Full wwPDB EM Validation Report

Dec 6, 2020 – 01:26 am GMT

PDB ID	:	5ARH
EMDB ID	:	EMD-3166
Title	:	Bovine mitochondrial ATP synthase state 2a
Authors	:	Zhou, A.; Rohou, A.; Schep, D.G.; Bason, J.V.; Montgomery, M.G.; Walker, J.E.; Grigorieff, N.; Rubinstein, J.L.
Deposited on	:	2015-09-24
Resolution	:	7.20 Å(reported)
Based on initial models	:	2CLY, 2XND, 2WSS

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

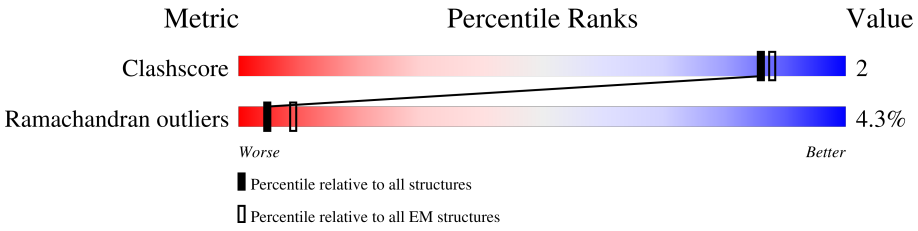
EMDB validation analysis	:	0.0.0.dev61
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.15.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 7.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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	510	90% 9%
1	B	510	87% 6% • 6%
1	C	510	85% 10% • 5%
2	D	482	88% 9% •
2	E	482	84% 12% •
2	F	482	90% 6% •
3	G	273	80% 15% • •
4	H	146	80% 10% 10%
5	I	50	82% 12% 6%

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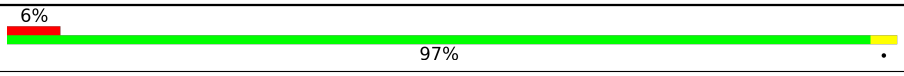
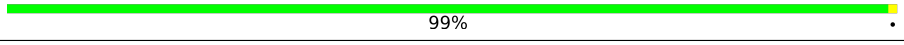
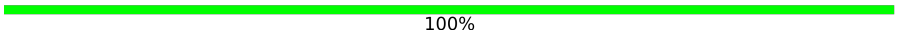
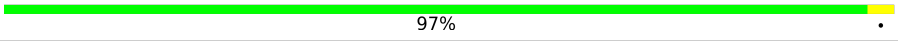
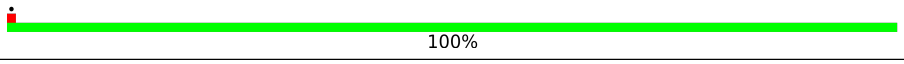
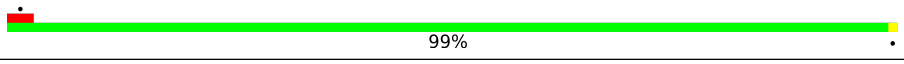
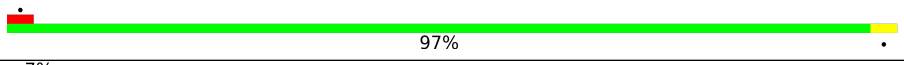
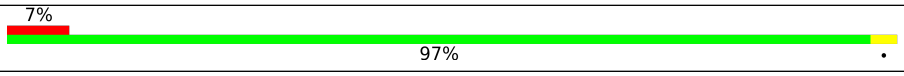
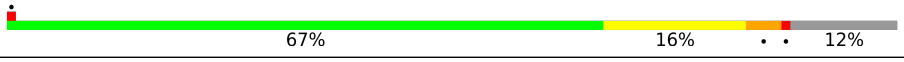
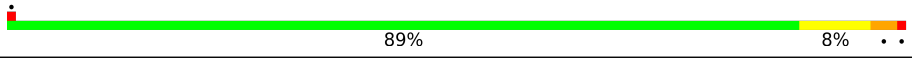
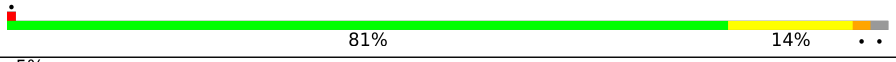
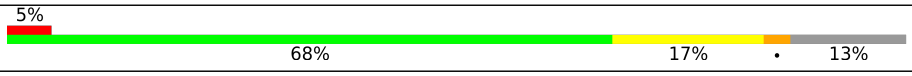
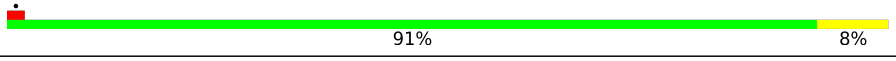
Mol	Chain	Length	Quality of chain
6	J	72	
6	K	72	
6	L	72	
6	M	72	
6	N	72	
6	O	72	
6	P	72	
6	Q	72	
7	S	190	
8	T	174	
9	U	124	
10	V	77	
11	W	217	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 18544 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 ALPHA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	509	Total 2035	C 1018	N 509	O 508	0	0
1	B	480	Total 1918	C 960	N 480	O 478	0	0
1	C	487	Total 1947	C 974	N 487	O 486	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	conflict	UNP P19483
B	481	GLY	SER	conflict	UNP P19483
C	481	GLY	SER	conflict	UNP P19483

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	467	Total 1867	C 934	N 467	O 466	0	0
2	E	466	Total 1863	C 932	N 466	O 465	0	0
2	F	466	Total 1863	C 932	N 466	O 465	0	0

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	264	Total 1053	C 528	N 264	O 261	0	0

- Molecule 4 is a protein called ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	131	Total	C	N	O	0	0
			523	262	131	130		

- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	47	Total	C	N	O	0	0
			187	94	47	46		

- Molecule 6 is a protein called ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	72	Total	C	N	O	0	0
			288	144	72	72		
6	K	72	Total	C	N	O	0	0
			288	144	72	72		
6	L	72	Total	C	N	O	0	0
			288	144	72	72		
6	M	72	Total	C	N	O	0	0
			288	144	72	72		
6	N	72	Total	C	N	O	0	0
			288	144	72	72		
6	O	72	Total	C	N	O	0	0
			288	144	72	72		
6	P	72	Total	C	N	O	0	0
			288	144	72	72		
6	Q	72	Total	C	N	O	0	0
			288	144	72	72		

- Molecule 7 is a protein called ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	S	168	Total	C	N	O	0	1
			669	334	168	167		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	129	THR	ALA	conflict	UNP P13621

- Molecule 8 is a protein called ATP SYNTHASE F(0) COMPLEX SUBUNIT B1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	T	174	Total 697	C 348	N 174	O 175	0	0

- Molecule 9 is a protein called ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	U	121	Total 484	C 242	N 121	O 121	0	0

- Molecule 10 is a protein called ATP SYNTHASE-COUPLING FACTOR 6, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	V	67	Total 265	C 132	N 67	O 66	0	1

- Molecule 11 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

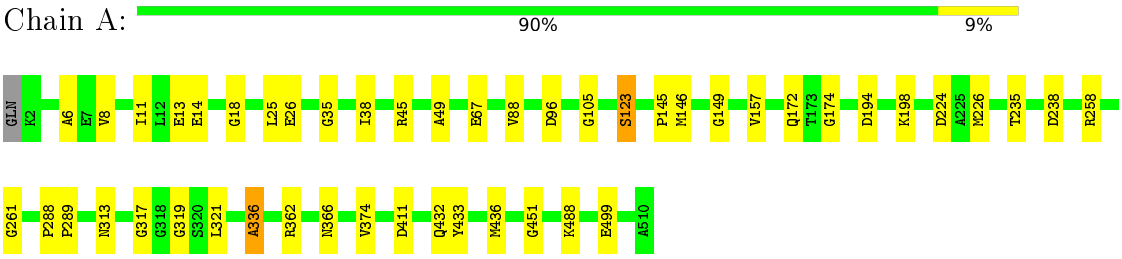
Mol	Chain	Residues	Atoms				AltConf	Trace
11	W	217	Total 869	C 434	N 217	O 218	0	0

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.

