



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 02:21 AM EST

PDB ID : 3J9U
EMDB ID : EMD-6285
Title : Yeast V-ATPase state 2
Authors : Zhao, J.; Benlekbir, S.; Rubinstein, J.L.
Deposited on : 2015-02-23
Resolution : 7.60 Å(reported)
Based on initial models : 4RND, 1HO8, 1U7L, 4DL0

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.dev43
MolProbity : 4.02b-467
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) : 2.31.3

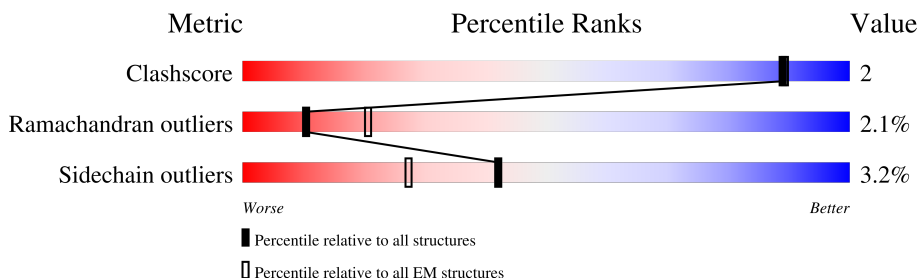
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.60 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	M	256	
2	N	118	
3	A	616	
3	C	616	
3	E	616	
4	B	517	
4	D	517	
4	F	517	

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Mol	Chain	Length	Quality of chain
5	Q	345	
6	H	114	
6	J	114	
6	L	114	
7	G	233	
7	I	233	
7	K	233	
8	P	478	
9	b	840	
10	O	392	
11	R	160	
11	S	160	
11	T	160	
11	U	160	
11	V	160	
11	W	160	
11	X	160	
11	Y	160	
11	Z	160	
11	a	160	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 57659 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 V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	210	Total	C	N	O	S	0	0
			1691	1061	305	321	4		

- Molecule 2 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	N	115	Total	C	N	O	0	0
			928	589	157	182		

- Molecule 3 is a protein called V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	593	Total	C	N	O	S	0	0
			4578	2904	760	894	20		
3	E	593	Total	C	N	O	S	0	0
			4578	2904	760	894	20		
3	A	593	Total	C	N	O	S	0	0
			4578	2904	760	894	20		

- Molecule 4 is a protein called V-type proton ATPase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	457	Total	C	N	O	S	0	0
			3585	2266	612	695	12		
4	F	457	Total	C	N	O	S	0	0
			3585	2266	612	695	12		
4	B	457	Total	C	N	O	S	0	0
			3585	2266	612	695	12		

- Molecule 5 is a protein called V-type proton ATPase subunit d.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	345	Total	C	N	O	S	0	0
			2802	1779	454	555	14		

- Molecule 6 is a protein called V-type proton ATPase subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	105	Total	C	N	O		0	0
			824	517	144	163			
6	H	105	Total	C	N	O		0	0
			824	517	144	163			
6	J	105	Total	C	N	O		0	0
			824	517	144	163			

- Molecule 7 is a protein called V-type proton ATPase subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	217	Total	C	N	O	S	0	0
			1731	1083	296	347	5		
7	G	217	Total	C	N	O	S	0	0
			1731	1083	296	347	5		
7	I	217	Total	C	N	O	S	0	0
			1731	1083	296	347	5		

- Molecule 8 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	461	Total	C	N	O	S	0	0
			3712	2373	623	704	12		

- Molecule 9 is a protein called V-type proton ATPase subunit a, vacuolar isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	b	312	Total	C	N	O	S	0	0
			2540	1614	434	489	3		

- Molecule 10 is a protein called V-type proton ATPase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	392	Total	C	N	O	S	0	0
			3122	2005	516	596	5		

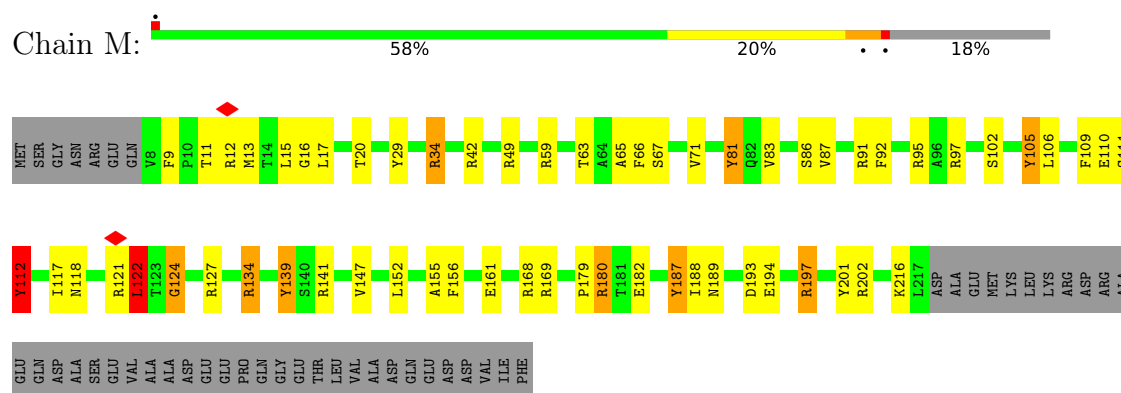
- Molecule 11 is a protein called V-type proton ATPase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	U	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	X	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	a	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	R	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	Z	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	S	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	Y	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	T	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	V	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	W	150	Total 1071	C 704	N 173	O 187	S 7	0	0

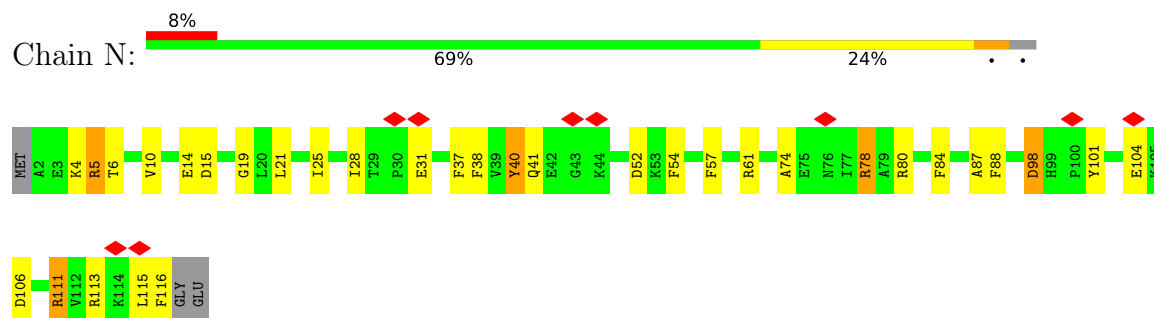
3 Residue-property plots

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.

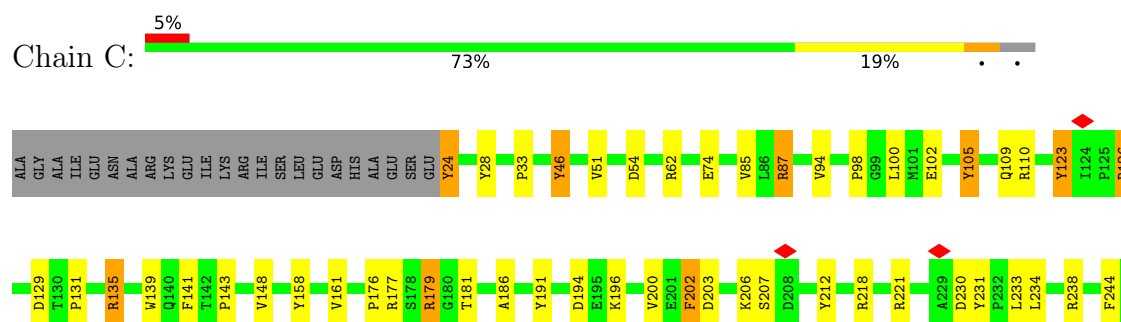
• Molecule 1: V-type proton ATPase subunit D

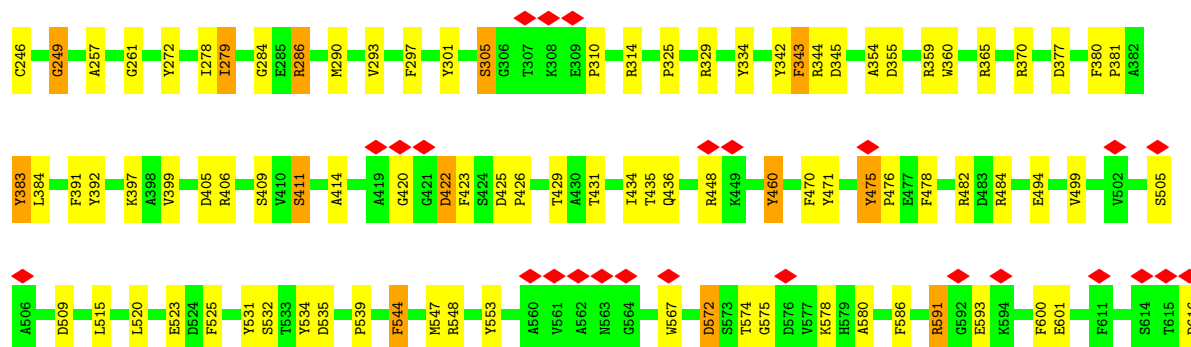


• Molecule 2: V-type proton ATPase subunit F



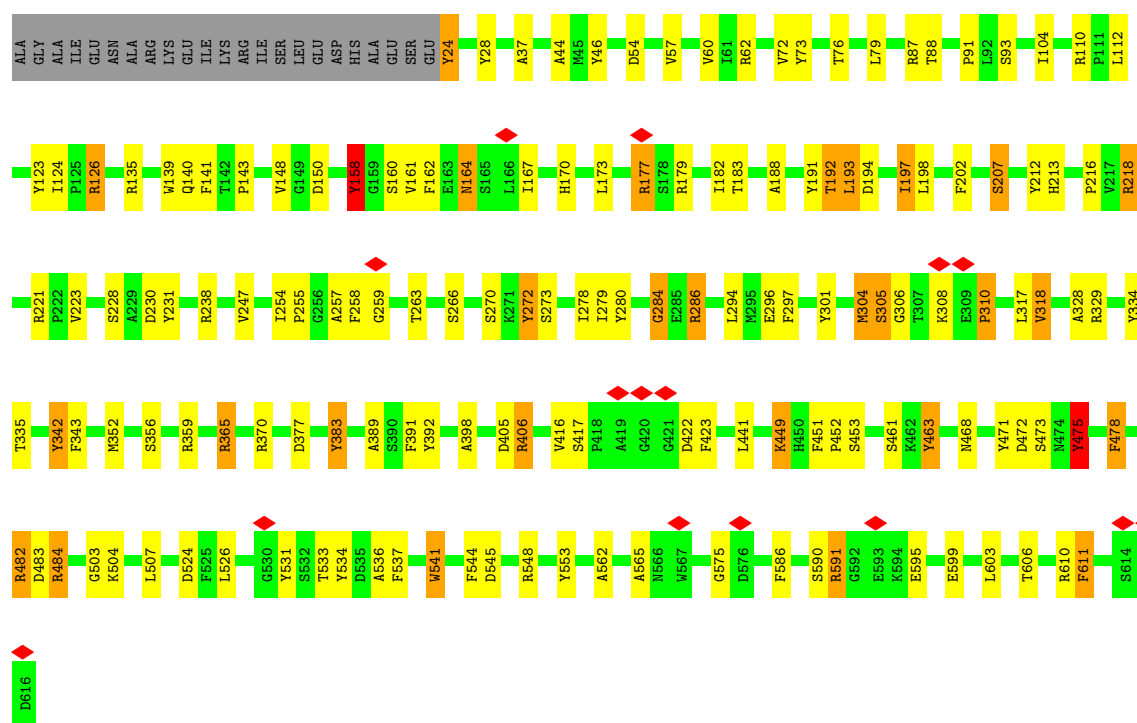
• Molecule 3: V-type proton ATPase catalytic subunit A





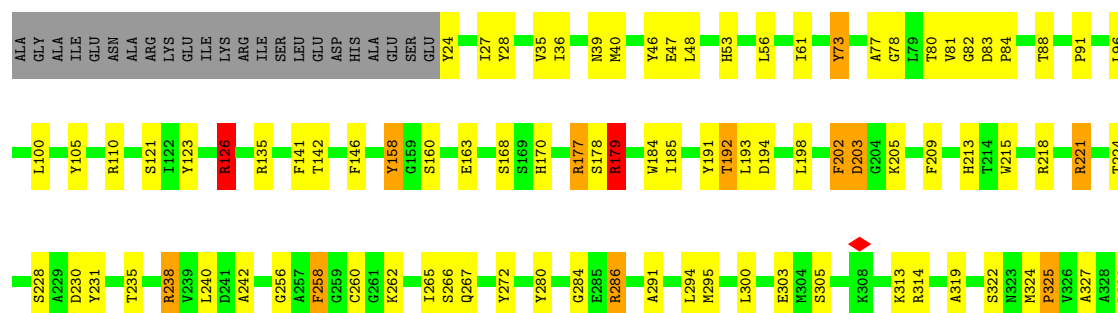
• Molecule 3: V-type proton ATPase catalytic subunit A

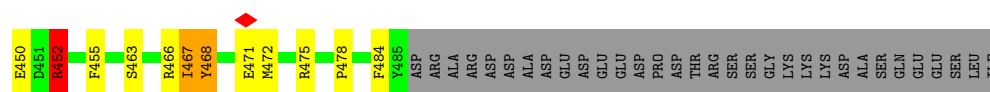
Chain E: 71% 20% 5% .



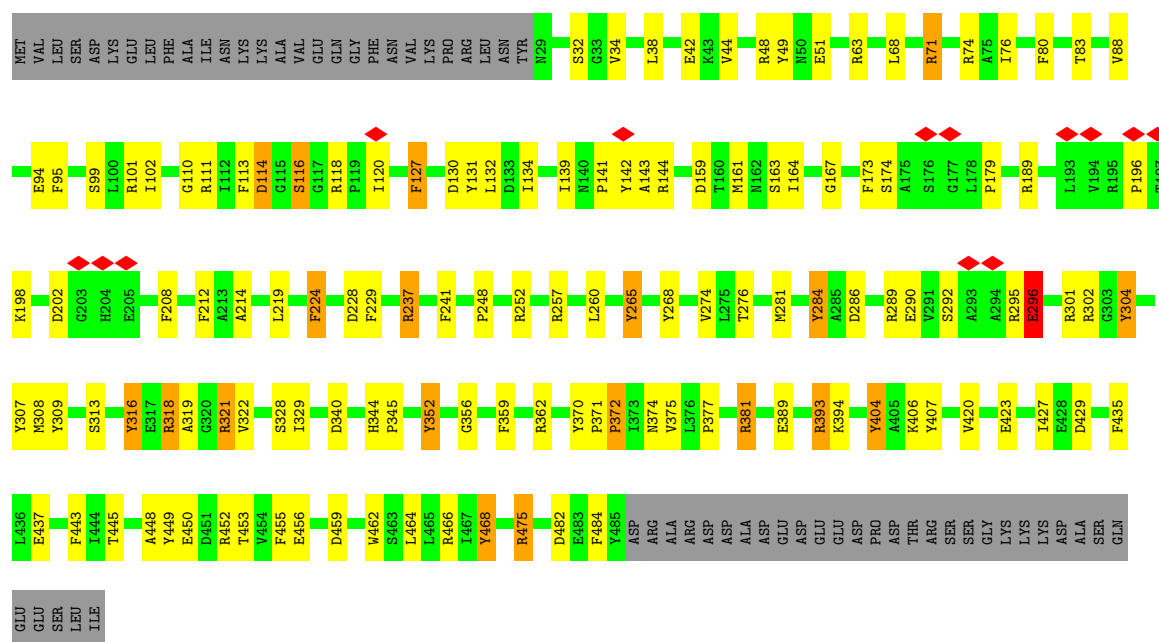
• Molecule 3: V-type proton ATPase catalytic subunit A

Chain A: 69% 23% . . .

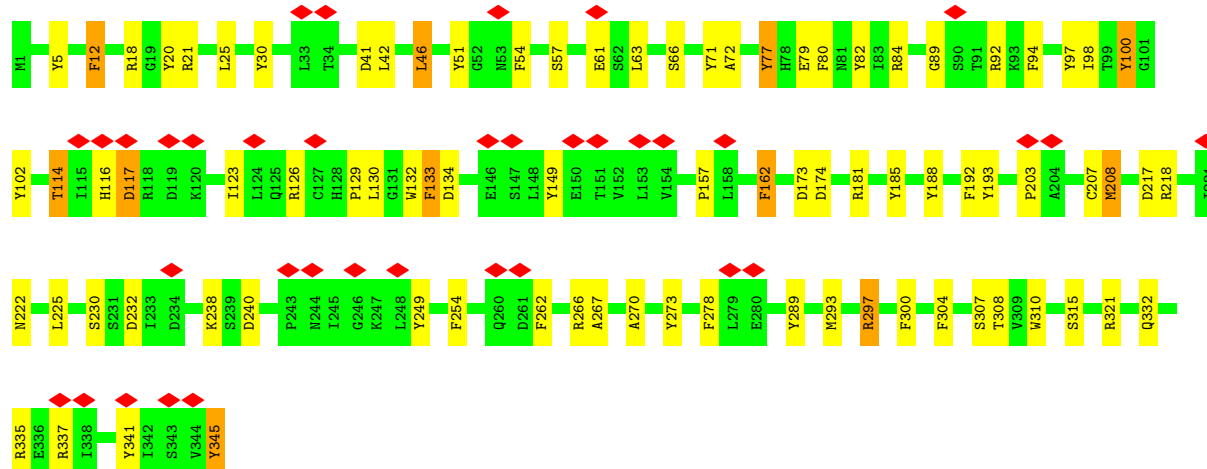
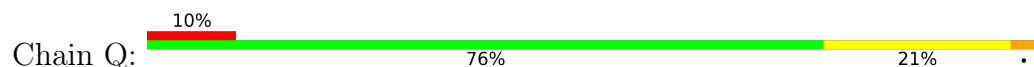




• Molecule 4: V-type proton ATPase subunit B

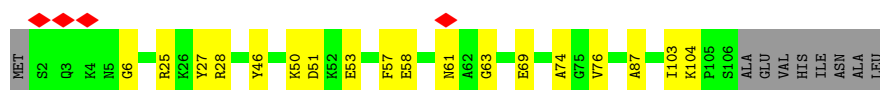


• Molecule 5: V-type proton ATPase subunit d

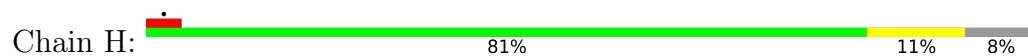


• Molecule 6: V-type proton ATPase subunit G

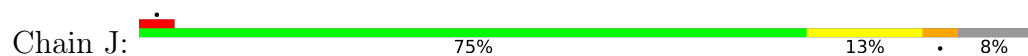




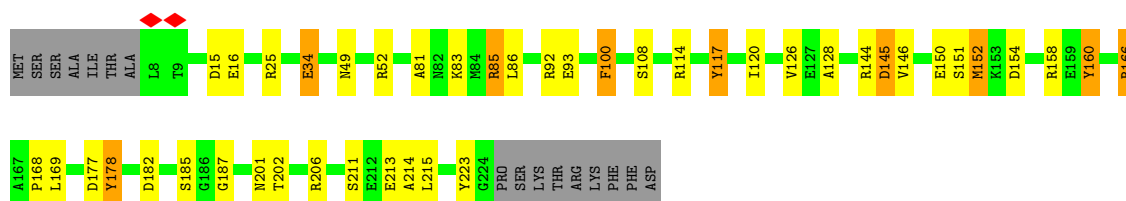
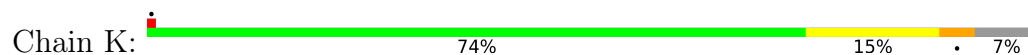
- Molecule 6: V-type proton ATPase subunit G



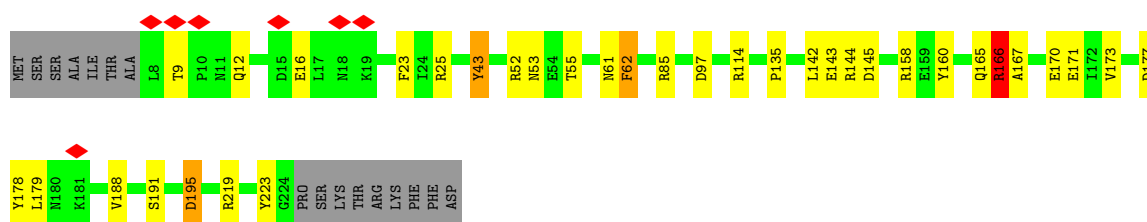
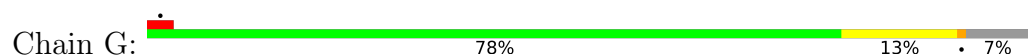
- Molecule 6: V-type proton ATPase subunit G



- Molecule 7: V-type proton ATPase subunit E



- Molecule 7: V-type proton ATPase subunit E

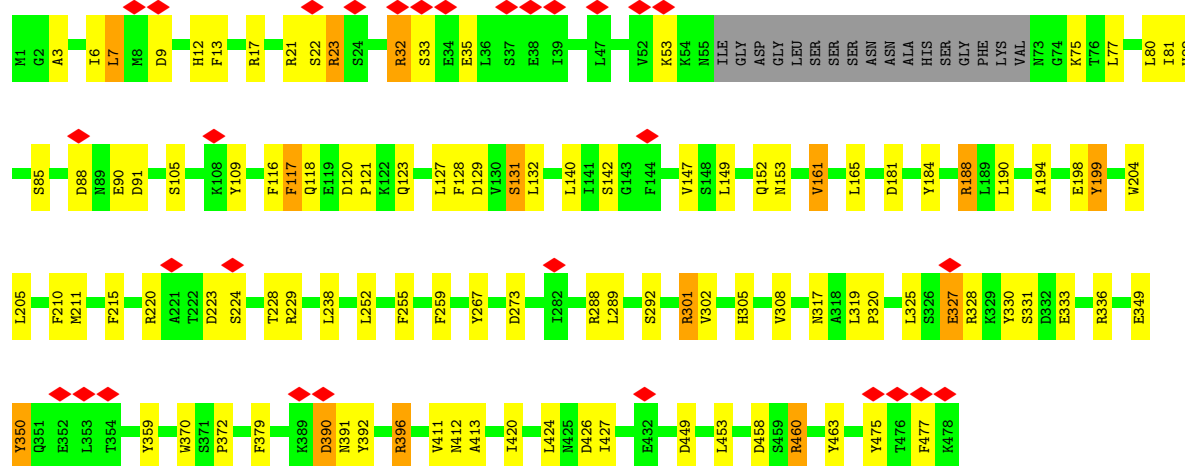
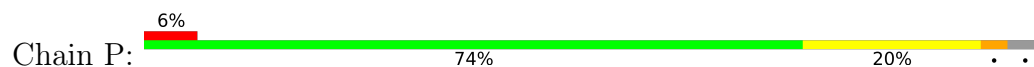


- Molecule 7: V-type proton ATPase subunit E

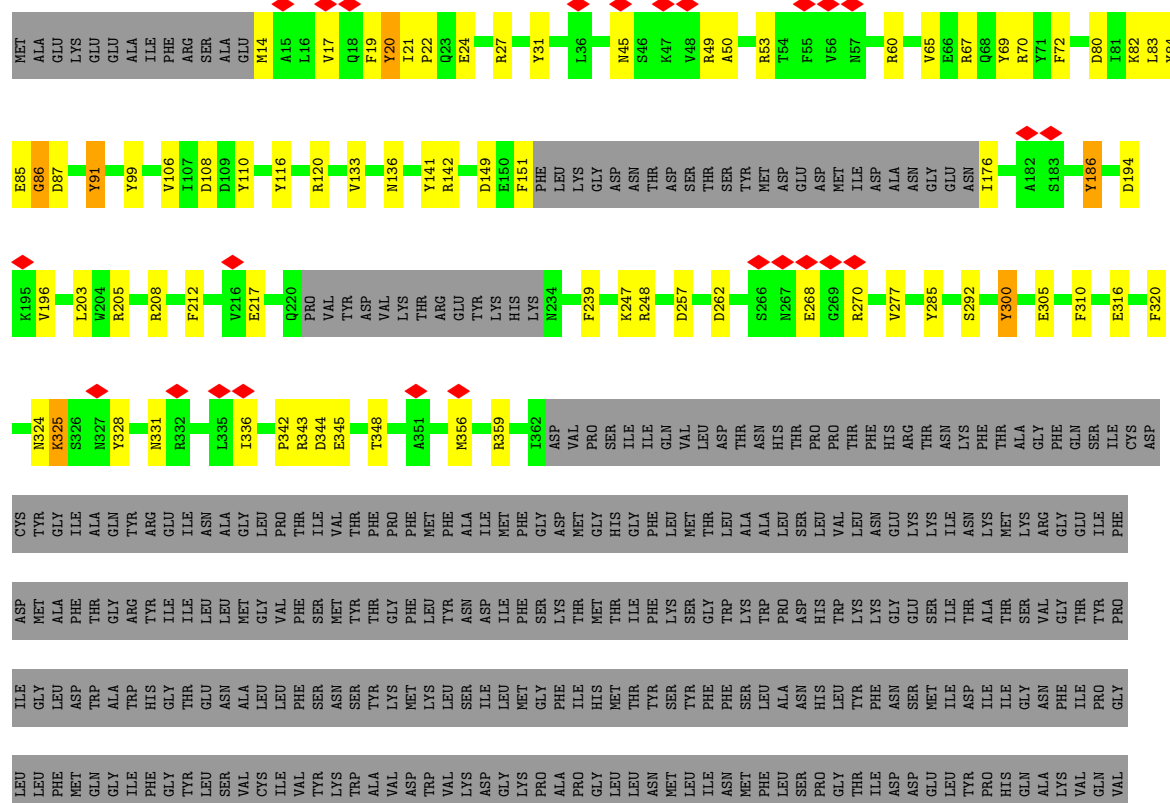


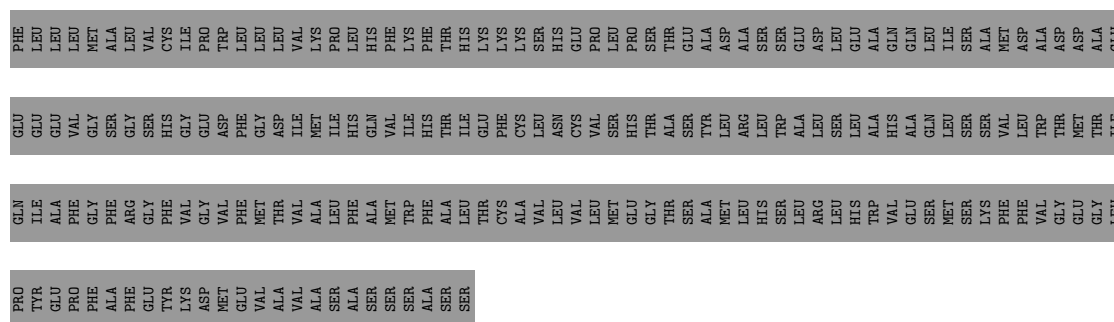


• Molecule 8: V-type proton ATPase subunit H

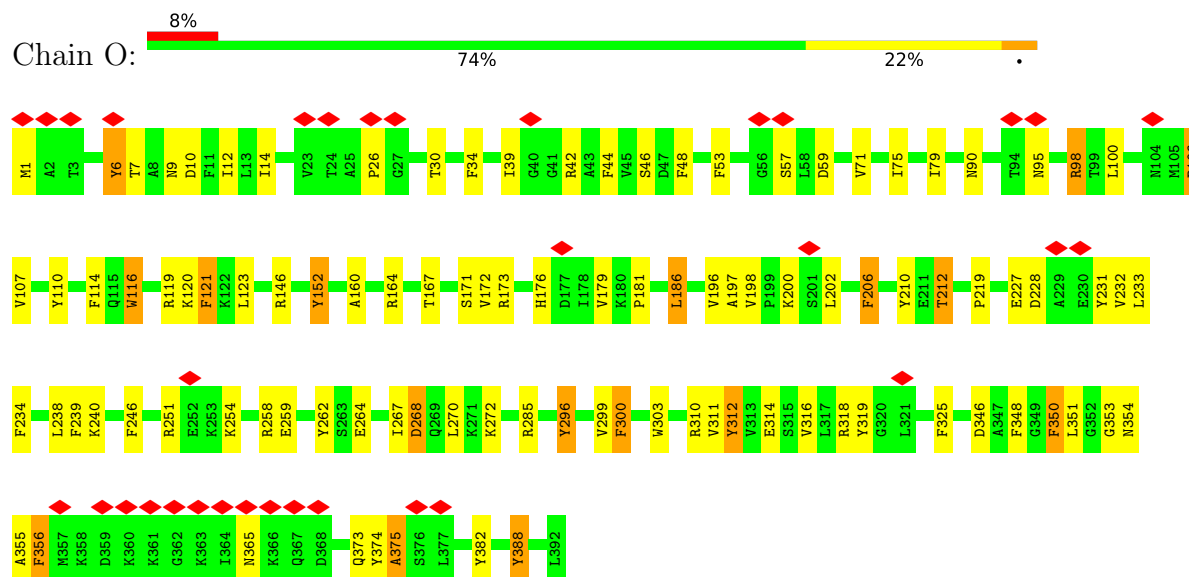


• Molecule 9: V-type proton ATPase subunit a, vacuolar isoform

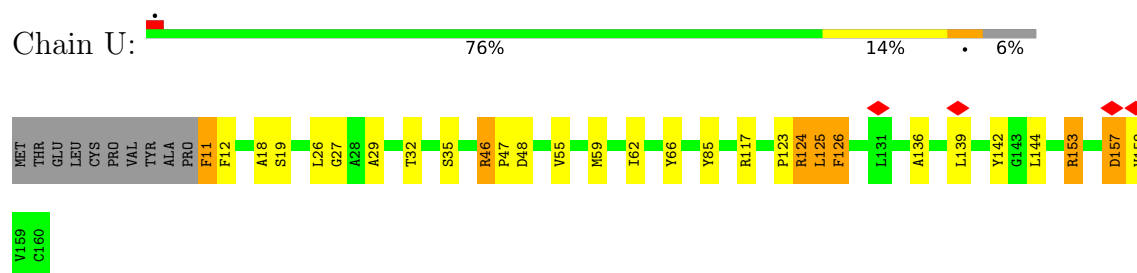




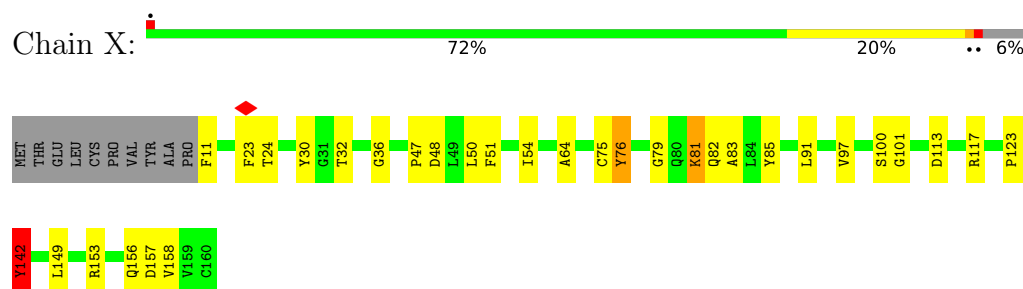
- Molecule 10: V-type proton ATPase subunit C



