



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 01:56 AM UTC

PDB ID : 9YUY / pdb_00009yuy
EMDB ID : EMD-73509
Title : Structure of the Plasmodium falciparum 20S proteasome in complex with a beta5-selective covalent syringolin analogue inhibitor.
Authors : Yan, N.L.; Gu, X.; Fajtova, P.; Tse, E.; Melo, A.; Southworth, D.R.; O'Donoghue, A.; Sello, J.K.; Gestwicki, J.E.
Deposited on : 2025-10-23
Resolution : 2.70 Å (reported)
Based on initial model : 6MUW

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:

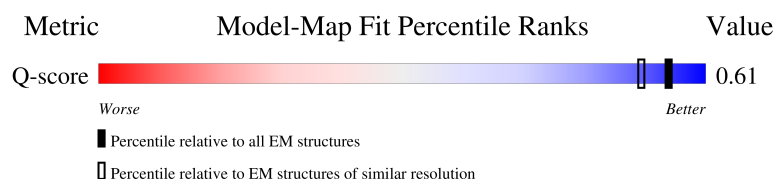
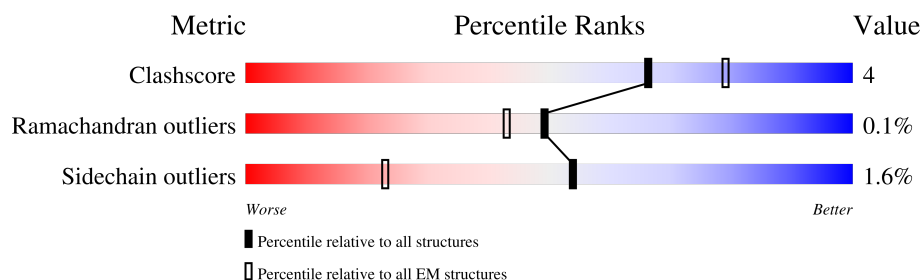
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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.









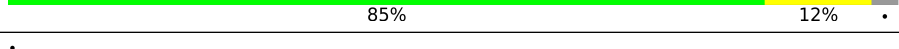
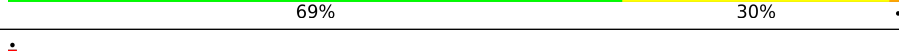
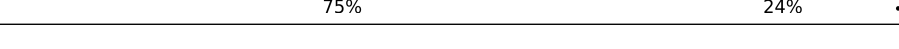
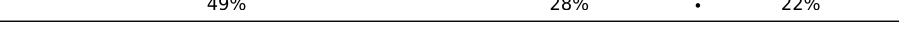
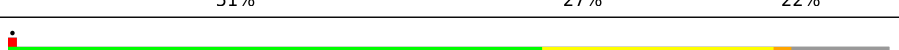

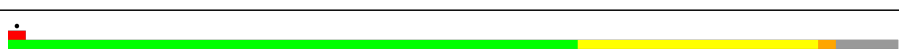

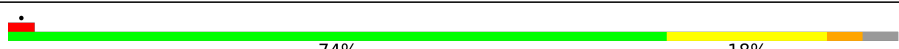





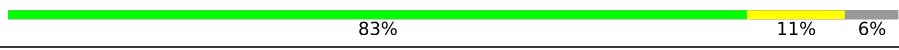
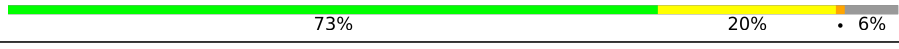



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	C	246	
1	Q	246	
2	D	241	

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Mol	Chain	Length	Quality of chain
2	R	241	
3	E	256	
3	S	256	
4	F	254	
4	T	254	
5	G	252	
5	U	252	
6	K	195	
6	Y	195	
7	L	271	
7	Z	271	
8	M	240	
8	a	240	
9	A	260	
9	O	260	
10	B	235	
10	P	235	
11	H	282	
11	V	282	
12	I	270	
12	W	270	
13	J	218	
13	X	218	
14	N	265	
14	b	265	

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 100048 atoms, of which 49886 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 Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	C	240	Total	C	H	N	O	S	0	0
			3828	1226	1911	312	376	3		
1	Q	240	Total	C	H	N	O	S	0	0
			3828	1226	1911	312	376	3		

- Molecule 2 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	233	Total	C	H	N	O	S	0	0
			3724	1178	1879	312	347	8		
2	R	233	Total	C	H	N	O	S	0	0
			3724	1178	1879	312	347	8		

- Molecule 3 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	240	Total	C	H	N	O	S	0	0
			3728	1170	1868	311	368	11		
3	S	240	Total	C	H	N	O	S	0	0
			3728	1170	1868	311	368	11		

- Molecule 4 is a protein called Proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	F	237	Total	C	H	N	O	S	0	0
			3758	1194	1879	310	364	11		
4	T	237	Total	C	H	N	O	S	0	0
			3758	1194	1879	310	364	11		

- Molecule 5 is a protein called Proteasome subunit alpha type-3, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	G	245	Total	C	H	N	O	S	0	0
			3958	1277	1950	335	383	13		
5	U	245	Total	C	H	N	O	S	0	0
			3958	1277	1950	335	383	13		

- Molecule 6 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	K	195	Total	C	H	N	O	S	0	0
			3198	1042	1584	266	298	8		
6	Y	195	Total	C	H	N	O	S	0	0
			3198	1042	1584	266	298	8		

- Molecule 7 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	L	211	Total	C	H	N	O	S	0	0
			3277	1060	1615	275	319	8		
7	Z	211	Total	C	H	N	O	S	0	0
			3277	1060	1615	275	319	8		

- Molecule 8 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	M	213	Total	C	H	N	O	S	0	0
			3404	1085	1708	283	321	7		
8	a	213	Total	C	H	N	O	S	0	0
			3404	1085	1708	283	321	7		

- Molecule 9 is a protein called Proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	A	242	Total	C	H	N	O	S	0	0
			3809	1201	1899	318	377	14		
9	O	242	Total	C	H	N	O	S	0	0
			3809	1201	1899	318	377	14		

- Molecule 10 is a protein called Proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	B	225	Total	C	H	N	O	S	0	0
			3614	1157	1816	294	341	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	P	225	Total	C	H	N	O	S	0	0
			3614	1157	1816	294	341	6		

- Molecule 11 is a protein called Proteasome subunit beta type-6, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	H	214	Total	C	H	N	O	S	0	0
			3461	1096	1739	297	318	11		
11	V	214	Total	C	H	N	O	S	0	0
			3461	1096	1739	297	318	11		

- Molecule 12 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	I	218	Total	C	H	N	O	S	0	0
			3336	1055	1668	289	311	13		
12	W	218	Total	C	H	N	O	S	0	0
			3336	1055	1668	289	311	13		

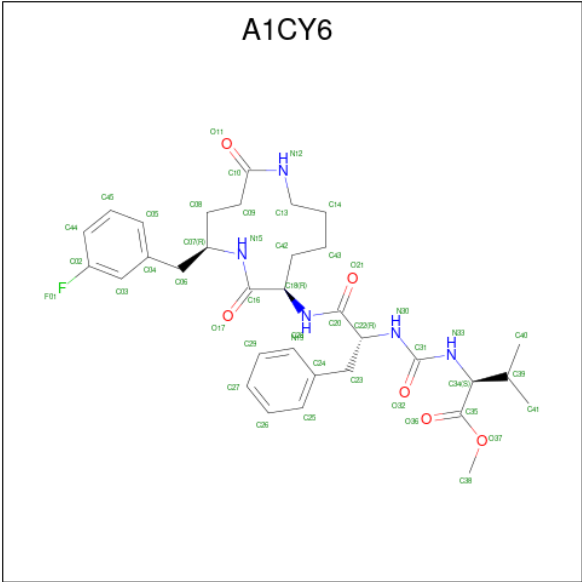
- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	J	205	Total	C	H	N	O	S	0	0
			3222	1029	1610	261	308	14		
13	X	205	Total	C	H	N	O	S	0	0
			3222	1029	1610	261	308	14		

- Molecule 14 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	224	Total	C	H	N	O	S	0	0
			3662	1177	1817	313	348	7		
14	b	224	Total	C	H	N	O	S	0	0
			3662	1177	1817	313	348	7		

- Molecule 15 is methyl N-{[(2R)-1-({(5R,8R)-5-[(3-fluorophenyl)methyl]-2,7-dioxo-1,6-diazacyclododecan-8-yl}amino)-1-oxo-3-phenylpropan-2-yl]carbonyl}-L-valinate (CCD ID: A1CY6) (formula: C₃₃H₄₄FN₅O₆) (labeled as "Ligand of Interest" by depositor).

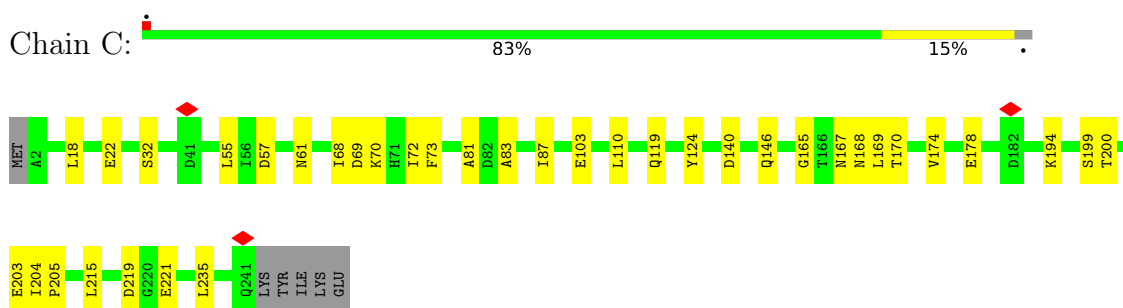


Mol	Chain	Residues	Atoms					AltConf
15	L	1	Total	C	F	N	O	0
			45	33	1	5	6	
15	Z	1	Total	C	F	N	O	0
			45	33	1	5	6	

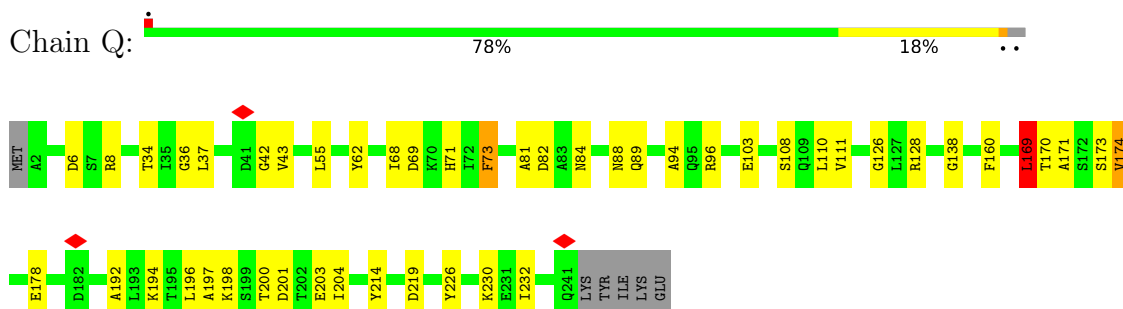
3 Residue-property plots [i](#)

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.

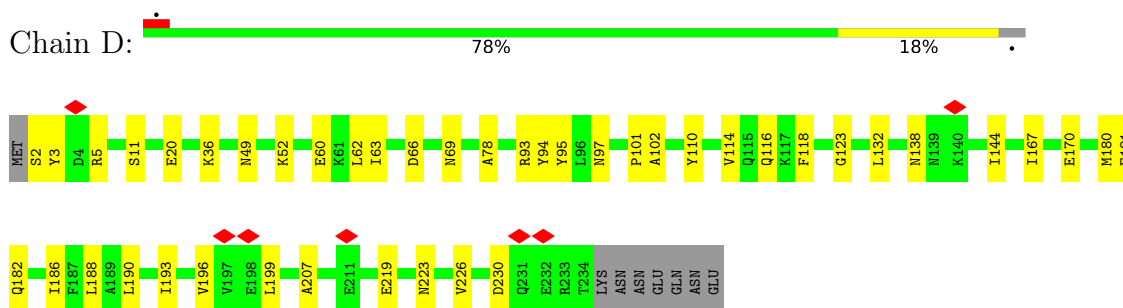
- Molecule 1: Proteasome subunit alpha type



- Molecule 1: Proteasome subunit alpha type

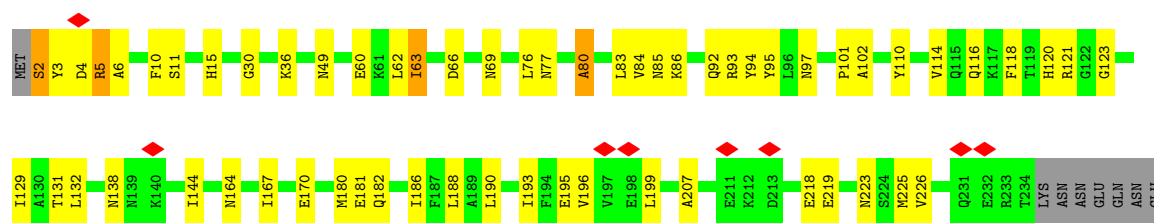


- Molecule 2: Proteasome subunit alpha type

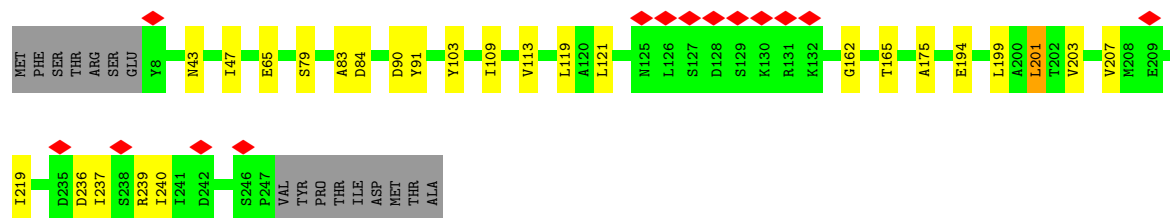
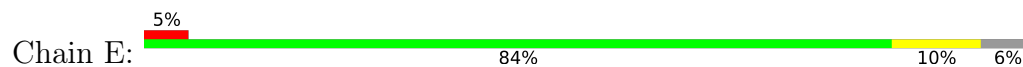


- Molecule 2: Proteasome subunit alpha type

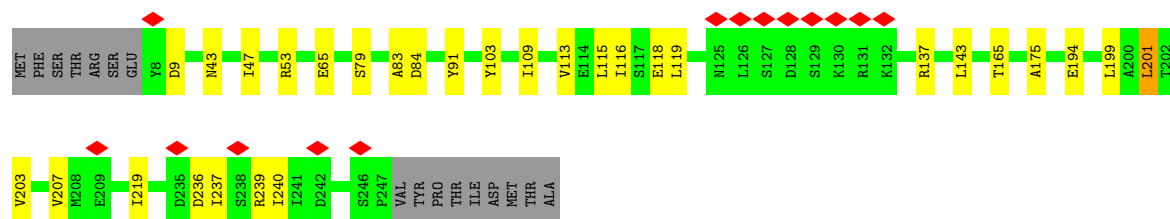
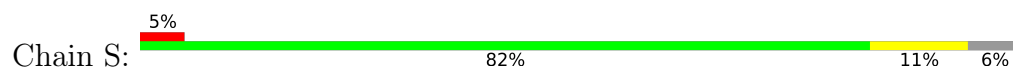




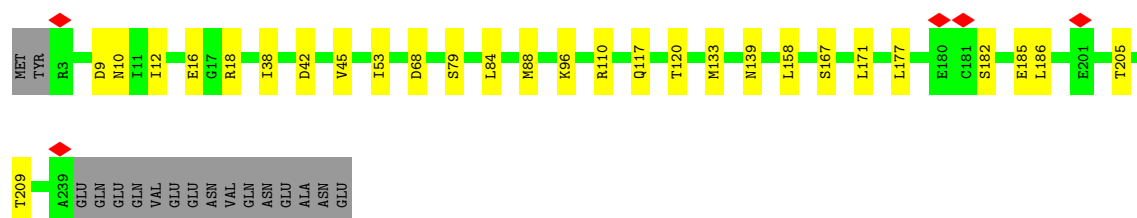
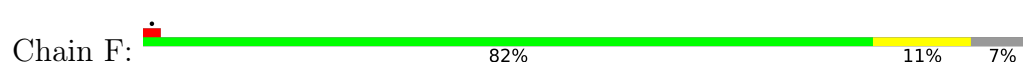
• Molecule 3: Proteasome subunit alpha type



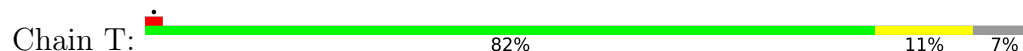
• Molecule 3: Proteasome subunit alpha type

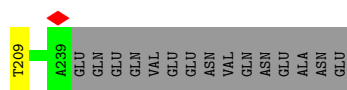


• Molecule 4: Proteasome endopeptidase complex

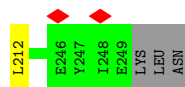
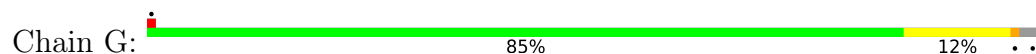


• Molecule 4: Proteasome endopeptidase complex

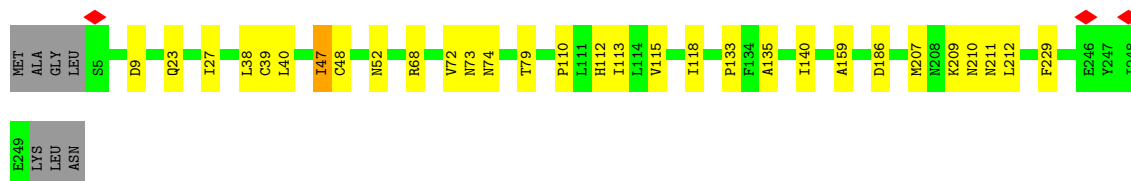
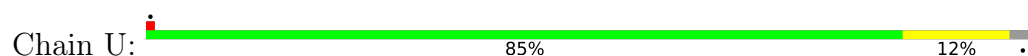




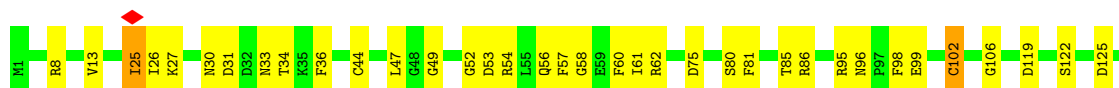
- Molecule 5: Proteasome subunit alpha type-3, putative



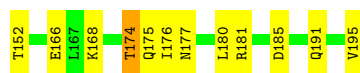
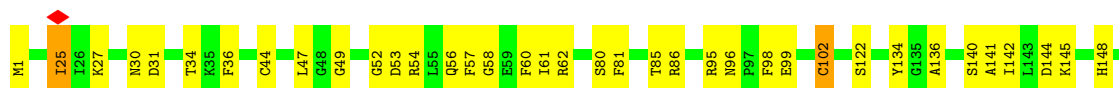
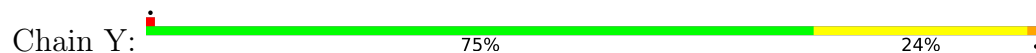
- Molecule 5: Proteasome subunit alpha type-3, putative



- Molecule 6: Proteasome subunit beta

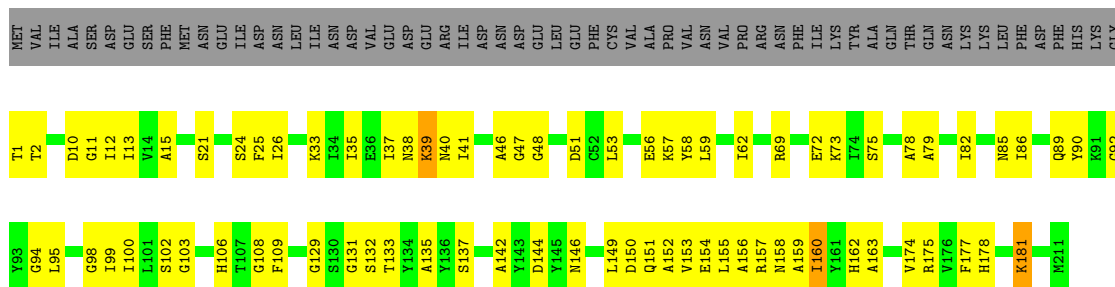


- Molecule 6: Proteasome subunit beta

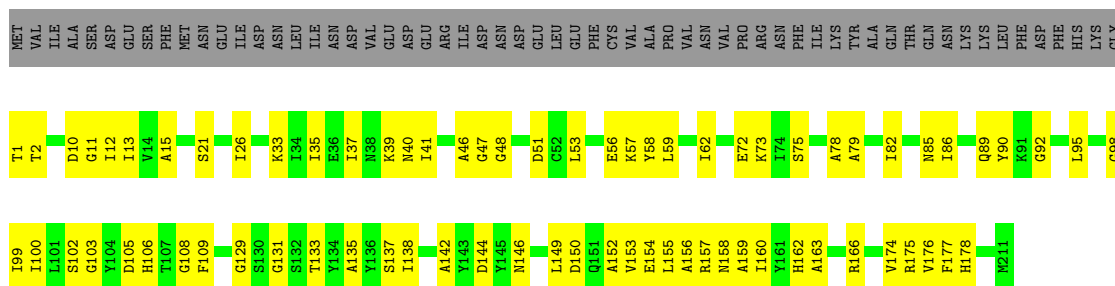


- Molecule 7: Proteasome subunit beta

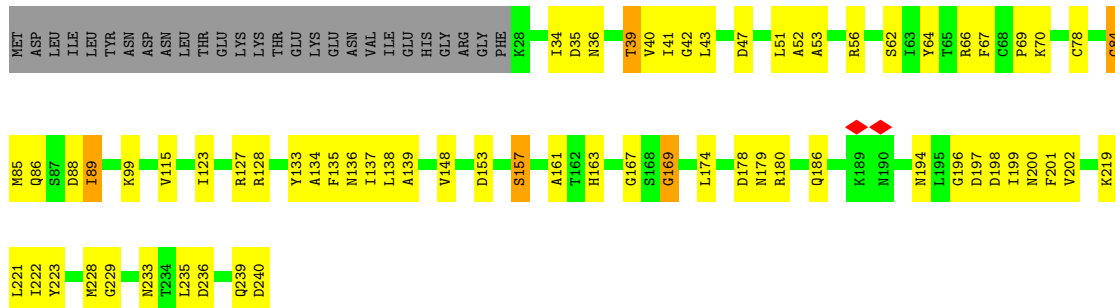




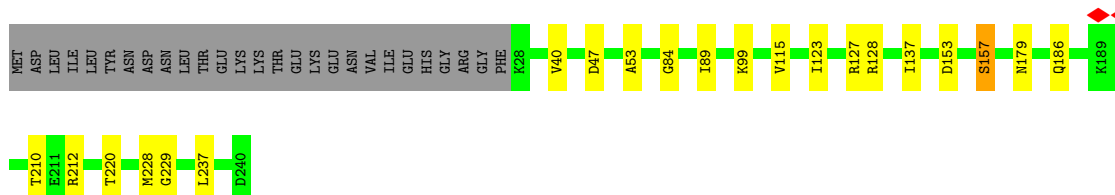
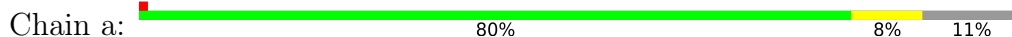
- Molecule 7: Proteasome subunit beta



- Molecule 8: Proteasome subunit beta

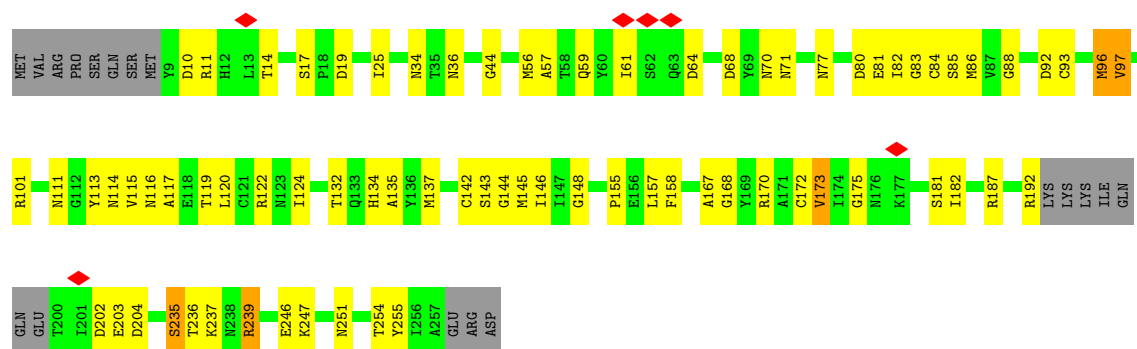


- Molecule 8: Proteasome subunit beta



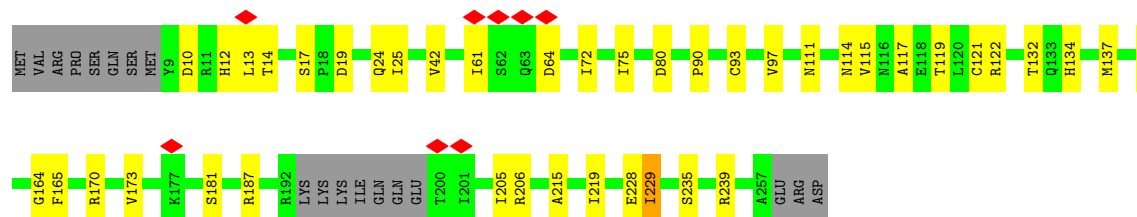
- Molecule 9: Proteasome endopeptidase complex





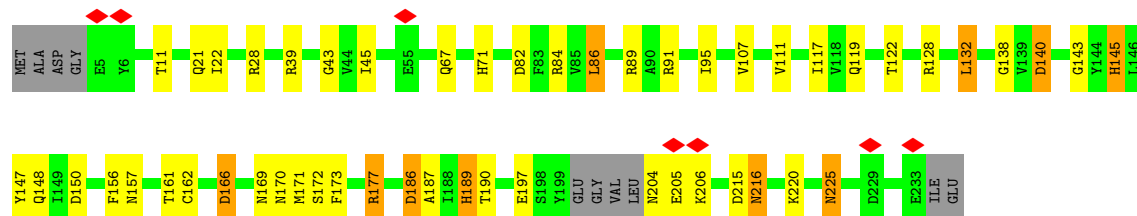
- Molecule 9: Proteasome endopeptidase complex

