



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Jul 24, 2017 – 02:02 PM EDT

PDB ID : 5MPE
EMDB ID: : EMD-3535
Title : 26S proteasome in presence of ATP (s2)
Authors : Wehmer, M.; Rudack, T.; Beck, F.; Aufderheide, A.; Pfeifer, G.; Plitzko, J.M.;
Foerster, F.; Schulten, K.; Baumeister, W.; Sakata, E.
Deposited on : unknown
Resolution : 4.50 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

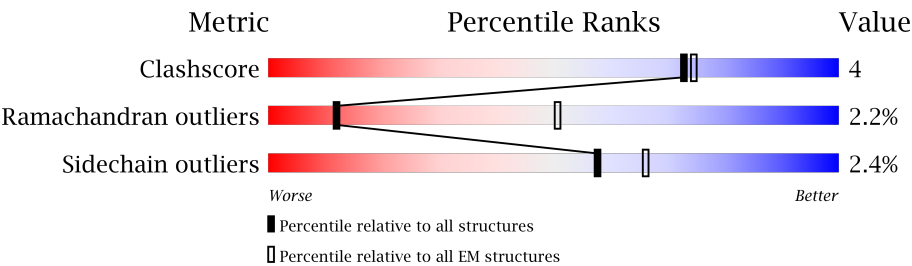
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	W	268	<div><div>57%</div><div>16%</div><div>26%</div></div>
2	V	306	<div><div>72%</div><div>20%</div><div>• 6%</div></div>
3	T	274	<div><div>76%</div><div>17%</div><div>• •</div></div>
4	X	156	<div><div>60%</div><div>17%</div><div>• • 19%</div></div>
5	Y	89	<div><div>36%</div><div>18%</div><div>• 43%</div></div>
6	Z	993	<div><div>72%</div><div>16%</div><div>• 9%</div></div>
7	N	945	<div><div>78%</div><div>14%</div><div>• 6%</div></div>
8	S	523	<div><div>70%</div><div>17%</div><div>• 9%</div></div>
9	P	445	<div><div>76%</div><div>20%</div><div>• •</div></div>

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Mol	Chain	Length	Quality of chain
10	Q	434	<div><div></div><div>76%</div><div>19%</div><div>• •</div></div>
11	R	429	<div><div></div><div>63%</div><div>20%</div><div>5% • 11%</div></div>
12	U	338	<div><div></div><div>70%</div><div>17%</div><div>• 12%</div></div>
13	O	393	<div><div></div><div>73%</div><div>20%</div><div>5% • •</div></div>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 40974 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 26S proteasome regulatory subunit RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	W	197	Total	C	N	O	S	0	0
			1534	962	269	300	3		

- Molecule 2 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	289	Total	C	N	O	S	0	0
			2274	1425	389	446	14		

- Molecule 3 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	266	Total	C	N	O	S	0	0
			2192	1405	349	432	6		

- Molecule 4 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	127	Total	C	N	O	S	0	0
			1032	664	169	195	4		

- Molecule 5 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	Y	51	Total	C	N	O	0	0
			435	264	69	102		

- Molecule 6 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	906	Total	C	N	O	S	0	0
			7005	4416	1150	1409	30		

- Molecule 7 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	890	Total	C	N	O	S	0	0
			6882	4373	1156	1325	28		

- Molecule 8 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	475	Total	C	N	O	S	0	0
			3894	2488	653	738	15		

- Molecule 9 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	440	Total	C	N	O	S	0	0
			3608	2297	604	697	10		

- Molecule 10 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	434	Total	C	N	O	S	0	0
			3499	2225	577	681	16		

- Molecule 11 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	381	Total	C	N	O	S	0	0
			3060	1955	502	593	10		

- Molecule 12 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	298	Total	C	N	O	S	0	0
			2373	1496	404	466	7		

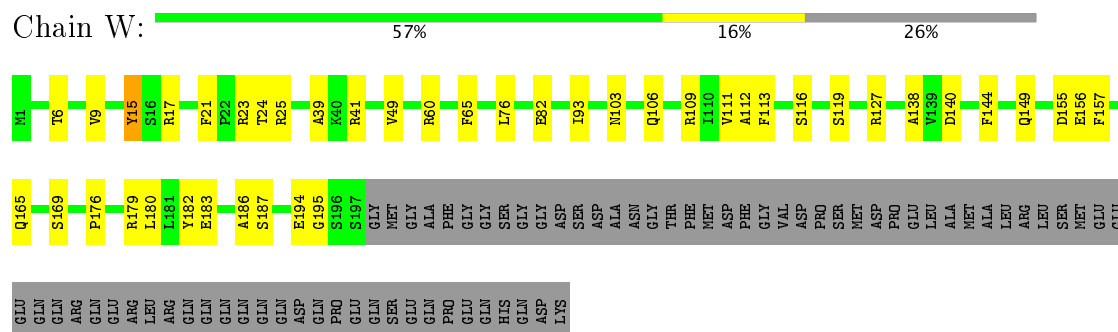
- Molecule 13 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	388	Total	C	N	O	S	0	0
			3186	2051	519	608	8		

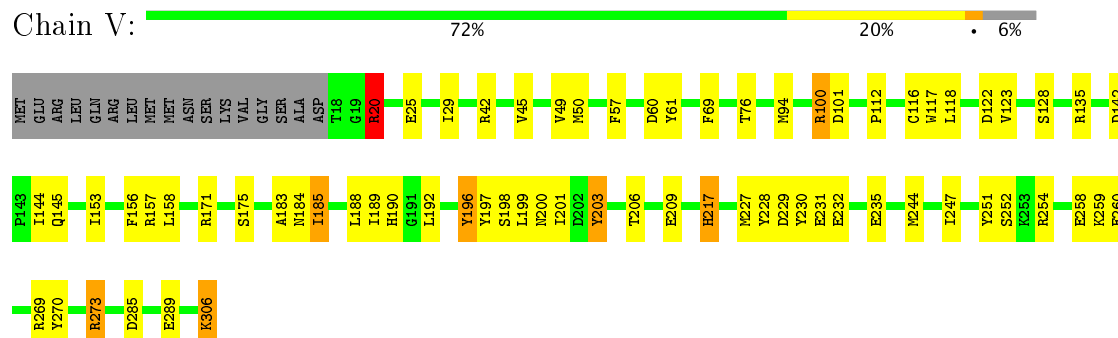
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

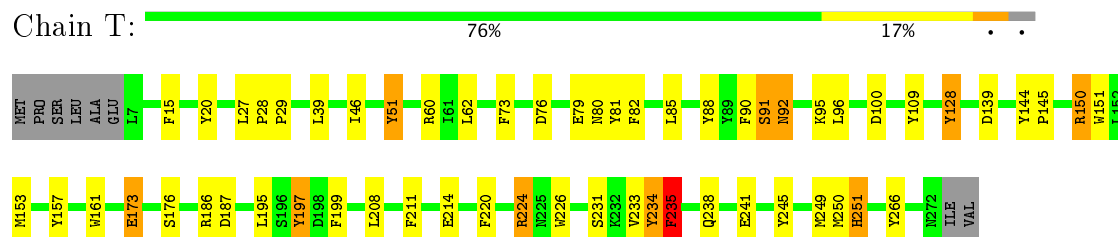
- Molecule 1: 26S proteasome regulatory subunit RPN10



- Molecule 2: Ubiquitin carboxyl-terminal hydrolase RPN11



- Molecule 3: 26S proteasome regulatory subunit RPN12

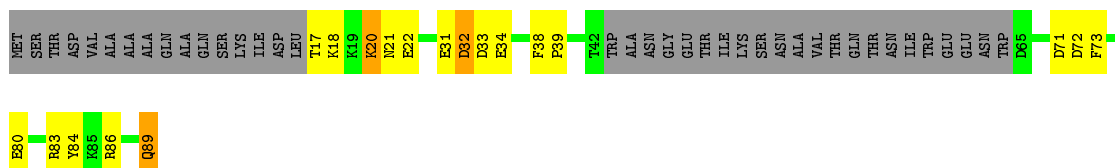


- Molecule 4: 26S proteasome regulatory subunit RPN13



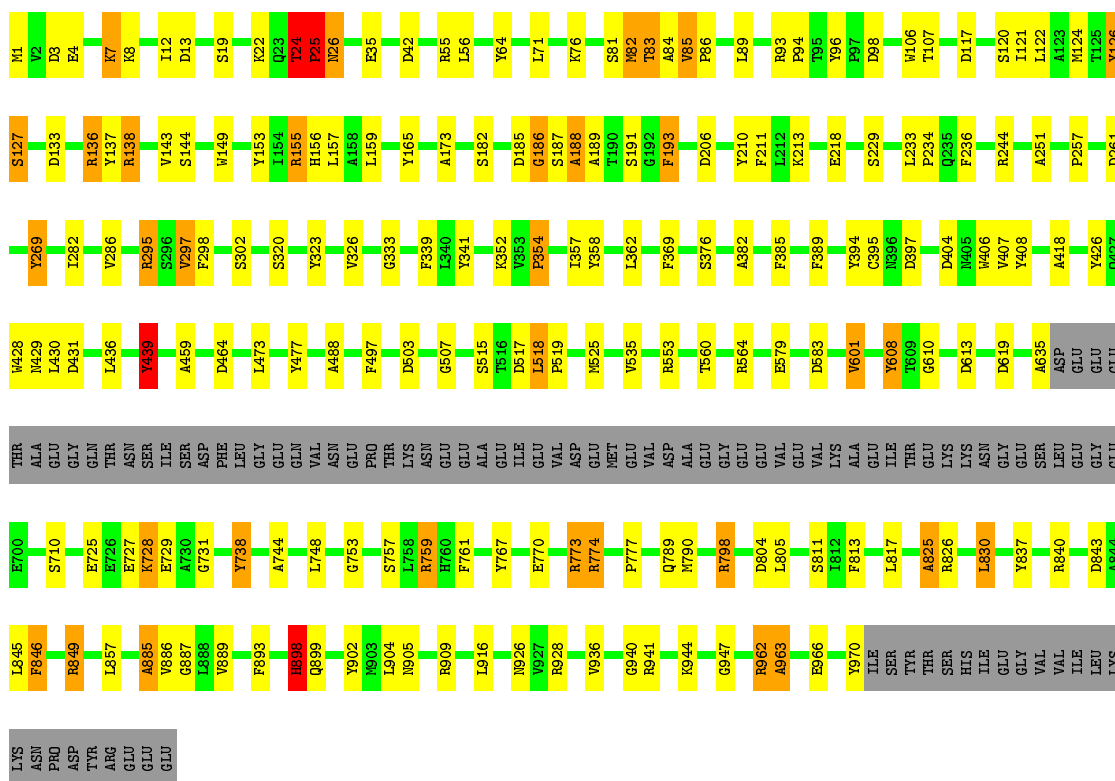
- Molecule 5: 26S proteasome complex subunit SEM1

Chain Y: 36% 18% . 43%



- Molecule 6: 26S proteasome regulatory subunit RPN1

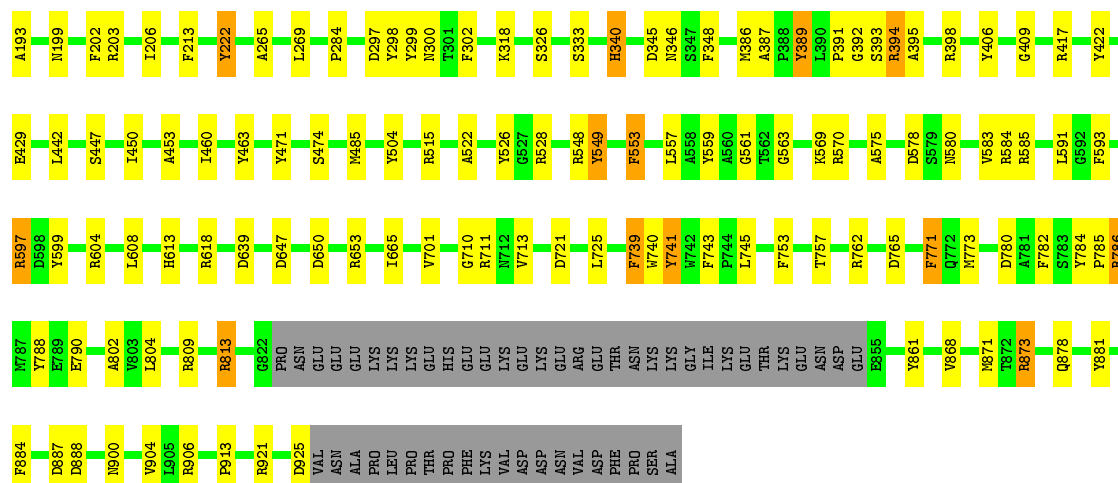
Chain Z: 72% 16% 0% 9%



- Molecule 7: 26S proteasome regulatory subunit RPN2

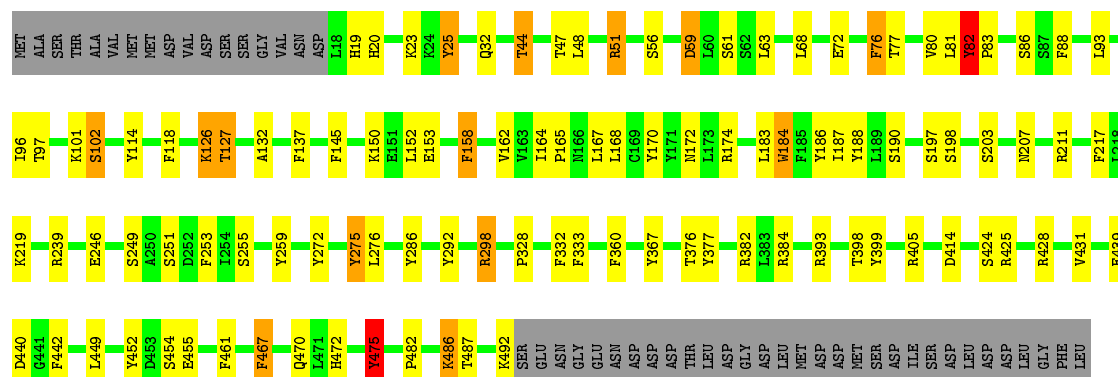
Chain N: 78% 14% 6%





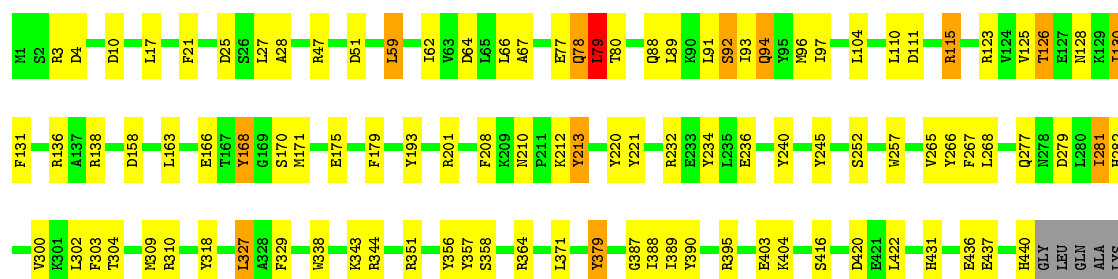
• Molecule 8: 26S proteasome regulatory subunit RPN3

Chain S: 70% 17% 9%



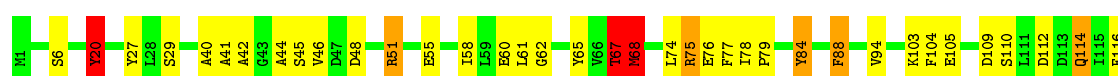
• Molecule 9: 26S proteasome regulatory subunit RPN5

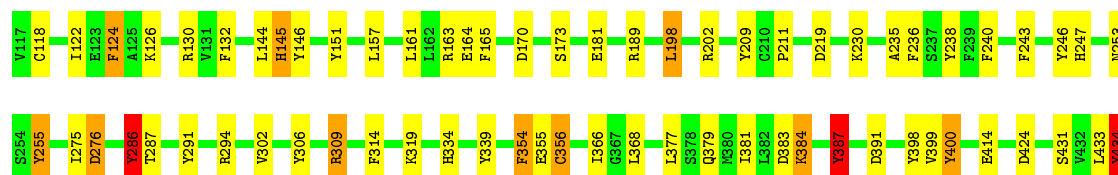
Chain P: 76% 20%



• Molecule 10: 26S proteasome regulatory subunit RPN6

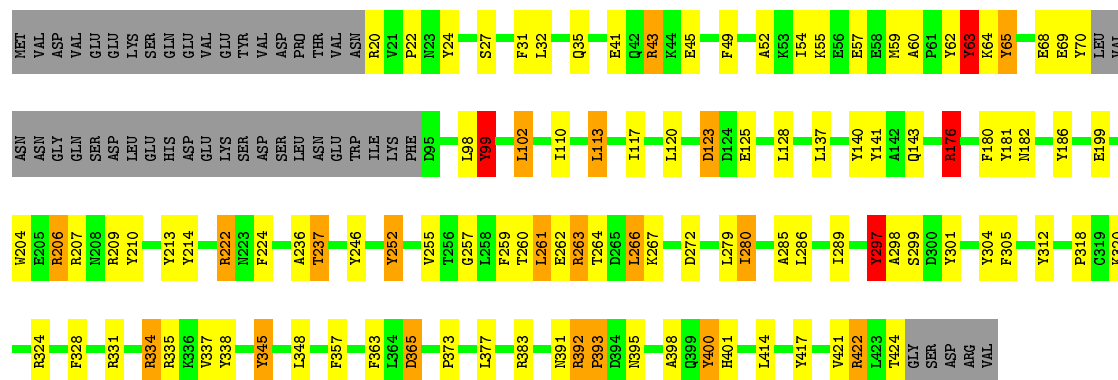
Chain Q: 76% 19%





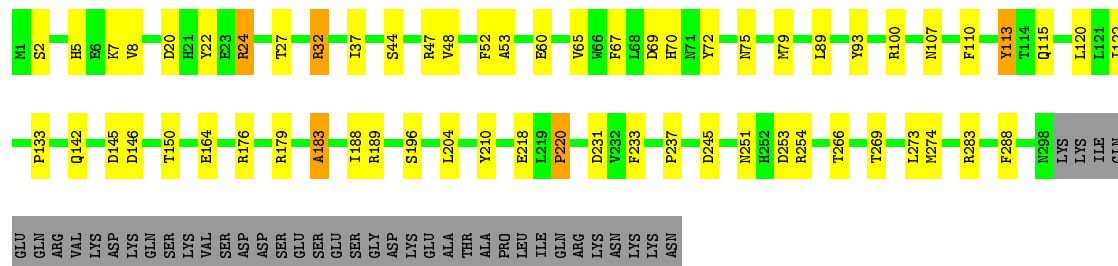
- Molecule 11: 26S proteasome regulatory subunit RPN7

