



Full wwPDB EM Validation Report ⓘ

Feb 13, 2024 – 08:08 PM EST

PDB ID : 3J1F
EMDB ID : EMD-5396
Title : Cryo-EM structure of 9-fold symmetric rATcpn-beta in ATP-binding state
Authors : Zhang, K.; Wang, L.; Liu, Y.X.; Wang, X.; Gao, B.; Hu, Z.J.; Ji, G.; Chan, K.Y.; Schulten, K.; Dong, Z.Y.; Sun, F.
Deposited on : 2012-02-06
Resolution : 6.20 Å(reported)
Based on initial model : 3K01

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

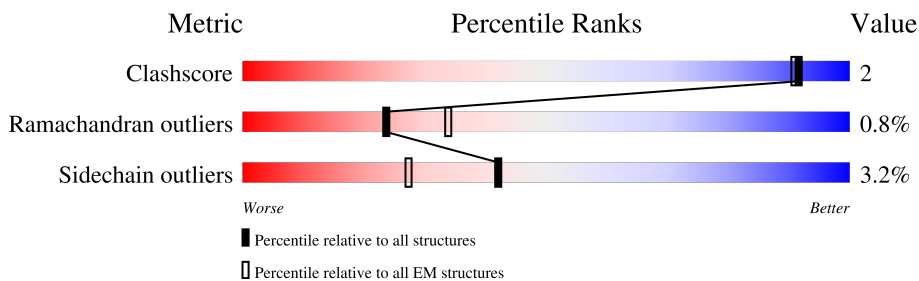
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	553	
1	B	553	
1	C	553	
1	D	553	
1	E	553	
1	F	553	
1	G	553	
1	H	553	

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Mol	Chain	Length	Quality of chain
1	I	553	<p>19% 72% 16% 9%</p>
1	K	553	<p>21% 72% 15% 9%</p>
1	L	553	<p>21% 73% 16% 9%</p>
1	M	553	<p>20% 70% 19% 9%</p>
1	N	553	<p>21% 68% 21% 9%</p>
1	O	553	<p>21% 70% 17% 9%</p>
1	P	553	<p>21% 72% 16% 9%</p>
1	Q	553	<p>20% 72% 16% 9%</p>
1	R	553	<p>20% 71% 17% 9%</p>
1	S	553	<p>19% 71% 18% 9%</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 69858 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 Chaperonin beta subunit.

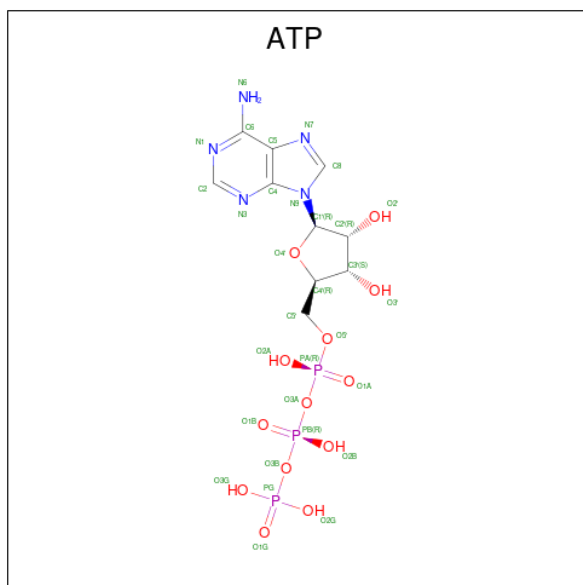
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	505	3849	2423	658	757	11	0	0
1	B	505	3849	2423	658	757	11	0	0
1	C	505	3849	2423	658	757	11	0	0
1	D	505	3849	2423	658	757	11	0	0
1	E	505	3849	2423	658	757	11	0	0
1	F	505	3849	2423	658	757	11	0	0
1	G	505	3849	2423	658	757	11	0	0
1	H	505	3849	2423	658	757	11	0	0
1	I	505	3849	2423	658	757	11	0	0
1	K	505	3849	2423	658	757	11	0	0
1	L	505	3849	2423	658	757	11	0	0
1	M	505	3849	2423	658	757	11	0	0
1	N	505	3849	2423	658	757	11	0	0
1	O	505	3849	2423	658	757	11	0	0
1	P	505	3849	2423	658	757	11	0	0
1	Q	505	3849	2423	658	757	11	0	0
1	R	505	3849	2423	658	757	11	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	S	505	3849	2423	658	757	11	0	0

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	Total 31	10	5	13	3	0
2	B	1	Total 31	10	5	13	3	0
2	C	1	Total 31	10	5	13	3	0
2	D	1	Total 31	10	5	13	3	0
2	E	1	Total 31	10	5	13	3	0
2	F	1	Total 31	10	5	13	3	0
2	G	1	Total 31	10	5	13	3	0
2	H	1	Total 31	10	5	13	3	0
2	I	1	Total 31	10	5	13	3	0
2	K	1	Total 31	10	5	13	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	L	1	31	10	5	13	3	0
2	M	1	31	10	5	13	3	0
2	N	1	31	10	5	13	3	0
2	O	1	31	10	5	13	3	0
2	P	1	31	10	5	13	3	0
2	Q	1	31	10	5	13	3	0
2	R	1	31	10	5	13	3	0
2	S	1	31	10	5	13	3	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
3	A	1	1	1	0
3	B	1	1	1	0
3	C	1	1	1	0
3	D	1	1	1	0
3	E	1	1	1	0
3	F	1	1	1	0
3	G	1	1	1	0
3	H	1	1	1	0
3	I	1	1	1	0
3	K	1	1	1	0
3	L	1	1	1	0

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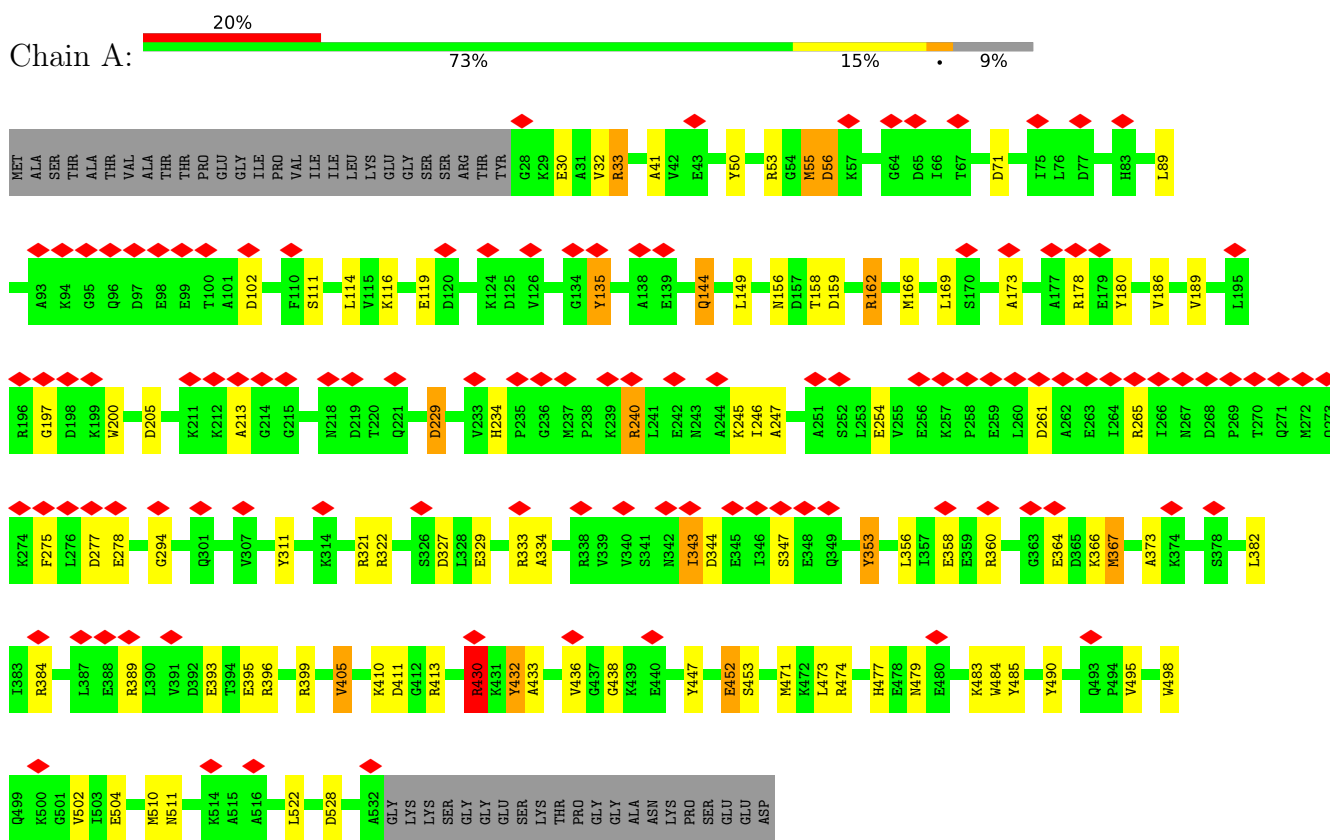
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Mol	Chain	Residues	Atoms		AltConf
3	M	1	Total 1	Mg 1	0
3	N	1	Total 1	Mg 1	0
3	O	1	Total 1	Mg 1	0
3	P	1	Total 1	Mg 1	0
3	Q	1	Total 1	Mg 1	0
3	R	1	Total 1	Mg 1	0
3	S	1	Total 1	Mg 1	0

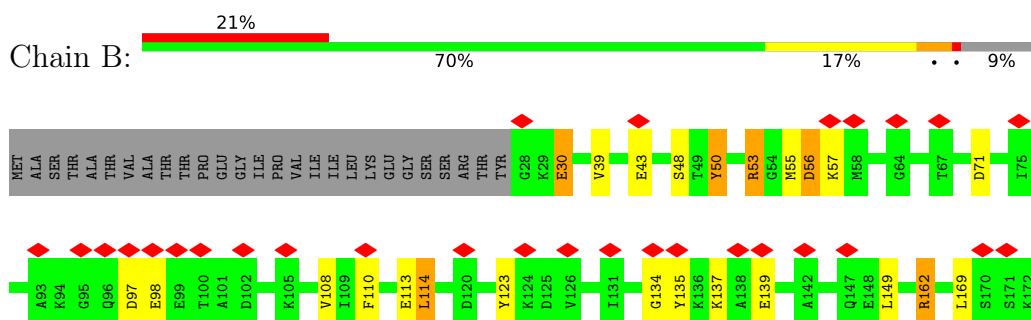
3 Residue-property plots

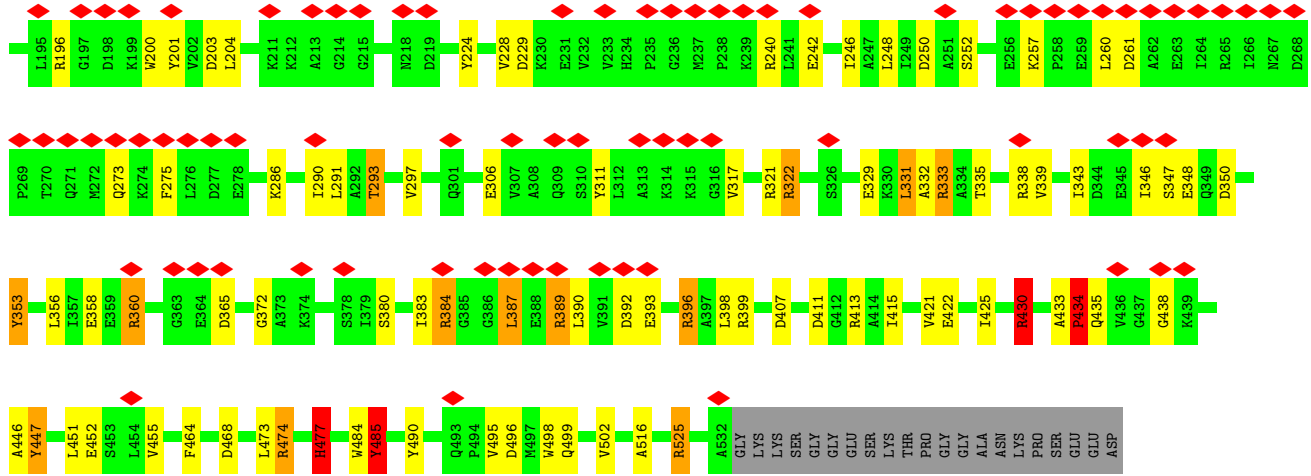
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Chaperonin beta subunit

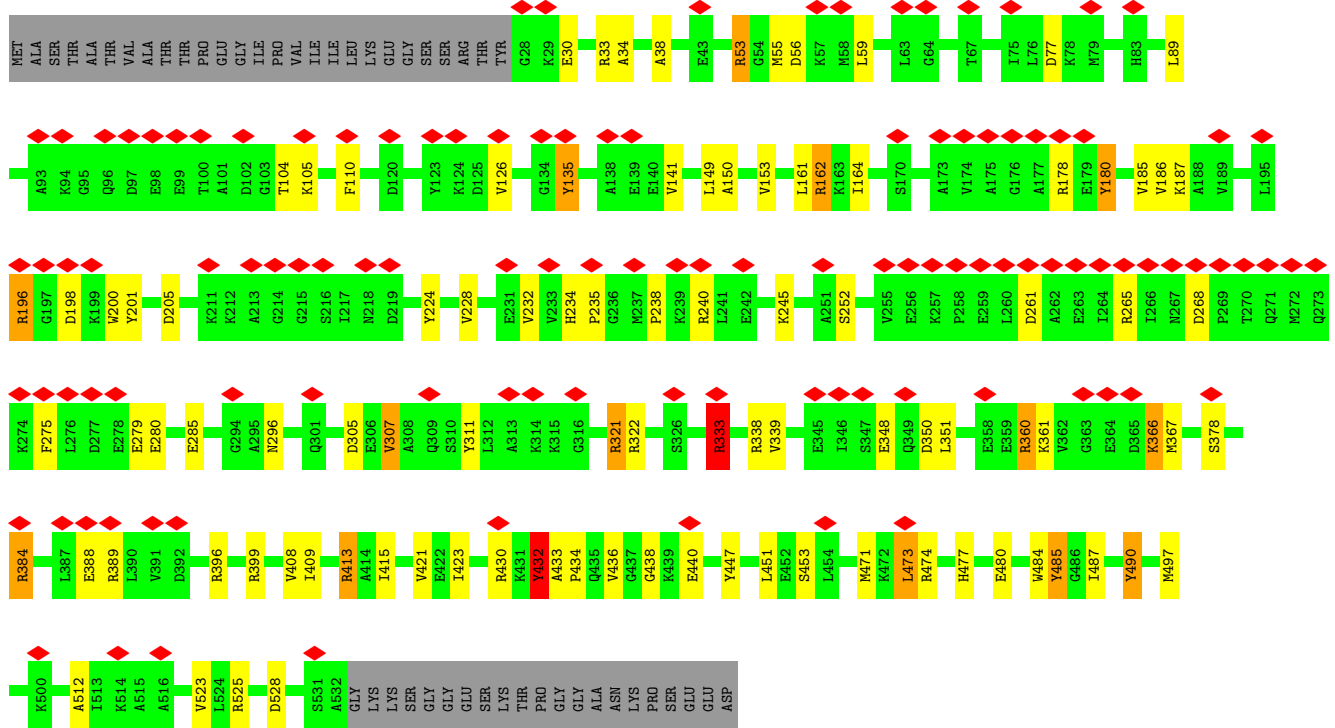
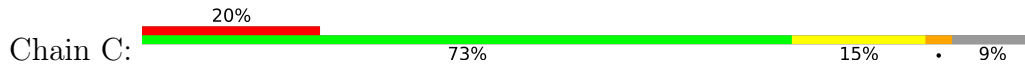


- Molecule 1: Chaperonin beta subunit

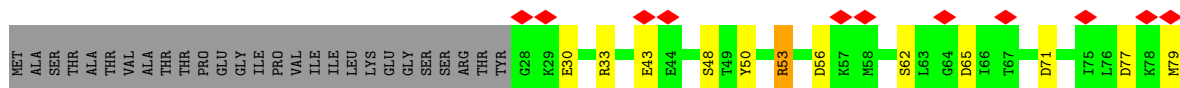
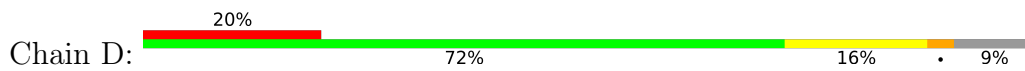


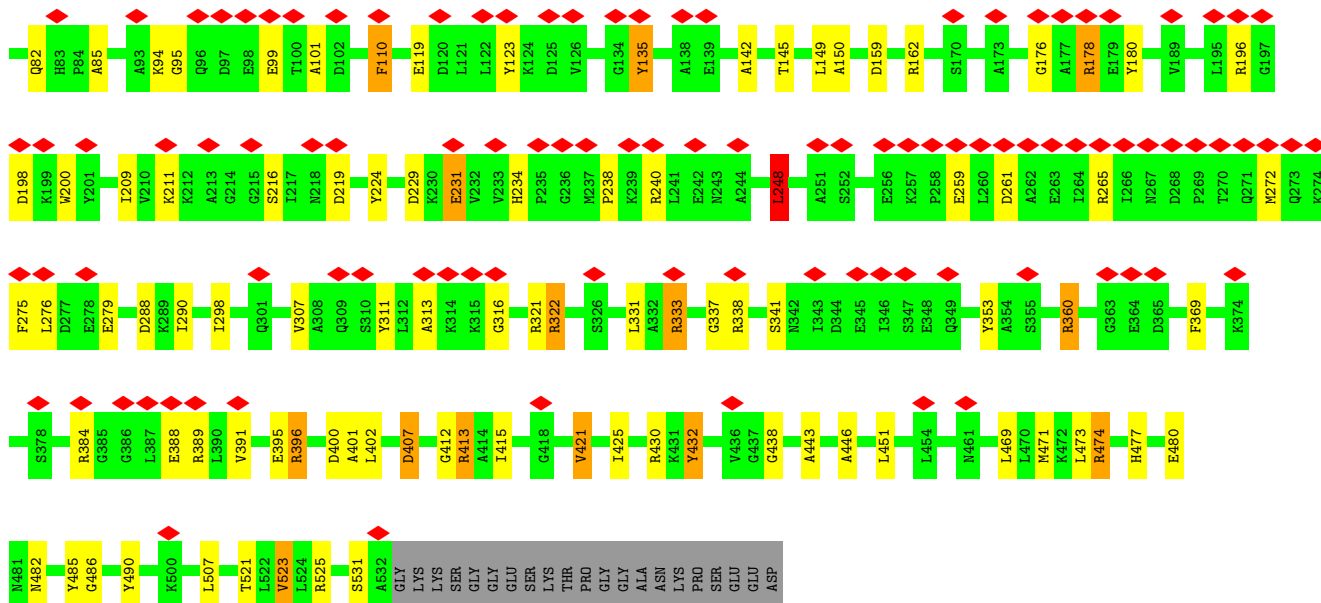


• Molecule 1: Chaperonin beta subunit

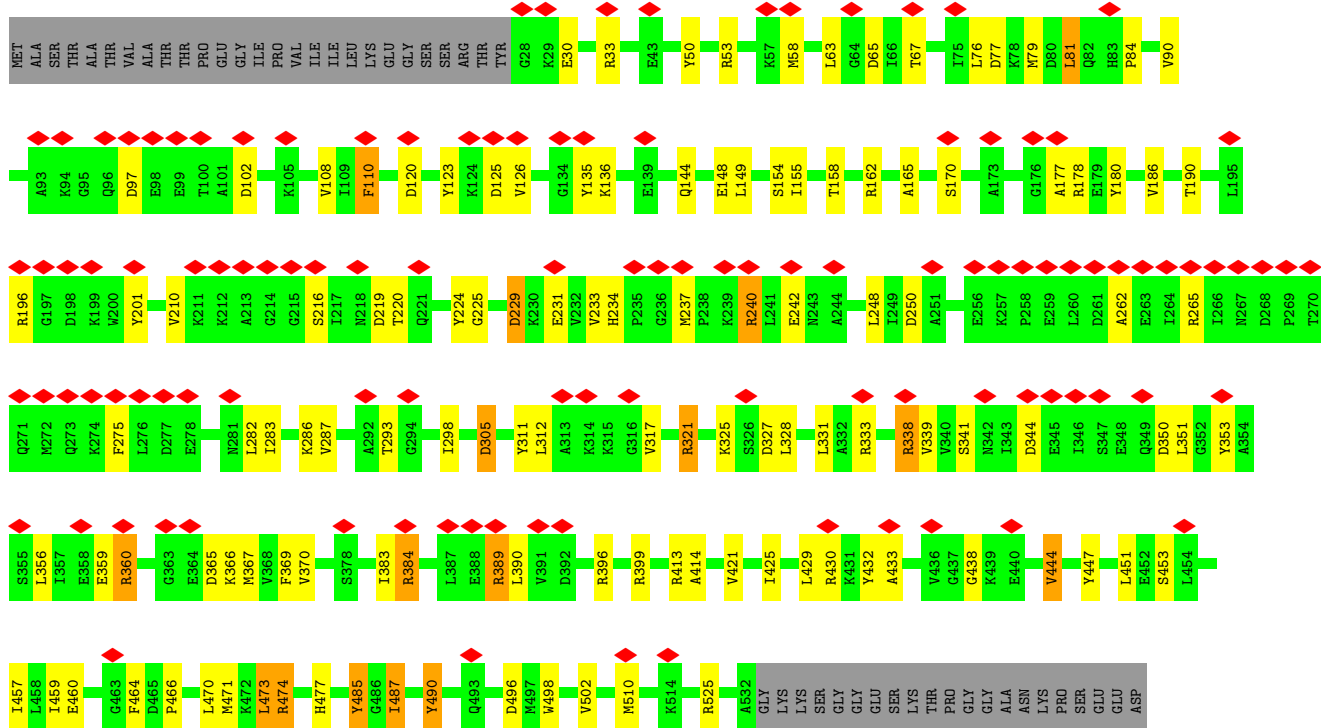


• Molecule 1: Chaperonin beta subunit



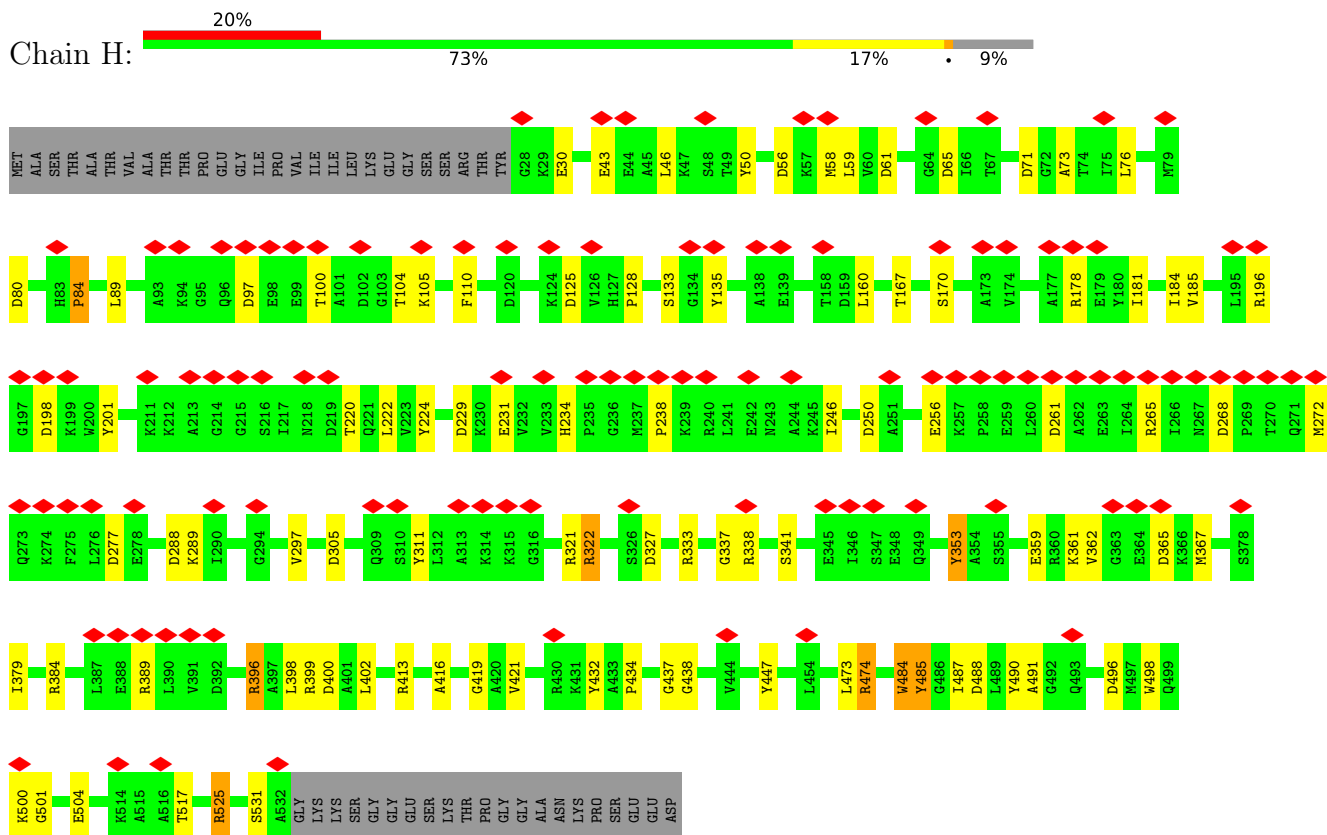


• Molecule 1: Chaperonin beta subunit

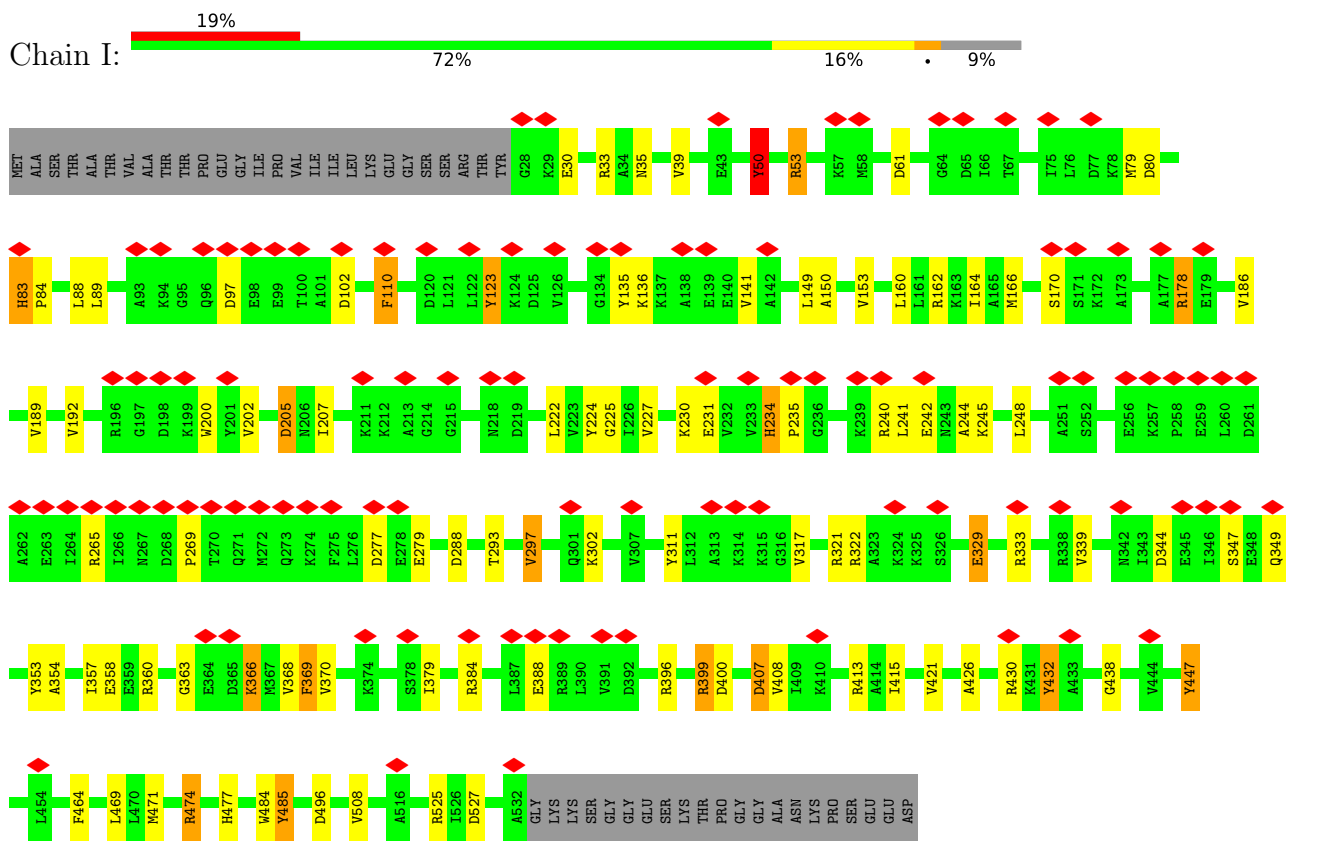


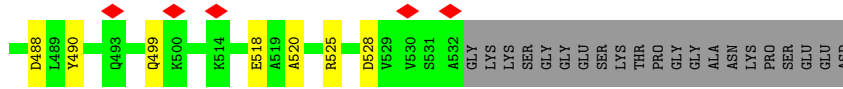
• Molecule 1: Chaperonin beta subunit



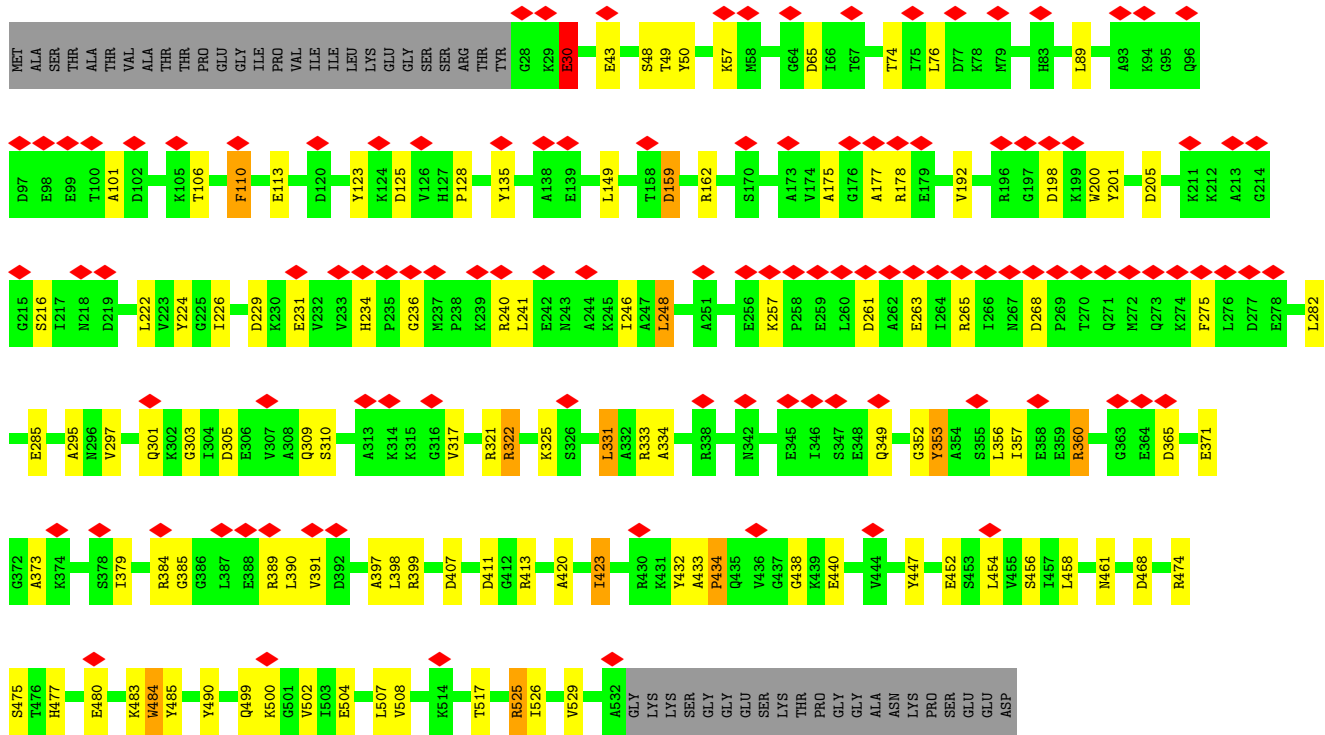


• Molecule 1: Chaperonin beta subunit

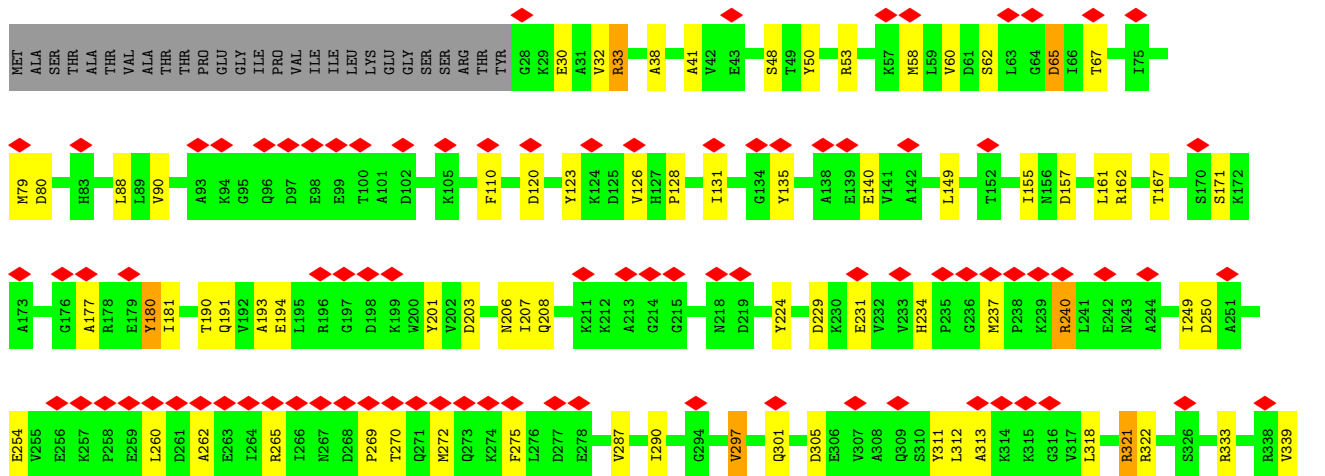


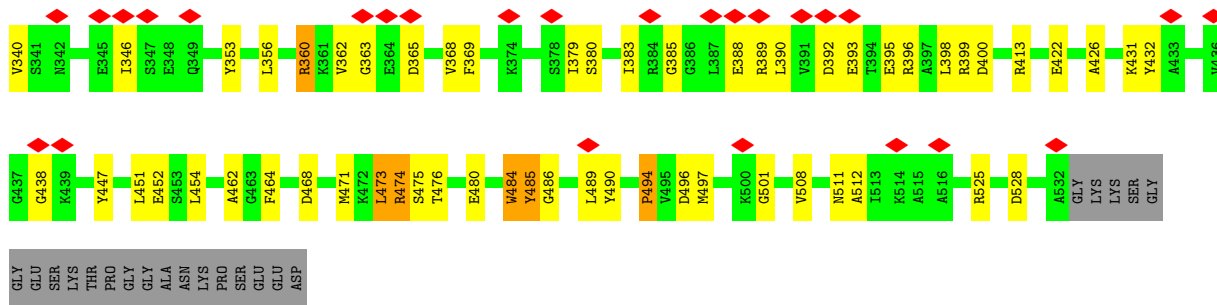


• Molecule 1: Chaperonin beta subunit

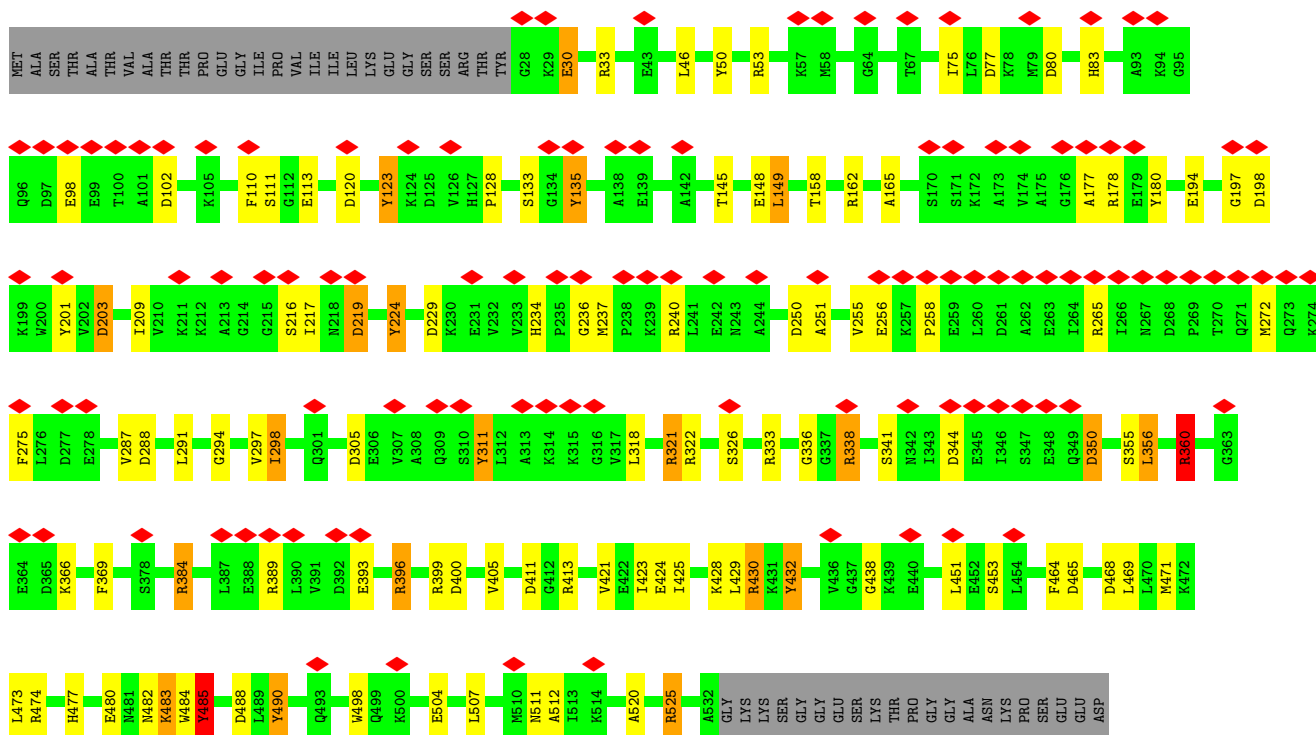


• Molecule 1: Chaperonin beta subunit

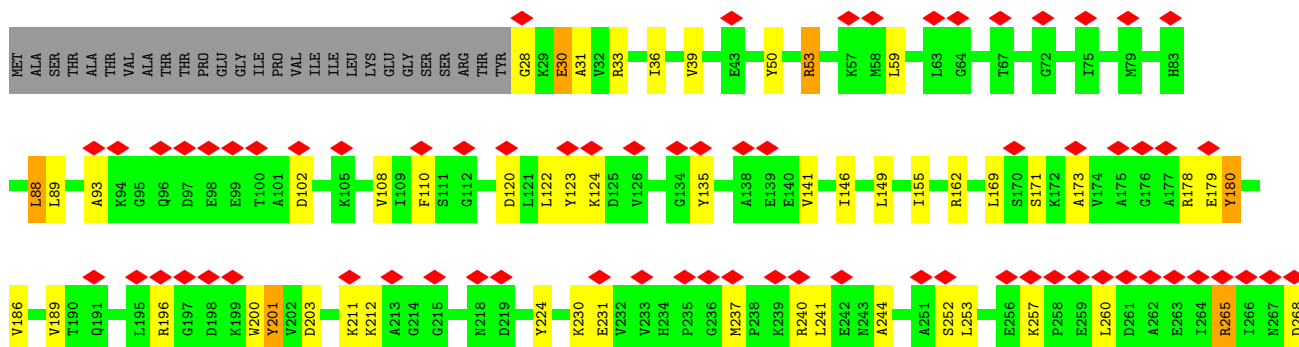


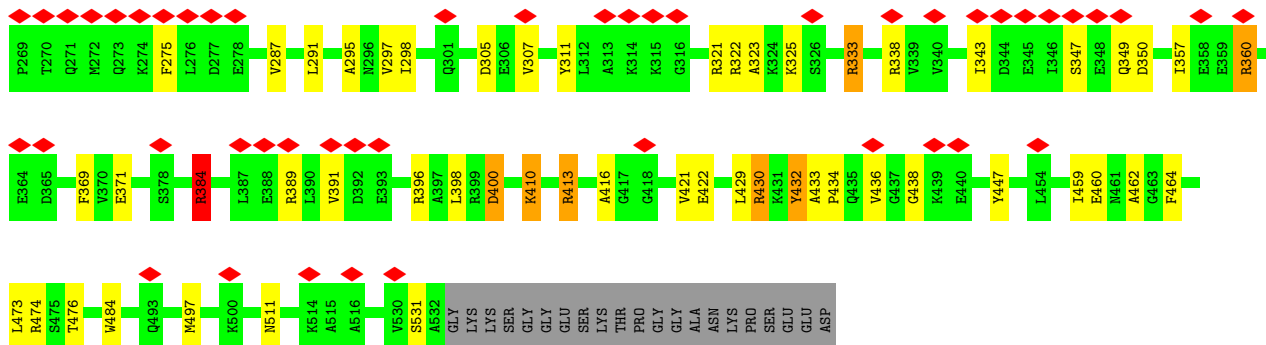


• Molecule 1: Chaperonin beta subunit

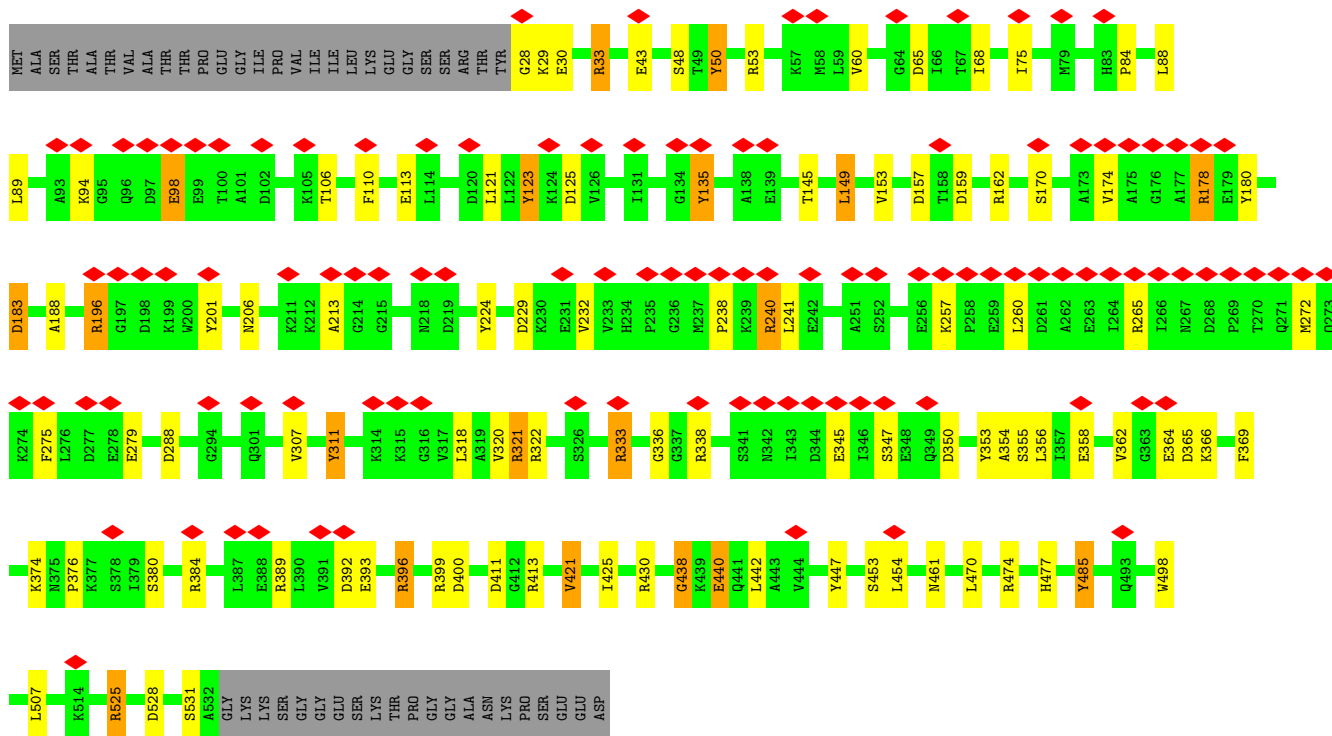
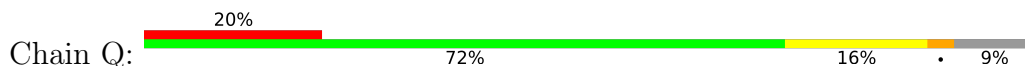


