Full wwPDB EM Validation Report ⓘ

Apr 30, 2024 – 08:30 pm BST

PDB ID	:	4CKG
EMDB ID	:	EMD-2546
Title	:	Helical reconstruction of ACAP1(BAR-PH domain) decorated membrane tubules by cryo-electron microscopy
Authors	:	Pang, X.Y.; Fan, J.; Zhang, Y.; Zhang, K.; Gao, B.Q.; Ma, J.; Li, J.; Deng, Y.C.; Zhou, Q.J.; Hsu, V.; Sun, F.
Deposited on	:	2014-01-06
Resolution	:	15.00 Å(reported)
Based on initial model	:	4NSW

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:

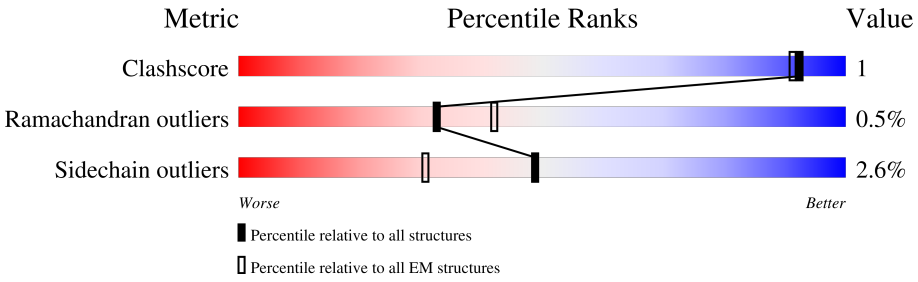
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 15.00 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
Sidechain outliers	154315	3826

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	382	70% 22%
1	B	382	73% 18% 5%
1	C	382	70% 23%
1	D	382	73% 17% 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 11682 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 ARF-GAP WITH COILED-COIL, ANK REPEAT AND PH DOMAIN-CONTAINING PROTEIN 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	369	Total	C	N	O	S	0	1
			2941	1841	539	548	13		
1	B	363	Total	C	N	O	S	0	1
			2900	1813	533	541	13		
1	C	369	Total	C	N	O	S	0	1
			2941	1841	539	548	13		
1	D	363	Total	C	N	O	S	0	1
			2900	1813	533	541	13		

There are 20 discrepancies between the modelled and reference sequences:

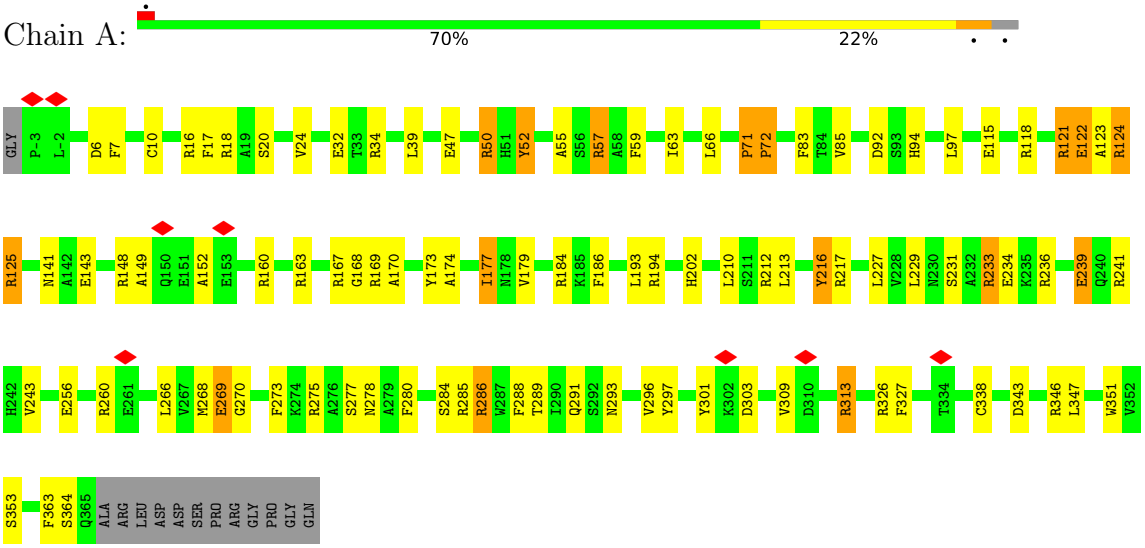
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q15027
A	-3	PRO	-	expression tag	UNP Q15027
A	-2	LEU	-	expression tag	UNP Q15027
A	-1	GLY	-	expression tag	UNP Q15027
A	0	SER	-	expression tag	UNP Q15027
B	-4	GLY	-	expression tag	UNP Q15027
B	-3	PRO	-	expression tag	UNP Q15027
B	-2	LEU	-	expression tag	UNP Q15027
B	-1	GLY	-	expression tag	UNP Q15027
B	0	SER	-	expression tag	UNP Q15027
C	-4	GLY	-	expression tag	UNP Q15027
C	-3	PRO	-	expression tag	UNP Q15027
C	-2	LEU	-	expression tag	UNP Q15027
C	-1	GLY	-	expression tag	UNP Q15027
C	0	SER	-	expression tag	UNP Q15027
D	-4	GLY	-	expression tag	UNP Q15027
D	-3	PRO	-	expression tag	UNP Q15027
D	-2	LEU	-	expression tag	UNP Q15027
D	-1	GLY	-	expression tag	UNP Q15027
D	0	SER	-	expression tag	UNP Q15027

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.

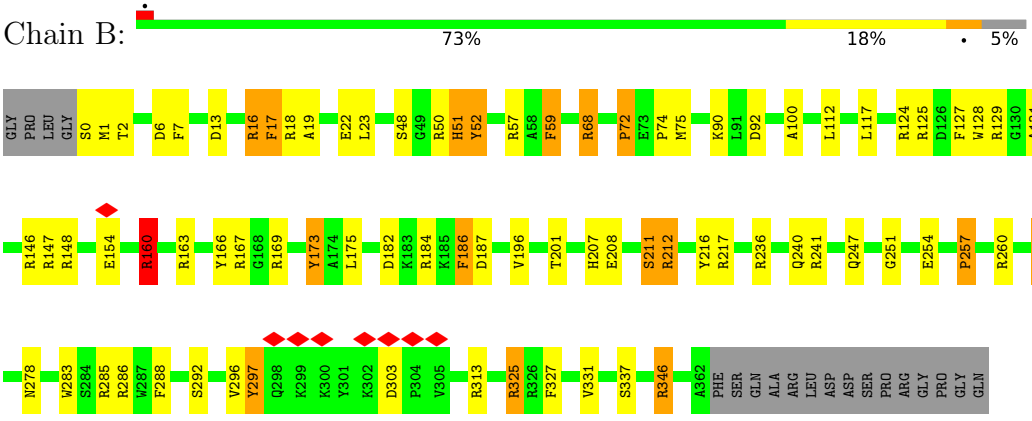
• Molecule 1: ARF-GAP WITH COILED-COIL, ANK REPEAT AND PH DOMAIN-CONTAINING PROTEIN 1

Chain A:



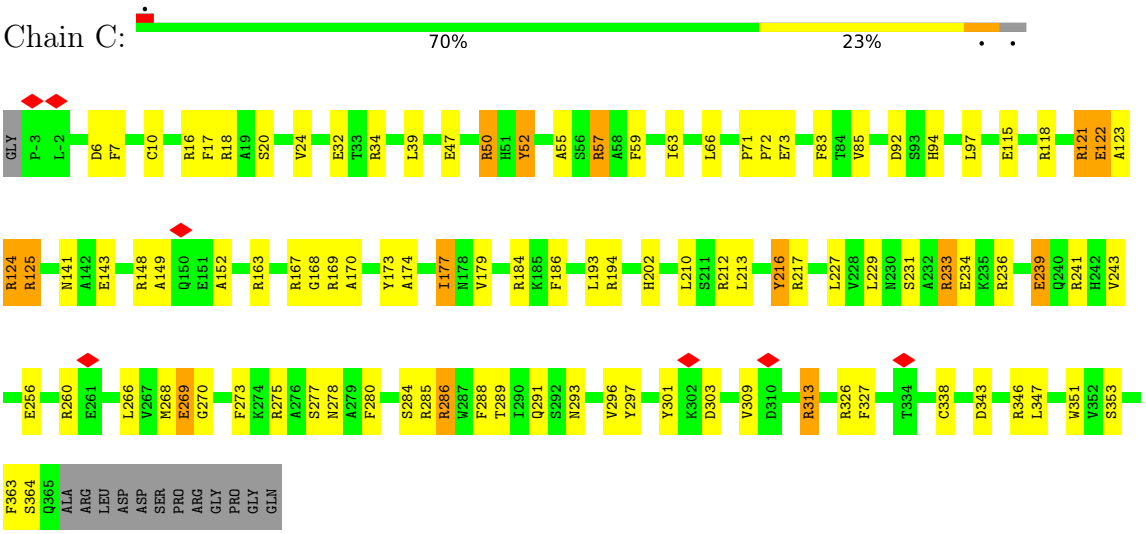
• Molecule 1: ARF-GAP WITH COILED-COIL, ANK REPEAT AND PH DOMAIN-CONTAINING PROTEIN 1

Chain B:



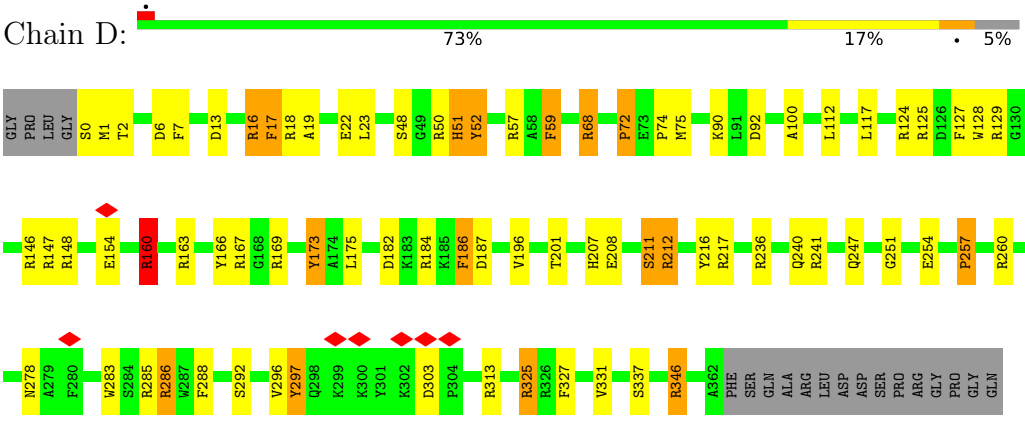
• Molecule 1: ARF-GAP WITH COILED-COIL, ANK REPEAT AND PH DOMAIN-CONTAINING PROTEIN 1

Chain C:



• Molecule 1: ARF-GAP WITH COILED-COIL, ANK REPEAT AND PH DOMAIN-CONTAINING PROTEIN 1

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	367	Depositor
Resolution determination method	Not provided	
CTF correction method	CTFFIND3	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	125418	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.00157	Depositor
Map size (Å)	720.0, 720.0, 720.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.6, 3.6, 3.6	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	1.69	26/2990 (0.9%)	2.00	82/4024 (2.0%)
1	B	1.69	18/2947 (0.6%)	2.00	74/3966 (1.9%)
1	C	1.69	27/2990 (0.9%)	2.00	82/4024 (2.0%)
1	D	1.69	20/2947 (0.7%)	2.00	75/3966 (1.9%)
All	All	1.69	91/11874 (0.8%)	2.00	313/15980 (2.0%)

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	12
1	B	0	15
1	C	0	12
1	D	0	15
All	All	0	54

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	337	SER	CA-CB	8.69	1.66	1.52
1	D	337	SER	CA-CB	8.60	1.65	1.52
1	A	280	PHE	CB-CG	-7.74	1.38	1.51
1	C	280	PHE	CB-CG	-7.72	1.38	1.51
1	A	297	TYR	CG-CD1	7.40	1.48	1.39
1	C	297	TYR	CG-CD1	7.36	1.48	1.39
1	C	239	GLU	CB-CG	7.13	1.65	1.52
1	A	239	GLU	CB-CG	7.10	1.65	1.52
1	D	211	SER	CA-CB	6.92	1.63	1.52
1	B	211	SER	CA-CB	6.86	1.63	1.52
1	A	168	GLY	N-CA	6.73	1.56	1.46
1	C	168	GLY	N-CA	6.71	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	GLU	CB-CG	6.56	1.64	1.52
1	C	47	GLU	CB-CG	6.56	1.64	1.52
1	A	194	ARG	CD-NE	6.45	1.57	1.46
1	A	327	PHE	CG-CD2	6.45	1.48	1.38
1	C	327	PHE	CG-CD2	6.42	1.48	1.38
1	C	194	ARG	CD-NE	6.39	1.57	1.46
1	D	48	SER	CA-CB	6.39	1.62	1.52
1	B	127	PHE	CG-CD1	6.36	1.48	1.38
1	B	146	ARG	CD-NE	6.36	1.57	1.46
1	D	127	PHE	CG-CD1	6.30	1.48	1.38
1	B	48	SER	CA-CB	6.29	1.62	1.52
1	D	146	ARG	CD-NE	6.26	1.57	1.46
1	B	154	GLU	CD-OE1	6.22	1.32	1.25
1	D	154	GLU	CD-OE1	6.21	1.32	1.25
1	A	269	GLU	CG-CD	6.21	1.61	1.51
1	C	269	GLU	CG-CD	6.20	1.61	1.51
1	C	285	ARG	CD-NE	6.17	1.56	1.46
1	A	285	ARG	CD-NE	6.15	1.56	1.46
1	A	256	GLU	C-N	6.10	1.45	1.34
1	C	256	GLU	C-N	6.09	1.45	1.34
1	B	22	GLU	CD-OE2	5.99	1.32	1.25
1	C	301	TYR	CE2-CZ	5.98	1.46	1.38
1	D	22	GLU	CD-OE2	5.97	1.32	1.25
1	D	124	ARG	CD-NE	5.96	1.56	1.46
1	B	124	ARG	CD-NE	5.96	1.56	1.46
1	D	254	GLU	CB-CG	5.96	1.63	1.52
1	C	173	TYR	CG-CD1	5.94	1.46	1.39
1	A	173	TYR	CG-CD1	5.91	1.46	1.39
1	B	254	GLU	CB-CG	5.90	1.63	1.52
1	B	288	PHE	CG-CD1	5.87	1.47	1.38
1	A	301	TYR	CE2-CZ	5.83	1.46	1.38
1	D	288	PHE	CG-CD1	5.81	1.47	1.38
1	C	270	GLY	CA-C	-5.81	1.42	1.51
1	A	270	GLY	CA-C	-5.78	1.42	1.51
1	A	338	CYS	CB-SG	5.75	1.92	1.82
1	C	338	CYS	CB-SG	5.75	1.92	1.82
1	A	326	ARG	CD-NE	5.72	1.56	1.46
1	C	326	ARG	CD-NE	5.71	1.56	1.46
1	A	297	TYR	CZ-OH	5.59	1.47	1.37
1	C	286	ARG	CD-NE	5.59	1.55	1.46
1	D	133	SER	CA-CB	5.59	1.61	1.52
1	B	169	ARG	CD-NE	5.58	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	133	SER	CA-CB	5.57	1.61	1.52
1	D	169	ARG	CD-NE	5.57	1.55	1.46
1	A	286	ARG	CD-NE	5.51	1.55	1.46
1	C	297	TYR	CZ-OH	5.49	1.47	1.37
1	A	233	ARG	CD-NE	5.49	1.55	1.46
1	A	216	TYR	CE2-CZ	5.46	1.45	1.38
1	C	233	ARG	CD-NE	5.41	1.55	1.46
1	D	74	PRO	CA-CB	5.39	1.64	1.53
1	C	123	ALA	CA-CB	5.37	1.63	1.52
1	C	216	TYR	CE2-CZ	5.35	1.45	1.38
1	A	234	GLU	CD-OE1	5.34	1.31	1.25
1	B	74	PRO	CA-CB	5.34	1.64	1.53
1	A	123	ALA	CA-CB	5.34	1.63	1.52
1	C	234	GLU	CD-OE1	5.33	1.31	1.25
1	B	211	SER	CB-OG	5.29	1.49	1.42
1	C	72	PRO	N-CA	-5.29	1.38	1.47
1	D	211	SER	CB-OG	5.28	1.49	1.42
1	A	72	PRO	N-CA	-5.26	1.38	1.47
1	C	167	ARG	CD-NE	5.25	1.55	1.46
1	A	353	SER	CA-CB	5.24	1.60	1.52
1	C	353	SER	CA-CB	5.21	1.60	1.52
1	A	167	ARG	CD-NE	5.21	1.55	1.46
1	B	128	TRP	CG-CD1	5.18	1.44	1.36
1	D	128	TRP	CG-CD1	5.18	1.44	1.36
1	B	208	GLU	CG-CD	-5.16	1.44	1.51
1	D	208	GLU	CG-CD	-5.16	1.44	1.51
1	D	251	GLY	N-CA	-5.15	1.38	1.46
1	A	59	PHE	CG-CD2	5.13	1.46	1.38
1	C	122	GLU	CG-CD	-5.13	1.44	1.51
1	B	251	GLY	N-CA	-5.12	1.38	1.46
1	D	236	ARG	CD-NE	5.11	1.55	1.46
1	C	59	PHE	CG-CD2	5.05	1.46	1.38
1	B	236	ARG	CD-NE	5.05	1.55	1.46
1	D	216	TYR	CZ-OH	5.04	1.46	1.37
1	C	73	GLU	CD-OE2	5.03	1.31	1.25
1	D	57	ARG	NE-CZ	5.02	1.39	1.33
1	A	122	GLU	CG-CD	-5.01	1.44	1.51