Chain R: 63% 20% 5% 11%



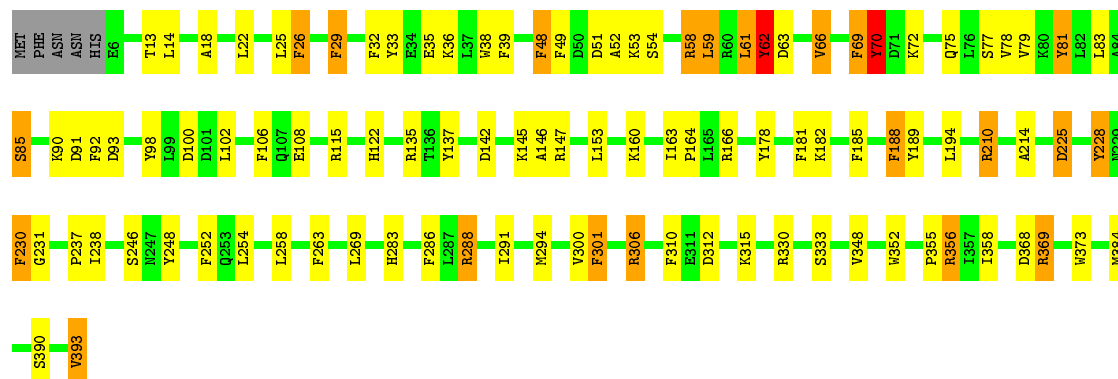
- Molecule 12: 26S proteasome regulatory subunit RPN8

Chain U: 70% 17% 12%



- Molecule 13: 26S proteasome regulatory subunit RPN9

Chain O: 73% 20% 5% 2%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	193337	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	W	1.69	17/1557 (1.1%)	1.87	34/2111 (1.6%)
10	Q	1.66	28/3556 (0.8%)	1.80	68/4787 (1.4%)
11	R	2.09	27/3110 (0.9%)	1.95	82/4193 (2.0%)
12	U	1.57	18/2407 (0.7%)	1.74	32/3258 (1.0%)
13	O	1.63	26/3247 (0.8%)	1.79	77/4380 (1.8%)
2	V	1.62	16/2309 (0.7%)	1.77	38/3115 (1.2%)
3	T	1.62	12/2235 (0.5%)	1.78	43/3017 (1.4%)
4	X	1.83	12/1058 (1.1%)	1.96	29/1432 (2.0%)
5	Y	1.83	7/438 (1.6%)	1.83	9/583 (1.5%)
6	Z	1.61	45/7122 (0.6%)	1.78	124/9645 (1.3%)
7	N	1.62	63/6994 (0.9%)	1.71	108/9455 (1.1%)
8	S	1.69	30/3966 (0.8%)	1.81	91/5355 (1.7%)
9	P	1.66	31/3663 (0.8%)	1.79	84/4940 (1.7%)
All	All	1.68	332/41662 (0.8%)	1.79	819/56271 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	W	0	2
10	Q	0	11
11	R	0	18
12	U	0	3
13	O	0	13
2	V	0	7
3	T	0	9
4	X	0	7
5	Y	0	1
6	Z	0	19
7	N	0	13
8	S	0	10

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	P	0	5
All	All	0	118

All (332) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	99	TYR	CE1-CZ	54.44	2.09	1.38
11	R	99	TYR	CZ-OH	39.26	2.04	1.37
8	S	59	ASP	CA-CB	-19.85	1.10	1.53
9	P	78	GLN	C-N	18.16	1.75	1.34
8	S	127	THR	CA-CB	17.50	1.98	1.53
13	O	393	VAL	C-OXT	-12.08	1.00	1.23
5	Y	89	GLN	C-O	-12.07	1.00	1.23
9	P	440	HIS	C-O	-12.06	1.00	1.23
8	S	492	LYS	C-O	-12.06	1.00	1.23
10	Q	434	TYR	C-OXT	-12.06	1.00	1.23
2	V	306	LYS	C-O	-12.06	1.00	1.23
5	Y	89	GLN	C-OXT	-12.06	1.00	1.23
2	V	306	LYS	C-OXT	-12.05	1.00	1.23
10	Q	434	TYR	C-O	-12.05	1.00	1.23
11	R	424	THR	C-O	-12.04	1.00	1.23
7	N	925	ASP	C-O	-12.03	1.00	1.23
13	O	393	VAL	C-O	-12.01	1.00	1.23
4	X	133	SER	C-O	-12.01	1.00	1.23
13	O	66	VAL	CA-CB	-9.59	1.34	1.54
9	P	3	ARG	NE-CZ	9.41	1.45	1.33
6	Z	25	PRO	CG-CD	-8.97	1.21	1.50
7	N	14	ARG	CZ-NH1	8.54	1.44	1.33
11	R	99	TYR	CD1-CE1	8.53	1.52	1.39
10	Q	163	ARG	CD-NE	8.19	1.60	1.46
1	W	17	ARG	NE-CZ	8.03	1.43	1.33
11	R	43	ARG	CZ-NH2	7.97	1.43	1.33
2	V	61	TYR	CE2-CZ	7.97	1.49	1.38
11	R	99	TYR	CG-CD1	7.84	1.49	1.39
7	N	653	ARG	NE-CZ	7.74	1.43	1.33
7	N	142	GLU	CD-OE2	7.71	1.34	1.25
10	Q	414	GLU	CG-CD	7.70	1.63	1.51
8	S	382	ARG	NE-CZ	7.67	1.43	1.33
7	N	585	ARG	NE-CZ	7.54	1.42	1.33
1	W	41	ARG	CZ-NH2	7.48	1.42	1.33
11	R	331	ARG	NE-CZ	7.24	1.42	1.33
9	P	252	SER	CA-CB	7.23	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	22	ARG	CD-NE	7.21	1.58	1.46
9	P	138	ARG	NE-CZ	7.20	1.42	1.33
1	W	25	ARG	CZ-NH2	7.20	1.42	1.33
10	Q	6	SER	CA-CB	-7.07	1.42	1.52
8	S	190	SER	CA-CB	7.05	1.63	1.52
11	R	331	ARG	CD-NE	7.03	1.58	1.46
6	Z	136	ARG	NE-CZ	6.98	1.42	1.33
11	R	209	ARG	CD-NE	6.98	1.58	1.46
11	R	70	TYR	CE1-CZ	6.97	1.47	1.38
7	N	584	ARG	NE-CZ	6.96	1.42	1.33
9	P	364	ARG	CD-NE	6.91	1.58	1.46
9	P	136	ARG	CZ-NH1	6.90	1.42	1.33
4	X	22	ARG	CZ-NH2	6.87	1.42	1.33
11	R	206	ARG	CZ-NH2	6.86	1.42	1.33
6	Z	826	ARG	NE-CZ	6.85	1.42	1.33
8	S	203	SER	CB-OG	6.84	1.51	1.42
7	N	40	SER	CA-CB	6.79	1.63	1.52
7	N	284	PRO	N-CD	-6.78	1.38	1.47
7	N	762	ARG	NE-CZ	6.75	1.41	1.33
10	Q	306	TYR	CD2-CE2	6.75	1.49	1.39
8	S	286	TYR	CG-CD2	6.74	1.48	1.39
9	P	193	TYR	CB-CG	-6.74	1.41	1.51
7	N	471	TYR	CG-CD1	6.66	1.47	1.39
9	P	364	ARG	NE-CZ	6.64	1.41	1.33
3	T	224	ARG	CZ-NH1	6.63	1.41	1.33
6	Z	138	ARG	NE-CZ	6.58	1.41	1.33
8	S	239	ARG	CD-NE	6.58	1.57	1.46
6	Z	408	TYR	CE2-CZ	6.54	1.47	1.38
7	N	809	ARG	CZ-NH1	6.52	1.41	1.33
9	P	221	TYR	CG-CD1	6.52	1.47	1.39
8	S	454	SER	CA-CB	6.52	1.62	1.52
6	Z	153	TYR	CE2-CZ	6.52	1.47	1.38
13	O	188	PHE	CE2-CZ	6.49	1.49	1.37
1	W	176	PRO	N-CA	-6.49	1.36	1.47
13	O	178	TYR	CE2-CZ	6.47	1.47	1.38
10	Q	165	PHE	CB-CG	-6.47	1.40	1.51
13	O	246	SER	CA-CB	6.43	1.62	1.52
7	N	515	ARG	NE-CZ	6.41	1.41	1.33
12	U	47	ARG	NE-CZ	6.38	1.41	1.33
7	N	333	SER	CA-CB	6.38	1.62	1.52
2	V	232	GLU	CG-CD	6.37	1.61	1.51
7	N	813	ARG	CZ-NH1	6.37	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	99	TYR	CE2-CZ	6.36	1.46	1.38
9	P	245	TYR	CZ-OH	6.34	1.48	1.37
7	N	873	ARG	NE-CZ	6.29	1.41	1.33
13	O	210	ARG	NE-CZ	6.28	1.41	1.33
6	Z	773	ARG	CZ-NH1	6.25	1.41	1.33
8	S	174	ARG	CD-NE	6.25	1.57	1.46
9	P	387	GLY	N-CA	-6.25	1.36	1.46
2	V	100	ARG	CD-NE	6.23	1.57	1.46
10	Q	211	PRO	CA-C	-6.22	1.40	1.52
7	N	474	SER	CA-CB	6.22	1.62	1.52
7	N	802	ALA	CA-CB	6.21	1.65	1.52
9	P	437	GLU	CD-OE1	6.20	1.32	1.25
7	N	921	ARG	CZ-NH1	6.20	1.41	1.33
9	P	123	ARG	NE-CZ	6.19	1.41	1.33
8	S	61	SER	CA-CB	6.18	1.62	1.52
6	Z	553	ARG	CZ-NH1	6.17	1.41	1.33
11	R	207	ARG	CZ-NH2	6.16	1.41	1.33
7	N	139	ARG	NE-CZ	6.16	1.41	1.33
3	T	60	ARG	CD-NE	6.14	1.56	1.46
10	Q	189	ARG	NE-CZ	6.12	1.41	1.33
13	O	178	TYR	CB-CG	-6.11	1.42	1.51
6	Z	840	ARG	NE-CZ	6.10	1.41	1.33
7	N	4	THR	N-CA	6.10	1.58	1.46
6	Z	394	TYR	CG-CD1	6.08	1.47	1.39
6	Z	710	SER	CA-CB	6.08	1.62	1.52
10	Q	309	ARG	CZ-NH2	6.08	1.41	1.33
11	R	334	ARG	NE-CZ	6.08	1.41	1.33
7	N	570	ARG	NE-CZ	6.05	1.41	1.33
8	S	255	SER	CA-CB	6.05	1.62	1.52
10	Q	309	ARG	NE-CZ	6.05	1.41	1.33
12	U	164	GLU	CD-OE2	6.04	1.32	1.25
6	Z	244	ARG	NE-CZ	6.04	1.41	1.33
7	N	117	TYR	CE1-CZ	6.04	1.46	1.38
11	R	383	ARG	CD-NE	6.03	1.56	1.46
3	T	157	TYR	CE2-CZ	6.03	1.46	1.38
1	W	169	SER	N-CA	-6.02	1.34	1.46
12	U	60	GLU	CB-CG	6.02	1.63	1.52
7	N	409	GLY	N-CA	-5.99	1.37	1.46
12	U	32	ARG	CZ-NH1	5.95	1.40	1.33
11	R	181	TYR	CG-CD1	5.94	1.46	1.39
2	V	116	CYS	CB-SG	-5.93	1.72	1.81
13	O	70	TYR	CE1-CZ	-5.93	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	98	ASP	CB-CG	5.91	1.64	1.51
13	O	355	PRO	N-CD	-5.91	1.39	1.47
8	S	188	TYR	CE2-CZ	5.91	1.46	1.38
10	Q	202	ARG	CZ-NH1	5.90	1.40	1.33
7	N	326	SER	CB-OG	5.89	1.50	1.42
6	Z	738	TYR	CE1-CZ	5.89	1.46	1.38
4	X	17	TYR	CE1-CZ	5.87	1.46	1.38
6	Z	759	ARG	NE-CZ	5.87	1.40	1.33
9	P	310	ARG	NE-CZ	5.87	1.40	1.33
6	Z	798	ARG	NE-CZ	5.87	1.40	1.33
12	U	100	ARG	CZ-NH1	5.86	1.40	1.33
2	V	231	GLU	CD-OE1	5.86	1.32	1.25
9	P	221	TYR	CZ-OH	5.83	1.47	1.37
12	U	189	ARG	CD-NE	5.83	1.56	1.46
7	N	597	ARG	NE-CZ	5.82	1.40	1.33
2	V	254	ARG	CZ-NH1	5.82	1.40	1.33
1	W	9	VAL	CB-CG1	5.82	1.65	1.52
7	N	299	TYR	CE2-CZ	5.81	1.46	1.38
7	N	584	ARG	CZ-NH2	5.81	1.40	1.33
13	O	356	ARG	CZ-NH2	5.79	1.40	1.33
4	X	42	GLU	CG-CD	5.78	1.60	1.51
10	Q	209	TYR	CE1-CZ	5.78	1.46	1.38
4	X	7	VAL	N-CA	5.77	1.57	1.46
2	V	135	ARG	CZ-NH1	5.76	1.40	1.33
8	S	455	GLU	CD-OE1	5.76	1.31	1.25
6	Z	564	ARG	CZ-NH1	5.75	1.40	1.33
11	R	57	GLU	CD-OE2	5.75	1.31	1.25
6	Z	729	GLU	CD-OE2	5.75	1.31	1.25
7	N	392	GLY	N-CA	-5.75	1.37	1.46
7	N	585	ARG	CD-NE	5.74	1.56	1.46
13	O	135	ARG	NE-CZ	5.74	1.40	1.33
3	T	186	ARG	CZ-NH1	5.74	1.40	1.33
4	X	59	ARG	CD-NE	5.73	1.56	1.46
13	O	77	SER	CA-CB	5.73	1.61	1.52
6	Z	849	ARG	NE-CZ	5.73	1.40	1.33
6	Z	553	ARG	CZ-NH2	5.72	1.40	1.33
9	P	123	ARG	CZ-NH2	5.72	1.40	1.33
10	Q	105	GLU	CD-OE2	5.71	1.31	1.25
12	U	196	SER	CA-CB	5.71	1.61	1.52
3	T	176	SER	CA-CB	5.70	1.61	1.52
4	X	59	ARG	CZ-NH1	5.70	1.40	1.33
6	Z	774	ARG	CZ-NH2	5.70	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	U	176	ARG	CZ-NH2	5.70	1.40	1.33
3	T	20	TYR	CG-CD1	5.69	1.46	1.39
7	N	559	TYR	CZ-OH	5.67	1.47	1.37
7	N	743	PHE	CB-CG	5.67	1.60	1.51
11	R	209	ARG	CZ-NH2	5.67	1.40	1.33
4	X	22	ARG	CZ-NH1	5.66	1.40	1.33
9	P	232	ARG	NE-CZ	5.66	1.40	1.33
3	T	144	TYR	CE1-CZ	5.65	1.45	1.38
3	T	161	TRP	CE3-CZ3	5.65	1.48	1.38
11	R	392	ARG	CA-CB	5.65	1.66	1.53
7	N	298	TYR	CG-CD1	5.64	1.46	1.39
7	N	394	ARG	CZ-NH2	5.64	1.40	1.33
6	Z	389	PHE	CG-CD2	5.64	1.47	1.38
4	X	72	GLU	CG-CD	5.64	1.60	1.51
9	P	338	TRP	CB-CG	5.63	1.60	1.50
8	S	333	PHE	CG-CD1	5.61	1.47	1.38
8	S	174	ARG	CZ-NH2	5.60	1.40	1.33
3	T	82	PHE	CG-CD1	5.59	1.47	1.38
13	O	210	ARG	CZ-NH1	5.57	1.40	1.33
6	Z	295	ARG	CD-NE	5.57	1.55	1.46
12	U	67	PHE	CB-CG	-5.56	1.41	1.51
7	N	463	TYR	CZ-OH	5.56	1.47	1.37
6	Z	408	TYR	CG-CD2	5.55	1.46	1.39
7	N	117	TYR	CZ-OH	5.54	1.47	1.37
10	Q	65	TYR	CG-CD1	5.54	1.46	1.39
10	Q	84	TYR	CE1-CZ	5.54	1.45	1.38
6	Z	295	ARG	CZ-NH2	5.53	1.40	1.33
1	W	15	TYR	CD1-CE1	5.52	1.47	1.39
1	W	23	ARG	NE-CZ	5.51	1.40	1.33
6	Z	302	SER	CB-OG	-5.51	1.35	1.42
7	N	102	VAL	CB-CG2	5.51	1.64	1.52
9	P	267	PHE	CG-CD1	5.50	1.47	1.38
7	N	618	ARG	NE-CZ	5.50	1.40	1.33
7	N	900	ASN	C-N	5.50	1.43	1.33
11	R	222	ARG	CZ-NH1	5.50	1.40	1.33
12	U	44	SER	CA-CB	5.50	1.61	1.52
6	Z	56	LEU	CA-CB	5.49	1.66	1.53
8	S	298	ARG	CZ-NH2	5.49	1.40	1.33
13	O	32	PHE	CG-CD2	5.48	1.47	1.38
7	N	139	ARG	CZ-NH1	5.48	1.40	1.33
1	W	41	ARG	NE-CZ	5.47	1.40	1.33
6	Z	635	ALA	CA-CB	5.47	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	P	201	ARG	CZ-NH2	5.47	1.40	1.33
7	N	597	ARG	CZ-NH1	5.47	1.40	1.33
5	Y	22	GLU	N-CA	-5.46	1.35	1.46
9	P	115	ARG	CZ-NH2	5.46	1.40	1.33
8	S	452	TYR	CE1-CZ	5.46	1.45	1.38
13	O	62	TYR	CA-CB	5.46	1.66	1.53
13	O	369	ARG	CZ-NH2	5.46	1.40	1.33
13	O	98	TYR	CZ-OH	5.45	1.47	1.37
8	S	424	SER	CB-OG	5.45	1.49	1.42
7	N	298	TYR	CZ-OH	5.45	1.47	1.37
7	N	460	ILE	N-CA	-5.44	1.35	1.46
2	V	252	SER	CA-CB	5.43	1.61	1.52
12	U	179	ARG	CD-NE	5.42	1.55	1.46
10	Q	84	TYR	CZ-OH	5.42	1.47	1.37
5	Y	86	ARG	NE-CZ	5.42	1.40	1.33
11	R	422	ARG	NE-CZ	5.42	1.40	1.33
2	V	61	TYR	CB-CG	5.42	1.59	1.51
13	O	231	GLY	N-CA	-5.42	1.38	1.46
10	Q	243	PHE	CB-CG	5.42	1.60	1.51
3	T	245	TYR	C-N	5.41	1.46	1.34
11	R	299	SER	CB-OG	5.39	1.49	1.42
2	V	235	GLU	CB-CG	5.39	1.62	1.52
7	N	429	GLU	CB-CG	5.39	1.62	1.52
9	P	170	SER	CA-CB	5.39	1.61	1.52
7	N	608	LEU	N-CA	-5.39	1.35	1.46
7	N	569	LYS	CD-CE	5.38	1.64	1.51
6	Z	127	SER	CA-CB	5.38	1.61	1.52
8	S	249	SER	CB-OG	-5.37	1.35	1.42
1	W	65	PHE	CB-CG	-5.36	1.42	1.51
12	U	47	ARG	CZ-NH1	5.35	1.40	1.33
8	S	428	ARG	NE-CZ	5.35	1.40	1.33
2	V	171	ARG	CZ-NH1	5.34	1.40	1.33
10	Q	62	GLY	CA-C	-5.34	1.43	1.51
5	Y	84	TYR	CE2-CZ	5.34	1.45	1.38
7	N	784	TYR	CE2-CZ	5.34	1.45	1.38
12	U	32	ARG	CD-NE	5.34	1.55	1.46
12	U	72	TYR	CB-CG	-5.34	1.43	1.51
8	S	276	LEU	CA-CB	5.33	1.66	1.53
5	Y	72	ASP	N-CA	-5.33	1.35	1.46
13	O	390	SER	N-CA	-5.33	1.35	1.46
7	N	72	LEU	C-N	5.33	1.42	1.33
7	N	762	ARG	CZ-NH2	5.32	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Q	246	TYR	CG-CD2	5.30	1.46	1.39
6	Z	966	GLU	CD-OE2	5.30	1.31	1.25
4	X	97	TYR	CZ-OH	5.29	1.46	1.37
8	S	170	TYR	CG-CD1	5.29	1.46	1.39
6	Z	339	PHE	CG-CD2	5.29	1.46	1.38
10	Q	51	ARG	CZ-NH1	5.28	1.40	1.33
11	R	63	TYR	CB-CG	-5.28	1.43	1.51
9	P	240	TYR	CE1-CZ	5.28	1.45	1.38
6	Z	138	ARG	CZ-NH1	5.27	1.40	1.33
11	R	176	ARG	NE-CZ	5.27	1.40	1.33
7	N	604	ARG	CZ-NH1	5.27	1.40	1.33
3	T	150	ARG	CZ-NH2	5.27	1.39	1.33
7	N	463	TYR	CE2-CZ	5.27	1.45	1.38
10	Q	246	TYR	CE1-CZ	5.27	1.45	1.38
6	Z	55	ARG	CZ-NH1	5.26	1.39	1.33
2	V	20	ARG	CZ-NH1	5.26	1.39	1.33
13	O	54	SER	C-N	5.25	1.46	1.34
9	P	240	TYR	CB-CG	-5.24	1.43	1.51
5	Y	39	PRO	CA-C	-5.24	1.42	1.52
8	S	86	SER	CA-CB	5.23	1.60	1.52
9	P	395	ARG	CZ-NH1	5.23	1.39	1.33
6	Z	579	GLU	CD-OE1	5.21	1.31	1.25
9	P	28	ALA	N-CA	-5.21	1.35	1.46
7	N	881	TYR	CB-CG	-5.20	1.43	1.51
8	S	51	ARG	CZ-NH1	5.19	1.39	1.33
6	Z	81	SER	CA-CB	5.19	1.60	1.52
1	W	116	SER	CA-CB	5.19	1.60	1.52
6	Z	757	SER	CA-CB	5.19	1.60	1.52
7	N	583	VAL	CA-CB	-5.18	1.43	1.54
11	R	180	PHE	CB-CG	-5.18	1.42	1.51
1	W	119	SER	CA-CB	5.18	1.60	1.52
10	Q	286	TYR	CZ-OH	5.18	1.46	1.37
1	W	60	ARG	NE-CZ	5.17	1.39	1.33
10	Q	61	LEU	C-N	5.17	1.42	1.33
13	O	283	HIS	CB-CG	5.17	1.59	1.50
7	N	563	GLY	CA-C	-5.17	1.43	1.51
1	W	195	GLY	C-O	5.16	1.31	1.23
12	U	24	ARG	CZ-NH2	5.14	1.39	1.33
7	N	784	TYR	CG-CD1	5.14	1.45	1.39
7	N	921	ARG	CZ-NH2	5.13	1.39	1.33
11	R	62	TYR	CB-CG	5.13	1.59	1.51
10	Q	77	PHE	CE1-CZ	5.12	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	106	TRP	CB-CG	5.12	1.59	1.50
6	Z	157	LEU	CA-C	-5.12	1.39	1.52
9	P	356	TYR	CG-CD1	5.12	1.45	1.39
3	T	241	GLU	CD-OE1	5.11	1.31	1.25
7	N	570	ARG	CZ-NH2	5.11	1.39	1.33
2	V	209	GLU	CG-CD	5.10	1.59	1.51
13	O	248	TYR	CE1-CZ	5.10	1.45	1.38
6	Z	837	TYR	CG-CD2	5.10	1.45	1.39
6	Z	886	VAL	CB-CG1	5.10	1.63	1.52
12	U	254	ARG	CD-NE	5.09	1.55	1.46
12	U	8	VAL	CB-CG2	5.09	1.63	1.52
7	N	561	GLY	CA-C	5.09	1.59	1.51
4	X	59	ARG	NE-CZ	5.08	1.39	1.33
2	V	259	LYS	CA-CB	5.08	1.65	1.53
7	N	906	ARG	NE-CZ	5.08	1.39	1.33
9	P	338	TRP	NE1-CE2	5.08	1.44	1.37
1	W	127	ARG	NE-CZ	5.07	1.39	1.33
10	Q	181	GLU	CG-CD	5.07	1.59	1.51
6	Z	725	GLU	CG-CD	5.06	1.59	1.51
8	S	184	TRP	CZ2-CH2	5.06	1.47	1.37
8	S	239	ARG	NE-CZ	5.06	1.39	1.33
8	S	298	ARG	CZ-NH1	5.06	1.39	1.33
6	Z	193	PHE	CG-CD2	5.06	1.46	1.38
1	W	155	ASP	CB-CG	5.05	1.62	1.51
7	N	913	PRO	CA-C	-5.05	1.42	1.52
6	Z	430	LEU	N-CA	-5.05	1.36	1.46
10	Q	60	GLU	CG-CD	5.05	1.59	1.51
7	N	406	TYR	N-CA	5.05	1.56	1.46
8	S	442	PHE	CG-CD1	5.05	1.46	1.38
11	R	199	GLU	CG-CD	5.05	1.59	1.51
7	N	873	ARG	CZ-NH1	5.04	1.39	1.33
7	N	653	ARG	CZ-NH1	5.04	1.39	1.33
13	O	66	VAL	CB-CG1	-5.04	1.42	1.52
13	O	108	GLU	CB-CG	5.04	1.61	1.52
10	Q	189	ARG	CD-NE	5.04	1.55	1.46
12	U	2	SER	CA-CB	5.04	1.60	1.52
13	O	263	PHE	CG-CD1	5.04	1.46	1.38
1	W	183	GLU	CD-OE1	-5.03	1.20	1.25
9	P	94	GLN	N-CA	-5.03	1.36	1.46
6	Z	928	ARG	CZ-NH2	5.03	1.39	1.33
6	Z	515	SER	CA-CB	5.01	1.60	1.52
7	N	548	ARG	CZ-NH2	5.01	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	P	282	HIS	CB-CG	5.00	1.59	1.50
8	S	360	PHE	CB-CG	5.00	1.59	1.51

