



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 03:06 PM UTC

PDB ID : 7TKA / pdb_00007tka
EMDB ID : EMD-25962
Title : Yeast ATP synthase State 1catalytic(e) with 10 mM ATP backbone model
Authors : Guo, H.; Rubinstein, J.L.
Deposited on : 2022-01-17
Resolution : 7.10 Å(reported)
Based on initial model : 2HLD

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

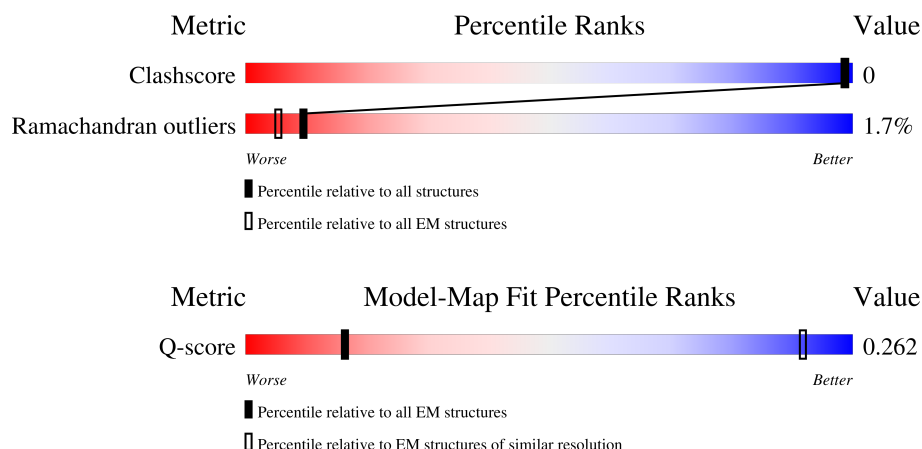
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 7.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	464 (6.60 - 7.60)

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

Mol	Chain	Length	Quality of chain
1	0	76	11% 91% 8%
1	1	76	22% 91% 8%
1	2	76	25% 93% 5%
1	3	76	5% 92% 5%
1	4	76	25% 93% 5%

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Mol	Chain	Length	Quality of chain
1	5	76	
1	6	76	
1	7	76	
1	8	76	
1	9	76	
2	A	510	
2	B	510	
2	C	510	
3	D	478	
3	E	478	
3	F	478	
4	G	278	
5	H	138	
6	I	61	
7	O	195	
8	T	249	
9	U	209	
10	V	173	
11	W	95	
12	X	92	
13	Y	59	
14	Z	48	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 20228 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	0	75	Total	C	N	O	0	0
			300	150	75	75		
1	1	75	Total	C	N	O	0	0
			300	150	75	75		
1	2	75	Total	C	N	O	0	0
			300	150	75	75		
1	3	74	Total	C	N	O	0	0
			296	148	74	74		
1	4	75	Total	C	N	O	0	0
			300	150	75	75		
1	5	75	Total	C	N	O	0	0
			300	150	75	75		
1	6	74	Total	C	N	O	0	0
			296	148	74	74		
1	7	73	Total	C	N	O	0	0
			292	146	73	73		
1	8	75	Total	C	N	O	0	0
			300	150	75	75		
1	9	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 2 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	A	499	Total	C	N	O	0	0
			1996	998	499	499		
2	B	505	Total	C	N	O	0	0
			2020	1010	505	505		
2	C	498	Total	C	N	O	0	0
			1992	996	498	498		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	470	Total	C	N	O	0	0
			1880	940	470	470		
3	E	468	Total	C	N	O	0	0
			1872	936	468	468		
3	F	469	Total	C	N	O	0	0
			1876	938	469	469		

- Molecule 4 is a protein called ATP synthase subunit gamma.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	265	Total	C	N	O	0	0
			1060	530	265	265		

- Molecule 5 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	120	Total	C	N	O	0	0
			480	240	120	120		

- Molecule 6 is a protein called ATP synthase subunit epsilon.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	I	48	Total	C	N	O	0	0
			193	96	48	49		

- Molecule 7 is a protein called ATP synthase subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	187	Total	C	N	O	0	0
			748	374	187	187		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	T	224	Total	C	N	O	0	0
			897	448	224	225		

- Molecule 9 is a protein called ATP synthase subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	U	155	Total	C	N	O	0	0
			620	310	155	155		

- Molecule 10 is a protein called ATP synthase subunit d.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	V	171	Total	C	N	O	0	0
			685	342	171	172		

- Molecule 11 is a protein called ATP synthase subunit f.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	W	85	Total	C	N	O	0	0
			340	170	85	85		

- Molecule 12 is a protein called ATP synthase subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	X	62	Total	C	N	O	0	0
			248	124	62	62		

- Molecule 13 is a protein called ATP synthase subunit J.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Y	37	Total	C	N	O	0	0
			148	74	37	37		

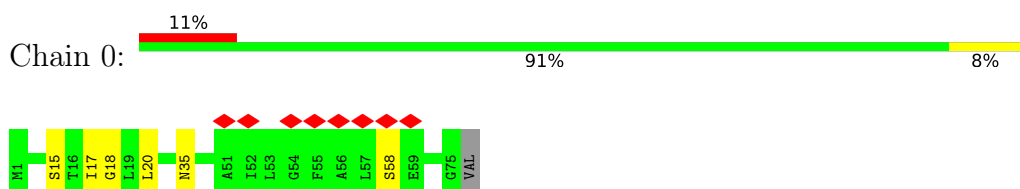
- Molecule 14 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	Z	48	Total	C	N	O	0	0
			193	96	48	49		

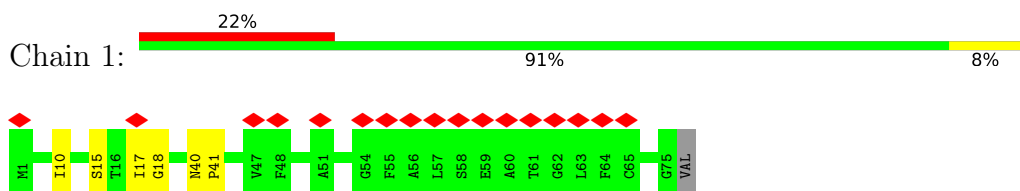
3 Residue-property plots [i](#)

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.

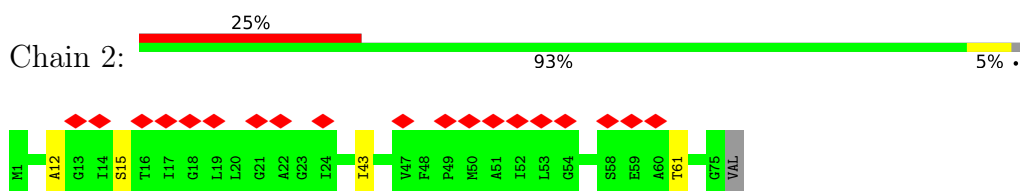
- Molecule 1: ATP synthase subunit 9, mitochondrial



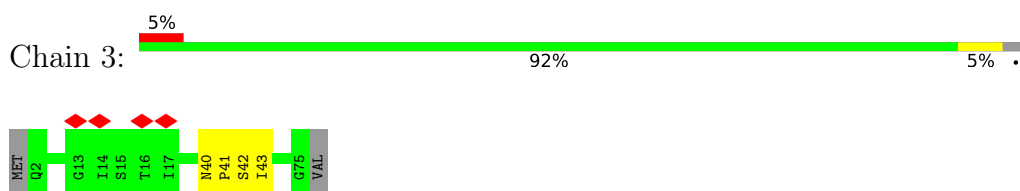
- Molecule 1: ATP synthase subunit 9, mitochondrial



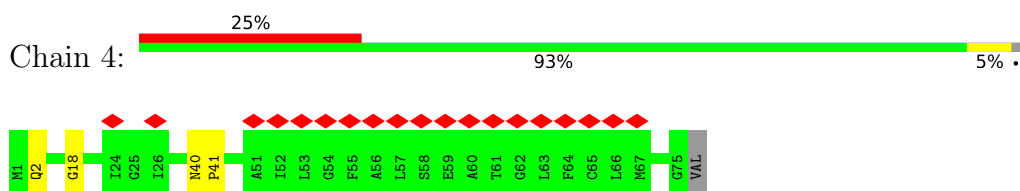
- Molecule 1: ATP synthase subunit 9, mitochondrial



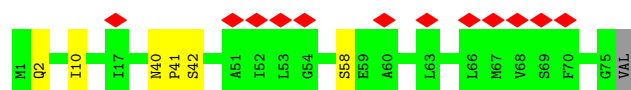
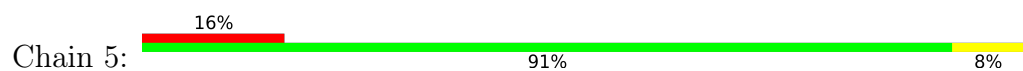
- Molecule 1: ATP synthase subunit 9, mitochondrial



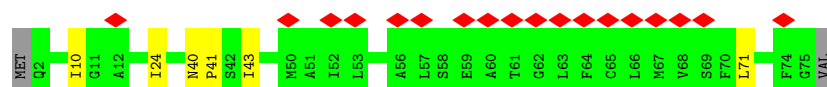
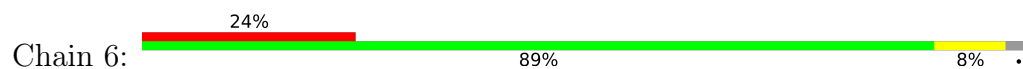
- Molecule 1: ATP synthase subunit 9, mitochondrial



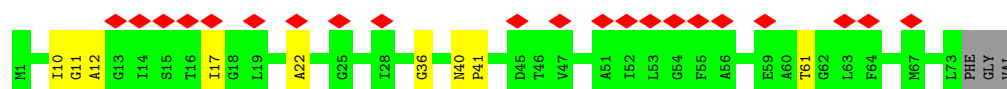
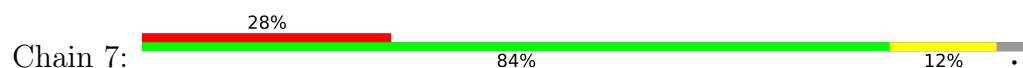
- Molecule 1: ATP synthase subunit 9, mitochondrial



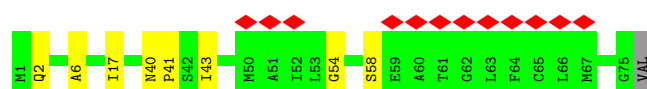
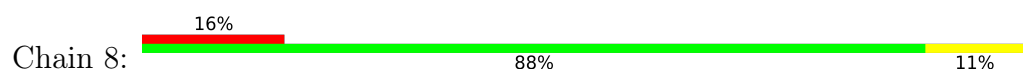
- Molecule 1: ATP synthase subunit 9, mitochondrial



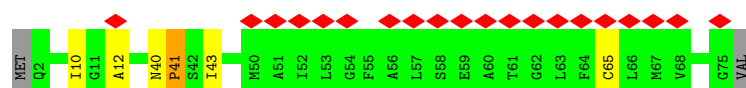
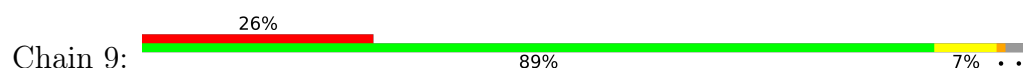
- Molecule 1: ATP synthase subunit 9, mitochondrial



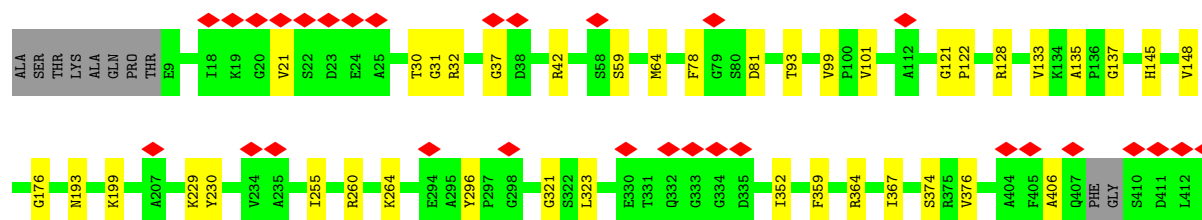
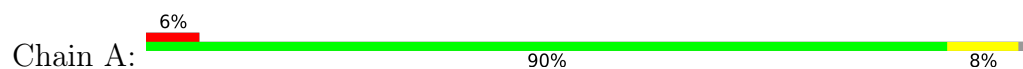
- Molecule 1: ATP synthase subunit 9, mitochondrial

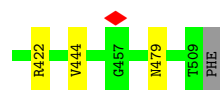


- Molecule 1: ATP synthase subunit 9, mitochondrial

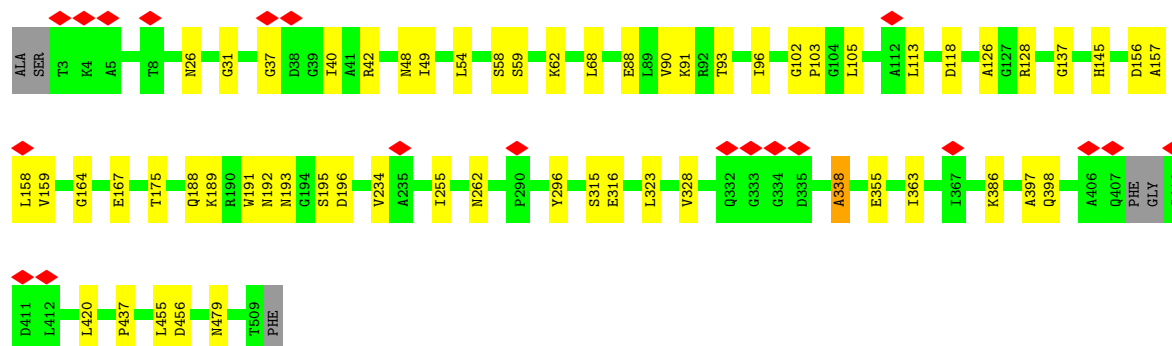
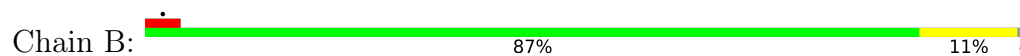


