Full wwPDB EM Validation Report

Dec 6, 2020 – 01:24 am GMT

PDB ID	:	5ARE
EMDB ID	:	EMD-3165
Title	:	Bovine mitochondrial ATP synthase state 1b
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	:	7.40 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:

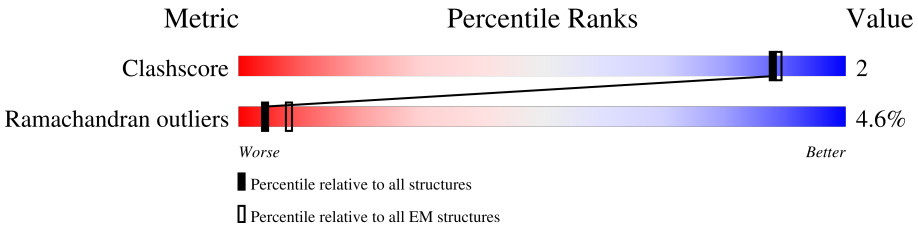
EMDB validation analysis	:	0.0.0.dev61
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.15.1

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 7.40 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	87% 12% •
1	B	510	83% 10% • 6%
1	C	510	86% 9% • 5%
2	D	482	86% 11% •
2	E	482	84% 11% • •
2	F	482	87% 10% •
3	G	273	85% 11% •• •
4	H	146	68% 21% 10%
5	I	50	86% 6% • 6%

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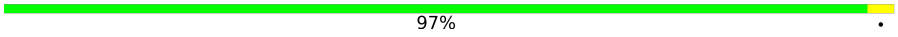
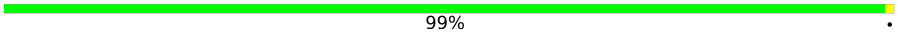
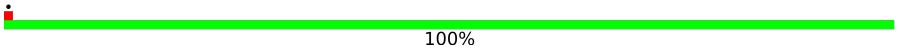
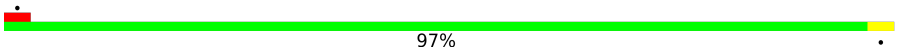
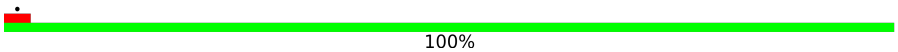
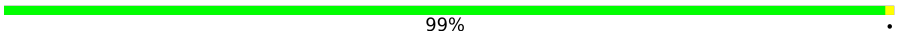
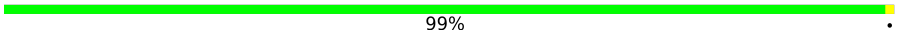
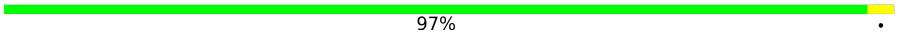
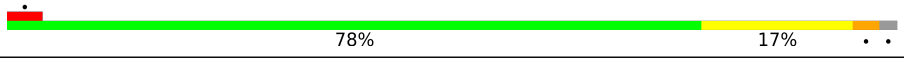
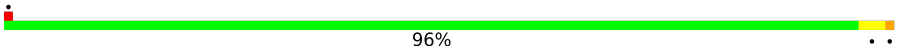
Mol	Chain	Length	Quality of chain
6	J	72	
6	K	72	
6	L	72	
6	M	72	
6	N	72	
6	O	72	
6	P	72	
6	Q	72	
7	S	190	
8	T	174	
9	U	124	
10	V	77	
11	W	217	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 18545 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	122	Total 485	C 242	N 122	O 121	0	1

- 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.

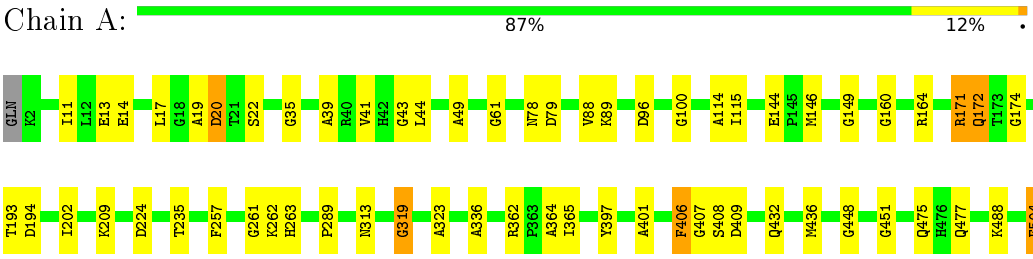
Mol	Chain	Residues	Atoms				AltConf	Trace
11	W	217	Total 869	C 434	N 217	O 218	0	0

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.

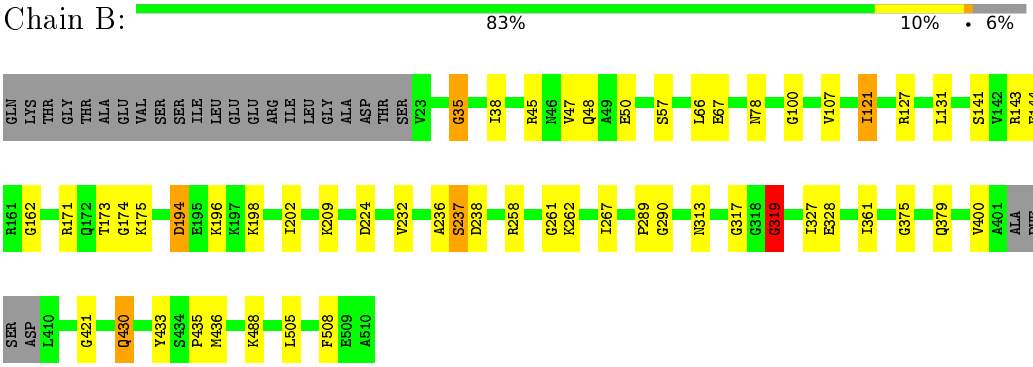
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain A:



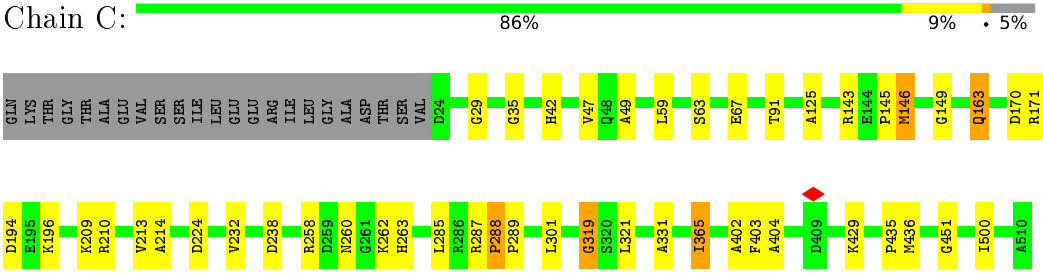
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain B:



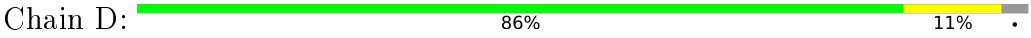
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

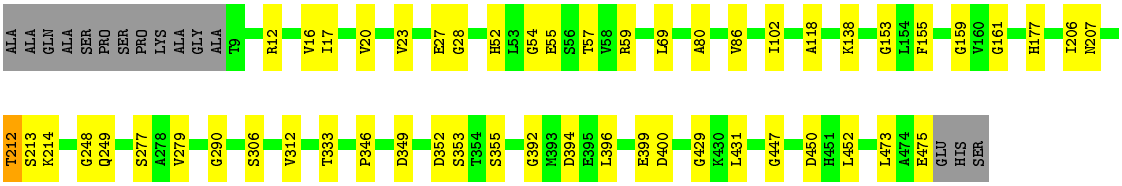
Chain C:



- Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

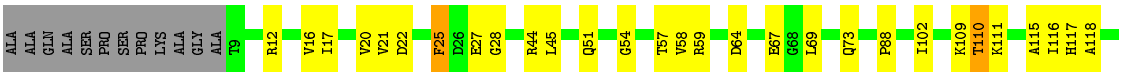
Chain D:





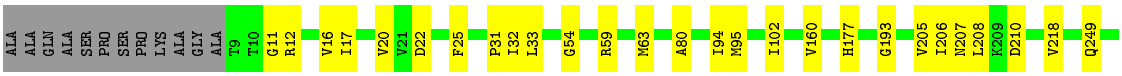
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

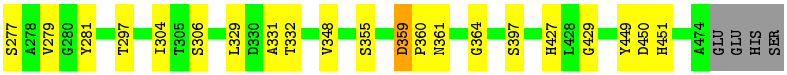
Chain E:



• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

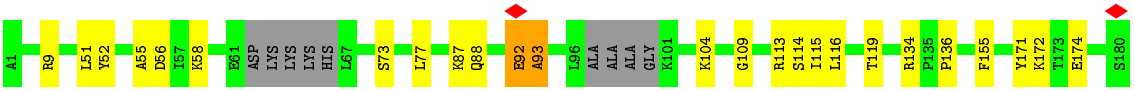
Chain F:

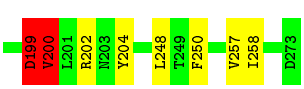




• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

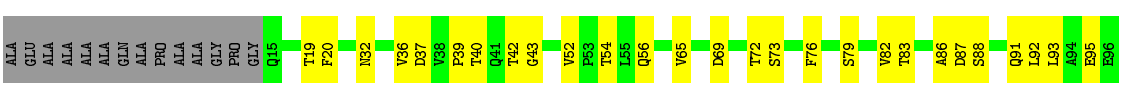
Chain G:

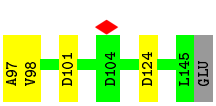




• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL

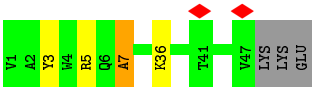
Chain H:





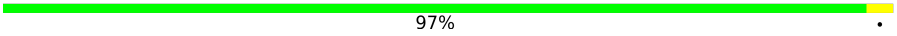
• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL

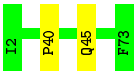
Chain I:



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

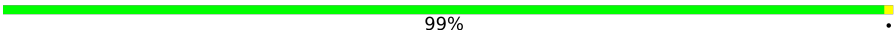
Chain J:





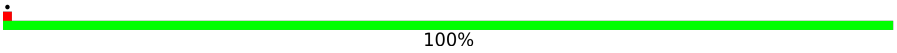
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

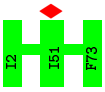
Chain K:



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

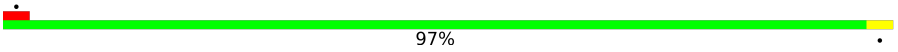
Chain L:

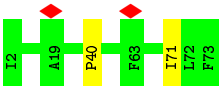




• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

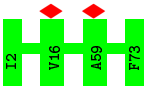
Chain M:





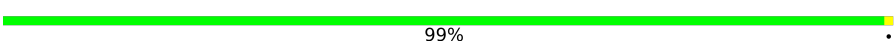
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain N:



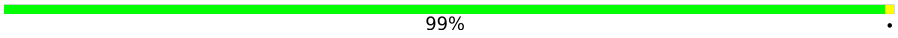
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain O:



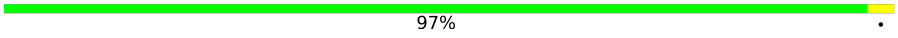
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

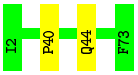
Chain P:



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

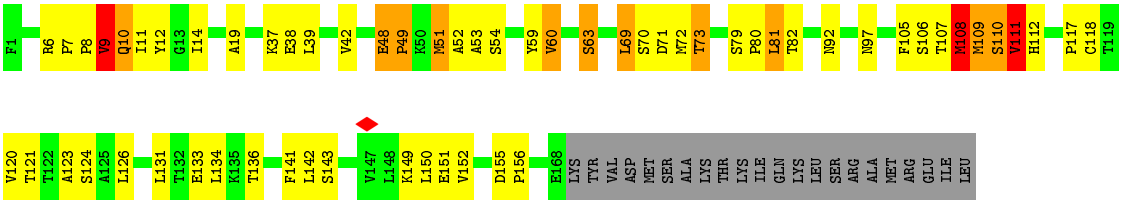
Chain Q:





• Molecule 7: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL

Chain S:

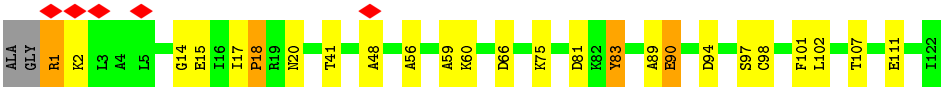


• Molecule 8: ATP SYNTHASE F(0) COMPLEX SUBUNIT B1, MITOCHONDRIAL

Chain T:

• Molecule 9: ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL

Chain U:

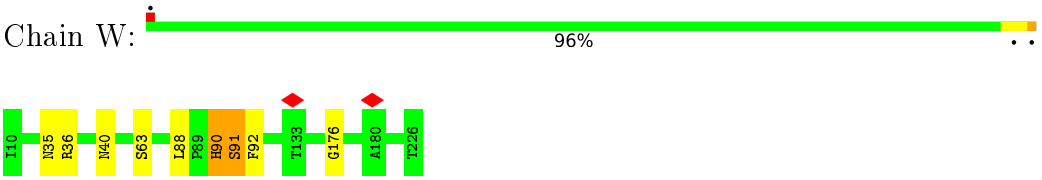


• Molecule 10: ATP SYNTHASE-COUPLING FACTOR 6, MITOCHONDRIAL

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	22935	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	0.411	Depositor
Minimum map value	-0.087	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	1.82	6/2034 (0.3%)	1.48	22/2541 (0.9%)
1	B	1.85	4/1916 (0.2%)	1.53	21/2392 (0.9%)
1	C	1.76	6/1946 (0.3%)	1.50	16/2431 (0.7%)
2	D	1.77	5/1866 (0.3%)	1.51	27/2331 (1.2%)
2	E	1.78	3/1862 (0.2%)	1.56	30/2326 (1.3%)
2	F	1.78	5/1862 (0.3%)	1.49	23/2326 (1.0%)
3	G	1.68	2/1050 (0.2%)	1.52	13/1308 (1.0%)
4	H	1.93	0/522	1.83	16/651 (2.5%)
5	I	1.68	0/186	1.35	1/231 (0.4%)
6	J	0.30	0/287	0.42	0/357
6	K	0.30	0/287	0.42	0/357
6	L	0.30	0/287	0.45	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	0.30	0/287	0.42	0/357
6	Q	0.30	0/287	0.44	0/357
7	S	1.01	5/668 (0.7%)	1.79	16/834 (1.9%)
8	T	0.87	2/696 (0.3%)	1.05	3/867 (0.3%)
9	U	0.77	0/484	1.18	1/604 (0.2%)
10	V	0.78	0/264	1.31	1/329 (0.3%)
11	W	0.44	0/868	0.72	1/1082 (0.1%)
All	All	1.55	38/18520 (0.2%)	1.39	191/23109 (0.8%)

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	4
1	B	0	3
1	C	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
2	E	0	5
2	F	0	4
3	G	0	5
4	H	0	2
7	S	0	38
8	T	0	16
9	U	0	30
10	V	0	16
11	W	0	5
All	All	0	132

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	T	93	ASP	N-CA	9.53	1.65	1.46
2	D	429	GLY	CA-C	-7.32	1.40	1.51
7	S	6	ARG	CA-C	6.89	1.70	1.52
1	C	35	GLY	CA-C	-6.80	1.41	1.51
7	S	6	ARG	C-N	6.77	1.47	1.34
7	S	7	PRO	N-CA	6.50	1.58	1.47
1	C	500	ILE	CA-C	-6.21	1.36	1.52
1	A	43	GLY	CA-C	-5.87	1.42	1.51
7	S	48	GLU	C-N	5.84	1.45	1.34
2	D	161	GLY	N-CA	-5.83	1.37	1.46
1	B	174	GLY	N-CA	-5.66	1.37	1.46
1	C	319	GLY	CA-C	-5.64	1.42	1.51
7	S	71	ASP	N-CA	5.63	1.57	1.46
1	A	319	GLY	CA-C	-5.49	1.43	1.51
1	A	257	PHE	CA-C	-5.48	1.38	1.52
2	D	290	GLY	CA-C	-5.46	1.43	1.51
2	D	153	GLY	CA-C	-5.46	1.43	1.51
2	F	11	GLY	CA-C	-5.45	1.43	1.51
2	E	12	ARG	CA-C	-5.42	1.38	1.52
1	A	451	GLY	CA-C	-5.38	1.43	1.51
1	B	319	GLY	CA-C	-5.38	1.43	1.51
2	E	58	VAL	N-CA	-5.37	1.35	1.46
1	C	35	GLY	N-CA	-5.36	1.38	1.46
2	F	429	GLY	CA-C	-5.27	1.43	1.51
2	F	193	GLY	CA-C	-5.25	1.43	1.51
1	B	35	GLY	CA-C	-5.20	1.43	1.51
2	E	51	GLN	CA-C	-5.17	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	448	GLY	CA-C	-5.15	1.43	1.51
2	D	400	ASP	N-CA	-5.11	1.36	1.46
1	A	174	GLY	N-CA	-5.09	1.38	1.46
2	F	95	MET	N-CA	-5.07	1.36	1.46
1	B	421	GLY	CA-C	-5.06	1.43	1.51
1	C	213	VAL	N-CA	-5.06	1.36	1.46
1	C	301	LEU	CA-C	-5.05	1.39	1.52
8	T	94	VAL	N-CA	-5.05	1.36	1.46
2	F	25	PHE	CA-C	-5.03	1.39	1.52
3	G	174	GLU	CA-C	-5.02	1.40	1.52
3	G	109	GLY	CA-C	-5.02	1.43	1.51

