



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jun 21, 2017 – 01:33 PM EDT

PDB ID : 5NBZ
EMDB ID: : EMD-3611
Title : Wzz dodecamer fitted by MDFF to the Wzz experimental map from cryo-EM
Authors : Ford, R.C.; Kargas, V.; Collins, R.F.; Whitfield, C.; Clarke, B.R.; Siebert, A.;
Bond, P.J.; Clare, D.K.
Deposited on : 2017-03-02
Resolution : 9.00 Å(reported)
Based on PDB ID : 4E29

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-20029077

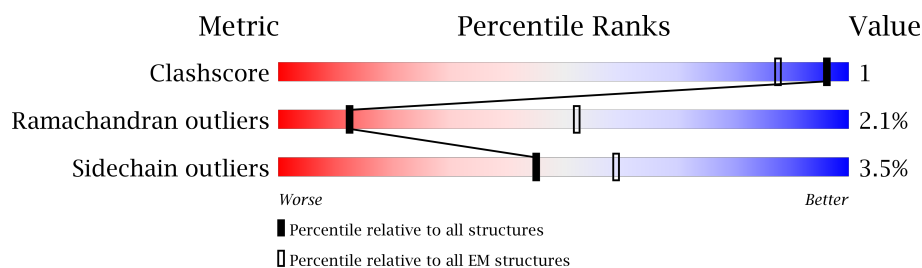
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	A	237	78% 18% .
1	B	237	74% 23% ..
1	C	237	78% 18% .
1	D	237	74% 22% .
1	E	237	75% 22% .
1	F	237	76% 20% ..
1	G	237	78% 18% 5%
1	H	237	74% 21% 5%
1	I	237	78% 17% ..

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Mol	Chain	Length	Quality of chain
1	J	237	<div><div></div><div>72%</div><div>22%</div><div>5%</div></div>
1	K	237	<div><div></div><div>76%</div><div>22%</div><div></div></div>
1	L	237	<div><div></div><div>83%</div><div>16%</div><div></div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 45252 atoms, of which 22704 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.

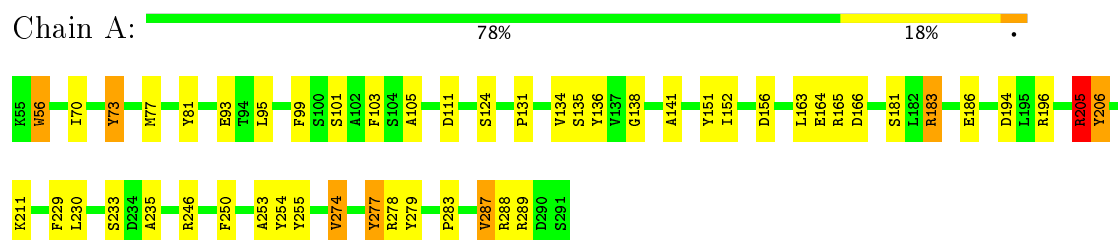
- Molecule 1 is a protein called WzzB.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0
1	B	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0
1	C	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0
1	D	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0
1	E	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0
1	F	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0
1	G	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0
1	H	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0
1	I	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0
1	J	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0
1	K	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0
1	L	237	Total 3771	C 1172	H 1892	N 325	O 377	S 5	0	0

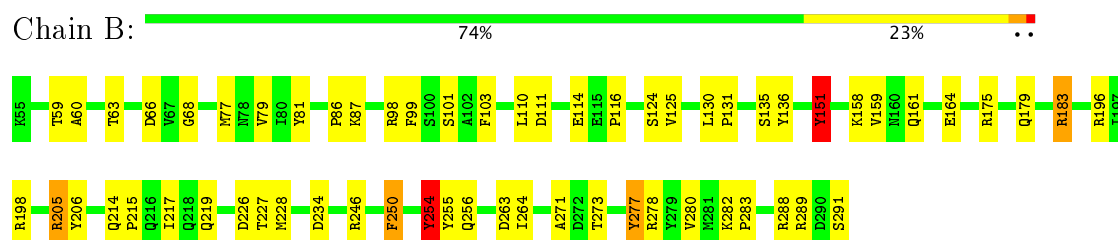
3 Residue-property plots [i](#)

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.