Chain O: 77% 16% 7%



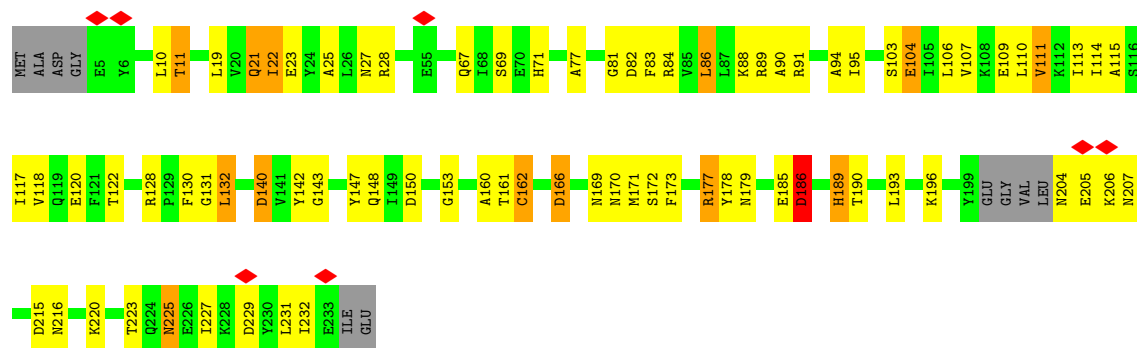
- Molecule 10: Proteasome endopeptidase complex

Chain B: 74% 18% 8%




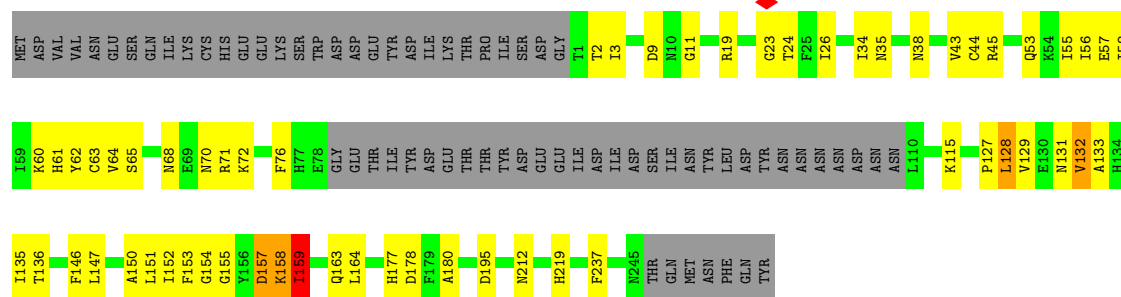
- Molecule 10: Proteasome endopeptidase complex

Chain P: 62% 28% 10%



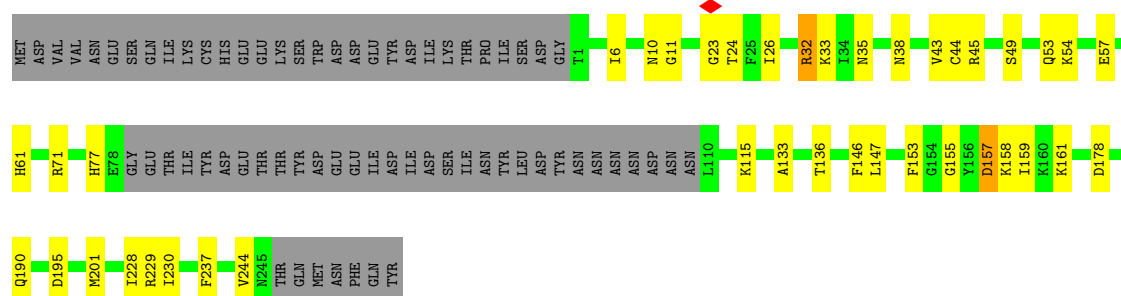
- Molecule 11: Proteasome subunit beta type-6, putative

Chain H:  55% 19% 24%



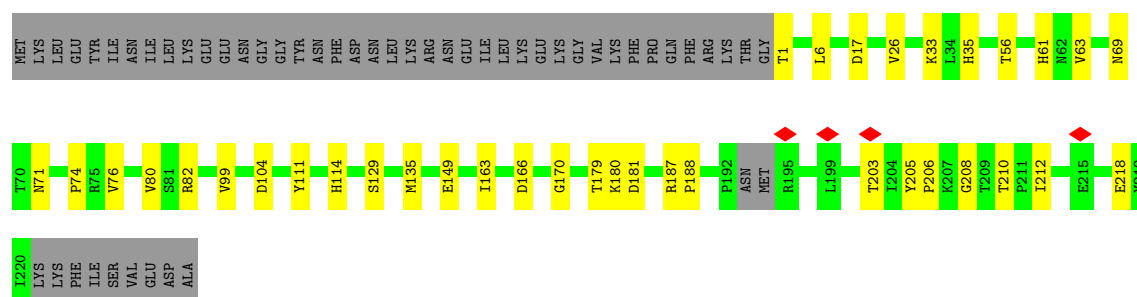
- Molecule 11: Proteasome subunit beta type-6, putative

Chain V:  62% 13% 24%



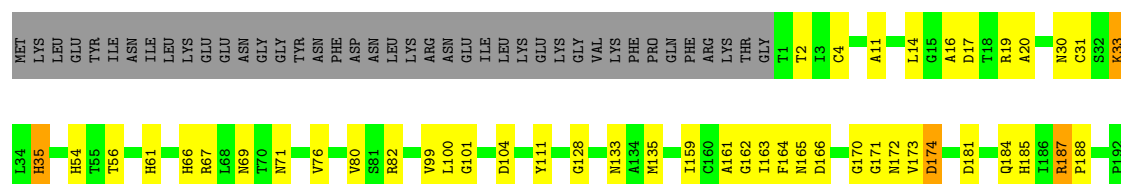
- Molecule 12: Proteasome subunit beta

Chain I:  67% 14% 19%



- Molecule 12: Proteasome subunit beta

Chain W:  59% 20% 19%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	36364	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.727	Depositor
Minimum map value	-2.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.159	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	333.6, 333.6, 333.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.112, 1.112, 1.112	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A1CY6

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	C	0.28	0/1952	0.45	1/2644 (0.0%)
1	Q	1.73	17/1952 (0.9%)	1.92	48/2644 (1.8%)
2	D	0.68	4/1875 (0.2%)	0.74	8/2530 (0.3%)
2	R	1.47	13/1875 (0.7%)	1.52	24/2530 (0.9%)
3	E	0.12	0/1886	0.39	0/2546
3	S	0.36	1/1886 (0.1%)	0.48	1/2546 (0.0%)
4	F	0.10	0/1913	0.32	0/2576
4	T	0.10	0/1913	0.33	0/2576
5	G	0.69	2/2052 (0.1%)	0.80	12/2774 (0.4%)
5	U	0.31	1/2052 (0.0%)	0.45	0/2774
6	K	1.79	11/1649 (0.7%)	2.01	70/2223 (3.1%)
6	Y	1.73	11/1649 (0.7%)	1.94	57/2223 (2.6%)
7	L	1.98	24/1696 (1.4%)	2.05	106/2286 (4.6%)
7	Z	1.94	26/1696 (1.5%)	2.01	101/2286 (4.4%)
8	M	1.74	21/1728 (1.2%)	1.83	85/2339 (3.6%)
8	a	0.36	3/1728 (0.2%)	0.43	2/2339 (0.1%)
9	A	1.82	24/1936 (1.2%)	1.98	90/2614 (3.4%)
9	O	1.03	5/1936 (0.3%)	1.12	14/2614 (0.5%)
10	B	1.78	13/1831 (0.7%)	1.97	47/2471 (1.9%)
10	P	2.16	26/1831 (1.4%)	2.34	120/2471 (4.9%)
11	H	1.76	15/1751 (0.9%)	1.98	70/2349 (3.0%)
11	V	1.49	7/1751 (0.4%)	1.68	23/2349 (1.0%)
12	I	0.59	1/1703 (0.1%)	0.68	2/2315 (0.1%)
12	W	1.87	27/1703 (1.6%)	1.89	53/2315 (2.3%)
13	J	0.42	0/1638	0.58	3/2211 (0.1%)
13	X	1.77	10/1638 (0.6%)	1.98	35/2211 (1.6%)
14	N	0.75	9/1882 (0.5%)	0.78	6/2538 (0.2%)
14	b	0.71	2/1882 (0.1%)	0.83	2/2538 (0.1%)
All	All	1.31	273/50984 (0.5%)	1.43	980/68832 (1.4%)

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	Q	0	2
6	K	0	2
6	Y	0	1
All	All	0	5

All (273) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	112	HIS	CE1-NE2	-8.86	1.23	1.32
7	Z	106	HIS	CE1-NE2	-8.86	1.23	1.32
7	L	162	HIS	CE1-NE2	-8.81	1.23	1.32
7	L	106	HIS	CE1-NE2	-8.79	1.23	1.32
10	P	71	HIS	ND1-CE1	-8.75	1.23	1.32
8	M	163	HIS	CE1-NE2	-8.74	1.23	1.32
12	W	198	HIS	CE1-NE2	-8.74	1.23	1.32
7	Z	162	HIS	CE1-NE2	-8.71	1.23	1.32
11	H	61	HIS	CE1-NE2	-8.71	1.23	1.32
10	P	189	HIS	CE1-NE2	-8.71	1.23	1.32
7	L	178	HIS	ND1-CE1	-8.70	1.23	1.32
12	W	201	HIS	CE1-NE2	-8.70	1.23	1.32
7	Z	178	HIS	ND1-CE1	-8.63	1.24	1.32
6	Y	181	ARG	CZ-NH2	-8.30	1.22	1.33
7	L	157	ARG	CZ-NH2	-8.26	1.22	1.33
8	a	128	ARG	CZ-NH2	-8.25	1.22	1.33
9	A	239	ARG	CZ-NH2	-8.24	1.22	1.33
11	H	45	ARG	CZ-NH2	-8.24	1.22	1.33
6	K	62	ARG	CZ-NH2	-8.24	1.22	1.33
8	M	128	ARG	CZ-NH2	-8.23	1.22	1.33
6	K	181	ARG	CZ-NH2	-8.22	1.22	1.33
12	W	187	ARG	CZ-NH2	-8.22	1.22	1.33
6	Y	62	ARG	CZ-NH2	-8.21	1.22	1.33
8	M	180	ARG	CZ-NH2	-8.21	1.22	1.33
8	M	66	ARG	CZ-NH2	-8.19	1.22	1.33
13	X	190	ARG	CZ-NH2	-8.19	1.22	1.33
12	W	195	ARG	CZ-NH2	-8.18	1.22	1.33
14	N	190	ARG	CZ-NH2	-8.17	1.22	1.33
14	N	182	ARG	CZ-NH2	-8.17	1.22	1.33
1	Q	128	ARG	CZ-NH2	-8.16	1.22	1.33
9	A	170	ARG	CZ-NH2	-8.15	1.22	1.33
9	A	101	ARG	CZ-NH2	-8.15	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	93	ARG	CZ-NH2	-8.13	1.22	1.33
1	Q	8	ARG	CZ-NH2	-8.13	1.22	1.33
7	Z	157	ARG	CZ-NH2	-8.12	1.22	1.33
2	R	93	ARG	CZ-NH2	-8.12	1.22	1.33
1	Q	71	HIS	CE1-NE2	-8.12	1.24	1.32
5	G	112	HIS	CD2-NE2	-8.08	1.28	1.37
12	W	198	HIS	CD2-NE2	-8.05	1.28	1.37
7	L	162	HIS	CD2-NE2	-8.03	1.29	1.37
7	L	106	HIS	CD2-NE2	-8.01	1.29	1.37
8	M	163	HIS	CD2-NE2	-8.01	1.29	1.37
7	Z	162	HIS	CD2-NE2	-8.00	1.29	1.37
7	Z	106	HIS	CD2-NE2	-7.98	1.29	1.37
11	H	61	HIS	CD2-NE2	-7.98	1.29	1.37
12	W	201	HIS	CD2-NE2	-7.97	1.29	1.37
10	P	189	HIS	CD2-NE2	-7.95	1.29	1.37
10	B	145	HIS	CE1-NE2	-7.91	1.24	1.32
10	P	91	ARG	CZ-NH2	-7.88	1.23	1.33
10	B	189	HIS	CE1-NE2	-7.84	1.24	1.32
8	M	139	ALA	CA-CB	-7.84	1.42	1.53
10	P	89	ARG	CZ-NH2	-7.81	1.23	1.33
10	P	28	ARG	CZ-NH2	-7.79	1.23	1.33
10	P	177	ARG	CZ-NH2	-7.78	1.23	1.33
10	B	71	HIS	ND1-CE1	-7.75	1.24	1.32
10	P	84	ARG	CZ-NH2	-7.75	1.23	1.33
9	O	122	ARG	CZ-NH2	-7.74	1.23	1.33
12	W	35	HIS	CE1-NE2	-7.64	1.25	1.32
12	W	54	HIS	CE1-NE2	-7.62	1.25	1.32
12	W	185	HIS	CE1-NE2	-7.62	1.25	1.32
1	Q	71	HIS	CD2-NE2	-7.36	1.29	1.37
12	W	171	GLY	N-CA	-7.33	1.38	1.45
10	B	145	HIS	CD2-NE2	-7.25	1.29	1.37
9	A	83	GLY	N-CA	-7.24	1.37	1.45
7	Z	163	ALA	CA-CB	-7.18	1.42	1.53
10	B	189	HIS	CD2-NE2	-7.16	1.29	1.37
9	A	187	ARG	CZ-NH2	-7.14	1.24	1.33
11	H	11	GLY	N-CA	-7.14	1.37	1.45
12	W	185	HIS	CD2-NE2	-7.14	1.29	1.37
2	R	102	ALA	CA-CB	-7.13	1.42	1.53
2	R	15	HIS	CE1-NE2	-7.12	1.25	1.32
7	Z	156	ALA	CA-CB	-7.11	1.42	1.53
6	Y	141	ALA	CA-CB	-7.10	1.42	1.53
2	R	120	HIS	CE1-NE2	-7.10	1.25	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Z	78	ALA	CA-CB	-7.09	1.42	1.53
7	L	163	ALA	CA-CB	-7.08	1.42	1.53
6	K	141	ALA	CA-CB	-7.08	1.42	1.53
11	H	133	ALA	CA-CB	-7.07	1.42	1.53
7	L	159	ALA	CA-CB	-7.06	1.42	1.53
7	L	156	ALA	CA-CB	-7.05	1.42	1.53
7	Z	135	ALA	CA-CB	-7.05	1.42	1.53
7	L	135	ALA	CA-CB	-7.04	1.42	1.53
7	L	152	ALA	CA-CB	-7.04	1.42	1.53
7	Z	152	ALA	CA-CB	-7.04	1.42	1.53
7	Z	79	ALA	CA-CB	-7.04	1.42	1.53
7	L	78	ALA	CA-CB	-7.03	1.42	1.53
1	Q	171	ALA	CA-CB	-7.03	1.42	1.53
2	D	102	ALA	CA-CB	-7.03	1.42	1.53
7	L	79	ALA	CA-CB	-7.03	1.42	1.53
11	H	177	HIS	CE1-NE2	-6.99	1.25	1.32
12	W	54	HIS	CD2-NE2	-6.99	1.30	1.37
7	Z	159	ALA	CA-CB	-6.99	1.42	1.53
9	A	144	GLY	N-CA	-6.98	1.37	1.44
12	W	161	ALA	CA-CB	-6.98	1.42	1.53
12	W	35	HIS	CD2-NE2	-6.98	1.30	1.37
1	Q	81	ALA	CA-CB	-6.95	1.42	1.53
13	X	187	ALA	CA-CB	-6.84	1.42	1.53
14	N	192	HIS	CE1-NE2	-6.83	1.25	1.32
1	Q	197	ALA	CA-CB	-6.82	1.42	1.53
9	A	101	ARG	CZ-NH1	-6.77	1.23	1.32
12	W	67	ARG	CZ-NH2	-6.75	1.24	1.33
10	P	115	ALA	CA-CB	-6.74	1.43	1.53
9	A	239	ARG	CZ-NH1	-6.73	1.23	1.32
8	M	128	ARG	CZ-NH1	-6.69	1.23	1.32
13	X	190	ARG	CZ-NH1	-6.67	1.23	1.32
1	Q	128	ARG	CZ-NH1	-6.66	1.23	1.32
14	N	182	ARG	CZ-NH1	-6.66	1.23	1.32
6	K	62	ARG	CZ-NH1	-6.65	1.23	1.32
6	Y	62	ARG	CZ-NH1	-6.65	1.23	1.32
14	N	190	ARG	CZ-NH1	-6.64	1.23	1.32
8	M	180	ARG	CZ-NH1	-6.64	1.23	1.32
2	R	93	ARG	CZ-NH1	-6.64	1.23	1.32
2	D	93	ARG	CZ-NH1	-6.63	1.23	1.32
7	Z	157	ARG	CZ-NH1	-6.63	1.23	1.32
12	W	195	ARG	CZ-NH1	-6.62	1.23	1.32
6	K	181	ARG	CZ-NH1	-6.61	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	66	ARG	CZ-NH1	-6.61	1.23	1.32
7	L	157	ARG	CZ-NH1	-6.61	1.23	1.32
1	Q	42	GLY	N-CA	-6.60	1.39	1.45
9	A	170	ARG	CZ-NH1	-6.60	1.23	1.32
6	Y	181	ARG	CZ-NH1	-6.60	1.23	1.32
12	W	187	ARG	CZ-NH1	-6.60	1.23	1.32
11	H	177	HIS	CD2-NE2	-6.59	1.30	1.37
11	H	45	ARG	CZ-NH1	-6.58	1.23	1.32
8	a	128	ARG	CZ-NH1	-6.58	1.23	1.32
1	Q	8	ARG	CZ-NH1	-6.58	1.23	1.32
12	W	16	ALA	CA-CB	-6.54	1.42	1.53
11	H	219	HIS	CE1-NE2	-6.52	1.26	1.32
2	R	15	HIS	CD2-NE2	-6.50	1.30	1.37
11	V	32	ARG	CZ-NH2	-6.49	1.25	1.33
10	B	43	GLY	N-CA	-6.47	1.39	1.45
12	I	114	HIS	ND1-CE1	-6.47	1.26	1.32
9	A	148	GLY	N-CA	-6.46	1.38	1.45
6	K	58	GLY	N-CA	-6.45	1.37	1.45
10	P	90	ALA	CA-CB	-6.44	1.43	1.53
6	Y	58	GLY	N-CA	-6.41	1.38	1.45
11	V	45	ARG	CZ-NH2	-6.40	1.25	1.33
2	R	120	HIS	CD2-NE2	-6.38	1.30	1.37
11	V	229	ARG	CZ-NH2	-6.38	1.25	1.33
9	A	117	ALA	CA-CB	-6.34	1.43	1.53
8	M	42	GLY	CA-C	-6.34	1.47	1.52
9	O	122	ARG	CZ-NH1	-6.34	1.23	1.32
11	H	155	GLY	N-CA	-6.33	1.38	1.45
12	W	162	GLY	N-CA	-6.29	1.38	1.45
10	P	143	GLY	N-CA	-6.29	1.38	1.45
9	A	57	ALA	CA-CB	-6.29	1.42	1.53
10	P	91	ARG	CZ-NH1	-6.28	1.24	1.32
10	P	89	ARG	CZ-NH1	-6.27	1.24	1.32
10	P	77	ALA	CA-CB	-6.26	1.43	1.52
10	P	177	ARG	CZ-NH1	-6.26	1.24	1.32
10	P	84	ARG	CZ-NH1	-6.25	1.24	1.32
12	W	170	GLY	N-CA	-6.24	1.38	1.45
10	P	28	ARG	CZ-NH1	-6.22	1.24	1.32
10	P	160	ALA	CA-CB	-6.21	1.43	1.53
7	Z	108	GLY	N-CA	-6.21	1.38	1.45
14	N	192	HIS	CD2-NE2	-6.19	1.31	1.37
13	X	9	GLY	N-CA	-6.18	1.39	1.45
8	M	196	GLY	N-CA	-6.11	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	52	ALA	CA-CB	-6.06	1.42	1.53
12	W	20	ALA	CA-CB	-6.04	1.42	1.53
9	A	167	ALA	CA-CB	-6.03	1.44	1.53
1	Q	138	GLY	N-CA	-6.01	1.39	1.45
8	M	42	GLY	N-CA	-5.97	1.38	1.46
11	V	11	GLY	N-CA	-5.96	1.39	1.45
7	Z	103	GLY	N-CA	-5.94	1.38	1.45
11	H	219	HIS	CD2-NE2	-5.94	1.31	1.37
6	K	106	GLY	N-CA	-5.93	1.39	1.45
10	P	81	GLY	N-CA	-5.89	1.38	1.45
10	B	89	ARG	CZ-NH2	-5.89	1.25	1.33
7	L	103	GLY	N-CA	-5.88	1.38	1.45
9	A	122	ARG	CZ-NH2	-5.88	1.25	1.33
10	B	28	ARG	CZ-NH2	-5.86	1.25	1.33
10	B	91	ARG	CZ-NH2	-5.85	1.25	1.33
7	L	142	ALA	CA-CB	-5.85	1.43	1.54
10	B	84	ARG	CZ-NH2	-5.80	1.25	1.33
7	Z	142	ALA	CA-CB	-5.80	1.43	1.54
2	R	80	ALA	CA-CB	-5.80	1.44	1.53
10	B	177	ARG	CZ-NH2	-5.78	1.25	1.33
6	Y	86	ARG	CZ-NH2	-5.76	1.25	1.33
10	B	39	ARG	CZ-NH2	-5.75	1.25	1.33
3	S	137	ARG	CZ-NH2	-5.67	1.26	1.33
2	R	6	ALA	CA-CB	-5.64	1.46	1.52
9	O	187	ARG	CZ-NH2	-5.63	1.26	1.33
2	R	5	ARG	CZ-NH2	-5.63	1.26	1.33
9	O	170	ARG	CZ-NH2	-5.59	1.26	1.33
13	X	113	GLY	N-CA	-5.59	1.39	1.45
9	A	239	ARG	CD-NE	-5.57	1.38	1.46
2	R	30	GLY	N-CA	-5.57	1.39	1.45
9	A	187	ARG	CZ-NH1	-5.56	1.25	1.32
1	Q	94	ALA	CA-CB	-5.55	1.44	1.53
9	A	170	ARG	CD-NE	-5.54	1.38	1.46
1	Q	128	ARG	CD-NE	-5.54	1.38	1.46
2	R	121	ARG	CZ-NH2	-5.54	1.26	1.33
8	M	128	ARG	CD-NE	-5.53	1.38	1.46
6	K	86	ARG	CZ-NH2	-5.51	1.26	1.33
1	Q	192	ALA	CA-CB	-5.51	1.44	1.53
6	Y	148	HIS	CE1-NE2	-5.51	1.27	1.32
8	M	167	GLY	N-CA	-5.50	1.37	1.45
2	D	93	ARG	CD-NE	-5.49	1.38	1.46
1	Q	36	GLY	N-CA	-5.48	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	45	ARG	CD-NE	-5.48	1.38	1.46
6	K	8	ARG	CZ-NH2	-5.47	1.26	1.33
8	a	128	ARG	CD-NE	-5.46	1.38	1.46
8	M	66	ARG	CD-NE	-5.43	1.38	1.46
7	Z	166	ARG	CZ-NH2	-5.42	1.26	1.33
2	R	93	ARG	CD-NE	-5.41	1.38	1.46
11	H	180	ALA	CA-CB	-5.41	1.44	1.53
13	X	79	ARG	CZ-NH2	-5.39	1.26	1.33
6	Y	181	ARG	CD-NE	-5.39	1.38	1.46
10	P	94	ALA	CA-CB	-5.37	1.45	1.53
5	U	112	HIS	CE1-NE2	-5.35	1.27	1.32
10	P	89	ARG	CD-NE	-5.35	1.38	1.46
12	W	67	ARG	CZ-NH1	-5.35	1.25	1.32
1	Q	8	ARG	CD-NE	-5.34	1.38	1.46
13	X	190	ARG	CD-NE	-5.34	1.38	1.46
9	O	122	ARG	CD-NE	-5.33	1.38	1.46
11	V	61	HIS	CE1-NE2	-5.33	1.27	1.32
7	L	157	ARG	CD-NE	-5.33	1.38	1.46
9	A	239	ARG	CA-CB	-5.33	1.48	1.54
7	L	46	ALA	CA-CB	-5.30	1.43	1.54
11	V	155	GLY	N-CA	-5.30	1.39	1.45
11	V	77	HIS	CE1-NE2	-5.30	1.27	1.32
1	Q	96	ARG	CZ-NH2	-5.30	1.26	1.33
7	L	129	GLY	N-CA	-5.29	1.38	1.45
7	Z	157	ARG	CD-NE	-5.29	1.38	1.46
7	Z	46	ALA	CA-CB	-5.28	1.43	1.54
12	W	187	ARG	CD-NE	-5.28	1.38	1.46
9	A	144	GLY	CA-C	-5.28	1.47	1.52
13	X	28	ARG	CZ-NH2	-5.27	1.26	1.33
12	W	195	ARG	CD-NE	-5.26	1.38	1.46
7	Z	129	GLY	N-CA	-5.26	1.38	1.45
7	L	48	GLY	N-CA	-5.25	1.37	1.45
6	K	62	ARG	CD-NE	-5.25	1.39	1.46
10	B	143	GLY	N-CA	-5.25	1.39	1.45
14	N	182	ARG	CD-NE	-5.25	1.39	1.46
6	K	181	ARG	CD-NE	-5.24	1.39	1.46
6	Y	62	ARG	CD-NE	-5.23	1.39	1.46
9	A	101	ARG	CD-NE	-5.23	1.39	1.46
14	N	190	ARG	CD-NE	-5.22	1.39	1.46
10	P	28	ARG	CD-NE	-5.21	1.39	1.46
9	A	59	GLN	CA-CB	-5.21	1.47	1.54
8	M	180	ARG	CD-NE	-5.20	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	P	84	ARG	CD-NE	-5.19	1.39	1.46
7	L	92	GLY	N-CA	-5.17	1.38	1.45
12	W	202	PRO	CA-CB	-5.17	1.46	1.53
7	Z	47	GLY	N-CA	-5.15	1.38	1.45
7	L	47	GLY	N-CA	-5.14	1.38	1.45
7	Z	48	GLY	N-CA	-5.13	1.38	1.45
7	Z	105	ASP	CA-CB	-5.13	1.47	1.53
13	X	197	GLY	N-CA	-5.13	1.39	1.45
9	A	88	GLY	N-CA	-5.12	1.38	1.45
11	H	154	GLY	N-CA	-5.12	1.38	1.45
7	Z	92	GLY	N-CA	-5.12	1.38	1.45
8	M	84	GLY	N-CA	-5.12	1.38	1.45
9	A	168	GLY	N-CA	-5.11	1.38	1.45
8	M	174	LEU	N-CA	-5.11	1.41	1.46
10	P	177	ARG	CD-NE	-5.10	1.39	1.46
12	W	67	ARG	CD-NE	-5.10	1.39	1.46
7	L	98	GLY	N-CA	-5.09	1.38	1.45
10	P	91	ARG	CD-NE	-5.08	1.39	1.46
13	X	10	GLY	N-CA	-5.08	1.39	1.45
12	W	101	GLY	N-CA	-5.07	1.40	1.45
14	N	211	ARG	CZ-NH2	-5.07	1.26	1.33
9	A	44	GLY	N-CA	-5.06	1.38	1.45
8	M	69	PRO	CA-CB	-5.06	1.47	1.53
11	H	127	PRO	CA-CB	-5.06	1.47	1.53
7	Z	98	GLY	N-CA	-5.05	1.38	1.45
14	b	211	ARG	CZ-NH2	-5.05	1.26	1.33
14	b	216	ARG	CZ-NH2	-5.04	1.26	1.33
6	Y	148	HIS	CD2-NE2	-5.03	1.32	1.37
10	P	131	GLY	N-CA	-5.03	1.38	1.45
7	L	94	GLY	N-CA	-5.01	1.38	1.45
8	M	174	LEU	CA-CB	-5.00	1.48	1.53

