



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:43 PM BST

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

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

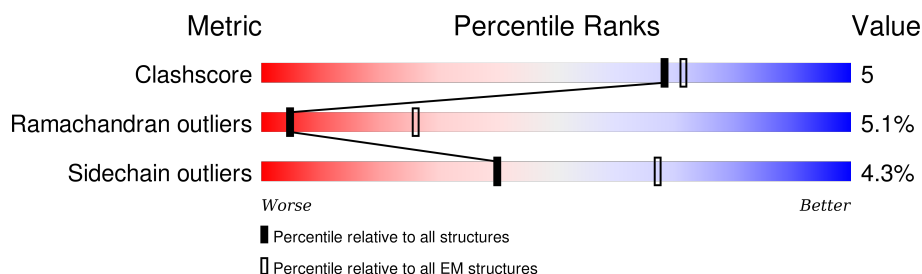
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	253	49% 15% . 32%
1	D	253	49% 15% . 32%
1	G	253	46% 18% . . 32%
1	J	253	49% 14% . 32%
2	B	427	67% 25% 6% .
2	E	427	69% 25% 5%
2	H	427	74% 20% 5% .
2	K	427	70% 24% 5% .
3	C	421	73% 22% . .

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Mol	Chain	Length	Quality of chain
3	F	421	<div><div></div><div>74%</div><div>22%</div><div>• •</div></div>
3	I	421	<div><div></div><div>70%</div><div>24%</div><div>5%</div></div>
3	L	421	<div><div></div><div>71%</div><div>25%</div><div>•</div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 31120 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CAPSID PROTEIN.

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

- Molecule 2 is a protein called E1 ENVELOPE GLYCOPROTEIN.

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

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	.	-	HIS	DELETION	UNP P89946
B	.	-	HIS	DELETION	UNP P89946
B	.	-	HIS	DELETION	UNP P89946
B	.	-	HIS	DELETION	UNP P89946
B	.	-	HIS	DELETION	UNP P89946
B	.	-	HIS	DELETION	UNP P89946
B	.	-	HIS	DELETION	UNP P89946
B	.	-	HIS	DELETION	UNP P89946
B	.	-	HIS	DELETION	UNP P89946

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Chain	Residue	Modelled	Actual	Comment	Reference
B	.	-	HIS	DELETION	UNP P89946
B	.	-	HIS	DELETION	UNP P89946
B	.	-	HIS	DELETION	UNP P89946
B	.	-	HIS	DELETION	UNP P89946
E	.	-	HIS	DELETION	UNP P89946
E	.	-	HIS	DELETION	UNP P89946
E	.	-	HIS	DELETION	UNP P89946
E	.	-	HIS	DELETION	UNP P89946
E	.	-	HIS	DELETION	UNP P89946
E	.	-	HIS	DELETION	UNP P89946
E	.	-	HIS	DELETION	UNP P89946
E	.	-	HIS	DELETION	UNP P89946
E	.	-	HIS	DELETION	UNP P89946
E	.	-	HIS	DELETION	UNP P89946
E	.	-	HIS	DELETION	UNP P89946
E	.	-	HIS	DELETION	UNP P89946
E	.	-	HIS	DELETION	UNP P89946
E	.	-	HIS	DELETION	UNP P89946
H	.	-	HIS	DELETION	UNP P89946
H	.	-	HIS	DELETION	UNP P89946
H	.	-	HIS	DELETION	UNP P89946
H	.	-	HIS	DELETION	UNP P89946
H	.	-	HIS	DELETION	UNP P89946
H	.	-	HIS	DELETION	UNP P89946
H	.	-	HIS	DELETION	UNP P89946
H	.	-	HIS	DELETION	UNP P89946
H	.	-	HIS	DELETION	UNP P89946
H	.	-	HIS	DELETION	UNP P89946
H	.	-	HIS	DELETION	UNP P89946
H	.	-	HIS	DELETION	UNP P89946
H	.	-	HIS	DELETION	UNP P89946
H	.	-	HIS	DELETION	UNP P89946
K	.	-	HIS	DELETION	UNP P89946
K	.	-	HIS	DELETION	UNP P89946
K	.	-	HIS	DELETION	UNP P89946
K	.	-	HIS	DELETION	UNP P89946
K	.	-	HIS	DELETION	UNP P89946
K	.	-	HIS	DELETION	UNP P89946
K	.	-	HIS	DELETION	UNP P89946
K	.	-	HIS	DELETION	UNP P89946
K	.	-	HIS	DELETION	UNP P89946
K	.	-	HIS	DELETION	UNP P89946
K	.	-	HIS	DELETION	UNP P89946
K	.	-	HIS	DELETION	UNP P89946
K	.	-	HIS	DELETION	UNP P89946
K	.	-	HIS	DELETION	UNP P89946
K	.	-	HIS	DELETION	UNP P89946

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Chain	Residue	Modelled	Actual	Comment	Reference
K	.	-	HIS	DELETION	UNP P89946

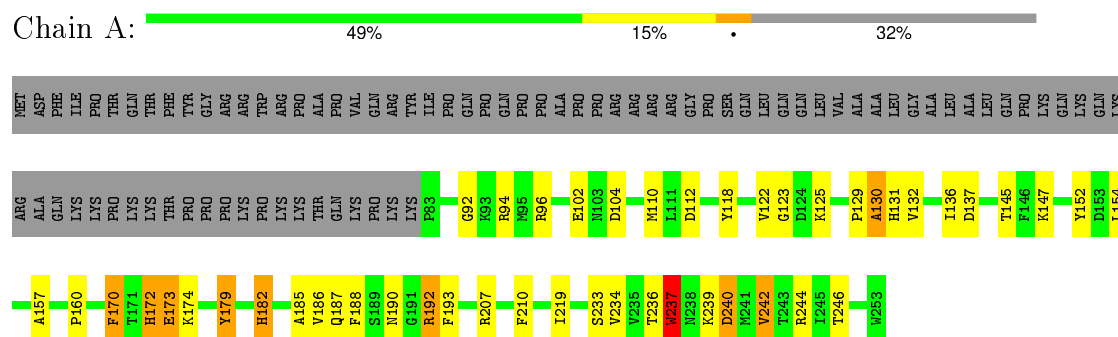
- Molecule 3 is a protein called E2 ENVELOPE GLYCOPROTEIN.

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

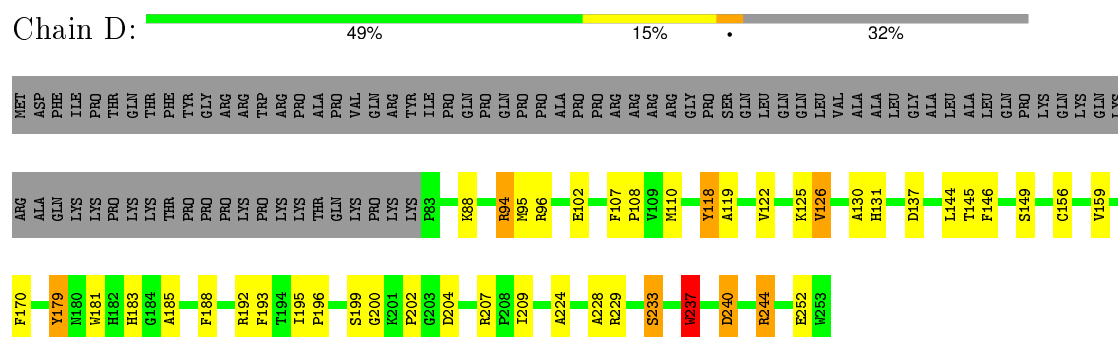
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