• Molecule 1: Chaperonin beta subunit

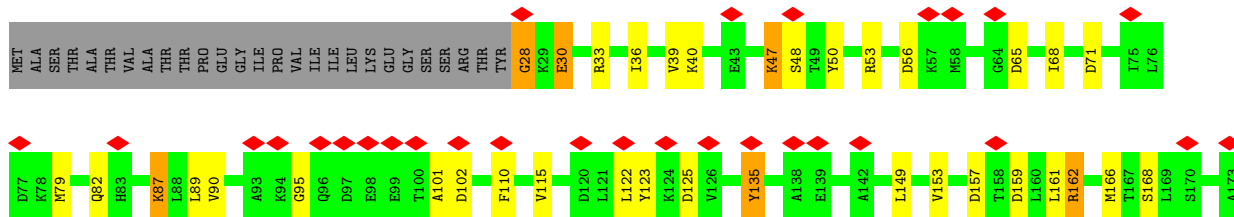


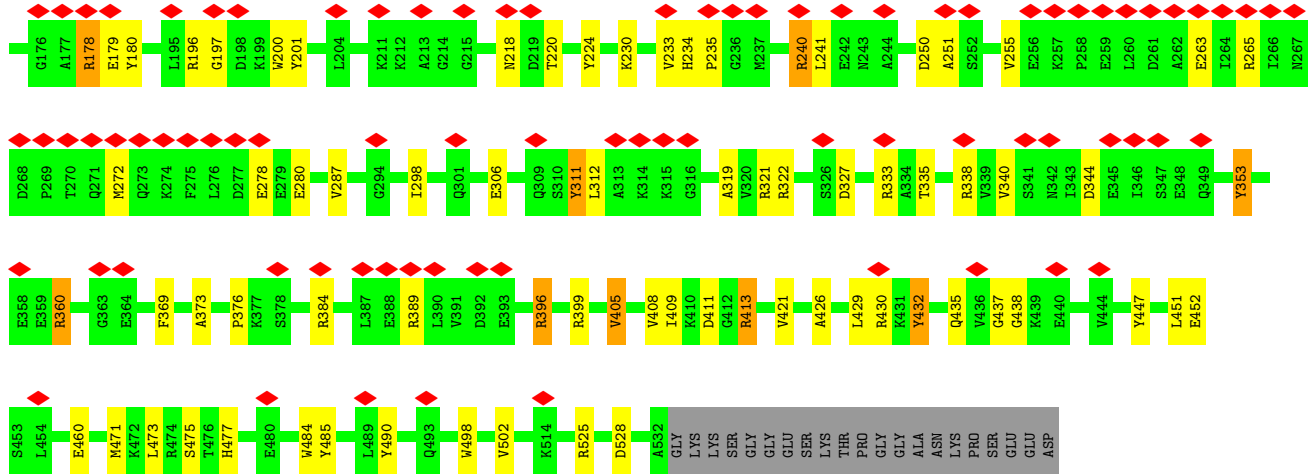


• Molecule 1: Chaperonin beta subunit

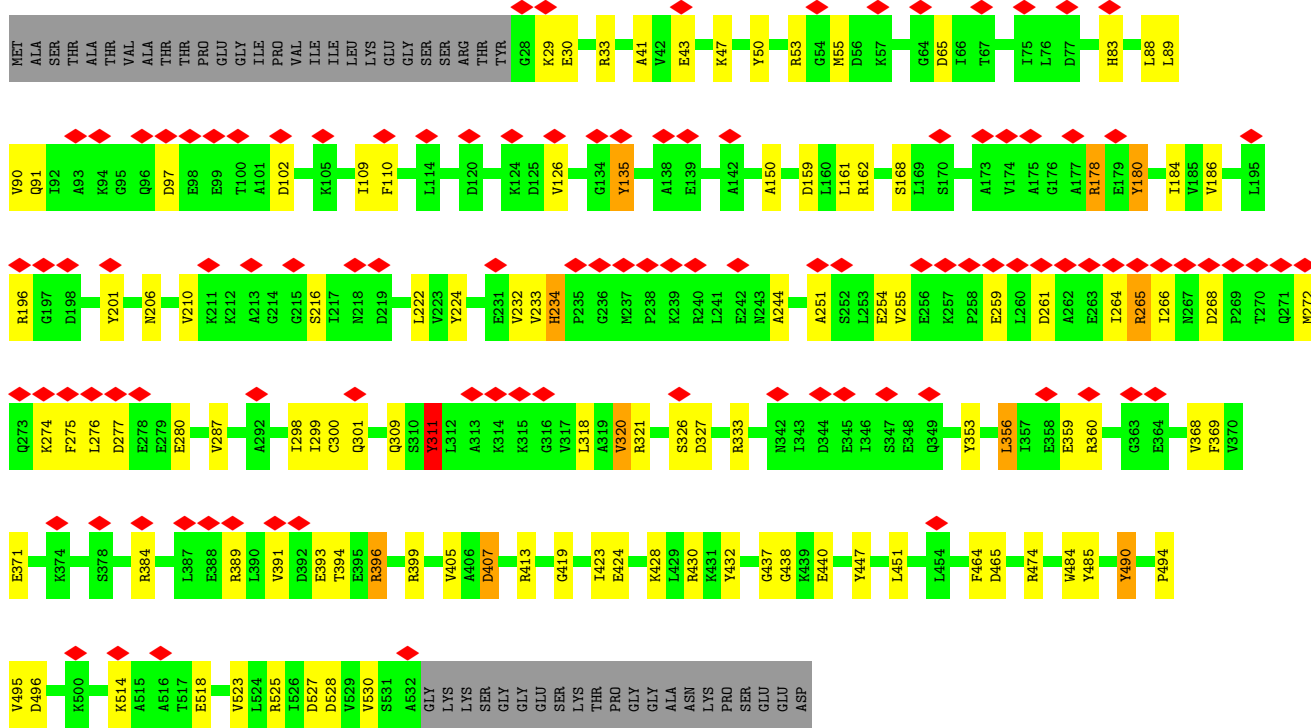


• Molecule 1: Chaperonin beta subunit





• Molecule 1: Chaperonin beta subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C9	Depositor
Number of particles used	28374	Depositor
Resolution determination method	Not provided	
CTF correction method	The whole micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	96000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	17.418	Depositor
Minimum map value	-16.157	Depositor
Average map value	-0.139	Depositor
Map value standard deviation	1.599	Depositor
Recommended contour level	4.0	Depositor
Map size (\AA)	298.56, 298.56, 298.56	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.8659999, 1.8659999, 1.8659999	Depositor

5 Model quality i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.59	16/3886 (0.4%)	1.94	81/5245 (1.5%)
1	B	1.59	20/3886 (0.5%)	1.94	87/5245 (1.7%)
1	C	1.59	15/3886 (0.4%)	1.94	82/5245 (1.6%)
1	D	1.57	21/3886 (0.5%)	1.94	81/5245 (1.5%)
1	E	1.58	19/3886 (0.5%)	1.97	97/5245 (1.8%)
1	F	1.63	25/3886 (0.6%)	1.92	74/5245 (1.4%)
1	G	1.59	25/3886 (0.6%)	1.91	83/5245 (1.6%)
1	H	1.57	13/3886 (0.3%)	1.91	79/5245 (1.5%)
1	I	1.63	19/3886 (0.5%)	1.90	81/5245 (1.5%)
1	K	1.60	18/3886 (0.5%)	1.90	78/5245 (1.5%)
1	L	1.58	21/3886 (0.5%)	1.99	88/5245 (1.7%)
1	M	1.57	18/3886 (0.5%)	1.92	79/5245 (1.5%)
1	N	1.59	15/3886 (0.4%)	1.96	104/5245 (2.0%)
1	O	1.57	16/3886 (0.4%)	1.95	106/5245 (2.0%)
1	P	1.54	13/3886 (0.3%)	1.91	80/5245 (1.5%)
1	Q	1.57	20/3886 (0.5%)	1.97	93/5245 (1.8%)
1	R	1.58	20/3886 (0.5%)	1.98	101/5245 (1.9%)
1	S	1.58	18/3886 (0.5%)	1.95	89/5245 (1.7%)
All	All	1.58	332/69948 (0.5%)	1.94	1563/94410 (1.7%)

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	9
1	B	0	16
1	C	0	15
1	D	0	12
1	E	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	9
1	G	0	14
1	H	0	13
1	I	0	12
1	K	0	14
1	L	0	13
1	M	0	8
1	N	0	6
1	O	0	13
1	P	0	10
1	Q	0	17
1	R	0	12
1	S	0	7
All	All	0	207

All (332) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	135	TYR	CG-CD2	9.30	1.51	1.39
1	N	494	PRO	N-CD	-8.56	1.35	1.47
1	K	113	GLU	CD-OE1	8.50	1.34	1.25
1	L	490	TYR	CZ-OH	8.11	1.51	1.37
1	A	432	TYR	CG-CD1	7.84	1.49	1.39
1	O	148	GLU	CD-OE1	7.73	1.34	1.25
1	B	474	ARG	CD-NE	7.67	1.59	1.46
1	Q	28	GLY	N-CA	7.65	1.57	1.46
1	C	453	SER	CA-CB	7.62	1.64	1.52
1	S	384	ARG	CD-NE	7.55	1.59	1.46
1	S	326	SER	CA-CB	7.28	1.63	1.52
1	D	99	GLU	CB-CG	7.23	1.65	1.52
1	D	110	PHE	CG-CD2	7.19	1.49	1.38
1	I	279	GLU	CG-CD	7.15	1.62	1.51
1	G	50	TYR	CG-CD1	7.14	1.48	1.39
1	S	216	SER	CA-CB	7.13	1.63	1.52
1	B	380	SER	CB-OG	7.11	1.51	1.42
1	N	485	TYR	CG-CD1	7.10	1.48	1.39
1	L	194	GLU	CG-CD	7.06	1.62	1.51
1	F	280	GLU	CD-OE2	7.03	1.33	1.25
1	A	360	ARG	CD-NE	6.95	1.58	1.46
1	P	50	TYR	CZ-OH	6.93	1.49	1.37
1	P	447	TYR	CE1-CZ	6.89	1.47	1.38
1	S	447	TYR	CG-CD2	6.89	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	311	TYR	CG-CD2	6.89	1.48	1.39
1	G	196	ARG	CD-NE	6.87	1.58	1.46
1	F	201	TYR	CB-CG	6.87	1.61	1.51
1	B	275	PHE	CB-CG	-6.86	1.39	1.51
1	E	216	SER	CA-CB	6.85	1.63	1.52
1	A	50	TYR	CB-CG	6.82	1.61	1.51
1	L	110	PHE	CG-CD2	6.78	1.49	1.38
1	N	395	GLU	CG-CD	6.75	1.62	1.51
1	I	369	PHE	CG-CD2	6.70	1.48	1.38
1	E	447	TYR	CG-CD1	6.70	1.47	1.39
1	S	440	GLU	CG-CD	6.67	1.61	1.51
1	S	50	TYR	CD1-CE1	6.59	1.49	1.39
1	I	265	ARG	NE-CZ	6.58	1.41	1.33
1	D	123	TYR	CG-CD1	6.56	1.47	1.39
1	D	95	GLY	CA-C	-6.55	1.41	1.51
1	E	201	TYR	CE1-CZ	6.55	1.47	1.38
1	R	353	TYR	CE1-CZ	6.52	1.47	1.38
1	Q	369	PHE	CG-CD1	6.50	1.48	1.38
1	P	28	GLY	N-CA	6.49	1.55	1.46
1	C	235	PRO	N-CD	-6.48	1.38	1.47
1	M	461	ASN	CB-CG	6.48	1.66	1.51
1	R	432	TYR	CG-CD2	6.48	1.47	1.39
1	O	30	GLU	CD-OE2	6.47	1.32	1.25
1	S	110	PHE	CG-CD2	6.47	1.48	1.38
1	F	28	GLY	N-CA	6.46	1.55	1.46
1	F	475	SER	CA-CB	6.46	1.62	1.52
1	B	123	TYR	CE2-CZ	6.45	1.47	1.38
1	B	358	GLU	CD-OE1	6.44	1.32	1.25
1	C	252	SER	CA-CB	6.43	1.62	1.52
1	O	498	TRP	CB-CG	6.41	1.61	1.50
1	B	347	SER	CA-CB	6.39	1.62	1.52
1	I	485	TYR	CB-CG	-6.39	1.42	1.51
1	M	352	GLY	CA-C	6.38	1.62	1.51
1	M	216	SER	CA-CB	6.35	1.62	1.52
1	M	456	SER	CA-CB	6.34	1.62	1.52
1	N	388	GLU	CD-OE2	-6.34	1.18	1.25
1	E	490	TYR	CB-CG	-6.33	1.42	1.51
1	Q	275	PHE	CE2-CZ	6.32	1.49	1.37
1	B	139	GLU	CD-OE1	6.30	1.32	1.25
1	G	200	TRP	NE1-CE2	6.27	1.45	1.37
1	E	231	GLU	CB-CG	6.26	1.64	1.52
1	N	50	TYR	CG-CD1	6.24	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	306	GLU	CD-OE2	6.22	1.32	1.25
1	F	225	GLY	CA-C	-6.22	1.41	1.51
1	M	224	TYR	CE1-CZ	6.20	1.46	1.38
1	M	224	TYR	CZ-OH	6.20	1.48	1.37
1	B	123	TYR	CZ-OH	6.18	1.48	1.37
1	R	376	PRO	N-CD	-6.18	1.39	1.47
1	E	50	TYR	CG-CD1	6.17	1.47	1.39
1	I	311	TYR	CE2-CZ	6.17	1.46	1.38
1	M	48	SER	CA-CB	6.16	1.62	1.52
1	H	498	TRP	CD1-NE1	6.14	1.48	1.38
1	F	447	TYR	CE1-CZ	6.13	1.46	1.38
1	G	485	TYR	CG-CD2	6.13	1.47	1.39
1	B	134	GLY	CA-C	6.13	1.61	1.51
1	P	135	TYR	CG-CD1	6.12	1.47	1.39
1	K	279	GLU	CG-CD	-6.11	1.42	1.51
1	A	41	ALA	CA-CB	6.09	1.65	1.52
1	H	337	GLY	CA-C	6.09	1.61	1.51
1	O	194	GLU	CD-OE2	6.08	1.32	1.25
1	L	180	TYR	CD1-CE1	6.08	1.48	1.39
1	K	326	SER	CA-CB	6.08	1.62	1.52
1	Q	531	SER	CA-CB	6.07	1.62	1.52
1	B	200	TRP	CD2-CE3	-6.04	1.31	1.40
1	F	422	GLU	CB-CG	6.03	1.63	1.52
1	M	360	ARG	CD-NE	6.00	1.56	1.46
1	F	531	SER	CA-CB	5.99	1.61	1.52
1	R	224	TYR	CG-CD1	5.99	1.47	1.39
1	H	73	ALA	N-CA	-5.98	1.34	1.46
1	C	162	ARG	CD-NE	5.96	1.56	1.46
1	M	135	TYR	CG-CD1	5.96	1.46	1.39
1	P	460	GLU	CG-CD	-5.96	1.43	1.51
1	K	154	SER	CA-CB	5.96	1.61	1.52
1	R	399	ARG	CD-NE	5.95	1.56	1.46
1	I	83	HIS	C-N	-5.95	1.23	1.34
1	E	154	SER	CA-CB	5.94	1.61	1.52
1	M	200	TRP	NE1-CE2	5.93	1.45	1.37
1	O	240	ARG	CD-NE	5.93	1.56	1.46
1	Q	333	ARG	NE-CZ	5.92	1.40	1.33
1	H	84	PRO	N-CD	-5.92	1.39	1.47
1	E	432	TYR	CZ-OH	5.91	1.47	1.37
1	K	30	GLU	CG-CD	-5.90	1.43	1.51
1	O	333	ARG	NE-CZ	5.90	1.40	1.33
1	P	338	ARG	CZ-NH2	5.89	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	378	SER	CA-CB	5.89	1.61	1.52
1	G	418	GLY	C-N	5.88	1.43	1.33
1	A	111	SER	CA-CB	5.87	1.61	1.52
1	B	114	LEU	CA-CB	5.87	1.67	1.53
1	H	201	TYR	CB-CG	5.86	1.60	1.51
1	S	432	TYR	CB-CG	-5.86	1.42	1.51
1	A	294	GLY	CA-C	-5.85	1.42	1.51
1	Q	311	TYR	CE2-CZ	5.85	1.46	1.38
1	Q	380	SER	CA-CB	5.83	1.61	1.52
1	I	347	SER	CA-CB	5.82	1.61	1.52
1	R	475	SER	CA-CB	5.82	1.61	1.52
1	D	388	GLU	CG-CD	5.81	1.60	1.51
1	N	385	GLY	N-CA	-5.80	1.37	1.46
1	Q	393	GLU	CD-OE2	5.80	1.32	1.25
1	O	111	SER	C-N	5.80	1.43	1.33
1	M	504	GLU	CD-OE2	5.80	1.32	1.25
1	C	413	ARG	CZ-NH1	-5.79	1.25	1.33
1	L	254	GLU	CG-CD	5.78	1.60	1.51
1	D	311	TYR	CZ-OH	5.78	1.47	1.37
1	K	28	GLY	N-CA	5.77	1.54	1.46
1	L	360	ARG	CD-NE	5.76	1.56	1.46
1	Q	113	GLU	CB-CG	5.75	1.63	1.52
1	R	48	SER	CA-CB	5.75	1.61	1.52
1	H	322	ARG	CD-NE	5.74	1.56	1.46
1	O	256	GLU	CD-OE2	5.74	1.31	1.25
1	A	275	PHE	CG-CD1	5.73	1.47	1.38
1	O	287	VAL	CA-CB	-5.73	1.42	1.54
1	C	200	TRP	CD2-CE3	5.72	1.49	1.40
1	N	53	ARG	C-N	5.71	1.43	1.33
1	B	490	TYR	CZ-OH	5.70	1.47	1.37
1	F	48	SER	CB-OG	5.70	1.49	1.42
1	L	33	ARG	NE-CZ	5.69	1.40	1.33
1	G	53	ARG	NE-CZ	5.69	1.40	1.33
1	S	300	CYS	CA-CB	5.69	1.66	1.53
1	P	178	ARG	CD-NE	5.69	1.56	1.46
1	R	353	TYR	CZ-OH	5.68	1.47	1.37
1	H	135	TYR	CG-CD1	5.68	1.46	1.39
1	O	123	TYR	CZ-OH	5.67	1.47	1.37
1	B	48	SER	CA-CB	5.67	1.61	1.52
1	G	154	SER	CA-CB	5.66	1.61	1.52
1	E	293	THR	N-CA	-5.66	1.35	1.46
1	N	50	TYR	CZ-OH	5.63	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	263	GLU	CD-OE1	5.62	1.31	1.25
1	S	518	GLU	CD-OE1	5.62	1.31	1.25
1	S	224	TYR	CZ-OH	5.62	1.47	1.37
1	K	504	GLU	CD-OE1	-5.61	1.19	1.25
1	K	358	GLU	CG-CD	5.61	1.60	1.51
1	N	501	GLY	CA-C	-5.61	1.42	1.51
1	Q	447	TYR	CE2-CZ	5.61	1.45	1.38
1	S	447	TYR	CA-CB	5.59	1.66	1.53
1	N	301	GLN	CG-CD	5.59	1.64	1.51
1	D	238	PRO	N-CA	-5.59	1.37	1.47
1	K	514	LYS	CD-CE	5.58	1.65	1.51
1	P	231	GLU	CG-CD	5.58	1.60	1.51
1	Q	358	GLU	CB-CG	5.57	1.62	1.52
1	N	126	VAL	CA-CB	-5.57	1.43	1.54
1	G	110	PHE	CG-CD1	5.56	1.47	1.38
1	E	148	GLU	CD-OE1	-5.55	1.19	1.25
1	K	224	TYR	CE2-CZ	5.54	1.45	1.38
1	F	326	SER	CA-CB	5.54	1.61	1.52
1	G	178	ARG	CD-NE	5.54	1.55	1.46
1	H	501	GLY	N-CA	-5.52	1.37	1.46
1	F	238	PRO	N-CA	5.52	1.56	1.47
1	G	430	ARG	CD-NE	5.52	1.55	1.46
1	L	474	ARG	CD-NE	5.51	1.55	1.46
1	O	484	TRP	N-CA	-5.51	1.35	1.46
1	F	240	ARG	CD-NE	5.51	1.55	1.46
1	D	265	ARG	CD-NE	5.50	1.55	1.46
1	O	389	ARG	NE-CZ	5.50	1.40	1.33
1	F	224	TYR	CZ-OH	5.49	1.47	1.37
1	C	440	GLU	CG-CD	5.49	1.60	1.51
1	B	242	GLU	CG-CD	-5.48	1.43	1.51
1	G	440	GLU	CG-CD	-5.47	1.43	1.51
1	L	432	TYR	CG-CD2	5.47	1.46	1.39
1	O	321	ARG	CZ-NH1	-5.47	1.25	1.33
1	P	311	TYR	CE2-CZ	5.47	1.45	1.38
1	M	128	PRO	N-CD	-5.46	1.40	1.47
1	D	316	GLY	CA-C	-5.46	1.43	1.51
1	F	256	GLU	CD-OE1	5.46	1.31	1.25
1	S	371	GLU	CG-CD	5.46	1.60	1.51
1	B	434	PRO	N-CD	-5.45	1.40	1.47
1	K	196	ARG	CD-NE	5.45	1.55	1.46
1	A	278	GLU	CB-CG	5.45	1.62	1.52
1	Q	438	GLY	N-CA	5.45	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	94	LYS	CA-CB	5.43	1.65	1.53
1	L	353	TYR	CZ-OH	5.43	1.47	1.37
1	G	475	SER	CA-CB	5.43	1.61	1.52
1	R	490	TYR	CE1-CZ	5.42	1.45	1.38
1	A	364	GLU	CD-OE2	5.41	1.31	1.25
1	E	180	TYR	CE1-CZ	5.41	1.45	1.38
1	L	28	GLY	N-CA	5.41	1.54	1.46
1	G	490	TYR	CE1-CZ	5.41	1.45	1.38
1	K	430	ARG	CD-NE	5.41	1.55	1.46
1	M	474	ARG	CD-NE	5.41	1.55	1.46
1	I	464	PHE	CB-CG	-5.40	1.42	1.51
1	G	518	GLU	CD-OE2	5.40	1.31	1.25
1	D	259	GLU	CB-CG	5.40	1.62	1.52
1	G	525	ARG	CD-NE	5.39	1.55	1.46
1	L	82	GLN	CB-CG	5.39	1.67	1.52
1	G	224	TYR	CZ-OH	5.38	1.47	1.37
1	C	311	TYR	CE2-CZ	5.38	1.45	1.38
1	F	135	TYR	CB-CG	5.38	1.59	1.51
1	I	225	GLY	CA-C	-5.37	1.43	1.51
1	K	364	GLU	CA-CB	5.37	1.65	1.53
1	I	265	ARG	CD-NE	5.37	1.55	1.46
1	F	353	TYR	CG-CD1	5.36	1.46	1.39
1	K	33	ARG	CD-NE	5.36	1.55	1.46
1	R	201	TYR	CE2-CZ	-5.36	1.31	1.38
1	R	525	ARG	CD-NE	5.36	1.55	1.46
1	Q	442	LEU	CA-CB	5.36	1.66	1.53
1	L	265	ARG	CD-NE	5.35	1.55	1.46
1	P	484	TRP	N-CA	-5.35	1.35	1.46
1	S	437	GLY	CA-C	-5.34	1.43	1.51
1	A	197	GLY	N-CA	5.33	1.54	1.46
1	N	447	TYR	CZ-OH	5.33	1.47	1.37
1	R	306	GLU	CB-CG	5.33	1.62	1.52
1	K	413	ARG	CD-NE	5.32	1.55	1.46
1	H	419	GLY	CA-C	-5.32	1.43	1.51
1	M	440	GLU	CD-OE2	5.32	1.31	1.25
1	H	43	GLU	CD-OE2	5.32	1.31	1.25
1	Q	485	TYR	CZ-OH	5.32	1.46	1.37
1	G	252	SER	CA-CB	5.31	1.60	1.52
1	D	412	GLY	CA-C	-5.31	1.43	1.51
1	E	444	VAL	CB-CG1	5.31	1.64	1.52
1	A	347	SER	CA-CB	5.30	1.60	1.52
1	I	186	VAL	CA-CB	-5.29	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	231	GLU	CB-CG	5.29	1.62	1.52
1	I	317	VAL	CB-CG1	5.28	1.64	1.52
1	R	235	PRO	N-CD	-5.28	1.40	1.47
1	C	285	GLU	CD-OE1	5.28	1.31	1.25
1	A	504	GLU	CD-OE1	5.27	1.31	1.25
1	H	504	GLU	N-CA	-5.27	1.35	1.46
1	Q	98	GLU	CD-OE2	5.27	1.31	1.25
1	K	311	TYR	CE1-CZ	5.26	1.45	1.38
1	I	363	GLY	CA-C	-5.26	1.43	1.51
1	G	369	PHE	CG-CD2	5.26	1.46	1.38
1	P	275	PHE	CE2-CZ	5.26	1.47	1.37
1	P	347	SER	CA-CB	5.25	1.60	1.52
1	L	103	GLY	CA-C	5.25	1.60	1.51
1	F	254	GLU	CB-CG	5.24	1.62	1.52
1	S	135	TYR	CG-CD1	5.24	1.46	1.39
1	O	294	GLY	CA-C	-5.24	1.43	1.51
1	D	337	GLY	N-CA	5.23	1.53	1.46
1	G	359	GLU	CD-OE1	5.23	1.31	1.25
1	B	252	SER	CB-OG	5.22	1.49	1.42
1	K	147	GLN	CA-CB	5.22	1.65	1.53
1	L	234	HIS	CB-CG	5.22	1.59	1.50
1	Q	110	PHE	CB-CG	5.22	1.60	1.51
1	H	485	TYR	CD2-CE2	5.22	1.47	1.39
1	C	187	LYS	CA-CB	5.21	1.65	1.53
1	F	259	GLU	CG-CD	5.21	1.59	1.51
1	E	84	PRO	N-CD	-5.21	1.40	1.47
1	I	339	VAL	CB-CG2	5.21	1.63	1.52
1	C	201	TYR	CD1-CE1	5.20	1.47	1.39
1	G	256	GLU	CB-CG	5.20	1.62	1.52
1	G	140	GLU	CD-OE1	5.20	1.31	1.25
1	D	279	GLU	CD-OE2	5.19	1.31	1.25
1	L	403	GLY	N-CA	-5.19	1.38	1.46
1	G	341	SER	CB-OG	5.18	1.49	1.42
1	M	385	GLY	N-CA	5.18	1.53	1.46
1	C	280	GLU	CB-CG	5.18	1.61	1.52
1	Q	224	TYR	CE2-CZ	5.18	1.45	1.38
1	I	447	TYR	CE1-CZ	5.17	1.45	1.38
1	N	48	SER	CA-CB	5.17	1.60	1.52
1	D	531	SER	CA-CB	5.17	1.60	1.52
1	G	214	GLY	CA-C	5.17	1.60	1.51
1	P	447	TYR	CD1-CE1	-5.17	1.31	1.39
1	G	355	SER	CA-CB	5.16	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	419	GLY	CA-C	-5.16	1.43	1.51
1	E	50	TYR	CG-CD2	-5.16	1.32	1.39
1	Q	345	GLU	CB-CG	5.16	1.61	1.52
1	D	341	SER	CA-CB	5.15	1.60	1.52
1	E	225	GLY	N-CA	5.15	1.53	1.46
1	A	484	TRP	CG-CD1	5.15	1.44	1.36
1	E	311	TYR	CZ-OH	5.15	1.46	1.37
1	R	322	ARG	CD-NE	5.14	1.55	1.46
1	E	136	LYS	CA-CB	5.14	1.65	1.53
1	F	33	ARG	NE-CZ	5.14	1.39	1.33
1	L	135	TYR	CG-CD1	5.14	1.45	1.39
1	O	133	SER	CA-CB	5.14	1.60	1.52
1	L	518	GLU	CG-CD	-5.14	1.44	1.51
1	R	28	GLY	N-CA	5.14	1.53	1.46
1	E	353	TYR	CE1-CZ	5.13	1.45	1.38
1	F	493	GLN	CA-CB	5.13	1.65	1.53
1	F	275	PHE	CG-CD2	5.13	1.46	1.38
1	C	105	LYS	N-CA	-5.12	1.36	1.46
1	G	460	GLU	N-CA	-5.12	1.36	1.46
1	L	333	ARG	CD-NE	5.12	1.55	1.46
1	Q	447	TYR	CG-CD1	5.12	1.45	1.39
1	D	142	ALA	CA-CB	5.11	1.63	1.52
1	D	486	GLY	N-CA	-5.11	1.38	1.46
1	H	178	ARG	CD-NE	5.11	1.55	1.46
1	I	269	PRO	N-CA	5.11	1.55	1.47
1	C	240	ARG	CD-NE	5.10	1.55	1.46
1	M	475	SER	CB-OG	5.10	1.48	1.42
1	R	71	ASP	C-N	5.09	1.42	1.33
1	F	285	GLU	CD-OE1	5.09	1.31	1.25
1	M	257	LYS	CA-CB	5.09	1.65	1.53
1	Q	170	SER	CA-CB	5.08	1.60	1.52
1	R	201	TYR	CE1-CZ	5.08	1.45	1.38
1	R	280	GLU	CD-OE1	5.08	1.31	1.25
1	E	148	GLU	CB-CG	5.08	1.61	1.52
1	C	480	GLU	CD-OE1	5.07	1.31	1.25
1	L	62	SER	CA-CB	5.07	1.60	1.52
1	I	50	TYR	CE1-CZ	5.06	1.45	1.38
1	N	490	TYR	CG-CD1	5.05	1.45	1.39
1	A	329	GLU	CD-OE1	5.05	1.31	1.25
1	A	213	ALA	C-N	5.05	1.42	1.33
1	B	372	GLY	CA-C	5.04	1.59	1.51
1	F	518	GLU	CG-CD	5.04	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	43	GLU	CD-OE1	5.03	1.31	1.25
1	A	358	GLU	CG-CD	-5.03	1.44	1.51
1	D	259	GLU	CG-CD	5.03	1.59	1.51
1	I	329	GLU	C-N	5.03	1.45	1.34
1	L	484	TRP	CG-CD1	-5.02	1.29	1.36
1	N	123	TYR	CG-CD1	5.02	1.45	1.39
1	S	280	GLU	CA-CB	5.02	1.65	1.53
1	D	402	LEU	C-N	5.02	1.42	1.33
1	K	369	PHE	CG-CD1	5.02	1.46	1.38
1	F	369	PHE	CG-CD1	5.02	1.46	1.38
1	R	437	GLY	CA-C	-5.02	1.43	1.51
1	B	273	GLN	CG-CD	5.01	1.62	1.51
1	D	401	ALA	CA-CB	5.01	1.62	1.52
1	M	285	GLU	CB-CG	5.01	1.61	1.52