All (980) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	143	SER	CA-C-N	8.58	128.96	121.58
9	A	143	SER	C-N-CA	8.58	128.96	121.58
9	A	82	ILE	CA-C-N	8.25	129.30	121.46
9	A	82	ILE	C-N-CA	8.25	129.30	121.46
6	Y	98	PHE	CA-CB-CG	7.89	121.69	113.80
6	K	98	PHE	CA-CB-CG	7.88	121.68	113.80
1	Q	73	PHE	CA-CB-CG	7.79	121.59	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	251	ASN	CA-CB-CG	7.75	120.35	112.60
10	P	140	ASP	CA-CB-CG	7.66	120.26	112.60
6	Y	136	ALA	CA-C-N	7.64	130.52	120.28
6	Y	136	ALA	C-N-CA	7.64	130.52	120.28
10	P	166	ASP	CA-CB-CG	7.61	120.21	112.60
7	Z	108	GLY	N-CA-C	7.58	119.21	111.56
6	K	136	ALA	CA-C-N	7.45	130.26	120.28
6	K	136	ALA	C-N-CA	7.45	130.26	120.28
11	H	70	ASN	CA-CB-CG	7.41	120.01	112.60
7	Z	10	ASP	CA-CB-CG	7.38	119.98	112.60
10	P	150	ASP	CA-CB-CG	7.34	119.94	112.60
9	A	77	ASN	CA-CB-CG	7.32	119.92	112.60
11	H	38	ASN	CA-CB-CG	7.31	119.91	112.60
9	A	64	ASP	CA-CB-CG	7.30	119.90	112.60
5	G	116	ASN	CA-CB-CG	7.29	119.89	112.60
8	M	200	ASN	CA-CB-CG	7.28	119.88	112.60
7	L	150	ASP	CA-CB-CG	7.28	119.88	112.60
7	Z	150	ASP	CA-CB-CG	7.28	119.88	112.60
12	W	170	GLY	CA-C-N	7.25	128.03	121.86
12	W	170	GLY	C-N-CA	7.25	128.03	121.86
8	M	233	ASN	CA-CB-CG	7.23	119.83	112.60
7	Z	177	PHE	CA-CB-CG	7.20	121.00	113.80
7	L	177	PHE	CA-CB-CG	7.20	121.00	113.80
10	P	143	GLY	N-CA-C	7.17	118.81	111.56
11	H	68	ASN	CA-CB-CG	7.16	119.76	112.60
12	W	30	ASN	CA-CB-CG	7.14	119.74	112.60
8	M	236	ASP	CA-CB-CG	7.13	119.73	112.60
11	H	153	PHE	CA-CB-CG	7.13	120.93	113.80
7	L	162	HIS	CA-CB-CG	7.09	120.89	113.80
10	P	225	ASN	CA-CB-CG	7.09	119.69	112.60
6	Y	31	ASP	CA-CB-CG	7.08	119.69	112.60
12	W	164	PHE	CA-CB-CG	7.06	120.86	113.80
6	K	31	ASP	CA-CB-CG	7.05	119.66	112.60
8	M	35	ASP	CA-CB-CG	7.05	119.65	112.60
9	A	80	ASP	CA-CB-CG	6.99	119.59	112.60
12	W	71	ASN	CA-CB-CG	6.97	119.58	112.60
7	Z	162	HIS	CA-CB-CG	6.97	120.77	113.80
7	L	10	ASP	CA-CB-CG	6.96	119.56	112.60
9	A	202	ASP	CA-CB-CG	6.94	119.54	112.60
7	Z	85	ASN	CA-CB-CG	6.93	119.53	112.60
11	H	212	ASN	CA-CB-CG	6.91	119.51	112.60
5	G	147	ASP	CA-CB-CG	6.91	119.51	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	53	ASP	CA-CB-CG	6.88	119.48	112.60
9	A	158	PHE	CA-CB-CG	6.88	120.68	113.80
7	L	85	ASN	CA-CB-CG	6.88	119.48	112.60
8	M	178	ASP	CA-CB-CG	6.88	119.48	112.60
8	M	197	ASP	CA-CB-CG	6.86	119.46	112.60
8	M	240	ASP	CA-CB-CG	6.86	119.46	112.60
6	Y	53	ASP	CA-CB-CG	6.85	119.45	112.60
6	K	36	PHE	CA-CB-CG	6.83	120.63	113.80
6	Y	36	PHE	CA-CB-CG	6.83	120.63	113.80
10	P	130	PHE	CA-CB-CG	6.82	120.62	113.80
7	L	158	ASN	CA-CB-CG	6.81	119.41	112.60
10	P	216	ASN	CA-CB-CG	6.80	119.40	112.60
8	M	198	ASP	CA-CB-CG	6.77	119.37	112.60
13	X	170	ASP	CA-CB-CG	6.77	119.37	112.60
7	Z	158	ASN	CA-CB-CG	6.76	119.36	112.60
7	L	109	PHE	CA-CB-CG	6.76	120.56	113.80
7	Z	109	PHE	CA-CB-CG	6.74	120.54	113.80
6	K	164	PHE	CA-CB-CG	6.72	120.52	113.80
7	L	25	PHE	CA-CB-CG	6.72	120.52	113.80
1	Q	82	ASP	CA-CB-CG	6.72	119.32	112.60
9	A	34	ASN	CA-CB-CG	6.71	119.31	112.60
9	A	204	ASP	CA-CB-CG	6.70	119.30	112.60
9	A	70	ASN	CA-CB-CG	6.67	119.27	112.60
10	P	189	HIS	CA-CB-CG	6.66	120.46	113.80
9	A	114	ASN	CA-CB-CG	6.64	119.24	112.60
12	W	165	ASN	CA-CB-CG	6.63	119.23	112.60
12	W	69	ASN	CA-CB-CG	6.62	119.22	112.60
7	Z	51	ASP	CA-CB-CG	6.61	119.21	112.60
7	L	51	ASP	CA-CB-CG	6.61	119.21	112.60
8	M	67	PHE	CA-CB-CG	6.60	120.40	113.80
10	P	173	PHE	CA-CB-CG	6.60	120.40	113.80
11	H	61	HIS	CA-CB-CG	6.59	120.39	113.80
12	W	166	ASP	CA-CB-CG	6.59	119.19	112.60
11	H	11	GLY	N-CA-C	6.58	119.44	110.69
7	Z	40	ASN	CA-CB-CG	6.57	119.17	112.60
6	K	96	ASN	CA-CB-CG	6.57	119.17	112.60
10	P	71	HIS	CA-CB-CG	6.56	120.36	113.80
8	M	135	PHE	CA-CB-CG	6.55	120.35	113.80
8	M	36	ASN	CA-CB-CG	6.54	119.14	112.60
7	L	40	ASN	CA-CB-CG	6.54	119.14	112.60
7	Z	146	ASN	CA-CB-CG	6.54	119.14	112.60
7	L	146	ASN	CA-CB-CG	6.54	119.14	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Y	96	ASN	CA-CB-CG	6.53	119.13	112.60
2	R	76	LEU	CA-C-N	6.50	128.99	120.28
2	R	76	LEU	C-N-CA	6.50	128.99	120.28
10	P	204	ASN	CA-CB-CG	6.50	119.10	112.60
12	W	198	HIS	CA-CB-CG	6.50	120.30	113.80
6	K	30	ASN	CA-CB-CG	6.50	119.09	112.60
9	A	71	ASN	CA-CB-CG	6.49	119.09	112.60
11	H	35	ASN	CA-CB-CG	6.49	119.09	112.60
10	P	170	ASN	CA-CB-CG	6.49	119.08	112.60
9	A	116	ASN	CA-CB-CG	6.46	119.06	112.60
8	M	70	LYS	CA-C-N	6.44	131.18	123.19
8	M	70	LYS	C-N-CA	6.44	131.18	123.19
1	Q	201	ASP	CA-CB-CG	6.43	119.03	112.60
10	P	220	LYS	CA-C-N	6.42	131.12	122.90
10	P	220	LYS	C-N-CA	6.42	131.12	122.90
11	H	131	ASN	CA-CB-CG	6.42	119.02	112.60
7	L	12	ILE	CA-C-N	6.42	131.15	123.19
7	L	12	ILE	C-N-CA	6.42	131.15	123.19
2	D	97	ASN	CA-CB-CG	6.41	119.01	112.60
10	P	82	ASP	CA-CB-CG	6.41	119.01	112.60
7	Z	144	ASP	CA-CB-CG	6.40	119.00	112.60
7	Z	12	ILE	CA-C-N	6.40	131.13	123.19
7	Z	12	ILE	C-N-CA	6.40	131.13	123.19
8	M	67	PHE	CA-C-N	6.39	131.02	123.16
8	M	67	PHE	C-N-CA	6.39	131.02	123.16
8	M	179	ASN	CA-CB-CG	6.39	118.99	112.60
7	L	144	ASP	CA-CB-CG	6.38	118.98	112.60
1	Q	69	ASP	CA-CB-CG	6.36	118.96	112.60
6	Y	30	ASN	CA-CB-CG	6.35	118.95	112.60
12	W	133	ASN	CA-CB-CG	6.35	118.95	112.60
2	R	97	ASN	CA-CB-CG	6.34	118.94	112.60
6	K	60	PHE	CA-CB-CG	6.32	120.12	113.80
11	H	11	GLY	CA-C-N	6.29	131.38	123.14
11	H	11	GLY	C-N-CA	6.29	131.38	123.14
6	Y	60	PHE	CA-CB-CG	6.29	120.09	113.80
6	K	57	PHE	CA-CB-CG	6.28	120.08	113.80
9	A	77	ASN	CA-C-N	6.28	129.72	120.74
9	A	77	ASN	C-N-CA	6.28	129.72	120.74
12	W	172	ASN	CA-CB-CG	6.28	118.88	112.60
6	Y	57	PHE	CA-CB-CG	6.27	120.07	113.80
7	Z	178	HIS	CA-CB-CG	6.27	120.07	113.80
11	H	157	ASP	CA-CB-CG	6.26	118.86	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	166	ASP	CA-CB-CG	6.25	118.85	112.60
12	W	174	ASP	CA-CB-CG	6.25	118.85	112.60
8	M	201	PHE	CA-CB-CG	6.24	120.04	113.80
6	Y	49	GLY	CA-C-N	6.24	129.70	120.90
6	Y	49	GLY	C-N-CA	6.24	129.70	120.90
9	A	36	ASN	CA-C-N	6.24	130.79	122.93
9	A	36	ASN	C-N-CA	6.24	130.79	122.93
2	D	101	PRO	CA-C-N	6.24	129.13	120.65
2	D	101	PRO	C-N-CA	6.24	129.13	120.65
11	H	71	ARG	NE-CZ-NH2	6.24	124.81	119.20
10	P	162	CYS	CA-C-N	6.23	129.59	122.36
10	P	162	CYS	C-N-CA	6.23	129.59	122.36
2	R	77	ASN	CA-CB-CG	6.23	118.83	112.60
2	R	101	PRO	CA-C-N	6.22	129.10	120.65
2	R	101	PRO	C-N-CA	6.22	129.10	120.65
7	L	178	HIS	CA-CB-CG	6.21	120.01	113.80
9	A	158	PHE	CA-C-N	6.20	131.92	122.93
9	A	158	PHE	C-N-CA	6.20	131.92	122.93
12	W	195	ARG	CD-NE-CZ	6.20	133.08	124.40
13	X	190	ARG	CD-NE-CZ	6.19	133.07	124.40
8	M	41	ILE	CA-C-N	6.19	128.80	122.80
8	M	41	ILE	C-N-CA	6.19	128.80	122.80
10	P	179	ASN	CA-CB-CG	6.18	118.78	112.60
6	K	95	ARG	CA-C-N	6.18	131.44	122.98
6	K	95	ARG	C-N-CA	6.18	131.44	122.98
10	P	10	LEU	CA-C-N	6.18	130.99	122.77
10	P	10	LEU	C-N-CA	6.18	130.99	122.77
6	Y	95	ARG	CA-C-N	6.17	131.44	122.98
6	Y	95	ARG	C-N-CA	6.17	131.44	122.98
6	Y	177	ASN	CA-CB-CG	6.16	118.76	112.60
8	M	180	ARG	CD-NE-CZ	6.15	133.01	124.40
12	W	19	ARG	NE-CZ-NH2	6.14	124.73	119.20
14	N	33	SER	CA-C-N	6.14	130.82	122.84
14	N	33	SER	C-N-CA	6.14	130.82	122.84
10	B	140	ASP	CA-CB-CG	6.13	118.73	112.60
7	L	24	SER	CA-C-N	6.12	130.82	122.19
7	L	24	SER	C-N-CA	6.12	130.82	122.19
14	N	190	ARG	CD-NE-CZ	6.11	132.96	124.40
12	W	100	LEU	CA-C-N	6.11	127.27	121.46
12	W	100	LEU	C-N-CA	6.11	127.27	121.46
12	W	187	ARG	CD-NE-CZ	6.11	132.95	124.40
7	L	33	LYS	CA-C-N	6.10	131.31	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	33	LYS	C-N-CA	6.10	131.31	123.13
9	A	101	ARG	CD-NE-CZ	6.10	132.94	124.40
9	A	148	GLY	CA-C-N	6.09	131.04	123.12
9	A	148	GLY	C-N-CA	6.09	131.04	123.12
9	O	165	PHE	CA-CB-CG	6.09	119.89	113.80
12	W	2	THR	CA-C-N	6.08	131.44	122.99
12	W	2	THR	C-N-CA	6.08	131.44	122.99
2	R	85	ASN	CA-CB-CG	6.07	118.67	112.60
9	A	173	VAL	CA-C-N	6.07	131.01	123.12
9	A	173	VAL	C-N-CA	6.07	131.01	123.12
11	H	76	PHE	CA-CB-CG	6.06	119.86	113.80
10	P	91	ARG	CD-NE-CZ	6.06	132.88	124.40
6	K	62	ARG	CD-NE-CZ	6.06	132.88	124.40
2	R	118	PHE	CA-CB-CG	6.05	119.85	113.80
7	L	157	ARG	CD-NE-CZ	6.05	132.86	124.40
9	A	68	ASP	CA-CB-CG	6.05	118.65	112.60
9	A	144	GLY	CA-C-N	6.04	132.04	122.74
9	A	144	GLY	C-N-CA	6.04	132.04	122.74
7	Z	157	ARG	CD-NE-CZ	6.04	132.85	124.40
12	W	172	ASN	CA-C-N	6.04	130.97	123.12
12	W	172	ASN	C-N-CA	6.04	130.97	123.12
10	P	186	ASP	CA-CB-CG	6.03	118.63	112.60
9	A	84	CYS	CA-C-N	6.02	131.48	122.99
9	A	84	CYS	C-N-CA	6.02	131.48	122.99
6	Y	62	ARG	CD-NE-CZ	6.02	132.83	124.40
1	Q	42	GLY	CA-C-N	6.01	130.51	122.93
1	Q	42	GLY	C-N-CA	6.01	130.51	122.93
11	V	38	ASN	CA-CB-CG	6.00	118.60	112.60
6	K	49	GLY	CA-C-N	6.00	129.36	120.90
6	K	49	GLY	C-N-CA	6.00	129.36	120.90
6	K	177	ASN	CA-CB-CG	5.99	118.59	112.60
7	Z	178	HIS	CA-C-N	5.99	130.56	122.90
7	Z	178	HIS	C-N-CA	5.99	130.56	122.90
10	P	67	GLN	CA-C-N	5.97	128.16	120.88
10	P	67	GLN	C-N-CA	5.97	128.16	120.88
11	V	71	ARG	NE-CZ-NH2	5.96	124.57	119.20
10	B	150	ASP	CA-CB-CG	5.96	118.56	112.60
10	P	84	ARG	CD-NE-CZ	5.96	132.74	124.40
10	P	147	TYR	CA-C-N	5.95	131.22	123.00
10	P	147	TYR	C-N-CA	5.95	131.22	123.00
6	K	31	ASP	CA-C-N	5.95	131.37	123.05
6	K	31	ASP	C-N-CA	5.95	131.37	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Y	31	ASP	CA-C-N	5.94	131.37	123.05
6	Y	31	ASP	C-N-CA	5.94	131.37	123.05
8	M	136	ASN	CA-C-N	5.93	131.23	122.99
8	M	136	ASN	C-N-CA	5.93	131.23	122.99
11	H	163	GLN	CA-C-N	5.92	131.34	122.99
11	H	163	GLN	C-N-CA	5.92	131.34	122.99
6	Y	175	GLN	CA-C-N	5.92	128.40	122.66
6	Y	175	GLN	C-N-CA	5.92	128.40	122.66
9	A	144	GLY	N-CA-C	5.91	120.28	111.18
7	Z	33	LYS	CA-C-N	5.91	131.26	123.11
7	Z	33	LYS	C-N-CA	5.91	131.26	123.11
9	A	86	MET	CA-C-N	5.91	130.88	123.14
9	A	86	MET	C-N-CA	5.91	130.88	123.14
1	Q	160	PHE	CA-CB-CG	5.90	119.70	113.80
7	Z	13	ILE	CA-C-N	5.89	130.94	123.10
7	Z	13	ILE	C-N-CA	5.89	130.94	123.10
6	Y	176	ILE	CA-C-N	5.89	130.85	122.72
6	Y	176	ILE	C-N-CA	5.89	130.85	122.72
13	X	191	ASP	CA-CB-CG	5.88	118.48	112.60
11	H	151	LEU	CA-C-N	5.88	131.33	122.98
11	H	151	LEU	C-N-CA	5.88	131.33	122.98
9	A	142	CYS	CA-C-N	5.87	131.27	122.99
9	A	142	CYS	C-N-CA	5.87	131.27	122.99
7	Z	102	SER	CA-C-N	5.87	128.89	120.56
7	Z	102	SER	C-N-CA	5.87	128.89	120.56
10	P	86	LEU	CA-C-N	5.86	128.06	120.44
10	P	86	LEU	C-N-CA	5.86	128.06	120.44
11	H	19	ARG	CA-C-N	5.86	131.76	122.74
11	H	19	ARG	C-N-CA	5.86	131.76	122.74
8	M	219	LYS	CA-C-N	5.86	131.08	123.00
8	M	219	LYS	C-N-CA	5.86	131.08	123.00
7	L	13	ILE	CA-C-N	5.85	130.88	123.10
7	L	13	ILE	C-N-CA	5.85	130.88	123.10
10	P	132	LEU	CA-C-N	5.84	131.22	122.99
10	P	132	LEU	C-N-CA	5.84	131.22	122.99
7	Z	177	PHE	CA-C-N	5.83	130.99	122.77
7	Z	177	PHE	C-N-CA	5.83	130.99	122.77
1	Q	37	LEU	CA-C-N	5.83	130.42	123.19
1	Q	37	LEU	C-N-CA	5.83	130.42	123.19
7	L	102	SER	CA-C-N	5.82	128.83	120.56
7	L	102	SER	C-N-CA	5.82	128.83	120.56
10	B	225	ASN	CA-CB-CG	5.82	118.42	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	43	VAL	CA-C-N	5.82	130.75	122.72
11	H	43	VAL	C-N-CA	5.82	130.75	122.72
11	H	159	ILE	CA-C-N	5.82	131.21	123.00
11	H	159	ILE	C-N-CA	5.82	131.21	123.00
6	K	176	ILE	CA-C-N	5.81	130.74	122.72
6	K	176	ILE	C-N-CA	5.81	130.74	122.72
10	B	143	GLY	N-CA-C	5.80	117.42	111.56
7	L	40	ASN	CA-C-N	5.79	130.73	123.14
7	L	40	ASN	C-N-CA	5.79	130.73	123.14
10	P	189	HIS	CA-C-N	5.79	127.96	120.44
10	P	189	HIS	C-N-CA	5.79	127.96	120.44
8	M	221	LEU	CA-C-N	5.78	130.50	122.93
8	M	221	LEU	C-N-CA	5.78	130.50	122.93
7	Z	103	GLY	CA-C-N	5.78	131.14	122.99
7	Z	103	GLY	C-N-CA	5.78	131.14	122.99
7	L	99	ILE	CA-C-N	5.77	131.18	123.10
7	L	99	ILE	C-N-CA	5.77	131.18	123.10
7	L	177	PHE	CA-C-N	5.77	130.91	122.77
7	L	177	PHE	C-N-CA	5.77	130.91	122.77
8	M	62	SER	CA-C-N	5.76	129.69	122.43
8	M	62	SER	C-N-CA	5.76	129.69	122.43
7	L	103	GLY	N-CA-C	5.76	118.92	110.80
12	W	162	GLY	CA-C-N	5.76	127.82	120.56
12	W	162	GLY	C-N-CA	5.76	127.82	120.56
7	Z	40	ASN	CA-C-N	5.76	130.68	123.14
7	Z	40	ASN	C-N-CA	5.76	130.68	123.14
7	Z	103	GLY	N-CA-C	5.76	118.92	110.80
8	M	222	ILE	CA-C-N	5.75	130.66	122.72
8	M	222	ILE	C-N-CA	5.75	130.66	122.72
10	B	220	LYS	CA-C-N	5.75	130.26	122.90
10	B	220	LYS	C-N-CA	5.75	130.26	122.90
12	W	173	VAL	CA-C-N	5.75	130.93	123.00
12	W	173	VAL	C-N-CA	5.75	130.93	123.00
7	L	11	GLY	CA-C-N	5.75	130.93	122.94
7	L	11	GLY	C-N-CA	5.75	130.93	122.94
11	V	10	ASN	CA-CB-CG	5.75	118.35	112.60
9	A	81	GLU	CA-C-N	5.74	130.74	123.10
9	A	81	GLU	C-N-CA	5.74	130.74	123.10
1	Q	201	ASP	CA-C-N	5.74	131.09	122.99
1	Q	201	ASP	C-N-CA	5.74	131.09	122.99
7	L	103	GLY	CA-C-N	5.74	131.08	122.99
7	L	103	GLY	C-N-CA	5.74	131.08	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	177	ARG	CD-NE-CZ	5.74	132.43	124.40
11	H	158	LYS	CA-C-N	5.73	127.89	120.56
11	H	158	LYS	C-N-CA	5.73	127.89	120.56
10	P	172	SER	CA-C-N	5.73	127.89	120.44
10	P	172	SER	C-N-CA	5.73	127.89	120.44
6	K	175	GLN	CA-C-N	5.73	129.11	122.35
6	K	175	GLN	C-N-CA	5.73	129.11	122.35
10	P	148	GLN	CA-C-N	5.72	130.89	123.11
10	P	148	GLN	C-N-CA	5.72	130.89	123.11
8	M	223	TYR	CA-C-N	5.72	130.79	123.13
8	M	223	TYR	C-N-CA	5.72	130.79	123.13
7	Z	11	GLY	CA-C-N	5.72	130.89	122.94
7	Z	11	GLY	C-N-CA	5.72	130.89	122.94
7	L	98	GLY	CA-C-N	5.71	130.62	123.14
7	L	98	GLY	C-N-CA	5.71	130.62	123.14
10	P	71	HIS	CA-C-N	5.71	130.69	123.10
10	P	71	HIS	C-N-CA	5.71	130.69	123.10
7	Z	98	GLY	CA-C-N	5.71	130.62	123.14
7	Z	98	GLY	C-N-CA	5.71	130.62	123.14
7	Z	99	ILE	CA-C-N	5.71	131.09	123.10
7	Z	99	ILE	C-N-CA	5.71	131.09	123.10
8	M	134	ALA	CA-C-N	5.70	131.03	123.05
8	M	134	ALA	C-N-CA	5.70	131.03	123.05
9	O	80	ASP	CA-CB-CG	5.70	118.30	112.60
7	Z	1	THR	CA-C-N	5.69	130.70	122.44
7	Z	1	THR	C-N-CA	5.69	130.70	122.44
10	P	185	GLU	CA-C-N	5.69	128.18	120.38
10	P	185	GLU	C-N-CA	5.69	128.18	120.38
13	X	113	GLY	N-CA-C	5.69	118.53	110.74
9	A	44	GLY	CA-C-N	5.68	130.32	122.77
9	A	44	GLY	C-N-CA	5.68	130.32	122.77
12	W	11	ALA	CA-C-N	5.67	130.57	123.14
12	W	11	ALA	C-N-CA	5.67	130.57	123.14
8	M	133	TYR	N-CA-CB	5.67	117.60	110.45
10	P	19	LEU	CA-C-N	5.67	128.22	120.46
10	P	19	LEU	C-N-CA	5.67	128.22	120.46
6	K	191	GLN	CA-C-N	5.67	130.99	123.00
6	K	191	GLN	C-N-CA	5.67	130.99	123.00
9	A	175	GLY	N-CA-C	5.66	118.22	110.58
7	L	1	THR	CA-C-N	5.66	130.64	122.44
7	L	1	THR	C-N-CA	5.66	130.64	122.44
10	P	161	THR	CA-C-N	5.64	131.87	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	161	THR	C-N-CA	5.64	131.87	122.73
12	W	14	LEU	CA-C-N	5.64	127.16	121.35
12	W	14	LEU	C-N-CA	5.64	127.16	121.35
1	Q	88	ASN	CA-CB-CG	5.63	118.23	112.60
10	P	229	ASP	CA-CB-CG	5.63	118.23	112.60
6	K	30	ASN	CA-C-N	5.63	131.87	121.52
6	K	30	ASN	C-N-CA	5.63	131.87	121.52
7	L	86	ILE	N-CA-CB	5.62	116.75	110.51
6	Y	180	LEU	CA-C-N	5.62	131.28	123.07
6	Y	180	LEU	C-N-CA	5.62	131.28	123.07
7	Z	86	ILE	N-CA-CB	5.62	116.75	110.51
11	H	131	ASN	CA-C-N	5.62	127.64	120.56
11	H	131	ASN	C-N-CA	5.62	127.64	120.56
1	Q	84	ASN	CA-C-N	5.62	127.64	120.56
1	Q	84	ASN	C-N-CA	5.62	127.64	120.56
7	Z	15	ALA	CA-C-N	5.62	129.87	122.51
7	Z	15	ALA	C-N-CA	5.62	129.87	122.51
10	P	83	PHE	N-CA-CB	5.62	118.15	110.01
6	K	180	LEU	CA-C-N	5.61	131.26	123.07
6	K	180	LEU	C-N-CA	5.61	131.26	123.07
7	L	15	ALA	CA-C-N	5.61	129.86	122.51
7	L	15	ALA	C-N-CA	5.61	129.86	122.51
6	K	25	ILE	CA-C-N	5.61	129.11	123.16
6	K	25	ILE	C-N-CA	5.61	129.11	123.16
6	Y	191	GLN	CA-C-N	5.61	130.91	123.00
6	Y	191	GLN	C-N-CA	5.61	130.91	123.00
13	X	22	ALA	CA-C-N	5.61	130.78	122.99
13	X	22	ALA	C-N-CA	5.61	130.78	122.99
1	Q	43	VAL	CA-C-N	5.60	130.55	123.10
1	Q	43	VAL	C-N-CA	5.60	130.55	123.10
12	I	71	ASN	CA-CB-CG	5.60	118.20	112.60
8	M	78	CYS	CA-C-N	5.60	130.65	122.69
8	M	78	CYS	C-N-CA	5.60	130.65	122.69
6	Y	30	ASN	CA-C-N	5.60	131.83	121.52
6	Y	30	ASN	C-N-CA	5.60	131.83	121.52
10	B	162	CYS	CA-C-N	5.60	128.86	122.36
10	B	162	CYS	C-N-CA	5.60	128.86	122.36
7	L	175	ARG	CA-C-N	5.59	130.63	123.13
7	L	175	ARG	C-N-CA	5.59	130.63	123.13
8	M	138	LEU	CA-C-N	5.59	130.88	123.05
8	M	138	LEU	C-N-CA	5.59	130.88	123.05
9	A	172	CYS	CA-C-N	5.59	130.76	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	172	CYS	C-N-CA	5.59	130.76	122.99
3	S	9	ASP	CA-CB-CG	5.59	118.19	112.60
6	Y	44	CYS	CA-C-N	5.59	131.04	123.11
6	Y	44	CYS	C-N-CA	5.59	131.04	123.11
11	H	152	ILE	CA-C-N	5.58	130.43	122.72
11	H	152	ILE	C-N-CA	5.58	130.43	122.72
10	P	117	ILE	CA-C-N	5.58	127.60	120.56
10	P	117	ILE	C-N-CA	5.58	127.60	120.56
7	Z	175	ARG	CA-C-N	5.58	130.61	123.13
7	Z	175	ARG	C-N-CA	5.58	130.61	123.13
9	A	192	ARG	NE-CZ-NH2	5.57	124.22	119.20
9	O	164	GLY	CA-C-N	5.57	130.85	123.05
9	O	164	GLY	C-N-CA	5.57	130.85	123.05
7	L	178	HIS	CA-C-N	5.57	130.03	122.90
7	L	178	HIS	C-N-CA	5.57	130.03	122.90
8	M	194	ASN	CA-C-N	5.57	127.68	120.44
8	M	194	ASN	C-N-CA	5.57	127.68	120.44
8	M	51	LEU	CA-C-N	5.57	130.84	122.99
8	M	51	LEU	C-N-CA	5.57	130.84	122.99
11	H	129	VAL	CA-C-N	5.57	127.74	120.28
11	H	129	VAL	C-N-CA	5.57	127.74	120.28
9	A	247	LYS	CA-C-N	5.56	127.67	120.44
9	A	247	LYS	C-N-CA	5.56	127.67	120.44
13	X	74	ASN	CA-CB-CG	5.56	118.16	112.60
6	K	44	CYS	CA-C-N	5.56	131.00	123.11
6	K	44	CYS	C-N-CA	5.56	131.00	123.11
11	H	62	TYR	CA-C-N	5.56	127.66	120.44
11	H	62	TYR	C-N-CA	5.56	127.66	120.44
8	M	220	THR	CA-C-N	5.54	130.98	123.11
8	M	220	THR	C-N-CA	5.54	130.98	123.11
1	Q	214	TYR	CA-C-N	5.54	130.82	123.00
1	Q	214	TYR	C-N-CA	5.54	130.82	123.00
10	P	110	LEU	CA-C-N	5.54	127.55	120.56
10	P	110	LEU	C-N-CA	5.54	127.55	120.56
2	R	83	LEU	CA-C-N	5.54	127.54	120.56
2	R	83	LEU	C-N-CA	5.54	127.54	120.56
6	Y	25	ILE	CA-C-N	5.53	129.03	123.16
6	Y	25	ILE	C-N-CA	5.53	129.03	123.16
8	M	169	GLY	CA-C-N	5.53	127.63	120.44
8	M	169	GLY	C-N-CA	5.53	127.63	120.44
1	Q	108	SER	CA-C-N	5.53	127.63	120.44
1	Q	108	SER	C-N-CA	5.53	127.63	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	34	ILE	CA-C-N	5.52	130.78	123.05
8	M	34	ILE	C-N-CA	5.52	130.78	123.05
10	P	89	ARG	CA-C-N	5.52	127.62	120.44
10	P	89	ARG	C-N-CA	5.52	127.62	120.44
7	Z	100	ILE	CA-C-N	5.52	129.72	121.72
7	Z	100	ILE	C-N-CA	5.52	129.72	121.72
9	A	182	ILE	N-CA-CB	5.52	116.64	110.51
11	H	3	ILE	CA-C-N	5.52	130.61	122.94
11	H	3	ILE	C-N-CA	5.52	130.61	122.94
13	X	114	PHE	CA-CB-CG	5.52	119.32	113.80
1	Q	171	ALA	CA-C-N	5.51	127.67	120.28
1	Q	171	ALA	C-N-CA	5.51	127.67	120.28
2	R	120	HIS	CA-CB-CG	5.51	119.31	113.80
13	X	49	ASN	CA-CB-CG	5.51	118.11	112.60
10	P	22	ILE	N-CA-CB	5.50	116.99	110.55
7	L	100	ILE	CA-C-N	5.50	129.70	121.72
7	L	100	ILE	C-N-CA	5.50	129.70	121.72
7	Z	90	TYR	CA-C-N	5.49	127.58	120.44
7	Z	90	TYR	C-N-CA	5.49	127.58	120.44
10	B	216	ASN	CA-CB-CG	5.49	118.09	112.60
10	P	170	ASN	CA-C-N	5.49	127.64	120.28
10	P	170	ASN	C-N-CA	5.49	127.64	120.28
7	L	2	THR	CA-C-N	5.49	130.51	122.77
7	L	2	THR	C-N-CA	5.49	130.51	122.77
10	P	223	THR	CA-C-N	5.48	128.17	120.28
10	P	223	THR	C-N-CA	5.48	128.17	120.28
7	Z	2	THR	CA-C-N	5.48	130.50	122.77
7	Z	2	THR	C-N-CA	5.48	130.50	122.77
12	W	19	ARG	CA-C-N	5.48	130.71	122.99
12	W	19	ARG	C-N-CA	5.48	130.71	122.99
11	V	6	ILE	CA-C-N	5.48	129.91	122.90
11	V	6	ILE	C-N-CA	5.48	129.91	122.90
8	M	88	ASP	CA-C-N	5.47	127.46	120.56
8	M	88	ASP	C-N-CA	5.47	127.46	120.56
9	A	117	ALA	CA-C-N	5.47	127.56	120.44
9	A	117	ALA	C-N-CA	5.47	127.56	120.44
7	L	90	TYR	CA-C-N	5.47	127.55	120.44
7	L	90	TYR	C-N-CA	5.47	127.55	120.44
11	H	164	LEU	CA-C-N	5.47	130.72	123.00
11	H	164	LEU	C-N-CA	5.47	130.72	123.00
13	J	36	THR	CA-C-N	5.46	128.01	121.84
13	J	36	THR	C-N-CA	5.46	128.01	121.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	196	LYS	CA-C-N	5.46	127.60	120.28
10	P	196	LYS	C-N-CA	5.46	127.60	120.28
12	W	185	HIS	CA-CB-CG	5.46	119.26	113.80
11	H	56	ILE	N-CA-CB	5.46	116.94	110.55
8	M	233	ASN	CA-C-N	5.45	130.77	122.65
8	M	233	ASN	C-N-CA	5.45	130.77	122.65
6	Y	52	GLY	CA-C-N	5.45	127.59	120.28
6	Y	52	GLY	C-N-CA	5.45	127.59	120.28
12	W	159	ILE	CA-C-N	5.44	127.52	120.44
12	W	159	ILE	C-N-CA	5.44	127.52	120.44
9	A	85	SER	CA-C-N	5.44	130.67	123.00
9	A	85	SER	C-N-CA	5.44	130.67	123.00
9	O	117	ALA	CA-C-N	5.43	127.50	120.44
9	O	117	ALA	C-N-CA	5.43	127.50	120.44
12	W	201	HIS	CA-CB-CG	5.43	119.23	113.80
6	K	60	PHE	CA-C-N	5.43	127.40	120.56
6	K	60	PHE	C-N-CA	5.43	127.40	120.56
7	L	95	LEU	CA-C-N	5.43	130.77	122.95
7	L	95	LEU	C-N-CA	5.43	130.77	122.95
10	B	157	ASN	CA-CB-CG	5.43	118.03	112.60
11	V	11	GLY	N-CA-C	5.42	117.90	110.69
7	L	178	HIS	CE1-NE2-CD2	-5.42	103.58	109.00
9	A	157	LEU	CA-C-N	5.42	130.63	122.99
9	A	157	LEU	C-N-CA	5.42	130.63	122.99
10	P	106	LEU	CA-C-N	5.42	127.39	120.56
10	P	106	LEU	C-N-CA	5.42	127.39	120.56
8	M	235	LEU	CA-C-N	5.42	129.82	122.19
8	M	235	LEU	C-N-CA	5.42	129.82	122.19
13	X	43	LYS	CA-C-N	5.41	130.15	123.12
13	X	43	LYS	C-N-CA	5.41	130.15	123.12
13	X	178	GLU	CA-C-N	5.41	127.47	120.44
13	X	178	GLU	C-N-CA	5.41	127.47	120.44
7	Z	178	HIS	CE1-NE2-CD2	-5.40	103.60	109.00
7	L	131	GLY	CA-C-N	5.40	127.46	120.44
7	L	131	GLY	C-N-CA	5.40	127.46	120.44
10	P	21	GLN	CA-C-N	5.40	127.36	120.56
10	P	21	GLN	C-N-CA	5.40	127.36	120.56
13	X	41	PHE	CA-CB-CG	5.40	119.20	113.80
13	X	129	ASN	CA-C-N	5.40	129.95	122.77
13	X	129	ASN	C-N-CA	5.40	129.95	122.77
11	H	128	LEU	CA-C-N	5.39	127.36	120.56
11	H	128	LEU	C-N-CA	5.39	127.36	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	36	ASN	CA-CB-CG	5.39	117.99	112.60
7	Z	95	LEU	CA-C-N	5.39	130.71	122.95
7	Z	95	LEU	C-N-CA	5.39	130.71	122.95
10	P	193	LEU	CA-C-N	5.39	127.44	120.44
10	P	193	LEU	C-N-CA	5.39	127.44	120.44
8	M	39	THR	CA-C-N	5.39	130.63	122.98
8	M	39	THR	C-N-CA	5.39	130.63	122.98
8	M	200	ASN	CA-C-N	5.38	127.44	120.44
8	M	200	ASN	C-N-CA	5.38	127.44	120.44
6	Y	60	PHE	CA-C-N	5.38	127.34	120.56
6	Y	60	PHE	C-N-CA	5.38	127.34	120.56
10	B	67	GLN	CA-C-N	5.38	127.44	120.88
10	B	67	GLN	C-N-CA	5.38	127.44	120.88
10	P	103	SER	CA-C-N	5.38	128.87	120.75
10	P	103	SER	C-N-CA	5.38	128.87	120.75
6	K	102	CYS	N-CA-C	5.37	117.43	108.99
9	O	114	ASN	CA-CB-CG	5.37	117.97	112.60
10	P	71	HIS	CE1-NE2-CD2	-5.37	103.63	109.00
13	X	102	PHE	CA-C-N	5.37	127.36	122.37
13	X	102	PHE	C-N-CA	5.37	127.36	122.37
7	Z	89	GLN	CA-C-N	5.37	131.07	122.86
7	Z	89	GLN	C-N-CA	5.37	131.07	122.86
11	V	230	ILE	CA-C-N	5.37	130.17	123.14
11	V	230	ILE	C-N-CA	5.37	130.17	123.14
12	W	165	ASN	CA-C-N	5.37	130.56	123.05
12	W	165	ASN	C-N-CA	5.37	130.56	123.05
7	Z	131	GLY	CA-C-N	5.36	127.47	120.28
7	Z	131	GLY	C-N-CA	5.36	127.47	120.28
5	G	151	ILE	CA-C-N	5.36	130.98	122.94
5	G	151	ILE	C-N-CA	5.36	130.98	122.94
8	M	127	ARG	CA-C-N	5.36	127.78	120.54
8	M	127	ARG	C-N-CA	5.36	127.78	120.54
12	I	69	ASN	CA-CB-CG	5.35	117.95	112.60
7	L	89	GLN	CA-C-N	5.35	131.04	122.86
7	L	89	GLN	C-N-CA	5.35	131.04	122.86
7	Z	152	ALA	CA-C-N	5.35	127.30	120.56
7	Z	152	ALA	C-N-CA	5.35	127.30	120.56
9	A	113	TYR	CA-C-N	5.35	128.46	120.87
9	A	113	TYR	C-N-CA	5.35	128.46	120.87
10	P	114	ILE	CA-C-N	5.35	127.39	120.44
10	P	114	ILE	C-N-CA	5.35	127.39	120.44
7	L	62	ILE	CA-C-N	5.34	127.78	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	62	ILE	C-N-CA	5.34	127.78	120.46
7	L	149	LEU	CA-C-N	5.34	127.39	120.44
7	L	149	LEU	C-N-CA	5.34	127.39	120.44
6	K	33	ASN	CA-C-N	5.34	129.78	122.84
6	K	33	ASN	C-N-CA	5.34	129.78	122.84
7	L	153	VAL	CA-C-N	5.34	127.38	120.44
7	L	153	VAL	C-N-CA	5.34	127.38	120.44
10	P	153	GLY	CA-C-N	5.34	130.09	122.72
10	P	153	GLY	C-N-CA	5.34	130.09	122.72
1	Q	81	ALA	CA-C-N	5.34	127.43	120.28
1	Q	81	ALA	C-N-CA	5.34	127.43	120.28
9	A	70	ASN	CA-C-N	5.34	127.87	120.29
9	A	70	ASN	C-N-CA	5.34	127.87	120.29
8	M	198	ASP	CA-C-N	5.33	127.28	120.56
8	M	198	ASP	C-N-CA	5.33	127.28	120.56
6	Y	141	ALA	CA-C-N	5.33	127.28	120.56
6	Y	141	ALA	C-N-CA	5.33	127.28	120.56
9	A	120	LEU	CA-C-N	5.33	127.37	120.44
9	A	120	LEU	C-N-CA	5.33	127.37	120.44
10	P	83	PHE	CA-CB-CG	5.33	119.13	113.80
7	L	152	ALA	CA-C-N	5.33	127.28	120.56
7	L	152	ALA	C-N-CA	5.33	127.28	120.56
7	Z	58	TYR	CA-C-N	5.33	127.37	120.44
7	Z	58	TYR	C-N-CA	5.33	127.37	120.44
10	B	147	TYR	CA-C-N	5.33	130.35	123.00
10	B	147	TYR	C-N-CA	5.33	130.35	123.00
1	Q	89	GLN	CA-C-N	5.33	127.36	120.44
1	Q	89	GLN	C-N-CA	5.33	127.36	120.44
1	C	57	ASP	CA-CB-CG	5.32	117.92	112.60
6	K	141	ALA	CA-C-N	5.32	127.27	120.56
6	K	141	ALA	C-N-CA	5.32	127.27	120.56
10	B	189	HIS	CA-CB-CG	5.32	119.12	113.80
7	Z	153	VAL	CA-C-N	5.32	127.36	120.44
7	Z	153	VAL	C-N-CA	5.32	127.36	120.44
12	W	35	HIS	CA-CB-CG	5.32	119.12	113.80
10	P	27	ASN	CA-C-N	5.32	127.36	120.44
10	P	27	ASN	C-N-CA	5.32	127.36	120.44
9	A	148	GLY	N-CA-C	5.32	118.34	110.42
10	B	86	LEU	CA-C-N	5.32	127.35	120.44
10	B	86	LEU	C-N-CA	5.32	127.35	120.44
13	X	167	TYR	CA-C-N	5.31	130.39	123.06
13	X	167	TYR	C-N-CA	5.31	130.39	123.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Z	39	LYS	CA-C-N	5.31	130.56	122.23
7	Z	39	LYS	C-N-CA	5.31	130.56	122.23
7	Z	149	LEU	CA-C-N	5.31	127.34	120.44
7	Z	149	LEU	C-N-CA	5.31	127.34	120.44
13	X	180	ILE	N-CA-CB	5.30	116.76	110.55
6	Y	168	LYS	N-CA-CB	5.30	117.70	110.01
11	H	61	HIS	CA-C-N	5.30	127.33	120.44
11	H	61	HIS	C-N-CA	5.30	127.33	120.44
6	K	62	ARG	N-CA-CB	5.30	117.70	110.01
10	B	148	GLN	CA-C-N	5.30	130.01	123.12
10	B	148	GLN	C-N-CA	5.30	130.01	123.12
9	O	42	VAL	CA-C-N	5.30	129.82	122.77
9	O	42	VAL	C-N-CA	5.30	129.82	122.77
11	V	11	GLY	CA-C-N	5.30	130.37	123.06
11	V	11	GLY	C-N-CA	5.30	130.37	123.06
7	Z	62	ILE	CA-C-N	5.29	127.71	120.46
7	Z	62	ILE	C-N-CA	5.29	127.71	120.46
7	Z	154	GLU	CA-C-N	5.29	127.31	120.44
7	Z	154	GLU	C-N-CA	5.29	127.31	120.44
10	B	169	ASN	CA-CB-CG	5.29	117.89	112.60
13	X	189	ASP	CA-C-N	5.29	130.69	122.49
13	X	189	ASP	C-N-CA	5.29	130.69	122.49
8	M	43	LEU	CA-C-N	5.29	130.53	122.65
8	M	43	LEU	C-N-CA	5.29	130.53	122.65
6	K	168	LYS	CA-C-N	5.28	127.62	120.44
6	K	168	LYS	C-N-CA	5.28	127.62	120.44
7	L	58	TYR	CA-C-N	5.28	127.30	120.44
7	L	58	TYR	C-N-CA	5.28	127.30	120.44
6	Y	62	ARG	N-CA-CB	5.28	117.67	110.01
10	B	132	LEU	CA-C-N	5.28	130.43	122.99
10	B	132	LEU	C-N-CA	5.28	130.43	122.99
7	L	156	ALA	CA-C-N	5.27	127.30	120.44
7	L	156	ALA	C-N-CA	5.27	127.30	120.44
9	A	92	ASP	CA-C-N	5.27	127.30	120.44
9	A	92	ASP	C-N-CA	5.27	127.30	120.44
10	P	25	ALA	CA-C-N	5.27	127.29	120.44
10	P	25	ALA	C-N-CA	5.27	127.29	120.44
8	M	201	PHE	CA-C-N	5.27	127.20	120.56
8	M	201	PHE	C-N-CA	5.27	127.20	120.56
13	X	48	ASN	CA-CB-CG	5.27	117.87	112.60
7	L	39	LYS	CA-C-N	5.26	130.50	122.23
7	L	39	LYS	C-N-CA	5.26	130.50	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	150	ASP	CA-C-N	5.26	127.28	120.44
7	L	150	ASP	C-N-CA	5.26	127.28	120.44
11	H	157	ASP	O-C-N	-5.26	117.25	123.41
8	a	127	ARG	CA-C-N	5.26	127.64	120.54
8	a	127	ARG	C-N-CA	5.26	127.64	120.54
1	Q	197	ALA	CA-C-N	5.26	127.28	120.44
1	Q	197	ALA	C-N-CA	5.26	127.28	120.44
11	V	35	ASN	CA-CB-CG	5.26	117.86	112.60
8	M	85	MET	CA-C-N	5.26	127.32	120.28
8	M	85	MET	C-N-CA	5.26	127.32	120.28
2	R	94	TYR	N-CA-CB	5.26	117.63	110.01
7	Z	178	HIS	ND1-CG-CD2	-5.26	100.84	106.10
10	B	204	ASN	CA-CB-CG	5.26	117.86	112.60
11	H	58	ILE	CA-C-N	5.26	127.66	120.46
11	H	58	ILE	C-N-CA	5.26	127.66	120.46
7	L	178	HIS	CG-CD2-NE2	5.25	112.45	107.20
7	Z	156	ALA	CA-C-N	5.25	127.27	120.44
7	Z	156	ALA	C-N-CA	5.25	127.27	120.44
9	A	155	PRO	CA-C-N	5.25	130.81	122.62
9	A	155	PRO	C-N-CA	5.25	130.81	122.62
6	K	145	LYS	N-CA-CB	5.25	117.58	109.91
6	Y	56	GLN	CA-C-N	5.25	127.26	120.44
6	Y	56	GLN	C-N-CA	5.25	127.26	120.44
7	Z	133	THR	CA-C-N	5.25	127.26	120.44
7	Z	133	THR	C-N-CA	5.25	127.26	120.44
10	B	173	PHE	CA-CB-CG	5.25	119.05	113.80
6	K	168	LYS	N-CA-CB	5.25	117.62	110.01
9	A	145	MET	CA-C-N	5.25	130.28	122.99
9	A	145	MET	C-N-CA	5.25	130.28	122.99
10	B	71	HIS	CA-CB-CG	5.25	119.05	113.80
7	Z	82	ILE	CA-C-N	5.25	127.26	120.44
7	Z	82	ILE	C-N-CA	5.25	127.26	120.44
7	Z	178	HIS	CG-CD2-NE2	5.24	112.44	107.20
6	K	162	LEU	CA-C-N	5.24	127.25	120.44
6	K	162	LEU	C-N-CA	5.24	127.25	120.44
11	H	55	ILE	CA-C-N	5.24	127.16	120.56
11	H	55	ILE	C-N-CA	5.24	127.16	120.56
10	P	231	LEU	CA-C-N	5.24	127.16	120.56
10	P	231	LEU	C-N-CA	5.24	127.16	120.56
8	M	178	ASP	CA-C-N	5.24	127.25	120.44
8	M	178	ASP	C-N-CA	5.24	127.25	120.44
6	K	52	GLY	CA-C-N	5.24	127.25	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	52	GLY	C-N-CA	5.24	127.25	120.44
7	L	41	ILE	CA-C-N	5.24	131.30	122.87
7	L	41	ILE	C-N-CA	5.24	131.30	122.87
7	L	133	THR	CA-C-N	5.23	127.24	120.44
7	L	133	THR	C-N-CA	5.23	127.24	120.44
12	W	128	GLY	CA-C-N	5.23	127.29	120.28
12	W	128	GLY	C-N-CA	5.23	127.29	120.28
2	R	10	PHE	CA-CB-CG	5.23	119.03	113.80
7	L	178	HIS	ND1-CG-CD2	-5.23	100.87	106.10
7	Z	150	ASP	CA-C-N	5.23	127.24	120.44
7	Z	150	ASP	C-N-CA	5.23	127.24	120.44
10	B	156	PHE	CA-C-N	5.23	129.73	122.77
10	B	156	PHE	C-N-CA	5.23	129.73	122.77
1	Q	174	VAL	CA-C-N	5.23	127.24	120.44
1	Q	174	VAL	C-N-CA	5.23	127.24	120.44
10	P	71	HIS	ND1-CG-CD2	-5.23	100.87	106.10
7	L	154	GLU	CA-C-N	5.23	127.23	120.44
7	L	154	GLU	C-N-CA	5.23	127.23	120.44
10	P	173	PHE	CA-C-N	5.23	127.28	120.28
10	P	173	PHE	C-N-CA	5.23	127.28	120.28
11	V	33	LYS	CA-C-N	5.23	129.78	122.93
11	V	33	LYS	C-N-CA	5.23	129.78	122.93
7	L	82	ILE	CA-C-N	5.22	127.23	120.44
7	L	82	ILE	C-N-CA	5.22	127.23	120.44
6	Y	102	CYS	N-CA-C	5.22	117.19	108.99
10	P	178	TYR	CA-C-N	5.22	131.19	122.73
10	P	178	TYR	C-N-CA	5.22	131.19	122.73
7	Z	41	ILE	CA-C-N	5.22	131.28	122.87
7	Z	41	ILE	C-N-CA	5.22	131.28	122.87
10	B	145	HIS	CA-CB-CG	5.22	119.02	113.80
7	L	137	SER	CA-C-N	5.22	127.14	120.56
7	L	137	SER	C-N-CA	5.22	127.14	120.56
7	Z	129	GLY	N-CA-C	5.22	118.36	111.52
2	R	93	ARG	CA-C-N	5.22	127.22	120.44
2	R	93	ARG	C-N-CA	5.22	127.22	120.44
12	W	66	HIS	CA-C-N	5.22	127.23	120.44
12	W	66	HIS	C-N-CA	5.22	127.23	120.44
6	Y	145	LYS	N-CA-CB	5.22	117.53	109.91
9	O	121	CYS	CA-C-N	5.22	127.22	120.44
9	O	121	CYS	C-N-CA	5.22	127.22	120.44
9	A	235	SER	CA-C-N	5.21	127.79	120.28
9	A	235	SER	C-N-CA	5.21	127.79	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	104	GLU	CA-CB-CG	5.21	124.53	114.10
13	X	113	GLY	CA-C-N	5.21	130.34	122.99
13	X	113	GLY	C-N-CA	5.21	130.34	122.99
10	P	88	LYS	CA-C-N	5.21	127.22	120.44
10	P	88	LYS	C-N-CA	5.21	127.22	120.44
6	K	56	GLN	CA-C-N	5.21	127.21	120.44
6	K	56	GLN	C-N-CA	5.21	127.21	120.44
10	B	91	ARG	CD-NE-CZ	5.21	131.69	124.40
11	V	195	ASP	CA-CB-CG	5.21	117.81	112.60
2	D	94	TYR	N-CA-CB	5.21	117.56	110.01
10	P	111	VAL	CA-C-N	5.20	127.20	120.44
10	P	111	VAL	C-N-CA	5.20	127.20	120.44
2	R	86	LYS	CA-C-N	5.20	127.20	120.44
2	R	86	LYS	C-N-CA	5.20	127.20	120.44
9	O	158	PHE	CA-C-N	5.19	130.72	122.94
9	O	158	PHE	C-N-CA	5.19	130.72	122.94
7	Z	137	SER	CA-C-N	5.19	127.10	120.56
7	Z	137	SER	C-N-CA	5.19	127.10	120.56
7	L	129	GLY	N-CA-C	5.19	118.31	111.52
6	Y	168	LYS	CA-C-N	5.19	127.49	120.44
6	Y	168	LYS	C-N-CA	5.19	127.49	120.44
10	P	71	HIS	CG-CD2-NE2	5.19	112.39	107.20
6	Y	57	PHE	N-CA-CB	5.19	117.53	110.01
13	J	32	ASN	CA-CB-CG	5.19	117.79	112.60
10	P	83	PHE	CA-C-N	5.19	127.18	120.44
10	P	83	PHE	C-N-CA	5.19	127.18	120.44
10	P	142	TYR	CA-C-N	5.18	129.47	122.42
10	P	142	TYR	C-N-CA	5.18	129.47	122.42
13	X	45	PHE	CA-CB-CG	5.18	118.98	113.80
6	Y	140	SER	CA-C-N	5.18	127.18	120.44
6	Y	140	SER	C-N-CA	5.18	127.18	120.44
9	A	96	MET	CA-C-N	5.18	127.09	120.56
9	A	96	MET	C-N-CA	5.18	127.09	120.56
10	B	189	HIS	CA-C-N	5.18	127.17	120.44
10	B	189	HIS	C-N-CA	5.18	127.17	120.44
8	M	161	ALA	CA-C-N	5.18	129.48	120.68
8	M	161	ALA	C-N-CA	5.18	129.48	120.68
7	Z	157	ARG	CA-C-N	5.18	127.17	120.44
7	Z	157	ARG	C-N-CA	5.18	127.17	120.44
11	H	34	ILE	CA-C-N	5.18	130.44	122.93
11	H	34	ILE	C-N-CA	5.18	130.44	122.93
11	H	195	ASP	CA-CB-CG	5.17	117.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	227	ILE	CA-C-N	5.17	127.17	120.44
10	P	227	ILE	C-N-CA	5.17	127.17	120.44
12	W	33	LYS	CB-CG-CD	5.17	123.20	111.30
11	H	65	SER	CA-C-N	5.17	127.17	120.44
11	H	65	SER	C-N-CA	5.17	127.17	120.44
11	H	132	VAL	CA-C-N	5.17	127.17	120.44
11	H	132	VAL	C-N-CA	5.17	127.17	120.44
6	Y	166	GLU	N-CA-CB	5.17	117.51	110.01
6	K	140	SER	CA-C-N	5.17	127.16	120.44
6	K	140	SER	C-N-CA	5.17	127.16	120.44
12	W	171	GLY	N-CA-C	5.17	117.81	111.45
6	K	57	PHE	N-CA-CB	5.17	117.50	110.01
1	Q	111	VAL	CA-C-N	5.17	127.07	120.56
1	Q	111	VAL	C-N-CA	5.17	127.07	120.56
11	H	212	ASN	CA-C-N	5.17	127.16	120.44
11	H	212	ASN	C-N-CA	5.17	127.16	120.44
10	P	113	ILE	N-CA-CB	5.17	116.59	110.55
1	Q	198	LYS	CA-C-N	5.16	127.20	120.28
1	Q	198	LYS	C-N-CA	5.16	127.20	120.28
10	B	161	THR	CA-C-N	5.16	131.09	122.73
10	B	161	THR	C-N-CA	5.16	131.09	122.73
13	X	6	ASN	CA-CB-CG	5.16	117.76	112.60
10	P	109	GLU	CA-C-N	5.16	127.15	120.44
10	P	109	GLU	C-N-CA	5.16	127.15	120.44
11	H	64	VAL	N-CA-CB	5.15	116.58	110.55
2	D	93	ARG	CA-C-N	5.15	127.14	120.44
2	D	93	ARG	C-N-CA	5.15	127.14	120.44
6	K	163	CYS	CA-C-N	5.15	127.14	120.44
6	K	163	CYS	C-N-CA	5.15	127.14	120.44
10	P	207	ASN	CA-CB-CG	5.15	117.75	112.60
11	H	72	LYS	CA-C-N	5.15	128.87	121.50
11	H	72	LYS	C-N-CA	5.15	128.87	121.50
7	L	73	LYS	CA-C-N	5.15	128.31	120.95
7	L	73	LYS	C-N-CA	5.15	128.31	120.95
7	L	75	SER	CA-C-N	5.14	127.50	120.46
7	L	75	SER	C-N-CA	5.14	127.50	120.46
1	Q	34	THR	CA-C-N	5.14	131.31	122.67
1	Q	34	THR	C-N-CA	5.14	131.31	122.67
11	V	157	ASP	CA-CB-CG	5.14	117.74	112.60
7	Z	155	LEU	N-CA-CB	5.14	117.47	110.01
9	A	246	GLU	CA-C-N	5.14	127.12	120.44
9	A	246	GLU	C-N-CA	5.14	127.12	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	142	ILE	N-CA-CB	5.14	116.56	110.55
14	N	39	ASN	CA-CB-CG	5.14	117.74	112.60
7	L	157	ARG	CA-C-N	5.14	127.12	120.44
7	L	157	ARG	C-N-CA	5.14	127.12	120.44
12	W	35	HIS	CA-C-N	5.14	129.60	122.77
12	W	35	HIS	C-N-CA	5.14	129.60	122.77
7	L	108	GLY	CA-C-N	5.13	129.16	121.72
7	L	108	GLY	C-N-CA	5.13	129.16	121.72
10	P	23	GLU	CA-C-N	5.13	127.16	120.28
10	P	23	GLU	C-N-CA	5.13	127.16	120.28
10	P	88	LYS	CA-CB-CG	5.13	124.37	114.10
5	G	101	TYR	N-CA-CB	5.13	117.45	110.01
6	K	166	GLU	N-CA-CB	5.13	117.45	110.01
9	A	145	MET	CA-CB-CG	5.13	124.36	114.10
11	H	178	ASP	CA-CB-CG	5.13	117.73	112.60
1	Q	126	GLY	CA-C-N	5.12	131.12	122.87
1	Q	126	GLY	C-N-CA	5.12	131.12	122.87
6	K	61	ILE	N-CA-CB	5.12	116.54	110.55
10	P	28	ARG	N-CA-CB	5.12	117.44	110.01
5	G	161	TYR	CA-C-N	5.12	129.67	122.09
5	G	161	TYR	C-N-CA	5.12	129.67	122.09
9	A	204	ASP	N-CA-CB	5.12	117.65	110.12
13	X	147	ARG	NE-CZ-NH2	5.12	123.81	119.20
13	X	190	ARG	CG-CD-NE	5.12	123.26	112.00
12	W	31	CYS	CA-C-N	5.12	129.21	122.30
12	W	31	CYS	C-N-CA	5.12	129.21	122.30
2	R	95	TYR	CA-C-N	5.12	127.09	120.44
2	R	95	TYR	C-N-CA	5.12	127.09	120.44
9	A	101	ARG	CG-CD-NE	5.12	123.25	112.00
10	B	170	ASN	CA-CB-CG	5.12	117.72	112.60
10	B	197	GLU	O-C-N	-5.12	116.70	122.12
10	P	178	TYR	N-CA-CB	5.12	117.78	110.06
8	M	56	ARG	NE-CZ-NH2	5.11	123.80	119.20
11	H	2	THR	CA-C-N	5.11	130.17	122.75
11	H	2	THR	C-N-CA	5.11	130.17	122.75
9	O	158	PHE	CA-CB-CG	5.11	118.91	113.80
7	Z	59	LEU	N-CA-CB	5.11	117.42	110.01
10	B	82	ASP	CA-CB-CG	5.11	117.71	112.60
7	Z	73	LYS	CA-C-N	5.11	128.25	120.95
7	Z	73	LYS	C-N-CA	5.11	128.25	120.95
7	Z	108	GLY	CA-C-N	5.11	129.13	121.72
7	Z	108	GLY	C-N-CA	5.11	129.13	121.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	155	LEU	N-CA-CB	5.11	117.41	110.01
8	M	148	VAL	CA-C-N	5.11	129.84	122.44
8	M	148	VAL	C-N-CA	5.11	129.84	122.44
14	b	213	LEU	CA-C-N	5.11	127.08	120.44
14	b	213	LEU	C-N-CA	5.11	127.08	120.44
1	Q	88	ASN	CA-C-N	5.10	127.07	120.44
1	Q	88	ASN	C-N-CA	5.10	127.07	120.44
1	Q	173	SER	CA-C-N	5.10	126.98	120.56
1	Q	173	SER	C-N-CA	5.10	126.98	120.56
8	M	196	GLY	CA-C-N	5.10	127.07	120.44
8	M	196	GLY	C-N-CA	5.10	127.07	120.44
9	A	236	THR	CA-C-N	5.10	127.07	120.44
9	A	236	THR	C-N-CA	5.10	127.07	120.44
6	Y	142	ILE	N-CA-CB	5.10	116.51	110.55
2	R	4	ASP	CA-CB-CG	5.09	117.69	112.60
6	Y	61	ILE	N-CA-CB	5.09	116.51	110.55
10	B	172	SER	CA-C-N	5.09	127.06	120.44
10	B	172	SER	C-N-CA	5.09	127.06	120.44
11	V	43	VAL	CA-C-N	5.09	129.75	122.72
11	V	43	VAL	C-N-CA	5.09	129.75	122.72
6	Y	144	ASP	CA-C-N	5.09	127.37	120.65
6	Y	144	ASP	C-N-CA	5.09	127.37	120.65
11	V	190	GLN	CA-C-N	5.09	127.10	120.28
11	V	190	GLN	C-N-CA	5.09	127.10	120.28
7	Z	75	SER	CA-C-N	5.09	127.43	120.46
7	Z	75	SER	C-N-CA	5.09	127.43	120.46
10	P	215	ASP	CA-C-N	5.09	129.43	121.08
10	P	215	ASP	C-N-CA	5.09	129.43	121.08
6	K	160	PHE	CA-CB-CG	5.09	118.89	113.80
6	Y	62	ARG	CA-C-N	5.09	127.05	120.44
6	Y	62	ARG	C-N-CA	5.09	127.05	120.44
11	H	63	CYS	N-CA-CB	5.09	117.39	110.01
8	M	89	ILE	N-CA-CB	5.08	116.50	110.55
11	V	244	VAL	N-CA-C	5.08	115.85	110.72
11	H	60	LYS	CA-CB-CG	5.08	124.26	114.10
11	H	155	GLY	N-CA-C	5.08	119.00	110.56
10	P	177	ARG	CA-C-N	5.08	128.69	121.42
10	P	177	ARG	C-N-CA	5.08	128.69	121.42
1	Q	196	LEU	CA-C-N	5.08	127.04	120.44
1	Q	196	LEU	C-N-CA	5.08	127.04	120.44
12	W	199	LEU	N-CA-CB	5.08	118.04	110.02
7	L	59	LEU	N-CA-CB	5.08	117.37	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Y	168	LYS	CB-CG-CD	5.08	122.97	111.30
10	B	138	GLY	CA-C-N	5.08	130.29	122.68
10	B	138	GLY	C-N-CA	5.08	130.29	122.68
10	P	118	VAL	CA-C-N	5.08	127.33	120.38
10	P	118	VAL	C-N-CA	5.08	127.33	120.38
6	K	164	PHE	CA-C-N	5.07	127.03	120.44
6	K	164	PHE	C-N-CA	5.07	127.03	120.44
13	X	8	ASN	CA-CB-CG	5.07	117.67	112.60
13	X	200	VAL	CA-C-N	5.07	130.15	123.05
13	X	200	VAL	C-N-CA	5.07	130.15	123.05
6	K	62	ARG	CA-C-N	5.07	127.03	120.44
6	K	62	ARG	C-N-CA	5.07	127.03	120.44
10	B	84	ARG	CD-NE-CZ	5.07	131.50	124.40
5	G	163	TYR	CA-C-N	5.07	130.58	121.66
5	G	163	TYR	C-N-CA	5.07	130.58	121.66
7	L	160	ILE	N-CA-CB	5.07	116.48	110.55
1	Q	6	ASP	CA-CB-CG	5.06	117.66	112.60
6	K	119	ASP	CA-CB-CG	5.06	117.66	112.60
13	X	129	ASN	CA-CB-CG	5.06	117.66	112.60
9	A	204	ASP	CA-C-N	5.06	127.13	120.60
9	A	204	ASP	C-N-CA	5.06	127.13	120.60
12	W	163	ILE	N-CA-CB	5.06	116.47	110.55
1	Q	169	LEU	CA-C-N	5.06	127.02	120.44
1	Q	169	LEU	C-N-CA	5.06	127.02	120.44
7	Z	86	ILE	CA-C-N	5.06	127.01	120.44
7	Z	86	ILE	C-N-CA	5.06	127.01	120.44
10	P	91	ARG	CB-CG-CD	5.06	122.93	111.30
8	M	179	ASN	N-CA-CB	5.06	117.34	110.01
5	G	115	VAL	CA-C-N	5.05	127.01	120.44
5	G	115	VAL	C-N-CA	5.05	127.01	120.44
14	N	181	ALA	CA-C-N	5.05	127.55	120.28
14	N	181	ALA	C-N-CA	5.05	127.55	120.28
10	P	232	ILE	N-CA-CB	5.05	116.46	110.55
2	R	164	ASN	CA-CB-CG	5.05	117.65	112.60
6	K	125	ASP	CA-CB-CG	5.04	117.64	112.60
9	A	254	THR	CA-C-N	5.04	127.00	120.44
9	A	254	THR	C-N-CA	5.04	127.00	120.44
2	D	95	TYR	CA-C-N	5.04	126.99	120.44
2	D	95	TYR	C-N-CA	5.04	126.99	120.44
7	Z	176	VAL	CA-C-N	5.04	130.69	122.07
7	Z	176	VAL	C-N-CA	5.04	130.69	122.07
9	A	203	GLU	CA-C-N	5.04	127.04	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	203	GLU	C-N-CA	5.04	127.04	120.28
10	P	110	LEU	N-CA-CB	5.04	117.32	110.01
13	X	176	LEU	N-CA-CB	5.04	117.32	110.01
10	P	169	ASN	CA-CB-CG	5.04	117.64	112.60
6	K	144	ASP	CA-C-N	5.03	127.29	120.65
6	K	144	ASP	C-N-CA	5.03	127.29	120.65
12	W	184	GLN	CA-C-N	5.03	129.38	122.84
12	W	184	GLN	C-N-CA	5.03	129.38	122.84
7	L	159	ALA	CA-C-N	5.03	126.90	120.56
7	L	159	ALA	C-N-CA	5.03	126.90	120.56
9	A	255	TYR	N-CA-CB	5.03	117.31	110.01
10	P	120	GLU	N-CA-CB	5.03	117.43	109.94
6	K	26	ILE	N-CA-CB	5.03	115.76	111.64
9	A	80	ASP	CA-C-N	5.03	130.12	122.23
9	A	80	ASP	C-N-CA	5.03	130.12	122.23
9	A	237	LYS	N-CA-CB	5.03	117.30	110.01
9	A	97	VAL	N-CA-CB	5.03	116.43	110.55
11	V	229	ARG	CD-NE-CZ	5.03	131.44	124.40
1	Q	8	ARG	CD-NE-CZ	5.02	131.43	124.40
8	M	199	ILE	N-CA-CB	5.02	116.43	110.55
11	V	228	ILE	CA-C-N	5.02	130.08	123.05
11	V	228	ILE	C-N-CA	5.02	130.08	123.05
5	G	113	ILE	N-CA-CB	5.01	116.42	110.55
6	K	168	LYS	CB-CG-CD	5.01	122.83	111.30
8	M	64	TYR	CA-CB-CG	5.01	122.92	113.90
7	L	151	GLN	CA-C-N	5.01	126.95	120.44
7	L	151	GLN	C-N-CA	5.01	126.95	120.44
10	B	187	ALA	CA-C-N	5.01	126.87	120.56
10	B	187	ALA	C-N-CA	5.01	126.87	120.56
11	H	9	ASP	CA-CB-CG	5.01	117.61	112.60
11	H	158	LYS	N-CA-C	5.01	117.47	111.71
2	R	92	GLN	CA-C-N	5.01	126.95	120.44
2	R	92	GLN	C-N-CA	5.01	126.95	120.44
7	L	181	LYS	CA-CB-CG	5.01	124.12	114.10
8	M	201	PHE	N-CA-CB	5.01	117.27	110.01
10	B	117	ILE	CA-C-N	5.01	126.87	120.56
10	B	117	ILE	C-N-CA	5.01	126.87	120.56
7	L	132	SER	CA-C-N	5.01	126.95	120.44
7	L	132	SER	C-N-CA	5.01	126.95	120.44
7	Z	138	ILE	N-CA-CB	5.01	116.41	110.55
12	W	170	GLY	N-CA-C	5.01	118.87	110.56
8	M	202	VAL	N-CA-CB	5.00	116.41	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	95	TYR	N-CA-CB	5.00	117.40	109.94
10	B	177	ARG	CD-NE-CZ	5.00	131.41	124.40
11	H	150	ALA	CA-C-N	5.00	130.43	122.62
11	H	150	ALA	C-N-CA	5.00	130.43	122.62
8	M	86	GLN	N-CA-CB	5.00	117.47	110.12
10	P	179	ASN	CA-C-N	5.00	126.98	120.28
10	P	179	ASN	C-N-CA	5.00	126.98	120.28

