



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 08:57 AM UTC

PDB ID : 4CKH / pdb_00004ckh
EMDB ID : EMD-2547
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 : 17.00 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

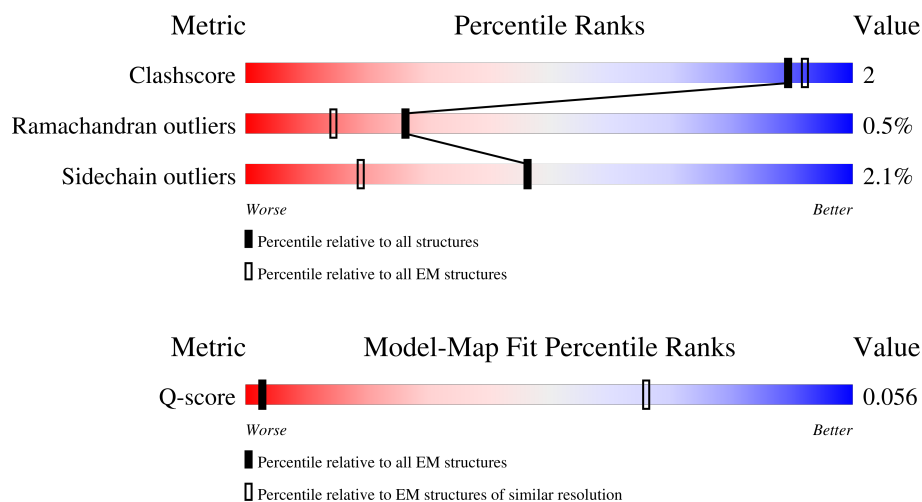
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 17.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	38 (16.50 - 17.50)

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	382	
1	B	382	
1	C	382	
1	D	382	

2 Entry composition

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		

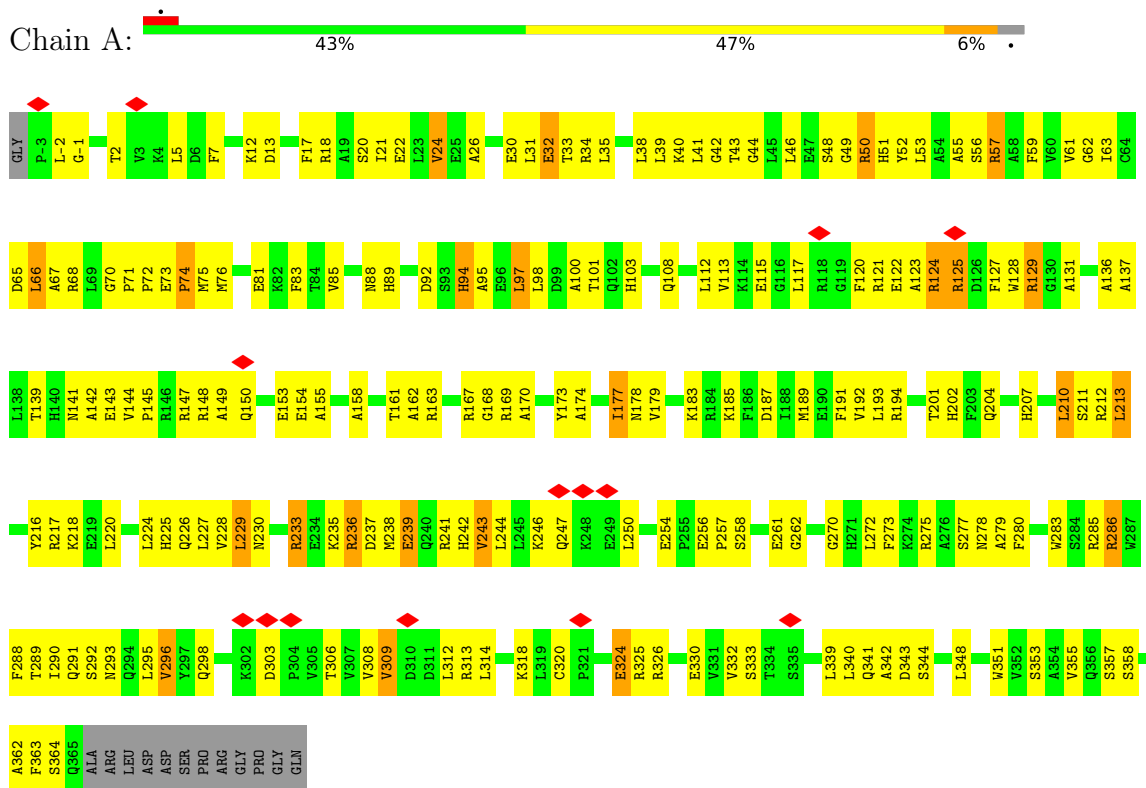
There are 20 discrepancies between the modelled and reference sequences:

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

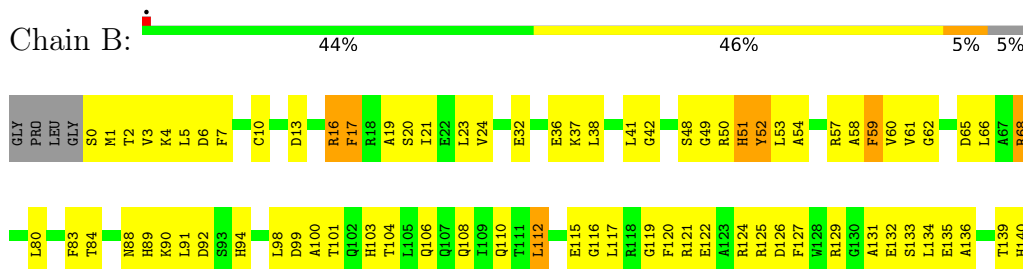
3 Residue-property plots

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.

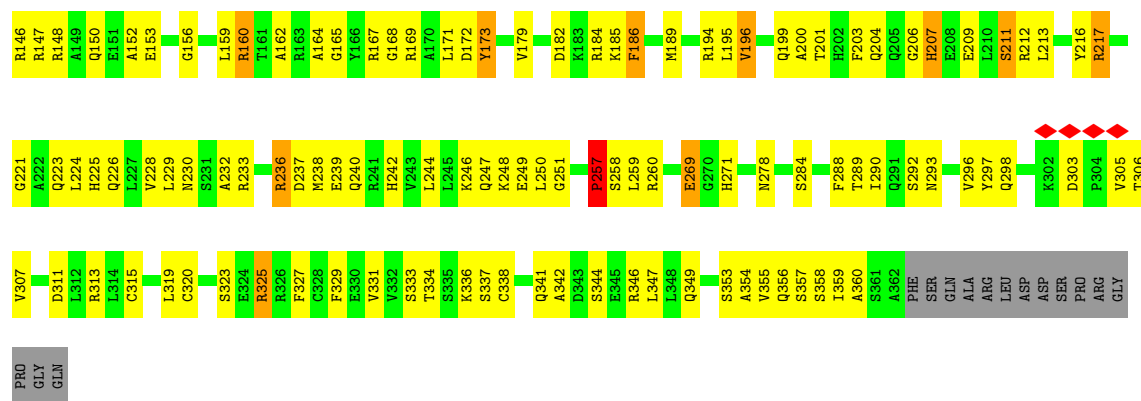
• Molecule 1: ARF-GAP WITH COILED-COIL, ANK REPEAT AND PH DOMAIN-CONTAINING PROTEIN 1



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







4 Experimental information

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	352	Depositor
Resolution determination method	Not provided	
CTF correction method	CTFFIND3	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	0.066	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0014	Depositor
Map size (Å)	720.0, 720.0, 720.0	wwPDB
Map dimensions	150, 150, 150	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	4.8, 4.8, 4.8	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	2.21	92/2990 (3.1%)	2.57	227/4024 (5.6%)
1	B	2.23	102/2947 (3.5%)	2.53	215/3966 (5.4%)
1	C	2.21	92/2990 (3.1%)	2.57	230/4024 (5.7%)
1	D	2.23	104/2947 (3.5%)	2.53	214/3966 (5.4%)
All	All	2.22	390/11874 (3.3%)	2.55	886/15980 (5.5%)