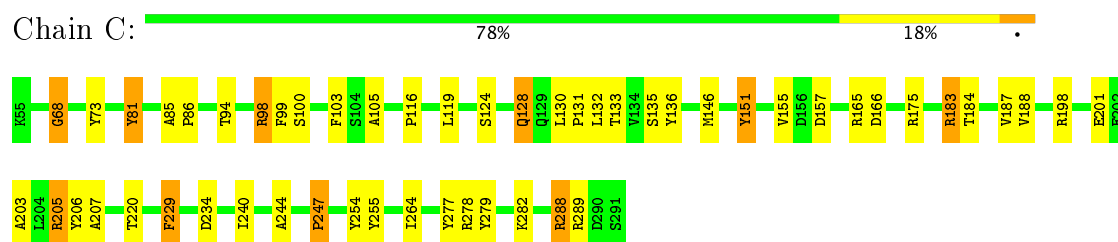
- Molecule 1: WzzB



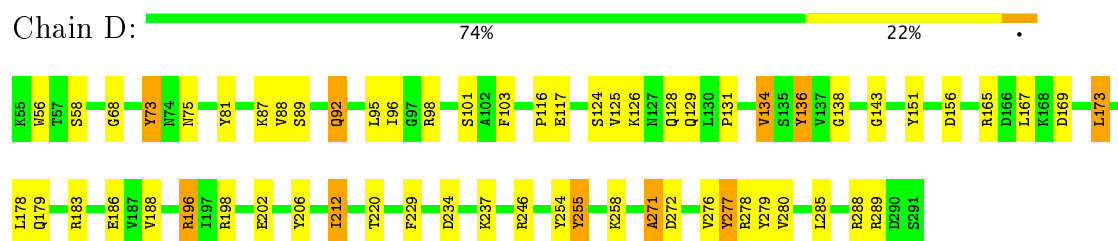
- Molecule 1: WzzB



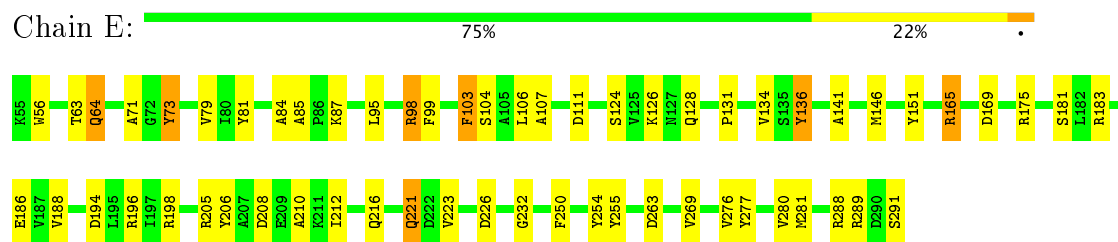
- Molecule 1: WzzB



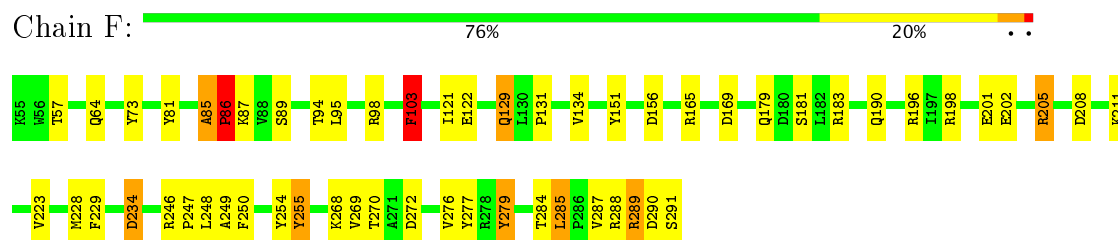
- Molecule 1: WzzB



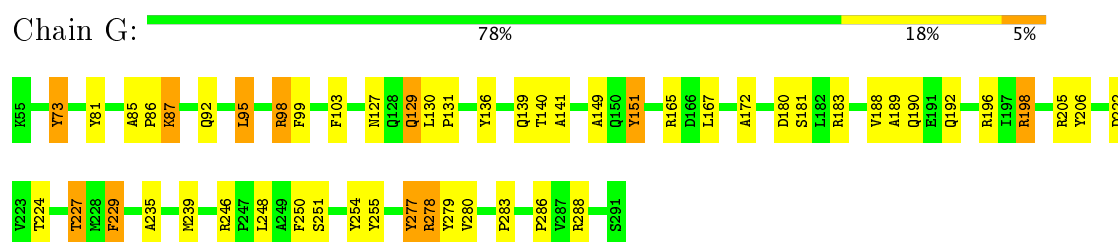
- Molecule 1: WzzB



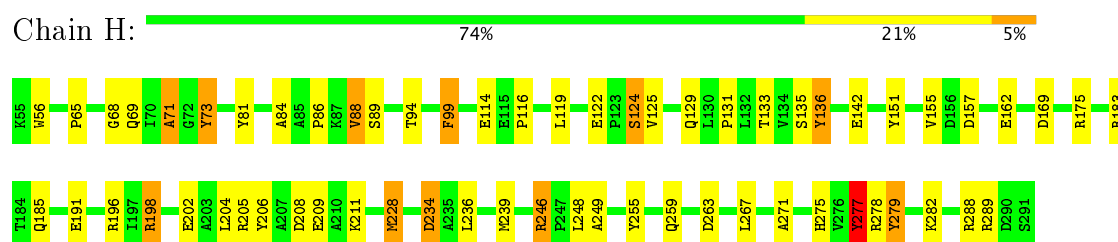
- Molecule 1: WzzB



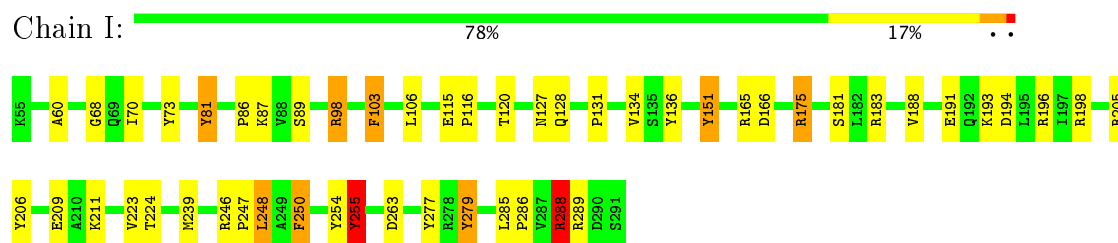
- Molecule 1: WzzB



- Molecule 1: WzzB

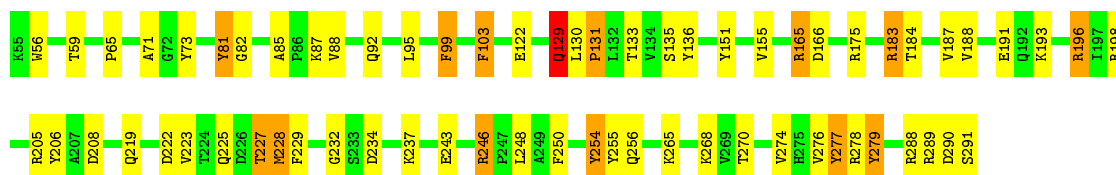


- Molecule 1: WzzB



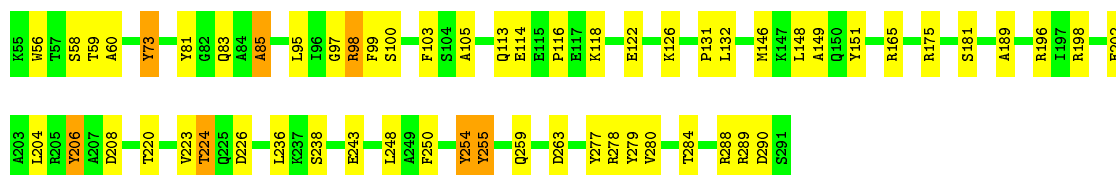
- Molecule 1: WzzB





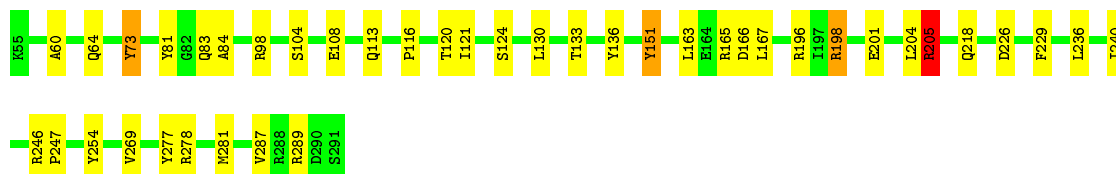
- Molecule 1: WzzB

Chain K: 76% 22% .



- Molecule 1: WzzB

Chain L: 83% 16% .



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	22000	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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	A	1.65	13/1904 (0.7%)	1.88	47/2580 (1.8%)
1	B	1.71	17/1904 (0.9%)	1.94	50/2580 (1.9%)
1	C	1.72	20/1904 (1.1%)	1.85	40/2580 (1.6%)
1	D	1.73	20/1904 (1.1%)	1.95	47/2580 (1.8%)
1	E	1.65	11/1904 (0.6%)	1.90	45/2580 (1.7%)
1	F	1.68	21/1904 (1.1%)	1.91	36/2580 (1.4%)
1	G	1.70	18/1904 (0.9%)	1.90	36/2580 (1.4%)
1	H	1.72	19/1904 (1.0%)	1.92	46/2580 (1.8%)
1	I	1.69	16/1904 (0.8%)	2.00	44/2580 (1.7%)
1	J	1.73	20/1904 (1.1%)	1.81	36/2580 (1.4%)
1	K	1.67	14/1904 (0.7%)	1.92	56/2580 (2.2%)
1	L	1.67	12/1904 (0.6%)	1.74	27/2580 (1.0%)
All	All	1.69	201/22848 (0.9%)	1.89	510/30960 (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	A	0	5
1	B	0	5
1	C	0	4
1	D	0	5
1	E	0	3
1	F	0	6
1	G	0	5
1	H	0	5
1	I	0	7
1	J	0	11
1	K	0	7
1	L	0	5
All	All	0	68