All (313) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	163	ARG	NE-CZ-NH1	16.76	128.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	163	ARG	NE-CZ-NH1	16.62	128.61	120.30
1	D	50	ARG	NE-CZ-NH2	14.46	127.53	120.30
1	A	18	ARG	NE-CZ-NH2	-14.37	113.12	120.30
1	C	18	ARG	NE-CZ-NH2	-14.32	113.14	120.30
1	B	50	ARG	NE-CZ-NH2	14.28	127.44	120.30
1	D	186	PHE	CB-CG-CD2	-14.03	110.98	120.80
1	B	186	PHE	CB-CG-CD2	-14.00	111.00	120.80
1	D	124	ARG	NE-CZ-NH2	-13.45	113.58	120.30
1	B	124	ARG	NE-CZ-NH2	-13.42	113.59	120.30
1	A	326	ARG	NE-CZ-NH2	-12.80	113.90	120.30
1	C	326	ARG	NE-CZ-NH2	-12.79	113.90	120.30
1	C	217	ARG	NE-CZ-NH1	12.47	126.53	120.30
1	A	217	ARG	NE-CZ-NH1	12.43	126.52	120.30
1	B	288	PHE	CB-CG-CD1	-12.34	112.16	120.80
1	D	288	PHE	CB-CG-CD1	-12.29	112.20	120.80
1	C	57	ARG	NE-CZ-NH2	-12.27	114.17	120.30
1	A	57	ARG	NE-CZ-NH2	-12.05	114.28	120.30
1	B	169	ARG	NE-CZ-NH1	11.69	126.14	120.30
1	D	169	ARG	NE-CZ-NH1	11.58	126.09	120.30
1	A	16	ARG	NE-CZ-NH1	11.50	126.05	120.30
1	B	68	ARG	NE-CZ-NH2	11.48	126.04	120.30
1	C	16	ARG	NE-CZ-NH1	11.40	126.00	120.30
1	D	68	ARG	NE-CZ-NH2	11.32	125.96	120.30
1	C	124	ARG	NE-CZ-NH2	-11.31	114.64	120.30
1	A	124	ARG	NE-CZ-NH2	-11.30	114.65	120.30
1	D	184	ARG	NE-CZ-NH1	11.22	125.91	120.30
1	B	184	ARG	NE-CZ-NH1	11.22	125.91	120.30
1	D	18	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	B	18	ARG	NE-CZ-NH1	10.82	125.71	120.30
1	D	127	PHE	CB-CG-CD2	-10.73	113.29	120.80
1	C	118	ARG	NE-CZ-NH1	10.73	125.67	120.30
1	D	325	ARG	NE-CZ-NH2	-10.69	114.96	120.30
1	B	325	ARG	NE-CZ-NH2	-10.65	114.97	120.30
1	D	325	ARG	NE-CZ-NH1	10.64	125.62	120.30
1	B	127	PHE	CB-CG-CD2	-10.63	113.36	120.80
1	A	118	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	B	325	ARG	NE-CZ-NH1	10.59	125.60	120.30
1	A	184	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	C	184	ARG	NE-CZ-NH1	10.40	125.50	120.30
1	A	217	ARG	NE-CZ-NH2	-10.23	115.19	120.30
1	C	217	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	D	124	ARG	NE-CZ-NH1	9.97	125.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	241	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	C	241	ARG	NE-CZ-NH1	9.91	125.26	120.30
1	D	186	PHE	CB-CG-CD1	9.87	127.71	120.80
1	B	124	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	B	186	PHE	CB-CG-CD1	9.83	127.68	120.80
1	A	18	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	C	18	ARG	NE-CZ-NH1	9.65	125.12	120.30
1	C	118	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	D	212	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	B	212	ARG	NE-CZ-NH2	-9.23	115.69	120.30
1	A	7	PHE	CB-CG-CD1	-9.16	114.39	120.80
1	C	326	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	C	7	PHE	CB-CG-CD1	-9.05	114.47	120.80
1	D	297	TYR	CB-CG-CD2	-9.03	115.58	121.00
1	A	148	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	A	118	ARG	NE-CZ-NH2	-9.01	115.79	120.30
1	D	173	TYR	CB-CG-CD2	-8.99	115.60	121.00
1	C	148	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	B	173	TYR	CB-CG-CD2	-8.96	115.63	121.00
1	A	326	ARG	NE-CZ-NH1	8.93	124.76	120.30
1	B	297	TYR	CB-CG-CD2	-8.91	115.66	121.00
1	D	241	ARG	NE-CZ-NH2	-8.79	115.90	120.30
1	C	313	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	A	169	ARG	NE-CZ-NH1	-8.66	115.97	120.30
1	B	241	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	C	169	ARG	NE-CZ-NH1	-8.57	116.01	120.30
1	A	313	ARG	NE-CZ-NH2	-8.45	116.07	120.30
1	C	125	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	A	163	ARG	NH1-CZ-NH2	-8.36	110.21	119.40
1	A	301	TYR	CB-CG-CD1	-8.34	115.99	121.00
1	A	125	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	C	301	TYR	CB-CG-CD1	-8.30	116.02	121.00
1	C	163	ARG	NH1-CZ-NH2	-8.30	110.27	119.40
1	B	313	ARG	NE-CZ-NH2	8.17	124.38	120.30
1	A	212	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	C	212	ARG	NE-CZ-NH2	-8.15	116.23	120.30
1	D	313	ARG	NE-CZ-NH2	8.05	124.33	120.30
1	C	6	ASP	CB-CG-OD2	8.02	125.52	118.30
1	A	6	ASP	CB-CG-OD2	8.01	125.51	118.30
1	D	7	PHE	CB-CG-CD2	7.93	126.35	120.80
1	B	7	PHE	CB-CG-CD2	7.86	126.30	120.80
1	B	285	ARG	NE-CZ-NH1	7.86	124.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	285	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	A	286	ARG	NE-CZ-NH2	-7.57	116.51	120.30
1	C	286	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	D	129	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	D	127	PHE	CG-CD1-CE1	-7.43	112.62	120.80
1	B	127	PHE	CG-CD1-CE1	-7.43	112.63	120.80
1	B	129	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	B	288	PHE	CG-CD2-CE2	-7.28	112.80	120.80
1	D	288	PHE	CG-CD2-CE2	-7.22	112.85	120.80
1	B	19	ALA	O-C-N	-7.17	111.22	122.70
1	C	288	PHE	CB-CG-CD2	-7.17	115.78	120.80
1	A	288	PHE	CB-CG-CD2	-7.15	115.80	120.80
1	D	19	ALA	O-C-N	-7.13	111.28	122.70
1	B	163	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	D	346	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	D	163	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	B	346	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	B	169	ARG	NH1-CZ-NH2	-7.01	111.69	119.40
1	D	50	ARG	NE-CZ-NH1	-6.97	116.81	120.30
1	D	169	ARG	NH1-CZ-NH2	-6.94	111.77	119.40
1	B	50	ARG	NE-CZ-NH1	-6.93	116.83	120.30
1	C	57	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	B	68	ARG	NH1-CZ-NH2	-6.91	111.80	119.40
1	B	182	ASP	CB-CG-OD1	6.90	124.51	118.30
1	B	187	ASP	CB-CG-OD1	6.88	124.49	118.30
1	B	327	PHE	CB-CG-CD2	-6.88	115.99	120.80
1	D	182	ASP	CB-CG-OD1	6.88	124.49	118.30
1	D	68	ARG	NH1-CZ-NH2	-6.87	111.85	119.40
1	D	212	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	B	288	PHE	CD1-CG-CD2	6.85	127.21	118.30
1	D	160	ARG	N-CA-CB	6.84	122.92	110.60
1	D	327	PHE	CB-CG-CD2	-6.84	116.01	120.80
1	D	288	PHE	CD1-CG-CD2	6.83	127.18	118.30
1	B	160	ARG	N-CA-CB	6.81	122.86	110.60
1	B	212	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	D	187	ASP	CB-CG-OD1	6.77	124.39	118.30
1	C	275	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	275	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	57	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	C	234	GLU	OE1-CD-OE2	-6.66	115.31	123.30
1	D	100	ALA	O-C-N	-6.64	112.08	122.70
1	B	100	ALA	O-C-N	-6.62	112.10	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	GLU	OE1-CD-OE2	-6.62	115.36	123.30
1	D	286	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	B	286	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	212	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	17	PHE	CB-CG-CD2	6.31	125.22	120.80
1	A	18	ARG	N-CA-CB	-6.30	99.25	110.60
1	C	18	ARG	N-CA-CB	-6.27	99.31	110.60
1	C	273	PHE	CB-CG-CD2	-6.27	116.41	120.80
1	C	212	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	A	83	PHE	CB-CG-CD1	6.21	125.15	120.80
1	A	266	LEU	CB-CG-CD1	6.21	121.55	111.00
1	D	52	TYR	CG-CD1-CE1	6.20	126.26	121.30
1	D	269	GLU	N-CA-CB	6.20	121.75	110.60
1	C	83	PHE	CB-CG-CD1	6.19	125.14	120.80
1	C	266	LEU	CB-CG-CD1	6.18	121.50	111.00
1	B	269	GLU	N-CA-CB	6.17	121.72	110.60
1	A	149	ALA	CB-CA-C	-6.16	100.86	110.10
1	C	149	ALA	CB-CA-C	-6.15	100.87	110.10
1	A	141	ASN	O-C-N	-6.14	112.87	122.70
1	C	141	ASN	O-C-N	-6.14	112.87	122.70
1	A	167	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	D	17	PHE	CB-CG-CD2	6.12	125.09	120.80
1	C	39	LEU	CB-CA-C	-6.12	98.58	110.20
1	C	167	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	52	TYR	CG-CD1-CE1	6.11	126.19	121.30
