



Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 08:53 am GMT

PDB ID : 5ARI
EMDB ID : EMD-3167
Title : Bovine mitochondrial ATP synthase state 2b
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 ⓘ symbol.

The types of validation reports are described at

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

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

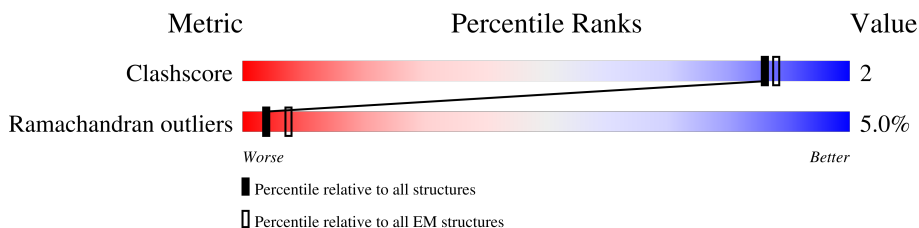
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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.



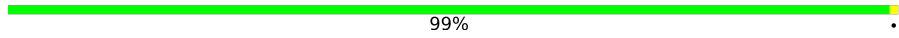
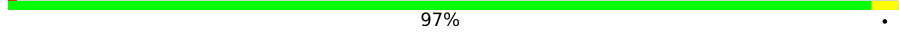
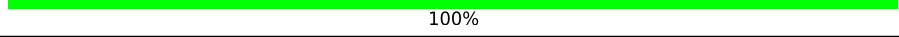
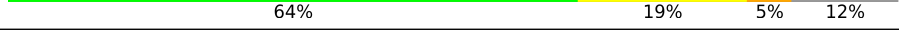
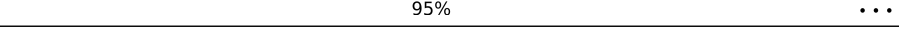
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	510	
1	B	510	
1	C	510	
2	D	482	
2	E	482	
2	F	482	
3	G	273	
4	H	146	
5	I	50	

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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% 19% 5% 12%
8	T	174	 87% 11% ..
9	U	124	 95% ...
10	V	77	 60% 23% . 13%
11	W	217	 96% .

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-COUPPLING FACTOR 6, MITOCHONDRIAL.

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

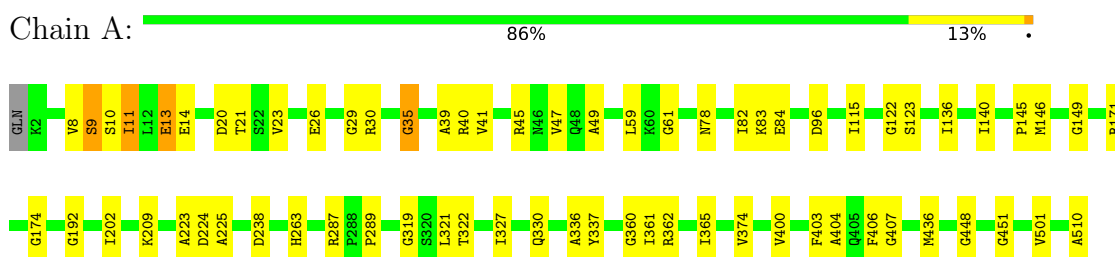
- Molecule 11 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

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

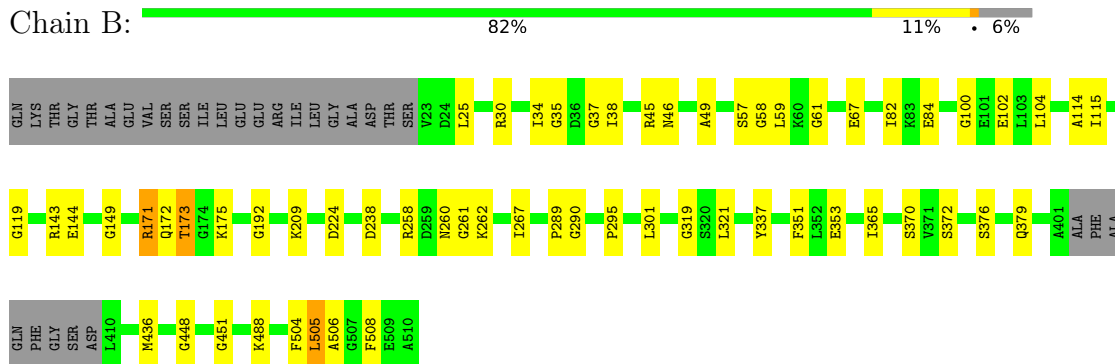
3 Residue-property plots [i](#)

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.

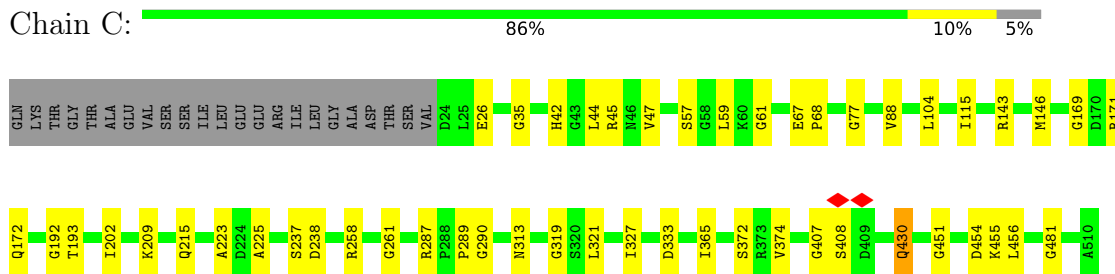
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



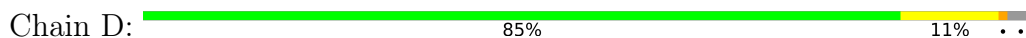
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

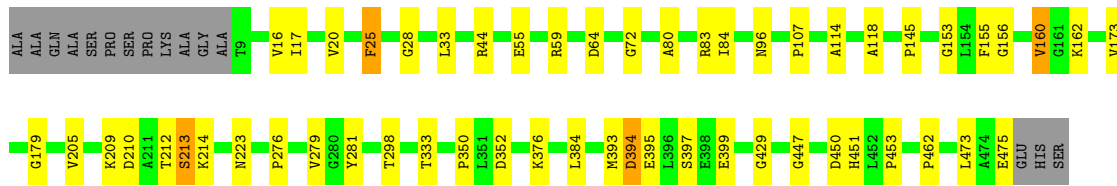


- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

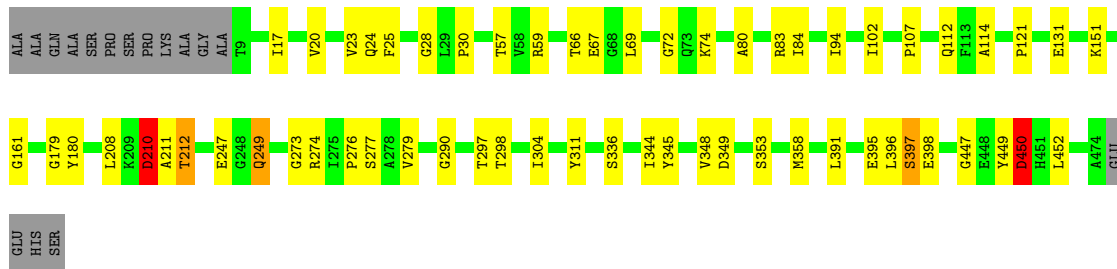
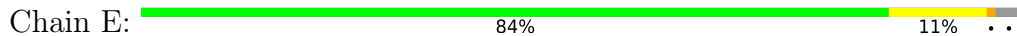


- Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

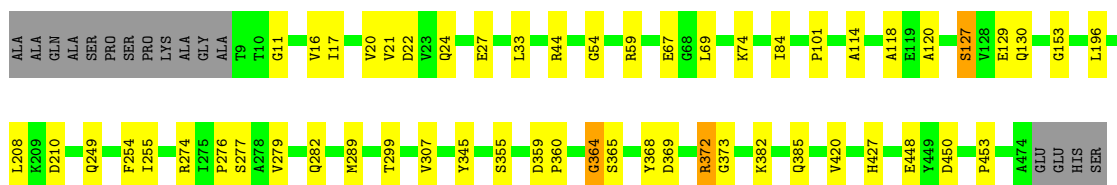
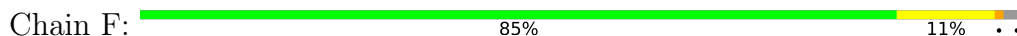




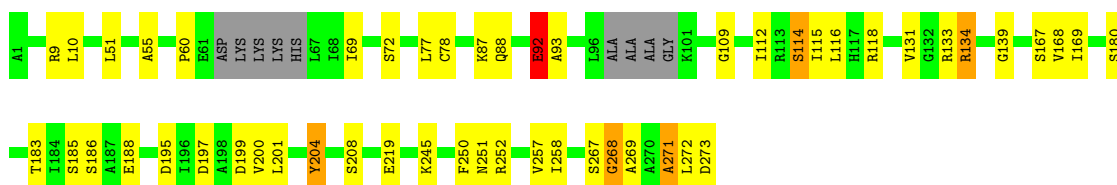
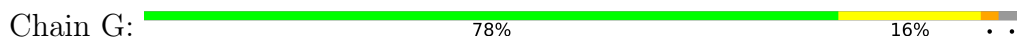
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



