



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:15 PM UTC

PDB ID : 5UP4 / pdb_00005up4
EMDB ID : EMD-8582
Title : Structure of the HIV-1 Capsid Protein and spacer peptide 1 by Cryo-EM
Authors : Perilla, J.R.; Schirra, R.; Zhang, P.; Schulten, K.
Deposited on : 2017-02-01
Resolution : 9.00 Å(reported)
Based on initial models : 2KOD, 3J34

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

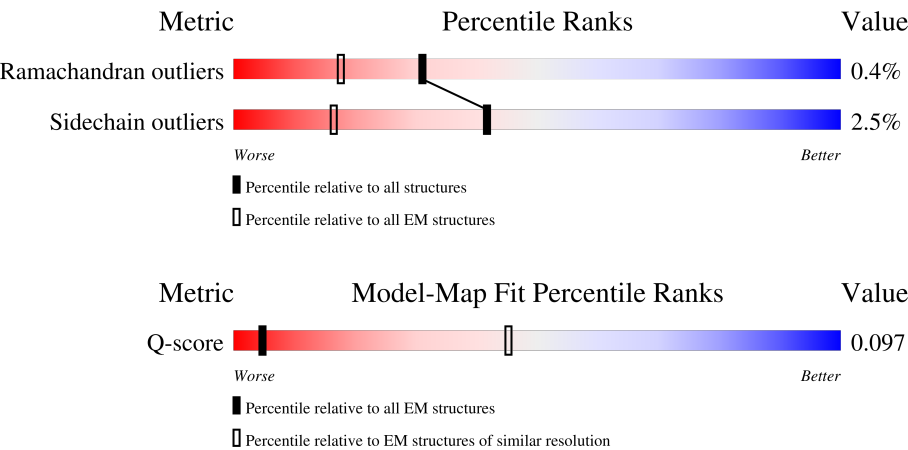
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 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.



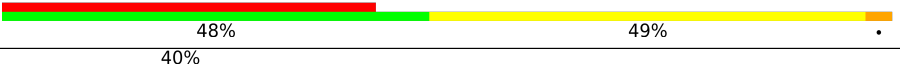
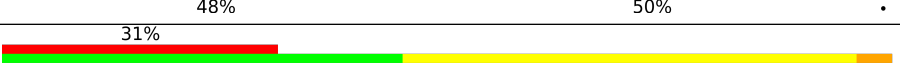
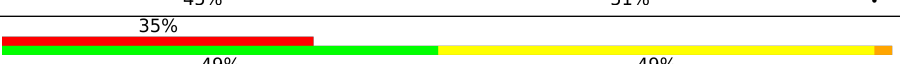
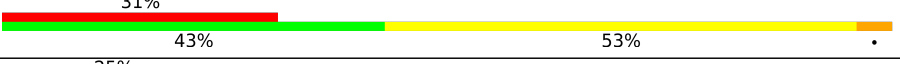
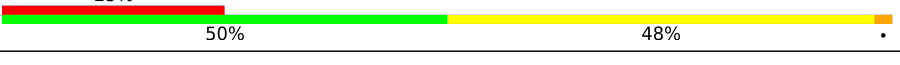
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	257 (8.50 - 9.50)

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	B	221	41% 44% 54% .
1	C	221	38% 43% 53% .
1	D	221	44% 55% 42% .
1	E	221	37% 48% 49% .
1	F	221	39% 52% 47% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	221	
1	H	221	
1	I	221	
1	J	221	
1	K	221	
1	L	221	
1	M	221	
1	N	221	
1	O	221	
1	P	221	
1	Q	221	
1	R	221	
1	S	221	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 31068 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HIV-1 Capsid Protein and spacer peptide 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	K	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	L	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	M	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	N	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	O	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	P	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	Q	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	R	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	S	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	C	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	D	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	E	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	F	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	G	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	H	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		
1	I	221	Total	C	N	O	S	0	0
			1726	1088	301	324	13		

Continued on next page...

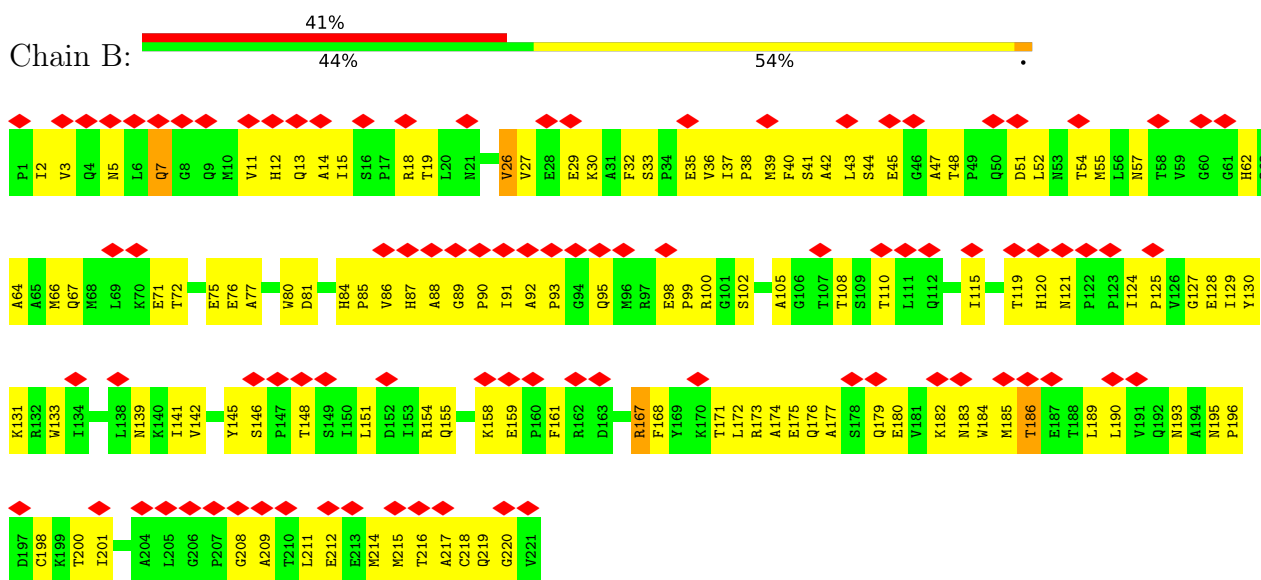
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	J	221	1726	1088	301	324	13	0	0

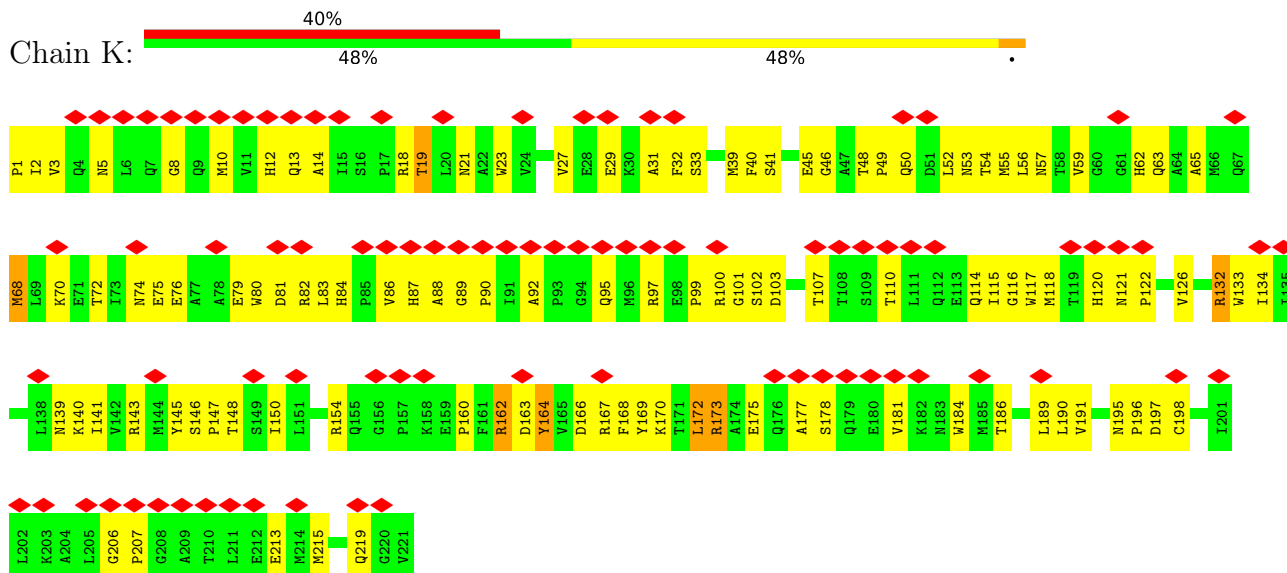
3 Residue-property plots

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.

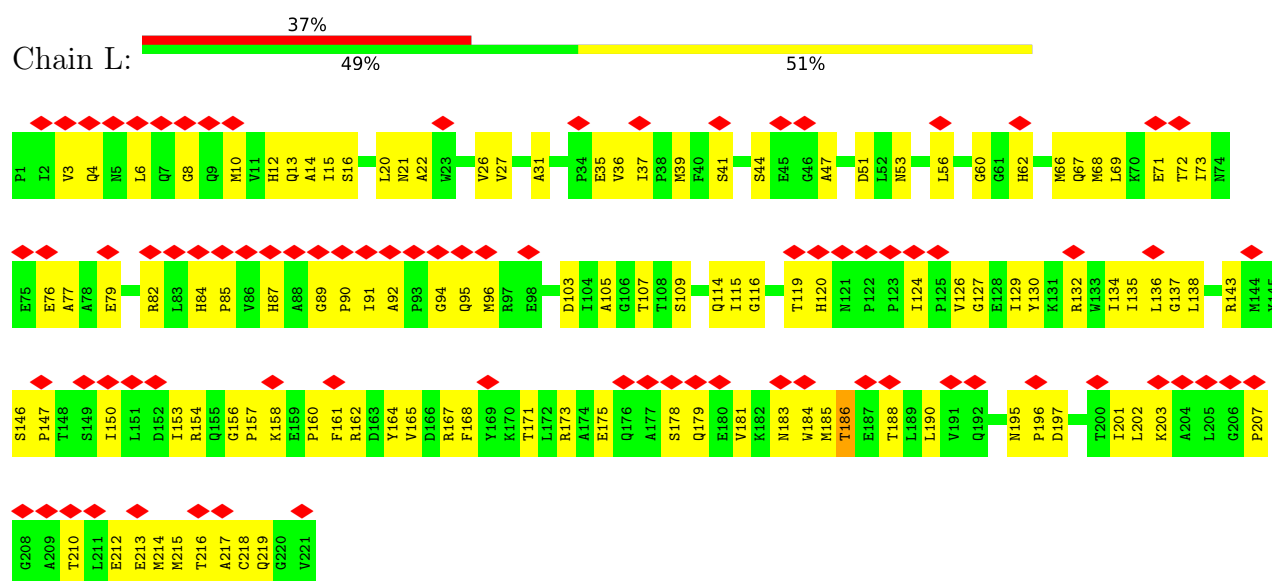
- Molecule 1: HIV-1 Capsid Protein and spacer peptide 1



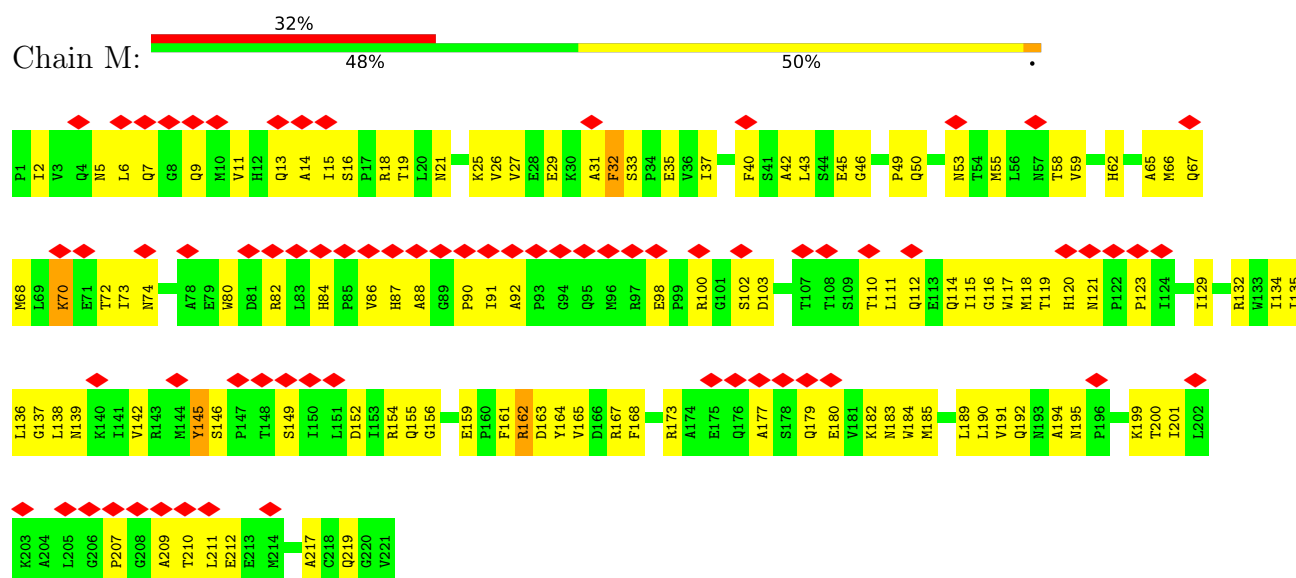
- Molecule 1: HIV-1 Capsid Protein and spacer peptide 1



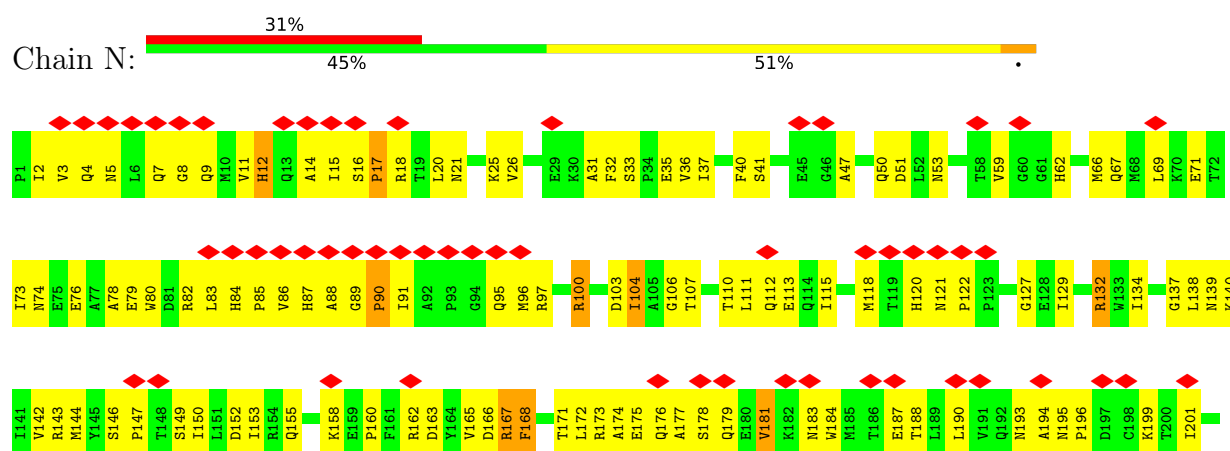
- Molecule 1: HIV-1 Capsid Protein and spacer peptide 1



• Molecule 1: HIV-1 Capsid Protein and spacer peptide 1

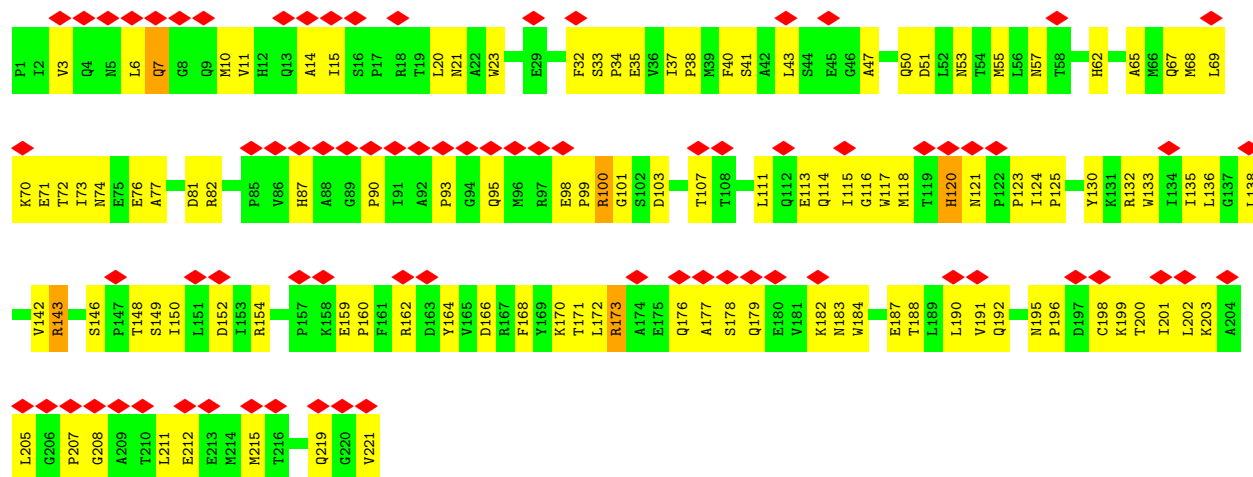


• Molecule 1: HIV-1 Capsid Protein and spacer peptide 1

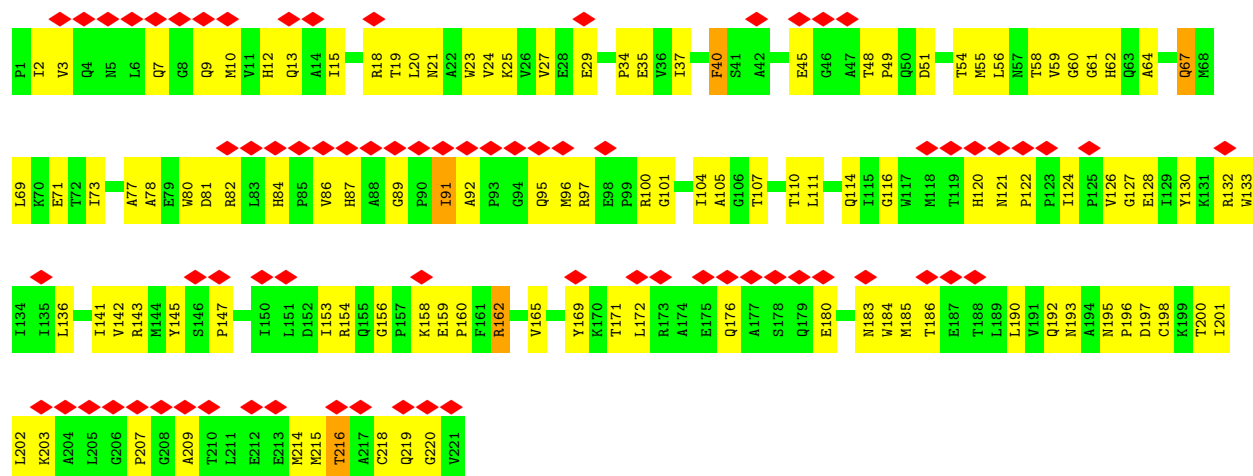




• Molecule 1: HIV-1 Capsid Protein and spacer peptide 1

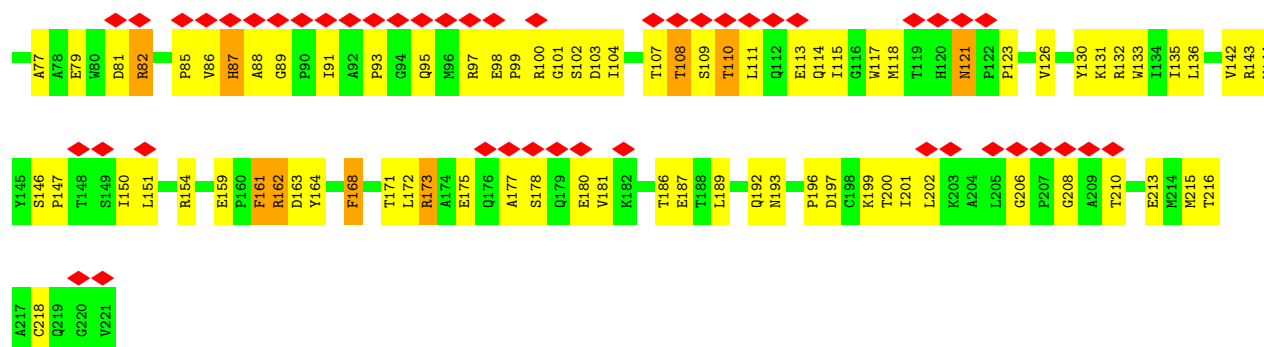


• Molecule 1: HIV-1 Capsid Protein and spacer peptide 1

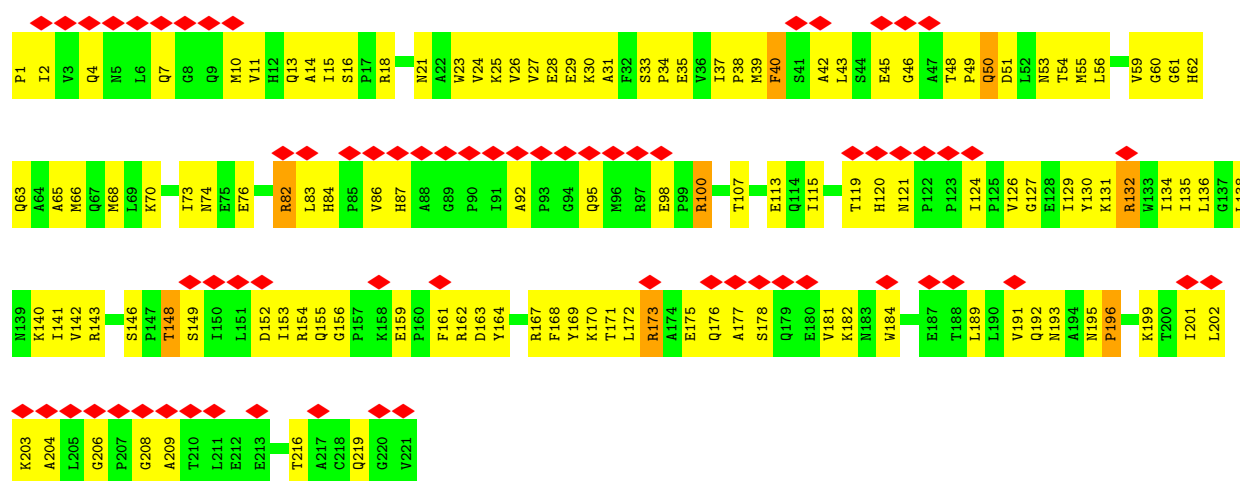
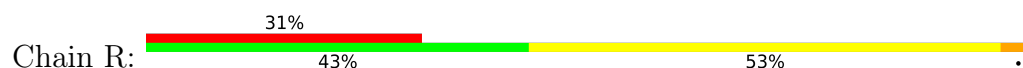


• Molecule 1: HIV-1 Capsid Protein and spacer peptide 1

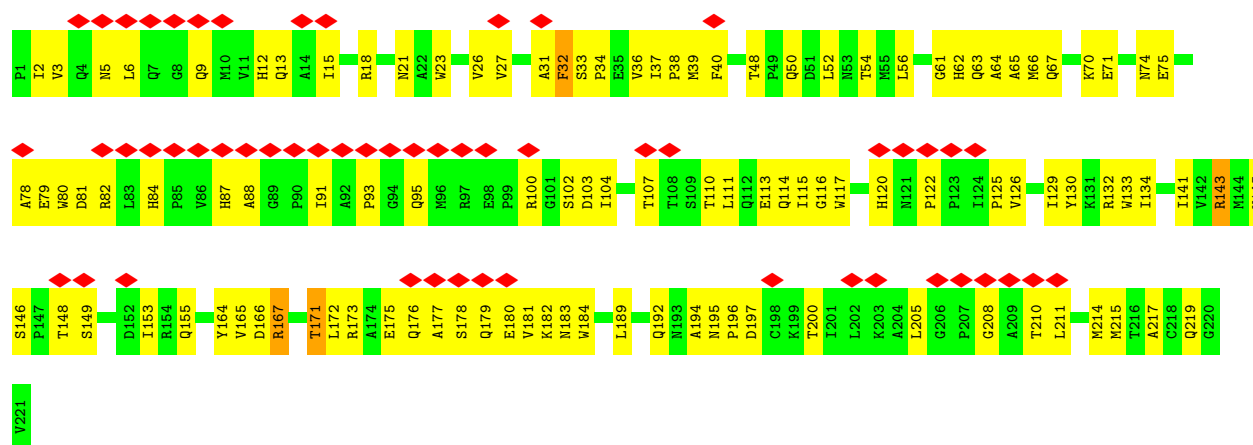




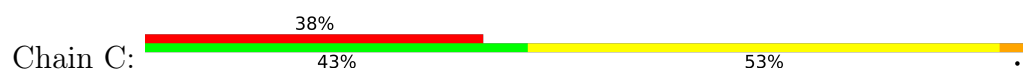
• Molecule 1: HIV-1 Capsid Protein and spacer peptide 1

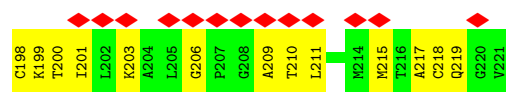


• Molecule 1: HIV-1 Capsid Protein and spacer peptide 1

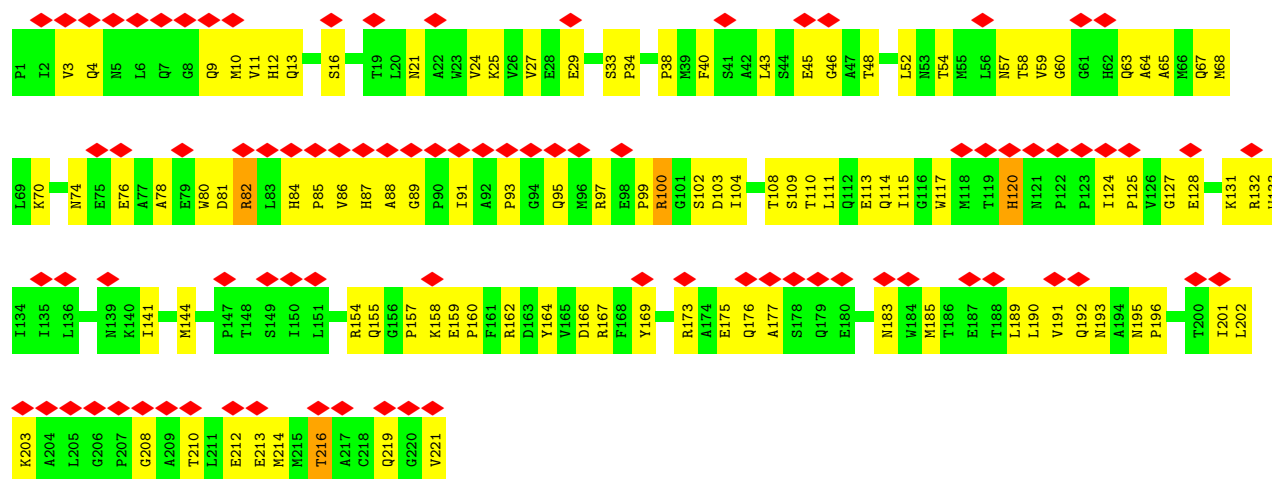
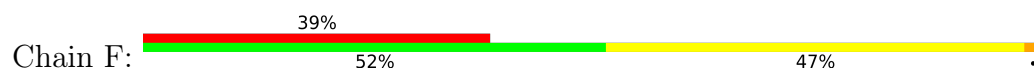


• Molecule 1: HIV-1 Capsid Protein and spacer peptide 1

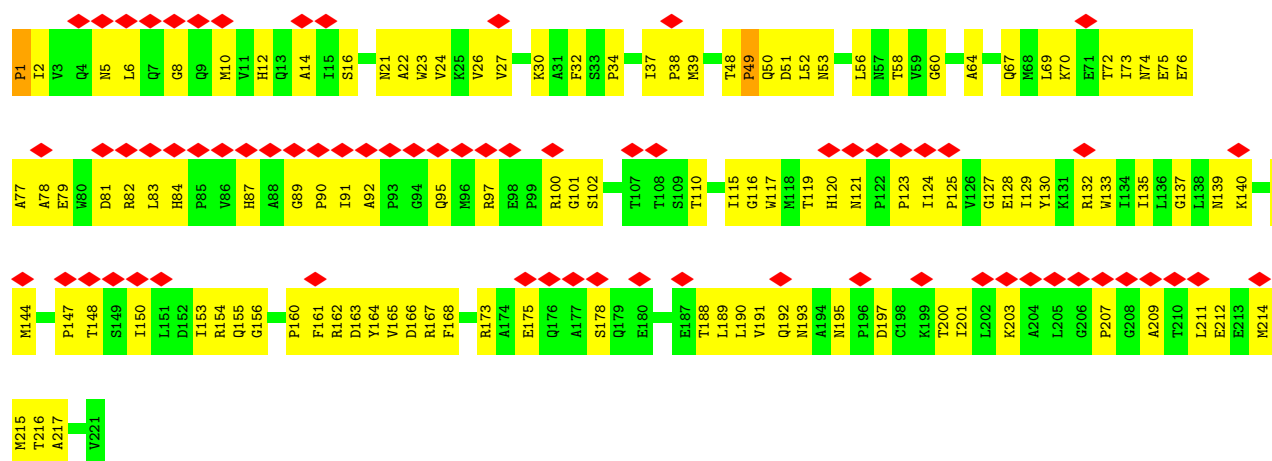




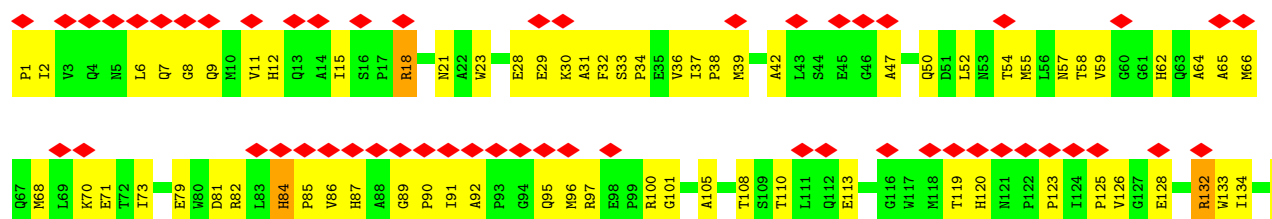
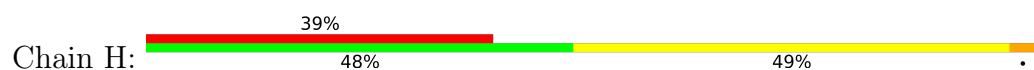
• Molecule 1: HIV-1 Capsid Protein and spacer peptide 1



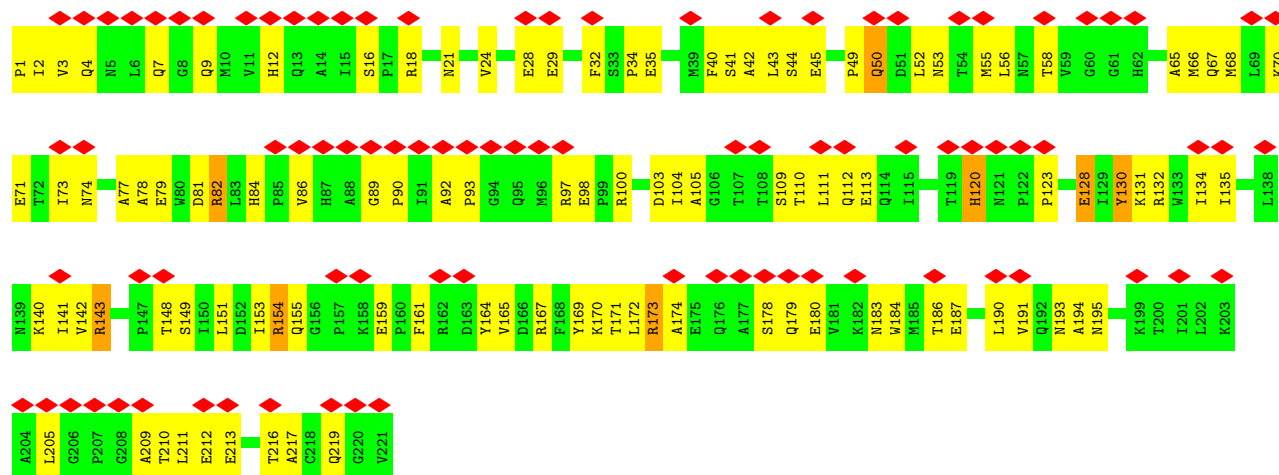
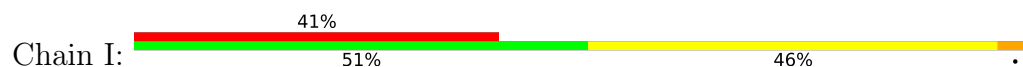
• Molecule 1: HIV-1 Capsid Protein and spacer peptide 1



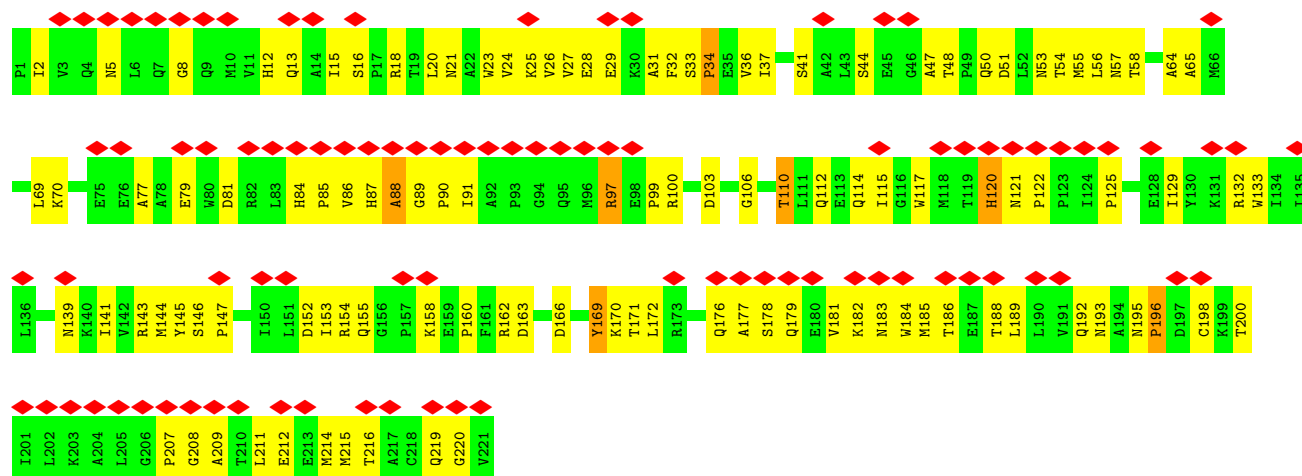
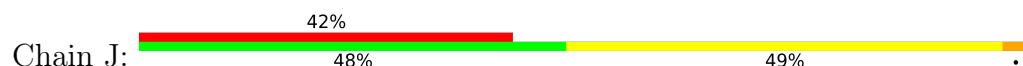
• Molecule 1: HIV-1 Capsid Protein and spacer peptide 1



- Molecule 1: HIV-1 Capsid Protein and spacer peptide 1



- Molecule 1: HIV-1 Capsid Protein and spacer peptide 1



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=128.88°, rise=13.46 Å, axial sym=C1	Depositor
Number of segments used	14000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	23	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.046	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	545.60004, 545.60004, 545.60004	wwPDB
Map dimensions	496, 496, 496	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	B	2.20	52/1765 (2.9%)	2.57	145/2398 (6.0%)
1	C	2.19	60/1765 (3.4%)	2.56	136/2398 (5.7%)
1	D	2.18	49/1765 (2.8%)	2.48	121/2398 (5.0%)
1	E	2.23	53/1765 (3.0%)	2.52	135/2398 (5.6%)
1	F	2.15	41/1765 (2.3%)	2.43	109/2398 (4.5%)
1	G	2.19	57/1765 (3.2%)	2.53	129/2398 (5.4%)
1	H	2.21	53/1765 (3.0%)	2.49	121/2398 (5.0%)
1	I	2.24	58/1765 (3.3%)	2.48	123/2398 (5.1%)
1	J	2.20	48/1765 (2.7%)	2.52	122/2398 (5.1%)
1	K	2.24	57/1765 (3.2%)	2.64	157/2398 (6.5%)
1	L	2.27	62/1765 (3.5%)	2.43	117/2398 (4.9%)
1	M	2.21	52/1765 (2.9%)	2.56	122/2398 (5.1%)
1	N	2.24	57/1765 (3.2%)	2.55	136/2398 (5.7%)
1	O	2.19	55/1765 (3.1%)	2.49	130/2398 (5.4%)
1	P	2.19	50/1765 (2.8%)	2.52	132/2398 (5.5%)
1	Q	2.13	60/1765 (3.4%)	2.55	129/2398 (5.4%)
1	R	2.24	61/1765 (3.5%)	2.47	133/2398 (5.5%)
1	S	2.18	50/1765 (2.8%)	2.54	129/2398 (5.4%)
All	All	2.20	975/31770 (3.1%)	2.52	2326/43164 (5.4%)

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	B	0	3
1	C	0	7
1	D	0	7
1	E	0	5
1	F	0	5
1	H	0	7
1	I	0	7

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	2
1	K	0	6
1	L	0	1
1	M	0	6
1	N	0	6
1	O	0	5
1	P	0	3
1	Q	0	8
1	R	0	6
1	S	0	3
All	All	0	87