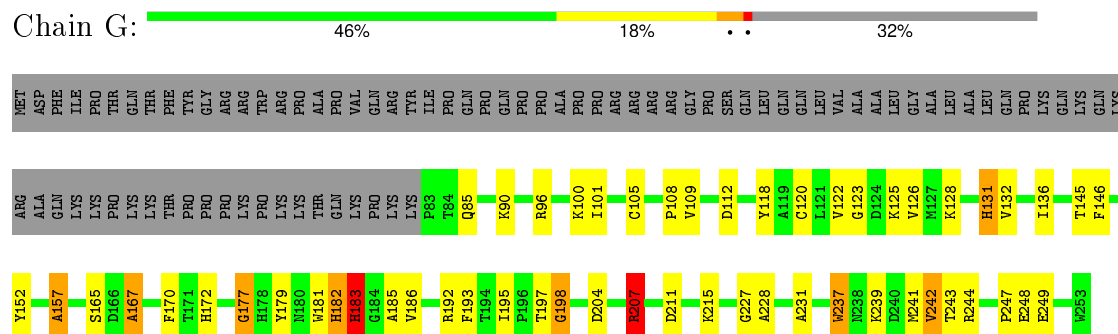
• Molecule 1: CAPSID PROTEIN



• Molecule 1: CAPSID PROTEIN

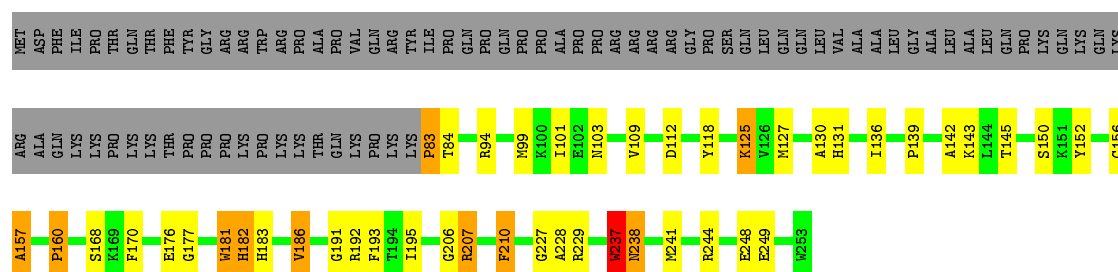


• Molecule 1: CAPSID PROTEIN



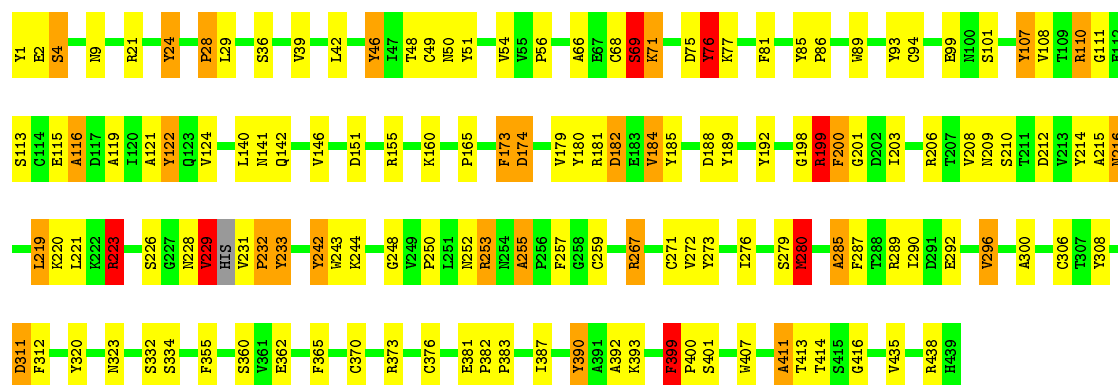
• Molecule 1: CAPSID PROTEIN





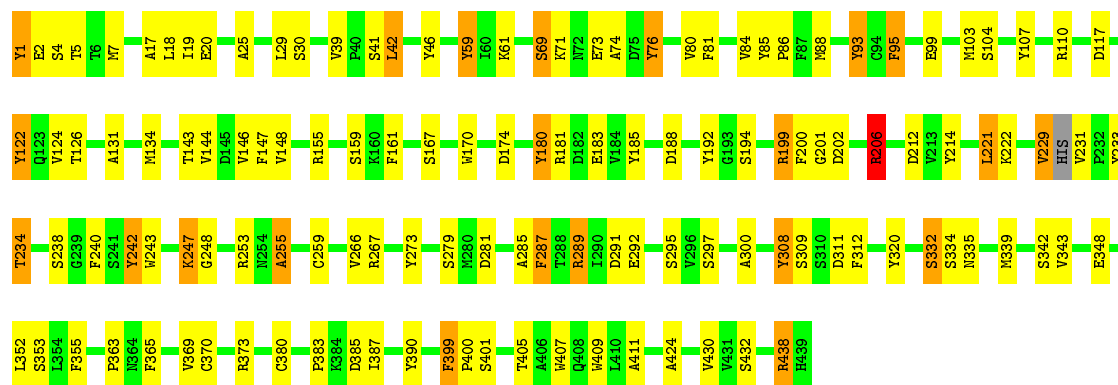
• Molecule 2: E1 ENVELOPE GLYCOPROTEIN

Chain B: 67% 25% 6% •



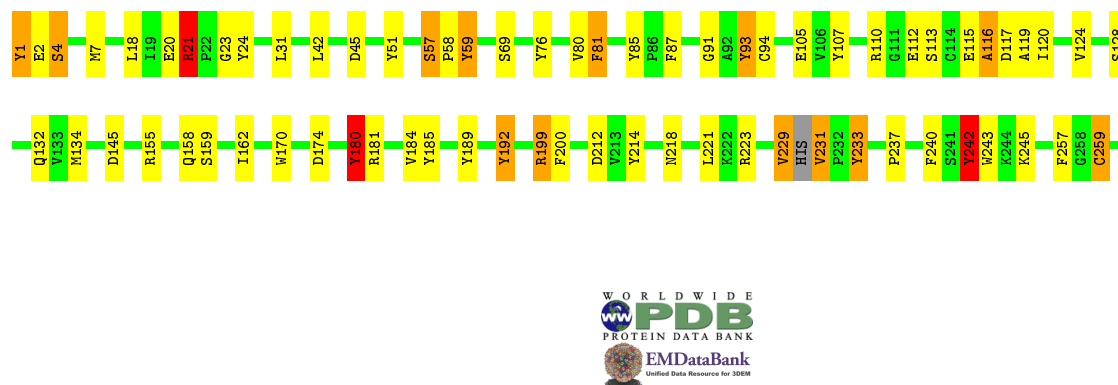
• Molecule 2: E1 ENVELOPE GLYCOPROTEIN

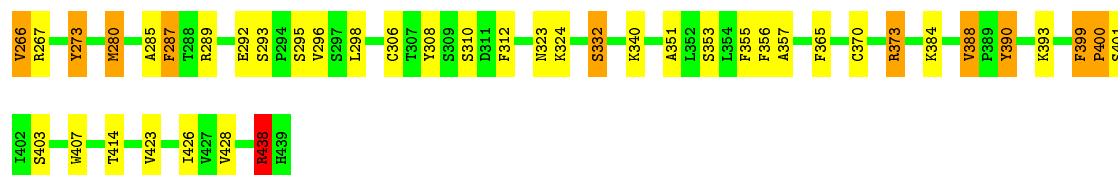
Chain E: 69% 25% 5% •



• Molecule 2: E1 ENVELOPE GLYCOPROTEIN

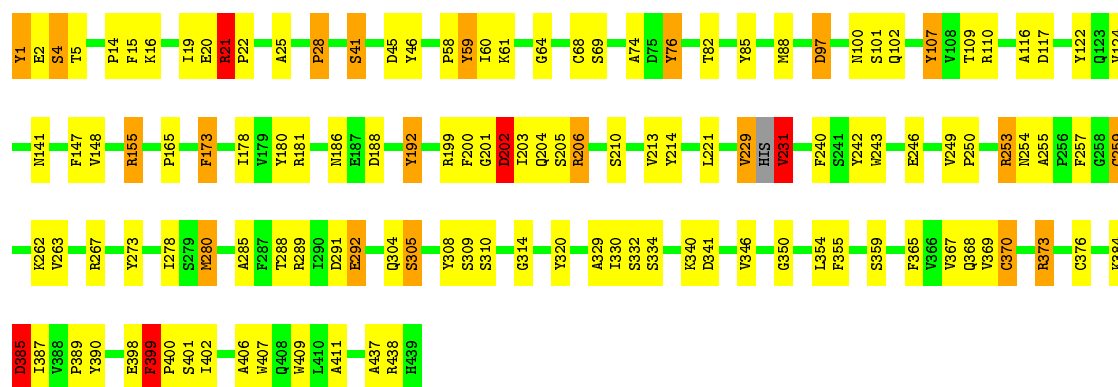
Chain H: 74% 20% 5% •





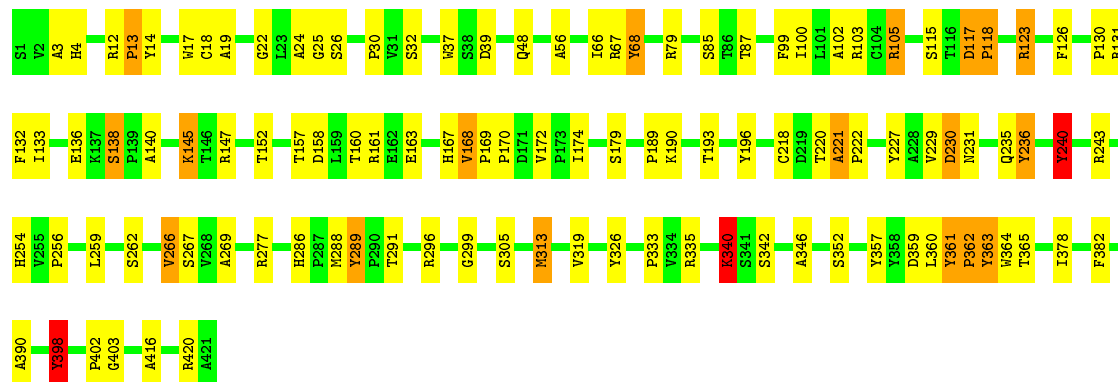
• Molecule 2: E1 ENVELOPE GLYCOPROTEIN

Chain K: 70% 24% 5%



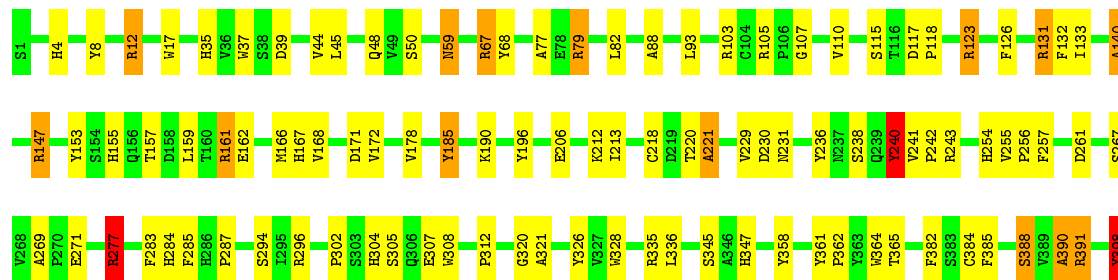
• Molecule 3: E2 ENVELOPE GLYCOPROTEIN

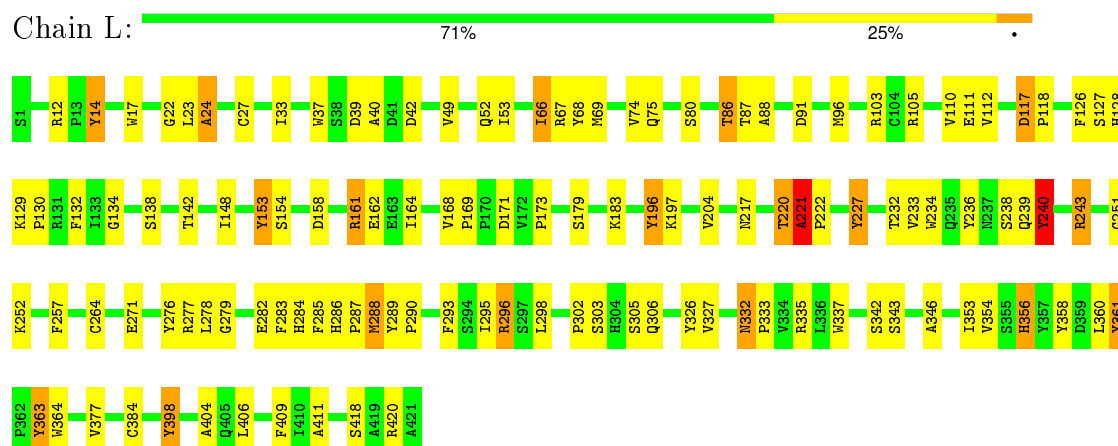
Chain C: 73% 22%



• Molecule 3: E2 ENVELOPE GLYCOPROTEIN

Chain F: 74% 22%





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	INDIVIDUAL PARTICLES	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	50000	Depositor
Image detector	GATAN CCD	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	3.19	16/1346 (1.2%)	2.07	35/1812 (1.9%)
1	D	3.19	11/1346 (0.8%)	2.09	43/1812 (2.4%)
1	G	3.16	17/1346 (1.3%)	2.03	33/1812 (1.8%)
1	J	3.19	18/1346 (1.3%)	2.09	31/1812 (1.7%)
2	B	1.75	29/3296 (0.9%)	2.05	102/4494 (2.3%)
2	E	1.75	28/3296 (0.8%)	1.98	84/4494 (1.9%)
2	H	1.74	26/3296 (0.8%)	2.05	93/4494 (2.1%)
2	K	1.78	29/3296 (0.9%)	1.99	83/4494 (1.8%)
3	C	2.79	40/3326 (1.2%)	1.94	75/4537 (1.7%)
3	F	2.71	44/3326 (1.3%)	1.99	82/4537 (1.8%)
3	I	2.80	48/3326 (1.4%)	2.00	80/4537 (1.8%)
3	L	2.77	35/3326 (1.1%)	2.01	95/4537 (2.1%)
All	All	2.49	341/31872 (1.1%)	2.01	836/43372 (1.9%)

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

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

All (341) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	237	TRP	CE2-CZ2	91.21	2.94	1.39
1	J	237	TRP	CE2-CZ2	88.72	2.90	1.39
1	G	237	TRP	CE2-CZ2	87.75	2.88	1.39
1	A	237	TRP	CE2-CZ2	87.70	2.88	1.39
3	I	398	TYR	CD2-CE2	78.02	2.56	1.39
3	L	398	TYR	CD2-CE2	77.17	2.55	1.39
3	C	398	TYR	CD2-CE2	77.03	2.54	1.39
3	F	398	TYR	CD2-CE2	76.70	2.54	1.39
3	I	240	TYR	CG-CD1	45.34	1.98	1.39
3	C	240	TYR	CE1-CZ	43.98	1.95	1.38
3	L	240	TYR	CE1-CZ	42.97	1.94	1.38
3	I	240	TYR	CG-CD2	41.53	1.93	1.39
3	C	240	TYR	CG-CD2	41.35	1.93	1.39
3	I	240	TYR	CE1-CZ	41.28	1.92	1.38
3	L	240	TYR	CG-CD2	41.08	1.92	1.39
3	C	240	TYR	CG-CD1	40.23	1.91	1.39
3	F	240	TYR	CE1-CZ	39.91	1.90	1.38
3	F	240	TYR	CE2-CZ	39.20	1.89	1.38
3	F	240	TYR	CG-CD1	38.80	1.89	1.39
3	L	240	TYR	CG-CD1	38.76	1.89	1.39
3	F	240	TYR	CG-CD2	37.93	1.88	1.39
3	L	240	TYR	CE2-CZ	37.68	1.87	1.38
3	I	240	TYR	CE2-CZ	37.56	1.87	1.38
3	C	240	TYR	CE2-CZ	36.20	1.85	1.38
3	F	240	TYR	CD1-CE1	34.64	1.91	1.39
3	L	240	TYR	CD2-CE2	34.60	1.91	1.39
3	C	240	TYR	CD1-CE1	33.47	1.89	1.39
3	C	240	TYR	CD2-CE2	32.48	1.88	1.39
3	L	240	TYR	CD1-CE1	28.72	1.82	1.39
3	I	240	TYR	CD1-CE1	28.05	1.81	1.39
1	A	237	TRP	CD2-CE3	27.84	1.82	1.40
3	I	240	TYR	CD2-CE2	27.33	1.80	1.39
3	F	240	TYR	CD2-CE2	26.74	1.79	1.39
1	J	237	TRP	CD2-CE2	24.17	1.70	1.41
3	I	398	TYR	CE2-CZ	23.42	1.69	1.38
1	G	237	TRP	CD2-CE3	22.97	1.74	1.40
1	G	237	TRP	CD2-CE2	22.63	1.68	1.41
1	A	237	TRP	CD2-CE2	21.88	1.67	1.41
3	C	398	TYR	CG-CD1	21.14	1.66	1.39
3	I	398	TYR	CG-CD2	20.37	1.65	1.39
1	D	237	TRP	CE3-CZ3	19.74	1.72	1.38
1	G	237	TRP	CE3-CZ3	19.56	1.71	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	237	TRP	CD2-CE3	19.50	1.69	1.40
1	J	237	TRP	CE3-CZ3	19.17	1.71	1.38
1	D	237	TRP	CD2-CE2	18.89	1.64	1.41
3	C	398	TYR	CE2-CZ	18.41	1.62	1.38
3	L	398	TYR	CG-CD1	18.25	1.62	1.39
1	A	237	TRP	CZ2-CH2	18.01	1.71	1.37
1	A	237	TRP	CE3-CZ3	17.78	1.68	1.38
3	L	398	TYR	CE1-CZ	17.77	1.61	1.38
1	G	237	TRP	CZ2-CH2	17.71	1.71	1.37
3	L	398	TYR	CE2-CZ	16.95	1.60	1.38
1	J	237	TRP	CZ2-CH2	16.38	1.68	1.37
1	J	237	TRP	CD2-CE3	16.33	1.64	1.40
1	D	237	TRP	CZ3-CH2	15.89	1.65	1.40
1	G	237	TRP	CZ3-CH2	15.80	1.65	1.40
3	F	398	TYR	CE1-CZ	15.69	1.58	1.38
3	F	398	TYR	CE2-CZ	15.58	1.58	1.38
1	D	237	TRP	CZ2-CH2	15.30	1.66	1.37
3	L	398	TYR	CG-CD2	14.80	1.58	1.39
1	J	237	TRP	CZ3-CH2	14.75	1.63	1.40
3	F	398	TYR	CG-CD2	14.72	1.58	1.39
3	C	398	TYR	CG-CD2	14.25	1.57	1.39
3	I	398	TYR	CD1-CE1	14.07	1.60	1.39
3	F	398	TYR	CG-CD1	13.82	1.57	1.39
3	I	398	TYR	CE1-CZ	13.80	1.56	1.38
3	C	398	TYR	CE1-CZ	13.02	1.55	1.38
3	I	398	TYR	CG-CD1	12.87	1.55	1.39
1	A	237	TRP	CZ3-CH2	11.70	1.58	1.40
3	F	398	TYR	CD1-CE1	11.37	1.56	1.39
3	C	398	TYR	CD1-CE1	11.16	1.56	1.39
3	L	398	TYR	CD1-CE1	9.83	1.54	1.39
2	K	21	ARG	CD-NE	9.35	1.62	1.46
2	E	59	TYR	CG-CD1	8.32	1.50	1.39
2	B	223	ARG	NE-CZ	8.15	1.43	1.33
3	C	416	ALA	CA-CB	8.08	1.69	1.52
2	K	390	TYR	CE1-CZ	7.99	1.49	1.38
3	C	79	ARG	CZ-NH1	7.99	1.43	1.33
3	C	277	ARG	NE-CZ	7.94	1.43	1.33
3	C	138	SER	CA-CB	7.70	1.64	1.52
3	F	50	SER	CA-CB	7.68	1.64	1.52
1	D	193	PHE	CG-CD2	7.63	1.50	1.38
3	I	380	SER	CA-CB	7.61	1.64	1.52
2	K	46	TYR	CE1-CZ	7.58	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	200	PHE	CG-CD1	7.47	1.50	1.38
2	K	181	ARG	CZ-NH1	7.38	1.42	1.33
3	L	305	SER	CA-CB	7.25	1.63	1.52
2	E	192	TYR	CG-CD2	7.23	1.48	1.39
2	H	312	PHE	C-N	7.19	1.46	1.33
2	E	309	SER	CA-CB	7.14	1.63	1.52
1	J	229	ARG	CZ-NH1	7.12	1.42	1.33
1	J	139	PRO	N-CD	-7.11	1.38	1.47
2	B	199	ARG	CZ-NH2	7.09	1.42	1.33
1	G	123	GLY	CA-C	-7.02	1.40	1.51
3	L	128	HIS	CB-CG	6.94	1.62	1.50
2	H	407	TRP	CD2-CE2	6.88	1.49	1.41
3	I	296	ARG	CD-NE	6.86	1.58	1.46
1	A	244	ARG	CZ-NH2	6.86	1.42	1.33
2	E	438	ARG	CZ-NH1	6.81	1.41	1.33
1	D	94	ARG	CZ-NH2	6.76	1.41	1.33
3	C	4	HIS	CB-CG	6.76	1.62	1.50
3	L	243	ARG	NE-CZ	6.73	1.41	1.33
2	K	76	TYR	CE1-CZ	6.71	1.47	1.38
3	F	103	ARG	CZ-NH2	6.71	1.41	1.33
2	B	320	TYR	CG-CD1	6.69	1.47	1.39
3	L	179	SER	CA-CB	6.68	1.62	1.52
3	I	296	ARG	NE-CZ	6.67	1.41	1.33
2	E	46	TYR	CG-CD2	6.66	1.47	1.39
2	B	69	SER	CA-CB	6.65	1.62	1.52
1	J	118	TYR	CE2-CZ	6.64	1.47	1.38
2	K	314	GLY	CA-C	-6.63	1.41	1.51
2	B	267	ARG	CZ-NH2	6.59	1.41	1.33
2	B	373	ARG	CZ-NH1	6.58	1.41	1.33
2	E	248	GLY	N-CA	-6.58	1.36	1.46
1	G	165	SER	CB-OG	6.55	1.50	1.42
2	B	267	ARG	CZ-NH1	6.54	1.41	1.33
2	B	232	PRO	N-CD	-6.52	1.38	1.47
1	G	207	ARG	CZ-NH1	6.46	1.41	1.33
2	K	173	PHE	CG-CD2	6.45	1.48	1.38
3	L	243	ARG	CZ-NH2	6.44	1.41	1.33
3	I	402	PRO	C-N	6.41	1.44	1.33
2	B	192	TYR	CG-CD1	6.39	1.47	1.39
2	K	246	GLU	CG-CD	6.38	1.61	1.51
3	L	356	HIS	CB-CG	6.38	1.61	1.50
2	K	257	PHE	CG-CD1	6.37	1.48	1.38
2	B	107	TYR	CE1-CZ	6.36	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	46	TYR	CZ-OH	6.35	1.48	1.37
2	K	21	ARG	CZ-NH2	6.34	1.41	1.33
1	A	192	ARG	NE-CZ	6.33	1.41	1.33
3	F	388	SER	CA-CB	6.32	1.62	1.52
1	G	198	GLY	N-CA	-6.30	1.36	1.46
3	L	67	ARG	NE-CZ	6.29	1.41	1.33
1	J	94	ARG	CZ-NH2	6.27	1.41	1.33
3	F	236	TYR	CG-CD2	6.26	1.47	1.39
2	H	76	TYR	CZ-OH	6.26	1.48	1.37
1	J	206	GLY	N-CA	-6.25	1.36	1.46
3	I	14	TYR	CZ-OH	6.21	1.48	1.37
2	B	1	TYR	CZ-OH	6.21	1.48	1.37
2	E	59	TYR	CB-CG	-6.20	1.42	1.51
3	I	131	ARG	CZ-NH1	6.18	1.41	1.33
3	L	134	GLY	CA-C	-6.18	1.42	1.51
3	I	163	GLU	CD-OE1	6.14	1.32	1.25
3	I	403	GLY	N-CA	6.14	1.55	1.46
2	H	306	CYS	CB-SG	-6.12	1.71	1.82
3	I	32	SER	CA-CB	6.12	1.62	1.52
1	G	108	PRO	N-CD	-6.12	1.39	1.47
3	I	153	TYR	CZ-OH	6.12	1.48	1.37
3	C	243	ARG	CD-NE	6.11	1.56	1.46
2	B	192	TYR	CB-CG	-6.11	1.42	1.51
2	E	159	SER	CA-CB	6.08	1.62	1.52
2	E	199	ARG	CZ-NH2	6.05	1.41	1.33
3	F	35	HIS	CA-CB	6.05	1.67	1.53
2	B	289	ARG	CZ-NH1	6.04	1.41	1.33
2	K	350	GLY	CA-C	-6.04	1.42	1.51
2	K	206	ARG	NE-CZ	6.04	1.41	1.33
3	C	179	SER	CA-CB	6.02	1.61	1.52
1	G	192	ARG	NE-CZ	6.01	1.40	1.33
2	E	253	ARG	CZ-NH1	5.97	1.40	1.33
2	E	373	ARG	CD-NE	5.97	1.56	1.46
3	F	271	GLU	CD-OE1	5.96	1.32	1.25
2	H	373	ARG	NE-CZ	5.94	1.40	1.33
1	A	173	GLU	CG-CD	5.93	1.60	1.51
3	I	147	ARG	CZ-NH2	5.93	1.40	1.33
3	L	279	GLY	CA-C	-5.93	1.42	1.51
3	F	79	ARG	CZ-NH1	5.93	1.40	1.33
3	I	85	SER	CA-CB	5.92	1.61	1.52
3	F	328	TRP	CB-CG	5.92	1.60	1.50
3	C	115	SER	CA-CB	5.92	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	420	ARG	NE-CZ	5.92	1.40	1.33
3	F	384	CYS	CB-SG	5.92	1.92	1.82
3	I	26	SER	CA-CB	5.91	1.61	1.52
3	I	290	PRO	CA-C	-5.89	1.41	1.52
2	B	56	PRO	N-CD	-5.87	1.39	1.47
3	L	130	PRO	N-CD	-5.87	1.39	1.47
2	B	226	SER	CA-CB	5.85	1.61	1.52
1	A	233	SER	CB-OG	-5.84	1.34	1.42
3	C	67	ARG	CD-NE	5.83	1.56	1.46
3	F	284	HIS	CB-CG	5.83	1.60	1.50
2	B	360	SER	CA-CB	5.82	1.61	1.52
3	C	32	SER	CA-CB	5.82	1.61	1.52
1	A	188	PHE	CG-CD1	5.81	1.47	1.38
2	E	332	SER	CA-CB	5.77	1.61	1.52
2	E	432	SER	CB-OG	5.76	1.49	1.42
2	H	105	GLU	CD-OE2	5.73	1.31	1.25
1	A	170	PHE	CG-CD2	5.73	1.47	1.38
3	I	196	TYR	CG-CD2	5.72	1.46	1.39
3	F	131	ARG	CZ-NH1	5.71	1.40	1.33
1	D	207	ARG	CD-NE	5.71	1.56	1.46
1	J	192	ARG	NE-CZ	5.71	1.40	1.33
3	F	105	ARG	CZ-NH1	5.71	1.40	1.33
2	H	353	SER	CB-OG	-5.69	1.34	1.42
3	C	163	GLU	CB-CG	5.69	1.62	1.52
3	I	17	TRP	NE1-CE2	5.69	1.45	1.37
1	D	149	SER	CA-CB	5.68	1.61	1.52
3	I	50	SER	CA-CB	5.68	1.61	1.52
3	C	357	TYR	CE1-CZ	5.67	1.46	1.38
3	C	103	ARG	CZ-NH2	5.67	1.40	1.33
1	G	165	SER	CA-CB	5.67	1.61	1.52
3	L	161	ARG	CZ-NH2	5.66	1.40	1.33
2	B	438	ARG	CD-NE	5.66	1.56	1.46
2	H	59	TYR	CZ-OH	5.65	1.47	1.37
2	E	279	SER	CA-CB	5.64	1.61	1.52
3	C	161	ARG	NE-CZ	5.64	1.40	1.33
2	E	181	ARG	NE-CZ	5.64	1.40	1.33
3	L	286	HIS	C-N	5.64	1.45	1.34
2	B	248	GLY	CA-C	-5.63	1.42	1.51
3	I	8	TYR	CE2-CZ	5.60	1.45	1.38
2	K	155	ARG	CZ-NH2	5.59	1.40	1.33
3	L	289	TYR	CE2-CZ	5.56	1.45	1.38
3	I	4	HIS	CB-CG	5.56	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	110	VAL	CB-CG1	5.56	1.64	1.52
2	E	238	SER	CA-CB	5.54	1.61	1.52
1	J	150	SER	CA-CB	5.54	1.61	1.52
2	H	332	SER	CA-CB	5.53	1.61	1.52
2	E	206	ARG	CD-NE	5.53	1.55	1.46
3	I	161	ARG	NE-CZ	5.53	1.40	1.33
2	H	76	TYR	CE1-CZ	5.52	1.45	1.38
3	I	409	PHE	CG-CD1	5.51	1.47	1.38
2	B	111	GLY	CA-C	-5.51	1.43	1.51
1	J	237	TRP	CG-CD1	5.50	1.44	1.36
2	H	85	TYR	CZ-OH	5.49	1.47	1.37
3	L	27	CYS	CB-SG	5.49	1.91	1.82
3	F	326	TYR	CE2-CZ	5.48	1.45	1.38
3	L	196	TYR	CG-CD1	5.47	1.46	1.39
2	H	428	VAL	N-CA	-5.47	1.35	1.46
3	I	131	ARG	CD-NE	5.46	1.55	1.46
2	K	438	ARG	N-CA	-5.46	1.35	1.46
2	B	181	ARG	CD-NE	5.45	1.55	1.46
2	B	407	TRP	CG-CD1	5.44	1.44	1.36
2	H	312	PHE	CE1-CZ	5.44	1.47	1.37
3	I	147	ARG	NE-CZ	5.44	1.40	1.33
2	K	101	SER	CB-OG	5.43	1.49	1.42
2	H	273	TYR	CE1-CZ	5.43	1.45	1.38
3	L	127	SER	CA-CB	5.42	1.61	1.52
2	E	201	GLY	CA-C	5.40	1.60	1.51
3	F	391	ARG	NE-CZ	5.40	1.40	1.33
2	H	438	ARG	N-CA	-5.40	1.35	1.46
1	A	94	ARG	NE-CZ	5.40	1.40	1.33
3	C	277	ARG	CD-NE	5.40	1.55	1.46
2	K	199	ARG	NE-CZ	5.39	1.40	1.33
2	E	76	TYR	CB-CG	5.38	1.59	1.51
3	I	20	ASP	N-CA	-5.38	1.35	1.46
3	I	227	TYR	CZ-OH	5.38	1.47	1.37
3	F	107	GLY	CA-C	-5.37	1.43	1.51
2	B	382	PRO	C-N	-5.37	1.24	1.34
1	J	83	PRO	N-CD	5.37	1.55	1.47
2	H	21	ARG	CZ-NH1	5.36	1.40	1.33
3	F	12	ARG	CD-NE	5.36	1.55	1.46
3	I	297	SER	N-CA	-5.36	1.35	1.46
3	F	420	ARG	CD-NE	5.36	1.55	1.46
2	K	205	SER	CA-CB	5.35	1.60	1.52
3	I	78	GLU	CD-OE2	5.35	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	292	GLU	CG-CD	5.35	1.59	1.51
1	G	193	PHE	CD1-CE1	5.34	1.50	1.39
3	F	166	MET	CG-SD	5.34	1.95	1.81
3	C	37	TRP	CE2-CZ2	5.34	1.48	1.39
2	B	21	ARG	CZ-NH2	5.33	1.40	1.33
3	F	123	ARG	CD-NE	5.33	1.55	1.46
3	F	12	ARG	NE-CZ	5.33	1.40	1.33
2	B	122	TYR	CG-CD2	5.32	1.46	1.39
2	H	110	ARG	CZ-NH2	5.31	1.40	1.33
2	K	165	PRO	N-CD	5.30	1.55	1.47
2	E	41	SER	CA-CB	5.30	1.60	1.52
3	L	276	TYR	CG-CD1	5.30	1.46	1.39
2	E	229	VAL	CA-C	5.30	1.66	1.52
3	I	276	TYR	CZ-OH	5.30	1.46	1.37
2	H	365	PHE	CG-CD1	5.29	1.46	1.38
3	F	409	PHE	CG-CD1	5.29	1.46	1.38
1	J	191	GLY	N-CA	-5.29	1.38	1.46
3	C	243	ARG	NE-CZ	5.29	1.40	1.33
3	C	326	TYR	CZ-OH	5.29	1.46	1.37
3	C	420	ARG	CZ-NH1	5.28	1.40	1.33
2	H	112	GLU	CB-CG	5.28	1.62	1.52
3	L	153	TYR	CD2-CE2	-5.28	1.31	1.39
2	K	155	ARG	NE-CZ	5.26	1.39	1.33
3	F	285	PHE	CB-CG	5.25	1.60	1.51
1	A	96	ARG	CD-NE	5.25	1.55	1.46
2	H	159	SER	CA-CB	5.25	1.60	1.52
3	I	170	PRO	N-CD	-5.24	1.40	1.47
2	E	185	TYR	CE1-CZ	5.24	1.45	1.38
3	C	163	GLU	CD-OE1	5.24	1.31	1.25
1	A	102	GLU	CB-CG	5.24	1.62	1.52
3	F	335	ARG	CD-NE	5.24	1.55	1.46
2	E	273	TYR	CE1-CZ	5.23	1.45	1.38
3	C	131	ARG	CZ-NH1	5.21	1.39	1.33
1	G	181	TRP	CB-CG	5.21	1.59	1.50
2	H	7	MET	N-CA	-5.21	1.35	1.46
3	I	113	SER	CA-CB	5.21	1.60	1.52
3	C	25	GLY	CA-C	-5.21	1.43	1.51
3	F	296	ARG	CZ-NH2	5.20	1.39	1.33
3	I	277	ARG	CZ-NH2	5.19	1.39	1.33
3	L	287	PRO	N-CD	-5.17	1.40	1.47
2	B	115	GLU	CD-OE1	5.17	1.31	1.25
3	F	123	ARG	CZ-NH1	5.17	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	267	ARG	CD-NE	5.16	1.55	1.46
1	A	187	GLN	CG-CD	5.16	1.62	1.51
2	K	14	PRO	N-CA	-5.16	1.38	1.47
3	I	24	ALA	C-N	5.15	1.42	1.33
2	E	390	TYR	CE2-CZ	5.15	1.45	1.38
1	J	176	GLU	CB-CG	5.14	1.61	1.52
2	B	296	VAL	CB-CG2	5.14	1.63	1.52
3	I	12	ARG	NE-CZ	5.14	1.39	1.33
2	B	399	PHE	CG-CD2	5.14	1.46	1.38
2	H	218	ASN	N-CA	-5.13	1.36	1.46
3	C	14	TYR	CZ-OH	5.13	1.46	1.37
2	K	64	GLY	N-CA	-5.12	1.38	1.46
2	K	201	GLY	CA-C	-5.12	1.43	1.51
3	L	12	ARG	CZ-NH2	5.12	1.39	1.33
1	G	177	GLY	N-CA	-5.12	1.38	1.46
3	C	333	PRO	CA-C	5.12	1.63	1.52
2	K	308	TYR	CE2-CZ	5.12	1.45	1.38
2	K	200	PHE	CG-CD2	5.11	1.46	1.38
3	C	163	GLU	CG-CD	5.11	1.59	1.51
3	C	152	THR	C-N	5.10	1.45	1.34
3	F	320	GLY	N-CA	5.10	1.53	1.46
2	H	59	TYR	CG-CD2	5.09	1.45	1.39
3	I	202	GLU	CG-CD	-5.09	1.44	1.51
3	F	409	PHE	CE2-CZ	5.09	1.47	1.37
3	F	304	HIS	CB-CG	5.07	1.59	1.50
1	J	181	TRP	NE1-CE2	-5.07	1.30	1.37
1	G	248	GLU	CA-CB	5.07	1.65	1.53
3	C	335	ARG	NE-CZ	5.06	1.39	1.33
2	E	110	ARG	NE-CZ	5.06	1.39	1.33
3	C	277	ARG	CZ-NH1	5.05	1.39	1.33
3	F	277	ARG	CZ-NH1	5.05	1.39	1.33
3	F	17	TRP	CE2-CZ2	5.05	1.48	1.39
3	L	75	GLN	CA-CB	5.04	1.65	1.53
2	H	189	TYR	CG-CD1	5.04	1.45	1.39
2	K	273	TYR	CB-CG	-5.04	1.44	1.51
2	B	312	PHE	CE2-CZ	5.03	1.47	1.37
3	L	420	ARG	NE-CZ	5.03	1.39	1.33
1	D	156	CYS	CA-CB	5.03	1.65	1.53
2	H	87	PHE	CG-CD2	5.02	1.46	1.38
3	I	289	TYR	CD2-CE2	5.02	1.46	1.39
2	E	107	TYR	CG-CD2	5.02	1.45	1.39
2	E	242	TYR	CE1-CZ	5.01	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	346	VAL	CA-CB	-5.01	1.44	1.54
2	K	82	THR	C-N	5.01	1.42	1.33
3	L	236	TYR	CB-CG	5.01	1.59	1.51
3	F	302	PRO	N-CD	-5.01	1.40	1.47
2	K	155	ARG	CD-NE	5.01	1.54	1.46

