Full wwPDB EM Validation Report (i)

May 1, 2024 – 12:08 am BST

PDB ID	:	5FIK
EMDB ID	:	EMD-3169
Title	:	Bovine mitochondrial ATP synthase state 3a
Authors	:	Zhou, A.; Rohou, A.; Schep, D.G.; Bason, J.V.; Montgomery, M.G.; Walker, J.E.; Grigorieff, N.; Rubinstein, J.L.
Deposited on	:	2015-09-28
Resolution	:	6.40 Å(reported)
Based on initial models	:	2WSS, 2XND, 2CLY

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

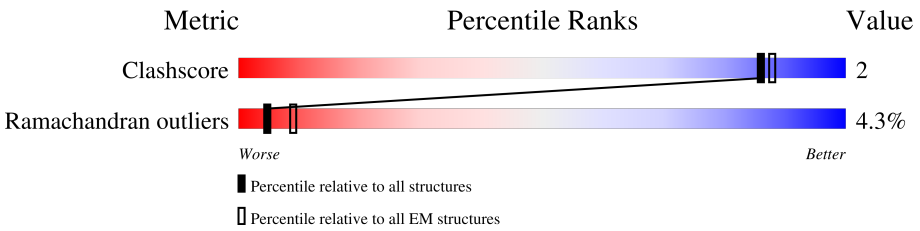
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 6.40 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	89% 10% •
1	B	510	85% 9% • 6%
1	C	510	88% 7% • 5%
2	D	482	89% 8% •
2	E	482	88% 8% • •
2	F	482	85% 11% • •
3	G	273	78% 17% • •
4	H	146	71% 19% 10%
5	I	50	• 86% 8% 6%

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Mol	Chain	Length	Quality of chain
6	J	72	97%
6	K	72	99%
6	L	72	100%
6	M	72	97%
6	N	72	100%
6	O	72	99%
6	P	72	99%
6	Q	72	97%
7	S	190	64% 22% 12%
8	T	174	83% 13%
9	U	124	82% 11%
10	V	77	74% 10% 13%
11	W	217	6% 92% 7%

2 Entry composition (i)

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
			Total	C	N	O		
1	A	509	2035	1018	509	508	0	0
1	B	480	1918	960	480	478	0	0
1	C	487	1947	974	487	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
			Total	C	N	O		
2	D	467	1867	934	467	466	0	0
2	E	466	1863	932	466	465	0	0
2	F	466	1863	932	466	465	0	0

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O		
8	T	174	697	348	174	175	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	U	122	485	242	122	121	0	1

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

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

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

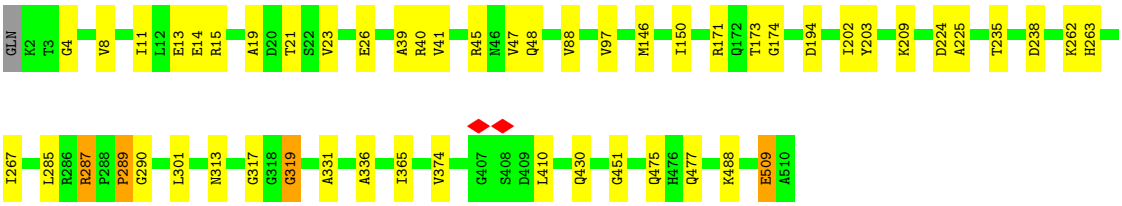
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	W	217	869	434	217	218	0	0

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.

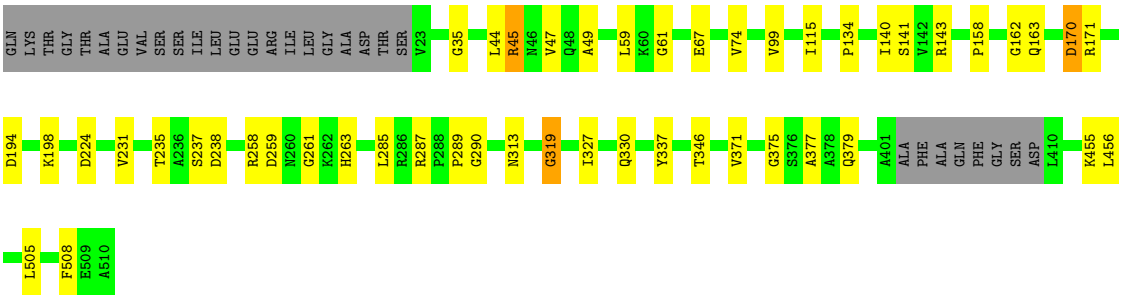
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain A:



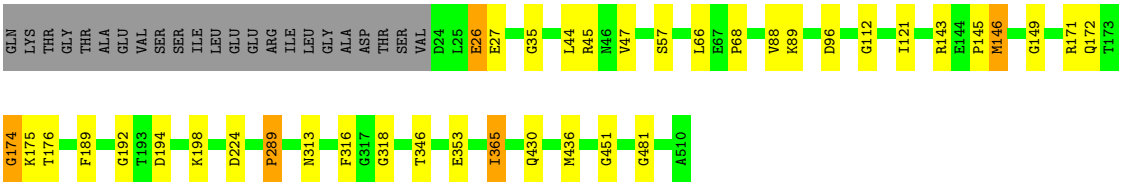
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain B:



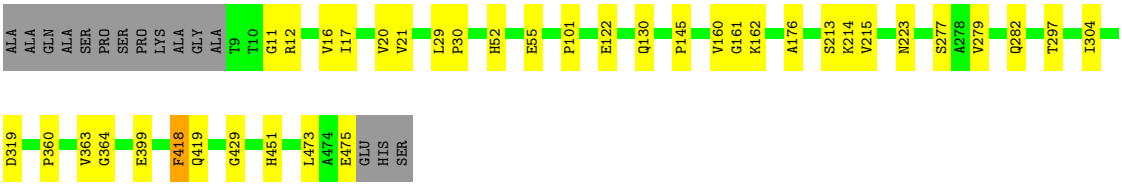
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain C:



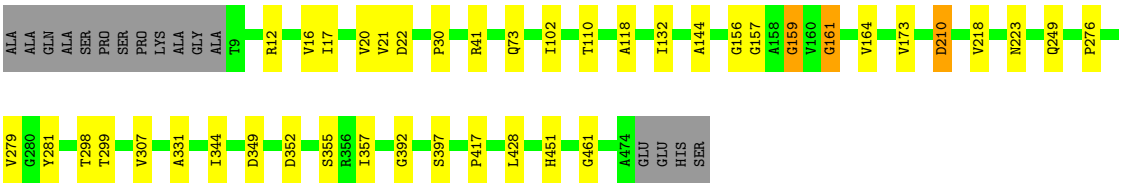
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain D:



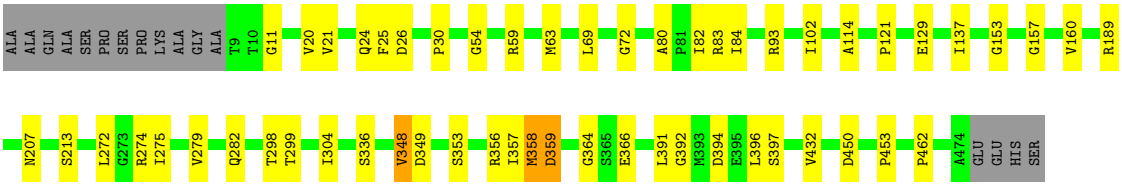
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain E:



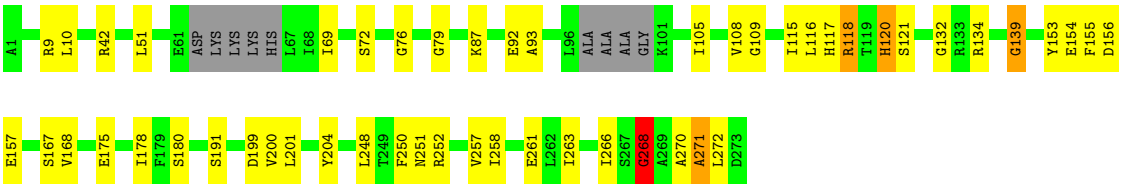
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain F:



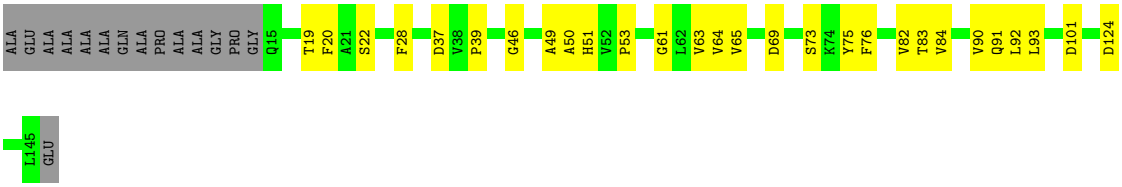
• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

Chain G:



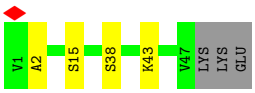
• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL

Chain H:

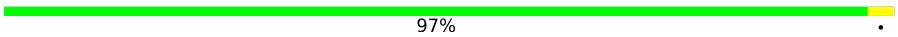


• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL

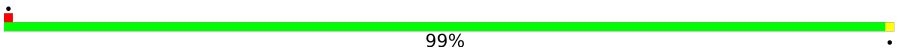
Chain I:

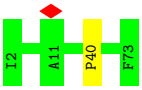


• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

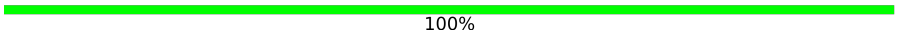
Chain J: 

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

Chain K: 

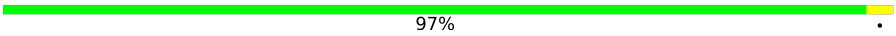


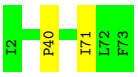
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain L: 

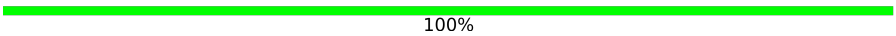
There are no outlier residues recorded for this chain.

