



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jul 24, 2017 – 02:01 PM EDT

PDB ID : 5MPD
EMDB ID: : EMD-3534
Title : 26S proteasome in presence of ATP (s1)
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 : 4.10 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

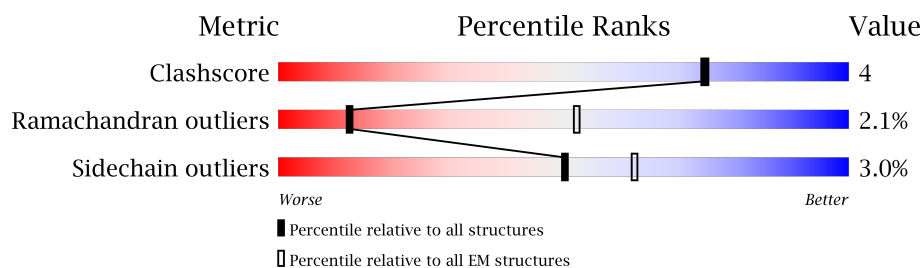
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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	
2	V	306	
3	T	274	
4	X	156	
5	Y	89	
6	Z	993	
7	N	945	
8	S	523	
9	P	445	

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Mol	Chain	Length	Quality of chain
10	Q	434	<div><div></div><div>76%</div><div>20%</div><div>.</div></div>
11	R	429	<div><div></div><div>67%</div><div>18%</div><div>.</div><div>11%</div></div>
12	U	338	<div><div></div><div>74%</div><div>13%</div><div>.</div><div>12%</div></div>
13	O	393	<div><div></div><div>74%</div><div>21%</div><div>.</div><div>..</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		

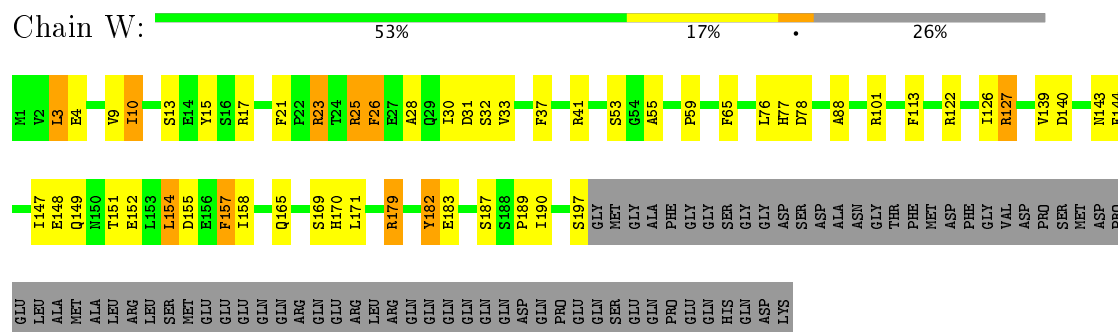
- Molecule 13 is a protein called 26S proteasome regulatory subunit RPN9.

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

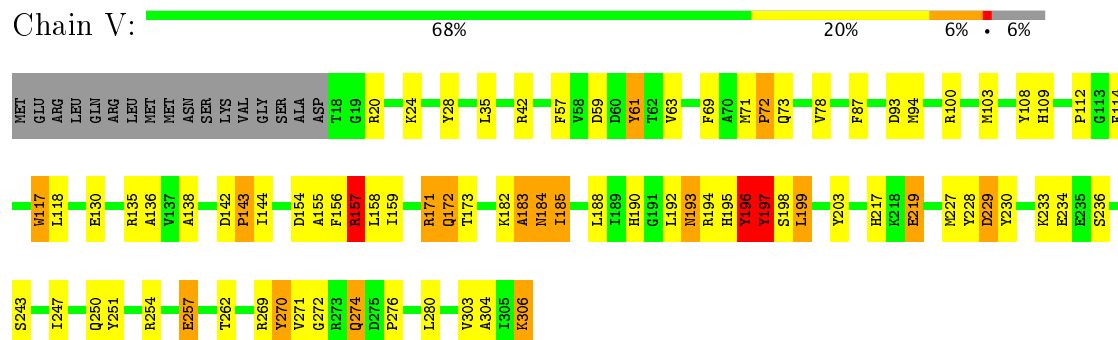
3 Residue-property plots

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.

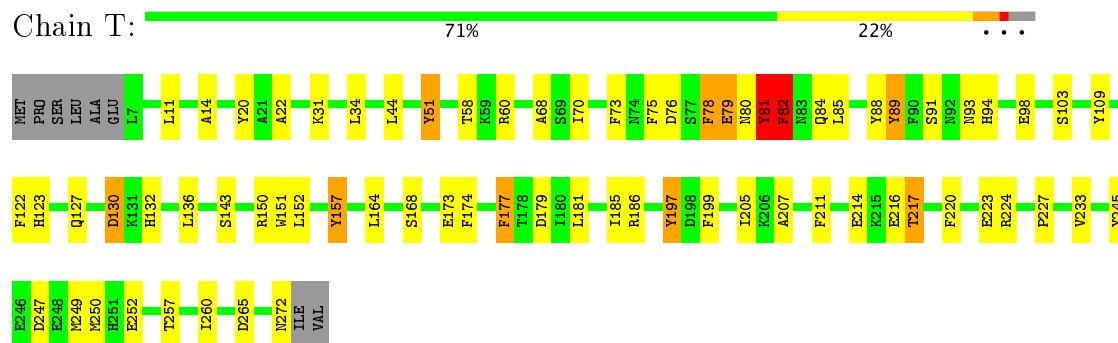
- Molecule 1: 26S proteasome regulatory subunit RPN10



- Molecule 2: Ubiquitin carboxyl-terminal hydrolase RPN11

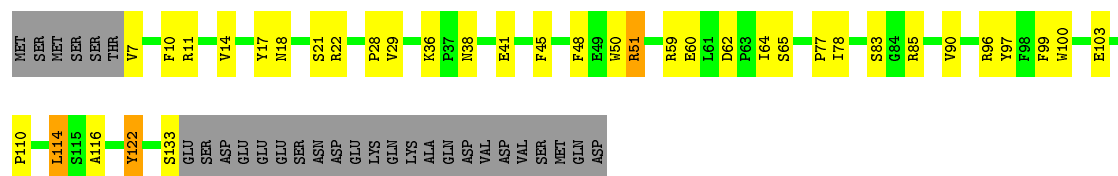


- Molecule 3: 26S proteasome regulatory subunit RPN12



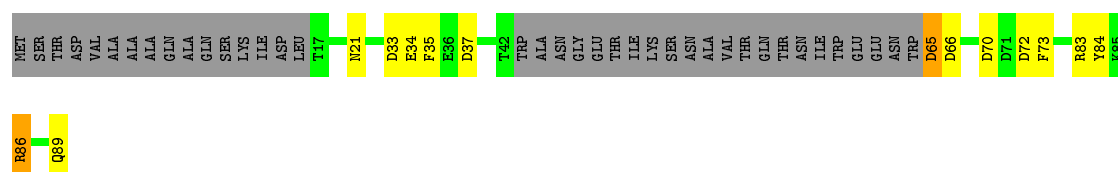
- Molecule 4: 26S proteasome regulatory subunit RPN13

Chain X: 



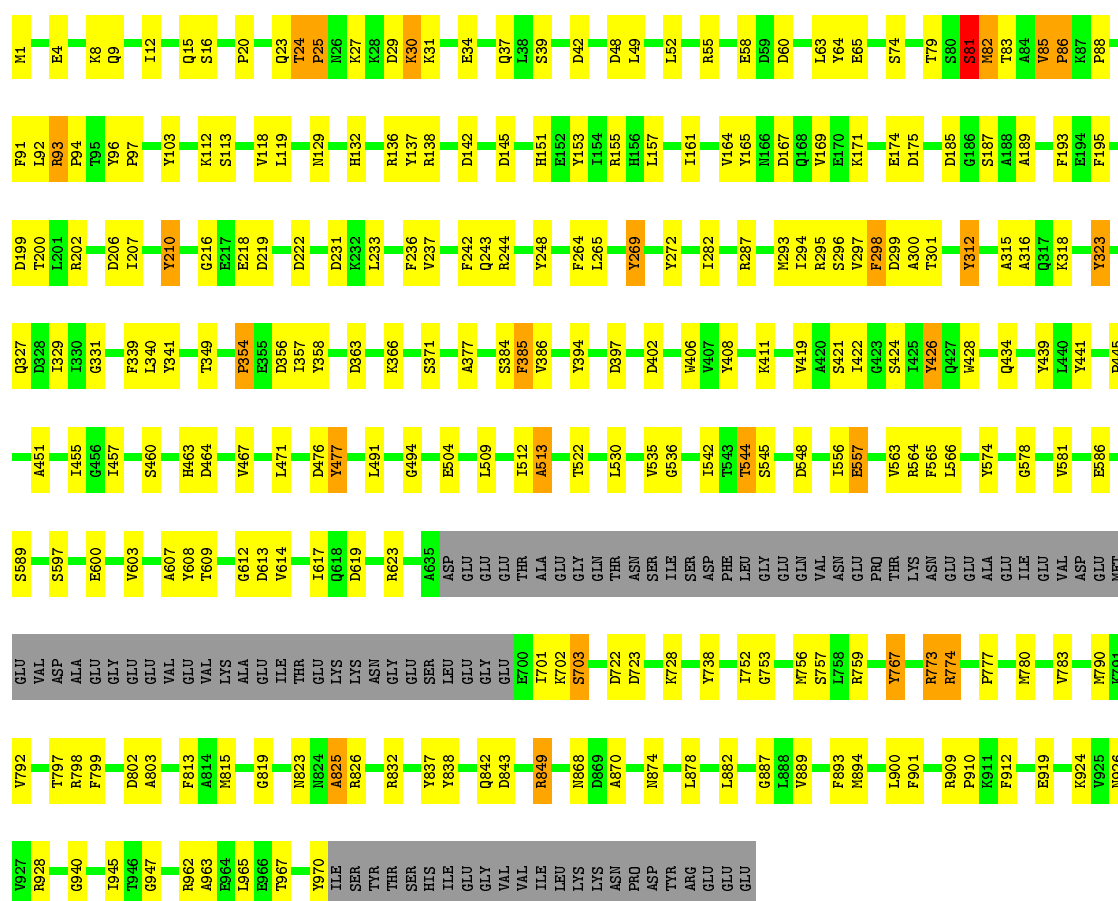
- Molecule 5: 26S proteasome complex subunit SEM1

Chain Y: 



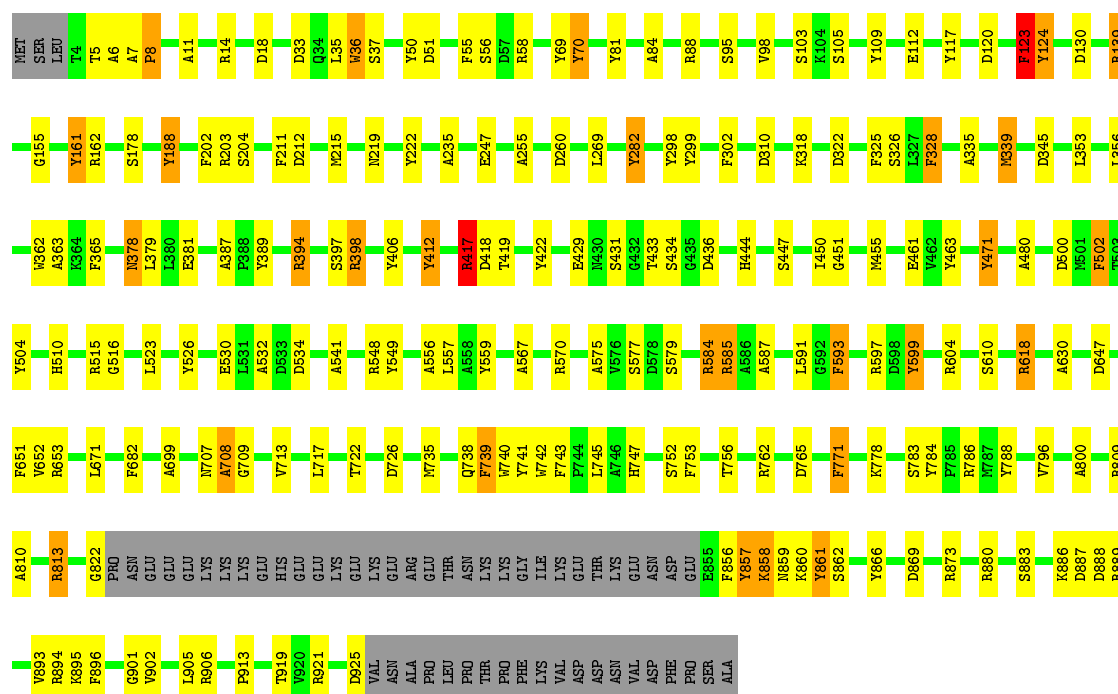
- Molecule 6: 26S proteasome regulatory subunit RPN1

Chain Z: 



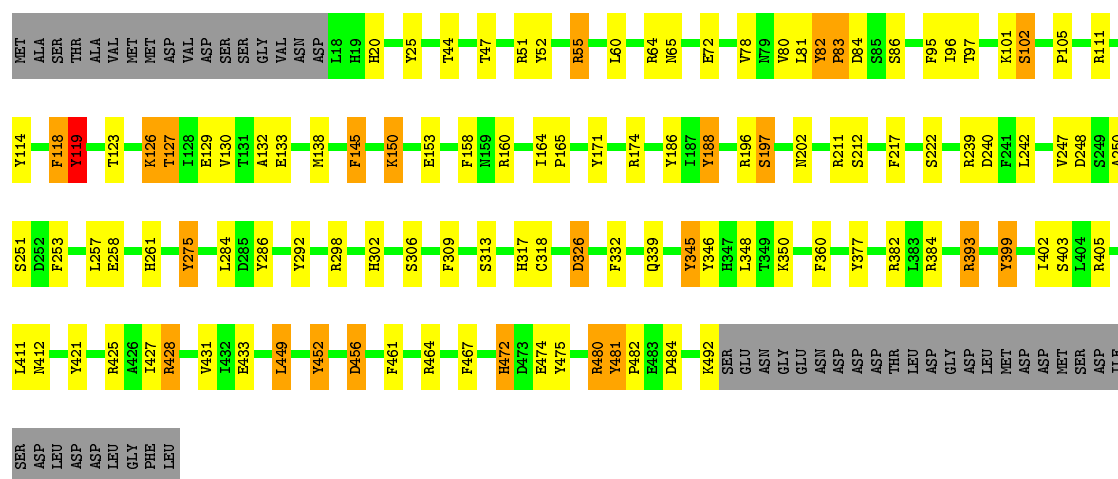
- Molecule 7: 26S proteasome regulatory subunit RPN2

Chain N: 



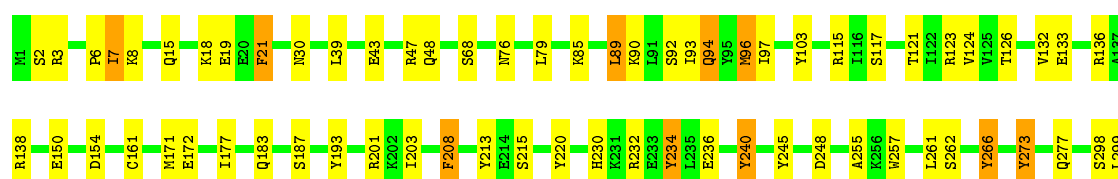
• Molecule 8: 26S proteasome regulatory subunit RPN3

Chain S: 



• Molecule 9: 26S proteasome regulatory subunit RPN5

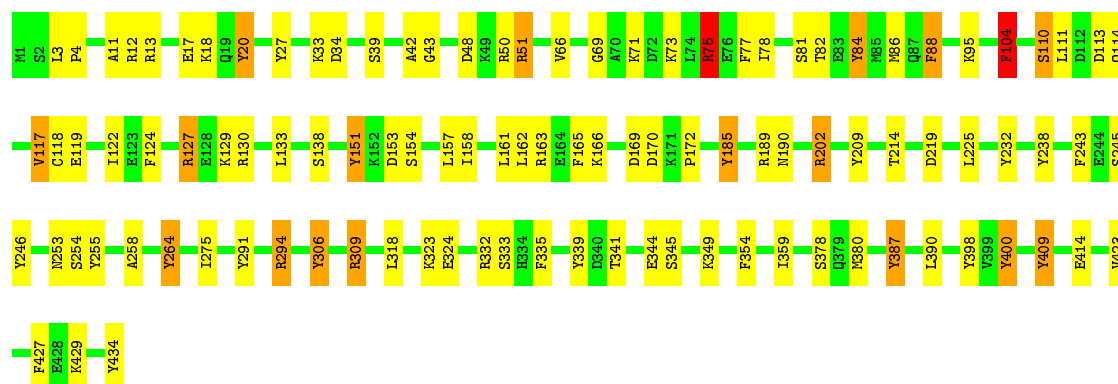
Chain P: 





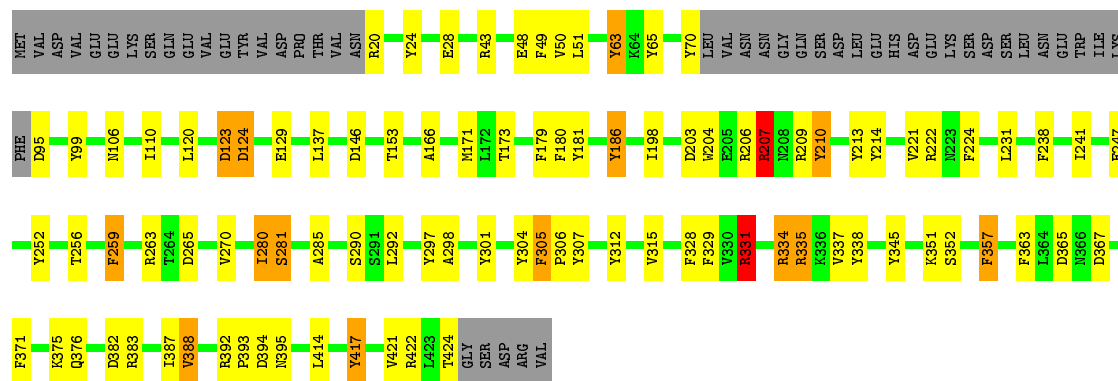
- Molecule 10: 26S proteasome regulatory subunit RPN6

Chain Q: 76% 20%



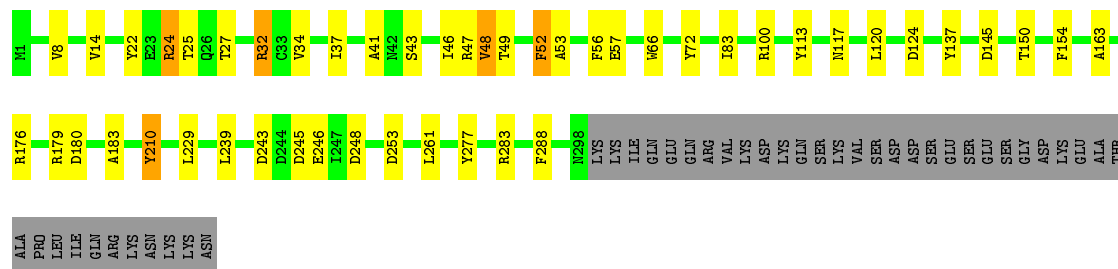
- Molecule 11: 26S proteasome regulatory subunit RPN7