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	S	48	GLU	O-C-N	13.96	147.63	121.10
7	S	48	GLU	CA-C-N	-11.40	85.17	117.10
7	S	6	ARG	CA-C-O	-9.20	100.79	120.10
7	S	108	MET	CA-C-O	-9.10	100.99	120.10
1	A	407	GLY	N-CA-C	-9.02	90.54	113.10
9	U	1	ARG	CA-C-O	-8.86	101.50	120.10
1	B	290	GLY	N-CA-C	-8.66	91.44	113.10
8	T	92	PHE	C-N-CA	8.47	142.87	121.70
2	D	355	SER	N-CA-C	-8.25	88.73	111.00
2	D	27	GLU	N-CA-C	-8.11	89.10	111.00
4	H	83	THR	N-CA-C	-7.95	89.55	111.00
7	S	9	VAL	O-C-N	-7.91	110.04	122.70
7	S	108	MET	C-N-CA	7.86	141.34	121.70
2	E	16	VAL	N-CA-C	-7.79	89.96	111.00
2	D	161	GLY	N-CA-C	-7.78	93.66	113.10
7	S	51	MET	C-N-CA	-7.72	102.40	121.70
2	D	312	VAL	N-CA-C	-7.69	90.23	111.00
1	C	172	GLN	C-N-CA	7.65	140.82	121.70
8	T	93	ASP	CA-C-N	-7.56	100.57	117.20
1	A	100	GLY	N-CA-C	-7.55	94.24	113.10
1	A	35	GLY	N-CA-C	-7.48	94.40	113.10
1	B	202	ILE	N-CA-C	-7.41	90.99	111.00
7	S	59	TYR	C-N-CA	7.39	140.18	121.70
1	C	35	GLY	N-CA-C	-7.33	94.78	113.10
2	E	59	ARG	N-CA-C	-7.27	91.36	111.00
1	B	198	LYS	N-CA-C	-7.06	91.94	111.00
1	B	327	ILE	N-CA-C	-7.00	92.10	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	95	MET	N-CA-C	-6.90	92.36	111.00
1	B	47	VAL	C-N-CA	6.90	138.94	121.70
2	D	20	VAL	N-CA-C	-6.86	92.47	111.00
2	F	449	TYR	N-CA-C	-6.86	92.47	111.00
11	W	88	LEU	CA-C-O	-6.85	105.72	120.10
1	C	172	GLN	CA-C-N	-6.84	102.16	117.20
2	F	20	VAL	N-CA-C	-6.73	92.83	111.00
4	H	93	LEU	N-CA-C	-6.72	92.86	111.00
2	E	345	TYR	N-CA-C	-6.69	92.94	111.00
3	G	172	LYS	N-CA-C	-6.61	93.16	111.00
2	F	332	THR	N-CA-C	-6.58	93.23	111.00
1	A	202	ILE	N-CA-C	-6.57	93.27	111.00
3	G	51	LEU	N-CA-C	-6.56	93.28	111.00
2	E	355	SER	N-CA-C	-6.50	93.46	111.00
7	S	51	MET	O-C-N	-6.46	112.36	122.70
2	E	54	GLY	N-CA-C	-6.45	96.99	113.10
2	E	20	VAL	N-CA-C	-6.44	93.61	111.00
2	F	17	ILE	N-CA-C	-6.41	93.70	111.00
1	B	488	LYS	N-CA-C	-6.37	93.79	111.00
1	A	20	ASP	N-CA-C	-6.36	93.82	111.00
2	E	45	LEU	N-CA-C	-6.32	93.92	111.00
7	S	110	SER	C-N-CA	6.32	137.51	121.70
2	F	94	ILE	N-CA-C	-6.32	93.93	111.00
2	D	349	ASP	N-CA-C	-6.31	93.97	111.00
1	B	121	ILE	N-CA-C	-6.30	93.98	111.00
4	H	72	THR	N-CA-C	-6.25	94.12	111.00
1	B	100	GLY	N-CA-C	-6.24	97.50	113.10
1	C	170	ASP	C-N-CA	6.24	137.29	121.70
2	E	21	VAL	N-CA-C	-6.18	94.32	111.00
2	D	54	GLY	N-CA-C	-6.15	97.72	113.10
7	S	108	MET	CA-C-N	6.15	130.73	117.20
1	C	67	GLU	N-CA-C	-6.14	94.41	111.00
2	D	212	THR	N-CA-C	-6.13	94.44	111.00
2	D	206	ILE	N-CA-C	-6.11	94.49	111.00
2	F	54	GLY	N-CA-C	-6.11	97.82	113.10
4	H	56	GLN	N-CA-C	-6.10	94.53	111.00
1	B	67	GLU	N-CA-C	-6.10	94.54	111.00
1	A	88	VAL	N-CA-C	-6.07	94.60	111.00
2	F	12	ARG	N-CA-C	-6.05	94.67	111.00
1	B	162	GLY	N-CA-C	-6.03	98.02	113.10
2	D	17	ILE	N-CA-C	-6.03	94.72	111.00
2	E	17	ILE	N-CA-C	-6.02	94.75	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	58	LYS	N-CA-C	-6.01	94.76	111.00
4	H	43	GLY	N-CA-C	-5.99	98.14	113.10
2	F	329	LEU	C-N-CA	5.97	136.63	121.70
1	A	362	ARG	N-CA-C	-5.97	94.88	111.00
1	C	174	GLY	N-CA-C	-5.96	98.20	113.10
2	E	116	ILE	C-N-CA	5.92	136.50	121.70
2	F	16	VAL	N-CA-C	-5.91	95.06	111.00
4	H	36	VAL	N-CA-C	-5.91	95.06	111.00
2	D	207	ASN	N-CA-C	-5.90	95.07	111.00
2	E	311	TYR	N-CA-C	-5.89	95.09	111.00
2	D	59	ARG	N-CA-C	-5.89	95.10	111.00
2	D	16	VAL	N-CA-C	-5.89	95.11	111.00
10	V	23	ARG	C-N-CA	5.88	136.40	121.70
3	G	171	TYR	N-CA-C	-5.88	95.13	111.00
1	A	194	ASP	N-CA-C	-5.87	95.14	111.00
2	D	52	HIS	N-CA-C	-5.86	95.17	111.00
2	D	306	SER	N-CA-C	-5.85	95.20	111.00
3	G	109	GLY	N-CA-C	-5.84	98.50	113.10
2	D	57	THR	N-CA-C	-5.84	95.24	111.00
2	E	110	THR	C-N-CA	5.81	136.23	121.70
1	A	61	GLY	N-CA-C	-5.81	98.57	113.10
2	F	364	GLY	N-CA-C	-5.77	98.68	113.10
2	E	161	GLY	N-CA-C	-5.75	98.73	113.10
2	E	276	PRO	N-CA-C	-5.74	97.17	112.10
1	B	232	VAL	N-CA-C	-5.74	95.52	111.00
2	E	130	GLN	N-CA-C	-5.73	95.53	111.00