All (1563) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	196	ARG	NE-CZ-NH1	-24.99	107.81	120.30
1	L	33	ARG	NE-CZ-NH1	21.31	130.95	120.30
1	F	430	ARG	NE-CZ-NH1	19.66	130.13	120.30
1	Q	135	TYR	CB-CG-CD1	-18.98	109.61	121.00
1	Q	178	ARG	NE-CZ-NH2	18.75	129.67	120.30
1	D	396	ARG	NE-CZ-NH1	18.61	129.60	120.30
1	I	321	ARG	NE-CZ-NH1	17.19	128.90	120.30
1	H	413	ARG	NE-CZ-NH2	17.13	128.87	120.30
1	N	360	ARG	NE-CZ-NH2	17.13	128.86	120.30
1	G	333	ARG	NE-CZ-NH1	16.70	128.65	120.30
1	F	240	ARG	NE-CZ-NH1	16.52	128.56	120.30
1	A	162	ARG	NE-CZ-NH1	16.49	128.54	120.30
1	C	399	ARG	NE-CZ-NH2	16.03	128.31	120.30
1	D	396	ARG	NE-CZ-NH2	-16.02	112.29	120.30
1	L	338	ARG	NE-CZ-NH2	-16.01	112.29	120.30
1	E	360	ARG	NE-CZ-NH2	15.84	128.22	120.30
1	D	413	ARG	NE-CZ-NH1	-15.67	112.46	120.30
1	G	196	ARG	NE-CZ-NH2	15.42	128.01	120.30
1	E	389	ARG	NE-CZ-NH1	15.39	127.99	120.30
1	H	413	ARG	NE-CZ-NH1	-15.14	112.73	120.30
1	R	50	TYR	CB-CG-CD1	-15.13	111.92	121.00
1	P	53	ARG	NE-CZ-NH1	15.04	127.82	120.30
1	I	50	TYR	CB-CG-CD1	15.00	130.00	121.00
1	K	430	ARG	NE-CZ-NH1	14.84	127.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	ARG	NE-CZ-NH2	-14.79	112.91	120.30
1	S	360	ARG	NE-CZ-NH2	14.78	127.69	120.30
1	C	360	ARG	NE-CZ-NH2	14.74	127.67	120.30
1	C	399	ARG	NE-CZ-NH1	-14.62	112.99	120.30
1	C	53	ARG	NE-CZ-NH1	14.54	127.57	120.30
1	S	490	TYR	CB-CG-CD2	-14.53	112.28	121.00
1	B	53	ARG	NE-CZ-NH1	14.52	127.56	120.30
1	S	389	ARG	NE-CZ-NH1	14.51	127.56	120.30
1	M	265	ARG	NE-CZ-NH2	14.39	127.49	120.30
1	E	384	ARG	NE-CZ-NH1	14.39	127.49	120.30
1	A	240	ARG	NE-CZ-NH1	14.37	127.48	120.30
1	E	430	ARG	NE-CZ-NH2	-14.32	113.14	120.30
1	D	240	ARG	NE-CZ-NH2	-14.17	113.22	120.30
1	N	275	PHE	CB-CG-CD2	14.16	130.71	120.80
1	K	321	ARG	NE-CZ-NH1	14.10	127.35	120.30
1	S	201	TYR	CB-CG-CD1	-13.99	112.61	121.00
1	O	162	ARG	NE-CZ-NH1	13.99	127.29	120.30
1	O	413	ARG	NE-CZ-NH1	-13.96	113.32	120.30
1	H	353	TYR	CB-CG-CD2	-13.89	112.67	121.00
1	F	430	ARG	NE-CZ-NH2	-13.82	113.39	120.30
1	E	162	ARG	NE-CZ-NH2	-13.78	113.41	120.30
1	L	389	ARG	NE-CZ-NH2	-13.76	113.42	120.30
1	S	311	TYR	CB-CG-CD2	13.74	129.25	121.00
1	O	488	ASP	CB-CG-OD2	-13.70	105.97	118.30
1	Q	135	TYR	CB-CG-CD2	13.63	129.18	121.00
1	M	413	ARG	NE-CZ-NH2	13.59	127.09	120.30
1	L	33	ARG	NE-CZ-NH2	-13.56	113.52	120.30
1	B	333	ARG	NE-CZ-NH1	13.53	127.07	120.30
1	A	265	ARG	NE-CZ-NH1	-13.52	113.54	120.30
1	Q	33	ARG	NE-CZ-NH2	-13.48	113.56	120.30
1	L	240	ARG	NE-CZ-NH2	-13.43	113.59	120.30
1	M	389	ARG	NE-CZ-NH1	13.40	127.00	120.30
1	I	396	ARG	NE-CZ-NH1	13.39	127.00	120.30
1	K	430	ARG	NE-CZ-NH2	-13.38	113.61	120.30
1	B	321	ARG	NE-CZ-NH2	-13.34	113.63	120.30
1	H	311	TYR	CB-CG-CD1	-13.32	113.01	121.00
1	D	265	ARG	NE-CZ-NH2	13.31	126.95	120.30
1	F	123	TYR	CB-CG-CD1	-13.21	113.07	121.00
1	M	135	TYR	CB-CG-CD2	13.17	128.90	121.00
1	N	389	ARG	NE-CZ-NH1	13.16	126.88	120.30
1	O	135	TYR	CB-CG-CD2	13.14	128.88	121.00
1	E	525	ARG	NE-CZ-NH1	13.12	126.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	344	ASP	CB-CG-OD2	13.10	130.09	118.30
1	P	384	ARG	NE-CZ-NH2	-13.09	113.75	120.30
1	H	178	ARG	NE-CZ-NH2	13.05	126.83	120.30
1	M	399	ARG	NE-CZ-NH2	13.02	126.81	120.30
1	M	447	TYR	CB-CG-CD1	-13.00	113.20	121.00
1	E	265	ARG	NE-CZ-NH2	12.99	126.80	120.30
1	N	389	ARG	NE-CZ-NH2	-12.99	113.81	120.30
1	A	384	ARG	NE-CZ-NH1	12.94	126.77	120.30
1	R	360	ARG	NE-CZ-NH1	12.88	126.74	120.30
1	R	485	TYR	CB-CG-CD1	12.75	128.65	121.00
1	D	240	ARG	NE-CZ-NH1	12.69	126.65	120.30
1	L	135	TYR	CB-CG-CD2	12.67	128.60	121.00
1	H	322	ARG	NE-CZ-NH2	-12.62	113.99	120.30
1	P	338	ARG	NE-CZ-NH1	12.57	126.59	120.30
1	K	485	TYR	CB-CG-CD1	-12.56	113.47	121.00
1	R	413	ARG	NE-CZ-NH2	12.48	126.54	120.30
1	S	196	ARG	NE-CZ-NH2	12.47	126.54	120.30
1	M	135	TYR	CB-CG-CD1	-12.40	113.56	121.00
1	B	180	TYR	CB-CG-CD1	-12.38	113.57	121.00
1	I	110	PHE	CB-CG-CD1	-12.38	112.13	120.80
1	L	338	ARG	NE-CZ-NH1	12.32	126.46	120.30
1	A	333	ARG	NE-CZ-NH1	12.32	126.46	120.30
1	F	33	ARG	NE-CZ-NH2	-12.29	114.16	120.30
1	C	135	TYR	CB-CG-CD2	12.25	128.35	121.00
1	R	485	TYR	CB-CG-CD2	-12.25	113.65	121.00
1	D	369	PHE	CB-CG-CD1	-12.22	112.24	120.80
1	A	321	ARG	NE-CZ-NH1	12.17	126.39	120.30
1	Q	525	ARG	NE-CZ-NH2	-12.14	114.23	120.30
1	D	430	ARG	NE-CZ-NH1	12.12	126.36	120.30
1	I	50	TYR	CB-CG-CD2	-12.08	113.75	121.00
1	I	240	ARG	NE-CZ-NH2	-12.08	114.26	120.30
1	M	474	ARG	NE-CZ-NH2	12.05	126.32	120.30
1	H	201	TYR	CB-CG-CD1	-11.97	113.82	121.00
1	E	474	ARG	NE-CZ-NH2	11.94	126.27	120.30
1	R	135	TYR	CB-CG-CD2	11.94	128.16	121.00
1	O	488	ASP	CB-CG-OD1	11.93	129.04	118.30
1	C	53	ARG	NE-CZ-NH2	-11.90	114.35	120.30
1	D	413	ARG	NE-CZ-NH2	11.84	126.22	120.30
1	N	321	ARG	NE-CZ-NH2	-11.84	114.38	120.30
1	L	322	ARG	NE-CZ-NH2	-11.82	114.39	120.30
1	K	338	ARG	NE-CZ-NH1	11.79	126.20	120.30
1	O	135	TYR	CB-CG-CD1	-11.78	113.93	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	311	TYR	CB-CG-CD1	-11.75	113.95	121.00
1	B	196	ARG	NE-CZ-NH2	11.64	126.12	120.30
1	E	471	MET	CG-SD-CE	-11.61	81.62	100.20
1	N	474	ARG	NE-CZ-NH1	11.60	126.10	120.30
1	M	224	TYR	CB-CG-CD1	-11.60	114.04	121.00
1	Q	53	ARG	NE-CZ-NH2	-11.55	114.53	120.30
1	P	384	ARG	NE-CZ-NH1	11.50	126.05	120.30
1	O	288	ASP	CB-CG-OD1	11.38	128.55	118.30
1	B	413	ARG	NE-CZ-NH1	11.37	125.99	120.30
1	H	353	TYR	CB-CG-CD1	11.34	127.80	121.00
1	M	384	ARG	NE-CZ-NH1	11.32	125.96	120.30
1	Q	474	ARG	NE-CZ-NH2	11.29	125.95	120.30
1	S	490	TYR	CB-CG-CD1	11.29	127.77	121.00
1	O	490	TYR	CB-CG-CD2	-11.27	114.24	121.00
1	E	240	ARG	NE-CZ-NH2	-11.26	114.67	120.30
1	R	135	TYR	CB-CG-CD1	-11.26	114.24	121.00
1	C	384	ARG	NE-CZ-NH2	-11.24	114.68	120.30
1	E	338	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	I	407	ASP	CB-CG-OD2	-11.19	108.23	118.30
1	A	311	TYR	CB-CG-CD1	-11.14	114.31	121.00
1	N	250	ASP	CB-CG-OD2	11.13	128.32	118.30
1	C	77	ASP	CB-CG-OD2	11.10	128.29	118.30
1	P	265	ARG	NE-CZ-NH2	11.08	125.84	120.30
1	H	485	TYR	CB-CG-CD1	-11.07	114.36	121.00
1	S	327	ASP	CB-CG-OD1	11.07	128.26	118.30
1	O	474	ARG	NE-CZ-NH1	-11.06	114.77	120.30
1	K	135	TYR	CB-CG-CD1	-11.02	114.39	121.00
1	P	240	ARG	NE-CZ-NH2	-11.02	114.79	120.30
1	P	360	ARG	NE-CZ-NH1	-11.01	114.79	120.30
1	H	525	ARG	NE-CZ-NH2	10.99	125.80	120.30
1	M	399	ARG	NE-CZ-NH1	-10.97	114.82	120.30
1	D	384	ARG	NE-CZ-NH2	-10.95	114.82	120.30
1	M	353	TYR	CB-CG-CD2	-10.95	114.43	121.00
1	R	338	ARG	NE-CZ-NH1	10.92	125.76	120.30
1	E	353	TYR	CB-CG-CD1	-10.91	114.45	121.00
1	R	396	ARG	NE-CZ-NH1	10.87	125.73	120.30
1	H	485	TYR	CG-CD1-CE1	-10.80	112.66	121.30
1	Q	201	TYR	CB-CG-CD1	-10.77	114.54	121.00
1	K	365	ASP	CB-CG-OD2	10.74	127.97	118.30
1	O	178	ARG	NE-CZ-NH2	10.74	125.67	120.30
1	F	447	TYR	CB-CG-CD2	-10.73	114.56	121.00
1	G	178	ARG	NE-CZ-NH2	10.73	125.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	110	PHE	CB-CG-CD1	-10.69	113.31	120.80
1	A	413	ARG	NE-CZ-NH2	10.68	125.64	120.30
1	H	447	TYR	CB-CG-CD1	10.57	127.34	121.00
1	G	389	ARG	NE-CZ-NH1	10.57	125.58	120.30
1	I	432	TYR	CB-CG-CD1	-10.56	114.66	121.00
1	E	135	TYR	CB-CG-CD1	-10.54	114.67	121.00
1	M	268	ASP	CB-CG-OD2	10.54	127.79	118.30
1	D	369	PHE	CB-CG-CD2	10.54	128.18	120.80
1	P	123	TYR	CB-CG-CD2	10.54	127.32	121.00
1	B	338	ARG	NE-CZ-NH1	10.53	125.57	120.30
1	S	180	TYR	CB-CG-CD2	-10.49	114.71	121.00
1	Q	396	ARG	NE-CZ-NH1	10.49	125.54	120.30
1	S	525	ARG	NE-CZ-NH1	10.43	125.52	120.30
1	C	110	PHE	CB-CG-CD1	-10.42	113.50	120.80
1	B	474	ARG	NE-CZ-NH2	10.39	125.50	120.30
1	N	265	ARG	NE-CZ-NH1	-10.38	115.11	120.30
1	O	333	ARG	NE-CZ-NH1	10.35	125.47	120.30
1	L	322	ARG	NE-CZ-NH1	10.33	125.47	120.30
1	O	399	ARG	NE-CZ-NH1	-10.33	115.14	120.30
1	E	275	PHE	CB-CG-CD1	-10.31	113.58	120.80
1	G	490	TYR	CB-CG-CD2	-10.28	114.83	121.00
1	I	322	ARG	NE-CZ-NH1	10.27	125.44	120.30
1	S	135	TYR	CB-CG-CD2	10.22	127.14	121.00
1	R	53	ARG	NE-CZ-NH1	10.21	125.41	120.30
1	B	389	ARG	NE-CZ-NH2	-10.18	115.21	120.30
1	F	432	TYR	CB-CG-CD1	-10.12	114.93	121.00
1	L	110	PHE	CB-CG-CD2	10.11	127.88	120.80
1	R	490	TYR	CB-CG-CD1	10.07	127.04	121.00
1	M	178	ARG	NE-CZ-NH2	10.06	125.33	120.30
1	E	369	PHE	CB-CG-CD2	10.01	127.81	120.80
1	R	490	TYR	CB-CG-CD2	-9.97	115.02	121.00
1	O	311	TYR	CB-CG-CD1	9.97	126.98	121.00
1	B	224	TYR	CB-CG-CD2	-9.96	115.03	121.00
1	G	447	TYR	CB-CG-CD2	-9.91	115.05	121.00
1	E	135	TYR	CB-CG-CD2	9.91	126.95	121.00
1	F	389	ARG	NE-CZ-NH1	9.89	125.25	120.30
1	K	369	PHE	CB-CG-CD2	9.84	127.69	120.80
1	S	333	ARG	NE-CZ-NH2	9.82	125.21	120.30
1	G	240	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	B	525	ARG	NE-CZ-NH2	-9.79	115.41	120.30
1	O	53	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	C	110	PHE	CB-CG-CD2	9.63	127.54	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	201	TYR	CB-CG-CD2	-9.63	115.22	121.00
1	R	353	TYR	CG-CD2-CE2	-9.62	113.60	121.30
1	R	353	TYR	CB-CG-CD2	-9.61	115.23	121.00
1	F	485	TYR	CB-CG-CD1	9.60	126.76	121.00
1	O	178	ARG	NE-CZ-NH1	-9.59	115.50	120.30
1	Q	33	ARG	NE-CZ-NH1	9.59	125.10	120.30
1	M	159	ASP	CB-CG-OD2	9.57	126.92	118.30
1	E	65	ASP	CB-CG-OD2	-9.55	109.70	118.30
1	Q	201	TYR	CB-CG-CD2	9.55	126.73	121.00
1	Q	365	ASP	CB-CG-OD2	-9.51	109.74	118.30
1	O	162	ARG	NE-CZ-NH2	-9.51	115.55	120.30
1	E	97	ASP	CB-CG-OD1	-9.47	109.77	118.30
1	A	265	ARG	NE-CZ-NH2	9.45	125.02	120.30
1	L	77	ASP	CB-CG-OD2	9.44	126.80	118.30
1	G	240	ARG	NE-CZ-NH2	-9.43	115.59	120.30
1	S	50	TYR	CB-CG-CD1	-9.42	115.35	121.00
1	C	474	ARG	NE-CZ-NH2	9.41	125.00	120.30
1	K	321	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	R	265	ARG	NE-CZ-NH1	-9.36	115.62	120.30
1	Q	400	ASP	CB-CG-OD1	9.35	126.72	118.30
1	R	311	TYR	CB-CG-CD1	-9.33	115.40	121.00
1	L	135	TYR	CB-CG-CD1	-9.31	115.42	121.00
1	P	396	ARG	NE-CZ-NH1	9.29	124.95	120.30
1	A	321	ARG	NE-CZ-NH2	-9.27	115.67	120.30
1	C	201	TYR	CB-CG-CD2	-9.27	115.44	121.00
1	P	203	ASP	CB-CG-OD1	9.21	126.59	118.30
1	H	396	ARG	NE-CZ-NH1	9.19	124.89	120.30
1	O	110	PHE	CB-CG-CD1	-9.16	114.39	120.80
1	H	474	ARG	NE-CZ-NH1	-9.16	115.72	120.30
1	K	322	ARG	NE-CZ-NH2	9.15	124.88	120.30
1	M	229	ASP	CB-CG-OD2	-9.15	110.06	118.30
1	F	123	TYR	CB-CG-CD2	9.14	126.48	121.00
1	D	333	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	F	525	ARG	NE-CZ-NH2	9.11	124.85	120.30
1	M	353	TYR	CB-CG-CD1	9.11	126.46	121.00
1	C	321	ARG	NE-CZ-NH2	-9.09	115.76	120.30
1	R	250	ASP	CB-CG-OD1	9.08	126.47	118.30
1	A	56	ASP	CB-CG-OD2	9.08	126.47	118.30
1	M	474	ARG	NE-CZ-NH1	-9.06	115.77	120.30
1	I	321	ARG	NE-CZ-NH2	-9.05	115.77	120.30
1	Q	196	ARG	NE-CZ-NH2	9.03	124.81	120.30
1	S	384	ARG	NE-CZ-NH1	9.00	124.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	525	ARG	NE-CZ-NH1	8.99	124.79	120.30
1	L	123	TYR	CB-CG-CD1	-8.98	115.61	121.00
1	D	490	TYR	CB-CG-CD2	-8.98	115.61	121.00
1	R	311	TYR	CB-CG-CD2	8.98	126.39	121.00
1	P	447	TYR	CB-CG-CD2	-8.98	115.61	121.00
1	B	353	TYR	CB-CG-CD2	-8.97	115.62	121.00
1	A	53	ARG	NE-CZ-NH2	8.97	124.79	120.30
1	H	250	ASP	CB-CG-OD1	-8.96	110.23	118.30
1	A	399	ARG	NE-CZ-NH2	8.96	124.78	120.30
1	M	192	VAL	CA-CB-CG2	-8.92	97.52	110.90
1	O	430	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	Q	123	TYR	CB-CG-CD2	-8.89	115.67	121.00
1	M	224	TYR	CB-CG-CD2	8.87	126.32	121.00
1	I	474	ARG	NE-CZ-NH2	8.87	124.73	120.30
1	P	338	ARG	NH1-CZ-NH2	-8.86	109.65	119.40
1	I	224	TYR	CB-CG-CD2	-8.86	115.69	121.00
1	F	399	ARG	NE-CZ-NH2	8.85	124.73	120.30
1	F	77	ASP	CB-CG-OD1	8.85	126.26	118.30
1	C	135	TYR	CB-CG-CD1	-8.85	115.69	121.00
1	N	65	ASP	CB-CG-OD2	8.84	126.26	118.30
1	F	224	TYR	CB-CG-CD1	-8.81	115.71	121.00
1	A	430	ARG	NE-CZ-NH2	-8.81	115.90	120.30
1	N	496	ASP	CB-CG-OD2	8.77	126.19	118.30
1	O	272	MET	CG-SD-CE	-8.77	86.17	100.20
1	N	79	MET	CG-SD-CE	-8.77	86.18	100.20
1	R	447	TYR	CB-CG-CD1	8.77	126.26	121.00
1	O	322	ARG	NE-CZ-NH2	-8.75	115.93	120.30
1	K	33	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	R	322	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	F	432	TYR	CB-CG-CD2	8.69	126.22	121.00
1	A	162	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	R	447	TYR	CB-CG-CD2	-8.69	115.79	121.00
1	P	447	TYR	CB-CG-CD1	8.68	126.21	121.00
1	O	203	ASP	CB-CG-OD1	-8.66	110.50	118.30
1	Q	240	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	C	311	TYR	CB-CG-CD2	-8.65	115.81	121.00
1	D	525	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	K	135	TYR	CB-CG-CD2	8.64	126.19	121.00
1	P	275	PHE	CB-CG-CD1	8.64	126.85	120.80
1	D	521	THR	CA-CB-CG2	-8.63	100.31	112.40
1	G	178	ARG	NE-CZ-NH1	-8.63	115.99	120.30
1	P	162	ARG	NE-CZ-NH2	-8.62	115.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	353	TYR	CB-CG-CD2	8.60	126.16	121.00
1	Q	411	ASP	CB-CG-OD2	-8.59	110.57	118.30
1	N	50	TYR	CB-CG-CD1	-8.58	115.85	121.00
1	M	229	ASP	CB-CG-OD1	8.56	126.01	118.30
1	R	53	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	E	311	TYR	CB-CG-CD1	-8.56	115.86	121.00
1	O	490	TYR	CB-CG-CD1	8.55	126.13	121.00
1	O	203	ASP	CB-CG-OD2	8.54	125.99	118.30
1	D	123	TYR	CB-CG-CD2	8.54	126.12	121.00
1	F	311	TYR	CB-CG-CD1	-8.53	115.88	121.00
1	F	497	MET	CG-SD-CE	-8.53	86.56	100.20
1	M	201	TYR	CB-CG-CD2	-8.52	115.89	121.00
1	S	275	PHE	CB-CG-CD2	-8.51	114.84	120.80
1	F	224	TYR	CG-CD2-CE2	-8.51	114.49	121.30
1	N	525	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	P	322	ARG	NE-CZ-NH2	8.48	124.54	120.30
1	S	162	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	G	338	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	G	311	TYR	CG-CD2-CE2	-8.45	114.54	121.30
1	O	321	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	B	135	TYR	CB-CG-CD2	8.43	126.06	121.00
1	G	65	ASP	CB-CG-OD2	8.43	125.88	118.30
1	I	485	TYR	CG-CD1-CE1	-8.43	114.56	121.30
1	A	229	ASP	CB-CG-OD1	8.41	125.87	118.30
1	N	413	ARG	NE-CZ-NH1	-8.41	116.09	120.30
1	A	166	MET	CG-SD-CE	-8.40	86.75	100.20
1	P	396	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	G	396	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	R	525	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	I	53	ARG	NE-CZ-NH2	-8.35	116.13	120.30
1	I	485	TYR	CD1-CE1-CZ	8.35	127.31	119.80
1	A	53	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	N	432	TYR	CB-CG-CD1	-8.33	116.00	121.00
1	F	162	ARG	NE-CZ-NH1	8.33	124.46	120.30
1	P	123	TYR	CB-CG-CD1	-8.33	116.00	121.00
1	Q	322	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	D	79	MET	CG-SD-CE	-8.32	86.89	100.20
1	Q	321	ARG	NE-CZ-NH1	-8.30	116.15	120.30
1	H	272	MET	CG-SD-CE	-8.30	86.92	100.20
1	P	474	ARG	NE-CZ-NH2	8.29	124.45	120.30
1	B	490	TYR	CB-CG-CD1	-8.29	116.03	121.00
1	N	471	MET	CG-SD-CE	-8.28	86.95	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	TYR	CB-CG-CD2	-8.28	116.03	121.00
1	E	53	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	C	268	ASP	CB-CG-OD2	-8.25	110.88	118.30
1	C	474	ARG	NE-CZ-NH1	-8.24	116.18	120.30
1	O	311	TYR	CB-CG-CD2	-8.22	116.06	121.00
1	R	115	VAL	CA-CB-CG2	-8.22	98.57	110.90
1	G	430	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	B	162	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	L	474	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	E	229	ASP	CB-CG-OD2	-8.19	110.93	118.30
1	G	360	ARG	NE-CZ-NH2	8.18	124.39	120.30
1	S	90	VAL	CA-CB-CG1	-8.18	98.64	110.90
1	B	240	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	R	50	TYR	CB-CG-CD2	8.16	125.89	121.00
1	I	407	ASP	CB-CG-OD1	8.14	125.63	118.30
1	C	432	TYR	CB-CG-CD1	-8.12	116.13	121.00
1	O	288	ASP	CB-CG-OD2	-8.12	110.99	118.30
1	E	33	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	A	490	TYR	CB-CG-CD2	-8.10	116.14	121.00
1	Q	48	SER	N-CA-CB	8.10	122.66	110.50
1	Q	389	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	L	53	ARG	NE-CZ-NH2	8.09	124.35	120.30
1	N	353	TYR	CB-CG-CD1	-8.09	116.15	121.00
1	N	157	ASP	CB-CG-OD1	8.09	125.58	118.30
1	G	430	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	F	396	ARG	NE-CZ-NH2	8.05	124.33	120.30
1	L	490	TYR	CB-CG-CD1	8.05	125.83	121.00
1	M	178	ARG	NE-CZ-NH1	-8.04	116.28	120.30
1	A	33	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	P	53	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	D	135	TYR	CB-CG-CD2	8.04	125.82	121.00
1	K	432	TYR	CB-CG-CD1	8.04	125.82	121.00
1	G	396	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	K	333	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	L	432	TYR	CB-CG-CD2	8.03	125.82	121.00
1	A	33	ARG	NE-CZ-NH2	-8.01	116.29	120.30
1	B	322	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	C	322	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	Q	353	TYR	CB-CG-CD2	-7.99	116.21	121.00
1	L	275	PHE	CB-CG-CD2	-7.98	115.21	120.80
1	B	224	TYR	CB-CG-CD1	7.95	125.77	121.00
1	G	311	TYR	CB-CG-CD1	-7.95	116.23	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	333	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	A	180	TYR	CB-CG-CD1	-7.93	116.24	121.00
1	A	53	ARG	NH1-CZ-NH2	-7.93	110.67	119.40
1	R	360	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	I	525	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	E	413	ARG	NE-CZ-NH2	7.92	124.26	120.30
1	E	102	ASP	CB-CG-OD1	7.90	125.41	118.30
1	K	369	PHE	CB-CG-CD1	-7.88	115.29	120.80
1	L	430	ARG	NE-CZ-NH1	7.87	124.24	120.30
1	H	333	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	O	411	ASP	CB-CG-OD2	-7.84	111.25	118.30
1	A	432	TYR	CB-CG-CD2	7.83	125.70	121.00
1	H	178	ARG	NE-CZ-NH1	-7.83	116.39	120.30
1	G	201	TYR	CB-CG-CD2	-7.82	116.31	121.00
1	M	447	TYR	CB-CG-CD2	7.82	125.69	121.00
1	P	333	ARG	NE-CZ-NH1	7.81	124.21	120.30
1	N	333	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	N	275	PHE	CB-CG-CD1	-7.80	115.34	120.80
1	B	485	TYR	CB-CG-CD2	-7.80	116.32	121.00
1	R	65	ASP	CB-CG-OD1	7.80	125.32	118.30
1	D	307	VAL	CA-CB-CG2	-7.79	99.21	110.90
1	E	474	ARG	NE-CZ-NH1	-7.79	116.40	120.30
1	Q	485	TYR	CB-CG-CD1	7.79	125.67	121.00
1	R	166	MET	CG-SD-CE	-7.78	87.75	100.20
1	L	224	TYR	CB-CG-CD1	-7.77	116.34	121.00
1	D	307	VAL	CA-CB-CG1	7.77	122.55	110.90
1	K	162	ARG	NE-CZ-NH1	-7.75	116.42	120.30
1	C	525	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	O	520	ALA	O-C-N	-7.74	110.31	122.70
1	F	399	ARG	NE-CZ-NH1	-7.74	116.43	120.30
1	Q	265	ARG	NE-CZ-NH1	-7.73	116.44	120.30
1	A	353	TYR	CB-CG-CD2	-7.72	116.37	121.00
1	M	360	ARG	NE-CZ-NH2	7.72	124.16	120.30
1	C	350	ASP	CB-CG-OD1	7.72	125.24	118.30
1	E	77	ASP	CB-CG-OD2	7.71	125.24	118.30
1	R	79	MET	N-CA-CB	-7.71	96.72	110.60
1	O	321	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	B	350	ASP	CB-CG-OD2	7.68	125.21	118.30
1	L	178	ARG	NE-CZ-NH2	7.67	124.13	120.30
1	G	224	TYR	CB-CG-CD2	-7.66	116.40	121.00
1	I	53	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	H	416	ALA	CB-CA-C	-7.64	98.64	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	50	TYR	CG-CD2-CE2	-7.63	115.19	121.30
1	A	360	ARG	NE-CZ-NH1	-7.63	116.49	120.30
1	D	110	PHE	CB-CG-CD1	-7.63	115.46	120.80
1	L	528	ASP	CB-CG-OD1	7.63	125.17	118.30
1	O	255	VAL	O-C-N	-7.61	110.52	122.70
1	H	525	ARG	NE-CZ-NH1	-7.61	116.50	120.30
1	A	180	TYR	CB-CG-CD2	7.60	125.56	121.00
1	C	389	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	D	53	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	M	321	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	K	240	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	C	196	ARG	NE-CZ-NH1	-7.59	116.50	120.30
1	A	135	TYR	CG-CD2-CE2	-7.59	115.23	121.30
1	R	178	ARG	NE-CZ-NH1	-7.58	116.51	120.30
1	O	471	MET	CG-SD-CE	-7.57	88.08	100.20
1	E	360	ARG	NH1-CZ-NH2	-7.56	111.08	119.40
1	N	464	PHE	CB-CG-CD1	-7.56	115.51	120.80
1	P	224	TYR	CB-CG-CD1	7.56	125.53	121.00
1	C	471	MET	CG-SD-CE	-7.52	88.17	100.20
1	A	135	TYR	CZ-CE2-CD2	7.52	126.57	119.80
1	R	338	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	L	389	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	N	496	ASP	CB-CG-OD1	-7.49	111.56	118.30
1	S	272	MET	CG-SD-CE	-7.49	88.22	100.20
1	Q	485	TYR	CB-CG-CD2	-7.47	116.52	121.00
1	B	399	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	I	399	ARG	NE-CZ-NH1	-7.45	116.57	120.30
1	K	399	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	O	111	SER	N-CA-CB	7.42	121.63	110.50
1	D	321	ARG	NE-CZ-NH2	7.41	124.01	120.30
1	E	389	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	H	322	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	S	159	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	I	396	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	M	50	TYR	CB-CG-CD2	-7.38	116.57	121.00
1	M	295	ALA	CB-CA-C	-7.38	99.04	110.10
1	K	392	ASP	CB-CG-OD1	7.37	124.94	118.30
1	N	110	PHE	CB-CG-CD2	7.37	125.96	120.80
1	S	65	ASP	CB-CG-OD1	7.36	124.92	118.30
1	P	53	ARG	NH1-CZ-NH2	-7.36	111.31	119.40
1	K	288	ASP	CB-CG-OD2	7.35	124.92	118.30
1	E	196	ARG	NE-CZ-NH2	7.34	123.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	TRP	CB-CG-CD2	-7.34	117.06	126.60
1	H	498	TRP	CG-CD2-CE3	-7.34	127.30	133.90
1	R	327	ASP	CB-CG-OD1	7.33	124.90	118.30
1	H	498	TRP	CE2-CD2-CG	7.32	113.16	107.30
1	R	123	TYR	CB-CG-CD1	-7.32	116.61	121.00
1	E	311	TYR	CB-CG-CD2	7.32	125.39	121.00
1	S	413	ARG	NE-CZ-NH1	-7.31	116.64	120.30
1	S	53	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	R	452	GLU	OE1-CD-OE2	-7.30	114.54	123.30
1	B	110	PHE	CB-CG-CD2	-7.29	115.69	120.80
1	C	485	TYR	CB-CG-CD1	-7.29	116.62	121.00
1	G	120	ASP	CB-CG-OD2	7.28	124.86	118.30
1	S	224	TYR	CB-CG-CD1	-7.28	116.63	121.00
1	A	169	LEU	CB-CG-CD2	7.28	123.37	111.00
1	G	368	VAL	CA-CB-CG2	-7.28	99.99	110.90
1	L	123	TYR	CB-CG-CD2	7.27	125.36	121.00
1	S	389	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	P	369	PHE	CB-CG-CD2	7.26	125.88	120.80
1	B	384	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	D	360	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	P	237	MET	CG-SD-CE	-7.23	88.63	100.20
1	F	77	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	H	485	TYR	CD1-CE1-CZ	7.22	126.30	119.80
1	I	33	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	E	162	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	R	240	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	B	196	ARG	NE-CZ-NH1	-7.20	116.70	120.30
1	H	311	TYR	CB-CG-CD2	7.20	125.32	121.00
1	Q	322	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	E	210	VAL	CA-CB-CG1	7.18	121.67	110.90
1	F	50	TYR	CG-CD2-CE2	7.18	127.05	121.30
1	L	219	ASP	N-CA-CB	-7.18	97.68	110.60
1	N	224	TYR	CB-CG-CD2	-7.17	116.70	121.00
1	F	485	TYR	CB-CG-CD2	-7.15	116.71	121.00
1	L	180	TYR	CB-CG-CD2	-7.14	116.71	121.00
1	Q	528	ASP	CB-CG-OD1	7.14	124.73	118.30
1	H	71	ASP	CB-CG-OD1	7.14	124.72	118.30
1	I	135	TYR	CB-CG-CD2	7.14	125.28	121.00
1	R	502	VAL	CA-CB-CG1	7.13	121.60	110.90
1	C	525	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	S	321	ARG	CD-NE-CZ	7.11	133.56	123.60
1	C	55	MET	CG-SD-CE	-7.11	88.83	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	201	TYR	CB-CG-CD1	7.10	125.26	121.00
1	F	391	VAL	CA-CB-CG1	7.10	121.55	110.90
1	S	530	VAL	CG1-CB-CG2	-7.10	99.55	110.90
1	D	265	ARG	NE-CZ-NH1	-7.09	116.75	120.30
1	L	471	MET	CG-SD-CE	-7.09	88.85	100.20
1	K	229	ASP	CB-CG-OD1	7.08	124.67	118.30
1	E	384	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	S	447	TYR	CB-CG-CD1	7.08	125.25	121.00
1	K	50	TYR	CB-CG-CD2	7.07	125.25	121.00
1	Q	279	GLU	OE1-CD-OE2	-7.07	114.81	123.30
1	R	178	ARG	NE-CZ-NH2	7.07	123.84	120.30
1	D	178	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	K	432	TYR	CB-CG-CD2	-7.06	116.76	121.00
1	E	110	PHE	CB-CG-CD1	-7.05	115.86	120.80
1	S	244	ALA	CB-CA-C	7.04	120.67	110.10
1	O	424	GLU	O-C-N	-7.04	111.44	122.70
1	F	88	LEU	CB-CG-CD2	7.03	122.96	111.00
1	I	240	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	P	135	TYR	CB-CG-CD2	7.02	125.21	121.00
1	P	122	LEU	CB-CG-CD1	-7.01	99.08	111.00
1	F	56	ASP	CB-CG-OD2	7.01	124.61	118.30
1	R	335	THR	CA-CB-CG2	-7.00	102.59	112.40
1	O	50	TYR	CB-CG-CD2	7.00	125.20	121.00
1	L	237	MET	CG-SD-CE	-6.99	89.01	100.20
1	I	344	ASP	CB-CG-OD1	-6.98	112.01	118.30
1	C	279	GLU	O-C-N	-6.98	111.53	122.70
1	D	322	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	C	396	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	D	389	ARG	CD-NE-CZ	6.97	133.35	123.60
1	H	488	ASP	CB-CG-OD1	6.95	124.56	118.30
1	S	525	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	R	56	ASP	CB-CG-OD2	6.94	124.55	118.30
1	B	333	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	G	384	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	Q	224	TYR	CB-CG-CD1	6.93	125.16	121.00
1	L	490	TYR	CB-CG-CD2	-6.93	116.84	121.00
1	D	485	TYR	CG-CD1-CE1	-6.93	115.76	121.30
1	L	61	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	E	433	ALA	CB-CA-C	6.91	120.47	110.10
1	Q	333	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	B	135	TYR	CG-CD2-CE2	6.89	126.81	121.30
1	G	365	ASP	CB-CG-OD1	6.89	124.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	272	MET	CG-SD-CE	-6.88	89.20	100.20
1	B	468	ASP	CB-CG-OD2	6.87	124.48	118.30
1	D	200	TRP	CB-CG-CD1	6.87	135.93	127.00
1	C	360	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	F	528	ASP	CB-CG-OD1	-6.86	112.13	118.30
1	L	196	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	Q	110	PHE	CB-CG-CD2	6.85	125.59	120.80
1	K	166	MET	CG-SD-CE	-6.84	89.26	100.20
1	P	244	ALA	N-CA-CB	-6.83	100.53	110.10
1	B	50	TYR	CB-CG-CD1	-6.83	116.90	121.00
1	C	200	TRP	CB-CG-CD1	6.83	135.88	127.00
1	C	201	TYR	CG-CD1-CE1	-6.82	115.84	121.30
1	A	510	MET	CG-SD-CE	-6.82	89.29	100.20
1	N	490	TYR	CB-CG-CD2	6.81	125.08	121.00
1	O	464	PHE	CB-CG-CD1	6.80	125.56	120.80
1	G	365	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	Q	311	TYR	CB-CG-CD1	-6.80	116.92	121.00
1	N	528	ASP	CB-CG-OD2	6.79	124.42	118.30
1	I	110	PHE	CB-CG-CD2	6.79	125.55	120.80
1	H	333	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	A	411	ASP	CB-CG-OD1	-6.79	112.19	118.30
1	K	180	TYR	CG-CD2-CE2	-6.78	115.88	121.30
1	P	196	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	D	485	TYR	CB-CG-CD1	-6.78	116.93	121.00
1	N	250	ASP	CB-CG-OD1	-6.78	112.20	118.30
1	E	50	TYR	CB-CG-CD1	-6.77	116.94	121.00
1	E	365	ASP	CB-CG-OD1	-6.77	112.20	118.30
1	L	159	ASP	CB-CG-OD2	-6.77	112.20	118.30
1	I	369	PHE	CB-CG-CD2	6.77	125.54	120.80
1	Q	430	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	R	432	TYR	CG-CD1-CE1	-6.76	115.89	121.30
1	M	413	ARG	NH1-CZ-NH2	-6.76	111.97	119.40
1	Q	355	SER	N-CA-CB	6.75	120.62	110.50
1	B	261	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	C	104	THR	CA-CB-CG2	-6.73	102.97	112.40
1	C	268	ASP	CB-CG-OD1	6.73	124.36	118.30
1	I	297	VAL	CA-CB-CG1	6.72	120.99	110.90
1	L	319	ALA	N-CA-CB	6.72	119.51	110.10
1	R	525	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	S	320	VAL	CA-CB-CG1	6.72	120.98	110.90
1	S	465	ASP	CB-CG-OD2	6.71	124.34	118.30
1	R	179	GLU	OE1-CD-OE2	-6.71	115.25	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ASP	CB-CG-OD1	6.71	124.34	118.30
1	I	399	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	S	150	ALA	N-CA-CB	-6.70	100.72	110.10
1	B	240	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	M	110	PHE	CB-CG-CD2	6.70	125.49	120.80
1	S	399	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	L	277	ASP	CB-CG-OD1	6.69	124.32	118.30
1	S	33	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	B	311	TYR	CB-CG-CD2	-6.69	116.99	121.00
1	C	396	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	G	111	SER	N-CA-CB	6.68	120.52	110.50
1	P	33	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	R	333	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	D	425	ILE	O-C-N	-6.68	112.01	122.70
1	O	298	ILE	CA-CB-CG1	6.68	123.69	111.00
1	N	432	TYR	CG-CD2-CE2	-6.68	115.96	121.30
1	L	203	ASP	CB-CG-OD2	6.67	124.30	118.30
1	E	125	ASP	CB-CG-OD1	6.67	124.30	118.30
1	L	484	TRP	CE2-CD2-CG	-6.66	101.97	107.30
1	S	527	ASP	CB-CG-OD1	6.66	124.29	118.30
1	S	464	PHE	CB-CG-CD2	-6.65	116.15	120.80
1	A	261	ASP	CB-CG-OD2	6.64	124.28	118.30
1	H	384	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	N	162	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	B	229	ASP	CB-CG-OD1	6.63	124.27	118.30
1	C	497	MET	CG-SD-CE	-6.63	89.59	100.20
1	N	32	VAL	CA-CB-CG1	6.63	120.84	110.90
1	D	313	ALA	CB-CA-C	-6.63	100.16	110.10
1	I	178	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	Q	188	ALA	O-C-N	-6.61	112.12	122.70
1	Q	461	ASN	CB-CA-C	-6.61	97.17	110.40
1	D	145	THR	O-C-N	-6.61	112.12	122.70
1	H	125	ASP	O-C-N	-6.61	112.13	122.70
1	H	261	ASP	CB-CG-OD1	-6.61	112.35	118.30
1	Q	474	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	E	65	ASP	N-CA-CB	-6.60	98.72	110.60
1	Q	65	ASP	CB-CG-OD2	6.60	124.24	118.30
1	H	104	THR	CA-CB-CG2	-6.57	103.21	112.40
1	O	298	ILE	O-C-N	-6.57	112.20	122.70
1	E	325	LYS	CA-CB-CG	6.56	127.83	113.40
1	H	65	ASP	CB-CG-OD2	6.56	124.20	118.30
1	L	180	TYR	CB-CG-CD1	6.56	124.94	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	102	ASP	CB-CG-OD1	-6.56	112.40	118.30
1	N	203	ASP	CB-CG-OD1	6.56	124.20	118.30
1	A	498	TRP	CB-CG-CD2	-6.55	118.08	126.60
1	Q	224	TYR	CA-CB-CG	-6.55	100.95	113.40
1	N	468	ASP	CB-CG-OD2	6.55	124.19	118.30
1	H	71	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	R	322	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	338	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	E	196	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	C	512	ALA	N-CA-CB	6.53	119.25	110.10
1	I	234	HIS	CA-CB-CG	6.53	124.70	113.60
1	K	445	GLU	OE1-CD-OE2	-6.53	115.47	123.30
1	L	482	ASN	N-CA-CB	6.52	122.34	110.60
1	N	474	ARG	NH1-CZ-NH2	-6.52	112.22	119.40
1	S	318	LEU	CB-CG-CD2	6.52	122.08	111.00
1	O	33	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	M	113	GLU	OE1-CD-OE2	-6.51	115.48	123.30
1	L	80	ASP	CB-CG-OD1	6.51	124.16	118.30
1	D	110	PHE	CB-CG-CD2	6.51	125.36	120.80
1	D	407	ASP	CB-CG-OD2	6.51	124.16	118.30
1	S	55	MET	CG-SD-CE	-6.51	89.79	100.20
1	C	240	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	F	169	LEU	CB-CG-CD2	6.50	122.05	111.00
1	G	159	ASP	CB-CG-OD2	6.50	124.15	118.30
1	Q	321	ARG	NE-CZ-NH2	6.49	123.55	120.30
1	B	286	LYS	O-C-N	-6.48	112.33	122.70
1	Q	240	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	S	261	ASP	CB-CG-OD1	6.48	124.13	118.30
1	G	433	ALA	CB-CA-C	6.48	119.82	110.10
1	D	485	TYR	CD1-CE1-CZ	6.48	125.63	119.80
1	I	432	TYR	CB-CG-CD2	6.47	124.89	121.00
1	O	405	VAL	CA-CB-CG1	6.47	120.61	110.90
1	K	196	ARG	NE-CZ-NH2	6.47	123.53	120.30
1	M	502	VAL	CA-CB-CG2	-6.46	101.20	110.90
1	N	360	ARG	NH1-CZ-NH2	-6.46	112.30	119.40
1	M	490	TYR	CB-CG-CD2	-6.46	117.13	121.00
1	R	411	ASP	CB-CG-OD1	6.45	124.11	118.30
1	F	50	TYR	CZ-CE2-CD2	-6.45	113.99	119.80
1	Q	392	ASP	CB-CG-OD1	6.45	124.11	118.30
1	C	265	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	Q	178	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	K	265	ARG	NE-CZ-NH2	6.44	123.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	413	ARG	NH1-CZ-NH2	-6.43	112.32	119.40
1	D	321	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	F	311	TYR	CG-CD1-CE1	-6.43	116.16	121.30
1	L	162	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	F	97	ASP	CB-CG-OD2	6.42	124.08	118.30
1	A	522	LEU	CB-CG-CD1	6.42	121.91	111.00
1	D	321	ARG	NH1-CZ-NH2	-6.42	112.34	119.40
1	P	371	GLU	OE1-CD-OE2	-6.41	115.61	123.30
1	A	32	VAL	CA-CB-CG2	6.41	120.51	110.90
1	O	110	PHE	CB-CG-CD2	6.40	125.28	120.80
1	Q	229	ASP	O-C-N	-6.40	112.46	122.70
1	C	275	PHE	CB-CG-CD1	6.40	125.28	120.80
1	A	405	VAL	CA-CB-CG1	6.39	120.48	110.90
1	K	338	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	D	77	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	D	432	TYR	CG-CD1-CE1	-6.38	116.20	121.30
1	O	411	ASP	CB-CG-OD1	6.38	124.04	118.30
1	C	447	TYR	CB-CG-CD2	6.37	124.82	121.00
1	F	367	MET	CG-SD-CE	6.37	110.39	100.20
1	L	145	THR	O-C-N	-6.37	112.51	122.70
1	Q	159	ASP	CB-CG-OD1	6.37	124.03	118.30
1	O	113	GLU	OE1-CD-OE2	-6.37	115.66	123.30
1	P	295	ALA	N-CA-CB	-6.37	101.19	110.10
1	R	421	VAL	CA-CB-CG2	-6.37	101.35	110.90
1	N	120	ASP	N-CA-CB	-6.36	99.16	110.60
1	E	399	ARG	CD-NE-CZ	-6.35	114.70	123.60
1	N	201	TYR	CB-CG-CD1	-6.35	117.19	121.00
1	E	180	TYR	CG-CD1-CE1	6.34	126.37	121.30
1	G	285	GLU	OE1-CD-OE2	-6.34	115.69	123.30
1	G	456	SER	N-CA-CB	6.34	120.01	110.50
1	H	389	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	N	392	ASP	O-C-N	-6.34	112.56	122.70
1	N	65	ASP	CB-CG-OD1	-6.33	112.60	118.30
1	O	389	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	G	162	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	D	71	ASP	CB-CG-OD2	6.32	123.98	118.30
1	A	396	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	R	33	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	K	42	VAL	CG1-CB-CG2	-6.31	100.81	110.90
1	K	322	ARG	CG-CD-NE	-6.30	98.56	111.80
1	Q	498	TRP	CB-CG-CD2	-6.29	118.42	126.60
1	K	219	ASP	CB-CG-OD2	6.29	123.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	120	ASP	N-CA-CB	-6.29	99.28	110.60
1	B	55	MET	CG-SD-CE	-6.28	90.16	100.20
1	I	245	LYS	N-CA-CB	6.28	121.90	110.60
1	L	321	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	H	100	THR	N-CA-CB	6.28	122.22	110.30
1	A	159	ASP	CB-CG-OD2	6.27	123.94	118.30
1	Q	94	LYS	CA-CB-CG	6.27	127.19	113.40
1	H	61	ASP	CB-CG-OD2	-6.26	112.66	118.30
1	E	123	TYR	CB-CG-CD2	6.26	124.76	121.00
1	O	400	ASP	CB-CG-OD2	6.26	123.93	118.30
1	H	399	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	S	407	ASP	CB-CG-OD1	-6.25	112.67	118.30
1	M	407	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	102	ASP	CB-CG-OD2	6.25	123.92	118.30
1	F	353	TYR	CG-CD2-CE2	-6.25	116.30	121.30
1	F	369	PHE	CB-CG-CD2	6.25	125.17	120.80
1	D	196	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	G	283	ILE	CB-CA-C	-6.24	99.12	111.60
1	K	322	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	G	408	VAL	CA-CB-CG1	6.23	120.25	110.90
1	L	465	ASP	CB-CG-OD2	6.23	123.91	118.30
1	E	265	ARG	NH1-CZ-NH2	-6.23	112.55	119.40
1	O	80	ASP	CB-CG-OD1	-6.23	112.69	118.30
1	P	416	ALA	N-CA-CB	-6.22	101.39	110.10
1	I	277	ASP	CB-CG-OD2	6.22	123.90	118.30
1	K	360	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	K	423	ILE	O-C-N	-6.22	112.75	122.70
1	G	353	TYR	CB-CG-CD1	-6.21	117.27	121.00
1	B	311	TYR	CG-CD1-CE1	-6.21	116.34	121.30
1	M	389	ARG	O-C-N	-6.20	112.78	122.70
1	I	162	ARG	CD-NE-CZ	6.19	132.27	123.60
1	G	237	MET	CG-SD-CE	-6.19	90.29	100.20
1	G	496	ASP	CB-CG-OD2	6.19	123.87	118.30
1	N	123	TYR	CB-CG-CD1	-6.19	117.29	121.00
1	R	369	PHE	CB-CG-CD2	6.19	125.13	120.80
1	M	365	ASP	CB-CG-OD2	6.18	123.87	118.30
1	A	327	ASP	CB-CG-OD2	6.18	123.86	118.30
1	B	321	ARG	NH1-CZ-NH2	6.18	126.20	119.40
1	C	490	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	F	338	ARG	CD-NE-CZ	6.17	132.24	123.60
1	Q	525	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	S	97	ASP	CB-CG-OD1	6.17	123.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	369	PHE	CB-CG-CD2	6.17	125.12	120.80
1	E	275	PHE	CB-CG-CD2	6.17	125.12	120.80
1	K	33	ARG	NH1-CZ-NH2	-6.17	112.61	119.40
1	A	156	ASN	CA-CB-CG	-6.16	99.85	113.40
1	P	169	LEU	O-C-N	-6.16	112.85	122.70
1	G	159	ASP	CB-CG-OD1	-6.16	112.76	118.30
1	O	507	LEU	O-C-N	-6.15	112.86	122.70
1	C	38	ALA	CB-CA-C	6.15	119.32	110.10
1	E	165	ALA	N-CA-CB	6.15	118.71	110.10
1	L	110	PHE	CB-CG-CD1	-6.15	116.50	120.80
1	O	430	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	C	185	VAL	CA-CB-CG1	6.12	120.08	110.90
1	L	432	TYR	CB-CG-CD1	-6.12	117.33	121.00
1	N	237	MET	CG-SD-CE	-6.12	90.41	100.20
1	O	384	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	P	287	VAL	CG1-CB-CG2	-6.12	101.11	110.90
1	B	123	TYR	CG-CD1-CE1	-6.11	116.41	121.30
1	M	373	ALA	N-CA-CB	6.11	118.65	110.10
1	B	311	TYR	CB-CG-CD1	6.11	124.66	121.00
1	B	516	ALA	CB-CA-C	6.11	119.26	110.10
1	K	322	ARG	O-C-N	-6.11	112.93	122.70
1	H	201	TYR	CB-CG-CD2	6.10	124.66	121.00
1	I	525	ARG	NH1-CZ-NH2	-6.10	112.69	119.40
1	M	322	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	L	391	VAL	CA-CB-CG2	-6.10	101.75	110.90
1	C	56	ASP	CB-CG-OD1	6.09	123.78	118.30
1	O	102	ASP	O-C-N	-6.09	112.85	123.20
1	S	276	LEU	CB-CA-C	-6.09	98.63	110.20
1	G	169	LEU	O-C-N	-6.08	112.97	122.70
1	O	344	ASP	O-C-N	-6.08	112.97	122.70
1	L	405	VAL	CA-CB-CG1	6.08	120.01	110.90
1	P	224	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	A	240	ARG	NH1-CZ-NH2	-6.07	112.73	119.40