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	K	170	ARG	Sidechain
6	K	54	ARG	Sidechain
1	Q	226	TYR	Sidechain
1	Q	62	TYR	Sidechain
6	Y	54	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1917	1911	1910	22	0
1	Q	1917	1911	1910	7	0
2	D	1845	1879	1878	26	0
2	R	1845	1879	1878	24	0
3	E	1860	1868	1867	23	0
3	S	1860	1868	1867	22	0
4	F	1879	1879	1878	19	0
4	T	1879	1879	1878	17	0
5	G	2008	1950	1949	15	0
5	U	2008	1950	1949	18	0
6	K	1614	1584	1584	10	0
6	Y	1614	1584	1584	8	0
7	L	1662	1615	1617	8	0
7	Z	1662	1615	1617	6	0
8	M	1696	1708	1707	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	a	1696	1708	1707	16	0
9	A	1910	1899	1897	14	0
9	O	1910	1899	1897	18	0
10	B	1798	1816	1814	15	0
10	P	1798	1816	1814	10	0
11	H	1722	1739	1740	10	0
11	V	1722	1739	1740	14	0
12	I	1668	1668	1669	26	0
12	W	1668	1668	1669	17	0
13	J	1612	1610	1608	15	0
13	X	1612	1610	1608	12	0
14	N	1845	1817	1814	11	0
14	b	1845	1817	1814	12	0
15	L	45	0	0	2	0
15	Z	45	0	0	2	0
All	All	50162	49886	49864	387	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 4.