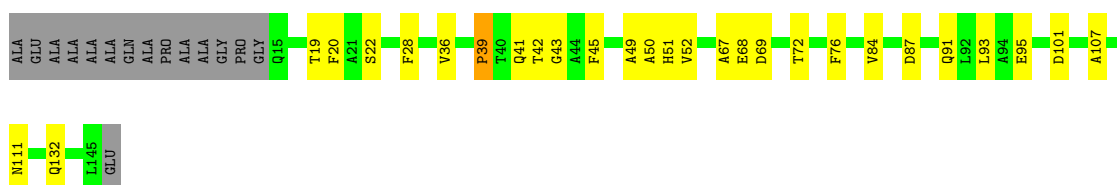
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL



• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL



• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL

Chain I:  76% 16% 6%



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

Chain J:  97%



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

Chain K:  99%



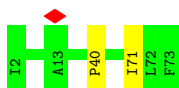
- Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain L:  100%

There are no outlier residues recorded for this chain.

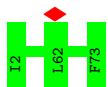
- Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain M:  97%



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

Chain N:  100%



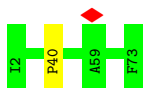
- Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain O:  99%



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

Chain P:  99%



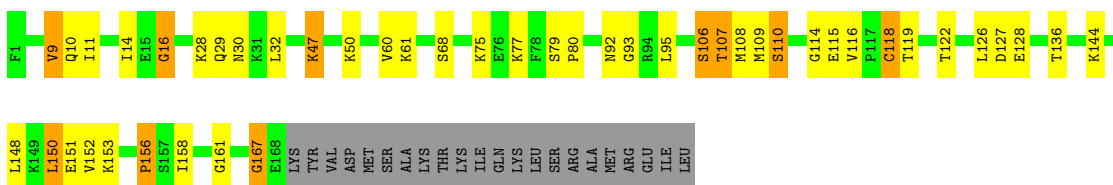
- Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain Q:  97%



- Molecule 7: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL

Chain S:  64% 19% 5% 12%



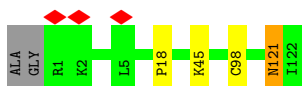
- Molecule 8: ATP SYNTHASE F(0) COMPLEX SUBUNIT B1, MITOCHONDRIAL

Chain T:  87% 11% ..



- Molecule 9: ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL

Chain U:  95% ...



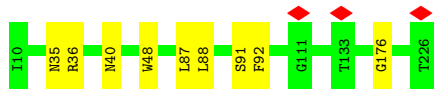
- Molecule 10: ATP SYNTHASE-COUPPLING FACTOR 6, MITOCHONDRIAL

Chain V:  60% 23% 13%



- Molecule 11: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain W:  96%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17610	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	0.395	Depositor
Minimum map value	-0.096	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.13	Depositor
Map size (\AA)	419.84, 419.84, 419.84	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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	1.83	9/2034 (0.4%)	1.55	29/2541 (1.1%)
1	B	1.90	7/1916 (0.4%)	1.53	19/2392 (0.8%)
1	C	1.85	4/1946 (0.2%)	1.50	23/2431 (0.9%)
2	D	1.84	4/1866 (0.2%)	1.55	20/2331 (0.9%)
2	E	1.81	3/1862 (0.2%)	1.54	27/2326 (1.2%)
2	F	1.82	9/1862 (0.5%)	1.53	18/2326 (0.8%)
3	G	1.98	7/1050 (0.7%)	1.58	10/1308 (0.8%)
4	H	2.09	5/522 (1.0%)	1.80	12/651 (1.8%)
5	I	1.91	1/186 (0.5%)	1.70	4/231 (1.7%)
6	J	0.30	0/287	0.41	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	0.31	0/287	0.41	0/357
6	P	0.29	0/287	0.42	0/357
6	Q	0.30	0/287	0.44	0/357
7	S	1.72	1/668 (0.1%)	2.43	11/834 (1.3%)
8	T	0.70	0/696	1.11	3/867 (0.3%)
9	U	0.56	0/484	2.57	1/604 (0.2%)
10	V	0.70	0/264	1.19	0/329
11	W	0.43	0/868	0.73	0/1082
All	All	1.63	50/18520 (0.3%)	1.49	177/23109 (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	6
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	3
2	F	0	2
3	G	0	2
7	S	0	11
8	T	0	18
9	U	0	2
10	V	0	20
11	W	0	5
All	All	0	78

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	35	GLY	N-CA	-7.25	1.35	1.46
3	G	252	ARG	CA-C	-6.38	1.36	1.52
1	C	261	GLY	CA-C	-5.94	1.42	1.51
4	H	28	PHE	CA-C	-5.93	1.37	1.52
1	A	451	GLY	CA-C	-5.92	1.42	1.51
1	C	215	GLN	N-CA	-5.92	1.34	1.46
2	E	74	LYS	CA-C	-5.64	1.38	1.52
2	F	364	GLY	CA-C	-5.63	1.42	1.51
1	A	174	GLY	N-CA	-5.62	1.37	1.46
1	A	35	GLY	CA-C	-5.61	1.42	1.51
1	B	451	GLY	CA-C	-5.57	1.43	1.51
3	G	109	GLY	N-CA	-5.46	1.37	1.46
1	C	481	GLY	CA-C	-5.46	1.43	1.51
3	G	268	GLY	CA-C	-5.41	1.43	1.51
2	D	153	GLY	CA-C	-5.39	1.43	1.51
2	F	373	GLY	CA-C	-5.39	1.43	1.51
7	S	16	GLY	N-CA	-5.37	1.38	1.46
3	G	252	ARG	N-CA	-5.36	1.35	1.46
2	D	173	VAL	CA-C	-5.34	1.39	1.52
1	A	448	GLY	CA-C	-5.34	1.43	1.51
4	H	132	GLN	N-CA	-5.32	1.35	1.46
2	F	373	GLY	N-CA	-5.31	1.38	1.46
2	E	290	GLY	CA-C	-5.31	1.43	1.51
2	F	196	LEU	CA-C	-5.25	1.39	1.52
1	B	35	GLY	CA-C	-5.22	1.43	1.51
1	B	337	TYR	CA-C	-5.19	1.39	1.52
4	H	19	THR	CA-C	-5.19	1.39	1.52
3	G	219	GLU	N-CA	-5.19	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	20	PHE	N-CA	-5.18	1.35	1.46
4	H	19	THR	N-CA	-5.18	1.35	1.46
1	A	319	GLY	CA-C	-5.18	1.43	1.51
1	A	501	VAL	CA-C	-5.18	1.39	1.52
2	E	72	GLY	N-CA	-5.13	1.38	1.46
2	D	447	GLY	CA-C	-5.11	1.43	1.51
3	G	251	ASN	CA-C	-5.11	1.39	1.52
1	B	261	GLY	CA-C	-5.10	1.43	1.51
2	F	153	GLY	CA-C	-5.10	1.43	1.51
1	B	448	GLY	CA-C	-5.09	1.43	1.51
1	C	451	GLY	CA-C	-5.08	1.43	1.51
1	A	337	TYR	CA-C	-5.07	1.39	1.52
2	F	369	ASP	CA-C	-5.05	1.39	1.52
3	G	245	LYS	CA-C	-5.05	1.39	1.52
5	I	14	TYR	N-CA	-5.05	1.36	1.46
2	D	376	LYS	N-CA	-5.05	1.36	1.46
2	F	74	LYS	CA-C	-5.04	1.39	1.52
2	F	372	ARG	CA-C	-5.04	1.39	1.52
1	A	26	GLU	CA-C	-5.03	1.39	1.52
1	B	301	LEU	CA-C	-5.03	1.39	1.52
2	F	289	MET	N-CA	-5.02	1.36	1.46
1	B	267	ILE	N-CA	-5.01	1.36	1.46