Chain R: 67% 18% 11%



- Molecule 12: 26S proteasome regulatory subunit RPN8

Chain U: 74% 13% 12%



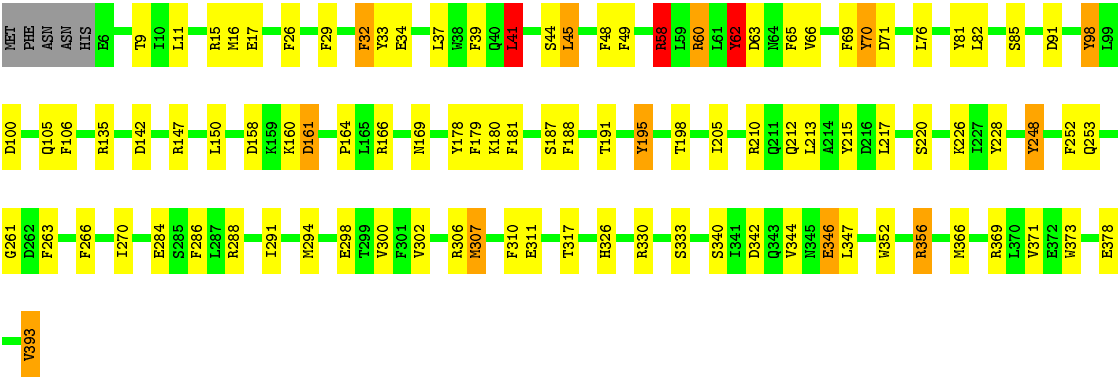
- Molecule 13: 26S proteasome regulatory subunit RPN9

Chain O:

74%

21%

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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	286500	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 QUANTUM (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	1.70	14/1557 (0.9%)	1.79	29/2111 (1.4%)
10	Q	1.68	28/3556 (0.8%)	1.89	77/4787 (1.6%)
11	R	1.73	31/3110 (1.0%)	1.95	83/4193 (2.0%)
12	U	1.58	11/2407 (0.5%)	1.76	41/3258 (1.3%)
13	O	1.68	36/3247 (1.1%)	1.93	86/4380 (2.0%)
2	V	1.74	22/2309 (1.0%)	2.02	64/3115 (2.1%)
3	T	1.71	27/2235 (1.2%)	1.82	45/3017 (1.5%)
4	X	1.75	12/1058 (1.1%)	1.90	24/1432 (1.7%)
5	Y	1.90	7/438 (1.6%)	1.92	10/583 (1.7%)
6	Z	1.66	59/7122 (0.8%)	1.88	169/9645 (1.8%)
7	N	1.74	61/6994 (0.9%)	1.84	142/9455 (1.5%)
8	S	1.68	33/3966 (0.8%)	1.84	98/5355 (1.8%)
9	P	1.67	29/3663 (0.8%)	1.77	60/4940 (1.2%)
All	All	1.69	370/41662 (0.9%)	1.86	928/56271 (1.6%)

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	6
10	Q	0	19
11	R	0	12
12	U	0	4
13	O	0	11
2	V	0	5
3	T	0	6
4	X	0	2
5	Y	0	1
6	Z	0	12
7	N	0	23
8	S	0	14

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	P	0	8
All	All	0	123

All (370) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	8	PRO	CA-CB	32.16	2.17	1.53
5	Y	89	GLN	C-OXT	-12.08	1.00	1.23
9	P	440	HIS	C-O	-12.08	1.00	1.23
3	T	272	ASN	C-O	-12.07	1.00	1.23
13	O	393	VAL	C-O	-12.07	1.00	1.23
10	Q	434	TYR	C-O	-12.06	1.00	1.23
2	V	306	LYS	C-O	-12.06	1.00	1.23
4	X	133	SER	C-O	-12.05	1.00	1.23
7	N	925	ASP	C-O	-12.05	1.00	1.23
1	W	197	SER	C-O	-12.04	1.00	1.23
10	Q	434	TYR	C-OXT	-12.05	1.00	1.23
11	R	424	THR	C-O	-12.04	1.00	1.23
13	O	393	VAL	C-OXT	-12.04	1.00	1.23
2	V	306	LYS	C-OXT	-12.04	1.00	1.23
8	S	492	LYS	C-O	-12.03	1.00	1.23
5	Y	89	GLN	C-O	-12.01	1.00	1.23
8	S	127	THR	CA-CB	10.47	1.80	1.53
7	N	604	ARG	CZ-NH2	10.40	1.46	1.33
1	W	25	ARG	NE-CZ	9.49	1.45	1.33
2	V	196	TYR	CA-CB	9.21	1.74	1.53
7	N	397	SER	CA-CB	8.76	1.66	1.52
9	P	357	TYR	CB-CG	-8.72	1.38	1.51
7	N	88	ARG	NE-CZ	8.58	1.44	1.33
7	N	155	GLY	N-CA	-8.35	1.33	1.46
6	Z	759	ARG	CZ-NH2	8.25	1.43	1.33
5	Y	65	ASP	CA-CB	-8.19	1.35	1.53
2	V	236	SER	CA-CB	8.14	1.65	1.52
1	W	101	ARG	CZ-NH2	8.13	1.43	1.33
3	T	186	ARG	NE-CZ	8.11	1.43	1.33
6	Z	753	GLY	CA-C	-8.07	1.39	1.51
7	N	889	ARG	NE-CZ	7.99	1.43	1.33
4	X	22	ARG	CZ-NH1	7.98	1.43	1.33
6	Z	371	SER	CA-CB	7.95	1.64	1.52
7	N	417	ARG	NE-CZ	7.94	1.43	1.33
10	Q	13	ARG	CZ-NH1	7.86	1.43	1.33
2	V	171	ARG	NE-CZ	7.66	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	196	TYR	CD1-CE1	7.65	1.50	1.39
1	W	179	ARG	CZ-NH1	7.63	1.43	1.33
9	P	47	ARG	NE-CZ	7.55	1.42	1.33
10	Q	50	ARG	CD-NE	7.52	1.59	1.46
7	N	584	ARG	CZ-NH2	7.50	1.42	1.33
2	V	20	ARG	CZ-NH1	7.47	1.42	1.33
8	S	382	ARG	CZ-NH2	7.44	1.42	1.33
7	N	752	SER	CA-CB	7.44	1.64	1.52
13	O	356	ARG	CZ-NH2	7.42	1.42	1.33
3	T	103	SER	CA-CB	7.29	1.63	1.52
4	X	122	TYR	CB-CG	7.29	1.62	1.51
3	T	224	ARG	CD-NE	7.28	1.58	1.46
7	N	786	ARG	NE-CZ	7.27	1.42	1.33
7	N	112	GLU	CD-OE1	7.24	1.33	1.25
6	Z	600	GLU	CG-CD	7.20	1.62	1.51
11	R	383	ARG	CZ-NH1	7.16	1.42	1.33
9	P	310	ARG	CD-NE	7.16	1.58	1.46
9	P	273	TYR	CB-CG	7.15	1.62	1.51
11	R	207	ARG	NE-CZ	7.10	1.42	1.33
11	R	392	ARG	CZ-NH1	7.07	1.42	1.33
11	R	207	ARG	CZ-NH1	7.06	1.42	1.33
6	Z	155	ARG	CZ-NH2	7.03	1.42	1.33
12	U	32	ARG	CD-NE	7.02	1.58	1.46
8	S	251	SER	CA-CB	6.97	1.63	1.52
7	N	906	ARG	NE-CZ	6.93	1.42	1.33
10	Q	332	ARG	CZ-NH2	6.93	1.42	1.33
11	R	209	ARG	CZ-NH2	6.90	1.42	1.33
11	R	222	ARG	CZ-NH2	6.89	1.42	1.33
2	V	196	TYR	CD2-CE2	-6.89	1.29	1.39
7	N	921	ARG	CZ-NH2	6.88	1.42	1.33
12	U	24	ARG	CZ-NH2	6.86	1.42	1.33
6	Z	826	ARG	CZ-NH2	6.85	1.42	1.33
13	O	135	ARG	NE-CZ	6.84	1.42	1.33
7	N	139	ARG	NE-CZ	6.81	1.42	1.33
11	R	247	GLU	CG-CD	6.80	1.62	1.51
10	Q	124	PHE	CE2-CZ	6.79	1.50	1.37
12	U	100	ARG	CZ-NH1	6.72	1.41	1.33
8	S	480	ARG	CD-NE	6.67	1.57	1.46
6	Z	928	ARG	CZ-NH2	6.66	1.41	1.33
12	U	179	ARG	CZ-NH2	6.66	1.41	1.33
6	Z	477	TYR	CE2-CZ	6.65	1.47	1.38
7	N	398	ARG	CZ-NH2	6.62	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	334	ARG	NE-CZ	6.59	1.41	1.33
8	S	211	ARG	NE-CZ	6.57	1.41	1.33
9	P	3	ARG	CZ-NH2	6.57	1.41	1.33
6	Z	849	ARG	NE-CZ	6.57	1.41	1.33
6	Z	138	ARG	CZ-NH1	6.55	1.41	1.33
7	N	14	ARG	CZ-NH2	6.55	1.41	1.33
7	N	883	SER	CA-CB	6.54	1.62	1.52
3	T	60	ARG	NE-CZ	6.54	1.41	1.33
8	S	171	TYR	CA-CB	-6.54	1.39	1.53
1	W	101	ARG	CD-NE	6.54	1.57	1.46
4	X	59	ARG	CZ-NH1	6.51	1.41	1.33
7	N	597	ARG	CZ-NH2	6.51	1.41	1.33
8	S	52	TYR	CE1-CZ	6.50	1.47	1.38
9	P	351	ARG	CZ-NH1	6.49	1.41	1.33
3	T	168	SER	CB-OG	6.49	1.50	1.42
8	S	474	GLU	CB-CG	6.48	1.64	1.52
6	Z	103	TYR	CG-CD1	6.47	1.47	1.39
8	S	86	SER	CA-CB	6.44	1.62	1.52
6	Z	919	GLU	CG-CD	6.42	1.61	1.51
6	Z	39	SER	CA-CB	6.41	1.62	1.52
13	O	306	ARG	NE-CZ	6.41	1.41	1.33
6	Z	16	SER	CB-OG	-6.41	1.33	1.42
7	N	516	GLY	CA-C	-6.41	1.41	1.51
13	O	288	ARG	CZ-NH2	6.39	1.41	1.33
6	Z	296	SER	CA-CB	6.39	1.62	1.52
7	N	394	ARG	NE-CZ	6.32	1.41	1.33
6	Z	385	PHE	CG-CD1	6.32	1.48	1.38
10	Q	51	ARG	CZ-NH1	6.29	1.41	1.33
6	Z	55	ARG	CZ-NH2	6.28	1.41	1.33
8	S	384	ARG	NE-CZ	6.27	1.41	1.33
4	X	59	ARG	CZ-NH2	6.26	1.41	1.33
6	Z	244	ARG	CZ-NH2	6.24	1.41	1.33
2	V	196	TYR	CE2-CZ	-6.23	1.30	1.38
6	Z	589	SER	CA-CB	6.22	1.62	1.52
1	W	41	ARG	CZ-NH2	6.21	1.41	1.33
9	P	136	ARG	NE-CZ	6.21	1.41	1.33
10	Q	344	GLU	CG-CD	6.20	1.61	1.51
2	V	269	ARG	NE-CZ	6.19	1.41	1.33
9	P	298	SER	CB-OG	6.19	1.50	1.42
6	Z	504	GLU	CD-OE2	6.18	1.32	1.25
6	Z	323	TYR	CB-CG	-6.15	1.42	1.51
8	S	51	ARG	CZ-NH2	6.15	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	U	277	TYR	CG-CD1	6.15	1.47	1.39
12	U	283	ARG	NE-CZ	6.14	1.41	1.33
4	X	22	ARG	CD-NE	6.14	1.56	1.46
10	Q	332	ARG	CZ-NH1	6.13	1.41	1.33
11	R	209	ARG	CZ-NH1	6.12	1.41	1.33
11	R	422	ARG	CZ-NH2	6.12	1.41	1.33
11	R	331	ARG	NE-CZ	6.09	1.41	1.33
3	T	265	ASP	N-CA	-6.08	1.34	1.46
10	Q	245	SER	CB-OG	6.08	1.50	1.42
7	N	282	TYR	CD1-CE1	6.07	1.48	1.39
7	N	56	SER	CA-CB	6.06	1.62	1.52
6	Z	703	SER	CA-CB	6.06	1.62	1.52
7	N	203	ARG	NE-CZ	6.05	1.41	1.33
7	N	14	ARG	NE-CZ	6.04	1.40	1.33
3	T	60	ARG	CZ-NH1	6.03	1.40	1.33
5	Y	86	ARG	CZ-NH2	6.03	1.40	1.33
6	Z	169	VAL	CB-CG1	6.02	1.65	1.52
6	Z	752	ILE	C-N	6.02	1.43	1.33
13	O	220	SER	CA-CB	6.01	1.61	1.52
7	N	682	PHE	CB-CG	-6.00	1.41	1.51
9	P	262	SER	CA-CB	6.00	1.61	1.52
7	N	738	GLN	CA-C	-6.00	1.37	1.52
6	Z	441	TYR	CZ-OH	5.99	1.48	1.37
6	Z	838	TYR	CZ-OH	5.99	1.48	1.37
7	N	894	ARG	NE-CZ	5.99	1.40	1.33
13	O	58	ARG	NE-CZ	5.98	1.40	1.33
7	N	579	SER	CA-CB	5.97	1.61	1.52
11	R	338	TYR	CG-CD2	5.96	1.46	1.39
1	W	148	GLU	CG-CD	5.96	1.60	1.51
10	Q	172	PRO	N-CD	-5.93	1.39	1.47
9	P	2	SER	CA-CB	5.93	1.61	1.52
8	S	405	ARG	NE-CZ	5.93	1.40	1.33
4	X	83	SER	CA-CB	5.92	1.61	1.52
7	N	247	GLU	CD-OE1	5.92	1.32	1.25
8	S	145	PHE	CG-CD2	5.91	1.47	1.38
12	U	253	ASP	CA-CB	5.90	1.67	1.53
6	Z	287	ARG	CZ-NH2	5.90	1.40	1.33
6	Z	623	ARG	CZ-NH2	5.90	1.40	1.33
9	P	3	ARG	NE-CZ	5.89	1.40	1.33
11	R	43	ARG	CZ-NH2	5.86	1.40	1.33
7	N	653	ARG	NE-CZ	5.86	1.40	1.33
2	V	135	ARG	NE-CZ	5.85	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	880	ARG	CZ-NH1	5.85	1.40	1.33
3	T	98	GLU	CG-CD	5.84	1.60	1.51
2	V	254	ARG	NE-CZ	5.84	1.40	1.33
11	R	252	TYR	CG-CD2	5.83	1.46	1.39
11	R	20	ARG	CZ-NH1	5.83	1.40	1.33
4	X	85	ARG	CZ-NH2	5.82	1.40	1.33
13	O	346	GLU	CD-OE1	5.81	1.32	1.25
3	T	186	ARG	CD-NE	5.81	1.56	1.46
8	S	119	TYR	CG-CD2	5.81	1.46	1.39
13	O	284	GLU	CG-CD	5.80	1.60	1.51
13	O	311	GLU	CG-CD	5.80	1.60	1.51
7	N	822	GLY	N-CA	5.79	1.54	1.46
10	Q	349	LYS	CA-CB	5.79	1.66	1.53
9	P	117	SER	CA-CB	5.78	1.61	1.52
7	N	901	GLY	N-CA	-5.77	1.37	1.46
9	P	261	LEU	C-N	5.77	1.47	1.34
11	R	65	TYR	CG-CD2	5.77	1.46	1.39
3	T	51	TYR	CB-CG	-5.76	1.43	1.51
10	Q	202	ARG	NE-CZ	5.75	1.40	1.33
11	R	63	TYR	CB-CG	-5.75	1.43	1.51
6	Z	773	ARG	CZ-NH2	5.74	1.40	1.33
11	R	290	SER	CA-CB	5.73	1.61	1.52
1	W	53	SER	CA-CB	-5.73	1.44	1.52
7	N	417	ARG	CD-NE	5.73	1.56	1.46
9	P	123	ARG	CZ-NH1	5.71	1.40	1.33
4	X	110	PRO	N-CD	-5.70	1.39	1.47
6	Z	962	ARG	NE-CZ	5.70	1.40	1.33
13	O	371	VAL	CB-CG1	5.69	1.64	1.52
6	Z	331	GLY	N-CA	-5.69	1.37	1.46
9	P	364	ARG	NE-CZ	5.69	1.40	1.33
2	V	198	SER	CA-CB	5.69	1.61	1.52
1	W	23	ARG	CZ-NH2	5.69	1.40	1.33
11	R	214	TYR	CG-CD1	5.69	1.46	1.39
11	R	24	TYR	CZ-OH	5.69	1.47	1.37
10	Q	117	VAL	CB-CG1	5.67	1.64	1.52
7	N	570	ARG	NE-CZ	5.66	1.40	1.33
6	Z	586	GLU	CD-OE2	5.66	1.31	1.25
2	V	272	GLY	N-CA	-5.65	1.37	1.46
10	Q	294	ARG	CZ-NH1	5.65	1.40	1.33
9	P	15	GLN	CG-CD	5.64	1.64	1.51
13	O	210	ARG	NE-CZ	5.64	1.40	1.33
13	O	166	ARG	CZ-NH1	5.64	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	130	GLU	CD-OE2	5.63	1.31	1.25
13	O	330	ARG	CZ-NH1	5.63	1.40	1.33
2	V	234	GLU	CB-CG	5.62	1.62	1.52
10	Q	294	ARG	NE-CZ	5.62	1.40	1.33
12	U	137	TYR	CZ-OH	5.62	1.47	1.37
6	Z	798	ARG	CZ-NH2	5.62	1.40	1.33
9	P	421	GLU	CD-OE2	5.59	1.31	1.25
7	N	222	TYR	CZ-OH	5.58	1.47	1.37
13	O	41	LEU	CA-CB	-5.58	1.41	1.53
6	Z	81	SER	CA-CB	5.58	1.61	1.52
8	S	286	TYR	CG-CD2	5.58	1.46	1.39
3	T	88	TYR	CE2-CZ	5.57	1.45	1.38
3	T	216	GLU	CG-CD	5.57	1.60	1.51
10	Q	378	SER	CA-CB	5.57	1.61	1.52
3	T	220	PHE	CB-CG	-5.56	1.42	1.51
4	X	11	ARG	CD-NE	5.56	1.55	1.46
6	Z	295	ARG	CD-NE	5.56	1.55	1.46
13	O	147	ARG	NE-CZ	5.55	1.40	1.33
6	Z	138	ARG	CZ-NH2	5.55	1.40	1.33
13	O	261	GLY	CA-C	5.55	1.60	1.51
6	Z	564	ARG	CZ-NH1	5.55	1.40	1.33
2	V	157	ARG	CZ-NH2	5.54	1.40	1.33
5	Y	83	ARG	NE-CZ	5.54	1.40	1.33
11	R	28	GLU	CG-CD	5.54	1.60	1.51
7	N	813	ARG	NE-CZ	5.53	1.40	1.33
7	N	585	ARG	CZ-NH2	5.53	1.40	1.33
8	S	188	TYR	CG-CD2	5.53	1.46	1.39
13	O	369	ARG	CZ-NH1	5.53	1.40	1.33
3	T	91	SER	CA-CB	5.52	1.61	1.52
7	N	103	SER	CA-CB	5.51	1.61	1.52
10	Q	324	GLU	CD-OE1	5.51	1.31	1.25
7	N	809	ARG	NE-CZ	5.51	1.40	1.33
10	Q	414	GLU	CB-CG	5.51	1.62	1.52
7	N	783	SER	CA-CB	5.50	1.61	1.52
8	S	461	PHE	CG-CD1	5.50	1.47	1.38
7	N	813	ARG	CZ-NH2	5.50	1.40	1.33
10	Q	246	TYR	CZ-OH	5.50	1.47	1.37
13	O	60	ARG	CZ-NH2	5.49	1.40	1.33
13	O	210	ARG	CZ-NH2	5.49	1.40	1.33
6	Z	494	GLY	N-CA	-5.49	1.37	1.46
12	U	120	LEU	N-CA	-5.49	1.35	1.46
8	S	298	ARG	CZ-NH2	5.49	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	O	106	PHE	CA-CB	5.48	1.66	1.53
6	Z	216	GLY	CA-C	-5.48	1.43	1.51
6	Z	623	ARG	NE-CZ	5.48	1.40	1.33
8	S	188	TYR	CG-CD1	5.48	1.46	1.39
10	Q	39	SER	CA-CB	5.47	1.61	1.52
7	N	921	ARG	CD-NE	5.46	1.55	1.46
6	Z	8	LYS	CA-CB	5.44	1.66	1.53
11	R	129	GLU	CB-CG	5.44	1.62	1.52
13	O	48	PHE	CB-CG	-5.44	1.42	1.51
13	O	34	GLU	CB-CG	5.43	1.62	1.52
13	O	44	SER	CB-OG	5.43	1.49	1.42
8	S	196	ARG	CD-NE	5.42	1.55	1.46
10	Q	294	ARG	CD-NE	5.42	1.55	1.46
6	Z	962	ARG	CD-NE	5.42	1.55	1.46
8	S	212	SER	CA-CB	5.41	1.61	1.52
7	N	610	SER	CA-CB	5.41	1.61	1.52
7	N	515	ARG	CD-NE	5.40	1.55	1.46
12	U	34	VAL	N-CA	-5.40	1.35	1.46
6	Z	64	TYR	CE2-CZ	5.39	1.45	1.38
7	N	431	SER	C-N	5.39	1.42	1.33
3	T	11	LEU	CA-CB	5.38	1.66	1.53
7	N	894	ARG	CZ-NH2	5.38	1.40	1.33
11	R	371	PHE	CB-CG	-5.38	1.42	1.51
7	N	422	TYR	CZ-OH	5.38	1.47	1.37
7	N	235	ALA	C-N	5.37	1.42	1.33
13	O	344	VAL	CB-CG1	5.36	1.64	1.52
9	P	310	ARG	NE-CZ	5.36	1.40	1.33
6	Z	832	ARG	CZ-NH2	5.36	1.40	1.33
10	Q	254	SER	CA-C	-5.36	1.39	1.52
8	S	382	ARG	CD-NE	5.34	1.55	1.46
7	N	422	TYR	CE2-CZ	5.33	1.45	1.38
9	P	172	GLU	CG-CD	5.33	1.59	1.51
3	T	89	TYR	CB-CG	-5.33	1.43	1.51
6	Z	819	GLY	CA-C	-5.33	1.43	1.51
11	R	263	ARG	CZ-NH1	5.32	1.40	1.33
5	Y	86	ARG	CZ-NH1	5.31	1.40	1.33
1	W	17	ARG	CZ-NH1	5.31	1.40	1.33
3	T	150	ARG	CZ-NH1	5.30	1.40	1.33
9	P	232	ARG	CZ-NH2	5.30	1.40	1.33
9	P	421	GLU	CG-CD	-5.30	1.44	1.51
3	T	60	ARG	CZ-NH2	5.30	1.40	1.33
13	O	41	LEU	N-CA	-5.29	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	86	ARG	NE-CZ	5.29	1.40	1.33
7	N	618	ARG	NE-CZ	5.28	1.40	1.33
2	V	257	GLU	CG-CD	5.27	1.59	1.51
7	N	913	PRO	N-CD	-5.27	1.40	1.47
1	W	182	TYR	CB-CG	-5.27	1.43	1.51
3	T	260	ILE	N-CA	-5.27	1.35	1.46
13	O	98	TYR	CG-CD2	5.27	1.46	1.39
7	N	139	ARG	CZ-NH1	5.25	1.39	1.33
13	O	373	TRP	CB-CG	-5.25	1.40	1.50
7	N	417	ARG	CZ-NH2	5.24	1.39	1.33
8	S	421	TYR	CG-CD2	5.24	1.46	1.39
4	X	22	ARG	CZ-NH2	5.23	1.39	1.33
2	V	243	SER	CA-CB	5.22	1.60	1.52
6	Z	202	ARG	CZ-NH2	5.22	1.39	1.33
6	Z	165	TYR	CE1-CZ	5.21	1.45	1.38
10	Q	17	GLU	N-CA	5.21	1.56	1.46
13	O	333	SER	CA-CB	5.20	1.60	1.52
2	V	230	TYR	N-CA	-5.20	1.35	1.46
9	P	161	CYS	N-CA	-5.20	1.35	1.46
3	T	157	TYR	CG-CD2	5.19	1.46	1.39
6	Z	113	SER	CA-CB	5.19	1.60	1.52
8	S	464	ARG	CZ-NH2	5.19	1.39	1.33
10	Q	232	TYR	CG-CD2	5.19	1.45	1.39
11	R	392	ARG	CZ-NH2	5.19	1.39	1.33
6	Z	174	GLU	CG-CD	5.18	1.59	1.51
3	T	233	VAL	N-CA	-5.18	1.35	1.46
13	O	32	PHE	CA-CB	5.17	1.65	1.53
1	W	37	PHE	CG-CD1	5.16	1.46	1.38
13	O	15	ARG	CZ-NH2	5.16	1.39	1.33
3	T	122	PHE	CG-CD2	5.16	1.46	1.38
6	Z	55	ARG	NE-CZ	5.16	1.39	1.33
6	Z	912	PHE	CG-CD1	5.15	1.46	1.38
8	S	95	PHE	CG-CD1	5.15	1.46	1.38
13	O	212	GLN	CG-CD	5.14	1.62	1.51
3	T	223	GLU	CD-OE1	-5.14	1.20	1.25
13	O	298	GLU	CB-CG	5.13	1.61	1.52
9	P	332	GLU	N-CA	-5.13	1.36	1.46
7	N	434	SER	CA-CB	5.12	1.60	1.52
6	Z	384	SER	CA-CB	5.12	1.60	1.52
11	R	48	GLU	CD-OE1	5.12	1.31	1.25
3	T	20	TYR	CE2-CZ	5.12	1.45	1.38
9	P	364	ARG	CZ-NH1	5.12	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	S	452	TYR	CG-CD2	5.11	1.45	1.39
10	Q	398	TYR	CZ-OH	5.11	1.46	1.37
6	Z	34	GLU	CD-OE2	5.10	1.31	1.25
7	N	604	ARG	NE-CZ	5.10	1.39	1.33
11	R	206	ARG	NE-CZ	5.10	1.39	1.33
8	S	425	ARG	CZ-NH2	5.10	1.39	1.33
1	W	4	GLU	CD-OE1	5.09	1.31	1.25
13	O	17	GLU	CG-CD	5.09	1.59	1.51
13	O	195	TYR	CG-CD2	5.08	1.45	1.39
8	S	428	ARG	CZ-NH2	5.08	1.39	1.33
2	V	304	ALA	CA-CB	5.08	1.63	1.52
8	S	393	ARG	CD-NE	5.07	1.55	1.46
8	S	82	TYR	CZ-OH	5.07	1.46	1.37
11	R	221	VAL	CA-CB	-5.07	1.44	1.54
2	V	28	TYR	CE2-CZ	5.06	1.45	1.38
6	Z	597	SER	CB-OG	5.06	1.48	1.42
6	Z	358	TYR	CE1-CZ	5.06	1.45	1.38
10	Q	104	PHE	CG-CD1	5.06	1.46	1.38
7	N	800	ALA	CA-CB	5.05	1.63	1.52
9	P	423	LEU	CA-C	-5.05	1.39	1.52
7	N	597	ARG	NE-CZ	5.05	1.39	1.33
11	R	328	PHE	CE2-CZ	5.04	1.47	1.37
10	Q	86	MET	CG-SD	-5.04	1.68	1.81
4	X	85	ARG	CZ-NH1	5.04	1.39	1.33
7	N	902	VAL	CA-CB	-5.04	1.44	1.54
8	S	275	TYR	CB-CG	-5.04	1.44	1.51
9	P	266	TYR	CG-CD1	5.03	1.45	1.39
11	R	331	ARG	CZ-NH1	5.03	1.39	1.33
1	W	21	PHE	CG-CD2	5.03	1.46	1.38
6	Z	136	ARG	CZ-NH2	5.03	1.39	1.33
9	P	94	GLN	N-CA	-5.03	1.36	1.46
12	U	57	GLU	CD-OE2	5.02	1.31	1.25
6	Z	408	TYR	CE1-CZ	5.02	1.45	1.38
8	S	160	ARG	CD-NE	5.02	1.54	1.46
7	N	893	VAL	N-CA	-5.02	1.36	1.46
9	P	437	GLU	CG-CD	5.02	1.59	1.51
3	T	151	TRP	NE1-CE2	-5.01	1.31	1.37
6	Z	55	ARG	CZ-NH1	5.01	1.39	1.33
6	Z	783	VAL	CB-CG2	5.01	1.63	1.52
3	T	252	GLU	N-CA	-5.01	1.36	1.46

