



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:32 PM UTC

PDB ID : 6SO3 / pdb_00006so3
EMDB ID : EMD-7029
Title : The interacting head motif in insect flight muscle myosin thick filaments
Authors : Morris, E.P.; Knupp, C.; Squire, J.M.
Deposited on : 2019-08-28
Resolution : 6.20 Å(reported)

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 : **NOT EXECUTED**
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

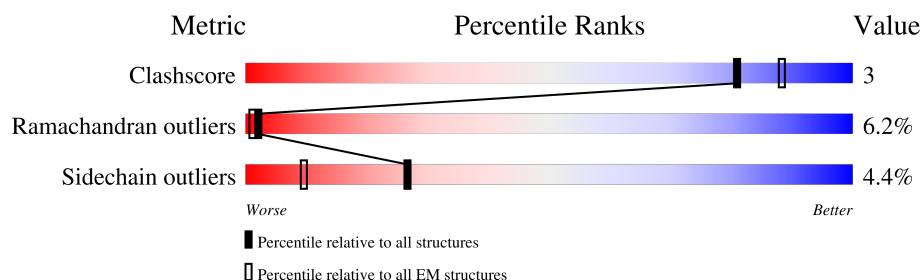
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	1953	43% 18% 20% . . 57%
1	B	1953	43% 16% 22% . 57%
2	C	156	100% 40% 48% 12%
2	D	156	100% 46% 46% 8%
3	E	196	100% 42% 47% 10% .
3	F	196	100% 34% 55% 10% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 37957 atoms, of which 18956 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 Myosin 2 heavy chain striated muscle.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	840	Total	C	H	N	O	S	0	0
			13499	4302	6760	1164	1245	28		
1	A	840	Total	C	H	N	O	S	0	0
			13498	4302	6760	1164	1244	28		

- Molecule 2 is a protein called Myosin 2 essential light chain striated muscle.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	156	Total	C	H	N	O	S	0	0
			2460	779	1227	199	247	8		
2	C	156	Total	C	H	N	O	S	0	0
			2460	779	1227	199	247	8		

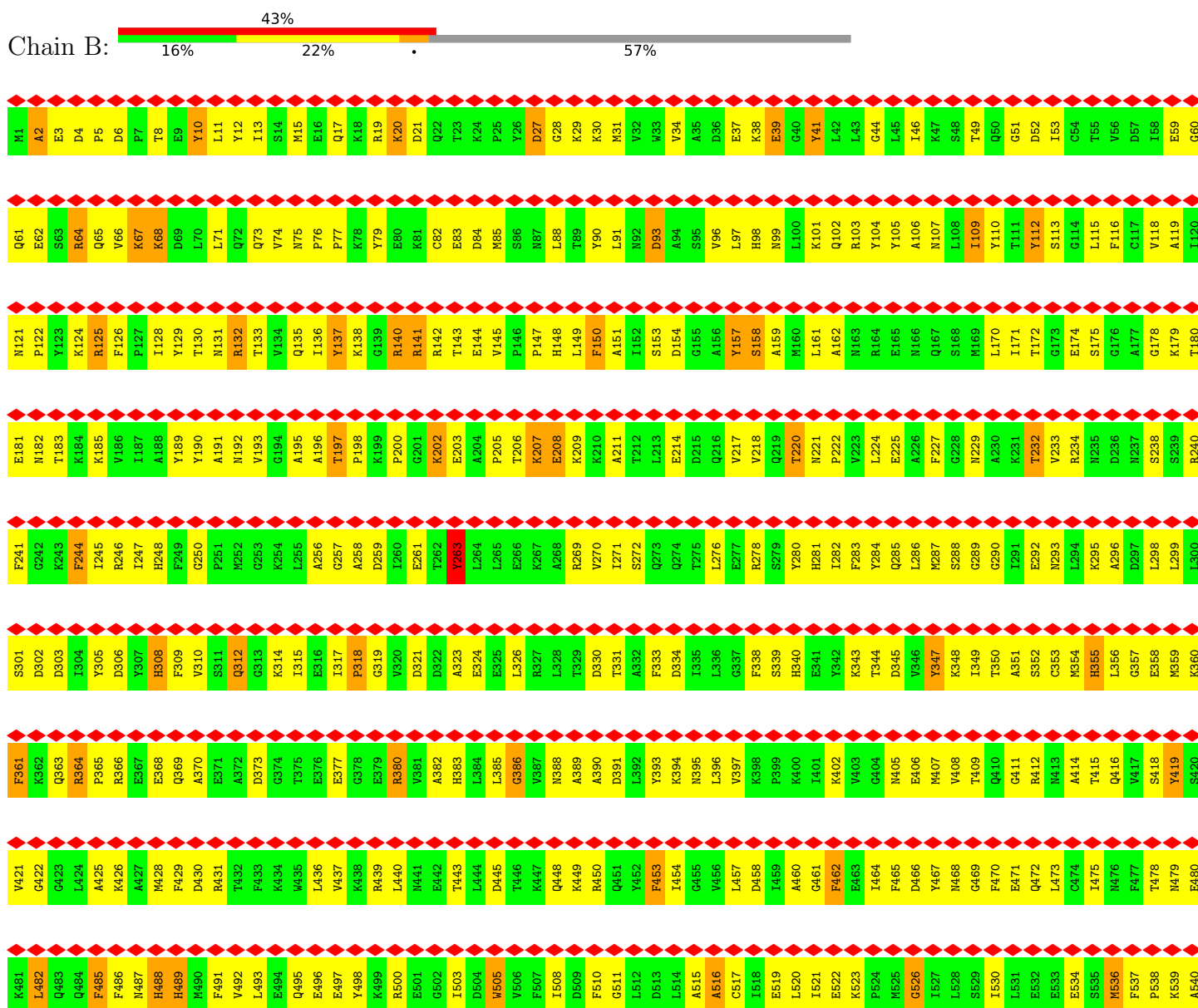
- Molecule 3 is a protein called Myosin 2 regulatory light chain striated muscle.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	F	196	Total	C	H	N	O	S	0	0
			3020	952	1491	257	314	6		
3	E	196	Total	C	H	N	O	S	0	0
			3020	952	1491	257	314	6		

3 Residue-property plots

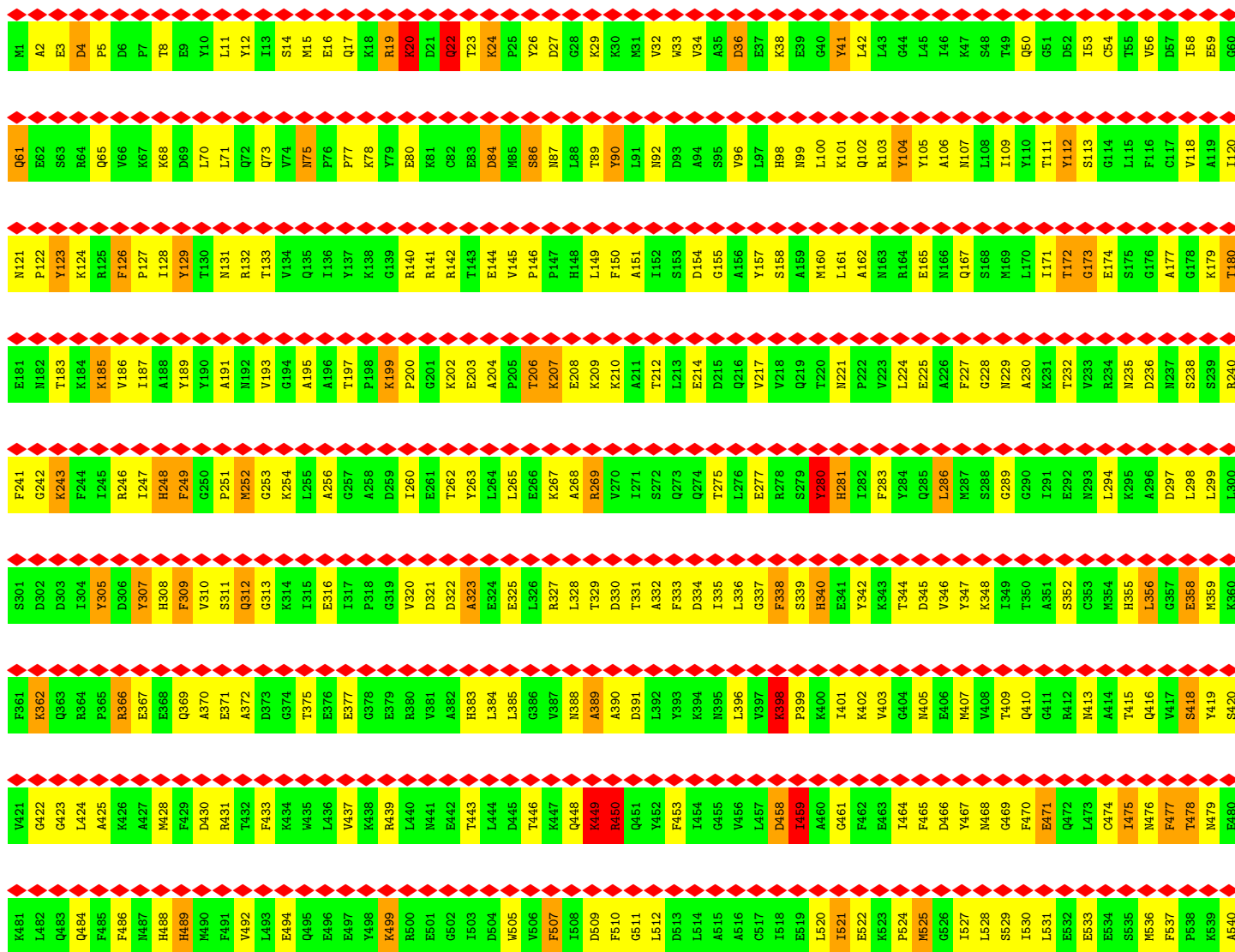
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Myosin 2 heavy chain striated muscle



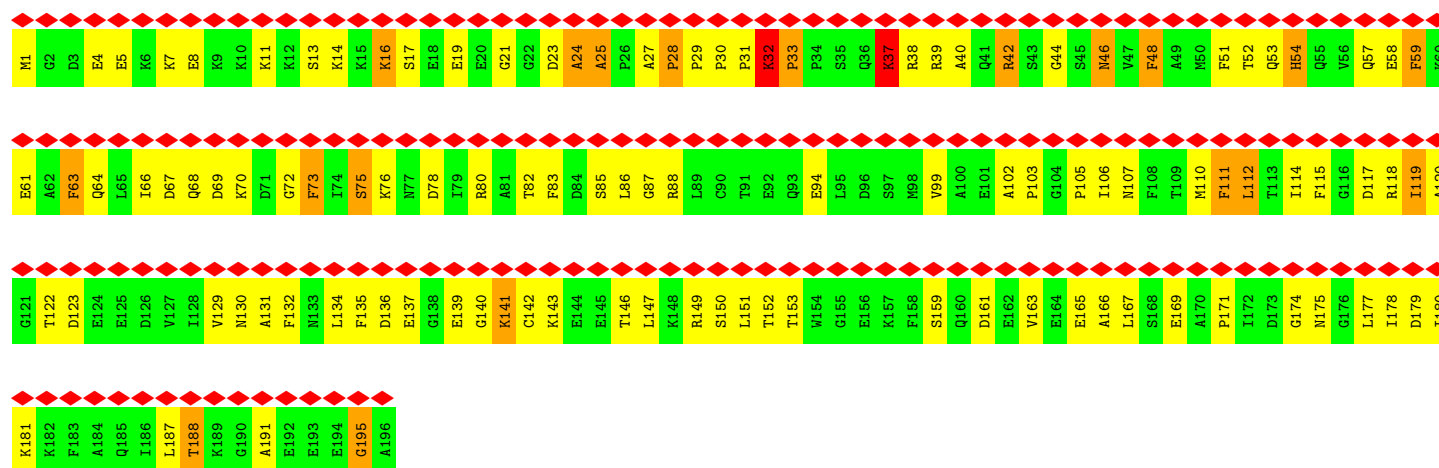


- Molecule 1: Myosin 2 heavy chain striated muscle





- Molecule 3: Myosin 2 regulatory light chain striated muscle



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=33.98°, rise=145 Å, axial sym=C4	Depositor
Number of segments used	24000	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 ($e^-/\text{Å}^2$)	65	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-20 (5k x 3k)	Depositor
Maximum map value	0.181	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	528.336, 528.336, 528.336	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.223, 1.223, 1.223	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.21	233/6882 (3.4%)	2.44	426/9279 (4.6%)
1	B	2.22	232/6883 (3.4%)	2.53	533/9280 (5.7%)
2	C	2.21	45/1251 (3.6%)	2.43	88/1674 (5.3%)
2	D	2.19	36/1251 (2.9%)	2.42	74/1674 (4.4%)
3	E	2.14	34/1554 (2.2%)	2.49	110/2081 (5.3%)
3	F	2.23	58/1554 (3.7%)	2.58	133/2081 (6.4%)
All	All	2.21	638/19375 (3.3%)	2.48	1364/26069 (5.2%)

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	18
1	B	0	31
2	C	0	6
2	D	0	1
3	E	0	3
3	F	0	3
All	All	0	62