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 (390) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	256	GLU	C-N	10.25	1.45	1.33
1	A	256	GLU	C-N	10.16	1.45	1.33
1	B	320	CYS	CA-CB	10.14	1.59	1.52
1	D	320	CYS	CA-CB	10.12	1.59	1.52
1	D	249	GLU	CA-C	9.34	1.64	1.52
1	B	249	GLU	CA-C	9.29	1.64	1.52
1	C	144	VAL	N-CA	-8.46	1.38	1.47
1	C	168	GLY	N-CA	8.44	1.56	1.45
1	A	144	VAL	N-CA	-8.40	1.38	1.47
1	A	168	GLY	N-CA	8.40	1.56	1.45
1	B	297	TYR	C-N	8.04	1.44	1.33
1	D	189	MET	C-N	7.99	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	297	TYR	C-N	7.99	1.44	1.33
1	D	189	MET	N-CA	7.98	1.55	1.46
1	B	189	MET	N-CA	7.98	1.55	1.46
1	A	161	THR	N-CA	7.95	1.55	1.46
1	A	194	ARG	CD-NE	7.94	1.57	1.46
1	B	146	ARG	CD-NE	7.94	1.57	1.46
1	D	146	ARG	CD-NE	7.93	1.57	1.46
1	B	189	MET	C-N	7.92	1.44	1.33
1	C	161	THR	N-CA	7.92	1.55	1.46
1	C	194	ARG	CD-NE	7.88	1.57	1.46
1	A	72	PRO	N-CA	-7.87	1.38	1.47
1	C	72	PRO	N-CA	-7.81	1.38	1.47
1	D	315	CYS	CA-C	7.76	1.64	1.53
1	B	315	CYS	CA-C	7.72	1.64	1.53
1	A	333	SER	N-CA	7.71	1.55	1.46
1	C	333	SER	N-CA	7.69	1.55	1.46
1	A	285	ARG	CD-NE	7.61	1.56	1.46
1	B	337	SER	CA-CB	7.60	1.66	1.53
1	C	285	ARG	CD-NE	7.59	1.56	1.46
1	D	337	SER	CA-CB	7.57	1.65	1.53
1	D	74	PRO	CA-CB	7.51	1.64	1.53
1	D	226	GLN	C-N	7.49	1.43	1.33
1	A	312	LEU	CA-CB	7.46	1.65	1.53
1	C	312	LEU	CA-CB	7.45	1.65	1.53
1	B	74	PRO	CA-CB	7.44	1.64	1.53
1	C	31	LEU	C-N	-7.43	1.24	1.33
1	C	155	ALA	CA-C	7.39	1.62	1.52
1	B	226	GLN	C-N	7.39	1.43	1.33
1	A	155	ALA	CA-C	7.37	1.62	1.52
1	A	254	GLU	CA-C	-7.33	1.45	1.53
1	D	213	LEU	C-N	7.31	1.43	1.33
1	C	254	GLU	CA-C	-7.31	1.45	1.53
1	B	124	ARG	CD-NE	7.29	1.56	1.46
1	D	124	ARG	CD-NE	7.28	1.56	1.46
1	A	31	LEU	C-N	-7.26	1.24	1.34
1	B	213	LEU	C-N	7.24	1.43	1.33
1	B	232	ALA	C-N	7.22	1.43	1.33
1	A	325	ARG	CA-C	7.20	1.61	1.52
1	C	325	ARG	CA-C	7.18	1.61	1.52
1	D	232	ALA	C-N	7.14	1.43	1.33
1	A	98	LEU	CA-C	-7.14	1.43	1.52
1	C	326	ARG	CD-NE	7.12	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	326	ARG	CD-NE	7.12	1.56	1.46
1	B	121	ARG	C-N	7.10	1.42	1.33
1	A	131	ALA	N-CA	-7.09	1.37	1.46
1	C	98	LEU	CA-C	-7.09	1.43	1.52
1	A	35	LEU	CA-CB	7.06	1.64	1.53
1	D	104	THR	CA-CB	-7.05	1.42	1.53
1	B	104	THR	CA-CB	-7.05	1.42	1.53
1	C	340	LEU	CA-C	7.05	1.61	1.52
1	D	121	ARG	C-N	7.05	1.42	1.33
1	C	131	ALA	N-CA	-7.04	1.37	1.46
1	B	150	GLN	CA-CB	7.04	1.64	1.53
1	D	150	GLN	CA-CB	7.04	1.64	1.53
1	C	163	ARG	CA-C	-7.01	1.44	1.52
1	C	314	LEU	CA-CB	7.00	1.63	1.53
1	A	241	ARG	N-CA	7.00	1.55	1.46
1	D	355	VAL	CA-CB	6.99	1.63	1.54
1	A	314	LEU	CA-CB	6.99	1.63	1.53
1	B	355	VAL	CA-CB	6.98	1.63	1.54
1	C	35	LEU	CA-CB	6.97	1.64	1.53
1	C	241	ARG	N-CA	6.97	1.55	1.46
1	A	340	LEU	CA-C	6.95	1.61	1.52
1	A	163	ARG	CA-C	-6.94	1.44	1.52
1	A	283	TRP	CA-C	6.93	1.61	1.52
1	C	286	ARG	CD-NE	6.92	1.55	1.46
1	D	242	HIS	C-N	-6.88	1.25	1.33
1	B	169	ARG	CD-NE	6.88	1.55	1.46
1	A	286	ARG	CD-NE	6.87	1.55	1.46
1	A	362	ALA	N-CA	-6.87	1.38	1.46
1	C	283	TRP	CA-C	6.84	1.61	1.52
1	C	362	ALA	N-CA	-6.84	1.38	1.46
1	B	242	HIS	C-N	-6.84	1.25	1.33
1	A	220	LEU	C-N	6.84	1.41	1.33
1	C	42	GLY	C-N	6.83	1.43	1.34
1	A	42	GLY	C-N	6.81	1.43	1.34
1	C	76	MET	N-CA	-6.81	1.37	1.46
1	C	220	LEU	C-N	6.81	1.41	1.33
1	D	169	ARG	CD-NE	6.80	1.55	1.46
1	A	59	PHE	CA-C	6.79	1.61	1.52
1	C	233	ARG	CD-NE	6.78	1.55	1.46
1	A	76	MET	N-CA	-6.76	1.37	1.46
1	C	59	PHE	CA-C	6.76	1.61	1.52
1	A	229	LEU	N-CA	-6.75	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	ARG	CD-NE	6.73	1.55	1.46
1	D	65	ASP	CA-CB	6.71	1.64	1.53
1	A	33	THR	C-N	6.70	1.42	1.33
1	A	236	ARG	N-CA	-6.70	1.38	1.46
1	C	257	PRO	N-CA	-6.69	1.39	1.47
1	A	257	PRO	N-CA	-6.69	1.39	1.47
1	D	84	THR	CA-C	6.68	1.61	1.52
1	B	84	THR	CA-C	6.65	1.61	1.52
1	C	236	ARG	N-CA	-6.64	1.38	1.46
1	C	66	LEU	CA-C	-6.62	1.44	1.52
1	B	65	ASP	CA-CB	6.62	1.64	1.53
1	B	307	VAL	CA-C	6.60	1.60	1.52
1	C	229	LEU	N-CA	-6.60	1.38	1.46
1	A	270	GLY	CA-C	-6.60	1.42	1.51
1	C	123	ALA	CA-CB	6.58	1.63	1.53
1	B	4	LYS	CA-C	6.57	1.61	1.53
1	D	307	VAL	CA-C	6.57	1.60	1.52
1	C	270	GLY	CA-C	-6.55	1.42	1.51
1	D	4	LYS	CA-C	6.55	1.61	1.53
1	D	88	ASN	N-CA	6.54	1.54	1.46
1	A	123	ALA	CA-CB	6.53	1.63	1.53
1	C	296	VAL	N-CA	6.53	1.53	1.46
1	C	343	ASP	N-CA	6.51	1.54	1.46
1	A	296	VAL	N-CA	6.50	1.53	1.46
1	C	32	GLU	N-CA	6.50	1.54	1.46
1	A	66	LEU	CA-C	-6.48	1.44	1.52
1	C	167	ARG	CD-NE	6.48	1.55	1.46
1	B	153	GLU	CA-CB	6.47	1.64	1.53
1	D	172	ASP	CA-CB	6.47	1.63	1.53
1	D	153	GLU	CA-CB	6.47	1.64	1.53
1	A	204	GLN	C-N	6.45	1.42	1.33
1	C	204	GLN	C-N	6.45	1.42	1.33
1	A	343	ASP	N-CA	6.44	1.54	1.46
1	B	172	ASP	CA-CB	6.43	1.63	1.53
1	C	33	THR	C-N	6.43	1.42	1.33
1	C	50	ARG	CA-C	6.43	1.61	1.52
1	A	167	ARG	CD-NE	6.42	1.55	1.46
1	D	94	HIS	N-CA	-6.42	1.38	1.46
1	B	88	ASN	N-CA	6.42	1.54	1.46
1	B	94	HIS	N-CA	-6.42	1.38	1.46
1	D	289	THR	C-O	-6.41	1.16	1.24
1	A	238	MET	CA-C	6.39	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	LEU	CA-CB	6.37	1.63	1.53
1	A	32	GLU	N-CA	6.35	1.54	1.46
1	C	238	MET	CA-C	6.34	1.61	1.52
1	A	50	ARG	CA-C	6.33	1.60	1.52
1	B	211	SER	CA-CB	6.33	1.63	1.53
1	B	289	THR	C-O	-6.33	1.16	1.24
1	D	236	ARG	CD-NE	6.32	1.55	1.46
1	A	66	LEU	CA-CB	6.31	1.63	1.53
1	D	211	SER	CA-CB	6.29	1.63	1.53
1	B	236	ARG	CD-NE	6.27	1.55	1.46
1	B	200	ALA	C-N	6.26	1.42	1.33
1	C	63	ILE	CA-C	-6.26	1.44	1.52
1	D	325	ARG	CD-NE	6.25	1.54	1.46
1	A	63	ILE	CA-C	-6.24	1.44	1.52
1	B	139	THR	N-CA	6.22	1.53	1.46
1	B	41	LEU	CA-C	6.21	1.60	1.52
1	A	41	LEU	CA-C	6.21	1.61	1.52
1	D	115	GLU	CA-C	6.18	1.58	1.52
1	C	41	LEU	CA-C	6.18	1.61	1.52
1	D	200	ALA	C-N	6.17	1.42	1.33
1	D	139	THR	N-CA	6.17	1.53	1.46
1	A	189	MET	CA-CB	6.17	1.63	1.53
1	D	41	LEU	CA-C	6.16	1.60	1.52
1	B	271	HIS	ND1-CE1	6.16	1.38	1.32
1	D	271	HIS	ND1-CE1	6.16	1.38	1.32
1	B	257	PRO	C-N	6.14	1.41	1.33
1	B	115	GLU	CA-C	6.09	1.58	1.52
1	D	260	ARG	CA-C	6.09	1.60	1.52
1	A	246	LYS	CA-C	6.08	1.60	1.52
1	D	257	PRO	C-N	6.08	1.41	1.33
1	B	68	ARG	C-O	6.06	1.31	1.24
1	B	325	ARG	CD-NE	6.06	1.54	1.46
1	D	68	ARG	C-O	6.05	1.31	1.24
1	B	200	ALA	N-CA	-6.05	1.39	1.46
1	D	341	GLN	CA-C	6.05	1.59	1.52
1	B	57	ARG	NE-CZ	6.03	1.39	1.33
1	C	189	MET	CA-CB	6.03	1.62	1.53
1	D	200	ALA	N-CA	-6.03	1.39	1.46
1	B	341	GLN	CA-C	6.00	1.59	1.52
1	B	62	GLY	C-N	5.99	1.41	1.33
1	B	260	ARG	CA-C	5.99	1.59	1.52
1	B	115	GLU	N-CA	-5.98	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	246	LYS	CA-C	5.97	1.60	1.52
1	D	57	ARG	NE-CZ	5.96	1.39	1.33
1	A	306	THR	N-CA	-5.96	1.38	1.46
1	A	74	PRO	CA-CB	-5.95	1.45	1.53
1	B	333	SER	N-CA	5.95	1.53	1.45
1	D	62	GLY	C-N	5.94	1.41	1.33
1	D	115	GLU	N-CA	-5.91	1.42	1.47
1	B	48	SER	CA-CB	5.89	1.62	1.53
1	C	74	PRO	CA-CB	-5.89	1.45	1.53
1	D	48	SER	CA-CB	5.86	1.62	1.53
1	D	133	SER	N-CA	-5.85	1.39	1.46
1	C	226	GLN	C-O	-5.84	1.17	1.24
1	D	122	GLU	C-N	5.84	1.41	1.33
1	D	333	SER	N-CA	5.83	1.53	1.45
1	D	164	ALA	CA-CB	5.82	1.62	1.53
1	B	338	CYS	CA-C	5.81	1.59	1.52
1	D	338	CYS	CA-C	5.81	1.59	1.52
1	C	148	ARG	CD-NE	5.80	1.54	1.46
1	B	171	LEU	CA-C	5.78	1.60	1.52
1	C	306	THR	N-CA	-5.78	1.38	1.46
1	B	122	GLU	C-N	5.78	1.41	1.33
1	A	262	GLY	C-N	-5.78	1.27	1.34
1	D	238	MET	N-CA	-5.78	1.39	1.46
1	B	303	ASP	CA-CB	5.77	1.62	1.54
1	D	196	VAL	N-CA	5.77	1.53	1.46
1	B	164	ALA	CA-CB	5.77	1.62	1.53
1	B	196	VAL	N-CA	5.77	1.53	1.46
1	C	262	GLY	C-N	-5.76	1.27	1.34
1	C	288	PHE	C-O	5.76	1.31	1.23
1	D	303	ASP	CA-CB	5.76	1.62	1.54
1	B	311	ASP	C-N	5.76	1.42	1.33
1	B	133	SER	N-CA	-5.74	1.39	1.46
1	D	59	PHE	C-N	5.73	1.40	1.33
1	C	44	GLY	CA-C	-5.73	1.45	1.52
1	C	218	LYS	C-O	-5.73	1.17	1.24
1	A	288	PHE	C-O	5.72	1.30	1.23
1	D	311	ASP	C-N	5.72	1.42	1.33
1	A	226	GLN	C-O	-5.71	1.17	1.24
1	C	185	LYS	CA-C	5.71	1.60	1.52
1	D	165	GLY	C-N	5.71	1.41	1.33
1	B	238	MET	N-CA	-5.70	1.39	1.46
1	C	49	GLY	CA-C	-5.70	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	59	PHE	C-N	5.69	1.40	1.33
1	A	185	LYS	CA-C	5.69	1.60	1.52
1	C	295	LEU	CA-CB	5.69	1.60	1.53
1	A	148	ARG	CD-NE	5.68	1.54	1.46
1	B	165	GLY	C-N	5.68	1.41	1.33
1	C	100	ALA	N-CA	-5.68	1.39	1.46
1	B	98	LEU	CA-CB	5.68	1.62	1.53
1	B	80	LEU	CA-C	5.67	1.60	1.52
1	A	218	LYS	C-O	-5.67	1.17	1.24
1	A	100	ALA	N-CA	-5.64	1.39	1.46
1	D	32	GLU	CA-C	-5.64	1.45	1.52
1	D	160	ARG	CD-NE	5.64	1.54	1.46
1	A	44	GLY	CA-C	-5.63	1.45	1.52
1	B	160	ARG	CD-NE	5.63	1.54	1.46
1	D	98	LEU	CA-CB	5.63	1.62	1.53
1	A	295	LEU	CA-CB	5.63	1.60	1.53
1	A	306	THR	C-O	-5.62	1.17	1.23
1	D	80	LEU	CA-C	5.62	1.60	1.52
1	D	171	LEU	CA-C	5.62	1.60	1.52
1	B	32	GLU	CA-C	-5.61	1.45	1.52
1	C	306	THR	C-O	-5.60	1.17	1.23
1	A	73	GLU	C-N	5.60	1.41	1.33
1	C	73	GLU	C-N	5.60	1.41	1.33
1	A	88	ASN	N-CA	5.59	1.53	1.46
1	C	353	SER	C-N	5.59	1.41	1.33
1	A	49	GLY	CA-C	-5.58	1.46	1.52
1	A	353	SER	C-N	5.58	1.41	1.33
1	C	88	ASN	N-CA	5.58	1.53	1.46
1	B	325	ARG	N-CA	-5.57	1.39	1.46
1	C	339	LEU	CB-CG	5.56	1.64	1.53
1	A	272	LEU	CA-C	5.56	1.59	1.52
1	D	325	ARG	N-CA	-5.56	1.39	1.46
1	C	272	LEU	CA-C	5.55	1.59	1.52
1	D	320	CYS	C-O	5.53	1.26	1.23
1	C	312	LEU	CA-C	5.53	1.59	1.52
1	C	351	TRP	C-N	5.51	1.40	1.33
1	A	193	LEU	N-CA	5.50	1.52	1.46
1	D	216	TYR	C-N	5.50	1.40	1.33
1	D	259	LEU	N-CA	-5.50	1.39	1.46
1	A	339	LEU	CB-CG	5.50	1.64	1.53
1	A	351	TRP	C-N	5.50	1.40	1.33
1	C	193	LEU	N-CA	5.50	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	LEU	N-CA	5.50	1.53	1.46
1	B	216	TYR	C-N	5.48	1.40	1.33
1	A	185	LYS	CA-CB	5.47	1.61	1.53
1	D	16	ARG	CA-C	5.47	1.59	1.52
1	A	247	GLN	C-N	5.46	1.41	1.33
1	A	312	LEU	CA-C	5.44	1.59	1.52
1	C	247	GLN	C-N	5.43	1.41	1.33
1	D	250	LEU	C-N	5.43	1.38	1.33
1	B	259	LEU	N-CA	-5.42	1.39	1.46
1	A	280	PHE	CB-CG	-5.42	1.38	1.50
1	C	185	LYS	CA-CB	5.41	1.61	1.53
1	D	5	LEU	N-CA	5.41	1.53	1.46
1	C	40	LYS	N-CA	-5.40	1.39	1.46
1	B	16	ARG	CA-C	5.40	1.59	1.52
1	C	239	GLU	N-CA	5.40	1.52	1.46
1	B	233	ARG	NE-CZ	5.39	1.39	1.33
1	D	90	LYS	CA-C	5.39	1.59	1.52
1	D	194	ARG	C-N	-5.39	1.27	1.33
1	B	20	SER	N-CA	5.38	1.53	1.46
1	C	95	ALA	N-CA	5.38	1.52	1.46
1	C	280	PHE	CB-CG	-5.38	1.38	1.50
1	B	358	SER	CA-C	5.37	1.59	1.52
1	D	53	LEU	CA-C	5.37	1.59	1.52
1	C	98	LEU	N-CA	5.37	1.52	1.46
1	B	90	LYS	C-O	-5.37	1.17	1.24
1	B	207	HIS	CE1-NE2	5.37	1.38	1.32
1	B	250	LEU	C-N	5.37	1.38	1.33
1	A	40	LYS	N-CA	-5.36	1.40	1.46
1	D	140	HIS	CA-CB	5.36	1.61	1.53
1	C	94	HIS	CB-CG	5.35	1.57	1.50
1	B	5	LEU	N-CA	5.35	1.53	1.46
1	D	90	LYS	C-O	-5.35	1.17	1.24
1	C	147	ARG	CA-C	5.34	1.59	1.52
1	A	306	THR	C-N	5.33	1.40	1.33
1	C	50	ARG	CD-NE	5.33	1.53	1.46
1	B	325	ARG	CA-CB	5.33	1.62	1.53
1	B	140	HIS	CA-CB	5.32	1.61	1.53
1	C	306	THR	C-N	5.31	1.40	1.33
1	D	358	SER	CA-C	5.31	1.59	1.52
1	A	147	ARG	CA-C	5.31	1.59	1.52
1	B	320	CYS	C-O	5.29	1.26	1.23
1	D	290	ILE	C-O	5.29	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	207	HIS	CE1-NE2	5.29	1.37	1.32
1	A	178	ASN	CA-C	5.29	1.59	1.52
1	A	95	ALA	N-CA	5.29	1.52	1.46
1	B	251	GLY	N-CA	-5.29	1.38	1.45
1	D	20	SER	N-CA	5.28	1.52	1.46
1	A	342	ALA	N-CA	-5.28	1.39	1.45
1	A	94	HIS	CB-CG	5.28	1.57	1.50
1	A	244	LEU	CA-CB	5.28	1.61	1.53
1	D	325	ARG	CA-CB	5.27	1.62	1.53
1	A	161	THR	C-N	5.27	1.40	1.33
1	D	251	GLY	N-CA	-5.27	1.38	1.45
1	B	194	ARG	C-N	-5.26	1.27	1.33
1	A	318	LYS	CA-CB	5.26	1.61	1.53
1	B	53	LEU	CA-C	5.25	1.59	1.52
1	D	233	ARG	NE-CZ	5.25	1.38	1.33
1	B	90	LYS	CA-C	5.25	1.59	1.52
1	D	112	LEU	CA-C	5.25	1.59	1.52
1	A	50	ARG	CD-NE	5.24	1.53	1.46
1	A	239	GLU	N-CA	5.24	1.52	1.46
1	C	161	THR	C-N	5.24	1.40	1.33
1	D	342	ALA	C-N	5.24	1.41	1.33
1	C	244	LEU	CA-CB	5.24	1.61	1.53
1	B	290	ILE	C-O	5.23	1.29	1.24
1	B	342	ALA	C-N	5.23	1.41	1.33
1	D	103	HIS	CD2-NE2	5.22	1.43	1.37
1	D	127	PHE	CA-C	5.22	1.59	1.52
1	B	320	CYS	N-CA	-5.21	1.42	1.46
1	C	178	ASN	CA-C	5.21	1.59	1.52
1	C	318	LYS	CA-CB	5.21	1.61	1.53
1	C	192	VAL	N-CA	5.19	1.52	1.46
1	C	342	ALA	N-CA	-5.18	1.39	1.45
1	D	147	ARG	NE-CZ	5.18	1.38	1.33
1	B	103	HIS	CD2-NE2	5.17	1.43	1.37
1	B	127	PHE	CA-C	5.17	1.59	1.52
1	B	112	LEU	CA-C	5.17	1.59	1.52
1	C	312	LEU	N-CA	-5.17	1.38	1.45
1	B	147	ARG	NE-CZ	5.17	1.38	1.33
1	A	192	VAL	N-CA	5.16	1.52	1.46
1	C	229	LEU	CA-CB	5.16	1.61	1.53
1	D	133	SER	CA-CB	5.14	1.61	1.53
1	D	156	GLY	CA-C	-5.14	1.45	1.52
1	A	50	ARG	NE-CZ	5.12	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	133	SER	CA-CB	5.12	1.61	1.53
1	B	143	GLU	CA-CB	5.12	1.58	1.52
1	C	193	LEU	C-N	5.11	1.40	1.33
1	A	61	VAL	C-O	-5.11	1.18	1.24
1	D	307	VAL	C-N	5.11	1.39	1.33
1	D	143	GLU	CA-CB	5.11	1.58	1.52
1	B	116	GLY	CA-C	5.10	1.59	1.51
1	D	116	GLY	CA-C	5.10	1.59	1.51
1	D	42	GLY	CA-C	-5.10	1.45	1.52
1	C	262	GLY	N-CA	5.10	1.51	1.44
1	D	217	ARG	NE-CZ	5.10	1.38	1.33
1	A	229	LEU	CA-CB	5.09	1.61	1.53
1	D	305	VAL	CA-CB	-5.09	1.47	1.54
1	D	127	PHE	CA-CB	5.09	1.61	1.53
1	D	126	ASP	CA-C	5.08	1.59	1.52
1	D	320	CYS	N-CA	-5.08	1.42	1.46
1	A	193	LEU	C-N	5.08	1.40	1.33
1	B	156	GLY	CA-C	-5.07	1.45	1.52
1	C	50	ARG	NE-CZ	5.07	1.38	1.33
1	B	42	GLY	CA-C	-5.07	1.45	1.52
1	C	61	VAL	C-O	-5.07	1.18	1.24
1	B	134	LEU	CA-CB	5.06	1.61	1.53
1	A	235	LYS	C-N	5.06	1.40	1.33
1	D	201	THR	N-CA	5.05	1.52	1.46
1	B	305	VAL	CA-CB	-5.05	1.47	1.54
1	A	312	LEU	N-CA	-5.04	1.39	1.45
1	B	140	HIS	C-N	5.04	1.41	1.33
1	B	298	GLN	N-CA	-5.04	1.39	1.46
1	D	184	ARG	NE-CZ	5.04	1.38	1.33
1	D	240	GLN	CA-C	5.04	1.59	1.52
1	D	159	LEU	C-O	5.04	1.30	1.24
1	B	127	PHE	CA-CB	5.04	1.61	1.53
1	D	325	ARG	C-N	5.04	1.40	1.33
1	D	122	GLU	CA-C	-5.03	1.46	1.52
1	B	307	VAL	C-N	5.03	1.39	1.33
1	B	184	ARG	NE-CZ	5.02	1.38	1.33
1	D	140	HIS	C-N	5.02	1.40	1.33
1	B	159	LEU	C-O	5.02	1.29	1.24
1	B	122	GLU	CA-C	-5.02	1.46	1.52
1	D	298	GLN	N-CA	-5.01	1.39	1.46
1	B	201	THR	N-CA	5.01	1.52	1.46
1	B	126	ASP	CA-C	5.01	1.59	1.52