All (975) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	8	GLY	CA-C	13.65	1.65	1.51
1	J	129	ILE	CA-CB	-12.79	1.39	1.54
1	L	127	GLY	CA-C	-11.54	1.39	1.52
1	R	124	ILE	CA-C	10.62	1.60	1.52
1	R	60	GLY	CA-C	-10.26	1.44	1.52
1	N	120	HIS	CE1-NE2	9.84	1.42	1.32
1	I	134	ILE	C-O	9.83	1.35	1.24
1	D	175	GLU	CA-C	9.60	1.65	1.52
1	K	115	ILE	CA-CB	-9.58	1.42	1.54
1	J	196	PRO	CA-C	-9.46	1.38	1.52
1	L	26	VAL	CA-CB	9.37	1.64	1.54
1	E	125	PRO	CA-C	-9.33	1.43	1.53
1	I	120	HIS	CA-CB	9.26	1.67	1.53
1	G	124	ILE	CA-C	9.20	1.61	1.53
1	R	120	HIS	CG-CD2	9.18	1.46	1.35
1	H	89	GLY	C-N	9.14	1.45	1.33
1	O	101	GLY	CA-C	-9.03	1.42	1.52
1	B	127	GLY	N-CA	9.01	1.57	1.45
1	J	8	GLY	CA-C	-9.00	1.40	1.51
1	Q	45	GLU	C-N	8.99	1.44	1.33
1	H	125	PRO	C-N	8.98	1.44	1.34
1	P	23	TRP	NE1-CE2	-8.98	1.27	1.37
1	K	87	HIS	CD2-NE2	8.95	1.47	1.37
1	I	111	LEU	CA-C	-8.94	1.41	1.52
1	H	38	PRO	N-CD	-8.84	1.35	1.47
1	R	61	GLY	N-CA	8.83	1.54	1.45
1	F	158	LYS	N-CA	-8.78	1.34	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	65	ALA	CA-C	-8.67	1.41	1.52
1	M	110	THR	CA-CB	8.65	1.67	1.53
1	O	43	LEU	CA-C	8.62	1.64	1.52
1	M	194	ALA	CA-C	8.57	1.63	1.52
1	C	85	PRO	C-N	8.56	1.44	1.33
1	H	2	ILE	CA-C	8.54	1.63	1.52
1	K	87	HIS	CG-ND1	8.46	1.47	1.38
1	I	68	MET	C-N	8.43	1.45	1.33
1	S	87	HIS	CA-CB	8.42	1.63	1.52
1	D	175	GLU	C-N	8.40	1.45	1.33
1	B	201	ILE	CA-CB	-8.38	1.44	1.54
1	J	26	VAL	CA-CB	8.35	1.65	1.54
1	O	120	HIS	ND1-CE1	8.32	1.40	1.32
1	S	91	ILE	CA-CB	8.31	1.65	1.54
1	I	29	GLU	CA-CB	8.30	1.66	1.53
1	E	44	SER	CA-CB	8.26	1.66	1.53
1	M	192	GLN	N-CA	8.25	1.56	1.46
1	I	141	ILE	N-CA	-8.22	1.36	1.46
1	G	73	ILE	CA-C	8.21	1.63	1.52
1	J	44	SER	N-CA	8.18	1.56	1.46
1	E	105	ALA	CA-C	8.14	1.64	1.52
1	N	17	PRO	N-CD	-8.12	1.36	1.47
1	F	120	HIS	ND1-CE1	8.11	1.40	1.32
1	P	48	THR	CA-C	8.03	1.62	1.52
1	O	125	PRO	CA-CB	8.02	1.61	1.53
1	E	64	ALA	C-N	7.96	1.44	1.33
1	P	100	ARG	CA-C	-7.95	1.42	1.53
1	N	199	LYS	CA-CB	7.95	1.65	1.53
1	K	101	GLY	CA-C	-7.93	1.43	1.52
1	L	60	GLY	CA-C	-7.93	1.42	1.52
1	Q	91	ILE	CA-C	-7.92	1.42	1.52
1	Q	107	THR	N-CA	7.89	1.56	1.46
1	N	160	PRO	CA-C	-7.88	1.41	1.52
1	N	88	ALA	N-CA	-7.85	1.36	1.46
1	M	91	ILE	CA-C	7.84	1.61	1.52
1	D	152	ASP	C-N	-7.84	1.26	1.33
1	L	202	LEU	C-N	7.81	1.44	1.34
1	C	135	ILE	CA-C	7.78	1.62	1.52
1	P	77	ALA	CA-C	7.76	1.62	1.52
1	S	40	PHE	CA-CB	7.75	1.65	1.53
1	S	6	LEU	CA-CB	7.75	1.66	1.53
1	L	91	ILE	CA-CB	-7.73	1.46	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	163	ASP	CA-CB	7.72	1.66	1.53
1	B	87	HIS	N-CA	-7.72	1.36	1.45
1	L	201	ILE	N-CA	-7.70	1.37	1.46
1	Q	123	PRO	N-CA	-7.70	1.38	1.47
1	P	87	HIS	CA-CB	7.68	1.64	1.53
1	M	138	LEU	CA-C	-7.67	1.43	1.52
1	R	204	ALA	C-N	7.67	1.44	1.33
1	E	65	ALA	CA-C	7.67	1.62	1.52
1	N	62	HIS	CE1-NE2	7.65	1.40	1.32
1	L	84	HIS	ND1-CE1	7.65	1.40	1.32
1	Q	131	LYS	CA-C	-7.65	1.42	1.52
1	Q	123	PRO	CA-C	-7.64	1.43	1.52
1	F	109	SER	N-CA	-7.64	1.36	1.45
1	I	141	ILE	C-N	7.64	1.43	1.33
1	G	175	GLU	CA-C	7.61	1.62	1.52
1	H	31	ALA	C-N	7.60	1.44	1.33
1	G	140	LYS	C-N	7.59	1.43	1.33
1	M	164	TYR	CA-CB	7.59	1.65	1.53
1	B	36	VAL	C-N	7.58	1.42	1.33
1	F	40	PHE	C-N	7.58	1.43	1.33
1	J	106	GLY	CA-C	-7.55	1.41	1.51
1	N	67	GLN	CA-CB	7.54	1.65	1.53
1	Q	101	GLY	CA-C	-7.53	1.43	1.52
1	I	79	GLU	CA-C	7.52	1.62	1.52
1	B	14	ALA	CA-C	7.50	1.62	1.52
1	S	34	PRO	N-CD	-7.49	1.37	1.47
1	I	43	LEU	CA-CB	7.48	1.66	1.53
1	P	45	GLU	CA-C	7.48	1.62	1.52
1	S	182	LYS	N-CA	7.47	1.55	1.46
1	O	179	GLN	C-N	7.47	1.44	1.33
1	I	79	GLU	C-N	7.46	1.43	1.33
1	D	153	ILE	CA-C	7.46	1.60	1.53
1	L	44	SER	CA-CB	7.45	1.63	1.53
1	R	154	ARG	CA-CB	7.44	1.67	1.53
1	B	98	GLU	C-N	-7.43	1.25	1.33
1	G	10	MET	CA-CB	7.43	1.63	1.53
1	P	132	ARG	CD-NE	7.43	1.56	1.46
1	B	91	ILE	C-N	7.43	1.43	1.33
1	L	132	ARG	CA-CB	7.42	1.64	1.53
1	G	39	MET	CA-CB	7.41	1.64	1.53
1	D	117	TRP	C-N	7.41	1.44	1.34
1	I	58	THR	CA-C	7.41	1.62	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1	PRO	N-CA	7.40	1.58	1.47
1	S	130	TYR	CA-C	7.39	1.62	1.52
1	D	59	VAL	CA-C	-7.39	1.44	1.52
1	N	115	ILE	CA-CB	-7.39	1.45	1.54
1	R	136	LEU	C-N	7.38	1.43	1.33
1	K	181	VAL	N-CA	-7.35	1.37	1.46
1	K	197	ASP	CA-C	7.34	1.62	1.52
1	I	53	ASN	N-CA	-7.33	1.37	1.46
1	I	134	ILE	C-N	7.32	1.43	1.33
1	I	174	ALA	C-N	7.30	1.44	1.33
1	I	151	LEU	N-CA	-7.29	1.37	1.46
1	R	42	ALA	CA-C	-7.29	1.43	1.52
1	G	125	PRO	CA-CB	7.28	1.62	1.53
1	M	87	HIS	C-N	7.28	1.42	1.33
1	O	124	ILE	CA-C	-7.27	1.46	1.52
1	C	152	ASP	N-CA	7.27	1.55	1.46
1	M	6	LEU	CA-C	7.27	1.62	1.52
1	L	6	LEU	N-CA	-7.26	1.37	1.46
1	S	164	TYR	C-N	7.25	1.42	1.33
1	D	188	THR	CA-C	-7.25	1.45	1.53
1	N	9	GLN	CA-CB	7.24	1.62	1.52
1	O	178	SER	CA-CB	7.23	1.64	1.53
1	M	58	THR	C-N	-7.21	1.25	1.33
1	R	84	HIS	CA-C	-7.21	1.43	1.52
1	E	10	MET	N-CA	7.21	1.55	1.46
1	H	18	ARG	C-N	7.21	1.43	1.33
1	M	210	THR	CA-C	-7.18	1.43	1.53
1	I	142	VAL	C-N	7.16	1.43	1.33
1	C	127	GLY	CA-C	-7.15	1.44	1.52
1	N	91	ILE	CA-CB	7.13	1.62	1.54
1	D	185	MET	C-N	7.12	1.42	1.33
1	H	87	HIS	ND1-CE1	7.12	1.39	1.32
1	R	127	GLY	CA-C	7.09	1.59	1.52
1	M	102	SER	CA-CB	7.09	1.65	1.53
1	N	91	ILE	CB-CG1	7.08	1.67	1.53
1	Q	197	ASP	C-O	7.08	1.32	1.24
1	F	103	ASP	C-N	7.07	1.42	1.33
1	O	143	ARG	CA-CB	7.05	1.64	1.53
1	E	117	TRP	CA-C	-7.04	1.43	1.52
1	K	114	GLN	CA-C	-7.02	1.43	1.52
1	N	59	VAL	CA-CB	7.02	1.61	1.53
1	D	124	ILE	CA-C	7.01	1.60	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	58	THR	CA-C	-7.01	1.43	1.52
1	B	119	THR	CA-CB	7.00	1.64	1.53
1	B	141	ILE	N-CA	7.00	1.54	1.46
1	P	40	PHE	N-CA	-6.99	1.38	1.46
1	R	206	GLY	CA-C	-6.99	1.42	1.51
1	E	23	TRP	CA-CB	6.97	1.64	1.53
1	P	184	TRP	NE1-CE2	-6.97	1.29	1.37
1	C	60	GLY	CA-C	-6.95	1.47	1.52
1	I	89	GLY	C-N	-6.95	1.25	1.33
1	K	87	HIS	CA-CB	6.94	1.62	1.53
1	G	12	HIS	ND1-CE1	6.94	1.39	1.32
1	S	33	SER	CA-C	-6.93	1.45	1.53
1	C	71	GLU	CA-C	6.93	1.61	1.52
1	D	13	GLN	C-N	6.92	1.43	1.33
1	D	120	HIS	ND1-CE1	6.92	1.39	1.32
1	O	73	ILE	CA-CB	6.91	1.63	1.54
1	J	146	SER	CA-CB	-6.91	1.43	1.53
1	I	131	LYS	C-O	-6.91	1.16	1.24
1	C	12	HIS	ND1-CE1	6.90	1.39	1.32
1	C	180	GLU	CA-CB	6.88	1.64	1.53
1	L	79	GLU	CA-C	6.88	1.61	1.52
1	L	39	MET	C-N	6.87	1.42	1.33
1	G	38	PRO	CA-C	6.87	1.62	1.52
1	H	71	GLU	CA-C	6.86	1.61	1.52
1	K	40	PHE	CA-C	6.86	1.61	1.52
1	K	45	GLU	CA-CB	6.85	1.65	1.53
1	M	145	TYR	N-CA	-6.85	1.37	1.46
1	K	120	HIS	ND1-CE1	6.84	1.39	1.32
1	C	152	ASP	CA-C	-6.83	1.43	1.52
1	R	59	VAL	C-N	6.83	1.40	1.33
1	C	155	GLN	CA-CB	6.83	1.63	1.53
1	O	62	HIS	CA-CB	6.83	1.64	1.53
1	Q	89	GLY	N-CA	6.82	1.54	1.44
1	C	141	ILE	CA-CB	-6.81	1.46	1.54
1	C	70	LYS	N-CA	6.80	1.54	1.46
1	R	84	HIS	CA-CB	6.80	1.62	1.53
1	N	178	SER	C-O	-6.79	1.15	1.24
1	R	7	GLN	CA-CB	6.79	1.63	1.53
1	D	120	HIS	CG-CD2	6.79	1.43	1.35
1	O	38	PRO	C-N	6.78	1.42	1.33
1	Q	208	GLY	N-CA	6.78	1.55	1.45
1	B	159	GLU	C-N	6.76	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	62	HIS	CD2-NE2	6.76	1.45	1.37
1	B	124	ILE	CA-CB	6.75	1.60	1.54
1	L	115	ILE	CA-C	-6.75	1.44	1.52
1	D	52	LEU	N-CA	-6.74	1.38	1.46
1	E	100	ARG	C-N	6.74	1.42	1.33
1	B	211	LEU	CA-CB	6.71	1.63	1.53
1	I	164	TYR	CA-CB	6.71	1.63	1.53
1	S	120	HIS	CA-C	-6.70	1.44	1.52
1	F	127	GLY	CA-C	-6.69	1.44	1.52
1	K	84	HIS	CG-CD2	6.68	1.43	1.35
1	C	70	LYS	CA-CB	6.67	1.63	1.53
1	M	119	THR	CA-C	-6.66	1.43	1.52
1	L	137	GLY	N-CA	6.66	1.54	1.45
1	H	59	VAL	CA-CB	-6.66	1.46	1.54
1	R	43	LEU	C-N	6.66	1.42	1.33
1	K	100	ARG	CA-CB	6.66	1.64	1.53
1	L	105	ALA	N-CA	-6.65	1.37	1.46
1	L	36	VAL	CA-C	-6.65	1.44	1.52
1	S	181	VAL	CA-C	6.64	1.61	1.52
1	I	187	GLU	C-N	-6.64	1.25	1.33
1	D	26	VAL	CA-CB	6.64	1.61	1.54
1	B	27	VAL	CA-CB	-6.63	1.45	1.54
1	R	35	GLU	CA-C	-6.63	1.43	1.52
1	O	111	LEU	CA-CB	6.62	1.63	1.53
1	K	178	SER	CA-CB	6.61	1.64	1.53
1	N	134	ILE	CA-C	6.60	1.60	1.52
1	G	5	ASN	CA-C	6.60	1.62	1.53
1	E	7	GLN	CA-CB	6.59	1.63	1.53
1	I	53	ASN	C-O	-6.59	1.16	1.24
1	M	62	HIS	CA-CB	6.58	1.63	1.53
1	N	96	MET	N-CA	-6.58	1.37	1.45
1	B	154	ARG	N-CA	6.58	1.53	1.45
1	R	16	SER	C-N	6.57	1.43	1.33
1	C	33	SER	CA-C	6.57	1.60	1.53
1	R	154	ARG	CD-NE	6.56	1.55	1.46
1	G	72	THR	CA-C	6.56	1.61	1.52
1	B	184	TRP	CA-CB	6.56	1.63	1.53
1	G	163	ASP	C-O	-6.55	1.15	1.24
1	L	85	PRO	N-CD	-6.53	1.38	1.47
1	E	63	GLN	N-CA	-6.53	1.37	1.46
1	C	196	PRO	C-N	6.53	1.42	1.33
1	P	81	ASP	CA-C	6.53	1.61	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	32	PHE	CA-C	6.53	1.61	1.53
1	M	132	ARG	CA-CB	6.52	1.63	1.53
1	K	1	PRO	C-N	6.51	1.41	1.33
1	P	202	LEU	N-CA	-6.51	1.38	1.46
1	O	7	GLN	CA-CB	6.51	1.63	1.53
1	Q	12	HIS	ND1-CE1	6.50	1.39	1.32
1	I	143	ARG	CA-C	-6.50	1.44	1.52
1	Q	62	HIS	CD2-NE2	6.50	1.45	1.37
1	N	12	HIS	CB-CG	6.50	1.59	1.50
1	E	176	GLN	CA-C	-6.50	1.44	1.52
1	J	27	VAL	C-N	6.49	1.42	1.33
1	E	117	TRP	CA-CB	6.48	1.63	1.53
1	P	55	MET	CA-C	6.48	1.61	1.52
1	G	37	ILE	CB-CG1	6.48	1.66	1.53
1	H	73	ILE	CA-C	6.48	1.61	1.52
1	Q	40	PHE	CA-CB	6.47	1.63	1.53
1	J	183	ASN	CA-C	-6.47	1.44	1.52
1	C	109	SER	N-CA	6.46	1.53	1.45
1	K	79	GLU	CA-CB	6.46	1.63	1.53
1	O	68	MET	CA-C	-6.45	1.44	1.52
1	F	120	HIS	CD2-NE2	6.45	1.45	1.37
1	S	182	LYS	CA-CB	6.45	1.63	1.53
1	P	128	GLU	CA-C	6.44	1.61	1.52
1	K	162	ARG	N-CA	-6.43	1.38	1.46
1	I	183	ASN	CA-C	-6.43	1.44	1.52
1	K	190	LEU	CA-C	-6.42	1.44	1.52
1	O	117	TRP	NE1-CE2	6.42	1.44	1.37
1	I	34	PRO	N-CD	6.41	1.56	1.47
1	S	175	GLU	CA-C	-6.41	1.44	1.53
1	L	173	ARG	N-CA	-6.41	1.38	1.46
1	M	33	SER	N-CA	-6.41	1.39	1.45
1	H	180	GLU	C-N	6.40	1.42	1.33
1	H	82	ARG	N-CA	-6.38	1.38	1.46
1	I	191	VAL	N-CA	-6.38	1.38	1.46
1	P	116	GLY	CA-C	-6.37	1.45	1.52
1	O	67	GLN	C-N	6.37	1.41	1.33
1	I	100	ARG	CA-CB	6.37	1.62	1.53
1	K	140	LYS	CA-C	6.36	1.61	1.52
1	E	144	MET	N-CA	-6.36	1.38	1.46
1	E	199	LYS	CA-CB	6.36	1.63	1.53
1	M	134	ILE	CA-C	6.35	1.60	1.52
1	D	66	MET	CA-CB	6.34	1.63	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	143	ARG	N-CA	6.34	1.54	1.46
1	C	199	LYS	C-N	6.33	1.42	1.33
1	L	90	PRO	N-CD	6.33	1.56	1.47
1	Q	180	GLU	CA-CB	6.32	1.63	1.53
1	O	40	PHE	CA-CB	6.31	1.63	1.53
1	R	155	GLN	CA-CB	6.31	1.62	1.53
1	G	95	GLN	CA-CB	6.31	1.62	1.53
1	S	180	GLU	C-N	6.31	1.41	1.33
1	O	196	PRO	N-CA	-6.31	1.39	1.47
1	R	208	GLY	CA-C	-6.30	1.45	1.51
1	Q	113	GLU	CA-C	-6.30	1.44	1.52
1	S	184	TRP	CA-CB	6.30	1.63	1.53
1	B	43	LEU	CA-C	6.30	1.61	1.52
1	K	72	THR	C-N	6.30	1.41	1.33
1	K	50	GLN	N-CA	6.29	1.53	1.46
1	O	198	CYS	C-N	6.29	1.41	1.33
1	N	79	GLU	C-N	6.29	1.41	1.33
1	K	148	THR	C-N	6.28	1.41	1.33
1	C	108	THR	CA-CB	6.28	1.63	1.53
1	C	63	GLN	CA-C	-6.28	1.44	1.52
1	F	124	ILE	CA-CB	6.28	1.60	1.53
1	P	143	ARG	CA-C	-6.28	1.44	1.52
1	J	2	ILE	C-N	6.28	1.42	1.33
1	K	168	PHE	C-O	-6.28	1.16	1.24
1	E	133	TRP	NE1-CE2	6.28	1.44	1.37
1	H	70	LYS	CA-C	6.28	1.60	1.52
1	G	81	ASP	CA-CB	6.27	1.63	1.53
1	E	59	VAL	N-CA	-6.27	1.39	1.46
1	H	120	HIS	CG-CD2	6.25	1.42	1.35
1	P	121	ASN	CA-CB	-6.25	1.42	1.53
1	C	162	ARG	CD-NE	6.25	1.54	1.46
1	L	197	ASP	C-O	-6.24	1.17	1.24
1	R	131	LYS	CA-CB	6.24	1.63	1.53
1	O	200	THR	CA-C	-6.24	1.44	1.52
1	I	167	ARG	CA-CB	6.23	1.63	1.53
1	P	201	ILE	N-CA	-6.23	1.39	1.46
1	G	128	GLU	CA-CB	6.22	1.63	1.53
1	M	111	LEU	N-CA	-6.22	1.38	1.46
1	S	26	VAL	CA-CB	6.22	1.61	1.54
1	M	182	LYS	N-CA	6.21	1.54	1.46
1	N	172	LEU	CA-CB	6.21	1.62	1.53
1	D	204	ALA	C-N	6.21	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	12	HIS	CG-ND1	6.20	1.45	1.38
1	I	16	SER	CA-CB	6.20	1.63	1.53
1	G	153	ILE	C-O	6.19	1.29	1.23
1	L	69	LEU	CA-C	6.19	1.60	1.52
1	E	21	ASN	C-N	6.19	1.42	1.33
1	H	215	MET	CA-C	6.19	1.60	1.52
1	L	73	ILE	CA-C	6.19	1.60	1.52
1	J	50	GLN	CA-CB	6.18	1.62	1.53
1	L	156	GLY	N-CA	6.18	1.53	1.44
1	J	77	ALA	CA-C	6.18	1.60	1.52
1	S	95	GLN	CA-C	-6.18	1.45	1.52
1	L	137	GLY	CA-C	-6.18	1.45	1.52
1	C	120	HIS	ND1-CE1	6.18	1.38	1.32
1	S	122	PRO	CA-CB	6.17	1.64	1.53
1	K	82	ARG	C-N	6.17	1.42	1.33
1	C	72	THR	CA-C	-6.17	1.45	1.52
1	R	37	ILE	CA-C	6.17	1.59	1.52
1	L	188	THR	C-O	-6.16	1.16	1.23
1	P	143	ARG	NE-CZ	6.16	1.39	1.33
1	B	133	TRP	CA-CB	6.16	1.62	1.53
1	J	87	HIS	ND1-CE1	6.16	1.38	1.32
1	E	168	PHE	C-O	-6.15	1.17	1.24
1	E	218	CYS	CA-C	6.15	1.61	1.52
1	D	54	THR	CA-C	-6.15	1.45	1.52
1	M	7	GLN	CA-C	6.14	1.60	1.52
1	M	123	PRO	N-CA	-6.14	1.40	1.46
1	P	89	GLY	CA-C	-6.14	1.43	1.51
1	M	43	LEU	CA-C	6.14	1.61	1.52
1	O	212	GLU	CA-C	-6.14	1.44	1.52
1	K	207	PRO	N-CA	6.13	1.55	1.47
1	N	153	ILE	C-N	6.13	1.41	1.33
1	J	220	GLY	N-CA	6.12	1.54	1.45
1	N	18	ARG	CA-CB	6.11	1.63	1.53
1	J	103	ASP	CA-C	-6.11	1.44	1.52
1	R	171	THR	CA-C	-6.11	1.45	1.52
1	K	133	TRP	N-CA	-6.10	1.39	1.46
1	S	177	ALA	CA-C	6.10	1.60	1.52
1	H	181	VAL	C-O	6.09	1.31	1.24
1	L	13	GLN	N-CA	-6.09	1.38	1.45
1	L	158	LYS	CA-C	6.09	1.60	1.53
1	N	195	ASN	C-O	6.09	1.31	1.23
1	S	5	ASN	CA-CB	6.09	1.62	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	34	PRO	C-N	6.08	1.42	1.33
1	I	7	GLN	CA-C	6.08	1.60	1.53
1	K	21	ASN	C-N	6.08	1.41	1.33
1	L	153	ILE	CA-CB	6.08	1.60	1.53
1	L	214	MET	CA-C	-6.08	1.45	1.52
1	G	207	PRO	CA-C	-6.08	1.46	1.52
1	R	113	GLU	C-N	6.07	1.41	1.33
1	M	31	ALA	CA-C	6.07	1.58	1.52
1	O	162	ARG	CD-NE	6.07	1.54	1.46
1	G	154	ARG	CD-NE	6.07	1.54	1.46
1	Q	162	ARG	CA-C	6.07	1.60	1.52
1	L	147	PRO	CA-C	6.06	1.61	1.52
1	M	183	ASN	N-CA	6.05	1.53	1.46
1	B	133	TRP	N-CA	6.05	1.53	1.46
1	B	35	GLU	N-CA	6.05	1.54	1.46
1	L	216	THR	C-O	6.04	1.31	1.24
1	R	141	ILE	CA-CB	-6.04	1.47	1.54
1	E	37	ILE	CA-CB	6.04	1.57	1.54
1	G	173	ARG	CA-CB	6.03	1.63	1.53
1	Q	8	GLY	C-N	6.03	1.41	1.33
1	R	153	ILE	C-N	6.03	1.41	1.33
1	B	219	GLN	N-CA	-6.03	1.39	1.46
1	I	73	ILE	CA-CB	-6.02	1.47	1.54
1	N	174	ALA	CA-C	6.02	1.61	1.52
1	D	82	ARG	CD-NE	6.01	1.54	1.46
1	K	55	MET	CA-C	6.01	1.60	1.52
1	G	143	ARG	CD-NE	6.01	1.54	1.46
1	C	214	MET	CA-C	-6.00	1.45	1.52
1	C	44	SER	C-N	6.00	1.41	1.33
1	F	60	GLY	CA-C	-6.00	1.46	1.52
1	K	19	THR	N-CA	6.00	1.53	1.46
1	R	15	ILE	C-O	6.00	1.31	1.24
1	R	163	ASP	CA-CB	6.00	1.63	1.53
1	C	194	ALA	CA-C	6.00	1.60	1.52
1	P	196	PRO	C-N	6.00	1.41	1.33
1	I	143	ARG	C-N	5.99	1.42	1.33
1	L	4	GLN	CA-CB	5.99	1.61	1.53
1	O	192	GLN	CA-C	-5.98	1.45	1.52
1	R	7	GLN	C-N	5.98	1.39	1.33
1	G	168	PHE	CB-CG	5.98	1.64	1.50
1	S	54	THR	CA-CB	5.97	1.62	1.53
1	E	56	LEU	N-CA	-5.97	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	107	THR	C-N	5.96	1.41	1.33
1	G	90	PRO	N-CA	-5.96	1.40	1.47
1	P	165	VAL	C-N	-5.96	1.26	1.33
1	E	113	GLU	C-N	5.96	1.41	1.33
1	J	26	VAL	C-O	-5.96	1.17	1.24
1	C	82	ARG	CD-NE	5.96	1.54	1.46
1	J	5	ASN	N-CA	-5.96	1.38	1.45
1	O	150	ILE	C-N	5.95	1.42	1.33
1	Q	87	HIS	ND1-CE1	5.95	1.38	1.32
1	G	100	ARG	CD-NE	5.95	1.54	1.46
1	N	184	TRP	CA-CB	5.95	1.62	1.53
1	K	23	TRP	N-CA	-5.95	1.39	1.46
1	J	198	CYS	N-CA	-5.95	1.38	1.46
1	H	12	HIS	N-CA	5.94	1.53	1.46
1	H	47	ALA	N-CA	-5.94	1.39	1.45
1	R	146	SER	CA-CB	5.94	1.62	1.53
1	K	195	ASN	C-N	5.94	1.42	1.33
1	P	130	TYR	C-N	5.94	1.41	1.33
1	J	147	PRO	N-CA	5.94	1.54	1.47
1	N	21	ASN	N-CA	-5.93	1.39	1.46
1	S	66	MET	CA-C	-5.93	1.45	1.52
1	L	12	HIS	ND1-CE1	5.93	1.38	1.32
1	H	132	ARG	CA-C	5.93	1.60	1.52
1	P	165	VAL	CA-C	5.92	1.60	1.52
1	F	167	ARG	CA-CB	5.92	1.62	1.53
1	K	90	PRO	C-O	-5.92	1.16	1.23
1	Q	46	GLY	C-N	5.92	1.41	1.33
1	H	55	MET	CA-C	5.92	1.60	1.52
1	I	28	GLU	C-N	5.92	1.42	1.33
1	Q	208	GLY	C-N	5.92	1.41	1.33
1	P	23	TRP	N-CA	5.92	1.53	1.46
1	O	107	THR	C-N	-5.91	1.25	1.33
1	B	84	HIS	N-CA	-5.91	1.40	1.46
1	E	65	ALA	N-CA	-5.91	1.39	1.46
1	G	191	VAL	CA-C	-5.91	1.45	1.52
1	B	40	PHE	CA-C	-5.90	1.45	1.52
1	Q	20	LEU	CA-CB	5.90	1.62	1.53
1	I	149	SER	CA-C	-5.90	1.44	1.53
1	K	53	ASN	C-N	5.90	1.41	1.33
1	O	55	MET	C-N	5.90	1.41	1.33
1	O	215	MET	N-CA	-5.90	1.39	1.46
1	R	66	MET	CA-CB	5.89	1.62	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	138	LEU	C-N	5.89	1.41	1.33
1	F	141	ILE	C-N	5.89	1.41	1.33
1	S	52	LEU	N-CA	5.88	1.53	1.46
1	D	98	GLU	CA-C	-5.88	1.46	1.52
1	H	95	GLN	CA-CB	5.87	1.62	1.53
1	K	41	SER	C-N	5.87	1.41	1.33
1	F	127	GLY	N-CA	5.87	1.53	1.45
1	N	188	THR	CA-C	-5.87	1.47	1.53
1	Q	65	ALA	CA-C	5.87	1.60	1.52
1	M	112	GLN	N-CA	-5.87	1.39	1.46
1	S	79	GLU	C-O	-5.87	1.17	1.24
1	B	130	TYR	CA-CB	5.86	1.62	1.53
1	F	212	GLU	N-CA	5.86	1.53	1.46
1	H	96	MET	N-CA	-5.86	1.38	1.46
1	Q	69	LEU	C-N	5.86	1.41	1.33
1	E	14	ALA	CA-C	5.86	1.60	1.52
1	Q	193	ASN	C-N	5.85	1.41	1.33
1	B	142	VAL	CA-C	5.85	1.59	1.52
1	J	144	MET	N-CA	-5.85	1.39	1.46
1	N	107	THR	CA-C	5.85	1.60	1.52
1	O	72	THR	C-N	5.85	1.41	1.33
1	R	49	PRO	C-N	5.84	1.41	1.33
1	M	37	ILE	N-CA	-5.84	1.39	1.46
1	S	211	LEU	C-N	5.84	1.41	1.33
1	E	206	GLY	CA-C	5.84	1.60	1.51
1	B	87	HIS	CA-C	-5.83	1.45	1.52
1	H	208	GLY	CA-C	-5.83	1.43	1.51
1	E	7	GLN	N-CA	5.83	1.54	1.46
1	N	103	ASP	CA-C	-5.83	1.45	1.52
1	S	143	ARG	CZ-NH2	-5.83	1.25	1.33
1	R	135	ILE	C-N	5.82	1.41	1.33
1	J	121	ASN	CA-C	5.82	1.59	1.52
1	B	108	THR	CA-C	-5.82	1.44	1.52
1	M	191	VAL	C-O	5.82	1.31	1.24
1	E	120	HIS	N-CA	-5.81	1.38	1.46
1	K	141	ILE	CA-CB	-5.81	1.47	1.54
1	H	120	HIS	C-N	-5.81	1.27	1.33
1	N	193	ASN	C-N	-5.81	1.25	1.33
1	H	142	VAL	N-CA	5.81	1.53	1.46
1	D	119	THR	CA-C	-5.81	1.44	1.52
1	F	59	VAL	CA-C	5.80	1.59	1.52
1	L	15	ILE	CA-CB	-5.80	1.48	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	160	PRO	N-CA	5.80	1.54	1.47
1	D	109	SER	CA-C	-5.80	1.45	1.52
1	K	83	LEU	N-CA	-5.79	1.39	1.46
1	Q	161	PHE	CA-C	-5.79	1.45	1.52
1	E	115	ILE	CA-CB	-5.79	1.47	1.54
1	C	111	LEU	CA-C	-5.79	1.45	1.52
1	D	164	TYR	CA-CB	5.79	1.62	1.53
1	G	191	VAL	N-CA	-5.78	1.39	1.46
1	L	31	ALA	CA-C	5.78	1.60	1.52
1	H	137	GLY	N-CA	5.78	1.52	1.45
1	J	184	TRP	N-CA	-5.78	1.39	1.46
1	C	196	PRO	CA-CB	5.77	1.62	1.53
1	D	73	ILE	CA-C	5.77	1.60	1.52
1	O	133	TRP	CA-C	5.77	1.60	1.52
1	H	173	ARG	N-CA	5.77	1.53	1.46
1	G	175	GLU	N-CA	-5.76	1.39	1.45
1	I	104	ILE	N-CA	5.75	1.53	1.46
1	N	194	ALA	CA-C	5.75	1.60	1.53
1	D	10	MET	CA-CB	5.75	1.61	1.53
1	F	176	GLN	N-CA	5.75	1.53	1.46
1	H	9	GLN	C-N	5.75	1.41	1.33
1	H	175	GLU	C-N	5.75	1.41	1.33
1	O	199	LYS	CA-C	-5.75	1.45	1.52
1	I	190	LEU	CA-C	5.75	1.60	1.52
1	J	18	ARG	CD-NE	5.75	1.54	1.46
1	F	185	MET	CA-CB	5.74	1.62	1.53
1	O	114	GLN	N-CA	-5.74	1.39	1.46
1	I	172	LEU	C-N	5.74	1.41	1.34
1	N	20	LEU	C-N	5.74	1.41	1.33
1	K	166	ASP	CA-CB	5.73	1.62	1.53
1	R	189	LEU	C-N	5.73	1.41	1.33
1	J	192	GLN	N-CA	5.73	1.53	1.46
1	Q	25	LYS	CA-C	-5.72	1.45	1.52
1	M	33	SER	CA-C	5.72	1.58	1.52
1	E	132	ARG	CA-C	5.71	1.60	1.52
1	B	45	GLU	C-N	5.71	1.41	1.33
1	H	167	ARG	CD-NE	5.71	1.54	1.46
1	M	155	GLN	CA-C	5.71	1.59	1.52
1	C	188	THR	N-CA	5.71	1.53	1.46
1	F	111	LEU	CA-CB	5.71	1.62	1.53
1	C	83	LEU	CA-C	5.71	1.60	1.52
1	D	134	ILE	CA-C	-5.71	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	178	SER	CA-CB	5.70	1.62	1.53
1	P	18	ARG	CD-NE	5.70	1.54	1.46
1	F	9	GLN	CA-CB	5.70	1.60	1.52
1	G	22	ALA	C-O	-5.69	1.17	1.24
1	J	189	LEU	C-N	5.69	1.40	1.33
1	L	10	MET	C-N	5.69	1.41	1.33
1	R	195	ASN	CA-C	5.68	1.60	1.53
1	C	201	ILE	CA-C	5.68	1.59	1.52
1	M	135	ILE	CA-C	-5.68	1.45	1.52
1	C	117	TRP	C-N	5.67	1.41	1.33
1	F	132	ARG	CD-NE	5.67	1.54	1.46
1	R	201	ILE	C-N	5.67	1.41	1.33
1	E	93	PRO	N-CA	5.67	1.53	1.47
1	N	150	ILE	CA-CB	-5.67	1.46	1.54
1	J	209	ALA	CA-C	-5.67	1.45	1.52
1	L	183	ASN	CA-CB	5.67	1.62	1.53
1	Q	175	GLU	CA-CB	5.67	1.61	1.53
1	D	192	GLN	CA-C	5.67	1.60	1.52
1	I	205	LEU	CA-C	5.67	1.60	1.52
1	R	13	GLN	CA-C	-5.66	1.45	1.52
1	C	201	ILE	CA-CB	5.66	1.60	1.54
1	P	202	LEU	C-N	-5.66	1.26	1.34
1	F	10	MET	C-N	5.66	1.41	1.33
1	N	37	ILE	C-N	5.66	1.41	1.34
1	G	124	ILE	CB-CG1	5.66	1.64	1.53
1	J	89	GLY	N-CA	5.65	1.52	1.44
1	Q	143	ARG	CD-NE	5.65	1.54	1.46
1	C	98	GLU	C-N	-5.65	1.27	1.33
1	R	100	ARG	CD-NE	5.65	1.54	1.46
1	N	87	HIS	C-N	5.64	1.41	1.33
1	M	177	ALA	CA-C	5.64	1.59	1.52
1	G	197	ASP	CA-C	5.64	1.59	1.52
1	H	23	TRP	CD2-CE2	5.64	1.50	1.41
1	L	8	GLY	N-CA	5.63	1.53	1.45
1	J	154	ARG	CZ-NH2	-5.63	1.26	1.33
1	C	49	PRO	CA-CB	-5.63	1.45	1.53
1	F	52	LEU	C-O	-5.63	1.17	1.24
1	O	160	PRO	CA-CB	5.63	1.61	1.53
1	B	130	TYR	CA-C	5.63	1.60	1.52
1	D	136	LEU	C-O	-5.63	1.17	1.24
1	L	116	GLY	N-CA	-5.62	1.39	1.45
1	O	135	ILE	CA-CB	-5.62	1.47	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	87	HIS	ND1-CE1	5.62	1.38	1.32
1	D	116	GLY	CA-C	5.62	1.58	1.51
1	P	133	TRP	C-N	5.61	1.40	1.33
1	G	102	SER	CA-C	-5.61	1.45	1.52
1	I	164	TYR	C-N	-5.61	1.26	1.33
1	C	70	LYS	CA-C	-5.61	1.45	1.52
1	Q	88	ALA	CA-C	5.60	1.60	1.52
1	B	214	MET	N-CA	-5.60	1.39	1.46
1	N	183	ASN	CA-C	5.60	1.60	1.52
1	I	167	ARG	CD-NE	5.60	1.54	1.46
1	C	87	HIS	ND1-CE1	5.60	1.38	1.32
1	I	71	GLU	CA-C	5.60	1.59	1.52
1	C	84	HIS	CA-C	5.59	1.59	1.52
1	H	86	VAL	CA-C	5.59	1.58	1.53
1	J	195	ASN	CA-CB	5.59	1.62	1.53
1	B	154	ARG	CD-NE	5.59	1.54	1.46
1	K	169	TYR	C-N	5.59	1.41	1.33
1	S	184	TRP	N-CA	-5.58	1.39	1.46
1	F	164	TYR	CA-C	-5.58	1.45	1.52
1	M	9	GLN	CA-CB	5.58	1.59	1.52
1	L	47	ALA	N-CA	-5.57	1.39	1.46
1	D	117	TRP	NE1-CE2	-5.57	1.31	1.37
1	G	14	ALA	C-N	5.57	1.40	1.33
1	L	37	ILE	CA-C	5.57	1.58	1.52
1	N	84	HIS	CA-CB	5.57	1.62	1.53
1	N	120	HIS	CD2-NE2	5.57	1.44	1.37
1	O	219	GLN	CA-C	5.56	1.60	1.52
1	D	174	ALA	N-CA	-5.56	1.38	1.46
1	R	27	VAL	C-N	5.55	1.41	1.33
1	S	125	PRO	C-N	-5.55	1.27	1.34
1	L	66	MET	CA-CB	5.55	1.61	1.53
1	M	116	GLY	N-CA	-5.55	1.39	1.45
1	M	189	LEU	CA-C	-5.55	1.45	1.52
1	G	8	GLY	C-N	5.55	1.41	1.33
1	N	213	GLU	CA-C	5.54	1.59	1.52
1	F	27	VAL	C-N	5.54	1.41	1.33
1	M	14	ALA	C-N	5.54	1.41	1.33
1	P	21	ASN	CA-C	-5.54	1.45	1.52
1	G	48	THR	CA-C	5.53	1.59	1.52
1	O	166	ASP	C-N	5.53	1.41	1.33
1	Q	43	LEU	CA-CB	5.53	1.63	1.53
1	M	32	PHE	CA-C	-5.53	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	200	THR	N-CA	5.53	1.52	1.46
1	Q	168	PHE	C-N	5.52	1.41	1.33
1	R	30	LYS	CA-C	-5.52	1.45	1.52
1	C	105	ALA	CA-CB	5.52	1.63	1.53
1	K	141	ILE	N-CA	-5.52	1.39	1.46
1	E	177	ALA	CA-C	-5.52	1.46	1.52
1	M	142	VAL	CA-C	5.52	1.59	1.52
1	S	56	LEU	CA-C	5.52	1.59	1.52
1	Q	144	MET	CA-C	5.52	1.59	1.52
1	C	82	ARG	CA-CB	5.51	1.61	1.53
1	E	148	THR	C-N	5.51	1.40	1.33
1	N	104	ILE	N-CA	-5.51	1.39	1.46
1	O	182	LYS	N-CA	5.51	1.53	1.46
1	I	170	LYS	C-N	5.50	1.41	1.33
1	S	12	HIS	CA-CB	5.50	1.62	1.53
1	F	201	ILE	N-CA	-5.50	1.40	1.46
1	F	65	ALA	N-CA	-5.50	1.39	1.46
1	F	144	MET	N-CA	5.50	1.53	1.46
1	J	15	ILE	N-CA	5.50	1.53	1.46
1	O	113	GLU	CA-CB	5.50	1.61	1.53
1	P	18	ARG	C-N	5.50	1.40	1.33
1	E	140	LYS	C-N	5.49	1.40	1.33
1	Q	50	GLN	CA-C	-5.49	1.45	1.52
1	Q	85	PRO	CA-C	5.49	1.59	1.52
1	Q	210	THR	C-N	5.48	1.41	1.33
1	P	216	THR	CB-OG1	-5.48	1.34	1.43
1	R	169	TYR	N-CA	-5.48	1.39	1.46
1	C	3	VAL	CA-CB	-5.48	1.47	1.54
1	C	215	MET	CA-CB	5.48	1.61	1.53
1	D	18	ARG	C-N	5.48	1.40	1.33
1	K	160	PRO	CA-C	5.47	1.58	1.52
1	O	116	GLY	CA-C	-5.47	1.45	1.51
1	E	113	GLU	C-O	-5.47	1.17	1.24
1	L	179	GLN	C-N	5.47	1.41	1.33
1	G	155	GLN	C-N	5.47	1.41	1.33
1	D	131	LYS	C-N	5.46	1.41	1.33
1	L	203	LYS	N-CA	-5.46	1.39	1.46
1	Q	107	THR	CA-C	-5.46	1.45	1.52
1	P	120	HIS	N-CA	-5.46	1.39	1.46
1	Q	117	TRP	CD2-CE3	-5.46	1.31	1.40
1	M	45	GLU	CA-C	-5.46	1.46	1.52
1	M	115	ILE	C-N	5.46	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	115	ILE	CA-CB	-5.45	1.47	1.54
1	P	24	VAL	C-N	5.45	1.41	1.33
1	R	196	PRO	N-CA	5.45	1.54	1.47
1	M	84	HIS	N-CA	5.45	1.53	1.46
1	L	171	THR	CA-C	-5.45	1.45	1.52
1	G	217	ALA	CA-CB	5.44	1.61	1.53
1	D	196	PRO	N-CA	5.44	1.54	1.47
1	P	84	HIS	ND1-CE1	5.44	1.38	1.32
1	H	91	ILE	CA-CB	5.44	1.61	1.54
1	S	189	LEU	CA-C	-5.43	1.45	1.52
1	C	35	GLU	CA-CB	5.43	1.63	1.53
1	I	165	VAL	CA-C	5.43	1.59	1.52
1	F	103	ASP	CA-C	5.43	1.59	1.52
1	G	84	HIS	CA-C	5.42	1.58	1.52
1	B	209	ALA	CA-C	5.42	1.59	1.52
1	I	49	PRO	N-CA	-5.42	1.40	1.47
1	L	94	GLY	N-CA	5.41	1.53	1.45
1	H	191	VAL	C-N	5.41	1.41	1.33
1	O	177	ALA	CA-CB	5.41	1.62	1.53
1	S	82	ARG	CD-NE	5.41	1.53	1.46
1	D	79	GLU	N-CA	5.41	1.52	1.46
1	B	12	HIS	CB-CG	5.40	1.57	1.50
1	P	3	VAL	CA-C	-5.40	1.46	1.52
1	O	40	PHE	N-CA	5.40	1.52	1.46
1	D	34	PRO	N-CD	-5.39	1.40	1.47
1	L	188	THR	CA-C	-5.39	1.47	1.53
1	D	117	TRP	CZ2-CH2	5.39	1.47	1.37
1	F	190	LEU	C-O	-5.39	1.17	1.24
1	G	100	ARG	CA-CB	5.39	1.60	1.53
1	E	179	GLN	N-CA	-5.39	1.39	1.46
1	L	212	GLU	C-O	-5.39	1.17	1.24
1	O	15	ILE	C-O	-5.38	1.18	1.24
1	O	90	PRO	CA-C	-5.38	1.46	1.52
1	H	29	GLU	N-CA	5.38	1.53	1.46
1	K	27	VAL	CA-C	5.38	1.59	1.52
1	L	173	ARG	CA-C	5.38	1.60	1.52
1	I	103	ASP	C-N	5.38	1.40	1.33
1	K	27	VAL	C-N	5.38	1.40	1.33
1	N	181	VAL	CA-CB	-5.38	1.47	1.54
1	Q	93	PRO	C-N	5.38	1.42	1.33
1	J	64	ALA	CA-CB	5.38	1.61	1.53
1	S	132	ARG	CD-NE	5.38	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	9	GLN	CA-CB	5.37	1.59	1.52
1	B	173	ARG	CD-NE	5.37	1.53	1.46
1	K	54	THR	CA-CB	5.37	1.61	1.53
1	E	177	ALA	C-N	5.37	1.40	1.33
1	N	84	HIS	ND1-CE1	5.37	1.38	1.32
1	N	193	ASN	N-CA	5.36	1.53	1.46
1	R	46	GLY	C-N	5.36	1.40	1.33
1	G	30	LYS	C-N	5.36	1.41	1.33
1	H	105	ALA	C-O	-5.36	1.16	1.24
1	G	5	ASN	N-CA	-5.36	1.39	1.45
1	D	184	TRP	C-O	-5.35	1.17	1.24
1	L	56	LEU	N-CA	5.35	1.52	1.46
1	D	54	THR	C-N	5.35	1.40	1.33
1	L	92	ALA	C-O	5.35	1.30	1.23
1	R	83	LEU	C-N	5.35	1.40	1.33
1	D	83	LEU	C-N	5.35	1.41	1.33
1	Q	196	PRO	CA-C	5.34	1.60	1.52
1	R	191	VAL	CA-CB	5.34	1.61	1.54
1	E	148	THR	N-CA	5.34	1.52	1.45
1	O	152	ASP	CA-C	5.34	1.60	1.52
1	N	18	ARG	CZ-NH1	5.34	1.40	1.32
1	K	172	LEU	N-CA	-5.34	1.39	1.46
1	J	166	ASP	CA-CB	5.34	1.61	1.53
1	F	190	LEU	CA-C	5.33	1.59	1.52
1	E	97	ARG	CZ-NH2	-5.33	1.26	1.33
1	K	46	GLY	C-N	5.33	1.40	1.33
1	P	84	HIS	C-N	5.33	1.40	1.33
1	B	217	ALA	N-CA	-5.33	1.40	1.46
1	J	211	LEU	CA-C	-5.33	1.45	1.52
1	K	74	ASN	C-N	5.33	1.40	1.33
1	S	104	ILE	CA-CB	5.33	1.61	1.54
1	D	38	PRO	C-N	5.33	1.40	1.33
1	I	216	THR	C-N	5.33	1.41	1.33
1	G	92	ALA	CA-CB	-5.32	1.44	1.53
1	L	71	GLU	C-N	5.32	1.40	1.33
1	Q	172	LEU	N-CA	5.32	1.52	1.46
1	O	107	THR	N-CA	5.32	1.52	1.45
1	B	214	MET	CA-C	-5.31	1.46	1.52
1	Q	132	ARG	C-N	5.31	1.40	1.33
1	B	120	HIS	CD2-NE2	5.31	1.43	1.37
1	H	7	GLN	CA-CB	5.31	1.61	1.53
1	H	95	GLN	N-CA	-5.31	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	20	LEU	C-N	5.31	1.40	1.33
1	S	36	VAL	CA-C	-5.31	1.45	1.52
1	G	24	VAL	CA-C	5.31	1.59	1.52
1	M	67	GLN	CA-CB	5.30	1.61	1.53
1	O	47	ALA	C-N	5.30	1.41	1.33
1	N	146	SER	CA-C	5.30	1.58	1.52
1	Q	186	THR	CA-CB	5.30	1.61	1.53
1	L	136	LEU	CA-C	5.30	1.59	1.52
1	C	60	GLY	N-CA	5.30	1.53	1.45
1	K	139	ASN	CA-CB	5.29	1.61	1.53
1	P	105	ALA	C-N	5.29	1.40	1.33
1	N	36	VAL	CA-C	-5.29	1.46	1.52
1	G	160	PRO	C-N	5.29	1.40	1.33
1	H	178	SER	N-CA	-5.29	1.38	1.45
1	O	113	GLU	C-N	-5.29	1.27	1.33
1	C	44	SER	CA-CB	5.29	1.60	1.53
1	H	150	ILE	N-CA	5.28	1.53	1.46
1	F	29	GLU	CA-C	5.28	1.59	1.52
1	L	96	MET	N-CA	5.28	1.52	1.45
1	C	189	LEU	C-N	5.28	1.40	1.33
1	P	59	VAL	CA-CB	5.28	1.60	1.54
1	B	38	PRO	C-O	5.27	1.30	1.24
1	E	131	LYS	CA-C	-5.27	1.46	1.52
1	M	118	MET	N-CA	-5.27	1.39	1.46
1	S	65	ALA	C-N	5.27	1.40	1.33
1	J	31	ALA	CA-CB	5.27	1.62	1.52
1	B	184	TRP	CA-C	5.27	1.59	1.52
1	F	85	PRO	N-CA	-5.27	1.41	1.47
1	I	32	PHE	CA-CB	5.27	1.62	1.53
1	J	114	GLN	C-N	5.27	1.40	1.33
1	B	2	ILE	CA-C	-5.27	1.45	1.52
1	N	113	GLU	CA-CB	5.26	1.61	1.53
1	N	132	ARG	CD-NE	5.26	1.53	1.46
1	N	153	ILE	CA-CB	5.26	1.59	1.53
1	B	183	ASN	C-N	5.26	1.40	1.33
1	E	173	ARG	NE-CZ	5.26	1.38	1.33
1	F	12	HIS	CD2-NE2	-5.26	1.32	1.37
1	G	128	GLU	CA-C	-5.26	1.45	1.52
1	P	145	TYR	N-CA	-5.26	1.39	1.46
1	S	167	ARG	CD-NE	5.26	1.53	1.46
1	H	39	MET	N-CA	5.26	1.52	1.46
1	B	99	PRO	C-N	5.25	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	23	TRP	CA-C	-5.25	1.46	1.52
1	S	18	ARG	CD-NE	5.25	1.53	1.46
1	S	141	ILE	C-N	5.25	1.40	1.33
1	G	1	PRO	N-CD	5.25	1.55	1.47
1	B	99	PRO	N-CD	5.25	1.55	1.47
1	O	188	THR	CA-CB	-5.25	1.45	1.53
1	S	62	HIS	CG-CD2	5.25	1.41	1.35
1	J	16	SER	CA-CB	5.25	1.61	1.53
1	Q	16	SER	CA-C	-5.25	1.47	1.53
1	H	59	VAL	CA-C	5.24	1.58	1.52
1	N	113	GLU	C-N	5.24	1.40	1.33
1	G	212	GLU	C-N	5.24	1.40	1.33
1	M	72	THR	N-CA	5.24	1.52	1.46
1	S	23	TRP	CA-CB	5.24	1.61	1.53
1	I	151	LEU	CA-CB	5.24	1.61	1.53
1	Q	103	ASP	N-CA	-5.24	1.40	1.46
1	C	97	ARG	CZ-NH1	-5.24	1.25	1.32
1	N	167	ARG	CA-CB	5.23	1.61	1.53
1	Q	12	HIS	CD2-NE2	5.22	1.43	1.37
1	E	138	LEU	CA-C	-5.22	1.46	1.52
1	J	154	ARG	NE-CZ	5.22	1.38	1.33
1	S	66	MET	C-O	-5.22	1.18	1.24
1	B	85	PRO	N-CA	5.22	1.53	1.47
1	R	132	ARG	CD-NE	5.22	1.53	1.46
1	Q	151	LEU	CA-CB	5.21	1.61	1.53
1	P	114	GLN	C-N	5.21	1.40	1.33
1	G	100	ARG	CZ-NH2	-5.21	1.26	1.33
1	Q	7	GLN	N-CA	5.21	1.54	1.46
1	Q	100	ARG	CD-NE	5.21	1.53	1.46
1	C	170	LYS	CA-C	5.21	1.59	1.52
1	Q	123	PRO	C-N	5.21	1.39	1.33
1	R	152	ASP	C-N	5.21	1.40	1.33
1	F	93	PRO	N-CD	-5.21	1.40	1.47
1	E	128	GLU	C-N	5.20	1.40	1.33
1	S	184	TRP	C-N	-5.20	1.27	1.33
1	D	92	ALA	C-O	-5.20	1.17	1.24
1	H	64	ALA	CA-C	-5.20	1.46	1.52
1	I	67	GLN	C-N	5.20	1.40	1.33
1	R	23	TRP	C-N	5.20	1.40	1.33
1	G	67	GLN	CA-C	5.20	1.59	1.52
1	L	135	ILE	N-CA	5.19	1.52	1.46
1	R	121	ASN	CA-C	5.19	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	86	VAL	CA-C	5.19	1.58	1.52
1	C	123	PRO	C-N	5.19	1.39	1.33
1	I	52	LEU	CA-C	-5.19	1.46	1.52
1	C	23	TRP	CA-C	5.19	1.59	1.52
1	S	13	GLN	CA-C	5.18	1.58	1.52
1	B	211	LEU	CA-C	-5.18	1.46	1.52
1	O	123	PRO	C-O	-5.18	1.18	1.23
1	P	220	GLY	C-N	5.18	1.40	1.33
1	S	145	TYR	CA-C	5.18	1.60	1.52
1	L	160	PRO	N-CD	-5.18	1.40	1.47
1	G	150	ILE	CA-C	-5.18	1.45	1.52
1	Q	154	ARG	C-N	5.18	1.40	1.33
1	B	71	GLU	CA-CB	5.18	1.61	1.53
1	S	48	THR	CA-CB	5.18	1.61	1.53
1	J	170	LYS	CA-CB	5.17	1.61	1.53
1	C	42	ALA	CA-C	5.17	1.59	1.52
1	B	54	THR	CB-OG1	-5.17	1.35	1.43
1	H	70	LYS	CA-CB	5.17	1.61	1.53
1	J	122	PRO	C-N	5.17	1.40	1.33
1	N	4	GLN	CA-CB	5.17	1.60	1.53
1	F	38	PRO	N-CA	-5.17	1.40	1.47
1	J	51	ASP	CA-C	5.17	1.59	1.52
1	G	189	LEU	C-N	5.17	1.40	1.33
1	H	186	THR	C-N	5.16	1.41	1.34
1	I	56	LEU	C-N	5.16	1.41	1.34
1	K	10	MET	CA-CB	5.16	1.60	1.53
1	K	49	PRO	N-CA	-5.16	1.40	1.47
1	C	38	PRO	CA-C	-5.16	1.44	1.52
1	N	36	VAL	C-N	5.16	1.39	1.33
1	N	78	ALA	CA-C	-5.16	1.46	1.52
1	R	175	GLU	N-CA	-5.16	1.39	1.45
1	G	56	LEU	CA-C	5.16	1.59	1.52
1	B	105	ALA	C-N	5.15	1.40	1.33
1	C	173	ARG	CD-NE	5.15	1.53	1.46
1	E	77	ALA	C-N	5.15	1.40	1.33
1	B	128	GLU	CA-CB	5.15	1.61	1.53
1	O	176	GLN	CA-CB	5.15	1.61	1.53
1	R	107	THR	C-N	5.15	1.40	1.33
1	F	68	MET	CA-C	5.15	1.59	1.52
1	B	99	PRO	C-O	5.15	1.29	1.23
1	R	55	MET	CA-CB	5.14	1.61	1.53
1	S	155	GLN	N-CA	-5.14	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	12	HIS	ND1-CE1	5.14	1.37	1.32
1	P	56	LEU	CA-C	5.13	1.59	1.52
1	R	138	LEU	C-O	-5.13	1.18	1.24
1	R	37	ILE	CA-CB	-5.13	1.47	1.54
1	R	177	ALA	CA-CB	5.13	1.62	1.53
1	O	10	MET	N-CA	-5.13	1.39	1.46
1	D	59	VAL	N-CA	-5.13	1.40	1.46
1	G	5	ASN	CA-CB	5.13	1.61	1.53
1	G	58	THR	N-CA	5.13	1.52	1.46
1	O	138	LEU	CA-CB	5.12	1.61	1.53
1	H	128	GLU	CA-C	5.12	1.59	1.52
1	I	167	ARG	CA-C	-5.12	1.46	1.52
1	J	24	VAL	N-CA	-5.12	1.40	1.46
1	K	150	ILE	N-CA	5.12	1.52	1.46
1	N	209	ALA	CA-C	-5.12	1.46	1.52
1	S	117	TRP	CG-CD2	-5.12	1.34	1.43
1	I	130	TYR	CA-CB	5.11	1.61	1.53
1	H	66	MET	CA-CB	5.11	1.61	1.53
1	J	181	VAL	CA-CB	5.11	1.61	1.54
1	Q	206	GLY	C-N	-5.11	1.28	1.34
1	D	190	LEU	CA-C	5.11	1.59	1.52
1	B	145	TYR	CA-CB	5.10	1.62	1.53
1	Q	23	TRP	CZ2-CH2	5.10	1.47	1.37
1	C	40	PHE	CA-CB	5.10	1.61	1.53
1	C	53	ASN	N-CA	5.10	1.52	1.46
1	N	158	LYS	CA-C	5.10	1.59	1.52
1	E	120	HIS	CD2-NE2	5.10	1.43	1.37
1	C	82	ARG	N-CA	5.10	1.52	1.46
1	J	147	PRO	C-O	-5.10	1.17	1.24
1	B	52	LEU	N-CA	-5.09	1.40	1.46
1	E	68	MET	N-CA	-5.09	1.40	1.46
1	F	70	LYS	CA-C	-5.09	1.46	1.52
1	F	95	GLN	N-CA	-5.09	1.39	1.46
1	J	133	TRP	C-O	-5.09	1.18	1.24
1	M	168	PHE	CA-C	-5.09	1.46	1.52
1	E	201	ILE	CA-CB	-5.09	1.48	1.54
1	L	184	TRP	NE1-CE2	5.09	1.43	1.37
1	K	52	LEU	C-O	-5.08	1.18	1.24
1	S	3	VAL	CA-C	-5.08	1.46	1.52
1	R	82	ARG	C-N	5.08	1.41	1.34
1	G	101	GLY	CA-C	-5.08	1.46	1.52
1	S	87	HIS	CB-CG	5.08	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	188	THR	C-N	5.08	1.40	1.33
1	M	88	ALA	CA-C	5.08	1.59	1.53
1	C	84	HIS	C-O	-5.08	1.17	1.24
1	R	119	THR	N-CA	5.08	1.52	1.46
1	M	59	VAL	CA-C	5.07	1.59	1.52
1	O	20	LEU	C-N	5.07	1.40	1.33
1	I	209	ALA	N-CA	-5.07	1.39	1.46
1	F	45	GLU	CA-CB	5.07	1.62	1.53
1	N	143	ARG	C-N	5.07	1.40	1.33
1	P	195	ASN	CA-C	5.07	1.59	1.53
1	R	54	THR	C-O	-5.07	1.18	1.24
1	H	81	ASP	C-O	-5.07	1.18	1.24
1	I	24	VAL	C-N	5.07	1.40	1.33
1	K	59	VAL	C-N	5.07	1.38	1.33
1	L	103	ASP	C-N	5.07	1.40	1.33
1	K	184	TRP	NE1-CE2	5.07	1.43	1.37
1	M	117	TRP	C-O	-5.07	1.18	1.24
1	H	144	MET	CA-CB	5.06	1.61	1.53
1	N	76	GLU	CA-CB	5.06	1.61	1.53
1	F	100	ARG	C-N	-5.05	1.27	1.33
1	P	207	PRO	CA-CB	5.05	1.60	1.53
1	D	120	HIS	N-CA	5.05	1.52	1.46
1	H	143	ARG	N-CA	-5.05	1.40	1.46
1	J	176	GLN	N-CA	5.05	1.52	1.46
1	O	172	LEU	C-O	-5.04	1.18	1.24
1	K	177	ALA	C-N	5.04	1.40	1.33
1	L	114	GLN	N-CA	-5.04	1.40	1.46
1	Q	82	ARG	CB-CG	5.04	1.67	1.52
1	E	101	GLY	N-CA	5.04	1.52	1.45
1	G	193	ASN	N-CA	5.04	1.52	1.46
1	I	90	PRO	N-CA	5.04	1.53	1.47
1	I	165	VAL	CA-CB	-5.04	1.48	1.54
1	B	88	ALA	C-O	-5.04	1.17	1.23
1	P	171	THR	C-O	-5.04	1.18	1.24
1	G	64	ALA	N-CA	-5.04	1.40	1.46
1	M	146	SER	C-O	-5.04	1.17	1.24
1	Q	50	GLN	CA-CB	5.04	1.61	1.53
1	Q	110	THR	CA-C	-5.04	1.45	1.53
1	F	108	THR	CB-OG1	-5.04	1.35	1.43
1	C	67	GLN	CA-CB	5.03	1.61	1.53
1	C	172	LEU	C-O	-5.03	1.18	1.24
1	M	152	ASP	CA-C	5.03	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	107	THR	C-N	5.03	1.40	1.33
1	E	55	MET	C-O	5.03	1.30	1.24
1	H	92	ALA	CA-C	5.03	1.58	1.52
1	M	31	ALA	C-N	5.03	1.40	1.33
1	P	97	ARG	CD-NE	5.03	1.53	1.46
1	I	217	ALA	C-N	5.03	1.40	1.33
1	D	151	LEU	N-CA	-5.02	1.39	1.46
1	R	173	ARG	CA-C	-5.02	1.45	1.52
1	J	171	THR	C-N	5.02	1.40	1.33
1	E	34	PRO	C-O	5.01	1.30	1.24
1	R	168	PHE	CA-C	5.01	1.59	1.52
1	E	80	TRP	NE1-CE2	-5.01	1.31	1.37
1	P	111	LEU	CA-C	5.01	1.59	1.52
1	D	141	ILE	C-O	-5.01	1.18	1.24
1	P	130	TYR	CA-CB	5.01	1.61	1.53
1	Q	136	LEU	C-N	5.01	1.40	1.33
1	D	214	MET	N-CA	5.01	1.52	1.46
1	E	97	ARG	CD-NE	5.01	1.53	1.46
1	L	218	CYS	CA-CB	5.00	1.60	1.53
1	N	155	GLN	CA-CB	5.00	1.60	1.53
1	Q	45	GLU	N-CA	-5.00	1.39	1.46
1	Q	121	ASN	CA-C	5.00	1.58	1.53
1	L	126	VAL	C-N	5.00	1.40	1.33
1	P	192	GLN	C-N	5.00	1.40	1.33