All (819) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	99	TYR	CE1-CZ-OH	-25.48	51.30	120.10
2	V	61	TYR	CB-CG-CD2	-19.36	109.39	121.00
6	Z	188	ALA	CB-CA-C	-18.32	82.62	110.10
13	O	62	TYR	CB-CA-C	-15.89	78.61	110.40
9	P	266	TYR	CB-CG-CD2	-15.64	111.62	121.00
2	V	61	TYR	CB-CG-CD1	15.12	130.07	121.00
9	P	78	GLN	O-C-N	-14.51	99.48	122.70
10	Q	163	ARG	NE-CZ-NH2	-14.28	113.16	120.30
11	R	99	TYR	CB-CG-CD2	-14.15	112.51	121.00
6	Z	188	ALA	N-CA-CB	-14.05	90.43	110.10
11	R	338	TYR	CB-CG-CD1	13.93	129.36	121.00
8	S	384	ARG	NE-CZ-NH1	13.71	127.16	120.30
1	W	41	ARG	NE-CZ-NH1	13.60	127.10	120.30
4	X	11	ARG	NE-CZ-NH1	13.58	127.09	120.30
5	Y	83	ARG	NE-CZ-NH1	13.50	127.05	120.30
12	U	113	TYR	CB-CG-CD1	-13.49	112.91	121.00
6	Z	295	ARG	NE-CZ-NH2	-13.45	113.58	120.30
9	P	266	TYR	CB-CG-CD1	13.40	129.04	121.00
13	O	62	TYR	CB-CG-CD2	-13.38	112.97	121.00
6	Z	25	PRO	N-CA-CB	-13.36	87.27	103.30
11	R	99	TYR	CD1-CE1-CZ	-13.21	107.91	119.80
12	U	113	TYR	CB-CG-CD2	13.21	128.93	121.00
6	Z	138	ARG	NE-CZ-NH2	-12.80	113.90	120.30
7	N	299	TYR	CB-CG-CD1	-12.79	113.33	121.00
2	V	254	ARG	NE-CZ-NH1	12.72	126.66	120.30
7	N	762	ARG	NE-CZ-NH1	12.60	126.60	120.30
3	T	266	TYR	CB-CG-CD1	12.49	128.50	121.00
6	Z	970	TYR	CB-CG-CD1	-12.45	113.53	121.00
13	O	330	ARG	NE-CZ-NH2	-12.32	114.14	120.30
11	R	334	ARG	NE-CZ-NH2	-12.31	114.14	120.30
8	S	382	ARG	NE-CZ-NH2	-12.25	114.18	120.30
1	W	23	ARG	NE-CZ-NH2	-12.14	114.23	120.30
10	Q	163	ARG	NE-CZ-NH1	11.98	126.29	120.30
11	R	99	TYR	OH-CZ-CE2	11.88	152.16	120.10
7	N	298	TYR	CB-CG-CD1	11.87	128.12	121.00
2	V	273	ARG	NE-CZ-NH1	-11.86	114.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	593	PHE	CB-CG-CD2	-11.82	112.53	120.80
11	R	207	ARG	NE-CZ-NH1	11.68	126.14	120.30
11	R	140	TYR	CB-CG-CD1	11.65	127.99	121.00
10	Q	387	TYR	CB-CG-CD2	-11.53	114.08	121.00
8	S	384	ARG	NE-CZ-NH2	-11.52	114.54	120.30
2	V	230	TYR	CB-CG-CD2	-11.46	114.12	121.00
6	Z	236	PHE	CB-CG-CD1	-11.30	112.89	120.80
1	W	23	ARG	NE-CZ-NH1	11.26	125.93	120.30
8	S	332	PHE	CB-CG-CD2	11.21	128.65	120.80
9	P	234	TYR	CB-CG-CD2	-11.12	114.33	121.00
7	N	906	ARG	NE-CZ-NH1	11.04	125.82	120.30
6	Z	941	ARG	NE-CZ-NH2	11.01	125.81	120.30
9	P	344	ARG	NE-CZ-NH2	-10.95	114.83	120.30
11	R	338	TYR	CB-CG-CD2	-10.90	114.46	121.00
3	T	100	ASP	CB-CG-OD1	10.86	128.07	118.30
11	R	345	TYR	CB-CG-CD2	-10.73	114.56	121.00
10	Q	124	PHE	CB-CG-CD1	10.69	128.28	120.80
2	V	230	TYR	CB-CG-CD1	10.68	127.41	121.00
10	Q	202	ARG	NE-CZ-NH1	10.65	125.62	120.30
8	S	382	ARG	NE-CZ-NH1	10.43	125.52	120.30
10	Q	387	TYR	CB-CG-CD1	10.37	127.22	121.00
13	O	330	ARG	NE-CZ-NH1	10.35	125.48	120.30
7	N	559	TYR	CB-CG-CD1	-10.32	114.81	121.00
11	R	24	TYR	CB-CG-CD1	10.29	127.17	121.00
8	S	405	ARG	NE-CZ-NH1	10.28	125.44	120.30
6	Z	24	THR	C-N-CD	-10.25	98.04	120.60
9	P	379	TYR	CB-CG-CD2	-10.25	114.85	121.00
1	W	157	PHE	CB-CG-CD1	10.23	127.96	120.80
7	N	549	TYR	CB-CG-CD1	-10.22	114.87	121.00
7	N	597	ARG	NE-CZ-NH2	-10.19	115.21	120.30
1	W	65	PHE	CB-CG-CD1	-10.16	113.69	120.80
9	P	21	PHE	CB-CG-CD2	10.15	127.90	120.80
10	Q	84	TYR	CB-CG-CD1	-10.12	114.92	121.00
4	X	59	ARG	NE-CZ-NH1	10.11	125.35	120.30
6	Z	394	TYR	CB-CG-CD1	-10.09	114.94	121.00
10	Q	339	TYR	CB-CG-CD1	-10.00	115.00	121.00
4	X	122	TYR	CB-CG-CD1	9.96	126.97	121.00
3	T	51	TYR	CB-CG-CD1	9.92	126.95	121.00
3	T	20	TYR	CB-CG-CD2	9.91	126.95	121.00
6	Z	583	ASP	CB-CG-OD1	-9.83	109.45	118.30
2	V	228	TYR	CB-CG-CD2	-9.79	115.13	121.00
10	Q	209	TYR	CB-CG-CD2	-9.74	115.16	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	363	PHE	CB-CG-CD1	9.64	127.55	120.80
5	Y	71	ASP	CB-CG-OD1	9.63	126.97	118.30
6	Z	497	PHE	CB-CG-CD2	-9.62	114.06	120.80
6	Z	962	ARG	NE-CZ-NH2	-9.61	115.50	120.30
3	T	128	TYR	CB-CG-CD1	-9.61	115.24	121.00
10	Q	354	PHE	CB-CA-C	-9.59	91.22	110.40
8	S	377	TYR	CG-CD1-CE1	-9.58	113.64	121.30
8	S	292	TYR	CB-CG-CD1	-9.57	115.26	121.00
12	U	233	PHE	CB-CG-CD2	9.54	127.48	120.80
3	T	51	TYR	CB-CG-CD2	-9.51	115.29	121.00
6	Z	408	TYR	CB-CG-CD1	9.51	126.71	121.00
9	P	78	GLN	CA-C-N	9.44	137.97	117.20
1	W	65	PHE	CB-CG-CD2	9.43	127.40	120.80
10	Q	27	TYR	CB-CG-CD2	-9.43	115.34	121.00
8	S	114	TYR	CB-CG-CD1	9.39	126.64	121.00
5	Y	73	PHE	CB-CG-CD2	-9.39	114.23	120.80
9	P	158	ASP	CB-CG-OD2	-9.39	109.85	118.30
9	P	356	TYR	CB-CG-CD2	-9.35	115.39	121.00
9	P	356	TYR	CB-CG-CD1	9.29	126.58	121.00
6	Z	418	ALA	CB-CA-C	-9.28	96.18	110.10
4	X	99	PHE	CB-CG-CD1	-9.20	114.36	120.80
10	Q	236	PHE	CB-CG-CD1	-9.18	114.38	120.80
10	Q	246	TYR	CB-CG-CD2	-9.16	115.50	121.00
7	N	887	ASP	CB-CG-OD1	-9.09	110.12	118.30
6	Z	426	TYR	CB-CG-CD1	9.06	126.44	121.00
4	X	59	ARG	NE-CZ-NH2	-9.02	115.79	120.30
9	P	232	ARG	NE-CZ-NH2	-9.00	115.80	120.30
8	S	127	THR	N-CA-CB	8.99	127.38	110.30
9	P	245	TYR	CB-CG-CD1	-8.93	115.64	121.00
10	Q	27	TYR	CB-CG-CD1	8.91	126.35	121.00
12	U	233	PHE	CB-CG-CD1	-8.88	114.59	120.80
12	U	283	ARG	NE-CZ-NH1	8.88	124.74	120.30
11	R	99	TYR	CG-CD2-CE2	8.87	128.40	121.30
3	T	128	TYR	CB-CG-CD2	8.84	126.31	121.00
9	P	221	TYR	CB-CG-CD1	8.82	126.29	121.00
11	R	363	PHE	CB-CG-CD2	-8.79	114.64	120.80
11	R	43	ARG	NE-CZ-NH1	8.75	124.68	120.30
6	Z	909	ARG	NE-CZ-NH1	8.74	124.67	120.30
11	R	43	ARG	NE-CZ-NH2	-8.73	115.93	120.30
9	P	303	PHE	CB-CG-CD1	-8.70	114.71	120.80
13	O	62	TYR	CB-CG-CD1	8.69	126.21	121.00
8	S	399	TYR	CB-CG-CD2	-8.64	115.81	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	U	69	ASP	CB-CG-OD1	8.64	126.08	118.30
8	S	137	PHE	CB-CG-CD2	-8.64	114.75	120.80
13	O	301	PHE	CB-CG-CD1	-8.61	114.77	120.80
7	N	762	ARG	NE-CZ-NH2	-8.61	116.00	120.30
10	Q	314	PHE	CB-CG-CD1	8.56	126.79	120.80
8	S	145	PHE	CB-CG-CD2	-8.55	114.81	120.80
7	N	753	PHE	CB-CG-CD1	-8.53	114.83	120.80
7	N	123	PHE	CG-CD1-CE1	8.50	130.15	120.80
11	R	113	LEU	CB-CG-CD1	8.48	125.42	111.00
13	O	66	VAL	CA-CB-CG2	-8.43	98.26	110.90
5	Y	73	PHE	CB-CG-CD1	8.40	126.68	120.80
9	P	163	LEU	CB-CG-CD1	8.39	125.27	111.00
6	Z	382	ALA	CB-CA-C	-8.39	97.52	110.10
13	O	62	TYR	CG-CD1-CE1	-8.38	114.60	121.30
8	S	332	PHE	CB-CG-CD1	-8.35	114.96	120.80
10	Q	151	TYR	CB-CG-CD1	8.34	126.00	121.00
10	Q	65	TYR	CB-CG-CD2	-8.32	116.01	121.00
8	S	186	TYR	CB-CG-CD2	8.32	125.99	121.00
6	Z	133	ASP	CB-CG-OD1	8.31	125.78	118.30
11	R	140	TYR	CB-CG-CD2	-8.27	116.04	121.00
6	Z	773	ARG	NE-CZ-NH2	-8.25	116.18	120.30
6	Z	155	ARG	NE-CZ-NH2	-8.23	116.18	120.30
7	N	188	TYR	CB-CG-CD2	8.22	125.93	121.00
9	P	364	ARG	NE-CZ-NH2	-8.22	116.19	120.30
10	Q	84	TYR	CB-CG-CD2	8.17	125.90	121.00
6	Z	408	TYR	CB-CG-CD2	-8.15	116.11	121.00
7	N	75	TYR	CB-CG-CD1	8.15	125.89	121.00
7	N	618	ARG	NE-CZ-NH1	8.14	124.37	120.30
7	N	548	ARG	NE-CZ-NH2	-8.13	116.24	120.30
11	R	261	LEU	CB-CA-C	8.12	125.62	110.20
11	R	335	ARG	NE-CZ-NH1	8.07	124.34	120.30
11	R	260	THR	O-C-N	-8.07	109.79	122.70
13	O	306	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	W	113	PHE	CB-CG-CD2	-8.04	115.17	120.80
9	P	21	PHE	CB-CG-CD1	-8.02	115.19	120.80
13	O	230	PHE	CB-CG-CD2	-8.01	115.19	120.80
11	R	24	TYR	CB-CG-CD2	-8.01	116.19	121.00
1	W	182	TYR	CG-CD1-CE1	-8.01	114.89	121.30
8	S	405	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	W	24	THR	N-CA-CB	7.99	125.48	110.30
9	P	279	ASP	CB-CG-OD2	-7.99	111.11	118.30
7	N	639	ASP	CB-CG-OD1	7.99	125.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	182	TYR	CB-CG-CD2	-7.98	116.21	121.00
12	U	100	ARG	NE-CZ-NH2	7.96	124.28	120.30
4	X	17	TYR	CB-CG-CD1	-7.95	116.23	121.00
8	S	298	ARG	NE-CZ-NH2	-7.93	116.33	120.30
7	N	559	TYR	CB-CG-CD2	7.93	125.76	121.00
10	Q	387	TYR	CG-CD2-CE2	-7.92	114.96	121.30
10	Q	68	MET	N-CA-CB	7.92	124.86	110.60
6	Z	837	TYR	CB-CG-CD2	7.91	125.74	121.00
6	Z	55	ARG	NE-CZ-NH1	7.89	124.25	120.30
8	S	442	PHE	CB-CG-CD1	7.89	126.32	120.80
10	Q	20	TYR	CZ-CE2-CD2	7.87	126.88	119.80
7	N	597	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	W	25	ARG	NE-CZ-NH1	7.85	124.22	120.30
6	Z	431	ASP	CB-CG-OD1	7.83	125.35	118.30
10	Q	286	TYR	CB-CG-CD2	7.83	125.70	121.00
8	S	145	PHE	CB-CG-CD1	7.82	126.27	120.80
8	S	82	TYR	CB-CG-CD1	7.82	125.69	121.00
13	O	48	PHE	CB-CG-CD2	-7.81	115.33	120.80
3	T	90	PHE	CB-CG-CD2	-7.80	115.34	120.80
7	N	213	PHE	CB-CG-CD2	-7.78	115.35	120.80
13	O	29	PHE	CB-CG-CD2	-7.74	115.38	120.80
8	S	25	TYR	CB-CG-CD2	-7.74	116.36	121.00
10	Q	65	TYR	CB-CG-CD1	7.74	125.64	121.00
13	O	70	TYR	CB-CG-CD1	-7.71	116.37	121.00
6	Z	738	TYR	CG-CD2-CE2	7.70	127.46	121.30
13	O	18	ALA	CB-CA-C	-7.67	98.60	110.10
13	O	147	ARG	NE-CZ-NH1	7.67	124.13	120.30
8	S	51	ARG	NE-CZ-NH1	-7.65	116.47	120.30
11	R	214	TYR	CB-CG-CD1	-7.63	116.42	121.00
4	X	17	TYR	CD1-CE1-CZ	-7.58	112.97	119.80
9	P	234	TYR	CB-CG-CD1	7.56	125.54	121.00
6	Z	55	ARG	NE-CZ-NH2	7.55	124.08	120.30
7	N	81	TYR	CB-CG-CD2	-7.55	116.47	121.00
1	W	17	ARG	NE-CZ-NH1	-7.55	116.53	120.30
7	N	743	PHE	CB-CG-CD2	-7.53	115.53	120.80
11	R	377	LEU	CB-CG-CD2	7.53	123.80	111.00
6	Z	608	TYR	CD1-CE1-CZ	7.53	126.58	119.80
11	R	305	PHE	CB-CG-CD1	7.52	126.06	120.80
9	P	327	LEU	N-CA-CB	7.50	125.40	110.40
7	N	188	TYR	CB-CG-CD1	-7.48	116.52	121.00
10	Q	434	TYR	CB-CG-CD1	-7.46	116.52	121.00
8	S	272	TYR	CB-CG-CD1	7.46	125.47	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	367	TYR	CB-CG-CD1	-7.45	116.53	121.00
7	N	593	PHE	CB-CG-CD1	7.45	126.02	120.80
13	O	286	PHE	CB-CG-CD1	7.44	126.01	120.80
11	R	345	TYR	CG-CD1-CE1	-7.43	115.36	121.30
10	Q	240	PHE	CB-CG-CD1	7.41	125.98	120.80
6	Z	439	TYR	CB-CG-CD1	7.40	125.44	121.00
4	X	48	PHE	CB-CG-CD2	-7.40	115.62	120.80
6	Z	619	ASP	CB-CG-OD2	-7.40	111.64	118.30
6	Z	439	TYR	CG-CD2-CE2	7.39	127.21	121.30
9	P	179	PHE	CB-CG-CD1	7.39	125.97	120.80
2	V	251	TYR	CB-CG-CD1	7.37	125.42	121.00
8	S	475	TYR	CB-CG-CD2	-7.37	116.58	121.00
7	N	784	TYR	CB-CG-CD1	7.35	125.41	121.00
13	O	100	ASP	CB-CG-OD2	7.35	124.92	118.30
7	N	19	SER	N-CA-CB	7.35	121.52	110.50
10	Q	124	PHE	CB-CG-CD2	-7.34	115.66	120.80
3	T	173	GLU	N-CA-CB	7.33	123.79	110.60
10	Q	291	TYR	CG-CD2-CE2	7.32	127.16	121.30
13	O	312	ASP	CB-CG-OD2	7.32	124.89	118.30
13	O	58	ARG	NE-CZ-NH1	-7.30	116.65	120.30
10	Q	400	TYR	CB-CG-CD1	7.30	125.38	121.00
6	Z	341	TYR	CB-CG-CD2	-7.29	116.62	121.00
8	S	286	TYR	CB-CG-CD1	-7.29	116.62	121.00
11	R	417	TYR	CB-CG-CD2	-7.28	116.63	121.00
8	S	259	TYR	CB-CG-CD1	-7.28	116.63	121.00
3	T	88	TYR	CB-CG-CD2	-7.27	116.64	121.00
9	P	78	GLN	C-N-CA	7.26	139.86	121.70
7	N	75	TYR	CB-CG-CD2	-7.25	116.65	121.00
3	T	266	TYR	CB-CG-CD2	-7.23	116.66	121.00
10	Q	88	PHE	CB-CG-CD1	-7.22	115.75	120.80
6	Z	193	PHE	CB-CG-CD2	-7.20	115.76	120.80
12	U	253	ASP	CB-CG-OD1	-7.18	111.83	118.30
7	N	109	TYR	CB-CG-CD1	-7.16	116.70	121.00
8	S	59	ASP	CA-CB-CG	-7.15	97.66	113.40
3	T	39	LEU	CB-CG-CD2	7.14	123.13	111.00
7	N	548	ARG	NE-CZ-NH1	7.13	123.86	120.30
13	O	33	TYR	CZ-CE2-CD2	-7.10	113.41	119.80
6	Z	431	ASP	CB-CG-OD2	-7.08	111.92	118.30
3	T	92	ASN	N-CA-C	-7.05	91.97	111.00
7	N	921	ARG	NE-CZ-NH2	-7.04	116.78	120.30
7	N	906	ARG	NH1-CZ-NH2	-7.03	111.66	119.40
10	Q	202	ARG	NH1-CZ-NH2	-7.03	111.66	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	20	TYR	CB-CG-CD1	-7.03	116.78	121.00
10	Q	400	TYR	CB-CG-CD2	-7.03	116.78	121.00
6	Z	55	ARG	NH1-CZ-NH2	-7.03	111.67	119.40
7	N	471	TYR	CB-CG-CD2	7.02	125.21	121.00
6	Z	26	ASN	CB-CA-C	-7.02	96.36	110.40
4	X	14	VAL	CG1-CB-CG2	7.01	122.12	110.90
6	Z	941	ARG	NE-CZ-NH1	-7.00	116.80	120.30
9	P	265	VAL	CA-CB-CG1	7.00	121.39	110.90
6	Z	759	ARG	NE-CZ-NH1	6.99	123.80	120.30
8	S	126	LYS	CB-CA-C	6.98	124.35	110.40
2	V	57	PHE	CB-CG-CD2	-6.97	115.92	120.80
7	N	721	ASP	CB-CG-OD2	6.96	124.57	118.30
7	N	213	PHE	CB-CG-CD1	6.96	125.67	120.80
7	N	453	ALA	CB-CA-C	-6.96	99.66	110.10
10	Q	116	PHE	CB-CG-CD2	-6.96	115.93	120.80
6	Z	138	ARG	NE-CZ-NH1	6.96	123.78	120.30
6	Z	269	TYR	CB-CG-CD2	-6.94	116.84	121.00
8	S	188	TYR	CB-CG-CD2	-6.94	116.84	121.00
7	N	591	LEU	CB-CA-C	-6.93	97.04	110.20
8	S	333	PHE	CB-CG-CD1	6.92	125.64	120.80
4	X	46	TRP	CE2-CD2-CG	-6.91	101.77	107.30
11	R	27	SER	N-CA-CB	6.90	120.86	110.50
9	P	25	ASP	CB-CG-OD1	-6.89	112.10	118.30