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	U	121	ASN	O-C-N	-59.23	27.93	122.70
7	S	167	GLY	O-C-N	-48.08	45.78	122.70
7	S	110	SER	C-N-CA	12.85	153.84	121.70
7	S	107	THR	C-N-CA	9.54	145.54	121.70
1	A	35	GLY	N-CA-C	-8.91	90.83	113.10
2	E	210	ASP	N-CA-C	-8.17	88.93	111.00
2	D	395	GLU	N-CA-C	-8.03	89.32	111.00
8	T	93	ASP	N-CA-C	-7.91	89.65	111.00
1	A	362	ARG	N-CA-C	-7.79	89.95	111.00
2	F	20	VAL	N-CA-C	-7.71	90.19	111.00
2	F	345	TYR	N-CA-C	-7.70	90.21	111.00
7	S	150	LEU	N-CA-C	-7.66	90.31	111.00
2	F	17	ILE	N-CA-C	-7.64	90.36	111.00
1	B	100	GLY	N-CA-C	-7.61	94.08	113.10
3	G	134	ARG	N-CA-C	-7.61	90.46	111.00
1	A	327	ILE	N-CA-C	-7.52	90.70	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	35	GLY	N-CA-C	-7.50	94.35	113.10
2	E	298	THR	N-CA-C	-7.07	91.90	111.00
1	A	140	ILE	N-CA-C	-6.96	92.22	111.00
2	E	349	ASP	N-CA-C	-6.90	92.37	111.00
2	D	429	GLY	N-CA-C	-6.88	95.89	113.10
2	D	17	ILE	N-CA-C	-6.84	92.53	111.00
1	C	407	GLY	N-CA-C	-6.80	96.11	113.10
3	G	109	GLY	N-CA-C	-6.77	96.17	113.10
5	I	42	ILE	N-CA-C	-6.77	92.71	111.00
1	C	67	GLU	N-CA-C	-6.71	92.88	111.00
1	A	123	SER	N-CA-C	-6.67	92.99	111.00
2	E	24	GLN	N-CA-C	-6.66	93.02	111.00
5	I	8	GLY	N-CA-C	-6.64	96.49	113.10
1	C	61	GLY	N-CA-C	-6.64	96.50	113.10
2	D	298	THR	N-CA-C	-6.63	93.09	111.00
1	B	488	LYS	N-CA-C	-6.63	93.09	111.00
1	B	25	LEU	N-CA-C	-6.63	93.11	111.00
4	H	36	VAL	N-CA-C	-6.60	93.18	111.00
1	C	146	MET	N-CA-C	-6.58	93.25	111.00
4	H	93	LEU	N-CA-C	-6.56	93.28	111.00
1	B	290	GLY	N-CA-C	-6.54	96.76	113.10
4	H	91	GLN	N-CA-C	-6.51	93.42	111.00
2	F	22	ASP	N-CA-C	-6.50	93.44	111.00
3	G	77	LEU	C-N-CA	6.50	137.95	121.70
1	C	42	HIS	C-N-CA	6.47	135.88	122.30
4	H	84	VAL	N-CA-C	-6.40	93.72	111.00
1	B	38	ILE	N-CA-C	-6.40	93.73	111.00
1	B	267	ILE	N-CA-C	-6.39	93.75	111.00
1	A	61	GLY	N-CA-C	-6.23	97.53	113.10
2	F	208	LEU	C-N-CA	6.21	137.22	121.70
2	E	397	SER	N-CA-C	-6.21	94.24	111.00
2	F	16	VAL	N-CA-C	-6.20	94.27	111.00
2	D	59	ARG	N-CA-C	-6.18	94.32	111.00
7	S	106	SER	C-N-CA	-6.16	106.30	121.70
2	E	345	TYR	N-CA-C	-6.15	94.39	111.00
2	F	255	ILE	N-CA-C	-6.13	94.44	111.00
2	E	80	ALA	N-CA-C	-6.13	94.46	111.00
2	E	450	ASP	N-CA-C	-6.12	94.47	111.00
2	E	273	GLY	N-CA-C	-6.09	97.89	113.10
2	E	23	VAL	N-CA-C	-6.08	94.60	111.00
1	B	35	GLY	N-CA-C	-6.07	97.93	113.10
3	G	139	GLY	C-N-CA	6.06	136.86	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	83	ARG	N-CA-C	-6.06	94.63	111.00
1	B	61	GLY	N-CA-C	-6.05	97.97	113.10
1	A	29	GLY	N-CA-C	-6.05	97.97	113.10
4	H	67	ALA	C-N-CA	6.05	136.82	121.70
1	B	192	GLY	N-CA-C	-6.04	98.00	113.10
2	F	307	VAL	N-CA-C	-6.04	94.70	111.00
2	D	20	VAL	N-CA-C	-6.03	94.73	111.00
4	H	76	PHE	N-CA-C	-6.01	94.78	111.00
1	C	287	ARG	N-CA-C	-5.99	94.83	111.00
1	C	430	GLN	N-CA-C	-5.97	94.88	111.00
2	D	399	GLU	N-CA-C	-5.94	94.96	111.00
1	B	506	ALA	C-N-CA	5.93	134.76	122.30
1	A	8	VAL	C-N-CA	5.93	136.51	121.70
2	E	17	ILE	N-CA-C	-5.93	95.00	111.00
2	D	393	MET	C-N-CA	5.92	136.50	121.70
2	F	127	SER	N-CA-C	-5.89	95.11	111.00
4	H	22	SER	N-CA-C	-5.88	95.11	111.00
2	D	394	ASP	CA-C-N	-5.88	104.26	117.20
1	A	263	HIS	N-CA-C	-5.88	95.12	111.00
1	A	287	ARG	N-CA-C	-5.82	95.29	111.00
7	S	118	CYS	N-CA-C	-5.82	95.29	111.00
1	A	330	GLN	N-CA-C	-5.82	95.30	111.00
3	G	204	TYR	N-CA-C	-5.81	95.32	111.00
2	E	57	THR	N-CA-C	-5.78	95.39	111.00
2	E	311	TYR	N-CA-C	-5.77	95.42	111.00
1	A	39	ALA	N-CA-C	-5.75	95.48	111.00
1	A	96	ASP	N-CA-C	-5.75	95.48	111.00
1	A	122	GLY	N-CA-C	-5.75	98.73	113.10
2	E	336	SER	N-CA-C	-5.74	95.50	111.00
2	F	355	SER	N-CA-C	-5.73	95.54	111.00
2	F	254	PHE	N-CA-C	-5.71	95.58	111.00
2	F	21	VAL	N-CA-C	-5.71	95.58	111.00
8	T	170	LEU	O-C-N	-5.70	113.58	122.70
4	H	39	PRO	N-CA-C	-5.69	97.30	112.10
1	C	192	GLY	N-CA-C	-5.68	98.89	113.10
1	A	224	ASP	C-N-CA	5.66	135.84	121.70
2	E	449	TYR	N-CA-C	-5.62	95.82	111.00
7	S	144	LYS	N-CA-C	-5.62	95.83	111.00
5	I	41	THR	C-N-CA	5.62	135.74	121.70
2	E	59	ARG	N-CA-C	-5.61	95.85	111.00
2	D	80	ALA	N-CA-C	-5.61	95.86	111.00
2	E	112	GLN	N-CA-C	-5.58	95.94	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	20	VAL	N-CA-C	-5.58	95.94	111.00
1	C	333	ASP	CA-C-N	-5.57	104.94	117.20
3	G	131	VAL	N-CA-C	-5.57	95.96	111.00
2	D	16	VAL	N-CA-C	-5.54	96.03	111.00
2	D	96	ASN	N-CA-C	-5.53	96.07	111.00
1	C	321	LEU	N-CA-C	-5.53	96.08	111.00
1	B	119	GLY	N-CA-C	-5.50	99.34	113.10
7	S	16	GLY	N-CA-C	-5.50	99.34	113.10
2	D	145	PRO	N-CA-C	-5.50	97.80	112.10
2	F	27	GLU	N-CA-C	-5.49	96.17	111.00
4	H	43	GLY	N-CA-C	-5.48	99.39	113.10
2	F	210	ASP	N-CA-C	-5.48	96.21	111.00
7	S	9	VAL	C-N-CA	5.48	135.39	121.70
3	G	114	SER	N-CA-C	-5.45	96.27	111.00
1	C	202	ILE	N-CA-C	-5.44	96.31	111.00
1	B	67	GLU	N-CA-C	-5.44	96.32	111.00
1	A	407	GLY	N-CA-C	5.43	126.68	113.10
1	A	35	GLY	CA-C-N	-5.42	105.27	117.20
3	G	273	ASP	N-CA-C	-5.42	96.36	111.00
1	A	202	ILE	N-CA-C	-5.42	96.36	111.00
1	A	30	ARG	N-CA-C	-5.42	96.37	111.00
1	C	372	SER	N-CA-C	-5.42	96.38	111.00
1	A	192	GLY	N-CA-C	-5.40	99.61	113.10
1	C	193	THR	N-CA-C	-5.38	96.47	111.00
2	E	391	LEU	CA-C-N	5.37	126.95	116.20
2	F	54	GLY	N-CA-C	-5.36	99.70	113.10
2	E	304	ILE	N-CA-C	-5.35	96.55	111.00
1	A	360	GLY	N-CA-C	-5.35	99.73	113.10
1	B	504	PHE	C-N-CA	5.34	135.06	121.70
2	E	211	ALA	C-N-CA	5.34	135.05	121.70
2	F	274	ARG	N-CA-C	-5.33	96.62	111.00
2	D	394	ASP	C-N-CA	5.32	134.99	121.70
3	G	271	ALA	N-CA-C	-5.31	96.66	111.00
2	F	59	ARG	N-CA-C	-5.31	96.66	111.00
1	A	83	LYS	N-CA-C	-5.30	96.69	111.00
2	D	213	SER	N-CA-C	-5.30	96.70	111.00
2	E	353	SER	N-CA-C	-5.29	96.71	111.00
5	I	43	LYS	CA-C-N	-5.29	105.57	117.20
1	B	34	ILE	N-CA-C	-5.28	96.75	111.00
2	E	83	ARG	N-CA-C	-5.25	96.82	111.00
1	B	173	THR	N-CA-C	-5.25	96.83	111.00
1	B	30	ARG	N-CA-C	-5.23	96.88	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	LEU	N-CA-C	-5.22	96.91	111.00
1	C	290	GLY	N-CA-C	-5.21	100.08	113.10
2	E	151	LYS	N-CA-C	-5.19	96.98	111.00
7	S	119	THR	N-CA-C	-5.19	96.99	111.00
1	A	510	ALA	N-CA-C	-5.19	97.00	111.00
1	C	237	SER	N-CA-C	-5.19	97.00	111.00
7	S	47	LYS	N-CA-C	5.18	124.99	111.00
2	D	210	ASP	N-CA-C	-5.18	97.02	111.00
1	A	8	VAL	O-C-N	5.18	130.98	122.70
1	C	327	ILE	N-CA-C	-5.17	97.03	111.00
2	D	118	ALA	N-CA-C	-5.17	97.04	111.00
4	H	72	THR	N-CA-C	-5.17	97.05	111.00
2	D	25	PHE	CA-C-N	-5.17	105.83	117.20
1	C	88	VAL	N-CA-C	-5.16	97.07	111.00
1	C	454	ASP	C-N-CA	5.16	134.59	121.70
4	H	41	GLN	N-CA-C	-5.13	97.14	111.00
2	D	156	GLY	N-CA-C	-5.13	100.28	113.10
1	C	313	ASN	C-N-CA	5.13	134.51	121.70
1	B	58	GLY	C-N-CA	5.11	134.48	121.70
2	E	66	THR	C-N-CA	5.10	134.45	121.70
2	F	365	SER	CA-C-N	5.10	128.41	117.20
1	C	104	LEU	N-CA-C	-5.09	97.24	111.00
1	A	403	PHE	N-CA-C	-5.08	97.27	111.00
1	A	40	ARG	N-CA-C	-5.08	97.28	111.00
1	C	77	GLY	N-CA-C	-5.08	100.41	113.10
8	T	170	LEU	CA-C-N	5.08	128.37	117.20
1	B	321	LEU	N-CA-C	-5.07	97.32	111.00
1	B	372	SER	N-CA-C	-5.07	97.32	111.00
3	G	92	GLU	C-N-CA	5.05	134.34	121.70
1	A	41	VAL	N-CA-C	-5.04	97.39	111.00
2	E	94	ILE	N-CA-C	-5.03	97.43	111.00
2	E	398	GLU	N-CA-C	5.03	124.58	111.00
1	C	407	GLY	C-N-CA	5.02	134.24	121.70
1	A	322	THR	N-CA-C	-5.01	97.48	111.00
4	H	20	PHE	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (78) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	THR	Peptide
1	A	336	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	A	35	GLY	Peptide
1	A	400	VAL	Mainchain
1	A	404	ALA	Mainchain
1	A	406	PHE	Mainchain
1	B	379	GLN	Peptide
1	B	505	LEU	Mainchain
1	C	169	GLY	Mainchain
2	D	160	VAL	Mainchain
2	D	205	VAL	Peptide
2	D	25	PHE	Mainchain
2	D	384	LEU	Mainchain
2	D	397	SER	Mainchain
2	D	72	GLY	Mainchain
2	E	249	GLN	Mainchain
2	E	25	PHE	Mainchain
2	E	397	SER	Mainchain
2	F	130	GLN	Mainchain
2	F	249	GLN	Peptide
3	G	92	GLU	Mainchain,Peptide
7	S	107	THR	Peptide
7	S	118	CYS	Mainchain
7	S	122	THR	Peptide
7	S	150	LEU	Mainchain,Peptide
7	S	151	GLU	Peptide
7	S	152	VAL	Peptide
7	S	156	PRO	Mainchain,Peptide
7	S	161	GLY	Mainchain
7	S	167	GLY	Mainchain
8	T	113	ARG	Mainchain
8	T	121	ARG	Mainchain
8	T	140	MET	Mainchain
8	T	144	VAL	Mainchain
8	T	149	VAL	Peptide
8	T	154	ALA	Peptide
8	T	155	GLN	Mainchain
8	T	158	LYS	Mainchain
8	T	166	ALA	Mainchain
8	T	168	LEU	Peptide
8	T	172	SER	Peptide
8	T	18	TYR	Mainchain
8	T	51	LYS	Mainchain
8	T	84	LEU	Mainchain