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

Chain M: 

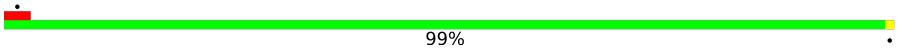


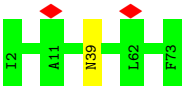
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain N: 

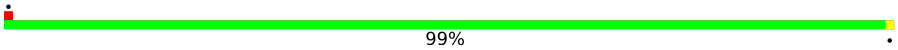
There are no outlier residues recorded for this chain.

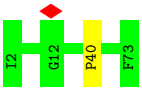
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain O: 



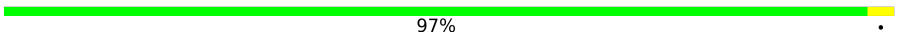
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain P: 



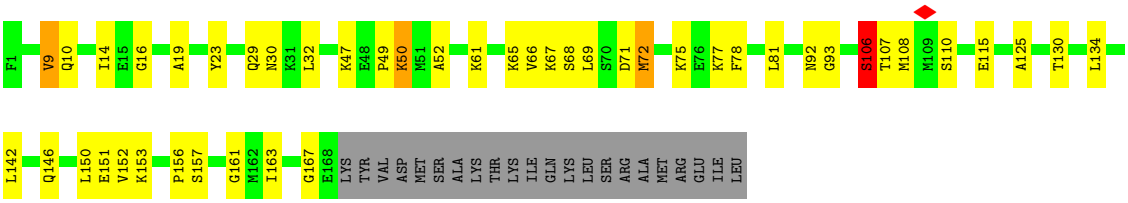
• Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain Q:



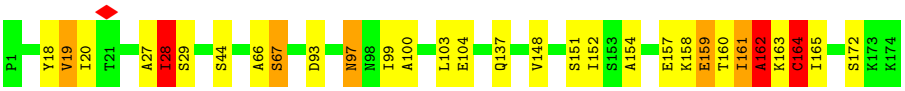
• Molecule 7: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL

Chain S:



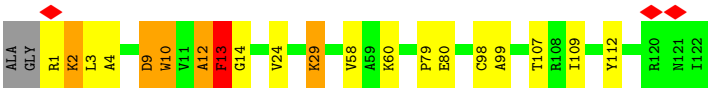
• Molecule 8: ATP SYNTHASE F(0) COMPLEX SUBUNIT B1, MITOCHONDRIAL

Chain T:



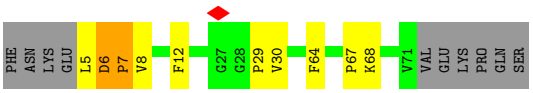
• Molecule 9: ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL

Chain U:



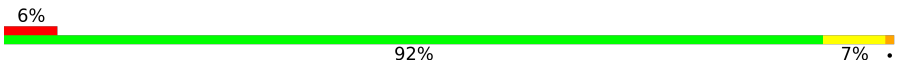
• Molecule 10: ATP SYNTHASE-COUPLING FACTOR 6, MITOCHONDRIAL

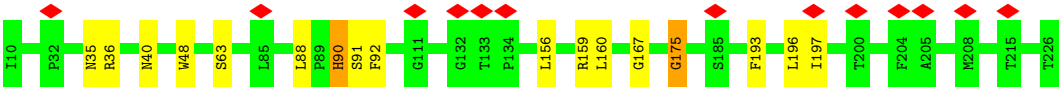
Chain V:



• Molecule 11: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain W:




I10
P32
N35
R36
N40
W48
S63
L85
L88
P89
H90
S91
F92
G111
G132
T133
P134
L156
R159
L160
G167
G175
S185
F193
L196
I197
T200
F204
A205
M208
T215
T226

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24140	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	0.515	Depositor
Minimum map value	-0.094	Depositor
Average map value	-0.001	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 (i)

5.1 Standard geometry (i)

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	1.79	2/2034 (0.1%)	1.43	19/2541 (0.7%)
1	B	1.80	1/1916 (0.1%)	1.42	19/2392 (0.8%)
1	C	1.84	7/1946 (0.4%)	1.39	14/2431 (0.6%)
2	D	1.78	3/1866 (0.2%)	1.39	12/2331 (0.5%)
2	E	1.81	1/1862 (0.1%)	1.49	21/2326 (0.9%)
2	F	1.84	4/1862 (0.2%)	1.50	24/2326 (1.0%)
3	G	2.04	5/1050 (0.5%)	1.56	16/1308 (1.2%)
4	H	2.18	7/522 (1.3%)	1.79	14/651 (2.2%)
5	I	1.96	1/186 (0.5%)	1.28	1/231 (0.4%)
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	0.45	0/357
6	M	0.29	0/287	0.44	0/357
6	N	0.28	0/287	0.40	0/357
6	O	0.31	0/287	0.41	0/357
6	P	0.29	0/287	0.43	0/357
6	Q	0.30	0/287	0.44	0/357
7	S	1.69	0/668	1.78	12/834 (1.4%)
8	T	1.10	4/696 (0.6%)	1.54	17/867 (2.0%)
9	U	0.99	3/484 (0.6%)	1.39	10/604 (1.7%)
10	V	0.81	1/264 (0.4%)	1.43	5/329 (1.5%)
11	W	0.86	4/868 (0.5%)	0.98	2/1082 (0.2%)
All	All	1.63	43/18520 (0.2%)	1.37	186/23109 (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	2
1	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	6
2	E	0	2
2	F	0	2
3	G	0	4
4	H	0	2
7	S	0	5
8	T	0	21
9	U	0	14
10	V	0	6
11	W	0	10
All	All	0	79

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	U	10	TRP	N-CA	8.48	1.63	1.46
8	T	28	ILE	CA-C	8.06	1.74	1.52
8	T	161	ILE	C-O	-7.20	1.09	1.23
3	G	261	GLU	CA-C	-7.02	1.34	1.52
3	G	139	GLY	CA-C	-6.24	1.41	1.51
1	C	174	GLY	N-CA	-6.18	1.36	1.46
2	F	364	GLY	N-CA	-6.13	1.36	1.46
1	A	451	GLY	CA-C	-6.03	1.42	1.51
4	H	28	PHE	CA-C	-5.97	1.37	1.52
1	C	174	GLY	CA-C	-5.85	1.42	1.51
2	E	159	GLY	CA-C	-5.82	1.42	1.51
4	H	46	GLY	CA-C	-5.82	1.42	1.51
1	C	481	GLY	CA-C	-5.76	1.42	1.51
11	W	88	LEU	N-CA	-5.70	1.34	1.46
2	F	366	GLU	CA-C	-5.67	1.38	1.52
8	T	158	LYS	CA-C	-5.62	1.38	1.52
1	C	451	GLY	CA-C	-5.57	1.43	1.51
9	U	13	PHE	N-CA	5.55	1.57	1.46
4	H	92	LEU	N-CA	-5.53	1.35	1.46
1	C	176	THR	N-CA	-5.47	1.35	1.46
4	H	91	GLN	CA-C	-5.44	1.38	1.52
10	V	6	ASP	C-O	-5.44	1.13	1.23
2	D	161	GLY	N-CA	-5.41	1.38	1.46
5	I	15	SER	CA-C	-5.33	1.39	1.52
1	C	35	GLY	N-CA	-5.32	1.38	1.46
4	H	19	THR	N-CA	-5.32	1.35	1.46
3	G	109	GLY	CA-C	-5.32	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	W	167	GLY	N-CA	-5.32	1.38	1.46
8	T	93	ASP	N-CA	-5.25	1.35	1.46
11	W	175	GLY	N-CA	-5.25	1.38	1.46
3	G	252	ARG	N-CA	-5.19	1.35	1.46
4	H	53	PRO	CA-C	-5.18	1.42	1.52
2	D	11	GLY	CA-C	-5.18	1.43	1.51
11	W	88	LEU	CA-C	5.16	1.66	1.52
9	U	13	PHE	CA-C	5.16	1.66	1.52
1	B	337	TYR	CA-C	-5.16	1.39	1.52
3	G	252	ARG	CA-C	-5.11	1.39	1.52
4	H	61	GLY	CA-C	-5.10	1.43	1.51
1	A	301	LEU	CA-C	-5.08	1.39	1.52
2	D	12	ARG	CA-C	-5.08	1.39	1.52
2	F	153	GLY	CA-C	-5.07	1.43	1.51
2	F	11	GLY	CA-C	-5.02	1.43	1.51
1	C	175	LYS	CA-C	-5.01	1.40	1.52