13	O	189	TYR	CB-CG-CD2	-6.89	116.86	121.00
6	Z	426	TYR	CB-CG-CD2	-6.89	116.87	121.00
8	S	198	SER	N-CA-CB	6.87	120.80	110.50
8	S	276	LEU	CB-CG-CD1	6.86	122.67	111.00
3	T	220	PHE	CB-CG-CD2	-6.86	116.00	120.80
9	P	329	PHE	CB-CG-CD1	6.86	125.60	120.80
13	O	288	ARG	NE-CZ-NH1	6.86	123.73	120.30
7	N	389	TYR	CB-CG-CD2	-6.84	116.89	121.00
8	S	174	ARG	NE-CZ-NH2	-6.83	116.88	120.30
9	P	379	TYR	CG-CD1-CE1	-6.82	115.85	121.30
4	X	46	TRP	CE2-CD2-CE3	6.81	126.88	118.70
10	Q	291	TYR	CB-CG-CD1	6.81	125.09	121.00
8	S	399	TYR	CG-CD1-CE1	-6.80	115.86	121.30
9	P	208	PHE	CB-CG-CD2	-6.80	116.04	120.80
1	W	25	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	W	60	ARG	NE-CZ-NH2	-6.78	116.91	120.30
12	U	20	ASP	CB-CG-OD2	-6.77	112.20	118.30
12	U	204	LEU	CB-CG-CD1	6.76	122.50	111.00
4	X	17	TYR	CG-CD1-CE1	6.74	126.69	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	254	ARG	NE-CZ-NH2	-6.73	116.94	120.30
6	Z	376	SER	N-CA-CB	6.73	120.59	110.50
11	R	214	TYR	CG-CD1-CE1	-6.71	115.93	121.30
12	U	189	ARG	NE-CZ-NH2	-6.71	116.94	120.30
8	S	82	TYR	CB-CG-CD2	-6.71	116.98	121.00
6	Z	165	TYR	O-C-N	-6.70	111.98	122.70
6	Z	261	ASP	CB-CG-OD2	-6.70	112.28	118.30
11	R	180	PHE	CB-CG-CD2	-6.69	116.12	120.80
10	Q	391	ASP	CB-CG-OD2	-6.68	112.29	118.30
8	S	23	LYS	N-CA-CB	6.67	122.61	110.60
5	Y	31	GLU	N-CA-CB	6.67	122.60	110.60
7	N	203	ARG	NE-CZ-NH1	6.66	123.63	120.30
8	S	158	PHE	CB-CG-CD1	-6.64	116.15	120.80
6	Z	8	LYS	N-CA-CB	6.64	122.56	110.60
13	O	26	PHE	CB-CG-CD1	-6.64	116.16	120.80
13	O	194	LEU	CB-CG-CD1	6.62	122.26	111.00
2	V	197	TYR	CB-CG-CD2	-6.62	117.03	121.00
7	N	639	ASP	CB-CG-OD2	-6.61	112.35	118.30
6	Z	404	ASP	CB-CG-OD1	6.61	124.25	118.30
2	V	273	ARG	NH1-CZ-NH2	6.61	126.67	119.40
10	Q	29	SER	CB-CA-C	6.60	122.64	110.10
11	R	246	TYR	CB-CG-CD1	-6.60	117.04	121.00
6	Z	107	THR	CA-CB-CG2	-6.59	103.17	112.40
12	U	22	TYR	CB-CG-CD1	-6.57	117.06	121.00
8	S	184	TRP	CE2-CD2-CE3	6.55	126.56	118.70
3	T	211	PHE	CZ-CE2-CD2	-6.55	112.24	120.10
11	R	99	TYR	CB-CA-C	6.54	123.49	110.40
11	R	123	ASP	CB-CG-OD1	-6.54	112.42	118.30
9	P	64	ASP	CB-CG-OD1	6.53	124.18	118.30
8	S	174	ARG	N-CA-CB	6.53	122.35	110.60
1	W	112	ALA	CB-CA-C	-6.52	100.31	110.10
11	R	297	TYR	CZ-CE2-CD2	-6.50	113.95	119.80
13	O	369	ARG	NE-CZ-NH1	6.50	123.55	120.30
7	N	442	LEU	CB-CG-CD2	6.49	122.03	111.00
4	X	47	ASP	N-CA-CB	6.48	122.27	110.60
7	N	721	ASP	CB-CG-OD1	-6.48	112.47	118.30
8	S	393	ARG	NE-CZ-NH2	-6.48	117.06	120.30
2	V	289	GLU	N-CA-CB	6.46	122.22	110.60
8	S	217	PHE	CB-CG-CD2	-6.45	116.29	120.80
3	T	139	ASP	CB-CG-OD2	-6.43	112.52	118.30
7	N	873	ARG	NE-CZ-NH2	-6.43	117.09	120.30
7	N	265	ALA	CB-CA-C	-6.42	100.47	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	323	TYR	CG-CD1-CE1	-6.40	116.18	121.30
13	O	122	HIS	CA-CB-CG	-6.40	102.73	113.60
8	S	76	PHE	CB-CG-CD2	-6.38	116.33	120.80
8	S	114	TYR	CB-CG-CD2	-6.38	117.17	121.00
11	R	260	THR	C-N-CA	-6.38	105.76	121.70
6	Z	837	TYR	CB-CG-CD1	-6.37	117.18	121.00
6	Z	7	LYS	N-CA-CB	6.37	122.07	110.60
4	X	17	TYR	CB-CG-CD2	6.36	124.82	121.00
11	R	331	ARG	NE-CZ-NH1	6.36	123.48	120.30
8	S	272	TYR	CB-CG-CD2	-6.36	117.19	121.00
10	Q	398	TYR	N-CA-CB	6.35	122.04	110.60
2	V	198	SER	N-CA-CB	6.35	120.03	110.50
7	N	741	TYR	CB-CG-CD2	-6.34	117.19	121.00
6	Z	7	LYS	CB-CA-C	-6.33	97.74	110.40
3	T	109	TYR	CB-CG-CD1	6.31	124.79	121.00
7	N	522	ALA	N-CA-CB	6.31	118.94	110.10
11	R	68	GLU	O-C-N	-6.31	112.61	122.70
1	W	138	ALA	N-CA-CB	6.30	118.92	110.10
4	X	65	SER	N-CA-CB	6.30	119.95	110.50
13	O	310	PHE	CB-CG-CD2	-6.29	116.40	120.80
3	T	234	TYR	CG-CD1-CE1	-6.28	116.28	121.30
7	N	417	ARG	NE-CZ-NH1	-6.28	117.16	120.30
6	Z	811	SER	O-C-N	-6.27	112.67	122.70
6	Z	825	ALA	N-CA-CB	6.27	118.87	110.10
7	N	584	ARG	NE-CZ-NH1	6.26	123.43	120.30
9	P	357	TYR	CB-CG-CD2	-6.25	117.25	121.00
9	P	220	TYR	CB-CG-CD2	-6.24	117.25	121.00
6	Z	970	TYR	CB-CG-CD2	6.24	124.74	121.00
7	N	417	ARG	NE-CZ-NH2	6.23	123.42	120.30
1	W	186	ALA	N-CA-CB	6.22	118.81	110.10
2	V	206	THR	CA-CB-CG2	-6.22	103.70	112.40
9	P	303	PHE	CB-CG-CD2	6.21	125.15	120.80
1	W	187	SER	O-C-N	-6.20	112.78	122.70
6	Z	963	ALA	CB-CA-C	-6.20	100.81	110.10
11	R	181	TYR	CZ-CE2-CD2	6.20	125.38	119.80
13	O	166	ARG	NE-CZ-NH1	6.19	123.40	120.30
4	X	22	ARG	N-CA-CB	6.19	121.75	110.60
10	Q	20	TYR	CG-CD2-CE2	-6.19	116.35	121.30
2	V	42	ARG	NE-CZ-NH2	-6.19	117.20	120.30
10	Q	94	VAL	CB-CA-C	-6.18	99.65	111.40
1	W	103	ASN	N-CA-CB	6.18	121.72	110.60
13	O	35	GLU	C-N-CA	6.17	137.14	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	608	TYR	CG-CD1-CE1	-6.17	116.36	121.30
9	P	356	TYR	CG-CD1-CE1	-6.17	116.37	121.30
6	Z	962	ARG	NE-CZ-NH1	6.17	123.38	120.30
13	O	189	TYR	CG-CD2-CE2	-6.16	116.37	121.30
13	O	59	LEU	CB-CA-C	-6.16	98.50	110.20
7	N	578	ASP	CB-CG-OD1	-6.15	112.77	118.30
8	S	377	TYR	CB-CG-CD1	-6.14	117.32	121.00
9	P	416	SER	N-CA-CB	6.11	119.67	110.50
7	N	653	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	W	157	PHE	CB-CG-CD2	-6.09	116.53	120.80
3	T	249	MET	CG-SD-CE	-6.09	90.45	100.20
9	P	47	ARG	NE-CZ-NH1	6.08	123.34	120.30
10	Q	110	SER	N-CA-CB	6.07	119.61	110.50
6	Z	358	TYR	CB-CG-CD2	-6.07	117.36	121.00
10	Q	103	LYS	N-CA-CB	6.06	121.51	110.60
10	Q	67	THR	C-N-CA	6.05	136.84	121.70
9	P	240	TYR	CB-CG-CD1	-6.05	117.37	121.00
12	U	176	ARG	NE-CZ-NH1	6.05	123.32	120.30
8	S	48	LEU	CB-CA-C	-6.03	98.73	110.20
12	U	274	MET	CG-SD-CE	-6.03	90.55	100.20
9	P	3	ARG	CG-CD-NE	-6.02	99.15	111.80
13	O	62	TYR	CD1-CE1-CZ	6.02	125.22	119.80
9	P	193	TYR	CA-CB-CG	-6.01	101.97	113.40
10	Q	132	PHE	CB-CG-CD1	6.01	125.01	120.80
11	R	398	ALA	N-CA-CB	6.01	118.51	110.10
3	T	60	ARG	NE-CZ-NH2	-6.01	117.30	120.30
9	P	431	HIS	CB-CA-C	-6.01	98.39	110.40
6	Z	885	ALA	CB-CA-C	-6.00	101.10	110.10
12	U	75	ASN	CB-CA-C	-6.00	98.39	110.40
11	R	324	ARG	NE-CZ-NH2	-5.99	117.31	120.30
6	Z	902	TYR	CB-CG-CD2	-5.98	117.41	121.00
10	Q	306	TYR	CG-CD1-CE1	5.98	126.08	121.30
2	V	157	ARG	NE-CZ-NH1	5.96	123.28	120.30
6	Z	193	PHE	CB-CG-CD1	5.96	124.97	120.80
6	Z	320	SER	N-CA-CB	5.96	119.43	110.50
13	O	228	TYR	CB-CG-CD1	-5.96	117.43	121.00
8	S	425	ARG	NE-CZ-NH2	-5.95	117.32	120.30
6	Z	369	PHE	CB-CG-CD1	5.95	124.96	120.80
6	Z	251	ALA	O-C-N	5.95	132.21	122.70
8	S	431	VAL	CA-CB-CG2	-5.94	101.99	110.90
7	N	202	PHE	CB-CG-CD2	-5.94	116.64	120.80
4	X	100	TRP	CG-CD2-CE3	-5.93	128.56	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	379	TYR	CD1-CE1-CZ	5.92	125.13	119.80
6	Z	323	TYR	CB-CG-CD2	-5.91	117.45	121.00
11	R	186	TYR	CB-CG-CD2	5.90	124.54	121.00
9	P	379	TYR	CB-CG-CD1	5.90	124.54	121.00
3	T	250	MET	CG-SD-CE	-5.88	90.79	100.20
8	S	168	LEU	CB-CA-C	-5.88	99.03	110.20
2	V	101	ASP	CB-CG-OD1	5.88	123.59	118.30
12	U	251	ASN	N-CA-CB	5.88	121.17	110.60
11	R	59	MET	CG-SD-CE	5.87	109.60	100.20
10	Q	309	ARG	NE-CZ-NH2	-5.86	117.37	120.30
11	R	272	ASP	CB-CG-OD1	5.86	123.57	118.30
11	R	213	TYR	CB-CG-CD1	-5.85	117.49	121.00
11	R	285	ALA	CB-CA-C	-5.85	101.32	110.10
6	Z	936	VAL	C-N-CA	5.85	134.58	122.30
7	N	406	TYR	CZ-CE2-CD2	-5.84	114.54	119.80
2	V	60	ASP	CB-CG-OD2	-5.84	113.04	118.30
7	N	58	ARG	NE-CZ-NH2	-5.84	117.38	120.30
7	N	300	ASN	CB-CG-OD1	-5.84	109.92	121.60
9	P	175	GLU	OE1-CD-OE2	5.83	130.30	123.30
12	U	7	LYS	CB-CA-C	-5.83	98.74	110.40
13	O	48	PHE	CB-CG-CD1	5.82	124.88	120.80
8	S	25	TYR	CB-CG-CD1	5.82	124.49	121.00
8	S	137	PHE	CB-CG-CD1	5.82	124.87	120.80
8	S	399	TYR	CD1-CE1-CZ	5.82	125.03	119.80
9	P	4	ASP	CB-CG-OD1	-5.82	113.06	118.30
6	Z	517	ASP	CB-CG-OD1	-5.82	113.07	118.30
6	Z	122	LEU	CB-CG-CD2	5.81	120.88	111.00
10	Q	189	ARG	NE-CZ-NH2	-5.81	117.39	120.30
13	O	142	ASP	N-CA-C	-5.81	95.31	111.00
8	S	186	TYR	CB-CG-CD1	-5.81	117.52	121.00
9	P	126	THR	CA-CB-CG2	-5.80	104.27	112.40
6	Z	753	GLY	C-N-CA	5.80	136.20	121.70
6	Z	473	LEU	CB-CG-CD2	5.80	120.86	111.00
9	P	318	TYR	CG-CD2-CE2	-5.80	116.66	121.30
7	N	913	PRO	N-CA-CB	5.80	110.25	103.30
11	R	213	TYR	CG-CD1-CE1	-5.79	116.67	121.30
2	V	94	MET	CA-CB-CG	5.79	123.15	113.30
6	Z	886	VAL	CA-CB-CG2	-5.79	102.22	110.90
7	N	557	LEU	CB-CG-CD2	5.79	120.84	111.00
8	S	162	VAL	CB-CA-C	5.78	122.38	111.40
6	Z	738	TYR	CZ-CE2-CD2	-5.78	114.60	119.80
9	P	21	PHE	CZ-CE2-CD2	-5.77	113.18	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	771	PHE	N-CA-CB	5.77	120.98	110.60
6	Z	944	LYS	N-CA-CB	5.76	120.98	110.60
11	R	204	TRP	CG-CD2-CE3	-5.76	128.72	133.90
7	N	804	LEU	CB-CA-C	-5.74	99.29	110.20
2	V	45	VAL	CA-CB-CG1	5.73	119.50	110.90
5	Y	83	ARG	NE-CZ-NH2	-5.73	117.44	120.30
7	N	599	TYR	CB-CG-CD2	-5.72	117.57	121.00
13	O	146	ALA	CB-CA-C	-5.72	101.52	110.10
10	Q	424	ASP	CB-CG-OD1	-5.71	113.16	118.30
7	N	203	ARG	NE-CZ-NH2	-5.71	117.44	120.30
7	N	743	PHE	CD1-CG-CD2	5.71	125.72	118.30
8	S	286	TYR	CB-CG-CD2	5.71	124.43	121.00
7	N	203	ARG	CD-NE-CZ	5.71	131.59	123.60
3	T	27	LEU	CA-C-N	5.70	133.07	117.10
8	S	167	LEU	CB-CG-CD2	5.70	120.69	111.00
6	Z	236	PHE	CG-CD1-CE1	-5.70	114.53	120.80
2	V	196	TYR	CB-CG-CD2	-5.70	117.58	121.00
11	R	214	TYR	CG-CD2-CE2	-5.70	116.74	121.30
11	R	252	TYR	CB-CG-CD1	5.69	124.42	121.00
10	Q	276	ASP	CB-CG-OD1	-5.69	113.18	118.30
13	O	39	PHE	CB-CG-CD2	5.69	124.78	120.80
11	R	422	ARG	NE-CZ-NH1	5.69	123.14	120.30
3	T	15	PHE	CB-CG-CD2	-5.69	116.82	120.80
8	S	440	ASP	CB-CG-OD1	5.69	123.42	118.30
13	O	92	PHE	CB-CG-CD1	5.69	124.78	120.80
6	Z	418	ALA	N-CA-CB	5.68	118.06	110.10
13	O	26	PHE	CB-CG-CD2	5.68	124.78	120.80
2	V	128	SER	CB-CA-C	-5.68	99.31	110.10
11	R	224	PHE	CB-CG-CD2	5.67	124.77	120.80
6	Z	126	TYR	CB-CG-CD1	-5.67	117.60	121.00
8	S	152	LEU	C-N-CA	5.67	135.87	121.70
6	Z	13	ASP	CB-CG-OD2	-5.66	113.21	118.30
10	Q	383	ASP	CB-CG-OD2	-5.65	113.21	118.30
6	Z	744	ALA	N-CA-CB	5.65	118.01	110.10
6	Z	899	GLN	N-CA-CB	5.65	120.77	110.60
11	R	237	THR	CA-CB-CG2	-5.65	104.49	112.40
6	Z	55	ARG	CD-NE-CZ	5.64	131.50	123.60
13	O	51	ASP	CB-CG-OD1	5.64	123.38	118.30
7	N	389	TYR	CB-CG-CD1	5.64	124.38	121.00
6	Z	813	PHE	CB-CG-CD2	-5.64	116.85	120.80
6	Z	507	GLY	O-C-N	-5.63	113.69	122.70
10	Q	68	MET	CA-CB-CG	5.63	122.87	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	535	VAL	CG1-CB-CG2	5.63	119.91	110.90
6	Z	126	TYR	CG-CD1-CE1	-5.63	116.80	121.30
12	U	231	ASP	N-CA-CB	-5.63	100.47	110.60
10	Q	399	VAL	CA-CB-CG2	-5.62	102.47	110.90
9	P	379	TYR	CA-CB-CG	-5.62	102.73	113.40
9	P	245	TYR	CB-CG-CD2	5.61	124.37	121.00
8	S	203	SER	CB-CA-C	-5.61	99.44	110.10
11	R	312	TYR	CD1-CE1-CZ	5.61	124.84	119.80
7	N	813	ARG	NE-CZ-NH2	-5.60	117.50	120.30
13	O	352	TRP	CD2-CE2-CZ2	-5.60	115.58	122.30
13	O	352	TRP	CE2-CD2-CG	-5.60	102.82	107.30
6	Z	497	PHE	CB-CG-CD1	5.59	124.72	120.80
9	P	220	TYR	CG-CD2-CE2	-5.59	116.83	121.30
11	R	365	ASP	CB-CG-OD1	5.59	123.33	118.30
6	Z	553	ARG	CD-NE-CZ	5.59	131.42	123.60
10	Q	198	LEU	CB-CG-CD1	5.59	120.50	111.00
12	U	79	MET	CA-CB-CG	5.58	122.79	113.30
9	P	257	TRP	CA-CB-CG	5.58	124.31	113.70
11	R	236	ALA	N-CA-CB	5.58	117.92	110.10
11	R	312	TYR	CG-CD2-CE2	5.58	125.77	121.30
8	S	442	PHE	CB-CG-CD2	-5.58	116.89	120.80
7	N	117	TYR	CB-CG-CD1	-5.58	117.65	121.00
9	P	4	ASP	CB-CG-OD2	5.58	123.32	118.30
9	P	431	HIS	N-CA-CB	5.58	120.64	110.60
2	V	285	ASP	CB-CG-OD1	5.56	123.31	118.30
7	N	740	TRP	CB-CG-CD2	-5.56	119.37	126.60
13	O	58	ARG	CA-CB-CG	5.56	125.64	113.40
11	R	373	PRO	C-N-CA	5.56	135.59	121.70
6	Z	761	PHE	O-C-N	-5.56	113.76	123.20
11	R	272	ASP	CB-CG-OD2	-5.55	113.31	118.30
12	U	288	PHE	CB-CG-CD2	-5.55	116.92	120.80
12	U	183	ALA	O-C-N	5.55	132.63	123.20
7	N	75	TYR	CA-CB-CG	-5.54	102.87	113.40
7	N	395	ALA	CB-CA-C	-5.54	101.79	110.10
11	R	301	TYR	CG-CD1-CE1	5.54	125.73	121.30
6	Z	613	ASP	CB-CG-OD2	-5.54	113.31	118.30
10	Q	145	HIS	CB-CA-C	-5.54	99.33	110.40
11	R	414	LEU	CB-CG-CD2	5.54	120.41	111.00
6	Z	117	ASP	CB-CG-OD1	-5.53	113.32	118.30
7	N	485	MET	O-C-N	-5.53	113.80	123.20
8	S	275	TYR	CD1-CE1-CZ	5.53	124.78	119.80
11	R	141	TYR	CB-CG-CD2	-5.53	117.68	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	U	53	ALA	N-CA-CB	5.53	117.84	110.10
13	O	358	ILE	N-CA-C	-5.52	96.11	111.00
6	Z	916	LEU	CB-CG-CD1	5.51	120.37	111.00
