



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:33 AM UTC

PDB ID : 9DXH / pdb_00009dxh
EMDB ID : EMD-47288
Title : attPmm and attBmm bound serine integrase complex in the pre-rotation state
Authors : Shin, H.; Rice, P.A.; Olorunniji, F.J.
Deposited on : 2024-10-11
Resolution : 4.69 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

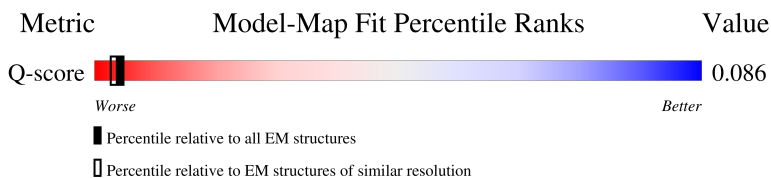
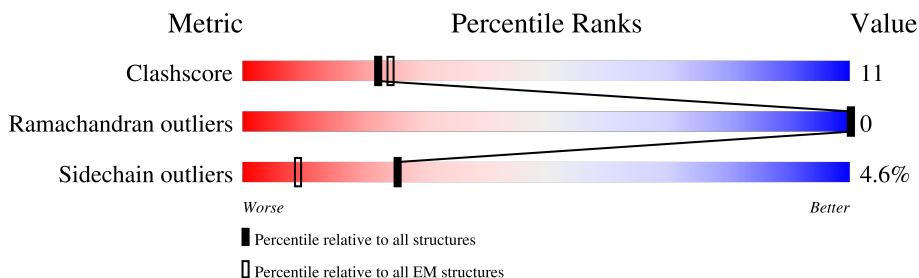
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.69 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	1970 (4.19 - 5.19)

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	545	<div> <div>8%</div> <div>43%</div> <div>43%</div> <div>11%</div> <div>..</div> </div>
1	C	545	<div> <div>7%</div> <div>48%</div> <div>40%</div> <div>10%</div> <div>..</div> </div>
1	I	545	<div> <div>6%</div> <div>43%</div> <div>42%</div> <div>11%</div> <div>..</div> </div>
1	K	545	<div> <div>7%</div> <div>47%</div> <div>40%</div> <div>10%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	34	
2	M	34	
3	F	33	
3	N	33	
4	G	25	
4	O	25	
5	H	24	
5	P	24	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 42532 atoms, of which 20350 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 Resolvase homolog YokA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	535	Total	C	H	N	O	S	0	0
			8781	2744	4425	753	841	18		
1	C	535	Total	C	H	N	O	S	0	0
			8781	2744	4425	753	841	18		
1	I	535	Total	C	H	N	O	S	0	0
			8781	2744	4425	753	841	18		
1	K	535	Total	C	H	N	O	S	0	0
			8781	2744	4425	753	841	18		

- Molecule 2 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	34	Total	C	H	N	O	P	0	0
			1087	337	393	110	213	34		
2	M	34	Total	C	H	N	O	P	0	0
			1087	337	393	110	213	34		

- Molecule 3 is a DNA chain called DNA (33-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
3	F	33	Total	C	H	N	O	P	0	0
			1052	326	373	130	190	33		
3	N	33	Total	C	H	N	O	P	0	0
			1052	326	373	130	190	33		

- Molecule 4 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
4	G	25	Total	C	H	N	O	P	0	0
			796	246	285	90	150	25		
4	O	25	Total	C	H	N	O	P	0	0
			796	246	285	90	150	25		

- Molecule 5 is a DNA chain called DNA (24-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
5	H	24	Total	C	H	N	O	P	0	0
			767	237	274	87	145	24		
5	P	24	Total	C	H	N	O	P	0	0
			767	237	274	87	145	24		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Zn	0
			1	1	
6	C	1	Total	Zn	0
			1	1	
6	I	1	Total	Zn	0
			1	1	
6	K	1	Total	Zn	0
			1	1	

3 Residue-property plots

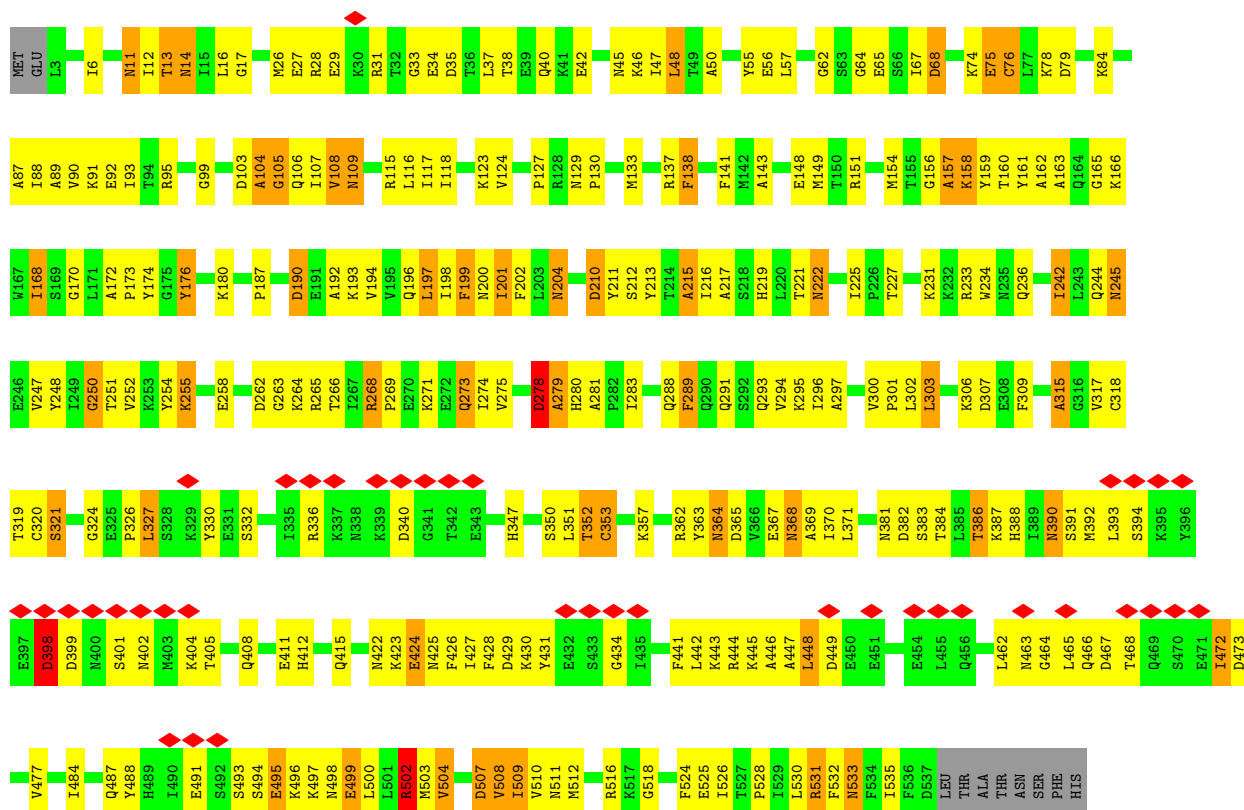
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

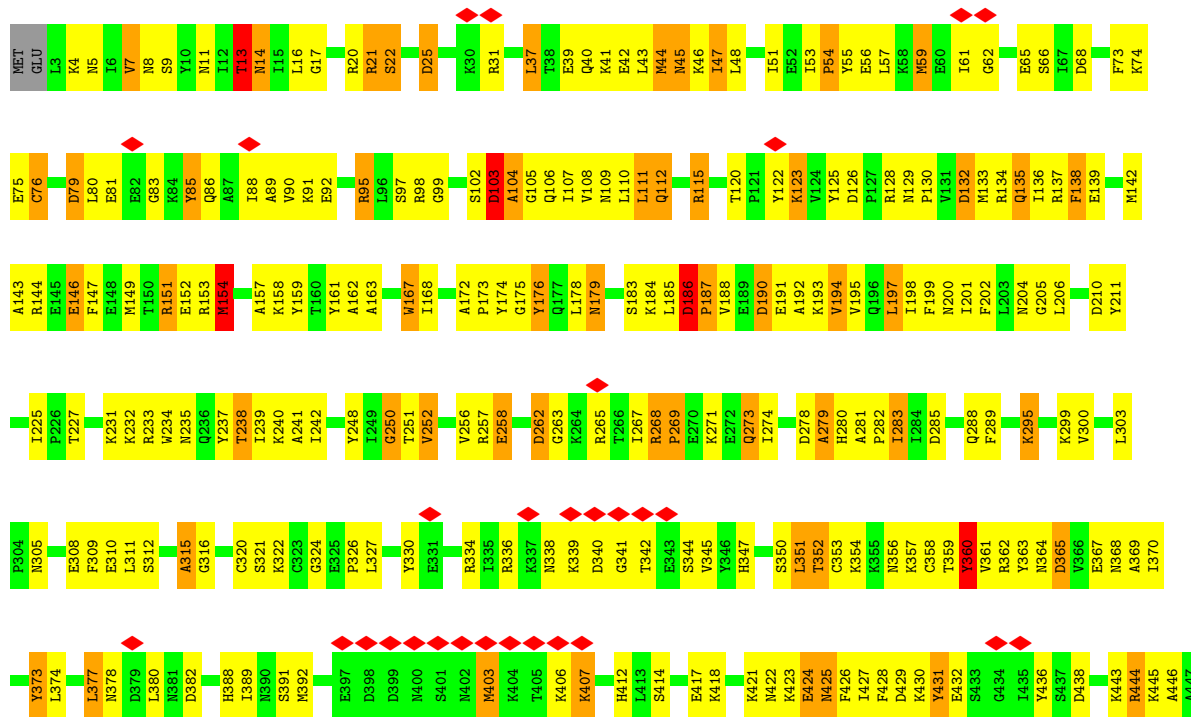


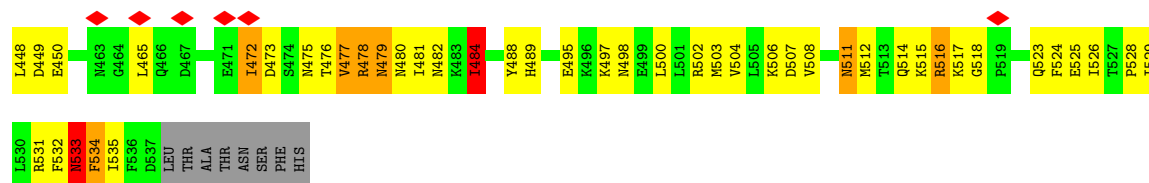
• Molecule 1: Resolvase homolog Yoka



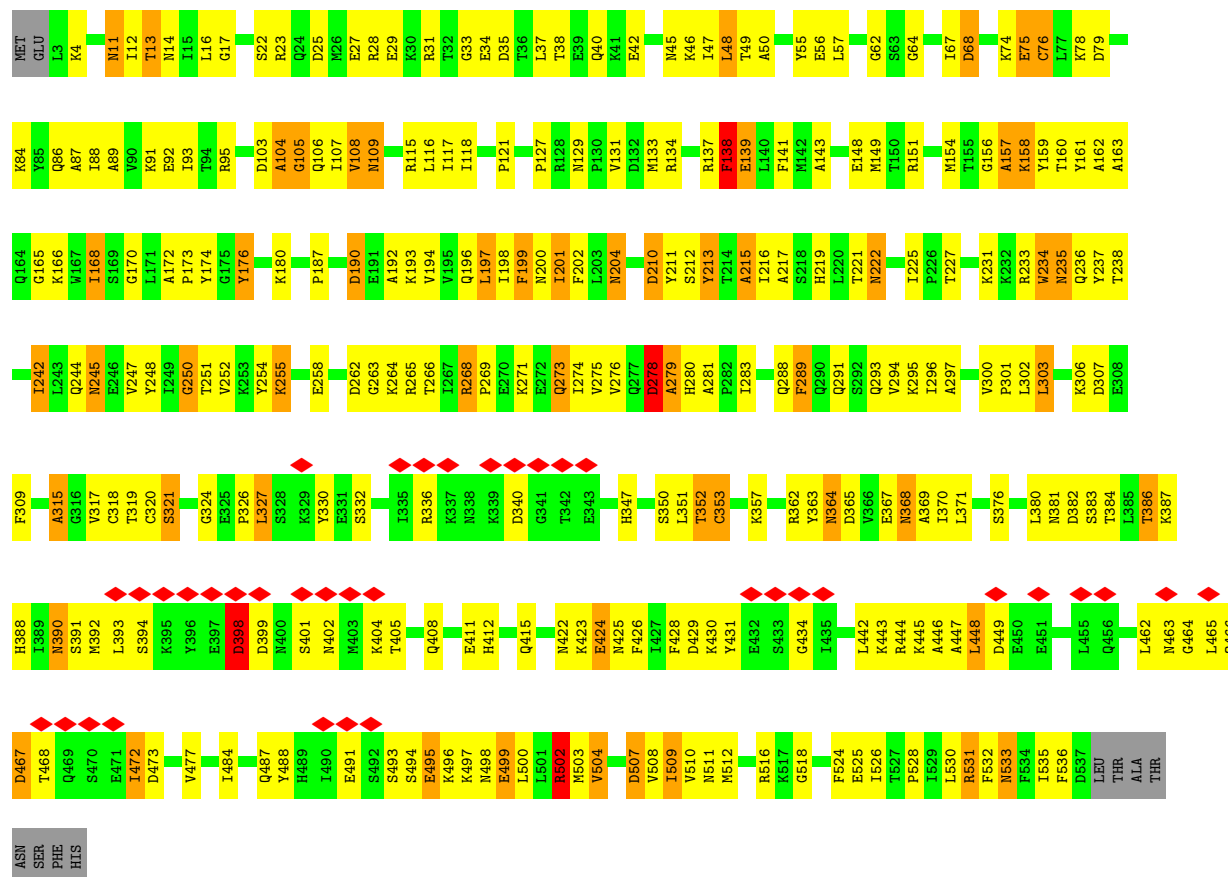


• Molecule 1: Resolvase homolog YokaA

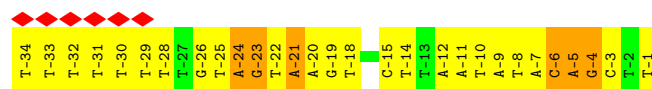




• Molecule 1: Resolvase homolog Yoka



• Molecule 2: DNA (34-MER)

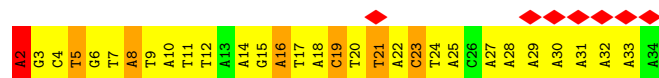
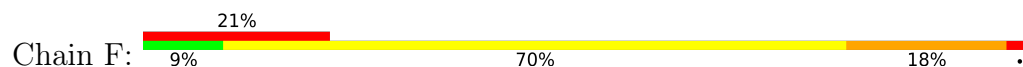


• Molecule 2: DNA (34-MER)

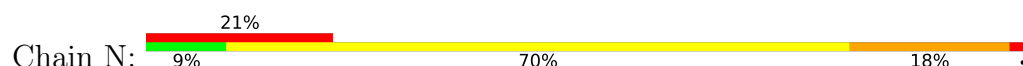




- Molecule 3: DNA (33-MER)



- Molecule 3: DNA (33-MER)



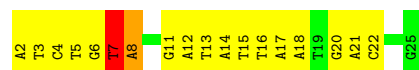
- Molecule 4: DNA (25-MER)



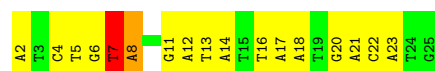
- Molecule 4: DNA (25-MER)



- Molecule 5: DNA (24-MER)



- Molecule 5: DNA (24-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	44115	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.642	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.01	Depositor
Map size (\AA)	463.27502, 482.44504, 412.15503	wwPDB
Map dimensions	435, 453, 387	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.065, 1.065, 1.065	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.39	88/4423 (2.0%)	2.44	376/5942 (6.3%)
1	C	2.39	80/4423 (1.8%)	2.43	364/5942 (6.1%)
1	I	2.42	91/4423 (2.1%)	2.45	386/5942 (6.5%)
1	K	2.43	83/4423 (1.9%)	2.47	383/5942 (6.4%)
2	E	1.40	7/774 (0.9%)	1.45	2/1193 (0.2%)
2	M	1.43	7/774 (0.9%)	1.46	2/1193 (0.2%)
3	F	1.49	5/764 (0.7%)	1.50	5/1176 (0.4%)
3	N	1.45	5/764 (0.7%)	1.47	6/1176 (0.5%)
4	G	1.75	9/572 (1.6%)	1.83	5/880 (0.6%)
4	O	1.76	10/572 (1.7%)	1.83	4/880 (0.5%)
5	H	1.70	9/552 (1.6%)	1.75	3/850 (0.4%)
5	P	1.70	10/552 (1.8%)	1.75	3/850 (0.4%)
All	All	2.24	404/23016 (1.8%)	2.26	1539/31966 (4.8%)

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	2
1	I	0	2
1	K	0	1
2	E	0	1
2	M	0	1
3	F	0	1
3	N	0	1
4	G	0	2
4	O	0	2
5	H	0	1
5	P	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	15

