



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:47 AM UTC

PDB ID : 4CKG / pdb_00004ckg
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:

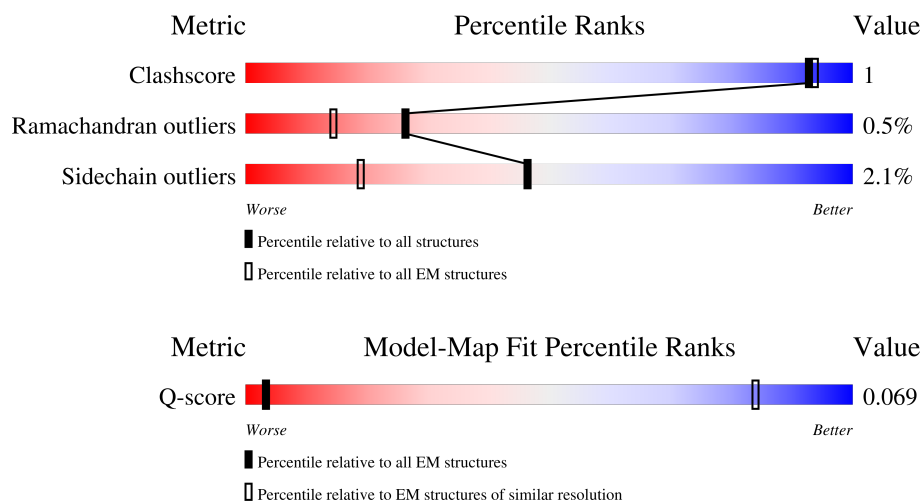
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	37 (14.50 - 15.50)

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		

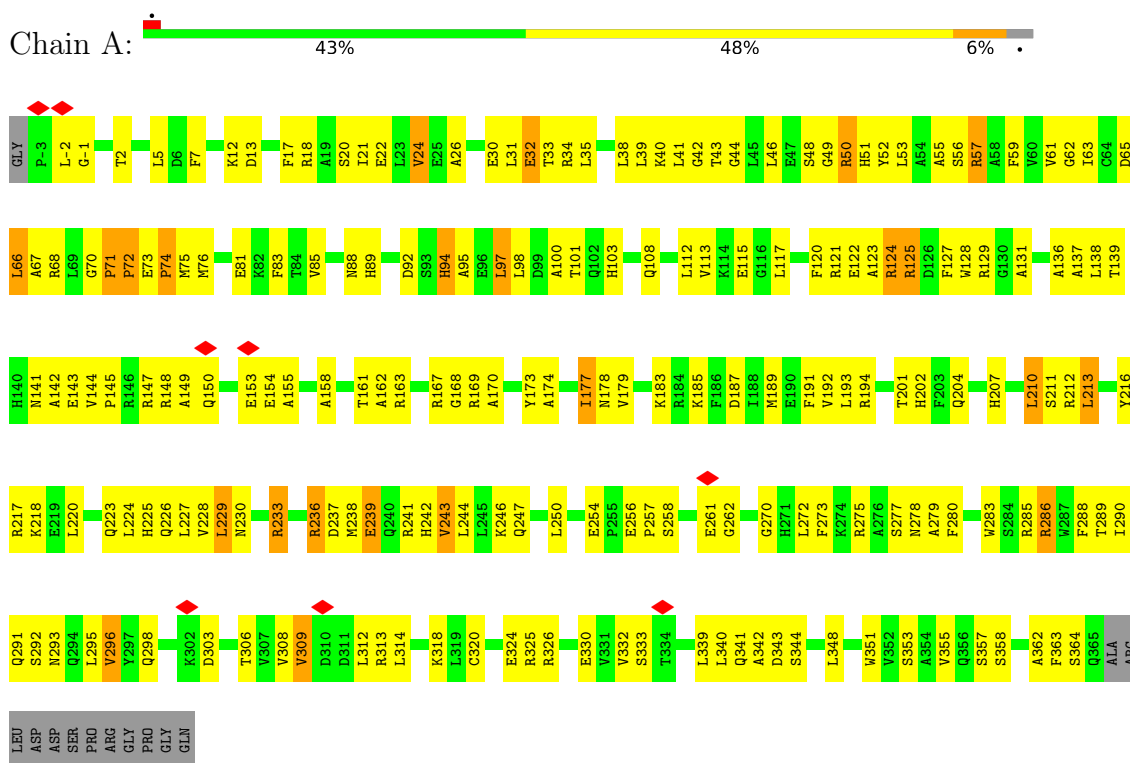
There are 20 discrepancies between the modelled and reference sequences:

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

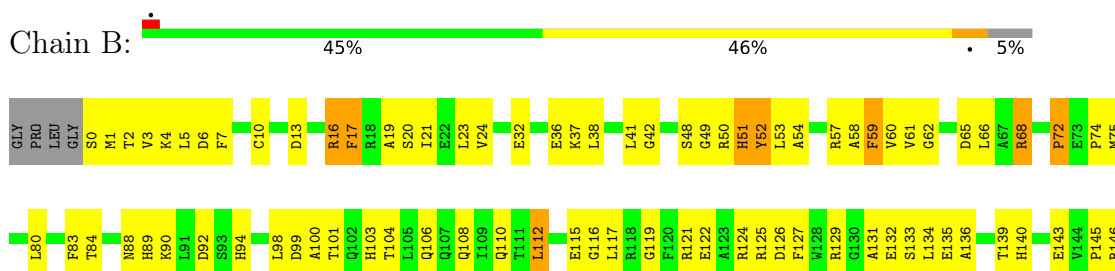
3 Residue-property plots

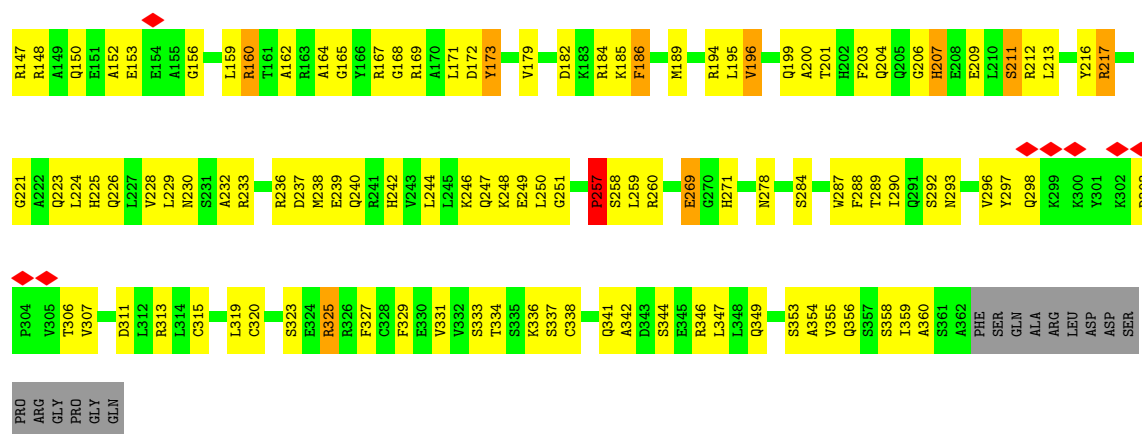
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

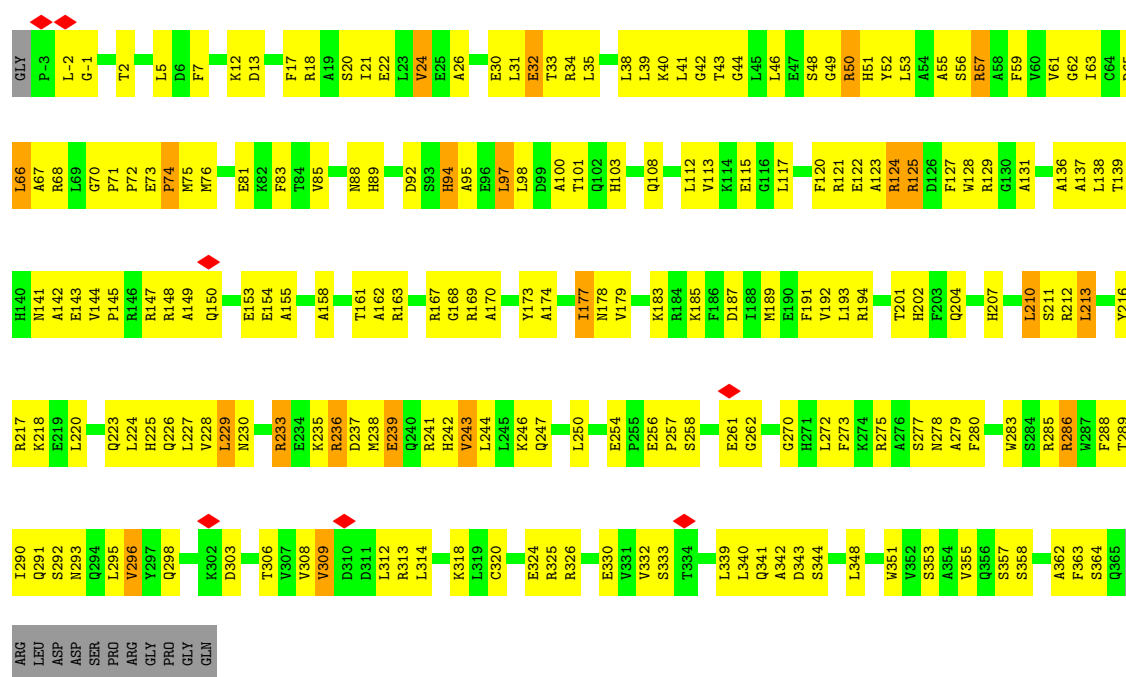


• Molecule 1: ARF-GAP WITH COILED-COIL, ANK REPEAT AND PH DOMAIN-CONTAINING PROTEIN 1

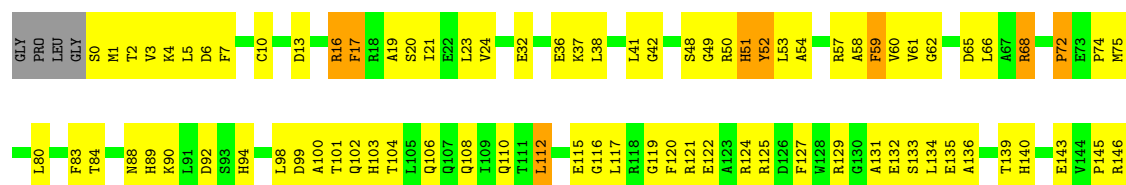


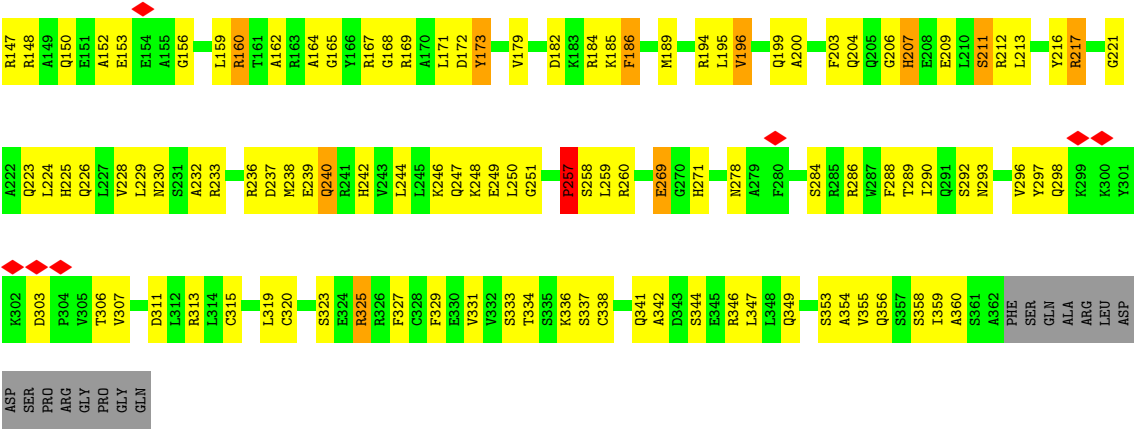


• Molecule 1: ARF-GAP WITH COILED-COIL, ANK REPEAT AND PH DOMAIN-CONTAINING PROTEIN 1



• 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	367	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	0.070	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	2.21	91/2990 (3.0%)	2.57	233/4024 (5.8%)
1	B	2.23	103/2947 (3.5%)	2.53	212/3966 (5.3%)
1	C	2.21	94/2990 (3.1%)	2.57	229/4024 (5.7%)
1	D	2.23	99/2947 (3.4%)	2.53	213/3966 (5.4%)
All	All	2.22	387/11874 (3.3%)	2.55	887/15980 (5.6%)

