



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 01:24 AM UTC

PDB ID : 5NBZ / pdb_00005nbz
EMDB ID : EMD-3611
Title : Wzz dodecamer fitted by MDFF to the Wzz experimental map from cryo-EM
Authors : Ford, R.C.; Kargas, V.; Collins, R.F.; Whitfield, C.; Clarke, B.R.; Siebert, A.;
Bond, P.J.; Clare, D.K.
Deposited on : 2017-03-02
Resolution : 9.00 Å(reported)
Based on initial model : 4E29

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

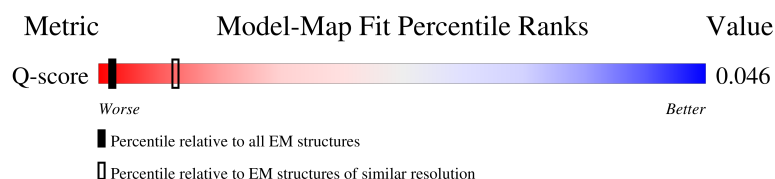
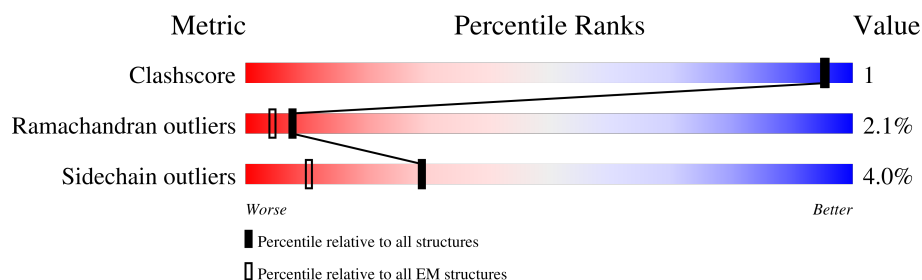
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 9.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	257 (8.50 - 9.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	237	18% 46% 49% 5%
1	B	237	16% 42% 53% ..
1	C	237	16% 43% 51% 6%
1	D	237	17% 43% 51% 6%

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Mol	Chain	Length	Quality of chain
1	E	237	
1	F	237	
1	G	237	
1	H	237	
1	I	237	
1	J	237	
1	K	237	
1	L	237	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 45252 atoms, of which 22704 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.

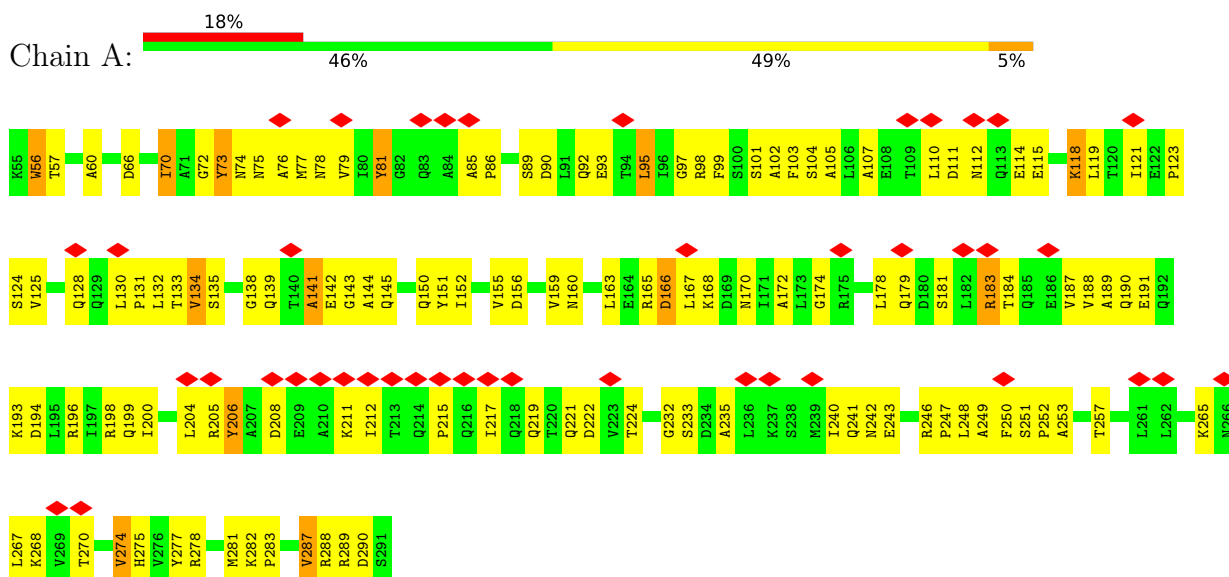
- Molecule 1 is a protein called WzzB.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0
1	B	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0
1	C	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0
1	D	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0
1	E	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0
1	F	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0
1	G	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0
1	H	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0
1	I	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0
1	J	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0
1	K	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0
1	L	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0

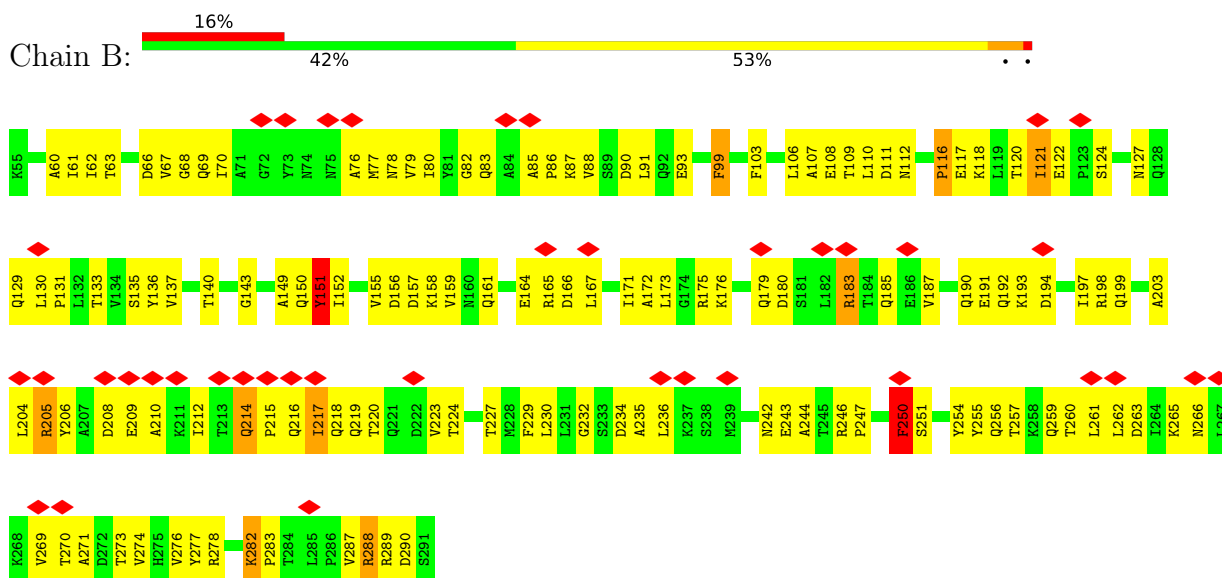
3 Residue-property plots

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.

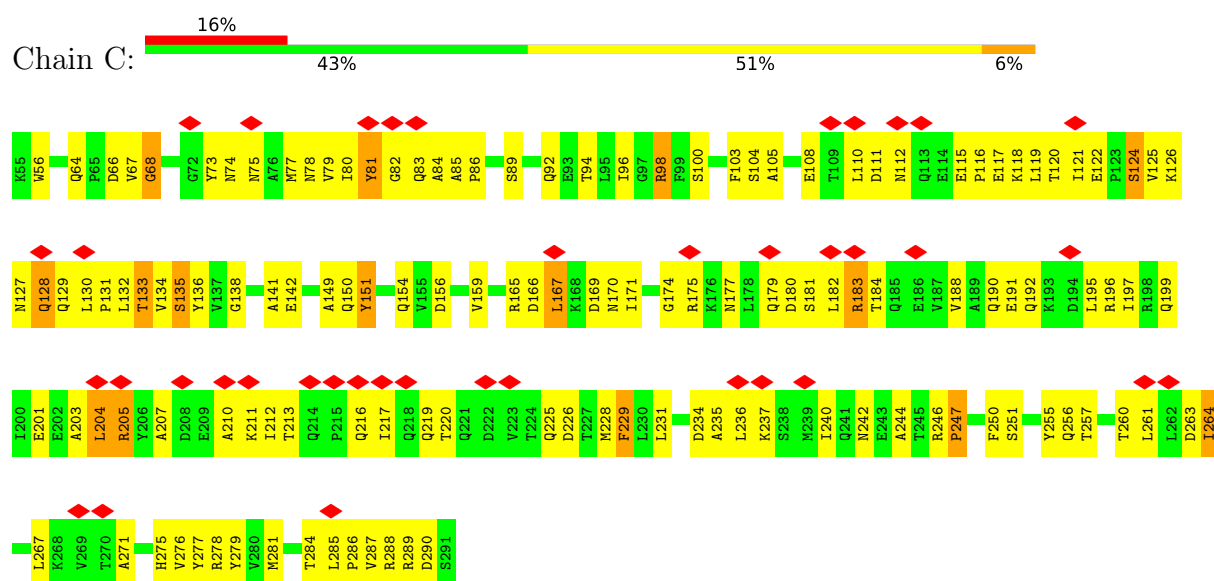
• Molecule 1: WzzB



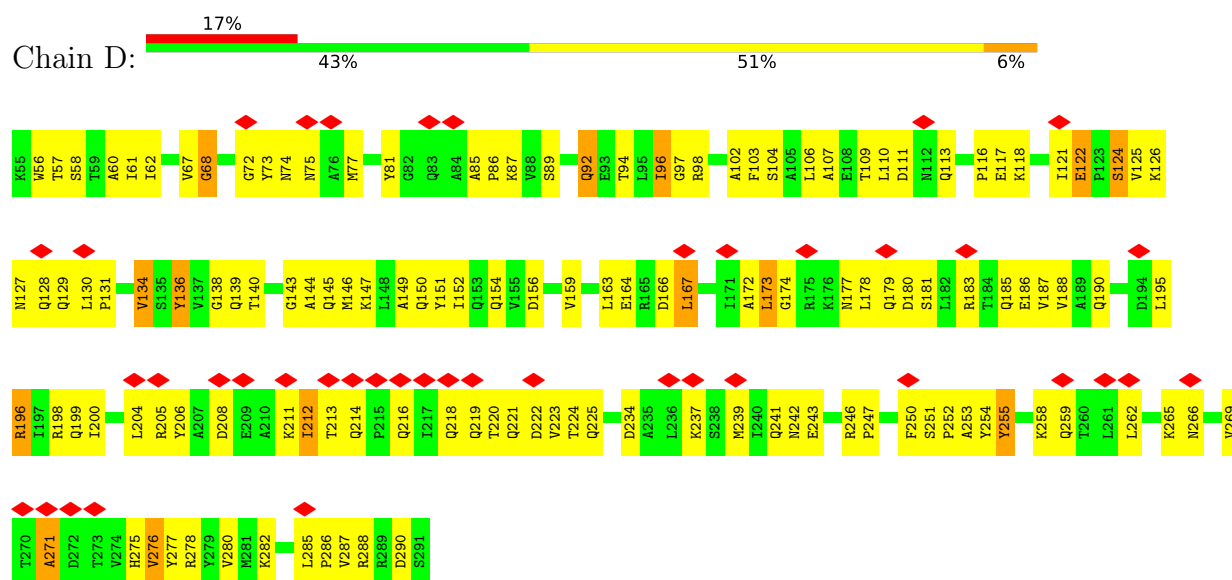
• Molecule 1: WzzB



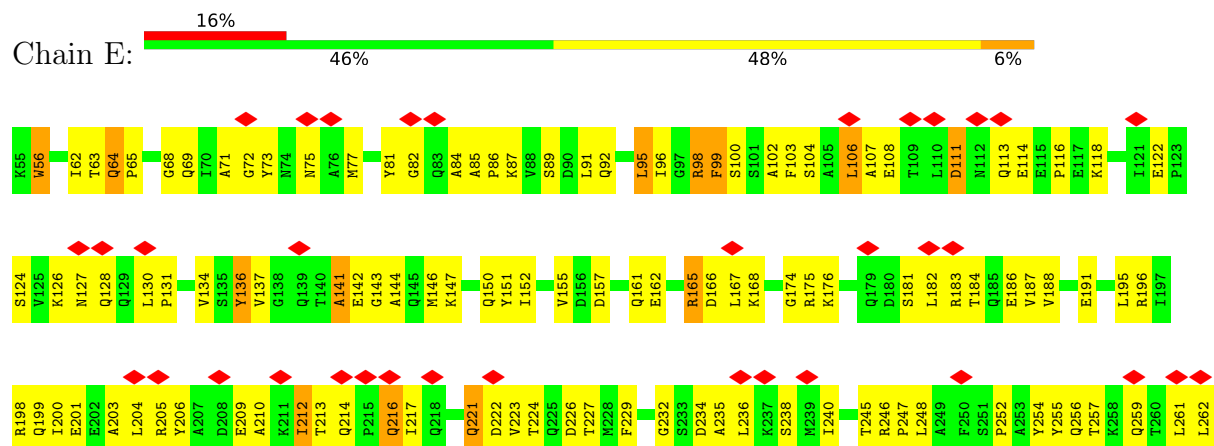
• Molecule 1: WzzB

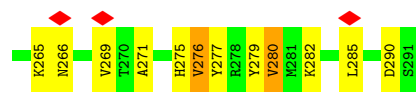


- Molecule 1: WzzB

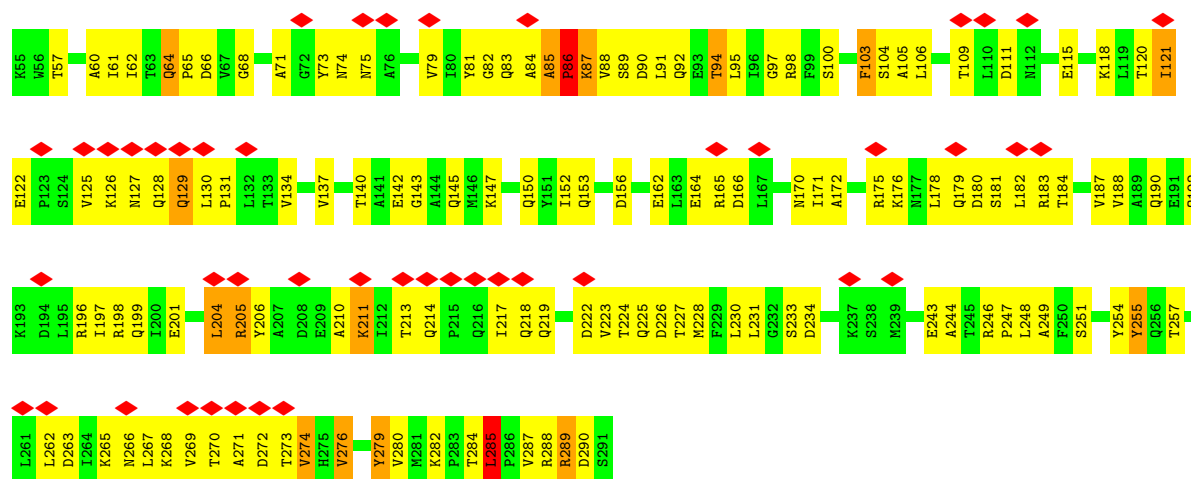
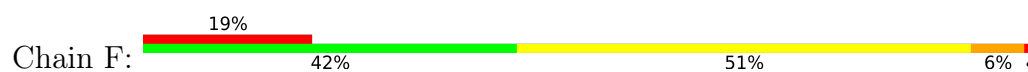


- Molecule 1: WzzB

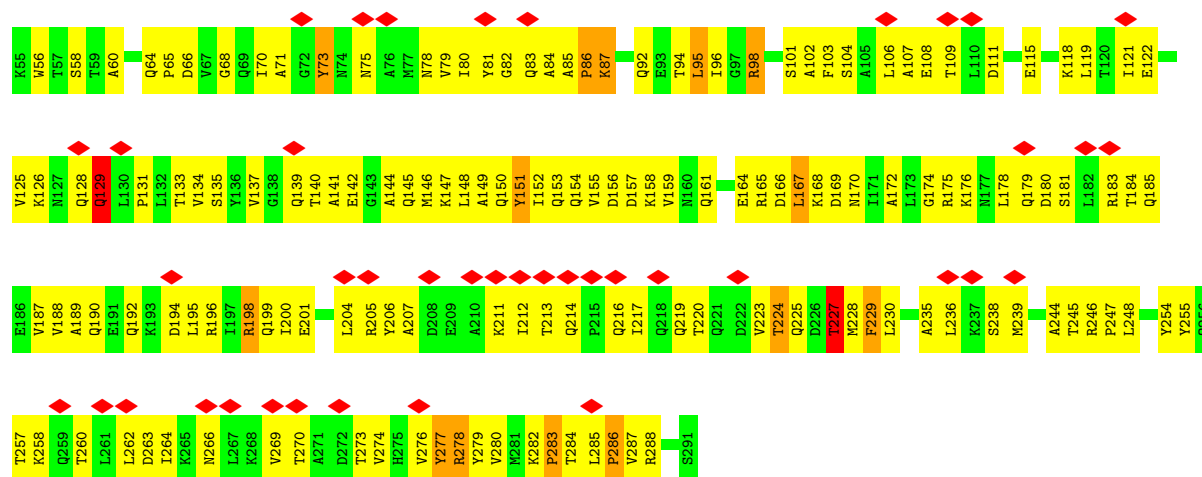




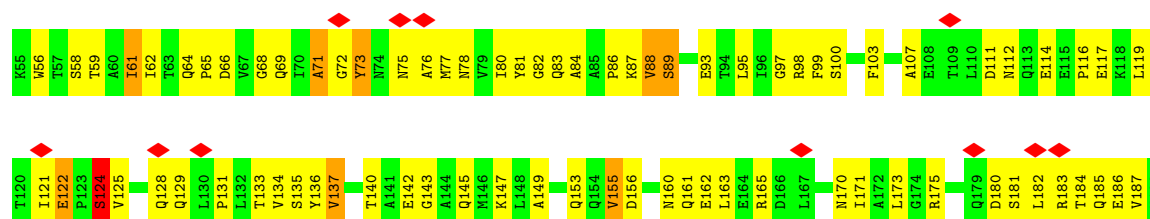
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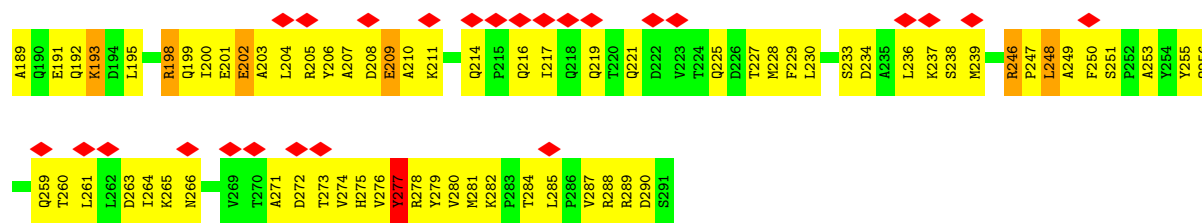


• Molecule 1: WzzB

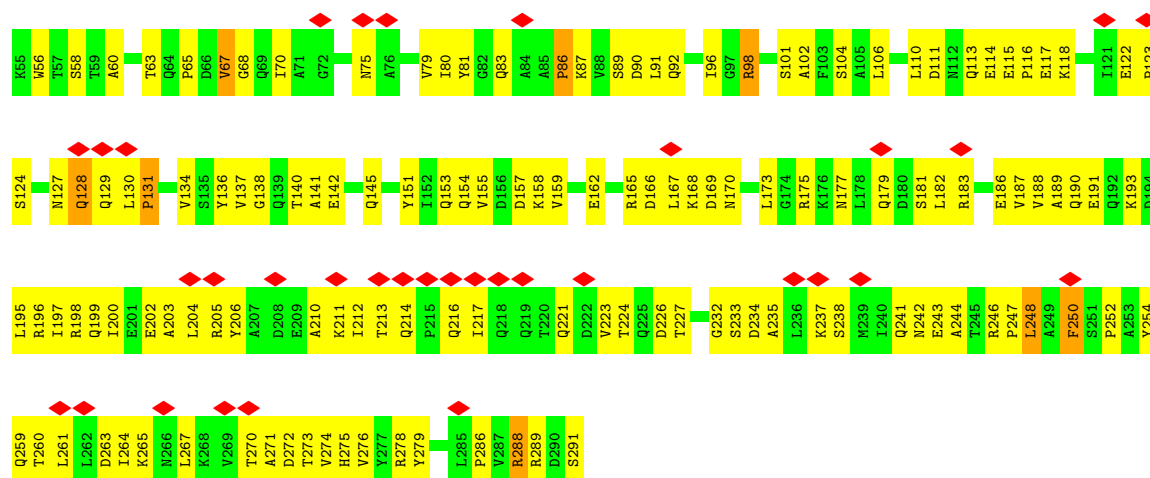


• Molecule 1: WzzB

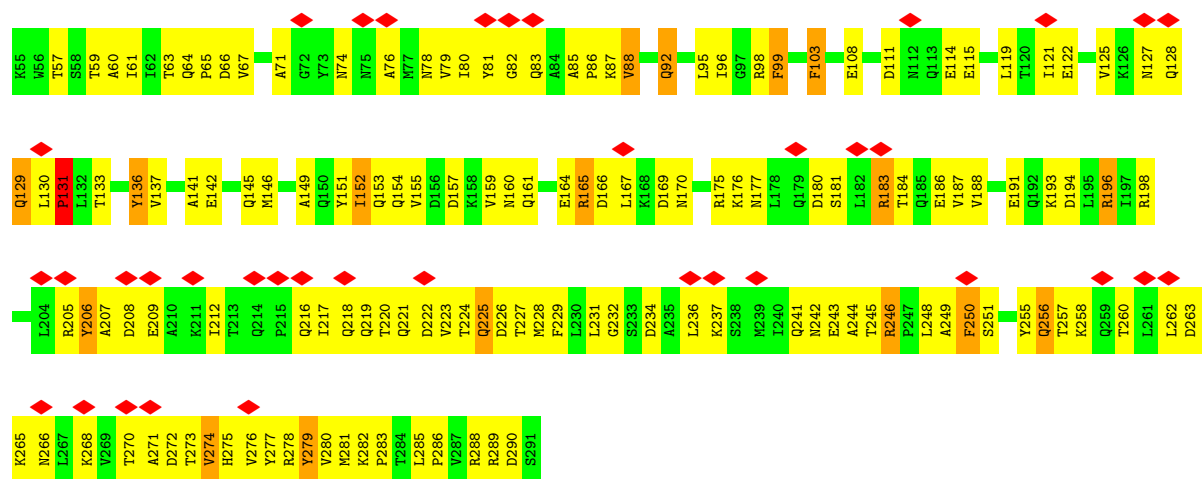




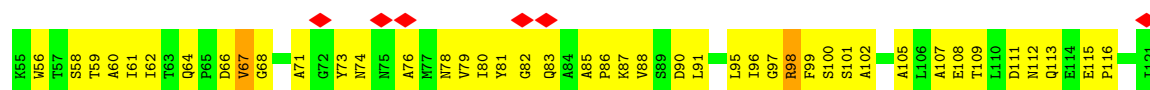
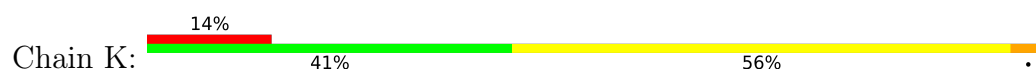
• Molecule 1: WzzB

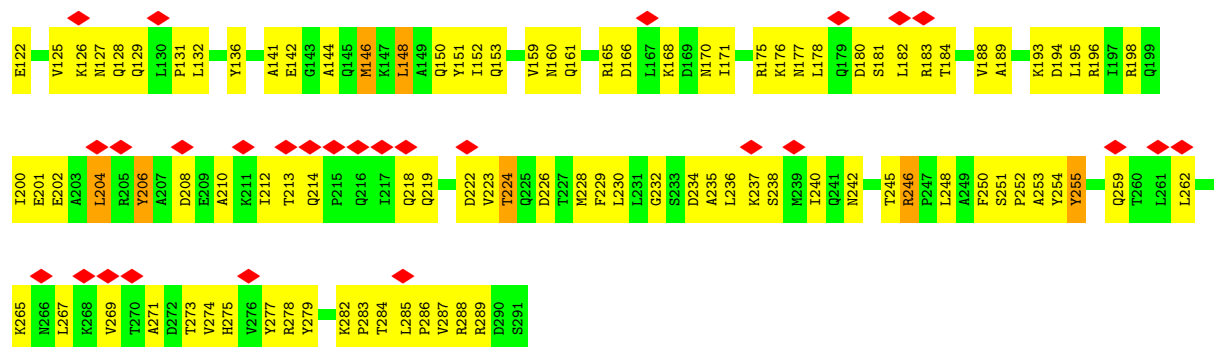


• Molecule 1: WzzB

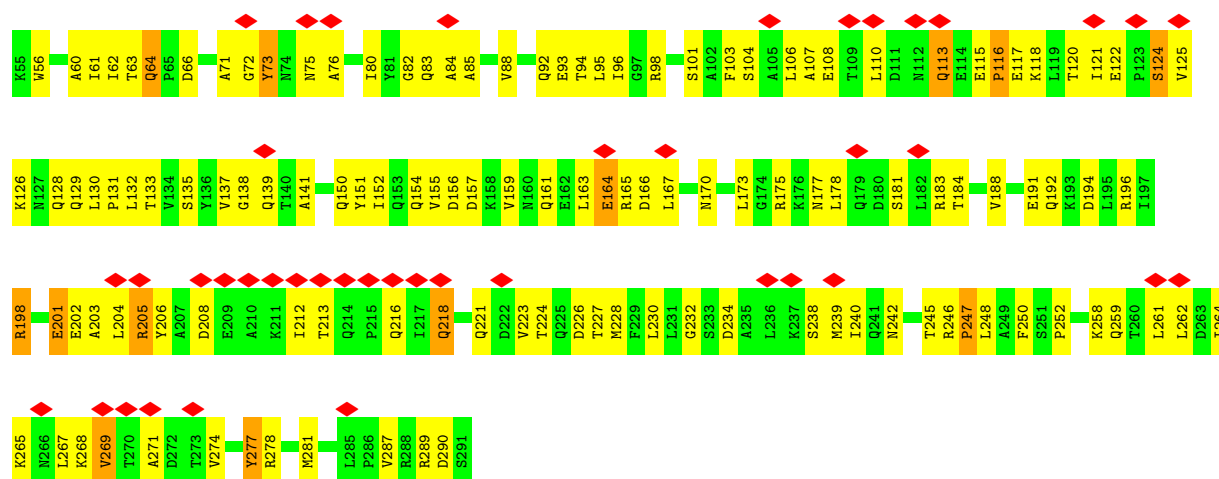


• Molecule 1: WzzB





• Molecule 1: WzzB



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22000	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.561	Depositor
Minimum map value	-3.224	Depositor
Average map value	0.027	Depositor
Map value standard deviation	0.209	Depositor
Recommended contour level	0.66	Depositor
Map size (Å)	371.2, 371.2, 371.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.45, 1.45, 1.45	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	2.22	68/1904 (3.6%)	2.46	128/2580 (5.0%)
1	B	2.28	64/1904 (3.4%)	2.66	171/2580 (6.6%)
1	C	2.29	67/1904 (3.5%)	2.52	136/2580 (5.3%)
1	D	2.29	65/1904 (3.4%)	2.59	142/2580 (5.5%)
1	E	2.24	62/1904 (3.3%)	2.58	132/2580 (5.1%)
1	F	2.27	72/1904 (3.8%)	2.50	132/2580 (5.1%)
1	G	2.33	83/1904 (4.4%)	2.56	159/2580 (6.2%)
1	H	2.28	70/1904 (3.7%)	2.52	141/2580 (5.5%)
1	I	2.26	73/1904 (3.8%)	2.54	149/2580 (5.8%)
1	J	2.29	81/1904 (4.3%)	2.54	147/2580 (5.7%)
1	K	2.25	74/1904 (3.9%)	2.54	138/2580 (5.3%)
1	L	2.25	63/1904 (3.3%)	2.42	125/2580 (4.8%)
All	All	2.27	842/22848 (3.7%)	2.54	1700/30960 (5.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
1	C	0	4
1	D	0	5
1	E	0	3
1	F	0	6
1	G	0	5
1	H	0	5
1	I	0	7
1	J	0	11
1	K	0	7
1	L	0	5
All	All	0	68