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Mol	Chain	Res	Type	Group
8	T	86	GLN	Mainchain
8	T	87	LYS	Mainchain
8	T	89	HIS	Mainchain
8	T	98	ASN	Mainchain
9	U	121	ASN	Mainchain
9	U	18	PRO	Mainchain
10	V	12	PHE	Mainchain
10	V	14	ASP	Mainchain
10	V	18	GLU	Mainchain
10	V	19	TYR	Mainchain
10	V	20	ARG	Mainchain
10	V	27	GLY	Peptide
10	V	29	PRO	Mainchain
10	V	32	ALA	Mainchain
10	V	33	GLY	Mainchain
10	V	35	GLU	Mainchain
10	V	49	GLN	Mainchain
10	V	50	MET	Peptide
10	V	54	ALA	Mainchain
10	V	56	MET	Mainchain
10	V	6	ASP	Mainchain,Peptide
10	V	63	THR	Mainchain
10	V	7	PRO	Mainchain,Peptide
10	V	70	GLU	Mainchain
11	W	176	GLY	Mainchain
11	W	35	ASN	Peptide
11	W	48	TRP	Mainchain
11	W	87	LEU	Mainchain
11	W	91	SER	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2035	0	589	6	0
1	B	1918	0	553	11	0
1	C	1947	0	563	2	0
2	D	1867	0	533	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1863	0	532	7	0
2	F	1863	0	532	7	0
3	G	1053	0	283	5	0
4	H	523	0	140	1	0
5	I	187	0	53	0	0
6	J	288	0	92	0	0
6	K	288	0	92	0	0
6	L	288	0	92	0	0
6	M	288	0	92	0	0
6	N	288	0	92	0	0
6	O	288	0	92	0	0
6	P	288	0	92	0	0
6	Q	288	0	92	0	0
7	S	669	0	178	5	0
8	T	697	0	182	1	0
9	U	485	0	121	0	0
10	V	265	0	68	0	0
11	W	869	0	226	0	0
All	All	18545	0	5289	49	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (49) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:267:SER:H	3:G:271:ALA:H	1.25	0.82
1:B:49:ALA:H	2:F:69:LEU:H	1.33	0.74
1:A:149:GLY:HA3	1:A:436:MET:H	1.54	0.72
1:B:149:GLY:HA3	1:B:436:MET:H	1.56	0.71
7:S:106:SER:O	7:S:108:MET:N	2.28	0.66
1:B:173:THR:N	1:B:175:LYS:H	1.96	0.63
3:G:267:SER:H	3:G:271:ALA:N	1.93	0.63
1:B:173:THR:H	1:B:175:LYS:H	1.51	0.59
7:S:30:ASN:C	7:S:32:LEU:H	2.06	0.57
2:D:160:VAL:H	2:D:162:LYS:H	1.52	0.56
3:G:167:SER:C	3:G:169:ILE:H	2.08	0.55
1:A:223:ALA:C	1:A:225:ALA:H	2.10	0.54
2:E:84:ILE:H	2:E:114:ALA:H	1.55	0.54
2:E:450:ASP:H	2:E:452:LEU:H	1.57	0.53
1:A:149:GLY:CA	1:A:436:MET:H	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:473:LEU:C	2:D:475:GLU:H	2.15	0.50
2:D:160:VAL:N	2:D:162:LYS:H	2.10	0.49
2:F:127:SER:C	2:F:129:GLU:H	2.15	0.49
7:S:28:LYS:C	7:S:30:ASN:H	2.15	0.49
2:E:210:ASP:C	2:E:212:THR:H	2.16	0.48
1:C:223:ALA:C	1:C:225:ALA:H	2.18	0.47
7:S:115:GLU:N	7:S:127:ASP:H	2.13	0.45
1:B:149:GLY:CA	1:B:436:MET:H	2.25	0.45
2:F:84:ILE:H	2:F:114:ALA:H	1.64	0.44
2:F:382:LYS:C	2:F:385:GLN:H	2.21	0.44
2:D:84:ILE:H	2:D:114:ALA:H	1.65	0.44
3:G:204:TYR:O	3:G:208:SER:N	2.50	0.44
7:S:93:GLY:C	7:S:95:LEU:H	2.21	0.43
1:A:49:ALA:H	2:E:69:LEU:N	2.16	0.43
2:F:448:GLU:C	2:F:450:ASP:H	2.21	0.43
1:A:9:SER:O	1:A:11:ILE:N	2.51	0.43
1:B:258:ARG:O	1:B:319:GLY:HA3	2.18	0.43
1:B:351:PHE:H	1:B:370:SER:CA	2.32	0.43
1:B:353:GLU:H	1:B:365:ILE:CA	2.32	0.43
1:C:258:ARG:O	1:C:319:GLY:HA3	2.19	0.42
2:E:208:LEU:C	2:E:210:ASP:H	2.22	0.42
2:E:247:GLU:C	2:E:249:GLN:H	2.22	0.42
2:E:450:ASP:H	2:E:452:LEU:N	2.17	0.42
8:T:166:ALA:O	8:T:170:LEU:N	2.51	0.42
1:A:9:SER:C	1:A:13:GLU:H	2.22	0.42
3:G:112:ILE:C	3:G:114:SER:H	2.22	0.42
2:F:368:TYR:O	2:F:372:ARG:N	2.51	0.41
1:B:260:ASN:C	1:B:262:LYS:H	2.23	0.41
1:B:102:GLU:C	1:B:104:LEU:H	2.23	0.41
2:D:350:PRO:C	2:D:352:ASP:H	2.24	0.41
4:H:107:ALA:O	4:H:111:ASN:N	2.53	0.41
2:D:155:PHE:N	2:D:333:THR:O	2.53	0.40
1:B:171:ARG:O	1:B:173:THR:N	2.54	0.40
2:F:11:GLY:HA2	2:F:24:GLN:O	2.22	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%)	442 (87%)	41 (8%)	24 (5%)	2	21
1	B	476/510 (93%)	425 (89%)	30 (6%)	21 (4%)	2	22
1	C	485/510 (95%)	434 (90%)	31 (6%)	20 (4%)	3	22
2	D	465/482 (96%)	407 (88%)	38 (8%)	20 (4%)	2	22
2	E	464/482 (96%)	406 (88%)	34 (7%)	24 (5%)	2	19
2	F	464/482 (96%)	416 (90%)	31 (7%)	17 (4%)	3	24
3	G	258/273 (94%)	191 (74%)	33 (13%)	34 (13%)	0	4
4	H	129/146 (88%)	105 (81%)	12 (9%)	12 (9%)	0	10
5	I	45/50 (90%)	32 (71%)	8 (18%)	5 (11%)	0	7
6	J	70/72 (97%)	62 (89%)	6 (9%)	2 (3%)	4	29
6	K	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	11	46
6	L	70/72 (97%)	57 (81%)	13 (19%)	0	100	100
6	M	70/72 (97%)	64 (91%)	4 (6%)	2 (3%)	4	29
6	N	70/72 (97%)	61 (87%)	9 (13%)	0	100	100
6	O	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	11	46
6	P	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	11	46
6	Q	70/72 (97%)	61 (87%)	7 (10%)	2 (3%)	4	29
7	S	166/190 (87%)	107 (64%)	32 (19%)	27 (16%)	0	3
8	T	172/174 (99%)	152 (88%)	16 (9%)	4 (2%)	6	34
9	U	120/124 (97%)	108 (90%)	10 (8%)	2 (2%)	9	42
10	V	65/77 (84%)	51 (78%)	8 (12%)	6 (9%)	1	11
11	W	215/217 (99%)	193 (90%)	18 (8%)	4 (2%)	8	38
All	All	4591/4803 (96%)	3966 (86%)	396 (9%)	229 (5%)	4	20