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 (387) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	GLU	C-N	10.22	1.45	1.33
1	D	320	CYS	CA-CB	10.22	1.59	1.52
1	C	256	GLU	C-N	10.22	1.45	1.33
1	B	320	CYS	CA-CB	10.15	1.59	1.52
1	D	249	GLU	CA-C	9.36	1.64	1.52
1	B	249	GLU	CA-C	9.23	1.64	1.52
1	C	144	VAL	N-CA	-8.45	1.38	1.47
1	A	168	GLY	N-CA	8.40	1.56	1.45
1	C	168	GLY	N-CA	8.38	1.56	1.45
1	A	144	VAL	N-CA	-8.36	1.38	1.47
1	D	297	TYR	C-N	8.09	1.45	1.33
1	B	297	TYR	C-N	8.01	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	189	MET	C-N	8.00	1.44	1.33
1	D	189	MET	N-CA	7.99	1.55	1.46
1	A	194	ARG	CD-NE	7.97	1.57	1.46
1	B	189	MET	C-N	7.94	1.44	1.33
1	C	161	THR	N-CA	7.91	1.55	1.46
1	C	194	ARG	CD-NE	7.90	1.57	1.46
1	C	72	PRO	N-CA	-7.89	1.38	1.47
1	A	161	THR	N-CA	7.88	1.55	1.46
1	B	146	ARG	CD-NE	7.86	1.57	1.46
1	B	189	MET	N-CA	7.85	1.55	1.46
1	A	72	PRO	N-CA	-7.84	1.38	1.47
1	B	315	CYS	CA-C	7.77	1.64	1.53
1	D	146	ARG	CD-NE	7.75	1.57	1.46
1	A	333	SER	N-CA	7.72	1.55	1.46
1	D	315	CYS	CA-C	7.70	1.64	1.53
1	C	333	SER	N-CA	7.68	1.55	1.46
1	B	337	SER	CA-CB	7.64	1.66	1.53
1	C	285	ARG	CD-NE	7.63	1.56	1.46
1	A	285	ARG	CD-NE	7.61	1.56	1.46
1	D	337	SER	CA-CB	7.57	1.65	1.53
1	C	312	LEU	CA-CB	7.49	1.65	1.53
1	A	312	LEU	CA-CB	7.48	1.65	1.53
1	D	226	GLN	C-N	7.47	1.43	1.33
1	C	31	LEU	C-N	-7.45	1.24	1.33
1	D	74	PRO	CA-CB	7.44	1.64	1.53
1	A	155	ALA	CA-C	7.42	1.62	1.52
1	A	31	LEU	C-N	-7.38	1.24	1.33
1	D	124	ARG	CD-NE	7.38	1.56	1.46
1	B	124	ARG	CD-NE	7.38	1.56	1.46
1	B	226	GLN	C-N	7.38	1.43	1.33
1	C	155	ALA	CA-C	7.37	1.62	1.52
1	D	213	LEU	C-N	7.37	1.43	1.33
1	B	74	PRO	CA-CB	7.37	1.64	1.53
1	A	254	GLU	CA-C	-7.34	1.45	1.53
1	B	213	LEU	C-N	7.30	1.43	1.33
1	C	254	GLU	CA-C	-7.29	1.45	1.53
1	A	325	ARG	CA-C	7.25	1.61	1.52
1	D	232	ALA	C-N	7.22	1.43	1.33
1	B	232	ALA	C-N	7.21	1.43	1.33
1	C	325	ARG	CA-C	7.20	1.61	1.52
1	D	121	ARG	C-N	7.16	1.42	1.33
1	C	98	LEU	CA-C	-7.14	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	121	ARG	C-N	7.14	1.42	1.33
1	A	98	LEU	CA-C	-7.11	1.43	1.52
1	B	150	GLN	CA-CB	7.10	1.65	1.53
1	A	326	ARG	CD-NE	7.09	1.56	1.46
1	B	104	THR	CA-CB	-7.08	1.42	1.53
1	C	326	ARG	CD-NE	7.08	1.56	1.46
1	C	35	LEU	CA-CB	7.07	1.64	1.53
1	A	131	ALA	N-CA	-7.06	1.37	1.46
1	B	355	VAL	CA-CB	7.05	1.63	1.54
1	A	35	LEU	CA-CB	7.05	1.64	1.53
1	C	340	LEU	CA-C	7.04	1.61	1.52
1	C	131	ALA	N-CA	-7.04	1.37	1.46
1	C	314	LEU	CA-CB	7.04	1.63	1.53
1	D	150	GLN	CA-CB	7.03	1.64	1.53
1	D	104	THR	CA-CB	-7.00	1.42	1.53
1	A	314	LEU	CA-CB	6.99	1.63	1.53
1	D	355	VAL	CA-CB	6.98	1.63	1.54
1	A	163	ARG	CA-C	-6.97	1.44	1.52
1	A	241	ARG	N-CA	6.96	1.55	1.46
1	C	163	ARG	CA-C	-6.96	1.44	1.52
1	C	241	ARG	N-CA	6.96	1.55	1.46
1	C	283	TRP	CA-C	6.94	1.61	1.52
1	C	286	ARG	CD-NE	6.93	1.55	1.46
1	A	59	PHE	CA-C	6.92	1.61	1.52
1	B	169	ARG	CD-NE	6.92	1.55	1.46
1	D	169	ARG	CD-NE	6.90	1.55	1.46
1	C	59	PHE	CA-C	6.90	1.61	1.52
1	A	340	LEU	CA-C	6.88	1.60	1.52
1	A	283	TRP	CA-C	6.85	1.61	1.52
1	C	257	PRO	N-CA	-6.84	1.39	1.47
1	A	286	ARG	CD-NE	6.84	1.55	1.46
1	B	242	HIS	C-N	-6.84	1.25	1.33
1	D	242	HIS	C-N	-6.84	1.25	1.33
1	A	233	ARG	CD-NE	6.81	1.55	1.46
1	A	42	GLY	C-N	6.81	1.43	1.34
1	C	42	GLY	C-N	6.80	1.43	1.34
1	C	362	ALA	N-CA	-6.76	1.38	1.46
1	C	76	MET	N-CA	-6.75	1.37	1.46
1	A	362	ALA	N-CA	-6.74	1.38	1.46
1	D	65	ASP	CA-CB	6.74	1.64	1.53
1	B	65	ASP	CA-CB	6.73	1.64	1.53
1	A	220	LEU	C-N	6.73	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	233	ARG	CD-NE	6.71	1.55	1.46
1	C	220	LEU	C-N	6.71	1.41	1.33
1	A	76	MET	N-CA	-6.71	1.37	1.46
1	B	84	THR	CA-C	6.70	1.61	1.52
1	A	257	PRO	N-CA	-6.70	1.39	1.47
1	A	33	THR	C-N	6.68	1.42	1.33
1	A	236	ARG	N-CA	-6.67	1.38	1.46
1	C	229	LEU	N-CA	-6.67	1.38	1.46
1	C	33	THR	C-N	6.66	1.42	1.33
1	C	32	GLU	N-CA	6.65	1.54	1.46
1	C	236	ARG	N-CA	-6.64	1.38	1.46
1	A	296	VAL	N-CA	6.63	1.53	1.46
1	A	229	LEU	N-CA	-6.62	1.38	1.46
1	C	270	GLY	CA-C	-6.61	1.42	1.51
1	D	84	THR	CA-C	6.60	1.61	1.52
1	B	4	LYS	CA-C	6.60	1.61	1.53
1	A	270	GLY	CA-C	-6.58	1.42	1.51
1	B	88	ASN	N-CA	6.58	1.54	1.46
1	C	123	ALA	CA-CB	6.57	1.63	1.53
1	B	307	VAL	CA-C	6.55	1.60	1.52
1	D	307	VAL	CA-C	6.54	1.60	1.52
1	D	88	ASN	N-CA	6.53	1.54	1.46
1	C	66	LEU	CA-C	-6.53	1.44	1.52
1	A	123	ALA	CA-CB	6.53	1.63	1.53
1	C	343	ASP	N-CA	6.52	1.54	1.46
1	C	167	ARG	CD-NE	6.52	1.55	1.46
1	D	4	LYS	CA-C	6.51	1.61	1.53
1	A	66	LEU	CA-C	-6.50	1.44	1.52
1	A	32	GLU	N-CA	6.48	1.54	1.46
1	A	167	ARG	CD-NE	6.46	1.55	1.46
1	C	238	MET	CA-C	6.46	1.61	1.52
1	C	50	ARG	CA-C	6.46	1.61	1.52
1	C	296	VAL	N-CA	6.46	1.53	1.46
1	A	343	ASP	N-CA	6.45	1.54	1.46
1	B	289	THR	C-O	-6.44	1.16	1.24
1	C	204	GLN	C-N	6.44	1.42	1.33
1	D	153	GLU	CA-CB	6.44	1.63	1.53
1	B	153	GLU	CA-CB	6.43	1.63	1.53
1	D	94	HIS	N-CA	-6.41	1.38	1.46
1	A	204	GLN	C-N	6.40	1.42	1.33
1	A	238	MET	CA-C	6.39	1.61	1.52
1	D	172	ASP	CA-CB	6.38	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	289	THR	C-O	-6.37	1.16	1.24
1	A	66	LEU	CA-CB	6.36	1.63	1.53
1	C	66	LEU	CA-CB	6.36	1.63	1.53
1	B	94	HIS	N-CA	-6.35	1.38	1.46
1	D	236	ARG	CD-NE	6.35	1.55	1.46
1	B	172	ASP	CA-CB	6.34	1.63	1.53
1	D	211	SER	CA-CB	6.32	1.63	1.53
1	A	50	ARG	CA-C	6.30	1.60	1.52
1	A	41	LEU	CA-C	6.28	1.61	1.52
1	B	236	ARG	CD-NE	6.27	1.55	1.46
1	B	211	SER	CA-CB	6.26	1.63	1.53
1	B	271	HIS	ND1-CE1	6.26	1.38	1.32
1	D	200	ALA	C-N	6.26	1.42	1.33
1	C	41	LEU	CA-C	6.25	1.61	1.52
1	A	63	ILE	CA-C	-6.24	1.44	1.52
1	B	41	LEU	CA-C	6.21	1.60	1.52
1	C	63	ILE	CA-C	-6.21	1.44	1.52
1	D	41	LEU	CA-C	6.20	1.60	1.52
1	B	115	GLU	CA-C	6.19	1.58	1.52
1	D	115	GLU	CA-C	6.18	1.58	1.52
1	B	200	ALA	C-N	6.17	1.42	1.33
1	D	139	THR	N-CA	6.16	1.53	1.46
1	D	271	HIS	ND1-CE1	6.15	1.38	1.32
1	A	189	MET	CA-CB	6.13	1.63	1.53
1	B	139	THR	N-CA	6.12	1.53	1.46
1	D	325	ARG	CD-NE	6.11	1.54	1.46
1	C	288	PHE	C-O	6.11	1.30	1.23
1	B	260	ARG	CA-C	6.10	1.60	1.52
1	D	68	ARG	C-O	6.10	1.31	1.24
1	C	189	MET	CA-CB	6.09	1.62	1.53
1	D	257	PRO	C-N	6.08	1.41	1.33
1	B	325	ARG	CD-NE	6.08	1.54	1.46
1	B	257	PRO	C-N	6.08	1.41	1.33
1	D	260	ARG	CA-C	6.08	1.60	1.52
1	B	341	GLN	CA-C	6.07	1.59	1.52
1	A	246	LYS	CA-C	6.04	1.60	1.52
1	D	341	GLN	CA-C	6.03	1.59	1.52
1	B	68	ARG	C-O	6.03	1.31	1.24
1	B	115	GLU	N-CA	-6.02	1.41	1.47
1	C	246	LYS	CA-C	6.00	1.60	1.52
1	A	74	PRO	CA-CB	-5.98	1.45	1.53
1	B	62	GLY	C-N	5.96	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	115	GLU	N-CA	-5.96	1.42	1.47
1	D	62	GLY	C-N	5.95	1.41	1.33
1	D	200	ALA	N-CA	-5.95	1.39	1.46
1	C	74	PRO	CA-CB	-5.95	1.45	1.53
1	C	306	THR	N-CA	-5.94	1.38	1.46
1	B	200	ALA	N-CA	-5.94	1.39	1.46
1	D	57	ARG	NE-CZ	5.93	1.39	1.33
1	D	48	SER	CA-CB	5.92	1.62	1.53
1	B	57	ARG	NE-CZ	5.91	1.39	1.33
1	B	333	SER	N-CA	5.88	1.53	1.45
1	B	338	CYS	CA-C	5.88	1.59	1.52
1	B	171	LEU	CA-C	5.88	1.60	1.52
1	D	122	GLU	C-N	5.88	1.41	1.33
1	B	133	SER	N-CA	-5.87	1.39	1.46
1	B	122	GLU	C-N	5.87	1.41	1.33
1	A	306	THR	N-CA	-5.84	1.38	1.46
1	B	164	ALA	CA-CB	5.83	1.62	1.53
1	B	48	SER	CA-CB	5.82	1.62	1.53
1	D	333	SER	N-CA	5.82	1.53	1.45
1	C	262	GLY	C-N	-5.82	1.27	1.34
1	D	303	ASP	CA-CB	5.82	1.62	1.54
1	D	338	CYS	CA-C	5.80	1.59	1.52
1	D	59	PHE	C-N	5.80	1.41	1.33
1	B	196	VAL	N-CA	5.80	1.53	1.46
1	D	164	ALA	CA-CB	5.80	1.62	1.53
1	A	262	GLY	C-N	-5.79	1.27	1.34
1	B	59	PHE	C-N	5.79	1.40	1.33
1	B	303	ASP	CA-CB	5.79	1.62	1.54
1	D	311	ASP	C-N	5.76	1.42	1.33
1	D	133	SER	N-CA	-5.76	1.39	1.46
1	C	44	GLY	CA-C	-5.76	1.45	1.52
1	C	148	ARG	CD-NE	5.76	1.54	1.46
1	B	165	GLY	C-N	5.73	1.41	1.33
1	A	226	GLN	C-O	-5.72	1.17	1.24
1	D	165	GLY	C-N	5.72	1.41	1.33
1	B	311	ASP	C-N	5.72	1.42	1.33
1	A	148	ARG	CD-NE	5.71	1.54	1.46
1	A	295	LEU	CA-CB	5.70	1.60	1.53
1	C	185	LYS	CA-C	5.70	1.60	1.52
1	D	171	LEU	CA-C	5.70	1.60	1.52
1	A	288	PHE	C-O	5.70	1.30	1.23
1	D	98	LEU	CA-CB	5.69	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	226	GLN	C-O	-5.68	1.17	1.24
1	D	80	LEU	CA-C	5.68	1.60	1.52
1	D	196	VAL	N-CA	5.68	1.53	1.46
1	B	80	LEU	CA-C	5.68	1.60	1.52
1	D	238	MET	N-CA	-5.68	1.39	1.46
1	A	185	LYS	CA-C	5.67	1.60	1.52
1	B	98	LEU	CA-CB	5.67	1.62	1.53
1	D	160	ARG	CD-NE	5.66	1.54	1.46
1	A	218	LYS	C-O	-5.65	1.17	1.24
1	C	295	LEU	CA-CB	5.64	1.60	1.53
1	C	73	GLU	C-N	5.64	1.41	1.33
1	B	238	MET	N-CA	-5.63	1.39	1.46
1	C	100	ALA	N-CA	-5.63	1.39	1.46
1	A	73	GLU	C-N	5.62	1.41	1.33
1	A	88	ASN	N-CA	5.61	1.53	1.46
1	B	32	GLU	CA-C	-5.61	1.45	1.52
1	A	49	GLY	CA-C	-5.61	1.46	1.52
1	B	160	ARG	CD-NE	5.60	1.54	1.46
1	D	325	ARG	N-CA	-5.59	1.39	1.46
1	C	353	SER	C-N	5.59	1.41	1.33
1	A	44	GLY	CA-C	-5.58	1.45	1.52
1	A	306	THR	C-O	-5.58	1.17	1.23
1	C	306	THR	C-O	-5.58	1.17	1.23
1	D	32	GLU	CA-C	-5.57	1.45	1.52
1	C	218	LYS	C-O	-5.57	1.17	1.24
1	A	100	ALA	N-CA	-5.56	1.39	1.46
1	A	353	SER	C-N	5.55	1.41	1.33
1	A	272	LEU	CA-C	5.55	1.59	1.52
1	C	272	LEU	CA-C	5.55	1.59	1.52
1	C	49	GLY	CA-C	-5.54	1.46	1.52
1	C	339	LEU	CB-CG	5.54	1.64	1.53
1	C	247	GLN	C-N	5.54	1.41	1.33
1	A	339	LEU	CB-CG	5.53	1.64	1.53
1	C	88	ASN	N-CA	5.53	1.53	1.46
1	C	312	LEU	CA-C	5.52	1.59	1.52
1	A	351	TRP	C-N	5.50	1.40	1.33
1	C	351	TRP	C-N	5.50	1.40	1.33
1	C	185	LYS	CA-CB	5.50	1.62	1.53
1	B	325	ARG	N-CA	-5.49	1.39	1.46
1	D	216	TYR	C-N	5.47	1.40	1.33
1	A	185	LYS	CA-CB	5.46	1.61	1.53
1	A	312	LEU	CA-C	5.46	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	306	THR	C-N	5.46	1.40	1.33
1	A	306	THR	C-N	5.46	1.40	1.33
1	C	98	LEU	N-CA	5.45	1.53	1.46
1	C	193	LEU	N-CA	5.45	1.52	1.46
1	A	247	GLN	C-N	5.44	1.41	1.33
1	D	90	LYS	C-O	-5.44	1.17	1.24
1	A	193	LEU	N-CA	5.44	1.52	1.46
1	B	90	LYS	C-O	-5.43	1.17	1.24
1	D	320	CYS	C-O	5.42	1.26	1.23
1	A	280	PHE	CB-CG	-5.41	1.38	1.50
1	B	216	TYR	C-N	5.41	1.40	1.33
1	B	233	ARG	NE-CZ	5.41	1.39	1.33
1	C	40	LYS	N-CA	-5.41	1.39	1.46
1	C	280	PHE	CB-CG	-5.41	1.38	1.50
1	D	259	LEU	N-CA	-5.40	1.39	1.46
1	B	5	LEU	N-CA	5.40	1.53	1.46
1	B	207	HIS	CE1-NE2	5.40	1.38	1.32
1	A	98	LEU	N-CA	5.39	1.52	1.46
1	B	259	LEU	N-CA	-5.39	1.39	1.46
1	D	90	LYS	CA-C	5.39	1.59	1.52
1	D	5	LEU	N-CA	5.38	1.53	1.46
1	B	320	CYS	C-O	5.37	1.26	1.23
1	D	16	ARG	CA-C	5.37	1.59	1.52
1	D	140	HIS	CA-CB	5.37	1.61	1.53
1	B	90	LYS	CA-C	5.36	1.59	1.52
1	D	358	SER	CA-C	5.36	1.59	1.52
1	D	207	HIS	CE1-NE2	5.36	1.38	1.32
1	B	16	ARG	CA-C	5.35	1.59	1.52
1	D	194	ARG	C-N	-5.34	1.27	1.33
1	A	147	ARG	CA-C	5.34	1.59	1.52
1	A	40	LYS	N-CA	-5.34	1.40	1.46
1	D	233	ARG	NE-CZ	5.34	1.39	1.33
1	D	20	SER	N-CA	5.33	1.53	1.46
1	D	290	ILE	C-O	5.32	1.30	1.24
1	A	239	GLU	N-CA	5.32	1.52	1.46
1	A	342	ALA	N-CA	-5.30	1.39	1.45
1	A	178	ASN	CA-C	5.30	1.59	1.52
1	A	50	ARG	CD-NE	5.30	1.53	1.46
1	A	161	THR	C-N	5.30	1.40	1.33
1	A	95	ALA	N-CA	5.30	1.52	1.46
1	C	244	LEU	CA-CB	5.29	1.61	1.53
1	D	53	LEU	CA-C	5.29	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	147	ARG	CA-C	5.29	1.59	1.52
1	A	94	HIS	CB-CG	5.29	1.57	1.50
1	B	20	SER	N-CA	5.29	1.53	1.46
1	B	194	ARG	C-N	-5.28	1.27	1.33
1	B	140	HIS	CA-CB	5.28	1.61	1.53
1	A	244	LEU	CA-CB	5.28	1.61	1.53
1	C	161	THR	C-N	5.28	1.40	1.33
1	A	318	LYS	CA-CB	5.27	1.61	1.53
1	D	250	LEU	C-N	5.27	1.38	1.33
1	B	290	ILE	C-O	5.27	1.29	1.24
1	D	251	GLY	N-CA	-5.26	1.38	1.45
1	D	325	ARG	CA-CB	5.26	1.62	1.53
1	C	239	GLU	N-CA	5.26	1.52	1.46
1	B	325	ARG	CA-CB	5.26	1.62	1.53
1	C	95	ALA	N-CA	5.25	1.52	1.46
1	C	50	ARG	CD-NE	5.25	1.53	1.46
1	B	53	LEU	CA-C	5.25	1.59	1.52
1	D	103	HIS	CD2-NE2	5.25	1.43	1.37
1	B	251	GLY	N-CA	-5.24	1.38	1.45
1	B	103	HIS	CD2-NE2	5.24	1.43	1.37
1	C	178	ASN	CA-C	5.23	1.59	1.52
1	C	94	HIS	CB-CG	5.22	1.57	1.50
1	C	318	LYS	CA-CB	5.22	1.61	1.53
1	B	358	SER	CA-C	5.22	1.59	1.52
1	C	342	ALA	N-CA	-5.21	1.39	1.45
1	D	320	CYS	N-CA	-5.20	1.42	1.46
1	C	192	VAL	N-CA	5.19	1.52	1.46
1	C	312	LEU	N-CA	-5.19	1.38	1.45
1	D	307	VAL	C-N	5.19	1.39	1.33
1	D	342	ALA	C-N	5.19	1.41	1.33
1	D	127	PHE	CA-C	5.18	1.59	1.52
1	D	42	GLY	CA-C	-5.17	1.45	1.52
1	B	116	GLY	CA-C	5.17	1.59	1.51
1	B	42	GLY	CA-C	-5.17	1.45	1.52
1	B	112	LEU	CA-C	5.17	1.59	1.52
1	B	143	GLU	CA-CB	5.16	1.59	1.52
1	B	250	LEU	C-N	5.16	1.37	1.33
1	B	127	PHE	CA-C	5.15	1.59	1.52
1	C	61	VAL	C-O	-5.15	1.18	1.24
1	D	133	SER	CA-CB	5.15	1.61	1.53
1	A	229	LEU	CA-CB	5.14	1.61	1.53
1	D	143	GLU	CA-CB	5.14	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	147	ARG	NE-CZ	5.14	1.38	1.33
1	B	133	SER	CA-CB	5.13	1.61	1.53
1	D	298	GLN	N-CA	-5.13	1.39	1.46
1	B	342	ALA	C-N	5.12	1.41	1.33
1	A	192	VAL	N-CA	5.12	1.52	1.46
1	B	126	ASP	CA-C	5.11	1.59	1.52
1	D	140	HIS	C-N	5.11	1.41	1.33
1	B	147	ARG	NE-CZ	5.11	1.38	1.33
1	B	298	GLN	N-CA	-5.10	1.39	1.46
1	A	262	GLY	N-CA	5.10	1.51	1.44
1	B	134	LEU	CA-CB	5.09	1.61	1.53
1	B	140	HIS	C-N	5.09	1.41	1.33
1	B	320	CYS	N-CA	-5.09	1.42	1.46
1	D	134	LEU	CA-CB	5.09	1.61	1.53
1	A	61	VAL	C-O	-5.09	1.18	1.24
1	B	307	VAL	C-N	5.08	1.39	1.33
1	C	193	LEU	C-N	5.08	1.40	1.33
1	D	127	PHE	CA-CB	5.08	1.61	1.53
1	D	156	GLY	CA-C	-5.08	1.45	1.52
1	A	50	ARG	NE-CZ	5.07	1.38	1.33
1	B	217	ARG	NE-CZ	5.07	1.38	1.33
1	D	217	ARG	NE-CZ	5.07	1.38	1.33
1	D	240	GLN	CA-C	5.07	1.59	1.52
1	B	159	LEU	C-O	5.07	1.30	1.24
1	B	156	GLY	CA-C	-5.07	1.45	1.52
1	C	262	GLY	N-CA	5.07	1.51	1.44
1	D	112	LEU	CA-C	5.06	1.59	1.52
1	B	122	GLU	CA-C	-5.04	1.46	1.52
1	C	50	ARG	NE-CZ	5.04	1.38	1.33
1	B	287	TRP	NE1-CE2	5.03	1.43	1.37
1	C	229	LEU	CA-CB	5.03	1.61	1.53
1	D	116	GLY	CA-C	5.03	1.58	1.51
1	A	312	LEU	N-CA	-5.02	1.39	1.45
1	C	235	LYS	C-N	5.02	1.40	1.33
1	D	122	GLU	CA-C	-5.01	1.46	1.52
1	B	24	VAL	C-N	5.01	1.40	1.33
1	C	303	ASP	C-N	5.01	1.40	1.33
1	B	127	PHE	CA-CB	5.00	1.61	1.53
1	B	201	THR	N-CA	5.00	1.52	1.46