All (886) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	220	LEU	CA-C-N	11.57	132.55	119.94
1	C	220	LEU	C-N-CA	11.57	132.55	119.94
1	A	220	LEU	CA-C-N	11.55	132.53	119.94
1	A	220	LEU	C-N-CA	11.55	132.53	119.94
1	B	179	VAL	N-CA-C	10.94	121.78	110.62
1	D	179	VAL	N-CA-C	10.93	121.77	110.62
1	A	55	ALA	CA-C-N	10.88	134.59	120.44
1	A	55	ALA	C-N-CA	10.88	134.59	120.44
1	C	55	ALA	CA-C-N	10.86	134.56	120.44
1	C	55	ALA	C-N-CA	10.86	134.56	120.44
1	C	278	ASN	CA-CB-CG	-10.43	102.17	112.60
1	A	278	ASN	CA-CB-CG	-10.36	102.24	112.60
1	C	63	ILE	N-CA-CB	10.20	124.42	110.54
1	A	63	ILE	N-CA-CB	10.15	124.34	110.54
1	C	103	HIS	N-CA-C	10.09	121.87	111.07
1	A	103	HIS	N-CA-C	10.05	121.83	111.07
1	A	279	ALA	N-CA-C	9.74	122.91	111.71
1	C	279	ALA	N-CA-C	9.72	122.89	111.71
1	A	141	ASN	CA-C-O	9.61	130.60	120.42
1	C	141	ASN	CA-C-O	9.60	130.60	120.42
1	A	211	SER	N-CA-C	9.44	122.44	111.11
1	C	211	SER	N-CA-C	9.42	122.41	111.11
1	C	207	HIS	CE1-NE2-CD2	-9.32	99.68	109.00
1	D	48	SER	CA-C-N	9.31	130.27	119.94
1	D	48	SER	C-N-CA	9.31	130.27	119.94
1	B	50	ARG	NE-CZ-NH2	9.29	127.56	119.20
1	B	48	SER	CA-C-N	9.25	130.21	119.94
1	B	48	SER	C-N-CA	9.25	130.21	119.94
1	A	207	HIS	CE1-NE2-CD2	-9.22	99.78	109.00
1	B	110	GLN	N-CA-C	9.22	121.33	111.28
1	D	303	ASP	CA-C-O	-9.22	110.51	119.91
1	B	303	ASP	CA-C-O	-9.22	110.51	119.91
1	D	110	GLN	N-CA-C	9.20	121.31	111.28
1	B	216	TYR	CA-C-N	9.19	132.78	120.65
1	B	216	TYR	C-N-CA	9.19	132.78	120.65
1	D	216	TYR	CA-C-N	9.17	132.76	120.65
1	D	216	TYR	C-N-CA	9.17	132.76	120.65
1	D	50	ARG	NE-CZ-NH2	9.15	127.44	119.20
1	A	242	HIS	CA-C-N	8.98	131.88	120.56
1	A	242	HIS	C-N-CA	8.98	131.88	120.56
1	C	242	HIS	CA-C-N	8.92	131.80	120.56
1	C	242	HIS	C-N-CA	8.92	131.80	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	ASP	CA-C-N	8.90	132.21	120.28
1	A	237	ASP	C-N-CA	8.90	132.21	120.28
1	A	92	ASP	CA-CB-CG	-8.88	103.72	112.60
1	C	237	ASP	CA-C-N	8.86	132.16	120.28
1	C	237	ASP	C-N-CA	8.86	132.16	120.28
1	C	92	ASP	CA-CB-CG	-8.84	103.76	112.60
1	B	92	ASP	CA-CB-CG	-8.83	103.77	112.60
1	D	92	ASP	CA-CB-CG	-8.81	103.79	112.60
1	D	100	ALA	O-C-N	-8.78	112.14	122.15
1	D	38	LEU	CA-C-N	8.77	132.98	120.79
1	D	38	LEU	C-N-CA	8.77	132.98	120.79
1	B	38	LEU	CA-C-N	8.76	132.97	120.79
1	B	38	LEU	C-N-CA	8.76	132.97	120.79
1	B	100	ALA	O-C-N	-8.76	112.17	122.15
1	B	160	ARG	N-CA-CB	8.72	122.94	109.94
1	D	160	ARG	N-CA-CB	8.70	122.91	109.94
1	D	284	SER	CA-C-O	8.66	130.42	120.89
1	B	284	SER	CA-C-O	8.65	130.41	120.89
1	A	332	VAL	N-CA-C	8.64	120.20	108.11
1	C	332	VAL	N-CA-C	8.61	120.17	108.11
1	C	85	VAL	CA-C-N	8.56	131.56	120.44
1	C	85	VAL	C-N-CA	8.56	131.56	120.44
1	A	85	VAL	CA-C-N	8.54	131.54	120.44
1	A	85	VAL	C-N-CA	8.54	131.54	120.44
1	A	127	PHE	CA-CB-CG	8.53	122.33	113.80
1	C	127	PHE	CA-CB-CG	8.44	122.24	113.80
1	C	100	ALA	N-CA-C	8.40	120.44	111.28
1	A	100	ALA	N-CA-C	8.38	120.42	111.28
1	B	19	ALA	O-C-N	-8.29	111.22	122.33
1	D	19	ALA	O-C-N	-8.26	111.26	122.33
1	D	182	ASP	CA-C-O	-8.21	111.12	120.24
1	B	246	LYS	CA-C-N	8.20	131.94	120.29
1	B	246	LYS	C-N-CA	8.20	131.94	120.29
1	C	129	ARG	CA-C-N	8.17	130.64	120.34
1	C	129	ARG	C-N-CA	8.17	130.64	120.34
1	C	241	ARG	CA-C-N	8.15	131.04	120.44
1	C	241	ARG	C-N-CA	8.15	131.04	120.44
1	B	182	ASP	CA-C-O	-8.15	111.19	120.24
1	D	246	LYS	CA-C-N	8.15	131.86	120.29
1	D	246	LYS	C-N-CA	8.15	131.86	120.29
1	C	141	ASN	O-C-N	-8.13	112.88	122.15
1	A	129	ARG	CA-C-N	8.11	130.56	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ARG	C-N-CA	8.11	130.56	120.34
1	A	141	ASN	O-C-N	-8.10	112.92	122.15
1	A	241	ARG	CA-C-N	8.08	130.95	120.44
1	A	241	ARG	C-N-CA	8.08	130.95	120.44
1	B	248	LYS	N-CA-C	8.02	123.54	113.43
1	B	297	TYR	CA-C-O	8.00	130.47	121.11
1	D	248	LYS	N-CA-C	7.99	123.50	113.43
1	D	297	TYR	CA-C-O	7.93	130.39	121.11
1	C	344	SER	CA-C-N	7.92	130.89	120.28
1	C	344	SER	C-N-CA	7.92	130.89	120.28
1	B	239	GLU	CA-C-N	7.91	131.53	120.29
1	B	239	GLU	C-N-CA	7.91	131.53	120.29
1	D	239	GLU	CA-C-N	7.90	131.51	120.29
1	D	239	GLU	C-N-CA	7.90	131.51	120.29
1	A	344	SER	CA-C-N	7.87	130.83	120.28
1	A	344	SER	C-N-CA	7.87	130.83	120.28
1	D	88	ASN	CA-C-N	7.87	130.68	120.44
1	D	88	ASN	C-N-CA	7.87	130.68	120.44
1	B	13	ASP	CB-CA-C	7.87	122.41	111.86
1	D	13	ASP	CB-CA-C	7.86	122.39	111.86
1	B	75	MET	CA-C-N	7.82	131.07	120.44
1	B	75	MET	C-N-CA	7.82	131.07	120.44
1	B	88	ASN	CA-C-N	7.80	130.59	120.44
1	B	88	ASN	C-N-CA	7.80	130.59	120.44
1	D	75	MET	CA-C-N	7.80	131.05	120.44
1	D	75	MET	C-N-CA	7.80	131.05	120.44
1	D	89	HIS	CA-CB-CG	-7.76	106.04	113.80
1	D	136	ALA	O-C-N	-7.75	114.08	122.07
1	A	225	HIS	N-CA-C	7.75	120.81	111.82
1	C	225	HIS	N-CA-C	7.74	120.79	111.82
1	A	233	ARG	CA-C-N	7.72	130.62	120.28
1	A	233	ARG	C-N-CA	7.72	130.62	120.28
1	D	207	HIS	CG-CD2-NE2	7.72	114.92	107.20
1	C	233	ARG	CA-C-N	7.71	130.62	120.28
1	C	233	ARG	C-N-CA	7.71	130.62	120.28
1	C	179	VAL	O-C-N	-7.70	114.40	121.87
1	B	89	HIS	CA-CB-CG	-7.70	106.10	113.80
1	A	324	GLU	CA-C-O	7.69	128.70	120.55
1	B	136	ALA	O-C-N	-7.69	114.15	122.07
1	B	207	HIS	CG-CD2-NE2	7.68	114.88	107.20
1	C	278	ASN	O-C-N	-7.63	113.85	122.86
1	C	324	GLU	CA-C-O	7.62	128.63	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	ASN	O-C-N	-7.62	113.87	122.86
1	C	177	ILE	O-C-N	-7.61	114.43	121.89
1	A	177	ILE	O-C-N	-7.61	114.43	121.89
1	A	179	VAL	O-C-N	-7.61	114.49	121.87
1	D	68	ARG	NE-CZ-NH2	7.58	126.03	119.20
1	B	195	LEU	CA-C-N	7.56	130.82	120.46
1	B	195	LEU	C-N-CA	7.56	130.82	120.46
1	D	50	ARG	CA-C-N	7.56	130.42	120.28
1	D	50	ARG	C-N-CA	7.56	130.42	120.28
1	D	195	LEU	CA-C-N	7.54	130.79	120.46
1	D	195	LEU	C-N-CA	7.54	130.79	120.46
1	A	167	ARG	CA-C-O	7.53	128.73	120.82
1	B	68	ARG	NE-CZ-NH2	7.52	125.97	119.20
1	B	50	ARG	CA-C-N	7.52	130.36	120.28
1	B	50	ARG	C-N-CA	7.52	130.36	120.28
1	C	167	ARG	CA-C-O	7.52	128.72	120.82
1	A	213	LEU	CA-C-N	7.46	130.89	120.29
1	A	213	LEU	C-N-CA	7.46	130.89	120.29
1	C	213	LEU	CA-C-N	7.45	130.88	120.29
1	C	213	LEU	C-N-CA	7.45	130.88	120.29
1	B	206	GLY	CA-C-N	7.43	130.24	120.28
1	B	206	GLY	C-N-CA	7.43	130.24	120.28
1	D	206	GLY	CA-C-N	7.42	130.23	120.28
1	D	206	GLY	C-N-CA	7.42	130.23	120.28
1	A	18	ARG	N-CA-CB	-7.39	99.25	110.12
1	A	39	LEU	CB-CA-C	-7.38	98.53	110.79
1	C	18	ARG	N-CA-CB	-7.38	99.28	110.12
1	C	39	LEU	CB-CA-C	-7.35	98.58	110.79
1	A	136	ALA	N-CA-C	7.27	120.26	111.82
1	D	89	HIS	CA-C-O	7.26	128.44	120.82
1	C	136	ALA	N-CA-C	7.25	120.22	111.82
1	B	89	HIS	CA-C-O	7.22	128.40	120.82
1	B	103	HIS	CA-C-N	7.19	130.25	120.54
1	B	103	HIS	C-N-CA	7.19	130.25	120.54
1	A	225	HIS	CA-CB-CG	7.18	120.98	113.80
1	C	225	HIS	CA-CB-CG	7.17	120.97	113.80
1	D	103	HIS	CA-C-N	7.17	130.22	120.54
1	D	103	HIS	C-N-CA	7.17	130.22	120.54
1	C	355	VAL	N-CA-CB	7.16	121.33	110.58
1	B	58	ALA	CA-C-N	7.16	129.75	120.44
1	B	58	ALA	C-N-CA	7.16	129.75	120.44
1	C	241	ARG	CA-C-O	7.15	128.19	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	ARG	NE-CZ-NH1	7.14	128.65	121.50
1	A	241	ARG	CA-C-O	7.14	128.19	119.97
1	B	140	HIS	CA-C-N	7.14	132.65	120.72
1	B	140	HIS	C-N-CA	7.14	132.65	120.72
1	D	58	ALA	CA-C-N	7.14	129.72	120.44
1	D	58	ALA	C-N-CA	7.14	129.72	120.44
1	C	61	VAL	N-CA-CB	7.14	119.39	110.47
1	D	140	HIS	CA-C-N	7.11	132.59	120.72
1	D	140	HIS	C-N-CA	7.11	132.59	120.72
1	C	112	LEU	N-CA-C	7.11	118.67	111.07
1	C	163	ARG	NE-CZ-NH1	7.10	128.60	121.50
1	A	112	LEU	N-CA-C	7.10	118.67	111.07
1	A	355	VAL	N-CA-CB	7.10	121.23	110.58
1	C	81	GLU	N-CA-C	7.09	119.01	111.28
1	B	17	PHE	CA-C-N	7.09	130.09	120.38
1	B	17	PHE	C-N-CA	7.09	130.09	120.38
1	C	187	ASP	CA-CB-CG	7.09	119.69	112.60
1	A	81	GLU	N-CA-C	7.06	118.98	111.28
1	D	94	HIS	CA-C-O	7.06	127.91	120.42
1	B	94	HIS	CA-C-O	7.05	127.89	120.42
1	A	167	ARG	CA-C-N	7.04	127.95	119.99
1	A	167	ARG	C-N-CA	7.04	127.95	119.99
1	A	187	ASP	CA-CB-CG	7.03	119.62	112.60
1	A	61	VAL	N-CA-CB	7.02	119.24	110.47
1	D	17	PHE	CA-C-N	7.01	129.98	120.38
1	D	17	PHE	C-N-CA	7.01	129.98	120.38
1	D	75	MET	O-C-N	-7.00	114.17	122.15
1	C	177	ILE	N-CA-CB	-6.97	101.76	110.47
1	D	224	LEU	O-C-N	-6.96	114.75	122.12
1	B	224	LEU	O-C-N	-6.95	114.75	122.12
1	A	163	ARG	NH1-CZ-NH2	-6.95	110.27	119.30
1	B	75	MET	O-C-N	-6.94	114.23	122.15
1	A	177	ILE	N-CA-CB	-6.93	101.80	110.47
1	C	150	GLN	CA-C-N	6.93	130.13	120.29
1	C	150	GLN	C-N-CA	6.93	130.13	120.29
1	C	167	ARG	CA-C-N	6.93	127.82	119.99
1	C	167	ARG	C-N-CA	6.93	127.82	119.99
1	A	150	GLN	CA-C-N	6.91	130.10	120.29
1	A	150	GLN	C-N-CA	6.91	130.10	120.29
1	C	218	LYS	O-C-N	-6.91	114.85	122.03
1	D	51	HIS	N-CA-CB	6.91	120.28	110.12
1	D	65	ASP	CA-C-N	6.90	129.53	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	65	ASP	C-N-CA	6.90	129.53	120.28
1	C	31	LEU	CA-C-N	6.88	129.50	120.28
1	C	31	LEU	C-N-CA	6.88	129.50	120.28
1	C	163	ARG	NH1-CZ-NH2	-6.87	110.36	119.30
1	A	218	LYS	O-C-N	-6.87	114.89	122.03
1	B	51	HIS	N-CA-CB	6.87	120.22	110.12
1	C	51	HIS	N-CA-C	6.86	118.83	111.36
1	B	229	LEU	CA-C-N	6.84	129.78	120.54
1	B	229	LEU	C-N-CA	6.84	129.78	120.54
1	A	51	HIS	N-CA-C	6.84	118.82	111.36
1	A	161	THR	CA-C-N	6.82	129.31	120.44
1	A	161	THR	C-N-CA	6.82	129.31	120.44
1	B	237	ASP	CA-CB-CG	-6.81	105.79	112.60
1	B	65	ASP	CA-C-N	6.80	129.40	120.28
1	B	65	ASP	C-N-CA	6.80	129.40	120.28
1	A	65	ASP	CA-C-N	6.80	129.95	120.29
1	A	65	ASP	C-N-CA	6.80	129.95	120.29
1	D	229	LEU	CA-C-N	6.80	129.72	120.54
1	D	229	LEU	C-N-CA	6.80	129.72	120.54
1	A	273	PHE	CA-CB-CG	-6.80	107.00	113.80
1	A	309	VAL	CA-C-N	6.79	129.69	120.38
1	A	309	VAL	C-N-CA	6.79	129.69	120.38
1	C	309	VAL	CA-C-N	6.79	129.69	120.38
1	C	309	VAL	C-N-CA	6.79	129.69	120.38
1	C	89	HIS	CE1-NE2-CD2	-6.79	102.21	109.00
1	D	72	PRO	N-CA-CB	-6.78	96.13	103.25
1	A	227	LEU	N-CA-C	6.78	119.24	111.11
1	B	303	ASP	N-CA-CB	-6.78	99.65	111.17
1	C	161	THR	CA-C-N	6.78	129.25	120.44
1	C	161	THR	C-N-CA	6.78	129.25	120.44
1	B	72	PRO	N-CA-CB	-6.77	96.14	103.25
1	D	303	ASP	N-CA-CB	-6.77	99.67	111.17
1	C	65	ASP	CA-C-N	6.76	129.90	120.29
1	C	65	ASP	C-N-CA	6.76	129.90	120.29
1	A	89	HIS	CE1-NE2-CD2	-6.76	102.24	109.00
1	D	237	ASP	CA-CB-CG	-6.75	105.85	112.60
1	C	273	PHE	CA-CB-CG	-6.73	107.07	113.80
1	A	149	ALA	N-CA-C	6.72	122.46	111.37
1	D	320	CYS	CA-C-O	-6.72	115.31	120.48
1	B	7	PHE	CA-CB-CG	6.71	120.51	113.80
1	C	233	ARG	N-CA-C	6.71	118.59	111.28
1	C	149	ALA	N-CA-C	6.71	122.44	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	137	ALA	CA-C-O	6.70	127.86	120.82
1	A	233	ARG	N-CA-C	6.70	118.58	111.28
1	C	227	LEU	N-CA-C	6.70	119.15	111.11
1	A	189	MET	CA-C-N	6.70	129.25	120.28
1	A	189	MET	C-N-CA	6.70	129.25	120.28
1	C	191	PHE	CA-CB-CG	-6.69	107.11	113.80
1	A	18	ARG	NE-CZ-NH2	-6.68	113.19	119.20
1	A	191	PHE	CA-CB-CG	-6.67	107.13	113.80
1	B	110	GLN	OE1-CD-NE2	-6.67	115.93	122.60
1	C	189	MET	CA-C-N	6.66	129.21	120.28
1	C	189	MET	C-N-CA	6.66	129.21	120.28
1	C	18	ARG	NE-CZ-NH2	-6.66	113.21	119.20
1	D	7	PHE	CA-CB-CG	6.65	120.45	113.80
1	B	127	PHE	N-CA-C	6.64	118.18	111.07
1	D	127	PHE	N-CA-C	6.64	118.18	111.07
1	B	292	SER	N-CA-C	6.63	120.31	111.30
1	A	137	ALA	CA-C-O	6.62	127.77	120.82
1	B	320	CYS	CA-C-O	-6.60	115.39	120.48
1	D	110	GLN	OE1-CD-NE2	-6.59	116.01	122.60
1	D	292	SER	N-CA-C	6.58	120.25	111.30
1	C	117	LEU	CA-C-N	6.58	129.34	120.65
1	C	117	LEU	C-N-CA	6.58	129.34	120.65
1	B	19	ALA	CA-C-O	6.58	127.55	119.79
1	C	108	GLN	CA-C-N	6.58	129.08	120.60
1	C	108	GLN	C-N-CA	6.58	129.08	120.60
1	D	209	GLU	N-CA-C	6.57	118.24	111.14
1	A	117	LEU	CA-C-N	6.57	129.32	120.65
1	A	117	LEU	C-N-CA	6.57	129.32	120.65
1	A	108	GLN	CA-C-N	6.56	129.07	120.60
1	A	108	GLN	C-N-CA	6.56	129.07	120.60
1	A	22	GLU	CA-C-N	6.55	129.06	120.28
1	A	22	GLU	C-N-CA	6.55	129.06	120.28
1	B	3	VAL	CB-CA-C	-6.55	104.38	111.59
1	D	19	ALA	CA-C-O	6.54	127.50	119.79
1	D	3	VAL	CB-CA-C	-6.52	104.42	111.59
1	B	258	SER	CA-C-N	6.51	131.59	122.41
1	B	258	SER	C-N-CA	6.51	131.59	122.41
1	D	356	GLN	N-CA-C	6.51	119.20	111.71
1	A	183	LYS	N-CA-C	6.51	118.37	111.28
1	C	22	GLU	CA-C-N	6.50	129.00	120.28
1	C	22	GLU	C-N-CA	6.50	129.00	120.28
1	B	209	GLU	N-CA-C	6.50	118.16	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	356	GLN	N-CA-C	6.50	119.19	111.71
1	C	183	LYS	N-CA-C	6.49	118.36	111.28