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	S	110	SER	C-N-CA	15.61	160.72	121.70
8	T	161	ILE	CA-C-O	-15.32	87.94	120.10
8	T	158	LYS	O-C-N	11.98	141.86	122.70
10	V	6	ASP	O-C-N	-11.58	99.10	121.10
8	T	162	ALA	N-CA-C	11.23	141.33	111.00
10	V	6	ASP	CA-C-O	-10.72	97.58	120.10
8	T	164	CYS	O-C-N	-10.22	106.34	122.70
1	A	4	GLY	N-CA-C	-9.45	89.47	113.10
10	V	5	LEU	C-N-CA	9.24	144.80	121.70
9	U	13	PHE	C-N-CA	9.11	141.43	122.30
8	T	158	LYS	CA-C-O	-8.93	101.35	120.10
7	S	106	SER	CA-C-N	-8.70	98.06	117.20
7	S	71	ASP	C-N-CA	8.59	143.18	121.70
2	D	161	GLY	N-CA-C	-8.24	92.51	113.10
1	C	174	GLY	N-CA-C	-8.12	92.81	113.10
4	H	20	PHE	N-CA-C	-8.07	89.22	111.00
7	S	150	LEU	N-CA-C	-8.07	89.22	111.00
2	F	83	ARG	N-CA-C	-8.06	89.24	111.00
2	F	304	ILE	N-CA-C	-7.99	89.44	111.00
3	G	154	GLU	N-CA-C	-7.91	89.65	111.00
1	A	290	GLY	N-CA-C	-7.77	93.67	113.10
1	B	198	LYS	N-CA-C	-7.68	90.26	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	T	19	VAL	CA-C-O	-7.54	104.26	120.10
4	H	64	VAL	N-CA-C	-7.44	90.92	111.00
2	F	391	LEU	N-CA-C	7.35	130.84	111.00
2	E	355	SER	N-CA-C	-7.31	91.27	111.00
4	H	93	LEU	N-CA-C	-7.13	91.76	111.00
1	A	509	GLU	N-CA-C	-7.09	91.86	111.00
1	C	313	ASN	C-N-CA	7.08	139.41	121.70
7	S	16	GLY	N-CA-C	-7.05	95.48	113.10
9	U	2	LYS	N-CA-C	7.03	129.98	111.00
8	T	161	ILE	C-N-CA	-7.02	104.16	121.70
1	C	35	GLY	N-CA-C	-7.02	95.56	113.10
8	T	158	LYS	C-N-CA	7.01	139.22	121.70
7	S	107	THR	C-N-CA	6.93	139.02	121.70
8	T	159	GLU	CA-C-N	-6.90	102.03	117.20
2	F	432	VAL	N-CA-C	-6.82	92.59	111.00
1	C	88	VAL	N-CA-C	-6.82	92.59	111.00
8	T	97	ASN	CA-C-N	-6.79	102.25	117.20
2	D	17	ILE	N-CA-C	-6.68	92.95	111.00
1	A	267	ILE	N-CA-C	-6.66	93.02	111.00
9	U	10	TRP	N-CA-C	-6.59	93.19	111.00
9	U	1	ARG	CA-C-O	-6.58	106.28	120.10
1	B	290	GLY	N-CA-C	-6.56	96.69	113.10
2	D	20	VAL	N-CA-C	-6.55	93.30	111.00
1	A	174	GLY	N-CA-C	-6.55	96.73	113.10
1	B	330	GLN	N-CA-C	-6.55	93.32	111.00
2	F	298	THR	N-CA-C	-6.51	93.41	111.00
2	E	349	ASP	N-CA-C	-6.51	93.43	111.00
3	G	272	LEU	N-CA-C	-6.49	93.47	111.00
2	E	20	VAL	N-CA-C	-6.44	93.61	111.00
2	E	16	VAL	N-CA-C	-6.42	93.66	111.00
10	V	5	LEU	O-C-N	6.42	132.98	122.70
1	C	112	GLY	N-CA-C	-6.41	97.07	113.10
2	E	159	GLY	N-CA-C	-6.37	97.17	113.10
8	T	28	ILE	N-CA-C	-6.35	93.86	111.00
2	E	17	ILE	N-CA-C	-6.34	93.87	111.00
1	C	26	GLU	N-CA-C	-6.31	93.97	111.00
2	E	307	VAL	N-CA-C	-6.27	94.07	111.00
8	T	28	ILE	O-C-N	-6.26	112.69	122.70
1	B	35	GLY	N-CA-C	-6.20	97.59	113.10
9	U	13	PHE	O-C-N	-6.20	112.66	123.20
2	E	392	GLY	N-CA-C	-6.18	97.64	113.10
1	A	289	PRO	N-CA-C	-6.18	96.04	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	116	LEU	N-CA-C	-6.15	94.39	111.00
3	G	157	GLU	N-CA-C	-6.12	94.47	111.00
4	H	82	VAL	N-CA-C	-6.11	94.52	111.00
1	B	44	LEU	C-N-CA	6.10	136.96	121.70
2	E	298	THR	N-CA-C	-6.10	94.53	111.00
4	H	63	VAL	N-CA-C	-6.07	94.62	111.00
2	E	156	GLY	C-N-CA	6.06	135.02	122.30
2	F	24	GLN	N-CA-C	-6.05	94.66	111.00
2	F	20	VAL	N-CA-C	-6.04	94.69	111.00
7	S	134	LEU	N-CA-C	-6.04	94.69	111.00
2	F	189	ARG	N-CA-C	-6.02	94.75	111.00
7	S	142	LEU	N-CA-C	-6.02	94.75	111.00
4	H	75	TYR	N-CA-C	-6.01	94.78	111.00
7	S	157	SER	N-CA-C	-6.00	94.80	111.00
2	E	461	GLY	N-CA-C	-5.90	98.36	113.10
9	U	13	PHE	CA-C-N	5.89	127.99	116.20
1	B	170	ASP	C-N-CA	5.88	136.41	121.70
2	D	16	VAL	N-CA-C	-5.88	95.11	111.00
1	A	88	VAL	N-CA-C	-5.88	95.14	111.00
2	F	349	ASP	N-CA-C	-5.87	95.15	111.00
1	A	39	ALA	N-CA-C	-5.86	95.18	111.00
2	F	275	ILE	N-CA-C	-5.83	95.25	111.00
2	D	399	GLU	N-CA-C	-5.80	95.33	111.00
4	H	92	LEU	N-CA-C	-5.79	95.36	111.00
2	F	391	LEU	CA-C-N	5.78	127.76	116.20
1	C	146	MET	N-CA-C	-5.77	95.43	111.00
1	C	198	LYS	N-CA-C	-5.75	95.46	111.00
7	S	106	SER	C-N-CA	5.74	136.04	121.70
7	S	9	VAL	C-N-CA	5.71	135.98	121.70
5	I	43	LYS	N-CA-C	-5.71	95.58	111.00
2	F	358	MET	C-N-CA	5.68	135.90	121.70
2	F	59	ARG	N-CA-C	-5.68	95.67	111.00
2	D	304	ILE	N-CA-C	-5.66	95.72	111.00
1	C	289	PRO	N-CA-C	-5.66	97.40	112.10
2	F	63	MET	C-N-CA	5.65	135.84	121.70
4	H	61	GLY	N-CA-C	-5.64	99.00	113.10
4	H	22	SER	N-CA-C	-5.64	95.77	111.00
1	A	430	GLN	N-CA-C	-5.64	95.78	111.00
2	E	12	ARG	N-CA-C	-5.62	95.83	111.00
1	B	67	GLU	N-CA-C	-5.61	95.85	111.00
4	H	76	PHE	N-CA-C	-5.61	95.85	111.00
2	E	173	VAL	N-CA-C	5.61	126.14	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	21	VAL	N-CA-C	-5.59	95.91	111.00
9	U	29	LYS	O-C-N	-5.58	113.77	122.70
1	B	455	LYS	N-CA-C	-5.58	95.94	111.00
2	F	54	GLY	N-CA-C	-5.58	99.16	113.10
2	F	207	ASN	N-CA-C	-5.57	95.95	111.00
8	T	19	VAL	CA-C-N	5.57	129.46	117.20
8	T	162	ALA	C-N-CA	-5.56	107.80	121.70
1	B	237	SER	C-N-CA	5.52	135.49	121.70
2	E	21	VAL	N-CA-C	-5.51	96.12	111.00
8	T	162	ALA	O-C-N	-5.51	113.89	122.70
1	B	140	ILE	C-N-CA	5.50	135.46	121.70
2	E	41	ARG	C-N-CA	5.49	135.44	121.70
3	G	132	GLY	N-CA-C	-5.49	99.37	113.10
1	C	66	LEU	N-CA-C	-5.48	96.20	111.00
1	C	89	LYS	N-CA-C	-5.48	96.20	111.00
1	A	40	ARG	N-CA-C	-5.47	96.23	111.00
3	G	42	ARG	CA-C-N	-5.47	105.17	117.20
3	G	204	TYR	N-CA-C	-5.46	96.25	111.00
2	E	210	ASP	N-CA-C	-5.46	96.25	111.00
4	H	83	THR	N-CA-C	-5.46	96.27	111.00
2	F	359	ASP	N-CA-C	-5.45	96.27	111.00
1	A	263	HIS	N-CA-C	-5.45	96.28	111.00
9	U	9	ASP	C-N-CA	5.45	135.33	121.70
9	U	4	ALA	O-C-N	-5.44	114.00	122.70
1	B	45	ARG	N-CA-C	5.44	125.68	111.00
1	A	225	ALA	C-N-CA	5.41	135.22	121.70
2	E	110	THR	N-CA-C	-5.39	96.44	111.00
3	G	121	SER	N-CA-C	-5.39	96.45	111.00
2	D	145	PRO	N-CA-C	-5.38	98.10	112.10
1	A	202	ILE	N-CA-C	-5.38	96.49	111.00
10	V	6	ASP	N-CA-C	5.37	125.50	111.00
1	C	45	ARG	C-N-CA	5.37	135.12	121.70
1	B	194	ASP	N-CA-C	-5.37	96.51	111.00
1	C	96	ASP	N-CA-C	-5.37	96.52	111.00
2	D	52	HIS	N-CA-C	-5.36	96.52	111.00
2	F	137	ILE	N-CA-C	-5.33	96.60	111.00
3	G	268	GLY	N-CA-C	-5.33	99.76	113.10
3	G	108	VAL	N-CA-C	-5.31	96.67	111.00
1	B	508	PHE	N-CA-C	-5.31	96.67	111.00
2	D	162	LYS	CA-C-N	-5.30	105.53	117.20
1	A	97	VAL	N-CA-C	-5.30	96.69	111.00
2	E	331	ALA	N-CA-C	-5.29	96.71	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	162	GLY	C-N-CA	5.27	134.89	121.70
4	H	46	GLY	N-CA-C	-5.27	99.92	113.10
1	A	203	TYR	N-CA-C	-5.26	96.80	111.00
3	G	248	LEU	C-N-CA	5.25	134.83	121.70
1	B	313	ASN	C-N-CA	5.25	134.83	121.70
8	T	67	SER	O-C-N	-5.25	114.31	122.70
2	F	353	SER	N-CA-C	-5.24	96.85	111.00
2	F	25	PHE	CA-C-N	-5.23	105.69	117.20
7	S	72	MET	C-N-CA	-5.23	108.62	121.70
2	F	392	GLY	N-CA-C	5.23	126.18	113.10
2	D	21	VAL	N-CA-C	-5.23	96.88	111.00
3	G	167	SER	N-CA-C	-5.22	96.89	111.00
11	W	90	HIS	CA-C-N	-5.22	105.71	117.20
1	B	263	HIS	N-CA-C	-5.22	96.92	111.00
3	G	42	ARG	C-N-CA	5.20	134.71	121.70
1	B	327	ILE	N-CA-C	-5.19	96.99	111.00
2	D	29	LEU	N-CA-C	-5.16	97.08	111.00
1	A	41	VAL	N-CA-C	-5.15	97.09	111.00
8	T	19	VAL	C-N-CA	5.15	134.57	121.70
1	A	313	ASN	C-N-CA	5.14	134.55	121.70
1	A	488	LYS	N-CA-C	-5.13	97.14	111.00
3	G	79	GLY	N-CA-C	-5.11	100.33	113.10
2	D	418	PHE	CA-C-N	-5.11	105.97	117.20
4	H	91	GLN	N-CA-C	-5.10	97.22	111.00
1	A	150	ILE	N-CA-C	-5.09	97.27	111.00
2	F	93	ARG	N-CA-C	-5.09	97.27	111.00
1	B	99	VAL	N-CA-C	-5.08	97.28	111.00
1	C	313	ASN	CA-C-N	-5.08	106.03	117.20
4	H	90	VAL	N-CA-C	-5.08	97.29	111.00
2	E	22	ASP	N-CA-C	-5.06	97.33	111.00
9	U	9	ASP	CA-C-O	-5.05	109.49	120.10
3	G	153	TYR	N-CA-C	-5.05	97.37	111.00
1	B	231	VAL	N-CA-C	-5.05	97.38	111.00
2	E	118	ALA	N-CA-C	-5.05	97.37	111.00
3	G	105	ILE	N-CA-C	-5.04	97.41	111.00
11	W	88	LEU	O-C-N	-5.03	111.54	121.10
2	E	218	VAL	N-CA-C	-5.02	97.45	111.00
2	F	80	ALA	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (79) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	THR	Mainchain,Peptide
1	A	287	ARG	Peptide
1	A	336	ALA	Peptide
1	B	371	VAL	Peptide
1	B	379	GLN	Peptide
1	C	194	ASP	Mainchain
2	D	122	GLU	Mainchain,Peptide
2	D	130	GLN	Mainchain
2	D	160	VAL	Mainchain
2	D	319	ASP	Mainchain
2	D	418	PHE	Mainchain
2	E	161	GLY	Mainchain
2	E	397	SER	Mainchain
2	F	26	ASP	Mainchain
2	F	397	SER	Mainchain
3	G	120	HIS	Mainchain
3	G	175	GLU	Mainchain
3	G	251	ASN	Mainchain
3	G	271	ALA	Mainchain
4	H	37	ASP	Peptide
4	H	84	VAL	Peptide
7	S	106	SER	Mainchain
7	S	152	VAL	Peptide
7	S	156	PRO	Peptide
7	S	161	GLY	Mainchain
7	S	49	PRO	Mainchain
8	T	103	LEU	Mainchain
8	T	104	GLU	Mainchain
8	T	137	GLN	Mainchain
8	T	148	VAL	Mainchain,Peptide
8	T	154	ALA	Peptide
8	T	161	ILE	Mainchain,Peptide
8	T	162	ALA	Mainchain,Peptide
8	T	163	LYS	Mainchain
8	T	164	CYS	Mainchain,Peptide
8	T	172	SER	Peptide
8	T	28	ILE	Mainchain,Peptide
8	T	29	SER	Mainchain
8	T	44	SER	Mainchain
8	T	66	ALA	Mainchain
8	T	67	SER	Mainchain
8	T	97	ASN	Mainchain
9	U	10	TRP	Mainchain