1	B	194	ASP	N-CA-C	-5.72	95.54	111.00
2	E	283	PRO	C-N-CA	5.70	135.96	121.70
4	H	20	PHE	N-CA-C	-5.69	95.64	111.00
1	B	328	GLU	N-CA-C	-5.69	95.64	111.00
4	H	54	THR	N-CA-C	-5.68	95.65	111.00
1	C	263	HIS	N-CA-C	-5.68	95.67	111.00
1	B	267	ILE	N-CA-C	-5.65	95.75	111.00
1	B	313	ASN	C-N-CA	5.65	135.82	121.70
2	E	88	PRO	N-CA-C	5.63	126.73	112.10
3	G	204	TYR	N-CA-C	-5.62	95.84	111.00
2	E	118	ALA	N-CA-C	-5.61	95.84	111.00
2	E	212	THR	N-CA-C	-5.60	95.88	111.00
2	E	110	THR	CA-C-N	-5.59	104.91	117.20
1	B	237	SER	C-N-CA	5.59	135.67	121.70
2	F	207	ASN	N-CA-C	-5.58	95.92	111.00
2	F	355	SER	N-CA-C	-5.58	95.93	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	504	PHE	C-N-CA	5.57	135.62	121.70
1	A	432	GLN	N-CA-C	-5.57	95.97	111.00
8	T	93	ASP	O-C-N	-5.57	113.79	122.70
2	E	25	PHE	CA-C-N	-5.55	104.98	117.20
2	D	392	GLY	N-CA-C	5.54	126.94	113.10
3	G	55	ALA	N-CA-C	-5.53	96.07	111.00
3	G	113	ARG	N-CA-C	-5.53	96.08	111.00
2	E	27	GLU	N-CA-C	-5.51	96.12	111.00
2	D	431	LEU	N-CA-C	-5.51	96.12	111.00
1	A	39	ALA	N-CA-C	-5.50	96.16	111.00
1	C	321	LEU	N-CA-C	-5.48	96.20	111.00
1	A	263	HIS	N-CA-C	-5.48	96.21	111.00
2	E	57	THR	CA-C-N	-5.48	105.15	117.20
2	F	59	ARG	N-CA-C	-5.45	96.28	111.00
4	H	91	GLN	N-CA-C	-5.44	96.31	111.00
3	G	248	LEU	C-N-CA	5.43	135.28	121.70
7	S	70	SER	C-N-CA	5.43	135.27	121.70
7	S	6	ARG	CA-C-N	5.41	132.24	117.10
2	F	331	ALA	N-CA-C	-5.40	96.42	111.00
2	E	129	GLU	N-CA-C	-5.40	96.42	111.00
1	A	164	ARG	N-CA-C	-5.38	96.46	111.00
2	E	394	ASP	N-CA-C	-5.38	96.46	111.00
2	F	22	ASP	N-CA-C	-5.37	96.49	111.00
1	A	406	PHE	N-CA-C	-5.35	96.55	111.00
2	F	32	ILE	N-CA-C	-5.34	96.57	111.00
2	E	22	ASP	N-CA-C	-5.34	96.58	111.00
2	D	12	ARG	N-CA-C	-5.34	96.59	111.00
2	F	218	VAL	N-CA-C	-5.33	96.59	111.00
4	H	76	PHE	N-CA-C	-5.32	96.63	111.00
2	E	182	VAL	N-CA-C	-5.32	96.64	111.00
2	F	80	ALA	N-CA-C	-5.31	96.65	111.00
7	S	111	VAL	C-N-CA	5.31	134.98	121.70
5	I	7	ALA	N-CA-C	-5.31	96.67	111.00
1	A	488	LYS	N-CA-C	-5.30	96.70	111.00
1	C	402	ALA	N-CA-C	5.30	125.30	111.00
1	B	430	GLN	N-CA-C	-5.29	96.71	111.00
1	A	406	PHE	CA-C-N	-5.29	105.62	116.20
2	D	80	ALA	N-CA-C	-5.28	96.73	111.00
2	D	23	VAL	N-CA-C	-5.28	96.75	111.00
2	F	206	ILE	C-N-CA	5.28	134.90	121.70
2	D	138	LYS	C-N-CA	5.27	134.88	121.70
4	H	19	THR	N-CA-C	-5.26	96.79	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	219	TYR	N-CA-C	-5.25	96.81	111.00
1	B	127	ARG	N-CA-C	-5.25	96.82	111.00
3	G	199	ASP	CA-C-N	5.24	128.73	117.20
1	A	364	ALA	C-N-CA	5.23	134.78	121.70
1	C	232	VAL	N-CA-C	-5.23	96.88	111.00
3	G	200	VAL	N-CA-C	5.22	125.10	111.00
3	G	104	LYS	N-CA-C	-5.20	96.97	111.00
1	C	63	SER	N-CA-C	-5.19	96.98	111.00
2	E	189	ARG	N-CA-C	-5.19	96.98	111.00
1	B	66	LEU	N-CA-C	-5.17	97.03	111.00
2	D	399	GLU	C-N-CA	5.17	134.63	121.70
1	A	96	ASP	N-CA-C	-5.17	97.05	111.00
1	C	146	MET	N-CA-C	-5.16	97.07	111.00
1	B	38	ILE	N-CA-C	-5.14	97.11	111.00
1	A	41	VAL	N-CA-C	-5.11	97.20	111.00
1	C	163	GLN	C-N-CA	5.11	134.47	121.70
2	D	396	LEU	C-N-CA	5.11	134.47	121.70
2	F	306	SER	N-CA-C	-5.10	97.23	111.00
4	H	92	LEU	N-CA-C	-5.10	97.23	111.00
1	C	125	ALA	N-CA-C	-5.09	97.26	111.00
1	C	288	PRO	N-CA-C	5.09	125.33	112.10
4	H	40	THR	N-CA-C	-5.08	97.28	111.00
4	H	98	VAL	N-CA-C	-5.08	97.28	111.00
1	A	323	ALA	N-CA-C	-5.07	97.33	111.00
4	H	32	ASN	C-N-CA	5.06	134.34	121.70
4	H	82	VAL	N-CA-C	-5.06	97.35	111.00
3	G	93	ALA	N-CA-C	5.06	124.65	111.00
2	E	25	PHE	N-CA-C	-5.05	97.35	111.00
7	S	72	MET	C-N-CA	5.05	134.32	121.70
2	D	248	GLY	C-N-CA	5.04	134.30	121.70
2	D	118	ALA	N-CA-C	-5.03	97.41	111.00
1	C	91	THR	N-CA-C	-5.03	97.42	111.00
2	D	353	SER	N-CA-C	-5.03	97.43	111.00
1	B	107	VAL	N-CA-C	-5.02	97.44	111.00
2	F	206	ILE	CA-C-N	-5.02	106.17	117.20
2	F	304	ILE	N-CA-C	-5.01	97.47	111.00
1	A	89	LYS	N-CA-C	-5.00	97.49	111.00
7	S	49	PRO	N-CA-C	5.00	125.10	112.10