1	B	132	GLU	O-C-N	6.48	129.09	122.09
1	D	258	SER	CA-C-N	6.48	131.54	122.41
1	D	258	SER	C-N-CA	6.48	131.54	122.41
1	D	23	LEU	N-CA-CB	-6.47	100.33	110.30
1	B	23	LEU	N-CA-CB	-6.45	100.36	110.30
1	B	115	GLU	O-C-N	-6.44	115.86	121.85
1	A	298	GLN	CA-C-N	6.44	129.55	120.28
1	A	298	GLN	C-N-CA	6.44	129.55	120.28
1	C	298	GLN	CA-C-N	6.42	129.53	120.28
1	C	298	GLN	C-N-CA	6.42	129.53	120.28
1	D	132	GLU	O-C-N	6.42	129.03	122.09
1	A	125	ARG	CA-C-N	6.42	128.88	120.28
1	A	125	ARG	C-N-CA	6.42	128.88	120.28
1	D	115	GLU	O-C-N	-6.42	115.88	121.85
1	B	199	GLN	O-C-N	-6.41	115.32	122.12
1	D	199	GLN	O-C-N	-6.41	115.33	122.12
1	C	125	ARG	CA-C-N	6.40	128.86	120.28
1	C	125	ARG	C-N-CA	6.40	128.86	120.28
1	B	94	HIS	CE1-NE2-CD2	-6.40	102.60	109.00
1	D	94	HIS	CE1-NE2-CD2	-6.39	102.61	109.00
1	B	199	GLN	CA-C-O	6.39	127.32	120.55
1	A	120	PHE	O-C-N	-6.38	115.50	122.07
1	A	139	THR	CA-C-O	6.37	127.30	120.55
1	A	293	ASN	OD1-CG-ND2	-6.37	116.23	122.60
1	D	207	HIS	CE1-NE2-CD2	-6.36	102.64	109.00
1	A	31	LEU	CA-C-N	6.35	129.43	120.28
1	A	31	LEU	C-N-CA	6.35	129.43	120.28
1	B	353	SER	O-C-N	-6.34	114.93	122.15
1	C	139	THR	CA-C-O	6.33	127.26	120.55
1	D	353	SER	O-C-N	-6.33	114.94	122.15
1	C	120	PHE	O-C-N	-6.33	115.55	122.07
1	D	185	LYS	N-CA-C	6.33	117.84	111.07
1	D	199	GLN	CA-C-O	6.33	127.26	120.55
1	C	293	ASN	OD1-CG-ND2	-6.32	116.28	122.60
1	B	185	LYS	N-CA-C	6.32	117.83	111.07
1	B	207	HIS	CE1-NE2-CD2	-6.32	102.69	109.00
1	D	184	ARG	O-C-N	-6.31	115.43	122.12
1	D	225	HIS	O-C-N	-6.30	114.97	122.15
1	B	184	ARG	O-C-N	-6.28	115.47	122.12
1	C	7	PHE	CA-C-N	6.27	129.31	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	7	PHE	C-N-CA	6.27	129.31	120.28
1	A	306	THR	N-CA-C	6.26	119.69	109.24
1	B	225	HIS	O-C-N	-6.26	115.02	122.15
1	A	7	PHE	CA-C-N	6.25	129.27	120.28
1	A	7	PHE	C-N-CA	6.25	129.27	120.28
1	C	207	HIS	CG-CD2-NE2	6.24	113.44	107.20
1	D	153	GLU	CA-C-N	6.24	129.15	120.29
1	D	153	GLU	C-N-CA	6.24	129.15	120.29
1	A	275	ARG	O-C-N	-6.23	115.75	123.36
1	B	124	ARG	NE-CZ-NH2	-6.23	113.60	119.20
1	B	153	GLU	CA-C-N	6.22	129.13	120.29
1	B	153	GLU	C-N-CA	6.22	129.13	120.29
1	C	108	GLN	OE1-CD-NE2	-6.22	116.38	122.60
1	C	306	THR	N-CA-C	6.22	119.62	109.24
1	D	146	ARG	N-CA-C	6.21	118.85	111.33
1	D	2	THR	CA-C-N	6.21	129.83	120.95
1	D	2	THR	C-N-CA	6.21	129.83	120.95
1	B	146	ARG	N-CA-C	6.21	118.84	111.33
1	A	26	ALA	CA-C-O	6.20	126.99	120.42
1	C	21	ILE	N-CA-CB	6.20	118.21	110.47
1	A	21	ILE	N-CA-CB	6.19	118.21	110.47
1	C	26	ALA	CA-C-O	6.19	126.98	120.42
1	A	293	ASN	CB-CA-C	6.18	121.44	111.36
1	C	293	ASN	CB-CA-C	6.18	121.43	111.36
1	A	108	GLN	OE1-CD-NE2	-6.17	116.43	122.60
1	A	207	HIS	CG-CD2-NE2	6.16	113.36	107.20
1	B	2	THR	CA-C-N	6.15	129.75	120.95
1	B	2	THR	C-N-CA	6.15	129.75	120.95
1	C	275	ARG	O-C-N	-6.15	115.86	123.36
1	D	124	ARG	NE-CZ-NH2	-6.14	113.67	119.20
1	B	101	THR	O-C-N	-6.14	115.61	122.12
1	B	248	LYS	CA-C-O	6.14	126.95	119.64
1	A	201	THR	N-CA-CB	6.14	119.25	110.16
1	D	248	LYS	CA-C-O	6.13	126.94	119.64
1	D	101	THR	O-C-N	-6.12	115.63	122.12
1	B	145	PRO	CA-C-O	-6.12	114.65	121.32
1	D	145	PRO	CA-C-O	-6.12	114.66	121.32
1	C	24	VAL	CA-C-N	6.11	129.07	120.28
1	C	24	VAL	C-N-CA	6.11	129.07	120.28
1	A	24	VAL	CA-C-N	6.10	129.06	120.28
1	A	24	VAL	C-N-CA	6.10	129.06	120.28
1	A	330	GLU	O-C-N	-6.10	115.83	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	GLU	CA-C-N	6.09	131.43	121.87
1	A	261	GLU	C-N-CA	6.09	131.43	121.87
1	A	256	GLU	N-CA-CB	-6.09	100.53	109.90
1	D	52	TYR	CB-CA-C	6.09	120.52	110.90
1	C	201	THR	N-CA-CB	6.08	119.17	110.16
1	B	52	TYR	CB-CA-C	6.08	120.51	110.90
1	C	261	GLU	CA-C-N	6.08	131.42	121.87
1	C	261	GLU	C-N-CA	6.08	131.42	121.87
1	A	330	GLU	CB-CG-CD	6.08	122.93	112.60
1	C	330	GLU	O-C-N	-6.07	115.87	123.27
1	C	330	GLU	CB-CG-CD	6.05	122.89	112.60
1	C	48	SER	CA-C-N	6.05	126.66	119.94
1	C	48	SER	C-N-CA	6.05	126.66	119.94
1	B	354	ALA	O-C-N	-6.04	115.26	122.15
1	C	129	ARG	N-CA-C	6.03	118.65	111.71
1	D	354	ALA	O-C-N	-6.03	115.27	122.15
1	C	256	GLU	N-CA-CB	-6.02	100.62	109.90
1	A	129	ARG	N-CA-C	6.02	118.63	111.71
1	A	228	VAL	O-C-N	-6.01	116.02	121.91
1	C	137	ALA	O-C-N	-6.00	115.89	122.07
1	B	104	THR	CA-C-N	6.00	128.59	120.44
1	B	104	THR	C-N-CA	6.00	128.59	120.44
1	B	140	HIS	CA-CB-CG	6.00	119.80	113.80
1	B	186	PHE	CA-C-O	5.98	126.85	119.79
1	D	36	GLU	O-C-N	-5.98	114.92	122.27
1	A	217	ARG	N-CA-C	-5.98	104.67	111.07
1	D	336	LYS	O-C-N	-5.98	116.42	123.41
1	C	149	ALA	CB-CA-C	-5.98	100.82	110.74
1	D	53	LEU	O-C-N	-5.97	115.79	122.12
1	A	5	LEU	CA-C-O	-5.97	113.91	120.36
1	D	313	ARG	CA-C-O	5.97	126.72	119.31
1	A	48	SER	CA-C-N	5.97	126.57	119.94
1	A	48	SER	C-N-CA	5.97	126.57	119.94
1	A	149	ALA	CB-CA-C	-5.97	100.84	110.74
1	C	43	THR	N-CA-C	5.97	118.74	111.82
1	C	326	ARG	NE-CZ-NH2	-5.97	113.83	119.20
1	B	313	ARG	CA-C-O	5.96	126.70	119.31
1	D	140	HIS	CA-CB-CG	5.96	119.76	113.80
1	B	53	LEU	O-C-N	-5.95	115.81	122.12
1	D	186	PHE	CA-C-O	5.95	126.81	119.79
1	B	36	GLU	O-C-N	-5.95	114.95	122.27
1	B	336	LYS	O-C-N	-5.95	116.45	123.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	5	LEU	CA-C-O	-5.95	113.94	120.36
1	C	194	ARG	CB-CA-C	-5.95	100.74	110.85
1	C	224	LEU	O-C-N	-5.94	115.82	122.12
1	A	224	LEU	O-C-N	-5.93	115.83	122.12
1	C	217	ARG	N-CA-C	-5.93	104.73	111.07
1	D	104	THR	CA-C-N	5.93	128.50	120.44
1	D	104	THR	C-N-CA	5.93	128.50	120.44
1	A	137	ALA	O-C-N	-5.92	115.97	122.07
1	C	207	HIS	ND1-CE1-NE2	5.92	114.32	108.40
1	D	54	ALA	N-CA-C	5.91	117.73	111.28
1	B	269	GLU	N-CA-CB	5.91	121.71	111.13
1	A	194	ARG	CB-CA-C	-5.91	100.81	110.85
1	D	269	GLU	N-CA-CB	5.91	121.70	111.13
1	A	43	THR	N-CA-C	5.91	118.67	111.82
1	C	247	GLN	CA-C-N	-5.90	110.27	121.54
1	C	247	GLN	C-N-CA	-5.90	110.27	121.54
1	B	54	ALA	N-CA-C	5.90	117.71	111.28
1	A	247	GLN	CA-C-N	-5.90	110.27	121.54
1	A	247	GLN	C-N-CA	-5.90	110.27	121.54
1	A	320	CYS	O-C-N	-5.90	115.22	121.30
1	D	90	LYS	CB-CA-C	5.90	120.58	110.79
1	D	169	ARG	NH1-CZ-NH2	-5.90	111.63	119.30
1	C	228	VAL	O-C-N	-5.89	116.13	121.91
1	A	61	VAL	N-CA-C	5.88	117.32	110.62
1	C	174	ALA	N-CA-C	5.88	117.69	111.28
1	D	173	TYR	CB-CA-C	5.88	120.19	110.90
1	B	90	LYS	CB-CA-C	5.87	120.54	110.79
1	B	173	TYR	CB-CA-C	5.87	120.18	110.90
1	C	320	CYS	O-C-N	-5.87	115.25	121.30
1	C	153	GLU	CA-C-N	5.86	128.06	120.44
1	C	153	GLU	C-N-CA	5.86	128.06	120.44
1	A	326	ARG	NE-CZ-NH2	-5.86	113.93	119.20
1	D	110	GLN	O-C-N	5.86	128.33	122.12
1	D	84	THR	CA-C-O	-5.85	113.75	120.24
1	D	327	PHE	N-CA-C	-5.85	106.09	113.23
1	A	207	HIS	ND1-CE1-NE2	5.84	114.24	108.40
1	B	84	THR	CA-C-O	-5.84	113.75	120.24
1	B	133	SER	N-CA-C	5.84	117.65	111.28
1	B	169	ARG	NH1-CZ-NH2	-5.83	111.72	119.30
1	D	133	SER	N-CA-C	5.83	117.63	111.28
1	A	153	GLU	CA-C-N	5.83	128.01	120.44
1	A	153	GLU	C-N-CA	5.83	128.01	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	ALA	CA-C-O	5.82	126.59	120.42
1	B	110	GLN	O-C-N	5.81	128.28	122.12
1	B	313	ARG	N-CA-C	-5.81	105.68	112.89
1	A	112	LEU	O-C-N	-5.81	116.09	122.07
1	B	327	PHE	N-CA-C	-5.81	106.15	113.23
1	A	20	SER	N-CA-CB	5.80	118.75	110.16
1	D	100	ALA	CA-C-O	5.80	126.57	120.42
1	A	13	ASP	CB-CA-C	5.79	119.62	111.86
1	B	74	PRO	N-CA-C	5.79	124.41	112.47
1	C	20	SER	N-CA-CB	5.79	118.73	110.16
1	A	243	VAL	N-CA-CB	5.79	117.32	110.55
1	D	313	ARG	N-CA-C	-5.79	105.72	112.89
1	C	13	ASP	CB-CA-C	5.78	119.61	111.86
1	C	72	PRO	CA-N-CD	5.78	120.09	112.00
1	A	211	SER	CA-C-N	5.78	128.02	120.28
1	A	211	SER	C-N-CA	5.78	128.02	120.28
1	A	70	GLY	N-CA-C	5.78	119.22	112.23
1	B	334	THR	N-CA-C	5.78	118.04	111.11
1	D	135	GLU	CA-C-N	5.77	127.95	120.44
1	D	135	GLU	C-N-CA	5.77	127.95	120.44
1	C	-2	LEU	N-CA-CB	-5.77	101.90	110.61
1	A	72	PRO	CA-N-CD	5.77	120.07	112.00
1	B	313	ARG	N-CA-CB	-5.77	101.00	110.40
1	A	-2	LEU	N-CA-CB	-5.76	101.91	110.61
1	C	61	VAL	N-CA-C	5.76	117.19	110.62
1	D	74	PRO	N-CA-C	5.76	124.34	112.47
1	B	68	ARG	NH1-CZ-NH2	-5.76	111.81	119.30
1	C	70	GLY	N-CA-C	5.76	119.20	112.23
1	C	243	VAL	N-CA-CB	5.76	117.29	110.55
1	D	89	HIS	CG-CD2-NE2	5.75	112.95	107.20
1	A	241	ARG	N-CA-C	5.75	118.49	111.82
1	C	343	ASP	O-C-N	-5.75	114.03	122.43
1	B	89	HIS	CG-CD2-NE2	5.75	112.95	107.20
1	D	50	ARG	N-CA-C	5.75	118.48	111.82
1	A	343	ASP	O-C-N	-5.74	114.04	122.43
1	C	187	ASP	CA-C-O	5.74	126.85	120.82
1	B	288	PHE	CD1-CG-CD2	5.74	127.21	118.60
1	D	313	ARG	N-CA-CB	-5.74	101.04	110.40
1	C	211	SER	CA-C-N	5.74	127.97	120.28
1	C	211	SER	C-N-CA	5.74	127.97	120.28
1	A	174	ALA	N-CA-C	5.74	117.53	111.28
1	D	334	THR	N-CA-C	5.72	117.98	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	ASP	N-CA-C	5.72	117.52	111.28
1	C	241	ARG	N-CA-C	5.72	118.46	111.82
1	B	135	GLU	CA-C-N	5.72	127.88	120.44
1	B	135	GLU	C-N-CA	5.72	127.88	120.44
1	B	313	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	D	92	ASP	N-CA-C	5.71	117.51	111.28
1	A	357	SER	O-C-N	-5.71	116.15	122.09
1	B	99	ASP	CA-CB-CG	-5.71	106.89	112.60
1	D	54	ALA	CA-C-N	5.70	128.24	120.54
1	D	54	ALA	C-N-CA	5.70	128.24	120.54
1	B	50	ARG	N-CA-C	5.70	118.43	111.82
1	B	186	PHE	CB-CG-CD2	-5.70	111.01	120.70
1	D	288	PHE	CD1-CG-CD2	5.70	127.15	118.60
1	D	313	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	D	323	SER	N-CA-C	5.69	118.09	110.35
1	D	186	PHE	CB-CG-CD2	-5.69	111.03	120.70
1	D	68	ARG	NH1-CZ-NH2	-5.68	111.91	119.30
1	C	68	ARG	N-CA-CB	5.68	118.47	110.12
1	D	99	ASP	CA-CB-CG	-5.68	106.92	112.60
1	C	145	PRO	O-C-N	-5.67	115.92	123.06
1	A	257	PRO	O-C-N	5.67	129.53	123.01
1	C	112	LEU	O-C-N	-5.66	116.24	122.07
1	C	257	PRO	O-C-N	5.66	129.52	123.01
1	A	187	ASP	CA-C-O	5.65	126.75	120.82
1	C	46	LEU	CA-C-N	5.65	127.79	120.44
1	C	46	LEU	C-N-CA	5.65	127.79	120.44
1	C	357	SER	O-C-N	-5.65	116.21	122.09
1	B	54	ALA	CA-C-N	5.65	128.16	120.54
1	B	54	ALA	C-N-CA	5.65	128.16	120.54
1	B	88	ASN	CA-CB-CG	-5.64	106.96	112.60
1	C	258	SER	N-CA-C	5.64	117.85	108.20
1	A	68	ARG	N-CA-CB	5.64	118.41	110.12
1	A	258	SER	N-CA-C	5.64	117.84	108.20
1	B	124	ARG	N-CA-C	5.64	117.10	111.07
1	D	24	VAL	O-C-N	-5.63	115.43	121.80
1	B	323	SER	N-CA-C	5.63	118.01	110.35
1	A	145	PRO	O-C-N	-5.63	115.97	123.06
1	B	159	LEU	CA-C-N	5.63	128.13	120.54
1	B	159	LEU	C-N-CA	5.63	128.13	120.54
1	C	169	ARG	NE-CZ-NH1	-5.63	115.87	121.50
1	D	124	ARG	N-CA-C	5.62	117.08	111.07
1	A	67	ALA	CA-C-O	-5.62	114.92	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	293	ASN	CA-CB-CG	-5.61	106.99	112.60
1	D	89	HIS	CE1-NE2-CD2	-5.61	103.39	109.00
1	D	293	ASN	CA-CB-CG	-5.61	106.99	112.60
1	D	159	LEU	CA-C-N	5.61	128.11	120.54
1	D	159	LEU	C-N-CA	5.61	128.11	120.54
1	A	46	LEU	CA-C-N	5.61	127.73	120.44
1	A	46	LEU	C-N-CA	5.61	127.73	120.44
1	C	288	PHE	N-CA-CB	5.61	119.31	110.56
1	C	63	ILE	CB-CA-C	-5.60	104.58	112.14
1	C	290	ILE	CB-CA-C	-5.60	103.31	110.98
1	A	63	ILE	CB-CA-C	-5.60	104.58	112.14
1	C	210	LEU	CB-CA-C	5.60	120.03	110.74
1	D	88	ASN	CA-CB-CG	-5.59	107.01	112.60
1	C	67	ALA	CA-C-O	-5.58	114.96	120.82
1	A	292	SER	CA-C-O	5.58	127.92	121.28
1	B	49	GLY	N-CA-C	-5.58	106.03	112.50
1	C	358	SER	CA-C-N	5.58	128.10	120.46
1	C	358	SER	C-N-CA	5.58	128.10	120.46
1	B	199	GLN	OE1-CD-NE2	-5.58	117.02	122.60
1	D	108	GLN	O-C-N	-5.58	115.61	122.19
1	B	89	HIS	CE1-NE2-CD2	-5.57	103.43	109.00
1	B	186	PHE	N-CA-C	5.57	119.25	112.23
1	A	288	PHE	N-CA-CB	5.57	119.25	110.56
1	B	24	VAL	O-C-N	-5.57	115.51	121.80
1	C	291	GLN	N-CA-CB	5.57	120.16	110.81
1	C	-1	GLY	N-CA-C	5.56	118.33	111.93
1	B	303	ASP	CA-C-N	5.56	126.79	119.84
1	B	303	ASP	C-N-CA	5.56	126.79	119.84
1	D	49	GLY	N-CA-C	-5.56	106.05	112.50
1	D	199	GLN	OE1-CD-NE2	-5.56	117.04	122.60
1	A	89	HIS	CA-CB-CG	5.56	119.36	113.80
1	A	210	LEU	CB-CA-C	5.55	119.96	110.74
1	A	290	ILE	CB-CA-C	-5.55	103.37	110.98
1	A	358	SER	CA-C-N	5.55	128.07	120.46
1	A	358	SER	C-N-CA	5.55	128.07	120.46
1	A	-1	GLY	N-CA-C	5.55	118.31	111.93
1	B	319	LEU	CB-CA-C	-5.54	100.83	110.09
1	D	37	LYS	O-C-N	-5.54	116.36	122.07
1	C	98	LEU	N-CA-CB	5.54	118.36	110.16
1	C	292	SER	CA-C-O	5.54	127.87	121.28
1	D	319	LEU	CB-CA-C	-5.54	100.84	110.09
1	A	291	GLN	N-CA-CB	5.54	120.11	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	186	PHE	N-CA-C	5.53	119.20	112.23
1	D	303	ASP	CA-C-N	5.53	126.75	119.84
1	D	303	ASP	C-N-CA	5.53	126.75	119.84
