



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:23 AM UTC

PDB ID : 7AOY / pdb_00007aoy
EMDB ID : EMD-11847
Title : Helical arrangement of Bunyamwera virus nucleocapsid protein within a native ribonucleoprotein
Authors : Hopkins, F.R.; Fontana, J.; Barr, J.N.
Deposited on : 2020-10-15
Resolution : 13.00 Å(reported)
Based on initial model : 3ZLA

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:

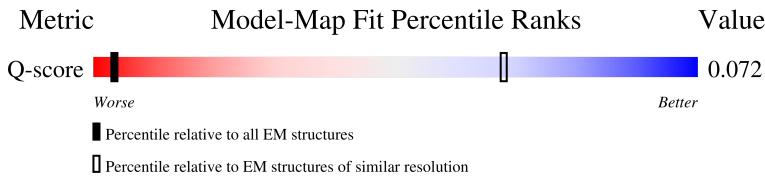
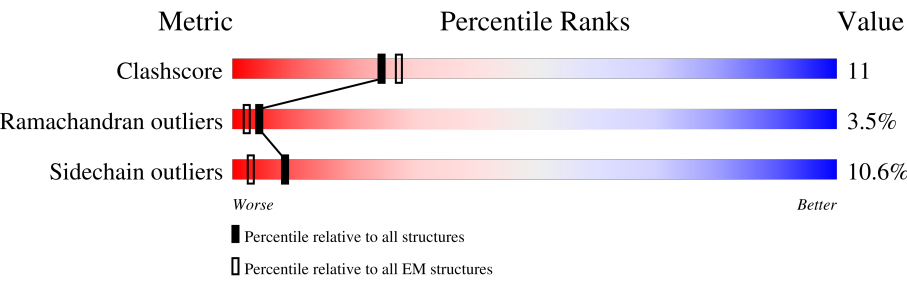
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 13.00 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	65 (12.50 - 13.50)

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	233	
1	B	233	
1	C	233	
1	D	233	

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Mol	Chain	Length	Quality of chain
1	E	233	33%45%18%..
1	F	233	33%47%17%..
1	G	233	33%45%18%..
1	H	233	34%45%18%..
1	I	233	6%34%45%17%..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16587 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.

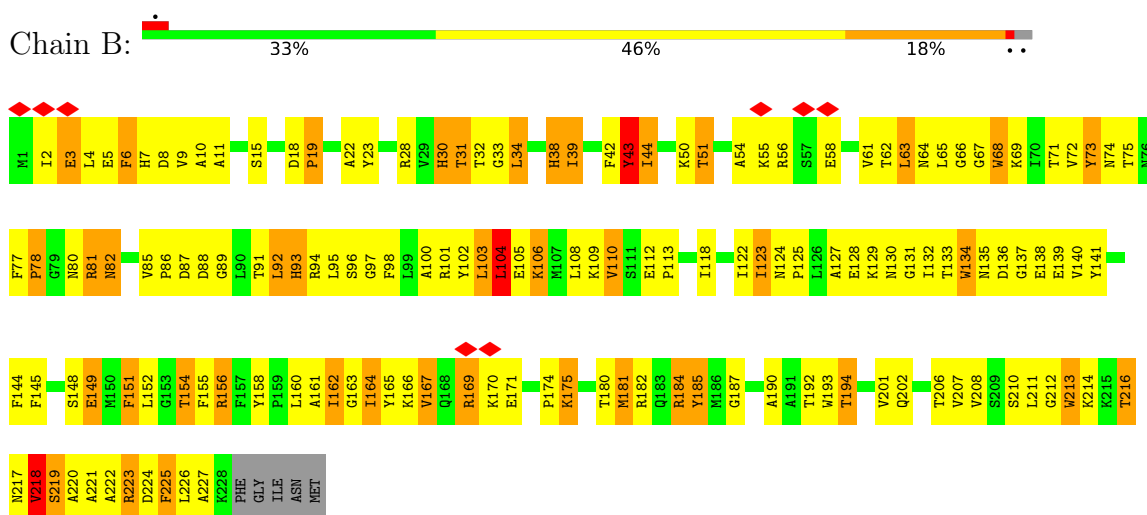
- Molecule 1 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	228	Total	C	N	O	S	0	0
			1843	1191	311	335	6		
1	A	228	Total	C	N	O	S	0	0
			1843	1191	311	335	6		
1	C	228	Total	C	N	O	S	0	0
			1843	1191	311	335	6		
1	D	228	Total	C	N	O	S	0	0
			1843	1191	311	335	6		
1	E	228	Total	C	N	O	S	0	0
			1843	1191	311	335	6		
1	F	228	Total	C	N	O	S	0	0
			1843	1191	311	335	6		
1	G	228	Total	C	N	O	S	0	0
			1843	1191	311	335	6		
1	H	228	Total	C	N	O	S	0	0
			1843	1191	311	335	6		
1	I	228	Total	C	N	O	S	0	0
			1843	1191	311	335	6		

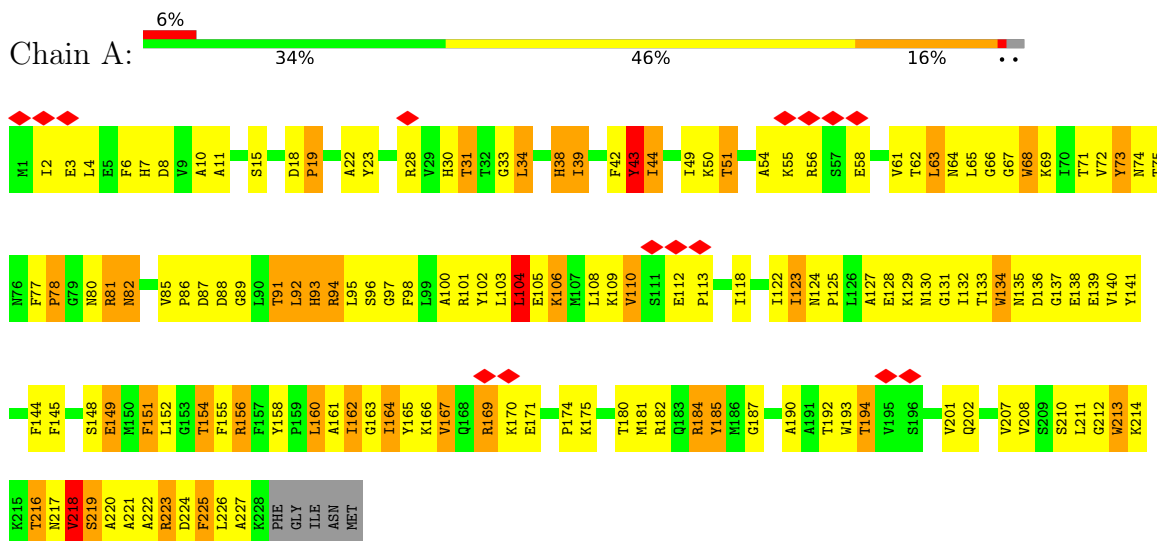
3 Residue-property plots

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: Nucleoprotein

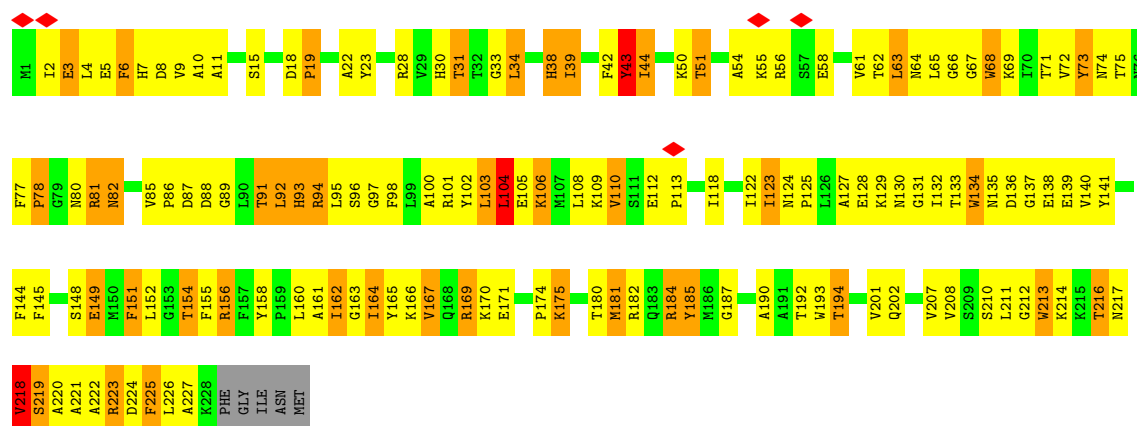


• Molecule 1: Nucleoprotein

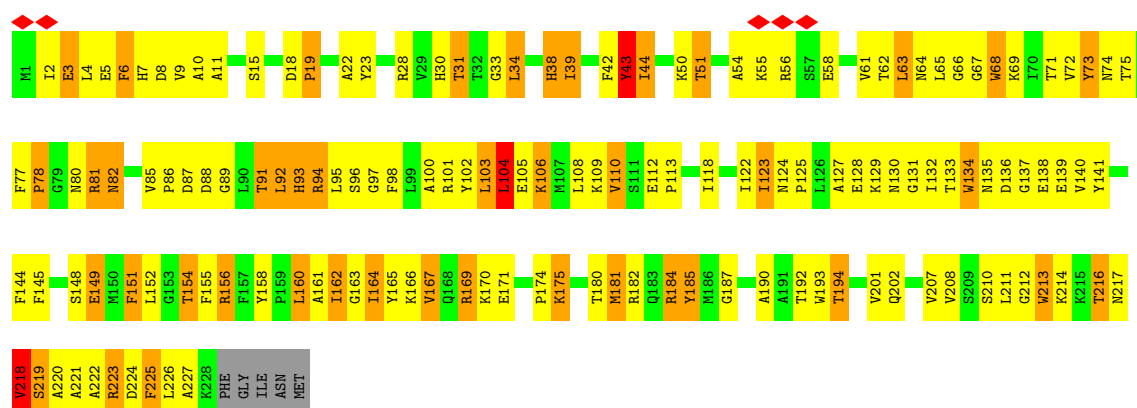


• Molecule 1: Nucleoprotein

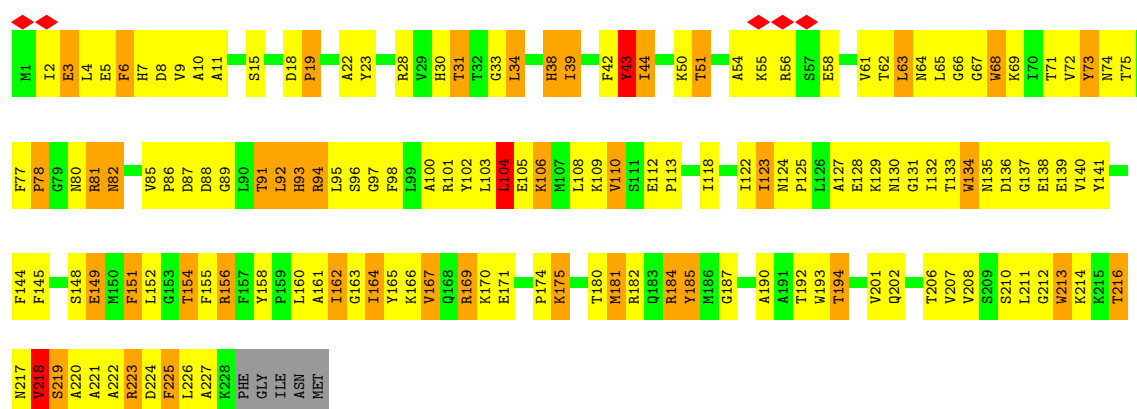




• Molecule 1: Nucleoprotein

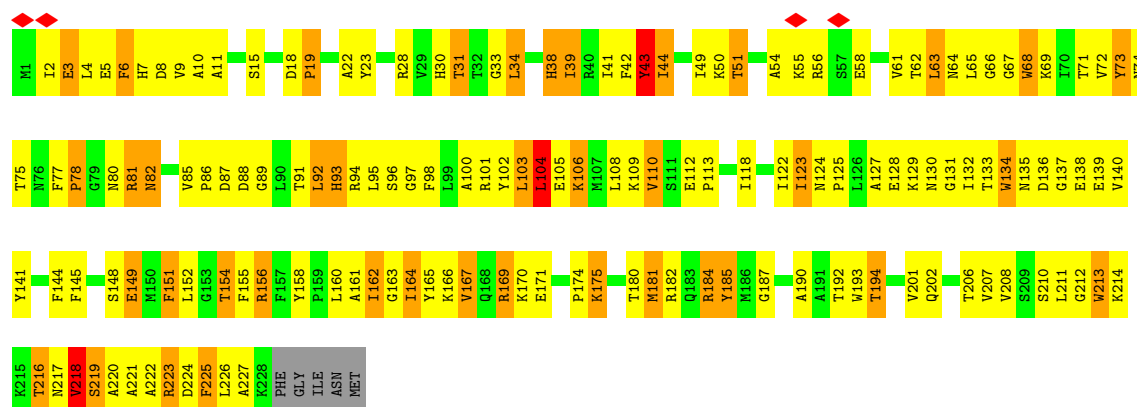


• Molecule 1: Nucleoprotein

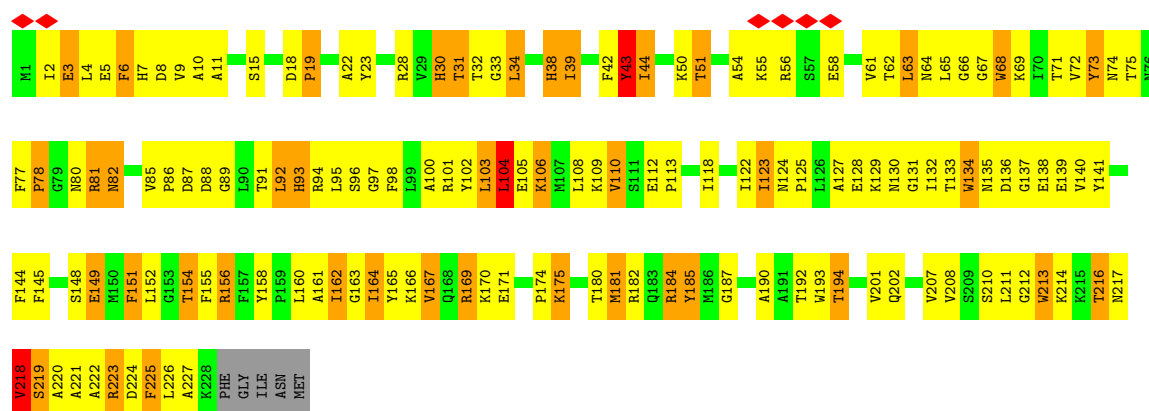


• Molecule 1: Nucleoprotein

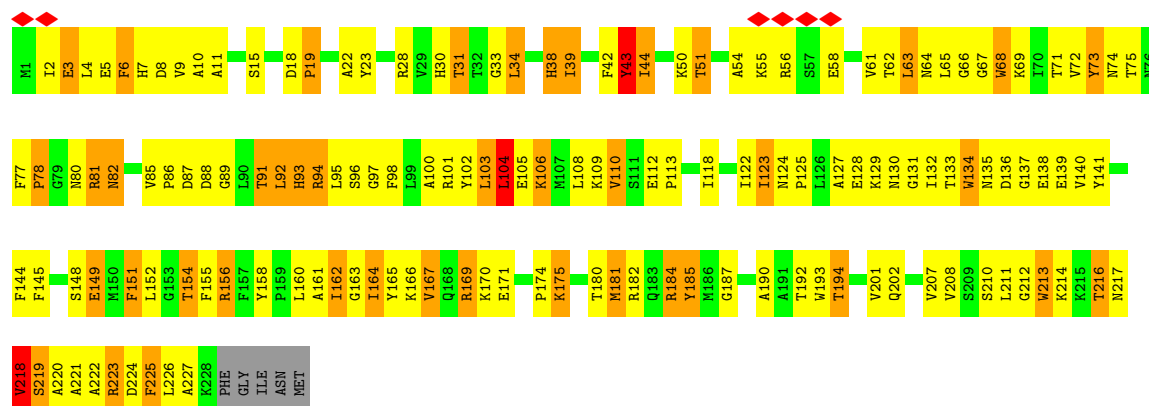




- Molecule 1: Nucleoprotein

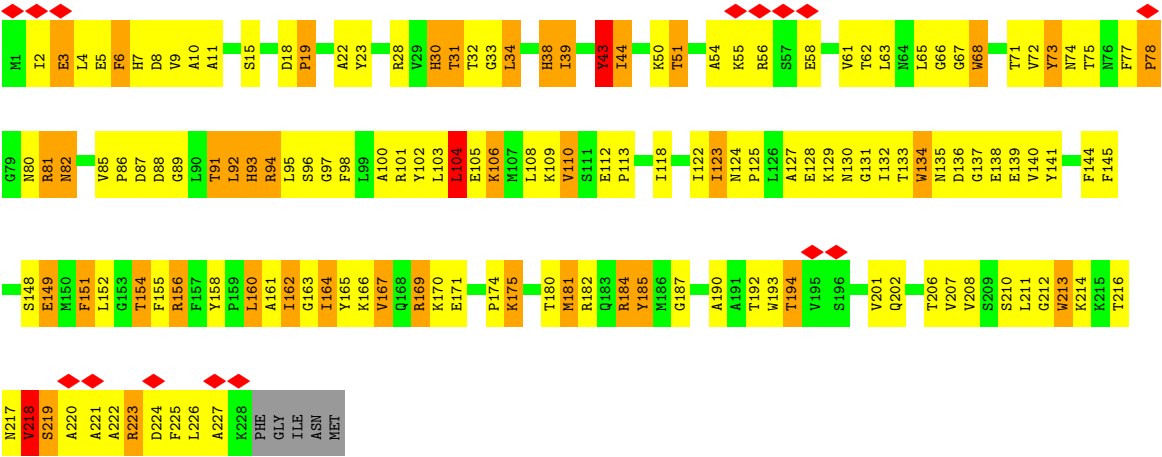


- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5077	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.146	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.056	Depositor
Map size (Å)	273.92, 273.92, 273.92	wwPDB
Map dimensions	64, 64, 64	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	4.28, 4.28, 4.28	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	2.26	76/1887 (4.0%)	2.53	143/2551 (5.6%)
1	B	2.26	76/1887 (4.0%)	2.53	140/2551 (5.5%)
1	C	2.26	76/1887 (4.0%)	2.53	140/2551 (5.5%)
1	D	2.26	76/1887 (4.0%)	2.53	140/2551 (5.5%)
1	E	2.26	77/1887 (4.1%)	2.53	142/2551 (5.6%)
1	F	2.26	77/1887 (4.1%)	2.53	143/2551 (5.6%)
1	G	2.26	76/1887 (4.0%)	2.53	140/2551 (5.5%)
1	H	2.26	77/1887 (4.1%)	2.53	141/2551 (5.5%)
1	I	2.26	76/1887 (4.0%)	2.53	142/2551 (5.6%)
All	All	2.26	687/16983 (4.0%)	2.53	1271/22959 (5.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	7
1	C	0	7
1	D	0	7
1	E	0	7
1	F	0	7
1	G	0	7
1	H	0	7
1	I	0	7
All	All	0	63

