



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:37 PM UTC

PDB ID : 2YEW / pdb_00002yew
EMDB ID : EMD-1886
Title : Modeling Barmah Forest virus structural proteins
Authors : Kostyuchenko, V.A.; Jakana, J.; Liu, X.; Haddow, A.D.; Aung, M.; Weaver, S.C.; Chiu, W.; Lok, S.M.
Deposited on : 2011-03-31
Resolution : 5.00 Å (reported)
Based on initial models : 2XFB, 1SVP, 2ALA

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:

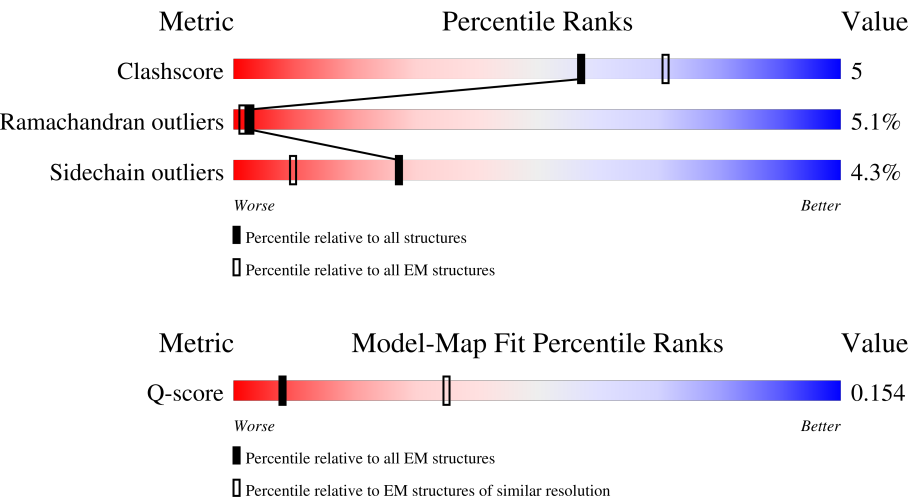
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 5.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	525 (5.50 - 6.50)

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

Mol	Chain	Length	Quality of chain
1	A	253	17% 28%33%7%32%
1	D	253	23% 28%36%.32%
1	G	253	22% 26%36%5%.32%
1	J	253	24% 23%38%6%.32%

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Mol	Chain	Length	Quality of chain
2	B	427	
2	E	427	
2	H	427	
2	K	427	
3	C	421	
3	F	421	
3	I	421	
3	L	421	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 31120 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 CAPSID PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	171	Total	C	N	O	S	0	0
			1316	827	234	244	11		
1	D	171	Total	C	N	O	S	0	0
			1316	827	234	244	11		
1	G	171	Total	C	N	O	S	0	0
			1316	827	234	244	11		
1	J	171	Total	C	N	O	S	0	0
			1316	827	234	244	11		

- Molecule 2 is a protein called E1 ENVELOPE GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	426	Total	C	N	O	S	0	1
			3225	2045	526	631	23		
2	E	426	Total	C	N	O	S	0	1
			3225	2045	526	631	23		
2	H	426	Total	C	N	O	S	0	1
			3225	2045	526	631	23		
2	K	426	Total	C	N	O	S	0	1
			3225	2045	526	631	23		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	HIS	deletion	UNP P89946
B	?	-	HIS	deletion	UNP P89946
B	?	-	HIS	deletion	UNP P89946
B	?	-	HIS	deletion	UNP P89946
B	?	-	HIS	deletion	UNP P89946
B	?	-	HIS	deletion	UNP P89946
B	?	-	HIS	deletion	UNP P89946
B	?	-	HIS	deletion	UNP P89946
B	?	-	HIS	deletion	UNP P89946

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	HIS	deletion	UNP P89946
B	?	-	HIS	deletion	UNP P89946
B	?	-	HIS	deletion	UNP P89946
B	?	-	HIS	deletion	UNP P89946
E	?	-	HIS	deletion	UNP P89946
E	?	-	HIS	deletion	UNP P89946
E	?	-	HIS	deletion	UNP P89946
E	?	-	HIS	deletion	UNP P89946
E	?	-	HIS	deletion	UNP P89946
E	?	-	HIS	deletion	UNP P89946
E	?	-	HIS	deletion	UNP P89946
E	?	-	HIS	deletion	UNP P89946
E	?	-	HIS	deletion	UNP P89946
E	?	-	HIS	deletion	UNP P89946
E	?	-	HIS	deletion	UNP P89946
E	?	-	HIS	deletion	UNP P89946
E	?	-	HIS	deletion	UNP P89946
E	?	-	HIS	deletion	UNP P89946
H	?	-	HIS	deletion	UNP P89946
H	?	-	HIS	deletion	UNP P89946
H	?	-	HIS	deletion	UNP P89946
H	?	-	HIS	deletion	UNP P89946
H	?	-	HIS	deletion	UNP P89946
H	?	-	HIS	deletion	UNP P89946
H	?	-	HIS	deletion	UNP P89946
H	?	-	HIS	deletion	UNP P89946
H	?	-	HIS	deletion	UNP P89946
H	?	-	HIS	deletion	UNP P89946
H	?	-	HIS	deletion	UNP P89946
H	?	-	HIS	deletion	UNP P89946
H	?	-	HIS	deletion	UNP P89946
H	?	-	HIS	deletion	UNP P89946
K	?	-	HIS	deletion	UNP P89946
K	?	-	HIS	deletion	UNP P89946
K	?	-	HIS	deletion	UNP P89946
K	?	-	HIS	deletion	UNP P89946
K	?	-	HIS	deletion	UNP P89946
K	?	-	HIS	deletion	UNP P89946
K	?	-	HIS	deletion	UNP P89946
K	?	-	HIS	deletion	UNP P89946
K	?	-	HIS	deletion	UNP P89946
K	?	-	HIS	deletion	UNP P89946
K	?	-	HIS	deletion	UNP P89946
K	?	-	HIS	deletion	UNP P89946
K	?	-	HIS	deletion	UNP P89946
K	?	-	HIS	deletion	UNP P89946

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Chain	Residue	Modelled	Actual	Comment	Reference
K	?	-	HIS	deletion	UNP P89946

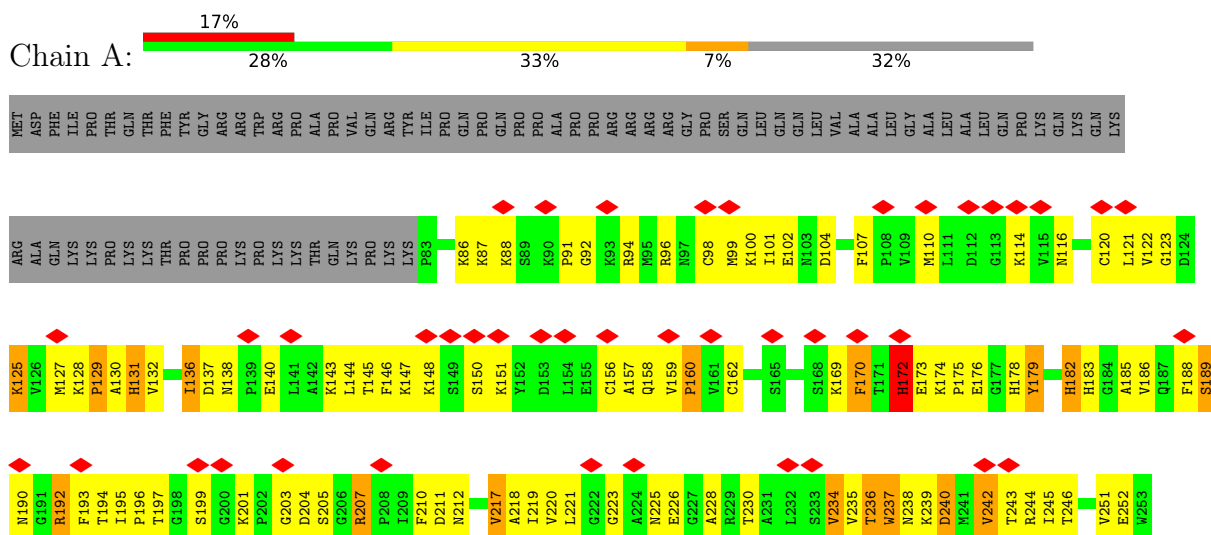
- Molecule 3 is a protein called E2 ENVELOPE GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	421	Total	C	N	O	S	0	0
			3239	2054	552	610	23		
3	F	421	Total	C	N	O	S	0	0
			3239	2054	552	610	23		
3	I	421	Total	C	N	O	S	0	0
			3239	2054	552	610	23		
3	L	421	Total	C	N	O	S	0	0
			3239	2054	552	610	23		

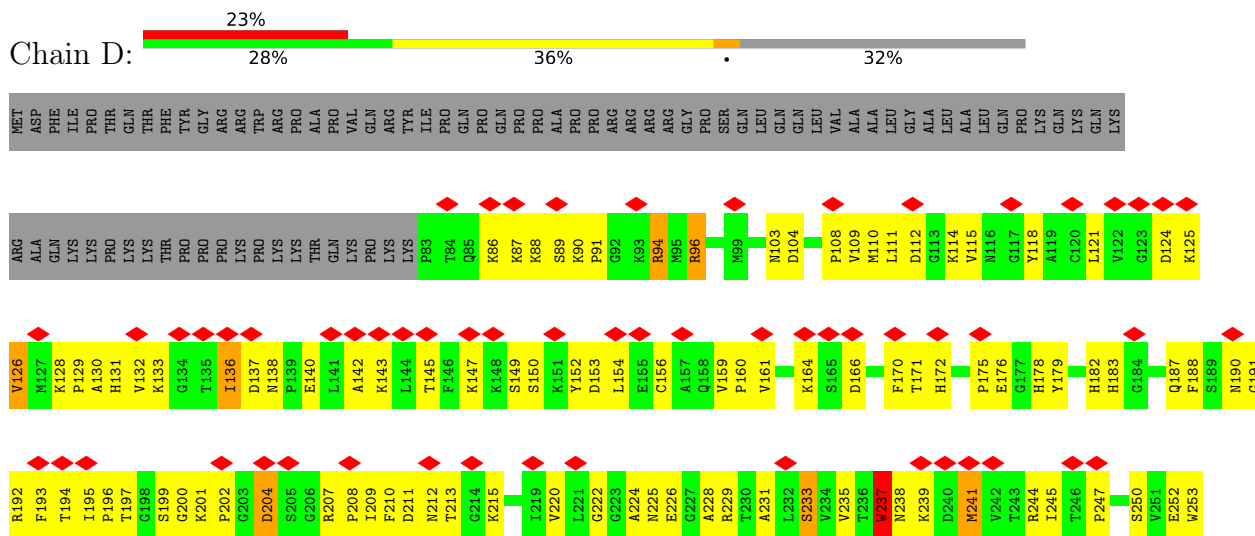
3 Residue-property plots

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.

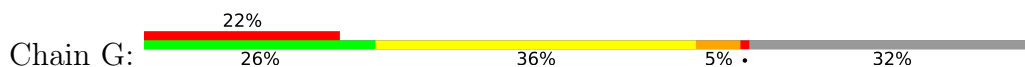
• Molecule 1: CAPSID PROTEIN

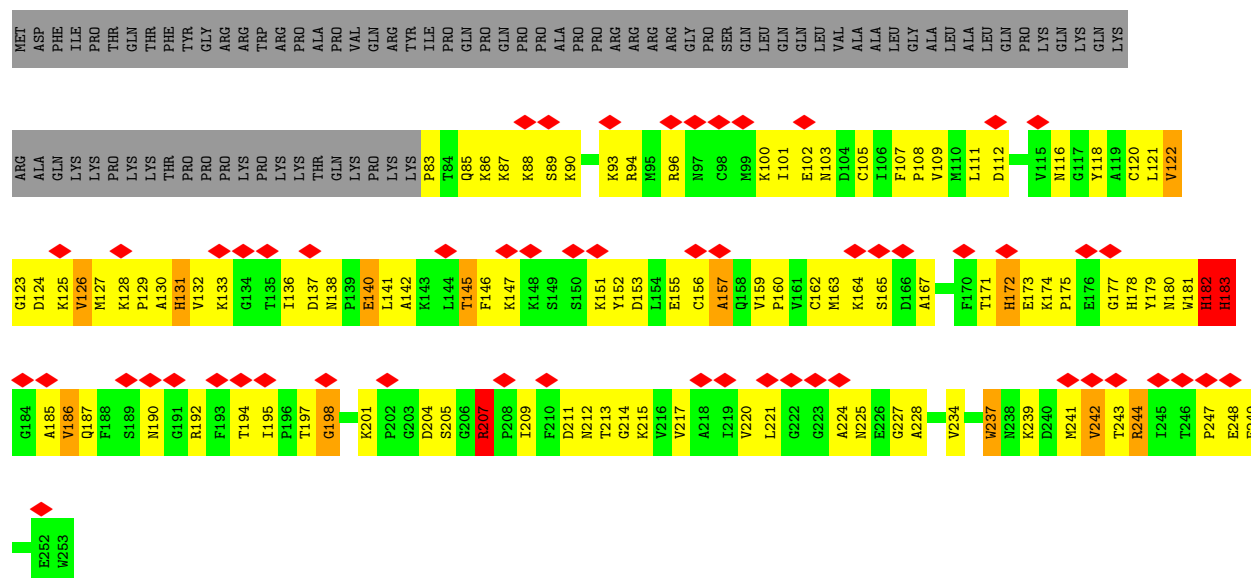


• Molecule 1: CAPSID PROTEIN

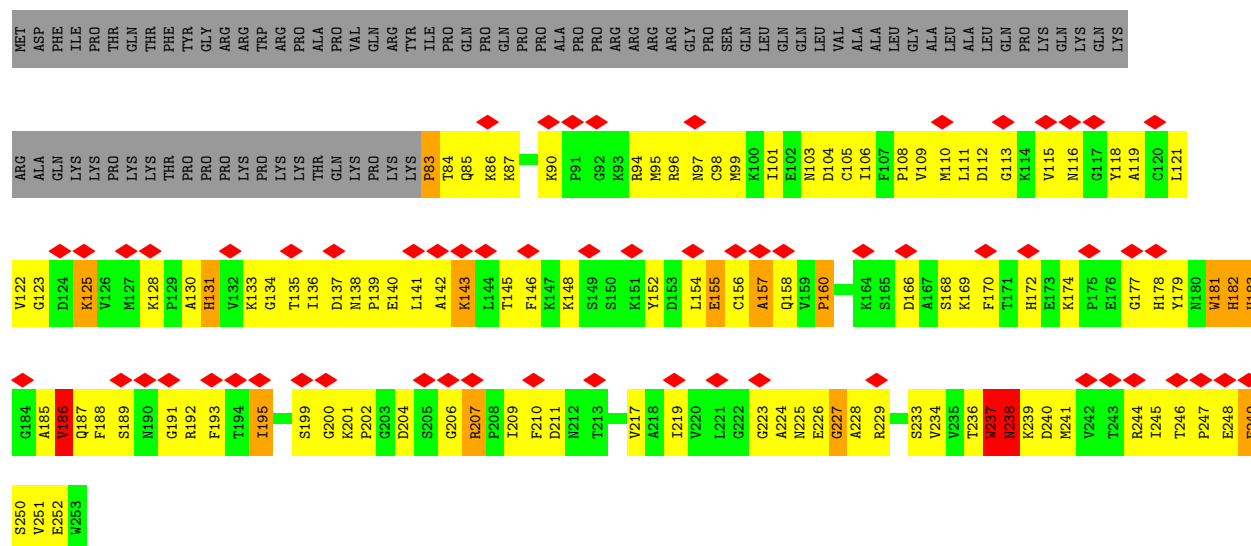
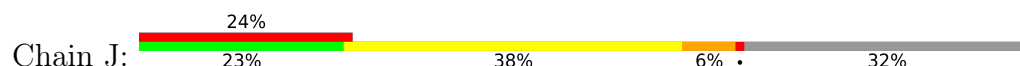


• Molecule 1: CAPSID PROTEIN

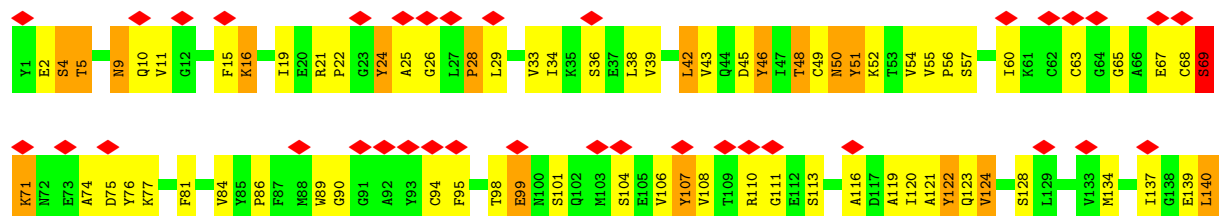


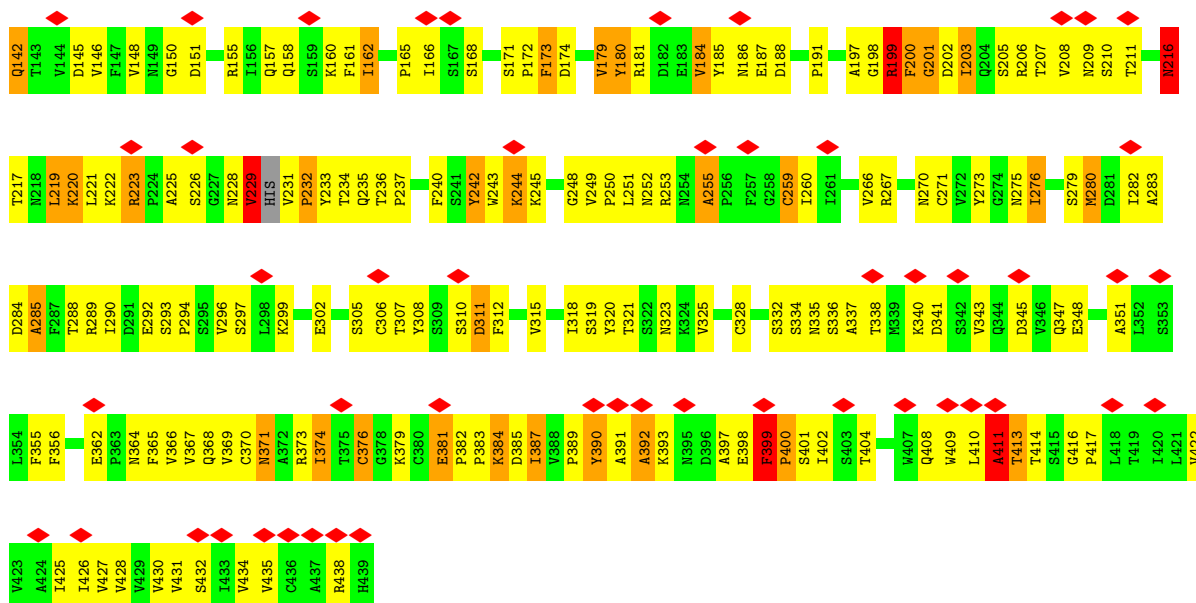


• Molecule 1: CAPSID PROTEIN

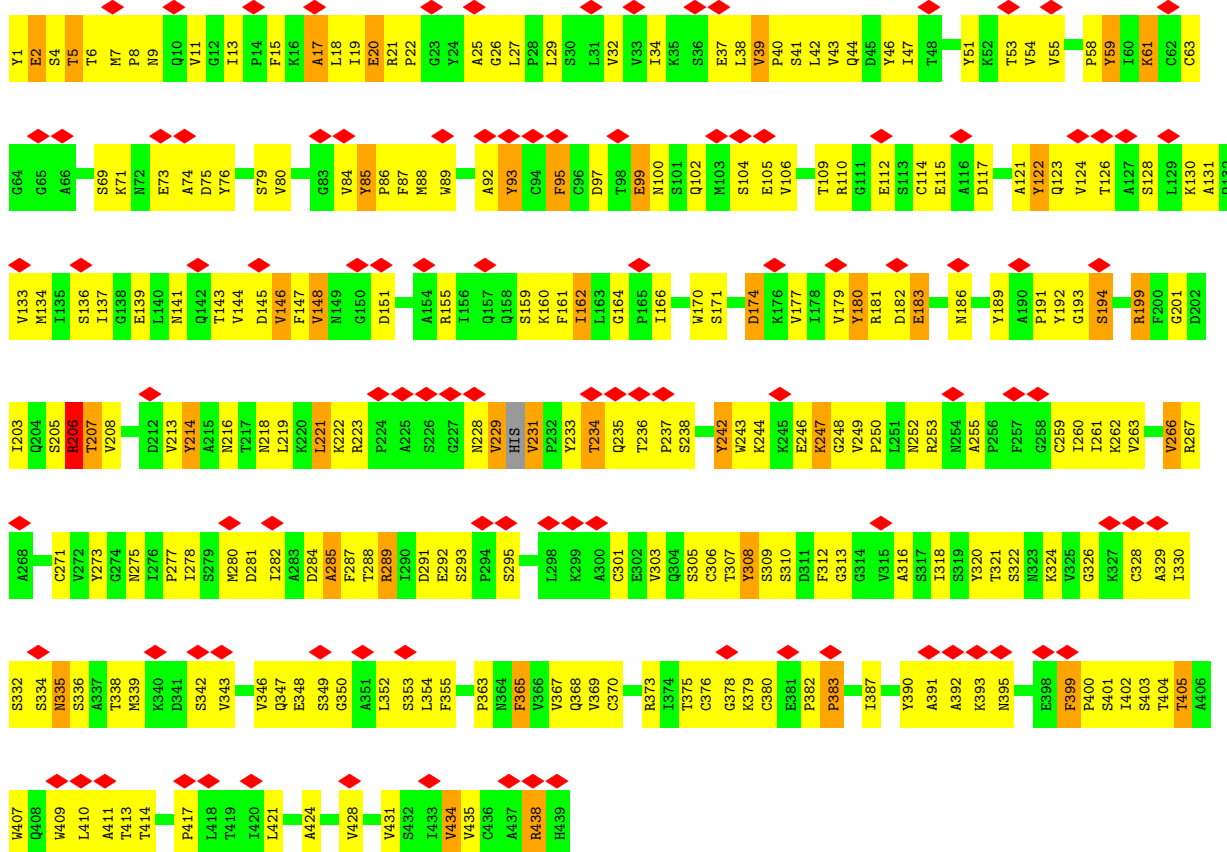


• Molecule 2: E1 ENVELOPE GLYCOPROTEIN

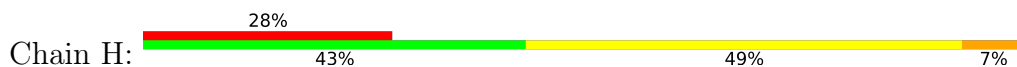


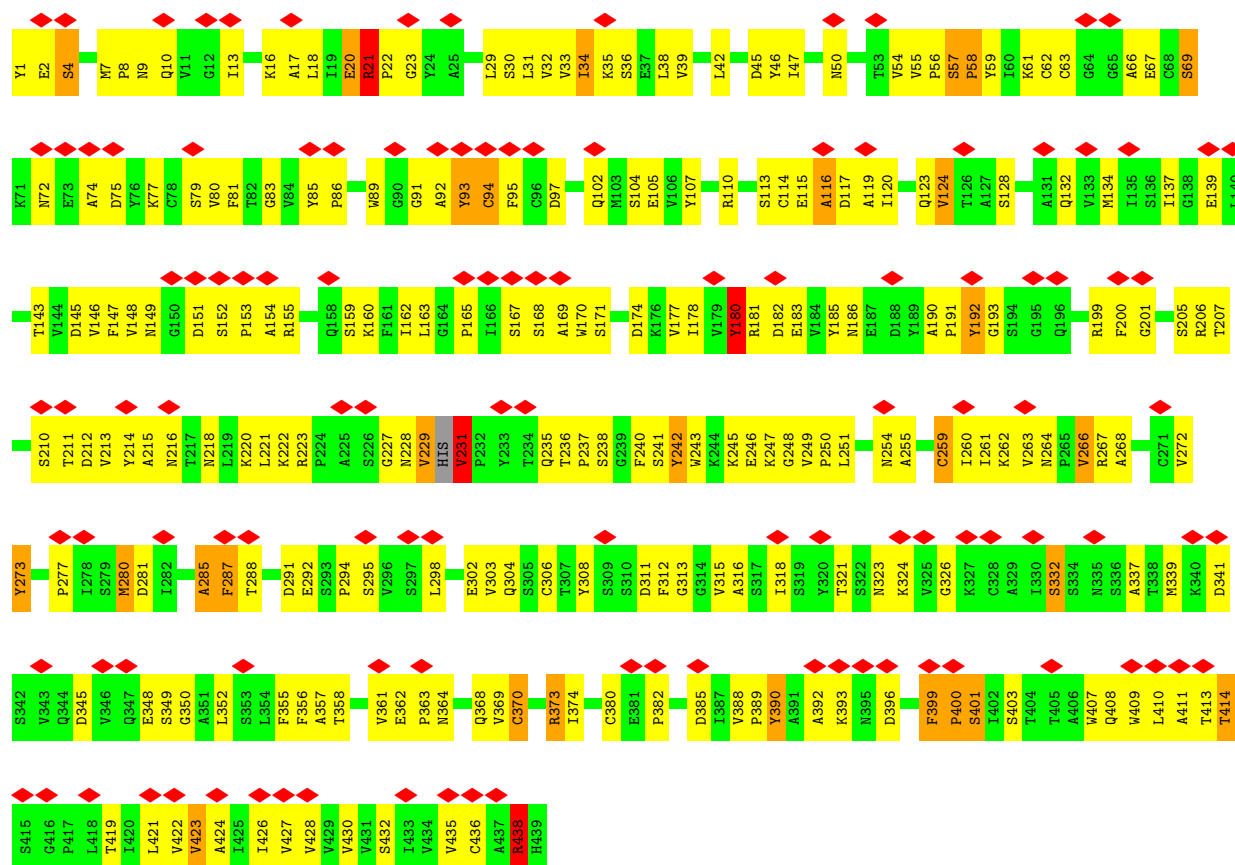


• Molecule 2: E1 ENVELOPE GLYCOPROTEIN

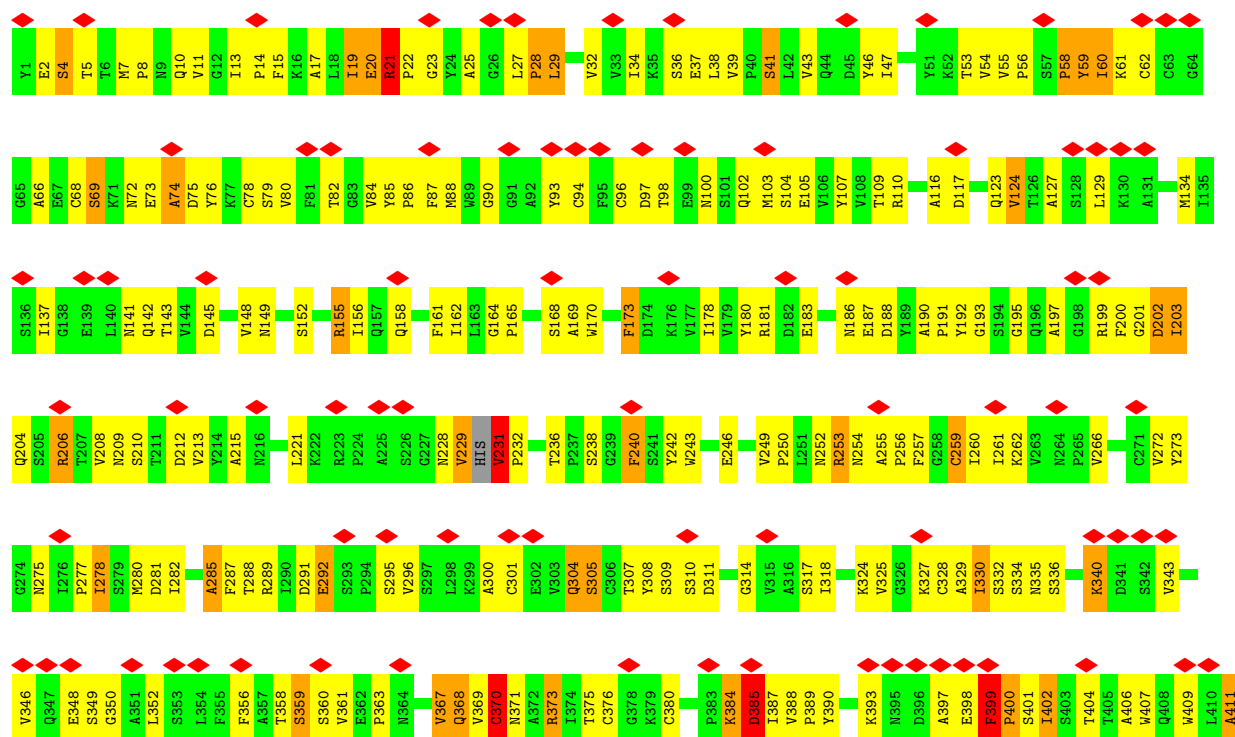
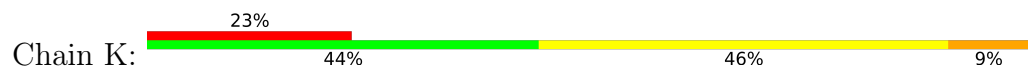


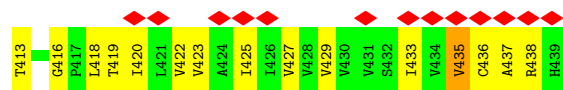
• Molecule 2: E1 ENVELOPE GLYCOPROTEIN



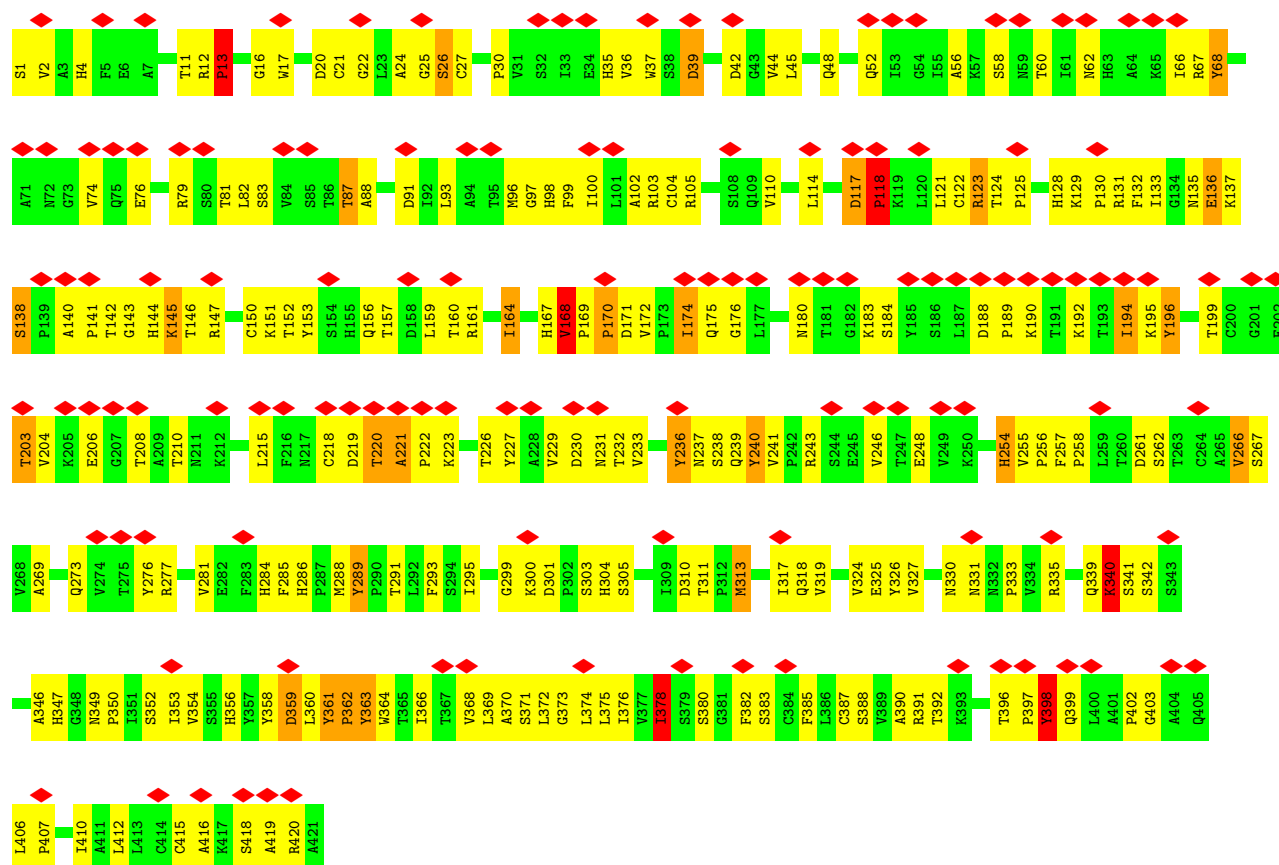


• Molecule 2: E1 ENVELOPE GLYCOPROTEIN

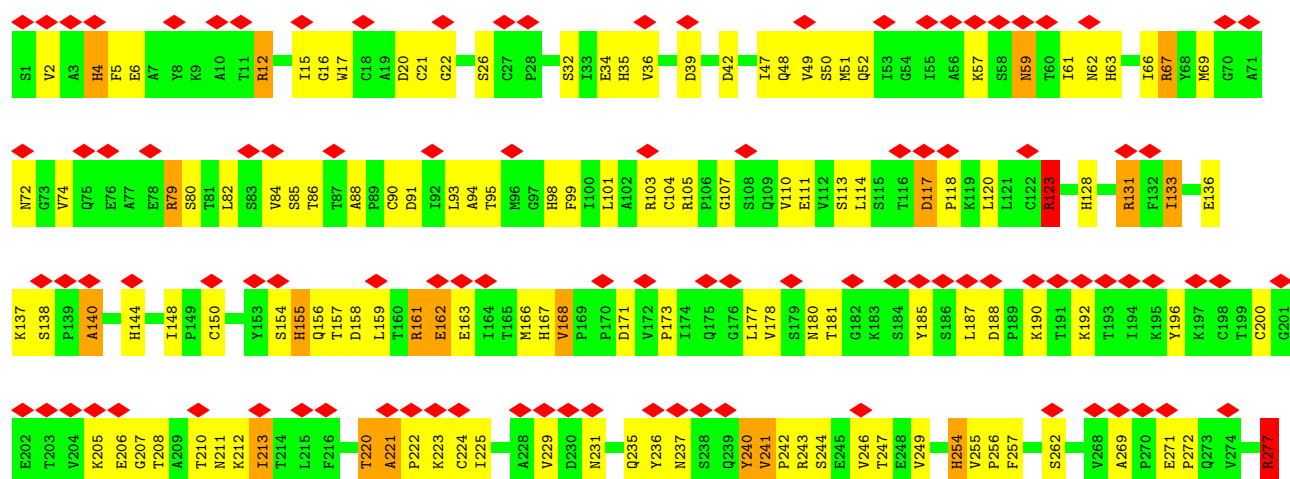




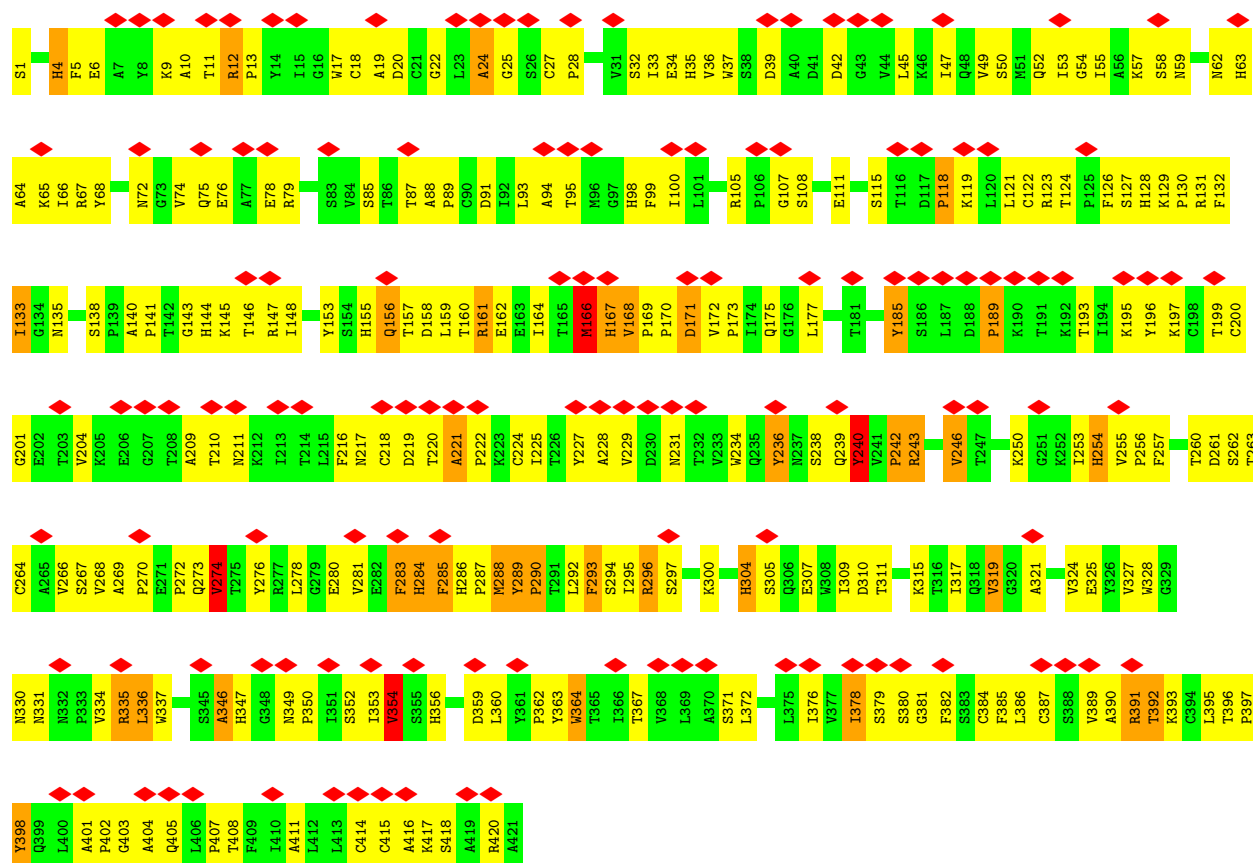
• Molecule 3: E2 ENVELOPE GLYCOPROTEIN



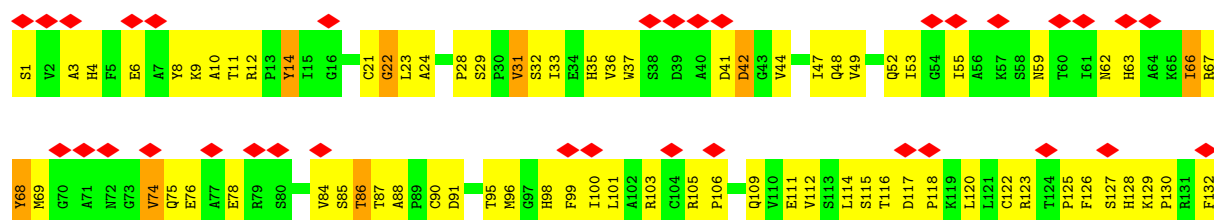
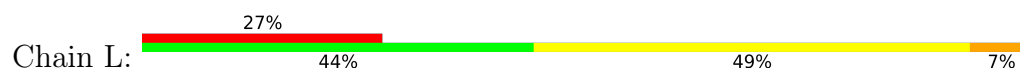
• Molecule 3: E2 ENVELOPE GLYCOPROTEIN

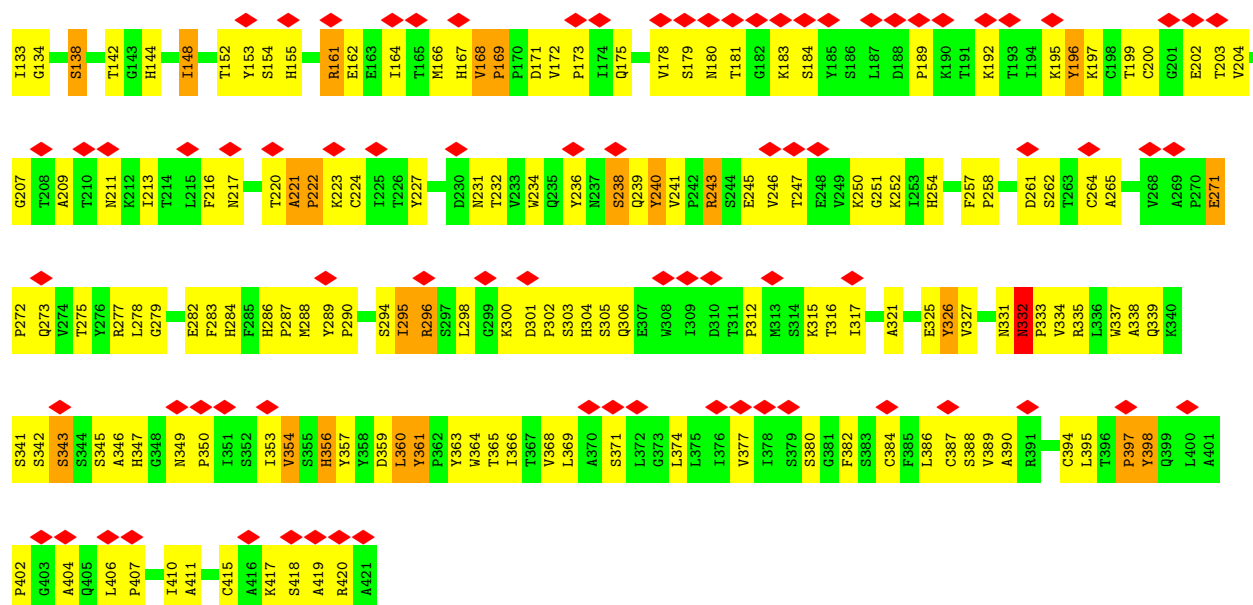


- Molecule 3: E2 ENVELOPE GLYCOPROTEIN



- Molecule 3: E2 ENVELOPE GLYCOPROTEIN





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	5169	Depositor
Resolution determination method	Not provided	
CTF correction method	INDIVIDUAL PARTICLES	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	50000	Depositor
Image detector	GENERIC GATAN	Depositor
Maximum map value	29.373	Depositor
Minimum map value	-20.788	Depositor
Average map value	0.000	Depositor
Map value standard deviation	2.501	Depositor
Recommended contour level	5	Depositor
Map size ($\text{\AA}$)	817.92, 817.92, 817.92	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.42, 1.42, 1.42	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	3.15	54/1346 (4.0%)	2.60	94/1812 (5.2%)
1	D	3.12	51/1346 (3.8%)	2.59	97/1812 (5.4%)
1	G	3.14	68/1346 (5.1%)	2.58	98/1812 (5.4%)
1	J	3.15	63/1346 (4.7%)	2.53	101/1812 (5.6%)
2	B	2.29	131/3296 (4.0%)	2.43	211/4494 (4.7%)
2	E	2.25	128/3296 (3.9%)	2.44	191/4494 (4.3%)
2	H	2.29	130/3296 (3.9%)	2.45	234/4494 (5.2%)
2	K	2.33	138/3296 (4.2%)	2.41	188/4494 (4.2%)
3	C	2.62	154/3326 (4.6%)	2.40	203/4537 (4.5%)
3	F	2.56	132/3326 (4.0%)	2.46	213/4537 (4.7%)
3	I	2.63	163/3326 (4.9%)	2.48	223/4537 (4.9%)
3	L	2.59	148/3326 (4.4%)	2.48	202/4537 (4.5%)
All	All	2.58	1360/31872 (4.3%)	2.46	2055/43372 (4.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	D	0	7
1	G	0	8
1	J	0	4
2	B	0	20
2	E	0	21
2	H	0	19
2	K	0	20
3	C	0	11
3	F	0	6
3	I	0	11
3	L	0	9
All	All	0	140