There are no chirality outliers.

All (132) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	406	PHE	Mainchain,Peptide
1	A	408	SER	Mainchain
1	A	509	GLU	Mainchain
1	B	379	GLN	Peptide
1	B	400	VAL	Mainchain
1	B	78	ASN	Mainchain
1	C	173	THR	Mainchain
1	C	365	ILE	Peptide
1	C	403	PHE	Mainchain
2	D	213	SER	Mainchain
2	E	110	THR	Mainchain
2	E	160	VAL	Mainchain
2	E	25	PHE	Mainchain
2	E	351	LEU	Mainchain
2	E	397	SER	Mainchain
2	F	205	VAL	Peptide
2	F	359	ASP	Mainchain
2	F	397	SER	Mainchain
2	F	63	MET	Mainchain
3	G	116	LEU	Mainchain
3	G	200	VAL	Mainchain
3	G	56	ASP	Mainchain
3	G	92	GLU	Mainchain,Peptide
4	H	37	ASP	Peptide
4	H	97	ALA	Mainchain
7	S	10	GLN	Mainchain
7	S	107	THR	Peptide
7	S	108	MET	Mainchain
7	S	109	MET	Mainchain
7	S	11	ILE	Mainchain
7	S	110	SER	Peptide
7	S	111	VAL	Mainchain
7	S	123	ALA	Mainchain
7	S	124	SER	Mainchain
7	S	126	LEU	Mainchain
7	S	131	LEU	Mainchain
7	S	133	GLU	Mainchain
7	S	134	LEU	Mainchain
7	S	136	THR	Mainchain
7	S	141	PHE	Mainchain
7	S	142	LEU	Peptide
7	S	150	LEU	Mainchain,Peptide
7	S	152	VAL	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
7	S	155	ASP	Mainchain
7	S	156	PRO	Mainchain,Peptide
7	S	19	ALA	Mainchain
7	S	37	LYS	Peptide
7	S	42	VAL	Mainchain
7	S	48	GLU	Mainchain
7	S	52	ALA	Peptide
7	S	60	VAL	Mainchain,Peptide
7	S	63	SER	Mainchain
7	S	69	LEU	Peptide
7	S	73	THR	Mainchain,Peptide
7	S	82	THR	Mainchain
7	S	9	VAL	Mainchain,Peptide
7	S	97	ASN	Mainchain
8	T	104	GLU	Mainchain
8	T	113	ARG	Mainchain
8	T	135	LYS	Mainchain
8	T	137	GLN	Mainchain
8	T	148	VAL	Peptide
8	T	155	GLN	Mainchain,Peptide
8	T	158	LYS	Mainchain
8	T	169	LYS	Mainchain
8	T	50	ASP	Peptide
8	T	86	GLN	Mainchain
8	T	87	LYS	Mainchain
8	T	88	ARG	Mainchain
8	T	89	HIS	Mainchain
8	T	93	ASP	Mainchain
8	T	98	ASN	Mainchain
9	U	1	ARG	Mainchain
9	U	101	PHE	Mainchain
9	U	107	THR	Mainchain
9	U	111	GLU	Mainchain
9	U	14	GLY	Peptide
9	U	15	GLU	Mainchain,Peptide
9	U	17	ILE	Mainchain,Peptide
9	U	18	PRO	Mainchain,Peptide
9	U	2	LYS	Mainchain
9	U	41	THR	Mainchain,Peptide
9	U	48	ALA	Mainchain,Peptide
9	U	56	ALA	Peptide
9	U	59	ALA	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
9	U	60	LYS	Mainchain,Peptide
9	U	66	ASP	Mainchain
9	U	75	LYS	Mainchain,Peptide
9	U	81	ASP	Peptide
9	U	83	TYR	Mainchain,Peptide
9	U	89	ALA	Peptide
9	U	90	GLU	Peptide
9	U	94	ASP	Mainchain
10	V	19	TYR	Mainchain
10	V	20	ARG	Mainchain
10	V	21	THR	Mainchain
10	V	22	LYS	Mainchain
10	V	29	PRO	Peptide
10	V	31	ASP	Mainchain,Peptide
10	V	32	ALA	Mainchain
10	V	5	LEU	Mainchain
10	V	51	TYR	Mainchain,Peptide
10	V	65	GLU	Mainchain
10	V	69	PHE	Peptide
10	V	7	PRO	Mainchain,Peptide
10	V	8	VAL	Mainchain
11	W	176	GLY	Mainchain
11	W	35	ASN	Peptide
11	W	63	SER	Mainchain
11	W	90	HIS	Mainchain
11	W	91	SER	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2035	0	589	10	0
1	B	1918	0	553	7	0
1	C	1947	0	562	8	0
2	D	1867	0	533	3	0
2	E	1863	0	532	8	0
2	F	1863	0	532	1	0
3	G	1053	0	283	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	0
6	Q	288	0	92	0	0
7	S	669	0	179	6	0
8	T	697	0	182	0	0
9	U	485	0	121	0	0
10	V	265	0	68	1	0
11	W	869	0	226	1	0
All	All	18545	0	5289	44	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 (44) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:CA	7:S:81:LEU:O	2.45	0.64
7:S:108:MET:O	7:S:112:HIS:CA	2.51	0.58
4:H:65:VAL:H	4:H:73:SER:H	1.55	0.55
7:S:106:SER:CA	7:S:109:MET:H	2.20	0.54
1:B:261:GLY:HA2	1:B:317:GLY:HA3	1.90	0.53
1:A:49:ALA:H	2:E:69:LEU:N	2.07	0.53
1:C:149:GLY:HA3	1:C:436:MET:H	1.74	0.52
1:C:258:ARG:O	1:C:319:GLY:HA3	2.10	0.52
2:F:208:LEU:C	2:F:210:ASP:H	2.12	0.52
10:V:20:ARG:O	10:V:24:GLN:N	2.44	0.49
2:E:159:GLY:C	2:E:161:GLY:H	2.17	0.48
1:B:194:ASP:C	1:B:196:LYS:H	2.15	0.48
1:A:149:GLY:HA3	1:A:436:MET:H	1.78	0.47
2:E:115:ALA:C	2:E:117:HIS:H	2.16	0.47
2:E:247:GLU:C	2:E:249:GLN:H	2.18	0.47
2:D:473:LEU:C	2:D:475:GLU:H	2.18	0.47
2:E:350:PRO:C	2:E:352:ASP:H	2.19	0.46
7:S:108:MET:O	7:S:112:HIS:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:272:LEU:C	2:E:274:ARG:H	2.19	0.46
1:A:261:GLY:O	1:A:319:GLY:HA2	2.16	0.45
2:E:210:ASP:C	2:E:212:THR:H	2.20	0.45
1:C:29:GLY:HA3	1:C:42:HIS:O	2.17	0.45
3:G:199:ASP:O	3:G:202:ARG:N	2.50	0.45
1:A:171:ARG:O	1:A:172:GLN:C	2.55	0.44
1:B:173:THR:N	1:B:175:LYS:H	2.15	0.44
1:B:258:ARG:O	1:B:319:GLY:CA	2.65	0.44
1:C:194:ASP:C	1:C:196:LYS:H	2.21	0.44
1:C:49:ALA:H	2:D:69:LEU:N	2.16	0.43
1:C:285:LEU:C	1:C:287:ARG:H	2.20	0.43
1:A:187:LYS:O	1:A:191:ASP:N	2.52	0.43
1:A:397:TYR:O	1:A:401:ALA:N	2.52	0.43
1:A:504:PHE:O	1:A:508:PHE:N	2.52	0.43
7:S:105:PHE:O	7:S:109:MET:N	2.52	0.43
2:E:277:SER:N	2:E:281:TYR:O	2.51	0.42
1:B:149:GLY:HA3	1:B:436:MET:H	1.84	0.42
2:D:155:PHE:N	2:D:333:THR:O	2.52	0.42
11:W:90:HIS:CA	11:W:91:SER:C	2.88	0.42
1:A:144:GLU:O	1:A:160:GLY:HA3	2.20	0.41
1:B:258:ARG:O	1:B:319:GLY:HA2	2.20	0.41
1:A:475:GLN:C	1:A:477:GLN:H	2.23	0.41
1:B:144:GLU:O	1:B:160:GLY:HA2	2.20	0.41
1:C:210:ARG:O	1:C:214:ALA:N	2.53	0.41
1:C:260:ASN:C	1:C:262:LYS:H	2.24	0.41
7:S:49:PRO:C	7:S:51:MET:N	2.70	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%)	441 (87%)	42 (8%)	24 (5%)	2 21
1	B	476/510 (93%)	420 (88%)	31 (6%)	25 (5%)	2 19
1	C	485/510 (95%)	433 (89%)	34 (7%)	18 (4%)	3 24
2	D	465/482 (96%)	404 (87%)	44 (10%)	17 (4%)	3 24
2	E	464/482 (96%)	413 (89%)	31 (7%)	20 (4%)	2 22
2	F	464/482 (96%)	414 (89%)	33 (7%)	17 (4%)	3 24
3	G	258/273 (94%)	204 (79%)	35 (14%)	19 (7%)	1 13
4	H	129/146 (88%)	110 (85%)	8 (6%)	11 (8%)	1 12
5	I	45/50 (90%)	34 (76%)	7 (16%)	4 (9%)	1 11
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%)	112 (68%)	28 (17%)	26 (16%)	0 3
8	T	172/174 (99%)	156 (91%)	9 (5%)	7 (4%)	3 22
9	U	120/124 (97%)	103 (86%)	10 (8%)	7 (6%)	1 18
10	V	65/77 (84%)	49 (75%)	10 (15%)	6 (9%)	1 11
11	W	215/217 (99%)	192 (89%)	20 (9%)	3 (1%)	11 46
All	All	4591/4803 (96%)	3982 (87%)	396 (9%)	213 (5%)	4 21

All (213) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	14	GLU
1	A	224	ASP
1	A	262	LYS
1	A	365	ILE
1	B	48	GLN
1	B	57	SER
1	B	141	SER

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Mol	Chain	Res	Type
1	B	171	ARG
1	B	224	ASP
1	B	237	SER
1	B	238	ASP
1	B	289	PRO
1	B	319	GLY
1	B	435	PRO
1	C	59	LEU
1	C	146	MET
1	C	163	GLN
1	C	171	ARG
1	C	224	ASP
1	C	238	ASP
1	C	289	PRO
1	C	365	ILE
2	D	177	HIS
2	D	214	LYS
2	D	249	GLN
2	D	352	ASP
2	D	394	ASP
2	E	109	LYS
2	F	277	SER
2	F	281	TYR
2	F	450	ASP
2	F	451	HIS
3	G	9	ARG
3	G	52	TYR
3	G	114	SER
3	G	119	THR
3	G	134	ARG
3	G	199	ASP
3	G	250	PHE
4	H	69	ASP
4	H	87	ASP
5	I	3	TYR
5	I	5	ARG
5	I	7	ALA
7	S	10	GLN
7	S	38	GLU
7	S	53	ALA
7	S	63	SER
7	S	73	THR

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Mol	Chain	Res	Type
7	S	111	VAL
7	S	117	PRO
7	S	118	CYS
9	U	90	GLU
9	U	98	CYS
10	V	6	ASP
10	V	7	PRO
10	V	30	VAL
1	A	11	ILE
1	A	19	ALA
1	A	20	ASP
1	A	44	LEU
1	A	78	ASN
1	A	172	GLN
1	A	193	THR
1	A	209	LYS
1	A	289	PRO
1	B	143	ARG
1	B	361	ILE
1	B	433	TYR
1	B	505	LEU
1	B	508	PHE
1	C	47	VAL
1	C	209	LYS
1	C	429	LYS
1	C	451	GLY
2	D	28	GLY
2	D	159	GLY
2	E	28	GLY
2	E	64	ASP
2	E	67	GLU
2	E	73	GLN
2	E	111	LYS
2	E	132	ILE
2	E	146	TYR
2	E	299	THR
2	E	394	ASP
2	F	31	PRO
2	F	102	ILE
2	F	249	GLN
2	F	348	VAL
2	F	427	HIS