All (842) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	115	GLU	C-N	11.06	1.43	1.33
1	D	196	ARG	NE-CZ	10.17	1.44	1.33
1	L	85	ALA	CA-C	-9.67	1.42	1.53
1	G	142	GLU	CA-C	-9.36	1.41	1.52
1	H	246	ARG	CA-C	-9.34	1.43	1.53
1	L	95	LEU	CA-C	-9.23	1.41	1.52
1	I	117	GLU	CA-CB	9.15	1.62	1.53
1	J	128	GLN	CA-CB	9.13	1.64	1.53
1	K	97	GLY	CA-C	-9.09	1.41	1.52
1	G	121	ILE	C-N	9.03	1.43	1.33
1	C	68	GLY	CA-C	-9.02	1.41	1.52
1	H	65	PRO	N-CA	-8.99	1.36	1.47
1	K	116	PRO	N-CA	-8.89	1.37	1.47
1	C	165	ARG	NE-CZ	8.87	1.42	1.33
1	J	289	ARG	NE-CZ	8.81	1.42	1.33
1	C	226	ASP	CA-C	-8.77	1.40	1.52
1	C	277	TYR	CA-C	-8.65	1.42	1.52
1	B	133	THR	CA-C	-8.64	1.42	1.52
1	K	234	ASP	CA-C	-8.52	1.42	1.52
1	H	137	VAL	CA-C	-8.51	1.42	1.52
1	B	256	GLN	N-CA	-8.50	1.36	1.46
1	F	98	ARG	CD-NE	8.49	1.58	1.46
1	B	191	GLU	CA-C	8.49	1.63	1.52
1	B	194	ASP	C-N	8.40	1.45	1.33
1	I	104	SER	CA-C	-8.39	1.41	1.52
1	J	80	ILE	CA-CB	8.37	1.64	1.54
1	E	201	GLU	CA-C	-8.36	1.42	1.52
1	G	196	ARG	CD-NE	8.36	1.57	1.46
1	F	62	ILE	CA-C	-8.32	1.42	1.52
1	K	62	ILE	N-CA	-8.32	1.36	1.46
1	C	92	GLN	CA-C	-8.30	1.42	1.52
1	F	122	GLU	C-N	8.25	1.44	1.33
1	G	214	GLN	CA-C	-8.17	1.44	1.52
1	J	59	THR	CA-C	-8.16	1.42	1.52
1	L	287	VAL	N-CA	-8.12	1.36	1.46
1	E	103	PHE	CA-C	-8.11	1.42	1.52
1	J	166	ASP	N-CA	8.08	1.56	1.46
1	J	251	SER	C-O	-8.06	1.17	1.24
1	C	289	ARG	CZ-NH2	8.04	1.44	1.33
1	F	246	ARG	NE-CZ	8.03	1.41	1.33
1	G	87	LYS	N-CA	-7.99	1.35	1.46
1	D	109	THR	CA-C	-7.96	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	205	ARG	CD-NE	7.93	1.57	1.46
1	B	68	GLY	CA-C	-7.92	1.42	1.52
1	J	198	ARG	NE-CZ	7.91	1.41	1.33
1	H	289	ARG	NE-CZ	7.90	1.41	1.33
1	G	278	ARG	NE-CZ	7.89	1.41	1.33
1	L	269	VAL	N-CA	-7.89	1.38	1.46
1	F	170	ASN	N-CA	-7.88	1.36	1.46
1	J	196	ARG	C-N	7.85	1.43	1.33
1	D	280	VAL	CA-CB	-7.84	1.43	1.54
1	H	183	ARG	CZ-NH2	7.83	1.43	1.33
1	D	173	LEU	CA-CB	7.82	1.65	1.53
1	C	205	ARG	NE-CZ	7.80	1.41	1.33
1	G	102	ALA	N-CA	-7.79	1.36	1.46
1	G	216	GLN	CA-C	-7.76	1.42	1.52
1	I	254	TYR	N-CA	-7.75	1.36	1.46
1	A	240	ILE	N-CA	7.74	1.55	1.46
1	J	71	ALA	CA-C	-7.73	1.42	1.52
1	C	290	ASP	N-CA	-7.72	1.41	1.46
1	L	196	ARG	NE-CZ	7.72	1.41	1.33
1	F	246	ARG	CZ-NH1	7.71	1.43	1.32
1	H	186	GLU	C-N	7.70	1.43	1.33
1	H	59	THR	CA-C	-7.69	1.43	1.52
1	I	191	GLU	C-N	7.65	1.44	1.33
1	K	213	THR	N-CA	-7.64	1.39	1.46
1	J	175	ARG	CZ-NH2	7.62	1.43	1.33
1	I	181	SER	CA-CB	7.62	1.65	1.53
1	K	250	PHE	CA-C	-7.61	1.43	1.52
1	H	76	ALA	CA-C	7.61	1.62	1.52
1	A	172	ALA	C-N	7.60	1.44	1.33
1	G	213	THR	CA-C	-7.59	1.42	1.52
1	I	195	LEU	C-N	7.58	1.43	1.33
1	E	98	ARG	CD-NE	7.58	1.56	1.46
1	F	187	VAL	C-N	7.57	1.43	1.33
1	E	75	ASN	CA-C	-7.55	1.43	1.52
1	A	247	PRO	CA-C	-7.54	1.44	1.52
1	D	110	LEU	CA-C	-7.54	1.43	1.52
1	H	205	ARG	CZ-NH2	7.53	1.43	1.33
1	E	209	GLU	N-CA	7.50	1.55	1.46
1	C	205	ARG	CD-NE	7.48	1.56	1.46
1	E	214	GLN	N-CA	-7.48	1.38	1.46
1	H	89	SER	CA-C	-7.47	1.43	1.52
1	G	168	LYS	N-CA	-7.47	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	280	VAL	N-CA	-7.45	1.37	1.46
1	F	210	ALA	CA-C	-7.42	1.42	1.52
1	F	178	LEU	CA-C	-7.41	1.43	1.52
1	A	184	THR	C-N	7.40	1.43	1.33
1	E	240	ILE	CA-CB	-7.40	1.45	1.54
1	D	198	ARG	CD-NE	7.37	1.56	1.46
1	F	190	GLN	CA-CB	7.37	1.65	1.53
1	I	104	SER	C-N	7.37	1.43	1.33
1	B	223	VAL	CA-C	-7.37	1.43	1.52
1	E	279	TYR	N-CA	-7.36	1.37	1.46
1	E	255	TYR	CA-CB	7.34	1.65	1.53
1	K	275	HIS	ND1-CE1	7.34	1.39	1.32
1	E	111	ASP	CA-CB	7.34	1.65	1.53
1	A	265	LYS	N-CA	-7.32	1.36	1.46
1	D	138	GLY	N-CA	-7.32	1.37	1.44
1	L	218	GLN	N-CA	-7.32	1.36	1.46
1	D	143	GLY	N-CA	7.31	1.55	1.45
1	H	248	LEU	CA-C	-7.31	1.43	1.52
1	J	186	GLU	CA-CB	7.30	1.64	1.53
1	C	98	ARG	CD-NE	7.29	1.56	1.46
1	G	104	SER	CA-C	-7.28	1.43	1.52
1	D	181	SER	N-CA	-7.26	1.37	1.46
1	G	147	LYS	CA-C	-7.26	1.43	1.52
1	I	205	ARG	NE-CZ	7.25	1.41	1.33
1	C	278	ARG	N-CA	-7.23	1.36	1.45
1	I	58	SER	CA-C	-7.23	1.44	1.52
1	G	155	VAL	CA-CB	-7.23	1.45	1.54
1	A	193	LYS	C-N	7.21	1.43	1.33
1	G	175	ARG	CA-C	-7.21	1.43	1.52
1	B	129	GLN	CA-C	-7.20	1.43	1.52
1	H	170	ASN	C-N	7.19	1.43	1.33
1	L	239	MET	C-N	7.19	1.42	1.33
1	A	144	ALA	CA-C	7.19	1.61	1.52
1	F	204	LEU	C-N	7.18	1.43	1.33
1	D	259	GLN	CA-C	-7.18	1.43	1.52
1	J	60	ALA	N-CA	-7.16	1.36	1.45
1	K	265	LYS	CA-C	-7.16	1.43	1.52
1	G	158	LYS	N-CA	-7.15	1.37	1.46
1	H	191	GLU	CA-CB	7.15	1.64	1.53
1	I	159	VAL	N-CA	-7.13	1.38	1.46
1	C	250	PHE	N-CA	-7.12	1.37	1.45
1	D	247	PRO	C-N	7.11	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	159	VAL	CA-CB	-7.06	1.45	1.54
1	C	138	GLY	CA-C	-7.06	1.46	1.52
1	E	238	SER	CA-C	-7.05	1.43	1.52
1	D	290	ASP	C-N	7.02	1.43	1.33
1	L	75	ASN	CA-CB	7.00	1.64	1.53
1	J	176	LYS	CA-CB	7.00	1.64	1.53
1	G	205	ARG	NE-CZ	6.99	1.40	1.33
1	I	286	PRO	CA-C	-6.97	1.42	1.52
1	L	223	VAL	CA-CB	-6.97	1.45	1.55
1	I	101	SER	CA-C	-6.96	1.43	1.52
1	G	134	VAL	N-CA	6.95	1.54	1.46
1	J	71	ALA	N-CA	-6.93	1.38	1.46
1	J	196	ARG	NE-CZ	6.92	1.40	1.33
1	H	216	GLN	C-N	6.92	1.42	1.33
1	I	159	VAL	CA-CB	-6.91	1.45	1.54
1	D	97	GLY	C-N	6.91	1.43	1.33
1	D	103	PHE	C-N	6.91	1.43	1.33
1	F	179	GLN	N-CA	-6.91	1.38	1.46
1	L	201	GLU	C-N	6.91	1.43	1.33
1	A	72	GLY	CA-C	-6.90	1.44	1.52
1	A	199	GLN	C-N	6.90	1.42	1.33
1	D	98	ARG	N-CA	-6.88	1.38	1.46
1	F	79	VAL	CA-C	6.88	1.61	1.52
1	A	204	LEU	C-N	6.87	1.43	1.33
1	C	89	SER	C-N	6.86	1.43	1.33
1	J	153	GLN	C-O	-6.85	1.16	1.24
1	L	117	GLU	CA-CB	6.84	1.61	1.53
1	B	199	GLN	CA-C	-6.84	1.44	1.52
1	F	121	ILE	C-N	6.84	1.41	1.33
1	G	164	GLU	CA-C	-6.84	1.44	1.52
1	F	120	THR	CA-C	6.84	1.60	1.52
1	J	208	ASP	C-N	6.83	1.43	1.33
1	C	256	GLN	C-O	-6.83	1.16	1.24
1	K	198	ARG	NE-CZ	6.83	1.40	1.33
1	I	186	GLU	N-CA	-6.82	1.38	1.46
1	J	266	ASN	C-N	6.82	1.43	1.33
1	H	56	TRP	CA-C	-6.81	1.44	1.52
1	C	134	VAL	CA-C	-6.81	1.44	1.52
1	E	229	PHE	CA-CB	6.81	1.64	1.53
1	F	205	ARG	NE-CZ	6.81	1.40	1.33
1	H	88	VAL	C-N	6.81	1.42	1.33
1	A	60	ALA	N-CA	-6.80	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	119	LEU	CA-C	-6.80	1.44	1.52
1	G	183	ARG	CD-NE	6.80	1.55	1.46
1	K	153	GLN	CA-CB	6.80	1.64	1.53
1	C	141	ALA	C-N	6.78	1.43	1.33
1	K	289	ARG	CZ-NH1	6.77	1.42	1.32
1	G	198	ARG	NE-CZ	6.76	1.40	1.33
1	J	88	VAL	CA-CB	-6.76	1.46	1.54
1	D	276	VAL	CA-CB	6.74	1.63	1.54
1	L	268	LYS	CA-C	-6.73	1.44	1.52
1	A	274	VAL	C-O	-6.71	1.16	1.24
1	A	275	HIS	ND1-CE1	6.68	1.39	1.32
1	F	211	LYS	N-CA	6.67	1.54	1.46
1	H	187	VAL	CA-C	-6.67	1.44	1.52
1	D	94	THR	C-N	6.67	1.42	1.33
1	C	211	LYS	C-N	6.67	1.41	1.33
1	E	205	ARG	NE-CZ	6.66	1.40	1.33
1	C	150	GLN	N-CA	-6.65	1.38	1.46
1	B	230	LEU	CA-C	-6.65	1.43	1.52
1	C	100	SER	CA-CB	6.64	1.63	1.53
1	E	72	GLY	C-N	6.63	1.42	1.33
1	B	289	ARG	CD-NE	6.63	1.55	1.46
1	L	198	ARG	CD-NE	6.63	1.55	1.46
1	I	198	ARG	CA-C	-6.62	1.44	1.52
1	A	77	MET	C-N	6.62	1.43	1.33
1	B	108	GLU	CA-CB	6.61	1.63	1.53
1	B	106	LEU	C-N	6.60	1.42	1.33
1	K	116	PRO	CA-C	-6.60	1.46	1.52
1	G	137	VAL	CA-CB	-6.59	1.46	1.54
1	I	288	ARG	NE-CZ	6.59	1.40	1.33
1	A	206	TYR	N-CA	-6.57	1.38	1.46
1	A	56	TRP	NE1-CE2	-6.57	1.30	1.37
1	K	267	LEU	CA-CB	6.57	1.64	1.53
1	J	256	GLN	CA-CB	6.56	1.63	1.53
1	B	60	ALA	CA-C	-6.56	1.44	1.52
1	L	118	LYS	N-CA	-6.56	1.38	1.46
1	K	198	ARG	CD-NE	6.55	1.55	1.46
1	C	108	GLU	N-CA	-6.55	1.38	1.46
1	H	263	ASP	N-CA	6.55	1.54	1.46
1	F	289	ARG	CD-NE	6.54	1.55	1.46
1	E	182	LEU	CA-CB	6.54	1.63	1.53
1	J	187	VAL	CA-CB	-6.54	1.46	1.54
1	F	196	ARG	CZ-NH1	6.53	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	270	THR	N-CA	-6.52	1.37	1.45
1	J	288	ARG	CD-NE	6.52	1.55	1.46
1	I	193	LYS	CA-C	-6.51	1.44	1.52
1	A	267	LEU	CA-C	-6.51	1.44	1.52
1	K	195	LEU	CA-C	-6.50	1.44	1.52
1	G	211	LYS	CA-CB	6.49	1.63	1.53
1	A	267	LEU	N-CA	6.49	1.54	1.46
1	G	64	GLN	CA-CB	6.49	1.63	1.53
1	H	276	VAL	CA-CB	-6.49	1.47	1.54
1	B	172	ALA	N-CA	-6.49	1.38	1.46
1	A	196	ARG	NE-CZ	6.48	1.40	1.33
1	E	73	TYR	N-CA	6.48	1.54	1.46
1	L	126	LYS	N-CA	-6.48	1.37	1.46
1	H	160	ASN	C-N	6.46	1.42	1.33
1	B	130	LEU	C-O	-6.44	1.16	1.24
1	A	235	ALA	C-N	6.43	1.42	1.33
1	D	187	VAL	CA-C	6.42	1.60	1.52
1	K	201	GLU	C-O	-6.41	1.16	1.24
1	J	151	TYR	CA-C	-6.41	1.44	1.52
1	J	92	GLN	N-CA	-6.41	1.38	1.46
1	D	188	VAL	CA-CB	-6.41	1.46	1.54
1	K	101	SER	N-CA	-6.40	1.38	1.46
1	F	222	ASP	CA-C	-6.39	1.44	1.52
1	D	251	SER	CA-C	-6.39	1.44	1.52
1	G	65	PRO	C-O	-6.38	1.15	1.23
1	K	240	ILE	C-N	6.38	1.42	1.33
1	A	128	GLN	CA-CB	6.38	1.62	1.53
1	J	157	ASP	N-CA	-6.38	1.38	1.46
1	E	206	TYR	N-CA	-6.38	1.38	1.46
1	I	79	VAL	C-N	6.37	1.41	1.33
1	B	192	GLN	CA-C	-6.37	1.44	1.52
1	C	175	ARG	CA-CB	6.36	1.63	1.53
1	E	167	LEU	CA-C	-6.36	1.44	1.52
1	K	129	GLN	CA-C	-6.34	1.44	1.52
1	I	271	ALA	N-CA	6.34	1.52	1.46
1	E	62	ILE	C-N	6.34	1.42	1.33
1	B	175	ARG	CD-NE	6.33	1.55	1.46
1	C	179	GLN	CA-CB	6.33	1.63	1.53
1	G	201	GLU	C-N	6.33	1.42	1.33
1	F	288	ARG	CD-NE	6.33	1.55	1.46
1	G	230	LEU	CA-CB	6.33	1.64	1.53
1	K	230	LEU	CA-CB	6.32	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	205	ARG	NE-CZ	6.32	1.40	1.33
1	B	69	GLN	C-N	6.30	1.41	1.33
1	F	125	VAL	CA-C	-6.30	1.44	1.52
1	K	68	GLY	CA-C	-6.30	1.45	1.52
1	G	135	SER	CA-C	-6.30	1.44	1.52
1	J	167	LEU	C-N	6.28	1.42	1.33
1	F	105	ALA	N-CA	-6.28	1.38	1.46
1	G	276	VAL	C-N	6.28	1.42	1.33
1	K	271	ALA	CA-C	-6.27	1.46	1.52
1	C	264	ILE	CA-C	-6.26	1.44	1.52
1	F	197	ILE	C-N	6.26	1.42	1.33
1	A	191	GLU	CA-CB	6.26	1.63	1.53
1	F	248	LEU	CA-C	-6.26	1.44	1.52
1	J	205	ARG	CZ-NH1	6.26	1.41	1.32
1	A	97	GLY	CA-C	-6.26	1.45	1.52
1	L	289	ARG	CD-NE	6.25	1.55	1.46
1	E	232	GLY	CA-C	6.25	1.60	1.51
1	I	134	VAL	C-N	6.25	1.41	1.33
1	I	289	ARG	CD-NE	6.24	1.54	1.46
1	G	137	VAL	C-N	6.24	1.39	1.33
1	G	246	ARG	NE-CZ	6.24	1.40	1.33
1	J	122	GLU	N-CA	-6.24	1.39	1.46
1	I	170	ASN	CA-CB	6.23	1.63	1.53
1	B	124	SER	CA-CB	6.23	1.63	1.53
1	G	277	TYR	N-CA	-6.22	1.37	1.45
1	L	290	ASP	CA-C	-6.22	1.45	1.52
1	A	95	LEU	C-N	6.21	1.41	1.33
1	E	195	LEU	C-N	6.21	1.42	1.33
1	I	129	GLN	CA-CB	6.21	1.62	1.53
1	J	154	GLN	CA-CB	6.21	1.62	1.53
1	A	138	GLY	CA-C	-6.20	1.46	1.52
1	K	269	VAL	CA-C	-6.20	1.44	1.52
1	F	270	THR	N-CA	-6.20	1.38	1.45
1	C	247	PRO	N-CD	6.19	1.56	1.47
1	H	58	SER	N-CA	-6.19	1.38	1.46
1	J	272	ASP	CA-CB	6.18	1.60	1.53
1	F	285	LEU	CA-C	6.18	1.60	1.52
1	D	136	TYR	N-CA	-6.18	1.38	1.46
1	B	260	THR	CA-C	-6.18	1.44	1.52
1	F	129	GLN	C-N	6.17	1.40	1.33
1	D	67	VAL	N-CA	-6.16	1.39	1.46
1	G	70	ILE	CA-CB	-6.16	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	289	ARG	CD-NE	6.16	1.54	1.46
1	K	218	GLN	CA-C	-6.16	1.44	1.52
1	G	98	ARG	CZ-NH1	6.15	1.41	1.32
1	D	196	ARG	CZ-NH1	6.15	1.41	1.32
1	B	288	ARG	CD-NE	6.15	1.54	1.46
1	E	266	ASN	CA-CB	6.15	1.63	1.53
1	I	273	THR	CA-C	-6.14	1.44	1.52
1	L	98	ARG	C-N	6.14	1.41	1.33
1	L	80	ILE	CA-C	-6.14	1.45	1.52
1	L	110	LEU	N-CA	-6.14	1.39	1.46
1	K	183	ARG	CA-C	6.14	1.60	1.52
1	B	278	ARG	CD-NE	6.13	1.54	1.46
1	A	257	THR	CA-C	-6.13	1.45	1.52
1	E	147	LYS	C-N	6.13	1.42	1.33
1	D	147	LYS	N-CA	-6.12	1.38	1.46
1	D	223	VAL	CA-CB	-6.12	1.46	1.54
1	D	275	HIS	ND1-CE1	6.12	1.38	1.32
1	A	283	PRO	N-CD	-6.12	1.39	1.47
1	F	98	ARG	NE-CZ	6.11	1.39	1.33
1	E	142	GLU	CA-C	-6.10	1.44	1.52
1	B	247	PRO	C-N	6.10	1.41	1.33
1	K	113	GLN	CA-C	-6.10	1.44	1.52
1	D	211	LYS	CA-CB	6.09	1.63	1.53
1	L	250	PHE	CA-C	6.09	1.60	1.52
1	J	121	ILE	C-N	6.09	1.40	1.33
1	D	56	TRP	NE1-CE2	-6.08	1.30	1.37
1	J	289	ARG	CA-C	-6.07	1.44	1.52
1	A	165	ARG	CD-NE	6.06	1.54	1.46
1	B	80	ILE	C-N	6.05	1.42	1.33
1	F	143	GLY	CA-C	-6.05	1.45	1.52
1	J	92	GLN	CA-CB	6.04	1.62	1.53
1	H	163	LEU	CA-CB	6.04	1.62	1.53
1	C	289	ARG	NE-CZ	6.04	1.39	1.33
1	C	286	PRO	C-N	6.03	1.39	1.33
1	J	83	GLN	N-CA	-6.03	1.39	1.46
1	H	185	GLN	CA-C	-6.02	1.45	1.52
1	I	221	GLN	N-CA	-6.01	1.39	1.46
1	K	74	ASN	N-CA	6.01	1.53	1.46
1	L	135	SER	C-N	6.01	1.42	1.33
1	F	142	GLU	CA-C	-6.01	1.45	1.52
1	H	289	ARG	C-O	-6.00	1.17	1.24
1	J	165	ARG	CD-NE	6.00	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	152	ILE	C-N	6.00	1.41	1.33
1	J	142	GLU	CA-CB	5.99	1.62	1.53
1	D	60	ALA	CA-C	-5.99	1.45	1.52
1	B	112	ASN	CA-CB	5.98	1.60	1.52
1	F	75	ASN	CA-C	-5.98	1.45	1.52
1	A	89	SER	CA-C	-5.97	1.45	1.52
1	I	111	ASP	N-CA	-5.97	1.39	1.46
1	H	107	ALA	C-N	5.97	1.41	1.33
1	F	288	ARG	NE-CZ	5.97	1.39	1.33
1	E	130	LEU	CA-CB	5.96	1.60	1.53
1	D	110	LEU	CB-CG	5.96	1.65	1.53
1	F	180	ASP	CA-CB	5.95	1.62	1.53
1	D	204	LEU	CA-CB	5.95	1.62	1.53
1	J	175	ARG	N-CA	-5.95	1.39	1.46
1	A	130	LEU	CA-CB	5.95	1.61	1.52
1	A	281	MET	CA-C	-5.93	1.45	1.52
1	D	218	GLN	CA-C	5.93	1.60	1.52
1	B	143	GLY	CA-C	-5.93	1.45	1.52
1	C	288	ARG	CD-NE	5.93	1.54	1.46
1	J	282	LYS	CA-C	5.93	1.59	1.53
1	I	154	GLN	C-N	5.93	1.41	1.33
1	E	187	VAL	C-O	-5.92	1.17	1.24
1	K	286	PRO	C-N	5.92	1.39	1.33
1	E	124	SER	CA-C	-5.92	1.45	1.52
1	B	265	LYS	CA-CB	5.92	1.63	1.53
1	G	220	THR	C-N	5.92	1.40	1.33
1	G	199	GLN	C-N	5.92	1.41	1.33
1	B	83	GLN	C-N	5.91	1.42	1.34
1	L	194	ASP	CA-C	-5.91	1.45	1.52
1	B	183	ARG	NE-CZ	5.91	1.39	1.33
1	C	246	ARG	CA-C	5.91	1.59	1.53
1	B	164	GLU	C-O	-5.91	1.17	1.24
1	H	173	LEU	CA-CB	5.90	1.62	1.53
1	K	238	SER	CA-CB	5.90	1.62	1.53
1	L	129	GLN	N-CA	-5.90	1.38	1.46
1	G	284	THR	CA-C	-5.90	1.45	1.53
1	L	103	PHE	N-CA	-5.90	1.39	1.46
1	F	266	ASN	CA-C	-5.90	1.45	1.52
1	E	224	THR	CA-C	-5.89	1.45	1.53
1	H	229	PHE	CA-C	-5.89	1.44	1.52
1	G	166	ASP	CA-C	-5.89	1.45	1.52
1	L	80	ILE	N-CA	-5.89	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	ARG	NE-CZ	5.89	1.39	1.33
1	I	130	LEU	N-CA	-5.89	1.40	1.46
1	K	214	GLN	CA-CB	5.89	1.61	1.53
1	C	133	THR	CA-C	-5.88	1.45	1.52
1	G	262	LEU	CA-CB	5.88	1.62	1.53
1	L	154	GLN	CA-C	-5.87	1.45	1.52
1	E	290	ASP	N-CA	-5.87	1.38	1.45
1	I	261	LEU	C-N	5.87	1.41	1.33
1	D	269	VAL	CA-C	5.87	1.60	1.52
1	C	271	ALA	C-N	5.86	1.41	1.33
1	D	254	TYR	CZ-OH	5.86	1.50	1.38
1	L	166	ASP	CA-CB	5.86	1.62	1.53
1	C	175	ARG	CZ-NH2	5.86	1.41	1.33
1	F	134	VAL	N-CA	-5.86	1.39	1.46
1	J	207	ALA	CA-CB	5.86	1.62	1.53
1	D	102	ALA	C-N	5.85	1.41	1.33
1	G	170	ASN	C-N	5.85	1.41	1.33
1	C	98	ARG	CZ-NH1	5.84	1.41	1.32
1	H	142	GLU	CA-C	-5.84	1.45	1.52
1	H	117	GLU	N-CA	-5.84	1.39	1.46
1	J	241	GLN	CA-C	-5.84	1.45	1.52
1	J	177	ASN	N-CA	-5.84	1.39	1.46
1	D	204	LEU	N-CA	-5.84	1.39	1.46
1	B	155	VAL	CA-CB	-5.83	1.46	1.54
1	F	274	VAL	C-N	5.83	1.41	1.33
1	C	125	VAL	C-N	5.81	1.41	1.33
1	K	67	VAL	CA-C	5.81	1.60	1.52
1	E	98	ARG	CA-CB	5.81	1.62	1.53
1	B	76	ALA	N-CA	-5.80	1.39	1.46
1	H	175	ARG	CD-NE	5.80	1.54	1.46
1	D	127	ASN	CA-CB	5.80	1.62	1.53
1	J	63	THR	CA-C	-5.80	1.45	1.52
1	J	246	ARG	CD-NE	5.79	1.54	1.46
1	I	158	LYS	CA-CB	5.79	1.62	1.53
1	I	91	LEU	C-N	5.79	1.41	1.33
1	K	151	TYR	C-N	5.79	1.41	1.33
1	B	116	PRO	N-CA	-5.79	1.40	1.47
1	C	170	ASN	CA-C	-5.78	1.45	1.52
1	L	274	VAL	C-N	5.78	1.41	1.33
1	C	276	VAL	C-N	5.77	1.40	1.33
1	H	76	ALA	CA-CB	-5.77	1.44	1.53
1	H	64	GLN	C-N	5.77	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	99	PHE	CA-C	-5.76	1.45	1.52
1	D	222	ASP	CA-CB	5.76	1.62	1.53
1	A	123	PRO	C-N	5.75	1.41	1.33
1	D	146	MET	CA-C	-5.75	1.45	1.52
1	F	198	ARG	CA-C	-5.75	1.45	1.52
1	K	223	VAL	C-N	5.74	1.41	1.33
1	H	198	ARG	NE-CZ	5.73	1.39	1.33
1	G	285	LEU	N-CA	-5.72	1.39	1.46
1	J	263	ASP	C-N	5.72	1.41	1.33
1	F	196	ARG	CD-NE	5.72	1.54	1.46
1	K	148	LEU	CA-C	-5.72	1.45	1.52
1	C	244	ALA	CA-C	-5.72	1.45	1.52
1	G	236	LEU	C-N	5.71	1.41	1.33
1	K	166	ASP	CA-CB	5.71	1.62	1.53
1	J	160	ASN	C-O	-5.71	1.17	1.24
1	G	183	ARG	CZ-NH2	5.71	1.40	1.33
1	J	278	ARG	C-N	5.70	1.41	1.33
1	D	251	SER	N-CA	-5.70	1.38	1.46
1	G	154	GLN	CA-C	-5.70	1.45	1.52
1	E	226	ASP	CA-C	-5.69	1.44	1.52
1	K	122	GLU	CA-C	-5.69	1.45	1.52
1	A	196	ARG	CA-C	5.69	1.60	1.52
1	J	216	GLN	CA-C	-5.68	1.45	1.52
1	J	278	ARG	CD-NE	5.68	1.54	1.46
1	A	166	ASP	CA-C	5.68	1.60	1.52
1	J	262	LEU	CA-C	-5.68	1.45	1.52
1	E	276	VAL	CA-CB	-5.68	1.46	1.54
1	F	150	GLN	CA-CB	5.68	1.62	1.53
1	H	217	ILE	C-N	5.67	1.40	1.33
1	D	262	LEU	CA-CB	5.67	1.62	1.53
1	I	213	THR	C-N	-5.67	1.26	1.33
1	L	208	ASP	C-N	5.67	1.41	1.33
1	G	223	VAL	CA-C	5.66	1.59	1.52
1	G	156	ASP	CA-C	5.66	1.60	1.52
1	K	96	ILE	CB-CG1	5.66	1.64	1.53
1	L	262	LEU	C-N	-5.66	1.26	1.33
1	D	121	ILE	C-N	5.66	1.40	1.33
1	F	153	GLN	C-O	-5.65	1.17	1.24
1	C	207	ALA	N-CA	-5.64	1.39	1.46
1	J	177	ASN	CA-C	-5.64	1.45	1.52
1	C	275	HIS	C-N	5.64	1.40	1.33
1	K	178	LEU	CA-CB	5.63	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	199	GLN	CA-CB	5.63	1.62	1.53
1	H	247	PRO	CA-CB	5.63	1.61	1.53
1	J	165	ARG	CZ-NH1	5.62	1.40	1.32
1	K	194	ASP	N-CA	5.62	1.53	1.46
1	J	260	THR	C-N	5.62	1.41	1.33
1	I	291	SER	CA-C	5.61	1.64	1.52
1	J	96	ILE	CA-C	-5.61	1.45	1.52
1	K	282	LYS	N-CA	-5.61	1.39	1.46
1	B	205	ARG	CD-NE	5.61	1.54	1.46
1	B	175	ARG	NE-CZ	5.61	1.39	1.33
1	H	207	ALA	C-N	5.61	1.41	1.33
1	I	246	ARG	CZ-NH1	5.61	1.40	1.32
1	I	260	THR	C-N	5.60	1.41	1.33
1	B	259	GLN	N-CA	-5.60	1.39	1.46
1	D	190	GLN	N-CA	-5.60	1.39	1.46
1	L	72	GLY	CA-C	-5.60	1.45	1.52
1	C	199	GLN	N-CA	5.60	1.53	1.46
1	I	288	ARG	CZ-NH2	5.59	1.40	1.33
1	G	122	GLU	CA-CB	5.59	1.62	1.54
1	J	275	HIS	CA-C	-5.59	1.45	1.52
1	K	81	TYR	CA-CB	5.59	1.62	1.53
1	E	166	ASP	CA-C	-5.59	1.45	1.52
1	B	164	GLU	C-N	5.58	1.41	1.33
1	L	98	ARG	NE-CZ	5.58	1.39	1.33
1	H	143	GLY	C-N	5.58	1.41	1.33
1	G	150	GLN	CA-C	-5.58	1.45	1.52
1	E	246	ARG	CD-NE	5.57	1.54	1.46
1	F	246	ARG	CZ-NH2	-5.57	1.26	1.33
1	L	60	ALA	CA-C	-5.56	1.45	1.52
1	F	82	GLY	C-N	5.56	1.41	1.34
1	B	187	VAL	C-N	5.56	1.41	1.33
1	J	98	ARG	NE-CZ	5.55	1.39	1.33
1	J	164	GLU	CA-C	-5.55	1.45	1.52
1	A	165	ARG	CA-C	-5.55	1.45	1.52
1	I	166	ASP	CA-C	-5.55	1.45	1.52
1	L	175	ARG	NE-CZ	5.55	1.39	1.33
1	L	183	ARG	CD-NE	5.55	1.54	1.46
1	G	64	GLN	C-N	5.54	1.40	1.33
1	K	129	GLN	C-N	5.54	1.40	1.33
1	E	155	VAL	CA-C	5.54	1.60	1.52
1	C	166	ASP	N-CA	-5.54	1.39	1.46
1	F	128	GLN	C-N	5.54	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	288	ARG	CA-C	-5.53	1.45	1.52
1	F	181	SER	CA-CB	5.53	1.62	1.53
1	G	288	ARG	CD-NE	5.52	1.53	1.46
1	C	279	TYR	CG-CD1	5.52	1.50	1.39
1	H	165	ARG	CD-NE	5.52	1.53	1.46
1	D	167	LEU	N-CA	-5.52	1.39	1.46
1	E	254	TYR	C-N	5.52	1.41	1.34
1	E	107	ALA	N-CA	-5.52	1.39	1.46
1	K	136	TYR	N-CA	-5.52	1.39	1.46
1	J	232	GLY	CA-C	-5.52	1.45	1.52
1	B	218	GLN	C-N	5.51	1.40	1.33
1	H	58	SER	CA-C	-5.51	1.46	1.52
1	F	176	LYS	C-N	5.51	1.41	1.33
1	F	183	ARG	CA-C	-5.51	1.45	1.52
1	B	246	ARG	CA-C	-5.51	1.45	1.52
1	D	61	ILE	N-CA	-5.51	1.39	1.46
1	H	277	TYR	CA-C	-5.51	1.46	1.52
1	I	110	LEU	CA-CB	5.51	1.61	1.53
1	B	244	ALA	N-CA	-5.50	1.39	1.46
1	C	225	GLN	CA-CB	5.50	1.62	1.53
1	G	279	TYR	CA-C	-5.50	1.46	1.52
1	A	198	ARG	CA-C	-5.50	1.45	1.52
1	H	290	ASP	N-CA	-5.50	1.38	1.46
1	B	93	GLU	C-N	5.50	1.41	1.33
1	H	98	ARG	CA-CB	5.49	1.62	1.53
1	A	233	SER	C-N	5.49	1.40	1.33
1	H	225	GLN	N-CA	5.49	1.53	1.46
1	F	205	ARG	C-N	5.48	1.40	1.33
1	K	141	ALA	CA-C	-5.48	1.45	1.52
1	D	225	GLN	N-CA	5.47	1.52	1.46
1	B	192	GLN	N-CA	-5.47	1.39	1.46
1	I	247	PRO	N-CA	-5.47	1.40	1.47
1	A	289	ARG	CZ-NH2	5.47	1.40	1.33
1	A	270	THR	CA-C	-5.46	1.46	1.52
1	E	162	GLU	N-CA	5.46	1.53	1.46
1	K	76	ALA	CA-C	-5.46	1.45	1.52
1	K	107	ALA	CA-C	-5.46	1.45	1.52
1	I	86	PRO	C-N	5.46	1.41	1.33
1	D	68	GLY	N-CA	5.45	1.52	1.45
1	H	87	LYS	CA-C	-5.45	1.45	1.53
1	H	117	GLU	CA-C	-5.45	1.46	1.52
1	E	114	GLU	CA-C	-5.44	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	66	ASP	N-CA	-5.44	1.39	1.46
1	G	58	SER	N-CA	-5.44	1.39	1.45
1	G	246	ARG	CD-NE	5.44	1.53	1.46
1	H	173	LEU	C-N	5.44	1.41	1.33
1	I	60	ALA	CA-C	-5.44	1.45	1.52
1	J	242	ASN	CA-CB	5.44	1.61	1.53
1	L	88	VAL	C-O	5.44	1.30	1.24
1	C	196	ARG	NE-CZ	5.44	1.39	1.33
1	H	221	GLN	CA-C	-5.44	1.45	1.53
1	I	75	ASN	CA-C	-5.44	1.45	1.52
1	I	200	ILE	N-CA	-5.43	1.39	1.46
1	K	196	ARG	NE-CZ	5.43	1.39	1.33
1	D	117	GLU	C-N	5.43	1.41	1.33
1	K	210	ALA	C-N	5.43	1.41	1.33
1	F	227	THR	N-CA	-5.43	1.40	1.46
1	K	289	ARG	CD-NE	5.43	1.53	1.46
1	K	175	ARG	C-N	5.42	1.41	1.33
1	I	106	LEU	CB-CG	5.42	1.64	1.53
1	I	136	TYR	CA-C	5.42	1.59	1.52
1	K	150	GLN	CA-C	-5.42	1.45	1.52
1	A	141	ALA	C-N	5.42	1.41	1.33
1	I	216	GLN	CA-CB	-5.42	1.44	1.53
1	A	130	LEU	CA-C	5.41	1.58	1.52
1	G	227	THR	C-N	5.41	1.41	1.34
1	A	75	ASN	N-CA	-5.40	1.39	1.46
1	D	138	GLY	C-N	5.40	1.41	1.33
1	L	71	ALA	C-N	5.40	1.41	1.33
1	L	183	ARG	NE-CZ	5.40	1.39	1.33
1	G	111	ASP	CA-C	-5.40	1.45	1.52
1	G	288	ARG	CZ-NH1	5.40	1.40	1.32
1	B	206	TYR	C-N	5.39	1.41	1.33
1	B	111	ASP	CA-CB	5.39	1.61	1.53
1	K	284	THR	C-O	5.39	1.30	1.23
1	L	94	THR	C-N	5.39	1.40	1.33
1	C	136	TYR	C-N	5.39	1.40	1.33
1	G	206	TYR	C-N	5.39	1.41	1.33
1	G	198	ARG	CD-NE	5.38	1.53	1.46
1	H	80	ILE	CA-C	-5.38	1.46	1.52
1	I	89	SER	N-CA	-5.38	1.39	1.46
1	D	92	GLN	CA-C	-5.38	1.45	1.52
1	G	176	LYS	CA-CB	5.38	1.61	1.53
1	I	80	ILE	N-CA	5.38	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	204	LEU	C-N	5.38	1.41	1.33
1	A	265	LYS	CA-CB	5.37	1.62	1.53
1	L	228	MET	CA-C	-5.37	1.45	1.52
1	A	178	LEU	C-N	5.37	1.41	1.33
1	B	266	ASN	CA-C	-5.37	1.45	1.52
1	F	175	ARG	C-N	5.37	1.41	1.33
1	C	231	LEU	N-CA	-5.37	1.39	1.46
1	H	61	ILE	CA-C	-5.37	1.46	1.52
1	G	107	ALA	CA-C	-5.37	1.45	1.52
1	G	269	VAL	CA-CB	-5.36	1.46	1.54
1	I	198	ARG	C-N	5.36	1.41	1.33
1	K	184	THR	CA-C	-5.36	1.45	1.52
1	G	219	GLN	CA-C	-5.36	1.46	1.52
1	J	286	PRO	N-CA	5.36	1.52	1.46
1	G	165	ARG	CZ-NH2	5.35	1.40	1.33
1	L	198	ARG	CZ-NH1	5.35	1.40	1.32
1	J	243	GLU	C-N	5.34	1.40	1.33
1	I	276	VAL	C-N	5.34	1.40	1.33
1	F	126	LYS	CA-CB	5.34	1.62	1.53
1	I	278	ARG	CD-NE	5.33	1.53	1.46
1	L	212	ILE	CA-C	-5.33	1.45	1.52
1	H	181	SER	C-O	-5.33	1.17	1.24
1	I	203	ALA	C-N	5.33	1.41	1.33
1	J	86	PRO	CA-C	-5.33	1.44	1.52
1	F	91	LEU	CA-CB	5.33	1.61	1.53
1	F	68	GLY	CA-C	-5.33	1.46	1.52
1	D	278	ARG	NE-CZ	5.33	1.39	1.33
1	K	58	SER	N-CA	-5.33	1.39	1.46
1	J	220	THR	CA-CB	-5.32	1.45	1.53
1	I	98	ARG	CA-CB	5.32	1.61	1.53
1	A	70	ILE	CA-C	-5.32	1.46	1.52
1	C	118	LYS	C-N	5.32	1.41	1.33
1	H	203	ALA	N-CA	-5.32	1.39	1.46
1	A	99	PHE	CA-C	-5.32	1.46	1.52
1	I	140	THR	C-N	5.32	1.40	1.33
1	K	109	THR	C-N	5.31	1.41	1.34
1	A	128	GLN	CA-C	-5.31	1.47	1.53
1	J	191	GLU	C-N	5.31	1.41	1.33
1	E	236	LEU	C-N	5.31	1.40	1.33
1	G	128	GLN	N-CA	5.31	1.52	1.46
1	B	107	ALA	CA-C	-5.30	1.45	1.52
1	E	186	GLU	C-N	5.29	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	192	GLN	C-N	5.29	1.40	1.33
1	F	218	GLN	CA-CB	5.29	1.62	1.54
1	A	163	LEU	CA-C	-5.29	1.46	1.52
1	J	278	ARG	C-O	-5.29	1.17	1.23
1	D	81	TYR	CZ-OH	5.29	1.49	1.38
1	H	149	ALA	CA-C	-5.29	1.46	1.52
1	I	102	ALA	CA-C	-5.29	1.46	1.52
1	F	74	ASN	CA-CB	5.28	1.61	1.53
1	K	193	LYS	CA-C	-5.28	1.46	1.52
1	A	133	THR	CA-C	-5.28	1.46	1.52
1	E	206	TYR	C-N	5.28	1.40	1.33
1	E	143	GLY	C-N	5.28	1.41	1.33
1	G	194	ASP	CA-C	-5.28	1.46	1.52
1	K	61	ILE	C-N	5.28	1.40	1.33
1	B	165	ARG	NE-CZ	5.27	1.38	1.33
1	D	106	LEU	CA-CB	-5.27	1.44	1.53
1	G	165	ARG	CZ-NH1	5.27	1.40	1.32
1	H	273	THR	CA-C	-5.27	1.46	1.52
1	E	176	LYS	CA-CB	5.27	1.61	1.53
1	I	102	ALA	C-N	5.27	1.41	1.33
1	E	175	ARG	CZ-NH2	5.27	1.40	1.33
1	C	275	HIS	CG-ND1	5.26	1.44	1.38
1	E	262	LEU	N-CA	-5.26	1.40	1.46
1	H	239	MET	C-N	5.26	1.40	1.33
1	I	289	ARG	C-N	5.26	1.40	1.33
1	D	89	SER	C-N	5.26	1.41	1.33
1	B	136	TYR	C-O	-5.26	1.17	1.23
1	A	150	GLN	CD-NE2	5.26	1.44	1.33
1	A	194	ASP	C-N	5.26	1.41	1.33
1	C	132	LEU	C-O	-5.26	1.17	1.24
1	I	242	ASN	CA-CB	5.25	1.60	1.52
1	I	288	ARG	C-N	5.25	1.40	1.33
1	G	183	ARG	C-O	-5.25	1.18	1.24
1	H	260	THR	C-N	5.25	1.40	1.33
1	A	196	ARG	CA-CB	5.25	1.61	1.53
1	C	74	ASN	C-N	5.25	1.40	1.33
1	J	232	GLY	N-CA	-5.25	1.38	1.45
1	D	205	ARG	NE-CZ	5.24	1.38	1.33
1	F	147	LYS	C-N	5.24	1.41	1.33
1	L	264	ILE	C-N	5.24	1.41	1.34
1	K	113	GLN	CA-CB	5.24	1.62	1.53
1	A	107	ALA	CA-C	5.24	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	61	ILE	C-N	5.24	1.40	1.33
1	B	278	ARG	CZ-NH2	5.24	1.40	1.33
1	K	283	PRO	CA-CB	5.24	1.60	1.53
1	G	115	GLU	CA-CB	5.24	1.61	1.53
1	H	128	GLN	CA-CB	5.24	1.61	1.53
1	C	67	VAL	CA-C	-5.23	1.46	1.52
1	H	142	GLU	C-N	5.23	1.40	1.33
1	F	118	LYS	N-CA	5.23	1.52	1.46
1	D	219	GLN	N-CA	-5.22	1.39	1.45
1	E	212	ILE	N-CA	-5.22	1.39	1.46
1	F	271	ALA	CA-C	-5.22	1.46	1.52
1	H	81	TYR	CZ-OH	5.22	1.49	1.38
1	H	278	ARG	CA-C	-5.22	1.46	1.52
1	L	173	LEU	C-N	5.22	1.40	1.33
1	J	183	ARG	NE-CZ	5.22	1.38	1.33
1	B	210	ALA	CA-C	-5.22	1.45	1.52
1	C	135	SER	N-CA	-5.22	1.39	1.45
1	K	109	THR	N-CA	-5.22	1.40	1.46
1	E	257	THR	C-N	5.22	1.40	1.33
1	L	61	ILE	CA-C	-5.22	1.46	1.52
1	E	261	LEU	C-N	5.21	1.40	1.33
1	L	157	ASP	C-N	5.21	1.40	1.33
1	A	242	ASN	CA-CB	5.21	1.60	1.52
1	F	266	ASN	C-N	5.20	1.40	1.33
1	K	87	LYS	CA-C	-5.20	1.45	1.52
1	J	64	GLN	N-CA	-5.20	1.38	1.46
1	C	182	LEU	C-N	5.20	1.40	1.33
1	B	109	THR	C-N	5.20	1.40	1.33
1	D	174	GLY	C-N	5.20	1.41	1.33
1	G	217	ILE	N-CA	-5.20	1.38	1.45
1	K	235	ALA	CA-C	-5.20	1.46	1.52
1	D	159	VAL	C-N	5.19	1.40	1.33
1	F	219	GLN	C-N	5.19	1.40	1.33
1	G	277	TYR	CA-C	-5.19	1.46	1.52
1	H	71	ALA	N-CA	-5.19	1.40	1.46
1	J	136	TYR	CA-C	5.18	1.58	1.52
1	F	276	VAL	CA-C	-5.18	1.46	1.52
1	L	248	LEU	N-CA	-5.18	1.39	1.46
1	L	278	ARG	CD-NE	5.18	1.53	1.46
1	K	165	ARG	CZ-NH1	5.17	1.40	1.32
1	J	288	ARG	CZ-NH1	5.17	1.40	1.32
1	K	90	ASP	C-N	5.17	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	184	THR	C-N	5.17	1.40	1.33
1	A	217	ILE	CA-C	-5.17	1.46	1.52
1	H	219	GLN	C-N	5.17	1.40	1.33
1	C	204	LEU	CA-CB	5.17	1.61	1.53
1	E	146	MET	CA-CB	5.16	1.61	1.53
1	I	289	ARG	CA-C	-5.16	1.46	1.52
1	K	196	ARG	CD-NE	5.16	1.53	1.46
1	E	162	GLU	CA-CB	-5.16	1.45	1.53
1	B	149	ALA	CA-C	-5.16	1.46	1.52
1	D	221	GLN	C-N	5.16	1.40	1.33
1	J	92	GLN	CA-C	-5.16	1.46	1.52
1	D	144	ALA	N-CA	-5.16	1.40	1.46
1	J	245	THR	C-N	5.16	1.41	1.33
1	E	165	ARG	CA-C	5.15	1.59	1.52
1	G	205	ARG	CD-NE	5.15	1.53	1.46
1	C	68	GLY	N-CA	-5.15	1.39	1.45
1	F	162	GLU	N-CA	5.15	1.52	1.46
1	C	267	LEU	CA-C	-5.15	1.46	1.52
1	G	148	LEU	CA-CB	5.15	1.61	1.53
1	A	135	SER	N-CA	-5.15	1.39	1.45
1	B	204	LEU	C-N	5.15	1.40	1.33
1	F	61	ILE	N-CA	5.14	1.52	1.46
1	H	162	GLU	CA-C	-5.14	1.46	1.52
1	A	219	GLN	CA-C	-5.14	1.46	1.52
1	C	210	ALA	N-CA	-5.14	1.39	1.46
1	F	178	LEU	C-N	5.14	1.40	1.33
1	K	100	SER	CA-CB	5.14	1.61	1.53
1	H	116	PRO	N-CD	-5.14	1.40	1.47
1	L	269	VAL	C-N	5.14	1.40	1.33
1	C	235	ALA	C-N	5.13	1.40	1.33
1	C	261	LEU	C-N	5.13	1.40	1.33
1	G	121	ILE	CA-C	-5.13	1.46	1.52
1	F	230	LEU	N-CA	-5.13	1.39	1.46
1	I	138	GLY	CA-C	-5.13	1.47	1.52
1	G	270	THR	CA-CB	-5.13	1.45	1.53
1	I	177	ASN	CA-CB	5.13	1.61	1.53
1	B	229	PHE	CA-C	5.13	1.59	1.52
1	I	56	TRP	C-O	5.13	1.30	1.23
1	A	150	GLN	C-O	-5.13	1.18	1.24
1	B	158	LYS	CA-C	-5.13	1.46	1.52
1	C	183	ARG	CZ-NH1	5.13	1.40	1.32
1	J	226	ASP	N-CA	-5.13	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	206	TYR	C-N	5.12	1.40	1.33
1	G	157	ASP	N-CA	5.12	1.52	1.46
1	K	176	LYS	CA-C	5.12	1.59	1.52
1	L	246	ARG	CA-C	5.12	1.58	1.53
1	J	161	GLN	C-N	5.12	1.40	1.33
1	K	285	LEU	C-N	5.12	1.39	1.33
1	C	167	LEU	C-N	5.12	1.40	1.33
1	B	246	ARG	CZ-NH1	5.11	1.40	1.32
1	I	183	ARG	C-N	5.11	1.40	1.33
1	H	111	ASP	N-CA	-5.11	1.40	1.46
1	B	287	VAL	CA-CB	-5.11	1.48	1.54
1	I	101	SER	N-CA	-5.11	1.40	1.46
1	J	131	PRO	CA-CB	-5.11	1.46	1.53
1	E	198	ARG	CZ-NH2	5.10	1.40	1.33
1	D	57	THR	C-O	-5.10	1.17	1.24
1	H	253	ALA	N-CA	-5.10	1.40	1.46
1	L	246	ARG	CA-CB	5.10	1.60	1.53
1	E	217	ILE	CA-C	-5.09	1.46	1.52
1	D	174	GLY	CA-C	-5.09	1.46	1.52
1	G	118	LYS	CA-C	-5.09	1.46	1.52
1	F	198	ARG	CZ-NH1	5.09	1.39	1.32
1	G	82	GLY	C-N	5.09	1.41	1.34
1	K	107	ALA	N-CA	-5.09	1.40	1.46
1	C	149	ALA	N-CA	-5.09	1.40	1.46
1	D	124	SER	N-CA	-5.09	1.39	1.46
1	I	177	ASN	C-O	-5.08	1.18	1.24
1	I	98	ARG	CD-NE	5.08	1.53	1.46
1	A	208	ASP	CA-CB	5.08	1.61	1.53
1	E	285	LEU	CA-CB	5.08	1.63	1.53
1	H	64	GLN	CA-CB	5.07	1.61	1.53
1	H	77	MET	C-N	5.07	1.40	1.33
1	K	112	ASN	CA-C	-5.07	1.46	1.52
1	L	175	ARG	CD-NE	5.07	1.53	1.46
1	L	137	VAL	N-CA	-5.07	1.40	1.46
1	C	281	MET	C-N	5.07	1.42	1.33
1	F	262	LEU	CA-CB	5.07	1.61	1.53
1	L	164	GLU	CA-CB	-5.07	1.45	1.53
1	A	215	PRO	CA-C	-5.06	1.46	1.52
1	E	89	SER	N-CA	-5.06	1.40	1.46
1	G	196	ARG	NE-CZ	5.06	1.38	1.33
1	L	115	GLU	CA-CB	5.06	1.59	1.53
1	E	77	MET	C-O	-5.06	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	227	THR	CA-CB	-5.06	1.47	1.54
1	C	191	GLU	C-N	5.06	1.40	1.33
1	F	184	THR	CA-C	-5.06	1.46	1.52
1	D	136	TYR	C-N	5.05	1.41	1.33
1	J	103	PHE	CA-CB	5.05	1.61	1.53
1	A	250	PHE	N-CA	-5.05	1.39	1.46
1	I	114	GLU	CA-C	-5.05	1.45	1.52
1	J	283	PRO	C-N	5.05	1.40	1.33
1	L	218	GLN	C-N	5.05	1.39	1.33
1	J	278	ARG	CZ-NH1	5.04	1.39	1.32
1	A	103	PHE	CA-CB	5.04	1.61	1.53
1	A	159	VAL	N-CA	-5.04	1.40	1.46
1	H	65	PRO	CA-C	-5.04	1.46	1.52
1	K	86	PRO	CA-CB	-5.04	1.45	1.53
1	K	102	ALA	C-N	5.04	1.40	1.33
1	L	234	ASP	CA-CB	5.04	1.61	1.53
1	A	79	VAL	CA-CB	5.03	1.60	1.54
1	G	235	ALA	CA-C	-5.03	1.46	1.52
1	I	183	ARG	NE-CZ	5.03	1.38	1.33
1	A	93	GLU	CA-C	-5.03	1.46	1.52
1	A	189	ALA	N-CA	-5.03	1.40	1.46
1	J	111	ASP	C-N	5.03	1.40	1.33
1	B	236	LEU	CA-C	-5.03	1.46	1.52
1	G	165	ARG	NE-CZ	5.03	1.38	1.33
1	L	226	ASP	N-CA	-5.03	1.39	1.46
1	L	269	VAL	CA-C	-5.03	1.46	1.52
1	G	56	TRP	C-N	5.02	1.40	1.33
1	L	181	SER	N-CA	5.02	1.52	1.46
1	A	132	LEU	C-O	-5.02	1.17	1.24
1	G	195	LEU	N-CA	5.02	1.52	1.46
1	E	209	GLU	CA-C	5.01	1.59	1.52
1	I	202	GLU	C-N	5.01	1.40	1.33
1	K	274	VAL	CA-C	-5.01	1.47	1.52
1	I	128	GLN	CA-C	-5.01	1.46	1.52
1	F	289	ARG	CZ-NH1	5.01	1.39	1.32
1	E	136	TYR	CA-C	-5.01	1.46	1.52
1	C	229	PHE	CA-C	-5.00	1.45	1.52
1	C	220	THR	C-N	5.00	1.40	1.33
1	E	91	LEU	C-N	5.00	1.40	1.33
1	A	155	VAL	C-O	-5.00	1.18	1.24
1	F	91	LEU	CA-C	-5.00	1.46	1.52
1	F	226	ASP	CA-CB	5.00	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	191	GLU	N-CA	-5.00	1.40	1.46
1	L	107	ALA	C-N	5.00	1.40	1.33