All (1360) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	237	TRP	CE2-CZ2	73.79	2.94	1.39
1	J	237	TRP	CE2-CZ2	71.77	2.90	1.39
1	G	237	TRP	CE2-CZ2	70.99	2.88	1.39
1	A	237	TRP	CE2-CZ2	70.95	2.88	1.39
3	I	398	TYR	CD2-CE2	39.24	2.56	1.38
3	L	398	TYR	CD2-CE2	38.82	2.55	1.38
3	C	398	TYR	CD2-CE2	38.75	2.54	1.38
3	F	398	TYR	CD2-CE2	38.58	2.54	1.38
3	I	240	TYR	CG-CD1	27.98	1.98	1.39
1	A	237	TRP	CD2-CE3	26.16	1.82	1.40
3	I	240	TYR	CG-CD2	25.61	1.93	1.39
3	C	240	TYR	CG-CD2	25.50	1.93	1.39
3	L	240	TYR	CG-CD2	25.34	1.92	1.39
3	C	240	TYR	CG-CD1	24.81	1.91	1.39
3	C	240	TYR	CE1-CZ	23.95	1.95	1.38
3	F	240	TYR	CG-CD1	23.92	1.89	1.39
3	L	240	TYR	CG-CD1	23.90	1.89	1.39
3	L	240	TYR	CE1-CZ	23.40	1.94	1.38
3	F	240	TYR	CG-CD2	23.39	1.88	1.39
3	I	240	TYR	CE1-CZ	22.49	1.92	1.38
3	F	240	TYR	CE1-CZ	21.75	1.90	1.38
1	G	237	TRP	CD2-CE3	21.59	1.74	1.40
3	F	240	TYR	CE2-CZ	21.36	1.89	1.38
3	L	240	TYR	CE2-CZ	20.54	1.87	1.38
3	I	240	TYR	CE2-CZ	20.47	1.87	1.38
3	C	240	TYR	CE2-CZ	19.73	1.85	1.38
1	D	237	TRP	CD2-CE3	18.34	1.69	1.40
1	A	237	TRP	CZ2-CH2	18.07	1.71	1.37
1	G	237	TRP	CZ2-CH2	17.77	1.71	1.37
3	F	240	TYR	CD1-CE1	17.55	1.91	1.38
3	L	240	TYR	CD2-CE2	17.54	1.91	1.38
1	J	237	TRP	CD2-CE2	17.06	1.70	1.41
3	C	240	TYR	CD1-CE1	16.97	1.89	1.38
3	C	240	TYR	CD2-CE2	16.47	1.88	1.38
1	J	237	TRP	CZ2-CH2	16.44	1.68	1.37
1	G	237	TRP	CD2-CE2	15.97	1.68	1.41
1	A	237	TRP	CD2-CE2	15.45	1.67	1.41
1	J	237	TRP	CD2-CE3	15.37	1.64	1.40
1	D	237	TRP	CZ2-CH2	15.36	1.66	1.37
3	L	240	TYR	CD1-CE1	14.59	1.82	1.38
3	I	240	TYR	CD1-CE1	14.26	1.81	1.38
3	I	240	TYR	CD2-CE2	13.90	1.80	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	240	TYR	CD2-CE2	13.60	1.79	1.38
1	D	237	TRP	CD2-CE2	13.33	1.64	1.41
3	C	398	TYR	CG-CD1	12.99	1.66	1.39
3	I	398	TYR	CE2-CZ	12.81	1.69	1.38
3	I	398	TYR	CG-CD2	12.52	1.65	1.39
2	K	21	ARG	CD-NE	11.49	1.62	1.46
3	L	398	TYR	CG-CD1	11.20	1.62	1.39
1	D	237	TRP	CE3-CZ3	11.12	1.72	1.38
1	G	237	TRP	CE3-CZ3	11.02	1.71	1.38
1	J	237	TRP	CE3-CZ3	10.80	1.71	1.38
2	E	229	VAL	CA-C	10.68	1.66	1.52
3	F	224	CYS	CA-C	-10.51	1.41	1.52
3	C	416	ALA	CA-CB	10.18	1.69	1.53
2	H	229	VAL	CA-C	10.15	1.64	1.52
3	C	398	TYR	CE2-CZ	10.10	1.62	1.38
1	A	237	TRP	CE3-CZ3	10.01	1.68	1.38
1	D	237	TRP	CZ3-CH2	10.01	1.65	1.40
3	F	123	ARG	C-N	10.01	1.45	1.33
2	H	92	ALA	CA-C	-9.99	1.40	1.52
3	C	215	LEU	CA-C	-9.97	1.40	1.52
1	G	237	TRP	CZ3-CH2	9.95	1.65	1.40
2	H	312	PHE	C-N	9.93	1.46	1.33
3	C	175	GLN	CA-C	9.87	1.65	1.52
2	E	123	GLN	CA-C	-9.85	1.40	1.52
2	H	54	VAL	C-N	9.78	1.40	1.33
3	L	172	VAL	CA-C	-9.76	1.45	1.53
3	C	121	LEU	CA-C	-9.75	1.40	1.52
3	L	398	TYR	CE1-CZ	9.75	1.61	1.38
2	B	223	ARG	NE-CZ	9.63	1.43	1.33
3	L	286	HIS	C-N	9.61	1.45	1.33
2	B	374	ILE	CA-C	-9.50	1.42	1.52
3	C	333	PRO	CA-C	9.43	1.63	1.52
3	C	277	ARG	NE-CZ	9.38	1.43	1.33
2	K	328	CYS	CA-C	-9.36	1.41	1.52
2	E	37	GLU	CA-C	-9.34	1.43	1.53
2	H	428	VAL	N-CA	-9.33	1.35	1.46
2	K	314	GLY	CA-C	-9.31	1.41	1.52
3	L	398	TYR	CE2-CZ	9.30	1.60	1.38
2	B	106	VAL	CA-C	-9.30	1.41	1.52
1	J	237	TRP	CZ3-CH2	9.28	1.63	1.40
3	F	286	HIS	CA-CB	9.24	1.61	1.53
3	L	316	THR	CA-C	-9.11	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	398	TYR	CG-CD2	9.07	1.58	1.39
3	F	398	TYR	CG-CD2	9.02	1.58	1.39
2	B	19	ILE	CA-C	-9.01	1.43	1.52
3	L	128	HIS	CB-CG	8.85	1.62	1.50
3	F	254	HIS	CE1-NE2	8.78	1.41	1.32
2	B	151	ASP	C-N	8.77	1.43	1.33
3	I	356	HIS	CA-C	-8.73	1.42	1.52
3	C	398	TYR	CG-CD2	8.73	1.57	1.39
2	H	148	VAL	N-CA	-8.70	1.36	1.46
3	C	310	ASP	C-N	8.68	1.43	1.32
3	I	20	ASP	N-CA	-8.67	1.35	1.46
3	I	240	TYR	C-N	8.67	1.41	1.33
2	E	13	ILE	CA-CB	-8.65	1.46	1.54
3	F	398	TYR	CE1-CZ	8.62	1.58	1.38
3	F	180	ASN	CA-C	-8.62	1.41	1.52
3	C	4	HIS	CB-CG	8.62	1.62	1.50
3	L	271	GLU	N-CA	8.61	1.55	1.45
1	G	175	PRO	C-N	8.58	1.44	1.33
3	F	398	TYR	CE2-CZ	8.57	1.58	1.38
3	C	364	TRP	CA-C	-8.56	1.40	1.52
3	L	76	GLU	CA-C	-8.54	1.41	1.52
2	K	346	VAL	CA-CB	-8.49	1.44	1.54
3	I	296	ARG	CD-NE	8.47	1.58	1.46
3	F	398	TYR	CG-CD1	8.46	1.57	1.39
3	C	152	THR	C-N	8.44	1.45	1.33
3	I	297	SER	N-CA	-8.42	1.35	1.46
3	L	371	SER	CA-C	-8.37	1.42	1.52
1	G	174	LYS	C-O	-8.35	1.17	1.25
2	H	352	LEU	N-CA	-8.29	1.36	1.46
2	K	307	THR	CA-C	-8.26	1.42	1.52
3	L	353	ILE	C-N	8.25	1.44	1.33
1	A	178	HIS	CE1-NE2	8.25	1.40	1.32
2	H	9	ASN	CA-CB	8.25	1.63	1.52
3	C	318	GLN	CA-C	-8.23	1.42	1.52
2	K	193	GLY	C-O	-8.23	1.18	1.24
1	G	121	LEU	C-N	8.22	1.44	1.33
3	C	210	THR	C-N	8.21	1.44	1.33
3	F	107	GLY	CA-C	-8.21	1.43	1.51
3	I	256	PRO	CA-C	-8.16	1.44	1.52
3	L	356	HIS	CB-CG	8.13	1.61	1.50
3	F	35	HIS	CA-CB	8.11	1.67	1.53
2	H	214	TYR	CA-CB	8.10	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	298	LEU	CA-C	-8.10	1.43	1.53
2	K	229	VAL	CA-C	8.09	1.62	1.52
3	F	329	GLY	C-N	8.08	1.42	1.33
1	D	147	LYS	CA-C	-8.08	1.42	1.52
2	H	218	ASN	N-CA	-8.08	1.36	1.46
2	K	390	TYR	C-N	8.07	1.43	1.33
1	J	189	SER	CA-C	-8.06	1.42	1.52
3	I	24	ALA	C-N	8.05	1.42	1.32
3	F	288	MET	CA-C	-8.03	1.42	1.52
3	I	402	PRO	C-N	8.02	1.44	1.33
2	B	299	LYS	CA-C	-8.01	1.42	1.52
1	G	123	GLY	CA-C	-7.99	1.40	1.51
3	I	290	PRO	CA-C	-7.98	1.41	1.52
1	D	94	ARG	CA-C	-7.96	1.43	1.52
3	L	243	ARG	NE-CZ	7.96	1.41	1.33
2	K	201	GLY	CA-C	-7.95	1.43	1.52
2	K	371	ASN	N-CA	-7.94	1.36	1.46
2	B	248	GLY	CA-C	-7.93	1.42	1.51
3	C	21	CYS	N-CA	-7.91	1.40	1.47
1	G	183	HIS	CE1-NE2	7.90	1.40	1.32
3	I	296	ARG	NE-CZ	7.88	1.41	1.33
3	I	315	LYS	CA-C	-7.88	1.43	1.52
3	I	398	TYR	CG-CD1	7.87	1.55	1.39
3	L	101	LEU	CA-C	-7.84	1.43	1.52
3	C	176	GLY	C-N	7.82	1.43	1.33
2	B	275	ASN	C-N	7.79	1.42	1.33
3	C	262	SER	CA-C	-7.79	1.43	1.52
3	F	315	LYS	CA-C	-7.78	1.43	1.52
2	B	237	PRO	CA-C	-7.75	1.44	1.52
3	C	1	SER	C-N	7.73	1.41	1.33
3	F	354	VAL	CA-C	-7.72	1.43	1.52
2	K	29	LEU	CA-C	-7.71	1.43	1.52
1	J	189	SER	C-N	7.70	1.44	1.33
2	E	249	VAL	N-CA	-7.68	1.37	1.46
2	H	407	TRP	C-N	7.67	1.44	1.33
2	E	402	ILE	N-CA	7.66	1.55	1.46
1	G	220	VAL	CA-C	-7.66	1.44	1.52
3	I	105	ARG	CA-CB	7.64	1.64	1.53
3	C	79	ARG	CZ-NH1	7.63	1.43	1.32
3	F	21	CYS	CA-CB	7.62	1.64	1.53
3	I	398	TYR	CE1-CZ	7.60	1.56	1.38
2	H	66	ALA	C-N	7.59	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	46	TYR	CA-C	7.58	1.61	1.52
3	F	374	LEU	CA-C	-7.58	1.43	1.52
2	E	214	TYR	CA-CB	7.57	1.63	1.53
3	C	243	ARG	CD-NE	7.57	1.56	1.46
2	B	104	SER	CA-C	-7.56	1.43	1.52
1	G	93	LYS	CA-C	7.56	1.61	1.52
2	H	413	THR	CA-C	-7.56	1.42	1.52
1	J	252	GLU	N-CA	-7.56	1.36	1.46
3	F	271	GLU	C-N	7.54	1.43	1.33
2	E	271	CYS	C-N	7.54	1.40	1.33
3	F	313	MET	CA-C	-7.54	1.42	1.52
1	D	136	ILE	N-CA	-7.53	1.37	1.46
3	L	178	VAL	N-CA	-7.53	1.37	1.46
2	E	336	SER	CA-C	-7.52	1.46	1.52
3	C	220	THR	N-CA	-7.51	1.37	1.46
3	F	324	VAL	CA-C	-7.51	1.43	1.52
2	B	42	LEU	C-N	7.50	1.43	1.33
3	L	103	ARG	CA-CB	7.50	1.64	1.53
2	K	221	LEU	CA-C	-7.50	1.43	1.52
1	A	192	ARG	NE-CZ	7.48	1.41	1.33
2	H	153	PRO	CA-CB	-7.46	1.44	1.53
2	H	261	ILE	N-CA	-7.46	1.37	1.46
3	F	286	HIS	CG-CD2	7.45	1.44	1.35
2	H	7	MET	N-CA	-7.45	1.35	1.45
2	K	373	ARG	CA-C	-7.45	1.43	1.52
3	L	67	ARG	NE-CZ	7.44	1.41	1.33
2	H	315	VAL	CA-C	-7.43	1.44	1.52
3	F	284	HIS	CB-CG	7.42	1.60	1.50
2	B	271	CYS	C-N	7.42	1.43	1.33
1	G	156	CYS	CA-C	-7.40	1.43	1.52
1	A	125	LYS	CA-C	-7.39	1.43	1.52
2	E	373	ARG	CD-NE	7.39	1.56	1.46
3	I	63	HIS	CE1-NE2	7.39	1.40	1.32
3	I	32	SER	CA-C	-7.38	1.43	1.52
3	C	326	TYR	C-N	7.38	1.42	1.33
3	F	16	GLY	CA-C	-7.37	1.45	1.52
3	I	173	PRO	N-CA	-7.37	1.40	1.47
1	A	147	LYS	CA-C	-7.34	1.43	1.52
1	G	204	ASP	N-CA	7.34	1.54	1.46
1	J	122	VAL	CA-CB	-7.34	1.45	1.54
2	E	338	THR	CA-C	-7.34	1.43	1.52
1	D	156	CYS	CA-CB	7.33	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	TRP	CZ3-CH2	7.33	1.58	1.40
1	G	172	HIS	CE1-NE2	7.33	1.39	1.32
1	J	98	CYS	CA-C	-7.32	1.43	1.53
2	K	285	ALA	C-N	7.32	1.44	1.33
2	B	185	TYR	CA-C	-7.32	1.43	1.52
2	E	288	THR	N-CA	-7.31	1.36	1.46
1	J	209	ILE	N-CA	-7.29	1.37	1.46
3	C	363	TYR	C-N	7.29	1.45	1.33
3	I	398	TYR	CD1-CE1	7.27	1.60	1.38
2	B	399	PHE	CA-CB	7.26	1.65	1.53
3	C	397	PRO	C-N	7.25	1.43	1.33
2	E	109	THR	CA-C	-7.24	1.43	1.52
3	I	119	LYS	C-N	7.24	1.41	1.33
3	L	21	CYS	CA-C	7.24	1.61	1.52
3	L	35	HIS	CE1-NE2	7.23	1.39	1.32
1	G	145	THR	N-CA	-7.23	1.37	1.46
2	H	218	ASN	C-N	7.23	1.44	1.33
2	B	310	SER	CA-C	-7.23	1.43	1.52
3	C	67	ARG	CD-NE	7.22	1.56	1.46
1	A	189	SER	CA-C	-7.22	1.43	1.52
2	B	293	SER	CA-C	-7.22	1.45	1.52
3	C	317	ILE	CB-CG1	7.21	1.67	1.53
3	C	128	HIS	CG-ND1	7.21	1.46	1.38
3	C	238	SER	CA-C	-7.21	1.42	1.53
3	C	246	VAL	N-CA	-7.20	1.38	1.46
2	H	272	VAL	N-CA	-7.20	1.37	1.46
2	K	109	THR	N-CA	-7.20	1.36	1.45
2	H	403	SER	CA-C	-7.18	1.44	1.52
3	C	398	TYR	CE1-CZ	7.18	1.55	1.38
2	K	325	VAL	CA-C	-7.17	1.44	1.52
2	E	136	SER	CA-C	-7.17	1.44	1.52
1	J	224	ALA	C-O	-7.17	1.16	1.23
3	F	381	GLY	C-N	7.16	1.43	1.33
3	I	276	TYR	CA-C	-7.16	1.43	1.52
2	B	24	TYR	CA-C	-7.16	1.44	1.52
3	I	59	ASN	CA-C	-7.16	1.43	1.52
1	J	148	LYS	CA-C	-7.14	1.43	1.52
2	K	206	ARG	NE-CZ	7.14	1.41	1.33
2	E	431	VAL	CA-C	-7.13	1.44	1.52
1	J	118	TYR	N-CA	-7.12	1.36	1.45
3	L	167	HIS	CE1-NE2	7.11	1.39	1.32
1	G	192	ARG	NE-CZ	7.11	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	360	LEU	N-CA	-7.11	1.37	1.46
3	F	225	ILE	CA-CB	7.10	1.63	1.53
2	B	60	ILE	CA-C	-7.09	1.43	1.52
2	K	246	GLU	C-N	7.08	1.43	1.33
3	L	224	CYS	C-N	7.08	1.42	1.33
1	D	207	ARG	CD-NE	7.08	1.56	1.46
2	H	280	MET	CA-C	-7.08	1.43	1.52
3	I	4	HIS	CB-CG	7.07	1.60	1.50
3	F	387	CYS	CA-C	-7.07	1.43	1.52
2	K	181	ARG	CZ-NH1	7.06	1.42	1.32
2	E	275	ASN	C-N	7.06	1.40	1.33
3	I	185	TYR	CA-C	-7.06	1.44	1.52
3	L	272	PRO	C-N	7.06	1.42	1.33
2	B	367	VAL	C-N	7.05	1.43	1.33
1	A	104	ASP	CA-C	-7.05	1.46	1.52
3	I	204	VAL	CA-C	-7.05	1.44	1.52
3	C	353	ILE	N-CA	-7.05	1.37	1.46
3	F	50	SER	CA-CB	7.04	1.64	1.53
1	J	139	PRO	N-CD	-7.03	1.38	1.47
3	L	134	GLY	CA-C	-7.03	1.42	1.51
2	E	128	SER	N-CA	-7.03	1.37	1.45
1	G	89	SER	C-N	7.03	1.41	1.33
1	A	199	SER	C-N	7.02	1.39	1.33
2	H	373	ARG	NE-CZ	7.02	1.40	1.33
2	B	438	ARG	CD-NE	7.01	1.56	1.46
3	I	294	SER	CA-C	-7.01	1.44	1.52
3	C	157	THR	CA-CB	-7.01	1.43	1.53
2	E	177	VAL	C-N	7.01	1.42	1.33
3	C	138	SER	CA-CB	7.00	1.64	1.53
3	L	302	PRO	C-N	7.00	1.43	1.33
2	K	373	ARG	C-N	7.00	1.42	1.33
3	F	420	ARG	NE-CZ	6.99	1.40	1.33
2	E	435	VAL	N-CA	-6.98	1.38	1.46
2	E	13	ILE	N-CA	-6.98	1.40	1.46
3	L	335	ARG	CA-C	-6.98	1.44	1.52
3	I	360	LEU	N-CA	6.97	1.54	1.46
3	I	380	SER	CA-CB	6.97	1.64	1.53
3	L	90	CYS	CA-C	-6.97	1.44	1.52
2	B	348	GLU	N-CA	-6.96	1.36	1.46
2	B	36	SER	N-CA	-6.95	1.37	1.45
3	C	45	LEU	CA-C	-6.95	1.44	1.52
1	G	122	VAL	N-CA	-6.95	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	79	SER	CA-C	-6.93	1.44	1.52
2	K	60	ILE	N-CA	-6.93	1.37	1.46
1	J	251	VAL	N-CA	-6.93	1.38	1.46
2	B	197	ALA	CA-C	-6.91	1.44	1.52
3	I	228	ALA	CA-C	-6.91	1.43	1.52
2	K	14	PRO	N-CA	-6.90	1.38	1.47
1	D	103	ASN	CA-C	-6.90	1.44	1.52
2	E	34	ILE	CA-C	-6.90	1.44	1.52
2	E	218	ASN	CA-C	-6.90	1.44	1.52
3	L	411	ALA	CA-C	-6.89	1.44	1.52
2	B	307	THR	N-CA	-6.89	1.36	1.45
2	B	229	VAL	CA-C	6.88	1.61	1.52
3	C	62	ASN	CA-C	-6.88	1.44	1.52
2	E	106	VAL	CA-C	-6.88	1.44	1.52
2	B	22	PRO	N-CA	-6.88	1.39	1.47
1	G	248	GLU	CA-CB	6.88	1.65	1.53
2	K	350	GLY	CA-C	-6.88	1.42	1.51
3	F	2	VAL	C-N	6.87	1.42	1.33
2	H	341	ASP	CA-CB	6.87	1.64	1.53
2	H	114	CYS	CA-C	-6.86	1.44	1.52
3	I	243	ARG	CA-C	-6.86	1.44	1.52
2	K	187	GLU	N-CA	-6.86	1.37	1.46
2	E	206	ARG	CD-NE	6.85	1.55	1.46
2	E	434	VAL	CA-CB	-6.85	1.46	1.54
3	I	254	HIS	CE1-NE2	6.85	1.39	1.32
3	F	99	PHE	CA-C	-6.84	1.44	1.52
3	I	53	ILE	CA-CB	-6.83	1.46	1.54
1	J	229	ARG	CZ-NH1	6.83	1.42	1.32
3	I	17	TRP	NE1-CE2	6.82	1.45	1.37
2	B	134	MET	CA-C	-6.79	1.44	1.52
2	B	199	ARG	CZ-NH2	6.78	1.42	1.33
3	F	94	ALA	C-N	6.78	1.42	1.33
3	I	131	ARG	CD-NE	6.77	1.55	1.46
2	B	282	ILE	N-CA	-6.77	1.38	1.46
2	K	93	TYR	CA-C	6.77	1.61	1.53
2	H	222	LYS	N-CA	-6.77	1.37	1.45
2	B	181	ARG	CD-NE	6.76	1.55	1.46
2	H	190	ALA	CA-CB	6.75	1.61	1.53
1	J	192	ARG	NE-CZ	6.75	1.40	1.33
2	K	69	SER	N-CA	-6.75	1.40	1.46
1	A	146	PHE	CA-CB	6.75	1.61	1.52
2	B	307	THR	CA-C	6.73	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	314	SER	CA-C	-6.73	1.44	1.52
3	I	229	VAL	CA-CB	-6.72	1.46	1.54
2	H	160	LYS	CA-C	-6.71	1.44	1.52
2	H	35	LYS	N-CA	-6.70	1.37	1.46
2	B	179	VAL	CA-CB	-6.70	1.45	1.53
3	C	277	ARG	CD-NE	6.70	1.55	1.46
2	K	134	MET	CA-C	-6.69	1.44	1.52
2	K	202	ASP	C-N	6.69	1.42	1.33
3	L	279	GLY	CA-C	-6.69	1.42	1.51
2	K	20	GLU	CA-CB	6.68	1.64	1.53
3	C	382	PHE	C-N	6.68	1.42	1.33
2	E	305	SER	CA-C	-6.68	1.45	1.53
3	L	357	TYR	CA-CB	6.68	1.62	1.53
2	H	22	PRO	C-N	6.67	1.42	1.32
3	C	161	ARG	NE-CZ	6.67	1.40	1.33
2	E	181	ARG	NE-CZ	6.67	1.40	1.33
3	L	10	ALA	C-N	6.66	1.41	1.33
1	J	121	LEU	CA-C	6.66	1.61	1.52
3	I	118	PRO	C-N	6.66	1.43	1.33
3	F	12	ARG	CD-NE	6.65	1.55	1.46
3	I	53	ILE	CA-C	-6.65	1.44	1.52
3	I	246	VAL	N-CA	-6.65	1.37	1.46
2	K	94	CYS	N-CA	-6.65	1.37	1.45
3	F	420	ARG	CD-NE	6.65	1.55	1.46
2	K	261	ILE	CA-CB	6.65	1.61	1.54
1	G	157	ALA	C-N	6.64	1.42	1.33
2	H	146	VAL	C-N	6.64	1.42	1.33
1	J	154	LEU	CA-C	-6.64	1.44	1.52
3	C	88	ALA	C-N	6.63	1.41	1.33
3	L	47	ILE	CA-C	-6.63	1.44	1.52
3	F	123	ARG	CD-NE	6.62	1.55	1.46
1	J	87	LYS	N-CA	-6.62	1.38	1.46
3	C	13	PRO	CA-CB	6.62	1.63	1.53
2	K	58	PRO	N-CA	-6.62	1.38	1.47
1	A	246	THR	CA-C	-6.61	1.45	1.52
2	E	402	ILE	C-N	6.61	1.41	1.33
3	F	284	HIS	CA-C	-6.61	1.44	1.52
1	J	166	ASP	CA-CB	6.61	1.64	1.53
2	K	38	LEU	C-N	6.61	1.40	1.33
3	I	47	ILE	N-CA	6.60	1.54	1.46
3	I	376	ILE	N-CA	-6.60	1.38	1.46
3	L	36	VAL	CA-C	-6.59	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	267	ARG	CA-C	-6.59	1.44	1.52
1	G	86	LYS	C-N	6.59	1.42	1.33
2	K	429	VAL	N-CA	-6.58	1.38	1.46
2	H	143	THR	C-N	6.58	1.41	1.33
2	E	346	VAL	CA-C	-6.58	1.44	1.52
3	I	396	THR	C-N	6.58	1.41	1.34
3	F	340	LYS	CA-C	-6.57	1.44	1.53
3	C	192	LYS	C-O	-6.57	1.16	1.23
2	B	65	GLY	C-N	6.56	1.41	1.33
2	K	232	PRO	C-N	6.56	1.41	1.33
2	B	428	VAL	N-CA	-6.55	1.38	1.46
3	L	6	GLU	N-CA	-6.55	1.38	1.46
2	E	85	TYR	CA-C	-6.55	1.44	1.52
2	H	264	ASN	CA-CB	6.55	1.62	1.53
3	C	104	CYS	CA-C	-6.55	1.44	1.52
1	A	244	ARG	CZ-NH2	6.55	1.42	1.33
3	F	171	ASP	CA-C	-6.54	1.44	1.52
3	L	366	ILE	CA-C	-6.54	1.44	1.52
2	E	438	ARG	CZ-NH1	6.54	1.41	1.32
3	L	296	ARG	CA-C	-6.54	1.44	1.52
3	I	9	LYS	N-CA	-6.53	1.38	1.46
1	A	182	HIS	CG-ND1	6.53	1.45	1.38
3	I	161	ARG	NE-CZ	6.53	1.40	1.33
1	A	96	ARG	CD-NE	6.52	1.55	1.46
1	J	140	GLU	N-CA	-6.52	1.38	1.46
2	B	137	ILE	CA-C	-6.51	1.44	1.52
2	E	277	PRO	CA-C	6.51	1.60	1.52
2	H	363	PRO	C-N	6.51	1.42	1.33
2	K	66	ALA	N-CA	-6.51	1.37	1.45
2	K	75	ASP	CA-C	-6.51	1.44	1.52
3	F	335	ARG	CD-NE	6.50	1.55	1.46
2	B	249	VAL	CA-C	6.50	1.59	1.52
2	B	305	SER	CA-C	-6.50	1.46	1.53
3	F	120	LEU	CA-CB	6.50	1.62	1.53
3	L	390	ALA	N-CA	-6.49	1.38	1.46
3	I	153	TYR	CA-C	-6.49	1.44	1.52
2	B	173	PHE	N-CA	-6.48	1.37	1.46
3	I	45	LEU	N-CA	-6.48	1.38	1.46
1	G	217	VAL	CA-C	6.48	1.61	1.52
3	I	159	LEU	CA-C	-6.48	1.44	1.52
1	J	143	LYS	CA-C	-6.47	1.44	1.52
3	F	192	LYS	CA-C	-6.47	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	234	VAL	N-CA	6.46	1.53	1.46
1	D	94	ARG	CZ-NH2	6.45	1.41	1.33
2	B	48	THR	CA-C	-6.45	1.44	1.52
3	F	304	HIS	CB-CG	6.45	1.59	1.50
2	E	324	LYS	C-N	6.45	1.40	1.33
3	F	15	ILE	CA-C	-6.45	1.45	1.52
2	B	232	PRO	N-CD	-6.45	1.38	1.47
3	L	99	PHE	N-CA	-6.45	1.38	1.46
3	I	68	TYR	CA-C	-6.44	1.44	1.52
2	K	191	PRO	CA-C	-6.44	1.44	1.52
2	K	301	CYS	C-N	6.44	1.42	1.33
2	H	134	MET	CA-C	-6.44	1.45	1.52
3	L	184	SER	CA-C	-6.44	1.44	1.52
3	I	148	ILE	CA-C	-6.43	1.46	1.52
3	I	147	ARG	NE-CZ	6.42	1.40	1.33
3	F	324	VAL	C-N	6.42	1.42	1.33
3	I	250	LYS	C-N	6.42	1.41	1.33
3	C	254	HIS	C-N	6.42	1.38	1.33
2	E	355	PHE	CA-CB	6.42	1.64	1.53
2	H	267	ARG	CD-NE	6.41	1.55	1.46
3	I	175	GLN	C-N	6.41	1.40	1.32
2	K	180	TYR	CA-C	-6.40	1.44	1.53
3	F	103	ARG	CZ-NH2	6.40	1.41	1.33
2	H	221	LEU	N-CA	-6.40	1.38	1.46
2	H	128	SER	C-N	6.39	1.41	1.33
2	K	27	LEU	C-O	-6.39	1.17	1.24
3	F	391	ARG	NE-CZ	6.39	1.40	1.33
3	F	332	ASN	C-N	6.38	1.41	1.33
1	A	94	ARG	NE-CZ	6.38	1.40	1.33
3	I	274	VAL	CA-C	-6.38	1.45	1.52
2	H	77	LYS	N-CA	-6.38	1.37	1.45
3	I	328	TRP	CA-C	-6.38	1.45	1.52
3	L	325	GLU	N-CA	-6.37	1.38	1.46
2	K	199	ARG	NE-CZ	6.37	1.40	1.33
3	L	114	LEU	CA-C	-6.37	1.44	1.52
3	F	298	LEU	CA-CB	6.37	1.64	1.53
3	C	360	LEU	C-N	6.37	1.42	1.33
3	C	39	ASP	N-CA	6.36	1.54	1.46
3	C	376	ILE	C-N	6.35	1.41	1.33
2	H	215	ALA	N-CA	-6.35	1.37	1.46
3	C	326	TYR	N-CA	-6.35	1.38	1.46
3	L	9	LYS	C-N	6.35	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	69	MET	N-CA	-6.34	1.38	1.46
2	B	216	ASN	CA-C	-6.34	1.44	1.52
2	B	208	VAL	C-O	-6.34	1.16	1.24
3	C	81	THR	CA-CB	-6.34	1.44	1.54
2	E	435	VAL	CA-CB	-6.34	1.46	1.54
2	B	200	PHE	C-N	6.33	1.41	1.33
3	I	171	ASP	N-CA	-6.33	1.38	1.46
2	E	248	GLY	N-CA	-6.33	1.36	1.45
1	D	211	ASP	CA-CB	6.33	1.64	1.53
2	B	373	ARG	CZ-NH1	6.33	1.41	1.32
3	L	11	THR	CA-C	-6.33	1.45	1.53
3	L	152	THR	C-N	6.33	1.42	1.33
2	H	268	ALA	CA-C	-6.32	1.45	1.52
2	K	360	SER	C-N	6.31	1.42	1.33
3	F	12	ARG	NE-CZ	6.30	1.40	1.33
3	F	397	PRO	C-N	6.30	1.42	1.33
3	C	318	GLN	N-CA	-6.30	1.38	1.46
2	E	22	PRO	CA-CB	6.29	1.61	1.53
2	E	61	LYS	N-CA	-6.29	1.38	1.46
1	D	89	SER	N-CA	6.29	1.52	1.46
3	L	95	THR	CA-CB	-6.29	1.43	1.53
2	K	129	LEU	N-CA	-6.29	1.38	1.46
3	C	196	TYR	CA-C	-6.29	1.45	1.52
1	D	114	LYS	C-N	6.29	1.39	1.33
1	G	194	THR	C-N	6.29	1.39	1.33
3	I	197	LYS	CA-C	-6.29	1.45	1.52
2	B	267	ARG	CZ-NH1	6.28	1.41	1.32
2	B	267	ARG	CZ-NH2	6.28	1.41	1.33
2	E	11	VAL	N-CA	-6.28	1.38	1.46
3	F	255	VAL	CA-CB	6.28	1.61	1.54
3	C	199	THR	CA-C	-6.28	1.44	1.52
3	C	25	GLY	CA-C	-6.27	1.43	1.51
2	B	111	GLY	CA-C	-6.27	1.43	1.51
3	I	108	SER	C-N	6.27	1.41	1.33
1	D	231	ALA	CA-C	-6.26	1.44	1.52
1	A	252	GLU	CA-CB	6.26	1.61	1.53
3	C	368	VAL	CA-CB	-6.26	1.46	1.54
2	K	340	LYS	C-N	6.26	1.42	1.33
1	D	245	ILE	CA-C	6.26	1.60	1.52
1	A	207	ARG	CA-C	6.25	1.59	1.53
3	F	196	TYR	CA-C	-6.25	1.45	1.52
2	K	273	TYR	CA-C	6.25	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	254	HIS	CD2-NE2	6.25	1.44	1.37
2	B	240	PHE	C-N	6.25	1.42	1.34
3	C	243	ARG	NE-CZ	6.25	1.40	1.33
2	H	262	LYS	CA-C	-6.25	1.45	1.52
2	E	58	PRO	CA-CB	6.24	1.62	1.53
2	E	105	GLU	N-CA	-6.24	1.38	1.46
2	K	74	ALA	C-N	6.23	1.41	1.33
2	B	234	THR	C-N	6.23	1.41	1.33
3	C	240	TYR	C-N	6.23	1.40	1.33
2	K	155	ARG	CD-NE	6.22	1.54	1.46
3	L	350	PRO	N-CA	6.22	1.55	1.47
1	G	207	ARG	CZ-NH1	6.22	1.41	1.32
3	F	90	CYS	N-CA	-6.21	1.38	1.45
2	H	137	ILE	N-CA	6.21	1.54	1.46
2	H	294	PRO	CA-C	6.21	1.59	1.52
3	I	382	PHE	CA-CB	6.21	1.62	1.53
2	K	155	ARG	NE-CZ	6.21	1.39	1.33
3	I	177	LEU	C-N	6.21	1.42	1.33
3	L	356	HIS	ND1-CE1	-6.21	1.26	1.32
3	F	103	ARG	N-CA	-6.21	1.38	1.46
3	L	369	LEU	CA-C	6.21	1.60	1.52
3	C	304	HIS	CE1-NE2	6.19	1.38	1.32
2	K	129	LEU	C-N	6.19	1.43	1.33
3	L	356	HIS	CE1-NE2	6.19	1.38	1.32
1	A	88	LYS	N-CA	-6.19	1.38	1.46
3	C	58	SER	C-N	6.19	1.41	1.33
2	H	193	GLY	C-N	6.18	1.41	1.33
3	C	266	VAL	C-O	-6.18	1.16	1.23
3	C	276	TYR	CA-C	-6.18	1.44	1.52
2	H	104	SER	C-N	6.18	1.41	1.33
3	I	28	PRO	C-N	6.18	1.43	1.33
2	K	38	LEU	N-CA	-6.18	1.38	1.46
3	L	223	LYS	C-N	6.17	1.41	1.33
2	K	90	GLY	C-N	6.17	1.41	1.33
2	K	206	ARG	CA-C	-6.16	1.44	1.52
1	D	128	LYS	C-N	-6.15	1.26	1.33
2	K	72	ASN	C-N	6.15	1.38	1.33
2	B	188	ASP	N-CA	-6.15	1.38	1.46
2	E	121	ALA	CA-C	-6.15	1.45	1.52
2	E	303	VAL	CA-C	-6.14	1.44	1.52
2	K	435	VAL	CA-C	-6.14	1.45	1.52
1	A	137	ASP	N-CA	-6.14	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	257	PHE	CA-C	-6.14	1.45	1.52
3	C	67	ARG	CA-C	-6.14	1.45	1.52
2	H	348	GLU	C-N	6.14	1.41	1.33
3	L	4	HIS	CB-CG	6.14	1.58	1.50
3	I	128	HIS	CG-ND1	6.14	1.45	1.38
3	I	411	ALA	N-CA	-6.13	1.38	1.46
3	L	243	ARG	CZ-NH2	6.13	1.41	1.33
3	C	359	ASP	CA-C	-6.12	1.44	1.52
3	I	392	THR	C-N	6.12	1.42	1.33
1	J	234	VAL	CA-C	-6.12	1.45	1.52
1	D	194	THR	C-N	6.11	1.39	1.33
2	E	201	GLY	CA-C	6.11	1.60	1.51
1	A	107	PHE	CA-C	-6.11	1.46	1.53
3	I	385	PHE	CA-C	-6.11	1.45	1.52
3	L	195	LYS	N-CA	-6.11	1.38	1.46
2	K	78	CYS	C-O	-6.10	1.16	1.23
2	E	328	CYS	CA-CB	6.10	1.63	1.53
3	I	115	SER	CA-C	-6.10	1.45	1.53
2	B	379	LYS	CA-C	6.09	1.60	1.53
1	G	146	PHE	N-CA	6.09	1.54	1.46
3	F	255	VAL	CA-C	6.09	1.58	1.53
3	I	309	ILE	CA-CB	-6.09	1.46	1.53
2	H	411	ALA	C-N	6.09	1.41	1.33
2	H	220	LYS	N-CA	-6.08	1.39	1.46
3	I	12	ARG	NE-CZ	6.08	1.39	1.33
2	E	180	TYR	N-CA	-6.07	1.37	1.45
3	I	403	GLY	N-CA	6.07	1.55	1.45
2	H	94	CYS	C-N	6.07	1.42	1.33
3	I	130	PRO	C-N	6.07	1.42	1.33
3	C	146	THR	CA-C	-6.06	1.45	1.52
3	I	91	ASP	C-O	-6.06	1.16	1.24
2	B	297	SER	C-N	6.06	1.41	1.33
1	J	106	ILE	N-CA	6.06	1.53	1.46
2	E	38	LEU	C-N	6.05	1.38	1.33
1	G	108	PRO	N-CD	-6.05	1.39	1.47
1	G	198	GLY	N-CA	-6.05	1.36	1.45
2	E	293	SER	C-N	-6.05	1.25	1.33
3	I	177	LEU	CA-CB	6.04	1.61	1.53
2	K	46	TYR	CA-CB	6.04	1.63	1.53
3	L	294	SER	CA-C	-6.04	1.45	1.52
3	I	74	VAL	N-CA	-6.04	1.39	1.46
3	I	337	TRP	C-O	6.04	1.27	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	340	LYS	CA-C	-6.04	1.44	1.52
1	D	197	THR	N-CA	6.04	1.53	1.46
2	K	243	TRP	C-N	6.04	1.41	1.33
2	E	336	SER	C-N	6.03	1.41	1.33
2	K	21	ARG	CZ-NH2	6.03	1.41	1.33
3	F	167	HIS	CE1-NE2	6.02	1.38	1.32
1	A	235	VAL	CA-C	-6.02	1.45	1.52
2	K	80	VAL	CA-C	6.02	1.60	1.52
1	D	96	ARG	CA-CB	6.01	1.63	1.53
3	L	387	CYS	CA-C	-6.01	1.45	1.52
1	D	137	ASP	CA-CB	6.01	1.62	1.53
3	I	39	ASP	N-CA	-6.01	1.39	1.46
2	K	197	ALA	N-CA	-6.01	1.38	1.45
3	L	418	SER	C-N	6.00	1.41	1.33
2	K	173	PHE	CA-CB	6.00	1.60	1.53
3	C	223	LYS	CA-CB	6.00	1.63	1.53
1	J	206	GLY	N-CA	-6.00	1.36	1.45
1	D	143	LYS	CA-C	-5.99	1.45	1.52
1	D	196	PRO	CA-C	-5.99	1.44	1.52
2	H	304	GLN	CA-C	5.99	1.59	1.52
2	K	277	PRO	N-CA	-5.99	1.40	1.47
3	C	335	ARG	NE-CZ	5.98	1.39	1.33
2	E	2	GLU	N-CA	-5.98	1.38	1.46
2	K	260	ILE	CA-C	-5.98	1.45	1.52
3	L	95	THR	C-N	5.98	1.41	1.33
3	L	397	PRO	N-CA	-5.98	1.39	1.47
2	E	110	ARG	NE-CZ	5.98	1.39	1.33
3	C	293	PHE	N-CA	-5.97	1.38	1.46
2	H	213	VAL	N-CA	-5.97	1.39	1.46
2	E	238	SER	C-N	5.97	1.41	1.33
1	J	94	ARG	CZ-NH2	5.97	1.41	1.33
3	I	240	TYR	CA-C	-5.96	1.46	1.52
2	E	203	ILE	C-N	5.96	1.41	1.33
1	J	188	PHE	N-CA	-5.96	1.38	1.46
3	L	246	VAL	CA-CB	-5.96	1.47	1.54
3	I	153	TYR	N-CA	5.96	1.53	1.46
3	L	155	HIS	CE1-NE2	5.96	1.38	1.32
2	K	402	ILE	CB-CG1	5.96	1.65	1.53
3	I	131	ARG	CZ-NH1	5.96	1.41	1.32
3	L	273	GLN	CA-CB	5.96	1.63	1.53
1	D	225	ASN	CA-C	-5.95	1.45	1.52
3	I	278	LEU	CA-C	-5.95	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	13	ILE	N-CA	-5.95	1.40	1.46
3	L	120	LEU	CA-C	-5.95	1.45	1.52
1	G	163	MET	N-CA	-5.94	1.39	1.46
3	F	409	PHE	N-CA	-5.94	1.39	1.46
2	K	291	ASP	C-N	5.94	1.42	1.33
3	L	420	ARG	NE-CZ	5.94	1.39	1.33
2	B	387	ILE	C-N	5.93	1.40	1.33
1	A	217	VAL	N-CA	-5.93	1.38	1.46
3	C	96	MET	CA-C	-5.93	1.45	1.52
3	I	317	ILE	N-CA	-5.93	1.39	1.46
2	K	422	VAL	C-N	5.93	1.41	1.33
2	E	213	VAL	CA-C	-5.93	1.45	1.52
2	K	61	LYS	CA-C	-5.92	1.45	1.52
2	K	335	ASN	CA-C	-5.92	1.44	1.52
3	C	254	HIS	CE1-NE2	5.92	1.38	1.32
2	H	93	TYR	CA-C	-5.92	1.45	1.53
2	H	132	GLN	CA-C	-5.92	1.43	1.53
3	I	257	PHE	CA-C	-5.92	1.45	1.52
3	I	319	VAL	CA-C	-5.92	1.45	1.52
3	F	398	TYR	CD1-CE1	5.92	1.56	1.38
2	H	16	LYS	CA-C	-5.92	1.45	1.52
2	H	369	VAL	C-N	5.91	1.42	1.33
3	L	98	HIS	CE1-NE2	5.91	1.38	1.32
1	A	131	HIS	CB-CG	5.91	1.58	1.50
1	D	178	HIS	CE1-NE2	5.90	1.38	1.32
3	I	47	ILE	CA-C	-5.90	1.45	1.52
2	H	263	VAL	N-CA	-5.90	1.39	1.46
1	J	181	TRP	NE1-CE2	-5.90	1.30	1.37
3	L	243	ARG	CD-NE	5.90	1.54	1.46
3	I	91	ASP	CA-C	-5.90	1.45	1.52
2	K	75	ASP	C-N	5.90	1.41	1.33
3	F	287	PRO	CA-CB	5.89	1.62	1.53
2	H	392	ALA	CA-C	-5.89	1.45	1.52
1	G	129	PRO	CA-C	5.89	1.59	1.52
1	A	170	PHE	N-CA	-5.89	1.38	1.46
2	K	36	SER	N-CA	5.88	1.53	1.45
3	I	10	ALA	CA-C	-5.88	1.44	1.52
3	F	302	PRO	CA-C	-5.88	1.45	1.52
3	I	362	PRO	C-N	5.88	1.42	1.33
2	E	383	PRO	C-O	5.87	1.31	1.24
2	K	343	VAL	CA-C	-5.87	1.45	1.52
3	C	170	PRO	CA-CB	5.87	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	200	CYS	N-CA	-5.87	1.38	1.45
3	F	277	ARG	NE-CZ	5.86	1.39	1.33
1	D	172	HIS	ND1-CE1	-5.86	1.26	1.32
3	I	390	ALA	CA-C	-5.86	1.45	1.52
2	E	208	VAL	N-CA	-5.85	1.38	1.46
2	H	77	LYS	CA-C	-5.85	1.45	1.52
2	H	155	ARG	CD-NE	5.85	1.54	1.46
3	C	219	ASP	C-N	5.85	1.41	1.33
3	L	296	ARG	CD-NE	5.84	1.54	1.46
1	D	235	VAL	CA-C	-5.84	1.45	1.52
3	I	266	VAL	C-N	5.84	1.41	1.33
3	L	168	VAL	CA-C	5.84	1.59	1.52
2	H	8	PRO	CA-C	-5.84	1.46	1.52
3	F	159	LEU	C-N	5.83	1.40	1.33
3	I	133	ILE	CA-C	-5.83	1.45	1.52
3	I	219	ASP	CA-C	-5.83	1.45	1.52
3	F	416	ALA	C-N	5.83	1.41	1.33
2	H	21	ARG	CA-CB	5.83	1.62	1.53
3	C	304	HIS	CD2-NE2	5.83	1.44	1.37
3	F	387	CYS	CA-CB	5.83	1.62	1.53
1	G	185	ALA	C-N	5.83	1.40	1.33
2	B	289	ARG	CZ-NH1	5.83	1.41	1.32
2	E	114	CYS	CA-C	-5.83	1.44	1.52
3	I	33	ILE	CA-CB	-5.82	1.47	1.54
2	B	168	SER	CA-C	-5.81	1.45	1.52
3	C	398	TYR	CD1-CE1	5.81	1.56	1.38
2	H	114	CYS	N-CA	-5.81	1.39	1.46
3	I	309	ILE	C-N	5.81	1.41	1.33
1	J	238	ASN	CA-C	5.81	1.60	1.52
2	K	82	THR	C-N	5.81	1.42	1.33
1	D	152	TYR	N-CA	-5.81	1.40	1.46
2	B	56	PRO	N-CD	-5.80	1.39	1.47
3	I	224	CYS	CA-C	-5.80	1.46	1.52
3	I	5	PHE	C-N	5.80	1.41	1.33
2	H	167	SER	CA-C	5.80	1.60	1.52
3	L	130	PRO	N-CD	-5.79	1.39	1.47
2	B	430	VAL	N-CA	-5.79	1.39	1.46
3	C	97	GLY	CA-C	-5.79	1.44	1.51
1	D	241	MET	N-CA	5.79	1.52	1.46
2	H	152	SER	CA-CB	5.79	1.60	1.53
2	E	191	PRO	CA-CB	5.79	1.61	1.53
2	B	355	PHE	CA-C	-5.79	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	20	GLU	CA-C	-5.79	1.45	1.52
3	I	217	ASN	CA-CB	5.79	1.62	1.53
3	L	47	ILE	N-CA	-5.79	1.39	1.46
2	B	253	ARG	NE-CZ	5.78	1.39	1.33
3	I	261	ASP	N-CA	-5.78	1.38	1.45
2	B	108	VAL	N-CA	-5.78	1.39	1.46
3	C	161	ARG	C-O	-5.78	1.16	1.24
3	F	311	THR	CA-C	-5.78	1.46	1.52
2	H	427	VAL	CA-C	-5.78	1.45	1.52
2	E	322	SER	N-CA	5.77	1.53	1.45
3	C	237	ASN	CA-CB	5.77	1.61	1.53
2	E	189	TYR	CA-CB	5.77	1.62	1.53
2	E	21	ARG	C-N	5.77	1.40	1.33
2	E	223	ARG	CD-NE	5.77	1.54	1.46
2	H	75	ASP	C-N	5.77	1.40	1.33
2	E	170	TRP	CA-C	-5.77	1.45	1.52
2	K	17	ALA	N-CA	-5.77	1.39	1.46
2	B	128	SER	CA-C	5.76	1.60	1.52
2	E	395	ASN	C-N	5.76	1.41	1.33
2	E	253	ARG	CZ-NH1	5.76	1.40	1.32
2	E	312	PHE	C-N	5.76	1.39	1.33
3	F	398	TYR	CA-C	-5.76	1.45	1.52
3	F	388	SER	CA-CB	5.75	1.62	1.53
2	H	74	ALA	N-CA	-5.75	1.38	1.46
2	B	38	LEU	CA-C	-5.75	1.45	1.52
2	E	229	VAL	CA-CB	5.75	1.61	1.54
3	F	5	PHE	CA-C	-5.75	1.45	1.52
3	F	301	ASP	CA-C	5.75	1.59	1.53
2	H	362	GLU	N-CA	5.75	1.51	1.45
3	L	304	HIS	CE1-NE2	5.75	1.38	1.32
2	H	137	ILE	CA-CB	-5.75	1.46	1.54
2	E	199	ARG	CZ-NH2	5.74	1.41	1.33
3	F	320	GLY	N-CA	5.74	1.53	1.45
3	L	342	SER	CA-C	-5.74	1.45	1.52
3	L	196	TYR	CA-C	-5.74	1.45	1.52
3	F	257	PHE	C-N	5.74	1.40	1.33
2	H	210	SER	CA-C	-5.74	1.45	1.52
3	I	37	TRP	C-N	5.74	1.42	1.33
2	H	62	CYS	C-N	5.73	1.42	1.33
1	D	229	ARG	NE-CZ	5.73	1.39	1.33
3	F	255	VAL	N-CA	-5.73	1.41	1.46
3	C	319	VAL	CA-C	-5.72	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	110	ARG	CD-NE	5.72	1.54	1.46
3	I	315	LYS	N-CA	-5.72	1.39	1.46
2	B	302	GLU	C-N	5.72	1.40	1.33
2	B	5	THR	CA-CB	-5.72	1.43	1.53
2	B	107	TYR	CA-C	-5.72	1.45	1.52
3	I	307	GLU	CA-C	-5.72	1.45	1.52
3	F	79	ARG	CZ-NH1	5.72	1.40	1.32
2	H	57	SER	CA-C	-5.72	1.45	1.52
2	B	11	VAL	C-O	-5.72	1.17	1.24
3	F	166	MET	CG-SD	5.72	1.95	1.80
3	C	98	HIS	CE1-NE2	5.71	1.38	1.32
2	E	375	THR	C-N	5.71	1.41	1.33
2	B	161	PHE	CA-C	-5.71	1.45	1.52
3	C	248	GLU	CA-C	-5.71	1.45	1.52
2	B	225	ALA	N-CA	-5.71	1.41	1.46
2	B	244	LYS	C-N	5.71	1.41	1.33
2	B	71	LYS	N-CA	-5.70	1.39	1.46
2	B	270	ASN	CA-CB	5.70	1.61	1.53
2	E	228	ASN	CA-C	-5.70	1.45	1.53
1	J	229	ARG	CD-NE	5.70	1.54	1.46
2	K	46	TYR	N-CA	-5.69	1.39	1.46
3	C	143	GLY	CA-C	-5.69	1.44	1.52
3	F	167	HIS	C-N	5.69	1.39	1.33
2	K	438	ARG	N-CA	-5.69	1.35	1.46
1	D	129	PRO	N-CA	-5.69	1.40	1.47
1	G	116	ASN	C-N	5.69	1.39	1.32
3	I	286	HIS	CD2-NE2	5.69	1.44	1.37
1	D	96	ARG	NE-CZ	5.69	1.39	1.33
3	I	19	ALA	N-CA	-5.69	1.38	1.46
2	H	374	ILE	C-N	5.68	1.41	1.33
3	I	243	ARG	CD-NE	5.68	1.54	1.46
2	K	110	ARG	C-N	5.68	1.39	1.33
3	I	126	PHE	CA-C	-5.68	1.45	1.52
2	B	343	VAL	CA-C	-5.68	1.45	1.52
3	L	68	TYR	N-CA	-5.68	1.38	1.45
2	H	339	MET	CA-C	-5.68	1.45	1.52
3	I	221	ALA	CA-CB	5.68	1.62	1.53
3	L	397	PRO	CA-CB	-5.68	1.45	1.53
2	H	380	CYS	CA-C	-5.68	1.45	1.52
3	C	110	VAL	N-CA	-5.67	1.39	1.46
1	G	152	TYR	CA-CB	5.67	1.63	1.53
3	L	222	PRO	N-CA	5.67	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	98	THR	C-N	5.67	1.41	1.33
3	I	334	VAL	N-CA	-5.67	1.39	1.46
1	A	169	LYS	N-CA	-5.67	1.38	1.45
2	B	19	ILE	CA-CB	5.67	1.60	1.54
2	H	178	ILE	N-CA	-5.67	1.39	1.46
2	K	289	ARG	NE-CZ	5.67	1.39	1.33
3	C	203	THR	CA-C	5.66	1.59	1.52
3	C	391	ARG	CD-NE	5.66	1.54	1.46
3	F	181	THR	C-N	5.66	1.41	1.33
3	C	208	THR	C-O	-5.66	1.17	1.24
2	H	154	ALA	N-CA	-5.66	1.39	1.46
2	B	285	ALA	CA-C	-5.66	1.46	1.52
2	H	370	CYS	CA-C	-5.66	1.45	1.52
2	E	238	SER	CA-CB	5.66	1.61	1.53
3	L	78	GLU	CA-C	-5.66	1.45	1.52
1	G	90	LYS	N-CA	-5.65	1.40	1.45
2	H	110	ARG	C-N	5.65	1.41	1.33
3	I	386	LEU	CA-CB	5.65	1.62	1.53
2	B	430	VAL	C-N	5.65	1.41	1.33
1	D	164	LYS	N-CA	-5.65	1.39	1.46
2	E	102	GLN	N-CA	-5.65	1.39	1.46
2	K	183	GLU	C-N	5.65	1.40	1.33
3	L	59	ASN	C-N	5.65	1.40	1.33
1	D	121	LEU	C-N	5.65	1.41	1.33
1	A	121	LEU	CA-C	-5.64	1.45	1.52
3	F	32	SER	C-N	5.64	1.40	1.33
2	H	67	GLU	N-CA	-5.64	1.39	1.45
2	H	436	CYS	N-CA	-5.64	1.39	1.46
2	K	300	ALA	CA-C	-5.64	1.45	1.52
3	C	354	VAL	C-N	5.64	1.41	1.33
2	K	278	ILE	N-CA	-5.64	1.39	1.46
2	K	317	SER	CA-C	-5.64	1.45	1.52
3	F	292	LEU	CA-CB	5.63	1.61	1.53
2	H	438	ARG	N-CA	-5.63	1.35	1.46
3	I	193	THR	C-N	5.63	1.40	1.33
3	I	199	THR	CA-CB	-5.63	1.44	1.53
3	L	181	THR	N-CA	-5.63	1.39	1.46
1	D	192	ARG	NE-CZ	5.63	1.39	1.33
3	F	300	LYS	CA-C	-5.63	1.45	1.52
2	E	44	GLN	CA-C	-5.63	1.45	1.52
2	E	285	ALA	CA-C	-5.63	1.48	1.53
2	K	256	PRO	CA-CB	5.63	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	410	ILE	CA-C	5.62	1.59	1.52
3	I	147	ARG	CZ-NH2	5.62	1.40	1.33
2	B	351	ALA	CA-C	-5.62	1.45	1.52
1	G	94	ARG	NE-CZ	5.62	1.39	1.33
2	H	298	LEU	CA-CB	5.62	1.61	1.53
2	E	424	ALA	N-CA	-5.62	1.39	1.46
3	I	126	PHE	N-CA	-5.62	1.39	1.46
2	K	304	GLN	C-N	5.62	1.41	1.33
2	B	398	GLU	C-N	5.62	1.45	1.33
3	I	171	ASP	CA-CB	5.62	1.63	1.53
2	B	220	LYS	CA-C	-5.61	1.46	1.52
3	C	419	ALA	CA-C	-5.61	1.45	1.52
3	F	49	VAL	N-CA	-5.61	1.40	1.46
2	E	160	LYS	CA-C	-5.61	1.45	1.52
2	K	300	ALA	N-CA	-5.61	1.38	1.45
3	L	132	PHE	CA-C	5.61	1.59	1.52
1	J	96	ARG	CD-NE	5.61	1.54	1.46
3	I	123	ARG	N-CA	5.60	1.53	1.46
3	C	132	PHE	N-CA	-5.60	1.39	1.46
2	B	69	SER	CA-CB	5.60	1.62	1.53
2	K	418	LEU	CA-C	-5.60	1.45	1.52
1	J	131	HIS	C-N	5.60	1.41	1.33
2	B	121	ALA	C-N	5.59	1.42	1.33
2	B	315	VAL	CA-C	-5.59	1.46	1.52
2	E	329	ALA	N-CA	-5.59	1.39	1.46
2	E	59	TYR	CA-C	-5.59	1.46	1.52
1	A	156	CYS	CA-C	-5.59	1.45	1.52
3	C	44	VAL	C-N	5.58	1.41	1.33
2	E	194	SER	N-CA	-5.58	1.39	1.45
2	B	184	VAL	CA-CB	-5.58	1.48	1.54
3	C	48	GLN	CA-C	-5.58	1.46	1.52
3	F	284	HIS	CE1-NE2	5.58	1.38	1.32
3	L	202	GLU	C-N	5.58	1.40	1.33
2	B	384	LYS	C-N	5.58	1.41	1.33
1	G	183	HIS	CA-C	-5.58	1.45	1.52
3	C	410	ILE	N-CA	-5.57	1.39	1.46
2	H	170	TRP	NE1-CE2	5.57	1.43	1.37
3	C	374	LEU	CA-C	-5.57	1.45	1.52
3	L	359	ASP	C-O	5.57	1.31	1.24
2	E	123	GLN	CA-CB	5.57	1.61	1.53
3	F	47	ILE	CB-CG1	5.57	1.64	1.53
3	L	317	ILE	C-N	5.57	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	11	THR	N-CA	-5.56	1.40	1.46
3	C	12	ARG	CA-C	5.56	1.59	1.52
2	B	390	TYR	C-N	5.56	1.41	1.33
2	H	9	ASN	N-CA	-5.56	1.39	1.46
3	I	85	SER	CA-C	-5.56	1.46	1.52
3	F	69	MET	N-CA	-5.55	1.39	1.46
2	B	427	VAL	C-N	5.55	1.41	1.33
3	F	67	ARG	N-CA	-5.55	1.39	1.46
3	L	63	HIS	CE1-NE2	5.55	1.38	1.32
3	L	209	ALA	CA-C	-5.55	1.46	1.52
2	H	8	PRO	CA-CB	-5.55	1.46	1.54
3	I	268	VAL	CA-CB	-5.55	1.48	1.54
2	B	148	VAL	N-CA	-5.55	1.39	1.46
3	C	226	THR	N-CA	-5.55	1.39	1.46
3	I	20	ASP	C-N	5.55	1.41	1.33
1	D	161	VAL	C-N	5.55	1.41	1.33
3	F	416	ALA	CA-CB	5.54	1.62	1.53
3	I	216	PHE	CA-C	-5.54	1.45	1.52
2	K	236	THR	CA-CB	5.54	1.61	1.53
2	H	211	THR	N-CA	5.54	1.53	1.46
3	L	305	SER	N-CA	5.54	1.53	1.45
1	D	115	VAL	N-CA	-5.54	1.39	1.46
3	L	28	PRO	CA-C	-5.54	1.47	1.52
2	E	285	ALA	C-N	5.53	1.41	1.33
3	C	16	GLY	CA-C	5.53	1.57	1.51
1	J	96	ARG	C-N	5.53	1.40	1.33
1	A	87	LYS	CA-C	5.52	1.59	1.52
2	K	397	ALA	C-N	5.52	1.41	1.33
3	L	62	ASN	CA-C	-5.52	1.45	1.52
2	B	101	SER	CA-C	-5.52	1.46	1.52
3	F	131	ARG	CZ-NH1	5.52	1.40	1.32
2	B	185	TYR	N-CA	-5.51	1.38	1.45
3	F	117	ASP	CA-CB	5.51	1.62	1.53
2	B	417	PRO	N-CA	-5.51	1.40	1.47
3	F	225	ILE	CA-C	-5.51	1.45	1.52
3	F	105	ARG	CZ-NH1	5.51	1.40	1.32
3	C	375	LEU	C-N	5.51	1.40	1.33
3	I	372	LEU	C-N	5.51	1.41	1.33
1	J	116	ASN	C-N	5.51	1.38	1.32
1	J	244	ARG	NE-CZ	5.51	1.39	1.33
2	K	411	ALA	N-CA	5.51	1.53	1.46
3	F	2	VAL	CA-C	-5.50	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	203	THR	CB-OG1	-5.50	1.34	1.43
3	I	4	HIS	CE1-NE2	5.50	1.38	1.32
3	I	371	SER	CA-C	-5.50	1.45	1.52
3	L	76	GLU	CA-CB	5.50	1.61	1.53
2	E	214	TYR	CA-C	-5.50	1.46	1.52
3	F	208	THR	CA-CB	-5.50	1.46	1.53
3	L	250	LYS	CA-CB	5.50	1.63	1.53
3	L	350	PRO	C-N	5.50	1.39	1.33
2	E	438	ARG	NE-CZ	5.49	1.39	1.33
1	G	185	ALA	CA-C	-5.49	1.45	1.52
2	E	262	LYS	N-CA	-5.49	1.39	1.46
1	G	195	ILE	N-CA	-5.49	1.41	1.46
3	L	78	GLU	CA-CB	5.49	1.61	1.53
3	F	94	ALA	CA-C	-5.48	1.45	1.52
2	B	255	ALA	CA-CB	5.48	1.62	1.53
2	H	423	VAL	CA-C	5.48	1.59	1.52
2	E	330	ILE	N-CA	-5.47	1.40	1.46
1	G	175	PRO	N-CA	5.47	1.52	1.46
3	L	347	HIS	CA-C	-5.47	1.46	1.52
2	B	410	LEU	C-O	-5.47	1.17	1.24
2	H	213	VAL	CA-CB	-5.47	1.47	1.54
1	A	218	ALA	CA-C	-5.47	1.46	1.52
3	C	83	SER	CA-C	-5.46	1.45	1.52
2	E	46	TYR	C-O	-5.46	1.17	1.23
1	J	238	ASN	C-N	5.46	1.41	1.33
3	F	326	TYR	CA-C	5.46	1.59	1.52
3	L	36	VAL	N-CA	-5.46	1.39	1.46
2	K	39	VAL	CA-C	5.46	1.57	1.52
1	G	130	ALA	N-CA	-5.46	1.39	1.46
2	B	52	LYS	CA-C	-5.46	1.46	1.52
2	H	183	GLU	CA-C	-5.46	1.45	1.52
1	A	148	LYS	CA-C	-5.45	1.45	1.52
3	C	136	GLU	C-N	5.45	1.41	1.33
3	C	152	THR	CA-C	-5.45	1.45	1.52
1	G	180	ASN	C-N	5.45	1.41	1.33
1	G	147	LYS	CA-C	5.45	1.59	1.52
2	E	148	VAL	CA-CB	-5.44	1.48	1.54
1	J	83	PRO	N-CD	5.44	1.55	1.47
3	L	125	PRO	N-CA	-5.44	1.40	1.47
2	E	17	ALA	N-CA	-5.43	1.39	1.46
2	K	73	GLU	CA-C	5.43	1.58	1.53
2	K	253	ARG	CA-C	-5.43	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	354	VAL	N-CA	-5.43	1.40	1.46
1	G	204	ASP	C-N	5.43	1.40	1.33
2	E	166	ILE	C-N	5.43	1.40	1.33
2	E	99	GLU	CA-C	-5.42	1.45	1.52
2	E	182	ASP	CA-CB	5.42	1.61	1.53
2	H	115	GLU	C-N	5.42	1.41	1.33
3	C	131	ARG	NE-CZ	5.42	1.39	1.33
2	H	316	ALA	C-N	5.42	1.41	1.33
2	K	201	GLY	N-CA	-5.42	1.39	1.45
3	I	335	ARG	CA-CB	5.42	1.63	1.53
3	I	385	PHE	C-O	-5.42	1.17	1.24
3	C	39	ASP	CA-CB	5.42	1.62	1.53
3	L	52	GLN	N-CA	-5.42	1.40	1.46
2	E	63	CYS	CA-CB	5.42	1.62	1.53
3	F	91	ASP	CA-CB	5.42	1.61	1.53
1	D	133	LYS	C-O	-5.42	1.17	1.24
2	B	157	GLN	C-N	5.41	1.41	1.33
1	J	110	MET	N-CA	-5.41	1.39	1.45
2	E	122	TYR	C-N	5.41	1.41	1.33
2	H	145	ASP	CA-C	5.41	1.59	1.52
3	L	192	LYS	CA-CB	5.41	1.62	1.53
3	L	245	GLU	C-N	5.41	1.40	1.34
3	F	286	HIS	CE1-NE2	5.41	1.38	1.32
3	F	305	SER	CA-C	-5.41	1.45	1.52
2	K	55	VAL	C-O	-5.40	1.18	1.24
1	D	193	PHE	CG-CD2	5.40	1.50	1.38
2	E	8	PRO	CA-C	-5.40	1.47	1.52
2	K	266	VAL	C-N	5.40	1.40	1.33
2	H	264	ASN	C-N	5.40	1.40	1.34
2	H	321	THR	N-CA	-5.39	1.39	1.46
3	I	270	PRO	CA-CB	-5.39	1.46	1.53
3	C	76	GLU	CA-C	-5.39	1.46	1.52
3	I	218	CYS	C-N	5.39	1.40	1.33
2	E	123	GLN	N-CA	-5.39	1.39	1.46
3	I	418	SER	C-N	5.39	1.40	1.33
2	B	302	GLU	CA-CB	5.39	1.63	1.53
2	E	20	GLU	N-CA	5.38	1.53	1.46
2	E	85	TYR	CA-CB	5.38	1.61	1.53
3	L	357	TYR	CA-C	-5.38	1.46	1.53
2	B	155	ARG	CD-NE	5.38	1.53	1.46
2	H	218	ASN	CA-C	-5.38	1.46	1.52
2	H	421	LEU	C-N	5.38	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	67	ARG	CA-C	-5.38	1.46	1.52
2	K	165	PRO	N-CD	5.38	1.55	1.47
2	E	322	SER	CA-C	-5.37	1.46	1.52
2	H	292	GLU	CA-C	5.37	1.60	1.53
2	H	149	ASN	CA-C	-5.37	1.46	1.52
1	D	195	ILE	CA-C	5.37	1.57	1.52
2	H	409	TRP	CA-C	5.37	1.59	1.52
1	A	104	ASP	C-O	-5.37	1.20	1.23
1	A	251	VAL	CA-C	-5.37	1.46	1.52
2	E	402	ILE	CA-C	-5.36	1.46	1.52
2	H	22	PRO	CA-CB	5.36	1.60	1.53
3	C	103	ARG	CZ-NH2	5.36	1.40	1.33
1	A	131	HIS	ND1-CE1	-5.36	1.27	1.32
1	J	137	ASP	C-N	5.36	1.39	1.32
3	F	306	GLN	C-O	5.36	1.30	1.23
2	B	211	THR	CA-C	5.36	1.60	1.52
3	C	324	VAL	N-CA	-5.36	1.39	1.46
3	L	161	ARG	CZ-NH2	5.36	1.40	1.33
3	C	372	LEU	CB-CG	5.35	1.64	1.53
1	G	228	ALA	N-CA	-5.35	1.41	1.46
1	G	112	ASP	C-N	5.35	1.41	1.33
3	L	257	PHE	CA-CB	5.35	1.61	1.53
3	F	385	PHE	CA-CB	5.35	1.61	1.53
1	J	202	PRO	CA-C	-5.35	1.45	1.52
3	I	209	ALA	N-CA	5.35	1.52	1.46
2	B	43	VAL	CA-CB	-5.35	1.48	1.54
3	L	315	LYS	N-CA	-5.35	1.39	1.46
2	K	69	SER	C-N	5.34	1.40	1.33
3	C	359	ASP	CA-CB	5.34	1.61	1.53
2	K	181	ARG	CD-NE	5.34	1.53	1.46
2	B	259	CYS	CA-C	-5.34	1.45	1.52
3	C	204	VAL	C-O	-5.34	1.17	1.23
2	H	102	GLN	CA-C	-5.34	1.46	1.52
2	K	317	SER	N-CA	-5.34	1.39	1.46
3	L	335	ARG	NE-CZ	5.34	1.39	1.33
3	F	363	TYR	N-CA	-5.34	1.39	1.46
2	B	389	PRO	C-N	5.34	1.41	1.33
3	F	207	GLY	C-N	5.34	1.41	1.33
1	G	234	VAL	N-CA	-5.34	1.40	1.46
2	H	313	GLY	C-N	5.34	1.38	1.33
3	L	275	THR	CA-C	-5.34	1.46	1.52
3	C	123	ARG	N-CA	-5.33	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	187	LEU	CA-CB	5.33	1.60	1.53
3	I	147	ARG	N-CA	-5.33	1.38	1.46
2	E	417	PRO	C-N	5.33	1.41	1.33
3	I	324	VAL	N-CA	-5.33	1.40	1.46
3	L	326	TYR	N-CA	5.33	1.52	1.46
2	B	219	LEU	N-CA	-5.33	1.39	1.46
2	B	267	ARG	CD-NE	5.33	1.53	1.46
1	D	110	MET	N-CA	-5.33	1.39	1.45
1	A	218	ALA	C-N	5.32	1.41	1.33
2	K	10	GLN	CA-C	-5.32	1.46	1.52
3	C	412	LEU	CA-CB	5.32	1.61	1.53
3	F	272	PRO	C-N	5.32	1.40	1.33
3	I	359	ASP	CA-C	5.32	1.59	1.52
2	B	99	GLU	CA-C	-5.32	1.45	1.52
2	E	266	VAL	CA-CB	5.32	1.61	1.54
2	B	397	ALA	CA-C	-5.31	1.45	1.53
3	F	154	SER	CA-C	-5.31	1.46	1.53
1	G	121	LEU	N-CA	-5.31	1.39	1.46
3	L	332	ASN	CA-CB	5.31	1.61	1.53
2	K	352	LEU	N-CA	-5.31	1.39	1.46
2	B	166	ILE	C-O	-5.31	1.17	1.24
3	C	150	CYS	CA-C	-5.31	1.46	1.52
2	H	249	VAL	CA-C	-5.30	1.47	1.52
3	L	75	GLN	CA-CB	5.30	1.65	1.54
1	A	86	LYS	CA-C	-5.30	1.45	1.52
3	C	375	LEU	CA-CB	5.30	1.61	1.53
3	C	313	MET	CA-C	-5.30	1.46	1.52
2	E	29	LEU	CB-CG	5.30	1.64	1.53
3	F	94	ALA	N-CA	-5.30	1.39	1.46
2	K	123	GLN	CA-C	-5.30	1.46	1.52
3	C	26	SER	C-N	5.29	1.39	1.33
2	B	253	ARG	CA-C	-5.29	1.45	1.52
2	E	403	SER	CA-C	-5.29	1.46	1.52
2	B	434	VAL	CA-C	-5.29	1.46	1.52
1	J	139	PRO	N-CA	-5.29	1.40	1.47
3	C	258	PRO	C-N	5.29	1.40	1.33
3	F	220	THR	CA-C	-5.29	1.46	1.52
2	K	155	ARG	CZ-NH2	5.29	1.40	1.33
2	K	200	PHE	CG-CD1	5.29	1.50	1.38
3	F	309	ILE	CA-C	-5.29	1.46	1.52
2	H	169	ALA	C-N	5.29	1.40	1.33
3	I	167	HIS	CG-ND1	5.29	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	12	ARG	NE-CZ	5.28	1.38	1.33
1	J	113	GLY	CA-C	5.28	1.58	1.51
2	E	267	ARG	CD-NE	5.28	1.53	1.46
3	F	223	LYS	N-CA	-5.28	1.39	1.46
2	B	392	ALA	CA-C	-5.28	1.45	1.52
2	H	4	SER	CA-C	-5.28	1.45	1.52
2	K	79	SER	CA-C	-5.28	1.46	1.52
2	H	421	LEU	CA-C	-5.28	1.46	1.52
3	I	111	GLU	N-CA	-5.28	1.39	1.46
1	J	185	ALA	CA-CB	5.28	1.62	1.53
1	J	207	ARG	CD-NE	5.28	1.53	1.46
1	A	172	HIS	N-CA	-5.27	1.39	1.46
2	E	235	GLN	CA-C	-5.27	1.46	1.52
3	L	29	SER	CA-C	-5.27	1.45	1.52
3	C	45	LEU	N-CA	-5.27	1.39	1.46
3	F	296	ARG	C-N	5.27	1.40	1.33
2	H	63	CYS	CA-CB	5.27	1.61	1.53
2	K	178	ILE	CA-C	-5.27	1.46	1.52
1	J	219	ILE	C-N	5.27	1.40	1.33
2	B	228	ASN	CA-C	-5.26	1.45	1.53
3	C	37	TRP	N-CA	5.26	1.52	1.46
2	K	296	VAL	CA-C	-5.26	1.46	1.52
3	L	55	ILE	C-O	-5.26	1.18	1.24
1	A	185	ALA	C-N	5.26	1.40	1.33
1	A	205	SER	CA-C	-5.26	1.46	1.52
2	B	226	SER	CA-C	-5.26	1.47	1.53
1	J	225	ASN	C-N	5.26	1.40	1.33
2	K	348	GLU	CA-C	-5.26	1.45	1.52
3	L	55	ILE	CA-CB	5.26	1.62	1.54
3	F	104	CYS	CA-CB	5.25	1.61	1.53
1	J	219	ILE	CB-CG1	5.25	1.64	1.53
2	B	216	ASN	CA-CB	5.25	1.62	1.53
2	H	345	ASP	N-CA	-5.25	1.39	1.46
3	I	273	GLN	N-CA	-5.25	1.39	1.46
2	K	289	ARG	C-N	5.25	1.40	1.33
2	K	384	LYS	N-CA	-5.25	1.39	1.46
2	B	226	SER	CA-CB	5.25	1.61	1.54
2	E	378	GLY	C-N	5.24	1.40	1.33
1	G	244	ARG	CA-C	-5.24	1.47	1.53
3	C	223	LYS	C-N	5.24	1.40	1.33
2	E	413	THR	CA-C	-5.24	1.45	1.52
1	J	186	VAL	C-O	-5.24	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	LEU	CB-CG	5.24	1.64	1.53
2	K	300	ALA	C-N	5.23	1.40	1.33
3	C	347	HIS	CG-CD2	5.23	1.41	1.35
3	I	395	LEU	C-O	-5.23	1.17	1.24
2	B	26	GLY	C-N	5.23	1.39	1.33
3	C	21	CYS	CA-C	-5.23	1.48	1.52
1	G	182	HIS	CA-C	-5.23	1.45	1.52
3	C	289	TYR	CA-CB	5.22	1.61	1.53
2	H	61	LYS	CA-C	-5.22	1.46	1.52
3	I	336	LEU	CA-C	-5.22	1.46	1.52
3	L	127	SER	CA-CB	5.22	1.61	1.53
3	C	137	LYS	N-CA	-5.22	1.39	1.46
1	G	165	SER	CA-CB	5.22	1.61	1.53
3	C	164	ILE	CB-CG1	5.22	1.63	1.53
3	I	292	LEU	CB-CG	5.22	1.63	1.53
2	B	180	TYR	CA-CB	5.22	1.61	1.53
3	C	122	CYS	CA-C	-5.22	1.46	1.52
2	K	127	ALA	N-CA	-5.21	1.39	1.45
2	K	349	SER	CA-C	-5.21	1.47	1.53
2	K	373	ARG	NE-CZ	5.21	1.38	1.33
3	I	161	ARG	CD-NE	5.21	1.53	1.46
2	K	190	ALA	CA-CB	5.21	1.61	1.53
2	E	347	GLN	C-N	5.21	1.40	1.33
1	G	155	GLU	CA-C	-5.21	1.46	1.52
2	H	370	CYS	N-CA	5.21	1.52	1.46
3	I	283	PHE	CA-C	-5.21	1.46	1.52
3	C	420	ARG	CD-NE	5.21	1.53	1.46
1	A	102	GLU	N-CA	-5.21	1.39	1.46
3	F	161	ARG	CD-NE	5.21	1.53	1.46
1	G	172	HIS	ND1-CE1	-5.21	1.27	1.32
1	D	229	ARG	CA-CB	5.20	1.62	1.54
2	E	146	VAL	N-CA	-5.20	1.40	1.46
1	G	190	ASN	CA-C	-5.20	1.46	1.53
2	H	430	VAL	CA-CB	5.20	1.60	1.54
3	F	26	SER	CA-C	-5.20	1.46	1.52
3	I	224	CYS	N-CA	-5.20	1.40	1.46
3	L	380	SER	C-N	5.20	1.40	1.33
1	A	196	PRO	CA-C	-5.20	1.46	1.52
3	I	57	LYS	CA-CB	5.20	1.61	1.53
3	C	311	THR	C-O	5.20	1.28	1.24
1	A	236	THR	N-CA	-5.20	1.39	1.45
1	D	171	THR	CA-C	5.20	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	21	ARG	CZ-NH1	5.20	1.40	1.32
3	L	271	GLU	CA-CB	5.20	1.60	1.53
3	C	206	GLU	N-CA	-5.19	1.40	1.46
2	K	69	SER	CA-C	-5.19	1.47	1.52
2	B	283	ALA	CA-C	-5.19	1.46	1.52
1	D	191	GLY	CA-C	-5.19	1.44	1.51
1	G	171	THR	C-N	5.19	1.41	1.33
2	K	168	SER	CA-C	-5.19	1.46	1.52
3	L	179	SER	CA-CB	5.19	1.62	1.53
3	I	156	GLN	C-N	5.19	1.40	1.33
3	L	305	SER	CA-CB	5.19	1.63	1.54
3	F	4	HIS	ND1-CE1	5.19	1.37	1.32
3	C	68	TYR	CA-C	-5.18	1.46	1.52
2	E	55	VAL	CA-C	-5.18	1.47	1.52
2	K	145	ASP	C-N	5.18	1.39	1.33
2	K	149	ASN	C-N	5.18	1.40	1.33
3	L	333	PRO	CA-CB	5.18	1.60	1.53
1	G	224	ALA	C-N	5.18	1.40	1.33
1	A	223	GLY	N-CA	-5.18	1.39	1.45
1	A	121	LEU	CB-CG	5.18	1.63	1.53
1	J	125	LYS	CA-C	-5.18	1.46	1.52
2	B	67	GLU	C-N	5.17	1.40	1.33
3	L	261	ASP	CA-C	-5.17	1.46	1.52
1	A	244	ARG	CD-NE	5.17	1.53	1.46
3	I	170	PRO	N-CD	-5.17	1.40	1.47
1	G	126	VAL	N-CA	-5.17	1.40	1.46
2	H	177	VAL	CA-C	-5.17	1.46	1.52
2	H	110	ARG	NE-CZ	5.17	1.38	1.33
3	F	79	ARG	CD-NE	5.17	1.53	1.46
1	D	194	THR	N-CA	-5.16	1.39	1.45
2	H	38	LEU	CB-CG	5.16	1.63	1.53
3	I	49	VAL	N-CA	-5.16	1.40	1.46
1	G	164	LYS	N-CA	-5.16	1.40	1.46
1	A	143	LYS	C-N	5.16	1.40	1.33
2	K	173	PHE	N-CA	-5.16	1.39	1.46
1	A	192	ARG	CD-NE	5.15	1.53	1.46
2	E	181	ARG	CD-NE	5.15	1.53	1.46
3	L	341	SER	C-N	5.15	1.41	1.33
3	I	50	SER	CA-CB	5.15	1.61	1.53
3	F	346	ALA	CA-C	-5.15	1.46	1.53
3	L	415	CYS	CA-C	-5.15	1.46	1.52
3	L	398	TYR	CD1-CE1	5.15	1.54	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	GLU	CA-CB	5.14	1.61	1.53
3	C	356	HIS	CE1-NE2	5.14	1.37	1.32
1	G	243	THR	CA-C	-5.14	1.46	1.52
3	F	205	LYS	N-CA	-5.14	1.39	1.46
3	I	391	ARG	CA-C	-5.14	1.46	1.52
1	J	227	GLY	CA-C	5.14	1.59	1.51
2	K	281	ASP	N-CA	5.14	1.52	1.46
3	L	128	HIS	CE1-NE2	5.14	1.37	1.32
2	B	122	TYR	CA-C	-5.14	1.46	1.52
2	B	187	GLU	C-N	5.14	1.40	1.33
3	C	118	PRO	C-N	5.13	1.41	1.33
1	J	179	TYR	C-N	5.13	1.41	1.33
3	C	407	PRO	N-CA	-5.13	1.40	1.47
1	G	186	VAL	CA-C	-5.13	1.46	1.52
3	L	265	ALA	CA-C	5.13	1.59	1.52
3	C	60	THR	N-CA	-5.13	1.39	1.45
2	H	410	LEU	N-CA	5.13	1.52	1.46
3	C	304	HIS	CA-C	-5.13	1.46	1.52
2	K	124	VAL	CA-CB	-5.13	1.48	1.54
3	L	347	HIS	CE1-NE2	5.13	1.37	1.32
2	E	308	TYR	C-N	5.12	1.41	1.33
2	B	371	ASN	C-N	5.12	1.40	1.33
3	I	263	THR	C-N	5.12	1.40	1.33
3	L	111	GLU	CA-C	5.12	1.58	1.52
1	G	209	ILE	N-CA	-5.12	1.40	1.46
3	C	420	ARG	CZ-NH1	5.12	1.40	1.32
1	D	220	VAL	C-N	5.12	1.40	1.33
2	H	419	THR	C-O	-5.12	1.18	1.24
1	J	123	GLY	CA-C	5.12	1.59	1.51
3	L	9	LYS	CA-C	-5.12	1.46	1.52
1	D	204	ASP	CA-C	-5.12	1.45	1.52
3	L	389	VAL	N-CA	5.12	1.52	1.46
3	C	144	HIS	CE1-NE2	5.11	1.37	1.32
2	H	85	TYR	CA-C	5.11	1.59	1.52
1	J	204	ASP	CA-C	-5.11	1.46	1.52
2	K	406	ALA	CA-C	-5.11	1.46	1.52
1	G	142	ALA	CA-C	-5.11	1.46	1.52
2	B	162	ILE	C-O	-5.11	1.18	1.24
3	C	239	GLN	CA-C	5.10	1.59	1.52
2	K	59	TYR	N-CA	5.10	1.52	1.46
3	L	287	PRO	N-CD	-5.10	1.40	1.47
2	B	95	PHE	CA-CB	5.10	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	233	VAL	CA-CB	-5.10	1.49	1.55
2	E	179	VAL	CA-C	-5.10	1.46	1.52
2	B	222	LYS	CA-CB	5.09	1.62	1.53
3	F	318	GLN	CA-C	-5.09	1.46	1.52
3	C	392	THR	C-N	5.09	1.40	1.33
2	E	271	CYS	CA-CB	5.09	1.60	1.53
2	K	102	GLN	CA-C	-5.09	1.46	1.52
2	E	368	GLN	CD-NE2	5.09	1.44	1.33
2	H	207	THR	C-N	-5.09	1.28	1.34
2	H	438	ARG	C-N	-5.09	1.26	1.33
3	L	312	PRO	CA-CB	-5.09	1.46	1.53
2	B	9	ASN	CA-CB	5.08	1.59	1.53
2	B	99	GLU	N-CA	-5.08	1.39	1.46
2	E	199	ARG	C-N	5.08	1.40	1.33
3	F	156	GLN	CD-NE2	5.08	1.44	1.33
1	G	152	TYR	CA-C	-5.08	1.46	1.52
3	L	204	VAL	C-N	5.08	1.40	1.33
3	L	338	ALA	N-CA	-5.08	1.39	1.46
3	I	327	VAL	CA-CB	-5.08	1.48	1.54
3	C	360	LEU	CA-CB	5.07	1.62	1.53
1	D	188	PHE	N-CA	-5.07	1.40	1.46
2	E	122	TYR	N-CA	-5.07	1.39	1.46
3	L	106	PRO	N-CA	-5.07	1.40	1.47
1	G	243	THR	N-CA	-5.07	1.39	1.45
1	J	245	ILE	CA-CB	-5.07	1.48	1.54
3	I	32	SER	C-O	-5.07	1.18	1.23
3	C	147	ARG	CD-NE	5.07	1.53	1.46
1	G	83	PRO	N-CD	5.07	1.54	1.47
2	K	215	ALA	CA-C	-5.07	1.46	1.52
2	K	361	VAL	C-N	5.07	1.40	1.33
2	B	140	LEU	CA-C	-5.07	1.46	1.52
1	J	115	VAL	CA-CB	5.07	1.58	1.53
2	H	180	TYR	CA-C	-5.06	1.46	1.53
3	I	42	ASP	C-N	5.06	1.41	1.33
2	K	148	VAL	CA-C	-5.06	1.46	1.52
2	H	206	ARG	CD-NE	5.06	1.53	1.46
3	I	162	GLU	CA-CB	5.06	1.61	1.53
3	C	124	THR	C-N	5.06	1.39	1.33
1	D	160	PRO	CA-C	-5.06	1.46	1.52
2	E	244	LYS	N-CA	-5.06	1.40	1.46
1	J	158	GLN	C-N	5.06	1.39	1.33
3	I	238	SER	CA-C	-5.06	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	83	SER	N-CA	-5.06	1.39	1.45
3	C	131	ARG	CZ-NH1	5.05	1.39	1.32
2	E	41	SER	N-CA	-5.05	1.40	1.46
2	E	59	TYR	CG-CD1	5.05	1.50	1.39
2	E	193	GLY	CA-C	-5.05	1.44	1.51
2	K	358	THR	CA-C	-5.05	1.46	1.52
2	B	46	TYR	CZ-OH	5.05	1.48	1.38
3	F	51	MET	CA-CB	5.05	1.61	1.53
3	I	287	PRO	CA-CB	5.05	1.60	1.53
2	K	23	GLY	N-CA	-5.05	1.40	1.45
3	F	211	ASN	CA-C	-5.05	1.46	1.52
3	F	67	ARG	NE-CZ	5.04	1.38	1.33
1	G	172	HIS	CD2-NE2	-5.04	1.32	1.37
3	I	371	SER	C-N	-5.04	1.27	1.33
2	B	432	SER	N-CA	-5.04	1.40	1.46
3	L	247	THR	C-N	5.04	1.40	1.33
3	C	388	SER	N-CA	-5.04	1.40	1.46
1	J	119	ALA	N-CA	-5.04	1.39	1.45
3	L	85	SER	CA-C	-5.04	1.46	1.52
2	B	19	ILE	C-N	5.04	1.40	1.33
2	E	79	SER	CA-C	-5.04	1.46	1.52
3	I	304	HIS	CG-CD2	-5.04	1.30	1.35
2	E	105	GLU	CA-CB	5.03	1.62	1.53
3	I	189	PRO	CA-CB	-5.03	1.46	1.53
2	B	21	ARG	CZ-NH2	5.03	1.40	1.33
2	E	6	THR	CA-C	-5.03	1.46	1.52
2	E	89	TRP	NE1-CE2	-5.03	1.31	1.37
3	F	376	ILE	CA-C	5.03	1.59	1.52
3	I	74	VAL	CA-CB	-5.03	1.48	1.54
3	I	123	ARG	NE-CZ	5.03	1.38	1.33
3	F	281	VAL	CA-C	-5.03	1.46	1.52
2	K	282	ILE	CA-C	-5.03	1.46	1.52
3	L	207	GLY	CA-C	-5.03	1.46	1.51
2	B	223	ARG	CA-C	5.02	1.59	1.52
2	H	165	PRO	C-O	-5.02	1.17	1.23
3	I	127	SER	N-CA	-5.02	1.40	1.46
1	J	201	LYS	C-N	-5.02	1.27	1.33
2	K	262	LYS	C-N	-5.02	1.27	1.33
3	F	72	ASN	CA-CB	5.02	1.61	1.53
1	G	140	GLU	CA-C	-5.02	1.46	1.52
2	K	200	PHE	CA-CB	5.02	1.61	1.53
2	K	253	ARG	NE-CZ	5.02	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	PHE	C-N	5.02	1.40	1.33
1	J	191	GLY	N-CA	-5.02	1.38	1.45
2	K	164	GLY	C-N	5.02	1.40	1.33
1	G	225	ASN	N-CA	-5.01	1.39	1.46
2	E	110	ARG	CD-NE	5.01	1.53	1.46
3	C	220	THR	CA-C	-5.01	1.46	1.52
3	C	233	VAL	C-N	5.01	1.40	1.33
2	E	58	PRO	CA-C	-5.01	1.45	1.52
3	F	123	ARG	CZ-NH1	5.01	1.39	1.32
2	H	298	LEU	N-CA	-5.01	1.39	1.46
2	K	287	PHE	CA-CB	5.01	1.61	1.53
1	A	158	GLN	C-N	5.01	1.37	1.33
3	L	115	SER	C-N	5.01	1.40	1.33
3	F	113	SER	C-N	5.01	1.40	1.33
2	K	17	ALA	CA-C	-5.01	1.46	1.52
3	C	295	ILE	CA-C	-5.00	1.46	1.52