1	C	384	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	B	455	VAL	CA-CB-CG1	-6.06	101.80	110.90
1	D	248	LEU	CB-CG-CD2	6.06	121.31	111.00
1	L	408	VAL	CG1-CB-CG2	-6.06	101.20	110.90
1	O	275	PHE	CB-CG-CD1	6.06	125.04	120.80
1	K	305	ASP	CB-CG-OD2	6.06	123.75	118.30
1	Q	149	LEU	CB-CG-CD1	6.06	121.30	111.00
1	F	396	ARG	NH1-CZ-NH2	-6.05	112.74	119.40
1	B	387	LEU	CB-CG-CD2	6.04	121.28	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	525	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	O	360	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	F	381	ILE	O-C-N	-6.03	113.05	122.70
1	E	33	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	389	ARG	CG-CD-NE	-6.03	99.14	111.80
1	F	299	ILE	CA-CB-CG1	6.03	122.46	111.00
1	M	507	LEU	CB-CG-CD1	6.03	121.25	111.00
1	P	173	ALA	N-CA-CB	-6.03	101.66	110.10
1	M	65	ASP	CB-CG-OD1	-6.03	112.87	118.30
1	N	53	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	D	48	SER	O-C-N	-6.03	113.06	122.70
1	A	114	LEU	CB-CA-C	6.02	121.64	110.20
1	O	464	PHE	CB-CG-CD2	-6.02	116.59	120.80
1	P	400	ASP	CB-CG-OD2	6.02	123.72	118.30
1	N	123	TYR	CG-CD1-CE1	-6.01	116.49	121.30
1	C	525	ARG	CD-NE-CZ	6.01	132.01	123.60
1	I	205	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	O	197	GLY	C-N-CA	6.00	136.71	121.70
1	G	434	PRO	N-CA-CB	6.00	110.50	103.30
1	A	55	MET	CG-SD-CE	-6.00	90.60	100.20
1	F	240	ARG	NH1-CZ-NH2	-6.00	112.80	119.40
1	S	369	PHE	CB-CG-CD1	6.00	125.00	120.80
1	O	240	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	Q	213	ALA	CB-CA-C	5.99	119.08	110.10
1	R	241	LEU	CB-CG-CD1	5.96	121.13	111.00
1	R	389	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	H	341	SER	CB-CA-C	-5.96	98.78	110.10
1	C	311	TYR	CG-CD1-CE1	-5.95	116.54	121.30
1	E	399	ARG	NE-CZ-NH2	5.95	123.27	120.30
1	Q	528	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	G	33	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	K	400	ASP	CB-CG-OD1	5.94	123.64	118.30
1	S	396	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	384	ARG	NH1-CZ-NH2	-5.93	112.87	119.40
1	E	490	TYR	CB-CG-CD2	5.93	124.56	121.00
1	N	333	ARG	NH1-CZ-NH2	-5.93	112.88	119.40
1	I	322	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	I	464	PHE	CB-CG-CD2	-5.92	116.65	120.80
1	N	206	ASN	O-C-N	-5.92	113.22	122.70
1	E	65	ASP	CB-CG-OD1	5.92	123.63	118.30
1	I	79	MET	CG-SD-CE	-5.92	90.72	100.20
1	N	454	LEU	CB-CG-CD2	-5.92	100.93	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	149	LEU	CB-CG-CD1	5.92	121.06	111.00
1	K	191	GLN	CA-CB-CG	5.92	126.42	113.40
1	O	512	ALA	N-CA-CB	5.92	118.38	110.10
1	F	468	ASP	CB-CG-OD1	5.91	123.62	118.30
1	B	396	ARG	CD-NE-CZ	5.91	131.87	123.60
1	N	65	ASP	N-CA-CB	5.91	121.23	110.60
1	F	489	LEU	CB-CG-CD1	5.91	121.04	111.00
1	N	272	MET	CG-SD-CE	-5.90	90.75	100.20
1	P	265	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	N	451	LEU	CB-CG-CD2	5.90	121.02	111.00
1	R	250	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	I	302	LYS	C-N-CA	5.89	134.68	122.30
1	D	272	MET	CG-SD-CE	-5.89	90.77	100.20
1	N	80	ASP	CB-CG-OD2	5.89	123.60	118.30
1	R	432	TYR	CG-CD2-CE2	-5.89	116.59	121.30
1	K	505	PRO	O-C-N	-5.88	113.30	122.70
1	G	229	ASP	N-CA-CB	-5.87	100.03	110.60
1	K	123	TYR	CB-CG-CD2	5.87	124.52	121.00
1	K	497	MET	CG-SD-CE	-5.87	90.81	100.20
1	R	180	TYR	CB-CG-CD2	5.87	124.52	121.00
1	G	489	LEU	CB-CG-CD2	-5.87	101.03	111.00
1	K	365	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	D	421	VAL	CG1-CB-CG2	-5.86	101.52	110.90
1	E	510	MET	CA-CB-CG	5.86	123.26	113.30
1	F	494	PRO	N-CD-CG	5.86	111.99	103.20
1	O	322	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	D	482	ASN	C-N-CA	5.86	136.34	121.70
1	L	430	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	H	61	ASP	O-C-N	-5.85	113.34	122.70
1	N	399	ARG	NE-CZ-NH2	5.85	123.22	120.30
1	E	53	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	N	447	TYR	CB-CG-CD1	5.84	124.51	121.00
1	I	200	TRP	CE2-CD2-CG	5.84	111.97	107.30
1	L	499	GLN	O-C-N	-5.84	113.36	122.70
1	E	327	ASP	CA-CB-CG	-5.83	100.56	113.40
1	R	159	ASP	CB-CG-OD2	5.83	123.55	118.30
1	E	305	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	H	484	TRP	CE3-CZ3-CH2	-5.83	114.79	121.20
1	G	135	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	G	268	ASP	CB-CG-OD2	5.82	123.53	118.30
1	D	159	ASP	O-C-N	-5.81	113.40	122.70
1	I	388	GLU	OE1-CD-OE2	-5.81	116.32	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	265	ARG	NE-CZ-NH2	5.81	123.21	120.30
1	I	349	GLN	N-CA-CB	-5.81	100.14	110.60
1	E	344	ASP	CB-CG-OD2	5.81	123.53	118.30
1	Q	183	ASP	CB-CG-OD1	5.81	123.53	118.30
1	E	58	MET	CG-SD-CE	-5.81	90.91	100.20
1	H	198	ASP	CB-CG-OD2	5.80	123.52	118.30
1	K	353	TYR	CB-CG-CD1	5.80	124.48	121.00
1	C	485	TYR	CG-CD2-CE2	-5.80	116.66	121.30
1	E	333	ARG	CD-NE-CZ	5.80	131.72	123.60
1	I	400	ASP	CB-CG-OD1	5.80	123.52	118.30
1	S	201	TYR	CD1-CG-CD2	5.80	124.28	117.90
1	G	333	ARG	NH1-CZ-NH2	-5.80	113.02	119.40
1	S	523	VAL	CA-CB-CG1	5.80	119.59	110.90
1	K	80	ASP	CB-CG-OD2	5.79	123.52	118.30
1	O	291	LEU	CB-CG-CD1	5.79	120.85	111.00
1	P	196	ARG	CG-CD-NE	-5.79	99.64	111.80
1	N	490	TYR	CG-CD2-CE2	5.79	125.93	121.30
1	H	268	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	S	210	VAL	CA-CB-CG2	-5.79	102.22	110.90
1	F	190	THR	O-C-N	-5.78	113.45	122.70
1	B	335	THR	CA-CB-OG1	5.78	121.14	109.00
1	K	396	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	384	ARG	NH1-CZ-NH2	-5.78	113.04	119.40
1	N	171	SER	O-C-N	-5.78	113.45	122.70
1	Q	123	TYR	CB-CG-CD1	5.78	124.47	121.00
1	R	451	LEU	CB-CG-CD2	-5.78	101.18	111.00
1	B	169	LEU	O-C-N	-5.78	113.46	122.70
1	H	327	ASP	CB-CG-OD2	5.77	123.50	118.30
1	F	287	VAL	CA-CB-CG1	-5.77	102.25	110.90
1	H	367	MET	CG-SD-CE	-5.77	90.97	100.20
1	D	353	TYR	CB-CG-CD2	-5.77	117.54	121.00
1	I	170	SER	O-C-N	-5.77	113.47	122.70
1	E	170	SER	O-C-N	-5.76	113.48	122.70
1	O	468	ASP	CB-CG-OD2	5.76	123.48	118.30
1	G	180	TYR	CG-CD2-CE2	-5.76	116.69	121.30
1	F	490	TYR	CB-CG-CD1	-5.76	117.55	121.00
1	S	277	ASP	CB-CG-OD2	5.76	123.48	118.30
1	S	353	TYR	CB-CG-CD1	-5.76	117.55	121.00
1	C	228	VAL	O-C-N	-5.75	113.49	122.70
1	R	460	GLU	OE1-CD-OE2	-5.75	116.40	123.30
1	S	424	GLU	CA-CB-CG	5.75	126.06	113.40
1	C	528	ASP	CB-CA-C	-5.75	98.90	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	205	ASP	CB-CG-OD1	5.75	123.47	118.30
1	O	350	ASP	O-C-N	-5.75	113.50	122.70
1	I	150	ALA	CB-CA-C	-5.75	101.48	110.10
1	E	177	ALA	O-C-N	-5.74	113.51	122.70
1	K	353	TYR	CB-CG-CD2	-5.74	117.55	121.00
1	B	228	VAL	O-C-N	-5.74	113.52	122.70
1	B	451	LEU	CB-CG-CD2	5.74	120.76	111.00
1	M	261	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	M	480	GLU	OE1-CD-OE2	-5.74	116.41	123.30
1	Q	396	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	E	396	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	I	162	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	F	205	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	L	401	ALA	CB-CA-C	-5.73	101.50	110.10
1	B	430	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	N	368	VAL	CG1-CB-CG2	-5.73	101.73	110.90
1	E	317	VAL	CA-CB-CG2	-5.73	102.31	110.90
1	L	94	LYS	C-N-CA	5.73	134.32	122.30
1	A	433	ALA	CB-CA-C	5.72	118.69	110.10
1	K	119	GLU	OE1-CD-OE2	-5.72	116.43	123.30
1	C	198	ASP	CB-CG-OD1	5.72	123.45	118.30
1	M	397	ALA	N-CA-CB	-5.71	102.10	110.10
1	P	186	VAL	CG1-CB-CG2	-5.71	101.76	110.90
1	D	101	ALA	N-CA-CB	-5.71	102.10	110.10
1	N	431	LYS	O-C-N	-5.71	113.56	122.70
1	E	502	VAL	CG1-CB-CG2	-5.71	101.77	110.90
1	K	392	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	G	232	VAL	CG1-CB-CG2	-5.71	101.77	110.90
1	L	347	SER	N-CA-CB	5.71	119.06	110.50
1	E	396	ARG	NH1-CZ-NH2	-5.70	113.13	119.40
1	O	429	LEU	CB-CG-CD1	5.70	120.69	111.00
1	O	255	VAL	CA-CB-CG1	5.70	119.45	110.90
1	N	180	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	F	141	VAL	CA-CB-CG1	-5.69	102.36	110.90
1	A	102	ASP	N-CA-CB	-5.69	100.36	110.60
1	N	162	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	R	340	VAL	O-C-N	-5.69	113.60	122.70
1	N	508	VAL	CA-CB-CG1	5.69	119.43	110.90
1	B	50	TYR	CZ-CE2-CD2	-5.69	114.68	119.80
1	C	367	MET	CG-SD-CE	-5.69	91.10	100.20
1	A	119	GLU	N-CA-CB	-5.68	100.37	110.60
1	P	171	SER	O-C-N	-5.68	113.61	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113	GLU	O-C-N	-5.68	113.61	122.70
1	B	392	ASP	CB-CG-OD1	5.67	123.41	118.30
1	G	62	SER	CB-CA-C	-5.67	99.32	110.10
1	H	80	ASP	CB-CG-OD1	5.67	123.41	118.30
1	E	333	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	E	430	ARG	NH1-CZ-NH2	5.67	125.64	119.40
1	F	263	GLU	OE1-CD-OE2	-5.67	116.50	123.30
1	N	123	TYR	CZ-CE2-CD2	5.67	124.90	119.80
1	N	400	ASP	CB-CA-C	5.67	121.73	110.40
1	A	502	VAL	O-C-N	-5.66	113.64	122.70
1	S	135	TYR	CB-CG-CD1	-5.66	117.60	121.00
1	A	452	GLU	O-C-N	-5.66	113.64	122.70
1	M	420	ALA	O-C-N	-5.66	113.64	122.70
1	L	389	ARG	CG-CD-NE	-5.66	99.92	111.80
1	E	473	LEU	CB-CG-CD1	-5.66	101.39	111.00
1	F	400	ASP	O-C-N	-5.65	113.66	122.70
1	P	240	ARG	NH1-CZ-NH2	5.65	125.62	119.40
1	C	33	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	D	333	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	Q	338	ARG	N-CA-CB	5.65	120.77	110.60
1	G	353	TYR	CD1-CE1-CZ	5.65	124.88	119.80
1	O	250	ASP	N-CA-CB	-5.65	100.44	110.60
1	Q	29	LYS	C-N-CA	5.64	135.81	121.70
1	M	391	VAL	CA-CB-CG1	5.64	119.36	110.90
1	R	429	LEU	N-CA-CB	5.64	121.67	110.40
1	R	498	TRP	CB-CG-CD1	5.64	134.33	127.00
1	P	389	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	102	ASP	CB-CG-OD1	-5.63	113.23	118.30
1	P	31	ALA	CB-CA-C	5.63	118.55	110.10
1	Q	178	ARG	NH1-CZ-NH2	-5.63	113.21	119.40
1	Q	338	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	413	ARG	NH1-CZ-NH2	-5.63	113.21	119.40
1	N	512	ALA	CB-CA-C	-5.63	101.66	110.10
1	O	484	TRP	CE2-CD2-CG	-5.63	102.80	107.30
1	E	470	LEU	CB-CG-CD1	-5.63	101.44	111.00
1	H	61	ASP	CA-C-O	5.63	131.92	120.10
1	S	495	VAL	CG1-CB-CG2	-5.63	101.90	110.90
1	K	293	THR	O-C-N	-5.62	113.64	123.20
1	M	440	GLU	N-CA-CB	-5.62	100.48	110.60
1	O	498	TRP	CG-CD2-CE3	-5.62	128.84	133.90
1	G	438	GLY	O-C-N	-5.62	113.70	122.70
1	N	269	PRO	N-CD-CG	5.62	111.63	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	413	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	S	178	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	H	97	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	479	ASN	N-CA-CB	5.62	120.71	110.60
1	N	480	GLU	OE1-CD-OE2	-5.61	116.56	123.30
1	R	265	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	S	168	SER	O-C-N	-5.61	113.72	122.70
1	E	464	PHE	O-C-N	-5.61	113.72	122.70
1	K	157	ASP	CB-CG-OD2	5.61	123.35	118.30
1	R	162	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	P	307	VAL	CA-CB-CG2	-5.61	102.49	110.90
1	H	58	MET	CG-SD-CE	-5.61	91.23	100.20
1	C	307	VAL	CA-CB-CG1	-5.60	102.49	110.90
1	R	200	TRP	CD1-NE1-CE2	5.60	114.04	109.00
1	G	474	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	L	275	PHE	CB-CG-CD1	5.60	124.72	120.80
1	M	432	TYR	CB-CG-CD1	5.60	124.36	121.00
1	Q	98	GLU	C-N-CA	5.60	135.70	121.70
1	I	430	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	N	475	SER	N-CA-CB	5.60	118.89	110.50
1	B	293	THR	CA-CB-CG2	-5.59	104.57	112.40
1	O	396	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	Q	485	TYR	CA-CB-CG	-5.59	102.78	113.40
1	C	307	VAL	CA-CB-CG2	5.59	119.28	110.90
1	L	302	LYS	O-C-N	-5.59	113.70	123.20
1	F	100	THR	CA-CB-CG2	5.58	120.22	112.40
1	G	344	ASP	O-C-N	-5.58	113.77	122.70
1	N	484	TRP	CA-CB-CG	5.58	124.31	113.70
1	B	275	PHE	CB-CG-CD1	-5.58	116.89	120.80
1	M	76	LEU	CB-CG-CD1	5.58	120.49	111.00
1	O	504	GLU	OE1-CD-OE2	-5.58	116.60	123.30
1	D	396	ARG	CD-NE-CZ	5.58	131.41	123.60
1	A	144	GLN	O-C-N	5.58	131.62	122.70
1	D	384	ARG	N-CA-CB	5.57	120.63	110.60
1	Q	498	TRP	CB-CG-CD1	5.57	134.25	127.00
1	S	91	GLN	CG-CD-OE1	5.57	132.75	121.60
1	I	368	VAL	CA-CB-CG1	5.57	119.26	110.90
1	L	144	GLN	O-C-N	-5.57	113.79	122.70
1	Q	174	VAL	CA-CB-CG1	-5.57	102.55	110.90
1	S	159	ASP	CB-CG-OD1	5.57	123.31	118.30
1	P	88	LEU	CB-CG-CD2	-5.57	101.53	111.00
1	R	122	LEU	CB-CG-CD2	5.57	120.46	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	262	ALA	O-C-N	-5.57	113.80	122.70
1	O	288	ASP	N-CA-CB	-5.57	100.58	110.60
1	G	208	GLN	O-C-N	-5.56	113.80	122.70
1	I	430	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	D	33	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	N	33	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	N	297	VAL	CA-CB-CG2	5.56	119.24	110.90
1	M	317	VAL	CG1-CB-CG2	-5.56	102.01	110.90
1	R	272	MET	CG-SD-CE	-5.55	91.32	100.20
1	C	339	VAL	CA-C-O	5.55	131.75	120.10
1	G	447	TYR	CB-CG-CD1	5.55	124.33	121.00
1	M	490	TYR	CG-CD2-CE2	-5.55	116.86	121.30
1	H	305	ASP	CB-CG-OD1	5.54	123.29	118.30
1	D	119	GLU	OE1-CD-OE2	5.54	129.95	123.30
1	F	338	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	R	421	VAL	CA-CB-CG1	5.54	119.21	110.90
1	G	264	ILE	O-C-N	-5.54	113.84	122.70
1	N	201	TYR	CG-CD1-CE1	-5.54	116.87	121.30
1	G	78	LYS	O-C-N	-5.54	113.84	122.70
1	D	176	GLY	CA-C-O	5.54	130.56	120.60
1	K	265	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	R	432	TYR	CB-CG-CD2	-5.54	117.68	121.00
1	F	213	ALA	CB-CA-C	-5.53	101.80	110.10
1	R	101	ALA	N-CA-CB	-5.53	102.36	110.10
1	S	368	VAL	CB-CA-C	5.53	121.91	111.40
1	L	484	TRP	CA-CB-CG	5.53	124.21	113.70
1	M	411	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	384	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	B	71	ASP	CB-CG-OD1	5.52	123.27	118.30
1	Q	389	ARG	NH1-CZ-NH2	-5.52	113.33	119.40
1	C	205	ASP	CB-CG-OD2	5.52	123.27	118.30
1	I	288	ASP	CB-CG-OD1	-5.52	113.33	118.30
1	P	200	TRP	CB-CG-CD2	-5.52	119.43	126.60
1	A	528	ASP	CB-CG-OD1	5.52	123.26	118.30
1	K	274	LYS	O-C-N	-5.51	113.88	122.70
1	S	474	ARG	CD-NE-CZ	5.51	131.32	123.60
1	G	443	ALA	O-C-N	-5.51	113.88	122.70
1	N	254	GLU	N-CA-CB	-5.51	100.68	110.60
1	Q	376	PRO	N-CD-CG	5.51	111.47	103.20
1	K	180	TYR	CB-CG-CD1	-5.51	117.69	121.00
1	S	391	VAL	CA-CB-CG1	5.51	119.16	110.90
1	M	331	LEU	CB-CG-CD1	-5.51	101.64	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	413	ARG	NE-CZ-NH2	5.51	123.05	120.30
1	Q	288	ASP	N-CA-CB	-5.51	100.69	110.60
1	E	351	LEU	CB-CG-CD1	-5.51	101.64	111.00
1	M	175	ALA	N-CA-CB	5.51	117.81	110.10
1	M	508	VAL	CA-CB-CG2	-5.51	102.64	110.90
1	R	528	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	Q	260	LEU	CB-CG-CD2	-5.50	101.65	111.00
1	F	205	ASP	CB-CG-OD1	5.50	123.25	118.30
1	P	325	LYS	C-N-CA	5.50	135.45	121.70
1	C	528	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	L	50	TYR	CG-CD1-CE1	-5.49	116.91	121.30
1	S	514	LYS	O-C-N	-5.49	113.91	122.70
1	O	135	TYR	CG-CD1-CE1	5.49	125.69	121.30
1	D	219	ASP	N-CA-CB	-5.49	100.72	110.60
1	F	159	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	F	400	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	415	ILE	CB-CA-C	-5.48	100.63	111.60
1	C	77	ASP	CB-CG-OD1	-5.48	113.36	118.30
1	S	369	PHE	CB-CG-CD2	-5.48	116.96	120.80
1	Q	121	LEU	CB-CG-CD1	-5.48	101.68	111.00
1	O	198	ASP	CB-CG-OD2	5.48	123.23	118.30
1	R	396	ARG	CD-NE-CZ	-5.48	115.93	123.60
1	O	33	ARG	CG-CD-NE	-5.47	100.31	111.80
1	O	229	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	D	400	ASP	CB-CG-OD2	5.47	123.22	118.30
1	L	126	VAL	CA-CB-CG2	5.47	119.11	110.90
1	L	270	THR	O-C-N	-5.47	113.95	122.70
1	P	430	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	S	423	ILE	CA-CB-CG2	-5.47	99.97	110.90
1	D	198	ASP	CB-CG-OD2	5.46	123.22	118.30
1	R	251	ALA	N-CA-CB	-5.46	102.45	110.10
1	P	497	MET	CG-SD-CE	-5.46	91.46	100.20
1	G	162	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	D	162	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	K	120	ASP	N-CA-CB	-5.46	100.77	110.60
1	M	282	LEU	CB-CG-CD1	5.46	120.28	111.00
1	S	268	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	F	219	ASP	CB-CG-OD1	5.46	123.21	118.30
1	N	161	LEU	N-CA-CB	-5.45	99.50	110.40
1	N	393	GLU	OE1-CD-OE2	-5.45	116.76	123.30
1	D	451	LEU	CB-CG-CD2	-5.45	101.73	111.00
1	H	229	ASP	CB-CG-OD1	5.45	123.20	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	384	ARG	CD-NE-CZ	5.45	131.23	123.60
1	M	198	ASP	CB-CG-OD1	5.45	123.20	118.30
1	N	270	THR	CA-CB-CG2	5.45	120.03	112.40
1	B	137	LYS	N-CA-CB	-5.45	100.80	110.60
1	C	348	GLU	OE1-CD-OE2	-5.44	116.77	123.30
1	Q	257	LYS	CA-CB-CG	-5.44	101.43	113.40
1	O	158	THR	O-C-N	-5.44	114.00	122.70
1	E	196	ARG	CD-NE-CZ	-5.44	115.99	123.60
1	R	477	HIS	O-C-N	-5.44	114.00	122.70
1	B	311	TYR	CG-CD2-CE2	5.43	125.65	121.30
1	E	359	GLU	OE1-CD-OE2	-5.43	116.78	123.30
1	I	80	ASP	CB-CG-OD2	5.43	123.19	118.30
1	M	525	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	N	88	LEU	CB-CG-CD2	-5.43	101.76	111.00
1	B	422	GLU	OE1-CD-OE2	-5.43	116.78	123.30
1	O	120	ASP	N-CA-CB	-5.43	100.82	110.60
1	A	158	THR	CA-CB-OG1	5.43	120.40	109.00
1	E	496	ASP	CB-CG-OD1	-5.43	113.41	118.30
1	I	178	ARG	N-CA-CB	-5.43	100.83	110.60
1	N	194	GLU	OE1-CD-OE2	-5.43	116.79	123.30
1	P	350	ASP	CB-CG-OD1	5.43	123.19	118.30
1	S	233	VAL	CA-CB-CG1	5.43	119.04	110.90
1	E	432	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	M	125	ASP	O-C-N	-5.42	114.02	122.70
1	A	389	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	196	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	E	90	VAL	CA-CB-CG2	5.42	119.03	110.90
1	K	305	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	R	157	ASP	CB-CG-OD1	5.42	123.18	118.30
1	N	123	TYR	CG-CD2-CE2	-5.41	116.97	121.30
1	S	274	LYS	CB-CA-C	-5.41	99.58	110.40
1	F	30	GLU	O-C-N	-5.41	114.04	122.70
1	F	186	VAL	CA-CB-CG1	5.41	119.02	110.90
1	N	362	VAL	CA-CB-CG1	5.41	119.02	110.90
1	S	413	ARG	CD-NE-CZ	5.41	131.17	123.60
1	C	178	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	L	399	ARG	CG-CD-NE	-5.41	100.44	111.80
1	M	389	ARG	NH1-CZ-NH2	-5.41	113.45	119.40
1	P	421	VAL	CA-CB-CG2	-5.41	102.79	110.90
1	N	193	ALA	O-C-N	5.40	131.35	122.70
1	N	497	MET	CA-CB-CG	-5.40	104.11	113.30
1	C	261	ASP	CB-CG-OD2	5.40	123.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	447	TYR	CB-CG-CD2	5.40	124.24	121.00
1	M	357	ILE	O-C-N	-5.40	114.06	122.70
1	S	496	ASP	CB-CG-OD1	5.40	123.16	118.30
1	N	240	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	P	120	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	317	VAL	CA-CB-CG2	-5.39	102.81	110.90
1	N	240	ARG	N-CA-CB	5.39	120.31	110.60
1	C	200	TRP	CH2-CZ2-CE2	5.39	122.79	117.40
1	P	291	LEU	O-C-N	-5.39	114.07	122.70
1	Q	362	VAL	CA-CB-CG2	-5.39	102.81	110.90
1	E	67	THR	CA-CB-CG2	5.39	119.94	112.40
1	G	287	VAL	O-C-N	-5.39	114.08	122.70
1	Q	364	GLU	OE1-CD-OE2	-5.39	116.84	123.30
1	A	364	GLU	O-C-N	-5.38	114.08	122.70
1	I	166	MET	O-C-N	-5.38	114.09	122.70
1	O	356	LEU	O-C-N	-5.38	114.08	122.70
1	Q	50	TYR	CB-CG-CD2	5.38	124.23	121.00
1	B	484	TRP	CE3-CZ3-CH2	-5.38	115.28	121.20
1	D	216	SER	N-CA-CB	5.38	118.57	110.50
1	D	490	TYR	CG-CD2-CE2	-5.38	117.00	121.30
1	C	232	VAL	CA-CB-CG2	5.38	118.97	110.90
1	E	525	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	L	141	VAL	CG1-CB-CG2	-5.38	102.30	110.90
1	A	229	ASP	CB-CG-OD2	-5.37	113.46	118.30
1	I	399	ARG	CG-CD-NE	-5.37	100.51	111.80
1	L	483	LYS	N-CA-C	5.37	125.51	111.00
1	R	278	GLU	OE1-CD-OE2	-5.37	116.85	123.30
1	R	484	TRP	CB-CG-CD2	5.37	133.59	126.60
1	I	88	LEU	CB-CG-CD2	-5.37	101.87	111.00
1	K	180	TYR	CA-CB-CG	-5.37	103.19	113.40
1	R	435	GLN	N-CA-CB	-5.37	100.93	110.60
1	A	116	LYS	N-CA-CB	-5.37	100.94	110.60
1	N	396	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	D	62	SER	N-CA-CB	5.37	118.55	110.50
1	S	394	THR	OG1-CB-CG2	-5.37	97.66	110.00
1	G	382	LEU	CB-CG-CD1	5.36	120.12	111.00
1	A	254	GLU	OE1-CD-OE2	-5.36	116.87	123.30
1	I	358	GLU	OE1-CD-OE2	-5.36	116.87	123.30
1	E	341	SER	CB-CA-C	-5.36	99.91	110.10
1	L	50	TYR	CG-CD2-CE2	-5.36	117.01	121.30
1	K	495	VAL	CB-CA-C	-5.36	101.22	111.40
1	Q	123	TYR	CA-CB-CG	-5.35	103.23	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	102	ASP	CB-CG-OD2	5.35	123.12	118.30
1	D	261	ASP	CB-CA-C	-5.35	99.70	110.40
1	H	400	ASP	CB-CG-OD1	5.35	123.12	118.30
1	O	483	LYS	N-CA-C	5.35	125.45	111.00
1	A	277	ASP	CB-CG-OD1	5.35	123.11	118.30
1	D	469	LEU	CB-CG-CD2	-5.35	101.91	111.00
1	L	274	LYS	N-CA-C	5.35	125.44	111.00
1	L	293	THR	N-CA-CB	5.35	120.46	110.30
1	O	421	VAL	CG1-CB-CG2	-5.35	102.34	110.90
1	F	278	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	I	384	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	C	265	ARG	O-C-N	-5.34	114.16	122.70
1	H	125	ASP	N-CA-CB	5.34	120.22	110.60
1	M	74	THR	CA-CB-CG2	5.34	119.87	112.40
1	F	192	VAL	CA-CB-CG2	-5.34	102.89	110.90
1	M	265	ARG	NH1-CZ-NH2	-5.34	113.53	119.40
1	B	322	ARG	CG-CD-NE	-5.33	100.60	111.80
1	G	224	TYR	C-N-CA	5.33	133.50	122.30
1	M	458	LEU	CB-CA-C	5.33	120.34	110.20
1	B	502	VAL	C-N-CA	5.33	135.03	121.70
1	H	485	TYR	CD1-CG-CD2	5.33	123.77	117.90
1	L	333	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	N	224	TYR	CG-CD2-CE2	-5.33	117.03	121.30
1	I	485	TYR	CG-CD2-CE2	-5.33	117.04	121.30
1	D	276	LEU	CB-CG-CD2	5.33	120.06	111.00
1	E	158	THR	CA-CB-CG2	-5.33	104.94	112.40
1	Q	350	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	G	329	GLU	O-C-N	-5.33	114.18	122.70
1	B	389	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	367	MET	CG-SD-CE	-5.32	91.68	100.20
1	E	344	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	P	179	GLU	OE1-CD-OE2	-5.32	116.91	123.30
1	D	229	ASP	CB-CG-OD1	5.32	123.09	118.30
1	M	205	ASP	O-C-N	-5.32	114.19	122.70
1	N	322	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	O	318	LEU	CB-CG-CD2	5.32	120.05	111.00
1	O	333	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	R	87	LYS	N-CA-CB	-5.32	101.03	110.60
1	B	57	LYS	CB-CA-C	-5.31	99.78	110.40
1	G	398	LEU	CB-CG-CD1	5.31	120.02	111.00
1	H	437	GLY	C-N-CA	5.30	133.44	122.30
1	N	131	ILE	CA-CB-CG2	-5.30	100.30	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	498	TRP	CB-CG-CD1	5.30	133.89	127.00
1	G	311	TYR	CZ-CE2-CD2	5.30	124.57	119.80
1	Q	43	GLU	CB-CA-C	5.30	121.00	110.40
1	N	525	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	P	241	LEU	CB-CG-CD2	5.30	120.01	111.00
1	F	269	PRO	N-CD-CG	5.30	111.14	103.20
1	P	432	TYR	CB-CG-CD1	-5.29	117.82	121.00
1	B	411	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	55	MET	C-N-CA	5.29	134.92	121.70
1	I	242	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	F	322	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	L	520	ALA	O-C-N	-5.28	114.25	122.70
1	N	140	GLU	O-C-N	-5.28	114.25	122.70
1	P	422	GLU	OE1-CD-OE2	-5.28	116.96	123.30
1	A	447	TYR	CB-CG-CD1	5.28	124.17	121.00
1	I	525	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	H	50	TYR	CB-CG-CD2	5.28	124.17	121.00
1	B	201	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	F	489	LEU	O-C-N	-5.28	114.26	122.70
1	H	288	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	O	366	LYS	N-CA-C	-5.28	96.76	111.00
1	Q	366	LYS	O-C-N	-5.28	114.26	122.70
1	A	477	HIS	CA-CB-CG	5.27	122.57	113.60
1	N	422	GLU	CG-CD-OE1	5.27	128.84	118.30
1	O	75	ILE	O-C-N	-5.27	114.26	122.70
1	I	61	ASP	O-C-N	-5.27	114.27	122.70
1	G	405	VAL	CA-CB-CG2	-5.27	103.00	110.90
1	Q	307	VAL	CA-CB-CG2	-5.27	103.00	110.90
1	S	224	TYR	CG-CD2-CE2	-5.27	117.09	121.30
1	F	229	ASP	CB-CG-OD2	5.26	123.04	118.30
1	D	216	SER	CB-CA-C	-5.26	100.10	110.10
1	E	321	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	E	414	ALA	N-CA-CB	-5.26	102.73	110.10
1	P	189	VAL	CG1-CB-CG2	-5.26	102.48	110.90
1	P	464	PHE	CB-CG-CD2	-5.26	117.12	120.80
1	Q	157	ASP	CB-CG-OD1	5.26	123.03	118.30
1	O	77	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	R	218	ASN	O-C-N	-5.26	114.29	122.70
1	G	192	VAL	CA-CB-CG1	5.25	118.78	110.90
1	H	289	LYS	O-C-N	-5.25	114.30	122.70
1	L	185	VAL	CA-CB-CG1	5.25	118.77	110.90
1	M	371	GLU	N-CA-CB	5.25	120.04	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	389	ARG	N-CA-CB	5.25	120.04	110.60
1	H	491	ALA	CB-CA-C	-5.25	102.23	110.10
1	C	126	VAL	CA-CB-CG2	-5.24	103.03	110.90
1	R	384	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	R	471	MET	CG-SD-CE	-5.24	91.81	100.20
1	D	523	VAL	CG1-CB-CG2	-5.24	102.52	110.90
1	P	59	LEU	CB-CA-C	5.24	120.16	110.20
1	P	124	LYS	C-N-CA	5.24	134.79	121.70
1	Q	364	GLU	CG-CD-OE2	5.24	128.78	118.30
1	S	485	TYR	CG-CD2-CE2	5.24	125.49	121.30
1	B	180	TYR	CB-CG-CD2	5.24	124.14	121.00
1	E	350	ASP	CB-CG-OD2	5.24	123.01	118.30
1	L	275	PHE	CG-CD2-CE2	5.24	126.56	120.80
1	P	50	TYR	CA-C-O	5.23	131.09	120.10
1	N	485	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	O	237	MET	N-CA-CB	-5.23	101.18	110.60
1	O	473	LEU	CB-CG-CD2	5.23	119.89	111.00
1	A	311	TYR	CG-CD1-CE1	-5.23	117.12	121.30
1	G	491	ALA	CB-CA-C	-5.23	102.25	110.10
1	M	57	LYS	O-C-N	-5.23	114.33	122.70
1	O	396	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	322	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	F	90	VAL	O-C-N	-5.23	114.33	122.70
1	K	253	LEU	N-CA-CB	5.23	120.85	110.40
1	B	204	LEU	CB-CG-CD2	5.23	119.88	111.00
1	F	75	ILE	O-C-N	-5.23	114.34	122.70
1	G	123	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	M	57	LYS	CA-C-O	5.22	131.07	120.10
1	O	389	ARG	CG-CD-NE	-5.22	100.83	111.80
1	P	50	TYR	CB-CG-CD1	5.22	124.13	121.00
1	G	502	VAL	CG1-CB-CG2	-5.22	102.55	110.90
1	H	361	LYS	O-C-N	-5.22	114.35	122.70
1	H	384	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	L	488	ASP	CB-CG-OD1	5.22	123.00	118.30
1	N	161	LEU	CB-CG-CD1	-5.22	102.13	111.00
1	P	410	LYS	O-C-N	-5.22	114.35	122.70
1	I	484	TRP	CD1-CG-CD2	-5.22	102.13	106.30
1	S	525	ARG	CD-NE-CZ	5.22	130.91	123.60
1	B	413	ARG	NH1-CZ-NH2	-5.22	113.66	119.40
1	D	77	ASP	CB-CG-OD1	5.22	123.00	118.30
1	F	155	ILE	CA-CB-CG2	5.22	121.33	110.90
1	K	55	MET	O-C-N	-5.22	114.35	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	356	LEU	CB-CG-CD2	5.22	119.87	111.00
1	R	255	VAL	CG1-CB-CG2	-5.21	102.56	110.90
1	A	411	ASP	CB-CG-OD2	5.21	122.99	118.30
1	K	309	GLN	O-C-N	-5.21	114.36	122.70
1	I	224	TYR	CG-CD1-CE1	-5.21	117.13	121.30
1	K	420	ALA	O-C-N	-5.21	114.36	122.70
1	K	490	TYR	CA-CB-CG	-5.21	103.50	113.40
1	L	50	TYR	CD1-CG-CD2	5.21	123.63	117.90
1	R	321	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	Q	470	LEU	CB-CG-CD1	5.21	119.85	111.00
1	R	110	PHE	CZ-CE2-CD2	-5.21	113.85	120.10
1	H	333	ARG	CB-CA-C	-5.21	99.99	110.40
1	M	517	THR	OG1-CB-CG2	-5.21	98.03	110.00
1	P	429	LEU	CB-CG-CD1	5.21	119.85	111.00
1	H	359	GLU	OE1-CD-OE2	-5.20	117.06	123.30
1	O	128	PRO	O-C-N	-5.20	114.38	122.70
1	E	298	ILE	O-C-N	-5.20	114.38	122.70
1	I	426	ALA	N-CA-CB	5.20	117.38	110.10
1	N	464	PHE	CB-CG-CD2	5.20	124.44	120.80
1	E	126	VAL	CA-CB-CG2	-5.20	103.10	110.90
1	G	149	LEU	CB-CA-C	-5.20	100.32	110.20
1	O	224	TYR	CG-CD2-CE2	-5.20	117.14	121.30
1	R	287	VAL	CG1-CB-CG2	-5.20	102.58	110.90
1	G	275	PHE	CB-CG-CD1	-5.20	117.16	120.80
1	H	160	LEU	CB-CA-C	5.20	120.07	110.20
1	K	452	GLU	OE1-CD-OE2	-5.20	117.07	123.30
1	A	395	GLU	OE1-CD-OE2	-5.19	117.07	123.30
1	I	265	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	K	248	LEU	CB-CG-CD1	5.19	119.82	111.00
1	Q	135	TYR	CD1-CE1-CZ	-5.19	115.13	119.80
1	S	41	ALA	N-CA-CB	5.19	117.36	110.10
1	B	97	ASP	CB-CG-OD1	5.18	122.97	118.30
1	O	180	TYR	CB-CG-CD2	5.18	124.11	121.00
1	A	452	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	F	447	TYR	CB-CG-CD1	5.18	124.11	121.00
1	H	256	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	B	356	LEU	CB-CA-C	-5.18	100.36	110.20
1	C	384	ARG	CG-CD-NE	-5.18	100.92	111.80
1	O	384	ARG	CG-CD-NE	-5.18	100.92	111.80
1	K	104	THR	CA-CB-CG2	5.18	119.65	112.40
1	N	369	PHE	CB-CG-CD2	-5.18	117.17	120.80
1	E	490	TYR	CG-CD1-CE1	5.18	125.44	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	265	ARG	CG-CD-NE	-5.18	100.93	111.80
1	Q	206	ASN	O-C-N	-5.18	114.42	122.70
1	R	353	TYR	CD1-CG-CD2	5.18	123.59	117.90
1	S	356	LEU	CB-CG-CD1	5.18	119.80	111.00
1	P	146	ILE	CA-C-O	5.17	130.96	120.10
1	R	298	ILE	CB-CA-C	-5.17	101.25	111.60
1	F	114	LEU	CB-CG-CD1	5.17	119.79	111.00
1	I	141	VAL	CA-CB-CG2	-5.17	103.14	110.90
1	K	269	PRO	N-CA-CB	5.17	109.51	103.30
1	H	76	LEU	O-C-N	-5.17	114.43	122.70
1	L	169	LEU	O-C-N	-5.17	114.43	122.70
1	I	430	ARG	NH1-CZ-NH2	-5.17	113.72	119.40
1	L	50	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	C	311	TYR	CD1-CG-CD2	5.16	123.58	117.90
1	D	322	ARG	O-C-N	-5.16	114.44	122.70
1	E	224	TYR	CB-CG-CD1	-5.16	117.90	121.00
1	K	377	LYS	CB-CA-C	-5.16	100.07	110.40
1	L	445	GLU	N-CA-CB	5.16	119.89	110.60
1	S	298	ILE	O-C-N	-5.16	114.44	122.70
1	D	474	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	H	170	SER	N-CA-CB	5.16	118.24	110.50
1	L	174	VAL	CB-CA-C	-5.16	101.60	111.40
1	P	413	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	Q	440	GLU	CA-CB-CG	5.16	124.75	113.40
1	K	239	LYS	CA-CB-CG	5.16	124.75	113.40
1	C	339	VAL	CA-CB-CG2	-5.16	103.17	110.90
1	K	464	PHE	CD1-CE1-CZ	5.16	126.29	120.10
1	H	58	MET	O-C-N	-5.15	114.45	122.70
1	K	523	VAL	CG1-CB-CG2	-5.15	102.65	110.90
1	C	34	ALA	CB-CA-C	5.15	117.83	110.10
1	C	53	ARG	CD-NE-CZ	5.15	130.81	123.60
1	E	262	ALA	CB-CA-C	5.15	117.83	110.10
1	O	219	ASP	CB-CG-OD1	5.15	122.94	118.30
1	Q	162	ARG	CD-NE-CZ	5.15	130.81	123.60
1	B	498	TRP	CG-CD2-CE3	-5.15	129.26	133.90
1	D	56	ASP	CB-CG-OD1	5.15	122.94	118.30
1	H	365	ASP	CA-C-O	5.15	130.91	120.10
1	I	366	LYS	N-CA-CB	5.15	119.87	110.60
1	E	485	TYR	CG-CD2-CE2	-5.15	117.18	121.30
1	S	360	ARG	NH1-CZ-NH2	-5.15	113.74	119.40
1	S	265	ARG	CG-CD-NE	-5.15	100.99	111.80
1	L	250	ASP	N-CA-CB	-5.14	101.34	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	390	LEU	CB-CG-CD1	5.14	119.75	111.00
1	P	268	ASP	CB-CG-OD2	5.14	122.93	118.30
1	S	206	ASN	CB-CG-OD1	-5.14	111.31	121.60
1	M	529	VAL	CB-CA-C	-5.14	101.63	111.40
1	R	405	VAL	CA-CB-CG1	5.14	118.61	110.90
1	P	321	ARG	CD-NE-CZ	5.14	130.80	123.60
1	B	139	GLU	OE1-CD-OE2	-5.14	117.14	123.30
1	G	326	SER	CB-CA-C	-5.14	100.34	110.10
1	N	53	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	N	260	LEU	O-C-N	-5.13	114.49	122.70
1	Q	354	ALA	O-C-N	-5.13	114.48	122.70
1	E	180	TYR	CD1-CE1-CZ	-5.13	115.18	119.80
1	G	389	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	L	326	SER	CB-CA-C	-5.13	100.35	110.10
1	L	395	GLU	OE1-CD-OE2	-5.13	117.14	123.30
1	A	200	TRP	CH2-CZ2-CE2	5.13	122.53	117.40
1	F	496	ASP	CB-CG-OD2	5.13	122.92	118.30
1	S	259	GLU	OE1-CD-OE2	5.13	129.46	123.30
1	Q	145	THR	CA-CB-CG2	5.13	119.58	112.40
1	S	413	ARG	NH1-CZ-NH2	5.13	125.04	119.40
1	M	101	ALA	CB-CA-C	-5.12	102.41	110.10
1	O	258	PRO	N-CA-CB	-5.12	96.96	102.60
1	R	123	TYR	CB-CA-C	5.12	120.65	110.40
1	A	205	ASP	CB-CG-OD1	5.12	122.91	118.30
1	M	349	GLN	CG-CD-OE1	-5.12	111.36	121.60
1	F	473	LEU	O-C-N	-5.12	114.51	122.70
1	S	90	VAL	CG1-CB-CG2	5.12	119.09	110.90
1	I	83	HIS	CB-CA-C	-5.11	100.19	110.40
1	S	126	VAL	CA-CB-CG2	-5.11	103.24	110.90
1	O	336	GLY	C-N-CA	5.11	133.02	122.30
1	O	396	ARG	N-CA-CB	5.11	119.79	110.60
1	P	50	TYR	O-C-N	-5.11	114.52	123.20
1	B	477	HIS	O-C-N	-5.10	114.54	122.70
1	E	498	TRP	CB-CG-CD1	-5.10	120.37	127.00
1	K	288	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	Q	275	PHE	CB-CG-CD1	-5.10	117.23	120.80
1	B	135	TYR	CD1-CG-CD2	-5.10	112.29	117.90
1	I	123	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	M	303	GLY	CA-C-O	5.10	129.78	120.60
1	R	168	SER	N-CA-CB	5.10	118.15	110.50
1	G	510	MET	CA-CB-CG	5.10	121.97	113.30
1	O	53	ARG	NE-CZ-NH2	-5.10	117.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	186	VAL	O-C-N	-5.10	114.55	122.70
1	A	410	LYS	N-CA-CB	-5.09	101.43	110.60
1	C	436	VAL	O-C-N	-5.09	114.54	123.20
1	H	496	ASP	O-C-N	-5.09	114.55	122.70
1	K	171	SER	O-C-N	-5.09	114.55	122.70
1	R	344	ASP	N-CA-CB	-5.09	101.44	110.60
1	S	233	VAL	CG1-CB-CG2	-5.09	102.75	110.90
1	A	343	ILE	CA-CB-CG1	5.09	120.67	111.00
1	G	299	ILE	N-CA-C	-5.09	97.26	111.00
1	H	531	SER	N-CA-CB	5.09	118.14	110.50
1	C	238	PRO	N-CA-C	5.09	125.32	112.10
1	G	240	ARG	CG-CD-NE	-5.09	101.12	111.80
1	M	500	LYS	CA-CB-CG	5.08	124.59	113.40
1	R	373	ALA	N-CA-CB	-5.08	102.98	110.10
1	L	387	LEU	CB-CG-CD1	-5.08	102.36	111.00
1	N	426	ALA	N-CA-CB	5.08	117.22	110.10
1	P	180	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	R	153	VAL	CG1-CB-CG2	5.08	119.03	110.90
1	H	220	THR	O-C-N	-5.08	114.57	122.70
1	D	101	ALA	O-C-N	-5.08	114.58	122.70
1	G	311	TYR	CD1-CE1-CZ	-5.08	115.23	119.80
1	H	517	THR	O-C-N	-5.08	114.58	122.70
1	L	404	THR	O-C-N	-5.08	114.58	122.70
1	R	353	TYR	CZ-CE2-CD2	5.08	124.37	119.80
1	G	432	TYR	CB-CG-CD1	5.07	124.04	121.00
1	A	200	TRP	CZ3-CH2-CZ2	-5.07	115.51	121.60
1	L	317	VAL	CG1-CB-CG2	5.07	119.01	110.90
1	M	240	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	R	197	GLY	C-N-CA	5.07	134.37	121.70
1	R	396	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	O	265	ARG	CG-CD-NE	-5.07	101.16	111.80
1	H	201	TYR	CA-CB-CG	-5.07	103.78	113.40
1	I	153	VAL	CA-CB-CG1	5.06	118.50	110.90
1	C	399	ARG	CG-CD-NE	-5.06	101.17	111.80
1	D	391	VAL	CA-CB-CG2	-5.06	103.31	110.90
1	G	180	TYR	CZ-CE2-CD2	5.06	124.35	119.80
1	C	523	VAL	CA-CB-CG2	-5.06	103.31	110.90
1	E	396	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	Q	213	ALA	N-CA-CB	-5.06	103.02	110.10
1	S	428	LYS	CA-CB-CG	5.06	124.53	113.40
1	D	82	GLN	N-CA-CB	5.06	119.70	110.60
1	S	186	VAL	CA-CB-CG1	5.06	118.48	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	353	TYR	CB-CG-CD1	5.05	124.03	121.00
1	M	162	ARG	NE-CZ-NH2	5.05	122.83	120.30
1	A	495	VAL	O-C-N	-5.05	114.62	122.70
1	G	438	GLY	CA-C-O	5.05	129.70	120.60
1	E	369	PHE	CB-CG-CD1	-5.05	117.26	120.80
1	R	389	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	G	270	THR	CA-CB-CG2	5.05	119.47	112.40
1	H	362	VAL	CG1-CB-CG2	5.05	118.98	110.90
1	N	135	TYR	CB-CG-CD2	5.05	124.03	121.00
1	N	339	VAL	CA-CB-CG1	5.05	118.47	110.90
1	O	474	ARG	NE-CZ-NH2	5.05	122.83	120.30
1	P	421	VAL	CG1-CB-CG2	5.05	118.98	110.90
1	P	260	LEU	CB-CG-CD1	5.05	119.58	111.00
1	R	39	VAL	CG1-CB-CG2	-5.05	102.83	110.90
1	B	446	ALA	N-CA-CB	-5.04	103.04	110.10
1	Q	384	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	344	ASP	CA-CB-CG	-5.04	102.31	113.40
1	D	180	TYR	CD1-CE1-CZ	5.04	124.34	119.80
1	O	355	SER	CB-CA-C	-5.04	100.52	110.10
1	O	209	ILE	O-C-N	-5.04	114.64	122.70
1	O	485	TYR	CD1-CE1-CZ	5.04	124.33	119.80
1	M	452	GLU	OE1-CD-OE2	-5.04	117.26	123.30
1	B	365	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	E	219	ASP	CB-CG-OD1	5.04	122.83	118.30
1	I	230	LYS	C-N-CA	5.04	134.29	121.70
1	L	82	GLN	CB-CA-C	-5.04	100.33	110.40
1	R	220	THR	CA-CB-OG1	5.04	119.58	109.00
1	D	79	MET	CA-CB-CG	5.03	121.85	113.30
1	F	384	ARG	NE-CZ-NH2	5.03	122.81	120.30
1	H	396	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	R	125	ASP	CB-CG-OD1	5.03	122.83	118.30
1	M	484	TRP	CZ3-CH2-CZ2	-5.03	115.57	121.60
1	A	247	ALA	N-CA-CB	5.03	117.14	110.10
1	H	277	ASP	CB-CG-OD2	5.03	122.83	118.30
1	L	85	ALA	N-CA-CB	5.03	117.14	110.10
1	L	411	ASP	CA-CB-CG	-5.03	102.34	113.40
1	C	180	TYR	CD1-CE1-CZ	-5.02	115.28	119.80
1	B	291	LEU	CB-CG-CD1	5.02	119.54	111.00
1	C	484	TRP	CA-CB-CG	5.02	123.24	113.70
1	P	384	ARG	CG-CD-NE	-5.02	101.25	111.80
1	D	65	ASP	CB-CG-OD2	5.02	122.82	118.30
1	I	370	VAL	CG1-CB-CG2	-5.02	102.87	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	53	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	P	141	VAL	CB-CA-C	-5.02	101.86	111.40
1	I	496	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	B	447	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	F	167	THR	N-CA-CB	5.02	119.83	110.30
1	B	311	TYR	CA-CB-CG	-5.01	103.87	113.40
1	I	189	VAL	CA-CB-CG1	5.01	118.42	110.90
1	K	327	ASP	CB-CG-OD2	5.01	122.81	118.30
1	O	165	ALA	N-CA-CB	-5.01	103.08	110.10
1	I	110	PHE	CG-CD2-CE2	-5.01	115.29	120.80
1	O	465	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	C	480	GLU	O-C-N	-5.01	114.69	122.70
1	N	224	TYR	CG-CD1-CE1	-5.01	117.29	121.30
1	O	464	PHE	CZ-CE2-CD2	5.01	126.11	120.10
1	S	29	LYS	C-N-CA	5.01	134.22	121.70
1	N	90	VAL	O-C-N	-5.01	114.69	122.70
1	S	196	ARG	N-CA-C	-5.01	97.48	111.00
1	B	189	VAL	CG1-CB-CG2	-5.00	102.89	110.90
1	N	313	ALA	CB-CA-C	-5.00	102.59	110.10
1	E	165	ALA	CB-CA-C	-5.00	102.59	110.10
1	I	447	TYR	CG-CD2-CE2	-5.00	117.30	121.30
1	L	129	THR	CA-CB-CG2	5.00	119.41	112.40
1	M	310	SER	O-C-N	-5.00	114.69	122.70
1	Q	125	ASP	CB-CG-OD2	5.00	122.80	118.30
1	M	468	ASP	CB-CG-OD1	5.00	122.80	118.30
1	Q	89	LEU	CB-CG-CD1	5.00	119.50	111.00
1	R	426	ALA	N-CA-CB	5.00	117.10	110.10