1	A	273	PHE	CB-CG-CD2	-6.11	116.52	120.80
1	D	303	ASP	N-CA-CB	-6.09	99.63	110.60
1	A	39	LEU	CB-CA-C	-6.09	98.63	110.20
1	C	268	MET	CG-SD-CE	-6.09	90.46	100.20
1	B	303	ASP	N-CA-CB	-6.08	99.66	110.60
1	B	201	THR	CA-CB-CG2	-6.07	103.90	112.40
1	A	268	MET	CG-SD-CE	-6.05	90.51	100.20
1	D	275	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	285	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	D	201	THR	CA-CB-CG2	-6.03	103.96	112.40
1	D	13	ASP	CB-CA-C	6.01	122.42	110.40
1	C	16	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	72	PRO	CA-N-CD	5.99	120.09	111.70
1	C	72	PRO	CA-N-CD	5.98	120.08	111.70
1	B	13	ASP	CB-CA-C	5.98	122.36	110.40
1	B	275	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	16	ARG	NE-CZ-NH2	-5.96	117.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	72	PRO	N-CA-CB	-5.93	96.08	102.60
1	A	63	ILE	N-CA-CB	5.92	124.42	110.80
1	B	117	LEU	CB-CG-CD2	5.91	121.05	111.00
1	C	167	ARG	NE-CZ-NH1	-5.91	117.34	120.30
1	C	285	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	D	117	LEU	CB-CG-CD2	5.91	121.05	111.00
1	C	63	ILE	N-CA-CB	5.91	124.39	110.80
1	A	167	ARG	NE-CZ-NH1	-5.89	117.36	120.30
1	B	72	PRO	N-CA-CB	-5.89	96.12	102.60
1	C	184	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	A	184	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	D	216	TYR	CD1-CE1-CZ	-5.84	114.54	119.80
1	B	182	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	C	297	TYR	CZ-CE2-CD2	5.83	125.05	119.80
1	A	347	LEU	CB-CG-CD1	5.82	120.90	111.00
1	A	297	TYR	CZ-CE2-CD2	5.80	125.02	119.80
1	D	182	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	C	347	LEU	CB-CG-CD1	5.80	120.86	111.00
1	B	216	TYR	CD1-CE1-CZ	-5.76	114.62	119.80
1	B	131	ALA	N-CA-CB	-5.73	102.07	110.10
1	B	59	PHE	CB-CG-CD2	-5.72	116.79	120.80
1	D	131	ALA	N-CA-CB	-5.68	102.15	110.10
1	B	52	TYR	CD1-CE1-CZ	-5.67	114.70	119.80
1	D	52	TYR	CD1-CE1-CZ	-5.65	114.72	119.80
1	D	59	PHE	CB-CG-CD2	-5.65	116.85	120.80
1	D	296	VAL	CA-CB-CG2	5.64	119.36	110.90
1	A	186	PHE	CB-CG-CD1	5.62	124.74	120.80
1	D	147	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	C	52	TYR	CB-CG-CD1	5.61	124.37	121.00
1	C	186	PHE	CB-CG-CD1	5.60	124.72	120.80
1	A	256	GLU	N-CA-CB	-5.60	100.53	110.60
1	B	296	VAL	CA-CB-CG2	5.58	119.28	110.90
1	A	52	TYR	CB-CG-CD1	5.57	124.34	121.00
1	B	2	THR	CA-CB-CG2	-5.57	104.61	112.40
1	C	278	ASN	O-C-N	-5.57	113.79	122.70
1	C	256	GLU	N-CA-CB	-5.56	100.60	110.60
1	A	278	ASN	O-C-N	-5.55	113.81	122.70
1	D	16	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	D	166	TYR	CB-CG-CD2	-5.54	117.68	121.00
1	C	293	ASN	CB-CA-C	5.52	121.45	110.40
1	D	2	THR	CA-CB-CG2	-5.52	104.67	112.40
1	B	297	TYR	CB-CG-CD1	5.51	124.31	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	20	SER	N-CA-CB	5.51	118.77	110.50
1	D	273	PHE	CB-CG-CD2	5.51	124.66	120.80
1	C	273	PHE	CB-CG-CD1	5.51	124.65	120.80
1	A	293	ASN	CB-CA-C	5.50	121.39	110.40
1	D	297	TYR	CB-CG-CD1	5.49	124.29	121.00
1	B	166	TYR	CB-CG-CD2	-5.48	117.72	121.00
1	A	273	PHE	CB-CG-CD1	5.47	124.63	120.80
1	C	173	TYR	CB-CG-CD1	5.47	124.28	121.00
1	D	175	LEU	CB-CG-CD1	5.47	120.29	111.00
1	B	175	LEU	CB-CG-CD1	5.46	120.28	111.00
1	C	20	SER	N-CA-CB	5.46	118.68	110.50
1	C	343	ASP	O-C-N	-5.45	113.98	122.70
1	B	147	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	C	124	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	D	57	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	343	ASP	O-C-N	-5.43	114.02	122.70
1	B	273	PHE	CB-CG-CD2	5.42	124.60	120.80
1	A	303	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	B	16	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	C	92	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	50	ARG	CG-CD-NE	-5.39	100.47	111.80
1	B	136	ALA	O-C-N	-5.39	114.08	122.70
1	A	297	TYR	CD1-CE1-CZ	5.39	124.65	119.80
1	C	50	ARG	CG-CD-NE	-5.38	100.49	111.80
1	B	57	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	C	297	TYR	CD1-CE1-CZ	5.38	124.64	119.80
1	A	124	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	C	303	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	D	313	ARG	N-CA-CB	-5.35	100.96	110.60
1	D	51	HIS	N-CA-CB	5.35	120.24	110.60
1	B	51	HIS	N-CA-CB	5.35	120.23	110.60
1	D	136	ALA	O-C-N	-5.34	114.16	122.70
1	B	92	ASP	CB-CG-OD2	5.33	123.09	118.30
1	D	75	MET	O-C-N	-5.32	114.18	122.70
1	A	173	TYR	CB-CG-CD1	5.32	124.19	121.00
1	A	291	GLN	N-CA-CB	5.32	120.17	110.60
1	B	313	ARG	N-CA-CB	-5.32	101.03	110.60
1	C	291	GLN	N-CA-CB	5.31	120.16	110.60
1	A	92	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	6	ASP	CB-CG-OD1	5.30	123.07	118.30
1	C	174	ALA	N-CA-CB	-5.30	102.68	110.10
1	C	346	ARG	CD-NE-CZ	5.30	131.02	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	75	MET	O-C-N	-5.29	114.23	122.70
1	D	92	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	346	ARG	CD-NE-CZ	5.29	131.01	123.60
1	A	174	ALA	N-CA-CB	-5.28	102.70	110.10
1	C	227	LEU	CB-CG-CD2	5.26	119.94	111.00
1	C	170	ALA	N-CA-CB	5.25	117.46	110.10
1	C	167	ARG	NH1-CZ-NH2	5.24	125.17	119.40
1	A	167	ARG	NH1-CZ-NH2	5.24	125.16	119.40
1	A	170	ALA	N-CA-CB	5.24	117.43	110.10
1	B	297	TYR	CG-CD1-CE1	-5.24	117.11	121.30
1	C	52	TYR	CZ-CE2-CD2	5.24	124.51	119.80
1	A	227	LEU	CB-CG-CD2	5.22	119.88	111.00
1	C	363	PHE	CB-CG-CD2	-5.21	117.15	120.80
1	D	297	TYR	CG-CD1-CE1	-5.21	117.14	121.30
1	C	177	ILE	O-C-N	-5.20	114.38	122.70
1	C	85	VAL	CG1-CB-CG2	-5.20	102.58	110.90
1	D	6	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	85	VAL	CG1-CB-CG2	-5.18	102.62	110.90
1	A	363	PHE	CB-CG-CD2	-5.18	117.18	120.80
1	C	210	LEU	CB-CA-C	5.17	120.03	110.20
1	A	284	SER	N-CA-CB	5.17	118.26	110.50
1	B	50	ARG	CG-CD-NE	-5.17	100.95	111.80
1	C	179	VAL	O-C-N	-5.16	114.45	122.70
1	A	177	ILE	O-C-N	-5.16	114.45	122.70
1	A	179	VAL	O-C-N	-5.16	114.45	122.70
1	C	55	ALA	C-N-CA	5.16	134.59	121.70
1	C	284	SER	N-CA-CB	5.15	118.22	110.50
1	D	50	ARG	CG-CD-NE	-5.15	100.99	111.80
1	C	231	SER	N-CA-CB	-5.13	102.80	110.50
1	A	210	LEU	CB-CA-C	5.13	119.95	110.20
1	A	160	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	D	173	TYR	CG-CD2-CE2	-5.12	117.20	121.30
1	A	55	ALA	C-N-CA	5.12	134.50	121.70
1	A	231	SER	N-CA-CB	-5.12	102.82	110.50
1	A	278	ASN	CA-CB-CG	-5.12	102.14	113.40
1	B	292	SER	N-CA-CB	5.11	118.17	110.50
1	A	121	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	D	292	SER	N-CA-CB	5.11	118.16	110.50
1	A	52	TYR	CZ-CE2-CD2	5.10	124.39	119.80
1	B	90	LYS	CB-CA-C	5.10	120.60	110.40
1	D	90	LYS	CB-CA-C	5.09	120.58	110.40
1	C	278	ASN	CA-CB-CG	-5.09	102.21	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	351	TRP	CG-CD2-CE3	-5.08	129.32	133.90
1	A	193	LEU	CB-CG-CD1	-5.08	102.36	111.00
1	B	173	TYR	CG-CD2-CE2	-5.08	117.24	121.30
1	C	351	TRP	CG-CD2-CE3	-5.08	129.33	133.90
1	C	193	LEU	CB-CG-CD1	-5.07	102.39	111.00
1	D	52	TYR	CB-CA-C	5.05	120.50	110.40
1	D	283	TRP	CG-CD2-CE3	-5.05	129.35	133.90
1	B	23	LEU	N-CA-CB	-5.04	100.31	110.40
1	C	152	ALA	N-CA-CB	-5.04	103.04	110.10
1	C	256	GLU	OE1-CD-OE2	-5.04	117.25	123.30
1	B	52	TYR	CB-CA-C	5.04	120.48	110.40
1	D	128	TRP	CH2-CZ2-CE2	5.03	122.43	117.40
1	D	23	LEU	N-CA-CB	-5.03	100.34	110.40
1	A	141	ASN	CA-C-O	5.02	130.65	120.10
1	A	152	ALA	N-CA-CB	-5.02	103.07	110.10
1	C	141	ASN	CA-C-O	5.01	130.62	120.10
1	C	121	ARG	NE-CZ-NH1	-5.01	117.80	120.30
1	B	283	TRP	CG-CD2-CE3	-5.00	129.40	133.90