All (928) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	8	PRO	N-CA-CB	-29.24	68.21	103.30
2	V	196	TYR	CB-CA-C	-25.02	60.37	110.40
2	V	157	ARG	NE-CZ-NH1	16.47	128.53	120.30
13	O	330	ARG	NE-CZ-NH1	16.47	128.53	120.30
10	Q	409	TYR	CB-CG-CD2	-16.00	111.40	121.00
13	O	15	ARG	NE-CZ-NH1	15.89	128.24	120.30
6	Z	574	TYR	CB-CG-CD2	-15.65	111.61	121.00
6	Z	439	TYR	CB-CG-CD1	15.32	130.19	121.00
8	S	253	PHE	CB-CG-CD1	-15.12	110.22	120.80
5	Y	65	ASP	CB-CA-C	-14.87	80.67	110.40
10	Q	124	PHE	CB-CG-CD2	-14.75	110.47	120.80
10	Q	124	PHE	CB-CG-CD1	14.68	131.07	120.80
10	Q	77	PHE	CB-CG-CD1	14.20	130.74	120.80
6	Z	574	TYR	CB-CG-CD1	13.96	129.37	121.00
11	R	338	TYR	CB-CG-CD2	-13.80	112.72	121.00
10	Q	50	ARG	NE-CZ-NH1	13.66	127.13	120.30
8	S	158	PHE	CB-CG-CD2	13.53	130.27	120.80
7	N	81	TYR	CB-CG-CD1	13.39	129.03	121.00
13	O	65	PHE	CB-CG-CD1	13.35	130.14	120.80
10	Q	243	PHE	CB-CG-CD1	-13.34	111.46	120.80
6	Z	385	PHE	CB-CG-CD2	-13.18	111.58	120.80
2	V	157	ARG	NE-CZ-NH2	-13.17	113.71	120.30
2	V	196	TYR	N-CA-CB	13.07	134.13	110.60
7	N	282	TYR	CB-CG-CD2	12.96	128.78	121.00
11	R	305	PHE	CB-CG-CD2	-12.94	111.74	120.80
6	Z	269	TYR	CB-CG-CD2	-12.92	113.25	121.00
6	Z	264	PHE	CB-CG-CD2	-12.81	111.83	120.80
13	O	58	ARG	NE-CZ-NH1	-12.63	113.98	120.30
5	Y	73	PHE	CB-CG-CD2	12.58	129.61	120.80
11	R	224	PHE	CB-CG-CD1	-12.57	112.00	120.80
2	V	254	ARG	NE-CZ-NH1	12.55	126.57	120.30
6	Z	103	TYR	CB-CG-CD1	12.47	128.49	121.00
8	S	384	ARG	NE-CZ-NH2	-12.41	114.10	120.30
12	U	22	TYR	CB-CG-CD1	12.37	128.42	121.00
2	V	114	PHE	CB-CG-CD1	12.36	129.45	120.80
6	Z	738	TYR	CB-CG-CD1	12.24	128.35	121.00
8	S	158	PHE	CB-CG-CD1	-12.24	112.23	120.80
9	P	208	PHE	CB-CG-CD2	-12.24	112.23	120.80
6	Z	96	TYR	CB-CG-CD1	-12.18	113.69	121.00
11	R	417	TYR	CB-CG-CD2	-12.03	113.78	121.00
7	N	559	TYR	CB-CG-CD2	-11.93	113.84	121.00
13	O	98	TYR	CB-CG-CD2	-11.91	113.85	121.00
5	Y	84	TYR	CB-CG-CD2	-11.86	113.88	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	114	PHE	CB-CG-CD2	-11.81	112.53	120.80
7	N	906	ARG	NE-CZ-NH1	11.75	126.17	120.30
2	V	197	TYR	N-CA-CB	11.69	131.64	110.60
9	P	356	TYR	CB-CG-CD2	-11.66	114.00	121.00
11	R	222	ARG	NE-CZ-NH1	11.65	126.13	120.30
8	S	428	ARG	NE-CZ-NH2	-11.64	114.48	120.30
9	P	273	TYR	CB-CG-CD2	-11.61	114.04	121.00
7	N	463	TYR	CB-CG-CD1	11.55	127.93	121.00
6	Z	55	ARG	NE-CZ-NH1	11.36	125.98	120.30
10	Q	12	ARG	NE-CZ-NH2	-11.27	114.67	120.30
11	R	312	TYR	CB-CG-CD1	-11.26	114.24	121.00
6	Z	928	ARG	NE-CZ-NH2	-11.18	114.71	120.30
10	Q	77	PHE	CB-CG-CD2	-11.09	113.03	120.80
1	W	23	ARG	NE-CZ-NH2	-11.02	114.79	120.30
7	N	299	TYR	CB-CG-CD2	-10.92	114.44	121.00
7	N	162	ARG	NE-CZ-NH2	-10.92	114.84	120.30
8	S	196	ARG	NE-CZ-NH1	10.90	125.75	120.30
7	N	139	ARG	NE-CZ-NH1	10.89	125.74	120.30
13	O	179	PHE	CB-CG-CD1	10.84	128.39	120.80
11	R	207	ARG	NE-CZ-NH1	10.84	125.72	120.30
9	P	359	ARG	NE-CZ-NH2	-10.74	114.93	120.30
6	Z	843	ASP	CB-CG-OD2	-10.71	108.67	118.30
8	S	126	LYS	N-CA-CB	10.70	129.85	110.60
8	S	127	THR	N-CA-CB	-10.63	90.11	110.30
6	Z	137	TYR	CB-CG-CD1	10.56	127.34	121.00
4	X	122	TYR	CB-CG-CD2	-10.56	114.67	121.00
2	V	156	PHE	CB-CG-CD1	-10.50	113.45	120.80
2	V	228	TYR	CB-CG-CD1	-10.48	114.71	121.00
7	N	81	TYR	CB-CG-CD2	-10.45	114.73	121.00
6	Z	339	PHE	CB-CG-CD2	-10.44	113.49	120.80
7	N	896	PHE	CB-CG-CD1	10.39	128.07	120.80
11	R	392	ARG	NE-CZ-NH2	10.32	125.46	120.30
6	Z	970	TYR	CB-CG-CD1	-10.32	114.81	121.00
7	N	70	TYR	CB-CG-CD2	-10.31	114.81	121.00
6	Z	774	ARG	NE-CZ-NH1	10.25	125.43	120.30
11	R	186	TYR	CB-CG-CD1	-10.22	114.87	121.00
10	Q	34	ASP	CB-CG-OD1	10.22	127.50	118.30
8	S	425	ARG	NE-CZ-NH1	10.21	125.40	120.30
2	V	196	TYR	CD1-CE1-CZ	-10.03	110.77	119.80
13	O	98	TYR	CB-CG-CD1	10.03	127.02	121.00
7	N	282	TYR	CB-CG-CD1	-10.02	114.99	121.00
7	N	906	ARG	NE-CZ-NH2	-10.01	115.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	137	TYR	CB-CG-CD2	-9.99	115.00	121.00
4	X	96	ARG	NE-CZ-NH2	-9.98	115.31	120.30
3	T	150	ARG	NE-CZ-NH1	9.95	125.28	120.30
8	S	82	TYR	CB-CG-CD1	9.85	126.91	121.00
4	X	122	TYR	CB-CG-CD1	9.84	126.90	121.00
11	R	43	ARG	NE-CZ-NH2	-9.71	115.45	120.30
6	Z	248	TYR	CB-CG-CD2	-9.67	115.20	121.00
11	R	65	TYR	CB-CG-CD1	-9.66	115.20	121.00
9	P	245	TYR	CB-CG-CD1	9.52	126.71	121.00
13	O	147	ARG	NE-CZ-NH1	9.46	125.03	120.30
7	N	786	ARG	NE-CZ-NH1	-9.45	115.57	120.30
10	Q	294	ARG	NE-CZ-NH2	-9.44	115.58	120.30
6	Z	738	TYR	CB-CG-CD2	-9.42	115.35	121.00
6	Z	385	PHE	CB-CG-CD1	9.37	127.36	120.80
6	Z	759	ARG	NE-CZ-NH1	9.33	124.96	120.30
9	P	328	ALA	N-CA-CB	9.29	123.11	110.10
7	N	526	TYR	CB-CG-CD1	-9.27	115.44	121.00
13	O	356	ARG	NE-CZ-NH2	-9.27	115.66	120.30
11	R	224	PHE	CB-CG-CD2	9.26	127.28	120.80
9	P	356	TYR	CB-CG-CD1	9.25	126.55	121.00
11	R	338	TYR	CB-CG-CD1	9.25	126.55	121.00
11	R	206	ARG	NE-CZ-NH1	9.22	124.91	120.30
7	N	18	ASP	CB-CG-OD1	-9.21	110.01	118.30
6	Z	153	TYR	CB-CG-CD2	-9.21	115.47	121.00
8	S	286	TYR	CB-CG-CD2	9.21	126.53	121.00
9	P	245	TYR	CB-CG-CD2	-9.16	115.50	121.00
7	N	559	TYR	CB-CG-CD1	9.13	126.48	121.00
11	R	63	TYR	CB-CG-CD1	-9.12	115.53	121.00
6	Z	928	ARG	NE-CZ-NH1	9.12	124.86	120.30
13	O	65	PHE	CB-CG-CD2	-9.09	114.44	120.80
13	O	342	ASP	CB-CG-OD2	-9.03	110.17	118.30
5	Y	86	ARG	NE-CZ-NH2	-9.03	115.79	120.30
11	R	222	ARG	NE-CZ-NH2	-9.01	115.79	120.30
8	S	309	PHE	CB-CG-CD2	9.01	127.11	120.80
8	S	127	THR	CA-CB-CG2	9.00	125.00	112.40
11	R	357	PHE	CB-CG-CD1	-8.99	114.51	120.80
6	Z	103	TYR	CB-CG-CD2	-8.98	115.61	121.00
2	V	194	ARG	NE-CZ-NH1	8.95	124.78	120.30
8	S	332	PHE	CB-CG-CD2	-8.95	114.54	120.80
8	S	95	PHE	CB-CG-CD1	8.94	127.06	120.80
5	Y	84	TYR	CB-CG-CD1	8.94	126.36	121.00
6	Z	264	PHE	CB-CG-CD1	8.90	127.03	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	513	ALA	CB-CA-C	8.90	123.45	110.10
9	P	3	ARG	NE-CZ-NH2	-8.89	115.85	120.30
6	Z	298	PHE	CB-CG-CD1	8.88	127.01	120.80
4	X	45	PHE	CB-CG-CD1	8.88	127.01	120.80
13	O	41	LEU	N-CA-CB	-8.87	92.66	110.40
6	Z	912	PHE	CB-CG-CD2	8.84	126.98	120.80
10	Q	309	ARG	NE-CZ-NH1	8.82	124.71	120.30
2	V	155	ALA	N-CA-CB	8.80	122.42	110.10
5	Y	65	ASP	N-CA-CB	8.80	126.44	110.60
13	O	32	PHE	CB-CG-CD1	-8.80	114.64	120.80
9	P	138	ARG	NE-CZ-NH2	-8.74	115.93	120.30
6	Z	439	TYR	CB-CG-CD2	-8.74	115.76	121.00
2	V	135	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	W	26	PHE	CB-CG-CD2	-8.70	114.71	120.80
12	U	113	TYR	CB-CG-CD1	-8.68	115.80	121.00
10	Q	88	PHE	CB-CG-CD1	-8.67	114.73	120.80
13	O	41	LEU	CB-CA-C	8.67	126.67	110.20
13	O	26	PHE	CB-CG-CD2	8.66	126.86	120.80
13	O	166	ARG	NE-CZ-NH1	8.63	124.61	120.30
5	Y	83	ARG	NE-CZ-NH1	8.61	124.61	120.30
11	R	63	TYR	CB-CG-CD2	8.61	126.16	121.00
4	X	100	TRP	CG-CD2-CE3	-8.60	126.16	133.90
10	Q	423	VAL	CA-CB-CG2	8.59	123.78	110.90
8	S	52	TYR	CB-CG-CD2	-8.55	115.87	121.00
9	P	213	TYR	CB-CG-CD1	-8.54	115.87	121.00
7	N	299	TYR	CB-CG-CD1	8.54	126.12	121.00
1	W	113	PHE	CB-CG-CD1	8.53	126.77	120.80
7	N	584	ARG	NE-CZ-NH2	-8.52	116.04	120.30
13	O	29	PHE	CB-CG-CD2	-8.51	114.84	120.80
5	Y	73	PHE	CB-CG-CD1	-8.51	114.84	120.80
10	Q	88	PHE	CB-CG-CD2	8.51	126.75	120.80
6	Z	722	ASP	CB-CG-OD1	8.50	125.95	118.30
4	X	85	ARG	NE-CZ-NH2	-8.49	116.06	120.30
10	Q	409	TYR	CB-CG-CD1	8.48	126.09	121.00
8	S	186	TYR	CB-CG-CD1	-8.47	115.92	121.00
6	Z	4	GLU	N-CA-CB	8.42	125.75	110.60
6	Z	244	ARG	NE-CZ-NH1	8.40	124.50	120.30
10	Q	335	PHE	CB-CG-CD1	8.40	126.68	120.80
1	W	140	ASP	CB-CG-OD2	-8.37	110.77	118.30
1	W	179	ARG	NE-CZ-NH2	-8.36	116.12	120.30
11	R	304	TYR	CB-CG-CD2	8.34	126.01	121.00
3	T	157	TYR	CB-CG-CD1	8.32	125.99	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	306	ARG	NE-CZ-NH1	8.30	124.45	120.30
2	V	61	TYR	CB-CG-CD2	-8.28	116.03	121.00
13	O	69	PHE	CB-CG-CD2	-8.24	115.03	120.80
7	N	139	ARG	NE-CZ-NH2	-8.21	116.19	120.30
7	N	500	ASP	CB-CG-OD1	8.20	125.68	118.30
7	N	188	TYR	CB-CG-CD2	-8.20	116.08	121.00
2	V	183	ALA	C-N-CA	8.18	142.16	121.70
2	V	254	ARG	NE-CZ-NH2	-8.18	116.21	120.30
13	O	33	TYR	CB-CG-CD2	-8.16	116.10	121.00
9	P	3	ARG	NE-CZ-NH1	8.16	124.38	120.30
2	V	59	ASP	CB-CG-OD2	-8.16	110.96	118.30
7	N	604	ARG	NE-CZ-NH2	-8.16	116.22	120.30
13	O	15	ARG	NE-CZ-NH2	-8.16	116.22	120.30
3	T	73	PHE	CB-CG-CD1	-8.10	115.13	120.80
6	Z	272	TYR	CB-CG-CD2	8.09	125.85	121.00
7	N	162	ARG	NE-CZ-NH1	8.05	124.33	120.30
3	T	109	TYR	CB-CG-CD2	-8.01	116.19	121.00
2	V	270	TYR	CB-CG-CD1	-8.00	116.20	121.00
13	O	347	LEU	CB-CG-CD2	8.00	124.59	111.00
11	R	307	TYR	CB-CG-CD2	-7.98	116.21	121.00
8	S	345	TYR	CB-CG-CD1	-7.97	116.22	121.00
1	W	78	ASP	CB-CG-OD1	7.97	125.47	118.30
12	U	245	ASP	CB-CG-OD1	-7.97	111.13	118.30
11	R	124	ASP	CB-CG-OD2	7.94	125.45	118.30
3	T	60	ARG	NE-CZ-NH2	-7.94	116.33	120.30
10	Q	75	ARG	NE-CZ-NH1	-7.92	116.34	120.30
2	V	103	MET	CG-SD-CE	-7.90	87.56	100.20
3	T	51	TYR	CB-CG-CD1	7.89	125.73	121.00
6	Z	48	ASP	CB-CG-OD2	-7.88	111.21	118.30
1	W	182	TYR	CZ-CE2-CD2	-7.87	112.72	119.80
2	V	93	ASP	CB-CG-OD2	-7.86	111.23	118.30
2	V	228	TYR	CB-CG-CD2	7.86	125.71	121.00
11	R	329	PHE	CB-CG-CD1	7.86	126.30	120.80
11	R	179	PHE	CB-CG-CD2	-7.86	115.30	120.80
11	R	20	ARG	NE-CZ-NH1	7.85	124.23	120.30
12	U	179	ARG	N-CA-CB	7.85	124.72	110.60
6	Z	242	PHE	CB-CG-CD2	-7.83	115.32	120.80
11	R	180	PHE	CB-CG-CD2	-7.81	115.33	120.80
7	N	463	TYR	CB-CG-CD2	-7.81	116.31	121.00
7	N	739	PHE	CB-CG-CD2	-7.81	115.33	120.80
2	V	59	ASP	CB-CG-OD1	7.80	125.32	118.30
7	N	394	ARG	NE-CZ-NH2	7.78	124.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	441	TYR	CB-CG-CD1	7.77	125.67	121.00
10	Q	20	TYR	CB-CG-CD1	-7.74	116.36	121.00
7	N	894	ARG	NE-CZ-NH2	-7.73	116.43	120.30
13	O	48	PHE	CB-CG-CD1	7.72	126.20	120.80
13	O	181	PHE	CB-CG-CD2	-7.72	115.40	120.80
10	Q	20	TYR	CG-CD1-CE1	-7.71	115.13	121.30
2	V	156	PHE	CB-CG-CD2	7.71	126.20	120.80
9	P	359	ARG	NE-CZ-NH1	7.70	124.15	120.30
13	O	248	TYR	CB-CG-CD2	-7.70	116.38	121.00
6	Z	202	ARG	NE-CZ-NH2	-7.68	116.46	120.30
7	N	204	SER	N-CA-CB	7.68	122.03	110.50
6	Z	767	TYR	CB-CG-CD1	7.68	125.61	121.00
11	R	305	PHE	CB-CG-CD1	7.67	126.17	120.80
11	R	265	ASP	CB-CG-OD2	7.67	125.20	118.30
10	Q	13	ARG	NE-CZ-NH2	7.67	124.14	120.30
7	N	215	MET	CG-SD-CE	-7.67	87.93	100.20
7	N	742	TRP	CB-CG-CD2	-7.66	116.64	126.60
6	Z	175	ASP	CB-CG-OD2	-7.64	111.43	118.30
13	O	263	PHE	CB-CG-CD2	-7.62	115.46	120.80
2	V	57	PHE	CB-CG-CD2	-7.58	115.49	120.80
7	N	8	PRO	CA-N-CD	7.56	122.28	111.70
10	Q	219	ASP	CB-CG-OD1	7.55	125.10	118.30
7	N	463	TYR	CD1-CE1-CZ	7.55	126.59	119.80
8	S	298	ARG	NE-CZ-NH1	7.55	124.07	120.30
9	P	318	TYR	CB-CG-CD1	-7.53	116.48	121.00
11	R	179	PHE	CB-CG-CD1	7.53	126.07	120.80
2	V	155	ALA	CB-CA-C	-7.52	98.83	110.10
3	T	224	ARG	NE-CZ-NH1	7.51	124.06	120.30
2	V	69	PHE	CB-CG-CD1	-7.50	115.55	120.80
8	S	174	ARG	NE-CZ-NH2	-7.49	116.56	120.30
13	O	62	TYR	CB-CG-CD1	7.48	125.49	121.00
11	R	99	TYR	CB-CG-CD1	-7.46	116.52	121.00
10	Q	34	ASP	CB-CG-OD2	-7.45	111.59	118.30
8	S	484	ASP	CB-CG-OD1	-7.44	111.60	118.30
6	Z	408	TYR	CB-CG-CD1	7.43	125.46	121.00
6	Z	153	TYR	CB-CG-CD1	7.41	125.45	121.00
8	S	174	ARG	NE-CZ-NH1	7.40	124.00	120.30
9	P	344	ARG	NE-CZ-NH2	-7.40	116.60	120.30
12	U	113	TYR	CB-CG-CD2	7.40	125.44	121.00
1	W	41	ARG	NE-CZ-NH1	7.38	123.99	120.30
2	V	229	ASP	CB-CG-OD1	-7.36	111.68	118.30
7	N	896	PHE	CB-CG-CD2	-7.36	115.65	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	798	ARG	NE-CZ-NH2	-7.36	116.62	120.30
2	V	182	LYS	O-C-N	-7.34	110.95	122.70
11	R	65	TYR	CG-CD2-CE2	-7.32	115.44	121.30
3	T	245	TYR	CB-CG-CD1	-7.30	116.62	121.00
10	Q	339	TYR	CG-CD1-CE1	7.30	127.14	121.30
6	Z	603	VAL	CA-CB-CG2	-7.29	99.97	110.90
7	N	599	TYR	CB-CG-CD2	7.28	125.37	121.00
3	T	130	ASP	CB-CG-OD1	-7.28	111.75	118.30
11	R	335	ARG	NE-CZ-NH2	-7.28	116.66	120.30
7	N	584	ARG	NE-CZ-NH1	7.24	123.92	120.30
8	S	346	TYR	CB-CG-CD2	-7.24	116.66	121.00
8	S	253	PHE	CD1-CG-CD2	7.24	127.71	118.30
7	N	762	ARG	NE-CZ-NH2	-7.23	116.68	120.30
11	R	285	ALA	CB-CA-C	-7.23	99.25	110.10
6	Z	723	ASP	CB-CG-OD1	7.23	124.81	118.30
9	P	344	ARG	NE-CZ-NH1	7.23	123.91	120.30
7	N	783	SER	N-CA-CB	7.21	121.32	110.50
6	Z	231	ASP	CB-CG-OD2	-7.21	111.81	118.30
7	N	406	TYR	CB-CG-CD1	7.19	125.31	121.00
6	Z	574	TYR	CZ-CE2-CD2	7.18	126.26	119.80
7	N	888	ASP	CB-CG-OD1	-7.17	111.84	118.30
2	V	196	TYR	CZ-CE2-CD2	7.13	126.22	119.80
1	W	113	PHE	CB-CG-CD2	-7.13	115.81	120.80
7	N	599	TYR	CB-CG-CD1	-7.13	116.72	121.00
6	Z	565	PHE	CB-CG-CD2	-7.12	115.82	120.80
8	S	171	TYR	CB-CA-C	7.09	124.58	110.40
6	Z	613	ASP	CB-CG-OD2	7.09	124.68	118.30
11	R	335	ARG	NE-CZ-NH1	7.08	123.84	120.30
6	Z	843	ASP	CB-CG-OD1	7.08	124.67	118.30
3	T	122	PHE	CB-CG-CD2	7.07	125.75	120.80
8	S	360	PHE	CB-CG-CD1	7.07	125.75	120.80
13	O	179	PHE	CB-CG-CD2	-7.07	115.85	120.80
2	V	154	ASP	CB-CG-OD1	-7.07	111.94	118.30
8	S	197	SER	CA-C-O	-7.06	105.28	120.10
8	S	25	TYR	CD1-CE1-CZ	-7.05	113.45	119.80
7	N	212	ASP	CB-CG-OD1	7.04	124.64	118.30
4	X	51	ARG	NE-CZ-NH1	7.02	123.81	120.30
9	P	124	VAL	CA-CB-CG1	7.02	121.43	110.90
11	R	422	ARG	NE-CZ-NH1	7.02	123.81	120.30
4	X	48	PHE	CB-CG-CD2	-7.01	115.89	120.80
10	Q	434	TYR	CG-CD1-CE1	-7.00	115.70	121.30
9	P	345	VAL	CA-CB-CG1	6.99	121.39	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	735	MET	CG-SD-CE	-6.97	89.05	100.20
10	Q	82	THR	CA-CB-CG2	-6.97	102.64	112.40
7	N	567	ALA	N-CA-CB	6.96	119.85	110.10
10	Q	427	PHE	CB-CG-CD1	6.96	125.67	120.80
6	Z	564	ARG	NE-CZ-NH2	-6.96	116.82	120.30
10	Q	104	PHE	CB-CG-CD2	-6.95	115.93	120.80
13	O	302	VAL	CA-CB-CG1	-6.95	100.47	110.90
6	Z	826	ARG	NE-CZ-NH1	6.94	123.77	120.30
7	N	593	PHE	CB-CG-CD1	-6.94	115.94	120.80
10	Q	151	TYR	CB-CG-CD2	6.94	125.16	121.00
8	S	298	ARG	NE-CZ-NH2	-6.94	116.83	120.30
9	P	236	GLU	N-CA-CB	6.93	123.08	110.60
6	Z	825	ALA	N-CA-CB	6.93	119.80	110.10
2	V	251	TYR	CG-CD2-CE2	-6.90	115.78	121.30
7	N	69	TYR	CB-CG-CD2	-6.88	116.87	121.00
2	V	136	ALA	N-CA-CB	6.88	119.73	110.10
6	Z	912	PHE	CB-CG-CD1	-6.88	115.99	120.80
9	P	154	ASP	CB-CG-OD2	-6.87	112.11	118.30
11	R	292	LEU	CB-CG-CD1	6.86	122.66	111.00
11	R	312	TYR	CB-CG-CD2	6.85	125.11	121.00
9	P	397	ALA	N-CA-CB	6.85	119.69	110.10
7	N	178	SER	N-CA-CB	6.84	120.75	110.50
3	T	14	ALA	N-CA-CB	6.83	119.67	110.10
9	P	21	PHE	CB-CG-CD2	6.83	125.58	120.80
10	Q	185	TYR	CB-CG-CD2	-6.82	116.91	121.00
12	U	243	ASP	CB-CG-OD2	6.82	124.44	118.30
7	N	742	TRP	CE2-CD2-CG	-6.81	101.85	107.30
8	S	480	ARG	NE-CZ-NH1	6.81	123.71	120.30
7	N	556	ALA	N-CA-CB	6.79	119.61	110.10
1	W	127	ARG	NE-CZ-NH1	6.79	123.69	120.30
13	O	330	ARG	NH1-CZ-NH2	-6.79	111.93	119.40
7	N	302	PHE	CB-CG-CD1	-6.79	116.05	120.80
8	S	52	TYR	CB-CG-CD1	6.78	125.07	121.00
10	Q	162	LEU	N-CA-C	-6.76	92.75	111.00
7	N	526	TYR	CG-CD2-CE2	-6.75	115.90	121.30
9	P	333	ALA	CB-CA-C	-6.75	99.97	110.10
3	T	75	PHE	CB-CG-CD1	-6.75	116.08	120.80
13	O	288	ARG	NE-CZ-NH2	-6.74	116.93	120.30
4	X	97	TYR	CB-CG-CD1	6.74	125.05	121.00
3	T	82	PHE	CB-CG-CD1	6.74	125.52	120.80
3	T	265	ASP	CB-CG-OD1	6.73	124.36	118.30
13	O	71	ASP	CB-CG-OD2	-6.72	112.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	U	124	ASP	CB-CG-OD1	-6.71	112.26	118.30
6	Z	165	TYR	CB-CG-CD2	6.71	125.02	121.00
8	S	95	PHE	CB-CG-CD2	-6.68	116.12	120.80
6	Z	386	VAL	CA-CB-CG2	-6.67	100.89	110.90
11	R	124	ASP	CB-CG-OD1	-6.66	112.30	118.30
2	V	42	ARG	NE-CZ-NH1	6.66	123.63	120.30
3	T	82	PHE	CB-CG-CD2	-6.66	116.14	120.80
10	Q	151	TYR	CB-CG-CD1	-6.66	117.01	121.00
9	P	123	ARG	NE-CZ-NH2	-6.64	116.98	120.30
11	R	365	ASP	CB-CG-OD2	-6.63	112.33	118.30
6	Z	231	ASP	CB-CG-OD1	6.63	124.27	118.30
11	R	180	PHE	CB-CG-CD1	6.62	125.43	120.80
8	S	253	PHE	CG-CD1-CE1	-6.61	113.52	120.80
2	V	138	ALA	N-CA-CB	6.61	119.35	110.10
8	S	292	TYR	CB-CG-CD2	-6.60	117.04	121.00
2	V	172	GLN	N-CA-CB	6.60	122.47	110.60
6	Z	544	THR	CA-CB-CG2	-6.60	103.16	112.40
7	N	548	ARG	NE-CZ-NH1	6.60	123.60	120.30
3	T	217	THR	CA-CB-CG2	-6.59	103.17	112.40
7	N	671	LEU	O-C-N	-6.58	112.17	122.70
3	T	150	ARG	NE-CZ-NH2	-6.58	117.01	120.30
7	N	117	TYR	CB-CG-CD2	-6.57	117.06	121.00
9	P	310	ARG	NE-CZ-NH1	-6.56	117.02	120.30
2	V	87	PHE	CB-CG-CD2	-6.55	116.22	120.80
6	Z	312	TYR	CG-CD1-CE1	6.54	126.53	121.30
12	U	56	PHE	CB-CG-CD2	-6.53	116.23	120.80
11	R	210	TYR	CB-CG-CD2	-6.52	117.09	121.00
6	Z	837	TYR	CB-CG-CD1	6.52	124.91	121.00
13	O	26	PHE	CB-CG-CD1	-6.51	116.24	120.80
6	Z	167	ASP	CB-CG-OD2	6.51	124.16	118.30
2	V	171	ARG	NE-CZ-NH1	6.51	123.56	120.30
7	N	130	ASP	CB-CG-OD1	6.51	124.16	118.30
13	O	217	LEU	CB-CG-CD1	6.50	122.05	111.00
10	Q	345	SER	N-CA-CB	6.50	120.25	110.50
2	V	271	VAL	CA-CB-CG1	6.50	120.64	110.90
12	U	25	THR	CA-CB-CG2	-6.49	103.32	112.40
6	Z	767	TYR	CG-CD1-CE1	6.48	126.49	121.30
13	O	29	PHE	CB-CG-CD1	6.48	125.34	120.80
8	S	240	ASP	CB-CG-OD2	-6.48	112.47	118.30
12	U	22	TYR	CB-CG-CD2	-6.47	117.12	121.00
13	O	187	SER	N-CA-CB	6.46	120.18	110.50
6	Z	1	MET	CG-SD-CE	-6.45	89.88	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	189	PRO	N-CA-CB	6.44	111.03	103.30
7	N	722	THR	CA-CB-CG2	-6.44	103.39	112.40
6	Z	970	TYR	CB-CG-CD2	6.43	124.86	121.00
6	Z	790	MET	N-CA-CB	6.43	122.18	110.60
11	R	24	TYR	CD1-CE1-CZ	-6.43	114.02	119.80
8	S	248	ASP	CB-CG-OD1	-6.42	112.52	118.30
10	Q	104	PHE	CB-CG-CD1	6.42	125.30	120.80
2	V	274	GLN	N-CA-CB	6.42	122.16	110.60
9	P	234	TYR	CB-CG-CD2	-6.42	117.15	121.00
6	Z	780	MET	CG-SD-CE	-6.41	89.94	100.20
7	N	575	ALA	CB-CA-C	-6.41	100.48	110.10
13	O	178	TYR	CB-CG-CD2	-6.41	117.15	121.00
4	X	17	TYR	CB-CG-CD1	-6.41	117.16	121.00
10	Q	294	ARG	CD-NE-CZ	-6.40	114.64	123.60
7	N	109	TYR	CB-CG-CD1	-6.40	117.16	121.00
9	P	339	GLU	CB-CA-C	-6.39	97.62	110.40
6	Z	441	TYR	CA-CB-CG	-6.39	101.26	113.40
10	Q	434	TYR	CB-CG-CD1	-6.39	117.17	121.00
8	S	119	TYR	CB-CG-CD2	6.39	124.83	121.00
7	N	577	SER	CB-CA-C	-6.38	97.97	110.10
13	O	342	ASP	CB-CG-OD1	6.38	124.04	118.30
10	Q	294	ARG	NE-CZ-NH1	6.37	123.48	120.30
7	N	796	VAL	CG1-CB-CG2	6.36	121.08	110.90
7	N	869	ASP	CB-CG-OD1	-6.36	112.58	118.30
6	Z	608	TYR	CB-CG-CD2	-6.36	117.19	121.00
11	R	417	TYR	CB-CG-CD1	6.36	124.81	121.00
1	W	23	ARG	NE-CZ-NH1	6.35	123.47	120.30
9	P	213	TYR	CB-CG-CD2	6.35	124.81	121.00
4	X	10	PHE	CG-CD2-CE2	6.34	127.78	120.80
6	Z	58	GLU	N-CA-CB	6.32	121.98	110.60
11	R	417	TYR	CG-CD1-CE1	-6.31	116.25	121.30
4	X	100	TRP	CE2-CD2-CE3	6.30	126.26	118.70
7	N	260	ASP	CB-CG-OD1	6.30	123.97	118.30
12	U	248	ASP	CB-CG-OD2	-6.30	112.63	118.30
9	P	208	PHE	CB-CG-CD1	6.29	125.21	120.80
7	N	88	ARG	NE-CZ-NH1	-6.29	117.16	120.30
6	Z	210	TYR	CB-CG-CD1	6.28	124.77	121.00
6	Z	838	TYR	CG-CD1-CE1	6.28	126.32	121.30
3	T	51	TYR	CB-CG-CD2	-6.28	117.23	121.00
7	N	70	TYR	CB-CG-CD1	6.28	124.77	121.00
8	S	326	ASP	CB-CG-OD2	-6.27	112.66	118.30
10	Q	12	ARG	NE-CZ-NH1	6.27	123.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	78	PHE	CB-CG-CD1	6.27	125.19	120.80
11	R	173	THR	CA-CB-CG2	-6.27	103.62	112.40
7	N	406	TYR	CB-CG-CD2	-6.26	117.24	121.00
11	R	166	ALA	N-CA-CB	6.26	118.86	110.10
13	O	71	ASP	CB-CG-OD1	6.26	123.93	118.30
8	S	452	TYR	CD1-CE1-CZ	6.26	125.43	119.80
3	T	68	ALA	N-CA-CB	6.25	118.86	110.10
6	Z	426	TYR	CB-CG-CD1	6.25	124.75	121.00
13	O	253	GLN	N-CA-CB	6.25	121.85	110.60
2	V	35	LEU	CB-CG-CD1	6.24	121.61	111.00
3	T	245	TYR	CG-CD1-CE1	-6.24	116.31	121.30
3	T	81	TYR	CB-CG-CD1	6.24	124.74	121.00
11	R	337	VAL	CA-CB-CG1	6.23	120.25	110.90
6	Z	269	TYR	CG-CD2-CE2	-6.23	116.32	121.30
7	N	211	PHE	CB-CG-CD2	6.23	125.16	120.80
2	V	196	TYR	CA-CB-CG	-6.22	101.57	113.40
6	Z	476	ASP	CB-CG-OD1	6.22	123.90	118.30
8	S	399	TYR	CB-CG-CD1	6.22	124.73	121.00
4	X	29	VAL	CG1-CB-CG2	6.21	120.84	110.90
8	S	80	VAL	CA-CB-CG1	6.21	120.22	110.90
13	O	60	ARG	NE-CZ-NH2	6.21	123.40	120.30
6	Z	298	PHE	CG-CD2-CE2	6.20	127.62	120.80
9	P	187	SER	N-CA-CB	6.20	119.80	110.50
13	O	346	GLU	N-CA-CB	6.20	121.76	110.60
12	U	283	ARG	NE-CZ-NH1	6.20	123.40	120.30
3	T	44	LEU	N-CA-CB	6.19	122.78	110.40
11	R	270	VAL	CA-CB-CG1	6.18	120.17	110.90
3	T	75	PHE	CB-CG-CD2	6.18	125.12	120.80
1	W	10	ILE	N-CA-C	-6.17	94.33	111.00
13	O	210	ARG	NE-CZ-NH1	6.17	123.38	120.30
10	Q	219	ASP	CB-CG-OD2	-6.15	112.76	118.30
7	N	417	ARG	NE-CZ-NH1	-6.15	117.23	120.30
11	R	256	THR	CA-CB-CG2	-6.14	103.80	112.40
7	N	788	TYR	CB-CG-CD1	6.13	124.68	121.00
13	O	378	GLU	CA-CB-CG	6.12	126.86	113.40
11	R	363	PHE	CB-CG-CD1	6.12	125.08	120.80
2	V	100	ARG	CD-NE-CZ	6.11	132.16	123.60
13	O	150	LEU	N-CA-CB	6.11	122.62	110.40
8	S	382	ARG	NE-CZ-NH1	-6.11	117.25	120.30
7	N	515	ARG	NE-CZ-NH2	-6.10	117.25	120.30