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Mol	Chain	Res	Type
3	G	73	SER
3	G	87	LYS
3	G	93	ALA
3	G	155	PHE
3	G	200	VAL
4	H	42	THR
4	H	88	SER
5	I	36	LYS
7	S	8	PRO
7	S	60	VAL
7	S	80	PRO
7	S	92	ASN
7	S	108	MET
7	S	143	SER
8	T	155	GLN
9	U	18	PRO
10	V	61	ASN
1	A	115	ILE
1	A	171	ARG
1	A	313	ASN
1	B	35	GLY
1	B	45	ARG
1	B	209	LYS
1	B	236	ALA
1	B	262	LYS
1	B	375	GLY
1	C	143	ARG
1	C	145	PRO
1	C	331	ALA
2	D	55	GLU
2	D	212	THR
2	E	44	ARG
2	E	277	SER
2	E	350	PRO
2	E	351	LEU
2	F	297	THR
2	F	360	PRO
3	G	88	GLN
3	G	257	VAL
4	H	86	ALA
4	H	95	GLU
4	H	101	ASP

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Mol	Chain	Res	Type
6	J	45	GLN
7	S	12	TYR
7	S	69	LEU
7	S	120	VAL
7	S	149	LYS
7	S	151	GLU
8	T	171	LEU
9	U	20	ASN
9	U	83	TYR
9	U	102	LEU
10	V	29	PRO
11	W	92	PHE
1	A	22	SER
1	A	79	ASP
1	A	146	MET
1	A	336	ALA
1	B	50	GLU
1	B	131	LEU
1	C	435	PRO
2	E	210	ASP
2	E	297	THR
2	F	33	LEU
2	F	177	HIS
2	F	359	ASP
3	G	92	GLU
4	H	79	SER
6	P	40	PRO
6	Q	44	GLN
7	S	9	VAL
7	S	39	LEU
7	S	121	THR
8	T	99	ILE
9	U	97	SER
11	W	36	ARG
11	W	40	ASN
1	A	409	ASP
1	B	430	GLN
1	C	404	ALA
2	D	86	VAL
2	D	102	ILE
2	D	277	SER
2	D	450	ASP

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Mol	Chain	Res	Type
2	E	102	ILE
2	F	361	ASN
3	G	77	LEU
3	G	258	ILE
6	O	39	ASN
7	S	54	SER
7	S	81	LEU
8	T	147	ARG
10	V	55	ASP
1	A	114	ALA
1	A	235	THR
1	B	121	ILE
2	F	160	VAL
4	H	124	ASP
6	M	40	PRO
7	S	79	SER
8	T	121	ARG
2	D	279	VAL
2	D	452	LEU
2	E	160	VAL
2	E	279	VAL
2	F	279	VAL
3	G	136	PRO
4	H	52	VAL
2	D	447	GLY
3	G	115	ILE
1	C	288	PRO
2	E	460	VAL
4	H	39	PRO
6	J	40	PRO
6	M	71	ILE
8	T	148	VAL
8	T	149	VAL
7	S	14	ILE
6	K	40	PRO
2	D	346	PRO
6	Q	40	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

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

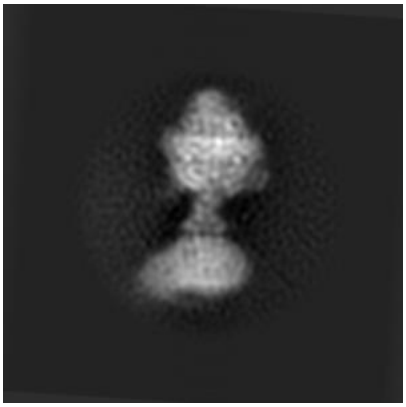
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3165. These allow visual inspection of the internal detail of the map and identification of artifacts.

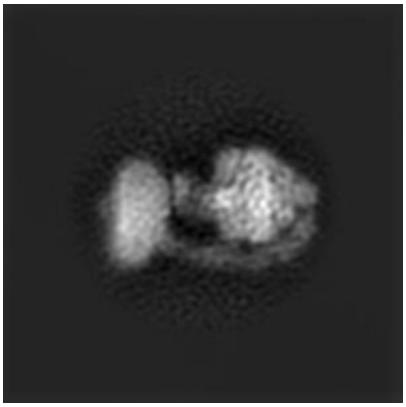
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

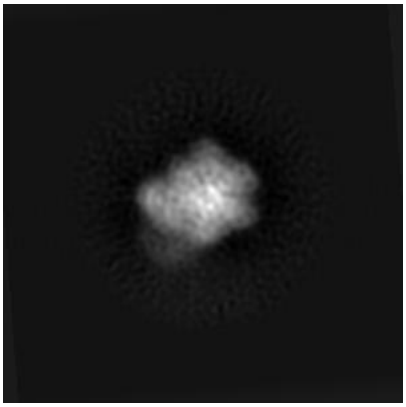
6.1.1 Primary map



X



Y



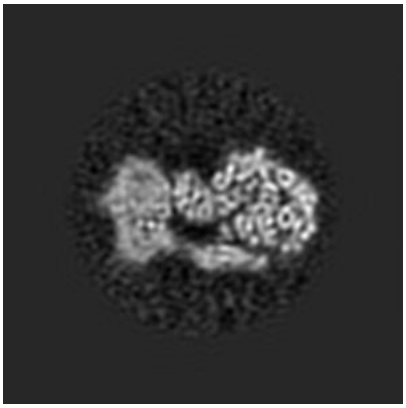
Z

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

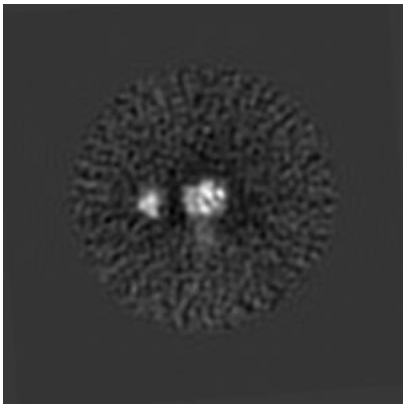
6.2 Central slices

6.2.1 Primary map

X Index: 128



Y Index: 128

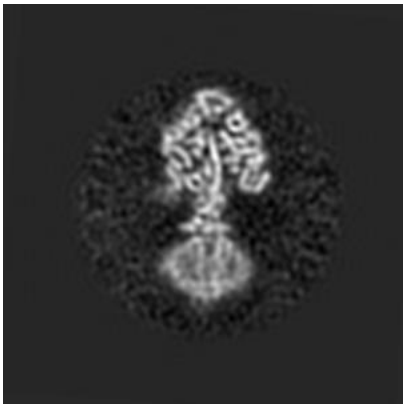


Z Index: 128

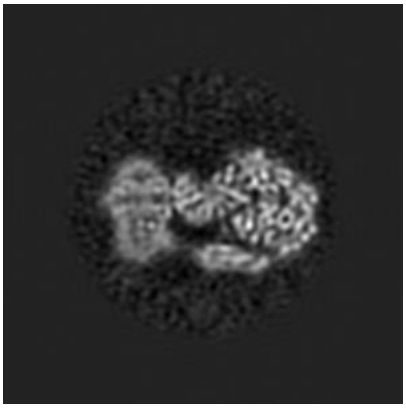
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

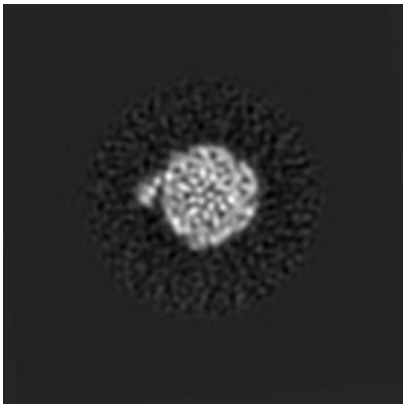
6.3.1 Primary map



X Index: 133



Y Index: 130

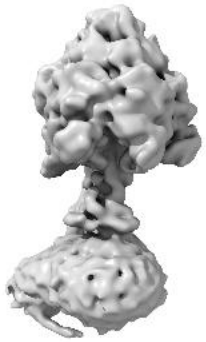


Z Index: 167

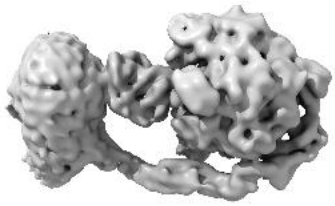
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

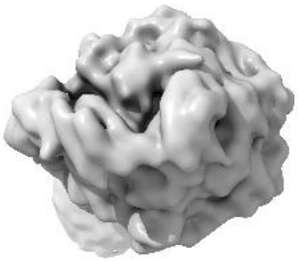
6.4.1 Primary map



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.