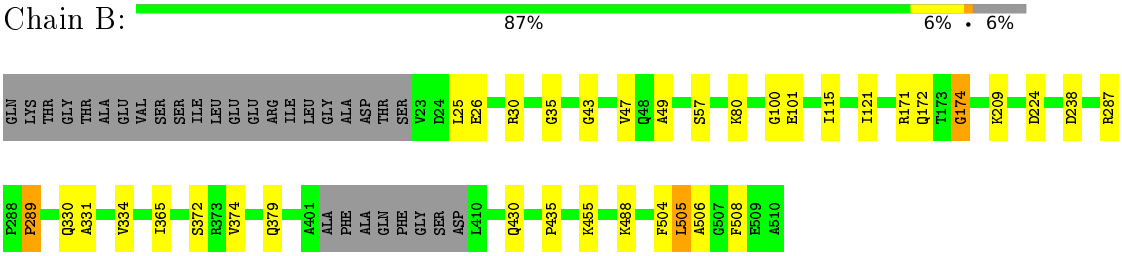
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain A:



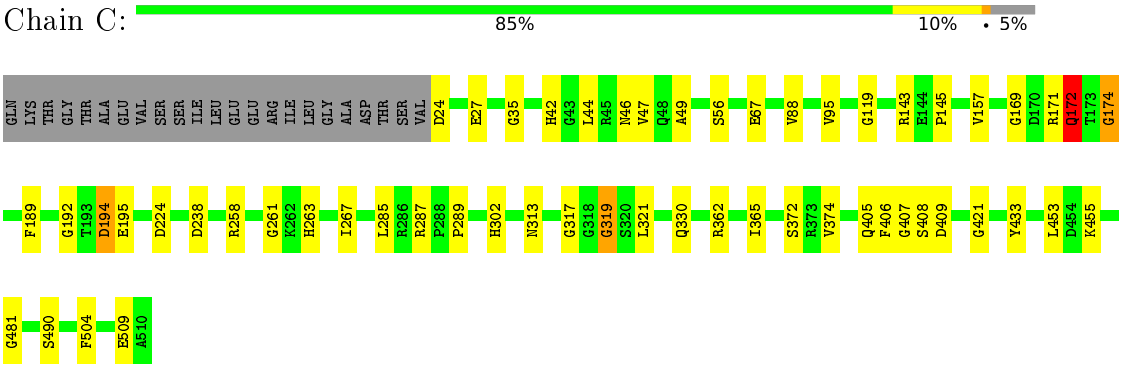
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain B:



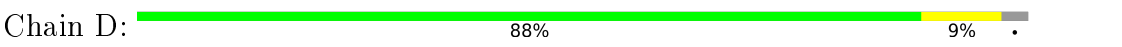
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

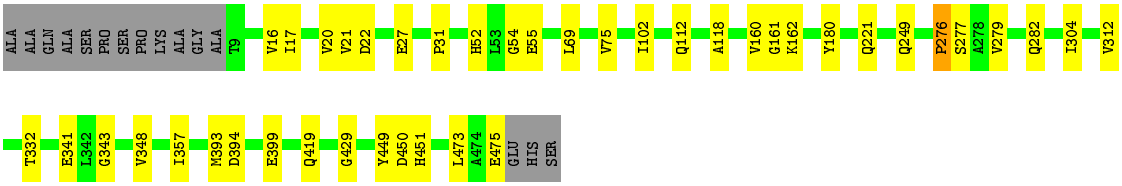
Chain C:



• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

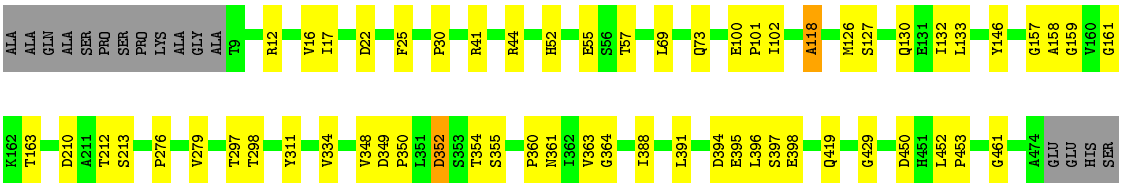
Chain D:





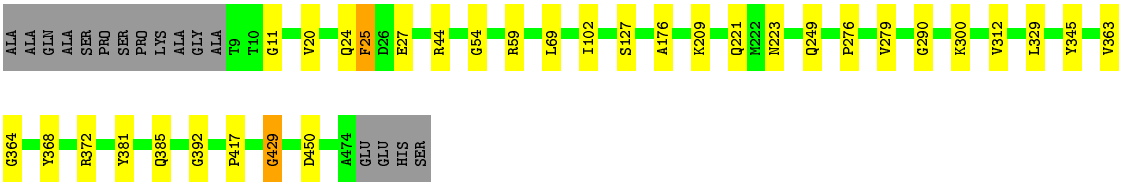
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain E:



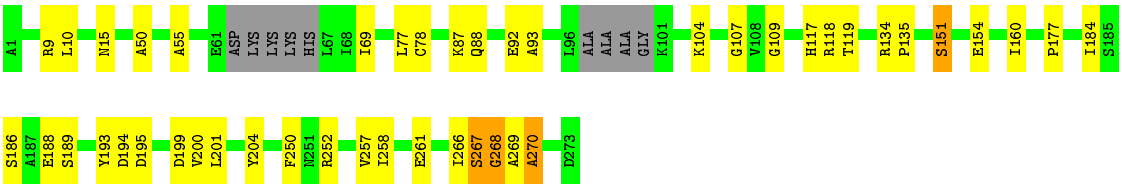
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain F:



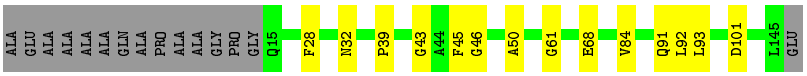
• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

Chain G:



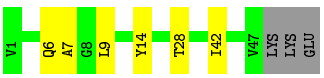
• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL

Chain H:



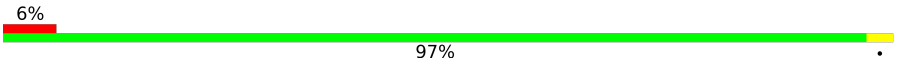
• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL

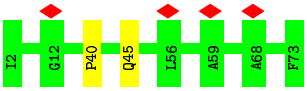
Chain I:



• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

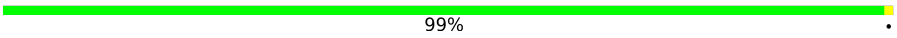
Chain J:





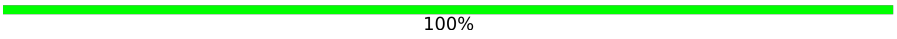
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain K:



• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

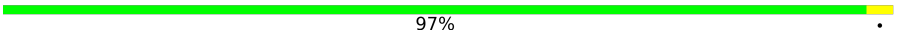
Chain L:

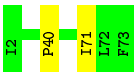


There are no outlier residues recorded for this chain.

• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

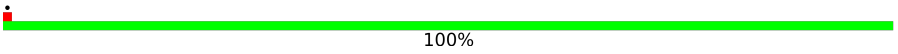
Chain M:

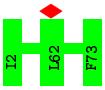




• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

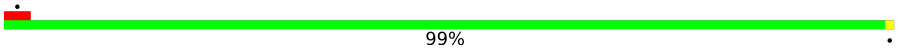
Chain N:

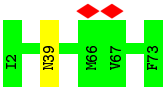




• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

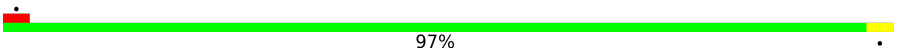
Chain O:

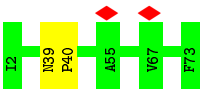




• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

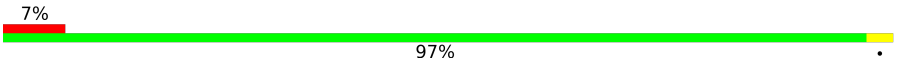
Chain P:

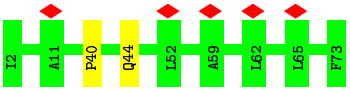




• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

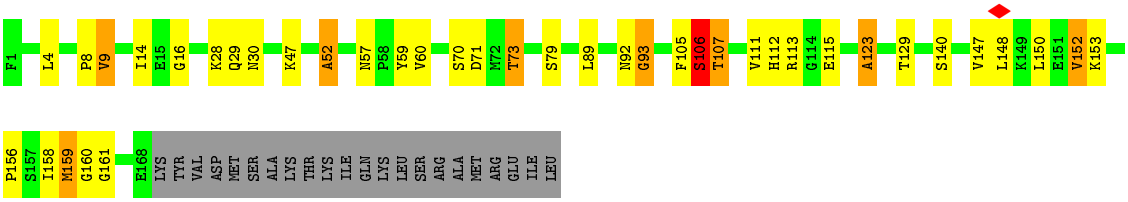
Chain Q:





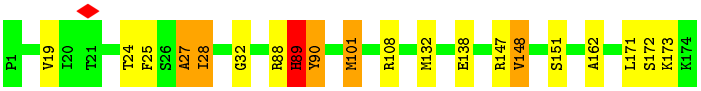
• Molecule 7: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL

Chain S:



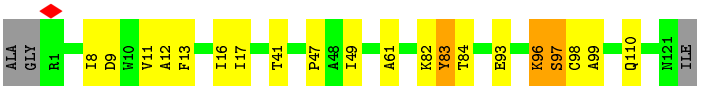
• Molecule 8: ATP SYNTHASE F(0) COMPLEX SUBUNIT B1, MITOCHONDRIAL

Chain T:



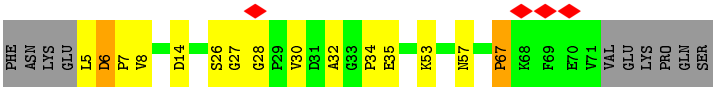
• Molecule 9: ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL

Chain U:



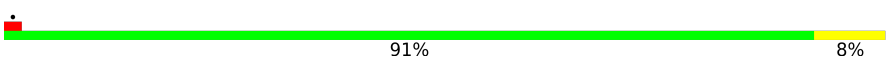
• Molecule 10: ATP SYNTHASE-COUPLING FACTOR 6, MITOCHONDRIAL

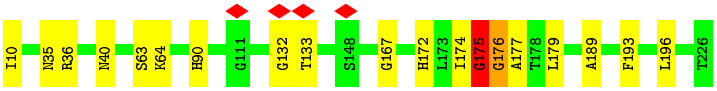
Chain V:



• Molecule 11: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain W:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	19250	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60.3	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4100	Depositor
Magnification	30487	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.469	Depositor
Minimum map value	-0.097	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	419.84, 419.84, 419.84	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.64, 1.64, 1.64	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	1.73	4/2034 (0.2%)	1.39	16/2541 (0.6%)
1	B	1.78	1/1916 (0.1%)	1.39	12/2392 (0.5%)
1	C	1.83	6/1946 (0.3%)	1.43	20/2431 (0.8%)
2	D	1.79	1/1866 (0.1%)	1.48	18/2331 (0.8%)
2	E	1.73	1/1862 (0.1%)	1.48	21/2326 (0.9%)
2	F	1.79	5/1862 (0.3%)	1.43	11/2326 (0.5%)
3	G	2.00	8/1050 (0.8%)	1.57	14/1308 (1.1%)
4	H	1.92	1/522 (0.2%)	1.67	9/651 (1.4%)
5	I	1.84	1/186 (0.5%)	1.47	2/231 (0.9%)
6	J	0.30	0/287	0.41	0/357
6	K	0.30	0/287	0.42	0/357
6	L	0.31	0/287	0.44	0/357
6	M	0.29	0/287	0.44	0/357
6	N	0.28	0/287	0.40	0/357
6	O	0.30	0/287	0.41	0/357
6	P	0.29	0/287	0.42	0/357
6	Q	0.30	0/287	0.44	0/357
7	S	1.78	3/668 (0.4%)	1.77	11/834 (1.3%)
8	T	0.84	2/696 (0.3%)	1.08	5/867 (0.6%)
9	U	0.64	1/483 (0.2%)	1.11	3/602 (0.5%)
10	V	0.70	0/264	1.05	2/329 (0.6%)
11	W	0.78	2/868 (0.2%)	1.01	0/1082
All	All	1.59	36/18519 (0.2%)	1.34	144/23107 (0.6%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	6
2	F	0	2
7	S	0	8
8	T	0	15
9	U	0	15
10	V	0	9
11	W	0	15
All	All	0	75

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	S	107	THR	CA-C	14.01	1.89	1.52
11	W	175	GLY	N-CA	-9.30	1.32	1.46
7	S	107	THR	N-CA	7.60	1.61	1.46
2	F	429	GLY	CA-C	-7.57	1.39	1.51
8	T	28	ILE	N-CA	7.47	1.61	1.46
3	G	261	GLU	CA-C	-6.58	1.35	1.52
3	G	252	ARG	CA-C	-6.39	1.36	1.52
1	C	174	GLY	N-CA	-6.32	1.36	1.46
2	F	364	GLY	N-CA	-6.05	1.36	1.46
4	H	28	PHE	CA-C	-6.05	1.37	1.52
3	G	266	ILE	CA-C	-5.84	1.37	1.52
1	C	481	GLY	CA-C	-5.78	1.42	1.51
2	F	364	GLY	CA-C	-5.69	1.42	1.51
1	C	172	GLN	CA-C	-5.62	1.38	1.52
1	A	499	GLU	CA-C	-5.59	1.38	1.52
3	G	109	GLY	CA-C	-5.59	1.43	1.51
2	D	161	GLY	N-CA	-5.57	1.37	1.46
1	C	35	GLY	CA-C	-5.53	1.43	1.51
1	C	421	GLY	CA-C	-5.53	1.43	1.51
2	E	12	ARG	CA-C	-5.40	1.39	1.52
1	B	174	GLY	N-CA	-5.39	1.38	1.46
3	G	261	GLU	N-CA	-5.39	1.35	1.46
1	C	302	HIS	CA-C	-5.34	1.39	1.52
3	G	107	GLY	CA-C	-5.29	1.43	1.51
1	A	174	GLY	N-CA	-5.20	1.38	1.46
3	G	15	ASN	CA-C	-5.17	1.39	1.52
5	I	14	TYR	N-CA	-5.17	1.36	1.46
9	U	97	SER	N-CA	-5.15	1.36	1.46
2	F	11	GLY	CA-C	-5.11	1.43	1.51
3	G	252	ARG	N-CA	-5.10	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	W	175	GLY	CA-C	-5.10	1.43	1.51
1	A	451	GLY	CA-C	-5.09	1.43	1.51
8	T	28	ILE	CA-C	-5.09	1.39	1.52
1	A	35	GLY	N-CA	-5.08	1.38	1.46
7	S	106	SER	C-N	-5.07	1.22	1.34
2	F	290	GLY	CA-C	-5.02	1.43	1.51

