



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:47 PM UTC

PDB ID : 5H3D / pdb_00005h3d
EMDB ID : EMD-2546
Title : Helical structure of membrane tubules decorated by ACAP1 (BARPH domain) protein by cryo-electron microscopy and MD simulation
Authors : Chan, C.; Pang, X.Y.; Zhang, Y.; Sun, F.; Fan, J.
Deposited on : 2016-10-22
Resolution : 14.00 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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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

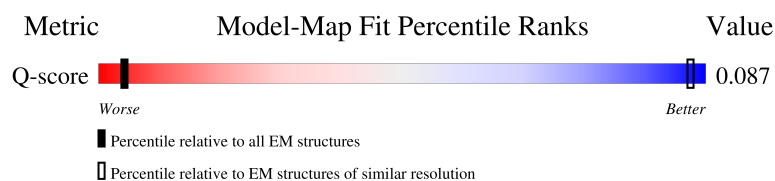
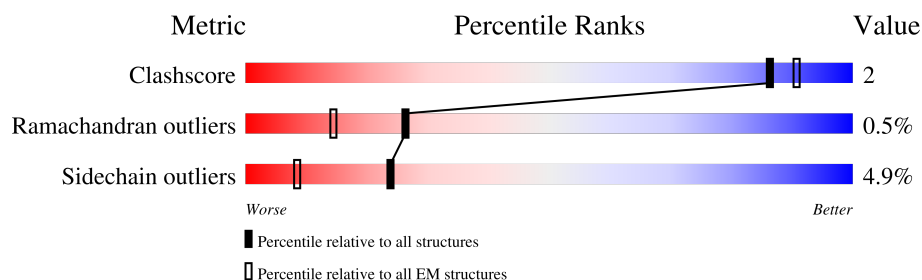
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 14.00 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 23314 atoms, of which 11698 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	364	Total	C	H	N	O	S	0	0
			5849	1825	2934	534	543	13		
1	B	361	Total	C	H	N	O	S	0	0
			5808	1810	2915	531	539	13		
1	C	364	Total	C	H	N	O	S	0	0
			5849	1825	2934	534	543	13		
1	D	361	Total	C	H	N	O	S	0	0
			5808	1810	2915	531	539	13		

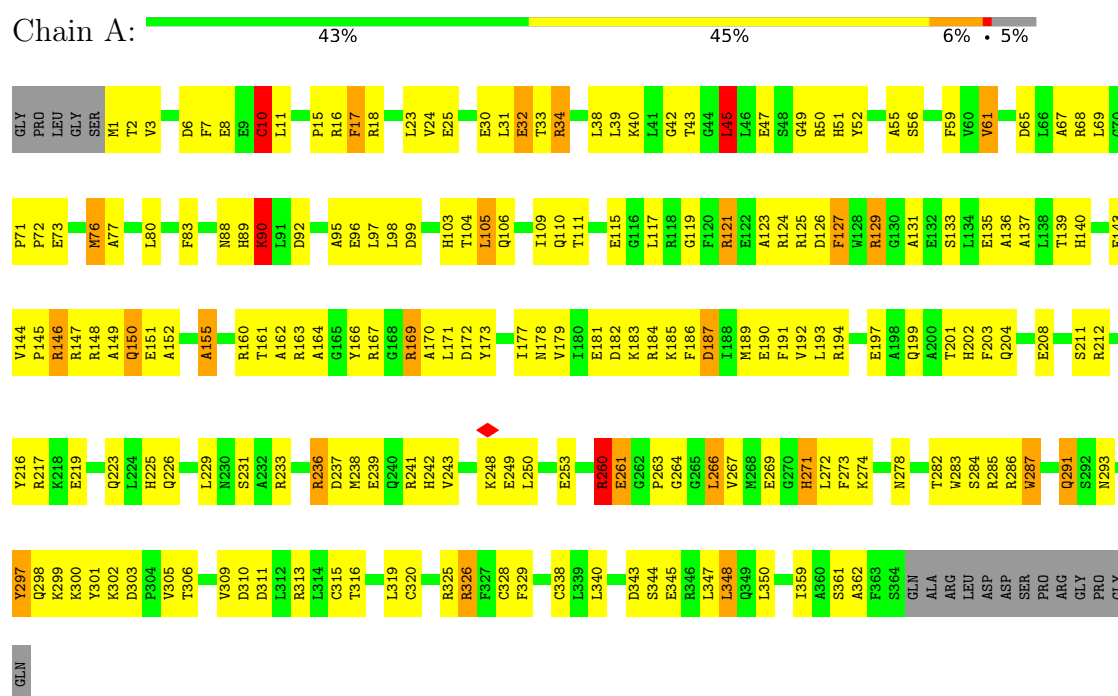
There are 20 discrepancies between the modelled and reference sequences:

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

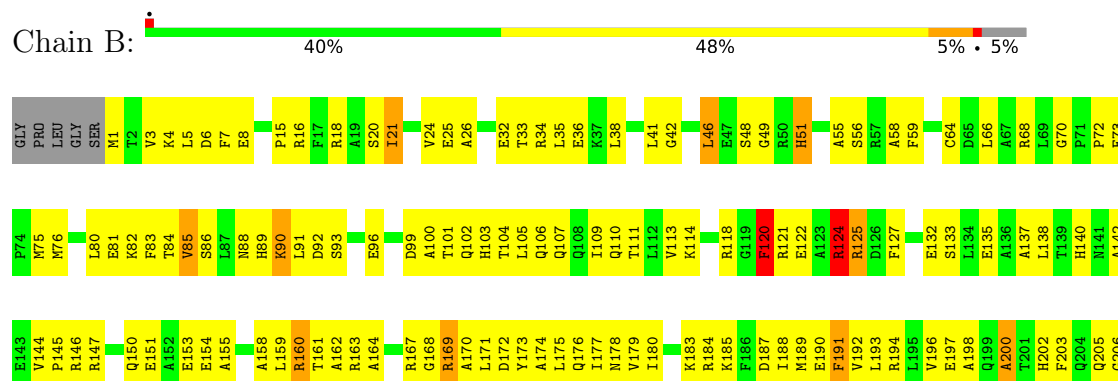
3 Residue-property plots

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

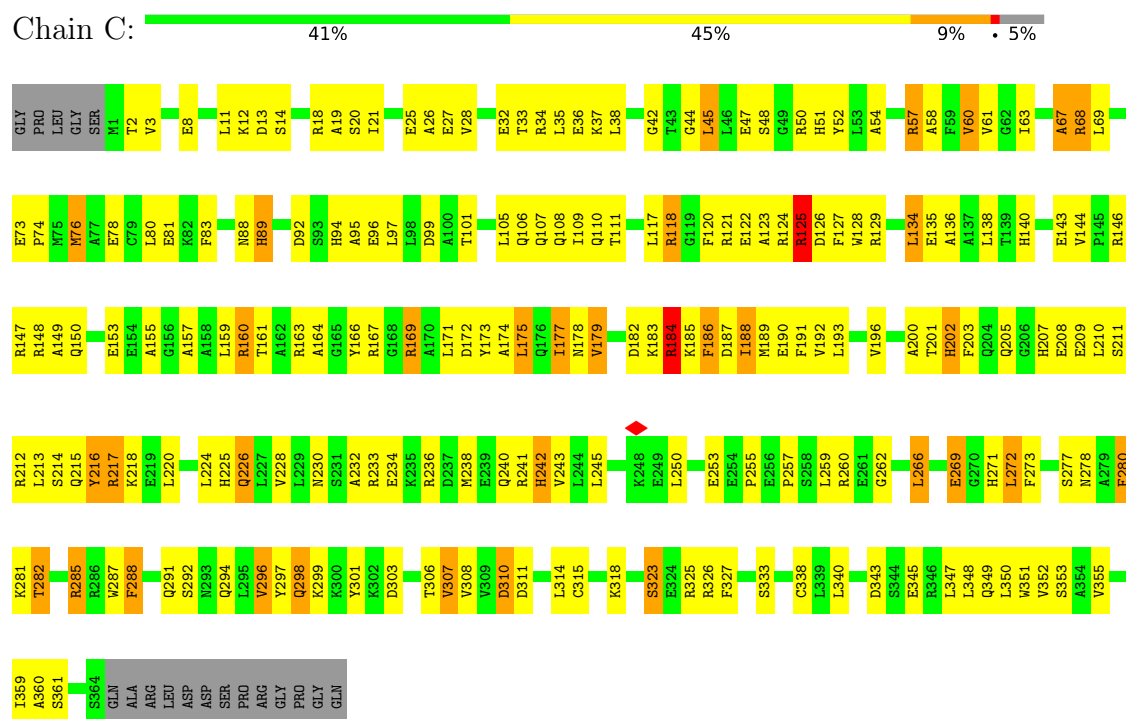


- Molecule 1: Arf-GAP with coiled-coil, ANK repeat and PH domain-containing protein 1

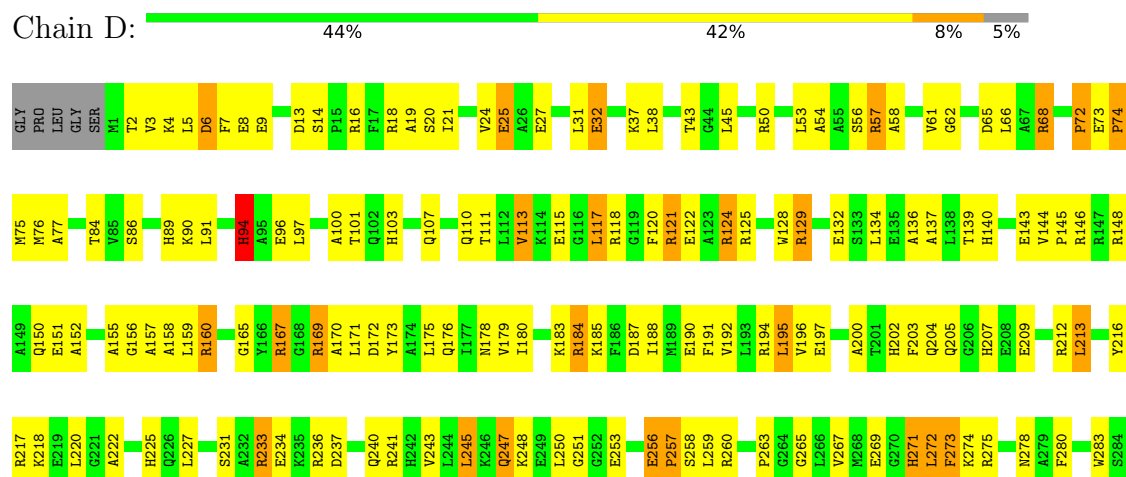




- Molecule 1: Arf-GAP with coiled-coil, ANK repeat and PH domain-containing protein 1



- 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=42.72°, rise=23.20 Å, axial sym=C3	Depositor
Number of segments used	304	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	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	75000	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	2.13	74/2963 (2.5%)	2.63	240/3987 (6.0%)
1	B	2.18	90/2940 (3.1%)	2.61	243/3956 (6.1%)
1	C	2.13	88/2963 (3.0%)	2.66	255/3987 (6.4%)
1	D	2.15	84/2940 (2.9%)	2.53	201/3956 (5.1%)
All	All	2.15	336/11806 (2.8%)	2.61	939/15886 (5.9%)

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	10
1	C	0	12
1	D	0	15
All	All	0	49