All (887) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	LEU	CA-C-N	11.57	132.55	119.94
1	A	220	LEU	C-N-CA	11.57	132.55	119.94
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	D	179	VAL	N-CA-C	10.92	121.76	110.62
1	B	179	VAL	N-CA-C	10.89	121.73	110.62
1	C	55	ALA	CA-C-N	10.88	134.59	120.44
1	C	55	ALA	C-N-CA	10.88	134.59	120.44
1	A	55	ALA	CA-C-N	10.82	134.50	120.44
1	A	55	ALA	C-N-CA	10.82	134.50	120.44
1	A	278	ASN	CA-CB-CG	-10.46	102.14	112.60
1	C	278	ASN	CA-CB-CG	-10.39	102.21	112.60
1	A	63	ILE	N-CA-CB	10.21	124.42	110.54
1	C	63	ILE	N-CA-CB	10.18	124.39	110.54
1	A	103	HIS	N-CA-C	10.10	121.88	111.07
1	C	103	HIS	N-CA-C	10.04	121.82	111.07
1	C	279	ALA	N-CA-C	9.74	122.91	111.71
1	A	279	ALA	N-CA-C	9.72	122.89	111.71
1	A	141	ASN	CA-C-O	9.65	130.65	120.42
1	C	141	ASN	CA-C-O	9.63	130.62	120.42
1	A	211	SER	N-CA-C	9.44	122.43	111.11
1	C	211	SER	N-CA-C	9.43	122.43	111.11
1	B	48	SER	CA-C-N	9.32	130.29	119.94
1	B	48	SER	C-N-CA	9.32	130.29	119.94
1	A	207	HIS	CE1-NE2-CD2	-9.27	99.73	109.00
1	D	48	SER	CA-C-N	9.26	130.22	119.94
1	D	48	SER	C-N-CA	9.26	130.22	119.94
1	D	50	ARG	NE-CZ-NH2	9.26	127.53	119.20
1	C	207	HIS	CE1-NE2-CD2	-9.22	99.78	109.00
1	D	303	ASP	CA-C-O	-9.22	110.51	119.91
1	D	216	TYR	CA-C-N	9.22	132.81	120.65
1	D	216	TYR	C-N-CA	9.22	132.81	120.65
1	B	216	TYR	CA-C-N	9.20	132.79	120.65
1	B	216	TYR	C-N-CA	9.20	132.79	120.65
1	B	303	ASP	CA-C-O	-9.19	110.54	119.91
1	B	50	ARG	NE-CZ-NH2	9.15	127.44	119.20
1	B	110	GLN	N-CA-C	9.12	121.22	111.28
1	D	110	GLN	N-CA-C	9.10	121.19	111.28
1	C	242	HIS	CA-C-N	8.99	131.88	120.56
1	C	242	HIS	C-N-CA	8.99	131.88	120.56
1	A	242	HIS	CA-C-N	8.98	131.87	120.56
1	A	242	HIS	C-N-CA	8.98	131.87	120.56
1	A	237	ASP	CA-C-N	8.88	132.18	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	ASP	C-N-CA	8.88	132.18	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	-8.86	103.75	112.60
1	D	92	ASP	CA-CB-CG	-8.85	103.75	112.60
1	D	100	ALA	O-C-N	-8.83	112.08	122.15
1	B	92	ASP	CA-CB-CG	-8.83	103.77	112.60
1	B	100	ALA	O-C-N	-8.81	112.10	122.15
1	B	38	LEU	CA-C-N	8.79	133.01	120.79
1	B	38	LEU	C-N-CA	8.79	133.01	120.79
1	D	38	LEU	CA-C-N	8.79	133.01	120.79
1	D	38	LEU	C-N-CA	8.79	133.01	120.79
1	D	160	ARG	N-CA-CB	8.71	122.92	109.94
1	D	284	SER	CA-C-O	8.69	130.45	120.89
1	B	160	ARG	N-CA-CB	8.67	122.86	109.94
1	B	284	SER	CA-C-O	8.67	130.43	120.89
1	A	332	VAL	N-CA-C	8.64	120.21	108.11
1	C	332	VAL	N-CA-C	8.63	120.19	108.11
1	C	85	VAL	CA-C-N	8.57	131.59	120.44
1	C	85	VAL	C-N-CA	8.57	131.59	120.44
1	A	85	VAL	CA-C-N	8.56	131.57	120.44
1	A	85	VAL	C-N-CA	8.56	131.57	120.44
1	A	127	PHE	CA-CB-CG	8.50	122.30	113.80
1	C	127	PHE	CA-CB-CG	8.44	122.24	113.80
1	C	100	ALA	N-CA-C	8.42	120.46	111.28
1	A	100	ALA	N-CA-C	8.42	120.46	111.28
1	B	19	ALA	O-C-N	-8.29	111.22	122.33
1	D	19	ALA	O-C-N	-8.24	111.28	122.33
1	D	182	ASP	CA-C-O	-8.21	111.13	120.24
1	D	246	LYS	CA-C-N	8.19	131.92	120.29
1	D	246	LYS	C-N-CA	8.19	131.92	120.29
1	B	182	ASP	CA-C-O	-8.18	111.16	120.24
1	A	129	ARG	CA-C-N	8.16	130.62	120.34
1	A	129	ARG	C-N-CA	8.16	130.62	120.34
1	C	129	ARG	CA-C-N	8.16	130.62	120.34
1	C	129	ARG	C-N-CA	8.16	130.62	120.34
1	A	141	ASN	O-C-N	-8.14	112.87	122.15
1	B	246	LYS	CA-C-N	8.14	131.85	120.29
1	B	246	LYS	C-N-CA	8.14	131.85	120.29
1	C	141	ASN	O-C-N	-8.14	112.87	122.15
1	C	241	ARG	CA-C-N	8.12	131.00	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	241	ARG	C-N-CA	8.12	131.00	120.44
1	A	241	ARG	CA-C-N	8.08	130.94	120.44
1	A	241	ARG	C-N-CA	8.08	130.94	120.44
1	B	248	LYS	N-CA-C	8.04	123.56	113.43
1	D	248	LYS	N-CA-C	8.03	123.55	113.43
1	D	297	TYR	CA-C-O	8.04	130.51	121.11
1	B	297	TYR	CA-C-O	7.96	130.43	121.11
1	A	344	SER	CA-C-N	7.92	130.89	120.28
1	A	344	SER	C-N-CA	7.92	130.89	120.28
1	D	13	ASP	CB-CA-C	7.88	122.42	111.86
1	B	239	GLU	CA-C-N	7.87	131.47	120.29
1	B	239	GLU	C-N-CA	7.87	131.47	120.29
1	D	239	GLU	CA-C-N	7.85	131.44	120.29
1	D	239	GLU	C-N-CA	7.85	131.44	120.29
1	D	88	ASN	CA-C-N	7.85	130.64	120.44
1	D	88	ASN	C-N-CA	7.85	130.64	120.44
1	B	13	ASP	CB-CA-C	7.84	122.36	111.86
1	C	344	SER	CA-C-N	7.83	130.78	120.28
1	C	344	SER	C-N-CA	7.83	130.78	120.28
1	D	75	MET	CA-C-N	7.83	131.09	120.44
1	D	75	MET	C-N-CA	7.83	131.09	120.44
1	B	75	MET	CA-C-N	7.82	131.08	120.44
1	B	75	MET	C-N-CA	7.82	131.08	120.44
1	B	88	ASN	CA-C-N	7.81	130.60	120.44
1	B	88	ASN	C-N-CA	7.81	130.60	120.44
1	D	89	HIS	CA-CB-CG	-7.79	106.01	113.80
1	B	89	HIS	CA-CB-CG	-7.78	106.03	113.80
1	B	136	ALA	O-C-N	-7.76	114.08	122.07
1	A	225	HIS	N-CA-C	7.75	120.81	111.82
1	D	207	HIS	CG-CD2-NE2	7.74	114.94	107.20
1	C	225	HIS	N-CA-C	7.72	120.78	111.82
1	A	233	ARG	CA-C-N	7.71	130.62	120.28
1	A	233	ARG	C-N-CA	7.71	130.62	120.28
1	C	233	ARG	CA-C-N	7.69	130.59	120.28
1	C	233	ARG	C-N-CA	7.69	130.59	120.28
1	C	278	ASN	O-C-N	-7.68	113.79	122.86
1	D	136	ALA	O-C-N	-7.68	114.16	122.07
1	C	324	GLU	CA-C-O	7.68	128.69	120.55
1	A	278	ASN	O-C-N	-7.67	113.81	122.86
1	C	177	ILE	O-C-N	-7.67	114.38	121.89
1	C	179	VAL	O-C-N	-7.65	114.45	121.87
1	A	179	VAL	O-C-N	-7.65	114.45	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	GLU	CA-C-O	7.63	128.64	120.55
1	B	207	HIS	CG-CD2-NE2	7.61	114.81	107.20
1	B	68	ARG	NE-CZ-NH2	7.60	126.04	119.20
1	A	177	ILE	O-C-N	-7.59	114.45	121.89
1	A	167	ARG	CA-C-O	7.56	128.76	120.82
1	B	195	LEU	CA-C-N	7.54	130.79	120.46
1	B	195	LEU	C-N-CA	7.54	130.79	120.46
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	C	167	ARG	CA-C-O	7.53	128.73	120.82
1	D	50	ARG	CA-C-N	7.53	130.37	120.28
1	D	50	ARG	C-N-CA	7.53	130.37	120.28
1	B	50	ARG	CA-C-N	7.53	130.37	120.28
1	B	50	ARG	C-N-CA	7.53	130.37	120.28
1	D	68	ARG	NE-CZ-NH2	7.51	125.96	119.20
1	C	213	LEU	CA-C-N	7.49	130.93	120.29
1	C	213	LEU	C-N-CA	7.49	130.93	120.29
1	A	213	LEU	CA-C-N	7.49	130.92	120.29
1	A	213	LEU	C-N-CA	7.49	130.92	120.29
1	D	206	GLY	CA-C-N	7.44	130.25	120.28
1	D	206	GLY	C-N-CA	7.44	130.25	120.28
1	B	206	GLY	CA-C-N	7.42	130.22	120.28
1	B	206	GLY	C-N-CA	7.42	130.22	120.28
1	A	18	ARG	N-CA-CB	-7.39	99.25	110.12
1	C	39	LEU	CB-CA-C	-7.36	98.58	110.79
1	C	18	ARG	N-CA-CB	-7.36	99.31	110.12
1	A	39	LEU	CB-CA-C	-7.33	98.63	110.79
1	B	89	HIS	CA-C-O	7.27	128.45	120.82
1	A	136	ALA	N-CA-C	7.25	120.23	111.82
1	A	225	HIS	CA-CB-CG	7.24	121.03	113.80
1	D	89	HIS	CA-C-O	7.23	128.41	120.82
1	C	136	ALA	N-CA-C	7.20	120.17	111.82
1	A	163	ARG	NE-CZ-NH1	7.18	128.68	121.50
1	A	355	VAL	N-CA-CB	7.17	121.33	110.58
1	C	225	HIS	CA-CB-CG	7.17	120.97	113.80
1	B	103	HIS	CA-C-N	7.16	130.21	120.54
1	B	103	HIS	C-N-CA	7.16	130.21	120.54
1	C	241	ARG	CA-C-O	7.14	128.18	119.97
1	C	81	GLU	N-CA-C	7.14	119.06	111.28
1	C	355	VAL	N-CA-CB	7.14	121.29	110.58
1	B	58	ALA	CA-C-N	7.13	129.71	120.44
1	B	58	ALA	C-N-CA	7.13	129.71	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	187	ASP	CA-CB-CG	7.13	119.73	112.60
1	A	61	VAL	N-CA-CB	7.12	119.37	110.47
1	D	140	HIS	CA-C-N	7.12	132.61	120.72
1	D	140	HIS	C-N-CA	7.12	132.61	120.72
1	B	140	HIS	CA-C-N	7.11	132.60	120.72
1	B	140	HIS	C-N-CA	7.11	132.60	120.72
1	A	241	ARG	CA-C-O	7.11	128.15	119.97
1	C	163	ARG	NE-CZ-NH1	7.11	128.61	121.50
1	D	94	HIS	CA-C-O	7.11	127.96	120.42
1	D	103	HIS	CA-C-N	7.11	130.13	120.54
1	D	103	HIS	C-N-CA	7.11	130.13	120.54
1	D	58	ALA	CA-C-N	7.10	129.67	120.44
1	D	58	ALA	C-N-CA	7.10	129.67	120.44
1	C	61	VAL	N-CA-CB	7.10	119.34	110.47
1	B	94	HIS	CA-C-O	7.08	127.93	120.42
1	A	112	LEU	N-CA-C	7.08	118.64	111.07
1	B	17	PHE	CA-C-N	7.07	130.06	120.38
1	B	17	PHE	C-N-CA	7.07	130.06	120.38
1	C	112	LEU	N-CA-C	7.07	118.63	111.07
1	A	81	GLU	N-CA-C	7.05	118.97	111.28
1	A	187	ASP	CA-CB-CG	7.05	119.65	112.60
1	D	17	PHE	CA-C-N	7.05	130.04	120.38
1	D	17	PHE	C-N-CA	7.05	130.04	120.38
1	A	167	ARG	CA-C-N	7.03	127.93	119.99
1	A	167	ARG	C-N-CA	7.03	127.93	119.99
1	A	177	ILE	N-CA-CB	-7.02	101.69	110.47
1	C	167	ARG	CA-C-N	7.00	127.90	119.99
1	C	167	ARG	C-N-CA	7.00	127.90	119.99
1	A	163	ARG	NH1-CZ-NH2	-6.99	110.21	119.30
1	D	75	MET	O-C-N	-6.99	114.18	122.15
1	C	177	ILE	N-CA-CB	-6.95	101.78	110.47
1	B	75	MET	O-C-N	-6.95	114.23	122.15
1	C	163	ARG	NH1-CZ-NH2	-6.95	110.27	119.30
1	A	218	LYS	O-C-N	-6.94	114.81	122.03
1	C	218	LYS	O-C-N	-6.93	114.82	122.03
1	B	224	LEU	O-C-N	-6.92	114.78	122.12
1	D	224	LEU	O-C-N	-6.91	114.80	122.12
1	C	150	GLN	CA-C-N	6.89	130.08	120.29
1	C	150	GLN	C-N-CA	6.89	130.08	120.29
1	A	150	GLN	CA-C-N	6.89	130.08	120.29
1	A	150	GLN	C-N-CA	6.89	130.08	120.29
1	D	51	HIS	N-CA-CB	6.88	120.24	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	HIS	N-CA-CB	6.88	120.23	110.12
1	A	31	LEU	CA-C-N	6.85	129.46	120.28
1	A	31	LEU	C-N-CA	6.85	129.46	120.28
1	C	51	HIS	N-CA-C	6.83	118.81	111.36
1	B	229	LEU	CA-C-N	6.83	129.76	120.54
1	B	229	LEU	C-N-CA	6.83	129.76	120.54
1	D	72	PRO	N-CA-CB	-6.83	96.08	103.25
1	A	51	HIS	N-CA-C	6.82	118.79	111.36
1	C	65	ASP	CA-C-N	6.81	129.96	120.29
1	C	65	ASP	C-N-CA	6.81	129.96	120.29
1	B	65	ASP	CA-C-N	6.81	129.40	120.28
1	B	65	ASP	C-N-CA	6.81	129.40	120.28
1	D	65	ASP	CA-C-N	6.81	129.40	120.28
1	D	65	ASP	C-N-CA	6.81	129.40	120.28
1	A	309	VAL	CA-C-N	6.80	129.69	120.38
1	A	309	VAL	C-N-CA	6.80	129.69	120.38
1	B	237	ASP	CA-CB-CG	-6.80	105.80	112.60
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	C	161	THR	CA-C-N	6.79	129.27	120.44
1	C	161	THR	C-N-CA	6.79	129.27	120.44
1	C	31	LEU	CA-C-N	6.79	129.38	120.28
1	C	31	LEU	C-N-CA	6.79	129.38	120.28
1	D	303	ASP	N-CA-CB	-6.79	99.63	111.17
1	C	233	ARG	N-CA-C	6.79	118.68	111.28
1	B	72	PRO	N-CA-CB	-6.79	96.12	103.25
1	A	65	ASP	CA-C-N	6.78	129.92	120.29
1	A	65	ASP	C-N-CA	6.78	129.92	120.29
1	B	303	ASP	N-CA-CB	-6.77	99.66	111.17
1	C	309	VAL	CA-C-N	6.77	129.65	120.38
1	C	309	VAL	C-N-CA	6.77	129.65	120.38
1	A	161	THR	CA-C-N	6.76	129.24	120.44
1	A	161	THR	C-N-CA	6.76	129.24	120.44
1	A	18	ARG	NE-CZ-NH2	-6.76	113.12	119.20
1	C	227	LEU	N-CA-C	6.75	119.22	111.11
1	D	237	ASP	CA-CB-CG	-6.75	105.85	112.60
1	A	273	PHE	CA-CB-CG	-6.73	107.07	113.80
1	C	18	ARG	NE-CZ-NH2	-6.73	113.14	119.20
1	C	89	HIS	CE1-NE2-CD2	-6.73	102.27	109.00
1	D	7	PHE	CA-CB-CG	6.73	120.53	113.80
1	C	273	PHE	CA-CB-CG	-6.72	107.08	113.80
1	A	227	LEU	N-CA-C	6.72	119.18	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	110	GLN	OE1-CD-NE2	-6.70	115.90	122.60
1	A	149	ALA	N-CA-C	6.70	122.42	111.37
1	A	189	MET	CA-C-N	6.70	129.26	120.28
1	A	189	MET	C-N-CA	6.70	129.26	120.28
1	C	189	MET	CA-C-N	6.70	129.26	120.28
1	C	189	MET	C-N-CA	6.70	129.26	120.28
1	A	233	ARG	N-CA-C	6.70	118.58	111.28
1	C	149	ALA	N-CA-C	6.70	122.42	111.37
1	A	191	PHE	CA-CB-CG	-6.69	107.11	113.80
1	B	110	GLN	OE1-CD-NE2	-6.68	115.92	122.60
1	A	137	ALA	CA-C-O	6.67	127.83	120.82
1	A	89	HIS	CE1-NE2-CD2	-6.67	102.33	109.00
1	C	191	PHE	CA-CB-CG	-6.67	107.13	113.80
1	B	320	CYS	CA-C-O	-6.66	115.35	120.48
1	B	127	PHE	N-CA-C	6.65	118.19	111.07
1	D	320	CYS	CA-C-O	-6.65	115.36	120.48
1	B	7	PHE	CA-CB-CG	6.64	120.44	113.80
1	D	127	PHE	N-CA-C	6.62	118.16	111.07
1	C	137	ALA	CA-C-O	6.62	127.77	120.82
1	D	292	SER	N-CA-C	6.61	120.29	111.30
1	A	117	LEU	CA-C-N	6.61	129.37	120.65
1	A	117	LEU	C-N-CA	6.61	129.37	120.65
1	B	209	GLU	N-CA-C	6.61	118.27	111.14
1	B	292	SER	N-CA-C	6.60	120.28	111.30
1	C	117	LEU	CA-C-N	6.60	129.36	120.65
1	C	117	LEU	C-N-CA	6.60	129.36	120.65
1	B	19	ALA	CA-C-O	6.57	127.54	119.79
1	C	22	GLU	CA-C-N	6.55	129.06	120.28
1	C	22	GLU	C-N-CA	6.55	129.06	120.28
1	D	19	ALA	CA-C-O	6.55	127.52	119.79
1	C	183	LYS	N-CA-C	6.55	118.42	111.28
1	B	3	VAL	CB-CA-C	-6.55	104.39	111.59
1	D	356	GLN	N-CA-C	6.54	119.23	111.71
1	C	108	GLN	CA-C-N	6.54	129.04	120.60
1	C	108	GLN	C-N-CA	6.54	129.04	120.60
1	D	3	VAL	CB-CA-C	-6.54	104.40	111.59
1	A	108	GLN	CA-C-N	6.54	129.03	120.60
1	A	108	GLN	C-N-CA	6.54	129.03	120.60
1	D	132	GLU	O-C-N	6.53	129.15	122.09
1	A	183	LYS	N-CA-C	6.53	118.40	111.28
1	B	356	GLN	N-CA-C	6.53	119.22	111.71
1	A	22	GLU	CA-C-N	6.52	129.02	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	GLU	C-N-CA	6.52	129.02	120.28
1	D	209	GLU	N-CA-C	6.51	118.18	111.14
1	B	23	LEU	N-CA-CB	-6.49	100.31	110.30