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	S	106	SER	C-N-CA	-16.48	80.49	121.70
7	S	106	SER	O-C-N	-13.22	101.55	122.70
4	H	43	GLY	N-CA-C	-9.82	88.56	113.10
1	C	35	GLY	N-CA-C	-8.97	90.68	113.10
7	S	107	THR	C-N-CA	8.30	142.45	121.70
1	C	194	ASP	N-CA-C	-8.29	88.63	111.00
2	D	449	TYR	N-CA-C	-7.92	89.63	111.00
2	D	16	VAL	N-CA-C	-7.91	89.63	111.00
7	S	52	ALA	C-N-CA	7.62	140.75	121.70
2	D	17	ILE	N-CA-C	-7.41	91.00	111.00
4	H	45	PHE	N-CA-C	-7.36	91.13	111.00
1	C	407	GLY	N-CA-C	-7.31	94.83	113.10
7	S	107	THR	N-CA-C	7.29	130.68	111.00
1	B	25	LEU	N-CA-C	-7.14	91.72	111.00
2	E	22	ASP	N-CA-C	-7.00	92.11	111.00
2	F	345	TYR	N-CA-C	-6.95	92.24	111.00
1	B	508	PHE	N-CA-C	-6.95	92.25	111.00
2	D	20	VAL	N-CA-C	-6.79	92.65	111.00
2	D	161	GLY	N-CA-C	-6.77	96.17	113.10
2	E	355	SER	N-CA-C	-6.65	93.05	111.00
2	E	213	SER	N-CA-C	-6.63	93.10	111.00
3	G	78	CYS	N-CA-C	-6.61	93.16	111.00
3	G	188	GLU	C-N-CA	6.57	138.13	121.70
1	C	119	GLY	N-CA-C	-6.55	96.71	113.10
2	E	349	ASP	N-CA-C	-6.45	93.58	111.00
1	A	35	GLY	N-CA-C	-6.42	97.04	113.10
1	C	42	HIS	C-N-CA	6.42	135.79	122.30
3	G	268	GLY	N-CA-C	-6.41	97.07	113.10
3	G	151	SER	N-CA-C	-6.40	93.72	111.00
1	A	123	SER	N-CA-C	-6.33	93.90	111.00
1	C	313	ASN	C-N-CA	6.32	137.50	121.70
1	A	321	LEU	N-CA-C	-6.30	93.99	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	T	88	ARG	O-C-N	6.28	132.74	122.70
8	T	89	HIS	N-CA-C	-6.28	94.05	111.00
1	C	330	GLN	N-CA-C	-6.25	94.12	111.00
8	T	27	ALA	C-N-CA	6.25	137.33	121.70
2	E	118	ALA	N-CA-C	-6.25	94.13	111.00
1	A	411	ASP	C-N-CA	6.18	137.15	121.70
2	F	59	ARG	N-CA-C	-6.09	94.55	111.00
2	E	311	TYR	N-CA-C	-6.04	94.68	111.00
8	T	101	MET	CA-C-N	-6.04	103.92	117.20
1	C	362	ARG	N-CA-C	-5.99	94.83	111.00
2	D	21	VAL	N-CA-C	-5.97	94.89	111.00
3	G	177	PRO	N-CA-C	-5.96	96.60	112.10
2	F	127	SER	N-CA-C	-5.93	94.99	111.00
2	F	25	PHE	N-CA-C	-5.90	95.08	111.00
2	E	398	GLU	N-CA-C	5.85	126.78	111.00
1	A	157	VAL	N-CA-C	-5.84	95.24	111.00
1	B	506	ALA	C-N-CA	5.83	134.55	122.30
1	A	194	ASP	N-CA-C	-5.82	95.28	111.00
2	F	249	GLN	CA-C-N	-5.82	104.40	117.20
10	V	7	PRO	O-C-N	-5.82	113.39	122.70
1	A	88	VAL	N-CA-C	-5.81	95.31	111.00
1	C	157	VAL	N-CA-C	-5.81	95.32	111.00
4	H	46	GLY	N-CA-C	-5.80	98.60	113.10
1	A	313	ASN	C-N-CA	5.77	136.13	121.70
1	A	67	GLU	N-CA-C	-5.76	95.44	111.00
2	E	212	THR	N-CA-C	-5.76	95.44	111.00
7	S	9	VAL	C-N-CA	5.76	136.10	121.70
9	U	9	ASP	CA-C-N	5.76	129.87	117.20
1	A	362	ARG	N-CA-C	-5.74	95.52	111.00
1	B	372	SER	N-CA-C	-5.73	95.53	111.00
2	D	399	GLU	N-CA-C	-5.68	95.67	111.00
2	F	24	GLN	N-CA-C	-5.68	95.67	111.00
3	G	193	TYR	N-CA-C	-5.66	95.72	111.00
8	T	28	ILE	CA-C-N	-5.65	104.76	117.20
2	E	461	GLY	N-CA-C	-5.65	98.97	113.10
7	S	160	GLY	N-CA-C	5.65	127.23	113.10
1	B	30	ARG	N-CA-C	-5.63	95.79	111.00
2	D	276	PRO	N-CA-C	-5.62	97.48	112.10
1	A	96	ASP	N-CA-C	-5.61	95.85	111.00
1	B	100	GLY	N-CA-C	-5.58	99.16	113.10
4	H	93	LEU	N-CA-C	-5.57	95.96	111.00
2	D	52	HIS	N-CA-C	-5.57	95.96	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	118	ARG	C-N-CA	5.56	135.60	121.70
2	D	22	ASP	N-CA-C	-5.55	96.02	111.00
10	V	67	PRO	N-CA-C	5.54	126.51	112.10
1	C	321	LEU	N-CA-C	-5.48	96.21	111.00
3	G	77	LEU	CA-C-N	-5.45	105.22	117.20
1	C	267	ILE	N-CA-C	-5.45	96.30	111.00
2	E	41	ARG	C-N-CA	5.45	135.31	121.70
9	U	96	LYS	CA-C-N	-5.44	105.23	117.20
9	U	8	ILE	N-CA-C	-5.44	96.31	111.00
2	D	304	ILE	N-CA-C	-5.43	96.33	111.00
2	E	133	LEU	N-CA-C	-5.42	96.36	111.00
1	B	287	ARG	N-CA-C	-5.42	96.38	111.00
2	D	118	ALA	N-CA-C	-5.41	96.40	111.00
2	E	364	GLY	N-CA-C	-5.41	99.58	113.10
3	G	154	GLU	N-CA-C	-5.41	96.40	111.00
1	C	408	SER	C-N-CA	5.41	135.21	121.70
2	D	332	THR	N-CA-C	-5.41	96.41	111.00
2	D	112	GLN	N-CA-C	-5.39	96.43	111.00
2	E	16	VAL	N-CA-C	-5.39	96.46	111.00
2	E	298	THR	N-CA-C	-5.38	96.47	111.00
1	B	43	GLY	N-CA-C	-5.38	99.65	113.10
1	C	263	HIS	N-CA-C	-5.37	96.51	111.00
7	S	73	THR	N-CA-C	5.35	125.44	111.00
2	F	364	GLY	C-N-CA	5.34	135.06	121.70
3	G	160	ILE	N-CA-C	-5.34	96.57	111.00
4	H	32	ASN	C-N-CA	5.34	135.06	121.70
2	F	54	GLY	N-CA-C	-5.34	99.75	113.10
3	G	104	LYS	N-CA-C	-5.33	96.61	111.00
2	E	17	ILE	N-CA-C	-5.33	96.61	111.00
4	H	84	VAL	N-CA-C	-5.33	96.62	111.00
2	E	57	THR	N-CA-C	-5.31	96.66	111.00
3	G	266	ILE	N-CA-C	-5.29	96.73	111.00
1	B	334	VAL	C-N-CA	5.27	134.87	121.70
3	G	77	LEU	C-N-CA	5.27	134.87	121.70
1	B	330	GLN	N-CA-C	-5.26	96.79	111.00
7	S	123	ALA	N-CA-C	-5.26	96.80	111.00
1	C	504	PHE	C-N-CA	5.25	134.82	121.70
2	D	27	GLU	N-CA-C	-5.24	96.86	111.00
2	F	20	VAL	N-CA-C	-5.23	96.87	111.00
1	C	372	SER	N-CA-C	-5.23	96.88	111.00
1	B	289	PRO	N-CA-C	-5.22	98.53	112.10
1	A	336	ALA	N-CA-C	-5.21	96.94	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	504	PHE	C-N-CA	5.19	134.68	121.70
2	E	130	GLN	N-CA-C	-5.19	96.99	111.00
4	H	92	LEU	N-CA-C	-5.19	97.00	111.00
2	E	52	HIS	N-CA-C	-5.16	97.06	111.00
7	S	158	ILE	N-CA-C	-5.16	97.06	111.00
1	A	198	LYS	N-CA-C	-5.15	97.08	111.00
2	E	334	VAL	N-CA-C	-5.13	97.14	111.00
5	I	7	ALA	N-CA-C	-5.13	97.16	111.00
1	C	88	VAL	N-CA-C	-5.13	97.16	111.00
5	I	28	THR	C-N-CA	5.12	134.50	121.70
1	C	195	GLU	C-N-CA	5.11	134.47	121.70
1	A	38	ILE	N-CA-C	-5.07	97.31	111.00
2	D	54	GLY	N-CA-C	-5.07	100.44	113.10
1	C	509	GLU	N-CA-C	-5.06	97.34	111.00
4	H	61	GLY	N-CA-C	-5.06	100.46	113.10
1	C	490	SER	C-N-CA	5.05	134.34	121.70
1	A	432	GLN	N-CA-C	-5.05	97.36	111.00
2	D	312	VAL	N-CA-C	-5.05	97.36	111.00
7	S	71	ASP	C-N-CA	5.04	134.31	121.70
3	G	204	TYR	N-CA-C	-5.04	97.39	111.00
2	D	75	VAL	N-CA-C	-5.03	97.42	111.00
4	H	91	GLN	N-CA-C	-5.03	97.42	111.00
1	C	67	GLU	N-CA-C	-5.03	97.42	111.00
2	F	221	GLN	C-N-CA	5.03	134.27	121.70
1	A	366	ASN	C-N-CA	5.02	134.25	121.70
2	F	392	GLY	N-CA-C	-5.02	100.54	113.10
2	E	25	PHE	N-CA-C	-5.02	97.45	111.00
2	E	157	GLY	N-CA-C	-5.00	100.59	113.10

There are no chirality outliers.