All (387) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:65:GLU:OE1	3:E:65:GLU:N	2.08	0.87
4:T:68:ASP:OD2	4:T:96:LYS:NZ	2.08	0.87
4:F:68:ASP:OD2	4:F:96:LYS:NZ	2.08	0.86
13:J:8:ASN:ND2	13:J:30:GLY:O	2.10	0.85
3:S:65:GLU:N	3:S:65:GLU:OE1	2.11	0.83
3:E:194:GLU:N	3:E:194:GLU:OE1	2.12	0.82
6:K:174:THR:OG1	6:Y:174:THR:OG1	1.97	0.81
2:R:66:ASP:OD1	2:R:69:ASN:ND2	2.14	0.80
12:W:218:GLU:N	12:W:218:GLU:OE1	2.14	0.80
12:I:218:GLU:N	12:I:218:GLU:OE1	2.14	0.79
13:X:8:ASN:ND2	13:X:30:GLY:O	2.16	0.79
3:S:194:GLU:N	3:S:194:GLU:OE1	2.15	0.79
14:N:10:THR:O	14:N:42:ARG:NH1	2.16	0.78
2:D:66:ASP:OD1	2:D:69:ASN:ND2	2.17	0.77
14:N:26:ASP:OD1	14:N:42:ARG:NH2	2.19	0.76
14:b:10:THR:O	14:b:42:ARG:NH1	2.19	0.75
15:Z:301:A1CY6:O36	8:a:157:SER:OG	2.04	0.74
15:L:301:A1CY6:O36	8:M:157:SER:OG	2.05	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:10:THR:HG22	14:b:11:SER:H	1.53	0.73
13:J:48:ASN:ND2	13:J:77:GLU:OE2	2.22	0.73
14:b:26:ASP:OD1	14:b:42:ARG:NH2	2.21	0.72
12:I:1:THR:HG23	12:I:1:THR:O	1.90	0.72
1:C:140:ASP:OD1	1:C:146:GLN:NE2	2.23	0.72
11:V:157:ASP:OD1	11:V:158:LYS:N	2.23	0.72
2:D:2:SER:OG	2:D:3:TYR:N	2.19	0.71
2:R:2:SER:OG	2:R:3:TYR:N	2.19	0.71
13:X:48:ASN:ND2	13:X:77:GLU:OE2	2.25	0.70
4:F:110:ARG:NH2	14:N:78:GLU:OE1	2.25	0.69
11:V:23:GLY:O	11:V:24:THR:OG1	2.10	0.69
2:D:116:GLN:NE2	3:E:84:ASP:OD1	2.25	0.68
13:J:65:LEU:HD22	13:J:107:VAL:HG11	1.76	0.68
3:E:121:LEU:HD11	3:E:162:GLY:HA3	1.76	0.67
11:V:158:LYS:O	11:V:161:LYS:NZ	2.22	0.67
8:a:228:MET:SD	8:a:229:GLY:N	2.68	0.66
2:D:186:ILE:O	2:D:190:LEU:HD12	1.95	0.66
11:H:23:GLY:O	11:H:24:THR:OG1	2.11	0.66
4:T:9:ASP:HB2	4:T:12:ILE:HD12	1.77	0.66
6:K:122:SER:OG	13:J:60:THR:OG1	2.11	0.65
8:M:228:MET:SD	8:M:229:GLY:N	2.70	0.65
4:F:9:ASP:HB2	4:F:12:ILE:HD12	1.78	0.65
2:D:5:ARG:O	2:D:123:GLY:N	2.30	0.64
12:I:35:HIS:HB3	12:I:56:THR:HG21	1.79	0.64
3:E:201:LEU:HD11	3:E:219:ILE:HD11	1.80	0.63
10:B:22:ILE:HD11	10:B:122:THR:HG23	1.79	0.63
9:O:228:GLU:O	9:O:229:ILE:HD12	1.98	0.63
2:R:116:GLN:NE2	3:S:84:ASP:OD1	2.31	0.62
8:M:40:VAL:HG12	8:M:53:ALA:HB2	1.80	0.62
14:b:6:VAL:HG23	14:b:7:VAL:HG23	1.80	0.62
14:N:6:VAL:HG23	14:N:7:VAL:HG23	1.80	0.62
4:T:53:ILE:HD12	4:T:53:ILE:H	1.66	0.61
8:a:84:GLY:H	8:a:89:ILE:HD11	1.66	0.61
2:R:132:LEU:HD12	2:R:132:LEU:O	2.01	0.61
6:Y:185:ASP:OD1	6:Y:185:ASP:O	2.18	0.61
3:S:201:LEU:HD11	3:S:219:ILE:HD11	1.82	0.60
4:F:53:ILE:H	4:F:53:ILE:HD12	1.66	0.60
2:R:186:ILE:O	2:R:190:LEU:HD12	2.02	0.60
3:S:91:TYR:CG	3:S:119:LEU:HD22	2.36	0.60
7:L:21:SER:O	15:L:301:A1CY6:N19	2.35	0.59
7:Z:21:SER:O	15:Z:301:A1CY6:N19	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:11:THR:HG23	10:B:21:GLN:HB2	1.83	0.59
10:B:86:LEU:HD12	10:B:132:LEU:HD21	1.84	0.59
3:E:91:TYR:CG	3:E:119:LEU:HD22	2.38	0.59
1:C:61:ASN:O	1:C:61:ASN:ND2	2.34	0.59
2:R:5:ARG:O	2:R:123:GLY:N	2.36	0.59
5:G:9:ASP:O	5:G:23:GLN:NE2	2.36	0.58
9:O:173:VAL:HG11	9:O:181:SER:CB	2.34	0.58
9:O:111:ASN:OD1	12:W:82:ARG:NH2	2.36	0.58
9:A:111:ASN:OD1	12:I:82:ARG:NH2	2.37	0.58
1:C:119:GLN:HG3	2:D:78:ALA:HB1	1.86	0.58
8:a:212:ARG:NH2	12:I:26:VAL:O	2.37	0.57
5:G:27:ILE:HD11	5:G:133:PRO:HG2	1.85	0.57
9:O:25:ILE:HD11	9:O:132:THR:HG23	1.86	0.57
5:U:9:ASP:O	5:U:23:GLN:NE2	2.37	0.57
5:U:27:ILE:HD11	5:U:133:PRO:HG2	1.85	0.57
5:G:211:ASN:OD1	5:G:212:LEU:N	2.38	0.57
5:U:211:ASN:OD1	5:U:212:LEU:N	2.37	0.57
14:N:10:THR:HG22	14:N:11:SER:H	1.70	0.57
1:Q:169:LEU:H	1:Q:169:LEU:HD22	1.68	0.57
8:a:40:VAL:HG12	8:a:53:ALA:CB	2.35	0.57
9:A:25:ILE:HD11	9:A:132:THR:HG23	1.87	0.56
1:C:170:THR:O	1:C:174:VAL:HG23	2.05	0.56
7:L:37:ILE:HD11	7:L:56:GLU:HG2	1.86	0.56
2:D:116:GLN:HG3	3:E:83:ALA:HB1	1.87	0.56
5:G:207:MET:HA	5:G:207:MET:HE2	1.86	0.56
4:T:53:ILE:HD12	4:T:53:ILE:N	2.21	0.56
12:I:35:HIS:CB	12:I:56:THR:HG21	2.36	0.56
10:B:215:ASP:OD1	10:B:216:ASN:N	2.36	0.56
8:M:153:ASP:OD2	8:M:157:SER:OG	2.23	0.55
10:P:86:LEU:HD12	10:P:132:LEU:HD21	1.87	0.55
4:F:53:ILE:HD12	4:F:53:ILE:N	2.21	0.55
2:R:180:MET:HE1	2:R:188:LEU:HD22	1.88	0.55
4:T:182:SER:OG	4:T:185:GLU:OE1	2.23	0.55
5:U:207:MET:HA	5:U:207:MET:HE2	1.88	0.55
8:a:40:VAL:HG12	8:a:53:ALA:HB2	1.88	0.55
9:O:235:SER:O	9:O:239:ARG:N	2.40	0.55
10:P:22:ILE:HD11	10:P:122:THR:HG23	1.89	0.55
8:a:84:GLY:N	8:a:89:ILE:HD11	2.21	0.55
3:S:201:LEU:CD1	3:S:219:ILE:HD11	2.38	0.54
12:W:35:HIS:HB3	12:W:56:THR:HG21	1.90	0.54
3:E:201:LEU:CD1	3:E:219:ILE:HD11	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:37:ILE:HD11	7:Z:56:GLU:HG2	1.88	0.54
1:C:178:GLU:OE2	1:C:194:LYS:NZ	2.35	0.54
11:H:26:ILE:O	14:b:216:ARG:NH1	2.40	0.54
1:C:205:PRO:O	1:C:235:LEU:HD21	2.08	0.54
12:I:179:THR:OG1	12:I:180:LYS:N	2.40	0.54
14:N:216:ARG:NH1	11:V:26:ILE:O	2.40	0.54
5:U:52:ASN:OD1	5:U:68:ARG:NH2	2.41	0.54
9:A:235:SER:O	9:A:239:ARG:N	2.41	0.54
1:C:68:ILE:HG21	1:C:110:LEU:HD21	1.91	0.53
11:V:178:ASP:OD1	11:V:178:ASP:N	2.41	0.53
5:U:110:PRO:HG2	5:U:113:ILE:HD12	1.91	0.53
8:a:153:ASP:OD2	8:a:157:SER:OG	2.26	0.53
5:G:110:PRO:HG2	5:G:113:ILE:HD12	1.91	0.53
8:a:40:VAL:HG23	8:a:137:ILE:HD12	1.90	0.52
1:Q:170:THR:O	1:Q:174:VAL:HG23	2.08	0.52
5:G:52:ASN:OD1	5:G:68:ARG:NH2	2.42	0.52
5:U:186:ASP:C	5:U:186:ASP:OD1	2.52	0.52
10:B:107:VAL:O	10:B:111:VAL:HG23	2.09	0.52
13:J:51:VAL:HG22	13:J:86:VAL:CG1	2.39	0.52
11:V:136:THR:HG21	11:V:153:PHE:CE1	2.44	0.52
10:P:107:VAL:O	10:P:111:VAL:HG23	2.09	0.52
1:C:165:GLY:N	1:C:168:ASN:OD1	2.43	0.52
5:G:186:ASP:OD1	5:G:186:ASP:C	2.53	0.52
8:M:40:VAL:HG12	8:M:53:ALA:CB	2.40	0.52
4:T:16:GLU:OE2	4:T:18:ARG:NH2	2.43	0.52
5:U:27:ILE:HG23	5:U:135:ALA:HA	1.93	0.51
1:Q:178:GLU:OE2	1:Q:194:LYS:NZ	2.40	0.51
4:F:16:GLU:OE2	4:F:18:ARG:NH2	2.44	0.51
6:Y:174:THR:OG1	6:Y:174:THR:O	2.29	0.51
2:R:62:LEU:HD21	2:R:207:ALA:HB3	1.91	0.51
12:I:104:ASP:N	12:I:104:ASP:OD1	2.43	0.51
12:I:203:THR:HG22	12:I:203:THR:O	2.11	0.51
12:I:187:ARG:HB2	12:I:188:PRO:HD3	1.93	0.50
2:D:230:ASP:OD1	2:D:230:ASP:C	2.53	0.50
11:H:132:VAL:O	11:H:136:THR:HG22	2.10	0.50
3:E:103:TYR:HB3	8:M:115:VAL:HG13	1.94	0.50
2:R:199:LEU:O	2:R:226:VAL:HG21	2.11	0.50
2:D:138:ASN:ND2	7:L:72:GLU:OE2	2.44	0.49
5:G:27:ILE:HG23	5:G:135:ALA:HA	1.93	0.49
12:I:187:ARG:CB	12:I:188:PRO:HD3	2.43	0.49
12:I:203:THR:HG21	13:J:168:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:17:ASP:OD1	12:I:33:LYS:NZ	2.40	0.49
12:I:80:VAL:HG21	12:I:111:TYR:CG	2.47	0.49
4:F:133:MET:HG3	4:F:158:LEU:HD23	1.94	0.49
10:P:11:THR:HG23	10:P:21:GLN:HB2	1.94	0.49
13:X:65:LEU:HD22	13:X:107:VAL:HG11	1.94	0.49
2:R:116:GLN:HG3	3:S:83:ALA:HB1	1.94	0.49
12:W:203:THR:HG22	12:W:203:THR:O	2.13	0.49
3:E:165:THR:HG21	4:F:53:ILE:HD13	1.93	0.49
3:S:103:TYR:HB3	8:a:115:VAL:HG13	1.93	0.49
2:R:60:GLU:CD	2:R:63:ILE:HG22	2.37	0.49
4:T:133:MET:HG3	4:T:158:LEU:HD23	1.94	0.49
12:I:129:SER:OG	12:I:166:ASP:OD2	2.23	0.49
11:V:136:THR:HG21	11:V:153:PHE:CZ	2.48	0.49
12:W:35:HIS:CB	12:W:56:THR:HG21	2.43	0.49
9:O:25:ILE:HD11	9:O:132:THR:CG2	2.43	0.48
9:O:215:ALA:O	9:O:219:ILE:HG12	2.13	0.48
12:W:80:VAL:HG21	12:W:111:TYR:CG	2.48	0.48
8:M:39:THR:CG2	8:M:169:GLY:H	2.26	0.48
12:W:104:ASP:N	12:W:104:ASP:OD1	2.46	0.48
2:D:180:MET:HE1	2:D:188:LEU:HD22	1.94	0.48
9:O:173:VAL:HG11	9:O:181:SER:HB3	1.94	0.48
4:T:42:ASP:N	4:T:42:ASP:OD1	2.46	0.48
8:a:47:ASP:OD1	8:a:47:ASP:N	2.46	0.48
6:K:149:GLU:HA	6:K:149:GLU:OE1	2.13	0.48
8:a:220:THR:OG1	8:a:237:LEU:HD11	2.14	0.48
10:P:205:GLU:N	10:P:205:GLU:OE1	2.47	0.48
11:V:133:ALA:O	11:V:136:THR:HG22	2.12	0.48
2:D:60:GLU:CD	2:D:63:ILE:HG22	2.39	0.48
2:D:62:LEU:HD21	2:D:207:ALA:HB3	1.96	0.48
3:S:91:TYR:CD2	3:S:119:LEU:HD22	2.49	0.48
4:F:42:ASP:OD1	4:F:42:ASP:N	2.46	0.48
9:A:25:ILE:HD11	9:A:132:THR:CG2	2.44	0.48
3:E:47:ILE:HD11	3:E:219:ILE:CG2	2.44	0.47
14:b:52:MET:HE3	14:b:64:LEU:HD23	1.96	0.47
3:E:121:LEU:HD13	4:F:79:SER:HB3	1.95	0.47
6:K:75:ASP:C	6:K:75:ASP:OD1	2.57	0.47
4:T:38:ILE:HG23	4:T:177:LEU:HD13	1.96	0.47
11:V:115:LYS:HE3	11:V:237:PHE:CD1	2.49	0.47
13:X:51:VAL:HG22	13:X:86:VAL:CG1	2.45	0.47
1:C:200:THR:HG22	1:C:200:THR:O	2.14	0.47
7:Z:26:ILE:O	13:J:190:ARG:NH2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:36:LYS:HB2	2:D:144:ILE:HD12	1.97	0.47
4:F:182:SER:OG	4:F:185:GLU:OE1	2.22	0.47
3:S:47:ILE:HD11	3:S:219:ILE:CG2	2.44	0.47
8:a:186:GLN:HA	8:a:186:GLN:OE1	2.14	0.47
2:D:193:ILE:HG21	2:D:199:LEU:HG	1.97	0.47
8:a:99:LYS:HD2	8:a:123:ILE:HD11	1.97	0.47
11:H:157:ASP:OD1	11:H:158:LYS:N	2.47	0.47
8:a:179:ASN:ND2	12:I:205:TYR:OH	2.41	0.47
11:V:147:LEU:HD12	11:V:147:LEU:O	2.15	0.47
2:D:223:ASN:O	2:D:226:VAL:HG12	2.16	0.46
5:U:210:ASN:OD1	5:U:210:ASN:C	2.59	0.46
8:M:186:GLN:OE1	8:M:186:GLN:HA	2.14	0.46
1:C:124:TYR:HH	2:D:118:PHE:HZ	1.61	0.46
6:K:174:THR:OG1	6:K:174:THR:O	2.28	0.46
8:M:99:LYS:HD2	8:M:123:ILE:HD11	1.97	0.46
2:R:36:LYS:HB2	2:R:144:ILE:HD12	1.97	0.46
6:K:47:LEU:HD23	6:K:102:CYS:HB3	1.98	0.46
9:O:14:THR:O	10:P:128:ARG:HB3	2.16	0.46
9:O:205:ILE:HG23	9:O:206:ARG:N	2.31	0.46
3:S:165:THR:HG21	4:T:53:ILE:HD13	1.97	0.46
14:N:46:ILE:HD11	14:N:50:THR:CG2	2.46	0.46
4:T:84:LEU:O	4:T:88:MET:HG3	2.16	0.46
10:B:177:ARG:HD2	10:B:190:THR:HG23	1.98	0.46
11:H:53:GLN:O	11:H:57:GLU:HG2	2.16	0.46
11:H:147:LEU:HD12	11:H:147:LEU:O	2.16	0.46
13:J:90:ALA:HB1	13:J:137:TYR:OH	2.16	0.46
1:C:167:ASN:ND2	1:C:199:SER:O	2.45	0.46
2:R:195:GLU:O	2:R:195:GLU:OE1	2.34	0.46
13:J:51:VAL:HG22	13:J:86:VAL:HG12	1.98	0.46
1:C:103:GLU:OE1	6:K:80:SER:OG	2.33	0.46
6:Y:47:LEU:HD23	6:Y:102:CYS:HB3	1.98	0.46
4:F:38:ILE:HG23	4:F:177:LEU:HD13	1.97	0.45
8:M:84:GLY:H	8:M:89:ILE:HD11	1.81	0.45
2:R:193:ILE:HG21	2:R:199:LEU:HG	1.98	0.45
12:I:181:ASP:OD1	12:I:181:ASP:N	2.49	0.45
2:D:199:LEU:O	2:D:226:VAL:HG21	2.16	0.45
5:G:210:ASN:C	5:G:210:ASN:OD1	2.58	0.45
11:V:53:GLN:O	11:V:57:GLU:HG2	2.16	0.45
8:M:47:ASP:OD1	8:M:47:ASP:N	2.47	0.45
5:U:40:LEU:HD23	5:U:47:ILE:HG23	1.99	0.45
10:P:69:SER:OG	10:P:104:GLU:OE2	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:40:LEU:HD23	5:G:47:ILE:HG23	1.97	0.45
6:K:182:ILE:HG22	6:K:184:TYR:CD1	2.52	0.45
11:H:159:ILE:N	11:H:159:ILE:HD13	2.30	0.45
13:J:24:ALA:HB1	13:J:184:LEU:HD22	1.99	0.45
1:C:169:LEU:HD22	1:C:169:LEU:H	1.80	0.45
3:S:43:ASN:OD1	3:S:43:ASN:N	2.49	0.45
5:U:115:VAL:HG22	5:U:140:ILE:HG21	1.98	0.45
10:B:95:ILE:HG23	12:I:61:HIS:HB3	1.98	0.45
10:B:122:THR:O	10:B:122:THR:HG22	2.17	0.45
9:A:10:ASP:N	9:A:10:ASP:OD1	2.51	0.44
11:H:115:LYS:HE3	11:H:237:PHE:CD1	2.51	0.44
4:T:45:VAL:HG23	4:T:186:LEU:HD23	2.00	0.44
9:A:173:VAL:HG11	9:A:181:SER:CB	2.47	0.44
12:W:206:PRO:O	12:W:208:GLY:N	2.50	0.44
9:O:173:VAL:HG11	9:O:181:SER:HB2	2.00	0.44
4:F:45:VAL:HG23	4:F:186:LEU:HD23	2.00	0.44
10:B:22:ILE:CD1	10:B:122:THR:HG23	2.46	0.44
11:V:159:ILE:HD13	11:V:159:ILE:N	2.31	0.44
12:W:99:VAL:O	12:W:99:VAL:HG13	2.17	0.44
5:G:115:VAL:HG22	5:G:140:ILE:HG21	1.98	0.44
13:J:15:MET:HB3	13:J:176:LEU:HD11	1.99	0.44
1:C:83:ALA:O	1:C:87:ILE:HG12	2.17	0.44
1:C:215:LEU:HD21	1:C:221:GLU:OE2	2.17	0.44
2:D:219:GLU:OE1	2:D:219:GLU:HA	2.18	0.44
3:E:175:ALA:CB	3:E:207:VAL:HG13	2.48	0.44
3:E:199:LEU:O	3:E:203:VAL:HG23	2.18	0.44
11:H:146:PHE:CD1	11:H:146:PHE:C	2.94	0.44
12:W:203:THR:HG21	13:X:168:VAL:HG12	2.00	0.44
4:F:10:ASN:OD1	4:F:10:ASN:C	2.61	0.44
12:I:163:ILE:HG23	12:I:170:GLY:HA2	2.00	0.44
13:J:155:THR:O	13:J:155:THR:OG1	2.31	0.44
1:Q:103:GLU:OE1	6:Y:80:SER:OG	2.32	0.44
2:R:181:GLU:HG2	2:R:182:GLN:N	2.33	0.44
11:H:132:VAL:O	11:H:135:ILE:HG22	2.18	0.44
3:S:175:ALA:CB	3:S:207:VAL:HG13	2.48	0.43
9:O:115:VAL:HG22	9:O:119:THR:HB	2.00	0.43
5:G:6:ALA:O	9:A:11:ARG:NH1	2.51	0.43
9:A:115:VAL:HG22	9:A:119:THR:HB	2.00	0.43
14:N:52:MET:HE3	14:N:64:LEU:HD23	1.98	0.43
2:D:116:GLN:CG	3:E:83:ALA:HB1	2.49	0.43
3:E:219:ILE:HD12	3:E:237:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:138:ASN:ND2	7:Z:72:GLU:OE2	2.44	0.43
1:C:81:ALA:HB1	10:B:119:GLN:CG	2.48	0.43
9:A:14:THR:OG1	9:A:135:ALA:HB2	2.18	0.43
9:A:14:THR:HG21	9:A:134:HIS:C	2.44	0.43
12:I:206:PRO:O	12:I:208:GLY:N	2.52	0.43
3:S:47:ILE:HG23	3:S:47:ILE:O	2.19	0.43
4:T:205:THR:O	4:T:209:THR:HG22	2.18	0.43
1:C:81:ALA:HB1	10:B:119:GLN:HG3	2.01	0.43
8:M:40:VAL:HG23	8:M:137:ILE:HD12	2.01	0.43
2:R:49:ASN:OD1	2:R:49:ASN:C	2.62	0.43
2:R:110:TYR:O	2:R:114:VAL:HG23	2.18	0.43
2:R:219:GLU:OE1	2:R:219:GLU:HA	2.18	0.43
14:N:128:ASP:OD1	14:N:128:ASP:N	2.52	0.43
2:D:181:GLU:HG2	2:D:182:GLN:N	2.34	0.43
4:F:167:SER:O	4:F:171:LEU:HG	2.19	0.43
10:P:95:ILE:HG23	12:W:61:HIS:HB3	2.01	0.43
1:C:72:ILE:HD13	1:C:110:LEU:HD23	2.01	0.43
4:F:205:THR:O	4:F:209:THR:HG22	2.18	0.43
1:C:69:ASP:OD1	1:C:70:LYS:N	2.42	0.43
14:N:198:THR:HG23	14:N:201:GLU:H	1.84	0.43
2:D:52:LYS:HG2	2:D:52:LYS:O	2.19	0.43
3:E:91:TYR:CD2	3:E:119:LEU:HD22	2.53	0.43
3:E:201:LEU:HD22	3:E:240:ILE:CG2	2.49	0.43
4:F:117:GLN:O	4:F:120:THR:OG1	2.37	0.43
12:I:99:VAL:O	12:I:99:VAL:HG13	2.19	0.43
3:E:43:ASN:OD1	3:E:43:ASN:N	2.49	0.42
3:E:236:ASP:HA	3:E:239:ARG:HG2	2.01	0.42
3:S:199:LEU:O	3:S:203:VAL:HG23	2.19	0.42
10:B:205:GLU:OE1	10:B:205:GLU:N	2.51	0.42
12:I:76:VAL:O	12:I:80:VAL:HG23	2.19	0.42
9:O:10:ASP:OD1	9:O:10:ASP:N	2.51	0.42
12:W:17:ASP:OD1	12:W:33:LYS:NZ	2.41	0.42
14:b:46:ILE:HD11	14:b:50:THR:CG2	2.48	0.42
5:G:209:LYS:O	5:G:210:ASN:CG	2.62	0.42
3:S:201:LEU:HD22	3:S:240:ILE:CG2	2.49	0.42
4:T:10:ASN:OD1	4:T:10:ASN:C	2.61	0.42
3:E:47:ILE:O	3:E:47:ILE:HG23	2.19	0.42
7:Z:160:ILE:HG21	7:Z:174:VAL:HG23	2.01	0.42
11:V:54:LYS:O	11:V:54:LYS:HD3	2.20	0.42
2:R:223:ASN:O	2:R:226:VAL:HG12	2.19	0.42
4:T:167:SER:O	4:T:171:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:72:VAL:HG23	5:U:73:ASN:N	2.35	0.42
9:A:17:SER:OG	9:A:19:ASP:OD1	2.34	0.42
12:W:198:HIS:O	12:W:198:HIS:ND1	2.51	0.42
14:b:47:ASN:OD1	14:b:47:ASN:C	2.63	0.42
4:F:84:LEU:O	4:F:88:MET:HG3	2.19	0.42
3:S:236:ASP:HA	3:S:239:ARG:HG2	2.01	0.42
8:a:210:THR:OG1	8:a:237:LEU:HD13	2.19	0.42
14:b:128:ASP:OD1	14:b:128:ASP:N	2.53	0.42
7:L:160:ILE:HG21	7:L:174:VAL:HG23	2.02	0.42
9:A:14:THR:O	10:B:128:ARG:HB3	2.19	0.42
9:O:17:SER:OG	9:O:19:ASP:OD1	2.37	0.42
11:V:146:PHE:CD1	11:V:146:PHE:C	2.98	0.42
3:S:201:LEU:HD22	3:S:240:ILE:HG21	2.02	0.42
5:U:159:ALA:HB2	9:O:90:PRO:HG2	2.02	0.42
5:U:209:LYS:O	5:U:210:ASN:CG	2.62	0.42
6:Y:122:SER:OG	13:X:60:THR:OG1	2.13	0.42
5:G:72:VAL:HG23	5:G:73:ASN:N	2.35	0.42
5:U:74:ASN:O	5:U:229:PHE:N	2.41	0.42
9:A:96:MET:HE2	9:A:124:ILE:HG23	2.01	0.42
2:D:193:ILE:HA	2:D:196:VAL:HG22	2.02	0.42
7:L:26:ILE:O	13:X:190:ARG:NH2	2.50	0.42
12:I:6:LEU:C	12:I:6:LEU:HD12	2.44	0.42
12:I:63:VAL:HG13	12:I:74:PRO:HB3	2.01	0.42
1:C:203:GLU:HG3	1:C:204:ILE:N	2.35	0.42
8:M:84:GLY:N	8:M:89:ILE:HD11	2.34	0.42
3:S:115:LEU:O	3:S:118:GLU:HG3	2.19	0.42
13:J:60:THR:HG23	13:J:61:ASP:N	2.35	0.42
13:X:31:ALA:HB2	13:X:37:VAL:HG11	2.02	0.42
10:B:107:VAL:HG11	10:B:145:HIS:HB2	2.02	0.41
9:O:93:CYS:O	9:O:97:VAL:HG23	2.20	0.41
14:b:198:THR:HG23	14:b:201:GLU:H	1.85	0.41
3:E:109:ILE:O	3:E:113:VAL:HG23	2.19	0.41
4:F:10:ASN:OD1	4:F:10:ASN:O	2.39	0.41
6:K:81:PHE:O	6:K:85:THR:HG22	2.20	0.41
3:S:109:ILE:O	3:S:113:VAL:HG23	2.20	0.41
9:O:14:THR:HG21	9:O:134:HIS:C	2.44	0.41
12:W:76:VAL:O	12:W:80:VAL:HG23	2.20	0.41
13:X:24:ALA:HB1	13:X:184:LEU:HD22	2.01	0.41
13:X:60:THR:HG23	13:X:61:ASP:N	2.35	0.41
1:C:18:LEU:O	1:C:22:GLU:HG2	2.20	0.41
10:B:186:ASP:OD1	10:B:186:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:ASN:OD1	2:D:49:ASN:C	2.62	0.41
2:D:132:LEU:O	2:D:132:LEU:HD12	2.21	0.41
5:G:48:CYS:SG	5:G:79:THR:HG21	2.61	0.41
4:T:117:GLN:O	4:T:120:THR:OG1	2.38	0.41
5:U:118:ILE:HD13	5:U:118:ILE:HA	1.91	0.41
2:R:80:ALA:O	2:R:84:VAL:HG23	2.20	0.41
12:W:212:ILE:HG23	13:X:214:LYS:HB2	2.03	0.41
6:Y:81:PHE:O	6:Y:85:THR:HG22	2.20	0.41
1:Q:203:GLU:HG3	1:Q:204:ILE:N	2.36	0.41
5:U:48:CYS:SG	5:U:79:THR:HG21	2.61	0.41
9:A:93:CYS:O	9:A:97:VAL:HG23	2.20	0.41
13:X:33:THR:O	13:X:193:ILE:HG22	2.21	0.41
2:D:110:TYR:O	2:D:114:VAL:HG23	2.20	0.41
2:D:167:ILE:O	2:D:170:GLU:HG2	2.20	0.41
1:Q:219:ASP:OD1	1:Q:219:ASP:N	2.54	0.41
7:Z:53:LEU:O	7:Z:57:LYS:HG2	2.21	0.41
12:I:212:ILE:HG23	13:J:214:LYS:HB2	2.02	0.41
14:N:124:ASP:O	14:N:125:ASN:HB2	2.21	0.41
9:O:13:LEU:HA	9:O:24:GLN:HG3	2.03	0.41
7:L:38:ASN:OD1	7:L:39:LYS:N	2.46	0.40
7:L:53:LEU:O	7:L:57:LYS:HG2	2.21	0.40
2:R:167:ILE:O	2:R:170:GLU:HG2	2.20	0.40
2:R:195:GLU:O	2:R:196:VAL:C	2.64	0.40
3:S:219:ILE:HD12	3:S:237:ILE:HG12	2.04	0.40
12:W:181:ASP:OD1	12:W:181:ASP:N	2.53	0.40
12:I:149:GLU:OE1	12:I:149:GLU:HA	2.20	0.40
10:P:177:ARG:HD2	10:P:190:THR:HG23	2.02	0.40
10:P:186:ASP:OD1	10:P:186:ASP:N	2.54	0.40
6:K:13:VAL:O	6:K:13:VAL:HG13	2.21	0.40
12:W:187:ARG:CB	12:W:188:PRO:HD3	2.51	0.40
1:C:219:ASP:OD1	1:C:219:ASP:N	2.52	0.40
3:E:90:ASP:OD1	7:L:69:ARG:HD3	2.21	0.40
1:Q:68:ILE:HG21	1:Q:110:LEU:HD21	2.04	0.40
3:S:116:ILE:HG21	3:S:143:LEU:HD12	2.04	0.40
4:T:10:ASN:OD1	4:T:10:ASN:O	2.39	0.40
5:U:38:LEU:HD23	5:U:39:CYS:N	2.36	0.40
6:Y:1:MET:HG2	6:Y:134:TYR:H	1.86	0.40
14:b:126:ASN:OD1	14:b:127:ASP:N	2.50	0.40
2:R:218:GLU:HA	2:R:218:GLU:OE1	2.22	0.40
13:J:148:ASP:OD1	13:J:148:ASP:N	2.54	0.40
14:b:124:ASP:O	14:b:125:ASN:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	238/246 (97%)	235 (99%)	3 (1%)	0	100	100
1	Q	238/246 (97%)	234 (98%)	4 (2%)	0	100	100
2	D	231/241 (96%)	222 (96%)	9 (4%)	0	100	100
2	R	231/241 (96%)	220 (95%)	11 (5%)	0	100	100
3	E	238/256 (93%)	231 (97%)	7 (3%)	0	100	100
3	S	238/256 (93%)	232 (98%)	6 (2%)	0	100	100
4	F	235/254 (92%)	230 (98%)	5 (2%)	0	100	100
4	T	235/254 (92%)	231 (98%)	4 (2%)	0	100	100
5	G	243/252 (96%)	232 (96%)	11 (4%)	0	100	100
5	U	243/252 (96%)	233 (96%)	10 (4%)	0	100	100
6	K	193/195 (99%)	184 (95%)	7 (4%)	2 (1%)	12	32
6	Y	193/195 (99%)	183 (95%)	8 (4%)	2 (1%)	12	32
7	L	209/271 (77%)	206 (99%)	3 (1%)	0	100	100
7	Z	209/271 (77%)	206 (99%)	3 (1%)	0	100	100
8	M	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
8	a	211/240 (88%)	205 (97%)	6 (3%)	0	100	100
9	A	238/260 (92%)	233 (98%)	4 (2%)	1 (0%)	30	54
9	O	238/260 (92%)	230 (97%)	7 (3%)	1 (0%)	30	54
10	B	221/235 (94%)	216 (98%)	4 (2%)	1 (0%)	24	48
10	P	221/235 (94%)	217 (98%)	3 (1%)	1 (0%)	24	48
11	H	210/282 (74%)	203 (97%)	7 (3%)	0	100	100
11	V	210/282 (74%)	204 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	I	214/270 (79%)	202 (94%)	12 (6%)	0	100	100
12	W	214/270 (79%)	200 (94%)	14 (6%)	0	100	100
13	J	201/218 (92%)	195 (97%)	6 (3%)	0	100	100
13	X	201/218 (92%)	194 (96%)	7 (4%)	0	100	100
14	N	220/265 (83%)	214 (97%)	6 (3%)	0	100	100
14	b	220/265 (83%)	214 (97%)	6 (3%)	0	100	100
All	All	6204/6970 (89%)	6009 (97%)	187 (3%)	8 (0%)	49	73