All (2055) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	229	VAL	CA-C-O	-22.83	97.21	120.27
2	K	229	VAL	CA-C-O	-20.49	98.76	120.48
2	H	229	VAL	CA-C-O	-19.39	98.79	121.28
2	E	229	VAL	CA-C-O	-18.93	101.76	120.31
1	J	237	TRP	CD2-CE2-CZ2	-15.78	106.62	122.40
1	G	237	TRP	CD2-CE2-CZ2	-15.66	106.74	122.40
1	A	237	TRP	CD2-CE2-CZ2	-15.64	106.76	122.40
1	D	237	TRP	CD2-CE2-CZ2	-14.82	107.58	122.40
3	I	200	CYS	CA-C-N	13.26	132.37	122.16
3	I	200	CYS	C-N-CA	13.26	132.37	122.16
3	F	80	SER	N-CA-C	-13.07	99.72	114.62
1	G	237	TRP	NE1-CE2-CZ2	12.99	149.59	130.10
2	B	312	PHE	CA-CB-CG	-12.50	101.30	113.80
1	A	101	ILE	N-CA-C	-12.38	101.72	112.12
2	K	34	ILE	N-CA-C	-11.92	100.36	111.45
2	B	34	ILE	N-CA-C	-11.89	100.39	111.45
2	E	238	SER	CA-C-N	11.88	135.30	120.22
2	E	238	SER	C-N-CA	11.88	135.30	120.22
2	B	382	PRO	CA-C-O	-11.64	111.53	120.73
1	G	131	HIS	ND1-CE1-NE2	11.63	120.03	108.40
2	B	311	ASP	CA-CB-CG	-11.50	101.10	112.60
1	D	237	TRP	NE1-CE2-CZ2	11.46	147.29	130.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	23	GLY	N-CA-C	-11.29	96.93	111.72
2	K	13	ILE	CA-C-O	-11.11	111.97	119.19
3	F	137	LYS	N-CA-C	-11.10	97.98	112.41
3	L	345	SER	N-CA-C	-11.08	101.99	114.62
2	K	15	PHE	CA-CB-CG	-10.90	102.90	113.80
2	E	137	ILE	N-CA-C	-10.87	101.84	112.17
1	A	237	TRP	NE1-CE2-CZ2	10.83	146.34	130.10
1	G	128	LYS	CA-C-O	-10.81	107.86	118.34
3	L	167	HIS	ND1-CE1-NE2	10.73	119.13	108.40
2	H	428	VAL	CB-CA-C	-10.64	97.77	112.14
1	J	237	TRP	NE1-CE2-CZ2	10.51	145.87	130.10
1	J	104	ASP	CA-CB-CG	10.47	123.07	112.60
2	H	57	SER	O-C-N	-10.43	109.33	121.32
2	H	356	PHE	CA-CB-CG	-10.41	103.39	113.80
3	L	91	ASP	CA-CB-CG	-10.40	102.19	112.60
3	F	82	LEU	N-CA-C	-10.36	92.73	108.99
1	G	159	VAL	CA-C-N	10.27	132.68	119.84
1	G	159	VAL	C-N-CA	10.27	132.68	119.84
3	L	42	ASP	N-CA-C	-10.20	100.33	113.17
2	H	162	ILE	N-CA-C	-10.18	92.61	107.78
3	I	140	ALA	CA-C-N	10.18	132.56	119.84
3	I	140	ALA	C-N-CA	10.18	132.56	119.84
1	D	195	ILE	N-CA-C	-10.17	96.24	108.45
3	L	216	PHE	CA-CB-CG	10.04	123.84	113.80
3	L	148	ILE	CA-C-N	9.95	129.71	119.76
3	L	148	ILE	C-N-CA	9.95	129.71	119.76
3	C	135	ASN	OD1-CG-ND2	9.87	132.47	122.60
2	E	151	ASP	CA-CB-CG	9.85	122.45	112.60
3	F	158	ASP	CA-CB-CG	-9.83	102.77	112.60
3	L	167	HIS	CE1-NE2-CD2	-9.82	99.18	109.00
1	G	147	LYS	CA-C-O	-9.81	110.02	121.11
2	H	228	ASN	CA-CB-CG	-9.77	102.83	112.60
1	D	190	ASN	OD1-CG-ND2	9.73	132.33	122.60
1	D	237	TRP	CH2-CZ2-CE2	-9.73	104.85	117.50
1	D	140	GLU	CA-C-N	9.70	133.28	120.28
1	D	140	GLU	C-N-CA	9.70	133.28	120.28
3	C	2	VAL	N-CA-C	-9.66	102.49	111.67
2	E	339	MET	N-CA-C	-9.63	95.08	109.81
2	H	34	ILE	N-CA-C	-9.54	102.58	111.45
3	L	173	PRO	CA-C-N	9.51	137.71	122.68
3	L	173	PRO	C-N-CA	9.51	137.71	122.68
1	G	220	VAL	N-CA-CB	9.51	121.60	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	138	ASN	O-C-N	-9.49	115.21	121.85
1	A	190	ASN	CA-CB-CG	-9.48	103.12	112.60
2	K	437	ALA	O-C-N	9.48	132.17	122.12
3	C	91	ASP	CA-CB-CG	-9.41	103.19	112.60
2	B	15	PHE	CA-CB-CG	-9.33	104.47	113.80
2	K	291	ASP	N-CA-C	-9.32	101.22	112.59
2	K	145	ASP	CA-CB-CG	-9.31	103.29	112.60
3	C	66	ILE	N-CA-C	-9.30	96.07	108.35
1	D	209	ILE	N-CA-C	-9.29	93.62	107.37
2	E	365	PHE	CA-CB-CG	9.27	123.07	113.80
1	A	237	TRP	CD2-CE3-CZ3	9.26	130.63	118.60
1	J	237	TRP	CH2-CZ2-CE2	-9.26	105.47	117.50
2	B	84	VAL	N-CA-C	9.25	121.86	109.37
3	F	20	ASP	CA-CB-CG	-9.24	103.36	112.60
2	E	34	ILE	N-CA-C	-9.23	102.34	110.74
2	K	72	ASN	CA-CB-CG	-9.22	103.38	112.60
1	A	182	HIS	CA-CB-CG	-9.16	104.64	113.80
1	A	196	PRO	CA-C-O	-9.12	110.98	121.56
2	K	231	VAL	N-CA-CB	9.07	126.92	111.50
2	H	435	VAL	CA-C-N	9.05	132.41	120.28
2	H	435	VAL	C-N-CA	9.05	132.41	120.28
2	E	282	ILE	N-CA-C	-9.04	103.79	112.29
1	G	124	ASP	N-CA-C	8.97	121.14	111.36
1	G	145	THR	CA-C-O	-8.97	111.46	120.70
1	D	190	ASN	N-CA-C	-8.96	101.64	112.58
3	I	371	SER	N-CA-C	8.95	120.65	111.07
3	C	21	CYS	N-CA-C	-8.90	100.75	113.21
3	L	398	TYR	CG-CD2-CE2	-8.90	107.85	121.20
1	G	195	ILE	CA-CB-CG1	8.88	125.50	110.40
2	E	434	VAL	N-CA-C	8.87	119.66	110.62
2	B	49	CYS	N-CA-C	-8.85	97.31	108.45
2	H	151	ASP	CA-C-N	8.81	133.26	122.42
2	H	151	ASP	C-N-CA	8.81	133.26	122.42
3	C	369	LEU	CA-C-N	8.80	131.89	120.44
3	C	369	LEU	C-N-CA	8.80	131.89	120.44
3	C	262	SER	N-CA-C	-8.80	97.36	108.45
2	K	425	ILE	CA-C-N	8.77	131.61	120.56
2	K	425	ILE	C-N-CA	8.77	131.61	120.56
2	H	362	GLU	O-C-N	-8.74	115.27	121.65
3	C	412	LEU	CA-C-N	8.70	132.64	120.29
3	C	412	LEU	C-N-CA	8.70	132.64	120.29
2	H	255	ALA	CA-C-N	8.69	129.02	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	255	ALA	C-N-CA	8.69	129.02	119.90
1	J	237	TRP	CE3-CZ3-CH2	8.64	132.34	121.10
3	I	75	GLN	OE1-CD-NE2	-8.62	113.98	122.60
3	I	360	LEU	N-CA-C	8.60	120.27	111.07
3	L	168	VAL	CA-C-N	8.60	129.23	120.38
3	L	168	VAL	C-N-CA	8.60	129.23	120.38
3	L	105	ARG	NE-CZ-NH1	8.59	130.09	121.50
1	D	200	GLY	N-CA-C	-8.56	92.89	113.18
1	D	237	TRP	CD2-CE3-CZ3	8.48	129.62	118.60
2	E	348	GLU	N-CA-C	-8.46	96.21	109.07
1	J	112	ASP	CA-CB-CG	-8.46	104.14	112.60
2	K	409	TRP	CA-C-N	8.42	131.56	120.28
2	K	409	TRP	C-N-CA	8.42	131.56	120.28
2	E	382	PRO	N-CA-C	-8.40	100.45	110.70
2	K	161	PHE	CA-CB-CG	-8.39	105.41	113.80
3	F	398	TYR	CG-CD2-CE2	-8.39	108.62	121.20
2	E	161	PHE	N-CA-C	-8.36	96.28	109.50
1	A	151	LYS	N-CA-C	-8.35	102.65	113.17
2	E	164	GLY	CA-C-N	8.35	128.41	119.89
2	E	164	GLY	C-N-CA	8.35	128.41	119.89
3	I	380	SER	CA-C-N	8.34	129.24	119.98
3	I	380	SER	C-N-CA	8.34	129.24	119.98
3	F	305	SER	O-C-N	-8.33	112.47	122.96
2	K	212	ASP	CA-CB-CG	-8.33	104.27	112.60
3	L	169	PRO	CA-C-N	8.32	130.24	119.84
3	L	169	PRO	C-N-CA	8.32	130.24	119.84
2	B	228	ASN	OD1-CG-ND2	8.30	130.90	122.60
2	B	207	THR	CA-C-N	8.26	131.77	120.46
2	B	207	THR	C-N-CA	8.26	131.77	120.46
1	A	237	TRP	CH2-CZ2-CE2	-8.26	106.77	117.50
1	J	204	ASP	N-CA-C	-8.20	102.03	114.16
1	G	116	ASN	CA-C-O	8.20	129.62	119.95
1	G	128	LYS	O-C-N	8.18	128.40	120.71
1	A	127	MET	N-CA-C	-8.15	102.89	112.92
2	E	21	ARG	CA-C-O	-8.15	111.81	120.70
3	I	398	TYR	CG-CD2-CE2	-8.15	108.98	121.20
1	G	162	CYS	CA-C-N	8.14	131.19	120.28
1	G	162	CYS	C-N-CA	8.14	131.19	120.28
3	I	253	ILE	CA-C-N	8.14	135.79	120.97
3	I	253	ILE	C-N-CA	8.14	135.79	120.97
3	F	255	VAL	N-CA-C	-8.14	98.45	107.73
3	I	66	ILE	N-CA-C	-8.13	96.42	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	131	HIS	CE1-NE2-CD2	-8.12	100.88	109.00
3	L	327	VAL	N-CA-C	-8.12	96.74	108.11
2	E	309	SER	N-CA-C	-8.11	96.75	109.72
2	K	436	CYS	CA-C-N	8.11	131.14	120.28
2	K	436	CYS	C-N-CA	8.11	131.14	120.28
2	K	98	THR	N-CA-C	-8.10	102.86	114.12
3	C	231	ASN	CA-C-N	8.10	137.01	121.54
3	C	231	ASN	C-N-CA	8.10	137.01	121.54
3	L	132	PHE	CA-CB-CG	-8.09	105.71	113.80
3	L	296	ARG	NE-CZ-NH2	8.08	126.48	119.20
3	L	112	VAL	N-CA-C	-8.08	96.80	108.11
1	J	172	HIS	N-CA-C	-8.08	102.20	114.16
2	E	221	LEU	N-CA-CB	8.06	123.35	110.46
2	E	84	VAL	O-C-N	8.05	131.36	122.75
3	C	402	PRO	CA-C-N	8.05	136.18	121.70
3	C	402	PRO	C-N-CA	8.05	136.18	121.70
1	G	243	THR	N-CA-CB	8.04	123.72	110.85
2	H	245	LYS	N-CA-CB	8.04	121.72	110.07
3	C	304	HIS	ND1-CE1-NE2	8.02	116.42	108.40
1	D	182	HIS	N-CA-C	-8.01	102.30	114.16
1	G	237	TRP	CH2-CZ2-CE2	-8.01	107.08	117.50
3	F	348	GLY	CA-C-N	8.01	132.85	120.68
3	F	348	GLY	C-N-CA	8.01	132.85	120.68
1	J	146	PHE	CA-CB-CG	8.01	121.81	113.80
1	A	138	ASN	N-CA-C	-8.00	98.97	108.25
1	G	183	HIS	N-CA-C	-7.99	96.84	109.23
3	F	221	ALA	CA-C-O	-7.98	109.22	120.16
2	E	100	ASN	CA-CB-CG	7.97	120.57	112.60
3	C	284	HIS	CA-CB-CG	-7.96	105.84	113.80
3	L	251	GLY	N-CA-C	-7.96	99.48	111.10
3	F	399	GLN	CA-C-N	7.95	133.83	121.19
3	F	399	GLN	C-N-CA	7.95	133.83	121.19
3	I	12	ARG	CA-C-N	7.95	129.78	119.84
3	I	12	ARG	C-N-CA	7.95	129.78	119.84
2	K	137	ILE	N-CA-C	-7.93	104.97	112.83
2	B	54	VAL	N-CA-C	-7.93	96.03	107.77
2	E	222	LYS	O-C-N	7.92	132.28	123.25
3	I	286	HIS	ND1-CE1-NE2	7.92	116.32	108.40
3	I	4	HIS	CA-C-N	7.92	130.89	120.28
3	I	4	HIS	C-N-CA	7.92	130.89	120.28
1	D	210	PHE	CA-CB-CG	7.91	121.71	113.80
2	E	424	ALA	CB-CA-C	-7.90	97.68	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	74	VAL	N-CA-CB	7.88	119.98	111.00
2	E	203	ILE	N-CA-CB	7.88	121.43	110.56
3	L	155	HIS	CB-CG-ND1	-7.88	110.89	122.70
2	K	385	ASP	CA-C-N	7.85	135.84	121.70
2	K	385	ASP	C-N-CA	7.85	135.84	121.70
3	C	194	ILE	CA-C-N	7.85	133.21	122.77
3	C	194	ILE	C-N-CA	7.85	133.21	122.77
2	B	209	ASN	N-CA-C	-7.84	95.48	108.34
1	A	221	LEU	N-CA-C	-7.84	104.24	113.88
1	D	90	LYS	CA-C-N	7.83	129.63	119.84
1	D	90	LYS	C-N-CA	7.83	129.63	119.84
1	J	183	HIS	ND1-CE1-NE2	7.83	116.23	108.40
1	J	237	TRP	CD2-CE3-CZ3	7.83	128.78	118.60
3	L	333	PRO	N-CA-CB	7.83	110.62	103.34
2	H	303	VAL	CA-C-O	-7.82	112.37	120.27
3	L	284	HIS	CA-CB-CG	7.82	121.62	113.80
2	E	431	VAL	N-CA-C	7.82	117.92	110.42
3	L	66	ILE	N-CA-C	-7.81	97.26	108.42
3	F	312	PRO	N-CA-CB	7.80	110.14	103.35
2	K	41	SER	CB-CA-C	-7.79	99.93	111.77
3	C	387	CYS	CA-C-O	-7.79	112.64	120.82
3	L	407	PRO	N-CA-C	-7.78	103.37	114.18
2	B	362	GLU	CB-CG-CD	-7.76	99.41	112.60
1	D	142	ALA	O-C-N	7.76	130.06	122.07
3	L	289	TYR	CA-C-N	7.76	129.54	119.84
3	L	289	TYR	C-N-CA	7.76	129.54	119.84
3	I	408	THR	N-CA-C	7.73	120.69	111.33
2	B	250	PRO	O-C-N	7.73	132.59	123.01
3	I	300	LYS	CA-C-O	-7.72	112.57	121.07
3	C	380	SER	CA-C-N	7.72	128.35	119.94
3	C	380	SER	C-N-CA	7.72	128.35	119.94
2	H	80	VAL	N-CA-C	-7.72	96.61	107.80
3	L	287	PRO	CA-C-O	-7.71	112.24	121.03
1	G	153	ASP	CA-CB-CG	-7.70	104.90	112.60
3	I	93	LEU	N-CA-CB	7.69	121.22	110.07
3	I	387	CYS	CB-CA-C	-7.69	98.81	110.88
1	D	229	ARG	NE-CZ-NH2	7.67	126.10	119.20
3	L	116	THR	N-CA-C	7.66	119.26	111.07
2	E	307	THR	N-CA-C	-7.65	97.69	109.24
1	A	107	PHE	CA-C-O	-7.65	112.76	119.72
2	K	370	CYS	CA-C-N	7.64	130.52	120.28
2	K	370	CYS	C-N-CA	7.64	130.52	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	PHE	CA-CB-CG	-7.63	106.17	113.80
3	I	72	ASN	CA-CB-CG	-7.63	104.97	112.60
2	B	336	SER	N-CA-C	-7.63	103.04	114.64
3	F	222	PRO	N-CA-C	-7.63	105.84	114.92
3	L	231	ASN	CA-CB-CG	-7.62	104.98	112.60
3	I	255	VAL	CA-C-O	-7.61	113.43	119.98
3	I	239	GLN	OE1-CD-NE2	-7.61	114.99	122.60
1	G	163	MET	N-CA-C	7.61	119.57	111.28
1	G	228	ALA	N-CA-C	-7.60	100.95	113.50
3	I	17	TRP	N-CA-C	7.60	121.42	110.10
3	L	138	SER	CA-C-O	-7.59	109.76	120.16
3	C	273	GLN	CA-C-O	-7.59	112.66	121.16
2	H	357	ALA	N-CA-C	-7.58	101.14	110.61
3	I	94	ALA	CB-CA-C	-7.58	97.70	110.43
3	L	302	PRO	CA-C-N	7.57	136.01	121.54
3	L	302	PRO	C-N-CA	7.57	136.01	121.54
1	D	124	ASP	N-CA-C	-7.57	101.47	111.24
3	F	188	ASP	CA-C-N	7.57	127.60	119.28
3	F	188	ASP	C-N-CA	7.57	127.60	119.28
2	K	208	VAL	CA-C-O	-7.57	112.47	120.57
3	L	118	PRO	O-C-N	7.57	131.69	122.23
2	K	109	THR	CA-C-O	-7.57	112.59	121.44
2	B	284	ASP	N-CA-C	-7.56	102.27	113.61
3	L	251	GLY	O-C-N	-7.55	116.70	123.65
1	A	204	ASP	N-CA-C	-7.55	103.14	112.88
3	F	374	LEU	CA-C-N	7.55	130.40	120.28
3	F	374	LEU	C-N-CA	7.55	130.40	120.28
3	I	264	CYS	CA-C-N	7.55	133.24	121.99
3	I	264	CYS	C-N-CA	7.55	133.24	121.99
2	H	216	ASN	OD1-CG-ND2	-7.55	115.05	122.60
3	L	286	HIS	N-CA-C	-7.53	101.47	110.13
3	F	271	GLU	CA-C-N	7.50	127.56	119.90
3	F	271	GLU	C-N-CA	7.50	127.56	119.90
3	I	269	ALA	CA-C-N	7.50	127.95	119.93
3	I	269	ALA	C-N-CA	7.50	127.95	119.93
3	L	283	PHE	N-CA-C	-7.50	96.68	108.90
3	F	150	CYS	CA-C-O	-7.48	113.44	121.45
1	J	138	ASN	CA-C-O	-7.48	113.23	120.64
2	E	280	MET	CA-C-N	7.48	133.99	123.07
2	E	280	MET	C-N-CA	7.48	133.99	123.07
2	K	257	PHE	CA-CB-CG	-7.48	106.32	113.80
3	I	398	TYR	CZ-CE2-CD2	-7.48	106.14	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	80	VAL	N-CA-CB	7.47	120.87	111.46
3	L	172	VAL	CA-C-N	7.47	127.52	119.90
3	L	172	VAL	C-N-CA	7.47	127.52	119.90
3	I	261	ASP	CA-CB-CG	7.46	120.06	112.60
1	A	207	ARG	CA-C-O	-7.46	112.19	120.25
3	F	332	ASN	OD1-CG-ND2	7.46	130.06	122.60
3	I	124	THR	O-C-N	-7.46	116.58	121.88
3	L	356	HIS	ND1-CE1-NE2	7.46	115.86	108.40
3	F	364	TRP	N-CA-C	-7.45	104.70	114.31
2	B	81	PHE	N-CA-CB	7.45	122.55	110.41
2	H	421	LEU	N-CA-C	7.45	119.04	111.07
2	B	364	ASN	N-CA-C	-7.45	97.55	109.76
1	A	121	LEU	CA-C-O	-7.44	112.50	120.46
1	G	173	GLU	CA-C-O	-7.43	113.19	121.51
2	B	285	ALA	N-CA-CB	7.42	121.21	110.37
1	D	88	LYS	N-CA-C	-7.42	97.80	109.07
3	I	25	GLY	O-C-N	7.41	130.09	122.75
1	J	200	GLY	N-CA-C	-7.41	104.26	114.64
2	K	28	PRO	N-CA-C	-7.41	97.20	112.47
2	K	420	ILE	CA-C-N	7.41	130.21	120.28
2	K	420	ILE	C-N-CA	7.41	130.21	120.28
2	H	428	VAL	N-CA-C	7.40	118.17	110.62
3	F	277	ARG	CA-C-O	-7.40	113.18	121.40
2	H	206	ARG	N-CA-C	-7.40	106.19	114.62
3	I	107	GLY	CA-C-O	7.40	128.91	121.29
2	B	307	THR	CA-C-N	7.40	131.69	120.82
2	B	307	THR	C-N-CA	7.40	131.69	120.82
3	C	373	GLY	CA-C-N	7.39	130.79	120.29
3	C	373	GLY	C-N-CA	7.39	130.79	120.29
3	I	128	HIS	ND1-CE1-NE2	7.39	115.80	108.40
2	K	152	SER	O-C-N	-7.39	115.36	121.27
2	E	414	THR	CA-C-N	7.38	130.16	120.28
2	E	414	THR	C-N-CA	7.38	130.16	120.28
1	G	237	TRP	CE3-CZ3-CH2	7.38	130.69	121.10
2	E	205	SER	CA-C-N	7.37	131.52	120.31
2	E	205	SER	C-N-CA	7.37	131.52	120.31
3	F	88	ALA	N-CA-CB	7.37	118.83	111.10
1	G	237	TRP	CD2-CE3-CZ3	7.36	128.17	118.60
2	H	396	ASP	N-CA-C	-7.36	102.68	114.09
3	I	236	TYR	N-CA-C	-7.36	99.59	110.48
2	B	5	THR	CA-C-O	-7.35	113.28	121.51
3	L	234	TRP	CD2-CE2-CZ2	-7.34	115.06	122.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	129	LYS	N-CA-C	-7.33	98.89	110.10
1	G	157	ALA	N-CA-CB	7.32	122.87	110.49
3	I	173	PRO	N-CA-CB	7.32	107.02	102.92
3	C	354	VAL	O-C-N	-7.32	114.75	123.02
2	H	220	LYS	CA-C-O	7.32	128.00	120.24
1	A	225	ASN	CA-CB-CG	-7.32	105.28	112.60
2	E	335	ASN	N-CA-C	-7.31	102.98	113.21
2	H	345	ASP	CA-CB-CG	-7.31	105.29	112.60
2	K	305	SER	N-CA-CB	7.31	122.84	110.49
3	C	304	HIS	ND1-CG-CD2	7.30	113.40	106.10
3	I	349	ASN	CA-C-O	-7.29	113.68	119.66
3	I	79	ARG	N-CA-C	-7.28	104.25	113.72
3	L	236	TYR	N-CA-C	-7.28	99.75	110.52
3	L	342	SER	N-CA-CB	7.28	122.79	110.49
2	K	210	SER	CB-CA-C	-7.28	99.68	110.16
3	C	339	GLN	OE1-CD-NE2	7.27	129.87	122.60
3	C	380	SER	O-C-N	7.27	129.82	122.12
2	H	407	TRP	CB-CA-C	-7.27	98.49	110.85
3	I	224	CYS	CB-CA-C	-7.27	101.64	110.94
1	D	150	SER	CA-C-N	7.26	130.01	120.28
1	D	150	SER	C-N-CA	7.26	130.01	120.28
2	H	236	THR	N-CA-C	-7.26	98.01	109.04
2	E	73	GLU	N-CA-CB	7.25	121.54	110.81
3	L	33	ILE	O-C-N	7.25	131.78	122.94
3	C	398	TYR	CG-CD2-CE2	-7.23	110.36	121.20
1	D	128	LYS	CA-C-O	-7.23	111.64	118.73
3	F	42	ASP	N-CA-C	-7.23	102.25	113.02
1	J	219	ILE	N-CA-C	-7.22	98.00	108.11
2	E	40	PRO	CA-C-O	-7.21	112.87	121.67
1	A	194	THR	CA-C-N	7.21	133.64	121.88
1	A	194	THR	C-N-CA	7.21	133.64	121.88
2	B	416	GLY	N-CA-C	7.21	127.04	112.34
2	K	423	VAL	CA-C-N	7.20	129.93	120.28
2	K	423	VAL	C-N-CA	7.20	129.93	120.28
1	A	94	ARG	NE-CZ-NH2	-7.20	112.72	119.20
2	E	7	MET	CA-C-O	-7.20	113.22	120.63
2	B	139	GLU	N-CA-C	-7.19	105.43	114.56
3	C	398	TYR	CB-CG-CD2	-7.19	110.02	120.80
3	F	241	VAL	N-CA-CB	7.18	121.27	111.21
2	E	324	LYS	O-C-N	-7.17	115.17	123.27
3	I	354	VAL	O-C-N	-7.16	115.32	122.76
2	H	57	SER	CA-C-N	7.16	126.92	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	57	SER	C-N-CA	7.16	126.92	119.76
1	D	111	LEU	CA-C-N	7.14	132.28	122.07
1	D	111	LEU	C-N-CA	7.14	132.28	122.07
3	C	359	ASP	CA-CB-CG	-7.14	105.46	112.60
1	J	181	TRP	CE2-CD2-CE3	7.14	125.94	118.80
3	F	286	HIS	CB-CG-ND1	-7.13	112.00	122.70
2	K	55	VAL	CB-CA-C	-7.13	102.98	111.18
1	J	239	LYS	O-C-N	7.12	130.27	122.15
3	C	392	THR	CA-C-N	7.12	129.82	120.28
3	C	392	THR	C-N-CA	7.12	129.82	120.28
1	D	237	TRP	CE3-CZ3-CH2	7.12	130.35	121.10
2	H	303	VAL	O-C-N	7.12	130.58	123.18
3	C	399	GLN	N-CA-C	7.11	119.03	111.28
3	F	231	ASN	CA-C-N	7.11	134.88	123.93
3	F	231	ASN	C-N-CA	7.11	134.88	123.93
1	J	99	MET	CB-CA-C	-7.11	98.41	110.64
1	A	246	THR	CA-C-O	-7.07	113.64	120.64
3	L	197	LYS	N-CA-C	-7.07	97.38	108.90
2	K	54	VAL	N-CA-C	-7.07	97.94	108.12
3	I	414	CYS	N-CA-C	7.06	118.97	111.28
3	L	394	CYS	CA-C-O	-7.05	113.41	120.82
3	F	359	ASP	CA-CB-CG	7.05	119.65	112.60
3	C	62	ASN	OD1-CG-ND2	7.05	129.65	122.60
2	H	72	ASN	CA-C-N	7.04	133.62	122.21
2	H	72	ASN	C-N-CA	7.04	133.62	122.21
3	I	304	HIS	ND1-CG-CD2	7.04	113.14	106.10
1	D	103	ASN	CA-CB-CG	-7.04	105.56	112.60
2	K	272	VAL	N-CA-CB	7.03	119.44	111.21
2	B	341	ASP	N-CA-C	-7.02	98.80	109.95
3	C	313	MET	CG-SD-CE	-7.01	85.48	100.90
3	F	200	CYS	O-C-N	7.01	130.72	122.24
3	I	287	PRO	N-CA-CB	-7.01	96.81	103.33
3	C	62	ASN	O-C-N	-7.00	114.82	123.36
3	I	376	ILE	CA-C-N	7.00	130.36	120.42
3	I	376	ILE	C-N-CA	7.00	130.36	120.42
2	K	336	SER	N-CA-C	-7.00	104.71	113.18
2	B	252	ASN	N-CA-CB	-7.00	99.80	110.16
3	F	405	GLN	N-CA-C	-7.00	103.80	114.16
3	C	60	THR	N-CA-C	-6.99	98.02	108.99
2	E	73	GLU	N-CA-C	-6.98	105.38	114.04
2	E	55	VAL	CA-C-N	6.98	127.01	119.89
2	E	55	VAL	C-N-CA	6.98	127.01	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	48	GLN	N-CA-CB	6.98	122.41	110.68
2	E	171	SER	CA-C-O	-6.98	114.15	119.59
2	H	259	CYS	N-CA-CB	6.98	122.28	110.49
2	B	68	CYS	CA-C-N	6.97	134.86	121.54
2	B	68	CYS	C-N-CA	6.97	134.86	121.54
2	H	264	ASN	OD1-CG-ND2	6.97	129.57	122.60
3	C	267	SER	O-C-N	-6.97	114.39	122.89
3	I	278	LEU	O-C-N	6.96	131.14	123.13
2	K	180	TYR	CA-C-O	-6.96	113.51	121.72
3	F	340	LYS	CA-C-O	6.96	129.53	121.32
2	B	191	PRO	CA-C-N	6.95	130.58	120.71
2	B	191	PRO	C-N-CA	6.95	130.58	120.71
3	F	286	HIS	CB-CA-C	-6.95	102.78	110.98
2	E	288	THR	N-CA-C	-6.95	102.21	110.41
3	F	357	TYR	CA-C-N	6.95	131.66	121.31
3	F	357	TYR	C-N-CA	6.95	131.66	121.31
3	I	385	PHE	CA-C-N	6.95	129.59	120.28
3	I	385	PHE	C-N-CA	6.95	129.59	120.28
3	L	172	VAL	O-C-N	-6.94	114.53	120.92
3	C	353	ILE	N-CA-C	-6.94	99.77	109.21
2	H	23	GLY	O-C-N	6.94	128.47	122.64
2	E	115	GLU	N-CA-C	-6.94	104.81	113.28
2	E	284	ASP	CA-C-O	-6.94	113.56	121.19
3	I	242	PRO	N-CA-C	6.94	120.93	111.22
3	L	295	ILE	N-CA-C	-6.94	97.50	107.77
3	C	129	LYS	CA-C-O	-6.93	113.78	120.64
2	B	385	ASP	CA-C-O	-6.93	113.76	120.90
1	D	178	HIS	CB-CG-CD2	-6.93	122.19	131.20
3	L	35	HIS	ND1-CG-CD2	6.93	113.03	106.10
2	B	315	VAL	N-CA-CB	6.92	120.59	112.35
2	K	169	ALA	CA-C-O	-6.92	113.08	120.42
1	G	180	ASN	CA-CB-CG	6.92	119.52	112.60
1	G	181	TRP	CB-CG-CD2	-6.92	117.11	126.80
2	B	416	GLY	CA-C-N	6.91	126.89	119.28
2	B	416	GLY	C-N-CA	6.91	126.89	119.28
1	G	90	LYS	CB-CA-C	-6.91	99.26	109.97
1	A	179	TYR	CA-C-O	6.90	126.11	118.52
2	E	339	MET	N-CA-CB	6.90	121.40	111.05
1	J	97	ASN	CA-CB-CG	-6.90	105.70	112.60
3	F	415	CYS	CA-C-N	6.89	130.08	120.29
3	F	415	CYS	C-N-CA	6.89	130.08	120.29
1	G	225	ASN	CA-CB-CG	-6.89	105.71	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	88	LYS	CA-C-N	6.89	129.81	120.44
1	G	88	LYS	C-N-CA	6.89	129.81	120.44
3	C	62	ASN	CA-C-O	6.89	128.75	120.28
3	C	141	PRO	CA-C-N	6.88	129.39	120.44
3	C	141	PRO	C-N-CA	6.88	129.39	120.44
2	E	38	LEU	CA-C-N	-6.88	112.44	123.46
2	E	38	LEU	C-N-CA	-6.88	112.44	123.46
1	G	118	TYR	O-C-N	6.88	131.65	123.33
2	H	321	THR	N-CA-C	-6.88	97.76	109.24
1	D	195	ILE	O-C-N	-6.87	115.45	121.57
1	J	195	ILE	O-C-N	-6.87	115.46	121.57
2	H	85	TYR	CA-C-O	-6.86	110.76	120.16
1	D	247	PRO	CA-C-N	6.86	129.77	120.38
1	D	247	PRO	C-N-CA	6.86	129.77	120.38
2	K	330	ILE	O-C-N	-6.86	115.44	123.05
3	F	399	GLN	OE1-CD-NE2	6.85	129.45	122.60
2	K	43	VAL	O-C-N	-6.85	115.86	123.26
1	G	93	LYS	N-CA-C	-6.84	98.67	109.07
2	E	301	CYS	CA-C-N	6.84	132.84	122.93
2	E	301	CYS	C-N-CA	6.84	132.84	122.93
2	B	404	THR	CA-C-N	6.83	129.44	120.28
2	B	404	THR	C-N-CA	6.83	129.44	120.28
2	B	422	VAL	N-CA-CB	6.83	118.54	110.55
2	B	228	ASN	N-CA-C	-6.83	101.33	110.55
1	D	109	VAL	N-CA-CB	6.83	120.83	111.41
2	E	55	VAL	O-C-N	-6.83	113.32	121.10
2	E	252	ASN	CA-CB-CG	-6.83	105.77	112.60
3	C	221	ALA	N-CA-CB	6.82	122.51	110.37
3	I	405	GLN	CB-CG-CD	-6.82	101.01	112.60
1	J	109	VAL	N-CA-CB	6.82	121.10	111.82
3	F	295	ILE	N-CA-C	-6.81	97.81	107.75
3	I	347	HIS	ND1-CG-CD2	6.81	112.91	106.10
3	F	366	ILE	CA-C-O	-6.80	113.64	120.85
2	B	250	PRO	CA-C-O	-6.79	113.68	121.56
3	L	8	TYR	N-CA-C	6.79	118.76	111.36
2	H	55	VAL	CA-C-N	6.79	128.32	119.84
2	H	55	VAL	C-N-CA	6.79	128.32	119.84
1	J	169	LYS	CA-C-N	6.79	130.51	120.87
1	J	169	LYS	C-N-CA	6.79	130.51	120.87
1	J	125	LYS	N-CA-CB	6.78	121.37	110.65
1	J	223	GLY	N-CA-C	6.78	120.53	110.42
3	I	155	HIS	CA-C-N	6.78	134.49	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	155	HIS	C-N-CA	6.78	134.49	121.54
3	C	188	ASP	N-CA-C	-6.78	101.52	110.40
3	L	1	SER	CA-C-N	6.78	130.04	120.42
3	L	1	SER	C-N-CA	6.78	130.04	120.42
3	I	350	PRO	N-CA-CB	6.77	106.71	102.92
1	J	85	GLN	OE1-CD-NE2	6.77	129.37	122.60
1	A	179	TYR	N-CA-C	-6.76	104.15	114.16
3	C	398	TYR	N-CA-C	-6.76	103.69	112.68
3	C	299	GLY	CA-C-N	6.75	134.59	122.64
3	C	299	GLY	C-N-CA	6.75	134.59	122.64
3	C	415	CYS	O-C-N	6.75	129.85	122.15
1	D	196	PRO	CA-C-N	6.75	134.42	121.54
1	D	196	PRO	C-N-CA	6.75	134.42	121.54
2	E	263	VAL	CA-C-N	6.75	128.14	119.78
2	E	263	VAL	C-N-CA	6.75	128.14	119.78
2	E	275	ASN	CA-CB-CG	-6.75	105.86	112.60
2	H	303	VAL	N-CA-CB	6.74	120.98	111.82
1	A	104	ASP	N-CA-C	-6.74	103.78	113.21
3	L	144	HIS	CA-CB-CG	6.74	120.54	113.80
1	D	224	ALA	N-CA-CB	6.73	121.89	110.71
2	E	159	SER	N-CA-C	-6.73	97.93	108.90
3	I	55	ILE	N-CA-C	-6.73	98.44	108.46
1	D	112	ASP	CA-CB-CG	-6.72	105.88	112.60
3	I	129	LYS	CA-C-N	6.72	126.17	118.85
3	I	129	LYS	C-N-CA	6.72	126.17	118.85
1	D	166	ASP	CA-CB-CG	-6.72	105.88	112.60
2	H	212	ASP	CA-C-N	6.71	132.79	122.25
2	H	212	ASP	C-N-CA	6.71	132.79	122.25
2	E	92	ALA	N-CA-C	-6.71	104.57	112.89
3	L	386	LEU	CA-C-N	6.71	129.16	120.44
3	L	386	LEU	C-N-CA	6.71	129.16	120.44
3	C	284	HIS	ND1-CG-CD2	6.71	112.81	106.10
3	F	88	ALA	CA-C-N	6.70	126.68	119.78
3	F	88	ALA	C-N-CA	6.70	126.68	119.78
3	I	315	LYS	N-CA-C	-6.70	97.98	108.90
3	L	4	HIS	CA-CB-CG	6.70	120.50	113.80
2	H	424	ALA	N-CA-C	6.70	118.58	111.28
3	L	271	GLU	CA-C-N	6.70	126.66	120.03
3	L	271	GLU	C-N-CA	6.70	126.66	120.03
2	E	390	TYR	CA-C-O	-6.69	114.02	121.51
2	K	87	PHE	N-CA-C	-6.69	106.06	114.56
2	E	15	PHE	CA-CB-CG	-6.68	107.12	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	284	HIS	CB-CG-CD2	-6.68	122.52	131.20
2	E	369	VAL	N-CA-C	-6.67	95.46	109.34
3	C	17	TRP	CE2-CD2-CE3	6.67	125.47	118.80
3	C	142	THR	CA-C-N	6.67	131.16	121.96
3	C	142	THR	C-N-CA	6.67	131.16	121.96
3	C	215	LEU	CA-C-O	-6.66	113.18	120.24
3	I	285	PHE	N-CA-CB	-6.66	100.00	110.06
2	H	264	ASN	O-C-N	-6.66	115.12	120.38
1	J	152	TYR	N-CA-C	-6.65	103.78	114.09
3	C	304	HIS	CE1-NE2-CD2	-6.65	102.35	109.00
2	B	382	PRO	O-C-N	6.65	124.27	121.15
2	E	43	VAL	O-C-N	-6.64	116.09	123.26
2	B	236	THR	N-CA-C	-6.64	100.01	109.24
3	C	291	THR	O-C-N	6.64	131.08	123.31
2	K	73	GLU	N-CA-C	-6.64	100.86	108.49
2	K	259	CYS	CB-CA-C	6.63	123.62	110.42
2	K	413	THR	CA-C-N	6.63	129.17	120.28
2	K	413	THR	C-N-CA	6.63	129.17	120.28
1	J	211	ASP	CA-CB-CG	-6.63	105.97	112.60
2	B	217	THR	N-CA-C	-6.63	99.43	108.38
2	E	424	ALA	CA-C-O	-6.63	113.52	120.55
2	K	68	CYS	N-CA-CB	6.63	119.84	109.83
2	E	393	LYS	CA-C-N	6.63	133.63	121.70
2	E	393	LYS	C-N-CA	6.63	133.63	121.70
3	L	368	VAL	O-C-N	-6.63	115.41	121.91
2	B	271	CYS	N-CA-CB	6.63	121.47	110.47
2	H	414	THR	O-C-N	-6.63	115.10	122.12
2	H	438	ARG	N-CA-CB	6.63	121.76	110.50
1	J	187	GLN	OE1-CD-NE2	-6.63	115.97	122.60
1	D	204	ASP	CA-C-O	6.62	127.06	119.18
3	C	27	CYS	CA-C-O	-6.62	113.97	120.26
3	I	325	GLU	N-CA-C	-6.62	98.61	109.40
2	B	150	GLY	CA-C-N	6.62	130.88	121.42
2	B	150	GLY	C-N-CA	6.62	130.88	121.42
2	B	294	PRO	N-CA-CB	6.61	108.85	103.36
3	F	398	TYR	CZ-CE2-CD2	-6.61	107.69	119.60
2	K	74	ALA	CA-C-O	-6.61	113.41	120.42
3	L	347	HIS	ND1-CE1-NE2	6.61	115.01	108.40
2	B	425	ILE	CA-C-N	6.61	128.89	120.56
2	B	425	ILE	C-N-CA	6.61	128.89	120.56
1	J	86	LYS	CA-C-N	6.61	132.02	122.44
1	J	86	LYS	C-N-CA	6.61	132.02	122.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	144	HIS	CA-C-O	-6.61	112.42	120.54
3	F	356	HIS	ND1-CE1-NE2	6.60	115.00	108.40
1	A	137	ASP	N-CA-C	-6.59	101.51	111.34
3	I	389	VAL	N-CA-CB	6.59	119.51	110.54
3	C	218	CYS	N-CA-CB	6.59	122.92	111.39
3	C	353	ILE	O-C-N	6.59	130.50	122.72
3	C	420	ARG	N-CA-C	6.59	118.25	111.14
2	K	209	ASN	CA-CB-CG	6.59	119.19	112.60
3	C	285	PHE	CA-CB-CG	-6.58	107.22	113.80
3	F	154	SER	CA-C-N	6.58	133.17	122.65
3	F	154	SER	C-N-CA	6.58	133.17	122.65
2	H	178	ILE	N-CA-C	-6.58	98.65	108.12
3	C	340	LYS	N-CA-CB	6.57	121.60	110.49
1	G	211	ASP	CA-C-N	6.56	129.07	120.28
1	G	211	ASP	C-N-CA	6.56	129.07	120.28
3	F	72	ASN	CA-CB-CG	6.56	119.16	112.60
2	H	220	LYS	N-CA-C	-6.56	97.58	108.34
2	H	304	GLN	CA-C-O	-6.56	113.75	120.71
2	K	409	TRP	CB-CG-CD2	-6.56	117.62	126.80
2	K	242	TYR	N-CA-CB	6.56	119.58	110.07
3	L	41	ASP	CA-CB-CG	-6.56	106.04	112.60
3	I	143	GLY	N-CA-C	-6.55	102.39	111.76
1	J	193	PHE	CB-CA-C	-6.55	98.72	109.53
3	F	269	ALA	N-CA-CB	-6.55	101.33	110.04
2	B	142	GLN	O-C-N	-6.54	115.94	123.33
3	L	334	VAL	CB-CA-C	6.54	120.21	110.98
2	E	293	SER	CA-C-N	6.54	126.56	119.89
2	E	293	SER	C-N-CA	6.54	126.56	119.89
3	I	78	GLU	O-C-N	-6.54	115.74	123.06
3	L	74	VAL	CB-CA-C	6.54	118.87	110.96
3	C	4	HIS	N-CA-CB	6.53	119.83	110.16
2	H	36	SER	N-CA-C	-6.53	99.65	110.17
3	I	337	TRP	N-CA-CB	6.53	117.67	111.59
2	K	288	THR	N-CA-C	-6.53	97.13	108.69
3	C	398	TYR	CZ-CE2-CD2	-6.53	107.84	119.60
1	A	110	MET	CG-SD-CE	-6.53	86.53	100.90
3	F	42	ASP	CA-CB-CG	-6.53	106.07	112.60
2	H	399	PHE	CA-C-O	6.53	129.10	120.16
3	C	277	ARG	N-CA-C	-6.52	99.42	109.14
2	H	250	PRO	N-CA-CB	6.52	109.11	103.31
3	C	17	TRP	CB-CG-CD2	-6.52	117.67	126.80
2	K	252	ASN	CA-CB-CG	6.52	119.12	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	311	ASP	CA-CB-CG	-6.51	106.09	112.60
3	L	184	SER	N-CA-C	-6.50	99.69	108.86
3	C	203	THR	N-CA-C	-6.50	107.21	114.62
3	L	402	PRO	O-C-N	-6.50	115.06	123.06
3	F	16	GLY	O-C-N	-6.50	117.67	123.65
3	L	317	ILE	N-CA-C	-6.50	98.78	108.46
2	B	69	SER	N-CA-CB	6.49	121.46	110.49
3	F	402	PRO	CA-C-N	6.49	133.38	121.70
3	F	402	PRO	C-N-CA	6.49	133.38	121.70
2	E	273	TYR	CB-CA-C	-6.49	98.29	110.16
3	C	74	VAL	CA-C-O	6.48	128.23	120.65
3	L	264	CYS	CA-C-N	6.48	131.11	121.72
3	L	264	CYS	C-N-CA	6.48	131.11	121.72
3	F	98	HIS	ND1-CG-CD2	6.47	112.57	106.10
3	L	211	ASN	OD1-CG-ND2	-6.47	116.13	122.60
3	F	308	TRP	N-CA-CB	6.47	120.83	110.16
3	I	122	CYS	N-CA-C	-6.47	97.25	108.69
3	C	145	LYS	N-CA-CB	6.46	121.42	110.49
3	F	213	ILE	N-CA-C	-6.46	98.17	108.90
2	H	32	VAL	N-CA-C	-6.46	98.34	108.86
3	L	332	ASN	CA-CB-CG	6.46	119.06	112.60
2	H	221	LEU	N-CA-C	-6.45	96.87	108.48
2	E	97	ASP	N-CA-C	-6.45	104.18	113.21
2	H	21	ARG	O-C-N	-6.45	113.90	121.32
2	E	141	ASN	OD1-CG-ND2	-6.44	116.16	122.60
3	I	193	THR	N-CA-CB	6.44	120.93	110.43
2	B	276	ILE	N-CA-CB	6.44	120.22	111.21
3	I	18	CYS	N-CA-C	-6.44	97.88	108.76
2	K	145	ASP	O-C-N	-6.44	115.10	123.02
2	E	234	THR	N-CA-CB	6.44	121.49	110.68
3	F	173	PRO	CA-C-N	6.44	129.32	122.11
3	F	173	PRO	C-N-CA	6.44	129.32	122.11
1	A	237	TRP	N-CA-C	-6.43	97.09	110.80
3	F	235	GLN	N-CA-C	6.43	119.60	110.14
3	L	301	ASP	N-CA-C	-6.43	100.79	108.25
1	A	240	ASP	N-CA-C	-6.43	106.65	114.75
2	E	39	VAL	N-CA-C	-6.43	100.40	107.73
3	F	243	ARG	N-CA-C	-6.43	104.21	113.21
3	F	244	SER	N-CA-C	6.43	119.10	111.71
1	G	133	LYS	O-C-N	-6.43	115.79	123.31
3	L	334	VAL	N-CA-C	-6.43	99.14	108.71
3	F	247	THR	N-CA-C	-6.41	99.89	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	410	LEU	CA-C-N	6.41	130.96	120.63
2	H	410	LEU	C-N-CA	6.41	130.96	120.63
3	I	144	HIS	ND1-CE1-NE2	6.41	114.81	108.40
1	A	193	PHE	N-CA-C	-6.41	99.19	109.96
3	C	232	THR	CB-CA-C	6.41	123.17	110.42
3	I	371	SER	CA-C-N	6.40	128.86	120.28
3	I	371	SER	C-N-CA	6.40	128.86	120.28
1	J	186	VAL	N-CA-CB	6.40	121.79	111.23
3	C	125	PRO	CB-CA-C	6.40	119.70	111.64
2	H	277	PRO	N-CA-CB	6.40	109.29	103.34
2	E	9	ASN	CA-C-O	6.39	127.59	120.43
2	K	178	ILE	CA-CB-CG2	-6.39	99.64	110.50
2	E	80	VAL	N-CA-C	-6.39	97.12	107.28
3	F	330	ASN	CA-CB-CG	-6.39	106.21	112.60
3	F	358	TYR	CA-C-N	6.39	129.47	120.28
3	F	358	TYR	C-N-CA	6.39	129.47	120.28
3	F	385	PHE	CA-C-N	6.38	129.13	120.38
3	F	385	PHE	C-N-CA	6.38	129.13	120.38
3	L	347	HIS	CA-CB-CG	-6.38	107.42	113.80
2	H	167	SER	N-CA-C	-6.38	104.41	111.36
2	H	363	PRO	CA-C-N	6.38	129.77	120.71
2	H	363	PRO	C-N-CA	6.38	129.77	120.71
2	E	201	GLY	O-C-N	6.38	130.99	122.70
3	F	86	THR	N-CA-CB	6.38	119.32	110.07
1	A	138	ASN	CA-C-N	6.37	126.13	119.05
1	A	138	ASN	C-N-CA	6.37	126.13	119.05
3	C	284	HIS	ND1-CE1-NE2	6.37	114.77	108.40
1	J	135	THR	CA-C-N	6.37	133.44	121.97
1	J	135	THR	C-N-CA	6.37	133.44	121.97
3	L	133	ILE	N-CA-C	-6.37	98.94	108.12
3	C	183	LYS	N-CA-C	-6.37	104.13	112.41