9	P	304	THR	CA-CB-CG2	-5.51	104.68	112.40
3	T	199	PHE	CZ-CE2-CD2	-5.50	113.50	120.10
1	W	156	GLU	CB-CG-CD	-5.50	99.35	114.20
7	N	739	PHE	CB-CG-CD2	-5.50	116.95	120.80
6	Z	295	ARG	NE-CZ-NH1	5.50	123.05	120.30
11	R	236	ALA	CB-CA-C	-5.50	101.86	110.10
13	O	115	ARG	CD-NE-CZ	5.50	131.29	123.60
6	Z	963	ALA	N-CA-CB	5.49	117.79	110.10
8	S	184	TRP	CD1-CG-CD2	5.49	110.69	106.30
12	U	110	PHE	CB-CG-CD2	-5.49	116.96	120.80
9	P	51	ASP	N-CA-CB	5.49	120.48	110.60
6	Z	518	LEU	CA-C-O	-5.48	108.58	120.10
1	W	6	THR	N-CA-CB	5.48	120.72	110.30
8	S	76	PHE	CD1-CE1-CZ	-5.48	113.52	120.10
9	P	115	ARG	NE-CZ-NH2	-5.48	117.56	120.30
7	N	386	MET	CG-SD-CE	5.47	108.96	100.20
8	S	328	PRO	N-CA-CB	5.47	109.87	103.30
7	N	584	ARG	NE-CZ-NH2	-5.47	117.56	120.30
7	N	782	PHE	CB-CG-CD2	-5.47	116.97	120.80
9	P	67	ALA	CB-CA-C	-5.47	101.89	110.10
10	Q	433	LEU	CB-CG-CD2	-5.47	101.71	111.00
9	P	128	ASN	N-CA-CB	5.46	120.44	110.60
11	R	143	GLN	N-CA-CB	5.46	120.44	110.60
7	N	900	ASN	O-C-N	-5.46	113.91	123.20
7	N	394	ARG	NE-CZ-NH2	-5.46	117.57	120.30
7	N	346	ASN	CA-CB-CG	-5.46	101.39	113.40
7	N	782	PHE	CG-CD2-CE2	-5.46	114.80	120.80
1	W	111	VAL	CA-CB-CG1	5.46	119.08	110.90
9	P	123	ARG	NE-CZ-NH1	5.45	123.03	120.30
3	T	157	TYR	CB-CG-CD2	5.45	124.27	121.00
9	P	358	SER	N-CA-CB	5.45	118.67	110.50
8	S	405	ARG	CD-NE-CZ	-5.45	115.97	123.60
9	P	213	TYR	CG-CD2-CE2	5.44	125.65	121.30
10	Q	68	MET	CB-CA-C	-5.44	99.52	110.40
13	O	178	TYR	CB-CG-CD1	-5.44	117.73	121.00
7	N	199	ASN	O-C-N	5.43	131.40	122.70
2	V	269	ARG	NE-CZ-NH2	-5.43	117.58	120.30
7	N	526	TYR	CB-CG-CD2	-5.43	117.74	121.00
11	R	99	TYR	O-C-N	-5.43	114.02	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	159	LEU	CB-CA-C	-5.43	99.89	110.20
10	Q	287	THR	CA-CB-CG2	-5.43	104.80	112.40
3	T	91	SER	N-CA-CB	5.42	118.64	110.50
13	O	91	ASP	CA-CB-CG	-5.42	101.47	113.40
8	S	461	PHE	N-CA-CB	5.42	120.36	110.60
3	T	211	PHE	CB-CG-CD1	-5.42	117.01	120.80
11	R	181	TYR	CG-CD2-CE2	-5.42	116.97	121.30
11	R	259	PHE	CG-CD2-CE2	-5.42	114.84	120.80
9	P	179	PHE	CB-CG-CD2	-5.41	117.01	120.80
11	R	52	ALA	N-CA-CB	5.41	117.67	110.10
8	S	102	SER	N-CA-CB	5.41	118.61	110.50
8	S	376	THR	CA-CB-CG2	-5.41	104.83	112.40
6	Z	503	ASP	CB-CG-OD1	5.40	123.16	118.30
1	W	182	TYR	CZ-CE2-CD2	-5.40	114.94	119.80
4	X	11	ARG	NE-CZ-NH2	-5.40	117.60	120.30
6	Z	790	MET	CG-SD-CE	-5.39	91.57	100.20
12	U	245	ASP	N-CA-CB	5.39	120.31	110.60
2	V	171	ARG	NE-CZ-NH2	-5.38	117.61	120.30
11	R	345	TYR	CB-CA-C	-5.38	99.63	110.40
6	Z	191	SER	CB-CA-C	-5.38	99.87	110.10
1	W	109	ARG	CD-NE-CZ	5.38	131.13	123.60
8	S	377	TYR	CD1-CG-CD2	5.38	123.81	117.90
11	R	328	PHE	CB-CG-CD1	-5.38	117.03	120.80
9	P	371	LEU	CB-CA-C	-5.38	99.98	110.20
10	Q	384	LYS	N-CA-CB	5.38	120.28	110.60
11	R	45	GLU	CG-CD-OE1	-5.37	107.55	118.30
2	V	197	TYR	CB-CG-CD1	5.37	124.22	121.00
11	R	102	LEU	CB-CG-CD1	5.37	120.13	111.00
1	W	194	GLU	OE1-CD-OE2	-5.37	116.86	123.30
7	N	871	MET	CB-CA-C	5.37	121.13	110.40
7	N	528	ARG	NE-CZ-NH2	5.36	122.98	120.30
13	O	58	ARG	NH1-CZ-NH2	5.36	125.30	119.40
8	S	467	PHE	CZ-CE2-CD2	-5.36	113.67	120.10
13	O	38	TRP	CE3-CZ3-CH2	5.36	127.09	121.20
7	N	580	ASN	N-CA-CB	5.36	120.24	110.60
13	O	352	TRP	CE2-CD2-CE3	5.36	125.13	118.70
6	Z	813	PHE	CG-CD2-CE2	-5.35	114.91	120.80
10	Q	130	ARG	C-N-CA	5.35	135.08	121.70
2	V	42	ARG	NE-CZ-NH1	5.35	122.97	120.30
8	S	360	PHE	CB-CG-CD1	-5.35	117.06	120.80
8	S	183	LEU	N-CA-CB	5.34	121.08	110.40
8	S	275	TYR	CG-CD1-CE1	-5.34	117.03	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	553	PHE	CB-CG-CD2	-5.34	117.06	120.80
13	O	181	PHE	N-CA-CB	5.33	120.20	110.60
7	N	318	LYS	CB-CA-C	-5.33	99.73	110.40
12	U	218	GLU	N-CA-CB	5.33	120.19	110.60
2	V	197	TYR	CA-CB-CG	5.33	123.52	113.40
9	P	130	ILE	O-C-N	-5.33	114.18	122.70
7	N	599	TYR	CD1-CE1-CZ	5.33	124.59	119.80
8	S	452	TYR	CB-CG-CD2	-5.33	117.81	121.00
5	Y	71	ASP	CB-CG-OD2	-5.32	113.51	118.30
9	P	213	TYR	CZ-CE2-CD2	-5.32	115.01	119.80
4	X	25	THR	N-CA-C	-5.32	96.64	111.00
10	Q	379	GLN	N-CA-CB	5.32	120.17	110.60
3	T	226	TRP	CB-CG-CD1	5.32	133.91	127.00
11	R	128	LEU	CB-CG-CD1	-5.31	101.97	111.00
1	W	82	GLU	OE1-CD-OE2	5.31	129.67	123.30
12	U	27	THR	CA-CB-OG1	5.31	120.15	109.00
13	O	81	TYR	CB-CG-CD2	-5.31	117.82	121.00
5	Y	89	GLN	CA-C-O	-5.31	108.96	120.10
2	V	228	TYR	CB-CG-CD1	5.30	124.18	121.00
6	Z	601	VAL	CA-CB-CG2	5.30	118.85	110.90
7	N	650	ASP	N-CA-CB	5.29	120.13	110.60
9	P	440	HIS	CA-C-O	-5.29	108.98	120.10
13	O	166	ARG	NE-CZ-NH2	-5.29	117.65	120.30
2	V	306	LYS	CA-C-O	-5.29	108.98	120.10
10	Q	434	TYR	CA-C-O	-5.29	108.99	120.10
4	X	51	ARG	CB-CA-C	-5.29	99.82	110.40
4	X	100	TRP	CE2-CD2-CE3	5.29	125.05	118.70
13	O	230	PHE	CG-CD2-CE2	-5.29	114.98	120.80
7	N	925	ASP	CA-C-O	-5.29	109.00	120.10
10	Q	286	TYR	CB-CG-CD1	-5.29	117.83	121.00
1	W	186	ALA	CB-CA-C	-5.29	102.17	110.10
4	X	133	SER	CA-C-O	-5.28	109.01	120.10
6	Z	464	ASP	CB-CG-OD2	-5.28	113.55	118.30
4	X	97	TYR	CG-CD1-CE1	5.28	125.52	121.30
7	N	745	LEU	CB-CG-CD2	5.28	119.97	111.00
11	R	424	THR	CA-C-O	-5.28	109.02	120.10
6	Z	298	PHE	CB-CG-CD1	5.28	124.49	120.80
6	Z	813	PHE	CZ-CE2-CD2	5.28	126.43	120.10
9	P	10	ASP	N-CA-CB	5.28	120.10	110.60
9	P	221	TYR	CB-CG-CD2	-5.28	117.83	121.00
6	Z	25	PRO	CB-CA-C	-5.27	98.82	112.00
8	S	492	LYS	CA-C-O	-5.27	109.03	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	393	VAL	CA-C-O	-5.27	109.03	120.10
7	N	904	VAL	CG1-CB-CG2	5.27	119.33	110.90
10	Q	309	ARG	N-CA-CB	5.27	120.08	110.60
9	P	240	TYR	CD1-CG-CD2	5.26	123.69	117.90
6	Z	397	ASP	CB-CG-OD2	-5.26	113.56	118.30
7	N	139	ARG	NE-CZ-NH1	-5.26	117.67	120.30
8	S	398	THR	CA-CB-CG2	-5.26	105.03	112.40
3	T	266	TYR	CG-CD2-CE2	5.25	125.50	121.30
6	Z	759	ARG	NE-CZ-NH2	-5.25	117.68	120.30
8	S	251	SER	N-CA-CB	5.24	118.36	110.50
8	S	253	PHE	CB-CG-CD2	5.24	124.47	120.80
6	Z	738	TYR	CG-CD1-CE1	-5.23	117.11	121.30
6	Z	218	GLU	OE1-CD-OE2	-5.23	117.02	123.30
11	R	255	VAL	CB-CA-C	-5.23	101.46	111.40
2	V	203	TYR	CA-CB-CG	-5.23	103.47	113.40
10	Q	219	ASP	CB-CG-OD2	-5.22	113.60	118.30
7	N	299	TYR	CG-CD1-CE1	-5.22	117.12	121.30
9	P	343	LYS	N-CA-CB	5.22	120.00	110.60
2	V	228	TYR	CG-CD1-CE1	-5.22	117.12	121.30
3	T	73	PHE	CB-CG-CD2	-5.22	117.15	120.80
7	N	780	ASP	CB-CG-OD1	5.21	122.99	118.30
12	U	24	ARG	NE-CZ-NH1	5.21	122.91	120.30
11	R	391	ASN	N-CA-CB	5.21	119.98	110.60
4	X	45	PHE	CB-CG-CD2	-5.21	117.15	120.80
7	N	174	LEU	O-C-N	5.21	131.03	122.70
3	T	76	ASP	CB-CG-OD2	5.20	122.98	118.30
3	T	82	PHE	CG-CD1-CE1	-5.20	115.08	120.80
11	R	357	PHE	CB-CG-CD1	-5.20	117.16	120.80
3	T	161	TRP	CB-CG-CD1	5.20	133.76	127.00
9	P	236	GLU	OE1-CD-OE2	5.20	129.54	123.30
9	P	436	GLU	OE1-CD-OE2	5.20	129.53	123.30
10	Q	334	HIS	CA-CB-CG	-5.20	104.77	113.60
7	N	713	VAL	CA-CB-CG2	5.19	118.69	110.90
7	N	193	ALA	CB-CA-C	-5.19	102.31	110.10
6	Z	436	LEU	CB-CG-CD1	5.19	119.82	111.00
7	N	504	TYR	CA-CB-CG	-5.19	103.54	113.40
13	O	356	ARG	NE-CZ-NH1	5.19	122.89	120.30
6	Z	525	MET	CG-SD-CE	-5.18	91.91	100.20
8	S	127	THR	CB-CA-C	-5.18	97.62	111.60
11	R	252	TYR	CB-CG-CD2	-5.18	117.89	121.00
13	O	368	ASP	CB-CG-OD1	-5.18	113.64	118.30
6	Z	149	TRP	CZ3-CH2-CZ2	-5.17	115.39	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	U	146	ASP	CB-CG-OD2	-5.17	113.64	118.30
9	P	329	PHE	CB-CG-CD2	-5.17	117.18	120.80
13	O	145	LYS	CB-CA-C	-5.17	100.05	110.40
7	N	701	VAL	CA-CB-CG1	5.17	118.66	110.90
13	O	373	TRP	CB-CG-CD2	-5.17	119.88	126.60
12	U	89	LEU	CB-CG-CD2	5.17	119.79	111.00
10	Q	238	TYR	CB-CG-CD1	5.17	124.10	121.00
4	X	10	PHE	CB-CG-CD1	-5.17	117.18	120.80
9	P	27	LEU	CB-CG-CD2	5.17	119.78	111.00
13	O	182	LYS	CB-CA-C	-5.17	100.07	110.40
4	X	22	ARG	NE-CZ-NH2	5.16	122.88	120.30
5	Y	80	GLU	CB-CA-C	-5.16	100.07	110.40
6	Z	352	LYS	N-CA-CB	5.16	119.89	110.60
1	W	109	ARG	NE-CZ-NH2	5.16	122.88	120.30
8	S	51	ARG	NE-CZ-NH2	5.16	122.88	120.30
13	O	288	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	W	113	PHE	CB-CG-CD1	5.16	124.41	120.80
6	Z	298	PHE	CB-CG-CD2	-5.15	117.19	120.80
13	O	188	PHE	CZ-CE2-CD2	-5.15	113.92	120.10
6	Z	406	TRP	CZ3-CH2-CZ2	-5.15	115.42	121.60
8	S	275	TYR	CB-CG-CD1	5.15	124.09	121.00
3	T	62	LEU	O-C-N	5.15	130.94	122.70
13	O	286	PHE	CG-CD1-CE1	5.15	126.46	120.80
8	S	72	GLU	CA-CB-CG	5.15	124.72	113.40
10	Q	387	TYR	CZ-CE2-CD2	5.15	124.43	119.80
6	Z	229	SER	N-CA-CB	5.14	118.22	110.50
7	N	647	ASP	CB-CG-OD2	-5.14	113.67	118.30
13	O	225	ASP	N-CA-CB	5.14	119.86	110.60
13	O	310	PHE	CB-CG-CD1	5.14	124.40	120.80
3	T	92	ASN	N-CA-CB	5.14	119.86	110.60
12	U	210	TYR	CB-CG-CD1	-5.14	117.91	121.00
13	O	85	SER	N-CA-CB	5.14	118.21	110.50
13	O	301	PHE	CB-CG-CD2	5.14	124.39	120.80
6	Z	173	ALA	CB-CA-C	5.13	117.80	110.10
1	W	106	GLN	CB-CA-C	-5.13	100.14	110.40
6	Z	904	LEU	C-N-CA	5.13	134.52	121.70
1	W	39	ALA	CB-CA-C	-5.12	102.41	110.10
8	S	170	TYR	CG-CD1-CE1	-5.12	117.20	121.30
3	T	226	TRP	CD1-CG-CD2	-5.12	102.20	106.30
9	P	66	LEU	CB-CG-CD1	5.12	119.71	111.00
13	O	248	TYR	CZ-CE2-CD2	-5.12	115.19	119.80
3	T	145	PRO	N-CD-CG	5.12	110.88	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	125	VAL	C-N-CA	5.12	134.50	121.70
3	T	234	TYR	CB-CG-CD2	-5.12	117.93	121.00
11	R	99	TYR	CD1-CG-CD2	5.11	123.52	117.90
4	X	98	PHE	CB-CG-CD1	-5.11	117.22	120.80
4	X	118	ASP	CB-CG-OD1	5.11	122.90	118.30
13	O	22	LEU	CB-CA-C	-5.11	100.50	110.20
7	N	299	TYR	CD1-CG-CD2	5.10	123.51	117.90
2	V	258	GLU	CB-CG-CD	-5.10	100.44	114.20
9	P	390	TYR	CA-CB-CG	-5.10	103.72	113.40
11	R	298	ALA	CB-CA-C	-5.09	102.46	110.10
13	O	368	ASP	CB-CG-OD2	5.09	122.88	118.30
8	S	25	TYR	CG-CD2-CE2	-5.09	117.23	121.30
6	Z	488	ALA	O-C-N	5.09	130.84	122.70
9	P	25	ASP	O-C-N	-5.09	114.56	122.70
11	R	41	GLU	CG-CD-OE2	5.08	128.47	118.30
4	X	23	LEU	CB-CG-CD2	5.08	119.64	111.00
8	S	184	TRP	CB-CG-CD1	-5.08	120.39	127.00
9	P	252	SER	CB-CA-C	-5.08	100.45	110.10
9	P	422	LEU	CB-CG-CD2	5.08	119.63	111.00
8	S	482	PRO	N-CA-CB	5.08	109.39	103.30
12	U	52	PHE	CB-CG-CD2	-5.08	117.25	120.80
8	S	486	LYS	CB-CG-CD	5.07	124.79	111.60
9	P	59	LEU	CB-CG-CD2	-5.07	102.38	111.00
1	W	49	VAL	CB-CA-C	-5.07	101.76	111.40
6	Z	459	ALA	CB-CA-C	-5.07	102.50	110.10
2	V	76	THR	O-C-N	-5.07	114.59	123.20
6	Z	42	ASP	CB-CG-OD2	-5.07	113.74	118.30
7	N	340	HIS	CB-CA-C	-5.07	100.27	110.40
9	P	166	GLU	CA-CB-CG	5.07	124.55	113.40
7	N	297	ASP	CB-CG-OD1	-5.06	113.74	118.30
8	S	68	LEU	N-CA-CB	5.06	120.52	110.40
12	U	107	ASN	C-N-CA	5.06	134.35	121.70
11	R	65	TYR	CB-CG-CD2	-5.06	117.97	121.00
3	T	151	TRP	CB-CA-C	-5.06	100.29	110.40
2	V	122	ASP	N-CA-CB	5.05	119.70	110.60
7	N	222	TYR	CB-CG-CD1	-5.05	117.97	121.00
7	N	345	ASP	O-C-N	5.05	130.78	122.70
3	T	81	TYR	N-CA-CB	5.05	119.69	110.60
6	Z	107	THR	N-CA-CB	5.05	119.89	110.30
7	N	387	ALA	N-CA-CB	5.05	117.17	110.10
13	O	333	SER	CB-CA-C	-5.05	100.51	110.10
3	T	208	LEU	CB-CG-CD2	5.04	119.57	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	575	ALA	CB-CA-C	-5.04	102.54	110.10
13	O	93	ASP	CB-CG-OD2	5.04	122.84	118.30
6	Z	297	VAL	O-C-N	5.04	130.76	122.70
13	O	384	MET	CG-SD-CE	-5.04	92.14	100.20
6	Z	26	ASN	CA-CB-CG	-5.03	102.33	113.40
7	N	386	MET	CB-CA-C	-5.03	100.34	110.40
10	Q	235	ALA	CB-CA-C	-5.03	102.56	110.10
1	W	24	THR	N-CA-C	-5.03	97.43	111.00
7	N	549	TYR	CD1-CG-CD2	5.03	123.43	117.90
10	Q	302	VAL	CG1-CB-CG2	-5.03	102.86	110.90
13	O	373	TRP	CE2-CD2-CE3	5.02	124.73	118.70
2	V	260	GLU	OE1-CD-OE2	5.02	129.33	123.30
6	Z	155	ARG	NE-CZ-NH1	5.02	122.81	120.30
6	Z	830	LEU	CB-CG-CD2	5.02	119.54	111.00
9	P	300	VAL	CA-CB-CG1	5.02	118.43	110.90
3	T	109	TYR	CG-CD1-CE1	5.02	125.31	121.30
8	S	217	PHE	CB-CG-CD1	5.02	124.31	120.80
8	S	207	ASN	CB-CG-OD1	-5.02	111.57	121.60
13	O	252	PHE	O-C-N	-5.01	114.68	122.70
10	Q	291	TYR	CD1-CG-CD2	-5.01	112.39	117.90
13	O	58	ARG	CB-CG-CD	5.01	124.63	111.60
2	V	244	MET	CG-SD-CE	5.01	108.21	100.20
7	N	298	TYR	CB-CG-CD2	-5.01	118.00	121.00
9	P	168	TYR	CB-CG-CD2	-5.01	118.00	121.00
11	R	69	GLU	N-CA-C	5.01	124.52	111.00
9	P	104	LEU	CB-CG-CD1	5.00	119.51	111.00
13	O	315	LYS	CA-CB-CG	5.00	124.41	113.40