All (229) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	10	SER
1	A	13	GLU
1	A	14	GLU
1	A	20	ASP
1	A	45	ARG
1	A	47	VAL
1	A	59	LEU
1	A	78	ASN
1	A	84	GLU
1	A	238	ASP
1	A	361	ILE
1	A	365	ILE
1	A	374	VAL
1	B	45	ARG
1	B	57	SER
1	B	59	LEU
1	B	114	ALA
1	B	144	GLU
1	B	171	ARG
1	B	172	GLN
1	B	238	ASP
1	B	376	SER
1	C	289	PRO
1	C	365	ILE
1	C	374	VAL
1	C	408	SER
1	C	455	LYS
1	C	456	LEU
2	D	214	LYS
2	D	281	TYR
2	D	450	ASP
2	D	451	HIS
2	E	180	TYR
2	E	210	ASP
2	E	274	ARG
2	E	344	ILE
2	E	348	VAL
2	E	358	MET
2	F	67	GLU
2	F	277	SER
2	F	299	THR
2	F	364	GLY

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Mol	Chain	Res	Type
3	G	55	ALA
3	G	60	PRO
3	G	78	CYS
3	G	93	ALA
3	G	115	ILE
3	G	134	ARG
3	G	183	THR
3	G	186	SER
3	G	199	ASP
3	G	250	PHE
4	H	42	THR
4	H	45	PHE
4	H	49	ALA
4	H	50	ALA
4	H	51	HIS
4	H	52	VAL
4	H	68	GLU
4	H	69	ASP
4	H	87	ASP
4	H	95	GLU
4	H	101	ASP
5	I	28	THR
5	I	41	THR
7	S	10	GLN
7	S	11	ILE
7	S	47	LYS
7	S	50	LYS
7	S	75	LYS
7	S	80	PRO
7	S	109	MET
7	S	110	SER
7	S	126	LEU
7	S	136	THR
7	S	153	LYS
9	U	98	CYS
10	V	54	ALA
10	V	67	PRO
10	V	70	GLU
1	A	11	ILE
1	A	23	VAL
1	A	82	ILE
1	A	171	ARG

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Mol	Chain	Res	Type
1	B	46	ASN
1	B	82	ILE
1	B	84	GLU
1	B	115	ILE
1	B	143	ARG
1	B	209	LYS
1	B	224	ASP
1	B	289	PRO
1	B	505	LEU
1	C	26	GLU
1	C	44	LEU
1	C	45	ARG
1	C	115	ILE
1	C	143	ARG
1	C	172	GLN
1	C	209	LYS
2	D	28	GLY
2	D	107	PRO
2	D	179	GLY
2	D	212	THR
2	D	276	PRO
2	D	394	ASP
2	E	28	GLY
2	E	67	GLU
2	E	102	ILE
2	E	450	ASP
2	F	420	VAL
2	F	453	PRO
3	G	9	ARG
3	G	51	LEU
3	G	69	ILE
3	G	87	LYS
3	G	116	LEU
3	G	180	SER
3	G	185	SER
3	G	200	VAL
3	G	257	VAL
3	G	272	LEU
7	S	68	SER
7	S	114	GLY
7	S	158	ILE
8	T	147	ARG

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Mol	Chain	Res	Type
1	A	146	MET
1	A	289	PRO
1	B	37	GLY
1	B	508	PHE
1	C	68	PRO
1	C	171	ARG
1	C	238	ASP
1	C	430	GLN
2	D	55	GLU
2	D	209	LYS
2	D	462	PRO
2	E	212	THR
2	E	395	GLU
2	F	44	ARG
2	F	118	ALA
2	F	282	GLN
2	F	359	ASP
2	F	427	HIS
3	G	88	GLN
3	G	195	ASP
3	G	197	ASP
3	G	268	GLY
3	G	269	ALA
6	J	45	GLN
7	S	16	GLY
7	S	29	GLN
7	S	79	SER
10	V	55	ASP
11	W	36	ARG
1	A	136	ILE
1	A	209	LYS
1	C	57	SER
2	D	44	ARG
2	D	453	PRO
2	E	277	SER
2	E	447	GLY
2	F	101	PRO
3	G	72	SER
3	G	92	GLU
3	G	188	GLU
5	I	33	ASN
5	I	38	SER

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Mol	Chain	Res	Type
6	P	40	PRO
6	Q	44	GLN
7	S	61	LYS
7	S	77	LYS
8	T	149	VAL
8	T	170	LEU
11	W	40	ASN
1	A	145	PRO
1	C	59	LEU
2	D	33	LEU
2	E	276	PRO
2	E	396	LEU
2	F	33	LEU
2	F	360	PRO
3	G	10	LEU
3	G	133	ARG
3	G	201	LEU
3	G	258	ILE
4	H	39	PRO
6	O	39	ASN
7	S	14	ILE
7	S	92	ASN
7	S	128	GLU
7	S	148	LEU
10	V	31	ASP
11	W	92	PHE
2	D	64	ASP
2	D	213	SER
2	D	223	ASN
2	D	279	VAL
2	E	107	PRO
2	E	131	GLU
2	E	179	GLY
2	E	297	THR
3	G	118	ARG
6	M	40	PRO
9	U	45	LYS
1	A	115	ILE
2	E	161	GLY
2	E	279	VAL
2	F	279	VAL
7	S	116	VAL

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Mol	Chain	Res	Type
10	V	6	ASP
1	B	295	PRO
2	E	30	PRO
2	E	121	PRO
7	S	156	PRO
2	F	120	ALA
3	G	168	VAL
7	S	9	VAL
8	T	19	VAL
1	C	47	VAL
2	F	276	PRO
6	J	40	PRO
6	M	71	ILE
11	W	88	LEU
5	I	39	GLY
7	S	60	VAL
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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

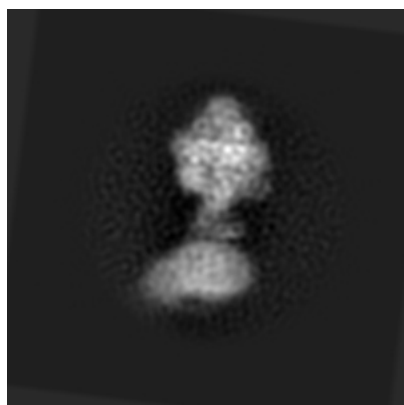
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3167. These allow visual inspection of the internal detail of the map and identification of artifacts.

