



Full wwPDB EM Validation Report ⓘ

Mar 9, 2024 – 01:25 PM EST

PDB ID : 6NRA
EMDB ID : EMD-0492
Title : hTRiC-hPFD Class1 (No PFD)
Authors : Gestaut, D.R.; Roh, S.H.; Ma, B.; Pintilie, G.; Joachimiak, L.A.; Leitner, A.; Walzthoeni, T.; Aebersold, R.; Chiu, W.; Frydman, J.
Deposited on : 2019-01-23
Resolution : 7.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

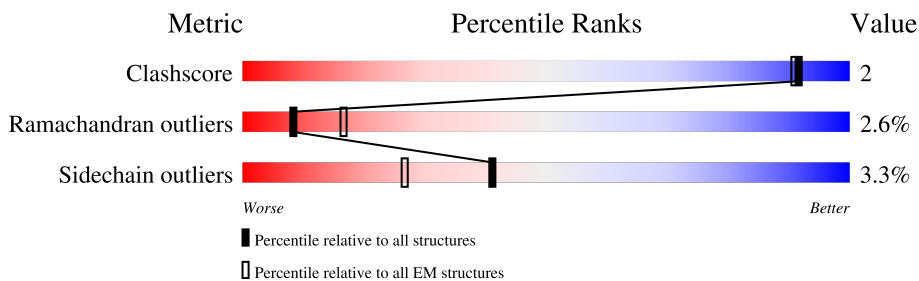
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	534	
1	I	534	
2	B	509	
2	J	509	
3	C	513	
3	K	513	
4	D	514	
4	L	514	

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Mol	Chain	Length	Quality of chain
5	E	517	
5	M	517	
6	F	515	
6	N	515	
7	G	514	
7	O	514	
8	H	514	
8	P	514	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 62802 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 T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	521	Total	C	N	O	S	0	0
			3956	2479	691	763	23		
1	I	534	Total	C	N	O	S	0	0
			4056	2540	709	783	24		

- Molecule 2 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	509	Total	C	N	O	S	0	0
			3829	2392	673	745	19		
2	J	508	Total	C	N	O	S	0	0
			3823	2389	672	743	19		

- Molecule 3 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	509	Total	C	N	O	S	0	0
			3956	2465	697	764	30		
3	K	513	Total	C	N	O	S	0	0
			3985	2481	703	771	30		

- Molecule 4 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	508	Total	C	N	O	S	0	0
			3832	2398	665	746	23		
4	L	513	Total	C	N	O	S	0	0
			3873	2422	674	754	23		

- Molecule 5 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	517	Total	C	N	O	S	0	0
			3974	2483	692	769	30		
5	M	517	Total	C	N	O	S	0	0
			3974	2483	692	769	30		

- Molecule 6 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	514	Total	C	N	O	S	0	0
			3945	2478	690	757	20		
6	N	513	Total	C	N	O	S	0	0
			3940	2476	689	755	20		

- Molecule 7 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	512	Total	C	N	O	S	0	0
			3936	2485	682	746	23		
7	O	514	Total	C	N	O	S	0	0
			3947	2490	684	750	23		

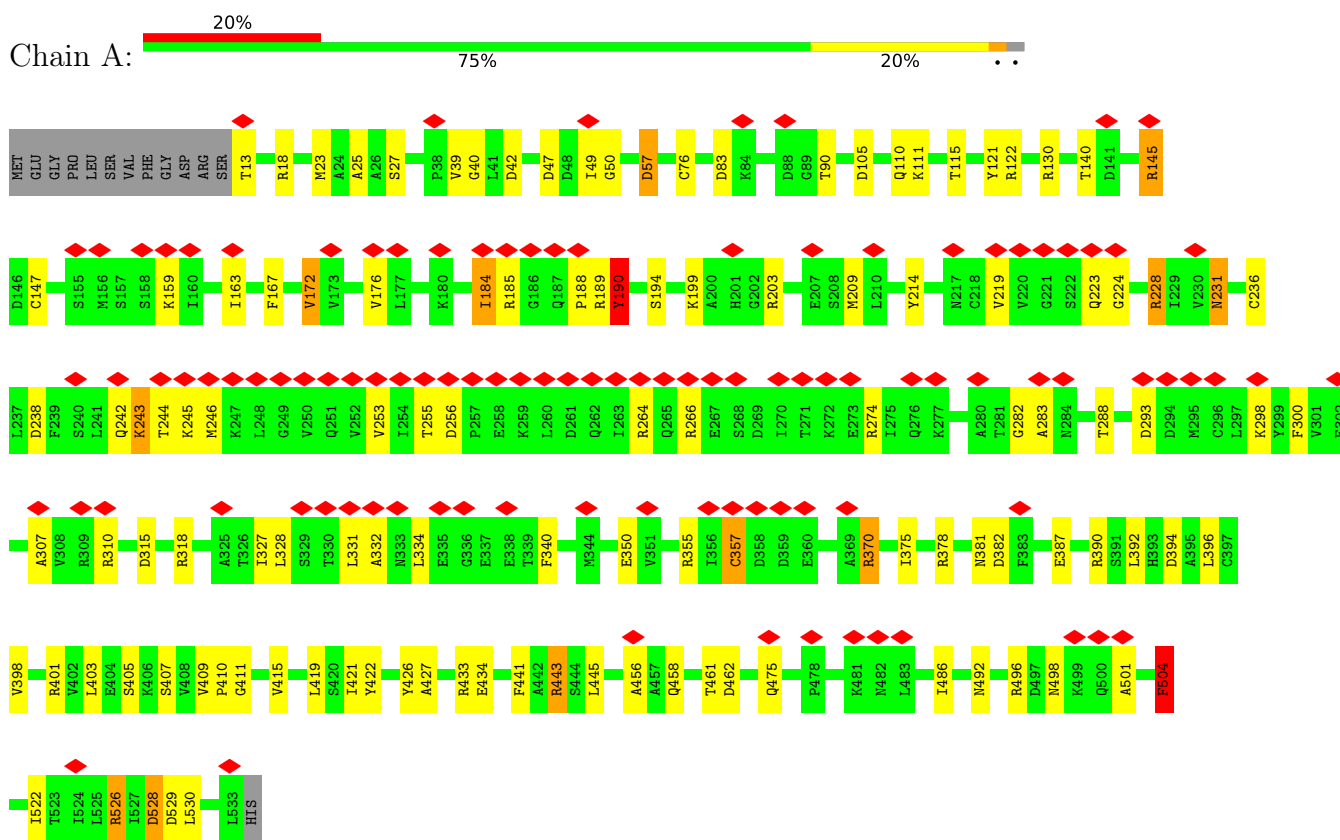
- Molecule 8 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	510	Total	C	N	O	S	0	0
			3892	2451	661	754	26		
8	P	509	Total	C	N	O	S	0	0
			3884	2447	659	752	26		

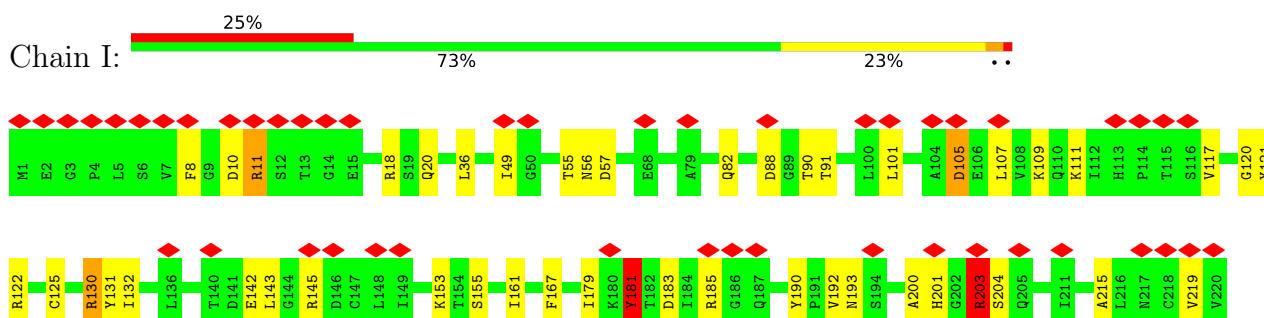
3 Residue-property plots [i](#)

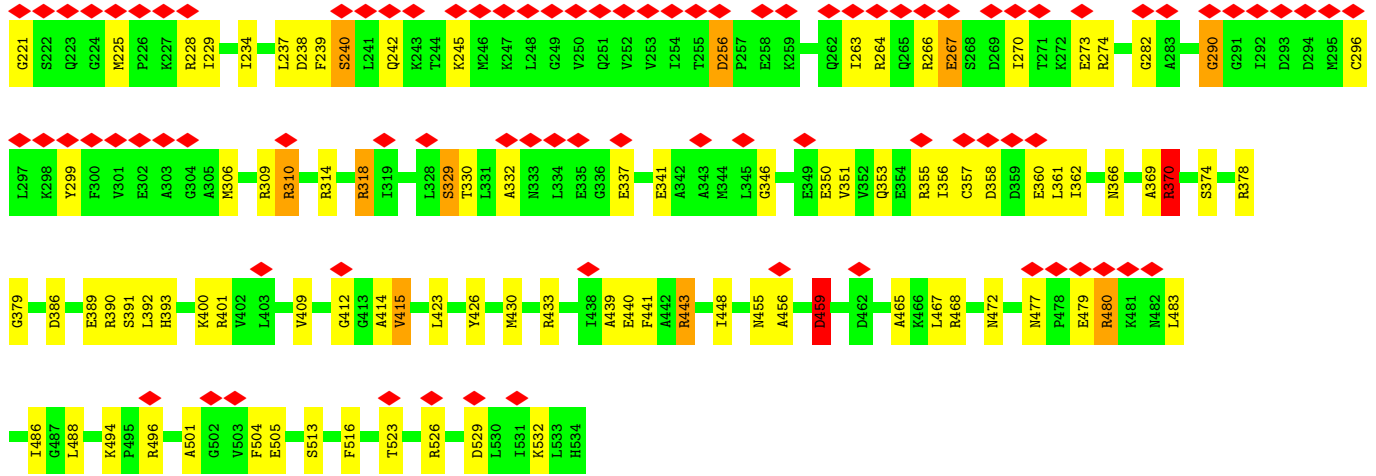
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: T-complex protein 1 subunit alpha

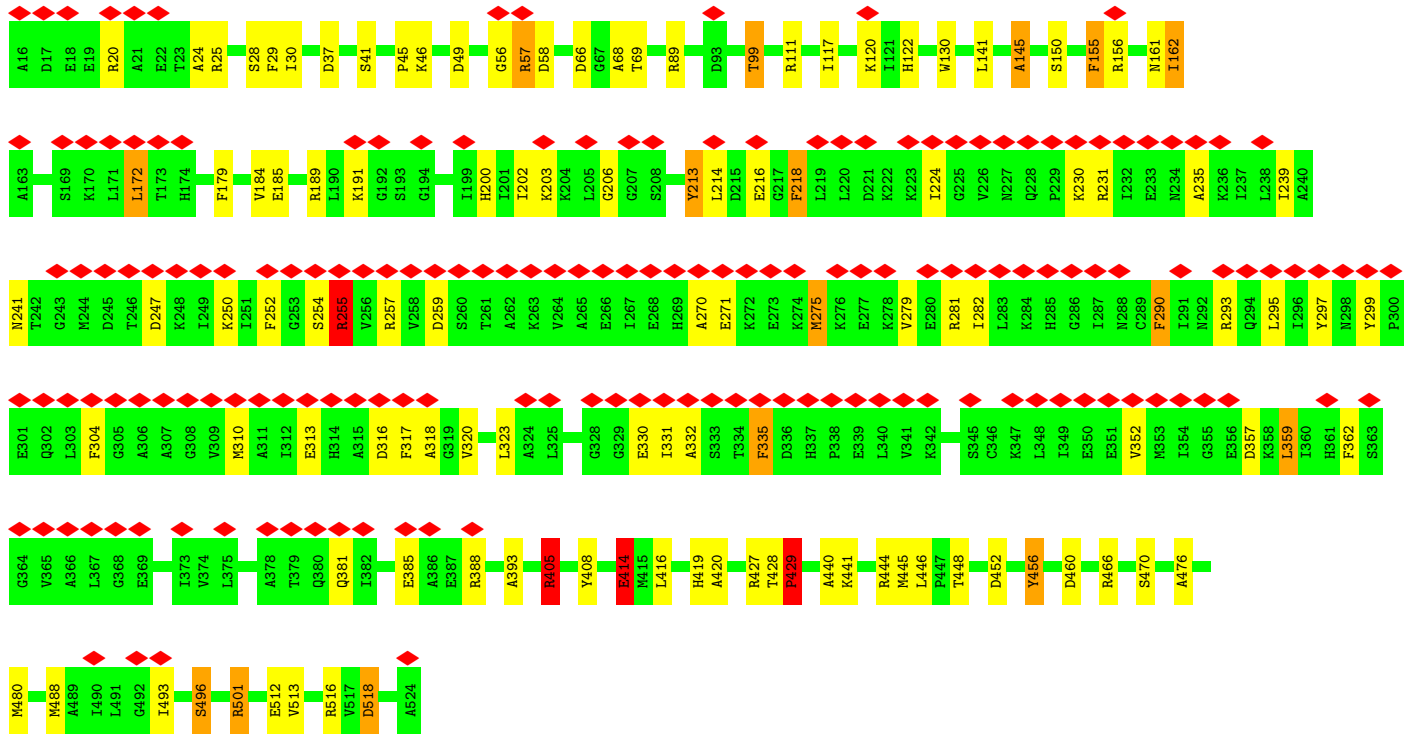
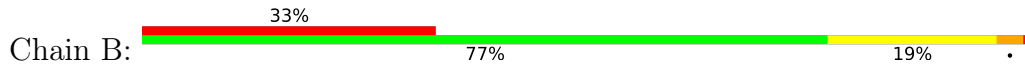


- Molecule 1: T-complex protein 1 subunit alpha

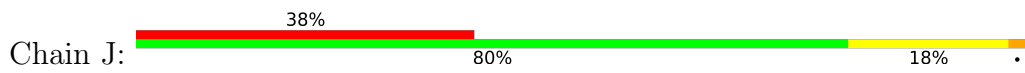


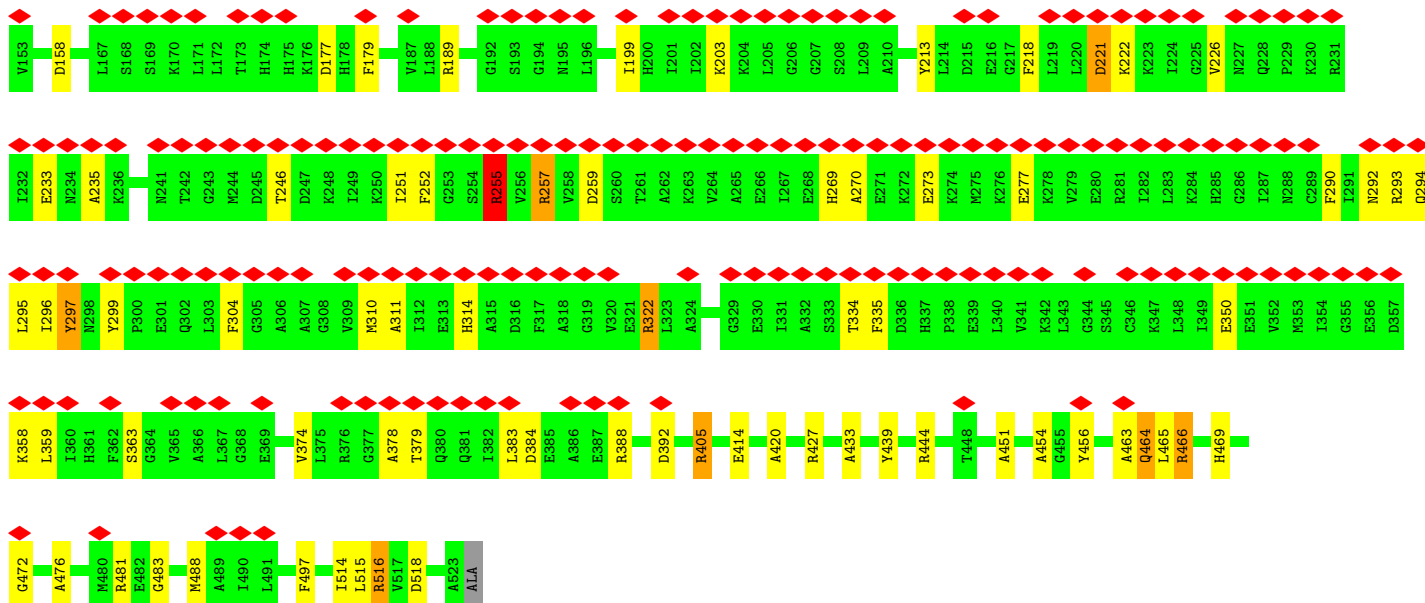


• Molecule 2: T-complex protein 1 subunit beta

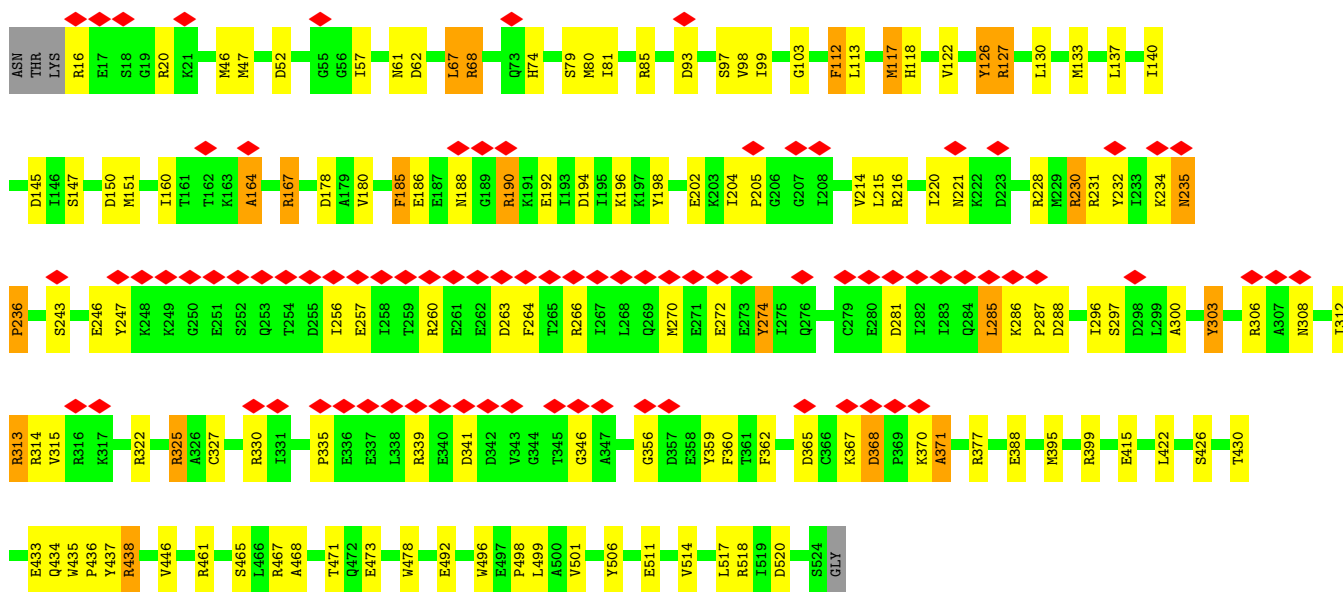


• Molecule 2: T-complex protein 1 subunit beta

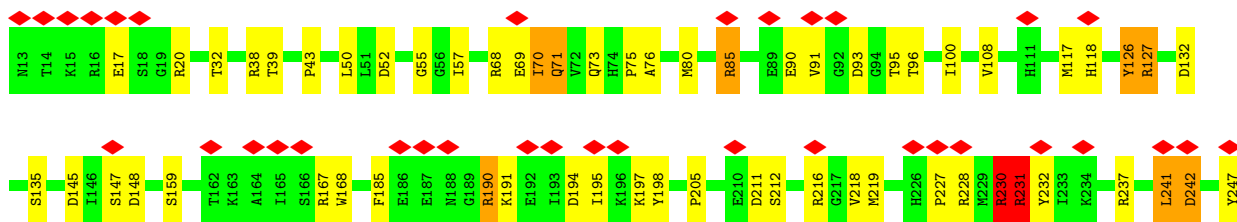
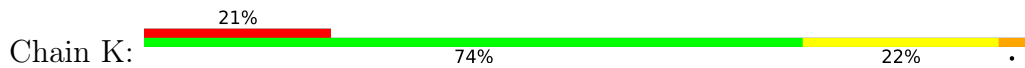


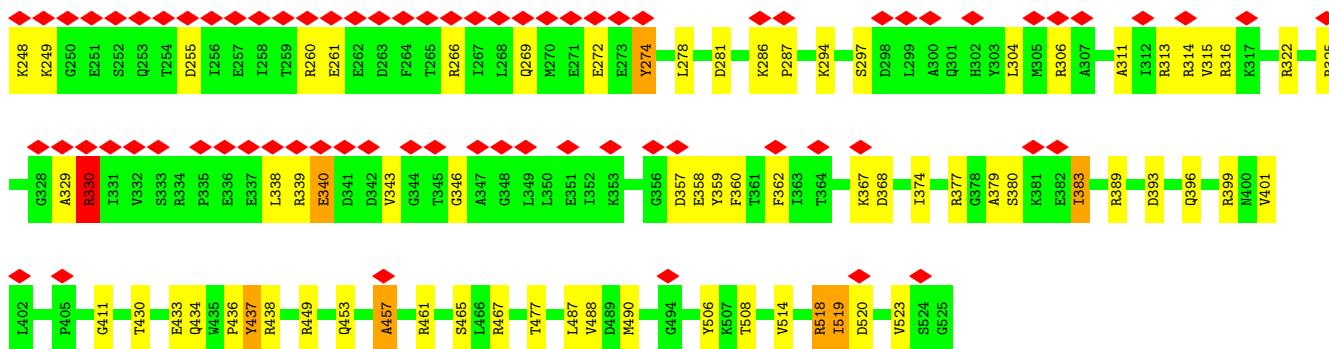


• Molecule 3: T-complex protein 1 subunit gamma

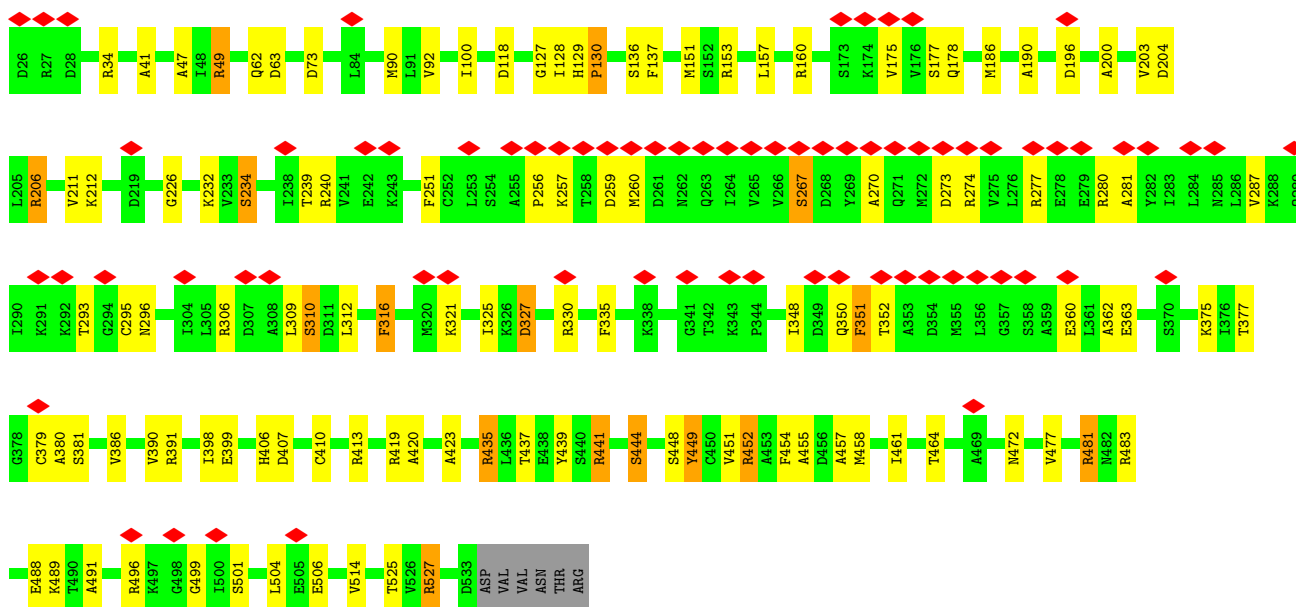
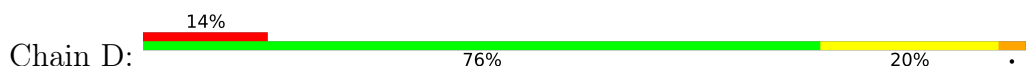


• Molecule 3: T-complex protein 1 subunit gamma

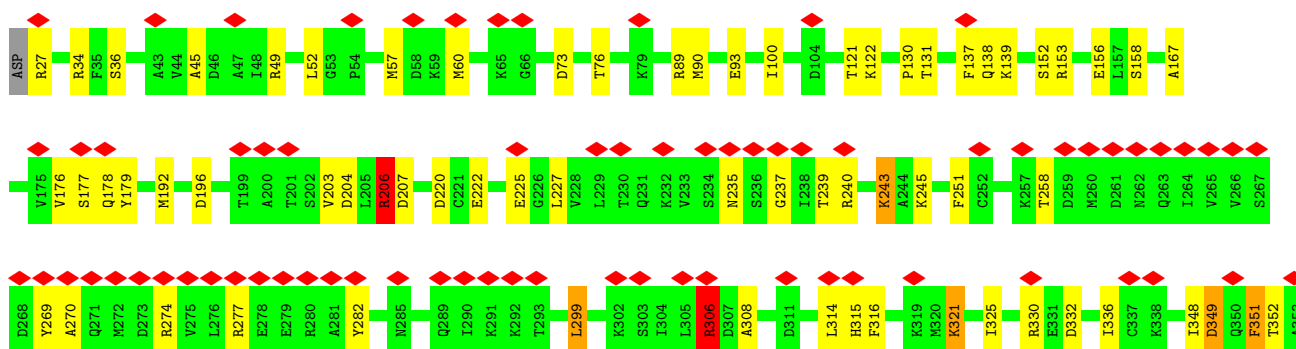
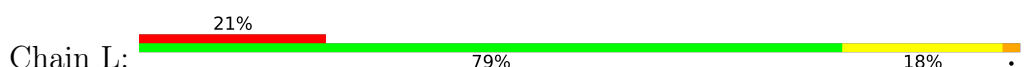


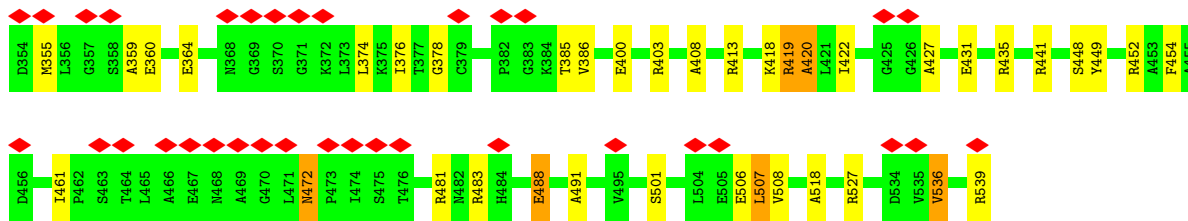


• Molecule 4: T-complex protein 1 subunit delta

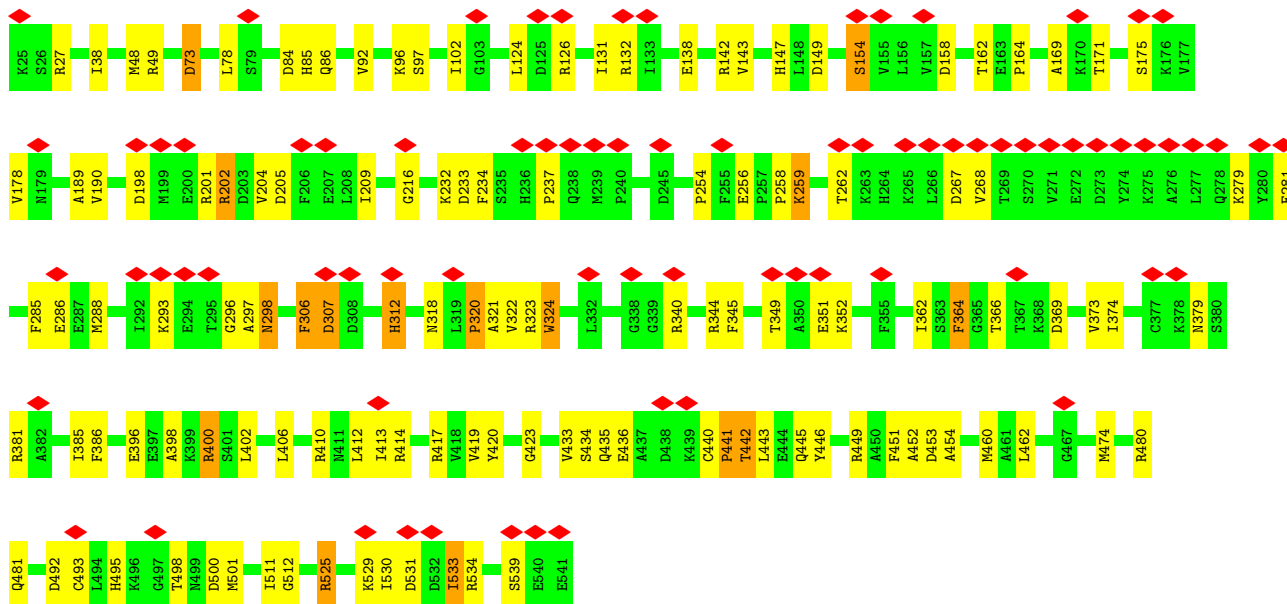
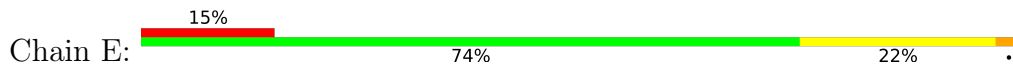


• Molecule 4: T-complex protein 1 subunit delta

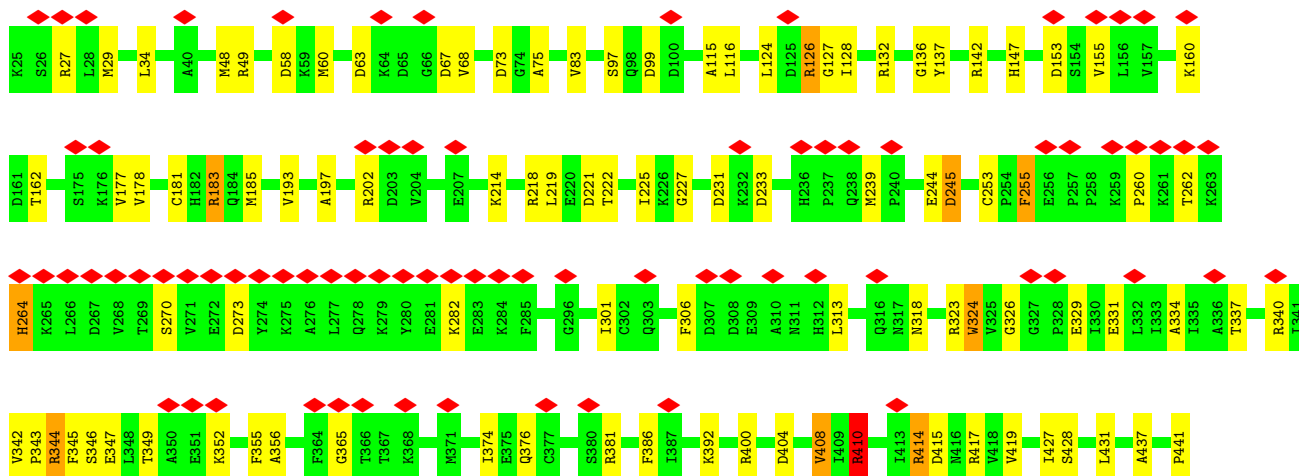
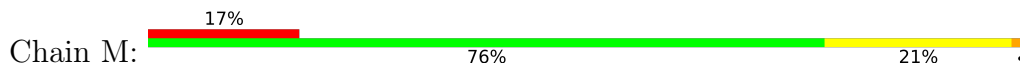