1	C	293	ASN	OD1-CG-ND2	-6.47	116.13	122.60
1	D	23	LEU	N-CA-CB	-6.47	100.34	110.30
1	B	258	SER	CA-C-N	6.45	131.51	122.41
1	B	258	SER	C-N-CA	6.45	131.51	122.41
1	D	199	GLN	O-C-N	-6.45	115.28	122.12
1	B	132	GLU	O-C-N	6.45	129.06	122.09
1	D	199	GLN	CA-C-O	6.44	127.38	120.55
1	A	298	GLN	CA-C-N	6.43	129.54	120.28
1	A	298	GLN	C-N-CA	6.43	129.54	120.28
1	A	125	ARG	CA-C-N	6.43	128.89	120.28
1	A	125	ARG	C-N-CA	6.43	128.89	120.28
1	B	115	GLU	O-C-N	-6.43	115.87	121.85
1	B	199	GLN	O-C-N	-6.41	115.32	122.12
1	D	258	SER	CA-C-N	6.41	131.44	122.41
1	D	258	SER	C-N-CA	6.41	131.44	122.41
1	C	125	ARG	CA-C-N	6.40	128.85	120.28
1	C	125	ARG	C-N-CA	6.40	128.85	120.28
1	A	139	THR	CA-C-O	6.39	127.32	120.55
1	A	120	PHE	O-C-N	-6.38	115.50	122.07
1	C	298	GLN	CA-C-N	6.38	129.47	120.28
1	C	298	GLN	C-N-CA	6.38	129.47	120.28
1	D	115	GLU	O-C-N	-6.38	115.92	121.85
1	C	139	THR	CA-C-O	6.38	127.31	120.55
1	B	199	GLN	CA-C-O	6.37	127.30	120.55
1	D	207	HIS	CE1-NE2-CD2	-6.36	102.64	109.00
1	D	94	HIS	CE1-NE2-CD2	-6.36	102.64	109.00
1	B	353	SER	O-C-N	-6.34	114.92	122.15
1	D	353	SER	O-C-N	-6.34	114.92	122.15
1	C	120	PHE	O-C-N	-6.33	115.55	122.07
1	A	293	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	B	94	HIS	CE1-NE2-CD2	-6.32	102.68	109.00
1	B	185	LYS	N-CA-C	6.32	117.83	111.07
1	B	184	ARG	O-C-N	-6.31	115.43	122.12
1	B	207	HIS	CE1-NE2-CD2	-6.29	102.71	109.00
1	A	7	PHE	CA-C-N	6.28	129.33	120.28
1	A	7	PHE	C-N-CA	6.28	129.33	120.28
1	D	185	LYS	N-CA-C	6.28	117.79	111.07
1	B	225	HIS	O-C-N	-6.28	114.99	122.15
1	C	306	THR	N-CA-C	6.28	119.72	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	184	ARG	O-C-N	-6.28	115.47	122.12
1	D	225	HIS	O-C-N	-6.27	115.00	122.15
1	C	7	PHE	CA-C-N	6.27	129.31	120.28
1	C	7	PHE	C-N-CA	6.27	129.31	120.28
1	A	21	ILE	N-CA-CB	6.26	118.29	110.47
1	C	26	ALA	CA-C-O	6.25	127.04	120.42
1	D	124	ARG	NE-CZ-NH2	-6.25	113.58	119.20
1	A	306	THR	N-CA-C	6.24	119.66	109.24
1	B	124	ARG	NE-CZ-NH2	-6.23	113.59	119.20
1	D	153	GLU	CA-C-N	6.22	129.12	120.29
1	D	153	GLU	C-N-CA	6.22	129.12	120.29
1	C	108	GLN	OE1-CD-NE2	-6.22	116.38	122.60
1	A	26	ALA	CA-C-O	6.21	127.01	120.42
1	B	153	GLU	CA-C-N	6.21	129.12	120.29
1	B	153	GLU	C-N-CA	6.21	129.12	120.29
1	C	21	ILE	N-CA-CB	6.21	118.23	110.47
1	C	207	HIS	CG-CD2-NE2	6.21	113.41	107.20
1	C	293	ASN	CB-CA-C	6.19	121.45	111.36
1	D	2	THR	CA-C-N	6.18	129.79	120.95
1	D	2	THR	C-N-CA	6.18	129.79	120.95
1	D	146	ARG	N-CA-C	6.18	118.81	111.33
1	B	145	PRO	CA-C-O	-6.18	114.58	121.32
1	A	108	GLN	OE1-CD-NE2	-6.17	116.43	122.60
1	B	146	ARG	N-CA-C	6.17	118.80	111.33
1	A	207	HIS	CG-CD2-NE2	6.17	113.37	107.20
1	C	275	ARG	O-C-N	-6.16	115.84	123.36
1	D	145	PRO	CA-C-O	-6.16	114.60	121.32
1	B	2	THR	CA-C-N	6.16	129.76	120.95
1	B	2	THR	C-N-CA	6.16	129.76	120.95
1	A	293	ASN	CB-CA-C	6.15	121.39	111.36
1	D	248	LYS	CA-C-O	6.14	126.94	119.64
1	B	248	LYS	CA-C-O	6.13	126.94	119.64
1	C	24	VAL	CA-C-N	6.11	129.08	120.28
1	C	24	VAL	C-N-CA	6.11	129.08	120.28
1	A	275	ARG	O-C-N	-6.11	115.91	123.36
1	A	201	THR	N-CA-CB	6.09	119.18	110.16
1	C	201	THR	N-CA-CB	6.09	119.17	110.16
1	D	101	THR	O-C-N	-6.09	115.67	122.12
1	A	256	GLU	N-CA-CB	-6.09	100.53	109.90
1	B	101	THR	O-C-N	-6.08	115.67	122.12
1	C	261	GLU	CA-C-N	6.08	131.41	121.87
1	C	261	GLU	C-N-CA	6.08	131.41	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	52	TYR	CB-CA-C	6.08	120.50	110.90
1	A	330	GLU	O-C-N	-6.07	115.86	123.27
1	D	354	ALA	O-C-N	-6.07	115.23	122.15
1	B	52	TYR	CB-CA-C	6.06	120.48	110.90
1	C	330	GLU	CB-CG-CD	6.06	122.90	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	A	261	GLU	CA-C-N	6.05	131.36	121.87
1	A	261	GLU	C-N-CA	6.05	131.36	121.87
1	C	256	GLU	N-CA-CB	-6.04	100.60	109.90
1	D	313	ARG	CA-C-O	6.04	126.80	119.31
1	A	217	ARG	N-CA-C	-6.03	104.61	111.07
1	C	330	GLU	O-C-N	-6.03	115.91	123.27
1	A	24	VAL	CA-C-N	6.03	128.97	120.28
1	A	24	VAL	C-N-CA	6.03	128.97	120.28
1	D	104	THR	CA-C-N	6.03	128.64	120.44
1	D	104	THR	C-N-CA	6.03	128.64	120.44
1	A	48	SER	CA-C-N	6.03	126.63	119.94
1	A	48	SER	C-N-CA	6.03	126.63	119.94
1	A	330	GLU	CB-CG-CD	6.03	122.84	112.60
1	B	104	THR	CA-C-N	6.02	128.63	120.44
1	B	104	THR	C-N-CA	6.02	128.63	120.44
1	A	137	ALA	O-C-N	-6.01	115.88	122.07
1	A	228	VAL	O-C-N	-6.01	116.02	121.91
1	B	140	HIS	CA-CB-CG	6.01	119.81	113.80
1	B	354	ALA	O-C-N	-6.00	115.31	122.15
1	A	224	LEU	O-C-N	-6.00	115.76	122.12
1	C	129	ARG	N-CA-C	6.00	118.61	111.71
1	C	137	ALA	O-C-N	-5.99	115.90	122.07
1	D	53	LEU	O-C-N	-5.99	115.77	122.12
1	A	129	ARG	N-CA-C	5.99	118.60	111.71
1	C	224	LEU	O-C-N	-5.98	115.78	122.12
1	C	228	VAL	O-C-N	-5.97	116.06	121.91
1	D	36	GLU	O-C-N	-5.97	114.93	122.27
1	B	36	GLU	O-C-N	-5.97	114.93	122.27
1	B	313	ARG	CA-C-O	5.96	126.70	119.31
1	C	217	ARG	N-CA-C	-5.96	104.69	111.07
1	D	336	LYS	O-C-N	-5.96	116.44	123.41
1	A	149	ALA	CB-CA-C	-5.95	100.86	110.74
1	B	53	LEU	O-C-N	-5.95	115.81	122.12
1	C	5	LEU	CA-C-O	-5.95	113.94	120.36
1	C	149	ALA	CB-CA-C	-5.95	100.87	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	43	THR	N-CA-C	5.94	118.71	111.82
1	C	247	GLN	CA-C-N	-5.93	110.20	121.54
1	C	247	GLN	C-N-CA	-5.93	110.20	121.54
1	D	269	GLU	N-CA-CB	5.93	121.75	111.13
1	D	140	HIS	CA-CB-CG	5.93	119.73	113.80
1	D	100	ALA	CA-C-O	5.92	126.70	120.42
1	B	186	PHE	CA-C-O	5.92	126.78	119.79
1	C	194	ARG	CB-CA-C	-5.92	100.79	110.85
1	A	194	ARG	CB-CA-C	-5.91	100.80	110.85
1	B	269	GLU	N-CA-CB	5.91	121.72	111.13
1	B	90	LYS	CB-CA-C	5.91	120.60	110.79
1	A	5	LEU	CA-C-O	-5.90	113.98	120.36
1	B	336	LYS	O-C-N	-5.90	116.50	123.41
1	A	43	THR	N-CA-C	5.90	118.66	111.82
1	D	90	LYS	CB-CA-C	5.90	120.58	110.79
1	C	320	CYS	O-C-N	-5.89	115.23	121.30
1	D	186	PHE	CA-C-O	5.89	126.74	119.79
1	A	320	CYS	O-C-N	-5.89	115.23	121.30
1	D	54	ALA	N-CA-C	5.89	117.70	111.28
1	A	326	ARG	NE-CZ-NH2	-5.89	113.90	119.20
1	D	173	TYR	CB-CA-C	5.89	120.20	110.90
1	C	326	ARG	NE-CZ-NH2	-5.88	113.90	119.20
1	A	247	GLN	CA-C-N	-5.88	110.30	121.54
1	A	247	GLN	C-N-CA	-5.88	110.30	121.54
1	B	54	ALA	N-CA-C	5.87	117.68	111.28
1	B	100	ALA	CA-C-O	5.87	126.64	120.42
1	D	327	PHE	N-CA-C	-5.87	106.07	113.23
1	C	174	ALA	N-CA-C	5.87	117.68	111.28
1	B	173	TYR	CB-CA-C	5.86	120.16	110.90
1	B	84	THR	CA-C-O	-5.86	113.74	120.24
1	B	133	SER	N-CA-C	5.86	117.67	111.28
1	A	207	HIS	ND1-CE1-NE2	5.85	114.25	108.40
1	B	169	ARG	NH1-CZ-NH2	-5.85	111.69	119.30
1	A	61	VAL	N-CA-C	5.85	117.28	110.62
1	C	153	GLU	CA-C-N	5.84	128.04	120.44
1	C	153	GLU	C-N-CA	5.84	128.04	120.44
1	B	327	PHE	N-CA-C	-5.84	106.11	113.23
1	C	13	ASP	CB-CA-C	5.83	119.68	111.86
1	D	133	SER	N-CA-C	5.83	117.63	111.28
1	A	13	ASP	CB-CA-C	5.82	119.66	111.86
1	A	20	SER	N-CA-CB	5.82	118.77	110.16
1	C	61	VAL	N-CA-C	5.81	117.25	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	ALA	N-CA-C	5.81	117.61	111.28
1	B	110	GLN	O-C-N	5.80	128.27	122.12
1	B	313	ARG	N-CA-C	-5.80	105.70	112.89
1	D	84	THR	CA-C-O	-5.80	113.80	120.24
1	C	207	HIS	ND1-CE1-NE2	5.80	114.20	108.40
1	D	169	ARG	NH1-CZ-NH2	-5.79	111.77	119.30
1	B	334	THR	N-CA-C	5.79	118.06	111.11
1	D	313	ARG	N-CA-CB	-5.79	100.96	110.40
1	C	70	GLY	N-CA-C	5.79	119.23	112.23
1	C	343	ASP	O-C-N	-5.78	113.98	122.43
1	C	-2	LEU	N-CA-CB	-5.78	101.88	110.61
1	B	74	PRO	N-CA-C	5.78	124.38	112.47
1	A	72	PRO	CA-N-CD	5.78	120.09	112.00
1	C	243	VAL	N-CA-CB	5.78	117.31	110.55
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	A	-2	LEU	N-CA-CB	-5.77	101.90	110.61
1	B	68	ARG	NH1-CZ-NH2	-5.77	111.80	119.30
1	C	72	PRO	CA-N-CD	5.77	120.08	112.00
1	A	153	GLU	CA-C-N	5.77	127.94	120.44
1	A	153	GLU	C-N-CA	5.77	127.94	120.44
1	B	92	ASP	N-CA-C	5.77	117.57	111.28
1	A	70	GLY	N-CA-C	5.76	119.20	112.23
1	A	343	ASP	O-C-N	-5.76	114.02	122.43
1	B	313	ARG	NE-CZ-NH2	5.76	124.38	119.20
1	C	20	SER	N-CA-CB	5.76	118.68	110.16
1	D	74	PRO	N-CA-C	5.76	124.33	112.47
1	D	92	ASP	N-CA-C	5.75	117.55	111.28
1	D	110	GLN	O-C-N	5.75	128.22	122.12
1	B	99	ASP	CA-CB-CG	-5.75	106.85	112.60
1	D	99	ASP	CA-CB-CG	-5.75	106.85	112.60
1	A	243	VAL	N-CA-CB	5.75	117.28	110.55
1	C	357	SER	O-C-N	-5.75	116.11	122.09
1	D	313	ARG	N-CA-C	-5.75	105.76	112.89
1	B	313	ARG	N-CA-CB	-5.75	101.03	110.40
1	D	334	THR	N-CA-C	5.75	118.00	111.11
1	A	211	SER	CA-C-N	5.74	127.98	120.28
1	A	211	SER	C-N-CA	5.74	127.98	120.28
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	B	288	PHE	CD1-CG-CD2	5.74	127.21	118.60
1	C	187	ASP	CA-C-O	5.73	126.84	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	ASP	CA-C-O	5.73	126.84	120.82
1	D	68	ARG	NH1-CZ-NH2	-5.73	111.85	119.30
1	A	357	SER	O-C-N	-5.73	116.13	122.09
1	B	135	GLU	CA-C-N	5.73	127.89	120.44
1	B	135	GLU	C-N-CA	5.73	127.89	120.44
1	D	288	PHE	CD1-CG-CD2	5.72	127.18	118.60
1	D	89	HIS	CG-CD2-NE2	5.72	112.92	107.20
1	D	186	PHE	CB-CG-CD2	-5.72	110.98	120.70
1	C	112	LEU	O-C-N	-5.71	116.19	122.07
1	A	112	LEU	O-C-N	-5.71	116.19	122.07
1	B	186	PHE	CB-CG-CD2	-5.71	111.00	120.70
1	C	241	ARG	N-CA-C	5.70	118.43	111.82
1	D	313	ARG	NE-CZ-NH2	5.69	124.33	119.20
1	D	54	ALA	CA-C-N	5.69	128.22	120.54
1	D	54	ALA	C-N-CA	5.69	128.22	120.54
1	A	241	ARG	N-CA-C	5.68	118.42	111.82
1	D	323	SER	N-CA-C	5.68	118.07	110.35
1	D	50	ARG	N-CA-C	5.68	118.41	111.82
1	B	50	ARG	N-CA-C	5.67	118.40	111.82
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	A	145	PRO	O-C-N	-5.66	115.92	123.06
1	C	258	SER	N-CA-C	5.66	117.87	108.20
1	A	46	LEU	CA-C-N	5.66	127.79	120.44
1	A	46	LEU	C-N-CA	5.66	127.79	120.44
1	B	89	HIS	CG-CD2-NE2	5.65	112.85	107.20
1	C	68	ARG	N-CA-CB	5.65	118.43	110.12
1	B	323	SER	N-CA-C	5.65	118.03	110.35
1	A	258	SER	N-CA-C	5.64	117.85	108.20
1	B	54	ALA	CA-C-N	5.63	128.15	120.54
1	B	54	ALA	C-N-CA	5.63	128.15	120.54
1	A	68	ARG	N-CA-CB	5.62	118.39	110.12
1	C	257	PRO	O-C-N	5.62	129.47	123.01
1	A	63	ILE	CB-CA-C	-5.62	104.56	112.14
1	B	124	ARG	N-CA-C	5.61	117.07	111.07
1	C	89	HIS	CA-CB-CG	5.61	119.41	113.80
1	D	24	VAL	O-C-N	-5.60	115.47	121.80
1	D	293	ASN	CA-CB-CG	-5.60	107.00	112.60
1	B	24	VAL	O-C-N	-5.60	115.47	121.80
1	C	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	159	LEU	CA-C-N	5.60	128.09	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	159	LEU	C-N-CA	5.60	128.09	120.54
1	C	57	ARG	NE-CZ-NH2	-5.59	114.17	119.20
1	D	124	ARG	N-CA-C	5.59	117.05	111.07
1	B	49	GLY	N-CA-C	-5.59	106.02	112.50
1	C	46	LEU	CA-C-N	5.59	127.70	120.44
1	C	46	LEU	C-N-CA	5.59	127.70	120.44
1	B	303	ASP	CA-C-N	5.58	126.82	119.84
1	B	303	ASP	C-N-CA	5.58	126.82	119.84
1	D	88	ASN	CA-CB-CG	-5.58	107.02	112.60
1	B	37	LYS	O-C-N	-5.58	116.33	122.07
1	A	-1	GLY	N-CA-C	5.58	118.34	111.93
1	A	288	PHE	N-CA-CB	5.57	119.26	110.56
1	A	291	GLN	N-CA-CB	5.57	120.17	110.81
1	C	292	SER	CA-C-O	5.57	127.91	121.28
1	D	89	HIS	CE1-NE2-CD2	-5.57	103.43	109.00
1	B	293	ASN	CA-CB-CG	-5.57	107.03	112.60
1	B	159	LEU	CA-C-N	5.57	128.06	120.54
1	B	159	LEU	C-N-CA	5.57	128.06	120.54
1	A	290	ILE	CB-CA-C	-5.57	103.35	110.98
1	B	127	PHE	CA-C-N	5.57	128.19	120.29
1	B	127	PHE	C-N-CA	5.57	128.19	120.29
1	C	67	ALA	CA-C-O	-5.57	114.97	120.82
1	C	291	GLN	N-CA-CB	5.57	120.16	110.81
1	D	303	ASP	CA-C-N	5.57	126.80	119.84
1	D	303	ASP	C-N-CA	5.57	126.80	119.84
1	C	290	ILE	CB-CA-C	-5.56	103.36	110.98
1	A	67	ALA	CA-C-O	-5.55	114.99	120.82
1	D	319	LEU	CB-CA-C	-5.55	100.82	110.09
1	A	210	LEU	CB-CA-C	5.55	119.95	110.74
1	B	199	GLN	OE1-CD-NE2	-5.55	117.05	122.60
1	A	358	SER	CA-C-N	5.55	128.06	120.46
1	A	358	SER	C-N-CA	5.55	128.06	120.46
1	B	88	ASN	CA-CB-CG	-5.54	107.06	112.60
1	C	98	LEU	N-CA-CB	5.54	118.36	110.16
1	A	89	HIS	CA-CB-CG	5.54	119.34	113.80
1	B	89	HIS	CE1-NE2-CD2	-5.54	103.46	109.00
1	D	49	GLY	N-CA-C	-5.54	106.08	112.50
1	D	127	PHE	CA-C-N	5.54	128.15	120.29
1	D	127	PHE	C-N-CA	5.54	128.15	120.29
1	A	169	ARG	NE-CZ-NH1	-5.53	115.97	121.50
1	B	319	LEU	CB-CA-C	-5.53	100.86	110.09
1	A	292	SER	CA-C-O	5.51	127.84	121.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	HIS	O-C-N	-5.51	115.86	122.15
1	D	199	GLN	OE1-CD-NE2	-5.51	117.09	122.60
1	C	358	SER	CA-C-N	5.51	128.01	120.46
1	C	358	SER	C-N-CA	5.51	128.01	120.46