7	N	810	ALA	CB-CA-C	-6.10	100.95	110.10
6	Z	623	ARG	NE-CZ-NH1	6.09	123.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	49	PHE	CB-CG-CD1	-6.09	116.54	120.80
7	N	887	ASP	CB-CG-OD2	-6.09	112.82	118.30
11	R	210	TYR	CB-CG-CD1	6.09	124.65	121.00
10	Q	111	LEU	O-C-N	6.08	132.43	122.70
8	S	384	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	W	170	HIS	CA-CB-CG	6.07	123.93	113.60
4	X	90	VAL	CA-CB-CG2	-6.07	101.79	110.90
7	N	365	PHE	CB-CG-CD1	-6.07	116.56	120.80
1	W	151	THR	CA-CB-CG2	-6.06	103.92	112.40
9	P	215	SER	N-CA-CB	6.06	119.59	110.50
7	N	120	ASP	CB-CA-C	-6.06	98.28	110.40
7	N	587	ALA	CB-CA-C	-6.06	101.02	110.10
8	S	449	LEU	CB-CA-C	6.05	121.70	110.20
9	P	123	ARG	NE-CZ-NH1	6.05	123.33	120.30
6	Z	803	ALA	N-CA-CB	6.05	118.57	110.10
8	S	411	LEU	CB-CG-CD2	6.04	121.28	111.00
12	U	72	TYR	CB-CG-CD2	-6.04	117.37	121.00
13	O	181	PHE	CB-CG-CD1	6.04	125.03	120.80
8	S	138	MET	CG-SD-CE	-6.04	90.54	100.20
12	U	239	LEU	CB-CG-CD2	6.03	121.25	111.00
1	W	78	ASP	CB-CG-OD2	-6.03	112.88	118.30
2	V	243	SER	N-CA-CB	6.02	119.54	110.50
6	Z	774	ARG	NE-CZ-NH2	-6.02	117.29	120.30
10	Q	153	ASP	CB-CA-C	-6.02	98.37	110.40
6	Z	406	TRP	CE2-CD2-CE3	6.01	125.91	118.70
2	V	274	GLN	N-CA-C	-6.01	94.78	111.00
6	Z	206	ASP	CB-CG-OD1	6.00	123.70	118.30
8	S	332	PHE	CD1-CE1-CZ	-6.00	112.90	120.10
13	O	85	SER	N-CA-CB	6.00	119.51	110.50
8	S	318	CYS	CB-CA-C	-6.00	98.40	110.40
13	O	215	TYR	CG-CD1-CE1	-5.99	116.50	121.30
11	R	50	VAL	CA-CB-CG2	-5.99	101.92	110.90
10	Q	43	GLY	N-CA-C	-5.98	98.15	113.10
11	R	231	LEU	CB-CA-C	-5.98	98.85	110.20
7	N	123	PHE	CB-CG-CD1	5.97	124.98	120.80
8	S	313	SER	N-CA-CB	5.97	119.45	110.50
9	P	333	ALA	N-CA-CB	5.97	118.45	110.10
8	S	306	SER	N-CA-CB	5.96	119.44	110.50
8	S	102	SER	N-CA-C	-5.96	94.91	111.00
6	Z	300	ALA	N-CA-CB	5.95	118.43	110.10
7	N	310	ASP	CB-CG-OD2	5.94	123.65	118.30
7	N	387	ALA	N-CA-CB	5.94	118.42	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	217	PHE	CG-CD1-CE1	5.93	127.32	120.80
10	Q	165	PHE	CG-CD2-CE2	5.93	127.32	120.80
10	Q	318	LEU	CB-CG-CD1	5.93	121.08	111.00
6	Z	63	LEU	CB-CG-CD1	5.92	121.07	111.00
11	R	203	ASP	CB-CG-OD1	5.92	123.63	118.30
10	Q	398	TYR	CB-CG-CD1	5.92	124.55	121.00
6	Z	777	PRO	N-CA-CB	5.92	110.40	103.30
7	N	422	TYR	CB-CG-CD2	-5.91	117.45	121.00
8	S	286	TYR	CG-CD2-CE2	5.91	126.03	121.30
7	N	389	TYR	CB-CG-CD1	-5.90	117.46	121.00
11	R	388	VAL	N-CA-C	-5.90	95.07	111.00
6	Z	301	THR	CA-CB-CG2	-5.89	104.16	112.40
7	N	652	VAL	CA-CB-CG2	-5.89	102.06	110.90
8	S	118	PHE	N-CA-CB	5.89	121.20	110.60
9	P	357	TYR	CB-CG-CD1	5.89	124.53	121.00
6	Z	894	MET	CG-SD-CE	5.88	109.62	100.20
2	V	114	PHE	CB-CA-C	-5.88	98.63	110.40
13	O	158	ASP	CB-CG-OD1	5.88	123.59	118.30
7	N	55	PHE	CB-CG-CD2	-5.88	116.68	120.80
10	Q	232	TYR	CB-CG-CD2	-5.88	117.47	121.00
9	P	124	VAL	CG1-CB-CG2	-5.87	101.50	110.90
7	N	418	ASP	CB-CA-C	-5.87	98.66	110.40
11	R	392	ARG	NH1-CZ-NH2	-5.87	112.95	119.40
7	N	14	ARG	NE-CZ-NH1	5.87	123.23	120.30
11	R	394	ASP	CB-CG-OD2	5.87	123.58	118.30
10	Q	258	ALA	N-CA-CB	5.86	118.30	110.10
13	O	306	ARG	NE-CZ-NH2	-5.85	117.37	120.30
11	R	49	PHE	N-CA-CB	5.85	121.13	110.60
1	W	28	ALA	N-CA-CB	5.84	118.27	110.10
6	Z	42	ASP	CB-CG-OD1	5.83	123.55	118.30
9	P	257	TRP	CB-CG-CD2	-5.83	119.02	126.60
8	S	399	TYR	CB-CG-CD2	-5.83	117.50	121.00
8	S	158	PHE	CG-CD2-CE2	-5.82	114.39	120.80
6	Z	565	PHE	CB-CA-C	-5.82	98.76	110.40
13	O	161	ASP	CB-CG-OD2	-5.82	113.06	118.30
6	Z	612	GLY	O-C-N	5.82	132.00	122.70
6	Z	815	MET	CG-SD-CE	5.81	109.50	100.20
8	S	309	PHE	CD1-CG-CD2	-5.81	110.74	118.30
6	Z	909	ARG	NE-CZ-NH2	5.81	123.21	120.30
6	Z	889	VAL	CA-CB-CG1	5.81	119.62	110.90
11	R	265	ASP	CB-CG-OD1	-5.80	113.08	118.30
12	U	47	ARG	NE-CZ-NH1	5.80	123.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	88	TYR	CB-CG-CD2	-5.80	117.52	121.00
3	T	250	MET	N-CA-CB	5.80	121.03	110.60
7	N	203	ARG	NE-CZ-NH2	5.79	123.20	120.30
7	N	784	TYR	CB-CG-CD1	-5.79	117.53	121.00
13	O	76	LEU	O-C-N	-5.79	113.44	122.70
8	S	481	TYR	CB-CG-CD1	-5.78	117.53	121.00
7	N	741	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	W	55	ALA	CB-CA-C	-5.77	101.44	110.10
6	Z	96	TYR	CB-CG-CD2	5.77	124.46	121.00
12	U	246	GLU	OE1-CD-OE2	-5.76	116.38	123.30
6	Z	218	GLU	N-CA-CB	5.76	120.97	110.60
2	V	229	ASP	CB-CG-OD2	5.75	123.47	118.30
10	Q	400	TYR	CZ-CE2-CD2	-5.75	114.63	119.80
6	Z	189	ALA	CB-CA-C	-5.75	101.48	110.10
6	Z	476	ASP	CB-CG-OD2	-5.74	113.13	118.30
4	X	10	PHE	CZ-CE2-CD2	-5.74	113.21	120.10
9	P	255	ALA	CB-CA-C	-5.74	101.50	110.10
6	Z	386	VAL	CG1-CB-CG2	5.73	120.07	110.90
3	T	122	PHE	CB-CG-CD1	-5.73	116.79	120.80
12	U	22	TYR	CG-CD2-CE2	5.73	125.88	121.30
10	Q	190	ASN	N-CA-CB	5.72	120.90	110.60
2	V	142	ASP	CB-CG-OD2	-5.72	113.15	118.30
10	Q	380	MET	CG-SD-CE	5.72	109.35	100.20
3	T	179	ASP	CB-CG-OD1	-5.72	113.15	118.30
8	S	317	HIS	CA-CB-CG	5.71	123.32	113.60
11	R	123	ASP	CB-CG-OD2	-5.71	113.16	118.30
9	P	96	MET	CG-SD-CE	5.71	109.34	100.20
13	O	300	VAL	CG1-CB-CG2	-5.71	101.76	110.90
8	S	20	HIS	N-CA-C	5.71	126.40	111.00
13	O	33	TYR	CG-CD2-CE2	-5.70	116.74	121.30
8	S	309	PHE	CG-CD1-CE1	5.70	127.07	120.80
12	U	113	TYR	CZ-CE2-CD2	-5.69	114.68	119.80
13	O	188	PHE	CB-CG-CD1	5.69	124.78	120.80
8	S	83	PRO	C-N-CA	5.69	135.91	121.70
7	N	726	ASP	N-CA-CB	5.68	120.83	110.60
7	N	325	PHE	CB-CG-CD1	-5.68	116.83	120.80
9	P	379	TYR	CG-CD1-CE1	-5.68	116.76	121.30
1	W	32	SER	N-CA-CB	5.68	119.02	110.50
6	Z	295	ARG	CD-NE-CZ	5.68	131.55	123.60
7	N	379	LEU	O-C-N	-5.67	113.62	122.70
10	Q	48	ASP	N-CA-CB	5.67	120.81	110.60
7	N	745	LEU	CB-CG-CD2	5.67	120.64	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	362	TRP	CE3-CZ3-CH2	-5.67	114.97	121.20
8	S	326	ASP	N-CA-CB	5.67	120.80	110.60
6	Z	206	ASP	CB-CG-OD2	-5.66	113.20	118.30
7	N	532	ALA	CB-CA-C	-5.66	101.61	110.10
2	V	251	TYR	CZ-CE2-CD2	5.66	124.89	119.80
6	Z	155	ARG	CD-NE-CZ	5.65	131.52	123.60
6	Z	23	GLN	CB-CG-CD	-5.65	96.92	111.60
6	Z	849	ARG	N-CA-CB	5.65	120.77	110.60
10	Q	323	LYS	CB-CA-C	-5.63	99.13	110.40
13	O	248	TYR	CB-CG-CD1	5.63	124.38	121.00
2	V	230	TYR	CG-CD1-CE1	5.63	125.81	121.30
6	Z	607	ALA	CB-CA-C	-5.63	101.66	110.10
6	Z	900	LEU	CB-CG-CD1	5.63	120.57	111.00
7	N	222	TYR	CB-CG-CD2	-5.63	117.62	121.00
10	Q	20	TYR	CD1-CE1-CZ	5.62	124.86	119.80
9	P	428	THR	N-CA-CB	5.62	120.98	110.30
6	Z	421	SER	N-CA-CB	5.62	118.92	110.50
8	S	302	HIS	CA-CB-CG	-5.62	104.05	113.60
13	O	366	MET	CG-SD-CE	-5.62	91.22	100.20
3	T	127	GLN	N-CA-CB	5.61	120.69	110.60
7	N	771	PHE	CB-CG-CD1	5.60	124.72	120.80
10	Q	243	PHE	CG-CD1-CE1	-5.60	114.64	120.80
6	Z	491	LEU	N-CA-CB	5.60	121.60	110.40
9	P	39	LEU	CB-CG-CD1	5.60	120.52	111.00
6	Z	97	PRO	N-CA-CB	5.59	110.01	103.30
9	P	103	TYR	CB-CG-CD2	-5.59	117.64	121.00
6	Z	151	HIS	CB-CA-C	-5.59	99.22	110.40
8	S	332	PHE	CB-CG-CD1	5.58	124.71	120.80
3	T	22	ALA	N-CA-CB	5.58	117.92	110.10
9	P	361	THR	N-CA-CB	5.58	120.91	110.30
10	Q	318	LEU	CB-CA-C	5.58	120.80	110.20
6	Z	175	ASP	CB-CG-OD1	5.58	123.32	118.30
6	Z	426	TYR	CD1-CE1-CZ	-5.58	114.78	119.80
9	P	273	TYR	CB-CG-CD1	5.58	124.35	121.00
6	Z	798	ARG	NE-CZ-NH1	5.57	123.09	120.30
10	Q	189	ARG	NE-CZ-NH2	-5.57	117.51	120.30
13	O	160	LYS	N-CA-CB	5.57	120.63	110.60
6	Z	339	PHE	CB-CG-CD1	5.57	124.70	120.80
7	N	339	MET	CG-SD-CE	-5.57	91.30	100.20
13	O	373	TRP	CB-CA-C	-5.57	99.27	110.40
6	Z	118	VAL	CA-CB-CG1	5.56	119.25	110.90
7	N	549	TYR	CB-CG-CD1	5.56	124.34	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	353	LEU	CB-CG-CD1	5.56	120.45	111.00
6	Z	564	ARG	NE-CZ-NH1	5.55	123.08	120.30
8	S	186	TYR	CG-CD2-CE2	-5.55	116.86	121.30
7	N	471	TYR	CB-CG-CD2	5.55	124.33	121.00
7	N	526	TYR	CD1-CG-CD2	5.55	124.00	117.90
12	U	43	SER	N-CA-CB	5.55	118.82	110.50
8	S	275	TYR	CB-CG-CD1	-5.54	117.67	121.00
12	U	137	TYR	CG-CD1-CE1	-5.54	116.86	121.30
13	O	300	VAL	CA-CB-CG1	5.54	119.21	110.90
1	W	170	HIS	CB-CA-C	-5.54	99.32	110.40
7	N	651	PHE	CB-CG-CD1	5.54	124.68	120.80
12	U	66	TRP	CG-CD2-CE3	-5.54	128.92	133.90
7	N	84	ALA	CB-CA-C	-5.53	101.80	110.10
6	Z	272	TYR	CG-CD1-CE1	5.53	125.73	121.30
5	Y	37	ASP	CB-CG-OD2	-5.53	113.33	118.30
6	Z	129	ASN	C-N-CA	5.53	133.91	122.30
13	O	32	PHE	CB-CG-CD2	5.53	124.67	120.80
7	N	161	TYR	CB-CG-CD2	-5.53	117.68	121.00
6	Z	889	VAL	CA-CB-CG2	-5.52	102.62	110.90
7	N	322	ASP	CB-CG-OD1	-5.52	113.33	118.30
6	Z	293	MET	CG-SD-CE	-5.52	91.37	100.20
11	R	120	LEU	N-CA-CB	5.52	121.44	110.40
6	Z	58	GLU	CB-CA-C	-5.52	99.37	110.40
6	Z	167	ASP	CB-CG-OD1	-5.51	113.34	118.30
12	U	66	TRP	CB-CG-CD2	-5.51	119.43	126.60
2	V	203	TYR	CA-CB-CG	-5.51	102.93	113.40
11	R	281	SER	N-CA-CB	5.51	118.76	110.50
13	O	215	TYR	CZ-CE2-CD2	-5.51	114.84	119.80
13	O	58	ARG	NH1-CZ-NH2	5.51	125.46	119.40
10	Q	246	TYR	CG-CD2-CE2	5.50	125.70	121.30
11	R	367	ASP	CB-CG-OD1	5.50	123.25	118.30
7	N	412	TYR	CZ-CE2-CD2	-5.50	114.85	119.80
11	R	259	PHE	CB-CG-CD1	5.50	124.65	120.80
6	Z	265	LEU	CB-CA-C	-5.50	99.76	110.20
6	Z	530	LEU	O-C-N	-5.49	113.91	122.70
6	Z	963	ALA	CB-CA-C	-5.49	101.87	110.10
8	S	55	ARG	NE-CZ-NH1	-5.49	117.56	120.30
9	P	273	TYR	CG-CD1-CE1	-5.49	116.91	121.30
7	N	433	THR	N-CA-CB	5.49	120.73	110.30
12	U	277	TYR	CG-CD2-CE2	-5.49	116.91	121.30
8	S	421	TYR	CB-CA-C	-5.48	99.43	110.40
6	Z	356	ASP	CB-CG-OD1	5.48	123.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	182	LYS	CA-C-N	5.48	129.25	117.20
7	N	412	TYR	CB-CG-CD2	-5.48	117.71	121.00
6	Z	349	THR	CA-CB-CG2	-5.48	104.73	112.40
1	W	9	VAL	CA-CB-CG1	5.47	119.11	110.90
7	N	591	LEU	CB-CG-CD1	5.47	120.30	111.00
2	V	251	TYR	CB-CG-CD2	-5.47	117.72	121.00
9	P	68	SER	N-CA-CB	5.47	118.71	110.50
10	Q	209	TYR	CB-CG-CD1	5.47	124.28	121.00
8	S	318	CYS	N-CA-CB	5.47	120.44	110.60
9	P	326	ASP	CB-CG-OD1	5.46	123.22	118.30
7	N	762	ARG	NE-CZ-NH1	5.46	123.03	120.30
7	N	461	GLU	OE1-CD-OE2	5.46	129.85	123.30
8	S	467	PHE	CB-CG-CD2	-5.46	116.98	120.80
4	X	41	GLU	OE1-CD-OE2	5.45	129.84	123.30
1	W	152	GLU	OE1-CD-OE2	5.45	129.84	123.30
2	V	138	ALA	CB-CA-C	-5.45	101.92	110.10
3	T	73	PHE	CB-CG-CD2	5.45	124.61	120.80
6	Z	619	ASP	CB-CG-OD2	-5.45	113.40	118.30
11	R	181	TYR	CA-CB-CG	-5.45	103.06	113.40
9	P	19	GLU	OE1-CD-OE2	5.44	129.83	123.30
7	N	739	PHE	CG-CD1-CE1	-5.44	114.81	120.80
13	O	288	ARG	NE-CZ-NH1	5.44	123.02	120.30
11	R	298	ALA	O-C-N	-5.44	114.00	122.70
10	Q	214	THR	CA-CB-CG2	-5.43	104.79	112.40
7	N	740	TRP	CH2-CZ2-CE2	5.43	122.83	117.40
6	Z	467	VAL	CA-CB-CG2	-5.43	102.75	110.90
6	Z	838	TYR	CB-CG-CD1	5.43	124.26	121.00
12	U	117	ASN	CA-CB-CG	-5.43	101.46	113.40
13	O	181	PHE	CB-CA-C	-5.42	99.55	110.40
10	Q	169	ASP	C-N-CA	5.42	135.24	121.70
3	T	227	PRO	CA-N-CD	5.42	119.28	111.70
10	Q	127	ARG	NE-CZ-NH2	-5.41	117.59	120.30
10	Q	232	TYR	CG-CD2-CE2	-5.41	116.97	121.30
6	Z	901	PHE	CB-CG-CD1	-5.41	117.01	120.80
7	N	95	SER	N-CA-CB	5.41	118.61	110.50
13	O	11	LEU	CB-CG-CD1	5.41	120.19	111.00
13	O	373	TRP	CB-CG-CD2	-5.41	119.57	126.60
9	P	299	LEU	CB-CG-CD1	5.40	120.19	111.00
4	X	41	GLU	N-CA-CB	5.40	120.32	110.60
12	U	288	PHE	CB-CG-CD2	5.40	124.58	120.80
13	O	340	SER	N-CA-CB	5.40	118.60	110.50
9	P	240	TYR	CB-CG-CD2	-5.40	117.76	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	108	TYR	CG-CD1-CE1	-5.39	116.98	121.30
13	O	191	THR	CA-CB-CG2	-5.39	104.85	112.40
4	X	96	ARG	NE-CZ-NH1	5.39	123.00	120.30
7	N	753	PHE	CB-CG-CD2	5.39	124.57	120.80
10	Q	333	SER	N-CA-CB	5.39	118.58	110.50
8	S	82	TYR	CD1-CG-CD2	-5.38	111.98	117.90
3	T	89	TYR	CG-CD1-CE1	-5.38	117.00	121.30
9	P	183	GLN	CB-CA-C	-5.38	99.65	110.40
10	Q	113	ASP	CB-CG-OD2	-5.38	113.46	118.30
11	R	28	GLU	OE1-CD-OE2	5.37	129.75	123.30
11	R	414	LEU	CA-CB-CG	-5.37	102.94	115.30
10	Q	429	LYS	O-C-N	-5.37	114.11	122.70
6	Z	15	GLN	CG-CD-OE1	-5.37	110.86	121.60
4	X	60	GLU	OE1-CD-OE2	-5.37	116.86	123.30
11	R	99	TYR	CA-CB-CG	-5.37	103.20	113.40
12	U	277	TYR	CZ-CE2-CD2	5.37	124.63	119.80
6	Z	60	ASP	N-CA-CB	5.36	120.26	110.60
11	R	315	VAL	CG1-CB-CG2	-5.36	102.32	110.90
6	Z	397	ASP	CB-CG-OD1	5.36	123.12	118.30
10	Q	264	TYR	CG-CD2-CE2	-5.36	117.01	121.30
8	S	403	SER	N-CA-CB	5.36	118.53	110.50
8	S	286	TYR	CD1-CE1-CZ	5.35	124.61	119.80
11	R	382	ASP	CB-CA-C	-5.35	99.70	110.40
6	Z	323	TYR	CB-CG-CD1	-5.35	117.79	121.00
3	T	177	PHE	CB-CG-CD1	-5.34	117.06	120.80
6	Z	428	TRP	CG-CD2-CE3	-5.34	129.09	133.90
12	U	34	VAL	CA-CB-CG1	5.34	118.92	110.90
3	T	93	ASN	C-N-CA	5.34	135.05	121.70
3	T	164	LEU	CB-CA-C	-5.34	100.06	110.20
8	S	431	VAL	CA-CB-CG2	-5.34	102.89	110.90
6	Z	112	LYS	CA-CB-CG	5.33	125.13	113.40
6	Z	269	TYR	CD1-CE1-CZ	-5.33	115.00	119.80
7	N	282	TYR	CZ-CE2-CD2	5.33	124.60	119.80
7	N	335	ALA	CB-CA-C	-5.33	102.10	110.10
7	N	880	ARG	CB-CG-CD	5.33	125.46	111.60
12	U	48	VAL	CA-CB-CG1	-5.33	102.91	110.90
1	W	31	ASP	CB-CG-OD2	5.32	123.09	118.30
6	Z	299	ASP	CB-CG-OD2	-5.32	113.51	118.30
2	V	233	LYS	CB-CA-C	-5.31	99.77	110.40
6	Z	316	ALA	N-CA-CB	5.31	117.53	110.10
8	S	425	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	W	140	ASP	CB-CA-C	-5.31	99.78	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	114	LEU	CB-CG-CD2	5.31	120.02	111.00
5	Y	89	GLN	CA-C-O	-5.30	108.96	120.10
7	N	630	ALA	CB-CA-C	-5.30	102.14	110.10
13	O	41	LEU	CB-CG-CD1	5.30	120.02	111.00
7	N	362	TRP	CZ3-CH2-CZ2	5.30	127.96	121.60
3	T	197	TYR	CB-CG-CD1	-5.29	117.82	121.00
6	Z	269	TYR	CD1-CG-CD2	5.29	123.72	117.90
11	R	301	TYR	CB-CG-CD2	-5.29	117.83	121.00
8	S	492	LYS	CA-C-O	-5.29	108.99	120.10
2	V	73	GLN	CB-CA-C	-5.29	99.82	110.40
6	Z	145	ASP	N-CA-CB	5.29	120.12	110.60
13	O	187	SER	CB-CA-C	-5.29	100.05	110.10
11	R	424	THR	CA-C-O	-5.29	109.00	120.10
10	Q	434	TYR	CA-C-O	-5.29	109.00	120.10
13	O	393	VAL	CA-C-O	-5.29	109.00	120.10
4	X	133	SER	CA-C-O	-5.28	109.01	120.10
3	T	174	PHE	CB-CA-C	-5.28	99.84	110.40
7	N	925	ASP	CA-C-O	-5.28	109.01	120.10
7	N	255	ALA	N-CA-CB	5.28	117.49	110.10
9	P	440	HIS	CA-C-O	-5.28	109.01	120.10
7	N	699	ALA	CB-CA-C	-5.28	102.18	110.10
8	S	111	ARG	NE-CZ-NH2	5.28	122.94	120.30
13	O	213	LEU	CB-CG-CD2	5.28	119.97	111.00
8	S	428	ARG	NH1-CZ-NH2	5.27	125.20	119.40
1	W	197	SER	CA-C-O	-5.27	109.03	120.10
1	W	101	ARG	CA-CB-CG	5.27	124.99	113.40
2	V	306	LYS	CA-C-O	-5.27	109.03	120.10
7	N	541	ALA	CB-CA-C	-5.27	102.20	110.10
6	Z	792	VAL	CA-CB-CG1	5.27	118.80	110.90
7	N	618	ARG	O-C-N	-5.27	114.27	122.70
10	Q	69	GLY	CA-C-O	5.27	130.08	120.60
9	P	220	TYR	CG-CD1-CE1	-5.27	117.09	121.30
13	O	164	PRO	CA-N-CD	5.26	119.07	111.70
3	T	272	ASN	CA-C-O	-5.26	109.06	120.10
3	T	207	ALA	N-CA-CB	5.26	117.46	110.10
10	Q	110	SER	O-C-N	5.25	131.11	122.70
13	O	147	ARG	CA-CB-CG	5.25	124.96	113.40
3	T	136	LEU	CB-CG-CD2	-5.25	102.07	111.00
8	S	275	TYR	CB-CG-CD2	5.25	124.15	121.00
11	R	297	TYR	CB-CG-CD2	-5.25	117.85	121.00
6	Z	868	ASN	CB-CA-C	-5.25	99.91	110.40
6	Z	893	PHE	CG-CD1-CE1	-5.24	115.03	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	252	TYR	CB-CA-C	-5.24	99.91	110.40
13	O	9	THR	N-CA-CB	5.24	120.26	110.30
13	O	180	LYS	CB-CA-C	-5.24	99.91	110.40
6	Z	757	SER	N-CA-CB	5.24	118.36	110.50
7	N	120	ASP	CB-CG-OD1	-5.23	113.59	118.30
11	R	171	MET	CG-SD-CE	-5.23	91.84	100.20
7	N	326	SER	N-CA-CB	5.22	118.34	110.50
13	O	307	MET	CG-SD-CE	-5.22	91.84	100.20
8	S	399	TYR	CG-CD1-CE1	5.22	125.48	121.30
12	U	53	ALA	CB-CA-C	-5.22	102.27	110.10
8	S	257	LEU	CB-CG-CD2	-5.22	102.13	111.00
7	N	429	GLU	N-CA-CB	5.21	119.98	110.60
12	U	49	THR	CA-CB-CG2	-5.21	105.11	112.40
8	S	150	LYS	N-CA-CB	5.21	119.97	110.60
11	R	213	TYR	CB-CG-CD1	-5.21	117.88	121.00
12	U	66	TRP	CB-CG-CD1	5.21	133.77	127.00
12	U	163	ALA	N-CA-CB	5.21	117.39	110.10
6	Z	145	ASP	CB-CG-OD2	5.20	122.98	118.30
7	N	526	TYR	CG-CD1-CE1	-5.20	117.14	121.30
9	P	248	ASP	CB-CG-OD1	-5.20	113.62	118.30
10	Q	162	LEU	CB-CA-C	5.20	120.08	110.20
9	P	18	LYS	N-CA-CB	5.20	119.96	110.60
11	R	24	TYR	CG-CD1-CE1	5.20	125.46	121.30
11	R	345	TYR	CB-CG-CD2	5.19	124.11	121.00
3	T	247	ASP	CB-CG-OD2	-5.19	113.63	118.30
4	X	50	TRP	CB-CG-CD2	-5.19	119.85	126.60
12	U	210	TYR	CB-CG-CD1	5.19	124.11	121.00
6	Z	200	THR	CA-CB-CG2	-5.19	105.14	112.40
6	Z	408	TYR	CG-CD2-CE2	5.19	125.45	121.30
8	S	472	HIS	N-CA-CB	5.18	119.93	110.60
10	Q	51	ARG	N-CA-CB	5.18	119.93	110.60
10	Q	238	TYR	CB-CG-CD1	-5.18	117.89	121.00
6	Z	837	TYR	CB-CG-CD2	-5.18	117.89	121.00
6	Z	823	ASN	CB-CG-OD1	-5.17	111.25	121.60
4	X	7	VAL	CG1-CB-CG2	-5.17	102.62	110.90
4	X	103	GLU	CB-CG-CD	-5.17	100.23	114.20
6	Z	164	VAL	O-C-N	-5.17	114.43	122.70
7	N	747	HIS	CB-CA-C	-5.17	100.06	110.40
7	N	647	ASP	CB-CG-OD2	-5.17	113.65	118.30
8	S	202	ASN	N-CA-CB	5.17	119.90	110.60
6	Z	195	PHE	CB-CG-CD1	5.16	124.41	120.80
8	S	72	GLU	C-N-CA	5.16	134.60	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	30	ASN	CA-CB-CG	-5.16	102.05	113.40
7	N	51	ASP	N-CA-CB	5.16	119.88	110.60
11	R	186	TYR	CG-CD2-CE2	-5.16	117.17	121.30
12	U	183	ALA	CB-CA-C	5.16	117.84	110.10
6	Z	340	LEU	N-CA-C	-5.15	97.09	111.00
6	Z	813	PHE	CB-CG-CD2	-5.15	117.19	120.80
6	Z	243	GLN	CG-CD-OE1	-5.15	111.30	121.60
7	N	742	TRP	CE2-CD2-CE3	5.15	124.88	118.70
2	V	114	PHE	N-CA-CB	5.14	119.86	110.60
13	O	142	ASP	N-CA-C	-5.14	97.11	111.00
6	Z	967	THR	CA-C-N	-5.14	105.89	117.20
9	P	329	PHE	CB-CG-CD2	-5.14	117.20	120.80
10	Q	339	TYR	CZ-CE2-CD2	5.14	124.43	119.80
6	Z	193	PHE	CB-CG-CD1	-5.14	117.20	120.80
2	V	69	PHE	N-CA-CB	5.13	119.84	110.60
13	O	62	TYR	CB-CG-CD2	-5.13	117.92	121.00
13	O	63	ASP	CB-CG-OD2	-5.13	113.68	118.30
7	N	356	LEU	CB-CG-CD2	-5.13	102.28	111.00
7	N	866	TYR	CD1-CE1-CZ	5.13	124.42	119.80
12	U	154	PHE	CB-CG-CD2	5.13	124.39	120.80
2	V	199	LEU	CB-CA-C	-5.12	100.46	110.20
7	N	740	TRP	CZ3-CH2-CZ2	-5.12	115.45	121.60
8	S	275	TYR	CG-CD1-CE1	5.12	125.39	121.30
6	Z	924	LYS	O-C-N	-5.11	114.52	122.70
6	Z	406	TRP	CG-CD2-CE3	-5.11	129.30	133.90
8	S	64	ARG	NE-CZ-NH2	-5.11	117.74	120.30
8	S	114	TYR	CB-CG-CD2	-5.11	117.93	121.00
8	S	350	LYS	N-CA-CB	5.11	119.80	110.60
13	O	317	THR	CA-CB-CG2	-5.11	105.25	112.40
6	Z	199	ASP	CB-CG-OD1	-5.11	113.70	118.30
3	T	199	PHE	CB-CG-CD2	-5.11	117.23	120.80
7	N	269	LEU	CB-CG-CD2	5.11	119.68	111.00
6	Z	219	ASP	CB-CG-OD2	5.10	122.89	118.30
11	R	351	LYS	CB-CG-CD	5.10	124.87	111.60
7	N	328	PHE	CB-CG-CD1	5.10	124.37	120.80
7	N	756	THR	N-CA-CB	5.10	119.99	110.30
8	S	348	LEU	CB-CG-CD2	5.10	119.67	111.00
12	U	32	ARG	NE-CZ-NH2	-5.10	117.75	120.30
6	Z	882	LEU	CB-CG-CD1	-5.10	102.34	111.00
10	Q	81	SER	N-CA-CB	5.09	118.14	110.50
10	Q	225	LEU	CB-CG-CD1	5.09	119.66	111.00
12	U	229	LEU	CB-CA-C	-5.09	100.52	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	76	ASN	O-C-N	5.09	130.85	122.70
8	S	188	TYR	CB-CG-CD1	-5.09	117.95	121.00
1	W	187	SER	CB-CA-C	-5.09	100.43	110.10
6	Z	363	ASP	CB-CG-OD2	-5.08	113.73	118.30
8	S	456	ASP	CB-CG-OD2	-5.08	113.73	118.30
11	R	421	VAL	CG1-CB-CG2	5.07	119.02	110.90
8	S	284	LEU	N-CA-CB	5.07	120.54	110.40
2	V	94	MET	CA-CB-CG	5.07	121.92	113.30
11	R	263	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	W	65	PHE	CB-CG-CD2	-5.07	117.25	120.80
12	U	27	THR	CA-CB-CG2	-5.07	105.31	112.40
6	Z	155	ARG	NE-CZ-NH1	-5.07	117.77	120.30
8	S	239	ARG	N-CA-CB	5.07	119.72	110.60
2	V	63	VAL	N-CA-CB	5.06	122.64	111.50
6	Z	74	SER	CB-CA-C	-5.06	100.48	110.10
6	Z	341	TYR	CG-CD1-CE1	-5.06	117.25	121.30
12	U	25	THR	N-CA-CB	5.06	119.92	110.30
10	Q	341	THR	CA-CB-CG2	-5.06	105.32	112.40
2	V	72	PRO	CA-N-CD	5.06	118.78	111.70
6	Z	491	LEU	O-C-N	-5.05	114.61	123.20
12	U	52	PHE	CB-CG-CD2	-5.05	117.26	120.80
13	O	69	PHE	CB-CG-CD1	5.05	124.34	120.80
8	S	250	ALA	CB-CA-C	-5.05	102.52	110.10
13	O	352	TRP	N-CA-CB	5.05	119.69	110.60
6	Z	460	SER	N-CA-CB	5.04	118.07	110.50
7	N	905	LEU	CB-CA-C	-5.04	100.62	110.20
9	P	327	LEU	CB-CG-CD2	5.04	119.57	111.00
10	Q	84	TYR	CG-CD1-CE1	-5.04	117.27	121.30
11	R	181	TYR	CD1-CE1-CZ	-5.04	115.26	119.80
3	T	123	HIS	CA-CB-CG	-5.04	105.03	113.60
8	S	452	TYR	CB-CG-CD1	5.04	124.02	121.00
13	O	286	PHE	N-CA-CB	5.04	119.66	110.60
3	T	143	SER	N-CA-CB	-5.03	102.96	110.50
7	N	786	ARG	NE-CZ-NH2	5.03	122.81	120.30
7	N	363	ALA	N-CA-CB	5.03	117.14	110.10
12	U	145	ASP	N-CA-CB	5.03	119.65	110.60
6	Z	799	PHE	CB-CG-CD2	-5.02	117.28	120.80
6	Z	522	THR	CA-CB-CG2	-5.02	105.37	112.40
6	Z	119	LEU	CB-CG-CD2	-5.02	102.47	111.00
6	Z	52	LEU	CB-CG-CD2	5.01	119.52	111.00
9	P	395	ARG	CA-C-N	5.01	131.13	117.10
10	Q	113	ASP	CB-CG-OD1	5.01	122.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	109	TYR	CG-CD1-CE1	-5.01	117.29	121.30
8	S	52	TYR	CZ-CE2-CD2	5.01	124.31	119.80
1	W	88	ALA	CB-CA-C	-5.00	102.59	110.10