There are no chirality outliers.

All (54) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	GLU	Peptide
1	A	124	ARG	Sidechain
1	A	202	HIS	Sidechain
1	A	216	TYR	Sidechain
1	A	236	ARG	Sidechain
1	A	286	ARG	Sidechain
1	A	313	ARG	Sidechain
1	A	34	ARG	Sidechain
1	A	50	ARG	Sidechain
1	A	52	TYR	Sidechain
1	A	57	ARG	Sidechain
1	A	71	PRO	Peptide
1	B	125	ARG	Sidechain
1	B	148	ARG	Sidechain
1	B	16	ARG	Sidechain
1	B	160	ARG	Sidechain
1	B	167	ARG	Sidechain
1	B	17	PHE	Sidechain
1	B	173	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	186	PHE	Sidechain
1	B	212	ARG	Sidechain
1	B	217	ARG	Sidechain
1	B	346	ARG	Sidechain
1	B	51	HIS	Sidechain
1	B	52	TYR	Sidechain
1	B	59	PHE	Sidechain
1	B	68	ARG	Sidechain
1	C	115	GLU	Peptide
1	C	124	ARG	Sidechain
1	C	202	HIS	Sidechain
1	C	216	TYR	Sidechain
1	C	236	ARG	Sidechain
1	C	286	ARG	Sidechain
1	C	313	ARG	Sidechain
1	C	34	ARG	Sidechain
1	C	50	ARG	Sidechain
1	C	52	TYR	Sidechain
1	C	57	ARG	Sidechain
1	C	71	PRO	Peptide
1	D	125	ARG	Sidechain
1	D	148	ARG	Sidechain
1	D	16	ARG	Sidechain
1	D	160	ARG	Sidechain
1	D	167	ARG	Sidechain
1	D	17	PHE	Sidechain
1	D	173	TYR	Sidechain
1	D	186	PHE	Sidechain
1	D	212	ARG	Sidechain
1	D	217	ARG	Sidechain
1	D	346	ARG	Sidechain
1	D	51	HIS	Sidechain
1	D	52	TYR	Sidechain
1	D	59	PHE	Sidechain
1	D	68	ARG	Sidechain

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	2941	0	2960	20	0
1	B	2900	0	2922	5	0
1	C	2941	0	2959	19	0
1	D	2900	0	2922	6	0
All	All	11682	0	11763	33	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 1.

All (33) 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:122:GLU:OE1	1:C:125:ARG:NH2	1.60	1.35
1:A:122:GLU:CD	1:C:125:ARG:NH2	1.91	1.20
1:A:125:ARG:NH2	1:C:122:GLU:OE1	1.72	1.20
1:A:122:GLU:OE1	1:C:122:GLU:OE1	1.60	1.20
1:A:125:ARG:NH2	1:C:122:GLU:CD	1.96	1.17
1:A:122:GLU:CD	1:C:125:ARG:HH22	1.52	1.10
1:A:125:ARG:HH22	1:C:122:GLU:CD	1.53	1.10
1:A:122:GLU:CG	1:C:125:ARG:HH22	1.93	0.81
1:B:247:GLN:OE1	1:D:240:GLN:NE2	2.16	0.78
1:A:125:ARG:HH22	1:C:122:GLU:CG	2.00	0.74
1:B:240:GLN:NE2	1:D:247:GLN:OE1	2.20	0.73
1:A:122:GLU:HG3	1:C:125:ARG:HH22	1.68	0.55
1:A:239:GLU:O	1:A:243:VAL:HG23	2.12	0.49
1:A:229:LEU:HD21	1:A:233:ARG:NH2	2.27	0.49
1:C:239:GLU:O	1:C:243:VAL:HG23	2.12	0.49
1:C:229:LEU:HD21	1:C:233:ARG:NH2	2.27	0.48
1:C:10:CYS:HG	1:C:17:PHE:HZ	1.65	0.45
1:A:213:LEU:HD21	1:B:196:VAL:HG13	1.99	0.44
1:C:213:LEU:HD21	1:D:196:VAL:HG13	1.99	0.44
1:B:207:HIS:CE1	1:B:211:SER:HB2	2.53	0.43
1:A:125:ARG:HH22	1:C:122:GLU:HG3	1.79	0.42
1:A:32:GLU:CD	1:A:121:ARG:HH12	2.22	0.42
1:C:94:HIS:O	1:C:97:LEU:HB3	2.20	0.42
1:C:32:GLU:CD	1:C:121:ARG:HH12	2.23	0.42
1:D:207:HIS:CE1	1:D:211:SER:HB2	2.53	0.42
1:C:143:GLU:CD	1:D:325:ARG:HH12	2.23	0.41
1:A:94:HIS:O	1:A:97:LEU:HB3	2.20	0.41
1:A:143:GLU:CD	1:B:325:ARG:HH12	2.24	0.41
1:C:289:THR:O	1:C:296:VAL:HG22	2.20	0.41
1:A:10:CYS:HG	1:A:17:PHE:HZ	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:PRO:HA	1:A:72:PRO:HD3	1.93	0.41
1:A:289:THR:O	1:A:296:VAL:HG22	2.20	0.41
1:D:286:ARG:HD3	1:D:286:ARG:HA	1.97	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	367/382 (96%)	354 (96%)	12 (3%)	1 (0%)	41	77
1	B	361/382 (94%)	347 (96%)	11 (3%)	3 (1%)	19	60
1	C	367/382 (96%)	354 (96%)	12 (3%)	1 (0%)	41	77
1	D	361/382 (94%)	347 (96%)	11 (3%)	3 (1%)	19	60
All	All	1456/1528 (95%)	1402 (96%)	46 (3%)	8 (0%)	32	69

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	SER
1	C	364	SER
1	B	278	ASN
1	D	278	ASN
1	B	257	PRO
1	D	257	PRO
1	B	72	PRO
1	D	72	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain 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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	315/325 (97%)	308 (98%)	7 (2%)	52	71
1	B	311/325 (96%)	302 (97%)	9 (3%)	42	64
1	C	315/325 (97%)	308 (98%)	7 (2%)	52	71
1	D	311/325 (96%)	302 (97%)	9 (3%)	42	64
All	All	1252/1300 (96%)	1220 (97%)	32 (3%)	49	66

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	66	LEU
1	A	177	ILE
1	A	260	ARG
1	A	269	GLU
1	A	277	SER
1	A	309	VAL
1	B	0	SER
1	B	1	MET
1	B	112	LEU
1	B	160	ARG
1	B	257	PRO
1	B	260	ARG
1	B	269	GLU
1	B	297	TYR
1	B	331	VAL
1	C	24	VAL
1	C	66	LEU
1	C	177	ILE
1	C	260	ARG
1	C	269	GLU
1	C	277	SER
1	C	309	VAL
1	D	0	SER

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Mol	Chain	Res	Type
1	D	1	MET
1	D	112	LEU
1	D	160	ARG
1	D	257	PRO
1	D	260	ARG
1	D	269	GLU
1	D	297	TYR
1	D	331	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	207	HIS
1	D	207	HIS

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.

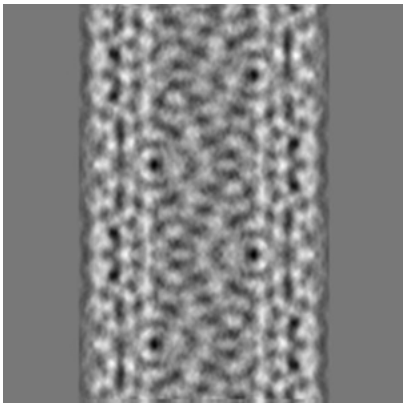
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2546. These allow visual inspection of the internal detail of the map and identification of artifacts.