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Mol	Chain	Res	Type	Group
9	U	107	THR	Mainchain
9	U	109	ILE	Mainchain
9	U	112	TYR	Mainchain
9	U	12	ALA	Peptide
9	U	13	PHE	Peptide
9	U	2	LYS	Mainchain
9	U	24	VAL	Mainchain
9	U	29	LYS	Mainchain
9	U	58	VAL	Mainchain
9	U	60	LYS	Mainchain
9	U	80	GLU	Mainchain
9	U	9	ASP	Mainchain,Peptide
10	V	12	PHE	Mainchain
10	V	29	PRO	Peptide
10	V	30	VAL	Mainchain
10	V	6	ASP	Mainchain
10	V	64	PHE	Peptide
10	V	7	PRO	Mainchain
11	W	159	ARG	Mainchain
11	W	175	GLY	Mainchain
11	W	193	PHE	Mainchain
11	W	196	LEU	Mainchain
11	W	197	ILE	Mainchain
11	W	35	ASN	Peptide
11	W	48	TRP	Mainchain
11	W	63	SER	Mainchain
11	W	90	HIS	Mainchain,Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2035	0	589	4	0
1	B	1918	0	553	8	0
1	C	1947	0	562	6	0
2	D	1867	0	533	3	0
2	E	1863	0	532	1	0
2	F	1863	0	532	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1053	0	283	6	0
4	H	523	0	140	1	0
5	I	187	0	53	2	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	178	9	0
8	T	697	0	182	7	0
9	U	485	0	121	0	0
10	V	265	0	68	0	0
11	W	869	0	226	3	0
All	All	18545	0	5288	50	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 (50) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:84:ILE:H	2:F:114:ALA:H	1.24	0.83
1:B:49:ALA:H	2:F:69:LEU:H	1.31	0.79
7:S:163:ILE:O	7:S:167:GLY:O	2.16	0.63
8:T:19:VAL:O	11:W:91:SER:N	2.32	0.62
1:C:149:GLY:HA3	1:C:436:MET:H	1.66	0.60
7:S:72:MET:N	7:S:75:LYS:H	2.00	0.59
2:F:356:ARG:C	2:F:358:MET:H	2.12	0.53
8:T:20:ILE:CA	11:W:91:SER:H	2.21	0.52
1:A:285:LEU:C	1:A:287:ARG:H	2.12	0.52
1:B:158:PRO:O	1:B:375:GLY:HA3	2.10	0.52
1:C:172:GLN:C	1:C:174:GLY:H	2.12	0.51
7:S:72:MET:CA	7:S:75:LYS:H	2.23	0.51
1:B:285:LEU:C	1:B:287:ARG:H	2.14	0.51
8:T:160:THR:C	8:T:162:ALA:N	2.59	0.51
7:S:69:LEU:O	7:S:72:MET:CA	2.59	0.51
4:H:65:VAL:H	4:H:73:SER:H	1.60	0.50
7:S:69:LEU:O	7:S:72:MET:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:118:ARG:H	3:G:120:HIS:H	1.60	0.49
2:E:159:GLY:HA2	2:E:164:VAL:H	1.76	0.49
7:S:50:LYS:C	7:S:52:ALA:H	2.16	0.49
8:T:27:ALA:O	8:T:28:ILE:C	2.51	0.49
8:T:157:GLU:C	8:T:159:GLU:H	2.16	0.48
1:B:49:ALA:N	2:F:69:LEU:H	2.04	0.47
3:G:139:GLY:H	5:I:38:SER:CA	2.28	0.47
7:S:30:ASN:C	7:S:32:LEU:H	2.16	0.46
1:A:475:GLN:C	1:A:477:GLN:H	2.18	0.46
1:C:353:GLU:H	1:C:365:ILE:N	2.13	0.46
2:F:336:SER:H	2:F:348:VAL:C	2.19	0.46
1:B:49:ALA:H	2:F:69:LEU:N	2.09	0.46
8:T:18:TYR:C	8:T:19:VAL:O	2.52	0.46
2:D:473:LEU:C	2:D:475:GLU:H	2.20	0.46
1:B:61:GLY:HA2	1:B:74:VAL:O	2.17	0.44
1:C:149:GLY:CA	1:C:436:MET:H	2.31	0.44
2:D:213:SER:C	2:D:215:VAL:H	2.22	0.44
1:B:258:ARG:O	1:B:319:GLY:HA2	2.18	0.43
8:T:99:ILE:O	8:T:100:ALA:C	2.56	0.43
2:F:272:LEU:C	2:F:274:ARG:H	2.22	0.43
1:C:316:PHE:C	1:C:318:GLY:H	2.22	0.42
11:W:156:LEU:O	11:W:160:LEU:N	2.53	0.42
2:D:419:GLN:CA	2:D:429:GLY:H	2.32	0.42
7:S:65:LYS:C	7:S:67:LYS:H	2.23	0.42
3:G:178:ILE:C	3:G:180:SER:H	2.23	0.41
3:G:263:ILE:O	3:G:266:ILE:O	2.38	0.41
1:A:15:ARG:CA	1:A:19:ALA:H	2.33	0.41
1:C:189:PHE:C	1:C:192:GLY:H	2.24	0.41
3:G:139:GLY:HA3	5:I:38:SER:O	2.20	0.41
3:G:268:GLY:H	3:G:270:ALA:H	1.69	0.41
1:A:317:GLY:C	1:A:319:GLY:H	2.23	0.41
1:B:259:ASP:C	1:B:261:GLY:H	2.23	0.40
7:S:19:ALA:O	7:S:23:TYR:N	2.55	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%)	452 (89%)	30 (6%)	25 (5%)	2	20
1	B	476/510 (93%)	419 (88%)	38 (8%)	19 (4%)	3	23
1	C	485/510 (95%)	443 (91%)	26 (5%)	16 (3%)	4	26
2	D	465/482 (96%)	418 (90%)	33 (7%)	14 (3%)	4	28
2	E	464/482 (96%)	409 (88%)	35 (8%)	20 (4%)	2	22
2	F	464/482 (96%)	417 (90%)	27 (6%)	20 (4%)	2	22
3	G	258/273 (94%)	199 (77%)	34 (13%)	25 (10%)	0	9
4	H	129/146 (88%)	114 (88%)	8 (6%)	7 (5%)	2	19
5	I	45/50 (90%)	38 (84%)	6 (13%)	1 (2%)	6	35
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%)	117 (70%)	27 (16%)	22 (13%)	0	4
8	T	172/174 (99%)	157 (91%)	10 (6%)	5 (3%)	4	29
9	U	120/124 (97%)	102 (85%)	11 (9%)	7 (6%)	1	18
10	V	65/77 (84%)	53 (82%)	8 (12%)	4 (6%)	1	16
11	W	215/217 (99%)	191 (89%)	21 (10%)	3 (1%)	11	46
All	All	4591/4803 (96%)	4026 (88%)	368 (8%)	197 (4%)	5	22