All (638) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	47	VAL	CA-CB	-11.37	1.40	1.54
3	F	81	ALA	CA-C	-10.23	1.43	1.52
1	B	289	GLY	C-N	10.12	1.42	1.33
1	A	171	ILE	CA-CB	10.01	1.66	1.53
1	B	317	ILE	CA-C	9.97	1.63	1.52
3	E	54	HIS	N-CA	-9.97	1.38	1.47
1	A	241	PHE	C-N	9.69	1.38	1.33
1	A	727	LEU	N-CA	9.32	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	174	GLY	CA-C	-9.31	1.43	1.52
1	B	755	ASN	CA-C	9.29	1.65	1.52
1	A	24	LYS	CA-CB	9.24	1.66	1.53
1	A	340	HIS	ND1-CE1	9.17	1.41	1.32
1	B	122	PRO	C-N	9.00	1.46	1.33
1	A	247	ILE	C-N	9.00	1.46	1.33
2	D	101	MET	CA-C	-8.85	1.42	1.52
1	B	540	ALA	CA-CB	8.82	1.65	1.53
1	B	44	GLY	CA-C	-8.71	1.45	1.52
1	B	408	VAL	CA-C	-8.71	1.43	1.53
1	A	232	THR	C-N	8.69	1.43	1.34
1	B	776	GLU	CA-C	-8.68	1.41	1.52
3	E	30	PRO	CA-C	-8.64	1.47	1.51
1	A	173	GLY	CA-C	-8.58	1.43	1.52
1	B	142	ARG	NE-CZ	8.50	1.42	1.33
1	B	412	ARG	CD-NE	8.50	1.58	1.46
1	A	783	GLY	CA-C	8.39	1.61	1.52
3	F	161	ASP	CA-CB	8.29	1.66	1.53
3	F	82	THR	CA-C	-8.24	1.42	1.52
3	E	150	SER	N-CA	-8.22	1.35	1.46
1	B	125	ARG	CD-NE	8.17	1.57	1.46
3	F	34	PRO	C-N	8.15	1.45	1.33
1	B	377	GLU	N-CA	-8.14	1.36	1.46
1	B	592	LEU	CA-C	-8.09	1.42	1.52
3	F	42	ARG	CZ-NH2	8.07	1.44	1.33
2	C	117	LEU	CA-C	-8.07	1.42	1.52
1	A	275	THR	CA-C	-8.03	1.42	1.52
1	A	492	VAL	C-N	7.97	1.45	1.34
1	B	269	ARG	NE-CZ	7.95	1.41	1.33
2	C	83	LEU	CA-C	-7.94	1.43	1.52
2	C	95	LYS	CA-C	-7.91	1.42	1.52
1	B	368	GLU	C-N	7.89	1.43	1.33
1	B	665	HIS	ND1-CE1	7.88	1.40	1.32
1	B	782	LEU	CA-C	-7.87	1.43	1.52
1	A	793	ILE	CA-C	-7.87	1.42	1.52
1	B	539	LYS	N-CA	-7.79	1.36	1.46
1	A	124	LYS	CA-C	-7.79	1.42	1.52
1	A	348	LYS	CA-C	-7.75	1.42	1.52
1	B	363	GLN	C-N	7.74	1.45	1.33
1	B	736	PHE	CA-CB	7.74	1.63	1.53
1	A	714	ARG	CA-C	-7.73	1.43	1.52
1	A	704	ILE	CA-CB	-7.71	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	ASN	CA-C	7.70	1.62	1.52
2	C	25	GLY	CA-C	-7.68	1.41	1.51
1	A	236	ASP	CA-CB	7.65	1.65	1.53
1	A	520	LEU	C-N	7.61	1.42	1.33
1	B	567	LYS	N-CA	-7.59	1.39	1.46
1	A	536	MET	N-CA	-7.56	1.36	1.46
1	A	775	GLU	C-N	7.49	1.44	1.33
1	A	510	PHE	CA-CB	7.47	1.64	1.53
1	A	694	GLN	CA-C	-7.44	1.42	1.52
1	A	685	VAL	C-N	7.38	1.42	1.33
3	F	13	SER	CA-CB	7.38	1.64	1.52
1	A	238	SER	CA-C	-7.37	1.43	1.52
1	A	553	HIS	CE1-NE2	-7.36	1.25	1.32
1	A	383	HIS	ND1-CE1	7.35	1.39	1.32
1	A	208	GLU	C-N	7.34	1.41	1.33
1	B	116	PHE	CA-CB	7.33	1.63	1.52
1	A	232	THR	CA-C	-7.31	1.44	1.53
2	D	118	THR	C-N	7.30	1.43	1.33
3	E	24	ALA	N-CA	-7.29	1.38	1.46
1	B	640	ARG	CD-NE	7.28	1.56	1.46
1	B	278	ARG	CD-NE	7.27	1.56	1.46
2	D	119	ASP	C-N	7.26	1.43	1.33
3	E	174	GLY	C-N	7.26	1.44	1.33
1	A	416	GLN	C-N	7.24	1.41	1.33
1	B	482	LEU	C-N	7.24	1.43	1.34
1	A	714	ARG	C-N	7.24	1.39	1.33
2	C	93	TYR	C-N	7.22	1.43	1.33
3	F	114	ILE	N-CA	-7.22	1.37	1.46
1	A	209	LYS	C-N	7.20	1.43	1.33
1	A	470	PHE	CA-C	-7.19	1.44	1.52
1	A	177	ALA	CA-C	-7.17	1.43	1.52
1	A	779	ASP	CA-C	-7.16	1.42	1.52
1	B	753	ASP	N-CA	-7.16	1.36	1.45
1	A	161	LEU	N-CA	-7.15	1.38	1.46
1	B	827	ASN	CA-C	-7.14	1.44	1.52
1	B	834	TYR	N-CA	-7.14	1.38	1.46
1	A	71	LEU	CA-C	-7.14	1.43	1.52
1	A	89	THR	N-CA	-7.13	1.36	1.46
1	A	708	ARG	NE-CZ	7.11	1.40	1.33
1	B	5	PRO	CA-CB	-7.10	1.44	1.53
1	A	488	HIS	ND1-CE1	7.10	1.39	1.32
1	B	800	LYS	N-CA	-7.08	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	401	ILE	C-N	7.05	1.45	1.33
1	A	366	ARG	CZ-NH1	7.05	1.42	1.32
1	B	51	GLY	CA-C	-7.03	1.43	1.52
1	B	826	ARG	NE-CZ	7.02	1.40	1.33
2	D	53	GLY	C-N	7.02	1.42	1.33
1	A	512	LEU	CA-C	-7.01	1.44	1.53
1	A	126	PHE	CA-CB	7.00	1.64	1.53
2	C	132	ASP	CA-C	-6.99	1.43	1.52
1	A	133	THR	C-N	6.98	1.43	1.33
3	E	86	LEU	CA-C	-6.97	1.43	1.52
1	B	12	TYR	CA-CB	6.95	1.63	1.53
1	A	75	ASN	CA-CB	6.95	1.63	1.53
1	B	142	ARG	C-N	6.93	1.43	1.33
2	D	108	HIS	ND1-CE1	6.92	1.39	1.32
1	B	147	PRO	C-N	6.92	1.42	1.33
3	F	160	GLN	C-N	6.91	1.42	1.33
2	C	84	GLU	CA-C	-6.91	1.43	1.52
1	A	778	ARG	N-CA	-6.90	1.37	1.46
3	F	42	ARG	N-CA	-6.89	1.37	1.45
3	F	8	GLU	CA-CB	6.88	1.64	1.53
1	B	115	LEU	C-N	6.88	1.42	1.33
2	D	4	LEU	CA-CB	6.88	1.62	1.53
1	B	839	PRO	CA-C	-6.87	1.42	1.52
1	B	301	SER	C-N	6.87	1.42	1.33
1	A	453	PHE	CA-C	-6.86	1.43	1.52
1	B	281	HIS	ND1-CE1	6.85	1.39	1.32
1	B	221	ASN	C-O	-6.83	1.18	1.24
1	A	499	LYS	C-N	6.79	1.42	1.33
3	F	25	ALA	CA-CB	6.79	1.64	1.53
1	B	356	LEU	CA-C	-6.78	1.43	1.52
1	B	801	GLU	C-N	6.78	1.42	1.33
1	A	803	LYS	CA-C	6.78	1.61	1.52
1	B	284	TYR	CA-C	-6.76	1.44	1.52
1	B	448	GLN	C-N	-6.75	1.27	1.33
3	F	7	LYS	CA-CB	6.75	1.63	1.53
1	A	11	LEU	C-N	6.74	1.42	1.33
1	A	765	PHE	CA-C	-6.74	1.44	1.52
1	A	56	VAL	C-N	6.73	1.42	1.33
1	B	810	VAL	CA-C	-6.72	1.44	1.52
1	B	121	ASN	CA-CB	6.72	1.61	1.53
3	F	18	GLU	CA-C	-6.71	1.45	1.52
2	D	142	PHE	C-N	6.70	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	388	ASN	CA-C	-6.70	1.44	1.52
2	C	27	ILE	C-N	6.69	1.42	1.33
1	B	595	ASN	N-CA	-6.69	1.38	1.46
1	A	735	GLY	N-CA	-6.69	1.35	1.45
2	D	142	PHE	CA-C	-6.68	1.44	1.52
3	F	54	HIS	ND1-CE1	6.67	1.39	1.32
1	B	402	LYS	C-N	6.67	1.42	1.33
1	B	583	THR	N-CA	-6.64	1.38	1.46
1	B	437	VAL	CA-CB	-6.63	1.46	1.54
1	B	734	LYS	CA-CB	6.63	1.63	1.54
3	E	120	ALA	CA-C	-6.63	1.44	1.52
3	F	128	ILE	N-CA	-6.62	1.38	1.46
1	B	17	GLN	CA-C	6.62	1.61	1.53
1	A	162	ALA	N-CA	-6.62	1.37	1.46
3	F	118	ARG	CA-CB	6.60	1.63	1.53
1	B	767	ARG	CA-C	-6.59	1.45	1.52
2	C	114	GLY	C-N	6.57	1.43	1.33
1	A	474	CYS	C-N	6.57	1.42	1.33
1	A	781	ARG	CZ-NH2	6.56	1.42	1.33
1	A	389	ALA	N-CA	-6.55	1.37	1.46
1	A	655	GLU	N-CA	-6.54	1.38	1.46
3	F	136	ASP	N-CA	6.54	1.54	1.46
1	A	509	ASP	CA-C	-6.52	1.44	1.52
1	A	141	ARG	NE-CZ	6.52	1.40	1.33
1	B	339	SER	CA-C	-6.51	1.44	1.52
1	B	109	ILE	N-CA	-6.51	1.38	1.46
2	D	21	TRP	CA-CB	6.50	1.64	1.53
1	A	549	LEU	C-N	6.50	1.43	1.33
1	A	107	ASN	CA-CB	6.50	1.63	1.53
1	A	450	ARG	CZ-NH2	6.49	1.41	1.33
1	A	415	THR	C-N	6.49	1.42	1.33
1	A	359	MET	C-N	6.46	1.42	1.33
2	D	74	ILE	C-N	6.46	1.42	1.33
3	E	58	GLU	CA-C	-6.46	1.42	1.52
1	B	365	PRO	CA-C	-6.45	1.45	1.52
1	B	305	TYR	CA-CB	6.45	1.62	1.53
1	B	707	CYS	N-CA	-6.45	1.37	1.46
1	A	345	ASP	CA-CB	6.45	1.64	1.53
1	B	450	ARG	NE-CZ	6.44	1.40	1.33
1	B	282	ILE	C-N	6.42	1.42	1.33
1	B	510	PHE	C-N	6.41	1.37	1.33
1	A	410	GLN	CA-C	6.41	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	685	VAL	CA-CB	-6.41	1.46	1.54
2	C	146	ILE	CA-C	-6.40	1.43	1.52
2	C	14	GLU	CA-C	-6.40	1.44	1.52
1	B	197	THR	C-N	6.39	1.41	1.33
1	A	111	THR	C-O	-6.39	1.16	1.23
2	D	112	SER	N-CA	-6.39	1.37	1.46
1	A	321	ASP	C-N	6.39	1.41	1.33
1	A	715	MET	CA-C	-6.39	1.47	1.53
3	E	129	VAL	CA-C	-6.38	1.45	1.52
1	B	621	ASP	CA-C	-6.38	1.44	1.52
1	B	364	ARG	CD-NE	6.37	1.55	1.46
1	B	772	GLY	CA-C	-6.34	1.45	1.52
3	E	28	PRO	CA-C	6.34	1.58	1.52
3	F	85	SER	CA-C	6.33	1.61	1.52
2	C	78	LYS	CA-C	-6.32	1.44	1.53
2	C	13	ARG	CD-NE	6.31	1.55	1.46
1	A	185	LYS	C-N	6.31	1.40	1.33
1	A	585	PRO	C-N	6.30	1.41	1.33
1	B	258	ALA	N-CA	-6.27	1.38	1.46
2	D	57	ARG	CD-NE	6.27	1.55	1.46
3	F	42	ARG	C-N	6.27	1.41	1.33
1	A	831	TYR	CA-CB	6.26	1.64	1.53
1	B	162	ALA	CA-CB	6.25	1.63	1.53
2	D	3	ASP	CA-CB	6.24	1.63	1.53
1	B	31	MET	CA-C	-6.24	1.45	1.52
1	A	704	ILE	CA-C	-6.24	1.44	1.52
2	D	83	LEU	N-CA	-6.24	1.38	1.46
2	D	46	ALA	N-CA	-6.23	1.38	1.46
1	B	258	ALA	CA-C	-6.23	1.45	1.52
1	A	466	ASP	CA-C	-6.23	1.44	1.52
1	A	552	ASN	CA-CB	6.21	1.61	1.53
1	A	582	GLY	C-N	6.20	1.41	1.33
1	A	671	PHE	CA-C	-6.20	1.44	1.52
1	B	389	ALA	CA-C	-6.19	1.44	1.52
1	A	431	ARG	C-O	-6.19	1.16	1.24
1	B	140	ARG	CD-NE	6.18	1.54	1.46
1	A	61	GLN	CA-C	-6.18	1.44	1.52
3	E	59	PHE	N-CA	-6.18	1.39	1.46
1	A	533	GLU	N-CA	-6.18	1.38	1.46
2	C	78	LYS	N-CA	-6.18	1.38	1.45
1	A	584	VAL	CA-CB	6.17	1.60	1.53
1	B	296	ALA	CA-C	-6.17	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217	VAL	CA-C	-6.17	1.44	1.52
1	A	391	ASP	C-N	6.16	1.42	1.33
1	B	811	ALA	CA-C	-6.15	1.45	1.52
1	B	102	GLN	CA-CB	6.14	1.64	1.53
1	B	436	LEU	CA-C	-6.14	1.45	1.52
1	B	238	SER	CA-CB	6.13	1.60	1.52
1	B	587	ASN	CA-C	6.13	1.59	1.52
1	B	503	ILE	C-O	6.12	1.31	1.24
1	B	373	ASP	C-N	6.11	1.42	1.33
1	A	203	GLU	CA-C	-6.10	1.45	1.52
1	B	261	GLU	C-N	6.08	1.43	1.33
1	B	340	HIS	CE1-NE2	6.08	1.38	1.32
1	A	537	PHE	N-CA	-6.08	1.40	1.45
1	A	70	LEU	CA-CB	6.08	1.65	1.54
1	B	373	ASP	CA-CB	6.07	1.64	1.53
3	F	101	GLU	CA-CB	6.07	1.63	1.53
1	A	385	LEU	C-N	6.06	1.41	1.33
1	A	262	THR	N-CA	6.05	1.53	1.46
1	A	618	ILE	CA-C	-6.04	1.45	1.52
1	A	422	GLY	C-N	6.03	1.41	1.33
3	F	148	LYS	CA-CB	6.03	1.62	1.53
1	B	91	LEU	CA-CB	6.03	1.63	1.53
2	C	59	GLU	C-N	6.02	1.41	1.33
1	B	172	THR	N-CA	-6.01	1.38	1.45
3	F	149	ARG	CD-NE	6.01	1.54	1.46
1	B	511	GLY	CA-C	6.00	1.58	1.52
1	B	130	THR	N-CA	-6.00	1.38	1.46
1	A	53	ILE	C-N	6.00	1.41	1.33
2	D	121	GLU	CA-C	-5.99	1.45	1.52
1	B	286	LEU	CA-C	-5.99	1.45	1.52
1	A	90	TYR	N-CA	-5.99	1.38	1.46
1	B	269	ARG	C-N	5.98	1.41	1.33
1	A	191	ALA	CA-CB	5.98	1.63	1.53
1	B	430	ASP	C-N	5.98	1.42	1.33
1	B	68	LYS	CA-C	-5.97	1.44	1.52
1	B	13	ILE	C-N	5.97	1.41	1.33
1	B	610	GLY	CA-C	-5.97	1.43	1.51
1	B	109	ILE	C-N	5.97	1.41	1.33
1	B	326	LEU	N-CA	5.96	1.53	1.46
1	B	113	SER	CA-C	-5.96	1.44	1.53
1	A	68	LYS	C-N	5.96	1.42	1.33
1	A	433	PHE	CA-C	-5.95	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	133	THR	N-CA	5.95	1.53	1.46
1	A	443	THR	N-CA	-5.95	1.38	1.46
1	A	210	LYS	C-N	5.95	1.41	1.33
3	F	53	GLN	CA-C	-5.94	1.44	1.52
1	B	170	LEU	N-CA	-5.94	1.39	1.46
1	B	796	TYR	CA-C	-5.93	1.45	1.52
1	B	720	PHE	C-N	5.93	1.41	1.33
2	D	125	ILE	N-CA	5.92	1.53	1.46
1	A	676	ILE	N-CA	-5.92	1.41	1.47
1	B	500	ARG	NE-CZ	5.92	1.39	1.33
2	C	29	ALA	C-N	5.92	1.42	1.34
1	A	246	ARG	CD-NE	5.92	1.54	1.46
2	D	44	THR	CA-C	-5.92	1.45	1.53
3	F	28	PRO	N-CA	5.92	1.54	1.46
1	A	253	GLY	C-N	5.91	1.42	1.33
1	B	39	GLU	C-N	5.91	1.38	1.32
3	F	32	LYS	CA-CB	5.91	1.60	1.53
1	B	505	TRP	C-N	5.91	1.40	1.33
3	F	148	LYS	CA-C	-5.90	1.45	1.52
3	F	80	ARG	C-N	5.90	1.41	1.33
3	F	93	GLN	CA-CB	5.90	1.63	1.53
2	C	100	THR	C-O	-5.90	1.16	1.23
1	A	576	SER	CA-CB	5.90	1.63	1.53
1	B	296	ALA	C-N	5.89	1.41	1.33
3	F	118	ARG	CD-NE	5.89	1.54	1.46
1	B	159	ALA	C-N	5.88	1.41	1.33
1	B	340	HIS	CA-CB	5.88	1.63	1.53
1	B	478	THR	CA-C	-5.88	1.46	1.52
1	A	624	GLY	C-N	5.88	1.41	1.33
1	A	559	ASN	CA-CB	5.87	1.63	1.53
1	A	579	HIS	CD2-NE2	5.87	1.44	1.37
3	F	175	ASN	C-N	5.86	1.42	1.33
1	B	752	LEU	C-N	5.85	1.41	1.33
1	A	390	ALA	CA-C	-5.85	1.45	1.52
2	C	67	PHE	N-CA	-5.85	1.38	1.46
2	D	88	GLU	C-N	5.84	1.42	1.33
2	C	80	VAL	CA-CB	-5.84	1.46	1.54
1	A	129	TYR	CA-CB	5.84	1.64	1.53
1	B	662	ALA	C-N	5.83	1.41	1.33
1	B	200	PRO	N-CA	-5.83	1.39	1.47
1	B	234	ARG	NE-CZ	5.83	1.39	1.33
1	A	308	HIS	CG-CD2	5.83	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	530	ILE	C-N	5.83	1.41	1.33
1	A	475	ILE	CA-CB	-5.81	1.49	1.55
3	F	171	PRO	N-CA	-5.81	1.40	1.47
1	B	391	ASP	CA-CB	5.80	1.62	1.53
1	A	151	ALA	C-N	5.80	1.41	1.33
1	B	151	ALA	CA-C	-5.79	1.45	1.52
1	A	391	ASP	CA-C	-5.79	1.45	1.52
1	B	136	ILE	CA-C	5.79	1.60	1.52
1	A	214	GLU	C-N	5.78	1.42	1.33
1	B	144	GLU	C-N	5.78	1.38	1.33
1	A	510	PHE	CA-C	-5.78	1.45	1.52
1	A	592	LEU	N-CA	-5.78	1.39	1.46
1	B	359	MET	N-CA	-5.77	1.39	1.46
2	D	10	GLU	N-CA	-5.76	1.39	1.46
1	A	202	LYS	C-N	5.76	1.41	1.33
1	B	101	LYS	N-CA	5.75	1.53	1.46
1	B	737	VAL	CA-CB	5.75	1.62	1.54
1	B	526	GLY	C-N	5.75	1.41	1.33
2	D	3	ASP	CA-C	-5.75	1.47	1.53
1	B	147	PRO	CA-C	-5.74	1.46	1.52
3	E	78	ASP	N-CA	-5.74	1.38	1.46
1	A	254	LYS	CA-C	-5.73	1.45	1.52
1	A	331	THR	CA-C	-5.73	1.45	1.52
2	C	29	ALA	CA-C	5.72	1.60	1.52
1	A	458	ASP	CA-CB	5.71	1.61	1.52
3	F	187	LEU	CA-CB	5.70	1.61	1.52
1	A	832	LYS	CA-CB	5.70	1.64	1.54
3	E	177	LEU	CA-C	-5.69	1.45	1.52
1	B	321	ASP	N-CA	5.68	1.53	1.45
2	C	17	GLU	CA-C	-5.68	1.44	1.52
3	E	66	ILE	C-N	5.68	1.43	1.33
1	B	159	ALA	CA-C	-5.68	1.45	1.52
2	C	85	ASP	CA-CB	5.68	1.61	1.53
3	F	192	GLU	N-CA	5.68	1.52	1.46
1	A	22	GLN	C-O	-5.67	1.16	1.24
1	A	320	VAL	C-N	5.67	1.41	1.33
1	A	572	GLU	CA-C	-5.66	1.45	1.53
1	B	516	ALA	N-CA	-5.65	1.39	1.46
2	C	8	GLU	CA-CB	5.65	1.62	1.53
1	B	665	HIS	CA-CB	5.65	1.62	1.53
1	A	59	GLU	C-N	5.65	1.40	1.33
1	A	371	GLU	C-N	5.65	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	92	VAL	C-O	-5.65	1.17	1.24
2	D	116	ARG	CD-NE	5.64	1.54	1.46
1	B	677	PRO	C-N	5.64	1.41	1.33
1	A	428	MET	C-N	5.64	1.41	1.33
1	A	671	PHE	N-CA	-5.64	1.39	1.45
1	B	158	SER	C-N	5.63	1.41	1.33
1	A	578	ALA	CA-C	-5.63	1.45	1.52
1	B	457	LEU	N-CA	-5.62	1.39	1.46
1	B	829	LEU	CA-C	-5.62	1.45	1.52
3	F	125	GLU	C-N	5.61	1.41	1.33
2	C	75	LYS	N-CA	-5.61	1.39	1.46
1	B	572	GLU	C-N	5.61	1.41	1.33
1	A	16	GLU	C-N	5.61	1.41	1.33
1	A	812	LEU	CA-C	-5.61	1.45	1.52
1	A	721	LYS	CA-C	-5.60	1.44	1.52
1	A	770	VAL	CA-CB	5.60	1.61	1.54
1	B	185	LYS	C-N	5.59	1.40	1.33
1	A	267	LYS	CA-C	-5.59	1.47	1.53
2	C	10	GLU	C-N	5.59	1.41	1.33
3	E	187	LEU	CA-C	-5.59	1.45	1.52
2	D	120	ILE	N-CA	-5.58	1.40	1.46
3	E	88	ARG	C-N	5.58	1.41	1.33
1	B	2	ALA	C-O	-5.58	1.17	1.24
1	A	741	LYS	C-O	-5.58	1.17	1.24
1	A	762	THR	N-CA	5.58	1.53	1.46
1	B	256	ALA	N-CA	-5.58	1.39	1.46
3	F	3	ASP	N-CA	-5.58	1.39	1.46
1	A	146	PRO	CA-C	5.58	1.57	1.52
3	E	54	HIS	ND1-CE1	5.58	1.38	1.32
1	B	439	ARG	CZ-NH1	5.58	1.40	1.32
3	F	73	PHE	C-N	5.57	1.41	1.33
2	D	15	HIS	CG-CD2	5.57	1.42	1.35
1	B	537	PHE	N-CA	-5.57	1.40	1.45
1	B	719	ASP	N-CA	5.57	1.52	1.46
1	B	15	MET	CA-CB	5.56	1.62	1.53
2	D	38	SER	C-N	5.55	1.41	1.33
1	B	370	ALA	CA-CB	5.55	1.59	1.53
1	B	390	ALA	C-N	5.55	1.41	1.33
1	A	461	GLY	C-N	5.55	1.41	1.33
1	A	335	ILE	C-N	5.55	1.41	1.34
1	A	420	SER	C-N	5.55	1.40	1.33
3	F	94	GLU	N-CA	-5.55	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	111	LEU	CA-C	-5.55	1.45	1.52
2	D	43	PRO	CA-C	-5.54	1.46	1.52
2	C	41	CYS	C-N	5.54	1.41	1.33
1	B	103	ARG	N-CA	-5.54	1.39	1.46
1	B	98	HIS	ND1-CE1	5.54	1.38	1.32
1	B	314	LYS	C-N	5.54	1.40	1.33
1	A	799	LYS	N-CA	-5.54	1.38	1.46
1	A	140	ARG	CZ-NH2	5.53	1.40	1.33
1	A	383	HIS	C-O	-5.53	1.17	1.24
1	A	281	HIS	ND1-CE1	5.53	1.38	1.32
1	A	615	VAL	C-N	5.53	1.41	1.33
2	C	89	GLY	C-N	5.53	1.41	1.33
1	B	2	ALA	CA-C	-5.52	1.45	1.52
1	B	11	LEU	CB-CG	5.52	1.64	1.53
1	B	560	PHE	CA-CB	5.52	1.61	1.53
1	B	827	ASN	C-N	5.52	1.39	1.33
2	D	40	ASP	CA-C	5.52	1.60	1.52
1	B	15	MET	CA-C	-5.51	1.45	1.53
1	A	38	LYS	C-N	5.50	1.40	1.33
3	F	45	SER	C-N	5.50	1.40	1.33
1	A	269	ARG	CD-NE	5.50	1.53	1.46
3	E	110	MET	CA-C	-5.50	1.46	1.53
2	D	139	TYR	CZ-OH	5.50	1.49	1.38
1	B	431	ARG	NE-CZ	5.49	1.39	1.33
3	F	108	PHE	CA-C	-5.49	1.45	1.52
2	C	118	THR	CA-C	5.49	1.60	1.52
1	B	366	ARG	NE-CZ	5.49	1.39	1.33
1	B	622	HIS	CB-CG	5.49	1.57	1.50
3	E	132	PHE	N-CA	-5.49	1.39	1.46
1	B	687	ASP	CA-C	-5.49	1.46	1.52
1	A	145	VAL	CA-CB	5.49	1.61	1.54
1	A	798	SER	CA-CB	5.49	1.62	1.53
1	A	783	GLY	N-CA	-5.48	1.38	1.45
1	A	34	VAL	N-CA	-5.47	1.39	1.46
2	C	79	GLU	C-O	-5.47	1.17	1.24
1	B	530	ILE	C-N	5.47	1.41	1.33
1	B	764	VAL	N-CA	-5.47	1.39	1.46
1	A	407	MET	CA-C	-5.47	1.46	1.53
1	A	728	ALA	C-N	5.47	1.41	1.33
1	B	812	LEU	C-N	5.47	1.41	1.33
3	F	72	GLY	CA-C	5.46	1.59	1.52
1	B	789	LEU	CA-CB	5.46	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	12	ALA	C-N	5.46	1.41	1.33
1	B	643	GLY	N-CA	-5.46	1.37	1.46
1	B	293	ASN	C-O	5.45	1.30	1.24
1	B	746	VAL	CA-C	5.45	1.58	1.52
1	B	654	ARG	C-N	5.45	1.40	1.33
1	B	62	GLU	CA-C	-5.45	1.46	1.52
1	B	350	THR	N-CA	-5.45	1.39	1.46
1	A	531	LEU	CA-CB	5.44	1.61	1.53
3	F	38	ARG	NE-CZ	5.43	1.39	1.33
2	C	116	ARG	CA-CB	5.43	1.62	1.53
1	B	299	LEU	CB-CG	5.43	1.64	1.53
1	B	244	PHE	N-CA	-5.43	1.39	1.46
1	A	626	GLY	CA-C	-5.42	1.44	1.52
3	F	97	SER	N-CA	-5.41	1.39	1.46
1	A	328	LEU	CA-CB	5.41	1.61	1.53
1	A	528	LEU	C-N	5.41	1.41	1.33
1	B	809	ARG	NE-CZ	5.41	1.39	1.33
1	A	200	PRO	C-N	5.41	1.41	1.33
3	F	183	PHE	N-CA	-5.41	1.39	1.46
1	B	745	ALA	CA-C	-5.40	1.45	1.52
1	B	833	LEU	CA-C	-5.40	1.46	1.52
2	C	70	ILE	CA-C	5.40	1.59	1.52
3	F	118	ARG	CZ-NH1	5.40	1.40	1.32
1	A	478	THR	C-N	5.40	1.41	1.34
2	D	108	HIS	CG-ND1	5.39	1.44	1.38
1	B	439	ARG	CD-NE	5.39	1.53	1.46
1	B	649	VAL	C-N	5.39	1.41	1.33
1	A	330	ASP	CA-CB	5.39	1.61	1.53
3	E	181	LYS	CA-C	-5.39	1.45	1.52
3	F	84	ASP	C-N	5.39	1.41	1.33
3	F	152	THR	CA-CB	-5.39	1.44	1.53
3	F	150	SER	C-N	5.38	1.41	1.34
1	B	347	TYR	CA-C	-5.38	1.45	1.52
1	A	600	ASN	N-CA	-5.38	1.39	1.46
1	A	724	TYR	CA-CB	5.38	1.60	1.53
3	E	48	PHE	N-CA	-5.38	1.39	1.46
1	B	79	TYR	CA-C	-5.37	1.45	1.52
1	A	172	THR	C-N	5.37	1.40	1.33
1	A	248	HIS	CA-C	-5.37	1.46	1.52
1	A	780	ASP	N-CA	5.37	1.52	1.46
1	B	137	TYR	CA-CB	5.37	1.60	1.53
1	B	107	ASN	C-N	5.37	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	349	ILE	N-CA	-5.36	1.40	1.46
1	B	98	HIS	CA-C	-5.36	1.45	1.52
3	E	7	LYS	C-N	5.36	1.41	1.33
1	B	460	ALA	C-N	5.36	1.40	1.33
3	F	74	ILE	N-CA	-5.36	1.39	1.46
1	B	105	TYR	N-CA	5.35	1.52	1.46
1	B	348	LYS	C-N	5.35	1.40	1.33
1	A	4	ASP	N-CA	-5.35	1.41	1.46
1	A	416	GLN	N-CA	-5.35	1.39	1.46
1	B	118	VAL	CA-C	-5.34	1.46	1.52
1	B	419	TYR	N-CA	-5.34	1.39	1.46
1	B	225	GLU	C-N	5.34	1.41	1.33
3	E	130	ASN	CA-CB	5.34	1.61	1.53
1	A	356	LEU	CA-C	-5.33	1.46	1.52
1	A	12	TYR	N-CA	-5.33	1.39	1.46
1	A	464	ILE	CA-C	-5.33	1.46	1.52
1	A	86	SER	N-CA	-5.33	1.39	1.46
2	C	59	GLU	CA-C	5.33	1.60	1.53
3	E	80	ARG	NE-CZ	5.33	1.39	1.33
1	B	789	LEU	CA-C	-5.32	1.46	1.52
1	A	142	ARG	CA-CB	5.32	1.61	1.53
1	A	145	VAL	C-N	-5.32	1.27	1.33
1	B	431	ARG	CD-NE	5.32	1.53	1.46
3	F	7	LYS	C-N	5.32	1.40	1.33
3	E	73	PHE	CA-CB	5.32	1.62	1.53
3	F	13	SER	C-N	5.32	1.40	1.33
1	B	600	ASN	CA-C	-5.32	1.45	1.52
1	A	383	HIS	CA-C	-5.32	1.46	1.52
2	C	72	SER	C-N	5.32	1.41	1.33
1	B	175	SER	N-CA	-5.32	1.39	1.46
1	B	225	GLU	CA-C	-5.32	1.46	1.52
3	E	167	LEU	CA-C	-5.32	1.45	1.52
1	B	464	ILE	C-N	5.31	1.40	1.33
1	A	263	TYR	CA-CB	5.31	1.62	1.53
1	A	667	THR	CA-C	-5.31	1.46	1.52
3	E	8	GLU	CA-C	-5.31	1.45	1.52
1	A	294	LEU	N-CA	5.31	1.53	1.46
1	B	604	VAL	CA-C	-5.31	1.46	1.52
1	B	492	VAL	CA-C	-5.30	1.46	1.52
1	A	748	GLY	N-CA	5.30	1.50	1.45
2	C	144	LYS	N-CA	-5.30	1.39	1.46
1	B	298	LEU	C-N	5.30	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	TYR	CZ-OH	5.30	1.49	1.38
1	B	2	ALA	C-N	5.30	1.41	1.33
1	A	653	TYR	CA-CB	5.29	1.62	1.53
1	B	27	ASP	C-N	5.29	1.40	1.33
1	A	58	ILE	CB-CG1	5.29	1.64	1.53
1	A	68	LYS	CA-C	-5.29	1.45	1.52
1	A	527	ILE	C-N	5.29	1.41	1.33
1	A	183	THR	CA-C	-5.29	1.45	1.52
1	A	720	PHE	N-CA	-5.28	1.38	1.45
1	B	233	VAL	N-CA	-5.28	1.40	1.46
1	A	579	HIS	CA-C	5.28	1.57	1.52
1	A	521	ILE	CB-CG1	5.28	1.64	1.53
1	B	276	LEU	C-N	5.27	1.40	1.33
1	A	665	HIS	CA-CB	5.27	1.62	1.53
1	A	683	PRO	CA-CB	5.27	1.60	1.53
1	B	583	THR	CA-C	-5.27	1.46	1.52
1	A	477	PHE	C-N	5.27	1.41	1.33
1	A	782	LEU	CA-CB	5.26	1.62	1.53
3	E	140	GLY	C-N	5.26	1.40	1.33
1	B	449	LYS	CA-C	5.26	1.58	1.53
1	A	527	ILE	CA-C	-5.26	1.46	1.52
1	B	755	ASN	CA-CB	5.25	1.62	1.53
1	B	348	LYS	N-CA	-5.25	1.40	1.46
2	C	48	VAL	C-N	5.25	1.41	1.34
3	E	42	ARG	CZ-NH1	5.25	1.40	1.32
1	B	106	ALA	C-N	5.25	1.40	1.33
3	F	28	PRO	C-N	-5.25	1.27	1.33
1	A	32	VAL	CA-C	-5.25	1.46	1.52
1	A	662	ALA	C-N	5.24	1.41	1.33
1	A	113	SER	CA-CB	5.24	1.58	1.53
2	C	74	ILE	N-CA	-5.24	1.39	1.46
2	C	153	ASP	CA-C	-5.23	1.46	1.53
1	B	730	SER	CA-CB	5.23	1.62	1.53
1	A	337	GLY	CA-C	-5.23	1.44	1.51
3	F	142	CYS	N-CA	-5.23	1.39	1.46
1	B	353	CYS	C-N	5.23	1.41	1.33
1	A	122	PRO	CA-C	5.21	1.59	1.52
3	E	134	LEU	N-CA	-5.21	1.39	1.46
1	A	322	ASP	CA-C	-5.21	1.46	1.52
2	C	145	THR	C-N	5.21	1.40	1.34
1	B	5	PRO	N-CA	-5.21	1.40	1.47
1	B	628	GLU	N-CA	-5.21	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	224	LEU	CA-C	-5.21	1.46	1.52
1	B	745	ALA	N-CA	5.20	1.52	1.46
1	B	769	GLY	CA-C	-5.20	1.44	1.51
2	C	48	VAL	CA-CB	-5.20	1.47	1.54
1	B	782	LEU	C-N	5.20	1.41	1.33
1	A	352	SER	CA-CB	5.19	1.61	1.53
2	C	35	LEU	CA-CB	5.19	1.61	1.53
2	D	65	GLU	N-CA	-5.19	1.39	1.46
1	A	123	TYR	CA-CB	5.19	1.62	1.53
2	C	111	LEU	N-CA	-5.19	1.38	1.45
1	B	195	ALA	C-N	5.18	1.40	1.33
1	B	747	LEU	N-CA	-5.18	1.40	1.46
3	F	50	MET	C-N	5.18	1.41	1.33
2	D	126	MET	N-CA	-5.18	1.39	1.46
1	A	521	ILE	CA-CB	5.18	1.60	1.54
1	B	576	SER	C-N	5.18	1.40	1.33
1	A	612	ASN	CA-C	-5.18	1.46	1.52
1	B	695	LEU	N-CA	-5.17	1.39	1.46
3	E	75	SER	CA-C	-5.17	1.46	1.53
1	B	453	PHE	CG-CD1	5.17	1.49	1.38
1	B	756	ASP	C-O	-5.16	1.18	1.24
1	A	54	CYS	CA-C	-5.16	1.47	1.52
1	A	792	TRP	NE1-CE2	-5.16	1.31	1.37
1	A	336	LEU	N-CA	-5.15	1.39	1.46
1	A	605	ASP	N-CA	-5.15	1.40	1.46
2	D	110	LEU	CA-C	-5.15	1.45	1.52
2	D	108	HIS	CB-CG	-5.14	1.43	1.50
1	B	781	ARG	CD-NE	5.14	1.53	1.46
1	B	660	LEU	N-CA	-5.14	1.39	1.46
1	A	370	ALA	CA-CB	5.14	1.61	1.53
1	A	430	ASP	C-N	5.14	1.41	1.34
1	A	313	GLY	N-CA	-5.13	1.38	1.45
1	A	308	HIS	ND1-CE1	5.12	1.37	1.32
1	B	431	ARG	CZ-NH1	5.12	1.40	1.32
1	A	675	ILE	C-N	5.12	1.39	1.33
1	B	834	TYR	C-N	5.12	1.40	1.33
1	A	333	PHE	CA-CB	5.12	1.61	1.53
1	B	422	GLY	C-N	5.11	1.40	1.33
1	B	545	PHE	CA-C	-5.11	1.46	1.52
1	A	242	GLY	N-CA	-5.11	1.37	1.44
1	B	461	GLY	CA-C	5.11	1.57	1.52
1	B	636	GLY	C-N	5.11	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	817	ARG	NE-CZ	5.11	1.38	1.33
1	B	566	PRO	N-CA	-5.10	1.42	1.47
1	A	15	MET	N-CA	-5.10	1.39	1.46
1	A	826	ARG	CA-C	-5.10	1.46	1.52
3	E	54	HIS	CA-C	-5.10	1.48	1.52
1	A	529	SER	CA-CB	5.10	1.61	1.53
1	B	555	GLY	CA-C	-5.10	1.44	1.51
1	B	41	TYR	N-CA	-5.08	1.39	1.46
1	B	669	PRO	CA-C	5.08	1.58	1.52
1	A	611	SER	CA-CB	5.08	1.61	1.54
1	A	206	THR	C-N	5.08	1.40	1.33
1	B	344	THR	CA-C	-5.07	1.45	1.52
1	A	673	ARG	CA-CB	5.07	1.60	1.53
3	F	126	ASP	C-N	5.07	1.40	1.33
3	E	122	THR	C-O	-5.07	1.17	1.23
1	B	563	PRO	C-N	5.06	1.39	1.33
1	B	52	ASP	CA-C	-5.06	1.45	1.52
2	D	109	VAL	C-O	-5.06	1.18	1.24
2	D	31	ASP	C-N	5.05	1.40	1.34
1	A	251	PRO	C-N	5.05	1.40	1.33
2	C	146	ILE	CA-CB	-5.05	1.47	1.54
1	A	128	ILE	CA-CB	-5.05	1.47	1.54
2	C	104	ALA	C-N	5.05	1.40	1.33
1	B	783	GLY	CA-C	-5.04	1.44	1.51
1	A	73	GLN	N-CA	-5.04	1.39	1.46
1	A	372	ALA	N-CA	-5.04	1.40	1.45
1	A	224	LEU	CA-CB	5.04	1.61	1.53
1	A	418	SER	CA-CB	5.04	1.61	1.53
3	E	13	SER	N-CA	-5.04	1.39	1.46
1	A	424	LEU	CA-CB	-5.04	1.45	1.53
1	A	726	ILE	CA-C	5.04	1.59	1.52
3	F	51	PHE	CA-C	-5.03	1.46	1.53
1	B	472	GLN	C-N	5.03	1.40	1.33
1	B	83	GLU	CA-C	-5.03	1.45	1.52
1	A	355	HIS	CD2-NE2	-5.02	1.32	1.37
1	A	723	ARG	NE-CZ	5.02	1.38	1.33
3	F	20	GLU	C-O	5.02	1.29	1.23
1	B	90	TYR	N-CA	-5.02	1.39	1.46
1	A	155	GLY	CA-C	-5.01	1.45	1.51
1	A	193	VAL	C-N	5.01	1.41	1.33
1	B	104	TYR	CZ-OH	5.01	1.48	1.38
1	A	794	ARG	NE-CZ	5.00	1.38	1.33