1	D	132	GLU	CB-CG-CD	-5.51	103.23	112.60
1	B	132	GLU	CB-CG-CD	-5.51	103.23	112.60
1	C	-1	GLY	N-CA-C	5.51	118.26	111.93
1	D	60	VAL	O-C-N	-5.51	115.58	121.80
1	B	160	ARG	CA-C-O	5.50	126.79	120.90
1	A	98	LEU	N-CA-CB	5.50	118.29	110.16
1	D	94	HIS	O-C-N	-5.50	115.88	122.15
1	D	160	ARG	CA-C-O	5.49	126.78	120.90
1	D	186	PHE	N-CA-C	5.49	119.15	112.23
1	C	169	ARG	NE-CZ-NH1	-5.49	116.01	121.50
1	B	186	PHE	N-CA-C	5.47	119.13	112.23
1	A	363	PHE	O-C-N	5.47	130.01	122.46
1	A	57	ARG	NE-CZ-NH2	-5.47	114.28	119.20
1	D	108	GLN	O-C-N	-5.47	115.73	122.19
1	D	37	LYS	O-C-N	-5.47	116.44	122.07
1	C	226	GLN	N-CA-CB	-5.46	102.07	110.16
1	C	83	PHE	N-CA-CB	5.46	117.93	110.01
1	C	38	LEU	O-C-N	-5.46	115.93	122.15
1	B	60	VAL	O-C-N	-5.45	115.64	121.80
1	C	51	HIS	CA-C-O	-5.45	114.65	120.42
1	A	226	GLN	N-CA-CB	-5.44	102.11	110.16
1	B	108	GLN	O-C-N	-5.44	115.77	122.19
1	A	83	PHE	N-CA-CB	5.43	117.89	110.01
1	C	363	PHE	O-C-N	5.43	129.96	122.46
1	A	343	ASP	CA-C-O	5.43	126.06	119.11
1	A	38	LEU	O-C-N	-5.43	115.96	122.15
1	A	51	HIS	CA-C-O	-5.43	114.67	120.42
1	D	354	ALA	CA-C-O	5.42	126.17	120.42
1	B	152	ALA	N-CA-C	5.41	117.18	111.28
1	B	249	GLU	O-C-N	-5.41	115.64	122.19
1	B	65	ASP	CA-CB-CG	-5.41	107.19	112.60
1	D	329	PHE	CA-CB-CG	5.41	119.21	113.80
1	D	66	LEU	CA-C-O	5.40	126.28	120.55
1	D	213	LEU	CA-C-N	5.40	127.52	120.28
1	D	213	LEU	C-N-CA	5.40	127.52	120.28
1	D	359	ILE	CB-CA-C	-5.40	103.79	112.16
1	C	17	PHE	CA-CB-CG	-5.40	108.40	113.80
1	D	152	ALA	N-CA-C	5.38	117.14	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	ALA	CA-C-O	-5.38	114.27	120.24
1	B	354	ALA	CA-C-O	5.38	126.12	120.42
1	D	162	ALA	CA-C-O	-5.38	114.82	120.63
1	B	66	LEU	CA-C-O	5.38	126.25	120.55
1	A	101	THR	CA-CB-OG1	5.37	117.66	109.60
1	A	230	ASN	CA-C-N	5.37	127.92	120.29
1	A	230	ASN	C-N-CA	5.37	127.92	120.29
1	C	343	ASP	CA-C-O	5.37	125.99	119.11
1	C	123	ALA	CA-C-N	5.37	127.48	120.28
1	C	123	ALA	C-N-CA	5.37	127.48	120.28
1	B	329	PHE	CA-CB-CG	5.37	119.17	113.80
1	A	17	PHE	CA-CB-CG	-5.37	108.43	113.80
1	A	312	LEU	N-CA-CB	-5.37	102.80	110.80
1	C	101	THR	CA-C-N	5.37	127.42	120.44
1	C	101	THR	C-N-CA	5.37	127.42	120.44
1	B	6	ASP	CA-C-N	5.36	130.53	121.14
1	B	6	ASP	C-N-CA	5.36	130.53	121.14
1	D	344	SER	CA-C-N	5.36	127.91	120.29
1	D	344	SER	C-N-CA	5.36	127.91	120.29
1	A	12	LYS	CA-C-N	5.36	129.79	122.34
1	A	12	LYS	C-N-CA	5.36	129.79	122.34
1	B	213	LEU	CA-C-N	5.36	127.46	120.28
1	B	213	LEU	C-N-CA	5.36	127.46	120.28
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	D	221	GLY	CA-C-N	5.36	127.90	120.29
1	D	221	GLY	C-N-CA	5.36	127.90	120.29
1	A	162	ALA	O-C-N	5.35	127.58	122.07
1	C	162	ALA	O-C-N	5.35	127.58	122.07
1	D	65	ASP	CA-CB-CG	-5.35	107.25	112.60
1	D	203	PHE	N-CA-C	5.35	117.11	111.28
1	B	115	GLU	CA-C-O	5.34	125.65	118.38
1	D	249	GLU	O-C-N	-5.34	115.72	122.19
1	B	230	ASN	CA-C-O	5.34	126.62	120.90
1	C	12	LYS	CA-C-N	5.34	129.76	122.34
1	C	12	LYS	C-N-CA	5.34	129.76	122.34
1	D	13	ASP	N-CA-CB	-5.34	103.79	111.91
1	C	158	ALA	O-C-N	-5.33	116.47	122.12
1	D	237	ASP	N-CA-CB	-5.33	102.29	110.12
1	B	237	ASP	N-CA-CB	-5.33	102.29	110.12
1	A	158	ALA	O-C-N	-5.33	116.47	122.12
1	B	13	ASP	N-CA-CB	-5.33	103.82	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	359	ILE	CB-CA-C	-5.33	103.91	112.16
1	C	312	LEU	N-CA-CB	-5.33	102.86	110.80
1	B	344	SER	CA-C-N	5.32	127.85	120.29
1	B	344	SER	C-N-CA	5.32	127.85	120.29
1	B	145	PRO	CA-C-N	5.32	127.67	120.38
1	B	145	PRO	C-N-CA	5.32	127.67	120.38
1	B	221	GLY	CA-C-N	5.32	127.85	120.29
1	B	221	GLY	C-N-CA	5.32	127.85	120.29
1	C	191	PHE	N-CA-C	-5.32	105.39	111.14
1	D	6	ASP	CA-C-N	5.32	130.45	121.14
1	D	6	ASP	C-N-CA	5.32	130.45	121.14
1	D	23	LEU	O-C-N	-5.32	115.20	122.33
1	D	145	PRO	CA-C-N	5.32	127.67	120.38
1	D	145	PRO	C-N-CA	5.32	127.67	120.38
1	B	203	PHE	N-CA-C	5.32	117.08	111.28
1	A	101	THR	CA-C-N	5.32	127.35	120.44
1	A	101	THR	C-N-CA	5.32	127.35	120.44
1	B	10	CYS	N-CA-C	5.32	117.08	111.28
1	C	101	THR	CA-CB-OG1	5.32	117.57	109.60
1	D	115	GLU	CA-C-O	5.32	125.61	118.38
1	A	97	LEU	O-C-N	-5.31	116.49	122.12
1	D	101	THR	CA-C-N	5.31	127.34	120.44
1	D	101	THR	C-N-CA	5.31	127.34	120.44
1	C	32	GLU	N-CA-C	5.31	117.07	111.28
1	A	123	ALA	CA-C-N	5.30	127.39	120.28
1	A	123	ALA	C-N-CA	5.30	127.39	120.28
1	B	139	THR	CA-C-O	5.30	126.17	120.55
1	C	288	PHE	N-CA-CB	5.30	119.28	110.63
1	A	62	GLY	CA-C-N	5.30	127.72	120.46
1	A	62	GLY	C-N-CA	5.30	127.72	120.46
1	B	204	GLN	CA-C-O	5.30	126.39	120.82
1	C	75	MET	N-CA-C	-5.30	105.67	111.82
1	B	101	THR	CA-C-N	5.30	127.33	120.44
1	B	101	THR	C-N-CA	5.30	127.33	120.44
1	C	97	LEU	O-C-N	-5.29	116.51	122.12
1	B	162	ALA	CA-C-O	-5.29	114.92	120.63
1	A	309	VAL	CA-C-O	-5.29	114.94	120.76
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	61	VAL	O-C-N	-5.29	116.74	121.87
1	C	308	VAL	N-CA-C	-5.29	105.38	110.72
1	D	347	LEU	N-CA-C	5.28	117.95	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	230	ASN	CA-C-O	5.28	126.55	120.90
1	B	228	VAL	CA-C-O	-5.28	114.55	120.25
1	B	61	VAL	O-C-N	-5.28	116.75	121.87
1	A	191	PHE	N-CA-C	-5.28	105.44	111.14
1	A	173	TYR	CA-C-N	5.27	127.35	120.28
1	A	173	TYR	C-N-CA	5.27	127.35	120.28
1	D	296	VAL	CA-CB-CG2	5.27	119.36	110.40
1	D	119	GLY	CA-C-O	5.27	125.73	120.09
1	B	23	LEU	O-C-N	-5.26	115.28	122.33
1	A	308	VAL	N-CA-C	-5.26	105.40	110.72
1	C	56	SER	O-C-N	-5.26	116.65	122.07
1	C	212	ARG	O-C-N	-5.26	116.55	122.12
1	D	199	GLN	CB-CG-CD	-5.26	103.66	112.60
1	C	142	ALA	CA-C-O	-5.26	114.41	120.24
1	D	103	HIS	CB-CG-CD2	5.26	138.03	131.20
1	A	75	MET	N-CA-C	-5.25	105.73	111.82
1	D	90	LYS	N-CA-C	5.25	117.00	111.28
1	D	139	THR	CA-C-O	5.25	126.12	120.55
1	B	347	LEU	N-CA-C	5.25	117.91	111.82
1	C	309	VAL	CA-C-O	-5.25	114.99	120.76
1	D	228	VAL	CA-C-O	-5.25	114.58	120.25
1	A	32	GLU	N-CA-C	5.25	117.00	111.28
1	B	199	GLN	CB-CG-CD	-5.25	103.68	112.60
1	C	225	HIS	O-C-N	-5.25	115.82	122.27
1	C	173	TYR	CA-C-N	5.24	127.31	120.28
1	C	173	TYR	C-N-CA	5.24	127.31	120.28
1	B	129	ARG	N-CA-CB	5.24	117.75	109.94
1	A	50	ARG	CG-CD-NE	-5.24	100.47	112.00
1	C	53	LEU	N-CA-C	5.24	118.83	112.23
1	C	303	ASP	N-CA-CB	-5.24	103.22	110.29
1	A	225	HIS	O-C-N	-5.23	115.83	122.27
1	D	10	CYS	N-CA-C	5.23	116.98	111.28
1	C	50	ARG	CG-CD-NE	-5.23	100.49	112.00
1	D	117	LEU	CA-C-N	5.23	127.72	120.29
1	D	117	LEU	C-N-CA	5.23	127.72	120.29
1	B	90	LYS	N-CA-C	5.23	116.98	111.28
1	B	117	LEU	CA-C-N	5.22	127.71	120.29
1	B	117	LEU	C-N-CA	5.22	127.71	120.29
1	A	333	SER	O-C-N	5.22	128.58	122.99
1	B	296	VAL	CA-CB-CG2	5.22	119.28	110.40
1	A	113	VAL	CA-C-N	5.22	127.73	120.63
1	A	113	VAL	C-N-CA	5.22	127.73	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	ASP	N-CA-CB	-5.22	103.25	110.29
1	A	179	VAL	CB-CA-C	-5.21	105.10	112.14
1	A	212	ARG	O-C-N	-5.21	116.60	122.12
1	D	106	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	B	103	HIS	CB-CG-CD2	5.21	137.97	131.20
1	D	21	ILE	CA-CB-CG1	5.21	119.25	110.40
1	D	204	GLN	CA-C-O	5.20	126.28	120.82
1	A	56	SER	O-C-N	-5.20	116.71	122.07
1	A	53	LEU	N-CA-C	5.20	118.78	112.23
1	A	154	GLU	N-CA-CB	-5.20	102.47	110.01
1	B	21	ILE	CA-CB-CG1	5.20	119.24	110.40
1	A	250	LEU	CA-C-N	5.20	131.60	121.41
1	A	250	LEU	C-N-CA	5.20	131.60	121.41
1	C	113	VAL	CA-C-N	5.20	127.70	120.63
1	C	113	VAL	C-N-CA	5.20	127.70	120.63
1	C	179	VAL	CB-CA-C	-5.20	105.12	112.14
1	C	250	LEU	CA-C-N	5.20	131.59	121.41
1	C	250	LEU	C-N-CA	5.20	131.59	121.41
1	C	212	ARG	N-CA-CB	5.20	117.76	110.12
1	D	106	GLN	N-CA-C	5.19	116.94	111.28
1	B	293	ASN	OD1-CG-ND2	5.19	127.79	122.60
1	C	131	ALA	CA-C-N	5.19	127.19	120.44
1	C	131	ALA	C-N-CA	5.19	127.19	120.44
1	B	119	GLY	CA-C-O	5.19	125.64	120.09
1	B	106	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	C	108	GLN	CB-CG-CD	5.18	121.41	112.60
1	C	48	SER	CA-CB-OG	5.18	121.46	111.10
1	D	129	ARG	N-CA-CB	5.17	117.65	109.94
1	C	2	THR	N-CA-CB	5.17	117.50	110.01
1	C	154	GLU	N-CA-CB	-5.17	102.52	110.01
1	A	128	TRP	CD2-CE2-CZ2	-5.17	117.23	122.40
1	B	106	GLN	N-CA-C	5.16	116.91	111.28
1	D	244	LEU	CA-C-N	5.16	127.15	120.44
1	D	244	LEU	C-N-CA	5.16	127.15	120.44
1	D	359	ILE	CA-CB-CG2	5.16	119.27	110.50
1	A	48	SER	CA-CB-OG	5.16	121.41	111.10
1	D	349	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	A	108	GLN	CB-CG-CD	5.15	121.36	112.60
1	C	169	ARG	CA-C-N	5.15	127.44	120.44
1	C	169	ARG	C-N-CA	5.15	127.44	120.44
1	C	333	SER	O-C-N	5.15	128.50	122.99
1	A	131	ALA	CA-C-N	5.15	127.13	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	ALA	C-N-CA	5.15	127.13	120.44
1	B	349	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	A	2	THR	N-CA-CB	5.13	117.45	110.01
1	A	103	HIS	CA-C-O	5.13	126.20	120.82
1	C	128	TRP	CD2-CE2-CZ2	-5.13	117.27	122.40
1	A	212	ARG	N-CA-CB	5.12	117.65	110.12
1	C	39	LEU	CA-C-N	5.12	127.40	120.44
1	C	39	LEU	C-N-CA	5.12	127.40	120.44
1	D	325	ARG	CA-CB-CG	5.12	124.33	114.10
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	C	314	LEU	CB-CA-C	-5.11	102.79	111.02
1	A	22	GLU	N-CA-C	5.11	116.93	111.36
1	B	131	ALA	N-CA-CB	-5.11	102.07	110.40
1	C	30	GLU	N-CA-C	5.11	116.53	111.07
1	A	314	LEU	CB-CA-C	-5.10	102.81	111.02
1	C	341	GLN	O-C-N	-5.10	117.16	123.33
1	D	293	ASN	OD1-CG-ND2	5.10	127.70	122.60
1	B	325	ARG	CA-CB-CG	5.09	124.29	114.10
1	C	170	ALA	N-CA-CB	5.09	117.46	110.07
1	B	359	ILE	CA-CB-CG2	5.09	119.16	110.50
1	B	203	PHE	CB-CA-C	-5.09	102.34	110.79
1	B	306	THR	CA-C-N	5.09	127.98	120.91
1	B	306	THR	C-N-CA	5.09	127.98	120.91
1	A	30	GLU	N-CA-C	5.09	116.51	111.07
1	B	83	PHE	O-C-N	-5.09	116.35	122.15
1	D	120	PHE	O-C-N	-5.08	116.73	122.12
1	A	341	GLN	O-C-N	-5.08	117.18	123.33
1	A	39	LEU	CA-C-N	5.08	127.35	120.44
1	A	39	LEU	C-N-CA	5.08	127.35	120.44
1	A	170	ALA	N-CA-CB	5.08	117.43	110.07
1	B	108	GLN	CA-C-O	5.08	127.93	120.42
1	D	203	PHE	CB-CA-C	-5.08	102.36	110.79
1	D	360	ALA	N-CA-C	5.08	119.19	113.15
1	B	223	GLN	O-C-N	-5.07	116.74	122.12
1	B	315	CYS	O-C-N	5.07	128.62	122.94
1	C	103	HIS	CA-C-O	5.07	126.15	120.82
1	C	223	GLN	CA-C-O	-5.07	115.04	120.42
1	C	95	ALA	CA-C-N	5.07	127.08	120.28
1	C	95	ALA	C-N-CA	5.07	127.08	120.28
1	D	108	GLN	CA-C-O	5.07	127.92	120.42
1	A	95	ALA	CA-C-N	5.06	127.07	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	ALA	C-N-CA	5.06	127.07	120.28
1	C	22	GLU	N-CA-C	5.06	116.88	111.36
1	D	131	ALA	N-CA-CB	-5.06	102.15	110.40
1	C	124	ARG	NE-CZ-NH2	-5.06	114.64	119.20
1	C	174	ALA	N-CA-CB	-5.06	102.68	110.12
1	B	168	GLY	CA-C-N	5.06	127.48	120.29
1	B	168	GLY	C-N-CA	5.06	127.48	120.29
1	B	360	ALA	N-CA-C	5.06	119.17	113.15
1	A	124	ARG	NE-CZ-NH2	-5.06	114.65	119.20
1	D	168	GLY	CA-C-N	5.05	127.47	120.29
1	D	168	GLY	C-N-CA	5.05	127.47	120.29
1	A	155	ALA	N-CA-C	5.05	116.87	111.36
1	B	244	LEU	CA-C-N	5.05	127.01	120.44
1	B	244	LEU	C-N-CA	5.05	127.01	120.44
1	C	38	LEU	CB-CA-C	5.05	119.44	110.85
1	A	38	LEU	CB-CA-C	5.05	119.43	110.85
1	A	223	GLN	CA-C-O	-5.05	115.07	120.42
1	D	83	PHE	O-C-N	-5.05	116.39	122.15
1	C	155	ALA	N-CA-C	5.05	116.86	111.36
1	A	174	ALA	N-CA-CB	-5.04	102.70	110.12
1	B	37	LYS	CA-C-N	5.04	127.04	120.28
1	B	37	LYS	C-N-CA	5.04	127.04	120.28
1	D	284	SER	O-C-N	-5.04	117.83	123.48
1	C	217	ARG	NE-CZ-NH1	5.03	126.53	121.50
1	D	223	GLN	O-C-N	-5.03	116.79	122.12
1	A	207	HIS	CA-C-N	5.02	127.42	120.29
1	A	207	HIS	C-N-CA	5.02	127.42	120.29
1	B	50	ARG	CG-CD-NE	-5.02	100.95	112.00
1	D	306	THR	CA-C-N	5.02	127.89	120.91
1	D	306	THR	C-N-CA	5.02	127.89	120.91
1	B	288	PHE	CB-CG-CD1	-5.02	112.16	120.70
1	B	284	SER	O-C-N	-5.02	117.86	123.48
1	C	138	LEU	CA-C-N	5.02	127.00	120.28
1	C	138	LEU	C-N-CA	5.02	127.00	120.28
1	D	296	VAL	N-CA-CB	-5.02	104.04	112.47
1	A	217	ARG	NE-CZ-NH1	5.01	126.52	121.50
1	B	296	VAL	N-CA-CB	-5.01	104.05	112.47
1	D	102	GLN	CA-C-N	5.01	126.95	120.44
1	D	102	GLN	C-N-CA	5.01	126.95	120.44
1	A	30	GLU	CA-C-N	5.01	126.99	120.28
1	A	30	GLU	C-N-CA	5.01	126.99	120.28
1	A	138	LEU	CA-C-N	5.00	126.99	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	LEU	C-N-CA	5.00	126.99	120.28
1	D	50	ARG	CG-CD-NE	-5.00	100.99	112.00
1	D	297	TYR	O-C-N	-5.00	117.08	123.24
1	D	288	PHE	CB-CG-CD1	-5.00	112.20	120.70