All (2326) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	120	HIS	CA-CB-CG	15.19	128.99	113.80
1	O	195	ASN	CA-CB-CG	14.71	127.31	112.60
1	F	120	HIS	CA-CB-CG	12.48	126.28	113.80
1	P	7	GLN	N-CA-C	12.30	128.36	111.39
1	I	97	ARG	NE-CZ-NH2	-12.14	108.27	119.20
1	O	82	ARG	NE-CZ-NH2	-11.61	108.75	119.20
1	J	25	LYS	N-CA-C	11.49	123.88	111.36
1	N	190	LEU	N-CA-C	11.00	124.44	111.02
1	O	21	ASN	CA-CB-CG	10.90	123.50	112.60
1	L	124	ILE	N-CA-C	-10.82	97.44	108.15
1	Q	162	ARG	N-CA-C	10.74	124.33	111.33
1	K	89	GLY	CA-C-N	10.71	130.81	119.78
1	K	89	GLY	C-N-CA	10.71	130.81	119.78
1	D	162	ARG	NE-CZ-NH1	10.51	132.01	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	173	ARG	NE-CZ-NH2	-10.46	109.79	119.20
1	Q	16	SER	CA-C-N	10.43	131.21	119.32
1	Q	16	SER	C-N-CA	10.43	131.21	119.32
1	M	163	ASP	CA-CB-CG	-10.39	102.21	112.60
1	D	143	ARG	NE-CZ-NH1	10.24	131.75	121.50
1	I	98	GLU	CA-C-N	10.24	130.17	120.03
1	I	98	GLU	C-N-CA	10.24	130.17	120.03
1	B	173	ARG	NE-CZ-NH1	10.21	131.71	121.50
1	Q	110	THR	CA-CB-OG1	10.19	124.88	109.60
1	J	8	GLY	O-C-N	-10.08	112.25	122.54
1	D	32	PHE	CA-CB-CG	-10.05	103.75	113.80
1	E	91	ILE	N-CA-C	-10.01	93.54	108.46
1	N	76	GLU	CA-C-N	10.01	133.45	120.44
1	N	76	GLU	C-N-CA	10.01	133.45	120.44
1	M	192	GLN	OE1-CD-NE2	-9.97	112.63	122.60
1	N	32	PHE	CA-CB-CG	-9.94	103.86	113.80
1	G	139	ASN	CB-CG-ND2	9.91	131.26	116.40
1	S	84	HIS	CE1-NE2-CD2	-9.87	99.13	109.00
1	E	82	ARG	NE-CZ-NH1	9.85	131.35	121.50
1	G	121	ASN	CB-CA-C	9.83	121.09	110.17
1	L	173	ARG	NE-CZ-NH1	9.81	131.31	121.50
1	N	139	ASN	CA-CB-CG	9.79	122.39	112.60
1	K	80	TRP	CA-C-O	9.73	130.86	120.55
1	J	51	ASP	CA-CB-CG	9.73	122.33	112.60
1	Q	143	ARG	CA-C-O	9.71	130.85	120.55
1	O	201	ILE	O-C-N	-9.71	112.45	121.87
1	M	86	VAL	CB-CA-C	9.61	122.59	110.96
1	P	126	VAL	CA-C-N	9.59	130.59	119.94
1	P	126	VAL	C-N-CA	9.59	130.59	119.94
1	N	168	PHE	CA-CB-CG	9.56	123.36	113.80
1	S	167	ARG	NE-CZ-NH2	-9.54	110.61	119.20
1	C	211	LEU	CA-C-N	9.50	133.36	120.54
1	C	211	LEU	C-N-CA	9.50	133.36	120.54
1	Q	154	ARG	NE-CZ-NH1	9.49	130.99	121.50
1	I	97	ARG	NE-CZ-NH1	9.49	130.99	121.50
1	E	53	ASN	CA-CB-CG	-9.48	103.12	112.60
1	M	199	LYS	CA-C-N	9.43	132.70	120.44
1	M	199	LYS	C-N-CA	9.43	132.70	120.44
1	M	165	VAL	CA-C-N	9.42	132.69	120.44
1	M	165	VAL	C-N-CA	9.42	132.69	120.44
1	G	209	ALA	N-CA-C	9.37	123.46	110.24
1	I	40	PHE	CA-C-N	9.30	132.74	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	40	PHE	C-N-CA	9.30	132.74	120.28
1	R	23	TRP	O-C-N	-9.28	112.07	122.09
1	D	39	MET	CA-C-N	9.27	133.05	120.54
1	D	39	MET	C-N-CA	9.27	133.05	120.54
1	S	217	ALA	N-CA-C	9.20	121.08	111.14
1	L	103	ASP	O-C-N	-9.18	111.68	122.15
1	S	167	ARG	NE-CZ-NH1	9.18	130.68	121.50
1	R	177	ALA	O-C-N	-9.18	113.83	123.56
1	B	7	GLN	N-CA-C	9.18	123.99	112.24
1	J	172	LEU	CA-C-N	9.18	132.58	120.28
1	J	172	LEU	C-N-CA	9.18	132.58	120.28
1	R	192	GLN	N-CA-C	9.18	121.28	111.28
1	K	82	ARG	N-CA-C	9.16	120.88	111.07
1	H	169	TYR	CA-C-N	9.14	132.88	120.44
1	H	169	TYR	C-N-CA	9.14	132.88	120.44
1	S	2	ILE	O-C-N	-9.12	113.70	123.18
1	L	132	ARG	NE-CZ-NH1	9.05	130.55	121.50
1	P	2	ILE	O-C-N	-9.02	113.80	123.18
1	D	162	ARG	NE-CZ-NH2	-8.97	111.12	119.20
1	R	195	ASN	CA-C-O	-8.96	111.41	120.64
1	Q	162	ARG	NE-CZ-NH2	-8.95	111.14	119.20
1	P	114	GLN	OE1-CD-NE2	8.95	131.55	122.60
1	D	195	ASN	CA-C-N	8.92	128.52	119.24
1	D	195	ASN	C-N-CA	8.92	128.52	119.24
1	D	120	HIS	CA-CB-CG	8.92	122.72	113.80
1	P	101	GLY	O-C-N	8.90	130.73	122.19
1	M	53	ASN	CA-CB-CG	-8.85	103.75	112.60
1	H	90	PRO	N-CA-C	8.83	124.91	111.14
1	I	66	MET	N-CA-C	8.78	120.85	111.28
1	P	82	ARG	NH1-CZ-NH2	-8.75	107.93	119.30
1	H	84	HIS	CA-CB-CG	-8.72	105.08	113.80
1	R	126	VAL	CA-C-N	8.71	129.61	119.94
1	R	126	VAL	C-N-CA	8.71	129.61	119.94
1	F	87	HIS	ND1-CE1-NE2	8.70	117.10	108.40
1	Q	104	ILE	O-C-N	-8.69	112.88	121.83
1	H	142	VAL	N-CA-C	8.68	119.47	110.36
1	G	84	HIS	CA-C-N	8.68	128.75	119.90
1	G	84	HIS	C-N-CA	8.68	128.75	119.90
1	S	23	TRP	CA-C-N	8.62	131.42	120.56
1	S	23	TRP	C-N-CA	8.62	131.42	120.56
1	S	100	ARG	NE-CZ-NH2	-8.59	111.47	119.20
1	K	23	TRP	N-CA-C	8.58	120.63	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	20	LEU	N-CA-C	8.57	121.39	111.11
1	E	76	GLU	CA-C-N	8.56	131.57	120.44
1	E	76	GLU	C-N-CA	8.56	131.57	120.44
1	N	47	ALA	N-CA-C	8.55	121.64	110.43
1	G	87	HIS	CA-CB-CG	-8.54	105.25	113.80
1	E	67	GLN	CA-C-O	-8.54	111.90	120.70
1	I	167	ARG	NE-CZ-NH1	8.51	130.01	121.50
1	B	200	THR	CA-C-N	8.47	131.24	120.56
1	B	200	THR	C-N-CA	8.47	131.24	120.56
1	E	37	ILE	O-C-N	8.46	125.84	120.42
1	C	144	MET	N-CA-C	8.45	120.58	111.36
1	F	81	ASP	CA-C-N	8.45	131.43	120.44
1	F	81	ASP	C-N-CA	8.45	131.43	120.44
1	P	193	ASN	CA-CB-CG	-8.44	104.16	112.60
1	Q	59	VAL	O-C-N	-8.43	112.97	122.66
1	C	115	ILE	CA-C-N	8.42	129.28	119.94
1	C	115	ILE	C-N-CA	8.42	129.28	119.94
1	O	81	ASP	CA-CB-CG	-8.41	104.19	112.60
1	G	139	ASN	OD1-CG-ND2	-8.41	114.19	122.60
1	G	189	LEU	CA-C-O	8.41	129.34	120.42
1	E	167	ARG	NE-CZ-NH1	8.40	129.90	121.50
1	H	36	VAL	N-CA-C	8.39	119.18	110.62
1	C	120	HIS	CG-CD2-NE2	8.36	115.56	107.20
1	D	216	THR	N-CA-C	8.37	121.33	111.71
1	N	14	ALA	O-C-N	-8.36	112.99	122.86
1	B	89	GLY	CA-C-N	8.34	128.40	119.89
1	B	89	GLY	C-N-CA	8.34	128.40	119.89
1	S	146	SER	O-C-N	-8.34	113.69	121.20
1	N	87	HIS	N-CA-CB	8.34	122.30	110.04
1	E	146	SER	O-C-N	-8.34	113.35	121.19
1	O	201	ILE	CA-C-O	8.33	129.61	120.95
1	E	35	GLU	CA-C-N	8.32	133.62	120.47
1	E	35	GLU	C-N-CA	8.32	133.62	120.47
1	S	100	ARG	NE-CZ-NH1	8.31	129.81	121.50
1	K	33	SER	CA-C-O	-8.29	111.71	119.76
1	C	146	SER	CA-C-O	-8.29	112.74	119.71
1	J	162	ARG	CA-C-O	8.28	129.57	120.63
1	Q	114	GLN	OE1-CD-NE2	-8.27	114.33	122.60
1	M	70	LYS	CA-C-N	8.26	131.18	120.44
1	M	70	LYS	C-N-CA	8.26	131.18	120.44
1	I	100	ARG	NE-CZ-NH1	8.25	129.75	121.50
1	I	82	ARG	NE-CZ-NH1	8.25	129.75	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	195	ASN	CA-C-O	-8.24	111.81	120.87
1	B	88	ALA	CA-C-N	8.22	134.78	121.87
1	B	88	ALA	C-N-CA	8.22	134.78	121.87
1	D	167	ARG	NE-CZ-NH1	8.20	129.70	121.50
1	O	142	VAL	N-CA-C	8.20	118.97	110.36
1	K	115	ILE	CA-C-O	8.19	129.47	120.95
1	E	5	ASN	CA-CB-CG	8.18	120.78	112.60
1	K	173	ARG	NE-CZ-NH2	-8.16	111.86	119.20
1	P	61	GLY	CA-C-O	-8.16	115.68	122.29
1	G	82	ARG	NH1-CZ-NH2	-8.14	108.72	119.30
1	Q	121	ASN	N-CA-C	8.13	119.97	109.64
1	H	179	GLN	OE1-CD-NE2	-8.13	114.47	122.60
1	B	121	ASN	O-C-N	-8.12	114.17	121.39
1	D	159	GLU	O-C-N	-8.11	114.08	121.30
1	H	195	ASN	CA-CB-CG	8.10	120.70	112.60
1	Q	162	ARG	NE-CZ-NH1	8.09	129.59	121.50
1	C	37	ILE	N-CA-CB	8.08	116.76	110.45
1	L	41	SER	CA-C-N	8.07	130.93	120.44
1	L	41	SER	C-N-CA	8.07	130.93	120.44
1	K	134	ILE	CA-C-N	8.06	131.51	120.46
1	K	134	ILE	C-N-CA	8.06	131.51	120.46
1	F	132	ARG	NE-CZ-NH2	-8.05	111.95	119.20
1	F	82	ARG	NH1-CZ-NH2	-8.04	108.85	119.30
1	I	81	ASP	CA-C-N	8.02	130.86	120.44
1	I	81	ASP	C-N-CA	8.02	130.86	120.44
1	M	114	GLN	O-C-N	8.01	130.61	122.12
1	P	195	ASN	CA-CB-CG	8.00	120.60	112.60
1	M	209	ALA	N-CA-C	8.00	122.29	110.30
1	J	195	ASN	CA-CB-CG	7.99	120.59	112.60
1	O	115	ILE	CA-C-N	7.97	129.00	119.99
1	O	115	ILE	C-N-CA	7.97	129.00	119.99
1	Q	85	PRO	N-CA-CB	7.96	110.26	103.25
1	O	177	ALA	N-CA-C	7.96	120.59	110.24
1	S	84	HIS	ND1-CE1-NE2	7.96	116.36	108.40
1	K	84	HIS	O-C-N	-7.96	112.39	120.83
1	S	214	MET	N-CA-C	7.95	119.95	111.28
1	B	173	ARG	NE-CZ-NH2	-7.95	112.05	119.20
1	M	179	GLN	N-CA-C	7.95	119.94	111.28
1	M	201	ILE	CA-CB-CG1	7.95	123.91	110.40
1	E	62	HIS	CE1-NE2-CD2	-7.93	101.06	109.00
1	E	189	LEU	N-CA-C	7.93	121.45	111.69
1	L	130	TYR	CA-C-O	7.93	128.95	120.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	219	GLN	N-CA-C	7.93	119.55	111.07
1	P	82	ARG	NE-CZ-NH1	7.92	129.42	121.50
1	D	40	PHE	N-CA-C	-7.92	101.60	111.11
1	E	25	LYS	O-C-N	-7.90	113.75	122.12
1	M	112	GLN	OE1-CD-NE2	-7.90	114.70	122.60
1	M	162	ARG	N-CA-C	7.90	120.89	111.33
1	M	154	ARG	O-C-N	-7.89	112.54	123.11
1	M	189	LEU	N-CA-C	7.89	119.96	111.36
1	I	81	ASP	CA-CB-CG	7.89	120.49	112.60
1	N	181	VAL	N-CA-CB	7.87	122.38	110.58
1	J	89	GLY	CA-C-N	7.86	127.91	119.89
1	J	89	GLY	C-N-CA	7.86	127.91	119.89
1	J	33	SER	O-C-N	-7.85	113.10	121.42
1	K	162	ARG	N-CA-C	7.84	120.82	111.33
1	L	72	THR	CA-C-N	7.84	131.21	120.46
1	L	72	THR	C-N-CA	7.84	131.21	120.46
1	P	29	GLU	CA-C-O	7.84	128.94	120.55
1	J	166	ASP	CA-CB-CG	7.84	120.44	112.60
1	I	53	ASN	CA-CB-CG	-7.84	104.76	112.60
1	N	76	GLU	N-CA-C	7.83	120.72	111.71
1	S	177	ALA	N-CA-C	7.83	120.42	110.24
1	R	2	ILE	CA-C-O	7.82	128.17	120.27
1	L	215	MET	N-CA-C	7.80	119.86	111.36
1	Q	196	PRO	CA-C-N	7.79	130.94	120.65
1	Q	196	PRO	C-N-CA	7.79	130.94	120.65
1	J	200	THR	CA-C-N	7.79	130.64	120.60
1	J	200	THR	C-N-CA	7.79	130.64	120.60
1	F	82	ARG	NE-CZ-NH2	7.78	126.20	119.20
1	H	50	GLN	OE1-CD-NE2	-7.77	114.83	122.60
1	Q	50	GLN	OE1-CD-NE2	-7.76	114.84	122.60
1	C	39	MET	CA-C-N	7.76	131.01	120.54
1	C	39	MET	C-N-CA	7.76	131.01	120.54
1	J	214	MET	CA-C-O	7.75	128.64	120.42
1	G	130	TYR	O-C-N	-7.75	113.90	122.12
1	N	8	GLY	CA-C-O	7.75	128.95	119.88
1	S	200	THR	CA-C-N	7.75	130.32	120.56
1	S	200	THR	C-N-CA	7.75	130.32	120.56
1	K	163	ASP	CA-C-N	7.75	130.66	120.28
1	K	163	ASP	C-N-CA	7.75	130.66	120.28
1	Q	46	GLY	CA-C-N	7.73	133.07	120.94
1	Q	46	GLY	C-N-CA	7.73	133.07	120.94
1	B	88	ALA	O-C-N	-7.71	114.31	123.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	32	PHE	N-CA-CB	7.71	123.52	110.49
1	C	142	VAL	CA-C-N	7.70	130.60	120.28
1	C	142	VAL	C-N-CA	7.70	130.60	120.28
1	L	195	ASN	CA-CB-CG	7.70	120.30	112.60
1	M	80	TRP	CB-CG-CD2	-7.69	116.03	126.80
1	C	55	MET	CA-C-O	7.69	128.70	120.55
1	O	57	ASN	OD1-CG-ND2	-7.69	114.91	122.60
1	E	134	ILE	CA-C-O	7.69	129.00	120.85
1	I	190	LEU	N-CA-C	7.69	120.33	111.11
1	K	115	ILE	CA-C-N	7.69	128.47	119.94
1	K	115	ILE	C-N-CA	7.69	128.47	119.94
1	P	100	ARG	CA-C-N	7.68	128.51	119.98
1	P	100	ARG	C-N-CA	7.68	128.51	119.98
1	M	192	GLN	N-CA-C	7.68	119.29	111.07
1	E	146	SER	CA-C-O	7.67	125.80	119.36
1	I	173	ARG	NE-CZ-NH1	7.66	129.16	121.50
1	M	68	MET	CA-C-O	7.65	128.89	120.63
1	C	79	GLU	N-CA-C	7.65	119.62	111.28
1	P	127	GLY	O-C-N	-7.64	114.85	122.18
1	H	161	PHE	CA-C-N	7.63	130.84	120.38
1	H	161	PHE	C-N-CA	7.63	130.84	120.38
1	M	29	GLU	O-C-N	-7.63	113.85	122.09
1	H	148	THR	N-CA-CB	7.62	121.21	109.85
1	H	163	ASP	CA-CB-CG	-7.62	104.98	112.60
1	C	36	VAL	CA-C-N	7.62	126.42	120.33
1	C	36	VAL	C-N-CA	7.62	126.42	120.33
1	G	135	ILE	N-CA-C	7.61	118.38	110.62
1	K	101	GLY	CA-C-N	7.61	131.88	120.31
1	K	101	GLY	C-N-CA	7.61	131.88	120.31
1	K	116	GLY	CA-C-N	7.60	130.46	120.28
1	K	116	GLY	C-N-CA	7.60	130.46	120.28
1	G	190	LEU	CA-C-N	7.58	131.18	120.42
1	G	190	LEU	C-N-CA	7.58	131.18	120.42
1	P	104	ILE	CA-C-O	7.58	128.88	120.85
1	F	87	HIS	CE1-NE2-CD2	-7.58	101.42	109.00
1	C	210	THR	CA-CB-OG1	7.57	120.96	109.60
1	E	117	TRP	O-C-N	-7.57	114.09	122.12
1	C	37	ILE	CA-C-O	7.57	123.76	118.69
1	B	195	ASN	CA-C-N	7.57	129.30	119.84
1	B	195	ASN	C-N-CA	7.57	129.30	119.84
1	H	155	GLN	OE1-CD-NE2	7.57	130.17	122.60
1	H	85	PRO	N-CA-C	7.56	122.94	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	73	ILE	N-CA-C	7.56	118.33	110.62
1	I	167	ARG	N-CA-C	7.54	119.50	111.28
1	D	81	ASP	CA-C-N	7.54	130.25	120.44
1	D	81	ASP	C-N-CA	7.54	130.25	120.44
1	I	171	THR	CA-C-N	7.54	130.38	120.28
1	I	171	THR	C-N-CA	7.54	130.38	120.28
1	P	126	VAL	N-CA-C	7.54	118.31	110.62
1	R	42	ALA	N-CA-C	7.54	119.13	111.07
1	S	2	ILE	CA-C-N	7.53	131.79	122.37
1	S	2	ILE	C-N-CA	7.53	131.79	122.37
1	G	70	LYS	CA-C-O	-7.53	112.92	120.82
1	H	138	LEU	N-CA-C	7.52	119.48	111.28
1	S	196	PRO	CA-C-N	7.51	130.21	120.44
1	S	196	PRO	C-N-CA	7.51	130.21	120.44
1	E	12	HIS	CE1-NE2-CD2	-7.50	101.50	109.00
1	L	22	ALA	CA-C-O	-7.50	112.95	120.82
1	M	137	GLY	CA-C-N	7.50	130.18	120.44
1	M	137	GLY	C-N-CA	7.50	130.18	120.44
1	E	69	LEU	O-C-N	-7.49	114.18	122.12
1	B	110	THR	CA-C-N	7.49	130.32	120.28
1	B	110	THR	C-N-CA	7.49	130.32	120.28
1	S	88	ALA	N-CA-C	7.49	121.06	110.50
1	K	12	HIS	CB-CG-CD2	-7.47	121.48	131.20
1	E	189	LEU	CA-C-N	7.47	130.62	120.54
1	E	189	LEU	C-N-CA	7.47	130.62	120.54
1	H	97	ARG	NE-CZ-NH2	-7.46	112.49	119.20
1	H	196	PRO	CA-C-N	7.45	130.13	120.44
1	H	196	PRO	C-N-CA	7.45	130.13	120.44
1	P	104	ILE	O-C-N	-7.45	114.16	121.83
1	Q	59	VAL	N-CA-C	7.42	118.64	108.84
1	L	150	ILE	CA-C-N	7.41	130.94	120.28
1	L	150	ILE	C-N-CA	7.41	130.94	120.28
1	L	126	VAL	CA-C-N	7.40	128.15	119.94
1	L	126	VAL	C-N-CA	7.40	128.15	119.94
1	O	164	TYR	N-CA-C	7.40	119.34	111.28
1	G	14	ALA	CA-C-N	7.39	131.57	120.77
1	G	14	ALA	C-N-CA	7.39	131.57	120.77
1	G	69	LEU	CA-C-N	7.39	130.05	120.44
1	G	69	LEU	C-N-CA	7.39	130.05	120.44
1	F	74	ASN	CA-C-O	7.38	128.25	120.42
1	R	189	LEU	N-CA-C	7.37	119.39	111.36
1	C	55	MET	O-C-N	-7.37	114.31	122.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	99	PRO	O-C-N	-7.37	113.88	123.01
1	F	175	GLU	N-CA-CB	7.37	120.80	109.97
1	N	122	PRO	N-CA-CB	7.36	110.70	102.60
1	I	9	GLN	CB-CG-CD	7.35	125.10	112.60
1	J	12	HIS	CE1-NE2-CD2	-7.35	101.65	109.00
1	J	188	THR	O-C-N	-7.34	113.53	122.19
1	D	162	ARG	N-CA-C	7.34	120.21	111.33
1	C	183	ASN	OD1-CG-ND2	-7.33	115.27	122.60
1	K	189	LEU	CA-C-N	7.33	130.43	120.54
1	K	189	LEU	C-N-CA	7.33	130.43	120.54
1	C	195	ASN	OD1-CG-ND2	-7.32	115.28	122.60
1	K	195	ASN	CA-C-O	-7.30	112.44	120.69
1	C	152	ASP	CA-CB-CG	7.30	119.90	112.60
1	C	193	ASN	CA-CB-CG	-7.29	105.31	112.60
1	C	131	LYS	N-CA-C	7.29	119.22	111.28
1	C	20	LEU	CA-C-N	7.28	130.03	120.28
1	C	20	LEU	C-N-CA	7.28	130.03	120.28
1	J	219	GLN	N-CA-C	7.28	120.27	111.82
1	R	23	TRP	CA-C-O	7.28	128.20	120.70
1	K	76	GLU	CA-C-N	7.28	129.90	120.44
1	K	76	GLU	C-N-CA	7.28	129.90	120.44
1	L	124	ILE	N-CA-CB	7.28	118.86	111.36
1	B	102	SER	CA-C-N	7.26	130.01	120.28
1	B	102	SER	C-N-CA	7.26	130.01	120.28
1	E	155	GLN	O-C-N	-7.26	115.07	123.27
1	R	176	GLN	OE1-CD-NE2	-7.25	115.35	122.60
1	R	92	ALA	CA-C-O	-7.25	112.42	120.25
1	L	76	GLU	O-C-N	-7.24	113.36	122.27
1	L	69	LEU	CA-C-N	7.24	129.98	120.28
1	L	69	LEU	C-N-CA	7.24	129.98	120.28
1	G	173	ARG	NE-CZ-NH2	-7.24	112.68	119.20
1	J	193	ASN	CA-CB-CG	7.24	119.84	112.60
1	E	53	ASN	N-CA-C	-7.24	103.39	111.28
1	I	110	THR	N-CA-CB	7.23	121.43	110.45
1	L	87	HIS	N-CA-C	7.22	119.87	108.67
1	K	147	PRO	N-CA-C	7.22	123.03	113.57
1	F	191	VAL	CB-CA-C	-7.22	102.25	112.22
1	I	210	THR	N-CA-C	7.22	119.29	110.41
1	M	114	GLN	N-CA-C	7.22	119.15	111.28
1	K	121	ASN	CA-CB-CG	7.21	119.81	112.60
1	C	36	VAL	N-CA-C	7.20	117.97	110.62
1	I	191	VAL	CA-C-N	7.20	129.93	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	191	VAL	C-N-CA	7.20	129.93	120.28
1	B	37	ILE	CA-C-N	7.20	127.04	119.05
1	B	37	ILE	C-N-CA	7.20	127.04	119.05
1	C	87	HIS	CE1-NE2-CD2	-7.20	101.80	109.00
1	B	146	SER	CB-CA-C	-7.20	103.05	110.17
1	O	14	ALA	O-C-N	-7.19	114.37	122.86
1	K	122	PRO	CA-C-N	7.19	127.17	119.76
1	K	122	PRO	C-N-CA	7.19	127.17	119.76
1	M	159	GLU	O-C-N	-7.19	113.80	121.42
1	M	207	PRO	CA-C-N	7.18	129.39	120.34
1	M	207	PRO	C-N-CA	7.18	129.39	120.34
1	F	33	SER	CA-C-O	-7.17	113.25	120.64
1	R	26	VAL	N-CA-C	7.17	117.89	110.36
1	F	133	TRP	CB-CG-CD2	-7.17	116.77	126.80
1	P	62	HIS	CG-CD2-NE2	7.16	114.36	107.20
1	G	51	ASP	CA-C-N	7.16	130.18	120.44
1	G	51	ASP	C-N-CA	7.16	130.18	120.44
1	E	15	ILE	O-C-N	-7.16	115.00	122.66
1	H	28	GLU	O-C-N	-7.15	114.70	122.07
1	B	42	ALA	N-CA-C	7.15	118.72	111.07
1	R	115	ILE	CA-C-N	7.15	128.07	119.99
1	R	115	ILE	C-N-CA	7.15	128.07	119.99
1	H	173	ARG	NE-CZ-NH1	7.15	128.65	121.50
1	I	35	GLU	CA-C-N	7.15	130.25	120.46
1	I	35	GLU	C-N-CA	7.15	130.25	120.46
1	Q	87	HIS	CE1-NE2-CD2	-7.15	101.85	109.00
1	E	112	GLN	O-C-N	-7.14	114.55	122.12
1	F	38	PRO	CA-C-N	7.13	129.71	120.44
1	F	38	PRO	C-N-CA	7.13	129.71	120.44
1	M	135	ILE	CA-C-N	7.13	129.71	120.44
1	M	135	ILE	C-N-CA	7.13	129.71	120.44
1	I	159	GLU	CA-C-O	-7.13	113.97	119.46
1	I	98	GLU	O-C-N	-7.12	114.79	121.20
1	B	131	LYS	O-C-N	-7.12	114.57	122.12
1	B	133	TRP	CD2-CE2-CZ2	-7.12	115.28	122.40
1	O	35	GLU	CA-C-O	7.12	128.14	119.38
1	R	120	HIS	ND1-CE1-NE2	7.12	115.52	108.40
1	H	185	MET	CA-C-N	7.12	130.04	120.65
1	H	185	MET	C-N-CA	7.12	130.04	120.65
1	O	120	HIS	CE1-NE2-CD2	-7.11	101.89	109.00
1	B	26	VAL	O-C-N	7.11	128.86	121.89
1	I	82	ARG	NE-CZ-NH2	-7.11	112.80	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	124	ILE	O-C-N	-7.11	113.00	121.10
1	K	206	GLY	O-C-N	-7.10	114.67	121.77
1	O	41	SER	O-C-N	7.10	129.65	122.12
1	H	52	LEU	O-C-N	7.10	129.38	122.07
1	K	70	LYS	N-CA-C	7.10	119.02	111.28
1	I	110	THR	N-CA-C	-7.10	100.97	110.55
1	B	171	THR	CA-C-O	7.10	128.07	120.55
1	N	51	ASP	CA-C-N	7.10	129.79	120.28
1	N	51	ASP	C-N-CA	7.10	129.79	120.28
1	N	100	ARG	O-C-N	-7.10	114.61	122.84
1	L	4	GLN	CA-C-O	7.09	128.37	120.43
1	C	183	ASN	CA-CB-CG	-7.09	105.51	112.60
1	P	195	ASN	CA-C-N	7.09	126.61	119.24
1	P	195	ASN	C-N-CA	7.09	126.61	119.24
1	C	160	PRO	CA-C-N	7.08	130.08	120.38
1	C	160	PRO	C-N-CA	7.08	130.08	120.38
1	H	101	GLY	CA-C-N	7.08	130.48	120.28
1	H	101	GLY	C-N-CA	7.08	130.48	120.28
1	O	11	VAL	CA-C-O	7.08	127.86	120.36
1	R	82	ARG	CA-C-O	7.07	128.25	120.82
1	M	91	ILE	CA-C-N	7.07	131.42	120.60
1	M	91	ILE	C-N-CA	7.07	131.42	120.60
1	O	51	ASP	CA-CB-CG	-7.07	105.53	112.60
1	M	19	THR	CB-CA-C	-7.05	100.10	110.96
1	K	118	MET	CA-C-O	7.05	128.08	119.97
1	Q	66	MET	N-CA-C	7.05	118.97	111.28
1	P	180	GLU	CA-C-N	7.05	130.43	120.42
1	P	180	GLU	C-N-CA	7.05	130.43	120.42
1	E	121	ASN	CA-C-O	-7.04	112.79	119.55
1	F	162	ARG	CG-CD-NE	-7.03	96.54	112.00
1	B	198	CYS	CA-C-O	7.03	128.05	119.97
1	G	89	GLY	CA-C-N	7.03	127.45	119.93
1	G	89	GLY	C-N-CA	7.03	127.45	119.93
1	B	175	GLU	CA-C-N	7.03	130.02	120.54
1	B	175	GLU	C-N-CA	7.03	130.02	120.54
1	F	85	PRO	N-CA-C	7.03	122.71	111.26
1	B	131	LYS	CA-C-N	7.02	129.69	120.28
1	B	131	LYS	C-N-CA	7.02	129.69	120.28
1	O	149	SER	CA-C-N	7.02	131.81	120.30
1	O	149	SER	C-N-CA	7.02	131.81	120.30
1	B	75	GLU	N-CA-C	7.01	118.93	111.28
1	S	38	PRO	CA-C-N	7.01	129.56	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	38	PRO	C-N-CA	7.01	129.56	120.44
1	J	184	TRP	CB-CG-CD1	-7.01	116.38	126.90
1	C	173	ARG	NE-CZ-NH1	7.01	128.51	121.50
1	B	159	GLU	CA-C-N	7.00	127.39	119.83
1	B	159	GLU	C-N-CA	7.00	127.39	119.83
1	D	119	THR	CA-CB-OG1	7.00	120.11	109.60
1	L	77	ALA	N-CA-C	6.99	118.90	111.28
1	E	172	LEU	N-CA-C	6.99	118.90	111.28
1	J	189	LEU	CA-C-N	6.99	130.50	120.79
1	J	189	LEU	C-N-CA	6.99	130.50	120.79
1	K	101	GLY	O-C-N	-6.99	115.48	122.19
1	R	4	GLN	OE1-CD-NE2	-6.98	115.62	122.60
1	H	143	ARG	N-CA-C	6.98	118.89	111.28
1	K	213	GLU	CA-C-N	6.98	129.63	120.28
1	K	213	GLU	C-N-CA	6.98	129.63	120.28
1	G	192	GLN	OE1-CD-NE2	-6.98	115.62	122.60
1	M	5	ASN	CA-C-N	6.98	131.29	120.75
1	M	5	ASN	C-N-CA	6.98	131.29	120.75
1	C	84	HIS	CE1-NE2-CD2	-6.97	102.03	109.00
1	N	178	SER	O-C-N	-6.97	113.33	122.59
1	R	74	ASN	CA-CB-CG	-6.97	105.63	112.60
1	R	39	MET	CA-C-N	6.96	129.93	120.54
1	R	39	MET	C-N-CA	6.96	129.93	120.54
1	I	100	ARG	NE-CZ-NH2	-6.96	112.94	119.20
1	C	37	ILE	O-C-N	-6.96	115.97	120.42
1	C	22	ALA	N-CA-C	6.95	118.85	111.28
1	E	20	LEU	N-CA-C	6.95	119.50	111.02
1	N	87	HIS	O-C-N	-6.95	114.27	122.81
1	H	64	ALA	O-C-N	-6.95	114.76	122.12
1	O	98	GLU	CA-C-N	6.94	126.93	119.78
1	O	98	GLU	C-N-CA	6.94	126.93	119.78
1	N	112	GLN	CA-C-N	6.93	129.57	120.28
1	N	112	GLN	C-N-CA	6.93	129.57	120.28
1	K	79	GLU	O-C-N	-6.92	114.94	122.07
1	Q	154	ARG	NH1-CZ-NH2	-6.92	110.30	119.30
1	B	5	ASN	CA-CB-CG	-6.92	105.68	112.60
1	S	208	GLY	CA-C-N	6.91	130.98	120.82
1	S	208	GLY	C-N-CA	6.91	130.98	120.82
1	J	31	ALA	N-CA-C	6.91	118.82	108.31
1	S	197	ASP	CA-CB-CG	-6.91	105.69	112.60
1	G	60	GLY	CA-C-O	-6.91	114.90	120.91
1	C	120	HIS	CE1-NE2-CD2	-6.90	102.10	109.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	160	PRO	CA-C-N	6.90	129.85	120.54
1	K	160	PRO	C-N-CA	6.90	129.85	120.54
1	P	35	GLU	CA-C-N	6.90	129.91	120.46
1	P	35	GLU	C-N-CA	6.90	129.91	120.46
1	G	163	ASP	CA-C-N	6.90	130.08	120.29
1	G	163	ASP	C-N-CA	6.90	130.08	120.29
1	J	132	ARG	NE-CZ-NH1	6.89	128.39	121.50
1	Q	104	ILE	CA-C-O	6.88	128.15	120.85
1	Q	111	LEU	O-C-N	-6.88	114.82	122.12
1	E	211	LEU	CA-C-N	6.88	129.38	120.44
1	E	211	LEU	C-N-CA	6.88	129.38	120.44
1	B	180	GLU	CA-C-N	6.88	129.23	120.56
1	B	180	GLU	C-N-CA	6.88	129.23	120.56
1	M	19	THR	N-CA-CB	6.88	119.95	109.91
1	O	32	PHE	CA-CB-CG	-6.88	106.92	113.80
1	O	170	LYS	CA-C-N	6.88	129.50	120.28
1	O	170	LYS	C-N-CA	6.88	129.50	120.28
1	D	120	HIS	O-C-N	-6.88	114.02	122.82
1	L	137	GLY	O-C-N	-6.87	115.52	122.19
1	J	32	PHE	CA-CB-CG	-6.87	106.93	113.80
1	J	100	ARG	NE-CZ-NH1	6.87	128.37	121.50
1	P	176	GLN	CA-C-N	6.87	130.58	120.90
1	P	176	GLN	C-N-CA	6.87	130.58	120.90
1	C	76	GLU	CA-C-N	6.86	129.35	120.44
1	C	76	GLU	C-N-CA	6.86	129.35	120.44
1	J	12	HIS	ND1-CE1-NE2	6.85	115.25	108.40
1	K	197	ASP	CA-CB-CG	6.84	119.44	112.60
1	K	215	MET	CG-SD-CE	-6.84	85.86	100.90
1	K	89	GLY	O-C-N	-6.83	114.94	121.77
1	M	200	THR	CA-CB-OG1	-6.83	99.35	109.60
1	E	153	ILE	N-CA-CB	6.82	119.30	111.39
1	R	195	ASN	CA-C-N	6.82	128.36	119.84
1	R	195	ASN	C-N-CA	6.82	128.36	119.84
1	O	33	SER	N-CA-C	6.81	117.43	109.60
1	D	21	ASN	O-C-N	6.81	129.34	122.12
1	E	120	HIS	N-CA-C	6.81	119.09	110.24
1	P	18	ARG	NE-CZ-NH1	6.80	128.30	121.50
1	L	96	MET	N-CA-C	6.80	119.50	110.53
1	S	52	LEU	CA-C-O	-6.80	113.22	120.42
1	Q	85	PRO	CB-CA-C	-6.79	102.93	111.56
1	C	114	GLN	CA-C-N	6.79	129.77	120.46
1	C	114	GLN	C-N-CA	6.79	129.77	120.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	65	ALA	N-CA-CB	-6.79	100.13	110.12
1	I	134	ILE	CA-C-N	6.79	129.77	120.46
1	I	134	ILE	C-N-CA	6.79	129.77	120.46
1	Q	41	SER	CA-C-N	6.79	129.38	120.28
1	Q	41	SER	C-N-CA	6.79	129.38	120.28
1	K	195	ASN	CB-CA-C	6.79	120.59	109.46
1	K	181	VAL	N-CA-C	6.79	117.57	110.72
1	B	72	THR	CA-C-N	6.78	129.75	120.46
1	B	72	THR	C-N-CA	6.78	129.75	120.46
1	K	126	VAL	CA-C-N	6.78	127.47	119.94
1	K	126	VAL	C-N-CA	6.78	127.47	119.94
1	J	20	LEU	CA-C-O	6.78	128.16	120.90
1	B	168	PHE	CA-CB-CG	-6.78	107.02	113.80
1	D	208	GLY	O-C-N	-6.78	113.89	122.70
1	I	193	ASN	OD1-CG-ND2	-6.78	115.82	122.60
1	L	161	PHE	CA-C-O	6.77	128.15	120.90
1	F	84	HIS	CA-C-N	6.77	127.17	119.93
1	F	84	HIS	C-N-CA	6.77	127.17	119.93
1	B	190	LEU	CA-C-O	-6.77	113.66	120.90
1	D	202	LEU	N-CA-C	-6.76	103.99	111.36
1	O	130	TYR	CA-C-N	6.75	129.33	120.28
1	O	130	TYR	C-N-CA	6.75	129.33	120.28
1	J	55	MET	N-CA-C	6.75	118.64	111.28
1	Q	32	PHE	CA-CB-CG	-6.74	107.06	113.80
1	H	140	LYS	N-CA-C	6.74	118.63	111.28
1	E	217	ALA	N-CA-C	6.74	118.71	111.36
1	H	79	GLU	N-CA-C	6.74	118.42	111.14
1	J	192	GLN	N-CA-C	6.74	118.63	111.28
1	K	68	MET	CA-C-N	6.74	129.20	120.44
1	K	68	MET	C-N-CA	6.74	129.20	120.44
1	M	149	SER	CA-C-N	6.74	131.35	120.30
1	M	149	SER	C-N-CA	6.74	131.35	120.30
1	L	87	HIS	CA-C-N	6.73	130.27	120.71
1	L	87	HIS	C-N-CA	6.73	130.27	120.71
1	I	3	VAL	N-CA-CB	6.73	119.08	111.21
1	O	136	LEU	O-C-N	-6.73	115.09	122.09
1	S	126	VAL	CA-C-O	-6.72	113.38	120.57
1	B	32	PHE	CA-CB-CG	-6.72	107.08	113.80
1	I	153	ILE	N-CA-C	6.72	117.71	108.84
1	Q	192	GLN	OE1-CD-NE2	6.71	129.31	122.60
1	C	140	LYS	CA-C-N	6.71	129.15	120.56
1	C	140	LYS	C-N-CA	6.71	129.15	120.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	70	LYS	N-CA-C	6.71	118.59	111.28
1	G	211	LEU	CA-C-N	6.71	129.60	120.54
1	G	211	LEU	C-N-CA	6.71	129.60	120.54
1	E	2	ILE	CA-C-N	6.71	130.75	122.37
1	E	2	ILE	C-N-CA	6.71	130.75	122.37
1	D	201	ILE	N-CA-C	6.71	116.86	110.42
1	O	50	GLN	CA-C-N	6.70	129.26	120.28
1	O	50	GLN	C-N-CA	6.70	129.26	120.28
1	F	78	ALA	N-CA-C	6.69	118.57	111.28
1	H	110	THR	O-C-N	-6.69	115.47	123.03
1	Q	69	LEU	CA-C-N	6.69	129.24	120.28
1	Q	69	LEU	C-N-CA	6.69	129.24	120.28
1	C	5	ASN	O-C-N	-6.69	113.27	121.83
1	N	69	LEU	CA-C-N	6.68	129.24	120.28
1	N	69	LEU	C-N-CA	6.68	129.24	120.28
1	E	48	THR	N-CA-CB	6.68	117.49	109.74
1	L	181	VAL	O-C-N	-6.68	114.95	121.83
1	H	66	MET	N-CA-C	6.68	118.56	111.28
1	S	166	ASP	CA-CB-CG	6.67	119.28	112.60
1	C	9	GLN	CA-C-N	-6.67	113.29	122.30
1	C	9	GLN	C-N-CA	-6.67	113.29	122.30
1	L	4	GLN	O-C-N	-6.67	115.46	123.13
1	E	209	ALA	CB-CA-C	6.67	120.79	109.72
1	S	120	HIS	ND1-CE1-NE2	6.67	115.06	108.40
1	B	92	ALA	N-CA-C	6.66	119.09	109.84
1	O	14	ALA	CA-C-N	6.65	129.48	120.63
1	O	14	ALA	C-N-CA	6.65	129.48	120.63
1	N	74	ASN	OD1-CG-ND2	-6.65	115.95	122.60
1	S	155	GLN	O-C-N	-6.65	115.64	123.22
1	M	40	PHE	O-C-N	6.65	129.00	122.09
1	F	113	GLU	N-CA-C	6.64	118.52	111.28
1	R	4	GLN	CA-C-N	6.64	134.57	122.02
1	R	4	GLN	C-N-CA	6.64	134.57	122.02
1	B	102	SER	CA-C-O	6.64	127.61	119.97
1	J	37	ILE	CA-C-N	6.64	126.42	119.05
1	J	37	ILE	C-N-CA	6.64	126.42	119.05
1	D	175	GLU	N-CA-CB	6.64	120.38	110.29
1	K	132	ARG	NE-CZ-NH2	-6.64	113.23	119.20
1	K	82	ARG	CA-C-N	6.63	129.71	120.29
1	K	82	ARG	C-N-CA	6.63	129.71	120.29
1	Q	25	LYS	N-CA-CB	-6.63	100.35	110.16
1	M	46	GLY	CA-C-O	6.62	127.96	119.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	80	TRP	CB-CG-CD1	6.62	136.83	126.90
1	Q	109	SER	O-C-N	-6.62	115.55	123.03
1	I	154	ARG	O-C-N	-6.62	115.85	123.33
1	F	76	GLU	N-CA-C	6.62	118.50	111.28
1	Q	147	PRO	CA-C-N	6.62	132.13	123.00
1	Q	147	PRO	C-N-CA	6.62	132.13	123.00
1	S	173	ARG	O-C-N	6.62	129.13	122.12
1	O	120	HIS	CG-CD2-NE2	6.62	113.81	107.20
1	N	53	ASN	CB-CG-ND2	6.61	126.32	116.40
1	O	168	PHE	CA-C-O	6.61	127.51	120.70
1	H	210	THR	O-C-N	-6.61	115.31	122.85
1	R	40	PHE	CA-CB-CG	-6.61	107.19	113.80
1	E	16	SER	CA-C-N	6.61	126.85	119.32
1	E	16	SER	C-N-CA	6.61	126.85	119.32
1	R	146	SER	O-C-N	-6.60	115.42	121.30
1	B	99	PRO	O-C-N	-6.60	115.57	123.03
1	G	153	ILE	N-CA-C	6.60	116.96	108.12
1	C	219	GLN	N-CA-CB	6.60	120.46	110.30
1	E	146	SER	CA-C-N	6.60	128.09	119.84
1	E	146	SER	C-N-CA	6.60	128.09	119.84
1	F	159	GLU	O-C-N	-6.60	115.43	121.30
1	S	9	GLN	N-CA-C	6.59	119.57	108.23
1	C	33	SER	CA-C-O	-6.59	113.13	120.25
1	S	71	GLU	CA-C-N	6.59	129.01	120.44
1	S	71	GLU	C-N-CA	6.59	129.01	120.44
1	I	161	PHE	CA-C-N	6.59	129.41	120.38
1	I	161	PHE	C-N-CA	6.59	129.41	120.38
1	B	84	HIS	CE1-NE2-CD2	-6.59	102.41	109.00
1	B	80	TRP	CA-C-N	6.58	129.10	120.28
1	B	80	TRP	C-N-CA	6.58	129.10	120.28
1	M	68	MET	O-C-N	-6.58	115.14	122.12
1	H	133	TRP	O-C-N	-6.58	115.15	122.12
1	B	40	PHE	N-CA-C	6.58	119.00	111.11
1	S	183	ASN	OD1-CG-ND2	-6.57	116.03	122.60
1	E	69	LEU	CA-C-N	6.57	129.41	120.54
1	E	69	LEU	C-N-CA	6.57	129.41	120.54
1	I	70	LYS	O-C-N	-6.57	115.15	122.12
1	L	173	ARG	NE-CZ-NH2	-6.57	113.29	119.20
1	E	27	VAL	O-C-N	-6.57	115.07	121.83
1	J	120	HIS	CE1-NE2-CD2	-6.56	102.44	109.00
1	S	183	ASN	CB-CA-C	-6.56	99.90	110.79
1	S	192	GLN	OE1-CD-NE2	6.56	129.16	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	132	ARG	O-C-N	-6.56	115.17	122.12
1	L	20	LEU	N-CA-C	6.55	119.01	111.02
1	M	161	PHE	N-CA-C	6.55	118.97	111.11
1	S	179	GLN	OE1-CD-NE2	-6.55	116.05	122.60
1	Q	154	ARG	O-C-N	-6.55	115.78	123.25
1	C	115	ILE	N-CA-C	-6.55	103.94	110.62
1	F	33	SER	CA-C-N	6.55	126.79	119.32
1	F	33	SER	C-N-CA	6.55	126.79	119.32
1	K	48	THR	CA-CB-OG1	6.54	119.41	109.60
1	C	183	ASN	CA-C-O	-6.54	113.61	120.55
1	S	153	ILE	N-CA-CB	-6.54	103.43	111.67
1	F	208	GLY	N-CA-C	6.54	122.77	114.66
1	B	190	LEU	N-CA-CB	-6.54	100.20	109.94
1	K	100	ARG	NE-CZ-NH1	6.54	128.03	121.50
1	M	129	ILE	N-CA-CB	6.53	118.93	110.57
1	R	219	GLN	N-CA-C	6.53	119.23	111.33
1	F	48	THR	O-C-N	-6.52	114.69	121.60
1	J	56	LEU	N-CA-CB	6.52	119.52	110.07
1	Q	77	ALA	CA-C-O	-6.52	113.98	120.82
1	K	99	PRO	N-CA-CB	-6.51	97.51	103.31
1	M	87	HIS	CE1-NE2-CD2	-6.51	102.48	109.00
1	C	134	ILE	CA-C-O	-6.51	113.82	121.05
1	I	213	GLU	CA-C-N	6.51	129.54	120.29
1	I	213	GLU	C-N-CA	6.51	129.54	120.29
1	K	167	ARG	CA-C-N	6.51	129.24	120.65
1	K	167	ARG	C-N-CA	6.51	129.24	120.65
1	D	193	ASN	OD1-CG-ND2	-6.51	116.09	122.60
1	E	203	LYS	CA-C-N	6.51	130.21	120.31
1	E	203	LYS	C-N-CA	6.51	130.21	120.31
1	F	34	PRO	N-CA-C	6.51	123.45	113.75
1	J	70	LYS	N-CA-C	6.51	118.04	111.07
1	R	51	ASP	CA-C-N	6.51	129.00	120.28
1	R	51	ASP	C-N-CA	6.51	129.00	120.28
1	B	81	ASP	CA-C-N	6.51	128.90	120.44
1	B	81	ASP	C-N-CA	6.51	128.90	120.44
1	Q	79	GLU	CA-C-N	6.50	129.00	120.28
1	Q	79	GLU	C-N-CA	6.50	129.00	120.28
1	S	102	SER	N-CA-C	6.50	119.36	111.82
1	H	33	SER	CA-C-N	6.50	126.73	119.32
1	H	33	SER	C-N-CA	6.50	126.73	119.32
1	N	155	GLN	CA-C-N	6.50	132.08	121.87
1	N	155	GLN	C-N-CA	6.50	132.08	121.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	117	TRP	CE2-CD2-CE3	6.50	125.30	118.80
1	J	85	PRO	N-CA-CB	-6.50	97.28	103.39
1	B	176	GLN	N-CA-C	6.50	118.91	111.11
1	K	133	TRP	O-C-N	-6.49	115.24	122.12
1	O	171	THR	O-C-N	-6.49	115.24	122.12
1	H	9	GLN	CA-C-N	6.49	131.06	122.30
1	H	9	GLN	C-N-CA	6.49	131.06	122.30
1	R	177	ALA	CA-C-O	6.49	128.02	120.75
1	I	84	HIS	CA-C-N	6.49	126.86	119.92
1	I	84	HIS	C-N-CA	6.49	126.86	119.92
1	E	80	TRP	CA-C-N	6.49	128.97	120.28
1	E	80	TRP	C-N-CA	6.49	128.97	120.28
1	J	29	GLU	CA-C-O	6.49	127.38	120.70
1	N	195	ASN	CA-C-O	-6.48	113.62	120.88
1	E	3	VAL	CA-C-N	-6.48	113.55	122.30
1	E	3	VAL	C-N-CA	-6.48	113.55	122.30
1	J	88	ALA	CA-C-N	6.48	132.05	121.87
1	J	88	ALA	C-N-CA	6.48	132.05	121.87
1	Q	215	MET	N-CA-C	6.48	118.14	111.14
1	C	212	GLU	CA-C-N	6.48	129.49	120.29
1	C	212	GLU	C-N-CA	6.48	129.49	120.29
1	H	163	ASP	N-CA-C	6.48	119.33	111.82
1	B	84	HIS	ND1-CE1-NE2	6.47	114.87	108.40
1	R	170	LYS	CA-C-O	6.47	127.36	120.70
1	C	159	GLU	CA-C-N	6.47	127.92	119.84
1	C	159	GLU	C-N-CA	6.47	127.92	119.84
1	M	65	ALA	CA-C-O	6.46	127.40	120.55
1	R	31	ALA	N-CA-C	6.46	117.56	108.00
1	M	2	ILE	CA-C-O	6.46	126.80	120.27
1	N	67	GLN	CA-C-N	6.46	128.93	120.28
1	N	67	GLN	C-N-CA	6.46	128.93	120.28
1	B	95	GLN	OE1-CD-NE2	-6.45	116.15	122.60
1	K	114	GLN	N-CA-C	6.45	118.31	111.28
1	N	87	HIS	CE1-NE2-CD2	-6.45	102.55	109.00
1	E	12	HIS	CG-CD2-NE2	6.45	113.64	107.20
1	J	56	LEU	O-C-N	-6.44	115.13	122.09
1	S	9	GLN	OE1-CD-NE2	-6.44	116.16	122.60
1	K	13	GLN	OE1-CD-NE2	6.44	129.04	122.60
1	L	87	HIS	ND1-CE1-NE2	6.44	114.84	108.40
1	E	176	GLN	CA-C-O	6.44	127.24	120.54
1	R	40	PHE	CA-C-O	6.43	127.78	120.90
1	H	210	THR	CA-C-N	6.43	128.90	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	210	THR	C-N-CA	6.43	128.90	120.28
1	S	13	GLN	O-C-N	-6.43	115.81	123.27
1	R	63	GLN	OE1-CD-NE2	-6.43	116.17	122.60
1	C	84	HIS	CG-CD2-NE2	6.43	113.63	107.20
1	E	183	ASN	OD1-CG-ND2	-6.43	116.17	122.60
1	G	147	PRO	CA-C-N	6.43	131.03	120.94
1	G	147	PRO	C-N-CA	6.43	131.03	120.94
1	N	129	ILE	O-C-N	-6.42	115.07	121.94
1	D	185	MET	CA-C-O	6.42	127.36	120.55
1	F	88	ALA	CA-C-N	6.42	131.96	121.87
1	F	88	ALA	C-N-CA	6.42	131.96	121.87
1	B	12	HIS	ND1-CE1-NE2	6.42	114.82	108.40
1	L	62	HIS	ND1-CE1-NE2	6.42	114.82	108.40
1	C	84	HIS	O-C-N	-6.42	113.94	121.32
1	G	76	GLU	N-CA-CB	6.42	119.56	110.12
1	K	100	ARG	CA-C-O	-6.42	114.56	121.94
1	M	165	VAL	N-CA-C	6.42	117.16	110.62
1	O	138	LEU	N-CA-CB	6.42	119.55	110.12
1	F	54	THR	N-CA-C	6.42	117.94	111.07
1	N	26	VAL	CA-C-N	6.41	129.53	120.42
1	N	26	VAL	C-N-CA	6.41	129.53	120.42
1	H	2	ILE	CA-C-O	6.41	126.75	120.27
1	R	84	HIS	CA-CB-CG	-6.41	107.39	113.80
1	N	171	THR	CA-C-N	6.41	128.87	120.28
1	N	171	THR	C-N-CA	6.41	128.87	120.28
1	K	95	GLN	CB-CG-CD	6.41	123.49	112.60
1	H	217	ALA	N-CA-C	6.41	118.34	111.36
1	G	23	TRP	CB-CA-C	6.40	121.42	110.79
1	K	115	ILE	O-C-N	-6.40	115.66	121.87
1	E	65	ALA	CA-C-N	6.40	128.86	120.28
1	E	65	ALA	C-N-CA	6.40	128.86	120.28
1	B	179	GLN	N-CA-C	6.40	118.25	111.28
1	O	148	THR	O-C-N	-6.40	116.57	123.42
1	G	27	VAL	O-C-N	-6.40	115.24	121.83
1	K	3	VAL	N-CA-CB	6.40	118.69	111.21
1	C	23	TRP	N-CA-C	6.39	118.25	111.28
1	B	33	SER	CA-C-N	6.39	126.88	119.47
1	B	33	SER	C-N-CA	6.39	126.88	119.47
1	M	68	MET	CA-C-N	6.39	128.74	120.44
1	M	68	MET	C-N-CA	6.39	128.74	120.44
1	P	197	ASP	CA-CB-CG	-6.39	106.21	112.60
1	G	82	ARG	NE-CZ-NH1	6.38	127.89	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	62	HIS	CE1-NE2-CD2	-6.38	102.62	109.00
1	B	84	HIS	CG-CD2-NE2	6.38	113.58	107.20
1	K	75	GLU	O-C-N	-6.38	115.50	122.07
1	M	16	SER	CA-C-N	6.38	126.59	119.32
1	M	16	SER	C-N-CA	6.38	126.59	119.32
1	J	33	SER	CA-C-N	6.38	127.81	119.84
1	J	33	SER	C-N-CA	6.38	127.81	119.84
1	B	102	SER	O-C-N	-6.38	114.43	122.27
1	K	82	ARG	NE-CZ-NH1	6.37	127.87	121.50
1	M	21	ASN	CB-CG-ND2	6.37	125.95	116.40
1	S	103	ASP	CA-CB-CG	-6.37	106.23	112.60
1	D	82	ARG	CA-C-N	6.37	129.99	120.31
1	D	82	ARG	C-N-CA	6.37	129.99	120.31
1	N	138	LEU	N-CA-C	6.37	118.22	111.28
1	I	18	ARG	NE-CZ-NH1	6.36	127.86	121.50
1	C	219	GLN	CA-C-N	6.36	128.09	120.14
1	C	219	GLN	C-N-CA	6.36	128.09	120.14
1	E	72	THR	O-C-N	-6.36	115.52	122.07
1	E	54	THR	CA-C-N	6.36	128.80	120.28
1	E	54	THR	C-N-CA	6.36	128.80	120.28
1	J	13	GLN	OE1-CD-NE2	-6.36	116.24	122.60
1	B	26	VAL	CA-C-O	-6.35	114.44	121.05
1	P	67	GLN	N-CA-CB	6.35	119.22	110.01
1	S	195	ASN	CA-C-O	-6.35	113.88	120.87
1	C	115	ILE	O-C-N	-6.35	115.71	121.87
1	H	62	HIS	CA-CB-CG	-6.35	107.45	113.80
1	G	144	MET	N-CA-C	6.34	118.27	111.36
1	N	216	THR	N-CA-C	6.34	119.17	111.82
1	D	195	ASN	CA-CB-CG	6.34	118.94	112.60
1	Q	102	SER	CA-C-N	6.34	129.29	120.29
1	Q	102	SER	C-N-CA	6.34	129.29	120.29
1	C	88	ALA	N-CA-C	6.34	120.02	110.64
1	G	216	THR	N-CA-CB	6.33	120.10	110.28
1	R	172	LEU	N-CA-C	6.33	118.18	111.28
1	E	33	SER	CA-C-N	6.33	126.54	119.32
1	E	33	SER	C-N-CA	6.33	126.54	119.32
1	N	53	ASN	CA-CB-CG	6.33	118.93	112.60
1	O	71	GLU	CA-C-N	6.33	128.66	120.44
1	O	71	GLU	C-N-CA	6.33	128.66	120.44
1	E	50	GLN	OE1-CD-NE2	-6.32	116.28	122.60
1	O	190	LEU	N-CA-C	6.32	118.73	111.02
1	E	195	ASN	N-CA-C	6.32	119.30	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	100	ARG	NH1-CZ-NH2	-6.32	111.09	119.30
1	D	210	THR	CA-C-N	6.31	128.65	120.44
1	D	210	THR	C-N-CA	6.31	128.65	120.44
1	G	110	THR	CA-CB-OG1	6.31	119.07	109.60
1	J	110	THR	CA-CB-OG1	6.31	119.06	109.60
1	B	27	VAL	O-C-N	-6.31	115.33	121.83
1	N	199	LYS	CA-C-N	6.31	128.64	120.44
1	N	199	LYS	C-N-CA	6.31	128.64	120.44
1	F	86	VAL	N-CA-CB	6.30	118.58	110.13
1	P	27	VAL	O-C-N	-6.30	115.34	121.83
1	B	3	VAL	N-CA-CB	6.30	118.18	111.00
1	O	93	PRO	N-CA-C	6.29	122.28	113.53
1	H	188	THR	CA-C-N	6.29	129.22	120.29
1	H	188	THR	C-N-CA	6.29	129.22	120.29
1	Q	108	THR	CB-CA-C	-6.29	98.99	109.55
1	F	63	GLN	N-CA-C	6.28	120.78	113.18
1	D	5	ASN	OD1-CG-ND2	-6.27	116.33	122.60
1	P	19	THR	CA-C-N	6.27	129.01	120.54
1	P	19	THR	C-N-CA	6.27	129.01	120.54
1	N	80	TRP	N-CA-C	-6.27	104.36	111.07
1	H	120	HIS	ND1-CE1-NE2	6.27	114.67	108.40
1	L	119	THR	CA-C-N	6.27	133.51	121.54
1	L	119	THR	C-N-CA	6.27	133.51	121.54
1	I	143	ARG	O-C-N	-6.26	115.48	122.12
1	P	60	GLY	CA-C-O	-6.26	114.47	121.23
1	O	7	GLN	CB-CG-CD	6.26	123.24	112.60
1	E	53	ASN	CB-CA-C	-6.26	100.40	110.79
1	O	135	ILE	CA-CB-CG2	6.25	121.13	110.50
1	P	84	HIS	CG-CD2-NE2	6.25	113.45	107.20
1	P	184	TRP	CA-C-N	6.25	129.17	120.29
1	P	184	TRP	C-N-CA	6.25	129.17	120.29
1	M	73	ILE	N-CA-C	6.25	117.00	110.62
1	R	203	LYS	N-CA-C	6.25	118.90	111.71
1	N	51	ASP	CA-CB-CG	-6.25	106.35	112.60
1	J	152	ASP	N-CA-C	-6.25	105.66	113.28
1	H	216	THR	CA-C-O	-6.25	112.78	119.97
1	S	111	LEU	CA-C-N	6.25	128.65	120.28
1	S	111	LEU	C-N-CA	6.25	128.65	120.28
1	B	200	THR	CA-C-O	-6.25	114.26	120.82
1	I	78	ALA	CA-C-O	6.24	127.17	120.55
1	O	207	PRO	N-CA-C	-6.24	108.19	114.68
1	I	42	ALA	N-CA-C	6.24	117.74	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	121	ASN	CB-CA-C	6.23	117.84	109.42
1	N	163	ASP	O-C-N	-6.23	114.13	122.23
1	K	31	ALA	N-CA-C	6.23	117.78	108.31
1	K	81	ASP	CA-CB-CG	-6.23	106.37	112.60
1	B	47	ALA	O-C-N	-6.23	115.94	123.16
1	K	117	TRP	CA-C-O	6.23	127.15	120.55
1	S	102	SER	O-C-N	-6.22	114.61	122.27
1	H	105	ALA	CA-C-O	6.22	127.27	119.12
1	K	5	ASN	CA-C-N	6.22	131.15	121.26
1	K	5	ASN	C-N-CA	6.22	131.15	121.26
1	M	7	GLN	O-C-N	6.22	129.77	122.00
1	K	5	ASN	OD1-CG-ND2	-6.22	116.38	122.60
1	P	87	HIS	CE1-NE2-CD2	-6.22	102.78	109.00
1	P	156	GLY	O-C-N	-6.21	115.56	121.77
1	O	50	GLN	O-C-N	-6.21	115.67	122.07
1	G	155	GLN	CA-C-N	6.21	131.61	121.87
1	G	155	GLN	C-N-CA	6.21	131.61	121.87
1	P	92	ALA	O-C-N	-6.20	116.29	121.38
1	R	182	LYS	O-C-N	-6.20	115.55	122.12
1	F	16	SER	CA-C-O	-6.20	113.72	120.17
1	S	200	THR	O-C-N	-6.20	115.65	122.09
1	J	169	TYR	CA-C-N	6.20	128.87	120.44
1	J	169	TYR	C-N-CA	6.20	128.87	120.44
1	B	13	GLN	N-CA-C	-6.19	99.92	109.52
1	Q	19	THR	N-CA-CB	6.19	118.95	109.98
1	I	123	PRO	N-CA-C	6.19	120.93	111.15
1	N	83	LEU	N-CA-C	6.19	118.11	111.36
1	F	183	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	Q	98	GLU	N-CA-CB	-6.19	102.13	110.23
1	D	166	ASP	CA-CB-CG	6.18	118.78	112.60
1	B	218	CYS	CA-C-N	6.18	128.56	120.28
1	B	218	CYS	C-N-CA	6.18	128.56	120.28
1	D	53	ASN	O-C-N	-6.18	115.57	122.12
1	Q	41	SER	N-CA-CB	6.18	119.20	110.12
1	K	32	PHE	CA-C-O	6.18	126.96	120.54
1	O	37	ILE	O-C-N	-6.18	114.06	121.10
1	S	21	ASN	O-C-N	-6.17	115.58	122.12
1	E	145	TYR	N-CA-C	-6.17	105.75	113.28
1	C	32	PHE	CA-C-N	6.17	129.25	120.49
1	C	32	PHE	C-N-CA	6.17	129.25	120.49
1	K	103	ASP	CA-CB-CG	6.17	118.77	112.60
1	P	23	TRP	N-CA-C	6.17	118.00	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	GLN	CA-C-N	6.17	133.32	121.54
1	B	176	GLN	C-N-CA	6.17	133.32	121.54
1	N	90	PRO	CA-C-N	6.16	129.48	120.91
1	N	90	PRO	C-N-CA	6.16	129.48	120.91
1	R	86	VAL	CA-C-O	6.16	128.48	120.78
1	B	19	THR	CA-C-N	6.16	128.85	120.54
1	B	19	THR	C-N-CA	6.16	128.85	120.54
1	B	212	GLU	CA-C-O	-6.16	114.36	120.82
1	E	25	LYS	CA-C-N	6.16	128.54	120.60
1	E	25	LYS	C-N-CA	6.16	128.54	120.60
1	F	84	HIS	CA-C-O	6.16	124.71	119.66
1	J	182	LYS	N-CA-C	6.15	118.07	111.36
1	S	50	GLN	CA-C-N	6.15	129.02	120.29
1	S	50	GLN	C-N-CA	6.15	129.02	120.29
1	C	131	LYS	CA-C-N	6.15	128.51	120.28
1	C	131	LYS	C-N-CA	6.15	128.51	120.28
1	D	81	ASP	O-C-N	6.14	128.63	122.12
1	J	54	THR	N-CA-CB	6.14	119.09	109.94
1	Q	171	THR	CA-C-N	6.14	128.79	120.38
1	Q	171	THR	C-N-CA	6.14	128.79	120.38
1	K	164	TYR	CA-C-N	6.14	129.14	120.42
1	K	164	TYR	C-N-CA	6.14	129.14	120.42
1	K	189	LEU	CB-CA-C	-6.14	100.42	110.85
1	H	153	ILE	N-CA-C	6.14	117.62	108.54
1	H	180	GLU	O-C-N	-6.13	115.16	122.15
1	F	9	GLN	OE1-CD-NE2	6.13	128.73	122.60
1	I	49	PRO	CA-C-N	6.13	128.41	120.44
1	I	49	PRO	C-N-CA	6.13	128.41	120.44
1	O	76	GLU	N-CA-C	6.13	118.76	111.71
1	F	214	MET	CA-C-N	6.13	128.99	120.29
1	F	214	MET	C-N-CA	6.13	128.99	120.29
1	Q	186	THR	CA-C-O	6.13	127.43	121.00
1	Q	150	ILE	CA-C-O	6.12	127.12	120.57
1	E	126	VAL	N-CA-C	6.12	116.86	110.62
1	E	210	THR	CA-C-N	6.12	128.48	120.28
1	E	210	THR	C-N-CA	6.12	128.48	120.28
1	H	196	PRO	O-C-N	-6.12	115.57	122.18
1	E	209	ALA	CA-C-O	6.12	127.92	121.19
1	G	216	THR	CA-C-N	6.11	128.97	120.29
1	G	216	THR	C-N-CA	6.11	128.97	120.29
1	F	82	ARG	O-C-N	-6.11	115.78	122.07
1	Q	218	CYS	CA-C-O	6.11	127.10	119.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	219	GLN	N-CA-C	6.11	118.91	111.82
1	S	56	LEU	CA-C-O	-6.10	113.95	120.42
1	Q	213	GLU	N-CA-C	6.10	117.93	111.28
1	K	198	CYS	CA-C-N	6.10	128.78	120.54
1	K	198	CYS	C-N-CA	6.10	128.78	120.54
1	Q	142	VAL	CA-C-N	6.10	128.46	120.28
1	Q	142	VAL	C-N-CA	6.10	128.46	120.28
1	R	4	GLN	CG-CD-NE2	6.10	125.55	116.40
1	I	18	ARG	NE-CZ-NH2	-6.10	113.71	119.20
1	J	88	ALA	N-CA-C	6.10	123.79	110.80
1	J	215	MET	CA-C-O	6.10	126.98	120.70
1	P	29	GLU	O-C-N	-6.10	114.79	122.17
1	P	153	ILE	O-C-N	-6.10	116.00	122.83
1	F	202	LEU	O-C-N	-6.10	115.20	122.15
1	I	68	MET	CG-SD-CE	-6.10	87.49	100.90
1	R	76	GLU	O-C-N	-6.09	115.09	122.22
1	K	107	THR	N-CA-C	-6.09	106.17	113.97
1	G	48	THR	N-CA-C	-6.09	102.20	110.36
1	M	156	GLY	CA-C-O	-6.09	112.81	121.52
1	B	51	ASP	CA-C-N	6.09	128.44	120.28
1	B	51	ASP	C-N-CA	6.09	128.44	120.28
1	N	97	ARG	NE-CZ-NH1	6.08	127.58	121.50
1	G	193	ASN	OD1-CG-ND2	-6.08	116.52	122.60
1	R	195	ASN	CB-CA-C	6.08	118.23	109.11
1	F	54	THR	CA-C-O	6.08	127.20	120.82
1	C	144	MET	N-CA-CB	-6.08	101.17	110.16
1	C	195	ASN	CA-C-N	6.07	125.55	119.24
1	C	195	ASN	C-N-CA	6.07	125.55	119.24
1	E	48	THR	O-C-N	-6.07	113.45	121.34
1	J	103	ASP	N-CA-C	6.07	117.89	111.28
1	R	191	VAL	CA-C-N	6.06	128.40	120.28
1	R	191	VAL	C-N-CA	6.06	128.40	120.28
1	L	129	ILE	N-CA-C	-6.06	104.83	110.53
1	S	23	TRP	CB-CG-CD1	-6.06	117.81	126.90
1	B	62	HIS	ND1-CE1-NE2	6.06	114.46	108.40
1	H	194	ALA	N-CA-CB	6.06	119.02	110.36
1	L	168	PHE	CA-C-O	-6.05	114.64	121.00
1	G	6	LEU	CA-C-N	6.05	133.25	123.93
1	G	6	LEU	C-N-CA	6.05	133.25	123.93
1	P	2	ILE	CA-C-O	6.05	126.38	120.27
1	J	160	PRO	CA-C-N	6.05	128.71	120.54
1	J	160	PRO	C-N-CA	6.05	128.71	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	196	PRO	CA-C-N	6.05	128.31	120.44
1	L	196	PRO	C-N-CA	6.05	128.31	120.44
1	P	95	GLN	OE1-CD-NE2	-6.05	116.55	122.60
1	L	134	ILE	CA-C-O	6.05	127.58	121.17
1	B	219	GLN	O-C-N	-6.05	115.71	122.12
1	L	178	SER	N-CA-C	6.04	117.84	110.41
1	M	200	THR	N-CA-CB	6.04	118.77	110.01
1	G	72	THR	O-C-N	-6.04	115.85	122.07
1	R	50	GLN	CB-CA-C	-6.04	100.76	110.79
1	R	192	GLN	CG-CD-NE2	-6.04	107.34	116.40
1	K	21	ASN	CB-CA-C	-6.04	100.77	110.79
1	R	208	GLY	O-C-N	6.03	127.70	121.97
1	G	34	PRO	N-CA-C	6.03	122.74	113.75
1	H	126	VAL	N-CA-C	6.03	118.59	111.05
1	S	171	THR	N-CA-CB	6.03	118.98	110.12
1	J	178	SER	N-CA-C	6.03	118.69	110.55
1	L	210	THR	CA-CB-OG1	6.02	118.63	109.60
1	R	134	ILE	CA-CB-CG1	-6.02	100.17	110.40
1	N	18	ARG	CA-C-O	-6.02	111.85	119.31
1	R	65	ALA	N-CA-C	6.02	117.92	111.36
1	D	185	MET	CA-C-N	6.02	128.59	120.65
1	D	185	MET	C-N-CA	6.02	128.59	120.65
1	G	77	ALA	O-C-N	-6.02	115.87	122.07
1	S	149	SER	N-CA-C	-6.01	101.56	110.46
1	M	103	ASP	CA-C-N	6.01	128.96	120.42
1	M	103	ASP	C-N-CA	6.01	128.96	120.42
1	J	21	ASN	CA-CB-CG	6.01	118.61	112.60
1	P	120	HIS	CE1-NE2-CD2	-6.01	102.99	109.00
1	P	197	ASP	O-C-N	-6.01	115.88	122.07
1	C	41	SER	CA-C-N	6.01	128.25	120.44
1	C	41	SER	C-N-CA	6.01	128.25	120.44
1	E	167	ARG	CA-C-N	6.01	128.80	120.63
1	E	167	ARG	C-N-CA	6.01	128.80	120.63
1	L	68	MET	O-C-N	-6.00	115.75	122.12
1	S	75	GLU	O-C-N	-6.00	115.75	122.12
1	L	37	ILE	CA-C-O	-6.00	111.90	119.95
1	G	195	ASN	CA-C-N	6.00	126.17	119.32
1	G	195	ASN	C-N-CA	6.00	126.17	119.32
1	O	11	VAL	O-C-N	-6.00	116.72	123.20
1	P	110	THR	O-C-N	-6.00	116.25	123.03
1	H	209	ALA	CA-C-O	6.00	127.91	121.55
1	H	134	ILE	N-CA-C	6.00	116.18	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	219	GLN	N-CA-C	6.00	118.93	110.23
1	K	82	ARG	O-C-N	-6.00	115.89	122.07
1	K	84	HIS	ND1-CG-CD2	-5.99	100.11	106.10
1	I	44	SER	O-C-N	-5.99	115.12	122.25
1	J	207	PRO	CA-C-N	5.99	127.83	120.22
1	J	207	PRO	C-N-CA	5.99	127.83	120.22
1	L	21	ASN	CA-C-O	-5.99	114.20	120.55
1	G	32	PHE	CA-CB-CG	-5.99	107.81	113.80
1	E	39	MET	CA-C-O	-5.99	114.53	120.82
1	N	12	HIS	ND1-CE1-NE2	5.99	114.39	108.40
1	E	173	ARG	N-CA-C	5.98	117.80	111.28
1	K	14	ALA	N-CA-C	5.98	119.33	110.48
1	S	74	ASN	OD1-CG-ND2	-5.98	116.62	122.60
1	O	70	LYS	CA-C-O	5.98	127.10	120.82
1	B	27	VAL	CA-C-N	5.98	128.21	120.44
1	B	27	VAL	C-N-CA	5.98	128.21	120.44
1	Q	25	LYS	N-CA-C	5.98	117.88	111.36
1	S	114	GLN	CA-C-O	5.98	127.10	120.82
1	K	72	THR	N-CA-C	5.97	118.28	111.11
1	P	215	MET	N-CA-C	5.97	117.87	111.36
1	S	39	MET	O-C-N	-5.97	115.92	122.07
1	G	78	ALA	CA-C-N	5.97	128.20	120.44
1	G	78	ALA	C-N-CA	5.97	128.20	120.44
1	D	25	LYS	CA-C-N	5.97	128.30	120.60
1	D	25	LYS	C-N-CA	5.97	128.30	120.60
1	N	8	GLY	O-C-N	-5.97	115.36	122.34
1	D	122	PRO	CA-C-N	5.97	126.44	119.99
1	D	122	PRO	C-N-CA	5.97	126.44	119.99
1	F	82	ARG	N-CA-C	5.97	117.46	111.07
1	G	52	LEU	N-CA-C	5.97	117.59	111.14
1	P	160	PRO	CA-C-N	5.97	128.60	120.54
1	P	160	PRO	C-N-CA	5.97	128.60	120.54
1	R	146	SER	CA-C-N	5.97	126.85	120.47
1	R	146	SER	C-N-CA	5.97	126.85	120.47
1	C	165	VAL	CA-C-N	5.97	128.20	120.44
1	C	165	VAL	C-N-CA	5.97	128.20	120.44
1	H	95	GLN	O-C-N	-5.97	116.06	123.04
1	E	191	VAL	CB-CA-C	-5.96	103.99	112.22
1	H	181	VAL	CA-C-O	-5.96	114.53	120.85
1	K	48	THR	N-CA-CB	5.96	118.01	109.78
1	M	179	GLN	OE1-CD-NE2	-5.96	116.64	122.60
1	C	59	VAL	CA-CB-CG2	-5.96	100.27	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	35	GLU	CA-C-N	5.96	128.62	120.46
1	M	35	GLU	C-N-CA	5.96	128.62	120.46
1	C	175	GLU	O-C-N	-5.96	115.71	122.68
1	M	146	SER	CA-C-N	5.96	125.58	119.56
1	M	146	SER	C-N-CA	5.96	125.58	119.56
1	B	139	ASN	CB-CA-C	5.95	120.67	110.79
1	N	179	GLN	CA-C-N	5.95	128.26	120.28
1	N	179	GLN	C-N-CA	5.95	128.26	120.28
1	D	137	GLY	CA-C-N	5.95	128.26	120.28
1	D	137	GLY	C-N-CA	5.95	128.26	120.28
1	K	101	GLY	CA-C-O	5.95	126.88	120.75
1	M	217	ALA	N-CA-C	5.95	117.84	111.36
1	J	141	ILE	N-CA-CB	5.95	118.18	110.57
1	D	143	ARG	CD-NE-CZ	5.95	132.72	124.40
1	N	175	GLU	CA-C-N	5.94	130.74	120.58
1	N	175	GLU	C-N-CA	5.94	130.74	120.58
1	H	120	HIS	CE1-NE2-CD2	-5.94	103.06	109.00
1	N	59	VAL	CB-CA-C	-5.94	104.81	111.23
1	G	203	LYS	N-CA-C	5.94	118.54	111.71
1	K	126	VAL	N-CA-C	5.94	118.47	111.05
1	M	26	VAL	N-CA-CB	5.94	117.50	110.55
1	N	167	ARG	CA-C-N	5.94	128.51	120.44
1	N	167	ARG	C-N-CA	5.94	128.51	120.44
1	P	219	GLN	N-CA-C	5.94	117.42	111.07
1	C	18	ARG	N-CA-C	-5.94	105.53	112.89
1	I	186	THR	N-CA-C	5.94	117.44	110.97
1	Q	95	GLN	O-C-N	5.94	130.11	123.05
1	F	162	ARG	N-CA-C	5.93	118.51	111.33
1	C	19	THR	OG1-CB-CG2	-5.93	97.44	109.30
1	I	92	ALA	CA-C-N	5.93	127.26	119.84
1	I	92	ALA	C-N-CA	5.93	127.26	119.84
1	L	162	ARG	CA-C-N	5.93	128.71	120.29
1	L	162	ARG	C-N-CA	5.93	128.71	120.29
1	N	120	HIS	CE1-NE2-CD2	-5.93	103.07	109.00
1	P	195	ASN	N-CA-CB	5.93	118.76	110.11
1	R	21	ASN	CA-CB-CG	5.93	118.53	112.60
1	O	190	LEU	N-CA-CB	-5.92	100.81	109.82
1	F	68	MET	CB-CA-C	5.92	120.75	110.68
1	N	106	GLY	CA-C-N	5.92	128.49	120.44
1	N	106	GLY	C-N-CA	5.92	128.49	120.44
1	O	95	GLN	OE1-CD-NE2	-5.92	116.68	122.60
1	K	121	ASN	O-C-N	-5.92	116.12	121.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	ARG	NE-CZ-NH1	5.92	127.42	121.50
1	D	167	ARG	CA-C-N	5.92	128.46	120.65
1	D	167	ARG	C-N-CA	5.92	128.46	120.65
1	D	70	LYS	CA-C-O	5.91	126.82	120.55
1	K	40	PHE	CA-C-O	5.91	127.22	120.90
1	L	217	ALA	N-CA-C	5.91	117.52	111.14
1	B	212	GLU	N-CA-CB	5.91	118.58	110.01
1	L	165	VAL	CA-C-N	5.91	128.12	120.44
1	L	165	VAL	C-N-CA	5.91	128.12	120.44
1	Q	111	LEU	CA-C-N	5.91	128.20	120.28
1	Q	111	LEU	C-N-CA	5.91	128.20	120.28
1	B	44	SER	N-CA-CB	5.91	119.53	110.61
1	H	146	SER	CB-CA-C	-5.91	100.34	109.85
1	I	135	ILE	N-CA-C	5.91	116.64	110.62
1	J	179	GLN	N-CA-C	5.91	117.72	111.28
1	L	68	MET	CA-C-O	5.90	126.81	120.55
1	Q	146	SER	CB-CA-C	-5.90	100.01	109.69
1	N	62	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	P	165	VAL	CA-C-N	5.89	128.10	120.44
1	P	165	VAL	C-N-CA	5.89	128.10	120.44
1	S	74	ASN	N-CA-C	-5.89	104.93	111.36
1	G	200	THR	CA-C-N	5.89	128.20	120.60
1	G	200	THR	C-N-CA	5.89	128.20	120.60
1	I	55	MET	N-CA-C	5.89	117.71	111.28
1	G	82	ARG	CB-CA-C	-5.89	101.63	110.88
1	D	155	GLN	N-CA-C	5.89	118.77	110.23
1	B	219	GLN	CA-C-O	5.89	126.79	120.55
1	L	156	GLY	CA-C-N	5.89	125.27	118.85
1	L	156	GLY	C-N-CA	5.89	125.27	118.85
1	D	82	ARG	CA-C-O	5.89	127.00	120.82
1	J	48	THR	CA-C-N	5.89	125.58	119.05
1	J	48	THR	C-N-CA	5.89	125.58	119.05
1	L	146	SER	CA-C-N	5.88	127.19	119.84
1	L	146	SER	C-N-CA	5.88	127.19	119.84
1	K	8	GLY	CA-C-O	-5.88	112.54	119.72
1	O	162	ARG	N-CA-C	5.88	118.45	111.33
1	Q	163	ASP	CA-CB-CG	5.88	118.48	112.60
1	F	11	VAL	O-C-N	-5.88	116.85	123.20
1	B	171	THR	O-C-N	-5.88	115.89	122.12
1	H	199	LYS	N-CA-C	5.88	117.69	111.28
1	G	49	PRO	CA-C-N	5.88	128.15	120.28
1	G	49	PRO	C-N-CA	5.88	128.15	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	176	GLN	O-C-N	-5.88	115.29	122.34
1	E	218	CYS	CA-C-O	5.88	126.77	119.78
1	M	98	GLU	O-C-N	-5.87	115.41	121.28
1	B	108	THR	CA-C-O	5.87	126.43	119.56
1	L	14	ALA	N-CA-CB	5.87	118.60	109.97
1	O	166	ASP	CA-C-N	5.87	128.15	120.28
1	O	166	ASP	C-N-CA	5.87	128.15	120.28
1	L	212	GLU	O-C-N	-5.87	115.99	122.09
1	O	203	LYS	N-CA-CB	5.87	118.75	110.12
1	L	92	ALA	CA-C-O	5.87	127.09	120.70
1	H	219	GLN	CA-C-O	5.87	126.58	119.31
1	I	212	GLU	CB-CA-C	-5.87	101.67	110.88
1	O	132	ARG	N-CA-C	5.86	117.67	111.28
1	P	64	ALA	O-C-N	-5.86	115.91	122.12
1	D	181	VAL	CA-C-N	5.86	128.13	120.28
1	D	181	VAL	C-N-CA	5.86	128.13	120.28
1	J	177	ALA	N-CA-C	5.86	118.18	108.99
1	R	193	ASN	N-CA-CB	-5.85	101.98	110.47