All (836) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	105	ARG	NE-CZ-NH1	19.59	130.09	120.30
3	C	398	TYR	CB-CG-CD2	-18.30	110.02	121.00
1	G	237	TRP	NE1-CE2-CZ2	17.45	149.59	130.40
3	L	398	TYR	CG-CD2-CE2	-16.81	107.85	121.30
3	F	398	TYR	CG-CD2-CE2	-15.85	108.62	121.30
3	I	276	TYR	CB-CG-CD1	-15.54	111.68	121.00
3	I	398	TYR	CG-CD2-CE2	-15.40	108.98	121.30
1	D	237	TRP	NE1-CE2-CZ2	15.36	147.29	130.40
3	I	398	TYR	CZ-CE2-CD2	-15.17	106.14	119.80
1	A	94	ARG	NE-CZ-NH2	-15.16	112.72	120.30
2	H	192	TYR	CB-CG-CD2	-15.12	111.93	121.00
1	A	237	TRP	NE1-CE2-CZ2	14.49	146.34	130.40
1	J	244	ARG	NE-CZ-NH1	14.14	127.37	120.30
1	J	237	TRP	NE1-CE2-CZ2	14.06	145.87	130.40
3	L	14	TYR	CB-CG-CD2	-13.94	112.64	121.00
3	C	289	TYR	CB-CG-CD2	13.73	129.24	121.00
3	C	398	TYR	CG-CD2-CE2	-13.68	110.36	121.30
3	F	398	TYR	CZ-CE2-CD2	-13.45	107.69	119.80
2	H	273	TYR	CB-CG-CD2	-13.37	112.98	121.00
3	C	398	TYR	CZ-CE2-CD2	-13.29	107.84	119.80
2	H	390	TYR	CB-CG-CD2	-13.24	113.06	121.00
1	J	237	TRP	CD2-CE2-CZ2	-13.06	106.62	122.30
1	G	237	TRP	CD2-CE2-CZ2	-12.97	106.74	122.30
1	A	237	TRP	CD2-CE2-CZ2	-12.95	106.76	122.30
2	H	93	TYR	CB-CG-CD2	-12.94	113.23	121.00
3	L	398	TYR	CZ-CE2-CD2	-12.72	108.35	119.80
2	H	155	ARG	NE-CZ-NH2	-12.69	113.96	120.30
2	H	192	TYR	CB-CG-CD1	12.60	128.56	121.00
1	D	237	TRP	CH2-CZ2-CE2	-12.55	104.85	117.40
2	B	189	TYR	CB-CG-CD1	-12.47	113.52	121.00
2	H	93	TYR	CB-CG-CD1	12.44	128.47	121.00
3	L	296	ARG	NE-CZ-NH2	12.35	126.48	120.30
2	K	173	PHE	CB-CG-CD2	12.35	129.44	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	237	TRP	CD2-CE2-CZ2	-12.26	107.58	122.30
1	J	237	TRP	CH2-CZ2-CE2	-11.93	105.47	117.40
2	B	253	ARG	NE-CZ-NH2	-11.72	114.44	120.30
3	F	398	TYR	CG-CD1-CE1	11.72	130.67	121.30
1	A	152	TYR	CB-CG-CD1	-11.67	114.00	121.00
1	D	229	ARG	NE-CZ-NH2	11.60	126.10	120.30
2	H	242	TYR	CB-CG-CD2	-11.58	114.05	121.00
2	K	214	TYR	CB-CG-CD2	-11.33	114.20	121.00
3	C	398	TYR	CG-CD1-CE1	11.31	130.35	121.30
2	B	122	TYR	CG-CD1-CE1	-11.23	112.32	121.30
3	C	382	PHE	CB-CG-CD2	-11.10	113.03	120.80
1	D	94	ARG	NE-CZ-NH1	11.10	125.85	120.30
2	B	200	PHE	CB-CG-CD2	-11.05	113.06	120.80
2	K	289	ARG	NE-CZ-NH2	-11.02	114.79	120.30
2	H	24	TYR	CB-CG-CD2	-11.00	114.40	121.00
1	J	207	ARG	NE-CZ-NH1	10.92	125.76	120.30
1	J	192	ARG	NE-CZ-NH2	-10.90	114.85	120.30
2	B	229	VAL	CA-C-O	-10.90	97.21	120.10
3	I	398	TYR	CD1-CE1-CZ	10.90	129.61	119.80
3	F	131	ARG	NE-CZ-NH2	-10.87	114.86	120.30
3	L	398	TYR	CG-CD1-CE1	10.72	129.87	121.30
1	A	237	TRP	CH2-CZ2-CE2	-10.63	106.77	117.40
2	B	24	TYR	CB-CG-CD1	-10.62	114.63	121.00
3	L	240	TYR	CB-CG-CD2	-10.59	114.64	121.00
3	F	283	PHE	CB-CG-CD1	-10.59	113.39	120.80
3	I	285	PHE	CB-CG-CD2	-10.58	113.39	120.80
3	F	243	ARG	NE-CZ-NH2	-10.57	115.02	120.30
3	C	289	TYR	CB-CG-CD1	-10.56	114.67	121.00
2	B	206	ARG	NE-CZ-NH1	10.53	125.56	120.30
2	E	161	PHE	CB-CG-CD1	10.52	128.17	120.80
3	I	276	TYR	CB-CG-CD2	10.41	127.24	121.00
1	G	237	TRP	CH2-CZ2-CE2	-10.32	107.08	117.40
3	I	185	TYR	CG-CD1-CE1	-10.28	113.08	121.30
2	E	1	TYR	CB-CG-CD2	-10.17	114.90	121.00
2	K	229	VAL	CA-C-O	-10.16	98.76	120.10
3	I	68	TYR	CB-CG-CD1	10.16	127.10	121.00
2	H	229	VAL	CA-C-O	-10.15	98.79	120.10
2	E	206	ARG	NE-CZ-NH1	10.13	125.37	120.30
1	J	237	TRP	CE3-CZ3-CH2	10.12	132.34	121.20
3	I	382	PHE	CB-CG-CD1	10.05	127.84	120.80
3	L	240	TYR	CB-CG-CD1	9.99	126.99	121.00
1	J	118	TYR	CB-CG-CD1	-9.94	115.04	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	202	ASP	CB-CG-OD1	-9.89	109.40	118.30
3	I	147	ARG	NE-CZ-NH2	-9.87	115.37	120.30
3	C	398	TYR	CB-CG-CD1	9.85	126.91	121.00
3	F	12	ARG	NE-CZ-NH2	-9.83	115.38	120.30
3	L	335	ARG	NE-CZ-NH2	-9.83	115.39	120.30
2	H	242	TYR	CB-CG-CD1	9.79	126.87	121.00
2	K	192	TYR	CB-CG-CD1	9.77	126.86	121.00
3	F	240	TYR	CB-CG-CD2	-9.76	115.14	121.00
2	B	200	PHE	CB-CG-CD1	9.73	127.61	120.80
2	H	373	ARG	NE-CZ-NH2	-9.72	115.44	120.30
2	E	312	PHE	CB-CG-CD2	-9.72	114.00	120.80
2	K	110	ARG	NE-CZ-NH1	9.63	125.12	120.30
3	I	363	TYR	CB-CG-CD2	9.53	126.72	121.00
2	H	180	TYR	CB-CG-CD2	-9.52	115.29	121.00
2	B	233	TYR	CB-CG-CD2	-9.52	115.29	121.00
1	A	179	TYR	CB-CG-CD1	9.50	126.70	121.00
3	I	293	PHE	CB-CG-CD2	-9.43	114.20	120.80
2	E	200	PHE	CB-CG-CD2	-9.41	114.21	120.80
1	D	146	PHE	CB-CG-CD2	-9.40	114.22	120.80
2	K	289	ARG	NE-CZ-NH1	9.39	124.99	120.30
3	L	420	ARG	NE-CZ-NH1	9.37	124.99	120.30
3	I	382	PHE	CB-CG-CD2	-9.36	114.25	120.80
2	K	214	TYR	CB-CG-CD1	9.35	126.61	121.00
1	D	244	ARG	NE-CZ-NH2	-9.34	115.63	120.30
2	B	242	TYR	CB-CG-CD2	-9.27	115.44	121.00
3	I	161	ARG	NE-CZ-NH2	-9.25	115.67	120.30
3	C	313	MET	CG-SD-CE	-9.20	85.48	100.20
1	D	94	ARG	NE-CZ-NH2	-9.16	115.72	120.30
3	F	103	ARG	NE-CZ-NH2	-9.16	115.72	120.30
2	B	185	TYR	CB-CG-CD2	9.15	126.49	121.00
3	I	398	TYR	CG-CD1-CE1	9.14	128.62	121.30
1	G	157	ALA	N-CA-CB	9.12	122.87	110.10
1	A	237	TRP	CD2-CE3-CZ3	9.10	130.63	118.80
2	H	267	ARG	NE-CZ-NH1	-9.08	115.76	120.30
3	L	12	ARG	NE-CZ-NH2	-9.04	115.78	120.30
3	C	398	TYR	CD1-CE1-CZ	9.00	127.90	119.80
3	F	277	ARG	NE-CZ-NH1	-8.98	115.81	120.30
3	I	105	ARG	NE-CZ-NH2	-8.89	115.86	120.30
3	C	221	ALA	N-CA-CB	8.87	122.51	110.10
2	B	173	PHE	CB-CG-CD1	8.84	126.98	120.80
3	F	385	PHE	CB-CG-CD1	8.82	126.97	120.80
2	E	188	ASP	CB-CG-OD1	-8.77	110.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	229	VAL	CA-C-O	-8.73	101.76	120.10
2	K	341	ASP	CB-CG-OD2	-8.71	110.46	118.30
1	G	237	TRP	CE3-CZ3-CH2	8.62	130.69	121.20
2	K	1	TYR	CB-CG-CD2	-8.62	115.83	121.00
3	L	14	TYR	CB-CG-CD1	8.61	126.17	121.00
1	A	96	ARG	NE-CZ-NH1	8.60	124.60	120.30
3	F	240	TYR	CB-CG-CD1	8.57	126.14	121.00
2	K	147	PHE	CB-CG-CD1	-8.56	114.81	120.80
2	E	122	TYR	CB-CG-CD1	8.56	126.14	121.00
1	A	110	MET	CG-SD-CE	-8.54	86.53	100.20
3	I	68	TYR	CB-CG-CD2	-8.51	115.90	121.00
1	D	192	ARG	NE-CZ-NH2	-8.49	116.06	120.30
3	F	185	TYR	CB-CG-CD2	-8.47	115.92	121.00
3	I	363	TYR	CB-CG-CD1	-8.42	115.95	121.00
1	D	224	ALA	N-CA-CB	8.42	121.89	110.10
2	H	212	ASP	CB-CG-OD2	8.42	125.88	118.30
3	F	126	PHE	CB-CG-CD1	-8.41	114.91	120.80
3	L	132	PHE	CB-CG-CD1	-8.40	114.92	120.80
2	B	242	TYR	CB-CG-CD1	8.38	126.03	121.00
2	H	199	ARG	NE-CZ-NH1	8.37	124.48	120.30
3	L	196	TYR	CB-CG-CD1	8.35	126.01	121.00
1	D	237	TRP	CE3-CZ3-CH2	8.32	130.35	121.20
1	D	237	TRP	CD2-CE3-CZ3	8.32	129.62	118.80
3	L	358	TYR	CB-CG-CD1	-8.30	116.02	121.00
3	F	8	TYR	CB-CG-CD1	-8.29	116.03	121.00
2	E	424	ALA	CB-CA-C	-8.28	97.68	110.10
3	I	94	ALA	CB-CA-C	-8.26	97.70	110.10
2	K	305	SER	N-CA-CB	8.23	122.84	110.50
3	C	12	ARG	NE-CZ-NH1	8.22	124.41	120.30
2	K	192	TYR	CB-CG-CD2	-8.21	116.08	121.00
3	L	342	SER	N-CA-CB	8.19	122.79	110.50
3	F	296	ARG	NE-CZ-NH2	-8.18	116.21	120.30
3	C	335	ARG	NE-CZ-NH2	-8.16	116.22	120.30
3	F	358	TYR	CZ-CE2-CD2	-8.15	112.46	119.80
1	D	200	GLY	N-CA-C	-8.08	92.89	113.10
1	A	237	TRP	CG-CD1-NE1	8.08	118.18	110.10
2	E	312	PHE	CB-CG-CD1	8.07	126.45	120.80
3	I	39	ASP	CB-CG-OD1	-8.05	111.05	118.30
3	F	185	TYR	CG-CD1-CE1	-8.05	114.86	121.30
2	B	253	ARG	NE-CZ-NH1	8.03	124.32	120.30
3	F	398	TYR	CB-CG-CD2	-8.03	116.18	121.00
2	K	308	TYR	CB-CG-CD1	8.03	125.81	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	68	TYR	CB-CG-CD2	-8.02	116.19	121.00
2	H	85	TYR	CB-CG-CD1	-8.00	116.20	121.00
2	K	85	TYR	CB-CG-CD1	-8.00	116.20	121.00
2	H	257	PHE	CB-CG-CD2	-7.98	115.22	120.80
2	B	155	ARG	NE-CZ-NH2	-7.96	116.32	120.30
3	I	185	TYR	CB-CG-CD2	-7.95	116.23	121.00
1	D	146	PHE	CB-CG-CD1	7.95	126.36	120.80
3	L	420	ARG	NE-CZ-NH2	-7.95	116.33	120.30
2	B	285	ALA	N-CA-CB	7.94	121.21	110.10
2	K	110	ARG	NE-CZ-NH2	-7.93	116.34	120.30
3	F	161	ARG	NE-CZ-NH1	7.91	124.25	120.30
2	E	287	PHE	CB-CG-CD1	7.89	126.32	120.80
3	I	12	ARG	NE-CZ-NH2	-7.88	116.36	120.30
3	F	103	ARG	NE-CZ-NH1	7.86	124.23	120.30
3	I	285	PHE	CB-CG-CD1	7.85	126.30	120.80
2	E	311	ASP	CB-CG-OD1	7.84	125.36	118.30
1	A	179	TYR	CB-CG-CD2	-7.84	116.30	121.00
3	F	285	PHE	CB-CG-CD1	7.82	126.28	120.80
3	C	132	PHE	CB-CG-CD1	-7.81	115.33	120.80
2	B	210	SER	N-CA-CB	7.80	122.20	110.50
3	C	382	PHE	CB-CG-CD1	7.78	126.25	120.80
2	K	267	ARG	NE-CZ-NH2	-7.77	116.41	120.30
1	G	170	PHE	CB-CG-CD1	-7.71	115.40	120.80
1	J	170	PHE	CB-CG-CD2	-7.68	115.42	120.80
1	J	237	TRP	CD2-CE3-CZ3	7.68	128.78	118.80
3	F	257	PHE	CB-CG-CD1	7.66	126.16	120.80
3	F	283	PHE	CB-CG-CD2	7.63	126.14	120.80
1	G	195	ILE	CA-CB-CG1	7.63	125.50	111.00
3	L	236	TYR	CB-CG-CD2	-7.63	116.42	121.00
2	H	390	TYR	CB-CG-CD1	7.62	125.57	121.00
2	E	289	ARG	NE-CZ-NH1	7.62	124.11	120.30
2	B	267	ARG	NE-CZ-NH1	7.61	124.11	120.30
3	I	357	TYR	CG-CD1-CE1	-7.58	115.24	121.30
1	J	192	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	E	373	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	K	202	ASP	CB-CG-OD2	-7.57	111.48	118.30
2	B	289	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	G	146	PHE	CB-CG-CD1	7.50	126.05	120.80
1	J	210	PHE	CB-CG-CD2	-7.49	115.56	120.80
3	F	398	TYR	CD1-CE1-CZ	7.47	126.52	119.80
2	B	93	TYR	CB-CG-CD1	-7.47	116.52	121.00
3	C	296	ARG	NE-CZ-NH2	-7.46	116.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	399	PHE	CB-CG-CD2	-7.42	115.60	120.80
2	B	182	ASP	CB-CG-OD1	-7.42	111.62	118.30
2	B	122	TYR	CB-CG-CD2	-7.39	116.57	121.00
2	H	357	ALA	N-CA-CB	7.38	120.44	110.10
3	L	398	TYR	CD1-CE1-CZ	7.36	126.42	119.80
3	C	68	TYR	CB-CG-CD1	-7.34	116.59	121.00
3	F	110	VAL	CG1-CB-CG2	-7.34	99.15	110.90
2	K	97	ASP	CB-CG-OD2	-7.32	111.71	118.30
2	B	69	SER	N-CA-CB	7.30	121.46	110.50
1	G	181	TRP	CB-CG-CD2	-7.30	117.11	126.60
1	G	152	TYR	CB-CG-CD1	-7.27	116.64	121.00
2	E	46	TYR	CB-CG-CD1	7.26	125.36	121.00
3	F	420	ARG	NE-CZ-NH2	-7.25	116.68	120.30
3	F	123	ARG	NE-CZ-NH2	-7.24	116.68	120.30
2	H	214	TYR	CB-CG-CD1	7.22	125.33	121.00
1	G	237	TRP	CD2-CE3-CZ3	7.21	128.17	118.80
3	I	12	ARG	NE-CZ-NH1	7.21	123.91	120.30
3	F	385	PHE	CB-CG-CD2	-7.20	115.76	120.80
2	E	308	TYR	CB-CG-CD1	-7.18	116.69	121.00
2	H	428	VAL	CB-CA-C	-7.17	97.77	111.40
2	K	59	TYR	CB-CG-CD1	7.17	125.31	121.00
2	E	161	PHE	CB-CG-CD2	-7.14	115.80	120.80
2	B	155	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	G	204	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	J	152	TYR	CB-CG-CD1	-7.11	116.74	121.00
3	I	283	PHE	CB-CG-CD1	-7.10	115.83	120.80
3	I	305	SER	N-CA-CB	7.09	121.14	110.50
2	B	208	VAL	CA-CB-CG1	-7.08	100.29	110.90
2	K	85	TYR	CB-CG-CD2	7.07	125.24	121.00
1	G	243	THR	N-CA-CB	7.06	123.72	110.30
2	H	117	ASP	CB-CG-OD2	-7.06	111.95	118.30
2	H	116	ALA	N-CA-CB	7.03	119.94	110.10
1	A	185	ALA	N-CA-CB	7.02	119.92	110.10
2	K	231	VAL	N-CA-CB	7.01	126.92	111.50
2	K	181	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	J	237	TRP	CG-CD1-NE1	6.98	117.08	110.10
2	H	117	ASP	CB-CG-OD1	6.97	124.58	118.30
2	B	108	VAL	CA-CB-CG2	-6.97	100.45	110.90
3	I	196	TYR	N-CA-CB	6.96	123.14	110.60
2	E	7	MET	CG-SD-CE	-6.96	89.06	100.20
3	L	12	ARG	NE-CZ-NH1	6.96	123.78	120.30
3	L	171	ASP	CB-CG-OD1	-6.95	112.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	174	ASP	CB-CG-OD2	-6.94	112.05	118.30
2	E	107	TYR	CB-CG-CD2	6.94	125.16	121.00
2	H	1	TYR	CB-CG-CD1	-6.93	116.84	121.00
2	E	385	ASP	CB-CG-OD2	-6.91	112.08	118.30
2	K	409	TRP	CB-CG-CD2	-6.91	117.62	126.60
2	B	76	TYR	CD1-CE1-CZ	-6.90	113.59	119.80
3	C	79	ARG	NE-CZ-NH1	-6.89	116.86	120.30
2	H	45	ASP	CB-CG-OD2	6.89	124.50	118.30
2	E	311	ASP	CB-CG-OD2	-6.87	112.12	118.30
3	C	17	TRP	CB-CG-CD2	-6.87	117.67	126.60
2	B	81	PHE	CD1-CE1-CZ	-6.86	111.87	120.10
3	C	236	TYR	CB-CG-CD2	-6.86	116.89	121.00
2	H	4	SER	N-CA-CB	6.86	120.78	110.50
3	C	218	CYS	N-CA-CB	6.85	122.92	110.60
2	E	253	ARG	NE-CZ-NH2	-6.84	116.88	120.30
2	H	162	ILE	N-CA-C	-6.81	92.61	111.00
2	K	1	TYR	CB-CG-CD1	6.81	125.08	121.00
2	K	280	MET	CG-SD-CE	6.79	111.07	100.20
2	H	85	TYR	CB-CG-CD2	6.78	125.07	121.00
1	A	237	TRP	CE3-CZ3-CH2	6.78	128.66	121.20
3	L	257	PHE	CB-CG-CD1	-6.77	116.06	120.80
2	K	438	ARG	NE-CZ-NH1	6.77	123.68	120.30
3	F	82	LEU	N-CA-C	-6.77	92.73	111.00
2	K	122	TYR	CG-CD2-CE2	-6.75	115.90	121.30
3	F	132	PHE	CB-CG-CD1	6.74	125.52	120.80
2	E	212	ASP	CB-CG-OD1	-6.74	112.23	118.30
3	L	105	ARG	NH1-CZ-NH2	-6.73	112.00	119.40
3	I	357	TYR	CZ-CE2-CD2	-6.72	113.75	119.80
1	D	107	PHE	CB-CG-CD2	-6.72	116.10	120.80
3	L	404	ALA	N-CA-CB	6.71	119.49	110.10
3	C	363	TYR	CB-CG-CD2	-6.70	116.98	121.00
2	H	257	PHE	CB-CG-CD1	6.69	125.48	120.80
3	L	196	TYR	CB-CG-CD2	-6.69	116.99	121.00
2	K	200	PHE	CB-CG-CD2	6.69	125.48	120.80
1	J	228	ALA	N-CA-CB	6.68	119.46	110.10
2	B	1	TYR	CB-CG-CD2	-6.66	117.00	121.00
3	L	69	MET	CG-SD-CE	-6.66	89.54	100.20
3	F	229	VAL	CG1-CB-CG2	6.65	121.55	110.90
2	E	267	ARG	NE-CZ-NH1	6.64	123.62	120.30
2	B	81	PHE	N-CA-CB	6.64	122.55	110.60
2	H	308	TYR	CB-CG-CD2	6.62	124.97	121.00
2	B	119	ALA	N-CA-CB	6.62	119.37	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	233	TYR	CB-CG-CD1	6.62	124.97	121.00
2	K	259	CYS	CB-CA-C	6.61	123.62	110.40
3	C	402	PRO	C-N-CA	6.61	136.18	122.30
3	I	385	PHE	CB-CG-CD1	-6.60	116.18	120.80
2	B	334	SER	N-CA-CB	6.59	120.39	110.50
3	L	411	ALA	CB-CA-C	-6.58	100.22	110.10
2	B	46	TYR	CB-CG-CD2	6.57	124.94	121.00
2	H	185	TYR	CB-CG-CD2	-6.57	117.06	121.00
2	B	243	TRP	CB-CG-CD2	-6.56	118.07	126.60
3	C	48	GLN	N-CA-CB	6.56	122.41	110.60
2	B	101	SER	N-CA-CB	6.55	120.33	110.50
3	C	138	SER	N-CA-CB	6.55	120.32	110.50
1	J	142	ALA	N-CA-CB	6.53	119.25	110.10
2	H	390	TYR	CG-CD1-CE1	-6.50	116.10	121.30
3	C	243	ARG	NE-CZ-NH1	-6.50	117.05	120.30
2	E	93	TYR	CB-CG-CD1	6.50	124.90	121.00
2	B	189	TYR	CZ-CE2-CD2	-6.49	113.96	119.80
2	H	259	CYS	N-CA-CB	6.49	122.28	110.60
2	E	221	LEU	N-CA-CB	6.47	123.35	110.40
3	C	390	ALA	N-CA-CB	6.47	119.16	110.10
2	H	23	GLY	N-CA-C	-6.47	96.93	113.10
2	B	192	TYR	CB-CG-CD2	6.46	124.88	121.00
2	K	148	VAL	CA-CB-CG1	-6.46	101.21	110.90
2	H	128	SER	N-CA-CB	6.46	120.19	110.50
2	H	24	TYR	CB-CG-CD1	6.45	124.87	121.00
2	B	279	SER	N-CA-CB	6.45	120.17	110.50
1	D	240	ASP	CB-CG-OD1	-6.45	112.50	118.30
1	G	197	THR	CA-CB-CG2	-6.45	103.38	112.40
2	E	240	PHE	CB-CG-CD2	-6.44	116.29	120.80
1	D	209	ILE	N-CA-C	-6.44	93.62	111.00
2	E	200	PHE	CB-CG-CD1	6.44	125.31	120.80
3	F	17	TRP	CG-CD2-CE3	-6.43	128.11	133.90
2	B	39	VAL	CG1-CB-CG2	-6.43	100.62	110.90
2	H	174	ASP	CB-CG-OD2	6.43	124.08	118.30
1	D	233	SER	N-CA-CB	6.42	120.14	110.50
2	H	312	PHE	CB-CG-CD2	-6.42	116.31	120.80
3	L	173	PRO	C-N-CA	6.40	137.71	121.70
3	F	305	SER	O-C-N	-6.39	112.47	122.70
3	F	115	SER	N-CA-CB	6.39	120.09	110.50
3	I	132	PHE	N-CA-CB	6.39	122.10	110.60
2	E	155	ARG	NE-CZ-NH1	6.38	123.49	120.30
3	I	346	ALA	N-CA-CB	6.38	119.03	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	TRP	CE2-CD2-CG	-6.38	102.20	107.30
2	E	170	TRP	CB-CG-CD2	-6.37	118.32	126.60
2	E	409	TRP	CG-CD2-CE3	-6.37	128.17	133.90
3	F	67	ARG	NE-CZ-NH1	6.36	123.48	120.30
2	B	46	TYR	CB-CG-CD1	-6.35	117.19	121.00
2	H	296	VAL	CG1-CB-CG2	-6.35	100.73	110.90
3	F	140	ALA	N-CA-CB	6.35	118.99	110.10
2	K	4	SER	N-CA-CB	6.34	120.01	110.50
2	K	243	TRP	CE2-CD2-CG	-6.34	102.23	107.30
2	E	95	PHE	CB-CG-CD1	-6.34	116.36	120.80
1	D	193	PHE	CB-CG-CD1	6.33	125.23	120.80
1	G	152	TYR	CG-CD1-CE1	-6.33	116.24	121.30
3	I	326	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	D	118	TYR	CG-CD1-CE1	6.32	126.36	121.30
2	H	87	PHE	CB-CG-CD1	-6.32	116.38	120.80
3	L	285	PHE	CG-CD2-CE2	-6.32	113.85	120.80
3	C	365	THR	CA-CB-CG2	-6.32	103.56	112.40
3	F	267	SER	N-CA-CB	6.31	119.96	110.50
3	C	326	TYR	CB-CG-CD2	6.30	124.78	121.00
3	F	132	PHE	CB-CG-CD2	-6.29	116.39	120.80
2	B	199	ARG	NE-CZ-NH1	6.29	123.45	120.30
3	C	140	ALA	N-CA-CB	6.29	118.91	110.10
1	G	228	ALA	N-CA-CB	6.29	118.90	110.10
2	K	21	ARG	NE-CZ-NH1	6.28	123.44	120.30
3	C	131	ARG	NE-CZ-NH2	6.28	123.44	120.30
2	K	206	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	A	104	ASP	CB-CG-OD2	-6.27	112.66	118.30
3	F	269	ALA	N-CA-CB	-6.26	101.33	110.10
2	B	151	ASP	CB-CG-OD1	-6.26	112.67	118.30
2	B	312	PHE	CB-CG-CD2	6.26	125.18	120.80
3	F	294	SER	N-CA-CB	6.25	119.87	110.50
3	F	196	TYR	CB-CG-CD2	-6.25	117.25	121.00
2	H	214	TYR	CB-CG-CD2	-6.25	117.25	121.00
2	K	173	PHE	CB-CG-CD1	-6.25	116.43	120.80
2	B	77	LYS	N-CA-CB	6.24	121.84	110.60
3	C	56	ALA	N-CA-CB	6.24	118.84	110.10
3	F	88	ALA	N-CA-CB	6.24	118.83	110.10
2	H	212	ASP	CB-CG-OD1	-6.22	112.70	118.30
3	L	335	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	K	122	TYR	CB-CG-CD1	-6.22	117.27	121.00
3	L	285	PHE	CB-CG-CD1	-6.22	116.45	120.80
3	L	257	PHE	CB-CG-CD2	6.21	125.15	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	109	THR	CA-CB-CG2	-6.20	103.71	112.40
2	H	438	ARG	N-CA-CB	6.20	121.76	110.60
3	L	96	MET	CG-SD-CE	-6.20	90.28	100.20
1	D	244	ARG	NE-CZ-NH1	6.20	123.40	120.30
2	H	57	SER	O-C-N	-6.20	109.33	121.10
2	E	238	SER	C-N-CA	6.19	135.30	122.30
3	L	384	CYS	CA-CB-SG	-6.19	102.85	114.00
2	E	202	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	193	PHE	CB-CG-CD2	6.18	125.13	120.80
2	B	250	PRO	O-C-N	6.18	132.59	122.70
3	C	361	TYR	CB-CG-CD1	-6.18	117.29	121.00
2	H	245	LYS	N-CA-CB	6.18	121.72	110.60
2	E	46	TYR	CB-CG-CD2	-6.16	117.30	121.00
2	K	263	VAL	CG1-CB-CG2	6.16	120.76	110.90
3	F	409	PHE	CB-CG-CD2	6.16	125.11	120.80
3	C	79	ARG	CG-CD-NE	-6.16	98.87	111.80
2	B	312	PHE	CB-CG-CD1	-6.15	116.49	120.80
3	F	45	LEU	CB-CG-CD2	6.14	121.43	111.00
3	C	231	ASN	C-N-CA	6.12	137.01	121.70
1	J	152	TYR	CG-CD1-CE1	-6.12	116.40	121.30
3	C	319	VAL	CA-CB-CG1	-6.12	101.72	110.90
2	B	212	ASP	CB-CG-OD1	6.11	123.80	118.30
2	K	262	LYS	N-CA-CB	6.11	121.60	110.60
3	C	340	LYS	N-CA-CB	6.11	121.60	110.60
3	I	131	ARG	NE-CZ-NH1	-6.11	117.25	120.30
3	C	390	ALA	CB-CA-C	-6.11	100.94	110.10
2	B	206	ARG	NH1-CZ-NH2	-6.10	112.69	119.40
3	C	288	MET	N-CA-CB	6.10	121.58	110.60
3	L	333	PRO	N-CA-CB	6.10	110.62	103.30
3	L	14	TYR	CZ-CE2-CD2	6.09	125.28	119.80
3	I	79	ARG	NE-CZ-NH1	6.09	123.34	120.30
3	C	335	ARG	NH1-CZ-NH2	6.08	126.09	119.40
2	B	414	THR	CA-CB-CG2	-6.08	103.89	112.40
2	E	122	TYR	CB-CG-CD2	-6.08	117.35	121.00
2	E	73	GLU	N-CA-CB	6.08	121.54	110.60
2	E	273	TYR	CB-CA-C	-6.05	98.29	110.40
2	E	144	VAL	CA-CB-CG1	6.05	119.98	110.90
3	I	358	TYR	CG-CD2-CE2	-6.05	116.46	121.30
2	B	271	CYS	N-CA-CB	6.04	121.47	110.60
3	I	324	VAL	CA-CB-CG1	-6.04	101.85	110.90
3	L	234	TRP	CD2-CE2-CZ2	-6.04	115.06	122.30
1	J	181	TRP	CE2-CD2-CE3	6.03	125.94	118.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	24	ALA	N-CA-CB	6.03	118.54	110.10
3	L	418	SER	N-CA-CB	6.03	119.54	110.50
2	H	132	GLN	N-CA-CB	6.02	121.44	110.60
2	B	4	SER	N-CA-CB	6.02	119.53	110.50
3	C	145	LYS	N-CA-CB	6.01	121.42	110.60
2	E	339	MET	N-CA-CB	6.00	121.40	110.60
2	B	252	ASN	N-CA-CB	-6.00	99.80	110.60
2	E	229	VAL	CG1-CB-CG2	6.00	120.50	110.90
1	J	244	ARG	NH1-CZ-NH2	-6.00	112.80	119.40
1	D	188	PHE	CB-CG-CD1	-5.99	116.61	120.80
1	J	99	MET	CB-CA-C	-5.99	98.41	110.40
2	E	222	LYS	O-C-N	5.99	132.28	122.70
1	D	126	VAL	CA-CB-CG1	5.98	119.87	110.90
2	E	167	SER	N-CA-CB	5.98	119.47	110.50
1	J	125	LYS	N-CA-CB	5.98	121.37	110.60
3	L	306	GLN	N-CA-CB	5.97	121.34	110.60
2	B	121	ALA	CB-CA-C	-5.96	101.16	110.10
2	E	255	ALA	N-CA-CB	5.96	118.44	110.10
3	I	293	PHE	CB-CG-CD1	5.96	124.97	120.80
3	F	44	VAL	CA-CB-CG2	-5.96	101.96	110.90
3	I	147	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	B	36	SER	N-CA-CB	5.95	119.43	110.50