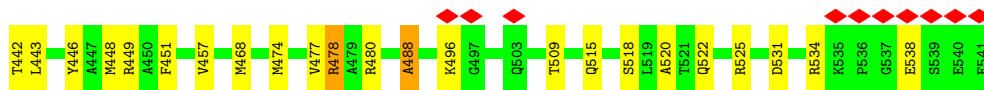


• Molecule 5: T-complex protein 1 subunit epsilon

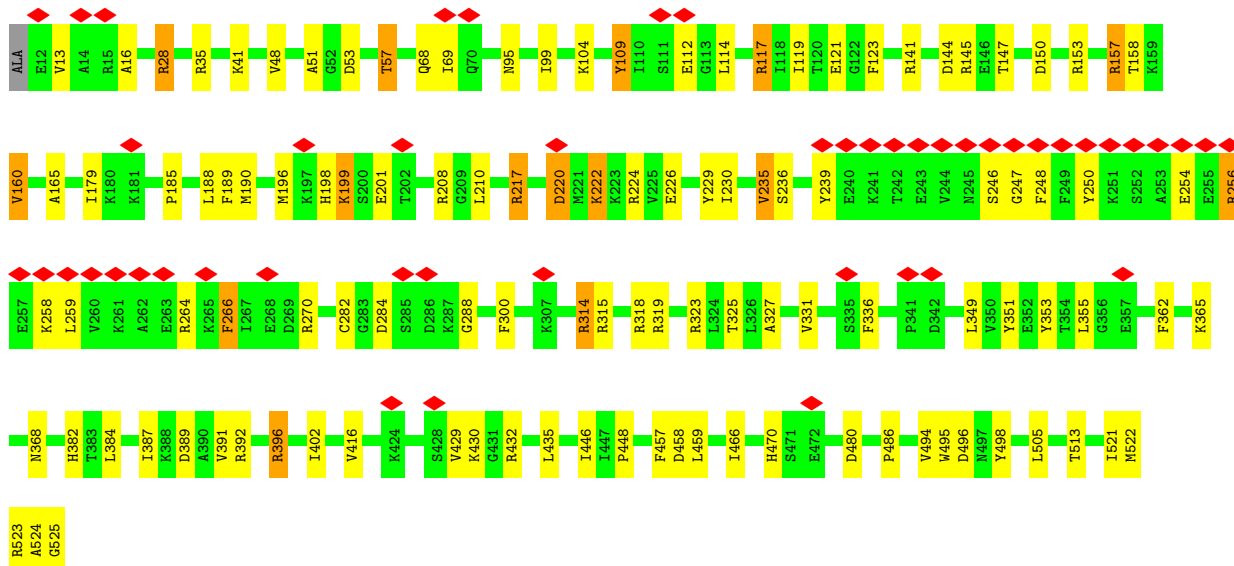
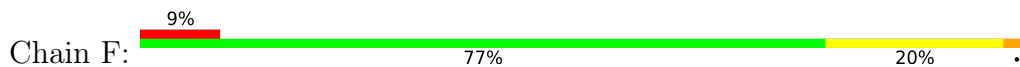


• Molecule 5: T-complex protein 1 subunit epsilon

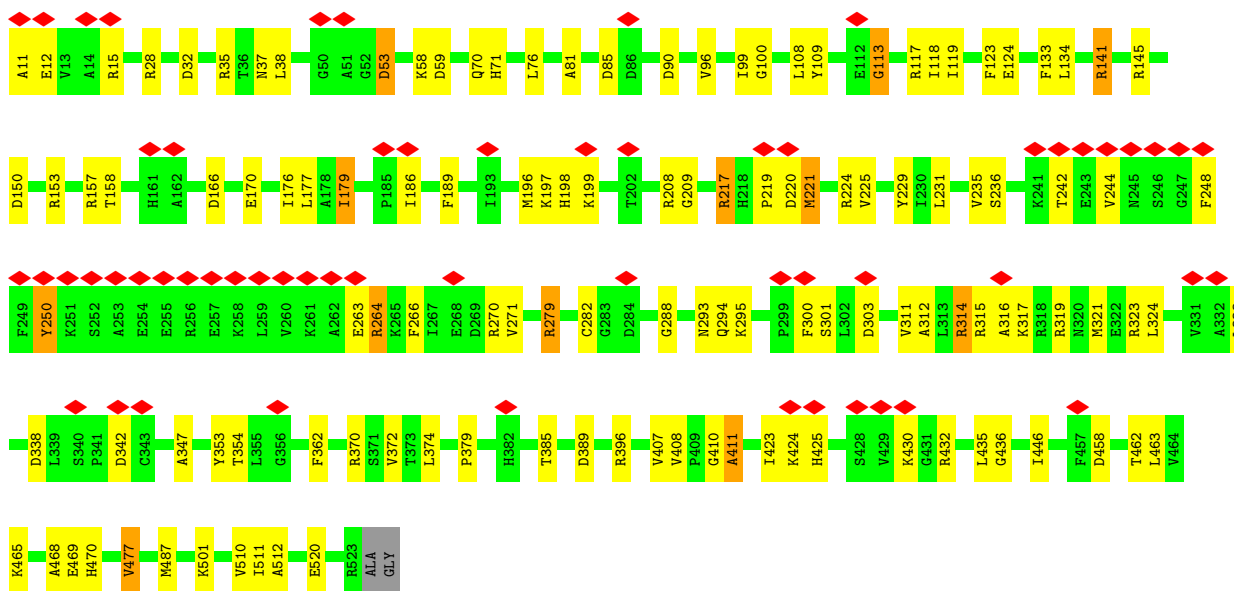
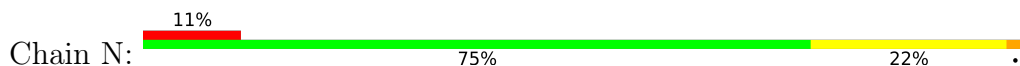




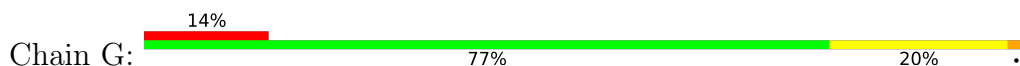
• Molecule 6: T-complex protein 1 subunit zeta

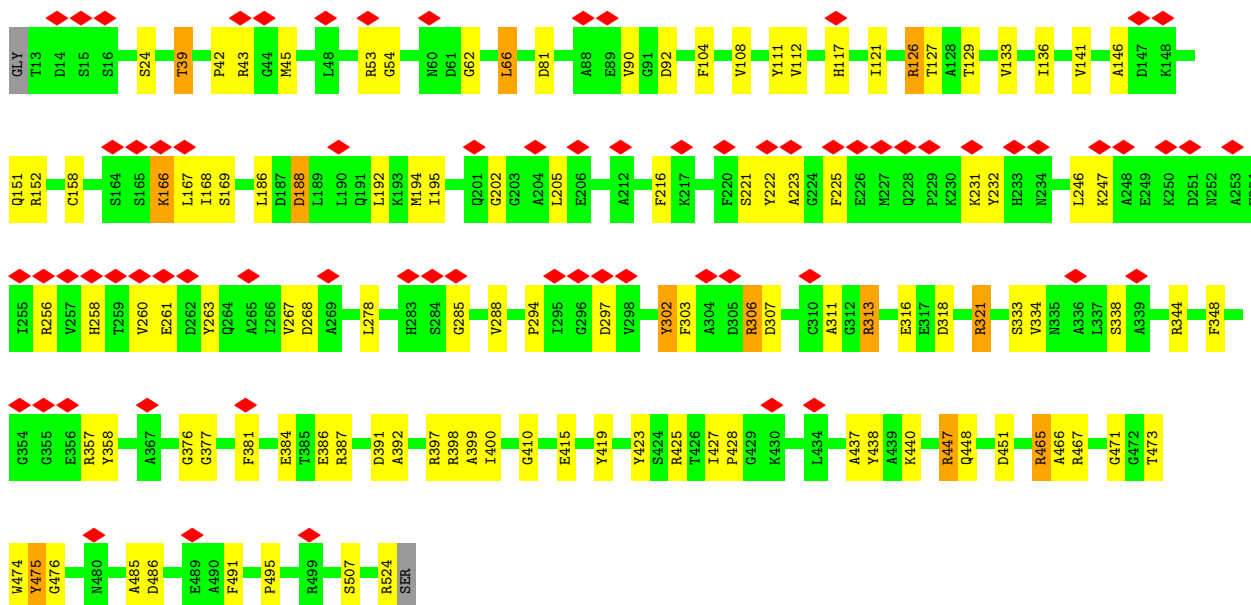


• Molecule 6: T-complex protein 1 subunit zeta

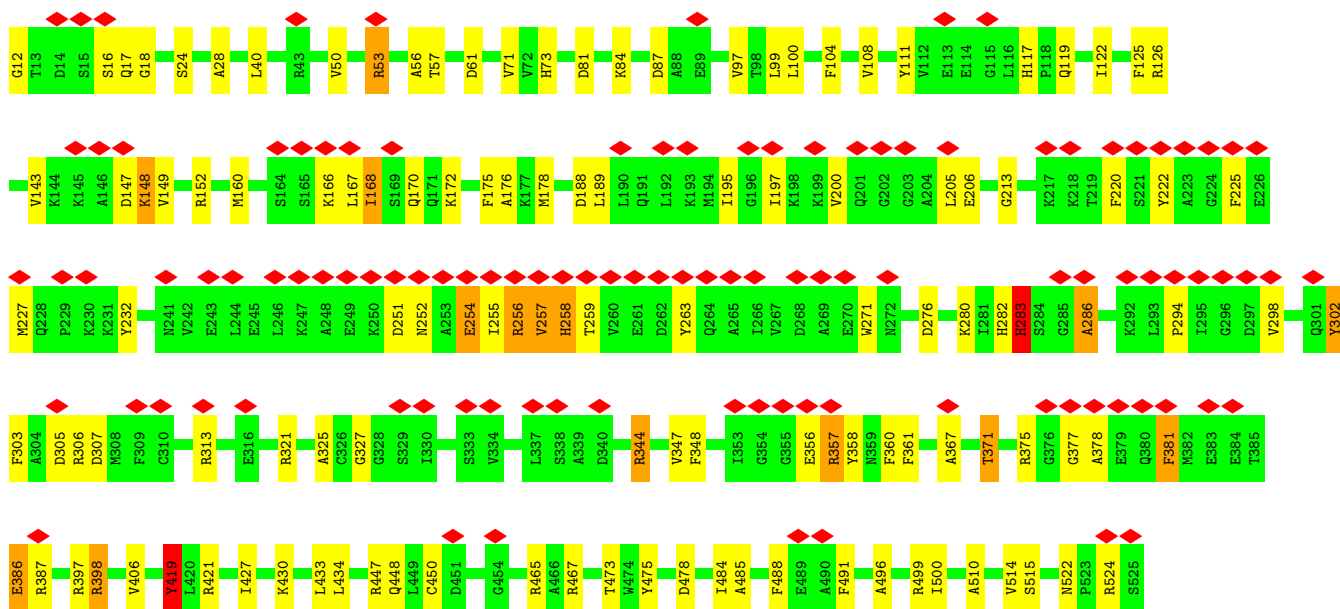
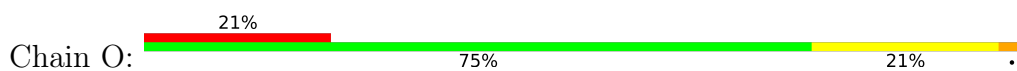


• Molecule 7: T-complex protein 1 subunit eta

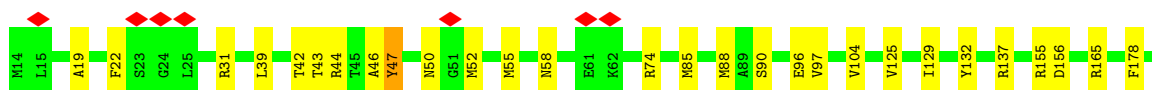
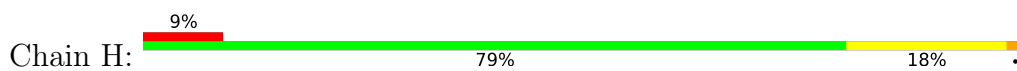


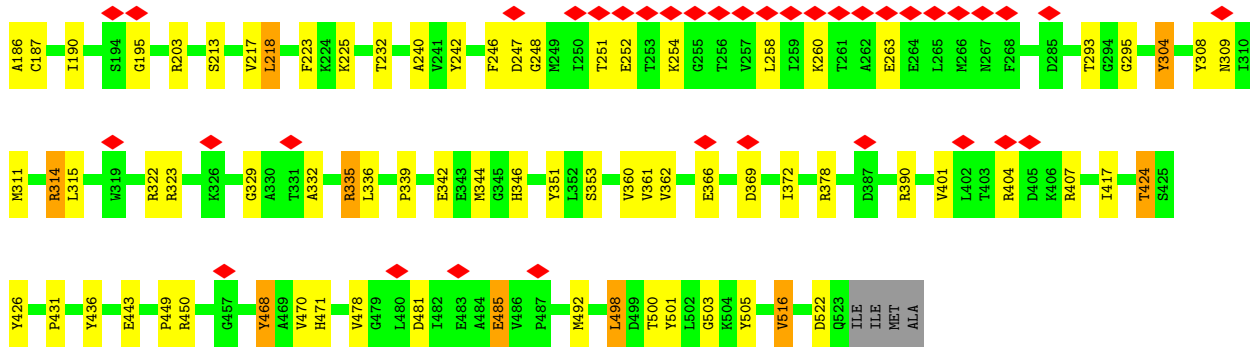


• Molecule 7: T-complex protein 1 subunit eta

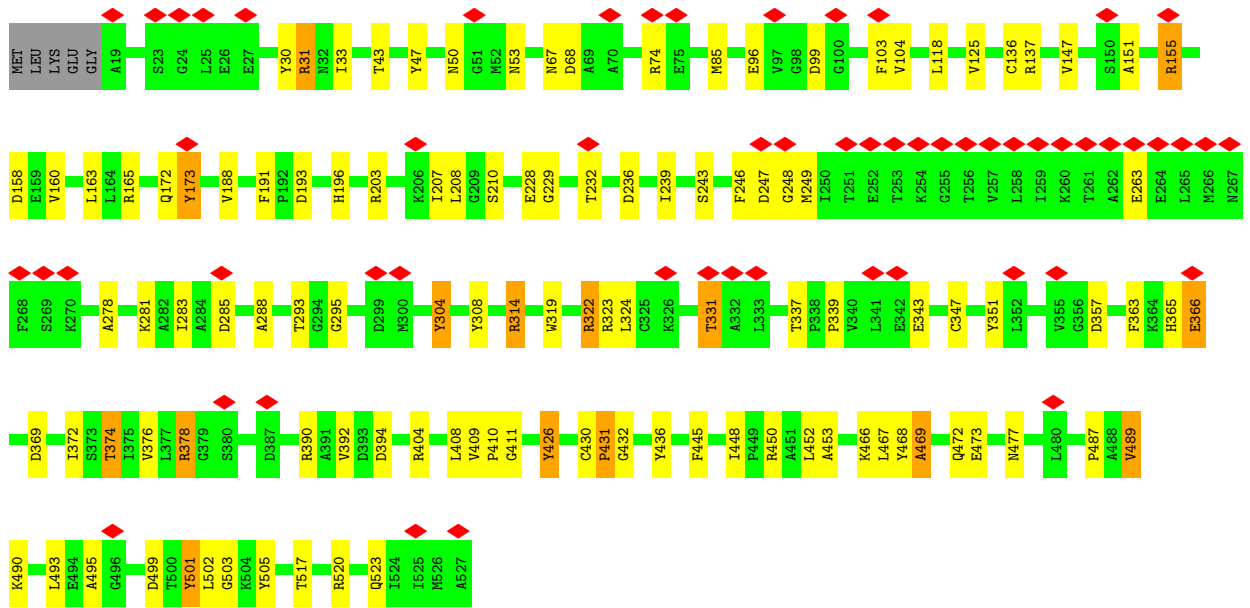
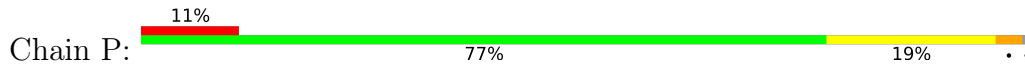


• Molecule 8: T-complex protein 1 subunit theta





• Molecule 8: T-complex protein 1 subunit theta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	38323	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.247	Depositor
Minimum map value	-0.081	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	408.0, 408.0, 408.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7, 1.7, 1.7	Depositor

5 Model quality i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.65	27/3992 (0.7%)	1.86	78/5389 (1.4%)
1	I	1.68	35/4095 (0.9%)	1.93	89/5526 (1.6%)
2	B	2.03	34/3869 (0.9%)	1.93	91/5214 (1.7%)
2	J	2.12	28/3863 (0.7%)	1.90	67/5207 (1.3%)
3	C	1.73	42/4000 (1.1%)	1.94	98/5397 (1.8%)
3	K	1.72	36/4029 (0.9%)	1.90	89/5434 (1.6%)
4	D	1.67	27/3863 (0.7%)	1.92	93/5214 (1.8%)
4	L	1.68	34/3904 (0.9%)	1.89	79/5269 (1.5%)
5	E	1.68	26/4020 (0.6%)	1.91	77/5414 (1.4%)
5	M	1.66	22/4020 (0.5%)	1.85	82/5414 (1.5%)
6	F	1.69	25/3991 (0.6%)	1.85	82/5379 (1.5%)
6	N	1.67	31/3986 (0.8%)	1.90	85/5374 (1.6%)
7	G	1.68	29/3991 (0.7%)	1.88	83/5386 (1.5%)
7	O	1.66	23/4002 (0.6%)	1.91	75/5399 (1.4%)
8	H	1.68	27/3945 (0.7%)	1.84	71/5331 (1.3%)
8	P	1.71	38/3937 (1.0%)	1.87	72/5321 (1.4%)
All	All	1.73	484/63507 (0.8%)	1.89	1311/85668 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	I	0	9
2	B	0	9
2	J	0	9
3	C	0	10
3	K	0	14
4	D	0	7
4	L	0	2
5	E	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	M	0	8
6	F	0	12
6	N	0	10
7	G	0	11
7	O	0	12
8	H	0	9
8	P	0	10
All	All	0	141