1	H	195	ASN	CA-C-N	5.85	125.33	119.24
1	H	195	ASN	C-N-CA	5.85	125.33	119.24
1	N	127	GLY	CA-C-O	-5.85	114.68	121.00
1	B	18	ARG	NE-CZ-NH2	5.85	124.46	119.20
1	Q	33	SER	CA-C-N	5.85	127.15	119.84
1	Q	33	SER	C-N-CA	5.85	127.15	119.84
1	C	214	MET	N-CA-C	5.85	117.45	111.14
1	S	194	ALA	CA-C-O	5.84	128.30	121.87
1	R	129	ILE	N-CA-CB	5.84	118.05	110.57
1	S	178	SER	N-CA-C	5.84	118.24	110.53
1	H	162	ARG	NE-CZ-NH2	5.84	124.46	119.20
1	J	65	ALA	N-CA-CB	-5.84	101.52	110.16
1	Q	126	VAL	CA-C-N	5.84	126.42	119.94
1	Q	126	VAL	C-N-CA	5.84	126.42	119.94
1	O	192	GLN	CA-C-O	5.84	126.74	120.55
1	E	12	HIS	ND1-CE1-NE2	5.84	114.24	108.40
1	L	181	VAL	CA-C-O	5.83	127.03	120.85
1	Q	2	ILE	CA-C-N	5.83	130.36	122.90
1	Q	2	ILE	C-N-CA	5.83	130.36	122.90
1	G	16	SER	N-CA-C	5.83	118.13	110.08
1	D	83	LEU	CA-C-O	-5.83	113.27	119.97
1	E	197	ASP	CA-CB-CG	-5.83	106.78	112.60
1	I	82	ARG	N-CA-C	5.83	117.30	111.07
1	G	95	GLN	CA-C-N	5.82	130.08	120.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	95	GLN	C-N-CA	5.82	130.08	120.94
1	J	112	GLN	OE1-CD-NE2	-5.82	116.78	122.60
1	J	216	THR	CA-CB-OG1	5.82	118.33	109.60
1	E	195	ASN	CA-C-O	-5.82	114.47	120.87
1	P	95	GLN	CA-C-N	-5.82	113.10	121.42
1	P	95	GLN	C-N-CA	-5.82	113.10	121.42
1	L	143	ARG	O-C-N	-5.82	115.95	122.12
1	R	143	ARG	CA-C-N	5.81	128.54	120.29
1	R	143	ARG	C-N-CA	5.81	128.54	120.29
1	L	203	LYS	CA-C-N	5.81	129.14	120.31
1	L	203	LYS	C-N-CA	5.81	129.14	120.31
1	O	6	LEU	CA-C-N	5.81	131.11	122.74
1	O	6	LEU	C-N-CA	5.81	131.11	122.74
1	S	172	LEU	CA-C-N	5.81	128.06	120.28
1	S	172	LEU	C-N-CA	5.81	128.06	120.28
1	L	56	LEU	CA-C-O	-5.81	114.72	120.70
1	B	215	MET	CA-C-O	-5.80	114.27	120.42
1	M	50	GLN	N-CA-C	5.80	117.61	111.28
1	B	67	GLN	OE1-CD-NE2	-5.80	116.80	122.60
1	Q	135	ILE	N-CA-C	5.80	116.54	110.62
1	E	39	MET	CG-SD-CE	-5.80	88.14	100.90
1	K	62	HIS	CB-CG-CD2	-5.80	123.66	131.20
1	Q	186	THR	O-C-N	-5.80	116.00	122.03
1	P	159	GLU	N-CA-C	5.80	117.83	109.48
1	R	140	LYS	CA-C-N	5.80	127.98	120.56
1	R	140	LYS	C-N-CA	5.80	127.98	120.56
1	O	136	LEU	CA-C-O	5.79	127.10	120.90
1	K	79	GLU	CA-C-O	5.79	126.90	120.82
1	N	84	HIS	CE1-NE2-CD2	-5.79	103.21	109.00
1	P	104	ILE	N-CA-C	-5.79	104.87	110.72
1	D	96	MET	CA-C-O	-5.79	114.00	120.54
1	J	90	PRO	N-CA-CB	5.79	108.18	103.32
1	J	34	PRO	CA-C-O	-5.78	110.08	120.60
1	C	125	PRO	CA-C-N	5.78	129.60	120.47
1	C	125	PRO	C-N-CA	5.78	129.60	120.47
1	O	212	GLU	N-CA-C	5.78	118.32	111.33
1	R	70	LYS	CA-C-O	5.78	126.67	120.55
1	D	178	SER	CA-C-N	5.78	128.02	120.28
1	D	178	SER	C-N-CA	5.78	128.02	120.28
1	G	21	ASN	N-CA-C	5.78	117.25	111.07
1	S	110	THR	N-CA-CB	5.77	118.70	110.44
1	R	4	GLN	O-C-N	-5.77	116.49	123.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	215	MET	CA-C-O	5.77	126.54	120.42
1	I	134	ILE	N-CA-CB	5.76	118.38	110.54
1	K	143	ARG	CA-C-N	5.76	128.47	120.29
1	K	143	ARG	C-N-CA	5.76	128.47	120.29
1	O	90	PRO	N-CA-C	5.76	119.29	111.22
1	C	15	ILE	O-C-N	-5.76	116.79	122.67
1	B	193	ASN	CA-C-O	5.76	126.40	119.43
1	O	176	GLN	CB-CG-CD	5.76	122.39	112.60
1	R	45	GLU	CA-C-N	5.76	131.38	121.07
1	R	45	GLU	C-N-CA	5.76	131.38	121.07
1	D	96	MET	N-CA-CB	5.76	119.66	110.16
1	B	48	THR	CA-C-N	5.76	125.88	119.32
1	B	48	THR	C-N-CA	5.76	125.88	119.32
1	R	83	LEU	N-CA-C	5.76	118.50	111.82
1	P	87	HIS	CA-C-O	5.75	126.65	120.32
1	P	69	LEU	CA-C-N	5.75	127.92	120.44
1	P	69	LEU	C-N-CA	5.75	127.92	120.44
1	C	176	GLN	O-C-N	-5.75	116.51	123.29
1	I	142	VAL	N-CA-C	5.75	116.40	110.36
1	J	125	PRO	N-CA-CB	5.75	106.56	102.65
1	P	10	MET	N-CA-C	5.75	118.10	108.96
1	Q	98	GLU	CA-C-N	5.75	125.68	119.76
1	Q	98	GLU	C-N-CA	5.75	125.68	119.76
1	C	19	THR	N-CA-CB	5.75	118.34	110.01
1	I	120	HIS	CA-CB-CG	5.75	119.55	113.80
1	Q	71	GLU	CA-C-N	5.74	127.91	120.44
1	Q	71	GLU	C-N-CA	5.74	127.91	120.44
1	D	155	GLN	CG-CD-NE2	5.74	125.02	116.40
1	D	188	THR	CA-C-N	5.74	128.44	120.29
1	D	188	THR	C-N-CA	5.74	128.44	120.29
1	M	103	ASP	N-CA-C	5.74	117.54	111.28
1	P	49	PRO	CA-C-N	5.74	127.97	120.28
1	P	49	PRO	C-N-CA	5.74	127.97	120.28
1	N	152	ASP	CA-C-O	5.74	126.01	119.18
1	I	53	ASN	O-C-N	5.74	128.20	122.12
1	F	213	GLU	CA-C-N	5.74	128.44	120.29
1	F	213	GLU	C-N-CA	5.74	128.44	120.29
1	J	208	GLY	N-CA-C	5.74	121.06	113.37
1	B	54	THR	O-C-N	-5.73	116.16	122.07
1	N	88	ALA	O-C-N	-5.73	115.82	122.87
1	C	74	ASN	CB-CG-OD1	5.73	132.26	120.80
1	G	167	ARG	N-CA-C	5.73	117.60	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	172	LEU	N-CA-C	5.73	117.52	111.28
1	D	104	ILE	O-C-N	5.72	127.73	121.83
1	D	161	PHE	CA-CB-CG	5.72	119.52	113.80
1	D	185	MET	N-CA-C	5.72	117.52	111.28
1	N	51	ASP	N-CA-C	5.72	117.59	111.36
1	D	120	HIS	N-CA-C	5.72	117.68	110.24
1	F	164	TYR	N-CA-C	5.72	117.52	111.28
1	L	27	VAL	O-C-N	-5.72	115.94	121.83
1	O	95	GLN	O-C-N	-5.72	116.21	122.84
1	H	160	PRO	N-CA-CB	5.72	108.66	103.34
1	B	174	ALA	N-CA-C	-5.71	105.89	112.92
1	P	20	LEU	CA-C-N	5.71	127.94	120.28
1	P	20	LEU	C-N-CA	5.71	127.94	120.28
1	Q	59	VAL	CA-C-O	5.71	127.86	120.95
1	S	80	TRP	CA-C-N	5.71	127.93	120.28
1	S	80	TRP	C-N-CA	5.71	127.93	120.28
1	G	53	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	I	90	PRO	N-CA-C	5.71	120.56	111.26
1	R	33	SER	CA-C-N	5.71	126.97	119.84
1	R	33	SER	C-N-CA	5.71	126.97	119.84
1	I	217	ALA	N-CA-C	5.71	117.58	111.36
1	P	35	GLU	CA-C-O	5.71	126.40	119.38
1	E	67	GLN	N-CA-C	5.71	117.30	111.14
1	P	51	ASP	CA-C-N	5.70	128.39	120.29
1	P	51	ASP	C-N-CA	5.70	128.39	120.29
1	Q	11	VAL	O-C-N	-5.70	117.04	123.20
1	B	11	VAL	N-CA-C	5.70	116.33	108.12
1	P	158	LYS	N-CA-C	-5.70	105.67	113.30
1	B	77	ALA	CA-C-N	5.70	127.91	120.28
1	B	77	ALA	C-N-CA	5.70	127.91	120.28
1	S	103	ASP	CA-C-N	5.70	128.51	120.42
1	S	103	ASP	C-N-CA	5.70	128.51	120.42
1	E	84	HIS	CA-C-N	5.70	126.96	119.84
1	E	84	HIS	C-N-CA	5.70	126.96	119.84
1	P	183	ASN	OD1-CG-ND2	-5.69	116.91	122.60
1	H	217	ALA	CA-C-O	5.69	126.46	120.42
1	K	84	HIS	CB-CA-C	-5.69	104.52	110.33
1	L	132	ARG	CD-NE-CZ	5.69	132.37	124.40
1	M	212	GLU	N-CA-C	5.69	117.94	111.11
1	O	33	SER	CA-C-O	-5.69	114.50	120.02
1	H	84	HIS	CE1-NE2-CD2	-5.69	103.31	109.00
1	H	91	ILE	CA-CB-CG1	5.69	120.07	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	THR	N-CA-C	5.69	117.34	109.15
1	M	53	ASN	CA-C-N	5.69	128.22	120.54
1	M	53	ASN	C-N-CA	5.69	128.22	120.54
1	H	18	ARG	CD-NE-CZ	5.69	132.36	124.40
1	M	180	GLU	CA-C-O	5.68	126.58	120.55
1	Q	215	MET	CG-SD-CE	-5.68	88.39	100.90
1	R	14	ALA	CA-C-N	5.68	128.12	120.50
1	R	14	ALA	C-N-CA	5.68	128.12	120.50
1	M	49	PRO	CA-C-N	5.68	127.89	120.28
1	M	49	PRO	C-N-CA	5.68	127.89	120.28
1	P	141	ILE	O-C-N	-5.68	115.99	121.90
1	S	120	HIS	CE1-NE2-CD2	-5.68	103.32	109.00
1	K	8	GLY	O-C-N	5.68	128.55	122.41
1	D	153	ILE	N-CA-C	5.68	115.44	107.37
1	F	189	LEU	CA-C-N	5.68	128.21	120.54
1	F	189	LEU	C-N-CA	5.68	128.21	120.54
1	L	109	SER	O-C-N	-5.68	116.57	123.10
1	M	201	ILE	CA-C-N	5.68	128.35	120.29
1	M	201	ILE	C-N-CA	5.68	128.35	120.29
1	G	95	GLN	N-CA-C	5.68	119.50	109.96
1	J	20	LEU	O-C-N	-5.68	116.18	122.09
1	N	47	ALA	CA-C-O	-5.68	115.62	121.87
1	S	205	LEU	CB-CA-C	-5.68	99.77	110.67
1	F	114	GLN	CA-C-N	5.68	128.24	120.46
1	F	114	GLN	C-N-CA	5.68	128.24	120.46
1	B	185	MET	CA-C-O	-5.67	114.54	120.55
1	M	53	ASN	CB-CG-ND2	5.67	124.91	116.40
1	N	173	ARG	NE-CZ-NH1	5.67	127.17	121.50
1	C	50	GLN	OE1-CD-NE2	-5.67	116.93	122.60
1	E	219	GLN	O-C-N	-5.67	116.11	122.12
1	M	32	PHE	N-CA-CB	-5.67	101.65	110.55
1	P	100	ARG	O-C-N	-5.67	114.77	122.36
1	Q	110	THR	CA-C-O	-5.67	115.03	121.72
1	B	66	MET	CG-SD-CE	-5.67	88.43	100.90
1	Q	115	ILE	CA-C-N	5.67	126.39	119.99
1	Q	115	ILE	C-N-CA	5.67	126.39	119.99
1	K	102	SER	CA-C-N	5.67	128.33	120.29
1	K	102	SER	C-N-CA	5.67	128.33	120.29
1	C	21	ASN	O-C-N	-5.67	116.11	122.12
1	C	70	LYS	CG-CD-CE	5.67	124.33	111.30
1	N	21	ASN	CA-CB-CG	5.66	118.26	112.60
1	N	82	ARG	CA-C-N	5.66	128.33	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	82	ARG	C-N-CA	5.66	128.33	120.29
1	E	198	CYS	CA-C-O	5.66	126.42	120.42
1	S	134	ILE	N-CA-CB	5.66	117.17	110.55
1	B	55	MET	CA-C-N	5.66	128.33	120.29
1	B	55	MET	C-N-CA	5.66	128.33	120.29
1	Q	199	LYS	O-C-N	5.66	127.97	122.09
1	R	129	ILE	N-CA-C	-5.66	105.21	110.53
1	L	36	VAL	N-CA-C	5.66	116.39	110.62
1	F	43	LEU	O-C-N	-5.66	114.66	122.46
1	J	192	GLN	CA-CB-CG	5.66	125.41	114.10
1	E	62	HIS	ND1-CE1-NE2	5.65	114.05	108.40
1	M	179	GLN	CA-C-N	5.65	127.85	120.28
1	M	179	GLN	C-N-CA	5.65	127.85	120.28
1	G	117	TRP	CD2-CE3-CZ3	-5.65	111.25	118.60
1	B	115	ILE	CA-C-N	5.65	126.38	119.99
1	B	115	ILE	C-N-CA	5.65	126.38	119.99
1	O	208	GLY	CA-C-N	5.65	128.74	120.71
1	O	208	GLY	C-N-CA	5.65	128.74	120.71
1	B	129	ILE	N-CA-C	5.65	115.84	110.53
1	F	84	HIS	O-C-N	-5.65	113.35	121.54
1	H	143	ARG	CA-C-N	5.65	128.31	120.29
1	H	143	ARG	C-N-CA	5.65	128.31	120.29
1	L	3	VAL	CB-CA-C	5.64	117.79	110.96
1	G	215	MET	CG-SD-CE	-5.64	88.48	100.90
1	S	196	PRO	N-CA-C	5.64	122.92	113.78
1	N	7	GLN	OE1-CD-NE2	-5.64	116.96	122.60
1	D	93	PRO	N-CA-C	5.64	122.15	113.75
1	D	167	ARG	N-CA-C	5.64	117.42	111.28
1	F	25	LYS	N-CA-C	5.64	117.42	111.28
1	K	92	ALA	N-CA-C	5.63	116.92	109.93
1	M	29	GLU	CA-C-O	5.63	126.50	120.70
1	S	215	MET	N-CA-C	5.63	117.23	111.14
1	C	11	VAL	N-CA-C	-5.63	100.01	108.12
1	I	209	ALA	N-CA-C	5.63	118.52	110.24
1	K	68	MET	CA-CB-CG	5.63	125.36	114.10
1	E	18	ARG	NE-CZ-NH2	-5.63	114.13	119.20
1	K	150	ILE	O-C-N	-5.63	116.18	121.87
1	G	178	SER	N-CA-C	5.62	117.59	110.33
1	K	39	MET	CA-C-N	5.62	128.13	120.54
1	K	39	MET	C-N-CA	5.62	128.13	120.54
1	L	134	ILE	N-CA-C	5.62	115.82	110.42
1	M	27	VAL	CA-C-N	5.62	127.82	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	27	VAL	C-N-CA	5.62	127.82	120.28
1	N	5	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	H	66	MET	CA-C-N	5.62	127.81	120.28
1	H	66	MET	C-N-CA	5.62	127.81	120.28
1	C	91	ILE	CA-C-N	5.62	129.19	120.60
1	C	91	ILE	C-N-CA	5.62	129.19	120.60
1	F	131	LYS	O-C-N	-5.62	116.17	122.12
1	O	65	ALA	N-CA-CB	-5.62	101.86	110.12
1	I	128	GLU	CA-C-O	5.62	126.43	119.97
1	O	159	GLU	O-C-N	-5.61	115.47	121.42
1	H	39	MET	CA-C-N	5.61	128.12	120.54
1	H	39	MET	C-N-CA	5.61	128.12	120.54
1	H	132	ARG	CA-C-N	5.61	127.80	120.28
1	H	132	ARG	C-N-CA	5.61	127.80	120.28
1	I	9	GLN	CA-C-N	5.61	130.24	122.77
1	I	9	GLN	C-N-CA	5.61	130.24	122.77
1	N	35	GLU	CA-C-N	5.61	128.15	120.46
1	N	35	GLU	C-N-CA	5.61	128.15	120.46
1	Q	118	MET	N-CA-CB	-5.61	101.86	110.16
1	D	3	VAL	O-C-N	-5.61	115.56	122.97
1	J	212	GLU	CA-C-N	5.61	127.80	120.28
1	J	212	GLU	C-N-CA	5.61	127.80	120.28
1	O	53	ASN	N-CA-C	5.61	117.39	111.28
1	N	129	ILE	CA-C-N	5.61	127.80	120.28
1	N	129	ILE	C-N-CA	5.61	127.80	120.28
1	S	141	ILE	CA-C-N	5.61	127.83	120.60
1	S	141	ILE	C-N-CA	5.61	127.83	120.60
1	S	179	GLN	N-CA-CB	-5.61	101.88	110.12
1	E	70	LYS	N-CA-CB	5.61	118.30	109.94
1	I	113	GLU	N-CA-C	5.61	117.39	111.28
1	I	45	GLU	N-CA-CB	5.60	118.26	109.69
1	D	175	GLU	CA-C-N	5.60	128.06	120.44
1	D	175	GLU	C-N-CA	5.60	128.06	120.44
1	J	186	THR	N-CA-CB	5.60	118.09	109.91
1	N	71	GLU	CA-C-N	5.60	127.72	120.44
1	N	71	GLU	C-N-CA	5.60	127.72	120.44
1	B	182	LYS	CA-C-N	5.60	127.78	120.28
1	B	182	LYS	C-N-CA	5.60	127.78	120.28
1	B	90	PRO	N-CA-CB	5.60	108.02	103.32
1	O	172	LEU	N-CA-C	5.60	117.38	111.28
1	P	54	THR	N-CA-CB	5.60	118.28	109.94
1	I	211	LEU	CA-C-N	5.60	127.72	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	211	LEU	C-N-CA	5.60	127.72	120.44
1	P	91	ILE	CA-C-N	5.59	128.83	120.83
1	P	91	ILE	C-N-CA	5.59	128.83	120.83
1	J	28	GLU	N-CA-CB	5.59	118.12	110.01
1	G	165	VAL	CG1-CB-CG2	-5.59	98.50	110.80
1	P	136	LEU	CA-C-O	-5.59	114.95	120.82
1	D	143	ARG	NH1-CZ-NH2	-5.59	112.04	119.30
1	J	91	ILE	CA-C-N	5.59	128.15	120.39
1	J	91	ILE	C-N-CA	5.59	128.15	120.39
1	B	158	LYS	CB-CA-C	-5.58	100.17	109.55
1	N	16	SER	O-C-N	-5.58	115.55	121.30
1	I	70	LYS	CA-C-N	5.58	127.70	120.44
1	I	70	LYS	C-N-CA	5.58	127.70	120.44
1	S	64	ALA	CA-C-N	5.58	128.03	120.44
1	S	64	ALA	C-N-CA	5.58	128.03	120.44
1	O	149	SER	O-C-N	-5.58	116.37	122.84
1	R	209	ALA	N-CA-C	5.58	118.32	110.23
1	K	72	THR	CA-C-O	5.58	126.87	120.90
1	P	15	ILE	CA-C-N	5.58	128.41	120.49
1	P	15	ILE	C-N-CA	5.58	128.41	120.49
1	Q	33	SER	CA-C-O	-5.58	113.36	119.61
1	C	121	ASN	CA-CB-CG	-5.58	107.02	112.60
1	J	115	ILE	CA-C-N	5.58	126.29	119.99
1	J	115	ILE	C-N-CA	5.58	126.29	119.99
1	S	134	ILE	CA-C-N	5.57	128.09	120.46
1	S	134	ILE	C-N-CA	5.57	128.09	120.46
1	E	126	VAL	CA-CB-CG1	-5.57	100.93	110.40
1	G	161	PHE	O-C-N	5.57	127.89	122.09
1	C	167	ARG	CG-CD-NE	-5.57	99.74	112.00
1	R	68	MET	CA-C-N	5.57	127.74	120.28
1	R	68	MET	C-N-CA	5.57	127.74	120.28
1	S	70	LYS	CA-C-O	5.57	126.45	120.55
1	B	155	GLN	CB-CA-C	-5.57	101.16	110.29
1	L	84	HIS	CA-C-O	-5.57	112.54	120.16
1	L	132	ARG	NE-CZ-NH2	-5.57	114.19	119.20
1	O	199	LYS	N-CA-C	5.57	117.03	111.07
1	I	32	PHE	CB-CG-CD2	5.57	130.16	120.70
1	J	51	ASP	N-CA-CB	-5.57	101.92	110.16
1	M	55	MET	O-C-N	-5.56	116.22	122.12
1	R	204	ALA	CA-C-O	5.56	126.37	119.97
1	Q	142	VAL	O-C-N	-5.56	116.38	121.94
1	M	45	GLU	CA-C-N	5.56	129.92	120.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	45	GLU	C-N-CA	5.56	129.92	120.91
1	D	13	GLN	O-C-N	-5.56	116.40	123.24
1	P	81	ASP	N-CA-CB	-5.56	101.95	110.12
1	R	65	ALA	CA-C-N	5.56	127.73	120.28
1	R	65	ALA	C-N-CA	5.56	127.73	120.28
1	B	87	HIS	O-C-N	-5.56	116.71	123.10
1	N	100	ARG	NH1-CZ-NH2	-5.56	112.07	119.30
1	O	34	PRO	N-CA-C	5.56	123.92	112.47
1	Q	114	GLN	CA-C-O	5.56	126.44	120.55
1	B	39	MET	O-C-N	-5.55	116.35	122.07
1	M	184	TRP	O-C-N	-5.55	116.23	122.12
1	N	74	ASN	O-C-N	-5.55	116.23	122.12
1	D	195	ASN	CB-CA-C	5.55	118.21	109.27
1	H	150	ILE	N-CA-C	5.55	117.99	111.05
1	K	86	VAL	N-CA-CB	5.55	116.98	110.82
1	N	144	MET	CA-C-O	5.55	126.44	120.55
1	I	50	GLN	OE1-CD-NE2	-5.55	117.05	122.60
1	P	58	THR	O-C-N	-5.55	114.18	122.39
1	M	62	HIS	O-C-N	-5.55	114.98	122.41
1	M	134	ILE	CA-C-N	5.54	128.29	120.42
1	M	134	ILE	C-N-CA	5.54	128.29	120.42
1	O	65	ALA	N-CA-C	5.54	117.32	111.28
1	O	67	GLN	N-CA-CB	5.54	118.11	110.07
1	O	196	PRO	CA-C-N	5.54	127.65	120.44
1	O	196	PRO	C-N-CA	5.54	127.65	120.44
1	E	143	ARG	NE-CZ-NH1	5.54	127.04	121.50
1	K	132	ARG	NE-CZ-NH1	5.54	127.04	121.50
1	O	176	GLN	CA-C-N	5.54	128.97	120.82
1	O	176	GLN	C-N-CA	5.54	128.97	120.82
1	P	59	VAL	N-CA-CB	5.54	117.16	110.95
1	C	10	MET	O-C-N	-5.54	116.76	123.13
1	N	187	GLU	N-CA-C	5.54	119.30	112.54
1	C	102	SER	CA-C-N	5.54	128.16	120.29
1	C	102	SER	C-N-CA	5.54	128.16	120.29
1	H	108	THR	CA-CB-CG2	5.54	119.92	110.50
1	G	215	MET	O-C-N	-5.54	115.84	122.15
1	R	38	PRO	CA-C-N	5.54	127.64	120.44
1	R	38	PRO	C-N-CA	5.54	127.64	120.44
1	L	53	ASN	CA-CB-CG	-5.53	107.07	112.60
1	N	66	MET	CG-SD-CE	-5.53	88.73	100.90
1	Q	111	LEU	CA-C-O	5.53	126.42	120.55
1	S	210	THR	CA-C-O	-5.53	115.42	121.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	205	LEU	O-C-N	5.53	129.07	122.27
1	P	18	ARG	CD-NE-CZ	-5.53	116.66	124.40
1	C	201	ILE	O-C-N	-5.53	116.41	121.94
1	G	156	GLY	N-CA-C	5.53	123.62	112.34
1	I	78	ALA	O-C-N	-5.53	116.26	122.12
1	N	220	GLY	N-CA-C	5.53	126.28	113.18
1	S	132	ARG	NE-CZ-NH2	-5.53	114.23	119.20
1	P	25	LYS	N-CA-C	5.52	117.38	111.36
1	I	112	GLN	OE1-CD-NE2	-5.52	117.08	122.60
1	I	180	GLU	CA-C-N	5.52	128.26	120.42
1	I	180	GLU	C-N-CA	5.52	128.26	120.42
1	S	197	ASP	N-CA-C	5.52	116.98	111.07
1	D	10	MET	O-C-N	-5.52	116.78	123.13
1	D	201	ILE	N-CA-CB	-5.52	104.09	110.55
1	J	117	TRP	CA-C-O	5.52	126.40	120.55
1	L	190	LEU	N-CA-C	5.52	117.73	111.11
1	L	202	LEU	N-CA-C	5.52	117.38	111.36
1	B	30	LYS	O-C-N	-5.52	115.56	122.24
1	B	41	SER	N-CA-C	-5.52	105.27	111.28
1	K	63	GLN	OE1-CD-NE2	-5.52	117.08	122.60
1	K	196	PRO	CA-C-N	5.51	127.61	120.44
1	K	196	PRO	C-N-CA	5.51	127.61	120.44
1	R	135	ILE	N-CA-C	5.51	116.24	110.62
1	D	62	HIS	CA-CB-CG	5.51	119.31	113.80
1	K	140	LYS	N-CA-C	5.51	117.28	111.28
1	S	148	THR	CA-CB-OG1	5.51	117.86	109.60
1	N	121	ASN	OD1-CG-ND2	-5.51	117.09	122.60
1	K	10	MET	N-CA-C	5.50	117.71	108.96
1	L	164	TYR	CA-C-N	5.50	128.24	120.42
1	L	164	TYR	C-N-CA	5.50	128.24	120.42
1	B	64	ALA	O-C-N	-5.50	115.88	122.15
1	J	198	CYS	CA-C-N	5.50	127.65	120.28
1	J	198	CYS	C-N-CA	5.50	127.65	120.28
1	P	209	ALA	N-CA-C	5.50	118.42	110.28
1	S	129	ILE	CB-CA-C	-5.50	104.81	112.02
1	E	181	VAL	CA-CB-CG2	-5.50	101.05	110.40
1	M	136	LEU	CA-C-O	-5.50	115.05	120.82
1	G	137	GLY	N-CA-C	5.50	120.74	113.37
1	M	82	ARG	NE-CZ-NH2	-5.50	114.25	119.20
1	N	90	PRO	N-CA-C	5.50	123.80	112.47
1	S	116	GLY	CA-C-O	-5.50	115.06	121.00
1	I	2	ILE	CB-CA-C	5.50	117.60	110.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	35	GLU	CA-C-O	5.50	126.14	119.38
1	G	2	ILE	N-CA-C	-5.50	99.64	107.77
1	Q	154	ARG	CA-C-O	5.49	127.26	121.33
1	R	149	SER	N-CA-CB	-5.49	101.45	110.52
1	F	4	GLN	CA-C-O	5.49	126.58	120.43
1	I	194	ALA	N-CA-C	5.49	117.97	110.55
1	B	98	GLU	CA-C-O	-5.49	114.31	119.80
1	Q	150	ILE	O-C-N	-5.49	116.32	121.87
1	Q	187	GLU	N-CA-C	5.49	118.19	111.82
1	Q	201	ILE	CA-C-O	5.49	126.99	121.17
1	D	117	TRP	CG-CD2-CE3	-5.49	128.41	133.90
1	J	100	ARG	NE-CZ-NH2	-5.49	114.26	119.20
1	C	120	HIS	CB-CG-ND1	5.49	130.93	122.70
1	D	220	GLY	O-C-N	-5.49	115.56	122.70
1	F	67	GLN	N-CA-C	5.49	116.94	111.07
1	O	53	ASN	CA-C-N	5.49	127.95	120.54
1	O	53	ASN	C-N-CA	5.49	127.95	120.54
1	G	167	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	K	12	HIS	ND1-CE1-NE2	5.49	113.89	108.40
1	Q	87	HIS	CG-CD2-NE2	5.49	112.69	107.20
1	P	169	TYR	CB-CG-CD1	-5.48	112.58	120.80
1	G	201	ILE	N-CA-C	5.48	116.11	110.36
1	H	21	ASN	CA-C-O	5.48	126.36	120.55
1	N	137	GLY	CA-C-O	5.48	126.47	120.66
1	Q	53	ASN	CA-C-N	5.48	127.93	120.54
1	Q	53	ASN	C-N-CA	5.48	127.93	120.54
1	G	39	MET	CA-C-N	5.48	127.93	120.54
1	G	39	MET	C-N-CA	5.48	127.93	120.54
1	B	30	LYS	CG-CD-CE	5.47	123.89	111.30
1	I	155	GLN	OE1-CD-NE2	-5.47	117.12	122.60
1	J	144	MET	CB-CA-C	5.47	119.88	110.79
1	C	64	ALA	CA-C-N	5.47	127.88	120.44
1	C	64	ALA	C-N-CA	5.47	127.88	120.44
1	D	87	HIS	N-CA-C	5.47	118.46	109.76
1	K	195	ASN	CA-C-N	5.47	124.93	119.24
1	K	195	ASN	C-N-CA	5.47	124.93	119.24
1	R	70	LYS	N-CA-C	5.47	117.24	111.28
1	E	84	HIS	CB-CG-CD2	-5.47	124.09	131.20
1	N	15	ILE	CA-C-N	5.47	127.99	120.39
1	N	15	ILE	C-N-CA	5.47	127.99	120.39
1	G	72	THR	CA-C-O	5.47	126.56	120.82
1	P	122	PRO	N-CD-CG	-5.46	97.24	103.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	24	VAL	CA-C-N	5.46	128.05	120.29
1	D	24	VAL	C-N-CA	5.46	128.05	120.29
1	E	37	ILE	N-CA-CB	5.46	114.71	110.45
1	G	51	ASP	N-CA-C	-5.46	105.40	111.36
1	G	123	PRO	N-CA-C	5.46	120.17	111.26
1	M	25	LYS	N-CA-C	5.46	117.31	111.36
1	H	201	ILE	N-CA-CB	-5.46	104.16	110.55
1	B	186	THR	CA-C-N	5.46	129.84	120.72
1	B	186	THR	C-N-CA	5.46	129.84	120.72
1	O	191	VAL	CB-CA-C	-5.46	104.69	112.22
1	O	77	ALA	N-CA-CB	-5.46	102.10	110.12
1	S	211	LEU	CA-C-O	-5.46	114.76	120.55
1	G	162	ARG	CA-CB-CG	5.46	125.02	114.10
1	P	7	GLN	O-C-N	-5.46	115.78	122.55
1	C	162	ARG	CD-NE-CZ	-5.46	116.76	124.40
1	G	175	GLU	O-C-N	-5.46	116.83	123.10
1	J	91	ILE	CB-CA-C	5.46	119.10	111.08
1	K	29	GLU	N-CA-C	5.46	117.31	111.36
1	M	86	VAL	N-CA-CB	-5.45	104.78	111.00
1	P	69	LEU	O-C-N	-5.45	116.34	122.12
1	C	192	GLN	N-CA-C	5.45	117.22	111.28
1	O	38	PRO	CA-C-N	5.45	127.53	120.44
1	O	38	PRO	C-N-CA	5.45	127.53	120.44
1	B	15	ILE	CB-CA-C	5.45	120.19	111.69
1	O	69	LEU	N-CA-C	5.45	117.22	111.28
1	O	183	ASN	CA-CB-CG	-5.45	107.15	112.60
1	Q	193	ASN	N-CA-C	-5.45	106.22	112.92
1	S	82	ARG	CD-NE-CZ	5.45	132.03	124.40
1	E	121	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	G	197	ASP	N-CA-C	5.45	116.90	111.07
1	O	203	LYS	O-C-N	-5.45	116.35	122.12
1	C	136	LEU	CA-C-N	5.45	125.99	120.00
1	C	136	LEU	C-N-CA	5.45	125.99	120.00
1	D	74	ASN	CA-C-N	5.45	127.84	120.44
1	D	74	ASN	C-N-CA	5.45	127.84	120.44
1	G	12	HIS	CE1-NE2-CD2	-5.45	103.56	109.00
1	G	214	MET	N-CA-C	5.45	117.22	111.28
1	P	87	HIS	ND1-CE1-NE2	5.44	113.84	108.40
1	C	156	GLY	O-C-N	-5.44	116.33	121.77
1	G	129	ILE	O-C-N	5.44	127.56	121.90
1	J	20	LEU	CA-C-N	5.44	127.57	120.28
1	J	20	LEU	C-N-CA	5.44	127.57	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	164	TYR	O-C-N	-5.44	116.36	122.12
1	R	62	HIS	CB-CA-C	-5.44	104.01	111.73
1	P	107	THR	CA-CB-OG1	5.44	117.75	109.60
1	Q	4	GLN	CA-C-O	5.44	126.52	120.43
1	D	104	ILE	CA-C-O	-5.44	115.09	120.85
1	D	187	GLU	CA-C-N	-5.44	113.99	122.42
1	D	187	GLU	C-N-CA	-5.44	113.99	122.42
1	H	42	ALA	CA-C-O	-5.44	115.11	120.82
1	L	186	THR	OG1-CB-CG2	-5.43	98.43	109.30
1	Q	114	GLN	O-C-N	-5.43	116.36	122.12
1	Q	173	ARG	NE-CZ-NH2	-5.43	114.31	119.20
1	C	72	THR	N-CA-C	5.43	116.88	111.07
1	H	173	ARG	NE-CZ-NH2	-5.43	114.31	119.20
1	Q	87	HIS	ND1-CE1-NE2	5.43	113.83	108.40
1	O	32	PHE	CA-C-N	5.43	128.38	120.51
1	O	32	PHE	C-N-CA	5.43	128.38	120.51
1	O	160	PRO	N-CA-C	5.43	119.39	111.03
1	K	18	ARG	N-CA-C	-5.43	106.16	112.89
1	L	136	LEU	O-C-N	5.43	127.66	122.07
1	Q	131	LYS	CB-CG-CD	5.43	123.78	111.30
1	N	2	ILE	CA-C-N	5.42	129.15	122.37
1	N	2	ILE	C-N-CA	5.42	129.15	122.37
1	D	26	VAL	CB-CA-C	-5.42	104.94	111.88
1	R	191	VAL	O-C-N	-5.42	116.25	121.83
1	K	57	ASN	CA-CB-CG	-5.42	107.18	112.60
1	D	2	ILE	N-CA-CB	5.42	119.19	111.82
1	D	176	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	E	109	SER	CA-C-O	-5.42	115.03	121.16
1	J	84	HIS	CE1-NE2-CD2	-5.42	103.58	109.00
1	M	139	ASN	O-C-N	-5.42	116.38	122.12
1	P	186	THR	O-C-N	-5.42	116.39	122.03
1	Q	161	PHE	CB-CA-C	-5.42	102.14	110.81
1	H	68	MET	CG-SD-CE	-5.42	88.98	100.90
1	H	36	VAL	CA-CB-CG1	5.42	119.61	110.40
1	K	12	HIS	CE1-NE2-CD2	-5.41	103.59	109.00
1	O	184	TRP	O-C-N	-5.41	116.38	122.12
1	C	26	VAL	CA-CB-CG2	-5.41	101.20	110.40
1	D	167	ARG	NE-CZ-NH2	-5.41	114.33	119.20
1	D	177	ALA	CA-C-N	5.41	128.92	120.75
1	D	177	ALA	C-N-CA	5.41	128.92	120.75
1	H	119	THR	N-CA-CB	5.41	118.45	110.33
1	M	74	ASN	N-CA-C	5.41	117.18	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	87	HIS	CG-CD2-NE2	5.41	112.61	107.20
1	S	15	ILE	N-CA-C	5.41	117.42	109.63
1	P	198	CYS	CB-CA-C	-5.41	101.66	110.85
1	L	89	GLY	CA-C-N	5.41	126.60	119.84
1	L	89	GLY	C-N-CA	5.41	126.60	119.84
1	R	167	ARG	O-C-N	5.41	127.85	122.12
1	C	145	TYR	CA-CB-CG	-5.41	104.17	113.90
1	E	137	GLY	CA-C-O	5.41	126.25	120.30
1	E	81	ASP	N-CA-C	5.41	117.17	111.28
1	J	183	ASN	N-CA-C	5.41	117.17	111.28
1	K	134	ILE	CB-CA-C	-5.40	105.05	111.97
1	N	112	GLN	N-CA-C	5.40	117.17	111.28
1	L	39	MET	CA-C-N	5.40	127.46	120.44
1	L	39	MET	C-N-CA	5.40	127.46	120.44
1	E	137	GLY	O-C-N	-5.40	116.39	122.28
1	K	97	ARG	CG-CD-NE	-5.40	100.12	112.00
1	O	182	LYS	CA-C-N	5.40	127.51	120.28
1	O	182	LYS	C-N-CA	5.40	127.51	120.28
1	P	71	GLU	N-CA-CB	5.39	117.83	110.01
1	P	114	GLN	CG-CD-OE1	-5.39	110.01	120.80
1	C	5	ASN	CB-CG-OD1	5.39	131.58	120.80
1	B	86	VAL	CA-CB-CG1	5.39	119.56	110.40
1	K	150	ILE	CA-C-N	5.39	128.04	120.28
1	K	150	ILE	C-N-CA	5.39	128.04	120.28
1	Q	130	TYR	CA-C-N	5.39	127.50	120.28
1	Q	130	TYR	C-N-CA	5.39	127.50	120.28
1	D	41	SER	N-CA-C	5.39	117.15	111.28
1	J	69	LEU	CA-C-N	5.39	127.44	120.44
1	J	69	LEU	C-N-CA	5.39	127.44	120.44
1	G	148	THR	N-CA-C	5.39	118.09	110.50
1	J	86	VAL	N-CA-C	5.39	116.00	108.89
1	K	88	ALA	O-C-N	-5.38	116.19	122.81
1	P	203	LYS	CA-C-N	5.38	128.50	120.31
1	P	203	LYS	C-N-CA	5.38	128.50	120.31
1	Q	159	GLU	CA-C-N	5.38	126.57	119.84
1	Q	159	GLU	C-N-CA	5.38	126.57	119.84
1	S	27	VAL	CA-C-N	5.38	127.44	120.44
1	S	27	VAL	C-N-CA	5.38	127.44	120.44
1	I	113	GLU	CA-C-O	-5.38	114.84	120.55
1	R	56	LEU	O-C-N	-5.38	116.01	122.15
1	J	18	ARG	NE-CZ-NH1	5.38	126.88	121.50
1	Q	16	SER	CA-CB-OG	5.38	121.86	111.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	GLY	CA-C-O	-5.38	111.21	120.57
1	Q	100	ARG	CD-NE-CZ	-5.38	116.87	124.40
1	C	127	GLY	O-C-N	-5.38	117.02	122.18
1	C	193	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	G	167	ARG	CG-CD-NE	-5.38	100.17	112.00
1	I	109	SER	N-CA-C	5.38	118.58	109.76
1	K	56	LEU	CB-CA-C	-5.37	101.87	110.79
1	O	202	LEU	CB-CA-C	-5.37	101.72	110.85
1	H	57	ASN	OD1-CG-ND2	-5.37	117.23	122.60
1	P	200	THR	N-CA-C	5.37	116.82	111.07
1	E	61	GLY	O-C-N	-5.37	117.52	123.05
1	R	130	TYR	O-C-N	-5.37	116.43	122.12
1	O	118	MET	N-CA-C	5.37	117.21	111.36
1	P	84	HIS	CA-C-N	5.37	126.12	120.11
1	P	84	HIS	C-N-CA	5.37	126.12	120.11
1	F	43	LEU	CA-C-O	5.37	126.03	119.05
1	B	76	GLU	N-CA-CB	5.37	118.10	110.16
1	M	167	ARG	CD-NE-CZ	5.37	131.91	124.40
1	S	40	PHE	CA-C-O	5.37	126.64	120.90
1	J	8	GLY	CA-C-O	5.37	125.94	119.82
1	B	108	THR	N-CA-CB	5.36	118.39	110.56
1	S	107	THR	CA-C-O	-5.36	113.50	119.67
1	E	10	MET	N-CA-C	5.36	117.04	108.41
1	I	74	ASN	CB-CG-ND2	-5.36	108.36	116.40
1	E	147	PRO	N-CA-CB	-5.36	97.62	103.25
1	M	185	MET	N-CA-C	5.36	117.12	111.28
1	N	31	ALA	CA-C-N	5.36	131.19	122.67
1	N	31	ALA	C-N-CA	5.36	131.19	122.67
1	O	172	LEU	CA-C-O	5.36	126.23	120.55
1	R	142	VAL	CA-C-N	5.36	127.46	120.28
1	R	142	VAL	C-N-CA	5.36	127.46	120.28
1	D	214	MET	CA-C-N	5.36	127.90	120.29
1	D	214	MET	C-N-CA	5.36	127.90	120.29
1	F	115	ILE	CA-C-N	5.36	126.05	119.99
1	F	115	ILE	C-N-CA	5.36	126.05	119.99
1	G	121	ASN	O-C-N	-5.36	115.01	121.12
1	B	161	PHE	CA-C-N	5.36	127.72	120.38
1	B	161	PHE	C-N-CA	5.36	127.72	120.38
1	B	29	GLU	N-CA-CB	-5.36	102.22	110.20
1	P	27	VAL	N-CA-C	5.36	116.13	110.72
1	R	132	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	C	132	ARG	NE-CZ-NH1	5.36	126.86	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	185	MET	CA-C-N	5.36	127.72	120.65
1	J	185	MET	C-N-CA	5.36	127.72	120.65
1	K	163	ASP	O-C-N	-5.36	115.68	122.27
1	P	185	MET	CA-C-N	5.36	127.72	120.65
1	P	185	MET	C-N-CA	5.36	127.72	120.65
1	I	164	TYR	CA-C-N	5.35	128.02	120.42
1	I	164	TYR	C-N-CA	5.35	128.02	120.42
1	R	178	SER	CA-CB-OG	5.35	121.81	111.10
1	H	81	ASP	CA-C-N	5.35	127.40	120.44
1	H	81	ASP	C-N-CA	5.35	127.40	120.44
1	N	17	PRO	N-CD-CG	5.35	111.23	103.20
1	Q	208	GLY	O-C-N	-5.35	116.65	122.54
1	E	144	MET	N-CA-C	5.35	117.19	111.36
1	D	11	VAL	O-C-N	-5.35	117.42	123.20
1	M	66	MET	N-CA-CB	5.35	117.98	110.12
1	O	3	VAL	N-CA-CB	5.35	117.47	111.21
1	D	177	ALA	N-CA-C	5.35	122.19	110.80
1	E	162	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	I	12	HIS	N-CA-CB	5.35	117.83	109.97
1	E	52	LEU	N-CA-C	5.35	117.19	111.36
1	B	167	ARG	CB-CA-C	-5.34	101.92	110.79
1	P	190	LEU	N-CA-C	5.34	117.52	111.11
1	M	195	ASN	CA-C-O	-5.34	114.88	120.70
1	J	23	TRP	O-C-N	-5.34	116.46	122.12
1	E	181	VAL	CA-C-O	-5.34	115.19	120.85
1	I	86	VAL	CA-C-N	-5.33	114.67	122.19
1	I	86	VAL	C-N-CA	-5.33	114.67	122.19
1	O	74	ASN	CB-CA-C	-5.33	101.78	110.85
1	G	23	TRP	O-C-N	-5.33	116.47	122.12
1	S	5	ASN	CA-C-N	5.33	129.31	120.94
1	S	5	ASN	C-N-CA	5.33	129.31	120.94
1	M	190	LEU	N-CA-C	5.33	117.51	111.11
1	N	85	PRO	CA-C-N	5.33	128.32	120.91
1	N	85	PRO	C-N-CA	5.33	128.32	120.91
1	F	80	TRP	CA-C-N	5.33	127.42	120.28
1	F	80	TRP	C-N-CA	5.33	127.42	120.28
1	F	21	ASN	N-CA-C	5.33	117.09	111.28
1	R	98	GLU	N-CA-C	5.33	117.30	109.42
1	G	129	ILE	CA-C-N	5.33	127.42	120.28
1	G	129	ILE	C-N-CA	5.33	127.42	120.28
1	G	132	ARG	N-CA-CB	5.33	117.95	110.12
1	L	212	GLU	CA-C-N	5.32	127.85	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	212	GLU	C-N-CA	5.32	127.85	120.29
1	N	89	GLY	O-C-N	5.32	127.09	121.77
1	O	82	ARG	CA-C-N	5.32	128.40	120.31
1	O	82	ARG	C-N-CA	5.32	128.40	120.31
1	C	108	THR	CA-CB-OG1	5.32	117.58	109.60
1	D	23	TRP	CA-C-O	5.32	126.19	120.55
1	D	74	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	L	103	ASP	CA-C-N	5.32	127.97	120.42
1	L	103	ASP	C-N-CA	5.32	127.97	120.42
1	B	148	THR	OG1-CB-CG2	-5.32	98.67	109.30
1	M	195	ASN	CA-CB-CG	5.32	117.92	112.60
1	C	171	THR	CA-C-N	5.32	127.40	120.28
1	C	171	THR	C-N-CA	5.32	127.40	120.28
1	S	32	PHE	CA-CB-CG	-5.31	108.49	113.80
1	C	133	TRP	CA-C-N	5.31	127.36	120.56
1	C	133	TRP	C-N-CA	5.31	127.36	120.56
1	G	211	LEU	CA-C-O	5.31	126.18	120.55
1	J	186	THR	O-C-N	-5.31	116.50	122.03
1	P	197	ASP	N-CA-C	5.31	116.75	111.07
1	G	116	GLY	CA-C-N	5.31	127.34	120.44
1	G	116	GLY	C-N-CA	5.31	127.34	120.44
1	J	81	ASP	N-CA-C	5.31	117.07	111.28
1	Q	39	MET	CA-C-N	5.31	127.70	120.54
1	Q	39	MET	C-N-CA	5.31	127.70	120.54
1	E	1	PRO	CB-CA-C	5.31	120.19	110.10
1	N	95	GLN	N-CA-C	5.31	117.53	110.53
1	Q	55	MET	CB-CA-C	-5.30	101.98	110.79
1	H	6	LEU	CA-C-O	5.30	127.17	121.55
1	H	28	GLU	CB-CA-C	-5.30	102.55	110.88
1	C	75	GLU	O-C-N	-5.30	116.61	122.07
1	L	16	SER	CA-C-O	-5.30	115.74	120.19
1	P	162	ARG	N-CA-C	5.30	117.74	111.33
1	H	119	THR	CA-CB-OG1	5.30	117.55	109.60
1	H	162	ARG	N-CA-C	5.30	117.74	111.33
1	K	97	ARG	CD-NE-CZ	5.30	131.82	124.40
1	L	213	GLU	CB-CA-C	-5.30	101.84	110.85
1	D	181	VAL	N-CA-C	5.30	116.07	110.72
1	J	158	LYS	CB-CG-CD	5.30	123.48	111.30
1	S	133	TRP	CE3-CZ3-CH2	-5.29	114.22	121.10
1	G	164	TYR	CB-CA-C	5.29	119.85	110.85
1	P	159	GLU	CA-C-N	5.29	125.54	119.83
1	P	159	GLU	C-N-CA	5.29	125.54	119.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	165	VAL	CA-CB-CG1	5.29	119.39	110.40
1	H	30	LYS	CG-CD-CE	5.29	123.47	111.30
1	E	82	ARG	NE-CZ-NH2	-5.29	114.44	119.20
1	H	59	VAL	CA-C-N	5.29	125.94	120.60
1	H	59	VAL	C-N-CA	5.29	125.94	120.60
1	K	70	LYS	CA-C-O	5.29	126.15	120.55
1	O	203	LYS	CA-C-O	5.29	126.15	120.55
1	R	159	GLU	CB-CA-C	5.29	116.23	110.15
1	S	217	ALA	CA-C-O	5.29	126.14	120.70
1	C	202	LEU	O-C-N	-5.29	116.12	122.15
1	J	47	ALA	N-CA-C	5.29	118.34	110.52
1	J	41	SER	N-CA-CB	5.28	117.73	110.07
1	K	41	SER	CA-C-O	-5.28	115.27	120.82
1	J	139	ASN	CA-C-N	5.28	127.36	120.28
1	J	139	ASN	C-N-CA	5.28	127.36	120.28
1	M	173	ARG	CA-C-N	5.28	131.94	122.38
1	M	173	ARG	C-N-CA	5.28	131.94	122.38
1	I	154	ARG	CA-C-O	5.28	126.90	120.99
1	J	57	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	B	12	HIS	CE1-NE2-CD2	-5.28	103.72	109.00
1	K	120	HIS	CG-CD2-NE2	5.28	112.48	107.20
1	M	84	HIS	CE1-NE2-CD2	-5.28	103.72	109.00
1	R	25	LYS	O-C-N	5.27	128.16	122.15
1	S	100	ARG	N-CA-C	-5.27	102.94	110.59
1	R	87	HIS	CA-CB-CG	-5.27	108.53	113.80
1	J	139	ASN	CB-CA-C	-5.27	102.05	110.79
1	G	97	ARG	N-CA-CB	5.27	117.89	110.36
1	L	13	GLN	CA-C-O	5.26	127.02	121.33
1	O	121	ASN	CA-CB-CG	-5.26	107.33	112.60
1	I	120	HIS	CE1-NE2-CD2	-5.26	103.74	109.00
1	L	62	HIS	CE1-NE2-CD2	-5.26	103.74	109.00
1	L	124	ILE	CA-C-O	5.26	124.46	120.88
1	M	219	GLN	CA-C-O	-5.26	114.97	120.55
1	Q	200	THR	O-C-N	-5.26	116.65	122.07
1	E	102	SER	CA-C-N	5.26	127.76	120.29
1	E	102	SER	C-N-CA	5.26	127.76	120.29
1	H	58	THR	N-CA-C	5.26	119.56	113.20
1	O	47	ALA	CA-C-N	5.26	130.34	121.92
1	O	47	ALA	C-N-CA	5.26	130.34	121.92
1	D	216	THR	CA-C-N	5.26	127.76	120.29
1	D	216	THR	C-N-CA	5.26	127.76	120.29
1	R	199	LYS	CA-C-O	5.26	126.12	120.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	15	ILE	CA-CB-CG1	5.26	119.33	110.40
1	I	173	ARG	NH1-CZ-NH2	-5.25	112.47	119.30
1	B	93	PRO	N-CA-C	5.25	121.58	113.75
1	P	3	VAL	CA-C-N	-5.25	115.21	122.30
1	P	3	VAL	C-N-CA	-5.25	115.21	122.30
1	R	216	THR	CA-C-N	5.25	127.32	120.28
1	R	216	THR	C-N-CA	5.25	127.32	120.28
1	E	160	PRO	N-CA-CB	5.25	108.00	103.27
1	E	200	THR	CA-C-N	5.25	127.38	120.60
1	E	200	THR	C-N-CA	5.25	127.38	120.60
1	L	210	THR	CA-C-N	5.25	127.31	120.28
1	L	210	THR	C-N-CA	5.25	127.31	120.28
1	H	32	PHE	N-CA-C	-5.25	103.73	111.81
1	K	191	VAL	CA-C-O	5.25	126.41	120.85
1	L	165	VAL	O-C-N	-5.25	116.42	121.83
1	N	177	ALA	N-CA-C	5.25	121.98	110.80
1	O	159	GLU	CA-C-N	5.25	125.50	119.83
1	O	159	GLU	C-N-CA	5.25	125.50	119.83
1	R	184	TRP	CA-C-N	5.25	127.31	120.28
1	R	184	TRP	C-N-CA	5.25	127.31	120.28
1	D	180	GLU	O-C-N	-5.25	116.56	122.12
1	S	153	ILE	N-CA-C	5.25	115.13	107.37
1	Q	32	PHE	N-CA-CB	5.25	117.06	110.45
1	Q	108	THR	N-CA-CB	5.25	118.36	110.65
1	P	153	ILE	CA-C-N	5.24	131.13	121.85
1	P	153	ILE	C-N-CA	5.24	131.13	121.85
1	C	87	HIS	CG-CD2-NE2	5.24	112.44	107.20
1	H	21	ASN	CA-CB-CG	5.24	117.84	112.60
1	L	130	TYR	CA-C-N	5.24	127.30	120.28
1	L	130	TYR	C-N-CA	5.24	127.30	120.28
1	L	185	MET	CG-SD-CE	-5.24	89.37	100.90
1	S	129	ILE	CA-CB-CG2	5.24	119.41	110.50
1	F	216	THR	CA-C-N	5.24	127.73	120.29
1	F	216	THR	C-N-CA	5.24	127.73	120.29
1	N	86	VAL	CA-CB-CG2	5.24	119.31	110.40
1	E	2	ILE	CA-CB-CG1	5.24	119.31	110.40
1	I	178	SER	CA-C-O	-5.24	115.91	121.94
1	N	25	LYS	CA-C-O	5.24	125.97	120.42
1	F	120	HIS	CE1-NE2-CD2	-5.24	103.76	109.00
1	B	64	ALA	N-CA-C	-5.24	105.65	111.36
1	H	7	GLN	N-CA-C	5.24	118.81	111.74
1	L	136	LEU	CA-C-N	-5.24	114.24	120.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	136	LEU	C-N-CA	-5.24	114.24	120.00
1	G	209	ALA	CB-CA-C	-5.24	101.27	109.70
1	I	179	GLN	CA-C-N	5.23	127.29	120.28
1	I	179	GLN	C-N-CA	5.23	127.29	120.28
1	B	208	GLY	CA-C-O	5.23	125.62	119.45
1	G	127	GLY	O-C-N	-5.23	117.16	122.18
1	R	131	LYS	CA-C-O	-5.23	115.00	120.55
1	S	87	HIS	N-CA-C	5.23	117.23	108.23
1	D	26	VAL	N-CA-CB	5.23	116.31	110.51
1	J	184	TRP	CB-CG-CD2	5.23	134.12	126.80
1	L	114	GLN	CA-C-O	5.23	126.09	120.55
1	J	99	PRO	N-CD-CG	5.23	111.04	103.20
1	F	11	VAL	CA-C-N	5.23	129.15	120.94
1	F	11	VAL	C-N-CA	5.23	129.15	120.94
1	P	58	THR	CA-C-O	5.22	125.96	119.12
1	I	49	PRO	CB-CA-C	5.22	121.73	112.64
1	J	211	LEU	N-CA-C	5.22	116.97	111.28
1	C	9	GLN	CB-CA-C	-5.22	102.22	111.05
1	O	173	ARG	NE-CZ-NH1	5.22	126.72	121.50
1	C	74	ASN	CA-CB-CG	-5.22	107.38	112.60
1	N	11	VAL	O-C-N	-5.22	117.52	123.10
1	S	126	VAL	O-C-N	5.22	127.14	121.87
1	E	67	GLN	CB-CA-C	-5.22	102.66	110.90
1	H	36	VAL	CA-CB-CG2	-5.22	101.53	110.40
1	S	117	TRP	CH2-CZ2-CE2	-5.22	110.72	117.50
1	D	62	HIS	ND1-CE1-NE2	5.22	113.62	108.40
1	D	145	TYR	N-CA-CB	5.22	118.42	110.44
1	G	133	TRP	O-C-N	-5.22	116.59	122.12
1	I	58	THR	N-CA-CB	5.22	119.52	110.39
1	P	172	LEU	CA-C-N	5.21	127.27	120.28
1	P	172	LEU	C-N-CA	5.21	127.27	120.28
1	I	105	ALA	N-CA-CB	-5.21	101.24	110.42
1	P	171	THR	N-CA-CB	5.21	117.78	110.12
1	M	121	ASN	CA-CB-CG	5.21	117.81	112.60
1	M	210	THR	CA-CB-OG1	5.21	117.42	109.60
1	S	115	ILE	CA-C-N	5.21	125.72	119.94
1	S	115	ILE	C-N-CA	5.21	125.72	119.94
1	E	113	GLU	CA-C-N	5.21	127.26	120.28
1	E	113	GLU	C-N-CA	5.21	127.26	120.28
1	I	21	ASN	CB-CG-ND2	5.21	124.22	116.40
1	K	48	THR	CA-C-O	-5.21	115.05	120.88
1	N	201	ILE	CA-C-N	5.21	127.69	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	201	ILE	C-N-CA	5.21	127.69	120.29
1	R	13	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	M	161	PHE	CA-C-O	-5.21	115.33	120.90
1	F	13	GLN	O-C-N	-5.21	117.45	123.33
1	G	12	HIS	ND1-CE1-NE2	5.21	113.61	108.40
1	J	53	ASN	CA-CB-CG	-5.21	107.39	112.60
1	L	95	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	O	135	ILE	N-CA-C	5.20	115.93	110.62
1	R	192	GLN	O-C-N	-5.20	116.60	122.12
1	D	69	LEU	O-C-N	-5.20	116.60	122.12
1	N	20	LEU	N-CA-C	5.20	116.64	111.07
1	P	80	TRP	CB-CG-CD1	5.20	134.70	126.90
1	Q	178	SER	N-CA-CB	5.20	117.80	110.36
1	D	160	PRO	CA-C-O	-5.20	115.81	121.27
1	J	153	ILE	N-CA-C	5.20	114.75	107.37
1	B	189	LEU	N-CA-C	5.20	118.08	111.69
1	F	74	ASN	O-C-N	-5.20	116.23	122.15
1	G	79	GLU	O-C-N	-5.20	116.72	122.07
1	K	114	GLN	O-C-N	-5.19	116.61	122.12
1	Q	114	GLN	N-CA-CB	-5.19	102.49	110.12
1	O	203	LYS	CA-C-N	5.19	128.20	120.31
1	O	203	LYS	C-N-CA	5.19	128.20	120.31
1	E	163	ASP	CA-C-O	-5.19	114.92	120.42
1	P	12	HIS	CE1-NE2-CD2	-5.19	103.81	109.00
1	R	176	GLN	N-CA-C	-5.19	100.84	109.46
1	J	58	THR	CA-C-O	5.19	125.92	119.12
1	Q	202	LEU	CA-C-N	5.19	127.23	120.28
1	Q	202	LEU	C-N-CA	5.19	127.23	120.28
1	I	52	LEU	N-CA-C	5.19	117.01	111.36
1	K	110	THR	N-CA-C	-5.18	103.55	110.55
1	H	123	PRO	CA-C-N	5.18	130.59	123.28
1	H	123	PRO	C-N-CA	5.18	130.59	123.28
1	M	180	GLU	N-CA-CB	-5.18	102.50	110.12
1	P	183	ASN	CA-C-O	-5.18	115.06	120.55
1	S	84	HIS	CG-CD2-NE2	5.18	112.38	107.20
1	L	207	PRO	N-CA-CB	-5.18	97.81	103.25
1	N	166	ASP	CA-CB-CG	5.18	117.78	112.60
1	S	37	ILE	CA-C-O	-5.18	113.01	119.95
1	N	140	LYS	CA-C-N	5.18	127.19	120.56
1	N	140	LYS	C-N-CA	5.18	127.19	120.56
1	C	170	LYS	N-CA-C	5.18	116.73	111.14
1	I	149	SER	O-C-N	-5.18	117.14	122.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	70	LYS	N-CA-C	5.17	116.92	111.28
1	R	163	ASP	CA-C-O	5.17	125.92	119.97
1	C	216	THR	O-C-N	-5.17	115.91	122.27
1	D	25	LYS	CB-CG-CD	5.17	123.20	111.30
1	B	105	ALA	N-CA-CB	-5.17	102.04	110.42
1	S	67	GLN	CA-C-N	5.17	127.16	120.44
1	S	67	GLN	C-N-CA	5.17	127.16	120.44
1	K	12	HIS	CB-CG-ND1	5.17	130.46	122.70
1	N	17	PRO	CA-N-CD	-5.17	104.76	112.00
1	R	4	GLN	CA-C-O	5.17	126.22	120.43
1	S	5	ASN	N-CA-C	5.17	117.87	109.86
1	G	91	ILE	CA-CB-CG1	5.17	119.19	110.40
1	I	191	VAL	O-C-N	-5.17	116.50	121.83
1	K	206	GLY	N-CA-C	5.17	122.89	112.34
1	C	5	ASN	CA-CB-CG	-5.17	107.44	112.60
1	M	167	ARG	NE-CZ-NH2	-5.16	114.55	119.20
1	O	184	TRP	CA-C-N	5.16	127.20	120.28
1	O	184	TRP	C-N-CA	5.16	127.20	120.28
1	F	125	PRO	CA-C-N	5.16	128.63	120.47
1	F	125	PRO	C-N-CA	5.16	128.63	120.47
1	F	128	GLU	N-CA-C	5.16	117.81	111.82
1	I	184	TRP	N-CA-C	5.16	116.91	111.28
1	M	42	ALA	CA-C-N	5.16	129.34	120.72
1	M	42	ALA	C-N-CA	5.16	129.34	120.72
1	O	205	LEU	CB-CA-C	-5.16	100.76	110.67
1	R	181	VAL	CA-CB-CG1	5.16	119.17	110.40
1	J	97	ARG	CA-C-O	-5.16	116.08	121.55
1	N	78	ALA	CA-C-N	5.16	127.62	120.29
1	N	78	ALA	C-N-CA	5.16	127.62	120.29
1	N	110	THR	CA-CB-CG2	5.16	119.27	110.50
1	N	146	SER	CB-CA-C	5.16	117.77	109.41
1	K	146	SER	CA-C-N	5.16	124.66	119.19
1	K	146	SER	C-N-CA	5.16	124.66	119.19
1	C	116	GLY	CA-C-N	5.16	127.19	120.28
1	C	116	GLY	C-N-CA	5.16	127.19	120.28
1	F	40	PHE	CA-CB-CG	5.16	118.96	113.80
1	F	110	THR	CA-CB-CG2	-5.16	101.73	110.50
1	R	195	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	G	188	THR	N-CA-C	5.16	119.23	111.96
1	Q	133	TRP	O-C-N	5.15	127.38	122.07
1	L	53	ASN	CA-C-O	5.15	126.01	120.55
1	L	167	ARG	N-CA-CB	-5.15	102.55	110.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	81	ASP	CA-C-O	5.15	126.01	120.55
1	F	195	ASN	CA-C-N	5.15	124.60	119.24
1	F	195	ASN	C-N-CA	5.15	124.60	119.24
1	I	120	HIS	CA-C-O	-5.15	116.21	122.03
1	K	175	GLU	CB-CA-C	5.15	118.25	109.75
1	P	142	VAL	N-CA-C	5.15	115.77	110.36
1	Q	54	THR	CA-CB-CG2	5.15	119.26	110.50
1	F	169	TYR	CA-C-N	5.15	127.45	120.44
1	F	169	TYR	C-N-CA	5.15	127.45	120.44
1	G	192	GLN	N-CA-C	5.15	116.89	111.28
1	I	65	ALA	O-C-N	-5.15	116.28	122.15
1	I	112	GLN	O-C-N	-5.15	116.66	122.12
1	S	31	ALA	N-CA-C	5.15	117.27	108.67
1	F	193	ASN	CA-CB-CG	-5.15	107.45	112.60
1	H	165	VAL	CA-C-N	5.15	127.13	120.44
1	H	165	VAL	C-N-CA	5.15	127.13	120.44
1	K	68	MET	N-CA-C	5.14	116.57	111.07
1	Q	67	GLN	CA-C-O	-5.14	115.40	120.70
1	S	93	PRO	O-C-N	-5.14	115.33	122.27
1	C	93	PRO	O-C-N	-5.14	115.70	122.64
1	D	194	ALA	O-C-N	-5.14	117.15	122.96
1	R	11	VAL	O-C-N	-5.14	117.65	123.20
1	E	18	ARG	CD-NE-CZ	5.14	131.60	124.40
1	G	75	GLU	N-CA-C	5.14	116.57	111.07
1	B	110	THR	CA-C-O	-5.14	115.20	121.78
1	N	142	VAL	N-CA-C	5.14	115.75	110.36
1	D	58	THR	CB-CA-C	-5.14	99.72	109.95
1	F	46	GLY	O-C-N	-5.14	115.99	122.41
1	R	168	PHE	CA-CB-CG	-5.13	108.67	113.80
1	S	103	ASP	O-C-N	-5.13	116.30	122.15
1	E	5	ASN	CA-C-N	5.13	128.00	120.71
1	E	5	ASN	C-N-CA	5.13	128.00	120.71
1	E	215	MET	N-CA-C	5.13	116.88	111.28
1	C	91	ILE	N-CA-C	5.13	116.63	109.80
1	I	140	LYS	N-CA-CB	5.13	117.67	110.12
1	L	164	TYR	CA-CB-CG	-5.13	104.66	113.90
1	P	18	ARG	NH1-CZ-NH2	-5.13	112.63	119.30
1	F	102	SER	CA-C-N	5.13	127.57	120.29
1	F	102	SER	C-N-CA	5.13	127.57	120.29
1	G	74	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	G	215	MET	CB-CA-C	-5.13	102.13	110.85
1	L	87	HIS	CE1-NE2-CD2	-5.13	103.87	109.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	61	GLY	CA-C-O	-5.13	116.05	122.61
1	J	129	ILE	CA-C-N	5.13	127.15	120.28
1	J	129	ILE	C-N-CA	5.13	127.15	120.28
1	Q	97	ARG	NE-CZ-NH2	5.13	123.81	119.20
1	H	6	LEU	N-CA-CB	5.13	117.58	110.04
1	R	202	LEU	CA-C-N	5.12	127.66	120.28
1	R	202	LEU	C-N-CA	5.12	127.66	120.28
1	J	158	LYS	CG-CD-CE	5.12	123.09	111.30
1	K	82	ARG	NH1-CZ-NH2	-5.12	112.64	119.30
1	Q	12	HIS	CE1-NE2-CD2	-5.12	103.88	109.00
1	E	39	MET	CA-C-N	5.12	127.45	120.54
1	E	39	MET	C-N-CA	5.12	127.45	120.54
1	S	81	ASP	CA-C-N	5.12	127.10	120.44
1	S	81	ASP	C-N-CA	5.12	127.10	120.44
1	E	100	ARG	N-CA-C	-5.12	103.93	110.53
1	N	118	MET	N-CA-C	5.12	116.94	111.36
1	P	214	MET	N-CA-C	5.12	116.86	111.28
1	D	53	ASN	N-CA-CB	5.12	117.64	110.12
1	F	102	SER	N-CA-C	5.12	117.76	111.82
1	O	221	VAL	CA-CB-CG1	5.12	119.10	110.40
1	P	87	HIS	O-C-N	-5.12	117.23	123.27
1	Q	73	ILE	CA-C-O	5.12	126.27	120.95
1	K	53	ASN	CA-C-N	5.12	127.09	120.44
1	K	53	ASN	C-N-CA	5.12	127.09	120.44
1	N	206	GLY	CA-C-N	5.12	126.13	120.45
1	N	206	GLY	C-N-CA	5.12	126.13	120.45
1	L	175	GLU	N-CA-C	5.11	118.15	109.76
1	L	107	THR	CB-CA-C	-5.11	102.21	110.79
1	N	149	SER	O-C-N	-5.11	116.83	122.86
1	Q	28	GLU	N-CA-C	5.11	116.54	111.07
1	G	73	ILE	O-C-N	5.11	126.83	121.87
1	J	29	GLU	CB-CG-CD	5.11	121.29	112.60
1	K	143	ARG	NH1-CZ-NH2	-5.11	112.66	119.30
1	O	62	HIS	CA-C-O	5.11	126.70	120.57
1	K	186	THR	O-C-N	-5.11	116.72	122.03
1	N	73	ILE	O-C-N	-5.11	116.92	121.87
1	F	155	GLN	O-C-N	-5.11	117.19	122.96
1	G	115	ILE	CA-C-O	5.11	126.26	120.95
1	M	120	HIS	ND1-CG-CD2	-5.11	101.00	106.10
1	B	161	PHE	N-CA-C	5.10	117.23	111.11
1	J	163	ASP	N-CA-C	5.10	118.66	112.23
1	K	84	HIS	CB-CG-ND1	5.10	130.35	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	103	ASP	CA-CB-CG	-5.10	107.50	112.60
1	D	3	VAL	CA-C-O	5.10	126.15	120.59
1	R	142	VAL	CA-CB-CG1	5.10	119.07	110.40
1	F	157	PRO	N-CA-C	5.10	120.23	113.40
1	I	77	ALA	CA-C-N	5.10	127.12	120.28
1	I	77	ALA	C-N-CA	5.10	127.12	120.28
1	M	121	ASN	O-C-N	-5.10	115.70	121.36
1	H	138	LEU	CA-C-N	5.10	127.11	120.28
1	H	138	LEU	C-N-CA	5.10	127.11	120.28
1	O	120	HIS	N-CA-C	5.10	121.66	110.80
1	S	63	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	C	180	GLU	N-CA-C	-5.10	105.72	111.28
1	J	145	TYR	CB-CG-CD2	5.10	128.44	120.80
1	K	82	ARG	CA-C-O	5.10	126.17	120.82
1	E	25	LYS	CA-C-O	5.10	125.95	120.55
1	H	37	ILE	O-C-N	-5.10	115.29	121.10
1	K	2	ILE	CA-C-N	5.09	129.42	122.90
1	K	2	ILE	C-N-CA	5.09	129.42	122.90
1	L	138	LEU	N-CA-C	5.09	116.83	111.28
1	D	87	HIS	CA-CB-CG	5.09	118.89	113.80
1	F	117	TRP	N-CA-C	5.09	116.83	111.28
1	B	32	PHE	N-CA-C	-5.09	104.33	110.44
1	C	139	ASN	N-CA-C	5.09	116.83	111.28
1	I	120	HIS	N-CA-C	5.09	116.89	110.33
1	G	26	VAL	N-CA-C	5.08	115.30	110.42
1	Q	99	PRO	CA-C-O	-5.08	115.54	121.34
1	P	78	ALA	O-C-N	5.08	127.51	122.12
1	B	151	LEU	CA-C-O	5.08	125.81	119.97
1	M	46	GLY	O-C-N	-5.08	116.39	122.33
1	R	143	ARG	CA-C-O	5.08	125.94	120.55
1	R	156	GLY	O-C-N	-5.08	116.69	121.77
1	N	209	ALA	CA-C-N	5.08	130.21	120.97
1	N	209	ALA	C-N-CA	5.08	130.21	120.97
1	D	172	LEU	CA-C-O	-5.08	115.17	120.55
1	E	76	GLU	N-CA-C	5.08	116.81	111.28
1	F	99	PRO	O-C-N	-5.08	116.72	123.01
1	F	84	HIS	ND1-CE1-NE2	5.08	113.47	108.40
1	F	124	ILE	CB-CA-C	5.08	117.02	111.18
1	N	33	SER	CA-C-O	-5.07	115.17	120.70
1	O	68	MET	CA-C-N	5.07	127.08	120.28
1	O	68	MET	C-N-CA	5.07	127.08	120.28
1	R	29	GLU	N-CA-C	5.07	116.62	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	62	HIS	CB-CG-ND1	5.07	130.31	122.70
1	R	120	HIS	CB-CG-ND1	5.07	130.31	122.70
1	B	172	LEU	O-C-N	-5.07	116.75	122.12
1	O	121	ASN	CA-C-O	-5.07	114.93	119.59
1	M	183	ASN	O-C-N	-5.07	116.75	122.12
1	G	56	LEU	CA-C-O	5.07	125.79	120.42
1	O	146	SER	CA-C-O	-5.07	114.99	119.75
1	D	110	THR	CA-CB-OG1	5.07	117.20	109.60
1	G	119	THR	CA-C-O	-5.07	113.67	119.60
1	H	84	HIS	CG-CD2-NE2	5.07	112.27	107.20
1	K	102	SER	N-CA-C	5.07	117.69	111.82
1	E	29	GLU	N-CA-C	5.07	116.88	111.36
1	F	192	GLN	N-CA-CB	-5.07	102.67	110.12
1	D	111	LEU	CA-C-N	5.06	127.07	120.28
1	D	111	LEU	C-N-CA	5.06	127.07	120.28
1	H	113	GLU	CA-C-N	5.06	127.48	120.29
1	H	113	GLU	C-N-CA	5.06	127.48	120.29
1	R	28	GLU	CA-C-N	5.06	127.33	120.44
1	R	28	GLU	C-N-CA	5.06	127.33	120.44
1	H	2	ILE	CB-CA-C	-5.06	103.58	110.42
1	J	155	GLN	O-C-N	-5.06	117.45	123.22
1	K	84	HIS	CG-CD2-NE2	5.06	112.26	107.20
1	N	168	PHE	CB-CG-CD1	5.06	129.30	120.70
1	F	210	THR	CA-C-O	-5.06	116.00	121.87
1	H	133	TRP	CA-C-O	5.06	125.91	120.55
1	F	3	VAL	O-C-N	-5.06	116.77	122.94
1	F	57	ASN	CB-CG-ND2	5.06	123.99	116.40
1	I	132	ARG	NH1-CZ-NH2	-5.06	112.72	119.30
1	E	160	PRO	CA-C-O	-5.06	115.82	121.23
1	H	1	PRO	N-CA-CB	5.06	108.56	103.00
1	N	3	VAL	N-CA-CB	5.05	116.76	111.00
1	N	162	ARG	O-C-N	5.05	127.48	122.12
1	P	25	LYS	N-CA-CB	5.05	117.64	110.16
1	R	86	VAL	O-C-N	-5.05	116.25	122.57
1	R	24	VAL	CA-C-O	-5.05	115.82	121.17
1	F	203	LYS	CG-CD-CE	5.05	122.92	111.30
1	I	195	ASN	CA-CB-CG	5.05	117.65	112.60
1	K	219	GLN	N-CA-CB	5.05	118.10	110.28
1	N	26	VAL	N-CA-C	5.05	115.66	110.36
1	Q	189	LEU	N-CA-CB	5.05	117.63	110.16
1	R	148	THR	O-C-N	-5.05	117.11	123.27
1	E	209	ALA	N-CA-C	5.05	117.55	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	157	PRO	CA-C-O	-5.04	112.42	119.74
1	R	73	ILE	CA-C-N	5.04	127.04	120.28
1	R	73	ILE	C-N-CA	5.04	127.04	120.28
1	S	102	SER	CA-C-O	5.04	125.77	119.97
1	K	80	TRP	N-CA-C	5.04	116.78	111.28
1	F	58	THR	CA-C-N	5.04	127.34	120.63
1	F	58	THR	C-N-CA	5.04	127.34	120.63
1	F	89	GLY	CA-C-N	5.04	124.94	119.85
1	F	89	GLY	C-N-CA	5.04	124.94	119.85
1	K	173	ARG	NE-CZ-NH1	5.04	126.54	121.50
1	N	165	VAL	O-C-N	5.04	127.02	121.83
1	Q	98	GLU	CB-CA-C	5.04	116.64	109.38
1	S	113	GLU	N-CA-C	5.04	116.78	111.28
1	C	59	VAL	CA-C-O	5.04	127.11	121.11
1	D	56	LEU	N-CA-C	5.04	116.59	111.14
1	L	21	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	R	92	ALA	CA-C-N	5.04	126.14	119.84
1	R	92	ALA	C-N-CA	5.04	126.14	119.84
1	F	64	ALA	CA-C-N	5.04	127.29	120.44
1	F	64	ALA	C-N-CA	5.04	127.29	120.44
1	N	168	PHE	N-CA-CB	5.04	117.37	110.07
1	B	77	ALA	O-C-N	-5.03	116.88	122.07
1	L	82	ARG	N-CA-C	5.03	116.46	111.07
1	M	92	ALA	O-C-N	-5.03	115.79	121.43
1	R	53	ASN	CA-C-N	5.03	126.98	120.44
1	R	53	ASN	C-N-CA	5.03	126.98	120.44
1	C	155	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	G	50	GLN	CA-C-N	5.03	127.44	120.29
1	G	50	GLN	C-N-CA	5.03	127.44	120.29
1	R	162	ARG	NE-CZ-NH2	-5.03	114.67	119.20
1	B	98	GLU	N-CA-C	5.03	116.89	109.50
1	S	78	ALA	N-CA-C	5.03	116.76	111.28
1	D	100	ARG	O-C-N	-5.03	116.46	122.65
1	E	211	LEU	O-C-N	-5.03	116.79	122.12
1	P	185	MET	CA-C-O	-5.03	115.09	120.42
1	I	184	TRP	CZ3-CH2-CZ2	-5.03	114.96	121.50
1	K	170	LYS	N-CA-C	5.03	116.57	111.14
1	N	50	GLN	CA-C-O	5.02	125.88	120.55
1	O	205	LEU	N-CA-C	-5.02	105.99	111.82
1	O	211	LEU	N-CA-C	5.02	116.75	111.28
1	Q	47	ALA	CA-C-O	-5.02	116.09	121.56
1	C	155	GLN	CA-C-N	5.02	129.76	121.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	155	GLN	C-N-CA	5.02	129.76	121.87
1	G	5	ASN	CA-C-N	5.02	127.90	120.82
1	G	5	ASN	C-N-CA	5.02	127.90	120.82
1	H	64	ALA	CA-C-O	5.02	125.87	120.55
1	P	132	ARG	N-CA-C	5.02	116.75	111.28
1	S	95	GLN	CA-C-N	5.02	127.98	120.90
1	S	95	GLN	C-N-CA	5.02	127.98	120.90
1	D	24	VAL	N-CA-C	5.02	115.74	110.62
1	G	173	ARG	N-CA-C	5.02	117.48	111.71
1	I	209	ALA	O-C-N	-5.02	117.03	123.06
1	K	184	TRP	CA-CB-CG	5.02	123.14	113.60
1	P	218	CYS	O-C-N	-5.02	115.94	122.37
1	R	48	THR	CA-C-O	-5.02	115.26	120.88
1	H	15	ILE	N-CA-C	5.02	115.71	108.93
1	B	201	ILE	N-CA-CB	-5.02	104.68	110.55
1	L	51	ASP	CA-CB-CG	-5.02	107.58	112.60
1	Q	181	VAL	CA-C-N	5.02	127.94	120.31
1	Q	181	VAL	C-N-CA	5.02	127.94	120.31
1	R	43	LEU	O-C-N	-5.02	115.54	122.46
1	I	4	GLN	N-CA-C	5.02	116.94	108.96
1	N	111	LEU	CA-C-O	5.02	125.87	120.55
1	P	96	MET	N-CA-C	5.01	118.12	110.20
1	R	10	MET	O-C-N	-5.01	117.36	123.13
1	C	165	VAL	O-C-N	-5.01	116.13	121.80
1	F	85	PRO	CA-C-N	5.01	127.30	120.63
1	F	85	PRO	C-N-CA	5.01	127.30	120.63
1	I	219	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	F	24	VAL	CA-C-N	5.01	127.00	120.28
1	F	24	VAL	C-N-CA	5.01	127.00	120.28
1	G	189	LEU	N-CA-C	5.01	116.82	111.36
1	J	57	ASN	CA-CB-CG	-5.01	107.59	112.60
1	N	193	ASN	CA-C-N	5.01	130.09	120.97
1	N	193	ASN	C-N-CA	5.01	130.09	120.97
1	S	196	PRO	O-C-N	-5.01	116.77	122.18
1	C	209	ALA	O-C-N	-5.01	117.50	123.11
1	G	83	LEU	N-CA-CB	-5.01	102.52	110.28
1	I	92	ALA	N-CA-CB	-5.00	103.94	109.74
1	B	57	ASN	OD1-CG-ND2	5.00	127.60	122.60
1	B	193	ASN	CA-C-N	5.00	128.80	120.94
1	B	193	ASN	C-N-CA	5.00	128.80	120.94
1	K	146	SER	N-CA-C	5.00	116.19	109.83
1	L	126	VAL	N-CA-C	5.00	117.30	111.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	190	LEU	CB-CA-C	-5.00	102.81	110.81
1	N	176	GLN	OE1-CD-NE2	-5.00	117.60	122.60