All (201) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	279	TYR	CG-CD1	9.08	1.50	1.39
1	D	196	ARG	NE-CZ	8.60	1.44	1.33
1	C	289	ARG	CZ-NH2	8.35	1.44	1.33
1	I	181	SER	CA-CB	8.29	1.65	1.52
1	H	151	TYR	CG-CD1	8.21	1.49	1.39
1	H	183	ARG	CZ-NH2	8.13	1.43	1.33
1	F	246	ARG	CZ-NH1	8.07	1.43	1.33
1	J	175	ARG	CZ-NH2	7.93	1.43	1.33
1	H	205	ARG	CZ-NH2	7.84	1.43	1.33
1	H	142	GLU	CG-CD	7.65	1.63	1.51
1	C	165	ARG	NE-CZ	7.51	1.42	1.33
1	F	73	TYR	CG-CD2	7.46	1.48	1.39
1	J	289	ARG	NE-CZ	7.45	1.42	1.33
1	D	254	TYR	CZ-OH	7.36	1.50	1.37
1	C	100	SER	CA-CB	7.14	1.63	1.52
1	K	289	ARG	CZ-NH1	7.06	1.42	1.33
1	B	81	TYR	CG-CD2	6.99	1.48	1.39
1	H	136	TYR	CE2-CZ	6.98	1.47	1.38
1	E	186	GLU	CG-CD	6.95	1.62	1.51
1	B	124	SER	CA-CB	6.92	1.63	1.52
1	F	98	ARG	CD-NE	6.88	1.58	1.46
1	J	135	SER	CA-CB	6.82	1.63	1.52
1	F	196	ARG	CZ-NH1	6.80	1.41	1.33
1	F	246	ARG	NE-CZ	6.79	1.41	1.33
1	G	196	ARG	CD-NE	6.76	1.57	1.46
1	J	198	ARG	NE-CZ	6.69	1.41	1.33
1	H	289	ARG	NE-CZ	6.69	1.41	1.33
1	G	278	ARG	NE-CZ	6.68	1.41	1.33
1	D	81	TYR	CZ-OH	6.65	1.49	1.37
1	C	205	ARG	NE-CZ	6.60	1.41	1.33
1	H	81	TYR	CZ-OH	6.57	1.49	1.37
1	L	196	ARG	NE-CZ	6.53	1.41	1.33
1	J	205	ARG	CZ-NH1	6.51	1.41	1.33
1	H	65	PRO	N-CA	-6.45	1.36	1.47
1	L	205	ARG	CD-NE	6.42	1.57	1.46
1	G	98	ARG	CZ-NH1	6.40	1.41	1.33
1	D	196	ARG	CZ-NH1	6.39	1.41	1.33
1	J	151	TYR	CE2-CZ	6.38	1.46	1.38
1	K	238	SER	CA-CB	6.37	1.62	1.52
1	A	164	GLU	CD-OE1	6.33	1.32	1.25
1	K	97	GLY	CA-C	-6.32	1.41	1.51
1	B	291	SER	CB-OG	6.30	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	73	TYR	CE2-CZ	6.30	1.46	1.38
1	C	68	GLY	CA-C	-6.26	1.41	1.51
1	D	117	GLU	CG-CD	6.26	1.61	1.51
1	A	277	TYR	CE1-CZ	6.24	1.46	1.38
1	D	277	TYR	CG-CD1	6.22	1.47	1.39
1	D	206	TYR	CG-CD2	6.21	1.47	1.39
1	A	255	TYR	CZ-OH	6.19	1.48	1.37
1	A	283	PRO	N-CD	-6.19	1.39	1.47
1	C	175	ARG	CZ-NH2	6.17	1.41	1.33
1	I	205	ARG	NE-CZ	6.14	1.41	1.33
1	D	143	GLY	N-CA	6.13	1.55	1.46
1	E	98	ARG	CD-NE	6.12	1.56	1.46
1	C	247	PRO	N-CD	6.12	1.56	1.47
1	F	181	SER	CA-CB	6.08	1.62	1.52
1	C	98	ARG	CZ-NH1	6.06	1.41	1.33
1	B	101	SER	CB-OG	6.05	1.50	1.42
1	C	205	ARG	CD-NE	6.05	1.56	1.46
1	A	250	PHE	CG-CD1	6.03	1.47	1.38
1	G	183	ARG	CZ-NH2	6.01	1.40	1.33
1	K	116	PRO	N-CA	-6.01	1.37	1.47
1	B	68	GLY	CA-C	-5.96	1.42	1.51
1	D	198	ARG	CD-NE	5.95	1.56	1.46
1	G	205	ARG	NE-CZ	5.91	1.40	1.33
1	D	279	TYR	CG-CD2	5.91	1.46	1.39
1	I	288	ARG	CZ-NH2	5.90	1.40	1.33
1	C	98	ARG	CD-NE	5.88	1.56	1.46
1	J	196	ARG	NE-CZ	5.86	1.40	1.33
1	I	277	TYR	CG-CD2	5.84	1.46	1.39
1	J	165	ARG	CZ-NH1	5.83	1.40	1.33
1	K	206	TYR	CG-CD1	5.83	1.46	1.39
1	L	73	TYR	CE2-CZ	5.82	1.46	1.38
1	C	279	TYR	CZ-OH	5.82	1.47	1.37
1	A	136	TYR	CE2-CZ	5.81	1.46	1.38
1	I	246	ARG	CZ-NH1	5.81	1.40	1.33
1	C	151	TYR	CD1-CE1	5.81	1.48	1.39
1	G	229	PHE	CG-CD2	5.79	1.47	1.38
1	K	198	ARG	NE-CZ	5.78	1.40	1.33
1	A	289	ARG	CZ-NH2	5.77	1.40	1.33
1	F	205	ARG	NE-CZ	5.76	1.40	1.33
1	H	114	GLU	CD-OE1	5.76	1.31	1.25
1	F	250	PHE	CE1-CZ	5.76	1.48	1.37
1	H	99	PHE	CG-CD2	5.76	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	73	TYR	CZ-OH	5.75	1.47	1.37
1	B	135	SER	CA-CB	5.75	1.61	1.52
1	I	209	GLU	CG-CD	5.74	1.60	1.51
1	G	198	ARG	NE-CZ	5.72	1.40	1.33
1	D	279	TYR	CZ-OH	5.71	1.47	1.37
1	F	291	SER	CA-CB	5.71	1.61	1.52
1	B	114	GLU	CD-OE2	5.68	1.31	1.25
1	B	136	TYR	CE2-CZ	5.66	1.46	1.38
1	G	165	ARG	CZ-NH2	5.66	1.40	1.33
1	K	206	TYR	CD1-CE1	5.65	1.47	1.39
1	F	202	GLU	CD-OE2	5.64	1.31	1.25
1	A	56	TRP	NE1-CE2	-5.64	1.30	1.37
1	E	205	ARG	NE-CZ	5.64	1.40	1.33
1	J	243	GLU	CG-CD	5.64	1.60	1.51
1	I	115	GLU	CD-OE1	5.61	1.31	1.25
1	D	138	GLY	N-CA	-5.59	1.37	1.46
1	G	288	ARG	CZ-NH1	5.58	1.40	1.33
1	I	288	ARG	NE-CZ	5.58	1.40	1.33
1	K	100	SER	CA-CB	5.58	1.61	1.52
1	E	175	ARG	CZ-NH2	5.57	1.40	1.33
1	B	278	ARG	CZ-NH2	5.55	1.40	1.33
1	H	56	TRP	CB-CG	5.55	1.60	1.50
1	J	191	GLU	CG-CD	5.55	1.60	1.51
1	E	232	GLY	CA-C	5.53	1.60	1.51
1	H	279	TYR	CE2-CZ	5.53	1.45	1.38
1	L	198	ARG	CZ-NH1	5.53	1.40	1.33
1	D	229	PHE	CD1-CE1	5.50	1.50	1.39
1	L	81	TYR	CE1-CZ	5.49	1.45	1.38
1	A	196	ARG	NE-CZ	5.49	1.40	1.33
1	G	183	ARG	CD-NE	5.48	1.55	1.46
1	A	181	SER	CA-CB	5.47	1.61	1.52
1	D	101	SER	CA-CB	5.45	1.61	1.52
1	G	165	ARG	CZ-NH1	5.45	1.40	1.33
1	C	277	TYR	CB-CG	5.42	1.59	1.51
1	B	151	TYR	CE2-CZ	5.41	1.45	1.38
1	E	198	ARG	CZ-NH2	5.41	1.40	1.33
1	I	255	TYR	CE2-CZ	5.37	1.45	1.38
1	E	291	SER	CA-CB	5.35	1.60	1.52
1	B	205	ARG	NE-CZ	5.35	1.40	1.33
1	H	191	GLU	CB-CG	5.35	1.62	1.52
1	L	254	TYR	CD1-CE1	5.35	1.47	1.39
1	J	288	ARG	CZ-NH1	5.34	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	165	ARG	CZ-NH1	5.34	1.40	1.33
1	B	289	ARG	CD-NE	5.34	1.55	1.46
1	L	198	ARG	CD-NE	5.34	1.55	1.46
1	A	73	TYR	CE2-CZ	5.30	1.45	1.38
1	F	122	GLU	C-N	5.29	1.44	1.34
1	C	183	ARG	CZ-NH1	5.29	1.40	1.33
1	A	233	SER	CA-CB	5.29	1.60	1.52
1	D	280	VAL	CA-CB	-5.28	1.43	1.54
1	J	99	PHE	CD2-CE2	5.28	1.49	1.39
1	G	246	ARG	NE-CZ	5.28	1.40	1.33
1	B	246	ARG	CZ-NH1	5.28	1.40	1.33
1	K	198	ARG	CD-NE	5.28	1.55	1.46
1	F	289	ARG	CD-NE	5.27	1.55	1.46
1	H	114	GLU	CB-CG	5.27	1.62	1.52
1	F	246	ARG	CZ-NH2	-5.26	1.26	1.33
1	H	277	TYR	CZ-OH	5.26	1.46	1.37
1	F	198	ARG	CZ-NH1	5.25	1.39	1.33
1	J	288	ARG	CD-NE	5.25	1.55	1.46
1	E	255	TYR	CA-CB	5.24	1.65	1.53
1	K	114	GLU	CD-OE1	5.24	1.31	1.25
1	G	87	LYS	N-CA	-5.24	1.35	1.46
1	C	229	PHE	CG-CD1	5.22	1.46	1.38
1	D	56	TRP	NE1-CE2	-5.22	1.30	1.37
1	I	151	TYR	CG-CD1	5.21	1.46	1.39
1	E	73	TYR	CG-CD2	5.21	1.46	1.39
1	H	116	PRO	N-CD	-5.21	1.40	1.47
1	F	103	PHE	CG-CD2	5.20	1.46	1.38
1	D	202	GLU	CB-CG	5.20	1.62	1.52
1	J	278	ARG	CZ-NH1	5.20	1.39	1.33
1	D	173	LEU	CA-CB	5.20	1.65	1.53
1	L	73	TYR	CB-CG	-5.19	1.43	1.51
1	G	277	TYR	CE2-CZ	5.19	1.45	1.38
1	D	255	TYR	CZ-OH	5.18	1.46	1.37
1	H	162	GLU	CD-OE2	5.18	1.31	1.25
1	I	279	TYR	CB-CG	-5.17	1.43	1.51
1	I	286	PRO	CA-C	-5.17	1.42	1.52
1	F	98	ARG	NE-CZ	5.17	1.39	1.33
1	I	103	PHE	CG-CD2	5.17	1.46	1.38
1	F	289	ARG	CZ-NH1	5.16	1.39	1.33
1	K	254	TYR	CZ-OH	5.16	1.46	1.37
1	H	246	ARG	CZ-NH1	5.15	1.39	1.33
1	B	256	GLN	N-CA	-5.14	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	278	ARG	CZ-NH2	5.14	1.39	1.33
1	G	127	ASN	CB-CG	5.13	1.62	1.51
1	H	81	TYR	CG-CD2	5.11	1.45	1.39
1	J	73	TYR	CB-CG	5.11	1.59	1.51
1	C	289	ARG	NE-CZ	5.11	1.39	1.33
1	K	175	ARG	CZ-NH1	5.10	1.39	1.33
1	B	175	ARG	CD-NE	5.10	1.55	1.46
1	F	288	ARG	CD-NE	5.09	1.55	1.46
1	L	287	VAL	N-CA	-5.07	1.36	1.46
1	B	164	GLU	CG-CD	5.07	1.59	1.51
1	C	206	TYR	CG-CD2	5.07	1.45	1.39
1	I	175	ARG	CZ-NH1	5.06	1.39	1.33
1	E	181	SER	CA-CB	5.06	1.60	1.52
1	J	82	GLY	CA-C	-5.06	1.43	1.51
1	J	187	VAL	CB-CG2	5.06	1.63	1.52
1	C	278	ARG	CZ-NH2	5.05	1.39	1.33
1	F	288	ARG	NE-CZ	5.05	1.39	1.33
1	I	89	SER	CA-CB	5.04	1.60	1.52
1	G	99	PHE	CG-CD1	5.04	1.46	1.38
1	G	251	SER	CA-CB	5.04	1.60	1.52
1	J	232	GLY	N-CA	-5.03	1.38	1.46
1	L	254	TYR	CD2-CE2	5.03	1.46	1.39
1	L	289	ARG	CD-NE	5.03	1.55	1.46
1	J	291	SER	CB-OG	5.03	1.48	1.42
1	C	254	TYR	CG-CD2	5.03	1.45	1.39
1	E	198	ARG	CZ-NH1	5.03	1.39	1.33
1	F	190	GLN	CA-CB	5.02	1.65	1.53
1	I	289	ARG	CD-NE	5.02	1.54	1.46
1	A	186	GLU	CD-OE2	-5.01	1.20	1.25
1	L	98	ARG	CZ-NH1	5.01	1.39	1.33
1	J	129	GLN	CG-CD	5.01	1.62	1.51
1	F	288	ARG	CZ-NH2	5.00	1.39	1.33
1	B	183	ARG	NE-CZ	5.00	1.39	1.33