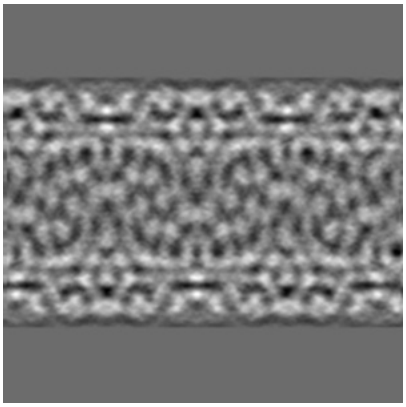
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map



X



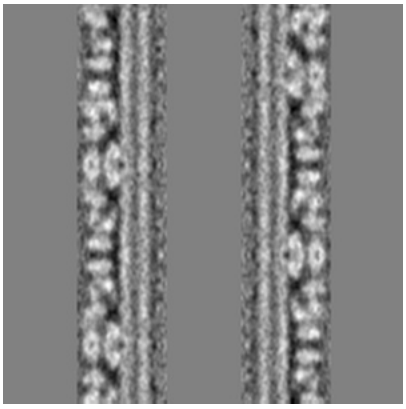
Y

Z

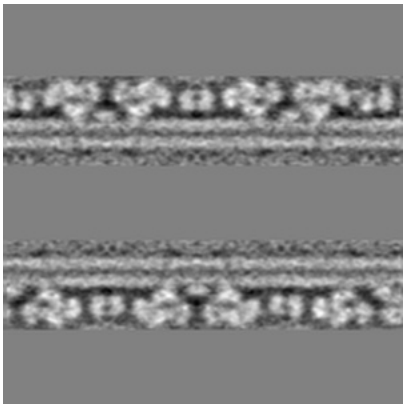
The images above show the map projected in three orthogonal directions.

6.2 Central slices

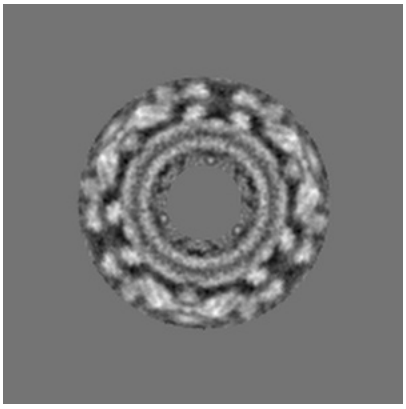
6.2.1 Primary map



X Index: 100



Y Index: 100

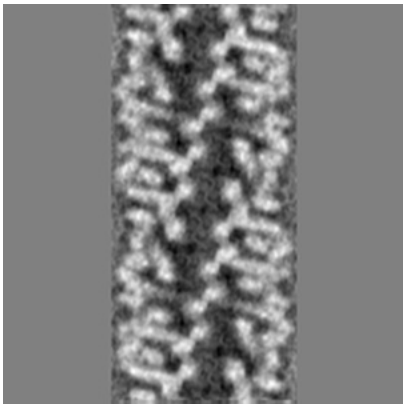


Z Index: 100

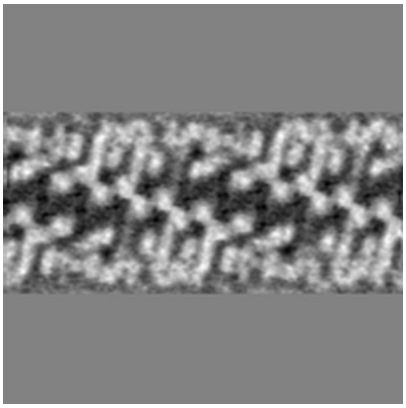
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

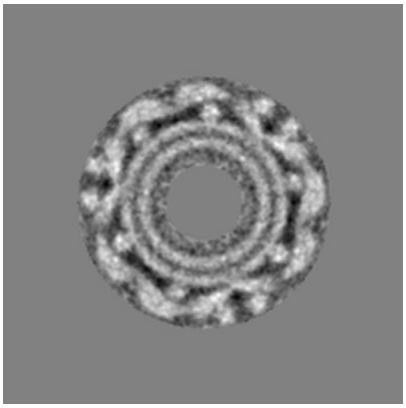
6.3.1 Primary map



X Index: 143



Y Index: 144

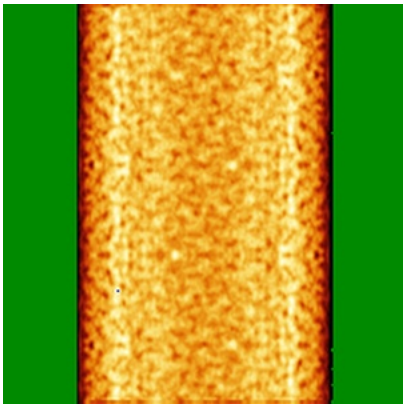


Z Index: 168

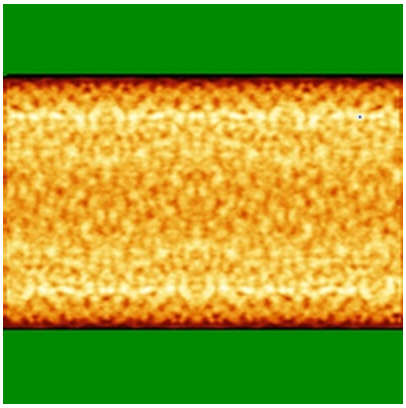
The images above show the largest variance slices of the map in three orthogonal directions.

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

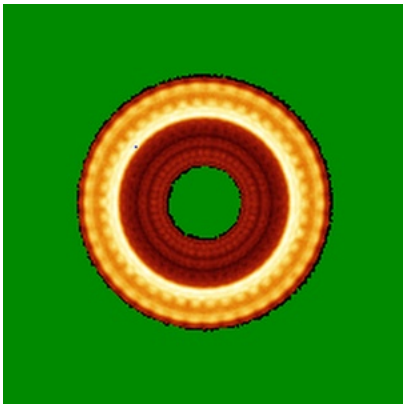
6.4.1 Primary map



X



Y

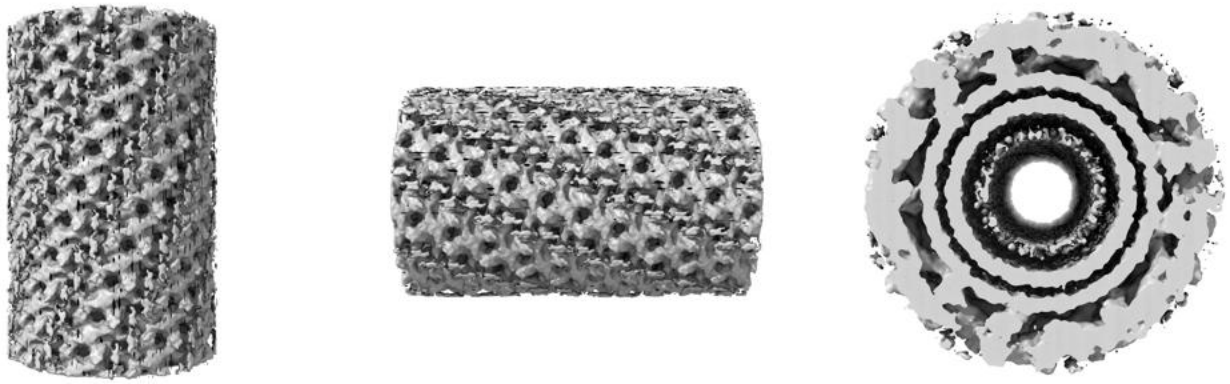


Z

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 0.00157. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

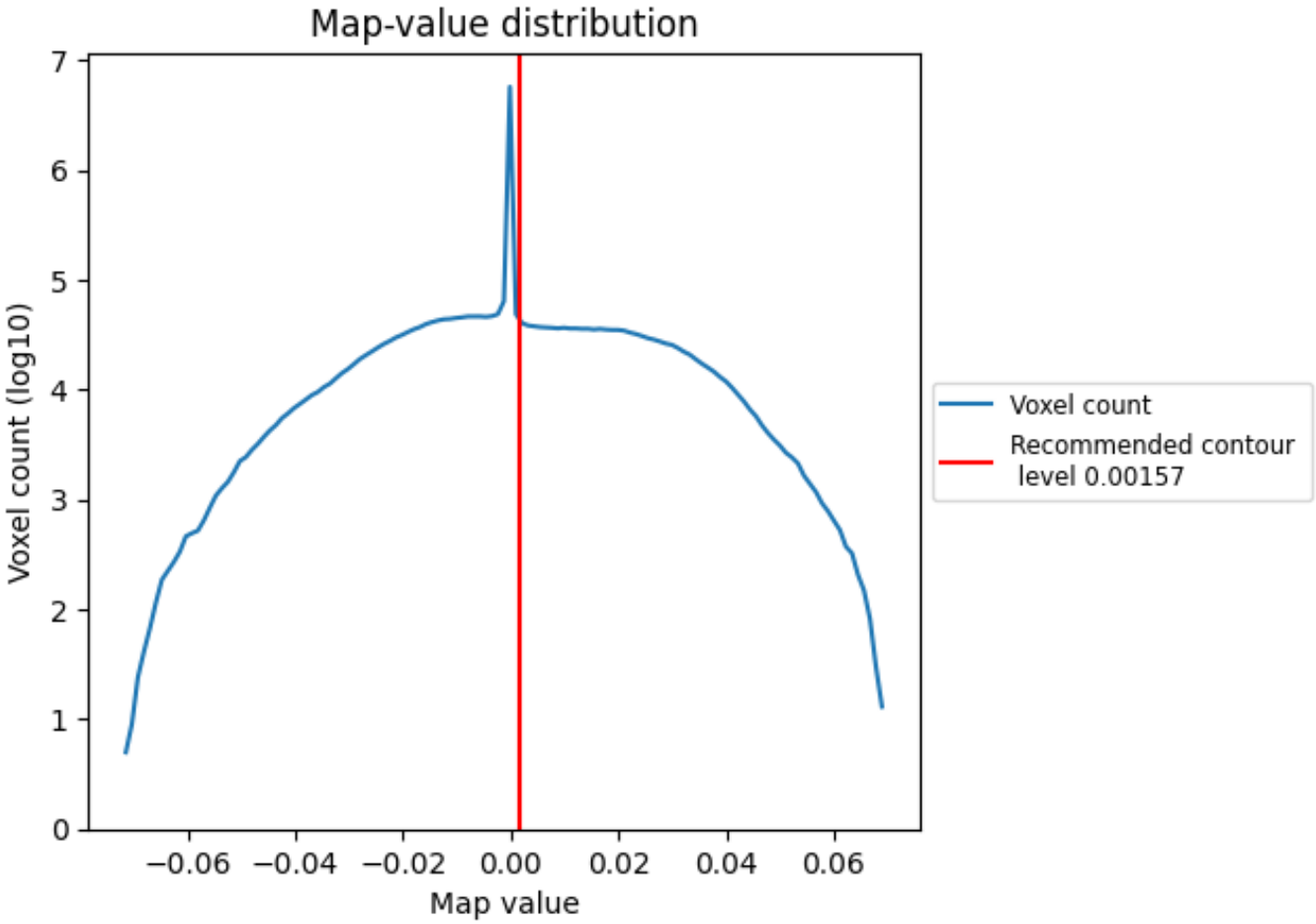
6.6 Mask visualisation (i)