1	C	89	HIS	CA-CB-CG	5.52	119.32	113.80
1	A	98	LEU	N-CA-CB	5.52	118.33	110.16
1	B	127	PHE	CA-C-N	5.52	128.13	120.29
1	B	127	PHE	C-N-CA	5.52	128.13	120.29
1	B	132	GLU	CB-CG-CD	-5.52	103.22	112.60
1	B	108	GLN	O-C-N	-5.52	115.68	122.19
1	D	127	PHE	CA-C-N	5.51	128.12	120.29
1	D	127	PHE	C-N-CA	5.51	128.12	120.29
1	A	57	ARG	NE-CZ-NH2	-5.50	114.25	119.20
1	A	51	HIS	CA-C-O	-5.49	114.60	120.42
1	D	132	GLU	CB-CG-CD	-5.49	103.26	112.60
1	C	38	LEU	O-C-N	-5.49	115.90	122.15
1	B	160	ARG	CA-C-O	5.48	126.77	120.90
1	D	94	HIS	O-C-N	-5.48	115.90	122.15
1	A	169	ARG	NE-CZ-NH1	-5.48	116.02	121.50
1	B	94	HIS	O-C-N	-5.48	115.91	122.15
1	D	160	ARG	CA-C-O	5.48	126.76	120.90
1	A	226	GLN	N-CA-CB	-5.47	102.06	110.16
1	B	37	LYS	O-C-N	-5.46	116.44	122.07
1	D	60	VAL	O-C-N	-5.46	115.63	121.80
1	A	38	LEU	O-C-N	-5.46	115.93	122.15
1	C	57	ARG	NE-CZ-NH2	-5.45	114.29	119.20
1	C	363	PHE	O-C-N	5.45	129.98	122.46
1	C	51	HIS	CA-C-O	-5.45	114.64	120.42
1	C	226	GLN	N-CA-CB	-5.44	102.18	110.07
1	A	83	PHE	N-CA-CB	5.44	117.90	110.01
1	B	66	LEU	CA-C-O	5.44	126.32	120.55
1	C	83	PHE	N-CA-CB	5.44	117.90	110.01
1	A	363	PHE	O-C-N	5.43	129.96	122.46
1	B	60	VAL	O-C-N	-5.42	115.68	121.80
1	A	230	ASN	CA-C-N	5.41	127.97	120.29
1	A	230	ASN	C-N-CA	5.41	127.97	120.29
1	B	329	PHE	CA-CB-CG	5.41	119.21	113.80
1	B	354	ALA	CA-C-O	5.41	126.15	120.42
1	D	344	SER	CA-C-N	5.40	127.95	120.29
1	D	344	SER	C-N-CA	5.40	127.95	120.29
1	D	66	LEU	CA-C-O	5.39	126.27	120.55
1	A	343	ASP	CA-C-O	5.39	126.01	119.11
1	A	123	ALA	CA-C-N	5.38	127.50	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	ALA	C-N-CA	5.38	127.50	120.28
1	B	152	ALA	N-CA-C	5.38	117.15	111.28
1	A	312	LEU	N-CA-CB	-5.38	102.78	110.80
1	D	329	PHE	CA-CB-CG	5.38	119.18	113.80
1	D	359	ILE	CB-CA-C	-5.38	103.82	112.16
1	A	17	PHE	CA-CB-CG	-5.38	108.42	113.80
1	C	17	PHE	CA-CB-CG	-5.38	108.42	113.80
1	B	249	GLU	O-C-N	-5.37	115.69	122.19
1	B	359	ILE	CB-CA-C	-5.37	103.83	112.16
1	B	213	LEU	CA-C-N	5.37	127.48	120.28
1	B	213	LEU	C-N-CA	5.37	127.48	120.28
1	B	101	THR	CA-C-N	5.37	127.42	120.44
1	B	101	THR	C-N-CA	5.37	127.42	120.44
1	C	343	ASP	CA-C-O	5.36	125.97	119.11
1	D	213	LEU	CA-C-N	5.36	127.47	120.28
1	D	213	LEU	C-N-CA	5.36	127.47	120.28
1	B	115	GLU	CA-C-O	5.36	125.67	118.38
1	D	65	ASP	CA-CB-CG	-5.36	107.24	112.60
1	C	230	ASN	CA-C-N	5.36	127.90	120.29
1	C	230	ASN	C-N-CA	5.36	127.90	120.29
1	B	23	LEU	O-C-N	-5.36	115.15	122.33
1	C	12	LYS	CA-C-N	5.36	129.79	122.34
1	C	12	LYS	C-N-CA	5.36	129.79	122.34
1	D	354	ALA	CA-C-O	5.36	126.10	120.42
1	A	101	THR	CA-C-N	5.36	127.40	120.44
1	A	101	THR	C-N-CA	5.36	127.40	120.44
1	A	162	ALA	O-C-N	5.36	127.59	122.07
1	D	101	THR	CA-C-N	5.35	127.40	120.44
1	D	101	THR	C-N-CA	5.35	127.40	120.44
1	D	152	ALA	N-CA-C	5.35	117.11	111.28
1	D	203	PHE	N-CA-C	5.35	117.11	111.28
1	B	344	SER	CA-C-N	5.35	127.88	120.29
1	B	344	SER	C-N-CA	5.35	127.88	120.29
1	D	6	ASP	CA-C-N	5.34	130.49	121.14
1	D	6	ASP	C-N-CA	5.34	130.49	121.14
1	D	115	GLU	CA-C-O	5.34	125.65	118.38
1	B	221	GLY	CA-C-N	5.34	127.88	120.29
1	B	221	GLY	C-N-CA	5.34	127.88	120.29
1	A	158	ALA	O-C-N	-5.34	116.46	122.12
1	C	162	ALA	O-C-N	5.34	127.57	122.07
1	B	237	ASP	N-CA-CB	-5.33	102.28	110.12
1	C	123	ALA	CA-C-N	5.33	127.43	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	123	ALA	C-N-CA	5.33	127.43	120.28
1	A	97	LEU	O-C-N	-5.33	116.47	122.12
1	B	6	ASP	CA-C-N	5.33	130.47	121.14
1	B	6	ASP	C-N-CA	5.33	130.47	121.14
1	D	145	PRO	CA-C-N	5.33	127.68	120.38
1	D	145	PRO	C-N-CA	5.33	127.68	120.38
1	D	237	ASP	N-CA-CB	-5.33	102.29	110.12
1	A	12	LYS	CA-C-N	5.33	129.74	122.34
1	A	12	LYS	C-N-CA	5.33	129.74	122.34
1	C	97	LEU	O-C-N	-5.33	116.48	122.12
1	D	230	ASN	CA-C-O	5.33	126.60	120.90
1	A	191	PHE	N-CA-C	-5.32	105.39	111.14
1	D	249	GLU	O-C-N	-5.32	115.75	122.19
1	C	101	THR	CA-CB-OG1	5.32	117.58	109.60
1	A	101	THR	CA-CB-OG1	5.32	117.58	109.60
1	B	230	ASN	CA-C-O	5.32	126.59	120.90
1	C	101	THR	CA-C-N	5.32	127.35	120.44
1	C	101	THR	C-N-CA	5.32	127.35	120.44
1	C	158	ALA	O-C-N	-5.32	116.48	122.12
1	C	308	VAL	N-CA-C	-5.32	105.35	110.72
1	A	142	ALA	CA-C-O	-5.32	114.34	120.24
1	B	162	ALA	CA-C-O	-5.32	114.89	120.63
1	B	65	ASP	CA-CB-CG	-5.31	107.29	112.60
1	B	203	PHE	N-CA-C	5.31	117.07	111.28
1	C	191	PHE	N-CA-C	-5.31	105.41	111.14
1	D	221	GLY	CA-C-N	5.31	127.83	120.29
1	D	221	GLY	C-N-CA	5.31	127.83	120.29
1	C	142	ALA	CA-C-O	-5.30	114.35	120.24
1	D	10	CYS	N-CA-C	5.30	117.06	111.28
1	D	23	LEU	O-C-N	-5.30	115.23	122.33
1	C	312	LEU	N-CA-CB	-5.30	102.91	110.80
1	A	113	VAL	CA-C-N	5.30	127.64	120.44
1	A	113	VAL	C-N-CA	5.30	127.64	120.44
1	B	145	PRO	CA-C-N	5.30	127.64	120.38
1	B	145	PRO	C-N-CA	5.30	127.64	120.38
1	C	56	SER	O-C-N	-5.30	116.61	122.07
1	C	62	GLY	CA-C-N	5.29	127.71	120.46
1	C	62	GLY	C-N-CA	5.29	127.71	120.46
1	D	13	ASP	N-CA-CB	-5.29	103.87	111.91
1	B	10	CYS	N-CA-C	5.29	117.04	111.28
1	B	13	ASP	N-CA-CB	-5.29	103.88	111.91
1	B	90	LYS	N-CA-C	5.29	117.04	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	VAL	CA-C-O	-5.29	114.54	120.25
1	D	162	ALA	CA-C-O	-5.29	114.92	120.63
1	A	309	VAL	CA-C-O	-5.28	114.95	120.76
1	B	119	GLY	CA-C-O	5.28	125.74	120.09
1	C	212	ARG	O-C-N	-5.28	116.52	122.12
1	D	228	VAL	CA-C-O	-5.28	114.55	120.25
1	A	308	VAL	N-CA-C	-5.28	105.39	110.72
1	A	225	HIS	O-C-N	-5.27	115.78	122.27
1	D	139	THR	CA-C-O	5.27	126.14	120.55
1	A	62	GLY	CA-C-N	5.26	127.67	120.46
1	A	62	GLY	C-N-CA	5.26	127.67	120.46
1	C	225	HIS	O-C-N	-5.26	115.81	122.27
1	B	139	THR	CA-C-O	5.25	126.11	120.55
1	C	32	GLU	N-CA-C	5.25	117.00	111.28
1	C	50	ARG	CG-CD-NE	-5.25	100.45	112.00
1	C	75	MET	N-CA-C	-5.25	105.62	112.23
1	D	204	GLN	CA-C-O	5.25	126.33	120.82
1	D	347	LEU	N-CA-C	5.25	117.91	111.82
1	D	199	GLN	CB-CG-CD	-5.25	103.68	112.60
1	A	131	ALA	CA-C-N	5.24	127.26	120.44
1	A	131	ALA	C-N-CA	5.24	127.26	120.44
1	A	56	SER	O-C-N	-5.24	116.67	122.07
1	D	61	VAL	O-C-N	-5.24	116.79	121.87
1	B	199	GLN	CB-CG-CD	-5.24	103.69	112.60
1	A	50	ARG	CG-CD-NE	-5.24	100.48	112.00
1	B	103	HIS	CB-CG-CD2	5.24	138.01	131.20
1	A	212	ARG	O-C-N	-5.24	116.57	122.12
1	D	90	LYS	N-CA-C	5.23	116.98	111.28
1	A	75	MET	N-CA-C	-5.23	105.64	112.23
1	B	21	ILE	CA-CB-CG1	5.23	119.29	110.40
1	D	21	ILE	CA-CB-CG1	5.23	119.29	110.40
1	D	349	GLN	OE1-CD-NE2	-5.23	117.37	122.60
1	D	296	VAL	CA-CB-CG2	5.23	119.29	110.40
1	A	173	TYR	CA-C-N	5.22	127.28	120.28
1	A	173	TYR	C-N-CA	5.22	127.28	120.28
1	D	103	HIS	CB-CG-CD2	5.22	137.99	131.20
1	B	347	LEU	N-CA-C	5.22	117.87	111.82
1	A	250	LEU	CA-C-N	5.22	131.63	121.41
1	A	250	LEU	C-N-CA	5.22	131.63	121.41
1	D	129	ARG	N-CA-CB	5.22	117.71	109.94
1	B	129	ARG	N-CA-CB	5.21	117.71	109.94
1	C	309	VAL	CA-C-O	-5.21	115.02	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	296	VAL	CA-CB-CG2	5.21	119.25	110.40
1	C	173	TYR	CA-C-N	5.20	127.25	120.28
1	C	173	TYR	C-N-CA	5.20	127.25	120.28
1	A	303	ASP	N-CA-CB	-5.20	103.27	110.29
1	B	61	VAL	O-C-N	-5.20	116.83	121.87
1	A	53	LEU	N-CA-C	5.20	118.78	112.23
1	B	106	GLN	OE1-CD-NE2	-5.20	117.41	122.60
1	C	303	ASP	N-CA-CB	-5.20	103.28	110.29
1	A	179	VAL	CB-CA-C	-5.19	105.13	112.14
1	D	119	GLY	CA-C-O	5.19	125.65	120.09
1	A	108	GLN	CB-CG-CD	5.18	121.41	112.60
1	C	53	LEU	N-CA-C	5.18	118.76	112.23
1	C	250	LEU	CA-C-N	5.18	131.56	121.41
1	C	250	LEU	C-N-CA	5.18	131.56	121.41
1	B	117	LEU	CA-C-N	5.18	127.64	120.29
1	B	117	LEU	C-N-CA	5.18	127.64	120.29
1	C	333	SER	O-C-N	5.18	128.53	122.99
1	D	117	LEU	CA-C-N	5.18	127.65	120.29
1	D	117	LEU	C-N-CA	5.18	127.65	120.29
1	A	212	ARG	N-CA-CB	5.17	117.73	110.12
1	C	179	VAL	CB-CA-C	-5.17	105.16	112.14
1	A	154	GLU	N-CA-CB	-5.17	102.52	110.01
1	A	128	TRP	CD2-CE2-CZ2	-5.16	117.24	122.40
1	C	108	GLN	CB-CG-CD	5.16	121.38	112.60
1	B	293	ASN	OD1-CG-ND2	5.16	127.76	122.60
1	C	2	THR	N-CA-CB	5.16	117.49	110.01
1	C	39	LEU	CA-C-N	5.16	127.45	120.44
1	C	39	LEU	C-N-CA	5.16	127.45	120.44
1	B	204	GLN	CA-C-O	5.16	126.23	120.82
1	C	113	VAL	CA-C-N	5.16	127.64	120.63
1	C	113	VAL	C-N-CA	5.16	127.64	120.63
1	C	128	TRP	CD2-CE2-CZ2	-5.16	117.24	122.40
1	D	106	GLN	N-CA-C	5.16	116.90	111.28
1	C	212	ARG	N-CA-CB	5.15	117.70	110.12
1	A	48	SER	CA-CB-OG	5.15	121.39	111.10
1	C	48	SER	CA-CB-OG	5.14	121.39	111.10
1	B	349	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	D	325	ARG	CA-CB-CG	5.14	124.39	114.10
1	A	341	GLN	O-C-N	-5.13	117.12	123.33
1	D	108	GLN	CA-C-O	5.13	128.02	120.42
1	D	106	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	B	106	GLN	N-CA-C	5.13	116.87	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	THR	CA-C-N	5.13	128.04	120.91
1	B	306	THR	C-N-CA	5.13	128.04	120.91
1	C	154	GLU	N-CA-CB	-5.13	102.57	110.01
1	D	244	LEU	CA-C-N	5.13	127.11	120.44
1	D	244	LEU	C-N-CA	5.13	127.11	120.44
1	D	359	ILE	CA-CB-CG2	5.13	119.22	110.50
1	A	2	THR	N-CA-CB	5.12	117.44	110.01
1	A	124	ARG	NE-CZ-NH2	-5.12	114.59	119.20
1	A	314	LEU	CB-CA-C	-5.12	102.77	111.02
1	B	359	ILE	CA-CB-CG2	5.12	119.21	110.50
1	C	169	ARG	CA-C-N	5.12	127.41	120.44
1	C	169	ARG	C-N-CA	5.12	127.41	120.44
1	A	39	LEU	CA-C-N	5.12	127.40	120.44
1	A	39	LEU	C-N-CA	5.12	127.40	120.44
1	B	325	ARG	CA-CB-CG	5.12	124.33	114.10
1	B	131	ALA	N-CA-CB	-5.12	102.06	110.40
1	D	203	PHE	CB-CA-C	-5.11	102.30	110.79
1	D	293	ASN	OD1-CG-ND2	5.11	127.71	122.60
1	B	244	LEU	CA-C-N	5.11	127.08	120.44
1	B	244	LEU	C-N-CA	5.11	127.08	120.44
1	B	360	ALA	N-CA-C	5.11	119.23	113.15
1	A	169	ARG	CA-C-N	5.11	127.39	120.44
1	A	169	ARG	C-N-CA	5.11	127.39	120.44
1	D	360	ALA	N-CA-C	5.11	119.23	113.15
1	D	37	LYS	CA-C-N	5.10	127.11	120.28
1	D	37	LYS	C-N-CA	5.10	127.11	120.28
1	B	108	GLN	CA-C-O	5.10	127.97	120.42
1	A	22	GLU	N-CA-C	5.09	116.91	111.36
1	C	131	ALA	CA-C-N	5.09	127.06	120.44
1	C	131	ALA	C-N-CA	5.09	127.06	120.44
1	A	30	GLU	N-CA-C	5.09	116.52	111.07
1	C	22	GLU	N-CA-C	5.09	116.91	111.36
1	A	170	ALA	N-CA-CB	5.09	117.45	110.07
1	A	95	ALA	CA-C-N	5.09	127.10	120.28
1	A	95	ALA	C-N-CA	5.09	127.10	120.28
1	C	314	LEU	CB-CA-C	-5.08	102.83	111.02
1	A	333	SER	O-C-N	5.08	128.42	122.99
1	B	203	PHE	CB-CA-C	-5.07	102.37	110.79
1	C	41	LEU	CA-C-N	5.07	125.47	119.94
1	C	41	LEU	C-N-CA	5.07	125.47	119.94
1	D	223	GLN	O-C-N	-5.07	116.75	122.12
1	B	315	CYS	O-C-N	5.07	128.62	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	SER	CA-C-N	5.07	127.07	120.28
1	B	357	SER	C-N-CA	5.07	127.07	120.28
1	C	30	GLU	N-CA-C	5.07	116.49	111.07
1	C	38	LEU	CB-CA-C	5.07	119.47	110.85
1	A	155	ALA	N-CA-C	5.07	116.88	111.36
1	D	131	ALA	N-CA-CB	-5.07	102.14	110.40
1	C	174	ALA	N-CA-CB	-5.06	102.68	110.12
1	A	41	LEU	CA-C-N	5.06	125.45	119.94
1	A	41	LEU	C-N-CA	5.06	125.45	119.94
1	C	124	ARG	NE-CZ-NH2	-5.05	114.65	119.20
1	A	174	ALA	N-CA-CB	-5.05	102.69	110.12
1	C	170	ALA	N-CA-CB	5.05	117.39	110.07
1	C	341	GLN	O-C-N	-5.05	117.22	123.33
1	A	38	LEU	CB-CA-C	5.04	119.42	110.85
1	D	315	CYS	O-C-N	5.04	128.59	122.94
1	C	217	ARG	NE-CZ-NH1	5.04	126.54	121.50
1	D	39	LEU	N-CA-C	5.04	117.17	111.02
1	D	50	ARG	CG-CD-NE	-5.04	100.92	112.00
1	C	95	ALA	CA-C-N	5.04	127.03	120.28
1	C	95	ALA	C-N-CA	5.04	127.03	120.28
1	C	223	GLN	CA-C-O	-5.03	115.08	120.42
1	D	83	PHE	O-C-N	-5.03	116.41	122.15
1	B	296	VAL	N-CA-CB	-5.03	104.02	112.47
1	A	103	HIS	CA-C-O	5.03	126.10	120.82
1	B	50	ARG	CG-CD-NE	-5.03	100.94	112.00
1	D	288	PHE	CB-CG-CD1	-5.03	112.15	120.70
1	D	306	THR	CA-C-N	5.03	127.90	120.91
1	D	306	THR	C-N-CA	5.03	127.90	120.91
1	D	296	VAL	N-CA-CB	-5.03	104.03	112.47
1	B	168	GLY	CA-C-N	5.02	127.42	120.29
1	B	168	GLY	C-N-CA	5.02	127.42	120.29
1	A	217	ARG	NE-CZ-NH1	5.02	126.52	121.50
1	B	288	PHE	CB-CG-CD1	-5.02	112.17	120.70
1	C	155	ALA	N-CA-C	5.02	116.83	111.36
1	B	37	LYS	CA-C-N	5.02	127.00	120.28
1	B	37	LYS	C-N-CA	5.02	127.00	120.28
1	B	120	PHE	O-C-N	-5.02	116.80	122.12
1	B	83	PHE	O-C-N	-5.02	116.43	122.15
1	D	168	GLY	CA-C-N	5.01	127.41	120.29
1	D	168	GLY	C-N-CA	5.01	127.41	120.29
1	C	231	SER	N-CA-CB	-5.01	102.74	110.16
1	D	357	SER	CA-C-N	5.01	126.99	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	357	SER	C-N-CA	5.01	126.99	120.28
1	C	110	GLN	CB-CG-CD	5.01	121.11	112.60
1	B	91	LEU	N-CA-CB	5.00	117.26	110.01
1	B	308	VAL	N-CA-C	-5.00	107.85	111.90