All (510) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	165	ARG	NE-CZ-NH1	20.65	130.62	120.30
1	I	250	PHE	CB-CG-CD1	15.40	131.58	120.80
1	H	206	TYR	CB-CG-CD1	15.32	130.19	121.00
1	I	206	TYR	CB-CG-CD1	14.36	129.61	121.00
1	I	183	ARG	NE-CZ-NH1	14.34	127.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	81	TYR	CB-CG-CD2	14.05	129.43	121.00
1	E	198	ARG	NE-CZ-NH2	-14.04	113.28	120.30
1	G	206	TYR	CB-CG-CD1	14.00	129.40	121.00
1	I	98	ARG	NE-CZ-NH1	13.81	127.20	120.30
1	I	288	ARG	NE-CZ-NH2	-13.80	113.40	120.30
1	D	151	TYR	CB-CG-CD2	-13.56	112.86	121.00
1	A	246	ARG	NE-CZ-NH1	13.35	126.98	120.30
1	E	165	ARG	NE-CZ-NH1	13.32	126.96	120.30
1	I	250	PHE	CB-CG-CD2	-13.12	111.61	120.80
1	G	279	TYR	CB-CG-CD2	-13.01	113.20	121.00
1	D	206	TYR	CB-CG-CD2	-12.99	113.20	121.00
1	K	255	TYR	CB-CG-CD1	12.93	128.76	121.00
1	F	103	PHE	CB-CG-CD1	-12.93	111.75	120.80
1	F	169	ASP	CB-CG-OD1	12.73	129.76	118.30
1	H	206	TYR	CB-CG-CD2	-12.18	113.69	121.00
1	D	206	TYR	CB-CG-CD1	11.62	127.97	121.00
1	D	289	ARG	NE-CZ-NH1	11.25	125.92	120.30
1	E	175	ARG	NE-CZ-NH1	11.21	125.90	120.30
1	C	136	TYR	CB-CG-CD1	11.11	127.66	121.00
1	F	289	ARG	NE-CZ-NH1	10.89	125.75	120.30
1	H	81	TYR	CB-CG-CD1	-10.69	114.59	121.00
1	F	228	MET	CG-SD-CE	-10.66	83.15	100.20
1	E	250	PHE	CB-CG-CD2	10.57	128.20	120.80
1	J	196	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	I	165	ARG	NE-CZ-NH2	-10.29	115.16	120.30
1	H	277	TYR	CB-CG-CD2	-10.21	114.87	121.00
1	G	165	ARG	NE-CZ-NH1	10.13	125.36	120.30
1	G	206	TYR	CB-CG-CD2	-10.09	114.95	121.00
1	I	198	ARG	NE-CZ-NH2	-10.07	115.27	120.30
1	K	255	TYR	CB-CG-CD2	-10.00	115.00	121.00
1	A	183	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	F	288	ARG	NE-CZ-NH2	-9.79	115.41	120.30
1	D	103	PHE	CB-CG-CD1	-9.73	113.99	120.80
1	C	151	TYR	CG-CD1-CE1	-9.72	113.52	121.30
1	C	198	ARG	NE-CZ-NH2	-9.71	115.44	120.30
1	H	198	ARG	NE-CZ-NH1	9.59	125.10	120.30
1	I	205	ARG	NE-CZ-NH2	-9.58	115.51	120.30
1	B	246	ARG	NE-CZ-NH1	9.57	125.08	120.30
1	E	205	ARG	NE-CZ-NH2	9.47	125.04	120.30
1	B	254	TYR	CB-CG-CD2	9.43	126.66	121.00
1	B	103	PHE	CB-CG-CD1	-9.39	114.23	120.80
1	C	136	TYR	CB-CG-CD2	-9.31	115.41	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	279	TYR	CB-CG-CD1	9.31	126.59	121.00
1	F	249	ALA	N-CA-CB	9.21	122.99	110.10
1	F	103	PHE	CB-CG-CD2	9.03	127.12	120.80
1	B	175	ARG	NE-CZ-NH2	-8.99	115.81	120.30
1	K	196	ARG	NE-CZ-NH2	8.86	124.73	120.30
1	B	206	TYR	CB-CG-CD2	8.74	126.25	121.00
1	A	151	TYR	CB-CG-CD2	-8.74	115.76	121.00
1	L	226	ASP	CB-CG-OD2	-8.68	110.49	118.30
1	D	196	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	I	196	ARG	NE-CZ-NH1	-8.60	116.00	120.30
1	K	98	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	C	289	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	J	254	TYR	CB-CG-CD1	8.45	126.07	121.00
1	E	250	PHE	CB-CG-CD1	-8.43	114.90	120.80
1	D	183	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	B	226	ASP	CB-CG-OD2	-8.39	110.75	118.30
1	D	165	ARG	NE-CZ-NH1	8.39	124.49	120.30
1	B	136	TYR	CB-CG-CD2	-8.30	116.02	121.00
1	I	279	TYR	CG-CD2-CE2	-8.30	114.66	121.30
1	G	140	THR	CA-CB-CG2	-8.22	100.89	112.40
1	I	206	TYR	CB-CG-CD2	-8.18	116.09	121.00
1	D	73	TYR	CB-CG-CD1	-8.14	116.11	121.00
1	D	136	TYR	CG-CD2-CE2	8.11	127.79	121.30
1	K	288	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	B	205	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	H	99	PHE	CB-CG-CD2	8.07	126.45	120.80
1	J	288	ARG	NE-CZ-NH1	-8.01	116.30	120.30
1	B	289	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	D	151	TYR	CB-CG-CD1	7.97	125.78	121.00
1	F	183	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	A	156	ASP	CB-CG-OD1	7.92	125.43	118.30
1	K	278	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	J	289	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	K	103	PHE	CB-CG-CD1	7.76	126.23	120.80
1	H	183	ARG	NE-CZ-NH1	-7.75	116.42	120.30
1	A	288	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	C	229	PHE	CB-CG-CD1	7.74	126.22	120.80
1	F	169	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	K	95	LEU	CB-CA-C	-7.69	95.59	110.20
1	D	288	ARG	NE-CZ-NH1	-7.67	116.46	120.30
1	E	206	TYR	CB-CG-CD1	7.63	125.58	121.00
1	C	151	TYR	CB-CG-CD1	-7.62	116.43	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	166	ASP	CB-CG-OD1	-7.62	111.44	118.30
1	L	254	TYR	CB-CG-CD1	-7.55	116.47	121.00
1	B	278	ARG	NE-CZ-NH1	7.55	124.07	120.30
1	A	206	TYR	CG-CD2-CE2	-7.54	115.27	121.30
1	B	277	TYR	CZ-CE2-CD2	-7.53	113.02	119.80
1	B	226	ASP	CB-CG-OD1	7.47	125.03	118.30
1	D	246	ARG	NE-CZ-NH1	-7.46	116.57	120.30
1	E	289	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	165	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	D	254	TYR	CB-CG-CD2	-7.36	116.58	121.00
1	L	81	TYR	CB-CG-CD1	7.31	125.39	121.00
1	A	151	TYR	CG-CD1-CE1	-7.30	115.46	121.30
1	A	253	ALA	N-CA-CB	7.28	120.29	110.10
1	A	255	TYR	CB-CG-CD2	-7.27	116.64	121.00
1	D	89	SER	N-CA-CB	7.26	121.39	110.50
1	L	289	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	L	104	SER	N-CA-CB	7.22	121.32	110.50
1	F	183	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	A	277	TYR	CB-CG-CD2	7.19	125.32	121.00
1	A	205	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	F	279	TYR	CB-CG-CD1	-7.18	116.69	121.00
1	I	288	ARG	NH1-CZ-NH2	7.18	127.30	119.40
1	L	136	TYR	CB-CG-CD2	-7.17	116.69	121.00
1	C	206	TYR	CB-CG-CD2	7.17	125.30	121.00
1	B	246	ARG	NH1-CZ-NH2	-7.16	111.52	119.40
1	F	208	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	D	234	ASP	CB-CG-OD1	-7.09	111.92	118.30
1	I	194	ASP	CB-CG-OD2	7.09	124.68	118.30
1	I	277	TYR	CB-CG-CD2	-7.09	116.75	121.00
1	K	73	TYR	CG-CD1-CE1	-7.08	115.64	121.30
1	L	246	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	G	103	PHE	CB-CG-CD2	7.07	125.75	120.80
1	B	205	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	C	203	ALA	CB-CA-C	-7.06	99.50	110.10
1	K	208	ASP	CB-CA-C	-7.06	96.28	110.40
1	A	278	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	K	277	TYR	CB-CG-CD1	-7.05	116.77	121.00
1	G	129	GLN	N-CA-CB	7.04	123.28	110.60
1	K	198	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	B	77	MET	CG-SD-CE	-7.02	88.97	100.20
1	L	60	ALA	N-CA-CB	7.02	119.92	110.10
1	C	255	TYR	CB-CG-CD1	7.01	125.21	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	289	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	G	136	TYR	CG-CD1-CE1	-6.99	115.71	121.30
1	A	73	TYR	CB-CG-CD2	-6.98	116.81	121.00
1	I	198	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	C	205	ARG	NE-CZ-NH1	-6.96	116.82	120.30
1	D	271	ALA	N-CA-CB	6.94	119.81	110.10
1	E	205	ARG	NE-CZ-NH1	-6.94	116.83	120.30
1	A	196	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	I	205	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	B	289	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	A	206	TYR	CB-CG-CD2	-6.90	116.86	121.00
1	I	183	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	I	285	LEU	CB-CG-CD2	6.88	122.70	111.00
1	H	279	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	E	196	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	H	196	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	I	194	ASP	CB-CG-OD1	-6.84	112.15	118.30
1	F	73	TYR	CG-CD2-CE2	-6.82	115.85	121.30
1	K	151	TYR	CB-CG-CD2	-6.79	116.92	121.00
1	D	73	TYR	CG-CD1-CE1	-6.79	115.87	121.30
1	A	73	TYR	CG-CD2-CE2	-6.79	115.87	121.30
1	D	103	PHE	CB-CG-CD2	6.78	125.55	120.80
1	B	161	GLN	CB-CA-C	-6.77	96.85	110.40
1	L	205	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	A	206	TYR	CB-CA-C	-6.76	96.88	110.40
1	E	165	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	G	151	TYR	CB-CG-CD1	6.75	125.05	121.00
1	I	136	TYR	CB-CG-CD1	6.75	125.05	121.00
1	F	277	TYR	CB-CG-CD2	-6.74	116.95	121.00
1	E	254	TYR	CB-CG-CD1	6.74	125.04	121.00
1	A	235	ALA	N-CA-CB	6.72	119.51	110.10
1	F	254	TYR	CB-CG-CD1	-6.72	116.97	121.00
1	I	151	TYR	CB-CG-CD2	6.72	125.03	121.00
1	B	196	ARG	NE-CZ-NH1	-6.71	116.95	120.30
1	D	289	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	C	207	ALA	N-CA-CB	6.69	119.47	110.10
1	I	98	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	F	198	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	H	71	ALA	N-CA-CB	6.68	119.45	110.10
1	G	172	ALA	N-CA-CB	6.65	119.41	110.10
1	I	254	TYR	CZ-CE2-CD2	6.62	125.76	119.80
1	I	277	TYR	CB-CG-CD1	6.60	124.96	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	103	PHE	CB-CG-CD2	6.60	125.42	120.80
1	J	219	GLN	N-CA-CB	6.58	122.45	110.60
1	G	95	LEU	N-CA-CB	6.57	123.55	110.40
1	H	73	TYR	CB-CG-CD1	6.57	124.94	121.00
1	K	56	TRP	CD1-NE1-CE2	6.57	114.91	109.00
1	A	229	PHE	CB-CG-CD2	-6.56	116.21	120.80
1	G	99	PHE	CB-CG-CD1	6.56	125.39	120.80
1	B	234	ASP	CB-CG-OD1	-6.54	112.42	118.30
1	H	205	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	B	255	TYR	CB-CG-CD2	6.52	124.91	121.00
1	L	136	TYR	CB-CG-CD1	6.51	124.91	121.00
1	D	237	LYS	N-CA-CB	6.51	122.32	110.60
1	E	226	ASP	CB-CG-OD2	6.51	124.16	118.30
1	D	73	TYR	CG-CD2-CE2	-6.50	116.10	121.30
1	A	288	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	H	263	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	G	103	PHE	CB-CG-CD1	-6.48	116.26	120.80
1	J	223	VAL	CG1-CB-CG2	6.48	121.27	110.90
1	K	278	ARG	NH1-CZ-NH2	6.48	126.53	119.40
1	H	208	ASP	CB-CG-OD1	-6.48	112.47	118.30
1	H	169	ASP	CB-CG-OD2	6.47	124.12	118.30
1	K	98	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	73	TYR	CD1-CE1-CZ	6.46	125.61	119.80
1	G	222	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	C	166	ASP	CB-CG-OD1	6.46	124.11	118.30
1	K	206	TYR	CD1-CE1-CZ	-6.45	114.00	119.80
1	H	255	TYR	CB-CG-CD2	-6.43	117.14	121.00
1	E	206	TYR	CZ-CE2-CD2	-6.42	114.02	119.80
1	A	101	SER	N-CA-CB	6.41	120.11	110.50
1	H	169	ASP	CB-CG-OD1	-6.40	112.54	118.30
1	H	239	MET	CG-SD-CE	-6.40	89.96	100.20
1	K	278	ARG	NE-CZ-NH1	-6.40	117.10	120.30
1	C	157	ASP	CB-CG-OD1	-6.37	112.56	118.30
1	F	85	ALA	CB-CA-C	-6.36	100.57	110.10
1	H	84	ALA	N-CA-CB	6.35	118.99	110.10
1	H	228	MET	CG-SD-CE	-6.35	90.04	100.20
1	K	255	TYR	CG-CD1-CE1	6.32	126.36	121.30
1	L	198	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	H	246	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	L	81	TYR	CB-CG-CD2	-6.32	117.21	121.00
1	G	81	TYR	CD1-CE1-CZ	6.32	125.48	119.80
1	L	151	TYR	CG-CD1-CE1	-6.31	116.25	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	103	PHE	CB-CG-CD2	-6.31	116.39	120.80
1	K	165	ARG	NE-CZ-NH2	6.29	123.44	120.30
1	C	198	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	G	206	TYR	CG-CD1-CE1	6.28	126.32	121.30
1	K	263	ASP	CB-CG-OD2	6.27	123.95	118.30
1	B	219	GLN	O-C-N	6.26	132.72	122.70
1	E	136	TYR	CB-CG-CD1	6.25	124.75	121.00
1	J	254	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	B	159	VAL	CA-CB-CG2	6.25	120.28	110.90
1	E	146	MET	CG-SD-CE	6.23	110.17	100.20
1	K	105	ALA	CB-CA-C	-6.23	100.75	110.10
1	A	111	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	151	TYR	CB-CG-CD1	6.21	124.73	121.00
1	C	244	ALA	CB-CA-C	-6.20	100.80	110.10
1	I	60	ALA	CB-CA-C	-6.20	100.80	110.10
1	C	99	PHE	CB-CG-CD2	6.20	125.14	120.80
1	E	73	TYR	CB-CG-CD2	6.18	124.71	121.00
1	B	246	ARG	NE-CZ-NH2	6.17	123.38	120.30
1	F	73	TYR	CB-CA-C	-6.17	98.07	110.40
1	A	105	ALA	CB-CA-C	-6.16	100.86	110.10
1	B	60	ALA	N-CA-CB	6.15	118.71	110.10
1	C	157	ASP	CB-CG-OD2	6.14	123.82	118.30
1	G	235	ALA	CB-CA-C	-6.12	100.91	110.10
1	A	194	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	279	TYR	CB-CG-CD1	-6.12	117.33	121.00
1	F	165	ARG	CD-NE-CZ	-6.12	115.04	123.60
1	E	194	ASP	CB-CG-OD1	-6.11	112.80	118.30
1	I	151	TYR	CB-CG-CD1	-6.09	117.34	121.00
1	K	259	GLN	O-C-N	6.08	132.43	122.70
1	B	183	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	F	234	ASP	CB-CG-OD1	6.07	123.76	118.30
1	F	229	PHE	CB-CG-CD2	-6.06	116.56	120.80