There are no chirality outliers.

All (118) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	N	117	TYR	Sidechain
7	N	14	ARG	Sidechain
7	N	222	TYR	Sidechain
7	N	302	PHE	Sidechain
7	N	389	TYR	Sidechain
7	N	394	ARG	Sidechain
7	N	398	ARG	Sidechain
7	N	422	TYR	Sidechain
7	N	553	PHE	Sidechain
7	N	597	ARG	Sidechain

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Mol	Chain	Res	Type	Group
7	N	613	HIS	Sidechain
7	N	788	TYR	Sidechain
7	N	813	ARG	Sidechain
13	O	106	PHE	Sidechain
13	O	137	TYR	Sidechain
13	O	185	PHE	Sidechain
13	O	188	PHE	Sidechain
13	O	210	ARG	Sidechain
13	O	288	ARG	Sidechain
13	O	301	PHE	Sidechain
13	O	306	ARG	Sidechain
13	O	356	ARG	Sidechain
13	O	369	ARG	Sidechain
13	O	48	PHE	Sidechain
13	O	62	TYR	Sidechain
13	O	70	TYR	Sidechain
9	P	110	LEU	Mainchain
9	P	115	ARG	Sidechain
9	P	168	TYR	Sidechain
9	P	379	TYR	Sidechain
9	P	79	LEU	Mainchain
10	Q	124	PHE	Peptide
10	Q	145	HIS	Sidechain
10	Q	146	TYR	Sidechain
10	Q	161	LEU	Peptide
10	Q	20	TYR	Sidechain
10	Q	255	TYR	Sidechain
10	Q	309	ARG	Sidechain
10	Q	387	TYR	Sidechain
10	Q	400	TYR	Sidechain
10	Q	434	TYR	Sidechain
10	Q	67	THR	Peptide
11	R	176	ARG	Sidechain
11	R	20	ARG	Sidechain
11	R	206	ARG	Sidechain
11	R	210	TYR	Sidechain
11	R	222	ARG	Sidechain
11	R	252	TYR	Sidechain
11	R	297	TYR	Sidechain
11	R	334	ARG	Sidechain
11	R	345	TYR	Sidechain
11	R	392	ARG	Sidechain

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Mol	Chain	Res	Type	Group
11	R	400	TYR	Sidechain
11	R	401	HIS	Sidechain
11	R	422	ARG	Sidechain
11	R	43	ARG	Sidechain
11	R	49	PHE	Sidechain
11	R	63	TYR	Sidechain
11	R	65	TYR	Sidechain
11	R	99	TYR	Sidechain
8	S	158	PHE	Sidechain
8	S	197	SER	Mainchain,Peptide
8	S	275	TYR	Sidechain
8	S	298	ARG	Sidechain
8	S	467	PHE	Sidechain
8	S	486	LYS	Mainchain
8	S	51	ARG	Sidechain
8	S	76	PHE	Sidechain
8	S	82	TYR	Sidechain
3	T	128	TYR	Sidechain
3	T	150	ARG	Sidechain
3	T	197	TYR	Sidechain
3	T	224	ARG	Sidechain
3	T	234	TYR	Sidechain
3	T	235	PHE	Sidechain
3	T	251	HIS	Peptide
3	T	51	TYR	Sidechain
3	T	91	SER	Peptide
12	U	113	TYR	Sidechain
12	U	24	ARG	Sidechain
12	U	32	ARG	Sidechain
2	V	100	ARG	Sidechain
2	V	156	PHE	Sidechain
2	V	20	ARG	Sidechain
2	V	217	HIS	Sidechain
2	V	229	ASP	Peptide
2	V	270	TYR	Sidechain
2	V	273	ARG	Sidechain
1	W	15	TYR	Sidechain
1	W	21	PHE	Sidechain
4	X	122	TYR	Sidechain
4	X	17	TYR	Sidechain
4	X	22	ARG	Sidechain
4	X	48	PHE	Sidechain

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Mol	Chain	Res	Type	Group
4	X	51	ARG	Sidechain
4	X	87	PHE	Sidechain
4	X	98	PHE	Sidechain
5	Y	38	PHE	Sidechain
6	Z	136	ARG	Sidechain
6	Z	137	TYR	Sidechain
6	Z	138	ARG	Sidechain
6	Z	155	ARG	Sidechain
6	Z	210	TYR	Sidechain
6	Z	269	TYR	Sidechain
6	Z	295	ARG	Sidechain
6	Z	439	TYR	Sidechain
6	Z	477	TYR	Sidechain
6	Z	608	TYR	Sidechain
6	Z	64	TYR	Sidechain
6	Z	738	TYR	Sidechain
6	Z	759	ARG	Sidechain
6	Z	774	ARG	Sidechain
6	Z	798	ARG	Sidechain
6	Z	849	ARG	Sidechain
6	Z	893	PHE	Sidechain
6	Z	898	HIS	Sidechain
6	Z	962	ARG	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	W	1534	0	1542	1	0
2	V	2274	0	2273	25	0
3	T	2192	0	2161	7	0
4	X	1032	0	1017	4	0
5	Y	435	0	393	9	0
6	Z	7005	0	6932	71	0
7	N	6882	0	6959	24	0
8	S	3894	0	3938	23	0
9	P	3608	0	3693	20	0
10	Q	3499	0	3524	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	R	3060	0	3083	50	0
12	U	2373	0	2403	16	0
13	O	3186	0	3213	58	0
All	All	40974	0	41131	318	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 4.