All (336) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	177	ILE	CA-CB	9.73	1.65	1.54
1	C	169	ARG	N-CA	-9.59	1.34	1.46
1	C	355	VAL	CA-CB	-8.99	1.42	1.54
1	D	144	VAL	N-CA	-8.73	1.39	1.45
1	B	51	HIS	ND1-CE1	8.72	1.41	1.32
1	D	192	VAL	CA-CB	8.34	1.64	1.54
1	B	89	HIS	ND1-CE1	8.22	1.40	1.32
1	D	236	ARG	C-N	8.15	1.44	1.33
1	C	57	ARG	CA-C	8.10	1.63	1.52
1	D	250	LEU	CA-CB	8.08	1.63	1.53
1	A	191	PHE	CA-C	7.97	1.62	1.52
1	D	172	ASP	CA-C	-7.96	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	248	LYS	CA-C	7.79	1.59	1.52
1	A	23	LEU	C-N	7.66	1.43	1.34
1	D	115	GLU	CA-C	7.60	1.59	1.52
1	C	166	TYR	CA-CB	7.56	1.65	1.53
1	A	166	TYR	CA-CB	7.56	1.65	1.53
1	B	300	LYS	N-CA	7.51	1.55	1.45
1	C	338	CYS	CA-C	7.51	1.61	1.52
1	C	201	THR	N-CA	-7.48	1.37	1.46
1	C	188	ILE	CA-C	7.47	1.62	1.52
1	B	100	ALA	C-N	7.43	1.43	1.33
1	B	317	VAL	CA-C	-7.42	1.43	1.52
1	B	41	LEU	C-N	7.35	1.43	1.33
1	C	353	SER	CA-C	-7.30	1.43	1.52
1	C	140	HIS	ND1-CE1	7.29	1.39	1.32
1	D	8	GLU	CA-C	7.27	1.62	1.52
1	A	223	GLN	N-CA	-7.26	1.37	1.46
1	A	49	GLY	CA-C	-7.25	1.43	1.51
1	C	326	ARG	CD-NE	7.21	1.56	1.46
1	C	44	GLY	CA-C	-7.15	1.44	1.52
1	D	101	THR	N-CA	7.13	1.54	1.46
1	B	240	GLN	C-N	7.12	1.43	1.33
1	D	128	TRP	CA-CB	7.11	1.64	1.53
1	C	25	GLU	N-CA	-7.10	1.37	1.46
1	C	143	GLU	CA-CB	7.09	1.66	1.53
1	C	308	VAL	CA-C	-7.03	1.43	1.52
1	A	8	GLU	CA-CB	7.03	1.64	1.53
1	D	225	HIS	ND1-CE1	7.03	1.39	1.32
1	B	228	VAL	CA-C	7.00	1.62	1.52
1	A	143	GLU	N-CA	7.00	1.55	1.46
1	A	186	PHE	N-CA	-6.96	1.38	1.46
1	D	303	ASP	CA-CB	6.95	1.62	1.54
1	D	348	LEU	CA-C	-6.92	1.44	1.52
1	C	209	GLU	CA-C	6.90	1.62	1.52
1	A	273	PHE	N-CA	-6.90	1.37	1.46
1	B	325	ARG	N-CA	-6.90	1.37	1.46
1	D	132	GLU	CA-C	-6.89	1.44	1.52
1	C	333	SER	N-CA	-6.89	1.36	1.45
1	C	155	ALA	CA-CB	6.86	1.64	1.53
1	B	105	LEU	CA-C	6.85	1.61	1.52
1	B	245	LEU	CA-C	-6.83	1.44	1.52
1	B	140	HIS	CE1-NE2	6.82	1.39	1.32
1	C	47	GLU	N-CA	6.82	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	CYS	N-CA	6.80	1.53	1.46
1	D	53	LEU	N-CA	-6.80	1.38	1.46
1	D	301	TYR	CA-C	6.76	1.61	1.52
1	B	32	GLU	CA-CB	6.75	1.64	1.53
1	B	202	HIS	CA-C	6.73	1.61	1.52
1	D	31	LEU	C-N	6.71	1.43	1.33
1	C	338	CYS	N-CA	-6.71	1.38	1.46
1	A	189	MET	C-N	6.67	1.42	1.33
1	B	188	ILE	CA-C	6.67	1.62	1.52
1	B	307	VAL	C-N	6.67	1.39	1.33
1	C	242	HIS	CA-CB	6.66	1.63	1.53
1	C	134	LEU	N-CA	-6.65	1.38	1.46
1	A	31	LEU	CA-CB	6.64	1.63	1.53
1	A	6	ASP	CA-C	6.62	1.61	1.52
1	B	283	TRP	N-CA	6.61	1.54	1.45
1	D	308	VAL	CA-C	6.58	1.59	1.52
1	B	170	ALA	CA-C	6.54	1.61	1.52
1	B	207	HIS	ND1-CE1	6.54	1.39	1.32
1	B	236	ARG	CD-NE	6.52	1.55	1.46
1	B	313	ARG	CD-NE	6.51	1.55	1.46
1	D	103	HIS	ND1-CE1	6.49	1.39	1.32
1	C	153	GLU	CA-C	6.49	1.61	1.52
1	B	169	ARG	CD-NE	6.48	1.55	1.46
1	C	149	ALA	N-CA	-6.47	1.38	1.46
1	B	295	LEU	N-CA	6.47	1.53	1.46
1	D	3	VAL	N-CA	-6.46	1.38	1.46
1	D	240	GLN	N-CA	6.45	1.54	1.46
1	B	173	TYR	C-N	6.44	1.42	1.33
1	A	160	ARG	CA-CB	6.44	1.63	1.53
1	C	348	LEU	CA-CB	6.44	1.63	1.53
1	C	207	HIS	ND1-CE1	6.43	1.39	1.32
1	A	45	LEU	C-N	6.41	1.42	1.33
1	A	239	GLU	N-CA	-6.38	1.38	1.46
1	C	262	GLY	N-CA	6.37	1.53	1.44
1	D	285	ARG	CA-CB	6.34	1.61	1.53
1	A	16	ARG	CA-CB	6.34	1.63	1.53
1	A	55	ALA	C-N	6.33	1.42	1.33
1	C	28	VAL	CA-CB	-6.33	1.47	1.54
1	B	81	GLU	CA-C	-6.32	1.44	1.52
1	D	96	GLU	C-O	-6.32	1.16	1.24
1	A	260	ARG	CA-CB	6.31	1.64	1.53
1	B	110	GLN	CA-C	-6.31	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	THR	CA-CB	6.28	1.63	1.53
1	C	101	THR	C-N	6.28	1.41	1.33
1	A	71	PRO	C-N	6.27	1.40	1.33
1	D	89	HIS	C-O	-6.27	1.16	1.24
1	A	59	PHE	C-N	6.26	1.41	1.33
1	C	243	VAL	CA-C	-6.25	1.45	1.52
1	D	9	GLU	CA-C	6.22	1.61	1.52
1	D	5	LEU	CA-CB	6.20	1.62	1.53
1	D	202	HIS	CA-C	-6.17	1.44	1.52
1	C	58	ALA	N-CA	-6.17	1.38	1.46
1	B	307	VAL	N-CA	-6.14	1.38	1.46
1	B	339	LEU	C-N	6.13	1.41	1.33
1	A	121	ARG	CD-NE	6.12	1.54	1.46
1	B	59	PHE	C-N	-6.12	1.26	1.33
1	D	349	GLN	CA-CB	6.12	1.63	1.53
1	D	6	ASP	CA-CB	6.10	1.63	1.53
1	C	163	ARG	CD-NE	6.10	1.54	1.46
1	C	327	PHE	CA-C	-6.09	1.45	1.53
1	B	106	GLN	CA-CB	6.09	1.62	1.53
1	D	307	VAL	CA-C	-6.08	1.46	1.52
1	A	237	ASP	C-N	6.08	1.42	1.33
1	B	48	SER	CA-CB	6.07	1.62	1.53
1	B	18	ARG	NE-CZ	6.06	1.39	1.33
1	B	346	ARG	CD-NE	6.06	1.54	1.46
1	D	323	SER	CA-C	-6.06	1.44	1.52
1	A	97	LEU	N-CA	6.03	1.53	1.46
1	D	334	THR	N-CA	6.02	1.53	1.46
1	A	231	SER	C-O	-6.02	1.17	1.24
1	D	188	ILE	CA-C	6.02	1.61	1.52
1	C	78	GLU	CA-CB	6.01	1.63	1.53
1	A	162	ALA	C-O	-5.98	1.17	1.24
1	C	128	TRP	NE1-CE2	-5.98	1.30	1.37
1	A	105	LEU	CA-CB	5.97	1.62	1.53
1	B	191	PHE	CA-CB	5.97	1.62	1.53
1	C	291	GLN	CA-CB	5.91	1.64	1.53
1	C	285	ARG	CZ-NH2	-5.91	1.25	1.33
1	D	73	GLU	CA-C	5.89	1.59	1.53
1	D	245	LEU	CA-C	-5.89	1.45	1.52
1	B	287	TRP	CA-CB	5.89	1.61	1.53
1	A	6	ASP	N-CA	5.89	1.54	1.46
1	B	133	SER	CA-CB	-5.88	1.44	1.53
1	A	225	HIS	CA-C	5.88	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	ASP	N-CA	-5.88	1.39	1.46
1	C	260	ARG	CA-CB	5.87	1.63	1.53
1	A	201	THR	CA-C	5.86	1.60	1.52
1	B	209	GLU	CA-C	-5.86	1.45	1.52
1	B	55	ALA	N-CA	-5.84	1.39	1.46
1	D	160	ARG	C-O	-5.84	1.17	1.24
1	A	286	ARG	CA-C	-5.83	1.45	1.52
1	A	264	GLY	C-N	5.83	1.41	1.33
1	D	57	ARG	N-CA	-5.83	1.39	1.46
1	B	168	GLY	CA-C	-5.82	1.45	1.52
1	A	45	LEU	C-O	-5.82	1.17	1.24
1	B	190	GLU	C-N	5.82	1.41	1.33
1	B	355	VAL	C-N	5.82	1.41	1.33
1	C	282	THR	N-CA	5.82	1.53	1.46
1	A	194	ARG	CA-CB	5.81	1.62	1.53
1	C	196	VAL	CA-C	-5.81	1.44	1.52
1	D	89	HIS	CE1-NE2	5.81	1.38	1.32
1	D	176	GLN	CA-C	5.81	1.60	1.52
1	B	103	HIS	ND1-CE1	5.80	1.38	1.32
1	A	282	THR	CA-C	-5.79	1.45	1.52
1	C	52	TYR	N-CA	5.79	1.53	1.46
1	B	4	LYS	CA-C	5.78	1.60	1.52
1	B	242	HIS	N-CA	5.77	1.53	1.46
1	B	58	ALA	CA-C	-5.77	1.45	1.52
1	D	61	VAL	N-CA	5.76	1.53	1.46
1	B	138	LEU	CA-CB	5.76	1.62	1.53
1	B	287	TRP	CD2-CE2	5.74	1.51	1.41
1	B	356	GLN	CA-CB	5.74	1.62	1.53
1	D	344	SER	N-CA	-5.73	1.39	1.46
1	C	228	VAL	CA-CB	-5.73	1.47	1.54
1	A	172	ASP	CA-C	-5.72	1.45	1.52
1	A	361	SER	CA-CB	5.72	1.62	1.53
1	B	158	ALA	C-N	5.72	1.41	1.33
1	B	198	ALA	N-CA	-5.71	1.39	1.46
1	D	124	ARG	CA-C	-5.71	1.45	1.52
1	A	163	ARG	CZ-NH2	-5.70	1.26	1.33
1	C	215	GLN	C-N	5.70	1.41	1.34
1	C	348	LEU	N-CA	-5.70	1.39	1.46
1	B	196	VAL	CA-CB	-5.69	1.47	1.54
1	B	91	LEU	CA-C	-5.69	1.45	1.52
1	A	161	THR	C-O	-5.68	1.17	1.24
1	B	322	ASP	N-CA	-5.67	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	233	ARG	CD-NE	5.67	1.54	1.46
1	D	205	GLN	CA-CB	5.66	1.62	1.53
1	B	138	LEU	CA-C	5.66	1.60	1.52
1	C	18	ARG	CD-NE	5.65	1.54	1.46
1	D	94	HIS	CD2-NE2	-5.64	1.31	1.37
1	B	243	VAL	C-N	5.64	1.41	1.33
1	A	303	ASP	C-N	5.63	1.40	1.33
1	D	258	SER	CA-C	5.63	1.59	1.52
1	D	293	ASN	CA-C	-5.60	1.44	1.52
1	A	345	GLU	N-CA	5.60	1.53	1.46
1	D	145	PRO	N-CD	-5.60	1.40	1.47
1	A	266	LEU	N-CA	5.59	1.53	1.46
1	A	71	PRO	CA-C	-5.59	1.47	1.52
1	A	126	ASP	CA-CB	5.59	1.62	1.53
1	D	32	GLU	C-N	5.59	1.41	1.33
1	D	156	GLY	CA-C	5.59	1.58	1.52
1	A	67	ALA	C-N	5.58	1.41	1.33
1	B	96	GLU	C-O	-5.58	1.17	1.24
1	B	213	LEU	C-O	-5.57	1.17	1.24
1	C	144	VAL	CA-C	5.56	1.57	1.53
1	B	103	HIS	CD2-NE2	5.55	1.44	1.37
1	C	240	GLN	CA-CB	5.54	1.62	1.53
1	D	165	GLY	CA-C	-5.54	1.45	1.52
1	D	54	ALA	CA-CB	5.53	1.62	1.53
1	B	175	LEU	C-O	-5.52	1.17	1.24
1	C	129	ARG	CD-NE	5.52	1.53	1.46
1	D	111	THR	CA-CB	5.52	1.61	1.53
1	B	326	ARG	CA-CB	5.52	1.61	1.53
1	C	63	ILE	CA-CB	5.50	1.61	1.54
1	C	287	TRP	CA-CB	5.49	1.60	1.53
1	C	345	GLU	N-CA	-5.49	1.39	1.46
1	D	344	SER	C-N	5.49	1.41	1.33
1	C	73	GLU	N-CA	-5.49	1.38	1.45
1	D	286	ARG	CD-NE	5.49	1.53	1.46
1	C	241	ARG	CD-NE	5.46	1.53	1.46
1	D	251	GLY	CA-C	5.46	1.58	1.52
1	A	147	ARG	CA-C	-5.46	1.45	1.52
1	C	314	LEU	CB-CG	5.45	1.64	1.53
1	A	72	PRO	N-CA	-5.45	1.40	1.47
1	B	73	GLU	CA-C	5.44	1.58	1.52
1	C	89	HIS	CA-CB	5.44	1.61	1.53
1	A	298	GLN	N-CA	-5.43	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	CYS	CA-CB	5.42	1.62	1.53
1	B	187	ASP	CA-CB	5.42	1.61	1.53
1	C	255	PRO	N-CA	-5.42	1.40	1.47
1	B	326	ARG	CZ-NH1	-5.41	1.25	1.32
1	D	140	HIS	C-O	-5.41	1.17	1.24
1	D	167	ARG	C-O	-5.41	1.17	1.24
1	B	155	ALA	CA-C	5.41	1.59	1.52
1	A	51	HIS	ND1-CE1	5.41	1.38	1.32
1	C	351	TRP	CA-C	5.39	1.59	1.52
1	B	283	TRP	NE1-CE2	5.39	1.43	1.37
1	C	200	ALA	N-CA	-5.39	1.39	1.46
1	B	64	CYS	CA-CB	5.38	1.62	1.53
1	D	169	ARG	CA-CB	5.37	1.61	1.53
1	B	322	ASP	CA-C	5.37	1.60	1.52
1	C	96	GLU	CA-C	-5.37	1.45	1.52
1	C	155	ALA	N-CA	-5.36	1.39	1.46
1	C	315	CYS	CA-C	-5.36	1.46	1.52
1	D	212	ARG	CA-C	-5.36	1.46	1.52
1	B	236	ARG	CA-CB	5.36	1.61	1.53
1	D	247	GLN	CA-C	5.35	1.59	1.52
1	B	207	HIS	C-N	5.35	1.40	1.33
1	B	146	ARG	CA-C	5.34	1.60	1.52
1	C	280	PHE	CA-CB	5.34	1.63	1.53
1	B	306	THR	CA-C	-5.33	1.46	1.52
1	B	34	ARG	CA-CB	5.33	1.61	1.53
1	A	11	LEU	CA-CB	5.32	1.61	1.53
1	C	95	ALA	CA-CB	5.32	1.61	1.53
1	B	48	SER	C-N	5.31	1.40	1.33
1	C	54	ALA	C-N	5.31	1.41	1.33
1	A	96	GLU	N-CA	-5.30	1.40	1.46
1	C	294	GLN	N-CA	5.30	1.52	1.46
1	D	169	ARG	CZ-NH1	-5.29	1.25	1.32
1	A	155	ALA	C-N	5.29	1.40	1.33
1	B	80	LEU	CA-CB	5.28	1.61	1.53
1	D	290	ILE	CA-CB	5.27	1.60	1.54
1	A	182	ASP	CA-CB	5.27	1.61	1.53
1	C	144	VAL	CA-CB	-5.27	1.47	1.54
1	C	148	ARG	CZ-NH1	-5.27	1.25	1.32
1	A	184	ARG	CD-NE	5.26	1.53	1.46
1	A	92	ASP	CA-CB	-5.26	1.45	1.53
1	A	238	MET	CA-C	-5.25	1.46	1.52
1	D	137	ALA	C-O	-5.25	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	260	ARG	N-CA	-5.25	1.39	1.46
1	C	14	SER	C-N	-5.24	1.26	1.33
1	C	292	SER	C-N	5.24	1.41	1.33
1	C	298	GLN	C-O	-5.24	1.17	1.23
1	B	241	ARG	CA-CB	5.23	1.61	1.53
1	D	327	PHE	C-N	5.23	1.40	1.33
1	D	9	GLU	N-CA	-5.23	1.39	1.46
1	C	13	ASP	CA-CB	5.21	1.61	1.53
1	C	135	GLU	CA-CB	5.21	1.61	1.53
1	C	148	ARG	CD-NE	5.20	1.53	1.46
1	A	104	THR	CA-CB	5.20	1.61	1.53
1	B	223	GLN	CA-C	5.19	1.59	1.52
1	D	237	ASP	CA-CB	5.18	1.61	1.53
1	C	164	ALA	C-N	5.18	1.40	1.34
1	B	213	LEU	CA-C	5.18	1.59	1.52
1	D	146	ARG	C-N	5.18	1.40	1.33
1	A	77	ALA	CA-CB	-5.16	1.45	1.53
1	D	307	VAL	C-N	5.16	1.39	1.33
1	D	204	GLN	C-N	5.15	1.40	1.34
1	A	217	ARG	CD-NE	5.15	1.53	1.46
1	D	61	VAL	C-N	5.15	1.41	1.33
1	C	307	VAL	CA-CB	5.14	1.60	1.54
1	D	8	GLU	N-CA	5.14	1.52	1.46
1	A	151	GLU	C-N	5.14	1.40	1.33
1	D	354	ALA	CA-C	5.13	1.59	1.52
1	D	103	HIS	CA-CB	5.13	1.61	1.53
1	C	19	ALA	CA-C	5.12	1.59	1.52
1	D	157	ALA	CA-C	5.12	1.59	1.52
1	A	283	TRP	CA-C	-5.12	1.46	1.52
1	C	311	ASP	CA-CB	5.12	1.62	1.53
1	A	239	GLU	CA-C	-5.12	1.46	1.52
1	C	352	VAL	CA-CB	-5.11	1.48	1.54
1	C	94	HIS	C-N	5.11	1.40	1.33
1	C	68	ARG	CD-NE	5.10	1.53	1.46
1	C	157	ALA	C-N	5.10	1.40	1.33
1	D	286	ARG	CA-C	-5.10	1.46	1.52
1	D	225	HIS	CA-CB	5.10	1.61	1.53
1	C	35	LEU	CA-C	-5.09	1.46	1.52
1	D	241	ARG	CD-NE	5.09	1.53	1.46
1	B	220	LEU	CA-C	5.09	1.59	1.52
1	D	202	HIS	ND1-CE1	5.09	1.37	1.32
1	A	187	ASP	CA-C	5.09	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	271	HIS	ND1-CE1	5.09	1.37	1.32
1	D	320	CYS	C-O	-5.08	1.17	1.24
1	C	177	ILE	CA-C	-5.08	1.46	1.52
1	C	224	LEU	CA-CB	5.08	1.61	1.53
1	A	301	TYR	CA-C	5.08	1.59	1.52
1	B	159	LEU	C-N	5.07	1.40	1.33
1	B	217	ARG	CA-C	-5.07	1.46	1.52
1	A	283	TRP	NE1-CE2	5.07	1.43	1.37
1	C	60	VAL	N-CA	5.07	1.52	1.46
1	B	107	GLN	CA-C	-5.06	1.46	1.52
1	C	236	ARG	CA-C	5.06	1.59	1.52
1	D	134	LEU	CA-CB	5.06	1.61	1.53
1	B	192	VAL	CA-C	5.06	1.59	1.52
1	A	211	SER	CA-C	-5.05	1.46	1.52
1	A	340	LEU	C-N	5.05	1.40	1.33
1	A	42	GLY	CA-C	-5.05	1.46	1.52
1	D	187	ASP	CA-CB	5.05	1.61	1.53
1	B	250	LEU	N-CA	5.04	1.52	1.46
1	B	150	GLN	CA-CB	-5.04	1.45	1.53
1	D	260	ARG	CD-NE	5.04	1.53	1.46
1	A	267	VAL	N-CA	-5.03	1.39	1.46
1	D	122	GLU	N-CA	-5.02	1.40	1.46
1	D	110	GLN	N-CA	-5.02	1.40	1.46
1	D	280	PHE	C-N	5.01	1.40	1.33
1	A	25	GLU	N-CA	-5.01	1.40	1.46
1	B	324	GLU	CA-C	5.01	1.59	1.52
1	C	271	HIS	C-O	-5.01	1.17	1.23
1	A	179	VAL	C-N	5.01	1.40	1.33
1	B	258	SER	CA-C	-5.01	1.46	1.52
1	B	246	LYS	N-CA	-5.00	1.40	1.46