1	J	279	TYR	CB-CG-CD2	-6.06	117.36	121.00
1	D	58	SER	N-CA-CB	6.06	119.59	110.50
1	K	196	ARG	NH1-CZ-NH2	-6.06	112.73	119.40
1	K	226	ASP	CB-CA-C	-6.04	98.31	110.40
1	H	157	ASP	CB-CG-OD1	-6.04	112.87	118.30
1	C	81	TYR	CB-CG-CD2	-6.01	117.39	121.00
1	I	103	PHE	CB-CG-CD1	-6.00	116.60	120.80
1	F	255	TYR	CB-CG-CD1	-5.99	117.40	121.00
1	E	277	TYR	CG-CD1-CE1	-5.99	116.51	121.30
1	F	270	THR	CA-CB-CG2	-5.97	104.04	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	277	TYR	N-CA-CB	5.97	121.34	110.60
1	A	136	TYR	CB-CG-CD2	-5.96	117.42	121.00
1	K	280	VAL	CA-CB-CG2	-5.96	101.96	110.90
1	D	198	ARG	NE-CZ-NH2	5.95	123.28	120.30
1	K	243	GLU	OE1-CD-OE2	5.95	130.44	123.30
1	I	136	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	D	169	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	B	135	SER	CB-CA-C	-5.94	98.82	110.10
1	A	163	LEU	CB-CA-C	-5.90	98.99	110.20
1	J	59	THR	CA-CB-CG2	-5.90	104.14	112.40
1	F	250	PHE	CB-CG-CD2	-5.90	116.67	120.80
1	B	111	ASP	CB-CG-OD1	5.88	123.59	118.30
1	F	95	LEU	CB-CG-CD1	5.88	121.00	111.00
1	G	136	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	J	246	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	E	71	ALA	O-C-N	-5.87	113.23	123.20
1	K	151	TYR	CB-CG-CD1	5.86	124.52	121.00
1	H	88	VAL	CA-CB-CG2	5.85	119.68	110.90
1	C	165	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	E	104	SER	N-CA-CB	5.81	119.21	110.50
1	F	205	ARG	NE-CZ-NH1	-5.81	117.40	120.30
1	B	79	VAL	CG1-CB-CG2	5.79	120.16	110.90
1	B	263	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	228	MET	CG-SD-CE	-5.77	90.97	100.20
1	H	249	ALA	N-CA-CB	5.77	118.17	110.10
1	I	98	ARG	CD-NE-CZ	-5.77	115.53	123.60
1	D	92	GLN	OE1-CD-NE2	5.76	135.16	121.90
1	E	106	LEU	C-N-CA	5.76	136.11	121.70
1	E	194	ASP	CB-CG-OD2	5.76	123.49	118.30
1	L	165	ARG	CD-NE-CZ	-5.76	115.53	123.60
1	K	56	TRP	CB-CA-C	-5.76	98.88	110.40
1	J	135	SER	CB-CA-C	-5.76	99.16	110.10
1	K	206	TYR	CG-CD1-CE1	5.76	125.91	121.30
1	L	226	ASP	CB-CG-OD1	5.76	123.48	118.30
1	I	106	LEU	N-CA-CB	-5.75	98.90	110.40
1	K	73	TYR	CB-CG-CD1	-5.75	117.55	121.00
1	I	247	PRO	N-CA-CB	5.74	110.19	103.30
1	D	95	LEU	CB-CG-CD1	5.73	120.75	111.00
1	E	79	VAL	CG1-CB-CG2	-5.72	101.75	110.90
1	K	81	TYR	N-CA-CB	5.72	120.89	110.60
1	C	73	TYR	CG-CD1-CE1	5.71	125.87	121.30
1	J	290	ASP	CB-CG-OD2	-5.70	113.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	151	TYR	CD1-CE1-CZ	5.69	124.92	119.80
1	L	108	GLU	CB-CG-CD	-5.69	98.84	114.20
1	D	98	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	J	208	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	L	130	LEU	CB-CA-C	5.66	120.95	110.20
1	D	116	PRO	N-CD-CG	5.65	111.68	103.20
1	D	188	VAL	CG1-CB-CG2	-5.65	101.86	110.90
1	I	239	MET	CG-SD-CE	-5.65	91.16	100.20
1	A	99	PHE	CB-CG-CD2	-5.65	116.84	120.80
1	B	175	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	H	151	TYR	CB-CG-CD1	5.64	124.39	121.00
1	D	285	LEU	N-CA-C	-5.64	95.78	111.00
1	F	134	VAL	CA-CB-CG1	5.63	119.35	110.90
1	H	278	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	C	220	THR	CA-CB-CG2	-5.62	104.53	112.40
1	C	234	ASP	CB-CG-OD1	-5.62	113.24	118.30
1	K	224	THR	N-CA-CB	5.60	120.95	110.30
1	E	151	TYR	CD1-CE1-CZ	5.60	124.84	119.80
1	E	208	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	C	155	VAL	CG1-CB-CG2	5.59	119.84	110.90
1	D	134	VAL	N-CA-C	-5.59	95.92	111.00
1	K	181	SER	N-CA-CB	5.59	118.88	110.50
1	C	116	PRO	N-CA-CB	5.58	110.00	103.30
1	L	121	ILE	N-CA-C	-5.58	95.94	111.00
1	F	277	TYR	CB-CG-CD1	5.57	124.34	121.00
1	G	250	PHE	CB-CG-CD2	-5.56	116.91	120.80
1	K	255	TYR	CD1-CE1-CZ	-5.56	114.79	119.80
1	H	94	THR	CA-CB-CG2	-5.55	104.63	112.40
1	J	265	LYS	N-CA-CB	5.54	120.58	110.60
1	B	66	ASP	N-CA-C	-5.54	96.03	111.00
1	D	81	TYR	CG-CD1-CE1	-5.54	116.86	121.30
1	J	227	THR	CA-CB-CG2	-5.54	104.64	112.40
1	G	190	GLN	O-C-N	-5.54	113.84	122.70
1	J	151	TYR	CB-CA-C	-5.54	99.32	110.40
1	K	220	THR	CA-CB-CG2	-5.54	104.65	112.40
1	K	224	THR	N-CA-C	-5.52	96.09	111.00
1	F	179	GLN	CA-CB-CG	5.52	125.53	113.40
1	J	133	THR	N-CA-CB	5.51	120.77	110.30
1	B	66	ASP	N-CA-CB	5.50	120.50	110.60
1	C	278	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	H	288	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	G	239	MET	CG-SD-CE	-5.50	91.41	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	136	TYR	CZ-CE2-CD2	-5.49	114.86	119.80
1	D	126	LYS	N-CA-CB	5.48	120.47	110.60
1	I	73	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	E	63	THR	CA-CB-OG1	5.47	120.49	109.00
1	E	84	ALA	N-CA-CB	-5.47	102.44	110.10
1	B	87	LYS	CB-CA-C	-5.47	99.46	110.40
1	E	126	LYS	N-CA-C	-5.47	96.24	111.00
1	K	56	TRP	CG-CD2-CE3	-5.46	128.98	133.90
1	I	81	TYR	CB-CG-CD1	-5.46	117.73	121.00
1	J	184	THR	N-CA-CB	5.45	120.66	110.30
1	C	103	PHE	N-CA-CB	5.45	120.41	110.60
1	E	175	ARG	CD-NE-CZ	-5.45	115.97	123.60
1	C	206	TYR	CB-CG-CD1	-5.44	117.73	121.00
1	H	125	VAL	CA-CB-CG2	5.44	119.06	110.90
1	E	169	ASP	CB-CG-OD2	5.44	123.19	118.30
1	J	279	TYR	N-CA-CB	5.43	120.38	110.60
1	D	75	ASN	N-CA-CB	5.42	120.36	110.60
1	G	149	ALA	CB-CA-C	-5.42	101.97	110.10
1	E	103	PHE	CB-CG-CD1	-5.42	117.01	120.80
1	H	288	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	I	120	THR	CA-CB-CG2	-5.42	104.81	112.40
1	A	183	ARG	NH1-CZ-NH2	-5.41	113.45	119.40
1	L	236	LEU	CB-CG-CD1	5.41	120.20	111.00
1	A	93	GLU	OE1-CD-OE2	5.40	129.78	123.30
1	G	255	TYR	CD1-CE1-CZ	-5.40	114.94	119.80
1	K	132	LEU	N-CA-CB	5.40	121.19	110.40
1	E	175	ARG	NH1-CZ-NH2	-5.40	113.46	119.40
1	D	212	ILE	N-CA-C	-5.39	96.43	111.00
1	K	250	PHE	CB-CG-CD1	-5.39	117.02	120.80
1	C	234	ASP	N-CA-CB	5.39	120.31	110.60
1	J	188	VAL	CA-CB-CG1	-5.39	102.81	110.90
1	J	228	MET	CG-SD-CE	-5.39	91.57	100.20
1	A	287	VAL	O-C-N	5.39	131.32	122.70
1	H	185	GLN	CB-CA-C	-5.38	99.63	110.40
1	A	105	ALA	N-CA-CB	5.37	117.61	110.10
1	C	99	PHE	CB-CG-CD1	-5.37	117.04	120.80
1	K	198	ARG	NH1-CZ-NH2	5.37	125.30	119.40
1	L	198	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	C	98	ARG	CB-CA-C	-5.36	99.67	110.40
1	E	206	TYR	CG-CD2-CE2	5.36	125.59	121.30
1	F	255	TYR	CD1-CE1-CZ	5.36	124.62	119.80
1	I	166	ASP	CB-CG-OD2	-5.35	113.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	183	ARG	CD-NE-CZ	-5.35	116.11	123.60
1	K	189	ALA	N-CA-CB	5.34	117.58	110.10
1	H	279	TYR	CG-CD2-CE2	-5.34	117.03	121.30
1	J	166	ASP	CB-CG-OD2	5.34	123.10	118.30
1	B	264	ILE	CG1-CB-CG2	-5.33	99.67	111.40
1	J	234	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	K	202	GLU	OE1-CD-OE2	-5.33	116.91	123.30
1	B	179	GLN	O-C-N	-5.33	114.17	122.70
1	F	201	GLU	N-CA-CB	5.33	120.19	110.60
1	G	130	LEU	CB-CG-CD1	5.33	120.06	111.00
1	E	255	TYR	CB-CG-CD2	5.32	124.19	121.00
1	G	280	VAL	CB-CA-C	-5.32	101.29	111.40
1	B	198	ARG	CB-CA-C	-5.32	99.76	110.40
1	G	192	GLN	N-CA-CB	5.32	120.17	110.60
1	J	237	LYS	N-CA-CB	-5.32	101.03	110.60
1	K	56	TRP	NE1-CE2-CZ2	5.31	136.25	130.40
1	J	81	TYR	CG-CD2-CE2	-5.30	117.06	121.30
1	B	125	VAL	CG1-CB-CG2	5.30	119.38	110.90
1	G	181	SER	N-CA-CB	5.30	118.44	110.50
1	A	135	SER	N-CA-CB	5.29	118.44	110.50
1	K	118	LYS	CD-CE-NZ	5.29	123.88	111.70
1	H	129	GLN	N-CA-CB	5.29	120.12	110.60
1	J	71	ALA	CB-CA-C	-5.28	102.17	110.10
1	J	81	TYR	CB-CG-CD1	-5.28	117.83	121.00
1	E	281	MET	CG-SD-CE	5.26	108.62	100.20
1	A	253	ALA	CB-CA-C	-5.26	102.21	110.10
1	B	130	LEU	CB-CA-C	-5.26	100.21	110.20
1	K	113	GLN	N-CA-CB	5.26	120.07	110.60
1	G	254	TYR	CB-CG-CD1	5.26	124.15	121.00
1	K	254	TYR	CB-CG-CD1	-5.26	117.85	121.00
1	C	187	VAL	CA-CB-CG2	-5.25	103.02	110.90
1	E	124	SER	N-CA-CB	5.25	118.38	110.50
1	D	98	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	C	146	MET	CA-CB-CG	5.25	122.22	113.30
1	D	220	THR	N-CA-CB	5.25	120.27	110.30
1	H	136	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	A	229	PHE	CB-CG-CD1	5.24	124.47	120.80
1	H	206	TYR	CG-CD1-CE1	5.24	125.49	121.30
1	E	280	VAL	O-C-N	-5.24	114.32	122.70
1	B	59	THR	CA-CB-CG2	-5.23	105.08	112.40
1	F	223	VAL	CA-CB-CG2	-5.23	103.06	110.90
1	C	288	ARG	NE-CZ-NH2	5.22	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	130	LEU	CA-C-N	5.22	131.73	117.10
1	E	64	GLN	N-CA-C	5.22	125.10	111.00
1	J	103	PHE	CD1-CE1-CZ	-5.22	113.83	120.10
1	L	281	MET	CB-CA-C	-5.22	99.96	110.40
1	D	183	ARG	CD-NE-CZ	5.22	130.91	123.60
1	A	254	TYR	CB-CG-CD2	-5.21	117.87	121.00
1	H	277	TYR	CG-CD1-CE1	-5.21	117.13	121.30
1	C	184	THR	CA-CB-CG2	-5.20	105.11	112.40
1	H	129	GLN	N-CA-C	-5.20	96.95	111.00
1	G	92	GLN	N-CA-CB	5.20	119.95	110.60
1	K	59	THR	N-CA-CB	5.19	120.17	110.30
1	D	81	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	K	284	THR	N-CA-C	-5.18	97.01	111.00
1	C	188	VAL	CA-CB-CG2	5.18	118.67	110.90
1	E	134	VAL	N-CA-C	-5.18	97.02	111.00
1	B	196	ARG	NH1-CZ-NH2	5.18	125.09	119.40
1	A	111	ASP	CB-CG-OD1	-5.17	113.64	118.30
1	D	186	GLU	CA-CB-CG	5.17	124.78	113.40
1	D	206	TYR	CB-CA-C	-5.17	100.06	110.40
1	A	77	MET	CG-SD-CE	-5.17	91.93	100.20
1	K	223	VAL	O-C-N	5.16	130.95	122.70
1	E	221	GLN	OE1-CD-NE2	5.16	133.75	121.90
1	D	178	LEU	N-CA-CB	5.15	120.71	110.40
1	J	277	TYR	CG-CD1-CE1	-5.15	117.18	121.30
1	B	198	ARG	N-CA-CB	5.15	119.87	110.60
1	E	98	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	C	105	ALA	CB-CA-C	-5.14	102.39	110.10
1	K	288	ARG	CB-CA-C	-5.14	100.12	110.40
1	C	229	PHE	CD1-CE1-CZ	5.14	126.27	120.10
1	G	189	ALA	CB-CA-C	-5.14	102.40	110.10
1	H	234	ASP	CB-CG-OD1	5.14	122.92	118.30
1	B	98	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	I	191	GLU	OE1-CD-OE2	-5.13	117.14	123.30
1	L	229	PHE	CB-CG-CD2	-5.12	117.21	120.80
1	G	180	ASP	CB-CG-OD2	5.12	122.91	118.30
1	J	222	ASP	CB-CG-OD1	5.12	122.91	118.30
1	K	85	ALA	CB-CA-C	5.12	117.78	110.10
1	A	206	TYR	CZ-CE2-CD2	5.12	124.40	119.80
1	B	63	THR	C-N-CA	5.11	134.47	121.70
1	I	263	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	D	56	TRP	CG-CD2-CE3	-5.11	129.30	133.90
1	H	267	LEU	CB-CG-CD2	5.11	119.68	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	95	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	B	283	PRO	CA-C-N	-5.10	105.97	117.20
1	J	56	TRP	NE1-CE2-CD2	5.10	112.40	107.30
1	H	259	GLN	CA-CB-CG	5.10	124.62	113.40
1	I	193	LYS	CA-CB-CG	5.10	124.62	113.40
1	L	83	GLN	N-CA-CB	5.10	119.78	110.60
1	E	107	ALA	N-CA-CB	5.10	117.24	110.10
1	K	58	SER	N-CA-C	-5.09	97.26	111.00
1	G	188	VAL	CB-CA-C	-5.09	101.73	111.40
1	E	288	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	H	185	GLN	CG-CD-OE1	5.08	131.75	121.60
1	G	188	VAL	CA-CB-CG1	5.07	118.51	110.90
1	A	230	LEU	CB-CA-C	-5.07	100.56	110.20
1	A	103	PHE	CB-CG-CD1	5.07	124.35	120.80
1	B	206	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	E	128	GLN	CA-CB-CG	5.07	124.56	113.40
1	H	56	TRP	CB-CG-CD2	-5.07	120.01	126.60
1	B	130	LEU	CB-CG-CD1	5.07	119.61	111.00
1	K	149	ALA	CB-CA-C	-5.07	102.50	110.10
1	H	56	TRP	CG-CD2-CE3	-5.06	129.34	133.90
1	J	81	TYR	CB-CG-CD2	5.06	124.04	121.00
1	H	69	GLN	CB-CA-C	-5.06	100.28	110.40
1	A	103	PHE	CB-CG-CD2	-5.05	117.26	120.80
1	L	278	ARG	CG-CD-NE	-5.05	101.19	111.80
1	L	84	ALA	C-N-CA	5.05	134.33	121.70
1	C	132	LEU	CB-CA-C	-5.05	100.60	110.20
1	I	134	VAL	N-CA-C	-5.05	97.36	111.00
1	F	129	GLN	N-CA-CB	5.05	119.68	110.60
1	C	128	GLN	N-CA-CB	5.04	119.68	110.60
1	F	89	SER	N-CA-CB	5.04	118.05	110.50
1	A	274	VAL	CB-CA-C	5.03	120.96	111.40
1	B	280	VAL	CA-CB-CG1	5.03	118.44	110.90
1	J	187	VAL	CB-CA-C	-5.03	101.85	111.40
1	J	268	LYS	N-CA-CB	5.03	119.65	110.60
1	B	255	TYR	CA-CB-CG	-5.02	103.86	113.40
1	H	175	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	D	88	VAL	CA-CB-CG1	5.01	118.42	110.90
1	G	140	THR	CA-CB-OG1	5.01	119.53	109.00
1	A	138	GLY	N-CA-C	-5.01	100.57	113.10
1	B	227	THR	C-N-CA	5.01	134.23	121.70
1	D	179	GLN	O-C-N	-5.01	114.69	122.70
1	G	229	PHE	CB-CG-CD2	-5.01	117.29	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	211	LYS	N-CA-CB	5.01	119.62	110.60