All (318) 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)
9:P:78:GLN:C	9:P:79:LEU:N	1.75	1.39
11:R:99:TYR:CE1	11:R:99:TYR:CZ	2.09	1.39
8:S:127:THR:CB	8:S:127:THR:CA	1.98	1.37
11:R:99:TYR:OH	11:R:99:TYR:CE1	1.79	1.32
9:P:212:LYS:O	9:P:213:TYR:CD1	1.92	1.22
11:R:64:LYS:NZ	11:R:99:TYR:CZ	2.10	1.18
6:Z:84:ALA:O	6:Z:86:PRO:HD3	1.45	1.16
6:Z:35:GLU:OE2	6:Z:83:THR:HG21	1.46	1.13
11:R:99:TYR:OH	11:R:99:TYR:CZ	2.04	1.10
11:R:60:ALA:O	11:R:99:TYR:CZ	2.04	1.09
11:R:60:ALA:HB1	11:R:99:TYR:CE1	1.89	1.07
11:R:60:ALA:HB1	11:R:99:TYR:CZ	1.88	1.06
13:O:69:PHE:HD1	13:O:72:LYS:HB2	1.18	1.02
11:R:60:ALA:CB	11:R:99:TYR:CE1	2.44	1.01
11:R:64:LYS:NZ	11:R:99:TYR:CE1	2.29	0.99
13:O:69:PHE:CD1	13:O:72:LYS:CB	2.36	0.99
13:O:69:PHE:CD1	13:O:72:LYS:HB2	1.99	0.97
11:R:60:ALA:C	11:R:99:TYR:CZ	2.39	0.96
12:U:37:ILE:CG2	12:U:48:VAL:CG1	2.44	0.94
13:O:69:PHE:HD1	13:O:72:LYS:CB	1.59	0.93
11:R:99:TYR:HH	11:R:99:TYR:HE1	1.00	0.89
6:Z:26:ASN:C	6:Z:26:ASN:OD1	2.08	0.88
8:S:219:LYS:HA	8:S:219:LYS:HE2	1.56	0.87
12:U:37:ILE:CG2	12:U:48:VAL:HG11	2.03	0.86
13:O:70:TYR:O	13:O:70:TYR:CD2	2.29	0.86
6:Z:26:ASN:O	6:Z:26:ASN:OD1	1.95	0.84
9:P:212:LYS:O	9:P:213:TYR:HD1	1.55	0.84
11:R:60:ALA:HB1	11:R:99:TYR:CE2	2.11	0.84
13:O:49:PHE:CZ	13:O:62:TYR:HB2	2.12	0.82
13:O:70:TYR:C	13:O:70:TYR:CD2	2.52	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:84:ALA:O	6:Z:86:PRO:CD	2.27	0.81
12:U:37:ILE:HG21	12:U:48:VAL:HG11	1.64	0.80
13:O:49:PHE:CE1	13:O:62:TYR:HB2	2.19	0.78
6:Z:127:SER:OG	6:Z:188:ALA:HA	1.83	0.78
13:O:49:PHE:CD1	13:O:58:ARG:HG2	2.18	0.78
13:O:14:LEU:HD21	13:O:61:LEU:HB2	1.66	0.76
11:R:60:ALA:CA	11:R:99:TYR:CE1	2.68	0.76
12:U:37:ILE:CG2	12:U:48:VAL:HG13	2.13	0.76
11:R:60:ALA:HB1	11:R:99:TYR:CD1	2.21	0.76
6:Z:124:MET:CA	6:Z:188:ALA:HB1	2.16	0.76
11:R:60:ALA:O	11:R:99:TYR:OH	2.06	0.73
9:P:212:LYS:C	9:P:213:TYR:CD1	2.62	0.73
11:R:64:LYS:NZ	11:R:99:TYR:CD1	2.56	0.73
2:V:29:ILE:HD12	2:V:201:ILE:HG21	1.71	0.72
11:R:60:ALA:CB	11:R:99:TYR:CZ	2.71	0.72
6:Z:1:MET:HA	6:Z:25:PRO:HG3	1.70	0.72
13:O:14:LEU:CD2	13:O:61:LEU:HB2	2.19	0.72
2:V:185:ILE:HA	2:V:189:ILE:HB	1.73	0.71
5:Y:17:THR:O	8:S:59:ASP:CB	2.38	0.71
12:U:37:ILE:HG22	12:U:48:VAL:HG13	1.72	0.71
11:R:60:ALA:CB	11:R:99:TYR:CD1	2.75	0.69
13:O:62:TYR:CD1	13:O:62:TYR:C	2.62	0.69
5:Y:17:THR:O	8:S:59:ASP:HB2	1.93	0.68
11:R:64:LYS:NZ	11:R:99:TYR:OH	2.21	0.68
11:R:60:ALA:HB1	11:R:99:TYR:CD2	2.30	0.67
6:Z:124:MET:HA	6:Z:188:ALA:HB1	1.77	0.67
6:Z:93:ARG:HB3	6:Z:94:PRO:HD3	1.76	0.67
13:O:62:TYR:CD1	13:O:62:TYR:O	2.48	0.66
13:O:62:TYR:CG	13:O:63:ASP:N	2.48	0.66
9:P:78:GLN:O	9:P:79:LEU:N	2.29	0.66
6:Z:124:MET:O	6:Z:188:ALA:CA	2.44	0.66
11:R:64:LYS:NZ	11:R:99:TYR:CG	2.64	0.66
13:O:26:PHE:HE1	13:O:61:LEU:HD22	1.62	0.65
6:Z:1:MET:CA	6:Z:25:PRO:HG3	2.25	0.65
10:Q:55:GLU:O	10:Q:58:ILE:HG22	1.97	0.64
6:Z:124:MET:SD	6:Z:182:SER:HB3	2.37	0.64
10:Q:366:ILE:HG23	10:Q:368:LEU:H	1.63	0.64
5:Y:89:GLN:OXT	5:Y:89:GLN:CG	2.45	0.64
11:R:55:LYS:HA	11:R:98:LEU:HD13	1.78	0.64
6:Z:1:MET:C	6:Z:25:PRO:HB3	2.17	0.64
8:S:127:THR:CB	8:S:127:THR:C	2.67	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:29:ILE:HD12	2:V:201:ILE:CG2	2.28	0.63
6:Z:1:MET:O	6:Z:25:PRO:HB3	1.99	0.63
6:Z:1:MET:O	6:Z:25:PRO:CB	2.46	0.63
6:Z:7:LYS:HB3	6:Z:26:ASN:ND2	2.13	0.63
11:R:64:LYS:NZ	11:R:99:TYR:CE2	2.52	0.63
13:O:70:TYR:CE1	13:O:78:VAL:HG11	2.34	0.62
2:V:142:ASP:OD1	2:V:144:ILE:HG22	1.99	0.62
6:Z:35:GLU:OE2	6:Z:83:THR:CG2	2.35	0.62
6:Z:35:GLU:CD	6:Z:83:THR:HG21	2.19	0.61
13:O:70:TYR:HD2	13:O:70:TYR:O	1.83	0.61
11:R:60:ALA:HA	11:R:99:TYR:CE1	2.35	0.61
12:U:37:ILE:HG23	12:U:48:VAL:CG1	2.27	0.61
6:Z:124:MET:CB	6:Z:188:ALA:HB1	2.31	0.60
13:O:70:TYR:C	13:O:70:TYR:HD2	2.04	0.60
10:Q:275:ILE:C	10:Q:275:ILE:HD12	2.21	0.60
6:Z:1:MET:O	6:Z:25:PRO:HG3	2.01	0.60
2:V:69:PHE:CD1	2:V:69:PHE:C	2.73	0.60
13:O:66:VAL:HG13	13:O:78:VAL:HG13	1.84	0.60
3:T:80:ASN:HA	7:N:11:ALA:HB1	1.84	0.60
10:Q:157:LEU:HD23	10:Q:157:LEU:C	2.22	0.60
6:Z:24:THR:HB	6:Z:25:PRO:HD3	1.83	0.59
13:O:52:ALA:O	13:O:58:ARG:HB2	2.02	0.59
13:O:66:VAL:CG1	13:O:78:VAL:HG13	2.32	0.59
9:P:93:ILE:O	9:P:96:MET:HB3	2.03	0.58
11:R:32:LEU:HA	11:R:35:GLN:HE21	1.69	0.58
11:R:257:GLY:O	11:R:266:LEU:HD13	2.04	0.58
6:Z:3:ASP:O	6:Z:26:ASN:HB2	2.04	0.58
11:R:113:LEU:HD13	11:R:137:LEU:HD22	1.86	0.58
13:O:49:PHE:HD1	13:O:58:ARG:HG2	1.69	0.57
5:Y:89:GLN:HG2	5:Y:89:GLN:OXT	2.05	0.57
11:R:64:LYS:NZ	11:R:99:TYR:CD2	2.72	0.57
9:P:59:LEU:O	9:P:62:ILE:HG12	2.04	0.57
6:Z:124:MET:O	6:Z:188:ALA:CB	2.52	0.57
10:Q:355:GLU:O	10:Q:356:CYS:CB	2.53	0.56
13:O:214:ALA:HB2	13:O:238:ILE:HG13	1.86	0.56
10:Q:118:CYS:SG	10:Q:144:LEU:HD13	2.45	0.56
6:Z:24:THR:CB	6:Z:25:PRO:CD	2.84	0.56
6:Z:82:MET:HG3	6:Z:82:MET:O	2.05	0.56
5:Y:18:LYS:HA	8:S:56:SER:HA	1.86	0.56
7:N:773:MET:HG2	7:N:884:PHE:CD1	2.41	0.55
13:O:258:LEU:HD23	13:O:291:ILE:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:70:TYR:OH	13:O:75:GLN:HG3	2.07	0.55
13:O:258:LEU:HD23	13:O:291:ILE:CD1	2.37	0.54
13:O:163:ILE:HG22	13:O:164:PRO:O	2.07	0.54
9:P:94:GLN:HB3	9:P:131:PHE:CD2	2.43	0.54
8:S:164:ILE:HB	8:S:165:PRO:CD	2.37	0.54
6:Z:185:ASP:O	6:Z:186:GLY:C	2.45	0.54
6:Z:124:MET:HB3	6:Z:188:ALA:CB	2.37	0.54
6:Z:84:ALA:C	6:Z:86:PRO:HD3	2.25	0.54
7:N:43:LEU:N	7:N:44:PRO:CD	2.70	0.54
6:Z:82:MET:HA	6:Z:85:VAL:HA	1.88	0.54
12:U:37:ILE:HD11	12:U:93:TYR:HB3	1.89	0.54
6:Z:24:THR:HB	6:Z:25:PRO:CD	2.37	0.54
2:V:306:LYS:OXT	2:V:306:LYS:HG3	2.07	0.53
8:S:19:HIS:CD2	8:S:19:HIS:H	2.26	0.53
3:T:28:PRO:HB2	3:T:29:PRO:HD3	1.89	0.53
6:Z:24:THR:N	6:Z:25:PRO:HD2	2.20	0.52
8:S:219:LYS:HE2	8:S:219:LYS:CA	2.34	0.52
7:N:665:ILE:O	7:N:665:ILE:HG23	2.10	0.52
10:Q:78:ILE:HB	10:Q:79:PRO:HD3	1.90	0.52
8:S:184:TRP:HA	8:S:187:ILE:HD12	1.92	0.52
9:P:268:LEU:HD21	9:P:281:ILE:HG13	1.92	0.52
11:R:279:LEU:O	11:R:280:ILE:HG12	2.10	0.51
2:V:117:TRP:HB3	2:V:188:LEU:HG	1.92	0.51
8:S:472:HIS:CE1	12:U:266:THR:HA	2.45	0.51
8:S:439:GLU:OE1	8:S:439:GLU:N	2.33	0.51
6:Z:124:MET:CA	6:Z:188:ALA:CB	2.88	0.51
6:Z:354:PRO:HA	6:Z:357:ILE:HG12	1.93	0.51
12:U:37:ILE:HG21	12:U:48:VAL:CG1	2.26	0.51
7:N:773:MET:HG3	7:N:884:PHE:HD1	1.76	0.51
11:R:286:LEU:O	11:R:289:ILE:HG22	2.11	0.50
13:O:49:PHE:CZ	13:O:62:TYR:CB	2.92	0.50
12:U:120:LEU:CD2	12:U:122:ILE:HG13	2.41	0.50
13:O:26:PHE:CE1	13:O:61:LEU:HD22	2.44	0.50
12:U:37:ILE:HG23	12:U:48:VAL:HG11	1.86	0.50
6:Z:845:LEU:HG	6:Z:846:PHE:CE1	2.47	0.50
2:V:192:LEU:HA	2:V:196:TYR:CZ	2.47	0.50
2:V:142:ASP:OD1	2:V:142:ASP:C	2.49	0.50
13:O:58:ARG:O	13:O:62:TYR:HB3	2.12	0.49
13:O:59:LEU:HD23	13:O:59:LEU:C	2.31	0.49
11:R:60:ALA:HB1	11:R:99:TYR:CG	2.47	0.49
6:Z:124:MET:SD	6:Z:182:SER:CB	3.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:393:VAL:OXT	13:O:393:VAL:HG12	2.11	0.49
10:Q:20:TYR:CZ	10:Q:68:MET:HG2	2.47	0.49
7:N:150:LEU:HD22	7:N:173:LYS:HG3	1.95	0.49
7:N:110:VAL:HG13	7:N:160:GLY:CA	2.42	0.49
8:S:77:THR:O	8:S:80:VAL:HG22	2.13	0.49
2:V:144:ILE:HG23	2:V:145:GLN:HG3	1.95	0.49
6:Z:728:LYS:HB2	6:Z:731:GLY:H	1.78	0.49
13:O:49:PHE:CE1	13:O:58:ARG:HG2	2.48	0.49
6:Z:1:MET:O	6:Z:25:PRO:CG	2.60	0.49
7:N:110:VAL:HG13	7:N:160:GLY:HA2	1.95	0.48
7:N:773:MET:CG	7:N:884:PHE:CD1	2.95	0.48
6:Z:428:TRP:CD1	6:Z:428:TRP:O	2.66	0.48
13:O:254:LEU:HG	13:O:269:LEU:HD13	1.96	0.48
10:Q:377:LEU:O	10:Q:381:ILE:HG13	2.14	0.48
5:Y:20:LYS:NZ	8:S:63:LEU:HD13	2.28	0.48
10:Q:275:ILE:HD12	10:Q:276:ASP:N	2.29	0.48
6:Z:84:ALA:C	6:Z:86:PRO:CD	2.82	0.48
2:V:29:ILE:CD1	2:V:201:ILE:HG21	2.41	0.48
13:O:258:LEU:HA	13:O:291:ILE:CD1	2.44	0.48
13:O:59:LEU:O	13:O:63:ASP:CB	2.62	0.48
11:R:261:LEU:CA	11:R:266:LEU:HB2	2.43	0.48
9:P:212:LYS:C	9:P:213:TYR:CG	2.86	0.48
2:V:117:TRP:CB	2:V:188:LEU:HG	2.44	0.47
10:Q:247:HIS:CE1	10:Q:286:TYR:CE2	3.02	0.47
2:V:183:ALA:O	2:V:184:ASN:HB2	2.14	0.47
6:Z:124:MET:C	6:Z:188:ALA:CB	2.83	0.47
6:Z:4:GLU:O	6:Z:26:ASN:ND2	2.47	0.47
3:T:80:ASN:CA	7:N:11:ALA:HB1	2.43	0.47
13:O:70:TYR:CE1	13:O:102:LEU:HD11	2.50	0.47
11:R:262:GLU:O	11:R:266:LEU:HB3	2.15	0.47
11:R:64:LYS:HG2	11:R:99:TYR:CZ	2.50	0.47
10:Q:255:TYR:H	10:Q:255:TYR:HD1	1.62	0.46
3:T:233:VAL:HG21	3:T:235:PHE:CE1	2.50	0.46
5:Y:32:ASP:HB3	5:Y:33:ASP:H	1.51	0.46
13:O:59:LEU:CG	13:O:85:SER:HB3	2.45	0.46
10:Q:67:THR:H	10:Q:68:MET:HG3	1.80	0.46
6:Z:124:MET:O	6:Z:188:ALA:HA	2.15	0.46
13:O:62:TYR:HE1	13:O:66:VAL:HG21	1.81	0.46
9:P:59:LEU:CG	9:P:96:MET:HG2	2.46	0.46
6:Z:124:MET:CB	6:Z:188:ALA:CB	2.94	0.46
2:V:118:LEU:HB2	2:V:196:TYR:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:113:LEU:HD13	11:R:137:LEU:CD2	2.46	0.46
8:S:475:TYR:CE2	12:U:269:THR:HB	2.51	0.46
3:T:80:ASN:HA	7:N:11:ALA:CB	2.46	0.46
7:N:773:MET:CG	7:N:884:PHE:HD1	2.28	0.45
11:R:60:ALA:HB2	11:R:99:TYR:CD1	2.49	0.45
3:T:85:LEU:HD13	3:T:85:LEU:HA	1.88	0.45
6:Z:1:MET:C	6:Z:25:PRO:HG3	2.36	0.45
13:O:258:LEU:HA	13:O:291:ILE:HD12	1.98	0.45
8:S:211:ARG:NH2	8:S:246:GLU:OE1	2.48	0.45
7:N:55:PHE:O	7:N:58:ARG:HG3	2.17	0.45
9:P:89:LEU:HD12	9:P:92:SER:HB2	1.98	0.45
2:V:29:ILE:CD1	2:V:201:ILE:CG2	2.95	0.45
6:Z:385:PHE:CD1	6:Z:385:PHE:N	2.81	0.45
13:O:214:ALA:HB2	13:O:238:ILE:CG1	2.47	0.45
10:Q:109:ASP:HB2	10:Q:114:GLN:HE22	1.82	0.44
11:R:304:TYR:CE2	11:R:337:VAL:HG11	2.52	0.44
13:O:58:ARG:O	13:O:62:TYR:CB	2.65	0.44
2:V:247:ILE:O	2:V:247:ILE:HG22	2.17	0.44
10:Q:74:LEU:C	10:Q:74:LEU:HD23	2.37	0.44
11:R:60:ALA:CA	11:R:99:TYR:CZ	2.99	0.44
3:T:80:ASN:CB	7:N:11:ALA:HB1	2.48	0.44
6:Z:185:ASP:O	6:Z:186:GLY:O	2.35	0.44
10:Q:431:SER:HA	10:Q:434:TYR:CD2	2.53	0.44
6:Z:189:ALA:O	6:Z:193:PHE:CG	2.70	0.44
9:P:59:LEU:HD21	9:P:96:MET:HG2	2.00	0.44
6:Z:362:LEU:HD13	6:Z:395:CYS:HA	2.00	0.44
13:O:25:LEU:HB3	13:O:29:PHE:CZ	2.53	0.44
11:R:60:ALA:HB3	11:R:102:LEU:HD22	1.98	0.44
7:N:83:LEU:HG	7:N:132:LYS:HG2	2.00	0.43
13:O:62:TYR:CD2	13:O:63:ASP:N	2.86	0.43
9:P:77:GLU:O	9:P:80:THR:HB	2.18	0.43
8:S:81:LEU:N	8:S:81:LEU:HD22	2.32	0.43
6:Z:407:VAL:HG11	6:Z:439:TYR:CE1	2.53	0.43
6:Z:767:TYR:CD2	6:Z:767:TYR:C	2.91	0.43
6:Z:898:HIS:CD2	6:Z:898:HIS:H	2.36	0.43
11:R:261:LEU:HB2	11:R:266:LEU:HB2	2.00	0.43
5:Y:21:ASN:N	8:S:59:ASP:OD2	2.51	0.43
2:V:189:ILE:HG13	2:V:189:ILE:O	2.17	0.43
6:Z:124:MET:HB3	6:Z:188:ALA:HB2	2.00	0.43
13:O:49:PHE:HZ	13:O:62:TYR:HB2	1.76	0.43
7:N:83:LEU:HG	7:N:132:LYS:CG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:160:LYS:HD3	13:O:163:ILE:CD1	2.48	0.43
9:P:93:ILE:HG22	9:P:97:ILE:HG13	2.00	0.43
4:X:17:TYR:CE1	4:X:96:ARG:HB2	2.53	0.43
11:R:279:LEU:O	11:R:280:ILE:CG1	2.66	0.43
6:Z:120:SER:O	6:Z:124:MET:HG3	2.18	0.43
7:N:447:SER:O	7:N:450:ILE:HG22	2.18	0.43
9:P:388:ILE:HG22	9:P:389:ILE:HG23	1.99	0.43
11:R:99:TYR:O	11:R:102:LEU:HB3	2.18	0.43
5:Y:21:ASN:HB2	8:S:59:ASP:OD2	2.19	0.43
2:V:196:TYR:N	2:V:196:TYR:CD2	2.86	0.43
7:N:711:ARG:NH1	7:N:786:ARG:O	2.52	0.43
12:U:120:LEU:HD22	12:U:122:ILE:HG13	2.01	0.43
6:Z:24:THR:CB	6:Z:25:PRO:HD3	2.46	0.43
2:V:153:ILE:HG21	2:V:203:TYR:OH	2.19	0.43
2:V:188:LEU:C	2:V:188:LEU:HD23	2.39	0.43
9:P:89:LEU:HB3	9:P:91:LEU:H	1.84	0.42
13:O:53:LYS:O	13:O:58:ARG:NH1	2.52	0.42
6:Z:1:MET:CA	6:Z:25:PRO:CG	2.95	0.42
2:V:123:VAL:HG13	2:V:158:LEU:HD11	2.01	0.42
6:Z:25:PRO:HB2	6:Z:26:ASN:H	1.43	0.42
9:P:351:ARG:HD3	9:P:388:ILE:CG2	2.49	0.42
10:Q:67:THR:H	10:Q:68:MET:CG	2.33	0.42
10:Q:78:ILE:N	10:Q:79:PRO:CD	2.83	0.42
11:R:257:GLY:O	11:R:266:LEU:CD1	2.67	0.42
6:Z:124:MET:O	6:Z:188:ALA:HB2	2.19	0.42
13:O:62:TYR:CE1	13:O:81:TYR:CB	3.03	0.42
4:X:17:TYR:HE1	4:X:96:ARG:HB2	1.84	0.42
4:X:88:ALA:HA	4:X:98:PHE:HD1	1.85	0.42
13:O:62:TYR:CE1	13:O:81:TYR:HB2	2.55	0.42
6:Z:93:ARG:HB3	6:Z:94:PRO:CD	2.48	0.42
6:Z:127:SER:OG	6:Z:188:ALA:CA	2.60	0.42
7:N:549:TYR:HH	7:N:741:TYR:HE2	1.67	0.41
7:N:710:GLY:O	7:N:711:ARG:HB2	2.20	0.41
13:O:49:PHE:HZ	13:O:62:TYR:CB	2.33	0.41
6:Z:82:MET:HB2	6:Z:85:VAL:HG22	2.01	0.41
4:X:64:ILE:HD13	4:X:97:TYR:CE1	2.54	0.41
6:Z:24:THR:HG23	6:Z:71:LEU:HB2	2.02	0.41
8:S:475:TYR:CD1	12:U:273:LEU:HB2	2.55	0.41
12:U:183:ALA:H	12:U:188:ILE:HG21	1.85	0.41
6:Z:518:LEU:HD23	6:Z:518:LEU:HA	1.92	0.41
13:O:79:VAL:O	13:O:83:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:354:PHE:CD1	10:Q:354:PHE:N	2.88	0.41
8:S:219:LYS:HA	8:S:219:LYS:CE	2.32	0.41
13:O:228:TYR:HA	13:O:230:PHE:CE2	2.55	0.41
11:R:31:PHE:CE2	11:R:320:LYS:HA	2.54	0.41
9:P:59:LEU:HG	9:P:96:MET:HG2	2.03	0.41
9:P:17:LEU:HD23	9:P:17:LEU:HA	1.82	0.41
6:Z:89:LEU:O	6:Z:126:TYR:CD1	2.74	0.41
13:O:66:VAL:HG11	13:O:78:VAL:HG13	2.03	0.41
11:R:60:ALA:O	11:R:99:TYR:CE1	2.73	0.41
2:V:69:PHE:CD1	2:V:69:PHE:O	2.73	0.41
13:O:70:TYR:HE1	13:O:102:LEU:HD11	1.86	0.41
10:Q:67:THR:N	10:Q:68:MET:HG3	2.35	0.41
10:Q:75:ARG:NH1	10:Q:76:GLU:OE2	2.54	0.41
13:O:393:VAL:OXT	13:O:393:VAL:CG1	2.69	0.41
2:V:192:LEU:O	2:V:196:TYR:O	2.39	0.41
2:V:49:VAL:HG12	2:V:50:MET:N	2.37	0.41
6:Z:804:ASP:O	6:Z:805:LEU:HB2	2.21	0.41
7:N:340:HIS:HE1	7:N:348:PHE:HB2	1.85	0.40
13:O:53:LYS:O	13:O:58:ARG:CZ	2.69	0.40
11:R:267:LYS:HG3	11:R:297:TYR:CE1	2.56	0.40
11:R:267:LYS:HG3	11:R:297:TYR:CD1	2.56	0.40
6:Z:76:LYS:HE2	6:Z:121:ILE:HG21	2.02	0.40
7:N:43:LEU:H	7:N:44:PRO:CD	2.35	0.40
13:O:58:ARG:CD	13:O:59:LEU:N	2.84	0.40
11:R:117:ILE:HA	11:R:120:LEU:HD12	2.02	0.40
1:W:93:ILE:HG13	12:U:65:VAL:HG13	2.04	0.40
6:Z:83:THR:HB	6:Z:84:ALA:H	1.76	0.40
10:Q:118:CYS:O	10:Q:122:ILE:HG13	2.21	0.40
8:S:164:ILE:HB	8:S:165:PRO:HD3	2.03	0.40
6:Z:354:PRO:O	6:Z:357:ILE:HG12	2.21	0.40
7:N:206:ILE:HD13	7:N:206:ILE:HA	1.88	0.40
7:N:87:ASP:O	7:N:88:ARG:HB2	2.21	0.40
10:Q:355:GLU:O	10:Q:356:CYS:HB3	2.22	0.40
11:R:261:LEU:CB	11:R:266:LEU:HB2	2.52	0.40
13:O:59:LEU:HG	13:O:85:SER:HB3	2.04	0.40
10:Q:356:CYS:SG	10:Q:356:CYS:O	2.79	0.40
11:R:54:ILE:HD13	11:R:63:TYR:CE1	2.57	0.40
8:S:19:HIS:CG	8:S:20:HIS:N	2.90	0.40
2:V:25:GLU:H	2:V:25:GLU:CD	2.24	0.40
6:Z:12:ILE:CG1	6:Z:22:LYS:HE3	2.51	0.40
6:Z:282:ILE:HB	6:Z:297:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:96:TYR:HE1	6:Z:156:HIS:CE1	2.40	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	W	195/268 (73%)	179 (92%)	12 (6%)	4 (2%)	8	47
2	V	287/306 (94%)	263 (92%)	18 (6%)	6 (2%)	8	47
3	T	264/274 (96%)	236 (89%)	21 (8%)	7 (3%)	6	42
4	X	125/156 (80%)	107 (86%)	12 (10%)	6 (5%)	2	29
5	Y	47/89 (53%)	43 (92%)	3 (6%)	1 (2%)	8	47
6	Z	902/993 (91%)	820 (91%)	55 (6%)	27 (3%)	5	39
7	N	886/945 (94%)	849 (96%)	30 (3%)	7 (1%)	22	66
8	S	473/523 (90%)	436 (92%)	24 (5%)	13 (3%)	6	42
9	P	438/445 (98%)	408 (93%)	22 (5%)	8 (2%)	10	50
10	Q	432/434 (100%)	388 (90%)	26 (6%)	18 (4%)	3	32
11	R	377/429 (88%)	352 (93%)	17 (4%)	8 (2%)	8	47
12	U	296/338 (88%)	280 (95%)	11 (4%)	5 (2%)	11	52
13	O	386/393 (98%)	368 (95%)	16 (4%)	2 (0%)	32	74
All	All	5108/5593 (91%)	4729 (93%)	267 (5%)	112 (2%)	12	46