All (484) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	464	GLN	N-CA	79.19	3.04	1.46
2	B	429	PRO	N-CD	41.36	2.05	1.47
2	B	429	PRO	CA-CB	35.04	2.23	1.53
2	B	429	PRO	N-CA	30.94	1.99	1.47
2	B	429	PRO	CG-CD	20.76	2.19	1.50
2	B	429	PRO	CB-CG	15.36	2.26	1.50
4	L	400	GLU	CD-OE2	8.79	1.35	1.25
1	A	310	ARG	NE-CZ	8.64	1.44	1.33
2	B	254	SER	CA-CB	8.56	1.65	1.52
8	H	90	SER	CA-CB	8.27	1.65	1.52
6	N	141	ARG	NE-CZ	8.16	1.43	1.33
3	C	313	ARG	NE-CZ	8.12	1.43	1.33
7	G	232	TYR	CE1-CZ	8.05	1.49	1.38
3	K	17	GLU	CG-CD	7.85	1.63	1.51
7	G	256	ARG	NE-CZ	7.75	1.43	1.33
3	K	127	ARG	CZ-NH1	7.70	1.43	1.33
1	I	309	ARG	NE-CZ	7.69	1.43	1.33
1	A	355	ARG	CZ-NH1	7.66	1.43	1.33
3	K	316	ARG	NE-CZ	7.66	1.43	1.33
3	K	449	ARG	CZ-NH2	7.66	1.43	1.33
2	B	111	ARG	CZ-NH1	7.62	1.43	1.33
6	F	254	GLU	CB-CG	7.61	1.66	1.52
2	J	57	ARG	CD-NE	7.59	1.59	1.46
1	I	310	ARG	NE-CZ	7.54	1.42	1.33
2	B	255	ARG	CZ-NH2	7.50	1.42	1.33
8	H	351	TYR	CE1-CZ	7.49	1.48	1.38
6	N	153	ARG	NE-CZ	7.42	1.42	1.33
2	B	293	ARG	NE-CZ	7.37	1.42	1.33
6	N	170	GLU	CD-OE2	7.36	1.33	1.25
8	P	165	ARG	CZ-NH1	7.35	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	527	ARG	CZ-NH1	7.35	1.42	1.33
7	G	261	GLU	CB-CG	7.33	1.66	1.52
3	K	185	PHE	CG-CD2	7.30	1.49	1.38
6	N	208	ARG	NE-CZ	7.24	1.42	1.33
7	G	111	TYR	CE2-CZ	7.20	1.48	1.38
8	H	295	GLY	CA-C	-7.14	1.40	1.51
7	O	321	ARG	NE-CZ	7.14	1.42	1.33
5	E	525	ARG	CD-NE	7.12	1.58	1.46
3	C	511	GLU	CD-OE2	7.09	1.33	1.25
3	C	147	SER	CB-OG	-7.07	1.33	1.42
1	I	389	GLU	CG-CD	7.07	1.62	1.51
3	K	216	ARG	NE-CZ	7.07	1.42	1.33
5	E	49	ARG	NE-CZ	7.05	1.42	1.33
8	P	137	ARG	CD-NE	7.04	1.58	1.46
5	E	126	ARG	CZ-NH2	7.02	1.42	1.33
3	C	16	ARG	CD-NE	7.01	1.58	1.46
2	B	516	ARG	NE-CZ	6.97	1.42	1.33
3	K	465	SER	CA-CB	6.97	1.63	1.52
2	J	111	ARG	CD-NE	6.96	1.58	1.46
1	A	122	ARG	CZ-NH2	6.93	1.42	1.33
3	K	322	ARG	NE-CZ	6.93	1.42	1.33
7	G	474	TRP	NE1-CE2	6.84	1.46	1.37
8	P	188	VAL	CB-CG1	6.83	1.67	1.52
2	J	131	ARG	NE-CZ	6.83	1.42	1.33
6	F	495	TRP	CD2-CE2	6.83	1.49	1.41
1	I	378	ARG	NE-CZ	6.80	1.41	1.33
6	F	121	GLU	CG-CD	6.80	1.62	1.51
6	F	323	ARG	CZ-NH2	6.79	1.41	1.33
4	L	378	GLY	CA-C	-6.79	1.41	1.51
2	B	156	ARG	CD-NE	6.76	1.57	1.46
2	B	427	ARG	CZ-NH2	6.76	1.41	1.33
4	D	419	ARG	NE-CZ	6.76	1.41	1.33
1	I	143	LEU	C-N	6.74	1.45	1.33
2	J	427	ARG	NE-CZ	6.74	1.41	1.33
5	E	175	SER	CA-CB	6.73	1.63	1.52
2	B	444	ARG	NE-CZ	6.72	1.41	1.33
4	L	34	ARG	NE-CZ	6.71	1.41	1.33
8	H	390	ARG	CZ-NH1	6.71	1.41	1.33
7	G	313	ARG	NE-CZ	6.70	1.41	1.33
5	M	340	ARG	CZ-NH2	6.68	1.41	1.33
3	C	231	ARG	CZ-NH2	6.68	1.41	1.33
4	L	138	GLN	CG-CD	6.67	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	310	SER	CA-CB	6.67	1.62	1.52
3	C	438	ARG	NE-CZ	6.67	1.41	1.33
4	L	330	ARG	NE-CZ	6.66	1.41	1.33
6	F	288	GLY	CA-C	-6.66	1.41	1.51
3	C	314	ARG	CZ-NH2	6.66	1.41	1.33
1	I	274	ARG	NE-CZ	6.65	1.41	1.33
6	N	264	ARG	CZ-NH1	6.65	1.41	1.33
4	D	360	GLU	CG-CD	6.62	1.61	1.51
3	C	127	ARG	CZ-NH1	6.62	1.41	1.33
8	H	426	TYR	CD2-CE2	-6.61	1.29	1.39
2	B	330	GLU	CG-CD	6.58	1.61	1.51
4	L	452	ARG	CD-NE	6.55	1.57	1.46
3	C	205	PRO	N-CA	-6.54	1.36	1.47
1	A	27	SER	CB-OG	-6.54	1.33	1.42
1	I	513	SER	CA-CB	6.54	1.62	1.52
6	N	117	ARG	CD-NE	6.53	1.57	1.46
6	N	319	ARG	CD-NE	6.53	1.57	1.46
2	B	56	GLY	CA-C	-6.46	1.41	1.51
4	L	364	GLU	CG-CD	6.44	1.61	1.51
6	N	250	TYR	CG-CD2	6.43	1.47	1.39
5	M	525	ARG	CZ-NH1	6.43	1.41	1.33
5	M	132	ARG	CZ-NH2	6.40	1.41	1.33
7	G	524	ARG	CD-NE	6.40	1.57	1.46
6	F	247	GLY	N-CA	-6.40	1.36	1.46
3	C	20	ARG	NE-CZ	6.40	1.41	1.33
3	C	216	ARG	CD-NE	6.39	1.57	1.46
8	P	50	ASN	C-N	6.38	1.44	1.33
4	L	452	ARG	NE-CZ	6.38	1.41	1.33
1	A	496	ARG	CZ-NH1	6.37	1.41	1.33
4	D	491	ALA	C-N	6.36	1.44	1.33
2	J	293	ARG	CZ-NH1	6.34	1.41	1.33
2	B	512	GLU	CD-OE2	6.33	1.32	1.25
1	I	346	GLY	N-CA	-6.33	1.36	1.46
6	N	315	ARG	NE-CZ	6.33	1.41	1.33
3	C	461	ARG	CZ-NH1	6.32	1.41	1.33
1	A	121	TYR	CG-CD1	6.31	1.47	1.39
1	I	370	ARG	NE-CZ	6.30	1.41	1.33
6	N	217	ARG	CZ-NH2	6.30	1.41	1.33
3	C	330	ARG	CZ-NH2	6.30	1.41	1.33
1	A	264	ARG	CD-NE	6.29	1.57	1.46
1	A	378	ARG	CZ-NH2	6.29	1.41	1.33
6	N	295	LYS	C-N	6.27	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	316	PHE	CG-CD1	6.27	1.48	1.38
4	D	330	ARG	CZ-NH2	6.26	1.41	1.33
7	O	195	ILE	N-CA	-6.26	1.33	1.46
7	O	254	GLU	CD-OE2	6.25	1.32	1.25
2	J	311	ALA	CA-CB	6.25	1.65	1.52
3	C	306	ARG	CZ-NH1	6.24	1.41	1.33
2	J	322	ARG	CZ-NH2	6.24	1.41	1.33
8	H	478	VAL	CB-CG1	6.22	1.66	1.52
4	L	137	PHE	CE2-CZ	6.22	1.49	1.37
8	P	137	ARG	N-CA	-6.22	1.33	1.46
7	G	306	ARG	CZ-NH2	6.22	1.41	1.33
8	H	96	GLU	CD-OE1	6.22	1.32	1.25
7	G	126	ARG	CD-NE	6.21	1.57	1.46
6	F	396	ARG	CZ-NH1	6.19	1.41	1.33
8	H	263	GLU	CD-OE2	6.19	1.32	1.25
8	P	450	ARG	CD-NE	6.18	1.56	1.46
4	L	179	TYR	CE1-CZ	6.15	1.46	1.38
5	M	478	ARG	NE-CZ	6.15	1.41	1.33
4	L	419	ARG	CZ-NH1	6.14	1.41	1.33
4	D	234	SER	CA-CB	6.14	1.62	1.52
6	N	219	PRO	N-CA	-6.13	1.36	1.47
8	P	432	GLY	N-CA	-6.13	1.36	1.46
2	B	206	GLY	CA-C	-6.12	1.42	1.51
7	O	104	PHE	CG-CD2	6.11	1.48	1.38
6	N	133	PHE	CE1-CZ	6.10	1.49	1.37
7	G	425	ARG	CZ-NH1	6.09	1.41	1.33
4	D	452	ARG	CZ-NH2	6.09	1.41	1.33
2	B	466	ARG	CZ-NH2	6.08	1.41	1.33
1	A	407	SER	CA-CB	6.08	1.62	1.52
6	N	432	ARG	NE-CZ	6.08	1.41	1.33
3	C	314	ARG	NE-CZ	6.07	1.41	1.33
8	P	314	ARG	CZ-NH1	6.06	1.41	1.33
1	I	443	ARG	CZ-NH1	6.06	1.41	1.33
8	P	243	SER	CA-CB	6.06	1.62	1.52
8	H	390	ARG	CD-NE	6.04	1.56	1.46
1	A	145	ARG	NE-CZ	6.04	1.41	1.33
5	M	347	GLU	CG-CD	6.01	1.60	1.51
5	M	400	ARG	CD-NE	6.01	1.56	1.46
8	P	47	TYR	CE2-CZ	6.00	1.46	1.38
4	L	239	THR	N-CA	-5.99	1.34	1.46
2	B	427	ARG	NE-CZ	5.99	1.40	1.33
6	F	270	ARG	CD-NE	5.98	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	53	ARG	NE-CZ	5.97	1.40	1.33
5	M	525	ARG	CD-NE	5.96	1.56	1.46
2	B	189	ARG	CZ-NH1	5.96	1.40	1.33
7	G	465	ARG	CZ-NH2	5.95	1.40	1.33
3	C	388	GLU	CG-CD	5.95	1.60	1.51
1	I	267	GLU	CD-OE1	5.94	1.32	1.25
5	M	480	ARG	CZ-NH1	5.93	1.40	1.33
5	E	142	ARG	CD-NE	5.92	1.56	1.46
2	B	130	TRP	CD2-CE2	-5.92	1.34	1.41
4	L	89	ARG	CZ-NH1	5.91	1.40	1.33
3	K	68	ARG	NE-CZ	5.91	1.40	1.33
8	P	390	ARG	CZ-NH2	5.91	1.40	1.33
1	I	215	ALA	CA-CB	5.90	1.64	1.52
6	F	224	ARG	NE-CZ	5.90	1.40	1.33
3	C	313	ARG	CZ-NH2	5.90	1.40	1.33
2	J	483	GLY	CA-C	-5.90	1.42	1.51
5	E	423	GLY	N-CA	-5.90	1.37	1.46
3	C	415	GLU	CB-CG	5.89	1.63	1.52
4	D	496	ARG	NE-CZ	5.87	1.40	1.33
3	K	457	ALA	CA-CB	5.86	1.64	1.52
8	P	96	GLU	CD-OE2	5.86	1.32	1.25
8	H	485	GLU	CD-OE1	5.85	1.32	1.25
7	G	423	TYR	CE1-CZ	5.85	1.46	1.38
5	M	518	SER	CB-OG	-5.85	1.34	1.42
6	F	246	SER	CA-CB	5.85	1.61	1.52
7	O	357	ARG	CD-NE	5.84	1.56	1.46
3	K	438	ARG	CZ-NH2	5.84	1.40	1.33
4	D	435	ARG	NE-CZ	5.83	1.40	1.33
3	K	230	ARG	NE-CZ	5.83	1.40	1.33
5	M	181	CYS	CB-SG	5.83	1.92	1.82
3	K	438	ARG	NE-CZ	5.82	1.40	1.33
6	N	28	ARG	CZ-NH1	5.81	1.40	1.33
4	D	49	ARG	NE-CZ	5.81	1.40	1.33
3	C	346	GLY	N-CA	-5.80	1.37	1.46
1	I	273	GLU	CG-CD	5.80	1.60	1.51
4	L	93	GLU	CD-OE1	5.80	1.32	1.25
5	M	538	GLU	CD-OE1	5.80	1.32	1.25
6	F	157	ARG	CD-NE	5.79	1.56	1.46
6	N	124	GLU	CD-OE1	5.79	1.32	1.25
6	F	35	ARG	NE-CZ	5.79	1.40	1.33
8	H	178	PHE	CG-CD2	-5.79	1.30	1.38
1	I	426	TYR	CE1-CZ	5.79	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	190	TYR	CE2-CZ	5.78	1.46	1.38
4	L	240	ARG	CZ-NH2	5.78	1.40	1.33
6	N	288	GLY	N-CA	-5.78	1.37	1.46
8	H	322	ARG	CD-NE	5.78	1.56	1.46
5	M	326	GLY	C-N	5.78	1.43	1.33
8	P	137	ARG	CZ-NH1	5.78	1.40	1.33
2	B	20	ARG	NE-CZ	5.77	1.40	1.33
3	C	79	SER	CA-CB	5.77	1.61	1.52
5	E	312	HIS	CB-CG	5.77	1.60	1.50
7	G	126	ARG	NE-CZ	5.76	1.40	1.33
8	H	203	ARG	CD-NE	5.76	1.56	1.46
7	O	306	ARG	CZ-NH1	5.75	1.40	1.33
2	B	290	PHE	CG-CD2	5.75	1.47	1.38
6	N	279	ARG	NE-CZ	5.75	1.40	1.33
7	G	524	ARG	CZ-NH2	5.75	1.40	1.33
2	J	414	GLU	CD-OE2	5.75	1.31	1.25
4	D	483	ARG	CZ-NH1	5.74	1.40	1.33
1	A	13	THR	C-N	5.74	1.43	1.33
4	L	501	SER	CA-CB	5.74	1.61	1.52
6	F	123	PHE	CG-CD2	5.74	1.47	1.38
1	A	441	PHE	CB-CG	5.73	1.61	1.51
5	E	493	CYS	CB-SG	-5.73	1.72	1.81
6	N	225	VAL	CB-CG2	5.73	1.64	1.52
1	A	378	ARG	CD-NE	5.72	1.56	1.46
5	M	126	ARG	CZ-NH2	5.72	1.40	1.33
4	D	360	GLU	CD-OE2	5.72	1.31	1.25
7	G	437	ALA	N-CA	-5.72	1.34	1.46
4	D	34	ARG	CZ-NH2	5.72	1.40	1.33
7	G	415	GLU	CB-CG	5.71	1.63	1.52
3	K	247	TYR	CZ-OH	5.71	1.47	1.37
3	K	20	ARG	CZ-NH2	5.70	1.40	1.33
1	A	274	ARG	CZ-NH2	5.68	1.40	1.33
8	H	314	ARG	CD-NE	5.68	1.56	1.46
7	O	356	GLU	CG-CD	5.68	1.60	1.51
2	J	476	ALA	CA-CB	5.67	1.64	1.52
3	K	228	ARG	CD-NE	5.67	1.56	1.46
3	C	496	TRP	CD1-NE1	5.66	1.47	1.38
3	C	518	ARG	NE-CZ	5.66	1.40	1.33
3	C	204	ILE	N-CA	-5.66	1.35	1.46
7	G	465	ARG	CZ-NH1	5.66	1.40	1.33
1	I	240	SER	CA-CB	5.65	1.61	1.52
2	B	352	VAL	CB-CG2	5.64	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	293	ARG	CZ-NH2	5.64	1.40	1.33
3	K	360	PHE	CB-CG	-5.64	1.41	1.51
4	L	137	PHE	CG-CD1	5.64	1.47	1.38
8	H	137	ARG	NE-CZ	5.63	1.40	1.33
3	C	399	ARG	CD-NE	5.62	1.56	1.46
4	D	128	ILE	N-CA	-5.62	1.35	1.46
6	N	436	GLY	N-CA	-5.62	1.37	1.46
1	I	296	CYS	CB-SG	5.62	1.91	1.82
6	N	113	GLY	CA-C	-5.62	1.42	1.51
4	L	269	TYR	CZ-OH	5.62	1.47	1.37
8	P	295	GLY	N-CA	-5.62	1.37	1.46
1	I	122	ARG	CD-NE	5.61	1.55	1.46
2	B	335	PHE	CG-CD1	5.61	1.47	1.38
3	K	159	SER	CA-CB	5.60	1.61	1.52
5	M	340	ARG	NE-CZ	5.60	1.40	1.33
2	B	318	ALA	C-N	5.60	1.43	1.33
5	M	344	ARG	NE-CZ	5.60	1.40	1.33
3	C	377	ARG	NE-CZ	5.60	1.40	1.33
4	D	127	GLY	CA-C	-5.59	1.42	1.51
4	D	280	ARG	CZ-NH2	5.59	1.40	1.33
2	J	96	GLY	CA-C	-5.59	1.43	1.51
3	C	228	ARG	CZ-NH2	5.58	1.40	1.33
5	E	345	PHE	CB-CG	5.58	1.60	1.51
7	O	302	TYR	CG-CD1	5.58	1.46	1.39
1	I	379	GLY	CA-C	-5.57	1.43	1.51
2	B	111	ARG	CZ-NH2	5.57	1.40	1.33
8	H	501	TYR	CE1-CZ	5.57	1.45	1.38
4	L	152	SER	CA-CB	5.56	1.61	1.52
1	A	130	ARG	CZ-NH2	5.56	1.40	1.33
8	H	329	GLY	CA-C	-5.55	1.43	1.51
7	G	410	GLY	CA-C	-5.55	1.43	1.51
1	A	315	ASP	CA-CB	5.54	1.66	1.53
1	I	526	ARG	NE-CZ	5.54	1.40	1.33
2	J	405	ARG	CZ-NH1	5.54	1.40	1.33
1	A	307	ALA	CA-C	5.54	1.67	1.52
2	J	213	TYR	CZ-OH	5.54	1.47	1.37
4	L	27	ARG	NE-CZ	5.53	1.40	1.33
2	B	313	GLU	N-CA	-5.53	1.35	1.46
5	M	183	ARG	NE-CZ	5.53	1.40	1.33
8	P	374	THR	N-CA	-5.53	1.35	1.46
1	A	422	TYR	CE2-CZ	5.52	1.45	1.38
7	O	213	GLY	CA-C	-5.52	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	475	TYR	CZ-OH	5.52	1.47	1.37
8	P	445	PHE	CB-CG	-5.51	1.42	1.51
2	B	257	ARG	NE-CZ	5.51	1.40	1.33
7	G	188	ASP	CA-CB	5.51	1.66	1.53
5	E	268	VAL	CB-CG1	5.51	1.64	1.52
2	J	277	GLU	CD-OE1	5.50	1.31	1.25
3	C	62	ASP	C-N	5.50	1.43	1.33
4	D	306	ARG	CD-NE	5.50	1.55	1.46
6	F	402	ILE	C-N	5.50	1.46	1.34
2	J	335	PHE	CG-CD2	5.49	1.47	1.38
8	P	319	TRP	CA-CB	5.49	1.66	1.53
2	B	385	GLU	CG-CD	5.49	1.60	1.51
6	N	410	GLY	CA-C	-5.48	1.43	1.51
6	F	201	GLU	CD-OE2	5.48	1.31	1.25
8	H	47	TYR	CG-CD2	5.48	1.46	1.39
5	M	270	SER	CA-CB	5.47	1.61	1.52
1	I	155	SER	CA-CB	5.47	1.61	1.52
6	N	236	SER	CA-CB	5.47	1.61	1.52
5	E	449	ARG	CA-CB	5.46	1.66	1.53
8	H	426	TYR	CD1-CE1	5.46	1.47	1.39
3	K	325	ARG	CZ-NH1	5.46	1.40	1.33
8	P	426	TYR	CZ-OH	5.46	1.47	1.37
4	D	399	GLU	CG-CD	5.46	1.60	1.51
6	F	121	GLU	C-N	5.46	1.42	1.33
4	L	277	ARG	CZ-NH2	5.44	1.40	1.33
5	E	132	ARG	NE-CZ	5.43	1.40	1.33
1	A	443	ARG	CZ-NH1	5.43	1.40	1.33
8	P	466	LYS	CA-CB	5.43	1.65	1.53
1	I	468	ARG	NE-CZ	5.42	1.40	1.33
3	K	272	GLU	CG-CD	5.42	1.60	1.51
4	L	49	ARG	CZ-NH1	5.42	1.40	1.33
8	P	33	ILE	C-N	5.42	1.46	1.34
5	M	326	GLY	CA-C	5.41	1.60	1.51
1	I	378	ARG	C-N	5.41	1.42	1.33
1	I	181	TYR	CE2-CZ	5.40	1.45	1.38
3	C	216	ARG	NE-CZ	5.40	1.40	1.33
2	J	405	ARG	CZ-NH2	5.40	1.40	1.33
8	H	155	ARG	NE-CZ	5.40	1.40	1.33
4	L	122	LYS	CA-CB	5.39	1.65	1.53
5	E	445	GLN	CG-CD	5.39	1.63	1.51
3	K	147	SER	CA-CB	5.38	1.61	1.52
7	O	500	ILE	N-CA	-5.38	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	480	ARG	CZ-NH2	5.38	1.40	1.33
2	B	414	GLU	CD-OE1	5.38	1.31	1.25
7	G	334	VAL	CB-CG1	5.38	1.64	1.52
7	G	54	GLY	N-CA	-5.38	1.38	1.46
2	J	111	ARG	CZ-NH1	5.37	1.40	1.33
7	O	12	GLY	N-CA	5.37	1.54	1.46
1	I	203	ARG	NE-CZ	5.36	1.40	1.33
5	E	400	ARG	CZ-NH1	5.36	1.40	1.33
5	E	286	GLU	CB-CG	5.35	1.62	1.52
6	F	448	PRO	N-CD	-5.35	1.40	1.47
8	P	304	TYR	CG-CD1	5.35	1.46	1.39
3	K	212	SER	CA-CB	5.35	1.60	1.52
6	F	318	ARG	CZ-NH1	5.35	1.40	1.33
5	E	410	ARG	CZ-NH2	5.34	1.40	1.33
7	G	387	ARG	CZ-NH1	5.33	1.40	1.33
2	J	60	SER	CA-CB	5.33	1.60	1.52
3	K	237	ARG	CZ-NH1	5.33	1.40	1.33
3	K	218	VAL	CB-CG2	5.32	1.64	1.52
7	O	126	ARG	CD-NE	5.32	1.55	1.46
5	E	412	LEU	CB-CG	5.31	1.68	1.52
1	I	480	ARG	CZ-NH1	5.31	1.40	1.33
7	G	491	PHE	CB-CG	-5.31	1.42	1.51
4	D	49	ARG	CD-NE	5.31	1.55	1.46
1	I	228	ARG	CZ-NH1	5.31	1.40	1.33
8	P	502	LEU	N-CA	-5.30	1.35	1.46
1	I	415	VAL	CB-CG1	5.30	1.64	1.52
8	P	47	TYR	CG-CD2	5.30	1.46	1.39
3	C	266	ARG	CZ-NH2	5.30	1.40	1.33
8	P	503	GLY	CA-C	-5.29	1.43	1.51
7	G	447	ARG	CZ-NH2	5.29	1.40	1.33
4	L	153	ARG	CZ-NH2	5.29	1.40	1.33
4	L	448	SER	CA-CB	5.28	1.60	1.52
8	H	322	ARG	NE-CZ	5.28	1.40	1.33
8	P	155	ARG	NE-CZ	5.28	1.40	1.33
1	A	504	PHE	CG-CD1	5.27	1.46	1.38
4	D	351	PHE	CB-CG	5.27	1.60	1.51
1	I	370	ARG	CZ-NH2	5.27	1.39	1.33
3	K	55	GLY	CA-C	-5.27	1.43	1.51
5	E	321	ALA	CA-CB	5.26	1.63	1.52
8	H	242	TYR	CB-CG	5.26	1.59	1.51
1	A	203	ARG	CZ-NH2	5.26	1.39	1.33
6	F	319	ARG	CZ-NH1	5.26	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	464	GLN	CA-CB	5.26	1.65	1.53
4	L	240	ARG	CZ-NH1	5.26	1.39	1.33
1	I	378	ARG	CA-CB	5.26	1.65	1.53
1	A	434	GLU	CG-CD	5.25	1.59	1.51
4	D	280	ARG	CZ-NH1	5.25	1.39	1.33
5	M	127	GLY	CA-C	-5.25	1.43	1.51
8	H	366	GLU	CG-CD	5.25	1.59	1.51
5	E	481	GLN	C-N	5.25	1.46	1.34
8	P	501	TYR	CD1-CE1	5.24	1.47	1.39
4	L	306	ARG	NE-CZ	5.24	1.39	1.33
1	I	314	ARG	CZ-NH1	5.24	1.39	1.33
3	C	274	TYR	CE1-CZ	5.23	1.45	1.38
6	N	11	ALA	C-N	5.23	1.46	1.34
1	A	411	GLY	C-N	5.22	1.42	1.33
6	F	315	ARG	CD-NE	5.22	1.55	1.46
6	F	315	ARG	NE-CZ	5.22	1.39	1.33
5	M	414	ARG	CD-NE	5.22	1.55	1.46
2	B	189	ARG	CZ-NH2	5.21	1.39	1.33
7	G	491	PHE	CG-CD2	5.21	1.46	1.38
6	F	266	PHE	CG-CD2	5.21	1.46	1.38
3	K	297	SER	CB-OG	5.20	1.49	1.42
2	J	304	PHE	CE2-CZ	5.20	1.47	1.37
8	P	322	ARG	CZ-NH1	5.19	1.39	1.33
7	O	206	GLU	CD-OE1	5.19	1.31	1.25
4	L	527	ARG	CD-NE	5.18	1.55	1.46
1	A	274	ARG	CZ-NH1	5.18	1.39	1.33
3	C	103	GLY	CA-C	-5.18	1.43	1.51
7	O	344	ARG	CZ-NH2	5.18	1.39	1.33
3	K	339	ARG	NE-CZ	5.17	1.39	1.33
8	P	339	PRO	CA-CB	5.17	1.63	1.53
2	J	62	MET	CA-CB	5.16	1.65	1.53
5	E	279	LYS	C-N	5.16	1.46	1.34
8	P	136	CYS	CB-SG	5.16	1.91	1.82
3	C	127	ARG	CD-NE	5.16	1.55	1.46
6	N	396	ARG	NE-CZ	5.16	1.39	1.33
3	C	322	ARG	CD-NE	5.15	1.55	1.46
1	I	412	GLY	CA-C	-5.15	1.43	1.51
2	J	138	ARG	CZ-NH1	5.15	1.39	1.33
5	M	67	ASP	CA-C	-5.15	1.39	1.52
3	K	274	TYR	CB-CG	-5.14	1.44	1.51
8	P	293	THR	C-N	5.14	1.42	1.33
5	E	154	SER	CA-CB	5.14	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	299	TYR	CD1-CE1	5.14	1.47	1.39
3	C	186	GLU	CG-CD	5.14	1.59	1.51
4	L	518	ALA	N-CA	-5.14	1.36	1.46
4	D	296	ASN	CB-CG	5.14	1.62	1.51
2	J	456	TYR	CG-CD2	5.13	1.45	1.39
6	F	117	ARG	NE-CZ	5.13	1.39	1.33
8	P	323	ARG	CD-NE	5.13	1.55	1.46
3	K	38	ARG	NE-CZ	5.13	1.39	1.33
6	N	263	GLU	CD-OE1	5.13	1.31	1.25
4	L	274	ARG	CZ-NH1	5.13	1.39	1.33
1	I	120	GLY	CA-C	-5.12	1.43	1.51
8	H	468	TYR	CZ-OH	5.12	1.46	1.37
5	E	201	ARG	CZ-NH2	5.12	1.39	1.33
4	D	363	GLU	CA-C	-5.12	1.39	1.52
7	G	344	ARG	CZ-NH2	5.12	1.39	1.33
6	N	408	VAL	CA-CB	-5.12	1.44	1.54
3	C	465	SER	N-CA	-5.12	1.36	1.46
7	G	495	PRO	N-CD	-5.11	1.40	1.47
5	M	443	LEU	N-CA	-5.11	1.36	1.46
8	P	487	PRO	N-CD	-5.11	1.40	1.47
8	H	505	TYR	CZ-OH	5.11	1.46	1.37
6	N	209	GLY	CA-C	-5.11	1.43	1.51
8	P	191	PHE	C-N	5.11	1.44	1.34
1	A	130	ARG	NE-CZ	5.10	1.39	1.33
2	B	271	GLU	CB-CG	5.10	1.61	1.52
8	H	378	ARG	CZ-NH1	5.10	1.39	1.33
3	C	202	GLU	CD-OE1	5.10	1.31	1.25
2	J	514	ILE	CA-CB	-5.10	1.43	1.54
3	K	126	TYR	CZ-OH	5.10	1.46	1.37
3	K	266	ARG	CZ-NH1	5.09	1.39	1.33
4	D	295	CYS	N-CA	-5.09	1.36	1.46
6	F	524	ALA	C-N	5.09	1.42	1.33
7	G	384	GLU	CB-CG	5.09	1.61	1.52
7	O	126	ARG	CZ-NH2	5.09	1.39	1.33
4	L	483	ARG	CZ-NH1	5.08	1.39	1.33
3	C	471	THR	N-CA	-5.08	1.36	1.46
4	D	499	GLY	N-CA	-5.07	1.38	1.46
3	K	168	TRP	CD2-CE2	5.07	1.47	1.41
7	O	386	GLU	CG-CD	5.07	1.59	1.51
7	O	325	ALA	N-CA	-5.07	1.36	1.46
3	C	322	ARG	CZ-NH1	5.07	1.39	1.33
8	P	430	CYS	C-N	5.07	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	50	VAL	CB-CG1	-5.07	1.42	1.52
8	P	450	ARG	CZ-NH2	5.07	1.39	1.33
5	E	435	GLN	CG-CD	5.07	1.62	1.51
3	C	520	ASP	CA-CB	5.06	1.65	1.53
7	O	524	ARG	CD-NE	5.06	1.55	1.46
7	G	425	ARG	CZ-NH2	5.06	1.39	1.33
1	I	142	GLU	CD-OE2	-5.06	1.20	1.25
2	J	121	ILE	N-CA	-5.06	1.36	1.46
6	N	15	ARG	NE-CZ	5.06	1.39	1.33
3	C	97	SER	CB-OG	-5.06	1.35	1.42
4	L	435	ARG	CZ-NH1	5.06	1.39	1.33
7	O	256	ARG	NE-CZ	5.06	1.39	1.33
3	K	260	ARG	NE-CZ	5.05	1.39	1.33
8	P	31	ARG	NE-CZ	5.05	1.39	1.33
3	C	498	PRO	N-CD	-5.05	1.40	1.47
3	K	237	ARG	CD-NE	5.05	1.55	1.46
1	A	40	GLY	CA-C	-5.04	1.43	1.51
6	N	436	GLY	CA-C	-5.04	1.43	1.51
5	E	234	PHE	CB-CG	5.03	1.59	1.51
6	F	201	GLU	CG-CD	-5.03	1.44	1.51
4	L	176	VAL	CB-CG1	5.03	1.63	1.52
8	P	263	GLU	CD-OE1	-5.03	1.20	1.25
8	P	155	ARG	CZ-NH1	5.02	1.39	1.33
6	N	100	GLY	N-CA	-5.02	1.38	1.46
8	H	132	TYR	CB-CG	-5.02	1.44	1.51
2	B	441	LYS	CA-CB	-5.02	1.43	1.53
1	A	228	ARG	CZ-NH1	5.01	1.39	1.33
3	K	389	ARG	NE-CZ	5.01	1.39	1.33
5	E	147	HIS	CB-CG	5.01	1.59	1.50
7	O	361	PHE	CA-C	-5.01	1.40	1.52
3	K	358	GLU	CB-CG	5.01	1.61	1.52
4	D	496	ARG	CD-NE	5.00	1.54	1.46
3	C	167	ARG	CZ-NH1	5.00	1.39	1.33
2	J	257	ARG	CZ-NH1	5.00	1.39	1.33