2	H	407	TRP	CB-CA-C	-5.95	98.49	110.40
1	A	152	TYR	CB-CG-CD2	5.95	124.57	121.00
2	B	75	ASP	CB-CG-OD2	5.95	123.65	118.30
1	D	192	ARG	NH1-CZ-NH2	5.93	125.92	119.40
3	C	335	ARG	NE-CZ-NH1	-5.92	117.34	120.30
3	F	126	PHE	CB-CG-CD2	5.92	124.94	120.80
2	K	437	ALA	O-C-N	5.92	132.17	122.70
2	B	24	TYR	CB-CG-CD2	5.92	124.55	121.00
2	E	292	GLU	N-CA-CB	5.92	121.25	110.60
2	H	51	TYR	CZ-CE2-CD2	5.92	125.12	119.80
1	J	229	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	94	ARG	NH1-CZ-NH2	5.90	125.89	119.40
3	L	74	VAL	CG1-CB-CG2	5.90	120.34	110.90
2	E	339	MET	N-CA-C	-5.90	95.08	111.00
2	E	234	THR	N-CA-CB	5.89	121.49	110.30
3	I	227	TYR	CB-CG-CD1	5.89	124.54	121.00
2	H	185	TYR	CB-CG-CD1	5.89	124.53	121.00
3	I	285	PHE	N-CA-CB	-5.89	100.00	110.60
1	A	210	PHE	N-CA-CB	5.88	121.18	110.60
2	H	400	PRO	N-CD-CG	5.87	112.01	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	TYR	CD1-CE1-CZ	5.87	125.08	119.80
2	K	355	PHE	CB-CG-CD2	5.87	124.91	120.80
3	F	153	TYR	CB-CG-CD1	5.86	124.52	121.00
2	B	199	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	G	231	ALA	N-CA-CB	5.86	118.31	110.10
2	H	1	TYR	CB-CG-CD2	5.86	124.52	121.00
1	A	154	LEU	CB-CG-CD1	5.86	120.96	111.00
3	F	59	ASN	N-CA-CB	5.86	121.15	110.60
2	K	409	TRP	CB-CG-CD1	5.86	134.61	127.00
2	E	155	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	J	193	PHE	CB-CA-C	-5.84	98.72	110.40
3	F	171	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	112	ASP	CB-CG-OD1	-5.83	113.05	118.30
1	G	128	LYS	CA-C-O	-5.83	107.86	120.10
3	L	293	PHE	CB-CG-CD2	5.83	124.88	120.80
1	G	167	ALA	CB-CA-C	5.82	118.83	110.10
2	K	373	ARG	NE-CZ-NH2	-5.81	117.39	120.30
3	C	123	ARG	NE-CZ-NH1	-5.81	117.40	120.30
3	C	37	TRP	NE1-CE2-CZ2	5.80	136.78	130.40
3	I	387	CYS	CB-CA-C	-5.79	98.81	110.40
2	H	181	ARG	NE-CZ-NH2	-5.79	117.40	120.30
2	E	103	MET	CG-SD-CE	-5.79	90.94	100.20
2	K	406	ALA	CB-CA-C	-5.79	101.42	110.10
3	I	166	MET	CA-CB-CG	5.78	123.13	113.30
1	D	144	LEU	CB-CG-CD2	-5.77	101.19	111.00
2	H	310	SER	N-CA-CB	5.77	119.15	110.50
2	E	369	VAL	N-CA-C	-5.75	95.46	111.00
2	H	81	PHE	CB-CG-CD1	-5.75	116.77	120.80
2	B	189	TYR	CD1-CG-CD2	5.75	124.23	117.90
2	B	209	ASN	N-CA-C	-5.75	95.48	111.00
1	G	185	ALA	N-CA-CB	5.75	118.15	110.10
3	L	337	TRP	CE3-CZ3-CH2	5.75	127.52	121.20
2	K	438	ARG	N-CA-CB	5.74	120.94	110.60
2	H	110	ARG	NE-CZ-NH1	5.74	123.17	120.30
3	F	221	ALA	CA-C-N	5.74	133.17	117.10
1	J	193	PHE	CB-CG-CD2	-5.74	116.78	120.80
2	B	355	PHE	CB-CG-CD2	-5.74	116.79	120.80
1	D	237	TRP	CG-CD1-NE1	5.74	115.83	110.10
1	D	179	TYR	CB-CG-CD2	5.73	124.44	121.00
2	E	353	SER	N-CA-CB	5.73	119.10	110.50
2	K	28	PRO	N-CA-C	-5.73	97.20	112.10
3	L	252	LYS	N-CA-CB	5.73	120.91	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	302	PRO	C-N-CA	5.72	136.01	121.70
2	B	273	TYR	CG-CD2-CE2	-5.72	116.72	121.30
3	F	12	ARG	NE-CZ-NH1	5.71	123.16	120.30
2	B	242	TYR	CZ-CE2-CD2	-5.71	114.66	119.80
2	B	272	VAL	CA-CB-CG2	-5.71	102.33	110.90
3	L	364	TRP	CB-CG-CD2	-5.71	119.18	126.60
1	A	210	PHE	CB-CG-CD2	5.70	124.79	120.80
3	F	312	PRO	N-CA-CB	5.70	110.14	103.30
3	F	308	TRP	N-CA-CB	5.68	120.83	110.60
3	L	361	TYR	CZ-CE2-CD2	-5.68	114.69	119.80
1	D	95	MET	CA-CB-CG	5.68	122.95	113.30
3	L	33	ILE	O-C-N	5.68	131.78	122.70
3	F	37	TRP	NE1-CE2-CZ2	5.67	136.64	130.40
1	A	240	ASP	CB-CG-OD1	-5.67	113.20	118.30
2	K	254	ASN	C-N-CA	5.67	135.86	121.70
1	G	211	ASP	CB-CG-OD2	5.66	123.40	118.30
2	B	308	TYR	CD1-CE1-CZ	5.66	124.89	119.80
2	E	170	TRP	CD1-CG-CD2	5.65	110.82	106.30
2	K	385	ASP	C-N-CA	5.65	135.84	121.70
3	L	164	ILE	N-CA-CB	5.65	123.78	110.80
2	H	308	TYR	CA-CB-CG	-5.64	102.68	113.40
2	B	255	ALA	N-CA-CB	5.64	118.00	110.10
3	C	17	TRP	CE2-CD2-CE3	5.64	125.47	118.70
2	E	243	TRP	CB-CG-CD2	-5.63	119.28	126.60
3	I	253	ILE	C-N-CA	5.63	135.79	121.70
2	B	75	ASP	CB-CG-OD1	-5.63	113.23	118.30
3	I	19	ALA	CB-CA-C	-5.63	101.65	110.10
2	K	178	ILE	CA-CB-CG2	-5.63	99.64	110.90
1	A	190	ASN	N-CA-CB	5.63	120.73	110.60
3	I	102	ALA	N-CA-CB	5.63	117.98	110.10
3	I	355	SER	N-CA-CB	5.62	118.94	110.50
3	F	48	GLN	N-CA-CB	5.62	120.72	110.60
3	L	118	PRO	O-C-N	5.62	131.69	122.70
3	C	161	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	G	85	GLN	N-CA-CB	5.61	120.70	110.60
2	B	110	ARG	NE-CZ-NH2	5.61	123.10	120.30
3	C	172	VAL	CG1-CB-CG2	-5.61	101.93	110.90
2	E	273	TYR	CG-CD1-CE1	-5.61	116.82	121.30
2	E	297	SER	N-CA-CB	5.60	118.90	110.50
2	H	399	PHE	CB-CG-CD1	-5.60	116.88	120.80
1	G	118	TYR	O-C-N	5.60	131.65	122.70
3	I	193	THR	N-CA-CB	5.59	120.93	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	337	TRP	CG-CD2-CE3	-5.59	128.87	133.90
2	B	311	ASP	CA-CB-CG	-5.59	101.10	113.40
3	L	204	VAL	CA-CB-CG2	5.59	119.29	110.90
2	K	354	LEU	CB-CG-CD2	5.59	120.50	111.00
2	H	266	VAL	CA-CB-CG1	-5.58	102.53	110.90
2	B	116	ALA	N-CA-CB	5.58	117.91	110.10
2	B	416	GLY	N-CA-C	5.58	127.04	113.10
1	G	90	LYS	CB-CA-C	-5.57	99.26	110.40
3	F	178	VAL	CA-CB-CG2	5.57	119.25	110.90
2	H	351	ALA	N-CA-CB	5.56	117.89	110.10
3	L	221	ALA	CB-CA-C	5.56	118.44	110.10
3	C	277	ARG	N-CA-CB	5.55	120.59	110.60
1	G	118	TYR	CD1-CE1-CZ	-5.55	114.81	119.80
3	L	67	ARG	CD-NE-CZ	-5.55	115.83	123.60
2	B	54	VAL	N-CA-C	-5.54	96.03	111.00
1	G	207	ARG	NE-CZ-NH1	-5.54	117.53	120.30
2	K	329	ALA	CB-CA-C	-5.54	101.79	110.10
2	B	370	CYS	CB-CA-C	5.54	121.47	110.40
3	L	87	THR	CA-CB-CG2	-5.54	104.65	112.40
3	I	413	LEU	CB-CG-CD1	5.53	120.40	111.00
3	C	66	ILE	N-CA-C	-5.53	96.07	111.00
3	C	230	ASP	CB-CG-OD1	-5.53	113.33	118.30
1	J	109	VAL	CA-CB-CG1	-5.53	102.61	110.90
2	H	403	SER	N-CA-CB	5.52	118.78	110.50
3	L	39	ASP	CB-CG-OD2	-5.52	113.33	118.30
3	L	103	ARG	NE-CZ-NH1	5.52	123.06	120.30
3	L	361	TYR	CB-CG-CD2	5.52	124.31	121.00
2	E	93	TYR	CB-CG-CD2	-5.51	117.69	121.00
3	F	161	ARG	NE-CZ-NH2	-5.51	117.54	120.30
3	F	382	PHE	CB-CG-CD1	5.50	124.65	120.80
2	H	323	ASN	N-CA-CB	5.50	120.51	110.60
2	K	369	VAL	N-CA-C	-5.50	96.14	111.00
2	E	180	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	A	246	THR	CA-CB-CG2	-5.50	104.70	112.40
2	H	233	TYR	CG-CD2-CE2	-5.50	116.90	121.30
2	K	373	ARG	NE-CZ-NH1	-5.50	117.55	120.30
3	I	357	TYR	CG-CD2-CE2	5.49	125.69	121.30
1	D	252	GLU	N-CA-CB	5.49	120.48	110.60
1	J	181	TRP	CG-CD2-CE3	-5.49	128.96	133.90
3	I	313	MET	CG-SD-CE	-5.48	91.42	100.20
2	K	210	SER	CB-CA-C	-5.48	99.68	110.10
3	L	111	GLU	OE1-CD-OE2	-5.48	116.72	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	362	GLU	CB-CG-CD	-5.48	99.41	114.20
2	E	348	GLU	N-CA-C	-5.48	96.21	111.00
2	E	30	SER	N-CA-CB	5.48	118.72	110.50
3	L	217	ASN	N-CA-CB	5.48	120.46	110.60
3	I	240	TYR	CB-CG-CD1	5.47	124.28	121.00
2	K	250	PRO	N-CD-CG	5.47	111.41	103.20
1	D	185	ALA	CB-CA-C	-5.47	101.90	110.10
1	D	195	ILE	N-CA-C	-5.47	96.24	111.00
2	H	59	TYR	CB-CG-CD1	5.46	124.28	121.00
3	L	126	PHE	N-CA-CB	5.46	120.43	110.60
3	L	234	TRP	CE2-CD2-CG	-5.45	102.94	107.30
2	E	161	PHE	N-CA-C	-5.45	96.28	111.00
3	C	363	TYR	CD1-CE1-CZ	-5.45	114.90	119.80
3	I	217	ASN	CB-CG-OD1	-5.45	110.70	121.60
3	L	251	GLY	N-CA-C	-5.45	99.48	113.10
3	C	102	ALA	N-CA-CB	5.43	117.70	110.10
2	B	308	TYR	CZ-CE2-CD2	5.43	124.68	119.80
1	D	88	LYS	N-CA-CB	5.43	120.37	110.60
3	L	284	HIS	N-CA-CB	5.42	120.36	110.60
2	H	240	PHE	CB-CG-CD1	5.42	124.59	120.80
3	C	227	TYR	N-CA-CB	5.42	120.35	110.60
2	B	390	TYR	CG-CD2-CE2	-5.41	116.97	121.30
3	C	193	THR	CA-CB-CG2	-5.41	104.82	112.40
2	E	84	VAL	O-C-N	5.41	131.36	122.70
2	B	300	ALA	N-CA-CB	5.41	117.68	110.10
3	I	93	LEU	N-CA-CB	5.41	121.22	110.40
1	J	103	ASN	CB-CG-OD1	-5.41	110.78	121.60
2	B	214	TYR	CG-CD1-CE1	-5.41	116.97	121.30
2	B	280	MET	CA-CB-CG	5.41	122.49	113.30
2	E	247	LYS	N-CA-CB	5.41	120.33	110.60
2	K	15	PHE	CB-CG-CD2	-5.41	117.02	120.80
3	I	66	ILE	N-CA-C	-5.40	96.42	111.00
3	C	147	ARG	N-CA-CB	5.39	120.31	110.60
3	L	110	VAL	CA-CB-CG2	-5.39	102.81	110.90
2	B	66	ALA	N-CA-CB	5.39	117.65	110.10
2	K	102	GLN	N-CA-CB	5.39	120.31	110.60
3	C	235	GLN	N-CA-CB	5.39	120.30	110.60
3	I	277	ARG	NE-CZ-NH1	5.39	122.99	120.30
2	E	81	PHE	CG-CD2-CE2	-5.39	114.88	120.80
2	B	199	ARG	N-CA-CB	5.38	120.29	110.60
3	F	68	TYR	N-CA-CB	5.38	120.29	110.60
2	H	199	ARG	NE-CZ-NH2	-5.38	117.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	19	ALA	CB-CA-C	-5.38	102.03	110.10
3	F	218	CYS	CA-CB-SG	-5.38	104.31	114.00
2	H	184	VAL	CA-CB-CG1	-5.38	102.83	110.90
3	F	159	LEU	CB-CG-CD2	5.38	120.14	111.00
2	B	308	TYR	CG-CD1-CE1	-5.38	117.00	121.30
3	I	131	ARG	N-CA-CB	5.38	120.28	110.60
1	D	181	TRP	CD1-CG-CD2	-5.37	102.00	106.30
2	K	308	TYR	CB-CG-CD2	-5.37	117.78	121.00
2	H	105	GLU	OE1-CD-OE2	-5.37	116.86	123.30
2	E	339	MET	CG-SD-CE	-5.37	91.61	100.20
3	L	37	TRP	CG-CD1-NE1	-5.37	104.73	110.10
3	I	221	ALA	CB-CA-C	5.36	118.14	110.10
2	B	188	ASP	CB-CG-OD1	-5.35	113.48	118.30
2	E	390	TYR	CD1-CE1-CZ	5.35	124.62	119.80
2	K	41	SER	CB-CA-C	-5.35	99.93	110.10
2	E	181	ARG	NE-CZ-NH2	-5.35	117.62	120.30
3	L	52	GLN	CG-CD-OE1	5.35	132.30	121.60
3	I	153	TYR	CZ-CE2-CD2	5.35	124.61	119.80
3	I	105	ARG	NE-CZ-NH1	5.34	122.97	120.30
3	F	238	SER	N-CA-CB	5.34	118.51	110.50
3	F	255	VAL	CG1-CB-CG2	5.34	119.44	110.90
2	H	115	GLU	N-CA-CB	5.34	120.20	110.60
1	J	181	TRP	CZ3-CH2-CZ2	-5.34	115.19	121.60
2	E	385	ASP	CB-CG-OD1	5.33	123.10	118.30
2	H	87	PHE	CB-CG-CD2	5.33	124.53	120.80
2	H	292	GLU	C-N-CA	5.33	135.03	121.70
3	I	41	ASP	CB-CG-OD1	5.33	123.10	118.30
2	K	242	TYR	CB-CG-CD2	-5.33	117.80	121.00
2	H	80	VAL	N-CA-C	-5.33	96.61	111.00
2	E	355	PHE	N-CA-CB	5.33	120.19	110.60
3	L	409	PHE	CB-CG-CD1	5.33	124.53	120.80
2	E	308	TYR	CB-CG-CD2	5.33	124.19	121.00
3	C	18	CYS	CA-CB-SG	-5.32	104.42	114.00
2	K	257	PHE	N-CA-CB	5.32	120.18	110.60
1	A	122	VAL	N-CA-C	-5.32	96.63	111.00
2	H	428	VAL	CA-CB-CG1	5.31	118.87	110.90
2	E	430	VAL	CA-CB-CG1	5.31	118.87	110.90
1	J	181	TRP	CD2-CE3-CZ3	-5.31	111.90	118.80
1	G	131	HIS	CG-ND1-CE1	-5.31	98.80	105.70
1	A	137	ASP	CB-CG-OD2	-5.30	113.53	118.30
2	B	215	ALA	N-CA-CB	5.30	117.53	110.10
3	I	257	PHE	CB-CG-CD2	5.30	124.51	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	283	PHE	N-CA-C	-5.30	96.68	111.00
2	K	320	TYR	CD1-CE1-CZ	-5.30	115.03	119.80
3	L	39	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	240	ASP	CB-CG-OD2	5.30	123.07	118.30
3	I	131	ARG	NE-CZ-NH2	5.30	122.95	120.30
3	F	361	TYR	CB-CG-CD2	5.29	124.18	121.00
3	L	88	ALA	CB-CA-C	-5.29	102.17	110.10
2	B	1	TYR	CB-CG-CD1	5.29	124.17	121.00
2	B	219	LEU	N-CA-CB	5.29	120.98	110.40
2	B	221	LEU	CB-CA-C	-5.29	100.16	110.20
3	F	296	ARG	NE-CZ-NH1	5.28	122.94	120.30
3	L	327	VAL	N-CA-C	-5.28	96.74	111.00
2	H	31	LEU	N-CA-CB	5.28	120.96	110.40
2	E	309	SER	N-CA-C	-5.28	96.75	111.00
3	F	402	PRO	C-N-CA	5.28	133.38	122.30
3	F	231	ASN	C-N-CA	5.27	134.88	121.70
3	I	274	VAL	CG1-CB-CG2	-5.27	102.46	110.90
3	C	360	LEU	CA-C-N	5.27	128.79	117.20
3	L	14	TYR	CG-CD2-CE2	-5.27	117.08	121.30
1	A	182	HIS	CA-CB-CG	-5.27	104.64	113.60
3	I	314	SER	N-CA-CB	5.27	118.40	110.50
2	B	68	CYS	C-N-CA	5.26	134.86	121.70
3	I	287	PRO	N-CA-CB	-5.26	96.81	102.60
1	D	149	SER	N-CA-C	-5.26	96.79	111.00
2	H	158	GLN	N-CA-CB	5.26	120.07	110.60
3	L	112	VAL	N-CA-C	-5.26	96.80	111.00
1	A	130	ALA	CB-CA-C	-5.26	102.22	110.10
2	K	291	ASP	CB-CG-OD1	-5.26	113.57	118.30
3	L	40	ALA	CB-CA-C	-5.26	102.22	110.10
3	F	77	ALA	CB-CA-C	-5.25	102.22	110.10
2	E	134	MET	CG-SD-CE	-5.25	91.80	100.20
2	B	312	PHE	CA-CB-CG	-5.25	101.30	113.90
2	E	409	TRP	CE2-CD2-CG	5.25	111.50	107.30
3	F	157	THR	CA-CB-CG2	-5.24	105.06	112.40
1	G	183	HIS	N-CA-C	-5.24	96.84	111.00
2	E	69	SER	N-CA-CB	5.24	118.36	110.50
2	H	223	ARG	NE-CZ-NH2	5.24	122.92	120.30
3	F	362	PRO	O-C-N	5.24	131.08	122.70
3	I	385	PHE	CZ-CE2-CD2	5.24	126.39	120.10
1	A	147	LYS	O-C-N	5.24	131.08	122.70
3	C	291	THR	O-C-N	5.24	131.08	122.70
1	G	157	ALA	CB-CA-C	-5.24	102.25	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	221	LEU	N-CA-C	-5.24	96.87	111.00
2	B	76	TYR	CG-CD1-CE1	5.23	125.49	121.30
3	F	420	ARG	CG-CD-NE	-5.23	100.81	111.80
3	I	37	TRP	CG-CD2-CE3	-5.23	129.19	133.90
2	B	296	VAL	CG1-CB-CG2	5.23	119.27	110.90
2	H	119	ALA	O-C-N	-5.23	114.33	122.70
2	E	387	ILE	O-C-N	-5.22	114.34	122.70
2	K	22	PRO	N-CA-CB	5.22	109.56	103.30
3	I	1	SER	CB-CA-C	5.22	120.02	110.10
3	C	32	SER	N-CA-CB	5.22	118.33	110.50
1	D	119	ALA	N-CA-CB	5.21	117.40	110.10
2	K	25	ALA	N-CA-CB	5.21	117.40	110.10
3	L	233	VAL	CG1-CB-CG2	-5.21	102.56	110.90
2	H	145	ASP	CB-CG-OD2	-5.21	113.61	118.30
3	I	268	VAL	CA-CB-CG2	5.21	118.71	110.90
3	L	234	TRP	CH2-CZ2-CE2	5.21	122.61	117.40
2	H	289	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	G	237	TRP	CB-CG-CD2	-5.20	119.83	126.60
3	C	3	ALA	N-CA-CB	5.20	117.38	110.10
1	G	181	TRP	CB-CG-CD1	5.20	133.76	127.00
3	C	267	SER	O-C-N	-5.20	114.39	122.70
1	D	110	MET	CG-SD-CE	-5.19	91.90	100.20
2	K	242	TYR	CZ-CE2-CD2	-5.18	115.13	119.80
2	K	257	PHE	CB-CG-CD1	-5.18	117.17	120.80
2	E	201	GLY	O-C-N	5.18	130.99	122.70
3	F	221	ALA	CA-C-O	-5.18	109.22	120.10
3	C	126	PHE	CB-CG-CD1	5.18	124.42	120.80
1	D	108	PRO	O-C-N	5.18	130.98	122.70
1	A	170	PHE	CB-CG-CD2	5.17	124.42	120.80
2	H	280	MET	N-CA-CB	5.17	119.91	110.60
2	H	295	SER	CB-CA-C	-5.17	100.27	110.10
2	B	71	LYS	CA-CB-CG	5.17	124.77	113.40
3	F	206	GLU	CA-CB-CG	5.17	124.77	113.40
3	C	266	VAL	CA-CB-CG1	-5.16	103.15	110.90
3	F	147	ARG	NE-CZ-NH2	5.16	122.88	120.30
3	C	299	GLY	C-N-CA	5.16	134.59	121.70
2	H	388	VAL	CG1-CB-CG2	5.16	119.15	110.90
3	I	290	PRO	N-CA-CB	5.16	109.49	103.30
3	C	259	LEU	CB-CG-CD1	5.15	119.76	111.00
3	L	363	TYR	CG-CD1-CE1	5.15	125.42	121.30
3	C	240	TYR	O-C-N	-5.15	114.45	122.70
1	A	237	TRP	N-CA-C	-5.15	97.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	17	TRP	CB-CG-CD2	-5.14	119.91	126.60
3	F	364	TRP	CG-CD2-CE3	-5.14	129.27	133.90
2	B	184	VAL	CG1-CB-CG2	-5.14	102.67	110.90
2	E	80	VAL	N-CA-C	-5.14	97.12	111.00
2	K	41	SER	N-CA-CB	5.14	118.21	110.50
2	K	288	THR	N-CA-C	-5.14	97.13	111.00
3	I	200	CYS	N-CA-CB	5.14	119.85	110.60
3	I	95	THR	CA-CB-CG2	-5.14	105.21	112.40
1	A	147	LYS	N-CA-CB	5.13	119.84	110.60
2	K	68	CYS	N-CA-CB	5.13	119.84	110.60
3	L	364	TRP	CB-CG-CD1	5.13	133.67	127.00
2	E	29	LEU	CB-CG-CD2	5.13	119.72	111.00
2	B	257	PHE	CG-CD2-CE2	5.13	126.44	120.80
3	C	4	HIS	N-CA-CB	5.13	119.83	110.60
2	K	180	TYR	CG-CD1-CE1	5.12	125.40	121.30
2	E	295	SER	N-CA-CB	5.12	118.19	110.50
3	I	32	SER	N-CA-CB	5.12	118.19	110.50
1	J	127	MET	CG-SD-CE	-5.12	92.00	100.20
2	B	308	TYR	CG-CD2-CE2	-5.12	117.20	121.30
2	B	320	TYR	N-CA-CB	5.12	119.81	110.60
3	L	264	CYS	N-CA-CB	5.12	119.81	110.60
3	C	227	TYR	CB-CG-CD1	5.12	124.07	121.00
2	H	293	SER	N-CA-CB	5.12	118.17	110.50
3	I	155	HIS	C-N-CA	5.12	134.49	121.70
3	L	80	SER	N-CA-CB	5.12	118.17	110.50
2	B	165	PRO	N-CD-CG	5.11	110.87	103.20
3	C	157	THR	CA-CB-CG2	-5.11	105.24	112.40
2	K	141	ASN	CB-CG-OD1	-5.11	111.38	121.60
2	K	409	TRP	CZ3-CH2-CZ2	-5.11	115.47	121.60
1	D	199	SER	N-CA-CB	5.11	118.16	110.50
3	F	326	TYR	CB-CG-CD2	-5.11	117.94	121.00
2	B	228	ASN	CB-CG-OD1	-5.11	111.39	121.60
2	H	298	LEU	CB-CG-CD2	5.11	119.68	111.00
2	K	107	TYR	CZ-CE2-CD2	-5.11	115.20	119.80
2	H	21	ARG	CD-NE-CZ	5.10	130.74	123.60
3	L	288	MET	CA-CB-CG	5.10	121.97	113.30
2	K	221	LEU	CB-CG-CD2	-5.10	102.33	111.00
2	B	243	TRP	CB-CG-CD1	5.10	133.63	127.00
3	C	364	TRP	CG-CD2-CE3	-5.10	129.31	133.90
1	D	122	VAL	CA-CB-CG1	-5.10	103.25	110.90
2	E	41	SER	N-CA-CB	5.10	118.15	110.50
3	I	216	PHE	CB-CG-CD1	-5.10	117.23	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	361	TYR	CD1-CE1-CZ	5.10	124.39	119.80
3	F	172	VAL	CA-CB-CG2	5.09	118.54	110.90
3	I	122	CYS	N-CA-C	-5.09	97.25	111.00
3	L	91	ASP	CA-CB-CG	-5.09	102.19	113.40
1	G	237	TRP	CE2-CD2-CG	-5.09	103.23	107.30
1	D	137	ASP	CB-CG-OD2	5.09	122.88	118.30
1	D	196	PRO	C-N-CA	5.09	134.42	121.70
1	J	112	ASP	CB-CG-OD1	5.09	122.88	118.30
3	L	66	ILE	N-CA-C	-5.09	97.26	111.00
3	L	220	THR	CA-CB-CG2	-5.08	105.28	112.40
2	H	355	PHE	CB-CG-CD2	-5.08	117.24	120.80
3	F	390	ALA	N-CA-CB	5.08	117.21	110.10
1	D	207	ARG	NE-CZ-NH2	5.08	122.84	120.30
2	B	49	CYS	N-CA-C	-5.07	97.31	111.00
2	K	61	LYS	N-CA-CB	5.07	119.73	110.60
3	I	310	ASP	CB-CG-OD2	-5.07	113.74	118.30
2	E	281	ASP	N-CA-C	-5.07	97.33	111.00
2	H	51	TYR	CB-CG-CD1	5.07	124.04	121.00
2	H	324	LYS	N-CA-CB	5.07	119.72	110.60
3	L	353	ILE	CA-CB-CG1	5.06	120.62	111.00
1	D	110	MET	CB-CA-C	-5.06	100.28	110.40
1	G	112	ASP	CB-CG-OD1	5.06	122.85	118.30
2	K	206	ARG	NE-CZ-NH1	5.06	122.83	120.30
3	L	105	ARG	NE-CZ-NH2	-5.05	117.77	120.30
3	C	262	SER	N-CA-C	-5.05	97.36	111.00
3	F	257	PHE	CB-CG-CD2	-5.05	117.26	120.80
3	C	305	SER	N-CA-CB	5.05	118.07	110.50
2	K	85	TYR	N-CA-CB	5.05	119.68	110.60
2	E	407	TRP	CG-CD2-CE3	-5.04	129.36	133.90
3	L	197	LYS	N-CA-C	-5.04	97.38	111.00
3	I	331	ASN	C-N-CA	5.04	134.30	121.70
3	F	185	TYR	CD1-CG-CD2	5.03	123.44	117.90
3	L	409	PHE	CB-CG-CD2	-5.03	117.28	120.80
3	I	234	TRP	CE3-CZ3-CH2	5.03	126.73	121.20
2	H	170	TRP	CB-CG-CD1	-5.02	120.47	127.00
2	H	356	PHE	CB-CG-CD2	-5.02	117.29	120.80
2	E	300	ALA	N-CA-CB	5.02	117.12	110.10
2	H	134	MET	CA-CB-CG	5.02	121.83	113.30
3	C	158	ASP	CB-CG-OD2	-5.01	113.79	118.30
2	K	365	PHE	CB-CG-CD2	5.01	124.31	120.80
3	L	398	TYR	CB-CG-CD2	-5.01	117.99	121.00
3	L	406	LEU	N-CA-C	-5.01	97.47	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	285	PHE	CD1-CG-CD2	5.01	124.81	118.30
2	K	188	ASP	N-CA-CB	5.01	119.61	110.60
2	B	85	TYR	CZ-CE2-CD2	5.00	124.30	119.80
2	K	292	GLU	N-CA-CB	5.00	119.61	110.60
3	L	117	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (140) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	LYS	Peptide
1	A	145	THR	Peptide
1	A	192	ARG	Sidechain
1	A	207	ARG	Sidechain
2	B	110	ARG	Sidechain
2	B	122	TYR	Sidechain
2	B	124	VAL	Peptide
2	B	173	PHE	Sidechain
2	B	174	ASP	Peptide
2	B	199	ARG	Sidechain
2	B	2	GLU	Peptide
2	B	223	ARG	Sidechain
2	B	233	TYR	Sidechain
2	B	242	TYR	Sidechain
2	B	285	ALA	Peptide
2	B	332	SER	Peptide
2	B	365	PHE	Sidechain
2	B	390	TYR	Sidechain
2	B	393	LYS	Peptide
2	B	399	PHE	Peptide
2	B	411	ALA	Peptide
2	B	46	TYR	Sidechain
2	B	51	TYR	Sidechain
2	B	69	SER	Peptide
3	C	105	ARG	Sidechain
3	C	123	ARG	Sidechain
3	C	196	TYR	Sidechain
3	C	220	THR	Peptide
3	C	236	TYR	Sidechain
3	C	286	HIS	Sidechain
3	C	289	TYR	Sidechain
3	C	361	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	C	363	TYR	Sidechain
3	C	398	TYR	Sidechain
3	C	99	PHE	Sidechain
1	D	118	TYR	Sidechain
1	D	125	LYS	Peptide
1	D	145	THR	Peptide
1	D	170	PHE	Sidechain
1	D	179	TYR	Sidechain
1	D	183	HIS	Peptide
1	D	94	ARG	Sidechain
2	E	1	TYR	Sidechain
2	E	117	ASP	Peptide
2	E	122	TYR	Sidechain
2	E	124	VAL	Peptide
2	E	147	PHE	Sidechain
2	E	180	TYR	Sidechain
2	E	2	GLU	Peptide
2	E	206	ARG	Sidechain
2	E	233	TYR	Sidechain
2	E	242	TYR	Sidechain
2	E	285	ALA	Peptide
2	E	289	ARG	Sidechain
2	E	332	SER	Peptide
2	E	365	PHE	Sidechain
2	E	399	PHE	Peptide
2	E	438	ARG	Sidechain
2	E	59	TYR	Sidechain
2	E	69	SER	Peptide
2	E	76	TYR	Sidechain
2	E	93	TYR	Sidechain
2	E	95	PHE	Sidechain
3	F	12	ARG	Sidechain
3	F	123	ARG	Sidechain
3	F	220	THR	Peptide
3	F	277	ARG	Sidechain
3	F	67	ARG	Sidechain
3	F	79	ARG	Sidechain
1	G	122	VAL	Peptide
1	G	125	LYS	Peptide
1	G	126	VAL	Peptide
1	G	145	THR	Peptide
1	G	183	HIS	Peptide