- Molecule 11: V-type proton ATPase subunit c

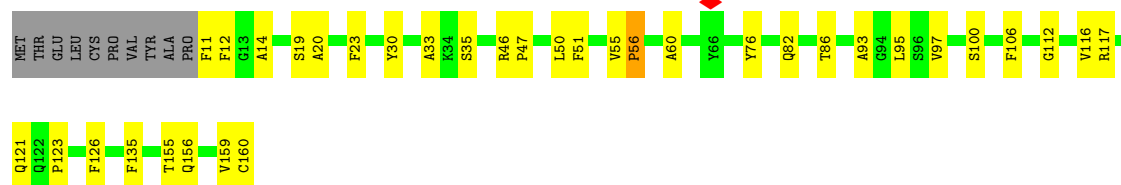


- Molecule 11: V-type proton ATPase subunit c



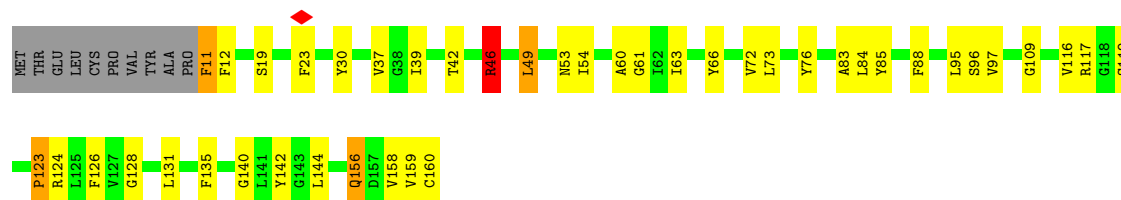
- Molecule 11: V-type proton ATPase subunit c

Chain a: 



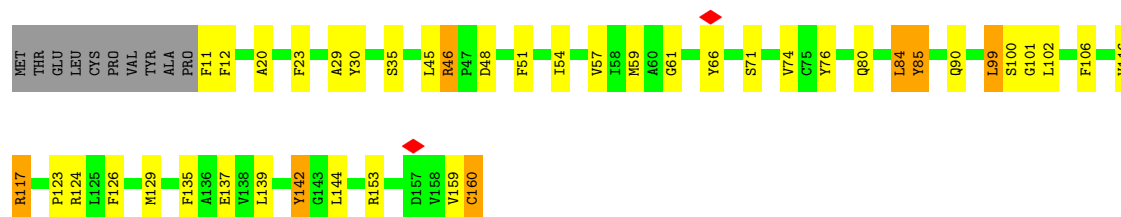
- Molecule 11: V-type proton ATPase subunit c

Chain R: 



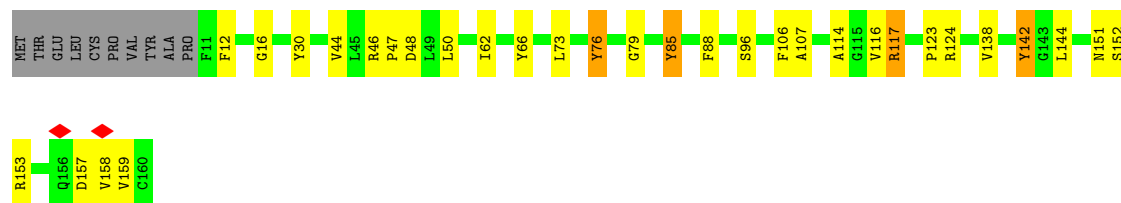
- Molecule 11: V-type proton ATPase subunit c

Chain Z: 



- Molecule 11: V-type proton ATPase subunit c

Chain S: 



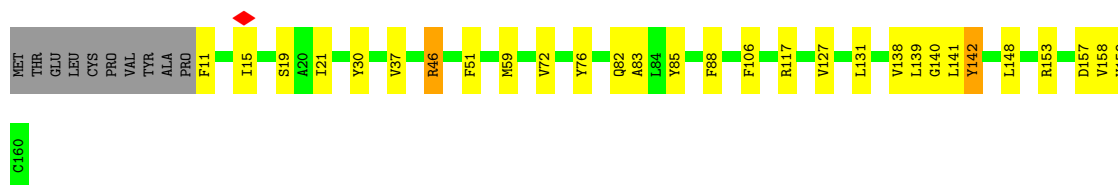
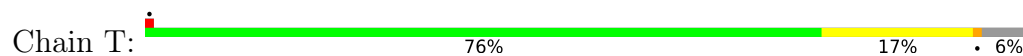
- Molecule 11: V-type proton ATPase subunit c

Chain Y: 

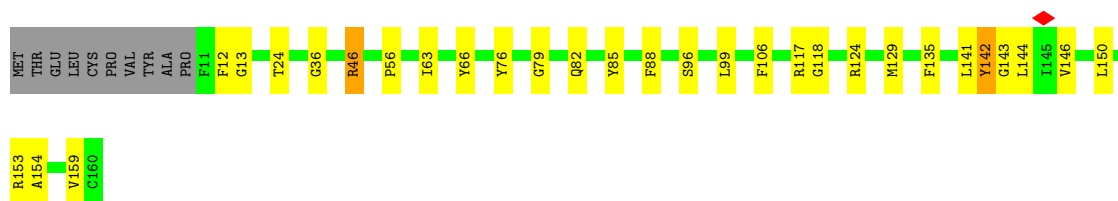
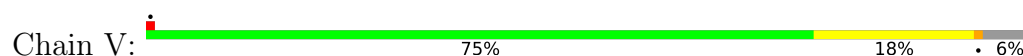




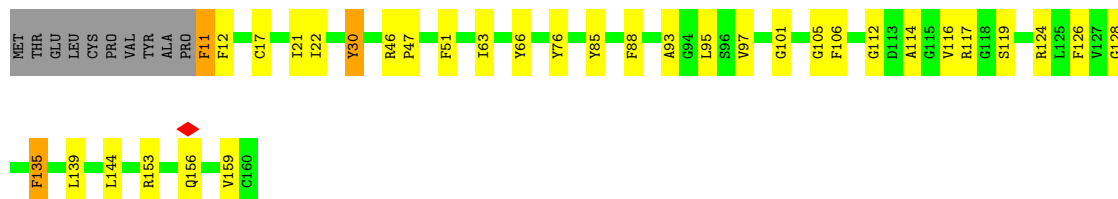
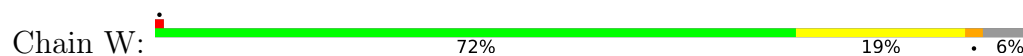
- Molecule 11: V-type proton ATPase subunit c



- Molecule 11: V-type proton ATPase subunit c



- Molecule 11: V-type proton ATPase subunit c



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	38347	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	7000	Depositor
Magnification	34483	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.131	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.03	Depositor
Map size (\AA)	371.2, 371.2, 371.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.45, 1.45, 1.45	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	M	1.80	24/1710 (1.4%)	2.05	49/2295 (2.1%)
2	N	1.77	11/944 (1.2%)	1.88	23/1277 (1.8%)
3	A	1.72	45/4677 (1.0%)	2.01	130/6339 (2.1%)
3	C	1.70	33/4677 (0.7%)	1.96	121/6339 (1.9%)
3	E	1.72	41/4677 (0.9%)	1.92	112/6339 (1.8%)
4	B	1.71	40/3654 (1.1%)	1.97	93/4953 (1.9%)
4	D	1.74	34/3654 (0.9%)	1.96	80/4953 (1.6%)
4	F	1.78	49/3654 (1.3%)	1.99	91/4953 (1.8%)
5	Q	1.71	23/2861 (0.8%)	2.02	73/3880 (1.9%)
6	H	1.55	2/828 (0.2%)	1.76	10/1098 (0.9%)
6	J	1.63	7/828 (0.8%)	1.70	9/1098 (0.8%)
6	L	1.64	4/828 (0.5%)	1.75	13/1098 (1.2%)
7	G	1.66	13/1743 (0.7%)	1.84	27/2338 (1.2%)
7	I	1.68	13/1743 (0.7%)	1.87	36/2338 (1.5%)
7	K	1.71	14/1743 (0.8%)	1.83	34/2338 (1.5%)
8	P	1.66	22/3766 (0.6%)	1.86	76/5087 (1.5%)
9	b	1.74	22/2578 (0.9%)	1.98	66/3479 (1.9%)
10	O	1.69	27/3185 (0.8%)	1.94	77/4314 (1.8%)
11	R	1.71	12/1086 (1.1%)	1.93	28/1472 (1.9%)
11	S	1.65	7/1086 (0.6%)	1.87	18/1472 (1.2%)
11	T	1.65	5/1086 (0.5%)	1.90	21/1472 (1.4%)
11	U	1.67	7/1086 (0.6%)	1.91	22/1472 (1.5%)
11	V	1.65	7/1086 (0.6%)	1.87	21/1472 (1.4%)
11	W	1.67	9/1086 (0.8%)	1.88	23/1472 (1.6%)
11	X	1.63	9/1086 (0.8%)	1.94	28/1472 (1.9%)
11	Y	1.69	9/1086 (0.8%)	1.80	23/1472 (1.6%)
11	Z	1.77	15/1086 (1.4%)	1.97	32/1472 (2.2%)
11	a	1.75	9/1086 (0.8%)	1.93	27/1472 (1.8%)
All	All	1.71	513/58610 (0.9%)	1.93	1363/79236 (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	M	0	9
2	N	0	4
3	A	0	12
3	C	0	13
3	E	0	15
4	B	0	17
4	D	0	13
4	F	0	14
5	Q	0	8
6	J	0	3
6	L	0	1
7	G	0	1
7	I	0	3
7	K	0	6
8	P	0	5
9	b	0	6
10	O	0	8
11	R	0	1
11	S	0	2
11	T	0	4
11	U	0	4
11	V	0	3
11	W	0	2
11	X	0	2
11	Y	0	2
11	Z	0	3
11	a	0	2
All	All	0	163

All (513) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Y	43	CYS	CB-SG	8.32	1.96	1.82
4	F	118	ARG	CZ-NH1	8.24	1.43	1.33
11	Z	101	GLY	CA-C	-8.09	1.39	1.51
3	E	365	ARG	CZ-NH2	7.91	1.43	1.33
1	M	97	ARG	CZ-NH2	7.89	1.43	1.33
3	E	417	SER	CA-CB	7.88	1.64	1.52
4	D	302	ARG	NE-CZ	7.83	1.43	1.33
7	K	117	TYR	CZ-OH	7.74	1.51	1.37
2	N	101	TYR	CB-CG	7.73	1.63	1.51
7	I	85	ARG	NE-CZ	7.61	1.43	1.33
4	F	309	TYR	CE2-CZ	7.57	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	482	ARG	CD-NE	7.54	1.59	1.46
3	C	74	GLU	CD-OE2	7.53	1.33	1.25
3	A	322	SER	CA-CB	7.49	1.64	1.52
4	D	205	GLU	CB-CG	7.44	1.66	1.52
9	b	316	GLU	CD-OE1	7.43	1.33	1.25
7	K	108	SER	CA-CB	7.42	1.64	1.52
1	M	112	TYR	CZ-OH	7.42	1.50	1.37
3	E	177	ARG	CZ-NH2	7.39	1.42	1.33
4	D	393	ARG	NE-CZ	7.31	1.42	1.33
11	X	36	GLY	CA-C	-7.28	1.40	1.51
10	O	259	GLU	CB-CG	7.27	1.66	1.52
4	B	301	ARG	CZ-NH1	7.27	1.42	1.33
3	C	544	PHE	CG-CD2	7.18	1.49	1.38
4	B	257	ARG	NE-CZ	7.18	1.42	1.33
11	U	123	PRO	N-CD	7.18	1.57	1.47
5	Q	266	ARG	CZ-NH1	7.17	1.42	1.33
3	C	344	ARG	NE-CZ	7.14	1.42	1.33
4	F	252	ARG	CD-NE	7.13	1.58	1.46
11	Z	30	TYR	CE2-CZ	7.12	1.47	1.38
4	D	195	ARG	NE-CZ	7.12	1.42	1.33
8	P	105	SER	CA-CB	7.12	1.63	1.52
9	b	31	TYR	CE1-CZ	7.11	1.47	1.38
4	B	237	ARG	CZ-NH1	7.09	1.42	1.33
11	Z	124	ARG	CZ-NH2	7.08	1.42	1.33
4	D	301	ARG	CD-NE	7.05	1.58	1.46
4	B	284	TYR	CB-CG	7.04	1.62	1.51
6	J	73	GLU	CD-OE2	7.03	1.33	1.25
3	A	336	GLY	N-CA	-7.01	1.35	1.46
3	A	574	THR	C-N	6.95	1.45	1.33
7	G	43	TYR	CE2-CZ	6.95	1.47	1.38
3	C	179	ARG	CZ-NH2	6.94	1.42	1.33
3	A	359	ARG	CD-NE	6.93	1.58	1.46
5	Q	89	GLY	N-CA	-6.91	1.35	1.46
11	a	112	GLY	CA-C	-6.89	1.40	1.51
3	C	593	GLU	CB-CG	6.87	1.65	1.52
4	B	295	ARG	CZ-NH1	6.86	1.42	1.33
3	A	406	ARG	NE-CZ	6.84	1.42	1.33
3	A	394	ARG	CD-NE	6.83	1.58	1.46
9	b	208	ARG	CZ-NH2	6.83	1.42	1.33
11	S	153	ARG	CD-NE	6.80	1.58	1.46
4	F	223	ARG	CZ-NH1	6.80	1.41	1.33
11	S	106	PHE	CG-CD1	6.79	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	144	ARG	CZ-NH1	6.78	1.41	1.33
3	C	334	TYR	CG-CD1	6.78	1.48	1.39
3	E	191	TYR	CG-CD1	6.76	1.48	1.39
3	C	46	TYR	CE1-CZ	6.75	1.47	1.38
9	b	60	ARG	NE-CZ	6.72	1.41	1.33
10	O	181	PRO	N-CA	-6.70	1.35	1.47
1	M	180	ARG	CZ-NH2	6.70	1.41	1.33
3	E	383	TYR	CE2-CZ	6.68	1.47	1.38
2	N	14	GLU	CG-CD	6.67	1.61	1.51
3	E	160	SER	CA-CB	6.67	1.62	1.52
11	R	23	PHE	CB-CG	6.67	1.62	1.51
4	B	455	PHE	CG-CD1	6.67	1.48	1.38
1	M	187	TYR	CZ-OH	6.65	1.49	1.37
3	E	221	ARG	NE-CZ	6.65	1.41	1.33
1	M	29	TYR	CE2-CZ	6.62	1.47	1.38
10	O	46	SER	CA-CB	6.61	1.62	1.52
5	Q	5	TYR	CE1-CZ	6.60	1.47	1.38
11	X	153	ARG	NE-CZ	6.60	1.41	1.33
3	C	525	PHE	CG-CD1	6.58	1.48	1.38
3	A	484	ARG	CZ-NH1	6.57	1.41	1.33
4	B	404	TYR	CG-CD2	6.57	1.47	1.39
3	A	123	TYR	CG-CD1	6.56	1.47	1.39
4	D	466	ARG	CZ-NH1	6.55	1.41	1.33
4	D	176	SER	CB-OG	6.55	1.50	1.42
10	O	42	ARG	CZ-NH1	6.53	1.41	1.33
3	C	392	TYR	CZ-OH	6.53	1.49	1.37
11	X	85	TYR	CB-CG	6.53	1.61	1.51
10	O	164	ARG	CZ-NH1	6.51	1.41	1.33
5	Q	77	TYR	CG-CD1	6.51	1.47	1.39
4	F	233	GLY	CA-C	-6.50	1.41	1.51
3	A	534	TYR	CE1-CZ	6.49	1.47	1.38
11	U	27	GLY	CA-C	-6.48	1.41	1.51
9	b	217	GLU	CG-CD	6.47	1.61	1.51
11	a	46	ARG	CZ-NH1	6.47	1.41	1.33
9	b	120	ARG	NE-CZ	6.47	1.41	1.33
11	X	117	ARG	CD-NE	6.47	1.57	1.46
11	U	142	TYR	CG-CD1	6.46	1.47	1.39
7	I	46	GLU	CG-CD	6.43	1.61	1.51
5	Q	273	TYR	CG-CD1	6.43	1.47	1.39
4	F	318	ARG	CD-NE	6.42	1.57	1.46
1	M	12	ARG	CZ-NH2	6.42	1.41	1.33
4	B	437	GLU	CD-OE2	6.41	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	5	ARG	NE-CZ	6.40	1.41	1.33
1	M	105	TYR	CG-CD2	6.39	1.47	1.39
6	J	46	TYR	CG-CD2	6.39	1.47	1.39
7	G	166	ARG	CD-NE	6.39	1.57	1.46
11	V	46	ARG	NE-CZ	6.39	1.41	1.33
3	C	286	ARG	CZ-NH2	6.39	1.41	1.33
4	B	304	TYR	CD1-CE1	6.39	1.49	1.39
7	I	158	ARG	CZ-NH2	6.39	1.41	1.33
11	Z	117	ARG	NE-CZ	6.38	1.41	1.33
8	P	336	ARG	CD-NE	6.38	1.57	1.46
4	F	362	ARG	CD-NE	6.38	1.57	1.46
8	P	184	TYR	CE2-CZ	6.37	1.46	1.38
4	B	321	ARG	NE-CZ	6.37	1.41	1.33
4	F	452	ARG	CZ-NH2	6.36	1.41	1.33
4	F	265	TYR	CE2-CZ	6.35	1.46	1.38
4	B	321	ARG	CZ-NH2	6.34	1.41	1.33
7	K	52	ARG	NE-CZ	6.34	1.41	1.33
4	F	381	ARG	CZ-NH2	6.33	1.41	1.33
10	O	314	GLU	CD-OE1	6.33	1.32	1.25
3	E	595	GLU	CG-CD	6.32	1.61	1.51
4	D	272	ARG	CZ-NH2	6.31	1.41	1.33
4	B	74	ARG	CD-NE	6.30	1.57	1.46
3	A	460	TYR	CB-CG	-6.30	1.42	1.51
3	A	110	ARG	CZ-NH1	6.29	1.41	1.33
3	E	370	ARG	CZ-NH2	6.27	1.41	1.33
3	C	342	TYR	CG-CD2	6.24	1.47	1.39
8	P	229	ARG	CZ-NH1	6.23	1.41	1.33
4	F	284	TYR	CZ-OH	6.22	1.48	1.37
9	b	22	PRO	N-CD	6.21	1.56	1.47
4	F	146	TYR	CB-CG	-6.20	1.42	1.51
3	E	126	ARG	CZ-NH2	6.19	1.41	1.33
4	B	393	ARG	NE-CZ	6.19	1.41	1.33
9	b	67	ARG	NE-CZ	6.19	1.41	1.33
3	E	123	TYR	CG-CD2	6.16	1.47	1.39
8	P	204	TRP	NE1-CE2	6.15	1.45	1.37
11	R	49	LEU	N-CA	-6.15	1.34	1.46
4	D	362	ARG	CZ-NH1	6.15	1.41	1.33
11	X	117	ARG	NE-CZ	6.14	1.41	1.33
5	Q	335	ARG	CA-C	-6.14	1.36	1.52
8	P	85	SER	CA-CB	6.14	1.62	1.52
7	K	166	ARG	NE-CZ	6.14	1.41	1.33
5	Q	72	ALA	CA-CB	6.13	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	b	205	ARG	NE-CZ	6.13	1.41	1.33
11	a	35	SER	CA-CB	6.13	1.62	1.52
3	E	471	TYR	CZ-OH	6.12	1.48	1.37
5	Q	321	ARG	CD-NE	6.12	1.56	1.46
3	E	610	ARG	CZ-NH1	6.12	1.41	1.33
11	X	142	TYR	CG-CD2	6.11	1.47	1.39
3	A	178	SER	CA-CB	6.08	1.62	1.52
10	O	319	TYR	CD2-CE2	6.06	1.48	1.39
6	J	66	GLY	CA-C	-6.06	1.42	1.51
11	S	46	ARG	CZ-NH2	6.05	1.41	1.33
8	P	17	ARG	CZ-NH2	6.05	1.41	1.33
4	D	404	TYR	CG-CD1	6.04	1.47	1.39
3	A	482	ARG	CZ-NH1	6.04	1.41	1.33
11	Z	76	TYR	CA-CB	6.04	1.67	1.53
11	T	142	TYR	CG-CD2	6.04	1.47	1.39
4	B	359	PHE	CG-CD1	6.03	1.47	1.38
8	P	372	PRO	CA-C	-6.03	1.40	1.52
11	Z	100	SER	C-N	6.03	1.43	1.33
3	A	215	TRP	CA-CB	6.02	1.67	1.53
4	F	284	TYR	CG-CD2	6.02	1.47	1.39
4	D	325	ARG	NE-CZ	6.02	1.40	1.33
1	M	110	GLU	CB-CG	6.01	1.63	1.52
3	C	436	GLN	N-CA	-6.01	1.34	1.46
4	B	94	GLU	CD-OE2	-6.00	1.19	1.25
4	B	475	ARG	CZ-NH1	6.00	1.40	1.33
4	F	475	ARG	CZ-NH1	6.00	1.40	1.33
11	Z	46	ARG	NE-CZ	5.99	1.40	1.33
11	a	30	TYR	CZ-OH	5.98	1.48	1.37
3	A	24	TYR	CE2-CZ	5.98	1.46	1.38
11	R	135	PHE	CG-CD1	5.98	1.47	1.38
1	M	169	ARG	CZ-NH1	5.97	1.40	1.33
4	B	296	GLU	CG-CD	5.97	1.60	1.51
8	P	292	SER	CA-CB	5.97	1.61	1.52
4	F	439	PHE	CG-CD1	5.96	1.47	1.38
3	C	314	ARG	CZ-NH1	5.96	1.40	1.33
11	a	106	PHE	CG-CD2	5.96	1.47	1.38
1	M	179	PRO	N-CA	-5.95	1.37	1.47
10	O	374	TYR	CG-CD1	5.95	1.46	1.39
3	A	417	SER	CA-CB	5.94	1.61	1.52
3	A	221	ARG	CZ-NH1	5.94	1.40	1.33
4	F	49	TYR	CZ-OH	5.93	1.48	1.37
5	Q	262	PHE	CG-CD2	5.93	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	252	ARG	NE-CZ	5.93	1.40	1.33
2	N	31	GLU	CG-CD	5.92	1.60	1.51
3	C	484	ARG	CZ-NH2	5.92	1.40	1.33
7	I	46	GLU	CD-OE1	5.92	1.32	1.25
11	W	106	PHE	CG-CD1	5.92	1.47	1.38
4	D	309	TYR	CD2-CE2	5.92	1.48	1.39
11	R	96	SER	CA-CB	5.91	1.61	1.52
11	W	76	TYR	CD1-CE1	5.91	1.48	1.39
4	D	166	ARG	CZ-NH2	5.90	1.40	1.33
3	C	523	GLU	CG-CD	5.90	1.60	1.51
10	O	254	LYS	N-CA	-5.90	1.34	1.46
4	B	313	SER	CA-CB	5.89	1.61	1.52
3	C	158	TYR	CE1-CZ	5.89	1.46	1.38
7	K	144	ARG	CZ-NH1	5.88	1.40	1.33
9	b	50	ALA	CA-CB	5.88	1.64	1.52
4	F	290	GLU	CG-CD	-5.87	1.43	1.51
11	Y	35	SER	CA-CB	5.87	1.61	1.52
3	A	325	PRO	N-CA	-5.87	1.37	1.47
7	G	16	GLU	CD-OE1	5.87	1.32	1.25
4	B	362	ARG	CZ-NH1	5.86	1.40	1.33
1	M	86	SER	CB-OG	-5.85	1.34	1.42
4	F	362	ARG	NE-CZ	5.85	1.40	1.33
5	Q	289	TYR	CE2-CZ	-5.85	1.30	1.38
10	O	348	PHE	CG-CD2	5.85	1.47	1.38
3	C	534	TYR	CE1-CZ	5.84	1.46	1.38
7	G	158	ARG	CZ-NH2	5.84	1.40	1.33
4	F	307	TYR	CG-CD1	5.83	1.46	1.39
1	M	16	GLY	N-CA	5.83	1.54	1.46
9	b	69	TYR	CE1-CZ	5.82	1.46	1.38
7	G	219	ARG	CZ-NH1	5.82	1.40	1.33
11	V	96	SER	CB-OG	5.82	1.49	1.42
5	Q	315	SER	CA-CB	5.81	1.61	1.52
10	O	388	TYR	CG-CD1	5.81	1.46	1.39
9	b	320	PHE	CG-CD2	5.81	1.47	1.38
1	M	141	ARG	CZ-NH2	5.80	1.40	1.33
2	N	111	ARG	CD-NE	5.80	1.56	1.46
3	E	255	PRO	C-N	5.79	1.43	1.33
7	K	150	GLU	CG-CD	5.79	1.60	1.51
7	I	93	GLU	CD-OE1	5.79	1.32	1.25
7	K	151	SER	CA-CB	5.79	1.61	1.52
11	T	30	TYR	CG-CD2	5.77	1.46	1.39
4	D	229	PHE	CG-CD2	5.77	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	b	53	ARG	CZ-NH1	5.77	1.40	1.33
3	C	548	ARG	CZ-NH1	5.76	1.40	1.33
3	A	218	ARG	CZ-NH1	5.76	1.40	1.33
3	A	303	GLU	CD-OE1	5.76	1.31	1.25
3	E	140	GLN	CG-CD	5.75	1.64	1.51
1	M	202	ARG	CZ-NH2	5.75	1.40	1.33
4	B	452	ARG	CZ-NH2	5.75	1.40	1.33
2	N	104	GLU	CB-CG	5.75	1.63	1.52
3	E	72	VAL	CA-CB	-5.75	1.42	1.54
3	E	228	SER	CA-CB	5.75	1.61	1.52
1	M	187	TYR	CG-CD1	5.74	1.46	1.39
3	E	286	ARG	NE-CZ	5.74	1.40	1.33
4	D	237	ARG	CZ-NH2	5.73	1.40	1.33
4	F	313	SER	CA-CB	5.73	1.61	1.52
9	b	142	ARG	NE-CZ	5.72	1.40	1.33
7	G	85	ARG	CZ-NH2	5.72	1.40	1.33
10	O	114	PHE	CG-CD1	5.71	1.47	1.38
4	D	475	ARG	NE-CZ	5.71	1.40	1.33
3	A	24	TYR	CD1-CE1	5.70	1.48	1.39
11	a	11	PHE	CE1-CZ	5.70	1.48	1.37
4	F	257	ARG	CZ-NH1	5.70	1.40	1.33
7	I	187	GLY	CA-C	-5.70	1.42	1.51
3	A	475	TYR	CZ-OH	5.69	1.47	1.37
11	Y	88	PHE	CE2-CZ	5.69	1.48	1.37
11	V	141	LEU	N-CA	-5.69	1.34	1.46
4	F	127	PHE	CB-CG	-5.68	1.41	1.51
10	O	227	GLU	CD-OE1	5.67	1.31	1.25
4	F	400	SER	CA-CB	5.67	1.61	1.52
3	C	409	SER	CB-OG	5.67	1.49	1.42
3	A	238	ARG	NE-CZ	5.67	1.40	1.33
11	Z	12	PHE	CB-CG	-5.66	1.41	1.51
3	A	499	VAL	CB-CG1	5.65	1.64	1.52
3	E	139	TRP	NE1-CE2	-5.65	1.30	1.37
3	E	356	SER	CA-CB	5.65	1.61	1.52
4	B	449	TYR	CZ-OH	5.65	1.47	1.37
4	D	298	VAL	CB-CG1	5.65	1.64	1.52
11	W	117	ARG	CD-NE	5.65	1.56	1.46
5	Q	84	ARG	CZ-NH2	5.64	1.40	1.33
4	F	84	SER	C-N	5.64	1.43	1.33
3	C	301	TYR	CE1-CZ	5.63	1.45	1.38
3	A	433	GLY	N-CA	-5.62	1.37	1.46
3	A	314	ARG	CD-NE	5.62	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	443	PHE	CG-CD2	5.61	1.47	1.38
11	R	76	TYR	CE2-CZ	5.61	1.45	1.38
11	T	76	TYR	CG-CD1	5.61	1.46	1.39
3	C	342	TYR	CE1-CZ	5.61	1.45	1.38
11	R	109	GLY	N-CA	-5.61	1.37	1.46
4	F	471	GLU	CD-OE2	5.61	1.31	1.25
8	P	288	ARG	NE-CZ	5.60	1.40	1.33
3	C	238	ARG	CD-NE	5.60	1.55	1.46
3	E	272	TYR	CG-CD2	5.60	1.46	1.39
4	B	356	GLY	N-CA	-5.60	1.37	1.46
4	F	220	GLU	CB-CG	5.59	1.62	1.52
11	Z	61	GLY	CA-C	5.58	1.60	1.51
3	A	357	SER	CA-CB	5.58	1.61	1.52
4	D	118	ARG	NE-CZ	5.57	1.40	1.33
4	B	450	GLU	CD-OE2	5.56	1.31	1.25
8	P	331	SER	CA-CB	5.54	1.61	1.52
4	B	49	TYR	CG-CD1	5.54	1.46	1.39
4	D	320	GLY	CA-C	-5.54	1.43	1.51
3	A	179	ARG	NE-CZ	5.54	1.40	1.33
11	Z	126	PHE	CG-CD1	5.54	1.47	1.38
9	b	359	ARG	CZ-NH2	5.54	1.40	1.33
11	V	36	GLY	CA-C	-5.54	1.43	1.51
2	N	78	ARG	CZ-NH1	5.53	1.40	1.33
7	I	16	GLU	CG-CD	5.53	1.60	1.51
4	F	43	LYS	N-CA	-5.53	1.35	1.46
10	O	107	VAL	CB-CG1	5.52	1.64	1.52
11	Y	13	GLY	N-CA	-5.52	1.37	1.46
11	a	121	GLN	CB-CG	5.52	1.67	1.52
2	N	6	THR	N-CA	-5.51	1.35	1.46
3	C	249	GLY	N-CA	-5.51	1.37	1.46
11	Y	87	GLY	CA-C	5.51	1.60	1.51
6	J	42	GLU	CD-OE2	5.50	1.31	1.25
4	D	456	GLU	CG-CD	5.49	1.60	1.51
8	P	327	GLU	CG-CD	5.49	1.60	1.51
9	b	136	ASN	CA-CB	5.47	1.67	1.53
4	D	98	GLU	CD-OE1	5.47	1.31	1.25
4	B	74	ARG	NE-CZ	5.47	1.40	1.33
6	L	74	ALA	C-N	5.46	1.42	1.33
7	I	52	ARG	CZ-NH1	5.46	1.40	1.33
7	I	43	TYR	CE2-CZ	5.46	1.45	1.38
3	A	358	SER	N-CA	-5.46	1.35	1.46
3	E	87	ARG	CZ-NH1	5.45	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	160	TYR	CE1-CZ	5.45	1.45	1.38
3	E	258	PHE	CE1-CZ	5.45	1.47	1.37
5	Q	278	PHE	CG-CD1	5.45	1.47	1.38
11	Z	71	SER	CA-CB	5.45	1.61	1.52
1	M	141	ARG	CD-NE	5.44	1.55	1.46
4	B	452	ARG	CD-NE	5.43	1.55	1.46
4	F	152	SER	CA-CB	5.43	1.61	1.52
11	a	20	ALA	C-N	5.43	1.46	1.34
10	O	210	TYR	CG-CD2	5.42	1.46	1.39
9	b	345	GLU	CG-CD	5.42	1.60	1.51
4	F	131	TYR	CG-CD1	5.42	1.46	1.39
10	O	318	ARG	CZ-NH1	5.42	1.40	1.33
4	D	289	ARG	CA-CB	5.41	1.65	1.53
7	G	52	ARG	NE-CZ	5.41	1.40	1.33
11	W	47	PRO	CA-CB	5.40	1.64	1.53
4	F	189	ARG	NE-CZ	5.40	1.40	1.33
7	G	25	ARG	CZ-NH1	5.40	1.40	1.33
3	C	359	ARG	CZ-NH1	5.40	1.40	1.33
11	Z	51	PHE	CA-CB	5.40	1.65	1.53
1	M	12	ARG	NE-CZ	5.39	1.40	1.33
3	E	218	ARG	CZ-NH1	5.38	1.40	1.33
4	B	328	SER	CA-CB	5.38	1.61	1.52
4	B	352	TYR	CD2-CE2	5.38	1.47	1.39
9	b	31	TYR	CE2-CZ	5.38	1.45	1.38
7	K	25	ARG	CD-NE	5.38	1.55	1.46
8	P	336	ARG	CZ-NH2	5.38	1.40	1.33
3	C	411	SER	CB-OG	5.37	1.49	1.42
4	F	431	LEU	CA-C	-5.37	1.39	1.52
6	L	6	GLY	N-CA	-5.37	1.38	1.46
11	X	124	ARG	NE-CZ	5.37	1.40	1.33
11	W	105	GLY	N-CA	5.37	1.54	1.46
1	M	124	GLY	CA-C	-5.37	1.43	1.51
3	E	463	TYR	CE1-CZ	5.37	1.45	1.38
7	K	85	ARG	CZ-NH2	5.37	1.40	1.33
10	O	262	TYR	CE1-CZ	5.37	1.45	1.38
4	F	352	TYR	CZ-OH	5.36	1.47	1.37
4	F	59	ASP	C-N	5.36	1.42	1.33
1	M	194	GLU	CB-CG	5.35	1.62	1.52
4	D	423	GLU	CB-CG	5.35	1.62	1.52
4	F	450	GLU	CB-CG	5.35	1.62	1.52
8	P	333	GLU	CD-OE2	5.35	1.31	1.25
9	b	305	GLU	CD-OE1	5.35	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	135	ARG	CZ-NH1	5.35	1.40	1.33
4	F	404	TYR	CE2-CZ	5.35	1.45	1.38
3	E	475	TYR	CG-CD2	5.35	1.46	1.39
4	F	208	PHE	CE2-CZ	5.35	1.47	1.37
4	F	149	GLU	CB-CG	5.34	1.62	1.52
7	K	25	ARG	NE-CZ	5.34	1.40	1.33
10	O	355	ALA	CA-CB	5.33	1.63	1.52
8	P	392	TYR	CE1-CZ	5.33	1.45	1.38
11	R	61	GLY	N-CA	-5.33	1.38	1.46
7	K	206	ARG	CZ-NH1	5.32	1.40	1.33
3	C	531	TYR	CE1-CZ	5.32	1.45	1.38
8	P	349	GLU	N-CA	-5.32	1.35	1.46
5	Q	321	ARG	NE-CZ	5.32	1.40	1.33
8	P	220	ARG	CZ-NH2	5.32	1.40	1.33
6	H	82	GLU	CG-CD	5.32	1.59	1.51
10	O	264	GLU	CB-CG	5.32	1.62	1.52
4	B	289	ARG	CD-NE	5.31	1.55	1.46
11	S	106	PHE	CE2-CZ	5.31	1.47	1.37
9	b	19	PHE	CG-CD2	5.31	1.46	1.38
4	F	252	ARG	CZ-NH1	5.31	1.40	1.33
4	B	295	ARG	CD-NE	5.31	1.55	1.46
9	b	343	ARG	CZ-NH2	5.30	1.40	1.33
4	D	289	ARG	CD-NE	5.30	1.55	1.46
11	Y	153	ARG	CD-NE	5.30	1.55	1.46
4	F	466	ARG	NE-CZ	5.30	1.40	1.33
7	G	114	ARG	CZ-NH1	5.30	1.40	1.33
11	U	117	ARG	CZ-NH1	5.30	1.40	1.33
11	W	101	GLY	CA-C	-5.29	1.43	1.51
11	S	16	GLY	N-CA	5.29	1.53	1.46
11	W	17	CYS	CB-SG	5.29	1.91	1.82
3	A	215	TRP	CZ2-CH2	5.28	1.47	1.37
5	Q	207	CYS	CA-CB	5.28	1.65	1.53
11	R	156	GLN	CG-CD	5.28	1.63	1.51
11	X	153	ARG	CZ-NH2	5.28	1.40	1.33
4	D	48	ARG	CZ-NH1	5.28	1.40	1.33
10	O	123	LEU	CA-CB	5.28	1.65	1.53
7	G	52	ARG	CZ-NH2	5.28	1.40	1.33
3	E	179	ARG	NE-CZ	5.27	1.39	1.33
7	I	25	ARG	CZ-NH1	5.27	1.39	1.33
5	Q	97	TYR	CB-CG	-5.27	1.43	1.51
4	F	428	GLU	CB-CG	5.27	1.62	1.52
4	D	189	ARG	NE-CZ	5.26	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	O	251	ARG	CZ-NH1	5.26	1.39	1.33
11	W	46	ARG	CZ-NH2	5.26	1.39	1.33
11	Y	100	SER	CB-OG	-5.26	1.35	1.42
4	F	166	ARG	CD-NE	5.26	1.55	1.46
9	b	359	ARG	NE-CZ	5.26	1.39	1.33
3	A	548	ARG	CD-NE	5.26	1.55	1.46
11	T	153	ARG	CZ-NH2	5.26	1.39	1.33
6	J	84	LYS	CE-NZ	5.25	1.62	1.49
7	K	85	ARG	CZ-NH1	5.25	1.39	1.33
3	E	553	TYR	CB-CG	5.25	1.59	1.51
11	Y	68	LEU	CA-CB	5.24	1.65	1.53
11	R	85	TYR	CG-CD1	5.23	1.46	1.39
5	Q	79	GLU	CG-CD	5.23	1.59	1.51
3	C	460	TYR	CE1-CZ	5.22	1.45	1.38
3	E	231	TYR	CA-CB	5.22	1.65	1.53
3	A	397	LYS	C-N	5.22	1.46	1.34
8	P	32	ARG	NE-CZ	5.22	1.39	1.33
6	H	53	GLU	CB-CG	5.22	1.62	1.52
4	D	454	VAL	CB-CG1	5.22	1.63	1.52
3	A	424	SER	CA-CB	5.22	1.60	1.52
3	C	177	ARG	CZ-NH2	5.21	1.39	1.33
3	E	73	TYR	CG-CD1	5.21	1.46	1.39
4	D	142	TYR	CG-CD2	5.21	1.46	1.39
11	S	117	ARG	NE-CZ	5.21	1.39	1.33
11	Y	60	ALA	C-N	5.21	1.42	1.33
8	P	23	ARG	CD-NE	5.21	1.55	1.46
10	O	382	TYR	CZ-OH	5.21	1.46	1.37
3	C	305	SER	CA-CB	5.21	1.60	1.52
4	F	440	GLU	CG-CD	5.20	1.59	1.51
11	Z	160	CYS	CB-SG	5.20	1.91	1.82
1	M	182	GLU	CG-CD	5.19	1.59	1.51
4	F	468	TYR	CZ-OH	5.19	1.46	1.37
4	D	362	ARG	CZ-NH2	5.18	1.39	1.33
5	Q	337	ARG	CZ-NH2	5.18	1.39	1.33
7	G	191	SER	CB-OG	5.18	1.49	1.42
4	B	374	ASN	CB-CG	5.18	1.62	1.51
7	I	167	ALA	CA-CB	5.18	1.63	1.52
3	E	57	VAL	C-N	5.18	1.42	1.33
11	V	118	GLY	N-CA	5.17	1.53	1.46
4	D	295	ARG	CZ-NH2	5.17	1.39	1.33
3	E	473	SER	CA-CB	5.17	1.60	1.52
3	E	365	ARG	CZ-NH1	5.17	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	O	310	ARG	CZ-NH1	5.17	1.39	1.33
4	F	367	LYS	C-N	5.16	1.42	1.33
5	Q	61	GLU	CB-CG	5.16	1.61	1.52
3	A	266	SER	CA-CB	5.16	1.60	1.52
10	O	146	ARG	CZ-NH1	5.16	1.39	1.33
6	J	27	TYR	CZ-OH	5.15	1.46	1.37
3	C	426	PRO	N-CD	5.15	1.55	1.47
11	U	124	ARG	CD-NE	5.15	1.55	1.46
11	U	126	PHE	CE2-CZ	5.15	1.47	1.37
4	B	102	ILE	C-N	-5.14	1.24	1.34
11	T	140	GLY	N-CA	-5.14	1.38	1.46
7	G	43	TYR	CG-CD2	5.14	1.45	1.39
11	W	128	GLY	CA-C	-5.14	1.43	1.51
3	E	62	ARG	CZ-NH1	5.14	1.39	1.33
3	A	121	SER	CA-CB	-5.14	1.45	1.52
6	J	16	GLU	CB-CG	5.14	1.61	1.52
3	A	319	ALA	CA-CB	5.14	1.63	1.52
5	Q	54	PHE	CE2-CZ	5.14	1.47	1.37
11	Z	12	PHE	CG-CD1	5.14	1.46	1.38
3	A	610	ARG	NE-CZ	5.13	1.39	1.33
7	K	185	SER	CA-CB	5.13	1.60	1.52
3	A	587	PHE	CG-CD1	5.13	1.46	1.38
7	K	160	TYR	CE1-CZ	5.13	1.45	1.38
2	N	101	TYR	CD2-CE2	5.12	1.47	1.39
3	A	534	TYR	CE2-CZ	-5.12	1.31	1.38
10	O	354	ASN	CB-CG	5.11	1.62	1.51
3	C	343	PHE	CG-CD2	5.11	1.46	1.38
8	P	117	PHE	CE2-CZ	5.11	1.47	1.37
4	D	323	GLU	CB-CG	5.11	1.61	1.52
4	F	146	TYR	CE1-CZ	5.11	1.45	1.38
11	R	85	TYR	CE1-CZ	5.11	1.45	1.38
3	A	423	PHE	CG-CD2	5.11	1.46	1.38
5	Q	297	ARG	CZ-NH2	5.10	1.39	1.33
11	R	160	CYS	CA-CB	5.10	1.65	1.53
11	V	153	ARG	NE-CZ	5.10	1.39	1.33
4	B	423	GLU	CG-CD	5.10	1.59	1.51
1	M	134	ARG	CZ-NH2	5.09	1.39	1.33
4	D	318	ARG	CZ-NH2	5.09	1.39	1.33
11	R	124	ARG	NE-CZ	5.08	1.39	1.33
10	O	71	VAL	CA-CB	-5.08	1.44	1.54
11	S	124	ARG	CZ-NH1	5.08	1.39	1.33
3	E	123	TYR	CE2-CZ	5.08	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	407	TYR	CG-CD1	5.08	1.45	1.39
3	A	126	ARG	CD-NE	5.08	1.55	1.46
4	D	96	THR	C-N	5.07	1.42	1.33
4	B	295	ARG	CZ-NH2	5.07	1.39	1.33
3	C	360	TRP	NE1-CE2	-5.07	1.30	1.37
11	a	51	PHE	CG-CD2	-5.07	1.31	1.38
11	V	79	GLY	CA-C	-5.07	1.43	1.51
2	N	87	ALA	N-CA	-5.06	1.36	1.46
3	A	185	ILE	CA-C	-5.06	1.39	1.52
4	D	286	ASP	CA-CB	5.05	1.65	1.53
4	F	449	TYR	CE2-CZ	5.05	1.45	1.38
3	A	370	ARG	CZ-NH1	5.05	1.39	1.33
3	E	342	TYR	CG-CD2	5.05	1.45	1.39
1	M	49	ARG	CD-NE	5.05	1.55	1.46
5	Q	345	TYR	CB-CG	-5.04	1.44	1.51
7	G	170	GLU	CB-CG	5.04	1.61	1.52
1	M	161	GLU	CG-CD	5.03	1.59	1.51
4	B	174	SER	CA-CB	5.03	1.60	1.52
3	E	599	GLU	CA-CB	5.03	1.65	1.53
2	N	54	PHE	CB-CG	-5.02	1.42	1.51
3	E	177	ARG	CD-NE	5.02	1.54	1.46
10	O	374	TYR	CG-CD2	5.02	1.45	1.39
11	U	46	ARG	NE-CZ	5.02	1.39	1.33
4	B	265	TYR	CG-CD2	5.02	1.45	1.39
5	Q	335	ARG	CZ-NH1	5.02	1.39	1.33
8	P	140	LEU	CA-CB	5.02	1.65	1.53
11	Z	139	LEU	C-N	5.02	1.42	1.33
4	F	144	ARG	CZ-NH2	5.02	1.39	1.33
4	B	116	SER	CA-CB	5.02	1.60	1.52
4	B	435	PHE	CB-CG	5.02	1.59	1.51
1	M	121	ARG	CD-NE	5.01	1.54	1.46
3	E	553	TYR	CG-CD2	5.01	1.45	1.39
6	L	58	GLU	CD-OE1	5.01	1.31	1.25
8	P	301	ARG	CD-NE	5.01	1.54	1.46
3	E	591	ARG	CZ-NH1	5.01	1.39	1.33
3	A	460	TYR	CG-CD2	5.01	1.45	1.39
3	A	329	ARG	NE-CZ	5.00	1.39	1.33
6	L	57	PHE	CE1-CZ	5.00	1.46	1.37
7	I	52	ARG	NE-CZ	5.00	1.39	1.33
11	X	30	TYR	CB-CG	-5.00	1.44	1.51