All (404) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	412	HIS	CE1-NE2	-8.98	1.23	1.32
1	A	412	HIS	CE1-NE2	-8.94	1.23	1.32
1	I	489	HIS	ND1-CE1	-8.88	1.23	1.32
1	K	412	HIS	CE1-NE2	-8.87	1.23	1.32
1	I	489	HIS	CE1-NE2	-8.86	1.23	1.32
1	A	388	HIS	CE1-NE2	-8.85	1.23	1.32
1	C	388	HIS	CE1-NE2	-8.83	1.23	1.32
1	I	388	HIS	CE1-NE2	-8.82	1.23	1.32
1	K	219	HIS	CE1-NE2	-8.82	1.23	1.32
1	A	347	HIS	ND1-CE1	-8.81	1.23	1.32
1	A	489	HIS	ND1-CE1	-8.81	1.23	1.32
1	A	489	HIS	CE1-NE2	-8.80	1.23	1.32
1	I	347	HIS	ND1-CE1	-8.80	1.23	1.32
1	C	219	HIS	CE1-NE2	-8.78	1.23	1.32
1	K	388	HIS	CE1-NE2	-8.78	1.23	1.32
1	C	280	HIS	CE1-NE2	-8.75	1.23	1.32
1	C	347	HIS	ND1-CE1	-8.75	1.23	1.32
1	K	280	HIS	CE1-NE2	-8.74	1.23	1.32
1	I	412	HIS	CE1-NE2	-8.71	1.23	1.32
1	C	137	ARG	CZ-NH2	-8.63	1.22	1.33
1	K	347	HIS	ND1-CE1	-8.62	1.24	1.32
1	K	444	ARG	CZ-NH2	-8.45	1.22	1.33
1	K	170	GLY	N-CA	-8.42	1.37	1.46
1	C	170	GLY	N-CA	-8.40	1.37	1.46
1	A	153	ARG	CZ-NH2	-8.36	1.22	1.33
1	I	137	ARG	CZ-NH2	-8.35	1.22	1.33
1	K	137	ARG	CZ-NH2	-8.35	1.22	1.33
1	I	134	ARG	CZ-NH2	-8.29	1.22	1.33
1	I	516	ARG	CZ-NH2	-8.27	1.22	1.33
1	A	516	ARG	CZ-NH2	-8.26	1.22	1.33
1	I	115	ARG	CZ-NH2	-8.26	1.22	1.33
1	A	115	ARG	CZ-NH2	-8.22	1.22	1.33
1	C	444	ARG	CZ-NH2	-8.19	1.22	1.33
1	K	115	ARG	CZ-NH2	-8.19	1.22	1.33
1	I	257	ARG	CZ-NH2	-8.18	1.22	1.33
1	I	128	ARG	CZ-NH2	-8.15	1.22	1.33
1	A	257	ARG	CZ-NH2	-8.15	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	334	ARG	CZ-NH2	-8.14	1.22	1.33
1	K	219	HIS	CD2-NE2	-8.13	1.28	1.37
1	K	134	ARG	CZ-NH2	-8.13	1.22	1.33
1	A	489	HIS	CD2-NE2	-8.12	1.28	1.37
1	C	151	ARG	CZ-NH2	-8.12	1.23	1.33
1	C	115	ARG	CZ-NH2	-8.11	1.23	1.33
1	I	531	ARG	CZ-NH2	-8.11	1.23	1.33
1	I	489	HIS	CD2-NE2	-8.10	1.28	1.37
1	A	144	ARG	CZ-NH2	-8.10	1.23	1.33
1	I	412	HIS	CD2-NE2	-8.09	1.28	1.37
1	K	151	ARG	CZ-NH2	-8.09	1.23	1.33
1	C	28	ARG	CZ-NH2	-8.08	1.23	1.33
1	I	388	HIS	CD2-NE2	-8.08	1.28	1.37
1	A	268	ARG	CZ-NH2	-8.07	1.23	1.33
1	I	144	ARG	CZ-NH2	-8.07	1.23	1.33
1	K	280	HIS	CD2-NE2	-8.07	1.28	1.37
1	A	334	ARG	CZ-NH2	-8.07	1.23	1.33
1	C	219	HIS	CD2-NE2	-8.06	1.28	1.37
1	K	28	ARG	CZ-NH2	-8.06	1.23	1.33
1	K	362	ARG	CZ-NH2	-8.05	1.23	1.33
1	K	516	ARG	CZ-NH2	-8.05	1.23	1.33
1	C	362	ARG	CZ-NH2	-8.04	1.23	1.33
1	C	233	ARG	CZ-NH2	-8.04	1.23	1.33
1	A	388	HIS	CD2-NE2	-8.04	1.29	1.37
1	K	412	HIS	CD2-NE2	-8.04	1.29	1.37
1	K	268	ARG	CZ-NH2	-8.04	1.23	1.33
1	A	98	ARG	CZ-NH2	-8.03	1.23	1.33
1	I	362	ARG	CZ-NH2	-8.03	1.23	1.33
1	I	98	ARG	CZ-NH2	-8.03	1.23	1.33
1	C	412	HIS	CD2-NE2	-8.02	1.29	1.37
1	A	31	ARG	CZ-NH2	-8.02	1.23	1.33
1	A	478	ARG	CZ-NH2	-8.01	1.23	1.33
1	A	531	ARG	CZ-NH2	-8.00	1.23	1.33
1	K	531	ARG	CZ-NH2	-8.00	1.23	1.33
1	C	268	ARG	CZ-NH2	-8.00	1.23	1.33
1	A	128	ARG	CZ-NH2	-8.00	1.23	1.33
1	K	502	ARG	CZ-NH2	-8.00	1.23	1.33
1	I	31	ARG	CZ-NH2	-8.00	1.23	1.33
1	C	280	HIS	CD2-NE2	-7.99	1.29	1.37
1	C	31	ARG	CZ-NH2	-7.99	1.23	1.33
1	C	531	ARG	CZ-NH2	-7.99	1.23	1.33
1	K	265	ARG	CZ-NH2	-7.98	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	412	HIS	CD2-NE2	-7.97	1.29	1.37
1	C	516	ARG	CZ-NH2	-7.97	1.23	1.33
1	C	502	ARG	CZ-NH2	-7.97	1.23	1.33
1	A	362	ARG	CZ-NH2	-7.96	1.23	1.33
1	C	388	HIS	CD2-NE2	-7.96	1.29	1.37
1	K	31	ARG	CZ-NH2	-7.95	1.23	1.33
1	I	478	ARG	CZ-NH2	-7.94	1.23	1.33
1	K	233	ARG	CZ-NH2	-7.94	1.23	1.33
1	C	265	ARG	CZ-NH2	-7.89	1.23	1.33
1	K	388	HIS	CD2-NE2	-7.89	1.29	1.37
1	A	444	ARG	CZ-NH2	-7.89	1.23	1.33
1	I	444	ARG	CZ-NH2	-7.89	1.23	1.33
1	I	268	ARG	CZ-NH2	-7.88	1.23	1.33
1	I	151	ARG	CZ-NH2	-7.84	1.23	1.33
1	I	233	ARG	CZ-NH2	-7.82	1.23	1.33
1	I	265	ARG	CZ-NH2	-7.79	1.23	1.33
1	A	151	ARG	CZ-NH2	-7.79	1.23	1.33
1	A	265	ARG	CZ-NH2	-7.76	1.23	1.33
1	I	153	ARG	CZ-NH2	-7.75	1.23	1.33
1	A	233	ARG	CZ-NH2	-7.74	1.23	1.33
1	C	104	ALA	CA-CB	-7.20	1.42	1.53
1	I	143	ALA	CA-CB	-7.10	1.42	1.53
1	I	62	GLY	N-CA	-7.04	1.37	1.45
1	A	62	GLY	N-CA	-7.04	1.37	1.45
1	K	89	ALA	CA-CB	-7.03	1.42	1.53
1	I	369	ALA	CA-CB	-7.01	1.42	1.53
1	A	104	ALA	CA-CB	-6.98	1.42	1.53
1	A	369	ALA	CA-CB	-6.95	1.42	1.53
1	K	281	ALA	CA-CB	-6.93	1.42	1.53
1	C	137	ARG	CZ-NH1	-6.91	1.23	1.32
1	C	447	ALA	CA-CB	-6.91	1.42	1.53
1	K	162	ALA	CA-CB	-6.88	1.42	1.53
1	C	89	ALA	CA-CB	-6.87	1.43	1.53
1	A	143	ALA	CA-CB	-6.87	1.42	1.53
1	I	137	ARG	CZ-NH1	-6.86	1.23	1.32
1	K	447	ALA	CA-CB	-6.86	1.42	1.53
1	A	446	ALA	CA-CB	-6.83	1.42	1.53
1	A	315	ALA	CA-CB	-6.83	1.42	1.53
1	C	446	ALA	CA-CB	-6.83	1.42	1.53
1	I	241	ALA	CA-CB	-6.83	1.42	1.53
1	I	134	ARG	CZ-NH1	-6.82	1.23	1.32
1	I	446	ALA	CA-CB	-6.82	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	217	ALA	CA-CB	-6.81	1.42	1.53
1	A	153	ARG	CZ-NH1	-6.77	1.23	1.32
1	I	315	ALA	CA-CB	-6.76	1.42	1.53
1	K	192	ALA	CA-CB	-6.76	1.42	1.53
1	A	241	ALA	CA-CB	-6.76	1.42	1.53
1	K	446	ALA	CA-CB	-6.76	1.42	1.53
1	I	162	ALA	CA-CB	-6.76	1.42	1.53
1	C	217	ALA	CA-CB	-6.75	1.42	1.53
1	C	143	ALA	CA-CB	-6.74	1.43	1.53
1	K	163	ALA	CA-CB	-6.73	1.43	1.53
1	A	516	ARG	CZ-NH1	-6.70	1.23	1.32
1	K	143	ALA	CA-CB	-6.70	1.43	1.53
1	A	157	ALA	CA-CB	-6.70	1.43	1.53
1	A	162	ALA	CA-CB	-6.69	1.43	1.53
1	C	163	ALA	CA-CB	-6.67	1.43	1.53
1	I	157	ALA	CA-CB	-6.67	1.43	1.53
1	I	516	ARG	CZ-NH1	-6.67	1.23	1.32
1	I	192	ALA	CA-CB	-6.65	1.43	1.53
1	A	172	ALA	CA-CB	-6.64	1.42	1.53
1	K	137	ARG	CZ-NH1	-6.64	1.23	1.32
1	I	172	ALA	CA-CB	-6.63	1.42	1.53
1	C	151	ARG	CZ-NH1	-6.62	1.23	1.32
1	A	192	ALA	CA-CB	-6.62	1.43	1.53
1	C	31	ARG	CZ-NH1	-6.62	1.23	1.32
1	C	50	ALA	CA-CB	-6.62	1.43	1.53
1	K	297	ALA	CA-CB	-6.61	1.43	1.53
1	A	268	ARG	CZ-NH1	-6.61	1.23	1.32
1	C	281	ALA	CA-CB	-6.61	1.43	1.53
1	C	162	ALA	CA-CB	-6.61	1.43	1.53
1	K	444	ARG	CZ-NH1	-6.60	1.23	1.32
1	K	151	ARG	CZ-NH1	-6.60	1.23	1.32
1	C	297	ALA	CA-CB	-6.59	1.43	1.53
1	K	31	ARG	CZ-NH1	-6.59	1.23	1.32
1	A	115	ARG	CZ-NH1	-6.58	1.23	1.32
1	C	444	ARG	CZ-NH1	-6.58	1.23	1.32
1	I	128	ARG	CZ-NH1	-6.58	1.23	1.32
1	C	516	ARG	CZ-NH1	-6.58	1.23	1.32
1	I	257	ARG	CZ-NH1	-6.58	1.23	1.32
1	A	281	ALA	CA-CB	-6.57	1.43	1.53
1	K	50	ALA	CA-CB	-6.57	1.43	1.53
1	C	502	ARG	CZ-NH1	-6.56	1.23	1.32
1	C	192	ALA	CA-CB	-6.56	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	362	ARG	CZ-NH1	-6.56	1.23	1.32
1	I	281	ALA	CA-CB	-6.55	1.43	1.53
1	K	531	ARG	CZ-NH1	-6.55	1.23	1.32
1	I	104	ALA	CA-CB	-6.55	1.43	1.53
1	A	334	ARG	CZ-NH1	-6.54	1.23	1.32
1	I	115	ARG	CZ-NH1	-6.54	1.23	1.32
1	C	362	ARG	CZ-NH1	-6.54	1.23	1.32
1	K	502	ARG	CZ-NH1	-6.53	1.23	1.32
1	C	531	ARG	CZ-NH1	-6.52	1.23	1.32
1	A	98	ARG	CZ-NH1	-6.52	1.23	1.32
1	A	362	ARG	CZ-NH1	-6.52	1.23	1.32
1	K	104	ALA	CA-CB	-6.52	1.43	1.53
1	K	516	ARG	CZ-NH1	-6.51	1.23	1.32
1	I	31	ARG	CZ-NH1	-6.51	1.23	1.32
1	K	28	ARG	CZ-NH1	-6.50	1.23	1.32
1	I	478	ARG	CZ-NH1	-6.50	1.23	1.32
1	K	115	ARG	CZ-NH1	-6.49	1.23	1.32
1	K	265	ARG	CZ-NH1	-6.48	1.23	1.32
1	A	531	ARG	CZ-NH1	-6.48	1.23	1.32
1	C	28	ARG	CZ-NH1	-6.48	1.23	1.32
1	A	478	ARG	CZ-NH1	-6.47	1.23	1.32
1	I	98	ARG	CZ-NH1	-6.47	1.23	1.32
1	A	105	GLY	N-CA	-6.46	1.37	1.45
1	I	362	ARG	CZ-NH1	-6.46	1.23	1.32
1	I	334	ARG	CZ-NH1	-6.45	1.23	1.32
1	A	31	ARG	CZ-NH1	-6.45	1.23	1.32
1	C	115	ARG	CZ-NH1	-6.45	1.23	1.32
1	K	279	ALA	CA-CB	-6.45	1.42	1.53
1	A	257	ARG	CZ-NH1	-6.44	1.23	1.32
1	K	157	ALA	CA-CB	-6.43	1.43	1.53
1	K	233	ARG	CZ-NH1	-6.43	1.23	1.32
1	A	128	ARG	CZ-NH1	-6.43	1.23	1.32
1	C	265	ARG	CZ-NH1	-6.43	1.23	1.32
1	K	134	ARG	CZ-NH1	-6.43	1.23	1.32
1	I	531	ARG	CZ-NH1	-6.42	1.23	1.32
1	C	233	ARG	CZ-NH1	-6.42	1.23	1.32
1	I	268	ARG	CZ-NH1	-6.41	1.23	1.32
1	A	144	ARG	CZ-NH1	-6.39	1.23	1.32
1	I	233	ARG	CZ-NH1	-6.39	1.23	1.32
1	I	105	GLY	N-CA	-6.39	1.38	1.45
1	C	268	ARG	CZ-NH1	-6.39	1.23	1.32
1	C	279	ALA	CA-CB	-6.38	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	ARG	CZ-NH1	-6.36	1.23	1.32
1	A	151	ARG	CZ-NH1	-6.36	1.23	1.32
1	C	157	ALA	CA-CB	-6.35	1.43	1.53
1	C	315	ALA	CA-CB	-6.35	1.42	1.53
1	A	444	ARG	CZ-NH1	-6.34	1.23	1.32
1	I	444	ARG	CZ-NH1	-6.34	1.23	1.32
1	I	144	ARG	CZ-NH1	-6.34	1.23	1.32
1	K	268	ARG	CZ-NH1	-6.34	1.23	1.32
1	I	265	ARG	CZ-NH1	-6.32	1.24	1.32
1	K	315	ALA	CA-CB	-6.31	1.42	1.53
1	A	163	ALA	CA-CB	-6.29	1.43	1.53
1	I	163	ALA	CA-CB	-6.26	1.43	1.53
1	A	265	ARG	CZ-NH1	-6.24	1.24	1.32
1	I	151	ARG	CZ-NH1	-6.24	1.24	1.32
1	C	170	GLY	CA-C	-6.18	1.47	1.53
1	K	87	ALA	CA-CB	-6.17	1.43	1.53
1	I	153	ARG	CZ-NH1	-6.14	1.24	1.32
1	A	156	GLY	N-CA	-6.13	1.38	1.45
1	K	170	GLY	CA-C	-6.13	1.47	1.53
1	C	105	GLY	N-CA	-6.06	1.38	1.45
1	C	87	ALA	CA-CB	-6.01	1.43	1.53
1	K	156	GLY	N-CA	-6.01	1.38	1.45
1	I	279	ALA	CA-CB	-6.00	1.42	1.53
1	A	279	ALA	CA-CB	-6.00	1.42	1.53
1	C	156	GLY	N-CA	-5.99	1.38	1.45
1	K	105	GLY	N-CA	-5.96	1.38	1.45
1	C	172	ALA	CA-CB	-5.93	1.42	1.52
1	K	172	ALA	CA-CB	-5.92	1.42	1.52
1	C	137	ARG	CD-NE	-5.85	1.38	1.46
1	A	170	GLY	N-CA	-5.79	1.38	1.45
1	K	137	ARG	CD-NE	-5.71	1.38	1.46
1	A	518	GLY	N-CA	-5.70	1.36	1.44
1	C	33	GLY	N-CA	-5.69	1.37	1.45
1	I	518	GLY	N-CA	-5.66	1.36	1.44
1	I	137	ARG	CD-NE	-5.66	1.38	1.46
1	K	33	GLY	N-CA	-5.62	1.37	1.45
1	A	31	ARG	CD-NE	-5.60	1.38	1.46
1	K	518	GLY	N-CA	-5.57	1.37	1.44
1	C	464	GLY	N-CA	-5.56	1.37	1.45
1	I	126	ASP	CA-CB	-5.55	1.46	1.53
1	C	518	GLY	N-CA	-5.54	1.37	1.44
1	K	31	ARG	CD-NE	-5.54	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	ARG	CD-NE	-5.53	1.38	1.46
1	I	31	ARG	CD-NE	-5.53	1.38	1.46
4	O	-6	DC	C4-N4	-5.51	1.23	1.34
1	K	464	GLY	N-CA	-5.51	1.37	1.45
5	H	4	DC	C4-N4	-5.50	1.23	1.34
1	A	153	ARG	CD-NE	-5.48	1.38	1.46
1	C	31	ARG	CD-NE	-5.48	1.38	1.46
1	I	257	ARG	CD-NE	-5.48	1.38	1.46
2	E	-5	DA	C6-N6	-5.48	1.23	1.34
5	P	22	DC	C4-N4	-5.47	1.23	1.34
1	A	126	ASP	CA-CB	-5.47	1.46	1.53
5	P	4	DC	C4-N4	-5.47	1.23	1.34
1	K	516	ARG	CD-NE	-5.46	1.38	1.46
3	F	4	DC	C4-N4	-5.45	1.23	1.34
1	K	263	GLY	N-CA	-5.45	1.37	1.45
1	C	516	ARG	CD-NE	-5.44	1.38	1.46
1	A	516	ARG	CD-NE	-5.44	1.38	1.46
4	G	-6	DC	C4-N4	-5.44	1.23	1.34
3	N	4	DC	C4-N4	-5.43	1.23	1.34
5	H	22	DC	C4-N4	-5.43	1.23	1.34
2	M	-5	DA	C6-N6	-5.43	1.23	1.34
1	C	531	ARG	CD-NE	-5.42	1.38	1.46
1	A	531	ARG	CD-NE	-5.42	1.38	1.46
1	I	516	ARG	CD-NE	-5.41	1.38	1.46
1	K	265	ARG	CD-NE	-5.41	1.38	1.46
1	I	531	ARG	CD-NE	-5.40	1.38	1.46
2	M	-6	DC	C4-N4	-5.39	1.23	1.34
1	K	502	ARG	CD-NE	-5.37	1.38	1.46
1	C	502	ARG	CD-NE	-5.37	1.38	1.46
1	C	28	ARG	CD-NE	-5.36	1.38	1.46
2	E	-21	DA	C6-N6	-5.36	1.23	1.34
4	G	-3	DA	C6-N6	-5.36	1.23	1.34
1	C	263	GLY	N-CA	-5.35	1.37	1.45
1	I	134	ARG	CD-NE	-5.35	1.38	1.46
2	E	-6	DC	C4-N4	-5.35	1.23	1.34
1	C	265	ARG	CD-NE	-5.35	1.38	1.46
1	K	151	ARG	CD-NE	-5.35	1.38	1.46
1	A	115	ARG	CD-NE	-5.34	1.38	1.46
1	I	478	ARG	CD-NE	-5.34	1.38	1.46
1	C	151	ARG	CD-NE	-5.34	1.38	1.46
3	F	23	DC	C4-N4	-5.33	1.23	1.34
1	A	265	ARG	CD-NE	-5.32	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	-3	DA	C6-N6	-5.32	1.23	1.34
1	I	153	ARG	CD-NE	-5.32	1.38	1.46
1	I	265	ARG	CD-NE	-5.31	1.38	1.46
1	I	128	ARG	CD-NE	-5.31	1.38	1.46
1	K	115	ARG	CD-NE	-5.31	1.38	1.46
1	C	115	ARG	CD-NE	-5.31	1.38	1.46
2	M	-21	DA	C6-N6	-5.31	1.23	1.34
3	N	23	DC	C4-N4	-5.31	1.23	1.34
1	K	531	ARG	CD-NE	-5.31	1.38	1.46
1	K	28	ARG	CD-NE	-5.31	1.38	1.46
1	C	303	LEU	N-CA	-5.29	1.41	1.46
4	G	-5	DA	C6-N6	-5.29	1.23	1.34
1	A	233	ARG	CD-NE	-5.28	1.38	1.46
1	I	115	ARG	CD-NE	-5.28	1.38	1.46
4	O	-5	DA	C6-N6	-5.28	1.23	1.34
4	O	-24	DA	C6-N6	-5.27	1.23	1.34
1	A	478	ARG	CD-NE	-5.26	1.38	1.46
4	G	-24	DA	C6-N6	-5.26	1.23	1.34
1	C	233	ARG	CD-NE	-5.25	1.38	1.46
1	K	134	ARG	CD-NE	-5.25	1.38	1.46
1	A	54	PRO	CA-CB	-5.25	1.46	1.53
2	E	-24	DA	C6-N6	-5.25	1.23	1.34
1	I	233	ARG	CD-NE	-5.25	1.38	1.46
1	K	444	ARG	CD-NE	-5.25	1.38	1.46
2	M	-24	DA	C6-N6	-5.24	1.23	1.34
5	H	21	DA	C6-N6	-5.24	1.23	1.34
5	P	21	DA	C6-N6	-5.24	1.23	1.34
1	K	303	LEU	N-CA	-5.24	1.41	1.46
1	I	54	PRO	CA-CB	-5.23	1.46	1.53
2	E	-26	DG	C2-N2	-5.22	1.24	1.34
1	I	362	ARG	CD-NE	-5.22	1.39	1.46
1	C	444	ARG	CD-NE	-5.22	1.39	1.46
1	K	165	GLY	N-CA	-5.22	1.37	1.45
1	C	268	ARG	CD-NE	-5.21	1.39	1.46
1	A	263	GLY	N-CA	-5.21	1.37	1.45
1	I	263	GLY	N-CA	-5.21	1.37	1.45
3	F	19	DC	C4-N4	-5.21	1.23	1.34
1	A	128	ARG	CD-NE	-5.20	1.39	1.46
1	A	83	GLY	N-CA	-5.20	1.37	1.45
1	I	83	GLY	N-CA	-5.20	1.37	1.45
1	A	98	ARG	CD-NE	-5.20	1.39	1.46
2	M	-26	DG	C2-N2	-5.19	1.24	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	151	ARG	CD-NE	-5.19	1.39	1.46
1	K	268	ARG	CD-NE	-5.19	1.39	1.46
5	H	8	DA	C6-N6	-5.18	1.23	1.34
1	K	233	ARG	CD-NE	-5.18	1.39	1.46
3	F	25	DA	C6-N6	-5.18	1.23	1.34
1	C	362	ARG	CD-NE	-5.18	1.39	1.46
1	K	362	ARG	CD-NE	-5.17	1.39	1.46
3	N	19	DC	C4-N4	-5.17	1.23	1.34
1	A	341	GLY	N-CA	-5.16	1.37	1.45
1	I	99	GLY	N-CA	-5.16	1.37	1.45
1	A	326	PRO	CA-CB	-5.16	1.46	1.53
4	O	-20	DC	C4-N4	-5.16	1.23	1.34
1	A	362	ARG	CD-NE	-5.15	1.39	1.46
1	I	98	ARG	CD-NE	-5.15	1.39	1.46
4	G	-16	DA	C6-N6	-5.15	1.23	1.34
1	I	268	ARG	CD-NE	-5.15	1.39	1.46
1	A	316	GLY	N-CA	-5.15	1.38	1.45
1	I	326	PRO	CA-CB	-5.14	1.46	1.53
3	N	8	DA	C6-N6	-5.14	1.23	1.34
4	O	-16	DA	C6-N6	-5.14	1.23	1.34
1	A	268	ARG	CD-NE	-5.14	1.39	1.46
1	C	130	PRO	CA-CB	-5.14	1.46	1.53
1	A	151	ARG	CD-NE	-5.14	1.39	1.46
1	A	175	GLY	N-CA	-5.13	1.38	1.45
2	M	-12	DA	C6-N6	-5.13	1.23	1.34
4	G	-20	DC	C4-N4	-5.13	1.23	1.34
4	O	-19	DA	C6-N6	-5.13	1.23	1.34
1	I	316	GLY	N-CA	-5.13	1.38	1.45
4	O	-7	DA	C6-N6	-5.12	1.24	1.34
1	C	326	PRO	CA-CB	-5.12	1.46	1.53
1	C	301	PRO	CA-CB	-5.12	1.47	1.53
4	G	-19	DA	C6-N6	-5.12	1.24	1.34
2	E	-12	DA	C6-N6	-5.12	1.24	1.34
1	A	269	PRO	CA-CB	-5.11	1.47	1.53
1	A	99	GLY	N-CA	-5.11	1.38	1.45
1	A	187	PRO	CA-CB	-5.11	1.47	1.53
1	A	334	ARG	CD-NE	-5.11	1.39	1.46
1	K	303	LEU	CA-CB	-5.11	1.47	1.53
1	C	64	GLY	N-CA	-5.10	1.38	1.45
3	N	25	DA	C6-N6	-5.10	1.24	1.34
4	G	-7	DA	C6-N6	-5.10	1.24	1.34
1	I	269	PRO	CA-CB	-5.10	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	18	DA	C6-N6	-5.09	1.24	1.34
1	I	175	GLY	N-CA	-5.09	1.38	1.45
5	P	8	DA	C6-N6	-5.09	1.24	1.34
5	P	18	DA	C6-N6	-5.09	1.24	1.34
1	K	301	PRO	CA-CB	-5.08	1.47	1.53
1	K	326	PRO	CA-CB	-5.08	1.46	1.53
1	C	165	GLY	N-CA	-5.08	1.38	1.45
1	K	64	GLY	N-CA	-5.07	1.38	1.45
5	H	12	DA	C6-N6	-5.07	1.24	1.34
5	P	14	DA	C6-N6	-5.07	1.24	1.34
1	A	179	ASN	CA-CB	-5.07	1.46	1.52
2	M	-4	DG	C2-N2	-5.06	1.24	1.34
5	P	12	DA	C6-N6	-5.06	1.24	1.34
5	H	14	DA	C6-N6	-5.06	1.24	1.34
1	I	341	GLY	N-CA	-5.05	1.37	1.45
4	G	-15	DA	C6-N6	-5.05	1.24	1.34
4	O	-15	DA	C6-N6	-5.05	1.24	1.34
5	P	17	DA	C6-N6	-5.05	1.24	1.34
2	E	-4	DG	C2-N2	-5.04	1.24	1.34
5	P	23	DA	C6-N6	-5.04	1.24	1.34
3	F	8	DA	C6-N6	-5.04	1.24	1.34
1	K	250	GLY	N-CA	-5.04	1.37	1.45
1	A	282	PRO	CA-CB	-5.04	1.46	1.53
1	I	179	ASN	CA-CB	-5.04	1.46	1.52
5	H	17	DA	C6-N6	-5.03	1.24	1.34
1	I	334	ARG	CD-NE	-5.02	1.39	1.46
4	O	-10	DA	C6-N6	-5.02	1.24	1.34
5	H	11	DG	C2-N2	-5.01	1.24	1.34
1	I	129	ASN	CG-ND2	-5.01	1.22	1.33
1	C	303	LEU	CA-CB	-5.00	1.47	1.53
5	P	11	DG	C2-N2	-5.00	1.24	1.34