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Mol	Chain	Res	Type	Group
1	G	207	ARG	Sidechain
1	G	244	ARG	Sidechain
1	G	96	ARG	Sidechain
2	H	1	TYR	Sidechain
2	H	107	TYR	Sidechain
2	H	124	VAL	Peptide
2	H	180	TYR	Sidechain
2	H	192	TYR	Sidechain
2	H	2	GLU	Peptide
2	H	242	TYR	Sidechain
2	H	273	TYR	Sidechain
2	H	285	ALA	Peptide
2	H	332	SER	Peptide
2	H	373	ARG	Sidechain
2	H	390	TYR	Sidechain
2	H	393	LYS	Peptide
2	H	399	PHE	Peptide
2	H	438	ARG	Sidechain
2	H	59	TYR	Sidechain
2	H	69	SER	Peptide
2	H	81	PHE	Sidechain
2	H	93	TYR	Sidechain
3	I	12	ARG	Sidechain
3	I	185	TYR	Sidechain
3	I	220	THR	Peptide
3	I	227	TYR	Sidechain
3	I	243	ARG	Sidechain
3	I	254	HIS	Sidechain
3	I	284	HIS	Sidechain
3	I	285	PHE	Sidechain
3	I	293	PHE	Sidechain
3	I	335	ARG	Sidechain
3	I	363	TYR	Sidechain
1	J	125	LYS	Peptide
1	J	145	THR	Peptide
1	J	183	HIS	Peptide
1	J	210	PHE	Sidechain
2	K	107	TYR	Sidechain
2	K	117	ASP	Peptide
2	K	124	VAL	Peptide
2	K	155	ARG	Sidechain
2	K	173	PHE	Sidechain