All (75) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	336	ALA	Peptide
1	B	379	GLN	Mainchain
1	B	505	LEU	Mainchain
1	C	169	GLY	Mainchain
1	C	24	ASP	Mainchain
2	E	101	PRO	Mainchain
2	E	354	THR	Mainchain,Peptide
2	E	397	SER	Mainchain
2	E	453	PRO	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
2	F	25	PHE	Mainchain
2	F	329	LEU	Mainchain
7	S	106	SER	Mainchain,Peptide
7	S	152	VAL	Peptide
7	S	156	PRO	Peptide
7	S	159	MET	Mainchain
7	S	161	GLY	Mainchain
7	S	70	SER	Peptide
7	S	73	THR	Peptide
8	T	101	MET	Mainchain
8	T	108	ARG	Mainchain
8	T	132	MET	Mainchain
8	T	138	GLU	Mainchain
8	T	148	VAL	Mainchain,Peptide
8	T	162	ALA	Mainchain
8	T	172	SER	Peptide
8	T	173	LYS	Peptide
8	T	25	PHE	Mainchain
8	T	27	ALA	Peptide
8	T	28	ILE	Mainchain
8	T	32	GLY	Mainchain
8	T	89	HIS	Mainchain
8	T	90	TYR	Mainchain
9	U	11	VAL	Mainchain
9	U	110	GLN	Mainchain
9	U	12	ALA	Mainchain
9	U	13	PHE	Mainchain,Peptide
9	U	16	ILE	Mainchain
9	U	17	ILE	Mainchain
9	U	41	THR	Mainchain
9	U	61	ALA	Mainchain
9	U	82	LYS	Mainchain,Peptide
9	U	83	TYR	Mainchain
9	U	93	GLU	Mainchain
9	U	96	LYS	Mainchain
9	U	97	SER	Mainchain
10	V	14	ASP	Mainchain
10	V	27	GLY	Peptide
10	V	28	GLY	Peptide
10	V	35	GLU	Mainchain
10	V	5	LEU	Mainchain
10	V	57	ASN	Mainchain

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Mol	Chain	Res	Type	Group
10	V	6	ASP	Mainchain,Peptide
10	V	8	VAL	Mainchain
11	W	10	ILE	Mainchain
11	W	132	GLY	Mainchain
11	W	133	THR	Mainchain
11	W	167	GLY	Mainchain
11	W	174	ILE	Peptide
11	W	175	GLY	Peptide
11	W	177	ALA	Mainchain
11	W	179	LEU	Mainchain
11	W	189	ALA	Mainchain
11	W	193	PHE	Mainchain
11	W	196	LEU	Mainchain
11	W	35	ASN	Peptide
11	W	63	SER	Mainchain
11	W	64	LYS	Mainchain
11	W	90	HIS	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2035	0	589	8	0
1	B	1918	0	553	3	0
1	C	1947	0	563	7	0
2	D	1867	0	533	6	0
2	E	1863	0	532	6	0
2	F	1863	0	532	5	0
3	G	1053	0	283	3	0
4	H	523	0	140	1	0
5	I	187	0	53	0	0
6	J	288	0	92	0	0
6	K	288	0	92	0	0
6	L	288	0	92	0	0
6	M	288	0	92	0	0
6	N	288	0	92	0	0
6	O	288	0	92	0	0
6	P	288	0	92	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Q	288	0	92	0	0
7	S	669	0	179	10	0
8	T	697	0	182	3	0
9	U	484	0	121	0	0
10	V	265	0	68	0	0
11	W	869	0	226	3	0
All	All	18544	0	5290	49	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 2.

All (49) 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)
7:S:107:THR:CA	7:S:107:THR:C	1.89	1.39
7:S:106:SER:O	7:S:107:THR:C	2.22	0.78
1:B:49:ALA:H	2:F:69:LEU:H	1.36	0.74
4:H:50:ALA:O	6:P:39:ASN:C	2.31	0.69
11:W:172:HIS:O	11:W:175:GLY:HA3	1.93	0.69
2:D:160:VAL:H	2:D:162:LYS:H	1.47	0.62
3:G:267:SER:H	3:G:270:ALA:H	1.52	0.58
3:G:267:SER:H	3:G:270:ALA:N	2.03	0.57
2:E:159:GLY:N	2:E:163:THR:H	2.06	0.54
1:C:261:GLY:HA2	1:C:317:GLY:HA3	1.89	0.54
1:A:49:ALA:H	2:E:69:LEU:N	2.08	0.52
2:F:417:PRO:C	2:F:429:GLY:HA2	2.31	0.51
2:D:473:LEU:C	2:D:475:GLU:H	2.14	0.51
1:A:6:ALA:C	1:A:8:VAL:H	2.14	0.49
8:T:24:THR:CA	11:W:176:GLY:HA2	2.42	0.49
1:A:261:GLY:HA3	1:A:317:GLY:HA3	1.94	0.48
1:A:26:GLU:CA	1:A:45:ARG:H	2.26	0.48
1:C:49:ALA:H	2:D:69:LEU:N	2.11	0.48
2:D:419:GLN:CA	2:D:429:GLY:H	2.27	0.48
7:S:107:THR:CA	7:S:112:HIS:CA	2.91	0.48
1:C:172:GLN:C	1:C:174:GLY:H	2.16	0.48
7:S:28:LYS:C	7:S:30:ASN:H	2.17	0.48
8:T:24:THR:C	11:W:176:GLY:HA2	2.35	0.47
1:C:285:LEU:C	1:C:287:ARG:H	2.19	0.46
1:A:261:GLY:CA	1:A:317:GLY:HA3	2.46	0.45
2:E:419:GLN:H	2:E:429:GLY:H	1.63	0.45
7:S:105:PHE:O	7:S:107:THR:CA	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:14:ILE:C	7:S:16:GLY:H	2.19	0.45
2:E:419:GLN:N	2:E:429:GLY:H	2.15	0.45
3:G:184:ILE:C	3:G:186:SER:H	2.19	0.45
8:T:89:HIS:O	8:T:90:TYR:C	2.55	0.45
2:F:368:TYR:O	2:F:372:ARG:N	2.51	0.43
2:D:160:VAL:N	2:D:162:LYS:H	2.14	0.43
1:B:49:ALA:H	2:F:69:LEU:N	2.11	0.43
1:C:189:PHE:C	1:C:192:GLY:H	2.23	0.42
2:F:381:TYR:O	2:F:385:GLN:N	2.51	0.42
7:S:105:PHE:O	7:S:107:THR:N	2.53	0.42
7:S:111:VAL:C	7:S:113:ARG:H	2.23	0.42
1:C:44:LEU:C	1:C:46:ASN:H	2.24	0.41
1:A:149:GLY:HA3	1:A:436:MET:H	1.85	0.41
1:A:105:GLY:HA2	1:A:226:MET:O	2.21	0.41
7:S:57:ASN:C	7:S:59:TYR:H	2.24	0.41
1:B:172:GLN:C	1:B:174:GLY:H	2.24	0.41
7:S:89:LEU:O	7:S:93:GLY:HA2	2.21	0.40
2:E:350:PRO:C	2:E:352:ASP:H	2.25	0.40
2:E:388:ILE:C	2:E:391:LEU:H	2.25	0.40
1:A:258:ARG:O	1:A:319:GLY:HA3	2.22	0.40
1:C:258:ARG:O	1:C:319:GLY:HA3	2.21	0.40
2:D:341:GLU:C	2:D:343:GLY:H	2.25	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	507/510 (99%)	455 (90%)	35 (7%)	17 (3%)	3 26
1	B	476/510 (93%)	428 (90%)	27 (6%)	21 (4%)	2 22
1	C	485/510 (95%)	431 (89%)	33 (7%)	21 (4%)	2 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	465/482 (96%)	418 (90%)	31 (7%)	16 (3%)	3 26
2	E	464/482 (96%)	411 (89%)	26 (6%)	27 (6%)	1 18
2	F	464/482 (96%)	419 (90%)	33 (7%)	12 (3%)	5 31
3	G	258/273 (94%)	198 (77%)	33 (13%)	27 (10%)	0 8
4	H	129/146 (88%)	115 (89%)	11 (8%)	3 (2%)	6 34
5	I	45/50 (90%)	31 (69%)	11 (24%)	3 (7%)	1 15
6	J	70/72 (97%)	62 (89%)	6 (9%)	2 (3%)	4 29
6	K	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	11 46
6	L	70/72 (97%)	57 (81%)	13 (19%)	0	100 100
6	M	70/72 (97%)	64 (91%)	4 (6%)	2 (3%)	4 29
6	N	70/72 (97%)	61 (87%)	9 (13%)	0	100 100
6	O	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	11 46
6	P	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	11 46
6	Q	70/72 (97%)	61 (87%)	7 (10%)	2 (3%)	4 29
7	S	166/190 (87%)	107 (64%)	38 (23%)	21 (13%)	0 5
8	T	172/174 (99%)	158 (92%)	9 (5%)	5 (3%)	4 29
9	U	119/124 (96%)	94 (79%)	19 (16%)	6 (5%)	2 20
10	V	65/77 (84%)	48 (74%)	10 (15%)	7 (11%)	0 8
11	W	215/217 (99%)	186 (86%)	25 (12%)	4 (2%)	8 38
All	All	4590/4803 (96%)	3996 (87%)	395 (9%)	199 (4%)	5 22

All (199) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	14	GLU
1	A	224	ASP
1	A	238	ASP
1	A	374	VAL
1	B	57	SER
1	B	171	ARG
1	B	289	PRO
1	B	331	ALA
1	B	455	LYS
1	C	27	GLU