There are no chirality outliers.

All (207) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	TYR	Sidechain
1	A	178	ARG	Sidechain
1	A	234	HIS	Sidechain
1	A	240	ARG	Sidechain
1	A	322	ARG	Sidechain
1	A	33	ARG	Sidechain
1	A	353	TYR	Sidechain
1	A	430	ARG	Sidechain
1	A	474	ARG	Sidechain
1	B	162	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	322	ARG	Sidechain
1	B	333	ARG	Sidechain
1	B	353	TYR	Sidechain
1	B	360	ARG	Sidechain
1	B	384	ARG	Sidechain
1	B	389	ARG	Sidechain
1	B	430	ARG	Sidechain
1	B	447	TYR	Sidechain
1	B	464	PHE	Sidechain
1	B	474	ARG	Sidechain
1	B	477	HIS	Sidechain
1	B	485	TYR	Sidechain
1	B	50	TYR	Sidechain
1	B	525	ARG	Sidechain
1	B	53	ARG	Sidechain
1	C	135	TYR	Sidechain
1	C	162	ARG	Sidechain
1	C	180	TYR	Sidechain
1	C	196	ARG	Sidechain
1	C	224	TYR	Sidechain
1	C	321	ARG	Sidechain
1	C	333	ARG	Sidechain
1	C	338	ARG	Sidechain
1	C	360	ARG	Sidechain
1	C	384	ARG	Sidechain
1	C	430	ARG	Sidechain
1	C	432	TYR	Sidechain
1	C	485	TYR	Sidechain
1	C	490	TYR	Sidechain
1	C	53	ARG	Sidechain
1	D	110	PHE	Sidechain
1	D	135	TYR	Sidechain
1	D	178	ARG	Sidechain
1	D	224	TYR	Sidechain
1	D	234	HIS	Sidechain
1	D	275	PHE	Sidechain
1	D	338	ARG	Sidechain
1	D	360	ARG	Sidechain
1	D	413	ARG	Sidechain
1	D	432	TYR	Sidechain
1	D	50	TYR	Sidechain
1	D	53	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	E	178	ARG	Sidechain
1	E	240	ARG	Sidechain
1	E	338	ARG	Sidechain
1	E	360	ARG	Sidechain
1	E	389	ARG	Sidechain
1	E	474	ARG	Sidechain
1	E	490	TYR	Sidechain
1	F	123	TYR	Sidechain
1	F	135	TYR	Sidechain
1	F	240	ARG	Sidechain
1	F	321	ARG	Sidechain
1	F	333	ARG	Sidechain
1	F	369	PHE	Sidechain
1	F	389	ARG	Sidechain
1	F	474	ARG	Sidechain
1	F	53	ARG	Sidechain
1	G	135	TYR	Sidechain
1	G	178	ARG	Sidechain
1	G	180	TYR	Sidechain
1	G	321	ARG	Sidechain
1	G	33	ARG	Sidechain
1	G	333	ARG	Sidechain
1	G	353	TYR	Sidechain
1	G	360	ARG	Sidechain
1	G	432	TYR	Sidechain
1	G	474	ARG	Sidechain
1	G	485	TYR	Sidechain
1	G	490	TYR	Sidechain
1	G	525	ARG	Sidechain
1	G	53	ARG	Sidechain
1	H	110	PHE	Sidechain
1	H	196	ARG	Sidechain
1	H	265	ARG	Sidechain
1	H	321	ARG	Sidechain
1	H	322	ARG	Sidechain
1	H	338	ARG	Sidechain
1	H	353	TYR	Sidechain
1	H	396	ARG	Sidechain
1	H	432	TYR	Sidechain
1	H	474	ARG	Sidechain
1	H	485	TYR	Sidechain
1	H	490	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	H	525	ARG	Sidechain
1	I	110	PHE	Sidechain
1	I	123	TYR	Sidechain
1	I	178	ARG	Sidechain
1	I	234	HIS	Sidechain
1	I	333	ARG	Sidechain
1	I	360	ARG	Sidechain
1	I	413	ARG	Sidechain
1	I	432	TYR	Sidechain
1	I	447	TYR	Sidechain
1	I	50	TYR	Sidechain
1	I	53	ARG	Sidechain
1	I	83	HIS	Sidechain
1	K	178	ARG	Sidechain
1	K	201	TYR	Sidechain
1	K	224	TYR	Sidechain
1	K	311	TYR	Sidechain
1	K	322	ARG	Sidechain
1	K	333	ARG	Sidechain
1	K	384	ARG	Sidechain
1	K	396	ARG	Sidechain
1	K	430	ARG	Sidechain
1	K	432	TYR	Sidechain
1	K	464	PHE	Sidechain
1	K	485	TYR	Sidechain
1	K	490	TYR	Sidechain
1	K	50	TYR	Sidechain
1	L	135	TYR	Sidechain
1	L	162	ARG	Sidechain
1	L	250	ASP	Mainchain
1	L	265	ARG	Sidechain
1	L	322	ARG	Sidechain
1	L	33	ARG	Sidechain
1	L	333	ARG	Sidechain
1	L	338	ARG	Sidechain
1	L	396	ARG	Sidechain
1	L	399	ARG	Sidechain
1	L	413	ARG	Sidechain
1	L	474	ARG	Mainchain
1	L	525	ARG	Sidechain
1	M	110	PHE	Sidechain
1	M	123	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	M	275	PHE	Sidechain
1	M	322	ARG	Sidechain
1	M	353	TYR	Sidechain
1	M	360	ARG	Sidechain
1	M	485	TYR	Sidechain
1	M	525	ARG	Sidechain
1	N	180	TYR	Sidechain
1	N	240	ARG	Sidechain
1	N	311	TYR	Sidechain
1	N	321	ARG	Sidechain
1	N	33	ARG	Sidechain
1	N	360	ARG	Sidechain
1	O	123	TYR	Sidechain
1	O	135	TYR	Sidechain
1	O	201	TYR	Sidechain
1	O	224	TYR	Sidechain
1	O	311	TYR	Sidechain
1	O	321	ARG	Sidechain
1	O	338	ARG	Sidechain
1	O	360	ARG	Sidechain
1	O	430	ARG	Sidechain
1	O	432	TYR	Sidechain
1	O	490	TYR	Sidechain
1	O	525	ARG	Sidechain
1	O	83	HIS	Sidechain
1	P	110	PHE	Sidechain
1	P	180	TYR	Sidechain
1	P	265	ARG	Sidechain
1	P	333	ARG	Sidechain
1	P	360	ARG	Sidechain
1	P	384	ARG	Sidechain
1	P	413	ARG	Sidechain
1	P	430	ARG	Sidechain
1	P	432	TYR	Sidechain
1	P	53	ARG	Sidechain
1	Q	123	TYR	Sidechain
1	Q	135	TYR	Sidechain
1	Q	178	ARG	Sidechain
1	Q	180	TYR	Sidechain
1	Q	196	ARG	Sidechain
1	Q	240	ARG	Sidechain
1	Q	311	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	Q	321	ARG	Sidechain
1	Q	33	ARG	Sidechain
1	Q	333	ARG	Sidechain
1	Q	396	ARG	Sidechain
1	Q	399	ARG	Sidechain
1	Q	413	ARG	Sidechain
1	Q	485	TYR	Sidechain
1	Q	50	TYR	Sidechain
1	Q	525	ARG	Sidechain
1	Q	98	GLU	Mainchain
1	R	135	TYR	Sidechain
1	R	162	ARG	Sidechain
1	R	178	ARG	Sidechain
1	R	196	ARG	Sidechain
1	R	240	ARG	Sidechain
1	R	311	TYR	Sidechain
1	R	353	TYR	Sidechain
1	R	360	ARG	Sidechain
1	R	396	ARG	Sidechain
1	R	413	ARG	Sidechain
1	R	430	ARG	Sidechain
1	R	432	TYR	Sidechain
1	S	135	TYR	Sidechain
1	S	180	TYR	Sidechain
1	S	265	ARG	Sidechain
1	S	311	TYR	Sidechain
1	S	430	ARG	Sidechain
1	S	490	TYR	Sidechain
1	S	83	HIS	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	3849	0	3995	8	0
1	B	3849	0	3995	17	0
1	C	3849	0	3995	12	0
1	D	3849	0	3995	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3849	0	3995	19	0
1	F	3849	0	3995	10	0
1	G	3849	0	3995	18	0
1	H	3849	0	3995	9	0
1	I	3849	0	3995	14	0
1	K	3849	0	3995	15	0
1	L	3849	0	3995	6	0
1	M	3849	0	3995	12	0
1	N	3849	0	3995	14	0
1	O	3849	0	3995	11	0
1	P	3849	0	3995	16	0
1	Q	3849	0	3995	12	0
1	R	3849	0	3995	7	0
1	S	3849	0	3995	10	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
2	D	31	0	12	0	0
2	E	31	0	12	0	0
2	F	31	0	12	0	0
2	G	31	0	12	0	0
2	H	31	0	12	0	0
2	I	31	0	12	0	0
2	K	31	0	12	0	0
2	L	31	0	12	0	0
2	M	31	0	12	0	0
2	N	31	0	12	0	0
2	O	31	0	12	0	0
2	P	31	0	12	0	0
2	Q	31	0	12	0	0
2	R	31	0	12	0	0
2	S	31	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
All	All	69858	0	72126	216	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 2.

All (216) 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:F:246:ILE:HA	1:F:297:VAL:HG13	1.62	0.79
1:P:88:LEU:HD13	1:Q:68:ILE:HD11	1.73	0.71
1:K:189:VAL:HG11	1:K:405:VAL:HG12	1.76	0.67
1:E:331:LEU:HD11	1:E:370:VAL:HG11	1.76	0.66
1:K:473:LEU:HD12	1:K:487:ILE:HG23	1.79	0.64
1:M:106:THR:HG23	1:M:454:LEU:HD21	1.79	0.62
1:M:222:LEU:HD11	1:M:379:ILE:HD12	1.80	0.62
1:F:240:ARG:HG2	1:F:240:ARG:HH11	1.64	0.61
1:K:104:THR:O	1:K:108:VAL:HG23	2.01	0.61
1:I:164:ILE:HG21	1:I:408:VAL:HG21	1.82	0.60
1:E:459:ILE:HD11	1:E:487:ILE:HB	1.87	0.57
1:G:222:LEU:HD11	1:G:379:ILE:HD12	1.85	0.56
1:Q:232:VAL:HG11	1:Q:318:LEU:HD11	1.87	0.56
1:D:507:LEU:HD23	1:D:507:LEU:H	1.71	0.56
1:D:85:ALA:HB1	1:D:523:VAL:HG13	1.89	0.55
1:I:241:LEU:HB3	1:I:244:ALA:HB2	1.88	0.54
1:H:46:LEU:HD21	1:H:105:LYS:HA	1.90	0.54
1:N:462:ALA:HB2	1:N:489:LEU:HD22	1.90	0.54
1:O:177:ALA:HB3	1:O:217:ILE:HG13	1.88	0.54
1:D:443:ALA:O	1:D:446:ALA:HB3	2.07	0.54
1:C:305:ASP:OD2	1:C:307:VAL:HG22	2.08	0.54
1:B:393:GLU:CD	1:B:396:ARG:HH22	2.11	0.54
1:O:393:GLU:CD	1:O:396:ARG:HH21	2.12	0.54
1:C:433:ALA:HB3	1:C:434:PRO:HD3	1.90	0.53
1:D:480:GLU:CD	1:D:480:GLU:H	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:30:GLU:H	1:M:30:GLU:CD	2.10	0.53
1:G:138:ALA:HB1	1:G:429:LEU:HD21	1.91	0.53
1:M:423:ILE:HD12	1:M:477:HIS:CG	2.44	0.53
1:E:233:VAL:HG12	1:E:237:MET:SD	2.49	0.53
1:A:162:ARG:HG3	1:A:186:VAL:HG21	1.91	0.53
1:O:145:THR:HG21	1:O:425:ILE:HA	1.91	0.53
1:O:234:HIS:CD2	1:O:236:GLY:H	2.28	0.52
1:I:248:LEU:N	1:I:248:LEU:HD22	2.25	0.52
1:N:155:ILE:HD12	1:N:190:THR:HG22	1.92	0.52
1:I:136:LYS:HA	1:I:136:LYS:HE2	1.92	0.51
1:H:473:LEU:HD11	1:H:487:ILE:HG23	1.91	0.51
1:O:360:ARG:HB2	1:O:369:PHE:CE2	2.45	0.51
1:Q:477:HIS:CG	1:Q:477:HIS:O	2.64	0.51
1:Q:75:ILE:HG22	1:Q:75:ILE:O	2.11	0.51
1:G:162:ARG:CG	1:G:186:VAL:HG21	2.41	0.50
1:H:224:TYR:HA	1:H:379:ILE:HG22	1.93	0.50
1:M:477:HIS:CG	1:M:477:HIS:O	2.63	0.50
1:L:185:VAL:HG13	1:L:402:LEU:HA	1.93	0.50
1:A:189:VAL:HG21	1:A:405:VAL:HG12	1.93	0.50
1:F:53:ARG:HH21	1:F:490:TYR:HA	1.77	0.49
1:K:327:ASP:O	1:K:331:LEU:HB2	2.12	0.49
1:H:184:ILE:HG23	1:H:222:LEU:HB2	1.94	0.49
1:N:38:ALA:O	1:N:41:ALA:HB3	2.13	0.49
1:Q:88:LEU:HD22	1:R:68:ILE:HD11	1.94	0.49
1:F:248:LEU:H	1:F:248:LEU:HD12	1.78	0.49
1:N:383:ILE:HD11	1:N:398:LEU:CD2	2.43	0.48
1:K:185:VAL:HG12	1:K:405:VAL:HG21	1.94	0.48
1:B:383:ILE:HD11	1:B:398:LEU:HD23	1.94	0.48
1:G:47:LYS:HA	1:G:109:ILE:HD11	1.96	0.48
1:I:222:LEU:HD11	1:I:379:ILE:HD12	1.95	0.48
1:O:251:ALA:HB2	1:O:341:SER:O	2.13	0.48
1:A:55:MET:HB3	1:I:527:ASP:HB2	1.96	0.47
1:C:161:LEU:HD11	1:C:409:ILE:HD11	1.95	0.47
1:I:192:VAL:HG21	1:I:207:ILE:HG12	1.96	0.47
1:B:248:LEU:HD21	1:B:331:LEU:HD13	1.94	0.47
1:K:244:ALA:HB1	1:K:297:VAL:HG23	1.96	0.47
1:K:423:ILE:HD12	1:K:477:HIS:CG	2.50	0.47
1:D:290:ILE:HG21	1:D:298:ILE:HD12	1.97	0.47
1:I:102:ASP:HB3	1:I:508:VAL:HG11	1.96	0.47
1:L:335:THR:HB	1:L:353:TYR:H	1.80	0.47
1:B:39:VAL:HG22	1:B:89:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:THR:HG22	1:F:49:THR:O	2.15	0.47
1:M:234:HIS:CD2	1:M:236:GLY:H	2.33	0.47
1:A:334:ALA:O	1:A:373:ALA:HB1	2.14	0.46
1:C:415:ILE:HD12	1:C:421:VAL:HG21	1.96	0.46
1:E:283:ILE:HD12	1:E:286:LYS:HD2	1.98	0.46
1:L:329:GLU:O	1:L:332:ALA:HB3	2.16	0.46
1:D:471:MET:HA	1:D:474:ARG:HG2	1.97	0.46
1:P:433:ALA:O	1:P:436:VAL:HG22	2.16	0.46
1:H:185:VAL:HG13	1:H:402:LEU:HA	1.97	0.46
1:S:184:ILE:HG23	1:S:222:LEU:HB2	1.98	0.46
1:Q:336:GLY:HA3	1:Q:374:LYS:HD3	1.98	0.45
1:D:248:LEU:HD22	1:D:248:LEU:H	1.82	0.45
1:N:473:LEU:HA	1:N:476:THR:HG22	1.98	0.45
1:F:246:ILE:HD13	1:F:331:LEU:HD21	1.97	0.45
1:G:162:ARG:HG2	1:G:186:VAL:HG21	1.97	0.45
1:P:253:LEU:HD11	1:P:298:ILE:HD11	1.98	0.45
1:R:161:LEU:HD22	1:R:405:VAL:HG13	1.99	0.45
1:D:477:HIS:CD2	1:D:477:HIS:O	2.70	0.45
1:D:231:GLU:CD	1:D:231:GLU:H	2.19	0.45
1:N:208:GLN:HB3	1:N:380:SER:HB3	1.99	0.45
1:E:242:GLU:HA	1:E:356:LEU:HD12	1.98	0.45
1:P:212:LYS:O	1:P:384:ARG:HA	2.17	0.45
1:E:155:ILE:HG13	1:E:190:THR:HG22	1.99	0.45
1:E:425:ILE:O	1:E:429:LEU:HB2	2.17	0.45
1:R:312:LEU:HD13	1:R:319:ALA:HB2	1.99	0.45
1:B:329:GLU:O	1:B:332:ALA:HB3	2.16	0.44
1:B:293:THR:HG21	1:B:346:ILE:HG22	1.98	0.44
1:K:208:GLN:OE1	1:K:226:ILE:HG23	2.18	0.44
1:P:531:SER:HA	1:Q:60:VAL:H	1.82	0.44
1:C:164:ILE:HG21	1:C:408:VAL:HG21	2.00	0.44
1:B:246:ILE:HA	1:B:297:VAL:HB	2.00	0.44
1:K:246:ILE:HD12	1:K:246:ILE:H	1.83	0.44
1:F:240:ARG:HG2	1:F:240:ARG:NH1	2.31	0.44
1:G:237:MET:HB3	1:G:238:PRO:HD2	2.00	0.44
1:Q:421:VAL:O	1:Q:425:ILE:HD12	2.18	0.44
1:B:387:LEU:H	1:B:390:LEU:HB3	1.83	0.44
1:B:76:LEU:HD11	1:B:108:VAL:HG21	1.98	0.44
1:L:443:ALA:O	1:L:446:ALA:HB3	2.17	0.43
1:E:76:LEU:HD11	1:E:108:VAL:HG21	2.00	0.43
1:E:229:ASP:HA	1:E:367:MET:SD	2.58	0.43
1:E:477:HIS:CG	1:E:477:HIS:O	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:ILE:HD12	1:C:473:LEU:HD22	1.99	0.43
1:S:161:LEU:HD22	1:S:405:VAL:HG13	2.01	0.43
1:D:209:ILE:HG21	1:D:395:GLU:HG3	2.00	0.43
1:E:250:ASP:HB2	1:E:339:VAL:CG1	2.49	0.43
1:E:287:VAL:HG13	1:E:312:LEU:HD21	2.00	0.43
1:E:453:SER:O	1:E:457:ILE:HG13	2.18	0.43
1:L:208:GLN:HE21	1:L:210:VAL:CG1	2.31	0.43
1:P:459:ILE:O	1:P:462:ALA:HB3	2.18	0.43
1:G:423:ILE:CD1	1:G:473:LEU:HD22	2.47	0.43
1:G:473:LEU:HD12	1:G:487:ILE:HB	2.00	0.43
1:M:526:ILE:HD13	1:N:58:MET:SD	2.59	0.43
1:N:383:ILE:HD11	1:N:398:LEU:HD23	2.01	0.43
1:A:430:ARG:HH21	1:A:452:GLU:CD	2.21	0.43
1:A:432:TYR:CZ	1:A:436:VAL:HG22	2.53	0.43
1:E:429:LEU:HD11	1:E:444:VAL:HG13	2.01	0.43
1:P:36:ILE:O	1:P:39:VAL:HB	2.19	0.43
1:S:232:VAL:HG22	1:S:359:GLU:OE1	2.18	0.43
1:C:477:HIS:O	1:C:477:HIS:CD2	2.71	0.43
1:M:226:ILE:HD11	1:M:334:ALA:HB2	2.01	0.43
1:N:207:ILE:HA	1:N:379:ILE:O	2.19	0.43
1:P:30:GLU:CD	1:P:30:GLU:H	2.22	0.43
1:F:226:ILE:HD11	1:F:378:SER:HB3	2.01	0.43
1:O:338:ARG:HH21	1:O:350:ASP:CG	2.22	0.43
1:B:430:ARG:HH21	1:B:452:GLU:CD	2.22	0.43
1:B:433:ALA:HB3	1:B:434:PRO:HD3	2.01	0.43
1:B:496:ASP:CG	1:B:499:GLN:HE21	2.22	0.43
1:I:192:VAL:HG12	1:I:202:VAL:HG23	2.01	0.43
1:N:249:ILE:HD11	1:N:290:ILE:HD13	2.01	0.43
1:P:88:LEU:CD1	1:Q:68:ILE:HD11	2.44	0.43
1:Q:238:PRO:HG2	1:Q:241:LEU:HD21	1.99	0.43
1:K:323:ALA:HB3	1:K:328:LEU:HD21	2.01	0.43
1:S:254:GLU:HG2	1:S:255:VAL:H	1.83	0.43
1:P:433:ALA:HB3	1:P:434:PRO:HD3	2.02	0.42
1:S:299:ILE:HG13	1:S:320:VAL:HB	2.01	0.42
1:K:415:ILE:HG12	1:K:506:ALA:HB2	2.01	0.42
1:L:213:ALA:HB2	1:L:391:VAL:HG11	2.01	0.42
1:M:49:THR:HG22	1:M:49:THR:O	2.20	0.42
1:K:232:VAL:HG11	1:K:318:LEU:HD11	2.02	0.42
1:F:185:VAL:HG13	1:F:402:LEU:HA	2.00	0.42
1:N:486:GLY:O	1:N:494:PRO:HA	2.20	0.42
1:G:290:ILE:HD13	1:G:298:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:248:LEU:H	1:M:248:LEU:HD22	1.85	0.42
1:Q:232:VAL:HA	1:Q:320:VAL:HG22	2.02	0.42
1:A:173:ALA:HB3	1:A:393:GLU:HG2	2.02	0.42
1:C:150:ALA:HB1	1:C:413:ARG:HB3	2.02	0.42
1:E:79:MET:HB3	1:E:81:LEU:HD21	2.02	0.42
1:G:526:ILE:HA	1:H:56:ASP:O	2.19	0.42
1:K:93:ALA:HB1	1:K:108:VAL:HG22	2.02	0.42
1:O:477:HIS:NE2	1:O:483:LYS:HA	2.34	0.42
1:M:433:ALA:HB3	1:M:434:PRO:HD3	2.01	0.41
1:N:452:GLU:CD	1:N:474:ARG:HH22	2.24	0.41
1:S:264:ILE:HD12	1:S:266:ILE:HD12	2.02	0.41
1:C:161:LEU:HB3	1:C:186:VAL:HG22	2.02	0.41
1:G:226:ILE:HG13	1:G:331:LEU:HA	2.01	0.41
1:G:234:HIS:CD2	1:G:236:GLY:H	2.38	0.41
1:K:42:VAL:O	1:K:45:ALA:HB3	2.21	0.41
1:G:291:LEU:HD21	1:G:317:VAL:HG21	2.01	0.41
1:S:47:LYS:HA	1:S:109:ILE:HD11	2.03	0.41
1:C:245:LYS:HB3	1:C:351:LEU:HD13	2.02	0.41
1:D:415:ILE:HB	1:D:421:VAL:HG21	2.03	0.41
1:G:249:ILE:O	1:G:300:CYS:HA	2.21	0.41
1:N:287:VAL:CG1	1:N:312:LEU:HD21	2.51	0.41
1:R:409:ILE:HD13	1:R:409:ILE:HA	1.96	0.41
1:S:287:VAL:HG11	1:S:311:TYR:CD2	2.56	0.41
1:G:162:ARG:HG3	1:G:186:VAL:HG21	2.03	0.41
1:C:141:VAL:HG21	1:C:432:TYR:CE1	2.55	0.41
1:H:181:ILE:CG2	1:H:398:LEU:HD23	2.51	0.41
1:H:500:LYS:HG2	1:H:500:LYS:O	2.20	0.41
1:O:46:LEU:HD23	1:O:46:LEU:HA	1.92	0.41
1:O:219:ASP:HB3	1:O:384:ARG:HD3	2.01	0.41
1:P:230:LYS:HG3	1:P:323:ALA:HA	2.02	0.41
1:P:297:VAL:HG21	1:P:357:ILE:HD13	2.02	0.41
1:S:393:GLU:CD	1:S:396:ARG:HH21	2.24	0.41
1:B:485:TYR:HA	1:B:495:VAL:O	2.20	0.41
1:E:248:LEU:HD12	1:E:328:LEU:HD23	2.02	0.41
1:G:30:GLU:CD	1:G:30:GLU:H	2.23	0.41
1:P:398:LEU:HD23	1:P:398:LEU:C	2.41	0.41
1:B:257:LYS:HB2	1:B:260:LEU:HD21	2.02	0.41
1:E:460:GLU:OE2	1:E:466:PRO:HG2	2.21	0.41
1:G:331:LEU:HD11	1:G:370:VAL:HG21	2.02	0.41
1:H:246:ILE:HA	1:H:297:VAL:HG13	2.02	0.41
1:I:227:VAL:HG22	1:I:369:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:354:ALA:HB3	1:I:357:ILE:HD11	2.02	0.41
1:K:416:ALA:HB3	1:K:484:TRP:CE3	2.56	0.41
1:P:201:TYR:CE1	1:P:410:LYS:HG2	2.56	0.41
1:E:110:PHE:CE2	1:E:451:LEU:HD22	2.56	0.41
1:G:312:LEU:HD13	1:G:319:ALA:HB2	2.03	0.41
1:I:415:ILE:HD12	1:I:421:VAL:HG21	2.02	0.41
1:M:246:ILE:HA	1:M:297:VAL:HG13	2.02	0.41
1:P:93:ALA:HB1	1:P:108:VAL:HG22	2.03	0.41
1:Q:106:THR:HG23	1:Q:454:LEU:HD21	2.01	0.41
1:B:250:ASP:HB2	1:B:339:VAL:HG12	2.03	0.40
1:B:290:ILE:HD11	1:B:343:ILE:HD12	2.03	0.40
1:B:425:ILE:HG21	1:B:425:ILE:HD13	1.81	0.40
1:D:477:HIS:O	1:D:477:HIS:CG	2.74	0.40
1:I:471:MET:HA	1:I:474:ARG:HG2	2.03	0.40
1:P:211:LYS:HD2	1:P:391:VAL:HG22	2.03	0.40
1:N:340:VAL:HG11	1:N:346:ILE:HB	2.04	0.40
1:R:36:ILE:HG22	1:R:40:LYS:HE2	2.03	0.40
1:S:234:HIS:CE1	1:S:309:GLN:OE1	2.74	0.40
1:A:229:ASP:HA	1:A:367:MET:HG2	2.04	0.40
1:D:150:ALA:HA	1:D:415:ILE:HG22	2.04	0.40
1:E:383:ILE:HG22	1:E:384:ARG:N	2.36	0.40
1:R:28:GLY:N	1:R:30:GLU:OE2	2.55	0.40
1:C:361:LYS:HG3	1:C:366:LYS:HG2	2.04	0.40
1:F:297:VAL:HG23	1:F:318:LEU:HD22	2.03	0.40
1:O:482:ASN:HB3	1:O:485:TYR:CD1	2.56	0.40
1:I:35:ASN:O	1:I:39:VAL:HG23	2.21	0.40
1:R:87:LYS:HA	1:R:90:VAL:HG22	2.02	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	503/553 (91%)	453 (90%)	46 (9%)	4 (1%)	19	60
1	B	503/553 (91%)	451 (90%)	44 (9%)	8 (2%)	9	44
1	C	503/553 (91%)	456 (91%)	44 (9%)	3 (1%)	25	66
1	D	503/553 (91%)	459 (91%)	41 (8%)	3 (1%)	25	66
1	E	503/553 (91%)	449 (89%)	50 (10%)	4 (1%)	19	60
1	F	503/553 (91%)	457 (91%)	42 (8%)	4 (1%)	19	60
1	G	503/553 (91%)	449 (89%)	50 (10%)	4 (1%)	19	60
1	H	503/553 (91%)	459 (91%)	42 (8%)	2 (0%)	34	72
1	I	503/553 (91%)	456 (91%)	44 (9%)	3 (1%)	25	66
1	K	503/553 (91%)	457 (91%)	44 (9%)	2 (0%)	34	72
1	L	503/553 (91%)	451 (90%)	46 (9%)	6 (1%)	13	50
1	M	503/553 (91%)	456 (91%)	42 (8%)	5 (1%)	15	54
1	N	503/553 (91%)	454 (90%)	43 (8%)	6 (1%)	13	50
1	O	503/553 (91%)	452 (90%)	46 (9%)	5 (1%)	15	54
1	P	503/553 (91%)	455 (90%)	43 (8%)	5 (1%)	15	54
1	Q	503/553 (91%)	450 (90%)	50 (10%)	3 (1%)	25	66
1	R	503/553 (91%)	455 (90%)	43 (8%)	5 (1%)	15	54
1	S	503/553 (91%)	451 (90%)	49 (10%)	3 (1%)	25	66
All	All	9054/9954 (91%)	8170 (90%)	809 (9%)	75 (1%)	24	60

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	213	ALA
1	B	30	GLU
1	C	30	GLU
1	D	30	GLU
1	F	30	GLU
1	H	30	GLU
1	H	438	GLY
1	I	30	GLU
1	K	30	GLU
1	L	95	GLY
1	L	203	ASP
1	M	177	ALA
1	O	30	GLU
1	P	30	GLU