There are no chirality outliers.

All (87) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	100	ARG	Sidechain
1	B	167	ARG	Sidechain
1	B	186	THR	Mainchain
1	C	130	TYR	Sidechain
1	C	132	ARG	Sidechain
1	C	162	ARG	Sidechain
1	C	164	TYR	Sidechain
1	C	168	PHE	Sidechain
1	C	169	TYR	Sidechain
1	C	82	ARG	Sidechain
1	D	100	ARG	Sidechain
1	D	120	HIS	Sidechain
1	D	130	TYR	Sidechain
1	D	145	TYR	Sidechain
1	D	154	ARG	Sidechain
1	D	162	ARG	Sidechain
1	D	84	HIS	Sidechain
1	E	100	ARG	Sidechain
1	E	169	TYR	Sidechain
1	E	173	ARG	Sidechain
1	E	18	ARG	Sidechain
1	E	84	HIS	Sidechain
1	F	100	ARG	Sidechain
1	F	154	ARG	Sidechain
1	F	173	ARG	Sidechain
1	F	82	ARG	Sidechain
1	F	97	ARG	Sidechain
1	H	100	ARG	Sidechain
1	H	132	ARG	Sidechain
1	H	143	ARG	Sidechain
1	H	145	TYR	Sidechain
1	H	154	ARG	Sidechain
1	H	18	ARG	Sidechain
1	H	84	HIS	Sidechain
1	I	130	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	I	143	ARG	Sidechain
1	I	154	ARG	Sidechain
1	I	169	TYR	Sidechain
1	I	173	ARG	Sidechain
1	I	41	SER	Mainchain
1	I	82	ARG	Sidechain
1	J	169	TYR	Sidechain
1	J	97	ARG	Sidechain
1	K	132	ARG	Sidechain
1	K	145	TYR	Sidechain
1	K	154	ARG	Sidechain
1	K	162	ARG	Sidechain
1	K	164	TYR	Sidechain
1	K	173	ARG	Sidechain
1	L	154	ARG	Sidechain
1	M	100	ARG	Sidechain
1	M	145	TYR	Sidechain
1	M	162	ARG	Sidechain
1	M	18	ARG	Sidechain
1	M	211	LEU	Mainchain
1	M	32	PHE	Sidechain
1	N	100	ARG	Sidechain
1	N	12	HIS	Sidechain
1	N	132	ARG	Sidechain
1	N	167	ARG	Sidechain
1	N	168	PHE	Sidechain
1	N	40	PHE	Sidechain
1	O	100	ARG	Sidechain
1	O	120	HIS	Sidechain
1	O	143	ARG	Sidechain
1	O	154	ARG	Sidechain
1	O	173	ARG	Sidechain
1	P	154	ARG	Sidechain
1	P	162	ARG	Sidechain
1	P	40	PHE	Sidechain
1	Q	161	PHE	Sidechain
1	Q	162	ARG	Sidechain
1	Q	164	TYR	Sidechain
1	Q	168	PHE	Sidechain
1	Q	173	ARG	Sidechain
1	Q	32	PHE	Sidechain
1	Q	82	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	Q	87	HIS	Sidechain
1	R	100	ARG	Sidechain
1	R	132	ARG	Sidechain
1	R	161	PHE	Sidechain
1	R	173	ARG	Sidechain
1	R	40	PHE	Sidechain
1	R	82	ARG	Sidechain
1	S	143	ARG	Sidechain
1	S	167	ARG	Sidechain
1	S	32	PHE	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	B	1726	0	1725	0	0
1	C	1726	0	1725	0	0
1	D	1726	0	1725	0	0
1	E	1726	0	1725	0	0
1	F	1726	0	1725	0	0
1	G	1726	0	1725	0	0
1	H	1726	0	1725	0	0
1	I	1726	0	1725	0	0
1	J	1726	0	1725	0	0
1	K	1726	0	1725	0	0
1	L	1726	0	1725	0	0
1	M	1726	0	1725	0	0
1	N	1726	0	1725	0	0
1	O	1726	0	1725	0	0
1	P	1726	0	1725	0	0
1	Q	1726	0	1725	0	0
1	R	1726	0	1725	0	0
1	S	1726	0	1725	0	0
All	All	31068	0	31050	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	219/221 (99%)	207 (94%)	10 (5%)	2 (1%)	14	51
1	C	219/221 (99%)	207 (94%)	11 (5%)	1 (0%)	24	63
1	D	219/221 (99%)	213 (97%)	4 (2%)	2 (1%)	14	51
1	E	219/221 (99%)	210 (96%)	9 (4%)	0	100	100
1	F	219/221 (99%)	209 (95%)	8 (4%)	2 (1%)	14	51
1	G	219/221 (99%)	209 (95%)	9 (4%)	1 (0%)	24	63
1	H	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
1	I	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
1	J	219/221 (99%)	210 (96%)	8 (4%)	1 (0%)	24	63
1	K	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
1	L	219/221 (99%)	210 (96%)	8 (4%)	1 (0%)	24	63
1	M	219/221 (99%)	207 (94%)	10 (5%)	2 (1%)	14	51
1	N	219/221 (99%)	207 (94%)	11 (5%)	1 (0%)	24	63
1	O	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
1	P	219/221 (99%)	206 (94%)	11 (5%)	2 (1%)	14	51
1	Q	219/221 (99%)	210 (96%)	8 (4%)	1 (0%)	24	63
1	R	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
1	S	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
All	All	3942/3978 (99%)	3783 (96%)	143 (4%)	16 (0%)	31	67