All (687) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217	ASN	CA-CB	9.13	1.67	1.53
1	G	217	ASN	CA-CB	9.11	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	217	ASN	CA-CB	9.11	1.67	1.53
1	F	217	ASN	CA-CB	9.11	1.67	1.53
1	B	217	ASN	CA-CB	9.10	1.67	1.53
1	I	217	ASN	CA-CB	9.10	1.67	1.53
1	C	217	ASN	CA-CB	9.09	1.67	1.53
1	E	217	ASN	CA-CB	9.08	1.67	1.53
1	H	217	ASN	CA-CB	9.07	1.67	1.53
1	G	80	ASN	CA-CB	8.15	1.67	1.53
1	F	80	ASN	CA-CB	8.13	1.67	1.53
1	C	80	ASN	CA-CB	8.12	1.67	1.53
1	I	80	ASN	CA-CB	8.12	1.67	1.53
1	B	80	ASN	CA-CB	8.12	1.67	1.53
1	E	80	ASN	CA-CB	8.12	1.67	1.53
1	A	80	ASN	CA-CB	8.12	1.67	1.53
1	D	80	ASN	CA-CB	8.11	1.67	1.53
1	H	80	ASN	CA-CB	8.08	1.67	1.53
1	F	219	SER	C-N	7.76	1.44	1.33
1	G	219	SER	C-N	7.76	1.44	1.33
1	B	219	SER	C-N	7.75	1.44	1.33
1	H	219	SER	C-N	7.75	1.44	1.33
1	I	219	SER	C-N	7.75	1.44	1.33
1	E	219	SER	C-N	7.75	1.44	1.33
1	A	219	SER	C-N	7.74	1.44	1.33
1	C	219	SER	C-N	7.74	1.44	1.33
1	D	219	SER	C-N	7.71	1.44	1.33
1	G	34	LEU	CA-CB	7.65	1.64	1.53
1	I	34	LEU	CA-CB	7.64	1.64	1.53
1	H	34	LEU	CA-CB	7.62	1.64	1.53
1	B	34	LEU	CA-CB	7.62	1.64	1.53
1	C	34	LEU	CA-CB	7.61	1.64	1.53
1	A	34	LEU	CA-CB	7.61	1.64	1.53
1	F	34	LEU	CA-CB	7.59	1.64	1.53
1	D	34	LEU	CA-CB	7.59	1.64	1.53
1	E	34	LEU	CA-CB	7.58	1.64	1.53
1	E	110	VAL	CA-C	-7.30	1.43	1.52
1	G	110	VAL	CA-C	-7.30	1.43	1.52
1	F	110	VAL	CA-C	-7.30	1.43	1.52
1	H	110	VAL	CA-C	-7.30	1.43	1.52
1	B	110	VAL	CA-C	-7.29	1.43	1.52
1	D	110	VAL	CA-C	-7.29	1.43	1.52
1	A	110	VAL	CA-C	-7.28	1.43	1.52
1	I	110	VAL	CA-C	-7.28	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	110	VAL	CA-C	-7.28	1.43	1.52
1	G	156	ARG	CZ-NH1	7.04	1.42	1.32
1	B	156	ARG	CZ-NH1	7.00	1.42	1.32
1	A	156	ARG	CZ-NH1	6.99	1.42	1.32
1	F	156	ARG	CZ-NH1	6.99	1.42	1.32
1	H	156	ARG	CZ-NH1	6.99	1.42	1.32
1	C	93	HIS	CD2-NE2	6.98	1.45	1.37
1	D	156	ARG	CZ-NH1	6.97	1.42	1.32
1	C	156	ARG	CZ-NH1	6.96	1.42	1.32
1	E	156	ARG	CZ-NH1	6.96	1.42	1.32
1	E	93	HIS	CD2-NE2	6.95	1.45	1.37
1	A	93	HIS	CD2-NE2	6.94	1.45	1.37
1	I	156	ARG	CZ-NH1	6.94	1.42	1.32
1	B	93	HIS	CD2-NE2	6.92	1.45	1.37
1	G	93	HIS	CD2-NE2	6.92	1.45	1.37
1	D	93	HIS	CD2-NE2	6.90	1.45	1.37
1	E	151	PHE	N-CA	-6.90	1.38	1.46
1	H	93	HIS	CD2-NE2	6.90	1.45	1.37
1	F	93	HIS	CD2-NE2	6.89	1.45	1.37
1	I	151	PHE	N-CA	-6.89	1.38	1.46
1	C	151	PHE	N-CA	-6.88	1.38	1.46
1	D	151	PHE	N-CA	-6.87	1.38	1.46
1	B	151	PHE	N-CA	-6.86	1.38	1.46
1	I	93	HIS	CD2-NE2	6.86	1.45	1.37
1	F	151	PHE	N-CA	-6.86	1.38	1.46
1	A	151	PHE	N-CA	-6.86	1.38	1.46
1	H	151	PHE	N-CA	-6.86	1.38	1.46
1	G	151	PHE	N-CA	-6.82	1.38	1.46
1	F	128	GLU	C-N	6.80	1.42	1.33
1	I	128	GLU	C-N	6.79	1.42	1.33
1	G	128	GLU	C-N	6.79	1.42	1.33
1	C	128	GLU	C-N	6.78	1.42	1.33
1	B	128	GLU	C-N	6.77	1.42	1.33
1	A	128	GLU	C-N	6.77	1.42	1.33
1	H	128	GLU	C-N	6.77	1.42	1.33
1	D	128	GLU	C-N	6.77	1.42	1.33
1	E	128	GLU	C-N	6.77	1.42	1.33
1	F	93	HIS	CA-C	-6.76	1.44	1.52
1	A	87	ASP	N-CA	-6.76	1.37	1.46
1	D	93	HIS	CA-C	-6.75	1.44	1.52
1	G	93	HIS	CA-C	-6.75	1.44	1.52
1	B	93	HIS	CA-C	-6.74	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	87	ASP	N-CA	-6.74	1.37	1.46
1	B	87	ASP	N-CA	-6.73	1.37	1.46
1	A	93	HIS	CA-C	-6.73	1.44	1.52
1	D	87	ASP	N-CA	-6.73	1.37	1.46
1	E	87	ASP	N-CA	-6.72	1.37	1.46
1	C	87	ASP	N-CA	-6.72	1.37	1.46
1	E	93	HIS	CA-C	-6.72	1.44	1.52
1	H	190	ALA	CA-C	-6.71	1.43	1.52
1	I	87	ASP	N-CA	-6.71	1.37	1.46
1	H	93	HIS	CA-C	-6.71	1.44	1.52
1	F	87	ASP	N-CA	-6.71	1.37	1.46
1	H	87	ASP	N-CA	-6.70	1.37	1.46
1	C	190	ALA	CA-C	-6.70	1.43	1.52
1	C	93	HIS	CA-C	-6.69	1.44	1.52
1	F	190	ALA	CA-C	-6.69	1.43	1.52
1	B	190	ALA	CA-C	-6.69	1.43	1.52
1	A	190	ALA	CA-C	-6.68	1.43	1.52
1	E	190	ALA	CA-C	-6.68	1.43	1.52
1	G	190	ALA	CA-C	-6.68	1.43	1.52
1	I	93	HIS	CA-C	-6.68	1.44	1.52
1	C	62	THR	C-N	6.67	1.42	1.33
1	E	62	THR	C-N	6.67	1.42	1.33
1	D	190	ALA	CA-C	-6.67	1.43	1.52
1	H	62	THR	C-N	6.67	1.42	1.33
1	F	62	THR	C-N	6.66	1.42	1.33
1	I	190	ALA	CA-C	-6.66	1.43	1.52
1	D	62	THR	C-N	6.66	1.42	1.33
1	I	62	THR	C-N	6.66	1.42	1.33
1	B	62	THR	C-N	6.66	1.42	1.33
1	G	62	THR	C-N	6.65	1.42	1.33
1	A	62	THR	C-N	6.64	1.42	1.33
1	E	55	LYS	C-N	6.46	1.42	1.33
1	F	55	LYS	C-N	6.45	1.42	1.33
1	C	44	ILE	CA-CB	-6.43	1.46	1.54
1	I	44	ILE	CA-CB	-6.43	1.46	1.54
1	I	131	GLY	C-N	6.43	1.42	1.33
1	C	55	LYS	C-N	6.43	1.42	1.33
1	B	44	ILE	CA-CB	-6.43	1.46	1.54
1	I	55	LYS	C-N	6.42	1.42	1.33
1	A	55	LYS	C-N	6.42	1.42	1.33
1	D	55	LYS	C-N	6.42	1.42	1.33
1	B	55	LYS	C-N	6.41	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	ILE	CA-CB	-6.41	1.47	1.54
1	A	131	GLY	C-N	6.41	1.42	1.33
1	D	44	ILE	CA-CB	-6.41	1.47	1.54
1	C	131	GLY	C-N	6.40	1.42	1.33
1	F	44	ILE	CA-CB	-6.40	1.47	1.54
1	F	131	GLY	C-N	6.40	1.42	1.33
1	H	44	ILE	CA-CB	-6.40	1.47	1.54
1	H	55	LYS	C-N	6.40	1.41	1.33
1	G	55	LYS	C-N	6.39	1.41	1.33
1	B	131	GLY	C-N	6.39	1.42	1.33
1	E	44	ILE	CA-CB	-6.39	1.47	1.54
1	E	131	GLY	C-N	6.37	1.42	1.33
1	G	44	ILE	CA-CB	-6.37	1.47	1.54
1	H	131	GLY	C-N	6.37	1.42	1.33
1	D	131	GLY	C-N	6.36	1.42	1.33
1	G	131	GLY	C-N	6.34	1.42	1.33
1	C	182	ARG	CA-CB	6.30	1.61	1.53
1	E	182	ARG	CA-CB	6.30	1.61	1.53
1	G	39	ILE	N-CA	-6.30	1.39	1.46
1	G	182	ARG	CA-CB	6.30	1.61	1.53
1	A	182	ARG	CA-CB	6.30	1.61	1.53
1	F	182	ARG	CA-CB	6.30	1.61	1.53
1	I	65	LEU	N-CA	-6.30	1.38	1.46
1	B	65	LEU	N-CA	-6.29	1.38	1.46
1	E	65	LEU	N-CA	-6.29	1.38	1.46
1	F	65	LEU	N-CA	-6.29	1.38	1.46
1	C	65	LEU	N-CA	-6.29	1.38	1.46
1	G	65	LEU	N-CA	-6.29	1.38	1.46
1	H	65	LEU	N-CA	-6.29	1.38	1.46
1	B	182	ARG	CA-CB	6.29	1.61	1.53
1	A	39	ILE	N-CA	-6.29	1.39	1.46
1	D	65	LEU	N-CA	-6.29	1.38	1.46
1	A	65	LEU	N-CA	-6.29	1.38	1.46
1	D	182	ARG	CA-CB	6.29	1.61	1.53
1	E	39	ILE	N-CA	-6.29	1.39	1.46
1	I	182	ARG	CA-CB	6.28	1.61	1.53
1	F	39	ILE	N-CA	-6.28	1.39	1.46
1	H	182	ARG	CA-CB	6.27	1.61	1.53
1	H	39	ILE	N-CA	-6.27	1.39	1.46
1	A	6	PHE	N-CA	-6.26	1.38	1.45
1	B	39	ILE	N-CA	-6.26	1.39	1.46
1	G	6	PHE	N-CA	-6.25	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	169	ARG	CZ-NH1	6.25	1.41	1.32
1	G	169	ARG	CZ-NH1	6.25	1.41	1.32
1	C	169	ARG	CZ-NH1	6.24	1.41	1.32
1	D	169	ARG	CZ-NH1	6.24	1.41	1.32
1	B	169	ARG	CZ-NH1	6.24	1.41	1.32
1	D	6	PHE	N-CA	-6.24	1.38	1.45
1	F	169	ARG	CZ-NH1	6.24	1.41	1.32
1	I	169	ARG	CZ-NH1	6.24	1.41	1.32
1	H	169	ARG	CZ-NH1	6.24	1.41	1.32
1	A	169	ARG	CZ-NH1	6.23	1.41	1.32
1	E	225	PHE	CA-CB	6.23	1.63	1.53
1	I	39	ILE	N-CA	-6.22	1.39	1.46
1	F	225	PHE	CA-CB	6.22	1.62	1.53
1	F	6	PHE	N-CA	-6.22	1.38	1.45
1	B	6	PHE	N-CA	-6.22	1.38	1.45
1	B	225	PHE	CA-CB	6.22	1.62	1.53
1	C	225	PHE	CA-CB	6.22	1.62	1.53
1	E	6	PHE	N-CA	-6.21	1.38	1.45
1	D	39	ILE	N-CA	-6.21	1.39	1.46
1	H	6	PHE	N-CA	-6.21	1.38	1.45
1	C	39	ILE	N-CA	-6.21	1.39	1.46
1	H	225	PHE	CA-CB	6.21	1.62	1.53
1	G	225	PHE	CA-CB	6.20	1.62	1.53
1	I	225	PHE	CA-CB	6.20	1.62	1.53
1	D	225	PHE	CA-CB	6.20	1.62	1.53
1	I	6	PHE	N-CA	-6.19	1.38	1.45
1	F	104	LEU	CA-CB	6.19	1.63	1.53
1	A	104	LEU	CA-CB	6.18	1.63	1.53
1	A	225	PHE	CA-CB	6.18	1.62	1.53
1	C	6	PHE	N-CA	-6.18	1.38	1.45
1	H	104	LEU	CA-CB	6.17	1.63	1.53
1	H	207	VAL	CA-CB	-6.16	1.47	1.54
1	G	207	VAL	CA-CB	-6.16	1.47	1.54
1	I	207	VAL	CA-CB	-6.16	1.47	1.54
1	G	104	LEU	CA-CB	6.15	1.63	1.53
1	B	104	LEU	CA-CB	6.15	1.63	1.53
1	E	104	LEU	CA-CB	6.15	1.63	1.53
1	C	104	LEU	CA-CB	6.14	1.63	1.53
1	C	207	VAL	CA-CB	-6.14	1.47	1.54
1	F	207	VAL	CA-CB	-6.14	1.47	1.54
1	I	104	LEU	CA-CB	6.14	1.63	1.53
1	A	63	LEU	N-CA	-6.13	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	112	GLU	N-CA	-6.13	1.40	1.46
1	E	66	GLY	C-N	6.13	1.41	1.33
1	C	63	LEU	N-CA	-6.13	1.38	1.46
1	D	104	LEU	CA-CB	6.13	1.63	1.53
1	H	66	GLY	C-N	6.13	1.41	1.33
1	B	63	LEU	N-CA	-6.12	1.38	1.46
1	G	112	GLU	N-CA	-6.12	1.40	1.46
1	B	207	VAL	CA-CB	-6.12	1.47	1.54
1	D	63	LEU	N-CA	-6.12	1.38	1.46
1	I	136	ASP	C-N	6.12	1.40	1.32
1	A	34	LEU	N-CA	-6.12	1.38	1.46
1	E	34	LEU	N-CA	-6.12	1.38	1.46
1	E	63	LEU	N-CA	-6.12	1.38	1.46
1	D	34	LEU	N-CA	-6.12	1.38	1.46
1	A	112	GLU	N-CA	-6.12	1.40	1.46
1	H	63	LEU	N-CA	-6.12	1.38	1.46
1	H	136	ASP	C-N	6.11	1.40	1.32
1	F	34	LEU	N-CA	-6.11	1.38	1.46
1	C	66	GLY	C-N	6.11	1.41	1.33
1	D	66	GLY	C-N	6.11	1.41	1.33
1	E	136	ASP	C-N	6.11	1.40	1.32
1	I	34	LEU	N-CA	-6.11	1.38	1.46
1	A	207	VAL	CA-CB	-6.11	1.47	1.54
1	C	34	LEU	N-CA	-6.10	1.38	1.46
1	F	63	LEU	N-CA	-6.10	1.38	1.46
1	E	207	VAL	CA-CB	-6.10	1.47	1.54
1	H	34	LEU	N-CA	-6.09	1.38	1.46
1	I	63	LEU	N-CA	-6.09	1.38	1.46
1	G	63	LEU	N-CA	-6.09	1.38	1.46
1	B	34	LEU	N-CA	-6.09	1.38	1.46
1	B	66	GLY	C-N	6.09	1.41	1.33
1	G	66	GLY	C-N	6.09	1.41	1.33
1	F	66	GLY	C-N	6.08	1.41	1.33
1	D	207	VAL	CA-CB	-6.08	1.47	1.54
1	A	136	ASP	C-N	6.08	1.40	1.32
1	G	34	LEU	N-CA	-6.08	1.38	1.46
1	A	66	GLY	C-N	6.08	1.41	1.33
1	D	136	ASP	C-N	6.08	1.40	1.32
1	F	136	ASP	C-N	6.08	1.40	1.32
1	B	136	ASP	C-N	6.07	1.40	1.32
1	H	112	GLU	N-CA	-6.07	1.40	1.46
1	B	112	GLU	N-CA	-6.07	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	112	GLU	N-CA	-6.07	1.40	1.46
1	C	136	ASP	C-N	6.07	1.40	1.32
1	E	112	GLU	N-CA	-6.07	1.40	1.46
1	C	112	GLU	N-CA	-6.05	1.40	1.46
1	G	136	ASP	C-N	6.04	1.40	1.32
1	I	66	GLY	C-N	6.04	1.41	1.33
1	F	112	GLU	N-CA	-6.02	1.40	1.46
1	H	182	ARG	N-CA	-5.97	1.39	1.46
1	E	182	ARG	N-CA	-5.96	1.39	1.46
1	C	182	ARG	N-CA	-5.95	1.39	1.46
1	B	182	ARG	N-CA	-5.94	1.39	1.46
1	I	182	ARG	N-CA	-5.93	1.39	1.46
1	C	67	GLY	C-N	5.93	1.41	1.33
1	G	182	ARG	N-CA	-5.93	1.39	1.46
1	D	93	HIS	CA-CB	5.92	1.62	1.53
1	F	182	ARG	N-CA	-5.92	1.39	1.46
1	F	93	HIS	CA-CB	5.92	1.62	1.53
1	A	93	HIS	CA-CB	5.91	1.62	1.53
1	B	93	HIS	CA-CB	5.91	1.62	1.53
1	D	182	ARG	N-CA	-5.91	1.39	1.46
1	H	93	HIS	CA-CB	5.91	1.62	1.53
1	A	67	GLY	C-N	5.91	1.41	1.33
1	E	67	GLY	C-N	5.91	1.41	1.33
1	A	182	ARG	N-CA	-5.90	1.39	1.46
1	A	15	SER	CA-C	-5.90	1.44	1.52
1	B	170	LYS	CA-C	5.90	1.61	1.52
1	G	93	HIS	CA-CB	5.90	1.62	1.53
1	I	15	SER	CA-C	-5.90	1.44	1.52
1	B	67	GLY	C-N	5.89	1.41	1.33
1	G	67	GLY	C-N	5.89	1.41	1.33
1	F	67	GLY	C-N	5.89	1.41	1.33
1	I	67	GLY	C-N	5.89	1.41	1.33
1	H	67	GLY	C-N	5.89	1.41	1.33
1	B	15	SER	CA-C	-5.88	1.45	1.52
1	E	15	SER	CA-C	-5.88	1.45	1.52
1	E	93	HIS	CA-CB	5.88	1.62	1.53
1	D	15	SER	CA-C	-5.88	1.45	1.52
1	C	170	LYS	CA-C	5.88	1.61	1.52
1	F	15	SER	CA-C	-5.88	1.45	1.52
1	C	15	SER	CA-C	-5.87	1.45	1.52
1	C	93	HIS	CA-CB	5.87	1.62	1.53
1	I	93	HIS	CA-CB	5.87	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	15	SER	CA-C	-5.87	1.45	1.52
1	G	170	LYS	CA-C	5.87	1.61	1.52
1	A	170	LYS	CA-C	5.87	1.61	1.52
1	G	15	SER	CA-C	-5.87	1.45	1.52
1	I	170	LYS	CA-C	5.87	1.61	1.52
1	F	15	SER	CA-CB	5.86	1.61	1.53
1	E	185	TYR	CA-CB	5.86	1.62	1.53
1	G	15	SER	CA-CB	5.86	1.61	1.53
1	G	218	VAL	C-N	5.85	1.41	1.33
1	D	15	SER	CA-CB	5.85	1.61	1.53
1	D	67	GLY	C-N	5.85	1.41	1.33
1	H	15	SER	CA-CB	5.85	1.61	1.53
1	A	28	ARG	NE-CZ	5.85	1.39	1.33
1	F	28	ARG	NE-CZ	5.84	1.39	1.33
1	H	28	ARG	NE-CZ	5.84	1.39	1.33
1	E	15	SER	CA-CB	5.84	1.61	1.53
1	I	185	TYR	CA-CB	5.84	1.62	1.53
1	A	15	SER	CA-CB	5.84	1.61	1.53
1	A	218	VAL	C-N	5.84	1.41	1.33
1	B	15	SER	CA-CB	5.84	1.61	1.53
1	D	28	ARG	NE-CZ	5.84	1.39	1.33
1	E	28	ARG	NE-CZ	5.83	1.39	1.33
1	G	28	ARG	NE-CZ	5.83	1.39	1.33
1	B	28	ARG	NE-CZ	5.83	1.39	1.33
1	E	218	VAL	C-N	5.83	1.41	1.33
1	F	185	TYR	CA-CB	5.82	1.62	1.53
1	D	185	TYR	CA-CB	5.82	1.62	1.53
1	D	218	VAL	C-N	5.82	1.41	1.33
1	B	185	TYR	CA-CB	5.82	1.62	1.53
1	A	185	TYR	CA-CB	5.82	1.62	1.53
1	I	15	SER	CA-CB	5.82	1.61	1.53
1	C	185	TYR	CA-CB	5.81	1.62	1.53
1	C	15	SER	CA-CB	5.81	1.61	1.53
1	I	28	ARG	NE-CZ	5.81	1.39	1.33
1	C	28	ARG	NE-CZ	5.81	1.39	1.33
1	B	218	VAL	C-N	5.80	1.41	1.33
1	H	185	TYR	CA-CB	5.80	1.62	1.53
1	H	30	HIS	ND1-CE1	5.80	1.38	1.32
1	I	218	VAL	C-N	5.80	1.41	1.33
1	I	30	HIS	ND1-CE1	5.79	1.38	1.32
1	G	185	TYR	CA-CB	5.79	1.62	1.53
1	C	30	HIS	ND1-CE1	5.79	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	218	VAL	C-N	5.79	1.41	1.33
1	G	30	HIS	ND1-CE1	5.79	1.38	1.32
1	A	30	HIS	ND1-CE1	5.78	1.38	1.32
1	A	65	LEU	CA-CB	5.78	1.60	1.52
1	C	218	VAL	C-N	5.78	1.41	1.33
1	E	65	LEU	CA-CB	5.78	1.60	1.52
1	B	30	HIS	ND1-CE1	5.78	1.38	1.32
1	H	65	LEU	CA-CB	5.77	1.60	1.52
1	F	65	LEU	CA-CB	5.77	1.60	1.52
1	I	65	LEU	CA-CB	5.76	1.60	1.52
1	D	65	LEU	CA-CB	5.76	1.60	1.52
1	E	30	HIS	ND1-CE1	5.76	1.38	1.32
1	D	30	HIS	ND1-CE1	5.76	1.38	1.32
1	B	65	LEU	CA-CB	5.76	1.60	1.52
1	C	65	LEU	CA-CB	5.75	1.60	1.52
1	H	218	VAL	C-N	5.75	1.41	1.33
1	A	144	PHE	C-N	5.75	1.41	1.33
1	F	30	HIS	ND1-CE1	5.75	1.38	1.32
1	G	65	LEU	CA-CB	5.75	1.60	1.52
1	C	123	ILE	N-CA	-5.74	1.39	1.46
1	E	144	PHE	C-N	5.74	1.41	1.33
1	B	81	ARG	CD-NE	5.74	1.54	1.46
1	E	123	ILE	N-CA	-5.74	1.39	1.46
1	D	144	PHE	C-N	5.74	1.41	1.33
1	F	81	ARG	CD-NE	5.74	1.54	1.46
1	H	81	ARG	CD-NE	5.74	1.54	1.46
1	H	123	ILE	N-CA	-5.74	1.39	1.46
1	B	144	PHE	C-N	5.73	1.41	1.33
1	F	144	PHE	C-N	5.73	1.41	1.33
1	H	144	PHE	C-N	5.73	1.41	1.33
1	G	81	ARG	CD-NE	5.73	1.54	1.46
1	G	123	ILE	N-CA	-5.72	1.39	1.46
1	H	227	ALA	C-N	5.72	1.41	1.33
1	I	123	ILE	N-CA	-5.72	1.39	1.46
1	I	144	PHE	C-N	5.72	1.41	1.33
1	F	123	ILE	N-CA	-5.72	1.39	1.46
1	D	81	ARG	CD-NE	5.72	1.54	1.46
1	B	123	ILE	N-CA	-5.71	1.39	1.46
1	C	144	PHE	C-N	5.71	1.41	1.33
1	D	123	ILE	N-CA	-5.71	1.39	1.46
1	C	81	ARG	CD-NE	5.71	1.54	1.46
1	A	123	ILE	N-CA	-5.71	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	ARG	CD-NE	5.70	1.54	1.46
1	F	227	ALA	C-N	5.70	1.41	1.33
1	E	81	ARG	CD-NE	5.70	1.54	1.46
1	G	227	ALA	C-N	5.70	1.41	1.33
1	I	81	ARG	CD-NE	5.70	1.54	1.46
1	A	227	ALA	C-N	5.69	1.41	1.33
1	B	227	ALA	C-N	5.68	1.41	1.33
1	E	227	ALA	C-N	5.68	1.41	1.33
1	G	144	PHE	C-N	5.67	1.41	1.33
1	C	227	ALA	C-N	5.65	1.41	1.33
1	D	187	GLY	C-N	5.64	1.41	1.33
1	A	187	GLY	C-N	5.64	1.41	1.33
1	D	227	ALA	C-N	5.64	1.41	1.33
1	H	223	ARG	CZ-NH2	5.63	1.40	1.33
1	C	187	GLY	C-N	5.63	1.40	1.33
1	B	187	GLY	C-N	5.63	1.40	1.33
1	I	227	ALA	C-N	5.63	1.41	1.33
1	D	182	ARG	NE-CZ	5.62	1.39	1.33
1	G	187	GLY	C-N	5.62	1.40	1.33
1	E	187	GLY	C-N	5.62	1.40	1.33
1	D	91	THR	CA-C	-5.61	1.45	1.53
1	H	187	GLY	C-N	5.61	1.40	1.33
1	I	91	THR	CA-C	-5.61	1.45	1.53
1	F	187	GLY	C-N	5.60	1.40	1.33
1	E	89	GLY	CA-C	-5.60	1.45	1.52
1	F	182	ARG	NE-CZ	5.60	1.39	1.33
1	I	187	GLY	C-N	5.60	1.40	1.33
1	C	182	ARG	NE-CZ	5.60	1.39	1.33
1	C	223	ARG	CZ-NH2	5.60	1.40	1.33
1	G	214	LYS	CA-CB	5.60	1.62	1.53
1	A	223	ARG	CZ-NH2	5.59	1.40	1.33
1	C	91	THR	CA-C	-5.59	1.45	1.53
1	A	91	THR	CA-C	-5.59	1.45	1.53
1	A	182	ARG	NE-CZ	5.59	1.39	1.33
1	G	91	THR	CA-C	-5.59	1.45	1.53
1	B	182	ARG	NE-CZ	5.59	1.39	1.33
1	F	223	ARG	CZ-NH2	5.58	1.40	1.33
1	I	89	GLY	CA-C	-5.58	1.45	1.52
1	I	214	LYS	CA-CB	5.58	1.62	1.53
1	G	182	ARG	NE-CZ	5.58	1.39	1.33
1	H	91	THR	CA-C	-5.58	1.45	1.53
1	B	91	THR	CA-C	-5.58	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	GLY	CA-C	-5.58	1.45	1.52
1	E	223	ARG	CZ-NH2	5.58	1.40	1.33
1	B	89	GLY	CA-C	-5.57	1.45	1.52
1	H	89	GLY	CA-C	-5.57	1.45	1.52
1	B	223	ARG	CZ-NH2	5.57	1.40	1.33
1	D	89	GLY	CA-C	-5.57	1.45	1.52
1	G	89	GLY	CA-C	-5.57	1.45	1.52
1	B	214	LYS	CA-CB	5.56	1.62	1.53
1	D	223	ARG	CZ-NH2	5.56	1.40	1.33
1	E	214	LYS	CA-CB	5.56	1.62	1.53
1	E	91	THR	CA-C	-5.56	1.45	1.53
1	E	182	ARG	NE-CZ	5.55	1.39	1.33
1	H	214	LYS	CA-CB	5.55	1.62	1.53
1	D	166	LYS	C-N	5.55	1.41	1.33
1	I	223	ARG	CZ-NH2	5.55	1.40	1.33
1	C	89	GLY	CA-C	-5.55	1.45	1.52
1	A	214	LYS	CA-CB	5.55	1.62	1.53
1	F	89	GLY	CA-C	-5.55	1.45	1.52
1	C	214	LYS	CA-CB	5.54	1.62	1.53
1	I	182	ARG	NE-CZ	5.54	1.39	1.33
1	H	182	ARG	NE-CZ	5.54	1.39	1.33
1	D	214	LYS	CA-CB	5.54	1.62	1.53
1	F	91	THR	CA-C	-5.54	1.45	1.53
1	F	214	LYS	CA-CB	5.53	1.62	1.53
1	G	223	ARG	CZ-NH2	5.53	1.40	1.33
1	H	166	LYS	C-N	5.53	1.40	1.33
1	D	170	LYS	CA-C	5.53	1.61	1.52
1	E	166	LYS	C-N	5.52	1.40	1.33
1	C	166	LYS	C-N	5.52	1.40	1.33
1	E	170	LYS	CA-C	5.52	1.61	1.52
1	F	170	LYS	CA-C	5.52	1.61	1.52
1	B	166	LYS	C-N	5.52	1.40	1.33
1	G	166	LYS	C-N	5.51	1.40	1.33
1	F	166	LYS	C-N	5.51	1.40	1.33
1	C	75	THR	CA-C	-5.50	1.45	1.52
1	H	170	LYS	CA-C	5.50	1.61	1.52
1	I	166	LYS	C-N	5.49	1.40	1.33
1	H	96	SER	CA-C	-5.47	1.45	1.52
1	C	96	SER	CA-C	-5.47	1.45	1.52
1	A	166	LYS	C-N	5.47	1.40	1.33
1	D	96	SER	CA-C	-5.47	1.45	1.52
1	A	96	SER	CA-C	-5.46	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	175	LYS	C-N	5.46	1.42	1.33
1	H	108	LEU	C-N	5.46	1.41	1.33
1	H	184	ARG	CZ-NH1	5.46	1.40	1.32
1	G	103	LEU	C-O	-5.46	1.17	1.24
1	F	103	LEU	C-O	-5.46	1.17	1.24
1	A	221	ALA	C-N	5.45	1.40	1.33
1	D	75	THR	CA-C	-5.45	1.45	1.52
1	G	108	LEU	C-N	5.45	1.41	1.33
1	E	96	SER	CA-C	-5.45	1.45	1.52
1	B	75	THR	CA-C	-5.45	1.45	1.52
1	D	108	LEU	C-N	5.45	1.41	1.33
1	C	108	LEU	C-N	5.45	1.41	1.33
1	C	221	ALA	C-N	5.45	1.40	1.33
1	H	175	LYS	C-N	5.45	1.41	1.33
1	B	96	SER	CA-C	-5.44	1.45	1.52
1	E	108	LEU	C-N	5.44	1.41	1.33
1	C	74	ASN	CA-C	-5.44	1.46	1.52
1	C	103	LEU	C-O	-5.44	1.17	1.24
1	F	175	LYS	C-N	5.44	1.41	1.33
1	I	108	LEU	C-N	5.44	1.41	1.33
1	H	221	ALA	C-N	5.44	1.40	1.33
1	B	184	ARG	CZ-NH1	5.43	1.40	1.32
1	E	74	ASN	CA-C	-5.43	1.46	1.52
1	F	96	SER	CA-C	-5.43	1.45	1.52
1	A	184	ARG	CZ-NH1	5.43	1.40	1.32
1	H	103	LEU	C-O	-5.43	1.17	1.24
1	E	184	ARG	CZ-NH1	5.43	1.40	1.32
1	B	103	LEU	C-O	-5.43	1.17	1.24
1	D	175	LYS	C-N	5.43	1.41	1.33
1	B	108	LEU	C-N	5.43	1.41	1.33
1	E	103	LEU	C-O	-5.43	1.17	1.24
1	B	175	LYS	C-N	5.42	1.41	1.33
1	A	175	LYS	C-N	5.42	1.41	1.33
1	G	74	ASN	CA-C	-5.42	1.46	1.52
1	I	103	LEU	C-O	-5.42	1.17	1.24
1	I	175	LYS	C-N	5.42	1.41	1.33
1	I	184	ARG	CZ-NH1	5.42	1.40	1.32
1	F	75	THR	CA-C	-5.42	1.45	1.52
1	D	184	ARG	CZ-NH1	5.42	1.40	1.32
1	F	56	ARG	CA-CB	5.42	1.62	1.53
1	F	221	ALA	C-N	5.42	1.40	1.33
1	H	75	THR	CA-C	-5.42	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	175	LYS	C-N	5.41	1.41	1.33
1	E	75	THR	CA-C	-5.41	1.45	1.52
1	F	184	ARG	CZ-NH1	5.41	1.40	1.32
1	F	108	LEU	C-N	5.41	1.41	1.33
1	G	221	ALA	C-N	5.41	1.40	1.33
1	G	227	ALA	CA-C	-5.41	1.45	1.52
1	B	227	ALA	CA-C	-5.41	1.45	1.52
1	E	227	ALA	CA-C	-5.41	1.45	1.52
1	G	184	ARG	CZ-NH1	5.41	1.40	1.32
1	C	227	ALA	CA-C	-5.41	1.45	1.52
1	E	221	ALA	C-N	5.41	1.40	1.33
1	D	227	ALA	CA-C	-5.41	1.45	1.52
1	F	227	ALA	CA-C	-5.41	1.45	1.52
1	I	227	ALA	CA-C	-5.41	1.45	1.52
1	A	227	ALA	CA-C	-5.40	1.45	1.52
1	D	103	LEU	C-O	-5.40	1.17	1.24
1	F	74	ASN	CA-C	-5.40	1.46	1.52
1	H	227	ALA	CA-C	-5.40	1.45	1.52
1	I	96	SER	CA-C	-5.40	1.45	1.52
1	B	221	ALA	C-N	5.40	1.40	1.33
1	C	184	ARG	CZ-NH1	5.40	1.40	1.32
1	B	74	ASN	CA-C	-5.40	1.46	1.52
1	A	56	ARG	CA-CB	5.40	1.62	1.53
1	A	75	THR	CA-C	-5.40	1.45	1.52
1	G	96	SER	CA-C	-5.40	1.45	1.52
1	A	103	LEU	C-O	-5.39	1.17	1.24
1	A	108	LEU	C-N	5.39	1.41	1.33
1	G	28	ARG	CA-CB	5.39	1.61	1.53
1	G	75	THR	CA-C	-5.39	1.45	1.52
1	H	56	ARG	CA-CB	5.39	1.62	1.53
1	A	74	ASN	CA-C	-5.39	1.46	1.52
1	I	74	ASN	CA-C	-5.39	1.46	1.52
1	E	175	LYS	C-N	5.38	1.41	1.33
1	H	74	ASN	CA-C	-5.38	1.46	1.52
1	I	221	ALA	C-N	5.38	1.40	1.33
1	C	56	ARG	CA-CB	5.38	1.62	1.53
1	D	221	ALA	C-N	5.38	1.40	1.33
1	G	152	LEU	CA-C	-5.38	1.45	1.52
1	G	182	ARG	CZ-NH2	5.38	1.40	1.33
1	I	56	ARG	CA-CB	5.38	1.62	1.53
1	I	75	THR	CA-C	-5.37	1.45	1.52
1	I	152	LEU	CA-C	-5.37	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	56	ARG	CA-CB	5.37	1.62	1.53
1	E	28	ARG	CA-CB	5.37	1.61	1.53
1	H	152	LEU	CA-C	-5.37	1.45	1.52
1	A	165	TYR	C-N	5.37	1.41	1.33
1	D	56	ARG	CA-CB	5.37	1.62	1.53
1	D	74	ASN	CA-C	-5.37	1.46	1.52
1	I	165	TYR	C-N	5.36	1.41	1.33
1	H	182	ARG	CZ-NH2	5.36	1.40	1.33
1	C	28	ARG	CA-CB	5.36	1.61	1.53
1	E	56	ARG	CA-CB	5.36	1.62	1.53
1	F	165	TYR	C-N	5.36	1.41	1.33
1	I	182	ARG	CZ-NH2	5.36	1.40	1.33
1	E	182	ARG	CZ-NH2	5.36	1.40	1.33
1	H	165	TYR	C-N	5.36	1.41	1.33
1	B	28	ARG	CA-CB	5.35	1.61	1.53
1	B	165	TYR	C-N	5.35	1.41	1.33
1	A	28	ARG	CA-CB	5.35	1.61	1.53
1	G	56	ARG	CA-CB	5.35	1.62	1.53
1	B	152	LEU	CA-C	-5.35	1.45	1.52
1	D	165	TYR	C-N	5.35	1.41	1.33
1	F	28	ARG	CA-CB	5.35	1.61	1.53
1	G	165	TYR	C-N	5.35	1.41	1.33
1	I	28	ARG	CA-CB	5.35	1.61	1.53
1	C	165	TYR	C-N	5.35	1.41	1.33
1	D	152	LEU	CA-C	-5.34	1.45	1.52
1	A	152	LEU	CA-C	-5.34	1.45	1.52
1	A	182	ARG	CZ-NH2	5.34	1.40	1.33
1	E	165	TYR	C-N	5.34	1.41	1.33
1	F	152	LEU	CA-C	-5.34	1.45	1.52
1	B	182	ARG	CZ-NH2	5.34	1.40	1.33
1	C	152	LEU	CA-C	-5.33	1.45	1.52
1	H	28	ARG	CA-CB	5.33	1.61	1.53
1	E	152	LEU	CA-C	-5.32	1.45	1.52
1	F	182	ARG	CZ-NH2	5.32	1.40	1.33
1	D	182	ARG	CZ-NH2	5.32	1.40	1.33
1	D	28	ARG	CA-CB	5.31	1.61	1.53
1	I	212	GLY	C-N	5.31	1.40	1.33
1	C	182	ARG	CZ-NH2	5.31	1.40	1.33
1	F	220	ALA	C-N	5.29	1.41	1.33
1	I	220	ALA	C-N	5.28	1.41	1.33
1	A	212	GLY	C-N	5.26	1.40	1.33
1	D	134	TRP	N-CA	-5.26	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	134	TRP	N-CA	-5.26	1.39	1.46
1	H	123	ILE	C-O	-5.26	1.18	1.24
1	C	220	ALA	C-N	5.26	1.41	1.33
1	E	212	GLY	C-N	5.26	1.40	1.33
1	D	123	ILE	C-O	-5.25	1.18	1.24
1	I	123	ILE	C-O	-5.25	1.18	1.24
1	G	123	ILE	C-O	-5.25	1.18	1.24
1	B	123	ILE	C-O	-5.25	1.18	1.24
1	B	212	GLY	C-N	5.25	1.40	1.33
1	A	123	ILE	C-O	-5.25	1.18	1.24
1	F	123	ILE	C-O	-5.24	1.18	1.24
1	C	123	ILE	C-O	-5.24	1.18	1.24
1	C	212	GLY	C-N	5.24	1.40	1.33
1	E	123	ILE	C-O	-5.24	1.18	1.24
1	G	97	GLY	C-N	-5.23	1.27	1.33
1	G	51	THR	CB-OG1	-5.23	1.35	1.43
1	B	220	ALA	C-N	5.23	1.41	1.33
1	H	51	THR	CB-OG1	-5.23	1.35	1.43
1	B	51	THR	CB-OG1	-5.23	1.35	1.43
1	C	51	THR	CB-OG1	-5.23	1.35	1.43
1	D	51	THR	CB-OG1	-5.23	1.35	1.43
1	F	51	THR	CB-OG1	-5.23	1.35	1.43
1	I	51	THR	CB-OG1	-5.23	1.35	1.43
1	A	51	THR	CB-OG1	-5.23	1.35	1.43
1	G	212	GLY	C-N	5.23	1.40	1.33
1	E	51	THR	CB-OG1	-5.22	1.35	1.43
1	B	134	TRP	N-CA	-5.21	1.40	1.46
1	H	220	ALA	C-N	5.21	1.41	1.33
1	I	134	TRP	N-CA	-5.21	1.40	1.46
1	F	212	GLY	C-N	5.21	1.40	1.33
1	H	124	ASN	CA-CB	5.21	1.60	1.53
1	H	212	GLY	C-N	5.21	1.40	1.33
1	D	220	ALA	C-N	5.21	1.41	1.33
1	A	97	GLY	C-N	-5.20	1.27	1.33
1	D	212	GLY	C-N	5.20	1.40	1.33
1	G	220	ALA	C-N	5.20	1.41	1.33
1	H	97	GLY	C-N	-5.20	1.27	1.33
1	F	97	GLY	C-N	-5.19	1.27	1.33
1	B	97	GLY	C-N	-5.19	1.27	1.33
1	E	97	GLY	C-N	-5.19	1.27	1.33
1	E	220	ALA	C-N	5.19	1.41	1.33
1	D	97	GLY	C-N	-5.19	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	134	TRP	N-CA	-5.18	1.40	1.46
1	I	124	ASN	CA-CB	5.18	1.60	1.53
1	C	97	GLY	C-N	-5.18	1.27	1.33
1	G	124	ASN	CA-CB	5.18	1.60	1.53
1	I	97	GLY	C-N	-5.18	1.27	1.33
1	B	124	ASN	CA-CB	5.17	1.60	1.53
1	C	124	ASN	CA-CB	5.17	1.60	1.53
1	D	124	ASN	CA-CB	5.17	1.60	1.53
1	H	134	TRP	N-CA	-5.17	1.40	1.46
1	C	134	TRP	N-CA	-5.17	1.40	1.46
1	E	134	TRP	N-CA	-5.17	1.40	1.46
1	A	220	ALA	C-N	5.17	1.41	1.33
1	E	124	ASN	CA-CB	5.17	1.60	1.53
1	A	22	ALA	CA-C	-5.16	1.46	1.52
1	A	134	TRP	N-CA	-5.15	1.40	1.46
1	F	124	ASN	CA-CB	5.14	1.60	1.53
1	I	22	ALA	CA-C	-5.14	1.46	1.52
1	E	33	GLY	CA-C	-5.13	1.44	1.51
1	B	22	ALA	CA-C	-5.12	1.46	1.52
1	A	124	ASN	CA-CB	5.12	1.60	1.53
1	C	33	GLY	CA-C	-5.12	1.44	1.51
1	D	33	GLY	CA-C	-5.12	1.44	1.51
1	G	33	GLY	CA-C	-5.12	1.44	1.51
1	D	22	ALA	CA-C	-5.12	1.46	1.52
1	I	33	GLY	CA-C	-5.11	1.44	1.51
1	F	33	GLY	CA-C	-5.11	1.44	1.51
1	C	22	ALA	CA-C	-5.11	1.46	1.52
1	E	22	ALA	CA-C	-5.11	1.46	1.52
1	B	33	GLY	CA-C	-5.10	1.44	1.51
1	G	22	ALA	CA-C	-5.10	1.46	1.52
1	H	22	ALA	CA-C	-5.10	1.46	1.52
1	D	103	LEU	CA-C	5.10	1.59	1.52
1	I	103	LEU	CA-C	5.09	1.59	1.52
1	A	33	GLY	CA-C	-5.09	1.44	1.51
1	A	103	LEU	CA-C	5.09	1.59	1.52
1	F	22	ALA	CA-C	-5.09	1.46	1.52
1	F	103	LEU	CA-C	5.08	1.59	1.52
1	B	103	LEU	CA-C	5.08	1.59	1.52
1	H	103	LEU	CA-C	5.08	1.59	1.52
1	C	103	LEU	CA-C	5.08	1.59	1.52
1	F	109	LYS	C-N	5.08	1.40	1.33
1	H	33	GLY	CA-C	-5.08	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	103	LEU	CA-C	5.06	1.59	1.52
1	E	109	LYS	C-N	5.05	1.40	1.33
1	C	109	LYS	C-N	5.05	1.40	1.33
1	G	103	LEU	CA-C	5.05	1.59	1.52
1	E	170	LYS	CA-CB	5.02	1.61	1.53
1	H	170	LYS	CA-CB	5.02	1.61	1.53
1	B	109	LYS	C-N	5.02	1.40	1.33
1	G	109	LYS	C-N	5.02	1.40	1.33
1	D	109	LYS	C-N	5.01	1.40	1.33
1	F	118	ILE	N-CA	-5.01	1.40	1.46
1	A	109	LYS	C-N	5.01	1.40	1.33
1	H	109	LYS	C-N	5.01	1.40	1.33
1	I	109	LYS	C-N	5.00	1.40	1.33