All (1700) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	276	VAL	N-CA-C	-13.10	100.38	112.43
1	D	92	GLN	OE1-CD-NE2	12.56	135.16	122.60
1	B	290	ASP	N-CA-C	-11.96	100.98	114.62
1	E	106	LEU	CA-C-N	11.81	136.11	120.28
1	E	106	LEU	C-N-CA	11.81	136.11	120.28
1	E	221	GLN	OE1-CD-NE2	11.15	133.75	122.60
1	L	130	LEU	CB-CA-C	10.89	120.95	110.71
1	F	266	ASN	N-CA-C	10.83	123.17	111.36
1	K	251	SER	CA-C-N	10.67	131.02	119.28
1	K	251	SER	C-N-CA	10.67	131.02	119.28
1	J	125	VAL	N-CA-C	-10.64	102.64	112.43
1	I	214	GLN	O-C-N	10.57	128.48	121.71
1	F	128	GLN	OE1-CD-NE2	10.52	133.12	122.60
1	K	259	GLN	CA-C-O	-10.48	109.81	120.82
1	I	122	GLU	O-C-N	-10.25	113.84	121.83
1	J	64	GLN	CA-C-N	10.25	132.65	119.84
1	J	64	GLN	C-N-CA	10.25	132.65	119.84
1	A	78	ASN	CA-CB-CG	-10.18	102.42	112.60
1	B	227	THR	CA-C-N	10.11	134.23	120.38
1	B	227	THR	C-N-CA	10.11	134.23	120.38
1	B	130	LEU	CB-CA-C	-10.06	100.21	110.17
1	K	259	GLN	O-C-N	10.06	132.43	122.07
1	H	103	PHE	CA-CB-CG	-9.97	103.83	113.80
1	B	224	THR	CA-C-N	9.93	133.59	120.28
1	B	224	THR	C-N-CA	9.93	133.59	120.28
1	J	111	ASP	CA-C-N	9.81	133.42	120.28
1	J	111	ASP	C-N-CA	9.81	133.42	120.28
1	K	95	LEU	CB-CA-C	-9.74	95.59	110.88
1	G	66	ASP	CA-CB-CG	-9.74	102.86	112.60
1	I	234	ASP	CA-CB-CG	-9.62	102.98	112.60
1	F	280	VAL	N-CA-C	-9.60	100.54	111.00
1	E	151	TYR	CA-C-O	-9.60	110.25	120.42
1	C	276	VAL	N-CA-C	-9.40	103.87	112.90
1	B	161	GLN	N-CA-C	9.29	121.41	111.28
1	G	95	LEU	N-CA-CB	9.29	123.55	110.07
1	B	283	PRO	CA-C-O	9.27	131.00	121.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	74	ASN	CA-CB-CG	9.26	121.86	112.60
1	K	273	THR	N-CA-C	-9.25	100.95	112.88
1	G	282	LYS	CA-C-O	-9.22	111.14	120.64
1	L	88	VAL	N-CA-C	9.18	119.99	110.62
1	J	223	VAL	CA-C-O	-9.15	113.59	121.09
1	I	165	ARG	NE-CZ-NH1	9.12	130.62	121.50
1	J	169	ASP	CA-CB-CG	8.99	121.59	112.60
1	E	229	PHE	CA-CB-CG	8.98	122.78	113.80
1	L	84	ALA	CA-C-N	8.97	134.33	120.60
1	L	84	ALA	C-N-CA	8.97	134.33	120.60
1	C	142	GLU	CA-C-N	8.88	129.84	119.98
1	C	142	GLU	C-N-CA	8.88	129.84	119.98
1	H	82	GLY	CA-C-N	8.88	133.06	120.28
1	H	82	GLY	C-N-CA	8.88	133.06	120.28
1	I	271	ALA	N-CA-C	-8.87	98.71	112.99
1	B	67	VAL	CA-C-N	8.83	131.18	120.14
1	B	67	VAL	C-N-CA	8.83	131.18	120.14
1	H	208	ASP	CA-CB-CG	8.83	121.43	112.60
1	A	76	ALA	CA-C-O	-8.77	111.67	120.70
1	H	124	SER	N-CA-C	8.75	122.60	110.35
1	I	142	GLU	CA-C-N	8.75	129.48	119.94
1	I	142	GLU	C-N-CA	8.75	129.48	119.94
1	K	208	ASP	CB-CA-C	-8.74	96.28	110.79
1	H	112	ASN	OD1-CG-ND2	8.72	131.32	122.60
1	E	175	ARG	CA-C-O	-8.71	111.31	120.55
1	B	219	GLN	O-C-N	8.71	132.72	122.79
1	I	232	GLY	CA-C-N	8.69	133.52	120.31
1	I	232	GLY	C-N-CA	8.69	133.52	120.31
1	C	115	GLU	CA-C-O	-8.68	112.04	119.76
1	C	154	GLN	CA-C-O	-8.61	111.42	120.55
1	I	242	ASN	CA-CB-CG	-8.60	104.00	112.60
1	E	71	ALA	CA-C-N	8.59	129.51	119.98
1	E	71	ALA	C-N-CA	8.59	129.51	119.98
1	D	177	ASN	CA-C-N	8.47	131.97	120.44
1	D	177	ASN	C-N-CA	8.47	131.97	120.44
1	L	121	ILE	N-CA-C	-8.45	95.94	108.45
1	K	234	ASP	CA-CB-CG	-8.45	104.15	112.60
1	E	275	HIS	CA-CB-CG	-8.44	105.36	113.80
1	B	66	ASP	CA-C-N	8.42	131.99	120.46
1	B	66	ASP	C-N-CA	8.42	131.99	120.46
1	J	273	THR	N-CA-C	-8.40	102.04	112.88
1	D	134	VAL	N-CA-C	-8.40	95.92	108.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	GLN	CB-CA-C	-8.39	96.85	110.79
1	K	218	GLN	N-CA-C	-8.39	102.05	112.88
1	E	71	ALA	O-C-N	-8.39	113.23	122.12
1	C	78	ASN	CA-CB-CG	-8.39	104.21	112.60
1	L	71	ALA	CA-C-N	8.39	129.29	119.98
1	L	71	ALA	C-N-CA	8.39	129.29	119.98
1	B	214	GLN	CA-C-N	8.36	128.67	119.90
1	B	214	GLN	C-N-CA	8.36	128.67	119.90
1	G	287	VAL	N-CA-C	-8.36	103.64	113.42
1	E	72	GLY	CA-C-N	8.35	131.80	120.44
1	E	72	GLY	C-N-CA	8.35	131.80	120.44
1	A	246	ARG	CA-C-N	8.32	128.38	119.89
1	A	246	ARG	C-N-CA	8.32	128.38	119.89
1	D	237	LYS	N-CA-CB	8.30	122.32	110.12
1	K	242	ASN	CA-CB-CG	-8.28	104.32	112.60
1	J	246	ARG	CA-C-N	8.28	130.19	119.84
1	J	246	ARG	C-N-CA	8.28	130.19	119.84
1	D	252	PRO	CA-C-N	8.26	131.35	120.28
1	D	252	PRO	C-N-CA	8.26	131.35	120.28
1	C	219	GLN	OE1-CD-NE2	8.24	130.84	122.60
1	A	125	VAL	N-CA-C	-8.22	105.17	113.47
1	H	206	TYR	CA-C-N	8.22	131.30	120.28
1	H	206	TYR	C-N-CA	8.22	131.30	120.28
1	A	206	TYR	CB-CA-C	-8.22	96.88	110.85
1	G	106	LEU	CA-C-N	8.20	131.26	120.28
1	G	106	LEU	C-N-CA	8.20	131.26	120.28
1	C	108	GLU	N-CA-C	8.18	119.82	111.07
1	G	280	VAL	CB-CA-C	-8.17	101.29	112.24
1	F	73	TYR	CB-CA-C	-8.16	98.07	110.88
1	C	290	ASP	CA-C-O	8.15	126.76	119.34
1	I	118	LYS	CA-C-O	-8.13	111.37	120.32
1	A	111	ASP	CA-C-O	-8.13	111.93	120.55
1	G	180	ASP	CA-CB-CG	8.13	120.73	112.60
1	I	96	ILE	CA-C-N	8.13	129.00	119.98
1	I	96	ILE	C-N-CA	8.13	129.00	119.98
1	E	157	ASP	CA-C-N	8.10	130.97	120.44
1	E	157	ASP	C-N-CA	8.10	130.97	120.44
1	K	284	THR	N-CA-C	-8.10	97.01	109.24
1	D	225	GLN	CA-C-N	8.10	131.13	120.28
1	D	225	GLN	C-N-CA	8.10	131.13	120.28
1	E	203	ALA	CA-C-N	8.10	130.96	120.44
1	E	203	ALA	C-N-CA	8.10	130.96	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	202	GLU	CA-C-N	8.09	131.12	120.28
1	K	202	GLU	C-N-CA	8.09	131.12	120.28
1	L	108	GLU	CB-CG-CD	-8.09	98.84	112.60
1	D	72	GLY	CA-C-N	8.08	131.76	120.29
1	D	72	GLY	C-N-CA	8.08	131.76	120.29
1	F	228	MET	CG-SD-CE	-8.07	83.15	100.90
1	B	208	ASP	CA-C-N	8.05	131.72	120.29
1	B	208	ASP	C-N-CA	8.05	131.72	120.29
1	E	166	ASP	CA-C-N	8.04	131.71	120.29
1	E	166	ASP	C-N-CA	8.04	131.71	120.29
1	G	179	GLN	OE1-CD-NE2	8.04	130.64	122.60
1	J	241	GLN	OE1-CD-NE2	-8.04	114.56	122.60
1	K	87	LYS	CA-C-N	8.04	131.47	120.46
1	K	87	LYS	C-N-CA	8.04	131.47	120.46
1	K	182	LEU	N-CA-C	-8.04	102.60	111.36
1	I	275	HIS	ND1-CE1-NE2	8.02	116.42	108.40
1	J	225	GLN	CA-C-N	8.00	131.35	120.38
1	J	225	GLN	C-N-CA	8.00	131.35	120.38
1	B	235	ALA	CA-C-N	8.00	131.00	120.28
1	B	235	ALA	C-N-CA	8.00	131.00	120.28
1	L	232	GLY	CA-C-N	8.00	131.80	120.28
1	L	232	GLY	C-N-CA	8.00	131.80	120.28
1	K	166	ASP	CA-C-O	8.00	128.90	120.42
1	H	214	GLN	O-C-N	-7.99	114.53	121.32
1	F	188	VAL	CA-C-N	7.98	130.98	120.28
1	F	188	VAL	C-N-CA	7.98	130.98	120.28
1	F	266	ASN	CA-CB-CG	7.98	120.58	112.60
1	L	152	ILE	CA-C-N	7.98	130.97	120.28
1	L	152	ILE	C-N-CA	7.98	130.97	120.28
1	K	141	ALA	CA-C-N	7.97	131.61	120.29
1	K	141	ALA	C-N-CA	7.97	131.61	120.29
1	F	115	GLU	CA-C-O	-7.96	112.11	120.87
1	E	82	GLY	CA-C-N	7.92	131.69	120.28
1	E	82	GLY	C-N-CA	7.92	131.69	120.28
1	J	232	GLY	CA-C-N	7.91	131.67	120.28
1	J	232	GLY	C-N-CA	7.91	131.67	120.28
1	J	187	VAL	CB-CA-C	-7.90	101.85	111.97
1	I	214	GLN	CA-C-N	7.89	129.71	119.84
1	I	214	GLN	C-N-CA	7.89	129.71	119.84
1	J	137	VAL	CA-C-O	-7.88	112.12	120.48
1	I	138	GLY	O-C-N	-7.88	116.74	123.60
1	J	96	ILE	CA-C-N	7.86	128.70	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	96	ILE	C-N-CA	7.86	128.70	119.98
1	G	185	GLN	N-CA-C	7.84	119.83	111.28
1	I	67	VAL	CA-C-N	7.84	128.68	119.98
1	I	67	VAL	C-N-CA	7.84	128.68	119.98
1	D	285	LEU	CA-C-N	7.83	128.30	119.92
1	D	285	LEU	C-N-CA	7.83	128.30	119.92
1	G	148	LEU	CA-C-O	-7.83	112.60	120.82
1	D	149	ALA	CA-C-N	7.82	130.76	120.28
1	D	149	ALA	C-N-CA	7.82	130.76	120.28
1	G	190	GLN	O-C-N	-7.81	113.84	122.12
1	K	79	VAL	O-C-N	7.80	129.56	121.91
1	F	255	TYR	CA-C-N	7.78	130.70	120.28
1	F	255	TYR	C-N-CA	7.78	130.70	120.28
1	F	249	ALA	N-CA-CB	7.78	122.99	110.16
1	B	290	ASP	CA-CB-CG	-7.76	104.84	112.60
1	C	244	ALA	CA-C-N	7.76	132.11	120.31
1	C	244	ALA	C-N-CA	7.76	132.11	120.31
1	K	159	VAL	N-CA-CB	7.75	121.08	110.54
1	D	212	ILE	N-CA-C	-7.75	96.43	107.75
1	B	106	LEU	CA-C-N	7.74	130.65	120.28
1	B	106	LEU	C-N-CA	7.74	130.65	120.28
1	E	96	ILE	N-CA-CB	7.73	121.06	110.54
1	F	199	GLN	CB-CG-CD	-7.72	99.47	112.60
1	K	66	ASP	CA-C-N	7.70	131.35	120.42
1	K	66	ASP	C-N-CA	7.70	131.35	120.42
1	C	226	ASP	N-CA-C	7.69	120.74	111.82
1	K	88	VAL	N-CA-CB	7.69	121.00	110.54
1	E	134	VAL	N-CA-C	-7.68	97.02	108.85
1	F	224	THR	CA-C-N	7.68	130.58	120.28
1	F	224	THR	C-N-CA	7.68	130.58	120.28
1	C	116	PRO	N-CA-CB	7.67	110.00	103.17
1	D	89	SER	N-CA-CB	7.67	121.39	110.12
1	G	200	ILE	CA-C-O	-7.66	112.73	120.85
1	H	200	ILE	N-CA-CB	7.64	120.93	110.54
1	E	277	TYR	O-C-N	-7.64	115.24	123.26
1	I	106	LEU	N-CA-CB	-7.63	98.90	110.12
1	L	227	THR	CA-C-N	7.63	131.26	120.28
1	L	227	THR	C-N-CA	7.63	131.26	120.28
1	K	58	SER	N-CA-C	-7.62	97.26	109.76
1	L	104	SER	N-CA-CB	7.62	121.32	110.12
1	C	116	PRO	CA-C-O	-7.61	113.28	121.27
1	G	188	VAL	CB-CA-C	-7.60	101.73	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	229	PHE	CA-C-N	7.60	131.22	120.28
1	H	229	PHE	C-N-CA	7.60	131.22	120.28
1	E	127	ASN	CA-CB-CG	-7.59	105.01	112.60
1	E	144	ALA	N-CA-C	-7.58	103.10	111.36
1	A	232	GLY	O-C-N	7.57	130.54	122.60
1	G	129	GLN	N-CA-CB	7.57	123.28	110.49
1	H	233	SER	CA-C-N	7.56	130.27	120.44
1	H	233	SER	C-N-CA	7.56	130.27	120.44
1	A	253	ALA	CA-C-N	7.56	130.41	120.28
1	A	253	ALA	C-N-CA	7.56	130.41	120.28
1	A	274	VAL	CB-CA-C	7.55	120.96	111.15
1	B	122	GLU	N-CA-C	7.54	115.01	108.22
1	J	250	PHE	N-CA-C	-7.54	97.61	109.07
1	E	282	LYS	CA-C-N	7.53	127.58	119.90
1	E	282	LYS	C-N-CA	7.53	127.58	119.90
1	D	252	PRO	CB-CA-C	-7.52	101.12	112.11
1	F	104	SER	CA-C-O	-7.52	112.45	120.42
1	H	184	THR	CA-C-N	7.52	130.35	120.28
1	H	184	THR	C-N-CA	7.52	130.35	120.28
1	I	110	LEU	CA-C-O	-7.51	112.59	120.55
1	D	139	GLN	N-CA-C	-7.49	103.73	113.17
1	A	66	ASP	CA-C-N	7.48	131.05	120.42
1	A	66	ASP	C-N-CA	7.48	131.05	120.42
1	K	214	GLN	CA-C-O	-7.48	113.45	120.34
1	B	61	ILE	N-CA-C	-7.48	97.64	108.11
1	D	246	ARG	CA-C-N	7.47	127.51	119.89
1	D	246	ARG	C-N-CA	7.47	127.51	119.89
1	I	134	VAL	N-CA-C	-7.46	97.36	108.85
1	L	271	ALA	N-CA-C	-7.46	104.03	113.43
1	I	137	VAL	CA-C-N	7.46	128.08	121.82
1	I	137	VAL	C-N-CA	7.46	128.08	121.82
1	K	68	GLY	CA-C-N	7.45	130.87	120.29
1	K	68	GLY	C-N-CA	7.45	130.87	120.29
1	E	73	TYR	N-CA-C	-7.44	103.11	111.14
1	G	235	ALA	CA-C-N	7.44	130.11	120.44
1	G	235	ALA	C-N-CA	7.44	130.11	120.44
1	B	133	THR	CB-CA-C	7.39	122.50	109.72
1	E	191	GLU	CA-C-N	7.38	130.17	120.28
1	E	191	GLU	C-N-CA	7.38	130.17	120.28
1	D	130	LEU	O-C-N	-7.38	118.14	121.53
1	E	214	GLN	CB-CA-C	-7.38	100.48	110.22
1	E	216	GLN	N-CA-C	-7.37	104.31	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	242	ASN	OD1-CG-ND2	-7.37	115.23	122.60
1	H	78	ASN	CA-CB-CG	7.37	119.97	112.60
1	J	218	GLN	N-CA-C	7.36	119.95	111.11
1	L	227	THR	N-CA-C	-7.36	103.72	114.39
1	I	275	HIS	CE1-NE2-CD2	-7.36	101.64	109.00
1	C	121	ILE	N-CA-C	-7.36	97.56	108.45
1	G	223	VAL	CA-C-O	7.36	128.91	121.63
1	D	110	LEU	N-CA-C	7.35	119.38	111.36
1	G	273	THR	CA-C-O	7.35	128.62	119.95
1	A	181	SER	CA-C-O	7.34	128.20	120.42
1	B	234	ASP	CA-CB-CG	-7.34	105.26	112.60
1	D	178	LEU	N-CA-CB	7.34	120.71	110.07
1	C	167	LEU	CA-C-N	7.33	129.97	120.44
1	C	167	LEU	C-N-CA	7.33	129.97	120.44
1	C	112	ASN	OD1-CG-ND2	7.32	129.92	122.60
1	E	162	GLU	CA-C-O	-7.31	112.67	120.42
1	A	110	LEU	N-CA-C	7.31	119.25	111.28
1	A	115	GLU	CA-C-O	-7.30	113.12	120.64
1	I	189	ALA	CA-C-N	7.30	130.06	120.28
1	I	189	ALA	C-N-CA	7.30	130.06	120.28
1	H	83	GLN	CA-C-N	7.29	130.78	120.28
1	H	83	GLN	C-N-CA	7.29	130.78	120.28
1	I	212	ILE	CB-CA-C	7.28	121.41	110.63
1	E	63	THR	CA-CB-OG1	7.26	120.49	109.60
1	A	90	ASP	CA-CB-CG	-7.26	105.34	112.60
1	G	122	GLU	CA-C-O	-7.24	113.38	120.26
1	A	138	GLY	N-CA-C	-7.24	100.57	111.14
1	H	153	GLN	CA-C-N	7.23	129.97	120.28
1	H	153	GLN	C-N-CA	7.23	129.97	120.28
1	J	226	ASP	CA-C-O	-7.23	112.83	120.63
1	G	287	VAL	CA-C-O	-7.21	112.55	118.90
1	F	65	PRO	CB-CA-C	-7.20	101.83	111.12
1	I	212	ILE	N-CA-C	-7.20	98.03	108.11
1	B	197	ILE	O-C-N	7.20	128.85	121.87
1	B	137	VAL	CA-C-N	7.18	128.86	122.47
1	B	137	VAL	C-N-CA	7.18	128.86	122.47
1	H	125	VAL	N-CA-C	-7.17	105.83	112.43
1	K	81	TYR	N-CA-CB	7.17	120.89	110.20
1	J	184	THR	N-CA-CB	7.17	120.66	110.12
1	B	243	GLU	CA-C-O	7.16	128.01	120.42
1	I	203	ALA	CA-C-N	7.16	129.87	120.28
1	I	203	ALA	C-N-CA	7.16	129.87	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	185	GLN	OE1-CD-NE2	7.15	129.75	122.60
1	L	267	LEU	N-CA-C	7.15	120.36	110.35
1	F	75	ASN	CA-C-N	7.14	129.85	120.28
1	F	75	ASN	C-N-CA	7.14	129.85	120.28
1	E	68	GLY	O-C-N	7.13	129.04	122.19
1	H	129	GLN	N-CA-C	-7.12	96.95	109.06
1	I	217	ILE	CA-C-N	7.12	131.13	120.31
1	I	217	ILE	C-N-CA	7.12	131.13	120.31
1	D	92	GLN	CA-C-N	7.11	130.39	120.29
1	D	92	GLN	C-N-CA	7.11	130.39	120.29
1	A	163	LEU	CB-CA-C	-7.11	98.99	110.79
1	C	234	ASP	N-CA-CB	7.10	120.31	110.01
1	H	66	ASP	CA-CB-CG	-7.08	105.52	112.60
1	K	237	LYS	CA-C-O	-7.06	113.07	120.55
1	C	96	ILE	CA-C-N	7.05	127.81	119.98
1	C	96	ILE	C-N-CA	7.05	127.81	119.98
1	B	180	ASP	CA-CB-CG	-7.05	105.55	112.60
1	H	195	LEU	CA-C-N	7.04	129.71	120.28
1	H	195	LEU	C-N-CA	7.04	129.71	120.28
1	J	57	THR	O-C-N	-7.04	114.93	123.30
1	C	142	GLU	CB-CG-CD	7.02	124.54	112.60
1	I	159	VAL	N-CA-CB	7.02	120.09	110.54
1	D	179	GLN	O-C-N	-7.01	114.69	122.12
1	G	145	GLN	CA-C-O	-7.01	113.46	120.82
1	L	139	GLN	CA-C-O	7.01	127.14	119.15
1	L	122	GLU	N-CA-C	-7.01	101.91	108.22
1	A	287	VAL	O-C-N	7.00	131.32	122.57
1	B	179	GLN	O-C-N	-7.00	114.17	122.15
1	G	96	ILE	N-CA-C	-7.00	103.65	110.72
1	F	127	ASN	N-CA-C	-6.99	102.60	113.02
1	J	108	GLU	CA-C-O	-6.99	113.02	120.42
1	B	251	SER	CA-C-O	-6.98	113.73	120.64
1	B	77	MET	O-C-N	-6.97	114.73	122.12
1	D	75	ASN	N-CA-CB	6.97	120.36	110.12
1	H	64	GLN	OE1-CD-NE2	6.97	129.57	122.60
1	E	222	ASP	CA-CB-CG	-6.96	105.64	112.60
1	F	246	ARG	CA-C-O	-6.96	110.63	120.16
1	B	223	VAL	CA-C-N	6.94	131.24	120.75
1	B	223	VAL	C-N-CA	6.94	131.24	120.75
1	F	206	TYR	CA-C-N	6.93	129.57	120.28
1	F	206	TYR	C-N-CA	6.93	129.57	120.28
1	K	194	ASP	O-C-N	6.93	129.47	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	103	PHE	N-CA-CB	6.92	120.41	110.16
1	E	111	ASP	CA-CB-CG	6.92	119.52	112.60
1	D	224	THR	CA-C-N	6.92	129.55	120.28
1	D	224	THR	C-N-CA	6.92	129.55	120.28
1	E	64	GLN	N-CA-C	6.92	125.10	109.81
1	G	200	ILE	CA-C-N	6.92	129.55	120.28
1	G	200	ILE	C-N-CA	6.92	129.55	120.28
1	C	242	ASN	CA-CB-CG	-6.91	105.69	112.60
1	K	224	THR	N-CA-C	-6.91	96.09	110.80
1	G	283	PRO	N-CA-C	6.91	122.52	111.26
1	F	263	ASP	N-CA-C	6.90	118.88	111.36
1	I	227	THR	N-CA-C	-6.90	106.06	114.75
1	J	263	ASP	CA-C-O	-6.90	113.11	120.42
1	C	246	ARG	CA-C-N	6.90	128.46	119.84
1	C	246	ARG	C-N-CA	6.90	128.46	119.84
1	K	168	LYS	CA-C-N	6.89	130.08	120.29
1	K	168	LYS	C-N-CA	6.89	130.08	120.29
1	C	64	GLN	N-CA-C	6.87	119.39	109.84
1	D	282	LYS	CA-C-N	6.86	126.90	119.90
1	D	282	LYS	C-N-CA	6.86	126.90	119.90
1	E	152	ILE	O-C-N	6.86	128.89	121.83
1	F	201	GLU	N-CA-CB	6.85	120.19	110.12
1	G	224	THR	CA-C-N	6.85	129.46	120.28
1	G	224	THR	C-N-CA	6.85	129.46	120.28
1	J	166	ASP	CA-CB-CG	6.85	119.45	112.60
1	E	126	LYS	N-CA-C	-6.84	96.24	110.80
1	G	198	ARG	N-CA-C	6.84	118.73	111.28
1	K	82	GLY	CA-C-N	6.83	130.12	120.28
1	K	82	GLY	C-N-CA	6.83	130.12	120.28
1	C	263	ASP	CA-CB-CG	-6.83	105.77	112.60
1	I	272	ASP	N-CA-C	-6.82	104.85	113.72
1	I	167	LEU	N-CA-C	-6.82	103.85	111.28
1	I	75	ASN	CA-C-N	6.81	129.96	120.29
1	I	75	ASN	C-N-CA	6.81	129.96	120.29
1	G	285	LEU	CA-C-N	6.80	127.20	119.93
1	G	285	LEU	C-N-CA	6.80	127.20	119.93
1	A	101	SER	N-CA-CB	6.79	120.11	110.12
1	I	243	GLU	CB-CG-CD	-6.79	101.05	112.60
1	J	127	ASN	CA-CB-CG	6.79	119.39	112.60
1	A	145	GLN	OE1-CD-NE2	-6.79	115.81	122.60
1	D	290	ASP	CA-CB-CG	-6.78	105.82	112.60
1	L	141	ALA	CA-C-N	6.78	129.92	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	141	ALA	C-N-CA	6.78	129.92	120.29
1	D	140	THR	CA-C-O	-6.78	113.19	121.06
1	J	151	TYR	CB-CA-C	-6.78	99.32	110.85
1	G	192	GLN	N-CA-CB	6.77	120.17	110.16
1	K	111	ASP	N-CA-C	6.76	118.73	111.36
1	C	159	VAL	N-CA-CB	6.76	119.74	110.54
1	D	234	ASP	N-CA-C	6.76	118.30	111.07
1	H	189	ALA	N-CA-C	-6.75	103.93	111.28
1	K	223	VAL	O-C-N	6.75	130.95	122.52
1	F	84	ALA	N-CA-C	6.73	119.45	111.71
1	C	213	THR	N-CA-C	-6.73	106.02	114.56
1	J	265	LYS	N-CA-CB	6.73	120.58	110.22
1	H	185	GLN	CB-CA-C	-6.72	99.63	110.79
1	H	265	LYS	CA-C-N	6.71	129.82	120.29
1	H	265	LYS	C-N-CA	6.71	129.82	120.29
1	C	192	GLN	CA-C-N	6.71	129.27	120.28
1	C	192	GLN	C-N-CA	6.71	129.27	120.28
1	L	170	ASN	O-C-N	6.71	129.23	122.12
1	K	222	ASP	N-CA-C	-6.70	100.04	110.42
1	G	92	GLN	N-CA-CB	6.69	119.95	110.12
1	F	165	ARG	CD-NE-CZ	-6.69	115.04	124.40
1	B	274	VAL	CA-C-N	6.68	132.22	123.00
1	B	274	VAL	C-N-CA	6.68	132.22	123.00
1	E	118	LYS	CA-C-O	-6.68	113.31	120.46
1	B	176	LYS	CA-C-N	6.68	129.77	120.29
1	B	176	LYS	C-N-CA	6.68	129.77	120.29
1	H	261	LEU	N-CA-CB	6.67	119.93	110.12
1	E	277	TYR	CA-C-O	6.67	128.45	121.38
1	G	213	THR	CB-CA-C	6.67	117.77	109.16
1	B	247	PRO	CA-C-N	6.66	130.17	120.71
1	B	247	PRO	C-N-CA	6.66	130.17	120.71
1	C	100	SER	O-C-N	6.65	129.17	122.12
1	F	227	THR	CA-C-N	6.65	129.19	120.28
1	F	227	THR	C-N-CA	6.65	129.19	120.28
1	H	272	ASP	CA-CB-CG	6.65	119.25	112.60
1	F	273	THR	CA-C-O	6.65	127.23	119.32
1	C	279	TYR	CA-C-O	-6.65	112.98	120.43
1	B	198	ARG	CB-CA-C	-6.65	99.76	110.79
1	D	187	VAL	N-CA-CB	6.64	118.33	110.55
1	G	180	ASP	CA-C-O	6.64	127.59	120.55
1	A	219	GLN	CA-C-N	6.64	130.78	120.75
1	A	219	GLN	C-N-CA	6.64	130.78	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	ILE	N-CA-CB	6.64	120.57	111.41
1	L	188	VAL	CA-C-N	6.64	129.72	120.29
1	L	188	VAL	C-N-CA	6.64	129.72	120.29
1	I	79	VAL	CA-C-N	6.64	129.06	120.56
1	I	79	VAL	C-N-CA	6.64	129.06	120.56
1	B	108	GLU	N-CA-C	6.63	118.17	111.07
1	B	198	ARG	N-CA-CB	6.63	119.87	110.12
1	G	133	THR	N-CA-C	-6.63	98.40	109.07
1	F	71	ALA	N-CA-C	6.63	118.50	111.28
1	C	226	ASP	CA-CB-CG	-6.62	105.98	112.60
1	E	174	GLY	CA-C-O	-6.62	113.64	120.66
1	G	140	THR	CA-CB-OG1	6.62	119.53	109.60
1	J	66	ASP	CA-CB-CG	-6.62	105.98	112.60
1	B	243	GLU	CA-C-N	6.61	129.14	120.28
1	B	243	GLU	C-N-CA	6.61	129.14	120.28
1	I	247	PRO	N-CA-CB	6.61	110.19	103.25
1	J	246	ARG	CA-C-O	-6.60	113.62	120.02
1	D	146	MET	N-CA-C	6.59	118.26	111.14
1	H	290	ASP	N-CA-C	-6.59	99.57	108.86
1	C	197	ILE	N-CA-C	-6.59	103.90	110.62
1	D	265	LYS	CA-C-N	6.58	129.64	120.29
1	D	265	LYS	C-N-CA	6.58	129.64	120.29
1	K	228	MET	N-CA-C	6.58	118.46	111.28
1	A	81	TYR	CA-C-N	6.58	127.86	120.42
1	A	81	TYR	C-N-CA	6.58	127.86	120.42
1	F	285	LEU	N-CA-C	6.58	124.35	109.81
1	G	245	THR	CA-CB-OG1	6.58	119.47	109.60
1	J	177	ASN	CA-CB-CG	6.58	119.18	112.60
1	E	198	ARG	NE-CZ-NH2	-6.58	113.28	119.20
1	A	287	VAL	CA-C-N	6.57	132.07	123.00
1	A	287	VAL	C-N-CA	6.57	132.07	123.00
1	C	98	ARG	CB-CA-C	-6.57	99.67	110.85
1	G	159	VAL	N-CA-CB	6.57	120.43	110.58
1	J	122	GLU	N-CA-CB	6.57	117.99	111.10
1	J	88	VAL	O-C-N	6.56	128.24	121.87
1	J	82	GLY	CA-C-N	6.56	129.07	120.28
1	J	82	GLY	C-N-CA	6.56	129.07	120.28
1	G	229	PHE	CA-CB-CG	6.55	120.36	113.80
1	K	59	THR	N-CA-C	-6.55	99.36	109.52
1	A	110	LEU	CA-C-N	6.54	129.05	120.28
1	A	110	LEU	C-N-CA	6.54	129.05	120.28
1	C	285	LEU	CA-C-N	6.54	126.50	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	LEU	C-N-CA	6.54	126.50	119.76
1	E	248	LEU	N-CA-C	6.54	120.16	109.76
1	B	229	PHE	CA-C-N	6.54	129.69	120.28
1	B	229	PHE	C-N-CA	6.54	129.69	120.28
1	D	258	LYS	O-C-N	6.53	129.04	122.12
1	B	227	THR	CA-C-O	6.52	126.22	119.05
1	K	278	ARG	N-CA-C	-6.52	99.13	109.23
1	I	264	ILE	N-CA-C	6.51	117.26	110.62
1	J	236	LEU	CA-C-N	6.51	129.01	120.28
1	J	236	LEU	C-N-CA	6.51	129.01	120.28
1	L	278	ARG	N-CA-C	-6.51	99.14	109.23
1	A	145	GLN	CA-C-N	6.51	128.90	120.44
1	A	145	GLN	C-N-CA	6.51	128.90	120.44
1	L	165	ARG	CA-C-N	6.50	128.99	120.28
1	L	165	ARG	C-N-CA	6.50	128.99	120.28
1	G	109	THR	N-CA-C	6.50	118.37	111.28
1	H	214	GLN	CA-C-N	6.50	127.97	119.84
1	H	214	GLN	C-N-CA	6.50	127.97	119.84
1	E	64	GLN	CA-C-N	6.49	127.38	120.11
1	E	64	GLN	C-N-CA	6.49	127.38	120.11
1	H	171	ILE	CA-C-N	6.49	128.98	120.28
1	H	171	ILE	C-N-CA	6.49	128.98	120.28
1	F	273	THR	N-CA-C	-6.49	104.60	113.30
1	E	205	ARG	NE-CZ-NH2	6.49	125.04	119.20
1	J	181	SER	CA-C-O	-6.48	113.68	120.55
1	H	203	ALA	CA-C-N	6.47	128.95	120.28
1	H	203	ALA	C-N-CA	6.47	128.95	120.28
1	I	234	ASP	CA-C-N	6.47	129.48	120.29
1	I	234	ASP	C-N-CA	6.47	129.48	120.29
1	L	192	GLN	CA-C-N	6.47	128.95	120.28
1	L	192	GLN	C-N-CA	6.47	128.95	120.28
1	D	206	TYR	CB-CA-C	-6.46	100.06	110.79
1	H	69	GLN	N-CA-C	6.46	118.32	111.28
1	I	205	ARG	N-CA-C	-6.46	104.32	111.36
1	A	253	ALA	N-CA-CB	6.46	120.29	110.28
1	B	140	THR	CA-C-N	6.46	128.83	120.44
1	B	140	THR	C-N-CA	6.46	128.83	120.44
1	J	83	GLN	OE1-CD-NE2	6.46	129.06	122.60
1	D	266	ASN	CA-C-N	6.45	129.87	120.71
1	D	266	ASN	C-N-CA	6.45	129.87	120.71
1	B	80	ILE	CA-C-O	-6.45	113.70	121.18
1	E	96	ILE	CA-C-N	6.44	127.13	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	96	ILE	C-N-CA	6.44	127.13	119.98
1	I	288	ARG	NE-CZ-NH2	-6.44	113.40	119.20
1	K	152	ILE	CA-C-N	6.44	129.44	120.29
1	K	152	ILE	C-N-CA	6.44	129.44	120.29
1	C	154	GLN	O-C-N	6.44	128.94	122.12
1	K	226	ASP	CB-CA-C	-6.44	98.31	110.67
1	C	66	ASP	CA-C-N	6.43	129.56	120.42
1	C	66	ASP	C-N-CA	6.43	129.56	120.42
1	I	260	THR	O-C-N	-6.43	114.82	122.15
1	G	174	GLY	CA-C-N	6.43	129.42	120.29
1	G	174	GLY	C-N-CA	6.43	129.42	120.29
1	I	263	ASP	CA-CB-CG	-6.42	106.18	112.60
1	G	274	VAL	N-CA-C	-6.42	99.88	108.35
1	F	243	GLU	CB-CG-CD	-6.42	101.69	112.60
1	I	242	ASN	OD1-CG-ND2	6.42	129.02	122.60
1	J	290	ASP	N-CA-C	-6.42	102.66	112.99
1	K	277	TYR	N-CA-CB	6.42	121.34	111.46
1	F	183	ARG	CA-C-N	6.41	128.78	120.44
1	F	183	ARG	C-N-CA	6.41	128.78	120.44
1	G	161	GLN	O-C-N	6.41	128.92	122.12
1	H	97	GLY	CA-C-N	6.41	129.40	120.29
1	H	97	GLY	C-N-CA	6.41	129.40	120.29
1	I	170	ASN	CA-C-N	6.41	129.24	120.46
1	I	170	ASN	C-N-CA	6.41	129.24	120.46
1	D	116	PRO	O-C-N	6.41	127.28	122.73
1	I	250	PHE	CB-CG-CD1	6.40	131.58	120.70
1	E	247	PRO	CA-C-N	-6.39	112.36	121.50
1	E	247	PRO	C-N-CA	-6.39	112.36	121.50
1	A	235	ALA	N-CA-CB	6.39	119.51	110.12
1	C	111	ASP	N-CA-CB	6.39	119.51	110.12
1	C	73	TYR	N-CA-C	-6.38	104.32	111.28
1	D	102	ALA	CA-C-N	6.38	129.12	120.44
1	D	102	ALA	C-N-CA	6.38	129.12	120.44
1	K	200	ILE	N-CA-CB	6.38	120.16	110.58
1	E	259	GLN	CA-C-N	6.38	129.35	120.29
1	E	259	GLN	C-N-CA	6.38	129.35	120.29
1	K	91	LEU	N-CA-CB	6.38	119.61	110.16
1	B	103	PHE	CA-C-O	-6.38	113.79	120.55
1	G	101	SER	N-CA-C	-6.38	104.33	111.28
1	F	152	ILE	N-CA-CB	6.38	118.01	110.55
1	A	128	GLN	N-CA-C	-6.38	100.72	109.71
1	C	129	GLN	N-CA-C	-6.38	106.46	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	235	ALA	N-CA-C	-6.38	104.41	111.36
1	J	170	ASN	CA-CB-CG	-6.37	106.23	112.60
1	J	218	GLN	CB-CA-C	-6.37	100.61	110.81
1	J	206	TYR	CA-C-N	6.37	128.82	120.28
1	J	206	TYR	C-N-CA	6.37	128.82	120.28
1	A	199	GLN	N-CA-C	6.37	118.22	111.28
1	I	250	PHE	CA-CB-CG	-6.37	107.43	113.80
1	K	208	ASP	CA-C-N	6.36	129.32	120.29
1	K	208	ASP	C-N-CA	6.36	129.32	120.29
1	D	222	ASP	N-CA-C	-6.36	100.42	109.96
1	B	117	GLU	CA-C-N	6.35	131.95	123.05
1	B	117	GLU	C-N-CA	6.35	131.95	123.05
1	F	217	ILE	N-CA-C	-6.35	99.07	108.85
1	D	200	ILE	CA-C-O	-6.35	114.35	120.95
1	E	265	LYS	N-CA-C	6.34	119.00	111.71
1	B	282	LYS	CA-C-N	6.34	127.33	119.98
1	B	282	LYS	C-N-CA	6.34	127.33	119.98
1	I	98	ARG	CD-NE-CZ	-6.34	115.53	124.40
1	B	88	VAL	CA-C-N	6.33	128.77	120.28
1	B	88	VAL	C-N-CA	6.33	128.77	120.28
1	G	216	GLN	OE1-CD-NE2	-6.33	116.27	122.60
1	H	250	PHE	N-CA-C	-6.33	99.49	109.50
1	H	69	GLN	CB-CA-C	-6.33	100.28	110.79
1	L	165	ARG	CD-NE-CZ	-6.33	115.53	124.40
1	J	251	SER	O-C-N	-6.33	115.94	121.32
1	L	277	TYR	N-CA-C	-6.33	99.53	108.96
1	B	192	GLN	OE1-CD-NE2	6.32	128.92	122.60
1	F	166	ASP	CA-CB-CG	6.32	118.92	112.60