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	147	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	177	ALA
1	F	177	ALA
1	G	120	HIS
1	B	177	ALA
1	L	120	HIS
1	Q	177	ALA
1	J	88	ALA
1	F	120	HIS
1	M	15	ILE
1	M	90	PRO
1	C	207	PRO
1	B	125	PRO
1	P	91	ILE
1	D	147	PRO
1	P	147	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	B	188/188 (100%)	184 (98%)	4 (2%)	47	65
1	C	188/188 (100%)	177 (94%)	11 (6%)	18	39
1	D	188/188 (100%)	186 (99%)	2 (1%)	65	76
1	E	188/188 (100%)	184 (98%)	4 (2%)	47	65
1	F	188/188 (100%)	182 (97%)	6 (3%)	34	56
1	G	188/188 (100%)	185 (98%)	3 (2%)	55	70
1	H	188/188 (100%)	182 (97%)	6 (3%)	34	56
1	I	188/188 (100%)	182 (97%)	6 (3%)	34	56
1	J	188/188 (100%)	182 (97%)	6 (3%)	34	56
1	K	188/188 (100%)	185 (98%)	3 (2%)	55	70
1	L	188/188 (100%)	186 (99%)	2 (1%)	65	76
1	M	188/188 (100%)	185 (98%)	3 (2%)	55	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	188/188 (100%)	182 (97%)	6 (3%)	34	56
1	O	188/188 (100%)	186 (99%)	2 (1%)	65	76
1	P	188/188 (100%)	182 (97%)	6 (3%)	34	56
1	Q	188/188 (100%)	182 (97%)	6 (3%)	34	56
1	R	188/188 (100%)	180 (96%)	8 (4%)	26	47
1	S	188/188 (100%)	186 (99%)	2 (1%)	65	76
All	All	3384/3384 (100%)	3298 (98%)	86 (2%)	42	63