All (1363) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	82	TYR	CB-CG-CD1	20.73	133.44	121.00
5	Q	82	TYR	CB-CG-CD2	-18.34	110.00	121.00
4	B	404	TYR	CB-CG-CD2	-16.36	111.19	121.00
3	A	272	TYR	CB-CG-CD2	-16.22	111.27	121.00
1	M	34	ARG	NE-CZ-NH1	15.89	128.25	120.30
7	I	85	ARG	NE-CZ-NH2	-15.40	112.60	120.30
3	E	383	TYR	CB-CG-CD1	-15.15	111.91	121.00
9	b	186	TYR	CB-CG-CD1	14.94	129.96	121.00
4	F	111	ARG	NE-CZ-NH2	14.70	127.65	120.30
11	R	124	ARG	NE-CZ-NH1	14.51	127.56	120.30
4	F	71	ARG	NE-CZ-NH2	-14.47	113.06	120.30
4	F	146	TYR	CB-CG-CD1	-14.44	112.33	121.00
11	Z	85	TYR	CB-CG-CD1	-14.31	112.41	121.00
1	M	92	PHE	CB-CG-CD2	-14.24	110.83	120.80
4	B	468	TYR	CB-CG-CD1	14.08	129.45	121.00
8	P	463	TYR	CB-CG-CD2	-13.81	112.71	121.00
7	K	92	ARG	NE-CZ-NH2	-13.81	113.39	120.30
5	Q	97	TYR	CB-CG-CD2	-13.57	112.86	121.00
5	Q	300	PHE	CB-CG-CD1	13.37	130.16	120.80
4	D	272	ARG	NE-CZ-NH1	13.29	126.94	120.30
1	M	97	ARG	NE-CZ-NH1	13.19	126.89	120.30
11	X	51	PHE	CB-CG-CD2	-13.12	111.61	120.80
4	B	49	TYR	CB-CG-CD2	13.06	128.84	121.00
4	B	468	TYR	CB-CG-CD2	-12.90	113.26	121.00
9	b	343	ARG	NE-CZ-NH1	12.89	126.75	120.30
10	O	296	TYR	CB-CG-CD2	-12.89	113.27	121.00
9	b	142	ARG	NE-CZ-NH2	-12.87	113.86	120.30
7	G	85	ARG	NE-CZ-NH2	-12.81	113.90	120.30
3	E	544	PHE	CB-CG-CD1	12.79	129.75	120.80
3	E	202	PHE	CB-CG-CD2	-12.77	111.86	120.80
4	D	475	ARG	NE-CZ-NH2	-12.55	114.03	120.30
3	C	383	TYR	CB-CG-CD1	-12.52	113.49	121.00
9	b	320	PHE	CB-CG-CD1	12.47	129.53	120.80
3	C	380	PHE	CB-CG-CD1	-12.26	112.22	120.80
3	C	365	ARG	NE-CZ-NH1	12.21	126.40	120.30
3	E	202	PHE	CB-CG-CD1	12.19	129.34	120.80
9	b	27	ARG	NE-CZ-NH2	-12.11	114.25	120.30
11	S	117	ARG	NE-CZ-NH2	-12.05	114.27	120.30
3	C	365	ARG	NE-CZ-NH2	-12.03	114.28	120.30
3	E	87	ARG	NE-CZ-NH1	-11.94	114.33	120.30
2	N	113	ARG	NE-CZ-NH2	-11.88	114.36	120.30
11	Z	124	ARG	NE-CZ-NH1	11.87	126.23	120.30
11	V	153	ARG	NE-CZ-NH2	-11.82	114.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	127	PHE	CB-CG-CD2	-11.78	112.56	120.80
4	F	195	ARG	NE-CZ-NH1	11.77	126.19	120.30
5	Q	97	TYR	CB-CG-CD1	11.77	128.06	121.00
4	B	268	TYR	CB-CG-CD2	-11.76	113.95	121.00
11	T	76	TYR	CB-CG-CD2	-11.70	113.98	121.00
10	O	173	ARG	NE-CZ-NH2	-11.62	114.49	120.30
1	M	34	ARG	NE-CZ-NH2	-11.56	114.52	120.30
1	M	42	ARG	NE-CZ-NH1	11.54	126.07	120.30
4	D	195	ARG	NE-CZ-NH1	11.54	126.07	120.30
4	F	404	TYR	CB-CG-CD1	11.53	127.92	121.00
10	O	173	ARG	NE-CZ-NH1	11.44	126.02	120.30
10	O	296	TYR	CB-CG-CD1	11.45	127.87	121.00
2	N	113	ARG	NE-CZ-NH1	11.44	126.02	120.30
6	L	28	ARG	NE-CZ-NH2	-11.30	114.65	120.30
3	E	24	TYR	CB-CG-CD2	-11.14	114.32	121.00
1	M	29	TYR	CB-CG-CD2	-11.08	114.35	121.00
5	Q	297	ARG	NE-CZ-NH1	11.04	125.82	120.30
11	T	76	TYR	CB-CG-CD1	11.00	127.60	121.00
1	M	92	PHE	CB-CG-CD1	10.96	128.47	120.80
9	b	186	TYR	CB-CG-CD2	-10.94	114.43	121.00
11	U	117	ARG	NE-CZ-NH2	-10.87	114.87	120.30
3	C	191	TYR	CB-CG-CD2	-10.86	114.49	121.00
11	R	117	ARG	NE-CZ-NH1	10.83	125.71	120.30
11	V	46	ARG	NE-CZ-NH1	-10.80	114.90	120.30
4	B	49	TYR	CB-CG-CD1	-10.78	114.53	121.00
4	F	318	ARG	NE-CZ-NH2	-10.78	114.91	120.30
4	F	111	ARG	NE-CZ-NH1	-10.73	114.94	120.30
3	C	286	ARG	NE-CZ-NH1	10.70	125.65	120.30
3	A	158	TYR	CB-CG-CD1	10.66	127.39	121.00
9	b	343	ARG	NE-CZ-NH2	-10.65	114.97	120.30
3	A	555	ASP	CB-CG-OD1	10.65	127.89	118.30
3	C	87	ARG	NE-CZ-NH2	10.64	125.62	120.30
5	Q	262	PHE	CB-CG-CD1	10.63	128.24	120.80
5	Q	345	TYR	CB-CG-CD1	10.55	127.33	121.00
3	A	334	TYR	CB-CG-CD2	-10.53	114.69	121.00
7	G	166	ARG	NE-CZ-NH2	-10.46	115.07	120.30
3	E	231	TYR	CG-CD1-CE1	-10.45	112.94	121.30
4	F	443	PHE	CB-CG-CD1	-10.41	113.51	120.80
4	B	404	TYR	CB-CG-CD1	10.39	127.23	121.00
3	A	286	ARG	NE-CZ-NH2	-10.36	115.12	120.30
4	B	309	TYR	CB-CG-CD2	-10.35	114.79	121.00
8	P	330	TYR	CB-CG-CD2	-10.34	114.79	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	343	PHE	CB-CG-CD1	10.33	128.03	120.80
1	M	156	PHE	CB-CG-CD2	-10.31	113.58	120.80
5	Q	297	ARG	NE-CZ-NH2	-10.31	115.14	120.30
7	I	43	TYR	CB-CG-CD2	-10.29	114.83	121.00
5	Q	188	TYR	CB-CG-CD1	10.25	127.15	121.00
3	C	553	TYR	CB-CG-CD2	-10.23	114.86	121.00
4	F	381	ARG	NE-CZ-NH1	10.18	125.39	120.30
4	B	48	ARG	NE-CZ-NH2	-10.11	115.25	120.30
10	O	356	PHE	CB-CG-CD1	-10.10	113.73	120.80
5	Q	51	TYR	CB-CG-CD1	-10.09	114.95	121.00
4	D	173	PHE	CB-CG-CD2	-10.04	113.77	120.80
9	b	151	PHE	CB-CG-CD1	10.03	127.82	120.80
3	A	194	ASP	CB-CG-OD2	10.01	127.31	118.30
4	F	166	ARG	NE-CZ-NH1	9.98	125.29	120.30
9	b	20	TYR	CB-CG-CD1	9.95	126.97	121.00
1	M	97	ARG	NE-CZ-NH2	-9.95	115.33	120.30
4	D	370	TYR	CB-CG-CD1	9.94	126.96	121.00
7	K	144	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	M	197	ARG	NE-CZ-NH1	9.90	125.25	120.30
11	S	30	TYR	CB-CG-CD2	-9.88	115.07	121.00
4	D	195	ARG	NE-CZ-NH2	-9.87	115.36	120.30
11	a	117	ARG	NE-CZ-NH1	-9.86	115.37	120.30
5	Q	149	TYR	CB-CG-CD1	-9.85	115.09	121.00
3	E	484	ARG	NE-CZ-NH2	-9.84	115.38	120.30
5	Q	300	PHE	CB-CG-CD2	-9.83	113.92	120.80
11	a	30	TYR	CB-CG-CD2	-9.82	115.11	121.00
3	E	537	PHE	CB-CG-CD2	-9.82	113.93	120.80
1	M	42	ARG	NE-CZ-NH2	-9.81	115.39	120.30
4	F	475	ARG	NE-CZ-NH1	9.79	125.19	120.30
11	a	12	PHE	CB-CG-CD2	9.78	127.64	120.80
3	A	203	ASP	CB-CG-OD1	-9.76	109.51	118.30
3	E	531	TYR	CB-CG-CD1	9.75	126.85	121.00
7	G	85	ARG	NE-CZ-NH1	9.75	125.17	120.30
3	E	135	ARG	NE-CZ-NH1	-9.74	115.43	120.30
11	Z	117	ARG	NE-CZ-NH1	-9.72	115.44	120.30
4	D	173	PHE	CB-CG-CD1	9.72	127.60	120.80
3	A	135	ARG	NE-CZ-NH2	9.69	125.15	120.30
4	B	127	PHE	CB-CG-CD1	9.68	127.57	120.80
3	C	123	TYR	CB-CG-CD1	9.67	126.80	121.00
11	X	135	PHE	CB-CG-CD2	-9.63	114.06	120.80
3	A	365	ARG	NE-CZ-NH2	9.62	125.11	120.30
9	b	72	PHE	CB-CG-CD2	-9.59	114.08	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	302	ARG	NE-CZ-NH2	-9.53	115.54	120.30
10	O	285	ARG	NE-CZ-NH1	9.52	125.06	120.30
7	I	25	ARG	NE-CZ-NH1	9.52	125.06	120.30
11	W	106	PHE	CB-CG-CD1	9.50	127.45	120.80
4	F	195	ARG	NE-CZ-NH2	-9.40	115.60	120.30
3	A	463	TYR	CB-CG-CD1	9.38	126.63	121.00
3	A	550	PHE	CB-CG-CD1	-9.38	114.23	120.80
11	U	157	ASP	CB-CG-OD2	-9.38	109.86	118.30
3	A	460	TYR	CB-CG-CD2	-9.36	115.38	121.00
3	A	544	PHE	CB-CG-CD1	9.36	127.36	120.80
3	C	177	ARG	NE-CZ-NH2	-9.36	115.62	120.30
7	G	144	ARG	NE-CZ-NH1	9.36	124.98	120.30
3	A	123	TYR	CB-CG-CD1	9.33	126.60	121.00
5	Q	254	PHE	CB-CG-CD2	-9.33	114.27	120.80
3	C	392	TYR	CB-CG-CD2	9.32	126.59	121.00
11	Y	23	PHE	CB-CG-CD2	-9.32	114.28	120.80
7	I	223	TYR	CB-CG-CD2	-9.32	115.41	121.00
3	C	177	ARG	NE-CZ-NH1	9.29	124.94	120.30
9	b	151	PHE	CB-CG-CD2	-9.28	114.30	120.80
3	E	231	TYR	CB-CG-CD1	-9.28	115.43	121.00
11	Z	135	PHE	CB-CG-CD2	-9.27	114.31	120.80
3	A	209	PHE	CB-CG-CD2	-9.26	114.32	120.80
11	W	11	PHE	CB-CG-CD2	-9.25	114.32	120.80
3	A	555	ASP	CB-CG-OD2	-9.24	109.98	118.30
3	C	110	ARG	NE-CZ-NH2	9.23	124.92	120.30
8	P	259	PHE	CB-CG-CD2	-9.19	114.36	120.80
5	Q	262	PHE	CB-CG-CD2	-9.17	114.38	120.80
7	I	100	PHE	CB-CG-CD1	9.16	127.21	120.80
8	P	273	ASP	CB-CG-OD1	9.16	126.54	118.30
3	C	105	TYR	CB-CG-CD1	9.12	126.47	121.00
5	Q	12	PHE	CB-CG-CD1	-9.12	114.41	120.80
11	X	23	PHE	CB-CG-CD2	-9.11	114.42	120.80
4	F	452	ARG	NE-CZ-NH2	-9.08	115.76	120.30
11	Z	59	MET	CG-SD-CE	-9.07	85.68	100.20
4	D	352	TYR	CB-CG-CD1	9.07	126.44	121.00
10	O	152	TYR	CB-CG-CD1	9.06	126.43	121.00
4	D	73	ASP	CB-CG-OD2	-9.06	110.15	118.30
11	a	155	THR	CA-CB-CG2	-9.05	99.72	112.40
3	E	280	TYR	CB-CG-CD2	-9.03	115.58	121.00
4	B	449	TYR	CB-CG-CD1	9.00	126.40	121.00
11	T	51	PHE	CB-CG-CD1	-9.00	114.50	120.80
11	W	106	PHE	CB-CG-CD2	-8.98	114.51	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	95	PHE	CB-CG-CD2	8.97	127.08	120.80
3	A	146	PHE	CB-CG-CD2	8.96	127.07	120.80
3	A	272	TYR	CB-CG-CD1	8.96	126.38	121.00
10	O	210	TYR	CB-CG-CD2	-8.96	115.62	121.00
3	C	471	TYR	CB-CG-CD1	-8.93	115.64	121.00
3	A	203	ASP	CB-CG-OD2	8.93	126.33	118.30
5	Q	5	TYR	CG-CD1-CE1	-8.92	114.16	121.30
7	I	223	TYR	CB-CG-CD1	8.92	126.36	121.00
4	B	134	ILE	CA-CB-CG1	8.92	127.94	111.00
3	C	126	ARG	NE-CZ-NH2	-8.91	115.84	120.30
9	b	141	TYR	CB-CG-CD1	-8.91	115.66	121.00
11	V	124	ARG	NE-CZ-NH2	8.88	124.74	120.30
8	P	188	ARG	NE-CZ-NH2	-8.87	115.87	120.30
4	D	225	PHE	CB-CG-CD2	8.85	126.99	120.80
4	D	268	TYR	CB-CG-CD1	8.83	126.30	121.00
6	J	25	ARG	NE-CZ-NH2	-8.82	115.89	120.30
3	A	610	ARG	NE-CZ-NH1	-8.81	115.89	120.30
1	M	59	ARG	NE-CZ-NH1	8.80	124.70	120.30
8	P	267	TYR	CB-CG-CD2	8.79	126.28	121.00
3	C	380	PHE	CB-CG-CD2	8.78	126.94	120.80
4	F	225	PHE	CB-CG-CD1	-8.77	114.66	120.80
3	A	545	ASP	CB-CG-OD2	-8.77	110.40	118.30
4	F	443	PHE	CB-CG-CD2	8.77	126.94	120.80
10	O	318	ARG	NE-CZ-NH2	-8.72	115.94	120.30
2	N	80	ARG	NE-CZ-NH2	-8.71	115.94	120.30
3	E	383	TYR	CB-CG-CD2	8.70	126.22	121.00
3	C	202	PHE	CB-CG-CD2	8.70	126.89	120.80
3	E	329	ARG	NE-CZ-NH1	8.68	124.64	120.30
3	C	126	ARG	NE-CZ-NH1	8.68	124.64	120.30
7	I	219	ARG	NE-CZ-NH2	-8.68	115.96	120.30
11	Z	85	TYR	CB-CG-CD2	8.68	126.20	121.00
11	Z	106	PHE	CB-CG-CD2	-8.67	114.73	120.80
4	F	404	TYR	CB-CG-CD2	-8.66	115.80	121.00
7	K	25	ARG	NE-CZ-NH2	8.65	124.62	120.30
3	A	508	SER	N-CA-CB	8.65	123.47	110.50
4	D	404	TYR	CB-CG-CD2	-8.64	115.82	121.00
3	A	380	PHE	CB-CG-CD2	-8.64	114.75	120.80
5	Q	30	TYR	CG-CD2-CE2	-8.64	114.39	121.30
3	E	126	ARG	NE-CZ-NH2	-8.61	116.00	120.30
4	B	449	TYR	CB-CG-CD2	-8.60	115.84	121.00
10	O	48	PHE	CB-CG-CD2	8.59	126.81	120.80
6	J	57	PHE	CB-CG-CD2	-8.57	114.80	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	74	ARG	N-CA-CB	8.57	126.03	110.60
11	U	12	PHE	CB-CG-CD2	-8.54	114.82	120.80
4	B	352	TYR	CB-CG-CD1	8.54	126.12	121.00
4	B	352	TYR	CB-CG-CD2	-8.53	115.88	121.00
11	R	135	PHE	CB-CG-CD2	-8.52	114.84	120.80
3	C	221	ARG	NE-CZ-NH1	8.49	124.55	120.30
4	F	80	PHE	CB-CG-CD1	8.46	126.72	120.80
4	D	268	TYR	CB-CG-CD2	-8.46	115.92	121.00
4	B	404	TYR	CG-CD2-CE2	-8.46	114.53	121.30
3	A	380	PHE	CB-CG-CD1	8.45	126.71	120.80
7	I	25	ARG	NE-CZ-NH2	-8.43	116.09	120.30
4	D	48	ARG	NE-CZ-NH1	8.41	124.51	120.30
11	a	76	TYR	CB-CG-CD2	-8.41	115.95	121.00
4	F	80	PHE	CB-CG-CD2	-8.40	114.92	120.80
6	J	28	ARG	NE-CZ-NH2	-8.39	116.10	120.30
8	P	460	ARG	NE-CZ-NH2	-8.38	116.11	120.30
3	C	54	ASP	CB-CG-OD2	-8.37	110.77	118.30
3	A	610	ARG	NE-CZ-NH2	8.36	124.48	120.30
11	R	135	PHE	CB-CG-CD1	8.35	126.64	120.80
4	B	131	TYR	CB-CG-CD2	-8.34	116.00	121.00
3	C	202	PHE	CB-CG-CD1	-8.34	114.97	120.80
4	B	48	ARG	NE-CZ-NH1	8.32	124.46	120.30
7	I	206	ARG	NE-CZ-NH1	8.32	124.46	120.30
4	F	224	PHE	CB-CG-CD2	8.31	126.62	120.80
11	T	142	TYR	CG-CD2-CE2	-8.30	114.66	121.30
11	W	51	PHE	CB-CG-CD2	-8.30	114.99	120.80
6	H	102	VAL	CA-CB-CG1	8.29	123.34	110.90
3	A	179	ARG	NE-CZ-NH2	-8.27	116.17	120.30
4	D	370	TYR	CB-CG-CD2	-8.25	116.05	121.00
11	X	142	TYR	CB-CG-CD1	8.25	125.95	121.00
5	Q	100	TYR	CB-CG-CD2	-8.22	116.07	121.00
1	M	168	ARG	NE-CZ-NH1	-8.21	116.19	120.30
3	A	484	ARG	NE-CZ-NH2	8.21	124.40	120.30
11	U	126	PHE	CB-CG-CD2	8.19	126.54	120.80
11	Z	142	TYR	CB-CG-CD2	-8.19	116.08	121.00
6	H	101	THR	CA-CB-CG2	-8.19	100.94	112.40
3	A	463	TYR	CB-CG-CD2	-8.17	116.10	121.00
3	C	471	TYR	CB-CG-CD2	8.17	125.90	121.00
11	X	153	ARG	NE-CZ-NH1	8.17	124.39	120.30
4	F	393	ARG	NE-CZ-NH1	8.16	124.38	120.30
3	C	392	TYR	CB-CG-CD1	-8.16	116.10	121.00
3	C	24	TYR	CB-CG-CD2	-8.16	116.11	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	X	113	ASP	CB-CG-OD1	-8.14	110.97	118.30
11	T	88	PHE	CB-CG-CD1	8.09	126.46	120.80
3	C	414	ALA	N-CA-CB	8.07	121.40	110.10
3	E	406	ARG	NE-CZ-NH1	8.05	124.33	120.30
3	A	600	PHE	CB-CG-CD2	-8.04	115.17	120.80
4	B	302	ARG	NE-CZ-NH1	8.04	124.32	120.30
3	A	146	PHE	CB-CG-CD1	-8.01	115.19	120.80
3	A	485	MET	CG-SD-CE	-8.01	87.38	100.20
1	M	193	ASP	CB-CG-OD1	8.01	125.51	118.30
3	A	158	TYR	CB-CG-CD2	-8.01	116.20	121.00
3	A	484	ARG	NE-CZ-NH1	-8.01	116.30	120.30
1	M	197	ARG	NE-CZ-NH2	-8.00	116.30	120.30
10	O	300	PHE	CB-CG-CD1	-8.00	115.20	120.80
3	C	221	ARG	NE-CZ-NH2	-8.00	116.30	120.30
3	A	576	ASP	CB-CG-OD2	-8.00	111.10	118.30
11	U	136	ALA	CB-CA-C	-8.00	98.10	110.10
1	M	201	TYR	CB-CG-CD2	-8.00	116.20	121.00
11	U	153	ARG	NE-CZ-NH1	7.98	124.29	120.30
7	K	85	ARG	NE-CZ-NH1	7.97	124.29	120.30
11	X	76	TYR	CB-CG-CD2	-7.96	116.22	121.00
4	F	455	PHE	CB-CG-CD2	-7.95	115.23	120.80
7	G	195	ASP	N-CA-CB	7.94	124.90	110.60
5	Q	92	ARG	NE-CZ-NH2	-7.94	116.33	120.30
11	S	142	TYR	CB-CG-CD1	7.93	125.76	121.00
9	b	262	ASP	CB-CG-OD2	-7.92	111.17	118.30
4	B	95	PHE	CB-CG-CD1	7.92	126.34	120.80
9	b	20	TYR	CB-CG-CD2	-7.89	116.26	121.00
10	O	375	ALA	N-CA-CB	7.89	121.15	110.10
11	U	153	ARG	NE-CZ-NH2	7.89	124.25	120.30
5	Q	249	TYR	CB-CG-CD1	-7.88	116.27	121.00
2	N	40	TYR	CB-CG-CD2	-7.87	116.28	121.00
8	P	463	TYR	CG-CD2-CE2	-7.87	115.00	121.30
4	F	131	TYR	CB-CG-CD1	7.86	125.71	121.00
5	Q	77	TYR	CB-CG-CD1	7.86	125.71	121.00
3	E	297	PHE	CB-CG-CD2	7.84	126.29	120.80
3	C	423	PHE	CB-CG-CD1	-7.84	115.31	120.80
3	A	342	TYR	CB-CG-CD1	7.80	125.68	121.00
7	I	23	PHE	CB-CG-CD1	-7.80	115.34	120.80
11	Z	76	TYR	CB-CG-CD2	-7.80	116.32	121.00
11	T	142	TYR	CB-CG-CD1	-7.79	116.33	121.00
7	G	167	ALA	N-CA-CB	7.78	121.00	110.10
5	Q	5	TYR	CB-CG-CD1	-7.78	116.33	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	129	ASP	CB-CG-OD2	-7.78	111.30	118.30
5	Q	218	ARG	NE-CZ-NH2	-7.75	116.42	120.30
4	F	59	ASP	CB-CG-OD2	-7.73	111.34	118.30
1	M	168	ARG	NE-CZ-NH2	7.73	124.16	120.30
11	R	46	ARG	NE-CZ-NH2	-7.72	116.44	120.30
8	P	420	ILE	CA-CB-CG1	-7.71	96.36	111.00
4	B	144	ARG	NE-CZ-NH2	7.70	124.15	120.30
3	C	238	ARG	NE-CZ-NH2	-7.69	116.46	120.30
4	F	146	TYR	CG-CD2-CE2	-7.68	115.15	121.30
11	Z	51	PHE	CB-CG-CD2	7.68	126.18	120.80
7	I	92	ARG	NE-CZ-NH1	7.67	124.13	120.30
3	E	76	THR	CA-CB-CG2	-7.65	101.69	112.40
8	P	215	PHE	CB-CG-CD2	-7.65	115.44	120.80
5	Q	94	PHE	CB-CG-CD1	-7.64	115.45	120.80
3	E	392	TYR	CB-CG-CD2	-7.63	116.42	121.00
8	P	109	TYR	CB-CG-CD1	-7.63	116.42	121.00
11	S	142	TYR	CB-CG-CD2	-7.61	116.43	121.00
7	G	160	TYR	CB-CG-CD1	7.61	125.56	121.00
3	C	470	PHE	CB-CG-CD2	7.60	126.12	120.80
9	b	67	ARG	NE-CZ-NH1	-7.60	116.50	120.30
4	B	118	ARG	NE-CZ-NH2	-7.59	116.50	120.30
9	b	110	TYR	CB-CG-CD2	-7.59	116.44	121.00
7	I	85	ARG	NE-CZ-NH1	7.57	124.09	120.30
8	P	463	TYR	CB-CG-CD1	7.54	125.53	121.00
8	P	223	ASP	CB-CG-OD2	7.54	125.08	118.30
11	a	35	SER	N-CA-CB	7.54	121.81	110.50
2	N	5	ARG	NE-CZ-NH1	-7.54	116.53	120.30
9	b	320	PHE	CB-CG-CD2	-7.54	115.53	120.80
4	D	284	TYR	CB-CG-CD2	-7.53	116.48	121.00
10	O	160	ALA	CB-CA-C	-7.52	98.82	110.10
9	b	292	SER	N-CA-CB	7.52	121.78	110.50
4	D	237	ARG	NE-CZ-NH2	7.51	124.05	120.30
3	E	482	ARG	NE-CZ-NH1	7.51	124.05	120.30
3	A	386	ALA	N-CA-CB	7.50	120.60	110.10
3	C	475	TYR	CB-CG-CD2	7.49	125.50	121.00
7	K	223	TYR	CB-CG-CD1	-7.49	116.51	121.00
3	E	422	ASP	CB-CG-OD1	-7.49	111.56	118.30
3	C	314	ARG	NE-CZ-NH1	7.46	124.03	120.30
11	V	88	PHE	CB-CG-CD1	7.45	126.02	120.80
4	B	321	ARG	NE-CZ-NH1	7.45	124.03	120.30
4	B	445	THR	CA-CB-CG2	-7.45	101.97	112.40
8	P	128	PHE	CB-CG-CD1	7.43	126.00	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	21	ARG	NE-CZ-NH2	7.43	124.02	120.30
8	P	392	TYR	CB-CG-CD2	-7.43	116.54	121.00
11	R	126	PHE	CB-CG-CD1	7.42	126.00	120.80
9	b	17	VAL	CA-CB-CG2	-7.42	99.77	110.90
11	U	35	SER	N-CA-CB	7.42	121.62	110.50
3	A	345	ASP	N-CA-CB	7.40	123.92	110.60
3	A	394	ARG	NE-CZ-NH2	-7.40	116.60	120.30
4	F	229	PHE	CB-CG-CD2	7.39	125.97	120.80
7	G	195	ASP	CB-CG-OD1	-7.38	111.66	118.30
3	C	425	ASP	CB-CG-OD2	-7.38	111.66	118.30
10	O	53	PHE	CB-CG-CD2	-7.36	115.64	120.80
11	a	30	TYR	CB-CG-CD1	7.36	125.42	121.00
4	B	71	ARG	NE-CZ-NH2	-7.35	116.62	120.30
5	Q	20	TYR	CB-CG-CD2	-7.35	116.59	121.00
6	H	22	SER	N-CA-CB	7.33	121.50	110.50
8	P	255	PHE	CB-CG-CD2	-7.33	115.67	120.80
4	B	142	TYR	CB-CG-CD1	-7.33	116.60	121.00
3	C	290	MET	CG-SD-CE	7.32	111.91	100.20
10	O	206	PHE	CB-CG-CD2	-7.32	115.68	120.80
11	V	106	PHE	CB-CG-CD2	-7.32	115.68	120.80
3	C	158	TYR	CB-CG-CD2	-7.31	116.61	121.00
4	F	180	HIS	CA-CB-CG	7.31	126.03	113.60
11	U	18	ALA	N-CA-CB	7.30	120.33	110.10
11	X	153	ARG	NE-CZ-NH2	-7.30	116.65	120.30
11	Z	30	TYR	CB-CG-CD1	-7.29	116.62	121.00
10	O	231	TYR	CB-CG-CD1	7.29	125.37	121.00
5	Q	341	TYR	CG-CD2-CE2	7.29	127.13	121.30
10	O	6	TYR	CG-CD1-CE1	-7.28	115.47	121.30
6	H	25	ARG	NE-CZ-NH1	-7.28	116.66	120.30
4	D	319	ALA	N-CA-CB	7.28	120.29	110.10
11	a	33	ALA	N-CA-CB	7.28	120.29	110.10
11	V	154	ALA	CB-CA-C	-7.28	99.19	110.10
3	E	304	MET	CG-SD-CE	-7.27	88.57	100.20
3	C	123	TYR	CB-CG-CD2	-7.27	116.64	121.00
11	Z	106	PHE	CB-CG-CD1	7.25	125.88	120.80
4	F	225	PHE	CB-CG-CD2	7.25	125.88	120.80
3	E	110	ARG	N-CA-CB	7.24	123.64	110.60
7	K	100	PHE	CB-CG-CD1	7.24	125.87	120.80
11	V	142	TYR	CG-CD1-CE1	-7.24	115.51	121.30
7	K	92	ARG	NE-CZ-NH1	7.22	123.91	120.30
9	b	270	ARG	NE-CZ-NH1	7.22	123.91	120.30
11	U	153	ARG	NH1-CZ-NH2	-7.21	111.46	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	273	TYR	N-CA-CB	7.21	123.58	110.60
1	M	134	ARG	NE-CZ-NH1	7.21	123.90	120.30
3	C	535	ASP	CB-CG-OD1	-7.20	111.82	118.30
4	F	484	PHE	CB-CG-CD2	-7.20	115.76	120.80
4	B	316	TYR	CB-CG-CD2	-7.19	116.68	121.00
5	Q	20	TYR	CG-CD2-CE2	-7.19	115.55	121.30
4	B	448	ALA	CB-CA-C	-7.19	99.32	110.10
11	X	51	PHE	CB-CG-CD1	7.18	125.83	120.80
4	F	354	THR	CA-CB-CG2	-7.17	102.36	112.40
3	A	448	ARG	NE-CZ-NH2	-7.17	116.72	120.30
11	a	12	PHE	CB-CG-CD1	-7.17	115.78	120.80
3	E	207	SER	N-CA-CB	7.16	121.25	110.50
3	E	284	GLY	N-CA-C	-7.16	95.20	113.10
7	K	178	TYR	CB-CG-CD1	-7.16	116.71	121.00
9	b	141	TYR	CB-CG-CD2	7.15	125.29	121.00
4	B	268	TYR	CB-CG-CD1	7.15	125.29	121.00
1	M	112	TYR	CG-CD1-CE1	7.15	127.02	121.30
4	B	370	TYR	CB-CG-CD1	-7.14	116.71	121.00
9	b	285	TYR	CB-CG-CD2	7.13	125.28	121.00
9	b	248	ARG	NE-CZ-NH2	-7.13	116.73	120.30
11	W	153	ARG	NE-CZ-NH2	-7.13	116.73	120.30
8	P	228	THR	CA-CB-CG2	-7.13	102.42	112.40
4	F	113	PHE	CB-CG-CD2	-7.11	115.82	120.80
3	A	177	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	M	65	ALA	N-CA-CB	7.10	120.04	110.10
3	A	141	PHE	CB-CG-CD2	-7.10	115.83	120.80
4	B	144	ARG	NE-CZ-NH1	-7.09	116.75	120.30
3	C	297	PHE	CB-CG-CD2	-7.09	115.84	120.80
7	K	166	ARG	NE-CZ-NH1	7.09	123.84	120.30
4	F	400	SER	N-CA-CB	-7.08	99.88	110.50
11	X	76	TYR	CB-CG-CD1	7.07	125.24	121.00
4	F	302	ARG	NE-CZ-NH1	-7.07	116.77	120.30
5	Q	100	TYR	CG-CD1-CE1	-7.06	115.65	121.30
3	E	334	TYR	CB-CG-CD2	-7.06	116.76	121.00
11	S	88	PHE	CB-CG-CD1	7.06	125.74	120.80
4	F	144	ARG	NE-CZ-NH1	7.06	123.83	120.30
8	P	475	TYR	CB-CG-CD2	-7.05	116.77	121.00
5	Q	218	ARG	NE-CZ-NH1	7.05	123.82	120.30
4	F	475	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	M	95	ARG	NE-CZ-NH2	-7.03	116.79	120.30
11	X	64	ALA	CB-CA-C	-7.01	99.58	110.10
10	O	346	ASP	CB-CG-OD2	7.01	124.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	71	ARG	NE-CZ-NH2	-7.00	116.80	120.30
6	H	80	LEU	CB-CG-CD2	7.00	122.90	111.00
3	E	301	TYR	CB-CG-CD2	7.00	125.20	121.00
4	F	435	PHE	CB-CG-CD1	7.00	125.70	120.80
3	A	460	TYR	CB-CG-CD1	6.99	125.19	121.00
3	C	212	TYR	CB-CG-CD1	6.98	125.19	121.00
9	b	116	TYR	CB-CG-CD1	6.97	125.18	121.00
10	O	388	TYR	CB-CG-CD2	6.97	125.18	121.00
5	Q	114	THR	CA-CB-CG2	-6.96	102.66	112.40
5	Q	188	TYR	CB-CG-CD2	-6.96	116.82	121.00
3	E	164	ASN	N-CA-CB	6.96	123.12	110.60
2	N	38	PHE	CB-CG-CD1	6.95	125.66	120.80
4	B	321	ARG	NE-CZ-NH2	-6.95	116.83	120.30
11	X	142	TYR	CB-CG-CD2	-6.95	116.83	121.00
11	W	119	SER	N-CA-CB	6.95	120.92	110.50
7	K	160	TYR	CB-CG-CD1	-6.94	116.84	121.00
11	R	60	ALA	CB-CA-C	-6.93	99.70	110.10
9	b	70	ARG	NE-CZ-NH2	-6.92	116.84	120.30
3	C	345	ASP	CB-CG-OD1	-6.92	112.07	118.30
1	M	17	LEU	CB-CG-CD2	6.91	122.75	111.00
3	A	272	TYR	CG-CD1-CE1	-6.91	115.77	121.30
1	M	13	MET	CG-SD-CE	-6.91	89.14	100.20
7	G	97	ASP	CB-CG-OD2	-6.89	112.09	118.30
3	C	520	LEU	CB-CG-CD2	6.88	122.70	111.00
4	F	309	TYR	CB-CG-CD2	-6.88	116.87	121.00
9	b	208	ARG	NE-CZ-NH1	6.88	123.74	120.30
2	N	52	ASP	CB-CG-OD1	6.88	124.49	118.30