All (1271) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	88	ASP	CA-CB-CG	10.36	122.96	112.60
1	D	88	ASP	CA-CB-CG	10.35	122.95	112.60
1	C	88	ASP	CA-CB-CG	10.35	122.95	112.60
1	A	88	ASP	CA-CB-CG	10.34	122.94	112.60
1	B	88	ASP	CA-CB-CG	10.33	122.93	112.60
1	H	88	ASP	CA-CB-CG	10.33	122.93	112.60
1	I	88	ASP	CA-CB-CG	10.32	122.92	112.60
1	G	88	ASP	CA-CB-CG	10.31	122.91	112.60
1	E	88	ASP	CA-CB-CG	10.30	122.90	112.60
1	F	100	ALA	CA-C-N	10.02	133.87	120.65
1	F	100	ALA	C-N-CA	10.02	133.87	120.65
1	E	100	ALA	CA-C-N	10.00	133.85	120.65
1	E	100	ALA	C-N-CA	10.00	133.85	120.65
1	D	100	ALA	CA-C-N	10.00	133.85	120.65
1	D	100	ALA	C-N-CA	10.00	133.85	120.65
1	C	100	ALA	CA-C-N	9.99	133.84	120.65
1	C	100	ALA	C-N-CA	9.99	133.84	120.65
1	B	100	ALA	CA-C-N	9.99	133.84	120.65
1	B	100	ALA	C-N-CA	9.99	133.84	120.65
1	G	100	ALA	CA-C-N	9.99	133.84	120.65
1	G	100	ALA	C-N-CA	9.99	133.84	120.65
1	H	100	ALA	CA-C-N	9.99	133.84	120.65
1	H	100	ALA	C-N-CA	9.99	133.84	120.65
1	I	100	ALA	CA-C-N	9.99	133.84	120.65
1	I	100	ALA	C-N-CA	9.99	133.84	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	ALA	CA-C-N	9.99	133.83	120.65
1	A	100	ALA	C-N-CA	9.99	133.83	120.65
1	E	110	VAL	CA-C-N	8.76	133.31	120.87
1	E	110	VAL	C-N-CA	8.76	133.31	120.87
1	G	110	VAL	CA-C-N	8.76	133.30	120.87
1	G	110	VAL	C-N-CA	8.76	133.30	120.87
1	H	110	VAL	CA-C-N	8.76	133.30	120.87
1	H	110	VAL	C-N-CA	8.76	133.30	120.87
1	A	110	VAL	CA-C-N	8.74	133.29	120.87
1	A	110	VAL	C-N-CA	8.74	133.29	120.87
1	B	110	VAL	CA-C-N	8.74	133.28	120.87
1	B	110	VAL	C-N-CA	8.74	133.28	120.87
1	I	110	VAL	CA-C-N	8.74	133.28	120.87
1	I	110	VAL	C-N-CA	8.74	133.28	120.87
1	D	110	VAL	CA-C-N	8.74	133.28	120.87
1	D	110	VAL	C-N-CA	8.74	133.28	120.87
1	C	110	VAL	CA-C-N	8.73	133.26	120.87
1	C	110	VAL	C-N-CA	8.73	133.26	120.87
1	D	225	PHE	CA-C-N	8.72	131.97	120.28
1	D	225	PHE	C-N-CA	8.72	131.97	120.28
1	G	225	PHE	CA-C-N	8.72	131.96	120.28
1	G	225	PHE	C-N-CA	8.72	131.96	120.28
1	E	225	PHE	CA-C-N	8.72	131.96	120.28
1	E	225	PHE	C-N-CA	8.72	131.96	120.28
1	A	225	PHE	CA-C-N	8.71	131.96	120.28
1	A	225	PHE	C-N-CA	8.71	131.96	120.28
1	B	225	PHE	CA-C-N	8.71	131.95	120.28
1	B	225	PHE	C-N-CA	8.71	131.95	120.28
1	F	110	VAL	CA-C-N	8.71	133.24	120.87
1	F	110	VAL	C-N-CA	8.71	133.24	120.87
1	H	225	PHE	CA-C-N	8.71	131.95	120.28
1	H	225	PHE	C-N-CA	8.71	131.95	120.28
1	F	225	PHE	CA-C-N	8.71	131.95	120.28
1	F	225	PHE	C-N-CA	8.71	131.95	120.28
1	C	225	PHE	CA-C-N	8.70	131.94	120.28
1	C	225	PHE	C-N-CA	8.70	131.94	120.28
1	I	225	PHE	CA-C-N	8.70	131.94	120.28
1	I	225	PHE	C-N-CA	8.70	131.94	120.28
1	H	124	ASN	CA-C-O	-8.51	112.58	119.99
1	I	124	ASN	CA-C-O	-8.48	112.61	119.99
1	A	124	ASN	CA-C-O	-8.48	112.61	119.99
1	C	124	ASN	CA-C-O	-8.48	112.61	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	124	ASN	CA-C-O	-8.46	112.63	119.99
1	B	124	ASN	CA-C-O	-8.46	112.63	119.99
1	E	124	ASN	CA-C-O	-8.46	112.63	119.99
1	D	124	ASN	CA-C-O	-8.45	112.64	119.99
1	G	124	ASN	CA-C-O	-8.44	112.65	119.99
1	H	193	TRP	CA-C-N	8.42	131.91	120.38
1	H	193	TRP	C-N-CA	8.42	131.91	120.38
1	C	193	TRP	CA-C-N	8.42	131.91	120.38
1	C	193	TRP	C-N-CA	8.42	131.91	120.38
1	E	193	TRP	CA-C-N	8.41	131.91	120.38
1	E	193	TRP	C-N-CA	8.41	131.91	120.38
1	B	193	TRP	CA-C-N	8.41	131.91	120.38
1	B	193	TRP	C-N-CA	8.41	131.91	120.38
1	A	193	TRP	CA-C-N	8.41	131.91	120.38
1	A	193	TRP	C-N-CA	8.41	131.91	120.38
1	I	193	TRP	CA-C-N	8.41	131.91	120.38
1	I	193	TRP	C-N-CA	8.41	131.91	120.38
1	F	193	TRP	CA-C-N	8.41	131.90	120.38
1	F	193	TRP	C-N-CA	8.41	131.90	120.38
1	G	193	TRP	CA-C-N	8.41	131.90	120.38
1	G	193	TRP	C-N-CA	8.41	131.90	120.38
1	D	193	TRP	CA-C-N	8.41	131.90	120.38
1	D	193	TRP	C-N-CA	8.41	131.90	120.38
1	I	93	HIS	CA-CB-CG	8.35	122.15	113.80
1	F	93	HIS	CA-CB-CG	8.33	122.13	113.80
1	D	93	HIS	CA-CB-CG	8.32	122.12	113.80
1	B	93	HIS	CA-CB-CG	8.31	122.11	113.80
1	E	93	HIS	CA-CB-CG	8.30	122.10	113.80
1	H	93	HIS	CA-CB-CG	8.28	122.08	113.80
1	F	184	ARG	NE-CZ-NH2	8.28	126.65	119.20
1	G	93	HIS	CA-CB-CG	8.28	122.08	113.80
1	A	93	HIS	CA-CB-CG	8.28	122.08	113.80
1	C	93	HIS	CA-CB-CG	8.28	122.08	113.80
1	A	184	ARG	NE-CZ-NH2	8.25	126.63	119.20
1	E	184	ARG	NE-CZ-NH2	8.25	126.63	119.20
1	C	184	ARG	NE-CZ-NH2	8.25	126.62	119.20
1	B	184	ARG	NE-CZ-NH2	8.24	126.62	119.20
1	H	184	ARG	NE-CZ-NH2	8.23	126.61	119.20
1	I	184	ARG	NE-CZ-NH2	8.23	126.61	119.20
1	D	184	ARG	NE-CZ-NH2	8.23	126.61	119.20
1	G	184	ARG	NE-CZ-NH2	8.20	126.58	119.20
1	E	78	PRO	CA-C-N	8.07	130.23	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	78	PRO	C-N-CA	8.07	130.23	120.14
1	D	78	PRO	CA-C-N	8.05	130.21	120.14
1	D	78	PRO	C-N-CA	8.05	130.21	120.14
1	D	158	TYR	CA-C-N	8.05	127.61	119.24
1	D	158	TYR	C-N-CA	8.05	127.61	119.24
1	E	158	TYR	CA-C-N	8.04	127.61	119.24
1	E	158	TYR	C-N-CA	8.04	127.61	119.24
1	C	78	PRO	CA-C-N	8.04	130.19	120.14
1	C	78	PRO	C-N-CA	8.04	130.19	120.14
1	B	78	PRO	CA-C-N	8.04	130.18	120.14
1	B	78	PRO	C-N-CA	8.04	130.18	120.14
1	C	158	TYR	CA-C-N	8.04	127.60	119.24
1	C	158	TYR	C-N-CA	8.04	127.60	119.24
1	F	78	PRO	CA-C-N	8.04	130.18	120.14
1	F	78	PRO	C-N-CA	8.04	130.18	120.14
1	A	78	PRO	CA-C-N	8.03	130.18	120.14
1	A	78	PRO	C-N-CA	8.03	130.18	120.14
1	G	78	PRO	CA-C-N	8.03	130.18	120.14
1	G	78	PRO	C-N-CA	8.03	130.18	120.14
1	G	158	TYR	CA-C-N	8.03	127.59	119.24
1	G	158	TYR	C-N-CA	8.03	127.59	119.24
1	B	158	TYR	CA-C-N	8.02	127.58	119.24
1	B	158	TYR	C-N-CA	8.02	127.58	119.24
1	I	78	PRO	CA-C-N	8.01	130.16	120.14
1	I	78	PRO	C-N-CA	8.01	130.16	120.14
1	I	158	TYR	CA-C-N	8.01	127.57	119.24
1	I	158	TYR	C-N-CA	8.01	127.57	119.24
1	H	158	TYR	CA-C-N	8.01	127.57	119.24
1	H	158	TYR	C-N-CA	8.01	127.57	119.24
1	A	158	TYR	CA-C-N	8.00	127.56	119.24
1	A	158	TYR	C-N-CA	8.00	127.56	119.24
1	H	78	PRO	CA-C-N	8.00	130.14	120.14
1	H	78	PRO	C-N-CA	8.00	130.14	120.14
1	F	158	TYR	CA-C-N	8.00	127.56	119.24
1	F	158	TYR	C-N-CA	8.00	127.56	119.24
1	F	43	TYR	O-C-N	7.98	131.25	122.15
1	I	43	TYR	O-C-N	7.95	131.21	122.15
1	B	43	TYR	O-C-N	7.94	131.21	122.15
1	G	43	TYR	O-C-N	7.94	131.21	122.15
1	D	43	TYR	O-C-N	7.92	131.18	122.15
1	A	43	TYR	O-C-N	7.92	131.17	122.15
1	C	43	TYR	O-C-N	7.91	131.17	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	43	TYR	O-C-N	7.91	131.17	122.15
1	H	43	TYR	O-C-N	7.88	131.13	122.15
1	I	95	LEU	CA-C-O	-7.69	112.74	120.82
1	A	95	LEU	CA-C-O	-7.69	112.74	120.82
1	H	149	GLU	CA-C-N	7.69	131.35	120.28
1	H	149	GLU	C-N-CA	7.69	131.35	120.28
1	D	95	LEU	CA-C-O	-7.69	112.75	120.82
1	F	95	LEU	CA-C-O	-7.69	112.75	120.82
1	E	149	GLU	CA-C-N	7.68	131.35	120.28
1	E	149	GLU	C-N-CA	7.68	131.35	120.28
1	B	95	LEU	CA-C-O	-7.68	112.76	120.82
1	C	95	LEU	CA-C-O	-7.68	112.76	120.82
1	B	149	GLU	CA-C-N	7.67	131.32	120.28
1	B	149	GLU	C-N-CA	7.67	131.32	120.28
1	D	149	GLU	CA-C-N	7.67	131.32	120.28
1	D	149	GLU	C-N-CA	7.67	131.32	120.28
1	H	95	LEU	CA-C-O	-7.67	112.77	120.82
1	G	149	GLU	CA-C-N	7.66	131.31	120.28
1	G	149	GLU	C-N-CA	7.66	131.31	120.28
1	A	149	GLU	CA-C-N	7.66	131.31	120.28
1	A	149	GLU	C-N-CA	7.66	131.31	120.28
1	E	95	LEU	CA-C-O	-7.66	112.78	120.82
1	G	95	LEU	CA-C-O	-7.65	112.78	120.82
1	I	149	GLU	CA-C-N	7.65	131.30	120.28
1	I	149	GLU	C-N-CA	7.65	131.30	120.28
1	C	149	GLU	CA-C-N	7.65	131.29	120.28
1	C	149	GLU	C-N-CA	7.65	131.29	120.28
1	F	149	GLU	CA-C-N	7.63	131.27	120.28
1	F	149	GLU	C-N-CA	7.63	131.27	120.28
1	G	73	TYR	N-CA-CB	7.59	121.40	109.71
1	D	210	SER	CA-C-N	7.59	136.03	121.54
1	D	210	SER	C-N-CA	7.59	136.03	121.54
1	I	210	SER	CA-C-N	7.58	136.02	121.54
1	I	210	SER	C-N-CA	7.58	136.02	121.54
1	H	210	SER	CA-C-N	7.57	136.00	121.54
1	H	210	SER	C-N-CA	7.57	136.00	121.54
1	E	210	SER	CA-C-N	7.57	135.99	121.54
1	E	210	SER	C-N-CA	7.57	135.99	121.54
1	B	210	SER	CA-C-N	7.57	135.99	121.54
1	B	210	SER	C-N-CA	7.57	135.99	121.54
1	B	73	TYR	N-CA-CB	7.56	121.36	109.71
1	F	73	TYR	N-CA-CB	7.56	121.35	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	73	TYR	N-CA-CB	7.56	121.35	109.71
1	F	210	SER	CA-C-N	7.56	135.98	121.54
1	F	210	SER	C-N-CA	7.56	135.98	121.54
1	A	210	SER	CA-C-N	7.55	135.97	121.54
1	A	210	SER	C-N-CA	7.55	135.97	121.54
1	C	210	SER	CA-C-N	7.55	135.96	121.54
1	C	210	SER	C-N-CA	7.55	135.96	121.54
1	H	73	TYR	N-CA-CB	7.55	121.34	109.71
1	C	73	TYR	N-CA-CB	7.55	121.33	109.71
1	I	73	TYR	N-CA-CB	7.55	121.33	109.71
1	D	73	TYR	N-CA-CB	7.55	121.33	109.71
1	G	210	SER	CA-C-N	7.54	135.94	121.54
1	G	210	SER	C-N-CA	7.54	135.94	121.54
1	A	73	TYR	N-CA-CB	7.53	121.30	109.71
1	D	43	TYR	CA-C-O	-7.50	112.47	120.42
1	I	43	TYR	CA-C-O	-7.49	112.48	120.42
1	B	43	TYR	CA-C-O	-7.49	112.48	120.42
1	C	43	TYR	CA-C-O	-7.48	112.49	120.42
1	D	74	ASN	CA-C-O	-7.48	112.15	120.60
1	F	43	TYR	CA-C-O	-7.48	112.49	120.42
1	G	43	TYR	CA-C-O	-7.45	112.52	120.42
1	H	74	ASN	CA-C-O	-7.45	112.18	120.60
1	B	74	ASN	CA-C-O	-7.45	112.18	120.60
1	F	74	ASN	CA-C-O	-7.45	112.18	120.60
1	E	43	TYR	CA-C-O	-7.45	112.53	120.42
1	D	218	VAL	CA-C-N	7.44	135.76	121.54
1	D	218	VAL	C-N-CA	7.44	135.76	121.54
1	A	43	TYR	CA-C-O	-7.44	112.53	120.42
1	H	43	TYR	CA-C-O	-7.44	112.53	120.42
1	A	74	ASN	CA-C-O	-7.44	112.20	120.60
1	I	74	ASN	CA-C-O	-7.44	112.20	120.60
1	E	218	VAL	CA-C-N	7.43	135.74	121.54
1	E	218	VAL	C-N-CA	7.43	135.74	121.54
1	G	74	ASN	CA-C-O	-7.43	112.20	120.60
1	F	218	VAL	CA-C-N	7.43	135.72	121.54
1	F	218	VAL	C-N-CA	7.43	135.72	121.54
1	H	218	VAL	CA-C-N	7.43	135.72	121.54
1	H	218	VAL	C-N-CA	7.43	135.72	121.54
1	I	218	VAL	CA-C-N	7.43	135.72	121.54
1	I	218	VAL	C-N-CA	7.43	135.72	121.54
1	C	218	VAL	CA-C-N	7.42	135.72	121.54
1	C	218	VAL	C-N-CA	7.42	135.72	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	VAL	CA-C-N	7.42	135.72	121.54
1	B	218	VAL	C-N-CA	7.42	135.72	121.54
1	C	74	ASN	CA-C-O	-7.42	112.22	120.60
1	G	218	VAL	CA-C-N	7.42	135.71	121.54
1	G	218	VAL	C-N-CA	7.42	135.71	121.54
1	H	98	PHE	N-CA-CB	7.42	120.76	110.01
1	I	98	PHE	N-CA-CB	7.41	120.76	110.01
1	A	218	VAL	CA-C-N	7.41	135.69	121.54
1	A	218	VAL	C-N-CA	7.41	135.69	121.54
1	D	98	PHE	N-CA-CB	7.41	120.75	110.01
1	E	74	ASN	CA-C-O	-7.41	112.23	120.60
1	C	98	PHE	N-CA-CB	7.41	120.75	110.01
1	G	98	PHE	N-CA-CB	7.41	120.75	110.01
1	B	98	PHE	N-CA-CB	7.40	120.74	110.01
1	F	98	PHE	N-CA-CB	7.40	120.74	110.01
1	H	155	PHE	N-CA-C	-7.40	104.40	113.50
1	E	98	PHE	N-CA-CB	7.40	120.74	110.01
1	A	98	PHE	N-CA-CB	7.40	120.74	110.01
1	D	155	PHE	N-CA-C	-7.39	104.41	113.50
1	E	155	PHE	N-CA-C	-7.39	104.41	113.50
1	F	155	PHE	N-CA-C	-7.39	104.42	113.50
1	C	155	PHE	N-CA-C	-7.38	104.43	113.50
1	B	155	PHE	N-CA-C	-7.37	104.43	113.50
1	A	155	PHE	N-CA-C	-7.37	104.43	113.50
1	I	155	PHE	N-CA-C	-7.37	104.44	113.50
1	G	155	PHE	N-CA-C	-7.36	104.45	113.50
1	E	105	GLU	CA-C-N	7.28	130.36	120.54
1	E	105	GLU	C-N-CA	7.28	130.36	120.54
1	C	105	GLU	CA-C-N	7.27	130.36	120.54
1	C	105	GLU	C-N-CA	7.27	130.36	120.54
1	D	105	GLU	CA-C-N	7.26	130.35	120.54
1	D	105	GLU	C-N-CA	7.26	130.35	120.54
1	I	105	GLU	CA-C-N	7.26	130.34	120.54
1	I	105	GLU	C-N-CA	7.26	130.34	120.54
1	B	105	GLU	CA-C-N	7.25	130.33	120.54
1	B	105	GLU	C-N-CA	7.25	130.33	120.54
1	A	105	GLU	CA-C-N	7.25	130.33	120.54
1	A	105	GLU	C-N-CA	7.25	130.33	120.54
1	H	105	GLU	CA-C-N	7.25	130.33	120.54
1	H	105	GLU	C-N-CA	7.25	130.33	120.54
1	F	105	GLU	CA-C-N	7.25	130.33	120.54
1	F	105	GLU	C-N-CA	7.25	130.33	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	105	GLU	CA-C-N	7.25	130.32	120.54
1	G	105	GLU	C-N-CA	7.25	130.32	120.54
1	C	137	GLY	O-C-N	7.23	129.91	122.75
1	D	137	GLY	O-C-N	7.23	129.91	122.75
1	F	137	GLY	O-C-N	7.22	129.90	122.75
1	E	137	GLY	O-C-N	7.21	129.89	122.75
1	B	137	GLY	O-C-N	7.21	129.89	122.75
1	A	137	GLY	O-C-N	7.21	129.89	122.75
1	H	137	GLY	O-C-N	7.21	129.89	122.75
1	G	137	GLY	O-C-N	7.21	129.89	122.75
1	I	137	GLY	O-C-N	7.20	129.88	122.75
1	H	134	TRP	N-CA-C	7.20	120.04	111.33
1	G	134	TRP	N-CA-C	7.19	120.03	111.33
1	E	134	TRP	N-CA-C	7.18	120.02	111.33
1	B	134	TRP	N-CA-C	7.18	120.01	111.33
1	A	134	TRP	N-CA-C	7.18	120.01	111.33
1	D	134	TRP	N-CA-C	7.18	120.01	111.33
1	I	134	TRP	N-CA-C	7.17	120.01	111.33
1	F	134	TRP	N-CA-C	7.16	119.99	111.33
1	C	134	TRP	N-CA-C	7.15	119.98	111.33
1	F	161	ALA	CA-C-N	7.07	130.14	120.46
1	F	161	ALA	C-N-CA	7.07	130.14	120.46
1	H	161	ALA	CA-C-N	7.05	130.12	120.46
1	H	161	ALA	C-N-CA	7.05	130.12	120.46
1	C	161	ALA	CA-C-N	7.05	130.12	120.46
1	C	161	ALA	C-N-CA	7.05	130.12	120.46
1	E	161	ALA	CA-C-N	7.04	130.11	120.46
1	E	161	ALA	C-N-CA	7.04	130.11	120.46
1	B	161	ALA	CA-C-N	7.02	130.08	120.46
1	B	161	ALA	C-N-CA	7.02	130.08	120.46
1	G	161	ALA	CA-C-N	7.02	130.08	120.46
1	G	161	ALA	C-N-CA	7.02	130.08	120.46
1	A	161	ALA	CA-C-N	7.01	130.07	120.46
1	A	161	ALA	C-N-CA	7.01	130.07	120.46
1	I	161	ALA	CA-C-N	7.01	130.06	120.46
1	I	161	ALA	C-N-CA	7.01	130.06	120.46
1	D	161	ALA	CA-C-N	6.99	130.03	120.46
1	D	161	ALA	C-N-CA	6.99	130.03	120.46
1	I	154	THR	N-CA-C	6.86	118.75	111.28
1	H	154	THR	N-CA-C	6.85	118.75	111.28
1	E	154	THR	N-CA-C	6.84	118.74	111.28
1	F	154	THR	N-CA-C	6.84	118.74	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	THR	N-CA-C	6.84	118.73	111.28
1	C	154	THR	N-CA-C	6.83	118.73	111.28
1	D	154	THR	N-CA-C	6.83	118.72	111.28
1	G	154	THR	N-CA-C	6.82	118.72	111.28
1	A	154	THR	N-CA-C	6.82	118.72	111.28
1	F	7	HIS	CE1-NE2-CD2	-6.80	102.20	109.00
1	D	58	GLU	N-CA-CB	6.77	119.92	110.17
1	A	7	HIS	CE1-NE2-CD2	-6.77	102.23	109.00
1	B	7	HIS	CE1-NE2-CD2	-6.77	102.23	109.00
1	G	7	HIS	CE1-NE2-CD2	-6.77	102.23	109.00
1	G	58	GLU	N-CA-CB	6.76	119.91	110.17
1	C	7	HIS	CE1-NE2-CD2	-6.76	102.24	109.00
1	H	7	HIS	CE1-NE2-CD2	-6.76	102.24	109.00
1	H	58	GLU	N-CA-CB	6.76	119.90	110.17
1	C	58	GLU	N-CA-CB	6.76	119.90	110.17
1	F	58	GLU	N-CA-CB	6.75	119.90	110.17
1	A	58	GLU	N-CA-CB	6.75	119.89	110.17
1	D	7	HIS	CE1-NE2-CD2	-6.75	102.25	109.00
1	E	58	GLU	N-CA-CB	6.75	119.89	110.17
1	E	7	HIS	CE1-NE2-CD2	-6.75	102.25	109.00
1	B	58	GLU	N-CA-CB	6.75	119.88	110.17
1	I	58	GLU	N-CA-CB	6.74	119.88	110.17
1	H	163	GLY	CA-C-N	6.73	129.68	120.46
1	H	163	GLY	C-N-CA	6.73	129.68	120.46
1	A	163	GLY	CA-C-N	6.73	129.68	120.46
1	A	163	GLY	C-N-CA	6.73	129.68	120.46
1	E	163	GLY	CA-C-N	6.72	129.67	120.46
1	E	163	GLY	C-N-CA	6.72	129.67	120.46
1	I	7	HIS	CE1-NE2-CD2	-6.72	102.28	109.00
1	B	163	GLY	CA-C-N	6.72	129.66	120.46
1	B	163	GLY	C-N-CA	6.72	129.66	120.46
1	D	163	GLY	CA-C-N	6.72	129.66	120.46
1	D	163	GLY	C-N-CA	6.72	129.66	120.46
1	C	163	GLY	CA-C-N	6.72	129.66	120.46
1	C	163	GLY	C-N-CA	6.72	129.66	120.46
1	G	163	GLY	CA-C-N	6.71	129.66	120.46
1	G	163	GLY	C-N-CA	6.71	129.66	120.46
1	F	163	GLY	CA-C-N	6.70	129.64	120.46
1	F	163	GLY	C-N-CA	6.70	129.64	120.46
1	I	163	GLY	CA-C-N	6.68	129.61	120.46
1	I	163	GLY	C-N-CA	6.68	129.61	120.46
1	A	224	ASP	CA-C-N	6.65	129.09	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	ASP	C-N-CA	6.65	129.09	120.44
1	D	224	ASP	CA-C-N	6.64	129.07	120.44
1	D	224	ASP	C-N-CA	6.64	129.07	120.44
1	F	224	ASP	CA-C-N	6.64	129.07	120.44
1	F	224	ASP	C-N-CA	6.64	129.07	120.44
1	H	224	ASP	CA-C-N	6.64	129.07	120.44
1	H	224	ASP	C-N-CA	6.64	129.07	120.44
1	E	224	ASP	CA-C-N	6.63	129.06	120.44
1	E	224	ASP	C-N-CA	6.63	129.06	120.44
1	G	224	ASP	CA-C-N	6.63	129.06	120.44
1	G	224	ASP	C-N-CA	6.63	129.06	120.44
1	B	224	ASP	CA-C-N	6.63	129.06	120.44
1	B	224	ASP	C-N-CA	6.63	129.06	120.44
1	I	224	ASP	CA-C-N	6.63	129.06	120.44
1	I	224	ASP	C-N-CA	6.63	129.06	120.44
1	C	224	ASP	CA-C-N	6.63	129.06	120.44
1	C	224	ASP	C-N-CA	6.63	129.06	120.44
1	H	130	ASN	CA-CB-CG	-6.62	105.98	112.60
1	B	130	ASN	CA-CB-CG	-6.61	105.99	112.60
1	D	130	ASN	CA-CB-CG	-6.60	106.00	112.60
1	E	130	ASN	CA-CB-CG	-6.60	106.00	112.60
1	F	130	ASN	CA-CB-CG	-6.59	106.01	112.60
1	I	130	ASN	CA-CB-CG	-6.59	106.01	112.60
1	C	130	ASN	CA-CB-CG	-6.58	106.02	112.60
1	A	130	ASN	CA-CB-CG	-6.58	106.02	112.60
1	E	137	GLY	CA-C-N	6.57	129.08	120.28
1	E	137	GLY	C-N-CA	6.57	129.08	120.28
1	G	130	ASN	CA-CB-CG	-6.57	106.03	112.60
1	G	137	GLY	CA-C-N	6.56	129.07	120.28
1	G	137	GLY	C-N-CA	6.56	129.07	120.28
1	F	71	THR	CA-CB-CG2	6.56	121.65	110.50
1	F	137	GLY	CA-C-N	6.56	129.07	120.28
1	F	137	GLY	C-N-CA	6.56	129.07	120.28
1	B	137	GLY	CA-C-N	6.56	129.07	120.28
1	B	137	GLY	C-N-CA	6.56	129.07	120.28
1	G	71	THR	CA-CB-CG2	6.56	121.65	110.50
1	I	71	THR	CA-CB-CG2	6.56	121.65	110.50
1	I	137	GLY	CA-C-N	6.56	129.07	120.28
1	I	137	GLY	C-N-CA	6.56	129.07	120.28
1	B	71	THR	CA-CB-CG2	6.55	121.64	110.50
1	E	71	THR	CA-CB-CG2	6.55	121.64	110.50
1	H	137	GLY	CA-C-N	6.55	129.06	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	137	GLY	C-N-CA	6.55	129.06	120.28
1	D	71	THR	CA-CB-CG2	6.55	121.63	110.50
1	A	71	THR	CA-CB-CG2	6.54	121.62	110.50
1	H	71	THR	CA-CB-CG2	6.54	121.62	110.50
1	C	71	THR	CA-CB-CG2	6.54	121.62	110.50
1	D	137	GLY	CA-C-N	6.54	129.05	120.28
1	D	137	GLY	C-N-CA	6.54	129.05	120.28
1	A	137	GLY	CA-C-N	6.54	129.04	120.28
1	A	137	GLY	C-N-CA	6.54	129.04	120.28
1	C	137	GLY	CA-C-N	6.53	129.03	120.28
1	C	137	GLY	C-N-CA	6.53	129.03	120.28
1	I	135	ASN	CA-CB-CG	6.53	119.13	112.60
1	H	135	ASN	CA-CB-CG	6.51	119.11	112.60
1	D	135	ASN	CA-CB-CG	6.51	119.11	112.60
1	E	135	ASN	CA-CB-CG	6.51	119.11	112.60
1	A	135	ASN	CA-CB-CG	6.51	119.11	112.60
1	B	135	ASN	CA-CB-CG	6.50	119.10	112.60
1	G	135	ASN	CA-CB-CG	6.50	119.10	112.60
1	F	135	ASN	CA-CB-CG	6.50	119.10	112.60
1	E	54	ALA	CA-C-N	6.49	129.46	120.63
1	E	54	ALA	C-N-CA	6.49	129.46	120.63
1	B	54	ALA	CA-C-N	6.48	129.44	120.63
1	B	54	ALA	C-N-CA	6.48	129.44	120.63
1	F	54	ALA	CA-C-N	6.48	129.44	120.63
1	F	54	ALA	C-N-CA	6.48	129.44	120.63
1	C	54	ALA	CA-C-N	6.47	129.44	120.63
1	C	54	ALA	C-N-CA	6.47	129.44	120.63
1	D	54	ALA	CA-C-N	6.47	129.43	120.63
1	D	54	ALA	C-N-CA	6.47	129.43	120.63
1	A	54	ALA	CA-C-N	6.47	129.43	120.63
1	A	54	ALA	C-N-CA	6.47	129.43	120.63
1	G	54	ALA	CA-C-N	6.47	129.42	120.63
1	G	54	ALA	C-N-CA	6.47	129.42	120.63
1	H	54	ALA	CA-C-N	6.47	129.43	120.63
1	H	54	ALA	C-N-CA	6.47	129.43	120.63
1	C	135	ASN	CA-CB-CG	6.46	119.06	112.60
1	I	54	ALA	CA-C-N	6.46	129.42	120.63
1	I	54	ALA	C-N-CA	6.46	129.42	120.63
1	A	7	HIS	N-CA-C	6.39	116.89	108.07
1	D	7	HIS	N-CA-C	6.39	116.88	108.07
1	F	18	ASP	CA-C-O	-6.38	113.72	119.59
1	C	7	HIS	N-CA-C	6.38	116.87	108.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	18	ASP	CA-C-O	-6.37	113.72	119.59
1	B	7	HIS	N-CA-C	6.37	116.86	108.07
1	B	18	ASP	CA-C-O	-6.37	113.73	119.59
1	G	18	ASP	CA-C-O	-6.37	113.73	119.59
1	A	18	ASP	CA-C-O	-6.37	113.73	119.59
1	E	18	ASP	CA-C-O	-6.37	113.73	119.59
1	H	7	HIS	N-CA-C	6.37	116.86	108.07
1	I	18	ASP	CA-C-O	-6.37	113.73	119.59
1	D	18	ASP	CA-C-O	-6.37	113.73	119.59
1	E	7	HIS	N-CA-C	6.37	116.86	108.07
1	F	7	HIS	N-CA-C	6.36	116.85	108.07
1	H	18	ASP	CA-C-O	-6.36	113.74	119.59
1	E	10	ALA	CA-C-N	6.36	132.16	122.37
1	E	10	ALA	C-N-CA	6.36	132.16	122.37
1	G	7	HIS	N-CA-C	6.36	116.84	108.07
1	G	10	ALA	CA-C-N	6.35	132.15	122.37
1	G	10	ALA	C-N-CA	6.35	132.15	122.37
1	D	10	ALA	CA-C-N	6.34	132.14	122.37
1	D	10	ALA	C-N-CA	6.34	132.14	122.37
1	C	10	ALA	CA-C-N	6.34	132.14	122.37
1	C	10	ALA	C-N-CA	6.34	132.14	122.37
1	I	7	HIS	N-CA-C	6.34	116.82	108.07
1	B	10	ALA	CA-C-N	6.34	132.13	122.37
1	B	10	ALA	C-N-CA	6.34	132.13	122.37
1	A	10	ALA	CA-C-N	6.34	132.13	122.37
1	A	10	ALA	C-N-CA	6.34	132.13	122.37
1	I	10	ALA	CA-C-N	6.34	132.13	122.37
1	I	10	ALA	C-N-CA	6.34	132.13	122.37
1	H	10	ALA	CA-C-N	6.33	132.12	122.37
1	H	10	ALA	C-N-CA	6.33	132.12	122.37
1	F	10	ALA	CA-C-N	6.32	132.10	122.37
1	F	10	ALA	C-N-CA	6.32	132.10	122.37
1	F	7	HIS	CG-CD2-NE2	6.32	113.52	107.20
1	D	7	HIS	CG-CD2-NE2	6.31	113.51	107.20
1	H	7	HIS	CG-CD2-NE2	6.31	113.51	107.20
1	C	7	HIS	CG-CD2-NE2	6.30	113.50	107.20
1	B	7	HIS	CG-CD2-NE2	6.29	113.48	107.20
1	G	7	HIS	CG-CD2-NE2	6.28	113.48	107.20
1	E	7	HIS	CG-CD2-NE2	6.28	113.48	107.20
1	A	7	HIS	CG-CD2-NE2	6.26	113.47	107.20
1	E	38	HIS	CG-CD2-NE2	6.26	113.46	107.20
1	G	38	HIS	CG-CD2-NE2	6.26	113.46	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	7	HIS	CG-CD2-NE2	6.26	113.46	107.20
1	C	38	HIS	CG-CD2-NE2	6.25	113.45	107.20
1	D	38	HIS	CG-CD2-NE2	6.25	113.45	107.20
1	B	38	HIS	CG-CD2-NE2	6.24	113.44	107.20
1	I	38	HIS	CG-CD2-NE2	6.24	113.44	107.20
1	F	184	ARG	NH1-CZ-NH2	-6.24	111.19	119.30
1	G	127	ALA	CB-CA-C	-6.24	101.05	110.90
1	E	184	ARG	NH1-CZ-NH2	-6.23	111.20	119.30
1	F	38	HIS	CG-CD2-NE2	6.23	113.43	107.20
1	C	184	ARG	NH1-CZ-NH2	-6.23	111.20	119.30
1	H	38	HIS	CG-CD2-NE2	6.22	113.42	107.20
1	A	184	ARG	NH1-CZ-NH2	-6.22	111.21	119.30
1	B	184	ARG	NH1-CZ-NH2	-6.22	111.21	119.30
1	D	184	ARG	NH1-CZ-NH2	-6.22	111.21	119.30
1	H	184	ARG	NH1-CZ-NH2	-6.22	111.22	119.30
1	I	184	ARG	NH1-CZ-NH2	-6.22	111.22	119.30
1	D	127	ALA	CB-CA-C	-6.21	101.09	110.90
1	G	184	ARG	NH1-CZ-NH2	-6.21	111.23	119.30
1	C	127	ALA	CB-CA-C	-6.21	101.10	110.90
1	E	127	ALA	CB-CA-C	-6.20	101.10	110.90
1	F	127	ALA	CB-CA-C	-6.20	101.10	110.90
1	B	127	ALA	CB-CA-C	-6.20	101.11	110.90
1	A	127	ALA	CB-CA-C	-6.20	101.11	110.90
1	H	127	ALA	CB-CA-C	-6.19	101.12	110.90
1	I	127	ALA	CB-CA-C	-6.19	101.12	110.90
1	A	38	HIS	CG-CD2-NE2	6.18	113.38	107.20
1	A	102	TYR	CA-C-N	6.16	128.82	120.44
1	A	102	TYR	C-N-CA	6.16	128.82	120.44
1	H	19	PRO	CA-C-N	6.15	128.80	120.38
1	H	19	PRO	C-N-CA	6.15	128.80	120.38
1	A	19	PRO	CA-C-N	6.14	128.80	120.38
1	A	19	PRO	C-N-CA	6.14	128.80	120.38
1	F	19	PRO	CA-C-N	6.14	128.80	120.38
1	F	19	PRO	C-N-CA	6.14	128.80	120.38
1	I	19	PRO	CA-C-N	6.14	128.79	120.38
1	I	19	PRO	C-N-CA	6.14	128.79	120.38
1	B	19	PRO	CA-C-N	6.13	128.78	120.38
1	B	19	PRO	C-N-CA	6.13	128.78	120.38
1	D	102	TYR	CA-C-N	6.13	128.78	120.44
1	D	102	TYR	C-N-CA	6.13	128.78	120.44
1	I	77	PHE	CA-C-O	-6.13	113.79	120.17
1	E	102	TYR	CA-C-N	6.13	128.78	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	102	TYR	C-N-CA	6.13	128.78	120.44
1	C	102	TYR	CA-C-N	6.13	128.77	120.44
1	C	102	TYR	C-N-CA	6.13	128.77	120.44
1	D	77	PHE	CA-C-O	-6.13	113.80	120.17
1	E	19	PRO	CA-C-N	6.12	128.77	120.38
1	E	19	PRO	C-N-CA	6.12	128.77	120.38
1	B	102	TYR	CA-C-N	6.12	128.76	120.44
1	B	102	TYR	C-N-CA	6.12	128.76	120.44
1	D	19	PRO	CA-C-N	6.12	128.76	120.38
1	D	19	PRO	C-N-CA	6.12	128.76	120.38
1	G	77	PHE	CA-C-O	-6.12	113.81	120.17
1	A	77	PHE	CA-C-O	-6.11	113.81	120.17
1	G	19	PRO	CA-C-N	6.10	128.74	120.38
1	G	19	PRO	C-N-CA	6.10	128.74	120.38
1	C	19	PRO	CA-C-N	6.10	128.74	120.38
1	C	19	PRO	C-N-CA	6.10	128.74	120.38
1	H	102	TYR	CA-C-N	6.10	128.74	120.44
1	H	102	TYR	C-N-CA	6.10	128.74	120.44
1	F	77	PHE	CA-C-O	-6.10	113.83	120.17
1	G	102	TYR	CA-C-N	6.10	128.74	120.44
1	G	102	TYR	C-N-CA	6.10	128.74	120.44
1	I	102	TYR	CA-C-N	6.10	128.74	120.44
1	I	102	TYR	C-N-CA	6.10	128.74	120.44
1	D	192	THR	N-CA-CB	6.10	118.85	110.01
1	F	102	TYR	CA-C-N	6.10	128.73	120.44
1	F	102	TYR	C-N-CA	6.10	128.73	120.44
1	B	77	PHE	CA-C-O	-6.10	113.83	120.17
1	D	158	TYR	O-C-N	-6.09	114.31	121.32
1	I	192	THR	N-CA-CB	6.09	118.84	110.01
1	E	192	THR	N-CA-CB	6.09	118.84	110.01
1	H	77	PHE	CA-C-O	-6.09	113.84	120.17
1	B	192	THR	N-CA-CB	6.08	118.83	110.01
1	A	192	THR	N-CA-CB	6.08	118.83	110.01
1	C	158	TYR	O-C-N	-6.08	114.33	121.32
1	C	192	THR	N-CA-CB	6.08	118.83	110.01
1	G	192	THR	N-CA-CB	6.08	118.83	110.01
1	E	77	PHE	CA-C-O	-6.08	113.85	120.17
1	F	192	THR	N-CA-CB	6.08	118.82	110.01
1	G	158	TYR	O-C-N	-6.08	114.33	121.32
1	E	158	TYR	O-C-N	-6.08	114.33	121.32
1	H	192	THR	N-CA-CB	6.07	118.81	110.01
1	B	158	TYR	O-C-N	-6.07	114.35	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	77	PHE	CA-C-O	-6.07	113.86	120.17
1	I	158	TYR	O-C-N	-6.06	114.35	121.32
1	H	158	TYR	O-C-N	-6.06	114.36	121.32
1	A	158	TYR	O-C-N	-6.05	114.36	121.32
1	D	8	ASP	CA-C-N	6.05	129.90	120.34
1	D	8	ASP	C-N-CA	6.05	129.90	120.34
1	F	158	TYR	O-C-N	-6.05	114.36	121.32
1	H	74	ASN	CA-CB-CG	6.05	118.65	112.60
1	C	74	ASN	CA-CB-CG	6.04	118.64	112.60
1	G	8	ASP	CA-C-N	6.04	129.88	120.34
1	G	8	ASP	C-N-CA	6.04	129.88	120.34
1	I	74	ASN	CA-CB-CG	6.04	118.64	112.60
1	A	8	ASP	CA-C-N	6.03	129.87	120.34
1	A	8	ASP	C-N-CA	6.03	129.87	120.34
1	H	8	ASP	CA-C-N	6.03	129.87	120.34
1	H	8	ASP	C-N-CA	6.03	129.87	120.34
1	B	8	ASP	CA-C-N	6.03	129.87	120.34
1	B	8	ASP	C-N-CA	6.03	129.87	120.34
1	E	74	ASN	CA-CB-CG	6.03	118.62	112.60
1	C	8	ASP	CA-C-N	6.02	129.85	120.34
1	C	8	ASP	C-N-CA	6.02	129.85	120.34
1	I	8	ASP	CA-C-N	6.02	129.85	120.34
1	I	8	ASP	C-N-CA	6.02	129.85	120.34
1	E	8	ASP	CA-C-N	6.02	129.85	120.34
1	E	8	ASP	C-N-CA	6.02	129.85	120.34
1	B	74	ASN	CA-CB-CG	6.02	118.62	112.60
1	F	8	ASP	CA-C-N	6.02	129.85	120.34
1	F	8	ASP	C-N-CA	6.02	129.85	120.34
1	F	74	ASN	CA-CB-CG	6.01	118.61	112.60
1	G	74	ASN	CA-CB-CG	6.01	118.61	112.60
1	A	74	ASN	CA-CB-CG	6.00	118.60	112.60
1	D	74	ASN	CA-CB-CG	5.99	118.59	112.60
1	I	110	VAL	CA-C-O	-5.98	114.69	121.75
1	A	110	VAL	CA-C-O	-5.97	114.71	121.75
1	H	30	HIS	ND1-CE1-NE2	5.96	114.36	108.40
1	G	30	HIS	ND1-CE1-NE2	5.95	114.35	108.40
1	I	30	HIS	ND1-CE1-NE2	5.95	114.35	108.40
1	F	30	HIS	ND1-CE1-NE2	5.95	114.35	108.40
1	A	30	HIS	ND1-CE1-NE2	5.95	114.35	108.40
1	C	110	VAL	CA-C-O	-5.95	114.73	121.75
1	C	30	HIS	ND1-CE1-NE2	5.94	114.34	108.40
1	I	118	ILE	N-CA-C	-5.94	104.53	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	HIS	ND1-CE1-NE2	5.94	114.34	108.40
1	D	30	HIS	ND1-CE1-NE2	5.94	114.34	108.40
1	E	110	VAL	CA-C-O	-5.94	114.74	121.75
1	C	118	ILE	N-CA-C	-5.93	104.54	110.30
1	D	110	VAL	CA-C-O	-5.93	114.75	121.75
1	D	118	ILE	N-CA-C	-5.93	104.54	110.30
1	H	110	VAL	CA-C-O	-5.93	114.75	121.75
1	H	118	ILE	N-CA-C	-5.93	104.55	110.30
1	B	110	VAL	CA-C-O	-5.93	114.75	121.75
1	G	118	ILE	N-CA-C	-5.93	104.55	110.30
1	B	118	ILE	N-CA-C	-5.93	104.55	110.30
1	H	225	PHE	CA-C-O	5.93	127.04	120.82
1	E	30	HIS	ND1-CE1-NE2	5.92	114.33	108.40
1	F	118	ILE	N-CA-C	-5.92	104.56	110.30
1	D	225	PHE	CA-C-O	5.92	127.04	120.82
1	G	225	PHE	CA-C-O	5.92	127.04	120.82
1	I	225	PHE	CA-C-O	5.92	127.03	120.82
1	E	118	ILE	N-CA-C	-5.92	104.56	110.30
1	B	225	PHE	CA-C-O	5.91	127.03	120.82
1	A	225	PHE	CA-C-O	5.91	127.03	120.82
1	A	118	ILE	N-CA-C	-5.91	104.57	110.30
1	C	225	PHE	CA-C-O	5.90	127.02	120.82
1	E	225	PHE	CA-C-O	5.90	127.01	120.82