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
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

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Mol	Chain	Res	Type	Group
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 ⓘ

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	2956	13	0
1	B	2900	0	2921	23	0
1	C	2941	0	2957	12	0
1	D	2900	0	2921	21	0
All	All	11682	0	11755	42	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 (42) 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:B:236:ARG:NH2	1:D:247:GLN:HB2	1.33	1.39
1:B:236:ARG:NH2	1:D:247:GLN:CB	1.92	1.30
1:B:236:ARG:HH21	1:D:247:GLN:CA	1.48	1.27
1:B:247:GLN:HB2	1:D:236:ARG:NH2	1.49	1.27
1:B:247:GLN:CA	1:D:236:ARG:HH21	1.57	1.17
1:B:236:ARG:HH21	1:D:247:GLN:HA	1.02	1.15
1:B:247:GLN:CB	1:D:236:ARG:NH2	2.09	1.15
1:B:247:GLN:HA	1:D:236:ARG:HH21	1.06	1.10
1:B:247:GLN:CA	1:D:236:ARG:NH2	2.25	0.98
1:B:236:ARG:NH2	1:D:247:GLN:CA	2.18	0.96
1:B:247:GLN:HB2	1:D:236:ARG:HH22	1.28	0.87
1:B:236:ARG:HH22	1:D:247:GLN:HB2	1.09	0.86
1:B:247:GLN:HA	1:D:236:ARG:NH2	1.91	0.83
1:B:236:ARG:NH2	1:D:247:GLN:HA	1.88	0.83
1:A:122:GLU:OE1	1:C:122:GLU:OE1	2.16	0.64
1:B:236:ARG:NH2	1:D:247:GLN:CG	2.67	0.54
1:A:125:ARG:NH2	1:C:125:ARG:NH2	2.57	0.52
1:A:129:ARG:CD	1:C:118:ARG:NE	2.72	0.51
1:A:239:GLU:O	1:A:243:VAL:HG23	2.12	0.49
1:C:229:LEU:HD21	1:C:233:ARG:NH2	2.27	0.49
1:C:239:GLU:O	1:C:243:VAL:HG23	2.12	0.49
1:A:229:LEU:HD21	1:A:233:ARG:NH2	2.28	0.48
1:B:236:ARG:HH21	1:D:247:GLN:CB	1.76	0.47
1:C:32:GLU:CD	1:C:121:ARG:HH12	2.23	0.47
1:A:32:GLU:CD	1:A:121:ARG:HH12	2.23	0.46
1:C:143:GLU:CD	1:D:325:ARG:HH12	2.24	0.45
1:A:143:GLU:CD	1:B:325:ARG:HH12	2.24	0.45
1:A:129:ARG:HD2	1:C:118:ARG:HE	1.82	0.45
1:B:247:GLN:N	1:D:236:ARG:NH2	2.64	0.45
1:A:213:LEU:HD21	1:B:196:VAL:HG13	2.00	0.44
1:C:213:LEU:HD21	1:D:196:VAL:HG13	1.99	0.43
1:B:207:HIS:CE1	1:B:211:SER:HB2	2.54	0.43
1:D:207:HIS:CE1	1:D:211:SER:HB2	2.54	0.42
1:B:236:ARG:CZ	1:D:247:GLN:HG3	2.50	0.42
1:A:289:THR:O	1:A:296:VAL:HG22	2.20	0.42
1:A:94:HIS:O	1:A:97:LEU:HB3	2.20	0.42
1:C:289:THR:O	1:C:296:VAL:HG22	2.20	0.41
1:A:348:LEU:HD13	1:A:348:LEU:C	2.46	0.41
1:B:286:ARG:HD3	1:B:286:ARG:HA	1.96	0.41
1:C:348:LEU:HD13	1:C:348:LEU:C	2.46	0.41
1:A:324:GLU:O	1:B:145:PRO:HA	2.22	0.40
1:C:94:HIS:O	1:C:97:LEU:HB3	2.20	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%)	36	72
1	B	361/382 (94%)	347 (96%)	11 (3%)	3 (1%)	16	54
1	C	367/382 (96%)	354 (96%)	12 (3%)	1 (0%)	36	72
1	D	361/382 (94%)	347 (96%)	11 (3%)	3 (1%)	16	54
All	All	1456/1528 (95%)	1402 (96%)	46 (3%)	8 (0%)	26	63