- Molecule 2: ATP synthase subunit alpha

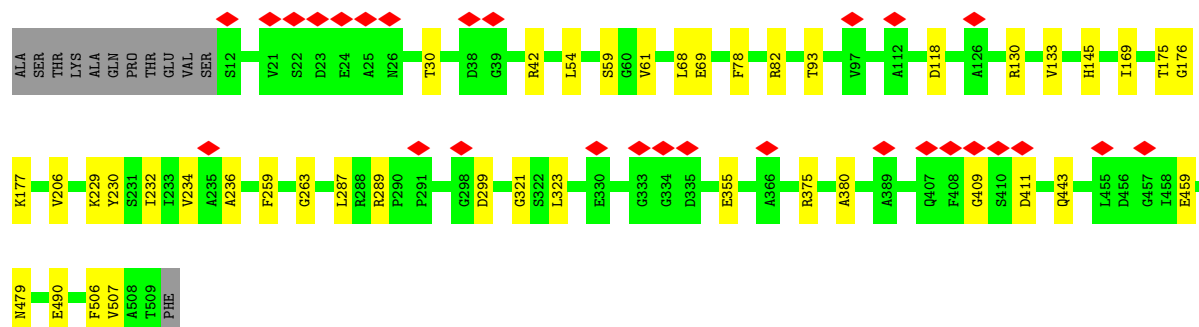
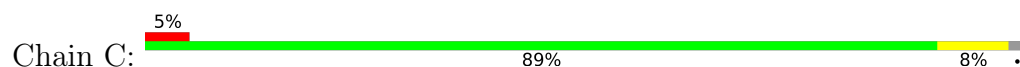




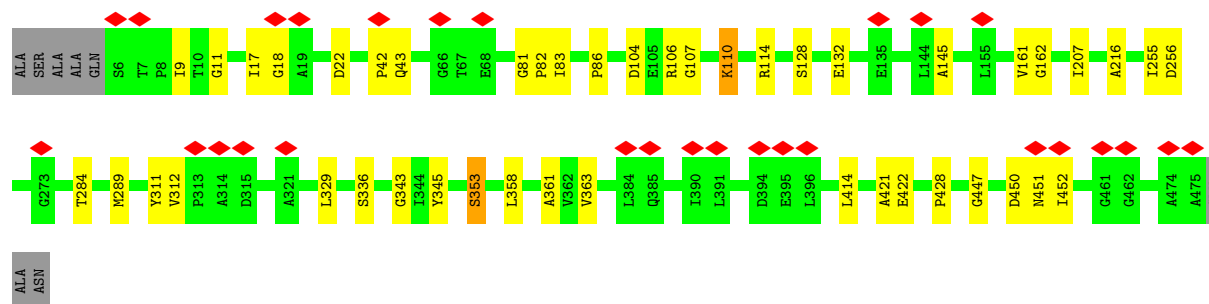
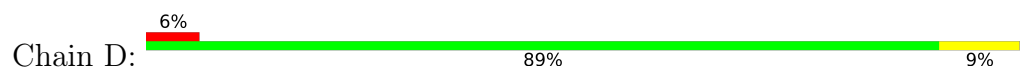
• Molecule 2: ATP synthase subunit alpha



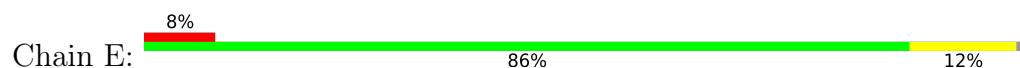
• Molecule 2: ATP synthase subunit alpha

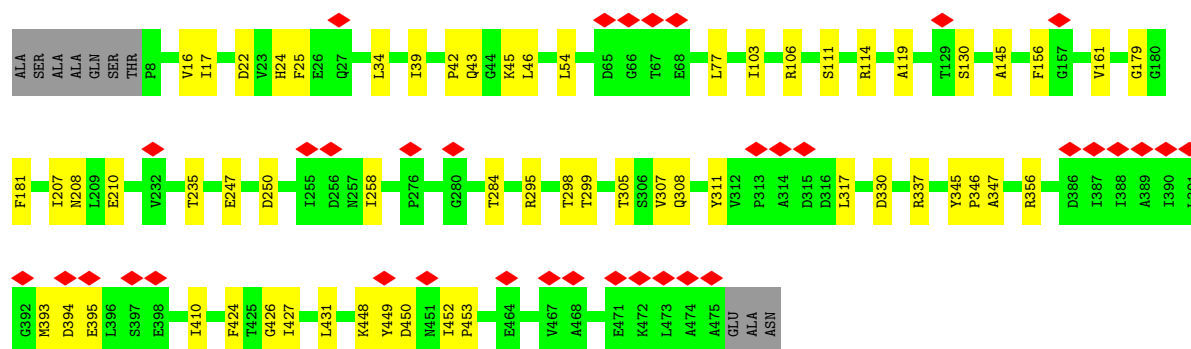


• Molecule 3: ATP synthase subunit beta



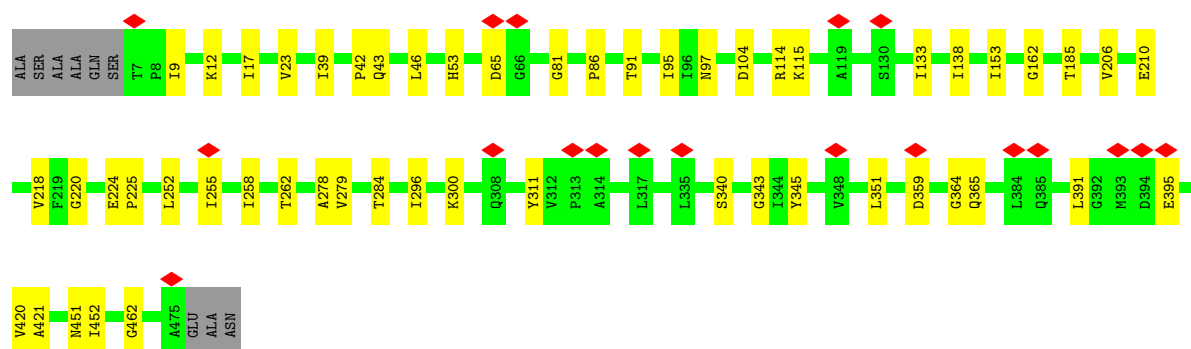
• Molecule 3: ATP synthase subunit beta





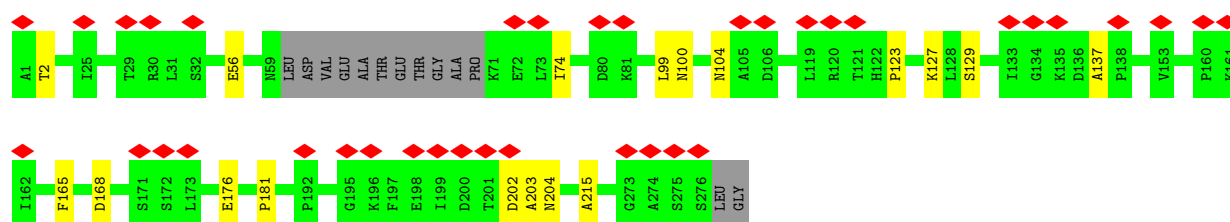
- Molecule 3: ATP synthase subunit beta

Chain F: 87% 11% .



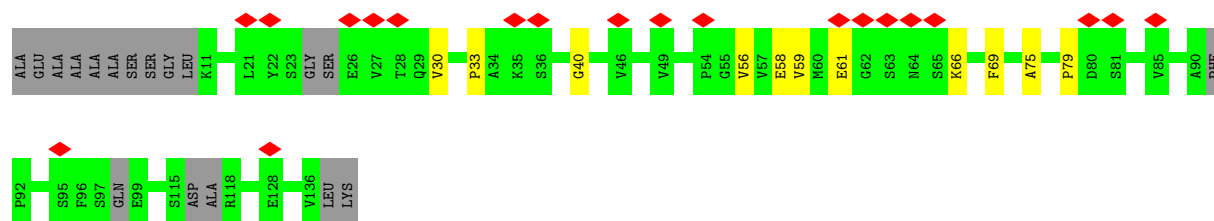
- Molecule 4: ATP synthase subunit gamma

Chain G: 13% 89% 6% 5%

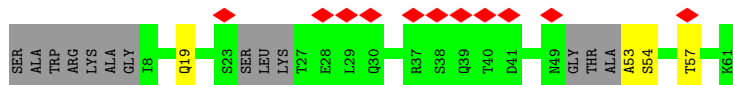


- Molecule 5: ATP synthase subunit delta

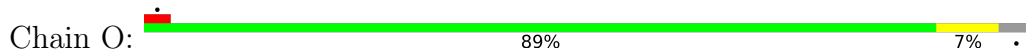
Chain H: 14% 79% 8% 13%



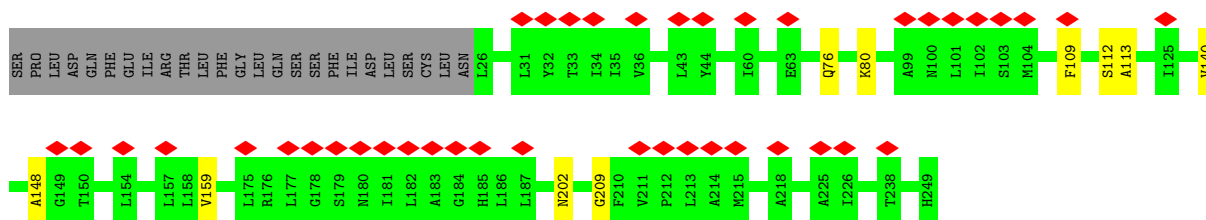
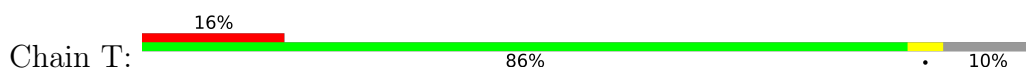
- Molecule 6: ATP synthase subunit epsilon



