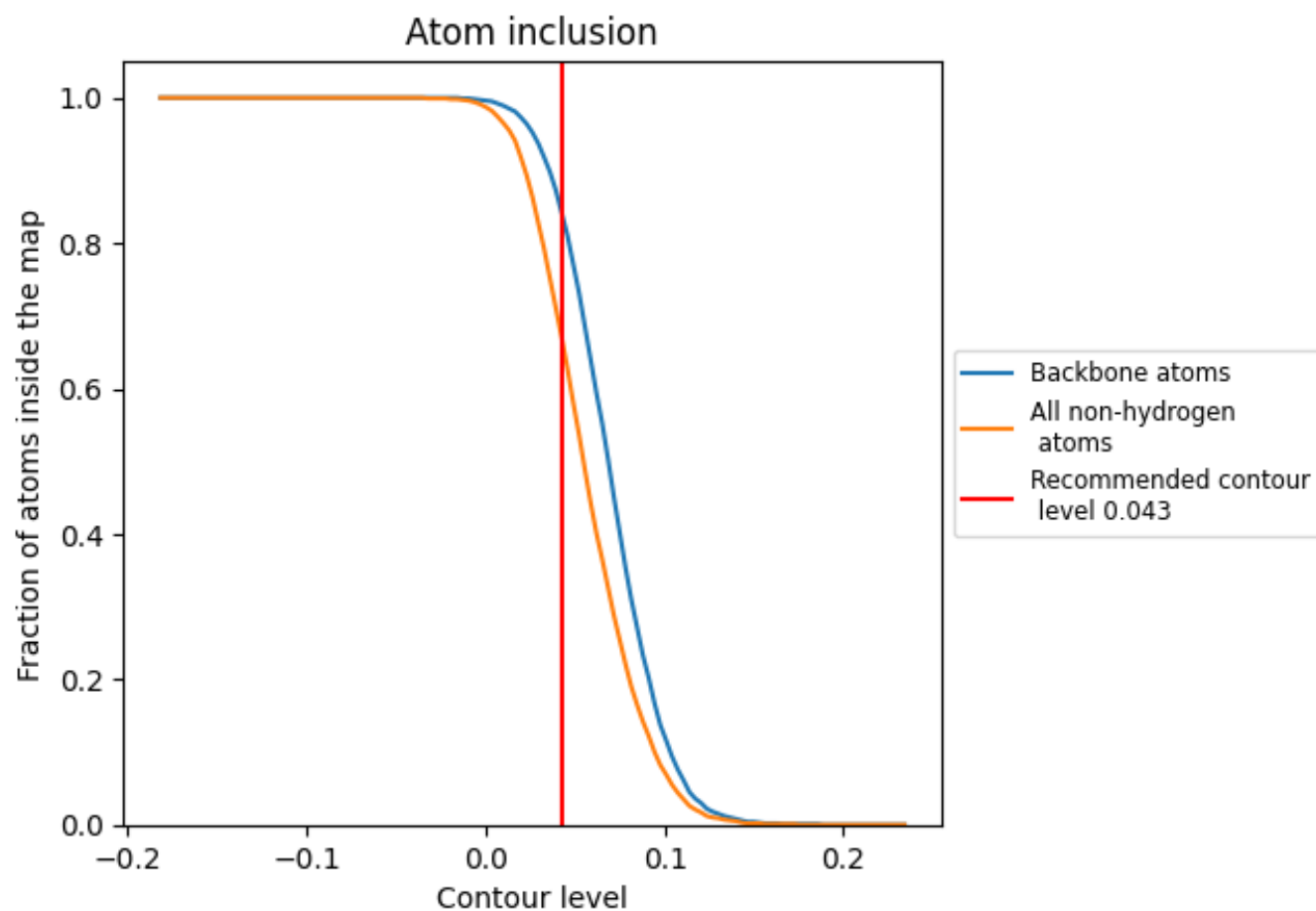


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 66% 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 (0.043) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6640	 0.3520
7	 0.6850	 0.3350
8	 0.7450	 0.3730
J	 0.5980	 0.3420
K	 0.6460	 0.3500
L	 0.6220	 0.3540
M	 0.6500	 0.3420
N	 0.6900	 0.3400
O	 0.6130	 0.3080
P	 0.6120	 0.3350
Q	 0.6710	 0.3740
R	 0.6990	 0.3680
S	 0.7070	 0.4240
T	 0.7030	 0.4100
U	 0.6790	 0.3430
X	 0.6510	 0.3370
Z	 0.6860	 0.3230