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Mol	Chain	Res	Type
1	P	305	ASP
1	Q	30	GLU
1	S	30	GLU
1	A	30	GLU
1	A	438	GLY
1	B	149	LEU
1	B	203	ASP
1	B	438	GLY
1	C	438	GLY
1	D	149	LEU
1	D	438	GLY
1	E	30	GLU
1	E	149	LEU
1	G	30	GLU
1	L	30	GLU
1	M	30	GLU
1	N	30	GLU
1	N	438	GLY
1	P	149	LEU
1	R	30	GLU
1	S	438	GLY
1	B	56	ASP
1	C	149	LEU
1	E	438	GLY
1	G	149	LEU
1	G	438	GLY
1	I	438	GLY
1	K	438	GLY
1	L	438	GLY
1	M	149	LEU
1	N	177	ALA
1	N	229	ASP
1	O	203	ASP
1	O	438	GLY
1	P	257	LYS
1	P	438	GLY
1	R	47	LYS
1	R	438	GLY
1	S	251	ALA
1	A	149	LEU
1	A	245	LYS
1	B	98	GLU

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Mol	Chain	Res	Type
1	F	216	SER
1	G	148	GLU
1	I	149	LEU
1	M	499	GLN
1	N	149	LEU
1	N	363	GLY
1	O	149	LEU
1	O	216	SER
1	R	149	LEU
1	E	81	LEU
1	F	149	LEU
1	M	438	GLY
1	Q	149	LEU
1	Q	438	GLY
1	B	176	GLY
1	B	434	PRO
1	L	202	VAL
1	R	95	GLY
1	F	438	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	410/447 (92%)	396 (97%)	14 (3%)	37	60
1	B	410/447 (92%)	397 (97%)	13 (3%)	39	61
1	C	410/447 (92%)	398 (97%)	12 (3%)	42	64
1	D	410/447 (92%)	399 (97%)	11 (3%)	44	65
1	E	410/447 (92%)	396 (97%)	14 (3%)	37	60
1	F	410/447 (92%)	397 (97%)	13 (3%)	39	61
1	G	410/447 (92%)	396 (97%)	14 (3%)	37	60
1	H	410/447 (92%)	398 (97%)	12 (3%)	42	64
1	I	410/447 (92%)	394 (96%)	16 (4%)	32	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	410/447 (92%)	397 (97%)	13 (3%)	39	61
1	L	410/447 (92%)	403 (98%)	7 (2%)	60	78
1	M	410/447 (92%)	389 (95%)	21 (5%)	24	48
1	N	410/447 (92%)	391 (95%)	19 (5%)	27	52
1	O	410/447 (92%)	395 (96%)	15 (4%)	34	58
1	P	410/447 (92%)	400 (98%)	10 (2%)	49	69
1	Q	410/447 (92%)	402 (98%)	8 (2%)	55	74
1	R	410/447 (92%)	401 (98%)	9 (2%)	52	71
1	S	410/447 (92%)	398 (97%)	12 (3%)	42	64
All	All	7380/8046 (92%)	7147 (97%)	233 (3%)	42	61

All (233) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ASP
1	A	89	LEU
1	A	144	GLN
1	A	246	ILE
1	A	343	ILE
1	A	356	LEU
1	A	366	LYS
1	A	382	LEU
1	A	453	SER
1	A	471	MET
1	A	473	LEU
1	A	483	LYS
1	A	485	TYR
1	A	511	ASN
1	B	30	GLU
1	B	56	ASP
1	B	89	LEU
1	B	114	LEU
1	B	183	ASP
1	B	331	LEU
1	B	348	GLU
1	B	360	ARG
1	B	407	ASP
1	B	421	VAL
1	B	435	GLN

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Mol	Chain	Res	Type
1	B	473	LEU
1	B	477	HIS
1	C	59	LEU
1	C	89	LEU
1	C	153	VAL
1	C	234	HIS
1	C	296	ASN
1	C	333	ARG
1	C	366	LYS
1	C	378	SER
1	C	388	GLU
1	C	451	LEU
1	C	473	LEU
1	C	487	ILE
1	D	43	GLU
1	D	211	LYS
1	D	231	GLU
1	D	248	LEU
1	D	288	ASP
1	D	322	ARG
1	D	331	LEU
1	D	333	ARG
1	D	396	ARG
1	D	407	ASP
1	D	473	LEU
1	E	63	LEU
1	E	120	ASP
1	E	144	GLN
1	E	220	THR
1	E	234	HIS
1	E	282	LEU
1	E	305	ASP
1	E	321	ARG
1	E	366	LYS
1	E	390	LEU
1	E	421	VAL
1	E	473	LEU
1	E	485	TYR
1	E	487	ILE
1	F	30	GLU
1	F	102	ASP
1	F	164	ILE

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Mol	Chain	Res	Type
1	F	167	THR
1	F	183	ASP
1	F	231	GLU
1	F	234	HIS
1	F	349	GLN
1	F	356	LEU
1	F	470	LEU
1	F	473	LEU
1	F	485	TYR
1	F	531	SER
1	G	47	LYS
1	G	83	HIS
1	G	89	LEU
1	G	167	THR
1	G	293	THR
1	G	301	GLN
1	G	311	TYR
1	G	429	LEU
1	G	432	TYR
1	G	453	SER
1	G	473	LEU
1	G	485	TYR
1	G	487	ILE
1	G	525	ARG
1	H	59	LEU
1	H	84	PRO
1	H	89	LEU
1	H	128	PRO
1	H	133	SER
1	H	167	THR
1	H	231	GLU
1	H	234	HIS
1	H	238	PRO
1	H	421	VAL
1	H	434	PRO
1	H	484	TRP
1	I	50	TYR
1	I	84	PRO
1	I	89	LEU
1	I	97	ASP
1	I	160	LEU
1	I	205	ASP

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Mol	Chain	Res	Type
1	I	235	PRO
1	I	293	THR
1	I	297	VAL
1	I	329	GLU
1	I	366	LYS
1	I	399	ARG
1	I	407	ASP
1	I	469	LEU
1	I	477	HIS
1	I	485	TYR
1	K	43	GLU
1	K	80	ASP
1	K	89	LEU
1	K	96	GLN
1	K	114	LEU
1	K	246	ILE
1	K	305	ASP
1	K	311	TYR
1	K	327	ASP
1	K	333	ARG
1	K	388	GLU
1	K	453	SER
1	K	473	LEU
1	L	84	PRO
1	L	102	ASP
1	L	195	LEU
1	L	341	SER
1	L	398	LEU
1	L	458	LEU
1	L	466	PRO
1	M	30	GLU
1	M	43	GLU
1	M	89	LEU
1	M	159	ASP
1	M	231	GLU
1	M	241	LEU
1	M	248	LEU
1	M	263	GLU
1	M	301	GLN
1	M	305	ASP
1	M	309	GLN
1	M	325	LYS

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Mol	Chain	Res	Type
1	M	331	LEU
1	M	333	ARG
1	M	356	LEU
1	M	390	LEU
1	M	398	LEU
1	M	423	ILE
1	M	434	PRO
1	M	483	LYS
1	M	484	TRP
1	N	60	VAL
1	N	62	SER
1	N	65	ASP
1	N	67	THR
1	N	128	PRO
1	N	167	THR
1	N	181	ILE
1	N	191	GLN
1	N	231	GLU
1	N	234	HIS
1	N	297	VAL
1	N	305	ASP
1	N	318	LEU
1	N	356	LEU
1	N	365	ASP
1	N	473	LEU
1	N	484	TRP
1	N	485	TYR
1	N	511	ASN
1	O	98	GLU
1	O	297	VAL
1	O	298	ILE
1	O	305	ASP
1	O	326	SER
1	O	356	LEU
1	O	423	ILE
1	O	428	LYS
1	O	432	TYR
1	O	451	LEU
1	O	453	SER
1	O	469	LEU
1	O	480	GLU
1	O	485	TYR

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Mol	Chain	Res	Type
1	O	511	ASN
1	P	89	LEU
1	P	102	ASP
1	P	155	ILE
1	P	252	SER
1	P	343	ILE
1	P	349	GLN
1	P	400	ASP
1	P	473	LEU
1	P	476	THR
1	P	511	ASN
1	Q	84	PRO
1	Q	153	VAL
1	Q	183	ASP
1	Q	347	SER
1	Q	421	VAL
1	Q	440	GLU
1	Q	453	SER
1	Q	507	LEU
1	R	47	LYS
1	R	82	GLN
1	R	89	LEU
1	R	102	ASP
1	R	230	LYS
1	R	233	VAL
1	R	234	HIS
1	R	408	VAL
1	R	473	LEU
1	S	43	GLU
1	S	88	LEU
1	S	89	LEU
1	S	178	ARG
1	S	234	HIS
1	S	301	GLN
1	S	356	LEU
1	S	407	ASP
1	S	451	LEU
1	S	484	TRP
1	S	494	PRO
1	S	528	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	HIS
1	A	309	GLN
1	A	499	GLN
1	B	441	GLN
1	B	499	GLN
1	F	147	GLN
1	F	441	GLN
1	G	234	HIS
1	G	441	GLN
1	I	191	GLN
1	L	147	GLN
1	L	441	GLN
1	M	144	GLN
1	M	206	ASN
1	M	234	HIS
1	N	441	GLN
1	N	499	GLN
1	O	234	HIS
1	P	435	GLN
1	P	441	GLN
1	Q	441	GLN
1	R	349	GLN
1	R	499	GLN
1	R	511	ASN
1	S	234	HIS
1	S	309	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 36 ligands modelled in this entry, 18 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	I	800	3	26,33,33	1.45	3 (11%)	31,52,52	1.74	5 (16%)
2	ATP	R	800	3	26,33,33	1.13	1 (3%)	31,52,52	2.40	7 (22%)
2	ATP	S	800	3	26,33,33	1.49	4 (15%)	31,52,52	1.86	6 (19%)
2	ATP	C	800	3	26,33,33	1.26	2 (7%)	31,52,52	1.51	3 (9%)
2	ATP	B	800	3	26,33,33	1.38	4 (15%)	31,52,52	1.76	6 (19%)
2	ATP	G	800	3	26,33,33	1.35	3 (11%)	31,52,52	1.85	8 (25%)
2	ATP	M	800	3	26,33,33	1.97	6 (23%)	31,52,52	1.79	3 (9%)
2	ATP	H	800	3	26,33,33	1.14	2 (7%)	31,52,52	1.60	3 (9%)
2	ATP	O	800	3	26,33,33	1.21	0	31,52,52	1.92	6 (19%)
2	ATP	L	800	3	26,33,33	1.61	3 (11%)	31,52,52	1.66	5 (16%)
2	ATP	F	800	3	26,33,33	1.24	3 (11%)	31,52,52	2.15	7 (22%)
2	ATP	A	800	3	26,33,33	1.06	2 (7%)	31,52,52	2.18	8 (25%)
2	ATP	Q	800	3	26,33,33	2.01	4 (15%)	31,52,52	2.15	6 (19%)
2	ATP	N	800	3	26,33,33	1.27	4 (15%)	31,52,52	2.25	9 (29%)
2	ATP	E	800	3	26,33,33	1.29	4 (15%)	31,52,52	1.94	7 (22%)
2	ATP	P	800	3	26,33,33	1.40	4 (15%)	31,52,52	2.05	6 (19%)
2	ATP	K	800	3	26,33,33	1.62	5 (19%)	31,52,52	1.62	4 (12%)
2	ATP	D	800	3	26,33,33	1.50	4 (15%)	31,52,52	1.85	6 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	I	800	3	-	3/18/38/38	0/3/3/3
2	ATP	R	800	3	-	4/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	S	800	3	-	3/18/38/38	0/3/3/3
2	ATP	C	800	3	-	3/18/38/38	0/3/3/3
2	ATP	B	800	3	-	4/18/38/38	0/3/3/3
2	ATP	G	800	3	-	5/18/38/38	0/3/3/3
2	ATP	M	800	3	-	3/18/38/38	0/3/3/3
2	ATP	H	800	3	-	8/18/38/38	0/3/3/3
2	ATP	O	800	3	-	3/18/38/38	0/3/3/3
2	ATP	L	800	3	-	3/18/38/38	0/3/3/3
2	ATP	F	800	3	-	4/18/38/38	0/3/3/3
2	ATP	A	800	3	-	5/18/38/38	0/3/3/3
2	ATP	Q	800	3	-	3/18/38/38	0/3/3/3
2	ATP	N	800	3	-	4/18/38/38	0/3/3/3
2	ATP	E	800	3	-	5/18/38/38	0/3/3/3
2	ATP	P	800	3	-	3/18/38/38	0/3/3/3
2	ATP	K	800	3	-	3/18/38/38	0/3/3/3
2	ATP	D	800	3	-	3/18/38/38	0/3/3/3

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	800	ATP	O4'-C1'	-7.75	1.30	1.41
2	M	800	ATP	C2'-C1'	-5.78	1.45	1.53
2	L	800	ATP	C8-N7	-4.74	1.26	1.34
2	I	800	ATP	C2'-C1'	-4.51	1.46	1.53
2	P	800	ATP	O4'-C1'	3.98	1.46	1.41
2	M	800	ATP	C2-N3	3.92	1.38	1.32
2	D	800	ATP	C2-N3	3.83	1.38	1.32
2	M	800	ATP	C8-N7	-3.81	1.27	1.34
2	S	800	ATP	C2'-C3'	3.79	1.63	1.53
2	S	800	ATP	C2'-C1'	-3.55	1.48	1.53
2	K	800	ATP	C2-N3	3.50	1.37	1.32
2	Q	800	ATP	C2-N3	3.37	1.37	1.32
2	Q	800	ATP	C8-N7	-3.34	1.28	1.34
2	B	800	ATP	C2'-C1'	-3.34	1.48	1.53
2	G	800	ATP	O4'-C4'	3.32	1.52	1.45
2	K	800	ATP	C8-N7	-3.29	1.28	1.34
2	Q	800	ATP	C4-N3	-3.28	1.31	1.35
2	K	800	ATP	C4-N3	-3.21	1.31	1.35
2	D	800	ATP	O4'-C1'	3.14	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	800	ATP	O4'-C1'	3.05	1.45	1.41
2	B	800	ATP	O4'-C1'	2.96	1.45	1.41
2	I	800	ATP	C8-N7	-2.95	1.29	1.34
2	G	800	ATP	C2-N3	2.80	1.36	1.32
2	E	800	ATP	O2'-C2'	2.74	1.49	1.43
2	B	800	ATP	C8-N7	-2.71	1.29	1.34
2	F	800	ATP	C5-C4	-2.69	1.33	1.40
2	M	800	ATP	C4-N3	2.66	1.39	1.35
2	P	800	ATP	C8-N7	-2.64	1.30	1.34
2	D	800	ATP	C2'-C1'	-2.60	1.49	1.53
2	R	800	ATP	C2'-C1'	-2.58	1.49	1.53
2	H	800	ATP	C5'-C4'	2.58	1.59	1.51
2	I	800	ATP	O4'-C1'	2.58	1.44	1.41
2	C	800	ATP	PA-O2A	-2.46	1.43	1.55
2	N	800	ATP	O3'-C3'	2.41	1.48	1.43
2	E	800	ATP	O3'-C3'	2.41	1.48	1.43
2	C	800	ATP	C8-N7	-2.39	1.30	1.34
2	N	800	ATP	C2'-C1'	-2.38	1.50	1.53
2	E	800	ATP	C8-N7	-2.35	1.30	1.34
2	E	800	ATP	C6-N6	2.34	1.42	1.34
2	L	800	ATP	C5'-C4'	2.32	1.58	1.51
2	F	800	ATP	C3'-C4'	-2.31	1.47	1.53
2	F	800	ATP	C2-N3	-2.25	1.28	1.32
2	D	800	ATP	C4-N3	-2.20	1.32	1.35
2	P	800	ATP	C3'-C4'	2.19	1.58	1.53
2	P	800	ATP	PB-O1B	2.17	1.58	1.50
2	N	800	ATP	C2-N3	2.13	1.35	1.32
2	H	800	ATP	PG-O2G	-2.13	1.46	1.54
2	K	800	ATP	C3'-C4'	2.12	1.58	1.53
2	K	800	ATP	C2'-C1'	-2.10	1.50	1.53
2	M	800	ATP	C3'-C4'	2.10	1.58	1.53
2	S	800	ATP	O4'-C4'	2.07	1.49	1.45
2	A	800	ATP	O4'-C1'	2.07	1.44	1.41
2	A	800	ATP	O3'-C3'	2.06	1.47	1.43
2	G	800	ATP	C4-N3	-2.05	1.32	1.35
2	N	800	ATP	C5-N7	-2.05	1.32	1.39
2	B	800	ATP	C4-N3	2.04	1.38	1.35
2	L	800	ATP	C2-N3	2.04	1.35	1.32
2	S	800	ATP	PG-O3G	-2.01	1.47	1.54

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	800	ATP	PB-O3B-PG	-7.73	106.30	132.83
2	O	800	ATP	PA-O3A-PB	-7.45	107.25	132.83
2	R	800	ATP	PA-O3A-PB	-7.22	108.05	132.83
2	F	800	ATP	PA-O3A-PB	-7.08	108.54	132.83
2	R	800	ATP	PB-O3B-PG	-6.76	109.64	132.83
2	P	800	ATP	PA-O3A-PB	-6.40	110.88	132.83
2	A	800	ATP	PA-O3A-PB	-6.39	110.92	132.83
2	P	800	ATP	PB-O3B-PG	-6.38	110.93	132.83
2	Q	800	ATP	PA-O3A-PB	-6.18	111.62	132.83
2	S	800	ATP	PA-O3A-PB	-6.08	111.95	132.83
2	E	800	ATP	PB-O3B-PG	-5.94	112.43	132.83
2	I	800	ATP	PA-O3A-PB	-5.86	112.73	132.83
2	G	800	ATP	PB-O3B-PG	-5.71	113.23	132.83
2	N	800	ATP	PA-O3A-PB	-5.71	113.25	132.83
2	M	800	ATP	PB-O3B-PG	-5.65	113.44	132.83
2	L	800	ATP	PA-O3A-PB	-5.55	113.79	132.83
2	F	800	ATP	PB-O3B-PG	-5.47	114.06	132.83
2	K	800	ATP	PA-O3A-PB	-5.46	114.10	132.83
2	Q	800	ATP	PB-O3B-PG	-5.45	114.11	132.83
2	C	800	ATP	PA-O3A-PB	-5.24	114.83	132.83
2	D	800	ATP	PA-O3A-PB	-5.07	115.44	132.83
2	B	800	ATP	PB-O3B-PG	-4.98	115.75	132.83
2	A	800	ATP	PB-O3B-PG	-4.94	115.89	132.83
2	M	800	ATP	C3'-C2'-C1'	4.88	108.33	100.98
2	D	800	ATP	PB-O3B-PG	-4.82	116.28	132.83
2	B	800	ATP	PA-O3A-PB	-4.72	116.63	132.83
2	A	800	ATP	C4-C5-N7	4.67	114.27	109.40
2	H	800	ATP	PB-O3B-PG	-4.64	116.89	132.83
2	Q	800	ATP	C5-C6-N6	4.39	127.02	120.35
2	A	800	ATP	N6-C6-N1	4.27	127.44	118.57
2	M	800	ATP	PA-O3A-PB	-4.26	118.19	132.83
2	E	800	ATP	PA-O3A-PB	-4.19	118.44	132.83
2	K	800	ATP	PB-O3B-PG	-4.15	118.60	132.83
2	R	800	ATP	C5-C6-N6	4.12	126.61	120.35
2	G	800	ATP	PA-O3A-PB	-4.05	118.93	132.83
2	F	800	ATP	C4-C5-N7	4.03	113.59	109.40
2	H	800	ATP	PA-O3A-PB	-3.95	119.26	132.83
2	R	800	ATP	C3'-C2'-C1'	3.65	106.47	100.98
2	Q	800	ATP	O4'-C4'-C3'	-3.65	97.90	105.11
2	I	800	ATP	PB-O3B-PG	-3.55	120.64	132.83
2	G	800	ATP	C4-C5-N7	3.53	113.07	109.40
2	S	800	ATP	PB-O3B-PG	-3.49	120.84	132.83
2	O	800	ATP	PB-O3B-PG	-3.49	120.85	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	800	ATP	N6-C6-N1	3.42	125.67	118.57
2	E	800	ATP	O2G-PG-O3B	3.36	115.90	104.64
2	C	800	ATP	PB-O3B-PG	-3.25	121.68	132.83
2	S	800	ATP	C5-C6-N6	-3.22	115.46	120.35
2	R	800	ATP	N6-C6-N1	-3.16	112.01	118.57
2	G	800	ATP	O3G-PG-O2G	3.03	119.22	107.64
2	D	800	ATP	N3-C2-N1	2.95	133.28	128.68
2	F	800	ATP	O4'-C1'-C2'	-2.91	102.67	106.93
2	K	800	ATP	C2-N1-C6	-2.88	113.82	118.75
2	S	800	ATP	O4'-C4'-C3'	-2.88	99.42	105.11
2	Q	800	ATP	C1'-N9-C4	-2.85	121.64	126.64
2	N	800	ATP	O2G-PG-O1G	2.83	121.75	110.68
2	S	800	ATP	O4'-C1'-C2'	2.78	110.99	106.93
2	L	800	ATP	C2-N1-C6	-2.74	114.06	118.75
2	L	800	ATP	PB-O3B-PG	-2.74	123.42	132.83
2	L	800	ATP	C4-C5-N7	2.72	112.23	109.40
2	P	800	ATP	C5-C6-N6	2.72	124.48	120.35
2	N	800	ATP	O3G-PG-O3B	-2.71	95.55	104.64
2	S	800	ATP	N6-C6-N1	2.68	124.14	118.57
2	N	800	ATP	C3'-C2'-C1'	2.64	104.96	100.98
2	E	800	ATP	O3B-PG-O1G	-2.63	96.59	111.19
2	N	800	ATP	C5-C6-N6	2.61	124.32	120.35
2	R	800	ATP	C4-C5-N7	2.58	112.09	109.40
2	H	800	ATP	O4'-C4'-C3'	-2.58	100.01	105.11
2	F	800	ATP	C3'-C2'-C1'	2.47	104.70	100.98
2	E	800	ATP	C5-C6-N6	-2.46	116.61	120.35
2	N	800	ATP	O3'-C3'-C2'	2.46	119.77	111.82
2	R	800	ATP	O4'-C4'-C5'	2.45	117.44	109.37
2	K	800	ATP	O5'-C5'-C4'	2.45	117.43	108.99
2	P	800	ATP	C4-C5-N7	2.45	111.95	109.40
2	I	800	ATP	O4'-C4'-C3'	-2.43	100.30	105.11
2	O	800	ATP	O4'-C4'-C5'	2.42	117.33	109.37
2	D	800	ATP	C5-C6-N6	2.42	124.02	120.35
2	O	800	ATP	O3'-C3'-C2'	2.41	119.62	111.82
2	A	800	ATP	C5-C6-N6	-2.38	116.73	120.35
2	F	800	ATP	O3G-PG-O2G	2.38	116.75	107.64
2	I	800	ATP	O3B-PG-O1G	-2.37	98.05	111.19
2	A	800	ATP	C3'-C2'-C1'	2.35	104.52	100.98
2	B	800	ATP	O4'-C4'-C5'	2.32	117.02	109.37
2	F	800	ATP	O3'-C3'-C4'	2.31	117.73	111.05
2	D	800	ATP	O3B-PG-O1G	-2.28	98.52	111.19
2	D	800	ATP	C3'-C2'-C1'	2.26	104.38	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	800	ATP	O4'-C4'-C3'	-2.24	100.69	105.11
2	B	800	ATP	C5-C6-N6	2.24	123.75	120.35
2	B	800	ATP	O3B-PG-O1G	-2.24	98.78	111.19
2	O	800	ATP	C4-C5-N7	2.23	111.72	109.40
2	P	800	ATP	C3'-C2'-C1'	2.23	104.33	100.98
2	B	800	ATP	C5-C6-N1	-2.23	115.30	120.35
2	L	800	ATP	O3'-C3'-C2'	2.22	119.01	111.82
2	Q	800	ATP	O3G-PG-O2G	2.15	115.86	107.64
2	N	800	ATP	O2G-PG-O3B	2.15	111.85	104.64
2	A	800	ATP	O2G-PG-O1G	2.13	119.03	110.68
2	N	800	ATP	C4-C5-N7	2.13	111.62	109.40
2	C	800	ATP	C4-C5-N7	2.12	111.61	109.40
2	G	800	ATP	C3'-C2'-C1'	2.12	104.16	100.98
2	O	800	ATP	O5'-PA-O1A	-2.09	100.88	109.07
2	P	800	ATP	C5'-C4'-C3'	2.07	122.93	115.18
2	A	800	ATP	C5-C6-N1	-2.04	115.73	120.35
2	G	800	ATP	C5-C6-N6	2.03	123.44	120.35
2	G	800	ATP	O3B-PG-O1G	-2.03	99.94	111.19
2	I	800	ATP	C5-C6-N6	2.02	123.42	120.35
2	G	800	ATP	C2-N1-C6	-2.01	115.32	118.75

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	ATP	C5'-O5'-PA-O1A
2	A	800	ATP	C5'-O5'-PA-O3A
2	B	800	ATP	C5'-O5'-PA-O1A
2	B	800	ATP	C5'-O5'-PA-O2A
2	B	800	ATP	C5'-O5'-PA-O3A
2	C	800	ATP	C5'-O5'-PA-O1A
2	C	800	ATP	C5'-O5'-PA-O2A
2	C	800	ATP	C5'-O5'-PA-O3A
2	D	800	ATP	C5'-O5'-PA-O1A
2	E	800	ATP	C5'-O5'-PA-O1A
2	E	800	ATP	C5'-O5'-PA-O2A
2	E	800	ATP	C5'-O5'-PA-O3A
2	F	800	ATP	C5'-O5'-PA-O1A
2	F	800	ATP	C5'-O5'-PA-O2A
2	F	800	ATP	C5'-O5'-PA-O3A
2	G	800	ATP	C5'-O5'-PA-O1A
2	G	800	ATP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
2	H	800	ATP	C5'-O5'-PA-O1A
2	H	800	ATP	C5'-O5'-PA-O2A
2	H	800	ATP	C5'-O5'-PA-O3A
2	H	800	ATP	O4'-C4'-C5'-O5'
2	I	800	ATP	C5'-O5'-PA-O1A
2	I	800	ATP	C5'-O5'-PA-O2A
2	I	800	ATP	C5'-O5'-PA-O3A
2	K	800	ATP	C5'-O5'-PA-O2A
2	K	800	ATP	C5'-O5'-PA-O3A
2	L	800	ATP	C5'-O5'-PA-O1A
2	L	800	ATP	C5'-O5'-PA-O2A
2	L	800	ATP	C5'-O5'-PA-O3A
2	M	800	ATP	C5'-O5'-PA-O3A
2	N	800	ATP	C5'-O5'-PA-O2A
2	N	800	ATP	C5'-O5'-PA-O3A
2	O	800	ATP	C5'-O5'-PA-O2A
2	O	800	ATP	C5'-O5'-PA-O3A
2	Q	800	ATP	C5'-O5'-PA-O2A
2	Q	800	ATP	C5'-O5'-PA-O3A
2	R	800	ATP	C5'-O5'-PA-O1A
2	R	800	ATP	C5'-O5'-PA-O2A
2	R	800	ATP	C5'-O5'-PA-O3A
2	S	800	ATP	C5'-O5'-PA-O3A
2	H	800	ATP	C3'-C4'-C5'-O5'
2	P	800	ATP	O4'-C4'-C5'-O5'
2	P	800	ATP	C3'-C4'-C5'-O5'
2	D	800	ATP	C5'-O5'-PA-O3A
2	P	800	ATP	C5'-O5'-PA-O3A
2	A	800	ATP	PB-O3A-PA-O2A
2	A	800	ATP	C5'-O5'-PA-O2A
2	K	800	ATP	C5'-O5'-PA-O1A
2	M	800	ATP	C5'-O5'-PA-O1A
2	M	800	ATP	C5'-O5'-PA-O2A
2	N	800	ATP	C5'-O5'-PA-O1A
2	O	800	ATP	C5'-O5'-PA-O1A
2	Q	800	ATP	C5'-O5'-PA-O1A
2	S	800	ATP	C5'-O5'-PA-O1A
2	S	800	ATP	C5'-O5'-PA-O2A
2	F	800	ATP	PG-O3B-PB-O2B
2	H	800	ATP	PG-O3B-PB-O2B
2	A	800	ATP	PB-O3A-PA-O1A
2	B	800	ATP	PG-O3B-PB-O2B

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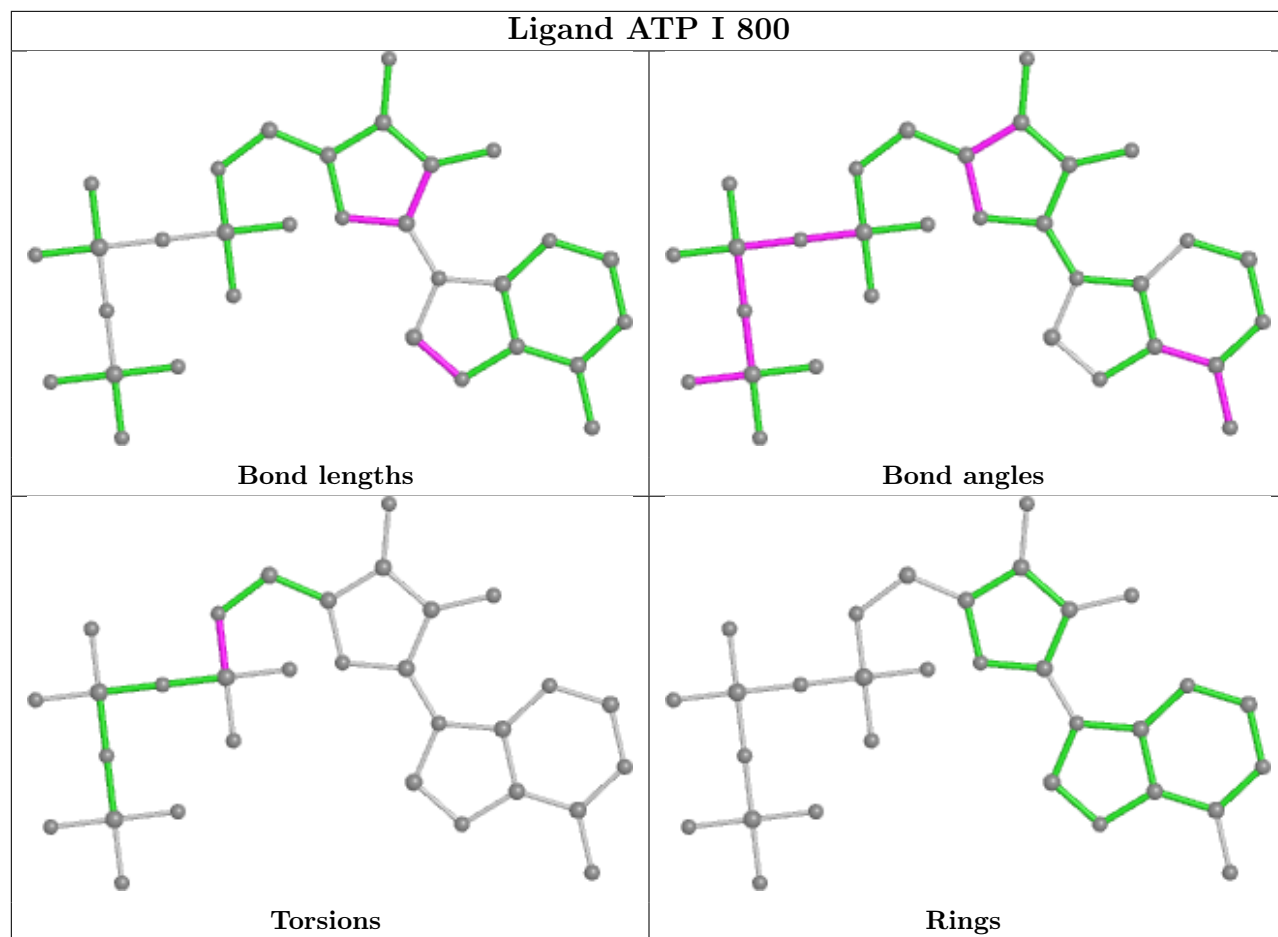
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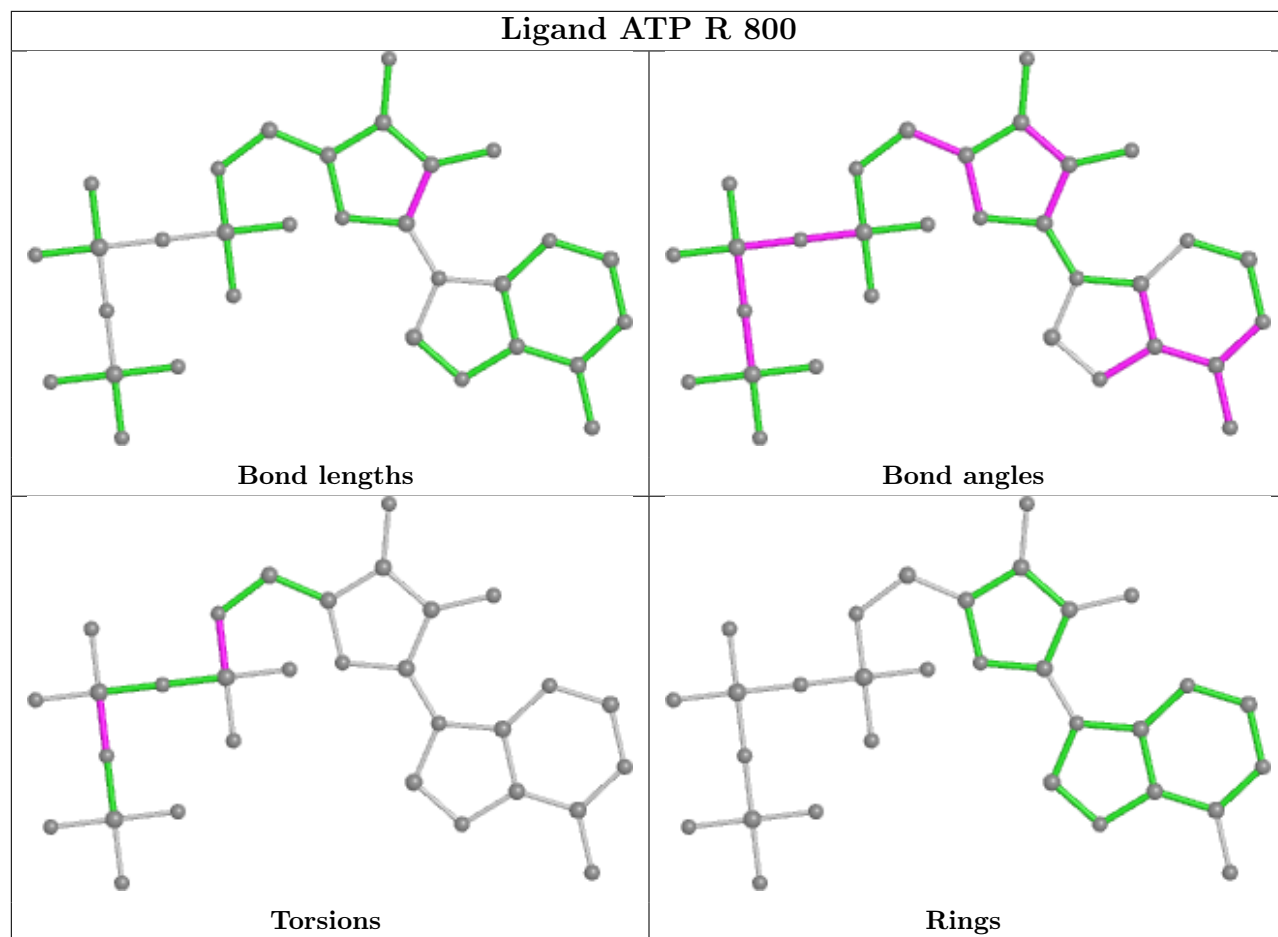
Mol	Chain	Res	Type	Atoms
2	D	800	ATP	PG-O3B-PB-O2B
2	E	800	ATP	PG-O3B-PB-O1B
2	E	800	ATP	PG-O3B-PB-O2B
2	G	800	ATP	PG-O3B-PB-O2B
2	G	800	ATP	PB-O3A-PA-O1A
2	H	800	ATP	PB-O3A-PA-O1A
2	H	800	ATP	PB-O3A-PA-O2A
2	N	800	ATP	PG-O3B-PB-O2B
2	R	800	ATP	PG-O3B-PB-O2B
2	G	800	ATP	C5'-O5'-PA-O2A

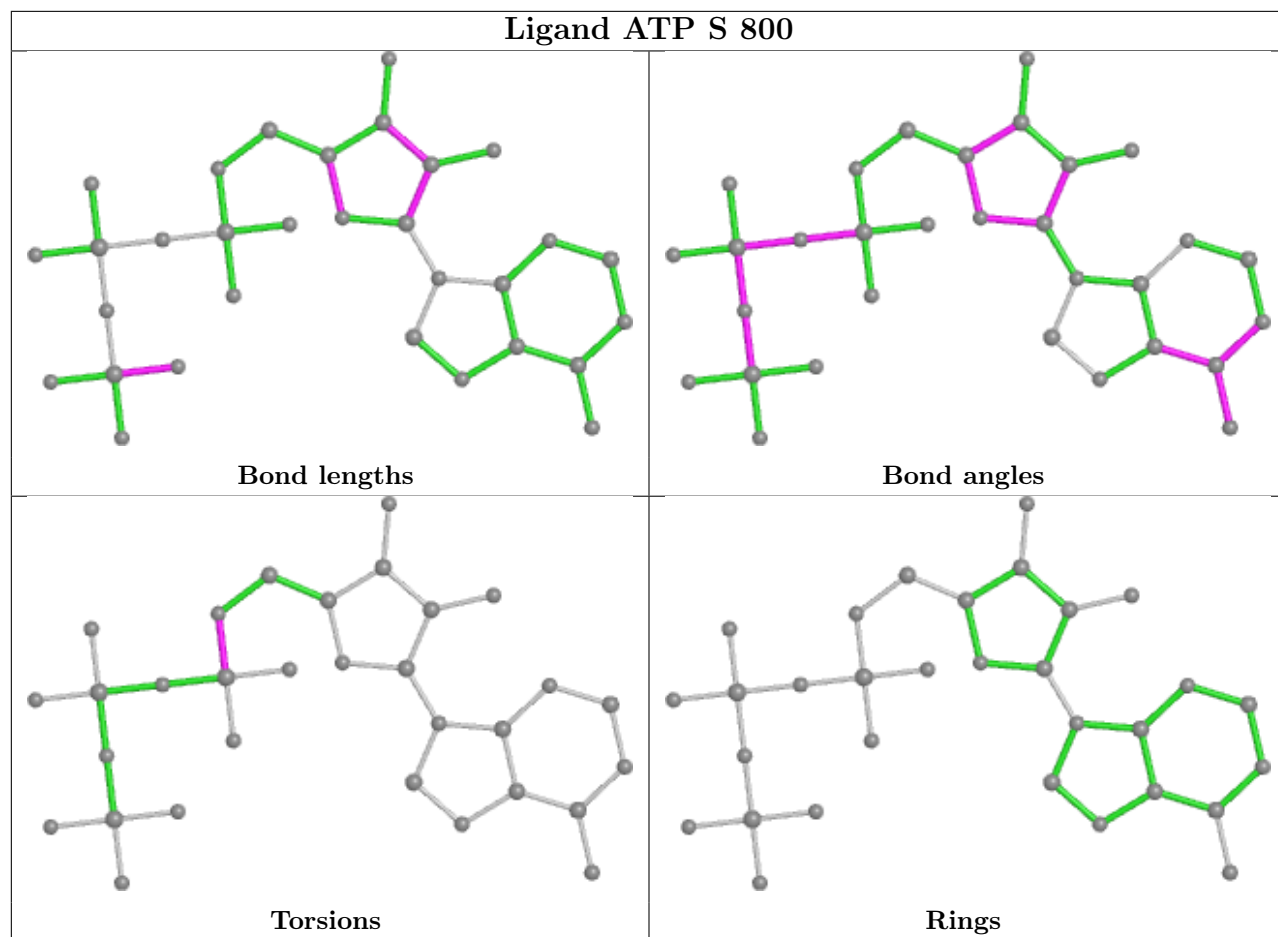
There are no ring outliers.

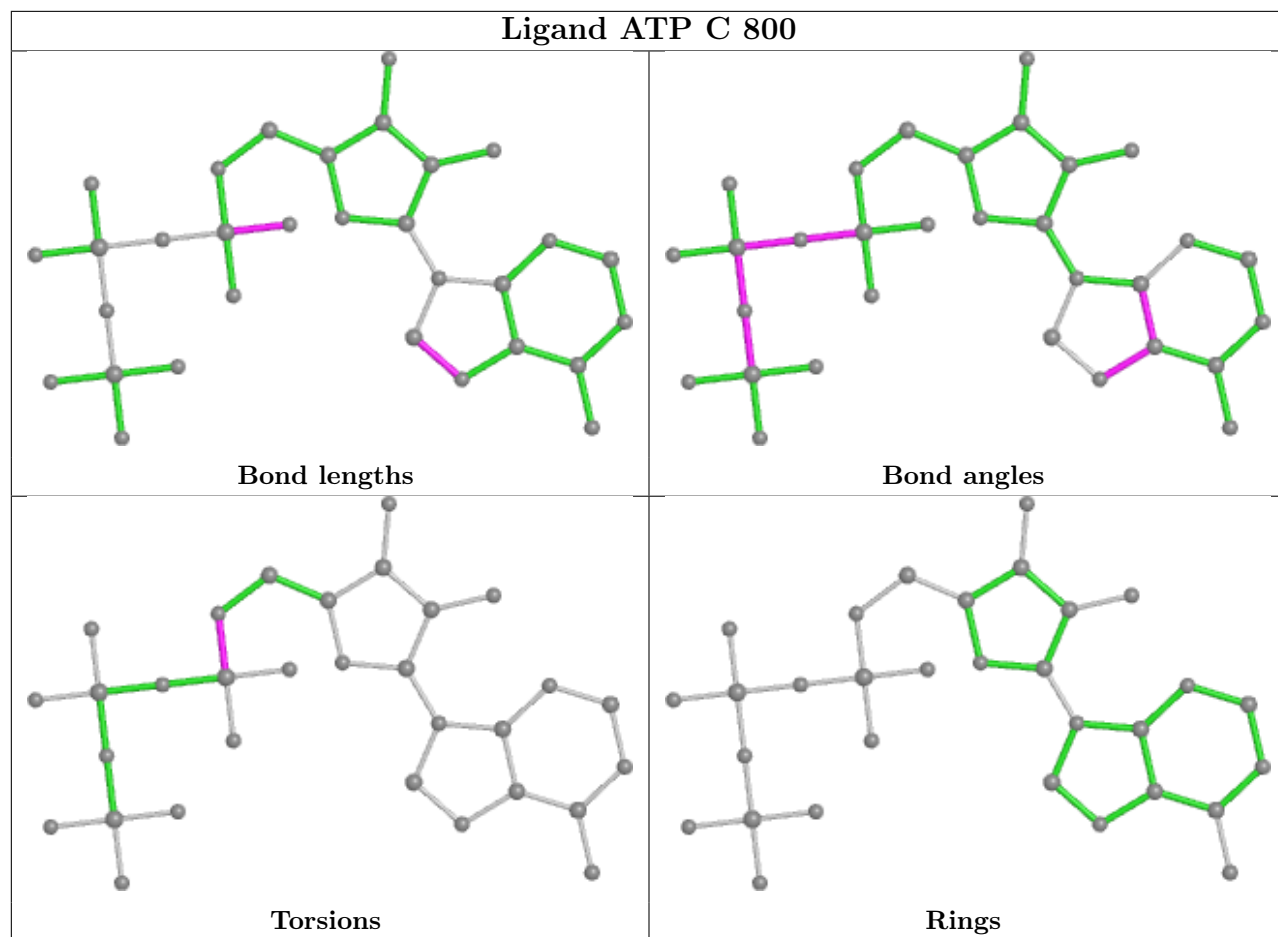
No monomer is involved in short contacts.