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	P	206	LYS
10	B	206	LYS
6	K	99	GLU
6	Y	99	GLU
9	A	61	ILE
9	O	61	ILE
6	Y	25	ILE
6	K	25	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	207/213 (97%)	204 (99%)	3 (1%)	59	82
1	Q	207/213 (97%)	201 (97%)	6 (3%)	37	67
2	D	199/207 (96%)	197 (99%)	2 (1%)	68	86
2	R	199/207 (96%)	193 (97%)	6 (3%)	36	66
3	E	208/223 (93%)	206 (99%)	2 (1%)	68	86
3	S	208/223 (93%)	205 (99%)	3 (1%)	59	82
4	F	211/227 (93%)	210 (100%)	1 (0%)	81	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	T	211/227 (93%)	208 (99%)	3 (1%)	59	82
5	G	224/229 (98%)	223 (100%)	1 (0%)	84	93
5	U	224/229 (98%)	223 (100%)	1 (0%)	84	93
6	K	174/174 (100%)	169 (97%)	5 (3%)	37	67
6	Y	174/174 (100%)	169 (97%)	5 (3%)	37	67
7	L	176/232 (76%)	174 (99%)	2 (1%)	65	85
7	Z	176/232 (76%)	175 (99%)	1 (1%)	78	91
8	M	191/216 (88%)	188 (98%)	3 (2%)	55	80
8	a	191/216 (88%)	190 (100%)	1 (0%)	81	92
9	A	213/231 (92%)	210 (99%)	3 (1%)	59	82
9	O	213/231 (92%)	207 (97%)	6 (3%)	38	68
10	B	198/205 (97%)	191 (96%)	7 (4%)	32	61
10	P	198/205 (97%)	190 (96%)	8 (4%)	28	56
11	H	194/260 (75%)	191 (98%)	3 (2%)	57	81
11	V	194/260 (75%)	190 (98%)	4 (2%)	47	75
12	I	184/231 (80%)	182 (99%)	2 (1%)	65	85
12	W	184/231 (80%)	178 (97%)	6 (3%)	33	63
13	J	180/191 (94%)	178 (99%)	2 (1%)	65	85
13	X	180/191 (94%)	179 (99%)	1 (1%)	78	91
14	N	201/239 (84%)	200 (100%)	1 (0%)	81	92
14	b	201/239 (84%)	199 (99%)	2 (1%)	68	86
All	All	5520/6156 (90%)	5430 (98%)	90 (2%)	54	80