All (1539) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	231	LYS	CA-C-N	9.10	133.01	120.63
1	I	231	LYS	C-N-CA	9.10	133.01	120.63
1	C	199	PHE	CA-CB-CG	8.66	122.46	113.80
1	K	199	PHE	CA-CB-CG	8.61	122.41	113.80
1	A	167	TRP	CA-C-N	8.55	132.22	123.16
1	A	167	TRP	C-N-CA	8.55	132.22	123.16
1	A	25	ASP	CA-CB-CG	8.46	121.06	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	LYS	CA-C-N	8.19	131.46	120.65
1	A	231	LYS	C-N-CA	8.19	131.46	120.65
1	I	25	ASP	CA-CB-CG	8.14	120.74	112.60
1	A	56	GLU	CA-C-N	7.87	133.58	122.72
1	A	56	GLU	C-N-CA	7.87	133.58	122.72
1	K	231	LYS	CA-C-N	7.87	131.14	120.44
1	K	231	LYS	C-N-CA	7.87	131.14	120.44
1	I	199	PHE	CA-CB-CG	7.75	121.55	113.80
1	I	56	GLU	CA-C-N	7.73	133.39	122.72
1	I	56	GLU	C-N-CA	7.73	133.39	122.72
1	A	199	PHE	CA-CB-CG	7.73	121.53	113.80
1	I	132	ASP	CA-CB-CG	7.62	120.22	112.60
1	I	428	PHE	CA-CB-CG	7.56	121.36	113.80
1	A	428	PHE	CA-CB-CG	7.53	121.33	113.80
1	C	467	ASP	CA-CB-CG	7.51	120.11	112.60
1	K	467	ASP	CA-CB-CG	7.46	120.06	112.60
1	A	132	ASP	CA-CB-CG	7.43	120.03	112.60
1	A	526	ILE	CA-C-N	7.41	131.19	122.89
1	A	526	ILE	C-N-CA	7.41	131.19	122.89
1	I	526	ILE	CA-C-N	7.36	131.13	122.89
1	I	526	ILE	C-N-CA	7.36	131.13	122.89
1	K	347	HIS	CA-CB-CG	7.24	121.04	113.80
1	C	347	HIS	CA-CB-CG	7.19	120.99	113.80
1	A	20	ARG	NE-CZ-NH2	7.18	125.67	119.20
1	I	344	SER	CA-C-N	7.13	131.42	122.43
1	I	344	SER	C-N-CA	7.13	131.42	122.43
1	A	344	SER	CA-C-N	7.13	131.41	122.43
1	A	344	SER	C-N-CA	7.13	131.41	122.43
1	K	180	LYS	CA-C-N	7.03	129.58	120.44
1	K	180	LYS	C-N-CA	7.03	129.58	120.44
1	I	282	PRO	CA-C-N	6.95	130.05	121.71
1	I	282	PRO	C-N-CA	6.95	130.05	121.71
1	A	282	PRO	CA-C-N	6.94	130.03	121.71
1	A	282	PRO	C-N-CA	6.94	130.03	121.71
1	A	426	PHE	CA-CB-CG	6.92	120.72	113.80
1	C	180	LYS	CA-C-N	6.92	129.43	120.44
1	C	180	LYS	C-N-CA	6.92	129.43	120.44
1	I	426	PHE	CA-CB-CG	6.89	120.69	113.80
1	C	402	ASN	CA-CB-CG	6.89	119.49	112.60
1	I	20	ARG	NE-CZ-NH2	6.89	125.40	119.20
1	K	402	ASN	CA-CB-CG	6.87	119.47	112.60
1	C	449	ASP	CA-CB-CG	6.84	119.44	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	273	GLN	CA-C-N	6.84	130.92	122.37
1	I	273	GLN	C-N-CA	6.84	130.92	122.37
1	I	95	ARG	NE-CZ-NH2	6.82	125.33	119.20
1	K	449	ASP	CA-CB-CG	6.81	119.41	112.60
1	C	45	ASN	CA-CB-CG	6.80	119.40	112.60
1	K	463	ASN	CA-CB-CG	6.80	119.40	112.60
1	A	273	GLN	CA-C-N	6.79	130.85	122.37
1	A	273	GLN	C-N-CA	6.79	130.85	122.37
1	C	388	HIS	CA-CB-CG	6.78	120.58	113.80
1	K	45	ASN	CA-CB-CG	6.78	119.38	112.60
1	K	388	HIS	CA-CB-CG	6.76	120.56	113.80
1	C	463	ASN	CA-CB-CG	6.74	119.34	112.60
1	K	429	ASP	CA-CB-CG	6.74	119.34	112.60
1	C	129	ASN	CA-CB-CG	6.74	119.34	112.60
1	C	429	ASP	CA-CB-CG	6.74	119.34	112.60
1	C	390	ASN	CA-CB-CG	6.71	119.31	112.60
1	I	129	ASN	CA-CB-CG	6.70	119.30	112.60
1	C	428	PHE	CA-CB-CG	6.70	120.50	113.80
1	K	390	ASN	CA-CB-CG	6.70	119.30	112.60
1	A	95	ARG	NE-CZ-NH2	6.69	125.22	119.20
1	C	231	LYS	CA-C-N	6.67	129.52	120.44
1	C	231	LYS	C-N-CA	6.67	129.52	120.44
1	K	498	ASN	CA-CB-CG	6.67	119.27	112.60
1	A	338	ASN	CA-CB-CG	6.66	119.26	112.60
1	K	103	ASP	CA-CB-CG	6.65	119.25	112.60
1	C	498	ASN	CA-CB-CG	6.63	119.23	112.60
1	I	347	HIS	CA-CB-CG	6.63	120.43	113.80
1	K	428	PHE	CA-CB-CG	6.63	120.43	113.80
1	I	338	ASN	CA-CB-CG	6.62	119.22	112.60
1	I	147	PHE	CA-CB-CG	6.62	120.42	113.80
1	A	147	PHE	CA-CB-CG	6.61	120.41	113.80
1	A	347	HIS	CA-CB-CG	6.61	120.41	113.80
1	K	129	ASN	CA-CB-CG	6.59	119.19	112.60
1	C	266	THR	CA-C-N	6.58	130.72	122.43
1	C	266	THR	C-N-CA	6.58	130.72	122.43
1	C	103	ASP	CA-CB-CG	6.56	119.16	112.60
1	I	438	ASP	CA-CB-CG	6.56	119.16	112.60
1	I	412	HIS	CA-CB-CG	6.55	120.36	113.80
1	K	35	ASP	CA-CB-CG	6.52	119.12	112.60
1	I	45	ASN	CA-CB-CG	6.52	119.12	112.60
1	A	412	HIS	CA-CB-CG	6.52	120.32	113.80
1	C	35	ASP	CA-CB-CG	6.51	119.11	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	179	ASN	CA-CB-CG	6.50	119.10	112.60
1	A	45	ASN	CA-CB-CG	6.49	119.09	112.60
1	K	509	ILE	CA-C-N	6.49	131.23	123.19
1	K	509	ILE	C-N-CA	6.49	131.23	123.19
1	K	266	THR	CA-C-N	6.48	130.59	122.43
1	K	266	THR	C-N-CA	6.48	130.59	122.43
1	A	179	ASN	CA-CB-CG	6.48	119.08	112.60
1	A	438	ASP	CA-CB-CG	6.47	119.08	112.60
1	C	509	ILE	CA-C-N	6.46	131.21	123.19
1	C	509	ILE	C-N-CA	6.46	131.21	123.19
1	A	129	ASN	CA-CB-CG	6.45	119.05	112.60
1	C	412	HIS	CA-CB-CG	6.45	120.25	113.80
1	A	68	ASP	CA-CB-CG	6.44	119.04	112.60
1	I	480	ASN	CA-CB-CG	6.43	119.03	112.60
1	A	449	ASP	CA-CB-CG	6.43	119.03	112.60
1	K	412	HIS	CA-CB-CG	6.43	120.23	113.80
1	I	449	ASP	CA-CB-CG	6.42	119.02	112.60
1	K	368	ASN	CA-CB-CG	6.41	119.01	112.60
1	C	425	ASN	CA-C-N	6.41	128.77	120.44
1	C	425	ASN	C-N-CA	6.41	128.77	120.44
1	I	340	ASP	CA-CB-CG	6.41	119.01	112.60
1	A	422	ASN	CA-CB-CG	6.40	119.00	112.60
1	I	422	ASN	CA-CB-CG	6.40	119.00	112.60
1	K	425	ASN	CA-C-N	6.40	128.76	120.44
1	K	425	ASN	C-N-CA	6.40	128.76	120.44
1	K	526	ILE	CA-C-N	6.40	130.89	123.15
1	K	526	ILE	C-N-CA	6.40	130.89	123.15
1	I	68	ASP	CA-CB-CG	6.39	119.00	112.60
1	A	480	ASN	CA-CB-CG	6.39	118.99	112.60
1	C	368	ASN	CA-CB-CG	6.39	118.99	112.60
1	A	73	PHE	CA-CB-CG	6.39	120.19	113.80
1	C	365	ASP	CA-CB-CG	6.38	118.98	112.60
1	C	526	ILE	CA-C-N	6.36	130.85	123.15
1	C	526	ILE	C-N-CA	6.36	130.85	123.15
1	A	187	PRO	CA-C-N	6.36	131.04	122.90
1	A	187	PRO	C-N-CA	6.36	131.04	122.90
1	I	14	ASN	CA-C-N	6.36	131.25	122.93
1	I	14	ASN	C-N-CA	6.36	131.25	122.93
1	K	245	ASN	CA-CB-CG	6.35	118.95	112.60
1	I	388	HIS	CA-CB-CG	6.35	120.15	113.80
1	I	73	PHE	CA-CB-CG	6.34	120.14	113.80
1	A	534	PHE	CA-CB-CG	6.34	120.14	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	ASP	CA-CB-CG	6.34	118.94	112.60
1	I	187	PRO	CA-C-N	6.34	131.01	122.90
1	I	187	PRO	C-N-CA	6.34	131.01	122.90
1	A	151	ARG	CD-NE-CZ	6.33	133.26	124.40
1	K	365	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	289	PHE	CA-CB-CG	6.33	120.12	113.80
1	A	14	ASN	CA-C-N	6.32	131.21	122.93
1	A	14	ASN	C-N-CA	6.32	131.21	122.93
1	K	210	ASP	CA-CB-CG	6.32	118.92	112.60
1	C	245	ASN	CA-CB-CG	6.30	118.91	112.60
1	A	342	THR	CA-C-N	6.30	131.03	122.84
1	A	342	THR	C-N-CA	6.30	131.03	122.84
1	A	388	HIS	CA-CB-CG	6.30	120.10	113.80
1	C	426	PHE	CA-CB-CG	6.30	120.10	113.80
1	C	251	THR	CA-C-N	6.29	130.99	123.19
1	C	251	THR	C-N-CA	6.29	130.99	123.19
1	C	511	ASN	CA-CB-CG	6.29	118.89	112.60
1	I	151	ARG	CD-NE-CZ	6.29	133.20	124.40
1	I	534	PHE	CA-CB-CG	6.29	120.09	113.80
1	K	251	THR	CA-C-N	6.29	130.99	123.19
1	K	251	THR	C-N-CA	6.29	130.99	123.19
1	K	426	PHE	CA-CB-CG	6.29	120.09	113.80
1	I	342	THR	CA-C-N	6.28	131.01	122.84
1	I	342	THR	C-N-CA	6.28	131.01	122.84
1	K	187	PRO	CA-C-N	6.28	130.93	122.90
1	K	187	PRO	C-N-CA	6.28	130.93	122.90
1	K	511	ASN	CA-CB-CG	6.27	118.87	112.60
1	K	190	ASP	CA-CB-CG	6.26	118.86	112.60
1	C	210	ASP	CA-CB-CG	6.26	118.86	112.60
1	C	166	LYS	CA-C-N	6.26	131.09	122.77
1	C	166	LYS	C-N-CA	6.26	131.09	122.77
1	C	190	ASP	CA-CB-CG	6.25	118.85	112.60
1	C	187	PRO	CA-C-N	6.24	130.89	122.90
1	C	187	PRO	C-N-CA	6.24	130.89	122.90
1	K	507	ASP	CA-CB-CG	6.24	118.84	112.60
1	K	289	PHE	CA-CB-CG	6.23	120.03	113.80
1	C	399	ASP	CA-CB-CG	6.23	118.83	112.60
1	I	289	PHE	CA-CB-CG	6.22	120.02	113.80
1	C	533	ASN	CA-CB-CG	6.22	118.82	112.60
1	C	507	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	144	ARG	CD-NE-CZ	6.21	133.09	124.40
1	A	356	ASN	CA-CB-CG	6.21	118.81	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	56	GLU	CA-C-N	6.21	131.34	121.66
1	C	56	GLU	C-N-CA	6.21	131.34	121.66
1	K	399	ASP	CA-CB-CG	6.21	118.81	112.60
1	K	166	LYS	CA-C-N	6.21	131.02	122.77
1	K	166	LYS	C-N-CA	6.21	131.02	122.77
1	C	289	PHE	CA-CB-CG	6.20	120.00	113.80
1	I	356	ASN	CA-CB-CG	6.20	118.80	112.60
1	I	511	ASN	CA-CB-CG	6.20	118.80	112.60
1	I	502	ARG	CA-C-N	6.19	128.86	120.38
1	I	502	ARG	C-N-CA	6.19	128.86	120.38
1	C	117	ILE	CA-C-N	6.19	130.10	122.37
1	C	117	ILE	C-N-CA	6.19	130.10	122.37
1	I	507	ASP	CA-CB-CG	6.19	118.79	112.60
1	C	14	ASN	CA-C-N	6.18	130.22	122.43
1	C	14	ASN	C-N-CA	6.18	130.22	122.43
1	C	42	GLU	CA-C-N	6.18	128.48	120.44
1	C	42	GLU	C-N-CA	6.18	128.48	120.44
1	A	507	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	511	ASN	CA-CB-CG	6.18	118.78	112.60
1	C	307	ASP	CA-CB-CG	6.18	118.78	112.60
1	I	190	ASP	CA-CB-CG	6.18	118.78	112.60
1	K	117	ILE	CA-C-N	6.18	130.09	122.37
1	K	117	ILE	C-N-CA	6.18	130.09	122.37
1	A	502	ARG	CA-C-N	6.17	128.84	120.38
1	A	502	ARG	C-N-CA	6.17	128.84	120.38
1	K	533	ASN	CA-CB-CG	6.17	118.77	112.60
1	I	144	ARG	CD-NE-CZ	6.17	133.04	124.40
1	I	14	ASN	CA-CB-CG	6.17	118.77	112.60
1	C	504	VAL	CA-C-N	6.16	130.62	122.42
1	C	504	VAL	C-N-CA	6.16	130.62	122.42
1	I	167	TRP	CA-C-N	6.16	129.69	123.16
1	I	167	TRP	C-N-CA	6.16	129.69	123.16
1	I	378	ASN	CA-CB-CG	6.16	118.76	112.60
1	K	14	ASN	CA-C-N	6.16	130.19	122.43
1	K	14	ASN	C-N-CA	6.16	130.19	122.43
1	A	378	ASN	CA-CB-CG	6.16	118.75	112.60
1	A	190	ASP	CA-CB-CG	6.15	118.75	112.60
1	I	125	TYR	CA-C-N	6.15	133.42	122.35
1	I	125	TYR	C-N-CA	6.15	133.42	122.35
1	K	42	GLU	CA-C-N	6.15	128.44	120.44
1	K	42	GLU	C-N-CA	6.15	128.44	120.44
1	A	14	ASN	CA-CB-CG	6.14	118.74	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	431	TYR	N-CA-CB	6.14	118.92	110.01
1	A	365	ASP	CA-CB-CG	6.13	118.73	112.60
1	C	116	LEU	CA-C-N	6.13	130.65	122.93
1	C	116	LEU	C-N-CA	6.13	130.65	122.93
1	C	431	TYR	N-CA-CB	6.13	118.90	110.01
1	K	504	VAL	CA-C-N	6.13	130.57	122.42
1	K	504	VAL	C-N-CA	6.13	130.57	122.42
1	A	489	HIS	CA-CB-CG	6.12	119.92	113.80
1	I	418	LYS	CA-CB-CG	6.12	126.34	114.10
1	C	109	ASN	CA-CB-CG	6.12	118.72	112.60
1	I	489	HIS	CA-CB-CG	6.10	119.90	113.80
1	I	426	PHE	CA-C-N	6.10	128.24	120.56
1	I	426	PHE	C-N-CA	6.10	128.24	120.56
1	A	115	ARG	CD-NE-CZ	6.10	132.93	124.40
1	K	307	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	79	ASP	CA-CB-CG	6.09	118.69	112.60
1	K	134	ARG	CD-NE-CZ	6.09	132.93	124.40
1	I	365	ASP	CA-CB-CG	6.08	118.68	112.60
1	K	116	LEU	CA-C-N	6.08	130.59	122.93
1	K	116	LEU	C-N-CA	6.08	130.59	122.93
1	K	273	GLN	CA-C-N	6.08	130.05	121.66
1	K	273	GLN	C-N-CA	6.08	130.05	121.66
1	A	426	PHE	CA-C-N	6.07	128.21	120.56
1	A	426	PHE	C-N-CA	6.07	128.21	120.56
1	A	418	LYS	CA-CB-CG	6.07	126.24	114.10
1	C	425	ASN	CA-CB-CG	6.07	118.67	112.60
1	C	273	GLN	CA-C-N	6.06	130.03	121.66
1	C	273	GLN	C-N-CA	6.06	130.03	121.66
1	C	264	LYS	CA-C-N	6.06	130.48	122.30
1	C	264	LYS	C-N-CA	6.06	130.48	122.30
1	K	264	LYS	CA-C-N	6.06	130.48	122.30
1	K	264	LYS	C-N-CA	6.06	130.48	122.30
1	I	134	ARG	CD-NE-CZ	6.05	132.87	124.40
1	K	425	ASN	CA-CB-CG	6.05	118.65	112.60
3	F	5	DT	O5'-C5'-C4'	6.05	119.87	110.80
1	I	115	ARG	CD-NE-CZ	6.05	132.87	124.40
1	I	109	ASN	CA-CB-CG	6.05	118.65	112.60
1	K	262	ASP	CA-CB-CG	6.04	118.64	112.60
1	C	398	ASP	CA-CB-CG	6.04	118.64	112.60
1	C	262	ASP	CA-CB-CG	6.04	118.64	112.60
1	K	398	ASP	CA-CB-CG	6.04	118.64	112.60
1	C	202	PHE	CA-C-N	6.03	128.84	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	202	PHE	C-N-CA	6.03	128.84	120.63
1	A	5	ASN	CA-CB-CG	6.03	118.63	112.60
1	I	79	ASP	CA-CB-CG	6.03	118.63	112.60
1	I	444	ARG	CD-NE-CZ	6.03	132.84	124.40
1	A	125	TYR	CA-C-N	6.03	133.20	122.35
1	A	125	TYR	C-N-CA	6.03	133.20	122.35
1	C	202	PHE	CA-CB-CG	6.03	119.83	113.80
1	A	109	ASN	CA-CB-CG	6.02	118.62	112.60
1	I	5	ASN	CA-CB-CG	6.02	118.62	112.60
1	K	25	ASP	CA-CB-CG	6.02	118.62	112.60
1	A	533	ASN	CA-CB-CG	6.02	118.62	112.60
1	I	533	ASN	CA-CB-CG	6.01	118.61	112.60
1	K	109	ASN	CA-CB-CG	6.01	118.61	112.60
1	K	362	ARG	CD-NE-CZ	6.01	132.82	124.40
1	K	141	PHE	CA-CB-CG	6.01	119.81	113.80
1	C	532	PHE	CA-CB-CG	6.00	119.81	113.80
1	A	444	ARG	CD-NE-CZ	6.00	132.81	124.40
1	A	480	ASN	CA-C-N	6.00	128.12	120.56
1	A	480	ASN	C-N-CA	6.00	128.12	120.56
1	C	362	ARG	CD-NE-CZ	6.00	132.79	124.40
1	I	128	ARG	CD-NE-CZ	5.99	132.78	124.40
1	I	480	ASN	CA-C-N	5.99	128.10	120.56
1	I	480	ASN	C-N-CA	5.99	128.10	120.56
3	N	5	DT	O5'-C5'-C4'	5.98	119.78	110.80
1	K	40	GLN	CA-C-N	5.98	128.22	120.44
1	K	40	GLN	C-N-CA	5.98	128.22	120.44
1	K	350	SER	CA-C-N	5.97	130.72	122.77
1	K	350	SER	C-N-CA	5.97	130.72	122.77
1	K	532	PHE	CA-CB-CG	5.97	119.77	113.80
1	A	431	TYR	N-CA-CB	5.97	118.89	110.12
1	I	61	ILE	CA-C-N	5.97	128.18	122.27
1	I	61	ILE	C-N-CA	5.97	128.18	122.27
1	A	61	ILE	CA-C-N	5.96	128.18	122.27
1	A	61	ILE	C-N-CA	5.96	128.18	122.27
1	C	40	GLN	CA-C-N	5.96	128.19	120.44
1	C	40	GLN	C-N-CA	5.96	128.19	120.44
1	K	202	PHE	CA-C-N	5.96	128.74	120.63
1	K	202	PHE	C-N-CA	5.96	128.74	120.63
1	C	141	PHE	CA-CB-CG	5.96	119.76	113.80
1	I	431	TYR	N-CA-CB	5.96	118.88	110.12
1	C	225	ILE	N-CA-CB	5.96	116.78	110.17
1	K	340	ASP	CA-CB-CG	5.96	118.56	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	ASN	CA-CB-CG	5.96	118.56	112.60
1	I	98	ARG	CD-NE-CZ	5.95	132.73	124.40
1	K	364	ASN	CA-CB-CG	5.95	118.55	112.60
1	C	340	ASP	CA-CB-CG	5.95	118.55	112.60
1	K	202	PHE	CA-CB-CG	5.95	119.75	113.80
1	A	334	ARG	CD-NE-CZ	5.95	132.72	124.40
1	C	364	ASN	CA-CB-CG	5.94	118.54	112.60
1	A	186	ASP	CA-CB-CG	5.94	118.54	112.60
1	A	285	ASP	CA-CB-CG	5.94	118.54	112.60
1	A	98	ARG	CD-NE-CZ	5.94	132.72	124.40
1	I	482	ASN	CA-CB-CG	5.93	118.53	112.60
1	A	128	ARG	CD-NE-CZ	5.93	132.71	124.40
1	I	11	ASN	CA-CB-CG	5.93	118.53	112.60
1	I	498	ASN	CA-CB-CG	5.92	118.53	112.60
1	I	40	GLN	CA-C-N	5.92	128.13	120.44
1	I	40	GLN	C-N-CA	5.92	128.13	120.44
1	I	186	ASP	CA-CB-CG	5.92	118.52	112.60
1	K	233	ARG	CD-NE-CZ	5.92	132.68	124.40
1	K	79	ASP	CA-CB-CG	5.91	118.51	112.60
1	C	233	ARG	CD-NE-CZ	5.91	132.67	124.40
1	A	482	ASN	CA-CB-CG	5.89	118.49	112.60
1	I	285	ASP	CA-CB-CG	5.89	118.49	112.60
1	A	103	ASP	CA-CB-CG	5.89	118.49	112.60
1	C	309	PHE	CA-CB-CG	5.89	119.69	113.80
1	I	425	ASN	CA-CB-CG	5.89	118.49	112.60
1	A	268	ARG	CD-NE-CZ	5.88	132.63	124.40
1	C	222	ASN	CA-CB-CG	5.88	118.48	112.60
1	I	262	ASP	CA-CB-CG	5.88	118.47	112.60
1	A	11	ASN	CA-CB-CG	5.87	118.47	112.60
1	K	512	MET	CA-C-N	5.87	128.62	120.29
1	K	512	MET	C-N-CA	5.87	128.62	120.29
1	A	368	ASN	CA-CB-CG	5.86	118.46	112.60
1	C	510	VAL	CA-C-N	5.86	131.26	123.00
1	C	510	VAL	C-N-CA	5.86	131.26	123.00
1	A	477	VAL	CA-C-N	5.85	128.05	120.44
1	A	477	VAL	C-N-CA	5.85	128.05	120.44
1	A	97	SER	CA-C-N	5.85	130.75	121.44
1	A	97	SER	C-N-CA	5.85	130.75	121.44
1	K	87	ALA	CA-C-N	5.85	131.12	122.99
1	K	87	ALA	C-N-CA	5.85	131.12	122.99
1	K	161	TYR	CA-C-N	5.85	128.05	120.44
1	K	161	TYR	C-N-CA	5.85	128.05	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	498	ASN	CA-CB-CG	5.85	118.45	112.60
1	C	512	MET	CA-C-N	5.85	128.60	120.29
1	C	512	MET	C-N-CA	5.85	128.60	120.29
1	I	334	ARG	CD-NE-CZ	5.85	132.59	124.40
1	C	507	ASP	CA-C-N	5.85	130.96	123.13
1	C	507	ASP	C-N-CA	5.85	130.96	123.13
1	I	103	ASP	CA-CB-CG	5.85	118.45	112.60
1	C	79	ASP	CA-CB-CG	5.84	118.44	112.60
1	K	510	VAL	CA-C-N	5.84	131.24	123.00
1	K	510	VAL	C-N-CA	5.84	131.24	123.00
1	I	477	VAL	CA-C-N	5.84	128.04	120.44
1	I	477	VAL	C-N-CA	5.84	128.04	120.44
1	I	368	ASN	CA-CB-CG	5.84	118.44	112.60
1	A	40	GLN	CA-C-N	5.83	128.10	120.28
1	A	40	GLN	C-N-CA	5.83	128.10	120.28
1	C	87	ALA	CA-C-N	5.83	131.10	122.99
1	C	87	ALA	C-N-CA	5.83	131.10	122.99
1	K	275	VAL	CA-C-N	5.83	130.64	123.17
1	K	275	VAL	C-N-CA	5.83	130.64	123.17
1	K	222	ASN	CA-CB-CG	5.83	118.43	112.60
1	I	97	SER	CA-C-N	5.83	130.71	121.44
1	I	97	SER	C-N-CA	5.83	130.71	121.44
1	I	268	ARG	CD-NE-CZ	5.83	132.56	124.40
1	C	14	ASN	CA-CB-CG	5.83	118.43	112.60
1	C	275	VAL	CA-C-N	5.82	130.62	123.17
1	C	275	VAL	C-N-CA	5.82	130.62	123.17
1	C	138	PHE	CA-CB-CG	5.82	119.61	113.80
1	I	336	ARG	NE-CZ-NH2	5.82	124.43	119.20
1	I	362	ARG	N-CA-CB	5.81	118.49	109.48
1	K	507	ASP	CA-C-N	5.81	130.92	123.13
1	K	507	ASP	C-N-CA	5.81	130.92	123.13
1	A	443	LYS	CA-C-N	5.81	127.99	120.44
1	A	443	LYS	C-N-CA	5.81	127.99	120.44
1	K	271	LYS	CA-C-N	5.81	127.99	120.44
1	K	271	LYS	C-N-CA	5.81	127.99	120.44
1	I	443	LYS	CA-C-N	5.81	127.99	120.44
1	I	443	LYS	C-N-CA	5.81	127.99	120.44
1	I	364	ASN	CA-CB-CG	5.79	118.39	112.60
1	A	80	LEU	CA-C-N	5.79	127.96	120.44
1	A	80	LEU	C-N-CA	5.79	127.96	120.44
1	C	250	GLY	CA-C-N	5.79	129.77	121.50
1	C	250	GLY	C-N-CA	5.79	129.77	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	271	LYS	CA-C-N	5.79	127.96	120.44
1	C	271	LYS	C-N-CA	5.79	127.96	120.44
1	K	250	GLY	CA-C-N	5.78	129.77	121.50
1	K	250	GLY	C-N-CA	5.78	129.77	121.50
1	A	362	ARG	N-CA-CB	5.78	118.44	109.48
1	C	106	GLN	CA-C-N	5.78	127.84	120.56
1	C	106	GLN	C-N-CA	5.78	127.84	120.56
1	A	138	PHE	CA-CB-CG	-5.78	108.03	113.80
1	K	309	PHE	CA-CB-CG	5.77	119.57	113.80
1	A	262	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	484	ILE	CA-C-N	5.77	127.83	120.56
1	A	484	ILE	C-N-CA	5.77	127.83	120.56
1	I	106	GLN	CA-C-N	5.77	127.83	120.56
1	I	106	GLN	C-N-CA	5.77	127.83	120.56
1	A	362	ARG	CD-NE-CZ	5.77	132.48	124.40
1	I	350	SER	CA-C-N	5.77	130.08	121.72
1	I	350	SER	C-N-CA	5.77	130.08	121.72
1	A	106	GLN	CA-C-N	5.76	127.82	120.56
1	A	106	GLN	C-N-CA	5.76	127.82	120.56
1	C	336	ARG	NE-CZ-NH2	5.76	124.38	119.20
1	I	362	ARG	CD-NE-CZ	5.76	132.46	124.40
1	I	528	PRO	CA-C-N	5.76	130.99	122.99
1	I	528	PRO	C-N-CA	5.76	130.99	122.99
1	A	8	ASN	CA-CB-CG	5.75	118.36	112.60
2	E	-23	DG	C5'-C4'-C3'	5.75	123.53	114.90
1	A	364	ASN	CA-CB-CG	5.75	118.35	112.60
3	N	16	DA	C2'-C3'-O3'	5.75	120.12	111.50
1	A	531	ARG	CA-C-N	5.75	127.98	120.28
1	A	531	ARG	C-N-CA	5.75	127.98	120.28
1	A	283	ILE	CA-C-N	5.74	130.92	122.94
1	A	283	ILE	C-N-CA	5.74	130.92	122.94
2	M	-23	DG	C5'-C4'-C3'	5.74	123.52	114.90
1	C	531	ARG	CD-NE-CZ	5.74	132.44	124.40
1	I	126	ASP	CA-CB-CG	5.74	118.34	112.60
1	I	283	ILE	CA-C-N	5.74	130.92	122.94
1	I	283	ILE	C-N-CA	5.74	130.92	122.94
1	I	80	LEU	CA-C-N	5.74	127.90	120.44
1	I	80	LEU	C-N-CA	5.74	127.90	120.44
1	I	484	ILE	CA-C-N	5.74	127.79	120.56
1	I	484	ILE	C-N-CA	5.74	127.79	120.56
1	I	8	ASN	CA-CB-CG	5.73	118.33	112.60
1	K	14	ASN	CA-CB-CG	5.73	118.33	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	89	ALA	CA-C-N	5.73	130.49	122.23
1	K	89	ALA	C-N-CA	5.73	130.49	122.23
1	K	106	GLN	CA-C-N	5.73	127.78	120.56
1	K	106	GLN	C-N-CA	5.73	127.78	120.56
1	C	326	PRO	CA-C-N	5.73	130.04	122.42
1	C	326	PRO	C-N-CA	5.73	130.04	122.42
1	K	326	PRO	CA-C-N	5.73	130.04	122.42
1	K	326	PRO	C-N-CA	5.73	130.04	122.42
1	I	531	ARG	CA-C-N	5.72	127.95	120.28
1	I	531	ARG	C-N-CA	5.72	127.95	120.28
1	I	360	TYR	CA-C-N	5.72	129.04	120.69
1	I	360	TYR	C-N-CA	5.72	129.04	120.69
1	A	350	SER	CA-C-N	5.72	130.01	121.72
1	A	350	SER	C-N-CA	5.72	130.01	121.72
3	F	16	DA	C2'-C3'-O3'	5.71	120.07	111.50
1	K	415	GLN	CA-C-N	5.71	127.87	120.44
1	K	415	GLN	C-N-CA	5.71	127.87	120.44
1	K	103	ASP	CA-C-N	5.71	127.86	120.44
1	K	103	ASP	C-N-CA	5.71	127.86	120.44
1	A	360	TYR	CA-C-N	5.71	129.03	120.69
1	A	360	TYR	C-N-CA	5.71	129.03	120.69
1	I	271	LYS	CA-C-N	5.71	128.39	120.29
1	I	271	LYS	C-N-CA	5.71	128.39	120.29
1	C	415	GLN	CA-C-N	5.71	127.86	120.44
1	C	415	GLN	C-N-CA	5.71	127.86	120.44
1	K	531	ARG	CD-NE-CZ	5.70	132.38	124.40
1	A	271	LYS	CA-C-N	5.70	128.38	120.29
1	A	271	LYS	C-N-CA	5.70	128.38	120.29
1	A	528	PRO	CA-C-N	5.70	130.91	122.99
1	A	528	PRO	C-N-CA	5.70	130.91	122.99
1	C	35	ASP	CA-C-N	5.70	127.84	120.44
1	C	35	ASP	C-N-CA	5.70	127.84	120.44
1	C	103	ASP	CA-C-N	5.69	127.83	120.44
1	C	103	ASP	C-N-CA	5.69	127.83	120.44
1	K	35	ASP	CA-C-N	5.68	127.83	120.44
1	K	35	ASP	C-N-CA	5.68	127.83	120.44
1	A	141	PHE	N-CA-CB	5.68	118.25	110.01
1	C	196	GLN	CA-C-N	5.68	127.82	120.44
1	C	196	GLN	C-N-CA	5.68	127.82	120.44
1	I	345	VAL	CA-C-N	5.68	130.75	122.85
1	I	345	VAL	C-N-CA	5.68	130.75	122.85
1	A	362	ARG	CA-C-N	5.67	127.82	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	ARG	C-N-CA	5.67	127.82	120.44
1	A	327	LEU	CA-C-N	5.67	130.55	122.72
1	A	327	LEU	C-N-CA	5.67	130.55	122.72
1	K	196	GLN	CA-C-N	5.67	127.81	120.44
1	K	196	GLN	C-N-CA	5.67	127.81	120.44
1	K	68	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	345	VAL	CA-C-N	5.67	130.73	122.85
1	A	345	VAL	C-N-CA	5.67	130.73	122.85
1	C	89	ALA	CA-C-N	5.67	130.39	122.23
1	C	89	ALA	C-N-CA	5.67	130.39	122.23
1	C	426	PHE	CA-C-N	5.67	127.70	120.56
1	C	426	PHE	C-N-CA	5.67	127.70	120.56
1	K	255	LYS	CA-C-N	5.66	129.42	120.47
1	K	255	LYS	C-N-CA	5.66	129.42	120.47
1	K	242	ILE	N-CA-CB	5.66	116.79	110.51
1	I	138	PHE	N-CA-CB	5.66	118.21	110.01
1	K	197	LEU	CA-C-N	5.65	127.68	120.56
1	K	197	LEU	C-N-CA	5.65	127.68	120.56
1	A	90	VAL	CA-C-N	5.65	127.79	120.44
1	A	90	VAL	C-N-CA	5.65	127.79	120.44
1	C	197	LEU	CA-C-N	5.65	127.68	120.56
1	C	197	LEU	C-N-CA	5.65	127.68	120.56
1	I	327	LEU	CA-C-N	5.65	130.52	122.72
1	I	327	LEU	C-N-CA	5.65	130.52	122.72
1	C	75	GLU	CA-C-N	5.65	127.78	120.44
1	C	75	GLU	C-N-CA	5.65	127.78	120.44
1	I	362	ARG	CA-C-N	5.65	127.78	120.44
1	I	362	ARG	C-N-CA	5.65	127.78	120.44
1	K	352	THR	CA-C-N	5.64	130.62	122.16
1	K	352	THR	C-N-CA	5.64	130.62	122.16
1	C	213	TYR	CA-C-N	5.64	127.77	120.44
1	C	213	TYR	C-N-CA	5.64	127.77	120.44
1	I	524	PHE	CA-C-N	5.64	131.60	122.29
1	I	524	PHE	C-N-CA	5.64	131.60	122.29
1	A	524	PHE	CA-C-N	5.64	131.59	122.29
1	A	524	PHE	C-N-CA	5.64	131.59	122.29
1	A	488	TYR	CA-C-N	5.64	127.77	120.44
1	A	488	TYR	C-N-CA	5.64	127.77	120.44
1	C	296	ILE	N-CA-CB	5.63	116.77	110.51
1	C	528	PRO	CA-C-N	5.63	130.88	123.11
1	C	528	PRO	C-N-CA	5.63	130.88	123.11