All (1364) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	458	ASP	CA-CB-CG	14.81	127.41	112.60
2	C	109	VAL	N-CA-C	-13.88	100.53	113.71
3	E	163	VAL	N-CA-C	-13.64	99.33	112.83
3	E	119	ILE	N-CA-C	-12.73	100.76	113.10
3	E	21	GLY	CA-C-N	11.30	133.30	120.53
3	E	21	GLY	C-N-CA	11.30	133.30	120.53
1	B	131	ASN	CA-CB-CG	11.18	123.78	112.60
2	D	20	ASP	CA-CB-CG	11.09	123.69	112.60
1	B	719	ASP	CA-C-N	11.07	135.54	120.38
1	B	719	ASP	C-N-CA	11.07	135.54	120.38
1	B	244	PHE	CA-CB-CG	11.00	124.80	113.80
3	F	38	ARG	NE-CZ-NH2	10.88	128.99	119.20
1	A	711	PHE	CA-CB-CG	-10.77	103.03	113.80
3	F	149	ARG	NE-CZ-NH2	10.65	128.78	119.20
1	A	767	ARG	NE-CZ-NH2	10.46	128.61	119.20
1	A	719	ASP	CA-CB-CG	10.36	122.96	112.60
1	B	730	SER	N-CA-C	-10.33	101.73	114.75
2	D	59	GLU	N-CA-C	-10.31	102.87	114.62
3	F	73	PHE	CA-CB-CG	-10.19	103.61	113.80
1	A	446	THR	N-CA-C	-10.18	101.92	114.75
1	B	209	LYS	N-CA-C	-10.16	101.66	114.56
1	B	21	ASP	CA-CB-CG	-10.03	102.57	112.60
1	A	84	ASP	CA-CB-CG	-9.92	102.68	112.60
1	A	405	ASN	N-CA-C	-9.88	100.38	114.12
1	A	732	VAL	CA-C-N	9.87	129.93	119.76
1	A	732	VAL	C-N-CA	9.87	129.93	119.76
1	B	622	HIS	CA-CB-CG	-9.82	103.98	113.80
1	B	232	THR	N-CA-C	-9.81	95.02	108.86
3	E	82	THR	N-CA-C	-9.79	101.09	113.43
1	B	193	VAL	N-CA-C	-9.75	101.59	112.80
1	B	221	ASN	CA-C-O	-9.74	109.83	119.08
1	B	145	VAL	O-C-N	-9.73	113.11	121.57
1	B	104	TYR	N-CA-CB	9.71	124.40	109.94
1	A	2	ALA	N-CA-C	-9.70	99.63	113.21
1	B	150	PHE	CA-C-N	9.68	133.03	120.44
1	B	150	PHE	C-N-CA	9.68	133.03	120.44
1	B	293	ASN	CA-CB-CG	-9.68	102.92	112.60
1	B	706	ILE	N-CA-C	-9.65	102.50	111.67
1	A	479	ASN	CA-CB-CG	9.60	122.19	112.60
1	A	383	HIS	CA-CB-CG	9.58	123.38	113.80
1	B	468	ASN	CA-C-N	9.52	130.82	120.44
1	B	468	ASN	C-N-CA	9.52	130.82	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	MET	N-CA-C	9.51	121.25	111.07
1	A	738	ASP	CA-CB-CG	9.41	122.01	112.60
3	F	87	GLY	CA-C-O	-9.37	112.93	121.18
1	A	553	HIS	CA-CB-CG	-9.34	104.46	113.80
1	A	232	THR	N-CA-C	-9.28	96.22	108.19
1	B	831	TYR	N-CA-CB	9.26	123.97	109.71
1	A	145	VAL	CA-C-N	9.23	129.89	120.38
1	A	145	VAL	C-N-CA	9.23	129.89	120.38
3	F	27	ALA	CA-C-N	9.20	126.28	119.66
3	F	27	ALA	C-N-CA	9.20	126.28	119.66
3	E	29	PRO	N-CA-C	9.17	121.89	110.70
1	A	150	PHE	CA-CB-CG	-9.15	104.64	113.80
3	E	161	ASP	N-CA-C	-9.15	100.73	114.64
3	E	123	ASP	CA-C-N	9.14	134.55	120.75
3	E	123	ASP	C-N-CA	9.14	134.55	120.75
1	B	478	THR	N-CA-C	-9.13	100.53	112.68
1	A	132	ARG	NE-CZ-NH2	9.10	127.39	119.20
1	B	698	ASN	CA-CB-CG	9.05	121.65	112.60
2	D	144	LYS	N-CA-C	8.97	121.06	111.28
1	A	488	HIS	N-CA-C	-8.97	101.23	112.72
1	A	252	MET	N-CA-C	-8.97	101.24	112.72
1	A	809	ARG	NE-CZ-NH2	8.95	127.26	119.20
1	A	720	PHE	N-CA-C	-8.94	102.10	113.72
1	A	827	ASN	CA-CB-CG	-8.89	103.71	112.60
1	B	767	ARG	NE-CZ-NH1	-8.85	112.65	121.50
2	D	34	ASP	CA-CB-CG	8.84	121.44	112.60
1	A	236	ASP	CA-CB-CG	8.81	121.41	112.60
2	C	113	LEU	N-CA-C	-8.80	96.59	108.74
1	B	66	VAL	CA-C-N	8.80	135.14	123.00
1	B	66	VAL	C-N-CA	8.80	135.14	123.00
1	A	367	GLU	CA-C-N	8.79	137.53	121.70
1	A	367	GLU	C-N-CA	8.79	137.53	121.70
1	B	575	PHE	CA-CB-CG	8.78	122.58	113.80
1	B	324	GLU	CA-C-N	8.73	132.85	120.28
1	B	324	GLU	C-N-CA	8.73	132.85	120.28
1	A	474	CYS	CA-C-N	8.69	131.49	122.97
1	A	474	CYS	C-N-CA	8.69	131.49	122.97
2	C	42	LYS	O-C-N	8.66	128.48	121.20
1	A	579	HIS	N-CA-C	-8.63	101.68	112.72
3	F	136	ASP	CA-CB-CG	-8.62	103.97	112.60
1	B	542	ASP	CA-C-N	8.61	132.01	120.65
1	B	542	ASP	C-N-CA	8.61	132.01	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	57	GLN	N-CA-C	-8.60	96.25	109.24
2	C	99	GLY	N-CA-C	-8.58	102.62	115.32
1	B	758	ARG	NE-CZ-NH1	-8.56	112.94	121.50
1	A	696	THR	N-CA-CB	8.55	122.80	110.40
3	E	64	GLN	OE1-CD-NE2	8.54	131.15	122.60
1	B	572	GLU	CA-C-N	8.48	133.28	120.82
1	B	572	GLU	C-N-CA	8.48	133.28	120.82
1	A	767	ARG	NE-CZ-NH1	-8.42	113.08	121.50
1	A	756	ASP	CA-CB-CG	8.42	121.02	112.60
2	C	132	ASP	CA-CB-CG	8.41	121.01	112.60
1	B	523	LYS	CA-C-O	-8.38	111.12	119.08
3	F	30	PRO	O-C-N	-8.36	117.22	121.15
1	A	557	SER	N-CA-C	-8.36	100.70	108.22
1	B	65	GLN	N-CA-CB	8.34	124.18	110.17
1	A	783	GLY	N-CA-C	8.33	123.00	112.83
3	E	102	ALA	CA-C-N	8.32	130.24	119.84
3	E	102	ALA	C-N-CA	8.32	130.24	119.84
1	B	128	ILE	N-CA-C	-8.28	104.95	112.90
1	B	458	ASP	CA-CB-CG	8.28	120.88	112.60
1	B	321	ASP	CA-CB-CG	-8.27	104.33	112.60
3	F	180	ILE	O-C-N	8.27	130.01	121.91
1	B	306	ASP	N-CA-C	-8.26	102.52	112.59
3	F	184	ALA	CA-C-N	8.24	132.15	120.28
3	F	184	ALA	C-N-CA	8.24	132.15	120.28
1	B	333	PHE	CA-CB-CG	-8.22	105.58	113.80
1	A	588	ILE	N-CA-C	8.19	118.99	110.72
3	E	4	GLU	N-CA-C	-8.14	102.66	112.59
1	A	268	ALA	CA-C-N	8.14	136.35	121.70
1	A	268	ALA	C-N-CA	8.14	136.35	121.70
1	A	327	ARG	NE-CZ-NH1	-8.12	113.38	121.50
1	B	416	GLN	CA-C-N	8.11	130.78	120.56
1	B	416	GLN	C-N-CA	8.11	130.78	120.56
1	B	761	ASN	CA-CB-CG	8.11	120.71	112.60
1	B	471	GLU	CA-C-N	8.10	131.94	120.28
1	B	471	GLU	C-N-CA	8.10	131.94	120.28
1	B	599	VAL	CA-C-O	8.10	127.42	120.22
1	B	227	PHE	CA-CB-CG	-8.09	105.71	113.80
2	C	141	PRO	N-CA-C	8.09	123.98	113.86
2	C	16	PHE	CA-CB-CG	8.09	121.89	113.80
1	B	290	GLY	O-C-N	8.08	130.93	122.93
3	E	33	PRO	N-CA-C	8.07	120.55	110.70
1	A	87	ASN	CA-CB-CG	8.04	120.64	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	LYS	CA-C-O	-8.03	113.28	119.46
1	A	665	HIS	N-CA-C	-8.02	103.07	113.17
1	A	202	LYS	N-CA-C	-8.00	101.69	112.26
1	B	618	ILE	O-C-N	-8.00	112.58	122.57
1	A	707	CYS	N-CA-C	-7.98	103.34	113.23
2	C	26	LYS	CA-C-N	7.95	133.10	121.18
2	C	26	LYS	C-N-CA	7.95	133.10	121.18
1	B	822	PHE	CA-CB-CG	7.92	121.72	113.80
1	A	838	LYS	CA-C-O	-7.92	109.31	120.16
1	A	778	ARG	NE-CZ-NH2	7.91	126.32	119.20
3	F	129	VAL	N-CA-C	-7.89	103.56	110.74
2	C	44	THR	CA-C-O	7.89	130.79	121.88
3	F	144	GLU	CA-C-N	7.87	131.62	120.28
3	F	144	GLU	C-N-CA	7.87	131.62	120.28
1	B	141	ARG	NE-CZ-NH2	7.86	126.28	119.20
1	B	330	ASP	CA-C-N	7.86	130.81	120.28
1	B	330	ASP	C-N-CA	7.86	130.81	120.28
1	A	467	TYR	O-C-N	7.85	132.35	122.93
1	B	462	PHE	N-CA-C	-7.83	94.12	110.80
1	A	537	PHE	CA-CB-CG	-7.83	105.97	113.80
1	B	703	GLY	CA-C-N	7.82	132.83	121.02
1	B	703	GLY	C-N-CA	7.82	132.83	121.02
1	A	283	PHE	N-CA-C	-7.82	103.76	113.38
1	A	294	LEU	N-CA-C	-7.82	103.32	113.17
1	B	418	SER	CA-C-N	7.81	131.38	120.29
1	B	418	SER	C-N-CA	7.81	131.38	120.29
1	A	199	LYS	CA-C-N	7.81	129.60	119.84
1	A	199	LYS	C-N-CA	7.81	129.60	119.84
1	B	489	HIS	CE1-NE2-CD2	-7.79	101.21	109.00
2	D	37	ARG	NE-CZ-NH2	7.77	126.19	119.20
2	D	154	GLU	N-CA-CB	7.75	124.18	111.62
1	A	475	ILE	N-CA-C	-7.75	104.20	111.48
2	D	28	ASP	CA-C-N	7.74	130.99	120.38
2	D	28	ASP	C-N-CA	7.74	130.99	120.38
1	B	536	MET	CA-C-N	7.74	135.76	122.38
1	B	536	MET	C-N-CA	7.74	135.76	122.38
1	B	259	ASP	N-CA-CB	7.72	122.48	110.21
2	C	108	HIS	CE1-NE2-CD2	-7.69	101.31	109.00
2	C	4	LEU	CB-CA-C	-7.67	96.54	109.65
1	B	809	ARG	NE-CZ-NH2	-7.67	112.30	119.20
2	C	153	ASP	CA-CB-CG	7.65	120.25	112.60
3	F	32	LYS	CA-C-O	-7.65	111.59	118.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	VAL	CA-C-N	7.64	132.29	120.75
1	A	320	VAL	C-N-CA	7.64	132.29	120.75
1	B	497	GLU	CA-C-O	-7.64	112.45	120.55
1	A	17	GLN	OE1-CD-NE2	-7.64	114.96	122.60
1	B	827	ASN	CA-CB-CG	7.62	120.22	112.60
1	A	323	ALA	N-CA-CB	7.61	123.35	110.49
1	A	565	PRO	N-CA-C	7.60	119.98	110.70
3	F	28	PRO	CA-C-N	7.60	128.21	120.38
3	F	28	PRO	C-N-CA	7.60	128.21	120.38
1	A	308	HIS	CA-CB-CG	7.60	121.40	113.80
1	A	489	HIS	CA-CB-CG	7.60	121.40	113.80
1	B	60	GLY	N-CA-C	-7.59	103.19	113.37
3	E	137	GLU	N-CA-C	-7.59	94.64	110.80
1	B	809	ARG	NE-CZ-NH1	7.58	129.08	121.50
3	F	55	GLN	N-CA-C	-7.57	104.09	112.72
1	B	574	HIS	ND1-CE1-NE2	7.57	115.97	108.40
3	F	130	ASN	N-CA-C	7.57	120.41	111.71
1	B	290	GLY	CA-C-O	-7.54	114.77	121.41
1	B	116	PHE	CA-C-O	-7.54	113.29	122.41
1	B	600	ASN	CA-C-N	7.53	135.93	121.54
1	B	600	ASN	C-N-CA	7.53	135.93	121.54
1	B	654	ARG	N-CA-C	-7.53	101.20	112.04
2	D	140	GLU	CA-C-N	7.52	127.55	119.28
2	D	140	GLU	C-N-CA	7.52	127.55	119.28
3	F	183	PHE	CA-CB-CG	-7.52	106.28	113.80
1	B	129	TYR	CA-C-N	7.51	132.09	120.75
1	B	129	TYR	C-N-CA	7.51	132.09	120.75
3	F	54	HIS	CA-CB-CG	-7.49	106.31	113.80
1	B	599	VAL	CA-C-N	7.48	135.83	121.54
1	B	599	VAL	C-N-CA	7.48	135.83	121.54
1	B	64	ARG	NE-CZ-NH2	7.48	125.93	119.20
3	E	142	CYS	O-C-N	-7.47	114.56	123.31
1	B	217	VAL	N-CA-C	7.47	119.14	110.62
1	B	670	HIS	N-CA-C	-7.47	97.23	109.40
1	B	814	VAL	CA-C-N	7.45	130.21	120.60
1	B	814	VAL	C-N-CA	7.45	130.21	120.60
1	A	377	GLU	O-C-N	-7.44	112.69	122.59
1	A	265	LEU	N-CA-C	-7.44	97.09	109.07
1	B	93	ASP	CA-C-N	7.44	130.57	120.38
1	B	93	ASP	C-N-CA	7.44	130.57	120.38
1	B	787	THR	CA-CB-OG1	7.44	120.76	109.60
1	B	723	ARG	N-CA-C	-7.43	103.67	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	338	PHE	CA-C-N	7.43	131.26	120.71
1	B	338	PHE	C-N-CA	7.43	131.26	120.71
1	B	439	ARG	NE-CZ-NH2	7.43	125.88	119.20
2	D	112	SER	N-CA-C	-7.43	103.35	113.30
3	E	175	ASN	CA-C-O	7.43	130.24	121.40
1	B	364	ARG	NE-CZ-NH2	7.42	125.88	119.20
3	E	106	ILE	CA-C-N	7.42	131.72	120.82
3	E	106	ILE	C-N-CA	7.42	131.72	120.82
1	B	668	GLN	CA-C-N	7.41	127.68	119.90
1	B	668	GLN	C-N-CA	7.41	127.68	119.90
1	A	599	VAL	N-CA-C	-7.41	105.90	112.12
1	A	601	ASP	CA-CB-CG	7.41	120.01	112.60
1	A	105	TYR	O-C-N	7.39	131.36	122.27
2	C	70	ILE	O-C-N	7.39	129.59	121.90
1	B	470	PHE	CA-C-N	7.39	130.05	120.44
1	B	470	PHE	C-N-CA	7.39	130.05	120.44
1	A	439	ARG	NE-CZ-NH2	7.39	125.85	119.20
1	B	537	PHE	N-CA-C	-7.38	99.69	108.25
3	F	15	LYS	N-CA-C	-7.37	96.26	108.34
3	F	166	ALA	N-CA-C	7.36	119.31	111.28
1	B	646	PHE	CA-C-N	7.36	131.28	120.90
1	B	646	PHE	C-N-CA	7.36	131.28	120.90
3	E	94	GLU	N-CA-C	-7.34	102.98	112.23
1	B	789	LEU	N-CA-C	-7.33	103.23	111.14
1	B	645	SER	N-CA-C	-7.30	104.50	113.41
2	D	51	ASN	CA-CB-CG	-7.29	105.31	112.60
1	B	138	LYS	N-CA-C	-7.29	103.70	112.59
2	D	104	ALA	O-C-N	7.29	129.96	122.09
1	B	96	VAL	N-CA-C	-7.28	103.06	111.00
1	A	344	THR	O-C-N	7.28	130.45	122.15
1	A	186	VAL	CA-C-N	7.26	130.41	120.46
1	A	186	VAL	C-N-CA	7.26	130.41	120.46
3	F	173	ASP	CA-C-O	7.26	126.73	118.97
1	B	582	GLY	CA-C-N	7.25	131.16	120.87
1	B	582	GLY	C-N-CA	7.25	131.16	120.87
2	D	109	VAL	CB-CA-C	-7.25	100.92	112.16
1	B	126	PHE	N-CA-CB	7.25	118.80	110.03
2	D	122	CYS	O-C-N	-7.25	114.44	122.12
1	B	436	LEU	N-CA-C	7.24	118.96	111.14
3	E	112	LEU	N-CA-CB	7.22	122.38	110.39
1	B	287	MET	CB-CA-C	-7.22	99.54	110.88
1	B	85	MET	CA-C-N	7.20	132.74	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	MET	C-N-CA	7.20	132.74	120.72
1	B	584	VAL	CA-C-O	-7.19	113.80	119.98
1	A	227	PHE	CA-CB-CG	-7.18	106.62	113.80
1	B	711	PHE	CA-CB-CG	-7.17	106.63	113.80
1	B	148	HIS	CA-C-N	7.17	135.23	121.54
1	B	148	HIS	C-N-CA	7.17	135.23	121.54
1	A	612	ASN	N-CA-C	-7.16	99.04	110.14
1	B	145	VAL	N-CA-C	-7.16	100.53	107.76
1	B	633	GLY	CA-C-N	7.16	132.44	122.06
1	B	633	GLY	C-N-CA	7.16	132.44	122.06
1	B	574	HIS	CE1-NE2-CD2	-7.16	101.84	109.00
1	B	793	ILE	CB-CA-C	-7.15	101.08	112.16
1	B	319	GLY	N-CA-C	-7.14	105.21	115.64
1	B	480	GLU	CA-C-N	7.12	131.13	120.31
1	B	480	GLU	C-N-CA	7.12	131.13	120.31
1	A	749	ALA	N-CA-C	-7.12	102.70	112.03
1	B	309	PHE	N-CA-C	-7.11	104.48	113.72
1	A	471	GLU	CA-C-N	7.09	134.00	122.65
1	A	471	GLU	C-N-CA	7.09	134.00	122.65
1	B	29	LYS	CA-C-N	7.09	129.78	120.28
1	B	29	LYS	C-N-CA	7.09	129.78	120.28
1	A	179	LYS	N-CA-C	-7.07	103.52	112.93
3	F	118	ARG	NE-CZ-NH1	-7.06	114.44	121.50
3	F	28	PRO	CA-C-O	-7.06	115.15	120.73
1	A	646	PHE	N-CA-C	-7.06	103.34	112.23
1	B	396	LEU	N-CA-C	7.05	119.58	111.11
1	B	179	LYS	CA-C-N	7.04	130.29	120.29
1	B	179	LYS	C-N-CA	7.04	130.29	120.29
1	A	596	LYS	N-CA-C	-7.02	104.18	112.89
1	A	346	VAL	O-C-N	7.02	129.20	121.90
3	E	114	ILE	N-CA-CB	7.02	118.28	110.62
1	B	650	SER	O-C-N	-7.02	113.03	122.43
1	A	646	PHE	CA-CB-CG	-7.02	106.78	113.80
1	A	281	HIS	CB-CG-ND1	7.01	133.22	122.70
1	B	12	TYR	CA-C-N	7.01	130.09	120.35
1	B	12	TYR	C-N-CA	7.01	130.09	120.35
1	A	803	LYS	CA-C-N	6.98	130.92	120.31
1	A	803	LYS	C-N-CA	6.98	130.92	120.31
1	A	560	PHE	CA-C-N	6.98	132.91	122.58
1	A	560	PHE	C-N-CA	6.98	132.91	122.58
1	B	192	ASN	CA-CB-CG	-6.96	105.64	112.60
1	B	421	VAL	N-CA-C	-6.96	103.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	602	THR	N-CA-C	-6.96	96.37	108.69
1	B	97	LEU	CA-C-N	6.96	129.93	120.54
1	B	97	LEU	C-N-CA	6.96	129.93	120.54
1	A	537	PHE	CA-C-N	6.96	128.53	119.84
1	A	537	PHE	C-N-CA	6.96	128.53	119.84
2	D	2	ALA	O-C-N	6.95	131.84	122.59
1	B	397	VAL	N-CA-C	6.95	117.74	110.72
1	B	180	THR	CA-C-N	6.95	129.59	120.28
1	B	180	THR	C-N-CA	6.95	129.59	120.28
1	B	572	GLU	N-CA-C	-6.93	102.88	112.30
1	A	665	HIS	N-CA-CB	6.91	120.72	110.49
2	C	86	PHE	CA-CB-CG	-6.91	106.89	113.80
3	F	159	SER	N-CA-C	6.91	120.66	110.30
1	A	437	VAL	CB-CA-C	-6.91	102.69	112.22
1	B	218	VAL	CA-C-N	6.90	129.53	120.28
1	B	218	VAL	C-N-CA	6.90	129.53	120.28
1	A	158	SER	CA-C-O	-6.89	112.59	120.24
1	A	685	VAL	N-CA-C	-6.89	95.00	109.34
3	E	179	ASP	CA-CB-CG	6.89	119.49	112.60
2	D	127	ARG	CA-C-N	6.89	129.49	120.60
2	D	127	ARG	C-N-CA	6.89	129.49	120.60
1	A	431	ARG	NE-CZ-NH1	-6.89	114.61	121.50
1	B	221	ASN	N-CA-CB	6.89	120.03	110.11
1	B	801	GLU	CA-C-N	6.88	129.39	120.44
1	B	801	GLU	C-N-CA	6.88	129.39	120.44
1	A	389	ALA	N-CA-CB	6.88	122.12	110.49
1	A	308	HIS	ND1-CE1-NE2	6.88	115.28	108.40
1	B	31	MET	CG-SD-CE	-6.87	85.79	100.90
3	E	59	PHE	CA-C-O	6.87	126.07	118.52
1	B	278	ARG	N-CA-C	-6.86	99.04	109.95
2	D	71	PHE	N-CA-C	6.86	118.42	111.07
1	A	413	ASN	N-CA-C	-6.86	99.73	110.36
3	E	122	THR	N-CA-CB	6.86	120.19	109.83
3	F	170	ALA	CA-C-N	6.86	126.32	118.85
3	F	170	ALA	C-N-CA	6.86	126.32	118.85
1	A	827	ASN	N-CA-C	-6.85	104.22	114.64
1	A	92	ASN	CA-CB-CG	-6.85	105.75	112.60
1	A	651	ALA	CA-C-O	6.84	127.27	119.27
1	B	622	HIS	CA-C-O	-6.82	112.05	118.73
1	B	815	ILE	CA-C-N	6.82	129.41	120.28
1	B	815	ILE	C-N-CA	6.82	129.41	120.28
2	C	22	GLU	CA-C-N	6.82	130.94	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	22	GLU	C-N-CA	6.82	130.94	121.26
1	B	183	THR	O-C-N	-6.81	114.90	122.12
1	A	773	ARG	NE-CZ-NH2	6.81	125.33	119.20
3	F	175	ASN	N-CA-C	-6.80	103.28	112.26
2	C	108	HIS	ND1-CE1-NE2	6.80	115.20	108.40
1	B	778	ARG	NE-CZ-NH2	6.80	125.32	119.20
1	B	289	GLY	CA-C-N	6.80	126.44	119.92
1	B	289	GLY	C-N-CA	6.80	126.44	119.92
1	B	159	ALA	CA-C-N	6.79	129.27	120.44
1	B	159	ALA	C-N-CA	6.79	129.27	120.44
1	B	244	PHE	CA-C-N	6.78	132.22	123.13
1	B	244	PHE	C-N-CA	6.78	132.22	123.13
3	F	177	LEU	CA-C-N	6.78	131.05	120.34
3	F	177	LEU	C-N-CA	6.78	131.05	120.34
3	E	111	PHE	CA-C-O	6.78	127.53	119.06
1	B	786	VAL	CA-C-O	-6.76	114.00	121.17
1	A	99	ASN	N-CA-C	-6.76	103.99	111.36
2	C	116	ARG	NE-CZ-NH1	-6.76	114.74	121.50
2	C	145	THR	CA-C-N	6.75	131.14	120.47
2	C	145	THR	C-N-CA	6.75	131.14	120.47
1	B	689	GLY	CA-C-N	6.75	129.56	120.65
1	B	689	GLY	C-N-CA	6.75	129.56	120.65
1	B	768	ALA	N-CA-C	6.75	119.01	110.24
1	B	130	THR	CA-C-O	-6.73	114.41	121.55
3	E	63	PHE	CA-CB-CG	-6.73	107.07	113.80
1	B	214	GLU	CA-C-N	6.73	129.84	120.29
1	B	214	GLU	C-N-CA	6.73	129.84	120.29
3	F	24	ALA	N-CA-CB	6.73	121.86	110.49
2	C	115	GLU	N-CA-C	-6.72	104.56	112.89
1	B	380	ARG	CA-C-O	-6.72	111.36	119.49
1	A	740	LYS	CA-C-N	6.72	130.52	120.31
1	A	740	LYS	C-N-CA	6.72	130.52	120.31
1	B	708	ARG	NE-CZ-NH1	6.71	128.21	121.50
2	C	3	ASP	CA-CB-CG	-6.71	105.89	112.60
1	B	511	GLY	O-C-N	6.70	128.31	123.35
1	A	241	PHE	O-C-N	-6.69	115.07	123.17
1	A	390	ALA	N-CA-C	-6.68	104.26	112.88
1	A	510	PHE	N-CA-CB	6.68	121.07	110.65
1	A	510	PHE	CB-CA-C	-6.67	99.08	110.16
3	E	68	GLN	N-CA-C	-6.67	105.02	113.02
3	E	103	PRO	N-CA-CB	6.67	110.25	103.25
1	B	344	THR	CA-C-N	6.65	129.48	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	THR	C-N-CA	6.65	129.48	120.44
1	B	614	LEU	CA-C-N	6.65	129.57	120.46
1	B	614	LEU	C-N-CA	6.65	129.57	120.46
1	B	488	HIS	CE1-NE2-CD2	-6.64	102.36	109.00
3	F	58	GLU	O-C-N	-6.64	113.76	122.59
1	A	129	TYR	CA-C-N	6.63	130.57	120.82
1	A	129	TYR	C-N-CA	6.63	130.57	120.82
2	C	130	ASP	N-CA-CB	6.61	119.75	110.04
1	B	181	GLU	CA-C-N	6.60	129.42	120.44
1	B	181	GLU	C-N-CA	6.60	129.42	120.44
2	C	29	ALA	N-CA-C	6.59	118.47	111.28
1	A	627	ALA	N-CA-C	6.59	119.54	110.24
1	B	771	LEU	N-CA-C	6.59	118.15	110.97
2	D	30	ARG	NE-CZ-NH2	6.59	125.13	119.20
1	A	229	ASN	CA-CB-CG	-6.59	106.01	112.60
1	B	388	ASN	CA-C-N	6.58	129.10	120.28
1	B	388	ASN	C-N-CA	6.58	129.10	120.28
1	B	229	ASN	N-CA-CB	6.58	120.00	110.06
1	A	165	GLU	N-CA-C	-6.58	99.66	108.74
3	E	119	ILE	O-C-N	-6.58	115.55	122.06
1	B	59	GLU	CA-C-N	6.57	128.57	120.22
1	B	59	GLU	C-N-CA	6.57	128.57	120.22
1	A	820	ARG	CA-C-N	6.57	134.39	121.58
1	A	820	ARG	C-N-CA	6.57	134.39	121.58
1	A	157	TYR	CA-C-O	6.57	127.38	120.42
1	A	468	ASN	O-C-N	-6.56	116.13	123.48
1	B	571	GLN	N-CA-C	6.56	119.49	110.24
1	A	620	GLU	CB-CG-CD	-6.55	101.46	112.60
1	B	766	PHE	CA-C-N	6.55	133.41	122.87
1	B	766	PHE	C-N-CA	6.55	133.41	122.87
1	B	469	GLY	CA-C-N	6.54	130.25	120.31
1	B	469	GLY	C-N-CA	6.54	130.25	120.31
1	A	833	LEU	N-CA-C	-6.54	96.87	110.80
2	D	2	ALA	N-CA-CB	6.54	121.54	110.49
1	A	129	TYR	N-CA-C	6.54	121.27	113.16
3	F	49	ALA	CA-C-N	6.53	132.38	122.65
3	F	49	ALA	C-N-CA	6.53	132.38	122.65
1	B	208	GLU	N-CA-CB	6.52	121.52	110.49
2	C	117	LEU	CA-C-N	6.52	134.00	121.54
2	C	117	LEU	C-N-CA	6.52	134.00	121.54
1	B	310	VAL	CA-C-N	6.51	133.02	121.75
1	B	310	VAL	C-N-CA	6.51	133.02	121.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	822	PHE	CA-C-N	6.51	129.66	120.28
1	B	822	PHE	C-N-CA	6.51	129.66	120.28
1	B	250	GLY	O-C-N	6.51	128.28	121.77
2	C	21	TRP	CA-C-N	6.50	133.96	121.54
2	C	21	TRP	C-N-CA	6.50	133.96	121.54
3	F	188	THR	N-CA-CB	6.50	121.48	110.49
3	E	135	PHE	N-CA-C	-6.50	99.28	108.96
1	B	257	GLY	CA-C-O	-6.50	115.05	121.48
1	B	720	PHE	CA-CB-CG	-6.49	107.31	113.80
1	A	670	HIS	CE1-NE2-CD2	-6.49	102.51	109.00
1	B	415	THR	CA-C-N	6.49	128.87	120.44
1	B	415	THR	C-N-CA	6.49	128.87	120.44
1	B	734	LYS	CA-C-O	6.48	126.15	118.69
3	F	33	PRO	N-CA-CB	6.48	109.36	103.08
1	B	131	ASN	CA-C-N	6.48	129.25	120.44
1	B	131	ASN	C-N-CA	6.48	129.25	120.44
2	D	36	LEU	CA-C-N	6.47	128.85	120.44
2	D	36	LEU	C-N-CA	6.47	128.85	120.44
1	B	792	TRP	CG-CD2-CE3	6.47	140.37	133.90
2	C	141	PRO	CB-CA-C	-6.46	102.24	111.68
1	A	759	LEU	CA-C-N	6.46	129.41	122.69
1	A	759	LEU	C-N-CA	6.46	129.41	122.69
3	F	22	GLY	O-C-N	6.46	128.45	122.90
3	F	87	GLY	CA-C-N	6.46	131.30	122.07
3	F	87	GLY	C-N-CA	6.46	131.30	122.07
2	D	146	ILE	CA-C-O	-6.46	114.38	121.29
3	E	118	ARG	NE-CZ-NH1	-6.45	115.05	121.50
1	B	817	ARG	CA-C-O	6.45	127.29	119.49
1	B	817	ARG	O-C-N	-6.45	114.01	122.39
1	B	354	MET	CA-C-N	6.43	129.77	120.38
1	B	354	MET	C-N-CA	6.43	129.77	120.38
1	A	98	HIS	CE1-NE2-CD2	-6.43	102.57	109.00
1	A	458	ASP	CA-C-O	6.42	129.14	120.47
1	A	469	GLY	N-CA-C	-6.42	97.96	113.18
1	B	574	HIS	CG-CD2-NE2	6.42	113.62	107.20