All (939) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	CYS	O-C-N	-14.95	109.81	121.47
1	A	148	ARG	NE-CZ-NH2	12.92	130.83	119.20
1	D	16	ARG	NE-CZ-NH2	12.38	130.34	119.20
1	A	163	ARG	NE-CZ-NH2	11.23	129.31	119.20
1	A	241	ARG	NE-CZ-NH1	11.11	132.60	121.50
1	A	51	HIS	CA-CB-CG	10.99	124.79	113.80
1	D	91	LEU	CA-C-N	10.98	135.00	120.28
1	D	91	LEU	C-N-CA	10.98	135.00	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	ILE	N-CA-C	10.86	121.77	110.36
1	C	169	ARG	N-CA-C	10.65	123.95	111.71
1	C	35	LEU	N-CA-C	10.49	122.72	111.28
1	C	271	HIS	CA-CB-CG	10.49	124.29	113.80
1	C	50	ARG	NE-CZ-NH2	10.21	128.39	119.20
1	C	92	ASP	CA-CB-CG	-10.20	102.40	112.60
1	C	73	GLU	O-C-N	-10.19	113.52	121.47
1	A	43	THR	CA-C-N	9.93	130.92	120.00
1	A	43	THR	C-N-CA	9.93	130.92	120.00
1	A	7	PHE	CA-C-N	9.91	133.56	120.28
1	A	7	PHE	C-N-CA	9.91	133.56	120.28
1	B	203	PHE	CA-CB-CG	-9.82	103.98	113.80
1	A	217	ARG	CA-C-N	9.75	133.11	120.44
1	A	217	ARG	C-N-CA	9.75	133.11	120.44
1	A	211	SER	N-CA-C	9.71	121.46	111.07
1	A	167	ARG	NE-CZ-NH2	9.62	127.86	119.20
1	B	75	MET	N-CA-C	9.56	121.78	111.36
1	C	18	ARG	N-CA-C	9.54	121.67	111.28
1	D	159	LEU	N-CA-C	9.53	121.67	111.28
1	A	226	GLN	N-CA-C	9.52	121.42	111.14
1	B	326	ARG	NH1-CZ-NH2	-9.51	106.94	119.30
1	C	147	ARG	NE-CZ-NH2	9.49	127.74	119.20
1	B	233	ARG	NE-CZ-NH2	9.46	127.71	119.20
1	A	177	ILE	N-CA-C	9.42	120.25	110.36
1	B	144	VAL	CA-C-N	9.42	131.61	119.84
1	B	144	VAL	C-N-CA	9.42	131.61	119.84
1	C	282	THR	N-CA-C	9.41	124.73	109.40
1	C	184	ARG	N-CA-C	9.34	122.31	111.11
1	A	181	GLU	O-C-N	9.27	131.62	122.07
1	B	51	HIS	CB-CG-CD2	-9.17	119.28	131.20
1	D	124	ARG	NE-CZ-NH1	9.16	130.66	121.50
1	C	225	HIS	CE1-NE2-CD2	-9.15	99.85	109.00
1	A	293	ASN	CA-CB-CG	9.11	121.71	112.60
1	B	326	ARG	NE-CZ-NH2	9.05	127.35	119.20
1	B	184	ARG	NE-CZ-NH2	9.05	127.34	119.20
1	B	55	ALA	N-CA-C	9.05	120.75	111.07
1	A	328	CYS	O-C-N	-8.94	111.61	123.23
1	C	160	ARG	NE-CZ-NH2	8.91	127.22	119.20
1	C	220	LEU	CA-C-N	8.90	129.64	119.94
1	C	220	LEU	C-N-CA	8.90	129.64	119.94
1	C	278	ASN	CA-CB-CG	8.90	121.50	112.60
1	C	226	GLN	OE1-CD-NE2	-8.88	113.72	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	VAL	N-CA-C	8.80	119.59	110.62
1	D	308	VAL	CB-CA-C	-8.77	102.88	111.30
1	A	278	ASN	O-C-N	-8.74	113.05	123.10
1	D	175	LEU	N-CA-C	8.73	120.79	111.28
1	C	325	ARG	NE-CZ-NH1	8.70	130.20	121.50
1	B	231	SER	N-CA-C	8.70	120.76	111.28
1	B	180	ILE	CA-C-N	8.69	132.63	120.29
1	B	180	ILE	C-N-CA	8.69	132.63	120.29
1	C	159	LEU	CA-C-O	-8.64	111.40	120.55
1	D	117	LEU	CA-C-N	8.59	132.49	120.29
1	D	117	LEU	C-N-CA	8.59	132.49	120.29
1	D	86	SER	N-CA-C	8.59	120.64	111.28
1	C	345	GLU	CB-CG-CD	8.58	127.19	112.60
1	B	83	PHE	CA-CB-CG	-8.54	105.26	113.80
1	D	307	VAL	N-CA-C	8.52	119.95	109.30
1	B	275	ARG	NE-CZ-NH1	8.46	129.97	121.50
1	D	124	ARG	NE-CZ-NH2	-8.44	111.60	119.20
1	D	73	GLU	CA-C-N	8.43	130.38	119.84
1	D	73	GLU	C-N-CA	8.43	130.38	119.84
1	C	225	HIS	CG-CD2-NE2	8.43	115.63	107.20
1	D	6	ASP	CA-CB-CG	8.40	121.00	112.60
1	D	172	ASP	O-C-N	-8.36	113.26	122.12
1	C	108	GLN	CA-C-N	8.30	131.01	120.56
1	C	108	GLN	C-N-CA	8.30	131.01	120.56
1	C	48	SER	CA-C-N	8.28	129.35	119.99
1	C	48	SER	C-N-CA	8.28	129.35	119.99
1	B	160	ARG	NE-CZ-NH2	8.28	126.65	119.20
1	D	14	SER	CA-C-O	-8.28	111.56	120.17
1	C	68	ARG	NE-CZ-NH2	8.27	126.64	119.20
1	D	256	GLU	CA-C-N	8.25	130.15	119.84
1	D	256	GLU	C-N-CA	8.25	130.15	119.84
1	B	35	LEU	N-CA-C	8.23	119.88	111.07
1	C	125	ARG	N-CA-C	8.20	120.00	111.14
1	B	179	VAL	CA-C-N	8.20	131.69	120.46
1	B	179	VAL	C-N-CA	8.20	131.69	120.46
1	C	333	SER	CA-C-O	8.15	130.64	121.51
1	C	179	VAL	N-CA-C	8.14	118.92	110.62
1	C	253	GLU	CA-C-N	8.09	132.24	120.51
1	C	253	GLU	C-N-CA	8.09	132.24	120.51
1	B	190	GLU	N-CA-C	8.08	119.72	111.07
1	A	147	ARG	NE-CZ-NH1	-8.07	113.43	121.50
1	B	163	ARG	CA-C-N	8.05	131.07	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	ARG	C-N-CA	8.05	131.07	120.28
1	D	200	ALA	CA-C-N	8.04	131.06	120.28
1	D	200	ALA	C-N-CA	8.04	131.06	120.28
1	A	32	GLU	CA-C-O	8.03	129.06	120.55
1	B	32	GLU	N-CA-CB	-8.02	98.29	110.16
1	B	20	SER	N-CA-C	8.02	120.10	111.36
1	A	89	HIS	CG-CD2-NE2	8.00	115.20	107.20
1	A	129	ARG	N-CA-C	7.99	119.99	111.28
1	B	317	VAL	CB-CA-C	7.99	119.52	110.41
1	D	50	ARG	NE-CZ-NH2	-7.99	112.01	119.20
1	A	285	ARG	NE-CZ-NH2	-7.97	112.02	119.20
1	B	236	ARG	CA-C-O	-7.95	111.99	120.42
1	C	233	ARG	N-CA-C	7.95	119.94	111.28
1	D	265	GLY	CA-C-N	7.91	131.95	120.71
1	D	265	GLY	C-N-CA	7.91	131.95	120.71
1	B	135	GLU	O-C-N	-7.91	113.74	122.12
1	A	6	ASP	CA-C-O	7.90	129.51	120.98
1	C	182	ASP	CA-C-N	7.88	130.84	120.28
1	C	182	ASP	C-N-CA	7.88	130.84	120.28
1	A	328	CYS	CA-C-O	7.88	129.21	120.70
1	A	55	ALA	CA-C-N	7.86	130.66	120.44
1	A	55	ALA	C-N-CA	7.86	130.66	120.44
1	D	329	PHE	CA-CB-CG	7.84	121.64	113.80
1	C	262	GLY	CA-C-N	7.84	127.75	119.05
1	C	262	GLY	C-N-CA	7.84	127.75	119.05
1	B	313	ARG	CD-NE-CZ	-7.83	113.44	124.40
1	D	151	GLU	CA-C-N	7.82	130.76	120.28
1	D	151	GLU	C-N-CA	7.82	130.76	120.28
1	A	187	ASP	N-CA-CB	7.80	121.59	110.12
1	D	231	SER	O-C-N	-7.80	113.85	122.12
1	A	229	LEU	N-CA-C	7.79	119.77	111.28
1	C	211	SER	N-CA-C	7.79	119.40	111.07
1	C	177	ILE	O-C-N	-7.78	114.16	121.94
1	B	178	ASN	N-CA-C	7.76	119.74	111.28
1	B	169	ARG	CA-C-O	7.74	128.88	119.97
1	B	172	ASP	CA-C-O	-7.74	112.34	120.55
1	A	343	ASP	CA-CB-CG	-7.74	104.86	112.60
1	B	209	GLU	N-CA-C	7.73	119.34	111.07
1	A	47	GLU	N-CA-C	7.73	119.34	111.07
1	B	118	ARG	N-CA-C	7.73	119.78	111.36
1	B	237	ASP	N-CA-C	7.72	119.70	111.28
1	B	125	ARG	NE-CZ-NH2	-7.72	112.25	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	136	ALA	CA-C-O	7.68	128.57	120.42
1	A	144	VAL	O-C-N	-7.68	114.89	121.57
1	C	202	HIS	CA-CB-CG	7.68	121.48	113.80
1	B	142	ALA	CB-CA-C	7.66	121.21	109.34
1	D	222	ALA	O-C-N	-7.64	112.30	122.23
1	A	178	ASN	OD1-CG-ND2	-7.62	114.98	122.60
1	B	5	LEU	O-C-N	-7.62	114.52	123.06
1	D	57	ARG	CA-C-N	7.60	130.47	120.28
1	D	57	ARG	C-N-CA	7.60	130.47	120.28
1	B	151	GLU	CA-C-N	7.60	130.46	120.28
1	B	151	GLU	C-N-CA	7.60	130.46	120.28
1	D	353	SER	N-CA-C	7.60	119.64	111.36
1	C	12	LYS	N-CA-C	7.59	121.47	111.75
1	B	107	GLN	N-CA-C	7.58	119.23	110.97
1	B	162	ALA	N-CA-C	7.55	120.47	111.33
1	D	9	GLU	CA-C-N	7.53	130.68	120.44
1	D	9	GLU	C-N-CA	7.53	130.68	120.44
1	C	296	VAL	O-C-N	-7.51	114.44	123.00
1	B	171	LEU	O-C-N	-7.50	114.34	122.07
1	A	160	ARG	NE-CZ-NH2	7.48	125.94	119.20
1	D	65	ASP	CA-CB-CG	-7.47	105.13	112.60
1	D	150	GLN	OE1-CD-NE2	-7.47	115.13	122.60
1	C	211	SER	O-C-N	-7.47	114.38	122.07
1	C	136	ALA	CA-C-N	7.43	130.11	120.44
1	C	136	ALA	C-N-CA	7.43	130.11	120.44
1	A	121	ARG	NE-CZ-NH1	7.39	128.89	121.50
1	B	209	GLU	CA-C-O	7.39	128.58	120.82
1	C	54	ALA	CA-C-N	7.39	130.78	120.29
1	C	54	ALA	C-N-CA	7.39	130.78	120.29
1	D	169	ARG	NE-CZ-NH1	7.38	128.88	121.50
1	A	152	ALA	O-C-N	-7.38	114.30	122.12
1	B	329	PHE	CA-C-N	7.36	134.07	122.74
1	B	329	PHE	C-N-CA	7.36	134.07	122.74
1	B	308	VAL	CA-C-N	7.35	133.41	122.75
1	B	308	VAL	C-N-CA	7.35	133.41	122.75
1	B	135	GLU	CA-C-O	7.35	128.34	120.55
1	D	62	GLY	O-C-N	-7.34	114.46	122.24
1	B	144	VAL	CA-C-O	-7.34	116.12	119.94
1	B	122	GLU	N-CA-C	7.34	119.92	111.11
1	A	99	ASP	CA-CB-CG	7.33	119.93	112.60
1	D	243	VAL	CA-C-N	7.32	130.69	120.29
1	D	243	VAL	C-N-CA	7.32	130.69	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	ARG	N-CA-C	7.32	120.13	111.71
1	A	263	PRO	N-CA-C	-7.32	104.41	114.80
1	A	24	VAL	O-C-N	-7.30	114.49	121.87
1	C	89	HIS	CE1-NE2-CD2	-7.30	101.70	109.00
1	A	173	TYR	CA-C-N	7.30	130.07	120.28
1	A	173	TYR	C-N-CA	7.30	130.07	120.28
1	B	300	LYS	O-C-N	-7.29	115.09	123.33
1	A	117	LEU	CA-C-N	7.28	130.26	120.65
1	A	117	LEU	C-N-CA	7.28	130.26	120.65
1	D	140	HIS	CA-CB-CG	-7.28	106.52	113.80
1	C	217	ARG	NE-CZ-NH1	-7.26	114.24	121.50
1	A	123	ALA	N-CA-C	7.26	119.27	111.36
1	B	142	ALA	N-CA-CB	-7.26	99.88	110.40
1	C	294	GLN	CB-CG-CD	-7.23	100.31	112.60
1	D	309	VAL	CA-CB-CG2	7.21	122.66	110.40
1	C	111	THR	N-CA-C	7.20	120.04	111.33
1	A	305	VAL	N-CA-C	7.19	119.47	109.55
1	A	212	ARG	NE-CZ-NH2	7.18	125.67	119.20
1	D	43	THR	CA-CB-OG1	7.18	120.38	109.60
1	C	124	ARG	NE-CZ-NH1	7.18	128.68	121.50
1	C	144	VAL	O-C-N	-7.18	114.44	121.12
1	A	315	CYS	O-C-N	-7.17	113.82	122.65
1	A	135	GLU	N-CA-C	7.15	118.72	111.07
1	A	172	ASP	O-C-N	7.15	130.31	122.15
1	B	88	ASN	CB-CA-C	7.14	123.77	110.70
1	C	157	ALA	CA-C-O	7.13	128.31	120.82
1	A	148	ARG	NE-CZ-NH1	-7.10	114.40	121.50
1	C	212	ARG	NE-CZ-NH1	7.08	128.58	121.50
1	A	362	ALA	O-C-N	-7.08	114.62	122.12
1	A	30	GLU	CA-C-N	7.07	129.63	120.44
1	A	30	GLU	C-N-CA	7.07	129.63	120.44
1	A	348	LEU	CA-C-N	7.06	129.62	120.44
1	A	348	LEU	C-N-CA	7.06	129.62	120.44
1	D	190	GLU	N-CA-C	7.05	118.97	111.28
1	D	43	THR	N-CA-CB	7.04	120.22	110.01
1	B	147	ARG	O-C-N	-7.01	113.65	122.27
1	B	205	GLN	CA-C-N	7.00	127.57	119.94
1	B	205	GLN	C-N-CA	7.00	127.57	119.94
1	D	145	PRO	CA-C-N	6.99	129.97	120.54
1	D	145	PRO	C-N-CA	6.99	129.97	120.54
1	D	18	ARG	NE-CZ-NH1	6.98	128.48	121.50
1	D	209	GLU	CB-CA-C	6.98	121.93	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	186	PHE	CA-CB-CG	6.98	120.78	113.80
1	D	61	VAL	N-CA-C	6.95	117.71	110.62
1	A	147	ARG	NE-CZ-NH2	6.94	125.45	119.20
1	A	121	ARG	NE-CZ-NH2	-6.94	112.95	119.20
1	A	248	LYS	N-CA-C	6.94	122.92	113.21
1	D	45	LEU	N-CA-CB	-6.93	99.96	110.01
1	A	95	ALA	CA-C-N	6.93	129.45	120.44
1	A	95	ALA	C-N-CA	6.93	129.45	120.44
1	D	118	ARG	CA-C-N	6.93	129.07	120.34
1	D	118	ARG	C-N-CA	6.93	129.07	120.34
1	D	194	ARG	NE-CZ-NH1	6.93	128.43	121.50
1	C	323	SER	N-CA-CB	6.92	122.18	110.49
1	B	66	LEU	CA-C-N	6.91	130.10	120.29
1	B	66	LEU	C-N-CA	6.91	130.10	120.29
1	A	136	ALA	N-CA-C	6.90	118.89	111.36
1	A	243	VAL	O-C-N	-6.90	115.04	121.94
1	C	2	THR	O-C-N	-6.89	114.92	122.09
1	D	356	GLN	OE1-CD-NE2	-6.88	115.72	122.60
1	B	307	VAL	N-CA-C	6.88	118.45	109.58
1	C	257	PRO	CA-C-N	6.88	132.52	122.41
1	C	257	PRO	C-N-CA	6.88	132.52	122.41
1	D	107	GLN	N-CA-C	6.88	118.46	110.97
1	C	210	LEU	CA-C-N	6.87	129.38	120.44
1	C	210	LEU	C-N-CA	6.87	129.38	120.44
1	B	89	HIS	CE1-NE2-CD2	-6.86	102.14	109.00
1	B	158	ALA	CA-C-O	6.85	127.81	120.55
1	B	8	GLU	N-CA-C	6.85	118.40	111.07
1	B	355	VAL	CA-C-N	6.84	129.45	120.28
1	B	355	VAL	C-N-CA	6.84	129.45	120.28
1	C	110	GLN	OE1-CD-NE2	-6.84	115.76	122.60
1	B	229	LEU	CA-C-O	6.83	127.99	120.82
1	A	267	VAL	N-CA-CB	6.83	120.51	111.64
1	B	90	LYS	CA-C-O	-6.82	113.32	120.55
1	C	37	LYS	CA-C-N	6.82	129.97	120.29
1	C	37	LYS	C-N-CA	6.82	129.97	120.29
1	D	179	VAL	O-C-N	-6.82	115.25	121.87
1	C	159	LEU	O-C-N	6.82	129.34	122.12
1	A	152	ALA	CA-C-N	6.81	129.40	120.28
1	A	152	ALA	C-N-CA	6.81	129.40	120.28
1	B	269	GLU	N-CA-CB	6.81	123.32	111.13
1	B	46	LEU	CA-C-N	6.80	129.28	120.44
1	B	46	LEU	C-N-CA	6.80	129.28	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	THR	N-CA-C	6.80	118.69	111.28
1	B	338	CYS	CA-C-O	6.79	128.42	120.14
1	C	161	THR	CA-C-N	6.79	129.26	120.44
1	C	161	THR	C-N-CA	6.79	129.26	120.44
1	A	166	TYR	N-CA-C	6.78	118.67	111.28
1	A	291	GLN	OE1-CD-NE2	-6.77	115.83	122.60
1	C	124	ARG	NH1-CZ-NH2	-6.77	110.50	119.30
1	D	217	ARG	CD-NE-CZ	-6.76	114.94	124.40
1	A	11	LEU	CA-C-N	6.76	132.00	120.71
1	A	11	LEU	C-N-CA	6.76	132.00	120.71
1	D	326	ARG	O-C-N	6.76	130.90	123.13
1	D	260	ARG	NE-CZ-NH2	6.76	125.28	119.20
1	B	58	ALA	CA-C-N	6.75	129.22	120.44
1	B	58	ALA	C-N-CA	6.75	129.22	120.44
1	A	319	LEU	CA-C-O	6.74	127.93	120.92
1	C	123	ALA	N-CA-C	6.74	118.71	111.36
1	C	32	GLU	N-CA-C	6.74	118.63	111.28
1	A	89	HIS	CE1-NE2-CD2	-6.74	102.26	109.00
1	D	236	ARG	NE-CZ-NH2	-6.72	113.15	119.20
1	D	233	ARG	NE-CZ-NH2	6.71	125.24	119.20
1	D	196	VAL	N-CA-C	6.69	117.44	110.62
1	C	3	VAL	O-C-N	-6.69	114.71	122.07
1	A	204	GLN	OE1-CD-NE2	-6.69	115.91	122.60
1	C	147	ARG	NE-CZ-NH1	-6.66	114.84	121.50
1	B	319	LEU	CA-C-O	6.66	127.71	119.05
1	B	137	ALA	CA-C-N	6.65	129.19	120.28
1	B	137	ALA	C-N-CA	6.65	129.19	120.28
1	C	242	HIS	CE1-NE2-CD2	-6.65	102.35	109.00
1	A	80	LEU	CA-C-N	6.65	129.19	120.28
1	A	80	LEU	C-N-CA	6.65	129.19	120.28
1	B	223	GLN	CA-C-N	6.64	129.18	120.28
1	B	223	GLN	C-N-CA	6.64	129.18	120.28
1	C	36	GLU	CA-C-O	6.64	127.46	120.42
1	C	232	ALA	N-CA-CB	-6.63	99.75	109.82
1	D	124	ARG	N-CA-C	6.62	118.15	111.07
1	B	101	THR	N-CA-C	6.62	119.05	111.11
1	C	117	LEU	CA-C-N	6.62	129.04	120.44
1	C	117	LEU	C-N-CA	6.62	129.04	120.44
1	A	110	GLN	OE1-CD-NE2	-6.61	115.99	122.60
1	A	73	GLU	CA-C-N	6.61	126.19	119.19
1	A	73	GLU	C-N-CA	6.61	126.19	119.19
1	C	127	PHE	CA-CB-CG	6.60	120.40	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	331	VAL	N-CA-CB	6.59	119.77	111.46
1	C	172	ASP	CA-C-N	6.58	128.99	120.44
1	C	172	ASP	C-N-CA	6.58	128.99	120.44
1	A	76	MET	CG-SD-CE	-6.57	86.44	100.90
1	D	37	LYS	N-CA-C	6.57	118.10	111.07
1	B	118	ARG	NE-CZ-NH1	6.55	128.05	121.50
1	D	170	ALA	N-CA-C	6.55	118.08	111.07
1	D	77	ALA	N-CA-C	6.55	118.42	111.28
1	B	308	VAL	CB-CA-C	-6.54	104.03	111.55
1	B	328	CYS	O-C-N	-6.54	115.58	123.10
1	A	260	ARG	NE-CZ-NH1	6.54	128.04	121.50