1	I	238	THR	CA-C-N	5.63	127.66	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	238	THR	C-N-CA	5.63	127.66	120.56
1	A	232	LYS	CA-C-N	5.63	128.76	120.82
1	A	232	LYS	C-N-CA	5.63	128.76	120.82
1	A	238	THR	CA-C-N	5.63	127.66	120.56
1	A	238	THR	C-N-CA	5.63	127.66	120.56
1	I	295	LYS	CA-C-N	5.63	127.66	120.56
1	I	295	LYS	C-N-CA	5.63	127.66	120.56
1	K	426	PHE	CA-C-N	5.63	127.66	120.56
1	K	426	PHE	C-N-CA	5.63	127.66	120.56
1	K	75	GLU	CA-C-N	5.63	127.76	120.44
1	K	75	GLU	C-N-CA	5.63	127.76	120.44
1	K	62	GLY	CA-C-N	5.63	129.60	120.60
1	K	62	GLY	C-N-CA	5.63	129.60	120.60
1	K	219	HIS	N-CA-CB	5.62	118.12	109.91
1	K	296	ILE	N-CA-CB	5.62	116.75	110.51
1	K	336	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	I	251	THR	CA-C-N	5.62	130.09	122.90
1	I	251	THR	C-N-CA	5.62	130.09	122.90
1	K	274	ILE	CA-C-N	5.62	130.50	123.14
1	K	274	ILE	C-N-CA	5.62	130.50	123.14
1	C	487	GLN	CA-C-N	5.62	127.75	120.44
1	C	487	GLN	C-N-CA	5.62	127.75	120.44
1	A	295	LYS	CA-C-N	5.62	127.64	120.56
1	A	295	LYS	C-N-CA	5.62	127.64	120.56
1	A	336	ARG	NE-CZ-NH2	5.62	124.25	119.20
1	K	200	ASN	CA-C-N	5.61	127.63	120.56
1	K	200	ASN	C-N-CA	5.61	127.63	120.56
1	K	213	TYR	CA-C-N	5.61	127.74	120.44
1	K	213	TYR	C-N-CA	5.61	127.74	120.44
1	C	219	HIS	N-CA-CB	5.61	118.10	109.91
1	C	352	THR	CA-C-N	5.61	130.57	122.16
1	C	352	THR	C-N-CA	5.61	130.57	122.16
1	K	149	MET	CA-C-N	5.61	127.73	120.44
1	K	149	MET	C-N-CA	5.61	127.73	120.44
1	A	429	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	126	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	242	ILE	CA-C-N	5.61	127.79	120.28
1	A	242	ILE	C-N-CA	5.61	127.79	120.28
1	C	274	ILE	CA-C-N	5.61	130.49	123.14
1	C	274	ILE	C-N-CA	5.61	130.49	123.14
1	I	46	LYS	CA-C-N	5.61	127.71	120.70
1	I	46	LYS	C-N-CA	5.61	127.71	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	ARG	CA-C-N	5.61	130.89	122.99
1	A	265	ARG	C-N-CA	5.61	130.89	122.99
1	I	90	VAL	CA-C-N	5.61	127.73	120.44
1	I	90	VAL	C-N-CA	5.61	127.73	120.44
1	K	487	GLN	CA-C-N	5.61	127.73	120.44
1	K	487	GLN	C-N-CA	5.61	127.73	120.44
1	A	251	THR	CA-C-N	5.60	130.07	122.90
1	A	251	THR	C-N-CA	5.60	130.07	122.90
1	K	528	PRO	CA-C-N	5.60	130.84	123.11
1	K	528	PRO	C-N-CA	5.60	130.84	123.11
1	A	533	ASN	CA-C-N	5.60	127.78	120.28
1	A	533	ASN	C-N-CA	5.60	127.78	120.28
1	A	250	GLY	CA-C-N	5.59	128.78	120.95
1	A	250	GLY	C-N-CA	5.59	128.78	120.95
1	I	278	ASP	CA-CB-CG	5.59	118.19	112.60
1	I	232	LYS	CA-C-N	5.59	128.70	120.82
1	I	232	LYS	C-N-CA	5.59	128.70	120.82
1	I	352	THR	CA-C-N	5.59	130.32	122.05
1	I	352	THR	C-N-CA	5.59	130.32	122.05
1	K	139	GLU	CA-C-N	5.59	127.70	120.44
1	K	139	GLU	C-N-CA	5.59	127.70	120.44
1	A	258	GLU	N-CA-CB	5.58	118.23	109.69
1	I	250	GLY	CA-C-N	5.58	128.77	120.95
1	I	250	GLY	C-N-CA	5.58	128.77	120.95
1	A	46	LYS	CA-C-N	5.58	127.68	120.70
1	A	46	LYS	C-N-CA	5.58	127.68	120.70
1	I	242	ILE	CA-C-N	5.58	127.76	120.28
1	I	242	ILE	C-N-CA	5.58	127.76	120.28
1	A	373	TYR	N-CA-CB	5.57	118.09	110.01
1	I	309	PHE	CA-C-N	5.57	130.05	122.19
1	I	309	PHE	C-N-CA	5.57	130.05	122.19
1	K	76	CYS	CA-C-N	5.57	127.68	120.44
1	K	76	CYS	C-N-CA	5.57	127.68	120.44
1	I	479	ASN	CA-CB-CG	5.57	118.17	112.60
1	A	197	LEU	CA-C-N	5.57	127.57	120.56
1	A	197	LEU	C-N-CA	5.57	127.57	120.56
1	C	88	ILE	CA-C-N	5.57	130.68	123.00
1	C	88	ILE	C-N-CA	5.57	130.68	123.00
1	C	327	LEU	CA-C-N	5.57	130.94	122.65
1	C	327	LEU	C-N-CA	5.57	130.94	122.65
1	A	309	PHE	CA-C-N	5.56	130.03	122.19
1	A	309	PHE	C-N-CA	5.56	130.03	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	265	ARG	CA-C-N	5.56	130.83	122.99
1	I	265	ARG	C-N-CA	5.56	130.83	122.99
1	K	46	LYS	CA-C-N	5.56	127.65	120.70
1	K	46	LYS	C-N-CA	5.56	127.65	120.70
1	I	373	TYR	N-CA-CB	5.56	118.07	110.01
1	A	352	THR	CA-C-N	5.56	130.27	122.05
1	A	352	THR	C-N-CA	5.56	130.27	122.05
1	I	429	ASP	CA-CB-CG	5.55	118.15	112.60
1	I	258	GLU	N-CA-CB	5.55	118.19	109.69
1	A	503	MET	CA-C-N	5.55	129.43	120.55
1	A	503	MET	C-N-CA	5.55	129.43	120.55
1	A	278	ASP	CA-CB-CG	5.55	118.15	112.60
1	C	161	TYR	CA-C-N	5.54	127.98	120.44
1	C	161	TYR	C-N-CA	5.54	127.98	120.44
1	A	280	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	K	138	PHE	CA-C-N	5.54	128.02	120.54
1	K	138	PHE	C-N-CA	5.54	128.02	120.54
1	A	391	SER	CA-C-N	5.54	127.64	120.44
1	A	391	SER	C-N-CA	5.54	127.64	120.44
1	I	533	ASN	CA-C-N	5.54	127.70	120.28
1	I	533	ASN	C-N-CA	5.54	127.70	120.28
1	C	362	ARG	CA-C-N	5.54	127.64	120.44
1	C	362	ARG	C-N-CA	5.54	127.64	120.44
1	K	327	LEU	CA-C-N	5.54	130.90	122.65
1	K	327	LEU	C-N-CA	5.54	130.90	122.65
3	F	2	DA	O5'-C5'-C4'	5.54	119.10	110.80
1	C	200	ASN	CA-C-N	5.53	127.53	120.56
1	C	200	ASN	C-N-CA	5.53	127.53	120.56
1	C	350	SER	CA-C-N	5.53	130.80	123.05
1	C	350	SER	C-N-CA	5.53	130.80	123.05
1	I	422	ASN	CA-C-N	5.53	128.01	120.54
1	I	422	ASN	C-N-CA	5.53	128.01	120.54
1	C	398	ASP	CA-C-N	5.53	127.63	120.44
1	C	398	ASP	C-N-CA	5.53	127.63	120.44
1	K	362	ARG	CA-C-N	5.53	127.63	120.44
1	K	362	ARG	C-N-CA	5.53	127.63	120.44
1	K	200	ASN	CA-CB-CG	5.53	118.13	112.60
1	I	197	LEU	CA-C-N	5.53	127.53	120.56
1	I	197	LEU	C-N-CA	5.53	127.53	120.56
1	K	398	ASP	CA-C-N	5.53	127.63	120.44
1	K	398	ASP	C-N-CA	5.53	127.63	120.44
1	C	76	CYS	CA-C-N	5.52	127.62	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	76	CYS	C-N-CA	5.52	127.62	120.44
1	I	391	SER	CA-C-N	5.52	127.61	120.44
1	I	391	SER	C-N-CA	5.52	127.61	120.44
1	C	78	LYS	CA-C-N	5.52	127.61	120.44
1	C	78	LYS	C-N-CA	5.52	127.61	120.44
1	K	237	TYR	CA-C-N	5.52	127.61	120.44
1	K	237	TYR	C-N-CA	5.52	127.61	120.44
1	C	46	LYS	CA-C-N	5.51	127.59	120.70
1	C	46	LYS	C-N-CA	5.51	127.59	120.70
1	A	479	ASN	CA-CB-CG	5.51	118.11	112.60
5	H	5	DT	P-O3'-C3'	5.51	128.47	120.20
1	A	422	ASN	CA-C-N	5.51	127.98	120.54
1	A	422	ASN	C-N-CA	5.51	127.98	120.54
1	K	92	GLU	CA-C-N	5.51	127.50	120.56
1	K	92	GLU	C-N-CA	5.51	127.50	120.56
3	N	2	DA	O5'-C5'-C4'	5.50	119.06	110.80
1	I	503	MET	CA-C-N	5.50	129.35	120.55
1	I	503	MET	C-N-CA	5.50	129.35	120.55
1	A	377	LEU	CA-C-N	5.50	127.65	120.28
1	A	377	LEU	C-N-CA	5.50	127.65	120.28
1	I	377	LEU	CA-C-N	5.50	127.65	120.28
1	I	377	LEU	C-N-CA	5.50	127.65	120.28
1	C	13	THR	CA-C-N	5.50	130.75	123.00
1	C	13	THR	C-N-CA	5.50	130.75	123.00
1	A	353	CYS	N-CA-CB	5.49	117.23	110.53
1	C	62	GLY	CA-C-N	5.49	129.39	120.60
1	C	62	GLY	C-N-CA	5.49	129.39	120.60
1	I	75	GLU	CA-C-N	5.49	127.58	120.44
1	I	75	GLU	C-N-CA	5.49	127.58	120.44
1	A	7	VAL	N-CA-CB	5.49	116.60	110.51
1	K	434	GLY	CA-C-N	5.49	127.48	120.56
1	K	434	GLY	C-N-CA	5.49	127.48	120.56
1	A	141	PHE	CA-CB-CG	5.49	119.28	113.80
1	I	418	LYS	CA-C-N	5.48	127.63	120.28
1	I	418	LYS	C-N-CA	5.48	127.63	120.28
1	K	88	ILE	CA-C-N	5.48	130.56	123.00
1	K	88	ILE	C-N-CA	5.48	130.56	123.00
1	I	445	LYS	N-CA-CB	5.48	117.95	110.01
1	A	321	SER	CA-C-N	5.48	127.62	120.28
1	A	321	SER	C-N-CA	5.48	127.62	120.28
1	C	200	ASN	CA-CB-CG	5.48	118.08	112.60
1	K	278	ASP	CA-CB-CG	5.48	118.08	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	193	LYS	CA-C-N	5.48	127.46	120.56
1	K	193	LYS	C-N-CA	5.48	127.46	120.56
1	C	105	GLY	CA-C-N	5.47	127.56	120.44
1	C	105	GLY	C-N-CA	5.47	127.56	120.44
1	C	278	ASP	CA-CB-CG	5.47	118.07	112.60
1	C	462	LEU	CA-C-N	5.47	128.16	120.28
1	C	462	LEU	C-N-CA	5.47	128.16	120.28
1	K	13	THR	CA-C-N	5.47	130.72	123.00
1	K	13	THR	C-N-CA	5.47	130.72	123.00
1	K	363	TYR	CA-C-N	5.47	127.56	120.44
1	K	363	TYR	C-N-CA	5.47	127.56	120.44
1	C	363	TYR	CA-C-N	5.47	127.55	120.44
1	C	363	TYR	C-N-CA	5.47	127.55	120.44
1	C	92	GLU	CA-C-N	5.47	127.45	120.56
1	C	92	GLU	C-N-CA	5.47	127.45	120.56
1	A	91	LYS	CA-C-N	5.47	130.70	122.99
1	A	91	LYS	C-N-CA	5.47	130.70	122.99
1	A	418	LYS	CA-C-N	5.47	127.61	120.28
1	A	418	LYS	C-N-CA	5.47	127.61	120.28
1	A	75	GLU	CA-C-N	5.47	127.55	120.44
1	A	75	GLU	C-N-CA	5.47	127.55	120.44
1	C	174	TYR	N-CA-CB	5.47	118.08	110.04
1	C	68	ASP	CA-CB-CG	5.46	118.06	112.60
1	K	154	MET	CA-C-N	5.46	127.54	120.44
1	K	154	MET	C-N-CA	5.46	127.54	120.44
1	I	353	CYS	N-CA-CB	5.46	117.19	110.53
1	C	367	GLU	N-CA-CB	5.45	117.92	110.01
1	C	109	ASN	CA-C-N	5.45	127.53	120.44
1	C	109	ASN	C-N-CA	5.45	127.53	120.44
1	C	210	ASP	N-CA-CB	5.45	118.06	109.83
1	I	66	SER	CA-C-N	5.45	127.93	120.46
1	I	66	SER	C-N-CA	5.45	127.93	120.46
1	K	210	ASP	N-CA-CB	5.45	118.06	109.83
1	K	274	ILE	N-CA-CB	5.45	116.47	110.53
1	A	153	ARG	N-CA-CB	5.45	117.91	110.01
1	I	417	GLU	CA-C-N	5.45	127.89	120.54
1	I	417	GLU	C-N-CA	5.45	127.89	120.54
1	I	61	ILE	N-CA-CB	5.45	116.34	110.62
1	I	91	LYS	CA-C-N	5.44	130.66	122.99
1	I	91	LYS	C-N-CA	5.44	130.66	122.99
1	C	215	ALA	CA-C-N	5.44	127.42	120.56
1	C	215	ALA	C-N-CA	5.44	127.42	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	105	GLY	CA-C-N	5.44	127.52	120.44
1	K	105	GLY	C-N-CA	5.44	127.52	120.44
1	K	497	LYS	CA-C-N	5.44	127.51	120.44
1	K	497	LYS	C-N-CA	5.44	127.51	120.44
1	A	132	ASP	CA-C-N	5.44	127.51	120.44
1	A	132	ASP	C-N-CA	5.44	127.51	120.44
1	C	193	LYS	CA-C-N	5.43	127.41	120.56
1	C	193	LYS	C-N-CA	5.43	127.41	120.56
1	K	462	LEU	CA-C-N	5.43	128.11	120.28
1	K	462	LEU	C-N-CA	5.43	128.11	120.28
1	C	274	ILE	N-CA-CB	5.43	116.45	110.53
1	K	174	TYR	N-CA-CB	5.43	118.02	110.04
1	I	280	HIS	CB-CG-CD2	-5.43	124.14	131.20
1	K	151	ARG	CA-C-N	5.43	127.55	120.28
1	K	151	ARG	C-N-CA	5.43	127.55	120.28
1	A	240	LYS	CA-C-N	5.42	127.49	120.44
1	A	240	LYS	C-N-CA	5.42	127.49	120.44
1	I	321	SER	CA-C-N	5.42	127.55	120.28
1	I	321	SER	C-N-CA	5.42	127.55	120.28
1	A	76	CYS	CA-C-N	5.42	127.86	120.54
1	A	76	CYS	C-N-CA	5.42	127.86	120.54
1	A	73	PHE	N-CA-CB	5.42	118.09	110.12
1	I	73	PHE	N-CA-CB	5.42	118.09	110.12
1	K	365	ASP	CA-C-N	5.42	127.39	120.56
1	K	365	ASP	C-N-CA	5.42	127.39	120.56
1	C	365	ASP	CA-C-N	5.42	127.39	120.56
1	C	365	ASP	C-N-CA	5.42	127.39	120.56
1	I	7	VAL	N-CA-CB	5.42	116.52	110.51
1	I	240	LYS	CA-C-N	5.42	127.48	120.44
1	I	240	LYS	C-N-CA	5.42	127.48	120.44
1	A	152	GLU	N-CA-CB	5.41	117.86	110.01
1	C	244	GLN	CA-C-N	5.41	129.62	122.42
1	C	244	GLN	C-N-CA	5.41	129.62	122.42
1	K	109	ASN	CA-C-N	5.41	127.48	120.44
1	K	109	ASN	C-N-CA	5.41	127.48	120.44
1	C	497	LYS	CA-C-N	5.41	127.48	120.44
1	C	497	LYS	C-N-CA	5.41	127.48	120.44
1	I	532	PHE	CA-CB-CG	5.41	119.21	113.80
1	A	417	GLU	CA-C-N	5.41	127.84	120.54
1	A	417	GLU	C-N-CA	5.41	127.84	120.54
1	A	508	VAL	CA-C-N	5.41	129.25	122.43
1	A	508	VAL	C-N-CA	5.41	129.25	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	118	ILE	N-CA-CB	5.41	117.17	111.00
1	K	118	ILE	N-CA-CB	5.41	117.17	111.00
1	A	66	SER	CA-C-N	5.41	127.87	120.46
1	A	66	SER	C-N-CA	5.41	127.87	120.46
1	A	92	GLU	CA-CB-CG	5.41	124.91	114.10
1	K	215	ALA	CA-C-N	5.41	127.37	120.56
1	K	215	ALA	C-N-CA	5.41	127.37	120.56
1	I	76	CYS	CA-C-N	5.40	127.83	120.54
1	I	76	CYS	C-N-CA	5.40	127.83	120.54
1	A	423	LYS	CA-C-N	5.40	128.30	120.79
1	A	423	LYS	C-N-CA	5.40	128.30	120.79
1	A	445	LYS	N-CA-CB	5.40	117.84	110.01
1	K	367	GLU	N-CA-CB	5.40	117.84	110.01
1	I	363	TYR	CA-C-N	5.40	127.46	120.44
1	I	363	TYR	C-N-CA	5.40	127.46	120.44
1	K	141	PHE	N-CA-CB	5.40	117.84	110.01
1	K	445	LYS	CA-C-N	5.40	127.46	120.44
1	K	445	LYS	C-N-CA	5.40	127.46	120.44
1	A	425	ASN	CA-C-N	5.39	127.82	120.54
1	A	425	ASN	C-N-CA	5.39	127.82	120.54
1	I	92	GLU	CA-CB-CG	5.39	124.88	114.10
1	K	265	ARG	CA-C-N	5.39	130.69	122.65
1	K	265	ARG	C-N-CA	5.39	130.69	122.65
1	A	194	VAL	CA-C-N	5.39	127.35	120.56
1	A	194	VAL	C-N-CA	5.39	127.35	120.56
1	C	445	LYS	CA-C-N	5.39	127.45	120.44
1	C	445	LYS	C-N-CA	5.39	127.45	120.44
1	A	532	PHE	CA-CB-CG	5.39	119.19	113.80
1	A	61	ILE	N-CA-CB	5.39	116.28	110.62
1	I	508	VAL	CA-C-N	5.39	129.22	122.43
1	I	508	VAL	C-N-CA	5.39	129.22	122.43
1	A	484	ILE	N-CA-CB	5.39	116.85	110.55
1	K	121	PRO	CA-C-N	5.38	130.75	122.42
1	K	121	PRO	C-N-CA	5.38	130.75	122.42
1	K	244	GLN	CA-C-N	5.38	129.57	122.42
1	K	244	GLN	C-N-CA	5.38	129.57	122.42
4	O	-19	DA	O5'-C5'-C4'	5.38	118.86	110.80
1	C	265	ARG	CA-C-N	5.37	130.65	122.65
1	C	265	ARG	C-N-CA	5.37	130.65	122.65
1	I	488	TYR	CA-C-N	5.37	127.42	120.44
1	I	488	TYR	C-N-CA	5.37	127.42	120.44
1	I	267	ILE	CA-C-N	5.37	128.84	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	267	ILE	C-N-CA	5.37	128.84	120.68
1	A	363	TYR	CA-C-N	5.37	127.42	120.44
1	A	363	TYR	C-N-CA	5.37	127.42	120.44
4	G	-19	DA	O5'-C5'-C4'	5.37	118.85	110.80
1	C	524	PHE	CA-C-N	5.37	131.34	122.33
1	C	524	PHE	C-N-CA	5.37	131.34	122.33
1	K	387	LYS	CA-C-N	5.37	127.42	120.44
1	K	387	LYS	C-N-CA	5.37	127.42	120.44
1	I	484	ILE	N-CA-CB	5.36	116.83	110.55
1	K	48	LEU	CA-C-N	5.36	127.41	120.44
1	K	48	LEU	C-N-CA	5.36	127.41	120.44
1	A	13	THR	CA-C-N	5.36	130.55	123.05
1	A	13	THR	C-N-CA	5.36	130.55	123.05
1	C	387	LYS	CA-C-N	5.36	127.41	120.44
1	C	387	LYS	C-N-CA	5.36	127.41	120.44
1	I	347	HIS	CE1-NE2-CD2	-5.36	103.64	109.00
1	I	13	THR	CA-C-N	5.36	130.55	123.05
1	I	13	THR	C-N-CA	5.36	130.55	123.05
1	A	316	GLY	CA-C-N	5.36	127.80	120.46
1	A	316	GLY	C-N-CA	5.36	127.80	120.46
1	C	347	HIS	CE1-NE2-CD2	-5.36	103.64	109.00
1	I	423	LYS	CA-C-N	5.36	128.24	120.79
1	I	423	LYS	C-N-CA	5.36	128.24	120.79
1	K	422	ASN	CA-C-N	5.36	127.41	120.44
1	K	422	ASN	C-N-CA	5.36	127.41	120.44
1	A	267	ILE	CA-C-N	5.36	128.82	120.68
1	A	267	ILE	C-N-CA	5.36	128.82	120.68
1	K	40	GLN	CA-CB-CG	5.36	124.81	114.10
1	K	347	HIS	CE1-NE2-CD2	-5.36	103.64	109.00
1	C	141	PHE	N-CA-CB	5.35	117.77	110.01
1	C	242	ILE	N-CA-CB	5.35	116.81	110.55
1	I	135	GLN	CA-C-N	5.35	127.30	120.56
1	I	135	GLN	C-N-CA	5.35	127.30	120.56
1	I	425	ASN	CA-C-N	5.35	127.76	120.54
1	I	425	ASN	C-N-CA	5.35	127.76	120.54
1	I	43	LEU	CA-C-N	5.35	127.45	120.28
1	I	43	LEU	C-N-CA	5.35	127.45	120.28
1	I	194	VAL	CA-C-N	5.35	127.30	120.56
1	I	194	VAL	C-N-CA	5.35	127.30	120.56
1	I	153	ARG	N-CA-CB	5.35	117.76	110.01
1	C	48	LEU	CA-C-N	5.34	127.39	120.44
1	C	48	LEU	C-N-CA	5.34	127.39	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	411	GLU	CA-C-N	5.34	127.38	120.44
1	K	411	GLU	C-N-CA	5.34	127.38	120.44
1	A	347	HIS	CE1-NE2-CD2	-5.34	103.66	109.00
1	C	40	GLN	CA-CB-CG	5.34	124.77	114.10
1	I	288	GLN	CA-CB-CG	5.34	124.78	114.10
1	K	524	PHE	CA-C-N	5.34	131.30	122.33
1	K	524	PHE	C-N-CA	5.34	131.30	122.33
1	A	198	ILE	CA-C-N	5.33	127.37	120.44
1	A	198	ILE	C-N-CA	5.33	127.37	120.44
1	K	444	ARG	CA-C-N	5.33	127.74	120.54
1	K	444	ARG	C-N-CA	5.33	127.74	120.54
1	A	144	ARG	CA-C-N	5.33	127.37	120.44
1	A	144	ARG	C-N-CA	5.33	127.37	120.44
1	C	422	ASN	CA-C-N	5.33	127.37	120.44
1	C	422	ASN	C-N-CA	5.33	127.37	120.44
1	I	316	GLY	CA-C-N	5.33	127.77	120.46
1	I	316	GLY	C-N-CA	5.33	127.77	120.46
1	K	107	ILE	CA-C-N	5.33	127.28	120.56
1	K	107	ILE	C-N-CA	5.33	127.28	120.56
1	K	148	GLU	N-CA-CB	5.33	117.96	110.12
1	C	255	LYS	CA-C-N	5.33	128.89	120.47
1	C	255	LYS	C-N-CA	5.33	128.89	120.47
1	A	149	MET	CA-C-N	5.33	127.36	120.44
1	A	149	MET	C-N-CA	5.33	127.36	120.44
1	C	411	GLU	CA-C-N	5.33	127.36	120.44
1	C	411	GLU	C-N-CA	5.33	127.36	120.44
1	I	239	ILE	CA-C-N	5.32	127.36	120.44
1	I	239	ILE	C-N-CA	5.32	127.36	120.44
5	P	5	DT	P-O3'-C3'	5.32	128.19	120.20
1	A	257	ARG	CA-C-N	5.32	128.32	120.82
1	A	257	ARG	C-N-CA	5.32	128.32	120.82
1	C	108	VAL	CA-C-N	5.32	127.36	120.44
1	C	108	VAL	C-N-CA	5.32	127.36	120.44
1	A	239	ILE	CA-C-N	5.32	127.35	120.44
1	A	239	ILE	C-N-CA	5.32	127.35	120.44
1	C	154	MET	CA-C-N	5.31	127.71	120.54
1	C	154	MET	C-N-CA	5.31	127.71	120.54
1	C	508	VAL	CA-C-N	5.31	129.01	122.37
1	C	508	VAL	C-N-CA	5.31	129.01	122.37
1	K	370	ILE	N-CA-CB	5.31	116.77	110.55
1	I	152	GLU	N-CA-CB	5.31	117.71	110.01
1	C	12	ILE	CA-C-N	5.31	130.53	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	12	ILE	C-N-CA	5.31	130.53	122.56
1	K	176	TYR	CA-C-N	5.31	131.25	122.33
1	K	176	TYR	C-N-CA	5.31	131.25	122.33
1	A	43	LEU	CA-C-N	5.31	127.39	120.28
1	A	43	LEU	C-N-CA	5.31	127.39	120.28
1	A	288	GLN	CA-C-N	5.31	127.34	120.44
1	A	288	GLN	C-N-CA	5.31	127.34	120.44
5	P	7	DT	C5'-C4'-C3'	-5.31	106.94	114.90
1	A	157	ALA	CA-C-N	5.31	127.34	120.44
1	A	157	ALA	C-N-CA	5.31	127.34	120.44
1	A	421	LYS	CA-CB-CG	5.30	124.71	114.10
1	A	21	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	I	175	GLY	N-CA-C	5.30	121.05	114.37
1	K	12	ILE	CA-C-N	5.30	130.51	122.56
1	K	12	ILE	C-N-CA	5.30	130.51	122.56
1	C	217	ALA	CA-C-N	5.30	127.33	120.44
1	C	217	ALA	C-N-CA	5.30	127.33	120.44
1	C	502	ARG	CA-C-N	5.30	127.64	120.38
1	C	502	ARG	C-N-CA	5.30	127.64	120.38
1	I	257	ARG	CA-C-N	5.30	128.29	120.82
1	I	257	ARG	C-N-CA	5.30	128.29	120.82
1	K	157	ALA	CA-C-N	5.30	127.33	120.44
1	K	157	ALA	C-N-CA	5.30	127.33	120.44
1	C	291	GLN	CA-C-N	5.30	127.33	120.44
1	C	291	GLN	C-N-CA	5.30	127.33	120.44
1	C	91	LYS	N-CA-CB	5.30	117.69	110.01
1	C	443	LYS	N-CA-CB	5.30	117.69	110.01
1	I	11	ASN	CA-C-N	5.30	128.99	122.37
1	I	11	ASN	C-N-CA	5.30	128.99	122.37
1	I	365	ASP	CA-C-N	5.30	127.23	120.56
1	I	365	ASP	C-N-CA	5.30	127.23	120.56
1	K	108	VAL	CA-C-N	5.30	127.33	120.44
1	K	108	VAL	C-N-CA	5.30	127.33	120.44
1	K	491	GLU	CA-C-N	5.30	131.47	122.36
1	K	491	GLU	C-N-CA	5.30	131.47	122.36
1	K	217	ALA	CA-C-N	5.29	127.32	120.44
1	K	217	ALA	C-N-CA	5.29	127.32	120.44
1	C	495	GLU	CA-C-N	5.29	127.31	120.44
1	C	495	GLU	C-N-CA	5.29	127.31	120.44
1	I	130	PRO	CA-C-N	5.29	127.22	120.56
1	I	130	PRO	C-N-CA	5.29	127.22	120.56
1	I	149	MET	CA-C-N	5.29	127.32	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	149	MET	C-N-CA	5.29	127.32	120.44
1	A	288	GLN	CA-CB-CG	5.29	124.67	114.10
1	C	95	ARG	CA-C-N	5.29	127.63	120.65
1	C	95	ARG	C-N-CA	5.29	127.63	120.65
1	C	157	ALA	CA-C-N	5.29	127.31	120.44
1	C	157	ALA	C-N-CA	5.29	127.31	120.44
1	C	491	GLU	CA-C-N	5.29	131.45	122.36
1	C	491	GLU	C-N-CA	5.29	131.45	122.36
1	I	138	PHE	CA-CB-CG	5.29	119.08	113.80
1	K	446	ALA	CA-C-N	5.29	127.31	120.44
1	K	446	ALA	C-N-CA	5.29	127.31	120.44
1	A	347	HIS	ND1-CG-CD2	-5.28	100.82	106.10
1	I	374	LEU	CA-C-N	5.28	127.36	120.28
1	I	374	LEU	C-N-CA	5.28	127.36	120.28
1	K	291	GLN	CA-C-N	5.28	127.31	120.44
1	K	291	GLN	C-N-CA	5.28	127.31	120.44
1	C	38	THR	CA-C-N	5.28	127.36	120.28
1	C	38	THR	C-N-CA	5.28	127.36	120.28
1	C	37	LEU	N-CA-CB	5.28	117.88	110.12
1	I	444	ARG	CA-C-N	5.28	127.30	120.44
1	I	444	ARG	C-N-CA	5.28	127.30	120.44
1	K	508	VAL	CA-C-N	5.28	128.97	122.37
1	K	508	VAL	C-N-CA	5.28	128.97	122.37
1	A	175	GLY	N-CA-C	5.28	121.02	114.37
1	I	421	LYS	CA-CB-CG	5.28	124.66	114.10
1	A	374	LEU	CA-C-N	5.28	127.35	120.28
1	A	374	LEU	C-N-CA	5.28	127.35	120.28
1	K	219	HIS	CA-CB-CG	5.28	119.08	113.80
1	K	347	HIS	ND1-CG-CD2	-5.28	100.82	106.10
1	C	347	HIS	ND1-CG-CD2	-5.28	100.82	106.10
1	C	370	ILE	N-CA-CB	5.28	116.72	110.55
1	I	37	LEU	CA-C-N	5.28	127.30	120.44
1	I	37	LEU	C-N-CA	5.28	127.30	120.44
1	C	176	TYR	CA-C-N	5.27	131.19	122.33
1	C	176	TYR	C-N-CA	5.27	131.19	122.33
1	C	321	SER	CA-C-N	5.27	127.61	120.38
1	C	321	SER	C-N-CA	5.27	127.61	120.38
1	I	123	LYS	CG-CD-CE	5.27	123.43	111.30
1	I	388	HIS	N-CA-CB	5.27	117.87	110.12
1	C	148	GLU	N-CA-CB	5.27	117.87	110.12
1	I	367	GLU	N-CA-CB	5.27	117.83	109.82
1	A	428	PHE	CA-C-N	5.27	127.29	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	PHE	C-N-CA	5.27	127.29	120.44
1	I	47	ILE	CA-C-N	5.27	127.87	120.28
1	I	47	ILE	C-N-CA	5.27	127.87	120.28
1	I	428	PHE	CA-C-N	5.27	127.29	120.44
1	I	428	PHE	C-N-CA	5.27	127.29	120.44
1	C	219	HIS	CA-CB-CG	5.27	119.07	113.80
1	I	288	GLN	CA-C-N	5.27	127.29	120.44
1	I	288	GLN	C-N-CA	5.27	127.29	120.44
1	K	78	LYS	CA-C-N	5.27	127.60	120.65
1	K	78	LYS	C-N-CA	5.27	127.60	120.65
1	K	495	GLU	CA-C-N	5.27	127.29	120.44
1	K	495	GLU	C-N-CA	5.27	127.29	120.44
1	A	130	PRO	CA-C-N	5.26	127.19	120.56
1	A	130	PRO	C-N-CA	5.26	127.19	120.56
1	C	442	LEU	CA-C-N	5.26	127.28	120.44
1	C	442	LEU	C-N-CA	5.26	127.28	120.44
1	I	179	ASN	N-CA-CB	5.26	118.20	109.88
1	I	347	HIS	ND1-CG-CD2	-5.26	100.84	106.10
1	K	216	ILE	CA-C-N	5.26	127.28	120.44
1	K	216	ILE	C-N-CA	5.26	127.28	120.44
1	I	144	ARG	CA-C-N	5.26	127.28	120.44
1	I	144	ARG	C-N-CA	5.26	127.28	120.44
1	C	444	ARG	CA-C-N	5.26	127.64	120.54
1	C	444	ARG	C-N-CA	5.26	127.64	120.54
1	K	289	PHE	N-CA-CB	5.26	117.64	110.01
1	K	317	VAL	CA-C-N	5.26	130.56	122.93
1	K	317	VAL	C-N-CA	5.26	130.56	122.93
1	A	159	TYR	CA-C-N	5.26	127.28	120.44
1	A	159	TYR	C-N-CA	5.26	127.28	120.44
1	C	446	ALA	CA-C-N	5.26	127.28	120.44
1	C	446	ALA	C-N-CA	5.26	127.28	120.44
1	A	516	ARG	N-CA-CB	5.26	117.82	109.51
1	K	91	LYS	N-CA-CB	5.26	117.63	110.01
1	K	502	ARG	CA-C-N	5.26	127.58	120.38
1	K	502	ARG	C-N-CA	5.26	127.58	120.38
1	K	321	SER	CA-C-N	5.25	127.58	120.38
1	K	321	SER	C-N-CA	5.25	127.58	120.38
1	C	289	PHE	N-CA-CB	5.25	117.63	110.01
1	I	198	ILE	CA-C-N	5.25	127.27	120.44
1	I	198	ILE	C-N-CA	5.25	127.27	120.44
1	I	310	GLU	CA-C-N	5.25	128.31	120.95
1	I	310	GLU	C-N-CA	5.25	128.31	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	4	LYS	CA-C-N	5.25	127.27	120.44
1	I	4	LYS	C-N-CA	5.25	127.27	120.44
1	A	357	LYS	CB-CG-CD	5.25	123.37	111.30
1	A	367	GLU	N-CA-CB	5.25	117.80	109.82
1	K	443	LYS	N-CA-CB	5.25	117.62	110.01
1	A	79	ASP	CA-C-N	5.25	127.31	120.28
1	A	79	ASP	C-N-CA	5.25	127.31	120.28
1	A	91	LYS	CA-CB-CG	5.25	124.59	114.10
1	K	318	CYS	CA-C-N	5.25	131.23	122.73
1	K	318	CYS	C-N-CA	5.25	131.23	122.73
1	A	47	ILE	CA-C-N	5.24	127.83	120.28
1	A	47	ILE	C-N-CA	5.24	127.83	120.28