All (197) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	14	GLU
1	A	45	ARG
1	A	48	GLN
1	A	171	ARG
1	A	194	ASP
1	A	224	ASP
1	A	262	LYS
1	A	289	PRO
1	A	319	GLY
1	A	509	GLU
1	B	45	ARG
1	B	143	ARG
1	B	163	GLN
1	B	171	ARG
1	B	224	ASP
1	B	238	ASP
1	B	346	THR
1	B	505	LEU
1	C	57	SER
1	C	121	ILE
1	C	146	MET
1	C	289	PRO
1	C	365	ILE
2	D	277	SER
2	D	364	GLY
2	D	451	HIS
2	E	132	ILE
2	E	276	PRO
2	E	281	TYR
2	E	344	ILE
2	E	352	ASP
2	E	428	LEU
2	F	30	PRO
2	F	282	GLN
2	F	348	VAL
2	F	396	LEU
3	G	51	LEU
3	G	118	ARG
3	G	156	ASP
3	G	199	ASP
3	G	250	PHE
3	G	271	ALA

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Mol	Chain	Res	Type
4	H	49	ALA
4	H	50	ALA
4	H	51	HIS
7	S	47	LYS
7	S	50	LYS
7	S	78	PHE
7	S	81	LEU
7	S	106	SER
7	S	108	MET
7	S	115	GLU
7	S	125	ALA
7	S	146	GLN
7	S	151	GLU
8	T	164	CYS
8	T	165	ILE
9	U	13	PHE
9	U	14	GLY
10	V	7	PRO
10	V	8	VAL
10	V	67	PRO
1	A	21	THR
1	A	238	ASP
1	A	331	ALA
1	A	374	VAL
1	B	319	GLY
1	C	26	GLU
1	C	44	LEU
1	C	47	VAL
1	C	224	ASP
1	C	346	THR
1	C	430	GLN
2	D	223	ASN
2	D	297	THR
2	D	363	VAL
2	E	73	GLN
2	E	157	GLY
2	E	210	ASP
2	E	451	HIS
2	F	82	ILE
2	F	299	THR
2	F	450	ASP
3	G	9	ARG

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Mol	Chain	Res	Type
3	G	76	GLY
3	G	87	LYS
3	G	93	ALA
3	G	155	PHE
3	G	191	SER
3	G	257	VAL
4	H	69	ASP
5	I	2	ALA
7	S	14	ILE
7	S	29	GLN
8	T	151	SER
9	U	3	LEU
9	U	12	ALA
9	U	98	CYS
10	V	68	LYS
1	A	11	ILE
1	A	146	MET
1	A	235	THR
1	A	410	LEU
1	B	141	SER
1	C	145	PRO
1	C	171	ARG
2	D	55	GLU
2	D	176	ALA
2	D	214	LYS
2	E	249	GLN
2	E	299	THR
2	F	72	GLY
2	F	102	ILE
2	F	129	GLU
2	F	213	SER
2	F	359	ASP
2	F	453	PRO
3	G	10	LEU
3	G	72	SER
3	G	92	GLU
3	G	117	HIS
3	G	134	ARG
3	G	168	VAL
3	G	200	VAL
3	G	258	ILE
4	H	101	ASP

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Mol	Chain	Res	Type
4	H	124	ASP
6	J	45	GLN
7	S	77	LYS
7	S	153	LYS
9	U	99	ALA
11	W	40	ASN
1	A	23	VAL
1	A	26	GLU
1	A	209	LYS
1	B	235	THR
1	B	289	PRO
1	B	377	ALA
1	B	456	LEU
1	C	27	GLU
2	D	360	PRO
2	E	223	ASN
2	F	160	VAL
2	F	394	ASP
6	P	40	PRO
6	Q	44	GLN
7	S	10	GLN
7	S	61	LYS
7	S	92	ASN
7	S	130	THR
11	W	36	ARG
1	A	8	VAL
1	B	59	LEU
1	B	170	ASP
2	D	101	PRO
2	D	279	VAL
2	E	357	ILE
2	F	157	GLY
2	F	357	ILE
3	G	201	LEU
3	G	268	GLY
4	H	39	PRO
6	O	39	ASN
7	S	68	SER
7	S	93	GLY
11	W	92	PHE
1	C	143	ARG
7	S	9	VAL