All (1311) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	179	PHE	CB-CG-CD1	-16.76	109.07	120.80
5	E	126	ARG	NE-CZ-NH2	-16.45	112.08	120.30
8	H	304	TYR	CB-CG-CD2	-15.96	111.42	121.00
2	J	179	PHE	CB-CG-CD2	15.96	131.97	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	357	ARG	NE-CZ-NH2	-15.58	112.51	120.30
4	D	206	ARG	NE-CZ-NH1	15.18	127.89	120.30
3	K	438	ARG	NE-CZ-NH2	-15.15	112.73	120.30
1	I	378	ARG	NE-CZ-NH2	-15.04	112.78	120.30
2	J	29	PHE	CB-CG-CD2	-15.00	110.30	120.80
7	O	398	ARG	NE-CZ-NH1	14.88	127.74	120.30
2	B	155	PHE	CB-CG-CD2	-14.04	110.97	120.80
1	I	390	ARG	NE-CZ-NH1	-14.04	113.28	120.30
1	I	11	ARG	NE-CZ-NH2	-13.78	113.41	120.30
2	B	218	PHE	CB-CG-CD1	-13.73	111.19	120.80
2	B	281	ARG	NE-CZ-NH1	13.73	127.17	120.30
6	F	314	ARG	NE-CZ-NH2	-13.66	113.47	120.30
3	C	325	ARG	NE-CZ-NH2	-13.60	113.50	120.30
4	D	527	ARG	NE-CZ-NH2	-13.45	113.58	120.30
7	O	313	ARG	NE-CZ-NH2	-13.05	113.78	120.30
4	D	277	ARG	NE-CZ-NH1	12.93	126.76	120.30
8	P	468	TYR	CB-CG-CD1	-12.91	113.26	121.00
2	B	218	PHE	CB-CG-CD2	12.88	129.82	120.80
6	N	109	TYR	CB-CG-CD2	-12.87	113.28	121.00
2	B	189	ARG	NE-CZ-NH2	-12.79	113.91	120.30
4	D	527	ARG	NE-CZ-NH1	12.67	126.63	120.30
1	I	433	ARG	NE-CZ-NH2	-12.61	114.00	120.30
5	E	27	ARG	NE-CZ-NH2	-12.53	114.03	120.30
3	K	20	ARG	NE-CZ-NH2	-12.53	114.04	120.30
5	E	49	ARG	NE-CZ-NH2	12.48	126.54	120.30
8	H	304	TYR	CB-CG-CD1	12.42	128.45	121.00
4	L	316	PHE	CB-CG-CD1	-12.35	112.16	120.80
2	B	516	ARG	NE-CZ-NH2	-12.30	114.15	120.30
1	A	390	ARG	NE-CZ-NH2	-12.20	114.20	120.30
3	K	461	ARG	NE-CZ-NH1	12.15	126.38	120.30
4	D	277	ARG	NE-CZ-NH2	-12.14	114.23	120.30
8	P	137	ARG	NE-CZ-NH2	12.11	126.36	120.30
3	C	399	ARG	NE-CZ-NH1	12.03	126.31	120.30
2	J	463	ALA	C-N-CA	11.84	151.29	121.70
7	G	225	PHE	CB-CG-CD2	11.82	129.07	120.80
4	D	481	ARG	NE-CZ-NH1	-11.81	114.39	120.30
1	A	228	ARG	NE-CZ-NH1	11.78	126.19	120.30
4	D	280	ARG	NE-CZ-NH1	11.69	126.15	120.30
8	P	468	TYR	CB-CG-CD2	11.67	128.00	121.00
6	F	35	ARG	NE-CZ-NH2	-11.61	114.50	120.30
2	J	57	ARG	NE-CZ-NH2	-11.60	114.50	120.30
3	C	362	PHE	CB-CG-CD2	11.48	128.84	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	111	TYR	CB-CG-CD2	-11.46	114.13	121.00
4	L	483	ARG	NE-CZ-NH2	11.42	126.01	120.30
6	N	279	ARG	NE-CZ-NH1	11.37	125.98	120.30
1	I	121	TYR	CB-CG-CD2	11.35	127.81	121.00
6	N	15	ARG	NE-CZ-NH1	11.30	125.95	120.30
2	J	464	GLN	N-CA-CB	11.26	130.86	110.60
1	I	526	ARG	NE-CZ-NH2	-11.19	114.70	120.30
2	J	464	GLN	CB-CA-C	-11.17	88.06	110.40
4	D	330	ARG	NE-CZ-NH2	-11.09	114.75	120.30
5	E	306	PHE	CB-CG-CD1	11.09	128.56	120.80
2	B	466	ARG	NE-CZ-NH2	-11.07	114.76	120.30
3	C	362	PHE	CB-CG-CD1	-11.07	113.05	120.80
7	O	178	MET	CG-SD-CE	-10.99	82.61	100.20
3	K	330	ARG	NE-CZ-NH2	-10.94	114.83	120.30
7	O	256	ARG	NE-CZ-NH2	-10.91	114.84	120.30
8	P	501	TYR	CB-CG-CD2	-10.91	114.45	121.00
7	G	387	ARG	NE-CZ-NH1	10.87	125.74	120.30
1	I	318	ARG	NE-CZ-NH1	10.86	125.73	120.30
7	O	175	PHE	CB-CG-CD2	-10.85	113.21	120.80
3	K	316	ARG	NE-CZ-NH1	10.84	125.72	120.30
7	G	111	TYR	CB-CG-CD1	10.83	127.50	121.00
1	I	390	ARG	NE-CZ-NH2	10.80	125.70	120.30
3	C	264	PHE	CB-CG-CD2	-10.70	113.31	120.80
4	L	153	ARG	NE-CZ-NH2	10.67	125.63	120.30
3	K	339	ARG	NE-CZ-NH2	-10.65	114.97	120.30
8	H	31	ARG	NE-CZ-NH1	10.64	125.62	120.30
5	M	417	ARG	NE-CZ-NH1	10.62	125.61	120.30
6	N	224	ARG	NE-CZ-NH2	10.61	125.61	120.30
3	C	438	ARG	NE-CZ-NH1	10.60	125.60	120.30
2	B	25	ARG	NE-CZ-NH2	-10.50	115.05	120.30
6	N	157	ARG	NE-CZ-NH1	10.48	125.54	120.30
1	A	504	PHE	CB-CG-CD2	10.41	128.09	120.80
3	K	20	ARG	NE-CZ-NH1	10.39	125.50	120.30
6	F	314	ARG	NE-CZ-NH1	10.38	125.49	120.30
6	N	315	ARG	NE-CZ-NH1	10.38	125.49	120.30
3	C	20	ARG	NE-CZ-NH2	-10.37	115.11	120.30
2	B	189	ARG	NE-CZ-NH1	10.37	125.48	120.30
5	E	417	ARG	NE-CZ-NH1	10.36	125.48	120.30
5	E	149	ASP	CB-CG-OD2	10.35	127.61	118.30
3	K	518	ARG	NE-CZ-NH1	10.35	125.47	120.30
2	B	317	PHE	CB-CG-CD1	-10.28	113.61	120.80
3	C	126	TYR	CB-CG-CD1	10.27	127.16	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	49	ARG	NE-CZ-NH1	-10.21	115.19	120.30
7	O	175	PHE	CB-CG-CD1	10.21	127.95	120.80
5	M	417	ARG	NE-CZ-NH2	-10.18	115.21	120.30
4	D	49	ARG	NE-CZ-NH2	10.17	125.39	120.30
8	P	378	ARG	NE-CZ-NH2	-10.15	115.23	120.30
8	P	30	TYR	CB-CG-CD2	-10.14	114.92	121.00
7	G	419	TYR	CB-CG-CD2	-10.13	114.92	121.00
4	L	527	ARG	NE-CZ-NH1	-10.11	115.24	120.30
3	K	216	ARG	NE-CZ-NH2	-10.10	115.25	120.30
7	G	397	ARG	NE-CZ-NH1	10.05	125.33	120.30
3	C	467	ARG	NE-CZ-NH2	-10.04	115.28	120.30
5	E	285	PHE	CB-CG-CD1	10.02	127.82	120.80
3	C	264	PHE	CB-CG-CD1	10.02	127.81	120.80
8	H	31	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	I	441	PHE	CB-CG-CD1	9.99	127.80	120.80
3	C	127	ARG	NE-CZ-NH2	-9.94	115.33	120.30
1	I	145	ARG	NE-CZ-NH2	-9.94	115.33	120.30
6	N	157	ARG	NE-CZ-NH2	-9.94	115.33	120.30
6	F	432	ARG	NE-CZ-NH2	-9.93	115.34	120.30
6	N	300	PHE	CB-CG-CD2	9.92	127.75	120.80
8	P	304	TYR	CG-CD1-CE1	-9.90	113.38	121.30
1	I	401	ARG	NE-CZ-NH2	-9.89	115.35	120.30
5	M	221	ASP	CB-CG-OD2	-9.80	109.47	118.30
8	H	155	ARG	NE-CZ-NH1	9.79	125.19	120.30
2	J	213	TYR	CB-CG-CD1	-9.79	115.13	121.00
3	K	230	ARG	NE-CZ-NH1	-9.73	115.43	120.30
5	E	344	ARG	NE-CZ-NH2	-9.73	115.44	120.30
3	C	260	ARG	NE-CZ-NH1	9.71	125.16	120.30
1	A	209	MET	CG-SD-CE	-9.66	84.74	100.20
4	L	420	ALA	N-CA-CB	9.66	123.62	110.10
2	B	388	ARG	NE-CZ-NH1	9.65	125.13	120.30
3	C	16	ARG	NE-CZ-NH1	9.65	125.13	120.30
4	D	330	ARG	NE-CZ-NH1	9.64	125.12	120.30
5	M	381	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	I	378	ARG	NE-CZ-NH1	9.63	125.12	120.30
1	I	266	ARG	NE-CZ-NH1	9.63	125.11	120.30
1	A	293	ASP	CB-CG-OD1	9.62	126.96	118.30
1	I	181	TYR	CB-CG-CD2	9.62	126.77	121.00
1	A	526	ARG	NE-CZ-NH1	-9.60	115.50	120.30
1	A	293	ASP	CB-CG-OD2	-9.58	109.67	118.30
1	I	441	PHE	CB-CG-CD2	-9.55	114.11	120.80
1	I	496	ARG	NE-CZ-NH2	-9.55	115.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	111	TYR	CB-CG-CD2	-9.53	115.28	121.00
8	H	47	TYR	CB-CG-CD2	9.52	126.71	121.00
1	I	203	ARG	NE-CZ-NH2	-9.51	115.54	120.30
7	O	419	TYR	CB-CG-CD2	9.51	126.70	121.00
3	K	274	TYR	CB-CG-CD1	9.50	126.70	121.00
8	P	520	ARG	NE-CZ-NH1	9.48	125.04	120.30
7	O	306	ARG	NE-CZ-NH1	9.45	125.02	120.30
1	I	310	ARG	NE-CZ-NH2	-9.45	115.58	120.30
7	G	263	TYR	CB-CG-CD2	-9.43	115.34	121.00
5	M	323	ARG	NE-CZ-NH1	9.42	125.01	120.30
5	M	414	ARG	NE-CZ-NH2	9.39	124.99	120.30
6	N	342	ASP	CB-CG-OD2	-9.38	109.86	118.30
4	L	206	ARG	NE-CZ-NH2	-9.38	115.61	120.30
6	N	196	MET	CG-SD-CE	-9.37	85.21	100.20
5	E	306	PHE	CB-CG-CD2	-9.36	114.25	120.80
3	K	306	ARG	NE-CZ-NH1	-9.34	115.63	120.30
3	C	266	ARG	NE-CZ-NH2	-9.33	115.64	120.30
2	J	439	TYR	CB-CG-CD2	9.31	126.58	121.00
8	H	468	TYR	CB-CG-CD2	9.29	126.57	121.00
6	N	319	ARG	NE-CZ-NH2	-9.27	115.67	120.30
2	J	392	ASP	CB-CG-OD2	9.25	126.63	118.30
4	L	277	ARG	NE-CZ-NH1	9.25	124.92	120.30
7	G	313	ARG	NE-CZ-NH2	-9.25	115.68	120.30
2	B	155	PHE	CB-CG-CD1	9.24	127.27	120.80
3	C	93	ASP	CB-CG-OD1	9.24	126.62	118.30
3	K	438	ARG	NE-CZ-NH1	9.22	124.91	120.30
3	K	461	ARG	NE-CZ-NH2	-9.21	115.70	120.30
3	C	359	TYR	CB-CG-CD2	-9.16	115.50	121.00
3	C	263	ASP	N-CA-CB	9.14	127.06	110.60
8	H	74	ARG	NE-CZ-NH2	-9.14	115.73	120.30
5	M	446	TYR	CB-CG-CD2	-9.12	115.53	121.00
4	L	441	ARG	NE-CZ-NH1	9.12	124.86	120.30
5	E	414	ARG	NE-CZ-NH2	-9.08	115.76	120.30
4	D	413	ARG	NE-CZ-NH1	9.07	124.83	120.30
5	E	49	ARG	NE-CZ-NH1	-9.07	115.77	120.30
7	O	419	TYR	CB-CG-CD1	-9.05	115.57	121.00
6	N	396	ARG	NE-CZ-NH2	-9.05	115.77	120.30
3	K	190	ARG	NE-CZ-NH1	9.04	124.82	120.30
2	B	362	PHE	CB-CG-CD1	9.03	127.12	120.80
2	J	488	MET	CG-SD-CE	9.02	114.64	100.20
6	F	256	ARG	NE-CZ-NH1	-9.02	115.79	120.30
6	N	279	ARG	NE-CZ-NH2	-8.99	115.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	151	MET	CG-SD-CE	-8.98	85.83	100.20
3	C	314	ARG	NE-CZ-NH1	-8.97	115.81	120.30
7	G	474	TRP	CB-CG-CD2	-8.93	115.00	126.60
8	P	165	ARG	NE-CZ-NH2	8.91	124.75	120.30
4	L	34	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	A	504	PHE	CB-CG-CD1	-8.90	114.57	120.80
5	E	480	ARG	NE-CZ-NH1	8.90	124.75	120.30
2	B	231	ARG	NE-CZ-NH1	8.89	124.75	120.30
6	N	353	TYR	CB-CG-CD1	-8.89	115.67	121.00
6	N	303	ASP	CB-CG-OD1	-8.89	110.30	118.30
4	D	435	ARG	NE-CZ-NH2	-8.88	115.86	120.30
3	K	330	ARG	NE-CZ-NH1	8.87	124.73	120.30
6	N	217	ARG	NE-CZ-NH2	-8.81	115.90	120.30
8	H	436	TYR	CB-CG-CD1	-8.81	115.72	121.00
8	P	173	TYR	CB-CG-CD2	8.81	126.28	121.00
4	D	449	TYR	CB-CG-CD2	8.80	126.28	121.00
5	M	245	ASP	CB-CG-OD2	8.78	126.20	118.30
8	P	247	ASP	CB-CG-OD1	-8.78	110.40	118.30
6	F	210	LEU	CB-CG-CD2	8.77	125.91	111.00
7	G	225	PHE	CB-CG-CD1	-8.77	114.67	120.80
4	L	89	ARG	NE-CZ-NH2	8.76	124.68	120.30
3	K	449	ARG	NE-CZ-NH1	-8.76	115.92	120.30
7	O	381	PHE	CB-CG-CD2	-8.75	114.67	120.80
5	E	285	PHE	CB-CG-CD2	-8.75	114.67	120.80
7	O	111	TYR	CB-CG-CD1	8.75	126.25	121.00
5	M	49	ARG	NE-CZ-NH1	8.75	124.67	120.30
8	H	426	TYR	CB-CG-CD1	-8.73	115.76	121.00
1	A	122	ARG	NE-CZ-NH1	8.71	124.65	120.30
5	M	488	ALA	N-CA-CB	8.62	122.17	110.10
8	H	314	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	A	526	ARG	NE-CZ-NH2	-8.59	116.01	120.30
8	H	137	ARG	NE-CZ-NH2	-8.59	116.01	120.30
7	O	263	TYR	CB-CG-CD2	-8.58	115.85	121.00
8	P	30	TYR	CB-CG-CD1	8.50	126.10	121.00
7	O	367	ALA	N-CA-CB	8.47	121.97	110.10
1	I	228	ARG	NE-CZ-NH2	8.46	124.53	120.30
6	F	392	ARG	NE-CZ-NH2	8.45	124.52	120.30
6	N	342	ASP	CB-CG-OD1	8.44	125.90	118.30
5	E	149	ASP	CB-CG-OD1	-8.43	110.71	118.30
6	F	217	ARG	NE-CZ-NH1	8.43	124.51	120.30
2	B	25	ARG	NE-CZ-NH1	8.42	124.51	120.30
3	K	359	TYR	CB-CG-CD1	-8.39	115.96	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	274	ARG	NE-CZ-NH2	-8.39	116.10	120.30
6	N	300	PHE	CB-CG-CD1	-8.36	114.94	120.80
2	J	427	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	A	266	ARG	NE-CZ-NH1	-8.35	116.13	120.30
1	I	266	ARG	NE-CZ-NH2	-8.34	116.13	120.30
7	G	321	ARG	NE-CZ-NH1	-8.31	116.15	120.30
4	D	439	TYR	CB-CG-CD2	8.30	125.98	121.00
5	M	415	ASP	CB-CG-OD2	8.29	125.76	118.30
8	H	468	TYR	CB-CG-CD1	-8.29	116.03	121.00
7	O	358	TYR	CB-CG-CD2	-8.28	116.03	121.00
6	F	396	ARG	NE-CZ-NH2	-8.27	116.16	120.30
6	N	145	ARG	NE-CZ-NH2	-8.27	116.16	120.30
8	H	47	TYR	CB-CG-CD1	-8.26	116.04	121.00
5	M	185	MET	CG-SD-CE	-8.26	86.98	100.20
5	E	201	ARG	NE-CZ-NH1	8.25	124.43	120.30
7	O	510	ALA	N-CA-CB	8.25	121.65	110.10
3	K	96	THR	CA-CB-CG2	-8.24	100.86	112.40
7	G	524	ARG	NE-CZ-NH2	-8.24	116.18	120.30
5	M	63	ASP	CB-CG-OD1	-8.24	110.88	118.30
1	I	504	PHE	CB-CG-CD1	8.24	126.57	120.80
6	F	264	ARG	NE-CZ-NH2	8.24	124.42	120.30
5	M	468	MET	CG-SD-CE	8.23	113.36	100.20
3	C	164	ALA	N-CA-CB	8.22	121.61	110.10
6	N	321	MET	CG-SD-CE	-8.22	87.06	100.20
2	J	392	ASP	CB-CG-OD1	-8.21	110.91	118.30
1	I	318	ARG	NE-CZ-NH2	-8.20	116.20	120.30
5	E	138	GLU	OE1-CD-OE2	8.15	133.09	123.30
6	F	351	TYR	CB-CG-CD1	-8.15	116.11	121.00
1	I	480	ARG	NE-CZ-NH1	8.14	124.37	120.30
2	B	66	ASP	CB-CG-OD2	-8.14	110.98	118.30
1	I	8	PHE	CB-CG-CD2	8.09	126.46	120.80
6	N	396	ARG	NE-CZ-NH1	8.08	124.34	120.30
2	J	454	ALA	CB-CA-C	-8.06	98.02	110.10
7	O	421	ARG	NE-CZ-NH2	-8.05	116.27	120.30
3	C	266	ARG	NE-CZ-NH1	8.03	124.31	120.30
6	N	189	PHE	CB-CG-CD2	-8.03	115.18	120.80
1	A	370	ARG	NE-CZ-NH2	-8.01	116.29	120.30
1	A	185	ARG	NE-CZ-NH2	-8.00	116.30	120.30
3	K	274	TYR	CB-CG-CD2	-8.00	116.20	121.00
4	D	441	ARG	NE-CZ-NH2	-8.00	116.30	120.30
6	F	109	TYR	CB-CG-CD1	-7.99	116.20	121.00
7	O	220	PHE	CB-CG-CD2	-7.98	115.22	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	29	MET	CG-SD-CE	-7.97	87.45	100.20
3	C	506	TYR	CB-CG-CD1	-7.94	116.23	121.00
4	D	444	SER	N-CA-CB	7.94	122.41	110.50
6	F	208	ARG	NE-CZ-NH2	7.92	124.26	120.30
5	E	417	ARG	NE-CZ-NH2	-7.92	116.34	120.30
2	J	427	ARG	NE-CZ-NH1	7.91	124.26	120.30
4	L	454	PHE	CB-CG-CD2	7.91	126.33	120.80
2	J	252	PHE	CB-CG-CD2	7.90	126.33	120.80
5	E	474	MET	CG-SD-CE	7.90	112.84	100.20
6	N	141	ARG	NE-CZ-NH1	7.89	124.24	120.30
4	D	287	VAL	CA-CB-CG2	-7.87	99.09	110.90
3	C	85	ARG	NE-CZ-NH2	7.83	124.22	120.30
8	P	404	ARG	NE-CZ-NH2	7.83	124.22	120.30
1	I	526	ARG	NE-CZ-NH1	7.83	124.22	120.30
5	M	155	VAL	N-CA-C	-7.80	89.94	111.00
7	O	357	ARG	NE-CZ-NH1	7.79	124.19	120.30
4	L	481	ARG	NE-CZ-NH1	7.78	124.19	120.30
2	B	476	ALA	N-CA-CB	7.78	120.99	110.10
5	E	126	ARG	NE-CZ-NH1	7.78	124.19	120.30
8	H	155	ARG	NE-CZ-NH2	-7.77	116.41	120.30
1	I	181	TYR	CB-CG-CD1	-7.77	116.34	121.00
3	K	306	ARG	NE-CZ-NH2	7.77	124.19	120.30
6	N	315	ARG	N-CA-CB	7.77	124.59	110.60
2	B	452	ASP	CB-CG-OD1	-7.76	111.31	118.30
3	K	316	ARG	NE-CZ-NH2	-7.74	116.43	120.30
4	D	274	ARG	NE-CZ-NH1	-7.74	116.43	120.30
5	E	27	ARG	NE-CZ-NH1	7.73	124.16	120.30
8	H	232	THR	CA-CB-CG2	-7.71	101.60	112.40
2	J	297	TYR	CB-CG-CD2	7.70	125.62	121.00
8	P	331	THR	CA-CB-CG2	-7.70	101.62	112.40
4	D	380	ALA	N-CA-CB	7.70	120.88	110.10
6	N	150	ASP	CB-CG-OD2	-7.70	111.37	118.30
4	L	316	PHE	CG-CD1-CE1	-7.68	112.36	120.80
3	C	339	ARG	NE-CZ-NH2	-7.67	116.46	120.30
4	D	153	ARG	NE-CZ-NH1	7.67	124.14	120.30
7	G	306	ARG	NE-CZ-NH1	7.66	124.13	120.30
2	J	464	GLN	N-CA-C	7.64	131.63	111.00
8	P	450	ARG	NE-CZ-NH2	-7.64	116.48	120.30
3	C	126	TYR	CB-CG-CD2	-7.64	116.42	121.00
6	F	222	LYS	N-CA-C	-7.64	90.38	111.00
8	H	246	PHE	CB-CG-CD1	-7.63	115.46	120.80
4	D	34	ARG	NE-CZ-NH1	-7.61	116.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ARG	NH1-CZ-NH2	-7.60	111.04	119.40
6	N	133	PHE	CB-CG-CD2	-7.59	115.48	120.80
1	A	167	PHE	CB-CG-CD2	7.59	126.11	120.80
2	J	138	ARG	NE-CZ-NH1	7.58	124.09	120.30
3	C	190	ARG	NE-CZ-NH1	7.58	124.09	120.30
8	H	47	TYR	N-CA-CB	7.57	124.23	110.60
5	M	400	ARG	NE-CZ-NH2	7.54	124.07	120.30
3	C	228	ARG	NE-CZ-NH2	7.53	124.06	120.30
3	K	357	ASP	CB-CG-OD1	-7.53	111.53	118.30
2	B	20	ARG	NE-CZ-NH2	7.52	124.06	120.30
4	L	481	ARG	NE-CZ-NH2	-7.52	116.54	120.30
5	E	449	ARG	NE-CZ-NH1	7.50	124.05	120.30
3	K	167	ARG	CG-CD-NE	-7.50	96.06	111.80
8	P	85	MET	CG-SD-CE	-7.49	88.21	100.20
5	M	255	PHE	CB-CG-CD2	-7.49	115.56	120.80
6	F	315	ARG	NE-CZ-NH1	-7.49	116.56	120.30
6	N	229	TYR	CB-CG-CD1	7.48	125.49	121.00
3	K	68	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	A	390	ARG	NE-CZ-NH1	7.46	124.03	120.30
7	O	348	PHE	CB-CG-CD2	7.46	126.03	120.80
6	N	28	ARG	NE-CZ-NH2	7.46	124.03	120.30
6	N	177	LEU	CB-CG-CD1	7.46	123.67	111.00
4	L	449	TYR	CB-CG-CD1	7.45	125.47	121.00
6	F	327	ALA	CB-CA-C	-7.43	98.95	110.10
1	I	190	TYR	CB-CG-CD1	-7.43	116.54	121.00
3	K	228	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	I	256	ASP	CB-CG-OD2	-7.42	111.62	118.30
8	P	304	TYR	CD1-CE1-CZ	7.42	126.48	119.80
2	B	304	PHE	CB-CG-CD2	-7.42	115.61	120.80
7	O	478	ASP	CB-CG-OD1	-7.41	111.63	118.30
1	A	228	ARG	NE-CZ-NH2	-7.40	116.60	120.30
6	F	495	TRP	CB-CG-CD2	-7.40	116.98	126.60
1	A	340	PHE	CB-CG-CD2	-7.40	115.62	120.80
7	O	232	TYR	CD1-CE1-CZ	-7.39	113.15	119.80
1	A	190	TYR	CB-CG-CD1	-7.38	116.57	121.00
4	L	76	THR	CA-CB-CG2	-7.38	102.07	112.40
1	A	121	TYR	CB-CG-CD1	7.38	125.42	121.00
5	E	364	PHE	CB-CG-CD2	-7.35	115.66	120.80
7	G	232	TYR	CB-CG-CD1	-7.34	116.59	121.00
8	P	322	ARG	NE-CZ-NH1	-7.32	116.64	120.30
3	C	325	ARG	NE-CZ-NH1	7.32	123.96	120.30
7	G	466	ALA	N-CA-CB	7.32	120.35	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	438	ARG	NE-CZ-NH2	-7.31	116.65	120.30
1	A	189	ARG	N-CA-CB	7.30	123.74	110.60
2	J	29	PHE	CB-CG-CD1	7.30	125.91	120.80
3	C	272	GLU	OE1-CD-OE2	7.29	132.05	123.30
1	A	256	ASP	CB-CG-OD1	7.29	124.86	118.30
3	C	133	MET	CG-SD-CE	-7.28	88.55	100.20
4	L	330	ARG	NE-CZ-NH2	-7.28	116.66	120.30
5	E	190	VAL	CA-CB-CG1	-7.28	99.99	110.90
3	C	499	LEU	CB-CG-CD2	7.26	123.34	111.00
7	O	227	MET	CG-SD-CE	7.25	111.81	100.20
5	M	414	ARG	NH1-CZ-NH2	-7.25	111.43	119.40
2	B	427	ARG	NE-CZ-NH1	7.24	123.92	120.30
5	E	396	GLU	OE1-CD-OE2	7.22	131.96	123.30
5	M	67	ASP	CB-CG-OD2	7.22	124.80	118.30
4	D	200	ALA	N-CA-CB	7.21	120.20	110.10
5	M	218	ARG	NE-CZ-NH2	7.20	123.90	120.30
3	C	52	ASP	CB-CG-OD2	7.18	124.77	118.30
7	G	268	ASP	CB-CG-OD1	-7.17	111.84	118.30
6	F	486	PRO	O-C-N	7.17	134.17	122.70
2	B	488	MET	CG-SD-CE	-7.16	88.75	100.20
4	L	403	ARG	NE-CZ-NH1	7.16	123.88	120.30
5	M	415	ASP	CB-CG-OD1	-7.15	111.86	118.30
6	F	145	ARG	NE-CZ-NH1	7.15	123.88	120.30
3	K	393	ASP	CB-CG-OD1	-7.15	111.86	118.30
1	I	18	ARG	NE-CZ-NH1	-7.15	116.72	120.30
1	I	121	TYR	CB-CG-CD1	-7.13	116.72	121.00
8	H	492	MET	CG-SD-CE	-7.13	88.80	100.20
2	B	130	TRP	CG-CD2-CE3	-7.12	127.49	133.90
7	G	117	HIS	N-CA-CB	7.11	123.40	110.60
4	L	269	TYR	CB-CG-CD2	7.11	125.27	121.00
8	H	308	TYR	CB-CG-CD2	7.11	125.27	121.00
2	J	93	ASP	CB-CG-OD2	7.11	124.70	118.30
4	L	251	PHE	CB-CG-CD1	-7.10	115.83	120.80
6	F	505	LEU	CB-CG-CD1	7.10	123.06	111.00
7	G	53	ARG	NE-CZ-NH1	-7.10	116.75	120.30
2	B	359	LEU	CB-CG-CD2	7.09	123.05	111.00
1	A	441	PHE	CB-CG-CD2	-7.08	115.84	120.80
7	O	465	ARG	NE-CZ-NH2	-7.08	116.76	120.30
6	F	522	MET	CG-SD-CE	-7.07	88.88	100.20
1	A	340	PHE	CB-CG-CD1	7.07	125.75	120.80
3	C	145	ASP	CB-CG-OD2	-7.06	111.95	118.30
5	E	500	ASP	CB-CG-OD1	7.05	124.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	286	ALA	N-CA-CB	7.05	119.97	110.10
4	L	240	ARG	NE-CZ-NH1	7.04	123.82	120.30
4	D	454	PHE	CB-CG-CD2	-7.02	115.88	120.80
4	D	137	PHE	CB-CG-CD1	7.02	125.71	120.80
2	J	516	ARG	NE-CZ-NH1	7.01	123.80	120.30
2	J	57	ARG	NH1-CZ-NH2	6.99	127.09	119.40
4	L	349	ASP	CB-CG-OD2	6.99	124.59	118.30
7	O	276	ASP	CB-CG-OD1	-6.99	112.01	118.30
4	L	258	THR	CA-CB-CG2	-6.98	102.62	112.40
7	G	486	ASP	CB-CG-OD1	6.97	124.58	118.30
3	C	360	PHE	CB-CG-CD2	-6.97	115.92	120.80
1	I	131	TYR	CD1-CE1-CZ	6.97	126.07	119.80
1	A	443	ARG	NE-CZ-NH2	6.97	123.78	120.30
3	C	247	TYR	CG-CD2-CE2	6.97	126.87	121.30
1	I	526	ARG	N-CA-CB	6.96	123.13	110.60
7	O	152	ARG	NE-CZ-NH1	6.96	123.78	120.30
5	E	386	PHE	CB-CG-CD1	-6.96	115.93	120.80
2	J	257	ARG	NE-CZ-NH2	6.95	123.77	120.30
8	P	285	ASP	N-CA-CB	6.95	123.10	110.60
6	F	53	ASP	N-CA-CB	6.94	123.10	110.60
6	F	336	PHE	CB-CG-CD2	6.94	125.66	120.80
8	H	242	TYR	CB-CG-CD2	-6.94	116.83	121.00
5	E	296	GLY	N-CA-C	-6.93	95.76	113.10
3	K	198	TYR	CD1-CE1-CZ	-6.93	113.56	119.80
6	F	123	PHE	CB-CG-CD1	6.92	125.65	120.80
6	N	250	TYR	CB-CG-CD1	6.92	125.15	121.00
2	J	299	TYR	CB-CG-CD2	6.92	125.15	121.00
1	A	526	ARG	NH1-CZ-NH2	6.91	127.00	119.40
2	B	448	THR	CA-CB-CG2	-6.91	102.72	112.40
1	A	300	PHE	CB-CG-CD1	-6.90	115.97	120.80
6	N	158	THR	CA-CB-CG2	-6.90	102.74	112.40
6	N	250	TYR	CB-CG-CD2	-6.90	116.86	121.00
6	N	362	PHE	CB-CG-CD1	6.89	125.63	120.80
2	J	466	ARG	NE-CZ-NH1	6.89	123.74	120.30
2	J	299	TYR	CB-CG-CD1	-6.89	116.87	121.00
4	D	362	ALA	N-CA-CB	6.88	119.74	110.10
5	M	128	ILE	CA-CB-CG1	-6.88	97.93	111.00
4	L	413	ARG	NE-CZ-NH2	6.86	123.73	120.30
3	K	359	TYR	CB-CG-CD2	6.86	125.11	121.00
2	B	66	ASP	CB-CG-OD1	6.85	124.47	118.30
3	C	228	ARG	NH1-CZ-NH2	-6.84	111.87	119.40
1	A	394	ASP	CB-CG-OD2	-6.84	112.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	63	ASP	CB-CG-OD1	-6.83	112.15	118.30
1	A	122	ARG	NE-CZ-NH2	6.83	123.71	120.30
3	C	185	PHE	CB-CG-CD2	-6.82	116.02	120.80
3	K	380	SER	N-CA-CB	6.82	120.73	110.50
4	D	441	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	I	355	ARG	NE-CZ-NH2	-6.81	116.89	120.30
4	L	355	MET	CG-SD-CE	-6.81	89.31	100.20
7	G	321	ARG	NE-CZ-NH2	6.80	123.70	120.30
2	B	405	ARG	NE-CZ-NH2	-6.80	116.90	120.30
7	G	391	ASP	CB-CG-OD2	-6.80	112.18	118.30
5	M	355	PHE	CB-CG-CD2	6.80	125.56	120.80
8	H	516	VAL	CA-CB-CG2	-6.79	100.71	110.90
2	B	456	TYR	CB-CG-CD1	-6.79	116.92	121.00
7	O	87	ASP	CB-CG-OD1	6.79	124.41	118.30
3	C	281	ASP	CB-CG-OD2	-6.78	112.19	118.30
4	L	27	ARG	NE-CZ-NH2	-6.78	116.91	120.30
2	B	57	ARG	NE-CZ-NH1	6.76	123.68	120.30
7	G	357	ARG	NE-CZ-NH1	6.76	123.68	120.30
3	K	198	TYR	CG-CD2-CE2	-6.75	115.90	121.30
1	I	456	ALA	CB-CA-C	-6.75	99.98	110.10
2	B	259	ASP	CB-CG-OD2	-6.75	112.23	118.30
8	H	436	TYR	CG-CD1-CE1	-6.74	115.91	121.30
4	L	27	ARG	NE-CZ-NH1	6.74	123.67	120.30
7	G	486	ASP	CB-CG-OD2	-6.74	112.23	118.30
8	P	469	ALA	CB-CA-C	-6.73	100.00	110.10
3	K	242	ASP	CB-CG-OD2	6.73	124.36	118.30
5	M	343	PRO	N-CA-CB	6.73	111.37	103.30
5	E	460	MET	CG-SD-CE	6.72	110.96	100.20
8	P	323	ARG	NE-CZ-NH1	6.71	123.66	120.30
5	M	48	MET	CG-SD-CE	-6.71	89.46	100.20
4	D	153	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	I	468	ARG	NE-CZ-NH2	-6.71	116.95	120.30
4	D	118	ASP	CB-CG-OD1	-6.71	112.26	118.30
1	A	357	CYS	N-CA-CB	6.70	122.66	110.60
6	N	220	ASP	CB-CG-OD1	6.70	124.33	118.30
4	L	282	TYR	CB-CG-CD2	-6.68	116.99	121.00
7	G	333	SER	N-CA-CB	6.67	120.51	110.50
1	I	90	THR	CA-CB-CG2	-6.67	103.06	112.40
5	M	478	ARG	NE-CZ-NH2	-6.66	116.97	120.30
4	L	507	LEU	N-CA-CB	6.65	123.69	110.40
5	M	534	ARG	NE-CZ-NH1	6.65	123.62	120.30
3	C	228	ARG	NE-CZ-NH1	6.64	123.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	501	TYR	CB-CG-CD1	6.64	124.99	121.00
2	B	275	MET	CG-SD-CE	-6.64	89.57	100.20
3	C	232	TYR	CB-CG-CD1	6.64	124.98	121.00
6	F	457	PHE	CB-CG-CD2	-6.63	116.16	120.80
3	K	76	ALA	CB-CA-C	-6.63	100.16	110.10
4	L	227	LEU	CB-CG-CD1	6.62	122.26	111.00
2	B	518	ASP	CB-CG-OD2	-6.62	112.34	118.30
8	H	88	MET	CG-SD-CE	-6.61	89.62	100.20
2	B	297	TYR	CB-CG-CD1	-6.60	117.04	121.00
3	K	518	ARG	CD-NE-CZ	-6.59	114.37	123.60
4	D	281	ALA	N-CA-CB	-6.59	100.87	110.10
7	G	216	PHE	CB-CG-CD2	-6.59	116.19	120.80
2	J	293	ARG	NE-CZ-NH1	6.59	123.59	120.30
6	N	458	ASP	CB-CG-OD2	6.58	124.22	118.30
3	C	198	TYR	CB-CG-CD1	-6.58	117.05	121.00
6	F	389	ASP	CB-CG-OD1	-6.58	112.38	118.30
7	O	344	ARG	NE-CZ-NH1	6.57	123.59	120.30
2	J	516	ARG	NE-CZ-NH2	-6.57	117.02	120.30
5	M	451	PHE	CB-CG-CD1	6.56	125.39	120.80
8	P	314	ARG	NE-CZ-NH1	6.56	123.58	120.30
3	C	467	ARG	CD-NE-CZ	6.56	132.78	123.60
1	A	426	TYR	CB-CG-CD2	-6.55	117.07	121.00
5	E	198	ASP	CB-CG-OD2	-6.55	112.40	118.30
3	K	211	ASP	CB-CG-OD2	6.55	124.20	118.30
4	D	413	ARG	NE-CZ-NH2	-6.54	117.03	120.30
6	N	468	ALA	CB-CA-C	-6.54	100.29	110.10
2	B	316	ASP	CB-CG-OD2	-6.52	112.43	118.30
2	B	460	ASP	CB-CG-OD1	6.52	124.17	118.30
2	B	445	MET	CG-SD-CE	-6.51	89.78	100.20
6	F	229	TYR	CB-CG-CD1	6.51	124.91	121.00
4	L	131	THR	CA-CB-CG2	-6.51	103.29	112.40
8	P	453	ALA	N-CA-CB	6.51	119.21	110.10
6	F	513	THR	CA-CB-CG2	-6.50	103.30	112.40
6	N	141	ARG	NE-CZ-NH2	-6.50	117.05	120.30
6	N	510	VAL	CG1-CB-CG2	6.50	121.31	110.90
5	M	60	MET	CA-CB-CG	6.50	124.35	113.30
1	A	528	ASP	CB-CG-OD2	-6.49	112.46	118.30
2	B	29	PHE	CB-CG-CD1	6.49	125.34	120.80
6	N	134	LEU	CB-CG-CD2	6.48	122.02	111.00
1	A	231	ASN	N-CA-CB	6.48	122.27	110.60
2	B	216	GLU	CG-CD-OE1	-6.48	105.34	118.30
3	K	80	MET	CG-SD-CE	-6.48	89.83	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	329	ALA	N-CA-CB	6.48	119.17	110.10
4	D	316	PHE	CB-CG-CD1	-6.47	116.27	120.80
8	P	351	TYR	CB-CG-CD1	-6.47	117.12	121.00
7	O	108	VAL	CG1-CB-CG2	-6.47	100.56	110.90
5	M	63	ASP	CB-CG-OD2	6.46	124.12	118.30
6	N	109	TYR	CG-CD1-CE1	-6.46	116.13	121.30
6	N	264	ARG	NE-CZ-NH2	-6.46	117.07	120.30
7	O	386	GLU	OE1-CD-OE2	6.46	131.05	123.30
2	B	513	VAL	CA-CB-CG2	-6.46	101.21	110.90
1	I	341	GLU	OE1-CD-OE2	6.46	131.05	123.30
7	O	302	TYR	CB-CG-CD1	6.45	124.87	121.00
6	F	235	VAL	CA-CB-CG1	-6.44	101.24	110.90
5	M	408	VAL	CA-CB-CG1	6.44	120.56	110.90
6	N	264	ARG	NE-CZ-NH1	6.44	123.52	120.30
8	H	323	ARG	NE-CZ-NH2	-6.43	117.08	120.30
8	P	151	ALA	CB-CA-C	-6.43	100.45	110.10
3	C	257	GLU	N-CA-CB	6.42	122.16	110.60
3	C	461	ARG	NE-CZ-NH2	6.42	123.51	120.30
7	G	321	ARG	CD-NE-CZ	-6.42	114.62	123.60
1	A	298	LYS	O-C-N	-6.41	112.44	122.70
5	E	531	ASP	CB-CG-OD1	-6.41	112.53	118.30
3	C	67	LEU	CB-CG-CD2	6.41	121.89	111.00
7	G	112	VAL	CA-CB-CG2	-6.40	101.30	110.90
5	E	84	ASP	CB-CG-OD1	6.40	124.06	118.30
2	B	362	PHE	CB-CG-CD2	-6.40	116.32	120.80
1	A	25	ALA	CB-CA-C	-6.39	100.51	110.10
5	M	446	TYR	CG-CD2-CE2	-6.38	116.20	121.30
4	L	316	PHE	CB-CG-CD2	6.38	125.27	120.80
6	N	109	TYR	CB-CG-CD1	6.38	124.83	121.00
8	P	236	ASP	CB-CG-OD2	-6.37	112.57	118.30
7	O	271	TRP	CB-CG-CD1	6.36	135.26	127.00
8	H	213	SER	N-CA-CB	6.35	120.02	110.50
4	D	309	LEU	N-CA-CB	6.34	123.08	110.40
5	E	374	ILE	N-CA-C	-6.34	93.88	111.00
6	N	314	ARG	NE-CZ-NH1	6.34	123.47	120.30
3	C	230	ARG	NE-CZ-NH2	6.33	123.47	120.30
3	C	435	TRP	CB-CG-CD2	-6.32	118.38	126.60
5	M	451	PHE	CB-CG-CD2	-6.32	116.37	120.80
5	E	178	VAL	CA-CB-CG1	-6.32	101.43	110.90
7	O	305	ASP	CB-CG-OD2	-6.32	112.62	118.30
4	D	449	TYR	CG-CD1-CE1	6.31	126.35	121.30
7	O	433	LEU	CB-CG-CD2	6.31	121.73	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	97	SER	N-CA-CB	6.30	119.96	110.50
6	N	90	ASP	CB-CG-OD1	-6.30	112.63	118.30
1	I	386	ASP	N-CA-CB	6.30	121.94	110.60
5	E	162	THR	CA-CB-CG2	-6.29	103.59	112.40
2	J	158	ASP	CB-CG-OD1	-6.29	112.64	118.30
5	M	446	TYR	CZ-CE2-CD2	6.29	125.46	119.80
4	D	206	ARG	NE-CZ-NH2	-6.29	117.16	120.30
8	P	173	TYR	CB-CG-CD1	-6.28	117.23	121.00
4	D	496	ARG	NE-CZ-NH1	6.28	123.44	120.30
4	L	351	PHE	CB-CG-CD1	-6.28	116.41	120.80
6	N	85	ASP	CB-CG-OD2	6.28	123.95	118.30
1	I	472	ASN	N-CA-CB	6.27	121.89	110.60
3	C	185	PHE	CB-CG-CD1	6.27	125.19	120.80
8	H	293	THR	N-CA-CB	6.27	122.22	110.30
7	O	271	TRP	CB-CG-CD2	-6.27	118.44	126.60
6	F	256	ARG	NH1-CZ-NH2	6.27	126.29	119.40
4	D	504	LEU	CB-CG-CD1	6.26	121.65	111.00
2	B	184	VAL	CA-CB-CG2	6.26	120.29	110.90
6	F	259	LEU	CB-CG-CD2	6.26	121.64	111.00
2	J	257	ARG	NH1-CZ-NH2	-6.26	112.51	119.40
7	O	447	ARG	NE-CZ-NH2	6.26	123.43	120.30
4	D	130	PRO	O-C-N	6.25	132.71	122.70
3	K	118	HIS	CA-CB-CG	6.25	124.23	113.60
3	C	461	ARG	NH1-CZ-NH2	-6.25	112.52	119.40
8	P	450	ARG	NE-CZ-NH1	6.25	123.43	120.30
2	J	111	ARG	NE-CZ-NH1	-6.25	117.18	120.30
6	N	293	ASN	N-CA-CB	6.25	121.84	110.60
6	F	362	PHE	CB-CG-CD1	6.24	125.17	120.80
5	M	324	TRP	C-N-CA	6.24	137.30	121.70
5	M	374	ILE	N-CA-C	-6.24	94.15	111.00
6	N	28	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	I	391	SER	N-CA-CB	6.23	119.85	110.50
5	M	153	ASP	CB-CA-C	-6.23	97.93	110.40
5	E	158	ASP	CB-CG-OD1	-6.23	112.69	118.30
6	F	270	ARG	NE-CZ-NH2	6.23	123.42	120.30
3	K	108	VAL	CA-CB-CG2	-6.23	101.55	110.90
1	I	465	ALA	CB-CA-C	-6.23	100.76	110.10
5	M	337	THR	CA-CB-CG2	-6.22	103.69	112.40
5	M	414	ARG	NE-CZ-NH1	6.22	123.41	120.30
3	K	95	THR	CA-CB-CG2	-6.22	103.70	112.40
6	F	189	PHE	CG-CD1-CE1	6.21	127.63	120.80
4	L	461	ILE	CA-C-N	6.21	134.48	117.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	448	GLN	N-CA-CB	6.21	121.77	110.60
5	E	531	ASP	CB-CG-OD2	6.20	123.88	118.30
4	L	243	LYS	N-CA-CB	6.20	121.76	110.60
8	P	499	ASP	CB-CG-OD1	6.20	123.88	118.30
4	L	435	ARG	NE-CZ-NH1	-6.20	117.20	120.30
7	O	327	GLY	C-N-CA	6.20	135.31	122.30
5	M	239	MET	CG-SD-CE	-6.19	90.29	100.20
1	A	415	VAL	CA-CB-CG2	-6.19	101.61	110.90
8	H	52	MET	CG-SD-CE	-6.18	90.31	100.20
8	H	344	MET	N-CA-CB	6.18	121.72	110.60
7	G	474	TRP	CB-CG-CD1	6.17	135.03	127.00
6	F	158	THR	N-CA-CB	6.17	122.02	110.30
7	O	387	ARG	NE-CZ-NH1	-6.16	117.22	120.30
7	G	465	ARG	NE-CZ-NH1	6.16	123.38	120.30
2	B	429	PRO	CB-CA-C	6.15	127.38	112.00
1	I	516	PHE	CB-CG-CD2	-6.15	116.50	120.80
1	I	423	LEU	CB-CG-CD1	6.13	121.42	111.00
5	E	84	ASP	CB-CG-OD2	-6.13	112.78	118.30
4	L	45	ALA	N-CA-CB	6.13	118.68	110.10
4	D	92	VAL	CA-CB-CG2	6.12	120.08	110.90
5	M	202	ARG	NE-CZ-NH2	6.12	123.36	120.30
2	B	66	ASP	O-C-N	6.12	133.60	123.20
4	D	92	VAL	CA-CB-CG1	-6.11	101.73	110.90
8	H	426	TYR	CG-CD1-CE1	-6.11	116.41	121.30
1	I	105	ASP	CB-CG-OD2	-6.10	112.81	118.30
6	N	432	ARG	NE-CZ-NH1	-6.09	117.25	120.30
7	O	313	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	266	ARG	CD-NE-CZ	-6.09	115.08	123.60
5	M	73	ASP	CB-CG-OD2	-6.09	112.82	118.30
6	F	119	ILE	CA-CB-CG1	-6.08	99.44	111.00
3	C	246	GLU	OE1-CD-OE2	6.07	130.59	123.30
3	K	85	ARG	NE-CZ-NH1	6.07	123.33	120.30
7	O	57	THR	CA-CB-OG1	6.07	121.75	109.00
1	A	461	THR	CA-CB-CG2	-6.07	103.90	112.40
2	B	69	THR	CA-CB-OG1	6.07	121.74	109.00
1	I	496	ARG	NE-CZ-NH1	6.07	123.33	120.30
4	L	472	ASN	N-CA-CB	6.06	121.52	110.60
2	B	316	ASP	CB-CG-OD1	6.06	123.76	118.30
3	C	341	ASP	CB-CG-OD1	-6.06	112.85	118.30
6	F	495	TRP	CB-CG-CD1	6.05	134.87	127.00
1	A	76	CYS	CA-CB-SG	6.05	124.89	114.00
5	E	492	ASP	CB-CG-OD2	-6.05	112.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	480	ASP	CB-CG-OD1	-6.05	112.85	118.30
3	C	360	PHE	CB-CG-CD1	6.05	125.03	120.80
2	J	91	GLN	CA-CB-CG	-6.05	100.10	113.40
8	H	378	ARG	NE-CZ-NH1	6.04	123.32	120.30
4	D	211	VAL	CA-CB-CG2	-6.04	101.84	110.90
8	H	203	ARG	NE-CZ-NH1	-6.04	117.28	120.30
7	G	221	SER	N-CA-CB	6.04	119.56	110.50
1	I	430	MET	CG-SD-CE	-6.04	90.54	100.20
6	N	411	ALA	N-CA-CB	6.04	118.55	110.10
8	P	203	ARG	NE-CZ-NH2	-6.04	117.28	120.30
8	H	369	ASP	CB-CG-OD2	6.03	123.73	118.30
1	I	532	LYS	CA-CB-CG	6.03	126.66	113.40
1	I	57	ASP	CB-CG-OD2	-6.03	112.88	118.30
4	D	316	PHE	CG-CD2-CE2	-6.02	114.18	120.80
1	A	246	MET	N-CA-C	-6.02	94.75	111.00