1	A	179	ASN	N-CA-CB	5.24	118.16	109.88
1	A	365	ASP	CA-C-N	5.24	127.17	120.56
1	A	365	ASP	C-N-CA	5.24	127.17	120.56
1	A	414	SER	CA-C-N	5.24	127.26	120.44
1	A	414	SER	C-N-CA	5.24	127.26	120.44
1	A	388	HIS	N-CA-CB	5.24	117.83	110.12
1	C	317	VAL	CA-C-N	5.24	130.53	122.93
1	C	317	VAL	C-N-CA	5.24	130.53	122.93
1	I	132	ASP	CA-C-N	5.24	127.56	120.38
1	I	132	ASP	C-N-CA	5.24	127.56	120.38
1	I	357	LYS	CB-CG-CD	5.24	123.36	111.30
1	I	91	LYS	CA-CB-CG	5.24	124.58	114.10
1	I	159	TYR	CA-C-N	5.24	127.25	120.44
1	I	159	TYR	C-N-CA	5.24	127.25	120.44
1	K	37	LEU	N-CA-CB	5.24	117.82	110.12
1	C	107	ILE	CA-C-N	5.24	127.16	120.56
1	C	107	ILE	C-N-CA	5.24	127.16	120.56
1	C	302	LEU	N-CA-CB	5.24	117.91	110.16
4	G	-10	DA	O5'-C5'-C4'	5.23	118.65	110.80
1	C	347	HIS	CG-CD2-NE2	5.23	112.43	107.20
1	K	423	LYS	CA-C-N	5.23	127.24	120.44
1	K	423	LYS	C-N-CA	5.23	127.24	120.44
1	K	370	ILE	CA-C-N	5.23	127.24	120.44
1	K	370	ILE	C-N-CA	5.23	127.24	120.44
4	O	-10	DA	O5'-C5'-C4'	5.23	118.65	110.80
1	C	370	ILE	CA-C-N	5.23	127.24	120.44
1	C	370	ILE	C-N-CA	5.23	127.24	120.44
1	I	176	TYR	CA-C-N	5.23	131.11	122.33
1	I	176	TYR	C-N-CA	5.23	131.11	122.33
1	I	225	ILE	N-CA-CB	5.23	115.97	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	516	ARG	N-CA-CB	5.23	117.77	109.51
1	K	67	ILE	CA-C-N	5.23	127.55	120.65
1	K	67	ILE	C-N-CA	5.23	127.55	120.65
1	A	444	ARG	CA-C-N	5.23	127.23	120.44
1	A	444	ARG	C-N-CA	5.23	127.23	120.44
1	K	494	SER	CA-C-N	5.23	127.23	120.44
1	K	494	SER	C-N-CA	5.23	127.23	120.44
1	A	74	LYS	CA-C-N	5.22	127.23	120.44
1	A	74	LYS	C-N-CA	5.22	127.23	120.44
1	A	158	LYS	CA-C-N	5.22	127.23	120.44
1	A	158	LYS	C-N-CA	5.22	127.23	120.44
1	A	176	TYR	CA-C-N	5.22	131.11	122.33
1	A	176	TYR	C-N-CA	5.22	131.11	122.33
1	C	141	PHE	CA-C-N	5.22	127.23	120.44
1	C	141	PHE	C-N-CA	5.22	127.23	120.44
1	C	387	LYS	N-CA-CB	5.22	117.59	110.01
1	I	111	LEU	CA-C-N	5.22	127.23	120.44
1	I	111	LEU	C-N-CA	5.22	127.23	120.44
1	K	300	VAL	N-CA-CB	5.22	115.97	110.17
1	K	390	ASN	CA-C-N	5.22	127.23	120.44
1	K	390	ASN	C-N-CA	5.22	127.23	120.44
1	C	318	CYS	CA-C-N	5.22	131.19	122.73
1	C	318	CYS	C-N-CA	5.22	131.19	122.73
1	K	347	HIS	CG-CD2-NE2	5.22	112.42	107.20
1	A	339	LYS	CA-C-N	5.22	129.44	120.72
1	A	339	LYS	C-N-CA	5.22	129.44	120.72
1	C	423	LYS	CA-C-N	5.22	127.23	120.44
1	C	423	LYS	C-N-CA	5.22	127.23	120.44
1	I	110	LEU	CA-C-N	5.22	127.23	120.44
1	I	110	LEU	C-N-CA	5.22	127.23	120.44
1	I	79	ASP	CA-C-N	5.22	127.27	120.28
1	I	79	ASP	C-N-CA	5.22	127.27	120.28
1	A	111	LEU	CA-C-N	5.22	127.22	120.44
1	A	111	LEU	C-N-CA	5.22	127.22	120.44
1	C	390	ASN	CA-C-N	5.22	127.22	120.44
1	C	390	ASN	C-N-CA	5.22	127.22	120.44
1	C	216	ILE	CA-C-N	5.21	127.22	120.44
1	C	216	ILE	C-N-CA	5.21	127.22	120.44
1	C	494	SER	CA-C-N	5.21	127.22	120.44
1	C	494	SER	C-N-CA	5.21	127.22	120.44
1	I	478	ARG	CA-C-N	5.21	127.22	120.44
1	I	478	ARG	C-N-CA	5.21	127.22	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	448	LEU	N-CA-CB	5.21	117.88	110.16
1	K	392	MET	CA-C-N	5.21	127.22	120.44
1	K	392	MET	C-N-CA	5.21	127.22	120.44
1	K	525	GLU	CA-C-N	5.21	130.50	122.68
1	K	525	GLU	C-N-CA	5.21	130.50	122.68
1	C	525	GLU	CA-C-N	5.21	130.50	122.68
1	C	525	GLU	C-N-CA	5.21	130.50	122.68
1	K	302	LEU	N-CA-CB	5.21	117.87	110.16
1	K	309	PHE	CA-C-N	5.21	130.19	123.00
1	K	309	PHE	C-N-CA	5.21	130.19	123.00
1	K	141	PHE	CA-C-N	5.21	127.21	120.44
1	K	141	PHE	C-N-CA	5.21	127.21	120.44
1	A	512	MET	N-CA-CB	5.21	117.66	109.69
3	F	21	DT	C3'-C2'-C1'	5.21	109.41	101.60
1	K	387	LYS	N-CA-CB	5.21	117.56	110.01
1	A	153	ARG	CB-CG-CD	5.21	123.27	111.30
1	I	347	HIS	CG-CD2-NE2	5.21	112.41	107.20
1	I	418	LYS	CG-CD-CE	5.21	123.27	111.30
3	N	21	DT	C3'-C2'-C1'	5.21	109.41	101.60
1	I	339	LYS	CA-C-N	5.20	129.41	120.72
1	I	339	LYS	C-N-CA	5.20	129.41	120.72
1	K	428	PHE	N-CA-CB	5.20	117.56	110.01
1	C	392	MET	CA-C-N	5.20	127.20	120.44
1	C	392	MET	C-N-CA	5.20	127.20	120.44
1	A	418	LYS	CG-CD-CE	5.20	123.26	111.30
1	I	133	MET	CA-C-N	5.20	127.20	120.44
1	I	133	MET	C-N-CA	5.20	127.20	120.44
1	K	38	THR	CA-C-N	5.20	127.25	120.28
1	K	38	THR	C-N-CA	5.20	127.25	120.28
1	A	310	GLU	CA-C-N	5.20	128.23	120.95
1	A	310	GLU	C-N-CA	5.20	128.23	120.95
1	I	512	MET	N-CA-CB	5.20	117.64	109.69
1	A	11	ASN	CA-C-N	5.19	128.86	122.37
1	A	11	ASN	C-N-CA	5.19	128.86	122.37
1	A	88	ILE	CB-CA-C	5.19	116.86	111.09
1	C	67	ILE	CA-C-N	5.19	127.50	120.65
1	C	67	ILE	C-N-CA	5.19	127.50	120.65
1	I	158	LYS	CA-C-N	5.19	127.19	120.44
1	I	158	LYS	C-N-CA	5.19	127.19	120.44
1	K	95	ARG	CA-C-N	5.19	127.50	120.65
1	K	95	ARG	C-N-CA	5.19	127.50	120.65
1	C	428	PHE	N-CA-CB	5.19	117.53	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	302	LEU	CA-C-N	5.19	129.39	123.21
1	K	302	LEU	C-N-CA	5.19	129.39	123.21
1	A	347	HIS	CG-CD2-NE2	5.19	112.39	107.20
1	A	489	HIS	ND1-CG-CD2	-5.19	100.91	106.10
1	K	442	LEU	CA-C-N	5.19	127.19	120.44
1	K	442	LEU	C-N-CA	5.19	127.19	120.44
1	A	225	ILE	N-CA-CB	5.19	115.93	110.17
5	H	7	DT	C5'-C4'-C3'	-5.19	107.12	114.90
1	A	478	ARG	CA-C-N	5.19	127.18	120.44
1	A	478	ARG	C-N-CA	5.19	127.18	120.44
1	A	4	LYS	CA-C-N	5.18	127.18	120.44
1	A	4	LYS	C-N-CA	5.18	127.18	120.44
1	C	509	ILE	N-CA-CB	5.18	116.91	111.00
1	K	499	GLU	CA-C-N	5.18	127.18	120.44
1	K	499	GLU	C-N-CA	5.18	127.18	120.44
1	K	493	SER	CA-C-N	5.18	127.22	120.28
1	K	493	SER	C-N-CA	5.18	127.22	120.28
1	A	445	LYS	CA-C-N	5.18	127.22	120.28
1	A	445	LYS	C-N-CA	5.18	127.22	120.28
1	I	143	ALA	CA-C-N	5.18	127.17	120.44
1	I	143	ALA	C-N-CA	5.18	127.17	120.44
1	I	193	LYS	CA-C-N	5.18	127.09	120.56
1	I	193	LYS	C-N-CA	5.18	127.09	120.56
1	I	414	SER	CA-C-N	5.18	127.17	120.44
1	I	414	SER	C-N-CA	5.18	127.17	120.44
1	K	56	GLU	CA-C-N	5.18	130.87	122.07
1	K	56	GLU	C-N-CA	5.18	130.87	122.07
1	C	198	ILE	CA-C-N	5.18	127.17	120.44
1	C	198	ILE	C-N-CA	5.18	127.17	120.44
1	I	274	ILE	N-CA-CB	5.18	116.90	111.00
1	I	367	GLU	CA-C-N	5.18	127.17	120.44
1	I	367	GLU	C-N-CA	5.18	127.17	120.44
1	I	489	HIS	ND1-CG-CD2	-5.18	100.92	106.10
1	K	47	ILE	CA-C-N	5.17	127.22	120.28
1	K	47	ILE	C-N-CA	5.17	127.22	120.28
1	I	74	LYS	CA-C-N	5.17	127.17	120.44
1	I	74	LYS	C-N-CA	5.17	127.17	120.44
1	A	193	LYS	CA-C-N	5.17	127.08	120.56
1	A	193	LYS	C-N-CA	5.17	127.08	120.56
1	C	159	TYR	CA-C-N	5.17	127.16	120.44
1	C	159	TYR	C-N-CA	5.17	127.16	120.44
1	I	280	HIS	CA-C-N	5.17	127.68	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	280	HIS	C-N-CA	5.17	127.68	120.65
1	C	499	GLU	CA-C-N	5.17	127.16	120.44
1	C	499	GLU	C-N-CA	5.17	127.16	120.44
1	I	42	GLU	CA-C-N	5.17	127.16	120.44
1	I	42	GLU	C-N-CA	5.17	127.16	120.44
1	K	295	LYS	N-CA-CB	5.17	117.51	110.01
1	A	143	ALA	CA-C-N	5.17	127.16	120.44
1	A	143	ALA	C-N-CA	5.17	127.16	120.44
1	I	107	ILE	CA-C-N	5.17	127.07	120.56
1	I	107	ILE	C-N-CA	5.17	127.07	120.56
1	A	300	VAL	N-CA-CB	5.16	115.90	110.17
1	C	309	PHE	CA-C-N	5.16	130.12	123.00
1	C	309	PHE	C-N-CA	5.16	130.12	123.00
1	C	448	LEU	N-CA-CB	5.16	117.80	110.16
1	I	444	ARG	CG-CD-NE	5.16	123.36	112.00
1	A	367	GLU	CA-C-N	5.16	127.15	120.44
1	A	367	GLU	C-N-CA	5.16	127.15	120.44
1	C	369	ALA	CA-C-N	5.16	127.06	120.56
1	C	369	ALA	C-N-CA	5.16	127.06	120.56
1	C	493	SER	CA-C-N	5.16	127.20	120.28
1	C	493	SER	C-N-CA	5.16	127.20	120.28
1	I	478	ARG	CA-CB-CG	5.16	124.42	114.10
1	A	444	ARG	CG-CD-NE	5.16	123.35	112.00
1	K	424	GLU	CA-C-N	5.16	127.15	120.44
1	K	424	GLU	C-N-CA	5.16	127.15	120.44
1	K	509	ILE	N-CA-CB	5.16	116.88	111.00
1	I	351	LEU	N-CA-CB	5.16	118.28	109.87
1	K	138	PHE	CA-CB-CG	5.16	118.96	113.80
1	A	478	ARG	CA-CB-CG	5.16	124.41	114.10
4	G	-2	DT	C2'-C3'-O3'	-5.16	103.77	111.50
1	C	353	CYS	N-CA-CB	5.15	117.53	110.57
1	K	386	THR	CA-C-N	5.15	127.14	120.44
1	K	386	THR	C-N-CA	5.15	127.14	120.44
1	K	462	LEU	N-CA-CB	5.15	117.62	109.94
1	C	300	VAL	N-CA-CB	5.15	115.89	110.17
1	I	495	GLU	CA-C-N	5.15	127.18	120.28
1	I	495	GLU	C-N-CA	5.15	127.18	120.28
1	A	123	LYS	CG-CD-CE	5.15	123.14	111.30
1	K	271	LYS	CA-CB-CG	5.15	124.40	114.10
1	C	295	LYS	N-CA-CB	5.15	117.48	110.01
1	C	302	LEU	CA-C-N	5.15	129.34	123.21
1	C	302	LEU	C-N-CA	5.15	129.34	123.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	198	ILE	CA-C-N	5.14	127.13	120.44
1	K	198	ILE	C-N-CA	5.14	127.13	120.44
1	I	136	ILE	CA-C-N	5.14	127.48	120.54
1	I	136	ILE	C-N-CA	5.14	127.48	120.54
1	K	353	CYS	N-CA-CB	5.14	117.51	110.57
1	A	423	LYS	CA-CB-CG	5.14	124.38	114.10
1	C	394	SER	N-CA-CB	5.14	117.46	110.01
1	I	445	LYS	CA-C-N	5.14	127.16	120.28
1	I	445	LYS	C-N-CA	5.14	127.16	120.28
1	A	110	LEU	CA-C-N	5.13	127.11	120.44
1	A	110	LEU	C-N-CA	5.13	127.11	120.44
1	A	151	ARG	CA-C-N	5.13	127.11	120.44
1	A	151	ARG	C-N-CA	5.13	127.11	120.44
1	C	258	GLU	O-C-N	-5.13	116.61	122.93
1	C	503	MET	CA-CB-CG	5.13	124.37	114.10
1	I	88	ILE	CB-CA-C	5.13	116.79	111.09
1	K	159	TYR	CA-C-N	5.13	127.11	120.44
1	K	159	TYR	C-N-CA	5.13	127.11	120.44
1	C	424	GLU	CA-C-N	5.13	127.11	120.44
1	C	424	GLU	C-N-CA	5.13	127.11	120.44
1	K	503	MET	CA-CB-CG	5.13	124.37	114.10
1	I	300	VAL	N-CA-CB	5.13	115.87	110.17
1	A	326	PRO	CA-C-N	5.13	129.59	122.77
1	A	326	PRO	C-N-CA	5.13	129.59	122.77
1	C	386	THR	CA-C-N	5.13	127.11	120.44
1	C	386	THR	C-N-CA	5.13	127.11	120.44
1	I	475	ASN	CA-C-N	5.13	127.11	120.44
1	I	475	ASN	C-N-CA	5.13	127.11	120.44
1	I	274	ILE	CA-C-N	5.13	130.18	122.75
1	I	274	ILE	C-N-CA	5.13	130.18	122.75
1	I	431	TYR	CA-C-N	5.13	127.15	120.28
1	I	431	TYR	C-N-CA	5.13	127.15	120.28
1	I	256	VAL	CA-C-N	5.12	130.54	122.34
1	I	256	VAL	C-N-CA	5.12	130.54	122.34
1	A	450	GLU	CA-C-N	5.12	127.10	120.44
1	A	450	GLU	C-N-CA	5.12	127.10	120.44
1	A	42	GLU	CA-C-N	5.12	127.10	120.44
1	A	42	GLU	C-N-CA	5.12	127.10	120.44
1	I	450	GLU	CA-C-N	5.12	127.09	120.44
1	I	450	GLU	C-N-CA	5.12	127.09	120.44
1	I	432	GLU	CB-CG-CD	5.12	121.30	112.60
1	K	93	ILE	N-CA-CB	5.12	116.54	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	369	ALA	CA-C-N	5.12	127.01	120.56
1	K	369	ALA	C-N-CA	5.12	127.01	120.56
1	A	133	MET	CA-C-N	5.12	127.14	120.28
1	A	133	MET	C-N-CA	5.12	127.14	120.28
1	A	351	LEU	N-CA-CB	5.12	118.21	109.87
1	A	475	ASN	CA-C-N	5.12	127.09	120.44
1	A	475	ASN	C-N-CA	5.12	127.09	120.44
1	C	149	MET	CA-C-N	5.12	127.09	120.44
1	C	149	MET	C-N-CA	5.12	127.09	120.44
1	K	148	GLU	CA-C-N	5.12	127.45	120.54
1	K	148	GLU	C-N-CA	5.12	127.45	120.54
1	K	394	SER	N-CA-CB	5.12	117.43	110.01
1	K	498	ASN	N-CA-CB	5.11	117.42	110.01
1	K	47	ILE	N-CA-CB	5.11	116.19	110.62
1	C	84	LYS	CA-C-N	5.11	130.59	122.62
1	C	84	LYS	C-N-CA	5.11	130.59	122.62
1	I	102	SER	CA-C-N	5.11	127.08	120.44
1	I	102	SER	C-N-CA	5.11	127.08	120.44
1	A	103	ASP	CA-C-N	5.11	127.08	120.44
1	A	103	ASP	C-N-CA	5.11	127.08	120.44
1	C	263	GLY	CA-C-N	5.11	127.96	120.71
1	C	263	GLY	C-N-CA	5.11	127.96	120.71
1	I	112	GLN	CA-C-N	5.11	127.39	120.65
1	I	112	GLN	C-N-CA	5.11	127.39	120.65
1	K	258	GLU	O-C-N	-5.11	116.65	122.93
1	C	462	LEU	N-CA-CB	5.10	117.55	109.94
1	I	154	MET	CA-C-N	5.10	127.08	120.44
1	I	154	MET	C-N-CA	5.10	127.08	120.44
1	C	198	ILE	N-CA-CB	5.10	116.52	110.55
1	I	137	ARG	CA-CB-CG	5.10	124.31	114.10
1	I	423	LYS	CA-CB-CG	5.10	124.31	114.10
1	C	408	GLN	CA-C-N	5.10	127.07	120.44
1	C	408	GLN	C-N-CA	5.10	127.07	120.44
1	I	81	GLU	CA-CB-CG	5.10	124.30	114.10
1	A	115	ARG	CA-C-N	5.10	127.95	120.71
1	A	115	ARG	C-N-CA	5.10	127.95	120.71
1	A	154	MET	CA-C-N	5.10	127.07	120.44
1	A	154	MET	C-N-CA	5.10	127.07	120.44
1	A	432	GLU	CB-CG-CD	5.10	121.27	112.60
1	C	93	ILE	N-CA-CB	5.10	116.52	110.55
1	I	5	ASN	CA-C-N	5.10	126.98	120.56
1	I	5	ASN	C-N-CA	5.10	126.98	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	198	ILE	N-CA-CB	5.10	116.51	110.55
1	I	151	ARG	CA-C-N	5.10	127.06	120.44
1	I	151	ARG	C-N-CA	5.10	127.06	120.44
1	K	84	LYS	CA-C-N	5.10	130.57	122.62
1	K	84	LYS	C-N-CA	5.10	130.57	122.62
1	K	408	GLN	CA-C-N	5.10	127.06	120.44
1	K	408	GLN	C-N-CA	5.10	127.06	120.44
1	A	81	GLU	CA-CB-CG	5.09	124.29	114.10
1	K	11	ASN	CA-CB-CG	5.09	117.69	112.60
1	A	146	GLU	CA-C-N	5.09	127.37	120.65
1	A	146	GLU	C-N-CA	5.09	127.37	120.65
1	K	79	ASP	CA-C-N	5.09	127.06	120.44
1	K	79	ASP	C-N-CA	5.09	127.06	120.44
1	K	173	PRO	CA-C-N	5.09	128.44	120.75
1	K	173	PRO	C-N-CA	5.09	128.44	120.75
1	A	256	VAL	CA-C-N	5.09	130.49	122.34
1	A	256	VAL	C-N-CA	5.09	130.49	122.34
1	A	431	TYR	CA-C-N	5.09	127.10	120.28
1	A	431	TYR	C-N-CA	5.09	127.10	120.28
1	C	288	GLN	CA-C-N	5.09	127.06	120.44
1	C	288	GLN	C-N-CA	5.09	127.06	120.44
1	K	158	LYS	CA-C-N	5.09	127.10	120.28
1	K	158	LYS	C-N-CA	5.09	127.10	120.28
1	A	102	SER	CA-C-N	5.09	127.05	120.44
1	A	102	SER	C-N-CA	5.09	127.05	120.44
1	A	107	ILE	CA-C-N	5.09	126.97	120.56
1	A	107	ILE	C-N-CA	5.09	126.97	120.56
1	C	531	ARG	CG-CD-NE	5.09	123.19	112.00
1	I	481	ILE	CA-C-N	5.09	127.06	120.44
1	I	481	ILE	C-N-CA	5.09	127.06	120.44
1	K	288	GLN	CA-C-N	5.09	127.05	120.44
1	K	288	GLN	C-N-CA	5.09	127.05	120.44
1	C	332	SER	CA-C-N	5.09	130.85	123.12
1	C	332	SER	C-N-CA	5.09	130.85	123.12
3	F	21	DT	O5'-C5'-C4'	5.09	118.43	110.80
1	I	103	ASP	CA-C-N	5.09	127.05	120.44
1	I	103	ASP	C-N-CA	5.09	127.05	120.44
1	I	326	PRO	CA-C-N	5.09	129.54	122.77
1	I	326	PRO	C-N-CA	5.09	129.54	122.77
1	K	332	SER	CA-C-N	5.09	130.85	123.12
1	K	332	SER	C-N-CA	5.09	130.85	123.12
1	A	174	TYR	CA-C-N	5.08	129.94	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	TYR	C-N-CA	5.08	129.94	123.08
1	A	299	LYS	CA-CB-CG	5.08	124.27	114.10
1	K	263	GLY	CA-C-N	5.08	127.93	120.71
1	K	263	GLY	C-N-CA	5.08	127.93	120.71
1	C	271	LYS	CA-CB-CG	5.08	124.27	114.10
1	C	173	PRO	CA-C-N	5.08	128.42	120.75
1	C	173	PRO	C-N-CA	5.08	128.42	120.75
1	I	497	LYS	CA-C-N	5.08	127.09	120.28
1	I	497	LYS	C-N-CA	5.08	127.09	120.28
1	K	234	TRP	CA-C-N	5.08	130.16	122.99
1	K	234	TRP	C-N-CA	5.08	130.16	122.99
1	A	5	ASN	CA-C-N	5.08	126.96	120.56
1	A	5	ASN	C-N-CA	5.08	126.96	120.56
1	A	9	SER	CA-C-N	5.08	130.75	122.07
1	A	9	SER	C-N-CA	5.08	130.75	122.07
1	A	289	PHE	CA-C-N	5.08	127.04	120.44
1	A	289	PHE	C-N-CA	5.08	127.04	120.44
1	A	289	PHE	N-CA-CB	5.08	117.37	110.01
1	C	428	PHE	CA-C-N	5.08	127.04	120.44
1	C	428	PHE	C-N-CA	5.08	127.04	120.44
1	C	498	ASN	N-CA-CB	5.08	117.37	110.01
1	C	158	LYS	CA-C-N	5.08	127.08	120.28
1	C	158	LYS	C-N-CA	5.08	127.08	120.28
1	C	269	PRO	CA-C-N	5.08	127.04	120.44
1	C	269	PRO	C-N-CA	5.08	127.04	120.44
1	I	184	LYS	CA-C-N	5.07	129.08	121.72
1	I	184	LYS	C-N-CA	5.07	129.08	121.72
1	I	299	LYS	CA-CB-CG	5.07	124.25	114.10
1	A	495	GLU	CA-C-N	5.07	127.07	120.28
1	A	495	GLU	C-N-CA	5.07	127.07	120.28
1	C	201	ILE	CA-C-N	5.07	127.03	120.44
1	C	201	ILE	C-N-CA	5.07	127.03	120.44
1	I	9	SER	CA-C-N	5.07	130.74	122.07
1	I	9	SER	C-N-CA	5.07	130.74	122.07
1	I	115	ARG	CA-C-N	5.07	127.91	120.71
1	I	115	ARG	C-N-CA	5.07	127.91	120.71
3	N	21	DT	O5'-C5'-C4'	5.07	118.40	110.80
1	I	242	ILE	N-CA-CB	5.07	116.47	110.55
1	K	235	ASN	CA-C-N	5.07	127.38	120.54
1	K	235	ASN	C-N-CA	5.07	127.38	120.54
1	I	91	LYS	CG-CD-CE	5.06	122.95	111.30
1	A	341	GLY	N-CA-C	5.06	121.50	114.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	464	GLY	CA-C-N	5.06	127.57	120.28
1	C	464	GLY	C-N-CA	5.06	127.57	120.28
2	M	-21	DA	N9-C1'-C2'	5.06	121.09	113.50
4	O	-14	DT	C2'-C3'-O3'	5.06	119.09	111.50
1	A	112	GLN	CA-C-N	5.06	127.33	120.65
1	A	112	GLN	C-N-CA	5.06	127.33	120.65
1	A	191	GLU	CA-C-N	5.06	127.02	120.44
1	A	191	GLU	C-N-CA	5.06	127.02	120.44
1	C	79	ASP	CA-C-N	5.06	127.02	120.44
1	C	79	ASP	C-N-CA	5.06	127.02	120.44
1	I	367	GLU	CB-CG-CD	5.06	121.20	112.60
1	K	464	GLY	CA-C-N	5.06	127.57	120.28
1	K	464	GLY	C-N-CA	5.06	127.57	120.28
1	K	269	PRO	CA-C-N	5.06	127.02	120.44
1	K	269	PRO	C-N-CA	5.06	127.02	120.44
1	A	195	VAL	N-CA-CB	5.06	116.47	110.55
1	A	245	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	A	274	ILE	CA-C-N	5.06	130.08	122.75
1	A	274	ILE	C-N-CA	5.06	130.08	122.75
1	A	370	ILE	N-CA-CB	5.06	116.47	110.55
1	I	146	GLU	CA-C-N	5.06	127.32	120.65
1	I	146	GLU	C-N-CA	5.06	127.32	120.65
1	A	367	GLU	CB-CG-CD	5.05	121.19	112.60
1	I	174	TYR	CA-C-N	5.05	129.90	123.08
1	I	174	TYR	C-N-CA	5.05	129.90	123.08
1	I	373	TYR	CA-C-N	5.05	127.00	120.44
1	I	373	TYR	C-N-CA	5.05	127.00	120.44
1	C	393	LEU	CA-C-N	5.05	127.00	120.44
1	C	393	LEU	C-N-CA	5.05	127.00	120.44
1	A	91	LYS	CG-CD-CE	5.05	122.91	111.30
1	C	391	SER	CA-C-N	5.05	127.00	120.44
1	C	391	SER	C-N-CA	5.05	127.00	120.44
1	K	4	LYS	CA-C-N	5.05	127.81	120.79
1	K	4	LYS	C-N-CA	5.05	127.81	120.79
1	I	195	VAL	N-CA-CB	5.04	116.45	110.55
1	C	99	GLY	CA-C-N	5.04	131.17	121.54
1	C	99	GLY	C-N-CA	5.04	131.17	121.54
1	C	221	THR	CA-C-N	5.04	127.00	120.44
1	C	221	THR	C-N-CA	5.04	127.00	120.44
1	C	434	GLY	CA-C-N	5.04	127.37	120.46
1	C	434	GLY	C-N-CA	5.04	127.37	120.46
1	K	531	ARG	CG-CD-NE	5.04	123.10	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	2	DA	C3'-C2'-C1'	5.04	109.16	101.60
1	A	184	LYS	CA-C-N	5.04	129.03	121.72
1	A	184	LYS	C-N-CA	5.04	129.03	121.72
1	C	11	ASN	CA-CB-CG	5.04	117.64	112.60
1	I	421	LYS	CA-C-N	5.04	127.80	120.79
1	I	421	LYS	C-N-CA	5.04	127.80	120.79
1	K	134	ARG	CG-CD-NE	5.04	123.09	112.00
1	C	367	GLU	CA-C-N	5.04	127.03	120.28
1	C	367	GLU	C-N-CA	5.04	127.03	120.28
2	E	-21	DA	N9-C1'-C2'	5.04	121.06	113.50
1	I	134	ARG	N-CA-CB	5.04	117.32	110.01
1	I	370	ILE	N-CA-CB	5.04	116.45	110.55
1	K	210	ASP	CA-C-N	5.04	130.74	123.13
1	K	210	ASP	C-N-CA	5.04	130.74	123.13
4	O	-7	DA	C3'-C2'-C1'	5.04	109.16	101.60
1	C	255	LYS	CB-CG-CD	5.04	122.89	111.30
1	I	40	GLN	CA-CB-CG	5.04	124.17	114.10
1	K	278	ASP	CA-C-N	5.03	127.53	120.28
1	K	278	ASP	C-N-CA	5.03	127.53	120.28
1	K	367	GLU	CA-C-N	5.03	127.02	120.28
1	K	367	GLU	C-N-CA	5.03	127.02	120.28
1	A	274	ILE	N-CA-CB	5.03	116.73	111.00
1	C	91	LYS	CB-CG-CD	5.03	122.87	111.30
1	C	388	HIS	CA-C-N	5.03	127.35	120.46
1	C	388	HIS	C-N-CA	5.03	127.35	120.46
4	G	-7	DA	C3'-C2'-C1'	5.03	109.15	101.60
1	I	289	PHE	N-CA-CB	5.03	117.31	110.01
1	K	391	SER	CA-C-N	5.03	126.98	120.44
1	K	391	SER	C-N-CA	5.03	126.98	120.44
1	A	481	ILE	CA-C-N	5.03	126.98	120.44
1	A	481	ILE	C-N-CA	5.03	126.98	120.44
1	I	289	PHE	CA-C-N	5.03	126.97	120.44
1	I	289	PHE	C-N-CA	5.03	126.97	120.44
1	K	221	THR	CA-C-N	5.03	126.98	120.44
1	K	221	THR	C-N-CA	5.03	126.98	120.44
1	I	424	GLU	CA-C-N	5.03	127.02	120.28
1	I	424	GLU	C-N-CA	5.03	127.02	120.28
1	I	506	LYS	CA-CB-CG	5.03	124.15	114.10
1	A	240	LYS	CA-CB-CG	5.02	124.15	114.10
1	I	102	SER	N-CA-CB	5.02	117.25	109.91
1	K	295	LYS	CA-C-N	5.02	127.08	120.60
1	K	295	LYS	C-N-CA	5.02	127.08	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	27	GLU	CB-CG-CD	5.02	121.14	112.60
1	K	74	LYS	CA-C-N	5.02	126.97	120.44
1	K	74	LYS	C-N-CA	5.02	126.97	120.44
1	K	201	ILE	CA-C-N	5.02	126.97	120.44
1	K	201	ILE	C-N-CA	5.02	126.97	120.44
1	K	255	LYS	CB-CG-CD	5.02	122.85	111.30
1	A	102	SER	N-CA-CB	5.02	117.24	109.91
1	C	29	GLU	CB-CG-CD	5.02	121.13	112.60
1	C	47	ILE	N-CA-CB	5.02	116.09	110.62
1	C	74	LYS	CA-C-N	5.02	126.97	120.44
1	C	74	LYS	C-N-CA	5.02	126.97	120.44
1	C	90	VAL	CA-C-N	5.02	126.97	120.44
1	C	90	VAL	C-N-CA	5.02	126.97	120.44
1	C	210	ASP	CA-C-N	5.02	130.71	123.13
1	C	210	ASP	C-N-CA	5.02	130.71	123.13
1	A	369	ALA	CA-C-N	5.02	126.88	120.56
1	A	369	ALA	C-N-CA	5.02	126.88	120.56
1	K	401	SER	CA-C-N	5.02	129.21	120.68
1	K	401	SER	C-N-CA	5.02	129.21	120.68
3	N	19	DC	C5'-C4'-C3'	5.02	122.42	114.90
1	C	401	SER	CA-C-N	5.01	129.20	120.68
1	C	401	SER	C-N-CA	5.01	129.20	120.68
1	I	369	ALA	CA-C-N	5.01	126.88	120.56
1	I	369	ALA	C-N-CA	5.01	126.88	120.56
1	A	284	ILE	CA-C-N	5.01	127.99	120.87
1	A	284	ILE	C-N-CA	5.01	127.99	120.87
4	G	-14	DT	C2'-C3'-O3'	5.01	119.02	111.50
1	I	252	VAL	CA-C-N	5.01	130.46	122.74
1	I	252	VAL	C-N-CA	5.01	130.46	122.74
1	I	354	LYS	CG-CD-CE	5.01	122.83	111.30
1	I	498	ASN	N-CA-CB	5.01	117.49	110.12
1	K	393	LEU	CA-C-N	5.01	126.96	120.44
1	K	393	LEU	C-N-CA	5.01	126.96	120.44
1	A	252	VAL	CA-C-N	5.01	130.46	122.74
1	A	252	VAL	C-N-CA	5.01	130.46	122.74
1	I	4	LYS	CA-CB-CG	5.01	124.12	114.10
1	A	506	LYS	CA-CB-CG	5.01	124.12	114.10
1	C	295	LYS	CA-C-N	5.01	127.06	120.60
1	C	295	LYS	C-N-CA	5.01	127.06	120.60
1	I	341	GLY	N-CA-C	5.01	121.43	114.92
1	A	40	GLN	CA-CB-CG	5.01	124.11	114.10
5	H	18	DA	O5'-C5'-C4'	5.01	118.31	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	29	GLU	CB-CG-CD	5.01	121.11	112.60
1	I	44	MET	CA-C-N	5.00	126.95	120.44
1	I	44	MET	C-N-CA	5.00	126.95	120.44
1	K	27	GLU	CB-CG-CD	5.00	121.11	112.60
1	I	191	GLU	CA-C-N	5.00	126.94	120.44
1	I	191	GLU	C-N-CA	5.00	126.94	120.44
1	K	91	LYS	CB-CG-CD	5.00	122.81	111.30
1	K	294	VAL	CA-C-N	5.00	126.94	120.44
1	K	294	VAL	C-N-CA	5.00	126.94	120.44
1	K	428	PHE	CA-C-N	5.00	126.94	120.44
1	K	428	PHE	C-N-CA	5.00	126.94	120.44
1	A	242	ILE	N-CA-CB	5.00	116.40	110.55
1	A	368	ASN	CA-C-N	5.00	126.94	120.44
1	A	368	ASN	C-N-CA	5.00	126.94	120.44
1	A	421	LYS	CA-C-N	5.00	127.74	120.79
1	A	421	LYS	C-N-CA	5.00	127.74	120.79
1	A	430	LYS	CG-CD-CE	5.00	122.80	111.30
1	C	294	VAL	CA-C-N	5.00	126.94	120.44
1	C	294	VAL	C-N-CA	5.00	126.94	120.44
1	K	158	LYS	CB-CG-CD	5.00	122.80	111.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ARG	Sidechain
1	A	248	TYR	Sidechain
2	E	-1	DT	Sidechain
3	F	2	DA	Sidechain
4	G	-12	DT	Sidechain
4	G	-2	DT	Sidechain
5	H	7	DT	Sidechain
1	I	248	TYR	Sidechain
1	I	95	ARG	Sidechain
1	K	23	ARG	Sidechain
2	M	-1	DT	Sidechain