1	C	212	ARG	N-CA-C	6.54	118.40	111.28
1	B	169	ARG	O-C-N	-6.53	114.24	122.27
1	D	303	ASP	CA-C-N	6.52	127.98	119.84
1	D	303	ASP	C-N-CA	6.52	127.98	119.84
1	A	121	ARG	CA-C-N	6.51	129.00	120.28
1	A	121	ARG	C-N-CA	6.51	129.00	120.28
1	C	213	LEU	CA-C-N	6.51	128.90	120.44
1	C	213	LEU	C-N-CA	6.51	128.90	120.44
1	C	166	TYR	N-CA-C	6.50	118.36	111.28
1	A	344	SER	N-CA-CB	-6.49	101.50	111.56
1	D	220	LEU	N-CA-C	6.49	118.35	111.28
1	B	285	ARG	CD-NE-CZ	-6.49	115.32	124.40
1	C	140	HIS	CE1-NE2-CD2	-6.48	102.52	109.00
1	A	97	LEU	O-C-N	-6.48	115.25	122.12
1	B	135	GLU	CA-C-N	6.47	129.48	120.29
1	B	135	GLU	C-N-CA	6.47	129.48	120.29
1	C	196	VAL	CA-C-N	6.47	128.85	120.44
1	C	196	VAL	C-N-CA	6.47	128.85	120.44
1	D	68	ARG	NE-CZ-NH1	6.47	127.97	121.50
1	A	311	ASP	CA-CB-CG	6.47	119.07	112.60
1	C	187	ASP	O-C-N	-6.46	115.42	122.07
1	A	241	ARG	NE-CZ-NH2	-6.46	113.39	119.20
1	C	57	ARG	NE-CZ-NH1	6.46	127.96	121.50
1	C	108	GLN	CB-CG-CD	6.45	123.56	112.60
1	C	150	GLN	N-CA-CB	6.44	119.35	110.01
1	C	299	LYS	N-CA-C	6.44	119.12	111.33
1	A	67	ALA	N-CA-C	6.43	118.29	111.28
1	C	121	ARG	NE-CZ-NH2	-6.43	113.41	119.20
1	A	17	PHE	CA-CB-CG	-6.43	107.37	113.80
1	B	154	GLU	N-CA-C	6.42	118.36	111.36
1	D	157	ALA	CA-C-N	6.42	128.88	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	157	ALA	C-N-CA	6.42	128.88	120.28
1	C	242	HIS	CA-C-O	-6.42	114.08	120.82
1	B	206	GLY	CA-C-N	6.40	128.86	120.28
1	B	206	GLY	C-N-CA	6.40	128.86	120.28
1	C	83	PHE	CA-CB-CG	-6.40	107.40	113.80
1	C	57	ARG	NE-CZ-NH2	-6.39	113.44	119.20
1	D	346	ARG	N-CA-C	6.39	117.91	111.07
1	C	211	SER	CA-C-O	6.39	127.53	120.82
1	C	260	ARG	NE-CZ-NH1	6.39	127.89	121.50
1	D	152	ALA	CA-C-O	6.38	127.32	120.55
1	C	18	ARG	CA-C-O	6.37	127.30	120.55
1	B	312	LEU	O-C-N	-6.37	112.23	122.41
1	B	215	GLN	CA-C-N	6.36	128.81	120.28
1	B	215	GLN	C-N-CA	6.36	128.81	120.28
1	C	18	ARG	NE-CZ-NH2	-6.36	113.48	119.20
1	A	149	ALA	N-CA-C	6.36	121.86	111.37
1	D	213	LEU	N-CA-C	6.35	118.20	111.28
1	C	217	ARG	NE-CZ-NH2	6.34	124.91	119.20
1	D	303	ASP	CA-CB-CG	6.34	118.94	112.60
1	D	169	ARG	NE-CZ-NH2	-6.34	113.50	119.20
1	C	108	GLN	O-C-N	-6.33	114.17	122.59
1	B	120	PHE	CB-CA-C	6.33	121.30	110.79
1	D	241	ARG	N-CA-C	6.31	118.16	111.28
1	A	71	PRO	N-CA-C	6.31	118.40	110.70
1	A	347	LEU	O-C-N	6.31	128.57	122.07
1	B	356	GLN	CA-C-N	6.31	129.25	120.29
1	B	356	GLN	C-N-CA	6.31	129.25	120.29
1	C	273	PHE	N-CA-C	-6.30	98.93	109.07
1	C	214	SER	N-CA-C	-6.29	104.34	111.07
1	C	243	VAL	N-CA-C	6.28	116.45	110.42
1	D	56	SER	CA-C-N	6.28	128.61	120.44
1	D	56	SER	C-N-CA	6.28	128.61	120.44
1	B	353	SER	CA-C-N	6.28	129.21	120.29
1	B	353	SER	C-N-CA	6.28	129.21	120.29
1	D	183	LYS	N-CA-C	6.28	118.13	111.28
1	A	249	GLU	CB-CG-CD	6.28	123.27	112.60
1	A	194	ARG	CB-CA-C	-6.27	98.62	110.67
1	C	140	HIS	ND1-CE1-NE2	6.27	114.67	108.40
1	A	65	ASP	CA-C-N	6.27	128.97	120.44
1	A	65	ASP	C-N-CA	6.27	128.97	120.44
1	D	184	ARG	CA-C-N	-6.27	112.29	120.44
1	D	184	ARG	C-N-CA	-6.27	112.29	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	356	GLN	N-CA-C	6.27	119.09	111.82
1	C	171	LEU	N-CA-C	6.27	118.91	111.33
1	C	190	GLU	O-C-N	-6.26	115.48	122.12
1	C	63	ILE	N-CA-CB	6.25	119.04	110.54
1	B	355	VAL	N-CA-C	6.24	117.03	110.72
1	C	234	GLU	N-CA-C	6.24	118.08	111.28
1	C	45	LEU	N-CA-C	6.24	118.16	111.36
1	C	160	ARG	NE-CZ-NH1	-6.24	115.26	121.50
1	C	285	ARG	NH1-CZ-NH2	-6.24	111.19	119.30
1	D	121	ARG	CG-CD-NE	-6.24	98.28	112.00
1	A	71	PRO	O-C-N	-6.23	114.11	121.46
1	D	58	ALA	CA-C-N	6.23	128.63	120.28
1	D	58	ALA	C-N-CA	6.23	128.63	120.28
1	C	83	PHE	N-CA-CB	6.23	119.04	110.01
1	D	27	GLU	CB-CG-CD	-6.22	102.02	112.60
1	B	51	HIS	ND1-CE1-NE2	6.21	114.61	108.40
1	C	21	ILE	N-CA-CB	6.21	118.99	110.54
1	C	125	ARG	CA-C-N	6.21	128.60	120.28
1	C	125	ARG	C-N-CA	6.21	128.60	120.28
1	C	110	GLN	CB-CA-C	-6.21	100.30	110.85
1	A	348	LEU	O-C-N	-6.20	115.69	122.07
1	B	160	ARG	NH1-CZ-NH2	-6.20	111.25	119.30
1	B	259	LEU	N-CA-CB	6.20	119.58	110.35
1	A	216	TYR	CA-CB-CG	-6.19	102.75	113.90
1	B	7	PHE	N-CA-C	6.19	120.09	112.54
1	C	148	ARG	CA-C-N	6.18	130.09	120.82
1	C	148	ARG	C-N-CA	6.18	130.09	120.82
1	B	113	VAL	N-CA-C	6.17	116.92	110.62
1	B	144	VAL	O-C-N	-6.17	114.54	120.59
1	B	241	ARG	NH1-CZ-NH2	-6.17	111.28	119.30
1	A	194	ARG	NE-CZ-NH2	-6.17	113.64	119.20
1	C	188	ILE	N-CA-CB	6.16	119.82	110.58
1	B	159	LEU	CA-C-O	6.16	127.08	120.55
1	A	155	ALA	CA-C-O	6.15	126.94	120.42
1	C	174	ALA	N-CA-CB	-6.15	101.08	110.12
1	C	272	LEU	N-CA-C	-6.14	99.81	108.96
1	C	214	SER	O-C-N	-6.14	115.75	122.07
1	D	128	TRP	CB-CA-C	6.13	120.97	110.79
1	B	262	GLY	O-C-N	-6.13	115.64	121.77
1	D	125	ARG	CD-NE-CZ	-6.13	115.82	124.40
1	A	38	LEU	CA-C-N	6.13	128.49	120.28
1	A	38	LEU	C-N-CA	6.13	128.49	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	241	ARG	NE-CZ-NH1	6.13	127.63	121.50
1	B	49	GLY	O-C-N	-6.10	116.33	122.19
1	B	132	GLU	CA-C-O	6.09	127.21	120.82
1	A	127	PHE	N-CA-C	6.09	117.91	111.28
1	A	186	PHE	CA-C-N	6.08	128.43	120.28
1	A	186	PHE	C-N-CA	6.08	128.43	120.28
1	B	164	ALA	CA-C-O	6.07	126.98	120.55
1	B	147	ARG	CA-C-N	6.07	130.10	121.42
1	B	147	ARG	C-N-CA	6.07	130.10	121.42
1	A	40	LYS	O-C-N	-6.07	115.23	122.15
1	A	18	ARG	NE-CZ-NH2	-6.06	113.74	119.20
1	D	337	SER	N-CA-CB	6.06	120.19	110.85
1	B	248	LYS	CA-C-O	-6.06	112.43	119.64
1	D	4	LYS	CA-C-N	6.05	130.15	121.50
1	D	4	LYS	C-N-CA	6.05	130.15	121.50
1	D	293	ASN	CA-CB-CG	-6.05	106.55	112.60
1	D	207	HIS	N-CA-C	6.05	117.87	111.28
1	B	127	PHE	CA-C-N	6.05	128.88	120.29
1	B	127	PHE	C-N-CA	6.05	128.88	120.29
1	A	171	LEU	N-CA-C	6.04	118.63	111.33
1	B	260	ARG	NE-CZ-NH1	6.03	127.53	121.50
1	A	199	GLN	OE1-CD-NE2	6.03	128.63	122.60
1	C	136	ALA	O-C-N	-6.03	114.86	122.27
1	D	113	VAL	O-C-N	6.02	127.81	121.91
1	A	103	HIS	CA-CB-CG	-6.02	107.78	113.80
1	C	105	LEU	CA-C-N	6.02	128.62	120.44
1	C	105	LEU	C-N-CA	6.02	128.62	120.44
1	C	355	VAL	CA-C-N	6.01	128.34	120.28
1	C	355	VAL	C-N-CA	6.01	128.34	120.28
1	C	50	ARG	N-CA-CB	6.01	119.06	110.16
1	C	89	HIS	CG-CD2-NE2	6.01	113.21	107.20
1	A	106	GLN	N-CA-C	6.01	117.63	111.14
1	D	94	HIS	CA-C-O	6.00	126.92	120.55
1	B	114	LYS	CA-C-O	-6.00	114.06	120.42
1	D	167	ARG	CA-C-O	6.00	126.78	120.42
1	A	15	PRO	CA-C-N	6.00	128.63	120.54
1	A	15	PRO	C-N-CA	6.00	128.63	120.54
1	B	172	ASP	CA-CB-CG	5.99	118.59	112.60
1	A	68	ARG	N-CA-C	5.99	117.81	111.28
1	A	272	LEU	CA-C-N	5.99	130.99	122.72
1	A	272	LEU	C-N-CA	5.99	130.99	122.72
1	B	83	PHE	O-C-N	-5.99	115.32	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	236	ARG	NE-CZ-NH1	5.98	127.48	121.50
1	A	166	TYR	CB-CG-CD2	-5.98	111.83	120.80
1	C	11	LEU	CA-C-N	5.96	129.09	120.38
1	C	11	LEU	C-N-CA	5.96	129.09	120.38
1	A	133	SER	N-CA-CB	5.96	118.66	110.01
1	B	70	GLY	O-C-N	-5.96	115.81	121.77
1	A	184	ARG	NE-CZ-NH1	5.96	127.46	121.50
1	A	197	GLU	CA-C-N	5.96	128.86	120.28
1	A	197	GLU	C-N-CA	5.96	128.86	120.28
1	A	145	PRO	CA-C-N	5.95	128.54	120.38
1	A	145	PRO	C-N-CA	5.95	128.54	120.38
1	B	273	PHE	CA-CB-CG	-5.95	107.86	113.80
1	A	47	GLU	CA-C-O	-5.94	114.58	120.82
1	A	203	PHE	CA-C-N	5.94	128.73	120.29
1	A	203	PHE	C-N-CA	5.94	128.73	120.29
1	C	106	GLN	OE1-CD-NE2	-5.94	116.66	122.60
1	B	200	ALA	CA-C-N	5.93	128.23	120.28
1	B	200	ALA	C-N-CA	5.93	128.23	120.28
1	C	262	GLY	O-C-N	-5.93	115.84	121.77
1	D	307	VAL	CA-C-N	-5.92	116.92	122.66
1	D	307	VAL	C-N-CA	-5.92	116.92	122.66
1	C	236	ARG	CA-C-O	-5.91	114.61	120.82
1	A	88	ASN	N-CA-CB	-5.91	101.12	110.28
1	B	93	SER	CA-C-O	5.91	126.68	120.42
1	B	68	ARG	NE-CZ-NH2	-5.90	113.89	119.20
1	C	310	ASP	CA-CB-CG	5.90	118.50	112.60
1	C	76	MET	N-CA-C	-5.90	104.80	112.23
1	C	355	VAL	O-C-N	-5.89	115.76	121.83
1	C	51	HIS	CA-C-O	-5.89	114.31	120.55
1	D	137	ALA	O-C-N	-5.89	115.03	122.27
1	A	52	TYR	N-CA-C	5.88	117.69	111.28
1	A	56	SER	N-CA-CB	5.88	118.54	110.01
1	B	6	ASP	CA-C-O	-5.88	114.76	121.58
1	C	144	VAL	CB-CA-C	5.88	117.61	110.85
1	D	259	LEU	O-C-N	-5.87	116.17	123.04
1	C	343	ASP	CA-CB-CG	-5.87	106.73	112.60
1	A	325	ARG	CA-C-N	5.87	131.65	120.97
1	A	325	ARG	C-N-CA	5.87	131.65	120.97
1	D	184	ARG	CA-CB-CG	5.87	125.84	114.10
1	D	103	HIS	CG-CD2-NE2	5.87	113.07	107.20
1	A	242	HIS	CA-C-N	5.87	128.16	120.60
1	A	242	HIS	C-N-CA	5.87	128.16	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	306	THR	CA-CB-OG1	5.86	118.39	109.60
1	B	160	ARG	N-CA-CB	5.86	118.67	109.94
1	C	241	ARG	CD-NE-CZ	5.86	132.60	124.40
1	B	185	LYS	CA-C-O	-5.85	114.85	121.00
1	D	89	HIS	CE1-NE2-CD2	-5.85	103.15	109.00
1	D	94	HIS	O-C-N	-5.85	115.92	122.12
1	B	202	HIS	ND1-CE1-NE2	5.85	114.25	108.40
1	B	254	GLU	CA-C-N	5.85	127.15	119.84
1	B	254	GLU	C-N-CA	5.85	127.15	119.84
1	A	89	HIS	CA-CB-CG	5.85	119.65	113.80
1	A	88	ASN	N-CA-C	5.84	118.60	111.82
1	C	8	GLU	CB-CG-CD	5.84	122.53	112.60
1	D	16	ARG	NH1-CZ-NH2	-5.84	111.70	119.30
1	A	89	HIS	CA-C-N	5.84	128.11	120.28
1	A	89	HIS	C-N-CA	5.84	128.11	120.28
1	D	231	SER	CA-C-N	5.84	128.03	120.44
1	D	231	SER	C-N-CA	5.84	128.03	120.44
1	A	83	PHE	N-CA-C	5.84	117.32	111.07
1	A	131	ALA	CA-C-N	5.84	128.03	120.44
1	A	131	ALA	C-N-CA	5.84	128.03	120.44
1	A	309	VAL	CA-C-N	5.83	128.37	120.44
1	A	309	VAL	C-N-CA	5.83	128.37	120.44
1	C	253	GLU	O-C-N	-5.83	116.22	123.04
1	B	274	LYS	O-C-N	-5.83	116.39	123.10
1	C	301	TYR	CA-C-O	5.83	126.73	120.20
1	D	323	SER	O-C-N	-5.82	116.54	123.06
1	A	163	ARG	NE-CZ-NH1	-5.82	115.69	121.50
1	D	234	GLU	CA-C-O	-5.82	114.68	120.90
1	C	186	PHE	CA-C-N	5.81	128.00	120.44
1	C	186	PHE	C-N-CA	5.81	128.00	120.44
1	B	89	HIS	CB-CG-CD2	-5.81	123.64	131.20
1	B	113	VAL	CA-C-N	5.81	128.54	120.29
1	B	113	VAL	C-N-CA	5.81	128.54	120.29
1	A	311	ASP	CA-C-O	5.80	127.67	120.54
1	D	54	ALA	CA-C-N	5.80	127.98	120.44
1	D	54	ALA	C-N-CA	5.80	127.98	120.44
1	B	241	ARG	NE-CZ-NH2	5.79	124.42	119.20
1	D	216	TYR	CA-C-N	5.79	128.36	120.54
1	D	216	TYR	C-N-CA	5.79	128.36	120.54
1	B	227	LEU	O-C-N	-5.79	116.11	122.07
1	D	120	PHE	CA-CB-CG	-5.78	108.02	113.80
1	C	242	HIS	CA-CB-CG	5.78	119.58	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	VAL	CA-C-O	5.78	127.28	121.27
1	B	34	ARG	NE-CZ-NH2	5.77	124.39	119.20
1	B	229	LEU	CA-C-N	5.77	128.33	120.54
1	B	229	LEU	C-N-CA	5.77	128.33	120.54
1	D	222	ALA	CA-C-O	5.77	126.65	120.24
1	A	239	GLU	N-CA-C	5.77	117.64	111.36
1	C	269	GLU	O-C-N	-5.77	116.15	123.24
1	A	73	GLU	O-C-N	-5.76	114.69	121.32
1	D	348	LEU	N-CA-CB	-5.76	101.66	110.01
1	C	281	LYS	CB-CA-C	5.75	119.71	109.65
1	C	360	ALA	CA-C-N	5.75	127.91	120.44
1	C	360	ALA	C-N-CA	5.75	127.91	120.44
1	A	192	VAL	N-CA-CB	5.74	119.20	110.58
1	A	90	LYS	N-CA-CB	5.74	118.56	110.12
1	D	19	ALA	N-CA-CB	-5.74	101.46	110.30
1	C	349	GLN	CG-CD-OE1	-5.74	109.32	120.80
1	C	208	GLU	O-C-N	-5.74	116.04	122.12
1	D	158	ALA	N-CA-C	5.74	117.53	111.28
1	A	320	CYS	CA-C-O	5.73	124.58	119.59
1	C	52	TYR	O-C-N	-5.73	116.05	122.12
1	C	185	LYS	CA-C-O	5.73	126.49	120.42
1	D	278	ASN	CB-CG-ND2	-5.73	107.81	116.40
1	C	140	HIS	CB-CG-CD2	-5.72	123.76	131.20
1	A	310	ASP	CA-CB-CG	5.72	118.32	112.60
1	C	126	ASP	N-CA-C	5.72	117.52	111.28
1	C	233	ARG	CD-NE-CZ	5.72	132.41	124.40
1	A	219	GLU	N-CA-C	5.72	117.59	111.36
1	D	231	SER	N-CA-C	5.72	117.51	111.28
1	D	278	ASN	CA-C-N	5.72	132.46	121.54
1	D	278	ASN	C-N-CA	5.72	132.46	121.54
1	D	25	GLU	N-CA-C	5.72	117.59	111.36
1	C	95	ALA	CA-C-N	5.71	127.93	120.28
1	C	95	ALA	C-N-CA	5.71	127.93	120.28
1	B	229	LEU	O-C-N	-5.71	116.19	122.07
1	B	86	SER	CB-CA-C	-5.70	101.33	110.79
1	D	253	GLU	O-C-N	-5.70	116.35	122.85
1	C	202	HIS	N-CA-C	5.70	117.49	111.28
1	B	146	ARG	N-CA-C	5.69	119.04	111.75
1	B	103	HIS	CA-C-N	5.69	128.22	120.54
1	B	103	HIS	C-N-CA	5.69	128.22	120.54
1	C	124	ARG	N-CA-C	5.69	117.48	111.28
1	B	21	ILE	CA-C-N	5.69	127.90	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	21	ILE	C-N-CA	5.69	127.90	120.28
1	D	38	LEU	N-CA-C	5.68	117.47	111.28
1	A	193	LEU	O-C-N	-5.68	116.22	122.07
1	A	164	ALA	N-CA-C	5.68	117.15	111.07
1	C	203	PHE	CA-C-O	5.68	126.50	119.97
1	A	61	VAL	N-CA-CB	5.67	117.56	110.47
1	C	350	LEU	CA-C-O	-5.67	114.41	120.42
1	B	91	LEU	N-CA-C	5.67	117.14	111.07
1	B	194	ARG	NE-CZ-NH2	-5.67	114.10	119.20
1	D	352	VAL	CB-CA-C	5.67	120.05	112.22
1	C	359	ILE	N-CA-CB	5.67	118.25	110.54
1	B	341	GLN	CA-C-O	5.67	127.86	120.21
1	A	211	SER	CA-C-N	5.66	127.87	120.28
1	A	211	SER	C-N-CA	5.66	127.87	120.28
1	A	326	ARG	NE-CZ-NH2	-5.66	114.11	119.20
1	A	124	ARG	N-CA-C	5.65	117.44	111.28
1	B	246	LYS	N-CA-C	5.64	117.43	111.28
1	C	207	HIS	N-CA-C	-5.64	106.24	113.23
1	A	250	LEU	N-CA-C	5.63	117.50	111.36
1	D	100	ALA	CB-CA-C	-5.63	101.28	110.85
1	B	68	ARG	NE-CZ-NH1	5.63	127.13	121.50
1	D	14	SER	N-CA-C	5.63	116.79	109.64
1	B	68	ARG	O-C-N	-5.61	114.91	122.43
1	D	160	ARG	CA-C-N	5.61	130.18	120.58
1	D	160	ARG	C-N-CA	5.61	130.18	120.58
1	A	190	GLU	CA-C-N	5.61	128.07	120.44
1	A	190	GLU	C-N-CA	5.61	128.07	120.44
1	A	146	ARG	NE-CZ-NH1	5.61	127.11	121.50
1	C	143	GLU	CA-C-O	5.61	126.07	119.28
1	A	242	HIS	CG-CD2-NE2	5.61	112.81	107.20
1	D	160	ARG	NH1-CZ-NH2	-5.61	112.01	119.30
1	A	260	ARG	NH1-CZ-NH2	-5.60	112.02	119.30