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

7 Map analysis

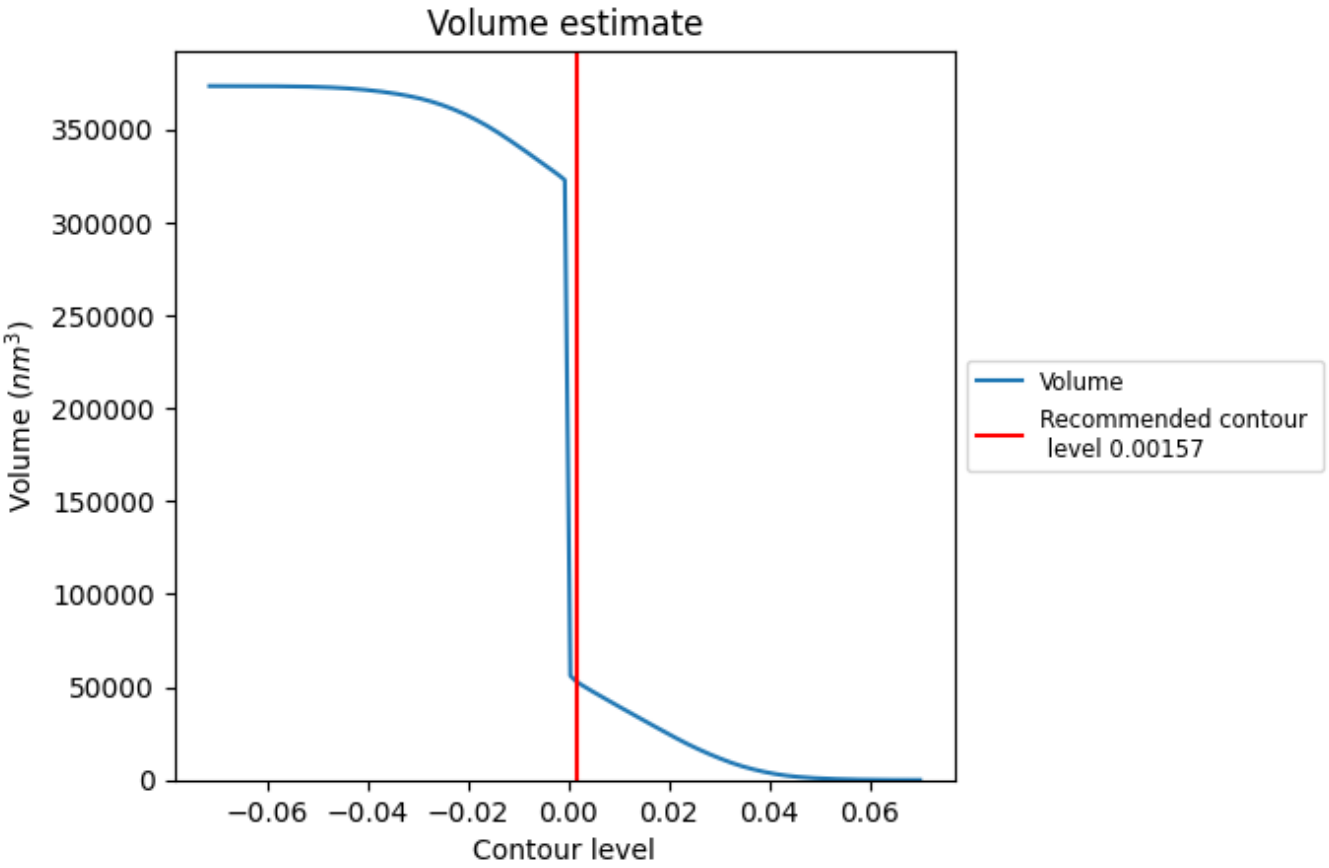
This section contains the results of statistical analysis of the map.

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.

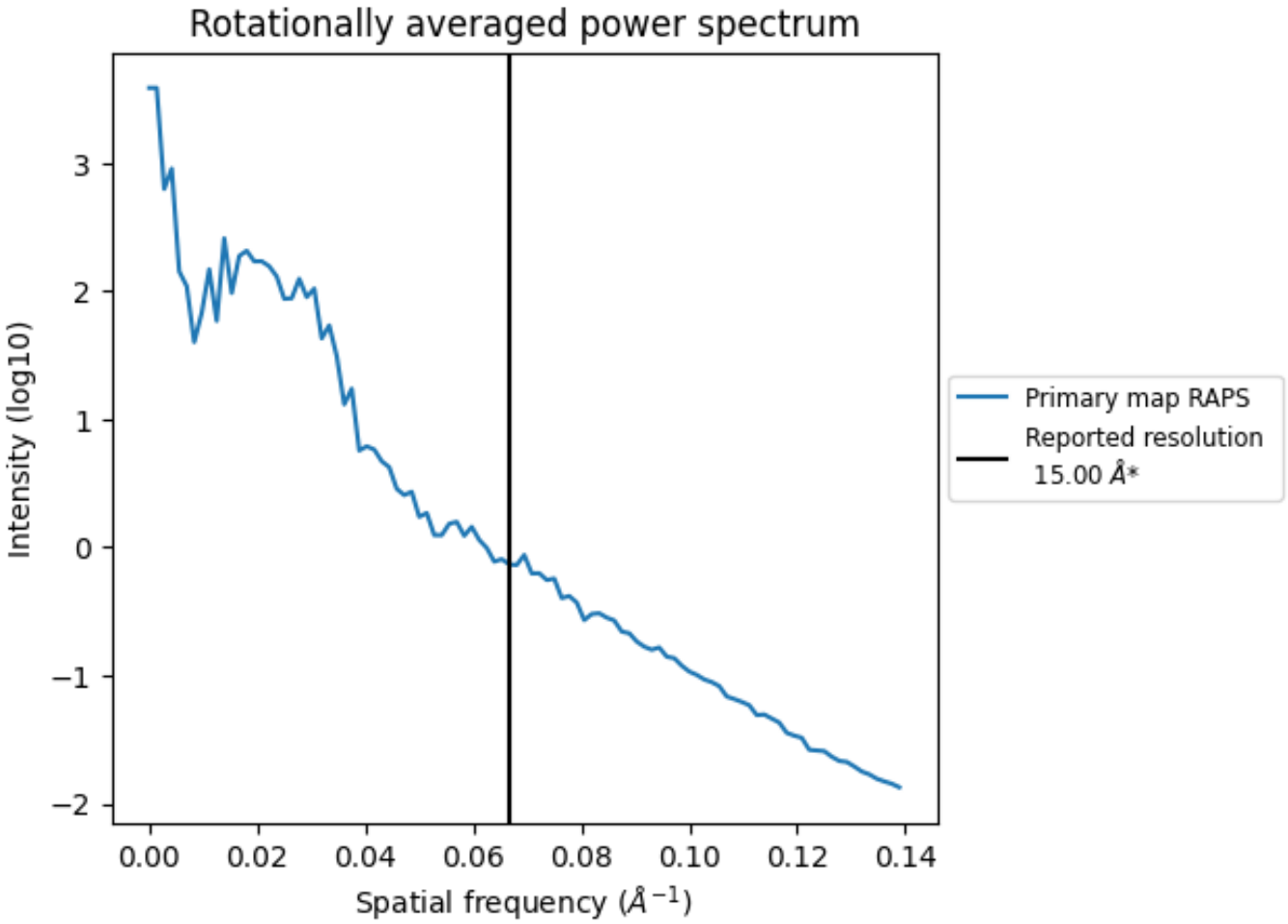
7.2 Volume estimate



The volume at the recommended contour level is 53038 nm^3; this corresponds to an approximate mass of 47910 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 0.067 Å^{-1}