1	J	142	ALA	N-CA-CB	6.37	119.25	110.01
2	E	133	VAL	CA-C-N	6.37	131.96	123.05
2	E	133	VAL	C-N-CA	6.37	131.96	123.05
2	E	391	ALA	N-CA-C	-6.37	102.09	110.43
3	I	166	MET	N-CA-C	-6.36	99.63	109.24
3	L	87	THR	N-CA-C	-6.36	103.84	113.89
2	B	305	SER	CA-C-N	6.36	133.68	121.54
2	B	305	SER	C-N-CA	6.36	133.68	121.54
2	K	39	VAL	CA-C-O	-6.36	114.52	119.98
3	F	140	ALA	CA-C-O	-6.35	111.46	120.16
3	C	303	SER	N-CA-C	-6.35	98.73	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	237	PRO	CA-C-N	6.35	130.38	121.24
2	E	237	PRO	C-N-CA	6.35	130.38	121.24
2	K	369	VAL	N-CA-C	-6.35	96.14	109.34
3	L	164	ILE	N-CA-CB	6.34	123.78	111.92
2	E	278	ILE	CA-C-O	-6.34	113.93	121.28
3	L	418	SER	N-CA-CB	6.34	119.54	110.16
2	E	404	THR	CA-CB-OG1	6.33	119.10	109.60
3	L	37	TRP	CA-C-O	-6.33	113.52	120.36
1	A	137	ASP	CA-CB-CG	-6.33	106.27	112.60
2	K	162	ILE	O-C-N	6.33	129.55	123.03
2	H	33	VAL	CA-C-O	6.33	127.19	120.48
2	B	172	PRO	CA-C-N	6.32	129.74	120.82
2	B	172	PRO	C-N-CA	6.32	129.74	120.82
3	F	148	ILE	N-CA-CB	6.32	120.06	111.21
2	H	13	ILE	O-C-N	-6.32	114.30	121.57
2	K	56	PRO	N-CA-CB	6.32	109.22	103.34
1	G	162	CYS	N-CA-C	6.32	117.83	111.07
3	F	398	TYR	CG-CD1-CE1	6.32	130.67	121.20
3	F	155	HIS	ND1-CE1-NE2	6.31	114.71	108.40
3	F	59	ASN	N-CA-CB	6.30	121.15	110.49
3	I	231	ASN	CA-CB-CG	-6.30	106.30	112.60
3	F	337	TRP	N-CA-C	-6.29	104.92	112.59
1	J	109	VAL	N-CA-C	-6.29	98.47	107.77
1	D	178	HIS	ND1-CG-CD2	6.28	112.38	106.10
3	I	210	THR	N-CA-C	-6.28	103.14	113.50
2	H	185	TYR	N-CA-C	-6.28	99.49	109.23
1	J	183	HIS	ND1-CG-CD2	6.28	112.38	106.10
1	G	178	HIS	CB-CG-CD2	-6.28	123.04	131.20
3	F	136	GLU	N-CA-C	-6.28	101.23	110.52
3	F	389	VAL	CA-C-O	-6.28	114.42	120.95
3	L	411	ALA	CA-C-N	6.28	129.85	120.31
3	L	411	ALA	C-N-CA	6.28	129.85	120.31
2	E	47	ILE	N-CA-C	-6.28	99.44	108.48
2	H	357	ALA	N-CA-CB	6.28	120.44	111.65
3	C	172	VAL	O-C-N	-6.27	113.95	121.10
1	J	95	MET	N-CA-C	-6.27	104.21	113.61
3	C	93	LEU	N-CA-C	6.27	117.91	111.14
1	G	121	LEU	N-CA-C	6.26	119.70	110.30
2	H	392	ALA	O-C-N	-6.26	116.69	123.26
3	C	300	LYS	N-CA-C	-6.26	100.72	110.17
3	L	231	ASN	CA-C-N	6.26	133.49	121.54
3	L	231	ASN	C-N-CA	6.26	133.49	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	362	PRO	O-C-N	6.25	131.08	122.64
1	G	237	TRP	N-CA-C	-6.25	103.84	112.03
3	C	360	LEU	CA-C-O	-6.25	111.57	120.51
2	H	392	ALA	CA-C-O	6.25	128.01	121.38
3	L	411	ALA	CB-CA-C	-6.25	100.22	110.85
3	C	233	VAL	CB-CA-C	-6.25	102.18	111.80
3	I	284	HIS	ND1-CE1-NE2	6.25	114.65	108.40
3	L	398	TYR	CZ-CE2-CD2	-6.25	108.35	119.60
1	J	217	VAL	CA-C-O	-6.25	113.36	119.92
3	C	151	LYS	N-CA-C	-6.25	99.73	109.72
2	E	405	THR	N-CA-CB	6.24	119.06	110.01
1	A	86	LYS	O-C-N	-6.24	114.84	122.20
3	I	196	TYR	N-CA-CB	6.24	123.14	111.53
2	B	243	TRP	CB-CG-CD2	-6.24	118.07	126.80
2	H	385	ASP	CA-CB-CG	-6.24	106.36	112.60
3	L	304	HIS	CA-CB-CG	6.24	120.04	113.80
1	D	132	VAL	N-CA-C	-6.24	105.27	111.88
2	H	308	TYR	CA-CB-CG	-6.24	102.68	113.90
1	D	108	PRO	O-C-N	6.23	130.98	123.13
3	I	27	CYS	N-CA-C	6.23	113.62	108.07
3	L	245	GLU	CB-CG-CD	-6.23	102.01	112.60
3	C	147	ARG	N-CA-CB	6.22	120.31	110.23
1	A	234	VAL	CA-C-N	6.22	131.80	122.91
1	A	234	VAL	C-N-CA	6.22	131.80	122.91
2	K	141	ASN	CA-CB-CG	-6.22	106.38	112.60
3	F	379	SER	CA-C-N	6.21	128.89	120.44
3	F	379	SER	C-N-CA	6.21	128.89	120.44
2	H	427	VAL	N-CA-CB	6.21	117.81	110.55
2	H	401	SER	CA-C-N	6.20	130.49	121.18
2	H	401	SER	C-N-CA	6.20	130.49	121.18
3	L	3	ALA	CA-C-N	6.20	128.59	120.28
3	L	3	ALA	C-N-CA	6.20	128.59	120.28
3	F	35	HIS	CA-CB-CG	6.20	120.00	113.80
1	D	153	ASP	N-CA-C	6.20	119.65	111.28
2	H	32	VAL	CA-C-O	-6.20	114.09	121.28
2	B	376	CYS	N-CA-C	-6.19	99.92	109.14
1	G	133	LYS	N-CA-C	-6.19	98.30	108.76
2	H	227	GLY	N-CA-C	-6.19	107.21	115.32
2	K	102	GLN	N-CA-CB	6.19	120.31	110.65
2	K	262	LYS	N-CA-CB	6.19	121.60	110.83
2	H	382	PRO	N-CA-C	-6.18	103.16	110.70
3	I	35	HIS	ND1-CE1-NE2	6.18	114.58	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	128	LYS	N-CA-C	6.18	121.94	113.16
3	C	347	HIS	CA-C-N	6.18	130.40	121.44
3	C	347	HIS	C-N-CA	6.18	130.40	121.44
2	B	77	LYS	N-CA-C	-6.18	99.74	109.50
2	B	210	SER	N-CA-CB	6.18	122.20	111.39
1	G	131	HIS	CG-ND1-CE1	-6.18	98.80	109.30
2	E	13	ILE	CB-CA-C	6.17	117.37	110.52
3	L	78	GLU	CA-C-O	-6.17	113.95	121.36
3	L	387	CYS	O-C-N	-6.17	115.72	122.07
3	F	322	GLU	O-C-N	6.17	130.79	122.59
1	D	212	ASN	CA-CB-CG	-6.17	106.44	112.60
2	H	262	LYS	CA-C-N	6.16	128.40	120.88
2	H	262	LYS	C-N-CA	6.16	128.40	120.88
2	H	288	THR	N-CA-C	-6.16	98.34	108.76
3	I	276	TYR	CA-C-N	6.16	132.45	122.53
3	I	276	TYR	C-N-CA	6.16	132.45	122.53
2	H	201	GLY	CA-C-N	6.16	128.82	120.44
2	H	201	GLY	C-N-CA	6.16	128.82	120.44
3	L	356	HIS	CE1-NE2-CD2	-6.16	102.84	109.00
3	I	356	HIS	N-CA-C	-6.16	99.69	109.23
2	B	221	LEU	CA-C-N	6.16	132.74	121.85
2	B	221	LEU	C-N-CA	6.16	132.74	121.85
2	B	232	PRO	N-CA-C	-6.16	99.79	112.47
2	E	216	ASN	CA-CB-CG	-6.16	106.44	112.60
3	F	231	ASN	OD1-CG-ND2	6.16	128.75	122.60
3	C	288	MET	N-CA-CB	6.15	121.58	111.31
3	C	390	ALA	N-CA-CB	6.15	119.16	110.12
3	F	262	SER	N-CA-C	-6.15	100.70	108.45
2	B	369	VAL	N-CA-CB	6.15	121.37	111.23
2	B	275	ASN	CA-CB-CG	-6.14	106.45	112.60
3	L	41	ASP	N-CA-C	-6.14	104.96	112.88
3	C	153	TYR	CA-C-O	6.14	126.93	120.36
2	K	438	ARG	N-CA-CB	6.14	120.94	110.50
1	A	237	TRP	CG-CD1-NE1	6.14	118.18	110.20
2	K	295	SER	N-CA-C	-6.14	102.27	110.55
3	C	68	TYR	CA-C-O	6.13	128.17	121.06
3	I	417	LYS	N-CA-CB	6.13	118.90	110.01
3	L	168	VAL	N-CA-CB	6.13	119.79	111.21
3	C	255	VAL	N-CA-C	-6.12	100.32	107.61
3	L	67	ARG	CD-NE-CZ	-6.12	115.83	124.40
3	C	240	TYR	O-C-N	-6.12	114.45	122.59
3	F	128	HIS	CA-CB-CG	6.12	119.92	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	66	ILE	N-CA-C	-6.12	100.28	108.35
3	F	312	PRO	CB-CA-C	-6.12	103.40	111.23
2	H	264	ASN	CA-C-N	6.12	125.52	118.85
2	H	264	ASN	C-N-CA	6.12	125.52	118.85
1	D	252	GLU	N-CA-CB	6.11	120.48	110.39
2	E	281	ASP	N-CA-C	-6.11	97.33	108.02
1	A	122	VAL	N-CA-C	-6.11	96.63	109.34
2	B	325	VAL	N-CA-C	-6.11	99.08	107.99
1	D	142	ALA	CA-C-N	6.11	128.46	120.28
1	D	142	ALA	C-N-CA	6.11	128.46	120.28
1	D	129	PRO	N-CA-CB	6.10	108.73	103.36
3	C	398	TYR	CG-CD1-CE1	6.10	130.35	121.20
2	E	208	VAL	CA-C-O	-6.10	113.88	120.47
3	F	289	TYR	CA-C-O	-6.10	114.89	120.50
2	B	335	ASN	OD1-CG-ND2	6.10	128.70	122.60
2	K	275	ASN	OD1-CG-ND2	6.10	128.70	122.60
2	E	174	ASP	N-CA-C	-6.10	97.82	110.80
1	D	208	PRO	CA-C-N	6.09	131.40	123.11
1	D	208	PRO	C-N-CA	6.09	131.40	123.11
3	C	371	SER	CA-C-O	6.09	127.01	120.55
2	H	4	SER	N-CA-CB	6.09	120.78	110.49
1	A	129	PRO	N-CA-CB	6.09	108.41	103.36
2	K	104	SER	N-CA-C	-6.08	100.37	110.17
3	I	276	TYR	CB-CG-CD1	-6.08	111.68	120.80
3	C	35	HIS	O-C-N	-6.08	117.11	123.56
3	L	171	ASP	N-CA-C	-6.08	97.86	110.80
3	C	156	GLN	OE1-CD-NE2	6.07	128.67	122.60
2	B	310	SER	CA-C-N	6.07	133.13	121.54
2	B	310	SER	C-N-CA	6.07	133.13	121.54
2	H	168	SER	O-C-N	-6.07	116.68	123.48
1	D	250	SER	CA-C-O	6.07	127.79	120.99
3	F	393	LYS	N-CA-CB	6.06	119.03	110.12
2	E	151	ASP	N-CA-C	-6.06	98.65	108.52
2	E	170	TRP	CB-CG-CD2	-6.06	118.32	126.80
2	K	96	CYS	CA-C-O	6.05	128.16	121.56
3	L	415	CYS	CA-C-N	6.05	128.31	120.44
3	L	415	CYS	C-N-CA	6.05	128.31	120.44
3	C	140	ALA	N-CA-CB	6.05	118.91	111.23
2	H	17	ALA	O-C-N	-6.05	116.10	123.30
3	I	267	SER	CA-C-O	6.05	127.12	120.71
3	L	62	ASN	CA-CB-CG	-6.05	106.55	112.60
3	L	361	TYR	CA-C-N	6.04	127.40	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	361	TYR	C-N-CA	6.04	127.40	119.84
2	H	163	LEU	N-CA-C	-6.04	99.35	108.96
1	G	85	GLN	N-CA-CB	6.04	120.70	110.49
2	K	393	LYS	N-CA-C	-6.04	99.15	109.24
3	I	283	PHE	CA-CB-CG	-6.04	107.76	113.80
1	A	147	LYS	O-C-N	6.04	131.08	123.23
2	K	143	THR	N-CA-C	-6.03	99.97	109.50
2	B	308	TYR	CA-C-O	-6.03	114.93	121.44
2	H	246	GLU	CA-C-O	-6.03	114.16	120.55
1	G	214	GLY	CA-C-N	6.03	133.05	121.54
1	G	214	GLY	C-N-CA	6.03	133.05	121.54
3	I	356	HIS	ND1-CE1-NE2	6.02	114.42	108.40
3	I	415	CYS	CA-C-O	-6.02	114.04	120.42
2	E	392	ALA	CA-C-N	6.02	131.96	122.21
2	E	392	ALA	C-N-CA	6.02	131.96	122.21
2	H	39	VAL	CB-CA-C	-6.01	103.93	110.85
3	I	161	ARG	N-CA-C	-6.01	102.36	111.56
3	L	353	ILE	CA-CB-CG1	6.01	120.62	110.40
2	B	245	LYS	CA-C-O	6.01	126.89	120.70
2	H	241	SER	CA-C-N	6.01	128.62	120.44
2	H	241	SER	C-N-CA	6.01	128.62	120.44
2	E	231	VAL	N-CA-CB	6.01	121.72	111.50
3	L	407	PRO	N-CA-CB	6.01	109.05	103.46
3	C	142	THR	O-C-N	6.01	128.26	122.07
3	L	349	ASN	N-CA-C	-6.01	99.18	108.55
2	E	75	ASP	N-CA-C	-6.00	99.40	108.52
3	F	95	THR	CA-C-O	-6.00	112.89	120.28
3	F	286	HIS	ND1-CE1-NE2	6.00	114.40	108.40
3	C	406	LEU	N-CA-C	-6.00	102.03	110.31
1	D	138	ASN	N-CA-C	-6.00	98.51	108.23
3	F	185	TYR	N-CA-C	-6.00	98.74	108.52
3	F	247	THR	CA-C-O	6.00	127.72	121.36
1	A	195	ILE	N-CA-C	-6.00	101.25	108.45
2	K	330	ILE	N-CA-C	-6.00	99.58	108.45
2	B	98	THR	N-CA-C	-5.99	104.62	113.61
3	I	234	TRP	N-CA-C	-5.99	101.59	110.46
3	I	330	ASN	CA-CB-CG	-5.99	106.61	112.60
3	I	337	TRP	N-CA-C	-5.99	99.54	108.34
2	B	390	TYR	N-CA-C	-5.99	100.42	108.86
2	B	431	VAL	CB-CA-C	5.99	120.48	112.22
2	B	171	SER	N-CA-C	-5.98	99.16	109.15
3	I	132	PHE	N-CA-CB	5.98	122.10	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	116	THR	CA-C-O	5.98	127.10	120.82
2	K	156	ILE	CA-C-N	5.98	130.87	122.08
2	K	156	ILE	C-N-CA	5.98	130.87	122.08
3	L	394	CYS	N-CA-C	5.98	117.47	111.07
2	B	119	ALA	N-CA-CB	5.98	119.37	110.40
3	C	21	CYS	O-C-N	-5.98	116.29	121.85
2	H	408	GLN	CG-CD-NE2	5.97	125.36	116.40
2	E	373	ARG	N-CA-C	5.97	118.15	109.07
3	F	177	LEU	CA-C-N	5.97	128.50	120.50
3	F	177	LEU	C-N-CA	5.97	128.50	120.50
3	F	286	HIS	ND1-CG-CD2	5.97	112.07	106.10
3	I	281	VAL	N-CA-C	-5.97	99.52	108.12
3	F	51	MET	N-CA-C	5.97	118.41	110.53
3	C	79	ARG	CG-CD-NE	-5.97	98.87	112.00
1	A	148	LYS	CA-C-N	5.97	133.12	123.33
1	A	148	LYS	C-N-CA	5.97	133.12	123.33
1	D	215	LYS	N-CA-CB	5.96	119.36	110.29
3	F	144	HIS	ND1-CG-CD2	5.96	112.06	106.10
3	I	281	VAL	N-CA-CB	5.96	120.22	111.52
2	K	400	PRO	N-CA-C	-5.96	100.20	112.47
3	L	284	HIS	N-CA-CB	5.96	120.36	110.47
2	E	285	ALA	N-CA-C	-5.96	103.94	110.91
1	J	199	SER	CA-C-N	5.96	132.16	122.69
1	J	199	SER	C-N-CA	5.96	132.16	122.69
2	K	427	VAL	N-CA-C	-5.96	104.70	110.72
3	L	59	ASN	CA-CB-CG	-5.96	106.64	112.60
2	E	236	THR	N-CA-C	-5.95	100.97	109.24
3	F	229	VAL	CB-CA-C	5.95	119.63	110.82
2	H	55	VAL	CA-C-O	-5.95	115.82	119.51
1	A	91	PRO	N-CA-CB	5.95	108.88	103.34
2	H	421	LEU	CA-C-N	5.95	128.06	120.56
2	H	421	LEU	C-N-CA	5.95	128.06	120.56
1	J	166	ASP	CA-C-N	5.95	129.29	120.90
1	J	166	ASP	C-N-CA	5.95	129.29	120.90
3	L	4	HIS	CA-C-O	-5.95	114.24	120.55
2	B	208	VAL	CA-CB-CG1	-5.95	100.29	110.40
3	C	220	THR	O-C-N	5.95	130.55	122.82
3	I	124	THR	CA-C-N	5.95	126.14	119.90
3	I	124	THR	C-N-CA	5.95	126.14	119.90
2	B	50	ASN	N-CA-CB	5.94	118.72	110.17
3	I	290	PRO	N-CA-CB	5.94	109.49	103.25
3	F	34	GLU	CB-CA-C	-5.94	100.81	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	241	VAL	CA-C-O	-5.94	115.65	119.15
1	A	150	SER	N-CA-C	-5.93	105.95	112.72
3	C	390	ALA	CB-CA-C	-5.93	100.94	110.79
2	E	32	VAL	CB-CA-C	5.93	119.46	110.62
2	K	318	ILE	N-CA-CB	5.93	120.18	111.52
2	K	368	GLN	N-CA-C	-5.93	100.23	109.72
2	E	347	GLN	CA-C-N	5.93	132.01	121.75
2	E	347	GLN	C-N-CA	5.93	132.01	121.75
2	B	347	GLN	CA-C-O	5.93	128.99	120.51
3	I	379	SER	CA-C-N	5.93	128.71	120.29
3	I	379	SER	C-N-CA	5.93	128.71	120.29
3	I	278	LEU	CA-C-O	-5.93	113.79	120.43
1	J	237	TRP	N-CA-C	-5.92	98.18	110.80
1	A	91	PRO	O-C-N	5.92	130.21	123.10
2	B	122	TYR	CG-CD1-CE1	-5.92	112.32	121.20
1	G	138	ASN	CA-C-O	-5.92	113.21	119.13
3	I	195	LYS	N-CA-C	-5.92	99.59	109.24
1	A	176	GLU	CA-C-N	5.92	127.53	120.14
1	A	176	GLU	C-N-CA	5.92	127.53	120.14
3	L	333	PRO	CB-CA-C	-5.92	103.34	111.21
2	H	192	TYR	CB-CG-CD2	-5.91	111.93	120.80
2	H	288	THR	O-C-N	-5.91	116.39	123.31
3	I	401	ALA	CA-C-N	5.91	126.06	119.32
3	I	401	ALA	C-N-CA	5.91	126.06	119.32
3	L	222	PRO	N-CA-C	-5.91	107.11	114.68
3	I	387	CYS	N-CA-CB	5.91	118.57	110.01
1	A	210	PHE	N-CA-CB	5.90	121.18	111.08
1	A	121	LEU	O-C-N	5.90	130.57	123.13
2	H	174	ASP	N-CA-C	-5.90	98.23	110.80
2	H	323	ASN	N-CA-CB	5.90	120.51	110.71
3	I	177	LEU	N-CA-C	-5.90	105.39	112.59
2	E	289	ARG	O-C-N	-5.90	115.69	122.89
1	A	204	ASP	CA-C-O	5.90	126.55	119.59
2	K	103	MET	N-CA-C	-5.90	99.58	108.96
3	L	217	ASN	N-CA-CB	5.90	120.46	110.49
2	B	347	GLN	O-C-N	-5.90	114.75	122.59
3	C	349	ASN	N-CA-C	-5.89	98.83	109.09
3	C	399	GLN	O-C-N	5.89	128.37	122.12
3	I	100	ILE	N-CA-C	-5.89	99.64	108.12
3	C	135	ASN	N-CA-C	-5.89	105.75	113.17
2	E	242	TYR	N-CA-CB	5.89	118.61	110.07
2	H	50	ASN	OD1-CG-ND2	5.88	128.49	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	21	ARG	CA-C-N	5.88	126.22	119.93
2	B	21	ARG	C-N-CA	5.88	126.22	119.93
2	B	260	ILE	N-CA-C	-5.88	99.17	107.75
2	B	285	ALA	O-C-N	-5.88	116.31	123.36
2	H	115	GLU	N-CA-CB	5.88	120.20	110.33
2	H	223	ARG	O-C-N	5.88	126.42	121.31
3	I	384	CYS	CB-CA-C	-5.88	100.86	110.85
2	K	134	MET	N-CA-C	-5.88	99.61	109.07
2	H	400	PRO	N-CD-CG	5.87	112.01	103.20
2	E	216	ASN	N-CA-C	-5.87	104.66	112.94
1	J	244	ARG	NE-CZ-NH1	5.87	127.37	121.50
1	D	233	SER	N-CA-CB	5.87	120.14	110.69
2	B	210	SER	O-C-N	-5.86	116.91	123.48
2	H	128	SER	N-CA-CB	5.86	120.19	110.63
2	K	8	PRO	N-CA-C	-5.86	101.98	111.77
2	H	432	SER	CA-C-N	5.86	128.49	120.46
2	H	432	SER	C-N-CA	5.86	128.49	120.46
3	I	4	HIS	N-CA-CB	5.86	118.83	110.16
3	L	122	CYS	N-CA-C	-5.86	98.32	108.69
2	B	334	SER	N-CA-CB	5.86	120.39	110.49
1	D	176	GLU	CA-C-O	5.85	125.11	119.08
3	L	126	PHE	N-CA-CB	5.85	120.43	110.71
2	B	108	VAL	CA-CB-CG2	-5.85	100.45	110.40
3	C	418	SER	CA-C-N	5.85	128.40	120.44
3	C	418	SER	C-N-CA	5.85	128.40	120.44
2	E	410	LEU	CA-C-N	5.85	132.72	121.54
2	E	410	LEU	C-N-CA	5.85	132.72	121.54
1	A	138	ASN	CA-C-O	-5.85	114.96	120.34
2	B	33	VAL	N-CA-C	-5.85	99.45	107.99
3	I	254	HIS	CB-CG-CD2	-5.85	123.60	131.20
3	L	382	PHE	CB-CA-C	-5.85	100.91	110.85
1	J	137	ASP	N-CA-C	-5.84	102.63	111.34
1	J	225	ASN	CA-C-N	5.84	130.35	120.88
1	J	225	ASN	C-N-CA	5.84	130.35	120.88
3	L	84	VAL	N-CA-C	-5.84	99.34	108.86
2	E	355	PHE	N-CA-CB	5.84	120.19	110.85
2	B	288	THR	CA-C-O	-5.84	115.20	121.56
2	B	310	SER	CA-C-O	-5.84	114.99	121.23
3	C	20	ASP	CA-C-N	5.84	129.15	119.35
3	C	20	ASP	C-N-CA	5.84	129.15	119.35
3	I	107	GLY	O-C-N	-5.84	118.33	123.76
2	K	404	THR	O-C-N	5.84	128.08	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	345	ASP	CB-CA-C	-5.83	101.03	110.77
2	B	245	LYS	N-CA-CB	5.83	118.52	110.07
2	E	284	ASP	CA-C-N	5.83	131.73	122.93
2	E	284	ASP	C-N-CA	5.83	131.73	122.93
1	G	244	ARG	CB-CA-C	-5.83	103.60	112.11
2	H	210	SER	CA-C-O	5.83	127.52	120.99
3	I	35	HIS	CA-CB-CG	5.83	119.63	113.80
2	H	155	ARG	NE-CZ-NH2	-5.83	113.96	119.20
2	H	272	VAL	CA-C-N	5.83	128.98	120.71
2	H	272	VAL	C-N-CA	5.83	128.98	120.71
2	B	98	THR	CA-C-O	-5.82	112.31	119.18
2	B	201	GLY	CA-C-N	5.82	132.93	121.58
2	B	201	GLY	C-N-CA	5.82	132.93	121.58
2	E	247	LYS	N-CA-CB	5.82	120.33	110.49
3	I	54	GLY	O-C-N	5.82	129.25	122.45
1	A	237	TRP	CE3-CZ3-CH2	5.81	128.66	121.10
3	L	78	GLU	O-C-N	5.81	129.57	123.06
1	A	116	ASN	CA-CB-CG	-5.81	106.79	112.60
2	B	399	PHE	CA-C-N	-5.81	112.58	119.84
2	B	399	PHE	C-N-CA	-5.81	112.58	119.84
3	L	4	HIS	N-CA-CB	5.81	118.66	110.12
1	D	211	ASP	CA-CB-CG	-5.81	106.79	112.60
1	A	160	PRO	CA-C-N	5.80	129.64	120.47
1	A	160	PRO	C-N-CA	5.80	129.64	120.47
2	B	408	GLN	CB-CA-C	-5.80	101.15	110.79
3	F	409	PHE	CA-C-N	5.80	128.41	120.46
3	F	409	PHE	C-N-CA	5.80	128.41	120.46
1	G	160	PRO	CA-C-N	5.80	129.64	120.47
1	G	160	PRO	C-N-CA	5.80	129.64	120.47
1	G	201	LYS	CA-C-N	5.80	126.13	119.92
1	G	201	LYS	C-N-CA	5.80	126.13	119.92
3	C	370	ALA	CA-C-O	-5.80	114.73	120.82
1	G	107	PHE	CA-C-N	5.80	126.29	120.14
1	G	107	PHE	C-N-CA	5.80	126.29	120.14
2	H	75	ASP	CA-CB-CG	-5.80	106.80	112.60
3	L	22	GLY	CA-C-N	5.80	132.62	121.54
3	L	22	GLY	C-N-CA	5.80	132.62	121.54
1	A	220	VAL	N-CA-CB	5.80	117.45	110.95
3	C	341	SER	N-CA-C	5.80	118.42	110.24
2	E	183	GLU	CA-C-N	5.80	128.41	120.35
2	E	183	GLU	C-N-CA	5.80	128.41	120.35
3	F	211	ASN	N-CA-C	5.80	118.51	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	62	ASN	CA-C-N	5.80	129.13	120.31
3	I	62	ASN	C-N-CA	5.80	129.13	120.31
3	I	280	GLU	N-CA-C	-5.80	98.84	108.75
2	H	171	SER	CA-C-N	5.79	126.88	120.45
2	H	171	SER	C-N-CA	5.79	126.88	120.45
3	I	131	ARG	N-CA-CB	5.79	120.28	110.49
3	F	17	TRP	CG-CD2-CE3	-5.79	128.11	133.90
2	H	242	TYR	N-CA-C	-5.79	104.89	111.14
2	E	260	ILE	CB-CA-C	5.79	118.99	110.77
2	E	390	TYR	CA-C-N	5.79	130.65	120.87
2	E	390	TYR	C-N-CA	5.79	130.65	120.87
3	I	270	PRO	CA-C-N	5.79	128.90	120.51
3	I	270	PRO	C-N-CA	5.79	128.90	120.51
2	B	39	VAL	CB-CA-C	-5.78	104.20	110.85
2	K	195	GLY	N-CA-C	-5.78	106.67	115.00
3	L	398	TYR	CG-CD1-CE1	5.78	129.87	121.20
3	I	168	VAL	CA-C-N	5.78	126.33	120.38
3	I	168	VAL	C-N-CA	5.78	126.33	120.38
2	E	54	VAL	O-C-N	-5.78	117.17	123.18
2	E	133	VAL	CA-C-O	5.78	128.59	121.54
2	K	25	ALA	N-CA-C	-5.78	100.56	109.52
3	L	109	GLN	O-C-N	5.78	130.16	123.17
2	B	75	ASP	CA-C-O	-5.78	114.54	120.89
2	B	166	ILE	CA-C-O	-5.77	114.24	121.11
2	H	205	SER	O-C-N	-5.77	116.14	123.24
2	B	232	PRO	N-CA-CB	-5.77	97.19	103.25
2	H	308	TYR	CA-C-N	5.77	129.30	121.05
2	H	308	TYR	C-N-CA	5.77	129.30	121.05
3	C	184	SER	N-CA-C	-5.77	100.64	109.41
3	I	396	THR	CA-C-O	-5.77	113.25	118.79
1	J	172	HIS	ND1-CG-CD2	5.77	111.87	106.10
3	I	58	SER	CA-C-N	5.77	132.81	123.93
3	I	58	SER	C-N-CA	5.77	132.81	123.93
2	K	254	ASN	CA-C-N	5.76	135.86	121.80
2	K	254	ASN	C-N-CA	5.76	135.86	121.80
2	B	202	ASP	CA-CB-CG	5.76	118.36	112.60
2	E	316	ALA	CA-C-N	5.76	131.61	122.62
2	E	316	ALA	C-N-CA	5.76	131.61	122.62
2	B	315	VAL	O-C-N	-5.76	117.13	122.71
1	J	236	THR	N-CA-C	-5.76	100.66	109.41
2	B	77	LYS	N-CA-CB	5.75	121.84	111.37
1	G	239	LYS	CB-CA-C	-5.75	101.45	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	207	ARG	CA-C-O	-5.75	114.64	119.76
3	L	52	GLN	CG-CD-OE1	5.75	132.30	120.80
3	C	327	VAL	N-CA-C	5.74	116.21	108.17
2	H	245	LYS	CA-C-O	5.74	126.62	120.70
2	H	267	ARG	NE-CZ-NH1	-5.74	115.76	121.50
2	K	257	PHE	N-CA-CB	5.74	120.18	110.49
2	E	409	TRP	CG-CD2-CE3	-5.73	128.17	133.90
1	J	143	LYS	CA-C-N	5.73	128.24	120.44
1	J	143	LYS	C-N-CA	5.73	128.24	120.44
2	B	242	TYR	O-C-N	5.73	128.28	122.09
2	H	355	PHE	CA-CB-CG	-5.73	108.07	113.80
2	H	132	GLN	N-CA-CB	5.73	121.44	110.90
2	H	72	ASN	OD1-CG-ND2	-5.72	116.88	122.60
2	B	10	GLN	N-CA-C	-5.72	99.09	108.76
1	D	90	LYS	CA-C-O	-5.72	115.36	120.56
1	D	164	LYS	N-CA-C	5.72	117.59	111.36
2	K	188	ASP	N-CA-CB	5.72	119.61	110.46
2	K	399	PHE	CA-C-N	-5.72	112.69	119.84
2	K	399	PHE	C-N-CA	-5.72	112.69	119.84
3	C	81	THR	N-CA-C	-5.72	106.29	113.72
2	K	161	PHE	N-CA-C	-5.71	100.37	109.23
3	L	128	HIS	N-CA-C	-5.71	98.97	108.34
3	I	100	ILE	N-CA-CB	5.71	119.86	111.52
3	I	155	HIS	CA-CB-CG	5.71	119.51	113.80
3	F	98	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	G	141	LEU	CA-C-N	5.71	127.86	120.44
1	G	141	LEU	C-N-CA	5.71	127.86	120.44
3	I	367	THR	CA-C-N	5.70	128.27	120.46
3	I	367	THR	C-N-CA	5.70	128.27	120.46
3	L	88	ALA	CB-CA-C	-5.70	102.17	109.92
3	F	351	ILE	CA-C-N	5.70	129.80	121.31
3	F	351	ILE	C-N-CA	5.70	129.80	121.31
1	D	201	LYS	CA-C-N	5.70	125.71	119.90
1	D	201	LYS	C-N-CA	5.70	125.71	119.90
3	L	300	LYS	N-CA-C	-5.70	108.12	114.62
2	B	289	ARG	CA-C-N	5.70	131.95	121.70
2	B	289	ARG	C-N-CA	5.70	131.95	121.70
2	B	54	VAL	CA-C-O	5.69	126.02	120.27
1	G	205	SER	O-C-N	-5.69	115.48	122.25
2	H	115	GLU	N-CA-C	-5.69	105.11	112.68
3	F	277	ARG	NE-CZ-NH1	-5.69	115.81	121.50
1	G	207	ARG	CA-C-O	-5.69	113.51	120.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	406	LEU	N-CA-C	-5.69	97.47	108.45
2	B	36	SER	N-CA-CB	5.69	119.43	110.56
3	F	48	GLN	N-CA-CB	5.68	120.72	110.83
1	G	107	PHE	CB-CA-C	-5.68	101.49	110.02
1	G	111	LEU	CA-C-N	5.68	130.47	122.46
1	G	111	LEU	C-N-CA	5.68	130.47	122.46
3	I	100	ILE	CB-CA-C	-5.68	102.03	110.33
3	I	6	GLU	CA-C-N	5.68	127.89	120.28
3	I	6	GLU	C-N-CA	5.68	127.89	120.28
3	I	65	LYS	N-CA-CB	5.68	119.42	110.56
3	F	114	LEU	O-C-N	5.68	129.63	123.10
2	B	173	PHE	CA-C-O	-5.68	114.45	120.92
2	K	416	GLY	CA-C-O	-5.68	113.40	121.52
2	B	285	ALA	N-CA-C	-5.67	97.62	107.49
2	H	231	VAL	N-CA-CB	5.67	121.15	111.50
1	A	178	HIS	ND1-CG-CD2	5.67	111.77	106.10
2	K	87	PHE	CA-C-N	5.67	132.37	121.54
2	K	87	PHE	C-N-CA	5.67	132.37	121.54
2	E	281	ASP	CA-CB-CG	-5.67	106.93	112.60
2	K	84	VAL	N-CA-C	5.67	118.59	110.09
1	A	100	LYS	CA-C-O	-5.67	114.29	120.81
2	H	56	PRO	N-CA-CB	5.67	109.20	103.25
2	H	254	ASN	CA-CB-CG	5.67	118.27	112.60
3	L	264	CYS	N-CA-CB	5.67	119.81	110.69
2	B	45	ASP	CB-CA-C	-5.66	101.51	110.86
3	C	378	ILE	N-CA-CB	5.66	119.07	110.58
1	G	152	TYR	N-CA-C	-5.66	98.75	110.80
2	K	69	SER	CA-C-N	5.66	128.75	120.71
2	K	69	SER	C-N-CA	5.66	128.75	120.71
2	B	409	TRP	N-CA-C	5.66	117.53	111.36
2	B	426	ILE	N-CA-CB	5.66	117.17	110.55
2	E	292	GLU	N-CA-CB	5.66	121.25	111.13
2	E	336	SER	N-CA-C	-5.66	105.29	113.21
3	L	98	HIS	CA-CB-CG	5.66	119.45	113.80
3	C	410	ILE	CA-C-N	5.65	127.85	120.28
3	C	410	ILE	C-N-CA	5.65	127.85	120.28
1	J	178	HIS	ND1-CE1-NE2	5.65	114.05	108.40
2	B	137	ILE	CA-C-O	5.65	125.11	119.97
1	D	137	ASP	N-CA-C	-5.65	102.92	111.56
1	D	233	SER	N-CA-C	-5.65	100.50	109.59
2	K	435	VAL	CB-CA-C	-5.65	104.52	112.14
1	A	197	THR	O-C-N	5.64	129.75	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	171	ASP	CA-CB-CG	5.64	118.24	112.60
1	G	112	ASP	O-C-N	-5.64	115.52	122.57
2	K	406	ALA	CB-CA-C	-5.64	101.42	110.79
2	E	207	THR	CA-CB-OG1	5.64	118.06	109.60
2	H	288	THR	CA-C-O	5.64	126.58	120.32
2	K	47	ILE	CA-C-O	5.64	127.27	120.67
1	J	134	GLY	N-CA-C	-5.64	106.27	115.46
1	A	211	ASP	N-CA-C	-5.64	98.79	110.80
1	D	213	THR	N-CA-C	-5.64	104.63	112.30
2	E	393	LYS	N-CA-C	-5.64	100.73	109.24
2	B	293	SER	CA-C-N	5.64	126.50	120.13
2	B	293	SER	C-N-CA	5.64	126.50	120.13
2	E	26	GLY	CA-C-O	-5.64	115.58	121.67
3	F	300	LYS	CA-C-N	5.64	128.23	120.39
3	F	300	LYS	C-N-CA	5.64	128.23	120.39
3	I	420	ARG	CA-C-O	-5.64	114.90	120.82
2	B	90	GLY	N-CA-C	-5.63	107.54	115.32
2	B	199	ARG	N-CA-CB	5.63	120.29	111.56
3	C	231	ASN	CA-C-O	-5.63	115.20	121.23
2	E	144	VAL	CA-CB-CG1	5.63	119.98	110.40
2	K	4	SER	N-CA-CB	5.63	120.01	110.49
3	L	360	LEU	N-CA-C	-5.63	100.22	109.40
3	I	350	PRO	CB-CA-C	-5.63	107.14	111.87
2	H	238	SER	CA-C-N	5.63	127.37	120.22
2	H	238	SER	C-N-CA	5.63	127.37	120.22
2	H	10	GLN	CA-C-O	5.63	126.57	120.32
2	K	170	TRP	O-C-N	-5.63	117.66	123.29
3	C	289	TYR	CB-CG-CD2	5.62	129.24	120.80
3	L	262	SER	N-CA-C	-5.62	100.98	108.74
3	L	155	HIS	ND1-CG-CD2	5.62	111.72	106.10
3	L	166	MET	N-CA-C	-5.62	100.81	109.52
3	C	406	LEU	CA-C-O	-5.62	114.96	120.19
1	A	136	ILE	CA-CB-CG1	5.62	119.95	110.40
3	C	318	GLN	CA-C-N	5.62	131.01	122.92
3	C	318	GLN	C-N-CA	5.62	131.01	122.92
2	E	249	VAL	CA-C-N	5.62	125.55	119.76
2	E	249	VAL	C-N-CA	5.62	125.55	119.76
1	G	164	LYS	CA-C-N	5.62	127.81	120.28
1	G	164	LYS	C-N-CA	5.62	127.81	120.28
3	I	356	HIS	ND1-CG-CD2	5.62	111.72	106.10
3	I	378	ILE	CA-CB-CG1	5.62	119.95	110.40
2	K	178	ILE	N-CA-CB	5.62	119.16	111.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	164	ILE	N-CA-C	-5.62	99.71	108.81
2	B	414	THR	N-CA-C	5.61	118.12	111.33
2	H	29	LEU	N-CA-C	-5.61	100.09	109.24
3	L	105	ARG	NH1-CZ-NH2	-5.61	112.00	119.30
3	F	6	GLU	O-C-N	-5.61	116.17	122.12
2	H	248	GLY	CA-C-O	-5.61	116.67	122.28
3	L	148	ILE	N-CA-CB	5.61	119.07	111.21
2	K	37	GLU	CA-C-N	5.61	130.35	121.99
2	K	37	GLU	C-N-CA	5.61	130.35	121.99
3	C	397	PRO	N-CA-C	5.61	121.21	113.98
2	K	158	GLN	CB-CG-CD	-5.61	103.07	112.60
3	F	91	ASP	N-CA-C	-5.60	100.05	109.07
1	G	131	HIS	ND1-CG-CD2	5.60	111.70	106.10
1	G	213	THR	N-CA-C	-5.60	104.66	112.45
3	C	87	THR	N-CA-C	-5.60	98.88	110.80
3	I	231	ASN	O-C-N	5.60	129.23	122.85
3	F	352	SER	N-CA-C	5.60	118.18	110.35
2	B	391	ALA	CA-C-N	5.59	132.22	121.54
2	B	391	ALA	C-N-CA	5.59	132.22	121.54
3	I	135	ASN	CA-CB-CG	5.59	118.19	112.60
2	H	116	ALA	N-CA-CB	5.59	119.94	110.49
3	C	138	SER	N-CA-CB	5.59	120.32	110.37
1	J	181	TRP	O-C-N	5.59	130.02	122.59
2	E	20	GLU	O-C-N	5.59	130.02	122.59
3	I	289	TYR	CA-C-O	-5.59	115.57	120.60
3	L	100	ILE	CA-C-N	5.59	131.03	122.93
3	L	100	ILE	C-N-CA	5.59	131.03	122.93
2	B	21	ARG	N-CA-C	-5.58	103.10	108.07
1	G	207	ARG	N-CA-C	-5.58	101.89	110.32
3	F	88	ALA	N-CA-C	-5.58	103.19	108.22
1	A	185	ALA	N-CA-CB	5.58	119.92	110.49
2	E	162	ILE	N-CA-C	-5.58	99.51	107.77
2	E	393	LYS	O-C-N	-5.58	116.42	123.17
2	E	310	SER	CA-C-O	5.58	126.34	120.54
2	B	121	ALA	CB-CA-C	-5.58	101.16	110.19
3	I	218	CYS	CA-C-O	-5.58	115.31	121.28
2	B	279	SER	N-CA-C	-5.57	99.58	109.06
1	D	126	VAL	CA-CB-CG1	5.57	119.87	110.40
2	H	95	PHE	CB-CA-C	-5.57	101.38	110.85
3	I	353	ILE	O-C-N	5.57	129.20	123.18
1	J	146	PHE	N-CA-CB	5.57	118.86	109.94
1	J	183	HIS	CG-ND1-CE1	-5.57	99.83	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	45	ASP	CA-C-O	-5.57	114.95	120.80
1	J	250	SER	N-CA-C	-5.57	101.05	109.85
1	D	86	LYS	N-CA-C	-5.57	105.70	112.88
1	D	195	ILE	CA-C-N	5.56	125.47	119.85
1	D	195	ILE	C-N-CA	5.56	125.47	119.85
1	G	118	TYR	CA-C-O	-5.56	113.92	120.60
2	H	251	LEU	N-CA-C	-5.56	106.16	113.17
2	B	205	SER	O-C-N	-5.56	116.49	123.27
2	B	355	PHE	CA-C-O	5.56	127.44	121.16
3	I	398	TYR	CD1-CE1-CZ	5.56	129.61	119.60
2	K	238	SER	CA-C-N	5.56	126.11	120.00
2	K	238	SER	C-N-CA	5.56	126.11	120.00
3	L	128	HIS	O-C-N	-5.56	116.77	123.27
3	L	365	THR	N-CA-C	-5.56	106.34	113.23
3	I	267	SER	O-C-N	-5.56	116.15	123.21
2	B	370	CYS	CB-CA-C	5.55	121.47	110.42
3	L	343	SER	O-C-N	5.55	129.98	122.59
1	D	199	SER	N-CA-CB	5.55	118.16	110.17
1	A	172	HIS	ND1-CG-CD2	5.55	111.65	106.10
3	C	331	ASN	N-CA-CB	5.55	117.98	110.38
2	K	53	THR	N-CA-C	-5.55	100.64	109.96
3	I	257	PHE	N-CA-CB	5.55	118.00	110.79
2	B	315	VAL	CB-CA-C	5.55	117.25	111.09
3	I	64	ALA	N-CA-C	5.54	117.32	111.28
3	F	310	ASP	N-CA-C	-5.54	106.69	113.50
3	F	332	ASN	N-CA-C	5.54	116.68	109.64
3	C	311	THR	CA-C-O	-5.54	115.35	120.94
3	F	105	ARG	CA-C-O	-5.54	116.15	121.08
3	F	211	ASN	CA-C-O	-5.54	114.96	121.44
1	G	234	VAL	N-CA-C	5.54	116.34	108.42
3	I	289	TYR	N-CA-CB	5.54	116.73	110.03
1	J	138	ASN	CA-C-N	5.54	125.20	119.05
1	J	138	ASN	C-N-CA	5.54	125.20	119.05
2	B	11	VAL	N-CA-CB	5.54	116.56	110.53
3	C	277	ARG	N-CA-CB	5.54	120.59	111.62
2	K	186	ASN	CA-CB-CG	5.54	118.14	112.60
3	C	236	TYR	CA-C-N	5.54	129.75	121.72
3	C	236	TYR	C-N-CA	5.54	129.75	121.72
3	F	293	PHE	CA-CB-CG	5.54	119.34	113.80
2	E	189	TYR	CA-C-O	-5.53	115.39	121.31
3	F	79	ARG	CD-NE-CZ	-5.53	116.65	124.40
3	F	347	HIS	ND1-CE1-NE2	5.53	113.93	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	134	MET	CA-C-O	5.53	126.40	120.32
2	E	306	CYS	N-CA-CB	5.53	119.50	110.37
3	L	339	GLN	CB-CA-C	-5.53	100.98	110.16
1	G	103	ASN	CA-C-N	5.53	129.33	121.42
1	G	103	ASN	C-N-CA	5.53	129.33	121.42
2	H	285	ALA	N-CA-C	-5.53	98.62	108.13
2	H	9	ASN	CA-C-O	-5.53	115.17	120.92
1	J	233	SER	N-CA-C	-5.53	100.17	109.07
2	E	182	ASP	CA-CB-CG	5.53	118.13	112.60
2	H	413	THR	CA-C-N	5.53	127.69	120.28
2	H	413	THR	C-N-CA	5.53	127.69	120.28
3	I	17	TRP	CA-C-N	5.53	131.25	122.74
3	I	17	TRP	C-N-CA	5.53	131.25	122.74
1	D	222	GLY	O-C-N	-5.52	117.34	123.58
2	K	329	ALA	CB-CA-C	-5.52	101.79	110.79
3	C	102	ALA	N-CA-C	-5.52	100.32	108.99
2	E	139	GLU	N-CA-C	-5.52	107.79	114.75
3	I	224	CYS	O-C-N	-5.52	116.73	123.36
3	I	39	ASP	CA-C-N	5.52	129.31	121.42
3	I	39	ASP	C-N-CA	5.52	129.31	121.42
3	I	257	PHE	CB-CA-C	-5.52	103.16	111.27
3	C	153	TYR	N-CA-CB	5.52	119.41	110.42
3	C	331	ASN	CA-CB-CG	-5.52	107.08	112.60
3	C	378	ILE	CB-CA-C	-5.51	104.61	112.22
2	H	263	VAL	CA-C-N	5.51	126.62	119.78
2	H	263	VAL	C-N-CA	5.51	126.62	119.78
3	F	351	ILE	O-C-N	-5.51	117.39	123.18
2	B	242	TYR	CA-C-O	-5.51	115.02	120.70
3	I	305	SER	N-CA-CB	5.51	121.14	111.55
1	J	83	PRO	CA-C-N	5.51	129.52	121.31
1	J	83	PRO	C-N-CA	5.51	129.52	121.31
1	D	91	PRO	O-C-N	5.51	130.08	122.64
3	C	103	ARG	CD-NE-CZ	-5.50	116.69	124.40
2	K	86	PRO	CA-C-N	5.50	130.50	122.08
2	K	86	PRO	C-N-CA	5.50	130.50	122.08
2	B	16	LYS	N-CA-C	5.50	117.37	108.41
2	B	187	GLU	N-CA-C	-5.50	99.09	110.80
3	C	68	TYR	N-CA-C	-5.50	100.71	109.23
3	F	4	HIS	CA-CB-CG	5.50	119.30	113.80
1	J	186	VAL	N-CA-C	-5.50	97.90	109.34
2	B	382	PRO	CB-CA-C	-5.50	106.00	111.17
2	K	324	LYS	CA-C-N	5.50	130.00	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	324	LYS	C-N-CA	5.50	130.00	123.19
2	E	5	THR	N-CA-C	-5.49	100.95	109.14
1	G	172	HIS	ND1-CE1-NE2	5.49	113.89	108.40
2	H	31	LEU	N-CA-CB	5.49	120.96	111.13