1	I	141	ALA	N-CA-C	6.32	117.83	111.07
1	F	213	THR	N-CA-C	-6.32	105.61	113.38
1	H	255	TYR	N-CA-CB	6.32	119.51	110.16
1	J	114	GLU	CA-C-N	6.31	129.12	120.67
1	J	114	GLU	C-N-CA	6.31	129.12	120.67
1	F	282	LYS	N-CA-C	-6.31	102.11	109.93
1	B	66	ASP	N-CA-C	-6.30	96.03	107.75
1	B	152	ILE	CA-C-N	6.29	129.23	120.29
1	B	152	ILE	C-N-CA	6.29	129.23	120.29
1	E	168	LYS	O-C-N	6.29	128.79	122.12
1	B	78	ASN	CA-CB-CG	6.29	118.89	112.60
1	C	207	ALA	N-CA-CB	6.29	119.47	110.16
1	F	171	ILE	CA-C-O	-6.29	114.18	120.85
1	L	216	GLN	CA-C-N	6.29	129.17	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	216	GLN	C-N-CA	6.29	129.17	120.49
1	E	92	GLN	N-CA-C	-6.29	104.43	111.28
1	C	156	ASP	CA-C-N	6.28	128.70	120.28
1	C	156	ASP	C-N-CA	6.28	128.70	120.28
1	E	266	ASN	OD1-CG-ND2	-6.28	116.32	122.60
1	H	134	VAL	CA-C-O	-6.28	114.00	121.28
1	J	167	LEU	CA-C-N	6.28	128.69	120.28
1	J	167	LEU	C-N-CA	6.28	128.69	120.28
1	B	194	ASP	N-CA-CB	6.27	119.34	110.12
1	B	232	GLY	CA-C-N	6.26	128.67	120.28
1	B	232	GLY	C-N-CA	6.26	128.67	120.28
1	B	220	THR	N-CA-C	-6.26	99.61	109.50
1	C	81	TYR	N-CA-C	-6.26	104.34	112.23
1	H	71	ALA	N-CA-CB	6.26	119.45	110.06
1	H	206	TYR	CB-CG-CD1	6.26	130.19	120.80
1	G	73	TYR	N-CA-C	-6.26	104.54	111.36
1	J	133	THR	N-CA-CB	6.26	120.77	110.69
1	J	268	LYS	N-CA-C	-6.25	98.06	108.75
1	D	96	ILE	CA-C-N	6.25	126.92	119.98
1	D	96	ILE	C-N-CA	6.25	126.92	119.98
1	G	172	ALA	N-CA-CB	6.25	119.41	110.16
1	G	257	THR	CA-C-N	-6.25	111.90	120.28
1	G	257	THR	C-N-CA	-6.25	111.90	120.28
1	G	228	MET	CA-C-N	6.25	129.50	120.38
1	G	228	MET	C-N-CA	6.25	129.50	120.38
1	A	139	GLN	N-CA-C	-6.25	105.66	113.28
1	D	111	ASP	N-CA-CB	6.25	119.30	110.12
1	E	255	TYR	CA-C-N	6.25	128.65	120.28
1	E	255	TYR	C-N-CA	6.25	128.65	120.28
1	G	103	PHE	CA-CB-CG	6.24	120.04	113.80
1	G	75	ASN	CA-CB-CG	-6.23	106.37	112.60
1	H	171	ILE	CB-CA-C	6.23	120.55	112.14
1	I	79	VAL	CA-C-O	-6.23	114.47	120.95
1	J	219	GLN	N-CA-CB	6.23	122.45	111.49
1	C	195	LEU	O-C-N	6.22	128.71	122.12
1	H	193	LYS	CA-C-N	6.22	128.61	120.28
1	H	193	LYS	C-N-CA	6.22	128.61	120.28
1	A	183	ARG	CA-C-N	6.22	128.61	120.28
1	A	183	ARG	C-N-CA	6.22	128.61	120.28
1	A	219	GLN	OE1-CD-NE2	-6.22	116.38	122.60
1	A	85	ALA	CA-C-N	6.21	126.13	119.85
1	A	85	ALA	C-N-CA	6.21	126.13	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	ASN	CA-CB-CG	6.21	118.81	112.60
1	J	264	ILE	CA-C-O	-6.21	114.49	120.95
1	B	278	ARG	N-CA-C	-6.21	99.60	109.23
1	I	233	SER	CA-C-N	6.21	128.51	120.44
1	I	233	SER	C-N-CA	6.21	128.51	120.44
1	E	69	GLN	CA-C-O	-6.21	113.97	120.55
1	B	193	LYS	CA-C-N	6.21	128.60	120.28
1	B	193	LYS	C-N-CA	6.21	128.60	120.28
1	C	79	VAL	CA-C-O	6.21	127.40	120.95
1	L	83	GLN	N-CA-CB	6.21	119.78	110.22
1	B	107	ALA	CA-C-N	6.20	128.50	120.44
1	B	107	ALA	C-N-CA	6.20	128.50	120.44
1	L	250	PHE	CA-CB-CG	-6.20	107.60	113.80
1	C	170	ASN	CA-CB-CG	-6.20	106.40	112.60
1	B	224	THR	CA-CB-OG1	6.20	118.90	109.60
1	G	286	PRO	CA-C-N	6.20	129.22	121.85
1	G	286	PRO	C-N-CA	6.20	129.22	121.85
1	I	124	SER	CA-CB-OG	6.19	123.49	111.10
1	E	137	VAL	CA-C-N	6.19	127.02	121.82
1	E	137	VAL	C-N-CA	6.19	127.02	121.82
1	B	85	ALA	CA-C-N	6.19	126.20	119.89
1	B	85	ALA	C-N-CA	6.19	126.20	119.89
1	K	224	THR	N-CA-CB	6.19	120.95	110.49
1	D	110	LEU	CA-C-N	6.18	128.57	120.28
1	D	110	LEU	C-N-CA	6.18	128.57	120.28
1	E	104	SER	N-CA-CB	6.18	119.21	110.12
1	H	100	SER	CA-CB-OG	6.18	123.47	111.10
1	J	237	LYS	N-CA-CB	-6.18	101.03	110.12
1	J	222	ASP	CA-C-N	-6.18	115.19	122.11
1	J	222	ASP	C-N-CA	-6.18	115.19	122.11
1	C	204	LEU	CA-C-N	6.18	128.56	120.28
1	C	204	LEU	C-N-CA	6.18	128.56	120.28
1	E	102	ALA	N-CA-C	6.18	118.01	111.28
1	J	191	GLU	CA-C-N	6.18	128.56	120.28
1	J	191	GLU	C-N-CA	6.18	128.56	120.28
1	K	74	ASN	CA-CB-CG	6.17	118.77	112.60
1	D	174	GLY	CA-C-N	6.17	129.05	120.29
1	D	174	GLY	C-N-CA	6.17	129.05	120.29
1	L	159	VAL	N-CA-CB	6.17	118.93	110.54
1	F	192	GLN	O-C-N	6.17	128.66	122.12
1	I	273	THR	N-CA-C	-6.16	104.37	113.61
1	I	288	ARG	NH1-CZ-NH2	6.15	127.30	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	173	LEU	CA-C-N	6.15	126.77	119.94
1	I	173	LEU	C-N-CA	6.15	126.77	119.94
1	J	157	ASP	CA-C-N	6.15	128.44	120.44
1	J	157	ASP	C-N-CA	6.15	128.44	120.44
1	F	243	GLU	N-CA-CB	6.15	119.26	110.16
1	K	196	ARG	NE-CZ-NH2	6.14	124.73	119.20
1	C	80	ILE	CA-C-O	-6.14	114.23	121.05
1	B	90	ASP	CA-CB-CG	-6.14	106.46	112.60
1	G	266	ASN	CA-CB-CG	-6.14	106.46	112.60
1	C	110	LEU	CA-C-O	-6.13	114.05	120.55
1	A	247	PRO	N-CA-C	6.13	120.85	111.11
1	B	66	ASP	N-CA-CB	6.13	120.50	110.39
1	B	218	GLN	OE1-CD-NE2	6.13	128.73	122.60
1	H	239	MET	N-CA-C	-6.13	104.60	111.28
1	I	154	GLN	OE1-CD-NE2	6.13	128.73	122.60
1	B	219	GLN	CG-CD-NE2	-6.12	107.21	116.40
1	C	242	ASN	N-CA-C	-6.12	103.16	111.55
1	E	150	GLN	CA-C-N	6.12	128.98	120.29
1	E	150	GLN	C-N-CA	6.12	128.98	120.29
1	B	127	ASN	OD1-CG-ND2	6.12	128.72	122.60
1	C	228	MET	CA-C-N	6.12	129.09	120.28
1	C	228	MET	C-N-CA	6.12	129.09	120.28
1	A	156	ASP	CA-CB-CG	6.11	118.71	112.60
1	C	154	GLN	CB-CA-C	-6.11	100.64	110.79
1	J	279	TYR	N-CA-CB	6.11	120.38	110.42
1	F	121	ILE	N-CA-CB	6.11	121.47	111.58
1	G	94	THR	CA-C-O	-6.11	113.94	120.42
1	D	290	ASP	N-CA-C	-6.11	99.24	109.07
1	L	129	GLN	CA-C-N	6.10	128.96	123.10
1	L	129	GLN	C-N-CA	6.10	128.96	123.10
1	I	187	VAL	CB-CA-C	-6.10	104.17	111.97
1	A	190	GLN	CA-C-N	6.09	128.45	120.28
1	A	190	GLN	C-N-CA	6.09	128.45	120.28
1	B	99	PHE	CA-CB-CG	6.09	119.89	113.80
1	E	89	SER	CA-C-O	6.09	127.01	120.55
1	F	94	THR	CA-C-N	6.09	128.36	120.44
1	F	94	THR	C-N-CA	6.09	128.36	120.44
1	D	166	ASP	N-CA-CB	6.09	119.17	110.16
1	B	210	ALA	CA-C-O	6.08	126.98	120.10
1	K	153	GLN	CA-C-N	6.08	128.93	120.29
1	K	153	GLN	C-N-CA	6.08	128.93	120.29
1	A	188	VAL	CA-C-N	6.08	128.43	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	VAL	C-N-CA	6.08	128.43	120.28
1	G	263	ASP	N-CA-C	-6.08	104.74	111.36
1	F	282	LYS	CA-C-O	-6.07	114.03	120.23
1	H	251	SER	N-CA-C	-6.07	102.50	110.39
1	K	204	LEU	N-CA-C	6.07	117.90	111.28
1	L	82	GLY	O-C-N	6.07	130.00	122.90
1	A	222	ASP	CA-CB-CG	-6.06	106.54	112.60
1	B	212	ILE	N-CA-C	-6.06	98.27	107.73
1	H	209	GLU	CA-C-N	6.06	130.85	120.72
1	H	209	GLU	C-N-CA	6.06	130.85	120.72
1	J	194	ASP	CA-CB-CG	-6.06	106.54	112.60
1	F	198	ARG	O-C-N	6.06	128.54	122.12
1	A	114	GLU	N-CA-C	-6.05	105.54	113.17
1	C	73	TYR	O-C-N	6.05	128.54	122.12
1	K	105	ALA	CB-CA-C	-6.05	100.75	110.79
1	G	60	ALA	O-C-N	6.04	130.14	123.25
1	K	200	ILE	CB-CA-C	-6.04	103.88	112.22
1	K	232	GLY	CA-C-N	6.04	128.98	120.28
1	K	232	GLY	C-N-CA	6.04	128.98	120.28
1	L	124	SER	CA-C-N	6.04	132.84	121.97
1	L	124	SER	C-N-CA	6.04	132.84	121.97
1	G	285	LEU	CB-CA-C	-6.04	105.01	110.44
1	L	131	PRO	N-CA-C	6.03	120.66	111.19
1	H	140	THR	N-CA-C	-6.03	99.24	108.76
1	K	107	ALA	N-CA-C	6.03	117.85	111.28
1	B	112	ASN	OD1-CG-ND2	6.02	128.62	122.60
1	C	244	ALA	CB-CA-C	-6.02	100.80	110.79
1	E	175	ARG	CD-NE-CZ	-6.02	115.97	124.40
1	K	166	ASP	CA-CB-CG	6.02	118.62	112.60
1	E	245	THR	CA-CB-OG1	6.02	118.62	109.60
1	C	203	ALA	CB-CA-C	-6.01	99.50	110.63
1	F	145	GLN	CA-C-N	6.01	128.33	120.28
1	F	145	GLN	C-N-CA	6.01	128.33	120.28
1	A	241	GLN	OE1-CD-NE2	6.01	128.61	122.60
1	D	183	ARG	CA-C-N	6.01	128.82	120.29
1	D	183	ARG	C-N-CA	6.01	128.82	120.29
1	I	142	GLU	N-CA-CB	6.00	119.05	110.16
1	J	221	GLN	O-C-N	-6.00	117.00	123.42
1	L	116	PRO	N-CA-C	-6.00	100.10	112.47
1	G	146	MET	N-CA-CB	6.00	119.04	110.16
1	C	121	ILE	CA-C-O	6.00	127.35	120.76
1	H	182	LEU	CA-C-N	5.99	128.23	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	182	LEU	C-N-CA	5.99	128.23	120.44
1	A	200	ILE	N-CA-CB	-5.99	102.40	110.54
1	G	196	ARG	CA-C-N	5.99	128.66	120.46
1	G	196	ARG	C-N-CA	5.99	128.66	120.46
1	L	96	ILE	O-C-N	-5.99	116.06	121.87
1	I	123	PRO	CA-C-O	-5.99	114.12	121.31
1	J	160	ASN	CB-CA-C	-5.99	100.86	110.79
1	K	208	ASP	N-CA-CB	5.99	118.92	110.12
1	B	246	ARG	NH1-CZ-NH2	-5.98	111.52	119.30
1	G	161	GLN	CB-CG-CD	-5.98	102.43	112.60
1	H	149	ALA	CA-C-N	5.98	128.22	120.44
1	H	149	ALA	C-N-CA	5.98	128.22	120.44
1	I	210	ALA	CA-C-O	-5.98	112.25	119.49
1	A	105	ALA	CB-CA-C	-5.98	100.86	110.79
1	F	122	GLU	N-CA-C	5.98	113.60	108.22
1	A	143	GLY	O-C-N	5.98	127.93	122.19
1	J	188	VAL	CA-C-N	5.97	128.21	120.44
1	J	188	VAL	C-N-CA	5.97	128.21	120.44
1	C	82	GLY	N-CA-C	5.97	121.10	110.95
1	C	73	TYR	CA-C-O	-5.97	114.22	120.55
1	G	167	LEU	CA-C-N	5.97	128.77	120.29
1	G	167	LEU	C-N-CA	5.97	128.77	120.29
1	H	137	VAL	CA-C-N	5.97	127.78	122.47
1	H	137	VAL	C-N-CA	5.97	127.78	122.47
1	I	183	ARG	NE-CZ-NH1	5.97	127.47	121.50
1	I	162	GLU	N-CA-CB	5.97	118.99	110.16
1	C	77	MET	CB-CA-C	-5.97	100.89	110.79
1	F	150	GLN	O-C-N	-5.97	115.92	122.07
1	D	285	LEU	N-CA-C	-5.96	95.78	108.66
1	K	181	SER	N-CA-CB	5.96	118.88	110.12
1	D	68	GLY	CA-C-N	5.96	128.75	120.29
1	D	68	GLY	C-N-CA	5.96	128.75	120.29
1	A	70	ILE	CA-C-N	5.96	128.54	120.38
1	A	70	ILE	C-N-CA	5.96	128.54	120.38
1	F	244	ALA	CA-C-N	5.96	129.36	120.31
1	F	244	ALA	C-N-CA	5.96	129.36	120.31
1	G	244	ALA	CA-C-N	5.96	128.75	120.29
1	G	244	ALA	C-N-CA	5.96	128.75	120.29
1	K	132	LEU	N-CA-CB	5.96	121.19	110.83
1	C	251	SER	CA-C-O	-5.95	115.08	121.27
1	J	234	ASP	O-C-N	-5.95	115.94	122.07
1	J	74	ASN	OD1-CG-ND2	5.95	128.55	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	221	GLN	N-CA-C	-5.95	99.69	108.79
1	E	235	ALA	CA-C-N	5.94	128.24	120.28
1	E	235	ALA	C-N-CA	5.94	128.24	120.28
1	L	72	GLY	O-C-N	5.94	127.89	122.19
1	C	83	GLN	CA-C-N	5.94	129.33	120.31
1	C	83	GLN	C-N-CA	5.94	129.33	120.31
1	H	284	THR	N-CA-C	-5.94	100.51	109.95
1	H	62	ILE	CA-C-O	5.93	127.90	121.67
1	I	153	GLN	N-CA-CB	5.93	118.84	110.12
1	J	74	ASN	CA-CB-CG	-5.93	106.67	112.60
1	G	126	LYS	N-CA-C	-5.93	100.50	108.86
1	L	157	ASP	CA-CB-CG	5.93	118.53	112.60
1	J	183	ARG	CD-NE-CZ	-5.92	116.11	124.40
1	K	67	VAL	O-C-N	-5.92	115.73	121.83
1	K	108	GLU	CA-C-N	5.92	128.22	120.28
1	K	108	GLU	C-N-CA	5.92	128.22	120.28
1	K	128	GLN	CA-C-N	5.92	129.28	120.87
1	K	128	GLN	C-N-CA	5.92	129.28	120.87
1	C	171	ILE	N-CA-C	5.92	116.66	110.62
1	F	128	GLN	N-CA-C	-5.92	105.36	113.30
1	G	263	ASP	CA-C-N	5.92	128.82	120.42
1	G	263	ASP	C-N-CA	5.92	128.82	120.42
1	A	191	GLU	CA-C-N	5.92	128.69	120.29
1	A	191	GLU	C-N-CA	5.92	128.69	120.29
1	K	56	TRP	CB-CA-C	-5.92	98.88	109.71
1	C	124	SER	N-CA-C	5.91	123.39	110.80
1	F	122	GLU	CA-C-N	5.91	125.82	119.85
1	F	122	GLU	C-N-CA	5.91	125.82	119.85
1	J	257	THR	O-C-N	5.91	128.39	122.12
1	L	245	THR	N-CA-C	5.91	118.68	111.82
1	J	221	GLN	N-CA-C	-5.91	99.75	108.79
1	H	266	ASN	N-CA-CB	5.91	118.90	110.16
1	E	182	LEU	N-CA-C	5.90	117.72	111.28
1	H	249	ALA	N-CA-C	-5.90	100.94	110.32
1	J	275	HIS	ND1-CE1-NE2	5.90	114.30	108.40
1	K	166	ASP	CA-C-N	5.90	128.19	120.28
1	K	166	ASP	C-N-CA	5.90	128.19	120.28
1	B	262	LEU	CA-C-N	5.90	128.19	120.28
1	B	262	LEU	C-N-CA	5.90	128.19	120.28
1	J	149	ALA	CA-C-N	5.90	128.11	120.44
1	J	149	ALA	C-N-CA	5.90	128.11	120.44
1	F	87	LYS	CA-C-O	-5.89	115.16	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	116	PRO	N-CA-CB	-5.89	99.62	102.92
1	E	234	ASP	N-CA-CB	5.88	118.77	110.12
1	L	64	GLN	N-CA-C	5.88	122.81	109.81
1	A	75	ASN	CA-CB-CG	-5.88	106.72	112.60
1	F	223	VAL	CA-C-O	-5.88	115.56	121.49
1	I	206	TYR	CB-CG-CD1	5.88	129.61	120.80
1	E	174	GLY	CA-C-N	5.87	128.15	120.28
1	E	174	GLY	C-N-CA	5.87	128.15	120.28
1	I	213	THR	CA-C-N	5.87	133.62	123.11
1	I	213	THR	C-N-CA	5.87	133.62	123.11
1	E	69	GLN	O-C-N	5.87	128.34	122.12
1	K	237	LYS	CA-C-N	5.87	128.14	120.28
1	K	237	LYS	C-N-CA	5.87	128.14	120.28
1	K	206	TYR	N-CA-C	-5.86	104.97	111.36
1	K	252	PRO	N-CA-C	-5.86	105.73	113.65
1	C	228	MET	N-CA-C	5.86	117.67	111.28
1	G	219	GLN	CA-C-O	-5.86	114.96	121.23
1	F	95	LEU	CB-CA-C	-5.86	101.69	110.88
1	K	277	TYR	N-CA-C	-5.85	100.06	108.60
1	B	157	ASP	CA-C-N	5.85	128.60	120.29
1	B	157	ASP	C-N-CA	5.85	128.60	120.29
1	K	88	VAL	N-CA-C	-5.85	104.65	110.62
1	E	95	LEU	CA-C-N	5.85	128.47	120.46
1	E	95	LEU	C-N-CA	5.85	128.47	120.46
1	C	122	GLU	CB-CG-CD	-5.84	102.66	112.60
1	G	235	ALA	CB-CA-C	-5.84	100.91	110.85
1	H	227	THR	CA-C-N	5.84	128.69	120.28
1	H	227	THR	C-N-CA	5.84	128.69	120.28
1	I	213	THR	N-CA-C	-5.84	107.39	114.75
1	C	244	ALA	N-CA-C	5.84	117.64	111.28
1	F	198	ARG	CA-C-O	-5.84	114.36	120.55
1	I	237	LYS	CB-CA-C	-5.84	101.10	110.79
1	A	132	LEU	CA-C-O	-5.83	114.40	120.70
1	E	116	PRO	O-C-N	5.83	130.52	122.64
1	D	180	ASP	CA-CB-CG	-5.83	106.77	112.60
1	G	260	THR	N-CA-C	-5.83	105.00	111.36
1	C	290	ASP	CA-CB-CG	-5.83	106.77	112.60
1	A	92	GLN	CB-CA-C	-5.83	101.12	110.79
1	C	287	VAL	N-CA-C	-5.83	107.61	113.20
1	H	156	ASP	CA-C-N	5.82	128.56	120.29
1	H	156	ASP	C-N-CA	5.82	128.56	120.29
1	H	265	LYS	CA-C-O	5.82	126.68	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	ALA	CA-C-N	5.82	128.08	120.28
1	A	102	ALA	C-N-CA	5.82	128.08	120.28
1	A	168	LYS	CA-C-O	-5.82	114.38	120.55
1	J	76	ALA	O-C-N	-5.82	115.95	122.12
1	B	151	TYR	CB-CA-C	-5.81	100.97	110.85
1	B	216	GLN	N-CA-C	-5.81	104.90	112.23
1	D	214	GLN	CA-C-N	5.81	126.11	119.83
1	D	214	GLN	C-N-CA	5.81	126.11	119.83
1	H	238	SER	CA-C-N	5.81	128.07	120.28
1	H	238	SER	C-N-CA	5.81	128.07	120.28
1	B	159	VAL	CA-CB-CG2	5.81	120.28	110.40
1	B	243	GLU	O-C-N	-5.81	115.53	122.15
1	K	78	ASN	CB-CA-C	-5.81	101.15	110.79
1	H	75	ASN	CB-CA-C	-5.81	100.98	110.85
1	C	260	THR	CA-C-O	-5.80	114.27	120.42
1	D	243	GLU	CA-C-N	5.80	128.06	120.28
1	D	243	GLU	C-N-CA	5.80	128.06	120.28
1	F	109	THR	CA-C-N	5.80	128.06	120.28
1	F	109	THR	C-N-CA	5.80	128.06	120.28
1	E	205	ARG	CA-C-N	5.80	128.33	120.44
1	E	205	ARG	C-N-CA	5.80	128.33	120.44
1	C	288	ARG	CA-C-O	5.80	126.51	120.30
1	E	199	GLN	CA-C-N	5.80	128.41	120.46
1	E	199	GLN	C-N-CA	5.80	128.41	120.46
1	H	147	LYS	N-CA-C	-5.80	105.04	111.36
1	A	130	LEU	O-C-N	5.80	128.20	121.47
1	F	106	LEU	CA-C-N	5.79	128.04	120.28
1	F	106	LEU	C-N-CA	5.79	128.04	120.28
1	I	267	LEU	CA-C-N	5.79	131.15	122.99
1	I	267	LEU	C-N-CA	5.79	131.15	122.99
1	J	146	MET	CB-CA-C	-5.79	101.01	110.85
1	I	242	ASN	CB-CA-C	-5.78	103.94	111.40
1	J	184	THR	CA-C-N	5.78	128.03	120.28
1	J	184	THR	C-N-CA	5.78	128.03	120.28
1	G	247	PRO	O-C-N	5.78	130.18	123.01
1	D	216	GLN	OE1-CD-NE2	5.78	128.38	122.60
1	J	176	LYS	CA-C-N	5.78	127.95	120.44
1	J	176	LYS	C-N-CA	5.78	127.95	120.44
1	C	75	ASN	N-CA-CB	5.78	118.61	110.12
1	B	149	ALA	CA-C-N	5.77	128.02	120.28
1	B	149	ALA	C-N-CA	5.77	128.02	120.28
1	L	218	GLN	N-CA-C	-5.77	98.50	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	170	ASN	CA-C-N	5.77	128.36	120.46
1	K	170	ASN	C-N-CA	5.77	128.36	120.46
1	F	103	PHE	O-C-N	5.76	128.72	122.15
1	K	287	VAL	N-CA-C	-5.76	107.65	113.47
1	C	177	ASN	N-CA-CB	5.76	118.36	110.01
1	B	197	ILE	N-CA-C	-5.76	104.75	110.62
1	L	216	GLN	OE1-CD-NE2	5.75	128.35	122.60
1	C	217	ILE	CB-CA-C	5.75	120.21	110.95
1	H	81	TYR	CB-CG-CD2	5.75	129.43	120.80
1	L	64	GLN	CA-C-N	5.75	126.08	119.92
1	L	64	GLN	C-N-CA	5.75	126.08	119.92
1	H	88	VAL	N-CA-C	5.75	116.49	110.62
1	H	183	ARG	N-CA-C	5.75	117.22	111.07
1	H	201	GLU	CA-C-N	5.75	128.25	120.44
1	H	201	GLU	C-N-CA	5.75	128.25	120.44
1	F	266	ASN	OD1-CG-ND2	5.74	128.34	122.60
1	J	188	VAL	N-CA-CB	5.74	118.35	110.54
1	C	128	GLN	N-CA-C	-5.74	98.58	110.80
1	G	151	TYR	CB-CA-C	-5.74	101.09	110.85
1	G	266	ASN	CA-C-O	-5.74	114.47	120.55
1	G	157	ASP	CA-C-N	5.74	127.90	120.44
1	G	157	ASP	C-N-CA	5.74	127.90	120.44
1	B	194	ASP	N-CA-C	-5.74	105.03	111.28
1	L	150	GLN	N-CA-CB	5.74	118.33	110.01
1	A	163	LEU	CA-C-N	5.73	128.43	120.29
1	A	163	LEU	C-N-CA	5.73	128.43	120.29
1	E	100	SER	O-C-N	5.73	127.98	122.07
1	G	206	TYR	CB-CG-CD1	5.73	129.40	120.80
1	L	258	LYS	CB-CA-C	-5.73	101.28	110.79
1	I	265	LYS	CA-C-N	5.73	128.42	120.29
1	I	265	LYS	C-N-CA	5.73	128.42	120.29
1	J	280	VAL	CB-CA-C	-5.73	104.57	112.24
1	K	219	GLN	N-CA-C	-5.73	100.61	109.14
1	F	172	ALA	CA-C-O	5.73	126.83	120.82
1	H	280	VAL	N-CA-C	-5.72	104.76	111.00
1	J	244	ALA	CA-C-N	5.72	128.52	120.28
1	J	244	ALA	C-N-CA	5.72	128.52	120.28
1	A	142	GLU	CA-C-N	5.72	126.33	119.98
1	A	142	GLU	C-N-CA	5.72	126.33	119.98
1	B	166	ASP	N-CA-CB	5.72	118.53	110.12
1	D	185	GLN	CA-C-N	5.72	127.94	120.28
1	D	185	GLN	C-N-CA	5.72	127.94	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	229	PHE	CA-CB-CG	5.72	119.52	113.80
1	F	179	GLN	CA-CB-CG	5.72	125.53	114.10
1	F	143	GLY	CA-C-O	-5.72	114.86	120.75
1	B	185	GLN	CA-C-O	-5.71	113.64	120.10
1	J	141	ALA	CA-C-N	5.71	128.40	120.29
1	J	141	ALA	C-N-CA	5.71	128.40	120.29
1	I	98	ARG	NE-CZ-NH1	5.71	127.20	121.50
1	D	251	SER	CA-C-N	5.70	125.23	119.19
1	D	251	SER	C-N-CA	5.70	125.23	119.19
1	C	257	THR	CA-CB-OG1	-5.70	101.05	109.60
1	G	155	VAL	CB-CA-C	5.70	120.08	112.22
1	H	84	ALA	N-CA-CB	5.70	118.99	110.22
1	C	151	TYR	N-CA-C	5.70	117.57	111.36
1	E	280	VAL	O-C-N	-5.69	114.32	121.84
1	H	103	PHE	CA-C-N	5.69	128.37	120.29
1	H	103	PHE	C-N-CA	5.69	128.37	120.29
1	L	265	LYS	N-CA-C	5.69	118.25	111.71
1	H	153	GLN	CA-C-O	-5.69	114.39	120.42
1	E	261	LEU	N-CA-C	-5.68	105.17	111.36
1	I	190	GLN	CA-C-N	5.68	127.90	120.28
1	I	190	GLN	C-N-CA	5.68	127.90	120.28
1	I	115	GLU	N-CA-CB	5.68	117.62	109.78
1	C	237	LYS	CA-C-O	-5.68	114.53	120.55
1	K	188	VAL	O-C-N	5.68	127.68	121.83
1	L	290	ASP	CA-CB-CG	5.68	118.28	112.60
1	B	173	LEU	O-C-N	5.68	128.62	122.15
1	A	74	ASN	N-CA-C	5.68	117.14	111.07
1	I	177	ASN	N-CA-CB	5.68	118.47	110.12
1	E	86	PRO	CB-CA-C	-5.67	102.47	111.04
1	F	228	MET	O-C-N	5.67	128.13	122.12
1	L	104	SER	CB-CA-C	-5.67	101.37	110.79
1	E	141	ALA	CA-C-N	5.67	127.88	120.28
1	E	141	ALA	C-N-CA	5.67	127.88	120.28
1	I	113	GLN	OE1-CD-NE2	5.67	128.27	122.60
1	K	150	GLN	CB-CA-C	-5.67	101.37	110.79
1	A	119	LEU	N-CA-C	-5.67	100.16	109.40
1	B	137	VAL	O-C-N	5.67	129.13	123.18
1	I	102	ALA	O-C-N	-5.67	115.96	122.09
1	K	262	LEU	O-C-N	5.67	128.13	122.12
1	L	113	GLN	CA-C-N	5.67	128.93	120.31
1	L	113	GLN	C-N-CA	5.67	128.93	120.31
1	G	247	PRO	CA-C-O	-5.67	114.99	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	113	GLN	N-CA-CB	5.67	120.07	110.49
1	G	96	ILE	CA-C-N	5.66	126.27	119.98
1	G	96	ILE	C-N-CA	5.66	126.27	119.98
1	I	89	SER	CB-CA-C	-5.66	101.22	110.85
1	J	166	ASP	CA-C-N	5.66	127.80	120.44
1	J	166	ASP	C-N-CA	5.66	127.80	120.44
1	C	207	ALA	CA-C-N	5.66	127.86	120.28
1	C	207	ALA	C-N-CA	5.66	127.86	120.28
1	D	122	GLU	O-C-N	-5.66	117.42	121.83
1	F	225	GLN	O-C-N	5.66	128.12	122.12
1	K	83	GLN	CA-C-N	5.66	128.91	120.31
1	K	83	GLN	C-N-CA	5.66	128.91	120.31
1	A	76	ALA	O-C-N	5.65	128.20	122.09
1	D	116	PRO	N-CD-CG	5.65	111.68	103.20
1	E	56	TRP	N-CA-C	-5.65	99.80	109.24
1	G	140	THR	CA-CB-CG2	-5.65	100.89	110.50
1	J	180	ASP	CA-C-O	-5.65	114.43	120.42
1	I	206	TYR	N-CA-C	-5.65	105.20	111.36
1	F	231	LEU	N-CA-CB	5.65	118.92	110.22
1	B	227	THR	CA-CB-OG1	5.65	118.07	109.60
1	L	92	GLN	CA-C-N	5.64	128.31	120.29
1	L	92	GLN	C-N-CA	5.64	128.31	120.29
1	A	184	THR	N-CA-CB	5.64	118.41	110.12
1	G	81	TYR	CB-CA-C	-5.64	101.26	110.85
1	L	106	LEU	N-CA-CB	5.64	118.42	110.12
1	C	231	LEU	CA-C-N	5.64	131.62	121.92
1	C	231	LEU	C-N-CA	5.64	131.62	121.92
1	B	223	VAL	CB-CA-C	5.63	119.63	111.80
1	I	131	PRO	N-CA-CB	-5.63	97.33	103.25
1	C	80	ILE	O-C-N	5.63	127.76	121.90
1	D	145	GLN	N-CA-C	-5.63	105.22	111.36
1	C	251	SER	N-CA-C	-5.63	103.55	110.31
1	B	216	GLN	OE1-CD-NE2	5.63	128.23	122.60
1	B	265	LYS	N-CA-C	5.63	118.35	111.82
1	F	83	GLN	OE1-CD-NE2	5.63	128.23	122.60
1	J	208	ASP	N-CA-C	5.62	117.41	111.28
1	J	160	ASN	N-CA-CB	5.62	118.39	110.12
1	I	115	GLU	CA-C-O	-5.62	114.58	120.88
1	J	119	LEU	N-CA-C	-5.62	100.24	109.40
1	L	161	GLN	CA-C-O	-5.62	114.47	120.42
1	E	150	GLN	O-C-N	-5.61	116.17	122.12
1	D	150	GLN	CB-CA-C	-5.61	101.48	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	202	GLU	CA-C-N	5.61	128.35	120.28
1	L	202	GLU	C-N-CA	5.61	128.35	120.28
1	C	284	THR	CA-CB-OG1	5.61	118.01	109.60
1	H	285	LEU	CA-C-N	5.60	125.61	119.89
1	H	285	LEU	C-N-CA	5.60	125.61	119.89
1	D	221	GLN	O-C-N	-5.60	116.86	123.25
1	L	191	GLU	N-CA-C	-5.60	105.17	111.28
1	B	99	PHE	CA-C-N	5.60	127.72	120.44
1	B	99	PHE	C-N-CA	5.60	127.72	120.44
1	G	144	ALA	O-C-N	-5.60	116.19	122.12
1	F	270	THR	CA-CB-OG1	5.60	118.00	109.60
1	G	181	SER	N-CA-CB	5.60	118.44	110.16
1	L	175	ARG	CA-C-O	-5.60	114.62	120.55
1	D	172	ALA	CA-C-N	5.59	128.05	120.44
1	D	172	ALA	C-N-CA	5.59	128.05	120.44
1	B	120	THR	CA-CB-OG1	5.59	117.99	109.60
1	E	65	PRO	CA-C-O	-5.59	114.26	122.31
1	E	212	ILE	N-CA-C	-5.59	99.59	107.75
1	I	258	LYS	N-CA-C	5.58	117.37	111.28
1	J	99	PHE	CA-CB-CG	-5.58	108.22	113.80
1	G	236	LEU	CA-C-O	-5.58	114.96	120.82
1	A	160	ASN	OD1-CG-ND2	5.58	128.18	122.60
1	B	255	TYR	CA-CB-CG	-5.58	103.86	113.90
1	K	246	ARG	CA-C-O	-5.58	112.52	120.16
1	G	239	MET	CA-C-N	5.58	128.34	120.42
1	G	239	MET	C-N-CA	5.58	128.34	120.42
1	A	104	SER	CA-C-O	-5.58	114.51	120.42
1	E	200	ILE	N-CA-CB	5.57	118.12	110.54
1	F	130	LEU	CB-CA-C	5.57	119.55	111.02
1	J	281	MET	CA-C-N	5.57	128.40	120.49
1	J	281	MET	C-N-CA	5.57	128.40	120.49
1	H	225	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	K	116	PRO	CA-C-O	-5.57	112.57	118.92
1	L	177	ASN	OD1-CG-ND2	5.57	128.17	122.60
1	F	85	ALA	CB-CA-C	-5.57	100.57	109.08
1	E	282	LYS	N-CA-C	-5.56	102.61	110.29
1	H	56	TRP	CE2-CD2-CE3	5.56	124.36	118.80
1	L	212	ILE	N-CA-C	-5.56	99.63	107.75
1	K	278	ARG	NH1-CZ-NH2	5.56	126.53	119.30
1	L	177	ASN	CB-CG-ND2	-5.56	108.06	116.40
1	A	130	LEU	CB-CA-C	-5.56	102.20	110.71
1	H	263	ASP	CA-CB-CG	-5.56	107.04	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	184	THR	N-CA-CB	5.55	118.28	110.12
1	I	241	GLN	CA-C-O	-5.55	114.67	120.55
1	A	219	GLN	N-CA-C	-5.55	100.86	109.24
1	B	263	ASP	CA-C-O	-5.55	114.67	120.55
1	E	266	ASN	CA-C-N	5.55	128.72	120.90
1	E	266	ASN	C-N-CA	5.55	128.72	120.90
1	F	66	ASP	N-CA-CB	5.54	119.02	110.21
1	A	257	THR	CA-C-N	5.54	127.71	120.28
1	A	257	THR	C-N-CA	5.54	127.71	120.28
1	F	126	LYS	N-CA-CB	5.54	119.33	110.46
1	F	233	SER	CA-C-N	5.54	127.64	120.44
1	F	233	SER	C-N-CA	5.54	127.64	120.44
1	L	238	SER	CA-C-N	5.54	127.71	120.28
1	L	238	SER	C-N-CA	5.54	127.71	120.28
1	A	278	ARG	O-C-N	5.54	129.87	123.17
1	B	165	ARG	CB-CA-C	5.54	119.98	110.79
1	I	104	SER	N-CA-C	5.54	117.32	111.28
1	K	166	ASP	O-C-N	-5.54	115.84	122.15
1	L	281	MET	CB-CA-C	-5.54	99.96	109.65
1	D	77	MET	CB-CA-C	-5.54	101.60	110.79
1	D	195	LEU	O-C-N	-5.54	116.25	122.12
1	E	196	ARG	CA-C-N	5.54	128.05	120.46
1	E	196	ARG	C-N-CA	5.54	128.05	120.46
1	F	282	LYS	CA-C-N	5.53	125.85	119.93
1	F	282	LYS	C-N-CA	5.53	125.85	119.93
1	E	108	GLU	N-CA-CB	5.53	118.09	110.07
1	E	255	TYR	CA-C-O	5.53	126.33	119.97
1	D	58	SER	N-CA-CB	5.53	119.59	110.69
1	E	128	GLN	O-C-N	-5.53	116.16	121.85
1	H	264	ILE	N-CA-C	5.53	116.26	110.62
1	J	231	LEU	N-CA-CB	5.53	118.24	110.12
1	D	259	GLN	CA-C-O	-5.53	115.02	120.82
1	H	219	GLN	OE1-CD-NE2	5.53	128.13	122.60
1	L	150	GLN	CB-CA-C	-5.52	102.21	110.88
1	B	217	ILE	O-C-N	-5.52	116.69	123.09
1	D	58	SER	N-CA-C	-5.52	100.70	109.59
1	D	271	ALA	N-CA-CB	5.52	119.81	110.49
1	L	73	TYR	N-CA-C	-5.52	105.27	111.28
1	H	184	THR	N-CA-CB	5.52	118.32	110.16
1	A	251	SER	CA-C-N	5.51	125.18	119.56
1	A	251	SER	C-N-CA	5.51	125.18	119.56
1	I	275	HIS	CG-CD2-NE2	5.51	112.72	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	196	ARG	CA-C-N	5.51	128.01	120.46
1	J	196	ARG	C-N-CA	5.51	128.01	120.46
1	D	234	ASP	CA-CB-CG	5.51	118.11	112.60
1	I	179	GLN	CB-CG-CD	-5.51	103.23	112.60
1	H	287	VAL	CA-C-O	5.51	127.67	120.78
1	L	213	THR	N-CA-C	-5.51	104.12	112.99