2	D	102	LEU	CB-CA-C	-6.42	99.62	109.89
1	B	190	TYR	CA-C-N	6.42	132.92	120.99
1	B	190	TYR	C-N-CA	6.42	132.92	120.99
1	A	399	PRO	CB-CA-C	6.41	119.70	111.56
1	A	212	THR	N-CA-C	-6.41	98.92	108.99
1	A	691	VAL	CA-C-N	6.41	129.51	120.28
1	A	691	VAL	C-N-CA	6.41	129.51	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	TYR	CA-C-O	-6.41	112.61	119.97
1	A	248	HIS	CB-CG-CD2	-6.38	122.90	131.20
1	B	343	LYS	CA-C-O	-6.38	114.05	121.07
3	E	118	ARG	NE-CZ-NH2	6.38	124.94	119.20
1	A	391	ASP	CA-CB-CG	-6.37	106.23	112.60
1	A	331	THR	CA-C-O	-6.37	113.67	120.42
3	F	142	CYS	N-CA-C	-6.37	98.14	108.52
1	B	669	PRO	N-CA-CB	6.37	108.97	103.36
3	F	31	PRO	CA-C-N	6.37	130.40	120.97
3	F	31	PRO	C-N-CA	6.37	130.40	120.97
1	A	687	ASP	N-CA-C	-6.37	96.88	108.02
2	C	63	THR	CA-CB-CG2	-6.36	99.68	110.50
3	F	166	ALA	O-C-N	-6.36	115.38	122.12
1	B	649	VAL	CA-C-N	6.36	131.34	120.72
1	B	649	VAL	C-N-CA	6.36	131.34	120.72
1	B	391	ASP	O-C-N	6.36	128.86	122.12
3	F	109	THR	CA-C-N	6.35	132.84	121.66
3	F	109	THR	C-N-CA	6.35	132.84	121.66
1	A	806	GLN	N-CA-C	-6.35	104.58	112.90
1	B	171	ILE	O-C-N	-6.34	116.52	123.18
1	B	505	TRP	CE2-CD2-CE3	6.34	125.14	118.80
1	B	783	GLY	N-CA-C	-6.34	98.15	113.18
1	A	593	GLU	CA-C-N	6.34	132.13	122.37
1	A	593	GLU	C-N-CA	6.34	132.13	122.37
1	A	468	ASN	N-CA-C	-6.34	98.74	108.76
1	B	30	LYS	O-C-N	6.34	128.84	122.12
1	A	830	TRP	N-CA-CB	6.33	121.20	110.49
2	D	153	ASP	N-CA-CB	6.33	121.19	110.49
1	B	20	LYS	N-CA-C	-6.33	99.36	108.60
1	A	131	ASN	OD1-CG-ND2	6.33	128.93	122.60
1	B	150	PHE	CA-CB-CG	-6.33	107.47	113.80
1	B	488	HIS	ND1-CE1-NE2	6.32	114.72	108.40
1	B	625	LEU	CA-C-O	-6.32	113.88	121.40
1	B	792	TRP	CA-C-O	-6.32	113.85	120.55
1	B	651	ALA	N-CA-CB	6.32	119.67	110.26
1	A	225	GLU	CA-C-O	6.32	127.15	119.38
1	B	774	LEU	N-CA-CB	6.31	120.87	110.39
1	B	440	LEU	CA-C-N	6.31	129.37	120.28
1	B	440	LEU	C-N-CA	6.31	129.37	120.28
1	B	651	ALA	CA-C-N	6.30	129.36	120.28
1	B	651	ALA	C-N-CA	6.30	129.36	120.28
3	F	127	VAL	CA-C-O	6.30	128.66	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	654	ARG	NE-CZ-NH1	-6.29	115.21	121.50
1	B	126	PHE	N-CA-C	-6.29	101.61	110.29
1	B	561	VAL	N-CA-CB	6.29	119.80	111.25
1	A	494	GLU	CB-CA-C	-6.29	98.59	110.67
1	B	285	GLN	CA-C-N	6.29	128.70	120.28
1	B	285	GLN	C-N-CA	6.29	128.70	120.28
2	C	54	SER	CA-C-O	-6.28	114.72	121.38
3	E	142	CYS	N-CA-C	-6.28	98.14	108.76
1	A	758	ARG	CB-CA-C	6.28	120.11	109.75
3	F	29	PRO	CA-C-O	-6.28	111.45	120.56
1	A	320	VAL	N-CA-C	-6.28	101.48	109.58
1	A	499	LYS	N-CA-C	-6.28	97.43	110.80
1	A	183	THR	CA-C-N	6.28	129.85	120.31
1	A	183	THR	C-N-CA	6.28	129.85	120.31
2	C	7	ALA	N-CA-CB	6.27	120.63	110.40
1	B	693	HIS	CA-C-N	6.27	128.69	120.28
1	B	693	HIS	C-N-CA	6.27	128.69	120.28
1	B	792	TRP	CE2-CD2-CE3	-6.27	112.53	118.80
1	A	597	ASP	CA-C-N	6.27	126.62	119.92
1	A	597	ASP	C-N-CA	6.27	126.62	119.92
1	A	711	PHE	CB-CA-C	-6.27	101.50	109.65
1	B	98	HIS	CA-CB-CG	6.26	120.06	113.80
1	A	568	PRO	CA-C-O	-6.25	114.44	122.13
2	C	63	THR	N-CA-C	-6.25	100.95	110.14
1	A	782	LEU	CA-C-N	6.24	127.02	120.03
1	A	782	LEU	C-N-CA	6.24	127.02	120.03
1	B	74	VAL	CA-C-N	6.24	129.03	120.67
1	B	74	VAL	C-N-CA	6.24	129.03	120.67
1	B	750	ILE	CB-CA-C	6.23	118.14	110.73
3	F	24	ALA	N-CA-C	-6.22	97.55	110.80
1	B	278	ARG	N-CA-CB	6.22	120.80	110.85
1	A	398	LYS	CA-C-N	6.22	126.24	119.90
1	A	398	LYS	C-N-CA	6.22	126.24	119.90
1	B	132	ARG	CA-C-N	6.22	128.61	120.28
1	B	132	ARG	C-N-CA	6.22	128.61	120.28
1	A	242	GLY	CA-C-O	-6.22	115.46	120.81
1	B	241	PHE	N-CA-C	-6.21	97.56	110.80
3	E	68	GLN	CB-CG-CD	-6.21	102.03	112.60
2	D	73	GLN	OE1-CD-NE2	6.21	128.81	122.60
3	F	134	LEU	N-CA-C	6.21	120.46	113.01
2	C	134	ASP	N-CA-C	-6.21	105.74	113.38
1	B	178	GLY	CA-C-N	6.21	128.88	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	178	GLY	C-N-CA	6.21	128.88	120.38
3	F	166	ALA	CA-C-O	6.20	127.13	120.55
1	A	232	THR	O-C-N	-6.20	114.92	122.68
1	A	574	HIS	CE1-NE2-CD2	-6.20	102.80	109.00
1	A	717	TYR	N-CA-CB	6.19	117.72	110.42
1	A	673	ARG	O-C-N	-6.18	115.81	123.04
1	B	443	THR	N-CA-CB	6.17	119.85	110.28
3	E	54	HIS	CA-CB-CG	6.17	119.97	113.80
1	B	12	TYR	CB-CA-C	-6.17	99.57	109.75
2	D	6	ALA	CA-C-N	6.17	128.55	120.28
2	D	6	ALA	C-N-CA	6.17	128.55	120.28
1	A	197	THR	CA-CB-OG1	6.17	118.85	109.60
1	B	473	LEU	CA-C-O	6.16	126.95	120.42
1	B	76	PRO	CA-C-N	6.16	127.54	119.84
1	B	76	PRO	C-N-CA	6.16	127.54	119.84
1	B	816	GLN	OE1-CD-NE2	6.16	128.76	122.60
1	A	622	HIS	CA-CB-CG	-6.15	107.65	113.80
1	B	6	ASP	CA-C-O	-6.14	114.77	119.32
1	A	8	THR	N-CA-C	-6.14	105.36	112.92
1	A	834	TYR	N-CA-C	-6.14	99.81	108.96
1	B	10	TYR	N-CA-CB	6.14	119.22	110.44
1	B	770	VAL	CA-C-N	6.14	128.75	120.65
1	B	770	VAL	C-N-CA	6.14	128.75	120.65
1	B	116	PHE	CA-CB-CG	-6.14	107.66	113.80
1	A	673	ARG	NE-CZ-NH2	6.14	124.72	119.20
1	A	830	TRP	O-C-N	6.13	130.75	122.59
3	E	40	ALA	N-CA-C	-6.13	105.89	113.19
1	A	289	GLY	CA-C-N	6.13	132.21	120.07
1	A	289	GLY	C-N-CA	6.13	132.21	120.07
3	E	52	THR	O-C-N	-6.13	116.86	123.42
1	B	621	ASP	N-CA-CB	6.12	121.09	110.81
1	A	608	LYS	CA-C-O	6.12	126.46	119.18
1	B	782	LEU	CA-C-N	6.11	133.39	121.41
1	B	782	LEU	C-N-CA	6.11	133.39	121.41
1	A	589	THR	N-CA-C	-6.11	100.23	109.95
1	B	326	LEU	CA-C-N	6.11	128.96	120.29
1	B	326	LEU	C-N-CA	6.11	128.96	120.29
1	A	413	ASN	N-CA-CB	6.11	119.83	110.49
1	A	431	ARG	NE-CZ-NH2	6.10	124.69	119.20
1	A	579	HIS	CA-CB-CG	-6.10	107.70	113.80
3	F	142	CYS	CA-C-N	6.10	132.09	122.21
3	F	142	CYS	C-N-CA	6.10	132.09	122.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	139	TYR	N-CA-C	-6.10	106.48	114.04
2	C	31	ASP	CA-C-N	6.09	128.94	120.29
2	C	31	ASP	C-N-CA	6.09	128.94	120.29
3	F	72	GLY	CA-C-N	6.09	131.01	122.36
3	F	72	GLY	C-N-CA	6.09	131.01	122.36
1	B	257	GLY	O-C-N	6.09	129.99	123.96
1	A	158	SER	O-C-N	6.09	130.15	122.23
2	C	115	GLU	CA-C-N	6.09	133.17	121.54
2	C	115	GLU	C-N-CA	6.09	133.17	121.54
1	B	386	GLY	CA-C-N	6.09	128.81	120.35
1	B	386	GLY	C-N-CA	6.09	128.81	120.35
3	F	13	SER	O-C-N	-6.09	117.90	123.50
2	C	70	ILE	N-CA-C	-6.09	104.81	110.53
1	A	242	GLY	CA-C-N	6.09	131.40	123.00
1	A	242	GLY	C-N-CA	6.09	131.40	123.00
1	A	180	THR	CA-C-N	6.08	128.92	120.29
1	A	180	THR	C-N-CA	6.08	128.92	120.29
2	D	79	GLU	N-CA-CB	6.07	121.99	111.00
3	E	153	THR	N-CA-C	-6.07	106.20	113.97
3	F	108	PHE	CA-C-O	-6.07	114.08	120.63
3	F	175	ASN	CB-CA-C	6.07	120.90	111.13
1	A	678	ASN	CA-CB-CG	6.07	118.67	112.60
1	B	534	GLU	CA-C-N	-6.06	114.97	122.84
1	B	534	GLU	C-N-CA	-6.06	114.97	122.84
1	A	766	PHE	CA-C-N	6.06	128.89	120.29
1	A	766	PHE	C-N-CA	6.06	128.89	120.29
3	E	30	PRO	O-C-N	-6.06	118.52	121.31
3	E	141	LYS	CA-C-O	6.05	127.92	121.45
1	A	102	GLN	CA-C-O	6.05	126.93	119.79
1	A	649	VAL	CA-C-N	6.05	130.82	120.72
1	A	649	VAL	C-N-CA	6.05	130.82	120.72
1	A	829	LEU	CA-C-O	-6.04	114.86	121.87
1	A	573	ALA	N-CA-CB	6.04	120.70	110.49
1	A	717	TYR	CA-C-O	-6.04	112.99	118.79
1	A	507	PHE	CA-CB-CG	-6.03	107.77	113.80
1	B	794	ARG	NE-CZ-NH1	-6.03	115.47	121.50
1	B	103	ARG	NE-CZ-NH2	6.03	124.62	119.20
1	B	758	ARG	NE-CZ-NH2	6.03	124.62	119.20
1	B	431	ARG	NE-CZ-NH1	-6.03	115.47	121.50
1	B	802	PHE	N-CA-C	-6.03	104.62	111.07
2	C	26	LYS	N-CA-CB	6.02	120.67	110.49
1	B	352	SER	N-CA-C	-6.02	104.64	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	15	HIS	CA-C-N	6.02	128.84	120.29
2	C	15	HIS	C-N-CA	6.02	128.84	120.29
3	E	149	ARG	N-CA-C	-6.02	105.90	113.18
1	B	783	GLY	CA-C-N	6.01	133.03	121.54
1	B	783	GLY	C-N-CA	6.01	133.03	121.54
1	B	323	ALA	N-CA-CB	6.01	119.03	110.13
1	A	705	ARG	NE-CZ-NH1	-6.01	115.49	121.50
1	B	143	THR	N-CA-C	-6.01	107.18	114.75
1	B	520	LEU	N-CA-C	-6.00	105.88	112.72
2	D	19	TYR	N-CA-CB	5.99	120.33	110.39
1	A	195	ALA	CA-C-O	5.99	126.25	119.18
1	A	544	SER	N-CA-C	-5.99	104.87	111.82
2	D	105	GLU	CA-C-O	5.99	126.87	120.10
2	D	119	ASP	CA-C-N	5.99	128.11	120.56
2	D	119	ASP	C-N-CA	5.99	128.11	120.56
1	A	575	PHE	N-CA-CB	5.99	119.00	110.44
1	B	792	TRP	CD2-CE3-CZ3	5.99	126.38	118.60
1	A	802	PHE	CA-C-N	5.99	128.30	120.28
1	A	802	PHE	C-N-CA	5.99	128.30	120.28
3	E	135	PHE	O-C-N	-5.98	116.22	123.10
1	B	288	SER	CA-C-N	5.98	131.43	120.79
1	B	288	SER	C-N-CA	5.98	131.43	120.79
3	F	33	PRO	N-CA-C	5.98	117.99	110.70
3	F	115	PHE	CA-CB-CG	5.98	119.78	113.80
1	A	307	TYR	N-CA-CB	5.97	120.59	110.49
1	B	363	GLN	N-CA-C	-5.97	104.65	113.61
1	B	411	GLY	CA-C-O	-5.97	115.37	120.98
1	A	777	MET	CG-SD-CE	-5.97	87.77	100.90
1	B	840	LEU	N-CA-CB	5.97	120.64	110.50
1	B	357	GLY	CA-C-O	-5.96	116.21	121.58
2	D	116	ARG	NE-CZ-NH1	-5.96	115.53	121.50
3	F	144	GLU	N-CA-C	5.96	123.50	110.80
1	A	533	GLU	N-CA-CB	5.96	119.48	110.30
1	A	84	ASP	N-CA-CB	5.96	120.56	110.49
3	F	59	PHE	N-CA-C	-5.96	104.86	111.71
3	F	52	THR	N-CA-C	-5.96	105.84	114.12
1	A	635	LYS	CA-C-N	5.96	130.18	121.96
1	A	635	LYS	C-N-CA	5.96	130.18	121.96
3	E	30	PRO	N-CA-C	5.96	116.19	110.47
1	A	103	ARG	NE-CZ-NH2	5.96	124.56	119.20
2	D	153	ASP	N-CA-C	-5.95	98.12	110.80
1	B	355	HIS	CE1-NE2-CD2	-5.95	103.05	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	TYR	CB-CG-CD1	-5.95	111.88	120.80
1	B	394	LYS	N-CA-CB	-5.94	101.33	110.07
2	D	110	LEU	CA-C-N	5.94	128.24	120.28
2	D	110	LEU	C-N-CA	5.94	128.24	120.28
1	B	465	PHE	CA-CB-CG	-5.93	107.87	113.80
2	C	73	GLN	OE1-CD-NE2	5.93	128.53	122.60
1	B	340	HIS	CG-CD2-NE2	5.92	113.12	107.20
1	A	560	PHE	N-CA-CB	5.91	120.48	110.49
3	E	136	ASP	CA-C-O	5.91	127.81	120.54
1	B	203	GLU	N-CA-C	5.91	117.65	109.15
1	B	360	LYS	N-CA-CB	5.91	121.44	110.99
1	B	521	ILE	CA-C-N	5.90	128.51	120.54
1	B	521	ILE	C-N-CA	5.90	128.51	120.54
1	B	150	PHE	O-C-N	-5.90	115.42	122.15
1	A	384	LEU	N-CA-C	5.90	120.76	113.50
1	A	736	PHE	CA-CB-CG	-5.90	107.90	113.80
1	A	367	GLU	N-CA-C	-5.90	98.67	108.34
3	E	4	GLU	CB-CG-CD	5.90	122.63	112.60
1	B	333	PHE	CA-C-N	5.88	128.48	120.54
1	B	333	PHE	C-N-CA	5.88	128.48	120.54
1	A	305	TYR	CB-CG-CD2	5.88	129.62	120.80
1	B	629	GLU	N-CA-C	-5.88	106.11	113.28
1	A	157	TYR	N-CA-C	-5.88	104.95	111.36
2	C	41	CYS	N-CA-C	-5.88	98.03	108.13
3	F	3	ASP	CA-C-N	5.87	128.62	120.29
3	F	3	ASP	C-N-CA	5.87	128.62	120.29
1	B	552	ASN	CA-CB-CG	5.87	118.47	112.60
3	F	1	MET	CA-C-N	5.87	128.69	121.06
3	F	1	MET	C-N-CA	5.87	128.69	121.06
2	C	41	CYS	N-CA-CB	5.87	120.27	110.59
1	B	789	LEU	CA-C-O	-5.87	114.66	120.70
1	A	574	HIS	CB-CG-CD2	-5.86	123.58	131.20
1	A	795	TRP	CA-CB-CG	5.86	124.73	113.60
1	A	763	LYS	N-CA-C	5.86	119.02	108.48
1	B	64	ARG	NE-CZ-NH1	-5.85	115.65	121.50
3	F	59	PHE	CA-CB-CG	-5.85	107.95	113.80
2	D	117	LEU	N-CA-CB	5.85	118.66	109.83
1	B	806	GLN	O-C-N	-5.85	114.81	122.59
1	B	777	MET	N-CA-C	5.84	118.43	111.71
1	A	36	ASP	N-CA-CB	5.84	119.43	110.49
1	B	767	ARG	CA-C-N	5.84	129.41	120.82
1	B	767	ARG	C-N-CA	5.84	129.41	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	LYS	N-CA-C	-5.84	100.19	109.07
1	B	492	VAL	N-CA-CB	5.84	120.87	111.23
1	B	632	GLY	N-CA-C	-5.84	103.67	112.60
3	F	4	GLU	CA-C-N	5.84	128.10	120.28
3	F	4	GLU	C-N-CA	5.84	128.10	120.28
1	A	154	ASP	CA-C-N	5.84	127.63	120.22
1	A	154	ASP	C-N-CA	5.84	127.63	120.22
1	A	623	PRO	CA-C-N	-5.83	115.71	122.77
1	A	623	PRO	C-N-CA	-5.83	115.71	122.77
3	F	62	ALA	CA-C-N	5.83	132.68	121.54
3	F	62	ALA	C-N-CA	5.83	132.68	121.54
1	B	282	ILE	N-CA-CB	5.83	117.76	110.47
1	B	497	GLU	CA-C-N	5.83	128.09	120.28
1	B	497	GLU	C-N-CA	5.83	128.09	120.28
1	A	106	ALA	CB-CA-C	-5.83	101.32	110.94
1	A	433	PHE	CA-CB-CG	5.83	119.63	113.80
1	A	298	LEU	CA-C-N	5.83	132.67	121.54
1	A	298	LEU	C-N-CA	5.83	132.67	121.54
1	A	673	ARG	NE-CZ-NH1	-5.83	115.67	121.50
1	A	488	HIS	CG-CD2-NE2	5.83	113.03	107.20
3	F	110	MET	N-CA-C	-5.82	106.01	113.23
1	B	38	LYS	CA-C-N	5.82	132.66	121.54
1	B	38	LYS	C-N-CA	5.82	132.66	121.54
1	A	155	GLY	CA-C-O	5.82	126.70	120.30
1	B	488	HIS	N-CA-C	5.82	119.99	113.01
1	B	495	GLN	CB-CG-CD	-5.82	102.71	112.60
1	A	390	ALA	CA-C-N	5.82	131.33	122.37
1	A	390	ALA	C-N-CA	5.82	131.33	122.37
3	E	46	ASN	CB-CG-ND2	-5.82	107.68	116.40
1	B	295	LYS	N-CA-C	5.81	118.36	111.33
1	A	730	SER	N-CA-C	-5.81	106.03	113.23
1	A	732	VAL	O-C-N	-5.81	114.48	121.10
1	B	4	ASP	CA-C-N	5.81	125.72	119.85
1	B	4	ASP	C-N-CA	5.81	125.72	119.85
3	E	195	GLY	N-CA-C	5.81	126.94	113.18
3	E	53	GLN	N-CA-C	-5.81	105.57	114.16
1	A	5	PRO	N-CA-C	5.80	124.42	112.47
1	B	788	TRP	CA-C-N	5.80	128.33	120.44
1	B	788	TRP	C-N-CA	5.80	128.33	120.44
1	A	19	ARG	N-CA-CB	5.80	120.30	110.49
2	C	124	GLU	CA-C-O	-5.79	112.95	119.79
3	E	13	SER	N-CA-C	-5.79	98.84	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	317	ILE	CA-C-N	5.79	127.08	119.84
1	B	317	ILE	C-N-CA	5.79	127.08	119.84
1	A	331	THR	CA-CB-CG2	5.79	120.35	110.50
1	A	371	GLU	N-CA-C	-5.79	99.34	108.14
1	A	459	ILE	CA-CB-CG2	-5.79	100.66	110.50
3	E	118	ARG	N-CA-CB	5.79	119.31	109.87
2	C	55	ASP	N-CA-C	-5.79	105.59	114.16
1	B	121	ASN	CA-CB-CG	5.79	118.39	112.60
1	B	345	ASP	CA-CB-CG	-5.79	106.81	112.60
1	A	705	ARG	CA-C-N	5.78	130.12	120.64
1	A	705	ARG	C-N-CA	5.78	130.12	120.64
1	B	281	HIS	CA-CB-CG	5.78	119.58	113.80
1	B	639	GLY	CA-C-N	-5.76	114.29	122.94
1	B	639	GLY	C-N-CA	-5.76	114.29	122.94
1	B	734	LYS	N-CA-C	-5.76	106.04	114.39
2	D	121	GLU	N-CA-C	5.76	117.56	111.28
1	B	73	GLN	CA-C-N	5.76	128.29	120.63
1	B	73	GLN	C-N-CA	5.76	128.29	120.63
1	B	627	ALA	N-CA-CB	5.76	121.19	110.99
1	B	383	HIS	CA-CB-CG	5.76	119.56	113.80
1	B	489	HIS	CG-CD2-NE2	5.75	112.95	107.20
1	B	198	PRO	CA-C-O	-5.75	114.86	121.36
3	E	191	ALA	N-CA-C	-5.75	106.31	113.38
1	B	816	GLN	N-CA-C	5.75	117.55	111.28
3	E	37	LYS	CB-CG-CD	5.75	124.52	111.30
1	A	664	LEU	N-CA-CB	5.75	119.48	110.46
1	B	685	VAL	N-CA-C	-5.74	99.85	108.12
1	A	340	HIS	CG-CD2-NE2	5.74	112.94	107.20
1	A	280	TYR	N-CA-C	-5.74	98.58	110.80
1	B	132	ARG	NE-CZ-NH2	5.74	124.36	119.20
1	B	493	LEU	N-CA-CB	5.74	119.91	110.39
1	B	665	HIS	CE1-NE2-CD2	-5.74	103.26	109.00
1	B	220	THR	CB-CA-C	-5.73	100.94	110.68
3	E	11	LYS	N-CA-C	-5.73	106.28	113.72
1	A	565	PRO	CA-C-N	5.73	125.41	119.05
1	A	565	PRO	C-N-CA	5.73	125.41	119.05
2	C	68	LEU	CA-C-N	5.72	125.25	119.19
2	C	68	LEU	C-N-CA	5.72	125.25	119.19
1	A	286	LEU	O-C-N	5.72	129.11	122.19
1	A	269	ARG	CA-C-N	5.71	132.25	121.97
1	A	269	ARG	C-N-CA	5.71	132.25	121.97
1	B	644	ALA	N-CA-C	-5.71	97.94	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	665	HIS	CG-CD2-NE2	5.71	112.91	107.20
1	B	19	ARG	NE-CZ-NH1	-5.70	115.80	121.50
1	A	836	LYS	N-CA-C	-5.70	98.67	110.80
3	E	83	PHE	N-CA-C	-5.69	105.60	112.54
2	C	151	PHE	CA-C-N	5.69	126.07	119.47
2	C	151	PHE	C-N-CA	5.69	126.07	119.47
2	D	40	ASP	N-CA-CB	5.68	120.10	110.49
1	A	33	TRP	N-CA-CB	5.68	119.60	110.85
1	B	125	ARG	CB-CG-CD	5.68	124.37	111.30
1	A	574	HIS	CA-C-O	5.68	127.08	120.49
1	B	758	ARG	O-C-N	5.67	129.95	123.48
1	B	27	ASP	N-CA-C	-5.67	98.72	110.80
1	B	205	PRO	N-CA-CB	5.67	108.28	103.35
3	E	19	GLU	N-CA-C	-5.67	107.01	114.04
1	B	385	LEU	N-CA-C	-5.67	106.49	113.41
3	F	171	PRO	CA-C-N	5.67	132.17	121.97
3	F	171	PRO	C-N-CA	5.67	132.17	121.97
1	A	564	LYS	CA-C-N	5.67	126.22	120.38
1	A	564	LYS	C-N-CA	5.67	126.22	120.38
2	D	35	LEU	N-CA-CB	5.67	118.20	109.98
1	A	50	GLN	OE1-CD-NE2	5.66	128.26	122.60
1	A	77	PRO	O-C-N	5.66	128.75	122.24
1	B	428	MET	N-CA-CB	5.66	118.28	110.07
3	F	110	MET	CA-C-N	5.66	132.35	121.54
3	F	110	MET	C-N-CA	5.66	132.35	121.54
1	A	332	ALA	N-CA-C	5.66	119.44	112.54
1	B	150	PHE	CA-C-O	5.66	126.41	120.42
1	B	590	GLY	N-CA-C	-5.66	107.86	115.21
3	F	118	ARG	NE-CZ-NH2	5.65	124.29	119.20
1	B	743	THR	CA-C-N	5.65	128.90	120.31
1	B	743	THR	C-N-CA	5.65	128.90	120.31
3	E	130	ASN	O-C-N	-5.65	116.43	123.04
1	B	690	LEU	CA-C-N	5.65	128.20	120.46
1	B	690	LEU	C-N-CA	5.65	128.20	120.46
1	B	537	PHE	O-C-N	-5.64	117.53	121.65
1	A	755	ASN	OD1-CG-ND2	5.64	128.25	122.60
3	E	29	PRO	CA-C-N	5.64	123.78	119.66
3	E	29	PRO	C-N-CA	5.64	123.78	119.66
1	A	676	ILE	CA-C-O	-5.64	114.54	119.62
3	E	117	ASP	CA-CB-CG	5.64	118.24	112.60
1	B	97	LEU	N-CA-C	5.63	117.87	111.11
1	B	318	PRO	N-CA-CB	5.63	109.16	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	10	LYS	N-CA-C	-5.63	104.53	111.40
3	E	57	GLN	OE1-CD-NE2	5.63	128.23	122.60
3	F	53	GLN	OE1-CD-NE2	-5.63	116.97	122.60
1	B	591	TRP	CA-C-N	5.62	132.28	121.54
1	B	591	TRP	C-N-CA	5.62	132.28	121.54
1	B	485	PHE	N-CA-CB	5.62	118.99	110.28
1	B	466	ASP	O-C-N	5.62	128.07	122.12
1	A	415	THR	CA-C-N	5.62	131.36	122.60
1	A	415	THR	C-N-CA	5.62	131.36	122.60
1	B	667	THR	N-CA-CB	5.62	118.54	110.06
1	A	674	CYS	N-CA-C	-5.62	99.75	108.90
1	A	174	GLU	O-C-N	-5.61	116.67	123.29
3	E	64	GLN	CA-C-N	5.61	132.26	121.54
3	E	64	GLN	C-N-CA	5.61	132.26	121.54
3	F	118	ARG	N-CA-CB	5.61	118.14	110.01
1	B	79	TYR	CA-CB-CG	-5.61	103.81	113.90
3	F	56	VAL	CA-CB-CG1	5.60	119.93	110.40
1	B	838	LYS	CA-C-O	-5.60	112.91	118.34
2	C	23	GLY	CA-C-O	5.60	126.07	119.46
1	B	425	ALA	N-CA-C	5.60	117.38	111.28
1	B	351	ALA	CA-C-O	5.60	126.27	119.11
1	B	439	ARG	NH1-CZ-NH2	-5.60	112.02	119.30
1	A	17	GLN	N-CA-C	-5.59	105.05	112.94
3	F	23	ASP	N-CA-C	-5.59	106.35	114.12
3	E	181	LYS	O-C-N	-5.59	115.39	122.27
1	A	422	GLY	O-C-N	-5.59	116.14	122.96
1	A	622	HIS	CA-C-O	-5.59	112.50	120.16
1	A	348	LYS	CA-C-O	5.59	126.34	120.42
1	B	498	TYR	CA-C-N	5.59	127.70	120.44
1	B	498	TYR	C-N-CA	5.59	127.70	120.44
1	B	738	ASP	CA-C-O	-5.58	115.39	121.87
1	B	762	THR	CA-CB-OG1	-5.58	101.23	109.60
3	F	58	GLU	CA-C-N	5.58	128.31	120.28
3	F	58	GLU	C-N-CA	5.58	128.31	120.28
2	C	133	ASP	N-CA-C	-5.58	105.78	112.59
1	A	297	ASP	CA-CB-CG	-5.58	107.02	112.60
1	B	837	VAL	CA-C-N	5.57	127.06	120.09
1	B	837	VAL	C-N-CA	5.57	127.06	120.09
1	A	260	ILE	N-CA-C	-5.57	99.70	108.23
1	A	383	HIS	CE1-NE2-CD2	-5.57	103.43	109.00
1	B	83	GLU	CA-C-N	5.57	128.75	120.90
1	B	83	GLU	C-N-CA	5.57	128.75	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	163	VAL	N-CA-C	5.57	115.77	110.53
2	D	10	GLU	O-C-N	5.57	128.02	122.12
3	E	137	GLU	O-C-N	-5.57	115.18	122.59
1	B	676	ILE	N-CA-CB	5.57	119.00	111.21
1	B	250	GLY	CA-C-N	5.56	124.91	118.85
1	B	250	GLY	C-N-CA	5.56	124.91	118.85
1	B	695	LEU	N-CA-C	5.56	118.27	111.82
1	A	672	VAL	O-C-N	-5.56	117.64	123.03
2	D	86	PHE	CB-CG-CD2	5.56	130.15	120.70
3	F	13	SER	CB-CA-C	-5.56	103.84	111.51
1	A	778	ARG	NE-CZ-NH1	-5.56	115.94	121.50
3	F	149	ARG	NE-CZ-NH1	-5.56	115.94	121.50
2	D	146	ILE	O-C-N	5.56	127.66	121.94
1	A	505	TRP	N-CA-C	-5.55	104.27	111.71
3	E	59	PHE	N-CA-CB	5.55	121.32	110.88
1	A	132	ARG	NE-CZ-NH1	-5.55	115.95	121.50
3	F	68	GLN	O-C-N	-5.55	116.24	122.12
1	B	795	TRP	CA-C-N	5.55	127.97	120.65
1	B	795	TRP	C-N-CA	5.55	127.97	120.65
2	C	116	ARG	NE-CZ-NH2	5.55	124.19	119.20
1	B	21	ASP	N-CA-C	5.54	118.85	111.75
1	B	82	CYS	CA-C-O	-5.54	115.14	121.40
1	A	550	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	B	131	ASN	N-CA-C	-5.54	106.52	113.28
1	A	355	HIS	CB-CG-ND1	5.54	131.01	122.70
1	B	383	HIS	CE1-NE2-CD2	-5.54	103.46	109.00
1	B	767	ARG	NE-CZ-NH2	5.54	124.18	119.20
2	D	68	LEU	N-CA-C	5.54	122.05	109.81