3	C	98	PRO	N-CA-CB	6.87	111.55	103.30
7	K	114	ARG	NE-CZ-NH1	-6.86	116.87	120.30
9	b	133	VAL	CA-CB-CG1	6.86	121.19	110.90
11	S	48	ASP	CB-CG-OD1	6.86	124.47	118.30
3	C	429	THR	CA-CB-CG2	-6.85	102.81	112.40
4	B	74	ARG	NE-CZ-NH1	6.85	123.72	120.30
3	C	431	THR	CA-CB-CG2	-6.84	102.82	112.40
4	F	223	ARG	NE-CZ-NH2	6.84	123.72	120.30
3	A	48	LEU	CB-CG-CD1	6.84	122.62	111.00
3	E	478	PHE	CB-CG-CD2	6.82	125.58	120.80
3	E	591	ARG	NE-CZ-NH2	-6.82	116.89	120.30
4	B	319	ALA	CB-CA-C	-6.82	99.87	110.10
8	P	109	TYR	CB-CG-CD2	6.82	125.09	121.00
10	O	268	ASP	CB-CG-OD2	6.81	124.43	118.30
7	G	160	TYR	CB-CG-CD2	-6.80	116.92	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	362	ARG	NE-CZ-NH1	6.80	123.70	120.30
3	A	423	PHE	CB-CG-CD2	-6.79	116.05	120.80
3	A	471	TYR	CB-CG-CD1	-6.79	116.93	121.00
3	E	342	TYR	CB-CG-CD2	-6.79	116.93	121.00
3	A	482	ARG	NE-CZ-NH2	6.77	123.69	120.30
11	U	32	THR	CA-CB-CG2	-6.77	102.92	112.40
11	V	88	PHE	CB-CG-CD2	-6.77	116.06	120.80
4	F	295	ARG	NE-CZ-NH2	6.76	123.68	120.30
3	E	406	ARG	NE-CZ-NH2	-6.75	116.92	120.30
10	O	196	VAL	CA-CB-CG2	-6.75	100.77	110.90
4	D	393	ARG	NE-CZ-NH1	-6.74	116.93	120.30
3	E	141	PHE	CB-CG-CD1	-6.74	116.08	120.80
3	E	266	SER	CB-CA-C	-6.74	97.30	110.10
3	E	46	TYR	CB-CA-C	-6.73	96.93	110.40
11	R	124	ARG	NE-CZ-NH2	-6.72	116.94	120.30
3	E	544	PHE	CB-CG-CD2	-6.72	116.10	120.80
4	F	46	PHE	CB-CG-CD2	-6.72	116.10	120.80
7	G	145	ASP	CB-CG-OD1	-6.71	112.26	118.30
3	C	203	ASP	CB-CG-OD1	-6.69	112.28	118.30
10	O	231	TYR	CB-CG-CD2	-6.69	116.99	121.00
3	C	515	LEU	CB-CG-CD2	6.68	122.36	111.00
11	U	126	PHE	CB-CG-CD1	-6.68	116.12	120.80
9	b	300	TYR	CB-CG-CD1	6.68	125.01	121.00
4	B	74	ARG	NE-CZ-NH2	-6.68	116.96	120.30
8	P	210	PHE	CB-CG-CD1	6.67	125.47	120.80
8	P	259	PHE	CB-CG-CD1	6.67	125.47	120.80
10	O	350	PHE	CB-CG-CD2	-6.67	116.13	120.80
11	V	153	ARG	NE-CZ-NH1	6.67	123.64	120.30
3	C	586	PHE	CB-CG-CD1	-6.67	116.13	120.80
11	U	12	PHE	CB-CG-CD1	6.66	125.46	120.80
3	A	46	TYR	CB-CG-CD2	6.66	125.00	121.00
2	N	61	ARG	NE-CZ-NH2	6.66	123.63	120.30
11	U	11	PHE	CB-CG-CD1	-6.66	116.14	120.80
1	M	63	THR	CA-CB-CG2	-6.65	103.09	112.40
4	B	257	ARG	NE-CZ-NH2	-6.65	116.97	120.30
7	I	43	TYR	CG-CD2-CE2	-6.65	115.98	121.30
4	F	229	PHE	CB-CG-CD1	-6.65	116.15	120.80
3	A	168	SER	N-CA-CB	6.64	120.47	110.50
9	b	108	ASP	CB-CG-OD2	-6.64	112.32	118.30
11	R	54	ILE	O-C-N	-6.64	112.07	122.70
3	E	370	ARG	NE-CZ-NH1	6.64	123.62	120.30
4	F	370	TYR	CB-CG-CD1	-6.64	117.02	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	88	VAL	CG1-CB-CG2	-6.64	100.28	110.90
3	C	334	TYR	CB-CG-CD1	-6.63	117.02	121.00
11	S	50	LEU	CB-CG-CD2	6.63	122.28	111.00
11	R	12	PHE	CB-CG-CD1	6.63	125.44	120.80
5	Q	126	ARG	NE-CZ-NH1	6.62	123.61	120.30
9	b	67	ARG	NE-CZ-NH2	6.62	123.61	120.30
4	F	272	ARG	NE-CZ-NH2	6.62	123.61	120.30
10	O	303	TRP	CG-CD2-CE3	-6.60	127.96	133.90
4	D	270	THR	CA-CB-CG2	-6.60	103.16	112.40
3	C	244	PHE	CD1-CE1-CZ	6.60	128.01	120.10
3	A	591	ARG	NE-CZ-NH1	6.60	123.60	120.30
4	B	111	ARG	NE-CZ-NH1	6.59	123.60	120.30
9	b	27	ARG	NE-CZ-NH1	6.59	123.60	120.30
3	E	162	PHE	CB-CG-CD2	6.59	125.41	120.80
11	a	19	SER	N-CA-CB	6.59	120.39	110.50
3	C	186	ALA	N-CA-CB	6.59	119.32	110.10
5	Q	217	ASP	CB-CG-OD2	-6.58	112.38	118.30
11	X	11	PHE	CB-CG-CD2	-6.57	116.20	120.80
3	E	553	TYR	CB-CG-CD1	6.57	124.94	121.00
11	W	126	PHE	CB-CG-CD2	6.57	125.40	120.80
4	F	256	PRO	N-CA-CB	6.57	111.18	103.30
3	A	235	THR	CA-CB-CG2	-6.57	103.20	112.40
10	O	231	TYR	CZ-CE2-CD2	6.57	125.71	119.80
7	I	195	ASP	CB-CG-OD1	6.57	124.21	118.30
11	W	85	TYR	CB-CG-CD1	6.56	124.94	121.00
11	V	46	ARG	NE-CZ-NH2	6.56	123.58	120.30
3	C	129	ASP	CB-CG-OD2	-6.55	112.40	118.30
3	A	531	TYR	CG-CD2-CE2	-6.55	116.06	121.30
10	O	388	TYR	CA-CB-CG	-6.55	100.95	113.40
5	Q	162	PHE	CB-CG-CD1	-6.55	116.22	120.80
8	P	328	ARG	NE-CZ-NH2	6.55	123.58	120.30
4	D	223	ARG	NE-CZ-NH2	6.55	123.57	120.30
3	C	329	ARG	NE-CZ-NH2	-6.55	117.03	120.30
11	W	12	PHE	CB-CA-C	-6.53	97.33	110.40
11	X	32	THR	CA-CB-CG2	-6.53	103.25	112.40
4	D	404	TYR	CG-CD1-CE1	-6.53	116.08	121.30
11	W	126	PHE	CB-CG-CD1	-6.53	116.23	120.80
1	M	182	GLU	OE1-CD-OE2	6.53	131.13	123.30
11	Z	135	PHE	CB-CG-CD1	6.52	125.37	120.80
3	E	139	TRP	CB-CG-CD1	6.52	135.48	127.00
8	P	350	TYR	CB-CG-CD1	-6.52	117.09	121.00
11	W	76	TYR	CG-CD1-CE1	-6.52	116.08	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	420	VAL	CA-CB-CG2	6.51	120.67	110.90
3	A	525	PHE	CB-CG-CD1	6.51	125.36	120.80
7	I	211	SER	N-CA-CB	6.50	120.25	110.50
8	P	267	TYR	CB-CG-CD1	-6.49	117.11	121.00
7	I	62	PHE	CB-CG-CD1	6.47	125.33	120.80
7	K	178	TYR	CB-CG-CD2	6.47	124.88	121.00
11	a	100	SER	N-CA-CB	6.47	120.21	110.50
10	O	98	ARG	NE-CZ-NH2	-6.47	117.07	120.30
5	Q	149	TYR	CB-CG-CD2	6.46	124.88	121.00
11	Y	51	PHE	CB-CG-CD1	6.46	125.32	120.80
10	O	1	MET	CG-SD-CE	-6.45	89.88	100.20
9	b	176	ILE	CA-CB-CG1	6.45	123.25	111.00
4	F	127	PHE	CB-CG-CD1	6.45	125.31	120.80
3	A	472	ASP	CB-CG-OD1	6.45	124.10	118.30
10	O	299	VAL	CA-CB-CG2	-6.44	101.23	110.90
8	P	463	TYR	CZ-CE2-CD2	6.44	125.60	119.80
3	C	329	ARG	NE-CZ-NH1	6.44	123.52	120.30
4	B	80	PHE	CB-CG-CD2	-6.44	116.29	120.80
1	M	67	SER	N-CA-CB	6.44	120.16	110.50
3	C	354	ALA	N-CA-CB	6.44	119.11	110.10
4	F	354	THR	N-CA-CB	6.43	122.52	110.30
10	O	353	GLY	O-C-N	6.43	132.99	122.70
3	A	468	ASN	CB-CA-C	6.43	123.25	110.40
11	X	142	TYR	CA-CB-CG	6.43	125.61	113.40
11	Z	126	PHE	N-CA-CB	6.43	122.17	110.60
3	E	270	SER	CB-CA-C	-6.42	97.89	110.10
3	C	148	VAL	CA-CB-CG1	-6.42	101.27	110.90
11	a	160	CYS	CA-CB-SG	-6.42	102.45	114.00
3	C	244	PHE	CG-CD1-CE1	-6.41	113.74	120.80
3	E	352	MET	CG-SD-CE	-6.41	89.94	100.20
3	A	365	ARG	NE-CZ-NH1	-6.41	117.10	120.30
3	E	329	ARG	NE-CZ-NH2	-6.40	117.10	120.30
7	I	114	ARG	NE-CZ-NH2	-6.38	117.11	120.30
10	O	365	ASN	N-CA-CB	6.38	122.09	110.60
11	W	153	ARG	CD-NE-CZ	-6.38	114.67	123.60
3	A	565	ALA	CB-CA-C	-6.38	100.53	110.10
8	P	33	SER	N-CA-CB	6.38	120.07	110.50
3	E	37	ALA	N-CA-CB	6.38	119.03	110.10
3	C	102	GLU	N-CA-CB	6.37	122.06	110.60
1	M	81	TYR	CB-CG-CD2	-6.36	117.18	121.00
3	A	509	ASP	CB-CG-OD1	6.36	124.02	118.30
4	B	393	ARG	NE-CZ-NH2	-6.35	117.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	535	ASP	CB-CG-OD2	6.35	124.01	118.30
8	P	152	GLN	N-CA-CB	6.35	122.02	110.60
3	C	344	ARG	NE-CZ-NH1	6.35	123.47	120.30
11	Y	155	THR	CA-CB-CG2	-6.34	103.53	112.40
8	P	255	PHE	CB-CG-CD1	6.33	125.23	120.80
3	A	442	ASP	CB-CG-OD1	-6.33	112.60	118.30
5	Q	335	ARG	NE-CZ-NH2	6.33	123.47	120.30
8	P	370	TRP	CE2-CD2-CG	-6.33	102.24	107.30
1	M	66	PHE	CB-CG-CD1	6.33	125.23	120.80
3	C	94	VAL	CA-CB-CG2	-6.32	101.42	110.90
7	I	165	GLN	C-N-CA	6.32	137.50	121.70
10	O	350	PHE	CB-CG-CD1	6.32	125.22	120.80
3	E	73	TYR	CZ-CE2-CD2	6.32	125.48	119.80
5	Q	30	TYR	CZ-CE2-CD2	6.32	125.49	119.80
9	b	110	TYR	CB-CG-CD1	6.32	124.79	121.00
7	I	97	ASP	CB-CG-OD2	-6.32	112.61	118.30
10	O	246	PHE	CB-CG-CD1	6.31	125.22	120.80
5	Q	345	TYR	N-CA-CB	6.31	121.95	110.60
10	O	98	ARG	NE-CZ-NH1	6.30	123.45	120.30
11	Z	126	PHE	CB-CG-CD2	6.30	125.21	120.80
3	E	548	ARG	NE-CZ-NH2	-6.30	117.15	120.30
10	O	348	PHE	CB-CG-CD1	6.30	125.21	120.80
3	C	377	ASP	C-N-CA	6.29	137.42	121.70
5	Q	71	TYR	CG-CD2-CE2	-6.29	116.27	121.30
7	G	188	VAL	CA-CB-CG1	-6.29	101.47	110.90
4	B	173	PHE	CB-CG-CD1	-6.29	116.40	120.80
4	F	30	THR	CA-CB-CG2	-6.29	103.60	112.40
4	D	63	ARG	NE-CZ-NH2	6.28	123.44	120.30
2	N	101	TYR	CZ-CE2-CD2	-6.28	114.15	119.80
4	D	448	ALA	CB-CA-C	6.28	119.52	110.10
4	D	295	ARG	NE-CZ-NH1	6.28	123.44	120.30
11	Z	35	SER	N-CA-CB	6.28	119.92	110.50
4	B	316	TYR	CB-CG-CD1	6.27	124.76	121.00
1	M	156	PHE	CB-CG-CD1	6.27	125.19	120.80
3	A	334	TYR	CG-CD2-CE2	-6.27	116.28	121.30
3	A	383	TYR	CB-CG-CD1	-6.27	117.24	121.00
7	K	85	ARG	NE-CZ-NH2	-6.27	117.17	120.30
3	E	88	THR	CA-CB-CG2	-6.26	103.64	112.40
3	E	280	TYR	CB-CG-CD1	6.26	124.76	121.00
7	K	154	ASP	CB-CG-OD2	6.26	123.93	118.30
11	X	23	PHE	CB-CG-CD1	6.25	125.17	120.80
4	F	455	PHE	CB-CG-CD1	6.23	125.16	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	117	TYR	CB-CG-CD1	-6.22	117.27	121.00
3	A	343	PHE	CB-CG-CD2	-6.22	116.45	120.80
4	F	335	LEU	CB-CG-CD2	-6.22	100.43	111.00
11	T	19	SER	N-CA-CB	6.21	119.82	110.50
2	N	57	PHE	CB-CG-CD2	-6.21	116.45	120.80
1	M	193	ASP	CB-CG-OD2	-6.21	112.71	118.30
4	B	404	TYR	CZ-CE2-CD2	6.21	125.39	119.80
11	Z	45	LEU	CB-CG-CD2	6.21	121.55	111.00
4	D	462	TRP	CG-CD2-CE3	-6.20	128.32	133.90
4	F	146	TYR	CD1-CG-CD2	6.20	124.72	117.90
11	U	29	ALA	N-CA-CB	6.20	118.78	110.10
4	F	463	SER	N-CA-CB	6.20	119.80	110.50
10	O	202	LEU	CB-CG-CD2	6.20	121.54	111.00
11	R	126	PHE	N-CA-CB	6.20	121.75	110.60
4	D	229	PHE	CB-CG-CD2	-6.19	116.46	120.80
4	B	443	PHE	CB-CG-CD2	-6.19	116.46	120.80
11	V	150	LEU	CB-CG-CD1	6.19	121.53	111.00
4	B	374	ASN	N-CA-CB	6.19	121.74	110.60
7	G	53	ASN	C-N-CA	6.19	137.17	121.70
7	G	165	GLN	C-N-CA	6.19	137.17	121.70
3	E	304	MET	CA-CB-CG	6.19	123.82	113.30
10	O	48	PHE	CB-CG-CD1	-6.19	116.47	120.80
10	O	42	ARG	NE-CZ-NH2	-6.18	117.21	120.30
11	R	76	TYR	CB-CG-CD2	6.18	124.71	121.00
3	C	279	ILE	CA-CB-CG1	6.18	122.74	111.00
11	Y	76	TYR	CB-CG-CD1	-6.18	117.29	121.00
3	E	452	PRO	N-CA-CB	6.17	110.71	103.30
3	A	525	PHE	CB-CG-CD2	-6.17	116.48	120.80
5	Q	304	PHE	CB-CG-CD2	6.17	125.12	120.80
3	A	439	TRP	CB-CG-CD2	-6.17	118.58	126.60
10	O	258	ARG	NE-CZ-NH1	-6.17	117.22	120.30
5	Q	133	PHE	CB-CG-CD2	-6.17	116.48	120.80
11	V	85	TYR	CB-CG-CD1	6.17	124.70	121.00
3	A	456	THR	CA-CB-CG2	-6.16	103.78	112.40
4	B	295	ARG	NE-CZ-NH1	6.15	123.38	120.30
8	P	22	SER	N-CA-CB	6.15	119.73	110.50
9	b	348	THR	CA-CB-CG2	-6.15	103.79	112.40
11	U	26	LEU	CB-CG-CD2	6.15	121.45	111.00
3	A	541	TRP	CZ3-CH2-CZ2	-6.15	114.22	121.60
9	b	324	ASN	CB-CG-OD1	-6.15	109.31	121.60
9	b	149	ASP	CB-CG-OD1	6.13	123.82	118.30
7	K	169	LEU	CB-CG-CD1	6.13	121.42	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	355	ASP	CB-CG-OD2	-6.12	112.79	118.30
9	b	82	LYS	O-C-N	6.12	132.49	122.70
2	N	111	ARG	NE-CZ-NH2	6.11	123.36	120.30
11	X	113	ASP	CB-CG-OD2	6.11	123.80	118.30
7	I	158	ARG	NE-CZ-NH2	-6.11	117.25	120.30
8	P	330	TYR	CB-CG-CD1	6.10	124.66	121.00
4	D	80	PHE	CB-CG-CD1	-6.09	116.53	120.80
3	C	293	VAL	CG1-CB-CG2	6.09	120.64	110.90
7	K	83	LYS	CB-CA-C	-6.09	98.22	110.40
11	X	135	PHE	CG-CD2-CE2	-6.08	114.11	120.80
4	F	468	TYR	CG-CD1-CE1	-6.08	116.44	121.30
6	L	87	ALA	O-C-N	-6.08	112.97	122.70
8	P	116	PHE	CB-CG-CD1	-6.08	116.55	120.80
4	D	261	THR	O-C-N	-6.08	112.98	122.70
4	B	114	ASP	CB-CG-OD1	-6.08	112.83	118.30
3	E	87	ARG	NH1-CZ-NH2	6.07	126.07	119.40
5	Q	254	PHE	CB-CG-CD1	6.07	125.05	120.80
6	J	27	TYR	CB-CG-CD2	-6.07	117.36	121.00
11	Y	60	ALA	CB-CA-C	-6.06	101.01	110.10
3	E	365	ARG	NE-CZ-NH2	6.06	123.33	120.30
4	F	370	TYR	CG-CD2-CE2	-6.06	116.46	121.30
4	D	272	ARG	NH1-CZ-NH2	-6.05	112.74	119.40
7	I	129	LEU	CB-CG-CD2	6.04	121.28	111.00
5	Q	345	TYR	CB-CG-CD2	-6.04	117.38	121.00
9	b	194	ASP	CB-CG-OD2	6.03	123.73	118.30
4	D	95	PHE	CB-CG-CD1	-6.03	116.58	120.80
4	B	286	ASP	CB-CG-OD2	6.03	123.73	118.30
3	C	305	SER	N-CA-CB	6.03	119.54	110.50
4	B	196	PRO	N-CA-CB	6.03	110.53	103.30
11	Z	99	LEU	CB-CG-CD2	6.02	121.24	111.00
3	C	423	PHE	CB-CG-CD2	6.02	125.01	120.80
3	A	567	TRP	CG-CD2-CE3	-6.01	128.49	133.90
5	Q	332	GLN	C-N-CA	6.01	136.73	121.70
5	Q	341	TYR	CZ-CE2-CD2	-6.01	114.39	119.80
6	J	95	VAL	CA-CB-CG2	-6.01	101.89	110.90
11	Z	84	LEU	CB-CG-CD2	-6.01	100.79	111.00
4	F	449	TYR	CZ-CE2-CD2	-6.01	114.39	119.80
3	E	423	PHE	CB-CG-CD1	6.00	125.00	120.80
3	A	191	TYR	CD1-CE1-CZ	6.00	125.20	119.80
3	C	544	PHE	CB-CG-CD2	6.00	125.00	120.80
4	D	337	MET	CG-SD-CE	-6.00	90.60	100.20
4	F	357	GLN	N-CA-CB	6.00	121.40	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	304	TYR	CB-CG-CD1	-6.00	117.40	121.00
1	M	122	LEU	CB-CA-C	-6.00	98.81	110.20
4	D	339	ASN	N-CA-CB	5.99	121.39	110.60
9	b	14	MET	CG-SD-CE	5.99	109.79	100.20
3	C	460	TYR	CG-CD2-CE2	-5.99	116.51	121.30
4	F	121	ASP	CB-CG-OD2	-5.99	112.91	118.30
4	B	407	TYR	CB-CG-CD2	5.99	124.59	121.00
11	T	141	LEU	CB-CG-CD2	5.99	121.17	111.00
3	E	179	ARG	NE-CZ-NH1	-5.98	117.31	120.30
3	E	534	TYR	CG-CD1-CE1	-5.98	116.52	121.30
3	A	511	ASP	O-C-N	-5.98	113.13	122.70
4	D	265	TYR	CB-CG-CD2	-5.98	117.41	121.00
3	C	422	ASP	CB-CG-OD1	-5.97	112.92	118.30
3	E	231	TYR	CD1-CG-CD2	5.97	124.47	117.90
3	E	533	THR	CA-CB-CG2	-5.97	104.04	112.40
4	F	189	ARG	NE-CZ-NH2	-5.97	117.31	120.30
8	P	211	MET	CA-C-O	-5.97	107.56	120.10
3	A	305	SER	N-CA-CB	5.97	119.45	110.50
3	A	534	TYR	CD1-CE1-CZ	-5.96	114.43	119.80
3	E	193	LEU	CB-CG-CD2	5.96	121.13	111.00
7	I	43	TYR	CD1-CG-CD2	5.96	124.45	117.90
11	X	135	PHE	N-CA-CB	5.95	121.32	110.60
4	F	223	ARG	NE-CZ-NH1	-5.95	117.32	120.30
5	Q	102	TYR	CG-CD2-CE2	-5.95	116.54	121.30
4	F	362	ARG	NE-CZ-NH2	-5.95	117.33	120.30
3	E	297	PHE	CG-CD1-CE1	5.94	127.34	120.80
3	A	202	PHE	CB-CG-CD1	-5.94	116.64	120.80
1	M	71	VAL	CA-CB-CG2	-5.94	101.99	110.90
4	D	215	MET	CG-SD-CE	-5.94	90.69	100.20
7	K	214	ALA	CB-CA-C	-5.94	101.19	110.10
2	N	74	ALA	CB-CA-C	-5.94	101.19	110.10
10	O	197	ALA	N-CA-CB	5.94	118.41	110.10
3	E	278	ILE	CB-CA-C	5.94	123.47	111.60
4	D	468	TYR	CG-CD2-CE2	-5.93	116.56	121.30
3	C	85	VAL	CG1-CB-CG2	5.93	120.39	110.90
5	Q	341	TYR	CD1-CE1-CZ	5.93	125.14	119.80
1	M	112	TYR	CB-CG-CD2	5.93	124.56	121.00
4	F	321	ARG	NE-CZ-NH2	-5.93	117.34	120.30
11	T	46	ARG	NE-CZ-NH1	5.92	123.26	120.30
3	C	567	TRP	CE2-CD2-CE3	5.92	125.81	118.70
3	E	73	TYR	CB-CG-CD1	5.92	124.55	121.00
3	A	531	TYR	CB-CG-CD2	-5.92	117.45	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	81	LYS	N-CA-C	-5.92	95.02	111.00
3	C	203	ASP	CB-CG-OD2	5.91	123.62	118.30
3	A	557	ALA	CB-CA-C	-5.91	101.23	110.10
10	O	246	PHE	CB-CG-CD2	-5.91	116.66	120.80
4	F	161	MET	CG-SD-CE	-5.91	90.74	100.20
4	D	144	ARG	NE-CZ-NH1	5.91	123.25	120.30
7	G	219	ARG	NE-CZ-NH1	5.91	123.25	120.30
3	C	141	PHE	O-C-N	5.91	132.15	122.70
11	Z	124	ARG	NE-CZ-NH2	-5.90	117.35	120.30
10	O	119	ARG	NE-CZ-NH1	5.90	123.25	120.30
4	F	237	ARG	NE-CZ-NH2	-5.90	117.35	120.30
5	Q	80	PHE	CB-CG-CD1	-5.89	116.67	120.80
11	Y	125	LEU	CB-CG-CD2	-5.89	100.98	111.00
8	P	91	ASP	CB-CG-OD2	-5.89	113.00	118.30
2	N	98	ASP	N-CA-CB	5.88	121.19	110.60
11	a	46	ARG	NE-CZ-NH2	-5.88	117.36	120.30
4	B	228	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	M	109	PHE	CA-CB-CG	-5.88	99.80	113.90
8	P	13	PHE	CB-CG-CD1	-5.88	116.69	120.80
3	A	295	MET	CG-SD-CE	5.87	109.59	100.20
3	A	377	ASP	CB-CG-OD1	5.87	123.58	118.30
3	C	470	PHE	CG-CD2-CE2	5.87	127.26	120.80
11	R	83	ALA	CB-CA-C	-5.87	101.30	110.10
3	C	448	ARG	N-CA-CB	5.86	121.15	110.60
3	C	460	TYR	CB-CG-CD2	-5.86	117.48	121.00
8	P	7	LEU	N-CA-CB	5.86	122.12	110.40
10	O	312	TYR	CG-CD1-CE1	-5.86	116.61	121.30
3	C	448	ARG	NE-CZ-NH1	5.86	123.23	120.30
11	a	86	THR	CA-CB-CG2	-5.86	104.19	112.40
11	S	85	TYR	N-CA-CB	-5.86	100.06	110.60
4	D	478	PRO	N-CD-CG	5.85	111.98	103.20
11	T	72	VAL	CA-CB-CG1	5.85	119.68	110.90
4	D	240	LEU	CB-CA-C	-5.85	99.09	110.20
8	P	379	PHE	CB-CG-CD2	-5.85	116.71	120.80
11	a	93	ALA	N-CA-CB	5.85	118.29	110.10
5	Q	273	TYR	CB-CG-CD1	-5.84	117.49	121.00
7	G	177	ASP	CB-CG-OD1	-5.84	113.05	118.30
4	D	340	ASP	CB-CG-OD2	5.84	123.55	118.30
4	F	59	ASP	CB-CG-OD1	5.84	123.55	118.30
3	A	135	ARG	NE-CZ-NH1	-5.84	117.38	120.30
3	E	606	THR	CA-CB-CG2	-5.83	104.23	112.40
11	T	106	PHE	CB-CG-CD2	-5.83	116.72	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	219	LEU	CB-CG-CD1	5.83	120.90	111.00
4	B	452	ARG	NE-CZ-NH1	5.82	123.21	120.30
7	I	137	ALA	CB-CA-C	-5.82	101.37	110.10
3	A	110	ARG	NE-CZ-NH2	-5.82	117.39	120.30
8	P	273	ASP	CB-CG-OD2	-5.82	113.06	118.30
3	E	475	TYR	N-CA-CB	5.82	121.07	110.60
5	Q	270	ALA	N-CA-CB	5.81	118.24	110.10
3	C	139	TRP	CG-CD2-CE3	-5.81	128.67	133.90
9	b	194	ASP	CB-CG-OD1	-5.80	113.08	118.30
2	N	40	TYR	CG-CD1-CE1	-5.80	116.66	121.30
4	B	309	TYR	CG-CD1-CE1	-5.80	116.66	121.30
4	B	142	TYR	CG-CD2-CE2	-5.80	116.66	121.30
10	O	119	ARG	NE-CZ-NH2	-5.80	117.40	120.30
3	A	123	TYR	CG-CD2-CE2	5.79	125.93	121.30
9	b	45	ASN	N-CA-C	-5.79	95.36	111.00
4	B	113	PHE	O-C-N	-5.79	113.44	122.70
10	O	212	THR	CA-CB-CG2	-5.79	104.30	112.40
3	E	273	SER	N-CA-CB	5.79	119.18	110.50
3	C	377	ASP	CB-CG-OD1	-5.79	113.09	118.30
8	P	9	ASP	CB-CG-OD2	-5.79	113.09	118.30
7	K	16	GLU	CB-CA-C	-5.78	98.83	110.40
8	P	120	ASP	CB-CA-C	-5.78	98.83	110.40
9	b	277	VAL	CG1-CB-CG2	-5.78	101.65	110.90
3	A	110	ARG	NE-CZ-NH1	5.78	123.19	120.30
6	J	74	ALA	N-CA-CB	5.78	118.19	110.10
1	M	20	THR	N-CA-CB	-5.78	99.32	110.30
3	C	591	ARG	CD-NE-CZ	-5.78	115.51	123.60
11	Y	11	PHE	CB-CG-CD1	5.78	124.84	120.80
3	C	342	TYR	CB-CG-CD2	-5.77	117.54	121.00
4	B	132	LEU	CB-CG-CD2	5.77	120.81	111.00
5	Q	12	PHE	CB-CG-CD2	5.77	124.84	120.80
3	C	397	LYS	CB-CG-CD	5.77	126.60	111.60
3	E	46	TYR	CB-CG-CD2	5.77	124.46	121.00
4	D	119	PRO	N-CD-CG	5.76	111.85	103.20
3	E	586	PHE	CB-CG-CD2	-5.76	116.77	120.80
4	F	113	PHE	CB-CG-CD1	5.76	124.83	120.80
11	W	124	ARG	NE-CZ-NH2	5.76	123.18	120.30
4	F	370	TYR	CD1-CG-CD2	5.76	124.23	117.90
11	R	12	PHE	CB-CG-CD2	-5.75	116.77	120.80
3	E	471	TYR	CG-CD2-CE2	-5.75	116.70	121.30
7	K	86	LEU	CB-CG-CD2	5.75	120.78	111.00
10	O	6	TYR	CB-CG-CD1	-5.74	117.56	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	95	ARG	NE-CZ-NH1	5.73	123.17	120.30
10	O	75	ILE	CA-CB-CG1	-5.73	100.11	111.00
4	F	318	ARG	NE-CZ-NH1	5.73	123.17	120.30
7	I	141	ALA	N-CA-CB	5.73	118.13	110.10
4	B	144	ARG	N-CA-CB	5.73	120.91	110.60
9	b	45	ASN	CB-CA-C	-5.73	98.94	110.40
3	A	531	TYR	CG-CD1-CE1	-5.72	116.72	121.30
11	Z	116	VAL	CG1-CB-CG2	5.72	120.06	110.90
8	P	413	ALA	N-CA-CB	5.72	118.11	110.10
4	B	118	ARG	NH1-CZ-NH2	5.72	125.69	119.40
4	D	246	ASN	N-CA-CB	5.72	120.89	110.60
4	B	101	ARG	NE-CZ-NH2	-5.72	117.44	120.30
3	A	548	ARG	NE-CZ-NH1	-5.72	117.44	120.30
11	Z	51	PHE	CB-CG-CD1	-5.72	116.80	120.80
4	D	49	TYR	CB-CG-CD1	5.71	124.43	121.00
1	M	29	TYR	CB-CG-CD1	5.71	124.43	121.00
11	R	11	PHE	CB-CG-CD1	5.71	124.80	120.80
3	C	272	TYR	CG-CD1-CE1	-5.70	116.74	121.30
3	E	611	PHE	CB-CG-CD2	-5.70	116.81	120.80
7	I	16	GLU	N-CA-CB	5.70	120.86	110.60
11	a	97	VAL	CB-CA-C	-5.70	100.57	111.40
5	Q	71	TYR	CB-CG-CD2	-5.70	117.58	121.00
11	Y	35	SER	C-N-CA	5.68	134.24	122.30
4	B	482	ASP	CB-CG-OD2	-5.68	113.19	118.30
11	V	129	MET	CG-SD-CE	-5.68	91.11	100.20
9	b	310	PHE	CB-CG-CD1	5.68	124.78	120.80
8	P	302	VAL	CA-CB-CG2	-5.68	102.38	110.90
3	E	54	ASP	CB-CG-OD2	5.68	123.41	118.30
10	O	152	TYR	CB-CG-CD2	-5.68	117.59	121.00
3	C	212	TYR	CB-CG-CD2	-5.67	117.59	121.00
3	C	435	THR	CA-CB-CG2	-5.67	104.45	112.40
3	E	422	ASP	CB-CG-OD2	5.67	123.41	118.30
5	Q	80	PHE	CB-CG-CD2	5.67	124.77	120.80
10	O	303	TRP	CH2-CZ2-CE2	5.67	123.08	117.40
11	U	19	SER	N-CA-CB	5.67	119.01	110.50
4	D	359	PHE	CB-CG-CD2	5.67	124.77	120.80
3	C	181	THR	N-CA-C	-5.67	95.69	111.00
3	C	355	ASP	CB-CG-OD1	5.67	123.40	118.30
7	K	117	TYR	CZ-CE2-CD2	5.67	124.90	119.80
11	R	76	TYR	CZ-CE2-CD2	5.67	124.90	119.80
4	F	347	PRO	N-CA-CB	5.67	110.10	103.30
11	S	158	VAL	O-C-N	5.67	131.77	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	63	ARG	NE-CZ-NH1	5.66	123.13	120.30
7	G	85	ARG	CA-CB-CG	5.65	125.83	113.40
11	R	30	TYR	CB-CG-CD1	5.65	124.39	121.00
3	A	592	GLY	N-CA-C	-5.65	98.97	113.10
7	G	43	TYR	CB-CG-CD2	5.64	124.39	121.00
3	C	509	ASP	CB-CG-OD2	-5.64	113.22	118.30
3	E	212	TYR	N-CA-CB	5.64	120.75	110.60
7	G	12	GLN	CG-CD-OE1	-5.64	110.32	121.60
3	A	35	VAL	CA-CB-CG1	5.64	119.36	110.90
11	a	56	PRO	CA-N-CD	-5.64	103.60	111.50
11	V	135	PHE	CB-CG-CD1	-5.64	116.85	120.80
7	I	166	ARG	NE-CZ-NH2	-5.64	117.48	120.30
3	C	161	VAL	CA-CB-CG2	-5.63	102.45	110.90
3	A	294	LEU	CB-CG-CD2	-5.63	101.42	111.00
8	P	129	ASP	N-CA-CB	5.63	120.73	110.60
11	R	117	ARG	NE-CZ-NH2	-5.63	117.49	120.30
11	Y	147	ALA	N-CA-CB	5.63	117.98	110.10
11	a	95	LEU	CB-CG-CD1	-5.62	101.44	111.00
10	O	44	PHE	CZ-CE2-CD2	5.62	126.84	120.10
3	E	296	GLU	CB-CG-CD	-5.62	99.03	114.20
3	A	160	SER	N-CA-CB	5.62	118.92	110.50