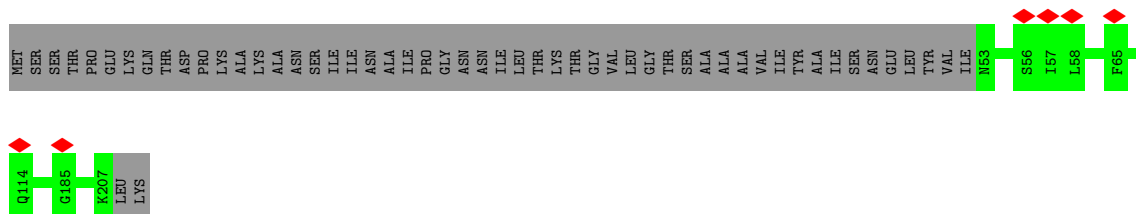
• Molecule 7: ATP synthase subunit 5



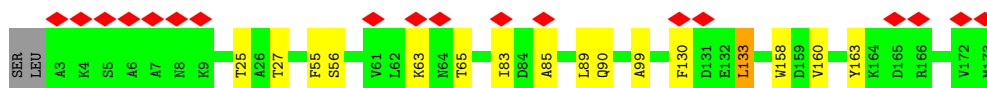
• Molecule 8: ATP synthase subunit a



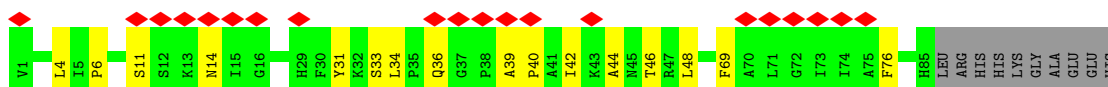
• Molecule 9: ATP synthase subunit 4



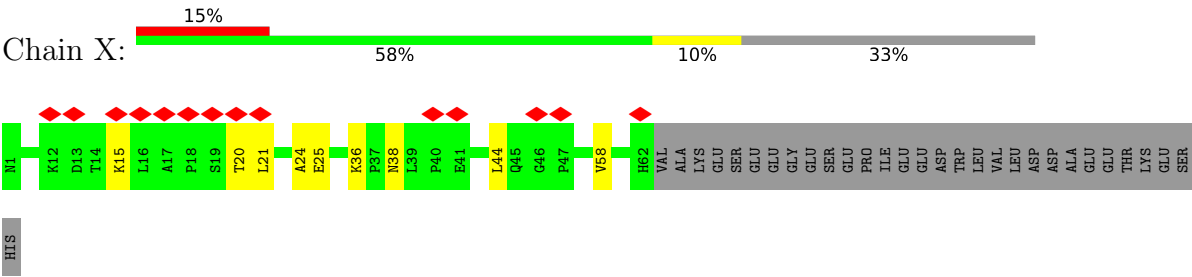
• Molecule 10: ATP synthase subunit d



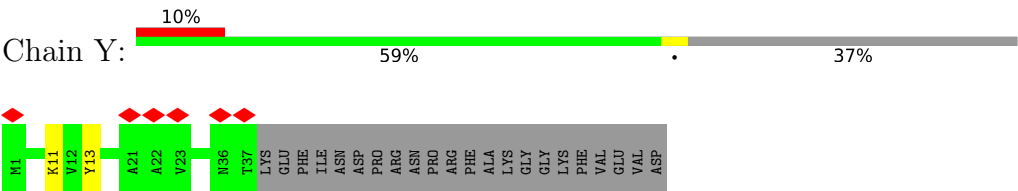
• Molecule 11: ATP synthase subunit f



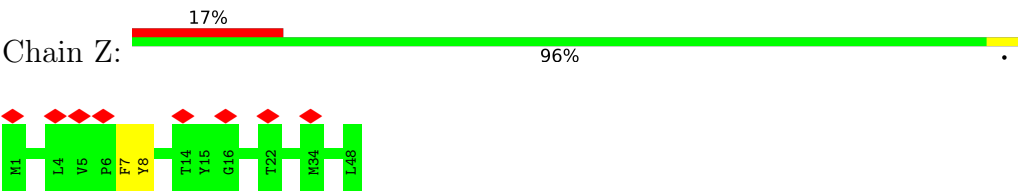
● Molecule 12: ATP synthase subunit H



● Molecule 13: ATP synthase subunit J



● Molecule 14: ATP synthase protein 8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	9849	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	103896	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.648	Depositor
Minimum map value	-0.508	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	0.62	Depositor
Map size (Å)	344.96, 344.96, 344.96	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3475, 1.3475, 1.3475	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	0	1.27	0/299	2.19	11/372 (3.0%)
1	1	1.22	0/299	2.10	8/372 (2.2%)
1	2	1.21	0/299	2.19	8/372 (2.2%)
1	3	1.23	0/295	2.00	2/367 (0.5%)
1	4	1.23	0/299	2.09	4/372 (1.1%)
1	5	1.22	0/299	2.12	7/372 (1.9%)
1	6	1.24	0/295	2.27	8/367 (2.2%)
1	7	1.20	0/291	2.30	14/362 (3.9%)
1	8	1.24	0/299	2.32	12/372 (3.2%)
1	9	1.22	0/295	2.20	9/367 (2.5%)
2	A	1.56	1/1994 (0.1%)	1.92	46/2489 (1.8%)
2	B	1.55	1/2018 (0.0%)	1.92	58/2519 (2.3%)
2	C	1.55	0/1991	1.92	40/2487 (1.6%)
3	D	1.55	1/1879 (0.1%)	1.92	44/2347 (1.9%)
3	E	1.56	0/1871	2.00	62/2337 (2.7%)
3	F	1.54	1/1875 (0.1%)	1.96	51/2342 (2.2%)
4	G	1.45	0/1058	2.01	17/1319 (1.3%)
5	H	1.53	0/475	1.95	10/585 (1.7%)
6	I	1.31	0/190	1.85	4/231 (1.7%)
7	O	1.55	0/747	1.94	10/932 (1.1%)
8	T	1.26	0/896	1.70	7/1117 (0.6%)
9	U	1.32	0/619	1.82	0/772
10	V	1.41	0/684	1.82	9/852 (1.1%)
11	W	1.30	0/339	1.93	14/422 (3.3%)
12	X	1.41	0/247	2.16	9/307 (2.9%)
13	Y	1.37	0/147	1.88	2/182 (1.1%)
14	Z	1.30	0/192	1.86	3/237 (1.3%)
All	All	1.47	4/20192 (0.0%)	1.96	469/25172 (1.9%)

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	1	0	1
1	3	0	1
1	4	0	1
1	5	0	1
1	6	0	1
1	7	0	1
1	8	0	1
1	9	0	1
3	D	0	1
3	F	0	1
All	All	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	391	LEU	CA-C	-7.51	1.49	1.53
2	A	321	GLY	CA-C	-6.50	1.45	1.52
3	D	11	GLY	CA-C	-6.01	1.46	1.51
2	B	323	LEU	CA-C	-5.12	1.48	1.53