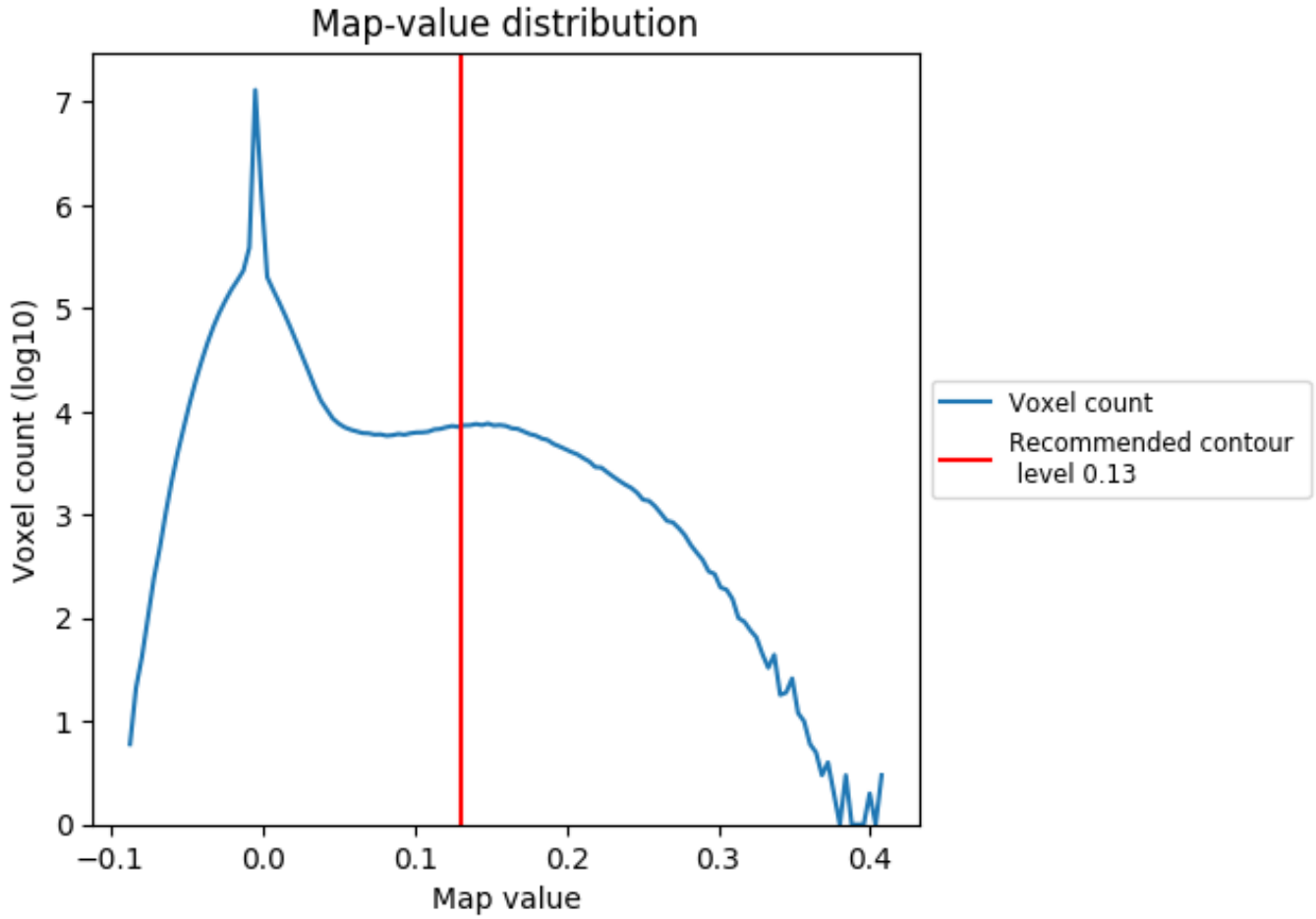
6.5 Mask visualisation (i)

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

7 Map analysis

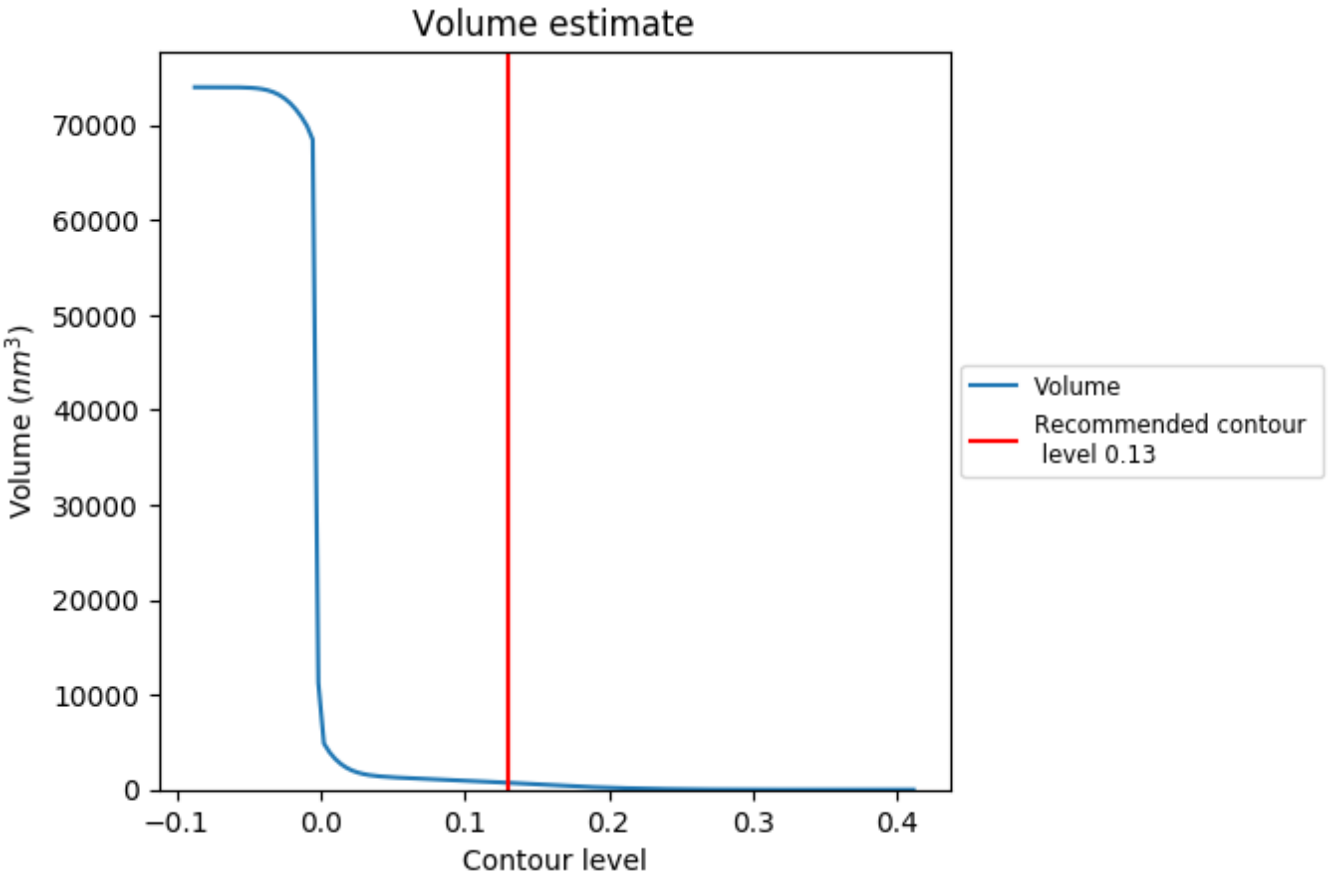
This section contains the results of statistical analysis of the map.

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.