7	I	39	ALA	CB-CA-C	-5.62	101.68	110.10
3	C	110	ARG	N-CA-CB	5.61	120.70	110.60
10	O	382	TYR	CZ-CE2-CD2	5.61	124.85	119.80
3	A	550	PHE	CZ-CE2-CD2	-5.61	113.37	120.10
7	K	160	TYR	CD1-CE1-CZ	5.61	124.85	119.80
1	M	121	ARG	NE-CZ-NH2	-5.61	117.50	120.30
3	A	508	SER	CB-CA-C	-5.61	99.45	110.10
11	X	149	LEU	CB-CG-CD1	-5.60	101.47	111.00
11	R	76	TYR	CB-CG-CD1	-5.60	117.64	121.00
10	O	42	ARG	NE-CZ-NH1	5.60	123.10	120.30
11	X	123	PRO	N-CA-CB	5.60	110.02	103.30
6	L	50	LYS	N-CA-CB	5.59	120.67	110.60
8	P	411	VAL	CB-CA-C	5.59	122.03	111.40
8	P	350	TYR	CG-CD1-CE1	-5.59	116.83	121.30
10	O	210	TYR	CD1-CE1-CZ	5.59	124.83	119.80
4	D	413	ALA	N-CA-CB	5.59	117.92	110.10
3	E	297	PHE	CD1-CG-CD2	-5.59	111.04	118.30
6	J	72	ALA	N-CA-CB	5.59	117.92	110.10
8	P	359	TYR	CG-CD2-CE2	-5.58	116.83	121.30
6	J	95	VAL	CA-CB-CG1	5.58	119.28	110.90
8	P	317	ASN	N-CA-CB	5.58	120.65	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	b	91	TYR	CG-CD2-CE2	-5.58	116.84	121.30
4	F	214	ALA	N-CA-CB	5.57	117.90	110.10
8	P	153	ASN	CA-CB-CG	-5.57	101.14	113.40
4	B	38	LEU	CB-CG-CD2	5.57	120.47	111.00
9	b	120	ARG	NE-CZ-NH2	5.57	123.08	120.30
7	K	34	GLU	N-CA-CB	5.57	120.62	110.60
9	b	72	PHE	CB-CG-CD1	5.57	124.70	120.80
6	L	51	ASP	CB-CG-OD2	-5.57	113.29	118.30
7	K	152	MET	CG-SD-CE	-5.57	91.30	100.20
11	X	100	SER	N-CA-CB	5.57	118.85	110.50
4	B	130	ASP	N-CA-C	-5.56	95.98	111.00
8	P	460	ARG	NE-CZ-NH1	5.56	123.08	120.30
11	a	56	PRO	N-CD-CG	5.56	111.54	103.20
11	X	11	PHE	CB-CG-CD1	5.56	124.69	120.80
3	C	62	ARG	NE-CZ-NH2	-5.56	117.52	120.30
11	S	117	ARG	NE-CZ-NH1	5.56	123.08	120.30
4	B	208	PHE	CG-CD1-CE1	-5.55	114.69	120.80
7	K	15	ASP	CB-CG-OD1	-5.55	113.31	118.30
11	S	46	ARG	NE-CZ-NH1	5.55	123.07	120.30
3	A	88	THR	CA-CB-CG2	-5.54	104.64	112.40
3	E	318	VAL	CG1-CB-CG2	5.53	119.75	110.90
5	Q	157	PRO	N-CA-CB	5.53	109.94	103.30
3	C	482	ARG	NE-CZ-NH1	5.53	123.06	120.30
3	A	591	ARG	NH1-CZ-NH2	-5.53	113.32	119.40
4	D	326	ASN	N-CA-CB	5.53	120.55	110.60
3	E	328	ALA	CB-CA-C	-5.53	101.81	110.10
4	B	286	ASP	CB-CG-OD1	-5.53	113.33	118.30
4	B	189	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	M	112	TYR	N-CA-CB	5.52	120.54	110.60
3	A	36	ILE	N-CA-C	-5.52	96.10	111.00
3	E	162	PHE	CB-CG-CD1	-5.52	116.94	120.80
3	E	228	SER	CB-CA-C	-5.52	99.62	110.10
3	E	377	ASP	CB-CG-OD1	-5.52	113.33	118.30
6	J	27	TYR	N-CA-CB	5.52	120.53	110.60
4	D	307	TYR	CB-CG-CD1	-5.51	117.69	121.00
4	F	272	ARG	NE-CZ-NH1	-5.51	117.54	120.30
3	A	394	ARG	NH1-CZ-NH2	5.51	125.47	119.40
11	U	142	TYR	CG-CD2-CE2	5.51	125.71	121.30
3	A	242	ALA	N-CA-CB	5.51	117.82	110.10
4	D	94	GLU	N-CA-C	-5.51	96.12	111.00
3	E	461	SER	N-CA-CB	5.51	118.76	110.50
11	V	154	ALA	N-CA-CB	5.51	117.81	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	8	ALA	CB-CA-C	-5.51	101.84	110.10
4	B	464	LEU	CB-CG-CD1	5.50	120.36	111.00
11	R	42	THR	CA-CB-CG2	5.50	120.11	112.40
5	Q	267	ALA	N-CA-CB	5.50	117.81	110.10
8	P	142	SER	N-CA-CB	5.50	118.75	110.50
8	P	17	ARG	NE-CZ-NH2	-5.50	117.55	120.30
11	U	48	ASP	CB-CG-OD1	5.50	123.25	118.30
4	B	302	ARG	NE-CZ-NH2	-5.50	117.55	120.30
3	E	586	PHE	CG-CD1-CE1	-5.49	114.76	120.80
3	C	384	LEU	CB-CG-CD1	5.48	120.32	111.00
3	A	398	ALA	CB-CA-C	-5.48	101.89	110.10
10	O	373	GLN	N-CA-CB	5.47	120.45	110.60
11	W	46	ARG	CB-CA-C	-5.47	99.45	110.40
4	D	466	ARG	NE-CZ-NH1	-5.47	117.56	120.30
8	P	390	ASP	N-CA-C	-5.47	96.23	111.00
4	D	334	ILE	N-CA-C	-5.47	96.24	111.00
8	P	328	ARG	NE-CZ-NH1	-5.47	117.57	120.30
3	C	601	GLU	CB-CA-C	-5.46	99.47	110.40
2	N	10	VAL	CA-CB-CG2	-5.46	102.71	110.90
3	A	324	MET	CG-SD-CE	-5.46	91.46	100.20
4	B	110	GLY	C-N-CA	5.46	135.36	121.70
2	N	111	ARG	NE-CZ-NH1	-5.46	117.57	120.30
3	E	416	VAL	CG1-CB-CG2	5.46	119.64	110.90
4	F	163	SER	N-CA-CB	5.46	118.69	110.50
4	B	370	TYR	CG-CD2-CE2	-5.46	116.93	121.30
2	N	116	PHE	CB-CG-CD1	5.46	124.62	120.80
11	W	30	TYR	CB-CG-CD2	-5.46	117.73	121.00
3	E	57	VAL	CA-CB-CG2	5.46	119.08	110.90
3	C	391	PHE	CG-CD1-CE1	5.45	126.80	120.80
3	A	286	ARG	CB-CA-C	-5.45	99.49	110.40
7	I	223	TYR	CG-CD1-CE1	-5.45	116.94	121.30
7	I	53	ASN	CB-CA-C	-5.45	99.50	110.40
4	D	439	PHE	CB-CG-CD1	5.44	124.61	120.80
9	b	110	TYR	CG-CD1-CE1	-5.44	116.95	121.30
9	b	212	PHE	CG-CD1-CE1	-5.44	114.81	120.80
6	H	37	THR	CA-CB-CG2	-5.44	104.79	112.40
7	K	25	ARG	NE-CZ-NH1	-5.44	117.58	120.30
3	E	475	TYR	CA-C-N	5.43	132.31	117.10
4	F	46	PHE	CB-CG-CD1	5.43	124.60	120.80
6	L	57	PHE	CB-CG-CD2	-5.43	117.00	120.80
3	A	398	ALA	N-CA-CB	5.43	117.70	110.10
4	B	212	PHE	CB-CG-CD1	5.43	124.60	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	76	VAL	CA-CB-CG1	-5.43	102.76	110.90
4	B	118	ARG	NE-CZ-NH1	-5.43	117.59	120.30
9	b	17	VAL	CA-CB-CG1	5.43	119.04	110.90
4	D	407	TYR	CZ-CE2-CD2	5.43	124.68	119.80
11	U	85	TYR	CB-CG-CD2	-5.42	117.75	121.00
7	K	126	VAL	CA-CB-CG1	5.42	119.03	110.90
7	G	158	ARG	NE-CZ-NH1	5.42	123.01	120.30
7	G	223	TYR	C-N-CA	-5.41	110.93	122.30
3	C	100	LEU	CB-CA-C	-5.41	99.92	110.20
11	R	72	VAL	CG1-CB-CG2	5.41	119.56	110.90
11	R	95	LEU	CB-CG-CD1	-5.41	101.80	111.00
11	Y	106	PHE	CB-CG-CD2	5.41	124.59	120.80
1	M	118	ASN	N-CA-CB	5.40	120.33	110.60
8	P	350	TYR	CD1-CE1-CZ	5.40	124.66	119.80
7	K	144	ARG	NH1-CZ-NH2	-5.40	113.46	119.40
11	Z	117	ARG	CB-CG-CD	5.40	125.64	111.60
6	L	27	TYR	CG-CD2-CE2	-5.40	116.98	121.30
8	P	336	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	M	81	TYR	CG-CD2-CE2	-5.40	116.98	121.30
4	B	370	TYR	CG-CD1-CE1	-5.40	116.98	121.30
4	D	34	VAL	CA-CB-CG1	-5.40	102.81	110.90
4	B	214	ALA	CB-CA-C	-5.40	102.01	110.10
3	E	54	ASP	CB-CG-OD1	-5.39	113.45	118.30
4	B	276	THR	N-CA-CB	5.39	120.55	110.30
3	C	246	CYS	N-CA-C	-5.39	96.44	111.00
6	L	104	LYS	N-CA-CB	5.39	120.31	110.60
7	G	55	THR	O-C-N	-5.39	114.07	122.70
4	B	241	PHE	CB-CG-CD2	-5.39	117.03	120.80
7	K	146	VAL	CA-CB-CG1	-5.39	102.82	110.90
11	S	12	PHE	CG-CD2-CE2	-5.39	114.87	120.80
4	B	420	VAL	CA-CB-CG2	-5.39	102.82	110.90
3	A	429	THR	CA-CB-CG2	-5.38	104.86	112.40
10	O	228	ASP	CB-CG-OD1	-5.38	113.45	118.30
3	E	44	ALA	N-CA-CB	5.38	117.64	110.10
5	Q	254	PHE	N-CA-CB	5.38	120.29	110.60
10	O	210	TYR	CG-CD1-CE1	-5.38	116.99	121.30
3	C	580	ALA	N-CA-CB	5.38	117.63	110.10
3	E	526	LEU	CB-CG-CD1	5.38	120.14	111.00
3	E	562	ALA	N-CA-CB	5.38	117.63	110.10
11	W	85	TYR	CB-CG-CD2	-5.38	117.78	121.00
7	K	177	ASP	CB-CG-OD2	-5.37	113.46	118.30
1	M	91	ARG	NE-CZ-NH2	-5.37	117.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	84	PHE	CB-CG-CD1	-5.37	117.04	120.80
3	C	548	ARG	NE-CZ-NH1	-5.37	117.61	120.30
11	a	50	LEU	CB-CG-CD1	5.37	120.13	111.00
4	D	210	ILE	CB-CA-C	-5.37	100.86	111.60
7	G	173	VAL	CA-CB-CG2	-5.37	102.85	110.90
11	S	157	ASP	N-CA-CB	5.37	120.26	110.60
4	F	478	PRO	N-CA-CB	5.36	109.73	103.30
11	V	135	PHE	CB-CG-CD2	5.36	124.55	120.80
5	Q	46	LEU	CB-CG-CD2	5.36	120.11	111.00
11	R	142	TYR	CG-CD2-CE2	-5.36	117.01	121.30
4	B	42	GLU	N-CA-C	-5.36	96.54	111.00
8	P	426	ASP	CB-CG-OD2	5.36	123.12	118.30
11	R	19	SER	O-C-N	-5.35	114.14	122.70
11	Y	30	TYR	CB-CG-CD1	-5.35	117.79	121.00
11	T	83	ALA	O-C-N	-5.35	114.14	122.70
4	D	142	TYR	C-N-CA	5.35	135.08	121.70
3	E	392	TYR	CB-CG-CD1	5.35	124.21	121.00
4	F	189	ARG	CD-NE-CZ	-5.35	116.11	123.60
4	B	322	VAL	N-CA-C	-5.35	96.56	111.00
11	Y	93	ALA	N-CA-CB	5.35	117.59	110.10
11	W	93	ALA	N-CA-CB	5.35	117.59	110.10
4	D	453	THR	N-CA-C	-5.35	96.57	111.00
10	O	116	TRP	N-CA-CB	5.34	120.22	110.60
10	O	239	PHE	CB-CG-CD2	-5.34	117.06	120.80
4	F	202	ASP	N-CA-CB	5.34	120.22	110.60
4	D	118	ARG	NE-CZ-NH2	5.34	122.97	120.30
11	X	30	TYR	CG-CD2-CE2	-5.34	117.03	121.30
11	Y	82	GLN	N-CA-CB	5.34	120.21	110.60
3	C	572	ASP	CB-CG-OD2	-5.34	113.50	118.30
3	E	545	ASP	CB-CA-C	-5.34	99.73	110.40
10	O	57	SER	CB-CA-C	-5.34	99.96	110.10
11	Y	132	ILE	O-C-N	5.34	131.24	122.70
7	G	171	GLU	N-CA-CB	-5.33	101.00	110.60
4	F	108	MET	CG-SD-CE	-5.33	91.67	100.20
7	G	223	TYR	CB-CG-CD1	-5.33	117.80	121.00
4	F	343	THR	CA-CB-CG2	-5.33	104.94	112.40
11	a	51	PHE	CG-CD2-CE2	5.33	126.67	120.80
11	Y	11	PHE	CB-CG-CD2	-5.33	117.07	120.80
11	Z	153	ARG	NE-CZ-NH2	-5.33	117.64	120.30
3	C	399	VAL	N-CA-C	-5.33	96.61	111.00
11	a	55	VAL	CA-CB-CG2	-5.33	102.91	110.90
7	K	81	ALA	CB-CA-C	-5.33	102.11	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	313	LYS	CB-CA-C	-5.32	99.75	110.40
11	W	85	TYR	CD1-CE1-CZ	-5.32	115.01	119.80
4	D	381	ARG	NE-CZ-NH1	5.32	122.96	120.30
4	F	374	ASN	N-CA-CB	5.32	120.17	110.60
8	P	82	HIS	CA-CB-CG	-5.32	104.56	113.60
11	T	138	VAL	N-CA-CB	5.31	123.19	111.50
3	E	238	ARG	NE-CZ-NH2	-5.31	117.64	120.30
3	A	567	TRP	CD1-CG-CD2	-5.31	102.05	106.30
3	A	550	PHE	CB-CG-CD2	5.31	124.52	120.80
9	b	196	VAL	CG1-CB-CG2	-5.30	102.41	110.90
11	Z	29	ALA	CB-CA-C	-5.30	102.15	110.10
7	K	160	TYR	CG-CD1-CE1	-5.30	117.06	121.30
9	b	328	TYR	CB-CG-CD2	-5.30	117.82	121.00
3	E	305	SER	N-CA-CB	5.30	118.45	110.50
3	A	286	ARG	NE-CZ-NH1	5.30	122.95	120.30
3	A	231	TYR	CD1-CE1-CZ	5.29	124.56	119.80
4	B	63	ARG	NE-CZ-NH2	-5.29	117.65	120.30
8	P	75	LYS	C-N-CA	5.29	134.93	121.70
6	L	53	GLU	O-C-N	-5.29	114.24	122.70
10	O	114	PHE	CB-CG-CD2	-5.29	117.10	120.80
3	E	483	ASP	CB-CG-OD1	-5.29	113.54	118.30
5	Q	98	ILE	O-C-N	-5.29	114.24	122.70
10	O	196	VAL	N-CA-C	-5.29	96.73	111.00
11	V	96	SER	CB-CA-C	-5.29	100.06	110.10
8	P	120	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	M	59	ARG	NE-CZ-NH2	-5.28	117.66	120.30
3	E	135	ARG	NH1-CZ-NH2	5.28	125.21	119.40
3	E	468	ASN	N-CA-CB	5.28	120.11	110.60
3	E	599	GLU	OE1-CD-OE2	5.28	129.64	123.30
3	E	150	ASP	CB-CG-OD2	5.28	123.05	118.30
4	F	86	ILE	CA-CB-CG1	-5.28	100.97	111.00
4	B	224	PHE	CB-CG-CD1	5.28	124.50	120.80
11	R	116	VAL	CB-CA-C	5.27	121.42	111.40
3	A	105	TYR	CB-CG-CD2	5.27	124.16	121.00
6	L	25	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	M	17	LEU	CB-CG-CD1	-5.27	102.04	111.00
3	E	507	LEU	CB-CG-CD1	5.27	119.96	111.00
10	O	303	TRP	CE2-CD2-CE3	5.27	125.02	118.70
3	C	200	VAL	CA-CB-CG2	-5.27	103.00	110.90
9	b	208	ARG	NE-CZ-NH2	-5.26	117.67	120.30
11	Y	84	LEU	CB-CG-CD2	5.26	119.95	111.00
8	P	127	LEU	CB-CG-CD1	5.26	119.95	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	23	ARG	NE-CZ-NH2	-5.26	117.67	120.30
3	A	537	PHE	CB-CG-CD2	-5.26	117.12	120.80
10	O	234	PHE	CB-CG-CD1	5.26	124.48	120.80
3	A	177	ARG	NE-CZ-NH2	-5.26	117.67	120.30
4	D	419	VAL	CA-CB-CG2	-5.25	103.02	110.90
11	Z	102	LEU	CB-CG-CD1	5.25	119.92	111.00
10	O	121	PHE	CB-CG-CD2	5.25	124.47	120.80
10	O	231	TYR	CE1-CZ-CE2	-5.25	111.40	119.80
3	E	472	ASP	CB-CG-OD1	5.25	123.02	118.30
7	G	178	TYR	CB-CG-CD1	-5.25	117.85	121.00
11	V	146	VAL	CA-CB-CG2	-5.25	103.03	110.90
6	H	51	ASP	N-CA-CB	5.24	120.04	110.60
9	b	80	ASP	CB-CA-C	5.24	120.88	110.40
3	C	194	ASP	CB-CG-OD2	5.24	123.02	118.30
4	F	69	GLU	OE1-CD-OE2	-5.24	117.01	123.30
3	A	81	VAL	CA-CB-CG2	-5.24	103.04	110.90
8	P	205	LEU	CB-CG-CD2	5.24	119.91	111.00
9	b	300	TYR	CD1-CE1-CZ	-5.24	115.08	119.80
3	C	28	TYR	CB-CG-CD1	5.24	124.14	121.00
11	Y	99	LEU	CB-CG-CD1	5.24	119.90	111.00
11	V	56	PRO	N-CD-CG	5.24	111.06	103.20
3	C	383	TYR	CG-CD2-CE2	-5.24	117.11	121.30
3	E	231	TYR	CD1-CE1-CZ	5.24	124.51	119.80
3	A	40	MET	CG-SD-CE	-5.24	91.82	100.20
11	W	95	LEU	N-CA-CB	5.24	120.87	110.40
1	M	15	LEU	CA-C-N	5.23	126.67	116.20
2	N	28	ILE	N-CA-C	-5.23	96.87	111.00
3	A	609	GLU	O-C-N	-5.23	114.33	122.70
4	D	281	MET	N-CA-CB	5.23	120.01	110.60
10	O	233	LEU	CB-CG-CD1	5.23	119.89	111.00
4	D	50	ASN	N-CA-CB	5.23	120.01	110.60
4	D	229	PHE	CB-CG-CD1	5.23	124.46	120.80
11	Y	60	ALA	N-CA-CB	5.23	117.42	110.10
3	C	567	TRP	CG-CD2-CE3	-5.22	129.20	133.90
4	D	459	ASP	CB-CG-OD1	-5.22	113.60	118.30
4	B	224	PHE	CB-CG-CD2	-5.22	117.14	120.80
8	P	199	TYR	CZ-CE2-CD2	-5.22	115.10	119.80
10	O	351	LEU	CB-CA-C	-5.22	100.29	110.20
4	D	485	TYR	CB-CG-CD2	-5.21	117.87	121.00
3	E	158	TYR	CG-CD1-CE1	-5.21	117.13	121.30
8	P	413	ALA	N-CA-C	-5.21	96.93	111.00
3	C	360	TRP	CZ3-CH2-CZ2	5.21	127.85	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	V	142	TYR	CD1-CE1-CZ	5.21	124.49	119.80
5	Q	225	LEU	CB-CG-CD2	-5.21	102.15	111.00
2	N	37	PHE	N-CA-CB	5.20	119.97	110.60
5	Q	232	ASP	CB-CG-OD2	-5.20	113.62	118.30
7	K	145	ASP	O-C-N	-5.20	114.37	122.70
7	K	126	VAL	CA-CB-CG2	-5.20	103.10	110.90
8	P	121	PRO	N-CA-CB	5.20	109.54	103.30
11	T	51	PHE	CB-CG-CD2	5.20	124.44	120.80
11	a	82	GLN	O-C-N	5.20	131.02	122.70
11	W	135	PHE	N-CA-CB	5.20	119.96	110.60
11	T	59	MET	CG-SD-CE	-5.20	91.89	100.20
3	E	451	PHE	CB-CG-CD2	-5.20	117.16	120.80
3	A	123	TYR	CB-CG-CD2	-5.20	117.88	121.00
11	T	148	LEU	N-CA-CB	5.20	120.79	110.40
5	Q	192	PHE	O-C-N	-5.19	114.39	122.70
4	D	391	MET	CG-SD-CE	-5.19	91.89	100.20
3	A	439	TRP	CB-CG-CD1	5.19	133.75	127.00
3	C	525	PHE	CB-CG-CD1	-5.19	117.17	120.80
4	F	29	ASN	N-CA-C	-5.19	96.99	111.00
7	I	208	LYS	N-CA-CB	5.19	119.94	110.60
5	Q	132	TRP	CG-CD2-CE3	-5.19	129.23	133.90
3	A	191	TYR	CB-CG-CD1	5.19	124.11	121.00
5	Q	66	SER	N-CA-CB	5.18	118.28	110.50
8	P	88	ASP	CB-CG-OD2	-5.18	113.63	118.30
10	O	219	PRO	N-CA-CB	5.18	109.52	103.30
4	F	156	SER	C-N-CA	5.18	134.66	121.70
3	C	434	ILE	C-N-CA	5.18	134.65	121.70
8	P	390	ASP	N-CA-CB	5.18	119.92	110.60
4	D	225	PHE	CB-CG-CD1	-5.18	117.17	120.80
4	B	159	ASP	CB-CA-C	-5.18	100.05	110.40
11	X	81	LYS	CA-CB-CG	5.18	124.79	113.40
11	Y	76	TYR	CG-CD2-CE2	-5.18	117.16	121.30
3	A	194	ASP	CB-CG-OD1	-5.17	113.64	118.30
9	b	196	VAL	CA-CB-CG2	-5.17	103.14	110.90
9	b	328	TYR	CG-CD2-CE2	-5.17	117.16	121.30
4	D	279	THR	N-CA-C	-5.17	97.04	111.00
11	X	131	LEU	CB-CG-CD1	5.17	119.78	111.00
10	O	146	ARG	NE-CZ-NH1	5.17	122.88	120.30
4	B	111	ARG	NH1-CZ-NH2	-5.16	113.72	119.40
6	L	61	ASN	CA-CB-CG	-5.16	102.04	113.40
3	C	87	ARG	NH1-CZ-NH2	-5.16	113.72	119.40
8	P	370	TRP	CD2-CE2-CZ2	-5.16	116.11	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	b	325	LYS	O-C-N	-5.16	114.44	122.70
9	b	336	ILE	N-CA-C	-5.16	97.06	111.00
10	O	10	ASP	N-CA-C	-5.16	97.07	111.00
1	M	9	PHE	CB-CG-CD1	5.16	124.41	120.80
3	C	33	PRO	N-CD-CG	5.15	110.93	103.20
4	F	67	VAL	O-C-N	-5.15	114.46	122.70
4	B	252	ARG	NE-CZ-NH2	-5.15	117.72	120.30
10	O	9	ASN	N-CA-CB	5.15	119.86	110.60
7	I	49	ASN	CB-CA-C	-5.15	100.10	110.40
5	Q	188	TYR	CG-CD1-CE1	5.14	125.42	121.30
4	D	331	GLN	CG-CD-OE1	-5.14	111.31	121.60
3	A	600	PHE	CB-CG-CD1	5.14	124.40	120.80
8	P	131	SER	N-CA-CB	5.14	118.21	110.50
11	Y	76	TYR	CZ-CE2-CD2	5.14	124.43	119.80
3	C	218	ARG	NE-CZ-NH2	-5.14	117.73	120.30
6	L	69	GLU	CB-CA-C	-5.14	100.12	110.40
11	X	85	TYR	CB-CG-CD1	5.14	124.08	121.00
4	D	420	VAL	C-N-CA	5.14	133.09	122.30
10	O	239	PHE	CZ-CE2-CD2	-5.14	113.93	120.10
11	S	138	VAL	CA-CB-CG1	-5.14	103.19	110.90
3	E	611	PHE	CB-CG-CD1	5.14	124.40	120.80
9	b	239	PHE	O-C-N	-5.14	114.48	122.70
11	S	107	ALA	N-CA-CB	5.14	117.29	110.10
11	T	37	VAL	CA-CB-CG1	5.14	118.61	110.90
3	A	231	TYR	CB-CG-CD1	5.13	124.08	121.00
4	B	406	LYS	CB-CG-CD	5.13	124.95	111.60
11	a	14	ALA	CB-CA-C	-5.13	102.40	110.10
3	C	51	VAL	N-CA-CB	5.13	122.79	111.50
4	D	452	ARG	NE-CZ-NH2	-5.13	117.73	120.30
11	Z	48	ASP	O-C-N	-5.13	114.49	122.70
4	D	304	TYR	CB-CG-CD1	5.13	124.08	121.00
10	O	319	TYR	CB-CG-CD2	-5.13	117.92	121.00
2	N	41	GLN	O-C-N	5.13	130.91	122.70
3	C	176	PRO	N-CA-CB	5.13	109.45	103.30
3	A	422	ASP	CB-CG-OD2	5.13	122.92	118.30
11	S	76	TYR	CA-CB-CG	-5.13	103.66	113.40
3	C	499	VAL	CG1-CB-CG2	5.13	119.10	110.90
10	O	251	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	M	141	ARG	NE-CZ-NH1	5.12	122.86	120.30
3	A	426	PRO	N-CA-CB	5.12	109.44	103.30
5	Q	126	ARG	N-CA-C	-5.12	97.17	111.00
3	A	516	ASP	CB-CA-C	-5.12	100.16	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	b	49	ARG	CD-NE-CZ	-5.12	116.43	123.60
3	E	294	LEU	O-C-N	-5.12	114.51	122.70
11	Z	23	PHE	CB-CG-CD2	5.12	124.38	120.80
3	E	247	VAL	CA-CB-CG1	5.12	118.57	110.90
3	E	548	ARG	CA-CB-CG	5.11	124.65	113.40
4	B	281	MET	CA-CB-CG	5.11	121.99	113.30
6	H	27	TYR	CG-CD1-CE1	-5.11	117.21	121.30
4	F	468	TYR	CB-CG-CD1	-5.11	117.93	121.00
10	O	270	LEU	CB-CG-CD2	5.11	119.69	111.00
2	N	57	PHE	CZ-CE2-CD2	5.11	126.23	120.10
8	P	267	TYR	CA-CB-CG	-5.11	103.69	113.40
11	a	60	ALA	N-CA-CB	5.11	117.25	110.10
11	a	156	GLN	CB-CA-C	5.11	120.61	110.40
5	Q	130	LEU	N-CA-CB	5.11	120.61	110.40
4	D	439	PHE	CG-CD2-CE2	5.10	126.41	120.80
11	W	114	ALA	CB-CA-C	-5.10	102.44	110.10
11	U	125	LEU	CB-CG-CD2	5.10	119.67	111.00
11	R	63	ILE	CA-CB-CG1	5.10	120.70	111.00
4	F	322	VAL	CA-CB-CG1	5.10	118.55	110.90
4	F	265	TYR	CD1-CE1-CZ	5.10	124.39	119.80
7	I	63	LYS	CB-CG-CD	5.10	124.86	111.60
4	D	484	PHE	CB-CG-CD1	-5.10	117.23	120.80
3	A	383	TYR	CB-CG-CD2	5.10	124.06	121.00
1	M	87	VAL	CA-CB-CG2	-5.09	103.26	110.90
3	E	308	LYS	N-CA-CB	5.09	119.77	110.60
3	C	46	TYR	CB-CG-CD1	5.09	124.06	121.00
3	C	616	ASP	N-CA-CB	5.09	119.77	110.60
10	O	210	TYR	CG-CD2-CE2	-5.09	117.23	121.30
7	I	15	ASP	CA-CB-CG	-5.09	102.20	113.40
9	b	20	TYR	CG-CD1-CE1	5.09	125.37	121.30
10	O	316	VAL	O-C-N	-5.09	114.56	122.70
4	B	274	VAL	CG1-CB-CG2	5.08	119.04	110.90
11	S	44	VAL	CA-CB-CG1	-5.08	103.27	110.90
3	A	531	TYR	CB-CG-CD1	-5.08	117.95	121.00
11	a	95	LEU	CB-CA-C	-5.08	100.55	110.20
7	K	177	ASP	CB-CG-OD1	5.08	122.87	118.30
3	A	56	LEU	CB-CG-CD2	5.08	119.63	111.00
3	A	429	THR	N-CA-CB	5.08	119.95	110.30
8	P	147	VAL	CA-CB-CG1	5.08	118.52	110.90
11	Y	19	SER	N-CA-CB	5.08	118.11	110.50
5	Q	222	ASN	CB-CA-C	-5.07	100.26	110.40
11	Z	20	ALA	CB-CA-C	-5.07	102.49	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Z	137	GLU	OE1-CD-OE2	-5.07	117.21	123.30
3	C	494	GLU	CB-CA-C	-5.07	100.26	110.40
11	T	15	ILE	CG1-CB-CG2	-5.07	100.25	111.40
1	M	152	LEU	CB-CG-CD2	5.07	119.62	111.00
4	D	485	TYR	CA-CB-CG	5.07	123.03	113.40
11	U	55	VAL	O-C-N	-5.07	111.47	121.10
4	F	159	ASP	N-CA-CB	5.07	119.72	110.60
3	E	453	SER	C-N-CA	5.07	134.37	121.70
9	b	91	TYR	CB-CA-C	-5.06	100.28	110.40
7	G	166	ARG	NH1-CZ-NH2	5.06	124.97	119.40
7	I	85	ARG	N-CA-CB	5.06	119.71	110.60
4	F	131	TYR	CB-CG-CD2	-5.06	117.97	121.00
5	Q	117	ASP	N-CA-CB	5.06	119.70	110.60
8	P	161	VAL	CG1-CB-CG2	5.05	118.98	110.90
3	A	163	GLU	N-CA-CB	-5.05	101.51	110.60
11	Z	23	PHE	CB-CG-CD1	-5.05	117.26	120.80
2	N	61	ARG	N-CA-CB	5.05	119.69	110.60
4	F	49	TYR	CB-CG-CD2	5.05	124.03	121.00
3	A	142	THR	CA-CB-OG1	5.05	119.61	109.00
9	b	106	VAL	N-CA-C	-5.05	97.37	111.00
3	C	279	ILE	N-CA-C	-5.05	97.37	111.00
9	b	85	GLU	C-N-CA	-5.05	111.70	122.30
11	W	76	TYR	CA-CB-CG	-5.04	103.81	113.40
4	B	381	ARG	CD-NE-CZ	5.04	130.66	123.60
5	Q	123	ILE	N-CA-C	-5.04	97.38	111.00
5	Q	238	LYS	CB-CA-C	-5.04	100.32	110.40
6	L	27	TYR	CB-CG-CD1	-5.04	117.97	121.00
11	T	139	LEU	O-C-N	-5.04	114.63	123.20
3	A	228	SER	N-CA-CB	5.04	118.05	110.50
4	B	459	ASP	N-CA-CB	5.04	119.66	110.60
9	b	344	ASP	CA-CB-CG	-5.04	102.32	113.40
11	X	83	ALA	N-CA-CB	5.04	117.15	110.10
11	R	73	LEU	CB-CG-CD1	-5.04	102.44	111.00
11	R	88	PHE	CB-CG-CD2	-5.03	117.28	120.80
11	W	88	PHE	CD1-CE1-CZ	-5.03	114.06	120.10
4	B	319	ALA	N-CA-CB	5.03	117.14	110.10
3	C	547	MET	CG-SD-CE	-5.03	92.15	100.20
11	Z	30	TYR	CG-CD1-CE1	-5.03	117.28	121.30
6	H	27	TYR	CB-CG-CD2	-5.02	117.99	121.00
11	V	141	LEU	CB-CG-CD2	5.02	119.54	111.00
3	E	553	TYR	CG-CD1-CE1	5.02	125.32	121.30
5	Q	267	ALA	CB-CA-C	-5.02	102.57	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	T	131	LEU	CB-CG-CD2	5.02	119.53	111.00
3	C	553	TYR	CG-CD1-CE1	-5.02	117.29	121.30
3	E	161	VAL	N-CA-C	-5.02	97.45	111.00
3	A	224	THR	N-CA-CB	5.02	119.83	110.30
11	S	123	PRO	N-CA-CB	5.02	109.32	103.30
4	D	404	TYR	CB-CG-CD1	-5.01	117.99	121.00
8	P	210	PHE	CB-CG-CD2	-5.01	117.29	120.80
3	A	184	TRP	N-CA-CB	5.01	119.62	110.60
8	P	80	LEU	CB-CG-CD1	-5.01	102.48	111.00
11	Y	139	LEU	CB-CG-CD2	5.01	119.52	111.00
4	F	400	SER	O-C-N	5.01	130.71	122.70
4	F	124	PRO	N-CD-CG	5.01	110.71	103.20
3	A	291	ALA	CB-CA-C	-5.01	102.59	110.10
11	T	82	GLN	CG-CD-OE1	-5.00	111.59	121.60
3	E	541	TRP	CG-CD2-CE3	-5.00	129.40	133.90
4	F	195	ARG	CA-C-N	5.00	131.11	117.10
3	E	343	PHE	CB-CG-CD1	-5.00	117.30	120.80
3	A	215	TRP	CZ3-CH2-CZ2	-5.00	115.60	121.60