3	N	2	DA	Sidechain
4	O	-12	DT	Sidechain
4	O	-2	DT	Sidechain
5	P	7	DT	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	4356	4425	4420	96	0
1	C	4356	4425	4420	70	0
1	I	4356	4425	4420	103	0
1	K	4356	4425	4420	74	0
2	E	694	393	361	35	0
2	M	694	393	360	36	0
3	F	679	373	339	36	0
3	N	679	373	340	32	0
4	G	511	285	247	16	0
4	O	511	285	247	16	0
5	H	493	274	242	9	0
5	P	493	274	242	6	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	I	1	0	0	0	0
6	K	1	0	0	0	0
All	All	22182	20350	20058	470	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (470) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:LYS:O	1:C:405:THR:OG1	1.98	0.82
1:K:404:LYS:O	1:K:405:THR:OG1	1.98	0.81
1:I:403:MET:HE2	1:I:403:MET:O	1.82	0.80
4:O:-25:DC:N3	4:O:-24:DA:N6	2.30	0.80
4:G:-25:DC:N3	4:G:-24:DA:N6	2.30	0.79
1:A:403:MET:SD	1:A:403:MET:N	2.56	0.79
1:I:403:MET:SD	1:I:403:MET:N	2.56	0.79
1:A:403:MET:HE2	1:A:403:MET:O	1.82	0.78
1:C:477:VAL:HG13	1:C:535:ILE:HG23	1.66	0.77
1:C:473:ASP:O	1:C:477:VAL:HG23	1.86	0.76
1:K:473:ASP:O	1:K:477:VAL:HG23	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:477:VAL:HG13	1:K:535:ILE:HG23	1.65	0.75
1:A:122:TYR:CE2	1:K:131:VAL:HG21	2.24	0.72
1:A:59:MET:SD	1:A:59:MET:N	2.65	0.70
1:A:235:ASN:ND2	1:A:238:THR:OG1	2.25	0.70
1:I:235:ASN:ND2	1:I:238:THR:OG1	2.25	0.70
1:C:190:ASP:O	1:C:194:VAL:HG23	1.92	0.69
1:A:122:TYR:CD2	1:K:131:VAL:HG21	2.28	0.69
1:I:59:MET:SD	1:I:59:MET:N	2.65	0.69
1:A:201:ILE:O	1:A:205:GLY:N	2.26	0.69
1:I:201:ILE:O	1:I:205:GLY:N	2.26	0.68
1:I:484:ILE:HG21	1:I:504:VAL:HG21	1.76	0.68
1:K:190:ASP:O	1:K:194:VAL:HG23	1.92	0.68
1:A:484:ILE:HG21	1:A:504:VAL:HG21	1.76	0.68
1:C:245:ASN:OD1	1:C:247:VAL:HG23	1.96	0.65
1:K:245:ASN:OD1	1:K:247:VAL:HG23	1.96	0.65
2:M:-29:DT:H2''	2:M:-28:DT:C5	2.32	0.65
1:A:122:TYR:CE2	1:K:131:VAL:CG2	2.80	0.65
2:E:-29:DT:H2''	2:E:-28:DT:C5	2.32	0.64
1:A:146:GLU:HG2	1:I:146:GLU:HG2	1.80	0.63
1:A:431:TYR:OH	1:C:430:LYS:NZ	2.28	0.63
1:C:303:LEU:HD12	4:G:-13:DA:C2	2.33	0.63
1:K:303:LEU:HD12	4:O:-13:DA:C2	2.33	0.63
1:K:353:CYS:O	1:K:357:LYS:N	2.30	0.63
1:C:353:CYS:O	1:C:357:LYS:N	2.30	0.63
2:E:-15:DC:H2'	2:E:-14:DT:H71	1.79	0.63
1:I:154:MET:SD	1:I:154:MET:N	2.72	0.63
1:C:255:LYS:O	1:C:268:ARG:NE	2.29	0.63
1:A:154:MET:SD	1:A:154:MET:N	2.72	0.63
1:K:530:LEU:HB3	1:K:535:ILE:HD11	1.81	0.63
1:I:250:GLY:O	1:I:279:ALA:N	2.33	0.62
1:I:308:GLU:OE1	1:I:308:GLU:N	2.32	0.62
1:A:202:PHE:O	1:A:295:LYS:NZ	2.29	0.62
1:K:255:LYS:O	1:K:268:ARG:NE	2.29	0.62
1:I:167:TRP:CD1	1:I:185:LEU:HD21	2.35	0.61
1:C:530:LEU:HB3	1:C:535:ILE:HD11	1.81	0.61
2:E:-31:DT:C6	2:E:-30:DT:H72	2.35	0.61
1:I:202:PHE:O	1:I:295:LYS:NZ	2.29	0.61
2:M:-31:DT:C6	2:M:-30:DT:H72	2.35	0.61
1:A:250:GLY:O	1:A:279:ALA:N	2.33	0.61
1:C:138:PHE:CB	1:I:138:PHE:CE1	2.82	0.61
1:C:138:PHE:HB3	1:I:138:PHE:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:-23:DG:H2'	2:E:-22:DT:H71	1.83	0.61
1:C:320:CYS:O	1:C:324:GLY:N	2.34	0.61
1:C:502:ARG:O	1:C:531:ARG:NE	2.34	0.61
1:K:320:CYS:O	1:K:324:GLY:N	2.34	0.61
1:K:215:ALA:N	4:O:-14:DT:OP2	2.34	0.61
1:K:502:ARG:O	1:K:531:ARG:NE	2.34	0.60
1:A:48:LEU:HD13	1:A:55:TYR:CD1	2.37	0.60
1:K:176:TYR:CE1	1:K:283:ILE:HD12	2.37	0.60
1:C:215:ALA:N	4:G:-14:DT:OP2	2.34	0.60
1:C:176:TYR:CE1	1:C:283:ILE:HD12	2.37	0.60
2:M:-28:DT:C2	3:N:28:DA:C2	2.90	0.59
1:C:138:PHE:CB	1:I:138:PHE:CD1	2.85	0.59
1:K:381:ASN:ND2	1:K:382:ASP:OD1	2.35	0.59
1:C:381:ASN:ND2	1:C:382:ASP:OD1	2.36	0.59
2:E:-28:DT:C2	3:F:28:DA:C2	2.90	0.59
2:M:-23:DG:H2'	2:M:-22:DT:H71	1.83	0.59
1:I:48:LEU:HD13	1:I:55:TYR:CD1	2.37	0.59
1:C:227:THR:HA	1:C:234:TRP:CZ2	2.38	0.59
1:C:371:LEU:HD21	1:C:488:TYR:CE1	2.38	0.59
1:A:151:ARG:NH2	3:F:3:DG:O4'	2.35	0.58
1:I:504:VAL:HG22	1:I:534:PHE:CZ	2.38	0.58
1:I:235:ASN:ND2	3:N:9:DT:OP2	2.36	0.58
1:A:504:VAL:HG22	1:A:534:PHE:CZ	2.38	0.58
1:I:392:MET:HE1	1:I:529:ILE:HG23	1.86	0.58
1:I:151:ARG:NH2	3:N:3:DG:O4'	2.35	0.58
1:I:190:ASP:O	1:I:194:VAL:HG23	2.02	0.58
1:A:190:ASP:O	1:A:194:VAL:HG23	2.02	0.58
1:A:235:ASN:ND2	3:F:9:DT:OP2	2.36	0.58
1:A:392:MET:HE1	1:A:529:ILE:HG23	1.86	0.58
1:I:515:LYS:NZ	2:M:-21:DA:OP1	2.31	0.58
1:I:403:MET:HE3	1:I:407:LYS:CG	2.34	0.58
1:A:403:MET:HE3	1:A:407:LYS:CG	2.34	0.58
1:K:386:THR:O	1:K:390:ASN:ND2	2.37	0.58
1:A:477:VAL:HG22	1:A:535:ILE:O	2.04	0.57
1:C:386:THR:O	1:C:390:ASN:ND2	2.37	0.57
1:K:364:ASN:O	1:K:368:ASN:ND2	2.37	0.57
1:K:371:LEU:HD21	1:K:488:TYR:CE1	2.38	0.57
1:C:364:ASN:O	1:C:368:ASN:ND2	2.37	0.57
1:I:179:ASN:O	1:I:183:SER:N	2.37	0.57
1:K:17:GLY:HA3	1:K:57:LEU:HD23	1.86	0.57
1:K:235:ASN:OD1	1:K:238:THR:N	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:477:VAL:HG22	1:I:535:ILE:O	2.04	0.57
1:I:22:SER:HB3	3:N:2:DA:P	2.45	0.56
1:I:237:TYR:OH	2:M:-11:DA:N7	2.31	0.56
1:A:179:ASN:O	1:A:183:SER:N	2.37	0.56
1:C:138:PHE:HB2	1:I:138:PHE:CD1	2.40	0.56
1:K:227:THR:HA	1:K:234:TRP:CH2	2.40	0.56
1:C:17:GLY:HA3	1:C:57:LEU:HD23	1.87	0.56
1:A:22:SER:HB3	3:F:2:DA:P	2.45	0.55
1:C:138:PHE:HB2	1:I:138:PHE:CE1	2.42	0.55
1:A:235:ASN:OD1	1:A:237:TYR:N	2.40	0.55
1:I:235:ASN:OD1	1:I:237:TYR:N	2.39	0.55
1:A:308:GLU:OE1	1:A:308:GLU:N	2.32	0.54
1:A:427:ILE:HD12	1:A:448:LEU:HD11	1.89	0.54
1:K:386:THR:HG23	1:K:472:ILE:HB	1.89	0.54
1:A:515:LYS:NZ	2:E:-21:DA:OP1	2.31	0.54
1:A:161:TYR:HB2	1:A:168:ILE:HD11	1.90	0.54
1:I:431:TYR:OH	1:K:430:LYS:NZ	2.28	0.54
1:C:386:THR:HG23	1:C:472:ILE:HB	1.89	0.54
1:K:138:PHE:CD1	1:K:138:PHE:C	2.86	0.53
1:I:427:ILE:HD12	1:I:448:LEU:HD11	1.89	0.53
1:I:382:ASP:OD1	1:I:478:ARG:NE	2.40	0.53
1:A:48:LEU:HD11	1:A:57:LEU:HD21	1.91	0.53
1:K:225:ILE:O	1:K:234:TRP:NE1	2.41	0.53
1:A:7:VAL:HG11	1:A:51:ILE:HG21	1.91	0.53
1:I:7:VAL:HG11	1:I:51:ILE:HG21	1.91	0.52
1:A:382:ASP:OD1	1:A:478:ARG:NE	2.40	0.52
1:I:167:TRP:CE2	1:I:185:LEU:HD11	2.45	0.52
1:K:16:LEU:HD21	1:K:76:CYS:HB3	1.92	0.52
1:A:48:LEU:HD13	1:A:55:TYR:CE1	2.45	0.52
1:A:53:ILE:HG23	1:A:54:PRO:HD2	1.92	0.52
2:E:-29:DT:H2''	2:E:-28:DT:C4	2.45	0.52
1:K:530:LEU:CB	1:K:535:ILE:HD11	2.40	0.52
1:A:359:THR:HG23	1:A:361:VAL:HG13	1.92	0.51
1:I:48:LEU:HD11	1:I:57:LEU:HD21	1.91	0.51
1:I:359:THR:HG23	1:I:361:VAL:HG13	1.92	0.51
2:M:-29:DT:H2''	2:M:-28:DT:C4	2.45	0.51
1:C:530:LEU:CB	1:C:535:ILE:HD11	2.40	0.51
1:I:48:LEU:HD13	1:I:55:TYR:CE1	2.46	0.51
2:M:-33:DT:H2''	2:M:-32:DT:C5'	2.41	0.51
1:I:167:TRP:CD2	1:I:185:LEU:HD11	2.46	0.51
1:K:381:ASN:OD1	1:K:383:SER:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:-33:DT:H2''	2:E:-32:DT:C5'	2.41	0.51
1:I:53:ILE:HG23	1:I:54:PRO:HD2	1.92	0.51
1:C:381:ASN:OD1	1:C:383:SER:N	2.44	0.50
3:F:8:DA:H2''	3:F:9:DT:H71	1.93	0.50
2:M:-30:DT:H2''	2:M:-29:DT:C6	2.46	0.50
4:G:-19:DA:H2'	4:G:-18:DT:H71	1.93	0.50
1:I:269:PRO:O	1:I:273:GLN:N	2.43	0.50
1:A:305:ASN:HB2	1:A:311:LEU:HD21	1.94	0.50
1:I:41:LYS:O	1:I:45:ASN:ND2	2.44	0.50
1:A:392:MET:HE1	1:A:529:ILE:HA	1.94	0.50
1:I:305:ASN:HB2	1:I:311:LEU:HD21	1.94	0.50
1:A:41:LYS:O	1:A:45:ASN:ND2	2.44	0.50
1:A:377:LEU:HD23	1:A:380:LEU:HD11	1.94	0.50
2:E:-30:DT:H2''	2:E:-29:DT:C6	2.46	0.50
1:A:269:PRO:O	1:A:273:GLN:N	2.43	0.50
1:I:258:GLU:OE1	1:I:268:ARG:NH2	2.45	0.50
1:A:258:GLU:OE1	1:A:268:ARG:NH2	2.45	0.49
1:C:278:ASP:OD1	1:C:278:ASP:N	2.43	0.49
1:K:210:ASP:OD1	1:K:211:TYR:N	2.46	0.49
1:C:158:LYS:HA	1:C:168:ILE:HD12	1.94	0.49
1:I:392:MET:HE1	1:I:529:ILE:HA	1.94	0.49
3:N:8:DA:H2''	3:N:9:DT:H71	1.93	0.49
1:C:210:ASP:OD1	1:C:211:TYR:N	2.46	0.49
1:C:227:THR:HG22	1:C:234:TRP:CD2	2.48	0.49
3:F:29:DA:H2''	3:F:30:DA:C8	2.48	0.49
1:A:210:ASP:OD1	1:A:211:TYR:N	2.46	0.49
1:I:161:TYR:HB2	1:I:168:ILE:HD11	1.94	0.49
1:A:322:LYS:NZ	1:A:358:CYS:O	2.42	0.49
1:C:16:LEU:HD21	1:C:76:CYS:HB3	1.94	0.49
1:A:252:VAL:HG23	1:A:279:ALA:HB3	1.95	0.48
1:K:204:ASN:OD1	1:K:204:ASN:N	2.46	0.48
4:O:-19:DA:H2'	4:O:-18:DT:H71	1.93	0.48
1:A:176:TYR:C	1:A:188:VAL:HG23	2.38	0.48
2:E:-31:DT:H2'	2:E:-30:DT:C6	2.48	0.48
1:I:377:LEU:HD23	1:I:380:LEU:HD11	1.94	0.48
4:O:-4:DG:C4	4:O:-3:DA:C8	3.01	0.48
1:A:330:TYR:OH	3:F:19:DC:N4	2.45	0.48
1:C:204:ASN:OD1	1:C:204:ASN:N	2.47	0.48
4:G:-4:DG:C4	4:G:-3:DA:C8	3.01	0.48
1:I:330:TYR:OH	3:N:19:DC:N4	2.45	0.48
2:E:-8:DT:H2''	2:E:-7:DA:N7	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:268:ARG:O	1:K:273:GLN:NE2	2.46	0.48
3:N:29:DA:H2''	3:N:30:DA:C8	2.48	0.48
4:G:-25:DC:C2	4:G:-24:DA:N6	2.82	0.48
1:I:252:VAL:HG23	1:I:279:ALA:HB3	1.95	0.48
1:A:373:TYR:CZ	1:A:377:LEU:HD21	2.48	0.48
1:C:268:ARG:O	1:C:273:GLN:NE2	2.47	0.48
3:F:11:DT:H2'	3:F:12:DT:H71	1.95	0.48
3:N:5:DT:H4'	3:N:5:DT:OP1	2.13	0.48
1:C:13:THR:HG1	1:C:14:ASN:H	1.62	0.48
3:F:16:DA:H3'	3:F:17:DT:H71	1.96	0.48
1:I:210:ASP:OD1	1:I:211:TYR:N	2.46	0.48
1:K:157:ALA:O	1:K:160:THR:OG1	2.27	0.48
1:K:278:ASP:N	1:K:278:ASP:OD1	2.43	0.48
2:M:-8:DT:H2''	2:M:-7:DA:N7	2.28	0.48
3:N:27:DA:H2''	3:N:28:DA:C5	2.49	0.48
1:A:120:THR:OG1	1:A:123:LYS:O	2.29	0.48
3:F:27:DA:H2''	3:F:28:DA:C5	2.49	0.48
1:I:360:TYR:CD1	2:M:-21:DA:OP2	2.67	0.48
1:K:158:LYS:HA	1:K:168:ILE:HD12	1.94	0.48
2:M:-31:DT:H2'	2:M:-30:DT:C6	2.48	0.48
1:I:176:TYR:C	1:I:188:VAL:HG23	2.38	0.48
2:M:-19:DG:H2'	2:M:-18:DT:H71	1.96	0.48
1:I:373:TYR:CZ	1:I:377:LEU:HD21	2.48	0.47
1:K:13:THR:HG1	1:K:86:GLN:CD	2.21	0.47
1:K:319:THR:HG23	1:K:507:ASP:OD1	2.14	0.47
1:A:473:ASP:O	1:A:476:THR:N	2.47	0.47
2:E:-19:DG:H2'	2:E:-18:DT:H71	1.96	0.47
2:M:-25:DT:H2''	2:M:-24:DA:O4'	2.14	0.47
1:A:392:MET:SD	1:A:529:ILE:HG23	2.55	0.47
1:I:322:LYS:NZ	1:I:358:CYS:O	2.42	0.47
1:I:477:VAL:HG21	1:I:535:ILE:HG23	1.96	0.47
1:A:86:GLN:N	1:A:86:GLN:OE1	2.47	0.47
3:F:5:DT:H4'	3:F:5:DT:OP1	2.13	0.47
1:I:86:GLN:N	1:I:86:GLN:OE1	2.47	0.47
1:K:104:ALA:O	1:K:108:VAL:HG23	2.14	0.47
1:I:392:MET:SD	1:I:529:ILE:HG23	2.55	0.47
3:N:16:DA:H3'	3:N:17:DT:H71	1.96	0.47
4:O:-25:DC:C2	4:O:-24:DA:N6	2.82	0.47
1:A:427:ILE:HD13	1:A:444:ARG:HB3	1.96	0.47
1:C:319:THR:HG23	1:C:507:ASP:OD1	2.14	0.47
2:E:-25:DT:H2''	2:E:-24:DA:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:312:SER:OG	1:I:315:ALA:HB2	2.15	0.47
1:I:431:TYR:HH	1:K:430:LYS:HZ1	1.56	0.47
2:M:-20:DA:H2''	2:M:-19:DG:O4'	2.14	0.47
1:A:514:GLN:OE1	1:A:517:LYS:NZ	2.32	0.47
2:E:-9:DA:C2	3:F:10:DA:C2	3.02	0.47
1:A:511:ASN:O	1:A:525:GLU:N	2.47	0.47
1:I:373:TYR:CE1	1:I:377:LEU:HD21	2.50	0.47
1:I:514:GLN:OE1	1:I:517:LYS:NZ	2.32	0.47
1:C:104:ALA:O	1:C:108:VAL:HG23	2.14	0.47
1:I:473:ASP:O	1:I:476:THR:N	2.47	0.47
2:M:-3:DC:H2'	2:M:-2:DT:C6	2.50	0.47
1:A:360:TYR:CD1	2:E:-21:DA:OP2	2.67	0.46
3:N:11:DT:H2'	3:N:12:DT:H71	1.97	0.46
2:E:-20:DA:H2''	2:E:-19:DG:O4'	2.14	0.46
2:M:-9:DA:C2	3:N:10:DA:C2	3.02	0.46
1:A:187:PRO:HB3	1:A:283:ILE:HD11	1.98	0.46
1:A:176:TYR:CE1	1:A:283:ILE:HD12	2.51	0.46
1:I:187:PRO:HB3	1:I:283:ILE:HD11	1.98	0.46
1:I:403:MET:HE3	1:I:407:LYS:HG3	1.97	0.46
1:K:235:ASN:ND2	1:K:238:THR:OG1	2.47	0.46
1:A:431:TYR:HH	1:C:430:LYS:HZ2	1.58	0.46
1:A:477:VAL:HG21	1:A:535:ILE:HG23	1.97	0.46
1:A:312:SER:OG	1:A:315:ALA:HB2	2.15	0.46
1:A:373:TYR:CE1	1:A:377:LEU:HD21	2.50	0.46
3:F:27:DA:H2''	3:F:28:DA:N7	2.31	0.46
1:I:161:TYR:CB	1:I:168:ILE:HD11	2.45	0.46
1:I:427:ILE:HD13	1:I:444:ARG:HB3	1.97	0.46
2:E:-30:DT:C5	2:E:-29:DT:C4	3.04	0.46
1:K:321:SER:HA	1:K:509:ILE:HG23	1.98	0.46
2:M:-4:DG:C4	2:M:-3:DC:C5	3.04	0.46
2:E:-4:DG:C4	2:E:-3:DC:C5	3.04	0.46
1:K:466:GLN:O	1:K:533:ASN:ND2	2.49	0.46
2:E:-28:DT:N3	3:F:28:DA:C6	2.84	0.46
1:C:466:GLN:O	1:C:533:ASN:ND2	2.49	0.45
3:F:22:DA:H1'	3:F:23:DC:O4'	2.16	0.45
3:N:22:DA:H1'	3:N:23:DC:O4'	2.16	0.45
1:A:227:THR:HA	1:A:234:TRP:CZ3	2.51	0.45
1:A:303:LEU:HD12	1:A:311:LEU:HD22	1.98	0.45
1:I:201:ILE:HG23	1:I:206:LEU:HB2	1.99	0.45
2:M:-28:DT:N3	3:N:28:DA:C6	2.84	0.45
3:N:27:DA:H2''	3:N:28:DA:N7	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:MET:HE3	1:A:407:LYS:HG3	1.97	0.45
1:C:477:VAL:HG13	1:C:535:ILE:CG2	2.43	0.45
1:I:303:LEU:HD12	1:I:311:LEU:HD22	1.98	0.45
3:N:17:DT:H2''	3:N:18:DA:C8	2.51	0.45
1:C:138:PHE:HB3	1:I:138:PHE:CZ	2.52	0.45
4:G:-19:DA:C2	5:H:20:DG:C2	3.04	0.45
3:F:17:DT:H2''	3:F:18:DA:C8	2.51	0.45
1:I:406:LYS:HE2	1:I:465:LEU:HD23	1.98	0.45
2:M:-30:DT:C5	2:M:-29:DT:C4	3.04	0.45
1:A:533:ASN:OD1	1:A:533:ASN:N	2.50	0.45
4:G:-18:DT:C6	4:G:-17:DT:H72	2.51	0.45
1:I:176:TYR:CE1	1:I:283:ILE:HD12	2.51	0.45
4:O:-25:DC:H4'	4:O:-24:DA:OP1	2.17	0.45
4:O:-17:DT:H2''	4:O:-16:DA:O5'	2.17	0.45
1:C:321:SER:HA	1:C:509:ILE:HG23	1.97	0.45
1:I:120:THR:OG1	1:I:123:LYS:O	2.29	0.45
4:O:-7:DA:C2	5:P:8:DA:C2	3.05	0.45
4:O:-20:DC:H2''	4:O:-19:DA:O4'	2.17	0.45
2:M:-22:DT:C2	2:M:-21:DA:C8	3.05	0.45
4:O:-18:DT:C6	4:O:-17:DT:H72	2.51	0.45
1:A:178:LEU:HA	1:A:185:LEU:HD23	1.99	0.45
1:A:13:THR:OG1	1:A:14:ASN:N	2.51	0.44
1:A:406:LYS:HE2	1:A:465:LEU:HD23	1.98	0.44
3:F:23:DC:H2''	3:F:24:DT:H5'	1.99	0.44
4:G:-17:DT:H2''	4:G:-16:DA:O5'	2.17	0.44
1:I:123:LYS:NZ	1:I:132:ASP:OD1	2.46	0.44
4:O:-19:DA:C2	5:P:20:DG:C2	3.04	0.44
1:C:250:GLY:O	1:C:279:ALA:N	2.50	0.44
1:C:327:LEU:O	1:C:351:LEU:HD11	2.18	0.44
4:G:-7:DA:C2	5:H:8:DA:C2	3.05	0.44
5:H:6:DG:C5	5:H:7:DT:C4	3.05	0.44
1:I:227:THR:HA	1:I:234:TRP:CZ3	2.52	0.44
3:N:27:DA:C2	3:N:28:DA:C2	3.05	0.44
1:C:157:ALA:O	1:C:160:THR:OG1	2.27	0.44
4:G:-25:DC:H4'	4:G:-24:DA:OP1	2.17	0.44
4:G:-20:DC:H2''	4:G:-19:DA:O4'	2.17	0.44
1:I:178:LEU:HA	1:I:185:LEU:HD23	1.99	0.44
1:K:227:THR:HA	1:K:234:TRP:CZ3	2.52	0.44
1:K:250:GLY:O	1:K:279:ALA:N	2.50	0.44
3:F:27:DA:C2	3:F:28:DA:C2	3.05	0.44
1:I:37:LEU:HD23	1:I:37:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:-9:DG:H2'	4:O:-8:DT:H71	2.00	0.44
2:E:-22:DT:C2	2:E:-21:DA:C8	3.05	0.44
4:G:-9:DG:H2'	4:G:-8:DT:H71	2.00	0.44
1:I:13:THR:OG1	1:I:14:ASN:N	2.51	0.44
1:A:37:LEU:O	1:A:37:LEU:HD23	2.18	0.44
1:A:201:ILE:HG23	1:A:206:LEU:HB2	1.99	0.44
4:G:-20:DC:C2	4:G:-19:DA:C8	3.06	0.44
1:I:44:MET:HA	1:I:47:ILE:HD12	1.99	0.44
1:K:138:PHE:CG	1:K:139:GLU:N	2.78	0.44
1:K:477:VAL:HG13	1:K:535:ILE:CG2	2.42	0.44
2:E:-28:DT:C4	3:F:28:DA:N1	2.86	0.44
1:K:327:LEU:O	1:K:351:LEU:HD11	2.18	0.44
1:C:242:ILE:HG23	1:C:248:TYR:OH	2.18	0.44
1:I:139:GLU:HA	1:I:142:MET:HE3	2.00	0.44
1:K:213:TYR:HB2	1:K:236:GLN:HB2	2.00	0.44
1:K:330:TYR:OH	5:P:16:DT:H71	2.17	0.44
2:M:-30:DT:H2''	2:M:-29:DT:H6	1.83	0.44
1:I:511:ASN:O	1:I:525:GLU:N	2.47	0.43
1:K:242:ILE:HG23	1:K:248:TYR:OH	2.18	0.43
1:K:248:TYR:O	1:K:283:ILE:N	2.48	0.43
3:N:23:DC:H2''	3:N:24:DT:H5'	1.99	0.43
1:I:111:LEU:O	1:I:115:ARG:N	2.51	0.43
1:K:105:GLY:O	1:K:109:ASN:ND2	2.51	0.43
1:A:7:VAL:HG11	1:A:51:ILE:CG2	2.49	0.43
3:F:17:DT:C2	3:F:18:DA:N7	2.86	0.43
2:M:-30:DT:C2'	2:M:-29:DT:C6	3.01	0.43
5:P:6:DG:C5	5:P:7:DT:C4	3.06	0.43
1:A:44:MET:HA	1:A:47:ILE:HD12	1.99	0.43
1:A:167:TRP:CD2	1:A:185:LEU:HD11	2.53	0.43
3:F:23:DC:H2''	3:F:24:DT:C5'	2.48	0.43
2:M:-31:DT:C2'	2:M:-30:DT:C6	3.01	0.43
1:A:29:GLU:HG2	1:A:36:THR:H	1.83	0.43
1:A:111:LEU:O	1:A:115:ARG:N	2.51	0.43
1:C:105:GLY:O	1:C:109:ASN:ND2	2.52	0.43
1:C:289:PHE:O	1:C:293:GLN:NE2	2.50	0.43
1:I:16:LEU:HD21	1:I:76:CYS:HB3	2.01	0.43
1:K:127:PRO:HA	1:K:133:MET:SD	2.58	0.43
1:K:227:THR:HG22	1:K:234:TRP:CE3	2.53	0.43
1:K:254:TYR:CD2	5:P:6:DG:H5''	2.54	0.43
3:N:23:DC:H2''	3:N:24:DT:C5'	2.48	0.43
2:E:-31:DT:C2'	2:E:-30:DT:C6	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:-28:DT:C4	3:N:28:DA:N1	2.86	0.43
1:C:315:ALA:HB2	5:H:13:DT:OP1	2.19	0.43
1:A:389:ILE:HG22	1:A:472:ILE:HD13	2.01	0.43
2:E:-30:DT:C2'	2:E:-29:DT:C6	3.01	0.43
1:I:352:THR:HG21	1:I:360:TYR:CE1	2.54	0.43
1:A:352:THR:HG21	1:A:360:TYR:CE1	2.54	0.43
1:K:289:PHE:O	1:K:293:GLN:NE2	2.50	0.43
1:A:17:GLY:HA2	1:A:89:ALA:O	2.18	0.43
2:E:-32:DT:H2''	2:E:-31:DT:O4'	2.19	0.43
1:I:351:LEU:O	1:I:361:VAL:O	2.37	0.43
1:A:16:LEU:HD21	1:A:76:CYS:HB3	2.01	0.42
1:I:17:GLY:HA2	1:I:89:ALA:O	2.18	0.42
1:K:197:LEU:CD1	1:K:201:ILE:HD11	2.49	0.42
2:M:-32:DT:H2''	2:M:-31:DT:O4'	2.19	0.42
3:N:17:DT:C2	3:N:18:DA:N7	2.86	0.42
1:A:104:ALA:O	1:A:108:VAL:HG23	2.20	0.42
1:C:248:TYR:O	1:C:283:ILE:N	2.48	0.42
3:N:6:DG:C5	3:N:7:DT:C4	3.07	0.42
4:O:-20:DC:C2	4:O:-19:DA:C8	3.06	0.42
1:A:21:ARG:CZ	1:A:37:LEU:HB2	2.49	0.42
1:A:351:LEU:O	1:A:361:VAL:O	2.37	0.42
1:C:127:PRO:HA	1:C:133:MET:SD	2.60	0.42
4:G:-17:DT:H4'	4:G:-16:DA:OP1	2.20	0.42
1:I:104:ALA:O	1:I:108:VAL:HG23	2.20	0.42
1:I:430:LYS:NZ	1:K:49:THR:OG1	2.43	0.42
1:A:200:ASN:OD1	1:A:204:ASN:ND2	2.53	0.42
2:E:-11:DA:H2'	2:E:-10:DT:H72	2.02	0.42
3:F:14:DA:C4	3:F:15:DG:C8	3.07	0.42
1:I:7:VAL:HG11	1:I:51:ILE:CG2	2.49	0.42
1:I:200:ASN:OD1	1:I:204:ASN:ND2	2.53	0.42
1:K:472:ILE:HD13	1:K:473:ASP:H	1.84	0.42
4:O:-17:DT:H4'	4:O:-16:DA:OP1	2.20	0.42
1:C:197:LEU:CD1	1:C:201:ILE:HD11	2.49	0.42
1:I:533:ASN:N	1:I:533:ASN:OD1	2.50	0.42
2:E:-7:DA:C5	2:E:-6:DC:C4	3.08	0.42
3:F:6:DG:C5	3:F:7:DT:C4	3.07	0.42
3:N:14:DA:C4	3:N:15:DG:C8	3.07	0.42
1:C:330:TYR:OH	5:H:16:DT:H71	2.19	0.42
1:C:386:THR:OG1	1:C:472:ILE:HG13	2.20	0.42
2:E:-22:DT:N3	2:E:-21:DA:C5	2.88	0.42
1:I:389:ILE:HG22	1:I:472:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:ILE:HD13	1:C:473:ASP:H	1.84	0.42
1:C:496:LYS:O	1:C:500:LEU:HD13	2.20	0.42
1:K:386:THR:OG1	1:K:472:ILE:HG13	2.20	0.42
2:M:-34:DT:H2''	2:M:-33:DT:H5'	2.01	0.42
1:A:36:THR:HA	1:A:39:GLU:CD	2.44	0.42
3:N:32:DA:H2''	3:N:33:DA:C5'	2.50	0.42
1:A:16:LEU:HB2	1:A:85:TYR:CG	2.55	0.41
1:A:184:LYS:NZ	1:A:279:ALA:O	2.51	0.41
1:C:254:TYR:CD2	5:H:6:DG:H5''	2.55	0.41
2:E:-30:DT:H2''	2:E:-29:DT:H6	1.83	0.41
2:M:-22:DT:N3	2:M:-21:DA:C5	2.88	0.41
2:M:-19:DG:H2'	2:M:-18:DT:C6	2.55	0.41
2:M:-19:DG:H2''	2:M:-18:DT:O5'	2.20	0.41
2:M:-7:DA:C5	2:M:-6:DC:C4	3.08	0.41
3:N:20:DT:H4'	3:N:21:DT:OP1	2.20	0.41
1:A:123:LYS:NZ	1:A:132:ASP:OD1	2.46	0.41
1:K:398:ASP:OD1	1:K:398:ASP:N	2.53	0.41
1:K:477:VAL:HG22	1:K:535:ILE:HG22	2.02	0.41
1:A:197:LEU:HD11	1:A:201:ILE:HD11	2.01	0.41
1:A:227:THR:HB	1:A:228:PRO:CD	2.51	0.41
1:A:500:LEU:O	1:A:504:VAL:HG23	2.20	0.41
1:C:398:ASP:N	1:C:398:ASP:OD1	2.53	0.41
3:F:31:DA:C4	3:F:32:DA:C8	3.09	0.41
1:K:404:LYS:O	1:K:405:THR:CB	2.68	0.41
2:E:-34:DT:H2''	2:E:-33:DT:H5'	2.01	0.41
1:C:65:GLU:OE2	5:H:2:DA:H5''	2.20	0.41
5:H:2:DA:C8	5:H:3:DT:C5	3.09	0.41
1:K:48:LEU:HD13	1:K:55:TYR:CD2	2.56	0.41
1:A:403:MET:HE2	1:A:403:MET:C	2.46	0.41
1:A:516:ARG:HB2	2:E:-22:DT:OP1	2.20	0.41
1:C:495:GLU:O	1:C:499:GLU:HG2	2.21	0.41
3:F:32:DA:H2''	3:F:33:DA:O4'	2.21	0.41
3:N:18:DA:H2'	3:N:19:DC:O4'	2.21	0.41
3:N:32:DA:H2''	3:N:33:DA:O4'	2.21	0.41
1:A:186:ASP:N	1:A:186:ASP:OD1	2.53	0.41
1:C:48:LEU:HD13	1:C:55:TYR:CD2	2.56	0.41
2:M:-32:DT:H2''	2:M:-31:DT:C5'	2.51	0.41
4:O:-18:DT:C4	4:O:-17:DT:C4	3.09	0.41
1:C:427:ILE:HG22	1:C:441:PHE:CE1	2.56	0.41
2:E:-19:DG:H2'	2:E:-18:DT:C6	2.55	0.41
3:F:18:DA:H2'	3:F:19:DC:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:32:DA:H2''	3:F:33:DA:C5'	2.50	0.41
1:I:197:LEU:HD11	1:I:201:ILE:HD11	2.01	0.41
1:K:276:VAL:HG12	1:K:279:ALA:HB2	2.02	0.41
1:K:315:ALA:HB2	5:P:13:DT:OP1	2.20	0.41
1:K:424:GLU:OE1	1:K:448:LEU:HD23	2.21	0.41
1:K:495:GLU:O	1:K:499:GLU:HG2	2.21	0.41
1:A:320:CYS:O	1:A:324:GLY:HA2	2.21	0.41
1:C:252:VAL:HG23	1:C:279:ALA:HB3	2.02	0.41
1:C:477:VAL:HG22	1:C:535:ILE:HG22	2.02	0.41
1:C:484:ILE:HG21	1:C:504:VAL:HG21	2.03	0.41
2:E:-28:DT:N3	3:F:28:DA:C2	2.88	0.41
2:E:-19:DG:H2''	2:E:-18:DT:O5'	2.20	0.41
4:G:-18:DT:C4	4:G:-17:DT:C4	3.09	0.41
1:I:186:ASP:OD1	1:I:186:ASP:N	2.53	0.41
1:I:516:ARG:HB2	2:M:-22:DT:OP1	2.20	0.41
2:M:-28:DT:N3	3:N:28:DA:C2	2.88	0.41
2:M:-5:DA:C2	3:N:6:DG:C2	3.08	0.41
1:C:404:LYS:O	1:C:405:THR:CB	2.68	0.41
1:C:424:GLU:OE1	1:C:448:LEU:HD23	2.21	0.41
2:E:-5:DA:C2	3:F:6:DG:C2	3.08	0.41
5:H:15:DT:H2''	5:H:16:DT:C6	2.56	0.41
1:K:496:LYS:O	1:K:500:LEU:HD13	2.20	0.41
3:F:21:DT:H2'	3:F:22:DA:C8	2.56	0.40
1:I:16:LEU:HB2	1:I:85:TYR:CG	2.55	0.40
1:I:320:CYS:O	1:I:324:GLY:HA2	2.20	0.40
1:I:427:ILE:HG23	1:I:436:TYR:HE2	1.86	0.40
2:E:-29:DT:O2	3:F:29:DA:C2	2.74	0.40
1:I:103:ASP:N	1:I:103:ASP:OD1	2.53	0.40
1:K:252:VAL:HG23	1:K:279:ALA:HB3	2.02	0.40
3:N:20:DT:H2''	3:N:21:DT:C5'	2.51	0.40
3:F:14:DA:H2''	3:F:15:DG:C5'	2.52	0.40
1:I:21:ARG:CZ	1:I:37:LEU:HB2	2.51	0.40
1:I:500:LEU:O	1:I:504:VAL:HG23	2.21	0.40
1:K:376:SER:O	1:K:380:LEU:N	2.48	0.40
3:N:31:DA:C4	3:N:32:DA:C8	3.09	0.40
1:A:427:ILE:HG23	1:A:436:TYR:HE2	1.86	0.40
1:A:507:ASP:OD1	1:A:508:VAL:N	2.55	0.40
1:C:123:LYS:CG	1:C:124:VAL:N	2.85	0.40
3:F:6:DG:C8	3:F:7:DT:H72	2.57	0.40
3:F:20:DT:H2''	3:F:21:DT:C5'	2.51	0.40
3:F:20:DT:H4'	3:F:21:DT:OP1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:65:GLU:HG2	3:N:2:DA:H3'	2.04	0.40
1:I:108:VAL:HG12	1:I:112:GLN:CD	2.47	0.40
1:K:467:ASP:OD2	1:K:536:PHE:CD2	2.75	0.40
1:K:484:ILE:HG21	1:K:504:VAL:HG21	2.03	0.40
2:M:-11:DA:H2'	2:M:-10:DT:H72	2.02	0.40
1:C:319:THR:N	1:C:508:VAL:O	2.44	0.40
3:F:22:DA:H2''	3:F:23:DC:O5'	2.22	0.40
1:I:173:PRO:HD2	1:I:185:LEU:HD13	2.04	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	533/545 (98%)	494 (93%)	39 (7%)	0	100	100
1	C	533/545 (98%)	495 (93%)	38 (7%)	0	100	100
1	I	533/545 (98%)	493 (92%)	40 (8%)	0	100	100
1	K	533/545 (98%)	498 (93%)	35 (7%)	0	100	100
All	All	2132/2180 (98%)	1980 (93%)	152 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	490/499 (98%)	465 (95%)	25 (5%)	21	43
1	C	490/499 (98%)	469 (96%)	21 (4%)	26	48
1	I	490/499 (98%)	465 (95%)	25 (5%)	21	43
1	K	490/499 (98%)	470 (96%)	20 (4%)	27	49
All	All	1960/1996 (98%)	1869 (95%)	91 (5%)	25	46