3	C	190	ARG	NH1-CZ-NH2	-6.02	112.78	119.40
7	G	386	GLU	CB-CG-CD	-6.01	97.96	114.20
4	L	454	PHE	CB-CG-CD1	-6.01	116.59	120.80
7	O	360	PHE	CB-CG-CD2	6.01	125.01	120.80
8	H	293	THR	CA-CB-CG2	-6.01	103.99	112.40
5	E	267	ASP	CB-CG-OD1	6.01	123.71	118.30
4	D	309	LEU	N-CA-C	-6.00	94.79	111.00
7	O	222	TYR	CB-CG-CD1	-6.00	117.40	121.00
4	L	351	PHE	CB-CG-CD2	6.00	125.00	120.80
1	I	11	ARG	NE-CZ-NH1	5.99	123.30	120.30
4	D	352	THR	N-CA-C	-5.99	94.82	111.00
8	P	390	ARG	NE-CZ-NH1	5.99	123.29	120.30
3	C	312	ILE	N-CA-C	-5.98	94.84	111.00
7	O	305	ASP	CB-CG-OD1	5.98	123.68	118.30
2	J	235	ALA	CB-CA-C	-5.98	101.13	110.10
4	L	277	ARG	NE-CZ-NH2	-5.98	117.31	120.30
4	L	418	LYS	N-CA-CB	5.97	121.35	110.60
3	C	422	LEU	N-CA-CB	5.97	122.34	110.40
4	D	186	MET	CG-SD-CE	-5.97	90.65	100.20
2	J	257	ARG	NE-CZ-NH1	5.97	123.28	120.30
5	E	410	ARG	NE-CZ-NH1	5.96	123.28	120.30
3	C	80	MET	CG-SD-CE	-5.96	90.66	100.20
3	K	255	ASP	CB-CG-OD1	-5.95	112.94	118.30
1	A	401	ARG	NE-CZ-NH1	-5.95	117.33	120.30
4	L	36	SER	N-CA-CB	5.95	119.43	110.50
6	N	224	ARG	NH1-CZ-NH2	-5.94	112.86	119.40
1	I	414	ALA	CB-CA-C	-5.94	101.19	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	435	TRP	CG-CD2-CE3	-5.93	128.56	133.90
7	G	152	ARG	NE-CZ-NH2	-5.93	117.34	120.30
8	H	426	TYR	CB-CG-CD2	5.93	124.56	121.00
6	N	250	TYR	CA-CB-CG	5.92	124.65	113.40
1	A	381	ASN	N-CA-C	-5.92	95.02	111.00
6	F	229	TYR	CB-CG-CD2	-5.92	117.45	121.00
3	C	68	ARG	NE-CZ-NH2	-5.91	117.34	120.30
4	L	308	ALA	N-CA-CB	5.91	118.38	110.10
5	E	320	PRO	CA-N-CD	-5.91	103.22	111.50
7	G	104	PHE	CB-CA-C	-5.91	98.58	110.40
7	O	71	VAL	CA-CB-CG1	-5.91	102.04	110.90
7	O	283	HIS	CA-CB-CG	5.91	123.64	113.60
2	B	41	SER	N-CA-CB	5.90	119.36	110.50
4	D	239	THR	CA-CB-CG2	-5.90	104.14	112.40
8	P	104	VAL	CA-CB-CG2	-5.90	102.05	110.90
7	G	146	ALA	CB-CA-C	-5.90	101.25	110.10
7	O	122	ILE	CA-CB-CG1	5.90	122.21	111.00
3	K	132	ASP	CB-CG-OD1	5.90	123.61	118.30
3	C	285	LEU	C-N-CA	5.90	136.44	121.70
1	I	125	CYS	O-C-N	-5.89	113.27	122.70
4	L	207	ASP	CB-CG-OD2	-5.89	113.00	118.30
3	C	16	ARG	CD-NE-CZ	-5.89	115.36	123.60
7	O	61	ASP	N-CA-C	-5.89	95.10	111.00
7	G	348	PHE	CB-CG-CD1	5.88	124.92	120.80
2	J	290	PHE	CB-CG-CD1	5.88	124.92	120.80
4	D	212	LYS	N-CA-CB	5.88	121.19	110.60
6	N	179	ILE	CG1-CB-CG2	5.88	124.34	111.40
3	K	430	THR	N-CA-CB	5.88	121.47	110.30
2	B	257	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	J	292	ASN	N-CA-CB	5.88	121.17	110.60
5	E	398	ALA	CB-CA-C	-5.87	101.29	110.10
6	N	316	ALA	N-CA-CB	5.87	118.32	110.10
7	O	100	LEU	CB-CG-CD1	5.87	120.98	111.00
8	P	501	TYR	CG-CD1-CE1	-5.87	116.60	121.30
2	B	270	ALA	N-CA-CB	5.87	118.31	110.10
5	E	171	THR	CA-CB-CG2	5.87	120.62	112.40
1	I	238	ASP	N-CA-CB	5.86	121.16	110.60
3	K	368	ASP	CB-CG-OD2	-5.86	113.02	118.30
5	M	214	LYS	CB-CA-C	-5.86	98.68	110.40
7	G	419	TYR	CG-CD2-CE2	-5.86	116.61	121.30
6	N	81	ALA	N-CA-CB	5.86	118.30	110.10
8	P	160	VAL	CA-CB-CG2	-5.86	102.12	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	470	VAL	CG1-CB-CG2	5.85	120.26	110.90
5	M	323	ARG	NE-CZ-NH2	-5.85	117.38	120.30
7	G	438	TYR	CB-CG-CD2	-5.85	117.49	121.00
1	I	229	ILE	N-CA-C	-5.85	95.21	111.00
3	C	160	ILE	CA-CB-CG2	-5.84	99.21	110.90
8	P	158	ASP	CB-CG-OD2	5.84	123.56	118.30
7	G	387	ARG	NE-CZ-NH2	-5.84	117.38	120.30
4	D	63	ASP	CB-CG-OD2	5.84	123.55	118.30
3	K	278	LEU	CB-CA-C	-5.84	99.11	110.20
4	L	449	TYR	CB-CG-CD2	-5.84	117.50	121.00
5	M	474	MET	CB-CA-C	-5.83	98.74	110.40
4	D	73	ASP	N-CA-C	-5.83	95.26	111.00
7	O	361	PHE	CB-CG-CD1	-5.83	116.72	120.80
4	D	327	ASP	N-CA-CB	5.83	121.08	110.60
4	D	256	PRO	O-C-N	5.82	132.01	122.70
8	H	426	TYR	CG-CD2-CE2	5.82	125.96	121.30
1	I	131	TYR	CE1-CZ-CE2	-5.82	110.49	119.80
4	L	245	LYS	N-CA-C	-5.82	95.29	111.00
7	G	92	ASP	CB-CG-OD2	5.82	123.53	118.30
3	C	446	VAL	CA-CB-CG2	-5.81	102.18	110.90
5	E	233	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	398	VAL	CA-CB-CG2	-5.81	102.18	110.90
5	E	420	TYR	CG-CD1-CE1	5.81	125.95	121.30
6	N	425	HIS	N-CA-CB	5.81	121.05	110.60
2	B	452	ASP	CB-CG-OD2	5.80	123.52	118.30
2	B	420	ALA	CB-CA-C	5.80	118.81	110.10
7	G	467	ARG	NE-CZ-NH1	5.80	123.20	120.30
6	F	165	ALA	N-CA-CB	5.80	118.22	110.10
6	N	35	ARG	NE-CZ-NH1	5.80	123.20	120.30
4	D	437	THR	CA-CB-CG2	-5.80	104.28	112.40
8	P	520	ARG	NE-CZ-NH2	-5.79	117.40	120.30
2	B	57	ARG	NE-CZ-NH2	-5.79	117.40	120.30
8	P	363	PHE	CB-CG-CD1	-5.79	116.75	120.80
6	N	370	ARG	CD-NE-CZ	5.79	131.71	123.60
5	E	436	GLU	OE1-CD-OE2	5.79	130.24	123.30
1	A	172	VAL	O-C-N	-5.78	113.44	122.70
1	A	47	ASP	CB-CG-OD1	5.77	123.50	118.30
6	N	389	ASP	CB-CG-OD2	5.77	123.49	118.30
8	P	324	LEU	CB-CG-CD1	5.77	120.81	111.00
5	E	256	GLU	CA-C-N	5.76	133.24	117.10
7	O	294	PRO	N-CD-CG	5.76	111.85	103.20
2	B	252	PHE	CB-CG-CD2	5.76	124.83	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	476	GLY	N-CA-C	-5.76	98.69	113.10
2	B	235	ALA	N-CA-CB	5.76	118.17	110.10
1	I	153	LYS	N-CA-CB	-5.76	100.23	110.60
5	M	83	VAL	CA-CB-CG1	5.76	119.54	110.90
3	C	446	VAL	CG1-CB-CG2	5.76	120.11	110.90
7	G	316	GLU	N-CA-CB	5.76	120.97	110.60
1	A	492	ASN	N-CA-CB	5.76	120.96	110.60
6	N	15	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	I	351	VAL	N-CA-C	-5.76	95.46	111.00
4	D	251	PHE	CB-CG-CD1	-5.75	116.77	120.80
2	J	233	GLU	N-CA-CB	5.75	120.96	110.60
4	D	398	ILE	N-CA-CB	5.75	124.02	110.80
6	F	217	ARG	NE-CZ-NH2	-5.75	117.42	120.30
4	L	299	LEU	CB-CA-C	-5.75	99.28	110.20
4	L	130	PRO	N-CD-CG	5.74	111.81	103.20
5	E	462	LEU	CB-CG-CD2	5.74	120.76	111.00
7	O	143	VAL	CA-CB-CG2	5.74	119.50	110.90
3	K	198	TYR	CB-CG-CD2	-5.73	117.56	121.00
3	C	461	ARG	NE-CZ-NH1	5.73	123.17	120.30
7	G	475	TYR	CB-CG-CD1	-5.73	117.56	121.00
7	O	371	THR	N-CA-CB	5.73	121.19	110.30
4	D	240	ARG	NE-CZ-NH2	-5.73	117.44	120.30
7	G	108	VAL	CA-CB-CG2	-5.73	102.31	110.90
7	O	485	ALA	N-CA-CB	5.73	118.12	110.10
4	L	386	VAL	CG1-CB-CG2	5.72	120.05	110.90
6	F	432	ARG	NE-CZ-NH1	5.71	123.16	120.30
2	B	29	PHE	CB-CG-CD2	-5.71	116.80	120.80
6	F	355	LEU	CB-CA-C	-5.71	99.36	110.20
3	C	473	GLU	OE1-CD-OE2	5.70	130.14	123.30
1	A	90	THR	CA-CB-CG2	-5.70	104.42	112.40
3	K	367	LYS	N-CA-CB	5.70	120.85	110.60
1	I	183	ASP	CB-CG-OD1	-5.69	113.17	118.30
2	J	218	PHE	N-CA-C	-5.69	95.63	111.00
4	L	204	ASP	CB-CG-OD1	-5.69	113.18	118.30
5	M	355	PHE	CB-CG-CD1	-5.69	116.81	120.80
4	D	204	ASP	CB-CG-OD2	-5.69	113.18	118.30
3	C	433	GLU	OE1-CD-OE2	5.68	130.12	123.30
6	F	153	ARG	N-CA-CB	5.68	120.83	110.60
7	O	251	ASP	N-CA-CB	5.68	120.83	110.60
7	O	467	ARG	NE-CZ-NH2	-5.68	117.46	120.30
5	M	231	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	I	459	ASP	O-C-N	5.68	131.79	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	391	ARG	NE-CZ-NH2	-5.68	117.46	120.30
3	K	360	PHE	CB-CG-CD2	-5.67	116.83	120.80
7	G	263	TYR	CG-CD2-CE2	-5.67	116.76	121.30
8	P	351	TYR	CB-CG-CD2	5.67	124.40	121.00
6	F	165	ALA	CB-CA-C	-5.67	101.60	110.10
8	H	104	VAL	CB-CA-C	-5.66	100.64	111.40
5	M	345	PHE	CB-CG-CD2	-5.66	116.84	120.80
1	I	337	GLU	OE1-CD-OE2	5.66	130.09	123.30
7	G	419	TYR	CG-CD1-CE1	-5.66	116.77	121.30
4	D	454	PHE	CB-CG-CD1	5.66	124.76	120.80
8	P	68	ASP	CB-CG-OD2	-5.65	113.21	118.30
2	B	150	SER	N-CA-CB	-5.65	102.03	110.50
2	B	440	ALA	CB-CA-C	-5.65	101.63	110.10
3	K	374	ILE	CB-CA-C	5.65	122.90	111.60
4	D	335	PHE	CB-CG-CD2	5.65	124.75	120.80
8	H	450	ARG	NE-CZ-NH1	5.64	123.12	120.30
5	M	334	ALA	CB-CA-C	-5.64	101.64	110.10
3	C	117	MET	N-CA-CB	5.64	120.75	110.60
5	E	446	TYR	CG-CD1-CE1	-5.64	116.79	121.30
3	K	145	ASP	CB-CG-OD1	5.64	123.37	118.30
4	L	483	ARG	NH1-CZ-NH2	-5.63	113.20	119.40
6	N	32	ASP	CB-CG-OD1	5.63	123.37	118.30
8	H	258	LEU	N-CA-C	-5.63	95.80	111.00
7	O	252	ASN	C-N-CA	5.63	135.77	121.70
3	C	150	ASP	CB-CG-OD2	-5.63	113.24	118.30
7	O	205	LEU	CB-CG-CD1	5.63	120.56	111.00
7	G	303	PHE	CB-CG-CD1	-5.62	116.86	120.80
8	H	85	MET	CG-SD-CE	5.62	109.20	100.20
3	C	190	ARG	NE-CZ-NH2	5.62	123.11	120.30
5	E	97	SER	CB-CA-C	-5.62	99.43	110.10
2	J	177	ASP	CB-CG-OD2	-5.62	113.24	118.30
7	G	267	VAL	CA-CB-CG1	-5.61	102.48	110.90
2	J	121	ILE	N-CA-C	-5.61	95.84	111.00
1	A	23	MET	CB-CG-SD	5.61	129.24	112.40
2	J	363	SER	N-CA-CB	5.61	118.92	110.50
5	E	324	TRP	N-CA-CB	5.61	120.69	110.60
3	C	98	VAL	CA-CB-CG1	-5.61	102.49	110.90
2	B	145	ALA	N-CA-CB	5.60	117.94	110.10
6	F	392	ARG	NH1-CZ-NH2	-5.60	113.24	119.40
3	K	362	PHE	CZ-CE2-CD2	-5.60	113.38	120.10
5	M	142	ARG	CB-CA-C	-5.60	99.21	110.40
5	M	531	ASP	CB-CG-OD2	-5.60	113.26	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	112	PHE	CB-CG-CD1	-5.59	116.88	120.80
7	G	194	MET	CB-CA-C	-5.59	99.22	110.40
4	L	270	ALA	N-CA-CB	5.59	117.93	110.10
7	O	176	ALA	CB-CA-C	-5.59	101.72	110.10
6	N	317	LYS	O-C-N	-5.59	113.76	122.70
7	G	302	TYR	CB-CG-CD1	5.58	124.35	121.00
3	C	46	MET	N-CA-CB	5.58	120.64	110.60
3	K	231	ARG	CG-CD-NE	-5.58	100.09	111.80
7	G	313	ARG	CD-NE-CZ	-5.58	115.80	123.60
3	K	93	ASP	CB-CG-OD2	-5.57	113.28	118.30
5	E	73	ASP	N-CA-CB	5.57	120.63	110.60
4	L	60	MET	N-CA-C	-5.57	95.96	111.00
5	M	222	THR	CA-CB-CG2	-5.57	104.60	112.40
5	M	301	ILE	CA-CB-CG2	-5.57	99.76	110.90
5	E	446	TYR	CZ-CE2-CD2	5.57	124.81	119.80
1	I	329	SER	N-CA-CB	5.57	118.85	110.50
7	G	438	TYR	CG-CD2-CE2	-5.56	116.85	121.30
1	I	131	TYR	CZ-CE2-CD2	5.56	124.81	119.80
8	H	522	ASP	CB-CG-OD1	5.56	123.31	118.30
7	G	381	PHE	CB-CG-CD1	-5.56	116.91	120.80
8	P	74	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	190	TYR	CB-CG-CD2	5.55	124.33	121.00
4	D	423	ALA	N-CA-CB	5.55	117.87	110.10
8	P	125	VAL	CA-CB-CG1	5.55	119.23	110.90
6	N	179	ILE	CA-CB-CG2	-5.54	99.81	110.90
3	C	468	ALA	N-CA-CB	5.54	117.86	110.10
2	J	433	ALA	N-CA-CB	5.54	117.86	110.10
8	H	22	PHE	CB-CG-CD1	-5.54	116.92	120.80
6	F	523	ARG	NE-CZ-NH1	-5.54	117.53	120.30
7	G	485	ALA	N-CA-CB	5.54	117.85	110.10
2	J	120	LYS	N-CA-CB	5.54	120.56	110.60
3	C	496	TRP	CE3-CZ3-CH2	-5.53	115.11	121.20
3	C	501	VAL	CA-CB-CG2	-5.53	102.60	110.90
2	J	405	ARG	NE-CZ-NH2	5.53	123.07	120.30
5	M	273	ASP	CB-CG-OD1	5.53	123.28	118.30
2	B	332	ALA	CB-CA-C	-5.53	101.81	110.10
2	B	444	ARG	NE-CZ-NH1	-5.53	117.54	120.30
5	M	329	GLU	CB-CG-CD	-5.53	99.27	114.20
8	P	376	VAL	CG1-CB-CG2	5.53	119.75	110.90
8	H	424	THR	CA-CB-CG2	-5.53	104.66	112.40
5	E	451	PHE	O-C-N	-5.52	113.86	122.70
4	L	167	ALA	N-CA-CB	5.52	117.83	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	281	ASP	CB-CG-OD1	-5.52	113.33	118.30
5	M	68	VAL	CG1-CB-CG2	-5.52	102.07	110.90
7	G	260	VAL	CA-CB-CG2	5.51	119.17	110.90
1	I	468	ARG	NE-CZ-NH1	5.51	123.06	120.30
3	K	185	PHE	N-CA-C	-5.51	96.11	111.00
4	L	167	ALA	CB-CA-C	-5.51	101.83	110.10
8	P	314	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	I	443	ARG	NE-CZ-NH2	-5.51	117.55	120.30
2	J	213	TYR	CB-CG-CD2	5.51	124.31	121.00
3	C	330	ARG	NE-CZ-NH2	-5.51	117.55	120.30
4	D	157	LEU	CB-CG-CD1	-5.51	101.64	111.00
5	E	48	MET	CG-SD-CE	-5.50	91.39	100.20
1	A	433	ARG	NE-CZ-NH2	5.50	123.05	120.30
3	C	231	ARG	NE-CZ-NH1	-5.50	117.55	120.30
8	H	443	GLU	O-C-N	-5.50	113.90	122.70
1	I	355	ARG	NE-CZ-NH1	5.50	123.05	120.30
4	D	273	ASP	CB-CG-OD2	-5.50	113.35	118.30
8	H	353	SER	N-CA-CB	5.50	118.75	110.50
4	L	314	LEU	CB-CA-C	-5.50	99.75	110.20
4	L	57	MET	N-CA-CB	5.49	120.49	110.60
5	M	233	ASP	CB-CG-OD2	-5.49	113.36	118.30
8	P	517	THR	CA-CB-CG2	5.49	120.09	112.40
5	M	181	CYS	N-CA-CB	5.49	120.49	110.60
6	F	466	ILE	O-C-N	5.49	131.48	122.70
5	M	520	ALA	CB-CA-C	-5.49	101.87	110.10
6	N	294	GLN	CG-CD-OE1	5.49	132.58	121.60
8	P	158	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	A	427	ALA	CB-CA-C	-5.49	101.87	110.10
6	F	190	MET	CG-SD-CE	-5.49	91.42	100.20
6	F	525	GLY	CA-C-O	-5.49	110.72	120.60
4	D	41	ALA	N-CA-CB	5.48	117.78	110.10
4	D	501	SER	N-CA-CB	5.48	118.72	110.50
1	A	318	ARG	NE-CZ-NH1	5.48	123.04	120.30
2	B	213	TYR	CB-CG-CD2	5.48	124.29	121.00
7	O	478	ASP	CB-CG-OD2	5.48	123.23	118.30
5	E	364	PHE	CB-CG-CD1	5.48	124.63	120.80
2	J	269	HIS	N-CA-CB	5.48	120.46	110.60
5	E	366	THR	CA-CB-CG2	-5.47	104.74	112.40
4	L	49	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	A	422	TYR	CG-CD2-CE2	-5.46	116.93	121.30
3	K	343	VAL	N-CA-C	-5.46	96.25	111.00
3	C	270	MET	CG-SD-CE	5.46	108.94	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	448	SER	N-CA-CB	5.46	118.69	110.50
3	C	356	GLY	N-CA-C	-5.46	99.45	113.10
7	O	303	PHE	O-C-N	-5.46	113.96	122.70
6	F	282	CYS	N-CA-CB	5.46	120.42	110.60
1	I	290	GLY	C-N-CA	5.46	133.76	122.30
6	N	53	ASP	CB-CG-OD2	5.45	123.21	118.30
8	P	281	LYS	CB-CA-C	-5.45	99.49	110.40
1	I	392	LEU	CB-CG-CD1	-5.45	101.74	111.00
2	B	393	ALA	N-CA-CB	5.45	117.73	110.10
3	K	508	THR	CA-CB-CG2	-5.45	104.77	112.40
6	F	496	ASP	N-CA-CB	5.45	120.41	110.60
1	A	426	TYR	CB-CG-CD1	5.45	124.27	121.00
5	M	386	PHE	CB-CG-CD2	-5.45	116.99	120.80
5	M	534	ARG	N-CA-C	-5.45	96.30	111.00
6	N	338	ASP	CB-CA-C	-5.44	99.51	110.40
2	B	428	THR	CA-CB-CG2	-5.44	104.78	112.40
4	D	457	ALA	N-CA-CB	5.44	117.72	110.10
4	D	379	CYS	N-CA-CB	5.44	120.39	110.60
1	I	440	GLU	OE1-CD-OE2	-5.44	116.77	123.30
8	P	196	HIS	N-CA-CB	5.44	120.39	110.60
7	G	399	ALA	CB-CA-C	-5.44	101.94	110.10
6	F	112	GLU	OE1-CD-OE2	5.44	129.82	123.30
8	P	453	ALA	CB-CA-C	-5.44	101.94	110.10
5	E	178	VAL	CG1-CB-CG2	5.43	119.60	110.90
5	M	99	ASP	CB-CG-OD2	5.43	123.19	118.30
6	N	312	ALA	N-CA-CB	5.43	117.71	110.10
8	P	147	VAL	CA-CB-CG2	-5.43	102.75	110.90
1	A	288	THR	CA-CB-CG2	-5.43	104.80	112.40
8	H	332	ALA	N-CA-CB	5.43	117.70	110.10
2	J	310	MET	CG-SD-CE	-5.43	91.51	100.20
2	J	359	LEU	N-CA-CB	5.43	121.26	110.40
4	L	220	ASP	CB-CG-OD2	-5.43	113.41	118.30
8	H	74	ARG	NE-CZ-NH1	5.43	123.01	120.30
7	G	127	THR	CA-CB-CG2	-5.42	104.81	112.40
1	I	393	HIS	N-CA-CB	5.42	120.36	110.60
2	B	496	SER	CA-C-N	-5.42	105.28	117.20
2	J	469	HIS	CA-CB-CG	5.42	122.81	113.60
4	D	260	MET	CG-SD-CE	-5.41	91.54	100.20
4	L	269	TYR	CG-CD1-CE1	5.41	125.63	121.30
6	F	498	TYR	CB-CG-CD2	-5.41	117.75	121.00
6	F	147	THR	O-C-N	-5.41	114.05	122.70
2	J	497	PHE	CB-CG-CD1	-5.41	117.01	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	131	TYR	C-N-CA	5.41	135.21	121.70
6	N	333	LEU	N-CA-C	-5.41	96.40	111.00
8	P	118	LEU	CB-CG-CD2	5.40	120.19	111.00
1	A	387	GLU	O-C-N	-5.40	114.06	122.70
1	I	117	VAL	CA-CB-CG2	-5.40	102.81	110.90
1	I	200	ALA	N-CA-CB	5.39	117.65	110.10
1	A	219	VAL	CA-CB-CG2	5.39	118.98	110.90
6	F	150	ASP	CB-CG-OD1	-5.39	113.45	118.30
7	G	141	VAL	CA-CB-CG2	-5.39	102.82	110.90
4	D	464	THR	N-CA-CB	5.39	120.54	110.30
6	N	347	ALA	N-CA-CB	5.39	117.64	110.10
2	J	296	ILE	N-CA-C	-5.38	96.46	111.00
7	O	160	MET	CA-CB-CG	5.38	122.45	113.30
3	C	368	ASP	N-CA-CB	5.38	120.28	110.60
6	F	396	ARG	NE-CZ-NH1	5.38	122.99	120.30
3	K	100	ILE	CA-CB-CG2	-5.38	100.15	110.90
3	K	194	ASP	CB-CG-OD1	5.38	123.14	118.30
4	L	408	ALA	CB-CA-C	-5.38	102.04	110.10
2	J	322	ARG	NE-CZ-NH1	-5.37	117.61	120.30
6	F	208	ARG	CD-NE-CZ	5.37	131.12	123.60
8	H	132	TYR	CG-CD2-CE2	-5.37	117.00	121.30
6	F	196	MET	CA-CB-CG	5.37	122.43	113.30
6	F	68	GLN	CG-CD-OE1	-5.37	110.86	121.60
7	G	104	PHE	CB-CG-CD1	5.37	124.56	120.80
8	H	96	GLU	OE1-CD-OE2	5.37	129.74	123.30
1	I	350	GLU	N-CA-CB	5.37	120.26	110.60
4	D	137	PHE	CB-CG-CD2	-5.37	117.05	120.80
5	M	162	THR	CA-CB-CG2	-5.36	104.89	112.40
3	K	294	LYS	CB-CA-C	-5.36	99.68	110.40
2	J	384	ASP	CB-CG-OD2	-5.36	113.47	118.30
3	C	359	TYR	CB-CG-CD1	5.36	124.22	121.00
3	K	523	VAL	N-CA-C	-5.36	96.53	111.00
8	P	378	ARG	NE-CZ-NH1	5.36	122.98	120.30
7	G	24	SER	N-CA-CB	5.36	118.53	110.50
6	N	231	LEU	N-CA-C	-5.36	96.54	111.00
7	O	99	LEU	CB-CG-CD2	5.36	120.11	111.00
3	K	434	GLN	CG-CD-OE1	5.35	132.31	121.60
2	B	28	SER	N-CA-CB	5.35	118.52	110.50
5	E	281	GLU	CB-CA-C	-5.35	99.70	110.40
1	A	194	SER	N-CA-CB	5.34	118.52	110.50
8	H	360	VAL	CA-CB-CG1	5.34	118.92	110.90
1	I	361	LEU	N-CA-CB	5.34	121.09	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	386	PHE	N-CA-CB	5.34	120.22	110.60
7	G	313	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	B	37	ASP	CB-CG-OD1	-5.34	113.49	118.30
7	G	108	VAL	CA-CB-CG1	5.34	118.91	110.90
1	I	501	ALA	O-C-N	-5.34	114.12	123.20
2	B	501	ARG	NE-CZ-NH2	-5.34	117.63	120.30
6	F	323	ARG	CD-NE-CZ	5.34	131.07	123.60
3	K	274	TYR	CG-CD1-CE1	-5.34	117.03	121.30
4	L	491	ALA	N-CA-CB	5.34	117.57	110.10
4	L	403	ARG	CD-NE-CZ	-5.33	116.13	123.60
1	A	23	MET	CG-SD-CE	-5.33	91.67	100.20
1	A	57	ASP	CB-CG-OD2	5.33	123.10	118.30
3	C	151	MET	CG-SD-CE	-5.33	91.67	100.20
8	H	351	TYR	CB-CG-CD2	-5.33	117.80	121.00
5	M	115	ALA	N-CA-CB	5.33	117.56	110.10
7	G	268	ASP	CB-CG-OD2	5.33	123.09	118.30
8	P	246	PHE	CB-CG-CD2	-5.33	117.07	120.80
4	L	153	ARG	NH1-CZ-NH2	-5.32	113.55	119.40
6	N	244	VAL	CA-CB-CG2	5.32	118.88	110.90
8	P	207	ILE	C-N-CA	5.32	135.01	121.70
3	C	371	ALA	N-CA-CB	5.32	117.55	110.10
4	D	335	PHE	CB-CG-CD1	-5.32	117.08	120.80
5	E	169	ALA	CB-CA-C	-5.32	102.12	110.10
5	M	75	ALA	CB-CA-C	-5.32	102.12	110.10
1	A	238	ASP	CB-CG-OD2	-5.32	113.52	118.30
4	D	481	ARG	NE-CZ-NH2	5.32	122.96	120.30
8	H	44	ARG	NE-CZ-NH1	5.32	122.96	120.30
8	H	361	VAL	CA-CB-CG1	5.32	118.87	110.90
6	N	12	GLU	N-CA-CB	5.31	120.17	110.60
6	N	271	VAL	CG1-CB-CG2	5.31	119.40	110.90
1	A	145	ARG	NE-CZ-NH2	-5.31	117.65	120.30
2	B	297	TYR	CB-CG-CD2	5.31	124.19	121.00
6	F	258	LYS	CB-CA-C	-5.31	99.78	110.40
1	I	505	GLU	N-CA-CB	5.31	120.16	110.60
2	B	405	ARG	NE-CZ-NH1	5.31	122.95	120.30
3	K	490	MET	CB-CA-C	-5.31	99.78	110.40
4	L	508	VAL	N-CA-C	-5.31	96.67	111.00
7	O	16	SER	N-CA-CB	5.31	118.46	110.50
5	E	254	PRO	N-CA-CB	5.31	109.67	103.30
7	G	303	PHE	CB-CG-CD2	5.31	124.51	120.80
1	I	467	LEU	CB-CG-CD2	-5.31	101.98	111.00
1	A	405	SER	N-CA-CB	5.30	118.45	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	118	HIS	N-CA-CB	5.30	120.14	110.60
2	B	156	ARG	CA-CB-CG	5.30	125.06	113.40
3	K	519	ILE	N-CA-CB	5.30	122.99	110.80
5	E	259	LYS	N-CA-C	-5.29	96.70	111.00
6	F	248	PHE	CB-CG-CD2	5.29	124.51	120.80
2	B	317	PHE	CD1-CG-CD2	5.29	125.18	118.30
4	L	488	GLU	CB-CA-C	5.29	120.98	110.40
5	M	477	VAL	O-C-N	-5.29	114.23	122.70
7	G	307	ASP	N-CA-CB	5.29	120.12	110.60
4	D	407	ASP	CA-CB-CG	-5.29	101.77	113.40
5	E	189	ALA	CB-CA-C	-5.29	102.17	110.10
6	F	325	THR	O-C-N	-5.29	114.24	122.70
5	M	342	VAL	N-CA-C	-5.29	96.72	111.00
6	N	372	VAL	CG1-CB-CG2	-5.29	102.44	110.90
8	P	203	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	462	ASP	CA-CB-CG	-5.29	101.77	113.40
8	P	246	PHE	CB-CG-CD1	5.29	124.50	120.80
3	K	383	ILE	CA-CB-CG1	-5.28	100.96	111.00
5	M	437	ALA	CB-CA-C	-5.28	102.18	110.10
7	G	92	ASP	CB-CG-OD1	-5.28	113.55	118.30
2	J	51	ILE	N-CA-C	-5.28	96.75	111.00
7	O	232	TYR	CG-CD2-CE2	-5.28	117.08	121.30
4	D	280	ARG	NH1-CZ-NH2	-5.27	113.60	119.40
8	H	401	VAL	C-N-CA	5.27	134.88	121.70
3	K	52	ASP	CB-CA-C	-5.27	99.86	110.40
1	A	396	LEU	CB-CA-C	-5.27	100.19	110.20
4	D	377	THR	CA-CB-CG2	-5.27	105.02	112.40
2	J	379	THR	N-CA-C	-5.27	96.77	111.00
3	C	478	TRP	CG-CD2-CE3	-5.27	129.16	133.90
4	L	196	ASP	CB-CG-OD2	5.27	123.04	118.30
2	B	362	PHE	CG-CD2-CE2	5.26	126.59	120.80
7	O	24	SER	N-CA-CB	5.26	118.39	110.50
4	D	514	VAL	N-CA-CB	5.26	123.07	111.50
5	E	323	ARG	NE-CZ-NH1	-5.26	117.67	120.30
7	G	205	LEU	N-CA-CB	5.26	120.92	110.40
8	H	156	ASP	CB-CG-OD1	-5.26	113.57	118.30
8	H	407	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	I	374	SER	N-CA-C	-5.26	96.80	111.00
4	L	90	MET	N-CA-CB	5.26	120.06	110.60
5	M	142	ARG	NE-CZ-NH2	-5.26	117.67	120.30
6	N	108	LEU	CB-CG-CD1	-5.26	102.06	111.00
2	B	456	TYR	CB-CG-CD2	-5.26	117.85	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	357	CYS	CA-C-O	-5.26	109.06	120.10
2	J	420	ALA	CB-CA-C	5.26	117.98	110.10
5	E	419	VAL	CA-CB-CG1	5.25	118.78	110.90
8	H	247	ASP	CB-CG-OD1	-5.25	113.57	118.30
2	J	518	ASP	CB-CA-C	-5.25	99.90	110.40
6	F	349	LEU	CB-CG-CD1	5.25	119.92	111.00
7	G	288	VAL	CA-CB-CG2	-5.24	103.04	110.90
4	D	136	SER	CB-CA-C	5.24	120.05	110.10
8	P	247	ASP	CB-CG-OD2	5.24	123.01	118.30
2	B	310	MET	CA-CB-CG	5.24	122.20	113.30
3	K	467	ARG	NE-CZ-NH2	-5.24	117.68	120.30
6	N	354	THR	N-CA-C	-5.24	96.87	111.00
8	P	339	PRO	O-C-N	5.24	131.08	122.70
1	I	439	ALA	N-CA-CB	5.23	117.43	110.10
3	K	219	MET	CA-CB-CG	5.23	122.19	113.30
3	C	178	ASP	CB-CG-OD1	5.23	123.01	118.30
3	C	359	TYR	CD1-CE1-CZ	5.23	124.51	119.80
8	H	311	MET	CA-CB-CG	5.23	122.19	113.30
5	M	27	ARG	NE-CZ-NH1	5.23	122.91	120.30
4	D	350	GLN	O-C-N	-5.22	114.34	122.70
6	F	300	PHE	CB-CG-CD1	-5.22	117.14	120.80
8	H	471	HIS	N-CA-CB	5.22	120.00	110.60
7	O	56	ALA	N-CA-CB	5.22	117.41	110.10
8	P	208	LEU	O-C-N	-5.22	114.33	123.20
4	D	240	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	529	ASP	CB-CG-OD2	5.21	122.99	118.30
4	D	270	ALA	CB-CA-C	-5.21	102.28	110.10
3	K	255	ASP	CB-CG-OD2	5.21	122.99	118.30
6	N	221	MET	CG-SD-CE	5.21	108.54	100.20
4	D	100	ILE	CA-CB-CG1	5.21	120.90	111.00
1	A	409	VAL	CA-CB-CG2	-5.21	103.09	110.90
4	D	381	SER	CB-CA-C	-5.21	100.20	110.10
7	G	392	ALA	CB-CA-C	-5.21	102.29	110.10
7	O	347	VAL	CA-CB-CG1	-5.21	103.09	110.90
4	D	420	ALA	CB-CA-C	5.21	117.91	110.10
7	O	450	CYS	CA-CB-SG	5.21	123.37	114.00
7	O	522	ASN	CA-CB-CG	-5.21	101.95	113.40
2	B	281	ARG	NE-CZ-NH2	-5.20	117.70	120.30
8	H	42	THR	CA-CB-CG2	-5.20	105.12	112.40
7	O	148	LYS	CB-CA-C	5.20	120.81	110.40
6	F	144	ASP	CB-CG-OD2	-5.20	113.62	118.30
2	B	161	ASN	N-CA-CB	5.20	119.96	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	426	SER	N-CA-CB	5.20	118.30	110.50
5	M	419	VAL	CG1-CB-CG2	5.20	119.22	110.90
8	P	436	TYR	CB-CG-CD2	5.20	124.12	121.00
8	H	332	ALA	N-CA-C	-5.20	96.97	111.00
3	K	477	THR	CA-CB-CG2	-5.20	105.13	112.40
5	M	245	ASP	CB-CG-OD1	-5.19	113.62	118.30
1	A	501	ALA	N-CA-CB	5.19	117.37	110.10
1	A	422	TYR	CZ-CE2-CD2	5.19	124.47	119.80
2	B	30	ILE	CA-CB-CG2	-5.19	100.53	110.90
2	J	466	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	57	ASP	N-CA-CB	5.18	119.93	110.60
6	F	336	PHE	CB-CG-CD1	-5.18	117.17	120.80
6	F	284	ASP	CB-CG-OD1	-5.18	113.64	118.30
4	L	315	HIS	N-CA-CB	5.18	119.92	110.60
2	B	117	ILE	N-CA-CB	-5.18	98.89	110.80
8	H	47	TYR	O-C-N	-5.18	114.40	123.20
2	J	28	SER	N-CA-CB	5.18	118.26	110.50
6	N	166	ASP	CB-CG-OD2	5.18	122.96	118.30
3	C	359	TYR	CG-CD1-CE1	-5.17	117.16	121.30
4	L	359	ALA	N-CA-CB	5.17	117.34	110.10
6	N	463	LEU	O-C-N	-5.17	114.42	122.70
7	G	318	ASP	CB-CG-OD1	5.17	122.95	118.30
1	I	130	ARG	NE-CZ-NH1	5.17	122.89	120.30
3	K	230	ARG	NH1-CZ-NH2	5.17	125.09	119.40
5	M	331	GLU	CB-CG-CD	-5.17	100.24	114.20
6	F	220	ASP	N-CA-CB	5.17	119.90	110.60
6	N	315	ARG	NE-CZ-NH2	-5.17	117.72	120.30
6	F	351	TYR	CD1-CG-CD2	5.17	123.58	117.90
4	L	352	THR	N-CA-CB	5.17	120.12	110.30
1	I	370	ARG	CB-CA-C	-5.16	100.07	110.40
3	K	232	TYR	CB-CG-CD1	5.16	124.10	121.00
3	K	314	ARG	NE-CZ-NH1	-5.16	117.72	120.30
2	B	213	TYR	CB-CG-CD1	-5.16	117.90	121.00
8	H	335	ARG	N-CA-CB	5.16	119.89	110.60
2	B	99	THR	CA-CB-CG2	-5.16	105.18	112.40
6	N	208	ARG	NE-CZ-NH1	5.16	122.88	120.30
3	K	198	TYR	CG-CD1-CE1	5.16	125.42	121.30
4	D	489	LYS	N-CA-CB	5.15	119.88	110.60
2	B	46	LYS	N-CA-CB	5.15	119.87	110.60
7	G	133	VAL	CA-CB-CG1	-5.15	103.17	110.90
7	G	318	ASP	CB-CA-C	-5.15	100.10	110.40
3	K	191	LYS	C-N-CA	5.15	134.58	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	216	ARG	CD-NE-CZ	-5.15	116.39	123.60
7	G	158	CYS	CB-CA-C	-5.15	100.11	110.40
4	D	47	ALA	CB-CA-C	-5.15	102.38	110.10
1	A	214	TYR	N-CA-CB	5.14	119.86	110.60
6	F	351	TYR	CG-CD1-CE1	-5.14	117.18	121.30
2	J	255	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	B	393	ALA	CB-CA-C	-5.14	102.39	110.10
6	F	236	SER	N-CA-CB	5.14	118.21	110.50
6	F	365	LYS	N-CA-CB	5.14	119.86	110.60
7	G	448	GLN	CB-CA-C	-5.14	100.11	110.40
3	K	269	GLN	CA-CB-CG	5.14	124.70	113.40
8	P	337	THR	N-CA-C	-5.14	97.12	111.00
2	J	273	GLU	OE1-CD-OE2	5.14	129.47	123.30
1	I	8	PHE	CB-CG-CD1	-5.13	117.21	120.80
7	O	166	LYS	N-CA-CB	5.13	119.84	110.60
8	H	246	PHE	CB-CG-CD2	5.13	124.39	120.80
2	J	221	ASP	N-CA-CB	5.13	119.84	110.60
3	K	32	THR	CA-CB-CG2	-5.13	105.22	112.40
6	F	446	ILE	CA-CB-CG1	5.13	120.75	111.00
7	O	377	GLY	N-CA-C	-5.13	100.28	113.10
8	H	308	TYR	CA-CB-CG	-5.13	103.66	113.40
3	K	50	LEU	CB-CG-CD1	5.13	119.72	111.00
6	N	477	VAL	CG1-CB-CG2	5.13	119.10	110.90
4	D	160	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	A	375	ILE	N-CA-C	-5.12	97.17	111.00
5	E	454	ALA	N-CA-CB	5.12	117.27	110.10
5	M	142	ARG	NE-CZ-NH1	5.12	122.86	120.30
2	J	374	VAL	CA-CB-CG2	-5.12	103.22	110.90
3	K	248	LYS	N-CA-CB	5.12	119.82	110.60
3	K	359	TYR	N-CA-C	-5.12	97.17	111.00
6	F	430	LYS	N-CA-CB	5.12	119.82	110.60
3	K	437	TYR	CA-CB-CG	5.12	123.12	113.40
4	L	427	ALA	N-CA-CB	5.12	117.27	110.10
4	L	36	SER	CB-CA-C	-5.12	100.38	110.10
4	L	222	GLU	O-C-N	5.12	130.89	122.70
2	B	216	GLU	CG-CD-OE2	5.12	128.53	118.30
4	L	321	LYS	N-CA-CB	5.11	119.80	110.60
1	A	105	ASP	CB-CG-OD2	5.11	122.90	118.30
3	C	308	ASN	N-CA-CB	5.11	119.79	110.60
8	H	240	ALA	N-CA-CB	5.11	117.25	110.10
1	I	88	ASP	N-CA-C	-5.11	97.21	111.00
7	G	263	TYR	CD1-CG-CD2	5.10	123.51	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	81	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	266	ARG	NE-CZ-NH2	5.10	122.85	120.30
6	N	324	LEU	N-CA-CB	5.09	120.59	110.40
2	B	185	GLU	OE1-CD-OE2	5.09	129.41	123.30
7	G	136	ILE	CG1-CB-CG2	-5.09	100.20	111.40
8	P	445	PHE	CB-CA-C	-5.09	100.22	110.40
1	A	282	GLY	N-CA-C	-5.09	100.38	113.10
4	L	121	THR	CA-CB-CG2	-5.09	105.28	112.40
6	F	28	ARG	NE-CZ-NH2	-5.09	117.76	120.30
5	M	400	ARG	NE-CZ-NH1	-5.09	117.76	120.30
8	P	53	ASN	CB-CA-C	-5.08	100.23	110.40
2	B	255	ARG	CA-CB-CG	5.08	124.58	113.40
2	B	357	ASP	CB-CG-OD2	5.08	122.87	118.30
2	B	408	TYR	CA-CB-CG	-5.08	103.74	113.40
2	J	189	ARG	CD-NE-CZ	-5.08	116.49	123.60
5	E	349	THR	N-CA-C	-5.07	97.30	111.00
6	F	266	PHE	CZ-CE2-CD2	5.07	126.19	120.10
8	P	172	GLN	CB-CG-CD	-5.07	98.41	111.60
2	B	172	LEU	N-CA-C	-5.07	97.31	111.00
7	G	311	ALA	N-CA-CB	5.07	117.20	110.10
1	A	496	ARG	NE-CZ-NH2	5.07	122.83	120.30
5	E	452	ALA	CB-CA-C	-5.07	102.50	110.10
5	M	386	PHE	CZ-CE2-CD2	-5.07	114.02	120.10
4	D	375	LYS	N-CA-C	-5.07	97.32	111.00
5	E	344	ARG	CB-CA-C	-5.07	100.27	110.40
7	O	125	PHE	N-CA-CB	5.07	119.72	110.60
8	P	489	VAL	N-CA-CB	5.07	122.64	111.50
4	D	293	THR	CA-CB-CG2	-5.06	105.31	112.40
8	P	193	ASP	CB-CA-C	-5.06	100.27	110.40
3	C	130	LEU	O-C-N	5.06	130.80	122.70
7	G	231	LYS	N-CA-CB	5.06	119.71	110.60
2	B	381	GLN	N-CA-CB	-5.06	101.50	110.60
6	F	389	ASP	CB-CG-OD2	5.06	122.85	118.30
8	H	450	ARG	NE-CZ-NH2	-5.06	117.77	120.30
8	P	278	ALA	N-CA-CB	5.06	117.18	110.10
3	C	435	TRP	CB-CG-CD1	5.06	133.57	127.00
3	C	122	VAL	CA-CB-CG1	-5.05	103.32	110.90
8	H	248	GLY	N-CA-C	-5.05	100.46	113.10
2	B	257	ARG	NE-CZ-NH2	-5.05	117.77	120.30
3	C	330	ARG	NE-CZ-NH1	5.05	122.83	120.30
5	E	298	ASN	CB-CA-C	-5.05	100.30	110.40
8	P	308	TYR	CD1-CE1-CZ	-5.05	115.25	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	351	GLU	CB-CA-C	-5.05	100.30	110.40
1	I	225	MET	CA-CB-CG	5.05	121.88	113.30
3	K	261	GLU	CB-CA-C	-5.05	100.30	110.40
1	A	243	LYS	N-CA-CB	5.05	119.69	110.60
3	K	340	GLU	OE1-CD-OE2	5.05	129.36	123.30
8	P	172	GLN	N-CA-CB	5.05	119.68	110.60
5	E	434	SER	N-CA-CB	5.04	118.07	110.50
5	E	369	ASP	CB-CG-OD2	-5.04	113.76	118.30
5	E	385	ILE	CA-CB-CG2	-5.04	100.81	110.90
6	F	226	GLU	O-C-N	5.04	130.77	122.70
1	I	448	ILE	CA-CB-CG1	-5.04	101.43	111.00
3	K	260	ARG	NE-CZ-NH1	5.04	122.82	120.30
4	L	431	GLU	C-N-CA	5.04	134.30	121.70
3	C	93	ASP	CB-CG-OD2	-5.04	113.77	118.30
5	E	164	PRO	N-CD-CG	5.04	110.75	103.20
4	D	451	VAL	CA-CB-CG2	-5.03	103.35	110.90
6	F	16	ALA	N-CA-CB	5.03	117.15	110.10
3	C	215	LEU	CB-CG-CD2	-5.03	102.45	111.00
7	G	474	TRP	CG-CD2-CE3	-5.03	129.37	133.90
2	J	451	ALA	CB-CA-C	-5.03	102.56	110.10
1	I	263	ILE	O-C-N	-5.03	114.66	122.70
5	M	264	HIS	CB-CA-C	-5.02	100.35	110.40
8	H	125	VAL	CA-CB-CG2	-5.02	103.37	110.90
3	C	296	ILE	CA-CB-CG2	5.02	120.94	110.90
7	G	133	VAL	CG1-CB-CG2	-5.02	102.87	110.90
4	D	506	GLU	OE1-CD-OE2	-5.02	117.28	123.30
8	H	39	LEU	CB-CA-C	-5.02	100.67	110.20
2	J	89	ARG	N-CA-CB	5.02	119.63	110.60
3	K	401	VAL	CA-CB-CG1	5.02	118.43	110.90
6	N	512	ALA	N-CA-CB	5.02	117.12	110.10
5	E	293	LYS	CD-CE-NZ	5.02	123.24	111.70
6	F	57	THR	O-C-N	-5.02	114.67	122.70
8	P	392	VAL	CA-CB-CG2	5.02	118.42	110.90
4	L	488	GLU	N-CA-CB	5.01	119.62	110.60
2	B	45	PRO	N-CD-CG	5.01	110.71	103.20
8	P	172	GLN	CB-CA-C	-5.01	100.38	110.40
4	D	226	GLY	O-C-N	-5.01	114.69	122.70
1	A	253	VAL	CG1-CB-CG2	5.00	118.91	110.90
3	C	234	LYS	N-CA-CB	5.00	119.61	110.60
7	G	466	ALA	CB-CA-C	-5.00	102.59	110.10
1	I	494	LYS	N-CA-CB	5.00	119.61	110.60
2	B	24	ALA	N-CA-CB	5.00	117.11	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	511	GLU	CB-CA-C	-5.00	100.39	110.40
1	I	358	ASP	CB-CG-OD2	5.00	122.80	118.30
5	M	410	ARG	NE-CZ-NH1	5.00	122.80	120.30
5	E	453	ASP	N-CA-CB	5.00	119.60	110.60
6	N	385	THR	CA-CB-CG2	-5.00	105.40	112.40