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	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	1.25
1:A:125:ARG:NH2	1:C:122:GLU:CD	1.96	1.21
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:122:GLU:CD	1:C:125:ARG:HH22	1.52	1.15
1:A:125:ARG:HH22	1:C:122:GLU:CD	1.53	1.15
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:A:32:GLU:CD	1:A:121:ARG:HH12	2.22	0.47
1:C:32:GLU:CD	1:C:121:ARG:HH12	2.23	0.47
1:C:143:GLU:CD	1:D:325:ARG:HH12	2.23	0.46
1:A:143:GLU:CD	1:B:325:ARG:HH12	2.24	0.46
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:C:94:HIS:O	1:C:97:LEU:HB3	2.20	0.42
1:D:207:HIS:CE1	1:D:211:SER:HB2	2.53	0.42
1:A:94:HIS:O	1:A:97:LEU:HB3	2.20	0.41
1:C:289:THR:O	1:C:296:VAL:HG22	2.20	0.41
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:C:348:LEU:HD13	1:C:348:LEU:C	2.46	0.41
1:D:286:ARG:HD3	1:D:286:ARG:HA	1.97	0.40
1:A:348:LEU:C	1:A:348:LEU:HD13	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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 ⓘ

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 (19) such sidechains are listed below:

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	205	GLN
1	C	207	HIS
1	C	240	GLN
1	C	298	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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.