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	21	ARG
1	A	22	SER
1	A	25	ASP
1	A	39	GLU
1	A	59	MET
1	A	79	ASP
1	A	85	TYR
1	A	103	ASP
1	A	122	TYR
1	A	142	MET
1	A	154	MET
1	A	186	ASP
1	A	262	ASP
1	A	360	TYR
1	A	365	ASP
1	A	403	MET
1	A	407	LYS
1	A	424	GLU
1	A	425	ASN
1	A	472	ILE
1	A	479	ASN
1	A	484	ILE
1	A	523	GLN
1	A	533	ASN
1	C	6	ILE
1	C	11	ASN
1	C	26	MET
1	C	34	GLU
1	C	68	ASP
1	C	75	GLU
1	C	168	ILE
1	C	199	PHE

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Mol	Chain	Res	Type
1	C	204	ASN
1	C	212	SER
1	C	222	ASN
1	C	236	GLN
1	C	278	ASP
1	C	306	LYS
1	C	352	THR
1	C	384	THR
1	C	398	ASP
1	C	465	LEU
1	C	468	THR
1	C	472	ILE
1	C	502	ARG
1	I	13	THR
1	I	21	ARG
1	I	22	SER
1	I	25	ASP
1	I	39	GLU
1	I	59	MET
1	I	79	ASP
1	I	85	TYR
1	I	103	ASP
1	I	122	TYR
1	I	135	GLN
1	I	154	MET
1	I	186	ASP
1	I	262	ASP
1	I	360	TYR
1	I	365	ASP
1	I	403	MET
1	I	407	LYS
1	I	424	GLU
1	I	425	ASN
1	I	472	ILE
1	I	479	ASN
1	I	484	ILE
1	I	523	GLN
1	I	533	ASN
1	K	11	ASN
1	K	22	SER
1	K	34	GLU
1	K	68	ASP