There are no chirality outliers.

All (141) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	ARG	Sidechain
1	A	242	GLN	Peptide
1	A	283	ALA	Peptide
1	A	443	ARG	Sidechain
2	B	122	HIS	Sidechain
2	B	179	PHE	Sidechain
2	B	213	TYR	Sidechain
2	B	299	TYR	Sidechain
2	B	335	PHE	Sidechain
2	B	405	ARG	Sidechain
2	B	456	TYR	Sidechain
2	B	501	ARG	Sidechain
2	B	89	ARG	Sidechain
3	C	112	PHE	Sidechain
3	C	126	TYR	Sidechain
3	C	243	SER	Peptide
3	C	274	TYR	Sidechain
3	C	303	TYR	Sidechain
3	C	325	ARG	Sidechain
3	C	367	LYS	Peptide
3	C	437	TYR	Sidechain
3	C	68	ARG	Sidechain
3	C	74	HIS	Sidechain
4	D	206	ARG	Sidechain
4	D	267	SER	Mainchain
4	D	435	ARG	Sidechain
4	D	452	ARG	Sidechain
4	D	481	ARG	Sidechain
4	D	49	ARG	Sidechain
4	D	527	ARG	Sidechain
5	E	202	ARG	Sidechain
5	E	400	ARG	Sidechain

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Mol	Chain	Res	Type	Group
5	E	440	CYS	Peptide
5	E	525	ARG	Sidechain
5	E	534	ARG	Sidechain
6	F	109	TYR	Sidechain
6	F	117	ARG	Sidechain
6	F	141	ARG	Sidechain
6	F	157	ARG	Sidechain
6	F	217	ARG	Sidechain
6	F	239	TYR	Peptide
6	F	250	TYR	Sidechain
6	F	256	ARG	Sidechain
6	F	266	PHE	Sidechain
6	F	353	TYR	Sidechain
6	F	396	ARG	Sidechain
6	F	57	THR	Mainchain
7	G	126	ARG	Sidechain
7	G	166	LYS	Peptide
7	G	167	LEU	Peptide
7	G	222	TYR	Sidechain
7	G	302	TYR	Sidechain
7	G	306	ARG	Sidechain
7	G	321	ARG	Sidechain
7	G	427	ILE	Peptide
7	G	43	ARG	Sidechain
7	G	447	ARG	Sidechain
7	G	465	ARG	Sidechain
8	H	165	ARG	Sidechain
8	H	223	PHE	Sidechain
8	H	252	GLU	Peptide
8	H	260	LYS	Peptide
8	H	304	TYR	Sidechain
8	H	314	ARG	Sidechain
8	H	335	ARG	Sidechain
8	H	404	ARG	Sidechain
8	H	468	TYR	Sidechain
1	I	11	ARG	Sidechain
1	I	111	LYS	Peptide
1	I	130	ARG	Sidechain
1	I	167	PHE	Sidechain
1	I	181	TYR	Sidechain
1	I	185	ARG	Sidechain
1	I	237	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	I	318	ARG	Sidechain
1	I	370	ARG	Sidechain
2	J	255	ARG	Sidechain
2	J	257	ARG	Sidechain
2	J	297	TYR	Sidechain
2	J	405	ARG	Sidechain
2	J	444	ARG	Sidechain
2	J	466	ARG	Sidechain
2	J	481	ARG	Sidechain
2	J	516	ARG	Sidechain
2	J	89	ARG	Sidechain
3	K	126	TYR	Sidechain
3	K	190	ARG	Peptide
3	K	230	ARG	Sidechain
3	K	231	ARG	Sidechain
3	K	241	LEU	Peptide
3	K	274	TYR	Sidechain
3	K	286	LYS	Peptide
3	K	313	ARG	Sidechain
3	K	377	ARG	Sidechain
3	K	399	ARG	Sidechain
3	K	437	TYR	Sidechain
3	K	506	TYR	Sidechain
3	K	518	ARG	Sidechain
3	K	85	ARG	Sidechain
4	L	306	ARG	Sidechain
4	L	419	ARG	Sidechain
5	M	126	ARG	Sidechain
5	M	147	HIS	Sidechain
5	M	262	THR	Peptide
5	M	264	HIS	Sidechain
5	M	306	PHE	Sidechain
5	M	410	ARG	Sidechain
5	M	414	ARG	Sidechain
5	M	449	ARG	Sidechain
6	N	217	ARG	Sidechain
6	N	235	VAL	Peptide
6	N	248	PHE	Sidechain
6	N	264	ARG	Sidechain
6	N	266	PHE	Sidechain
6	N	270	ARG	Sidechain
6	N	282	CYS	Peptide

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Mol	Chain	Res	Type	Group
6	N	314	ARG	Sidechain
6	N	323	ARG	Sidechain
6	N	470	HIS	Sidechain
7	O	256	ARG	Sidechain
7	O	257	VAL	Peptide
7	O	258	HIS	Peptide
7	O	302	TYR	Sidechain
7	O	357	ARG	Sidechain
7	O	397	ARG	Sidechain
7	O	398	ARG	Sidechain
7	O	419	TYR	Sidechain
7	O	427	ILE	Peptide
7	O	491	PHE	Sidechain
7	O	499	ARG	Sidechain
7	O	53	ARG	Sidechain
8	P	103	PHE	Sidechain
8	P	173	TYR	Sidechain
8	P	228	GLU	Peptide
8	P	304	TYR	Sidechain
8	P	314	ARG	Sidechain
8	P	322	ARG	Sidechain
8	P	378	ARG	Sidechain
8	P	426	TYR	Sidechain
8	P	472	GLN	Peptide
8	P	505	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	A	3956	0	4124	19	0
1	I	4056	0	4218	11	0
2	B	3829	0	3932	38	0
2	J	3823	0	3927	27	0
3	C	3956	0	4079	14	0
3	K	3985	0	4108	8	0
4	D	3832	0	4042	9	0
4	L	3873	0	4086	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	3974	0	4084	16	0
5	M	3974	0	4084	15	0
6	F	3945	0	4071	8	0
6	N	3940	0	4068	14	0
7	G	3936	0	4029	9	0
7	O	3947	0	4037	15	0
8	H	3892	0	3949	9	0
8	P	3884	0	3943	10	0
All	All	62802	0	64781	195	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 (195) 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)
2:B:429:PRO:CD	2:J:464:GLN:HA	1.60	1.30
2:B:429:PRO:CA	2:B:429:PRO:N	1.99	1.25
2:B:429:PRO:CD	2:B:429:PRO:N	2.05	1.20
2:B:429:PRO:CD	2:B:429:PRO:CG	2.19	1.19
2:B:429:PRO:CA	2:B:429:PRO:CB	2.23	1.15
2:B:429:PRO:CG	2:B:429:PRO:CB	2.26	1.13
2:B:429:PRO:N	2:J:464:GLN:HA	1.68	1.09
2:B:429:PRO:CB	2:J:464:GLN:CA	2.39	0.99
2:B:429:PRO:CA	2:J:464:GLN:CA	2.41	0.98
2:B:429:PRO:CD	2:J:464:GLN:CA	2.43	0.97
2:B:429:PRO:CG	2:J:464:GLN:CA	2.43	0.96
2:B:429:PRO:CA	2:J:464:GLN:N	2.32	0.92
2:B:429:PRO:CG	2:J:464:GLN:N	2.35	0.89
2:B:429:PRO:N	2:J:464:GLN:CA	2.38	0.86
2:B:429:PRO:CB	2:J:464:GLN:N	2.38	0.86
2:B:429:PRO:CD	2:J:464:GLN:N	2.39	0.86
2:B:429:PRO:N	2:J:464:GLN:N	2.29	0.81
2:B:429:PRO:CA	2:J:464:GLN:H	1.95	0.78
2:B:200:HIS:CE1	2:B:202:ILE:HD11	2.28	0.69
6:N:37:ASN:HD22	6:N:58:LYS:HG3	1.59	0.67
2:B:429:PRO:HD2	2:J:464:GLN:HA	1.74	0.67
2:B:429:PRO:CA	2:J:464:GLN:CB	2.73	0.66
5:E:204:VAL:HG12	5:E:413:ILE:HD11	1.77	0.65
2:B:419:HIS:CE1	2:B:470:SER:HA	2.33	0.63
8:P:410:PRO:HB3	8:P:493:LEU:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:ASN:HD21	2:B:331:ILE:HD11	1.64	0.61
6:N:198:HIS:CD2	6:N:199:LYS:H	2.18	0.61
2:B:429:PRO:CA	2:J:464:GLN:HB2	2.31	0.60
4:D:441:ARG:HE	5:M:431:LEU:HD23	1.66	0.59
8:H:129:ILE:HG23	8:H:516:VAL:HG13	1.83	0.59
5:M:225:ILE:HG22	5:M:227:GLY:H	1.68	0.59
6:F:198:HIS:CD2	6:F:199:LYS:H	2.20	0.59
3:C:297:SER:H	3:C:300:ALA:HB3	1.68	0.59
4:D:129:HIS:CD2	4:D:130:PRO:HD2	2.38	0.58
2:B:255:ARG:HE	2:B:255:ARG:H	1.50	0.58
7:G:202:GLY:H	7:G:377:GLY:HA2	1.69	0.57
3:K:330:ARG:HH22	3:K:338:LEU:HD13	1.70	0.57
3:C:47:MET:HG3	3:C:61:ASN:HD21	1.68	0.56
4:D:190:ALA:HB1	4:D:386:VAL:HG21	1.88	0.55
7:G:39:THR:HG21	7:G:62:GLY:H	1.71	0.55
2:B:429:PRO:CG	2:J:464:GLN:C	2.74	0.55
2:J:74:ILE:CD1	4:L:536:VAL:HG12	2.37	0.55
5:E:533:ILE:H	5:E:533:ILE:HD13	1.72	0.54
7:O:28:ALA:HB1	7:O:73:HIS:CD2	2.43	0.54
8:P:347:CYS:SG	8:P:365:HIS:CE1	3.01	0.54
5:E:204:VAL:HG22	5:E:205:ASP:N	2.22	0.54
4:L:332:ASP:O	4:L:336:ILE:HG22	2.07	0.54
6:N:70:GLN:O	6:N:71:HIS:CD2	2.60	0.54
5:E:85:HIS:CD2	5:E:86:GLN:H	2.26	0.54
2:B:429:PRO:HG2	2:J:464:GLN:C	2.29	0.53
2:B:275:MET:O	2:B:279:VAL:HG23	2.09	0.53
1:A:228:ARG:HH12	1:A:350:GLU:HB2	1.73	0.53
5:E:340:ARG:HE	5:E:352:LYS:HA	1.75	0.52
5:E:204:VAL:HG22	5:E:205:ASP:H	1.74	0.51
7:G:90:VAL:HG13	7:G:398:ARG:HD2	1.93	0.51
7:O:282:HIS:HA	7:O:286:ALA:HB3	1.91	0.51
8:P:331:THR:H	8:P:343:GLU:HA	1.75	0.51
3:C:137:LEU:HA	3:C:140:ILE:HG22	1.93	0.50
1:I:179:ILE:HG22	1:I:181:TYR:H	1.77	0.50
1:A:522:ILE:O	1:A:526:ARG:HG2	2.11	0.50
6:N:221:MET:SD	6:N:311:VAL:HG13	2.51	0.50
6:F:416:VAL:HG23	6:F:470:HIS:CE1	2.46	0.50
2:B:429:PRO:HB2	2:J:465:LEU:H	1.76	0.49
7:G:294:PRO:HB3	7:G:313:ARG:HE	1.77	0.49
2:B:429:PRO:CB	2:J:464:GLN:H	2.21	0.49
6:N:141:ARG:HH11	6:N:407:VAL:HG23	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LYS:H	3:C:335:PRO:HG2	1.77	0.49
4:D:461:ILE:H	4:D:461:ILE:HD12	1.78	0.49
3:K:57:ILE:HD13	6:N:76:LEU:HD23	1.95	0.49
4:L:374:LEU:HD11	4:L:376:ILE:HD11	1.95	0.49
8:H:43:THR:HA	8:H:46:ALA:HB3	1.95	0.49
2:B:145:ALA:HB1	2:B:405:ARG:HE	1.78	0.48
2:J:130:TRP:CH2	2:J:515:LEU:HD22	2.47	0.48
3:K:330:ARG:HD3	3:K:330:ARG:H	1.78	0.48
5:E:85:HIS:CG	5:E:86:GLN:H	2.30	0.48
1:I:242:GLN:HG2	1:I:245:LYS:H	1.78	0.48
4:L:299:LEU:HD21	4:L:374:LEU:HD22	1.96	0.48
5:M:349:THR:HG21	5:M:352:LYS:HG3	1.96	0.48
1:A:243:LYS:HG2	1:A:244:THR:H	1.79	0.48
2:B:414:GLU:HG2	2:B:446:LEU:HD23	1.96	0.48
1:I:219:VAL:HG13	1:I:310:ARG:HH11	1.79	0.48
7:O:168:ILE:H	7:O:168:ILE:HD13	1.79	0.48
2:B:429:PRO:C	2:J:464:GLN:HB2	2.33	0.48
3:C:127:ARG:HH21	3:C:514:VAL:HG11	1.79	0.47
1:A:382:ASP:H	3:C:190:ARG:HH11	1.61	0.47
1:A:382:ASP:H	3:C:190:ARG:NH1	2.11	0.47
5:E:131:ILE:HG21	7:G:451:ASP:O	2.15	0.47
5:M:522:GLN:OE1	7:O:378:ALA:HB2	2.15	0.47
8:P:448:ILE:HD12	8:P:448:ILE:H	1.79	0.47
1:A:328:LEU:HD12	1:A:331:LEU:HB2	1.96	0.47
1:I:132:ILE:HG12	1:I:415:VAL:HG21	1.96	0.47
5:M:356:ALA:HA	5:M:376:GLN:HE22	1.80	0.47
5:E:143:VAL:HG23	5:E:433:VAL:HG22	1.96	0.47
7:O:81:ASP:HA	7:O:84:LYS:HE3	1.97	0.47
2:B:162:ILE:HD13	2:B:496:SER:HB3	1.97	0.47
1:A:115:THR:HG22	1:A:526:ARG:HH12	1.80	0.47
5:E:232:LYS:HG3	5:E:322:VAL:HG22	1.96	0.47
1:I:267:GLU:HA	1:I:270:ILE:HG12	1.97	0.47
6:F:384:LEU:HD12	6:F:387:ILE:HD11	1.96	0.47
8:H:500:THR:HG23	8:H:503:GLY:H	1.80	0.46
6:N:198:HIS:CG	6:N:199:LYS:N	2.84	0.46
7:O:117:HIS:CE1	7:O:514:VAL:HG12	2.51	0.46
2:J:116:LEU:O	2:J:119:LYS:HB2	2.14	0.46
3:K:71:GLN:HE21	3:K:73:GLN:HE21	1.64	0.46
3:C:434:GLN:HE21	3:C:438:ARG:CZ	2.29	0.45
5:E:209:ILE:HB	5:E:406:LEU:HD23	1.98	0.45
7:O:378:ALA:H	7:O:381:PHE:HB3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:402:LEU:O	5:E:406:LEU:HD13	2.15	0.45
8:H:225:LYS:HG3	8:H:315:LEU:O	2.16	0.45
4:L:156:GLU:HG2	4:L:158:SER:H	1.82	0.45
7:O:119:GLN:HE22	7:O:515:SER:HA	1.82	0.45
8:P:163:LEU:HD23	8:P:408:LEU:HD11	1.98	0.45
5:E:102:ILE:HD12	5:E:512:GLY:HA2	1.99	0.45
3:K:304:LEU:HD12	3:K:311:ALA:HB2	1.98	0.45
3:C:188:ASN:HD21	3:C:192:GLU:HB2	1.82	0.44
8:P:365:HIS:O	8:P:366:GLU:HG3	2.18	0.44
5:M:34:LEU:HD13	5:M:124:LEU:HD22	2.00	0.44
1:I:203:ARG:HH12	1:I:356:ILE:HD11	1.82	0.44
2:B:68:ALA:HB2	2:B:99:THR:HG21	1.99	0.44
1:A:530:LEU:HD11	4:D:62:GLN:HE21	1.82	0.44
8:P:409:VAL:HG21	8:P:501:TYR:HA	2.00	0.44
2:B:282:ILE:HD13	2:B:290:PHE:CZ	2.52	0.44
7:O:17:GLN:HG2	7:O:18:GLY:H	1.83	0.44
1:A:190:TYR:HB2	1:A:403:LEU:HD22	2.00	0.43
8:H:218:LEU:HD11	8:H:362:VAL:HG13	1.99	0.43
8:P:283:ILE:HG22	8:P:288:ALA:HB2	1.98	0.43
2:J:100:THR:O	2:J:104:VAL:HG23	2.18	0.43
5:M:260:PRO:HG3	7:O:257:VAL:HG21	1.99	0.43
6:F:114:LEU:HD11	6:F:435:LEU:HD13	2.01	0.43
3:C:180:VAL:CG2	3:C:395:MET:HB2	2.48	0.43
8:H:218:LEU:HD22	8:H:218:LEU:HA	1.93	0.43
1:A:190:TYR:CB	1:A:403:LEU:HD22	2.49	0.43
3:C:235:ASN:HB3	3:C:236:PRO:HD3	2.01	0.43
5:M:427:ILE:HG21	5:M:478:ARG:HA	2.01	0.43
1:A:419:LEU:HB3	1:A:445:LEU:HD13	2.01	0.43
7:G:151:GLN:HE21	7:G:400:ILE:HD12	1.84	0.43
6:F:416:VAL:CG2	6:F:470:HIS:CE1	3.02	0.43
3:K:127:ARG:HH21	3:K:514:VAL:HG21	1.84	0.43
1:I:179:ILE:HA	1:I:370:ARG:HH22	1.84	0.42
4:L:100:ILE:HG23	4:L:206:ARG:HH12	1.84	0.42
4:D:348:ILE:H	4:D:348:ILE:HG12	1.63	0.42
6:F:95:ASN:O	6:F:99:ILE:HG13	2.19	0.42
5:M:136:GLY:O	5:M:448:MET:HG2	2.19	0.42
1:A:145:ARG:HG2	1:A:504:PHE:HB2	2.01	0.42
5:E:442:THR:HG23	5:E:443:LEU:H	1.84	0.42
5:E:78:LEU:HB3	5:E:92:VAL:HG22	2.02	0.42
7:O:406:VAL:HG13	7:O:496:ALA:HB2	2.01	0.42
1:A:410:PRO:HB3	1:A:498:ASN:HD21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:36:LEU:HB3	1:I:455:ASN:HD21	1.85	0.42
6:N:462:THR:HA	6:N:465:LYS:HE2	2.02	0.42
6:N:469:GLU:HB2	6:N:477:VAL:HG21	2.01	0.42
1:A:145:ARG:HG2	1:A:504:PHE:CB	2.49	0.42
8:H:186:ALA:HA	8:H:217:VAL:HG13	2.01	0.42
3:C:67:LEU:HB3	3:C:81:ILE:HG12	2.02	0.42
6:N:462:THR:HA	6:N:465:LYS:CE	2.50	0.42
5:M:116:LEU:HB3	5:M:137:TYR:CE2	2.55	0.41
5:M:344:ARG:CZ	7:O:298:VAL:HG11	2.51	0.41
3:C:113:LEU:HD22	3:C:118:HIS:CE1	2.55	0.41
6:F:69:ILE:HG22	8:H:19:ALA:H	1.85	0.41
5:M:193:VAL:O	5:M:197:ALA:HB3	2.20	0.41
3:C:430:THR:HG21	8:P:469:ALA:HA	2.03	0.41
2:J:203:LYS:HB3	2:J:383:LEU:HD13	2.02	0.41
6:N:197:LYS:HA	6:N:379:PRO:HA	2.02	0.41
6:N:96:VAL:O	6:N:99:ILE:HG12	2.20	0.41
1:A:172:VAL:O	1:A:176:VAL:HG23	2.20	0.41
1:A:236:CYS:H	1:A:327:ILE:HD11	1.86	0.41
4:D:90:MET:HB3	4:D:525:THR:HG23	2.03	0.41
5:M:253:CYS:HG	5:M:255:PHE:HE2	1.68	0.41
8:P:452:LEU:CD1	8:P:477:ASN:HD21	2.32	0.41
6:F:382:HIS:CD2	6:F:382:HIS:H	2.38	0.41
5:M:408:VAL:HG13	5:M:509:THR:HG22	2.03	0.41
1:A:456:ALA:CB	1:A:458:GLN:HG2	2.51	0.41
2:B:218:PHE:CD2	2:B:323:LEU:HD13	2.56	0.41
4:D:455:ALA:O	4:D:458:MET:HB2	2.21	0.41
5:E:362:ILE:HG13	5:E:373:VAL:HG21	2.02	0.41
3:K:69:GLU:O	3:K:70:ILE:HB	2.20	0.41
7:G:246:LEU:HG	7:G:247:LYS:HG2	2.03	0.41
1:I:483:LEU:HD23	1:I:483:LEU:HA	1.96	0.41
7:O:280:LYS:HD3	7:O:283:HIS:CE1	2.55	0.41
2:B:239:ILE:HG23	2:B:320:VAL:HG22	2.03	0.40
7:G:66:LEU:HD22	7:G:66:LEU:HA	1.99	0.40
1:I:192:VAL:HG22	1:I:400:LYS:HD3	2.03	0.40
4:L:348:ILE:HD12	4:L:348:ILE:HA	1.96	0.40
6:N:118:ILE:HD12	6:N:435:LEU:CD1	2.51	0.40
1:A:370:ARG:HH11	1:A:370:ARG:HD2	1.73	0.40
7:O:28:ALA:HB1	7:O:73:HIS:CG	2.56	0.40
8:H:498:LEU:HD13	8:H:498:LEU:HA	1.90	0.40
1:I:353:GLN:HG3	1:I:362:ILE:HG12	2.04	0.40
7:O:197:ILE:HB	7:O:386:GLU:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:406:HIS:CE1	4:D:410:CYS:SG	3.14	0.40
7:G:186:LEU:HD12	7:G:195:ILE:HD13	2.04	0.40
5:M:282:LYS:HG3	5:M:313:LEU:HD21	2.04	0.40
2:J:255:ARG:HE	2:J:270:ALA:HB1	1.86	0.40
3:K:379:ALA:H	3:K:383:ILE:HB	1.86	0.40
6:N:119:ILE:HG22	6:N:123:PHE:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	519/534 (97%)	461 (89%)	39 (8%)	19 (4%)	3	24
1	I	532/534 (100%)	474 (89%)	40 (8%)	18 (3%)	3	26
2	B	507/509 (100%)	473 (93%)	25 (5%)	9 (2%)	8	40
2	J	506/509 (99%)	464 (92%)	32 (6%)	10 (2%)	7	38
3	C	507/513 (99%)	465 (92%)	28 (6%)	14 (3%)	5	30
3	K	511/513 (100%)	462 (90%)	29 (6%)	20 (4%)	3	23
4	D	506/514 (98%)	470 (93%)	24 (5%)	12 (2%)	6	33
4	L	511/514 (99%)	458 (90%)	35 (7%)	18 (4%)	3	25
5	E	515/517 (100%)	461 (90%)	36 (7%)	18 (4%)	3	25
5	M	515/517 (100%)	480 (93%)	25 (5%)	10 (2%)	8	38
6	F	512/515 (99%)	474 (93%)	32 (6%)	6 (1%)	13	50
6	N	511/515 (99%)	483 (94%)	20 (4%)	8 (2%)	9	44
7	G	510/514 (99%)	464 (91%)	33 (6%)	13 (2%)	5	32
7	O	512/514 (100%)	471 (92%)	28 (6%)	13 (2%)	5	32
8	H	508/514 (99%)	466 (92%)	31 (6%)	11 (2%)	6	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	P	507/514 (99%)	463 (91%)	29 (6%)	15 (3%)	4	28
All	All	8189/8260 (99%)	7489 (92%)	486 (6%)	214 (3%)	8	31