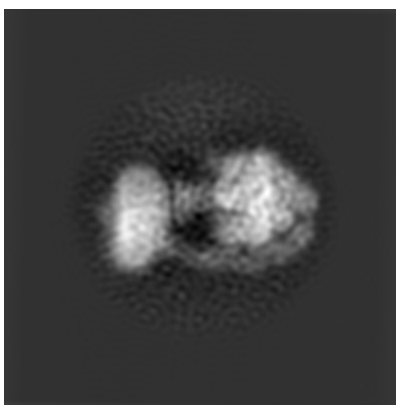
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

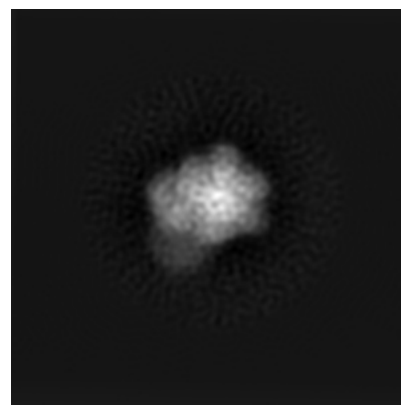
6.1.1 Primary map



X



Y



Z

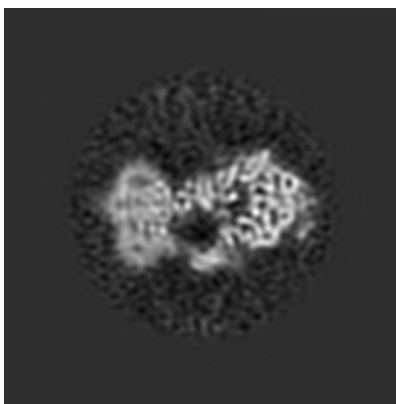
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

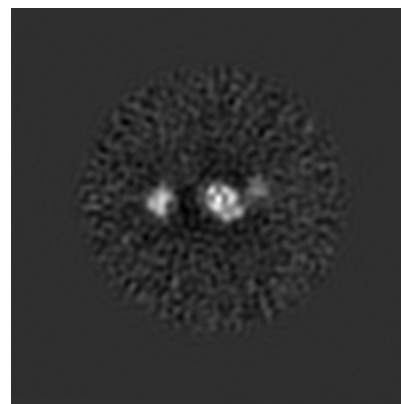
6.2.1 Primary map



X Index: 128



Y Index: 128

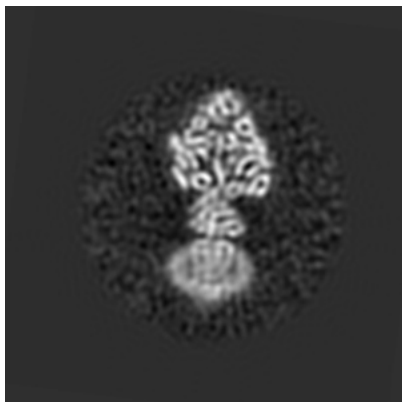


Z Index: 128

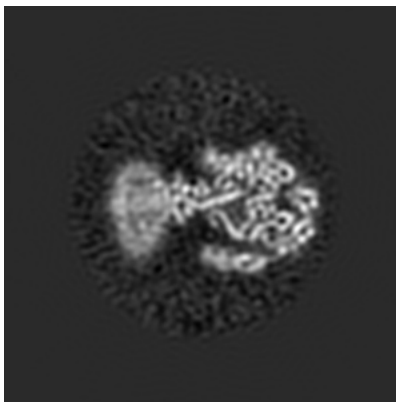
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

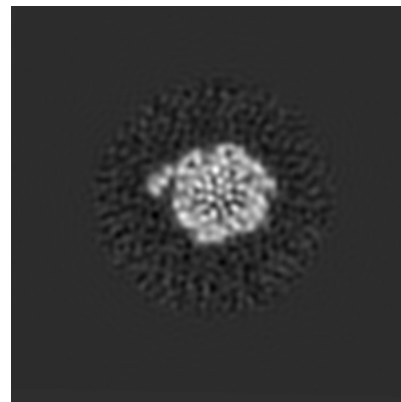
6.3.1 Primary map



X Index: 135



Y Index: 138



Z Index: 165

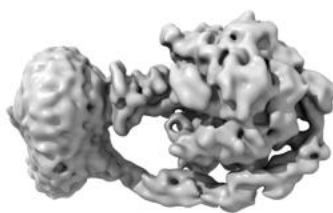
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

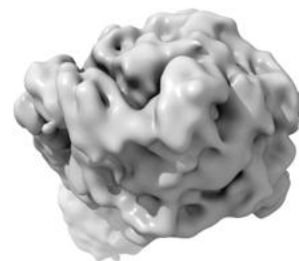
6.4.1 Primary map



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.