1	F	110	VAL	CA-C-O	-5.90	114.79	121.75
1	G	110	VAL	CA-C-O	-5.89	114.79	121.75
1	F	225	PHE	CA-C-O	5.88	127.00	120.82
1	C	82	ASN	N-CA-CB	5.88	120.43	110.49
1	B	82	ASN	N-CA-CB	5.87	120.40	110.49
1	G	82	ASN	N-CA-CB	5.87	120.40	110.49
1	H	82	ASN	N-CA-CB	5.86	120.40	110.49
1	I	82	ASN	N-CA-CB	5.86	120.39	110.49
1	A	82	ASN	N-CA-CB	5.86	120.39	110.49
1	D	82	ASN	N-CA-CB	5.85	120.38	110.49
1	F	82	ASN	N-CA-CB	5.85	120.38	110.49
1	E	82	ASN	N-CA-CB	5.84	120.36	110.49
1	E	210	SER	N-CA-CB	5.84	118.39	110.10
1	H	210	SER	N-CA-CB	5.83	118.39	110.10
1	A	210	SER	N-CA-CB	5.83	118.38	110.10
1	B	210	SER	N-CA-CB	5.83	118.37	110.10
1	D	210	SER	N-CA-CB	5.81	118.36	110.10
1	G	210	SER	N-CA-CB	5.81	118.35	110.10
1	C	210	SER	N-CA-CB	5.80	118.34	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	210	SER	N-CA-CB	5.80	118.34	110.10
1	A	68	TRP	CB-CG-CD2	-5.79	118.69	126.80
1	I	210	SER	N-CA-CB	5.79	118.32	110.10
1	E	51	THR	CA-C-N	5.78	128.02	120.28
1	E	51	THR	C-N-CA	5.78	128.02	120.28
1	F	75	THR	N-CA-C	-5.77	105.56	113.30
1	E	68	TRP	CB-CG-CD2	-5.77	118.72	126.80
1	E	75	THR	N-CA-C	-5.77	105.57	113.30
1	I	75	THR	N-CA-C	-5.77	105.57	113.30
1	B	68	TRP	CB-CG-CD2	-5.76	118.73	126.80
1	I	51	THR	CA-C-N	5.76	128.00	120.28
1	I	51	THR	C-N-CA	5.76	128.00	120.28
1	B	51	THR	CA-C-N	5.76	127.99	120.28
1	B	51	THR	C-N-CA	5.76	127.99	120.28
1	F	51	THR	CA-C-N	5.76	127.99	120.28
1	F	51	THR	C-N-CA	5.76	127.99	120.28
1	F	68	TRP	CB-CG-CD2	-5.76	118.74	126.80
1	D	51	THR	CA-C-N	5.75	127.99	120.28
1	D	51	THR	C-N-CA	5.75	127.99	120.28
1	D	75	THR	N-CA-C	-5.75	105.59	113.30
1	G	51	THR	CA-C-N	5.75	127.99	120.28
1	G	51	THR	C-N-CA	5.75	127.99	120.28
1	A	75	THR	N-CA-C	-5.75	105.59	113.30
1	C	68	TRP	CB-CG-CD2	-5.75	118.75	126.80
1	B	75	THR	N-CA-C	-5.75	105.59	113.30
1	H	51	THR	CA-C-N	5.75	127.98	120.28
1	H	51	THR	C-N-CA	5.75	127.98	120.28
1	C	51	THR	CA-C-N	5.75	127.98	120.28
1	C	51	THR	C-N-CA	5.75	127.98	120.28
1	G	68	TRP	CB-CG-CD2	-5.75	118.75	126.80
1	A	51	THR	CA-C-N	5.75	127.98	120.28
1	A	51	THR	C-N-CA	5.75	127.98	120.28
1	A	219	SER	N-CA-CB	5.75	120.20	110.49
1	I	68	TRP	CB-CG-CD2	-5.74	118.76	126.80
1	G	75	THR	N-CA-C	-5.74	105.61	113.30
1	C	75	THR	N-CA-C	-5.74	105.61	113.30
1	H	75	THR	N-CA-C	-5.73	105.62	113.30
1	D	68	TRP	CB-CG-CD2	-5.73	118.78	126.80
1	H	68	TRP	CB-CG-CD2	-5.73	118.78	126.80
1	H	219	SER	N-CA-CB	5.71	120.15	110.49
1	B	219	SER	N-CA-CB	5.71	120.14	110.49
1	C	219	SER	N-CA-CB	5.71	120.14	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	219	SER	N-CA-CB	5.71	120.14	110.49
1	G	210	SER	CA-C-O	5.70	126.88	120.89
1	I	219	SER	N-CA-CB	5.70	120.12	110.49
1	E	219	SER	N-CA-CB	5.70	120.12	110.49
1	H	222	ALA	CA-C-N	5.70	128.71	120.79
1	H	222	ALA	C-N-CA	5.70	128.71	120.79
1	F	219	SER	N-CA-CB	5.70	120.11	110.49
1	I	222	ALA	CA-C-N	5.69	128.71	120.79
1	I	222	ALA	C-N-CA	5.69	128.71	120.79
1	D	222	ALA	CA-C-N	5.69	128.70	120.79
1	D	222	ALA	C-N-CA	5.69	128.70	120.79
1	D	219	SER	N-CA-CB	5.69	120.11	110.49
1	G	219	SER	N-CA-C	-5.69	98.68	110.80
1	G	222	ALA	CA-C-N	5.69	128.69	120.79
1	G	222	ALA	C-N-CA	5.69	128.69	120.79
1	I	219	SER	N-CA-C	-5.68	98.69	110.80
1	B	222	ALA	CA-C-N	5.68	128.69	120.79
1	B	222	ALA	C-N-CA	5.68	128.69	120.79
1	C	222	ALA	CA-C-N	5.68	128.69	120.79
1	C	222	ALA	C-N-CA	5.68	128.69	120.79
1	E	222	ALA	CA-C-N	5.68	128.69	120.79
1	E	222	ALA	C-N-CA	5.68	128.69	120.79
1	F	219	SER	N-CA-C	-5.68	98.70	110.80
1	B	219	SER	N-CA-C	-5.68	98.71	110.80
1	A	222	ALA	CA-C-N	5.68	128.68	120.79
1	A	222	ALA	C-N-CA	5.68	128.68	120.79
1	A	219	SER	N-CA-C	-5.67	98.71	110.80
1	C	65	LEU	CA-C-O	-5.67	115.84	122.37
1	H	219	SER	N-CA-C	-5.67	98.71	110.80
1	A	61	VAL	N-CA-C	-5.67	99.61	108.86
1	F	222	ALA	CA-C-N	5.67	128.68	120.79
1	F	222	ALA	C-N-CA	5.67	128.68	120.79
1	D	65	LEU	CA-C-O	-5.67	115.85	122.37
1	G	65	LEU	CA-C-O	-5.67	115.85	122.37
1	I	50	LYS	O-C-N	5.67	127.91	122.07
1	A	65	LEU	CA-C-O	-5.66	115.86	122.37
1	C	219	SER	N-CA-C	-5.66	98.74	110.80
1	E	219	SER	N-CA-C	-5.66	98.74	110.80
1	G	2	ILE	O-C-N	-5.66	117.23	123.18
1	H	65	LEU	CA-C-O	-5.66	115.86	122.37
1	H	61	VAL	N-CA-C	-5.66	99.63	108.86
1	B	65	LEU	CA-C-O	-5.66	115.86	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	61	VAL	N-CA-C	-5.65	99.65	108.86
1	H	210	SER	CA-C-O	5.65	126.83	120.89
1	D	61	VAL	N-CA-C	-5.65	99.65	108.86
1	D	219	SER	N-CA-C	-5.65	98.77	110.80
1	G	61	VAL	N-CA-C	-5.65	99.65	108.86
1	B	61	VAL	N-CA-C	-5.65	99.66	108.86
1	I	61	VAL	N-CA-C	-5.65	99.66	108.86
1	C	50	LYS	O-C-N	5.64	127.88	122.07
1	C	61	VAL	N-CA-C	-5.64	99.66	108.86
1	F	210	SER	CA-C-O	5.64	126.81	120.89
1	E	210	SER	CA-C-O	5.64	126.81	120.89
1	I	65	LEU	CA-C-O	-5.64	115.88	122.37
1	B	210	SER	CA-C-O	5.64	126.81	120.89
1	F	65	LEU	CA-C-O	-5.63	115.89	122.37
1	F	61	VAL	N-CA-C	-5.63	99.68	108.86
1	G	50	LYS	O-C-N	5.63	127.87	122.07
1	A	210	SER	CA-C-O	5.62	126.79	120.89
1	E	65	LEU	CA-C-O	-5.62	115.91	122.37
1	F	2	ILE	O-C-N	-5.62	117.28	123.18
1	C	2	ILE	O-C-N	-5.62	117.28	123.18
1	I	210	SER	CA-C-O	5.62	126.79	120.89
1	B	50	LYS	O-C-N	5.61	127.85	122.07
1	I	2	ILE	O-C-N	-5.61	117.29	123.18
1	A	50	LYS	O-C-N	5.61	127.85	122.07
1	F	50	LYS	O-C-N	5.61	127.85	122.07
1	G	31	THR	CA-CB-OG1	5.61	118.02	109.60
1	H	2	ILE	O-C-N	-5.61	117.29	123.18
1	E	50	LYS	O-C-N	5.61	127.84	122.07
1	B	2	ILE	O-C-N	-5.61	117.29	123.18
1	C	31	THR	CA-CB-OG1	5.61	118.01	109.60
1	I	31	THR	CA-CB-OG1	5.61	118.01	109.60
1	C	23	TYR	N-CA-C	-5.60	105.09	111.14
1	B	31	THR	CA-CB-OG1	5.59	117.99	109.60
1	F	23	TYR	N-CA-C	-5.59	105.10	111.14
1	C	93	HIS	CE1-NE2-CD2	-5.59	103.41	109.00
1	A	2	ILE	O-C-N	-5.59	117.31	123.18
1	C	210	SER	CA-C-O	5.59	126.76	120.89
1	D	31	THR	CA-CB-OG1	5.59	117.99	109.60
1	D	50	LYS	O-C-N	5.59	127.83	122.07
1	E	23	TYR	N-CA-C	-5.59	105.11	111.14
1	E	2	ILE	O-C-N	-5.59	117.31	123.18
1	H	31	THR	CA-CB-OG1	5.59	117.98	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2	ILE	O-C-N	-5.58	117.32	123.18
1	B	93	HIS	CE1-NE2-CD2	-5.58	103.42	109.00
1	A	31	THR	CA-CB-OG1	5.58	117.97	109.60
1	G	93	HIS	CE1-NE2-CD2	-5.58	103.42	109.00
1	I	93	HIS	CE1-NE2-CD2	-5.58	103.42	109.00
1	F	31	THR	CA-CB-OG1	5.58	117.97	109.60
1	H	23	TYR	N-CA-C	-5.58	105.11	111.14
1	E	31	THR	CA-CB-OG1	5.58	117.97	109.60
1	F	93	HIS	CE1-NE2-CD2	-5.58	103.42	109.00
1	D	210	SER	CA-C-O	5.57	126.74	120.89
1	I	23	TYR	N-CA-C	-5.57	105.12	111.14
1	B	23	TYR	N-CA-C	-5.57	105.13	111.14
1	A	129	LYS	CA-C-O	-5.57	114.62	120.63
1	A	93	HIS	CE1-NE2-CD2	-5.56	103.44	109.00
1	D	23	TYR	N-CA-C	-5.56	105.13	111.14
1	E	93	HIS	CE1-NE2-CD2	-5.56	103.44	109.00
1	H	50	LYS	O-C-N	5.56	127.80	122.07
1	G	192	THR	N-CA-C	5.56	117.02	111.07
1	A	23	TYR	N-CA-C	-5.55	105.14	111.14
1	H	192	THR	N-CA-C	5.55	117.01	111.07
1	B	129	LYS	CA-C-O	-5.55	114.63	120.63
1	A	192	THR	N-CA-C	5.55	117.01	111.07
1	H	93	HIS	CE1-NE2-CD2	-5.55	103.45	109.00
1	E	213	TRP	N-CA-C	-5.55	100.50	108.60
1	G	23	TYR	N-CA-C	-5.55	105.15	111.14
1	D	129	LYS	CA-C-O	-5.55	114.64	120.63
1	F	192	THR	N-CA-C	5.55	117.00	111.07
1	H	129	LYS	CA-C-O	-5.55	114.64	120.63
1	D	93	HIS	CE1-NE2-CD2	-5.54	103.45	109.00
1	E	192	THR	N-CA-C	5.54	117.00	111.07
1	B	192	THR	N-CA-C	5.54	117.00	111.07
1	F	129	LYS	CA-C-O	-5.54	114.65	120.63
1	D	213	TRP	N-CA-C	-5.54	100.52	108.60
1	E	129	LYS	CA-C-O	-5.53	114.65	120.63
1	F	213	TRP	N-CA-C	-5.53	100.52	108.60
1	B	213	TRP	N-CA-C	-5.53	100.52	108.60
1	G	129	LYS	CA-C-O	-5.53	114.66	120.63
1	I	213	TRP	N-CA-C	-5.53	100.53	108.60
1	I	129	LYS	CA-C-O	-5.52	114.66	120.63
1	G	213	TRP	N-CA-C	-5.52	100.54	108.60
1	C	129	LYS	CA-C-O	-5.52	114.67	120.63
1	E	81	ARG	CB-CG-CD	5.52	124.00	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	213	TRP	N-CA-C	-5.52	100.54	108.60
1	A	213	TRP	N-CA-C	-5.52	100.54	108.60
1	C	192	THR	N-CA-C	5.52	116.97	111.07
1	C	81	ARG	CB-CG-CD	5.52	123.99	111.30
1	F	81	ARG	CB-CG-CD	5.51	123.98	111.30
1	G	81	ARG	CB-CG-CD	5.51	123.98	111.30
1	D	81	ARG	CB-CG-CD	5.51	123.97	111.30
1	I	81	ARG	CB-CG-CD	5.51	123.97	111.30
1	B	81	ARG	CB-CG-CD	5.51	123.97	111.30
1	H	81	ARG	CB-CG-CD	5.51	123.97	111.30
1	A	81	ARG	CB-CG-CD	5.51	123.96	111.30
1	C	213	TRP	N-CA-C	-5.51	100.56	108.60
1	I	192	THR	N-CA-C	5.51	116.96	111.07
1	G	124	ASN	CA-C-N	5.50	126.71	119.84
1	G	124	ASN	C-N-CA	5.50	126.71	119.84
1	I	113	PRO	CA-C-O	-5.50	111.77	119.74
1	C	113	PRO	CA-C-O	-5.50	111.77	119.74
1	H	3	GLU	CB-CG-CD	-5.50	103.26	112.60
1	D	3	GLU	CB-CG-CD	-5.49	103.27	112.60
1	G	3	GLU	CB-CG-CD	-5.49	103.27	112.60
1	A	3	GLU	CB-CG-CD	-5.49	103.27	112.60
1	A	113	PRO	CA-C-O	-5.49	111.79	119.74
1	D	192	THR	N-CA-C	5.49	116.94	111.07
1	B	3	GLU	CB-CG-CD	-5.48	103.28	112.60
1	D	124	ASN	CA-C-N	5.48	126.69	119.84
1	D	124	ASN	C-N-CA	5.48	126.69	119.84
1	F	3	GLU	CB-CG-CD	-5.48	103.28	112.60
1	G	167	VAL	CA-CB-CG2	5.48	119.72	110.40
1	H	167	VAL	CA-CB-CG2	5.48	119.72	110.40
1	E	167	VAL	CA-CB-CG2	5.48	119.71	110.40
1	F	167	VAL	CA-CB-CG2	5.48	119.71	110.40
1	B	167	VAL	CA-CB-CG2	5.48	119.71	110.40
1	I	3	GLU	CB-CG-CD	-5.48	103.29	112.60
1	B	113	PRO	CA-C-O	-5.47	111.80	119.74
1	C	167	VAL	CA-CB-CG2	5.47	119.70	110.40
1	D	113	PRO	CA-C-O	-5.47	111.80	119.74
1	H	124	ASN	CA-C-N	5.47	126.68	119.84
1	H	124	ASN	C-N-CA	5.47	126.68	119.84
1	A	167	VAL	CA-CB-CG2	5.47	119.70	110.40
1	D	167	VAL	CA-CB-CG2	5.47	119.70	110.40
1	D	194	THR	CA-C-O	5.47	126.54	120.63
1	E	3	GLU	CB-CG-CD	-5.47	103.30	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	113	PRO	CA-C-O	-5.47	111.81	119.74
1	I	167	VAL	CA-CB-CG2	5.47	119.70	110.40
1	H	113	PRO	CA-C-O	-5.47	111.81	119.74
1	E	124	ASN	CA-C-N	5.46	126.67	119.84
1	E	124	ASN	C-N-CA	5.46	126.67	119.84
1	B	124	ASN	CA-C-N	5.46	126.67	119.84
1	B	124	ASN	C-N-CA	5.46	126.67	119.84
1	E	194	THR	CA-C-O	5.46	126.53	120.63
1	E	113	PRO	CA-C-O	-5.46	111.82	119.74
1	G	113	PRO	CA-C-O	-5.46	111.83	119.74
1	I	124	ASN	CA-C-N	5.46	126.66	119.84
1	I	124	ASN	C-N-CA	5.46	126.66	119.84
1	F	124	ASN	CA-C-N	5.46	126.66	119.84
1	F	124	ASN	C-N-CA	5.46	126.66	119.84
1	C	124	ASN	CA-C-N	5.46	126.66	119.84
1	C	124	ASN	C-N-CA	5.46	126.66	119.84
1	A	124	ASN	CA-C-N	5.45	126.66	119.84
1	A	124	ASN	C-N-CA	5.45	126.66	119.84
1	C	3	GLU	CB-CG-CD	-5.45	103.33	112.60
1	G	194	THR	CA-C-O	5.45	126.51	120.63
1	C	194	THR	CA-C-O	5.44	126.50	120.63
1	H	194	THR	CA-C-O	5.43	126.49	120.63
1	I	194	THR	CA-C-O	5.42	126.49	120.63
1	B	194	THR	CA-C-O	5.42	126.48	120.63
1	A	194	THR	CA-C-O	5.42	126.48	120.63
1	F	194	THR	CA-C-O	5.42	126.48	120.63
1	D	166	LYS	CB-CG-CD	5.41	123.75	111.30
1	E	166	LYS	CB-CG-CD	5.41	123.74	111.30
1	A	166	LYS	CB-CG-CD	5.41	123.74	111.30
1	G	166	LYS	CB-CG-CD	5.41	123.74	111.30
1	C	166	LYS	CB-CG-CD	5.41	123.73	111.30
1	F	166	LYS	CB-CG-CD	5.41	123.73	111.30
1	B	166	LYS	CB-CG-CD	5.40	123.73	111.30
1	I	166	LYS	CB-CG-CD	5.40	123.73	111.30
1	D	148	SER	CA-C-N	5.40	129.25	120.60
1	D	148	SER	C-N-CA	5.40	129.25	120.60
1	H	148	SER	CA-C-N	5.40	129.24	120.60
1	H	148	SER	C-N-CA	5.40	129.24	120.60
1	H	166	LYS	CB-CG-CD	5.40	123.72	111.30
1	I	148	SER	CA-C-N	5.40	129.24	120.60
1	I	148	SER	C-N-CA	5.40	129.24	120.60
1	H	213	TRP	O-C-N	-5.39	117.60	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	148	SER	CA-C-N	5.39	129.22	120.60
1	E	148	SER	C-N-CA	5.39	129.22	120.60
1	H	223	ARG	N-CA-CB	5.39	118.01	109.82
1	B	148	SER	CA-C-N	5.38	129.22	120.60
1	B	148	SER	C-N-CA	5.38	129.22	120.60
1	I	213	TRP	O-C-N	-5.38	117.61	123.26
1	C	223	ARG	N-CA-CB	5.38	118.00	109.82
1	F	223	ARG	N-CA-CB	5.38	118.00	109.82
1	I	223	ARG	N-CA-CB	5.38	118.00	109.82
1	C	213	TRP	O-C-N	-5.38	117.62	123.26
1	E	223	ARG	N-CA-CB	5.38	117.99	109.82
1	G	148	SER	CA-C-N	5.38	129.20	120.60
1	G	148	SER	C-N-CA	5.38	129.20	120.60
1	B	213	TRP	O-C-N	-5.37	117.62	123.26
1	B	223	ARG	N-CA-CB	5.37	117.99	109.82
1	C	148	SER	CA-C-N	5.37	129.20	120.60
1	C	148	SER	C-N-CA	5.37	129.20	120.60
1	F	148	SER	CA-C-N	5.37	129.20	120.60
1	F	148	SER	C-N-CA	5.37	129.20	120.60
1	A	148	SER	CA-C-N	5.37	129.19	120.60
1	A	148	SER	C-N-CA	5.37	129.19	120.60
1	G	223	ARG	N-CA-CB	5.37	117.98	109.82
1	F	213	TRP	O-C-N	-5.37	117.62	123.26
1	A	223	ARG	N-CA-CB	5.37	117.98	109.82
1	D	223	ARG	N-CA-CB	5.37	117.98	109.82
1	D	213	TRP	O-C-N	-5.36	117.63	123.26
1	A	213	TRP	O-C-N	-5.36	117.64	123.26
1	A	221	ALA	CA-C-N	5.36	127.40	120.44
1	A	221	ALA	C-N-CA	5.36	127.40	120.44
1	C	221	ALA	CA-C-N	5.36	127.40	120.44
1	C	221	ALA	C-N-CA	5.36	127.40	120.44
1	E	213	TRP	O-C-N	-5.35	117.64	123.26
1	H	221	ALA	CA-C-N	5.35	127.40	120.44
1	H	221	ALA	C-N-CA	5.35	127.40	120.44
1	F	129	LYS	CG-CD-CE	5.35	123.61	111.30
1	G	213	TRP	O-C-N	-5.35	117.64	123.26
1	E	129	LYS	CG-CD-CE	5.35	123.61	111.30
1	F	221	ALA	CA-C-N	5.35	127.39	120.44
1	F	221	ALA	C-N-CA	5.35	127.39	120.44
1	G	129	LYS	CG-CD-CE	5.35	123.60	111.30
1	B	129	LYS	CG-CD-CE	5.34	123.59	111.30
1	A	129	LYS	CG-CD-CE	5.34	123.59	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	129	LYS	CG-CD-CE	5.34	123.59	111.30
1	D	129	LYS	CG-CD-CE	5.34	123.59	111.30
1	G	221	ALA	CA-C-N	5.34	127.39	120.44
1	G	221	ALA	C-N-CA	5.34	127.39	120.44
1	B	221	ALA	CA-C-N	5.34	127.38	120.44
1	B	221	ALA	C-N-CA	5.34	127.38	120.44
1	C	129	LYS	CG-CD-CE	5.34	123.58	111.30
1	E	221	ALA	CA-C-N	5.34	127.38	120.44
1	E	221	ALA	C-N-CA	5.34	127.38	120.44
1	I	221	ALA	CA-C-N	5.34	127.38	120.44
1	I	221	ALA	C-N-CA	5.34	127.38	120.44
1	D	221	ALA	CA-C-N	5.33	127.37	120.44
1	D	221	ALA	C-N-CA	5.33	127.37	120.44
1	H	129	LYS	CG-CD-CE	5.33	123.56	111.30
1	G	151	PHE	N-CA-C	-5.33	98.58	107.80
1	H	151	PHE	N-CA-C	-5.32	98.60	107.80
1	C	11	ALA	N-CA-C	-5.32	105.44	112.94
1	F	151	PHE	N-CA-C	-5.32	98.61	107.80
1	H	11	ALA	N-CA-C	-5.32	105.45	112.94
1	B	151	PHE	N-CA-C	-5.31	98.61	107.80
1	A	151	PHE	N-CA-C	-5.31	98.61	107.80
1	D	151	PHE	N-CA-C	-5.31	98.61	107.80
1	A	11	ALA	N-CA-C	-5.31	105.45	112.94
1	G	181	MET	CA-C-O	-5.31	112.15	119.05
1	A	181	MET	CA-C-O	-5.31	112.15	119.05
1	F	11	ALA	N-CA-C	-5.31	105.45	112.94
1	E	181	MET	CA-C-O	-5.31	112.15	119.05
1	E	151	PHE	N-CA-C	-5.30	98.62	107.80
1	C	151	PHE	N-CA-C	-5.30	98.63	107.80
1	B	11	ALA	N-CA-C	-5.30	105.47	112.94
1	C	181	MET	CA-C-O	-5.30	112.17	119.05
1	F	181	MET	CA-C-O	-5.30	112.16	119.05
1	G	11	ALA	N-CA-C	-5.29	105.47	112.94
1	B	181	MET	CA-C-O	-5.29	112.17	119.05
1	I	151	PHE	N-CA-C	-5.29	98.64	107.80
1	I	181	MET	CA-C-O	-5.29	112.17	119.05
1	H	181	MET	CA-C-O	-5.29	112.17	119.05
1	D	11	ALA	N-CA-C	-5.29	105.48	112.94
1	E	11	ALA	N-CA-C	-5.29	105.48	112.94
1	I	72	VAL	CA-CB-CG1	5.29	119.39	110.40
1	D	72	VAL	CA-CB-CG1	5.28	119.38	110.40
1	D	181	MET	CA-C-O	-5.28	112.18	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	72	VAL	CA-CB-CG1	5.28	119.38	110.40
1	B	72	VAL	CA-CB-CG1	5.28	119.38	110.40
1	F	72	VAL	CA-CB-CG1	5.28	119.38	110.40
1	A	72	VAL	CA-CB-CG1	5.28	119.37	110.40
1	D	30	HIS	CE1-NE2-CD2	-5.28	103.72	109.00
1	I	11	ALA	N-CA-C	-5.28	105.50	112.94
1	C	72	VAL	CA-CB-CG1	5.27	119.36	110.40
1	E	30	HIS	CE1-NE2-CD2	-5.27	103.73	109.00
1	H	72	VAL	CA-CB-CG1	5.27	119.36	110.40
1	H	226	LEU	CA-C-N	5.27	127.34	120.28
1	H	226	LEU	C-N-CA	5.27	127.34	120.28
1	A	67	GLY	CA-C-N	5.27	128.19	120.71
1	A	67	GLY	C-N-CA	5.27	128.19	120.71
1	G	72	VAL	CA-CB-CG1	5.27	119.36	110.40
1	C	67	GLY	CA-C-N	5.27	128.19	120.71
1	C	67	GLY	C-N-CA	5.27	128.19	120.71
1	E	67	GLY	CA-C-N	5.26	128.19	120.71
1	E	67	GLY	C-N-CA	5.26	128.19	120.71
1	F	67	GLY	CA-C-N	5.26	128.19	120.71
1	F	67	GLY	C-N-CA	5.26	128.19	120.71
1	G	67	GLY	CA-C-N	5.26	128.19	120.71
1	G	67	GLY	C-N-CA	5.26	128.19	120.71
1	H	67	GLY	CA-C-N	5.26	128.18	120.71
1	H	67	GLY	C-N-CA	5.26	128.18	120.71
1	B	67	GLY	CA-C-N	5.26	128.18	120.71
1	B	67	GLY	C-N-CA	5.26	128.18	120.71
1	F	30	HIS	CE1-NE2-CD2	-5.26	103.74	109.00
1	I	67	GLY	CA-C-N	5.26	128.18	120.71
1	I	67	GLY	C-N-CA	5.26	128.18	120.71
1	B	30	HIS	CE1-NE2-CD2	-5.26	103.74	109.00
1	D	112	GLU	N-CA-CB	5.26	118.58	110.43
1	G	112	GLU	N-CA-CB	5.26	118.58	110.43
1	I	30	HIS	CE1-NE2-CD2	-5.25	103.75	109.00
1	G	30	HIS	CE1-NE2-CD2	-5.25	103.75	109.00
1	D	101	ARG	CA-C-N	5.25	128.69	120.82
1	D	101	ARG	C-N-CA	5.25	128.69	120.82
1	E	226	LEU	CA-C-N	5.25	127.31	120.28
1	E	226	LEU	C-N-CA	5.25	127.31	120.28
1	I	101	ARG	CA-C-N	5.25	128.69	120.82
1	I	101	ARG	C-N-CA	5.25	128.69	120.82
1	B	226	LEU	CA-C-N	5.25	127.31	120.28
1	B	226	LEU	C-N-CA	5.25	127.31	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	226	LEU	CA-C-N	5.25	127.31	120.28
1	C	226	LEU	C-N-CA	5.25	127.31	120.28
1	A	30	HIS	CE1-NE2-CD2	-5.25	103.75	109.00
1	D	67	GLY	CA-C-N	5.24	128.16	120.71
1	D	67	GLY	C-N-CA	5.24	128.16	120.71
1	C	30	HIS	CE1-NE2-CD2	-5.24	103.76	109.00
1	F	226	LEU	CA-C-N	5.24	127.30	120.28
1	F	226	LEU	C-N-CA	5.24	127.30	120.28
1	E	112	GLU	N-CA-CB	5.24	118.55	110.43
1	H	30	HIS	CE1-NE2-CD2	-5.24	103.76	109.00
1	H	101	ARG	CA-C-N	5.24	128.68	120.82
1	H	101	ARG	C-N-CA	5.24	128.68	120.82
1	D	226	LEU	CA-C-N	5.24	127.30	120.28
1	D	226	LEU	C-N-CA	5.24	127.30	120.28
1	E	101	ARG	CA-C-N	5.24	128.68	120.82
1	E	101	ARG	C-N-CA	5.24	128.68	120.82
1	I	112	GLU	N-CA-CB	5.24	118.55	110.43
1	B	112	GLU	N-CA-CB	5.24	118.55	110.43
1	A	226	LEU	CA-C-N	5.24	127.30	120.28
1	A	226	LEU	C-N-CA	5.24	127.30	120.28
1	A	112	GLU	N-CA-CB	5.23	118.54	110.43
1	B	101	ARG	CA-C-N	5.23	128.66	120.82
1	B	101	ARG	C-N-CA	5.23	128.66	120.82
1	C	101	ARG	CA-C-N	5.23	128.66	120.82
1	C	101	ARG	C-N-CA	5.23	128.66	120.82
1	F	112	GLU	N-CA-CB	5.22	118.53	110.43
1	G	226	LEU	CA-C-N	5.22	127.28	120.28
1	G	226	LEU	C-N-CA	5.22	127.28	120.28
1	C	112	GLU	N-CA-CB	5.22	118.52	110.43
1	A	101	ARG	CA-C-N	5.22	128.65	120.82
1	A	101	ARG	C-N-CA	5.22	128.65	120.82
1	F	101	ARG	CA-C-N	5.22	128.65	120.82
1	F	101	ARG	C-N-CA	5.22	128.65	120.82
1	H	112	GLU	N-CA-CB	5.22	118.52	110.43
1	G	101	ARG	CA-C-N	5.21	128.64	120.82
1	G	101	ARG	C-N-CA	5.21	128.64	120.82
1	I	226	LEU	CA-C-N	5.21	127.26	120.28
1	I	226	LEU	C-N-CA	5.21	127.26	120.28
1	E	201	VAL	CB-CA-C	-5.19	104.12	112.16
1	F	201	VAL	CB-CA-C	-5.18	104.13	112.16
1	C	201	VAL	CB-CA-C	-5.18	104.14	112.16
1	G	85	VAL	CA-C-N	5.18	126.31	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	85	VAL	C-N-CA	5.18	126.31	119.84
1	B	201	VAL	CB-CA-C	-5.17	104.14	112.16
1	H	135	ASN	CA-C-N	5.17	131.43	121.18
1	H	135	ASN	C-N-CA	5.17	131.43	121.18
1	A	135	ASN	CA-C-N	5.17	131.42	121.18
1	A	135	ASN	C-N-CA	5.17	131.42	121.18
1	G	201	VAL	CB-CA-C	-5.17	104.14	112.16
1	A	201	VAL	CB-CA-C	-5.17	104.15	112.16
1	F	135	ASN	CA-C-N	5.17	131.42	121.18
1	F	135	ASN	C-N-CA	5.17	131.42	121.18
1	B	135	ASN	CA-C-N	5.17	131.41	121.18
1	B	135	ASN	C-N-CA	5.17	131.41	121.18
1	D	201	VAL	CB-CA-C	-5.17	104.15	112.16
1	G	135	ASN	CA-C-N	5.17	131.41	121.18
1	G	135	ASN	C-N-CA	5.17	131.41	121.18
1	I	135	ASN	CA-C-N	5.17	131.41	121.18
1	I	135	ASN	C-N-CA	5.17	131.41	121.18
1	D	135	ASN	CA-C-N	5.17	131.41	121.18
1	D	135	ASN	C-N-CA	5.17	131.41	121.18
1	I	201	VAL	CB-CA-C	-5.17	104.16	112.16
1	H	201	VAL	CB-CA-C	-5.16	104.16	112.16
1	C	135	ASN	CA-C-N	5.16	131.39	121.18
1	C	135	ASN	C-N-CA	5.16	131.39	121.18
1	D	95	LEU	CA-C-N	5.16	127.19	120.28
1	D	95	LEU	C-N-CA	5.16	127.19	120.28
1	E	135	ASN	CA-C-N	5.16	131.39	121.18
1	E	135	ASN	C-N-CA	5.16	131.39	121.18
1	F	95	LEU	CA-C-N	5.16	127.19	120.28
1	F	95	LEU	C-N-CA	5.16	127.19	120.28
1	A	95	LEU	CA-C-N	5.15	127.18	120.28
1	A	95	LEU	C-N-CA	5.15	127.18	120.28
1	C	139	GLU	CA-C-N	5.15	127.00	120.72
1	C	139	GLU	C-N-CA	5.15	127.00	120.72
1	G	95	LEU	CA-C-N	5.15	127.18	120.28
1	G	95	LEU	C-N-CA	5.15	127.18	120.28
1	H	85	VAL	CA-C-N	5.15	126.27	119.84
1	H	85	VAL	C-N-CA	5.15	126.27	119.84
1	B	85	VAL	CA-C-N	5.14	126.27	119.84
1	B	85	VAL	C-N-CA	5.14	126.27	119.84
1	B	95	LEU	CA-C-N	5.14	127.17	120.28
1	B	95	LEU	C-N-CA	5.14	127.17	120.28
1	E	124	ASN	CB-CA-C	5.14	115.58	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	95	LEU	CA-C-N	5.14	127.17	120.28
1	H	95	LEU	C-N-CA	5.14	127.17	120.28
1	F	85	VAL	CA-C-N	5.14	126.27	119.84
1	F	85	VAL	C-N-CA	5.14	126.27	119.84
1	D	85	VAL	CA-C-N	5.14	126.27	119.84
1	D	85	VAL	C-N-CA	5.14	126.27	119.84
1	E	95	LEU	CA-C-N	5.14	127.17	120.28
1	E	95	LEU	C-N-CA	5.14	127.17	120.28
1	A	85	VAL	CA-C-N	5.13	126.26	119.84
1	A	85	VAL	C-N-CA	5.13	126.26	119.84
1	A	162	ILE	O-C-N	5.13	126.85	121.87
1	E	139	GLU	CA-C-N	5.13	126.98	120.72
1	E	139	GLU	C-N-CA	5.13	126.98	120.72
1	I	139	GLU	CA-C-N	5.13	126.98	120.72
1	I	139	GLU	C-N-CA	5.13	126.98	120.72
1	D	139	GLU	CA-C-N	5.13	126.98	120.72
1	D	139	GLU	C-N-CA	5.13	126.98	120.72
1	A	124	ASN	CB-CA-C	5.13	115.56	110.33
1	B	139	GLU	CA-C-N	5.13	126.97	120.72
1	B	139	GLU	C-N-CA	5.13	126.97	120.72
1	A	139	GLU	CA-C-N	5.13	126.97	120.72
1	A	139	GLU	C-N-CA	5.13	126.97	120.72
1	I	85	VAL	CA-C-N	5.13	126.25	119.84
1	I	85	VAL	C-N-CA	5.13	126.25	119.84
1	C	95	LEU	CA-C-N	5.12	127.15	120.28
1	C	95	LEU	C-N-CA	5.12	127.15	120.28
1	I	95	LEU	CA-C-N	5.12	127.14	120.28
1	I	95	LEU	C-N-CA	5.12	127.14	120.28
1	H	124	ASN	CB-CA-C	5.12	115.56	110.33
1	I	162	ILE	O-C-N	5.12	126.84	121.87
1	H	162	ILE	O-C-N	5.12	126.83	121.87
1	F	139	GLU	CA-C-N	5.12	126.96	120.72
1	F	139	GLU	C-N-CA	5.12	126.96	120.72
1	B	124	ASN	CB-CA-C	5.12	115.55	110.33
1	H	139	GLU	CA-C-N	5.12	126.96	120.72
1	H	139	GLU	C-N-CA	5.12	126.96	120.72
1	B	162	ILE	O-C-N	5.11	126.83	121.87
1	C	124	ASN	CB-CA-C	5.11	115.55	110.33
1	C	85	VAL	CA-C-N	5.11	126.23	119.84
1	C	85	VAL	C-N-CA	5.11	126.23	119.84
1	D	124	ASN	CB-CA-C	5.11	115.54	110.33
1	G	124	ASN	CB-CA-C	5.11	115.54	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	HIS	ND1-CE1-NE2	5.11	113.51	108.40
1	G	171	GLU	CA-C-O	-5.11	113.77	120.00
1	I	61	VAL	CA-CB-CG2	-5.11	101.72	110.40
1	A	61	VAL	CA-CB-CG2	-5.10	101.72	110.40
1	E	162	ILE	O-C-N	5.10	126.82	121.87
1	H	61	VAL	CA-CB-CG2	-5.10	101.72	110.40
1	E	85	VAL	CA-C-N	5.10	126.22	119.84
1	E	85	VAL	C-N-CA	5.10	126.22	119.84
1	F	124	ASN	CB-CA-C	5.10	115.53	110.33
1	G	139	GLU	CA-C-N	5.10	126.94	120.72
1	G	139	GLU	C-N-CA	5.10	126.94	120.72
1	B	61	VAL	CA-CB-CG2	-5.10	101.73	110.40
1	G	61	VAL	CA-CB-CG2	-5.10	101.73	110.40
1	C	61	VAL	CA-CB-CG2	-5.10	101.73	110.40
1	C	162	ILE	O-C-N	5.10	126.82	121.87
1	F	61	VAL	CA-CB-CG2	-5.10	101.74	110.40
1	A	108	LEU	CA-C-O	-5.09	114.52	120.53
1	D	61	VAL	CA-CB-CG2	-5.09	101.74	110.40
1	E	61	VAL	CA-CB-CG2	-5.09	101.74	110.40
1	G	30	HIS	CA-CB-CG	-5.09	108.71	113.80
1	G	162	ILE	O-C-N	5.09	126.81	121.87
1	H	30	HIS	CA-CB-CG	-5.09	108.71	113.80
1	B	7	HIS	ND1-CE1-NE2	5.09	113.49	108.40
1	F	7	HIS	ND1-CE1-NE2	5.09	113.49	108.40
1	G	7	HIS	ND1-CE1-NE2	5.09	113.49	108.40
1	H	171	GLU	CA-C-O	-5.09	113.79	120.00
1	I	124	ASN	CB-CA-C	5.09	115.52	110.33
1	C	7	HIS	ND1-CE1-NE2	5.08	113.48	108.40
1	A	30	HIS	CA-CB-CG	-5.08	108.72	113.80
1	F	30	HIS	CA-CB-CG	-5.08	108.72	113.80
1	I	30	HIS	CA-CB-CG	-5.08	108.72	113.80
1	C	97	GLY	CA-C-N	5.08	127.05	120.44
1	C	97	GLY	C-N-CA	5.08	127.05	120.44
1	E	30	HIS	CA-CB-CG	-5.08	108.72	113.80
1	I	97	GLY	CA-C-N	5.08	127.05	120.44
1	I	97	GLY	C-N-CA	5.08	127.05	120.44
1	D	162	ILE	O-C-N	5.08	126.80	121.87
1	F	108	LEU	CA-C-O	-5.08	114.54	120.53
1	F	162	ILE	O-C-N	5.08	126.80	121.87
1	B	30	HIS	CA-CB-CG	-5.08	108.72	113.80
1	B	171	GLU	CA-C-O	-5.08	113.81	120.00
1	D	97	GLY	CA-C-N	5.08	127.04	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	97	GLY	C-N-CA	5.08	127.04	120.44
1	F	97	GLY	CA-C-N	5.08	127.04	120.44
1	F	97	GLY	C-N-CA	5.08	127.04	120.44
1	F	171	GLU	CA-C-O	-5.08	113.80	120.00
1	E	97	GLY	CA-C-N	5.08	127.04	120.44
1	E	97	GLY	C-N-CA	5.08	127.04	120.44
1	B	97	GLY	CA-C-N	5.07	127.04	120.44
1	B	97	GLY	C-N-CA	5.07	127.04	120.44
1	E	7	HIS	ND1-CE1-NE2	5.07	113.47	108.40
1	C	108	LEU	CA-C-O	-5.07	114.55	120.53
1	B	108	LEU	CA-C-O	-5.07	114.55	120.53
1	I	108	LEU	CA-C-O	-5.07	114.55	120.53
1	C	171	GLU	CA-C-O	-5.07	113.82	120.00
1	D	7	HIS	ND1-CE1-NE2	5.07	113.47	108.40
1	D	30	HIS	CA-CB-CG	-5.07	108.73	113.80
1	I	156	ARG	N-CA-CB	5.07	119.05	110.49
1	I	171	GLU	CA-C-O	-5.07	113.82	120.00
1	A	97	GLY	CA-C-N	5.06	127.02	120.44
1	A	97	GLY	C-N-CA	5.06	127.02	120.44
1	E	108	LEU	CA-C-O	-5.06	114.56	120.53
1	H	156	ARG	N-CA-CB	5.06	119.05	110.49
1	F	156	ARG	N-CA-CB	5.06	119.05	110.49
1	H	97	GLY	CA-C-N	5.06	127.02	120.44
1	H	97	GLY	C-N-CA	5.06	127.02	120.44
1	G	108	LEU	CA-C-O	-5.06	114.56	120.53
1	D	171	GLU	CA-C-O	-5.06	113.83	120.00
1	E	171	GLU	CA-C-O	-5.06	113.83	120.00
1	C	30	HIS	CA-CB-CG	-5.06	108.74	113.80
1	A	171	GLU	CA-C-O	-5.05	113.83	120.00
1	H	7	HIS	ND1-CE1-NE2	5.05	113.45	108.40
1	D	108	LEU	CA-C-O	-5.05	114.57	120.53
1	D	156	ARG	N-CA-CB	5.05	119.02	110.49
1	H	108	LEU	CA-C-O	-5.05	114.57	120.53
1	I	7	HIS	ND1-CE1-NE2	5.05	113.45	108.40
1	A	156	ARG	N-CA-CB	5.05	119.02	110.49
1	C	156	ARG	N-CA-CB	5.05	119.02	110.49
1	B	156	ARG	N-CA-CB	5.04	119.01	110.49
1	G	97	GLY	CA-C-N	5.04	127.00	120.44
1	G	97	GLY	C-N-CA	5.04	127.00	120.44
1	H	73	TYR	CA-C-O	5.04	126.42	120.58
1	E	206	THR	N-CA-C	5.03	116.76	111.28
1	H	167	VAL	N-CA-C	5.02	115.74	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	TYR	CA-C-O	5.02	126.40	120.58
1	G	156	ARG	N-CA-CB	5.02	118.97	110.49
1	H	185	TYR	N-CA-C	-5.02	100.23	108.41
1	E	167	VAL	N-CA-C	5.02	115.74	110.62
1	F	206	THR	N-CA-C	5.02	116.75	111.28
1	C	167	VAL	N-CA-C	5.01	115.73	110.62
1	E	156	ARG	N-CA-CB	5.01	118.96	110.49
1	I	167	VAL	N-CA-C	5.01	115.73	110.62
1	A	160	LEU	CA-C-N	5.01	126.99	120.28
1	A	160	LEU	C-N-CA	5.01	126.99	120.28
1	F	41	ILE	CA-C-N	5.01	126.99	120.28
1	F	41	ILE	C-N-CA	5.01	126.99	120.28
1	B	167	VAL	N-CA-C	5.01	115.73	110.62
1	G	185	TYR	N-CA-C	-5.01	100.25	108.41
1	D	160	LEU	CA-C-N	5.01	126.99	120.28
1	D	160	LEU	C-N-CA	5.01	126.99	120.28
1	G	73	TYR	CA-C-O	5.01	126.39	120.58
1	I	206	THR	N-CA-C	5.01	116.74	111.28
1	I	160	LEU	CA-C-N	5.00	126.99	120.28
1	I	160	LEU	C-N-CA	5.00	126.99	120.28
1	A	49	ILE	CA-C-N	5.00	126.94	120.44
1	A	49	ILE	C-N-CA	5.00	126.94	120.44
1	A	167	VAL	N-CA-C	5.00	115.72	110.62
1	E	73	TYR	CA-C-O	5.00	126.38	120.58
1	E	185	TYR	N-CA-C	-5.00	100.25	108.41
1	B	206	THR	N-CA-C	5.00	116.73	111.28
1	F	49	ILE	CA-C-N	5.00	126.94	120.44
1	F	49	ILE	C-N-CA	5.00	126.94	120.44