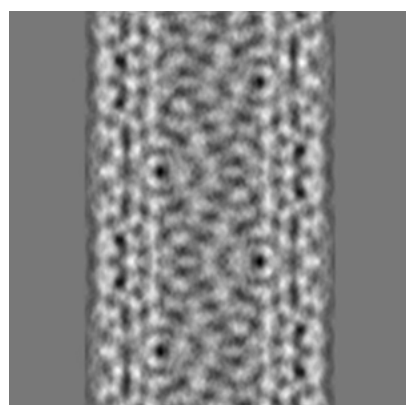
6 Map visualisation [i](#)

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

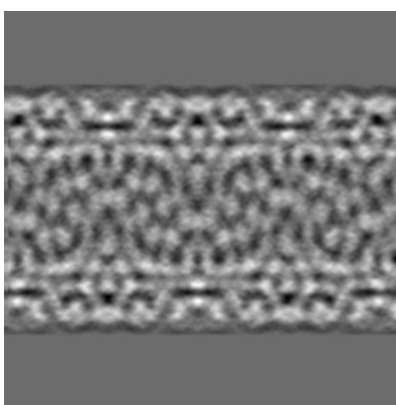
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

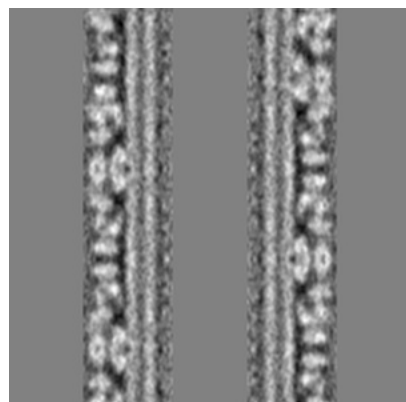


Z

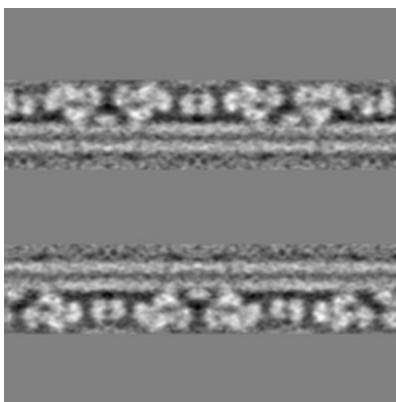
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

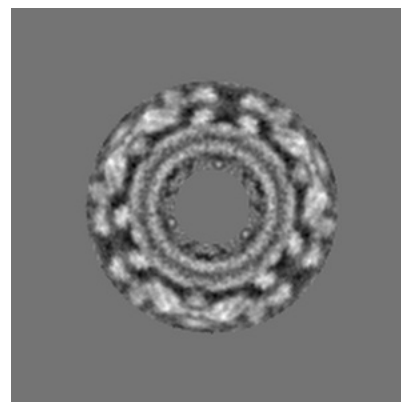
6.2.1 Primary map



X Index: 100



Y Index: 100

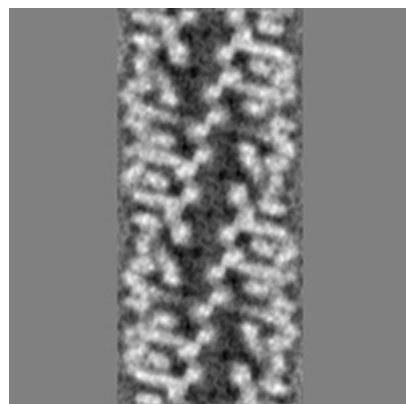


Z Index: 100

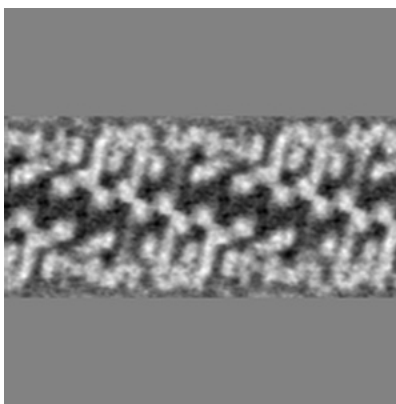
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

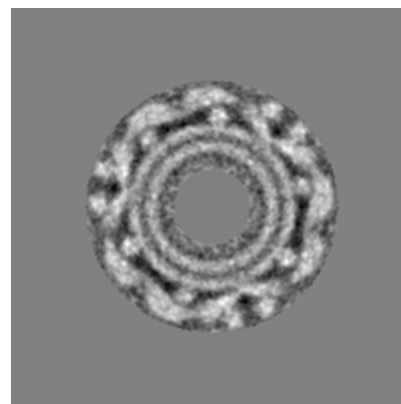
6.3.1 Primary map



X Index: 143



Y Index: 144

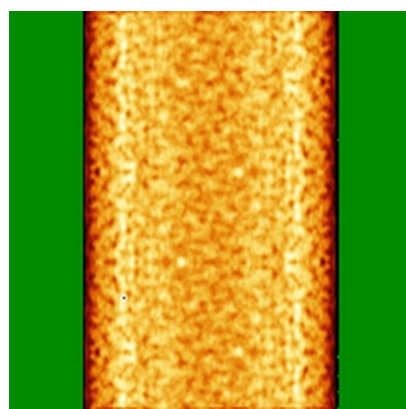


Z Index: 168

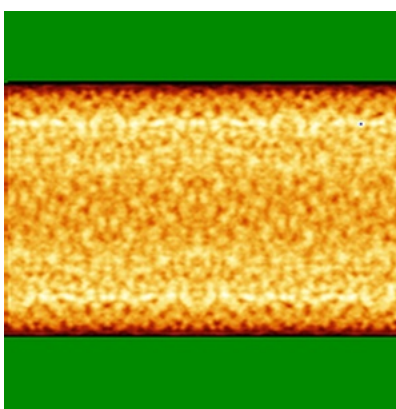
The images above show the largest variance slices of the map in three orthogonal directions.

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

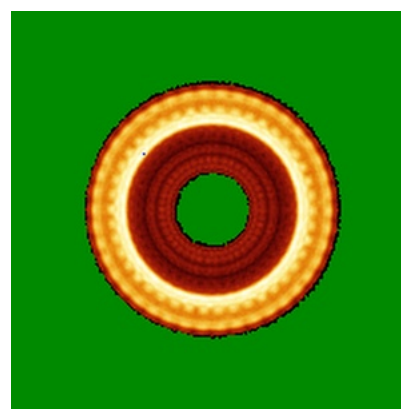
6.4.1 Primary map



X



Y

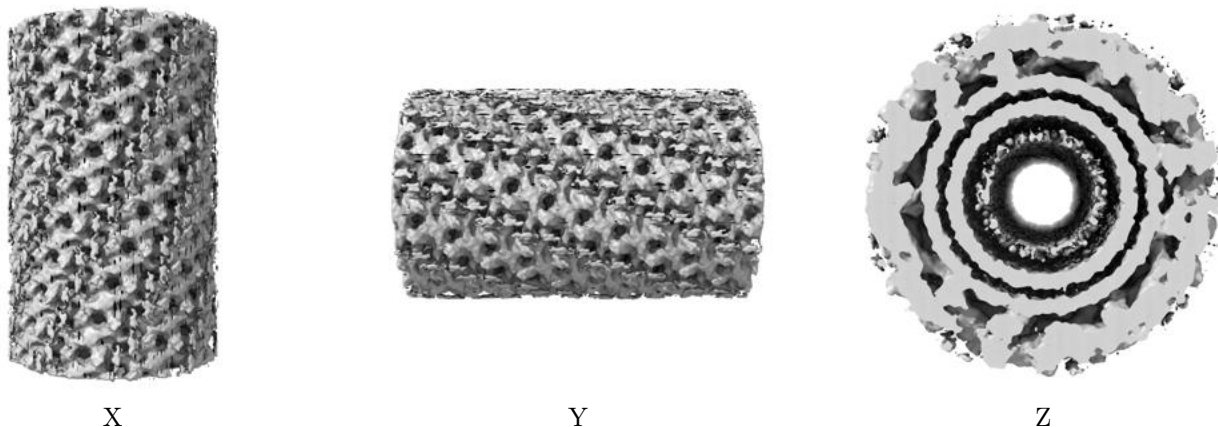


Z

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



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.

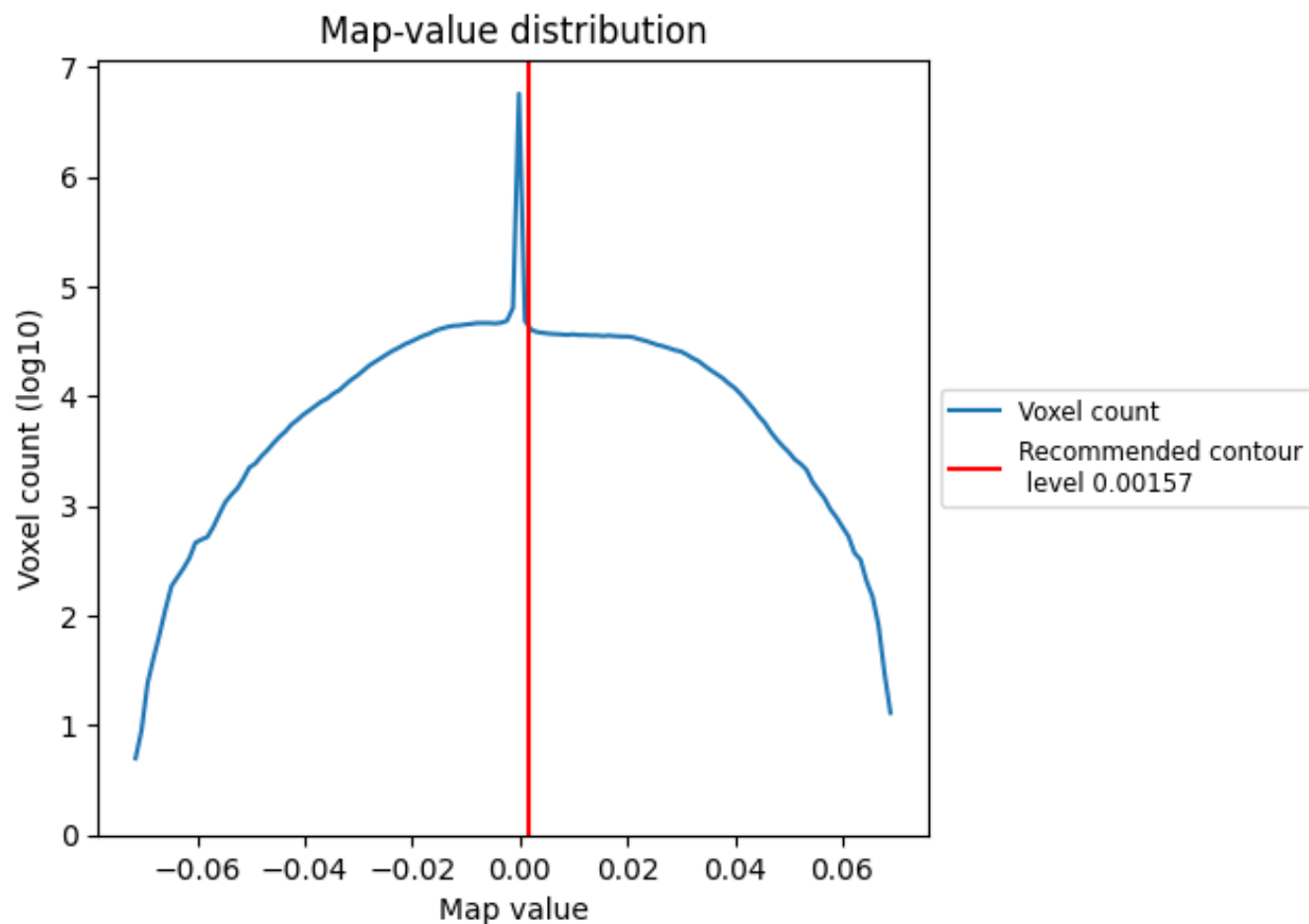
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

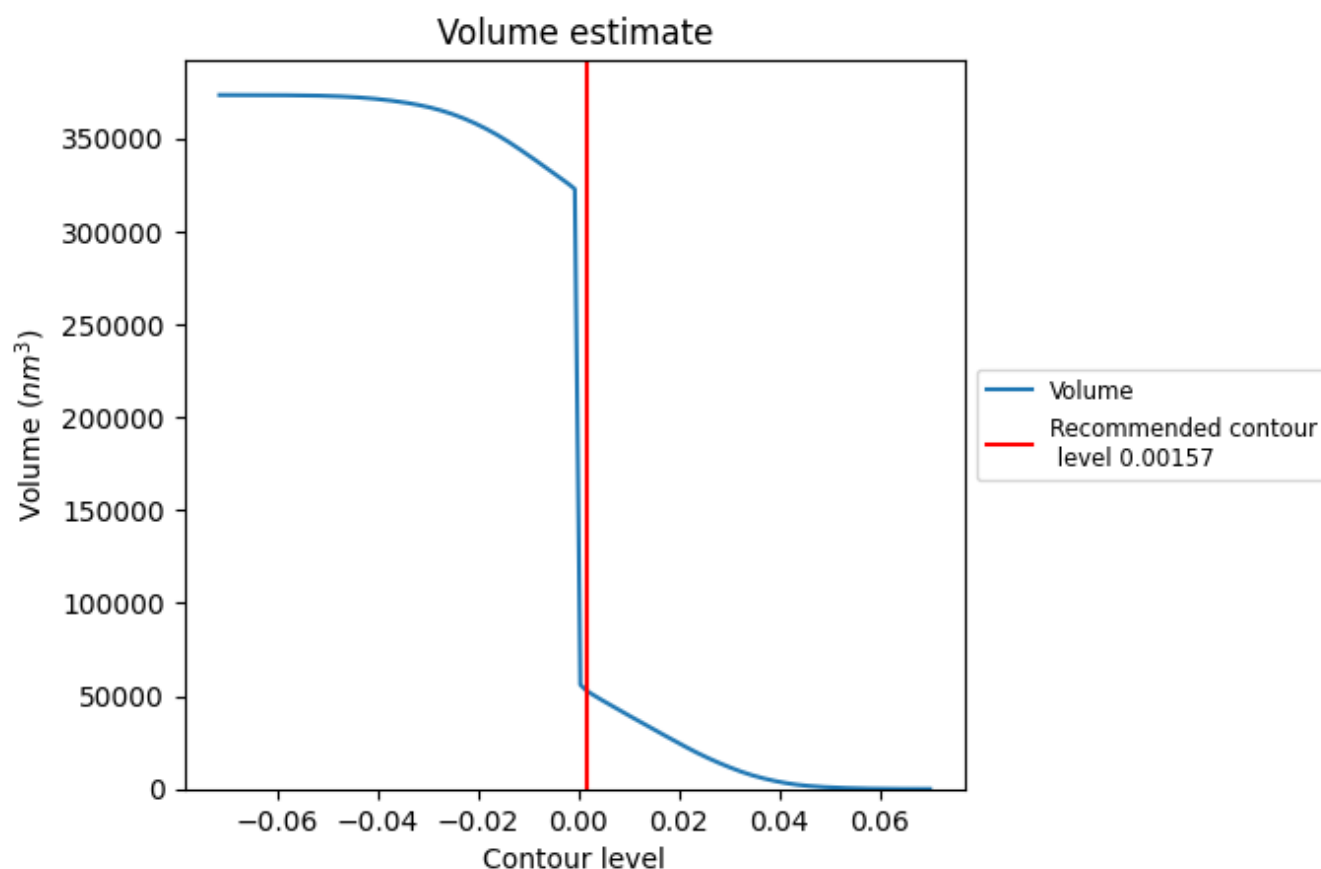
This section contains the results of statistical analysis of the map.