All (469) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	204	ASN	CA-C-N	10.55	126.89	120.24
4	G	204	ASN	C-N-CA	10.55	126.89	120.24
2	B	398	GLN	N-CA-C	-9.87	101.38	113.41
2	A	376	VAL	N-CA-C	-9.71	103.96	112.12
3	F	95	ILE	N-CA-C	-9.38	94.98	108.11
3	D	361	ALA	N-CA-C	-9.28	104.04	114.62
3	F	225	PRO	CA-C-O	-8.47	114.80	120.90
3	D	311	TYR	N-CA-C	-8.34	95.31	108.90
3	D	9	ILE	N-CA-C	-8.26	95.20	107.51
3	E	103	ILE	N-CA-C	-8.15	104.93	112.43
3	E	208	ASN	N-CA-C	-8.13	95.03	108.76
3	F	162	GLY	N-CA-C	-8.10	104.68	115.21
7	O	98	LEU	N-CA-C	-7.99	102.57	112.88
2	C	355	GLU	CA-C-N	7.97	130.96	120.28
2	C	355	GLU	C-N-CA	7.97	130.96	120.28
3	D	162	GLY	N-CA-C	-7.77	103.83	115.32
2	C	78	PHE	N-CA-C	-7.60	103.98	113.55
4	G	104	ASN	N-CA-C	-7.56	104.58	113.88
7	O	101	PHE	N-CA-C	-7.54	102.90	112.93
5	H	61	GLU	N-CA-C	-7.52	96.00	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	93	THR	N-CA-C	-7.48	103.21	111.36
3	E	356	ARG	N-CA-C	-7.36	104.44	113.50
7	O	179	SER	N-CA-C	-7.33	99.06	110.42
5	H	69	PHE	N-CA-C	-7.30	97.00	108.90
2	B	175	THR	N-CA-C	-7.24	105.30	112.97
1	9	43	ILE	CA-C-N	7.23	129.97	120.28
1	9	43	ILE	C-N-CA	7.23	129.97	120.28
2	A	255	ILE	CA-C-N	7.14	127.90	119.98
2	A	255	ILE	C-N-CA	7.14	127.90	119.98
2	C	93	THR	N-CA-C	-7.11	103.61	111.36
1	1	10	ILE	CA-C-N	7.10	129.01	120.14
1	1	10	ILE	C-N-CA	7.10	129.01	120.14
3	E	17	ILE	N-CA-C	-7.08	97.65	107.99
2	A	352	ILE	N-CA-C	-7.08	97.92	108.12
3	D	422	GLU	N-CA-C	-7.05	103.34	112.23
3	F	43	GLN	N-CA-C	-7.05	103.99	112.59
5	H	56	VAL	N-CA-C	-7.04	97.47	107.75
3	F	17	ILE	N-CA-C	-6.99	97.03	107.37
8	T	80	LYS	N-CA-C	-6.99	103.04	112.26
3	E	161	VAL	N-CA-C	-6.98	104.77	112.80
3	D	284	THR	N-CA-C	-6.98	104.76	112.72
2	B	188	GLN	N-CA-C	-6.95	104.72	112.57
2	C	234	VAL	N-CA-C	-6.92	98.48	108.17
2	C	230	TYR	N-CA-C	-6.91	105.13	113.97
2	B	128	ARG	N-CA-C	-6.90	98.60	109.50
3	D	414	LEU	N-CA-C	-6.85	104.92	113.55
10	V	163	TYR	N-CA-C	-6.84	104.97	113.38
2	B	323	LEU	N-CA-C	-6.83	95.32	107.28
2	A	30	THR	N-CA-C	-6.83	99.03	109.41
2	B	164	GLY	N-CA-C	-6.82	106.06	114.92
2	A	78	PHE	N-CA-C	-6.80	105.02	113.38
2	B	96	ILE	N-CA-C	-6.78	102.55	110.21
3	E	345	TYR	N-CA-C	-6.78	97.82	109.15
3	E	22	ASP	N-CA-C	-6.78	98.67	109.59
13	Y	11	LYS	N-CA-C	-6.77	106.91	114.62
2	B	455	LEU	N-CA-C	-6.73	104.69	113.17
2	C	206	VAL	N-CA-C	-6.71	98.71	108.11
1	8	43	ILE	CA-C-N	6.71	129.57	120.38
1	8	43	ILE	C-N-CA	6.71	129.57	120.38
4	G	168	ASP	N-CA-C	-6.71	101.20	109.65
7	O	176	VAL	N-CA-C	-6.66	98.54	108.12
3	F	39	ILE	N-CA-C	-6.64	98.86	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	71	LEU	CA-C-N	6.63	129.06	120.44
1	6	71	LEU	C-N-CA	6.63	129.06	120.44
2	C	42	ARG	N-CA-C	-6.63	96.54	108.48
5	H	66	LYS	N-CA-C	-6.63	98.16	109.24
1	6	10	ILE	CA-C-N	6.63	127.34	119.98
1	6	10	ILE	C-N-CA	6.63	127.34	119.98
7	O	154	LYS	N-CA-C	-6.63	98.40	109.07
3	E	24	HIS	N-CA-C	-6.62	98.41	109.07
2	C	69	GLU	N-CA-C	-6.61	99.98	110.10
5	H	79	PRO	N-CA-C	-6.60	107.81	114.68
2	C	82	ARG	N-CA-C	-6.60	104.85	113.17
1	5	2	GLN	N-CA-C	-6.59	104.02	111.14
2	C	30	THR	N-CA-C	-6.59	98.70	108.79
3	E	43	GLN	N-CA-C	-6.59	104.82	112.92
3	D	289	MET	CA-C-N	6.58	127.28	119.98
3	D	289	MET	C-N-CA	6.58	127.28	119.98
2	B	193	ASN	N-CA-C	-6.56	97.49	109.56
2	A	193	ASN	CA-C-N	6.55	126.21	119.92
2	A	193	ASN	C-N-CA	6.55	126.21	119.92
2	A	128	ARG	N-CA-C	-6.54	97.75	108.41
2	B	355	GLU	CA-C-N	6.53	129.03	120.28
2	B	355	GLU	C-N-CA	6.53	129.03	120.28
3	E	424	PHE	N-CA-C	6.47	118.41	111.36
3	F	224	GLU	CA-C-N	6.47	124.38	119.66
3	F	224	GLU	C-N-CA	6.47	124.38	119.66
2	C	133	VAL	N-CA-C	-6.46	99.42	108.27
2	B	40	ILE	N-CA-C	-6.46	98.35	108.81
3	F	421	ALA	N-CA-C	-6.45	104.03	112.41
2	C	507	VAL	N-CA-C	-6.44	103.55	112.50
2	B	62	LYS	N-CA-C	-6.41	99.37	109.50
4	G	74	ILE	N-CA-C	-6.40	98.90	108.12
3	F	206	VAL	N-CA-C	-6.36	104.29	110.72
3	E	337	ARG	N-CA-C	-6.36	105.35	113.23
3	D	22	ASP	N-CA-C	-6.32	99.91	109.95
12	X	21	LEU	CA-C-N	6.30	128.72	120.28
12	X	21	LEU	C-N-CA	6.30	128.72	120.28
2	A	479	ASN	N-CA-C	-6.30	105.59	113.28
3	E	250	ASP	N-CA-C	-6.30	99.01	109.46
2	B	90	VAL	N-CA-C	-6.28	99.38	108.17
3	E	179	GLY	N-CA-C	-6.27	105.73	116.01
1	7	12	ALA	CA-C-N	6.25	126.88	119.94
1	7	12	ALA	C-N-CA	6.25	126.88	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	25	PHE	N-CA-C	-6.25	99.71	109.72
3	F	114	ARG	N-CA-C	-6.25	99.02	109.07
3	F	53	HIS	N-CA-C	-6.22	99.06	109.07
3	F	104	ASP	N-CA-C	-6.22	105.34	113.17
3	F	46	LEU	N-CA-C	-6.21	98.26	108.76
2	C	177	LYS	N-CA-C	-6.21	104.51	111.28
11	W	42	ILE	N-CA-C	-6.21	107.81	113.71
3	F	420	VAL	N-CA-C	-6.21	105.30	111.88
7	O	55	HIS	N-CA-C	-6.20	106.94	114.75
2	A	42	ARG	N-CA-C	-6.20	98.31	108.41
3	F	252	LEU	N-CA-C	-6.19	99.74	108.96
3	E	114	ARG	N-CA-C	-6.18	99.95	109.52
3	E	207	ILE	N-CA-C	-6.16	99.55	108.17
10	V	27	THR	N-CA-C	-6.14	104.66	111.36
3	D	11	GLY	N-CA-C	-6.14	101.37	111.38
3	E	39	ILE	N-CA-C	-6.14	98.90	107.80
3	F	42	PRO	N-CA-C	-6.14	108.30	114.68
1	1	15	SER	CA-C-N	6.13	129.11	120.28
1	1	15	SER	C-N-CA	6.13	129.11	120.28
3	E	258	ILE	N-CA-C	-6.13	105.67	113.22
2	C	287	LEU	N-CA-C	-6.13	105.44	113.17
4	G	137	ALA	N-CA-C	-6.13	102.06	109.72
2	B	479	ASN	N-CA-C	-6.13	105.81	113.28
3	E	450	ASP	N-CA-C	-6.12	105.10	113.30
12	X	24	ALA	CA-C-N	6.12	128.48	120.28
12	X	24	ALA	C-N-CA	6.12	128.48	120.28
2	B	58	SER	N-CA-C	-6.12	105.39	112.92
3	D	43	GLN	N-CA-C	-6.12	104.19	112.26
3	E	77	LEU	N-CA-C	-6.12	99.03	109.24
3	E	394	ASP	N-CA-C	-6.11	105.47	113.17
3	E	235	THR	CA-C-N	6.11	126.76	119.98
3	E	235	THR	C-N-CA	6.11	126.76	119.98
4	G	100	ASN	N-CA-C	-6.09	104.92	112.90
2	B	195	SER	N-CA-C	-6.09	107.68	114.62
3	F	364	GLY	N-CA-C	-6.09	98.76	113.18
2	A	99	VAL	N-CA-C	-6.08	104.20	109.19
3	D	132	GLU	N-CA-C	-6.08	100.06	109.24
3	E	156	PHE	N-CA-C	-6.08	100.06	109.24
11	W	33	SER	N-CA-C	-6.08	102.99	110.65
2	C	54	LEU	N-CA-C	-6.06	99.32	109.07
3	E	54	LEU	N-CA-C	-6.05	105.75	113.02
2	C	232	ILE	N-CA-C	-6.03	99.79	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	453	PRO	CA-C-N	6.02	128.35	120.28
3	E	453	PRO	C-N-CA	6.02	128.35	120.28
3	E	181	PHE	N-CA-C	-6.01	100.38	108.86
3	D	363	VAL	N-CA-C	-6.01	106.88	113.43
2	C	479	ASN	N-CA-C	-6.01	105.78	113.23
2	C	118	ASP	N-CA-C	-6.01	105.78	113.23
3	F	351	LEU	N-CA-C	-5.99	105.62	113.17
2	A	296	TYR	N-CA-C	-5.98	99.83	109.40
2	B	420	LEU	CA-C-N	5.97	128.64	120.46
2	B	420	LEU	C-N-CA	5.97	128.64	120.46
3	E	42	PRO	N-CA-C	-5.96	108.49	114.68
2	B	189	LYS	N-CA-C	-5.95	104.73	112.23
3	E	305	THR	N-CA-C	-5.95	100.86	110.32
3	E	395	GLU	N-CA-C	-5.94	105.79	113.16
1	0	18	GLY	CA-C-N	5.93	128.82	120.28
1	0	18	GLY	C-N-CA	5.93	128.82	120.28
7	O	131	PRO	N-CA-C	-5.92	105.82	113.57
1	5	10	ILE	CA-C-N	5.91	126.54	119.98
1	5	10	ILE	C-N-CA	5.91	126.54	119.98
2	A	31	GLY	N-CA-C	-5.90	102.48	111.10
3	D	421	ALA	N-CA-C	-5.90	103.33	110.88
7	O	180	ILE	N-CA-C	-5.90	105.33	111.58
12	X	25	GLU	CA-C-N	5.89	126.51	119.98
12	X	25	GLU	C-N-CA	5.89	126.51	119.98
4	G	129	SER	N-CA-C	-5.88	100.13	109.07
10	V	133	LEU	N-CA-C	-5.87	98.29	110.80
2	C	169	ILE	N-CA-C	-5.86	99.43	107.99
2	A	364	ARG	N-CA-C	-5.86	97.83	108.85
3	E	106	ARG	N-CA-C	-5.86	106.37	112.93
3	E	452	ILE	CA-C-O	-5.84	115.89	119.51
3	D	17	ILE	N-CA-C	-5.83	97.20	109.34
3	D	104	ASP	N-CA-C	-5.83	106.17	113.28
5	H	59	VAL	N-CA-C	-5.83	99.73	108.12
2	C	409	GLY	N-CA-C	-5.83	107.22	115.43
3	D	312	VAL	N-CA-C	-5.82	96.32	108.88
3	E	452	ILE	CA-C-N	5.82	125.82	119.89
3	E	452	ILE	C-N-CA	5.82	125.82	119.89
2	B	456	ASP	N-CA-C	-5.81	104.91	112.23
11	W	39	ALA	CA-C-N	5.81	127.10	119.84
11	W	39	ALA	C-N-CA	5.81	127.10	119.84
1	0	35	ASN	CA-C-N	5.80	126.38	119.94
1	0	35	ASN	C-N-CA	5.80	126.38	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8	2	GLN	CA-C-N	5.80	128.05	120.28
1	8	2	GLN	C-N-CA	5.80	128.05	120.28
2	A	296	TYR	CA-C-N	5.80	127.09	119.84
2	A	296	TYR	C-N-CA	5.80	127.09	119.84
1	9	10	ILE	CA-C-N	5.79	126.41	119.98
1	9	10	ILE	C-N-CA	5.79	126.41	119.98
2	B	42	ARG	N-CA-C	-5.79	98.84	108.34
3	F	284	THR	N-CA-C	-5.77	105.55	112.59
3	E	448	LYS	N-CA-C	-5.77	106.00	113.16
2	A	422	ARG	CA-C-N	5.77	126.38	119.98
2	A	422	ARG	C-N-CA	5.77	126.38	119.98
2	B	363	ILE	N-CA-C	-5.77	99.27	107.98
3	F	300	LYS	N-CA-C	-5.77	106.01	113.16
12	X	15	LYS	N-CA-C	-5.76	101.16	110.32
3	F	185	THR	N-CA-C	-5.76	98.90	108.34
3	E	299	THR	N-CA-C	-5.74	101.50	110.17
3	E	410	ILE	CA-C-N	5.74	127.97	120.28
3	E	410	ILE	C-N-CA	5.74	127.97	120.28
3	E	46	LEU	N-CA-C	-5.72	99.09	108.76
2	A	264	LYS	N-CA-C	-5.71	102.31	110.59
2	C	443	GLN	N-CA-C	-5.71	106.85	113.88
2	C	380	ALA	N-CA-C	-5.70	105.53	112.88
3	F	138	ILE	N-CA-C	-5.70	100.13	108.11
2	A	148	VAL	N-CA-C	-5.69	100.28	108.48
3	F	218	VAL	N-CA-C	-5.69	99.92	108.12
2	B	164	GLY	CA-C-N	5.68	128.77	120.71
2	B	164	GLY	C-N-CA	5.68	128.77	120.71
2	C	68	LEU	N-CA-C	-5.67	98.10	108.02
2	A	176	GLY	N-CA-C	-5.67	105.07	114.48
6	I	53	ALA	CA-C-N	5.67	132.36	121.54
6	I	53	ALA	C-N-CA	5.67	132.36	121.54
3	F	12	LYS	N-CA-C	-5.66	100.74	109.52
2	B	196	ASP	N-CA-C	-5.66	100.02	109.24
3	D	82	PRO	CA-C-N	5.65	132.14	121.97
3	D	82	PRO	C-N-CA	5.65	132.14	121.97
11	W	6	PRO	N-CA-C	5.65	117.59	110.70
8	T	113	ALA	N-CA-C	-5.64	106.44	113.38
1	7	22	ALA	CA-C-N	5.64	126.24	119.98
1	7	22	ALA	C-N-CA	5.64	126.24	119.98
11	W	69	PHE	CA-C-N	5.63	127.83	120.28
11	W	69	PHE	C-N-CA	5.63	127.83	120.28
2	B	262	ASN	N-CA-C	-5.63	106.18	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	121	GLY	CA-C-N	5.62	126.87	119.84
2	A	121	GLY	C-N-CA	5.62	126.87	119.84
3	E	210	GLU	N-CA-C	-5.61	99.28	108.76
3	E	308	GLN	N-CA-C	-5.61	100.82	109.52
4	G	123	PRO	CA-C-N	5.61	127.73	120.44
4	G	123	PRO	C-N-CA	5.61	127.73	120.44
2	B	255	ILE	CA-C-N	5.60	126.16	120.00
2	B	255	ILE	C-N-CA	5.60	126.16	120.00
3	F	296	ILE	N-CA-C	-5.60	107.82	113.47
1	0	15	SER	CA-C-N	5.58	128.53	120.38
1	0	15	SER	C-N-CA	5.58	128.53	120.38
2	C	490	GLU	N-CA-C	-5.58	98.44	108.48
11	W	14	ASN	N-CA-C	-5.58	106.52	113.38
3	F	365	GLN	CA-C-N	5.58	127.75	120.28
3	F	365	GLN	C-N-CA	5.58	127.75	120.28
2	B	234	VAL	N-CA-C	-5.57	100.45	108.53
3	E	311	TYR	N-CA-C	-5.57	99.65	108.73
10	V	90	GLN	N-CA-C	-5.56	107.04	113.88
1	8	58	SER	CA-C-N	5.55	127.72	120.28
1	8	58	SER	C-N-CA	5.55	127.72	120.28
2	B	397	ALA	N-CA-C	-5.55	105.72	112.88
7	O	147	VAL	N-CA-C	-5.54	98.45	106.88
3	D	110	LYS	N-CA-C	-5.54	99.00	110.80
2	C	459	GLU	CA-C-N	5.53	127.69	120.28
2	C	459	GLU	C-N-CA	5.53	127.69	120.28
2	A	59	SER	N-CA-C	-5.53	106.31	113.16
8	T	76	GLN	N-CA-C	5.53	116.98	111.07
1	2	43	ILE	CA-C-N	5.52	127.94	120.38
1	2	43	ILE	C-N-CA	5.52	127.94	120.38
11	W	48	LEU	N-CA-C	-5.52	106.25	114.64
3	D	42	PRO	N-CA-C	-5.52	108.94	114.68
3	F	395	GLU	N-CA-C	-5.51	105.86	112.59
1	6	43	ILE	CA-C-N	5.50	127.92	120.38
1	6	43	ILE	C-N-CA	5.50	127.92	120.38
3	F	452	ILE	CA-C-N	5.50	125.50	119.89
3	F	452	ILE	C-N-CA	5.50	125.50	119.89
5	H	75	ALA	N-CA-C	-5.50	100.05	109.24
5	H	58	GLU	N-CA-C	-5.50	100.06	109.24
2	B	316	GLU	CA-C-N	5.49	127.64	120.28
2	B	316	GLU	C-N-CA	5.49	127.64	120.28
5	H	40	GLY	N-CA-C	-5.49	101.86	111.46
3	D	255	ILE	N-CA-C	-5.48	99.93	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	323	LEU	N-CA-C	-5.48	100.37	109.46
3	E	317	LEU	N-CA-C	-5.47	106.10	112.89
2	B	54	LEU	N-CA-C	-5.47	100.32	109.24
1	7	10	ILE	CA-C-N	5.47	126.05	119.98
1	7	10	ILE	C-N-CA	5.47	126.05	119.98
2	B	296	TYR	CA-C-N	5.47	125.47	119.89
2	B	296	TYR	C-N-CA	5.47	125.47	119.89
2	B	91	LYS	N-CA-C	-5.47	100.49	109.40
8	T	112	SER	N-CA-C	-5.46	106.66	113.38
3	E	45	LYS	N-CA-C	-5.46	101.00	109.24
3	D	336	SER	CA-C-N	5.44	127.57	120.28
3	D	336	SER	C-N-CA	5.44	127.57	120.28
2	A	93	THR	N-CA-C	-5.44	105.43	111.36
2	C	506	PHE	N-CA-C	-5.44	102.28	110.06
3	F	365	GLN	N-CA-C	-5.41	105.46	111.36
3	E	431	LEU	N-CA-C	-5.41	100.88	109.59
4	G	176	GLU	N-CA-C	-5.40	100.75	109.40
2	B	68	LEU	N-CA-C	-5.40	99.71	108.52
4	G	127	LYS	N-CA-C	-5.39	106.64	113.43
1	8	17	ILE	CA-C-N	5.38	126.06	120.03
1	8	17	ILE	C-N-CA	5.38	126.06	120.03
8	T	140	VAL	N-CA-C	-5.38	106.18	111.77
12	X	20	THR	CA-C-N	5.38	128.02	120.28
12	X	20	THR	C-N-CA	5.38	128.02	120.28
1	7	61	THR	CA-C-N	5.38	125.95	119.98
1	7	61	THR	C-N-CA	5.38	125.95	119.98
3	E	427	ILE	CA-C-N	5.37	125.38	119.90
3	E	427	ILE	C-N-CA	5.37	125.38	119.90
4	G	215	ALA	N-CA-C	-5.37	104.99	112.45
3	D	447	GLY	N-CA-C	-5.37	107.38	115.32
1	8	54	GLY	CA-C-N	5.36	127.41	120.44
1	8	54	GLY	C-N-CA	5.36	127.41	120.44
4	G	165	PHE	N-CA-C	-5.35	101.04	109.50
8	T	159	VAL	N-CA-C	-5.35	105.91	111.58
3	D	18	GLY	CA-C-N	5.35	127.45	120.28
3	D	18	GLY	C-N-CA	5.35	127.45	120.28
10	V	99	ALA	CA-C-N	5.35	127.45	120.28
10	V	99	ALA	C-N-CA	5.35	127.45	120.28
1	0	17	ILE	N-CA-C	5.35	116.08	110.62
3	E	347	ALA	CA-C-N	5.34	127.66	120.50
3	E	347	ALA	C-N-CA	5.34	127.66	120.50
3	F	311	TYR	N-CA-C	-5.34	102.18	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	W	33	SER	CA-C-N	5.33	134.81	121.80
11	W	33	SER	C-N-CA	5.33	134.81	121.80
3	E	284	THR	N-CA-C	-5.33	106.55	112.57
1	0	20	LEU	CA-C-N	5.33	125.89	119.98
1	0	20	LEU	C-N-CA	5.33	125.89	119.98
1	7	11	GLY	CA-C-N	5.32	127.41	120.28
1	7	11	GLY	C-N-CA	5.32	127.41	120.28
2	B	88	GLU	N-CA-C	-5.32	102.17	110.42
2	A	37	GLY	N-CA-C	-5.32	100.57	113.18
1	2	12	ALA	CA-C-N	5.32	125.84	119.94
1	2	12	ALA	C-N-CA	5.32	125.84	119.94
2	B	386	LYS	N-CA-C	-5.31	106.48	113.12
8	T	209	GLY	N-CA-C	-5.31	107.37	115.66
2	A	374	SER	N-CA-C	-5.31	99.79	108.76
2	C	175	THR	N-CA-C	-5.30	106.66	113.02
1	7	17	ILE	CA-C-N	5.30	125.86	119.98
1	7	17	ILE	C-N-CA	5.30	125.86	119.98
1	9	65	CYS	CA-C-N	5.30	127.38	120.28
1	9	65	CYS	C-N-CA	5.30	127.38	120.28
3	E	295	ARG	N-CA-C	-5.29	106.59	113.16
3	D	207	ILE	N-CA-C	-5.29	100.76	108.17
2	B	137	GLY	CA-C-N	5.29	127.23	120.56
2	B	137	GLY	C-N-CA	5.29	127.23	120.56
2	C	145	HIS	N-CA-C	-5.28	104.48	112.99
3	F	115	LYS	CA-C-N	5.28	125.20	119.76
3	F	115	LYS	C-N-CA	5.28	125.20	119.76
2	C	130	ARG	N-CA-C	-5.28	101.27	109.72
3	F	220	GLY	N-CA-C	-5.27	100.68	113.18
10	V	56	SER	N-CA-C	-5.27	104.44	111.24
2	B	158	LEU	N-CA-C	-5.26	106.90	113.38
3	D	106	ARG	CA-C-N	5.26	130.13	121.87
3	D	106	ARG	C-N-CA	5.26	130.13	121.87
2	A	199	LYS	N-CA-C	-5.25	106.92	113.38
3	F	262	THR	CA-C-N	5.25	127.31	120.28
3	F	262	THR	C-N-CA	5.25	127.31	120.28
3	F	210	GLU	N-CA-C	-5.24	101.23	109.50
2	A	64	MET	N-CA-C	-5.23	101.46	109.41
1	0	58	SER	CA-C-N	5.23	127.29	120.28
1	0	58	SER	C-N-CA	5.23	127.29	120.28
3	F	9	ILE	N-CA-C	-5.23	98.96	107.28
3	D	345	TYR	N-CA-C	-5.23	97.44	108.73
2	A	444	VAL	CA-C-O	-5.22	114.41	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	105	LEU	N-CA-C	-5.22	106.68	113.16
3	E	330	ASP	N-CA-C	-5.21	107.47	113.88
3	F	153	ILE	N-CA-C	-5.21	101.12	109.20
2	C	259	PHE	CA-C-N	5.21	127.26	120.28
2	C	259	PHE	C-N-CA	5.21	127.26	120.28
3	D	450	ASP	N-CA-C	-5.21	104.08	110.65
3	D	358	LEU	N-CA-C	-5.21	107.30	113.97
3	D	114	ARG	N-CA-C	-5.21	101.45	109.52
2	C	236	ALA	N-CA-C	-5.20	98.73	107.32
3	D	343	GLY	N-CA-C	-5.20	108.04	115.64
3	F	23	VAL	N-CA-C	-5.20	100.88	108.99
2	B	191	TRP	N-CA-C	-5.20	107.07	113.41
3	D	128	SER	N-CA-C	-5.20	99.73	110.80
2	B	59	SER	N-CA-C	-5.20	106.72	113.16
1	2	15	SER	CA-C-N	5.20	127.76	120.28
1	2	15	SER	C-N-CA	5.20	127.76	120.28
11	W	4	LEU	N-CA-C	-5.19	100.62	108.67
2	A	323	LEU	N-CA-C	-5.19	98.78	108.02
3	D	353	SER	N-CA-C	-5.19	99.74	110.80
3	F	343	GLY	N-CA-C	-5.19	107.84	114.85
2	B	192	ASN	N-CA-C	-5.19	106.63	113.17
2	A	133	VAL	N-CA-C	-5.19	101.50	108.35
2	B	31	GLY	N-CA-C	-5.19	103.57	111.14
2	B	159	VAL	N-CA-C	-5.19	97.68	108.88
7	O	123	VAL	N-CA-C	-5.18	98.56	109.34
2	A	21	VAL	N-CA-C	-5.18	107.67	112.43
1	5	2	GLN	CA-C-N	5.18	127.22	120.28
1	5	2	GLN	C-N-CA	5.18	127.22	120.28
2	A	359	PHE	CA-C-N	5.18	128.18	120.31
2	A	359	PHE	C-N-CA	5.18	128.18	120.31
3	E	111	SER	N-CA-C	-5.17	100.27	109.06
1	4	18	GLY	CA-C-N	5.17	127.72	120.28
1	4	18	GLY	C-N-CA	5.17	127.72	120.28
1	9	12	ALA	CA-C-N	5.17	125.67	119.94
1	9	12	ALA	C-N-CA	5.17	125.67	119.94
11	W	46	THR	N-CA-C	-5.16	104.98	113.50
2	B	118	ASP	N-CA-C	-5.16	106.76	113.16
3	D	329	LEU	CA-C-N	5.16	127.20	120.28
3	D	329	LEU	C-N-CA	5.16	127.20	120.28
3	E	145	ALA	CA-C-N	5.16	125.16	119.90
3	E	145	ALA	C-N-CA	5.16	125.16	119.90
1	1	17	ILE	CA-C-N	5.16	126.58	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	17	ILE	C-N-CA	5.16	126.58	120.14
11	W	76	PHE	N-CA-C	-5.14	104.61	111.24
3	F	91	THR	N-CA-C	-5.14	107.05	113.38
2	C	375	ARG	CA-C-N	5.14	127.04	120.56
2	C	375	ARG	C-N-CA	5.14	127.04	120.56
3	F	65	ASP	CA-C-N	5.14	126.04	120.44
3	F	65	ASP	C-N-CA	5.14	126.04	120.44
2	A	101	VAL	N-CA-C	-5.13	100.81	108.46
3	D	452	ILE	N-CA-C	-5.12	99.61	107.71
3	D	428	PRO	CA-C-N	5.12	126.32	120.53
3	D	428	PRO	C-N-CA	5.12	126.32	120.53
2	B	328	VAL	N-CA-C	-5.12	100.38	107.80
3	E	393	MET	N-CA-C	-5.11	106.82	113.16
4	G	2	THR	N-CA-C	-5.11	105.62	111.14
2	A	137	GLY	CA-C-N	5.10	126.99	120.56
2	A	137	GLY	C-N-CA	5.10	126.99	120.56
5	H	30	VAL	N-CA-C	-5.10	100.90	108.45
1	2	61	THR	CA-C-N	5.10	125.61	120.00
1	2	61	THR	C-N-CA	5.10	125.61	120.00
14	Z	8	TYR	CA-C-N	5.10	127.11	120.28
14	Z	8	TYR	C-N-CA	5.10	127.11	120.28
2	B	338	ALA	N-CA-C	-5.09	99.95	110.80
3	E	307	VAL	N-CA-C	-5.09	101.04	108.17
1	4	2	GLN	CA-C-N	5.09	127.10	120.28
1	4	2	GLN	C-N-CA	5.09	127.10	120.28
2	A	81	ASP	CA-C-N	5.09	127.05	120.44
2	A	81	ASP	C-N-CA	5.09	127.05	120.44
2	A	135	ALA	CA-C-N	5.09	125.36	119.92
2	A	135	ALA	C-N-CA	5.09	125.36	119.92
2	C	176	GLY	N-CA-C	-5.08	101.15	113.18
3	D	216	ALA	N-CA-C	-5.07	101.84	109.85
3	E	426	GLY	N-CA-C	-5.07	107.54	114.64
1	6	24	ILE	CA-C-N	5.07	125.57	119.94
1	6	24	ILE	C-N-CA	5.07	125.57	119.94
4	G	99	LEU	N-CA-C	-5.07	106.78	113.17
2	B	48	ASN	N-CA-C	-5.07	101.43	109.59
2	B	315	SER	CA-C-N	5.07	127.58	120.28
2	B	315	SER	C-N-CA	5.07	127.58	120.28
2	C	289	ARG	CA-C-N	5.07	125.60	120.38
2	C	289	ARG	C-N-CA	5.07	125.60	120.38
3	F	255	ILE	N-CA-C	-5.07	100.77	108.17
1	5	58	SER	CA-C-N	5.06	127.06	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	58	SER	C-N-CA	5.06	127.06	120.28
2	A	260	ARG	CA-C-N	5.06	127.48	120.29
2	A	260	ARG	C-N-CA	5.06	127.48	120.29
3	E	247	GLU	N-CA-C	-5.06	105.90	113.89
3	E	298	THR	N-CA-C	-5.05	100.50	108.73
6	I	19	GLN	CA-C-N	5.05	127.05	120.28
6	I	19	GLN	C-N-CA	5.05	127.05	120.28
3	E	449	TYR	N-CA-C	-5.04	104.87	112.99
10	V	160	VAL	N-CA-C	-5.04	102.40	107.89
1	9	41	PRO	N-CA-C	5.04	122.85	112.47
2	B	37	GLY	N-CA-C	-5.04	107.16	111.95
3	F	97	ASN	N-CA-C	-5.04	103.29	110.59
1	3	43	ILE	CA-C-N	5.04	127.73	120.38
1	3	43	ILE	C-N-CA	5.04	127.73	120.38
1	8	6	ALA	CA-C-N	5.03	127.02	120.28
1	8	6	ALA	C-N-CA	5.03	127.02	120.28
14	Z	7	PHE	N-CA-C	-5.03	105.85	112.94
3	F	258	ILE	N-CA-C	-5.02	107.86	112.83
4	G	202	ASP	N-CA-C	-5.02	107.00	112.72
1	1	18	GLY	CA-C-N	5.02	127.50	120.28
1	1	18	GLY	C-N-CA	5.02	127.50	120.28
2	B	113	LEU	N-CA-C	-5.01	106.41	112.88
3	F	340	SER	CA-C-N	5.01	127.92	120.31
3	F	340	SER	C-N-CA	5.01	127.92	120.31
10	V	63	LYS	N-CA-C	-5.01	106.68	112.89
2	A	32	ARG	N-CA-C	-5.01	99.83	108.69
1	7	36	GLY	CA-C-N	5.00	127.52	120.42
1	7	36	GLY	C-N-CA	5.00	127.52	120.42
13	Y	13	TYR	N-CA-C	-5.00	106.49	112.59