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Mol	Chain	Res	Type
1	K	75	GLU
1	K	138	PHE
1	K	168	ILE
1	K	199	PHE
1	K	204	ASN
1	K	212	SER
1	K	222	ASN
1	K	278	ASP
1	K	306	LYS
1	K	352	THR
1	K	384	THR
1	K	398	ASP
1	K	465	LEU
1	K	468	THR
1	K	472	ILE
1	K	502	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	109	ASN
1	A	204	ASN
1	A	207	ASN
1	A	293	GLN
1	A	356	ASN
1	A	388	HIS
1	A	412	HIS
1	A	466	GLN
1	A	469	GLN
1	C	109	ASN
1	C	244	GLN
1	C	273	GLN
1	C	293	GLN
1	C	408	GLN
1	I	24	GLN
1	I	109	ASN
1	I	204	ASN
1	I	293	GLN
1	I	356	ASN
1	I	388	HIS
1	I	412	HIS

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Mol	Chain	Res	Type
1	I	466	GLN
1	I	469	GLN
1	K	109	ASN
1	K	244	GLN
1	K	273	GLN
1	K	293	GLN
1	K	408	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

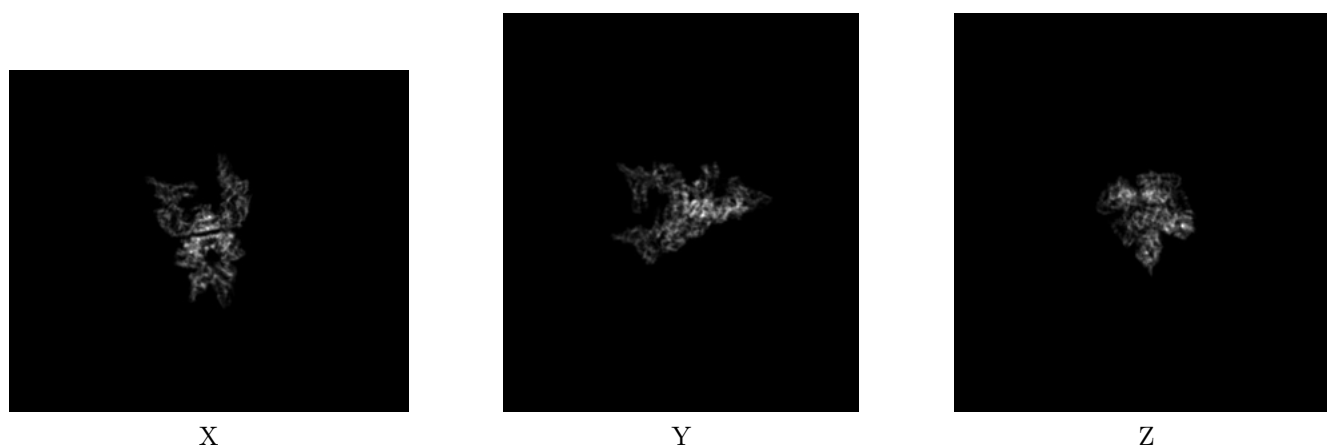
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47288. 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](#)

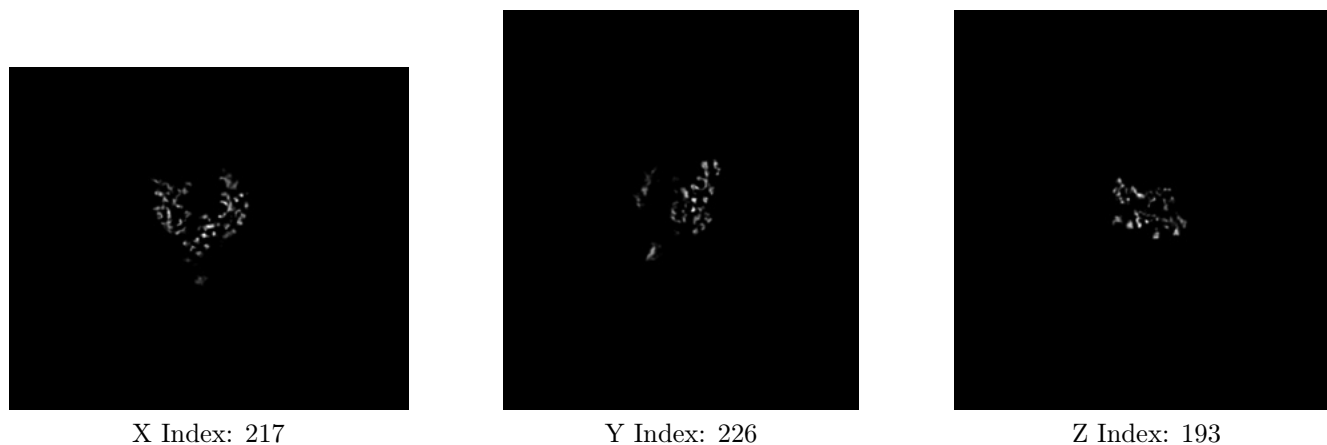
6.1.1 Primary map



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

6.2 Central slices [i](#)

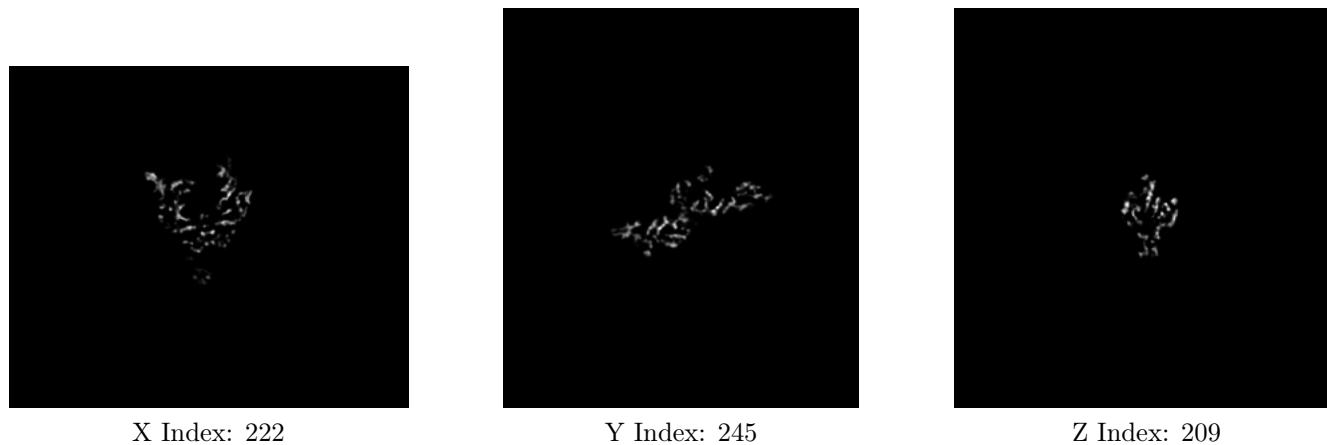
6.2.1 Primary map



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

6.3 Largest variance slices [i](#)

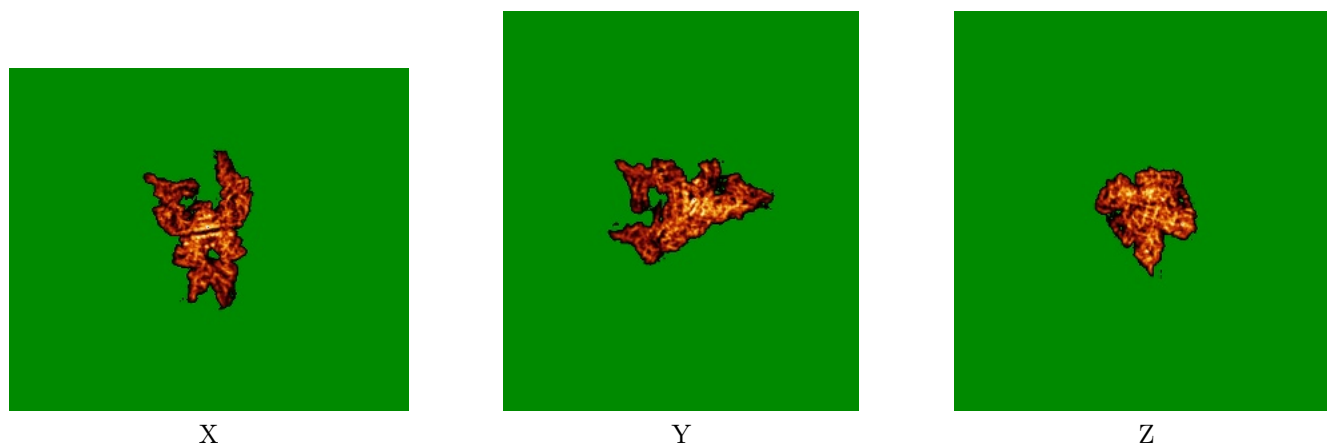
6.3.1 Primary map



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

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

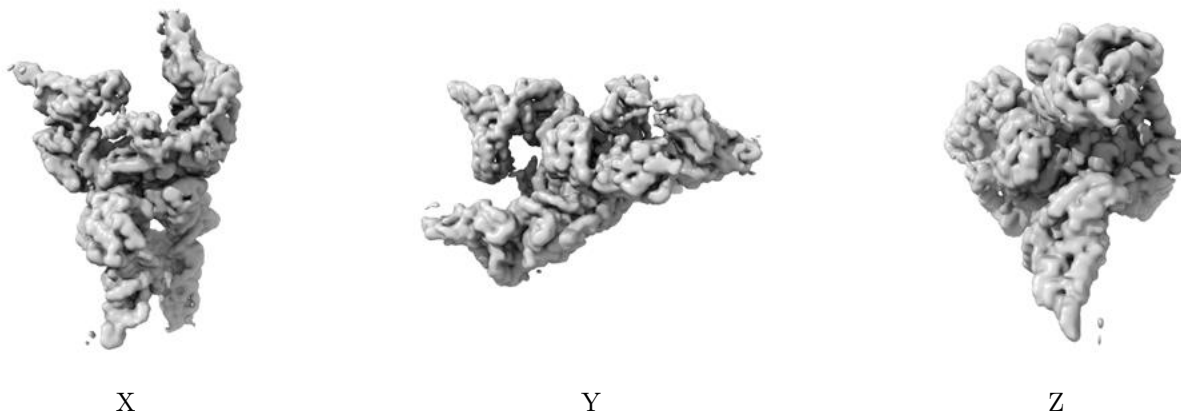
6.4.1 Primary map



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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

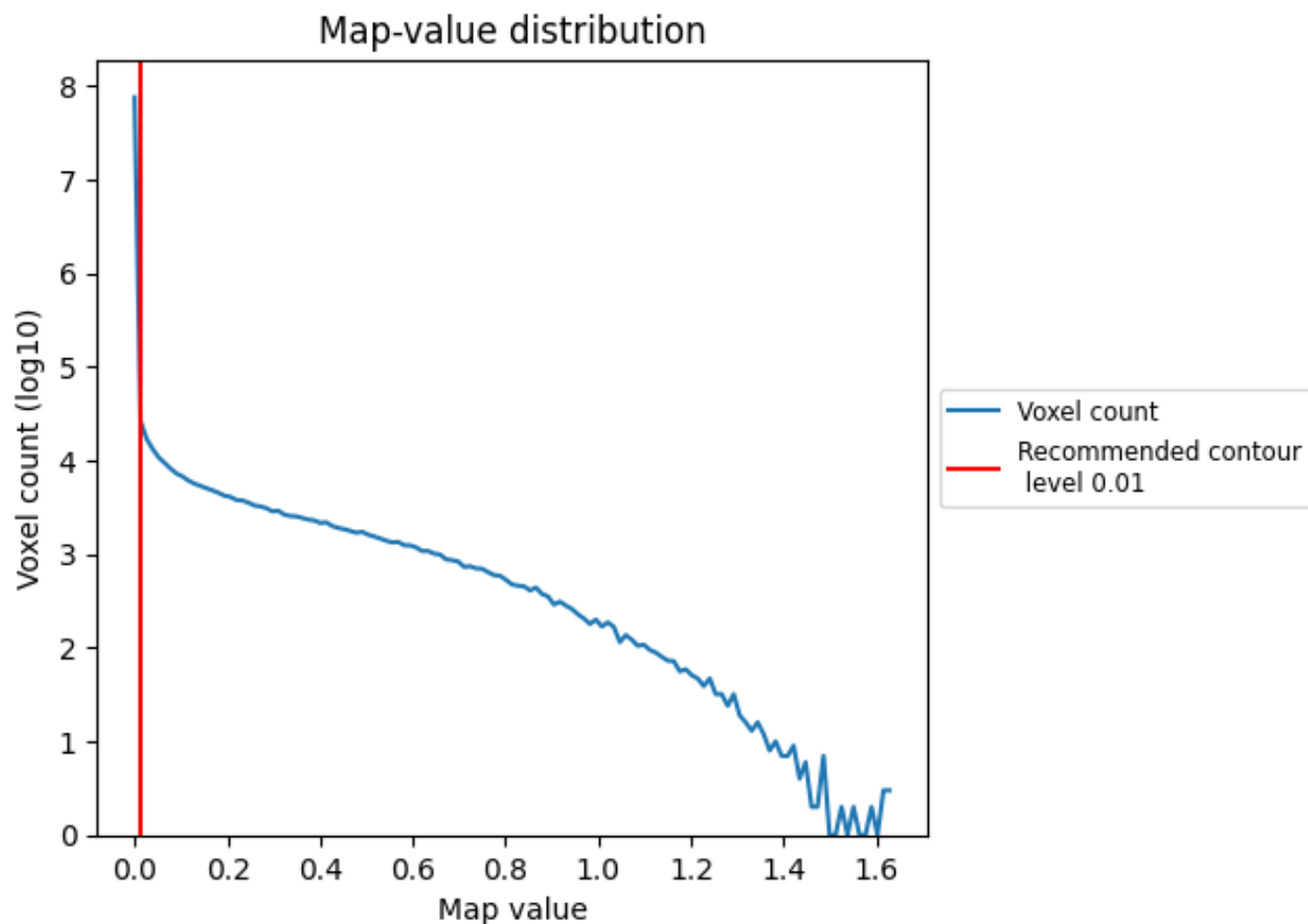
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

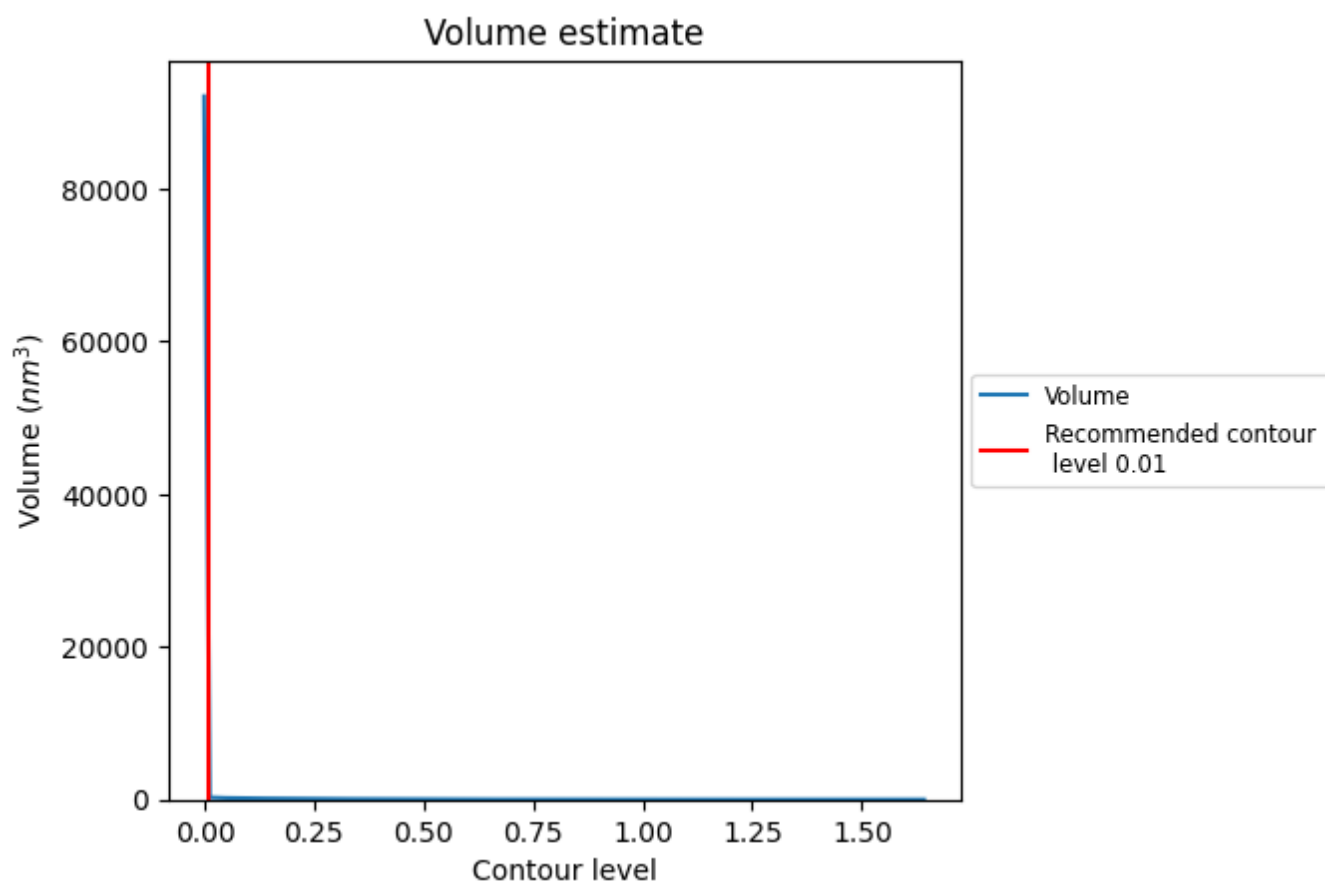
This section contains the results of statistical analysis of the map.

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 15136 nm³; this corresponds to an approximate mass of 13673 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 [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation ⓘ

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

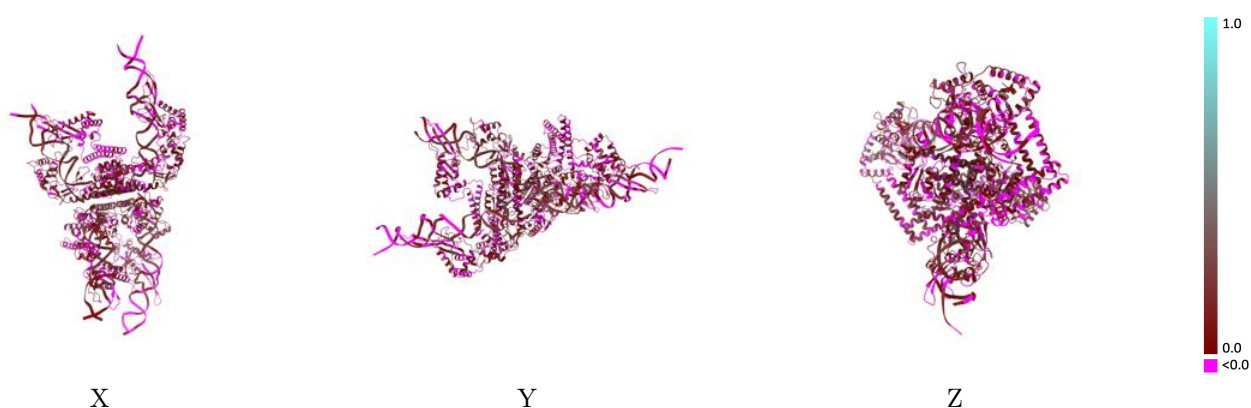
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47288 and PDB model 9DXH. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

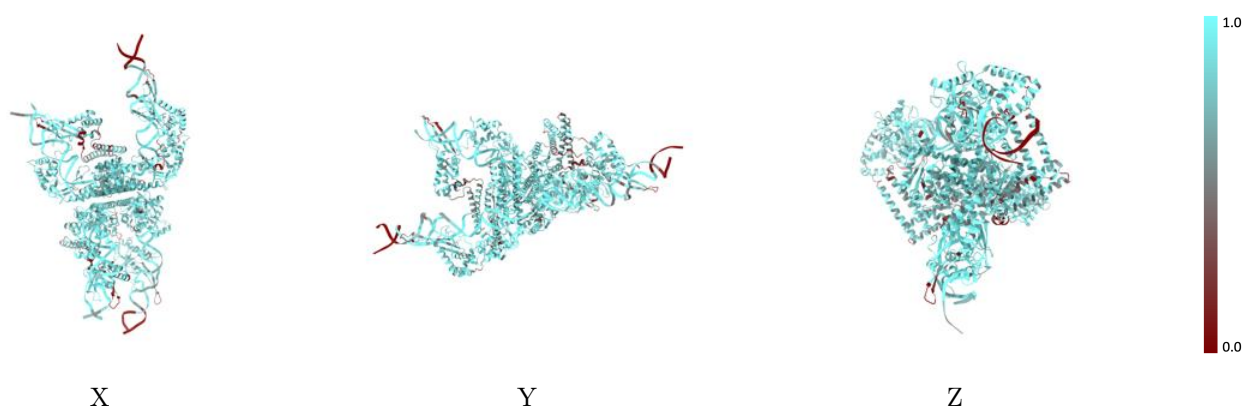
This section was not generated.

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



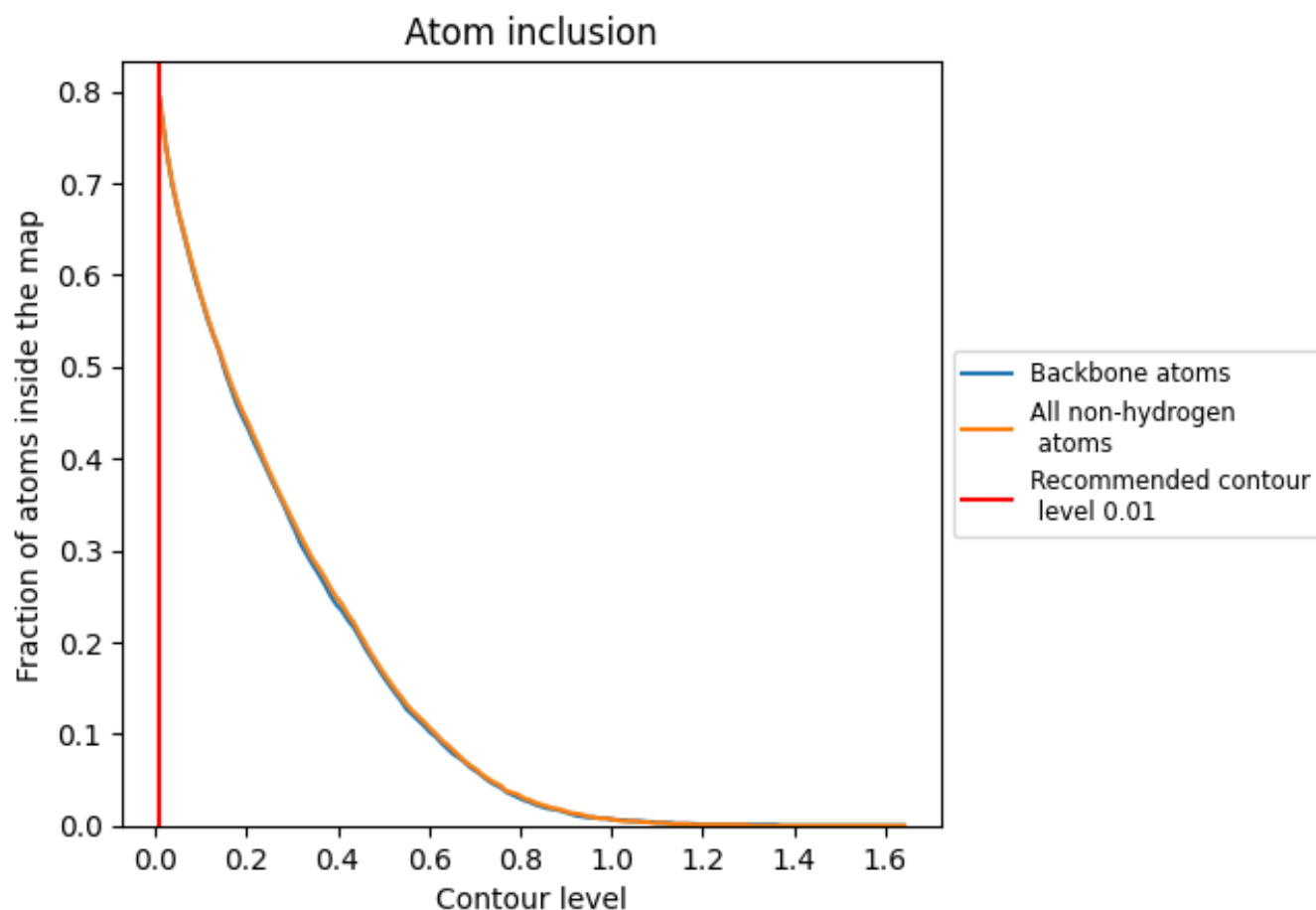
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7920	<div></div> 0.0860
A	<div></div> 0.7970	<div></div> 0.0720
C	<div></div> 0.7820	<div></div> 0.0710
E	<div></div> 0.7390	<div></div> 0.1040
F	<div></div> 0.7050	<div></div> 0.1110
G	<div></div> 0.9280	<div></div> 0.1660
H	<div></div> 0.8970	<div></div> 0.1690
I	<div></div> 0.8260	<div></div> 0.0770
K	<div></div> 0.8050	<div></div> 0.0760
M	<div></div> 0.7520	<div></div> 0.0960
N	<div></div> 0.7160	<div></div> 0.1130
O	<div></div> 0.9370	<div></div> 0.1730
P	<div></div> 0.9210	<div></div> 0.1720

1.0

0.0

<0.0