1	A	249	PHE	N-CA-CB	5.54	119.20	110.56
1	B	383	HIS	N-CA-C	5.53	117.31	111.28
1	B	113	SER	N-CA-C	-5.53	101.96	109.54
1	A	101	LYS	N-CA-CB	5.53	118.44	110.20
1	A	716	VAL	CA-C-N	5.53	126.64	119.78
1	A	716	VAL	C-N-CA	5.53	126.64	119.78
1	B	694	GLN	N-CA-C	-5.53	105.25	111.28
3	F	88	ARG	CA-C-N	5.52	132.09	121.54
3	F	88	ARG	C-N-CA	5.52	132.09	121.54
2	C	65	GLU	O-C-N	5.52	127.97	122.12
3	E	24	ALA	O-C-N	5.52	129.49	122.04
1	A	717	TYR	CA-C-N	5.52	126.74	119.84
1	A	717	TYR	C-N-CA	5.52	126.74	119.84
1	B	772	GLY	N-CA-C	5.52	118.90	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	159	SER	CB-CA-C	-5.52	102.39	110.06
1	B	445	ASP	N-CA-CB	5.51	118.65	110.49
1	B	545	PHE	CA-C-N	5.51	127.67	120.28
1	B	545	PHE	C-N-CA	5.51	127.67	120.28
1	A	688	SER	CA-C-N	5.51	126.06	120.00
1	A	688	SER	C-N-CA	5.51	126.06	120.00
1	B	347	TYR	N-CA-CB	5.51	118.32	110.16
1	A	545	PHE	CA-C-N	5.51	130.05	120.68
1	A	545	PHE	C-N-CA	5.51	130.05	120.68
2	C	4	LEU	N-CA-CB	5.51	118.07	109.97
2	C	7	ALA	N-CA-C	-5.51	106.06	112.89
1	A	488	HIS	CE1-NE2-CD2	-5.51	103.49	109.00
1	A	333	PHE	CB-CA-C	-5.51	101.49	110.85
1	A	541	THR	O-C-N	-5.51	116.80	123.13
1	B	688	SER	CA-C-N	5.50	126.09	119.98
1	B	688	SER	C-N-CA	5.50	126.09	119.98
1	A	277	GLU	N-CA-CB	5.50	119.78	110.49
1	A	327	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	A	675	ILE	CA-CB-CG2	-5.49	101.16	110.50
2	D	80	VAL	N-CA-C	-5.49	105.60	113.07
1	A	419	TYR	N-CA-C	-5.49	106.58	113.28
1	B	489	HIS	ND1-CE1-NE2	5.49	113.89	108.40
1	B	566	PRO	N-CA-CB	5.49	105.99	102.92
1	A	826	ARG	NE-CZ-NH1	-5.49	116.02	121.50
1	A	340	HIS	CE1-NE2-CD2	-5.48	103.52	109.00
3	E	171	PRO	N-CA-C	-5.48	103.24	111.57
1	B	283	PHE	CB-CG-CD2	5.48	130.02	120.70
1	B	654	ARG	N-CA-CB	5.48	118.68	110.19
1	B	99	ASN	CA-C-O	-5.48	114.61	120.42
3	E	67	ASP	CA-CB-CG	5.48	118.08	112.60
2	D	79	GLU	N-CA-C	-5.47	100.10	109.24
2	D	95	LYS	N-CA-C	-5.47	105.55	113.21
3	F	30	PRO	N-CA-CB	5.47	106.06	103.22
1	B	141	ARG	CB-CG-CD	5.47	123.88	111.30
3	F	15	LYS	CA-C-N	5.46	128.47	120.71
3	F	15	LYS	C-N-CA	5.46	128.47	120.71
2	C	48	VAL	N-CA-CB	5.46	118.77	110.58
2	C	145	THR	CA-C-O	5.46	126.21	120.42
1	A	811	ALA	CA-C-N	5.46	128.61	120.31
1	A	811	ALA	C-N-CA	5.46	128.61	120.31
1	B	46	ILE	N-CA-CB	-5.46	104.84	110.95
1	B	453	PHE	O-C-N	5.45	130.24	123.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	675	ILE	CA-CB-CG2	5.45	119.76	110.50
2	D	136	PHE	CB-CA-C	-5.45	99.73	109.71
1	B	75	ASN	N-CA-CB	5.45	119.65	109.68
1	B	132	ARG	NE-CZ-NH1	-5.45	116.06	121.50
1	A	15	MET	CA-C-O	-5.44	113.59	120.28
1	B	693	HIS	ND1-CE1-NE2	5.44	113.84	108.40
1	B	191	ALA	O-C-N	-5.44	115.20	122.43
1	B	105	TYR	O-C-N	5.43	127.88	122.12
1	B	110	TYR	CA-CB-CG	-5.43	104.12	113.90
1	B	600	ASN	OD1-CG-ND2	5.43	128.03	122.60
1	B	692	MET	O-C-N	5.43	127.67	122.07
1	A	77	PRO	CA-C-N	5.43	128.01	120.29
1	A	77	PRO	C-N-CA	5.43	128.01	120.29
2	D	78	LYS	CA-CB-CG	5.43	124.97	114.10
1	B	334	ASP	CA-CB-CG	-5.43	107.17	112.60
1	B	544	SER	CA-C-N	5.43	128.34	120.79
1	B	544	SER	C-N-CA	5.43	128.34	120.79
1	B	565	PRO	CB-CA-C	5.43	117.54	110.92
1	A	574	HIS	N-CA-CB	5.43	118.72	109.87
1	B	13	ILE	O-C-N	-5.43	117.03	122.62
1	A	767	ARG	N-CA-C	-5.43	105.44	111.36
3	E	85	SER	CA-C-N	5.43	129.06	121.24
3	E	85	SER	C-N-CA	5.43	129.06	121.24
1	B	640	ARG	NE-CZ-NH1	5.42	126.92	121.50
1	B	805	LEU	O-C-N	5.42	128.60	122.20
3	F	95	LEU	O-C-N	-5.42	115.38	122.59
1	A	804	LYS	CA-C-O	5.42	126.20	119.97
1	A	795	TRP	O-C-N	5.42	127.67	122.03
1	A	403	VAL	N-CA-C	-5.41	99.16	106.85
3	F	28	PRO	N-CA-C	-5.41	104.79	110.58
1	B	98	HIS	CE1-NE2-CD2	-5.41	103.59	109.00
1	A	449	LYS	N-CA-CB	5.41	119.63	110.49
1	A	682	GLN	CA-C-N	5.41	125.33	119.76
1	A	682	GLN	C-N-CA	5.41	125.33	119.76
1	B	472	GLN	CA-C-O	-5.41	113.99	120.10
1	B	752	LEU	O-C-N	5.41	129.78	122.59
2	D	147	ILE	CA-C-O	5.41	126.58	120.85
3	F	6	LYS	N-CA-C	-5.41	106.64	113.18
3	E	140	GLY	N-CA-C	-5.40	100.38	113.18
1	B	832	LYS	CA-C-O	5.40	124.84	118.90
2	C	120	ILE	CA-C-N	5.40	128.52	120.31
2	C	120	ILE	C-N-CA	5.40	128.52	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	LYS	CA-C-N	5.40	127.96	120.29
1	A	179	LYS	C-N-CA	5.40	127.96	120.29
3	F	98	MET	N-CA-C	5.40	118.08	111.82
1	A	199	LYS	O-C-N	-5.40	115.11	121.32
1	A	269	ARG	NE-CZ-NH1	-5.40	116.10	121.50
3	E	70	LYS	CA-C-N	5.39	128.90	120.75
3	E	70	LYS	C-N-CA	5.39	128.90	120.75
1	A	567	LYS	N-CA-CB	5.39	119.96	110.37
1	A	475	ILE	CB-CA-C	5.39	116.29	111.71
1	A	338	PHE	CA-CB-CG	-5.39	108.41	113.80
3	F	178	ILE	CA-C-N	5.38	128.03	120.28
3	F	178	ILE	C-N-CA	5.38	128.03	120.28
1	A	527	ILE	CA-C-N	5.38	129.71	120.72
1	A	527	ILE	C-N-CA	5.38	129.71	120.72
1	A	633	GLY	N-CA-C	-5.38	102.58	110.87
1	B	196	ALA	N-CA-C	-5.38	101.23	109.41
1	B	202	LYS	N-CA-CB	5.38	119.58	110.49
1	A	330	ASP	N-CA-C	5.38	117.22	111.36
3	E	72	GLY	CA-C-N	5.38	131.81	121.54
3	E	72	GLY	C-N-CA	5.38	131.81	121.54
1	B	828	TRP	N-CA-C	-5.38	101.67	108.45
1	A	690	LEU	CA-C-N	5.37	128.05	120.42
1	A	690	LEU	C-N-CA	5.37	128.05	120.42
3	E	28	PRO	CA-C-O	-5.37	112.77	120.56
2	C	90	LEU	CA-C-N	5.37	131.80	121.54
2	C	90	LEU	C-N-CA	5.37	131.80	121.54
1	B	541	THR	N-CA-C	-5.37	100.94	109.59
1	A	36	ASP	N-CA-C	-5.37	102.04	110.36
1	A	140	ARG	NE-CZ-NH1	-5.37	116.13	121.50
1	A	209	LYS	N-CA-C	-5.37	101.69	108.45
1	A	309	PHE	CA-C-N	5.37	131.63	121.97
1	A	309	PHE	C-N-CA	5.37	131.63	121.97
3	E	30	PRO	CA-C-N	5.37	125.69	119.47
3	E	30	PRO	C-N-CA	5.37	125.69	119.47
3	F	33	PRO	CA-C-O	-5.36	112.78	120.56
1	B	621	ASP	N-CA-C	-5.36	99.20	108.69
3	E	76	LYS	N-CA-C	-5.36	106.41	113.17
1	B	303	ASP	CA-C-N	5.36	130.17	122.45
1	B	303	ASP	C-N-CA	5.36	130.17	122.45
1	B	496	GLU	N-CA-C	-5.36	105.33	111.07
1	A	334	ASP	CA-C-N	5.36	128.03	120.42
1	A	334	ASP	C-N-CA	5.36	128.03	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	8	GLU	N-CA-C	-5.36	106.91	113.50
1	B	207	LYS	N-CA-CB	5.36	119.55	110.49
1	B	153	SER	N-CA-C	-5.36	105.48	112.23
3	F	192	GLU	CA-C-N	5.36	131.77	121.54
3	F	192	GLU	C-N-CA	5.36	131.77	121.54
3	E	107	ASN	N-CA-CB	5.36	118.49	109.92
1	A	744	GLU	CA-C-N	-5.36	112.25	122.53
1	A	744	GLU	C-N-CA	-5.36	112.25	122.53
1	A	792	TRP	CB-CG-CD2	-5.36	119.30	126.80
3	E	105	PRO	N-CA-C	-5.35	102.17	111.32
1	A	19	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	A	359	MET	N-CA-C	-5.35	99.40	110.80
1	B	343	LYS	CB-CA-C	-5.35	102.42	110.92
3	F	98	MET	CG-SD-CE	-5.35	89.13	100.90
1	A	241	PHE	N-CA-C	-5.35	101.16	109.24
1	A	794	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	A	823	LEU	N-CA-CB	5.34	117.70	110.59
1	B	88	LEU	N-CA-C	5.34	118.09	110.24
3	F	66	ILE	CA-C-N	5.34	131.74	121.54
3	F	66	ILE	C-N-CA	5.34	131.74	121.54
1	A	593	GLU	N-CA-C	-5.34	105.60	113.61
1	B	540	ALA	CA-C-O	-5.34	114.45	120.43
1	A	80	GLU	CB-CG-CD	-5.34	103.53	112.60
1	B	182	ASN	N-CA-CB	5.33	117.80	110.07
2	D	46	ALA	N-CA-C	5.33	117.51	111.11
1	A	96	VAL	CA-CB-CG1	-5.33	101.33	110.40
1	A	204	ALA	N-CA-C	-5.33	100.23	108.55
1	A	606	GLN	N-CA-C	-5.33	99.44	110.80
2	C	77	GLU	CB-CG-CD	-5.33	103.54	112.60
1	B	331	THR	N-CA-CB	5.33	117.95	110.12
1	B	508	ILE	N-CA-C	-5.33	100.39	108.17
1	A	790	GLN	CA-CB-CG	5.33	124.76	114.10
1	B	75	ASN	O-C-N	-5.32	115.96	121.28
1	A	98	HIS	ND1-CE1-NE2	5.32	113.72	108.40
1	A	78	LYS	N-CA-C	-5.32	105.56	111.36
1	A	453	PHE	CA-CB-CG	5.32	119.12	113.80
1	A	669	PRO	N-CA-C	5.32	119.21	110.55
1	A	313	GLY	CA-C-N	5.31	131.26	121.70
1	A	313	GLY	C-N-CA	5.31	131.26	121.70
1	A	579	HIS	CE1-NE2-CD2	-5.31	103.69	109.00
1	B	119	ALA	O-C-N	5.31	129.43	123.27
1	B	334	ASP	N-CA-CB	5.31	117.86	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	76	LYS	CA-C-O	5.31	125.90	119.31
1	B	271	ILE	CA-C-N	5.31	131.68	121.54
1	B	271	ILE	C-N-CA	5.31	131.68	121.54
1	A	525	MET	CA-C-O	-5.31	112.92	120.51
1	B	211	ALA	N-CA-CB	5.31	118.36	110.40
1	A	50	GLN	CA-C-N	5.31	128.00	119.98
1	A	50	GLN	C-N-CA	5.31	128.00	119.98
1	A	742	VAL	N-CA-C	5.31	116.08	110.72
1	B	105	TYR	CA-C-O	-5.31	114.90	120.63
1	A	733	PRO	CB-CA-C	5.30	118.30	111.46
1	A	409	THR	O-C-N	-5.30	116.35	122.87
3	E	129	VAL	CA-C-O	5.30	126.94	121.05
1	B	157	TYR	CA-C-N	5.30	127.64	120.38
1	B	157	TYR	C-N-CA	5.30	127.64	120.38
1	A	691	VAL	CA-C-O	5.30	126.47	120.85
1	A	217	VAL	CA-C-N	5.30	127.94	120.42
1	A	217	VAL	C-N-CA	5.30	127.94	120.42
1	A	73	GLN	N-CA-CB	5.29	120.71	111.13
1	B	284	TYR	CA-C-N	5.29	127.32	120.44
1	B	284	TYR	C-N-CA	5.29	127.32	120.44
2	D	9	VAL	CA-C-N	5.29	127.37	120.28
2	D	9	VAL	C-N-CA	5.29	127.37	120.28
1	B	259	ASP	N-CA-C	-5.29	99.89	108.41
1	A	207	LYS	CA-C-N	5.29	128.85	121.02
1	A	207	LYS	C-N-CA	5.29	128.85	121.02
1	A	615	VAL	N-CA-C	-5.29	104.89	112.35
1	B	53	ILE	N-CA-C	-5.29	101.03	109.17
1	B	796	TYR	CA-C-N	5.28	128.13	120.79
1	B	796	TYR	C-N-CA	5.28	128.13	120.79
3	F	89	LEU	CA-C-N	5.28	131.63	121.54
3	F	89	LEU	C-N-CA	5.28	131.63	121.54
1	B	224	LEU	CA-C-N	5.28	127.30	120.44
1	B	224	LEU	C-N-CA	5.28	127.30	120.44
3	E	87	GLY	CA-C-N	5.28	128.21	120.71
3	E	87	GLY	C-N-CA	5.28	128.21	120.71
1	A	22	GLN	N-CA-CB	5.28	119.41	110.49
3	F	82	THR	CA-CB-CG2	-5.28	101.53	110.50
1	A	396	LEU	CA-C-N	5.28	127.69	120.46
1	A	396	LEU	C-N-CA	5.28	127.69	120.46
1	A	591	TRP	N-CA-C	-5.27	99.57	110.80
2	C	68	LEU	N-CA-CB	-5.27	104.20	110.42
1	B	801	GLU	CB-CA-C	-5.27	102.53	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	486	PHE	CA-CB-CG	-5.27	108.53	113.80
2	C	98	ASN	CA-C-N	5.27	129.52	121.51
2	C	98	ASN	C-N-CA	5.27	129.52	121.51
1	B	189	TYR	O-C-N	5.27	127.51	122.03
3	F	57	GLN	CB-CG-CD	-5.27	103.64	112.60
2	D	108	HIS	N-CA-C	5.27	116.71	111.07
1	B	286	LEU	CA-C-N	5.26	127.28	120.44
1	B	286	LEU	C-N-CA	5.26	127.28	120.44
2	D	74	ILE	N-CA-C	5.26	116.62	110.62
2	C	18	ILE	CA-C-N	5.26	128.31	120.31
2	C	18	ILE	C-N-CA	5.26	128.31	120.31
3	F	155	GLY	O-C-N	-5.26	117.77	122.77
1	A	468	ASN	N-CA-CB	5.26	120.60	111.39
1	B	60	GLY	O-C-N	5.26	128.01	122.28
2	C	130	ASP	CA-C-O	5.26	127.12	121.55
3	F	195	GLY	CA-C-O	-5.25	117.74	122.57
1	A	780	ASP	CB-CA-C	-5.25	102.60	110.90
1	A	693	HIS	CE1-NE2-CD2	-5.25	103.75	109.00
1	B	157	TYR	CA-C-O	-5.25	115.31	120.82
1	B	422	GLY	O-C-N	-5.25	116.68	122.24
2	C	40	ASP	CA-C-O	-5.25	115.15	121.40
3	E	99	VAL	CA-CB-CG1	5.25	119.32	110.40
3	E	17	SER	O-C-N	-5.25	115.13	122.37
1	B	350	THR	CA-C-O	-5.24	115.31	120.82
2	C	38	SER	N-CA-C	-5.24	105.34	112.26
2	C	74	ILE	CA-CB-CG2	-5.24	101.59	110.50
1	B	109	ILE	CA-CB-CG1	5.24	119.31	110.40
1	A	611	SER	N-CA-C	-5.24	106.91	113.72
1	A	704	ILE	CA-C-N	5.24	128.27	120.31
1	A	704	ILE	C-N-CA	5.24	128.27	120.31
1	B	522	GLU	N-CA-C	5.23	117.39	111.11
1	A	281	HIS	CB-CG-CD2	-5.23	124.40	131.20
1	B	505	TRP	CD2-CE2-CZ2	-5.22	117.17	122.40
1	A	470	PHE	N-CA-C	-5.22	100.65	108.96
1	B	519	GLU	N-CA-C	-5.22	101.36	109.72
1	B	587	ASN	N-CA-C	-5.22	100.39	108.90
2	C	34	ASP	O-C-N	5.22	129.33	122.33
3	E	165	GLU	CB-CG-CD	5.22	121.47	112.60
1	B	740	LYS	N-CA-C	5.22	117.64	111.33
3	E	32	LYS	CA-C-N	5.22	125.75	120.38
3	E	32	LYS	C-N-CA	5.22	125.75	120.38
1	A	121	ASN	OD1-CG-ND2	-5.21	117.39	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	23	GLY	N-CA-C	-5.21	107.61	115.32
1	B	225	GLU	N-CA-C	5.21	116.64	111.07
1	B	534	GLU	CB-CG-CD	-5.21	103.75	112.60
1	B	75	ASN	CA-C-N	5.21	125.74	120.38
1	B	75	ASN	C-N-CA	5.21	125.74	120.38
1	B	684	GLY	N-CA-C	-5.21	108.04	115.64
1	A	146	PRO	CA-C-N	5.20	125.50	119.93
1	A	146	PRO	C-N-CA	5.20	125.50	119.93
1	A	355	HIS	CB-CG-CD2	-5.20	124.44	131.20
3	E	44	GLY	N-CA-C	-5.20	104.64	112.60
1	B	312	GLN	N-CA-CB	5.20	119.27	110.49
1	A	584	VAL	CA-C-O	-5.20	114.22	119.89
1	A	358	GLU	N-CA-CB	5.20	119.27	110.49
1	A	553	HIS	ND1-CE1-NE2	5.20	113.59	108.40
1	B	334	ASP	O-C-N	5.19	127.49	122.09
2	D	132	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	206	THR	CA-C-N	5.19	131.04	121.70
1	A	206	THR	C-N-CA	5.19	131.04	121.70
1	B	315	ILE	CA-C-O	5.19	125.84	120.39
2	D	115	GLU	CA-C-N	5.19	131.45	121.54
2	D	115	GLU	C-N-CA	5.19	131.45	121.54
1	B	811	ALA	CA-C-N	5.18	127.23	120.28
1	B	811	ALA	C-N-CA	5.18	127.23	120.28
1	B	28	GLY	O-C-N	-5.18	117.21	122.60
1	A	27	ASP	CA-C-N	5.18	129.08	121.67
1	A	27	ASP	C-N-CA	5.18	129.08	121.67
1	A	670	HIS	ND1-CE1-NE2	5.18	113.58	108.40
1	A	126	PHE	CA-CB-CG	-5.18	108.62	113.80
1	A	771	LEU	CA-C-O	-5.18	114.01	119.97
3	F	116	GLY	CA-C-N	5.18	132.30	121.94
3	F	116	GLY	C-N-CA	5.18	132.30	121.94
2	C	112	SER	O-C-N	-5.18	116.59	122.23
1	B	443	THR	N-CA-C	-5.17	105.82	111.82
1	B	462	PHE	CA-CB-CG	-5.17	108.62	113.80
1	B	631	GLY	CA-C-O	-5.17	117.21	122.59
1	A	42	LEU	CA-C-N	5.17	131.42	121.54
1	A	42	LEU	C-N-CA	5.17	131.42	121.54
1	A	817	ARG	CA-C-N	5.17	129.47	120.68
1	A	817	ARG	C-N-CA	5.17	129.47	120.68
1	A	785	ILE	N-CA-CB	5.17	117.82	112.65
3	F	167	LEU	CA-C-N	5.17	127.72	120.28
3	F	167	LEU	C-N-CA	5.17	127.72	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	448	GLN	CA-C-N	5.17	131.41	121.54
1	A	448	GLN	C-N-CA	5.17	131.41	121.54
1	B	151	ALA	N-CA-CB	5.16	117.50	110.01
1	B	308	HIS	CA-CB-CG	5.16	118.96	113.80
1	B	361	PHE	CA-C-O	5.16	127.89	120.51
1	B	538	PRO	N-CD-CG	5.16	110.94	103.20
2	D	87	MET	CA-C-N	5.16	127.45	120.38
2	D	87	MET	C-N-CA	5.16	127.45	120.38
3	F	67	ASP	N-CA-C	-5.16	99.81	110.80
3	E	76	LYS	CA-C-N	5.16	131.66	122.06
3	E	76	LYS	C-N-CA	5.16	131.66	122.06
2	C	110	LEU	N-CA-C	-5.16	106.99	113.28
2	D	31	ASP	CA-C-O	5.15	125.75	119.05
1	A	833	LEU	N-CA-CB	5.15	119.20	110.49
1	A	553	HIS	CB-CG-CD2	5.15	137.90	131.20
1	A	624	GLY	N-CA-C	-5.15	103.68	112.64
1	B	721	LYS	CA-C-N	5.15	128.14	120.31
1	B	721	LYS	C-N-CA	5.15	128.14	120.31
1	B	145	VAL	N-CA-CB	5.15	117.56	111.08
1	B	382	ALA	CA-C-O	-5.15	115.41	121.07
1	B	692	MET	CG-SD-CE	-5.15	89.58	100.90
1	B	110	TYR	N-CA-CB	5.15	117.58	110.17
3	F	25	ALA	N-CA-CB	5.14	119.53	110.37
3	F	172	ILE	CA-C-N	5.14	130.55	122.11
3	F	172	ILE	C-N-CA	5.14	130.55	122.11
1	A	80	GLU	N-CA-C	-5.14	101.77	109.95
1	B	340	HIS	N-CA-C	-5.14	106.51	112.89
3	E	7	LYS	CB-CG-CD	5.14	123.12	111.30
1	B	153	SER	N-CA-CB	5.14	118.21	110.30
1	A	740	LYS	N-CA-C	-5.14	106.17	112.90
2	C	32	LEU	N-CA-CB	5.14	117.77	110.16
3	E	27	ALA	CA-C-N	5.14	125.67	120.38
3	E	27	ALA	C-N-CA	5.14	125.67	120.38
1	B	640	ARG	CA-C-N	5.14	130.95	121.70
1	B	640	ARG	C-N-CA	5.14	130.95	121.70
1	A	722	GLN	N-CA-CB	5.14	119.17	110.49
2	C	33	GLY	N-CA-C	-5.14	106.16	113.86
2	C	100	THR	CA-C-N	5.14	130.80	122.53
2	C	100	THR	C-N-CA	5.14	130.80	122.53
1	B	607	PHE	CA-CB-CG	5.13	118.94	113.80
1	B	395	ASN	CA-C-N	5.13	127.47	120.54
1	B	395	ASN	C-N-CA	5.13	127.47	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	HIS	ND1-CE1-NE2	5.13	113.53	108.40
1	B	487	ASN	CA-CB-CG	-5.13	107.47	112.60
3	F	108	PHE	CA-C-N	5.13	127.15	120.28
3	F	108	PHE	C-N-CA	5.13	127.15	120.28
2	D	92	VAL	CG1-CB-CG2	-5.12	99.52	110.80
3	E	150	SER	N-CA-C	-5.12	106.43	113.30
1	A	522	GLU	CA-C-O	-5.12	113.44	119.48
1	B	573	ALA	N-CA-CB	5.11	118.10	109.92
1	B	303	ASP	CA-C-O	5.11	126.47	120.80
1	B	464	ILE	CA-CB-CG2	-5.11	101.81	110.50
1	B	486	PHE	CA-CB-CG	5.11	118.91	113.80
1	A	571	GLN	CB-CG-CD	-5.11	103.91	112.60
1	B	222	PRO	CA-C-O	-5.11	111.98	120.05
1	B	302	ASP	CA-C-O	5.11	125.62	119.59
1	B	488	HIS	CG-CD2-NE2	5.11	112.31	107.20
1	A	619	PHE	N-CA-CB	5.11	117.46	109.85
1	B	806	GLN	CB-CG-CD	-5.11	103.92	112.60
1	A	450	ARG	CA-C-O	5.11	127.81	120.51
2	C	135	GLY	N-CA-C	-5.11	106.71	115.08
3	E	141	LYS	O-C-N	-5.11	117.23	123.10
3	F	93	GLN	N-CA-CB	5.10	119.11	110.49
2	D	31	ASP	CA-C-N	5.10	127.62	120.28
2	D	31	ASP	C-N-CA	5.10	127.62	120.28
1	B	475	ILE	CA-CB-CG1	-5.10	101.73	110.40
1	A	765	PHE	CA-CB-CG	-5.10	108.70	113.80
2	C	49	LYS	CA-C-N	5.10	127.53	120.29
2	C	49	LYS	C-N-CA	5.10	127.53	120.29
3	E	147	LEU	CA-C-O	5.10	125.23	119.27
3	F	14	LYS	N-CA-CB	5.09	119.16	110.50
3	E	179	ASP	CA-C-O	-5.09	113.11	119.38
1	B	480	GLU	O-C-N	-5.09	116.83	122.07
1	A	26	TYR	CA-C-O	-5.09	115.28	121.28
1	A	450	ARG	N-CA-C	-5.09	99.97	110.80
1	B	37	GLU	CB-CG-CD	-5.08	103.95	112.60
3	F	40	ALA	N-CA-C	5.08	117.72	111.82
1	A	420	SER	N-CA-C	-5.08	105.82	112.23
3	F	56	VAL	CA-C-N	5.08	131.25	121.54
3	F	56	VAL	C-N-CA	5.08	131.25	121.54
1	B	280	TYR	O-C-N	5.08	129.18	122.93
1	B	584	VAL	CA-C-N	5.08	126.19	119.84
1	B	584	VAL	C-N-CA	5.08	126.19	119.84
1	A	339	SER	N-CA-CB	5.08	117.94	109.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	758	ARG	N-CA-C	-5.08	100.96	109.24
1	B	630	LYS	O-C-N	5.08	129.34	122.59
2	D	126	MET	CA-C-N	5.08	127.34	120.38
2	D	126	MET	C-N-CA	5.08	127.34	120.38
1	A	370	ALA	N-CA-CB	5.07	117.45	109.69
3	F	162	GLU	CB-CA-C	-5.07	102.06	110.68
2	D	66	GLU	CA-C-N	5.07	127.33	120.38
2	D	66	GLU	C-N-CA	5.07	127.33	120.38
1	A	423	GLY	N-CA-C	-5.07	98.59	113.30
3	F	80	ARG	NH1-CZ-NH2	-5.07	112.71	119.30
1	A	325	GLU	N-CA-C	-5.07	106.94	113.23
3	F	158	PHE	CA-CB-CG	-5.07	108.73	113.80
1	B	722	GLN	O-C-N	-5.07	116.04	122.27
3	E	143	LYS	CA-C-N	5.07	127.48	120.29
3	E	143	LYS	C-N-CA	5.07	127.48	120.29
1	A	575	PHE	CA-CB-CG	-5.06	108.74	113.80
1	A	11	LEU	O-C-N	-5.06	115.86	122.59
1	A	20	LYS	N-CA-C	-5.05	103.73	110.55
1	A	584	VAL	N-CA-CB	5.05	118.12	111.40
1	B	193	VAL	CA-C-N	-5.05	116.10	121.45
1	B	193	VAL	C-N-CA	-5.05	116.10	121.45
1	A	702	GLU	CA-C-N	5.05	129.78	120.79
1	A	702	GLU	C-N-CA	5.05	129.78	120.79
1	B	60	GLY	CA-C-O	-5.05	114.75	120.30
1	A	665	HIS	CB-CA-C	-5.04	101.67	110.09
3	E	30	PRO	N-CA-CB	5.04	106.01	103.19
3	E	5	GLU	CA-C-O	5.04	125.76	120.42
1	B	408	VAL	N-CA-CB	5.04	118.09	112.45
1	B	247	ILE	CA-C-O	-5.03	115.12	121.11
1	B	553	HIS	CA-CB-CG	-5.03	108.77	113.80
3	F	131	ALA	CB-CA-C	-5.03	100.41	110.42
1	A	559	ASN	CA-C-O	-5.03	113.31	120.51
1	B	246	ARG	CA-C-O	-5.03	115.41	120.84
1	B	154	ASP	CA-C-N	5.03	129.39	120.74
1	B	154	ASP	C-N-CA	5.03	129.39	120.74
1	B	816	GLN	O-C-N	5.03	127.45	122.12
2	D	49	LYS	CA-C-N	5.03	127.52	120.28
2	D	49	LYS	C-N-CA	5.03	127.52	120.28
1	B	708	ARG	NH1-CZ-NH2	-5.03	112.77	119.30
1	A	210	LYS	N-CA-CB	5.03	118.98	110.49
1	A	640	ARG	CA-C-N	5.03	127.02	120.28
1	A	640	ARG	C-N-CA	5.03	127.02	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	LYS	CA-C-N	5.02	130.13	123.10
1	A	402	LYS	C-N-CA	5.02	130.13	123.10
1	A	626	GLY	CA-C-N	5.02	127.98	120.90
1	A	626	GLY	C-N-CA	5.02	127.98	120.90
3	E	59	PHE	CB-CG-CD1	-5.02	112.17	120.70
1	B	568	PRO	O-C-N	5.02	129.26	122.89
1	A	668	GLN	CB-CG-CD	5.02	121.13	112.60
1	A	724	TYR	O-C-N	5.01	128.90	122.23
2	C	42	LYS	CA-C-O	-5.01	116.17	121.29
3	E	69	ASP	CA-C-N	5.01	131.12	121.54
3	E	69	ASP	C-N-CA	5.01	131.12	121.54
3	E	165	GLU	CA-C-O	-5.01	113.88	119.95
1	B	743	THR	N-CA-C	-5.01	106.01	111.82
1	B	49	THR	CA-CB-CG2	5.01	119.02	110.50
1	B	449	LYS	CB-CA-C	-5.01	102.89	114.41
1	A	540	ALA	CA-C-O	5.01	124.68	119.97
2	D	146	ILE	N-CA-C	5.01	115.16	110.30
2	C	87	MET	N-CA-CB	5.01	117.73	110.47
1	B	197	THR	CA-C-N	5.01	125.01	119.90
1	B	197	THR	C-N-CA	5.01	125.01	119.90