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Mol	Chain	Res	Type
7	S	66	VAL
2	D	30	PRO
2	E	279	VAL
2	F	279	VAL
3	G	69	ILE
6	M	40	PRO
8	T	152	ILE
2	E	102	ILE
9	U	79	PRO
1	B	47	VAL
1	B	115	ILE
1	C	68	PRO
2	E	30	PRO
2	E	161	GLY
2	E	417	PRO
2	F	121	PRO
2	F	462	PRO
3	G	115	ILE
6	J	40	PRO
6	M	71	ILE
8	T	28	ILE
1	A	47	VAL
1	A	365	ILE
1	B	134	PRO
2	D	282	GLN
2	E	144	ALA
6	K	40	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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation (i)

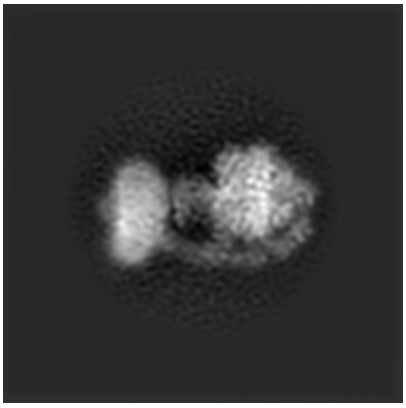
This section contains visualisations of the EMDB entry EMD-3169. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

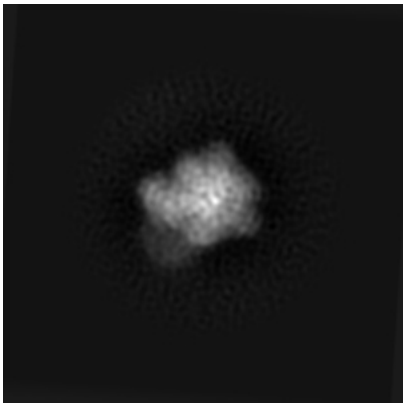
6.1 Orthogonal projections (i)

6.1.1 Primary map

X



Y



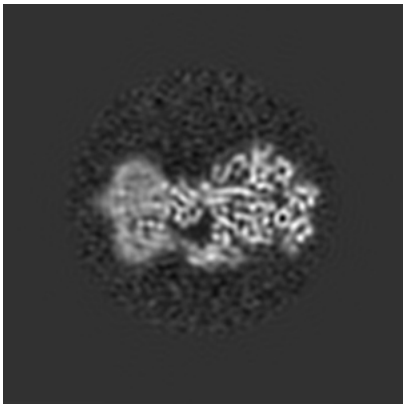
Z

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

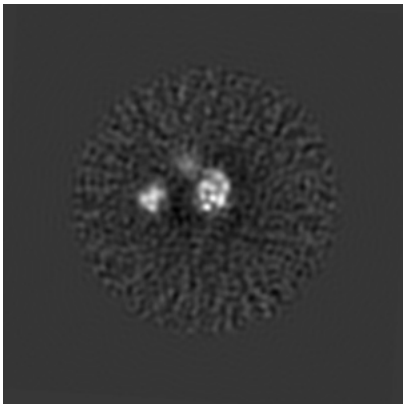
6.2 Central slices (i)

6.2.1 Primary map

X Index: 128



Y Index: 128



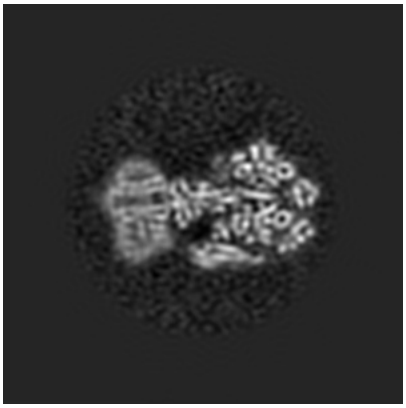
Z Index: 128

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

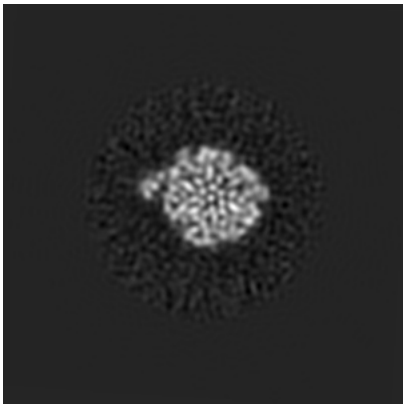
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 134



Y Index: 131

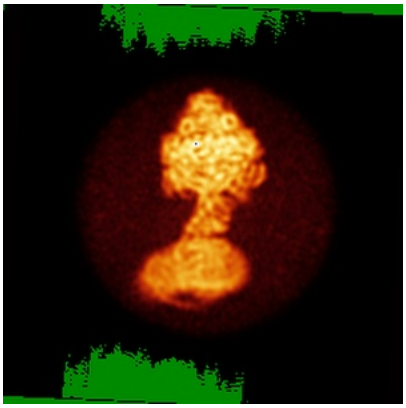


Z Index: 166

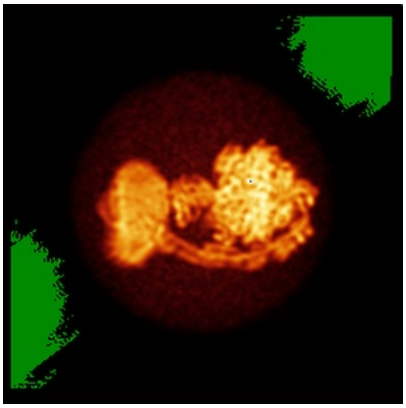
The images above show the largest variance slices of the map in three orthogonal directions.

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

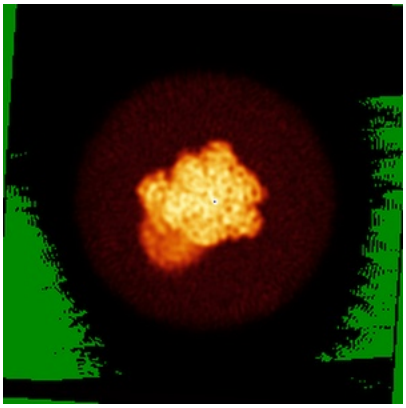
6.4.1 Primary map



X



Y

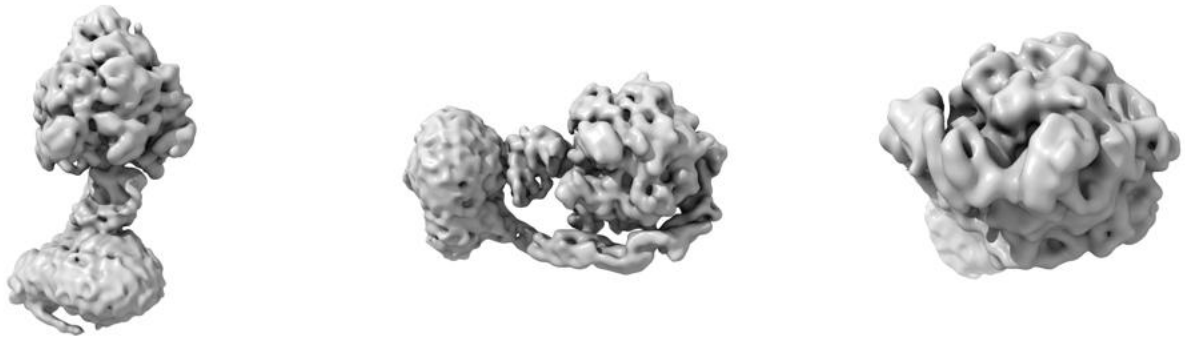


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



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.