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	32	SER
1	C	55	LEU
1	C	73	PHE
2	D	11	SER
2	D	20	GLU
3	E	79	SER
3	E	201	LEU
4	F	139	ASN
5	G	167	VAL

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Mol	Chain	Res	Type
6	K	27	LYS
6	K	34	THR
6	K	174	THR
6	K	190	THR
6	K	195	VAL
7	L	35	ILE
7	L	181	LYS
8	M	157	SER
8	M	220	THR
8	M	239	GLN
1	Q	55	LEU
1	Q	73	PHE
1	Q	169	LEU
1	Q	200	THR
1	Q	230	LYS
1	Q	232	ILE
2	R	2	SER
2	R	11	SER
2	R	63	ILE
2	R	129	ILE
2	R	131	THR
2	R	225	MET
3	S	53	ARG
3	S	79	SER
3	S	201	LEU
4	T	7	ASP
4	T	139	ASN
4	T	198	LEU
5	U	47	ILE
6	Y	27	LYS
6	Y	34	THR
6	Y	152	THR
6	Y	174	THR
6	Y	195	VAL
7	Z	35	ILE
8	a	157	SER
9	A	56	MET
9	A	137	MET
9	A	146	ILE
10	B	45	ILE
10	B	140	ASP
10	B	166	ASP

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Mol	Chain	Res	Type
10	B	171	MET
10	B	186	ASP
10	B	189	HIS
10	B	225	ASN
11	H	44	CYS
11	H	128	LEU
11	H	159	ILE
12	I	135	MET
12	I	210	THR
13	J	140	ILE
13	J	148	ASP
14	N	46	ILE
9	O	12	HIS
9	O	64	ASP
9	O	72	ILE
9	O	75	ILE
9	O	137	MET
9	O	229	ILE
10	P	11	THR
10	P	140	ASP
10	P	162	CYS
10	P	166	ASP
10	P	171	MET
10	P	186	ASP
10	P	189	HIS
10	P	225	ASN
11	V	32	ARG
11	V	44	CYS
11	V	49	SER
11	V	201	MET
12	W	4	CYS
12	W	135	MET
12	W	174	ASP
12	W	201	HIS
12	W	204	ILE
12	W	210	THR
13	X	108	ASN
14	b	10	THR
14	b	130	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	105	GLN
2	D	115	GLN
2	D	164	ASN
2	D	220	GLN
3	E	98	HIS
4	F	4	ASN
4	F	100	ASN
4	F	117	GLN
4	F	218	HIS
4	F	227	GLN
5	G	34	ASN
5	G	58	ASN
5	G	64	ASN
5	G	208	ASN
5	G	231	ASN
6	K	101	ASN
7	L	30	ASN
7	L	70	ASN
7	L	151	GLN
7	L	182	ASN
1	Q	61	ASN
1	Q	105	GLN
1	Q	113	GLN
2	R	115	GLN
2	R	220	GLN
3	S	98	HIS
4	T	4	ASN
4	T	117	GLN
4	T	227	GLN
5	U	34	ASN
5	U	58	ASN
5	U	64	ASN
5	U	208	ASN
6	Y	73	ASN
6	Y	101	ASN
7	Z	30	ASN
7	Z	70	ASN
7	Z	151	GLN
8	a	179	ASN
9	A	77	ASN
9	A	152	ASN
10	B	71	HIS
10	B	148	GLN

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Mol	Chain	Res	Type
10	B	207	ASN
11	H	38	ASN
11	H	194	GLN
11	H	219	HIS
11	H	232	ASN
12	I	30	ASN
12	I	62	ASN
13	J	171	GLN
14	N	155	HIS
9	O	152	ASN
10	P	71	HIS
10	P	148	GLN
10	P	157	ASN
11	V	38	ASN
11	V	194	GLN
11	V	219	HIS
12	W	30	ASN
12	W	73	GLN
13	X	108	ASN
14	b	155	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	A1CY6	Z	301	7	47,47,47	0.21	0	62,62,62	0.63	1 (1%)
15	A1CY6	L	301	7	47,47,47	0.22	0	62,62,62	0.62	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	A1CY6	Z	301	7	-	13/55/55/55	0/2/3/3
15	A1CY6	L	301	7	-	13/55/55/55	0/2/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	301	A1CY6	C13-N12-C10	2.42	127.33	122.82
15	Z	301	A1CY6	C13-N12-C10	2.40	127.29	122.82

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	L	301	A1CY6	C16-C18-C42-C43
15	Z	301	A1CY6	C16-C18-C42-C43
15	L	301	A1CY6	C14-C13-N12-C10
15	Z	301	A1CY6	C14-C13-N12-C10
15	L	301	A1CY6	N19-C18-C42-C43
15	Z	301	A1CY6	N19-C18-C42-C43
15	L	301	A1CY6	N15-C16-C18-C42
15	Z	301	A1CY6	N15-C16-C18-C42
15	L	301	A1CY6	O17-C16-C18-C42
15	Z	301	A1CY6	O17-C16-C18-C42
15	L	301	A1CY6	C08-C09-C10-N12
15	Z	301	A1CY6	C08-C09-C10-N12
15	L	301	A1CY6	C08-C09-C10-O11

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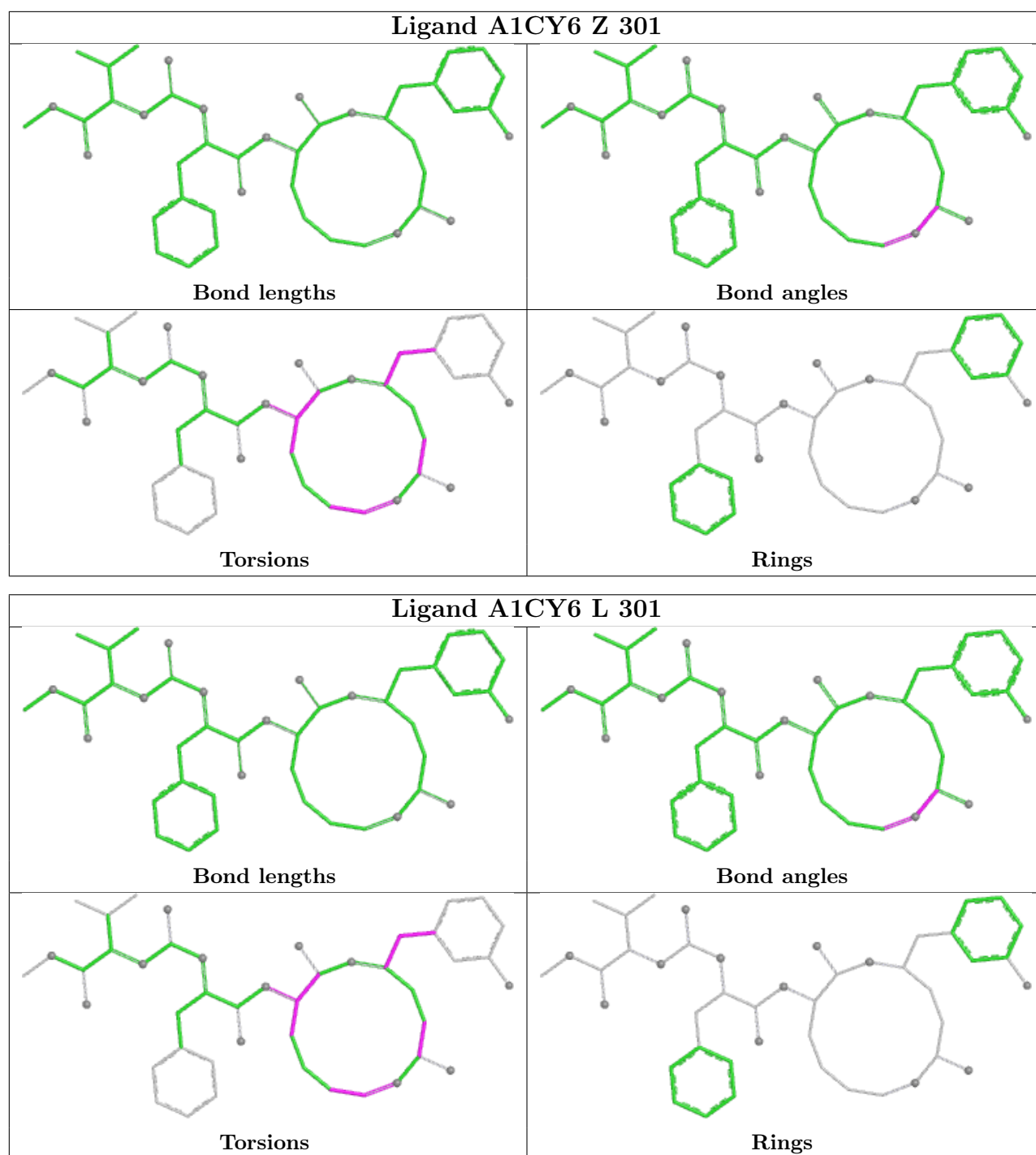
Mol	Chain	Res	Type	Atoms
15	Z	301	A1CY6	C08-C09-C10-O11
15	L	301	A1CY6	C04-C06-C07-C08
15	Z	301	A1CY6	C04-C06-C07-C08
15	L	301	A1CY6	C42-C18-N19-C20
15	Z	301	A1CY6	C42-C18-N19-C20
15	L	301	A1CY6	C03-C04-C06-C07
15	L	301	A1CY6	C04-C06-C07-N15
15	Z	301	A1CY6	C04-C06-C07-N15
15	L	301	A1CY6	C05-C04-C06-C07
15	L	301	A1CY6	N12-C13-C14-C43
15	Z	301	A1CY6	N12-C13-C14-C43
15	Z	301	A1CY6	C03-C04-C06-C07
15	Z	301	A1CY6	C05-C04-C06-C07

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	Z	301	A1CY6	2	0
15	L	301	A1CY6	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

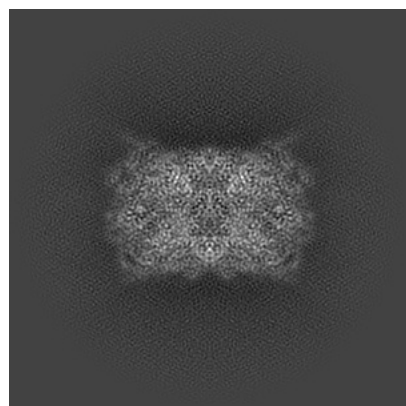
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73509. These allow visual inspection of the internal detail of the map and identification of artifacts.

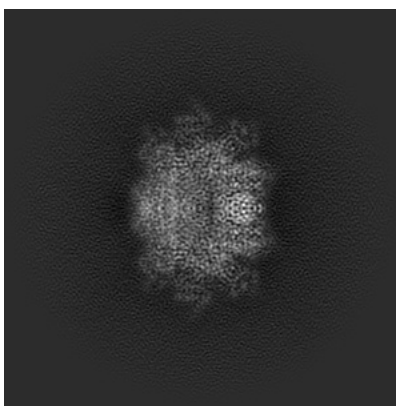
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

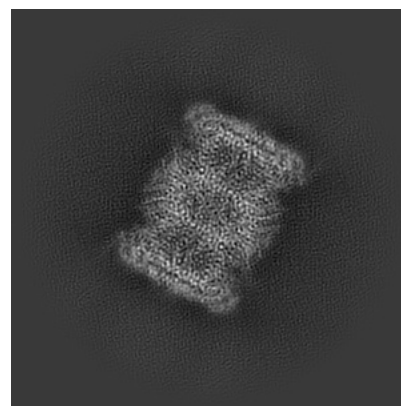
6.1.1 Primary map



X

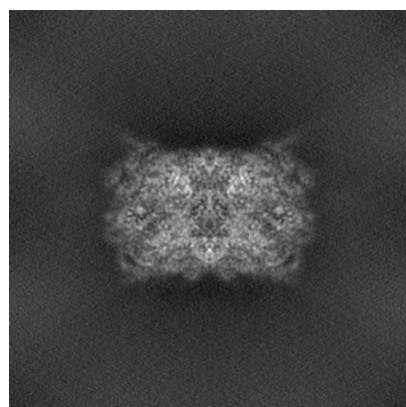


Y

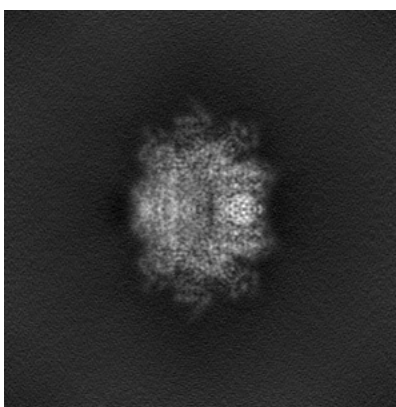


Z

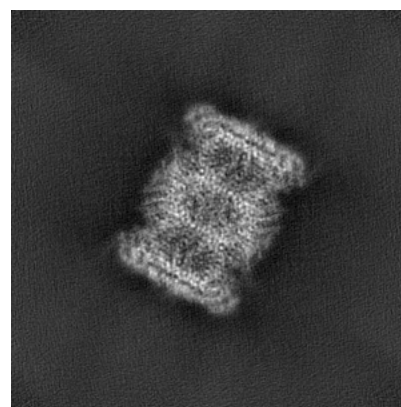
6.1.2 Raw map



X



Y

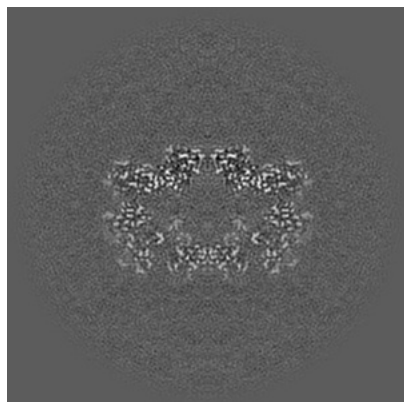


Z

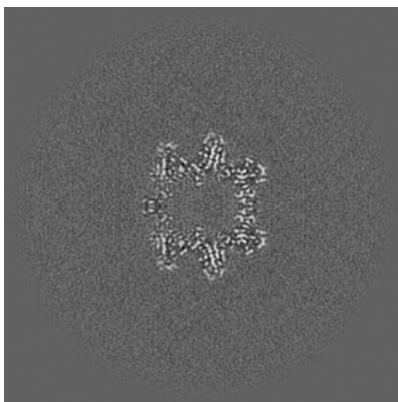
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

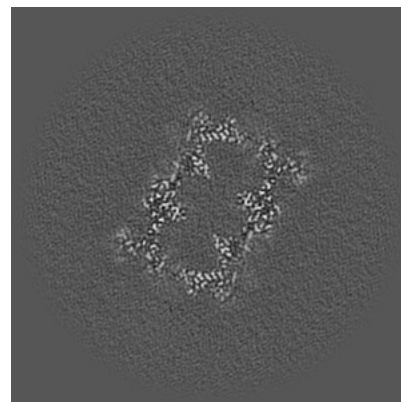
6.2.1 Primary map



X Index: 150

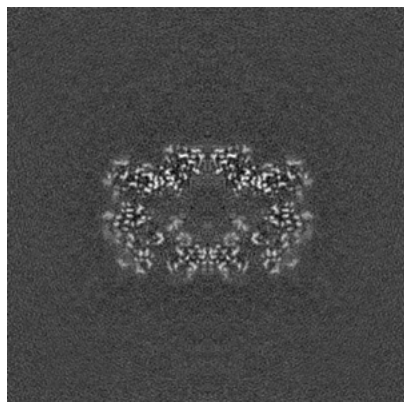


Y Index: 150

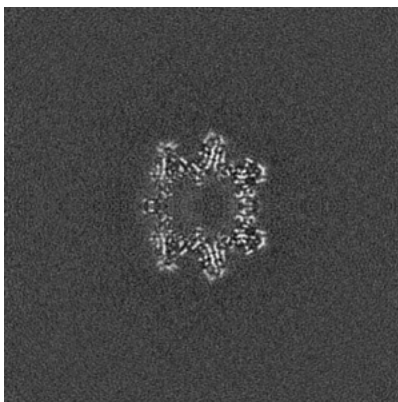


Z Index: 150

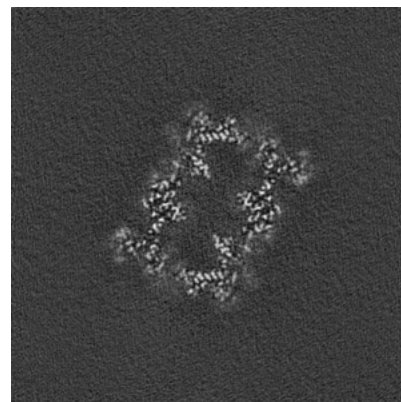
6.2.2 Raw map



X Index: 150



Y Index: 150

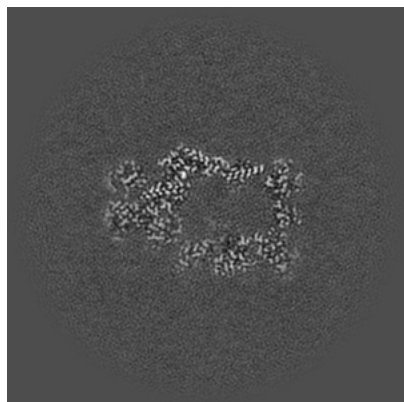


Z Index: 150

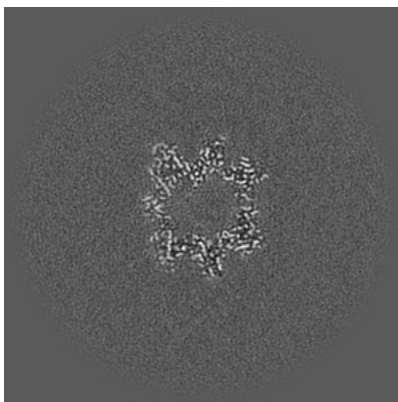
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

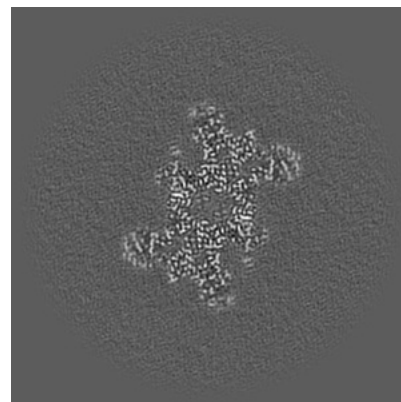
6.3.1 Primary map



X Index: 158

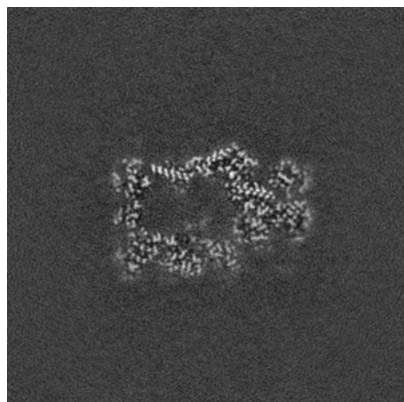


Y Index: 152

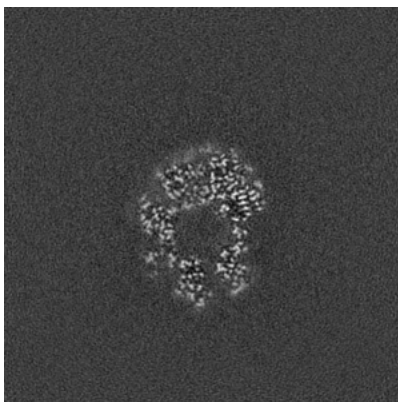


Z Index: 172

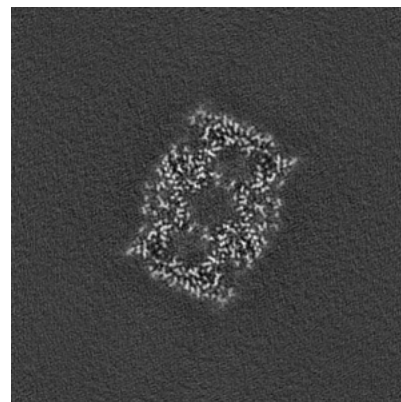
6.3.2 Raw map



X Index: 142



Y Index: 126

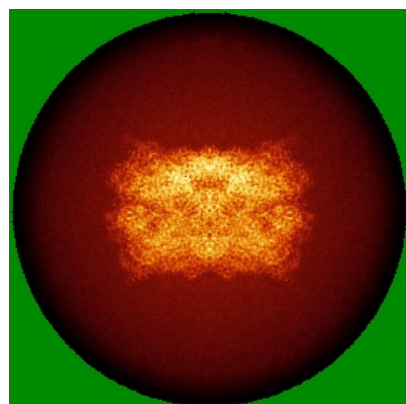


Z Index: 164

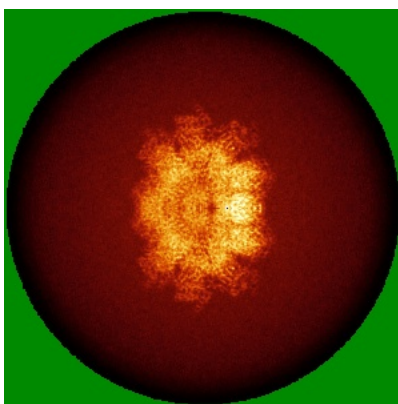
The images above show the largest variance slices of the map in three orthogonal directions.