1	B	180	ILE	N-CA-C	5.60	116.33	110.62
1	D	20	SER	N-CA-C	5.60	118.31	111.82
1	B	56	SER	N-CA-C	5.59	117.38	111.28
1	B	93	SER	O-C-N	-5.59	115.77	122.15
1	B	218	LYS	O-C-N	-5.59	116.19	122.12
1	B	89	HIS	CG-CD2-NE2	5.59	112.79	107.20
1	B	346	ARG	NE-CZ-NH2	-5.59	114.17	119.20
1	A	10	CYS	CA-C-O	-5.58	113.55	119.97
1	D	143	GLU	N-CA-CB	-5.58	103.42	110.45
1	C	271	HIS	ND1-CE1-NE2	5.58	113.98	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	150	GLN	O-C-N	-5.58	116.33	122.07
1	D	298	GLN	CB-CA-C	-5.57	100.12	109.48
1	C	69	LEU	CA-C-O	5.57	126.29	119.05
1	D	2	THR	N-CA-CB	5.57	118.16	109.97
1	B	298	GLN	CB-CG-CD	-5.57	103.14	112.60
1	B	310	ASP	CA-C-N	5.57	130.62	122.77
1	B	310	ASP	C-N-CA	5.57	130.62	122.77
1	A	68	ARG	NE-CZ-NH1	-5.56	115.94	121.50
1	B	81	GLU	N-CA-CB	-5.56	101.66	110.28
1	B	89	HIS	ND1-CE1-NE2	5.56	113.96	108.40
1	C	303	ASP	CA-CB-CG	-5.56	107.04	112.60
1	D	61	VAL	CB-CA-C	-5.56	104.63	112.14
1	D	325	ARG	N-CA-CB	-5.55	101.68	110.06
1	C	26	ALA	N-CA-CB	-5.55	101.68	110.28
1	C	44	GLY	O-C-N	-5.55	116.87	122.19
1	D	75	MET	O-C-N	-5.54	115.83	122.15
1	B	24	VAL	O-C-N	-5.54	115.54	121.80
1	A	34	ARG	N-CA-C	5.54	117.40	111.36
1	B	85	VAL	N-CA-C	5.54	116.31	110.72
1	C	67	ALA	N-CA-C	5.54	116.99	111.07
1	D	20	SER	N-CA-CB	5.54	118.86	110.28
1	A	146	ARG	NH1-CZ-NH2	-5.53	112.11	119.30
1	A	124	ARG	CG-CD-NE	-5.53	99.84	112.00
1	C	259	LEU	O-C-N	-5.52	116.92	123.22
1	A	253	GLU	N-CA-C	5.52	117.86	110.35
1	B	356	GLN	O-C-N	-5.52	116.27	122.12
1	A	191	PHE	CA-C-O	-5.51	115.02	120.70
1	B	216	TYR	O-C-N	5.51	127.97	122.12
1	C	33	THR	CA-C-O	5.51	126.26	120.42
1	A	202	HIS	CB-CG-CD2	-5.51	124.04	131.20
1	C	178	ASN	CA-C-N	5.51	128.00	120.46
1	C	178	ASN	C-N-CA	5.51	128.00	120.46
1	C	184	ARG	NE-CZ-NH1	5.51	127.01	121.50
1	B	243	VAL	CA-C-O	-5.50	114.53	120.47
1	A	65	ASP	N-CA-CB	-5.50	102.04	110.12
1	A	167	ARG	NH1-CZ-NH2	-5.50	112.15	119.30
1	B	110	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	C	74	PRO	CB-CA-C	-5.49	104.05	111.85
1	A	24	VAL	N-CA-C	5.49	117.91	111.05
1	A	111	THR	CA-C-O	-5.48	114.75	120.55
1	D	45	LEU	N-CA-C	5.48	116.93	111.07
1	B	193	LEU	CA-C-N	5.47	127.56	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	193	LEU	C-N-CA	5.47	127.56	120.44
1	C	318	LYS	O-C-N	-5.47	116.92	123.27
1	B	84	THR	CA-CB-OG1	5.46	117.79	109.60
1	C	80	LEU	O-C-N	-5.46	115.92	122.15
1	C	191	PHE	CA-CB-CG	5.46	119.26	113.80
1	B	80	LEU	CA-C-O	5.46	126.20	120.42
1	D	233	ARG	N-CA-C	5.44	116.89	111.07
1	D	195	LEU	CA-C-O	-5.44	115.11	120.82
1	A	361	SER	CA-C-N	5.43	127.56	120.28
1	A	361	SER	C-N-CA	5.43	127.56	120.28
1	B	153	GLU	CB-CG-CD	5.43	121.83	112.60
1	C	183	LYS	N-CA-CB	5.43	118.11	110.12
1	C	277	SER	N-CA-C	5.43	118.11	109.96
1	B	320	CYS	N-CA-C	5.42	121.79	109.81
1	A	194	ARG	CA-C-N	5.42	128.32	120.79
1	A	194	ARG	C-N-CA	5.42	128.32	120.79
1	C	361	SER	CA-C-N	5.42	127.54	120.28
1	C	361	SER	C-N-CA	5.42	127.54	120.28
1	B	38	LEU	N-CA-C	5.42	117.18	111.28
1	D	178	ASN	OD1-CG-ND2	5.41	128.01	122.60
1	A	185	LYS	CA-C-N	5.41	127.80	120.44
1	A	185	LYS	C-N-CA	5.41	127.80	120.44
1	C	285	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	A	119	GLY	CA-C-N	5.41	127.47	120.44
1	A	119	GLY	C-N-CA	5.41	127.47	120.44
1	A	160	ARG	NH1-CZ-NH2	-5.41	112.27	119.30
1	B	5	LEU	N-CA-C	5.41	118.92	110.32
1	C	109	ILE	N-CA-C	5.41	115.61	110.42
1	A	80	LEU	N-CA-CB	-5.40	101.91	110.28
1	B	26	ALA	O-C-N	-5.40	116.00	122.15
1	C	215	GLN	OE1-CD-NE2	-5.40	117.20	122.60
1	D	72	PRO	N-CA-CB	-5.40	96.50	102.17
1	D	260	ARG	NH1-CZ-NH2	-5.39	112.29	119.30
1	B	239	GLU	CA-C-N	5.39	127.77	120.44
1	B	239	GLU	C-N-CA	5.39	127.77	120.44
1	C	159	LEU	N-CA-C	5.39	117.15	111.28
1	C	325	ARG	NH1-CZ-NH2	-5.39	112.30	119.30
1	C	61	VAL	N-CA-C	5.38	116.76	110.62
1	D	13	ASP	CA-CB-CG	-5.38	107.22	112.60
1	A	202	HIS	N-CA-C	5.38	117.14	111.28
1	C	193	LEU	CA-C-N	5.38	127.93	120.29
1	C	193	LEU	C-N-CA	5.38	127.93	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	139	THR	N-CA-C	5.38	117.14	111.28
1	A	184	ARG	CD-NE-CZ	-5.38	116.88	124.40
1	D	313	ARG	CA-C-O	5.37	125.97	119.31
1	A	137	ALA	N-CA-CB	5.37	117.94	109.94
1	C	13	ASP	O-C-N	-5.37	116.52	122.91
1	D	267	VAL	N-CA-CB	5.37	118.82	111.41
1	A	173	TYR	N-CA-CB	-5.37	102.23	110.12
1	D	233	ARG	NE-CZ-NH1	-5.37	116.13	121.50
1	A	233	ARG	NE-CZ-NH2	-5.37	114.37	119.20
1	B	197	GLU	O-C-N	-5.36	116.30	122.09
1	C	301	TYR	O-C-N	-5.36	116.08	122.20
1	C	271	HIS	CE1-NE2-CD2	-5.36	103.64	109.00
1	D	315	CYS	CA-C-N	5.36	131.00	122.59
1	D	315	CYS	C-N-CA	5.36	131.00	122.59
1	B	15	PRO	CB-CA-C	5.36	119.93	112.11
1	C	200	ALA	N-CA-CB	-5.35	102.25	110.12
1	A	182	ASP	CA-C-N	5.35	127.45	120.28
1	A	182	ASP	C-N-CA	5.35	127.45	120.28
1	B	346	ARG	CA-C-O	-5.35	115.18	120.90
1	A	30	GLU	CA-C-O	5.34	126.43	120.82
1	A	217	ARG	O-C-N	-5.34	116.56	122.07
1	C	278	ASN	O-C-N	-5.34	117.71	123.42
1	D	191	PHE	N-CA-C	5.34	117.53	111.02
1	B	196	VAL	N-CA-C	5.34	116.06	110.62
1	D	56	SER	N-CA-C	5.33	117.09	111.28
1	C	217	ARG	CB-CA-C	-5.33	102.51	110.88
1	D	227	LEU	N-CA-C	5.33	117.09	111.28
1	A	236	ARG	NE-CZ-NH1	5.33	126.83	121.50
1	C	123	ALA	CA-C-O	-5.33	114.77	120.42
1	C	238	MET	N-CA-C	5.33	117.09	111.28
1	D	38	LEU	CA-C-N	5.33	128.20	120.79
1	D	38	LEU	C-N-CA	5.33	128.20	120.79
1	B	103	HIS	N-CA-C	5.33	116.77	111.07
1	D	218	LYS	N-CA-C	5.33	117.09	111.28
1	D	272	LEU	CA-C-O	-5.33	115.58	121.33
1	B	271	HIS	N-CA-CB	5.32	117.80	109.97
1	C	175	LEU	O-C-N	-5.32	116.48	122.12
1	C	177	ILE	N-CA-CB	5.32	116.42	110.51
1	C	187	ASP	CA-C-O	5.32	126.41	120.82
1	D	348	LEU	CA-C-N	5.32	127.84	120.29
1	D	348	LEU	C-N-CA	5.32	127.84	120.29
1	B	16	ARG	CA-C-O	-5.32	115.24	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	97	LEU	O-C-N	-5.31	116.49	122.12
1	D	218	LYS	O-C-N	-5.31	116.49	122.12
1	B	183	LYS	N-CA-C	5.31	117.06	111.28
1	A	111	THR	CA-CB-CG2	5.30	119.52	110.50
1	D	89	HIS	CA-C-N	5.30	127.39	120.28
1	D	89	HIS	C-N-CA	5.30	127.39	120.28
1	D	129	ARG	N-CA-C	5.29	116.73	111.07
1	D	86	SER	CA-C-O	5.29	126.16	120.55
1	B	346	ARG	NE-CZ-NH1	5.29	126.79	121.50
1	C	80	LEU	N-CA-C	5.29	117.12	111.36
1	C	218	LYS	O-C-N	-5.29	116.53	122.03
1	D	65	ASP	CA-C-N	5.29	127.36	120.28
1	D	65	ASP	C-N-CA	5.29	127.36	120.28
1	B	285	ARG	NE-CZ-NH1	5.28	126.78	121.50
1	D	273	PHE	CA-CB-CG	5.28	119.08	113.80
1	C	81	GLU	N-CA-C	5.28	117.03	111.28
1	B	133	SER	CB-CA-C	-5.27	102.04	110.79
1	C	192	VAL	N-CA-C	5.27	116.04	110.72
1	B	51	HIS	N-CA-C	5.27	117.02	111.28
1	C	189	MET	CG-SD-CE	-5.27	89.31	100.90
1	A	127	PHE	CA-C-O	-5.27	114.97	120.55
1	D	156	GLY	O-C-N	-5.27	116.66	122.24
1	D	271	HIS	CA-CB-CG	5.26	119.06	113.80
1	A	69	LEU	N-CA-C	5.26	118.96	112.54
1	A	69	LEU	CA-C-O	5.26	125.85	119.38
1	D	185	LYS	N-CA-CB	5.25	117.63	110.01
1	B	16	ARG	N-CA-C	5.25	116.69	111.07
1	D	86	SER	CB-CA-C	-5.25	102.08	110.79
1	A	284	SER	N-CA-CB	5.25	120.43	111.66
1	D	113	VAL	CA-C-O	-5.25	115.61	121.17
1	C	21	ILE	CA-CB-CG2	-5.24	101.59	110.50
1	C	44	GLY	CA-C-O	5.24	126.15	120.75
1	C	94	HIS	ND1-CE1-NE2	5.24	113.64	108.40
1	A	223	GLN	N-CA-C	5.24	117.07	111.36
1	D	299	LYS	N-CA-C	-5.24	99.64	110.80
1	D	308	VAL	N-CA-CB	-5.24	103.07	111.82
1	D	317	VAL	O-C-N	5.24	127.69	122.97
1	A	3	VAL	CA-CB-CG1	5.24	119.31	110.40
1	B	280	PHE	CA-CB-CG	-5.24	108.56	113.80
1	B	161	THR	CA-C-N	5.24	127.55	120.38
1	B	161	THR	C-N-CA	5.24	127.55	120.38
1	D	74	PRO	O-C-N	-5.23	115.57	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	269	GLU	CA-C-O	5.23	127.23	121.11
1	D	118	ARG	N-CA-C	5.23	117.06	111.36
1	D	207	HIS	CE1-NE2-CD2	-5.23	103.77	109.00
1	B	59	PHE	O-C-N	-5.22	116.69	122.07
1	C	3	VAL	CA-C-O	5.22	126.06	119.48
1	D	2	THR	CA-C-O	5.22	127.01	121.16
1	B	104	THR	N-CA-CB	5.22	117.72	109.94
1	D	263	PRO	CA-C-N	5.22	130.21	120.87
1	D	263	PRO	C-N-CA	5.22	130.21	120.87
1	B	99	ASP	O-C-N	-5.21	116.60	122.12
1	B	92	ASP	N-CA-C	5.21	116.96	111.28
1	A	104	THR	O-C-N	-5.21	116.60	122.12
1	B	101	THR	OG1-CB-CG2	-5.20	98.89	109.30
1	B	355	VAL	O-C-N	-5.20	116.47	121.83
1	C	107	GLN	CA-C-N	5.20	131.46	121.54
1	C	107	GLN	C-N-CA	5.20	131.46	121.54
1	B	21	ILE	CA-C-O	-5.19	114.86	120.47
1	A	150	GLN	CA-C-N	5.19	127.24	120.28
1	A	150	GLN	C-N-CA	5.19	127.24	120.28
1	B	169	ARG	CA-C-N	5.19	127.19	120.44
1	B	169	ARG	C-N-CA	5.19	127.19	120.44
1	C	27	GLU	CA-C-N	5.19	127.10	120.56
1	C	27	GLU	C-N-CA	5.19	127.10	120.56
1	C	88	ASN	CA-CB-CG	-5.19	107.41	112.60
1	A	199	GLN	N-CA-C	5.19	116.62	111.07
1	A	68	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	B	293	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	A	194	ARG	CD-NE-CZ	5.19	131.66	124.40
1	B	191	PHE	CB-CG-CD2	-5.18	111.89	120.70
1	C	200	ALA	N-CA-C	5.18	116.93	111.28
1	B	8	GLU	CB-CG-CD	-5.18	103.80	112.60
1	A	286	ARG	O-C-N	-5.18	116.91	123.17
1	B	167	ARG	N-CA-C	5.18	117.00	111.36
1	C	347	LEU	N-CA-C	5.17	116.60	111.07
1	C	20	SER	CA-C-N	5.17	127.54	120.46
1	C	20	SER	C-N-CA	5.17	127.54	120.46
1	C	99	ASP	CA-C-N	5.17	127.20	120.28
1	C	99	ASP	C-N-CA	5.17	127.20	120.28
1	A	49	GLY	CA-C-O	5.16	126.37	121.05
1	A	299	LYS	CA-C-N	5.16	132.39	121.91
1	A	299	LYS	C-N-CA	5.16	132.39	121.91
1	D	359	ILE	CA-CB-CG2	5.16	119.28	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ARG	CA-C-N	5.16	126.77	120.22
1	A	129	ARG	C-N-CA	5.16	126.77	120.22
1	C	37	LYS	CA-C-O	-5.16	114.04	119.97
1	A	208	GLU	N-CA-C	-5.15	105.75	111.36
1	A	89	HIS	ND1-CE1-NE2	5.15	113.55	108.40
1	A	162	ALA	O-C-N	-5.15	116.77	122.07
1	B	260	ARG	NH1-CZ-NH2	-5.15	112.61	119.30
1	A	92	ASP	CB-CA-C	-5.15	102.10	110.85
1	A	25	GLU	N-CA-C	5.14	117.62	111.71
1	D	159	LEU	CB-CA-C	-5.14	102.25	110.79
1	B	176	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	B	194	ARG	CB-CG-CD	5.14	123.11	111.30
1	B	333	SER	CA-C-N	5.13	129.35	121.19
1	B	333	SER	C-N-CA	5.13	129.35	121.19
1	B	353	SER	CA-C-O	-5.13	114.07	119.97
1	B	3	VAL	CA-CB-CG1	5.13	119.12	110.40
1	B	4	LYS	CA-C-N	5.13	130.85	122.07
1	B	4	LYS	C-N-CA	5.13	130.85	122.07
1	B	107	GLN	N-CA-CB	5.13	117.40	109.91
1	B	202	HIS	CA-C-N	5.12	127.14	120.28
1	B	202	HIS	C-N-CA	5.12	127.14	120.28
1	C	303	ASP	CA-C-N	5.12	125.84	120.11
1	C	303	ASP	C-N-CA	5.12	125.84	120.11
1	B	111	THR	CA-C-O	-5.12	115.13	120.55
1	B	83	PHE	CA-C-O	5.11	125.84	120.42
1	A	302	LYS	N-CA-C	5.11	119.21	112.92
1	D	256	GLU	O-C-N	-5.11	114.32	121.12
1	B	358	SER	N-CA-CB	5.11	117.63	110.12
1	B	132	GLU	CA-C-N	5.10	127.12	120.28
1	B	132	GLU	C-N-CA	5.10	127.12	120.28
1	C	138	LEU	O-C-N	-5.10	116.34	122.15
1	A	298	GLN	O-C-N	-5.10	117.61	123.42
1	C	146	ARG	N-CA-CB	5.09	117.61	110.12
1	B	174	ALA	CA-C-N	5.09	127.10	120.28
1	B	174	ALA	C-N-CA	5.09	127.10	120.28
1	A	24	VAL	CA-C-O	5.09	126.02	120.57
1	A	34	ARG	CG-CD-NE	-5.09	100.81	112.00
1	A	88	ASN	CA-C-N	5.09	127.51	120.29
1	A	88	ASN	C-N-CA	5.09	127.51	120.29
1	B	223	GLN	N-CA-C	5.08	116.82	111.28
1	C	241	ARG	CA-C-N	5.08	127.05	120.44
1	C	241	ARG	C-N-CA	5.08	127.05	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	HIS	CA-CB-CG	-5.08	108.72	113.80
1	B	315	CYS	CA-C-N	5.08	130.54	122.62
1	B	315	CYS	C-N-CA	5.08	130.54	122.62
1	B	124	ARG	N-CA-CB	-5.08	102.65	110.01
1	B	154	GLU	CA-C-N	5.08	127.04	120.44
1	B	154	GLU	C-N-CA	5.08	127.04	120.44
1	A	34	ARG	CA-C-N	5.08	127.08	120.28
1	A	34	ARG	C-N-CA	5.08	127.08	120.28
1	B	313	ARG	CA-C-O	5.08	125.29	119.35
1	C	167	ARG	N-CA-C	5.08	116.81	111.28
1	C	288	PHE	CA-C-O	5.07	126.89	121.16
1	C	255	PRO	N-CA-C	5.07	119.04	111.14
1	C	2	THR	CA-CB-CG2	5.06	119.11	110.50
1	C	118	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	D	301	TYR	O-C-N	5.06	129.15	122.93
1	A	300	LYS	O-C-N	5.06	128.47	123.46
1	D	155	ALA	CA-C-N	5.06	126.46	120.14
1	D	155	ALA	C-N-CA	5.06	126.46	120.14
1	C	110	GLN	N-CA-CB	5.05	117.64	110.16
1	C	230	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	A	8	GLU	O-C-N	-5.05	116.77	122.12
1	B	207	HIS	CB-CG-ND1	5.04	130.27	122.70
1	B	285	ARG	N-CA-C	5.04	116.98	108.96
1	D	107	GLN	CG-CD-NE2	5.04	123.97	116.40
1	A	106	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	B	84	THR	CA-C-O	5.04	125.50	119.60
1	C	42	GLY	N-CA-C	5.04	119.22	112.77
1	C	121	ARG	NE-CZ-NH1	5.04	126.54	121.50
1	D	290	ILE	N-CA-CB	-5.04	105.31	111.21
1	C	149	ALA	N-CA-C	5.03	119.67	111.37
1	A	201	THR	N-CA-CB	5.03	117.61	110.16
1	A	350	LEU	CA-C-O	-5.03	115.52	120.70
1	D	358	SER	CA-C-N	5.03	128.42	120.47
1	D	358	SER	C-N-CA	5.03	128.42	120.47
1	A	177	ILE	O-C-N	-5.03	116.91	121.94
1	A	300	LYS	CA-C-O	-5.03	115.57	121.10
1	D	57	ARG	CA-C-O	5.03	126.10	120.82
1	B	353	SER	N-CA-C	5.02	117.64	111.82
1	C	216	TYR	CA-C-N	5.02	126.97	120.44
1	C	216	TYR	C-N-CA	5.02	126.97	120.44
1	C	278	ASN	CA-C-N	5.02	127.26	120.38
1	C	278	ASN	C-N-CA	5.02	127.26	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	278	ASN	N-CA-C	5.02	118.39	109.96
1	B	345	GLU	CB-CG-CD	5.02	121.13	112.60
1	C	327	PHE	CB-CG-CD2	5.02	129.23	120.70
1	C	245	LEU	N-CA-C	5.01	116.75	111.28
1	B	233	ARG	NE-CZ-NH1	-5.01	116.49	121.50
1	C	36	GLU	O-C-N	-5.01	116.44	122.15
1	D	76	MET	CA-C-O	5.01	125.86	120.70