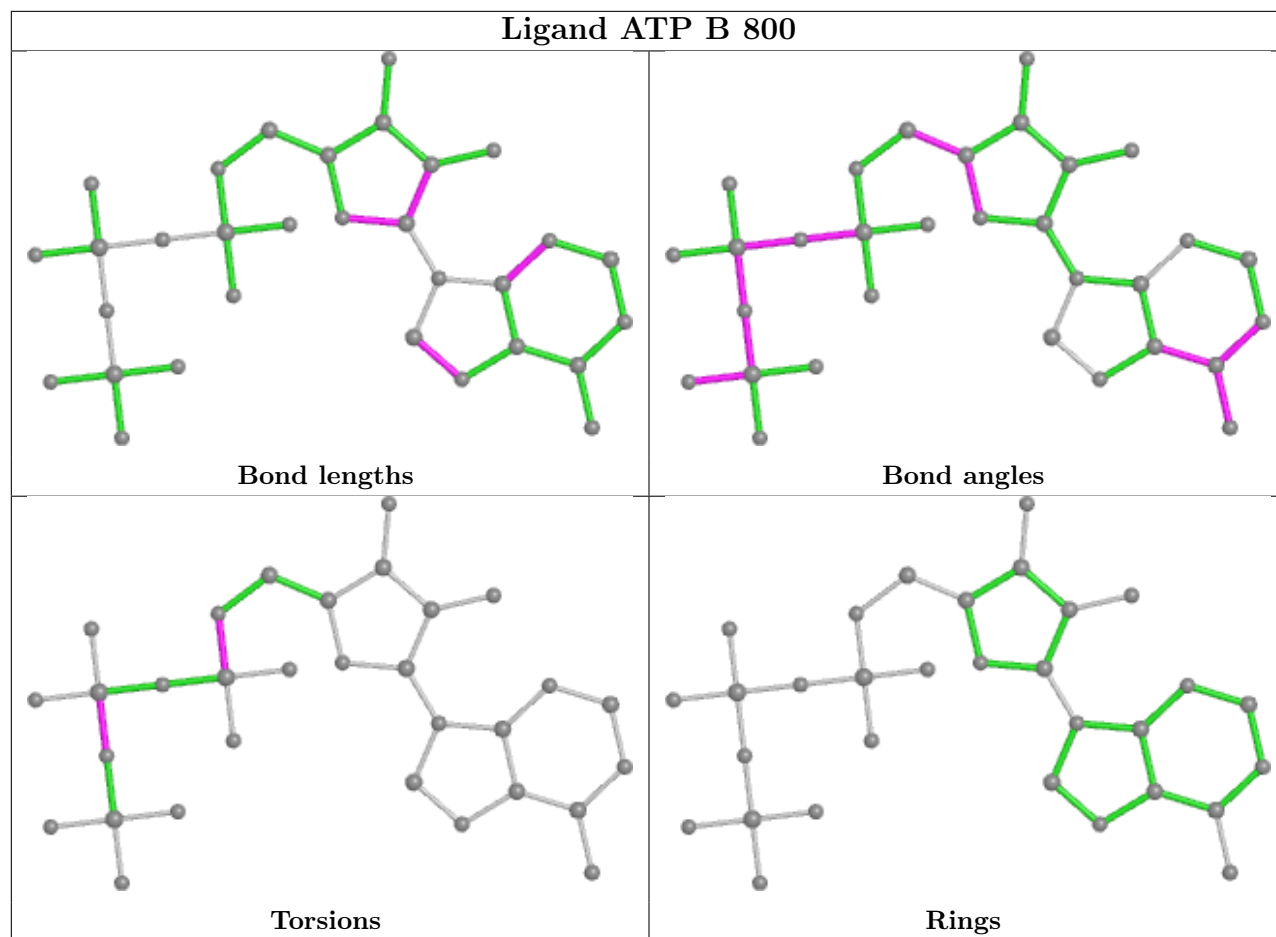
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