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Mol	Chain	Res	Type	Group
2	K	2	GLU	Peptide
2	K	206	ARG	Sidechain
2	K	21	ARG	Sidechain
2	K	240	PHE	Sidechain
2	K	253	ARG	Sidechain
2	K	285	ALA	Peptide
2	K	332	SER	Peptide
2	K	373	ARG	Sidechain
2	K	385	ASP	Peptide
2	K	399	PHE	Sidechain,Peptide
2	K	41	SER	Peptide
2	K	59	TYR	Sidechain
2	K	69	SER	Peptide
2	K	76	TYR	Sidechain
3	L	14	TYR	Sidechain
3	L	153	TYR	Sidechain
3	L	196	TYR	Sidechain
3	L	220	THR	Peptide
3	L	227	TYR	Sidechain
3	L	243	ARG	Sidechain
3	L	296	ARG	Sidechain
3	L	326	TYR	Sidechain
3	L	68	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1316	0	1322	30	0
1	D	1316	0	1322	23	0
1	G	1316	0	1322	28	0
1	J	1316	0	1322	26	0
2	B	3225	0	3161	34	0
2	E	3225	0	3161	33	0
2	H	3225	0	3161	29	0
2	K	3225	0	3161	32	0
3	C	3239	0	3208	57	0
3	F	3239	0	3208	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	3239	0	3208	58	0
3	L	3239	0	3208	58	0
All	All	31120	0	30764	289	0