There are no chirality outliers.

All (68) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	ARG	Sidechain
1	A	206	TYR	Sidechain
1	A	277	TYR	Sidechain
1	A	73	TYR	Sidechain
1	A	81	TYR	Sidechain
1	B	151	TYR	Sidechain
1	B	205	ARG	Sidechain
1	B	250	PHE	Sidechain
1	B	254	TYR	Sidechain
1	B	99	PHE	Sidechain
1	C	151	TYR	Sidechain
1	C	205	ARG	Sidechain
1	C	229	PHE	Sidechain
1	C	81	TYR	Sidechain
1	D	136	TYR	Sidechain
1	D	196	ARG	Sidechain
1	D	255	TYR	Sidechain
1	D	277	TYR	Sidechain
1	D	73	TYR	Sidechain
1	E	136	TYR	Sidechain
1	E	183	ARG	Sidechain
1	E	81	TYR	Sidechain
1	F	103	PHE	Sidechain
1	F	205	ARG	Sidechain
1	F	255	TYR	Sidechain
1	F	279	TYR	Sidechain
1	F	289	ARG	Sidechain
1	F	81	TYR	Sidechain
1	G	151	TYR	Sidechain
1	G	229	PHE	Sidechain
1	G	277	TYR	Sidechain
1	G	73	TYR	Sidechain
1	G	98	ARG	Sidechain
1	H	136	TYR	Sidechain
1	H	246	ARG	Sidechain
1	H	277	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	H	279	TYR	Sidechain
1	H	73	TYR	Sidechain
1	I	151	TYR	Sidechain
1	I	175	ARG	Sidechain
1	I	255	TYR	Sidechain
1	I	279	TYR	Sidechain
1	I	288	ARG	Sidechain
1	I	81	TYR	Sidechain
1	I	98	ARG	Sidechain
1	J	103	PHE	Sidechain
1	J	136	TYR	Sidechain
1	J	165	ARG	Sidechain
1	J	196	ARG	Sidechain
1	J	206	TYR	Sidechain
1	J	246	ARG	Sidechain
1	J	250	PHE	Sidechain
1	J	255	TYR	Sidechain
1	J	277	TYR	Sidechain
1	J	279	TYR	Sidechain
1	J	81	TYR	Sidechain
1	K	206	TYR	Sidechain
1	K	254	TYR	Sidechain
1	K	255	TYR	Sidechain
1	K	279	TYR	Sidechain
1	K	73	TYR	Sidechain
1	K	98	ARG	Sidechain
1	K	99	PHE	Sidechain
1	L	151	TYR	Sidechain
1	L	198	ARG	Sidechain
1	L	205	ARG	Sidechain
1	L	277	TYR	Sidechain
1	L	73	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1879	1892	1889	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1879	1892	1889	4	0
1	C	1879	1892	1889	7	0
1	D	1879	1892	1889	3	0
1	E	1879	1892	1889	6	0
1	F	1879	1892	1889	6	0
1	G	1879	1892	1889	2	0
1	H	1879	1892	1889	8	0
1	I	1879	1892	1889	3	0
1	J	1879	1892	1889	5	0
1	K	1879	1892	1889	2	0
1	L	1879	1892	1889	2	0
All	All	22548	22704	22668	43	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 1.