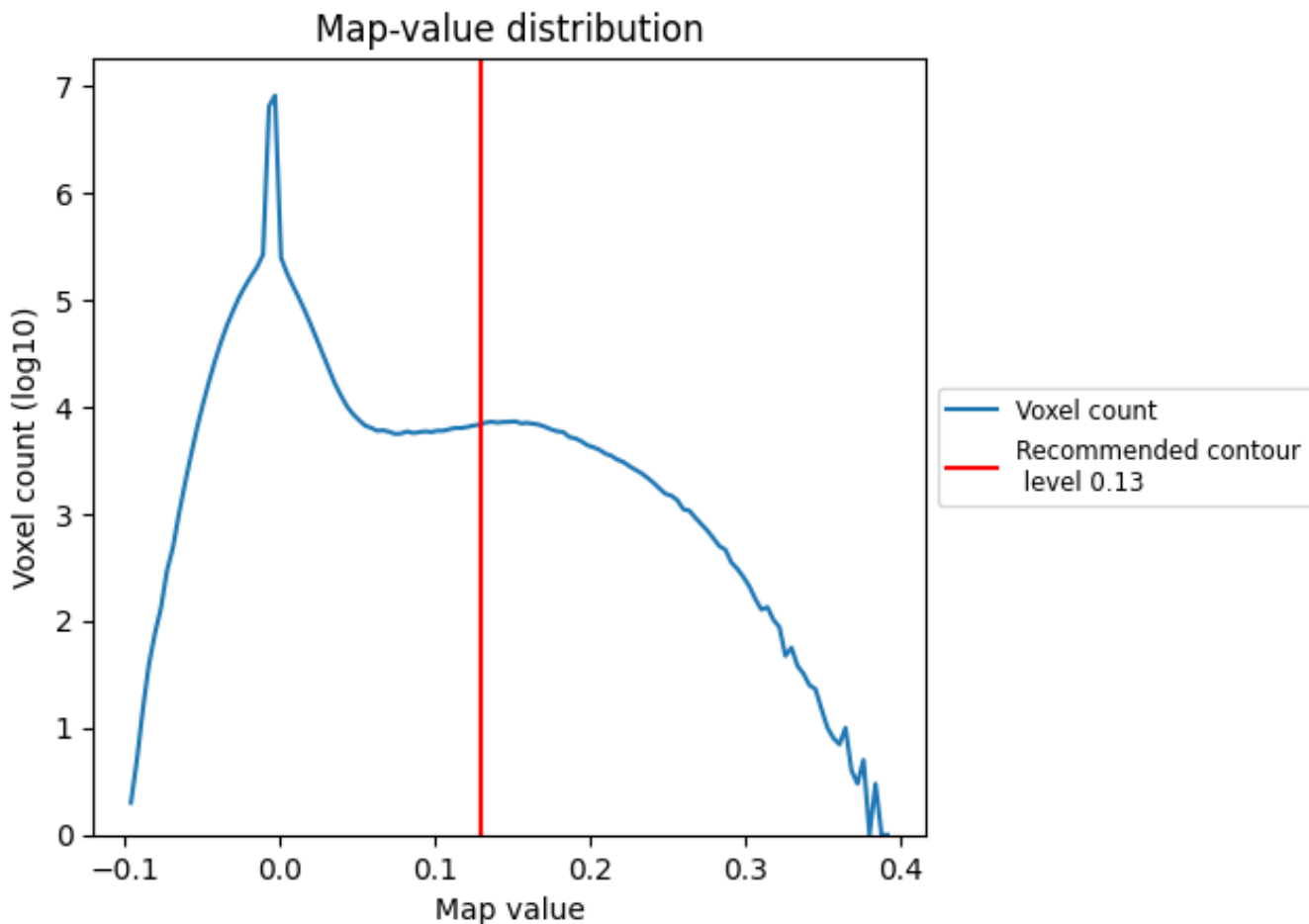
6.5 Mask visualisation

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

7 Map analysis [i](#)

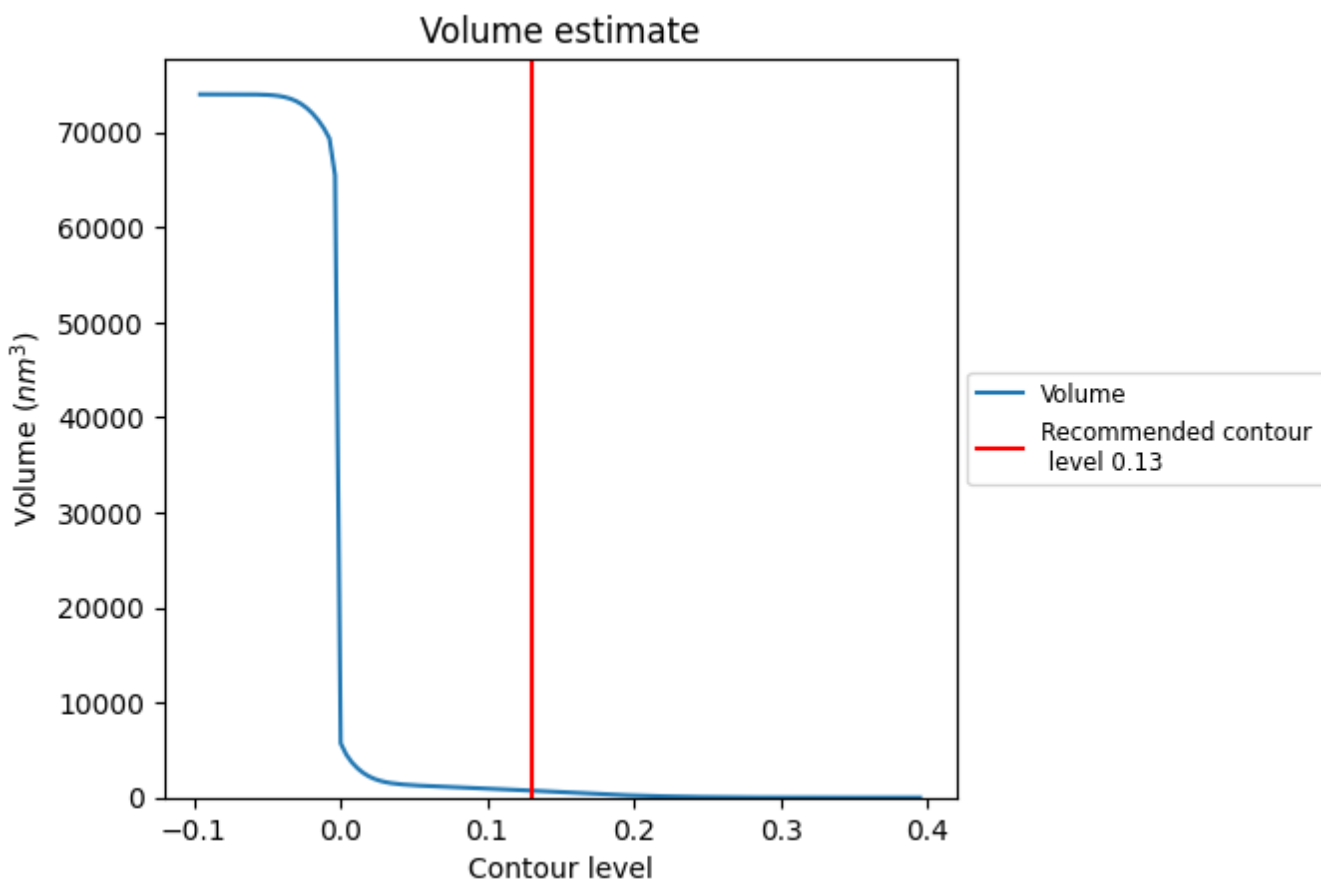
This section contains the results of statistical analysis of the map.

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.

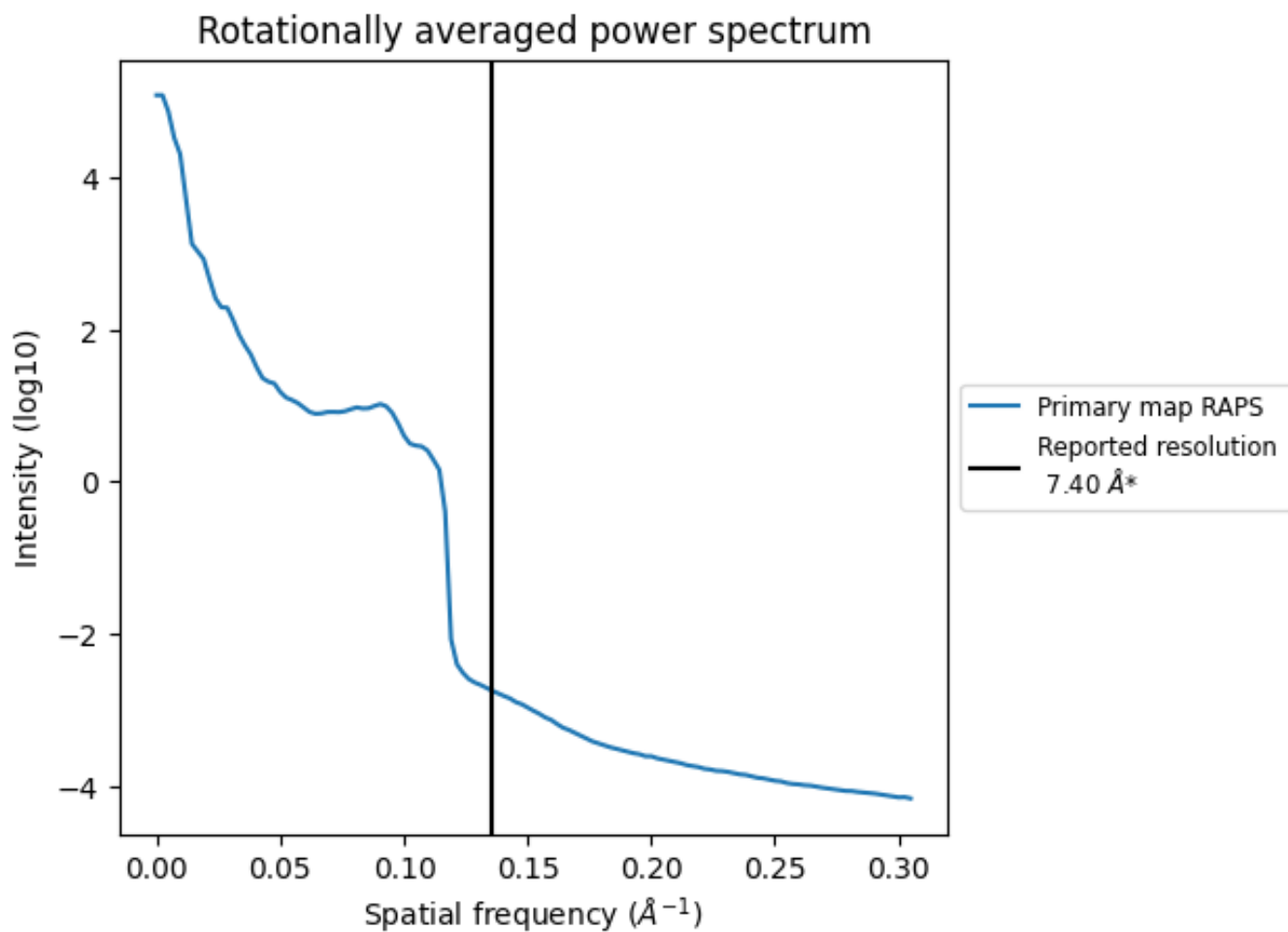
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 732 nm³; this corresponds to an approximate mass of 661 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\AA^{-1}