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

All (289) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:240:TYR:CD1	3:I:240:TYR:CE1	1.81	1.68
3:I:240:TYR:CD2	3:I:240:TYR:CE2	1.80	1.67
3:F:240:TYR:CE2	3:F:240:TYR:CD2	1.79	1.65
1:A:237:TRP:CD2	1:A:237:TRP:CE3	1.82	1.64
1:G:237:TRP:CD2	1:G:237:TRP:CE3	1.74	1.64
3:C:240:TYR:CD2	3:C:240:TYR:CE2	1.88	1.61
3:L:240:TYR:CD1	3:L:240:TYR:CE1	1.82	1.61
3:F:240:TYR:CD1	3:F:240:TYR:CG	1.89	1.60
3:C:240:TYR:CZ	3:C:240:TYR:CE2	1.85	1.60
3:F:240:TYR:CZ	3:F:240:TYR:CE2	1.89	1.59
3:F:240:TYR:CD2	3:F:240:TYR:CG	1.88	1.59
3:I:240:TYR:CE2	3:I:240:TYR:CZ	1.87	1.58
3:F:240:TYR:CE1	3:F:240:TYR:CD1	1.91	1.57
3:L:240:TYR:CD1	3:L:240:TYR:CG	1.89	1.57
3:F:240:TYR:CZ	3:F:240:TYR:CE1	1.90	1.56
3:C:240:TYR:CG	3:C:240:TYR:CD1	1.91	1.56
3:C:240:TYR:CE1	3:C:240:TYR:CD1	1.89	1.56
3:L:240:TYR:CE2	3:L:240:TYR:CD2	1.91	1.56
3:L:240:TYR:CZ	3:L:240:TYR:CE2	1.87	1.55
3:C:240:TYR:CG	3:C:240:TYR:CD2	1.92	1.55
3:I:240:TYR:CZ	3:I:240:TYR:CE1	1.92	1.54
3:C:240:TYR:CZ	3:C:240:TYR:CE1	1.95	1.54
3:L:240:TYR:CZ	3:L:240:TYR:CE1	1.94	1.53
3:L:240:TYR:CG	3:L:240:TYR:CD2	1.92	1.52
3:I:240:TYR:CD2	3:I:240:TYR:CG	1.93	1.51
3:I:240:TYR:CD1	3:I:240:TYR:CG	1.98	1.49
1:G:237:TRP:CE2	3:I:398:TYR:CD2	2.09	1.40
1:J:237:TRP:CE2	3:L:398:TYR:CD2	2.08	1.40
1:A:237:TRP:CE2	3:C:398:TYR:CD2	2.10	1.39
1:D:237:TRP:CE2	3:F:398:TYR:CD2	2.10	1.39
1:A:237:TRP:CE2	3:C:398:TYR:CE2	2.11	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:TRP:CE2	3:F:398:TYR:CE2	2.11	1.38
1:J:237:TRP:CE2	3:L:398:TYR:CE2	2.11	1.37
1:G:237:TRP:CE2	3:I:398:TYR:CE2	2.13	1.37
1:G:237:TRP:CZ2	3:I:398:TYR:CE2	2.19	1.30
1:J:237:TRP:CZ2	3:L:398:TYR:CD2	2.19	1.30
1:A:237:TRP:CZ2	3:C:398:TYR:CE2	2.18	1.30
1:G:237:TRP:CZ2	3:I:398:TYR:CD2	2.20	1.29
1:D:237:TRP:CZ2	3:F:398:TYR:CE2	2.21	1.29
1:J:237:TRP:CZ2	3:L:398:TYR:CE2	2.20	1.29
1:A:237:TRP:CZ2	3:C:398:TYR:CD2	2.20	1.28
1:D:237:TRP:CZ2	3:F:398:TYR:CD2	2.20	1.28
1:A:237:TRP:CE2	3:C:398:TYR:CZ	2.30	1.18
1:G:237:TRP:CD2	3:I:398:TYR:CD2	2.32	1.18
1:J:237:TRP:CE2	3:L:398:TYR:CG	2.31	1.18
1:D:237:TRP:CE2	3:F:398:TYR:CZ	2.30	1.17
1:A:237:TRP:CE2	3:C:398:TYR:CG	2.33	1.17
1:J:237:TRP:CE2	3:L:398:TYR:CZ	2.32	1.17
1:G:237:TRP:CE2	3:I:398:TYR:CZ	2.32	1.17
1:G:237:TRP:CE2	3:I:398:TYR:CG	2.32	1.16
1:D:237:TRP:CE2	3:F:398:TYR:CG	2.34	1.16
1:A:237:TRP:CE2	3:C:398:TYR:CE1	2.35	1.14
1:J:237:TRP:CD2	3:L:398:TYR:CD2	2.34	1.14
1:A:237:TRP:CD2	3:C:398:TYR:CD2	2.34	1.14
1:A:237:TRP:CD2	3:C:398:TYR:CE2	2.34	1.13
1:J:237:TRP:CZ2	3:L:398:TYR:CG	2.37	1.13
1:A:237:TRP:CE2	3:C:398:TYR:CD1	2.36	1.13
1:D:237:TRP:CD2	3:F:398:TYR:CD2	2.37	1.13
1:D:237:TRP:CD2	3:F:398:TYR:CE2	2.36	1.12
1:J:237:TRP:CD2	3:L:398:TYR:CE2	2.38	1.11
1:D:237:TRP:CE2	3:F:398:TYR:CD1	2.40	1.10
1:G:237:TRP:CD2	3:I:398:TYR:CE2	2.38	1.09
1:A:237:TRP:CZ2	3:C:398:TYR:CZ	2.41	1.09
1:D:237:TRP:CZ2	3:F:398:TYR:CG	2.40	1.08
1:D:237:TRP:CE2	3:F:398:TYR:CE1	2.41	1.08
1:J:237:TRP:CE2	3:L:398:TYR:CD1	2.42	1.08
1:D:237:TRP:CZ2	3:F:398:TYR:CZ	2.42	1.08
1:G:237:TRP:CZ2	3:I:398:TYR:CZ	2.43	1.07
1:G:237:TRP:CE2	3:I:398:TYR:CE1	2.43	1.06
1:G:237:TRP:CE2	3:I:398:TYR:CD1	2.43	1.06
1:J:237:TRP:CH2	3:L:398:TYR:CE2	2.43	1.06
1:J:237:TRP:CZ3	3:L:398:TYR:CE2	2.44	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:237:TRP:CZ2	3:L:398:TYR:CZ	2.43	1.06
1:D:237:TRP:CH2	3:F:398:TYR:CE2	2.43	1.05
1:D:237:TRP:CE3	3:F:398:TYR:CE2	2.44	1.05
1:A:237:TRP:CE3	3:C:398:TYR:CE2	2.43	1.05
1:A:237:TRP:CZ2	3:C:398:TYR:CG	2.44	1.05
1:D:237:TRP:CH2	3:F:398:TYR:CD2	2.44	1.05
1:G:237:TRP:CZ2	3:I:398:TYR:CG	2.45	1.04
1:A:237:TRP:CE3	3:C:398:TYR:CD2	2.46	1.04
1:A:237:TRP:CH2	3:C:398:TYR:CE2	2.45	1.03
2:K:231:VAL:N	3:L:240:TYR:CD2	2.26	1.03
1:D:237:TRP:CE3	3:F:398:TYR:CD2	2.46	1.03
1:J:237:TRP:CE2	3:L:398:TYR:CE1	2.47	1.03
1:G:237:TRP:CH2	3:I:398:TYR:CD2	2.46	1.03
2:K:231:VAL:N	3:L:240:TYR:CD1	2.27	1.03
1:A:237:TRP:CZ2	3:C:398:TYR:CD1	2.47	1.02
1:J:237:TRP:CE3	3:L:398:TYR:CE2	2.46	1.02
1:J:237:TRP:CH2	3:L:398:TYR:CD2	2.46	1.02
1:D:237:TRP:CZ3	3:F:398:TYR:CE2	2.48	1.02
2:B:229:VAL:C	3:C:240:TYR:CD1	2.33	1.02
2:B:231:VAL:N	3:C:240:TYR:CD2	2.27	1.01
1:D:237:TRP:CZ2	3:F:398:TYR:CD1	2.48	1.01
2:B:229:VAL:C	3:C:240:TYR:CZ	2.33	1.01
2:B:229:VAL:C	3:C:240:TYR:CE2	2.33	1.01
2:E:229:VAL:C	3:F:240:TYR:CZ	2.34	1.01
1:G:237:TRP:CE3	3:I:398:TYR:CD2	2.48	1.01
2:B:231:VAL:N	3:C:240:TYR:CE2	2.29	1.01
2:K:231:VAL:N	3:L:240:TYR:CE2	2.29	1.01
2:E:229:VAL:C	3:F:240:TYR:CE1	2.34	1.01
2:E:231:VAL:N	3:F:240:TYR:CZ	2.29	1.01
1:J:237:TRP:CZ2	3:L:398:TYR:CD1	2.48	1.01
1:J:237:TRP:CE3	3:L:398:TYR:CD2	2.47	1.01
1:D:237:TRP:CZ3	3:F:398:TYR:CD2	2.48	1.01
2:H:229:VAL:C	3:I:240:TYR:CD1	2.34	1.00
2:E:231:VAL:N	3:F:240:TYR:CE1	2.29	1.00
2:E:231:VAL:N	3:F:240:TYR:CE2	2.29	1.00
1:G:237:TRP:CZ3	3:I:398:TYR:CD2	2.49	1.00
2:B:229:VAL:C	3:C:240:TYR:CG	2.35	1.00
2:K:231:VAL:N	3:L:240:TYR:CZ	2.30	1.00
1:G:237:TRP:CE3	3:I:398:TYR:CE2	2.49	1.00
2:H:229:VAL:C	3:I:240:TYR:CE2	2.34	1.00
2:H:229:VAL:C	3:I:240:TYR:CG	2.35	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:TRP:CH2	3:C:398:TYR:CD2	2.48	1.00
1:J:237:TRP:CZ3	3:L:398:TYR:CD2	2.50	1.00
2:B:231:VAL:N	3:C:240:TYR:CD1	2.29	1.00
2:H:231:VAL:N	3:I:240:TYR:CE2	2.30	1.00
1:G:237:TRP:CH2	3:I:398:TYR:CE2	2.49	1.00
2:H:231:VAL:N	3:I:240:TYR:CD2	2.30	0.99
2:H:229:VAL:C	3:I:240:TYR:CD2	2.36	0.99
1:G:237:TRP:CZ2	3:I:398:TYR:CE1	2.50	0.99
2:K:229:VAL:C	3:L:240:TYR:CZ	2.35	0.99
2:B:231:VAL:N	3:C:240:TYR:CE1	2.30	0.99
2:H:231:VAL:N	3:I:240:TYR:CZ	2.31	0.99
2:H:229:VAL:C	3:I:240:TYR:CZ	2.36	0.99
2:E:229:VAL:C	3:F:240:TYR:CD2	2.35	0.99
2:B:231:VAL:N	3:C:240:TYR:CZ	2.30	0.99
2:K:229:VAL:C	3:L:240:TYR:CE1	2.36	0.99
2:H:231:VAL:N	3:I:240:TYR:CD1	2.31	0.99
2:K:229:VAL:C	3:L:240:TYR:CD2	2.36	0.98
2:E:229:VAL:C	3:F:240:TYR:CD1	2.37	0.98
2:E:231:VAL:N	3:F:240:TYR:CD2	2.30	0.98
2:K:231:VAL:N	3:L:240:TYR:CE1	2.31	0.98
2:K:229:VAL:C	3:L:240:TYR:CG	2.36	0.98
2:K:231:VAL:N	3:L:240:TYR:CG	2.31	0.98
2:E:229:VAL:C	3:F:240:TYR:CE2	2.37	0.98
2:H:229:VAL:C	3:I:240:TYR:CE1	2.37	0.97
2:K:229:VAL:C	3:L:240:TYR:CE2	2.37	0.97
2:B:231:VAL:N	3:C:240:TYR:CG	2.32	0.97
2:E:231:VAL:N	3:F:240:TYR:CG	2.33	0.97
2:B:229:VAL:C	3:C:240:TYR:CE1	2.38	0.97
2:H:231:VAL:N	3:I:240:TYR:CE1	2.31	0.97
1:J:237:TRP:CZ2	3:L:398:TYR:CE1	2.52	0.97
2:E:231:VAL:N	3:F:240:TYR:CD1	2.33	0.97
1:D:237:TRP:CZ2	3:F:398:TYR:CE1	2.53	0.96
2:H:231:VAL:N	3:I:240:TYR:CG	2.32	0.96
1:A:237:TRP:CZ3	3:C:398:TYR:CD2	2.53	0.96
2:K:229:VAL:C	3:L:240:TYR:CD1	2.38	0.96
1:G:237:TRP:CZ2	3:I:398:TYR:CD1	2.54	0.96
3:F:398:TYR:CE2	3:F:398:TYR:CD2	2.54	0.96
3:C:398:TYR:CD2	3:C:398:TYR:CE2	2.54	0.95
1:A:237:TRP:CZ2	3:C:398:TYR:CE1	2.54	0.95
3:L:398:TYR:CE2	3:L:398:TYR:CD2	2.55	0.95
3:I:398:TYR:CE2	3:I:398:TYR:CD2	2.56	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:VAL:C	3:C:240:TYR:CD2	2.41	0.94
2:E:229:VAL:C	3:F:240:TYR:CG	2.41	0.94
1:A:237:TRP:CZ3	3:C:398:TYR:CE2	2.56	0.93
1:G:237:TRP:CZ3	3:I:398:TYR:CE2	2.56	0.93
2:K:229:VAL:CA	3:L:240:TYR:CE1	2.65	0.80
2:E:229:VAL:CA	3:F:240:TYR:CZ	2.65	0.79
2:H:229:VAL:CA	3:I:240:TYR:CE1	2.66	0.77
2:B:229:VAL:CA	3:C:240:TYR:CE1	2.71	0.74
2:B:229:VAL:CA	3:C:240:TYR:CZ	2.71	0.74
2:E:229:VAL:O	3:F:240:TYR:CG	2.42	0.73
2:K:229:VAL:HA	3:L:240:TYR:CE1	2.24	0.73
2:K:385:ASP:H	2:K:387:ILE:HA	1.51	0.72
2:H:231:VAL:HA	3:I:240:TYR:CE1	2.25	0.72
2:H:229:VAL:O	3:I:240:TYR:CD2	2.44	0.70
2:H:231:VAL:CA	3:I:240:TYR:CE1	2.75	0.69
2:B:229:VAL:O	3:C:240:TYR:CG	2.45	0.69
3:I:354:VAL:H	3:I:364:TRP:HE1	1.41	0.69
2:K:229:VAL:CA	3:L:240:TYR:CZ	2.77	0.68
2:B:9:ASN:HD21	2:B:276:ILE:HD12	1.59	0.68
2:K:229:VAL:O	3:L:240:TYR:CD2	2.47	0.67
2:E:229:VAL:CA	3:F:240:TYR:CE1	2.79	0.66
2:K:229:VAL:HA	3:L:240:TYR:CZ	2.32	0.65
2:B:229:VAL:HA	3:C:240:TYR:CE1	2.31	0.65
2:K:231:VAL:CA	3:L:240:TYR:CE1	2.79	0.65
2:E:18:LEU:H	2:E:335:ASN:HD21	1.44	0.65
2:E:229:VAL:HA	3:F:240:TYR:CZ	2.32	0.64
2:B:229:VAL:HA	3:C:240:TYR:CZ	2.33	0.64
2:K:229:VAL:O	3:L:240:TYR:CG	2.51	0.64
2:E:229:VAL:HG12	3:F:240:TYR:CD1	2.33	0.63
2:H:229:VAL:O	3:I:240:TYR:CG	2.52	0.63
3:L:278:LEU:HD13	3:L:356:HIS:CE1	2.33	0.63
2:B:231:VAL:HA	3:C:240:TYR:CE1	2.33	0.63
2:H:229:VAL:CA	3:I:240:TYR:CZ	2.83	0.61
1:G:237:TRP:CE2	1:G:237:TRP:CZ2	2.88	0.61
1:A:237:TRP:CE2	1:A:237:TRP:CZ2	2.88	0.61
2:E:231:VAL:CA	3:F:240:TYR:CE1	2.84	0.60
2:B:231:VAL:CA	3:C:240:TYR:CE1	2.84	0.60
2:E:206:ARG:HH22	2:E:214:TYR:HB2	1.67	0.60
2:H:229:VAL:HA	3:I:240:TYR:CE1	2.37	0.59
1:J:237:TRP:CZ2	1:J:237:TRP:CE2	2.90	0.59
2:E:231:VAL:HG13	3:F:240:TYR:CD1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:VAL:O	3:C:240:TYR:CD2	2.55	0.58
2:K:231:VAL:HA	3:L:240:TYR:CE1	2.39	0.58
2:E:229:VAL:O	3:F:240:TYR:CD2	2.56	0.57
2:H:229:VAL:HA	3:I:240:TYR:CZ	2.39	0.56
2:K:402:ILE:HG23	2:K:407:TRP:HE1	1.71	0.56
1:D:237:TRP:CZ2	1:D:237:TRP:CE2	2.94	0.55
1:J:182:HIS:CD2	1:J:207:ARG:HH21	2.25	0.55
1:A:237:TRP:NE1	3:C:398:TYR:CE1	2.75	0.55
2:E:231:VAL:CA	3:F:240:TYR:CZ	2.89	0.55
2:E:131:ALA:HB2	2:E:148:VAL:HG11	1.88	0.54
3:F:388:SER:HA	3:F:391:ARG:HE	1.71	0.54
3:I:391:ARG:HG3	3:I:391:ARG:HH11	1.73	0.54
1:G:182:HIS:CE1	1:G:183:HIS:CE1	2.96	0.54
2:B:76:TYR:CE1	2:B:107:TYR:HB3	2.43	0.53
2:H:21:ARG:H	2:H:21:ARG:HD2	1.74	0.52
2:K:74:ALA:HB1	2:K:213:VAL:H	1.75	0.52
1:D:126:VAL:HG21	1:D:159:VAL:HG22	1.92	0.51
3:C:254:HIS:H	3:C:254:HIS:CD2	2.27	0.51
2:H:113:SER:HA	3:I:161:ARG:HH12	1.76	0.50
1:G:241:MET:HG2	1:G:242:VAL:H	1.77	0.50
3:L:332:ASN:HD22	3:L:332:ASN:H	1.60	0.50
2:E:229:VAL:HA	3:F:240:TYR:CE1	2.47	0.50
1:J:181:TRP:HE1	1:J:195:ILE:CD1	2.24	0.49
2:E:104:SER:HB3	2:E:221:LEU:HD22	1.94	0.49
2:B:24:TYR:H	2:B:290:ILE:HG22	1.77	0.49
1:G:182:HIS:CD2	1:G:207:ARG:HH12	2.30	0.49
3:L:53:ILE:HA	3:L:66:ILE:HG22	1.96	0.48
1:G:109:VAL:HG12	1:G:136:ILE:H	1.78	0.48
2:H:94:CYS:H	3:I:225:ILE:HG21	1.78	0.48
3:F:4:HIS:HA	3:F:254:HIS:CE1	2.48	0.48
2:B:203:ILE:HG22	2:B:216:ASN:H	1.77	0.48
3:I:296:ARG:HH21	3:I:304:HIS:CE1	2.33	0.47
2:K:330:ILE:HG21	2:K:370:CYS:H	1.78	0.47
2:B:229:VAL:C	2:B:231:VAL:N	2.68	0.47
2:E:194:SER:HA	2:E:199:ARG:HH11	1.79	0.47
3:C:117:ASP:H	3:C:118:PRO:CD	2.28	0.47
2:K:60:ILE:CG2	2:K:100:ASN:HD21	2.27	0.47
1:A:237:TRP:NE1	3:C:398:TYR:CD1	2.80	0.46
1:A:172:HIS:CD2	1:A:173:GLU:HG3	2.51	0.46
2:E:131:ALA:CB	2:E:148:VAL:HG11	2.46	0.46
1:J:181:TRP:HE1	1:J:195:ILE:HD12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:390:ALA:HB2	3:F:419:ALA:HB3	1.98	0.46
1:A:129:PRO:HA	1:A:132:VAL:HG23	1.97	0.45
1:G:182:HIS:CE1	1:G:183:HIS:HE1	2.34	0.45
3:C:229:VAL:HG22	3:C:230:ASP:N	2.31	0.45
2:H:423:VAL:HA	2:H:426:ILE:HD12	1.98	0.45
3:L:354:VAL:HG21	3:L:361:TYR:H	1.81	0.45
1:A:242:VAL:HG13	2:B:435:VAL:HA	1.98	0.45
1:J:237:TRP:NE1	3:L:398:TYR:CD1	2.84	0.45
2:B:50:ASN:HD22	2:B:113:SER:HB3	1.81	0.44
3:F:241:VAL:HB	3:F:242:PRO:HD2	1.99	0.44
2:E:42:LEU:O	2:E:42:LEU:HD12	2.16	0.44
3:I:393:LYS:O	3:I:397:PRO:HD2	2.17	0.44
2:B:29:LEU:HD22	2:B:280:MET:HG3	2.00	0.44
1:J:156:CYS:O	1:J:157:ALA:HB2	2.17	0.44
2:H:231:VAL:CA	3:I:240:TYR:CZ	3.00	0.44
2:K:229:VAL:C	2:K:231:VAL:N	2.70	0.44
2:E:320:TYR:CZ	2:E:352:LEU:HD12	2.53	0.44
2:K:398:GLU:H	2:K:401:SER:HA	1.82	0.43
3:L:221:ALA:HB3	3:L:222:PRO:HD3	2.00	0.43
1:A:219:ILE:O	1:A:234:VAL:HA	2.18	0.43
2:B:48:THR:HG21	2:B:201:GLY:HA2	1.99	0.43
2:K:192:TYR:HA	2:K:204:GLN:HE22	1.84	0.43
2:B:413:THR:HG23	3:C:378:ILE:HD11	2.00	0.43
2:H:58:PRO:O	3:I:242:PRO:HA	2.19	0.43
3:F:240:TYR:CB	3:F:240:TYR:CD2	2.88	0.43
2:E:231:VAL:HA	3:F:240:TYR:CE1	2.53	0.43
2:E:308:TYR:CE1	3:F:347:HIS:CE1	3.07	0.43
2:B:140:LEU:HD12	2:B:141:ASN:H	1.85	0.42
1:G:179:TYR:CE1	1:G:186:VAL:O	2.73	0.42
3:C:359:ASP:HA	3:C:362:PRO:HD3	2.01	0.42
2:E:5:THR:HG21	2:E:17:ALA:HB1	2.02	0.42
2:H:18:LEU:HD23	2:H:18:LEU:H	1.84	0.42
1:A:174:LYS:H	1:A:239:LYS:HE2	1.85	0.42
2:K:231:VAL:CA	3:L:240:TYR:CZ	3.01	0.42
3:I:288:MET:HB2	3:I:289:TYR:H	1.67	0.42
3:L:277:ARG:HG3	3:L:282:GLU:OE1	2.20	0.42
3:L:360:LEU:HA	3:L:360:LEU:HD23	1.92	0.42
2:K:231:VAL:CA	3:L:240:TYR:CD1	3.02	0.41
1:A:123:GLY:HA2	1:A:170:PHE:HA	2.01	0.41
3:I:274:VAL:HG13	3:I:283:PHE:CD1	2.55	0.41
1:D:237:TRP:NE1	3:F:398:TYR:CE1	2.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:93:LEU:HB3	3:F:155:HIS:CE1	2.55	0.41
3:I:52:GLN:HE21	3:I:98:HIS:CE1	2.38	0.41
2:H:229:VAL:C	2:H:231:VAL:N	2.74	0.41
3:L:238:SER:HB2	3:L:239:GLN:H	1.65	0.41
2:B:231:VAL:CA	3:C:240:TYR:CZ	3.02	0.41
2:K:58:PRO:HG2	2:K:231:VAL:HG11	2.02	0.41
2:B:9:ASN:HD21	2:B:276:ILE:CD1	2.32	0.40
2:K:385:ASP:N	2:K:387:ILE:HA	2.28	0.40
3:C:167:HIS:CD2	3:C:168:VAL:HG23	2.56	0.40
2:B:179:VAL:HG22	2:B:184:VAL:HG13	2.03	0.40
2:H:200:PHE:CD1	2:H:243:TRP:CD1	3.10	0.40
3:C:169:PRO:HA	3:C:170:PRO:HD3	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	169/253 (67%)	136 (80%)	24 (14%)	9 (5%)	2	30
1	D	169/253 (67%)	148 (88%)	15 (9%)	6 (4%)	4	40
1	G	169/253 (67%)	133 (79%)	21 (12%)	15 (9%)	1	16
1	J	169/253 (67%)	132 (78%)	22 (13%)	15 (9%)	1	16
2	B	422/427 (99%)	354 (84%)	47 (11%)	21 (5%)	3	31
2	E	422/427 (99%)	352 (83%)	42 (10%)	28 (7%)	1	24
2	H	422/427 (99%)	362 (86%)	47 (11%)	13 (3%)	5	43
2	K	422/427 (99%)	366 (87%)	33 (8%)	23 (6%)	2	29
3	C	419/421 (100%)	359 (86%)	36 (9%)	24 (6%)	2	28
3	F	419/421 (100%)	365 (87%)	38 (9%)	16 (4%)	4	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	419/421 (100%)	364 (87%)	38 (9%)	17 (4%)	3	35
3	L	419/421 (100%)	360 (86%)	40 (10%)	19 (4%)	3	33
All	All	4040/4404 (92%)	3431 (85%)	403 (10%)	206 (5%)	5	30