2	B	367	VAL	CB-CA-C	-5.48	104.11	110.91
2	H	228	ASN	O-C-N	-5.48	116.63	123.04
2	K	203	ILE	CB-CA-C	5.48	120.28	111.29
2	E	218	ASN	CA-CB-CG	-5.48	107.12	112.60
3	L	75	GLN	CA-C-N	5.48	131.44	122.07
3	L	75	GLN	C-N-CA	5.48	131.44	122.07
2	B	186	ASN	OD1-CG-ND2	5.48	128.08	122.60
2	B	253	ARG	O-C-N	5.47	129.18	122.34
2	E	353	SER	N-CA-CB	5.47	119.10	110.23
3	F	367	THR	O-C-N	-5.47	116.32	122.12
1	J	240	ASP	N-CA-C	-5.47	100.97	109.24
2	E	330	ILE	N-CA-C	-5.47	99.94	108.81
2	E	354	LEU	N-CA-C	-5.47	100.98	109.24
2	K	250	PRO	N-CD-CG	5.47	111.41	103.20
3	C	157	THR	CA-CB-OG1	5.47	117.81	109.60
3	F	168	VAL	CA-C-N	5.47	126.02	120.38
3	F	168	VAL	C-N-CA	5.47	126.02	120.38
2	B	221	LEU	CB-CA-C	-5.47	100.16	109.51
3	C	399	GLN	CA-C-O	-5.47	114.75	120.55
3	F	59	ASN	CA-CB-CG	5.47	118.07	112.60
2	K	186	ASN	N-CA-C	-5.47	99.82	108.73
3	F	98	HIS	ND1-CE1-NE2	5.47	113.87	108.40
3	I	123	ARG	CD-NE-CZ	-5.47	116.75	124.40
2	H	266	VAL	CA-C-O	-5.47	113.95	120.78
2	K	62	CYS	O-C-N	5.47	129.44	123.04
3	C	82	LEU	O-C-N	-5.46	116.22	122.89
2	K	288	THR	O-C-N	5.46	130.03	123.36
2	H	324	LYS	N-CA-CB	5.46	119.72	110.49
3	C	305	SER	N-CA-C	-5.46	101.00	109.24
2	K	259	CYS	CA-C-N	5.46	130.44	123.13
2	K	259	CYS	C-N-CA	5.46	130.44	123.13
1	D	238	ASN	CA-CB-CG	-5.46	107.14	112.60
2	B	381	GLU	N-CA-C	-5.45	97.76	109.81
1	G	155	GLU	CA-C-O	-5.45	114.84	121.28
2	K	191	PRO	CA-C-O	-5.45	114.77	121.31
3	F	63	HIS	ND1-CE1-NE2	5.45	113.85	108.40
1	A	212	ASN	CA-C-O	5.45	125.36	119.15
2	K	356	PHE	N-CA-C	-5.45	101.13	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	358	THR	N-CA-C	-5.45	102.94	110.35
2	B	351	ALA	CA-C-N	5.44	129.98	121.76
2	B	351	ALA	C-N-CA	5.44	129.98	121.76
3	F	407	PRO	N-CA-CB	5.44	109.29	103.52
3	L	14	TYR	CB-CG-CD2	-5.44	112.64	120.80
2	B	219	LEU	N-CA-CB	5.44	120.98	111.13
3	F	246	VAL	CA-C-O	-5.44	114.50	120.43
2	H	238	SER	N-CA-C	-5.44	102.70	110.59
3	L	364	TRP	CB-CG-CD2	-5.44	119.18	126.80
3	F	398	TYR	N-CA-CB	5.44	117.96	110.07
2	E	350	GLY	CA-C-N	5.44	129.27	121.50
2	E	350	GLY	C-N-CA	5.44	129.27	121.50
3	I	155	HIS	CE1-NE2-CD2	-5.44	103.56	109.00
2	H	235	GLN	CA-C-O	5.44	126.97	120.28
3	C	170	PRO	CA-C-O	-5.43	115.04	121.67
3	F	35	HIS	N-CA-C	-5.43	100.26	108.52
1	A	203	GLY	N-CA-C	-5.43	107.28	115.32
2	B	145	ASP	CA-CB-CG	-5.43	107.17	112.60
3	C	42	ASP	CA-CB-CG	5.43	118.03	112.60
1	D	87	LYS	N-CA-C	-5.43	100.87	108.96
3	L	31	VAL	CA-C-O	5.43	126.51	120.59
1	A	245	ILE	CB-CA-C	5.43	117.55	111.80
1	A	234	VAL	CA-C-O	5.43	126.78	121.19
2	B	320	TYR	N-CA-CB	5.43	119.81	111.24
2	E	130	LYS	N-CA-C	-5.43	101.04	109.72
2	E	347	GLN	CG-CD-NE2	-5.43	108.26	116.40
3	F	167	HIS	CA-C-O	5.43	127.09	121.28
2	K	87	PHE	N-CA-CB	5.43	118.22	111.00
2	K	427	VAL	N-CA-CB	5.43	118.72	110.58
2	H	123	GLN	N-CA-CB	5.42	119.28	110.17
3	C	195	LYS	N-CA-C	-5.42	99.89	108.73
2	H	151	ASP	N-CA-CB	5.42	118.36	109.95
2	H	292	GLU	CA-C-N	5.42	135.03	121.80
2	H	292	GLU	C-N-CA	5.42	135.03	121.80
3	I	99	PHE	CA-CB-CG	-5.42	108.38	113.80
2	B	345	ASP	N-CA-C	-5.42	100.27	108.67
2	B	390	TYR	O-C-N	5.42	129.99	122.78
3	F	376	ILE	N-CA-C	-5.42	105.25	110.72
3	C	128	HIS	N-CA-C	-5.42	99.46	108.34
1	D	226	GLU	CA-C-N	5.42	132.03	121.41
1	D	226	GLU	C-N-CA	5.42	132.03	121.41
2	H	119	ALA	O-C-N	-5.42	114.33	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	423	VAL	CA-C-N	5.42	127.54	120.28
2	H	423	VAL	C-N-CA	5.42	127.54	120.28
2	K	435	VAL	N-CA-CB	5.42	117.91	110.54
2	H	191	PRO	CA-C-O	-5.42	114.98	121.48
3	I	185	TYR	CG-CD1-CE1	-5.42	113.08	121.20
3	C	159	LEU	N-CA-C	-5.41	106.73	113.55
2	E	387	ILE	O-C-N	-5.41	114.34	123.00
3	C	385	PHE	CB-CA-C	-5.41	101.65	110.85
2	H	427	VAL	CB-CA-C	-5.41	105.05	111.97
1	J	170	PHE	N-CA-C	-5.41	102.28	110.28
1	J	217	VAL	N-CA-C	-5.41	104.73	112.35
2	H	326	GLY	CA-C-O	-5.41	116.36	121.60
2	K	148	VAL	CA-CB-CG1	-5.41	101.21	110.40
2	H	295	SER	CB-CA-C	-5.40	100.27	109.51
3	F	35	HIS	CB-CG-ND1	-5.40	114.60	122.70
2	E	192	TYR	CA-C-O	-5.40	115.33	121.65
3	F	52	GLN	CB-CG-CD	-5.40	103.42	112.60
3	F	210	THR	N-CA-C	-5.40	105.65	113.21
3	C	231	ASN	O-C-N	5.40	129.20	123.42
3	F	62	ASN	CA-C-O	5.40	126.92	120.28
2	K	292	GLU	N-CA-CB	5.39	119.61	110.49
1	A	148	LYS	N-CA-CB	-5.39	102.89	111.62
2	B	251	LEU	N-CA-C	-5.39	105.52	113.61
3	C	168	VAL	N-CA-CB	5.39	118.76	111.21
1	G	244	ARG	N-CA-C	5.39	118.56	111.28
2	H	147	PHE	CA-CB-CG	-5.39	108.41	113.80
2	H	266	VAL	O-C-N	5.39	129.31	122.57
1	D	253	TRP	CD2-CE2-CZ2	-5.39	117.01	122.40
1	G	90	LYS	N-CA-C	5.39	114.50	108.25
3	L	180	ASN	N-CA-C	-5.39	98.98	108.20
2	B	390	TYR	CA-CB-CG	-5.39	104.20	113.90
1	D	239	LYS	CA-C-N	5.39	131.46	122.73
1	D	239	LYS	C-N-CA	5.39	131.46	122.73
1	G	209	ILE	CA-CB-CG2	-5.39	101.34	110.50
3	L	395	LEU	CB-CA-C	-5.39	100.84	110.70
3	C	128	HIS	ND1-CE1-NE2	5.39	113.79	108.40
3	C	317	ILE	CB-CA-C	-5.39	102.20	110.50
2	E	421	LEU	N-CA-C	5.39	117.23	111.36
2	H	302	GLU	N-CA-C	-5.39	100.92	109.59
3	L	364	TRP	N-CA-C	-5.39	107.72	114.56
1	G	87	LYS	N-CA-C	-5.38	106.90	112.93
3	I	63	HIS	ND1-CG-CD2	5.38	111.48	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	415	CYS	CA-C-N	5.38	127.76	120.44
3	C	415	CYS	C-N-CA	5.38	127.76	120.44
1	D	239	LYS	CA-C-O	-5.38	113.13	119.05
2	E	7	MET	CG-SD-CE	-5.38	89.06	100.90
1	G	197	THR	N-CA-C	5.38	118.28	110.42
2	B	400	PRO	N-CA-CB	5.38	108.90	103.25
3	C	140	ALA	CA-C-O	-5.38	115.94	121.32
3	F	236	TYR	N-CA-CB	5.38	118.95	110.56
3	C	261	ASP	N-CA-C	-5.38	102.92	110.50
2	E	145	ASP	CA-CB-CG	5.38	117.98	112.60
3	L	252	LYS	N-CA-CB	5.38	120.91	111.55
3	F	22	GLY	O-C-N	5.38	128.47	122.50
3	F	86	THR	O-C-N	5.38	127.90	122.09
2	K	240	PHE	N-CA-CB	5.38	118.12	110.16
3	L	240	TYR	CA-C-N	5.38	126.46	122.59
3	L	240	TYR	C-N-CA	5.38	126.46	122.59
2	E	243	TRP	CB-CG-CD2	-5.38	119.28	126.80
3	F	105	ARG	CB-CA-C	-5.37	101.63	109.48
1	G	141	LEU	N-CA-C	5.37	116.82	111.07
3	I	138	SER	CA-C-N	5.37	126.56	119.84
3	I	138	SER	C-N-CA	5.37	126.56	119.84
2	B	173	PHE	N-CA-C	-5.37	102.09	110.10
3	I	404	ALA	CA-C-N	5.37	127.48	120.28
3	I	404	ALA	C-N-CA	5.37	127.48	120.28
2	E	321	THR	N-CA-C	-5.36	100.92	109.23
2	K	105	GLU	CA-C-N	5.36	129.15	121.96
2	K	105	GLU	C-N-CA	5.36	129.15	121.96
2	B	166	ILE	N-CA-CB	5.36	117.61	110.26
1	A	98	CYS	CA-C-N	5.36	128.43	120.17
1	A	98	CYS	C-N-CA	5.36	128.43	120.17
2	E	376	CYS	CA-C-N	5.36	131.35	121.70
2	E	376	CYS	C-N-CA	5.36	131.35	121.70
2	K	19	ILE	N-CA-CB	5.36	120.08	111.23
3	C	114	LEU	CA-C-O	-5.36	115.50	121.23
3	C	383	SER	CB-CA-C	-5.36	102.47	110.88
3	F	155	HIS	ND1-CG-CD2	5.36	111.46	106.10
2	K	188	ASP	CA-C-N	5.35	130.93	122.36
2	K	188	ASP	C-N-CA	5.35	130.93	122.36
2	B	337	ALA	N-CA-C	-5.35	101.16	109.72
1	D	138	ASN	CA-C-N	5.35	124.99	119.05
1	D	138	ASN	C-N-CA	5.35	124.99	119.05
1	D	187	GLN	O-C-N	-5.35	117.12	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	84	VAL	N-CA-C	-5.35	100.48	108.46
2	K	393	LYS	CG-CD-CE	5.35	123.61	111.30
3	L	155	HIS	N-CA-CB	5.35	118.17	110.20
2	B	273	TYR	CA-C-O	-5.35	115.51	121.23
2	H	86	PRO	CA-C-N	5.35	131.41	121.62
2	H	86	PRO	C-N-CA	5.35	131.41	121.62
1	J	96	ARG	N-CA-C	-5.35	99.60	108.75
1	J	108	PRO	CA-C-O	-5.35	115.33	121.86
1	D	220	VAL	N-CA-CB	5.35	116.36	110.53
1	G	102	GLU	N-CA-C	-5.35	102.61	110.52
3	I	11	THR	CA-CB-OG1	5.35	117.62	109.60
2	B	4	SER	N-CA-CB	5.35	119.53	110.49
3	I	33	ILE	CA-CB-CG2	-5.34	101.42	110.50
2	B	402	ILE	N-CA-C	-5.34	99.91	107.98
2	B	338	THR	N-CA-C	-5.34	100.62	108.79
3	L	321	ALA	CA-C-O	5.34	126.17	120.24
2	E	93	TYR	CA-CB-CG	-5.34	104.29	113.90
3	C	12	ARG	CB-CG-CD	5.34	123.57	111.30
2	H	67	GLU	CA-C-N	5.34	128.81	120.75
2	H	67	GLU	C-N-CA	5.34	128.81	120.75
2	B	216	ASN	CA-CB-CG	-5.33	107.27	112.60
3	L	419	ALA	CA-C-N	5.33	127.38	120.44
3	L	419	ALA	C-N-CA	5.33	127.38	120.44
3	F	105	ARG	CA-C-N	5.33	125.27	119.78
3	F	105	ARG	C-N-CA	5.33	125.27	119.78
3	F	206	GLU	CA-CB-CG	5.33	124.77	114.10
2	B	71	LYS	CA-CB-CG	5.33	124.77	114.10
2	H	291	ASP	CA-CB-CG	-5.33	107.27	112.60
3	I	74	VAL	CB-CA-C	-5.33	104.51	110.96
3	L	252	LYS	O-C-N	-5.33	116.22	123.15
1	J	133	LYS	N-CA-CB	5.33	118.20	110.26
2	B	328	CYS	N-CA-C	-5.33	101.88	110.14
3	L	175	GLN	OE1-CD-NE2	5.33	127.93	122.60
1	J	172	HIS	O-C-N	-5.33	116.36	121.85
2	B	385	ASP	CA-CB-CG	-5.33	107.27	112.60
2	E	428	VAL	N-CA-C	5.33	115.53	110.42
3	I	398	TYR	N-CA-C	-5.33	105.39	111.14
3	I	407	PRO	CA-C-O	-5.33	110.91	120.60
3	L	395	LEU	N-CA-C	5.33	118.24	111.69
2	E	219	LEU	N-CA-C	-5.32	100.01	109.06
2	H	318	ILE	N-CA-C	-5.32	100.66	108.11
3	L	189	PRO	O-C-N	5.32	129.83	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	48	THR	CB-CA-C	5.32	120.50	109.38
3	F	88	ALA	O-C-N	-5.32	116.87	121.71
2	B	25	ALA	CA-C-N	5.32	131.83	121.41
2	B	25	ALA	C-N-CA	5.32	131.83	121.41
3	F	306	GLN	CA-CB-CG	-5.32	103.46	114.10
3	F	419	ALA	N-CA-C	5.32	116.76	111.07
2	B	319	SER	N-CA-C	-5.31	101.05	109.76
3	C	156	GLN	CA-C-O	-5.31	115.92	121.55
3	C	407	PRO	N-CA-C	-5.31	106.79	114.18
2	B	141	ASN	N-CA-CB	5.31	118.92	110.84
2	H	89	TRP	CE2-CD2-CE3	5.31	124.11	118.80
2	B	57	SER	CA-C-N	5.31	125.57	119.83
2	B	57	SER	C-N-CA	5.31	125.57	119.83
2	B	210	SER	CA-C-O	5.31	126.73	120.89
2	E	404	THR	CA-C-N	5.31	127.34	120.44
2	E	404	THR	C-N-CA	5.31	127.34	120.44
2	K	61	LYS	N-CA-CB	5.31	119.73	110.81
3	C	241	VAL	O-C-N	-5.31	115.05	121.10
1	A	162	CYS	N-CA-C	-5.30	105.39	111.07
3	F	366	ILE	CA-C-N	5.30	127.39	120.28
3	F	366	ILE	C-N-CA	5.30	127.39	120.28
3	I	272	PRO	CA-C-N	5.30	128.40	120.87
3	I	272	PRO	C-N-CA	5.30	128.40	120.87
1	J	228	ALA	N-CA-CB	5.30	119.46	110.49
3	L	287	PRO	N-CA-CB	-5.30	98.69	103.36
2	B	402	ILE	N-CA-CB	5.30	117.54	111.39
2	E	261	ILE	N-CA-C	-5.30	100.78	108.36
1	D	193	PHE	CA-CB-CG	-5.30	108.50	113.80
3	F	257	PHE	CA-C-N	5.30	125.76	120.14
3	F	257	PHE	C-N-CA	5.30	125.76	120.14
3	C	62	ASN	N-CA-C	-5.30	99.31	108.69
3	F	110	VAL	CG1-CB-CG2	-5.30	99.15	110.80
3	F	412	LEU	O-C-N	5.30	128.78	122.27
2	H	139	GLU	N-CA-CB	5.30	119.44	110.49
2	H	311	ASP	CA-C-N	5.30	128.39	120.87
2	H	311	ASP	C-N-CA	5.30	128.39	120.87
2	B	207	THR	CA-C-O	5.29	127.28	121.40
2	B	356	PHE	N-CA-C	-5.29	101.36	109.41
3	L	96	MET	N-CA-C	-5.29	99.19	107.93
2	H	13	ILE	N-CA-CB	5.29	115.89	110.23
2	H	47	ILE	O-C-N	-5.29	117.46	123.18
2	H	306	CYS	CA-C-N	5.29	131.65	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	306	CYS	C-N-CA	5.29	131.65	121.54
1	J	237	TRP	CG-CD1-NE1	5.29	117.08	110.20
3	L	217	ASN	CA-CB-CG	-5.29	107.31	112.60
2	B	253	ARG	NE-CZ-NH2	-5.29	114.44	119.20
3	I	88	ALA	CA-C-N	5.29	126.45	119.84
3	I	88	ALA	C-N-CA	5.29	126.45	119.84
3	L	271	GLU	CA-C-O	-5.29	115.27	119.71
3	F	416	ALA	CA-C-N	5.29	127.31	120.44
3	F	416	ALA	C-N-CA	5.29	127.31	120.44
1	G	221	LEU	N-CA-C	-5.29	106.96	113.41
2	H	216	ASN	N-CA-C	-5.29	99.33	108.69
2	K	228	ASN	N-CA-C	-5.29	102.22	110.42
2	B	180	TYR	O-C-N	-5.29	116.15	122.65
3	F	148	ILE	CA-C-N	5.29	125.70	119.99
3	F	148	ILE	C-N-CA	5.29	125.70	119.99
1	G	153	ASP	N-CA-CB	5.29	119.42	110.49
2	H	368	GLN	CA-C-O	5.29	127.08	121.11
2	K	385	ASP	N-CA-CB	5.29	119.42	110.49
3	C	52	GLN	N-CA-C	-5.28	99.68	108.34
3	I	87	THR	CA-C-O	5.28	124.33	118.52
2	K	400	PRO	O-C-N	5.28	129.77	122.64
3	F	159	LEU	CA-C-O	-5.28	114.90	120.55
3	I	283	PHE	N-CA-C	-5.28	100.79	109.40
2	B	81	PHE	O-C-N	-5.28	117.15	123.06
2	K	363	PRO	CA-C-O	-5.28	111.53	119.55
3	F	171	ASP	N-CA-CB	5.28	119.47	110.71
2	K	411	ALA	N-CA-C	5.28	122.04	110.80
2	K	367	VAL	N-CA-CB	5.28	117.84	110.56
2	K	308	TYR	CA-C-N	5.27	131.61	121.54
2	K	308	TYR	C-N-CA	5.27	131.61	121.54
3	L	306	GLN	N-CA-CB	5.27	121.34	111.53
3	C	350	PRO	CA-C-N	5.27	127.68	120.46
3	C	350	PRO	C-N-CA	5.27	127.68	120.46
2	E	112	GLU	CB-CG-CD	-5.27	103.64	112.60
3	F	4	HIS	N-CA-C	5.27	117.03	111.28
3	F	61	ILE	N-CA-C	-5.27	100.15	107.80
3	I	274	VAL	O-C-N	5.27	128.52	123.14
3	C	237	ASN	O-C-N	5.27	129.50	123.02
1	J	219	ILE	N-CA-CB	5.27	118.68	111.41
3	L	213	ILE	N-CA-C	-5.27	100.15	108.90
3	C	210	THR	N-CA-C	-5.27	106.36	114.16
3	F	163	GLU	N-CA-C	-5.27	101.35	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	76	GLU	CB-CG-CD	-5.27	103.64	112.60
2	K	14	PRO	N-CA-CB	5.27	108.78	103.25
1	J	90	LYS	CB-CA-C	-5.27	101.28	109.55
2	K	32	VAL	CB-CA-C	-5.27	102.27	110.69
2	E	295	SER	N-CA-C	-5.26	101.36	109.52
2	E	402	ILE	N-CA-CB	5.26	117.00	111.00
1	A	228	ALA	CA-C-O	-5.26	112.98	120.51
3	F	57	LYS	CA-C-O	5.26	125.84	119.31
3	F	192	LYS	N-CA-C	-5.26	100.82	109.40
3	L	224	CYS	CB-CA-C	-5.26	104.21	110.94
2	E	250	PRO	N-CA-CB	-5.26	98.63	103.31
3	F	95	THR	CA-CB-OG1	5.26	117.49	109.60
2	E	155	ARG	CA-C-N	5.26	130.45	122.98
2	E	155	ARG	C-N-CA	5.26	130.45	122.98
1	G	201	LYS	N-CA-CB	5.26	116.39	110.03
1	J	141	LEU	CA-C-N	5.26	127.28	120.44
1	J	141	LEU	C-N-CA	5.26	127.28	120.44
2	K	380	CYS	CA-C-N	5.26	131.48	122.38
2	K	380	CYS	C-N-CA	5.26	131.48	122.38
3	L	199	THR	CA-CB-OG1	5.26	117.49	109.60
1	D	160	PRO	CA-C-N	5.26	128.78	120.47
1	D	160	PRO	C-N-CA	5.26	128.78	120.47
1	J	172	HIS	ND1-CE1-NE2	5.26	113.66	108.40
1	D	149	SER	N-CA-C	-5.25	96.79	107.41
2	E	405	THR	CB-CA-C	-5.25	102.63	110.88
3	F	17	TRP	CE2-CD2-CE3	5.25	124.06	118.80
2	E	367	VAL	N-CA-CB	5.25	116.45	110.72
1	A	234	VAL	O-C-N	-5.25	117.22	123.00
1	D	104	ASP	N-CA-CB	5.25	117.77	110.26
2	H	238	SER	CA-C-O	-5.25	115.75	121.89
3	I	371	SER	CB-CA-C	-5.25	102.64	110.88
2	K	388	VAL	CA-C-N	5.25	125.55	119.93
2	K	388	VAL	C-N-CA	5.25	125.55	119.93
1	A	183	HIS	ND1-CE1-NE2	5.25	113.65	108.40
3	L	374	LEU	N-CA-C	-5.25	105.47	111.14
1	G	204	ASP	CA-C-N	5.25	130.78	122.60
1	G	204	ASP	C-N-CA	5.25	130.78	122.60
2	K	155	ARG	N-CA-CB	5.25	119.50	110.68
3	L	304	HIS	ND1-CE1-NE2	5.25	113.65	108.40
1	A	99	MET	O-C-N	5.24	128.03	121.84
2	B	250	PRO	N-CA-C	5.24	119.55	111.21
3	C	188	ASP	N-CA-CB	5.24	117.33	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	347	HIS	CB-CG-CD2	-5.24	124.38	131.20
2	E	186	ASN	CA-CB-CG	5.24	117.84	112.60
3	I	290	PRO	CA-N-CD	-5.24	104.66	112.00
2	B	51	TYR	CA-C-O	-5.24	114.98	121.06
2	H	45	ASP	N-CA-CB	5.24	117.88	110.13
1	D	175	PRO	CA-C-N	5.24	129.77	121.18
1	D	175	PRO	C-N-CA	5.24	129.77	121.18
2	E	407	TRP	CE2-CD2-CE3	5.24	124.04	118.80
3	I	254	HIS	ND1-CE1-NE2	5.24	113.64	108.40
2	H	186	ASN	CA-CB-CG	-5.24	107.36	112.60
1	G	151	LYS	CB-CG-CD	5.23	123.34	111.30
2	B	15	PHE	N-CA-C	-5.23	101.18	109.76
2	B	321	THR	N-CA-C	-5.23	100.17	109.06
2	K	85	TYR	N-CA-CB	5.23	119.68	110.37
3	L	204	VAL	CA-CB-CG2	5.23	119.29	110.40
3	L	406	LEU	CA-C-O	-5.23	114.84	119.86
3	C	335	ARG	NH1-CZ-NH2	5.22	126.09	119.30
1	D	94	ARG	CA-C-O	5.22	127.12	121.06
2	K	23	GLY	N-CA-C	-5.22	105.01	111.70
2	K	307	THR	CA-C-O	5.22	126.97	120.54
2	B	404	THR	O-C-N	5.22	127.66	122.12
2	H	281	ASP	CA-CB-CG	-5.22	107.38	112.60
3	L	11	THR	CA-CB-OG1	5.22	117.44	109.60
3	F	48	GLN	OE1-CD-NE2	5.22	127.82	122.60
2	H	137	ILE	CA-C-N	5.22	130.22	120.87
2	H	137	ILE	C-N-CA	5.22	130.22	120.87
3	L	123	ARG	CB-CG-CD	5.22	123.31	111.30
3	C	81	THR	O-C-N	-5.22	115.93	122.35
3	C	129	LYS	CA-C-N	5.22	126.36	119.84
3	C	129	LYS	C-N-CA	5.22	126.36	119.84
2	H	69	SER	N-CA-C	-5.22	99.68	110.80
2	H	389	PRO	CA-C-O	-5.22	111.10	120.60
3	I	1	SER	CB-CA-C	5.22	120.02	110.10
1	J	226	GLU	N-CA-C	-5.22	104.51	111.24
2	K	36	SER	N-CA-C	-5.22	102.02	110.32
1	J	211	ASP	N-CA-CB	-5.22	102.64	110.73
1	J	249	GLU	N-CA-CB	5.22	119.31	110.49
2	K	165	PRO	O-C-N	5.22	129.63	123.06
2	K	262	LYS	CA-C-N	5.22	127.24	120.56
2	K	262	LYS	C-N-CA	5.22	127.24	120.56
1	A	238	ASN	O-C-N	5.21	129.52	122.59
1	D	88	LYS	N-CA-CB	5.21	120.37	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	8	PRO	N-CA-C	-5.21	103.06	111.77
2	H	273	TYR	CB-CG-CD2	-5.21	112.98	120.80
2	H	83	GLY	N-CA-C	-5.21	108.43	115.36
3	L	404	ALA	N-CA-CB	5.21	119.49	111.46
2	B	244	LYS	N-CA-C	5.21	117.70	111.71
2	K	429	VAL	N-CA-C	5.21	115.98	110.72
1	A	243	THR	N-CA-CB	5.21	118.37	110.45
2	H	33	VAL	CB-CA-C	-5.21	103.07	110.83
2	H	339	MET	O-C-N	-5.21	116.72	122.86
1	A	230	THR	N-CA-C	-5.21	99.93	108.41
1	D	172	HIS	N-CA-CB	5.21	119.29	110.49
3	F	162	GLU	N-CA-C	-5.21	99.71	110.80
3	F	178	VAL	CA-CB-CG2	5.21	119.25	110.40
3	F	418	SER	CA-C-O	-5.21	114.90	120.42
2	H	182	ASP	CA-CB-CG	5.21	117.81	112.60
2	B	366	VAL	N-CA-C	-5.20	99.46	106.85
2	H	337	ALA	N-CA-C	-5.20	101.00	108.60
3	I	234	TRP	O-C-N	5.20	128.88	122.84
3	I	262	SER	CA-C-O	-5.20	115.78	121.14
3	I	417	LYS	CB-CA-C	-5.20	102.71	110.88
2	K	311	ASP	N-CA-C	-5.20	106.78	113.02
3	L	286	HIS	ND1-CG-CD2	5.20	111.30	106.10
2	H	97	ASP	N-CA-C	-5.20	106.85	114.39
3	C	288	MET	N-CA-C	-5.20	101.53	108.86
3	F	85	SER	CA-C-O	5.20	126.32	119.98
3	F	144	HIS	CG-CD2-NE2	-5.20	102.00	107.20
2	B	409	TRP	CD2-CE2-CZ2	-5.20	117.20	122.40
3	I	34	GLU	CB-CG-CD	-5.20	103.77	112.60
3	I	128	HIS	CG-ND1-CE1	-5.20	100.46	109.30
2	B	219	LEU	CA-C-N	5.20	130.66	123.07
2	B	219	LEU	C-N-CA	5.20	130.66	123.07
2	H	55	VAL	N-CA-C	-5.20	101.43	107.61
2	H	21	ARG	CB-CG-CD	5.19	123.25	111.30
3	F	50	SER	N-CA-C	-5.19	105.70	111.36
2	H	93	TYR	CB-CA-C	-5.19	104.36	111.73
1	J	111	LEU	CA-C-N	5.19	131.41	123.47
1	J	111	LEU	C-N-CA	5.19	131.41	123.47
1	J	155	GLU	CA-C-O	-5.19	115.15	121.28
2	E	46	TYR	CA-C-N	5.19	130.22	123.06
2	E	46	TYR	C-N-CA	5.19	130.22	123.06
3	I	293	PHE	N-CA-C	-5.19	100.57	109.24
2	B	243	TRP	CE2-CD2-CE3	5.19	123.99	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	325	GLU	CA-C-O	-5.19	115.10	120.70
2	K	27	LEU	CB-CA-C	-5.19	103.18	110.13
1	A	128	LYS	CA-C-O	-5.18	113.06	120.16
1	G	187	GLN	OE1-CD-NE2	-5.18	117.42	122.60
2	H	350	GLY	N-CA-C	-5.18	100.89	113.18
3	L	258	PRO	CA-C-N	5.18	128.21	120.95
3	L	258	PRO	C-N-CA	5.18	128.21	120.95
3	L	286	HIS	N-CA-CB	5.18	115.35	109.49
2	B	328	CYS	CA-C-N	5.18	130.47	123.11
2	B	328	CYS	C-N-CA	5.18	130.47	123.11
2	H	236	THR	CA-C-N	5.18	126.32	119.84
2	H	236	THR	C-N-CA	5.18	126.32	119.84
1	A	147	LYS	N-CA-CB	5.18	119.84	110.83
1	A	148	LYS	CA-C-O	-5.18	115.71	121.51
1	J	247	PRO	CA-C-O	-5.18	112.23	119.74
3	C	392	THR	CA-CB-OG1	-5.18	101.83	109.60
2	K	142	GLN	O-C-N	-5.18	117.68	123.48
2	H	181	ARG	N-CA-C	-5.18	106.47	112.89
1	G	147	LYS	O-C-N	5.17	129.92	123.19
2	H	192	TYR	CB-CG-CD1	5.17	128.56	120.80
2	H	287	PHE	CA-C-N	5.17	130.71	122.74
2	H	287	PHE	C-N-CA	5.17	130.71	122.74
3	I	22	GLY	N-CA-C	-5.17	108.18	115.32
3	I	75	GLN	N-CA-C	-5.17	101.50	109.52
3	L	231	ASN	N-CA-C	5.17	117.53	110.55
3	C	35	HIS	CB-CG-CD2	-5.17	124.48	131.20
2	B	311	ASP	N-CA-CB	5.17	119.23	110.49
1	G	183	HIS	CE1-NE2-CD2	-5.17	103.83	109.00
1	J	246	THR	N-CA-C	-5.17	102.25	108.25
2	E	313	GLY	O-C-N	-5.17	118.68	122.71
3	I	270	PRO	CA-C-O	-5.17	115.69	121.32
2	K	58	PRO	CA-C-N	5.17	130.28	122.99
2	K	58	PRO	C-N-CA	5.17	130.28	122.99
3	L	32	SER	CA-C-N	5.17	128.83	122.37
3	L	32	SER	C-N-CA	5.17	128.83	122.37
2	K	7	MET	CA-C-O	-5.17	115.55	120.97
2	H	390	TYR	CB-CG-CD2	-5.16	113.06	120.80
3	L	69	MET	CG-SD-CE	-5.16	89.54	100.90
3	F	289	TYR	CA-C-N	5.16	126.29	119.84
3	F	289	TYR	C-N-CA	5.16	126.29	119.84
2	H	321	THR	CA-CB-CG2	5.16	119.27	110.50
2	B	158	GLN	OE1-CD-NE2	5.16	127.76	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	181	TRP	CD2-CE3-CZ3	-5.16	111.90	118.60
1	J	174	LYS	CA-C-O	-5.16	114.20	120.08
1	D	239	LYS	N-CA-C	-5.15	107.02	113.72
2	K	38	LEU	CA-C-N	5.15	130.54	123.28
2	K	38	LEU	C-N-CA	5.15	130.54	123.28
1	A	238	ASN	N-CA-CB	5.15	119.19	110.49
2	E	246	GLU	CA-C-O	-5.15	114.97	120.42
2	H	422	VAL	CA-C-N	5.14	127.73	120.42
2	H	422	VAL	C-N-CA	5.14	127.73	120.42
3	I	416	ALA	CA-C-N	5.14	127.13	120.44
3	I	416	ALA	C-N-CA	5.14	127.13	120.44
3	L	275	THR	N-CA-C	-5.14	101.37	109.50
2	B	259	CYS	CA-C-N	5.14	129.94	123.10
2	B	259	CYS	C-N-CA	5.14	129.94	123.10
3	C	396	THR	CA-C-N	5.14	124.86	119.82
3	C	396	THR	C-N-CA	5.14	124.86	119.82
3	F	140	ALA	CA-C-N	5.14	125.35	120.31
3	F	140	ALA	C-N-CA	5.14	125.35	120.31
2	K	173	PHE	CB-CG-CD2	5.14	129.44	120.70
3	F	240	TYR	CA-C-N	5.14	131.64	122.13
3	F	240	TYR	C-N-CA	5.14	131.64	122.13
3	I	201	GLY	N-CA-C	-5.14	102.11	111.16
3	I	381	GLY	O-C-N	5.14	127.12	122.19
2	K	409	TRP	CB-CG-CD1	5.14	134.61	126.90
2	B	411	ALA	N-CA-C	5.14	121.75	110.80
2	E	95	PHE	CA-CB-CG	5.14	118.94	113.80
3	F	331	ASN	CB-CG-ND2	-5.14	108.69	116.40
1	G	212	ASN	CB-CA-C	-5.14	102.26	110.79
1	D	250	SER	O-C-N	-5.14	117.52	123.33
2	B	318	ILE	CB-CA-C	5.14	118.23	110.63
2	H	332	SER	CA-C-N	5.14	131.72	122.89
2	H	332	SER	C-N-CA	5.14	131.72	122.89
3	I	254	HIS	O-C-N	5.14	128.65	122.79
2	K	359	SER	N-CA-C	-5.13	99.87	110.80
1	A	100	LYS	CA-C-N	5.13	128.16	122.77
1	A	100	LYS	C-N-CA	5.13	128.16	122.77
2	B	245	LYS	N-CA-C	-5.13	105.60	111.14
3	F	287	PRO	N-CA-CB	-5.13	97.86	103.25
3	F	349	ASN	O-C-N	-5.13	115.89	121.53
3	F	388	SER	N-CA-CB	5.13	117.75	110.16
2	B	124	VAL	N-CA-C	-5.13	101.09	108.53
2	H	247	LYS	CA-C-N	5.13	127.35	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	247	LYS	C-N-CA	5.13	127.35	122.27
2	H	364	ASN	CB-CG-ND2	-5.13	108.71	116.40
3	L	306	GLN	CB-CG-CD	-5.13	103.89	112.60
3	I	331	ASN	CA-C-N	5.12	134.30	121.80
3	I	331	ASN	C-N-CA	5.12	134.30	121.80
3	C	174	ILE	N-CA-CB	5.12	119.68	111.23
3	I	146	THR	N-CA-C	-5.12	100.95	108.99
3	L	283	PHE	CA-CB-CG	-5.12	108.68	113.80
3	I	364	TRP	N-CA-C	-5.12	107.69	114.04
3	L	410	ILE	CB-CA-C	-5.12	105.16	112.22
2	B	413	THR	OG1-CB-CG2	-5.12	99.06	109.30
1	G	127	MET	N-CA-C	-5.12	105.93	113.61
1	G	204	ASP	N-CA-C	-5.12	106.88	112.72
3	I	335	ARG	N-CA-C	-5.12	101.35	109.59
3	L	417	LYS	CA-C-N	5.12	127.56	120.29
3	L	417	LYS	C-N-CA	5.12	127.56	120.29
3	C	330	ASN	CB-CA-C	-5.12	101.84	110.44
2	H	260	ILE	N-CA-C	-5.12	100.28	107.75
3	I	330	ASN	CA-C-N	5.12	127.98	120.71
3	I	330	ASN	C-N-CA	5.12	127.98	120.71
2	H	86	PRO	CB-CA-C	-5.12	103.72	111.44
3	L	35	HIS	CB-CG-CD2	-5.11	124.55	131.20
2	B	55	VAL	N-CA-C	-5.11	102.13	107.60
2	B	165	PRO	N-CD-CG	5.11	110.87	103.20
3	F	247	THR	O-C-N	-5.11	116.94	122.92
2	H	93	TYR	CB-CG-CD1	5.11	128.47	120.80
2	H	240	PHE	N-CA-CB	5.11	117.48	110.07
1	A	131	HIS	ND1-CE1-NE2	5.11	113.51	108.40
3	C	124	THR	CA-C-O	-5.11	114.05	120.23
2	E	93	TYR	N-CA-C	-5.11	107.00	113.23
2	H	16	LYS	N-CA-CB	5.11	118.62	110.65
2	H	58	PRO	O-C-N	5.11	129.23	123.10
3	C	35	HIS	ND1-CG-CD2	5.11	111.21	106.10
2	E	326	GLY	CA-C-N	5.11	130.19	122.99
2	E	326	GLY	C-N-CA	5.11	130.19	122.99
3	F	356	HIS	CA-C-N	5.11	127.12	120.28
3	F	356	HIS	C-N-CA	5.11	127.12	120.28
3	I	155	HIS	ND1-CE1-NE2	5.11	113.50	108.40
1	J	202	PRO	O-C-N	-5.11	116.77	123.00
3	C	319	VAL	CA-CB-CG1	-5.10	101.72	110.40
3	F	133	ILE	CA-CB-CG2	-5.10	101.82	110.50
2	B	123	GLN	CG-CD-OE1	5.10	131.00	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	222	PRO	N-CA-CB	5.10	107.53	102.17
2	B	312	PHE	CA-C-O	5.10	127.41	121.44
3	C	361	TYR	CA-C-N	5.10	126.22	119.84
3	C	361	TYR	C-N-CA	5.10	126.22	119.84
1	J	138	ASN	CA-CB-CG	-5.10	107.50	112.60
3	F	67	ARG	CD-NE-CZ	-5.10	117.26	124.40
3	F	101	LEU	N-CA-C	-5.10	101.38	109.59
3	I	295	ILE	N-CA-C	-5.10	100.23	107.77
3	F	131	ARG	N-CA-C	-5.10	99.95	110.80
2	K	356	PHE	CA-CB-CG	-5.10	108.70	113.80
3	L	331	ASN	OD1-CG-ND2	5.10	127.70	122.60
2	B	425	ILE	CA-C-O	-5.09	115.65	120.95
2	E	53	THR	CA-CB-OG1	-5.09	101.96	109.60
3	I	157	THR	N-CA-C	-5.09	102.15	110.20
2	E	234	THR	N-CA-C	-5.09	100.60	108.90
3	C	227	TYR	N-CA-CB	5.09	120.35	111.13
1	D	192	ARG	NH1-CZ-NH2	5.09	125.92	119.30
2	E	27	LEU	N-CA-C	-5.09	101.70	109.64
3	I	172	VAL	O-C-N	5.09	126.91	121.10
2	B	371	ASN	CB-CA-C	-5.09	103.12	110.96
3	F	72	ASN	CA-C-O	5.09	125.49	119.48
1	G	195	ILE	CA-CB-CG2	-5.09	101.85	110.50
2	B	206	ARG	NH1-CZ-NH2	-5.09	112.69	119.30
3	C	341	SER	CA-C-N	5.09	131.26	121.54
3	C	341	SER	C-N-CA	5.09	131.26	121.54
2	E	100	ASN	CA-C-O	-5.09	116.16	121.55
2	E	303	VAL	N-CA-CB	5.09	118.25	111.64
3	F	347	HIS	ND1-CG-CD2	5.09	111.19	106.10
1	J	105	CYS	N-CA-CB	5.09	118.02	110.49
2	B	235	GLN	CB-CA-C	-5.09	102.31	110.14
3	C	91	ASP	N-CA-C	-5.09	100.88	109.07
3	F	420	ARG	CG-CD-NE	-5.09	100.81	112.00
2	H	348	GLU	N-CA-CB	5.08	117.36	109.48
2	B	74	ALA	CA-C-O	-5.08	115.16	120.55
1	D	193	PHE	CA-C-O	-5.08	115.08	120.92
3	F	35	HIS	ND1-CG-CD2	5.08	111.18	106.10
3	F	306	GLN	N-CA-C	-5.08	100.42	109.06
1	A	120	CYS	O-C-N	5.08	128.86	123.42
3	C	356	HIS	CA-CB-CG	-5.08	108.72	113.80
1	D	136	ILE	N-CA-CB	5.08	117.22	110.26
2	E	392	ALA	N-CA-C	-5.08	105.45	113.02
3	C	132	PHE	CA-C-N	5.08	131.11	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	132	PHE	C-N-CA	5.08	131.11	121.97
2	E	105	GLU	CB-CG-CD	-5.07	103.97	112.60
3	F	237	ASN	CA-CB-CG	5.07	117.67	112.60
2	H	191	PRO	CB-CA-C	-5.07	103.70	110.85
2	B	168	SER	N-CA-C	5.07	117.58	110.23
3	C	358	TYR	CA-C-N	5.07	128.30	121.05
3	C	358	TYR	C-N-CA	5.07	128.30	121.05
3	I	278	LEU	N-CA-C	-5.07	100.90	108.96
3	I	337	TRP	CB-CA-C	-5.07	109.14	116.54
1	A	94	ARG	NH1-CZ-NH2	5.07	125.89	119.30
2	H	9	ASN	O-C-N	5.07	129.12	122.68
2	H	117	ASP	CA-C-N	5.07	130.82	121.70
2	H	117	ASP	C-N-CA	5.07	130.82	121.70
3	I	211	ASN	CA-C-N	5.07	128.30	121.05
3	I	211	ASN	C-N-CA	5.07	128.30	121.05
2	K	62	CYS	CA-C-O	-5.07	114.91	120.69
1	J	83	PRO	CA-N-CD	-5.07	104.91	112.00
2	K	173	PHE	N-CA-CB	5.07	118.73	110.37
3	L	371	SER	CA-C-N	5.07	127.07	120.28
3	L	371	SER	C-N-CA	5.07	127.07	120.28
2	H	159	SER	CA-C-N	5.06	128.66	121.42
2	H	159	SER	C-N-CA	5.06	128.66	121.42
1	G	137	ASP	N-CA-C	-5.06	108.37	114.75
3	C	301	ASP	O-C-N	-5.06	116.80	121.30
2	E	51	TYR	CA-C-O	-5.06	115.19	121.06
3	F	247	THR	CA-C-N	5.06	130.33	122.49
3	F	247	THR	C-N-CA	5.06	130.33	122.49
2	K	169	ALA	O-C-N	5.06	127.92	122.15
3	L	33	ILE	CA-C-O	-5.06	114.73	120.65
3	L	388	SER	CB-CA-C	-5.06	102.25	110.85
2	E	318	ILE	N-CA-C	5.05	115.19	108.11
3	I	356	HIS	CA-CB-CG	5.05	118.86	113.80
2	K	22	PRO	N-CA-CB	5.05	109.56	103.45
2	B	279	SER	N-CA-CB	5.05	120.17	111.13
3	I	346	ALA	N-CA-CB	5.05	119.03	110.49
3	C	114	LEU	N-CA-C	-5.05	101.06	108.79
3	I	304	HIS	CB-CG-CD2	-5.05	124.64	131.20
3	I	217	ASN	CB-CG-OD1	-5.05	110.70	120.80
3	L	172	VAL	CA-C-O	5.05	125.39	119.89
2	H	361	VAL	N-CA-C	-5.05	98.84	109.34
1	J	236	THR	CA-C-N	5.05	131.18	121.54
1	J	236	THR	C-N-CA	5.05	131.18	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	419	THR	CA-C-O	-5.05	115.52	120.82
2	B	368	GLN	N-CA-C	-5.04	101.88	109.85
2	E	349	SER	CA-C-O	-5.04	115.83	121.23
3	I	284	HIS	CE1-NE2-CD2	-5.04	103.95	109.00
1	A	175	PRO	O-C-N	5.04	129.31	123.21
2	E	347	GLN	OE1-CD-NE2	5.04	127.64	122.60
2	H	93	TYR	CB-CG-CD2	-5.04	113.23	120.80
2	E	347	GLN	N-CA-C	-5.04	107.79	114.04
2	K	180	TYR	O-C-N	5.04	128.59	122.94
1	D	194	THR	O-C-N	5.04	129.27	123.17
3	F	36	VAL	N-CA-C	-5.04	101.06	108.11
2	H	30	SER	N-CA-C	-5.04	101.48	109.59
2	K	281	ASP	N-CA-CB	5.04	118.61	110.65
3	C	56	ALA	N-CA-CB	5.04	118.84	110.63
1	J	238	ASN	N-CA-C	-5.03	100.08	110.80
2	K	433	ILE	CA-C-N	5.03	127.36	120.46
2	K	433	ILE	C-N-CA	5.03	127.36	120.46
3	L	337	TRP	CG-CD2-CE3	-5.03	128.87	133.90
1	A	147	LYS	N-CA-C	-5.03	101.20	109.40
1	A	190	ASN	N-CA-CB	5.03	120.73	112.63
3	I	324	VAL	CA-CB-CG1	-5.03	101.85	110.40
2	E	87	PHE	CA-CB-CG	-5.03	108.77	113.80
3	L	238	SER	N-CA-C	-5.03	100.12	108.12
3	I	158	ASP	CA-CB-CG	-5.03	107.57	112.60
2	K	11	VAL	CA-C-N	5.03	131.43	121.53
2	K	11	VAL	C-N-CA	5.03	131.43	121.53
2	K	418	LEU	N-CA-CB	5.03	117.60	110.16
3	F	138	SER	CB-CA-C	-5.02	105.21	110.33
3	I	384	CYS	CA-C-O	-5.02	115.10	120.42
1	J	174	LYS	CA-C-N	5.02	125.01	119.89
1	J	174	LYS	C-N-CA	5.02	125.01	119.89
3	L	384	CYS	CA-CB-SG	-5.02	102.85	114.40
2	E	109	THR	CA-CB-OG1	5.02	117.13	109.60
3	F	161	ARG	CA-C-N	5.02	131.13	121.54
3	F	161	ARG	C-N-CA	5.02	131.13	121.54
2	H	228	ASN	CA-C-O	5.02	126.41	120.69
3	L	105	ARG	CA-C-O	-5.02	114.05	121.27
3	C	124	THR	N-CA-C	-5.01	100.71	109.48
3	C	281	VAL	CB-CA-C	5.01	118.22	110.50
2	K	327	LYS	CB-CA-C	-5.01	101.84	110.16
1	A	159	VAL	CA-C-N	5.01	126.11	119.84
1	A	159	VAL	C-N-CA	5.01	126.11	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	212	ASN	CB-CG-ND2	-5.01	108.88	116.40
2	H	349	SER	O-C-N	-5.01	118.00	123.26
2	K	273	TYR	N-CA-C	-5.01	100.43	108.55
3	C	180	ASN	N-CA-C	-5.01	99.63	108.20
3	F	330	ASN	CB-CA-C	-5.01	104.05	111.72
2	H	147	PHE	CA-C-O	5.01	127.23	121.47
3	I	93	LEU	N-CA-C	-5.01	105.73	111.14
3	I	364	TRP	O-C-N	5.01	128.26	122.25
1	J	105	CYS	N-CA-C	-5.01	106.86	113.17
3	C	366	ILE	CA-C-O	5.01	126.16	120.85
3	I	35	HIS	ND1-CG-CD2	5.01	111.11	106.10
1	J	103	ASN	CB-CG-OD1	-5.01	110.78	120.80
1	G	224	ALA	CA-C-O	-5.00	113.45	120.21
2	K	318	ILE	N-CA-C	-5.00	100.91	108.12
3	C	135	ASN	CA-CB-CG	-5.00	107.60	112.60
3	F	249	VAL	CA-C-O	5.00	126.04	120.59
1	A	201	LYS	CB-CA-C	-5.00	103.52	110.37