There are no chirality outliers.

All (63) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	TYR	Sidechain
1	A	169	ARG	Sidechain
1	A	184	ARG	Sidechain
1	A	185	TYR	Sidechain
1	A	43	TYR	Sidechain
1	A	73	TYR	Sidechain
1	A	94	ARG	Sidechain
1	B	141	TYR	Sidechain
1	B	169	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	184	ARG	Sidechain
1	B	185	TYR	Sidechain
1	B	43	TYR	Sidechain
1	B	73	TYR	Sidechain
1	B	94	ARG	Sidechain
1	C	141	TYR	Sidechain
1	C	169	ARG	Sidechain
1	C	184	ARG	Sidechain
1	C	185	TYR	Sidechain
1	C	43	TYR	Sidechain
1	C	73	TYR	Sidechain
1	C	94	ARG	Sidechain
1	D	141	TYR	Sidechain
1	D	169	ARG	Sidechain
1	D	184	ARG	Sidechain
1	D	185	TYR	Sidechain
1	D	43	TYR	Sidechain
1	D	73	TYR	Sidechain
1	D	94	ARG	Sidechain
1	E	141	TYR	Sidechain
1	E	169	ARG	Sidechain
1	E	184	ARG	Sidechain
1	E	185	TYR	Sidechain
1	E	43	TYR	Sidechain
1	E	73	TYR	Sidechain
1	E	94	ARG	Sidechain
1	F	141	TYR	Sidechain
1	F	169	ARG	Sidechain
1	F	184	ARG	Sidechain
1	F	185	TYR	Sidechain
1	F	43	TYR	Sidechain
1	F	73	TYR	Sidechain
1	F	94	ARG	Sidechain
1	G	141	TYR	Sidechain
1	G	169	ARG	Sidechain
1	G	184	ARG	Sidechain
1	G	185	TYR	Sidechain
1	G	43	TYR	Sidechain
1	G	73	TYR	Sidechain
1	G	94	ARG	Sidechain
1	H	141	TYR	Sidechain
1	H	169	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	H	184	ARG	Sidechain
1	H	185	TYR	Sidechain
1	H	43	TYR	Sidechain
1	H	73	TYR	Sidechain
1	H	94	ARG	Sidechain
1	I	141	TYR	Sidechain
1	I	169	ARG	Sidechain
1	I	184	ARG	Sidechain
1	I	185	TYR	Sidechain
1	I	43	TYR	Sidechain
1	I	73	TYR	Sidechain
1	I	94	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	1843	0	1863	41	0
1	B	1843	0	1863	67	0
1	C	1843	0	1863	68	0
1	D	1843	0	1863	67	0
1	E	1843	0	1863	65	0
1	F	1843	0	1863	66	0
1	G	1843	0	1863	67	0
1	H	1843	0	1863	66	0
1	I	1843	0	1863	41	0
All	All	16587	0	16767	353	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 11.