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	40	ASN	Peptide
1	3	40	ASN	Peptide
1	4	40	ASN	Peptide
1	5	40	ASN	Peptide
1	6	40	ASN	Peptide
1	7	40	ASN	Peptide
1	8	40	ASN	Peptide
1	9	40	ASN	Peptide

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Mol	Chain	Res	Type	Group
3	D	256	ASP	Peptide
3	F	345	TYR	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	0	300	0	95	0	0
1	1	300	0	95	0	0
1	2	300	0	95	0	0
1	3	296	0	91	0	0
1	4	300	0	95	0	0
1	5	300	0	95	0	0
1	6	296	0	91	0	0
1	7	292	0	91	0	0
1	8	300	0	95	0	0
1	9	296	0	91	0	0
2	A	1996	0	570	0	0
2	B	2020	0	575	1	0
2	C	1992	0	572	1	0
3	D	1880	0	538	0	0
3	E	1872	0	537	0	0
3	F	1876	0	537	0	0
4	G	1060	0	277	0	0
5	H	480	0	122	0	0
6	I	193	0	43	0	0
7	O	748	0	205	0	0
8	T	897	0	248	0	0
9	U	620	0	158	0	0
10	V	685	0	173	0	0
11	W	340	0	92	0	0
12	X	248	0	61	0	0
13	Y	148	0	40	0	0
14	Z	193	0	49	0	0
All	All	20228	0	5731	2	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 0.

All (2) 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:C:263:GLY:HA2	2:C:321:GLY:H	1.68	0.58
2:B:102:GLY:HA3	2:B:126:ALA:H	1.75	0.51

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	0	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
1	1	73/76 (96%)	71 (97%)	1 (1%)	1 (1%)	9	40
1	2	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
1	3	72/76 (95%)	69 (96%)	1 (1%)	2 (3%)	4	24
1	4	73/76 (96%)	71 (97%)	1 (1%)	1 (1%)	9	40
1	5	73/76 (96%)	70 (96%)	1 (1%)	2 (3%)	4	25
1	6	72/76 (95%)	70 (97%)	1 (1%)	1 (1%)	9	40
1	7	71/76 (93%)	69 (97%)	1 (1%)	1 (1%)	9	40
1	8	73/76 (96%)	70 (96%)	2 (3%)	1 (1%)	9	40
1	9	72/76 (95%)	69 (96%)	2 (3%)	1 (1%)	9	40
2	A	495/510 (97%)	464 (94%)	25 (5%)	6 (1%)	10	44
2	B	501/510 (98%)	469 (94%)	23 (5%)	9 (2%)	6	34
2	C	496/510 (97%)	470 (95%)	21 (4%)	5 (1%)	12	48
3	D	468/478 (98%)	432 (92%)	27 (6%)	9 (2%)	6	32
3	E	466/478 (98%)	439 (94%)	22 (5%)	5 (1%)	11	46
3	F	467/478 (98%)	429 (92%)	30 (6%)	8 (2%)	7	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	G	261/278 (94%)	252 (97%)	6 (2%)	3 (1%)	11	46
5	H	110/138 (80%)	104 (94%)	5 (4%)	1 (1%)	14	51
6	I	42/61 (69%)	37 (88%)	3 (7%)	2 (5%)	2	16
7	O	185/195 (95%)	168 (91%)	14 (8%)	3 (2%)	7	38
8	T	222/249 (89%)	208 (94%)	11 (5%)	3 (1%)	9	40
9	U	153/209 (73%)	152 (99%)	1 (1%)	0	100	100
10	V	169/173 (98%)	149 (88%)	11 (6%)	9 (5%)	1	15
11	W	83/95 (87%)	67 (81%)	10 (12%)	6 (7%)	1	11
12	X	60/92 (65%)	51 (85%)	5 (8%)	4 (7%)	1	12
13	Y	35/59 (59%)	32 (91%)	3 (9%)	0	100	100
14	Z	46/48 (96%)	43 (94%)	3 (6%)	0	100	100
All	All	4984/5321 (94%)	4669 (94%)	232 (5%)	83 (2%)	9	36

All (83) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	41	PRO
1	3	41	PRO
1	4	41	PRO
1	5	41	PRO
1	6	41	PRO
1	7	41	PRO
1	8	41	PRO
1	9	41	PRO
2	A	229	LYS
2	A	406	ALA
2	B	338	ALA
2	C	59	SER
2	C	299	ASP
3	F	359	ASP
3	F	451	ASN
6	I	54	SER
7	O	82	ASP
8	T	109	PHE
10	V	85	ALA
10	V	89	LEU
10	V	133	LEU
11	W	34	LEU

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Mol	Chain	Res	Type
12	X	38	ASN
12	X	58	VAL
2	B	49	ILE
2	B	156	ASP
2	C	61	VAL
3	D	83	ILE
3	D	110	LYS
3	E	130	SER
3	F	278	ALA
8	T	148	ALA
8	T	202	ASN
10	V	65	THR
10	V	130	PHE
11	W	31	TYR
11	W	44	ALA
12	X	44	LEU
2	B	26	ASN
2	B	167	GLU
3	D	81	GLY
3	D	107	GLY
3	D	451	ASN
3	E	119	ALA
3	F	81	GLY
3	F	86	PRO
4	G	203	ALA
5	H	33	PRO
7	O	61	ALA
10	V	83	ILE
11	W	11	SER
11	W	36	GLN
2	A	145	HIS
2	B	145	HIS
2	B	157	ALA
2	B	437	PRO
2	C	229	LYS
2	C	411	ASP
3	D	353	SER
3	F	279	VAL
4	G	56	GLU
6	I	57	THR
10	V	158	TRP
12	X	36	LYS

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Mol	Chain	Res	Type
1	3	42	SER
1	5	42	SER
2	A	230	TYR
2	A	367	ILE
3	E	16	VAL
3	E	34	LEU
3	F	462	GLY
10	V	55	PHE
3	F	133	ILE
7	O	171	LEU
10	V	25	THR
3	D	86	PRO
3	D	161	VAL
11	W	40	PRO
2	B	103	PRO
4	G	181	PRO
2	A	122	PRO
3	D	145	ALA
3	E	346	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

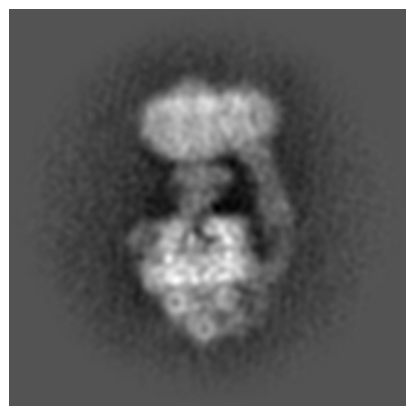
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25962. These allow visual inspection of the internal detail of the map and identification of artifacts.