There are no chirality outliers.

All (123) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	N	123	PHE	Sidechain
7	N	139	ARG	Sidechain
7	N	188	TYR	Sidechain
7	N	298	TYR	Sidechain
7	N	328	PHE	Sidechain
7	N	398	ARG	Sidechain
7	N	417	ARG	Sidechain
7	N	471	TYR	Sidechain
7	N	50	TYR	Sidechain
7	N	502	PHE	Sidechain
7	N	504	TYR	Sidechain
7	N	510	HIS	Sidechain
7	N	58	ARG	Sidechain
7	N	584	ARG	Sidechain
7	N	585	ARG	Sidechain
7	N	593	PHE	Sidechain
7	N	599	TYR	Sidechain
7	N	618	ARG	Sidechain
7	N	70	TYR	Sidechain
7	N	743	PHE	Sidechain
7	N	813	ARG	Sidechain
7	N	873	ARG	Sidechain
7	N	98	VAL	Peptide
13	O	228	TYR	Sidechain
13	O	248	TYR	Sidechain
13	O	252	PHE	Sidechain
13	O	310	PHE	Sidechain
13	O	356	ARG	Sidechain
13	O	58	ARG	Sidechain
13	O	60	ARG	Sidechain
13	O	62	TYR	Sidechain
13	O	70	TYR	Sidechain
13	O	81	TYR	Sidechain
13	O	98	TYR	Sidechain