All (353) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:PHE:CD2	1:C:181:MET:SD	2.65	0.90
1:H:225:PHE:CD2	1:I:181:MET:SD	2.65	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:PHE:CD2	1:F:181:MET:SD	2.65	0.90
1:D:225:PHE:CD2	1:E:181:MET:SD	2.65	0.90
1:F:225:PHE:CD2	1:G:181:MET:SD	2.65	0.90
1:G:225:PHE:CD2	1:H:181:MET:SD	2.65	0.90
1:B:181:MET:SD	1:A:225:PHE:CD2	2.65	0.89
1:C:225:PHE:CD2	1:D:181:MET:SD	2.65	0.89
1:B:181:MET:CE	1:A:225:PHE:CD2	2.57	0.88
1:H:225:PHE:CD2	1:I:181:MET:CE	2.57	0.88
1:B:225:PHE:CD2	1:C:181:MET:CE	2.57	0.88
1:D:225:PHE:CD2	1:E:181:MET:CE	2.57	0.88
1:F:225:PHE:CD2	1:G:181:MET:CE	2.56	0.88
1:C:225:PHE:CD2	1:D:181:MET:CE	2.57	0.87
1:E:225:PHE:CD2	1:F:181:MET:CE	2.56	0.87
1:G:225:PHE:CD2	1:H:181:MET:CE	2.56	0.86
1:E:225:PHE:HD2	1:F:181:MET:CE	1.92	0.82
1:G:225:PHE:HD2	1:H:181:MET:CE	1.92	0.82
1:F:225:PHE:HD2	1:G:181:MET:CE	1.92	0.82
1:C:225:PHE:HD2	1:D:181:MET:CE	1.92	0.82
1:B:181:MET:CE	1:A:225:PHE:HD2	1.92	0.81
1:B:225:PHE:HD2	1:C:181:MET:CE	1.92	0.81
1:H:225:PHE:HD2	1:I:181:MET:CE	1.92	0.81
1:D:225:PHE:HD2	1:E:181:MET:CE	1.92	0.80
1:C:225:PHE:CE2	1:D:181:MET:HE1	2.17	0.80
1:F:225:PHE:CE2	1:G:181:MET:HE1	2.17	0.79
1:G:225:PHE:CE2	1:H:181:MET:HE1	2.17	0.79
1:B:225:PHE:CE2	1:C:181:MET:HE1	2.17	0.79
1:D:225:PHE:CE2	1:E:181:MET:HE1	2.17	0.79
1:B:181:MET:HE1	1:A:225:PHE:CE2	2.17	0.79
1:H:225:PHE:CE2	1:I:181:MET:HE1	2.17	0.78
1:E:225:PHE:CE2	1:F:181:MET:HE1	2.17	0.78
1:B:160:LEU:HD21	1:A:225:PHE:CZ	2.20	0.77
1:F:225:PHE:CZ	1:G:160:LEU:HD21	2.20	0.77
1:C:225:PHE:CZ	1:D:160:LEU:HD21	2.20	0.77
1:G:225:PHE:CZ	1:H:160:LEU:HD21	2.20	0.77
1:H:225:PHE:CZ	1:I:160:LEU:HD21	2.20	0.77
1:D:225:PHE:CZ	1:E:160:LEU:HD21	2.20	0.77
1:E:225:PHE:CZ	1:F:160:LEU:HD21	2.20	0.76
1:G:225:PHE:CE2	1:H:181:MET:SD	2.79	0.76
1:H:225:PHE:CE2	1:I:181:MET:SD	2.79	0.76
1:B:225:PHE:CZ	1:C:160:LEU:HD21	2.20	0.76
1:B:181:MET:SD	1:A:225:PHE:CE2	2.79	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:PHE:CE2	1:D:181:MET:SD	2.79	0.76
1:D:225:PHE:CE2	1:E:181:MET:SD	2.79	0.75
1:B:225:PHE:CE2	1:C:181:MET:SD	2.79	0.75
1:E:225:PHE:CE2	1:F:181:MET:SD	2.79	0.74
1:F:225:PHE:CE2	1:G:181:MET:SD	2.79	0.74
1:B:216:THR:HG21	1:C:175:LYS:HG3	1.73	0.70
1:F:216:THR:HG21	1:G:175:LYS:HG3	1.73	0.70
1:E:216:THR:HG21	1:F:175:LYS:HG3	1.73	0.70
1:B:175:LYS:HG3	1:A:216:THR:HG21	1.73	0.70
1:H:216:THR:HG21	1:I:175:LYS:HG3	1.73	0.70
1:C:225:PHE:CE2	1:D:181:MET:CE	2.75	0.70
1:C:216:THR:HG21	1:D:175:LYS:HG3	1.73	0.69
1:D:225:PHE:CE2	1:E:181:MET:CE	2.75	0.69
1:B:181:MET:CE	1:A:225:PHE:CE2	2.75	0.69
1:B:225:PHE:CE2	1:C:181:MET:CE	2.75	0.69
1:G:216:THR:HG21	1:H:175:LYS:HG3	1.73	0.69
1:G:225:PHE:CE2	1:H:181:MET:CE	2.75	0.69
1:D:216:THR:HG21	1:E:175:LYS:HG3	1.73	0.69
1:H:225:PHE:HE2	1:I:181:MET:HE1	1.57	0.69
1:F:225:PHE:CE2	1:G:181:MET:CE	2.75	0.69
1:C:225:PHE:HE2	1:D:181:MET:HE1	1.57	0.69
1:E:225:PHE:HE2	1:F:181:MET:HE1	1.57	0.69
1:H:225:PHE:CE2	1:I:181:MET:CE	2.75	0.69
1:E:225:PHE:CE2	1:F:181:MET:CE	2.75	0.68
1:D:140:VAL:HG13	1:D:208:VAL:HG12	1.77	0.67
1:H:140:VAL:HG13	1:H:208:VAL:HG12	1.77	0.67
1:F:225:PHE:HE2	1:G:181:MET:HE1	1.57	0.67
1:B:225:PHE:HE2	1:C:181:MET:HE1	1.57	0.66
1:G:225:PHE:HE2	1:H:181:MET:HE1	1.57	0.66
1:D:225:PHE:HD2	1:E:181:MET:HE3	1.60	0.66
1:G:140:VAL:HG13	1:G:208:VAL:HG12	1.77	0.66
1:G:225:PHE:HD2	1:H:181:MET:HE3	1.60	0.66
1:B:181:MET:HE3	1:A:225:PHE:HD2	1.60	0.66
1:C:140:VAL:HG13	1:C:208:VAL:HG12	1.77	0.66
1:E:140:VAL:HG13	1:E:208:VAL:HG12	1.77	0.66
1:A:140:VAL:HG13	1:A:208:VAL:HG12	1.77	0.66
1:C:225:PHE:HD2	1:D:181:MET:HE3	1.60	0.66
1:I:140:VAL:HG13	1:I:208:VAL:HG12	1.77	0.66
1:B:140:VAL:HG13	1:B:208:VAL:HG12	1.77	0.66
1:B:181:MET:HE1	1:A:225:PHE:HE2	1.57	0.66
1:D:225:PHE:HE2	1:E:181:MET:HE1	1.57	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:PHE:HD2	1:F:181:MET:HE3	1.60	0.65
1:H:225:PHE:HD2	1:I:181:MET:HE3	1.60	0.65
1:B:225:PHE:HD2	1:C:181:MET:HE3	1.60	0.65
1:F:140:VAL:HG13	1:F:208:VAL:HG12	1.77	0.65
1:F:225:PHE:HD2	1:G:181:MET:HE3	1.60	0.65
1:H:106:LYS:O	1:H:110:VAL:HG22	1.98	0.65
1:B:216:THR:CG2	1:C:175:LYS:HG3	2.27	0.64
1:A:106:LYS:O	1:A:110:VAL:HG22	1.97	0.64
1:D:216:THR:CG2	1:E:175:LYS:HG3	2.27	0.64
1:B:175:LYS:HG3	1:A:216:THR:CG2	2.27	0.64
1:C:106:LYS:O	1:C:110:VAL:HG22	1.97	0.64
1:G:216:THR:CG2	1:H:175:LYS:HG3	2.27	0.64
1:H:216:THR:CG2	1:I:175:LYS:HG3	2.27	0.64
1:E:106:LYS:O	1:E:110:VAL:HG22	1.97	0.64
1:E:216:THR:CG2	1:F:175:LYS:HG3	2.27	0.64
1:F:216:THR:CG2	1:G:175:LYS:HG3	2.27	0.64
1:B:175:LYS:HD2	1:A:216:THR:CG2	2.28	0.64
1:I:106:LYS:O	1:I:110:VAL:HG22	1.97	0.64
1:G:106:LYS:O	1:G:110:VAL:HG22	1.98	0.64
1:G:216:THR:CG2	1:H:175:LYS:HD2	2.28	0.64
1:E:216:THR:CG2	1:F:175:LYS:HD2	2.28	0.63
1:F:216:THR:CG2	1:G:175:LYS:HD2	2.28	0.63
1:D:106:LYS:O	1:D:110:VAL:HG22	1.97	0.63
1:B:106:LYS:O	1:B:110:VAL:HG22	1.97	0.63
1:C:216:THR:CG2	1:D:175:LYS:HD2	2.28	0.63
1:B:216:THR:CG2	1:C:175:LYS:HD2	2.28	0.63
1:F:106:LYS:O	1:F:110:VAL:HG22	1.97	0.63
1:C:216:THR:CG2	1:D:175:LYS:HG3	2.27	0.63
1:H:216:THR:CG2	1:I:175:LYS:HD2	2.28	0.63
1:D:216:THR:CG2	1:E:175:LYS:HD2	2.28	0.63
1:B:225:PHE:CD2	1:C:181:MET:HE1	2.38	0.59
1:I:133:THR:HG22	1:I:134:TRP:H	1.68	0.59
1:B:133:THR:HG22	1:B:134:TRP:H	1.68	0.58
1:C:133:THR:HG22	1:C:134:TRP:H	1.68	0.58
1:F:133:THR:HG22	1:F:134:TRP:H	1.68	0.58
1:H:133:THR:HG22	1:H:134:TRP:H	1.68	0.58
1:E:133:THR:HG22	1:E:134:TRP:H	1.68	0.58
1:G:133:THR:HG22	1:G:134:TRP:H	1.68	0.57
1:D:133:THR:HG22	1:D:134:TRP:H	1.68	0.57
1:A:133:THR:HG22	1:A:134:TRP:H	1.68	0.56
1:D:216:THR:CG2	1:E:175:LYS:CG	2.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:PHE:CE2	1:C:160:LEU:HD21	2.41	0.56
1:F:225:PHE:CE2	1:G:160:LEU:HD21	2.41	0.56
1:H:225:PHE:CE2	1:I:160:LEU:HD21	2.41	0.56
1:G:216:THR:CG2	1:H:175:LYS:CG	2.84	0.55
1:B:216:THR:CG2	1:C:175:LYS:CG	2.84	0.55
1:C:216:THR:CG2	1:D:175:LYS:CG	2.84	0.55
1:E:216:THR:CG2	1:F:175:LYS:CG	2.84	0.55
1:H:216:THR:CG2	1:I:175:LYS:CG	2.84	0.55
1:E:225:PHE:CE2	1:F:160:LEU:HD21	2.41	0.55
1:B:175:LYS:CG	1:A:216:THR:CG2	2.84	0.55
1:F:216:THR:CG2	1:G:175:LYS:CG	2.84	0.55
1:D:225:PHE:CE2	1:E:160:LEU:HD21	2.41	0.55
1:G:225:PHE:CD2	1:H:181:MET:HE1	2.38	0.55
1:G:225:PHE:CE2	1:H:160:LEU:HD21	2.41	0.55
1:F:225:PHE:CD2	1:G:181:MET:HE1	2.38	0.54
1:B:160:LEU:HD21	1:A:225:PHE:CE2	2.41	0.54
1:C:225:PHE:CE2	1:D:160:LEU:HD21	2.41	0.54
1:G:216:THR:HG23	1:H:175:LYS:HD2	1.90	0.53
1:B:175:LYS:HD2	1:A:216:THR:HG23	1.90	0.53
1:C:216:THR:HG23	1:D:175:LYS:HD2	1.90	0.52
1:D:216:THR:HG23	1:E:175:LYS:HD2	1.90	0.52
1:H:216:THR:HG23	1:I:175:LYS:HD2	1.90	0.52
1:B:216:THR:HG23	1:C:175:LYS:HD2	1.90	0.52
1:F:216:THR:HG23	1:G:175:LYS:HD2	1.90	0.52
1:E:216:THR:HG23	1:F:175:LYS:HD2	1.90	0.52
1:F:44:ILE:HG21	1:G:9:VAL:HG13	1.92	0.52
1:B:9:VAL:HG13	1:A:44:ILE:HG21	1.92	0.52
1:D:225:PHE:CD2	1:E:181:MET:HE1	2.38	0.51
1:B:44:ILE:HG21	1:C:9:VAL:HG13	1.92	0.51
1:D:44:ILE:HG21	1:E:9:VAL:HG13	1.92	0.51
1:C:44:ILE:HG21	1:D:9:VAL:HG13	1.92	0.51
1:C:225:PHE:CD2	1:D:181:MET:HE1	2.38	0.51
1:G:44:ILE:HG21	1:H:9:VAL:HG13	1.92	0.51
1:B:225:PHE:HD2	1:C:181:MET:SD	2.29	0.51
1:E:44:ILE:HG21	1:F:9:VAL:HG13	1.92	0.50
1:H:44:ILE:HG21	1:I:9:VAL:HG13	1.92	0.50
1:E:225:PHE:CD2	1:F:181:MET:HE1	2.38	0.49
1:A:43:TYR:CG	1:A:145:PHE:CZ	3.01	0.48
1:D:43:TYR:CG	1:D:145:PHE:CZ	3.01	0.48
1:H:43:TYR:CG	1:H:145:PHE:CZ	3.01	0.48
1:E:43:TYR:CG	1:E:145:PHE:CZ	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:LEU:HD22	1:F:6:PHE:CE2	2.49	0.48
1:F:43:TYR:CG	1:F:145:PHE:CZ	3.01	0.48
1:G:43:TYR:CG	1:G:145:PHE:CZ	3.01	0.48
1:B:63:LEU:HD22	1:C:6:PHE:CE2	2.49	0.48
1:C:43:TYR:CG	1:C:145:PHE:CZ	3.01	0.48
1:B:223:ARG:HE	1:B:223:ARG:HA	1.79	0.48
1:H:223:ARG:HE	1:H:223:ARG:HA	1.79	0.48
1:I:43:TYR:CG	1:I:145:PHE:CZ	3.01	0.48
1:A:223:ARG:HE	1:A:223:ARG:HA	1.79	0.48
1:C:63:LEU:HD22	1:D:6:PHE:CE2	2.49	0.48
1:D:223:ARG:HE	1:D:223:ARG:HA	1.79	0.48
1:E:223:ARG:HE	1:E:223:ARG:HA	1.79	0.48
1:H:63:LEU:HD22	1:I:6:PHE:CE2	2.49	0.48
1:B:43:TYR:CG	1:B:145:PHE:CZ	3.01	0.48
1:G:223:ARG:HE	1:G:223:ARG:HA	1.79	0.48
1:B:6:PHE:CE2	1:A:63:LEU:HD22	2.49	0.47
1:G:63:LEU:HD22	1:H:6:PHE:CE2	2.49	0.47
1:C:223:ARG:HE	1:C:223:ARG:HA	1.79	0.47
1:D:63:LEU:HD22	1:E:6:PHE:CE2	2.49	0.47
1:F:63:LEU:HD22	1:G:6:PHE:CE2	2.49	0.47
1:F:223:ARG:HE	1:F:223:ARG:HA	1.79	0.47
1:I:223:ARG:HE	1:I:223:ARG:HA	1.79	0.47
1:C:223:ARG:HA	1:C:223:ARG:NE	2.31	0.46
1:F:223:ARG:HA	1:F:223:ARG:NE	2.31	0.46
1:I:223:ARG:HA	1:I:223:ARG:NE	2.31	0.46
1:B:223:ARG:HA	1:B:223:ARG:NE	2.31	0.46
1:G:223:ARG:HA	1:G:223:ARG:NE	2.31	0.46
1:E:216:THR:HG22	1:F:175:LYS:HD2	1.98	0.46
1:E:223:ARG:HA	1:E:223:ARG:NE	2.31	0.45
1:B:175:LYS:HD2	1:A:216:THR:HG22	1.98	0.45
1:E:92:LEU:HD13	1:E:92:LEU:C	2.42	0.45
1:F:225:PHE:HD2	1:G:181:MET:SD	2.29	0.45
1:D:223:ARG:HA	1:D:223:ARG:NE	2.31	0.45
1:G:69:LYS:HE2	1:H:3:GLU:OE1	2.17	0.45
1:H:216:THR:HG22	1:I:175:LYS:HD2	1.98	0.45
1:H:92:LEU:C	1:H:92:LEU:HD13	2.42	0.45
1:C:92:LEU:C	1:C:92:LEU:HD13	2.42	0.45
1:D:69:LYS:HE2	1:E:3:GLU:OE1	2.17	0.45
1:I:92:LEU:HD13	1:I:92:LEU:C	2.42	0.45
1:C:69:LYS:HE2	1:D:3:GLU:OE1	2.17	0.45
1:C:216:THR:CG2	1:D:175:LYS:CD	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:PHE:HE2	1:C:160:LEU:HD11	1.82	0.45
1:F:92:LEU:C	1:F:92:LEU:HD13	2.42	0.45
1:F:225:PHE:HE2	1:G:160:LEU:HD11	1.82	0.45
1:H:223:ARG:HA	1:H:223:ARG:NE	2.31	0.45
1:B:92:LEU:HD13	1:B:92:LEU:C	2.42	0.45
1:A:223:ARG:HA	1:A:223:ARG:NE	2.31	0.45
1:D:216:THR:CG2	1:E:175:LYS:CD	2.95	0.45
1:G:216:THR:CG2	1:H:175:LYS:CD	2.95	0.45
1:B:3:GLU:OE1	1:A:69:LYS:HE2	2.17	0.45
1:C:225:PHE:HE2	1:D:160:LEU:HD11	1.82	0.45
1:G:92:LEU:HD13	1:G:92:LEU:C	2.42	0.45
1:G:216:THR:HG22	1:H:175:LYS:HD2	1.98	0.45
1:H:69:LYS:HE2	1:I:3:GLU:OE1	2.17	0.45
1:B:181:MET:HE1	1:A:225:PHE:CD2	2.38	0.45
1:D:92:LEU:C	1:D:92:LEU:HD13	2.42	0.45
1:D:225:PHE:HE2	1:E:160:LEU:HD11	1.82	0.45
1:F:69:LYS:HE2	1:G:3:GLU:OE1	2.17	0.45
1:F:216:THR:HG22	1:G:175:LYS:HD2	1.98	0.45
1:G:225:PHE:HE2	1:H:160:LEU:HD11	1.82	0.45
1:I:38:HIS:CD2	1:I:68:TRP:HB2	2.52	0.44
1:B:160:LEU:HD11	1:A:225:PHE:HE2	1.82	0.44
1:E:225:PHE:HE2	1:F:160:LEU:HD11	1.82	0.44
1:B:38:HIS:CD2	1:B:68:TRP:HB2	2.52	0.44
1:D:216:THR:HG22	1:E:175:LYS:HD2	1.98	0.44
1:F:216:THR:CG2	1:G:175:LYS:CD	2.95	0.44
1:B:216:THR:HG22	1:C:175:LYS:HD2	1.98	0.44
1:A:38:HIS:CD2	1:A:68:TRP:HB2	2.52	0.44
1:G:38:HIS:CD2	1:G:68:TRP:HB2	2.52	0.44
1:H:225:PHE:HE2	1:I:160:LEU:HD11	1.82	0.44
1:B:69:LYS:HE2	1:C:3:GLU:OE1	2.17	0.44
1:A:92:LEU:C	1:A:92:LEU:HD13	2.42	0.44
1:C:216:THR:HG22	1:D:175:LYS:HD2	1.98	0.44
1:H:225:PHE:CD2	1:I:181:MET:HE1	2.38	0.44
1:B:44:ILE:HG21	1:C:9:VAL:CG1	2.48	0.44
1:E:31:THR:HA	1:E:34:LEU:HB3	1.99	0.44
1:E:38:HIS:CD2	1:E:68:TRP:HB2	2.52	0.44
1:E:69:LYS:HE2	1:F:3:GLU:OE1	2.17	0.44
1:D:38:HIS:CD2	1:D:68:TRP:HB2	2.52	0.44
1:C:31:THR:HA	1:C:34:LEU:HB3	1.99	0.44
1:C:164:ILE:HA	1:C:167:VAL:HG22	2.00	0.44
1:D:44:ILE:HG21	1:E:9:VAL:CG1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:THR:CG2	1:F:175:LYS:CD	2.95	0.44
1:F:38:HIS:CD2	1:F:68:TRP:HB2	2.52	0.44
1:G:164:ILE:HA	1:G:167:VAL:HG22	2.00	0.44
1:H:38:HIS:CD2	1:H:68:TRP:HB2	2.52	0.44
1:C:38:HIS:CD2	1:C:68:TRP:HB2	2.52	0.43
1:F:31:THR:HA	1:F:34:LEU:HB3	1.99	0.43
1:H:31:THR:HA	1:H:34:LEU:HB3	1.99	0.43
1:I:31:THR:HA	1:I:34:LEU:HB3	1.99	0.43
1:B:44:ILE:HD11	1:B:123:ILE:HB	2.00	0.43
1:D:31:THR:HA	1:D:34:LEU:HB3	1.99	0.43
1:G:31:THR:HA	1:G:34:LEU:HB3	1.99	0.43
1:B:216:THR:CG2	1:C:175:LYS:CD	2.95	0.43
1:E:44:ILE:HG21	1:F:9:VAL:CG1	2.48	0.43
1:F:44:ILE:HG21	1:G:9:VAL:CG1	2.48	0.43
1:F:44:ILE:HD11	1:F:123:ILE:HB	2.00	0.43
1:H:216:THR:CG2	1:I:175:LYS:CD	2.95	0.43
1:I:164:ILE:HA	1:I:167:VAL:HG22	2.00	0.43
1:B:164:ILE:HA	1:B:167:VAL:HG22	2.00	0.43
1:C:44:ILE:HD11	1:C:123:ILE:HB	2.01	0.43
1:G:44:ILE:HG21	1:H:9:VAL:CG1	2.48	0.43
1:H:164:ILE:HA	1:H:167:VAL:HG22	2.00	0.43
1:B:31:THR:HA	1:B:34:LEU:HB3	1.99	0.43
1:I:44:ILE:HD11	1:I:123:ILE:HB	2.01	0.43
1:A:164:ILE:HA	1:A:167:VAL:HG22	2.00	0.43
1:G:44:ILE:HD11	1:G:123:ILE:HB	2.00	0.43
1:A:31:THR:HA	1:A:34:LEU:HB3	1.99	0.43
1:D:164:ILE:HA	1:D:167:VAL:HG22	2.00	0.43
1:E:44:ILE:HD11	1:E:123:ILE:HB	2.01	0.43
1:F:164:ILE:HA	1:F:167:VAL:HG22	2.00	0.43
1:B:9:VAL:CG1	1:A:44:ILE:HG21	2.48	0.43
1:B:175:LYS:CD	1:A:216:THR:CG2	2.95	0.43
1:E:64:ASN:HB3	1:F:5:GLU:HA	2.01	0.43
1:H:44:ILE:HG21	1:I:9:VAL:CG1	2.48	0.43
1:C:44:ILE:HG21	1:D:9:VAL:CG1	2.48	0.42
1:A:39:ILE:HG22	1:A:43:TYR:CE2	2.55	0.42
1:D:44:ILE:HD11	1:D:123:ILE:HB	2.01	0.42
1:D:104:LEU:C	1:D:104:LEU:HD13	2.44	0.42
1:G:104:LEU:C	1:G:104:LEU:HD13	2.45	0.42
1:H:39:ILE:HG22	1:H:43:TYR:CE2	2.55	0.42
1:A:104:LEU:HD13	1:A:104:LEU:C	2.45	0.42
1:D:39:ILE:HG22	1:D:43:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:ILE:HG22	1:E:43:TYR:CE2	2.55	0.42
1:H:44:ILE:HD11	1:H:123:ILE:HB	2.00	0.42
1:H:104:LEU:HD13	1:H:104:LEU:C	2.45	0.42
1:I:39:ILE:HG22	1:I:43:TYR:CE2	2.55	0.42
1:A:44:ILE:HD11	1:A:123:ILE:HB	2.00	0.42
1:E:104:LEU:HD13	1:E:104:LEU:C	2.45	0.42
1:E:133:THR:HB	1:E:213:TRP:CD1	2.55	0.42
1:B:104:LEU:C	1:B:104:LEU:HD13	2.45	0.42
1:D:133:THR:HB	1:D:213:TRP:CD1	2.55	0.42
1:B:5:GLU:HA	1:A:64:ASN:HB3	2.01	0.42
1:C:104:LEU:HD13	1:C:104:LEU:C	2.45	0.42
1:C:133:THR:HB	1:C:213:TRP:CD1	2.55	0.42
1:F:104:LEU:HD13	1:F:104:LEU:C	2.44	0.42
1:G:133:THR:HB	1:G:213:TRP:CD1	2.55	0.42
1:I:104:LEU:C	1:I:104:LEU:HD13	2.45	0.42
1:I:133:THR:HB	1:I:213:TRP:CD1	2.55	0.42
1:B:133:THR:HB	1:B:213:TRP:CD1	2.55	0.42
1:F:39:ILE:HG22	1:F:43:TYR:CE2	2.55	0.42
1:G:64:ASN:HB3	1:H:5:GLU:HA	2.01	0.42
1:C:39:ILE:HG22	1:C:43:TYR:CE2	2.55	0.42
1:C:64:ASN:HB3	1:D:5:GLU:HA	2.01	0.42
1:B:39:ILE:HG22	1:B:43:TYR:CE2	2.55	0.42
1:E:164:ILE:HA	1:E:167:VAL:HG22	2.00	0.42
1:H:133:THR:HB	1:H:213:TRP:CD1	2.55	0.42
1:A:133:THR:HB	1:A:213:TRP:CD1	2.55	0.41
1:C:225:PHE:HD2	1:D:181:MET:SD	2.29	0.41
1:G:39:ILE:HG22	1:G:43:TYR:CE2	2.55	0.41
1:I:160:LEU:HD13	1:I:180:THR:HG21	2.02	0.41
1:C:160:LEU:HD13	1:C:180:THR:HG21	2.02	0.41
1:F:133:THR:HB	1:F:213:TRP:CD1	2.55	0.41
1:F:160:LEU:HD13	1:F:180:THR:HG21	2.02	0.41
1:G:160:LEU:HD13	1:G:180:THR:HG21	2.02	0.41
1:B:64:ASN:HB3	1:C:5:GLU:HA	2.01	0.41
1:A:160:LEU:HD13	1:A:180:THR:HG21	2.02	0.41
1:B:160:LEU:HD13	1:B:180:THR:HG21	2.02	0.41
1:F:64:ASN:HB3	1:G:5:GLU:HA	2.01	0.41
1:D:64:ASN:HB3	1:E:5:GLU:HA	2.01	0.41
1:H:160:LEU:HD13	1:H:180:THR:HG21	2.02	0.41
1:D:160:LEU:HD13	1:D:180:THR:HG21	2.02	0.41
1:E:160:LEU:HD13	1:E:180:THR:HG21	2.02	0.41
1:H:64:ASN:HB3	1:I:5:GLU:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ILE:HG21	1:B:103:LEU:HD11	2.03	0.41
1:A:42:PHE:CD2	1:A:42:PHE:C	2.99	0.41
1:C:39:ILE:HG21	1:C:103:LEU:HD11	2.03	0.41
1:H:42:PHE:CD2	1:H:42:PHE:C	2.99	0.41
1:H:91:THR:H	1:H:94:ARG:HB2	1.86	0.41
1:H:39:ILE:HG21	1:H:103:LEU:HD11	2.03	0.41
1:D:91:THR:H	1:D:94:ARG:HB2	1.86	0.40
1:E:42:PHE:CD2	1:E:42:PHE:C	2.99	0.40
1:G:30:HIS:C	1:G:32:THR:H	2.29	0.40
1:B:30:HIS:C	1:B:32:THR:H	2.29	0.40
1:A:91:THR:H	1:A:94:ARG:HB2	1.87	0.40
1:C:42:PHE:CD2	1:C:42:PHE:C	2.99	0.40
1:E:91:THR:H	1:E:94:ARG:HB2	1.86	0.40
1:G:39:ILE:HG21	1:G:103:LEU:HD11	2.03	0.40
1:G:42:PHE:C	1:G:42:PHE:CD2	2.99	0.40
1:I:30:HIS:C	1:I:32:THR:H	2.29	0.40
1:D:42:PHE:C	1:D:42:PHE:CD2	2.99	0.40
1:F:39:ILE:HG21	1:F:103:LEU:HD11	2.03	0.40
1:D:39:ILE:HG21	1:D:103:LEU:HD11	2.03	0.40
1:F:42:PHE:CD2	1:F:42:PHE:C	2.99	0.40
1:B:42:PHE:CD2	1:B:42:PHE:C	2.99	0.40
1:C:91:THR:H	1:C:94:ARG:HB2	1.87	0.40
1:I:91:THR:H	1:I:94:ARG:HB2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	226/233 (97%)	206 (91%)	12 (5%)	8 (4%)	3	20
1	B	226/233 (97%)	206 (91%)	12 (5%)	8 (4%)	3	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	226/233 (97%)	206 (91%)	12 (5%)	8 (4%)	3	20
1	D	226/233 (97%)	206 (91%)	12 (5%)	8 (4%)	3	20
1	E	226/233 (97%)	206 (91%)	12 (5%)	8 (4%)	3	20
1	F	226/233 (97%)	206 (91%)	12 (5%)	8 (4%)	3	20
1	G	226/233 (97%)	206 (91%)	12 (5%)	8 (4%)	3	20
1	H	226/233 (97%)	206 (91%)	12 (5%)	8 (4%)	3	20
1	I	226/233 (97%)	206 (91%)	12 (5%)	8 (4%)	3	20
All	All	2034/2097 (97%)	1854 (91%)	108 (5%)	72 (4%)	4	20