8 Fourier-Shell correlation (i)

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

9 Map-model fit

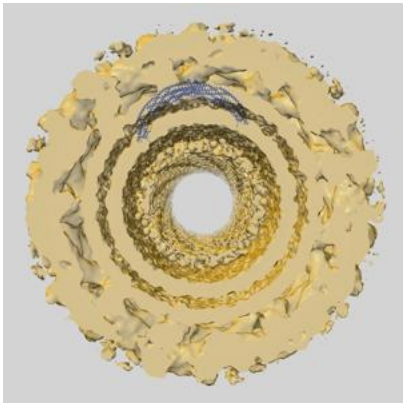
This section contains information regarding the fit between EMDB map EMD-2546 and PDB model 4CKG. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

9.1.1 Map-model overlay

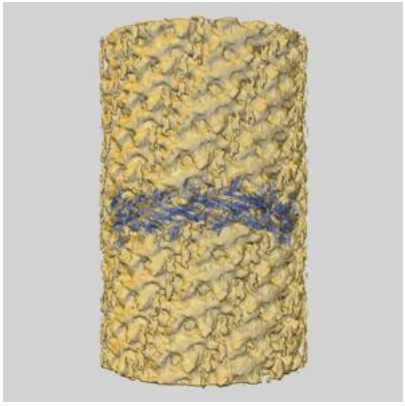
X

Y

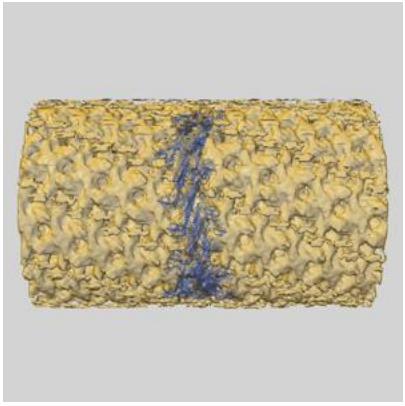


Z

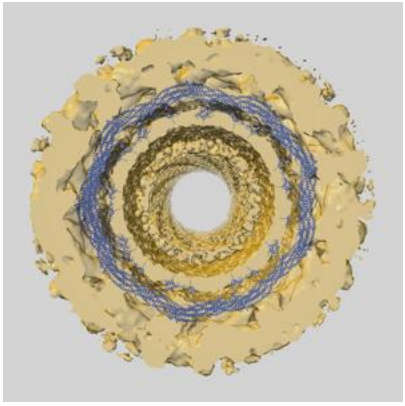
9.1.2 Map-model assembly overlay



X



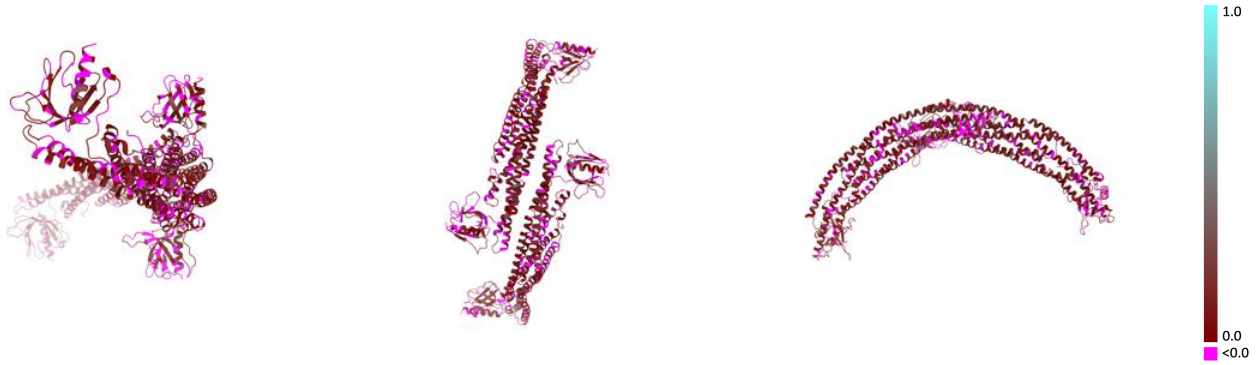
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00157 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.

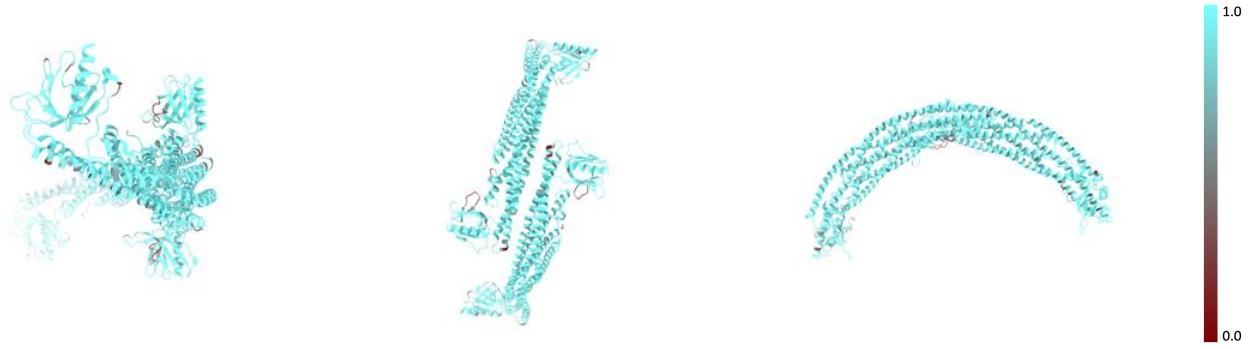
9.2 Q-score mapped to coordinate model



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.

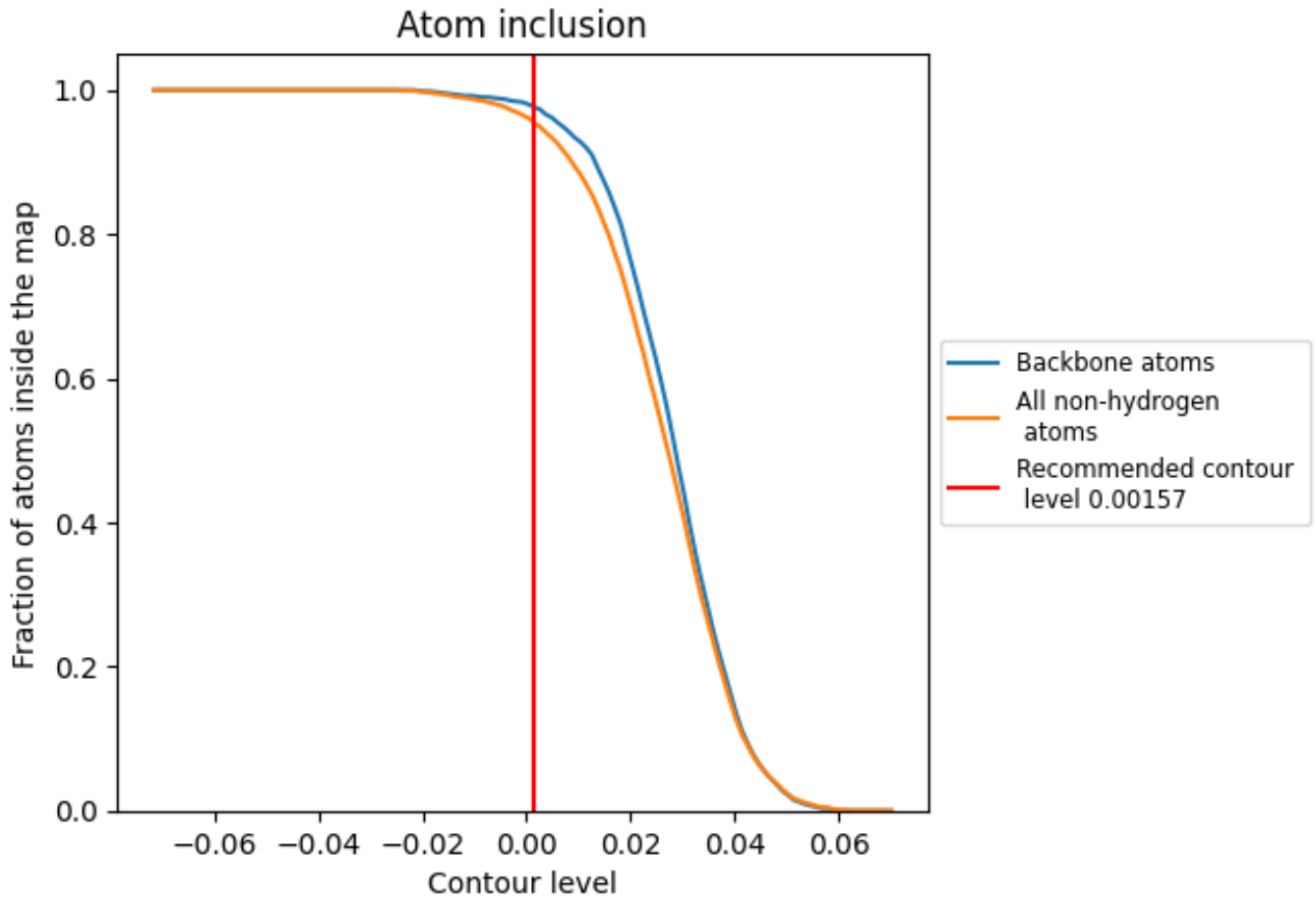
9.3 Atom inclusion mapped to coordinate model



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 (0.00157).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 95% 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 (0.00157) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9540	0.0690
A	0.9580	0.0700
B	0.9490	0.0710
C	0.9590	0.0760
D	0.9490	0.0570