All (214) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	ILE
1	A	486	ILE
2	B	172	LEU
2	B	250	LYS
2	B	429	PRO
3	C	164	ALA
3	C	371	ALA
4	D	234	SER
4	D	488	GLU
5	E	441	PRO
5	E	529	LYS
6	F	222	LYS
7	G	188	ASP
7	G	338	SER
8	H	58	ASN
8	H	481	ASP
1	I	49	ILE
1	I	369	ALA
2	J	120	LYS
2	J	222	LYS
2	J	226	VAL
3	K	75	PRO
3	K	241	LEU
3	K	242	ASP
4	L	321	LYS
4	L	325	ILE
4	L	420	ALA
4	L	488	GLU
4	L	506	GLU
6	N	423	ILE
7	O	188	ASP
7	O	189	LEU
7	O	258	HIS
8	P	431	PRO
8	P	523	GLN
1	A	140	THR

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Mol	Chain	Res	Type
1	A	147	CYS
1	A	159	LYS
1	A	231	ASN
1	A	332	ALA
1	A	475	GLN
2	B	120	LYS
2	B	224	ILE
2	B	247	ASP
3	C	117	MET
3	C	185	PHE
3	C	368	ASP
4	D	257	LYS
4	D	321	LYS
5	E	318	ASN
5	E	320	PRO
7	G	39	THR
8	H	47	TYR
1	I	239	PHE
1	I	332	ALA
1	I	370	ARG
1	I	479	GLU
2	J	259	ASP
2	J	378	ALA
3	K	197	LYS
3	K	249	LYS
4	L	203	VAL
4	L	237	GLY
5	M	178	VAL
5	M	318	ASN
5	M	488	ALA
6	N	38	LEU
6	N	179	ILE
6	N	250	TYR
6	N	430	LYS
7	O	149	VAL
7	O	430	LYS
8	P	232	THR
8	P	357	ASP
8	P	473	GLU
1	A	50	GLY
1	A	57	ASP
1	A	110	GLN

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Mol	Chain	Res	Type
1	A	224	GLY
1	A	334	LEU
2	B	191	LYS
3	C	235	ASN
3	C	288	ASP
3	C	365	ASP
3	C	370	LYS
4	D	177	SER
4	D	232	LYS
4	D	267	SER
4	D	327	ASP
5	E	154	SER
5	E	237	PRO
5	E	297	ALA
5	E	298	ASN
5	E	307	ASP
5	E	495	HIS
6	F	51	ALA
7	G	42	PRO
7	G	45	MET
7	G	258	HIS
7	G	285	GLY
7	G	471	GLY
7	G	473	THR
8	H	309	ASN
8	H	339	PRO
8	H	342	GLU
8	H	431	PRO
1	I	282	GLY
1	I	459	ASP
1	I	488	LEU
2	J	314	HIS
2	J	334	THR
3	K	71	GLN
3	K	90	GLU
3	K	117	MET
3	K	230	ARG
3	K	231	ARG
3	K	287	PRO
3	K	340	GLU
3	K	346	GLY
3	K	411	GLY

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Mol	Chain	Res	Type
3	K	457	ALA
4	L	235	ASN
4	L	243	LYS
4	L	306	ARG
4	L	351	PHE
4	L	385	THR
4	L	472	ASN
5	M	244	GLU
5	M	324	TRP
5	M	365	GLY
5	M	496	LYS
7	O	167	LEU
7	O	255	ILE
7	O	307	ASP
8	P	43	THR
8	P	99	ASP
8	P	210	SER
8	P	248	GLY
8	P	369	ASP
8	P	411	GLY
8	P	495	ALA
1	A	111	LYS
1	A	357	CYS
3	C	230	ARG
3	C	287	PRO
4	D	259	ASP
4	D	444	SER
5	E	202	ARG
5	E	324	TRP
5	E	539	SER
6	F	188	LEU
7	G	376	GLY
7	G	428	PRO
1	I	203	ARG
1	I	221	GLY
1	I	329	SER
1	I	366	ASN
4	L	52	LEU
4	L	177	SER
5	M	177	VAL
5	M	441	PRO
7	O	40	LEU

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Mol	Chain	Res	Type
7	O	473	THR
8	P	366	GLU
1	A	184	ILE
2	B	49	ASP
3	C	196	LYS
5	E	73	ASP
5	E	381	ARG
7	G	223	ALA
8	H	187	CYS
8	H	485	GLU
1	I	204	SER
2	J	246	THR
3	K	195	ILE
4	L	360	GLU
4	L	507	LEU
5	M	442	THR
7	O	148	LYS
7	O	225	PHE
7	O	254	GLU
8	P	229	GLY
8	P	372	ILE
1	A	223	GLN
1	A	255	THR
4	D	196	ASP
4	D	203	VAL
5	E	259	LYS
8	H	336	LEU
1	I	10	ASP
1	I	330	THR
2	J	199	ILE
2	J	472	GLY
3	K	43	PRO
4	L	73	ASP
6	N	53	ASP
6	N	411	ALA
6	F	160	VAL
1	I	290	GLY
2	B	493	ILE
7	G	168	ILE
3	K	205	PRO
3	C	286	LYS
5	E	258	PRO

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Mol	Chain	Res	Type
8	H	195	GLY
1	I	486	ILE
3	K	70	ILE
6	N	113	GLY
1	A	188	PRO
3	C	236	PRO
5	E	216	GLY
6	F	185	PRO
3	K	227	PRO
6	F	429	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	434/445 (98%)	423 (98%)	11 (2%)	47 68
1	I	445/445 (100%)	419 (94%)	26 (6%)	20 45
2	B	405/405 (100%)	390 (96%)	15 (4%)	34 58
2	J	405/405 (100%)	390 (96%)	15 (4%)	34 58
3	C	441/444 (99%)	425 (96%)	16 (4%)	35 59
3	K	444/444 (100%)	430 (97%)	14 (3%)	39 61
4	D	433/439 (99%)	422 (98%)	11 (2%)	47 68
4	L	438/439 (100%)	429 (98%)	9 (2%)	53 72
5	E	436/436 (100%)	419 (96%)	17 (4%)	32 56
5	M	436/436 (100%)	424 (97%)	12 (3%)	43 65
6	F	429/429 (100%)	410 (96%)	19 (4%)	28 53
6	N	429/429 (100%)	416 (97%)	13 (3%)	41 63
7	G	420/421 (100%)	408 (97%)	12 (3%)	42 64
7	O	421/421 (100%)	406 (96%)	15 (4%)	35 59
8	H	423/426 (99%)	410 (97%)	13 (3%)	40 62
8	P	422/426 (99%)	411 (97%)	11 (3%)	46 66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6861/6890 (100%)	6632 (97%)	229 (3%)	41 61

All (229) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	VAL
1	A	42	ASP
1	A	83	ASP
1	A	163	ILE
1	A	184	ILE
1	A	190	TYR
1	A	199	LYS
1	A	392	LEU
1	A	421	ILE
1	A	504	PHE
1	A	528	ASP
2	B	57	ARG
2	B	58	ASP
2	B	141	LEU
2	B	155	PHE
2	B	162	ILE
2	B	203	LYS
2	B	214	LEU
2	B	230	LYS
2	B	255	ARG
2	B	295	LEU
2	B	359	LEU
2	B	414	GLU
2	B	416	LEU
2	B	480	MET
2	B	518	ASP
3	C	57	ILE
3	C	99	ILE
3	C	167	ARG
3	C	194	ASP
3	C	214	VAL
3	C	220	ILE
3	C	221	ASN
3	C	256	ILE
3	C	285	LEU
3	C	303	TYR
3	C	313	ARG

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Mol	Chain	Res	Type
3	C	315	VAL
3	C	327	CYS
3	C	436	PRO
3	C	492	GLU
3	C	517	LEU
4	D	175	VAL
4	D	178	GLN
4	D	310	SER
4	D	312	LEU
4	D	316	PHE
4	D	325	ILE
4	D	351	PHE
4	D	390	VAL
4	D	449	TYR
4	D	472	ASN
4	D	477	VAL
5	E	38	ILE
5	E	96	LYS
5	E	124	LEU
5	E	262	THR
5	E	288	MET
5	E	306	PHE
5	E	307	ASP
5	E	312	HIS
5	E	364	PHE
5	E	379	ASN
5	E	441	PRO
5	E	442	THR
5	E	498	THR
5	E	501	MET
5	E	511	ILE
5	E	530	ILE
5	E	533	ILE
6	F	13	VAL
6	F	28	ARG
6	F	41	LYS
6	F	48	VAL
6	F	104	LYS
6	F	160	VAL
6	F	179	ILE
6	F	199	LYS
6	F	220	ASP

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Mol	Chain	Res	Type
6	F	230	ILE
6	F	235	VAL
6	F	314	ARG
6	F	331	VAL
6	F	368	ASN
6	F	391	VAL
6	F	458	ASP
6	F	459	LEU
6	F	494	VAL
6	F	521	ILE
7	G	66	LEU
7	G	121	ILE
7	G	129	THR
7	G	166	LYS
7	G	169	SER
7	G	192	LEU
7	G	278	LEU
7	G	297	ASP
7	G	358	TYR
7	G	440	LYS
7	G	475	TYR
7	G	507	SER
8	H	50	ASN
8	H	55	MET
8	H	97	VAL
8	H	190	ILE
8	H	218	LEU
8	H	251	THR
8	H	254	LYS
8	H	346	HIS
8	H	372	ILE
8	H	417	ILE
8	H	424	THR
8	H	449	PRO
8	H	498	LEU
1	I	20	GLN
1	I	55	THR
1	I	56	ASN
1	I	82	GLN
1	I	91	THR
1	I	101	LEU
1	I	105	ASP

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Mol	Chain	Res	Type
1	I	107	LEU
1	I	109	LYS
1	I	161	ILE
1	I	193	ASN
1	I	201	HIS
1	I	203	ARG
1	I	234	ILE
1	I	240	SER
1	I	256	ASP
1	I	264	ARG
1	I	306	MET
1	I	360	GLU
1	I	409	VAL
1	I	443	ARG
1	I	459	ASP
1	I	477	ASN
1	I	480	ARG
1	I	523	THR
1	I	529	ASP
2	J	39	VAL
2	J	50	LYS
2	J	76	VAL
2	J	77	ASP
2	J	99	THR
2	J	117	ILE
2	J	147	ASP
2	J	221	ASP
2	J	251	ILE
2	J	294	GLN
2	J	295	LEU
2	J	322	ARG
2	J	350	GLU
2	J	358	LYS
2	J	388	ARG
3	K	39	THR
3	K	91	VAL
3	K	135	SER
3	K	148	ASP
3	K	315	VAL
3	K	330	ARG
3	K	396	GLN
3	K	433	GLU

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Mol	Chain	Res	Type
3	K	436	PRO
3	K	453	GLN
3	K	487	LEU
3	K	488	VAL
3	K	519	ILE
3	K	520	ASP
4	L	139	LYS
4	L	178	GLN
4	L	192	MET
4	L	206	ARG
4	L	225	GLU
4	L	349	ASP
4	L	422	ILE
4	L	536	VAL
4	L	539	ARG
5	M	58	ASP
5	M	160	LYS
5	M	183	ARG
5	M	219	LEU
5	M	245	ASP
5	M	346	SER
5	M	392	LYS
5	M	404	ASP
5	M	410	ARG
5	M	428	SER
5	M	457	VAL
5	M	515	GLN
6	N	59	ASP
6	N	176	ILE
6	N	186	ILE
6	N	242	THR
6	N	279	ARG
6	N	301	SER
6	N	374	LEU
6	N	424	LYS
6	N	446	ILE
6	N	487	MET
6	N	501	LYS
6	N	511	ILE
6	N	520	GLU
7	O	97	VAL
7	O	147	ASP

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Mol	Chain	Res	Type
7	O	168	ILE
7	O	170	GLN
7	O	172	LYS
7	O	200	VAL
7	O	259	THR
7	O	283	HIS
7	O	344	ARG
7	O	371	THR
7	O	375	ARG
7	O	419	TYR
7	O	434	LEU
7	O	484	ILE
7	O	488	PHE
8	P	31	ARG
8	P	67	ASN
8	P	155	ARG
8	P	239	ILE
8	P	249	MET
8	P	374	THR
8	P	394	ASP
8	P	431	PRO
8	P	467	LEU
8	P	489	VAL
8	P	490	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	205	GLN
2	B	73	ASN
2	B	78	ASN
2	B	200	HIS
2	B	241	ASN
2	B	285	HIS
2	B	361	HIS
2	B	419	HIS
2	B	426	ASN
3	C	61	ASN
3	C	64	ASN
3	C	118	HIS
3	C	226	HIS

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Mol	Chain	Res	Type
3	C	434	GLN
4	D	32	GLN
4	D	62	GLN
4	D	138	GLN
4	D	178	GLN
4	D	366	ASN
4	D	406	HIS
4	D	494	ASN
5	E	46	ASN
5	E	55	ASN
5	E	85	HIS
5	E	236	HIS
5	E	411	ASN
6	F	198	HIS
6	F	320	ASN
6	F	382	HIS
6	F	438	GLN
6	F	503	GLN
7	G	30	GLN
7	G	151	GLN
7	G	191	GLN
7	G	282	HIS
7	G	468	HIS
8	H	346	HIS
8	H	365	HIS
8	H	435	GLN
1	I	196	ASN
1	I	333	ASN
1	I	435	GLN
1	I	455	ASN
2	J	91	GLN
2	J	361	HIS
2	J	391	HIS
3	K	64	ASN
3	K	73	GLN
3	K	184	GLN
3	K	221	ASN
3	K	302	HIS
3	K	470	HIS
4	L	129	HIS
4	L	301	GLN
4	L	484	HIS

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Mol	Chain	Res	Type
5	M	37	HIS
5	M	85	HIS
5	M	129	HIS
5	M	236	HIS
5	M	376	GLN
5	M	403	HIS
5	M	411	ASN
5	M	505	HIS
6	N	31	GLN
6	N	37	ASN
6	N	71	HIS
6	N	161	HIS
6	N	198	HIS
6	N	334	ASN
6	N	382	HIS
6	N	470	HIS
6	N	506	HIS
7	O	107	GLN
7	O	117	HIS
7	O	151	GLN
7	O	283	HIS
8	P	53	ASN
8	P	59	HIS
8	P	67	ASN
8	P	91	HIS
8	P	306	ASN
8	P	316	ASN
8	P	346	HIS
8	P	365	HIS
8	P	477	ASN

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 [i](#)

There are no chain breaks in this entry.

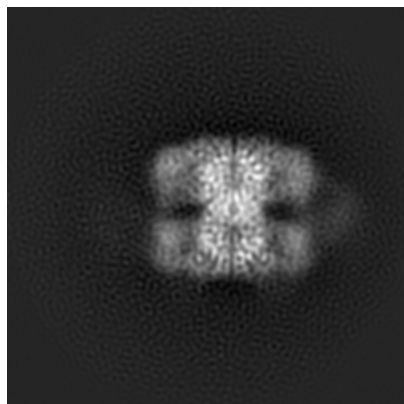
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0492. These allow visual inspection of the internal detail of the map and identification of artifacts.

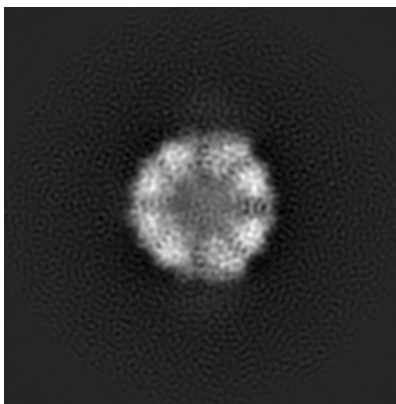
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

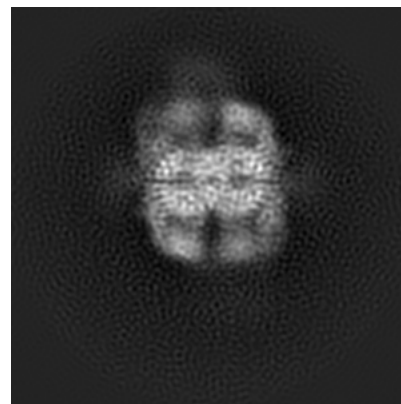
6.1.1 Primary map



X

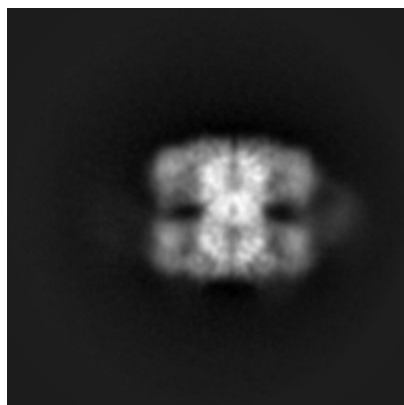


Y

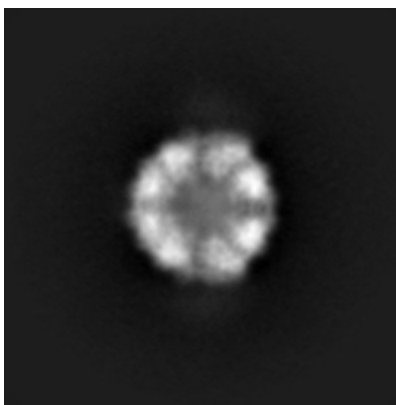


Z

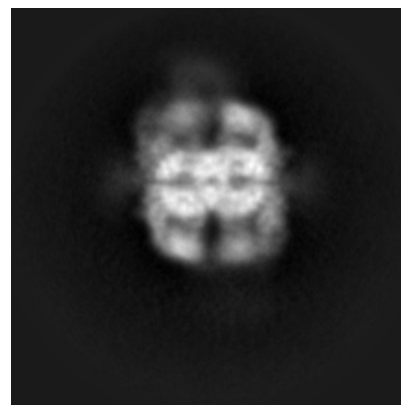
6.1.2 Raw map



X



Y

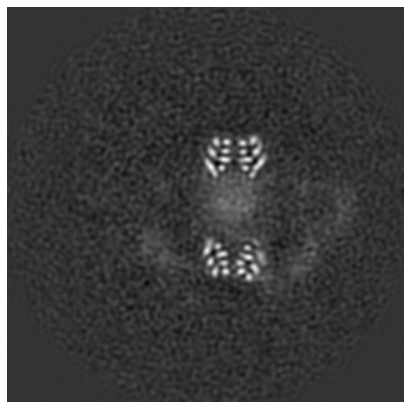


Z

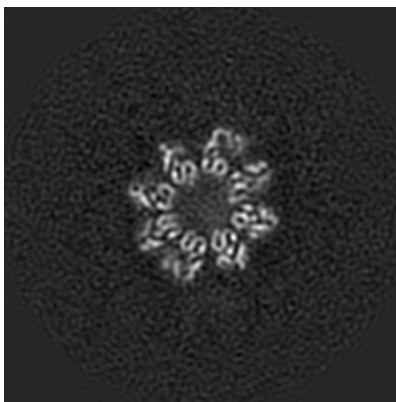
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

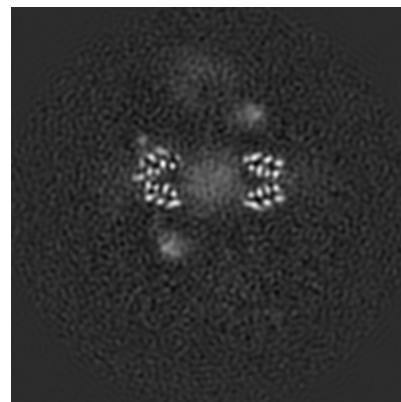
6.2.1 Primary map



X Index: 120

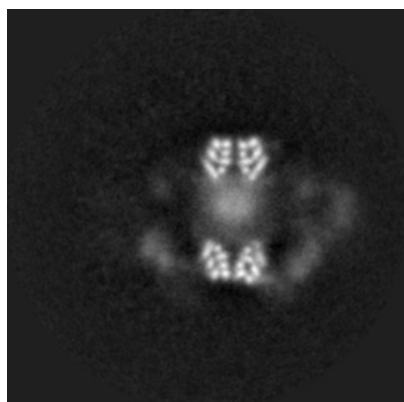


Y Index: 120

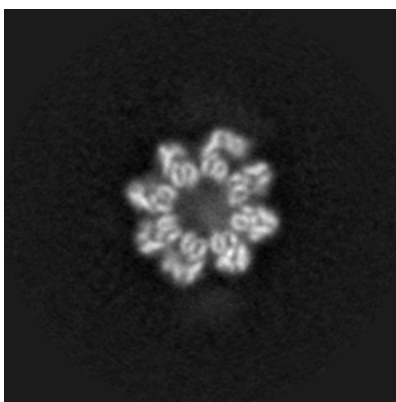


Z Index: 120

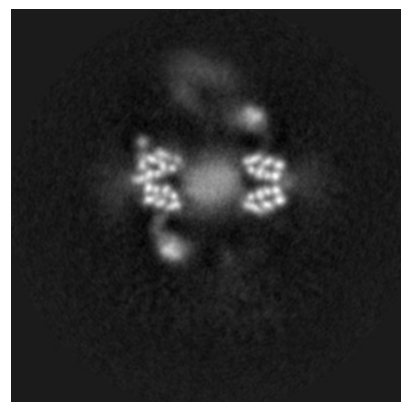
6.2.2 Raw map



X Index: 120



Y Index: 120

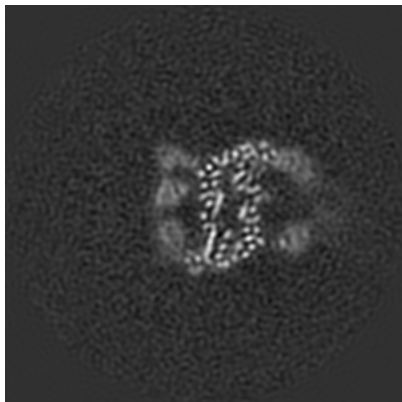


Z Index: 120

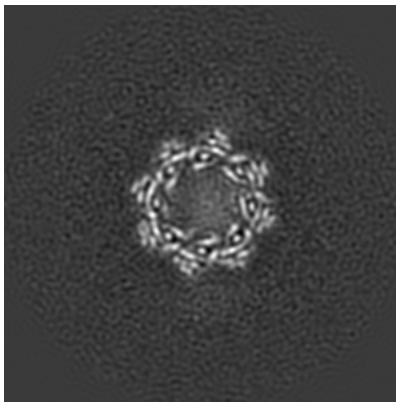
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