There are no chirality outliers.

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	GLU	Peptide
1	A	125	ARG	Sidechain
1	A	127	PHE	Sidechain
1	A	129	ARG	Sidechain
1	A	169	ARG	Sidechain
1	A	17	PHE	Sidechain
1	A	236	ARG	Sidechain
1	A	260	ARG	Sidechain
1	A	271	HIS	Sidechain
1	A	297	TYR	Sidechain
1	A	313	ARG	Sidechain
1	A	34	ARG	Sidechain
1	B	120	PHE	Sidechain
1	B	121	ARG	Sidechain
1	B	124	ARG	Sidechain
1	B	160	ARG	Sidechain
1	B	169	ARG	Sidechain
1	B	216	TYR	Sidechain
1	B	241	ARG	Sidechain
1	B	273	PHE	Sidechain
1	B	346	ARG	Sidechain
1	B	51	HIS	Sidechain
1	C	118	ARG	Sidechain
1	C	125	ARG	Sidechain
1	C	160	ARG	Sidechain
1	C	169	ARG	Sidechain
1	C	184	ARG	Sidechain
1	C	186	PHE	Sidechain
1	C	216	TYR	Sidechain
1	C	280	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	C	285	ARG	Sidechain
1	C	34	ARG	Sidechain
1	C	57	ARG	Sidechain
1	C	68	ARG	Sidechain
1	D	129	ARG	Sidechain
1	D	148	ARG	Sidechain
1	D	167	ARG	Sidechain
1	D	173	TYR	Sidechain
1	D	184	ARG	Sidechain
1	D	233	ARG	Sidechain
1	D	271	HIS	Sidechain
1	D	273	PHE	Sidechain
1	D	275	ARG	Sidechain
1	D	285	ARG	Sidechain
1	D	288	PHE	Sidechain
1	D	57	ARG	Sidechain
1	D	6	ASP	Peptide
1	D	68	ARG	Sidechain
1	D	7	PHE	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2915	2934	2936	14	0
1	B	2893	2915	2917	12	0
1	C	2915	2934	2936	15	0
1	D	2893	2915	2917	16	0
All	All	11616	11698	11706	50	0