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	GLN
1	B	26	VAL
1	B	196	PRO
1	B	216	THR
1	K	19	THR
1	K	68	MET
1	K	172	LEU
1	L	67	GLN
1	L	186	THR
1	M	11	VAL
1	M	13	GLN
1	M	70	LYS
1	N	17	PRO
1	N	41	SER
1	N	90	PRO
1	N	104	ILE
1	N	181	VAL
1	N	196	PRO
1	O	7	GLN
1	O	187	GLU
1	P	13	GLN
1	P	37	ILE
1	P	67	GLN
1	P	86	VAL
1	P	124	ILE
1	P	216	THR
1	Q	7	GLN
1	Q	70	LYS
1	Q	108	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Q	110	THR
1	Q	121	ASN
1	Q	216	THR
1	R	1	PRO
1	R	18	ARG
1	R	34	PRO
1	R	50	GLN
1	R	95	GLN
1	R	148	THR
1	R	164	TYR
1	R	196	PRO
1	S	171	THR
1	S	176	GLN
1	C	1	PRO
1	C	2	ILE
1	C	4	GLN
1	C	21	ASN
1	C	27	VAL
1	C	54	THR
1	C	79	GLU
1	C	90	PRO
1	C	176	GLN
1	C	207	PRO
1	C	210	THR
1	D	13	GLN
1	D	136	LEU
1	E	34	PRO
1	E	85	PRO
1	E	96	MET
1	E	166	ASP
1	F	91	ILE
1	F	104	ILE
1	F	166	ASP
1	F	196	PRO
1	F	216	THR
1	F	221	VAL
1	G	1	PRO
1	G	49	PRO
1	G	166	ASP
1	H	11	VAL
1	H	34	PRO
1	H	54	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	176	GLN
1	H	186	THR
1	H	218	CYS
1	I	1	PRO
1	I	50	GLN
1	I	93	PRO
1	I	120	HIS
1	I	128	GLU
1	I	148	THR
1	J	34	PRO
1	J	36	VAL
1	J	79	GLU
1	J	110	THR
1	J	120	HIS
1	J	196	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