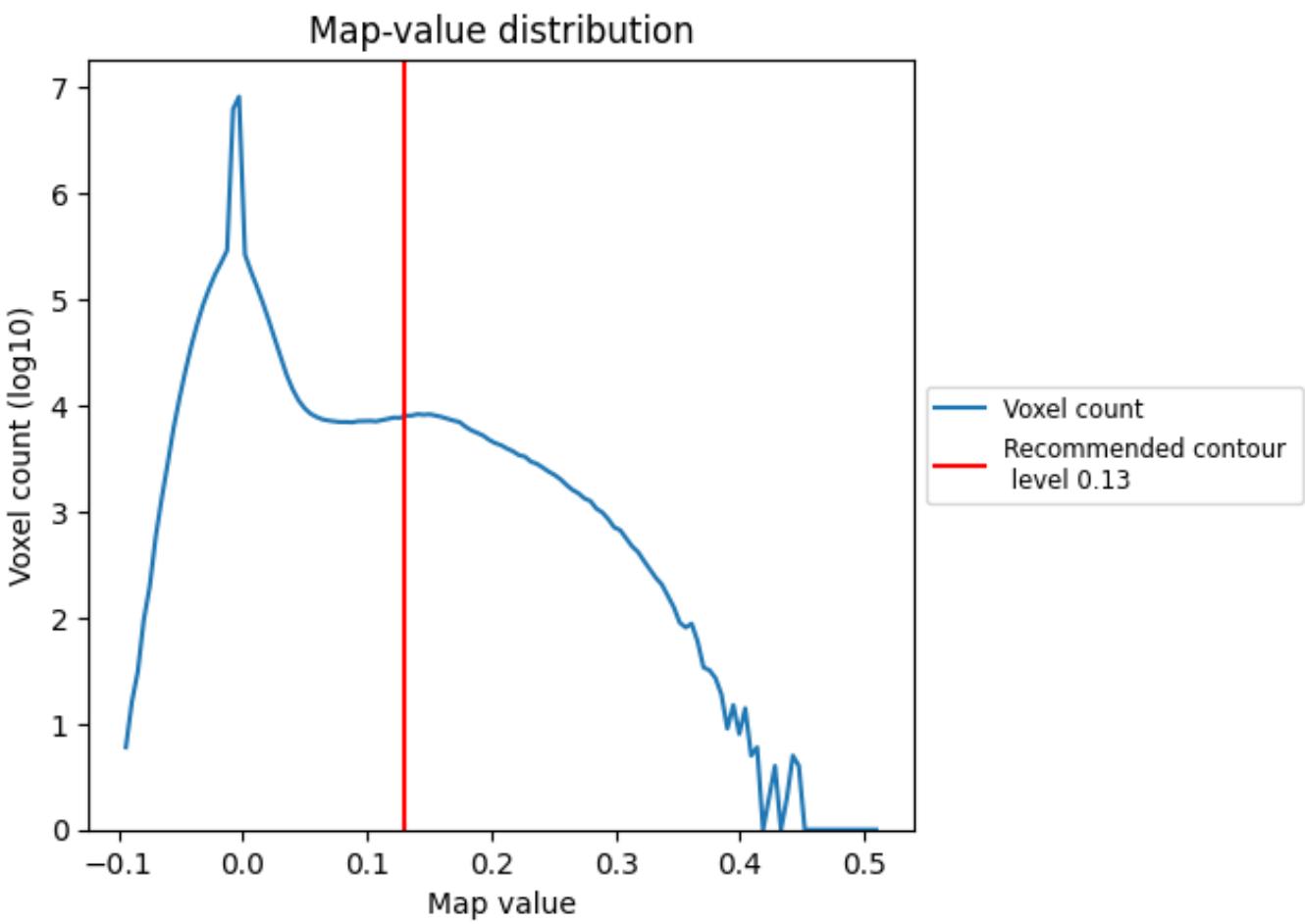
6.6 Mask visualisation (i)

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

7 Map analysis (i)

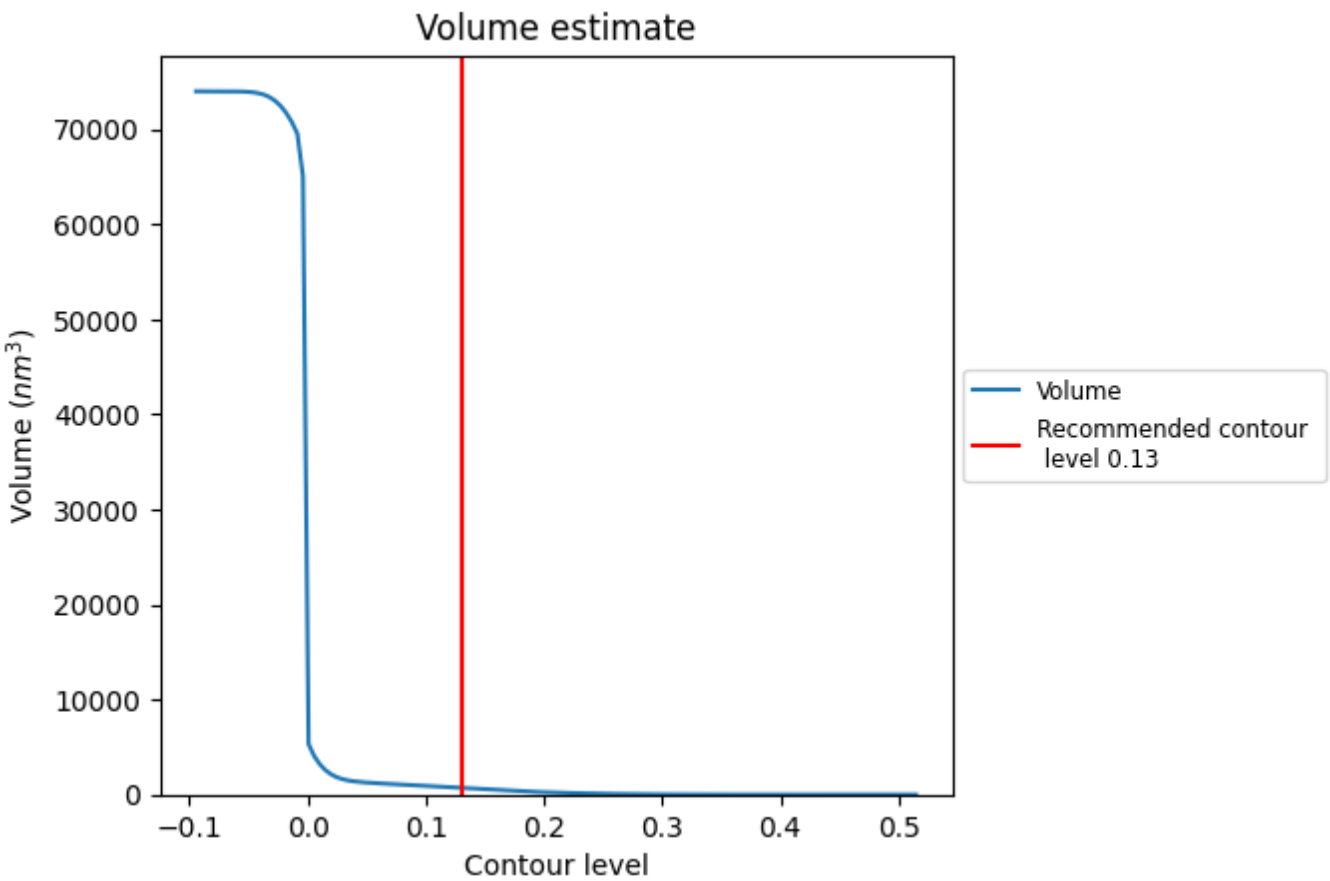
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

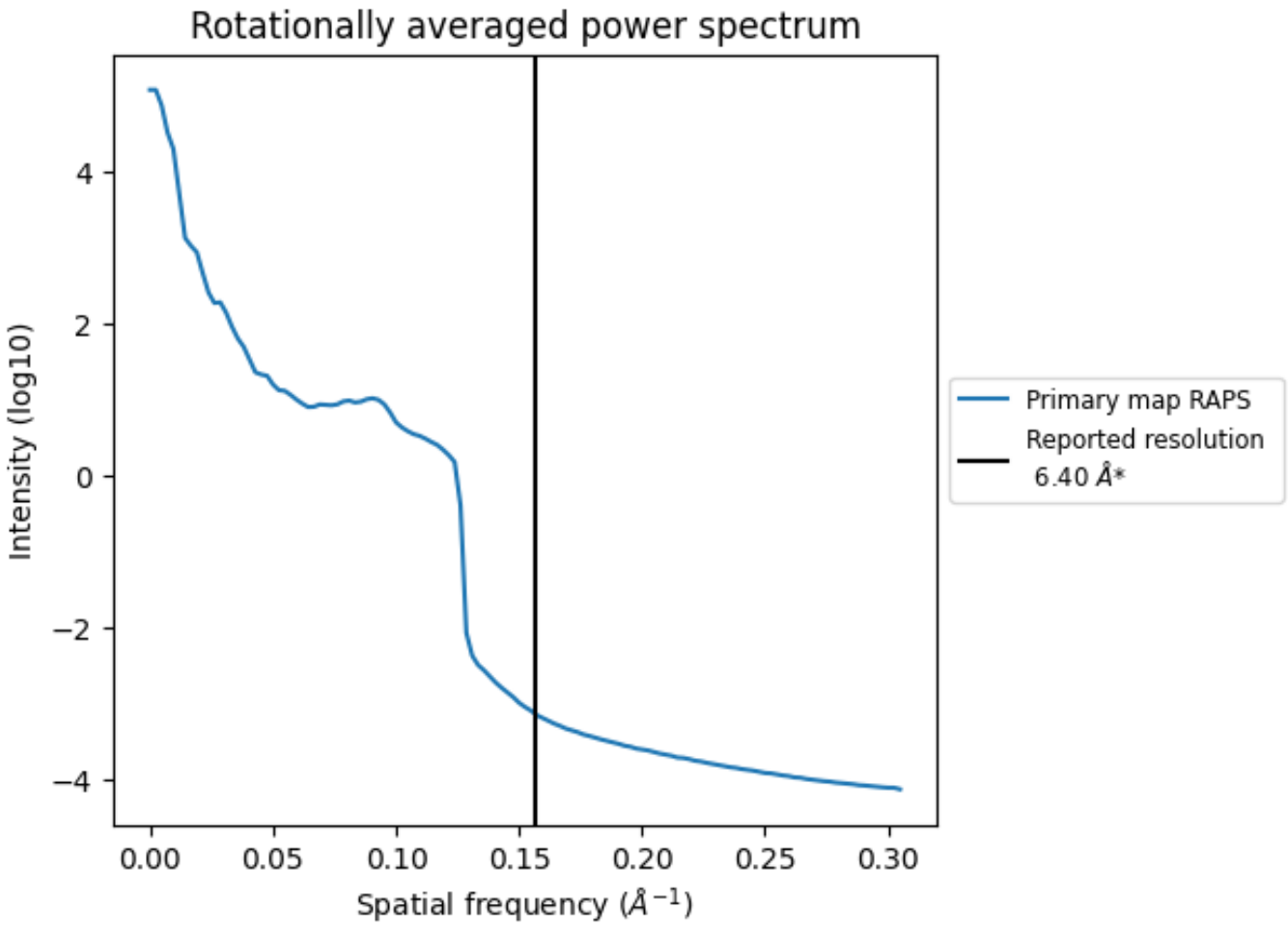
7.2 Volume estimate (i)