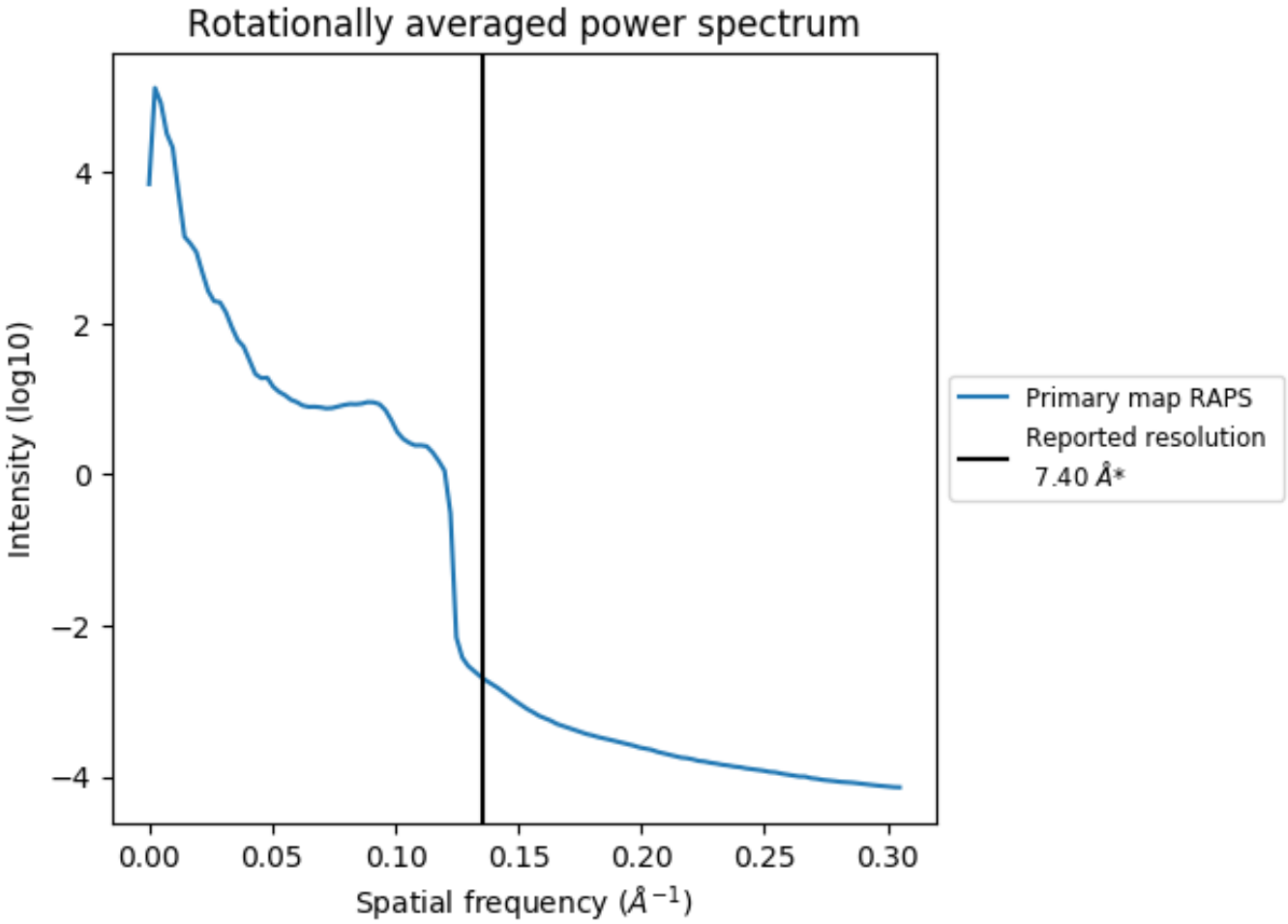
7.2 Volume estimate



The volume at the recommended contour level is 727 nm^3; this corresponds to an approximate mass of 656 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 0.135 Å^{-1}

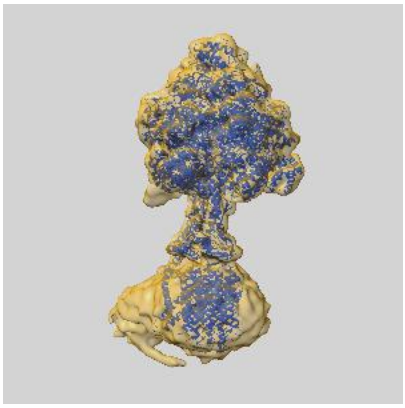
8 Fourier-Shell correlation

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

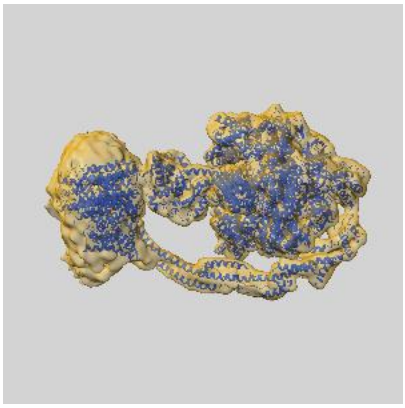
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3165 and PDB model 5ARE. Per-residue inclusion information can be found in section 3 on page 7.

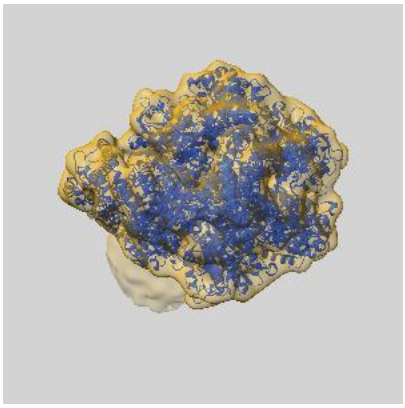
9.1 Map-model overlay



X



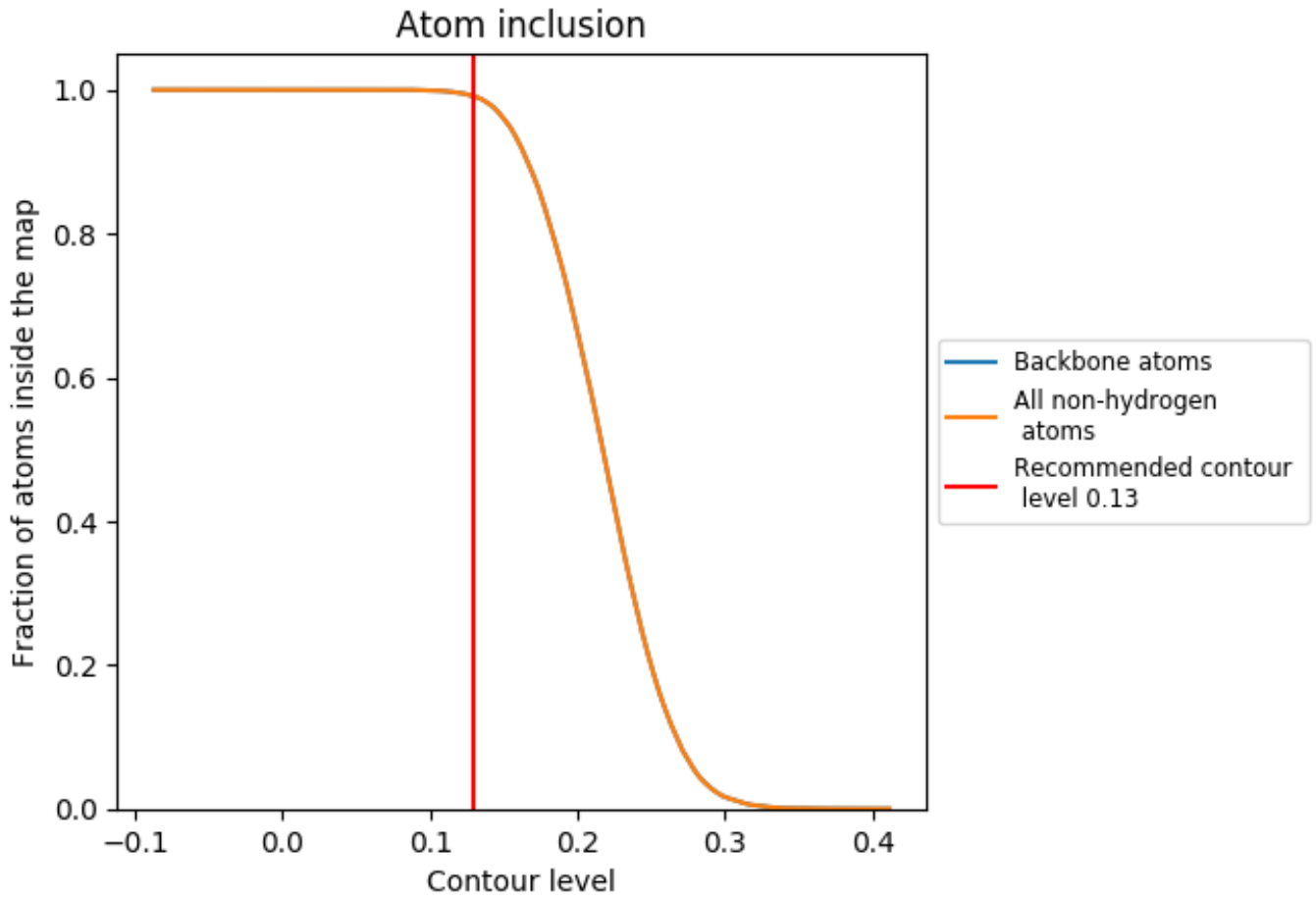
Y



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.