1	A	86	PRO	CB-CA-C	5.51	118.19	110.98
1	L	232	GLY	CA-C-O	-5.51	114.82	121.98
1	G	125	VAL	O-C-N	-5.50	115.69	122.57
1	I	196	ARG	NE-CZ-NH1	-5.50	116.00	121.50
1	K	128	GLN	O-C-N	5.50	127.74	122.07
1	L	161	GLN	CA-C-N	5.50	127.65	120.28
1	L	161	GLN	C-N-CA	5.50	127.65	120.28
1	E	257	THR	CA-C-N	5.50	127.65	120.28
1	E	257	THR	C-N-CA	5.50	127.65	120.28
1	G	64	GLN	CG-CD-NE2	-5.50	108.16	116.40
1	J	78	ASN	CB-CA-C	-5.50	101.67	110.79
1	A	243	GLU	N-CA-C	5.49	117.35	111.36
1	B	244	ALA	CA-C-N	5.49	128.66	120.31
1	B	244	ALA	C-N-CA	5.49	128.66	120.31
1	D	198	ARG	N-CA-CB	5.49	118.19	110.12
1	K	288	ARG	CB-CA-C	-5.49	100.12	109.51
1	J	246	ARG	N-CA-C	5.49	115.92	109.60
1	G	166	ASP	N-CA-CB	5.49	118.28	110.16
1	K	115	GLU	CA-C-O	-5.49	114.73	120.88
1	C	83	GLN	N-CA-C	-5.49	105.46	111.82
1	G	225	GLN	N-CA-C	5.49	117.26	111.28
1	J	115	GLU	CA-C-O	-5.49	114.31	119.80
1	B	80	ILE	O-C-N	5.48	127.81	121.94
1	D	164	GLU	CB-CA-C	-5.48	101.69	110.79
1	J	130	LEU	CA-C-O	-5.48	112.65	120.16
1	C	213	THR	N-CA-CB	5.48	118.29	111.00
1	D	163	LEU	CA-C-O	-5.48	114.61	120.42
1	I	238	SER	N-CA-C	5.48	117.25	111.28
1	G	255	TYR	CA-C-N	5.48	127.62	120.28
1	G	255	TYR	C-N-CA	5.48	127.62	120.28
1	H	122	GLU	O-C-N	-5.48	117.56	121.83
1	L	188	VAL	CB-CA-C	5.48	119.54	112.14
1	A	246	ARG	NE-CZ-NH1	5.48	126.98	121.50
1	G	263	ASP	N-CA-CB	5.48	118.27	110.16
1	G	287	VAL	O-C-N	5.48	128.19	122.17
1	H	185	GLN	CG-CD-OE1	5.48	131.75	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	145	GLN	CB-CA-C	-5.47	102.25	110.90
1	A	252	PRO	N-CA-CB	5.47	108.95	103.48
1	G	258	LYS	N-CA-C	5.47	117.24	111.28
1	H	161	GLN	OE1-CD-NE2	5.46	128.06	122.60
1	G	111	ASP	N-CA-C	5.46	117.23	111.28
1	E	165	ARG	NE-CZ-NH1	5.46	126.96	121.50
1	K	66	ASP	CA-C-O	5.46	126.22	120.54
1	G	207	ALA	CA-C-O	-5.46	114.76	120.55
1	H	88	VAL	CA-CB-CG2	5.46	119.68	110.40
1	K	161	GLN	CB-CG-CD	-5.46	103.32	112.60
1	K	271	ALA	N-CA-C	-5.46	104.49	113.50
1	C	56	TRP	CE2-CD2-CE3	5.46	124.26	118.80
1	F	267	LEU	O-C-N	5.46	129.58	122.87
1	B	276	VAL	N-CA-C	-5.45	100.60	108.89
1	L	117	GLU	N-CA-CB	5.45	119.39	110.39
1	K	177	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	B	171	ILE	CA-C-N	5.45	127.58	120.28
1	B	171	ILE	C-N-CA	5.45	127.58	120.28
1	G	214	GLN	N-CA-C	-5.45	100.70	109.58
1	B	166	ASP	CA-C-N	5.45	127.58	120.28
1	B	166	ASP	C-N-CA	5.45	127.58	120.28
1	H	221	GLN	N-CA-CB	5.45	119.09	110.87
1	H	155	VAL	CA-C-N	5.44	127.57	120.28
1	H	155	VAL	C-N-CA	5.44	127.57	120.28
1	C	127	ASN	CA-CB-CG	5.44	118.04	112.60
1	F	129	GLN	N-CA-CB	5.44	119.68	110.49
1	A	57	THR	CA-C-N	5.44	130.82	122.93
1	A	57	THR	C-N-CA	5.44	130.82	122.93
1	G	212	ILE	N-CA-C	-5.44	100.50	108.11
1	K	122	GLU	N-CA-C	5.44	113.11	108.22
1	C	128	GLN	N-CA-CB	5.44	119.68	110.49
1	G	122	GLU	CB-CA-C	-5.44	103.04	110.22
1	G	201	GLU	CA-C-O	5.44	126.31	120.55
1	B	118	LYS	CB-CG-CD	5.43	123.80	111.30
1	H	210	ALA	CA-C-N	5.43	131.92	121.54
1	H	210	ALA	C-N-CA	5.43	131.92	121.54
1	H	81	TYR	O-C-N	-5.43	115.06	122.33
1	A	151	TYR	N-CA-C	5.42	117.27	111.36
1	A	166	ASP	N-CA-C	-5.42	105.45	111.36
1	B	77	MET	CG-SD-CE	-5.42	88.97	100.90
1	K	274	VAL	O-C-N	-5.42	116.79	122.81
1	J	217	ILE	CA-C-N	5.42	127.86	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	217	ILE	C-N-CA	5.42	127.86	120.54
1	C	180	ASP	CA-C-N	5.42	127.54	120.28
1	C	180	ASP	C-N-CA	5.42	127.54	120.28
1	F	257	THR	CA-C-N	5.42	127.98	120.29
1	F	257	THR	C-N-CA	5.42	127.98	120.29
1	J	61	ILE	N-CA-C	-5.42	100.39	108.46
1	C	288	ARG	N-CA-C	-5.41	99.58	108.41
1	G	169	ASP	N-CA-CB	5.41	118.17	110.16
1	G	86	PRO	CA-C-N	5.41	131.88	121.54
1	G	86	PRO	C-N-CA	5.41	131.88	121.54
1	F	137	VAL	CA-C-N	5.41	126.36	121.82
1	F	137	VAL	C-N-CA	5.41	126.36	121.82
1	A	275	HIS	ND1-CE1-NE2	5.41	113.81	108.40
1	C	126	LYS	N-CA-C	-5.41	100.08	108.90
1	K	180	ASP	O-C-N	-5.41	116.39	122.12
1	G	247	PRO	CB-CA-C	5.41	118.15	111.23
1	I	90	ASP	CA-CB-CG	5.41	118.00	112.60
1	J	212	ILE	N-CA-C	-5.40	100.54	108.11
1	K	168	LYS	O-C-N	-5.40	115.99	122.15
1	F	65	PRO	CA-C-O	-5.40	115.20	121.95
1	I	211	LYS	N-CA-CB	5.40	119.62	110.49
1	I	270	THR	N-CA-C	-5.40	99.63	108.76
1	A	267	LEU	N-CA-C	5.40	118.18	110.24
1	J	266	ASN	CA-CB-CG	-5.40	107.20	112.60
1	F	64	GLN	CA-C-N	5.40	125.70	119.92
1	F	64	GLN	C-N-CA	5.40	125.70	119.92
1	J	188	VAL	O-C-N	-5.40	116.63	121.87
1	A	134	VAL	N-CA-C	-5.40	100.54	108.85
1	D	255	TYR	N-CA-C	-5.40	105.48	111.36
1	E	195	LEU	CB-CA-C	-5.40	101.83	110.79
1	F	89	SER	N-CA-CB	5.40	118.05	110.12
1	C	216	GLN	OE1-CD-NE2	5.40	128.00	122.60
1	B	261	LEU	CB-CA-C	-5.39	101.83	110.79
1	G	80	ILE	O-C-N	-5.39	116.29	121.90
1	A	265	LYS	CA-C-O	5.39	126.17	119.97
1	H	230	LEU	N-CA-CB	5.39	118.53	110.22
1	D	287	VAL	CA-C-N	5.39	128.74	120.82
1	D	287	VAL	C-N-CA	5.39	128.74	120.82
1	I	159	VAL	CA-C-N	5.39	127.50	120.28
1	I	159	VAL	C-N-CA	5.39	127.50	120.28
1	H	180	ASP	N-CA-CB	5.39	118.04	110.12
1	H	209	GLU	CA-C-O	5.39	126.13	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	GLN	N-CA-CB	5.38	119.58	110.49
1	C	177	ASN	CB-CA-C	-5.38	102.43	110.88
1	J	154	GLN	CA-C-O	-5.38	114.85	120.55
1	L	201	GLU	O-C-N	-5.38	116.42	122.12
1	A	200	ILE	CB-CA-C	5.38	119.40	112.14
1	H	202	GLU	N-CA-CB	5.38	117.86	110.07
1	B	164	GLU	CA-C-N	5.37	127.48	120.28
1	B	164	GLU	C-N-CA	5.37	127.48	120.28
1	J	272	ASP	CA-CB-CG	-5.37	107.23	112.60
1	A	265	LYS	CA-C-N	5.37	127.92	120.29
1	A	265	LYS	C-N-CA	5.37	127.92	120.29
1	F	100	SER	CA-C-O	-5.37	115.18	120.82
1	I	106	LEU	CA-C-N	5.37	127.48	120.28
1	I	106	LEU	C-N-CA	5.37	127.48	120.28
1	L	93	GLU	O-C-N	5.37	128.27	122.15
1	G	211	LYS	CA-C-N	-5.36	116.11	123.14
1	G	211	LYS	C-N-CA	-5.36	116.11	123.14
1	B	192	GLN	CB-CA-C	5.36	119.96	110.85
1	B	227	THR	O-C-N	-5.36	115.76	122.35
1	F	227	THR	CA-C-O	5.36	124.60	119.08
1	F	257	THR	N-CA-C	5.36	116.93	111.14
1	C	117	GLU	N-CA-C	-5.36	99.39	110.80
1	L	62	ILE	CA-CB-CG2	-5.36	101.40	110.50
1	A	101	SER	CB-CA-C	-5.35	101.90	110.79
1	J	114	GLU	N-CA-C	-5.35	106.70	113.18
1	A	212	ILE	N-CA-C	-5.35	97.93	107.18
1	G	254	TYR	N-CA-C	5.35	117.11	111.28
1	I	250	PHE	CB-CG-CD2	-5.34	111.61	120.70
1	J	221	GLN	OE1-CD-NE2	5.34	127.94	122.60
1	G	238	SER	CA-C-N	5.34	127.44	120.28
1	G	238	SER	C-N-CA	5.34	127.44	120.28
1	J	187	VAL	N-CA-CB	5.34	116.80	110.55
1	K	125	VAL	CB-CA-C	-5.34	103.55	111.19
1	H	73	TYR	N-CA-C	-5.34	105.54	111.36
1	D	186	GLU	CA-CB-CG	5.34	124.78	114.10
1	G	128	GLN	OE1-CD-NE2	-5.34	117.26	122.60
1	C	236	LEU	CA-C-N	5.34	127.43	120.28
1	C	236	LEU	C-N-CA	5.34	127.43	120.28
1	E	122	GLU	O-C-N	-5.34	116.85	121.71
1	D	152	ILE	N-CA-C	5.33	115.54	110.42
1	C	174	GLY	CA-C-N	5.33	127.43	120.28
1	C	174	GLY	C-N-CA	5.33	127.43	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	238	SER	CA-C-O	-5.33	114.90	120.55
1	I	252	PRO	CA-C-N	5.33	127.86	120.29
1	I	252	PRO	C-N-CA	5.33	127.86	120.29
1	C	181	SER	N-CA-C	-5.33	105.47	111.28
1	D	152	ILE	O-C-N	5.33	127.13	121.91
1	A	232	GLY	CA-C-N	5.33	128.41	120.31
1	A	232	GLY	C-N-CA	5.33	128.41	120.31
1	K	282	LYS	N-CA-CB	5.33	115.51	109.49
1	B	257	THR	CA-C-O	-5.32	115.22	120.70
1	J	224	THR	CB-CA-C	5.32	121.79	110.19
1	D	122	GLU	CA-C-N	5.32	125.49	119.90
1	D	122	GLU	C-N-CA	5.32	125.49	119.90
1	K	64	GLN	CA-C-N	5.32	126.49	119.84
1	K	64	GLN	C-N-CA	5.32	126.49	119.84
1	A	73	TYR	N-CA-CB	-5.32	102.36	110.07
1	A	121	ILE	N-CA-C	-5.32	100.58	108.45
1	C	271	ALA	N-CA-C	-5.32	99.48	110.80
1	G	149	ALA	CB-CA-C	-5.32	101.97	110.79
1	L	261	LEU	N-CA-CB	5.31	117.93	110.12
1	D	104	SER	CA-C-N	5.31	127.40	120.28
1	D	104	SER	C-N-CA	5.31	127.40	120.28
1	F	214	GLN	CA-C-O	-5.31	115.61	120.50
1	F	279	TYR	CB-CA-C	-5.31	101.35	110.22
1	J	66	ASP	CA-C-O	-5.31	114.48	120.43
1	D	208	ASP	CA-C-N	5.31	127.39	120.28
1	D	208	ASP	C-N-CA	5.31	127.39	120.28
1	I	272	ASP	CA-CB-CG	5.31	117.91	112.60
1	L	72	GLY	CA-C-N	5.31	127.39	120.28
1	L	72	GLY	C-N-CA	5.31	127.39	120.28
1	L	259	GLN	OE1-CD-NE2	5.31	127.91	122.60
1	K	255	TYR	CB-CG-CD1	5.31	128.76	120.80
1	B	216	GLN	CA-C-N	5.30	130.58	122.25
1	B	216	GLN	C-N-CA	5.30	130.58	122.25
1	F	280	VAL	CA-C-O	-5.30	115.03	120.71
1	D	86	PRO	CA-C-N	5.30	131.67	121.54
1	D	86	PRO	C-N-CA	5.30	131.67	121.54
1	A	92	GLN	OE1-CD-NE2	5.30	127.90	122.60
1	B	219	GLN	OE1-CD-NE2	5.30	127.90	122.60
1	L	138	GLY	O-C-N	-5.30	119.87	123.95
1	F	244	ALA	N-CA-C	5.30	117.05	111.28
1	H	112	ASN	CB-CG-ND2	-5.30	108.45	116.40
1	F	266	ASN	CA-C-N	5.29	128.22	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	266	ASN	C-N-CA	5.29	128.22	120.71
1	D	151	TYR	CB-CG-CD2	-5.29	112.86	120.80
1	J	181	SER	O-C-N	5.29	127.73	122.12
1	H	100	SER	N-CA-CB	5.29	117.68	110.01
1	B	183	ARG	N-CA-C	-5.29	105.43	111.14
1	K	153	GLN	N-CA-C	5.29	117.12	111.36
1	D	85	ALA	N-CA-C	5.29	121.49	109.81
1	I	259	GLN	CA-C-N	5.29	127.79	120.29
1	I	259	GLN	C-N-CA	5.29	127.79	120.29
1	B	87	LYS	CB-CA-C	-5.28	99.46	110.40
1	D	151	TYR	CB-CA-C	-5.28	101.87	110.85
1	K	80	ILE	CA-CB-CG1	5.28	119.38	110.40
1	K	253	ALA	N-CA-C	5.28	117.12	111.36
1	E	168	LYS	CA-C-O	-5.28	114.95	120.55
1	H	145	GLN	CA-C-O	-5.28	114.82	120.42
1	D	242	ASN	CA-CB-CG	-5.28	107.32	112.60
1	F	251	SER	CA-C-N	5.28	124.94	119.56
1	F	251	SER	C-N-CA	5.28	124.94	119.56
1	B	250	PHE	CA-CB-CG	-5.28	108.52	113.80
1	I	226	ASP	N-CA-C	-5.28	106.52	113.17
1	J	161	GLN	O-C-N	-5.28	116.13	122.15
1	B	60	ALA	O-C-N	-5.28	117.23	123.25
1	D	122	GLU	CB-CA-C	5.28	117.09	109.92
1	C	84	ALA	CA-C-O	-5.27	113.90	119.97
1	I	197	ILE	CA-C-N	5.27	127.35	120.28
1	I	197	ILE	C-N-CA	5.27	127.35	120.28
1	L	101	SER	CA-C-N	5.27	127.35	120.28
1	L	101	SER	C-N-CA	5.27	127.35	120.28
1	B	209	GLU	CA-C-N	5.27	127.87	120.28
1	B	209	GLU	C-N-CA	5.27	127.87	120.28
1	H	248	LEU	N-CA-CB	5.27	117.79	110.04
1	G	109	THR	CA-C-N	5.27	127.34	120.28
1	G	109	THR	C-N-CA	5.27	127.34	120.28
1	K	98	ARG	CB-CA-C	-5.27	102.57	110.90
1	E	271	ALA	N-CA-C	-5.27	105.83	113.21
1	H	95	LEU	CA-C-O	-5.27	115.28	120.70
1	I	169	ASP	CA-CB-CG	5.27	117.87	112.60
1	D	239	MET	O-C-N	5.26	127.70	122.12
1	F	103	PHE	CB-CG-CD1	-5.26	111.75	120.70
1	F	134	VAL	CA-CB-CG1	5.26	119.35	110.40
1	G	166	ASP	CA-CB-CG	-5.26	107.34	112.60
1	A	282	LYS	CA-C-O	-5.26	114.75	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	182	LEU	CB-CA-C	-5.26	102.06	110.79
1	H	259	GLN	CA-CB-CG	5.26	124.62	114.10
1	I	193	LYS	CA-CB-CG	5.26	124.62	114.10
1	B	269	VAL	N-CA-CB	5.26	116.78	110.31
1	L	128	GLN	N-CA-CB	5.26	117.51	109.94
1	I	157	ASP	N-CA-CB	5.25	117.94	110.16
1	I	214	GLN	CA-C-O	-5.25	115.67	120.50
1	L	203	ALA	CA-C-O	-5.25	114.16	120.10
1	B	255	TYR	CA-C-N	5.25	127.32	120.28
1	B	255	TYR	C-N-CA	5.25	127.32	120.28
1	H	260	THR	N-CA-CB	5.25	117.84	110.12
1	I	118	LYS	O-C-N	5.25	129.47	123.27
1	A	103	PHE	CA-C-N	5.25	127.75	120.29
1	A	103	PHE	C-N-CA	5.25	127.75	120.29
1	D	68	GLY	O-C-N	-5.25	117.15	122.19
1	G	184	THR	N-CA-C	5.25	117.08	111.36
1	G	266	ASN	O-C-N	5.25	127.69	122.12
1	L	252	PRO	CA-C-O	-5.25	111.67	119.18
1	D	150	GLN	CA-C-O	-5.25	114.99	120.55
1	J	273	THR	CA-CB-OG1	5.25	117.47	109.60
1	C	242	ASN	N-CA-CB	5.24	117.60	110.42
1	D	241	GLN	CA-C-O	-5.24	114.99	120.55
1	J	115	GLU	N-CA-CB	5.24	119.28	109.68
1	K	142	GLU	CA-C-N	5.24	125.80	119.98
1	K	142	GLU	C-N-CA	5.24	125.80	119.98
1	E	234	ASP	CA-C-O	-5.24	114.99	120.55
1	G	152	ILE	CA-C-O	5.24	126.40	120.95
1	G	187	VAL	CA-C-N	5.24	127.86	120.42
1	G	187	VAL	C-N-CA	5.24	127.86	120.42
1	A	174	GLY	CA-C-N	5.24	127.73	120.29
1	A	174	GLY	C-N-CA	5.24	127.73	120.29
1	B	217	ILE	CB-CA-C	-5.24	101.61	111.30
1	L	66	ASP	N-CA-C	-5.24	99.24	108.20
1	G	68	GLY	CA-C-N	5.24	127.72	120.29
1	G	68	GLY	C-N-CA	5.24	127.72	120.29
1	A	288	ARG	N-CA-C	-5.23	100.64	109.07
1	C	78	ASN	CA-C-N	5.23	127.63	120.46
1	C	78	ASN	C-N-CA	5.23	127.63	120.46
1	D	164	GLU	CA-C-N	5.23	127.29	120.28
1	D	164	GLU	C-N-CA	5.23	127.29	120.28
1	D	253	ALA	CA-C-O	-5.23	115.00	120.55
1	K	160	ASN	N-CA-C	5.23	116.98	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	128	GLN	CA-CB-CG	5.23	124.56	114.10
1	I	162	GLU	CB-CA-C	-5.23	101.96	110.85
1	K	146	MET	CA-C-N	5.23	127.71	120.29
1	K	146	MET	C-N-CA	5.23	127.71	120.29
1	B	82	GLY	CA-C-N	5.23	128.25	120.31
1	B	82	GLY	C-N-CA	5.23	128.25	120.31
1	K	196	ARG	O-C-N	-5.22	116.58	122.12
1	B	135	SER	CB-CA-C	-5.22	98.82	109.94
1	C	212	ILE	CB-CA-C	5.22	118.19	110.77
1	D	213	THR	N-CA-C	-5.22	105.24	113.02
1	K	189	ALA	N-CA-CB	5.22	117.58	110.01
1	D	154	GLN	CA-C-N	5.22	127.83	120.42
1	D	154	GLN	C-N-CA	5.22	127.83	120.42
1	G	179	GLN	CB-CG-CD	-5.22	103.73	112.60
1	G	278	ARG	CD-NE-CZ	-5.22	117.10	124.40
1	C	165	ARG	CA-C-N	5.21	127.69	120.29
1	C	165	ARG	C-N-CA	5.21	127.69	120.29
1	G	83	GLN	CB-CG-CD	-5.21	103.74	112.60
1	I	186	GLU	CA-C-N	5.21	127.13	120.56
1	I	186	GLU	C-N-CA	5.21	127.13	120.56
1	K	71	ALA	N-CA-C	5.21	116.96	111.28
1	C	255	TYR	CA-C-O	5.21	125.94	120.42
1	E	103	PHE	N-CA-C	5.21	117.04	111.36
1	F	218	GLN	CG-CD-NE2	-5.21	108.59	116.40
1	L	56	TRP	N-CA-C	-5.21	100.54	109.24
1	B	167	LEU	CA-C-N	5.21	127.68	120.29
1	B	167	LEU	C-N-CA	5.21	127.68	120.29
1	D	144	ALA	CA-C-N	5.21	127.68	120.29
1	D	144	ALA	C-N-CA	5.21	127.68	120.29
1	G	60	ALA	CA-C-O	-5.21	115.71	121.33
1	B	127	ASN	CA-C-O	-5.20	115.34	120.70
1	B	246	ARG	N-CA-C	5.20	121.31	109.81
1	J	288	ARG	NE-CZ-NH1	-5.20	116.30	121.50
1	L	132	LEU	CA-C-O	-5.20	115.08	120.70
1	L	156	ASP	CA-C-N	5.20	127.25	120.28
1	L	156	ASP	C-N-CA	5.20	127.25	120.28
1	J	279	TYR	CB-CA-C	-5.20	101.77	110.19
1	B	63	THR	CA-C-N	5.19	134.47	121.80
1	B	63	THR	C-N-CA	5.19	134.47	121.80
1	I	102	ALA	CA-C-O	5.19	126.05	120.70
1	L	224	THR	CA-CB-OG1	5.19	117.39	109.60
1	D	288	ARG	CA-C-O	-5.19	115.83	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	273	THR	O-C-N	-5.19	115.96	122.24
1	J	71	ALA	CB-CA-C	-5.19	102.17	110.79
1	J	88	VAL	CA-C-N	5.19	127.24	120.28
1	J	88	VAL	C-N-CA	5.19	127.24	120.28
1	K	109	THR	CA-C-N	5.19	128.20	120.31
1	K	109	THR	C-N-CA	5.19	128.20	120.31
1	I	214	GLN	N-CA-C	-5.19	100.46	108.55
1	B	70	ILE	CA-CB-CG2	-5.19	101.68	110.50
1	A	290	ASP	N-CA-C	-5.18	101.53	109.41
1	B	287	VAL	N-CA-C	-5.18	108.24	113.47
1	G	145	GLN	O-C-N	5.18	127.41	122.07
1	J	223	VAL	CA-C-N	5.18	130.80	121.06
1	J	223	VAL	C-N-CA	5.18	130.80	121.06
1	G	288	ARG	CA-C-N	5.18	130.15	123.00
1	G	288	ARG	C-N-CA	5.18	130.15	123.00
1	A	112	ASN	CA-CB-CG	-5.18	107.42	112.60
1	H	256	GLN	CG-CD-NE2	5.18	124.16	116.40
1	B	262	LEU	N-CA-C	5.17	116.92	111.28
1	G	70	ILE	O-C-N	-5.17	115.38	122.26
1	E	113	GLN	OE1-CD-NE2	5.17	127.77	122.60
1	H	72	GLY	CA-C-N	5.17	127.64	120.29
1	H	72	GLY	C-N-CA	5.17	127.64	120.29
1	K	81	TYR	CB-CA-C	-5.17	101.23	110.70
1	H	73	TYR	CA-CB-CG	-5.17	104.59	113.90
1	J	222	ASP	CA-CB-CG	5.17	117.77	112.60
1	H	251	SER	CB-CA-C	5.17	116.52	108.61
1	K	144	ALA	O-C-N	5.17	127.60	122.12
1	F	128	GLN	CB-CG-CD	-5.17	103.82	112.60
1	D	286	PRO	N-CA-CB	5.16	108.24	103.39
1	H	160	ASN	CA-CB-CG	5.16	117.76	112.60
1	H	198	ARG	N-CA-C	-5.16	105.65	111.28
1	K	109	THR	N-CA-CB	5.16	117.71	110.12
1	G	119	LEU	N-CA-C	-5.16	100.99	109.40
1	L	230	LEU	CA-C-N	5.16	128.16	120.31
1	L	230	LEU	C-N-CA	5.16	128.16	120.31
1	C	112	ASN	CA-C-N	5.16	128.04	120.71
1	C	112	ASN	C-N-CA	5.16	128.04	120.71
1	L	60	ALA	N-CA-C	-5.16	101.22	109.07
1	B	223	VAL	N-CA-C	-5.16	100.76	107.88
1	G	239	MET	N-CA-CB	5.15	117.69	110.12
1	I	274	VAL	CB-CA-C	5.15	118.74	111.63
1	A	251	SER	O-C-N	-5.15	115.76	121.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	214	GLN	CG-CD-NE2	5.15	124.13	116.40
1	I	92	GLN	CA-C-N	5.15	127.61	120.29
1	I	92	GLN	C-N-CA	5.15	127.61	120.29
1	A	248	LEU	N-CA-CB	5.15	117.49	110.38
1	I	123	PRO	N-CA-CB	5.15	108.13	103.34
1	H	214	GLN	N-CA-C	-5.15	99.90	109.06
1	C	188	VAL	N-CA-CB	5.15	118.30	110.58
1	D	62	ILE	O-C-N	5.15	128.75	123.04
1	D	107	ALA	O-C-N	5.14	127.57	122.12
1	G	274	VAL	N-CA-CB	5.14	119.79	111.36
1	H	237	LYS	N-CA-CB	-5.14	102.56	110.12
1	I	213	THR	CB-CA-C	-5.14	102.53	109.16
1	A	111	ASP	O-C-N	5.14	127.57	122.12
1	J	249	ALA	O-C-N	-5.14	116.33	122.65
1	H	114	GLU	N-CA-C	-5.14	106.79	113.16
1	G	108	GLU	CA-C-O	-5.14	114.97	120.42
1	G	154	GLN	CA-C-N	5.14	127.71	120.42
1	G	154	GLN	C-N-CA	5.14	127.71	120.42
1	A	179	GLN	O-C-N	5.13	127.56	122.12
1	B	190	GLN	OE1-CD-NE2	5.13	127.73	122.60
1	E	213	THR	N-CA-C	-5.13	105.78	113.89
1	I	182	LEU	N-CA-C	5.13	116.96	111.36
1	G	79	VAL	N-CA-CB	5.13	116.56	110.55
1	A	151	TYR	CB-CA-C	-5.13	102.13	110.85
1	F	90	ASP	CA-CB-CG	-5.13	107.47	112.60
1	J	159	VAL	N-CA-CB	5.13	117.52	110.54
1	J	258	LYS	CA-C-N	5.13	127.11	120.44
1	J	258	LYS	C-N-CA	5.13	127.11	120.44
1	H	199	GLN	CA-C-N	5.13	127.48	120.46
1	H	199	GLN	C-N-CA	5.13	127.48	120.46
1	J	209	GLU	N-CA-C	5.13	116.95	111.36
1	J	285	LEU	N-CA-CB	5.13	118.37	110.12
1	K	265	LYS	CA-C-N	5.13	127.15	120.28
1	K	265	LYS	C-N-CA	5.13	127.15	120.28
1	F	92	GLN	O-C-N	5.12	127.55	122.12
1	F	223	VAL	CB-CA-C	5.12	119.24	110.38
1	J	133	THR	CA-CB-OG1	5.12	117.28	109.60
1	C	256	GLN	N-CA-C	5.12	116.86	111.28
1	G	178	LEU	N-CA-CB	5.12	117.64	110.12
1	C	151	TYR	CG-CD1-CE1	-5.12	113.52	121.20
1	A	167	LEU	N-CA-CB	5.11	117.42	110.01
1	L	95	LEU	CB-CA-C	-5.11	102.86	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	252	PRO	O-C-N	5.11	129.09	122.24
1	F	145	GLN	CG-CD-NE2	-5.11	108.74	116.40
1	F	214	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	B	150	GLN	O-C-N	-5.11	116.71	122.12
1	D	219	GLN	CG-CD-NE2	-5.11	108.74	116.40
1	D	220	THR	N-CA-CB	5.11	120.27	111.13
1	K	180	ASP	CA-C-O	5.11	125.96	120.55
1	K	188	VAL	CB-CA-C	5.11	119.27	112.22
1	L	178	LEU	CA-C-O	-5.11	115.01	120.42
1	E	184	THR	CA-C-O	5.10	125.96	120.55
1	F	100	SER	N-CA-CB	5.10	117.41	110.01
1	F	182	LEU	CA-C-O	5.10	125.96	120.55
1	H	140	THR	CA-C-N	5.10	127.08	120.44
1	H	140	THR	C-N-CA	5.10	127.08	120.44
1	C	286	PRO	CB-CA-C	5.10	118.04	111.46
1	D	126	LYS	N-CA-CB	5.10	120.47	112.46
1	F	97	GLY	CA-C-N	5.10	127.53	120.29
1	F	97	GLY	C-N-CA	5.10	127.53	120.29
1	G	262	LEU	CA-C-N	5.10	127.53	120.29
1	G	262	LEU	C-N-CA	5.10	127.53	120.29
1	L	258	LYS	N-CA-C	5.10	116.84	111.28
1	A	105	ALA	N-CA-CB	5.10	117.61	110.12
1	B	156	ASP	CA-C-O	5.10	125.95	120.55
1	B	203	ALA	CA-C-N	5.10	127.53	120.29
1	B	203	ALA	C-N-CA	5.10	127.53	120.29
1	C	290	ASP	N-CA-CB	5.10	116.33	111.59
1	K	127	ASN	CA-C-N	5.10	127.07	120.44
1	K	127	ASN	C-N-CA	5.10	127.07	120.44
1	H	125	VAL	CA-CB-CG2	5.10	119.06	110.40
1	J	130	LEU	O-C-N	-5.10	115.46	121.32
1	A	118	LYS	N-CA-C	-5.09	100.22	108.52
1	D	113	GLN	CA-C-N	5.09	127.37	120.44
1	D	113	GLN	C-N-CA	5.09	127.37	120.44
1	H	274	VAL	N-CA-CB	5.09	117.59	110.56
1	A	249	ALA	CA-C-O	-5.09	115.48	121.44
1	L	164	GLU	N-CA-CB	5.09	117.70	110.16
1	I	102	ALA	N-CA-C	5.09	116.64	111.14
1	H	93	GLU	N-CA-C	-5.09	105.82	111.36
1	B	122	GLU	CA-C-N	5.08	124.84	119.76
1	B	122	GLU	C-N-CA	5.08	124.84	119.76
1	G	78	ASN	CA-C-O	-5.08	115.16	120.55
1	E	240	ILE	N-CA-C	-5.08	105.75	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	278	ARG	N-CA-C	-5.08	101.35	109.23
1	L	135	SER	N-CA-C	-5.08	101.35	109.07
1	D	250	PHE	CA-C-O	5.08	127.14	121.40
1	D	262	LEU	CB-CA-C	-5.08	102.91	110.88
1	J	145	GLN	N-CA-C	-5.08	105.82	111.36
1	H	183	ARG	NE-CZ-NH1	-5.08	116.42	121.50
1	A	268	LYS	CA-C-N	5.08	129.16	122.51
1	A	268	LYS	C-N-CA	5.08	129.16	122.51
1	E	277	TYR	N-CA-C	-5.08	101.19	108.60
1	G	214	GLN	CA-C-O	-5.08	114.72	120.46
1	B	121	ILE	CA-C-O	-5.07	115.18	120.76
1	C	120	THR	CA-CB-CG2	5.07	119.12	110.50
1	E	256	GLN	N-CA-CB	5.07	117.58	110.12
1	C	169	ASP	CA-CB-CG	5.07	117.67	112.60
1	F	254	TYR	N-CA-C	5.07	116.81	111.28
1	G	279	TYR	CB-CG-CD2	-5.07	113.20	120.80
1	J	271	ALA	CA-C-N	5.07	129.16	122.42
1	J	271	ALA	C-N-CA	5.07	129.16	122.42
1	E	205	ARG	N-CA-C	5.07	116.88	111.36
1	E	214	GLN	N-CA-C	-5.07	103.66	108.22
1	F	164	GLU	CA-C-N	5.07	127.33	120.44
1	F	164	GLU	C-N-CA	5.07	127.33	120.44
1	L	175	ARG	N-CA-CB	-5.07	102.67	110.12
1	C	237	LYS	N-CA-C	-5.06	105.76	111.28
1	D	206	TYR	CB-CG-CD2	-5.06	113.20	120.80
1	A	74	ASN	CA-C-O	-5.06	115.50	120.82
1	B	242	ASN	CA-C-N	5.06	127.48	120.29
1	B	242	ASN	C-N-CA	5.06	127.48	120.29
1	C	105	ALA	CB-CA-C	-5.06	102.39	110.79
1	H	107	ALA	CA-C-N	5.06	127.02	120.44
1	H	107	ALA	C-N-CA	5.06	127.02	120.44
1	B	91	LEU	CA-C-N	5.06	127.32	120.44
1	B	91	LEU	C-N-CA	5.06	127.32	120.44
1	C	67	VAL	N-CA-C	5.06	115.83	110.72
1	L	155	VAL	CB-CA-C	5.06	118.97	112.14
1	E	161	GLN	CA-C-N	5.06	127.47	120.29
1	E	161	GLN	C-N-CA	5.06	127.47	120.29
1	E	275	HIS	N-CA-C	-5.06	101.68	109.52
1	G	84	ALA	O-C-N	5.06	128.14	122.22
1	J	251	SER	CA-C-N	5.06	124.84	119.28
1	J	251	SER	C-N-CA	5.06	124.84	119.28
1	G	189	ALA	CB-CA-C	-5.06	102.40	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	206	TYR	O-C-N	5.06	127.48	122.12
1	I	197	ILE	N-CA-CB	5.06	117.42	110.54
1	D	74	ASN	CB-CA-C	-5.05	102.95	110.88
1	E	84	ALA	N-CA-CB	-5.05	102.44	110.22
1	I	155	VAL	O-C-N	-5.05	116.63	121.83
1	I	167	LEU	CA-C-N	5.05	127.05	120.28
1	I	167	LEU	C-N-CA	5.05	127.05	120.28
1	B	155	VAL	N-CA-C	-5.05	105.62	110.72
1	F	204	LEU	CA-C-O	5.05	125.81	120.10
1	K	196	ARG	NH1-CZ-NH2	-5.05	112.73	119.30
1	I	216	GLN	N-CA-C	-5.05	106.97	113.23
1	G	144	ALA	CA-C-O	5.05	125.90	120.55
1	D	247	PRO	O-C-N	5.04	129.40	122.99
1	K	74	ASN	CB-CA-C	-5.04	102.27	110.85
1	D	275	HIS	ND1-CE1-NE2	5.04	113.44	108.40
1	F	140	THR	N-CA-C	-5.04	100.12	108.75
1	L	63	THR	N-CA-C	-5.04	102.10	108.45
1	F	60	ALA	N-CA-C	-5.04	101.08	108.99
1	L	196	ARG	CA-C-N	5.04	127.36	120.46
1	L	196	ARG	C-N-CA	5.04	127.36	120.46
1	L	247	PRO	N-CA-CB	-5.04	97.96	103.25
1	C	104	SER	CA-C-N	5.04	127.03	120.28
1	C	104	SER	C-N-CA	5.04	127.03	120.28
1	D	288	ARG	NE-CZ-NH1	-5.04	116.46	121.50
1	H	202	GLU	CB-CA-C	-5.04	102.94	110.90
1	F	111	ASP	N-CA-CB	5.03	117.52	110.12
1	K	245	THR	CA-C-N	5.03	134.08	121.80
1	K	245	THR	C-N-CA	5.03	134.08	121.80
1	L	206	TYR	CA-C-N	5.03	127.44	120.29
1	L	206	TYR	C-N-CA	5.03	127.44	120.29
1	G	282	LYS	CA-C-N	5.03	125.31	119.93
1	G	282	LYS	C-N-CA	5.03	125.31	119.93
1	L	132	LEU	N-CA-C	-5.03	101.20	109.40
1	C	190	GLN	CA-C-N	5.03	127.43	120.29
1	C	190	GLN	C-N-CA	5.03	127.43	120.29
1	I	213	THR	O-C-N	5.03	127.82	121.64
1	I	255	TYR	CA-C-N	5.03	127.02	120.28
1	I	255	TYR	C-N-CA	5.03	127.02	120.28
1	A	196	ARG	N-CA-CB	5.03	117.51	110.12
1	E	162	GLU	N-CA-C	-5.03	105.88	111.36
1	F	265	LYS	CA-C-O	-5.03	114.19	119.97
1	J	268	LYS	CA-C-O	5.03	126.72	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	267	LEU	CA-C-N	5.02	130.48	122.59
1	F	267	LEU	C-N-CA	5.02	130.48	122.59
1	J	221	GLN	CA-CB-CG	5.02	124.15	114.10
1	H	129	GLN	N-CA-CB	5.02	120.12	111.13
1	I	244	ALA	N-CA-C	5.02	116.75	111.28
1	D	221	GLN	CB-CG-CD	-5.02	104.07	112.60
1	I	65	PRO	CA-C-N	5.02	128.47	121.24
1	I	65	PRO	C-N-CA	5.02	128.47	121.24
1	E	206	TYR	N-CA-C	-5.02	105.72	111.14
1	E	252	PRO	CA-C-N	5.01	127.41	120.29
1	E	252	PRO	C-N-CA	5.01	127.41	120.29
1	G	153	GLN	CA-C-O	-5.01	115.10	120.42
1	G	71	ALA	O-C-N	5.01	127.43	122.12
1	I	83	GLN	O-C-N	-5.01	116.11	122.27
1	L	76	ALA	CA-C-N	5.01	127.00	120.28
1	L	76	ALA	C-N-CA	5.01	127.00	120.28
1	A	66	ASP	O-C-N	5.01	128.74	122.63
1	C	100	SER	CA-C-O	-5.01	115.24	120.55
1	D	199	GLN	N-CA-CB	5.01	117.48	110.12
1	D	287	VAL	N-CA-C	-5.01	107.06	113.22
1	L	125	VAL	CB-CA-C	5.01	119.51	111.29
1	J	79	VAL	CB-CA-C	5.01	119.13	112.22
1	D	265	LYS	CA-C-O	5.01	125.73	119.97
1	E	181	SER	O-C-N	5.00	127.86	122.15
1	I	199	GLN	OE1-CD-NE2	-5.00	117.60	122.60
1	F	201	GLU	O-C-N	5.00	127.42	122.12