All (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:210:ALA:HA	1:F:234:ASP:HB3	1.85	0.58
1:E:111:ASP:OD1	1:F:285:LEU:HD13	2.06	0.55
1:J:88:VAL:HG22	1:J:92:GLN:HE21	1.71	0.55
1:B:214:GLN:HB3	1:B:215:PRO:HD2	1.90	0.54
1:F:94:THR:HG23	1:G:278:ARG:NH2	2.25	0.51
1:D:92:GLN:O	1:D:96:ILE:HG22	2.10	0.51
1:J:193:LYS:HD2	1:J:248:LEU:HD23	1.94	0.50
1:E:99:PHE:CD1	1:E:276:VAL:HG21	2.47	0.50
1:F:85:ALA:HB1	1:F:86:PRO:HD2	1.95	0.49
1:L:124:SER:HB2	1:L:133:THR:HB	1.95	0.49
1:A:56:TRP:CE3	1:A:141:ALA:HB2	2.48	0.48
1:K:204:LEU:HD23	1:K:236:LEU:HB2	1.95	0.47
1:D:156:ASP:OD2	1:D:276:VAL:HG22	2.15	0.47
1:J:129:GLN:HB2	1:J:131:PRO:HD3	1.97	0.46
1:I:248:LEU:HD12	1:I:250:PHE:CE1	2.50	0.46
1:H:68:GLY:O	1:H:71:ALA:HB3	2.17	0.45
1:K:60:ALA:HB2	1:K:148:LEU:HD21	1.97	0.45
1:L:201:GLU:HA	1:L:240:ILE:HD11	1.98	0.45
1:B:110:LEU:HD11	1:B:151:TYR:CE1	2.51	0.45
1:C:94:THR:HG22	1:C:98:ARG:HE	1.82	0.44
1:C:119:LEU:HD12	1:C:135:SER:O	2.17	0.44
1:E:56:TRP:CD2	1:E:141:ALA:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:THR:HG21	1:F:290:ASP:HB2	1.99	0.44
1:E:212:ILE:HD12	1:E:216:GLN:CG	2.48	0.44
1:H:86:PRO:HA	1:I:68:GLY:HA3	2.00	0.44
1:C:201:GLU:HA	1:C:240:ILE:HD11	2.01	0.43
1:J:225:GLN:HA	1:J:228:MET:HB2	2.01	0.43
1:H:275:HIS:HB2	1:H:277:TYR:H	1.83	0.43
1:H:119:LEU:HD12	1:H:135:SER:O	2.19	0.43
1:C:201:GLU:HG2	1:C:240:ILE:HG12	2.01	0.43
1:C:86:PRO:O	1:D:68:GLY:HA3	2.18	0.42
1:G:141:ALA:HB1	1:G:286:PRO:HD2	2.02	0.42
1:H:99:PHE:CD1	1:H:155:VAL:HG12	2.54	0.42
1:H:228:MET:HG2	1:H:236:LEU:HD21	2.02	0.42
1:H:88:VAL:HG13	1:H:89:SER:N	2.35	0.41
1:J:99:PHE:CE1	1:J:155:VAL:HG12	2.55	0.41
1:F:156:ASP:OD2	1:F:276:VAL:HG22	2.20	0.41
1:C:124:SER:HA	1:C:133:THR:HG22	2.02	0.41
1:B:86:PRO:HA	1:C:68:GLY:HA3	2.03	0.41
1:H:124:SER:HA	1:H:133:THR:HG22	2.02	0.41
1:I:223:VAL:HG22	1:I:224:THR:N	2.36	0.40
1:B:183:ARG:HD3	1:B:183:ARG:C	2.42	0.40
1:E:98:ARG:NH2	1:E:165:ARG:HH22	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/237 (99%)	221 (94%)	10 (4%)	4 (2%)	11	50
1	B	235/237 (99%)	223 (95%)	7 (3%)	5 (2%)	8	45
1	C	235/237 (99%)	219 (93%)	13 (6%)	3 (1%)	14	56
1	D	235/237 (99%)	217 (92%)	12 (5%)	6 (3%)	6	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	235/237 (99%)	222 (94%)	9 (4%)	4 (2%)	11	50
1	F	235/237 (99%)	222 (94%)	5 (2%)	8 (3%)	4	35
1	G	235/237 (99%)	217 (92%)	12 (5%)	6 (3%)	6	40
1	H	235/237 (99%)	225 (96%)	6 (3%)	4 (2%)	11	50
1	I	235/237 (99%)	220 (94%)	9 (4%)	6 (3%)	6	40
1	J	235/237 (99%)	216 (92%)	13 (6%)	6 (3%)	6	40
1	K	235/237 (99%)	219 (93%)	12 (5%)	4 (2%)	11	50
1	L	235/237 (99%)	217 (92%)	14 (6%)	4 (2%)	11	50
All	All	2820/2844 (99%)	2638 (94%)	122 (4%)	60 (2%)	12	45