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Mol	Chain	Res	Type
1	C	238	ASP
1	C	289	PRO
1	C	405	GLN
1	C	409	ASP
2	D	31	PRO
2	D	102	ILE
2	D	249	GLN
2	D	277	SER
2	D	282	GLN
2	D	393	MET
2	D	450	ASP
2	D	451	HIS
2	E	118	ALA
2	E	158	ALA
2	E	276	PRO
2	E	348	VAL
2	E	360	PRO
2	E	395	GLU
2	E	450	ASP
2	F	276	PRO
3	G	50	ALA
3	G	55	ALA
3	G	119	THR
3	G	151	SER
3	G	189	SER
3	G	199	ASP
3	G	250	PHE
4	H	68	GLU
4	H	101	ASP
5	I	9	LEU
7	S	29	GLN
7	S	47	LYS
7	S	79	SER
7	S	93	GLY
7	S	123	ALA
7	S	153	LYS
7	S	159	MET
8	T	151	SER
9	U	83	TYR
9	U	84	THR
9	U	98	CYS
10	V	26	SER

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Mol	Chain	Res	Type
10	V	67	PRO
11	W	175	GLY
11	W	176	GLY
1	A	488	LYS
1	B	80	LYS
1	B	224	ASP
1	B	238	ASP
1	B	374	VAL
1	B	430	GLN
1	B	488	LYS
1	B	505	LEU
1	C	47	VAL
1	C	172	GLN
1	C	224	ASP
1	C	319	GLY
1	C	365	ILE
1	C	374	VAL
1	C	433	TYR
1	C	455	LYS
2	D	55	GLU
2	D	348	VAL
2	E	132	ILE
2	E	210	ASP
2	E	297	THR
2	E	394	ASP
2	E	396	LEU
2	F	27	GLU
2	F	176	ALA
2	F	209	LYS
2	F	223	ASN
3	G	9	ARG
3	G	87	LYS
3	G	93	ALA
3	G	194	ASP
3	G	200	VAL
3	G	257	VAL
5	I	6	GLN
5	I	42	ILE
7	S	115	GLU
7	S	147	VAL
7	S	148	LEU
7	S	150	LEU

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Mol	Chain	Res	Type
8	T	147	ARG
9	U	49	ILE
10	V	30	VAL
10	V	32	ALA
1	A	11	ILE
1	A	25	LEU
1	A	123	SER
1	A	146	MET
1	B	26	GLU
1	B	35	GLY
1	B	101	GLU
1	C	406	PHE
1	C	453	LEU
2	E	44	ARG
2	E	73	GLN
2	E	100	GLU
2	E	361	ASN
2	F	102	ILE
2	F	300	LYS
2	F	450	ASP
3	G	10	LEU
3	G	134	ARG
3	G	267	SER
3	G	269	ALA
6	J	45	GLN
7	S	4	LEU
7	S	106	SER
7	S	129	THR
9	U	99	ALA
1	A	18	GLY
1	A	172	GLN
1	A	289	PRO
1	A	433	TYR
1	B	209	LYS
1	B	365	ILE
1	B	435	PRO
1	C	56	SER
1	C	95	VAL
1	C	143	ARG
1	C	145	PRO
1	C	171	ARG
2	D	180	TYR

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Mol	Chain	Res	Type
2	D	221	GLN
2	D	276	PRO
2	D	357	ILE
2	E	30	PRO
2	E	55	GLU
2	E	102	ILE
2	E	126	MET
2	E	146	TYR
2	E	352	ASP
3	G	88	GLN
3	G	92	GLU
3	G	117	HIS
3	G	135	PRO
3	G	195	ASP
3	G	258	ILE
3	G	268	GLY
3	G	270	ALA
6	P	40	PRO
6	Q	44	GLN
7	S	9	VAL
7	S	52	ALA
7	S	60	VAL
7	S	92	ASN
8	T	171	LEU
9	U	47	PRO
11	W	36	ARG
1	A	145	PRO
1	C	194	ASP
2	D	394	ASP
2	E	127	SER
2	E	161	GLY
2	E	452	LEU
2	F	44	ARG
2	F	279	VAL
2	F	312	VAL
2	F	363	VAL
3	G	201	LEU
6	O	39	ASN
7	S	140	SER
10	V	6	ASP
10	V	53	LYS
11	W	40	ASN

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Mol	Chain	Res	Type
1	A	235	THR
2	D	279	VAL
3	G	69	ILE
7	S	8	PRO
8	T	19	VAL
1	B	47	VAL
2	E	279	VAL
6	M	40	PRO
7	S	152	VAL
1	A	288	PRO
1	B	121	ILE
4	H	39	PRO
1	B	115	ILE
2	E	363	VAL
6	J	40	PRO
6	M	71	ILE
8	T	148	VAL
10	V	34	PRO
6	K	40	PRO
6	Q	40	PRO

5.3.2 Protein sidechains

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers (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

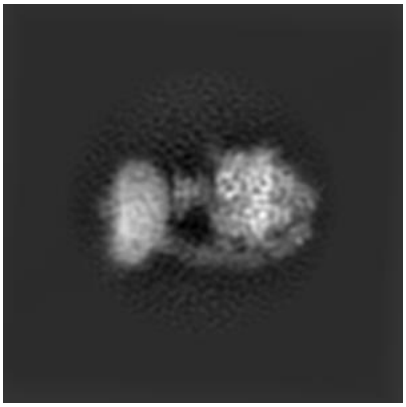
This section contains visualisations of the EMDB entry EMD-3166. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

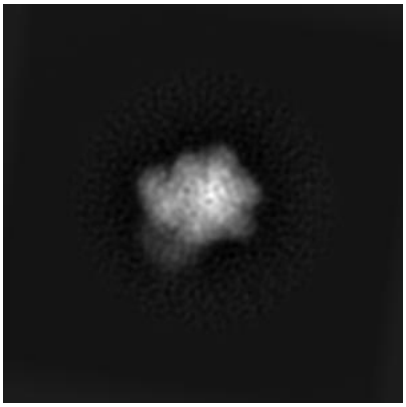
6.1 Orthogonal projections

6.1.1 Primary map

X



Y



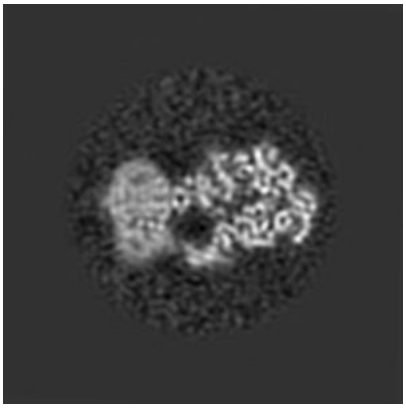
Z

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

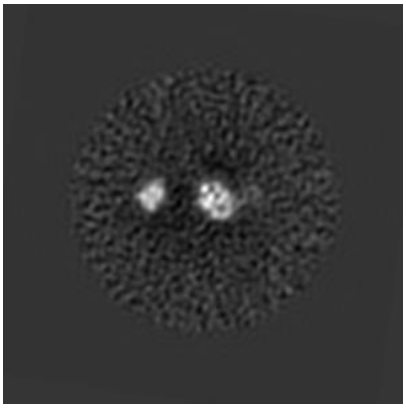
6.2 Central slices

6.2.1 Primary map

X Index: 128



Y Index: 128



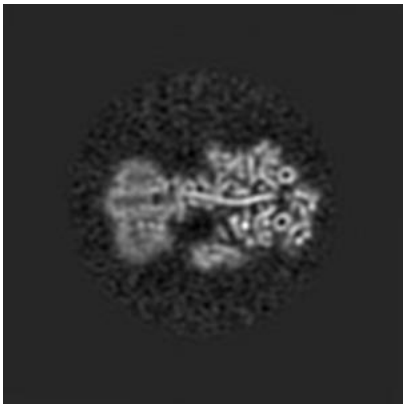
Z Index: 128

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

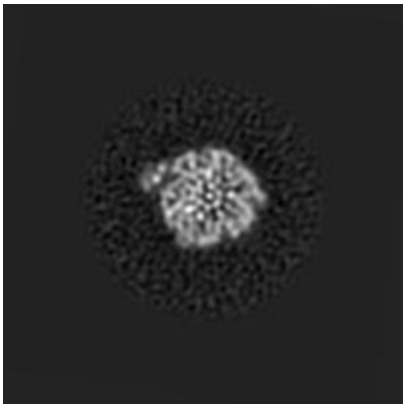
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 133



Y Index: 132

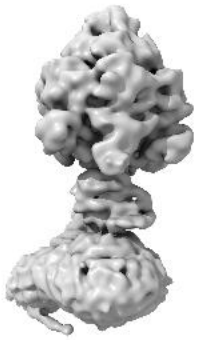


Z Index: 166

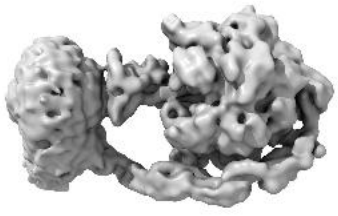
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