There are no chirality outliers.

All (68) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	ARG	Sidechain
1	A	206	TYR	Sidechain
1	A	277	TYR	Sidechain
1	A	73	TYR	Sidechain
1	A	81	TYR	Sidechain
1	B	151	TYR	Sidechain
1	B	205	ARG	Sidechain
1	B	250	PHE	Sidechain
1	B	254	TYR	Sidechain
1	B	99	PHE	Sidechain
1	C	151	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	C	205	ARG	Sidechain
1	C	229	PHE	Sidechain
1	C	81	TYR	Sidechain
1	D	136	TYR	Sidechain
1	D	196	ARG	Sidechain
1	D	255	TYR	Sidechain
1	D	277	TYR	Sidechain
1	D	73	TYR	Sidechain
1	E	136	TYR	Sidechain
1	E	183	ARG	Sidechain
1	E	81	TYR	Sidechain
1	F	103	PHE	Sidechain
1	F	205	ARG	Sidechain
1	F	255	TYR	Sidechain
1	F	279	TYR	Sidechain
1	F	289	ARG	Sidechain
1	F	81	TYR	Sidechain
1	G	151	TYR	Sidechain
1	G	229	PHE	Sidechain
1	G	277	TYR	Sidechain
1	G	73	TYR	Sidechain
1	G	98	ARG	Sidechain
1	H	136	TYR	Sidechain
1	H	246	ARG	Sidechain
1	H	277	TYR	Sidechain
1	H	279	TYR	Sidechain
1	H	73	TYR	Sidechain
1	I	151	TYR	Sidechain
1	I	175	ARG	Sidechain
1	I	255	TYR	Sidechain
1	I	279	TYR	Sidechain
1	I	288	ARG	Sidechain
1	I	81	TYR	Sidechain
1	I	98	ARG	Sidechain
1	J	103	PHE	Sidechain
1	J	136	TYR	Sidechain
1	J	165	ARG	Sidechain
1	J	196	ARG	Sidechain
1	J	206	TYR	Sidechain
1	J	246	ARG	Sidechain
1	J	250	PHE	Sidechain
1	J	255	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	J	277	TYR	Sidechain
1	J	279	TYR	Sidechain
1	J	81	TYR	Sidechain
1	K	206	TYR	Sidechain
1	K	254	TYR	Sidechain
1	K	255	TYR	Sidechain
1	K	279	TYR	Sidechain
1	K	73	TYR	Sidechain
1	K	98	ARG	Sidechain
1	K	99	PHE	Sidechain
1	L	151	TYR	Sidechain
1	L	198	ARG	Sidechain
1	L	205	ARG	Sidechain
1	L	277	TYR	Sidechain
1	L	73	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1879	1892	1889	1	0
1	B	1879	1892	1889	4	0
1	C	1879	1892	1889	7	0
1	D	1879	1892	1889	3	0
1	E	1879	1892	1889	6	0
1	F	1879	1892	1889	6	0
1	G	1879	1892	1889	2	0
1	H	1879	1892	1889	9	0
1	I	1879	1892	1889	3	0
1	J	1879	1892	1889	5	0
1	K	1879	1892	1889	2	0
1	L	1879	1892	1889	2	0
All	All	22548	22704	22668	44	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (44) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:210:ALA:HA	1:F:234:ASP:HB3	1.85	0.58
1:E:111:ASP:OD1	1:F:285:LEU:HD13	2.06	0.55
1:J:88:VAL:HG22	1:J:92:GLN:HE21	1.71	0.55
1:B:214:GLN:HB3	1:B:215:PRO:HD2	1.90	0.54
1:F:94:THR:HG23	1:G:278:ARG:NH2	2.25	0.51
1:D:92:GLN:O	1:D:96:ILE:HG22	2.10	0.51
1:J:193:LYS:HD2	1:J:248:LEU:HD23	1.94	0.50
1:E:99:PHE:CD1	1:E:276:VAL:HG21	2.47	0.50
1:F:85:ALA:HB1	1:F:86:PRO:HD2	1.95	0.49
1:L:124:SER:HB2	1:L:133:THR:HB	1.95	0.49
1:A:56:TRP:CE3	1:A:141:ALA:HB2	2.48	0.48
1:K:204:LEU:HD23	1:K:236:LEU:HB2	1.95	0.47
1:D:156:ASP:OD2	1:D:276:VAL:HG22	2.15	0.47
1:J:129:GLN:HB2	1:J:131:PRO:HD3	1.97	0.46
1:I:248:LEU:HD12	1:I:250:PHE:CE1	2.50	0.46
1:H:68:GLY:O	1:H:71:ALA:HB3	2.17	0.45
1:K:60:ALA:HB2	1:K:148:LEU:HD21	1.97	0.45
1:L:201:GLU:HA	1:L:240:ILE:HD11	1.98	0.45
1:B:183:ARG:HD3	1:B:183:ARG:C	2.42	0.45
1:B:110:LEU:HD11	1:B:151:TYR:CE1	2.51	0.45
1:C:94:THR:HG22	1:C:98:ARG:HE	1.82	0.44
1:C:119:LEU:HD12	1:C:135:SER:O	2.17	0.44
1:E:56:TRP:CD2	1:E:141:ALA:HB2	2.52	0.44
1:F:57:THR:HG21	1:F:290:ASP:HB2	1.99	0.44
1:E:212:ILE:HD12	1:E:216:GLN:CG	2.48	0.44
1:H:86:PRO:HA	1:I:68:GLY:HA3	2.00	0.44
1:C:201:GLU:HA	1:C:240:ILE:HD11	2.01	0.43
1:J:225:GLN:HA	1:J:228:MET:HB2	2.01	0.43
1:H:275:HIS:HB2	1:H:277:TYR:H	1.83	0.43
1:H:119:LEU:HD12	1:H:135:SER:O	2.19	0.43
1:C:201:GLU:HG2	1:C:240:ILE:HG12	2.01	0.43
1:C:86:PRO:O	1:D:68:GLY:HA3	2.18	0.42
1:G:141:ALA:HB1	1:G:286:PRO:HD2	2.02	0.42
1:H:99:PHE:CD1	1:H:155:VAL:HG12	2.54	0.42
1:H:228:MET:HG2	1:H:236:LEU:HD21	2.02	0.42
1:H:88:VAL:HG13	1:H:89:SER:N	2.35	0.41
1:J:99:PHE:CE1	1:J:155:VAL:HG12	2.55	0.41
1:F:156:ASP:OD2	1:F:276:VAL:HG22	2.20	0.41
1:C:124:SER:HA	1:C:133:THR:HG22	2.02	0.41
1:B:86:PRO:HA	1:C:68:GLY:HA3	2.03	0.41
1:H:124:SER:HA	1:H:133:THR:HG22	2.02	0.41
1:I:223:VAL:HG22	1:I:224:THR:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:ARG:NH2	1:E:165:ARG:HH22	2.19	0.40
1:H:61:ILE:HG13	1:H:281:MET:HE2	2.03	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	235/237 (99%)	221 (94%)	10 (4%)	4 (2%)	7	36
1	B	235/237 (99%)	223 (95%)	7 (3%)	5 (2%)	5	30
1	C	235/237 (99%)	219 (93%)	13 (6%)	3 (1%)	9	42
1	D	235/237 (99%)	217 (92%)	12 (5%)	6 (3%)	4	25
1	E	235/237 (99%)	222 (94%)	9 (4%)	4 (2%)	7	36
1	F	235/237 (99%)	222 (94%)	5 (2%)	8 (3%)	3	21
1	G	235/237 (99%)	217 (92%)	12 (5%)	6 (3%)	4	25
1	H	235/237 (99%)	225 (96%)	6 (3%)	4 (2%)	7	36
1	I	235/237 (99%)	220 (94%)	9 (4%)	6 (3%)	4	25
1	J	235/237 (99%)	216 (92%)	13 (6%)	6 (3%)	4	25
1	K	235/237 (99%)	219 (93%)	12 (5%)	4 (2%)	7	36
1	L	235/237 (99%)	217 (92%)	14 (6%)	4 (2%)	7	36
All	All	2820/2844 (99%)	2638 (94%)	122 (4%)	60 (2%)	8	30