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Mol	Chain	Res	Type	Group
9	P	115	ARG	Sidechain
9	P	201	ARG	Sidechain
9	P	234	TYR	Sidechain
9	P	240	TYR	Sidechain
9	P	273	TYR	Sidechain
9	P	310	ARG	Sidechain
9	P	351	ARG	Sidechain
9	P	79	LEU	Mainchain
10	Q	104	PHE	Sidechain
10	Q	127	ARG	Sidechain
10	Q	151	TYR	Sidechain
10	Q	161	LEU	Mainchain,Peptide
10	Q	163	ARG	Sidechain
10	Q	185	TYR	Sidechain
10	Q	20	TYR	Sidechain
10	Q	202	ARG	Sidechain
10	Q	255	TYR	Sidechain
10	Q	291	TYR	Sidechain
10	Q	294	ARG	Sidechain
10	Q	306	TYR	Sidechain
10	Q	309	ARG	Sidechain
10	Q	354	PHE	Peptide
10	Q	387	TYR	Sidechain
10	Q	400	TYR	Sidechain
10	Q	409	TYR	Sidechain
10	Q	84	TYR	Sidechain
11	R	123	ASP	Peptide
11	R	186	TYR	Sidechain
11	R	207	ARG	Sidechain
11	R	210	TYR	Sidechain
11	R	305	PHE	Sidechain
11	R	331	ARG	Sidechain
11	R	334	ARG	Sidechain
11	R	335	ARG	Sidechain
11	R	357	PHE	Sidechain
11	R	417	TYR	Sidechain
11	R	63	TYR	Sidechain
11	R	70	TYR	Sidechain
8	S	119	TYR	Sidechain
8	S	145	PHE	Sidechain
8	S	188	TYR	Sidechain
8	S	197	SER	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
8	S	261	HIS	Peptide
8	S	275	TYR	Sidechain
8	S	377	TYR	Sidechain
8	S	393	ARG	Sidechain
8	S	428	ARG	Sidechain
8	S	452	TYR	Sidechain
8	S	472	HIS	Sidechain
8	S	480	ARG	Sidechain
8	S	82	TYR	Sidechain
3	T	157	TYR	Sidechain
3	T	177	PHE	Sidechain
3	T	211	PHE	Sidechain
3	T	51	TYR	Sidechain
3	T	81	TYR	Sidechain
3	T	89	TYR	Sidechain
12	U	176	ARG	Sidechain
12	U	24	ARG	Sidechain
12	U	32	ARG	Sidechain
12	U	52	PHE	Sidechain
2	V	157	ARG	Sidechain
2	V	171	ARG	Sidechain
2	V	229	ASP	Peptide
2	V	270	TYR	Sidechain
2	V	61	TYR	Sidechain
1	W	122	ARG	Sidechain
1	W	127	ARG	Sidechain
1	W	182	TYR	Sidechain
1	W	23	ARG	Sidechain
1	W	25	ARG	Sidechain
1	W	77	HIS	Sidechain
4	X	51	ARG	Sidechain
4	X	99	PHE	Sidechain
5	Y	86	ARG	Sidechain
6	Z	132	HIS	Sidechain
6	Z	210	TYR	Sidechain
6	Z	269	TYR	Sidechain
6	Z	312	TYR	Sidechain
6	Z	323	TYR	Sidechain
6	Z	385	PHE	Sidechain
6	Z	394	TYR	Sidechain
6	Z	426	TYR	Sidechain
6	Z	477	TYR	Sidechain