There are no chirality outliers.

All (140) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	LYS	Peptide
1	A	145	THR	Peptide
1	A	192	ARG	Sidechain
1	A	207	ARG	Sidechain
2	B	110	ARG	Sidechain
2	B	122	TYR	Sidechain
2	B	124	VAL	Peptide
2	B	173	PHE	Sidechain
2	B	174	ASP	Peptide
2	B	199	ARG	Sidechain
2	B	2	GLU	Peptide
2	B	223	ARG	Sidechain
2	B	233	TYR	Sidechain
2	B	242	TYR	Sidechain
2	B	285	ALA	Peptide
2	B	332	SER	Peptide
2	B	365	PHE	Sidechain
2	B	390	TYR	Sidechain
2	B	393	LYS	Peptide
2	B	399	PHE	Peptide

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Mol	Chain	Res	Type	Group
2	B	411	ALA	Peptide
2	B	46	TYR	Sidechain
2	B	51	TYR	Sidechain
2	B	69	SER	Peptide
3	C	105	ARG	Sidechain
3	C	123	ARG	Sidechain
3	C	196	TYR	Sidechain
3	C	220	THR	Peptide
3	C	236	TYR	Sidechain
3	C	286	HIS	Sidechain
3	C	289	TYR	Sidechain
3	C	361	TYR	Sidechain
3	C	363	TYR	Sidechain
3	C	398	TYR	Sidechain
3	C	99	PHE	Sidechain
1	D	118	TYR	Sidechain
1	D	125	LYS	Peptide
1	D	145	THR	Peptide
1	D	170	PHE	Sidechain
1	D	179	TYR	Sidechain
1	D	183	HIS	Peptide
1	D	94	ARG	Sidechain
2	E	1	TYR	Sidechain
2	E	117	ASP	Peptide
2	E	122	TYR	Sidechain
2	E	124	VAL	Peptide
2	E	147	PHE	Sidechain
2	E	180	TYR	Sidechain
2	E	2	GLU	Peptide
2	E	206	ARG	Sidechain
2	E	233	TYR	Sidechain
2	E	242	TYR	Sidechain
2	E	285	ALA	Peptide
2	E	289	ARG	Sidechain
2	E	332	SER	Peptide
2	E	365	PHE	Sidechain
2	E	399	PHE	Peptide
2	E	438	ARG	Sidechain
2	E	59	TYR	Sidechain
2	E	69	SER	Peptide
2	E	76	TYR	Sidechain
2	E	93	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	E	95	PHE	Sidechain
3	F	12	ARG	Sidechain
3	F	123	ARG	Sidechain
3	F	220	THR	Peptide
3	F	277	ARG	Sidechain
3	F	67	ARG	Sidechain
3	F	79	ARG	Sidechain
1	G	122	VAL	Peptide
1	G	125	LYS	Peptide
1	G	126	VAL	Peptide
1	G	145	THR	Peptide
1	G	183	HIS	Peptide
1	G	207	ARG	Sidechain
1	G	244	ARG	Sidechain
1	G	96	ARG	Sidechain
2	H	1	TYR	Sidechain
2	H	107	TYR	Sidechain
2	H	124	VAL	Peptide
2	H	180	TYR	Sidechain
2	H	192	TYR	Sidechain
2	H	2	GLU	Peptide
2	H	242	TYR	Sidechain
2	H	273	TYR	Sidechain
2	H	285	ALA	Peptide
2	H	332	SER	Peptide
2	H	373	ARG	Sidechain
2	H	390	TYR	Sidechain
2	H	393	LYS	Peptide
2	H	399	PHE	Peptide
2	H	438	ARG	Sidechain
2	H	59	TYR	Sidechain
2	H	69	SER	Peptide
2	H	81	PHE	Sidechain
2	H	93	TYR	Sidechain
3	I	12	ARG	Sidechain
3	I	185	TYR	Sidechain
3	I	220	THR	Peptide
3	I	227	TYR	Sidechain
3	I	243	ARG	Sidechain
3	I	254	HIS	Sidechain
3	I	284	HIS	Sidechain
3	I	285	PHE	Sidechain