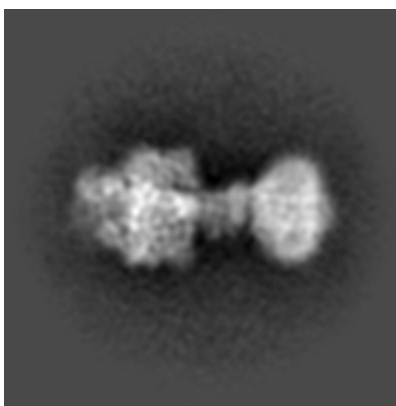
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

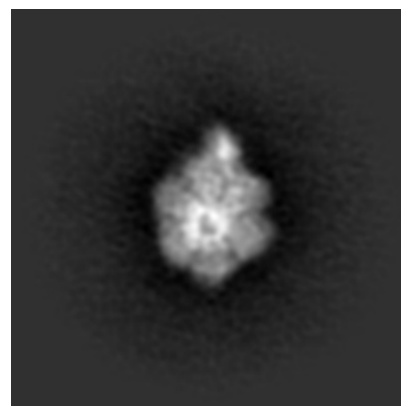
6.1.1 Primary map



X

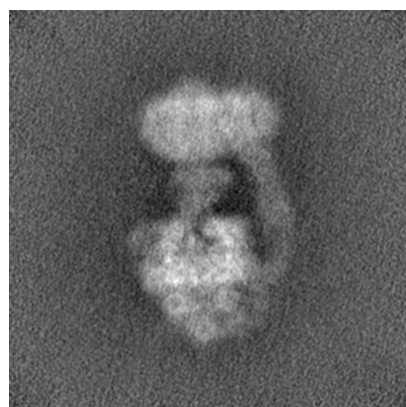


Y

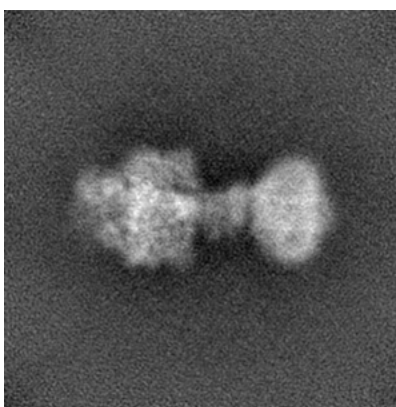


Z

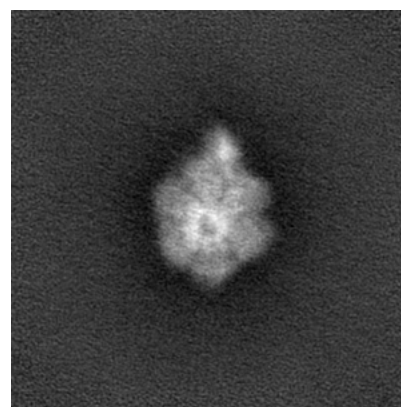
6.1.2 Raw map



X



Y



Z

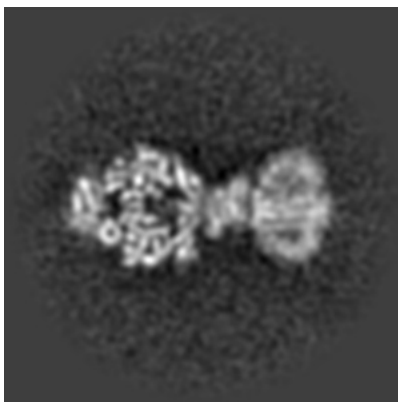
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

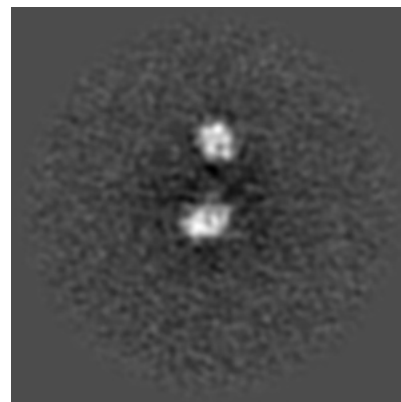
6.2.1 Primary map



X Index: 128

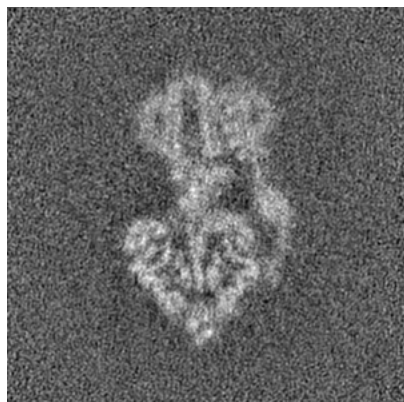


Y Index: 128

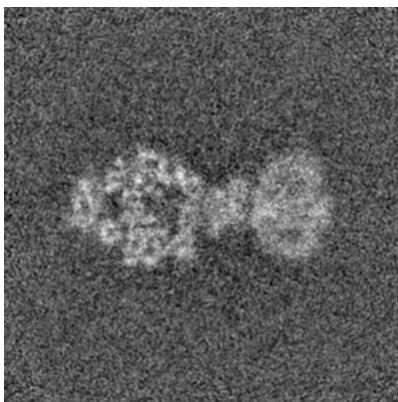


Z Index: 128

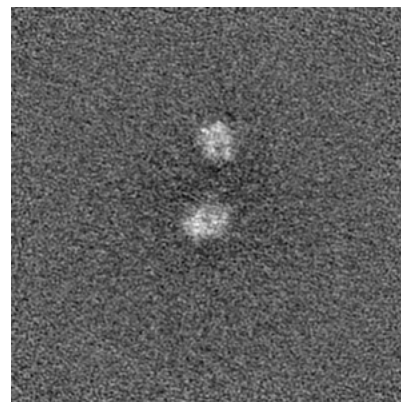
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

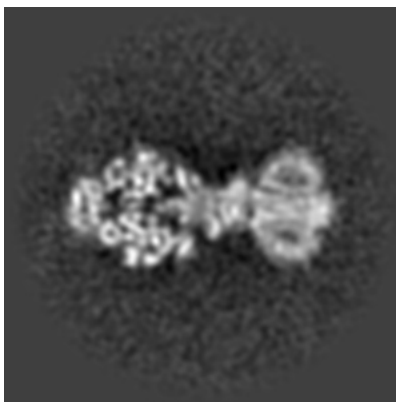
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

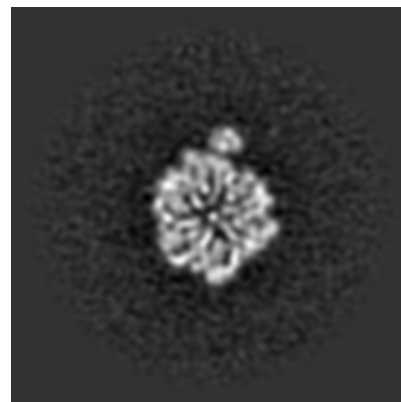
6.3.1 Primary map



X Index: 135

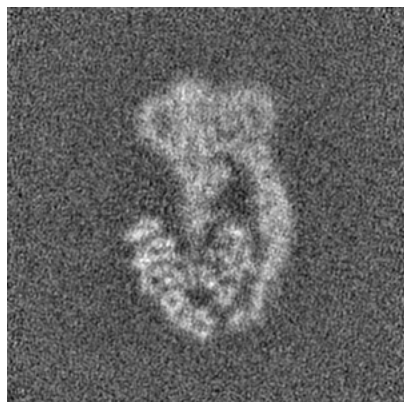


Y Index: 126

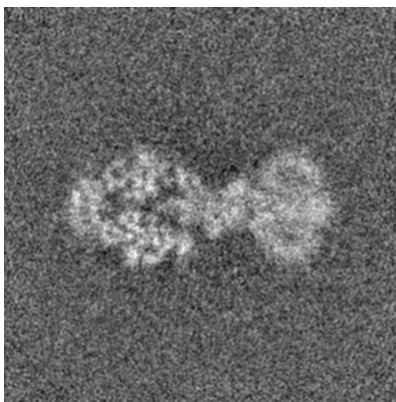


Z Index: 90

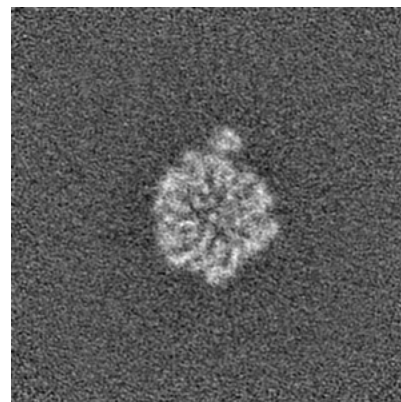
6.3.2 Raw map



X Index: 134



Y Index: 126

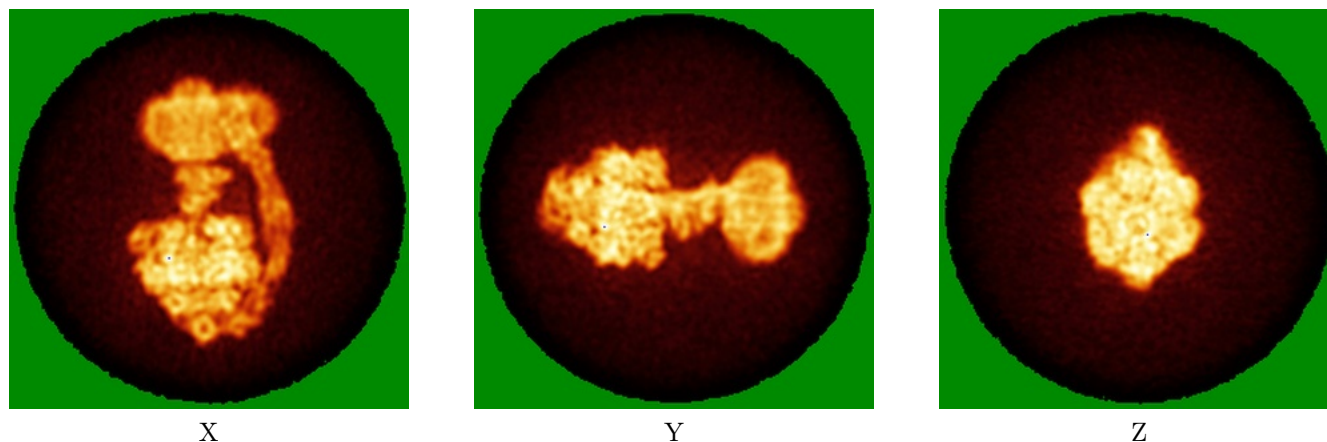


Z Index: 89

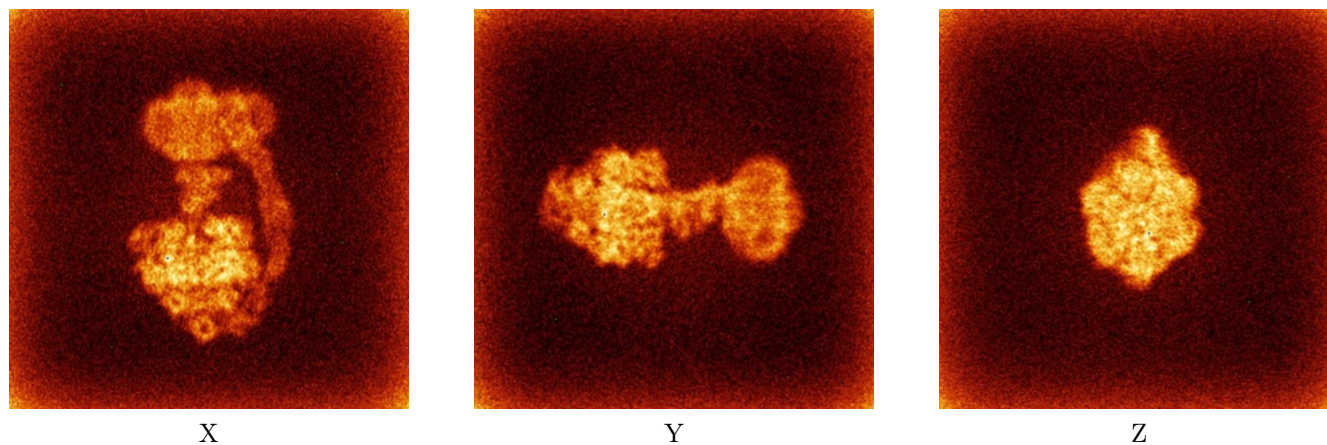
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



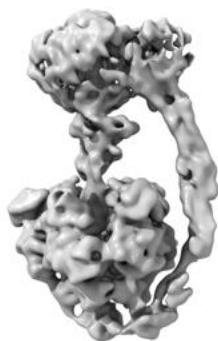
6.4.2 Raw map



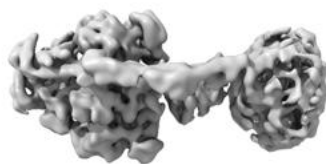
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

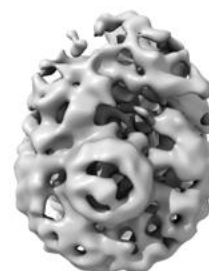
6.5.1 Primary map



X



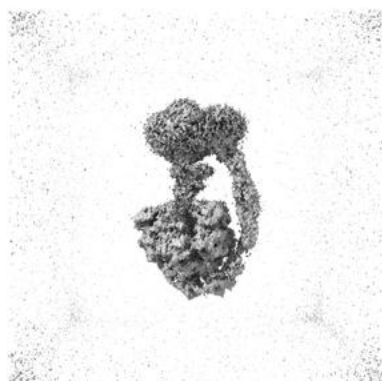
Y



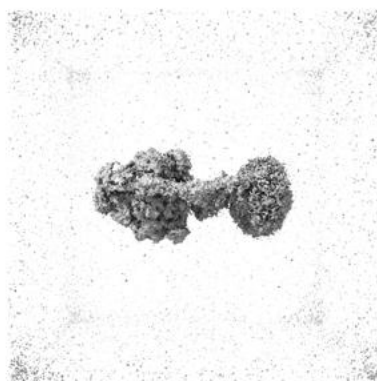
Z

The images above show the 3D surface view of the map at the recommended contour level 0.62. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

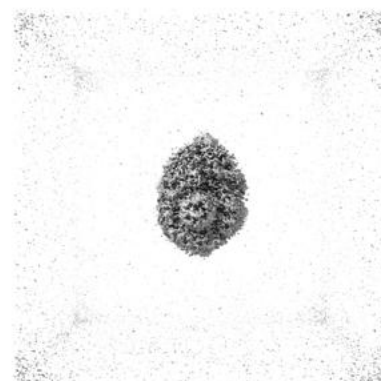
6.5.2 Raw map



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.