There are no chirality outliers.

All (163) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	126	ARG	Sidechain
3	A	177	ARG	Sidechain
3	A	179	ARG	Sidechain
3	A	28	TYR	Sidechain
3	A	280	TYR	Sidechain
3	A	359	ARG	Sidechain
3	A	460	TYR	Sidechain
3	A	478	PHE	Sidechain
3	A	531	TYR	Sidechain
3	A	553	TYR	Sidechain
3	A	610	ARG	Sidechain
3	A	73	TYR	Sidechain
4	B	224	PHE	Sidechain
4	B	229	PHE	Sidechain
4	B	237	ARG	Sidechain
4	B	265	TYR	Sidechain
4	B	284	TYR	Sidechain
4	B	307	TYR	Sidechain
4	B	316	TYR	Sidechain

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Mol	Chain	Res	Type	Group
4	B	318	ARG	Sidechain
4	B	321	ARG	Sidechain
4	B	352	TYR	Sidechain
4	B	381	ARG	Sidechain
4	B	393	ARG	Sidechain
4	B	404	TYR	Sidechain
4	B	44	VAL	Peptide
4	B	466	ARG	Sidechain
4	B	468	TYR	Sidechain
4	B	475	ARG	Sidechain
3	C	105	TYR	Sidechain
3	C	123	TYR	Sidechain
3	C	135	ARG	Sidechain
3	C	231	TYR	Sidechain
3	C	24	TYR	Sidechain
3	C	343	PHE	Sidechain
3	C	370	ARG	Sidechain
3	C	383	TYR	Sidechain
3	C	46	TYR	Sidechain
3	C	460	TYR	Sidechain
3	C	478	PHE	Sidechain
3	C	600	PHE	Sidechain
3	C	87	ARG	Sidechain
4	D	127	PHE	Sidechain
4	D	131	TYR	Sidechain
4	D	146	TYR	Sidechain
4	D	237	ARG	Sidechain
4	D	307	TYR	Sidechain
4	D	309	TYR	Sidechain
4	D	325	ARG	Sidechain
4	D	352	TYR	Sidechain
4	D	370	TYR	Sidechain
4	D	404	TYR	Sidechain
4	D	443	PHE	Sidechain
4	D	468	TYR	Sidechain
4	D	71	ARG	Sidechain
3	E	158	TYR	Sidechain
3	E	170	HIS	Sidechain
3	E	177	ARG	Sidechain
3	E	213	HIS	Sidechain
3	E	218	ARG	Sidechain
3	E	272	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	E	28	TYR	Sidechain
3	E	365	ARG	Sidechain
3	E	383	TYR	Sidechain
3	E	463	TYR	Sidechain
3	E	475	TYR	Sidechain
3	E	482	ARG	Sidechain
3	E	484	ARG	Sidechain
3	E	591	ARG	Sidechain
3	E	611	PHE	Sidechain
4	F	146	TYR	Sidechain
4	F	166	ARG	Sidechain
4	F	208	PHE	Sidechain
4	F	225	PHE	Sidechain
4	F	241	PHE	Sidechain
4	F	265	TYR	Sidechain
4	F	272	ARG	Sidechain
4	F	289	ARG	Sidechain
4	F	316	TYR	Sidechain
4	F	362	ARG	Sidechain
4	F	393	ARG	Sidechain
4	F	449	TYR	Sidechain
4	F	452	ARG	Sidechain
4	F	48	ARG	Sidechain
7	G	62	PHE	Sidechain
7	I	114	ARG	Sidechain
7	I	166	ARG	Sidechain
7	I	43	TYR	Sidechain
6	J	25	ARG	Sidechain
6	J	27	TYR	Sidechain
6	J	46	TYR	Sidechain
7	K	100	PHE	Sidechain
7	K	117	TYR	Sidechain
7	K	158	ARG	Sidechain
7	K	160	TYR	Sidechain
7	K	166	ARG	Sidechain
7	K	178	TYR	Sidechain
6	L	46	TYR	Sidechain
1	M	105	TYR	Sidechain
1	M	112	TYR	Sidechain
1	M	127	ARG	Sidechain
1	M	134	ARG	Sidechain
1	M	180	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	M	187	TYR	Sidechain
1	M	197	ARG	Sidechain
1	M	34	ARG	Sidechain
1	M	81	TYR	Sidechain
2	N	111	ARG	Sidechain
2	N	40	TYR	Sidechain
2	N	5	ARG	Sidechain
2	N	88	PHE	Sidechain
10	O	110	TYR	Sidechain
10	O	152	TYR	Sidechain
10	O	312	TYR	Sidechain
10	O	325	PHE	Sidechain
10	O	356	PHE	Sidechain
10	O	388	TYR	Sidechain
10	O	6	TYR	Sidechain
10	O	98	ARG	Sidechain
8	P	23	ARG	Sidechain
8	P	32	ARG	Sidechain
8	P	396	ARG	Sidechain
8	P	460	ARG	Sidechain
8	P	477	PHE	Sidechain
5	Q	100	TYR	Sidechain
5	Q	116	HIS	Sidechain
5	Q	12	PHE	Sidechain
5	Q	162	PHE	Sidechain
5	Q	18	ARG	Sidechain
5	Q	193	TYR	Sidechain
5	Q	297	ARG	Sidechain
5	Q	77	TYR	Sidechain
11	R	46	ARG	Sidechain
11	S	142	TYR	Sidechain
11	S	76	TYR	Sidechain
11	T	117	ARG	Sidechain
11	T	142	TYR	Sidechain
11	T	46	ARG	Sidechain
11	T	85	TYR	Sidechain
11	U	11	PHE	Sidechain
11	U	126	PHE	Sidechain
11	U	153	ARG	Sidechain
11	U	46	ARG	Sidechain
11	V	12	PHE	Sidechain
11	V	46	ARG	Sidechain