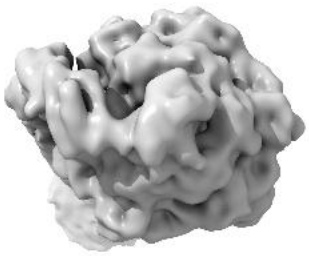
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

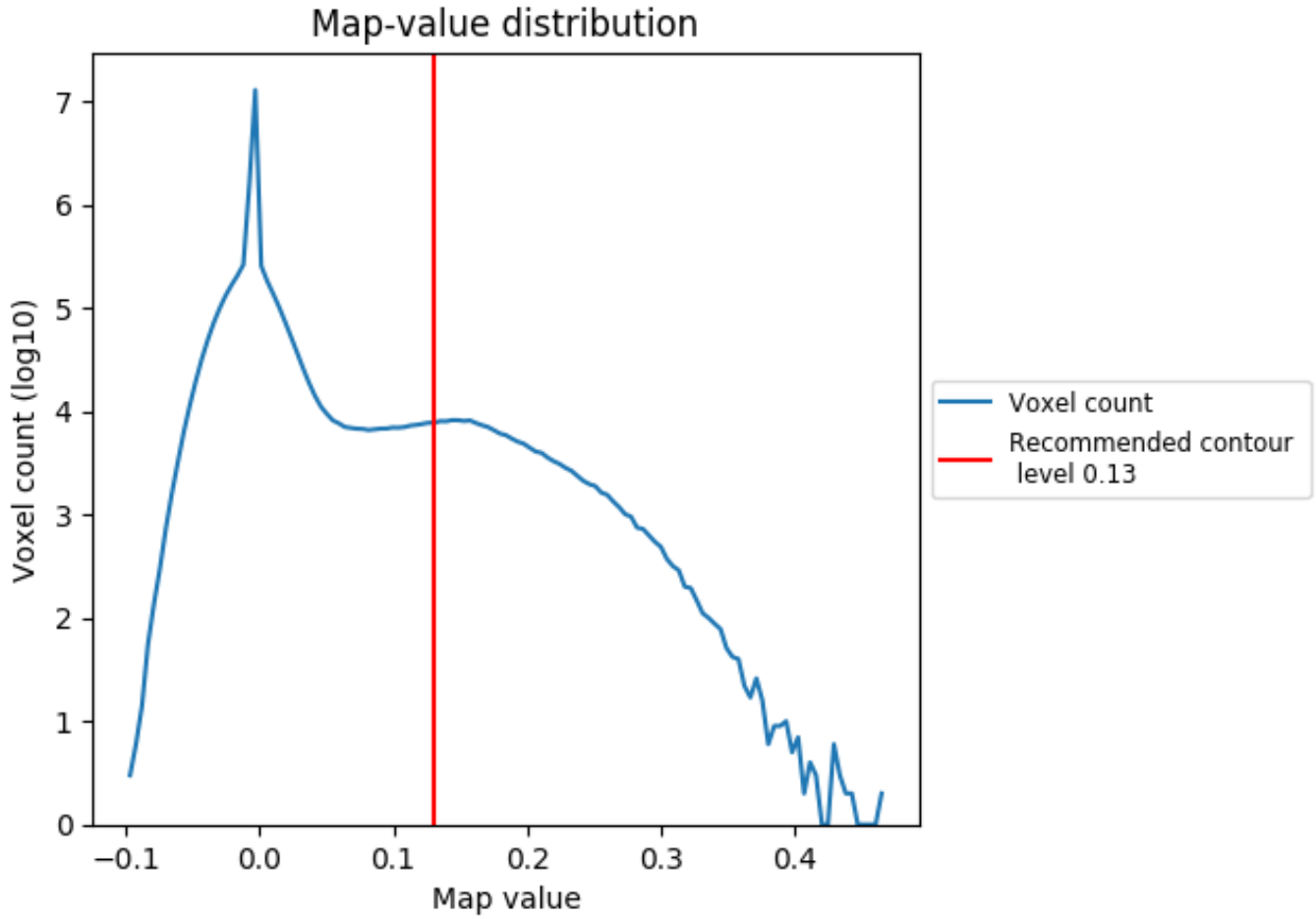
6.5 Mask visualisation (i)

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

7 Map analysis

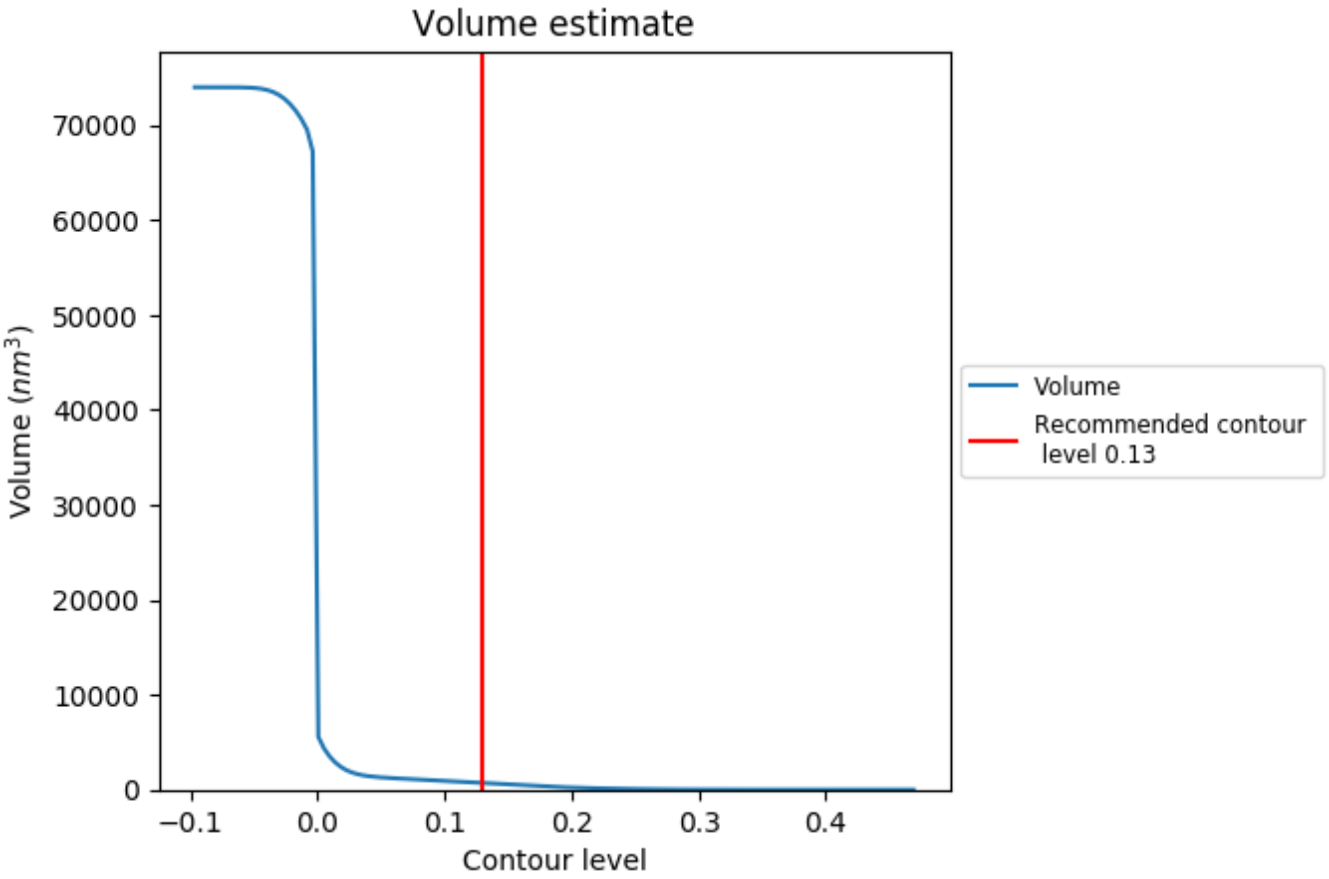
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