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

All (50) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:HIS:CD2	1:D:97:LEU:HD23	2.31	0.65
1:A:76:MET:HB2	1:B:189:MET:HE2	1.81	0.62
1:C:202:HIS:CE1	1:D:203:PHE:CE2	2.91	0.57
1:C:217:ARG:HH11	1:D:197:GLU:CD	2.17	0.53
1:C:202:HIS:CE1	1:D:203:PHE:CZ	2.97	0.52
1:A:271:HIS:CE1	1:A:287:TRP:CE3	3.00	0.49
1:C:296:VAL:HG12	1:C:307:VAL:HA	1.95	0.49
1:B:253:GLU:H	1:B:253:GLU:CD	2.21	0.49
1:C:38:LEU:CD2	1:D:66:LEU:HD11	2.43	0.48
1:B:109:ILE:HD11	1:B:191:PHE:CD2	2.48	0.48
1:C:45:LEU:C	1:C:45:LEU:HD23	2.39	0.47
1:C:120:PHE:CE2	1:C:177:ILE:HD11	2.48	0.47
1:D:288:PHE:HB3	1:D:295:LEU:HD11	1.97	0.47
1:D:272:LEU:HD21	1:D:351:TRP:CD1	2.49	0.47
1:A:140:HIS:CD2	1:A:155:ALA:HB2	2.50	0.47
1:D:25:GLU:CD	1:D:124:ARG:HE	2.23	0.47
1:C:307:VAL:HG11	1:C:310:ASP:HB3	1.97	0.47
1:A:39:LEU:HA	1:A:105:LEU:HD11	1.99	0.45
1:C:272:LEU:HB2	1:C:288:PHE:CE1	2.52	0.45
1:D:32:GLU:CD	1:D:121:ARG:HH22	2.24	0.45
1:D:289:THR:O	1:D:295:LEU:HD12	2.18	0.44
1:C:89:HIS:HE1	1:C:205:GLN:O	2.00	0.44
1:A:287:TRP:CD1	1:A:287:TRP:C	2.96	0.43
1:B:245:LEU:HA	1:B:249:GLU:HG2	2.00	0.43
1:D:169:ARG:CZ	1:D:169:ARG:HA	2.48	0.43
1:B:241:ARG:HH12	1:B:249:GLU:CD	2.27	0.43
1:C:175:LEU:O	1:C:179:VAL:HG23	2.19	0.43
1:B:76:MET:HA	1:B:76:MET:HE2	2.00	0.43
1:D:256:GLU:CD	1:D:346:ARG:HH21	2.26	0.43
1:A:50:ARG:HG3	1:A:98:LEU:HD13	2.00	0.42
1:A:90:LYS:HE2	1:B:200:ALA:HA	2.00	0.42
1:C:122:GLU:CD	1:C:125:ARG:HH22	2.27	0.42
1:C:340:LEU:HD23	1:C:340:LEU:HA	1.90	0.42
1:D:247:GLN:HG3	1:D:248:LYS:HG2	2.02	0.42
1:D:21:ILE:HA	1:D:24:VAL:HG12	2.02	0.42
1:A:183:LYS:HE3	1:A:187:ASP:OD1	2.20	0.41
1:B:42:GLY:O	1:B:46:LEU:HG	2.20	0.41
1:A:316:THR:HA	1:A:359:ILE:HD13	2.02	0.41
1:A:10:CYS:HB2	1:A:170:ALA:HB1	2.01	0.41
1:C:67:ALA:HB1	1:C:76:MET:HE3	2.01	0.41
1:A:45:LEU:HD23	1:A:45:LEU:C	2.46	0.41
1:B:25:GLU:CD	1:B:124:ARG:HH21	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:TYR:C	1:C:297:TYR:CD1	2.99	0.41
1:A:146:ARG:HG3	1:B:326:ARG:HA	2.02	0.41
1:D:274:LYS:O	1:D:283:TRP:HA	2.21	0.41
1:A:32:GLU:CD	1:A:121:ARG:HH12	2.30	0.40
1:B:21:ILE:HG22	1:B:177:ILE:CD1	2.50	0.40
1:B:82:LYS:HA	1:B:85:VAL:HG12	2.03	0.40
1:D:117:LEU:HA	1:D:180:ILE:HD12	2.02	0.40
1:A:260:ARG:O	1:A:261:GLU:HB2	2.21	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	362/382 (95%)	352 (97%)	8 (2%)	2 (1%)	21	59
1	B	359/382 (94%)	348 (97%)	9 (2%)	2 (1%)	21	59
1	C	362/382 (95%)	345 (95%)	15 (4%)	2 (1%)	21	59
1	D	359/382 (94%)	340 (95%)	18 (5%)	1 (0%)	36	72
All	All	1442/1528 (94%)	1385 (96%)	50 (4%)	7 (0%)	26	63

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	LEU
1	C	323	SER
1	B	257	PRO
1	C	266	LEU
1	D	257	PRO
1	A	261	GLU
1	B	255	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	312/325 (96%)	296 (95%)	16 (5%)	21	42
1	B	310/325 (95%)	292 (94%)	18 (6%)	18	40
1	C	312/325 (96%)	300 (96%)	12 (4%)	29	50
1	D	310/325 (95%)	295 (95%)	15 (5%)	23	44
All	All	1244/1300 (96%)	1183 (95%)	61 (5%)	24	43

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	THR
1	A	10	CYS
1	A	45	LEU
1	A	61	VAL
1	A	90	LYS
1	A	150	GLN
1	A	269	GLU
1	A	274	LYS
1	A	287	TRP
1	A	291	GLN
1	A	297	TYR
1	A	306	THR
1	A	326	ARG
1	A	329	PHE
1	A	348	LEU
1	B	1	MET
1	B	33	THR
1	B	36	GLU
1	B	72	PRO
1	B	90	LYS
1	B	102	GLN
1	B	120	PHE
1	B	125	ARG

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Mol	Chain	Res	Type
1	B	145	PRO
1	B	208	GLU
1	B	213	LEU
1	B	215	GLN
1	B	233	ARG
1	B	269	GLU
1	B	316	THR
1	B	329	PHE
1	B	331	VAL
1	B	343	ASP
1	C	60	VAL
1	C	134	LEU
1	C	173	TYR
1	C	184	ARG
1	C	188	ILE
1	C	226	GLN
1	C	242	HIS
1	C	250	LEU
1	C	266	LEU
1	C	269	GLU
1	C	282	THR
1	C	298	GLN
1	D	72	PRO
1	D	74	PRO
1	D	84	THR
1	D	90	LYS
1	D	94	HIS
1	D	113	VAL
1	D	160	ARG
1	D	171	LEU
1	D	195	LEU
1	D	213	LEU
1	D	245	LEU
1	D	257	PRO
1	D	269	GLU
1	D	299	LYS
1	D	303	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	GLN

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Mol	Chain	Res	Type
1	A	202	HIS
1	B	51	HIS
1	B	89	HIS
1	B	106	GLN
1	B	204	GLN
1	B	207	HIS
1	C	150	GLN
1	C	202	HIS
1	C	225	HIS
1	C	230	ASN
1	C	298	GLN
1	D	51	HIS
1	D	176	GLN
1	D	207	HIS
1	D	225	HIS
1	D	349	GLN

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 ⓘ

There are no chain breaks in this entry.

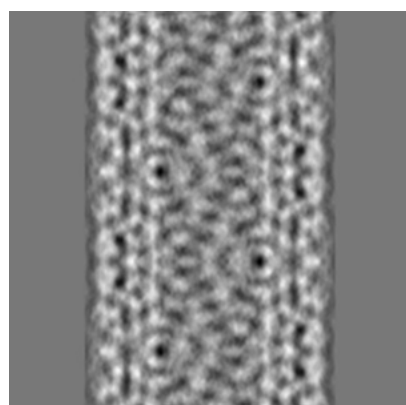
6 Map visualisation [i](#)

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.

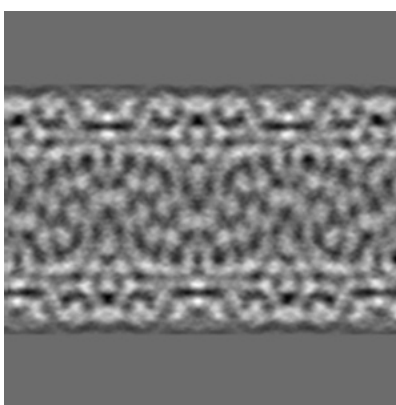
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

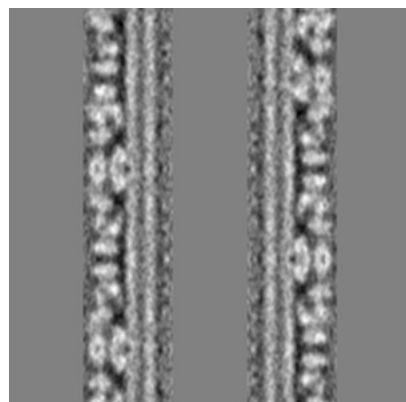


Z

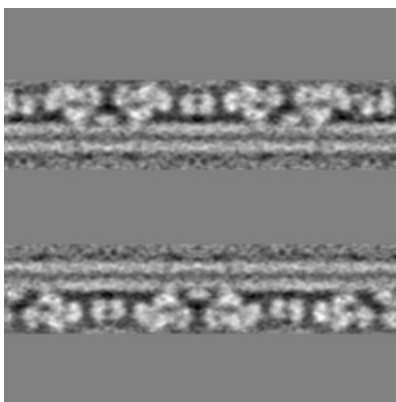
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

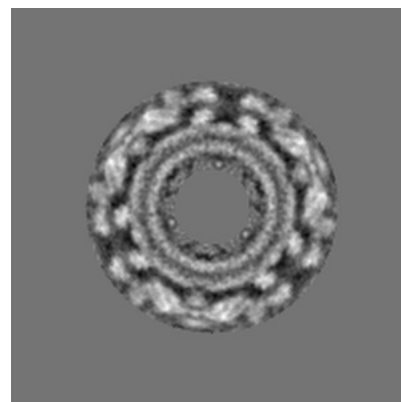
6.2.1 Primary map



X Index: 100



Y Index: 100

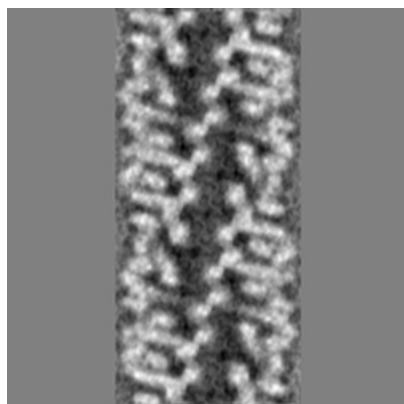


Z Index: 100

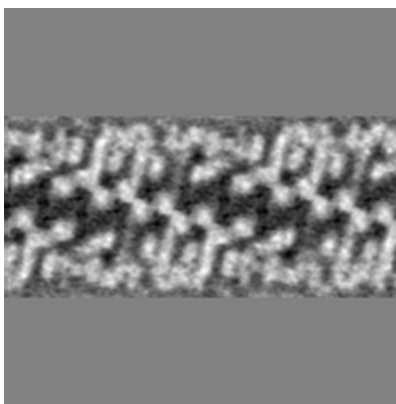
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

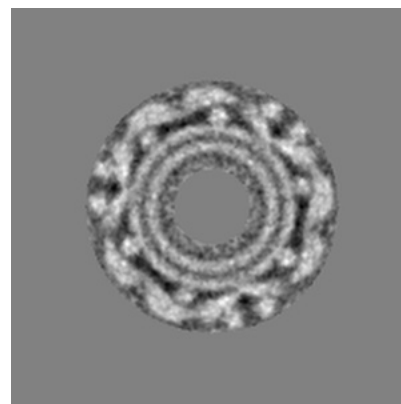
6.3.1 Primary map



X Index: 143



Y Index: 144

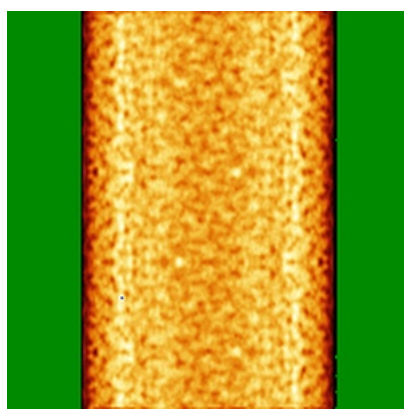


Z Index: 168

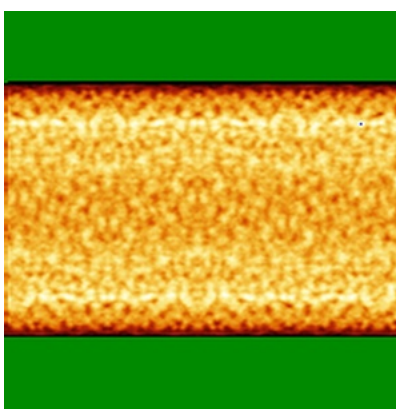
The images above show the largest variance slices of the map in three orthogonal directions.

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

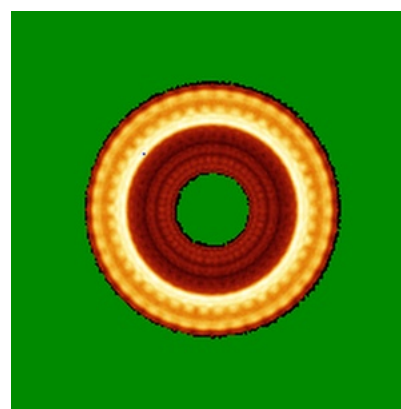
6.4.1 Primary map



X



Y

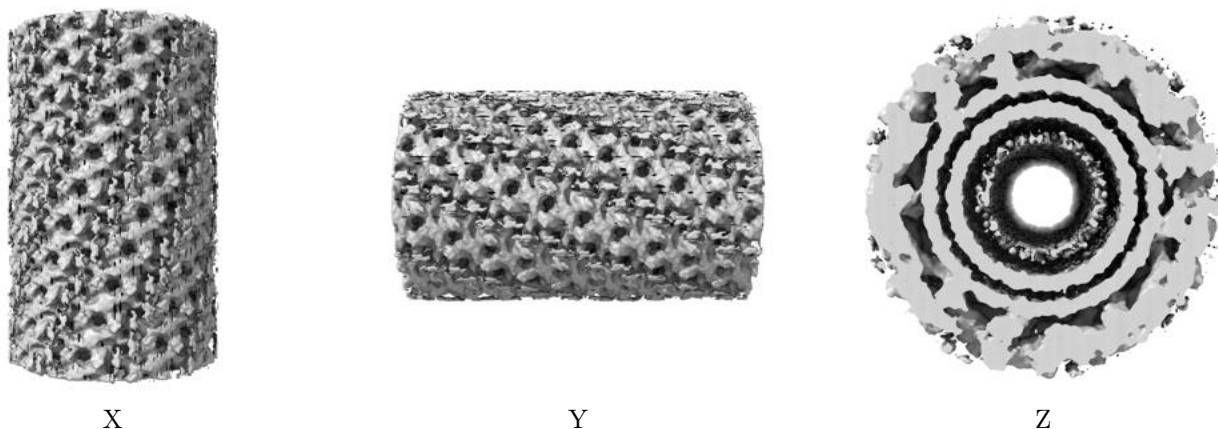


Z

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.

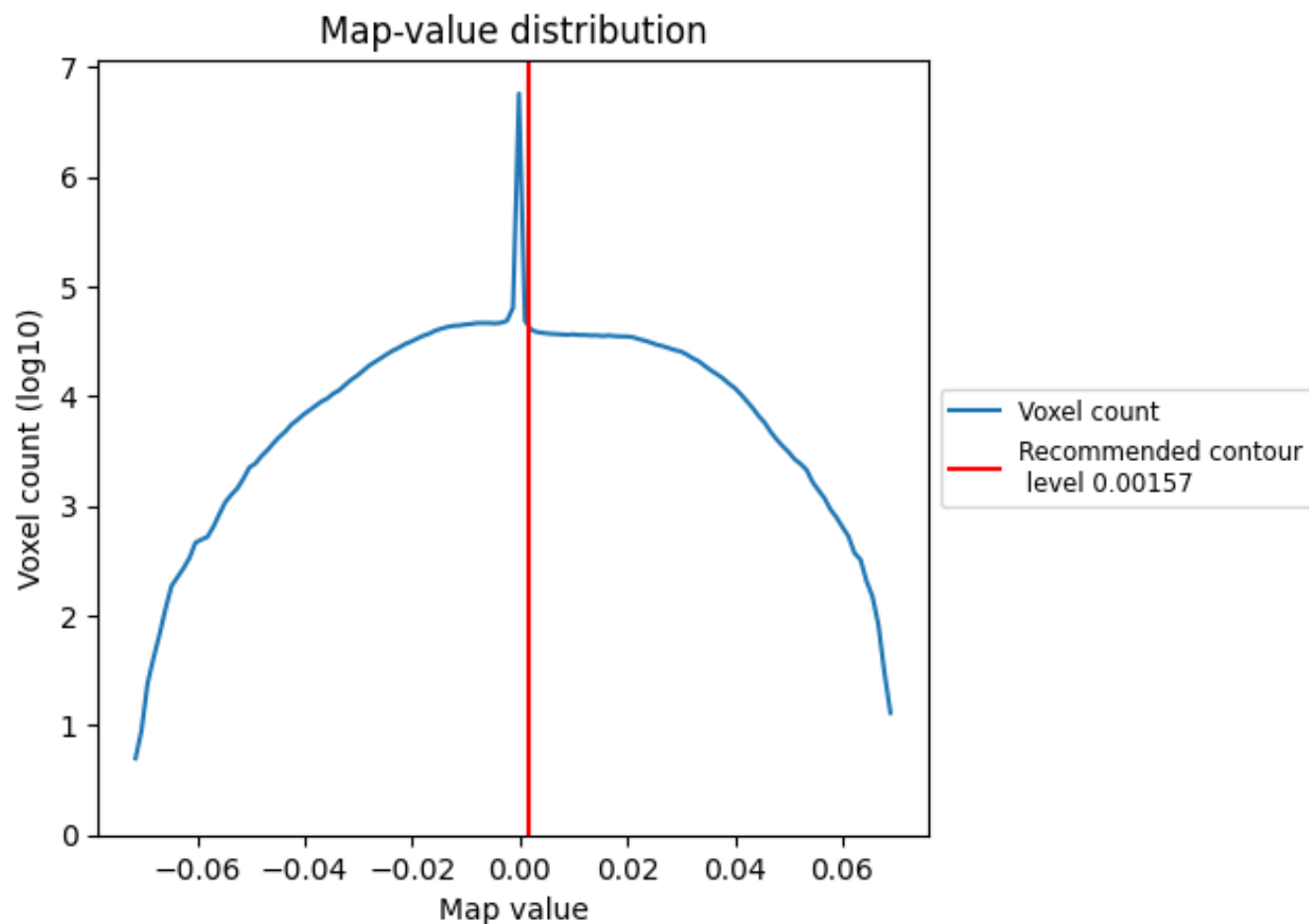
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