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	PRO
1	B	131	PRO

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Mol	Chain	Res	Type
1	B	271	ALA
1	C	131	PRO
1	D	271	ALA
1	E	87	LYS
1	E	131	PRO
1	G	131	PRO
1	H	131	PRO
1	K	131	PRO
1	K	224	THR
1	C	128	GLN
1	D	131	PRO
1	F	86	PRO
1	F	129	GLN
1	F	211	LYS
1	F	285	LEU
1	F	287	VAL
1	I	127	ASN
1	I	131	PRO
1	J	131	PRO
1	L	116	PRO
1	L	218	GLN
1	A	124	SER
1	D	87	LYS
1	D	124	SER
1	D	128	GLN
1	G	86	PRO
1	H	211	LYS
1	I	116	PRO
1	J	129	GLN
1	K	126	LYS
1	L	113	GLN
1	B	277	TYR
1	B	288	ARG
1	D	129	GLN
1	E	85	ALA
1	F	272	ASP
1	G	227	THR
1	I	87	LYS
1	I	128	GLN
1	J	65	PRO
1	J	85	ALA
1	K	85	ALA

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Mol	Chain	Res	Type
1	A	211	LYS
1	B	116	PRO
1	C	85	ALA
1	E	64	GLN
1	F	64	GLN
1	G	129	GLN
1	J	87	LYS
1	F	131	PRO
1	G	87	LYS
1	H	124	SER
1	H	271	ALA
1	L	64	GLN
1	G	85	ALA
1	J	274	VAL
1	A	287	VAL
1	I	86	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	208/208 (100%)	197 (95%)	11 (5%)	20	41
1	B	208/208 (100%)	201 (97%)	7 (3%)	32	54
1	C	208/208 (100%)	202 (97%)	6 (3%)	37	58
1	D	208/208 (100%)	201 (97%)	7 (3%)	32	54
1	E	208/208 (100%)	200 (96%)	8 (4%)	29	50
1	F	208/208 (100%)	198 (95%)	10 (5%)	23	44
1	G	208/208 (100%)	197 (95%)	11 (5%)	20	41
1	H	208/208 (100%)	197 (95%)	11 (5%)	20	41
1	I	208/208 (100%)	201 (97%)	7 (3%)	32	54
1	J	208/208 (100%)	198 (95%)	10 (5%)	23	44
1	K	208/208 (100%)	202 (97%)	6 (3%)	37	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	208/208 (100%)	201 (97%)	7 (3%)	32	54
All	All	2496/2496 (100%)	2395 (96%)	101 (4%)	29	49

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ILE
1	A	95	LEU
1	A	98	ARG
1	A	118	LYS
1	A	134	VAL
1	A	152	ILE
1	A	166	ASP
1	A	183	ARG
1	A	187	VAL
1	A	224	THR
1	A	274	VAL
1	B	62	ILE
1	B	79	VAL
1	B	121	ILE
1	B	217	ILE
1	B	250	PHE
1	B	273	THR
1	B	282	LYS
1	C	130	LEU
1	C	167	LEU
1	C	183	ARG
1	C	204	LEU
1	C	247	PRO
1	C	264	ILE
1	D	118	LYS
1	D	122	GLU
1	D	125	VAL
1	D	134	VAL
1	D	167	LEU
1	D	173	LEU
1	D	212	ILE
1	E	95	LEU
1	E	106	LEU
1	E	188	VAL
1	E	204	LEU
1	E	221	GLN

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Mol	Chain	Res	Type
1	E	223	VAL
1	E	269	VAL
1	E	280	VAL
1	F	86	PRO
1	F	87	LYS
1	F	88	VAL
1	F	121	ILE
1	F	204	LEU
1	F	247	PRO
1	F	268	LYS
1	F	269	VAL
1	F	274	VAL
1	F	284	THR
1	G	95	LEU
1	G	129	GLN
1	G	139	GLN
1	G	167	LEU
1	G	198	ARG
1	G	204	LEU
1	G	224	THR
1	G	227	THR
1	G	248	LEU
1	G	264	ILE
1	G	283	PRO
1	H	121	ILE
1	H	122	GLU
1	H	137	VAL
1	H	193	LYS
1	H	198	ARG
1	H	202	GLU
1	H	204	LEU
1	H	209	GLU
1	H	234	ASP
1	H	248	LEU
1	H	282	LYS
1	I	63	THR
1	I	67	VAL
1	I	70	ILE
1	I	168	LYS
1	I	188	VAL
1	I	248	LEU
1	I	255	TYR

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Mol	Chain	Res	Type
1	J	67	VAL
1	J	95	LEU
1	J	152	ILE
1	J	183	ARG
1	J	227	THR
1	J	229	PHE
1	J	256	GLN
1	J	270	THR
1	J	274	VAL
1	J	276	VAL
1	K	67	VAL
1	K	146	MET
1	K	171	ILE
1	K	212	ILE
1	K	246	ARG
1	K	248	LEU
1	L	120	THR
1	L	163	LEU
1	L	164	GLU
1	L	167	LEU
1	L	204	LEU
1	L	247	PRO
1	L	269	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	139	GLN
1	A	145	GLN
1	A	177	ASN
1	A	225	GLN
1	B	69	GLN
1	B	74	ASN
1	B	112	ASN
1	B	129	GLN
1	B	161	GLN
1	B	170	ASN
1	B	179	GLN
1	B	214	GLN
1	B	216	GLN
1	B	241	GLN

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Mol	Chain	Res	Type
1	B	266	ASN
1	C	75	ASN
1	C	83	GLN
1	C	92	GLN
1	C	113	GLN
1	C	127	ASN
1	C	139	GLN
1	C	145	GLN
1	C	154	GLN
1	C	177	ASN
1	C	179	GLN
1	C	256	GLN
1	D	75	ASN
1	D	113	GLN
1	D	128	GLN
1	D	153	GLN
1	D	160	ASN
1	D	219	GLN
1	E	69	GLN
1	E	75	ASN
1	E	145	GLN
1	E	160	ASN
1	E	192	GLN
1	E	219	GLN
1	E	221	GLN
1	E	266	ASN
1	F	75	ASN
1	F	154	GLN
1	F	177	ASN
1	F	185	GLN
1	F	199	GLN
1	F	214	GLN
1	F	266	ASN
1	G	92	GLN
1	G	127	ASN
1	G	128	GLN
1	G	139	GLN
1	G	160	ASN
1	G	170	ASN
1	G	214	GLN
1	G	219	GLN
1	G	259	GLN

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Mol	Chain	Res	Type
1	G	275	HIS
1	H	69	GLN
1	H	75	ASN
1	H	83	GLN
1	H	92	GLN
1	H	145	GLN
1	H	154	GLN
1	H	177	ASN
1	H	199	GLN
1	H	214	GLN
1	H	219	GLN
1	H	225	GLN
1	H	266	ASN
1	H	275	HIS
1	I	69	GLN
1	I	145	GLN
1	I	170	ASN
1	I	177	ASN
1	I	214	GLN
1	I	275	HIS
1	J	92	GLN
1	J	113	GLN
1	J	139	GLN
1	J	145	GLN
1	J	177	ASN
1	J	190	GLN
1	K	74	ASN
1	K	75	ASN
1	K	78	ASN
1	K	83	GLN
1	K	219	GLN
1	K	241	GLN
1	L	64	GLN
1	L	113	GLN
1	L	170	ASN
1	L	177	ASN
1	L	190	GLN
1	L	199	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3611. These allow visual inspection of the internal detail of the map and identification of artifacts.