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Mol	Chain	Res	Type	Group
6	Z	773	ARG	Sidechain
6	Z	774	ARG	Sidechain
6	Z	849	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	17	0
2	V	2274	0	2272	51	0
3	T	2192	0	2157	12	0
4	X	1032	0	1017	5	0
5	Y	435	0	394	17	0
6	Z	7005	0	6932	85	0
7	N	6882	0	6959	42	0
8	S	3894	0	3937	32	0
9	P	3608	0	3694	15	0
10	Q	3499	0	3524	18	0
11	R	3060	0	3083	12	0
12	U	2373	0	2403	6	0
13	O	3186	0	3213	11	0
All	All	40974	0	41127	301	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 (301) 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)
8:S:127:THR:CB	8:S:127:THR:CA	1.80	1.58
6:Z:30:LYS:CG	6:Z:37:GLN:HB3	1.22	1.55
6:Z:24:THR:HB	6:Z:25:PRO:CD	1.36	1.51
2:V:118:LEU:HB2	2:V:195:HIS:CD2	1.47	1.49
2:V:118:LEU:CB	2:V:195:HIS:NE2	1.80	1.44
5:Y:21:ASN:CG	8:S:55:ARG:NH1	1.68	1.39
6:Z:30:LYS:CG	6:Z:37:GLN:CB	2.03	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:85:VAL:CG1	6:Z:86:PRO:HD3	1.60	1.28
6:Z:30:LYS:CD	6:Z:37:GLN:HB3	1.64	1.26
5:Y:21:ASN:ND2	8:S:55:ARG:CZ	1.99	1.24
6:Z:30:LYS:HG3	6:Z:37:GLN:CB	1.63	1.24
6:Z:85:VAL:HG12	6:Z:86:PRO:CD	1.67	1.24
2:V:118:LEU:HB2	2:V:195:HIS:NE2	0.92	1.23
6:Z:85:VAL:CG1	6:Z:86:PRO:CD	2.18	1.19
7:N:36:TRP:O	7:N:36:TRP:CE3	1.95	1.19
6:Z:85:VAL:CB	6:Z:86:PRO:HD2	1.69	1.17
6:Z:24:THR:CB	6:Z:25:PRO:CD	2.22	1.17
6:Z:85:VAL:CB	6:Z:86:PRO:CD	2.22	1.17
6:Z:30:LYS:HG2	6:Z:37:GLN:HB3	1.23	1.15
7:N:856:PHE:O	7:N:857:TYR:O	1.64	1.14
6:Z:24:THR:HB	6:Z:25:PRO:HD2	1.20	1.14
7:N:708:ALA:HB1	7:N:713:VAL:HG22	1.30	1.13
6:Z:85:VAL:HB	6:Z:86:PRO:CD	1.77	1.13
1:W:126:ILE:HA	1:W:157:PHE:HZ	1.10	1.12
1:W:155:ASP:HB2	1:W:171:LEU:HD22	1.28	1.12
7:N:8:PRO:CB	7:N:8:PRO:CA	2.17	1.10
2:V:118:LEU:HD12	2:V:195:HIS:HD2	1.12	1.10
1:W:126:ILE:HA	1:W:157:PHE:CZ	1.86	1.09
6:Z:30:LYS:HG3	6:Z:37:GLN:CG	1.82	1.09
5:Y:65:ASP:HB2	11:R:331:ARG:CD	1.84	1.08
6:Z:85:VAL:HG12	6:Z:86:PRO:HD3	1.15	1.07
6:Z:24:THR:HB	6:Z:25:PRO:HD3	1.12	1.06
6:Z:282:ILE:HG13	6:Z:318:LYS:HD2	1.38	1.06
6:Z:85:VAL:O	6:Z:88:PRO:HD2	1.55	1.05
2:V:118:LEU:CB	2:V:195:HIS:CD2	2.32	1.04
6:Z:30:LYS:HG3	6:Z:37:GLN:CD	1.78	1.04
2:V:118:LEU:O	2:V:195:HIS:CE1	2.11	1.02
6:Z:282:ILE:HD11	6:Z:297:VAL:CG1	1.89	1.02
6:Z:24:THR:CB	6:Z:25:PRO:HD3	1.84	1.01
7:N:339:MET:HA	7:N:709:GLY:N	1.77	0.99
7:N:708:ALA:CB	7:N:713:VAL:HG22	1.93	0.97
7:N:36:TRP:CD2	7:N:36:TRP:O	2.17	0.97
6:Z:282:ILE:CD1	6:Z:297:VAL:HB	1.95	0.97
5:Y:65:ASP:HB2	11:R:331:ARG:HD3	1.47	0.95
6:Z:85:VAL:HB	6:Z:86:PRO:HD2	0.95	0.94
6:Z:49:LEU:HD21	6:Z:93:ARG:HG2	1.49	0.93
2:V:118:LEU:HD12	2:V:195:HIS:CD2	2.02	0.93
1:W:155:ASP:CB	1:W:171:LEU:HD22	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:118:LEU:CD1	2:V:195:HIS:HD2	1.83	0.92
6:Z:282:ILE:CD1	6:Z:297:VAL:CG1	2.49	0.91
8:S:127:THR:N	8:S:127:THR:CB	2.34	0.91
6:Z:85:VAL:HG12	6:Z:86:PRO:N	1.84	0.90
5:Y:65:ASP:HB2	11:R:331:ARG:HD2	1.51	0.90
7:N:707:ASN:O	7:N:709:GLY:N	2.05	0.88
6:Z:282:ILE:CD1	6:Z:297:VAL:HG11	2.05	0.87
7:N:6:ALA:HB2	7:N:35:LEU:CD1	2.06	0.86
2:V:157:ARG:O	2:V:196:TYR:CA	2.24	0.86
6:Z:282:ILE:CD1	6:Z:297:VAL:CB	2.54	0.85
5:Y:21:ASN:HD21	8:S:55:ARG:CZ	1.77	0.85
2:V:159:ILE:HD11	2:V:196:TYR:O	1.78	0.83
1:W:158:ILE:HG23	1:W:169:SER:HB2	1.61	0.82
2:V:159:ILE:HD11	2:V:196:TYR:CD1	2.15	0.82
7:N:708:ALA:HB1	7:N:713:VAL:CG2	2.10	0.82
2:V:24:LYS:HG3	2:V:196:TYR:CD1	2.14	0.81
6:Z:30:LYS:HD3	6:Z:37:GLN:HB3	1.61	0.81
2:V:157:ARG:H	2:V:196:TYR:HB2	1.46	0.81
5:Y:21:ASN:CG	8:S:55:ARG:CZ	2.45	0.79
2:V:118:LEU:O	2:V:195:HIS:HE1	1.65	0.79
6:Z:282:ILE:HD13	6:Z:297:VAL:CB	2.12	0.78
7:N:6:ALA:HB2	7:N:35:LEU:HD13	1.64	0.78
2:V:157:ARG:O	2:V:196:TYR:CB	2.32	0.76
2:V:24:LYS:HG3	2:V:196:TYR:CE1	2.20	0.76
2:V:158:LEU:HA	2:V:195:HIS:O	1.86	0.76
6:Z:30:LYS:HG2	6:Z:37:GLN:CB	1.91	0.75
11:R:280:ILE:HG13	11:R:281:SER:N	2.01	0.75
2:V:118:LEU:CG	2:V:195:HIS:CD2	2.70	0.75
6:Z:24:THR:CG2	6:Z:25:PRO:HD3	2.16	0.74
6:Z:282:ILE:HD11	6:Z:297:VAL:CB	2.18	0.73
6:Z:30:LYS:CD	6:Z:37:GLN:CB	2.53	0.73
6:Z:282:ILE:HD13	6:Z:297:VAL:HB	1.69	0.71
5:Y:33:ASP:C	5:Y:35:PHE:H	1.93	0.70
13:O:393:VAL:OXT	13:O:393:VAL:HG12	1.90	0.70
8:S:127:THR:HB	8:S:127:THR:CA	2.14	0.69
7:N:6:ALA:HB2	7:N:35:LEU:HD12	1.74	0.69
3:T:84:GLN:OE1	7:N:8:PRO:CB	2.41	0.69
2:V:196:TYR:HD1	2:V:197:TYR:HB3	1.59	0.68
6:Z:93:ARG:HB3	6:Z:94:PRO:CD	2.24	0.68
2:V:196:TYR:HD1	2:V:197:TYR:CB	2.07	0.68
6:Z:49:LEU:CD2	6:Z:93:ARG:HG2	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:84:GLN:NE2	7:N:8:PRO:CB	2.57	0.68
2:V:159:ILE:HD11	2:V:196:TYR:CE1	2.29	0.67
2:V:118:LEU:CD1	2:V:195:HIS:CD2	2.68	0.67
7:N:444:HIS:CD2	7:N:480:ALA:HB2	2.29	0.67
6:Z:30:LYS:HD3	6:Z:37:GLN:CB	2.21	0.67
13:O:32:PHE:HB2	13:O:41:LEU:HD13	1.75	0.67
1:W:155:ASP:HB2	1:W:171:LEU:CD2	2.16	0.67
4:X:18:ASN:HD21	4:X:21:SER:H	1.43	0.66
6:Z:85:VAL:HG11	6:Z:86:PRO:HD3	1.69	0.66
8:S:345:TYR:CD1	8:S:345:TYR:N	2.61	0.65
7:N:35:LEU:C	7:N:37:SER:H	1.98	0.65
5:Y:21:ASN:ND2	8:S:55:ARG:NH1	0.66	0.65
8:S:339:GLN:OE1	8:S:339:GLN:HA	1.96	0.65
6:Z:282:ILE:HD11	6:Z:297:VAL:HB	1.73	0.64
2:V:157:ARG:O	2:V:196:TYR:HB2	1.96	0.64
9:P:93:ILE:HG22	9:P:97:ILE:HG13	1.81	0.63
3:T:84:GLN:OE1	7:N:8:PRO:HB3	1.98	0.63
1:W:126:ILE:CA	1:W:157:PHE:HZ	1.98	0.62
1:W:155:ASP:CG	1:W:171:LEU:HD22	2.20	0.62
3:T:80:ASN:ND2	7:N:11:ALA:O	2.19	0.62
7:N:35:LEU:O	7:N:37:SER:N	2.33	0.62
8:S:127:THR:CB	8:S:127:THR:C	2.65	0.61
6:Z:282:ILE:HD11	6:Z:297:VAL:HG12	1.77	0.61
8:S:127:THR:H	8:S:127:THR:CB	2.12	0.61
11:R:241:ILE:HG23	11:R:241:ILE:O	1.99	0.61
7:N:36:TRP:C	7:N:36:TRP:CD2	2.71	0.61
5:Y:21:ASN:HD22	8:S:55:ARG:HH11	0.61	0.60
13:O:266:PHE:CZ	13:O:270:ILE:HG13	2.35	0.60
8:S:127:THR:N	8:S:127:THR:HB	2.17	0.60
6:Z:93:ARG:HB3	6:Z:94:PRO:HD3	1.83	0.60
5:Y:21:ASN:HD22	8:S:55:ARG:NH1	1.25	0.60
2:V:117:TRP:CH2	2:V:184:ASN:ND2	2.70	0.59
5:Y:33:ASP:C	5:Y:35:PHE:N	2.56	0.59
10:Q:78:ILE:CG2	10:Q:117:VAL:HG21	2.32	0.59
6:Z:509:LEU:HA	6:Z:512:ILE:HD11	1.83	0.59
2:V:157:ARG:O	2:V:196:TYR:HA	2.00	0.59
6:Z:329:ILE:HD13	6:Z:464:ASP:OD1	2.02	0.59
1:W:158:ILE:HG23	1:W:169:SER:CB	2.31	0.59
7:N:447:SER:O	7:N:450:ILE:HG22	2.02	0.58
6:Z:30:LYS:HA	6:Z:37:GLN:OE1	2.03	0.58
6:Z:31:LYS:HD2	6:Z:79:THR:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:393:VAL:OXT	13:O:393:VAL:CG1	2.53	0.56
2:V:118:LEU:CA	2:V:195:HIS:NE2	2.67	0.56
6:Z:24:THR:CB	6:Z:25:PRO:HD2	2.07	0.56
2:V:183:ALA:N	2:V:188:LEU:CD1	2.69	0.56
5:Y:21:ASN:HD21	8:S:55:ARG:NH1	0.65	0.56
10:Q:3:LEU:C	10:Q:3:LEU:HD23	2.26	0.56
6:Z:294:ILE:HD13	6:Z:327:GLN:HG2	1.89	0.55
7:N:707:ASN:C	7:N:709:GLY:N	2.59	0.55
2:V:196:TYR:CD1	2:V:197:TYR:HB3	2.39	0.55
6:Z:282:ILE:HD13	6:Z:297:VAL:CG2	2.37	0.55
7:N:856:PHE:O	7:N:857:TYR:C	2.41	0.55
8:S:164:ILE:HB	8:S:165:PRO:CD	2.37	0.54
8:S:427:ILE:HG22	8:S:427:ILE:O	2.07	0.54
6:Z:85:VAL:O	6:Z:88:PRO:CD	2.43	0.54
6:Z:282:ILE:HD13	6:Z:297:VAL:CG1	2.37	0.54
7:N:708:ALA:CB	7:N:713:VAL:CG2	2.75	0.54
2:V:303:VAL:O	2:V:306:LYS:O	2.24	0.54
10:Q:119:GLU:O	10:Q:122:ILE:HG22	2.07	0.54
8:S:481:TYR:HB2	8:S:482:PRO:HD3	1.89	0.54
12:U:14:VAL:HG21	12:U:48:VAL:HG12	1.90	0.54
6:Z:282:ILE:HD13	6:Z:297:VAL:HG21	1.89	0.54
7:N:707:ASN:C	7:N:709:GLY:H	2.10	0.53
10:Q:71:LYS:HG3	10:Q:73:LYS:H	1.74	0.53
2:V:157:ARG:N	2:V:196:TYR:HB2	2.20	0.53
2:V:159:ILE:CD1	2:V:196:TYR:O	2.55	0.53
1:W:30:ILE:HG23	1:W:76:LEU:HD21	1.89	0.53
6:Z:157:LEU:HB3	6:Z:207:ILE:HD12	1.91	0.53
1:W:126:ILE:CA	1:W:157:PHE:CZ	2.76	0.53
2:V:118:LEU:HB3	2:V:195:HIS:NE2	2.08	0.52
3:T:152:LEU:HD21	3:T:185:ILE:HD12	1.92	0.52
9:P:203:ILE:HG12	9:P:208:PHE:CZ	2.45	0.51
11:R:280:ILE:HG13	11:R:281:SER:H	1.76	0.51
7:N:6:ALA:CB	7:N:35:LEU:HD13	2.39	0.51
3:T:84:GLN:CD	7:N:8:PRO:CB	2.79	0.51
7:N:35:LEU:C	7:N:37:SER:N	2.60	0.51
8:S:123:THR:HG22	8:S:130:VAL:HG22	1.93	0.51
11:R:137:LEU:HB3	11:R:153:THR:HG21	1.91	0.51
6:Z:282:ILE:HD13	6:Z:297:VAL:HG11	1.91	0.51
2:V:250:GLN:HB3	2:V:276:PRO:HB3	1.92	0.51
6:Z:30:LYS:HG2	6:Z:37:GLN:HB2	1.87	0.51
9:P:48:GLN:HE22	9:P:89:LEU:HB3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:945:ILE:CG1	6:Z:965:LEU:HD21	2.41	0.50
8:S:127:THR:H	8:S:127:THR:HB	1.74	0.50
6:Z:9:GLN:HA	6:Z:12:ILE:HD12	1.94	0.50
2:V:143:PRO:HG2	2:V:144:ILE:HG23	1.93	0.50
2:V:183:ALA:C	2:V:188:LEU:HD12	2.32	0.50
7:N:7:ALA:HB3	7:N:8:PRO:HD2	1.94	0.50
10:Q:78:ILE:HG21	10:Q:117:VAL:HG21	1.93	0.50
8:S:345:TYR:H	8:S:345:TYR:HD1	1.51	0.50
6:Z:79:THR:O	6:Z:83:THR:HG23	2.12	0.50
6:Z:161:ILE:HD11	6:Z:207:ILE:HG13	1.95	0.49
5:Y:33:ASP:O	5:Y:35:PHE:N	2.46	0.49
8:S:164:ILE:HB	8:S:165:PRO:HD3	1.94	0.49
1:W:158:ILE:CG2	1:W:169:SER:HB2	2.40	0.49
6:Z:542:ILE:HG12	6:Z:544:THR:H	1.76	0.49
2:V:118:LEU:O	2:V:195:HIS:NE2	2.41	0.49
5:Y:65:ASP:CB	11:R:331:ARG:HD2	2.35	0.49
9:P:94:GLN:N	9:P:94:GLN:OE1	2.42	0.49
9:P:399:ILE:HG21	9:P:401:ASN:HD21	1.77	0.48
8:S:81:LEU:HD22	8:S:123:THR:HB	1.95	0.48
2:V:24:LYS:HG3	2:V:196:TYR:CZ	2.47	0.48
13:O:169:ASN:HD22	13:O:198:THR:HG23	1.78	0.48
6:Z:88:PRO:HA	6:Z:91:PHE:HB2	1.95	0.48
2:V:183:ALA:N	2:V:188:LEU:HD12	2.29	0.48
2:V:193:ASN:HD22	2:V:193:ASN:C	2.17	0.48
2:V:24:LYS:HG3	2:V:196:TYR:CG	2.48	0.48
13:O:41:LEU:O	13:O:45:LEU:CD2	2.62	0.48
2:V:159:ILE:HG12	2:V:196:TYR:CE2	2.48	0.48
2:V:172:GLN:HB3	2:V:196:TYR:OH	2.13	0.48
6:Z:354:PRO:HA	6:Z:357:ILE:HG12	1.96	0.48
6:Z:424:SER:HA	6:Z:457:ILE:HG21	1.94	0.48
7:N:7:ALA:N	7:N:8:PRO:HD2	2.28	0.47
2:V:184:ASN:HB2	2:V:188:LEU:HB2	1.95	0.47
6:Z:20:PRO:HB2	6:Z:24:THR:OG1	2.15	0.47
13:O:291:ILE:HA	13:O:291:ILE:HD13	1.66	0.47
4:X:36:LYS:C	4:X:38:ASN:H	2.17	0.47
2:V:157:ARG:O	2:V:196:TYR:CD2	2.68	0.47
7:N:860:LYS:O	7:N:861:TYR:C	2.54	0.47
7:N:860:LYS:O	7:N:861:TYR:O	2.32	0.47
9:P:349:ASN:O	9:P:353:ILE:HG13	2.15	0.47
10:Q:78:ILE:HG22	10:Q:117:VAL:CG2	2.44	0.47
8:S:399:TYR:CD2	8:S:402:ILE:HD13	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:117:TRP:CH2	2:V:184:ASN:CG	2.88	0.47
7:N:778:LYS:HB2	7:N:860:LYS:O	2.15	0.47
3:T:181:LEU:O	3:T:185:ILE:HG12	2.14	0.47
6:Z:542:ILE:HG23	6:Z:545:SER:H	1.80	0.47
2:V:196:TYR:HB3	2:V:197:TYR:O	2.15	0.46
10:Q:275:ILE:HD12	10:Q:275:ILE:C	2.36	0.46
10:Q:359:ILE:HD11	10:Q:390:LEU:HD21	1.97	0.46
1:W:10:ILE:HG22	1:W:33:VAL:HG22	1.98	0.46
6:Z:81:SER:O	6:Z:82:MET:HB3	2.16	0.46
6:Z:30:LYS:CG	6:Z:37:GLN:HB2	2.28	0.45
6:Z:282:ILE:CG1	6:Z:297:VAL:HG11	2.45	0.45
9:P:266:TYR:CD1	9:P:329:PHE:HE2	2.35	0.45
1:W:154:LEU:H	1:W:154:LEU:HG	1.53	0.45
5:Y:21:ASN:OD1	8:S:55:ARG:NH2	2.50	0.45
6:Z:581:VAL:O	6:Z:581:VAL:HG12	2.17	0.45
11:R:280:ILE:CG1	11:R:281:SER:H	2.30	0.45
5:Y:21:ASN:OD1	8:S:55:ARG:NH1	2.35	0.45
6:Z:945:ILE:HG12	6:Z:965:LEU:HD21	1.99	0.45
13:O:37:LEU:O	13:O:41:LEU:HB2	2.17	0.45
9:P:89:LEU:HG	9:P:90:LYS:H	1.82	0.44
10:Q:130:ARG:HG3	10:Q:133:LEU:H	1.82	0.44
9:P:193:TYR:CD1	9:P:230:HIS:CD2	3.06	0.44
6:Z:535:VAL:HG12	6:Z:536:GLY:N	2.32	0.44
6:Z:614:VAL:O	6:Z:617:ILE:HG12	2.17	0.44
1:W:143:ASN:OD1	1:W:147:ILE:HG23	2.17	0.44
6:Z:298:PHE:CE1	6:Z:315:ALA:HB1	2.53	0.44
6:Z:556:ILE:HD12	6:Z:556:ILE:C	2.38	0.44
3:T:79:GLU:O	3:T:82:PHE:HB3	2.18	0.43
10:Q:3:LEU:HB3	10:Q:4:PRO:HD3	2.00	0.43
8:S:427:ILE:CG2	8:S:427:ILE:O	2.65	0.43
10:Q:11:ALA:HB1	10:Q:27:TYR:CZ	2.54	0.43
9:P:177:ILE:HG12	9:P:203:ILE:CD1	2.48	0.43
2:V:159:ILE:HD11	2:V:196:TYR:CG	2.51	0.43
10:Q:95:LYS:C	10:Q:95:LYS:HD3	2.39	0.43
7:N:861:TYR:CG	7:N:862:SER:N	2.86	0.43
8:S:126:LYS:HD2	8:S:129:GLU:OE2	2.19	0.43
12:U:37:ILE:CG2	12:U:48:VAL:HG13	2.49	0.43
6:Z:701:ILE:HG13	6:Z:702:LYS:N	2.33	0.43
7:N:450:ILE:CG2	7:N:451:GLY:N	2.82	0.43
6:Z:419:VAL:HA	6:Z:422:ILE:HD12	2.01	0.43
7:N:5:THR:O	7:N:8:PRO:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:15:TYR:CE1	13:O:39:PHE:CE2	3.07	0.42
10:Q:264:TYR:CD1	10:Q:264:TYR:N	2.87	0.42
2:V:247:ILE:HG22	2:V:280:LEU:HG	2.01	0.42
6:Z:30:LYS:HB2	6:Z:30:LYS:HE2	1.48	0.42
7:N:707:ASN:O	7:N:708:ALA:C	2.58	0.42
9:P:7:ILE:HG22	9:P:8:LYS:N	2.34	0.42
9:P:93:ILE:O	9:P:96:MET:HB2	2.20	0.42
10:Q:154:SER:O	10:Q:158:ILE:HG13	2.19	0.42
3:T:70:ILE:HD11	3:T:78:PHE:CE1	2.53	0.42
12:U:8:VAL:HG22	12:U:46:ILE:HD12	2.01	0.42
4:X:78:ILE:HG12	4:X:114:LEU:O	2.19	0.42
13:O:41:LEU:HD12	13:O:41:LEU:HA	1.87	0.42
2:V:72:PRO:HA	12:U:83:ILE:HG12	2.01	0.42
2:V:217:HIS:CE1	2:V:219:GLU:C	2.93	0.42
6:Z:451:ALA:O	6:Z:455:ILE:HG13	2.19	0.42
7:N:450:ILE:HG23	7:N:451:GLY:N	2.34	0.42
4:X:77:PRO:C	4:X:78:ILE:HG13	2.40	0.42
13:O:62:TYR:CE1	13:O:82:LEU:HD13	2.55	0.42
7:N:124:TYR:N	7:N:124:TYR:CD1	2.88	0.42
7:N:161:TYR:HA	7:N:202:PHE:CZ	2.54	0.42
10:Q:66:VAL:HG12	10:Q:66:VAL:O	2.20	0.41
10:Q:3:LEU:HD22	10:Q:33:LYS:HG2	2.02	0.41
8:S:78:VAL:HA	8:S:105:PRO:HA	2.02	0.41
9:P:433:ILE:HD13	12:U:210:TYR:HB2	2.01	0.41
6:Z:471:LEU:HD13	6:Z:471:LEU:C	2.41	0.41
7:N:523:LEU:HA	7:N:557:LEU:HD13	2.02	0.41
10:Q:129:LYS:HB3	10:Q:130:ARG:H	1.74	0.41
4:X:64:ILE:HG12	4:X:65:SER:N	2.36	0.41
11:R:198:ILE:CG2	11:R:207:ARG:HG3	2.51	0.41
3:T:205:ILE:HG22	3:T:217:THR:HG21	2.03	0.41
2:V:193:ASN:C	2:V:193:ASN:ND2	2.73	0.41
9:P:177:ILE:HG12	9:P:203:ILE:HD13	2.02	0.41
6:Z:282:ILE:HG12	6:Z:297:VAL:HG11	2.02	0.41
11:R:198:ILE:HG23	11:R:207:ARG:HG3	2.03	0.41
3:T:31:LYS:HZ1	3:T:81:TYR:HE1	1.66	0.41
12:U:37:ILE:HG23	12:U:48:VAL:CG1	2.51	0.41
1:W:26:PHE:O	1:W:30:ILE:HG13	2.21	0.41
10:Q:129:LYS:N	10:Q:129:LYS:HD2	2.36	0.40
8:S:81:LEU:HD12	8:S:81:LEU:HA	1.93	0.40
3:T:70:ILE:HD11	3:T:78:PHE:CZ	2.56	0.40
6:Z:31:LYS:HE2	6:Z:31:LYS:HB2	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:88:PRO:O	6:Z:92:LEU:HG	2.21	0.40
6:Z:945:ILE:HG13	6:Z:965:LEU:HD21	2.04	0.40
11:R:387:ILE:HG22	11:R:388:VAL:N	2.36	0.40
6:Z:354:PRO:O	6:Z:357:ILE:HG12	2.21	0.40
7:N:7:ALA:N	7:N:8:PRO:CD	2.84	0.40
9:P:48:GLN:NE2	9:P:89:LEU:HD23	2.36	0.40
8:S:119:TYR:O	8:S:123:THR:HG23	2.21	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%)	175 (90%)	13 (7%)	7 (4%)	4	36
2	V	287/306 (94%)	262 (91%)	15 (5%)	10 (4%)	4	36
3	T	264/274 (96%)	240 (91%)	20 (8%)	4 (2%)	12	53
4	X	125/156 (80%)	105 (84%)	19 (15%)	1 (1%)	22	65
5	Y	47/89 (53%)	39 (83%)	6 (13%)	2 (4%)	3	31
6	Z	902/993 (91%)	813 (90%)	66 (7%)	23 (2%)	6	43
7	N	886/945 (94%)	842 (95%)	31 (4%)	13 (2%)	12	53
8	S	473/523 (90%)	441 (93%)	17 (4%)	15 (3%)	5	38
9	P	438/445 (98%)	405 (92%)	22 (5%)	11 (2%)	6	43
10	Q	432/434 (100%)	392 (91%)	32 (7%)	8 (2%)	9	49
11	R	377/429 (88%)	353 (94%)	16 (4%)	8 (2%)	8	47
12	U	296/338 (88%)	282 (95%)	12 (4%)	2 (1%)	25	67
13	O	386/393 (98%)	366 (95%)	17 (4%)	3 (1%)	22	65
All	All	5108/5593 (91%)	4715 (92%)	286 (6%)	107 (2%)	12	47