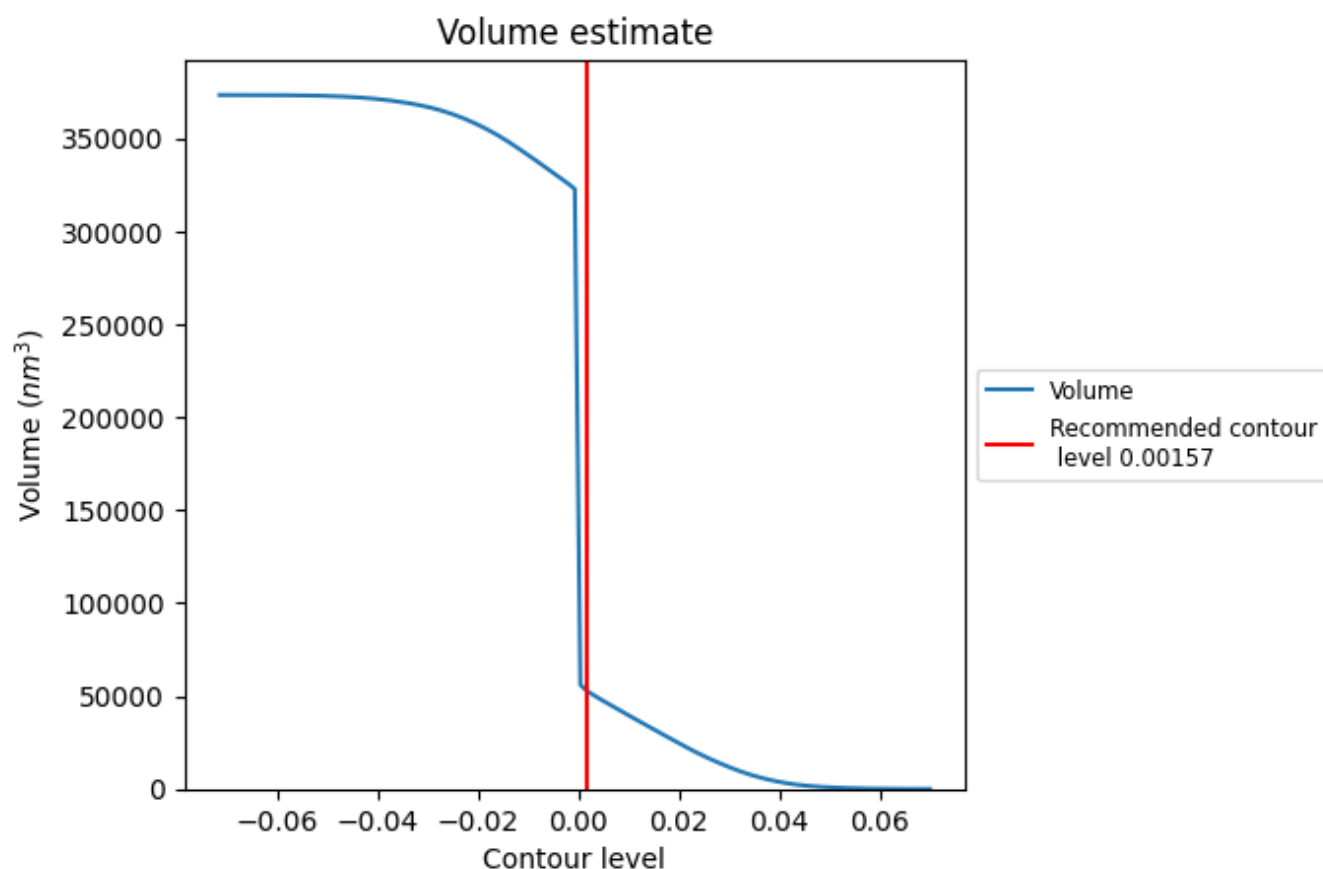
This section contains the results of statistical analysis of the map.

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.

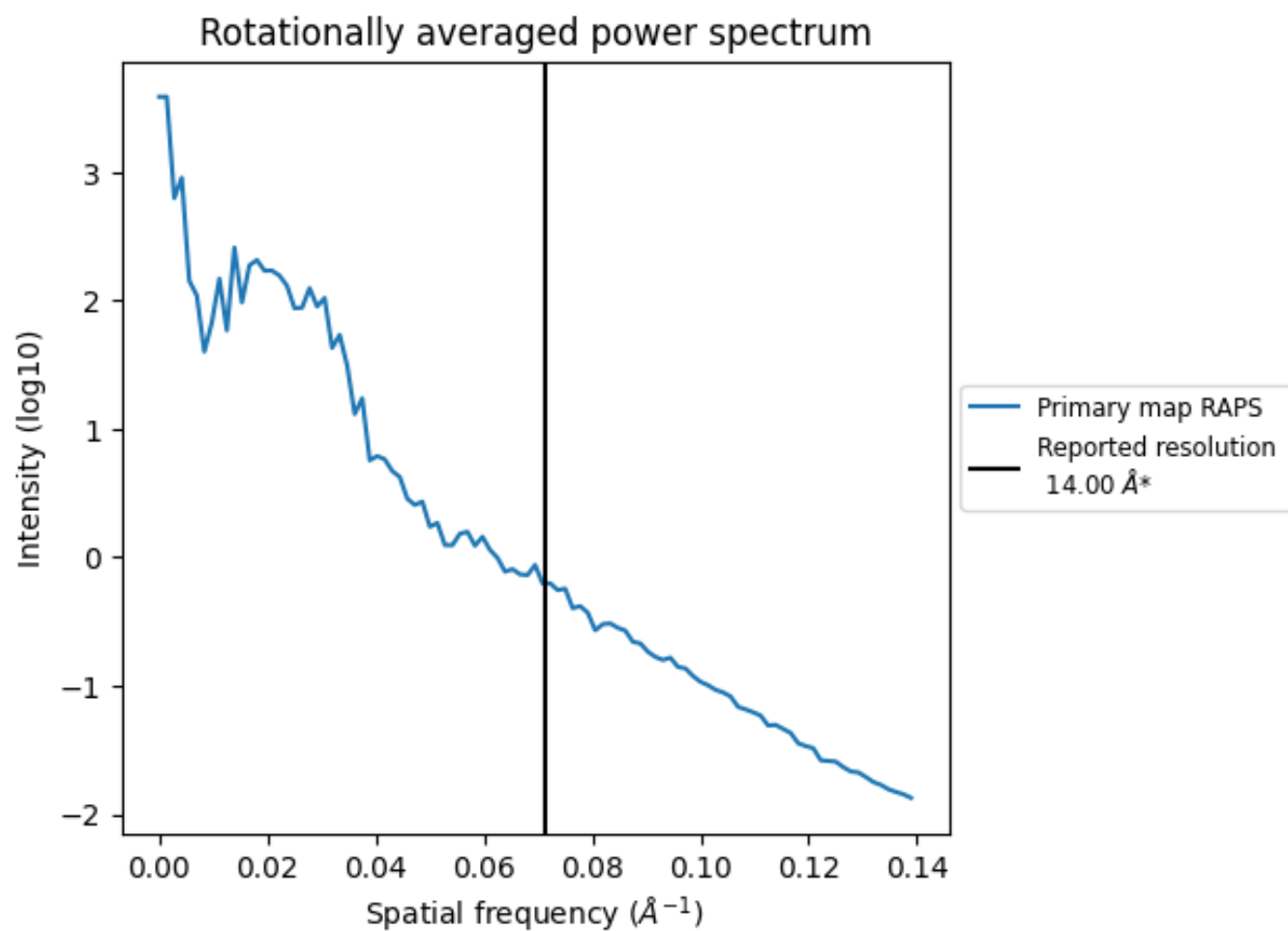
7.2 Volume estimate [i](#)



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 0.071 Å⁻¹

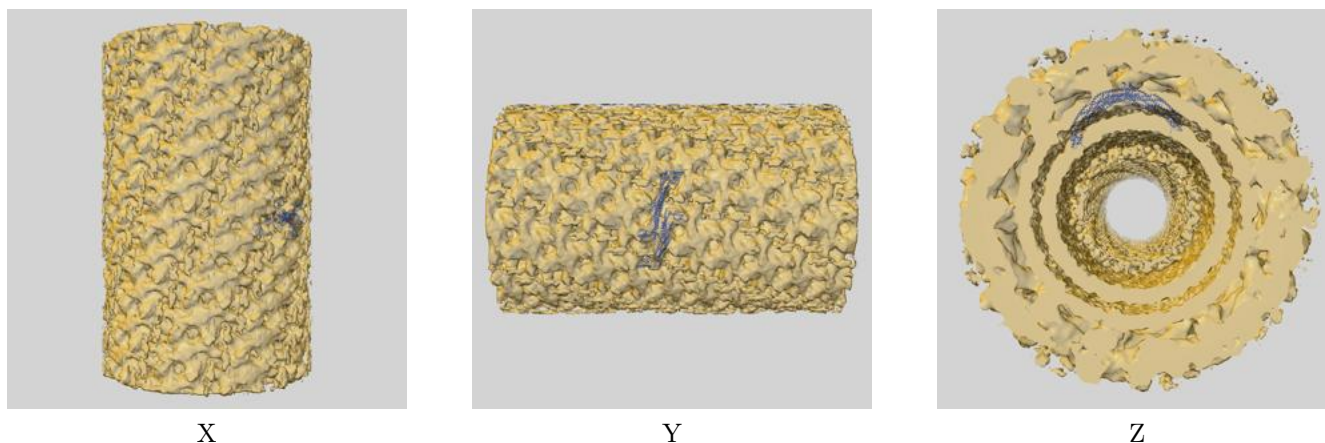
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

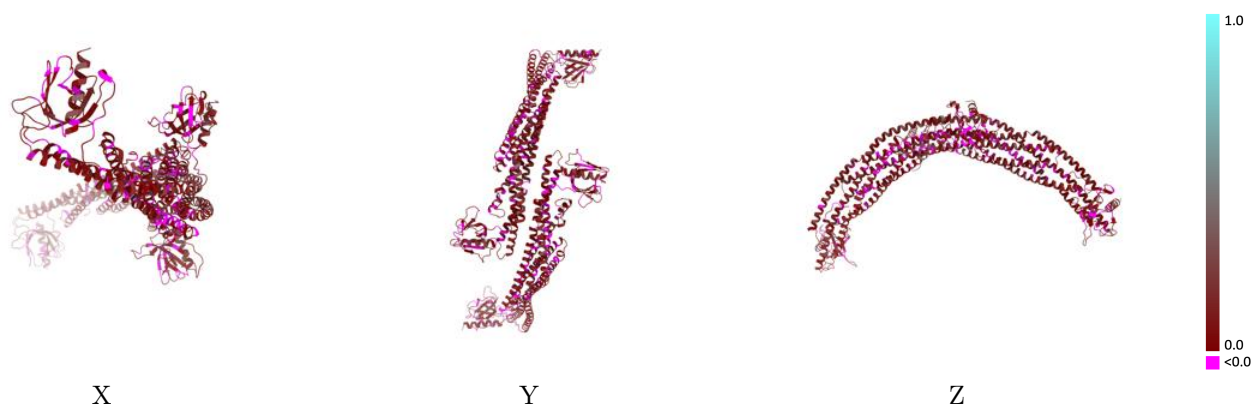
This section contains information regarding the fit between EMDB map EMD-2546 and PDB model 5H3D. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



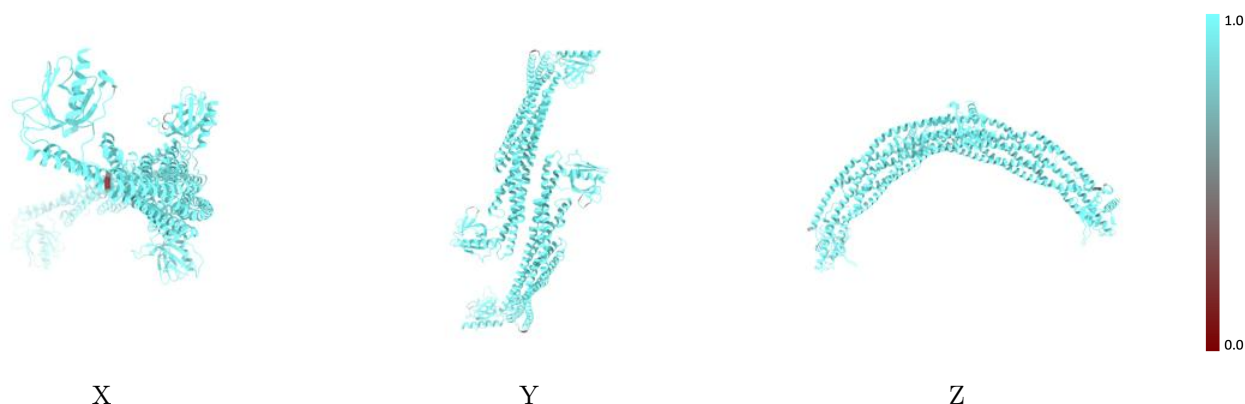
The images above show the 3D surface view of the map at the recommended contour level 0.00157 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



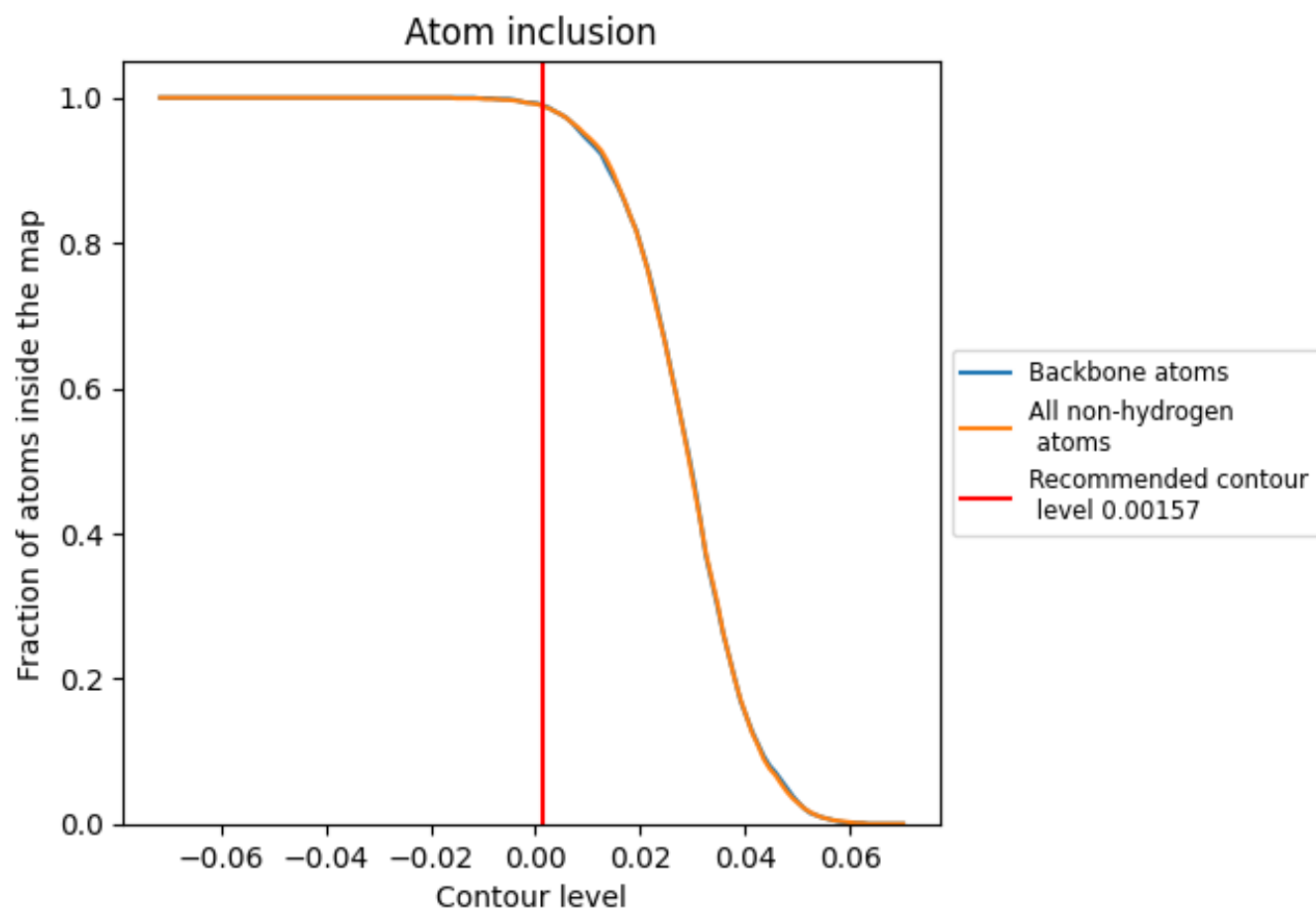
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.00157) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9880	0.0870
A	0.9870	0.0850
B	0.9850	0.0890
C	0.9870	0.0950
D	0.9920	0.0810