There are no chirality outliers.

All (62) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	TYR	Sidechain
1	A	112	TYR	Sidechain
1	A	123	TYR	Sidechain
1	A	129	TYR	Sidechain
1	A	189	TYR	Sidechain
1	A	240	ARG	Sidechain
1	A	249	PHE	Sidechain
1	A	338	PHE	Sidechain
1	A	340	HIS	Sidechain
1	A	342	TYR	Sidechain
1	A	347	TYR	Sidechain
1	A	477	PHE	Sidechain
1	A	489	HIS	Sidechain
1	A	567	LYS	Peptide
1	A	580	TYR	Sidechain
1	A	619	PHE	Sidechain
1	A	831	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	90	TYR	Sidechain
1	B	10	TYR	Sidechain
1	B	112	TYR	Sidechain
1	B	125	ARG	Sidechain
1	B	132	ARG	Sidechain
1	B	240	ARG	Peptide,Sidechain
1	B	263	TYR	Sidechain
1	B	318	PRO	Peptide
1	B	347	TYR	Sidechain
1	B	369	GLN	Mainchain
1	B	393	TYR	Sidechain
1	B	419	TYR	Sidechain
1	B	429	PHE	Sidechain
1	B	453	PHE	Sidechain
1	B	467	TYR	Peptide
1	B	491	PHE	Peptide
1	B	526	GLY	Peptide
1	B	621	ASP	Peptide
1	B	627	ALA	Peptide
1	B	639	GLY	Peptide
1	B	64	ARG	Sidechain
1	B	640	ARG	Sidechain
1	B	653	TYR	Sidechain
1	B	669	PRO	Peptide
1	B	670	HIS	Sidechain
1	B	714	ARG	Sidechain
1	B	724	TYR	Sidechain
1	B	757	TYR	Sidechain
1	B	796	TYR	Sidechain
1	B	831	TYR	Sidechain
1	B	84	ASP	Peptide
2	C	116	ARG	Sidechain
2	C	139	TYR	Sidechain
2	C	16	PHE	Sidechain
2	C	19	TYR	Sidechain
2	C	57	ARG	Sidechain
2	C	93	TYR	Sidechain
2	D	19	TYR	Sidechain
3	E	38	ARG	Sidechain
3	E	39	ARG	Sidechain
3	E	63	PHE	Sidechain
3	F	113	THR	Peptide