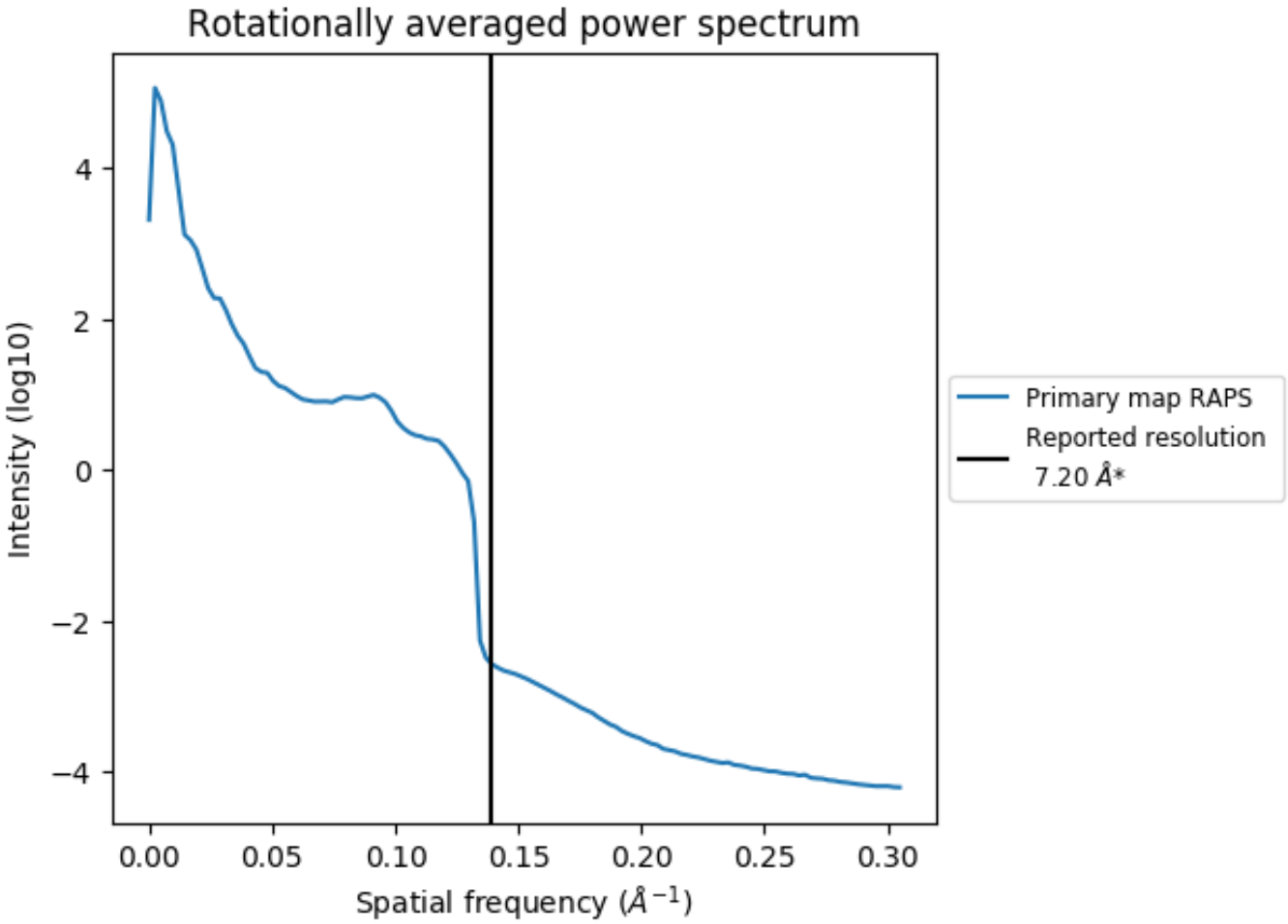
7.2 Volume estimate



The volume at the recommended contour level is 719 nm^3; this corresponds to an approximate mass of 649 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 0.139 Å^{-1}

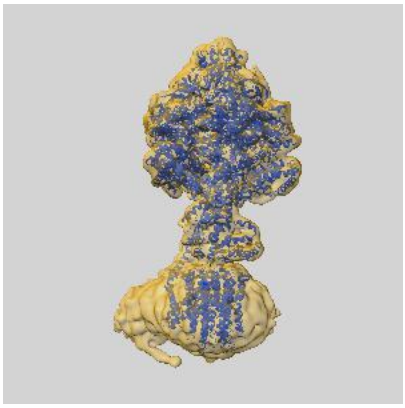
8 Fourier-Shell correlation

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

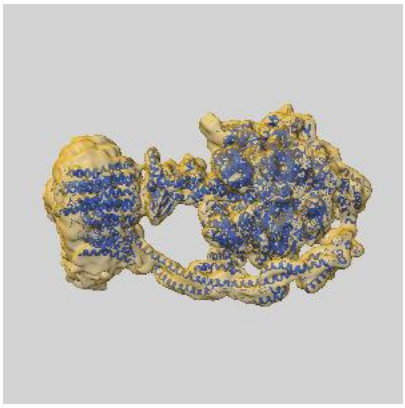
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3166 and PDB model 5ARH. Per-residue inclusion information can be found in section 3 on page 7.

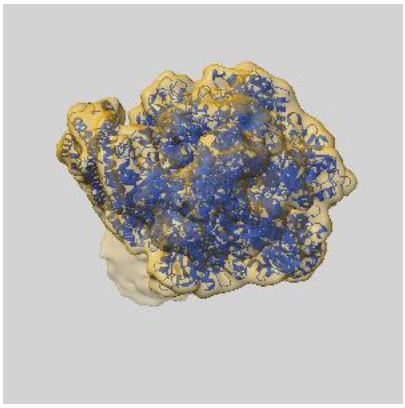
9.1 Map-model overlay



X



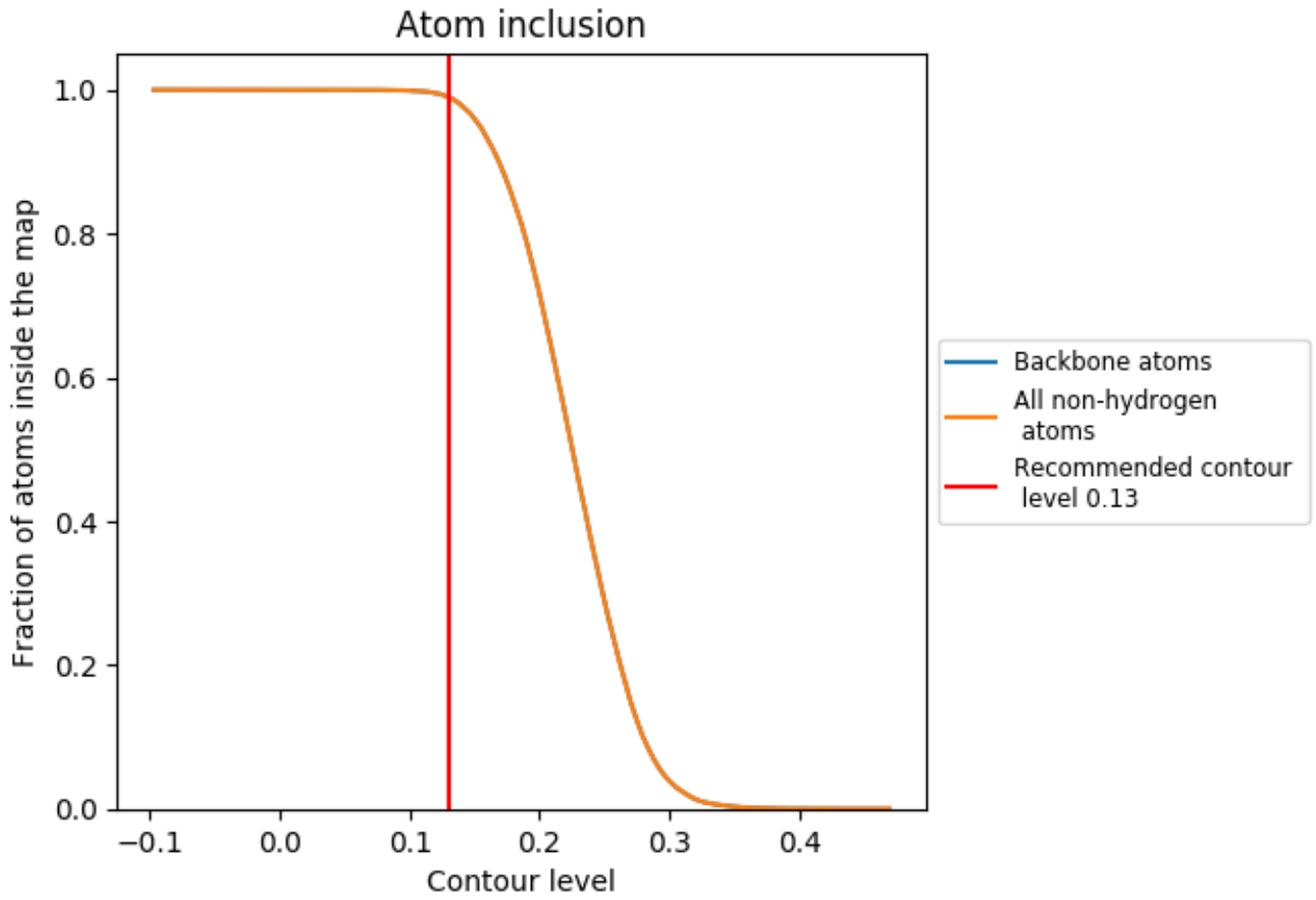
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13 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 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.