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

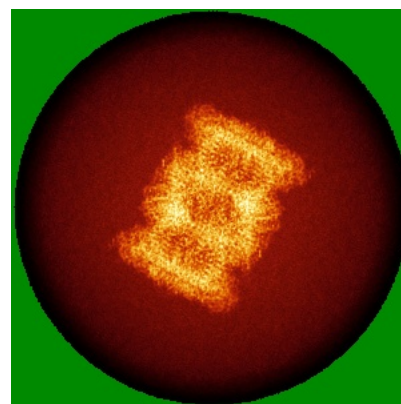
6.4.1 Primary map



X

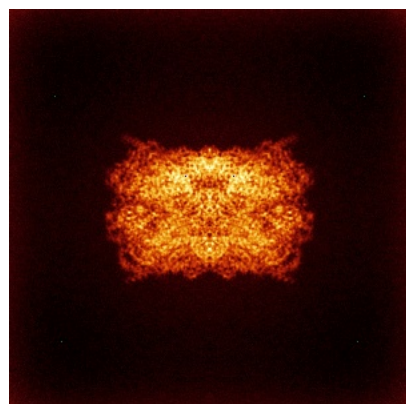


Y

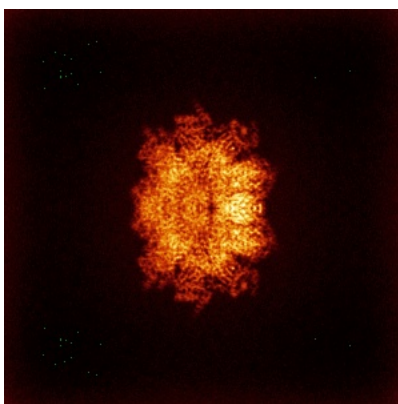


Z

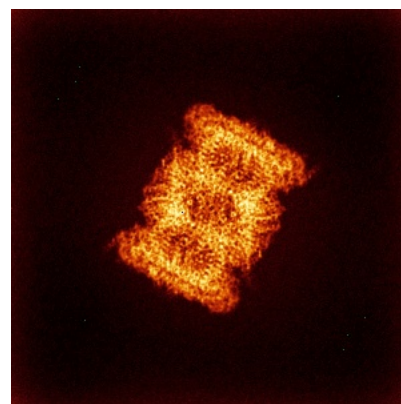
6.4.2 Raw map



X



Y

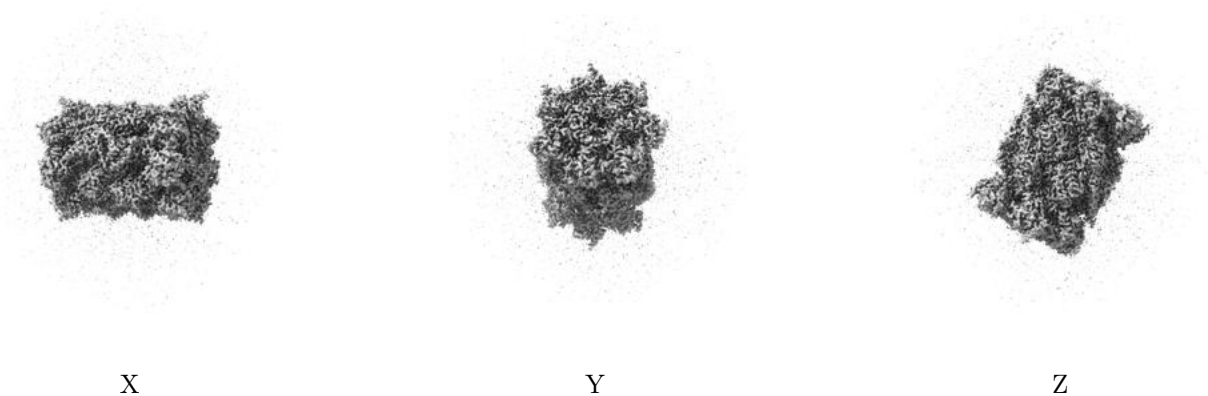


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

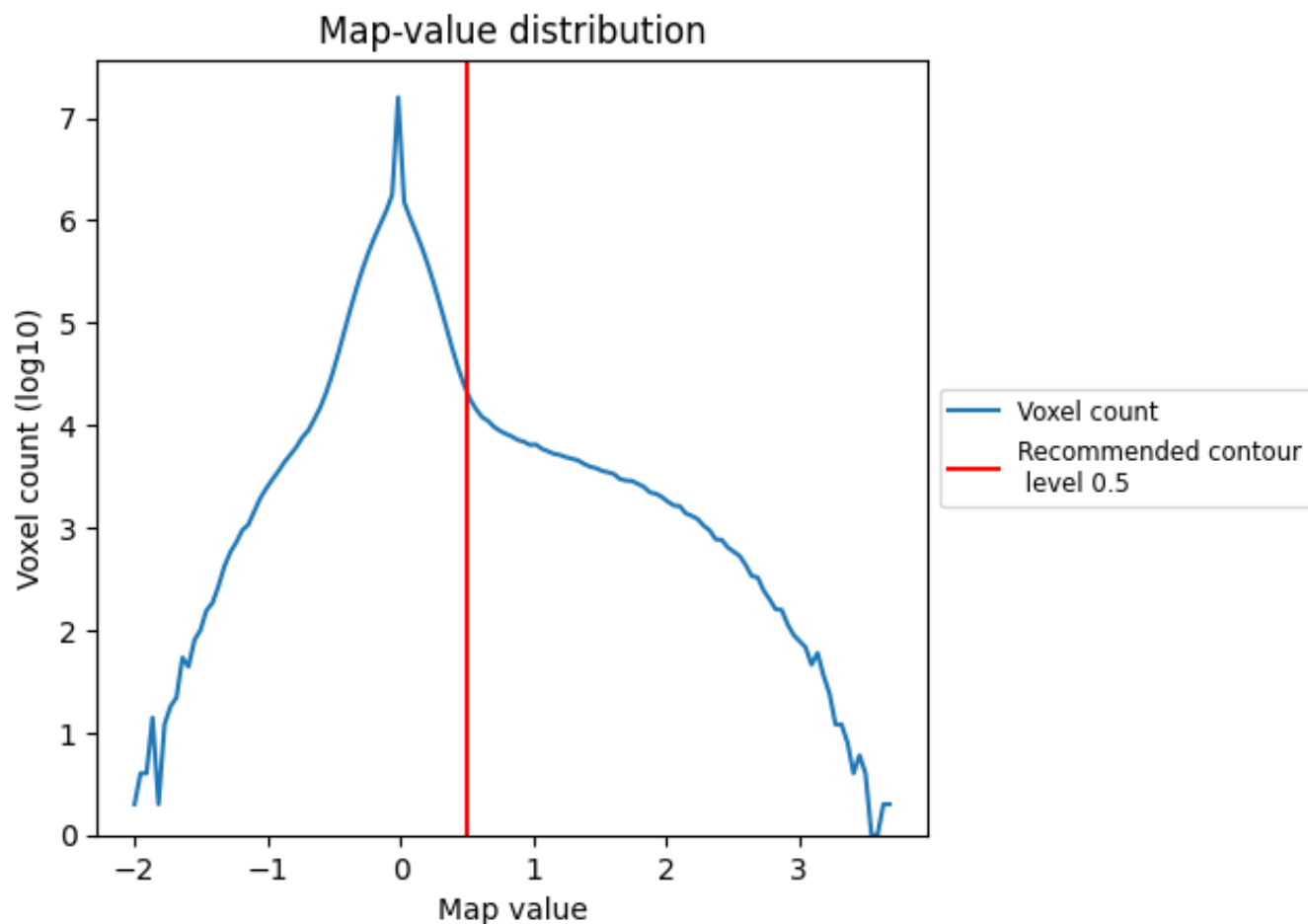
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

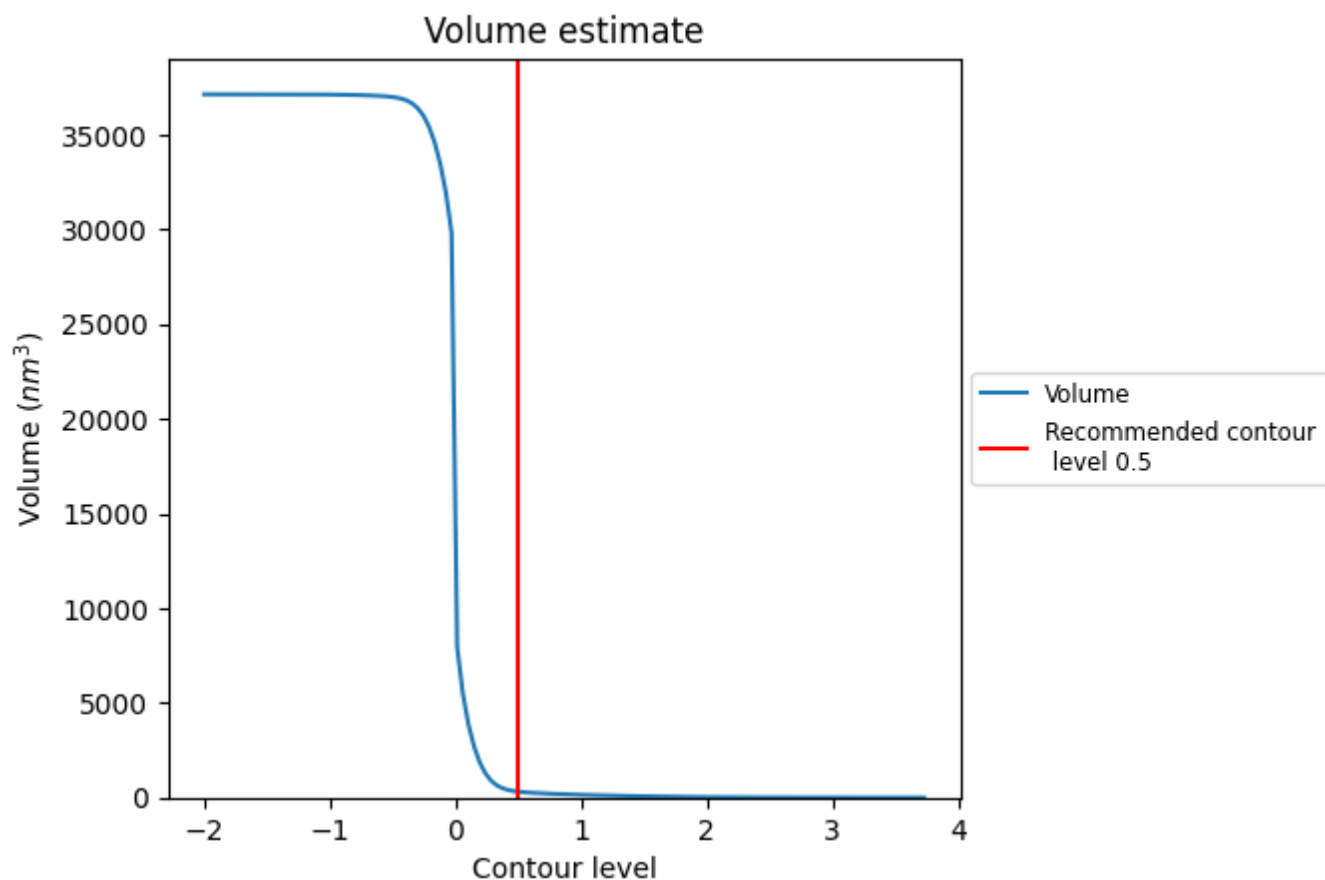
This section contains the results of statistical analysis of the map.

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.

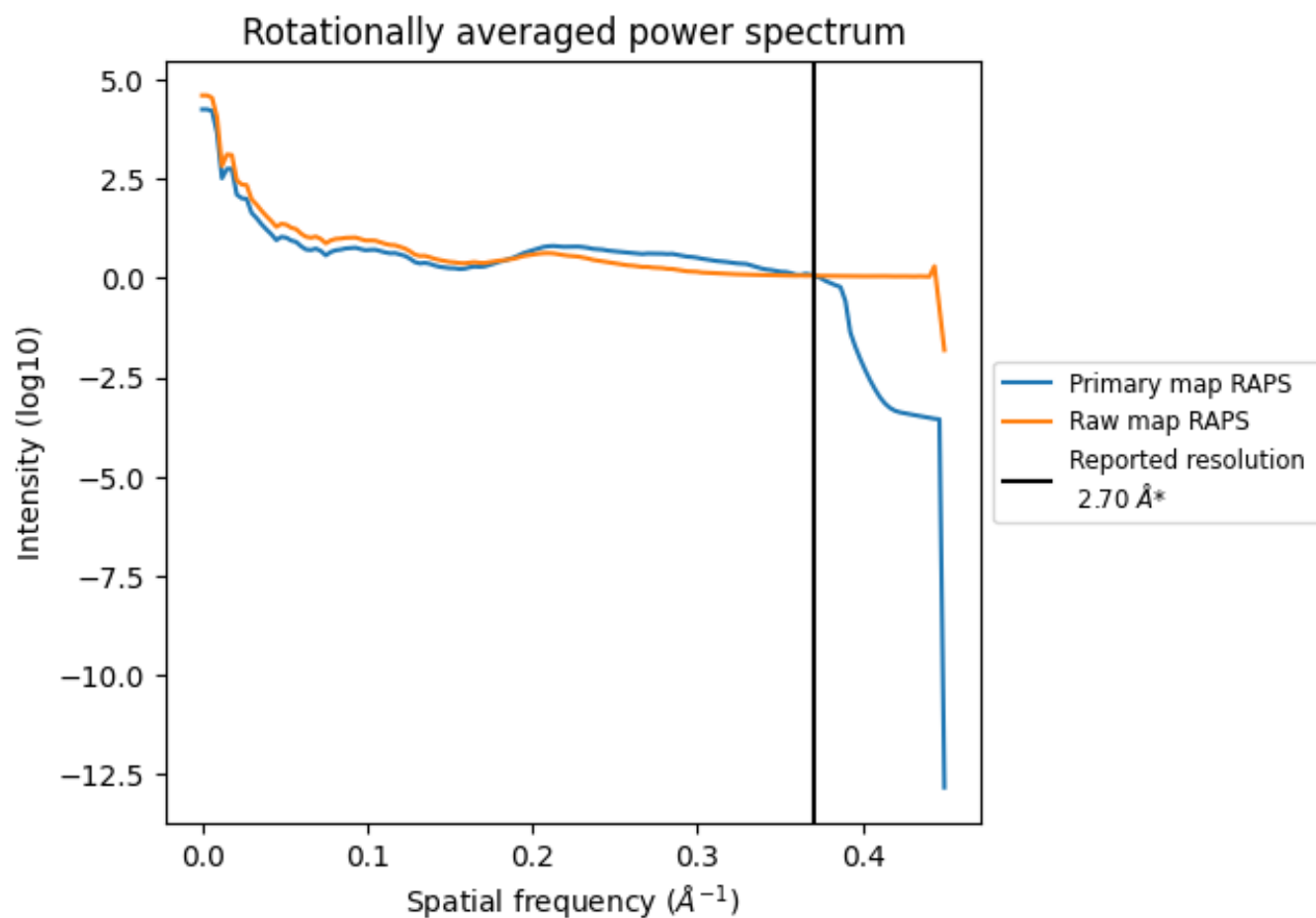
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 311 nm³; this corresponds to an approximate mass of 281 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

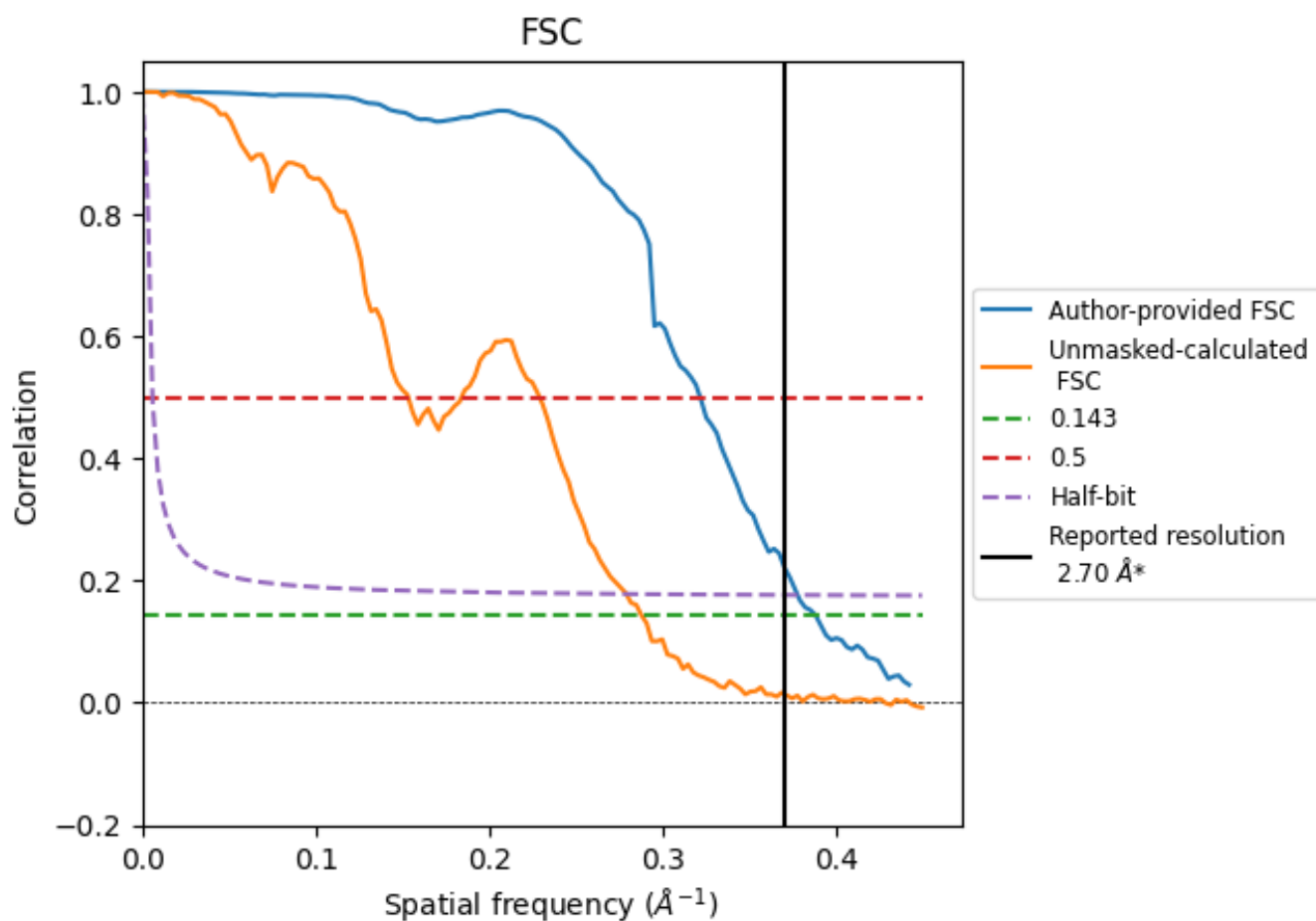


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

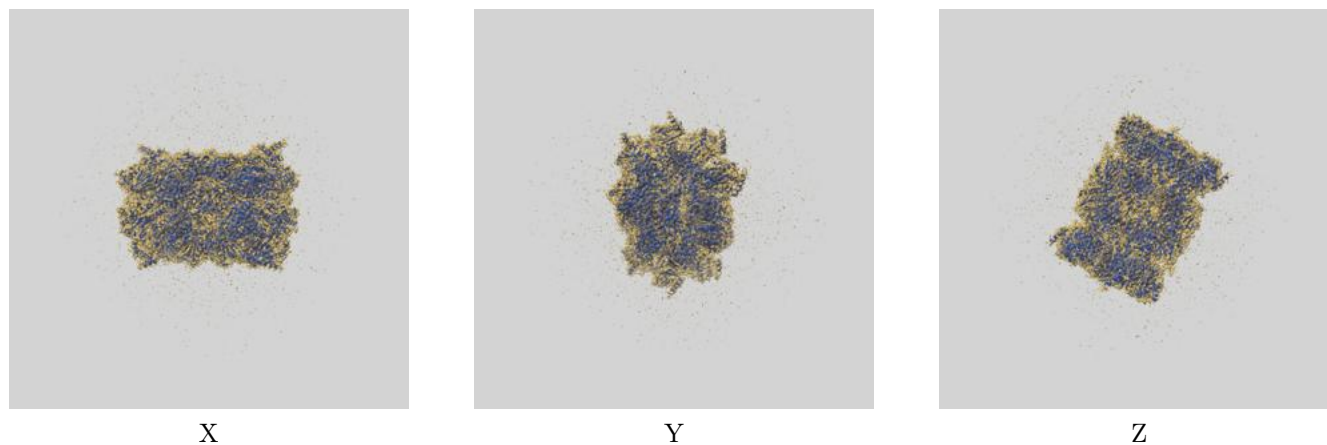
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.58	3.11	2.65
Unmasked-calculated*	3.47	6.52	3.58

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.47 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

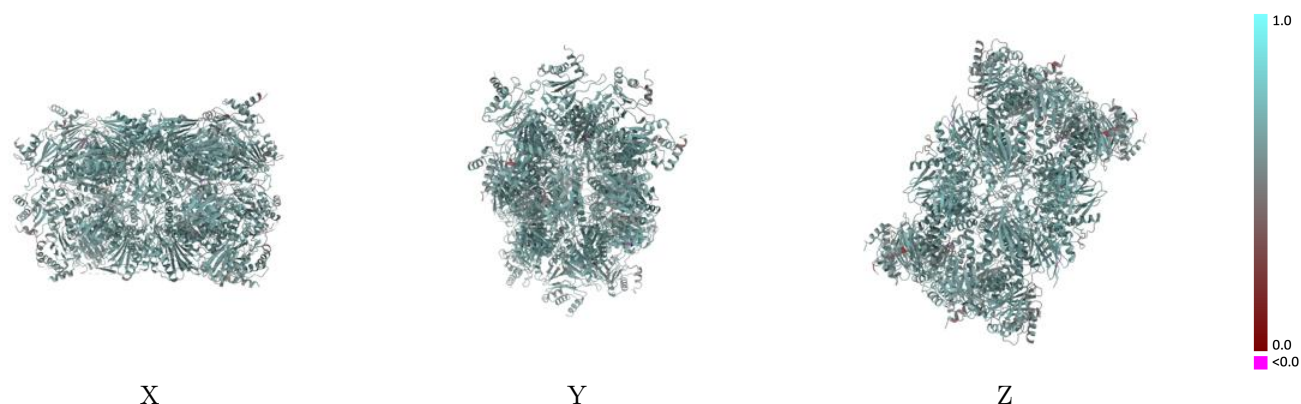
This section contains information regarding the fit between EMDB map EMD-73509 and PDB model 9YUY. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



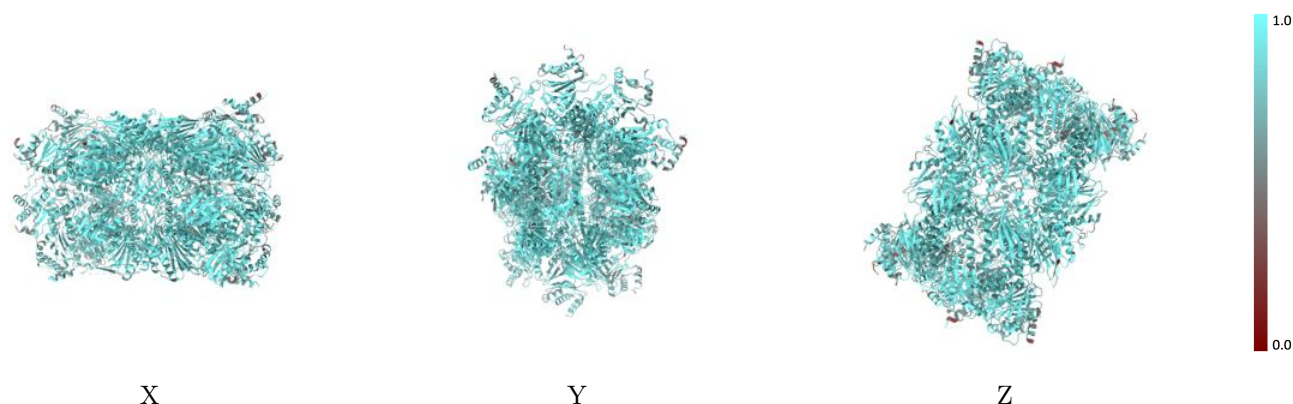
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



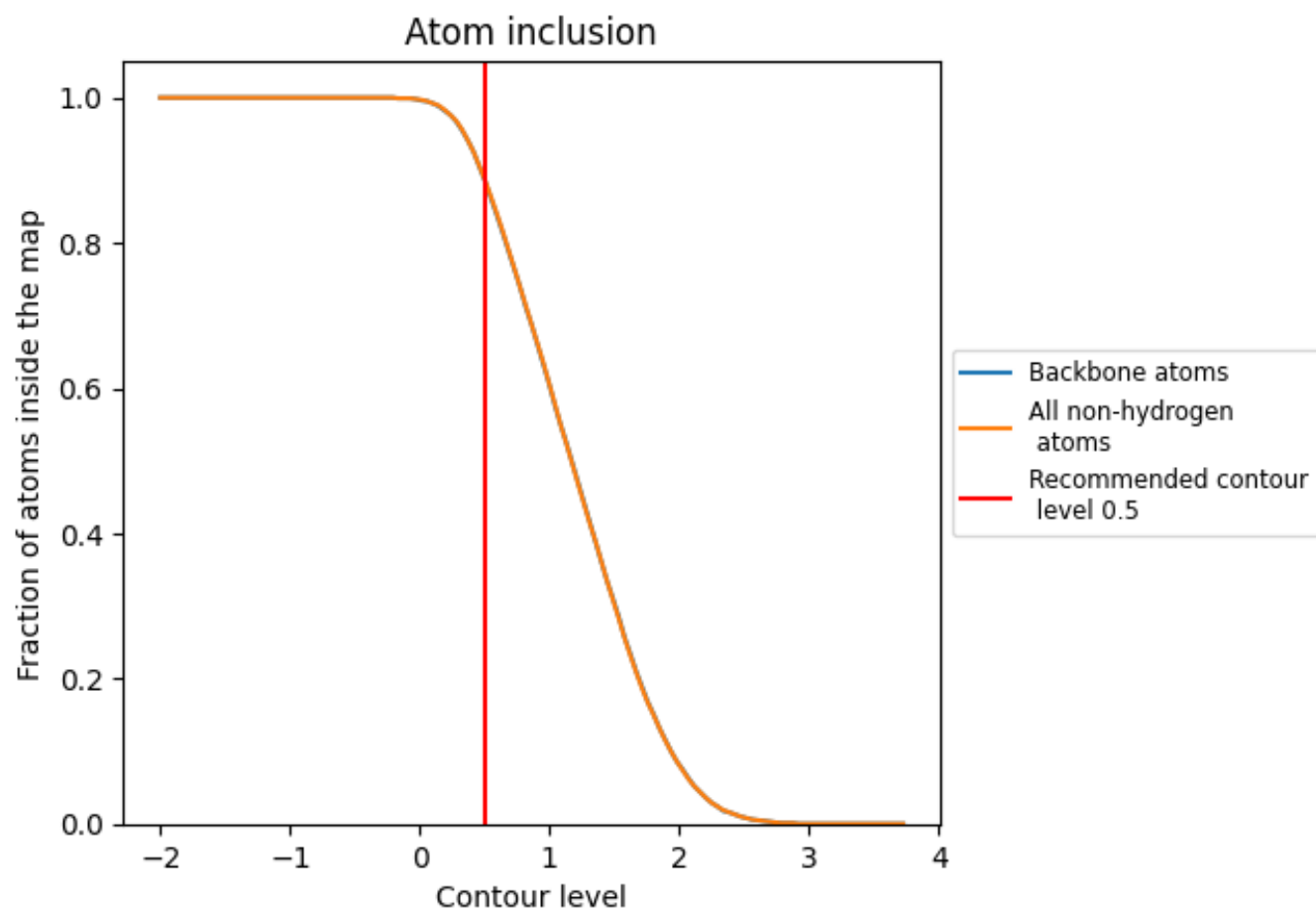
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8870	 0.6100
A	 0.8420	 0.5930
B	 0.8400	 0.5890
C	 0.8580	 0.5990
D	 0.8450	 0.5920
E	 0.8070	 0.5650
F	 0.8770	 0.6060
G	 0.8860	 0.6080
H	 0.8910	 0.6180
I	 0.8860	 0.5930
J	 0.9430	 0.6310
K	 0.9510	 0.6360
L	 0.9590	 0.6490
M	 0.9400	 0.6390
N	 0.9370	 0.6310
O	 0.8410	 0.5910
P	 0.8400	 0.5880
Q	 0.8630	 0.6010
R	 0.8480	 0.5970
S	 0.8050	 0.5650
T	 0.8770	 0.6080
U	 0.8860	 0.6060
V	 0.8910	 0.6170
W	 0.8870	 0.5930
X	 0.9420	 0.6340
Y	 0.9510	 0.6350
Z	 0.9610	 0.6500
a	 0.9360	 0.6340
b	 0.9380	 0.6330