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Mol	Chain	Res	Type	Group
3	I	293	PHE	Sidechain
3	I	335	ARG	Sidechain
3	I	363	TYR	Sidechain
1	J	125	LYS	Peptide
1	J	145	THR	Peptide
1	J	183	HIS	Peptide
1	J	210	PHE	Sidechain
2	K	107	TYR	Sidechain
2	K	117	ASP	Peptide
2	K	124	VAL	Peptide
2	K	155	ARG	Sidechain
2	K	173	PHE	Sidechain
2	K	2	GLU	Peptide
2	K	206	ARG	Sidechain
2	K	21	ARG	Sidechain
2	K	240	PHE	Sidechain
2	K	253	ARG	Sidechain
2	K	285	ALA	Peptide
2	K	332	SER	Peptide
2	K	373	ARG	Sidechain
2	K	385	ASP	Peptide
2	K	399	PHE	Sidechain,Peptide
2	K	41	SER	Peptide
2	K	59	TYR	Sidechain
2	K	69	SER	Peptide
2	K	76	TYR	Sidechain
3	L	14	TYR	Sidechain
3	L	153	TYR	Sidechain
3	L	196	TYR	Sidechain
3	L	220	THR	Peptide
3	L	227	TYR	Sidechain
3	L	243	ARG	Sidechain
3	L	296	ARG	Sidechain
3	L	326	TYR	Sidechain
3	L	68	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1316	0	1322	31	0
1	D	1316	0	1322	24	0
1	G	1316	0	1322	29	0
1	J	1316	0	1322	26	0
2	B	3225	0	3161	34	0
2	E	3225	0	3161	34	0
2	H	3225	0	3161	29	0
2	K	3225	0	3161	33	0
3	C	3239	0	3208	57	0
3	F	3239	0	3208	59	0
3	I	3239	0	3208	60	0
3	L	3239	0	3208	58	0
All	All	31120	0	30764	296	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (296) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:240:TYR:CE1	3:I:240:TYR:CD1	1.81	1.68
3:I:240:TYR:CE2	3:I:240:TYR:CD2	1.80	1.67
3:F:240:TYR:CD2	3:F:240:TYR:CE2	1.79	1.65
1:A:237:TRP:CE3	1:A:237:TRP:CD2	1.82	1.64
1:G:237:TRP:CE3	1:G:237:TRP:CD2	1.74	1.64
3:C:240:TYR:CE2	3:C:240:TYR:CD2	1.88	1.61
3:L:240:TYR:CE1	3:L:240:TYR:CD1	1.82	1.61
3:F:240:TYR:CD1	3:F:240:TYR:CG	1.89	1.60
3:C:240:TYR:CE2	3:C:240:TYR:CZ	1.85	1.60
3:F:240:TYR:CE2	3:F:240:TYR:CZ	1.89	1.59
3:F:240:TYR:CD2	3:F:240:TYR:CG	1.88	1.59
3:I:240:TYR:CE2	3:I:240:TYR:CZ	1.87	1.58
3:F:240:TYR:CD1	3:F:240:TYR:CE1	1.91	1.57
3:L:240:TYR:CD1	3:L:240:TYR:CG	1.89	1.57
3:F:240:TYR:CZ	3:F:240:TYR:CE1	1.90	1.56
3:C:240:TYR:CD1	3:C:240:TYR:CG	1.91	1.56
3:C:240:TYR:CD1	3:C:240:TYR:CE1	1.89	1.56
3:L:240:TYR:CE2	3:L:240:TYR:CD2	1.91	1.56
3:L:240:TYR:CE2	3:L:240:TYR:CZ	1.87	1.55
3:C:240:TYR:CD2	3:C:240:TYR:CG	1.92	1.55
3:I:240:TYR:CE1	3:I:240:TYR:CZ	1.92	1.54
3:C:240:TYR:CZ	3:C:240:TYR:CE1	1.95	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:240:TYR:CE1	3:L:240:TYR:CZ	1.94	1.53
3:L:240:TYR:CG	3:L:240:TYR:CD2	1.92	1.52
3:I:240:TYR:CD2	3:I:240:TYR:CG	1.93	1.51
3:I:240:TYR:CD1	3:I:240:TYR:CG	1.98	1.49
1:G:237:TRP:CE2	3:I:398:TYR:CD2	2.09	1.40
1:J:237:TRP:CE2	3:L:398:TYR:CD2	2.08	1.40
1:A:237:TRP:CE2	3:C:398:TYR:CD2	2.10	1.39
1:D:237:TRP:CE2	3:F:398:TYR:CD2	2.10	1.39
1:A:237:TRP:CE2	3:C:398:TYR:CE2	2.11	1.38
1:D:237:TRP:CE2	3:F:398:TYR:CE2	2.11	1.38
1:J:237:TRP:CE2	3:L:398:TYR:CE2	2.11	1.37
1:G:237:TRP:CE2	3:I:398:TYR:CE2	2.13	1.37
1:G:237:TRP:CZ2	3:I:398:TYR:CE2	2.19	1.30
1:J:237:TRP:CZ2	3:L:398:TYR:CD2	2.19	1.30
1:A:237:TRP:CZ2	3:C:398:TYR:CE2	2.18	1.30
1:G:237:TRP:CZ2	3:I:398:TYR:CD2	2.20	1.29
1:D:237:TRP:CZ2	3:F:398:TYR:CE2	2.21	1.29
1:J:237:TRP:CZ2	3:L:398:TYR:CE2	2.20	1.29
1:A:237:TRP:CZ2	3:C:398:TYR:CD2	2.20	1.28
1:D:237:TRP:CZ2	3:F:398:TYR:CD2	2.20	1.28
1:A:237:TRP:CE2	3:C:398:TYR:CZ	2.30	1.18
1:G:237:TRP:CD2	3:I:398:TYR:CD2	2.32	1.18
1:J:237:TRP:CE2	3:L:398:TYR:CG	2.31	1.18
1:D:237:TRP:CE2	3:F:398:TYR:CZ	2.30	1.17
1:A:237:TRP:CE2	3:C:398:TYR:CG	2.33	1.17
1:J:237:TRP:CE2	3:L:398:TYR:CZ	2.32	1.17
1:G:237:TRP:CE2	3:I:398:TYR:CZ	2.32	1.17
1:G:237:TRP:CE2	3:I:398:TYR:CG	2.32	1.16
1:D:237:TRP:CE2	3:F:398:TYR:CG	2.34	1.16
1:A:237:TRP:CE2	3:C:398:TYR:CE1	2.35	1.14
1:J:237:TRP:CD2	3:L:398:TYR:CD2	2.34	1.14
1:A:237:TRP:CD2	3:C:398:TYR:CD2	2.34	1.14
1:A:237:TRP:CD2	3:C:398:TYR:CE2	2.34	1.13
1:J:237:TRP:CZ2	3:L:398:TYR:CG	2.37	1.13
1:A:237:TRP:CE2	3:C:398:TYR:CD1	2.36	1.13
1:D:237:TRP:CD2	3:F:398:TYR:CD2	2.37	1.13
1:D:237:TRP:CD2	3:F:398:TYR:CE2	2.36	1.12
1:J:237:TRP:CD2	3:L:398:TYR:CE2	2.38	1.11
1:D:237:TRP:CE2	3:F:398:TYR:CD1	2.40	1.10
1:G:237:TRP:CD2	3:I:398:TYR:CE2	2.38	1.09
1:A:237:TRP:CZ2	3:C:398:TYR:CZ	2.41	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:TRP:CZ2	3:F:398:TYR:CG	2.40	1.08
1:D:237:TRP:CE2	3:F:398:TYR:CE1	2.41	1.08
1:J:237:TRP:CE2	3:L:398:TYR:CD1	2.42	1.08
1:D:237:TRP:CZ2	3:F:398:TYR:CZ	2.42	1.08
1:G:237:TRP:CZ2	3:I:398:TYR:CZ	2.43	1.07
2:B:229:VAL:C	3:C:240:TYR:CD1	2.33	1.06
1:G:237:TRP:CE2	3:I:398:TYR:CE1	2.43	1.06
1:G:237:TRP:CE2	3:I:398:TYR:CD1	2.43	1.06
1:J:237:TRP:CH2	3:L:398:TYR:CE2	2.43	1.06
1:J:237:TRP:CZ3	3:L:398:TYR:CE2	2.44	1.06
2:E:229:VAL:C	3:F:240:TYR:CE1	2.34	1.06
2:B:229:VAL:C	3:C:240:TYR:CZ	2.33	1.06
2:B:229:VAL:C	3:C:240:TYR:CE2	2.33	1.06
2:E:229:VAL:C	3:F:240:TYR:CZ	2.34	1.06
1:J:237:TRP:CZ2	3:L:398:TYR:CZ	2.43	1.06
2:H:229:VAL:C	3:I:240:TYR:CE2	2.34	1.05
1:D:237:TRP:CH2	3:F:398:TYR:CE2	2.43	1.05
1:D:237:TRP:CE3	3:F:398:TYR:CE2	2.44	1.05
2:H:229:VAL:C	3:I:240:TYR:CD1	2.34	1.05
1:A:237:TRP:CE3	3:C:398:TYR:CE2	2.43	1.05
1:A:237:TRP:CZ2	3:C:398:TYR:CG	2.44	1.05
2:B:229:VAL:C	3:C:240:TYR:CG	2.35	1.05
1:D:237:TRP:CH2	3:F:398:TYR:CD2	2.44	1.05
2:H:229:VAL:C	3:I:240:TYR:CG	2.35	1.05
1:G:237:TRP:CZ2	3:I:398:TYR:CG	2.45	1.04
2:H:229:VAL:C	3:I:240:TYR:CD2	2.36	1.04
2:K:229:VAL:C	3:L:240:TYR:CZ	2.35	1.04
1:A:237:TRP:CE3	3:C:398:TYR:CD2	2.46	1.04
2:E:229:VAL:C	3:F:240:TYR:CD2	2.35	1.03
2:H:229:VAL:C	3:I:240:TYR:CZ	2.36	1.03
2:K:229:VAL:C	3:L:240:TYR:CE1	2.36	1.03
1:A:237:TRP:CH2	3:C:398:TYR:CE2	2.45	1.03
1:D:237:TRP:CE3	3:F:398:TYR:CD2	2.46	1.03
2:K:229:VAL:C	3:L:240:TYR:CD2	2.36	1.03
2:K:231:VAL:N	3:L:240:TYR:CD2	2.26	1.03
1:J:237:TRP:CE2	3:L:398:TYR:CE1	2.47	1.03
2:K:229:VAL:C	3:L:240:TYR:CG	2.36	1.03
1:G:237:TRP:CH2	3:I:398:TYR:CD2	2.46	1.03
2:K:231:VAL:N	3:L:240:TYR:CD1	2.27	1.03
1:A:237:TRP:CZ2	3:C:398:TYR:CD1	2.47	1.02
1:J:237:TRP:CE3	3:L:398:TYR:CE2	2.46	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:VAL:C	3:C:240:TYR:CE1	2.38	1.02
2:E:229:VAL:C	3:F:240:TYR:CE2	2.37	1.02
2:H:229:VAL:C	3:I:240:TYR:CE1	2.37	1.02
2:E:229:VAL:C	3:F:240:TYR:CD1	2.37	1.02
1:J:237:TRP:CH2	3:L:398:TYR:CD2	2.46	1.02
2:K:229:VAL:C	3:L:240:TYR:CE2	2.37	1.02
1:D:237:TRP:CZ3	3:F:398:TYR:CE2	2.48	1.02
2:B:231:VAL:N	3:C:240:TYR:CD2	2.27	1.01
1:D:237:TRP:CZ2	3:F:398:TYR:CD1	2.48	1.01
2:B:231:VAL:N	3:C:240:TYR:CE2	2.29	1.01
1:G:237:TRP:CE3	3:I:398:TYR:CD2	2.48	1.01
2:K:231:VAL:N	3:L:240:TYR:CE2	2.29	1.01
1:D:237:TRP:CZ3	3:F:398:TYR:CD2	2.48	1.01
2:E:231:VAL:N	3:F:240:TYR:CZ	2.29	1.01
1:J:237:TRP:CZ2	3:L:398:TYR:CD1	2.48	1.01
1:J:237:TRP:CE3	3:L:398:TYR:CD2	2.47	1.01
2:K:229:VAL:C	3:L:240:TYR:CD1	2.38	1.01
2:E:231:VAL:N	3:F:240:TYR:CE1	2.29	1.00
2:E:231:VAL:N	3:F:240:TYR:CE2	2.29	1.00
1:G:237:TRP:CZ3	3:I:398:TYR:CD2	2.49	1.00
2:K:231:VAL:N	3:L:240:TYR:CZ	2.30	1.00
1:G:237:TRP:CE3	3:I:398:TYR:CE2	2.49	1.00
1:A:237:TRP:CH2	3:C:398:TYR:CD2	2.48	1.00
1:J:237:TRP:CZ3	3:L:398:TYR:CD2	2.50	1.00
2:B:231:VAL:N	3:C:240:TYR:CD1	2.29	1.00
1:G:237:TRP:CH2	3:I:398:TYR:CE2	2.49	1.00
2:H:231:VAL:N	3:I:240:TYR:CE2	2.30	1.00
2:H:231:VAL:N	3:I:240:TYR:CD2	2.30	0.99
1:G:237:TRP:CZ2	3:I:398:TYR:CE1	2.50	0.99
2:B:231:VAL:N	3:C:240:TYR:CE1	2.30	0.99
2:H:231:VAL:N	3:I:240:TYR:CZ	2.31	0.99
2:B:231:VAL:N	3:C:240:TYR:CZ	2.30	0.99
2:H:231:VAL:N	3:I:240:TYR:CD1	2.31	0.99
2:E:229:VAL:C	3:F:240:TYR:CG	2.41	0.98
2:E:231:VAL:N	3:F:240:TYR:CD2	2.30	0.98
2:K:231:VAL:N	3:L:240:TYR:CE1	2.31	0.98
2:B:229:VAL:C	3:C:240:TYR:CD2	2.41	0.98
2:K:231:VAL:N	3:L:240:TYR:CG	2.31	0.98
2:B:231:VAL:N	3:C:240:TYR:CG	2.32	0.97
2:E:231:VAL:N	3:F:240:TYR:CG	2.33	0.97
2:H:231:VAL:N	3:I:240:TYR:CE1	2.31	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:237:TRP:CZ2	3:L:398:TYR:CE1	2.52	0.97
2:E:231:VAL:N	3:F:240:TYR:CD1	2.33	0.97
1:D:237:TRP:CZ2	3:F:398:TYR:CE1	2.53	0.96
1:A:237:TRP:CZ3	3:C:398:TYR:CD2	2.53	0.96
2:H:231:VAL:N	3:I:240:TYR:CG	2.32	0.96
1:G:237:TRP:CZ2	3:I:398:TYR:CD1	2.54	0.96
3:F:398:TYR:CD2	3:F:398:TYR:CE2	2.54	0.96
3:C:398:TYR:CD2	3:C:398:TYR:CE2	2.54	0.95
1:A:237:TRP:CZ2	3:C:398:TYR:CE1	2.54	0.95
3:L:398:TYR:CD2	3:L:398:TYR:CE2	2.55	0.95
3:I:398:TYR:CD2	3:I:398:TYR:CE2	2.56	0.94
1:A:237:TRP:CZ3	3:C:398:TYR:CE2	2.56	0.93
1:G:237:TRP:CZ3	3:I:398:TYR:CE2	2.56	0.93
2:E:229:VAL:CA	3:F:240:TYR:CZ	2.65	0.79
2:K:229:VAL:CA	3:L:240:TYR:CE1	2.65	0.79
2:H:229:VAL:CA	3:I:240:TYR:CE1	2.66	0.77
2:B:229:VAL:CA	3:C:240:TYR:CZ	2.71	0.74
2:B:229:VAL:CA	3:C:240:TYR:CE1	2.71	0.73
2:E:229:VAL:O	3:F:240:TYR:CG	2.42	0.73
2:K:229:VAL:HA	3:L:240:TYR:CE1	2.24	0.73
2:K:385:ASP:H	2:K:387:ILE:HA	1.51	0.72
2:H:231:VAL:HA	3:I:240:TYR:CE1	2.25	0.72
2:H:229:VAL:O	3:I:240:TYR:CD2	2.44	0.70
2:H:231:VAL:CA	3:I:240:TYR:CE1	2.75	0.69
2:B:229:VAL:O	3:C:240:TYR:CG	2.45	0.69
3:I:354:VAL:H	3:I:364:TRP:HE1	1.41	0.69
2:K:229:VAL:CA	3:L:240:TYR:CZ	2.77	0.68
2:B:9:ASN:HD21	2:B:276:ILE:HD12	1.59	0.68
2:K:229:VAL:O	3:L:240:TYR:CD2	2.47	0.67
2:E:229:VAL:CA	3:F:240:TYR:CE1	2.79	0.66
2:K:229:VAL:HA	3:L:240:TYR:CZ	2.32	0.65
2:B:229:VAL:HA	3:C:240:TYR:CE1	2.31	0.65
2:K:231:VAL:CA	3:L:240:TYR:CE1	2.79	0.65
2:E:18:LEU:H	2:E:335:ASN:HD21	1.44	0.65
2:B:229:VAL:HA	3:C:240:TYR:CZ	2.33	0.64
2:E:229:VAL:HA	3:F:240:TYR:CZ	2.32	0.64
2:K:229:VAL:O	3:L:240:TYR:CG	2.51	0.64
2:E:229:VAL:HG12	3:F:240:TYR:CD1	2.33	0.63
2:H:229:VAL:O	3:I:240:TYR:CG	2.52	0.63
3:L:278:LEU:HD13	3:L:356:HIS:CE1	2.33	0.63
2:B:231:VAL:HA	3:C:240:TYR:CE1	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:237:TRP:CE2	1:G:237:TRP:CZ2	2.88	0.61
2:H:229:VAL:CA	3:I:240:TYR:CZ	2.83	0.61
1:A:237:TRP:CE2	1:A:237:TRP:CZ2	2.88	0.61
2:E:231:VAL:CA	3:F:240:TYR:CE1	2.84	0.60
2:B:231:VAL:CA	3:C:240:TYR:CE1	2.84	0.60
2:E:206:ARG:HH22	2:E:214:TYR:HB2	1.67	0.60
2:H:229:VAL:HA	3:I:240:TYR:CE1	2.37	0.59
1:J:237:TRP:CE2	1:J:237:TRP:CZ2	2.90	0.59
2:E:231:VAL:HG13	3:F:240:TYR:CD1	2.37	0.59
2:K:231:VAL:HA	3:L:240:TYR:CE1	2.39	0.58
2:B:229:VAL:O	3:C:240:TYR:CD2	2.55	0.58
1:D:154:LEU:HD21	1:D:241:MET:HE1	1.85	0.57
2:E:229:VAL:O	3:F:240:TYR:CD2	2.56	0.56
2:H:229:VAL:HA	3:I:240:TYR:CZ	2.39	0.56
3:I:354:VAL:H	3:I:364:TRP:NE1	2.04	0.56
2:K:402:ILE:HG23	2:K:407:TRP:HE1	1.71	0.56
1:D:237:TRP:CE2	1:D:237:TRP:CZ2	2.94	0.55
1:J:182:HIS:CD2	1:J:207:ARG:HH21	2.25	0.55
1:A:237:TRP:NE1	3:C:398:TYR:CE1	2.75	0.55
2:E:231:VAL:CA	3:F:240:TYR:CZ	2.89	0.55
2:E:131:ALA:HB2	2:E:148:VAL:HG11	1.88	0.54
3:F:388:SER:HA	3:F:391:ARG:HE	1.71	0.54
3:I:166:MET:HE2	3:I:236:TYR:CE1	2.42	0.54
3:I:391:ARG:HG3	3:I:391:ARG:HH11	1.73	0.54
1:G:182:HIS:CE1	1:G:183:HIS:CE1	2.96	0.54
2:B:76:TYR:CE1	2:B:107:TYR:HB3	2.43	0.53
2:B:229:VAL:C	2:B:231:VAL:N	2.68	0.52
2:H:21:ARG:H	2:H:21:ARG:HD2	1.74	0.52
2:K:74:ALA:HB1	2:K:213:VAL:H	1.75	0.52
1:D:126:VAL:HG21	1:D:159:VAL:HG22	1.92	0.51
3:C:254:HIS:CD2	3:C:254:HIS:H	2.27	0.51
2:H:113:SER:HA	3:I:161:ARG:HH12	1.76	0.50
1:G:241:MET:HG2	1:G:242:VAL:H	1.77	0.50
3:L:332:ASN:HD22	3:L:332:ASN:H	1.60	0.50
2:E:229:VAL:HA	3:F:240:TYR:CE1	2.47	0.50
1:J:181:TRP:HE1	1:J:195:ILE:CD1	2.24	0.49
2:E:104:SER:HB3	2:E:221:LEU:HD22	1.94	0.49
2:B:24:TYR:H	2:B:290:ILE:HG22	1.77	0.49
1:G:182:HIS:CD2	1:G:207:ARG:HH12	2.30	0.49
2:K:229:VAL:C	2:K:231:VAL:N	2.70	0.49
3:L:53:ILE:HA	3:L:66:ILE:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:109:VAL:HG12	1:G:136:ILE:H	1.78	0.48
2:H:94:CYS:H	3:I:225:ILE:HG21	1.78	0.48
3:F:4:HIS:HA	3:F:254:HIS:CE1	2.48	0.48
2:B:203:ILE:HG22	2:B:216:ASN:H	1.77	0.48
3:I:296:ARG:HH21	3:I:304:HIS:CE1	2.33	0.47
2:K:330:ILE:HG21	2:K:370:CYS:H	1.78	0.47
2:E:194:SER:HA	2:E:199:ARG:HH11	1.79	0.47
3:C:117:ASP:H	3:C:118:PRO:CD	2.28	0.47
2:K:60:ILE:CG2	2:K:100:ASN:HD21	2.27	0.47
1:A:172:HIS:CD2	1:A:173:GLU:HG3	2.51	0.46
1:A:237:TRP:NE1	3:C:398:TYR:CD1	2.80	0.46
2:E:131:ALA:CB	2:E:148:VAL:HG11	2.46	0.46
3:F:390:ALA:HB2	3:F:419:ALA:HB3	1.98	0.46
1:J:181:TRP:HE1	1:J:195:ILE:HD12	1.81	0.46
2:H:229:VAL:C	2:H:231:VAL:N	2.74	0.46
1:A:129:PRO:HA	1:A:132:VAL:HG23	1.97	0.45
3:C:229:VAL:HG22	3:C:230:ASP:N	2.31	0.45
1:G:182:HIS:CE1	1:G:183:HIS:HE1	2.34	0.45
2:H:423:VAL:HA	2:H:426:ILE:HD12	1.98	0.45
3:L:354:VAL:HG21	3:L:361:TYR:H	1.81	0.45
1:A:242:VAL:HG13	2:B:435:VAL:HA	1.98	0.45
2:K:29:LEU:CD2	2:K:280:MET:HE2	2.46	0.45
1:J:237:TRP:NE1	3:L:398:TYR:CD1	2.84	0.45
2:B:50:ASN:HD22	2:B:113:SER:HB3	1.81	0.44
3:F:241:VAL:HB	3:F:242:PRO:HD2	1.99	0.44
2:E:42:LEU:HD12	2:E:42:LEU:O	2.16	0.44
2:B:29:LEU:HD22	2:B:280:MET:HG3	2.00	0.44
3:I:393:LYS:O	3:I:397:PRO:HD2	2.17	0.44
1:J:156:CYS:O	1:J:157:ALA:HB2	2.17	0.44
2:E:320:TYR:CZ	2:E:352:LEU:HD12	2.53	0.44
2:H:231:VAL:CA	3:I:240:TYR:CZ	3.00	0.44
2:K:398:GLU:H	2:K:401:SER:HA	1.82	0.43
3:L:221:ALA:HB3	3:L:222:PRO:HD3	2.00	0.43
1:A:219:ILE:O	1:A:234:VAL:HA	2.18	0.43
2:B:48:THR:HG21	2:B:201:GLY:HA2	1.99	0.43
2:K:192:TYR:HA	2:K:204:GLN:HE22	1.84	0.43
1:A:114:LYS:HZ1	1:G:140:GLU:HG3	1.84	0.43
2:B:413:THR:HG23	3:C:378:ILE:HD11	2.00	0.43
2:E:229:VAL:C	2:E:231:VAL:N	2.77	0.43
2:H:58:PRO:O	3:I:242:PRO:HA	2.19	0.43
2:E:231:VAL:HA	3:F:240:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:308:TYR:CE1	3:F:347:HIS:CE1	3.07	0.43
3:F:240:TYR:CD2	3:F:240:TYR:CB	2.88	0.43
2:B:140:LEU:HD12	2:B:141:ASN:H	1.85	0.42
1:G:179:TYR:CE1	1:G:186:VAL:O	2.73	0.42
3:C:359:ASP:HA	3:C:362:PRO:HD3	2.01	0.42
2:E:5:THR:HG21	2:E:17:ALA:HB1	2.02	0.42
2:H:18:LEU:HD23	2:H:18:LEU:H	1.84	0.42
1:A:174:LYS:H	1:A:239:LYS:HE2	1.85	0.42
3:I:288:MET:HB2	3:I:289:TYR:H	1.67	0.42
2:K:231:VAL:CA	3:L:240:TYR:CZ	3.01	0.42
3:L:277:ARG:HG3	3:L:282:GLU:OE1	2.20	0.42
3:L:360:LEU:HD23	3:L:360:LEU:HA	1.92	0.42
1:A:123:GLY:HA2	1:A:170:PHE:HA	2.01	0.41
3:I:274:VAL:HG13	3:I:283:PHE:CD1	2.55	0.41
2:K:231:VAL:CA	3:L:240:TYR:CD1	3.02	0.41
1:D:237:TRP:NE1	3:F:398:TYR:CE1	2.85	0.41
3:F:93:LEU:HB3	3:F:155:HIS:CE1	2.55	0.41
3:I:52:GLN:HE21	3:I:98:HIS:CE1	2.38	0.41
3:F:111:GLU:CD	3:F:123:ARG:HH21	2.28	0.41
3:L:238:SER:HB2	3:L:239:GLN:H	1.65	0.41
2:B:231:VAL:CA	3:C:240:TYR:CZ	3.02	0.41
2:K:58:PRO:HG2	2:K:231:VAL:HG11	2.02	0.41
2:B:9:ASN:HD21	2:B:276:ILE:CD1	2.32	0.40
2:B:179:VAL:HG22	2:B:184:VAL:HG13	2.03	0.40
3:C:167:HIS:CD2	3:C:168:VAL:HG23	2.56	0.40
3:C:169:PRO:HA	3:C:170:PRO:HD3	1.93	0.40
2:H:200:PHE:CD1	2:H:243:TRP:CD1	3.10	0.40
2:K:385:ASP:N	2:K:387:ILE:HA	2.28	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	169/253 (67%)	136 (80%)	24 (14%)	9 (5%)	1	14
1	D	169/253 (67%)	148 (88%)	15 (9%)	6 (4%)	2	19
1	G	169/253 (67%)	133 (79%)	21 (12%)	15 (9%)	0	8
1	J	169/253 (67%)	132 (78%)	22 (13%)	15 (9%)	0	8
2	B	422/427 (99%)	354 (84%)	47 (11%)	21 (5%)	1	15
2	E	422/427 (99%)	352 (83%)	42 (10%)	28 (7%)	1	11
2	H	422/427 (99%)	362 (86%)	47 (11%)	13 (3%)	3	21
2	K	422/427 (99%)	366 (87%)	33 (8%)	23 (6%)	1	14
3	C	419/421 (100%)	359 (86%)	36 (9%)	24 (6%)	1	13
3	F	419/421 (100%)	365 (87%)	38 (9%)	16 (4%)	2	18
3	I	419/421 (100%)	364 (87%)	38 (9%)	17 (4%)	2	17
3	L	419/421 (100%)	360 (86%)	40 (10%)	19 (4%)	2	16
All	All	4040/4404 (92%)	3431 (85%)	403 (10%)	206 (5%)	3	14