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	82	ASN
1	B	211	LEU
1	B	218	VAL
1	B	219	SER
1	A	82	ASN
1	A	211	LEU
1	A	218	VAL
1	A	219	SER
1	C	82	ASN
1	C	211	LEU
1	C	218	VAL
1	C	219	SER
1	D	82	ASN
1	D	211	LEU
1	D	218	VAL
1	D	219	SER
1	E	82	ASN
1	E	211	LEU
1	E	218	VAL
1	E	219	SER
1	F	82	ASN
1	F	211	LEU
1	F	218	VAL
1	F	219	SER
1	G	82	ASN
1	G	211	LEU
1	G	218	VAL
1	G	219	SER

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Mol	Chain	Res	Type
1	H	82	ASN
1	H	211	LEU
1	H	218	VAL
1	H	219	SER
1	I	82	ASN
1	I	211	LEU
1	I	218	VAL
1	I	219	SER
1	B	132	ILE
1	B	156	ARG
1	A	132	ILE
1	A	156	ARG
1	C	132	ILE
1	C	156	ARG
1	D	132	ILE
1	D	156	ARG
1	E	132	ILE
1	E	156	ARG
1	F	132	ILE
1	F	156	ARG
1	G	132	ILE
1	G	156	ARG
1	H	132	ILE
1	H	156	ARG
1	I	132	ILE
1	I	156	ARG
1	B	86	PRO
1	A	86	PRO
1	C	86	PRO
1	D	86	PRO
1	E	86	PRO
1	F	86	PRO
1	G	86	PRO
1	H	86	PRO
1	I	86	PRO
1	B	19	PRO
1	A	19	PRO
1	C	19	PRO
1	D	19	PRO
1	E	19	PRO
1	F	19	PRO
1	G	19	PRO

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Mol	Chain	Res	Type
1	H	19	PRO
1	I	19	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	199/203 (98%)	178 (89%)	21 (11%)	6	21
1	B	199/203 (98%)	178 (89%)	21 (11%)	6	21
1	C	199/203 (98%)	178 (89%)	21 (11%)	6	21
1	D	199/203 (98%)	178 (89%)	21 (11%)	6	21
1	E	199/203 (98%)	178 (89%)	21 (11%)	6	21
1	F	199/203 (98%)	178 (89%)	21 (11%)	6	21
1	G	199/203 (98%)	178 (89%)	21 (11%)	6	21
1	H	199/203 (98%)	178 (89%)	21 (11%)	6	21
1	I	199/203 (98%)	178 (89%)	21 (11%)	6	21
All	All	1791/1827 (98%)	1602 (89%)	189 (11%)	9	21

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4	LEU
1	B	51	THR
1	B	78	PRO
1	B	81	ARG
1	B	92	LEU
1	B	93	HIS
1	B	104	LEU
1	B	106	LYS
1	B	122	ILE
1	B	125	PRO
1	B	138	GLU
1	B	149	GLU

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Mol	Chain	Res	Type
1	B	151	PHE
1	B	154	THR
1	B	162	ILE
1	B	164	ILE
1	B	174	PRO
1	B	194	THR
1	B	202	GLN
1	B	216	THR
1	B	218	VAL
1	A	4	LEU
1	A	51	THR
1	A	78	PRO
1	A	81	ARG
1	A	92	LEU
1	A	93	HIS
1	A	104	LEU
1	A	106	LYS
1	A	122	ILE
1	A	125	PRO
1	A	138	GLU
1	A	149	GLU
1	A	151	PHE
1	A	154	THR
1	A	162	ILE
1	A	164	ILE
1	A	174	PRO
1	A	194	THR
1	A	202	GLN
1	A	216	THR
1	A	218	VAL
1	C	4	LEU
1	C	51	THR
1	C	78	PRO
1	C	81	ARG
1	C	92	LEU
1	C	93	HIS
1	C	104	LEU
1	C	106	LYS
1	C	122	ILE
1	C	125	PRO
1	C	138	GLU
1	C	149	GLU

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Mol	Chain	Res	Type
1	C	151	PHE
1	C	154	THR
1	C	162	ILE
1	C	164	ILE
1	C	174	PRO
1	C	194	THR
1	C	202	GLN
1	C	216	THR
1	C	218	VAL
1	D	4	LEU
1	D	51	THR
1	D	78	PRO
1	D	81	ARG
1	D	92	LEU
1	D	93	HIS
1	D	104	LEU
1	D	106	LYS
1	D	122	ILE
1	D	125	PRO
1	D	138	GLU
1	D	149	GLU
1	D	151	PHE
1	D	154	THR
1	D	162	ILE
1	D	164	ILE
1	D	174	PRO
1	D	194	THR
1	D	202	GLN
1	D	216	THR
1	D	218	VAL
1	E	4	LEU
1	E	51	THR
1	E	78	PRO
1	E	81	ARG
1	E	92	LEU
1	E	93	HIS
1	E	104	LEU
1	E	106	LYS
1	E	122	ILE
1	E	125	PRO
1	E	138	GLU
1	E	149	GLU

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Mol	Chain	Res	Type
1	E	151	PHE
1	E	154	THR
1	E	162	ILE
1	E	164	ILE
1	E	174	PRO
1	E	194	THR
1	E	202	GLN
1	E	216	THR
1	E	218	VAL
1	F	4	LEU
1	F	51	THR
1	F	78	PRO
1	F	81	ARG
1	F	92	LEU
1	F	93	HIS
1	F	104	LEU
1	F	106	LYS
1	F	122	ILE
1	F	125	PRO
1	F	138	GLU
1	F	149	GLU
1	F	151	PHE
1	F	154	THR
1	F	162	ILE
1	F	164	ILE
1	F	174	PRO
1	F	194	THR
1	F	202	GLN
1	F	216	THR
1	F	218	VAL
1	G	4	LEU
1	G	51	THR
1	G	78	PRO
1	G	81	ARG
1	G	92	LEU
1	G	93	HIS
1	G	104	LEU
1	G	106	LYS
1	G	122	ILE
1	G	125	PRO
1	G	138	GLU
1	G	149	GLU

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Mol	Chain	Res	Type
1	G	151	PHE
1	G	154	THR
1	G	162	ILE
1	G	164	ILE
1	G	174	PRO
1	G	194	THR
1	G	202	GLN
1	G	216	THR
1	G	218	VAL
1	H	4	LEU
1	H	51	THR
1	H	78	PRO
1	H	81	ARG
1	H	92	LEU
1	H	93	HIS
1	H	104	LEU
1	H	106	LYS
1	H	122	ILE
1	H	125	PRO
1	H	138	GLU
1	H	149	GLU
1	H	151	PHE
1	H	154	THR
1	H	162	ILE
1	H	164	ILE
1	H	174	PRO
1	H	194	THR
1	H	202	GLN
1	H	216	THR
1	H	218	VAL
1	I	4	LEU
1	I	51	THR
1	I	78	PRO
1	I	81	ARG
1	I	92	LEU
1	I	93	HIS
1	I	104	LEU
1	I	106	LYS
1	I	122	ILE
1	I	125	PRO
1	I	138	GLU
1	I	149	GLU

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Mol	Chain	Res	Type
1	I	151	PHE
1	I	154	THR
1	I	162	ILE
1	I	164	ILE
1	I	174	PRO
1	I	194	THR
1	I	202	GLN
1	I	216	THR
1	I	218	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	7	HIS
1	B	38	HIS
1	B	64	ASN
1	B	217	ASN
1	A	38	HIS
1	A	64	ASN
1	A	217	ASN
1	C	7	HIS
1	C	38	HIS
1	C	64	ASN
1	C	217	ASN
1	D	7	HIS
1	D	38	HIS
1	D	64	ASN
1	D	217	ASN
1	E	7	HIS
1	E	38	HIS
1	E	64	ASN
1	E	217	ASN
1	F	38	HIS
1	F	64	ASN
1	F	217	ASN
1	G	7	HIS
1	G	38	HIS
1	G	64	ASN
1	G	217	ASN
1	H	7	HIS
1	H	38	HIS
1	H	64	ASN

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Mol	Chain	Res	Type
1	H	217	ASN
1	I	7	HIS
1	I	38	HIS
1	I	64	ASN
1	I	183	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 [i](#)

There are no chain breaks in this entry.

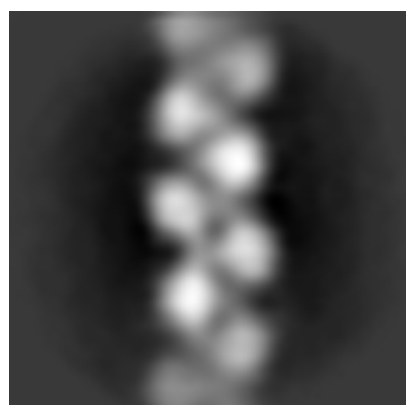
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11847. These allow visual inspection of the internal detail of the map and identification of artifacts.