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	184	ASN
2	V	197	TYR
2	V	274	GLN
4	X	116	ALA
6	Z	24	THR
6	Z	82	MET
6	Z	85	VAL
7	N	36	TRP
7	N	708	ALA
7	N	857	TYR
8	S	47	THR
8	S	102	SER
8	S	150	LYS
8	S	449	LEU
9	P	126	THR
9	P	397	ALA
10	Q	75	ARG
10	Q	170	ASP
1	W	13	SER
1	W	144	PHE
1	W	149	GLN
1	W	165	GLN
3	T	94	HIS
3	T	173	GLU
6	Z	142	ASP
6	Z	233	LEU
6	Z	802	ASP
6	Z	870	ALA
7	N	123	PHE
7	N	345	ASP
7	N	378	ASN
7	N	436	ASP
7	N	861	TYR
7	N	895	LYS
8	S	44	THR
8	S	118	PHE
8	S	132	ALA
8	S	153	GLU
8	S	433	GLU
9	P	89	LEU
9	P	327	LEU
10	Q	253	ASN

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Mol	Chain	Res	Type
11	R	238	PHE
11	R	393	PRO
1	W	3	LEU
2	V	185	ILE
2	V	262	THR
5	Y	70	ASP
6	Z	377	ALA
6	Z	513	ALA
6	Z	578	GLY
6	Z	887	GLY
6	Z	926	ASN
6	Z	940	GLY
6	Z	947	GLY
7	N	33	ASP
7	N	765	ASP
7	N	858	LYS
8	S	83	PRO
8	S	84	ASP
8	S	258	GLU
9	P	6	PRO
9	P	7	ILE
10	Q	18	LYS
10	Q	42	ALA
10	Q	51	ARG
10	Q	110	SER
11	R	124	ASP
13	O	226	LYS
1	W	179	ARG
2	V	143	PRO
2	V	196	TYR
2	V	257	GLU
5	Y	34	GLU
6	Z	25	PRO
6	Z	237	VAL
6	Z	366	LYS
6	Z	557	GLU
6	Z	825	ALA
7	N	859	ASN
8	S	65	ASN
8	S	97	THR
9	P	85	LYS
9	P	150	GLU

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Mol	Chain	Res	Type
9	P	171	MET
11	R	280	ILE
11	R	375	LYS
11	R	395	ASN
12	U	41	ALA
13	O	346	GLU
1	W	190	ILE
2	V	78	VAL
3	T	132	HIS
3	T	257	THR
6	Z	65	GLU
6	Z	463	HIS
9	P	92	SER
10	Q	387	TYR
11	R	376	GLN
12	U	150	THR
6	Z	728	LYS
11	R	106	ASN
2	V	112	PRO
6	Z	86	PRO
8	S	96	ILE
9	P	132	VAL
13	O	205	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%)	165 (96%)	6 (4%)	41	72
2	V	253/268 (94%)	242 (96%)	11 (4%)	33	68
3	T	249/256 (97%)	239 (96%)	10 (4%)	36	69
4	X	116/144 (81%)	112 (97%)	4 (3%)	42	73
5	Y	50/81 (62%)	48 (96%)	2 (4%)	36	69
6	Z	773/850 (91%)	745 (96%)	28 (4%)	40	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	N	745/797 (94%)	724 (97%)	21 (3%)	49	76
8	S	447/489 (91%)	436 (98%)	11 (2%)	53	78
9	P	412/415 (99%)	402 (98%)	10 (2%)	54	79
10	Q	391/391 (100%)	382 (98%)	9 (2%)	56	80
11	R	333/379 (88%)	325 (98%)	8 (2%)	54	79
12	U	271/308 (88%)	269 (99%)	2 (1%)	87	94
13	O	363/368 (99%)	349 (96%)	14 (4%)	37	70
All	All	4574/4976 (92%)	4438 (97%)	136 (3%)	50	74

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	3	LEU
1	W	59	PRO
1	W	139	VAL
1	W	154	LEU
1	W	157	PHE
1	W	183	GLU
2	V	71	MET
2	V	109	HIS
2	V	117	TRP
2	V	173	THR
2	V	185	ILE
2	V	190	HIS
2	V	192	LEU
2	V	193	ASN
2	V	199	LEU
2	V	219	GLU
2	V	227	MET
3	T	34	LEU
3	T	58	THR
3	T	76	ASP
3	T	79	GLU
3	T	82	PHE
3	T	85	LEU
3	T	130	ASP
3	T	197	TYR
3	T	214	GLU
3	T	249	MET
4	X	14	VAL

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Mol	Chain	Res	Type
4	X	28	PRO
4	X	62	ASP
4	X	122	TYR
5	Y	66	ASP
5	Y	72	ASP
6	Z	27	LYS
6	Z	29	ASP
6	Z	30	LYS
6	Z	81	SER
6	Z	93	ARG
6	Z	171	LYS
6	Z	185	ASP
6	Z	187	SER
6	Z	222	ASP
6	Z	236	PHE
6	Z	354	PRO
6	Z	402	ASP
6	Z	411	LYS
6	Z	434	GLN
6	Z	445	PRO
6	Z	548	ASP
6	Z	557	GLU
6	Z	563	VAL
6	Z	566	LEU
6	Z	609	THR
6	Z	703	SER
6	Z	756	MET
6	Z	767	TYR
6	Z	797	THR
6	Z	842	GLN
6	Z	874	ASN
6	Z	878	LEU
6	Z	910	PRO
7	N	105	SER
7	N	124	TYR
7	N	219	ASN
7	N	282	TYR
7	N	318	LYS
7	N	378	ASN
7	N	381	GLU
7	N	394	ARG
7	N	412	TYR

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Mol	Chain	Res	Type
7	N	417	ARG
7	N	419	THR
7	N	455	MET
7	N	502	PHE
7	N	530	GLU
7	N	534	ASP
7	N	717	LEU
7	N	739	PHE
7	N	771	PHE
7	N	858	LYS
7	N	886	LYS
7	N	919	THR
8	S	60	LEU
8	S	101	LYS
8	S	119	TYR
8	S	133	GLU
8	S	222	SER
8	S	242	LEU
8	S	247	VAL
8	S	326	ASP
8	S	412	ASN
8	S	456	ASP
8	S	475	TYR
9	P	21	PHE
9	P	43	GLU
9	P	121	THR
9	P	133	GLU
9	P	277	GLN
9	P	309	MET
9	P	312	PRO
9	P	368	LEU
9	P	403	GLU
9	P	416	SER
10	Q	75	ARG
10	Q	88	PHE
10	Q	104	PHE
10	Q	114	GLN
10	Q	118	CYS
10	Q	138	SER
10	Q	157	LEU
10	Q	166	LYS
10	Q	306	TYR

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Mol	Chain	Res	Type
11	R	51	LEU
11	R	95	ASP
11	R	110	ILE
11	R	146	ASP
11	R	204	TRP
11	R	259	PHE
11	R	306	PRO
11	R	352	SER
12	U	180	ASP
12	U	261	LEU
13	O	16	MET
13	O	41	LEU
13	O	45	LEU
13	O	58	ARG
13	O	66	VAL
13	O	70	TYR
13	O	91	ASP
13	O	100	ASP
13	O	105	GLN
13	O	161	ASP
13	O	195	TYR
13	O	294	MET
13	O	307	MET
13	O	326	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
2	V	40	HIS
2	V	195	HIS
2	V	217	HIS
2	V	220	GLN
4	X	18	ASN
6	Z	15	GLN
6	Z	129	ASN
6	Z	156	HIS
6	Z	215	ASN
6	Z	307	HIS
6	Z	317	GLN
6	Z	539	ASN
6	Z	823	ASN
6	Z	829	GLN

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Mol	Chain	Res	Type
7	N	240	GLN
7	N	256	GLN
7	N	288	ASN
7	N	300	ASN
7	N	444	HIS
7	N	666	GLN
7	N	703	GLN
7	N	747	HIS
8	S	19	HIS
8	S	112	ASN
8	S	139	HIS
8	S	172	ASN
8	S	290	ASN
8	S	314	ASN
8	S	317	HIS
8	S	334	HIS
8	S	470	GLN
9	P	230	HIS
9	P	296	GLN
9	P	385	ASN
9	P	401	ASN
9	P	431	HIS
10	Q	135	HIS
10	Q	247	HIS
11	R	100	ASN
11	R	143	GLN
11	R	287	GLN
12	U	77	ASN
12	U	156	HIS
12	U	230	GLN
13	O	169	ASN
13	O	273	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 [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](#)

There are no chain breaks in this entry.