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.

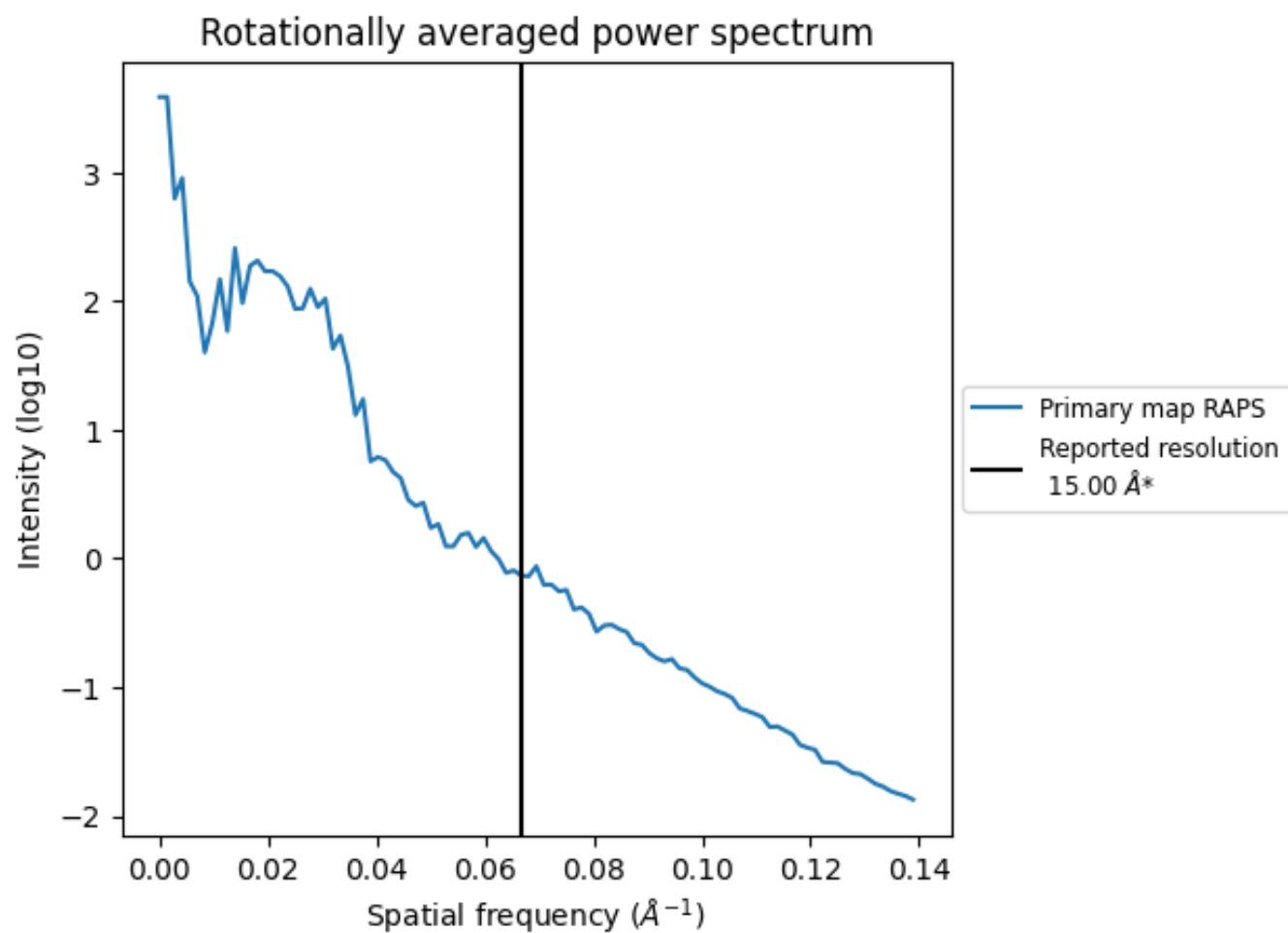
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 53038 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.067 Å⁻¹

8 Fourier-Shell correlation

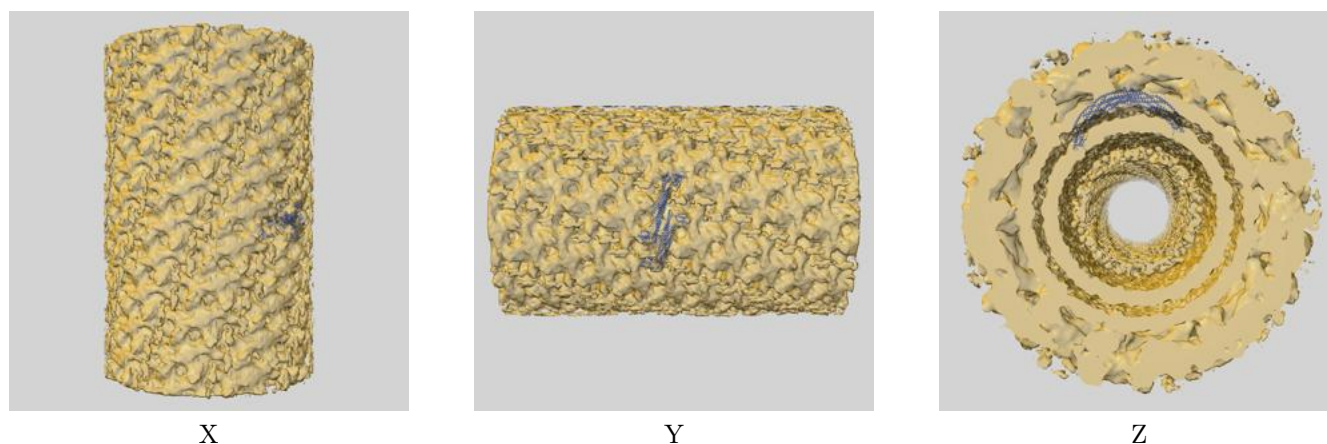
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

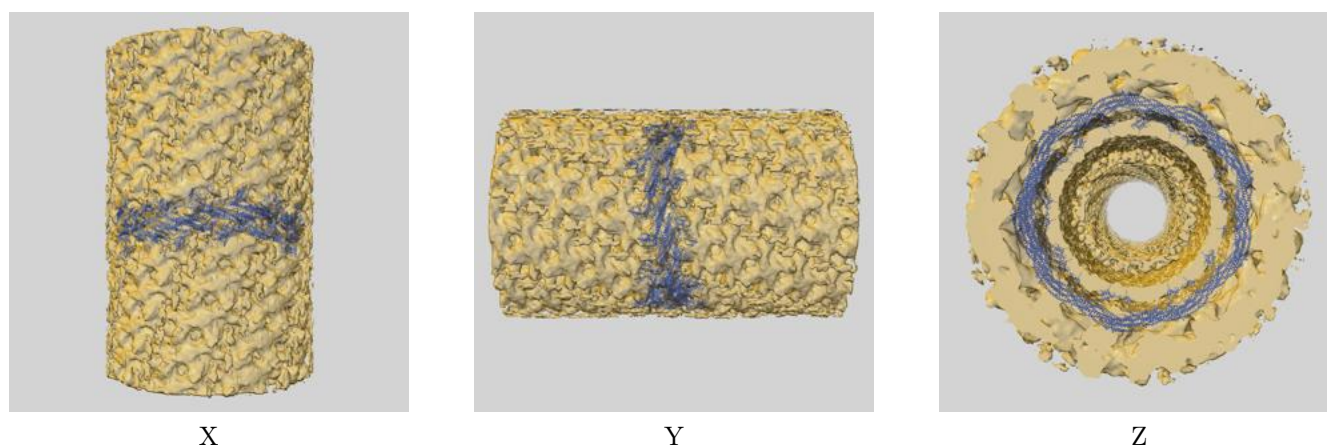
This section contains information regarding the fit between EMDB map EMD-2546 and PDB model 4CKG. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

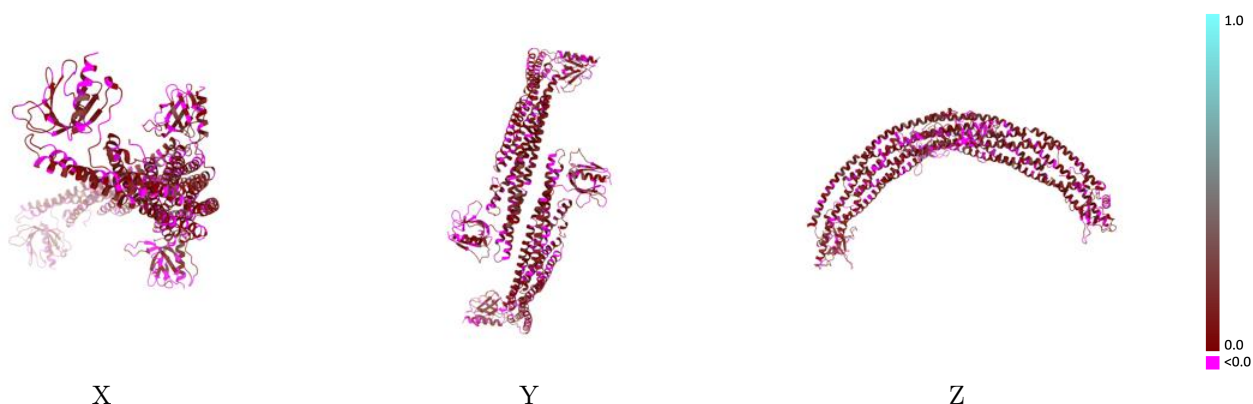


9.1.2 Map-model assembly overlay [i](#)



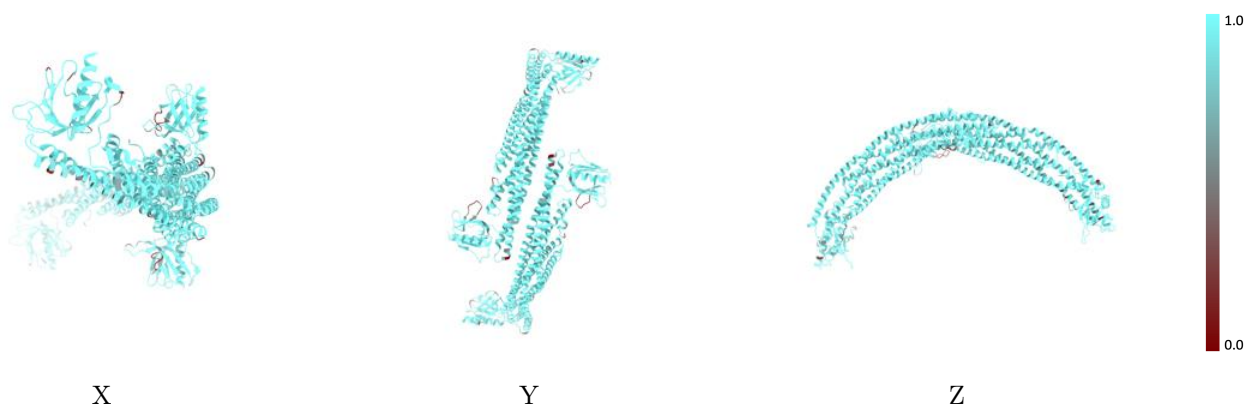
The images above show the 3D surface view of the map at the recommended contour level 0.00157 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



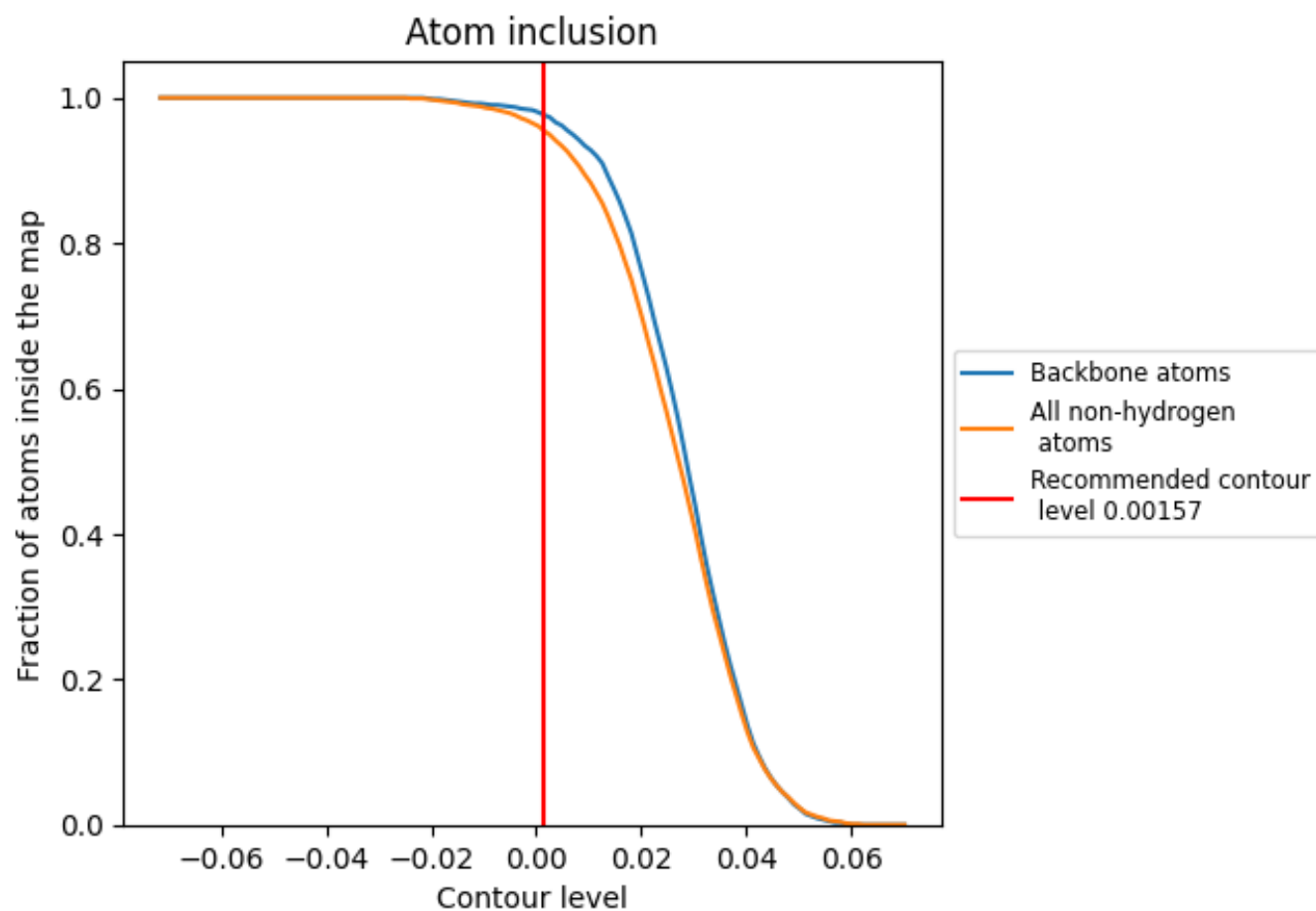
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00157).

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