All (206) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ILE
1	A	182	HIS
2	B	69	SER
2	B	86	PRO
2	B	89	TRP
2	B	232	PRO
2	B	306	CYS
2	B	381	GLU
2	B	383	PRO
2	B	400	PRO
3	C	117	ASP
3	C	138	SER
3	C	221	ALA
2	E	4	SER
2	E	86	PRO
2	E	255	ALA
2	E	383	PRO
2	E	399	PHE
3	F	140	ALA
3	F	221	ALA
1	G	100	LYS
1	G	215	LYS

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Mol	Chain	Res	Type
2	H	4	SER
2	H	287	PHE
2	H	400	PRO
3	I	221	ALA
3	I	346	ALA
1	J	136	ILE
1	J	157	ALA
1	J	182	HIS
1	J	237	TRP
2	K	4	SER
2	K	20	GLU
2	K	28	PRO
2	K	116	ALA
2	K	309	SER
2	K	400	PRO
3	L	221	ALA
3	L	303	SER
3	L	346	ALA
1	A	130	ALA
2	B	4	SER
2	B	28	PRO
2	B	292	GLU
2	B	401	SER
3	C	24	ALA
3	C	26	SER
3	C	340	LYS
3	C	346	ALA
1	D	96	ARG
1	D	237	TRP
2	E	19	ILE
2	E	20	GLU
2	E	71	LYS
2	E	287	PHE
2	E	334	SER
2	E	380	CYS
2	E	411	ALA
3	F	59	ASN
3	F	321	ALA
1	G	101	ILE
1	G	131	HIS
1	G	182	HIS
2	H	116	ALA

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Mol	Chain	Res	Type
2	H	401	SER
3	I	145	LYS
3	I	156	GLN
3	I	288	MET
3	I	310	ASP
3	I	321	ALA
1	J	101	ILE
1	J	130	ALA
1	J	249	GLU
2	K	411	ALA
3	L	24	ALA
3	L	117	ASP
3	L	161	ARG
3	L	162	GLU
3	L	290	PRO
1	A	92	GLY
1	A	157	ALA
2	B	116	ALA
2	B	392	ALA
3	C	13	PRO
3	C	87	THR
3	C	190	LYS
3	C	342	SER
3	C	352	SER
3	C	362	PRO
3	C	403	GLY
1	D	131	HIS
2	E	400	PRO
2	E	401	SER
3	F	39	ASP
3	F	131	ARG
3	F	190	LYS
3	F	345	SER
1	G	157	ALA
1	G	167	ALA
1	G	177	GLY
1	G	242	VAL
1	G	247	PRO
2	H	266	VAL
2	H	370	CYS
2	H	438	ARG
3	I	89	PRO

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Mol	Chain	Res	Type
3	I	160	THR
1	J	186	VAL
1	J	227	GLY
1	J	241	MET
2	K	19	ILE
2	K	202	ASP
2	K	292	GLU
2	K	334	SER
2	K	359	SER
2	K	370	CYS
2	K	384	LYS
2	K	385	ASP
3	L	22	GLY
3	L	23	LEU
3	L	86	THR
3	L	169	PRO
3	L	232	THR
2	B	255	ALA
2	B	259	CYS
2	B	411	ALA
3	C	22	GLY
3	C	145	LYS
3	C	174	ILE
1	D	130	ALA
1	D	228	ALA
2	E	74	ALA
2	E	88	MET
2	E	247	LYS
2	E	342	SER
2	E	363	PRO
2	E	370	CYS
3	F	168	VAL
1	G	105	CYS
1	G	120	CYS
1	G	172	HIS
1	G	198	GLY
2	H	91	GLY
2	H	199	ARG
3	I	141	PRO
3	I	168	VAL
3	I	169	PRO
1	J	131	HIS

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Mol	Chain	Res	Type
1	J	248	GLU
2	K	88	MET
2	K	97	ASP
2	K	259	CYS
2	K	310	SER
3	L	168	VAL
3	L	183	LYS
3	L	363	TYR
1	A	131	HIS
2	B	99	GLU
2	B	198	GLY
1	D	244	ARG
2	E	25	ALA
2	E	99	GLU
2	E	174	ASP
2	E	183	GLU
2	E	259	CYS
2	E	266	VAL
2	E	291	ASP
3	F	161	ARG
3	F	162	GLU
3	F	256	PRO
2	H	57	SER
2	H	237	PRO
2	H	259	CYS
3	I	24	ALA
3	I	189	PRO
3	I	352	SER
3	L	142	THR
3	L	154	SER
3	L	298	LEU
1	A	172	HIS
2	B	311	ASP
2	B	399	PHE
3	C	168	VAL
3	C	189	PRO
3	C	256	PRO
2	E	85	TYR
3	F	133	ILE
3	I	13	PRO
1	J	238	ASN
2	K	255	ALA

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Mol	Chain	Res	Type
2	K	305	SER
2	K	399	PHE
3	C	222	PRO
1	G	227	GLY
3	C	118	PRO
3	C	133	ILE
3	C	269	ALA
3	F	118	PRO
1	A	160	PRO
3	F	117	ASP
1	J	160	PRO
2	K	21	ARG
1	A	242	VAL
1	J	177	GLY
3	F	287	PRO
3	I	222	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	145/217 (67%)	138 (95%)	7 (5%)	23	45
1	D	145/217 (67%)	141 (97%)	4 (3%)	38	59
1	G	145/217 (67%)	143 (99%)	2 (1%)	59	72
1	J	145/217 (67%)	137 (94%)	8 (6%)	19	42
2	B	364/366 (100%)	334 (92%)	30 (8%)	10	31
2	E	364/366 (100%)	352 (97%)	12 (3%)	33	55
2	H	364/366 (100%)	352 (97%)	12 (3%)	33	55
2	K	364/366 (100%)	351 (96%)	13 (4%)	31	52
3	C	366/366 (100%)	350 (96%)	16 (4%)	25	47
3	F	366/366 (100%)	358 (98%)	8 (2%)	45	64
3	I	366/366 (100%)	345 (94%)	21 (6%)	18	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	366/366 (100%)	349 (95%)	17 (5%)	24	46
All	All	3500/3796 (92%)	3350 (96%)	150 (4%)	27	47

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	TYR
1	A	186	VAL
1	A	189	SER
1	A	217	VAL
1	A	226	GLU
1	A	236	THR
1	A	240	ASP
2	B	5	THR
2	B	16	LYS
2	B	28	PRO
2	B	42	LEU
2	B	63	CYS
2	B	71	LYS
2	B	94	CYS
2	B	120	ILE
2	B	142	GLN
2	B	146	VAL
2	B	160	LYS
2	B	162	ILE
2	B	180	TYR
2	B	199	ARG
2	B	200	PHE
2	B	203	ILE
2	B	216	ASN
2	B	219	LEU
2	B	220	LYS
2	B	229	VAL
2	B	244	LYS
2	B	266	VAL
2	B	280	MET
2	B	296	VAL
2	B	323	ASN
2	B	371	ASN
2	B	374	ILE
2	B	376	CYS
2	B	384	LYS

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Mol	Chain	Res	Type
2	B	387	ILE
3	C	13	PRO
3	C	30	PRO
3	C	36	VAL
3	C	39	ASP
3	C	68	TYR
3	C	100	ILE
3	C	130	PRO
3	C	136	GLU
3	C	160	THR
3	C	164	ILE
3	C	194	ILE
3	C	203	THR
3	C	266	VAL
3	C	313	MET
3	C	340	LYS
3	C	378	ILE
1	D	136	ILE
1	D	202	PRO
1	D	204	ASP
1	D	233	SER
2	E	39	VAL
2	E	61	LYS
2	E	126	THR
2	E	143	THR
2	E	146	VAL
2	E	162	ILE
2	E	207	THR
2	E	234	THR
2	E	343	VAL
2	E	379	LYS
2	E	405	THR
2	E	434	VAL
3	F	157	THR
3	F	212	LYS
3	F	213	ILE
3	F	277	ARG
3	F	298	LEU
3	F	336	LEU
3	F	365	THR
3	F	398	TYR
1	G	132	VAL

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Mol	Chain	Res	Type
1	G	249	GLU
2	H	20	GLU
2	H	21	ARG
2	H	34	ILE
2	H	42	LEU
2	H	105	GLU
2	H	120	ILE
2	H	124	VAL
2	H	180	TYR
2	H	231	VAL
2	H	280	MET
2	H	388	VAL
2	H	414	THR
3	I	4	HIS
3	I	36	VAL
3	I	95	THR
3	I	118	PRO
3	I	121	LEU
3	I	133	ILE
3	I	164	ILE
3	I	166	MET
3	I	167	HIS
3	I	171	ASP
3	I	240	TYR
3	I	246	VAL
3	I	260	THR
3	I	274	VAL
3	I	290	PRO
3	I	311	THR
3	I	319	VAL
3	I	336	LEU
3	I	354	VAL
3	I	378	ILE
3	I	392	THR
1	J	83	PRO
1	J	84	THR
1	J	143	LYS
1	J	155	GLU
1	J	160	PRO
1	J	168	SER
1	J	186	VAL
1	J	238	ASN

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Mol	Chain	Res	Type
2	K	5	THR
2	K	203	ILE
2	K	231	VAL
2	K	249	VAL
2	K	278	ILE
2	K	304	GLN
2	K	340	LYS
2	K	367	VAL
2	K	368	GLN
2	K	375	THR
2	K	376	CYS
2	K	389	PRO
2	K	435	VAL
3	L	31	VAL
3	L	42	ASP
3	L	44	VAL
3	L	48	GLN
3	L	49	VAL
3	L	74	VAL
3	L	86	THR
3	L	129	LYS
3	L	138	SER
3	L	148	ILE
3	L	271	GLU
3	L	288	MET
3	L	295	ILE
3	L	332	ASN
3	L	343	SER
3	L	377	VAL
3	L	397	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	131	HIS
1	A	172	HIS
1	A	182	HIS
2	B	9	ASN
2	B	50	ASN
2	B	132	GLN
2	B	141	ASN

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Mol	Chain	Res	Type
2	B	209	ASN
2	B	304	GLN
2	B	371	ASN
3	C	63	HIS
3	C	98	HIS
3	C	155	HIS
3	C	180	ASN
3	C	235	GLN
3	C	254	HIS
3	C	332	ASN
3	C	339	GLN
3	C	399	GLN
1	D	97	ASN
1	D	172	HIS
1	D	180	ASN
1	D	183	HIS
2	E	10	GLN
2	E	50	ASN
2	E	102	GLN
2	E	252	ASN
2	E	254	ASN
2	E	264	ASN
2	E	270	ASN
2	E	335	ASN
2	E	368	GLN
2	E	371	ASN
3	F	167	HIS
3	F	175	GLN
3	F	217	ASN
3	F	254	HIS
3	F	286	HIS
3	F	304	HIS
3	F	347	HIS
1	G	116	ASN
1	G	138	ASN
1	G	182	HIS
1	G	183	HIS
1	G	225	ASN
2	H	10	GLN
2	H	72	ASN
2	H	102	GLN
2	H	123	GLN

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Mol	Chain	Res	Type
2	H	186	ASN
2	H	209	ASN
3	I	35	HIS
3	I	52	GLN
3	I	109	GLN
3	I	217	ASN
3	I	235	GLN
3	I	237	ASN
3	I	254	HIS
3	I	284	HIS
3	I	286	HIS
3	I	318	GLN
3	I	330	ASN
3	I	347	HIS
3	I	349	ASN
3	I	356	HIS
1	J	103	ASN
1	J	182	HIS
1	J	190	ASN
1	J	225	ASN
2	K	100	ASN
2	K	102	GLN
2	K	123	GLN
2	K	186	ASN
2	K	204	GLN
2	K	335	ASN
2	K	344	GLN
2	K	368	GLN
2	K	371	ASN
3	L	4	HIS
3	L	35	HIS
3	L	52	GLN
3	L	98	HIS
3	L	109	GLN
3	L	175	GLN
3	L	217	ASN
3	L	235	GLN
3	L	237	ASN
3	L	273	GLN
3	L	284	HIS
3	L	286	HIS
3	L	332	ASN

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Mol	Chain	Res	Type
3	L	399	GLN
3	L	405	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

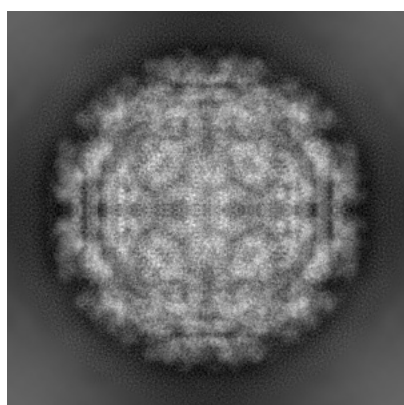
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1886. These allow visual inspection of the internal detail of the map and identification of artifacts.

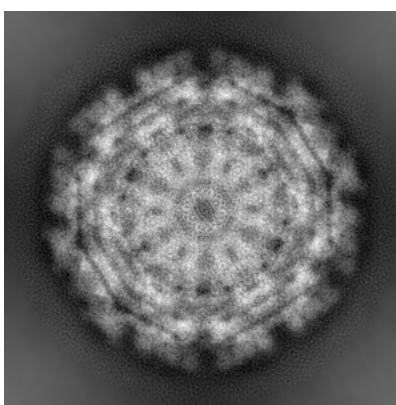
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

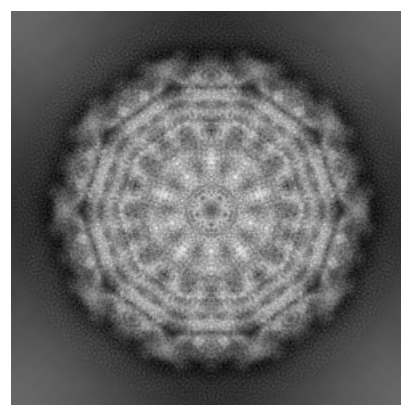
6.1.1 Primary map



X



Y

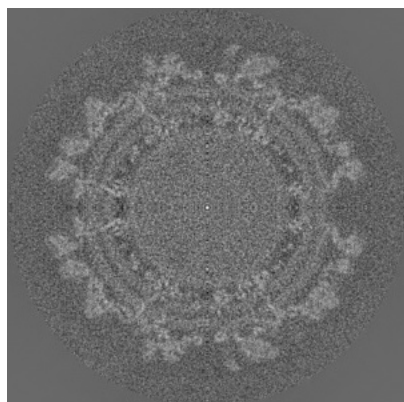


Z

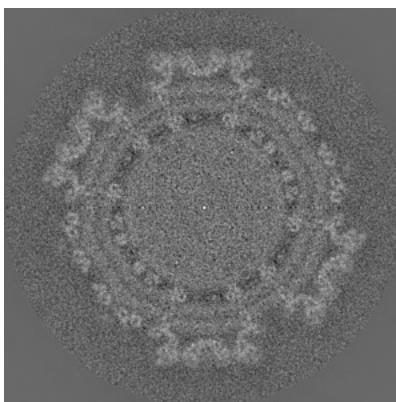
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

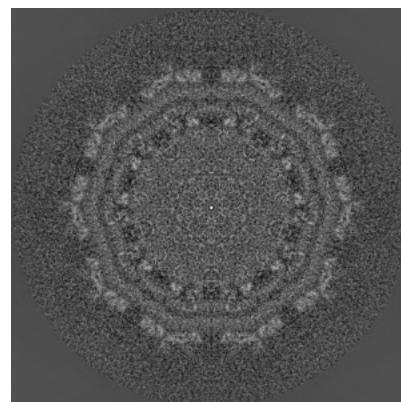
6.2.1 Primary map



X Index: 288



Y Index: 288

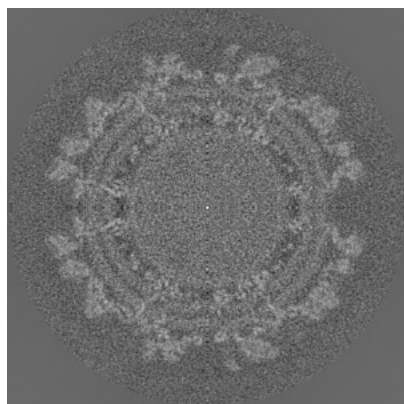


Z Index: 288

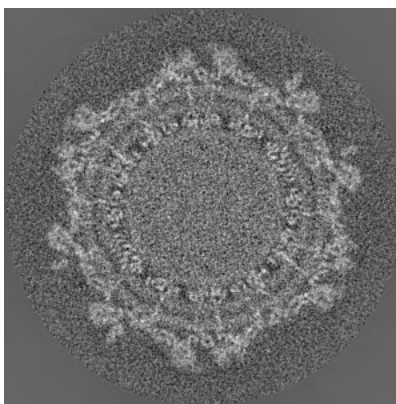
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

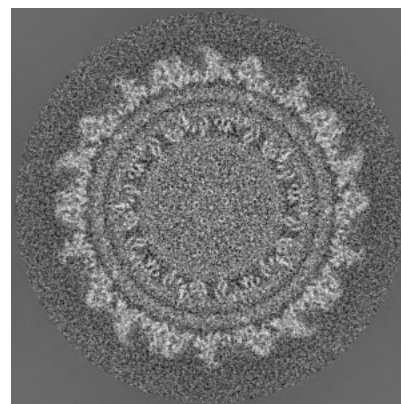
6.3.1 Primary map



X Index: 288



Y Index: 268

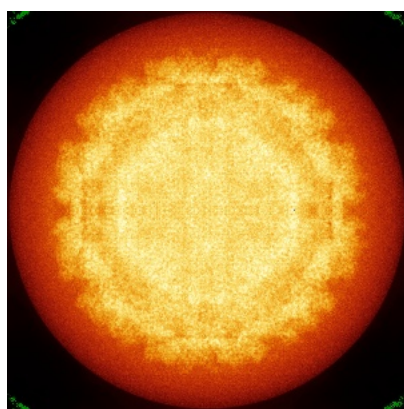


Z Index: 338

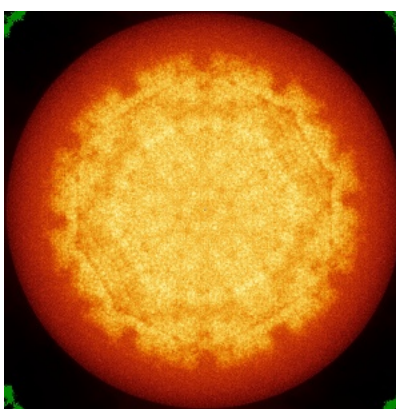
The images above show the largest variance slices of the map in three orthogonal directions.

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

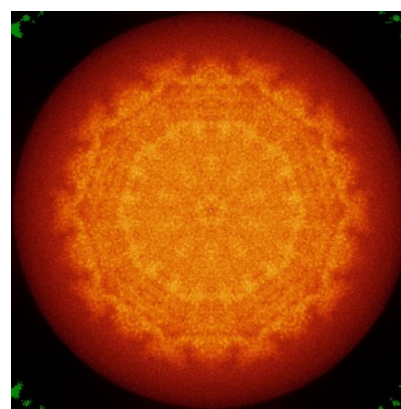
6.4.1 Primary map



X



Y

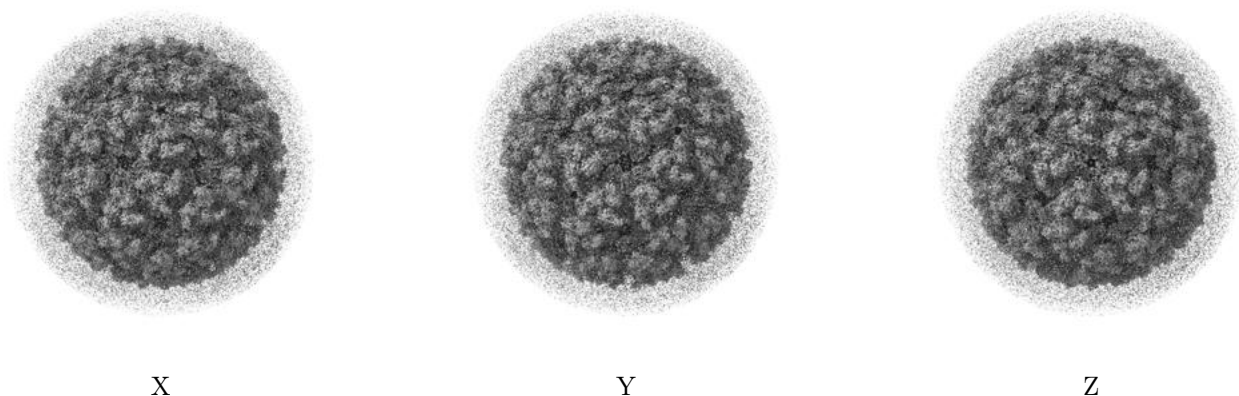


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

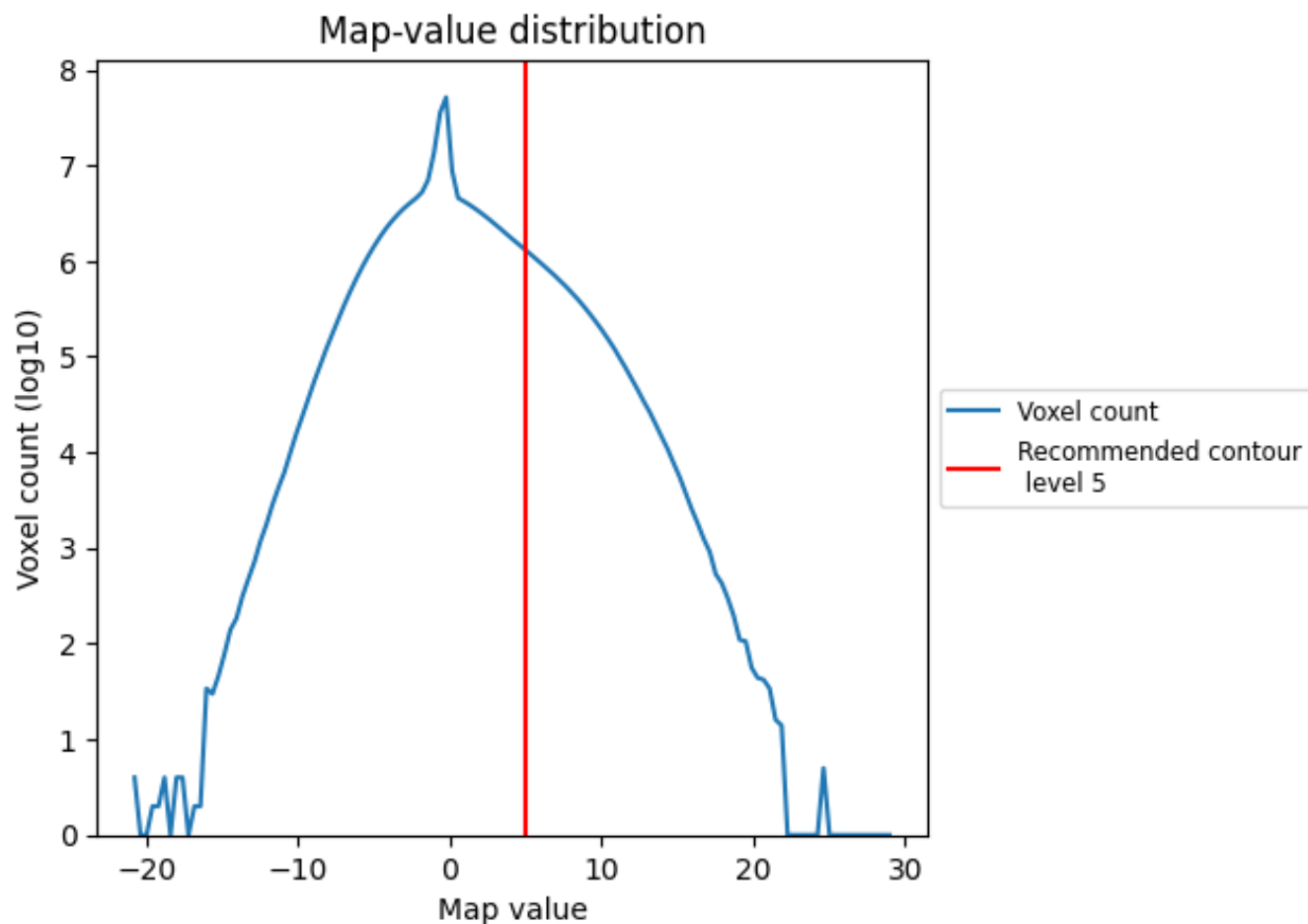
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

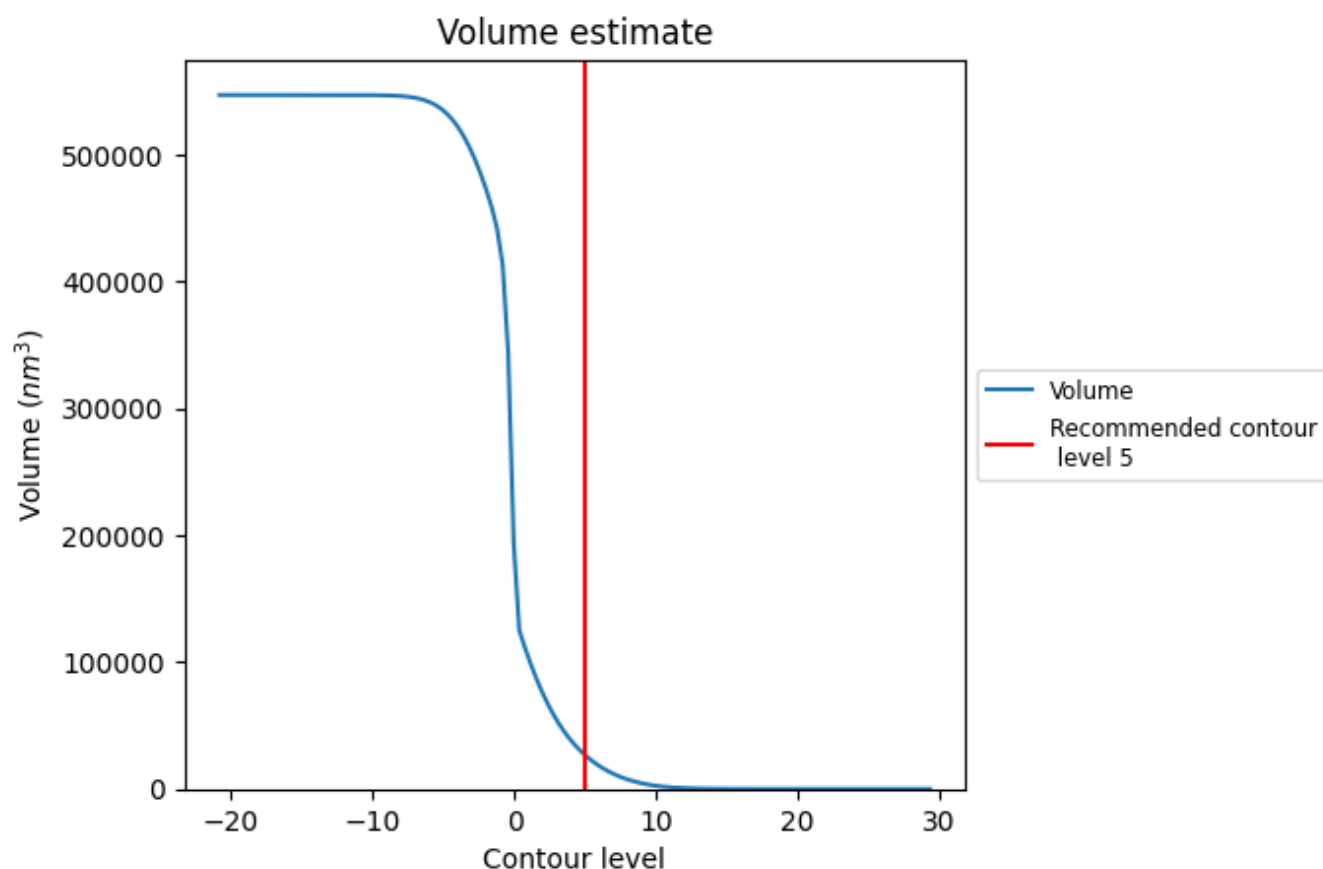
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

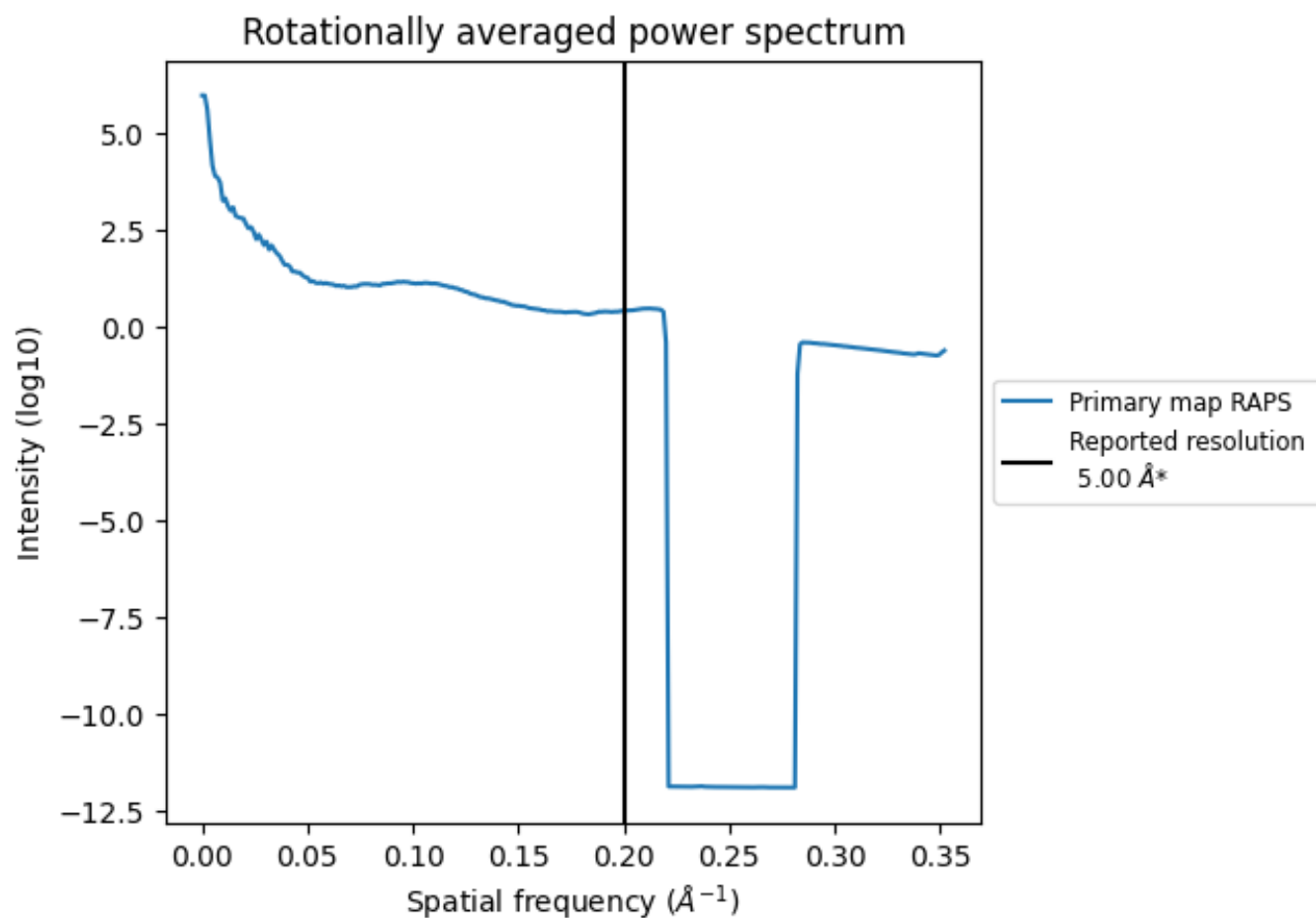
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 26924 nm^3 ; this corresponds to an approximate mass of 24321 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 0.200 Å⁻¹

8 Fourier-Shell correlation

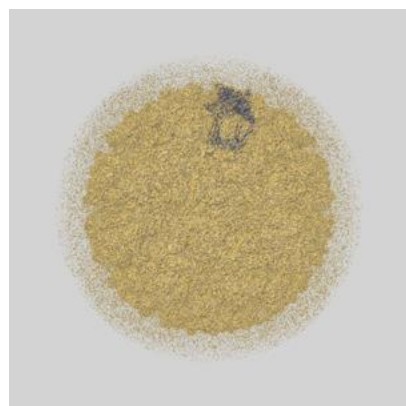
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

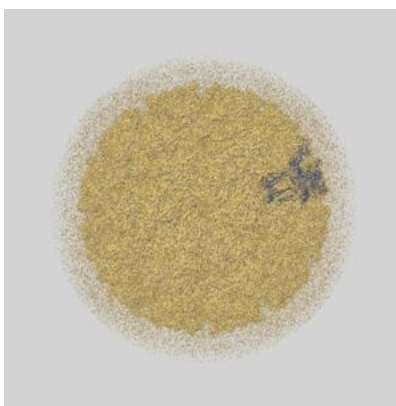
This section contains information regarding the fit between EMDB map EMD-1886 and PDB model 2YEW. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlays

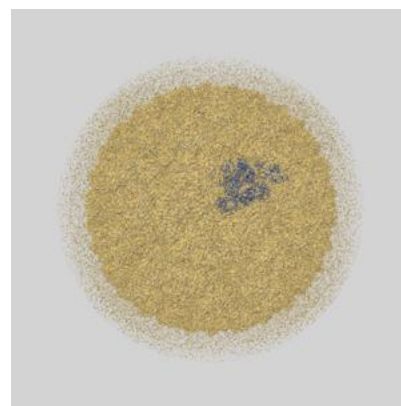
9.1.1 Map-model overlay [i](#)



X

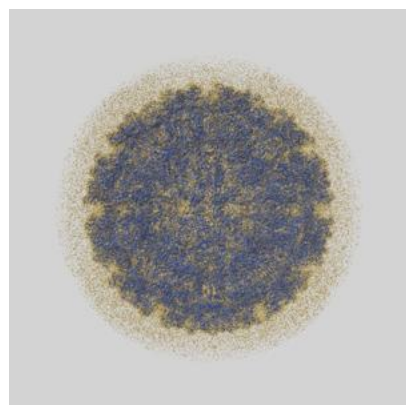


Y

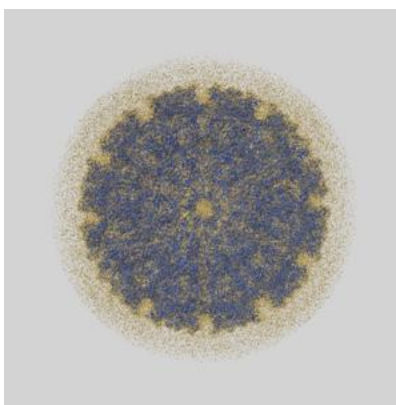


Z

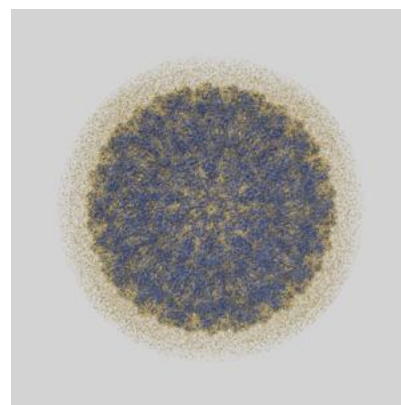
9.1.2 Map-model assembly overlay [i](#)



X



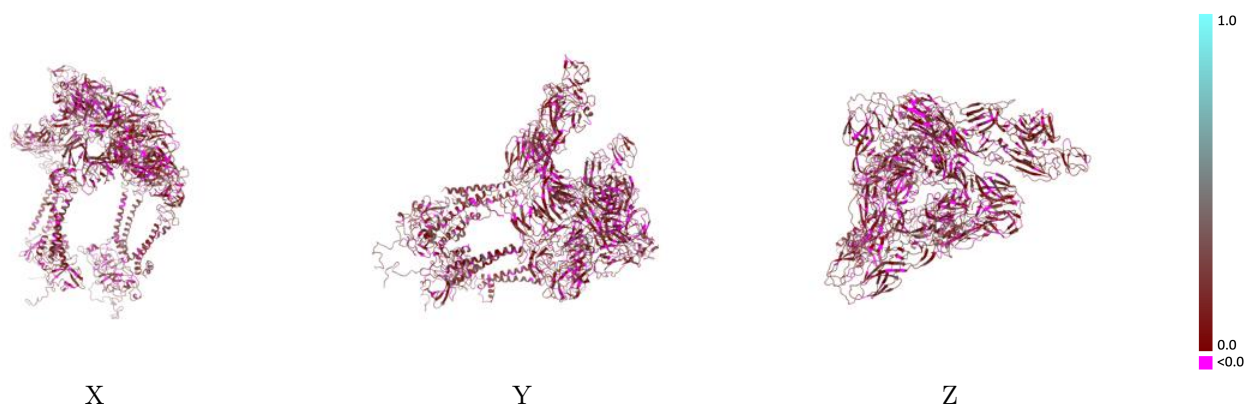
Y



Z

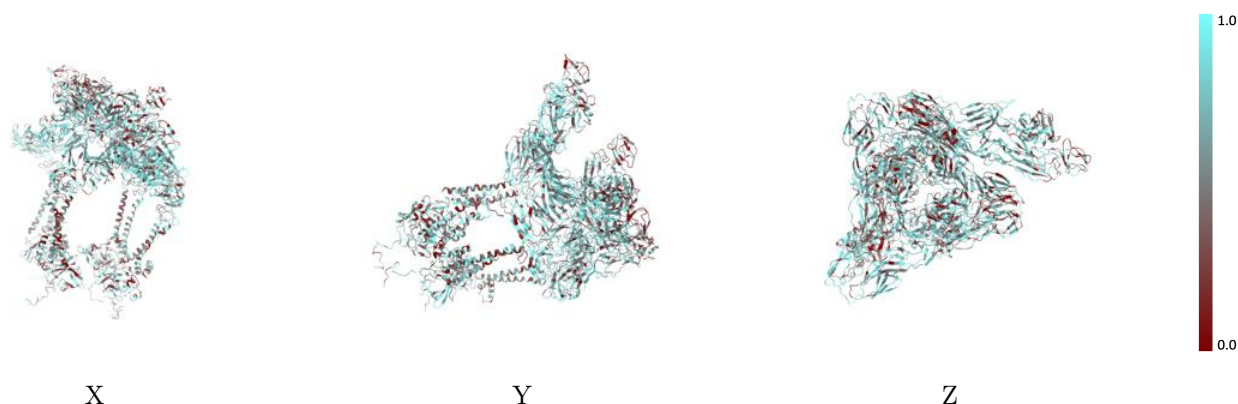
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



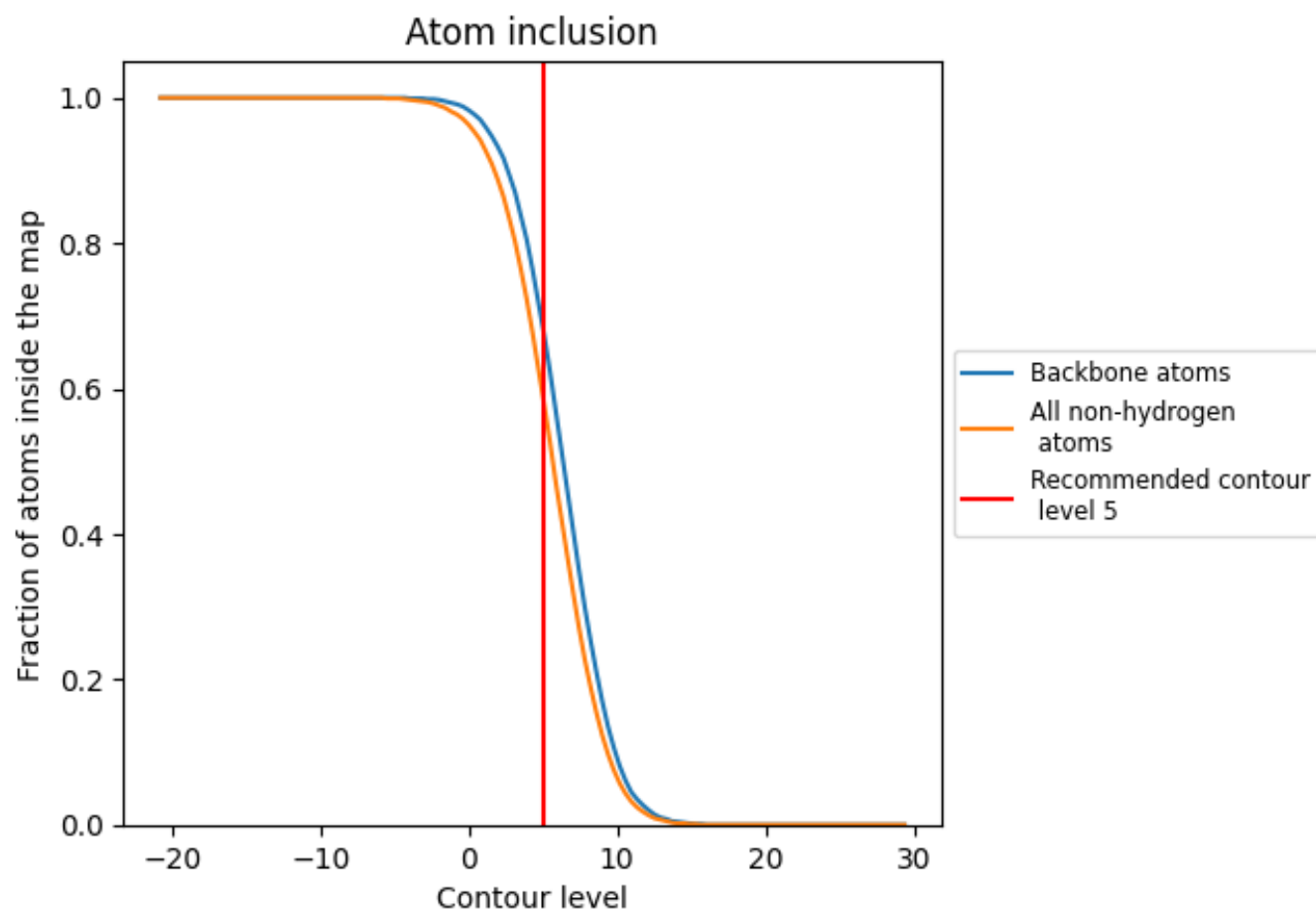
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 59% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5880	0.1540
A	0.5940	0.1610
B	0.6520	0.1800
C	0.5770	0.1520
D	0.5430	0.1610
E	0.6200	0.1580
F	0.5410	0.1270
G	0.5450	0.1880
H	0.5980	0.1490
I	0.5550	0.1360
J	0.5470	0.1750
K	0.6200	0.1480
L	0.5880	0.1490

1.0

0.0

<0.0