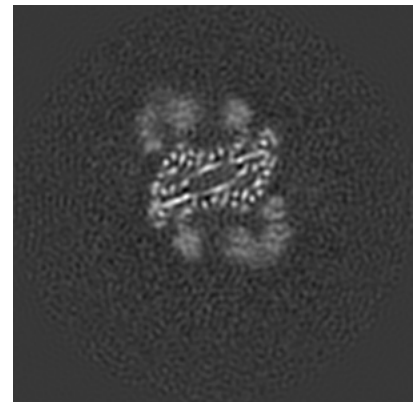
6.3.1 Primary map



X Index: 98

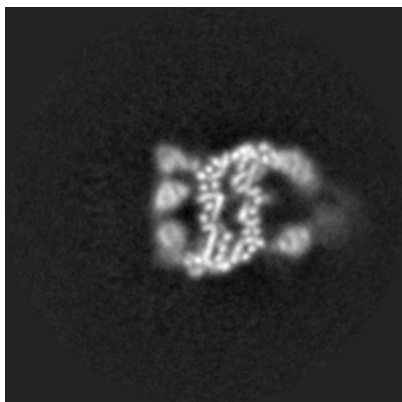


Y Index: 128

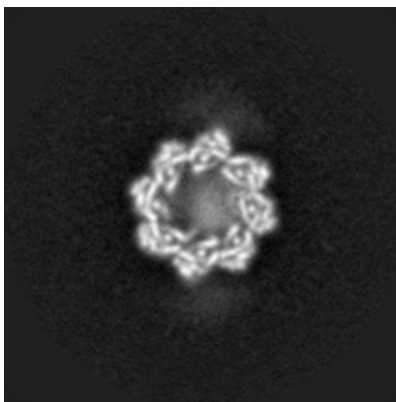


Z Index: 142

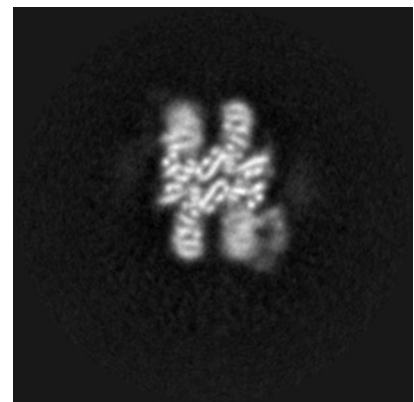
6.3.2 Raw map



X Index: 98



Y Index: 128

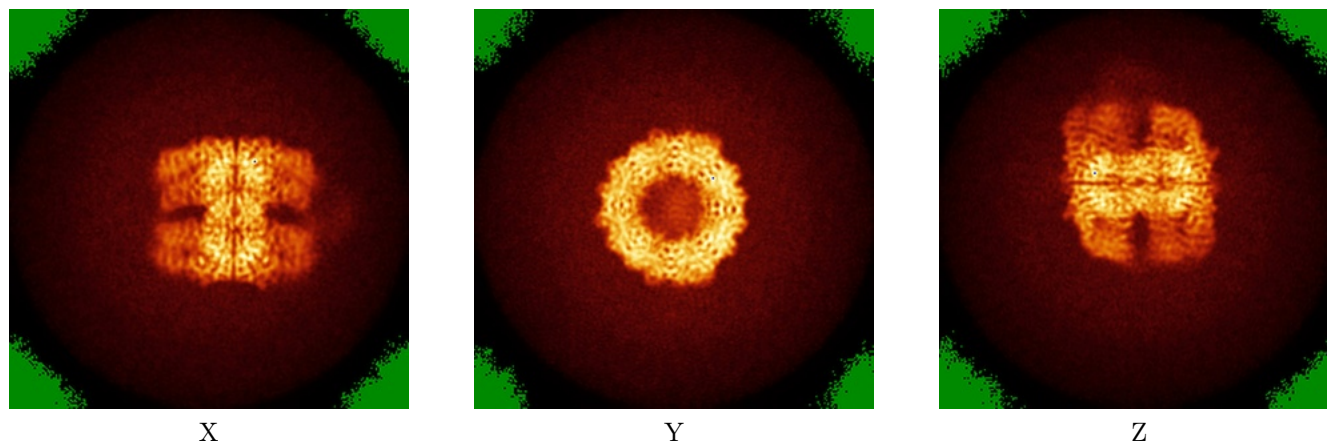


Z Index: 148

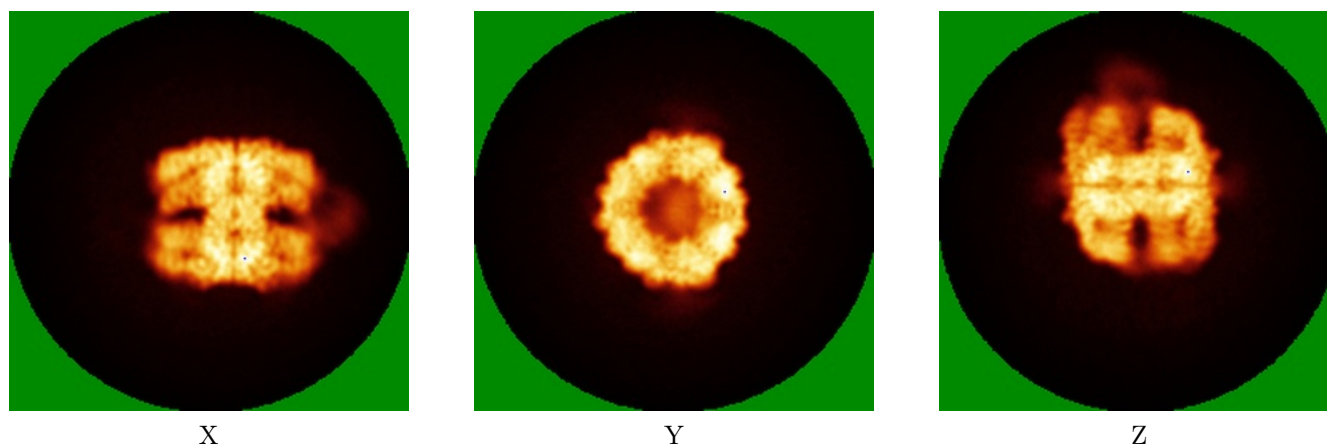
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



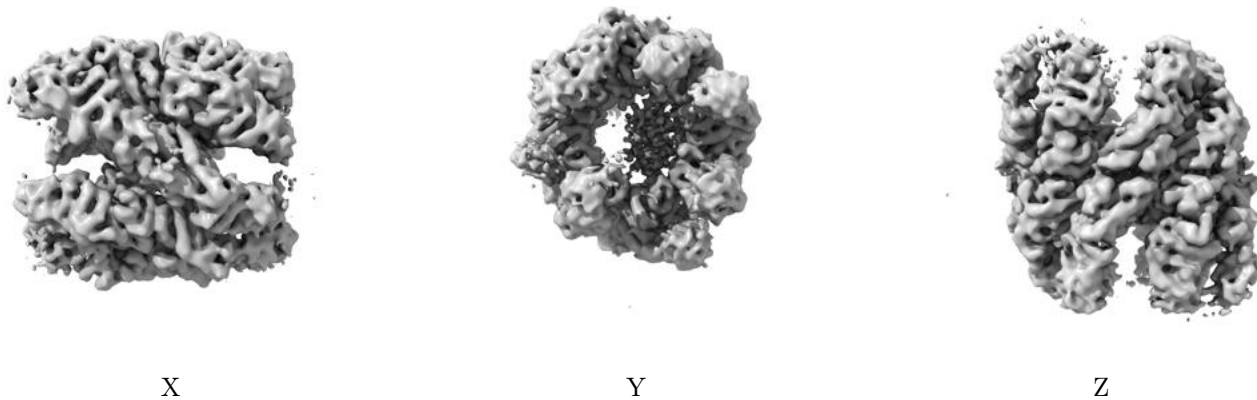
6.4.2 Raw map



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

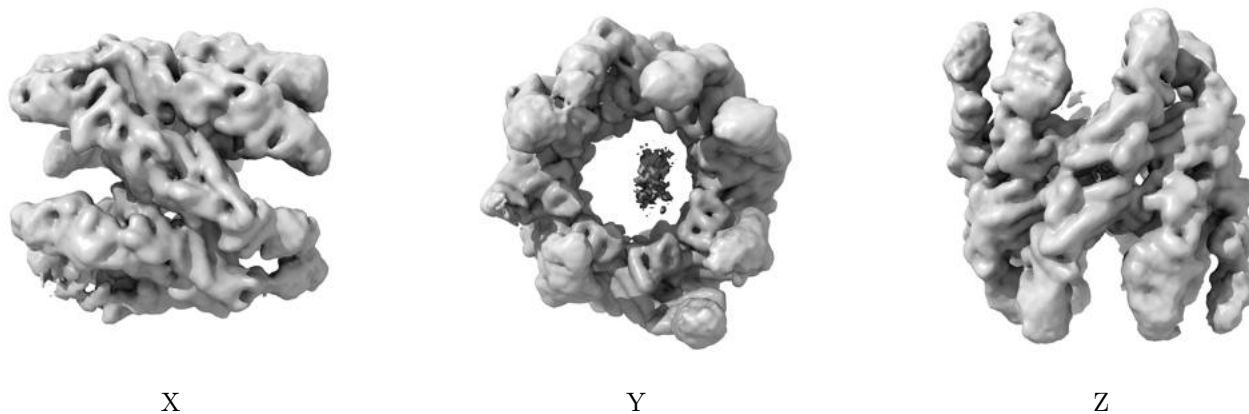
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

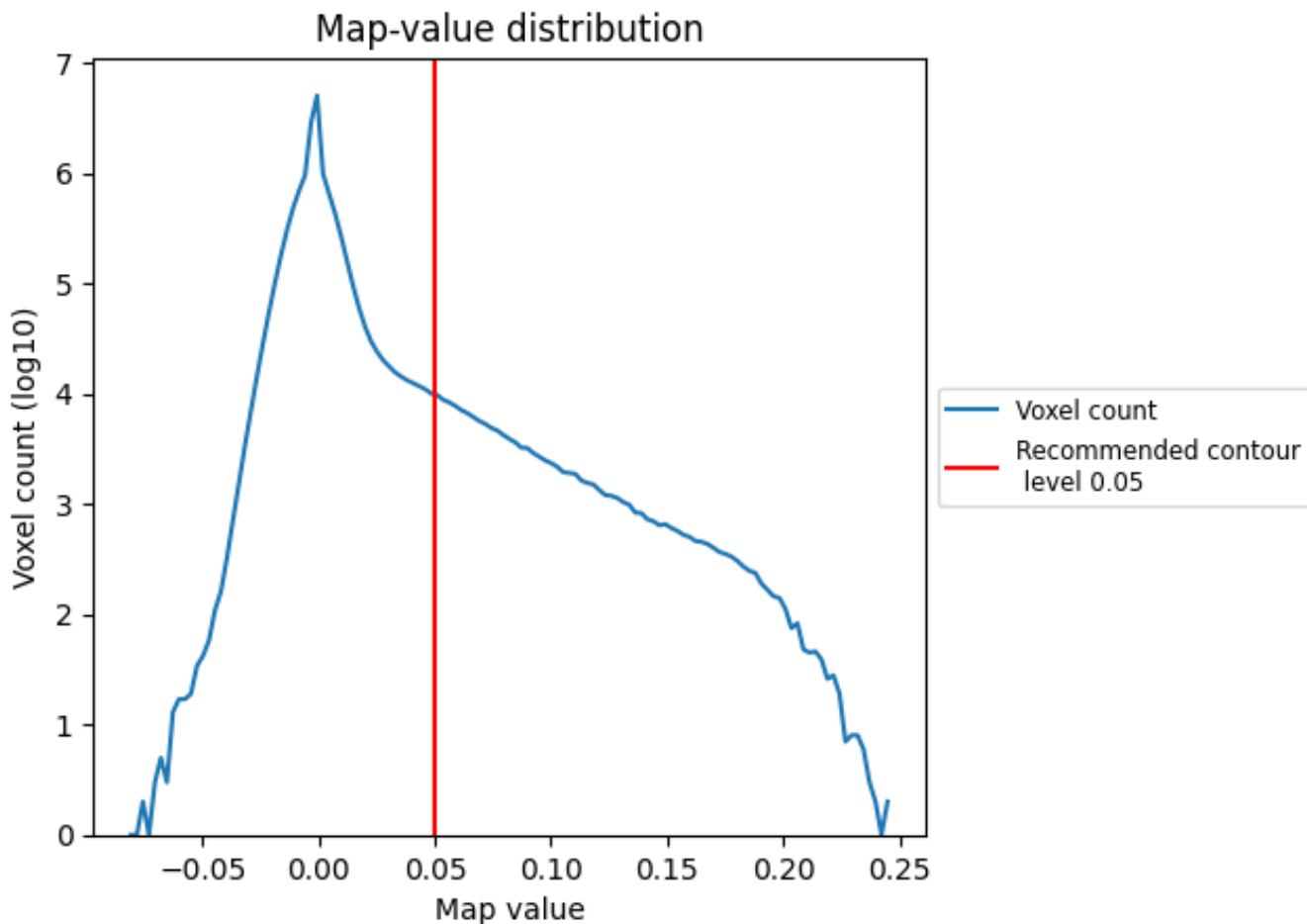
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

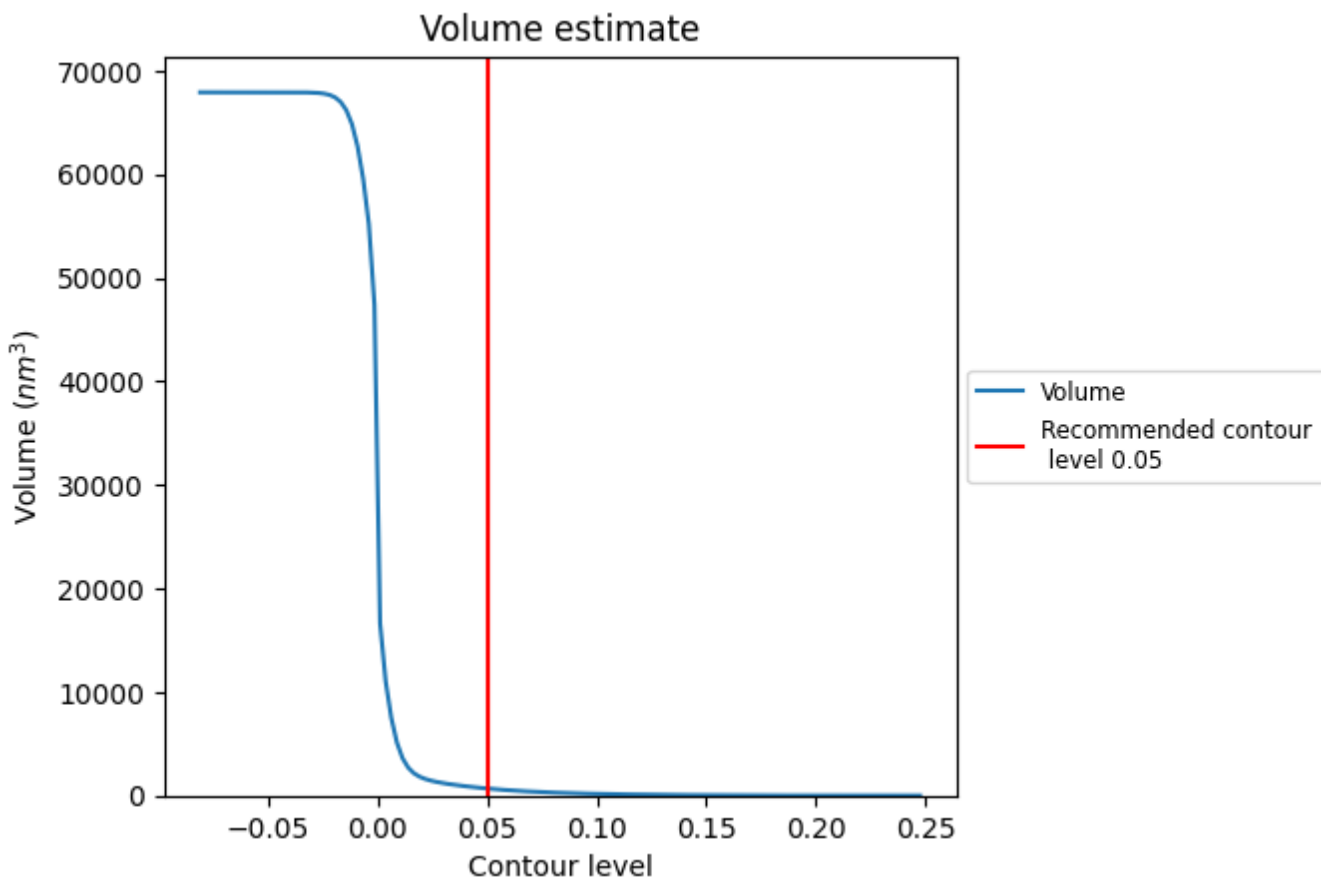
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

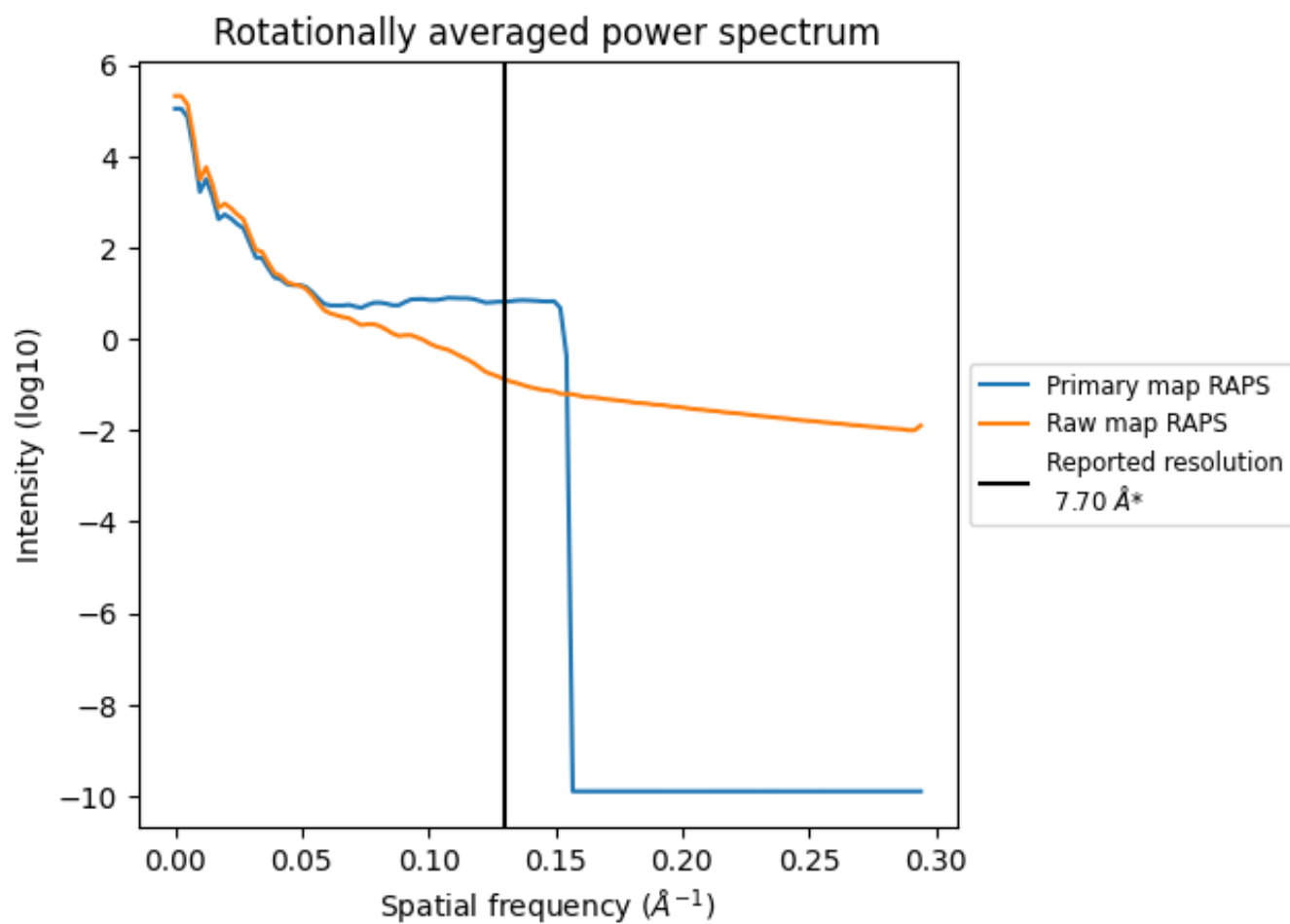
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 683 nm³; this corresponds to an approximate mass of 617 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

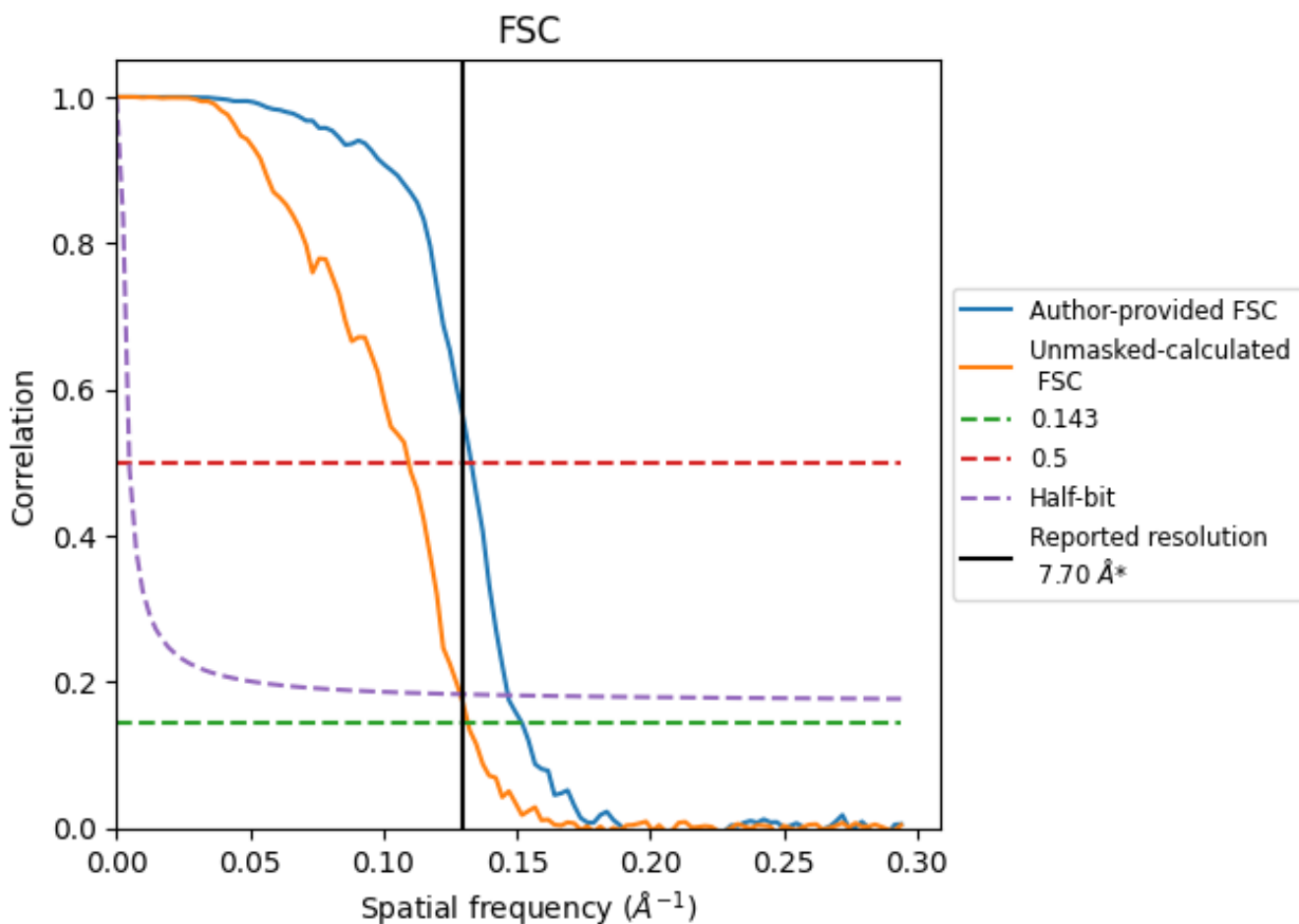


*Reported resolution corresponds to spatial frequency of 0.130 Å⁻¹

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 0.130 Å⁻¹

8.2 Resolution estimates [i](#)

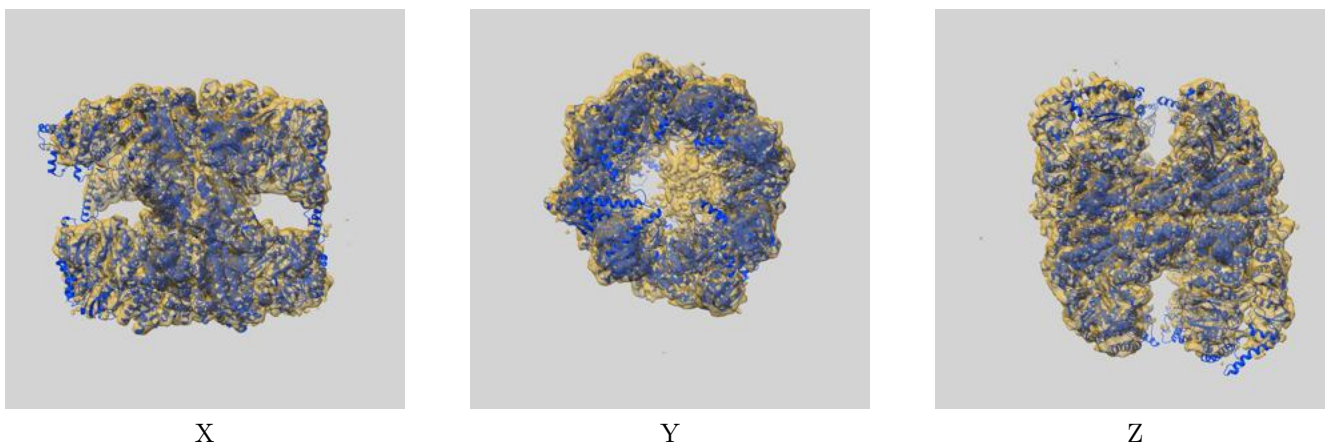
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.70	-	-
Author-provided FSC curve	6.58	7.52	6.82
Unmasked-calculated*	7.59	9.13	7.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.58 differs from the reported value 7.7 by more than 10 %

9 Map-model fit [i](#)

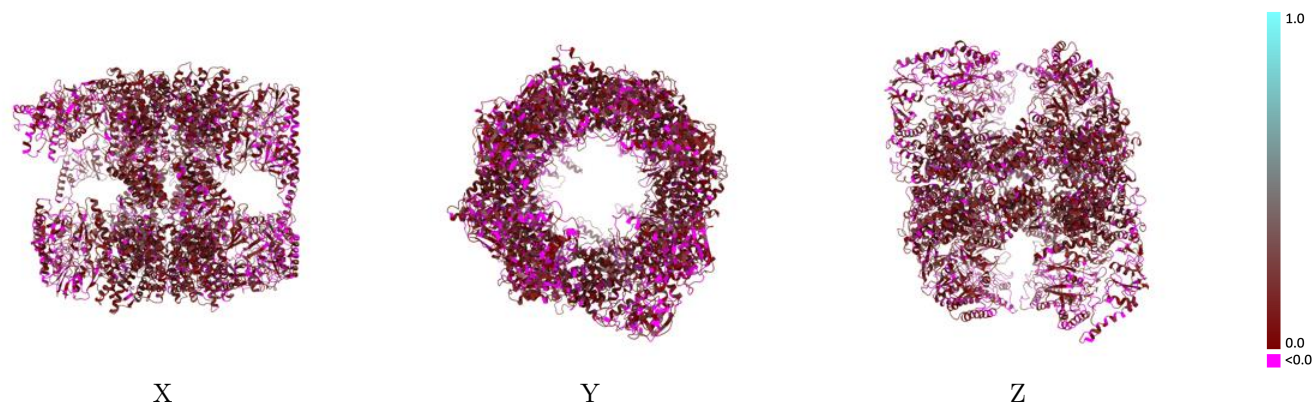
This section contains information regarding the fit between EMDB map EMD-0492 and PDB model 6NRA. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



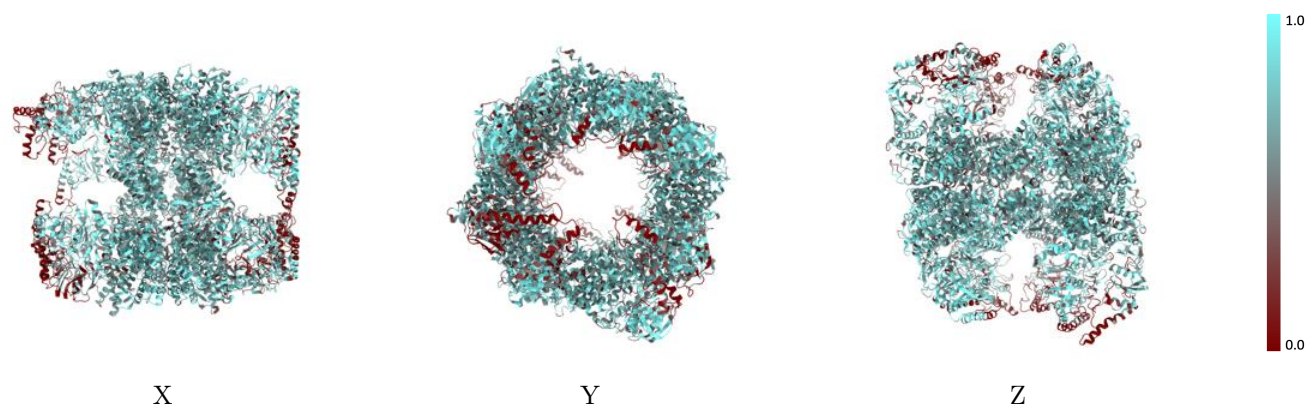
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



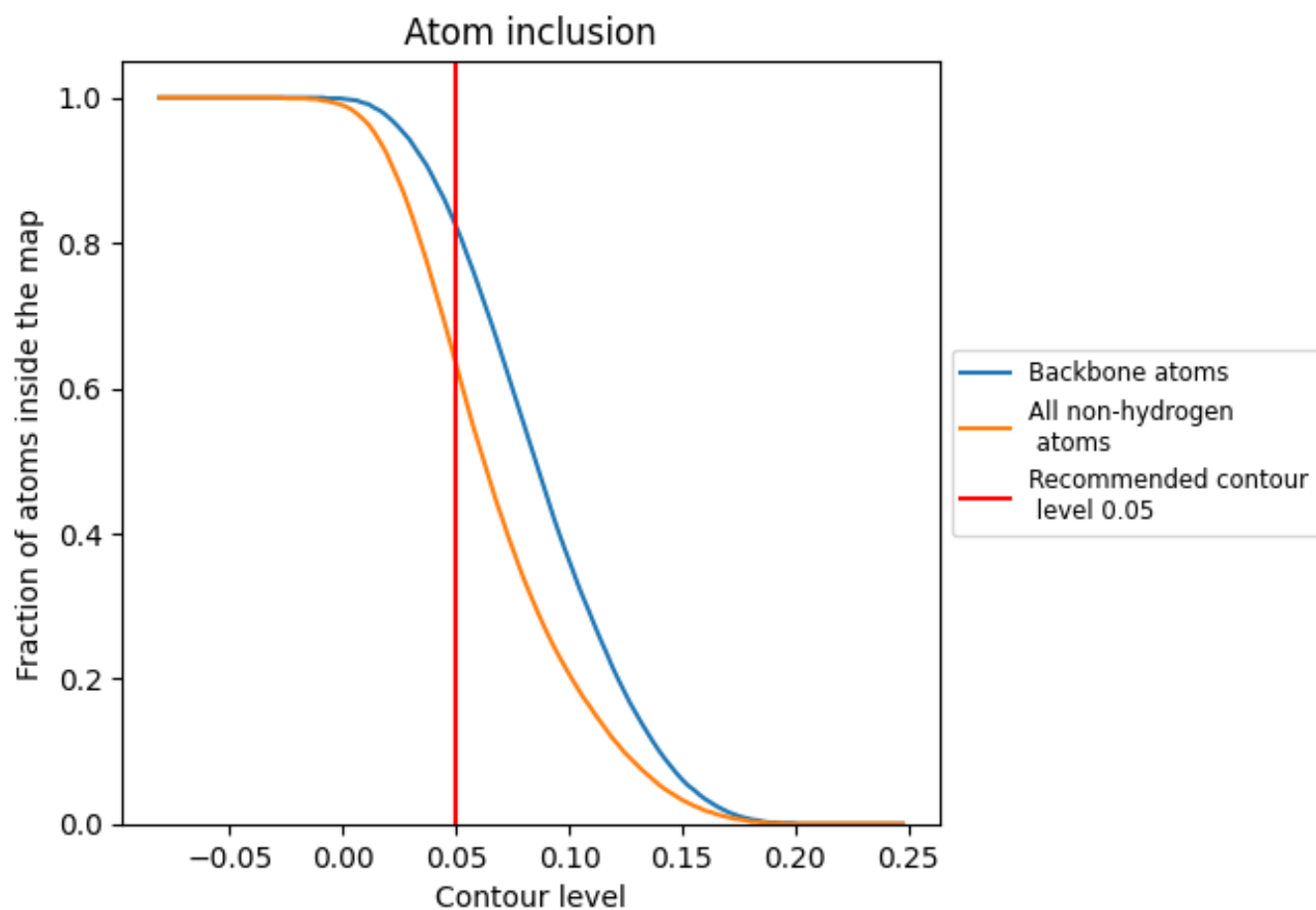
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 63% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6340	 0.1010
A	 0.6100	 0.0910
B	 0.5230	 0.0950
C	 0.6490	 0.1070
D	 0.6630	 0.1150
E	 0.6760	 0.0980
F	 0.7010	 0.1150
G	 0.6650	 0.1010
H	 0.7000	 0.1140
I	 0.6060	 0.0860
J	 0.4700	 0.0880
K	 0.6080	 0.0880
L	 0.6300	 0.1050
M	 0.6570	 0.1040
N	 0.6800	 0.1090
O	 0.6110	 0.0950
P	 0.6970	 0.1110