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	PRO
1	B	131	PRO
1	B	271	ALA
1	C	131	PRO
1	D	271	ALA
1	E	87	LYS
1	E	131	PRO
1	G	131	PRO
1	H	131	PRO
1	K	131	PRO
1	K	224	THR
1	C	128	GLN
1	D	131	PRO
1	F	86	PRO
1	F	129	GLN
1	F	211	LYS
1	F	285	LEU
1	F	287	VAL
1	I	127	ASN
1	I	131	PRO
1	J	131	PRO
1	L	116	PRO
1	L	218	GLN
1	A	124	SER
1	D	87	LYS
1	D	124	SER

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Mol	Chain	Res	Type
1	D	128	GLN
1	G	86	PRO
1	H	211	LYS
1	I	116	PRO
1	J	129	GLN
1	K	126	LYS
1	L	113	GLN
1	B	277	TYR
1	B	288	ARG
1	D	129	GLN
1	E	85	ALA
1	F	272	ASP
1	G	227	THR
1	I	87	LYS
1	I	128	GLN
1	J	65	PRO
1	J	85	ALA
1	K	85	ALA
1	A	211	LYS
1	B	116	PRO
1	C	85	ALA
1	E	64	GLN
1	F	64	GLN
1	G	129	GLN
1	J	87	LYS
1	F	131	PRO
1	G	87	LYS
1	H	124	SER
1	H	271	ALA
1	L	64	GLN
1	G	85	ALA
1	J	274	VAL
1	A	287	VAL
1	I	86	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/208 (100%)	200 (96%)	8 (4%)	38	67
1	B	208/208 (100%)	202 (97%)	6 (3%)	48	73
1	C	208/208 (100%)	202 (97%)	6 (3%)	48	73
1	D	208/208 (100%)	201 (97%)	7 (3%)	42	69
1	E	208/208 (100%)	200 (96%)	8 (4%)	38	67
1	F	208/208 (100%)	199 (96%)	9 (4%)	33	64
1	G	208/208 (100%)	200 (96%)	8 (4%)	38	67
1	H	208/208 (100%)	200 (96%)	8 (4%)	38	67
1	I	208/208 (100%)	202 (97%)	6 (3%)	48	73
1	J	208/208 (100%)	199 (96%)	9 (4%)	33	64
1	K	208/208 (100%)	203 (98%)	5 (2%)	54	78
1	L	208/208 (100%)	201 (97%)	7 (3%)	42	69
All	All	2496/2496 (100%)	2409 (96%)	87 (4%)	45	69

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ILE
1	A	95	LEU
1	A	134	VAL
1	A	152	ILE
1	A	166	ASP
1	A	183	ARG
1	A	205	ARG
1	A	274	VAL
1	B	158	LYS
1	B	217	ILE
1	B	250	PHE
1	B	254	TYR
1	B	273	THR
1	B	282	LYS
1	C	130	LEU
1	C	183	ARG
1	C	247	PRO
1	C	264	ILE
1	C	282	LYS
1	C	288	ARG
1	D	125	VAL
1	D	134	VAL

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Mol	Chain	Res	Type
1	D	167	LEU
1	D	173	LEU
1	D	212	ILE
1	D	258	LYS
1	D	272	ASP
1	E	73	TYR
1	E	95	LEU
1	E	103	PHE
1	E	188	VAL
1	E	221	GLN
1	E	223	VAL
1	E	263	ASP
1	E	269	VAL
1	F	86	PRO
1	F	87	LYS
1	F	103	PHE
1	F	121	ILE
1	F	247	PRO
1	F	248	LEU
1	F	268	LYS
1	F	269	VAL
1	F	284	THR
1	G	95	LEU
1	G	139	GLN
1	G	167	LEU
1	G	198	ARG
1	G	224	THR
1	G	227	THR
1	G	248	LEU
1	G	283	PRO
1	H	122	GLU
1	H	198	ARG
1	H	202	GLU
1	H	204	LEU
1	H	209	GLU
1	H	234	ASP
1	H	248	LEU
1	H	282	LYS
1	I	70	ILE
1	I	103	PHE
1	I	188	VAL
1	I	248	LEU

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Mol	Chain	Res	Type
1	I	255	TYR
1	I	288	ARG
1	J	95	LEU
1	J	122	GLU
1	J	183	ARG
1	J	227	THR
1	J	229	PHE
1	J	254	TYR
1	J	256	GLN
1	J	270	THR
1	J	276	VAL
1	K	83	GLN
1	K	122	GLU
1	K	146	MET
1	K	248	LEU
1	K	290	ASP
1	L	120	THR
1	L	163	LEU
1	L	167	LEU
1	L	204	LEU
1	L	205	ARG
1	L	247	PRO
1	L	269	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	216	GLN
1	B	241	GLN
1	C	170	ASN
1	C	179	GLN
1	D	160	ASN
1	D	199	GLN
1	F	112	ASN
1	F	113	GLN
1	F	199	GLN
1	G	170	ASN
1	G	214	GLN
1	H	78	ASN
1	H	154	GLN
1	I	225	GLN
1	I	242	ASN

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Mol	Chain	Res	Type
1	J	92	GLN
1	J	150	GLN
1	K	74	ASN
1	K	179	GLN
1	K	199	GLN
1	K	219	GLN
1	K	241	GLN
1	L	177	ASN
1	L	218	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](#)

There are no chain breaks in this entry.