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%)	45	64
1	B	311/325 (96%)	305 (98%)	6 (2%)	50	67
1	C	315/325 (97%)	308 (98%)	7 (2%)	45	64
1	D	311/325 (96%)	305 (98%)	6 (2%)	50	67
All	All	1252/1300 (96%)	1226 (98%)	26 (2%)	46	65

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	66	LEU
1	A	74	PRO
1	A	177	ILE
1	A	210	LEU
1	A	277	SER
1	A	309	VAL
1	B	0	SER
1	B	1	MET
1	B	112	LEU
1	B	257	PRO
1	B	269	GLU
1	B	331	VAL
1	C	24	VAL
1	C	66	LEU
1	C	74	PRO
1	C	177	ILE
1	C	210	LEU
1	C	277	SER
1	C	309	VAL
1	D	0	SER
1	D	1	MET
1	D	112	LEU
1	D	257	PRO
1	D	269	GLU
1	D	331	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	205	GLN
1	A	207	HIS
1	A	240	GLN
1	B	107	GLN
1	B	207	HIS
1	B	225	HIS
1	B	226	GLN
1	B	230	ASN
1	B	242	HIS
1	C	103	HIS
1	C	108	GLN
1	C	205	GLN
1	C	207	HIS
1	C	240	GLN
1	C	298	GLN
1	D	107	GLN
1	D	207	HIS
1	D	225	HIS
1	D	226	GLN
1	D	230	ASN
1	D	242	HIS

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 oligosaccharides 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.

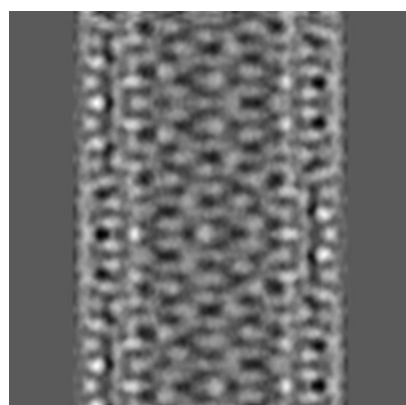
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2547. These allow visual inspection of the internal detail of the map and identification of artifacts.

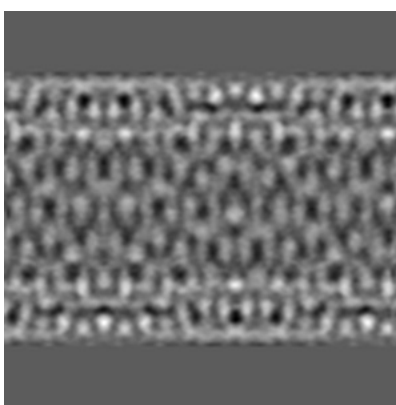
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

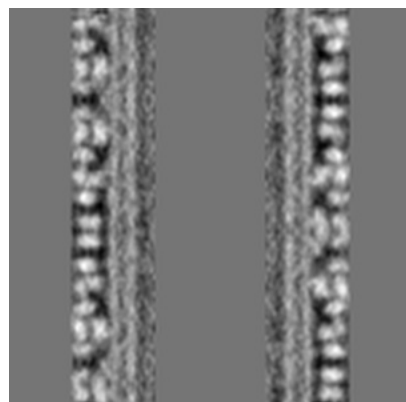


Z

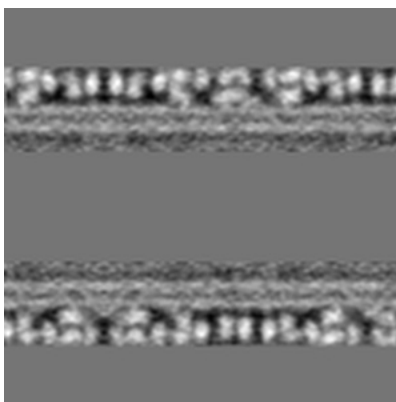
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

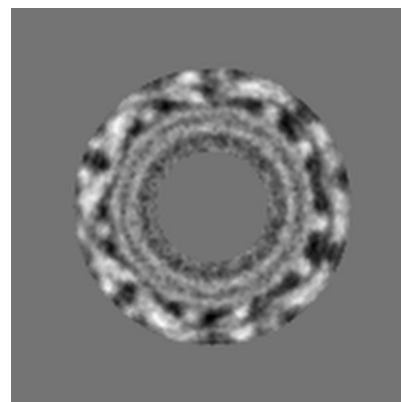
6.2.1 Primary map



X Index: 75



Y Index: 75

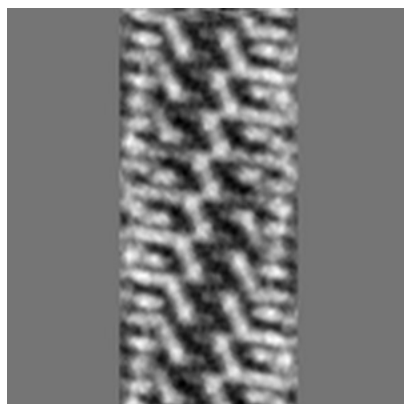


Z Index: 75

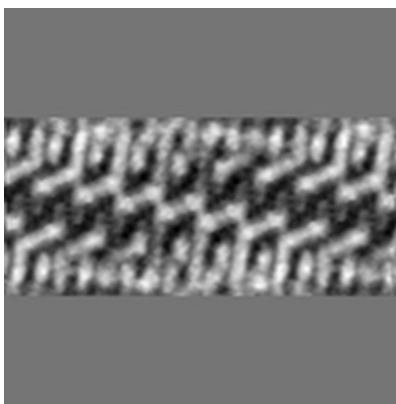
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

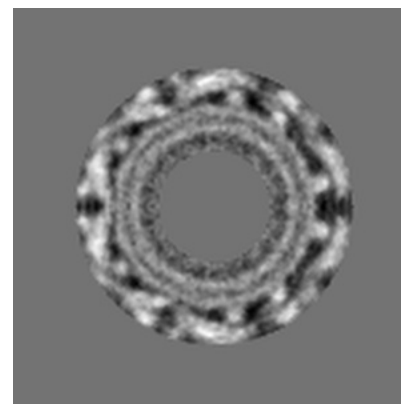
6.3.1 Primary map



X Index: 115



Y Index: 115

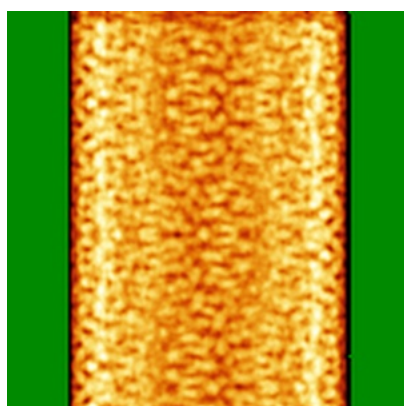


Z Index: 37

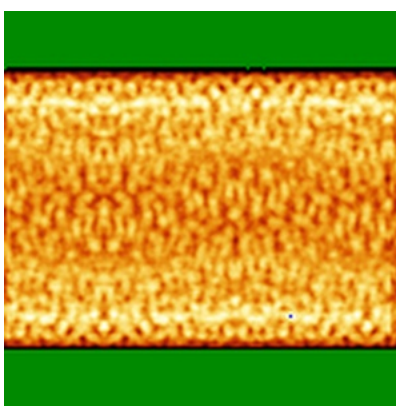
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



X



Y

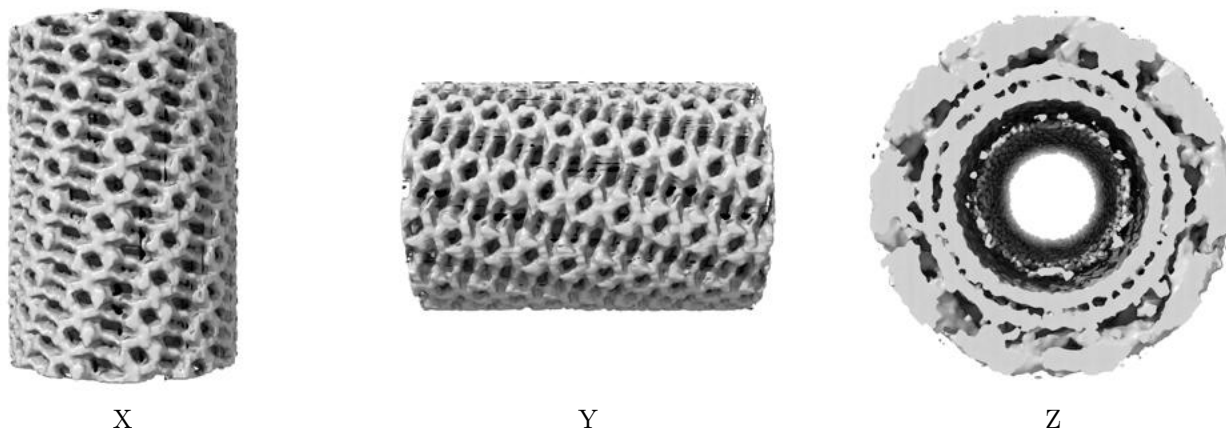


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.0014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

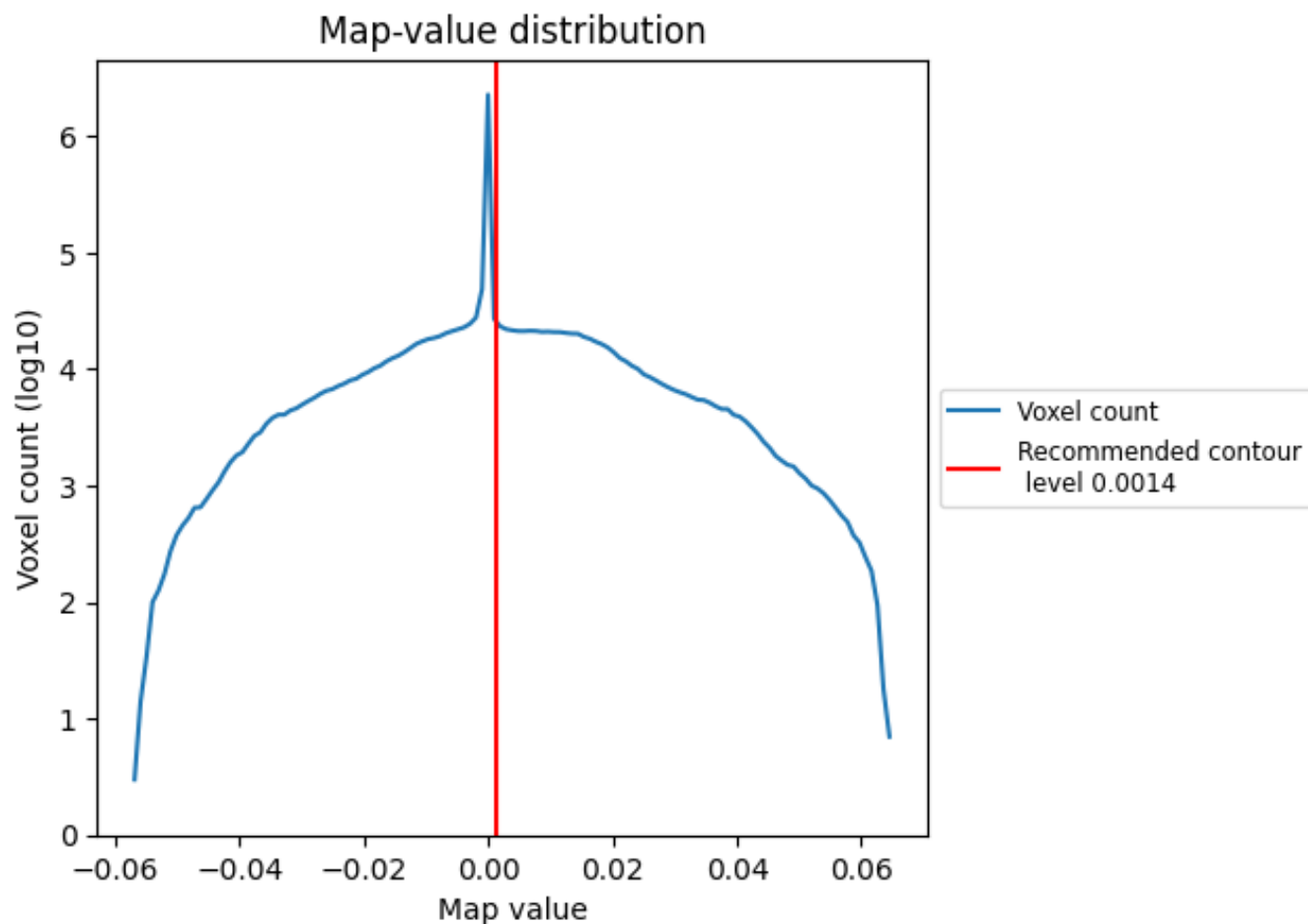
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

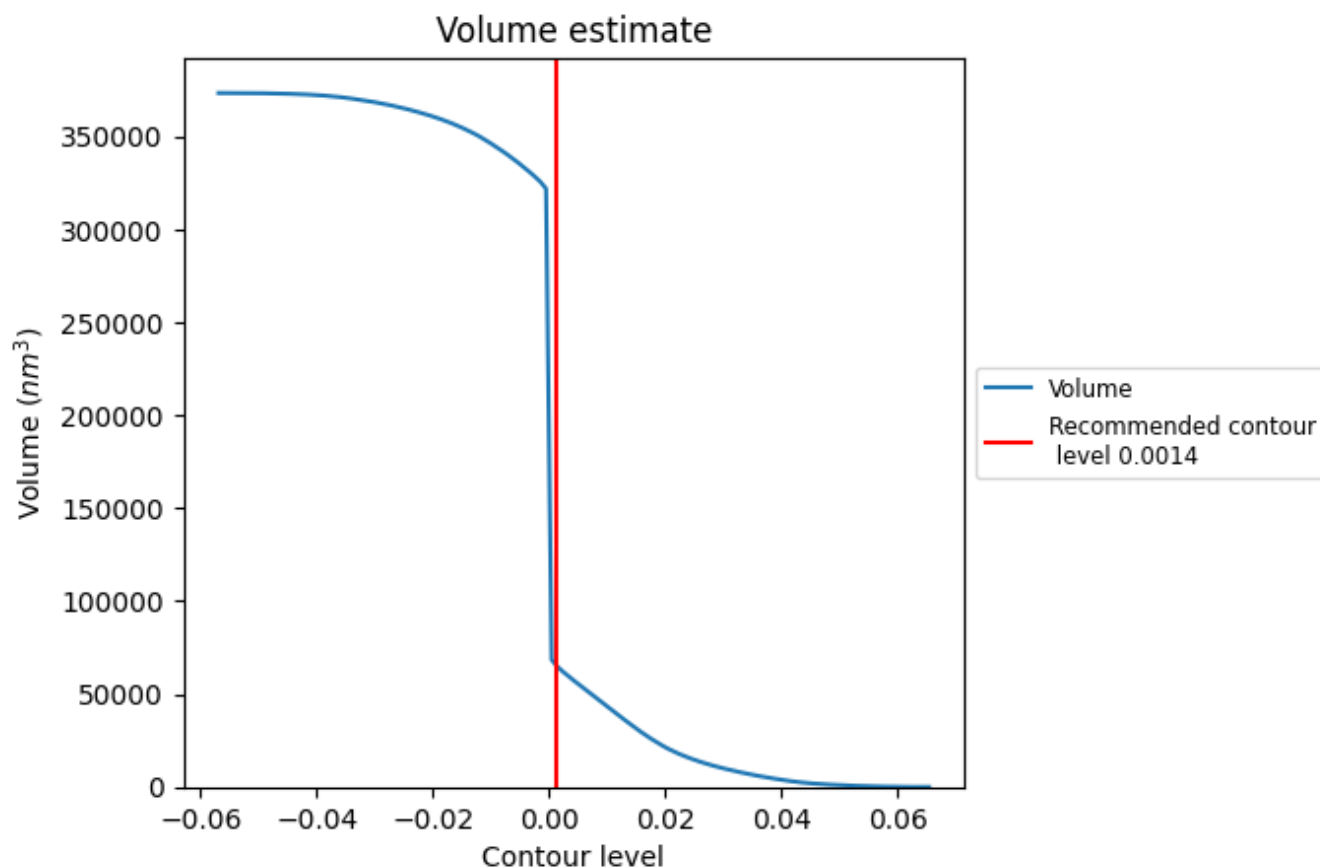
This section contains the results of statistical analysis of the map.