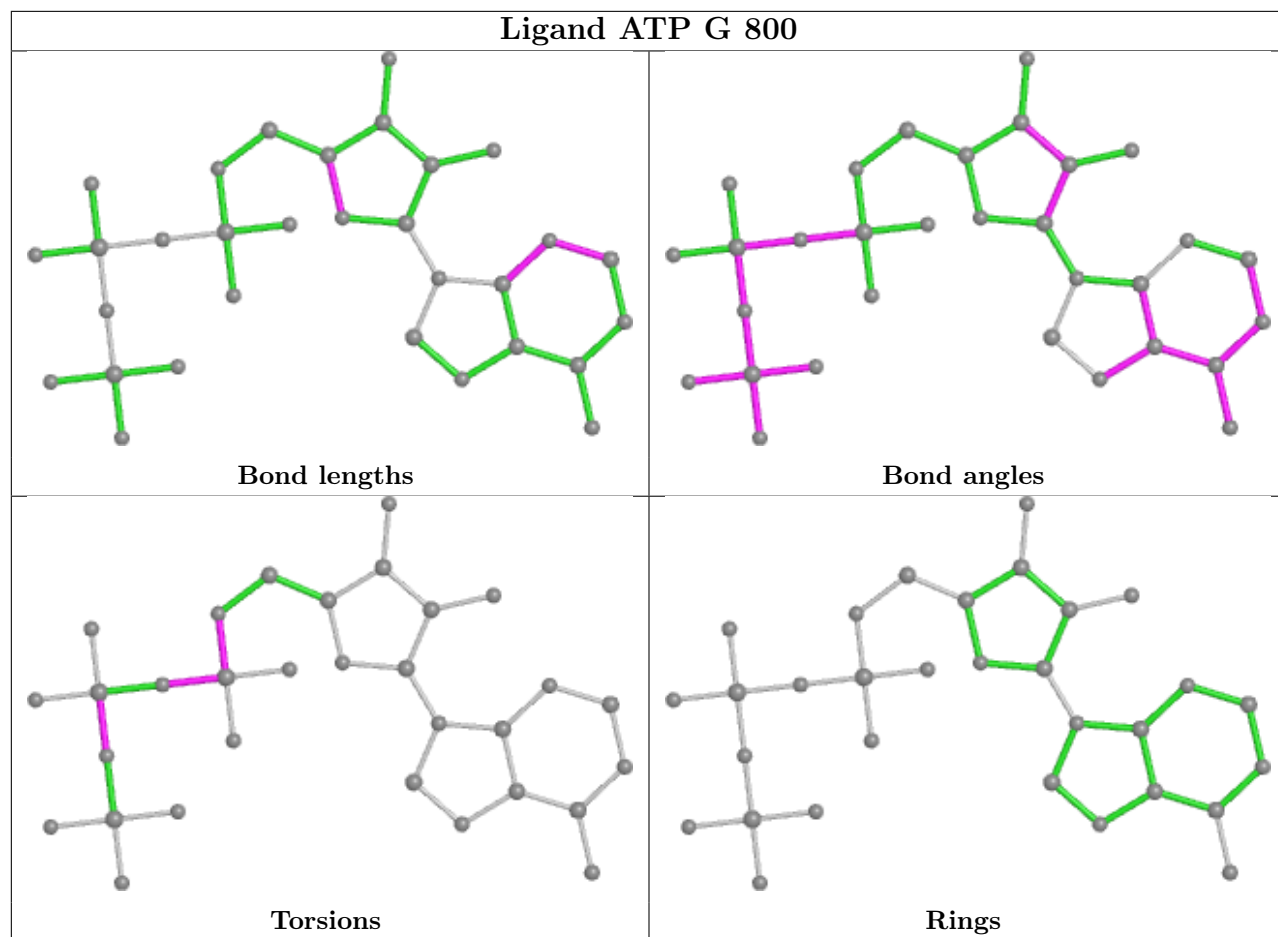


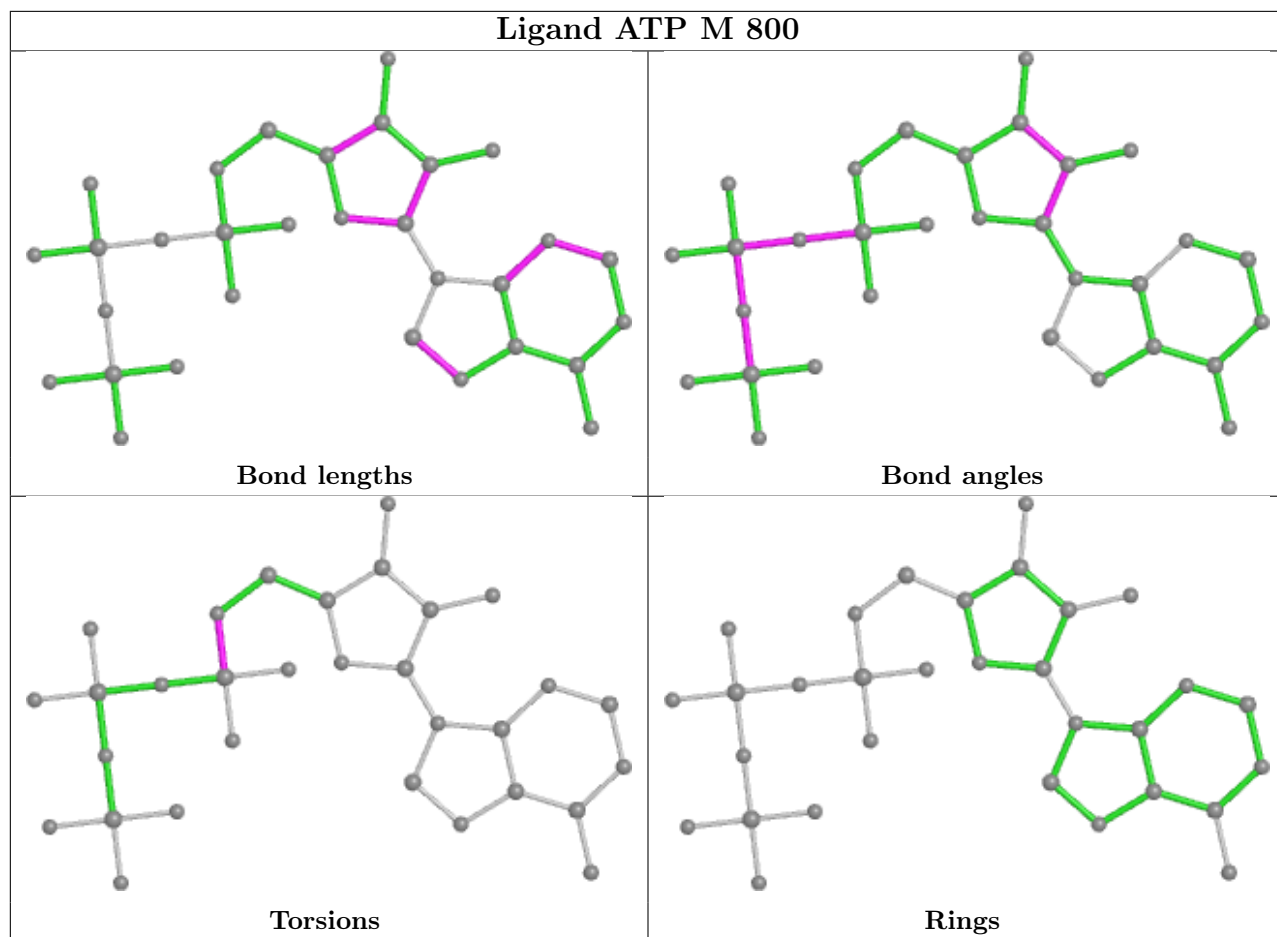


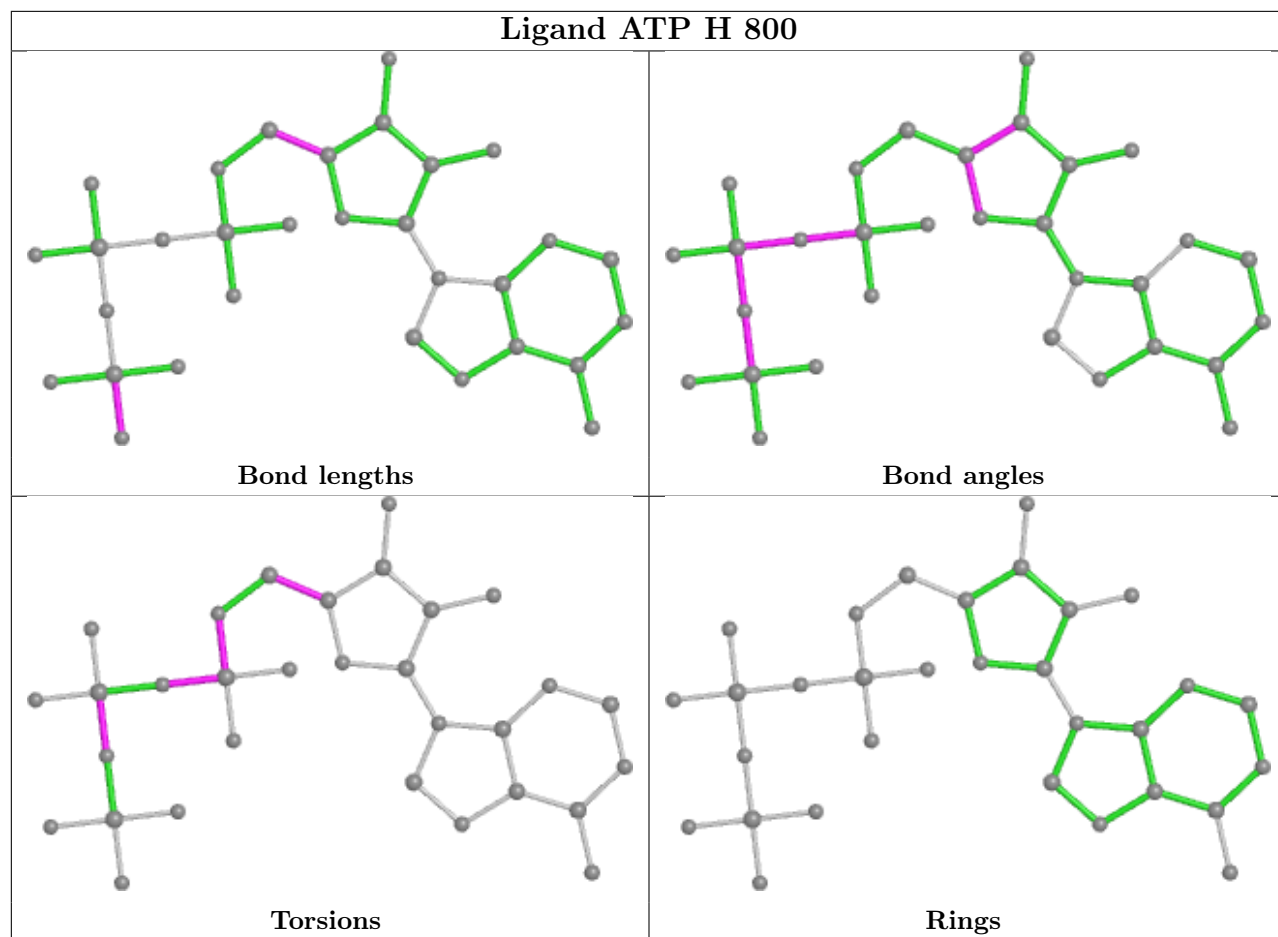


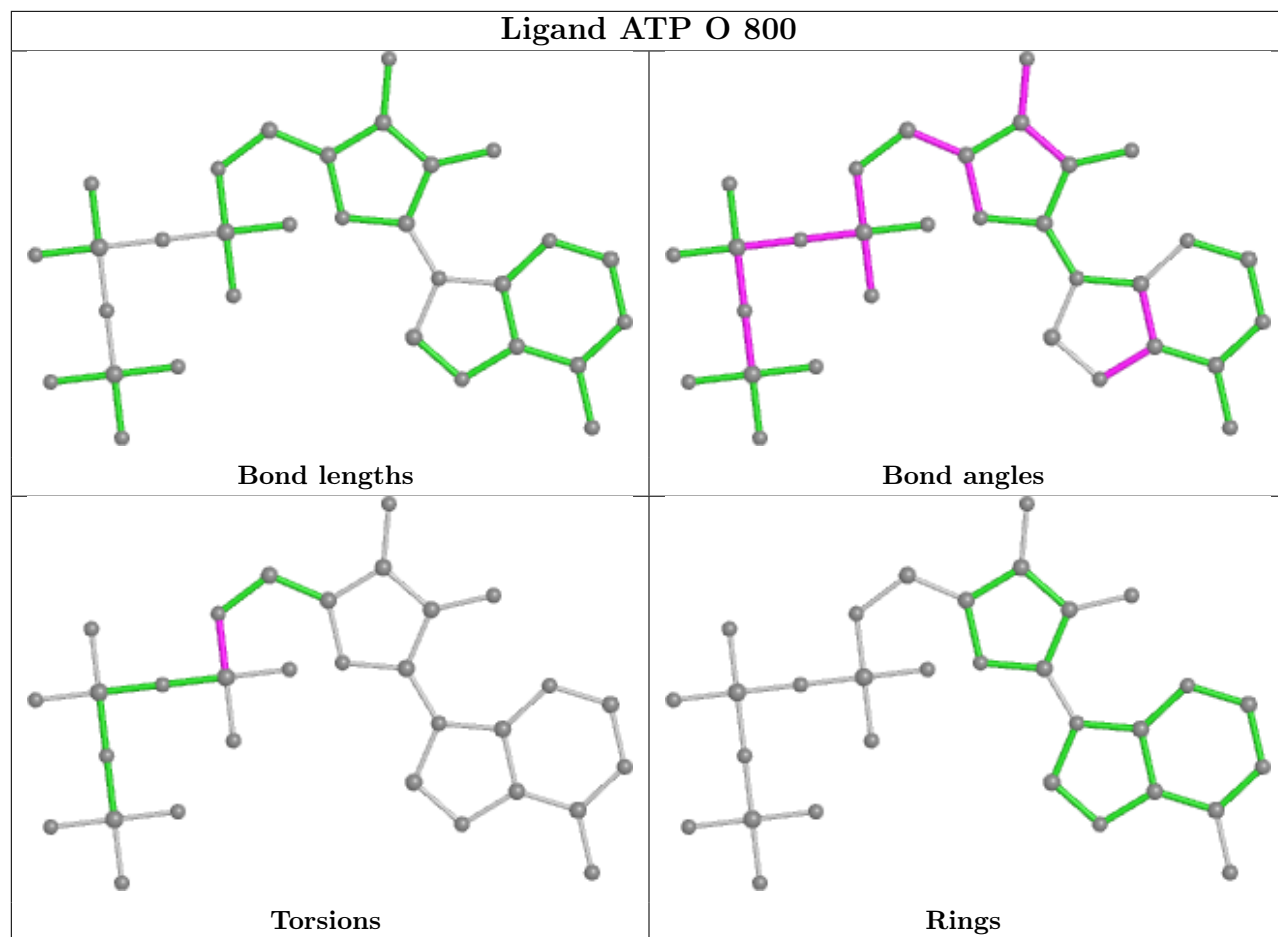


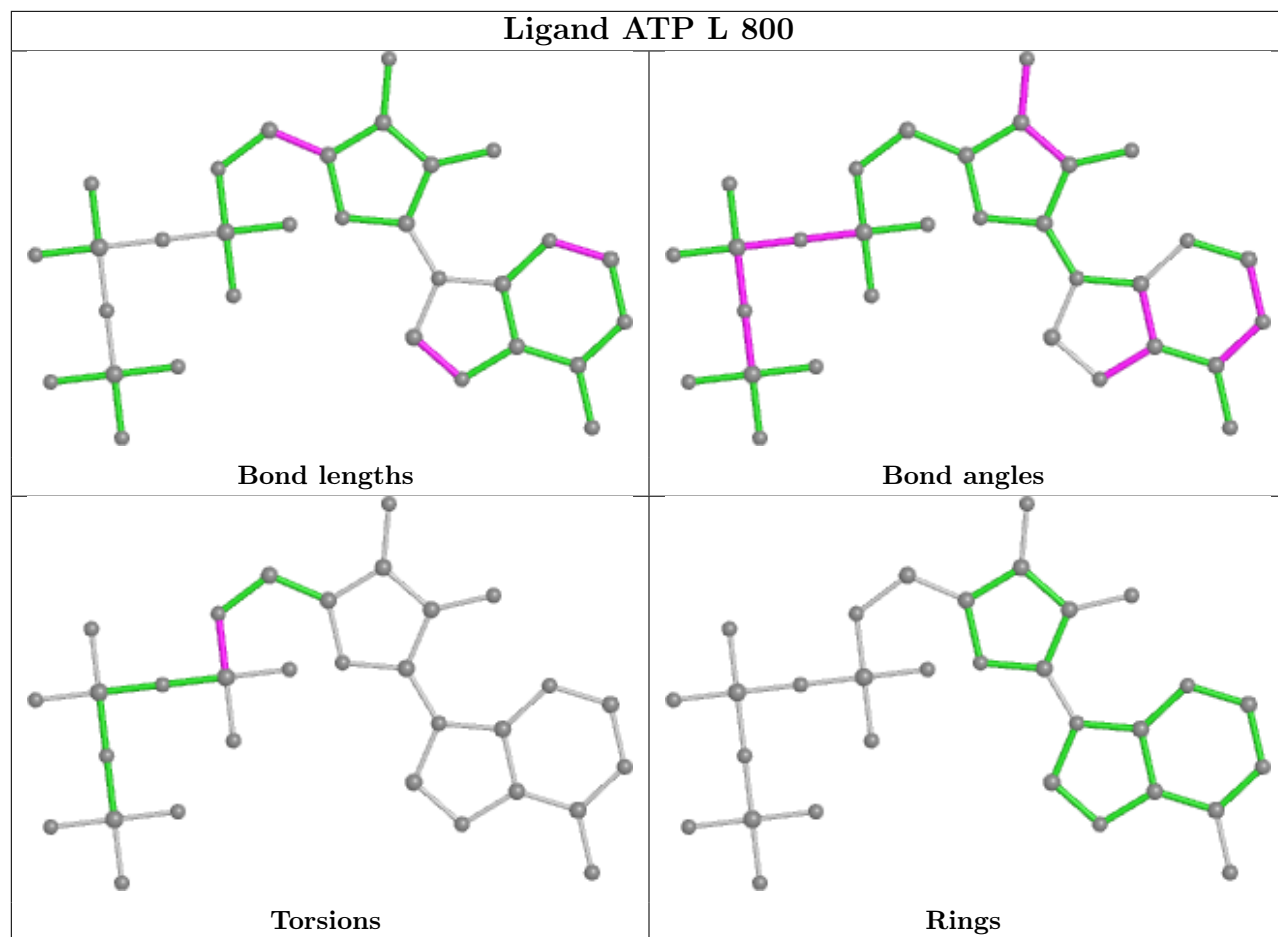


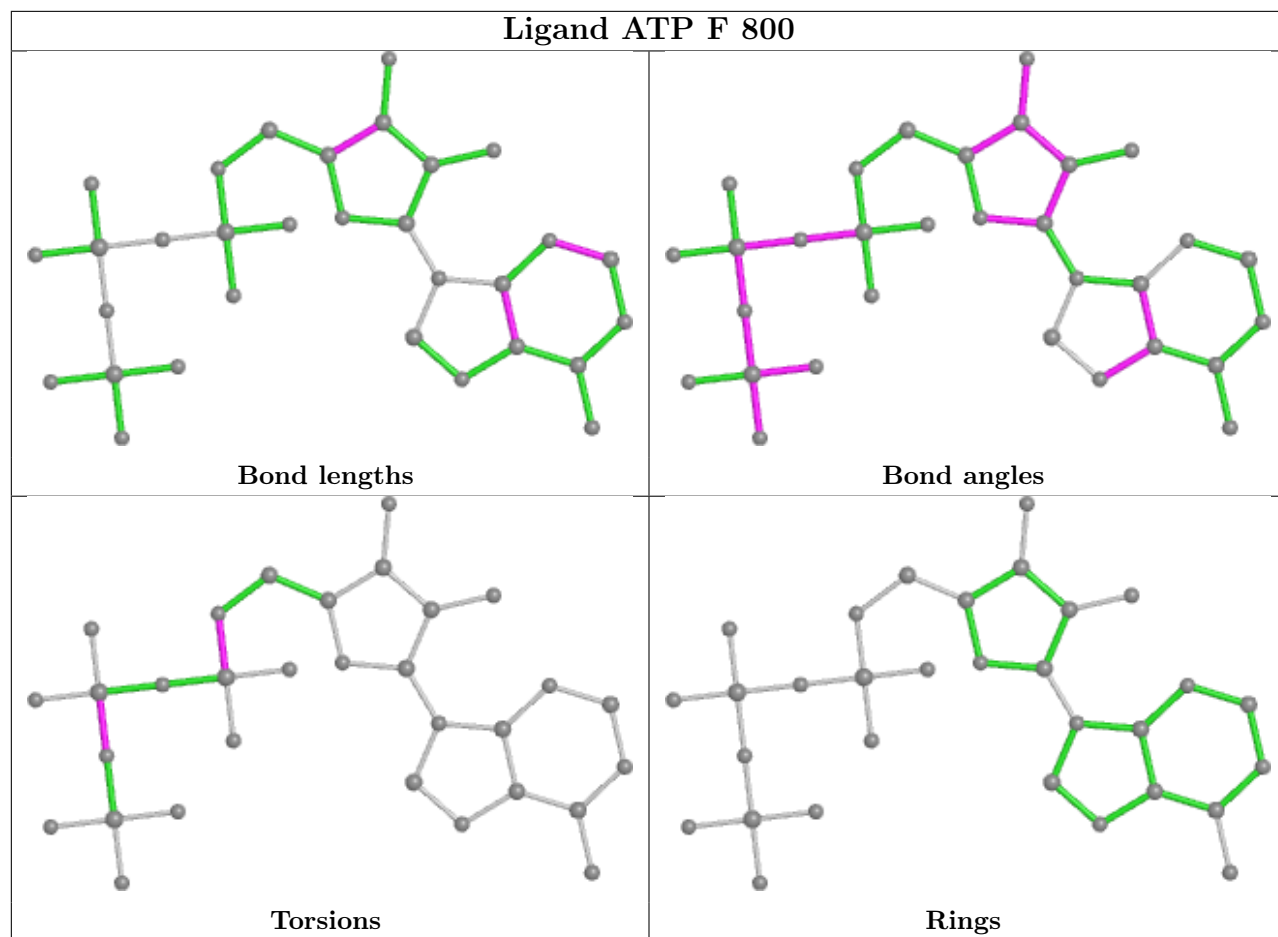


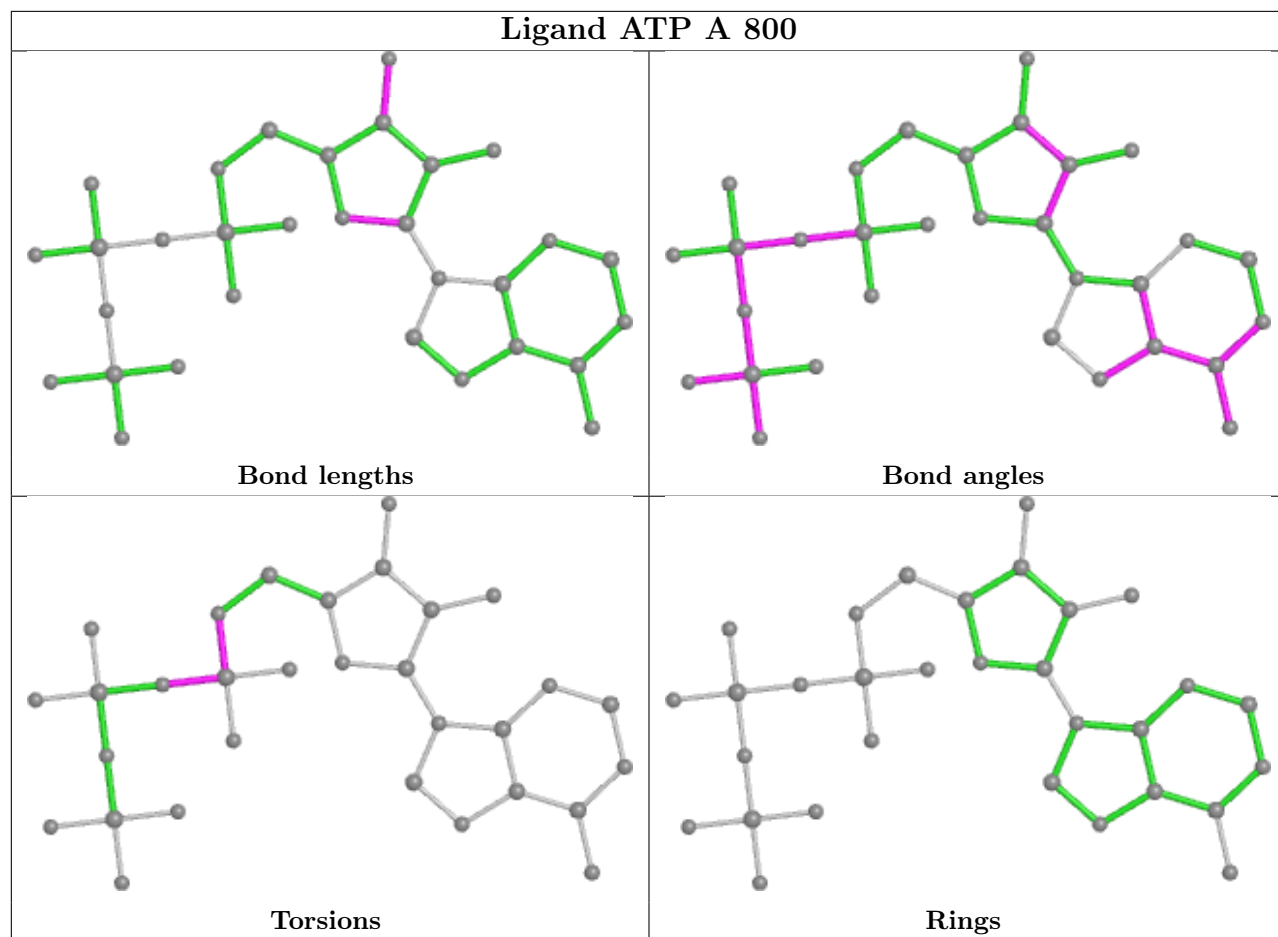


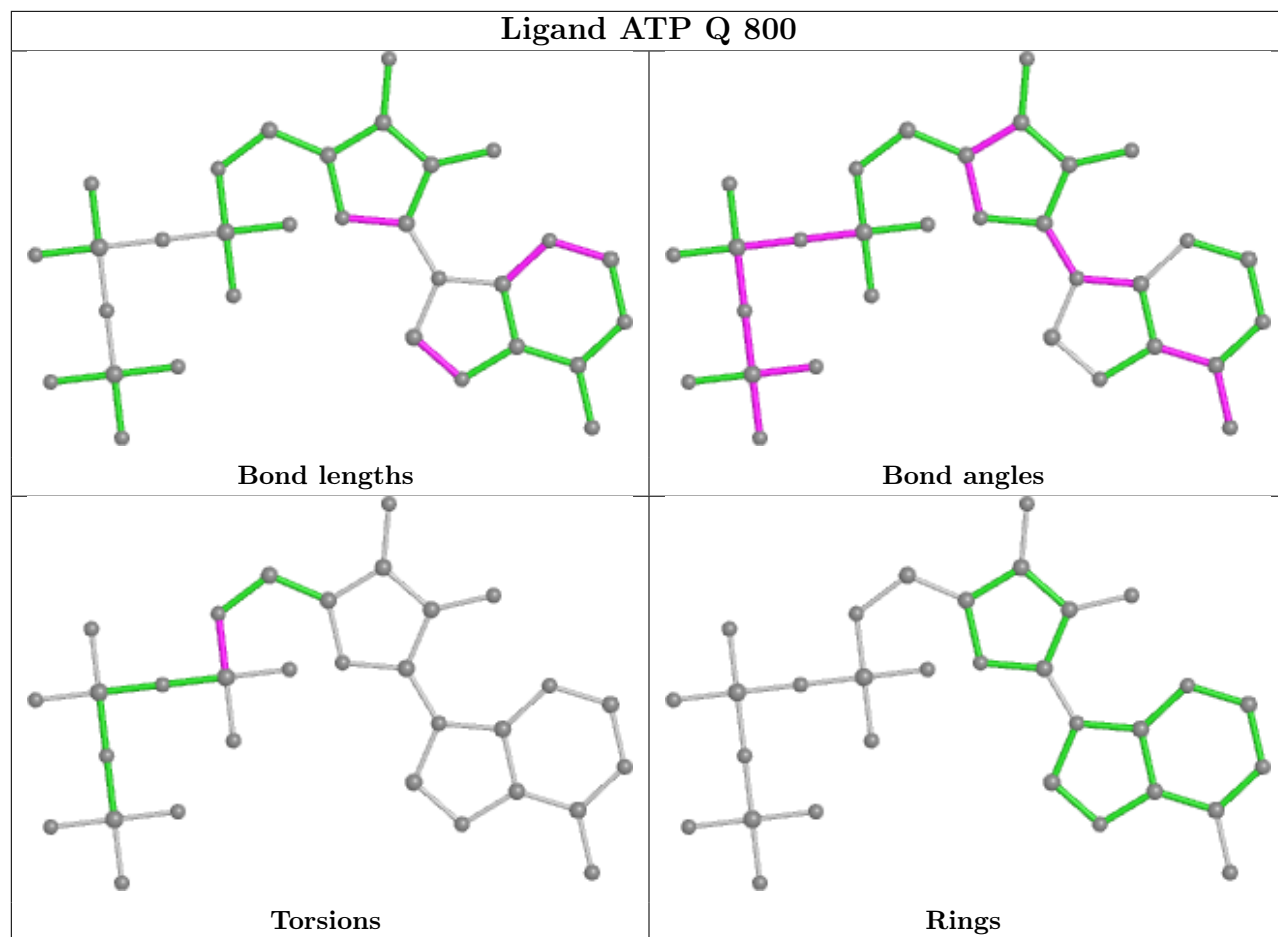


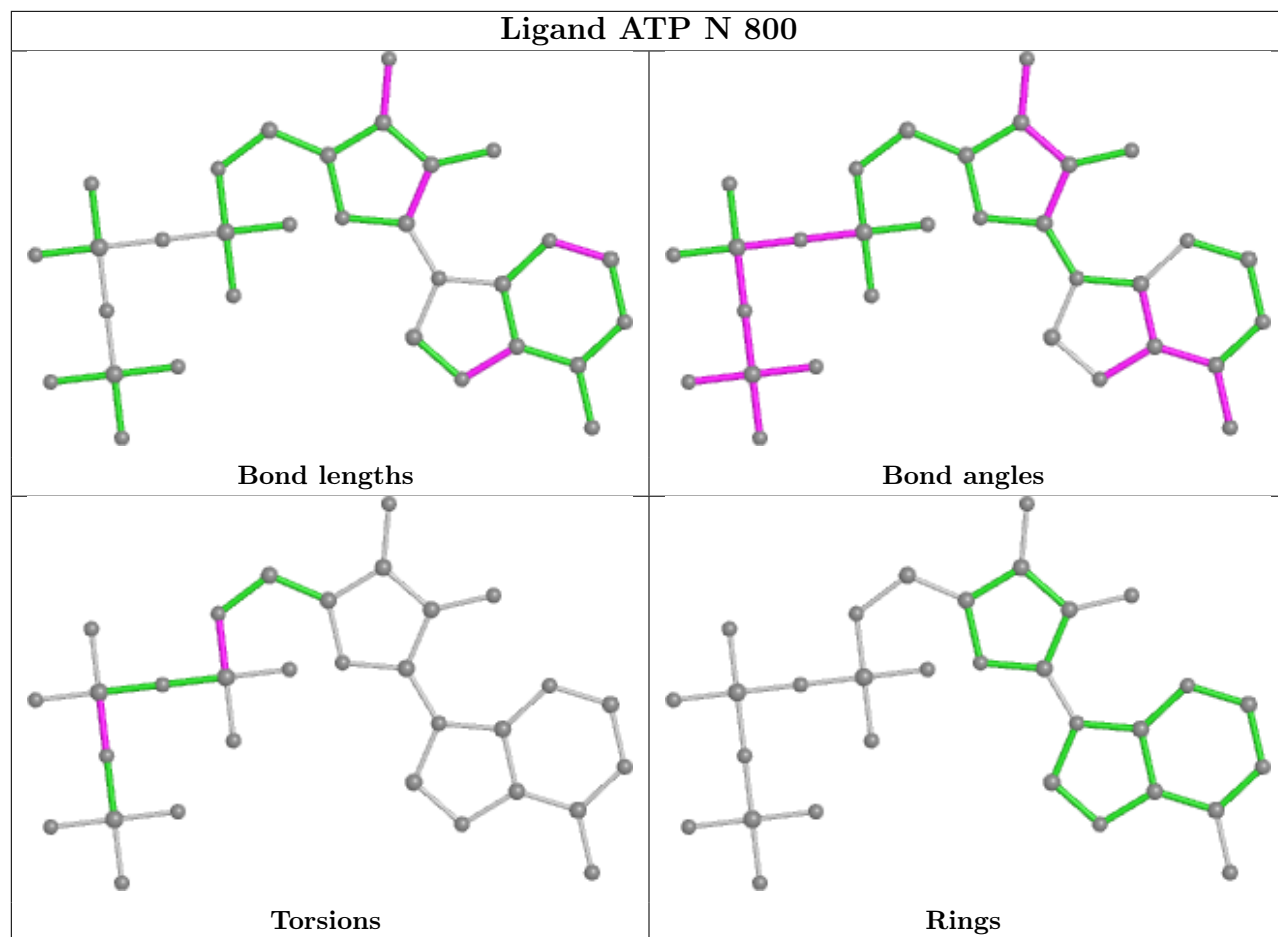


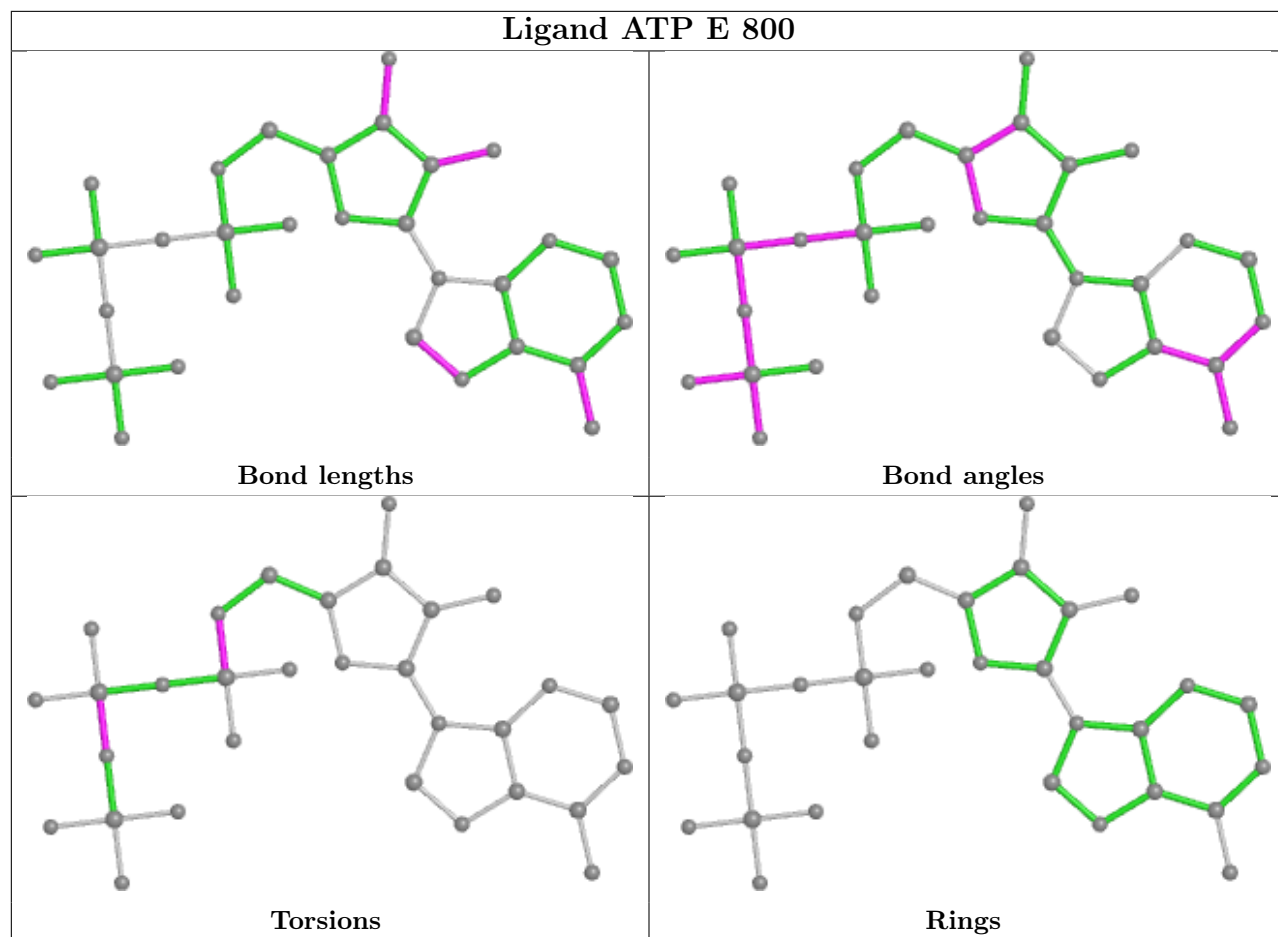


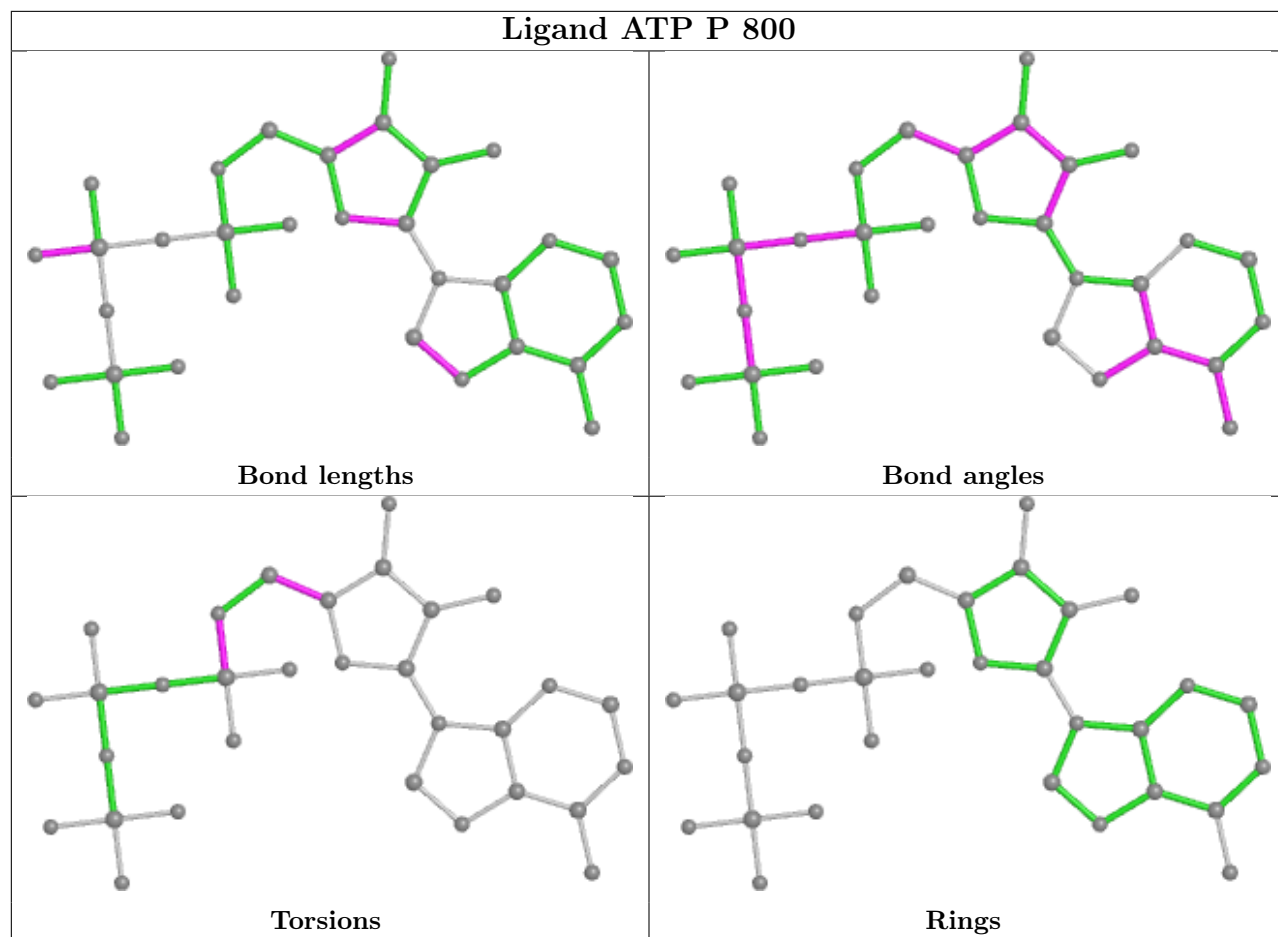


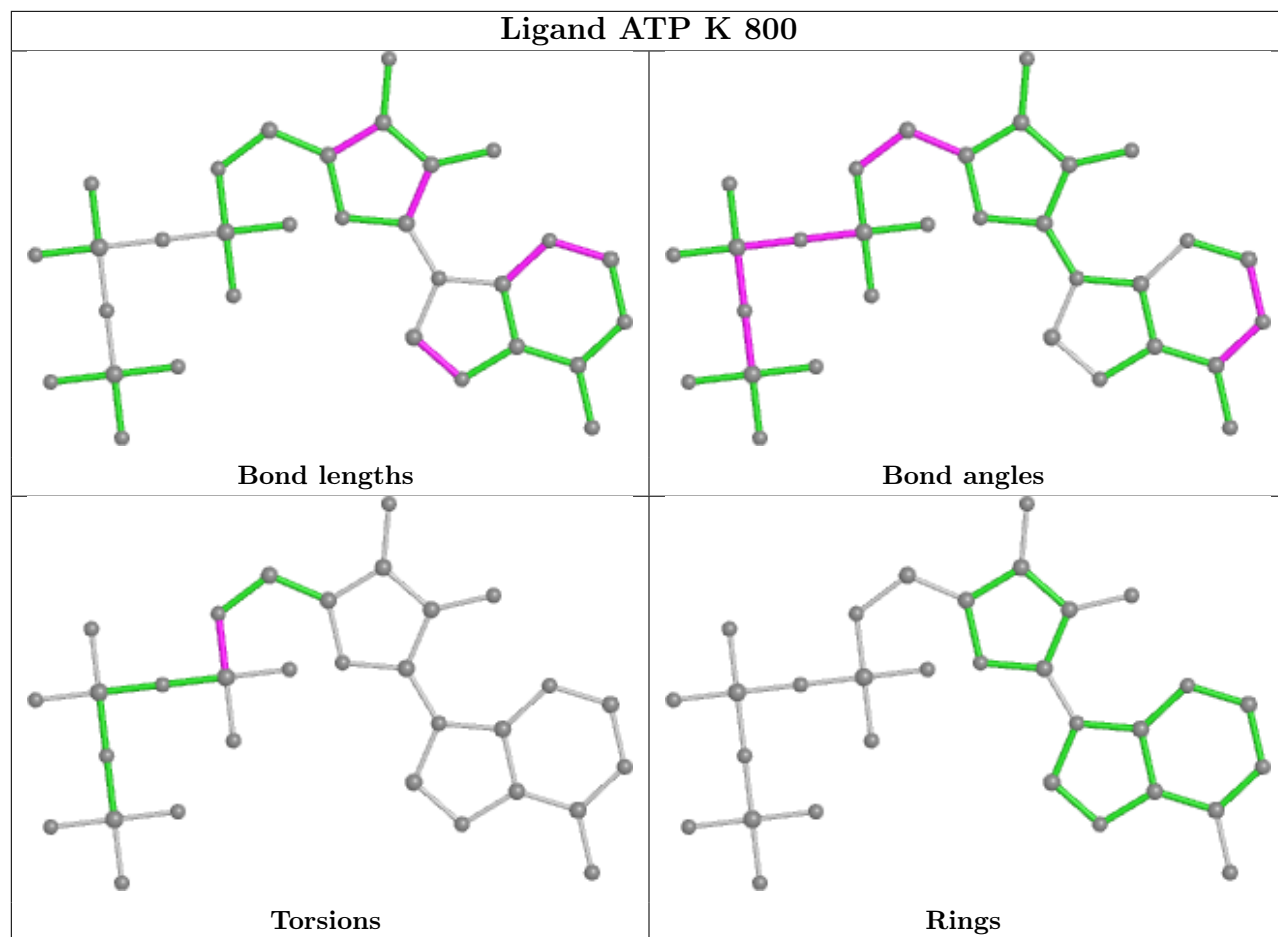


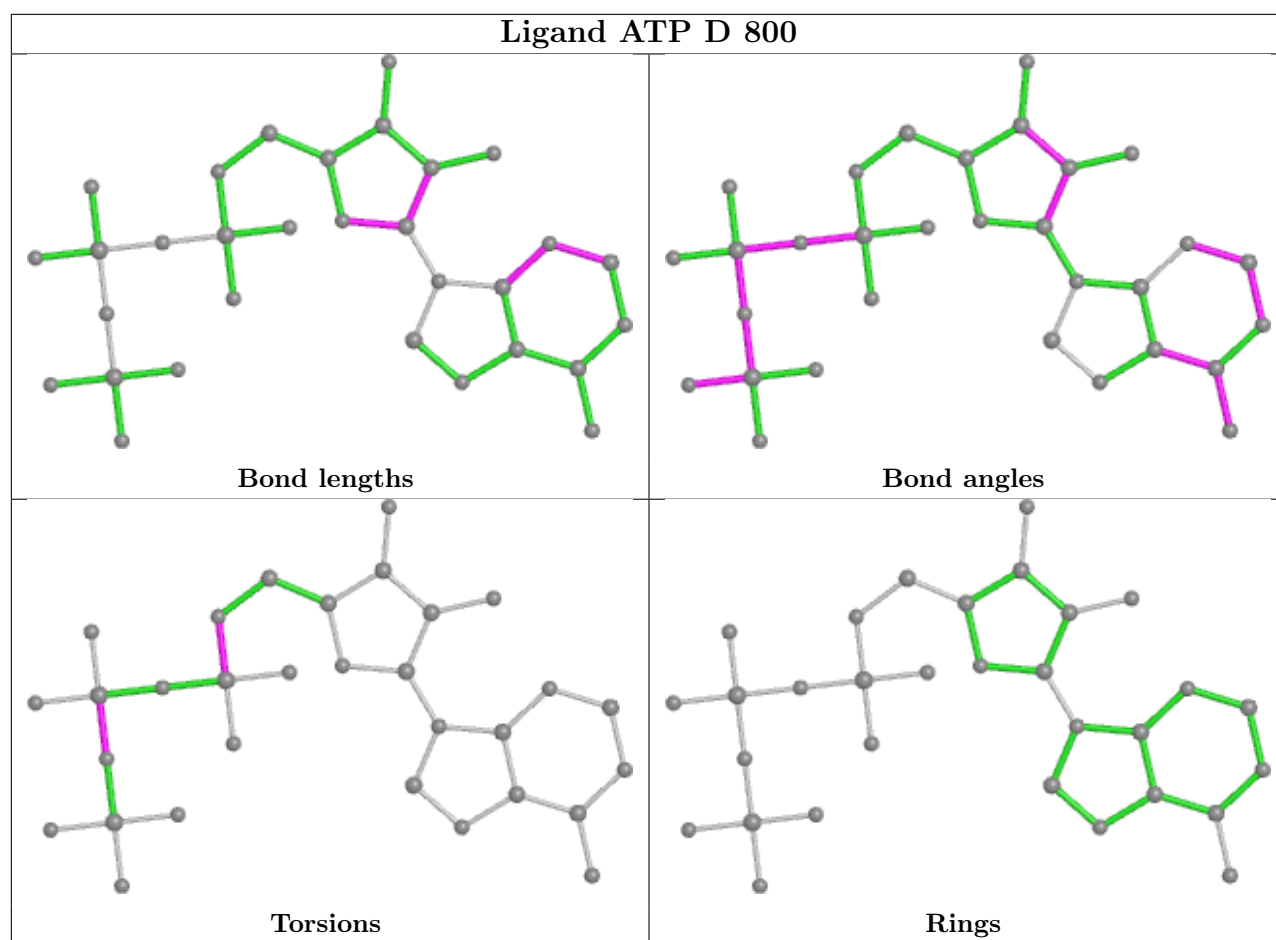












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

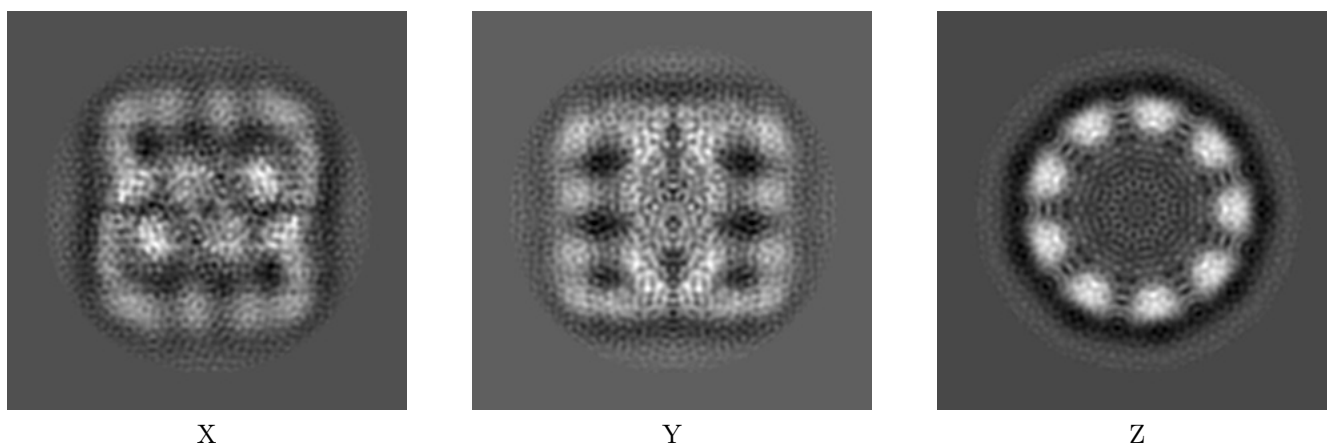
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5396. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

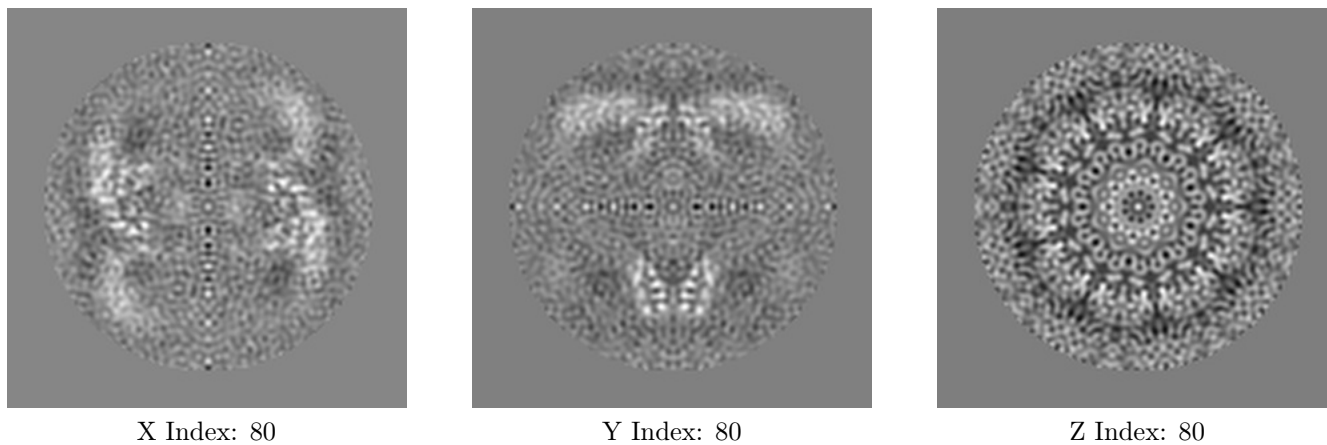
6.1.1 Primary map



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

6.2 Central slices [i](#)

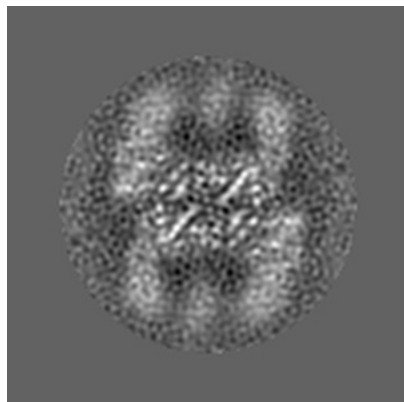
6.2.1 Primary map



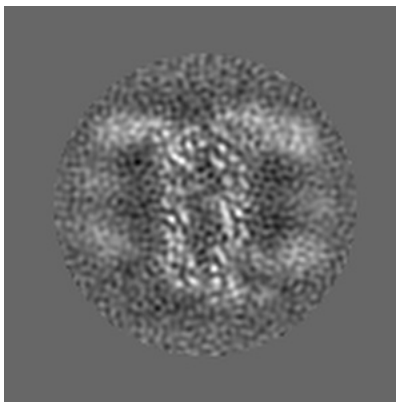
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

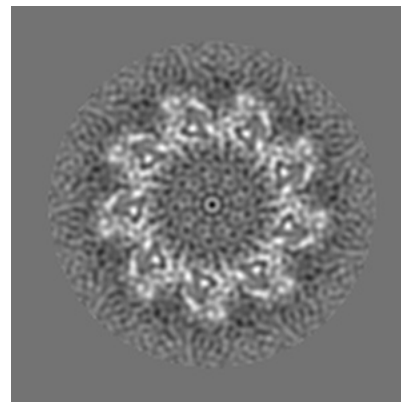
6.3.1 Primary map



X Index: 109



Y Index: 106

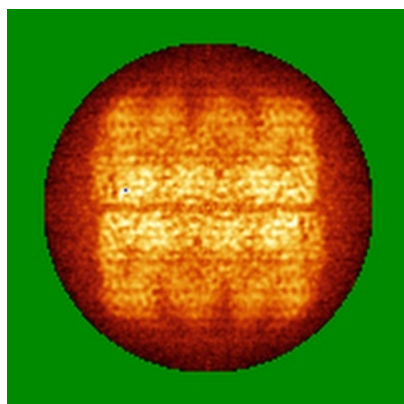


Z Index: 90

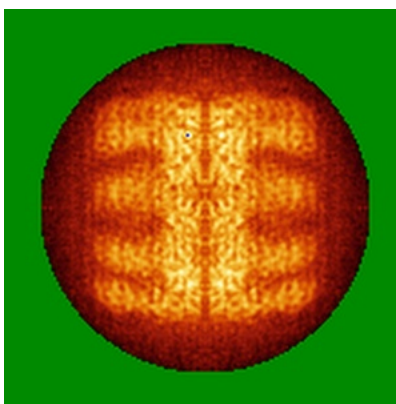
The images above show the largest variance slices of the map in three orthogonal directions.

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

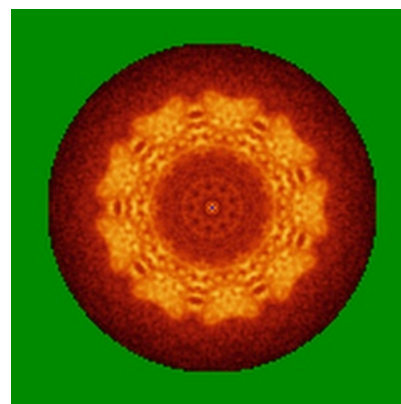
6.4.1 Primary map



X



Y

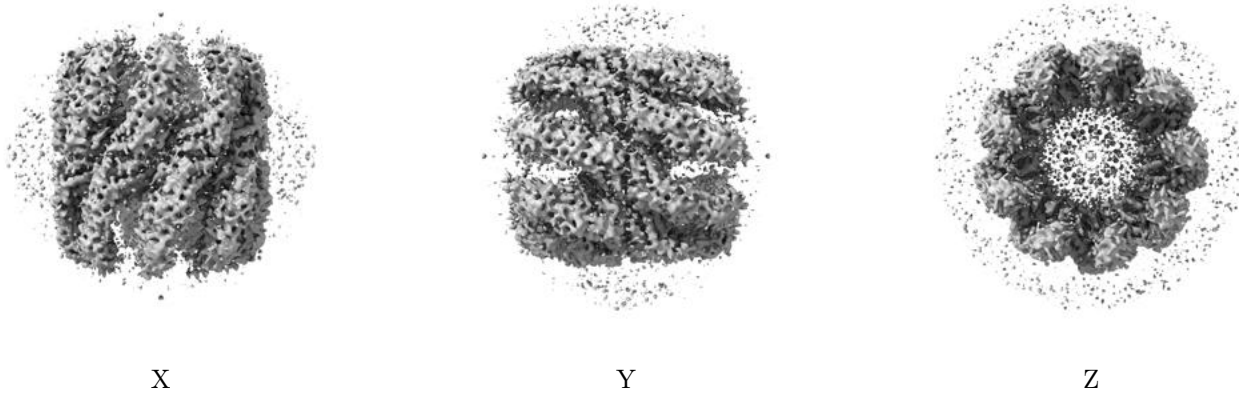


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

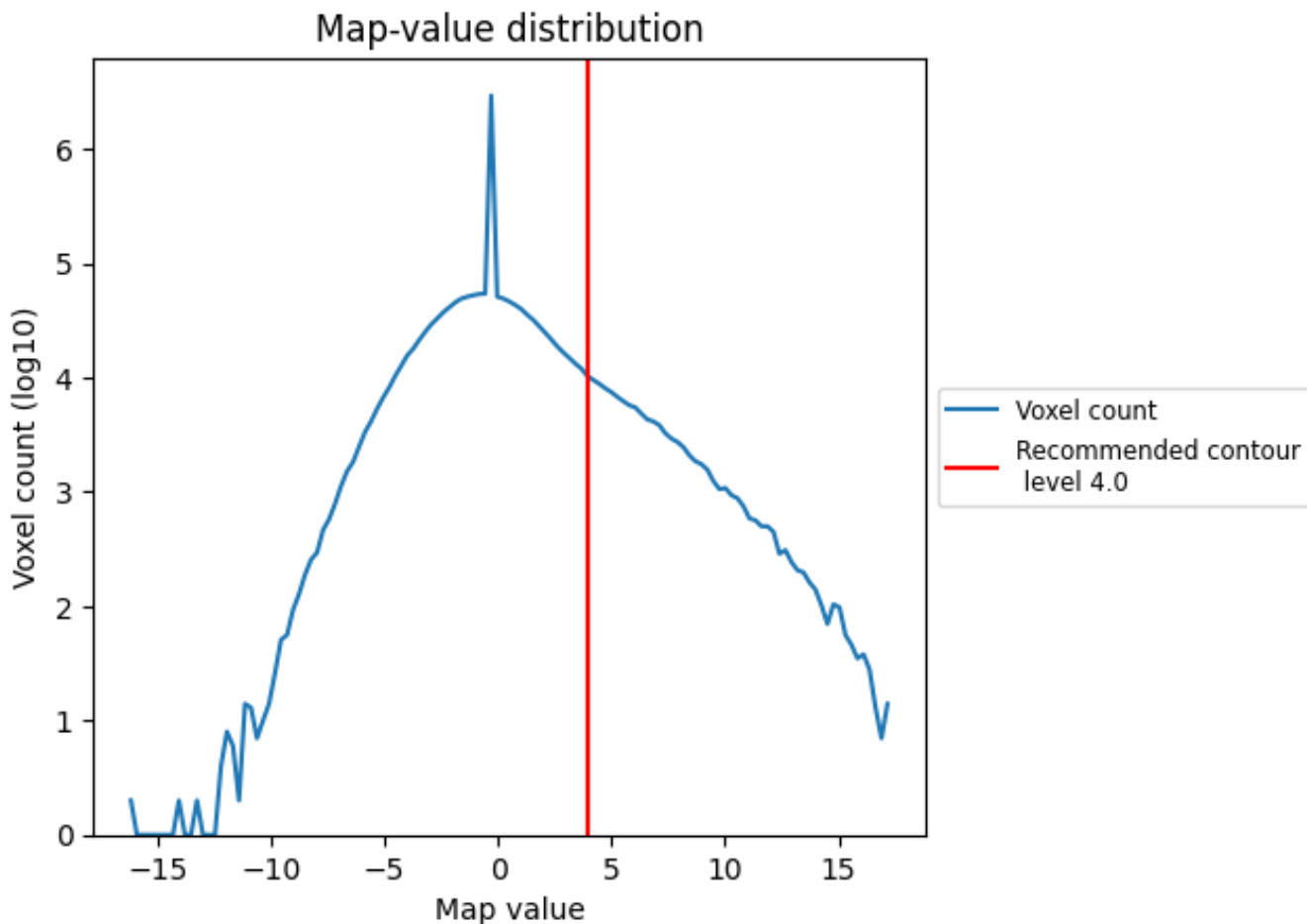
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

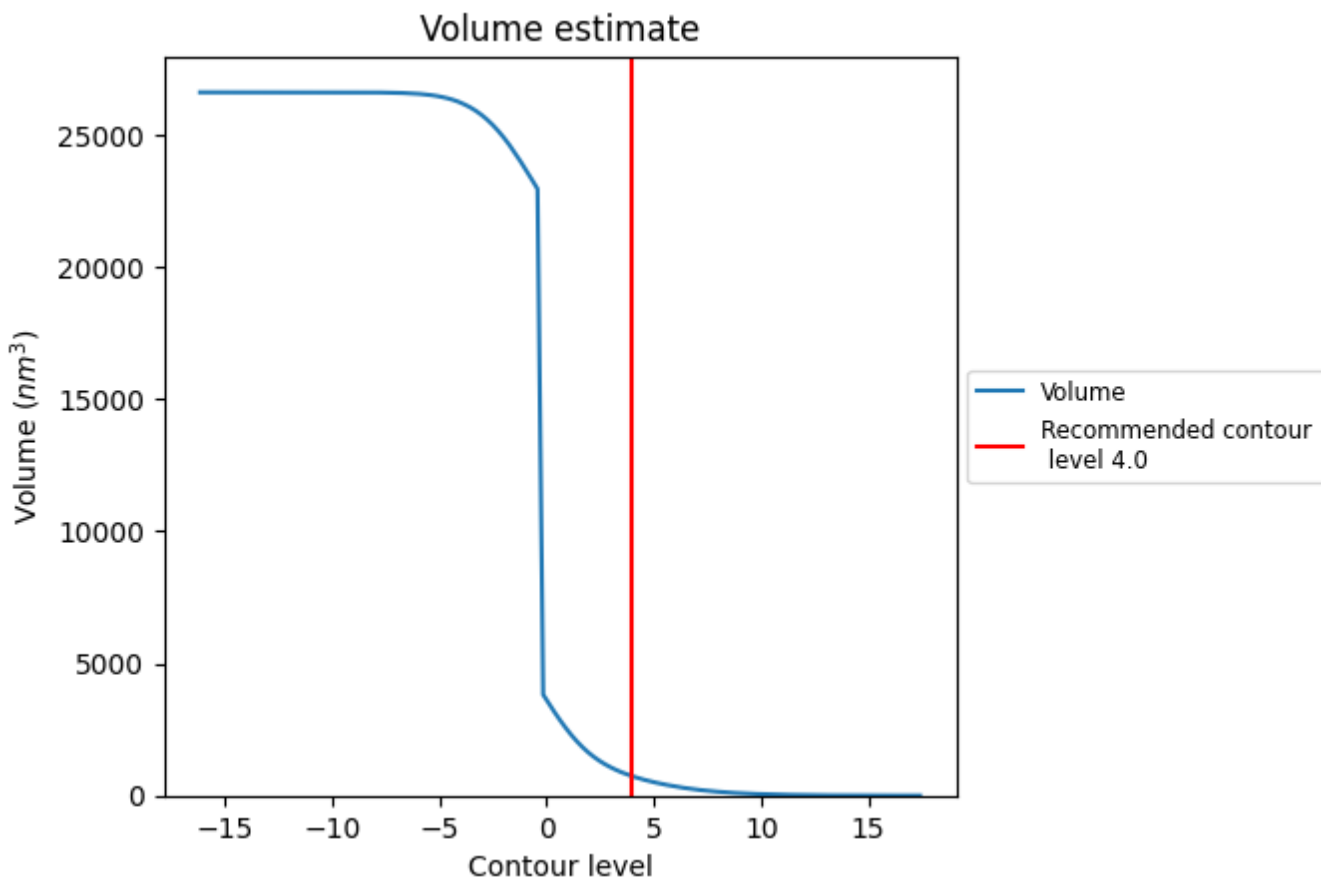
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

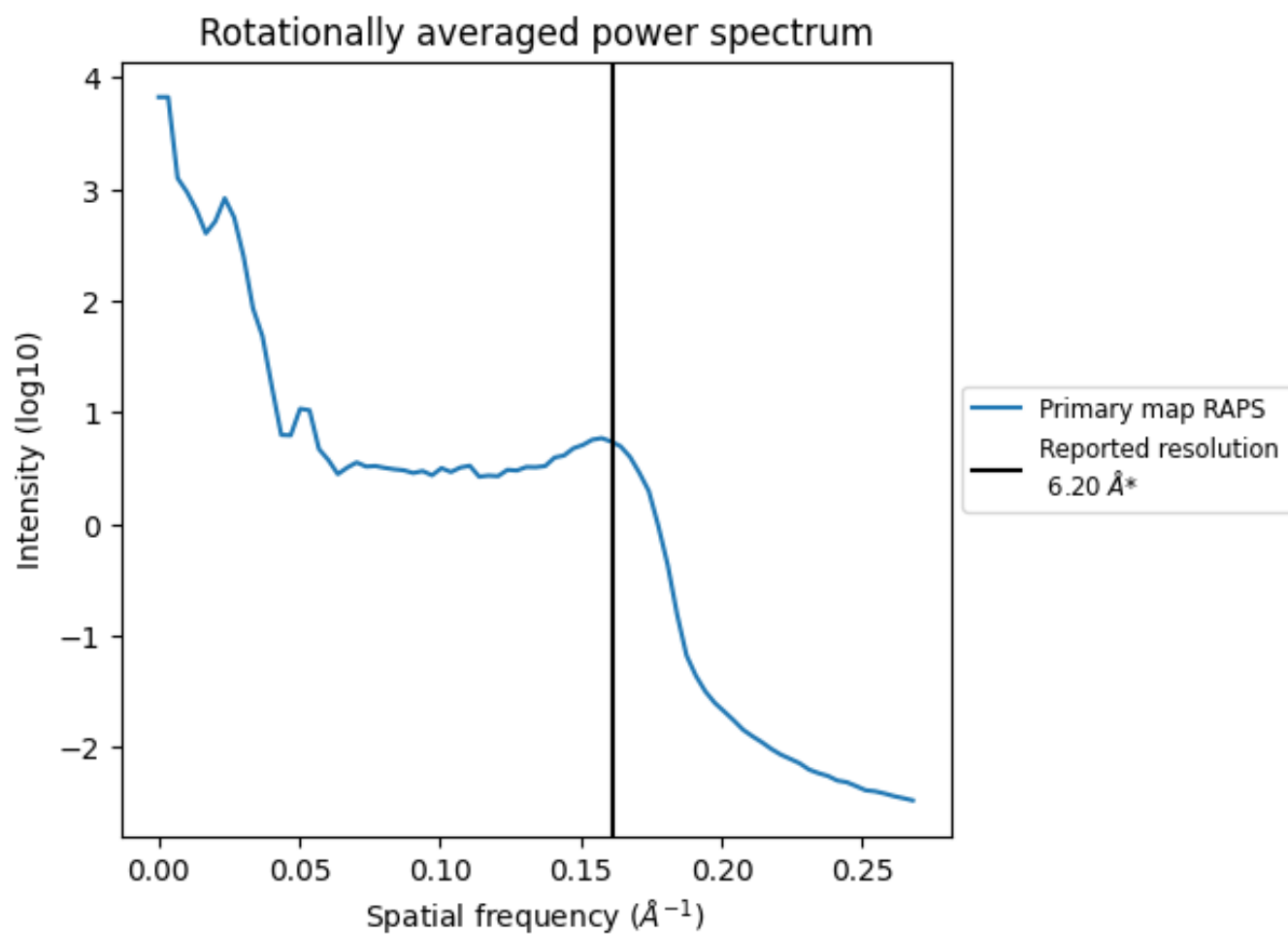
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 731 nm^3 ; this corresponds to an approximate mass of 660 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.161\AA^{-1}

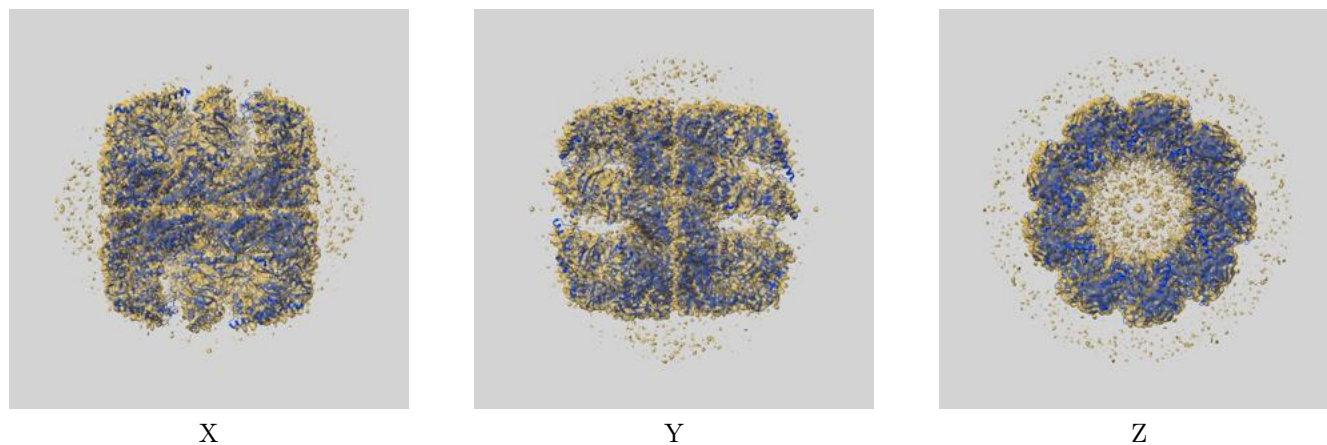
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

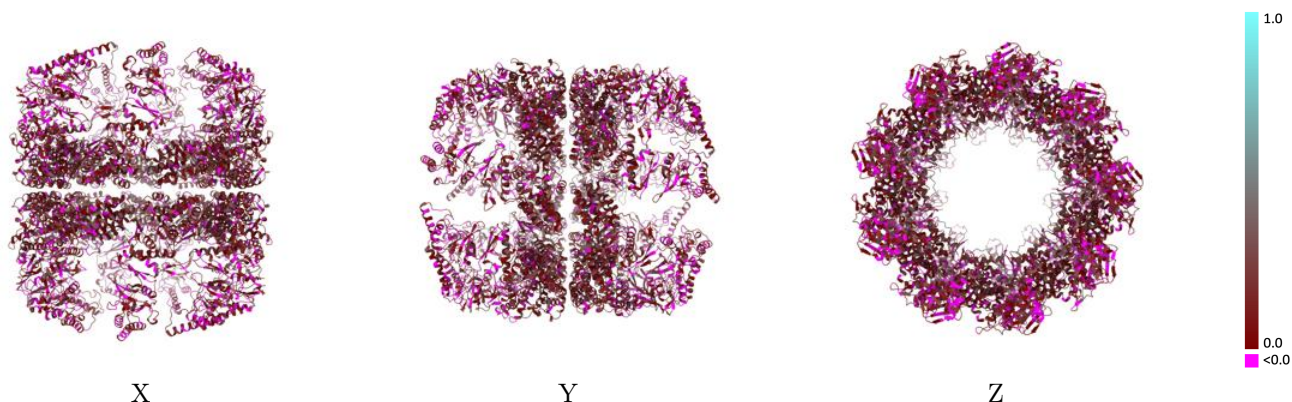
This section contains information regarding the fit between EMDB map EMD-5396 and PDB model 3J1F. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



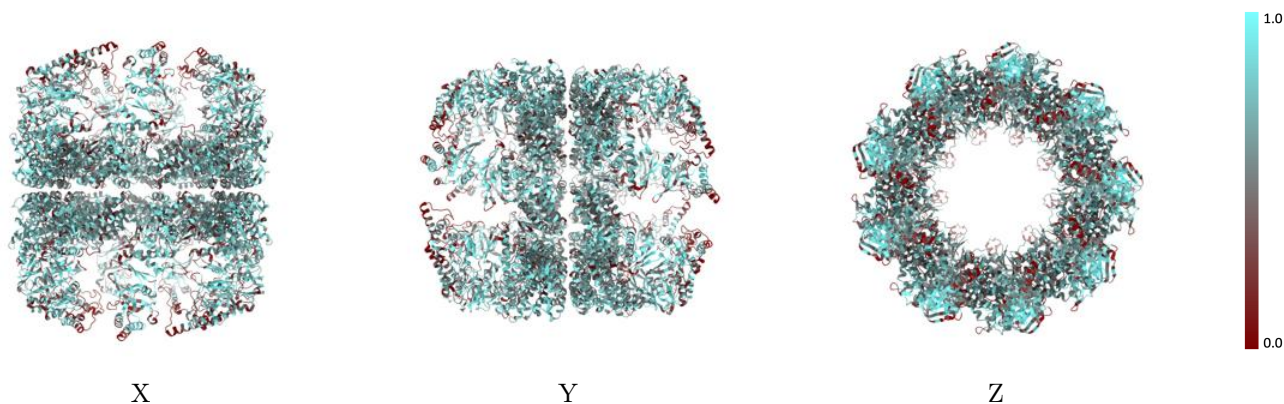
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



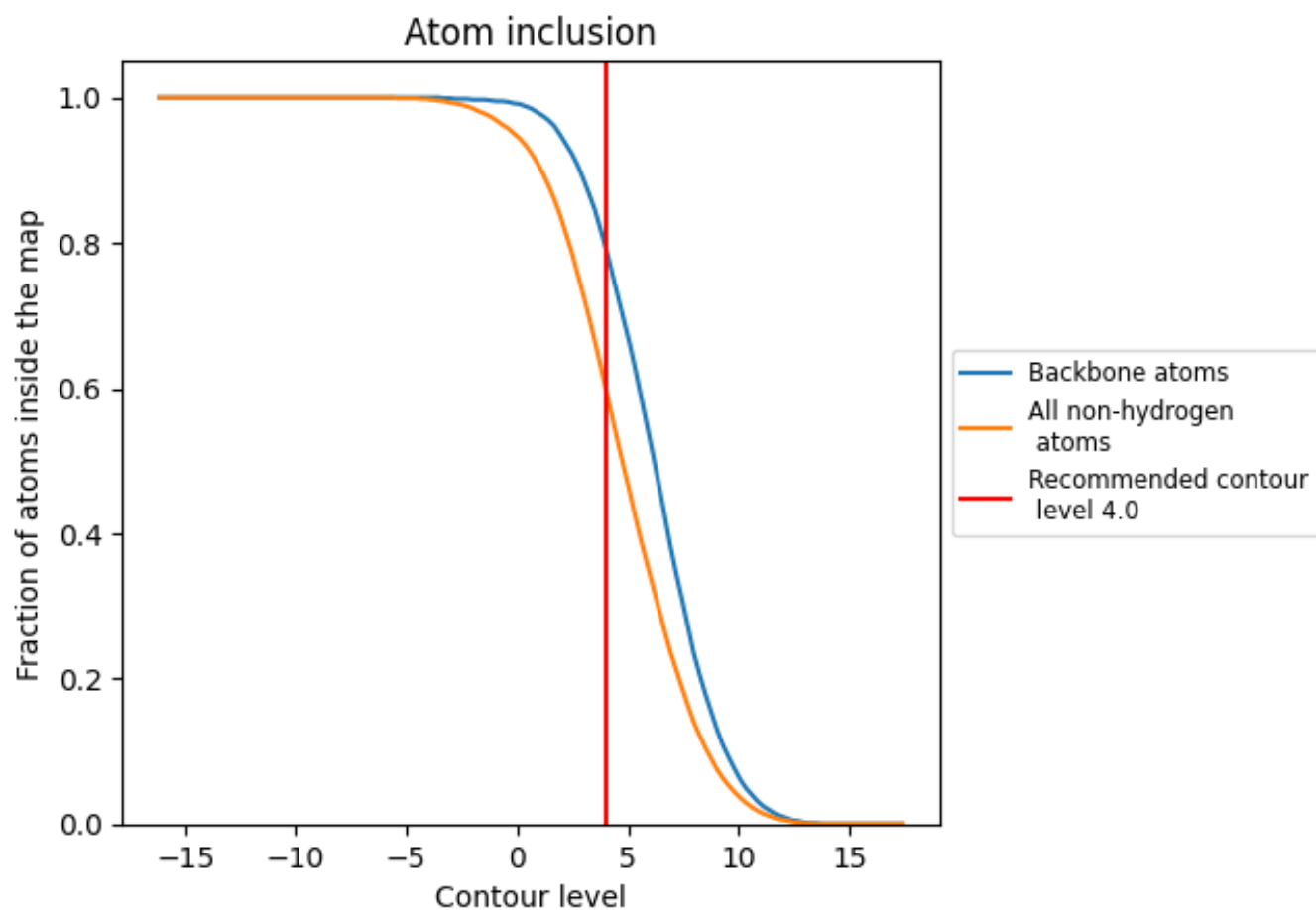
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.0).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6000	 0.1410
A	 0.6040	 0.1420
B	 0.5990	 0.1430
C	 0.6020	 0.1430
D	 0.6020	 0.1410
E	 0.6000	 0.1380
F	 0.6000	 0.1350
G	 0.6010	 0.1390
H	 0.5990	 0.1410
I	 0.6030	 0.1410
K	 0.5990	 0.1410
L	 0.6010	 0.1420
M	 0.6030	 0.1400
N	 0.6020	 0.1450
O	 0.5970	 0.1400
P	 0.5950	 0.1410
Q	 0.5990	 0.1410
R	 0.5990	 0.1450
S	 0.6000	 0.1420