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Mol	Chain	Res	Type	Group
3	F	88	ARG	Sidechain
3	F	9	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6738	6760	6760	40	0
1	B	6739	6760	6760	38	0
2	C	1233	1227	1227	5	0
2	D	1233	1227	1227	7	0
3	E	1529	1491	1491	12	0
3	F	1529	1491	1491	14	0
All	All	19001	18956	18956	99	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 3.

All (99) 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)
3:E:32:LYS:H	3:E:33:PRO:HD2	1.44	0.81
1:A:20:LYS:HG2	1:A:22:GLN:H	1.58	0.68
1:B:67:LYS:HD2	1:B:67:LYS:H	1.62	0.65
1:B:815:ILE:HG23	3:F:147:LEU:HD22	1.81	0.63
1:A:729:ALA:HB1	2:C:88:GLU:HG3	1.85	0.58
3:F:80:ARG:HE	3:F:99:VAL:HG23	1.69	0.58
1:B:773:ARG:HD3	1:B:773:ARG:H	1.69	0.58
3:E:23:ASP:H	3:E:31:PRO:HA	1.69	0.56
1:A:256:ALA:HB3	1:A:450:ARG:HH12	1.71	0.56
1:A:758:ARG:HE	1:A:759:LEU:H	1.53	0.55
1:B:197:THR:HG22	2:D:127:ARG:HH12	1.70	0.55
1:A:206:THR:HB	1:A:207:LYS:HB2	1.89	0.55
1:A:187:ILE:HD12	1:A:221:ASN:HD21	1.72	0.55
1:A:243:LYS:HZ2	1:A:243:LYS:HB3	1.72	0.54
1:B:135:GLN:HB3	1:B:140:ARG:HH11	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:814:VAL:HG21	3:F:39:ARG:HH21	1.73	0.54
1:B:773:ARG:H	1:B:773:ARG:CD	2.20	0.54
1:A:160:MET:HB2	1:A:167:GLN:HB2	1.89	0.54
3:E:32:LYS:H	3:E:33:PRO:CD	2.18	0.54
2:D:51:ASN:HD21	2:D:74:ILE:HD11	1.73	0.53
3:F:42:ARG:H	3:F:123:ASP:H	1.56	0.53
1:A:356:LEU:HD13	1:A:425:ALA:HB2	1.91	0.52
1:A:663:SER:O	1:A:667:THR:HG23	2.09	0.52
3:E:178:ILE:HG22	3:E:180:ILE:H	1.75	0.51
1:A:830:TRP:CH2	3:E:111:PHE:CE1	2.99	0.51
1:B:833:LEU:HD21	3:F:171:PRO:HB3	1.91	0.51
1:A:4:ASP:HB3	1:A:14:SER:HA	1.94	0.50
3:F:54:HIS:O	3:F:54:HIS:CG	2.65	0.48
1:A:248:HIS:CE1	1:A:449:LYS:HA	2.48	0.48
1:A:581:ALA:HA	1:A:697:CYS:SG	2.53	0.48
1:B:815:ILE:HG22	1:B:819:LEU:HD12	1.95	0.48
1:B:826:ARG:HH11	3:F:170:ALA:HA	1.79	0.47
1:B:244:PHE:CZ	1:B:664:LEU:HD21	2.49	0.47
3:F:44:GLY:H	3:F:120:ALA:HA	1.80	0.47
1:B:137:TYR:CE2	1:B:150:PHE:CE2	3.02	0.47
1:B:792:TRP:CH2	2:D:147:ILE:HD12	2.49	0.47
3:F:96:ASP:HA	3:F:99:VAL:HG12	1.96	0.47
1:A:100:LEU:HD22	1:A:118:VAL:HG23	1.96	0.47
2:C:15:HIS:HA	2:C:18:ILE:HD12	1.96	0.47
1:A:650:SER:HA	1:A:653:TYR:CD2	2.50	0.46
1:B:828:TRP:CD1	3:F:186:ILE:HG22	2.50	0.46
1:A:172:THR:HG22	1:A:173:GLY:H	1.81	0.45
3:E:24:ALA:O	3:E:25:ALA:HB2	2.17	0.45
1:A:356:LEU:HD12	1:A:356:LEU:H	1.82	0.45
1:B:386:GLY:HA3	1:A:736:PHE:HA	1.99	0.45
1:A:230:ALA:HB1	1:A:281:HIS:H	1.82	0.45
1:A:398:LYS:HB2	1:A:398:LYS:NZ	2.32	0.45
1:B:488:HIS:CD2	1:B:665:HIS:CE1	3.04	0.45
2:C:21:TRP:CG	3:E:146:THR:HG1	2.35	0.45
1:A:687:ASP:O	1:A:691:VAL:HG23	2.17	0.45
1:A:312:GLN:HE21	1:A:362:LYS:HB3	1.81	0.44
1:A:808:GLN:HE22	3:E:141:LYS:NZ	2.16	0.44
3:E:46:ASN:HD22	3:E:61:GLU:CD	2.25	0.44
1:A:751:GLN:HE21	1:A:751:GLN:HA	1.83	0.44
2:D:39:LEU:HD13	2:D:71:PHE:CZ	2.52	0.44
1:A:20:LYS:HA	1:A:24:LYS:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:HIS:O	1:B:488:HIS:CG	2.71	0.44
3:F:9:LYS:HA	3:F:12:LYS:HB2	2.00	0.44
1:A:104:TYR:CE1	1:A:120:ILE:HG22	2.52	0.43
1:B:579:HIS:CG	1:B:580:TYR:H	2.36	0.43
1:A:459:ILE:HD12	1:A:459:ILE:H	1.83	0.43
1:B:611:SER:HA	1:A:730:SER:HA	2.01	0.43
1:B:759:LEU:HD12	1:B:760:GLY:H	1.83	0.43
2:D:17:GLU:OE2	3:F:1:MET:HE3	2.19	0.43
1:B:827:ASN:HD21	1:B:831:TYR:HA	1.84	0.43
1:B:771:LEU:H	1:B:771:LEU:HD22	1.84	0.43
1:A:20:LYS:HA	1:A:24:LYS:CG	2.48	0.43
1:B:158:SER:HB3	1:B:715:MET:HA	2.00	0.43
1:A:230:ALA:HB3	1:A:280:TYR:HA	2.00	0.43
1:B:479:ASN:HA	1:B:482:LEU:HG	2.01	0.43
1:B:827:ASN:CG	1:B:828:TRP:H	2.26	0.43
1:B:833:LEU:HG	1:B:837:VAL:HG22	2.00	0.43
1:B:20:LYS:HZ2	1:B:773:ARG:HH11	1.65	0.42
3:F:86:LEU:HD21	3:E:31:PRO:HB2	2.01	0.42
1:B:361:PHE:HB2	1:B:414:ALA:HA	2.01	0.42
1:B:485:PHE:HB3	1:B:489:HIS:CE1	2.55	0.42
3:F:107:ASN:H	3:F:110:MET:HB2	1.84	0.42
3:E:151:LEU:HD23	3:E:151:LEU:HA	1.87	0.42
1:B:406:GLU:HG2	1:B:407:MET:H	1.85	0.42
1:A:230:ALA:CB	1:A:281:HIS:H	2.33	0.42
1:B:41:TYR:CE1	1:B:93:ASP:HB2	2.54	0.42
1:B:718:PRO:HB3	2:D:94:ASP:H	1.85	0.42
1:B:804:LYS:HA	1:B:808:GLN:HG3	2.01	0.41
1:A:459:ILE:HG21	1:A:478:THR:HB	2.02	0.41
1:A:561:VAL:HG12	1:A:562:LYS:N	2.34	0.41
2:C:19:TYR:CD2	2:C:31:ASP:HB3	2.55	0.41
1:A:831:TYR:HA	3:E:115:PHE:CE1	2.55	0.41
1:B:782:LEU:HD13	1:B:786:VAL:HG21	2.02	0.41
1:A:104:TYR:CD2	1:A:686:ILE:HD11	2.56	0.41
1:A:126:PHE:HB3	1:A:127:PRO:HD2	2.02	0.41
2:D:42:LYS:HZ1	2:D:81:GLY:HA3	1.85	0.41
1:A:41:TYR:CZ	1:A:688:SER:HB3	2.56	0.41
2:C:85:ASP:H	2:C:88:GLU:HB2	1.86	0.41
1:B:834:TYR:H	1:B:835:ILE:HG13	1.86	0.40
1:B:827:ASN:OD1	1:B:831:TYR:CE1	2.73	0.40
1:B:355:HIS:CG	1:B:380:ARG:HD2	2.56	0.40
1:B:157:TYR:CZ	1:B:161:LEU:HD22	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ASP:H	1:A:112:TYR:HB2	1.87	0.40
1:A:476:ASN:HB3	1:A:579:HIS:CD2	2.57	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	838/1953 (43%)	675 (80%)	106 (13%)	57 (7%)	1	11
1	B	838/1953 (43%)	705 (84%)	89 (11%)	44 (5%)	1	14
2	C	154/156 (99%)	130 (84%)	16 (10%)	8 (5%)	1	14
2	D	154/156 (99%)	132 (86%)	15 (10%)	7 (4%)	2	16
3	E	194/196 (99%)	148 (76%)	31 (16%)	15 (8%)	1	9
3	F	194/196 (99%)	149 (77%)	28 (14%)	17 (9%)	0	8
All	All	2372/4610 (52%)	1939 (82%)	285 (12%)	148 (6%)	2	12

All (148) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149	LEU
1	B	206	THR
1	B	208	GLU
1	B	270	VAL
1	B	358	GLU
1	B	462	PHE
1	B	505	TRP
1	B	515	ALA
1	B	536	MET
1	B	558	PRO

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Mol	Chain	Res	Type
1	B	600	ASN
1	B	731	ALA
1	B	759	LEU
1	B	806	GLN
1	B	836	LYS
3	F	24	ALA
3	F	93	GLN
3	F	127	VAL
3	F	136	ASP
3	F	144	GLU
1	A	369	GLN
1	A	418	SER
1	A	465	PHE
1	A	507	PHE
1	A	511	GLY
1	A	559	ASN
1	A	573	ALA
1	A	600	ASN
1	A	606	GLN
1	A	622	HIS
1	A	768	ALA
1	A	830	TRP
1	A	833	LEU
2	C	22	GLU
2	C	26	LYS
2	C	84	GLU
2	C	92	VAL
2	C	118	THR
3	E	25	ALA
3	E	32	LYS
3	E	139	GLU
3	E	188	THR
1	B	61	GLN
1	B	68	LYS
1	B	141	ARG
1	B	202	LYS
1	B	207	LYS
1	B	516	ALA
1	B	582	GLY
2	D	21	TRP
2	D	153	ASP
3	F	67	ASP

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Mol	Chain	Res	Type
3	F	86	LEU
1	A	3	GLU
1	A	65	GLN
1	A	86	SER
1	A	144	GLU
1	A	269	ARG
1	A	307	TYR
1	A	310	VAL
1	A	311	SER
1	A	316	GLU
1	A	323	ALA
1	A	366	ARG
1	A	471	GLU
1	A	499	LYS
1	A	556	LYS
1	A	560	PHE
1	A	723	ARG
3	E	51	PHE
3	E	159	SER
3	E	195	GLY
1	B	3	GLU
1	B	292	GLU
1	B	611	SER
1	B	646	PHE
1	B	677	PRO
1	B	712	PRO
1	B	839	PRO
2	D	2	ALA
2	D	96	ALA
3	F	45	SER
3	F	63	PHE
3	F	103	PRO
1	A	29	LYS
1	A	299	LEU
1	A	449	LYS
1	A	525	MET
1	A	567	LYS
1	A	580	TYR
1	A	635	LYS
1	A	719	ASP
1	A	722	GLN
1	A	754	ALA

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Mol	Chain	Res	Type
2	C	2	ALA
3	E	16	LYS
3	E	37	LYS
3	E	48	PHE
3	E	73	PHE
3	E	131	ALA
3	E	166	ALA
3	E	169	GLU
1	B	27	ASP
1	B	263	TYR
1	B	272	SER
1	B	308	HIS
1	B	405	ASN
1	B	597	ASP
1	B	725	THR
1	B	733	PRO
1	B	803	LYS
2	D	134	ASP
3	F	90	CYS
3	F	172	ILE
1	A	19	ARG
1	A	22	GLN
1	A	23	THR
1	A	199	LYS
1	A	235	ASN
1	A	309	PHE
1	A	389	ALA
1	A	682	GLN
2	C	107	ALA
3	E	152	THR
1	B	2	ALA
1	B	39	GLU
1	B	312	GLN
2	D	40	ASP
3	F	26	PRO
3	F	54	HIS
3	F	91	THR
3	F	95	LEU
1	A	61	GLN
1	A	358	GLU
1	A	450	ARG
1	A	582	GLY

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Mol	Chain	Res	Type
1	A	761	ASN
2	C	91	LYS
1	B	77	PRO
2	D	116	ARG
3	F	25	ALA
1	A	228	GLY
1	A	375	THR
1	A	571	GLN
1	B	623	PRO
1	A	712	PRO
1	B	737	VAL
1	A	524	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	721/1689 (43%)	688 (95%)	33 (5%)	24	45
1	B	721/1689 (43%)	693 (96%)	28 (4%)	28	49
2	C	132/132 (100%)	128 (97%)	4 (3%)	36	57
2	D	132/132 (100%)	126 (96%)	6 (4%)	24	46
3	E	164/164 (100%)	152 (93%)	12 (7%)	13	34
3	F	164/164 (100%)	157 (96%)	7 (4%)	26	47
All	All	2034/3970 (51%)	1944 (96%)	90 (4%)	27	47

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	8	THR
1	B	34	VAL
1	B	67	LYS
1	B	71	LEU
1	B	109	ILE
1	B	112	TYR

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Mol	Chain	Res	Type
1	B	174	GLU
1	B	220	THR
1	B	232	THR
1	B	245	ILE
1	B	364	ARG
1	B	409	THR
1	B	426	LYS
1	B	454	ILE
1	B	517	CYS
1	B	541	THR
1	B	678	ASN
1	B	681	LYS
1	B	758	ARG
1	B	771	LEU
1	B	773	ARG
1	B	812	LEU
1	B	818	ASN
1	B	831	TYR
1	B	832	LYS
1	B	836	LYS
1	B	837	VAL
1	B	840	LEU
2	D	32	LEU
2	D	35	LEU
2	D	54	SER
2	D	60	LYS
2	D	82	THR
2	D	139	TYR
3	F	64	GLN
3	F	93	GLN
3	F	99	VAL
3	F	106	ILE
3	F	141	LYS
3	F	182	LYS
3	F	186	ILE
1	A	20	LYS
1	A	36	ASP
1	A	75	ASN
1	A	109	ILE
1	A	149	LEU
1	A	180	THR
1	A	185	LYS

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Mol	Chain	Res	Type
1	A	243	LYS
1	A	252	MET
1	A	280	TYR
1	A	286	LEU
1	A	305	TYR
1	A	312	GLN
1	A	329	THR
1	A	362	LYS
1	A	398	LYS
1	A	458	ASP
1	A	459	ILE
1	A	475	ILE
1	A	484	GLN
1	A	521	ILE
1	A	599	VAL
1	A	600	ASN
1	A	702	GLU
1	A	722	GLN
1	A	725	THR
1	A	742	VAL
1	A	746	VAL
1	A	757	TYR
1	A	764	VAL
1	A	790	GLN
1	A	809	ARG
1	A	815	ILE
2	C	13	ARG
2	C	32	LEU
2	C	42	LYS
2	C	60	LYS
3	E	1	MET
3	E	14	LYS
3	E	16	LYS
3	E	28	PRO
3	E	37	LYS
3	E	42	ARG
3	E	54	HIS
3	E	59	PHE
3	E	75	SER
3	E	112	LEU
3	E	119	ILE
3	E	188	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	17	GLN
1	B	72	GLN
1	B	98	HIS
1	B	121	ASN
1	B	131	ASN
1	B	148	HIS
1	B	166	ASN
1	B	216	GLN
1	B	219	GLN
1	B	281	HIS
1	B	285	GLN
1	B	340	HIS
1	B	468	ASN
1	B	479	ASN
1	B	488	HIS
1	B	489	HIS
1	B	550	ASN
1	B	600	ASN
1	B	656	GLN
1	B	665	HIS
1	B	670	HIS
1	B	678	ASN
1	B	682	GLN
1	B	698	ASN
1	B	722	GLN
1	B	827	ASN
2	D	108	HIS
3	F	54	HIS
3	F	68	GLN
1	A	22	GLN
1	A	61	GLN
1	A	135	GLN
1	A	167	GLN
1	A	221	ASN
1	A	293	ASN
1	A	355	HIS
1	A	363	GLN
1	A	441	ASN
1	A	468	ASN
1	A	552	ASN
1	A	579	HIS

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Mol	Chain	Res	Type
1	A	587	ASN
1	A	622	HIS
1	A	656	GLN
1	A	658	ASN
1	A	665	HIS
1	A	678	ASN
1	A	713	ASN
1	A	751	GLN
1	A	808	GLN
1	A	816	GLN
2	C	15	HIS
3	E	46	ASN
3	E	55	GLN
3	E	57	GLN
3	E	64	GLN
3	E	93	GLN
3	E	160	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

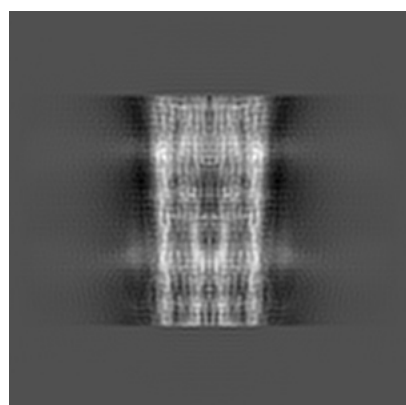
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7029. These allow visual inspection of the internal detail of the map and identification of artifacts.

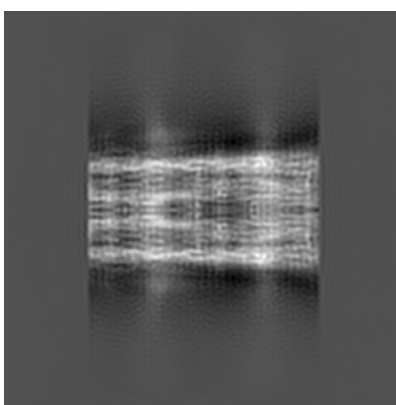
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

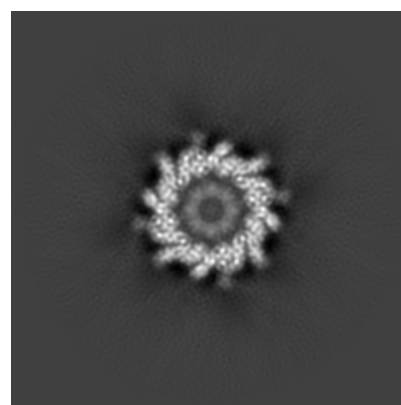
6.1.1 Primary map



X



Y

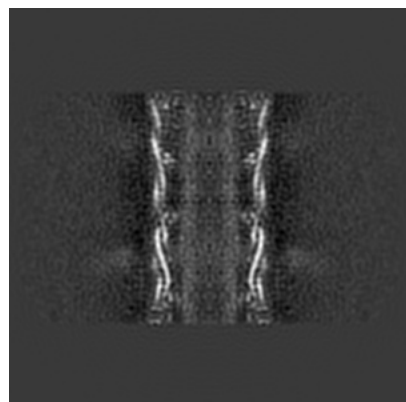


Z

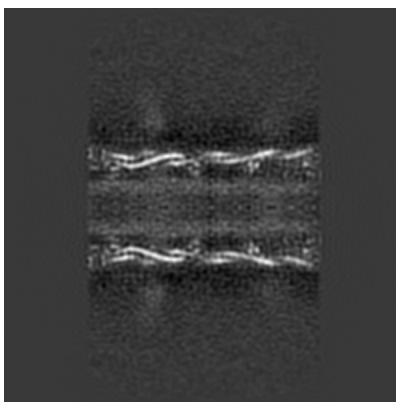
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

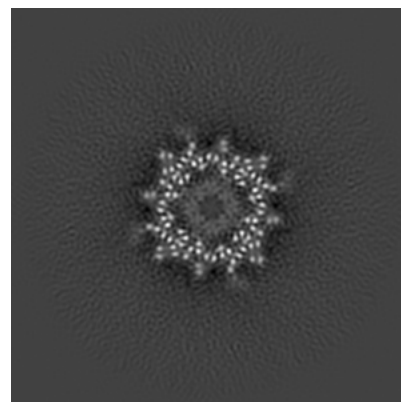
6.2.1 Primary map



X Index: 216



Y Index: 216

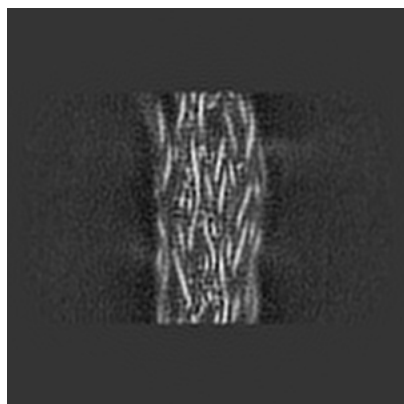


Z Index: 216

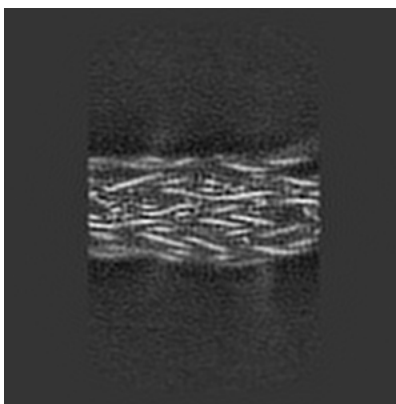
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

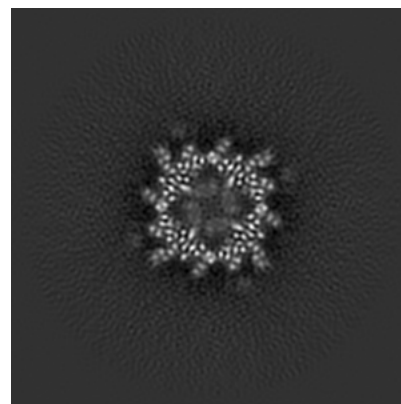
6.3.1 Primary map



X Index: 167



Y Index: 167

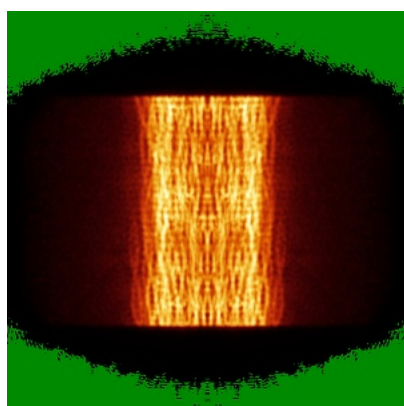


Z Index: 232

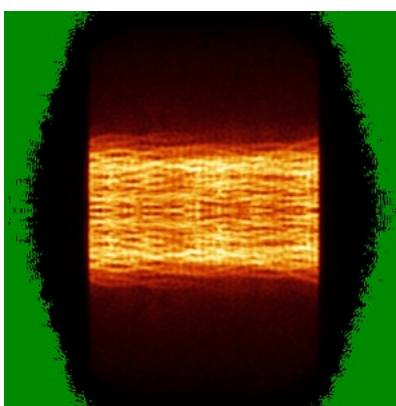
The images above show the largest variance slices of the map in three orthogonal directions.