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Mol	Chain	Res	Type	Group
11	V	76	TYR	Sidechain
11	W	11	PHE	Sidechain
11	W	30	TYR	Sidechain
11	X	142	TYR	Sidechain
11	X	76	TYR	Sidechain
11	Y	76	TYR	Sidechain
11	Y	85	TYR	Sidechain
11	Z	142	TYR	Sidechain
11	Z	46	ARG	Sidechain
11	Z	85	TYR	Sidechain
11	a	135	PHE	Sidechain
11	a	23	PHE	Sidechain
9	b	268	GLU	Peptide
9	b	300	TYR	Sidechain
9	b	84	TYR	Sidechain
9	b	86	GLY	Peptide
9	b	91	TYR	Sidechain
9	b	99	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	M	1691	0	1740	5	0
2	N	928	0	926	2	0
3	A	4578	0	4519	16	0
3	C	4578	0	4518	4	0
3	E	4578	0	4519	19	0
4	B	3585	0	3567	11	0
4	D	3585	0	3567	11	0
4	F	3585	0	3567	11	0
5	Q	2802	0	2689	5	0
6	H	824	0	877	0	0
6	J	824	0	877	4	0
6	L	824	0	877	2	0
7	G	1731	0	1797	2	0
7	I	1731	0	1797	4	0
7	K	1731	0	1797	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	P	3712	0	3829	17	0
9	b	2540	0	2537	0	0
10	O	3122	0	3155	7	0
11	R	1071	0	1141	18	0
11	S	1071	0	1141	8	0
11	T	1071	0	1141	2	0
11	U	1071	0	1141	4	0
11	V	1071	0	1141	9	0
11	W	1071	0	1141	10	0
11	X	1071	0	1141	5	0
11	Y	1071	0	1141	6	0
11	Z	1071	0	1141	5	0
11	a	1071	0	1141	0	0
All	All	57659	0	58565	178	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 (178) 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)
11:R:97:VAL:CG1	11:R:144:LEU:CD2	1.93	1.47
11:R:97:VAL:HG11	11:R:144:LEU:CD2	1.54	1.31
11:R:97:VAL:CG1	11:R:144:LEU:HD23	1.53	1.27
11:R:97:VAL:HG13	11:R:144:LEU:HD23	1.17	1.16
11:R:97:VAL:CG1	11:R:144:LEU:HD21	1.64	1.13
11:R:97:VAL:HG13	11:R:144:LEU:CD2	1.64	1.10
11:V:66:TYR:HB3	11:V:144:LEU:HD22	1.45	0.98
11:V:66:TYR:CB	11:V:144:LEU:HD22	2.06	0.85
11:V:66:TYR:HB3	11:V:144:LEU:CD2	2.09	0.83
11:S:66:TYR:HB3	11:S:144:LEU:HD22	1.60	0.82
11:R:97:VAL:HG11	11:R:144:LEU:HD21	1.36	0.81
11:V:66:TYR:CG	11:V:144:LEU:HD22	2.17	0.79
11:W:66:TYR:HB3	11:W:144:LEU:HD22	1.65	0.78
11:U:66:TYR:HB3	11:U:144:LEU:HD22	1.68	0.74
11:Y:62:ILE:HD12	11:Y:66:TYR:OH	1.92	0.70
4:D:263:ALA:HB3	4:D:329:ILE:HD12	1.77	0.66
3:E:124:ILE:H	3:E:124:ILE:HD12	1.61	0.64
11:R:66:TYR:HB3	11:R:144:LEU:HD13	1.82	0.61
8:P:6:ILE:HG22	8:P:7:LEU:HD22	1.84	0.60
11:Z:74:VAL:HG13	11:Z:90:GLN:HE21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:286:ARG:HE	4:F:381:ARG:HH21	1.50	0.59
3:A:77:ALA:H	3:A:126:ARG:HE	1.51	0.58
11:Z:80:GLN:HE21	11:Y:85:TYR:HA	1.68	0.58
4:B:71:ARG:HH22	4:B:76:ILE:HD11	1.67	0.58
8:P:12:HIS:NE2	8:P:238:LEU:HD22	2.18	0.58
3:E:192:THR:HG22	3:E:193:LEU:HD23	1.85	0.57
3:C:233:LEU:HD13	3:C:234:LEU:H	1.69	0.57
11:S:96:SER:HB3	11:T:21:ILE:HD11	1.86	0.57
11:R:66:TYR:CB	11:R:144:LEU:HD13	2.34	0.57
8:P:161:VAL:HG21	8:P:199:TYR:CE1	2.41	0.56
4:D:402:GLN:HA	4:D:475:ARG:HE	1.71	0.55
11:V:66:TYR:CG	11:V:144:LEU:CD2	2.87	0.55
3:E:503:GLY:HA2	4:F:424:ALA:HB2	1.87	0.55
11:R:140:GLY:O	11:R:144:LEU:HG	2.07	0.55
11:U:66:TYR:HB3	11:U:144:LEU:CD2	2.37	0.54
3:E:193:LEU:HD23	3:E:193:LEU:H	1.73	0.54
11:R:97:VAL:HG11	11:R:144:LEU:HD23	1.38	0.54
11:S:73:LEU:HD23	11:S:151:ASN:HD22	1.73	0.54
11:W:66:TYR:CB	11:W:144:LEU:HD22	2.36	0.54
4:D:462:TRP:CD2	4:D:484:PHE:HB3	2.44	0.53
3:A:406:ARG:N	3:A:406:ARG:HE	2.07	0.52
4:D:407:TYR:CE1	4:D:436:LEU:HD12	2.45	0.52
3:A:27:ILE:HD12	3:A:83:ASP:HB2	1.92	0.52
4:F:46:PHE:H	4:F:47:PRO:HD2	1.75	0.52
4:B:114:ASP:HB2	4:B:120:ILE:H	1.75	0.51
6:L:103:ILE:HG22	7:K:120:ILE:HG23	1.91	0.51
11:W:63:ILE:HA	11:W:66:TYR:CD2	2.46	0.51
11:W:66:TYR:CG	11:W:144:LEU:HD22	2.45	0.51
8:P:81:ILE:HG13	8:P:123:GLN:HE21	1.76	0.51
3:E:192:THR:HG22	3:E:193:LEU:H	1.74	0.51
11:S:62:ILE:HD12	11:S:66:TYR:OH	2.11	0.51
11:Y:31:GLY:HA2	11:Y:109:GLY:HA3	1.92	0.51
11:R:46:ARG:HE	11:R:49:LEU:HD11	1.76	0.51
3:A:158:TYR:CE1	3:A:198:LEU:HD13	2.46	0.51
3:A:27:ILE:HB	3:A:82:GLY:H	1.76	0.50
8:P:6:ILE:HG21	8:P:188:ARG:HE	1.77	0.50
10:O:179:VAL:HG11	10:O:267:ILE:HD13	1.95	0.49
4:F:236:GLU:H	4:F:236:GLU:CD	2.15	0.49
4:D:102:ILE:HD12	4:D:103:PRO:HD2	1.94	0.49
1:M:111:SER:HB2	1:M:147:VAL:HG11	1.95	0.49
7:K:211:SER:O	7:K:215:LEU:HD13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:84:LEU:HD12	11:R:84:LEU:H	1.78	0.48
11:X:50:LEU:H	11:X:50:LEU:HD12	1.78	0.48
3:A:213:HIS:HE1	3:A:221:ARG:HH12	1.60	0.48
10:O:200:LYS:HG2	10:O:232:VAL:HG13	1.95	0.48
11:U:66:TYR:CB	11:U:144:LEU:HD22	2.39	0.48
3:A:47:GLU:HA	3:A:91:PRO:HA	1.95	0.48
8:P:391:ASN:HB3	8:P:396:ARG:HH22	1.79	0.48
4:B:462:TRP:CZ2	4:B:484:PHE:HB2	2.49	0.48
3:C:202:PHE:HB3	3:C:206:LYS:HD2	1.95	0.48
3:A:262:LYS:HA	3:A:265:ILE:HG12	1.95	0.48
11:V:13:GLY:H	11:V:82:GLN:HE22	1.61	0.48
11:W:97:VAL:HG22	11:W:144:LEU:HA	1.96	0.48
3:E:306:GLY:H	3:E:310:PRO:HB3	1.78	0.47
3:C:574:THR:HG23	3:C:578:LYS:HB2	1.96	0.47
5:Q:293:MET:HG2	5:Q:345:TYR:CD2	2.49	0.47
5:Q:25:LEU:H	5:Q:25:LEU:HD12	1.78	0.47
3:C:249:GLY:H	3:C:411:SER:HB2	1.78	0.47
4:D:175:ALA:HB1	4:D:362:ARG:HH21	1.79	0.47
3:E:104:ILE:HG12	3:E:112:LEU:HD12	1.97	0.47
10:O:30:THR:HG22	10:O:34:PHE:CE2	2.50	0.47
11:V:99:LEU:HB2	11:W:22:ILE:HG12	1.95	0.47
7:G:166:ARG:HD3	7:G:166:ARG:H	1.80	0.47
3:E:143:PRO:HD3	3:E:188:ALA:HB2	1.97	0.47
4:D:440:GLU:HA	4:D:444:ILE:HD12	1.96	0.46
3:A:265:ILE:HG22	3:A:528:GLN:HE22	1.79	0.46
11:S:66:TYR:HB3	11:S:144:LEU:CD2	2.37	0.46
1:M:106:LEU:HD13	1:M:155:ALA:HB1	1.98	0.46
8:P:305:HIS:HA	8:P:308:VAL:HG22	1.96	0.46
11:R:97:VAL:HG12	11:R:144:LEU:HD21	1.82	0.46
4:F:467:ILE:HG23	4:F:468:TYR:CD2	2.51	0.46
8:P:301:ARG:HH11	8:P:301:ARG:HG3	1.79	0.46
11:X:54:ILE:HG23	11:W:135:PHE:CZ	2.50	0.45
11:X:24:THR:HG23	11:X:101:GLY:HA3	1.99	0.45
4:B:260:LEU:HD13	4:B:318:ARG:HD3	1.98	0.45
4:B:453:THR:HG23	4:B:456:GLU:H	1.80	0.45
11:Z:84:LEU:HD12	11:Z:84:LEU:H	1.82	0.45
3:A:192:THR:HG22	3:A:193:LEU:H	1.82	0.45
11:V:24:THR:HG21	11:V:63:ILE:HG22	1.98	0.45
11:V:143:GLY:HA2	11:W:21:ILE:HD11	1.99	0.45
4:B:51:GLU:HA	4:B:99:SER:HA	1.99	0.45
1:M:139:TYR:CE2	2:N:19:GLY:HA3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:54:ILE:HG23	11:W:135:PHE:HZ	1.83	0.44
11:S:66:TYR:CB	11:S:144:LEU:HD22	2.39	0.44
4:B:344:HIS:HA	4:B:345:PRO:HD3	1.88	0.44
10:O:12:ILE:HG22	10:O:14:ILE:HG23	1.99	0.44
10:O:268:ASP:O	10:O:272:LYS:HG3	2.17	0.44
3:E:124:ILE:H	3:E:124:ILE:CD1	2.30	0.44
4:D:245:ALA:HB1	3:E:389:ALA:HB1	1.99	0.44
3:E:93:SER:HA	3:E:216:PRO:HA	1.99	0.44
11:R:39:ILE:HG23	11:R:53:ASN:HB3	1.99	0.44
6:J:7:ILE:HD13	6:J:7:ILE:O	2.18	0.43
3:E:79:LEU:HD12	3:E:126:ARG:HH22	1.83	0.43
10:O:296:TYR:CE1	10:O:300:PHE:CE2	3.07	0.43
3:E:223:VAL:HG21	3:E:398:ALA:HB1	1.99	0.43
5:Q:21:ARG:HH12	5:Q:308:THR:CG2	2.32	0.43
6:J:65:VAL:HA	6:J:68:LEU:HB2	2.00	0.43
11:Z:66:TYR:CG	11:Z:144:LEU:HD22	2.53	0.43
3:E:158:TYR:CZ	3:E:198:LEU:HB2	2.54	0.43
8:P:131:SER:O	8:P:132:LEU:HB2	2.19	0.43
7:I:149:ILE:HG21	7:I:174:ILE:HD11	1.99	0.43
4:D:369:ILE:HG23	4:D:445:THR:OG1	2.18	0.43
8:P:319:LEU:HB3	8:P:320:PRO:HD3	2.00	0.43
8:P:424:LEU:HA	8:P:427:ILE:HG12	1.99	0.43
4:F:154:GLY:HA2	4:F:452:ARG:H	1.83	0.43
6:J:103:ILE:HG22	7:I:120:ILE:HD13	2.01	0.43
3:A:240:LEU:HD13	3:A:439:TRP:CH2	2.53	0.43
7:I:138:ILE:HG21	7:I:195:ASP:OD2	2.19	0.43
7:G:142:LEU:HG	7:G:179:LEU:HB2	1.99	0.43
11:Y:122:GLN:OE1	11:Y:122:GLN:HA	2.19	0.43
4:B:304:TYR:HB3	4:B:308:MET:SD	2.59	0.42
8:P:165:LEU:HD21	8:P:190:LEU:HD22	2.00	0.42
4:B:371:PRO:HA	4:B:372:PRO:HD3	1.83	0.42
8:P:12:HIS:HB3	8:P:181:ASP:HA	2.01	0.42
2:N:21:LEU:HD23	2:N:21:LEU:HA	1.92	0.42
5:Q:42:LEU:HD23	5:Q:63:LEU:HD22	2.01	0.42
6:L:103:ILE:CG2	7:K:120:ILE:HG23	2.49	0.42
4:F:360:VAL:HA	4:F:373:ILE:HA	2.01	0.42
11:W:112:GLY:O	11:W:116:VAL:HG23	2.19	0.42
1:M:11:THR:HA	1:M:188:ILE:HG23	2.01	0.42
11:Z:54:ILE:O	11:Z:57:VAL:HG12	2.19	0.42
3:A:53:HIS:CE1	3:A:84:PRO:CD	3.03	0.42
4:B:296:GLU:H	4:B:296:GLU:CD	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:73:TYR:HB3	3:A:327:ALA:H	1.85	0.42
7:K:34:GLU:HG2	8:P:289:LEU:HD21	2.02	0.42
7:K:128:ALA:HB2	7:K:201:ASN:OD1	2.20	0.42
8:P:424:LEU:HD21	8:P:453:LEU:HD13	2.01	0.42
3:E:148:VAL:HG13	3:E:183:THR:O	2.20	0.41
7:I:155:ASP:O	7:I:159:GLU:HB2	2.19	0.41
4:F:46:PHE:H	4:F:47:PRO:CD	2.32	0.41
3:A:256:GLY:H	3:A:418:PRO:HD3	1.86	0.41
3:A:526:LEU:N	3:A:526:LEU:HD12	2.35	0.41
4:B:161:MET:HG3	4:B:375:VAL:HG11	2.02	0.41
8:P:194:ALA:HB3	8:P:252:LEU:HD13	2.02	0.41
11:Y:46:ARG:HB2	11:Y:49:LEU:CD1	2.51	0.41
4:F:413:ALA:HB3	4:F:433:LEU:HG	2.03	0.41
11:X:79:GLY:H	11:X:158:VAL:HG22	1.84	0.41
4:F:138:PRO:O	4:F:139:ILE:HG23	2.20	0.41
7:K:187:GLY:HA3	7:K:202:THR:HA	2.03	0.41
5:Q:208:MET:HG2	5:Q:310:TRP:CE3	2.55	0.41
3:A:100:LEU:H	3:A:170:HIS:CE1	2.39	0.41
11:U:59:MET:O	11:U:62:ILE:HG12	2.20	0.41
11:Y:66:TYR:HB3	11:Y:144:LEU:HD22	2.02	0.41
3:E:318:VAL:HG21	3:E:335:THR:HG22	2.03	0.41
11:S:85:TYR:CE2	11:T:11:PHE:HB2	2.56	0.41
11:S:114:ALA:HB1	11:S:117:ARG:HH21	1.85	0.41
1:M:83:VAL:HG22	1:M:122:LEU:HD21	2.01	0.41
4:D:111:ARG:HH11	4:D:111:ARG:HD2	1.74	0.41
3:E:182:ILE:HG22	3:E:198:LEU:HD11	2.03	0.41
3:E:173:LEU:HD12	3:E:342:TYR:CE1	2.56	0.41
4:F:210:ILE:HA	4:F:275:LEU:O	2.21	0.41
6:J:91:LYS:O	6:J:95:VAL:HG23	2.21	0.41
11:R:97:VAL:HG13	11:R:144:LEU:CG	2.44	0.41
8:P:77:LEU:HD11	8:P:117:PHE:CZ	2.56	0.40
10:O:198:VAL:HG11	10:O:206:PHE:HB2	2.02	0.40
11:R:128:GLY:HA2	11:R:131:LEU:HD12	2.03	0.40
11:R:46:ARG:HH22	11:R:123:PRO:HD3	1.86	0.40
4:D:164:ILE:HG12	4:D:170:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	M	208/256 (81%)	202 (97%)	5 (2%)	1 (0%)	29	69
2	N	113/118 (96%)	102 (90%)	7 (6%)	4 (4%)	3	25
3	A	591/616 (96%)	551 (93%)	23 (4%)	17 (3%)	4	29
3	C	591/616 (96%)	545 (92%)	31 (5%)	15 (2%)	5	32
3	E	591/616 (96%)	544 (92%)	31 (5%)	16 (3%)	5	31
4	B	455/517 (88%)	415 (91%)	26 (6%)	14 (3%)	4	27
4	D	455/517 (88%)	410 (90%)	32 (7%)	13 (3%)	4	29
4	F	455/517 (88%)	425 (93%)	20 (4%)	10 (2%)	6	35
5	Q	343/345 (99%)	317 (92%)	18 (5%)	8 (2%)	6	34
6	H	103/114 (90%)	102 (99%)	0	1 (1%)	15	54
6	J	103/114 (90%)	100 (97%)	3 (3%)	0	100	100
6	L	103/114 (90%)	98 (95%)	4 (4%)	1 (1%)	15	54
7	G	215/233 (92%)	206 (96%)	7 (3%)	2 (1%)	17	57
7	I	215/233 (92%)	207 (96%)	6 (3%)	2 (1%)	17	57
7	K	215/233 (92%)	206 (96%)	8 (4%)	1 (0%)	29	69
8	P	457/478 (96%)	434 (95%)	18 (4%)	5 (1%)	14	52
9	b	306/840 (36%)	289 (94%)	11 (4%)	6 (2%)	7	38
10	O	390/392 (100%)	350 (90%)	26 (7%)	14 (4%)	3	25
11	R	148/160 (92%)	137 (93%)	7 (5%)	4 (3%)	5	31
11	S	148/160 (92%)	136 (92%)	9 (6%)	3 (2%)	7	38
11	T	148/160 (92%)	138 (93%)	7 (5%)	3 (2%)	7	38
11	U	148/160 (92%)	138 (93%)	7 (5%)	3 (2%)	7	38
11	V	148/160 (92%)	141 (95%)	6 (4%)	1 (1%)	22	63
11	W	148/160 (92%)	137 (93%)	9 (6%)	2 (1%)	11	46
11	X	148/160 (92%)	138 (93%)	5 (3%)	5 (3%)	3	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	Y	148/160 (92%)	139 (94%)	6 (4%)	3 (2%)	7	38
11	Z	148/160 (92%)	145 (98%)	2 (1%)	1 (1%)	22	63
11	a	148/160 (92%)	138 (93%)	7 (5%)	3 (2%)	7	38
All	All	7389/8469 (87%)	6890 (93%)	341 (5%)	158 (2%)	10	36

All (158) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	475	TYR
4	D	45	LYS
4	D	59	ASP
4	D	143	ALA
3	E	475	TYR
3	E	565	ALA
3	E	575	GLY
4	F	46	PHE
3	A	202	PHE
3	A	475	TYR
4	B	141	PRO
4	B	372	PRO
10	O	120	LYS
10	O	186	LEU
6	H	77	GLN
7	I	167	ALA
7	I	192	ASN
11	U	157	ASP
11	X	47	PRO
11	Y	158	VAL
11	T	158	VAL
2	N	115	LEU
3	C	575	GLY
4	D	319	ALA
4	D	372	PRO
3	E	164	ASN
4	F	467	ILE
3	A	230	ASP
3	A	258	PHE
3	A	532	SER
3	A	575	GLY
4	B	139	ILE
4	B	377	PRO

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Mol	Chain	Res	Type
5	Q	133	PHE
5	Q	240	ASP
8	P	3	ALA
9	b	24	GLU
9	b	87	ASP
9	b	356	MET
10	O	39	ILE
10	O	172	VAL
10	O	375	ALA
11	X	82	GLN
11	X	157	ASP
11	a	47	PRO
11	R	123	PRO
11	R	158	VAL
11	Y	156	GLN
11	T	157	ASP
11	T	159	VAL
11	W	156	GLN
1	M	124	GLY
2	N	98	ASP
3	C	230	ASP
3	C	261	GLY
3	C	310	PRO
4	D	58	PRO
4	D	141	PRO
4	D	149	GLU
3	E	405	ASP
3	E	449	LYS
3	E	536	ALA
4	F	299	PRO
3	A	39	ASN
3	A	203	ASP
3	A	284	GLY
3	A	441	LEU
3	A	565	ALA
6	L	63	GLY
8	P	35	GLU
9	b	83	LEU
9	b	86	GLY
9	b	257	ASP
10	O	90	ASN
10	O	167	THR

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Mol	Chain	Res	Type
10	O	176	HIS
11	X	156	GLN
11	a	123	PRO
11	R	156	GLN
11	R	159	VAL
11	S	47	PRO
11	W	159	VAL
3	C	257	ALA
3	C	305	SER
3	C	591	ARG
4	D	136	GLY
4	D	424	ALA
3	E	207	SER
3	E	257	ALA
4	F	83	THR
4	F	202	ASP
4	F	372	PRO
4	F	391	MET
3	A	325	PRO
3	A	405	ASP
3	A	531	TYR
3	A	590	SER
4	B	83	THR
4	B	116	SER
4	B	127	PHE
4	B	163	SER
4	B	167	GLY
4	B	292	SER
5	Q	134	ASP
5	Q	230	SER
10	O	171	SER
7	G	195	ASP
11	Y	159	VAL
3	C	207	SER
3	C	420	GLY
4	D	83	THR
3	E	230	ASP
3	E	305	SER
3	E	590	SER
4	F	123	GLY
4	F	125	LYS
4	F	360	VAL

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Mol	Chain	Res	Type
4	B	143	ALA
4	B	202	ASP
5	Q	117	ASP
5	Q	174	ASP
7	K	152	MET
8	P	458	ASP
10	O	7	THR
10	O	95	ASN
10	O	100	LEU
10	O	116	TRP
7	G	135	PRO
11	U	158	VAL
11	X	48	ASP
11	Z	159	VAL
11	S	159	VAL
11	V	159	VAL
2	N	4	LYS
3	C	109	GLN
3	C	405	ASP
4	D	50	ASN
4	D	137	SER
3	E	259	GLY
3	A	456	THR
5	Q	129	PRO
8	P	390	ASP
8	P	412	ASN
11	a	159	VAL
3	E	310	PRO
3	A	78	GLY
4	B	88	VAL
3	E	284	GLY
2	N	25	ILE
3	C	284	GLY
5	Q	203	PRO
11	S	79	GLY
10	O	106	PRO
3	C	381	PRO
3	C	539	PRO
3	E	197	ILE
4	B	179	PRO
11	U	47	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	183/221 (83%)	176 (96%)	7 (4%)	33	57
2	N	102/104 (98%)	99 (97%)	3 (3%)	42	64
3	A	497/515 (96%)	479 (96%)	18 (4%)	35	59
3	C	497/515 (96%)	481 (97%)	16 (3%)	39	61
3	E	497/515 (96%)	475 (96%)	22 (4%)	28	53
4	B	391/444 (88%)	377 (96%)	14 (4%)	35	59
4	D	391/444 (88%)	377 (96%)	14 (4%)	35	59
4	F	391/444 (88%)	375 (96%)	16 (4%)	30	55
5	Q	309/309 (100%)	300 (97%)	9 (3%)	42	64
6	H	87/94 (93%)	86 (99%)	1 (1%)	73	84
6	J	87/94 (93%)	84 (97%)	3 (3%)	37	60
6	L	87/94 (93%)	87 (100%)	0	100	100
7	G	194/208 (93%)	187 (96%)	7 (4%)	35	59
7	I	194/208 (93%)	190 (98%)	4 (2%)	53	72
7	K	194/208 (93%)	187 (96%)	7 (4%)	35	59
8	P	426/439 (97%)	416 (98%)	10 (2%)	50	70
9	b	275/728 (38%)	266 (97%)	9 (3%)	38	61
10	O	348/348 (100%)	337 (97%)	11 (3%)	39	61
11	R	110/119 (92%)	107 (97%)	3 (3%)	44	65
11	S	110/119 (92%)	108 (98%)	2 (2%)	59	77
11	T	110/119 (92%)	109 (99%)	1 (1%)	78	87
11	U	110/119 (92%)	107 (97%)	3 (3%)	44	65
11	V	110/119 (92%)	108 (98%)	2 (2%)	59	77
11	W	110/119 (92%)	109 (99%)	1 (1%)	78	87
11	X	110/119 (92%)	105 (96%)	5 (4%)	27	52
11	Y	110/119 (92%)	104 (94%)	6 (6%)	21	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	Z	110/119 (92%)	104 (94%)	6 (6%)	21	47
11	a	110/119 (92%)	107 (97%)	3 (3%)	44	65
All	All	6250/7122 (88%)	6047 (97%)	203 (3%)	42	61

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	102	SER
1	M	112	TYR
1	M	117	ILE
1	M	122	LEU
1	M	139	TYR
1	M	189	ASN
1	M	216	LYS
2	N	15	ASP
2	N	78	ARG
2	N	106	ASP
3	C	126	ARG
3	C	131	PRO
3	C	143	PRO
3	C	179	ARG
3	C	196	LYS
3	C	278	ILE
3	C	279	ILE
3	C	286	ARG
3	C	325	PRO
3	C	406	ARG
3	C	422	ASP
3	C	476	PRO
3	C	505	SER
3	C	532	SER
3	C	544	PHE
3	C	572	ASP
4	D	42	GLU
4	D	43	LYS
4	D	59	ASP
4	D	62	VAL
4	D	79	VAL
4	D	86	ILE
4	D	92	THR
4	D	243	ASN

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Mol	Chain	Res	Type
4	D	246	ASN
4	D	250	ILE
4	D	392	THR
4	D	443	PHE
4	D	467	ILE
4	D	474	ASN
3	E	24	TYR
3	E	60	VAL
3	E	91	PRO
3	E	167	ILE
3	E	192	THR
3	E	194	ASP
3	E	197	ILE
3	E	254	ILE
3	E	263	THR
3	E	279	ILE
3	E	304	MET
3	E	317	LEU
3	E	359	ARG
3	E	391	PHE
3	E	406	ARG
3	E	441	LEU
3	E	449	LYS
3	E	478	PHE
3	E	504	LYS
3	E	524	ASP
3	E	541	TRP
3	E	603	LEU
4	F	53	VAL
4	F	64	GLN
4	F	91	THR
4	F	95	PHE
4	F	118	ARG
4	F	169	LYS
4	F	198	LYS
4	F	219	LEU
4	F	250	ILE
4	F	297	GLU
4	F	299	PRO
4	F	305	PRO
4	F	329	ILE
4	F	337	MET

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Mol	Chain	Res	Type
4	F	357	GLN
4	F	472	MET
3	A	61	ILE
3	A	80	THR
3	A	96	LEU
3	A	179	ARG
3	A	192	THR
3	A	205	LYS
3	A	238	ARG
3	A	258	PHE
3	A	260	CYS
3	A	267	GLN
3	A	286	ARG
3	A	300	LEU
3	A	406	ARG
3	A	416	VAL
3	A	482	ARG
3	A	526	LEU
3	A	599	GLU
3	A	605	SER
4	B	32	SER
4	B	34	VAL
4	B	68	LEU
4	B	164	ILE
4	B	198	LYS
4	B	248	PRO
4	B	290	GLU
4	B	296	GLU
4	B	329	ILE
4	B	340	ASP
4	B	389	GLU
4	B	394	LYS
4	B	427	ILE
4	B	429	ASP
5	Q	41	ASP
5	Q	46	LEU
5	Q	57	SER
5	Q	114	THR
5	Q	173	ASP
5	Q	181	ARG
5	Q	185	TYR
5	Q	208	MET

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Mol	Chain	Res	Type
5	Q	307	SER
7	K	49	ASN
7	K	85	ARG
7	K	93	GLU
7	K	145	ASP
7	K	168	PRO
7	K	182	ASP
7	K	213	GLU
8	P	53	LYS
8	P	90	GLU
8	P	118	GLN
8	P	149	LEU
8	P	198	GLU
8	P	224	SER
8	P	325	LEU
8	P	327	GLU
8	P	350	TYR
8	P	449	ASP
9	b	20	TYR
9	b	21	ILE
9	b	65	VAL
9	b	186	TYR
9	b	203	LEU
9	b	247	LYS
9	b	325	LYS
9	b	331	ASN
9	b	342	PRO
10	O	26	PRO
10	O	59	ASP
10	O	79	ILE
10	O	106	PRO
10	O	121	PHE
10	O	186	LEU
10	O	212	THR
10	O	238	LEU
10	O	240	LYS
10	O	311	VAL
10	O	350	PHE
6	H	59	GLN
7	G	9	THR
7	G	23	PHE
7	G	43	TYR

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Mol	Chain	Res	Type
7	G	61	ASN
7	G	62	PHE
7	G	143	GLU
7	G	166	ARG
6	J	4	LYS
6	J	7	ILE
6	J	38	ASP
7	I	63	LYS
7	I	89	LEU
7	I	182	ASP
7	I	192	ASN
11	U	124	ARG
11	U	125	LEU
11	U	139	LEU
11	X	75	CYS
11	X	81	LYS
11	X	91	LEU
11	X	97	VAL
11	X	142	TYR
11	a	56	PRO
11	a	116	VAL
11	a	126	PHE
11	R	11	PHE
11	R	37	VAL
11	R	119	SER
11	Z	11	PHE
11	Z	99	LEU
11	Z	117	ARG
11	Z	123	PRO
11	Z	129	MET
11	Z	160	CYS
11	S	116	VAL
11	S	152	SER
11	Y	17	CYS
11	Y	34	LYS
11	Y	57	VAL
11	Y	81	LYS
11	Y	97	VAL
11	Y	120	SER
11	T	127	VAL
11	V	117	ARG
11	V	142	TYR

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Mol	Chain	Res	Type
11	W	139	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	98	GLN
2	N	55	ASN
3	C	320	ASN
3	C	474	ASN
4	D	50	ASN
4	D	78	GLN
3	E	147	GLN
3	E	151	HIS
3	E	164	ASN
3	E	267	GLN
3	E	447	GLN
3	E	465	ASN
4	F	273	HIS
4	F	396	HIS
3	A	53	HIS
3	A	213	HIS
3	A	288	ASN
3	A	528	GLN
3	A	558	GLN
4	B	207	ASN
4	B	331	GLN
4	B	396	HIS
5	Q	106	ASN
5	Q	287	HIS
6	L	3	GLN
7	K	113	ASN
7	K	200	ASN
8	P	123	GLN
8	P	374	HIS
8	P	425	ASN
8	P	429	HIS
8	P	456	HIS
9	b	79	HIS
9	b	146	GLN
9	b	185	ASN
9	b	210	ASN
9	b	220	GLN

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Mol	Chain	Res	Type
9	b	267	ASN
9	b	278	ASN
9	b	280	ASN
10	O	187	ASN
10	O	302	ASN
7	G	36	GLN
7	G	61	ASN
7	G	201	ASN
11	X	122	GLN
11	R	80	GLN
11	R	151	ASN
11	Z	80	GLN
11	Z	90	GLN
11	S	151	ASN
11	V	82	GLN
11	W	156	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 [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

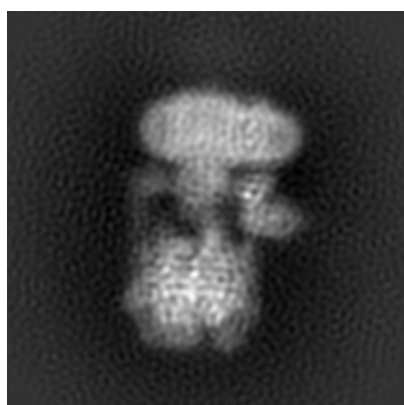
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6285. These allow visual inspection of the internal detail of the map and identification of artifacts.