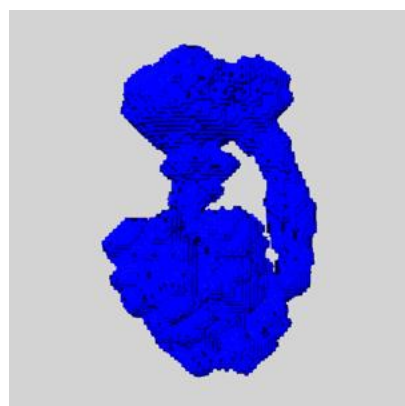
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

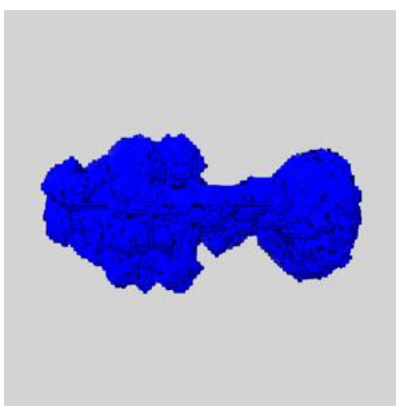
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

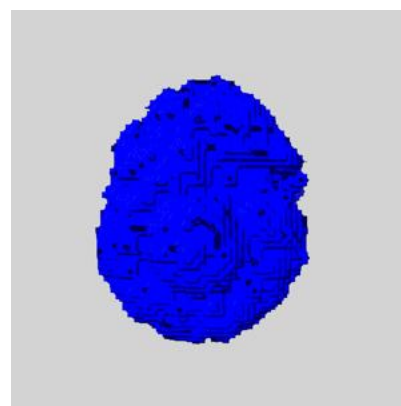
6.6.1 emd_25962_msk_1.map [i](#)



X



Y

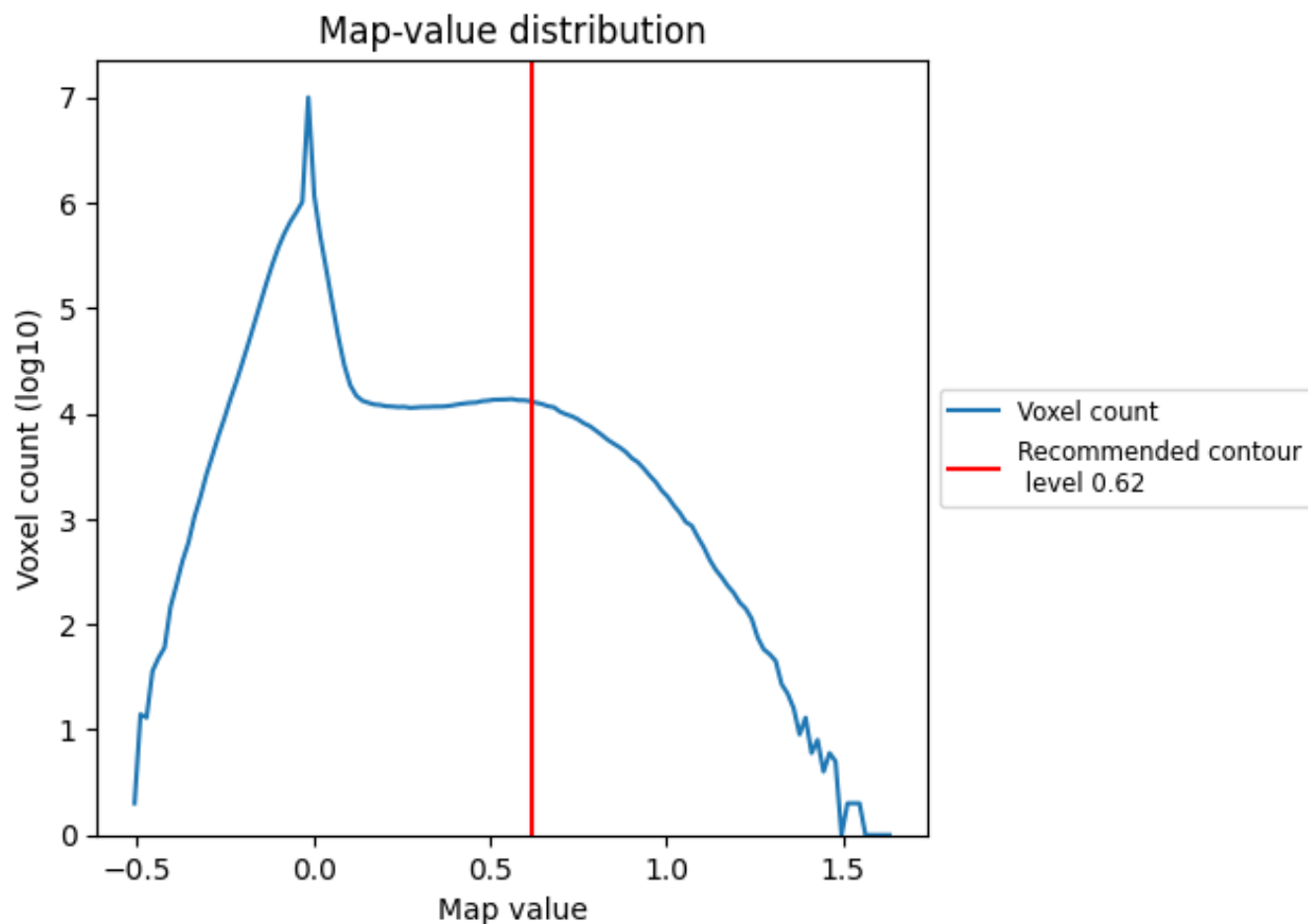


Z

7 Map analysis [i](#)

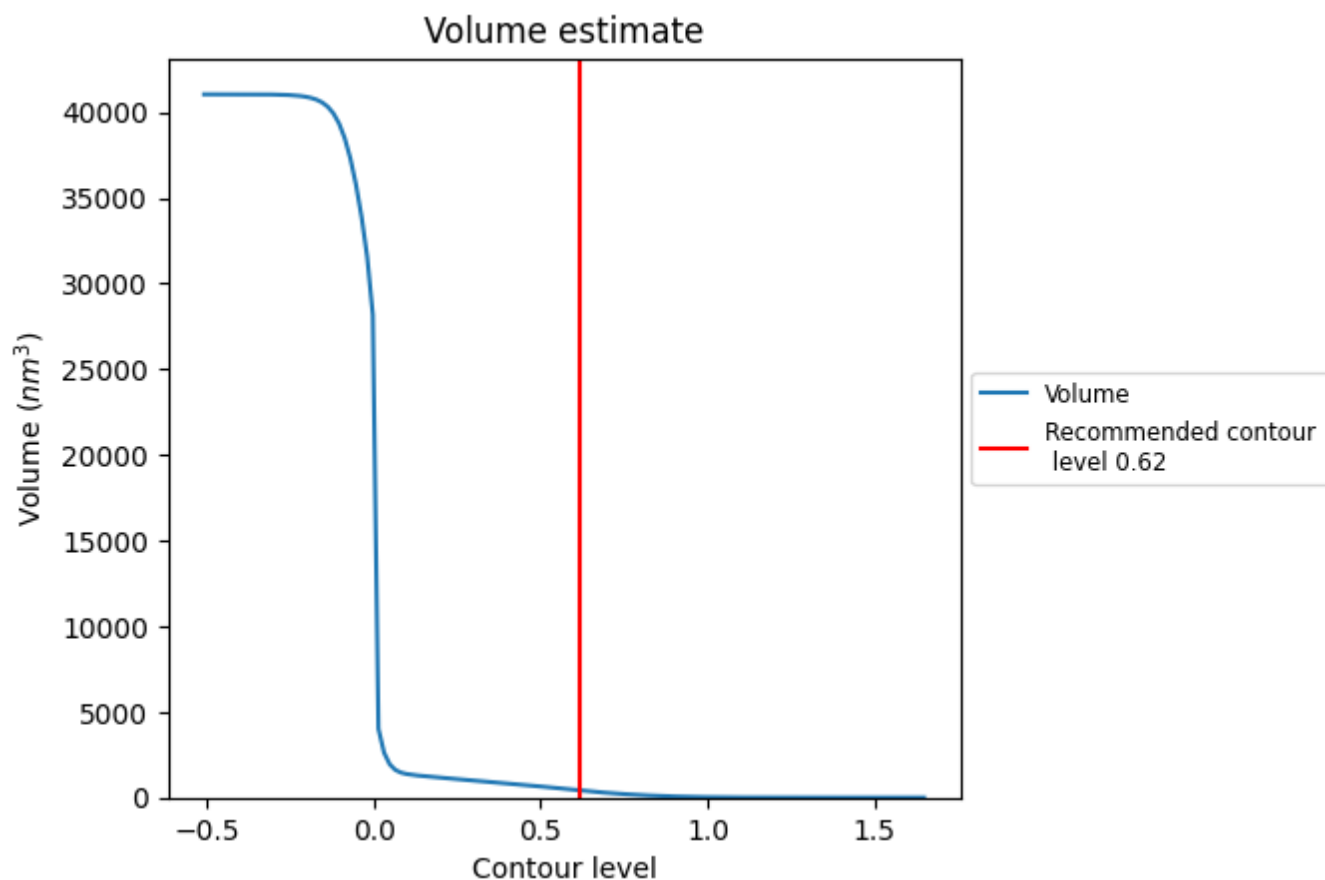
This section contains the results of statistical analysis of the map.

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.

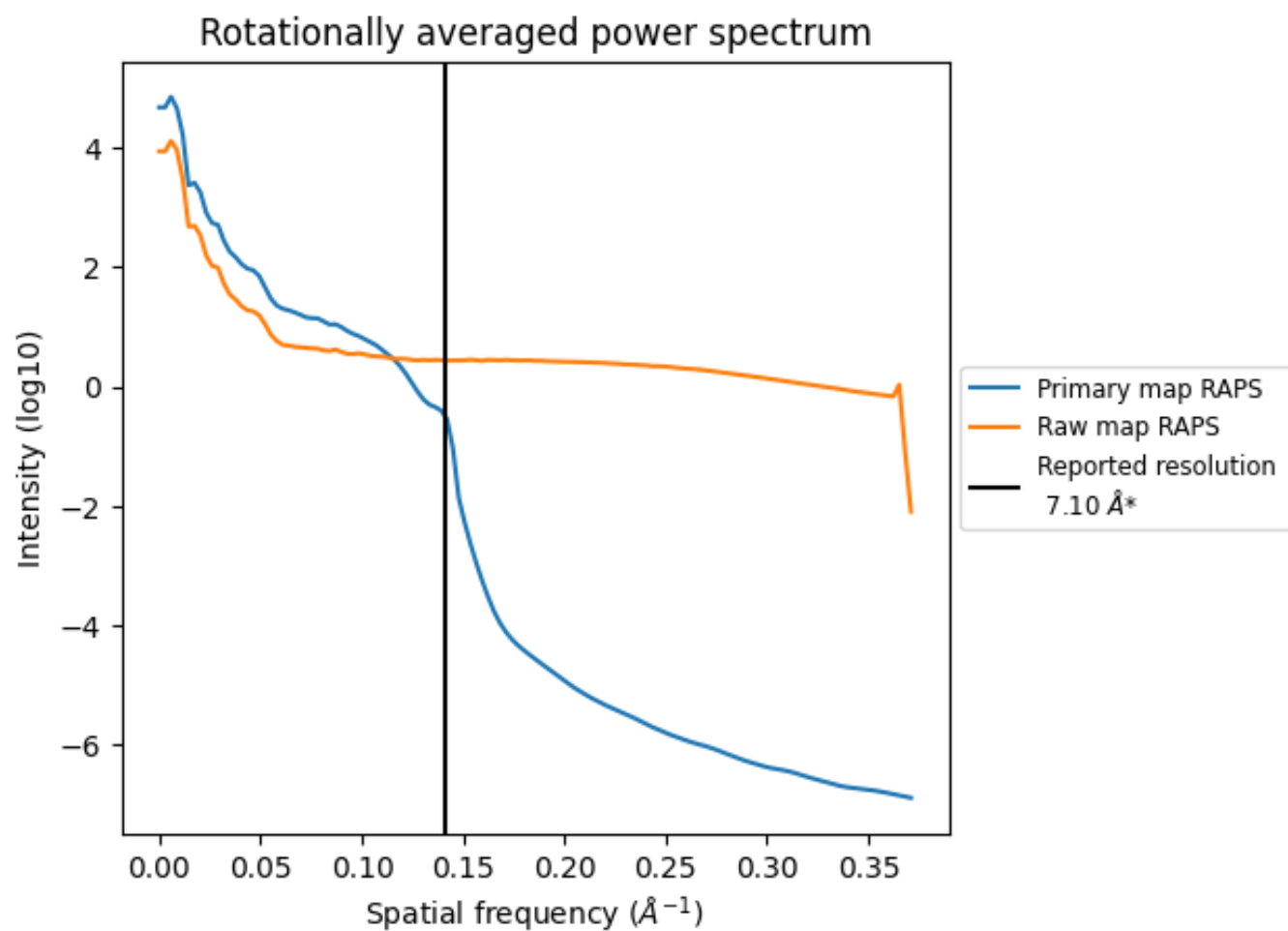
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 414 nm³; this corresponds to an approximate mass of 374 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 ⓘ