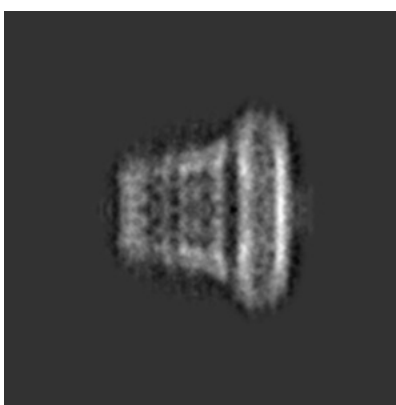
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

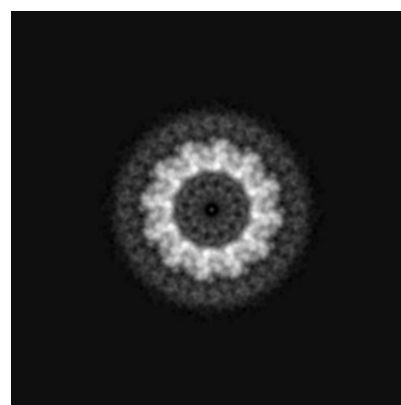
6.1.1 Primary map



X



Y

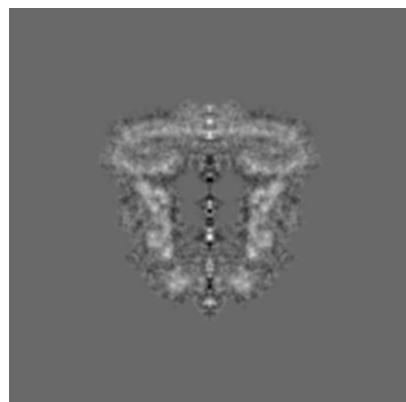


Z

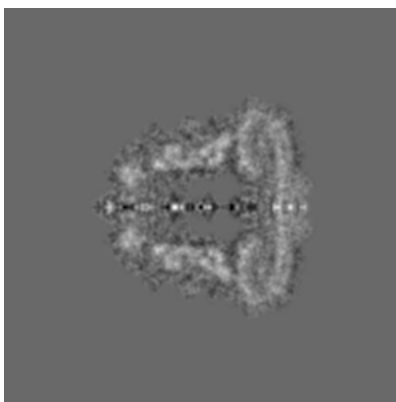
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

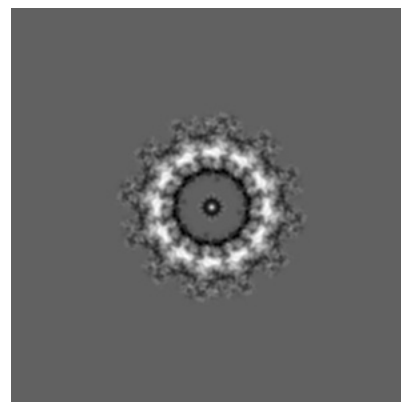
6.2.1 Primary map



X Index: 128



Y Index: 128

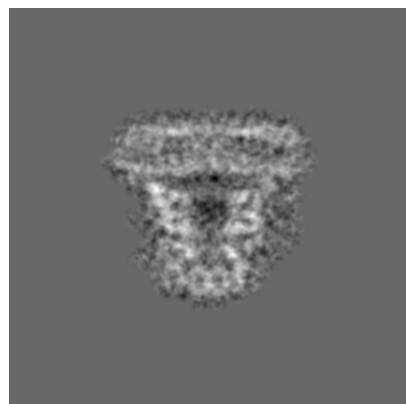


Z Index: 128

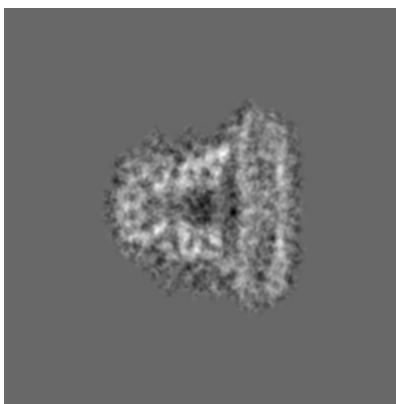
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

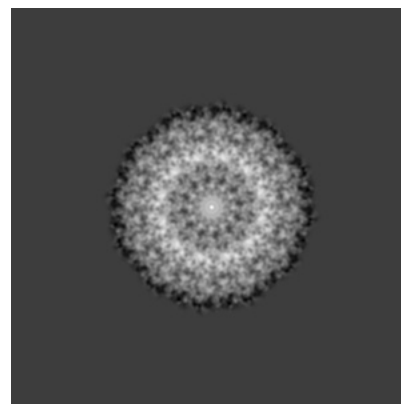
6.3.1 Primary map



X Index: 105



Y Index: 105

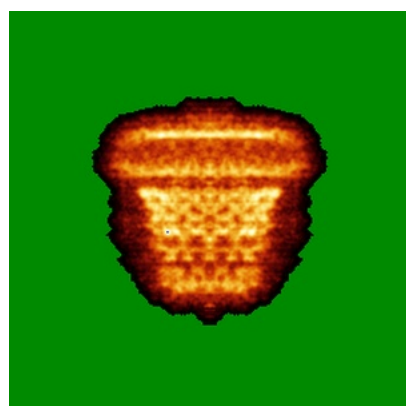


Z Index: 176

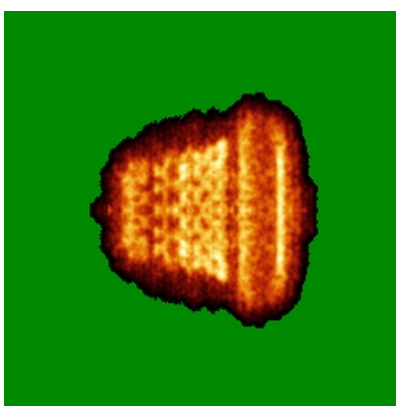
The images above show the largest variance slices of the map in three orthogonal directions.

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

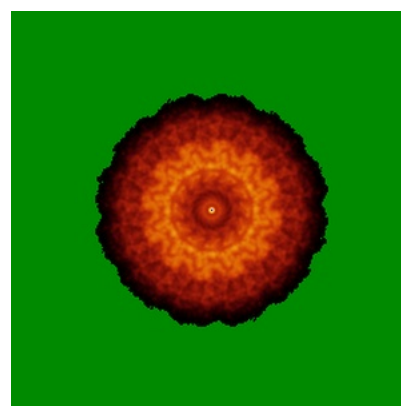
6.4.1 Primary map



X



Y

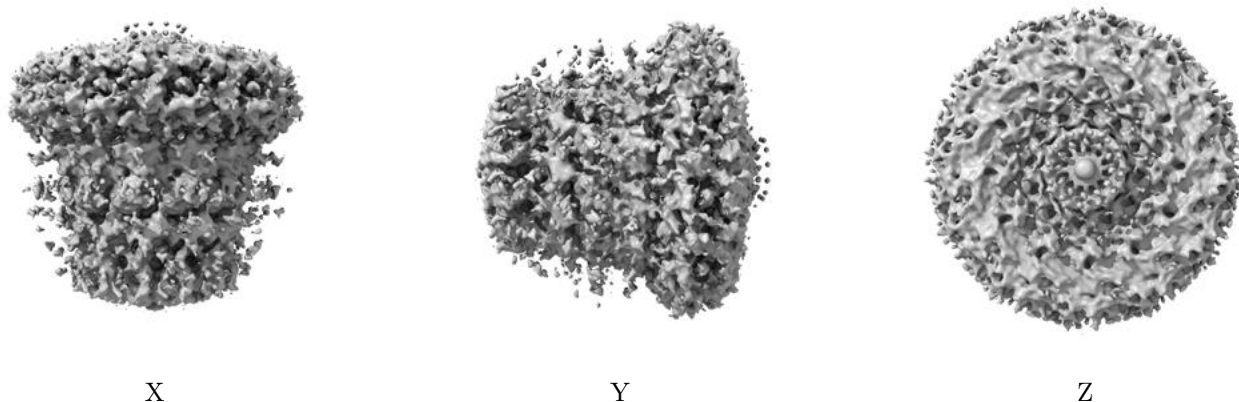


Z

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 0.66. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

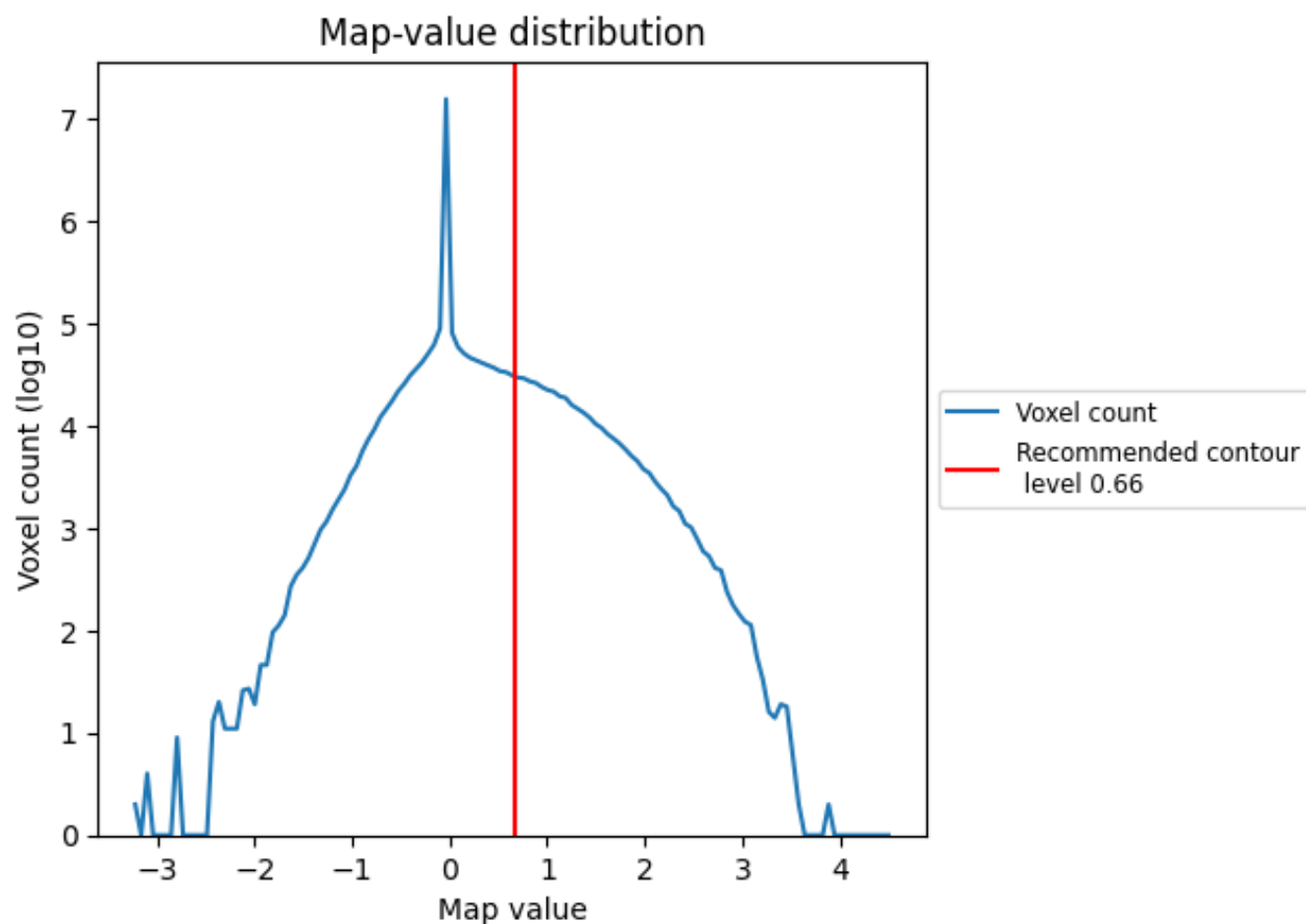
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

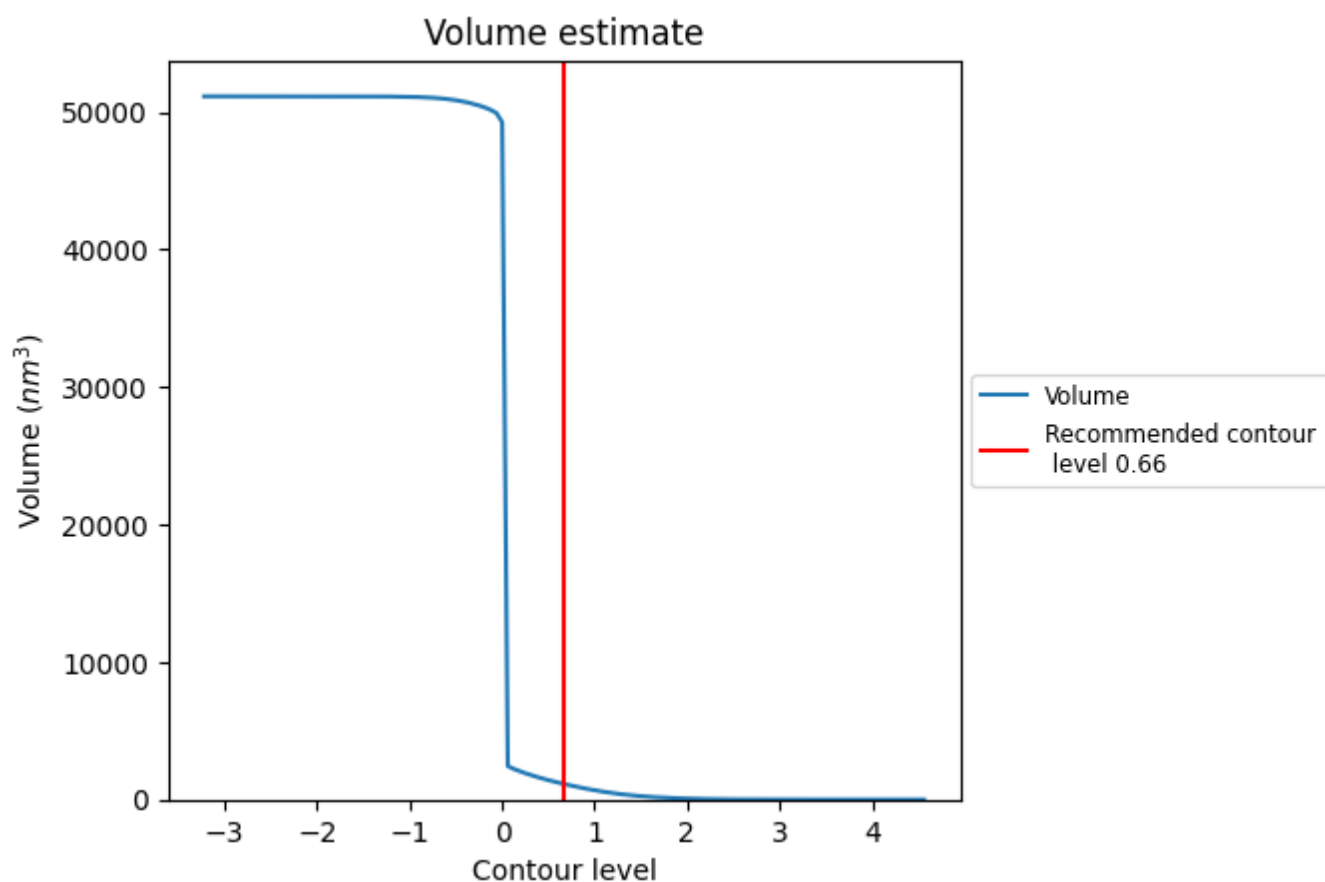
This section contains the results of statistical analysis of the map.

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.

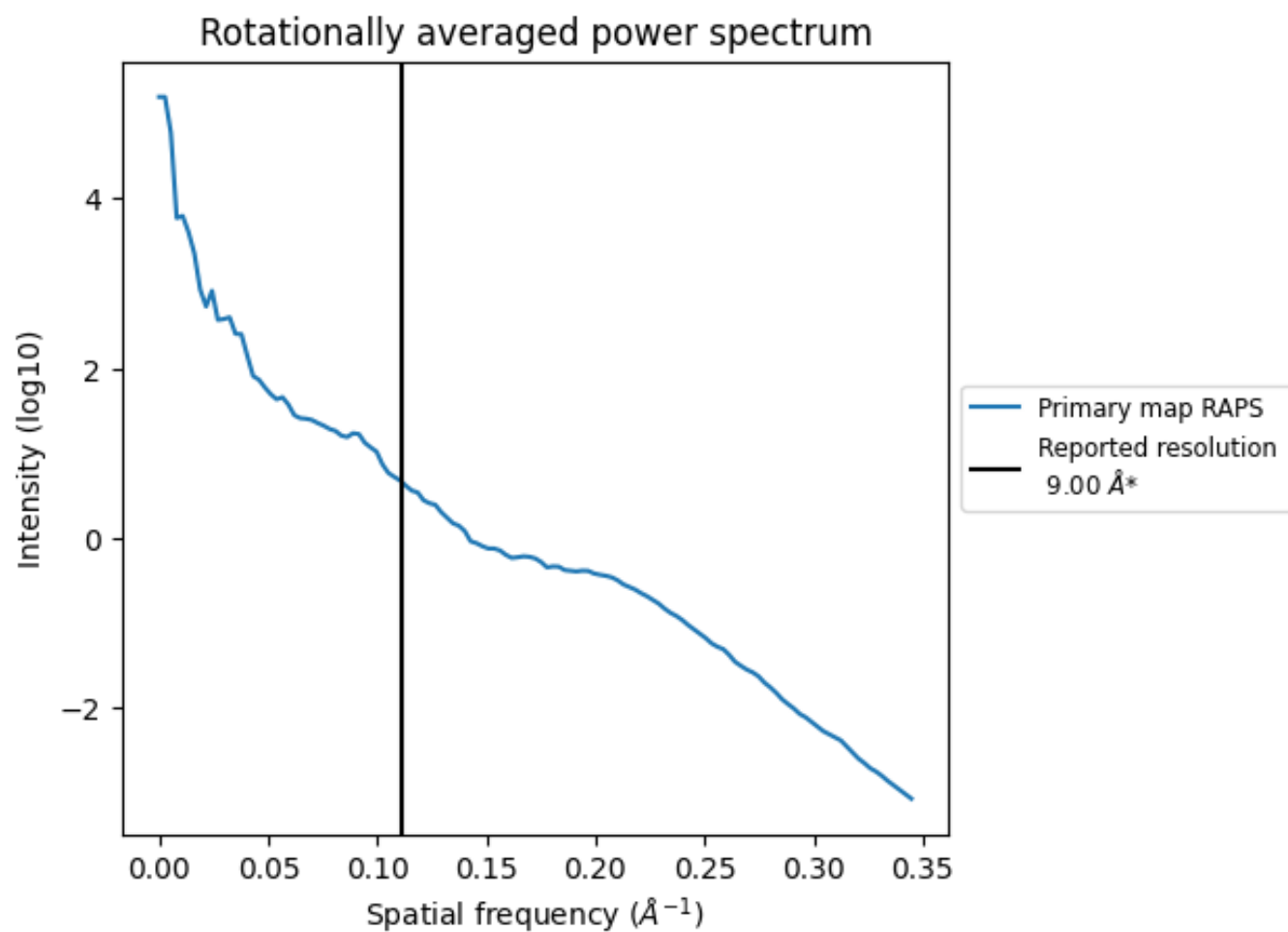
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1143 nm³; this corresponds to an approximate mass of 1032 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 0.111 Å⁻¹

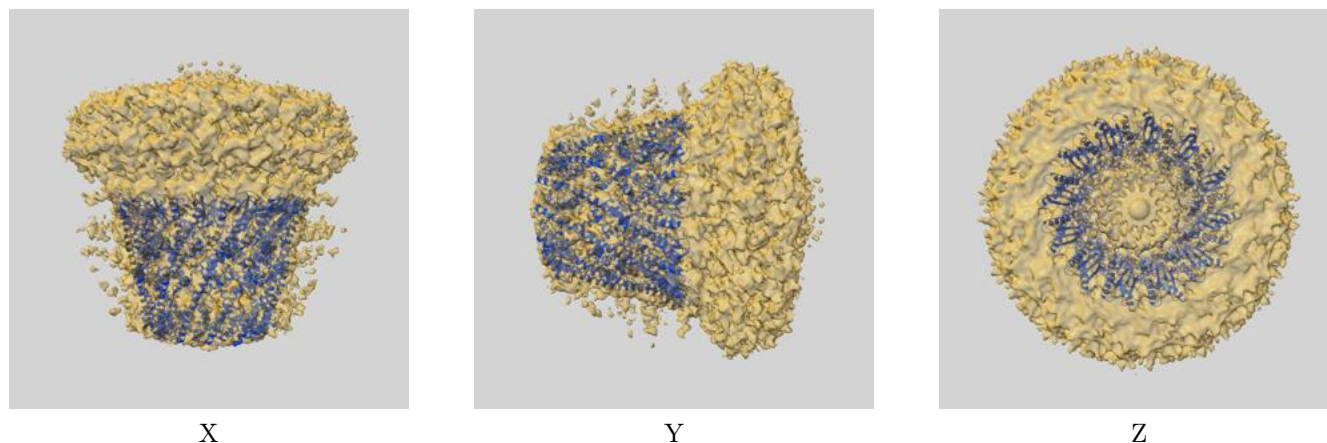
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

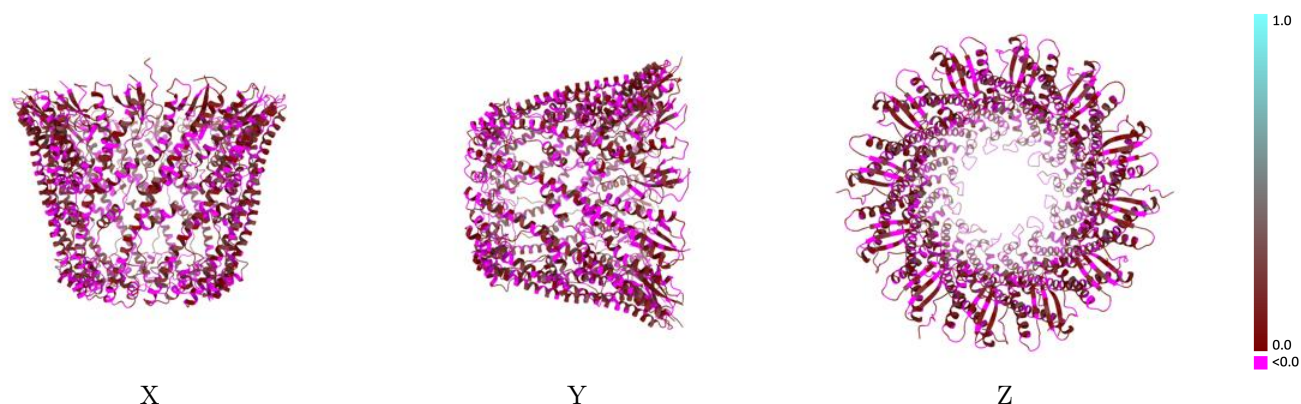
This section contains information regarding the fit between EMDB map EMD-3611 and PDB model 5NBZ. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



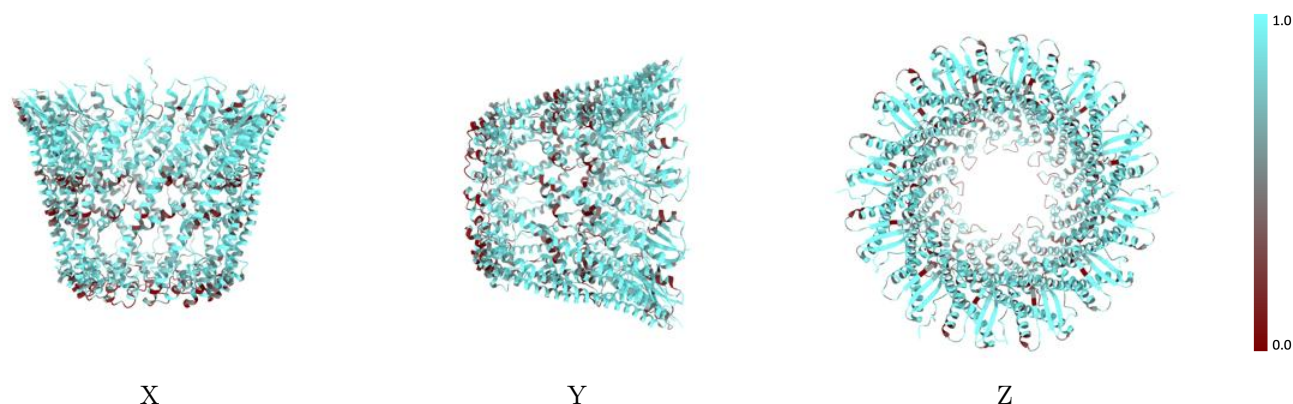
The images above show the 3D surface view of the map at the recommended contour level 0.66 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



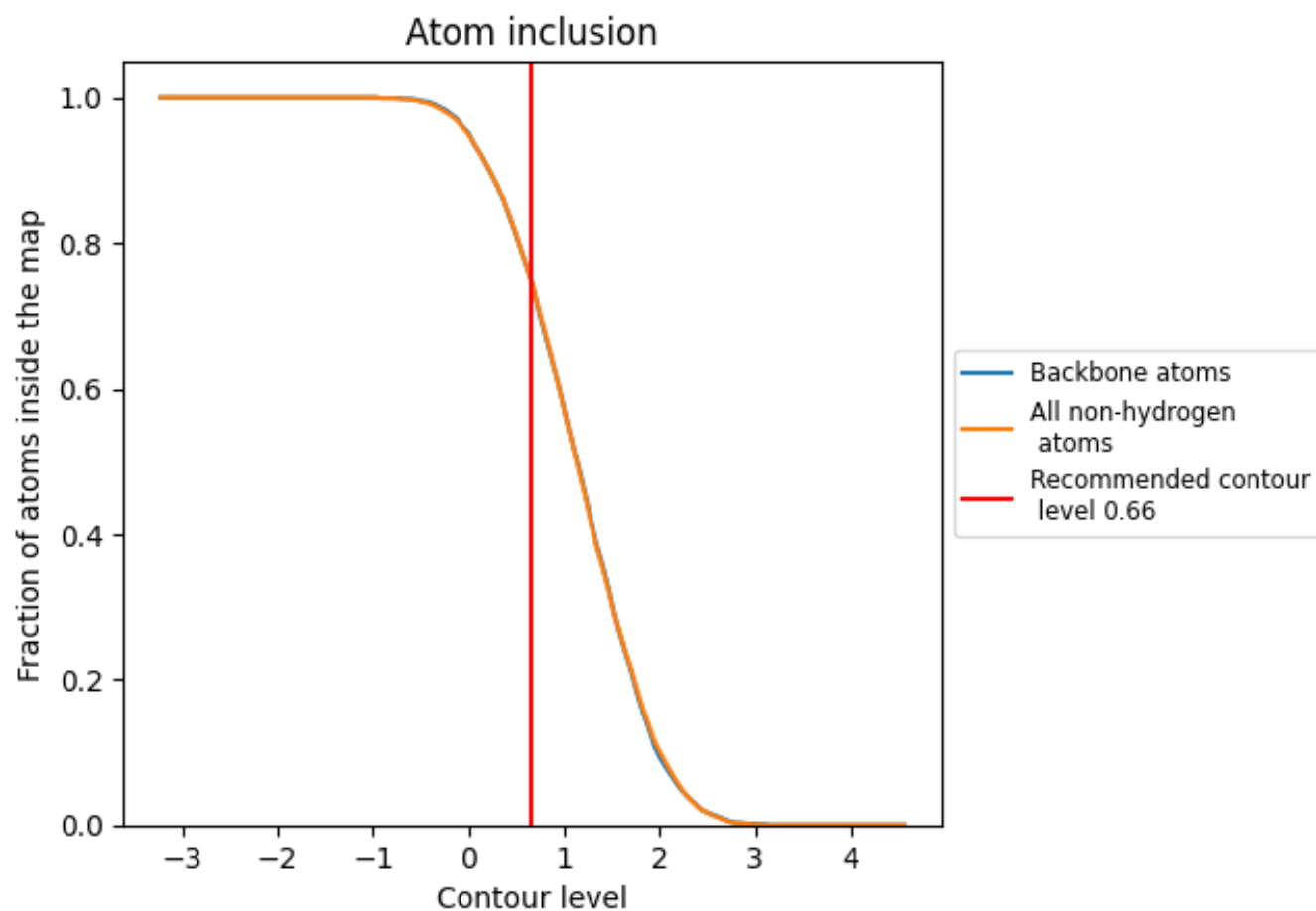
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.66).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 75% 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 (0.66) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7470	0.0460
A	0.7530	0.0440
B	0.7440	0.0390
C	0.7510	0.0580
D	0.7490	0.0460
E	0.7510	0.0500
F	0.7470	0.0360
G	0.7490	0.0460
H	0.7540	0.0450
I	0.7620	0.0430
J	0.7640	0.0470
K	0.7550	0.0440
L	0.7520	0.0510

1.0

0.0

<0.0