All (206) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ILE
1	A	182	HIS
2	B	69	SER
2	B	86	PRO
2	B	89	TRP
2	B	232	PRO
2	B	306	CYS
2	B	381	GLU
2	B	383	PRO
2	B	400	PRO
3	C	117	ASP
3	C	138	SER
3	C	221	ALA
2	E	4	SER
2	E	86	PRO
2	E	255	ALA
2	E	383	PRO
2	E	399	PHE
3	F	140	ALA
3	F	221	ALA
1	G	100	LYS
1	G	215	LYS
2	H	4	SER
2	H	287	PHE
2	H	400	PRO
3	I	221	ALA
3	I	346	ALA
1	J	136	ILE
1	J	157	ALA
1	J	182	HIS
1	J	237	TRP
2	K	4	SER
2	K	20	GLU
2	K	28	PRO

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Mol	Chain	Res	Type
2	K	116	ALA
2	K	309	SER
2	K	400	PRO
3	L	221	ALA
3	L	303	SER
3	L	346	ALA
1	A	130	ALA
2	B	4	SER
2	B	28	PRO
2	B	292	GLU
2	B	401	SER
3	C	24	ALA
3	C	26	SER
3	C	340	LYS
3	C	346	ALA
1	D	96	ARG
1	D	237	TRP
2	E	19	ILE
2	E	20	GLU
2	E	71	LYS
2	E	287	PHE
2	E	334	SER
2	E	380	CYS
2	E	411	ALA
3	F	59	ASN
3	F	321	ALA
1	G	101	ILE
1	G	131	HIS
1	G	182	HIS
2	H	116	ALA
2	H	401	SER
3	I	145	LYS
3	I	156	GLN
3	I	288	MET
3	I	310	ASP
3	I	321	ALA
1	J	101	ILE
1	J	130	ALA
1	J	249	GLU
2	K	411	ALA
3	L	24	ALA
3	L	117	ASP

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Mol	Chain	Res	Type
3	L	161	ARG
3	L	162	GLU
3	L	290	PRO
1	A	92	GLY
1	A	157	ALA
2	B	116	ALA
2	B	392	ALA
3	C	13	PRO
3	C	87	THR
3	C	190	LYS
3	C	342	SER
3	C	352	SER
3	C	362	PRO
3	C	403	GLY
1	D	131	HIS
2	E	400	PRO
2	E	401	SER
3	F	39	ASP
3	F	131	ARG
3	F	190	LYS
3	F	345	SER
1	G	157	ALA
1	G	167	ALA
1	G	177	GLY
1	G	242	VAL
1	G	247	PRO
2	H	266	VAL
2	H	370	CYS
2	H	438	ARG
3	I	89	PRO
3	I	160	THR
1	J	186	VAL
1	J	227	GLY
1	J	241	MET
2	K	19	ILE
2	K	202	ASP
2	K	292	GLU
2	K	334	SER
2	K	359	SER
2	K	370	CYS
2	K	384	LYS
2	K	385	ASP

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Mol	Chain	Res	Type
3	L	22	GLY
3	L	23	LEU
3	L	86	THR
3	L	169	PRO
3	L	232	THR
2	B	255	ALA
2	B	259	CYS
2	B	411	ALA
3	C	22	GLY
3	C	145	LYS
3	C	174	ILE
1	D	130	ALA
1	D	228	ALA
2	E	74	ALA
2	E	88	MET
2	E	247	LYS
2	E	342	SER
2	E	363	PRO
2	E	370	CYS
3	F	168	VAL
1	G	105	CYS
1	G	120	CYS
1	G	172	HIS
1	G	198	GLY
2	H	91	GLY
2	H	199	ARG
3	I	141	PRO
3	I	168	VAL
3	I	169	PRO
1	J	131	HIS
1	J	248	GLU
2	K	88	MET
2	K	97	ASP
2	K	259	CYS
2	K	310	SER
3	L	168	VAL
3	L	183	LYS
3	L	363	TYR
1	A	131	HIS
2	B	99	GLU
2	B	198	GLY
1	D	244	ARG

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Mol	Chain	Res	Type
2	E	25	ALA
2	E	99	GLU
2	E	174	ASP
2	E	183	GLU
2	E	259	CYS
2	E	266	VAL
2	E	291	ASP
3	F	161	ARG
3	F	162	GLU
3	F	256	PRO
2	H	57	SER
2	H	237	PRO
2	H	259	CYS
3	I	24	ALA
3	I	189	PRO
3	I	352	SER
3	L	142	THR
3	L	154	SER
3	L	298	LEU
1	A	172	HIS
2	B	311	ASP
2	B	399	PHE
3	C	168	VAL
3	C	189	PRO
3	C	256	PRO
2	E	85	TYR
3	F	133	ILE
3	I	13	PRO
1	J	238	ASN
2	K	255	ALA
2	K	305	SER
2	K	399	PHE
3	C	222	PRO
1	G	227	GLY
3	C	118	PRO
3	C	133	ILE
3	C	269	ALA
3	F	118	PRO
1	A	160	PRO
3	F	117	ASP
1	J	160	PRO
2	K	21	ARG

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Mol	Chain	Res	Type
1	A	242	VAL
1	J	177	GLY
3	F	287	PRO
3	I	222	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	145/217 (67%)	140 (97%)	5 (3%)	44	76
1	D	145/217 (67%)	140 (97%)	5 (3%)	44	76
1	G	145/217 (67%)	142 (98%)	3 (2%)	61	85
1	J	145/217 (67%)	138 (95%)	7 (5%)	31	68
2	B	364/366 (100%)	338 (93%)	26 (7%)	18	57
2	E	364/366 (100%)	355 (98%)	9 (2%)	55	82
2	H	364/366 (100%)	350 (96%)	14 (4%)	40	74
2	K	364/366 (100%)	346 (95%)	18 (5%)	31	68
3	C	366/366 (100%)	352 (96%)	14 (4%)	40	74
3	F	366/366 (100%)	353 (96%)	13 (4%)	42	75
3	I	366/366 (100%)	343 (94%)	23 (6%)	22	61
3	L	366/366 (100%)	351 (96%)	15 (4%)	37	72
All	All	3500/3796 (92%)	3348 (96%)	152 (4%)	40	71

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	TYR
1	A	186	VAL
1	A	236	THR
1	A	237	TRP
1	A	240	ASP
2	B	28	PRO

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Mol	Chain	Res	Type
2	B	42	LEU
2	B	71	LYS
2	B	76	TYR
2	B	94	CYS
2	B	142	GLN
2	B	146	VAL
2	B	160	LYS
2	B	180	TYR
2	B	182	ASP
2	B	199	ARG
2	B	200	PHE
2	B	216	ASN
2	B	219	LEU
2	B	220	LYS
2	B	223	ARG
2	B	229	VAL
2	B	244	LYS
2	B	253	ARG
2	B	267	ARG
2	B	280	MET
2	B	287	PHE
2	B	296	VAL
2	B	323	ASN
2	B	376	CYS
2	B	387	ILE
3	C	13	PRO
3	C	30	PRO
3	C	39	ASP
3	C	68	TYR
3	C	85	SER
3	C	100	ILE
3	C	105	ARG
3	C	130	PRO
3	C	136	GLU
3	C	160	THR
3	C	240	TYR
3	C	266	VAL
3	C	313	MET
3	C	340	LYS
1	D	102	GLU
1	D	202	PRO
1	D	204	ASP

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Mol	Chain	Res	Type
1	D	233	SER
1	D	240	ASP
2	E	39	VAL
2	E	42	LEU
2	E	61	LYS
2	E	126	THR
2	E	143	THR
2	E	146	VAL
2	E	234	THR
2	E	343	VAL
2	E	405	THR
3	F	147	ARG
3	F	167	HIS
3	F	185	TYR
3	F	212	LYS
3	F	213	ILE
3	F	230	ASP
3	F	240	TYR
3	F	261	ASP
3	F	277	ARG
3	F	307	GLU
3	F	336	LEU
3	F	365	THR
3	F	398	TYR
1	G	132	VAL
1	G	239	LYS
1	G	249	GLU
2	H	20	GLU
2	H	21	ARG
2	H	42	LEU
2	H	120	ILE
2	H	180	TYR
2	H	231	VAL
2	H	233	TYR
2	H	242	TYR
2	H	280	MET
2	H	287	PHE
2	H	340	LYS
2	H	384	LYS
2	H	388	VAL
2	H	414	THR
3	I	4	HIS

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Mol	Chain	Res	Type
3	I	36	VAL
3	I	67	ARG
3	I	79	ARG
3	I	82	LEU
3	I	95	THR
3	I	103	ARG
3	I	118	PRO
3	I	121	LEU
3	I	133	ILE
3	I	164	ILE
3	I	166	MET
3	I	167	HIS
3	I	171	ASP
3	I	240	TYR
3	I	246	VAL
3	I	260	THR
3	I	274	VAL
3	I	290	PRO
3	I	311	THR
3	I	319	VAL
3	I	354	VAL
3	I	392	THR
1	J	83	PRO
1	J	84	THR
1	J	143	LYS
1	J	160	PRO
1	J	168	SER
1	J	186	VAL
1	J	238	ASN
2	K	1	TYR
2	K	5	THR
2	K	16	LYS
2	K	45	ASP
2	K	186	ASN
2	K	202	ASP
2	K	203	ILE
2	K	231	VAL
2	K	249	VAL
2	K	253	ARG
2	K	278	ILE
2	K	280	MET
2	K	304	GLN

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Mol	Chain	Res	Type
2	K	340	LYS
2	K	367	VAL
2	K	368	GLN
2	K	376	CYS
2	K	389	PRO
3	L	42	ASP
3	L	49	VAL
3	L	86	THR
3	L	129	LYS
3	L	138	SER
3	L	148	ILE
3	L	158	ASP
3	L	227	TYR
3	L	240	TYR
3	L	271	GLU
3	L	288	MET
3	L	295	ILE
3	L	332	ASN
3	L	343	SER
3	L	377	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	HIS
2	B	9	ASN
2	B	50	ASN
3	C	109	GLN
3	C	128	HIS
3	C	144	HIS
3	C	167	HIS
3	C	175	GLN
3	C	180	ASN
3	C	239	GLN
3	C	254	HIS
2	E	254	ASN
2	E	335	ASN
3	F	217	ASN
3	F	254	HIS
3	F	284	HIS
3	F	347	HIS
1	G	138	ASN

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Mol	Chain	Res	Type
1	G	182	HIS
1	G	183	HIS
2	H	209	ASN
3	I	35	HIS
3	I	98	HIS
3	I	286	HIS
3	I	347	HIS
3	I	349	ASN
1	J	182	HIS
2	K	100	ASN
2	K	204	GLN
2	K	344	GLN
2	K	368	GLN
3	L	4	HIS
3	L	109	GLN
3	L	332	ASN
3	L	399	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 ⓘ

There are no chain breaks in this entry.