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

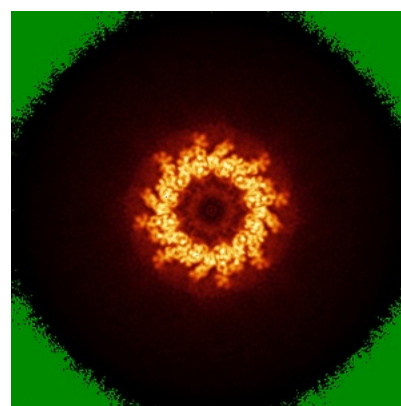
6.4.1 Primary map



X



Y

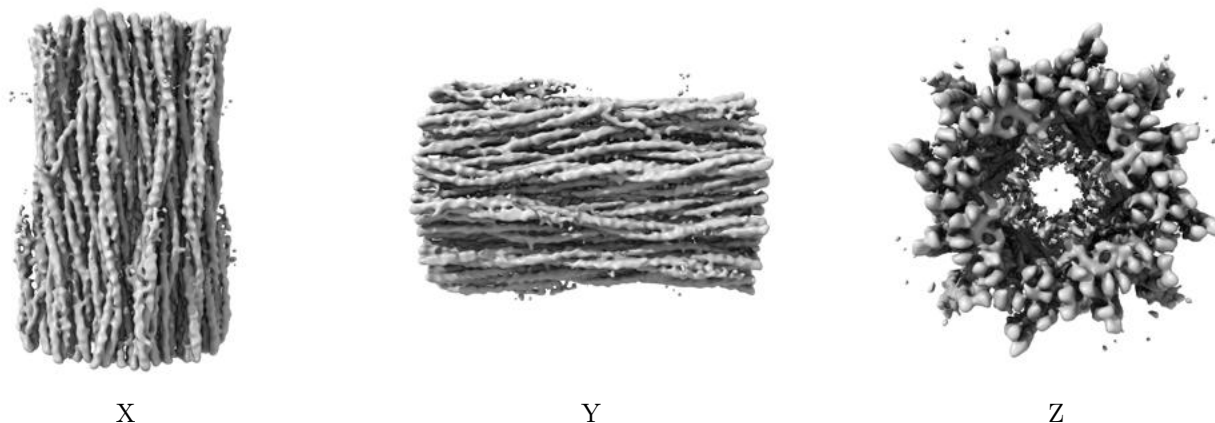


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

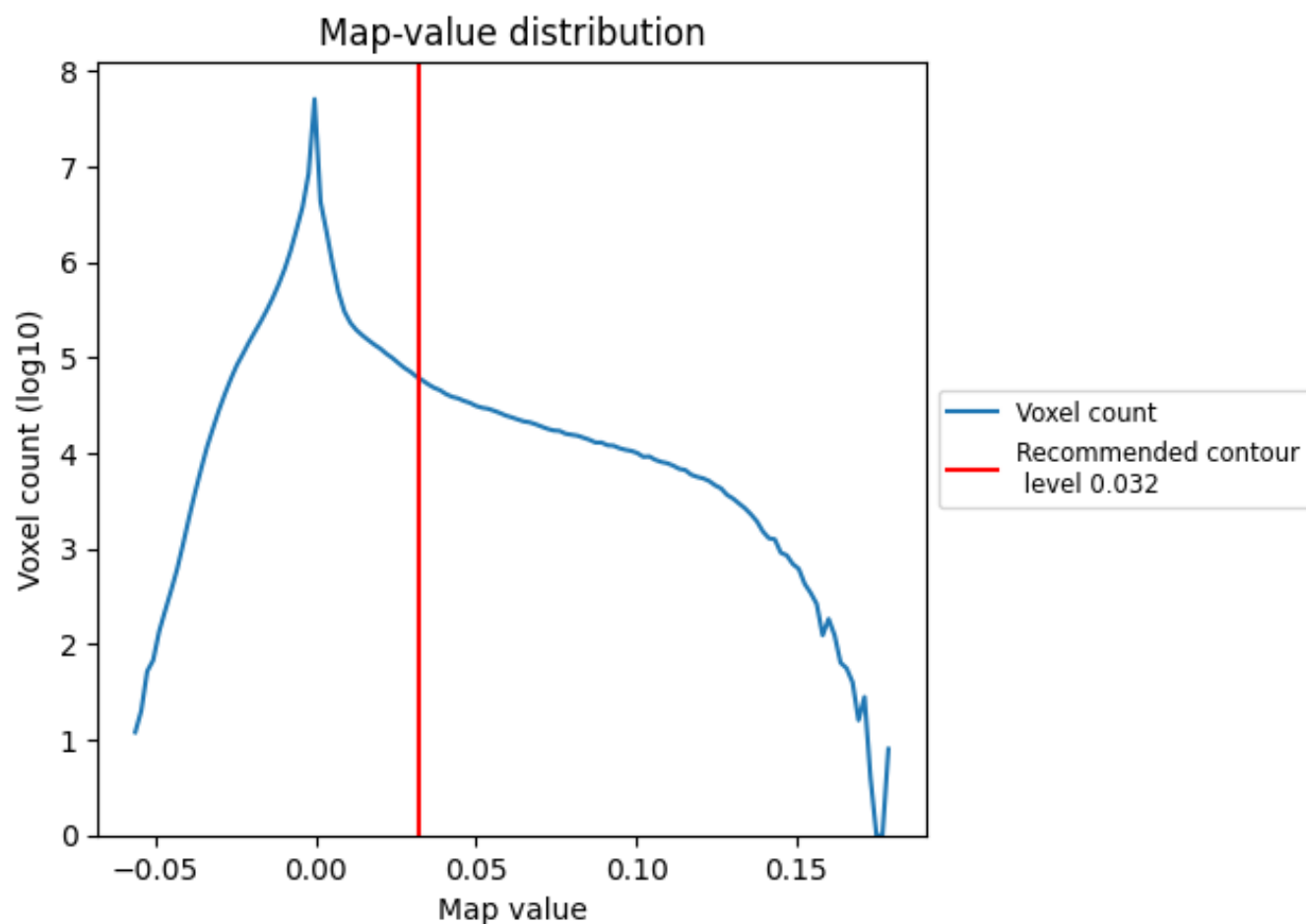
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

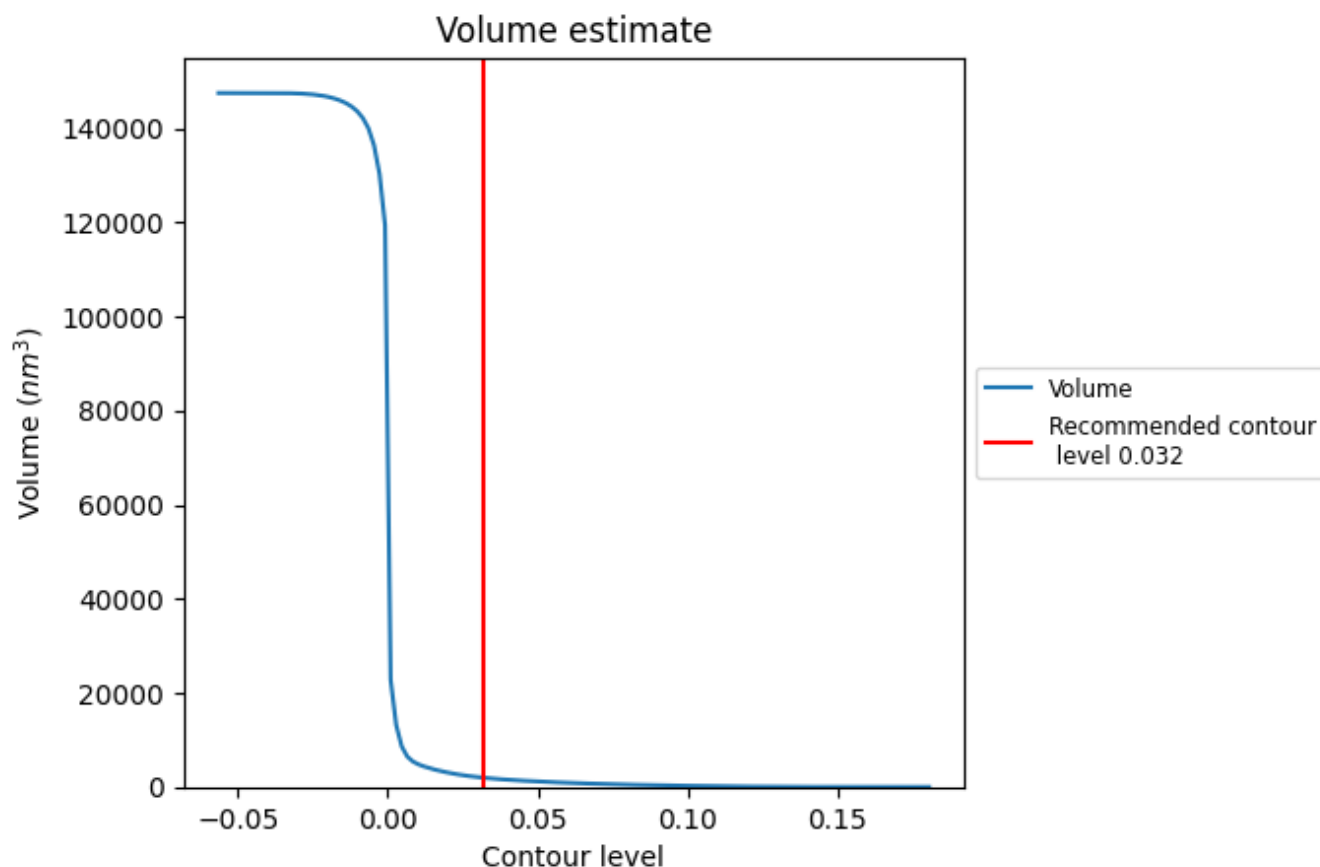
This section contains the results of statistical analysis of the map.

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.

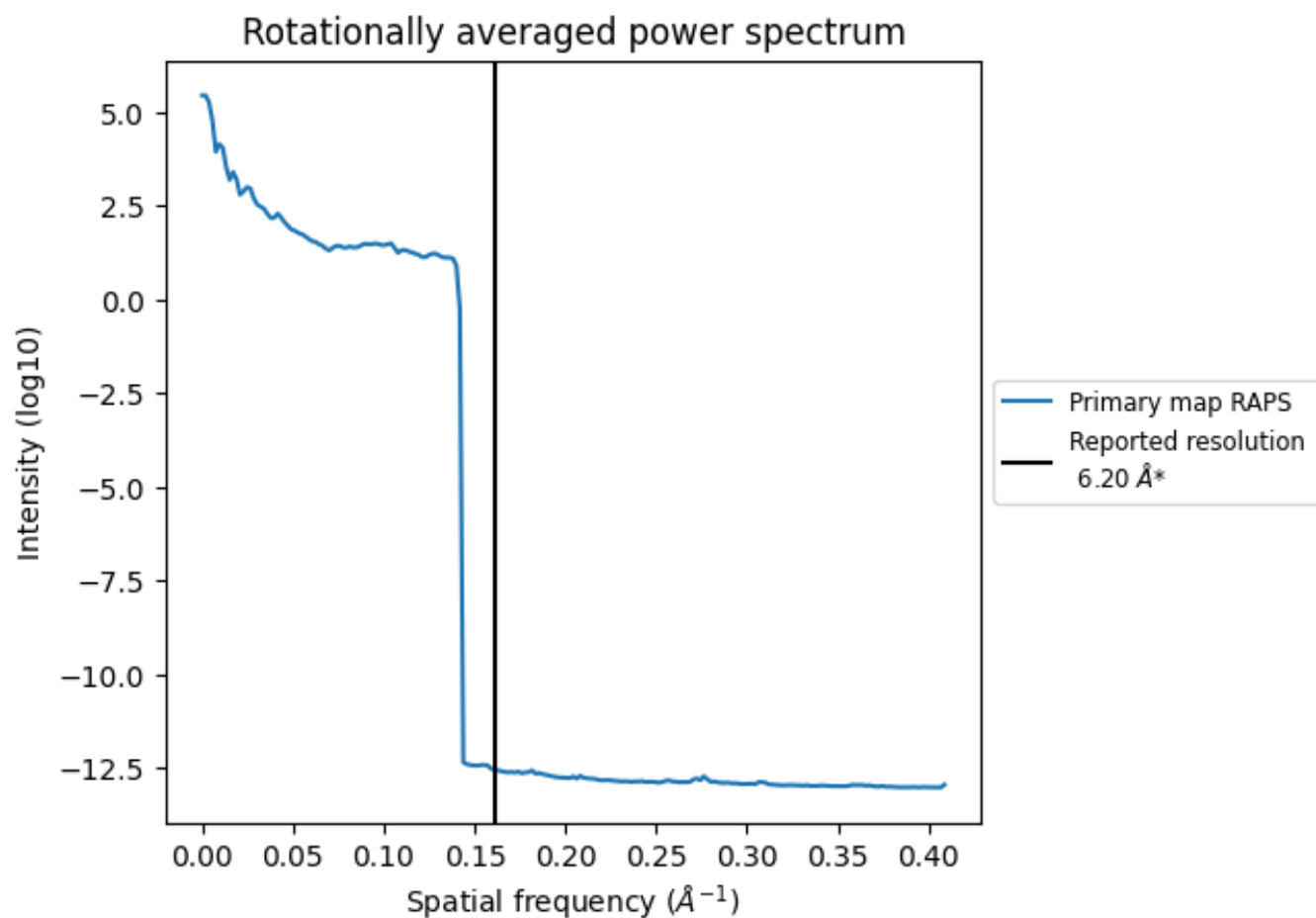
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1954 nm^3 ; this corresponds to an approximate mass of 1765 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 ⓘ

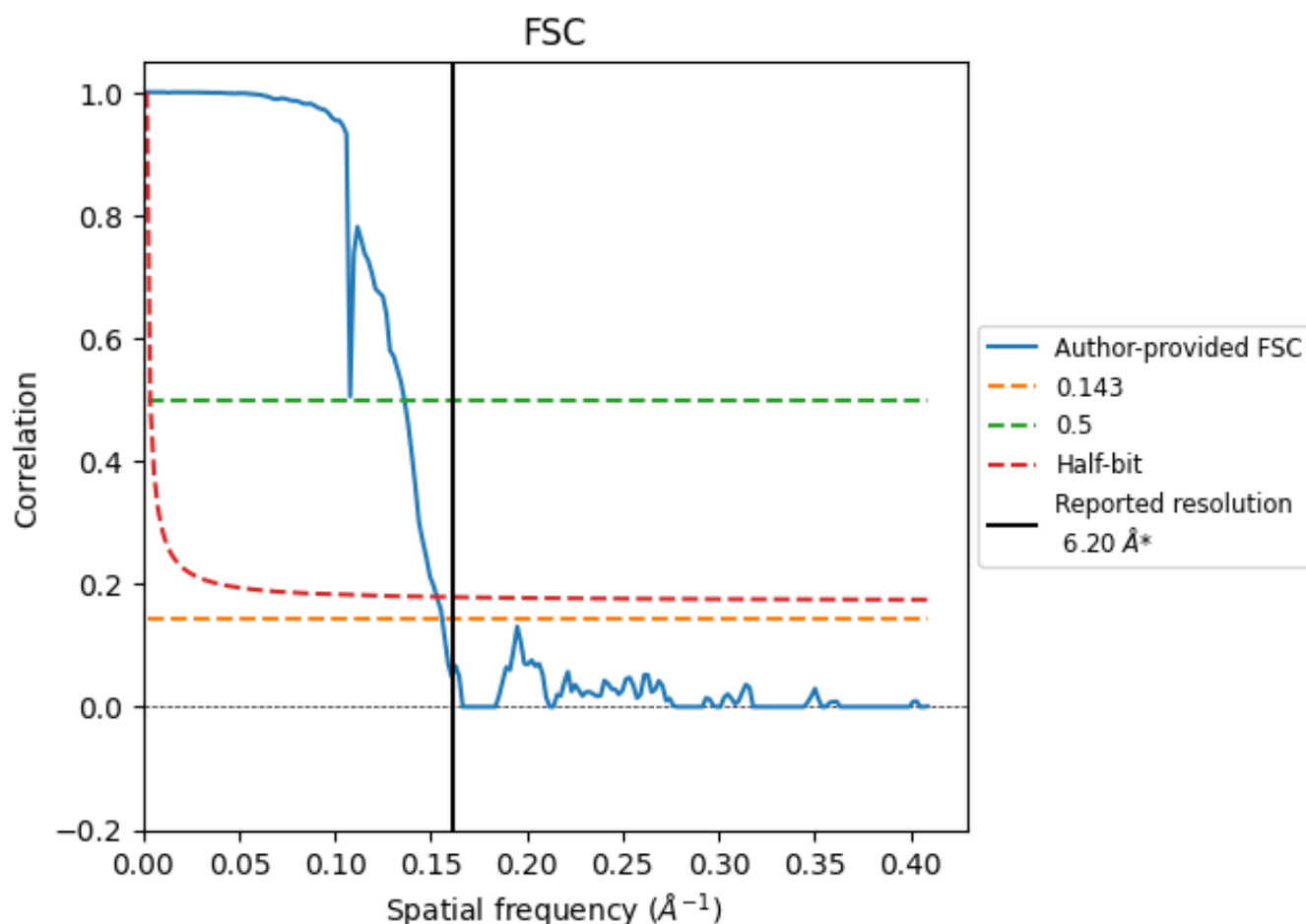


*Reported resolution corresponds to spatial frequency of 0.161 Å⁻¹

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 0.161 Å⁻¹

8.2 Resolution estimates [i](#)

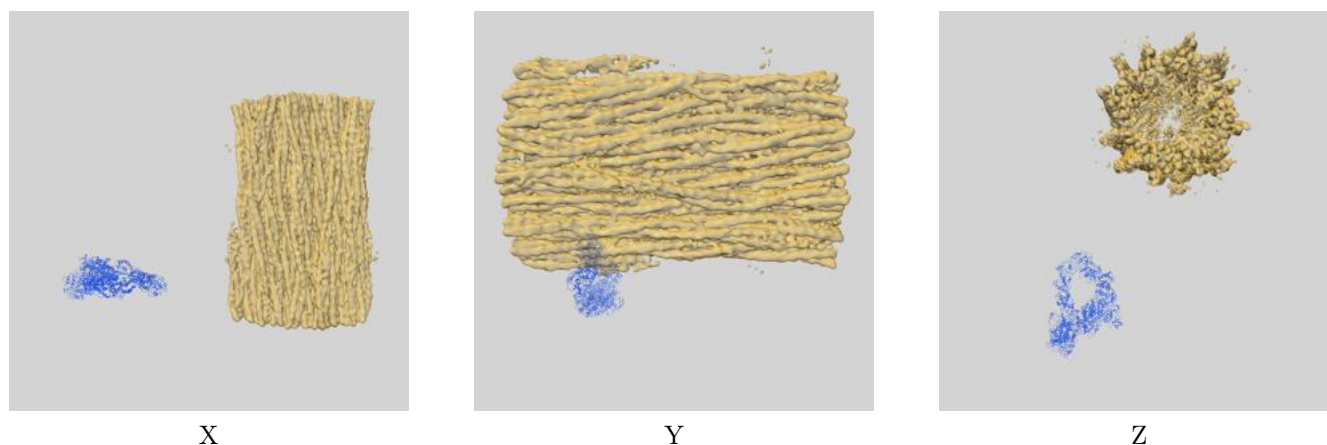
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.20	-	-
Author-provided FSC curve	6.41	7.35	6.53
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

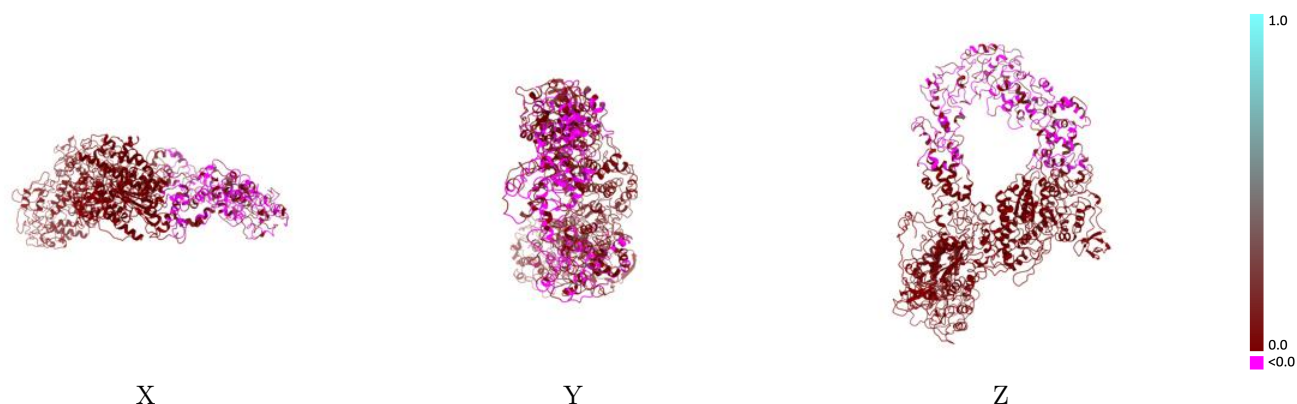
This section contains information regarding the fit between EMDB map EMD-7029 and PDB model 6SO3. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



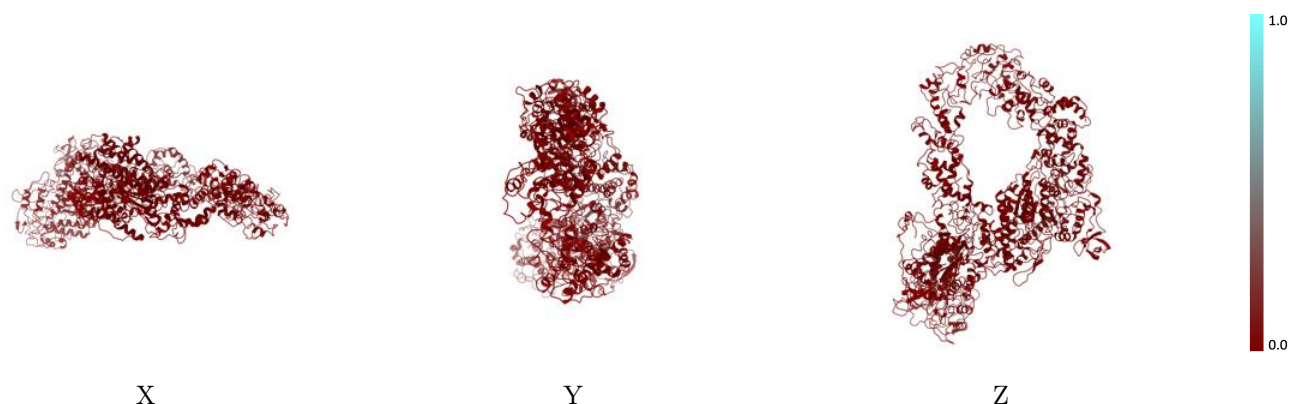
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



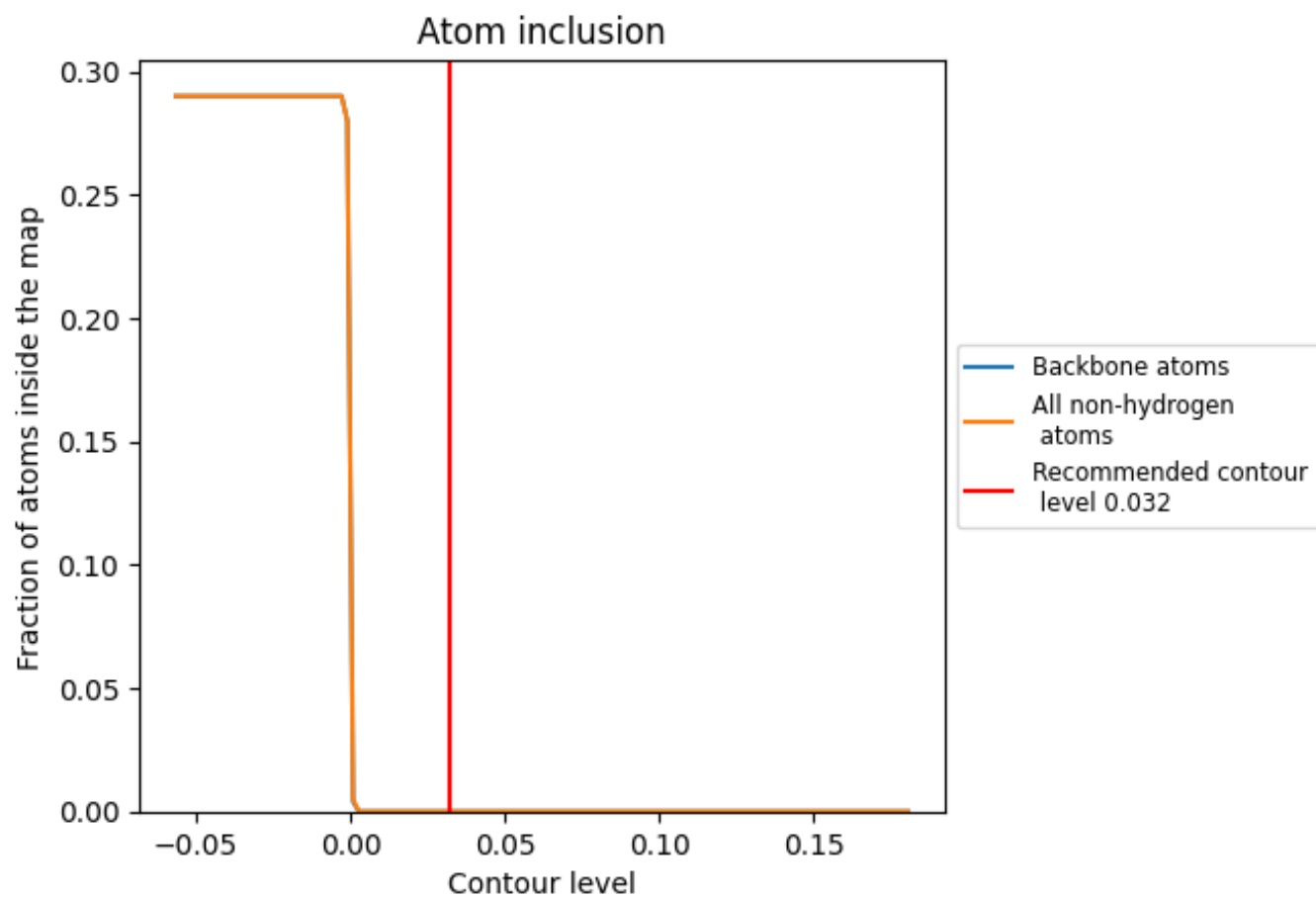
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.032).

9.4 Atom inclusion [i](#)



At the recommended contour level, 0% of all backbone atoms, 0% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0000	0.0000
A	0.0000	0.0010
B	0.0000	0.0010
C	0.0000	-0.0010
D	0.0000	-0.0070
E	0.0000	0.0250
F	0.0000	-0.0260

1.0
0.0
-0.0