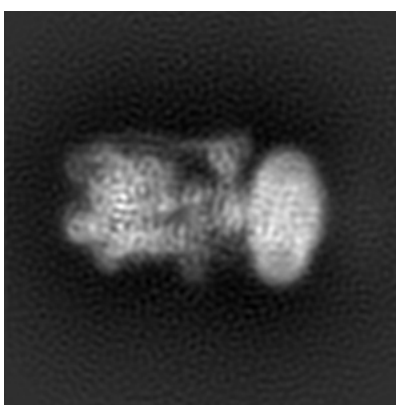
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

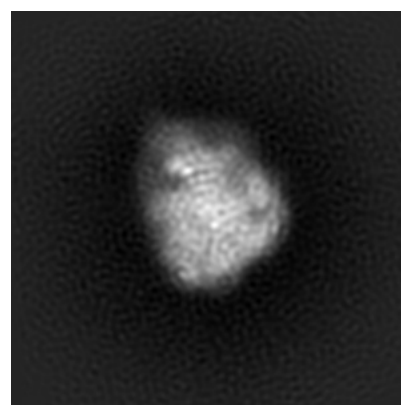
6.1.1 Primary map



X



Y

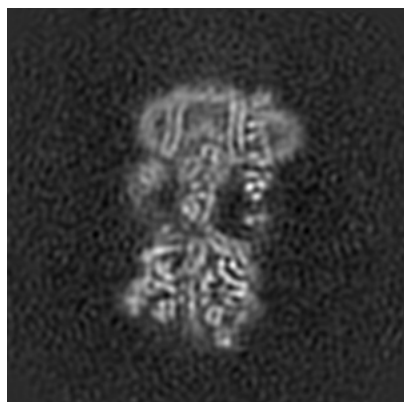


Z

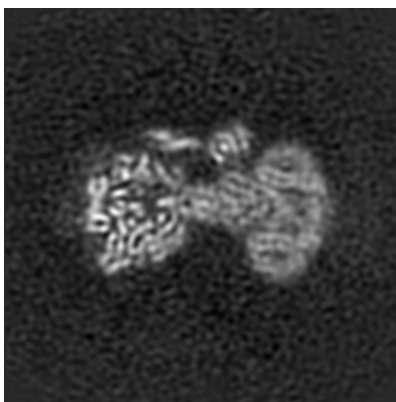
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

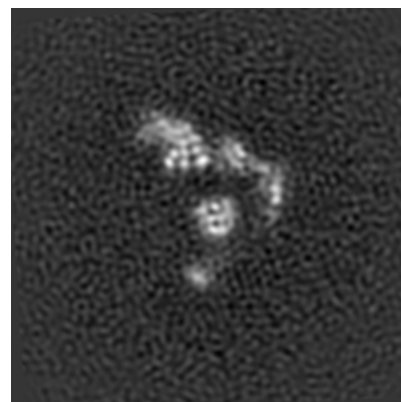
6.2.1 Primary map



X Index: 128



Y Index: 128

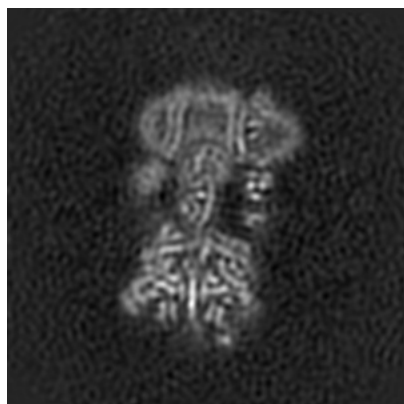


Z Index: 128

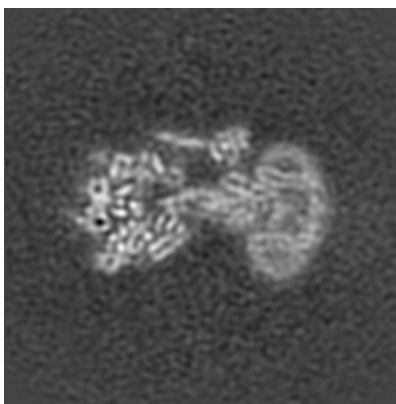
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

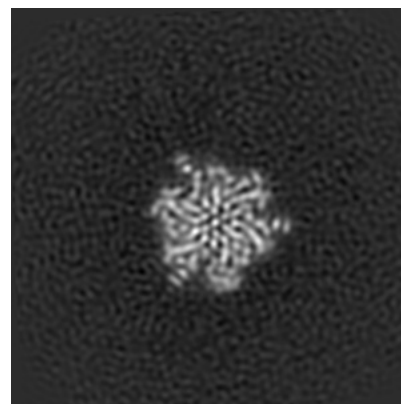
6.3.1 Primary map



X Index: 130



Y Index: 130



Z Index: 75

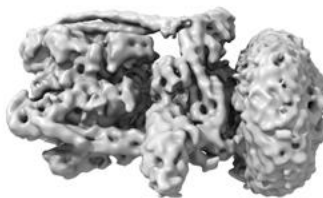
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

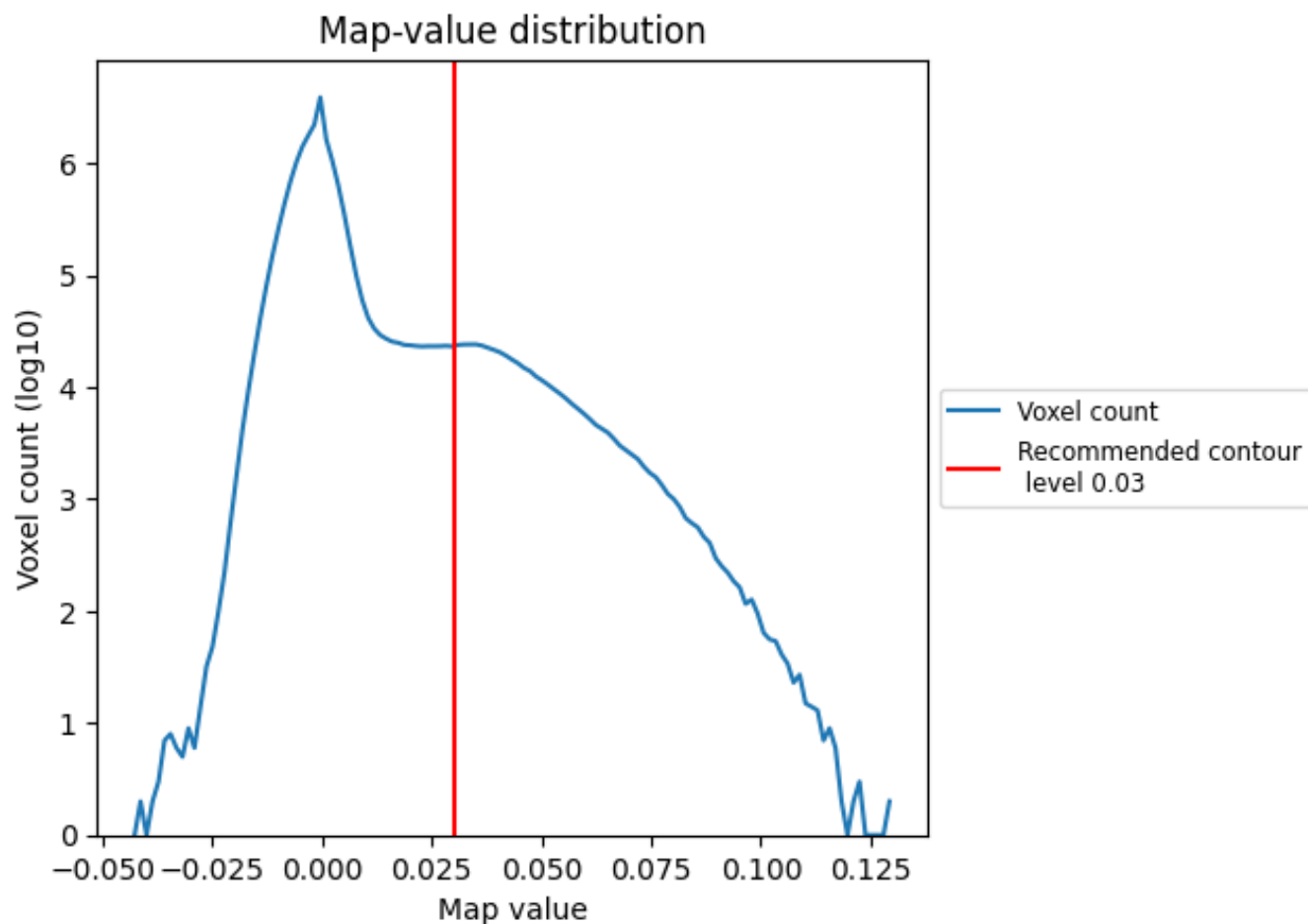
6.5 Mask visualisation

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

7 Map analysis [i](#)

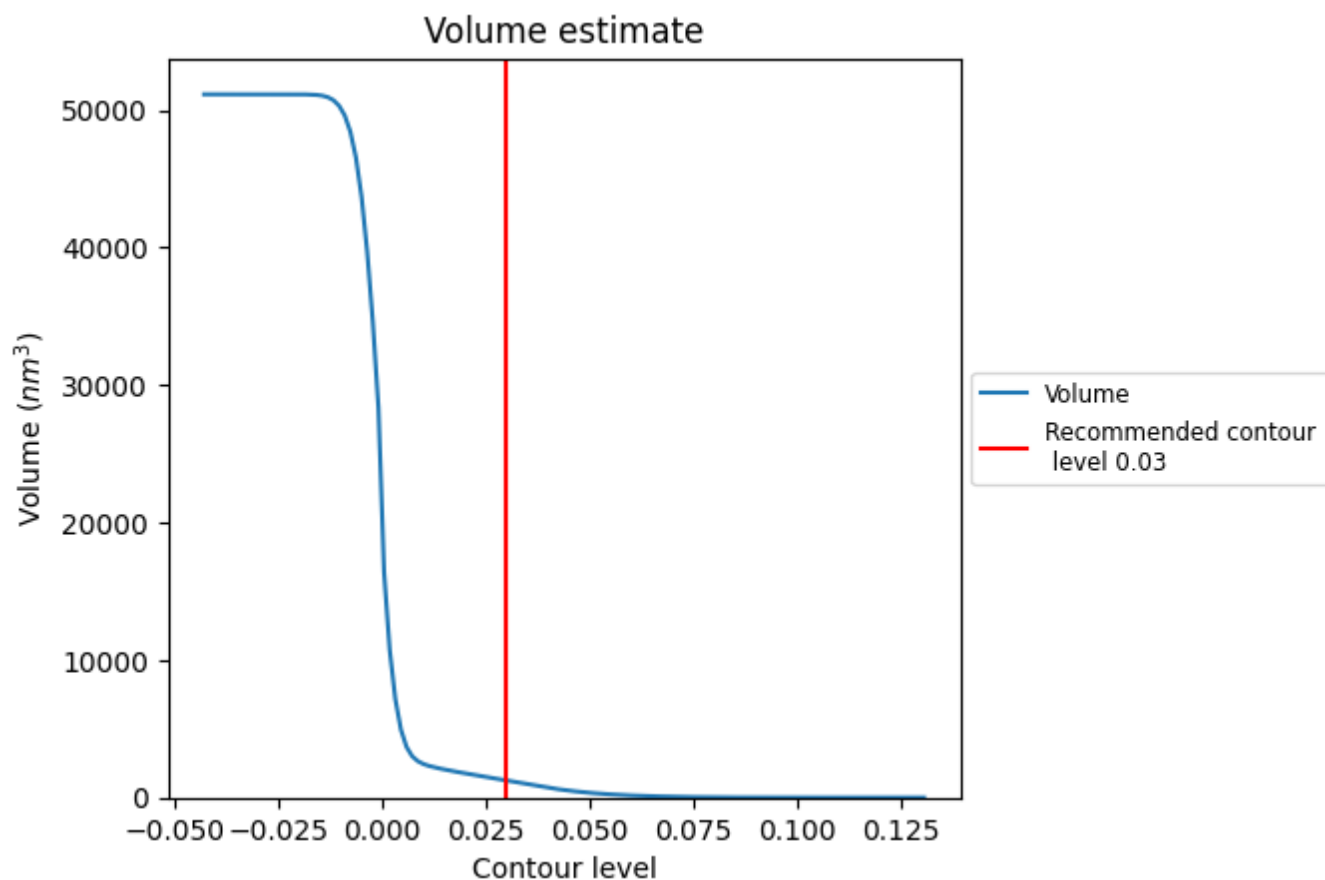
This section contains the results of statistical analysis of the map.

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.

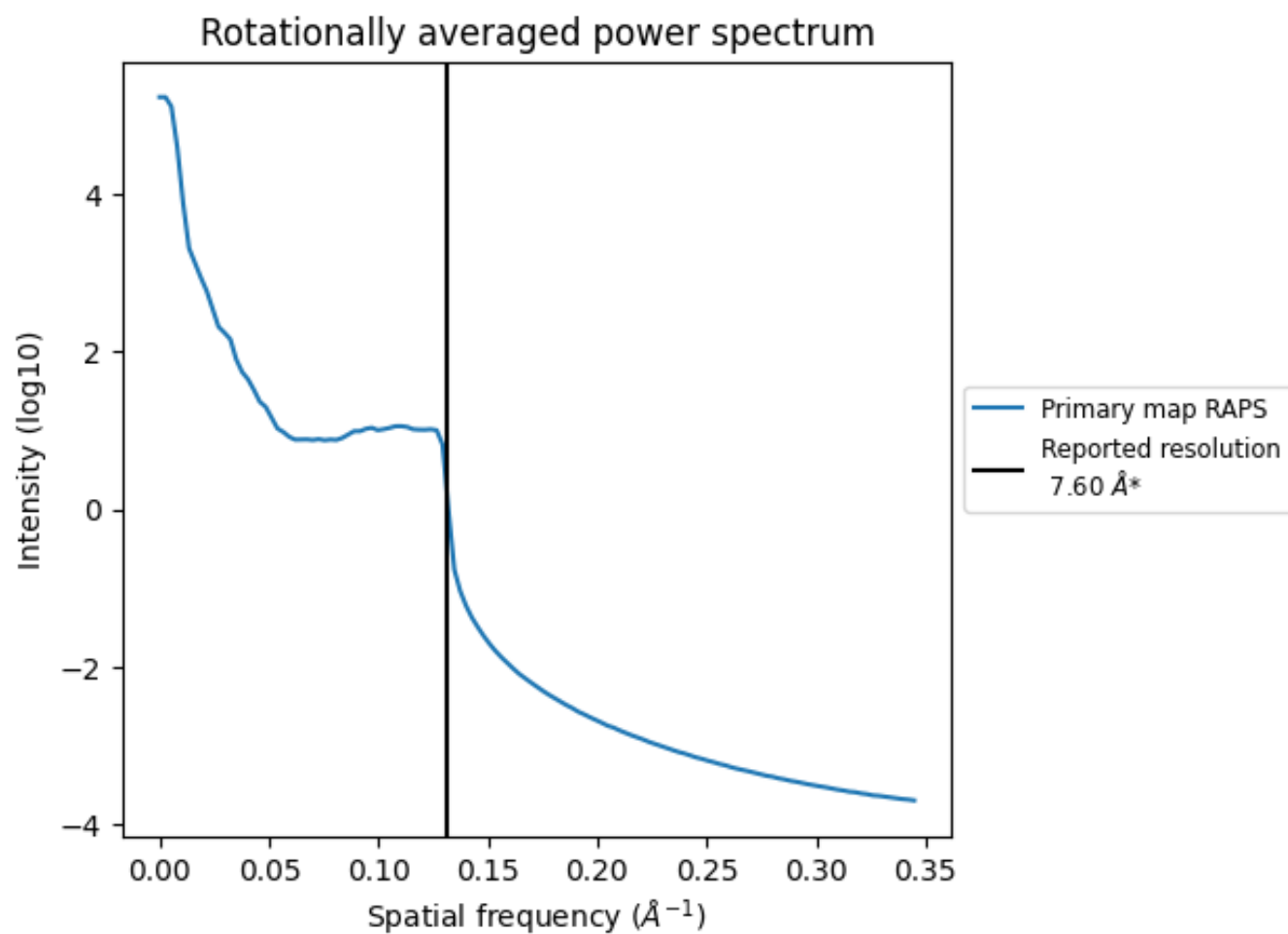
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1247 nm³; this corresponds to an approximate mass of 1126 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 ⓘ

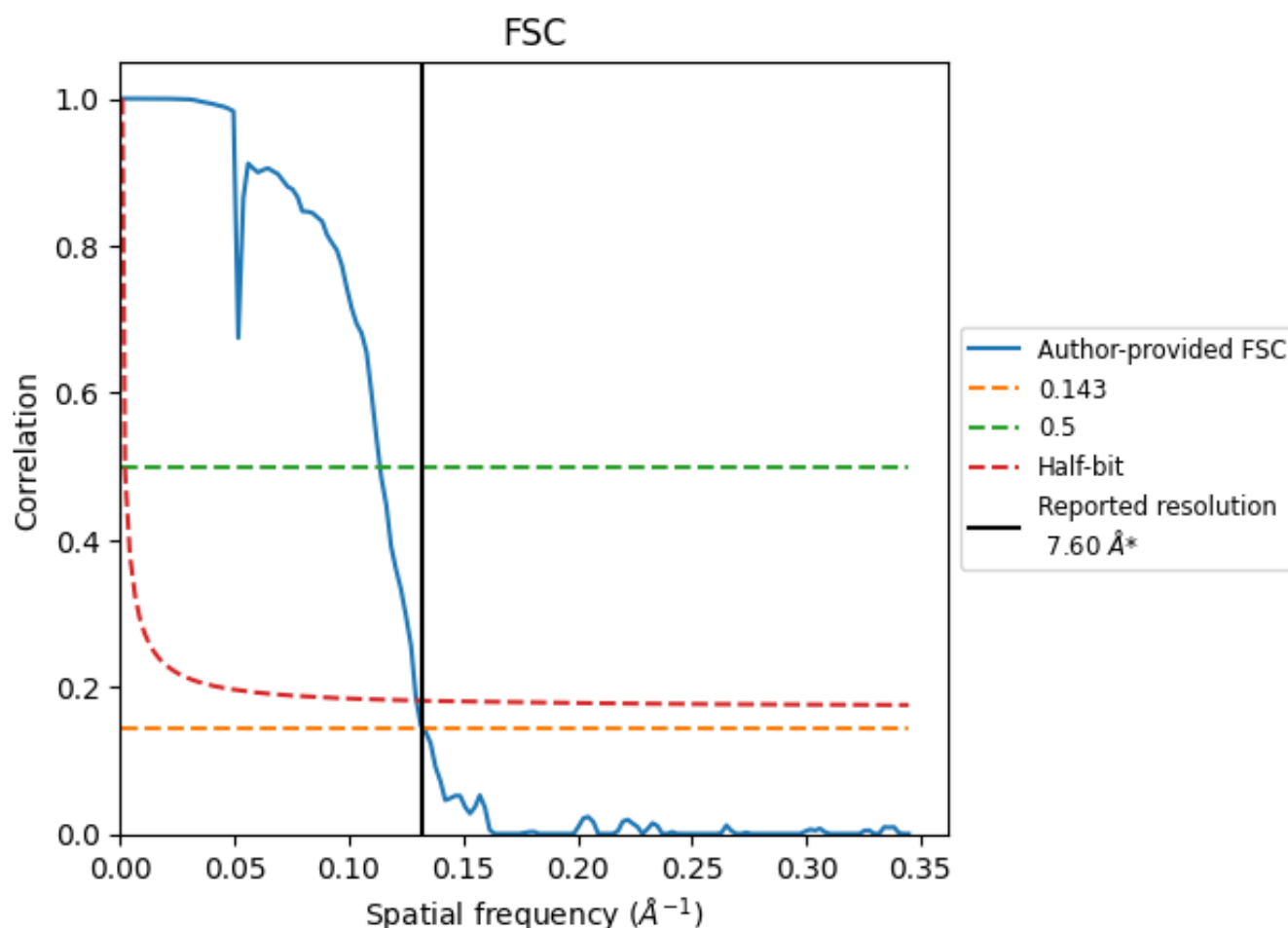


*Reported resolution corresponds to spatial frequency of 0.132 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.132 \AA^{-1}

8.2 Resolution estimates [i](#)

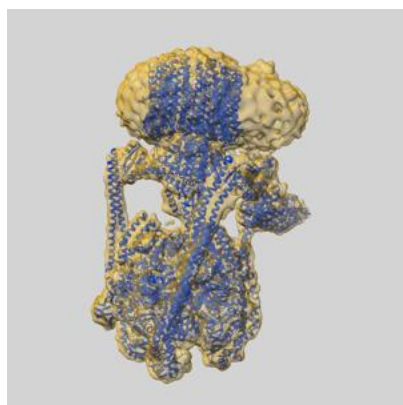
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.60	-	-
Author-provided FSC curve	7.54	8.80	7.72
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

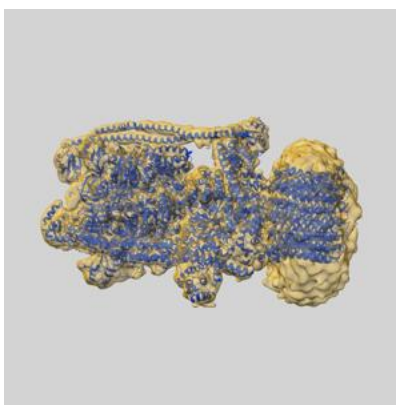
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6285 and PDB model 3J9U. Per-residue inclusion information can be found in section [3](#) on page [7](#).

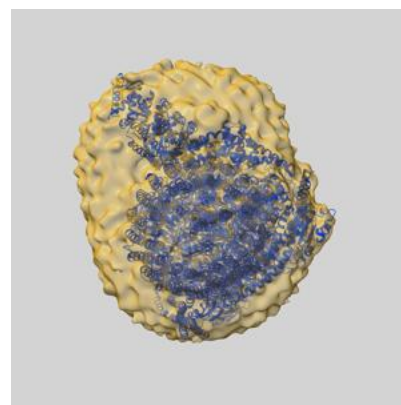
9.1 Map-model overlay [i](#)



X



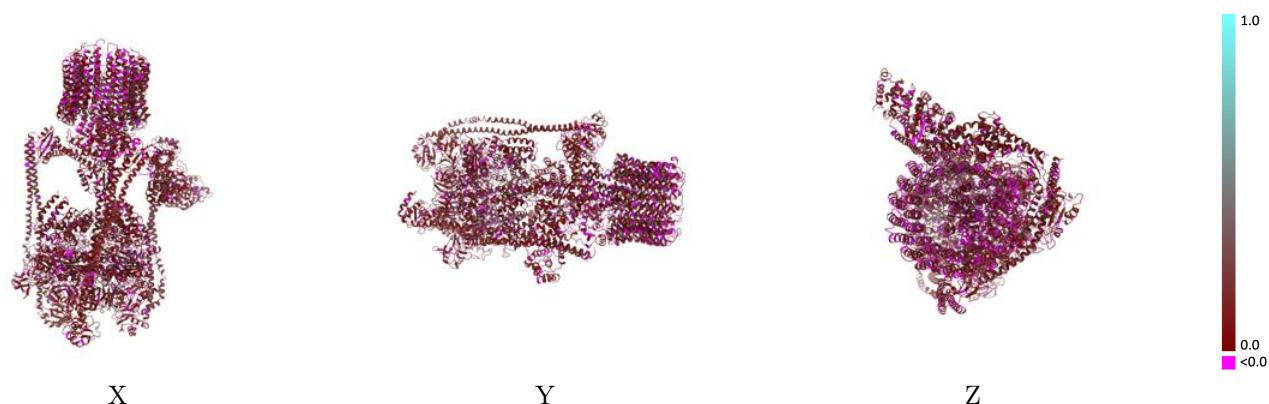
Y



Z

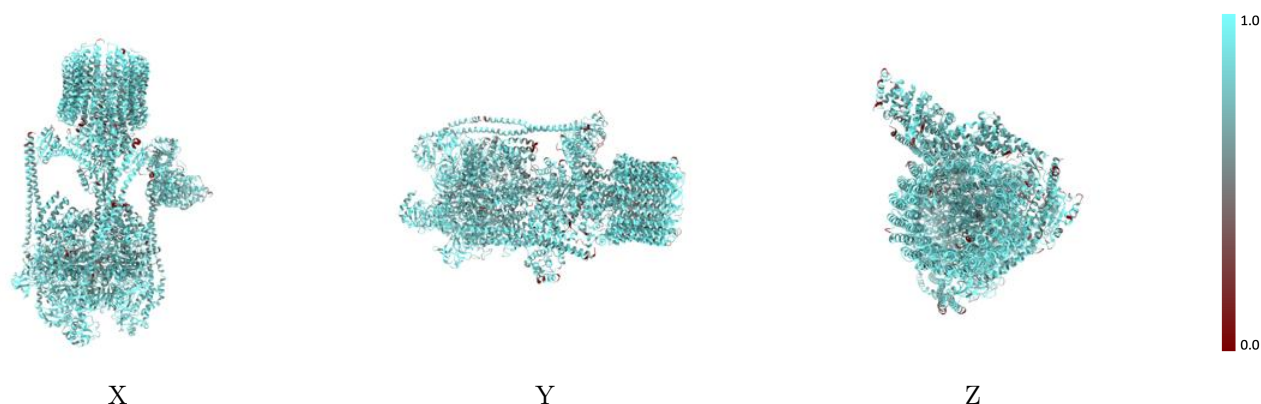
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



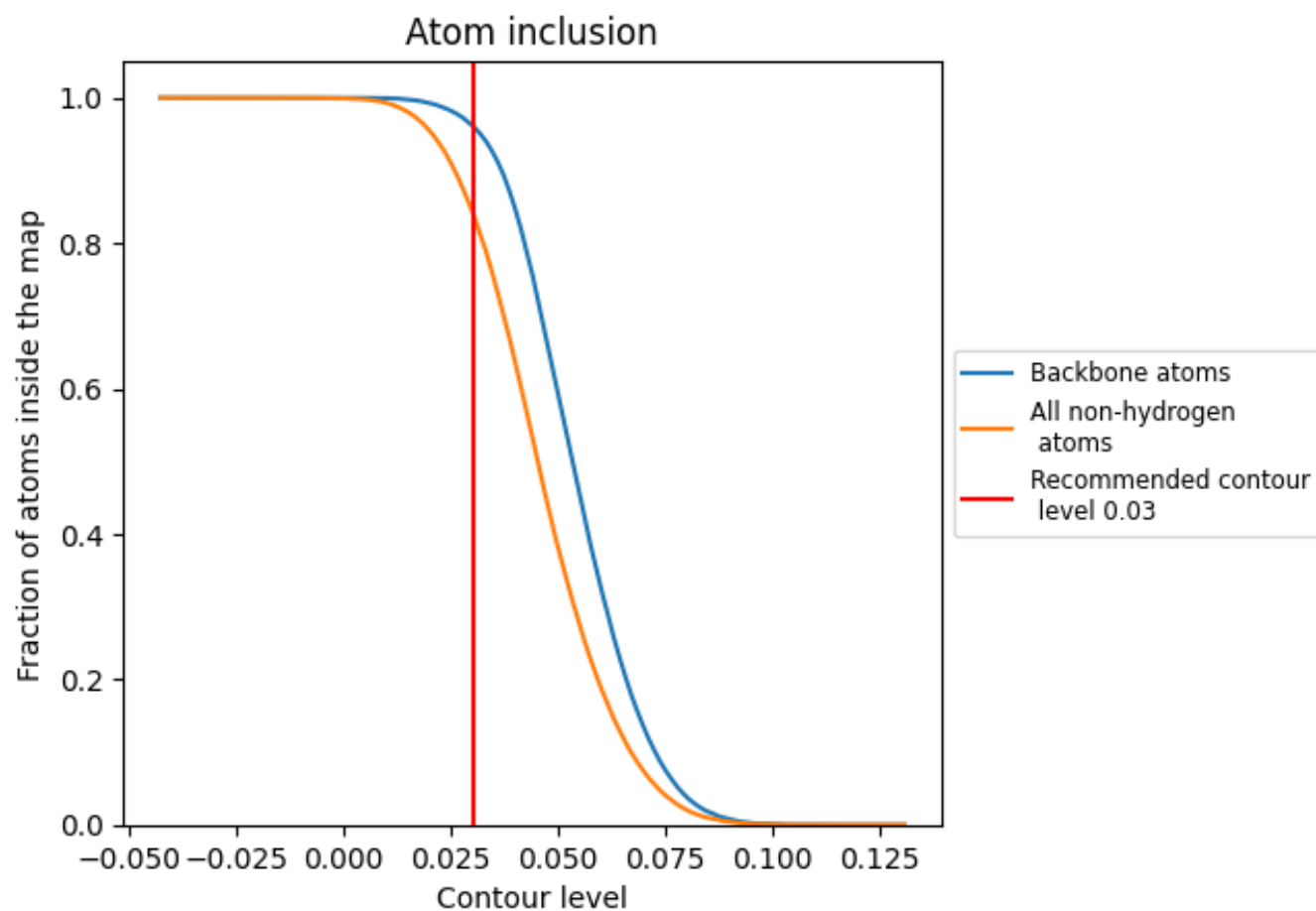
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8424	 0.1210
A	 0.8724	 0.1340
B	 0.8358	 0.1250
C	 0.8248	 0.1320
D	 0.8358	 0.1220
E	 0.8646	 0.1260
F	 0.8449	 0.1220
G	 0.8283	 0.1440
H	 0.7873	 0.1460
I	 0.8423	 0.1480
J	 0.7922	 0.1550
K	 0.8353	 0.1450
L	 0.7897	 0.1580
M	 0.8106	 0.1110
N	 0.7998	 0.1260
O	 0.8212	 0.1210
P	 0.7987	 0.1300
Q	 0.7870	 0.0840
R	 0.8507	 0.1240
S	 0.8724	 0.1180
T	 0.9282	 0.1010
U	 0.9036	 0.0840
V	 0.9272	 0.0980
W	 0.9093	 0.1000
X	 0.9149	 0.0860
Y	 0.9102	 0.0800
Z	 0.9074	 0.0810
a	 0.8941	 0.1120
b	 0.7985	 0.1090