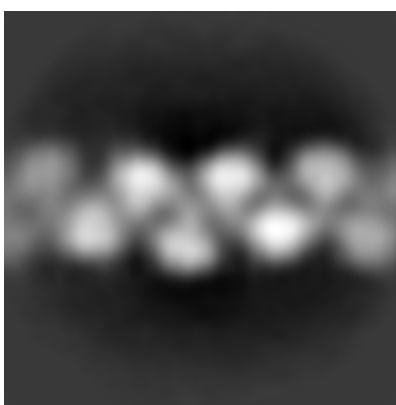
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

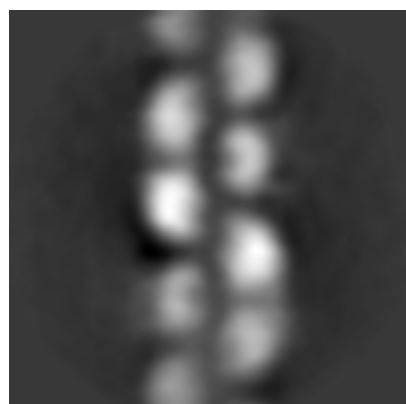


Z

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

6.2 Central slices [i](#)

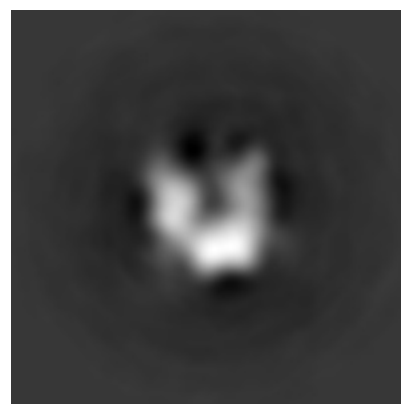
6.2.1 Primary map



X Index: 32



Y Index: 32

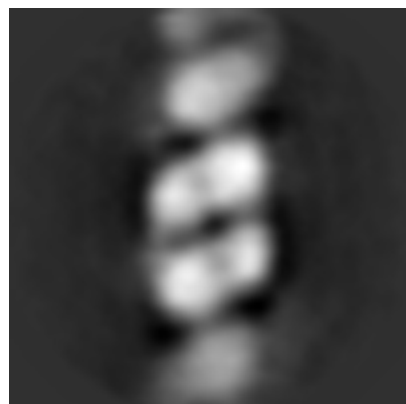


Z Index: 32

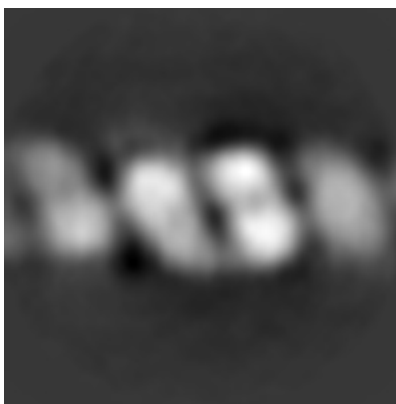
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

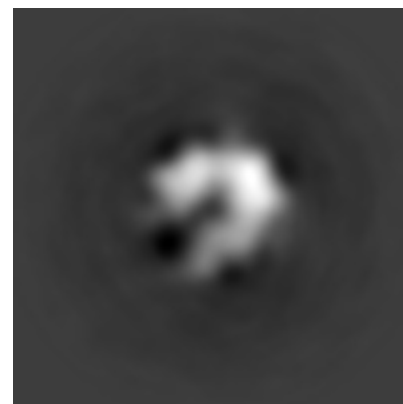
6.3.1 Primary map



X Index: 37



Y Index: 37

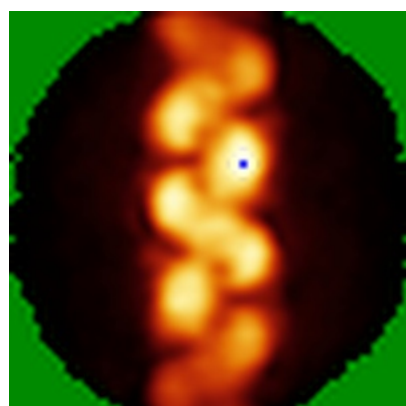


Z Index: 38

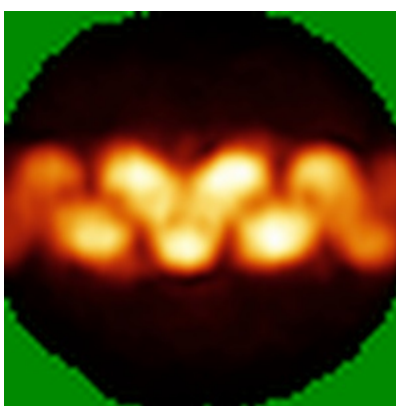
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.056. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

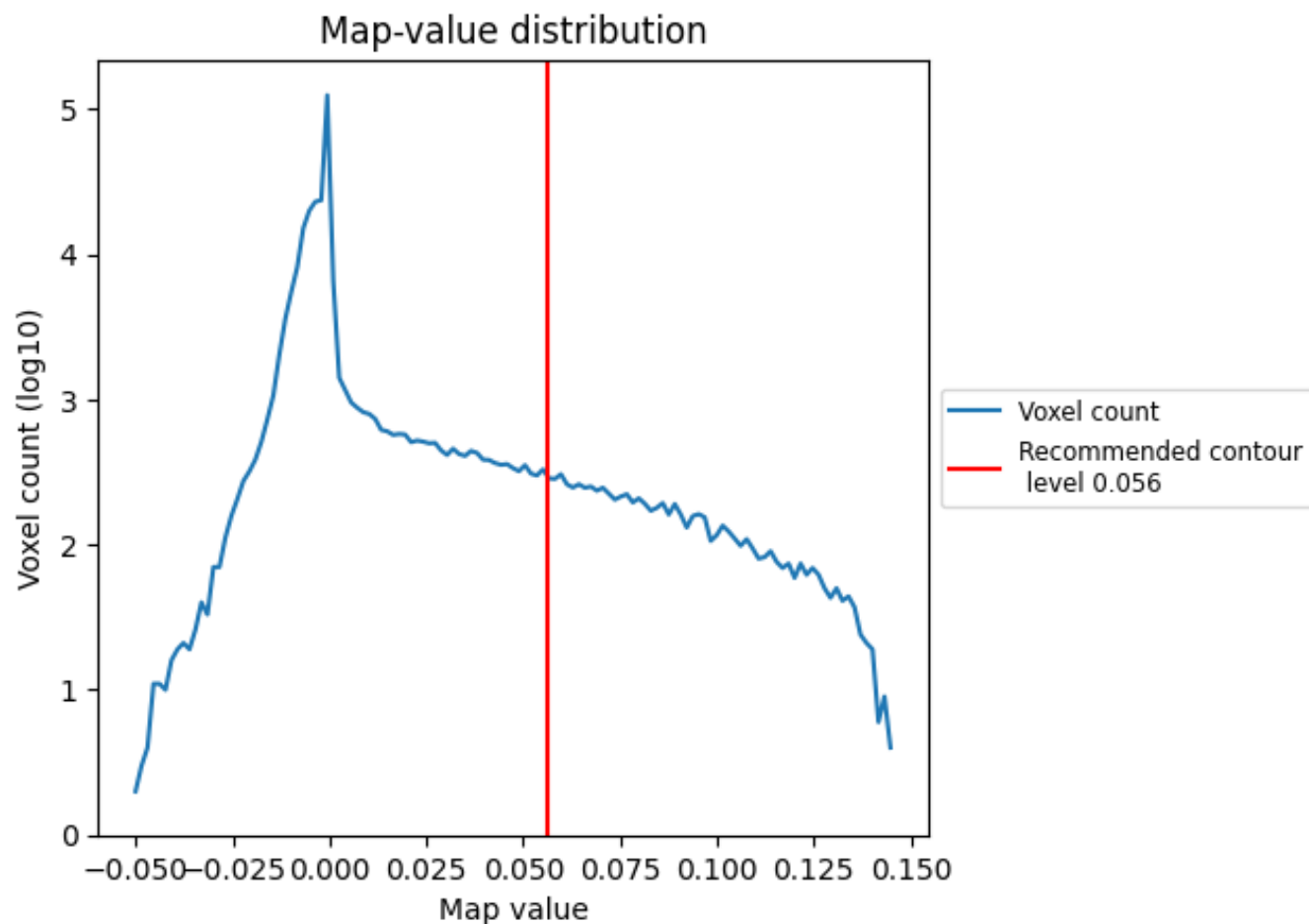
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

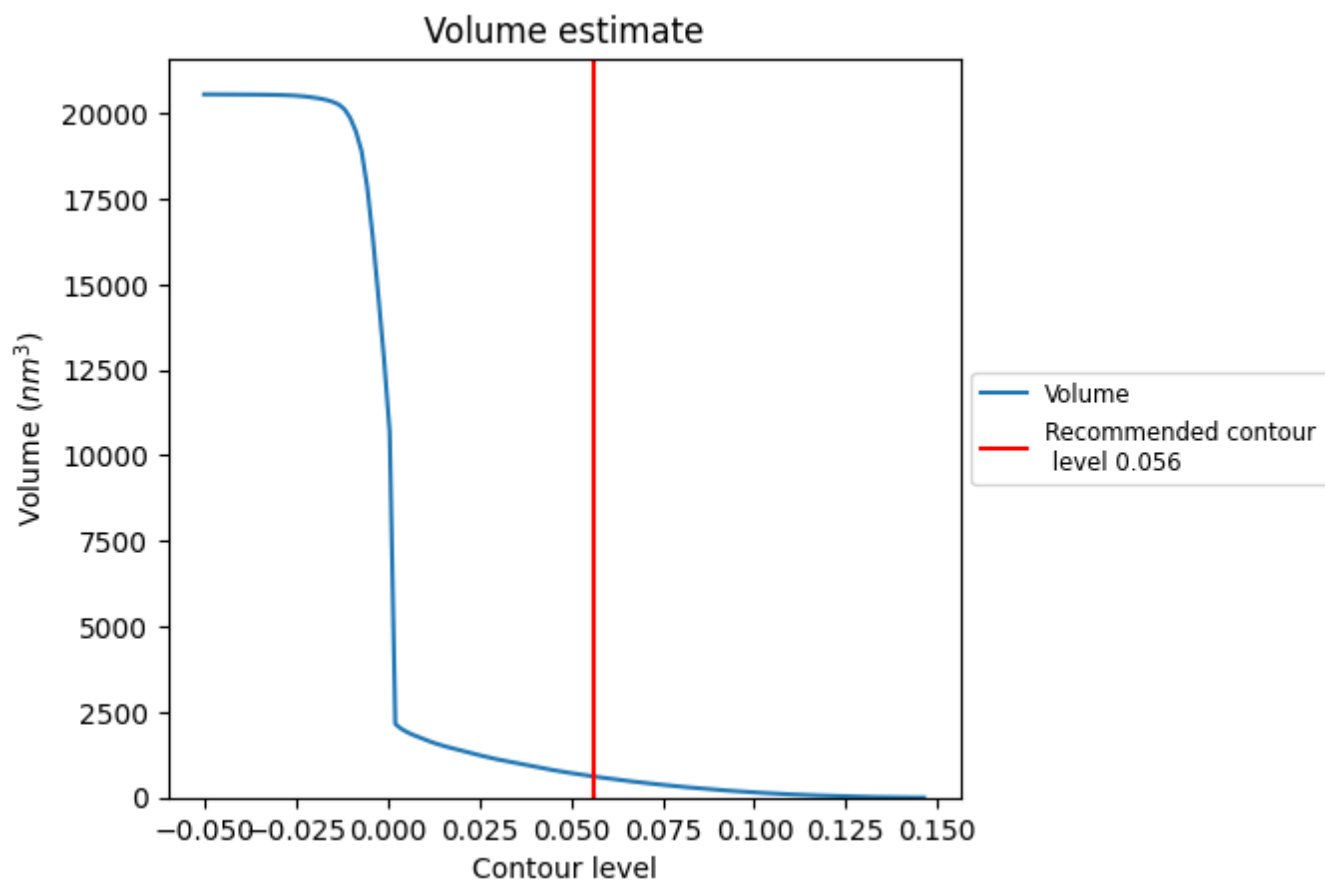
This section contains the results of statistical analysis of the map.

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.

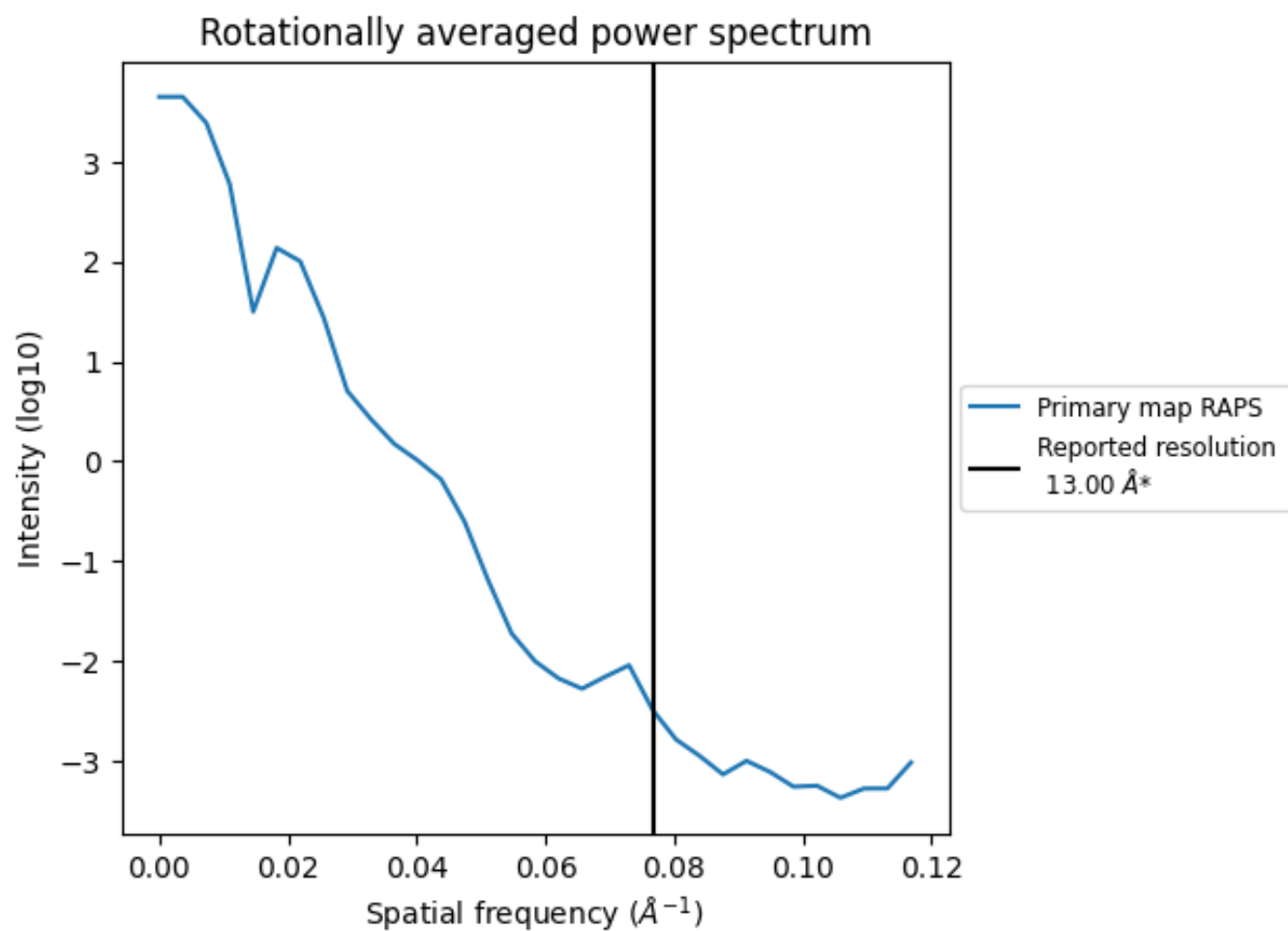
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 621 nm³; this corresponds to an approximate mass of 561 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 ⓘ

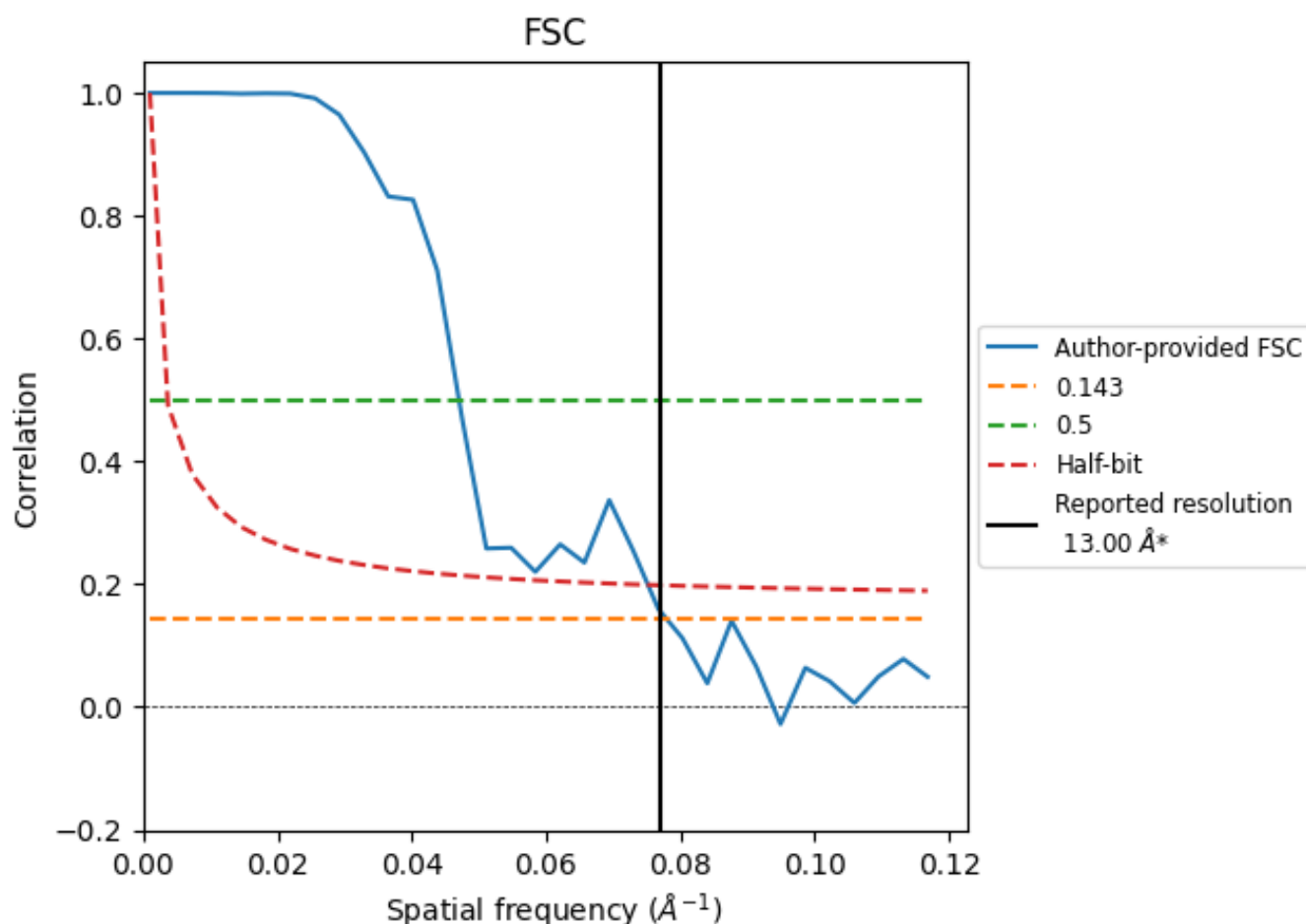


*Reported resolution corresponds to spatial frequency of 0.077 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.077 Å⁻¹

8.2 Resolution estimates [i](#)

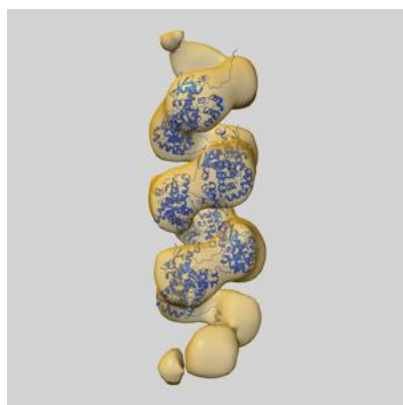
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	13.00	-	-
Author-provided FSC curve	12.84	21.28	13.32
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11847 and PDB model 7AOY. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

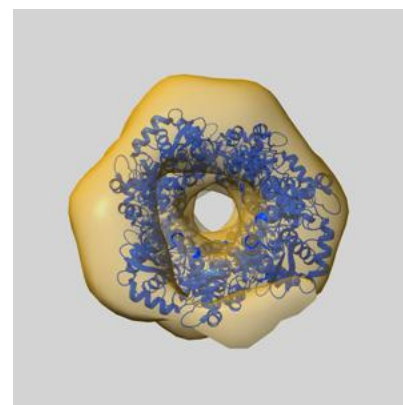
9.1 Map-model overlay [i](#)



X



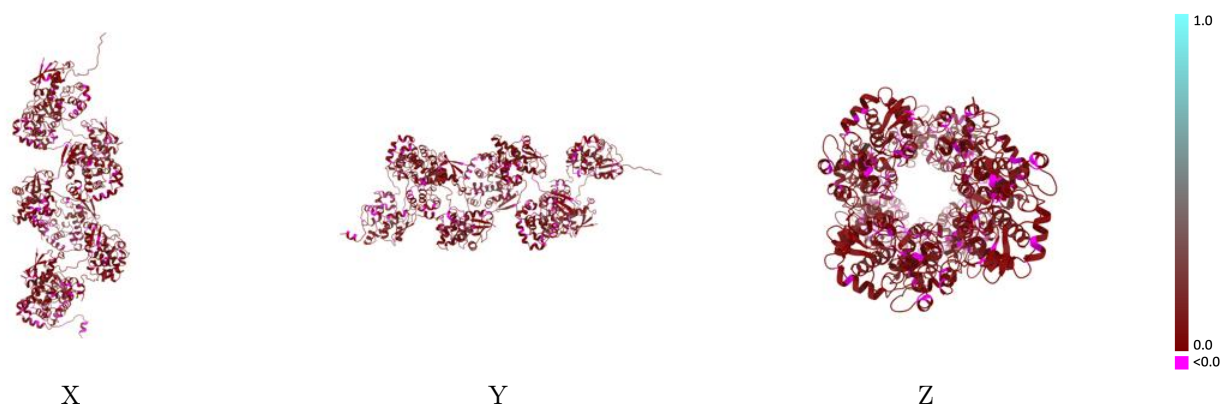
Y



Z

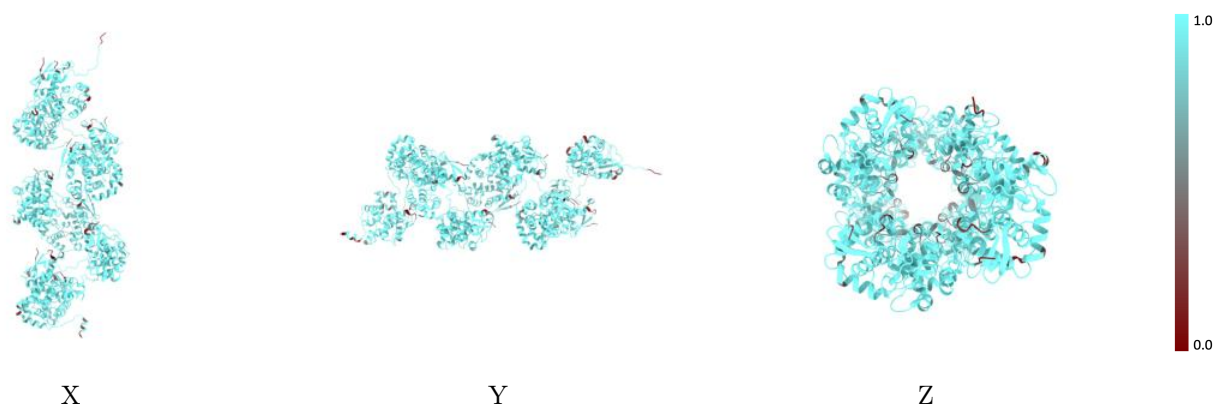
The images above show the 3D surface view of the map at the recommended contour level 0.056 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



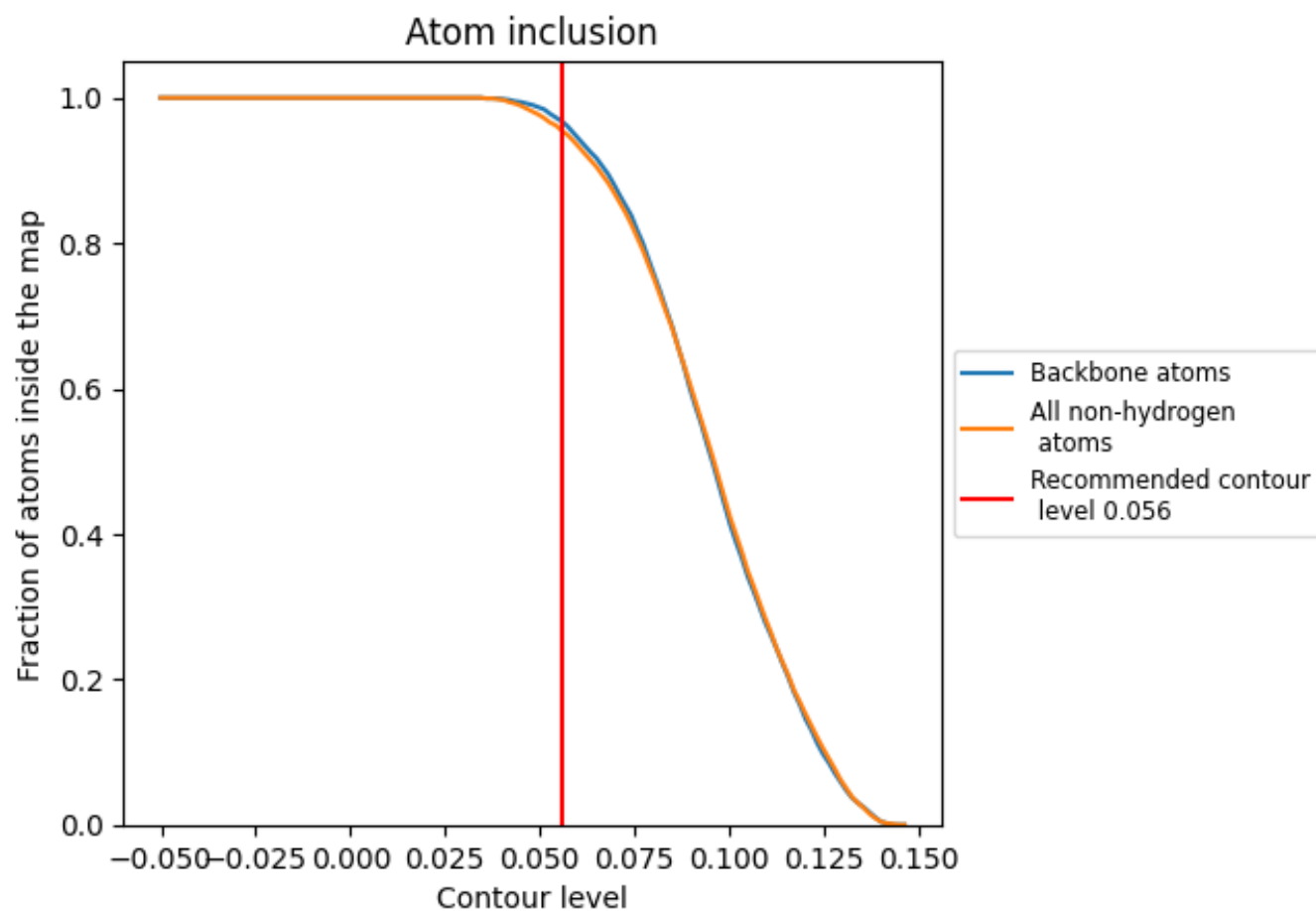
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.056).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% 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 (0.056) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9540	0.0720
A	0.9240	0.0730
B	0.9490	0.0760
C	0.9630	0.0720
D	0.9640	0.0710
E	0.9700	0.0720
F	0.9710	0.0710
G	0.9670	0.0720
H	0.9540	0.0740
I	0.9280	0.0710

1.0

0.0

<0.0