All (112) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	200	ASN
3	T	92	ASN

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Mol	Chain	Res	Type
3	T	96	LEU
3	T	173	GLU
4	X	116	ALA
5	Y	34	GLU
6	Z	24	THR
6	Z	25	PRO
6	Z	85	VAL
6	Z	519	PRO
6	Z	728	LYS
8	S	47	THR
8	S	83	PRO
8	S	172	ASN
9	P	88	GLN
10	Q	42	ALA
10	Q	75	ARG
10	Q	356	CYS
11	R	125	GLU
11	R	263	ARG
13	O	36	LYS
1	W	165	GLN
2	V	175	SER
4	X	38	ASN
6	Z	186	GLY
6	Z	187	SER
6	Z	727	GLU
6	Z	926	ASN
6	Z	963	ALA
7	N	175	ASP
8	S	44	THR
8	S	102	SER
8	S	126	LYS
8	S	132	ALA
8	S	150	LYS
8	S	153	GLU
9	P	79	LEU
9	P	111	ASP
9	P	126	THR
10	Q	51	ARG
10	Q	68	MET
10	Q	170	ASP
10	Q	387	TYR
11	R	123	ASP

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Mol	Chain	Res	Type
11	R	280	ILE
1	W	179	ARG
3	T	95	LYS
3	T	235	PHE
3	T	251	HIS
4	X	112	ASN
6	Z	234	PRO
6	Z	773	ARG
6	Z	885	ALA
6	Z	887	GLY
6	Z	905	ASN
6	Z	947	GLY
7	N	725	LEU
7	N	757	THR
7	N	786	ARG
8	S	118	PHE
9	P	130	ILE
9	P	171	MET
10	Q	44	ALA
10	Q	48	ASP
10	Q	230	LYS
10	Q	253	ASN
10	Q	286	TYR
12	U	133	PRO
1	W	144	PHE
2	V	112	PRO
2	V	217	HIS
4	X	19	GLU
4	X	63	PRO
6	Z	82	MET
6	Z	143	VAL
6	Z	144	SER
6	Z	770	GLU
6	Z	825	ALA
7	N	391	PRO
10	Q	46	VAL
10	Q	384	LYS
11	R	395	ASN
12	U	5	HIS
12	U	237	PRO
13	O	225	ASP
1	W	180	LEU

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Mol	Chain	Res	Type
2	V	20	ARG
6	Z	789	GLN
7	N	393	SER
8	S	82	TYR
8	S	97	THR
9	P	92	SER
9	P	327	LEU
10	Q	41	ALA
11	R	264	THR
12	U	150	THR
4	X	113	GLU
7	N	888	ASP
10	Q	40	ALA
10	Q	45	SER
10	Q	126	LYS
11	R	393	PRO
2	V	185	ILE
3	T	46	ILE
6	Z	940	GLY
11	R	110	ILE
12	U	220	PRO
6	Z	19	SER
6	Z	610	GLY
6	Z	233	LEU
6	Z	333	GLY
8	S	96	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	171/230 (74%)	168 (98%)	3 (2%)	64	84
2	V	253/268 (94%)	250 (99%)	3 (1%)	75	88
3	T	249/256 (97%)	241 (97%)	8 (3%)	44	71
4	X	116/144 (81%)	115 (99%)	1 (1%)	82	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Y	50/81 (62%)	48 (96%)	2 (4%)	36	66
6	Z	773/850 (91%)	753 (97%)	20 (3%)	51	76
7	N	745/797 (94%)	731 (98%)	14 (2%)	62	82
8	S	447/489 (91%)	436 (98%)	11 (2%)	53	77
9	P	412/415 (99%)	404 (98%)	8 (2%)	62	82
10	Q	391/391 (100%)	380 (97%)	11 (3%)	49	74
11	R	333/379 (88%)	321 (96%)	12 (4%)	40	69
12	U	271/308 (88%)	266 (98%)	5 (2%)	64	84
13	O	363/368 (99%)	353 (97%)	10 (3%)	49	74
All	All	4574/4976 (92%)	4466 (98%)	108 (2%)	58	78

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	76	LEU
1	W	140	ASP
1	W	149	GLN
2	V	190	HIS
2	V	199	LEU
2	V	227	MET
3	T	79	GLU
3	T	153	MET
3	T	187	ASP
3	T	195	LEU
3	T	197	TYR
3	T	214	GLU
3	T	231	SER
3	T	238	GLN
4	X	14	VAL
5	Y	20	LYS
5	Y	32	ASP
6	Z	83	THR
6	Z	206	ASP
6	Z	211	PHE
6	Z	213	LYS
6	Z	257	PRO
6	Z	286	VAL
6	Z	326	VAL
6	Z	354	PRO

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Mol	Chain	Res	Type
6	Z	429	ASN
6	Z	560	THR
6	Z	601	VAL
6	Z	748	LEU
6	Z	777	PRO
6	Z	817	LEU
6	Z	830	LEU
6	Z	843	ASP
6	Z	846	PHE
6	Z	857	LEU
6	Z	889	VAL
6	Z	898	HIS
7	N	63	LEU
7	N	70	TYR
7	N	142	GLU
7	N	175	ASP
7	N	269	LEU
7	N	739	PHE
7	N	765	ASP
7	N	771	PHE
7	N	785	PRO
7	N	790	GLU
7	N	861	TYR
7	N	868	VAL
7	N	873	ARG
7	N	878	GLN
8	S	25	TYR
8	S	32	GLN
8	S	44	THR
8	S	88	PHE
8	S	93	LEU
8	S	101	LYS
8	S	414	ASP
8	S	449	LEU
8	S	470	GLN
8	S	475	TYR
8	S	487	THR
9	P	210	ASN
9	P	277	GLN
9	P	281	ILE
9	P	302	LEU
9	P	309	MET

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Mol	Chain	Res	Type
9	P	403	GLU
9	P	404	LYS
9	P	420	ASP
10	Q	84	TYR
10	Q	88	PHE
10	Q	104	PHE
10	Q	112	ASP
10	Q	114	GLN
10	Q	164	GLU
10	Q	173	SER
10	Q	198	LEU
10	Q	294	ARG
10	Q	319	LYS
10	Q	387	TYR
11	R	22	PRO
11	R	176	ARG
11	R	182	ASN
11	R	237	THR
11	R	263	ARG
11	R	266	LEU
11	R	318	PRO
11	R	348	LEU
11	R	365	ASP
11	R	393	PRO
11	R	400	TYR
11	R	421	VAL
12	U	70	HIS
12	U	115	GLN
12	U	142	GLN
12	U	145	ASP
12	U	220	PRO
13	O	13	THR
13	O	61	LEU
13	O	62	TYR
13	O	69	PHE
13	O	90	LYS
13	O	153	LEU
13	O	237	PRO
13	O	294	MET
13	O	300	VAL
13	O	348	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such

sidechains are listed below:

Mol	Chain	Res	Type
1	W	162	ASN
2	V	73	GLN
2	V	181	ASN
2	V	200	ASN
2	V	279	HIS
3	T	230	ASN
6	Z	17	GLN
6	Z	275	GLN
6	Z	429	ASN
6	Z	763	HIS
6	Z	769	ASN
6	Z	833	GLN
6	Z	852	GLN
6	Z	898	HIS
6	Z	926	ASN
7	N	336	ASN
7	N	340	HIS
7	N	509	GLN
7	N	529	GLN
7	N	703	GLN
7	N	719	ASN
8	S	19	HIS
8	S	20	HIS
8	S	39	ASN
8	S	166	ASN
8	S	334	HIS
8	S	472	HIS
9	P	277	GLN
9	P	323	ASN
9	P	342	GLN
9	P	349	ASN
9	P	418	ASN
9	P	431	HIS
10	Q	87	GLN
10	Q	114	GLN
10	Q	247	HIS
10	Q	361	HIS
11	R	35	GLN
11	R	42	GLN
11	R	395	ASN
12	U	115	GLN
12	U	173	HIS

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Mol	Chain	Res	Type
12	U	230	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	78:GLN	C	79:LEU	N	1.75