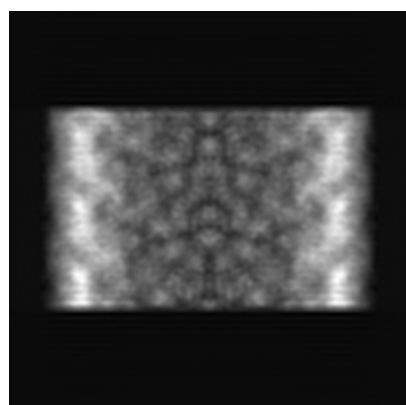
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8582. These allow visual inspection of the internal detail of the map and identification of artifacts.

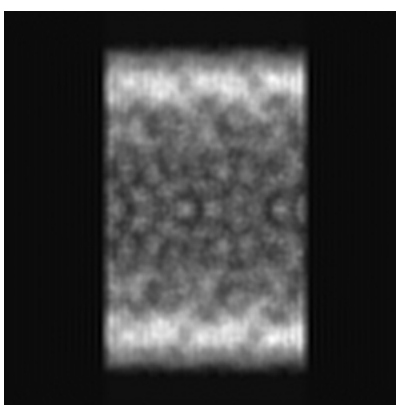
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

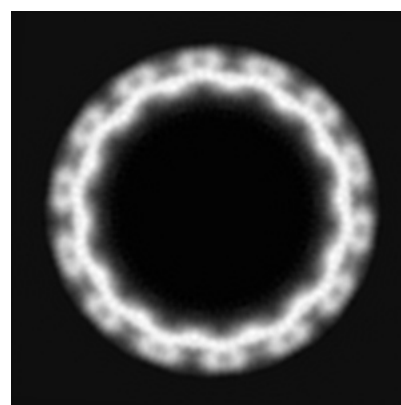
6.1.1 Primary map



X



Y

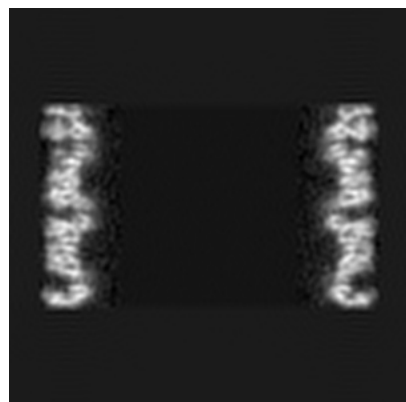


Z

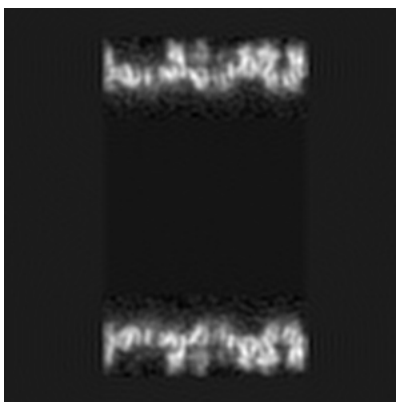
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

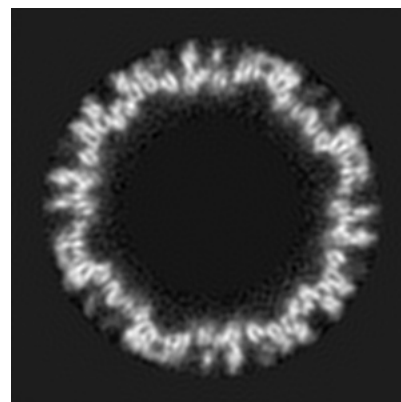
6.2.1 Primary map



X Index: 248



Y Index: 248

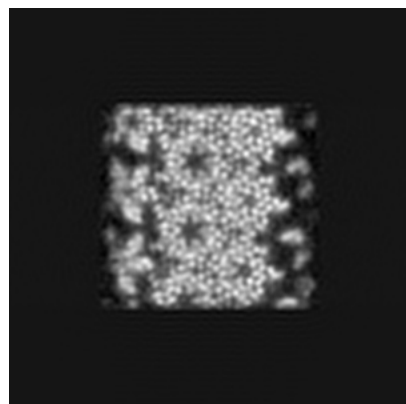


Z Index: 248

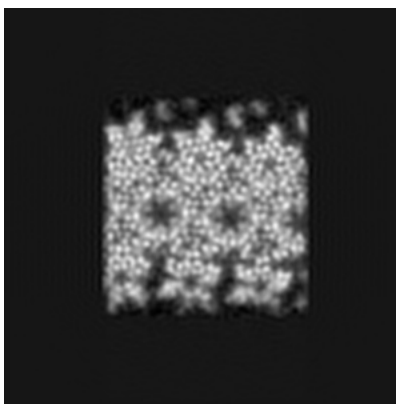
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

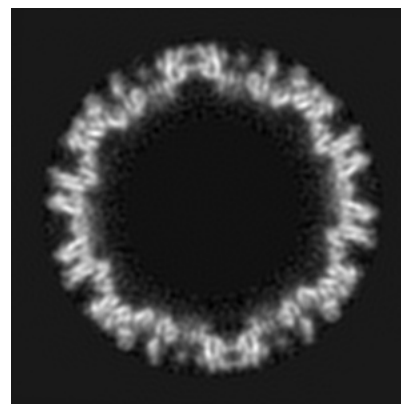
6.3.1 Primary map



X Index: 411



Y Index: 409

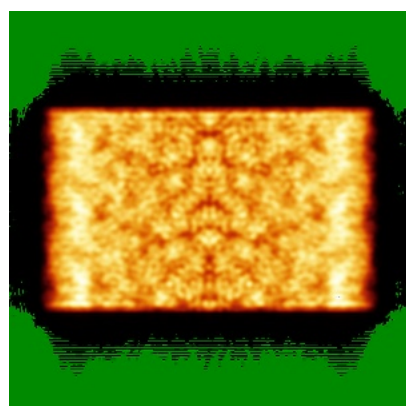


Z Index: 366

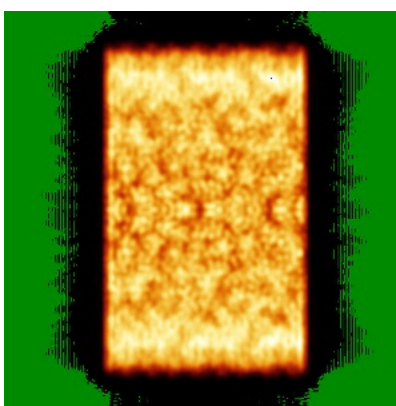
The images above show the largest variance slices of the map in three orthogonal directions.

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

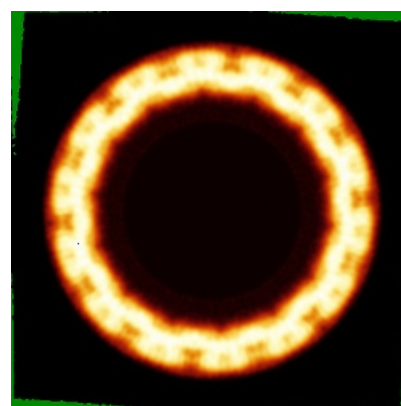
6.4.1 Primary map



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

This section was not generated.

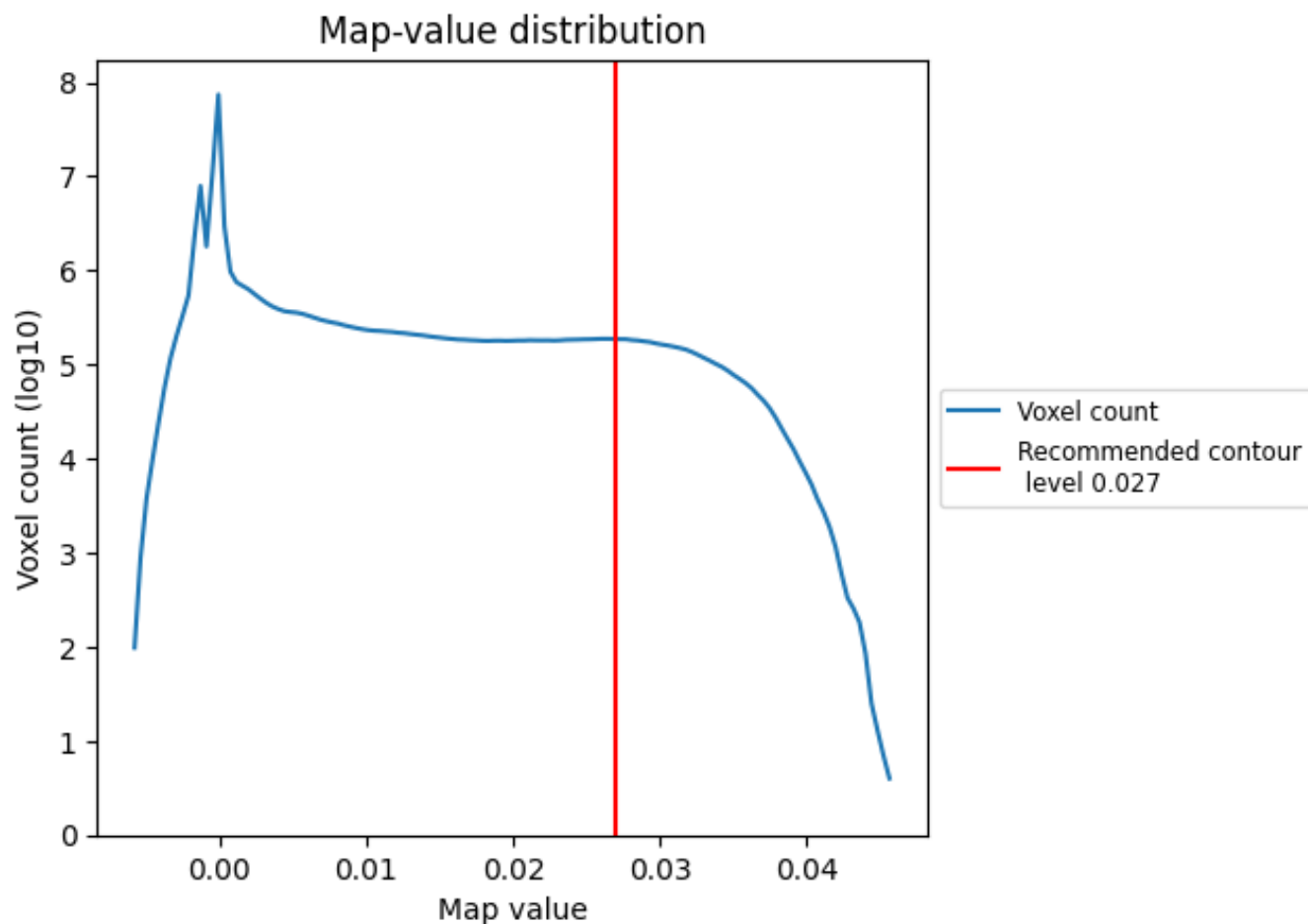
6.6 Mask visualisation

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

7 Map analysis [i](#)

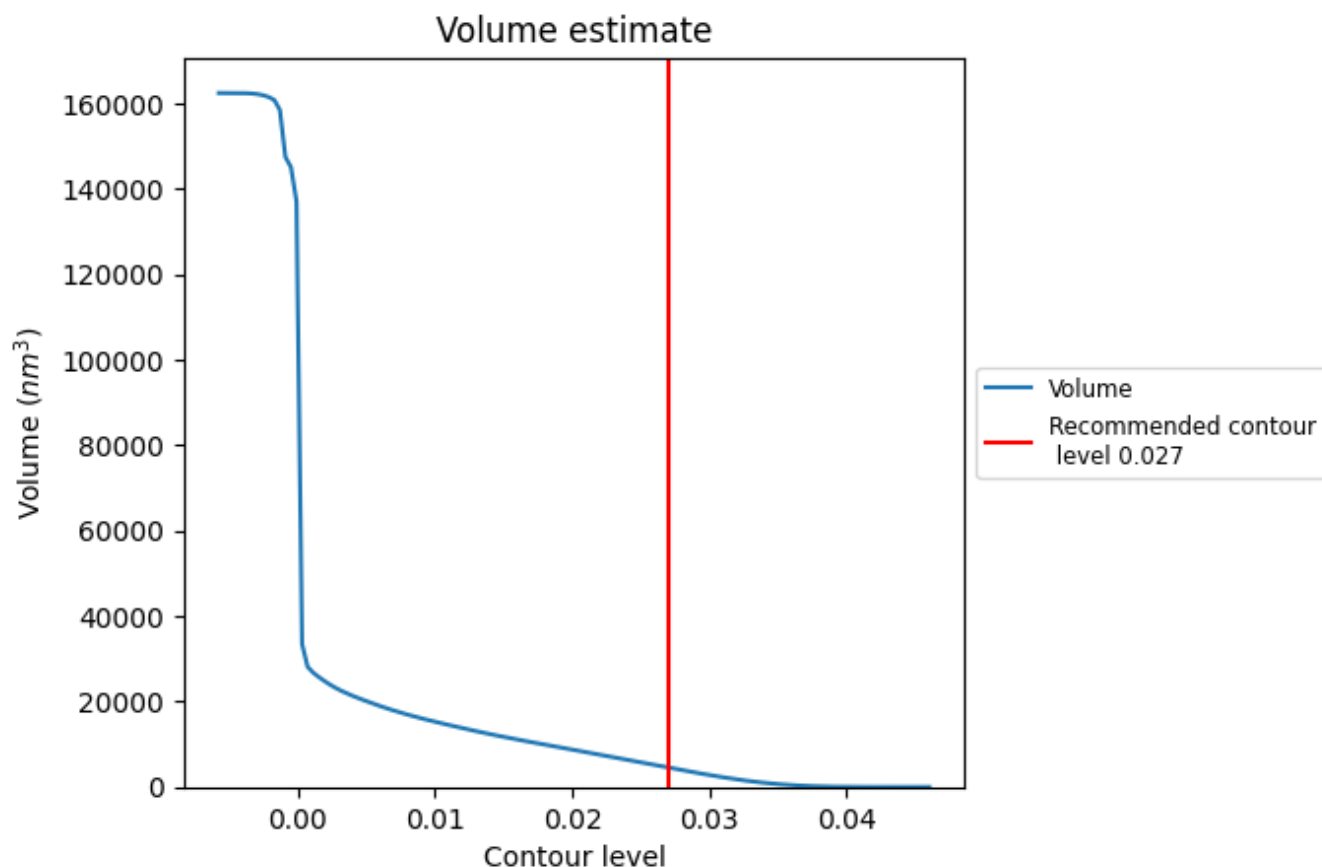
This section contains the results of statistical analysis of the map.

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.

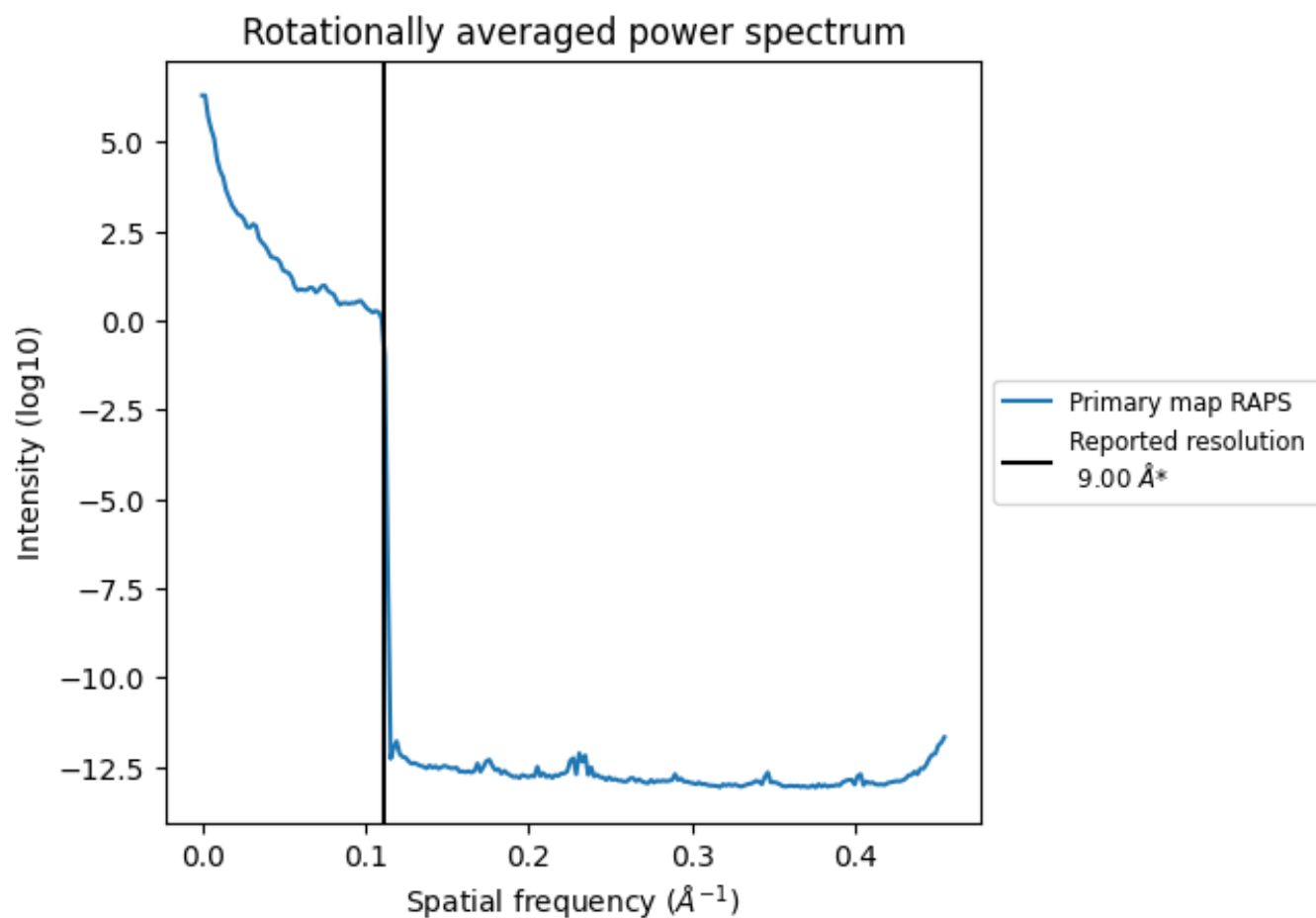
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4556 nm^3 ; this corresponds to an approximate mass of 4116 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 ⓘ

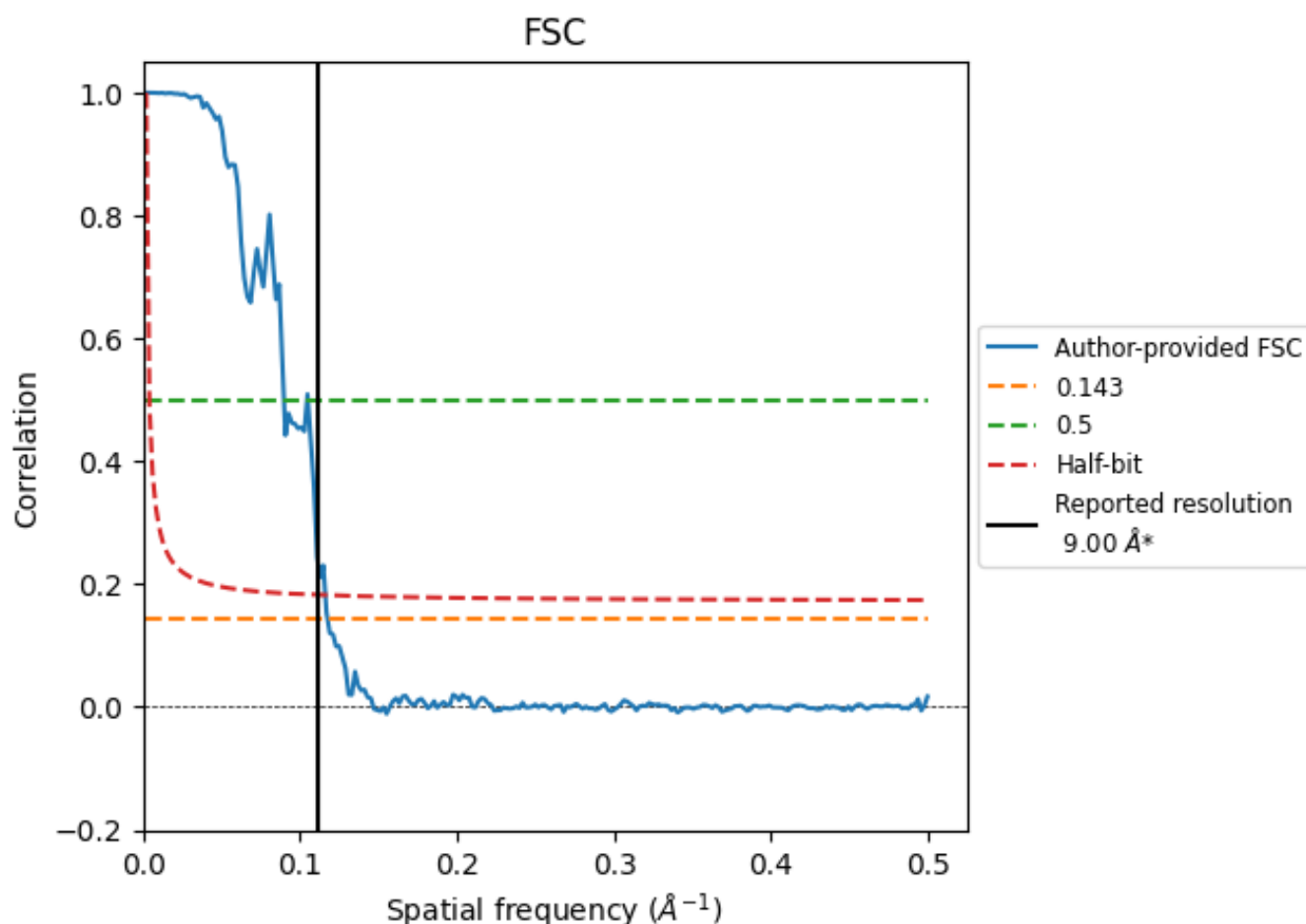


*Reported resolution corresponds to spatial frequency of 0.111 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.111 Å⁻¹

8.2 Resolution estimates [i](#)

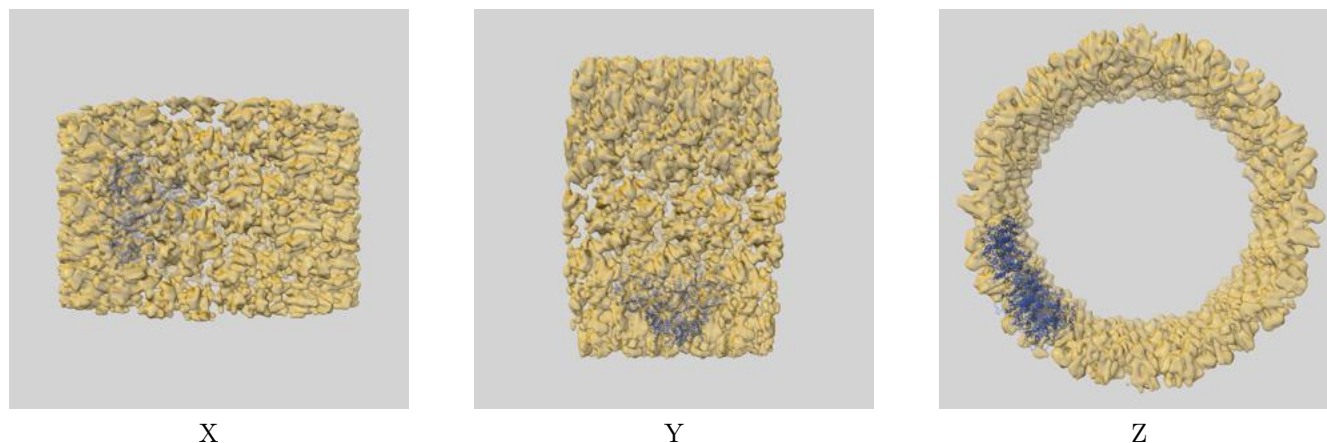
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.00	-	-
Author-provided FSC curve	8.50	11.14	8.61
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

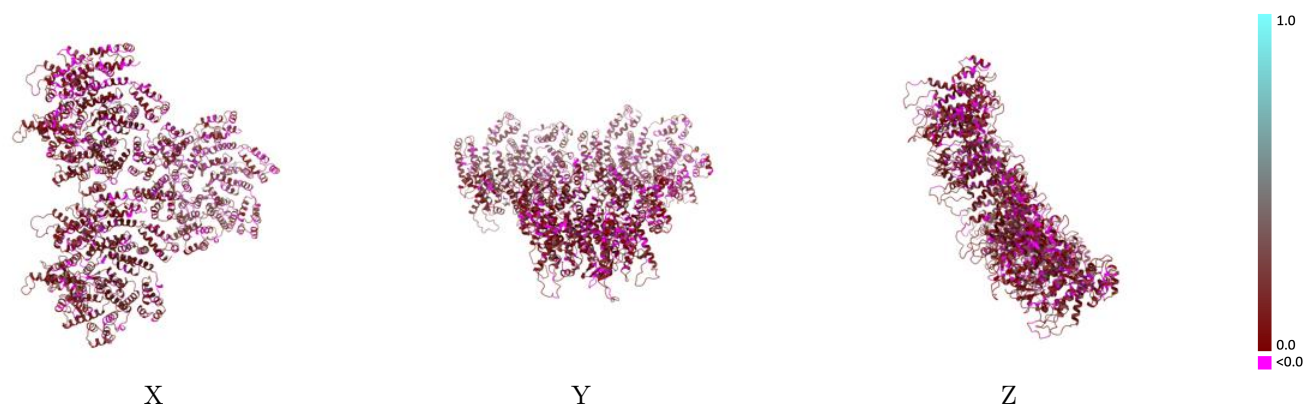
This section contains information regarding the fit between EMDB map EMD-8582 and PDB model 5UP4. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.027 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](#)

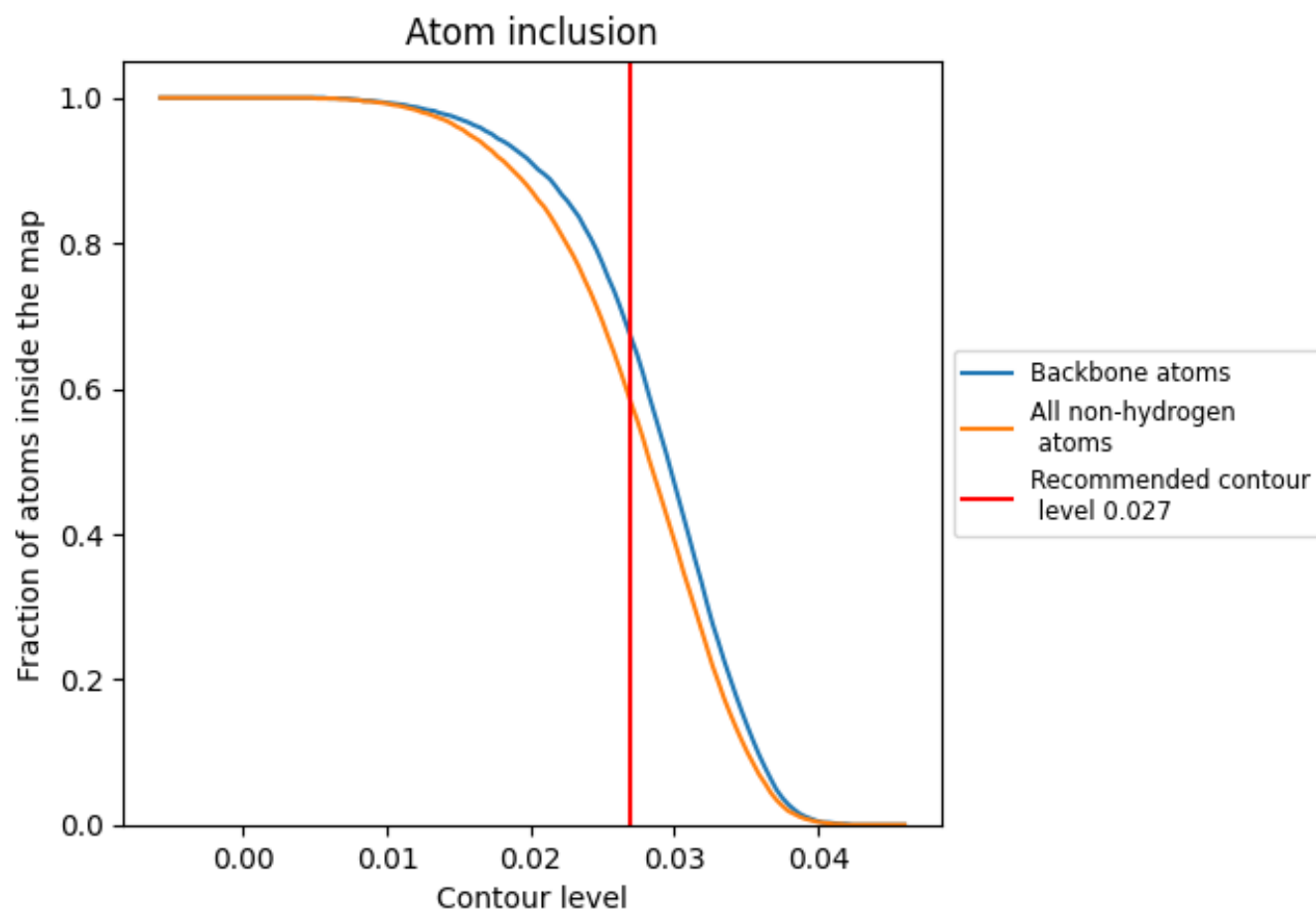


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 58% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5800	 0.0970
B	 0.5590	 0.0680
C	 0.5660	 0.0830
D	 0.5330	 0.0740
E	 0.5750	 0.0990
F	 0.5470	 0.0940
G	 0.6090	 0.1090
H	 0.5640	 0.0630
I	 0.5480	 0.0780
J	 0.5350	 0.0920
K	 0.5650	 0.0860
L	 0.5560	 0.1010
M	 0.6120	 0.1080
N	 0.6220	 0.1090
O	 0.5850	 0.0940
P	 0.5940	 0.1090
Q	 0.6120	 0.1230
R	 0.6020	 0.1260
S	 0.6540	 0.1340