The volume at the recommended contour level is 713 nm^3; this corresponds to an approximate mass of 644 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 0.156 Å^{-1}

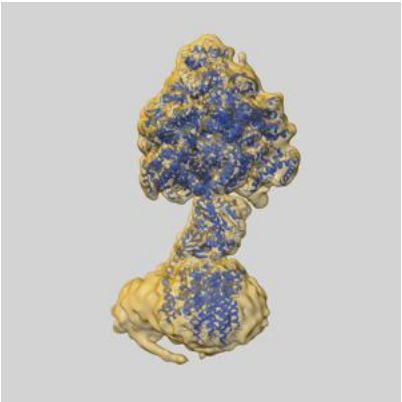
8 Fourier-Shell correlation (i)

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

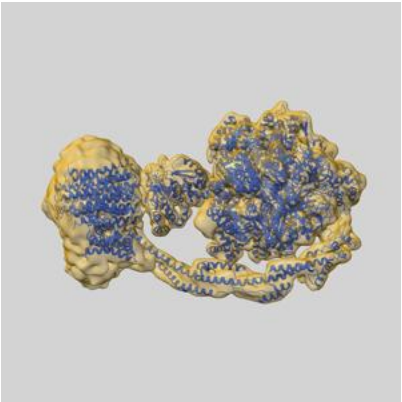
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3169 and PDB model 5FIK. Per-residue inclusion information can be found in section 3 on page 7.

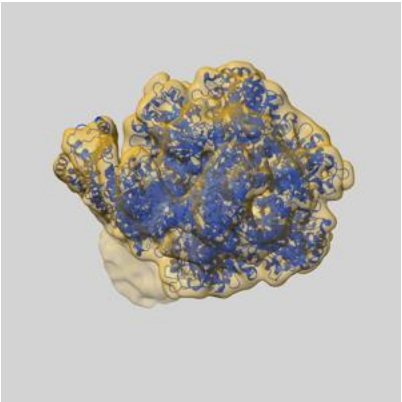
9.1 Map-model overlay (i)



X



Y



Z

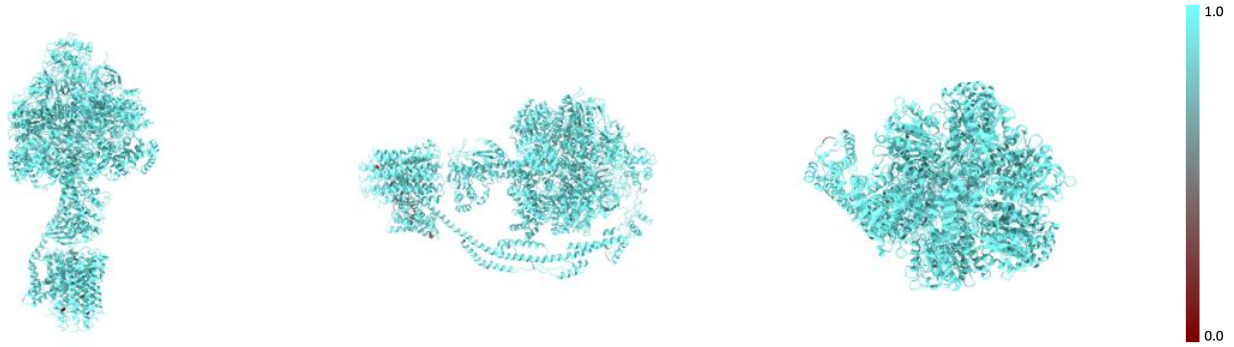
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

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

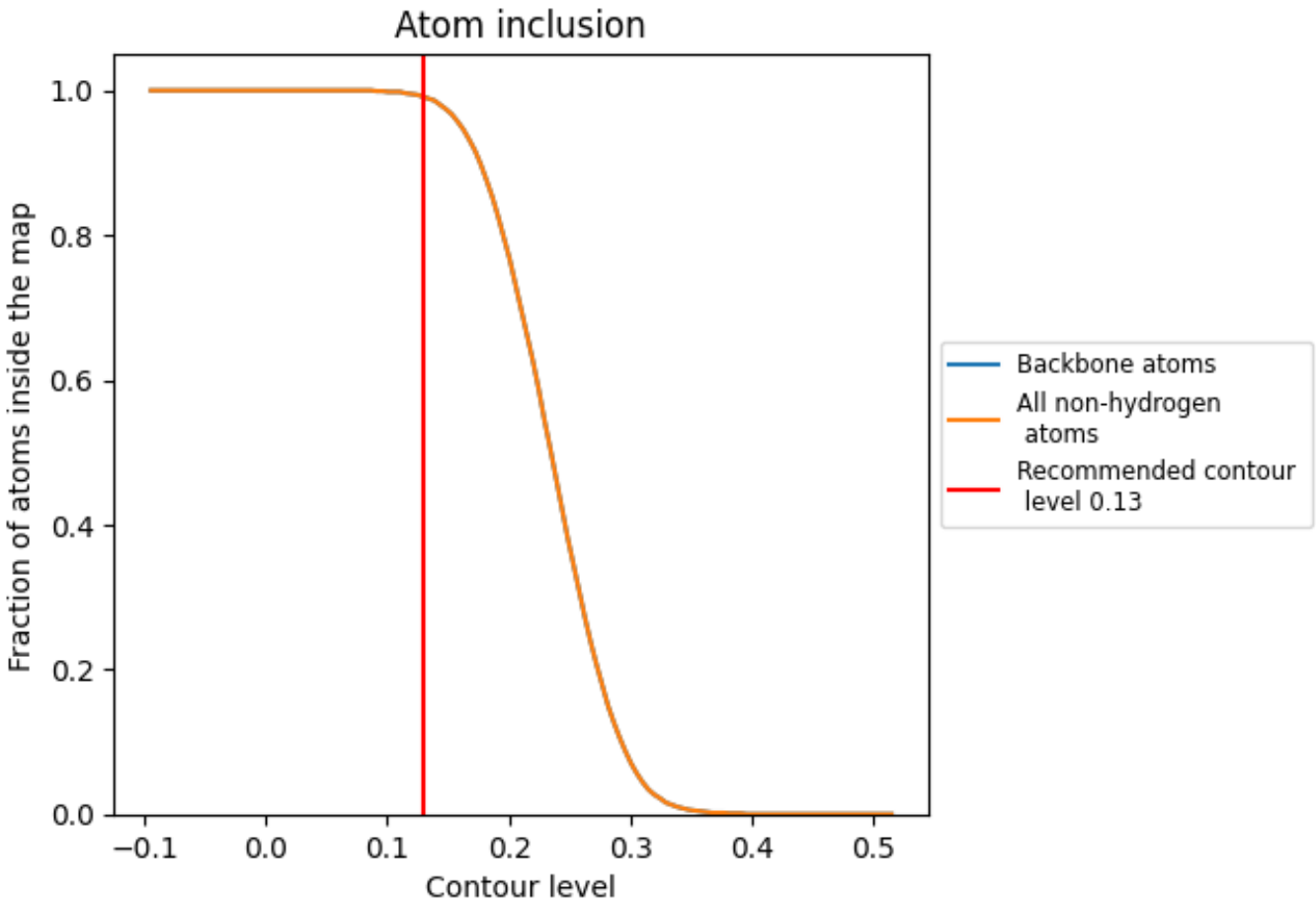
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).

9.4 Atom inclusion (i)



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

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9910	0.2850
A	0.9950	0.3020
B	1.0000	0.3090
C	1.0000	0.3170
D	1.0000	0.3070
E	1.0000	0.3100
F	1.0000	0.3040
G	0.9970	0.3150
H	1.0000	0.3090
I	0.9570	0.2930
J	1.0000	0.1950
K	0.9900	0.2250
L	0.9900	0.1760
M	0.9760	0.1740
N	0.9830	0.1930
O	0.9620	0.1990
P	0.9760	0.1590
Q	0.9900	0.1830
S	0.9910	0.3120
T	0.9910	0.2940
U	0.9570	0.2420
V	0.9740	0.2690
W	0.9270	0.1830