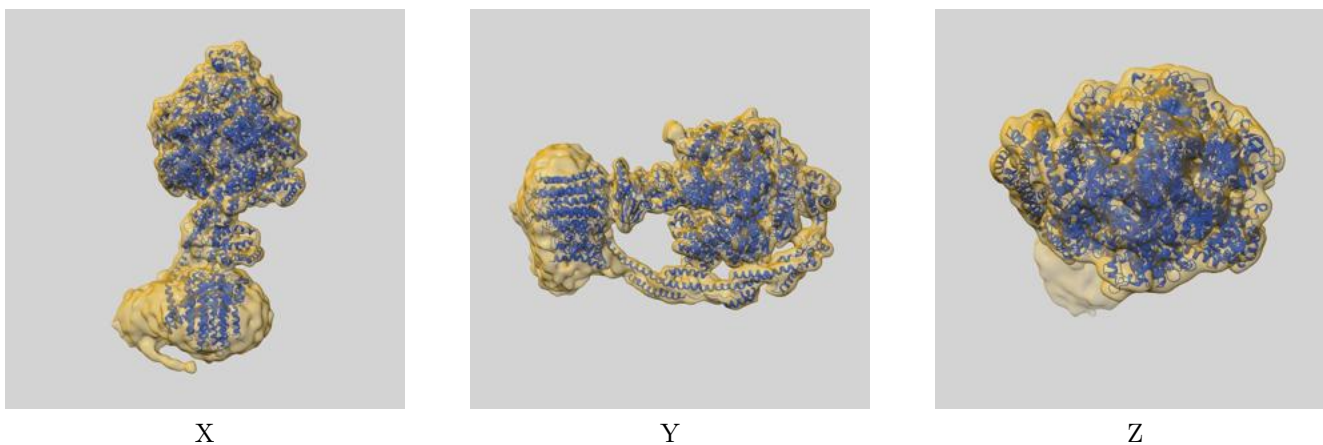
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

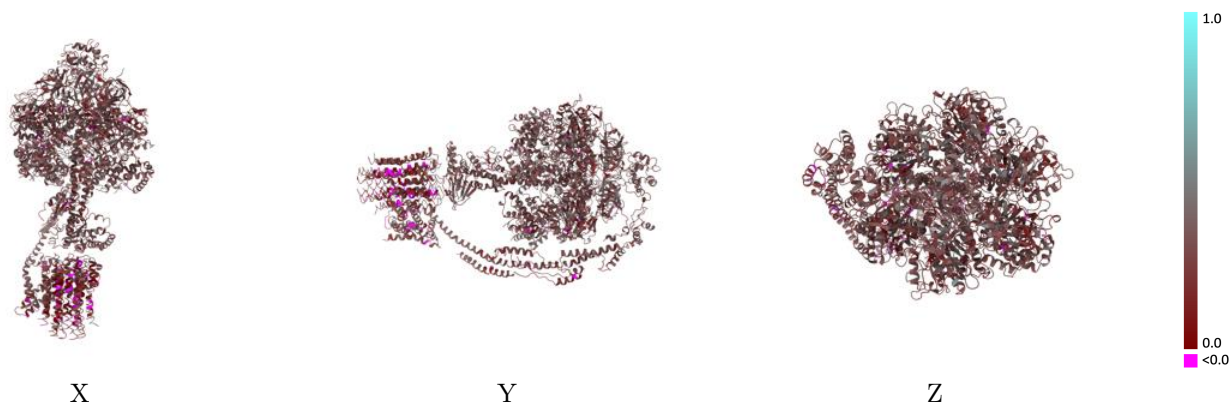
This section contains information regarding the fit between EMDB map EMD-3167 and PDB model 5ARI. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



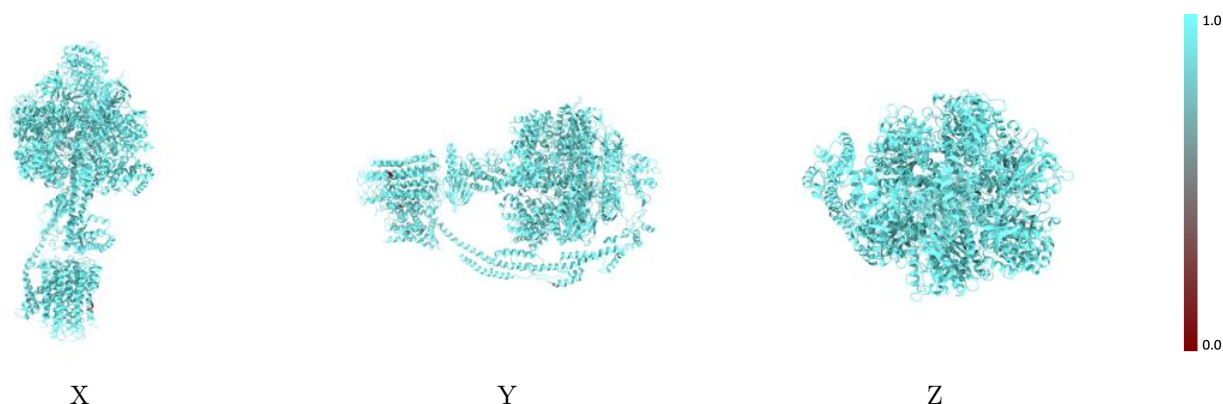
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



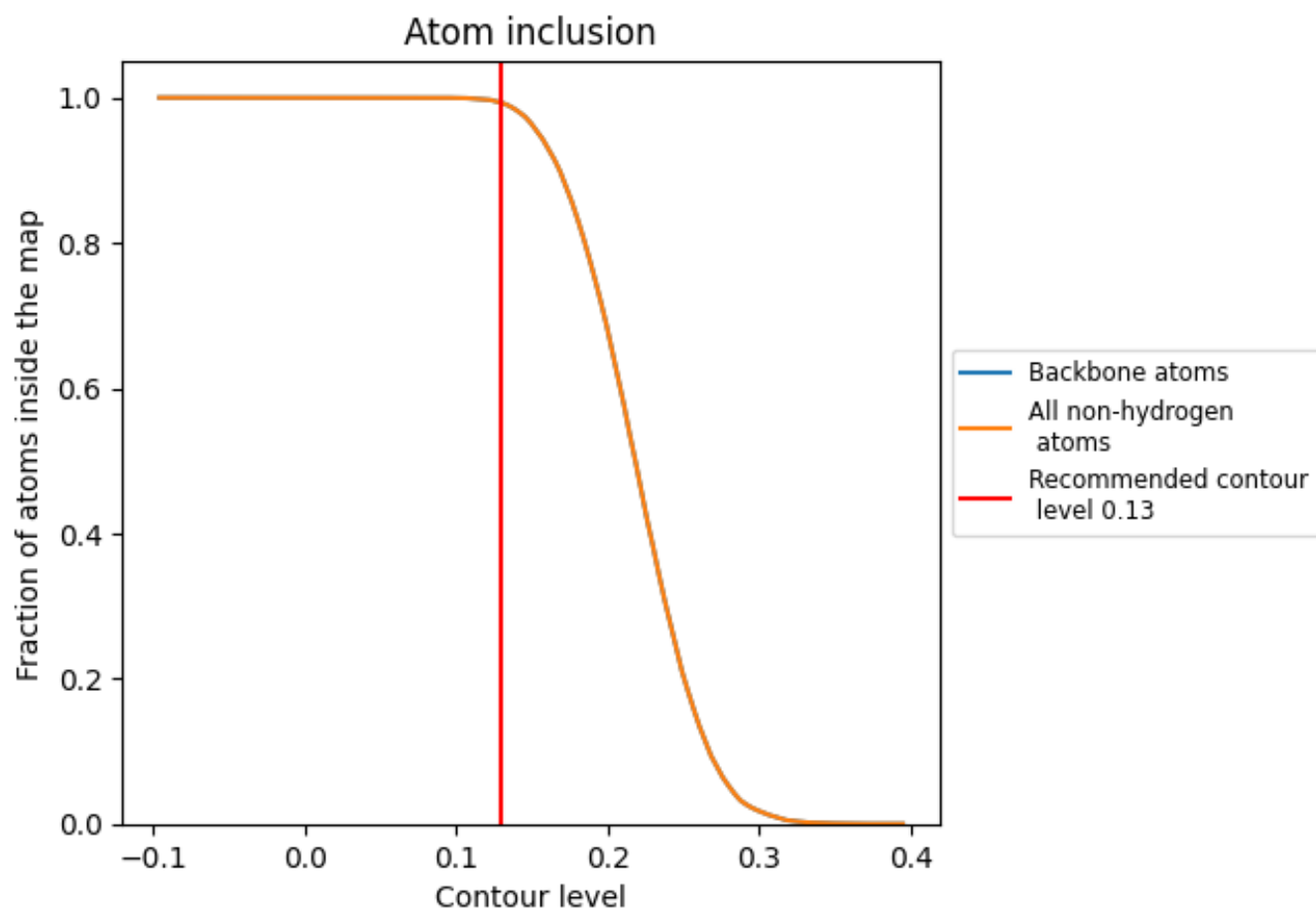
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [\(i\)](#)



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

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	 0.9929	 0.2700
A	 0.9971	 0.2870
B	 0.9984	 0.2970
C	 0.9923	 0.2920
D	 0.9984	 0.2900
E	 0.9989	 0.2860
F	 0.9979	 0.2870
G	 0.9953	 0.2950
H	 0.9981	 0.3040
I	 0.9893	 0.2960
J	 0.9826	 0.1860
K	 0.9861	 0.1580
L	 0.9757	 0.1520
M	 0.9722	 0.1700
N	 0.9757	 0.1970
O	 0.9792	 0.1130
P	 0.9757	 0.1570
Q	 0.9896	 0.1860
S	 0.9970	 0.3020
T	 0.9986	 0.2890
U	 0.9608	 0.2150
V	 0.9925	 0.2760
W	 0.9781	 0.2130