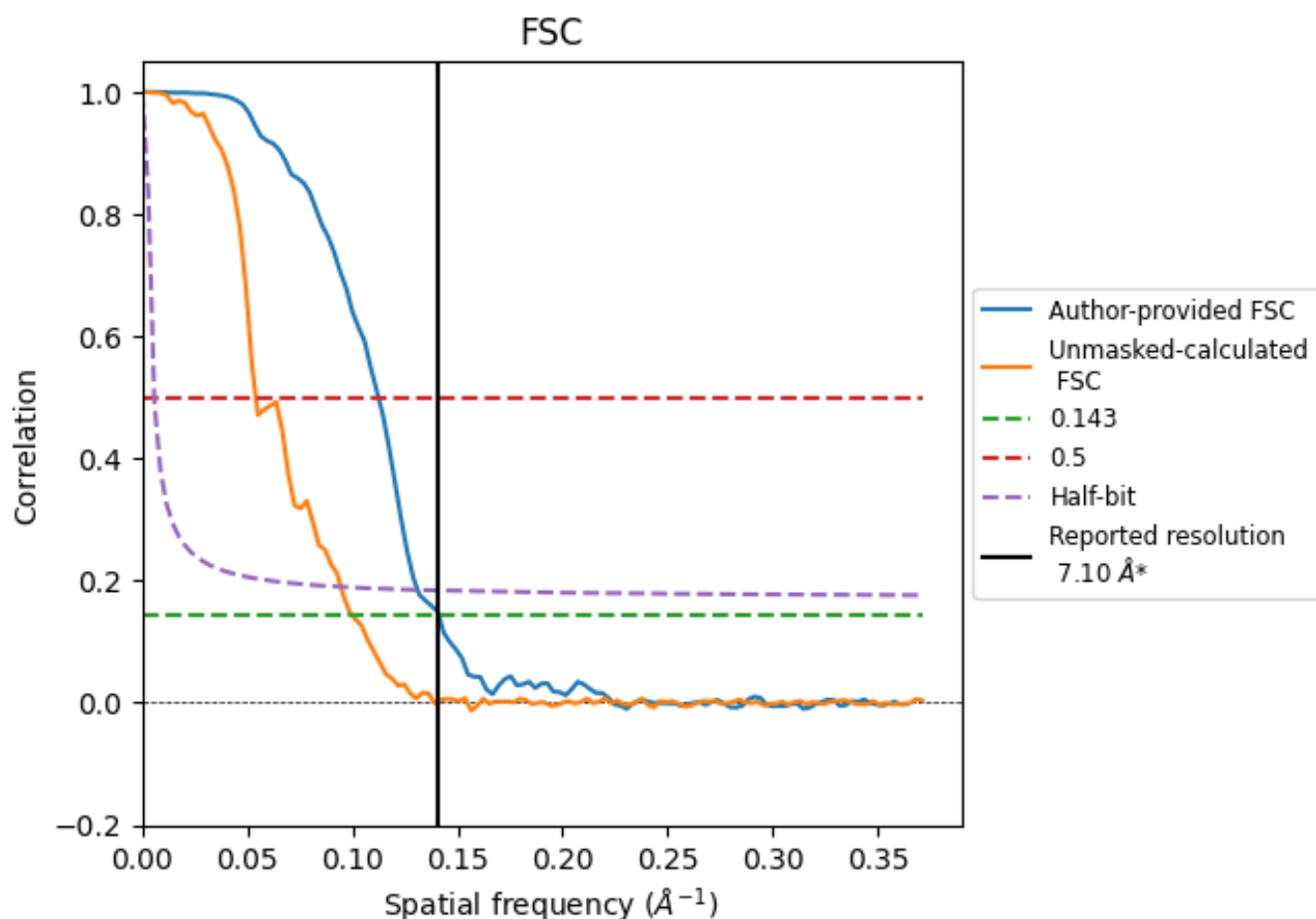


*Reported resolution corresponds to spatial frequency of 0.141 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.141 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

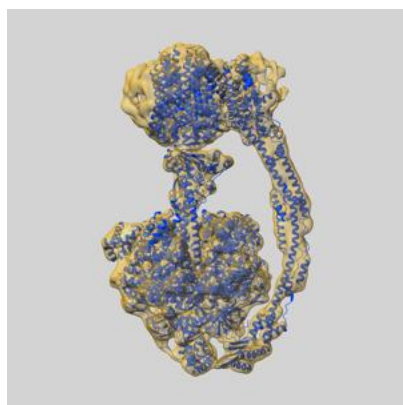
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.10	-	-
Author-provided FSC curve	7.09	8.90	7.63
Unmasked-calculated*	10.01	18.48	10.58

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 10.01 differs from the reported value 7.1 by more than 10 %

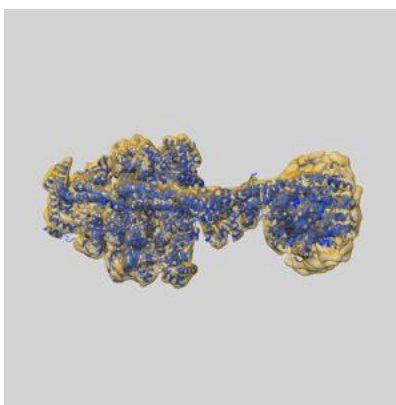
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25962 and PDB model 7TKA. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

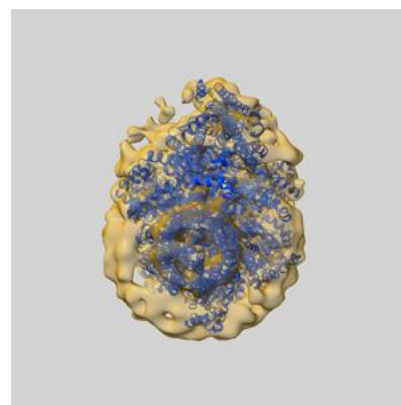
9.1 Map-model overlay [i](#)



X



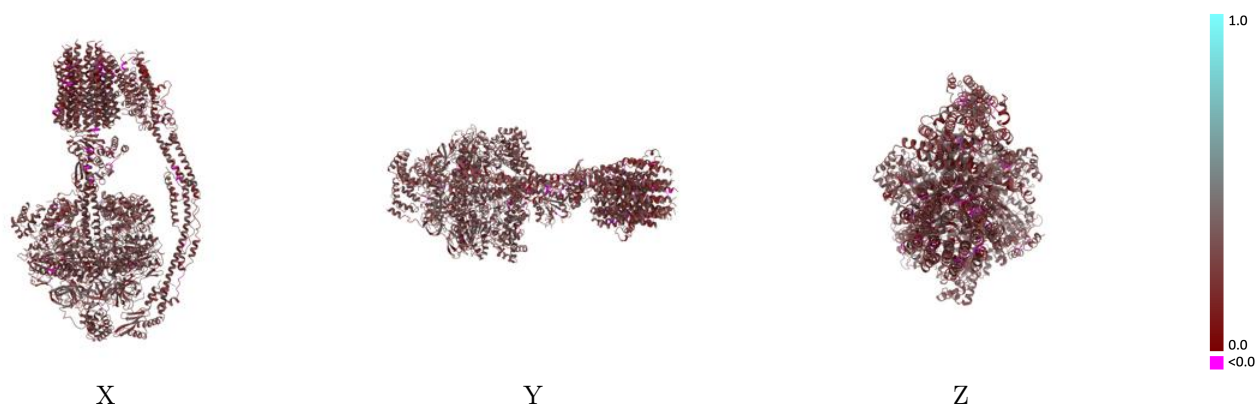
Y



Z

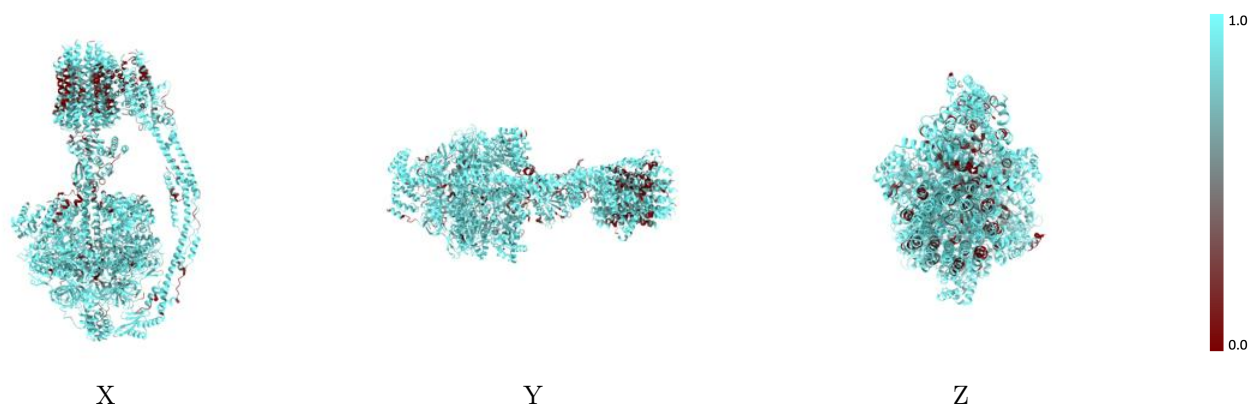
The images above show the 3D surface view of the map at the recommended contour level 0.62 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



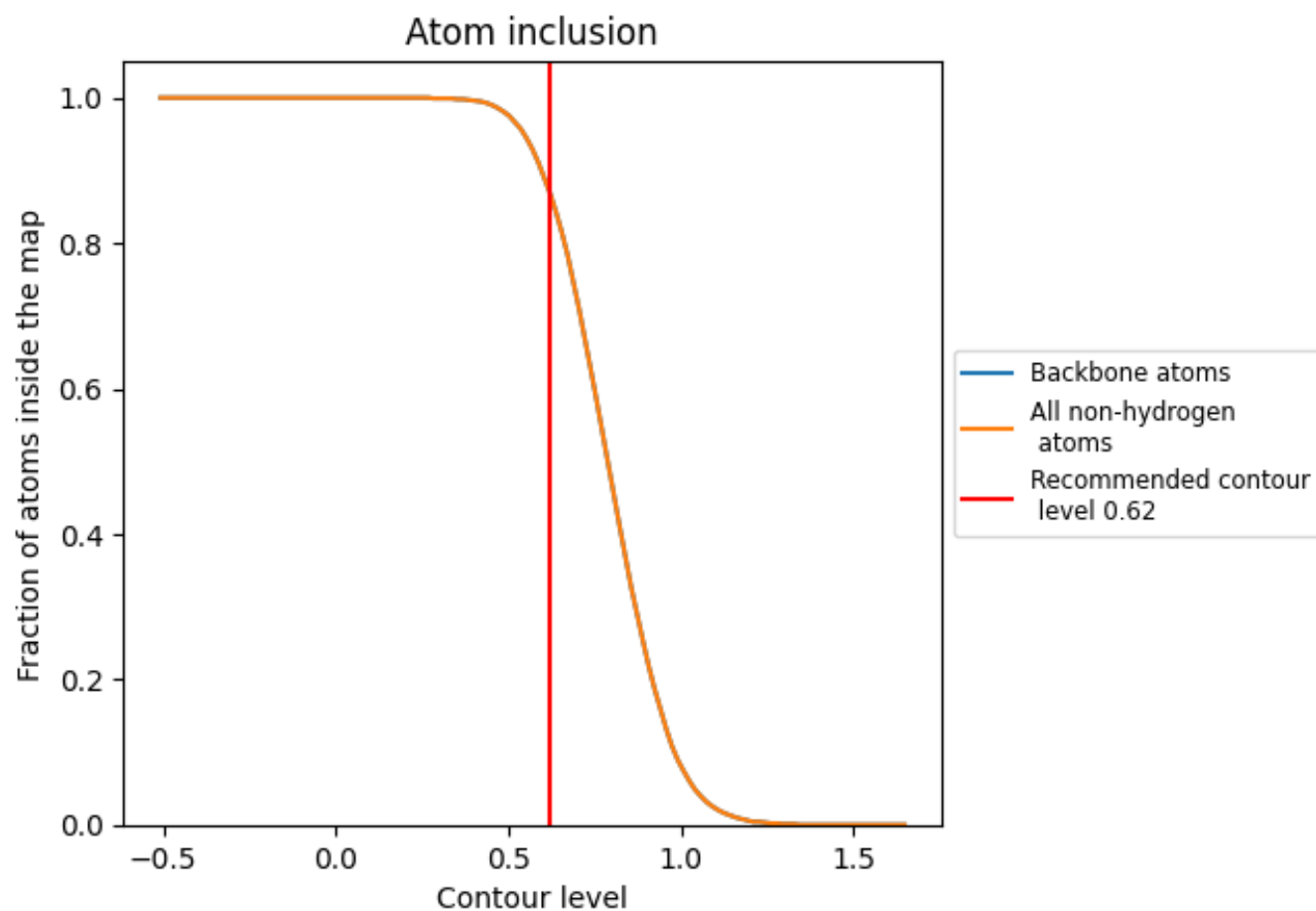
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.62).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (0.62) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8700	 0.2620
0	 0.8600	 0.2490
1	 0.7670	 0.2530
2	 0.7000	 0.2230
3	 0.8950	 0.2230
4	 0.7270	 0.2240
5	 0.8100	 0.2330
6	 0.7430	 0.2200
7	 0.6750	 0.1920
8	 0.7970	 0.2290
9	 0.7030	 0.1890
A	 0.9170	 0.2870
B	 0.9330	 0.2810
C	 0.9120	 0.2800
D	 0.9030	 0.2800
E	 0.8890	 0.2690
F	 0.9350	 0.2870
G	 0.8310	 0.2540
H	 0.7620	 0.2090
I	 0.7410	 0.2140
O	 0.9450	 0.2850
T	 0.7700	 0.2420
U	 0.9580	 0.2830
V	 0.8640	 0.2440
W	 0.7350	 0.1500
X	 0.7180	 0.2330
Y	 0.7700	 0.2300
Z	 0.7770	 0.2070