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.

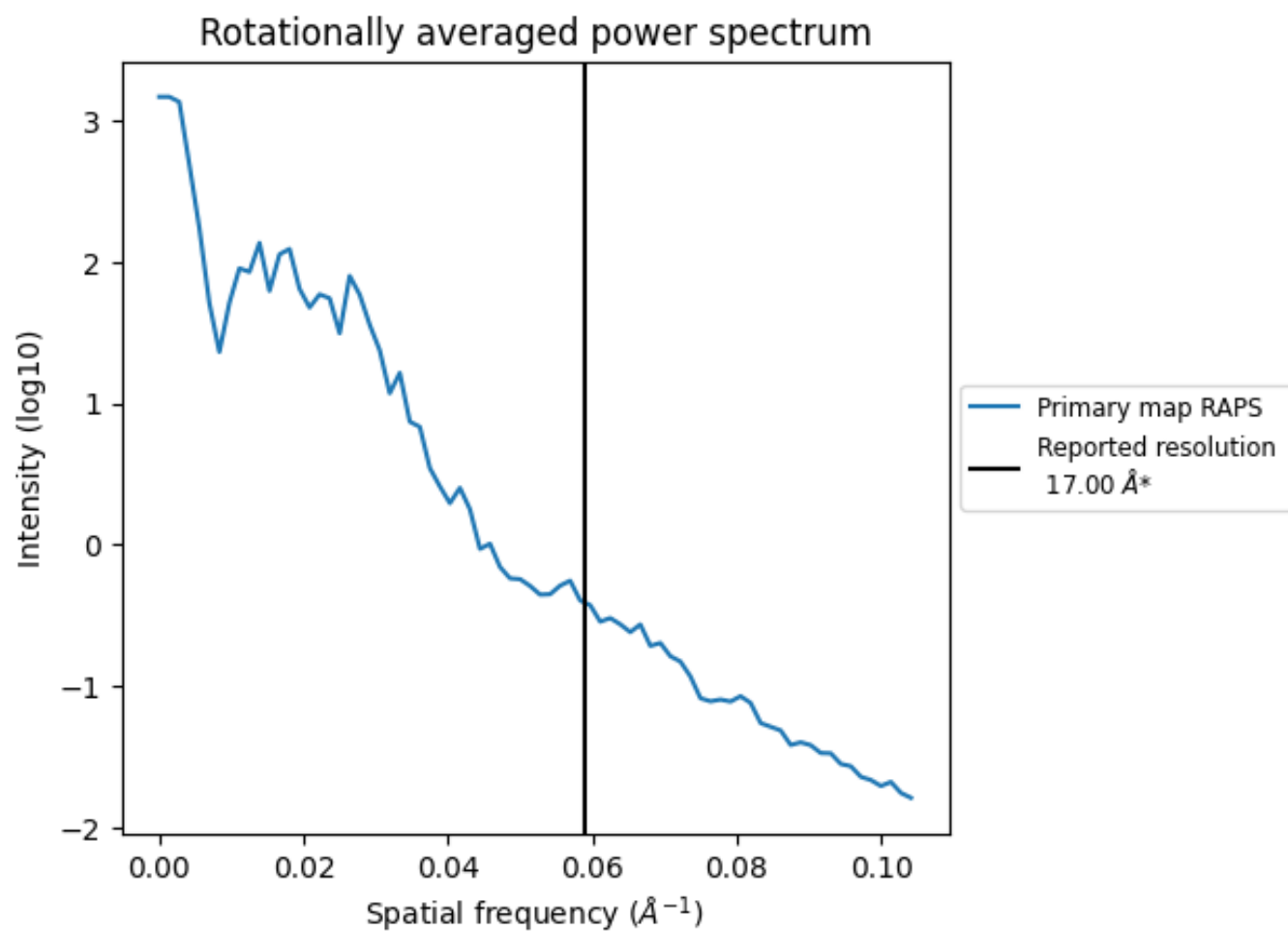
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 65012 nm^3 ; this corresponds to an approximate mass of 58727 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.059 Å⁻¹

8 Fourier-Shell correlation

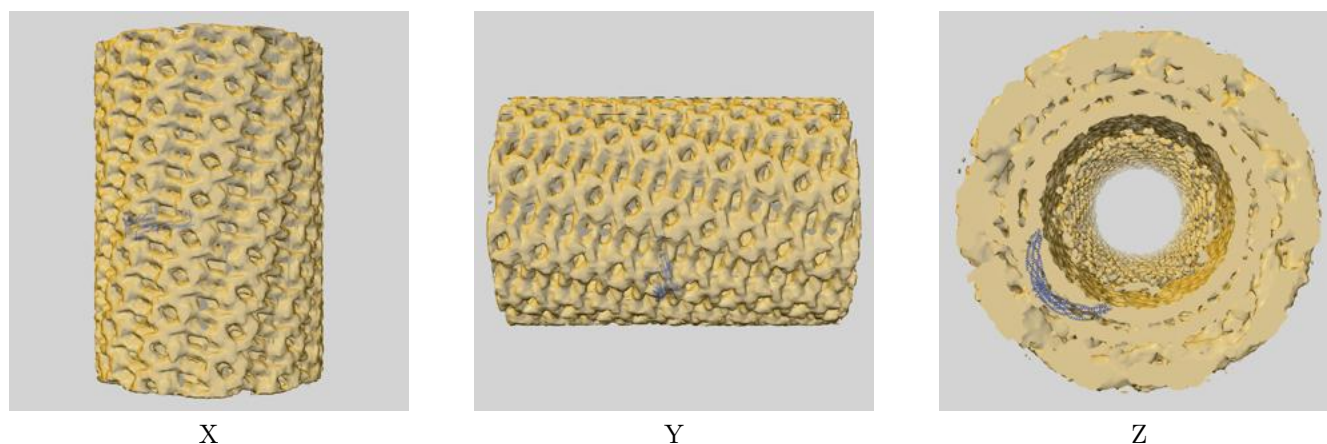
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

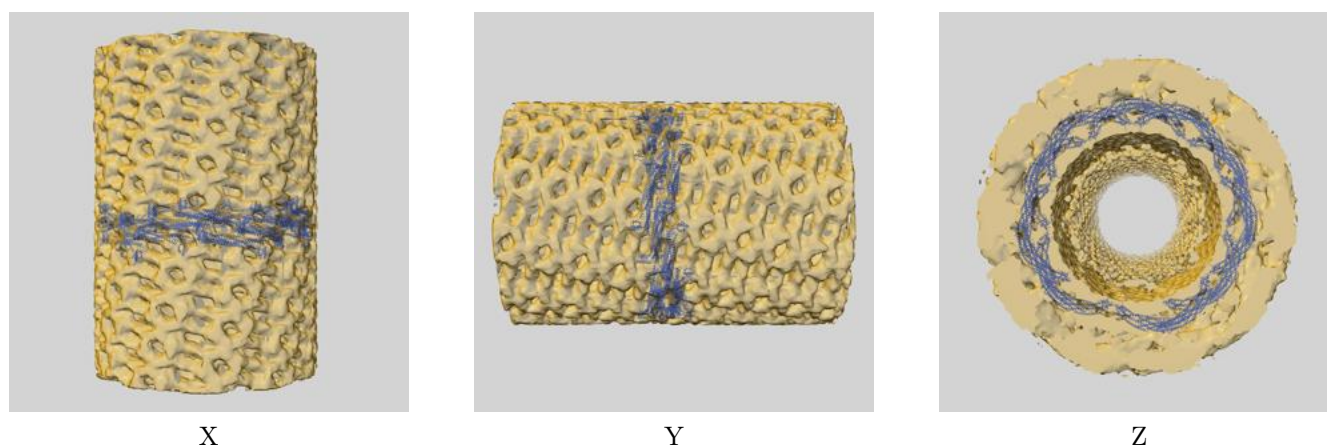
This section contains information regarding the fit between EMDB map EMD-2547 and PDB model 4CKH. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

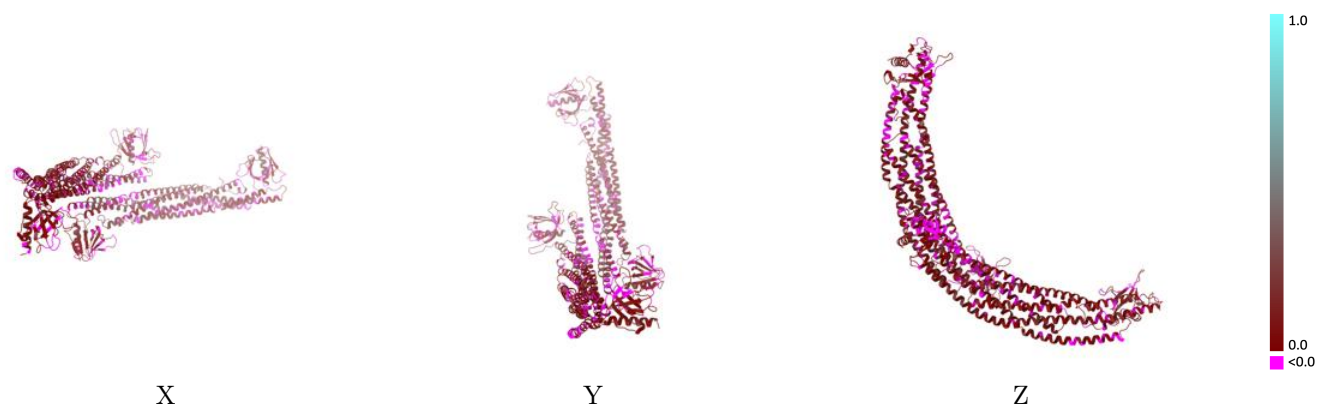


9.1.2 Map-model assembly overlay [i](#)



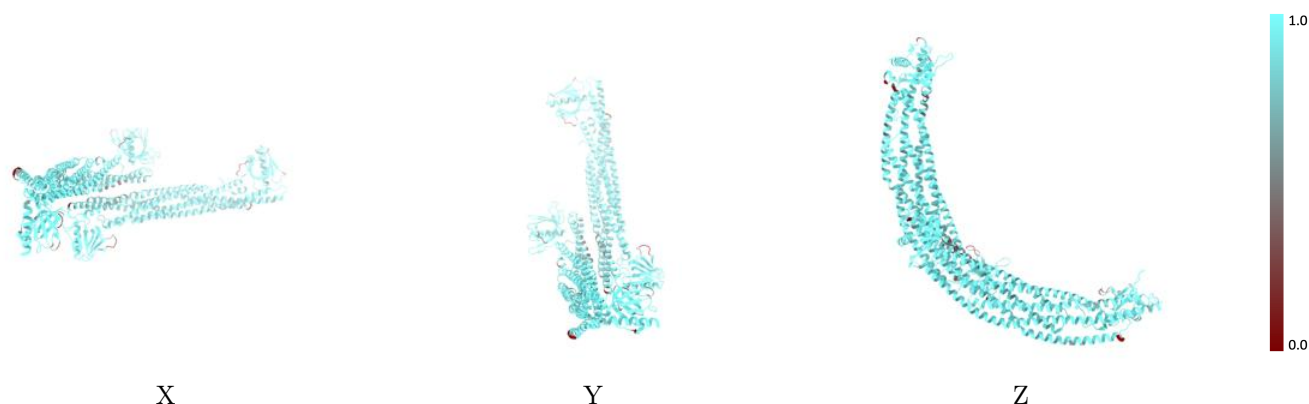
The images above show the 3D surface view of the map at the recommended contour level 0.0014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



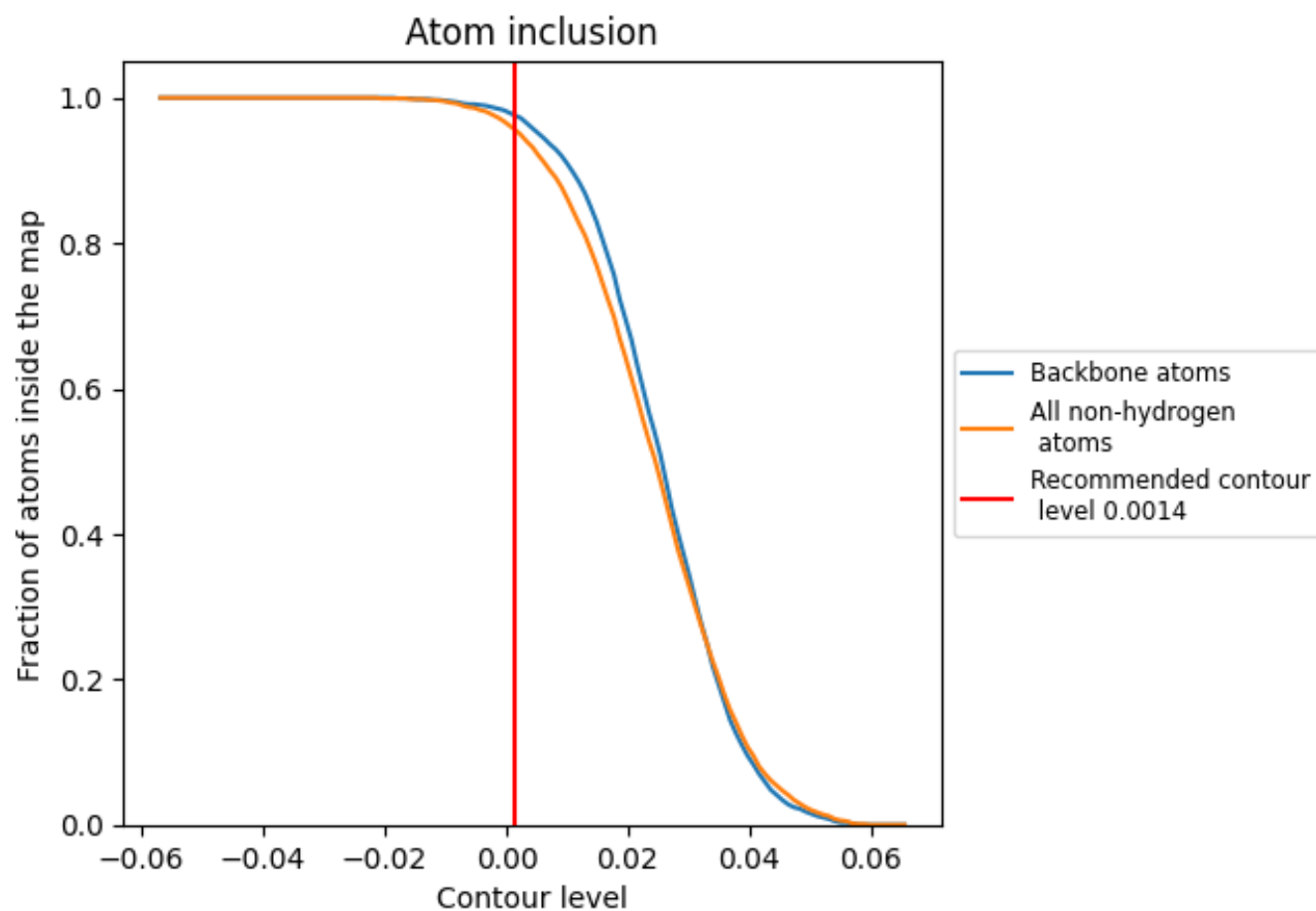
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.0014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9560	0.0560
A	0.9420	0.0470
B	0.9700	0.0670
C	0.9400	0.0540
D	0.9730	0.0560

