



Full wwPDB EM Validation Report ⓘ

Mar 3, 2024 – 09:54 AM EST

PDB ID : 6BNV
EMDB ID : EMD-7116
Title : CryoEM structure of MyosinVI-actin complex in the rigor (nucleotide-free) state, backbone-averaged with side chains truncated to alanine
Authors : Gurel, P.S.; Alushin, G.A.
Deposited on : 2017-11-17
Resolution : 4.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

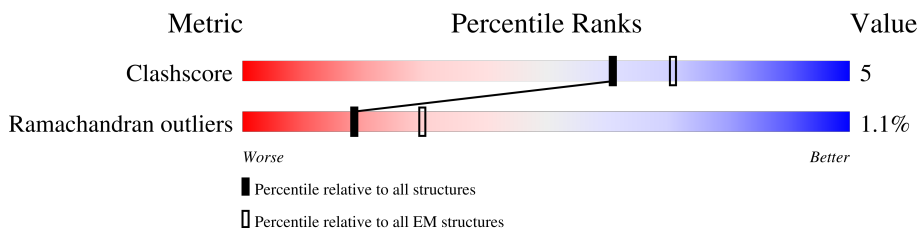
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.60 Å.

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



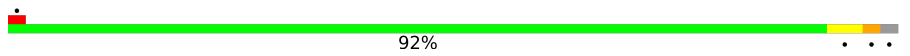
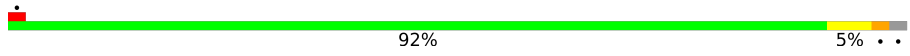
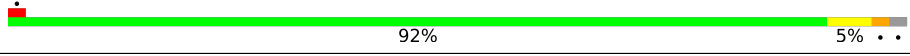
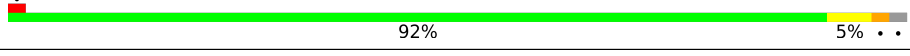
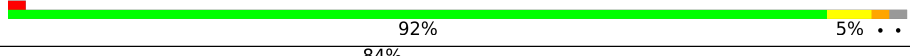
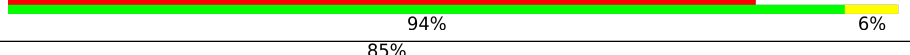
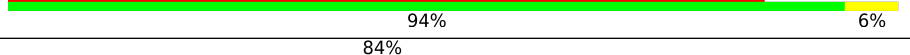
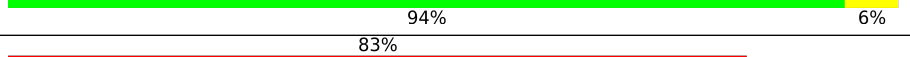
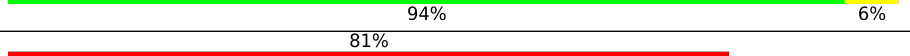
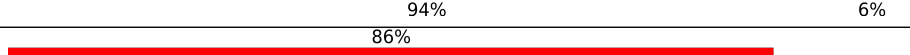
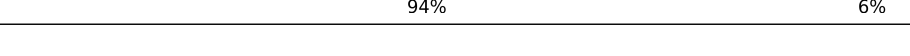
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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	I	816	16% 93% 5% 5%
1	J	816	16% 93% 5% 5%
1	K	816	16% 93% 5% 5%
1	L	816	17% 93% 5% 5%
1	M	816	16% 93% 5% 5%
1	N	816	17% 93% 5% 5%
2	A	373	1% 92% 5% 5%
2	B	373	1% 92% 5% 5%
2	C	373	1% 92% 5% 5%

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Mol	Chain	Length	Quality of chain
2	D	373	 92% . . .
2	E	373	 92% 5% . . .
2	F	373	 92% 5% . . .
2	G	373	 92% 5% . . .
2	H	373	 92% 5% . . .
3	O	145	 84% 94% 6%
3	P	145	 85% 94% 6%
3	Q	145	 84% 94% 6%
3	R	145	 83% 94% 6%
3	S	145	 81% 94% 6%
3	T	145	 86% 94% 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 42360 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Unconventional myosin-VI.

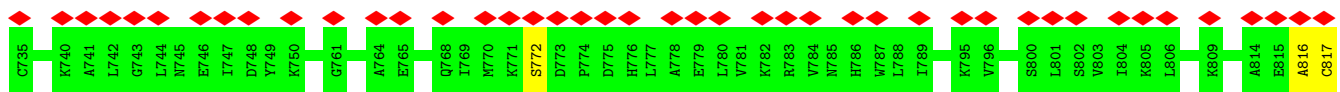
Mol	Chain	Residues	Atoms				AltConf	Trace
1	I	797	Total	C	N	O	0	0
			3939	2346	797	796		
1	J	797	Total	C	N	O	0	0
			3939	2346	797	796		
1	K	797	Total	C	N	O	0	0
			3939	2346	797	796		
1	L	797	Total	C	N	O	0	0
			3939	2346	797	796		
1	M	797	Total	C	N	O	0	0
			3939	2346	797	796		
1	N	797	Total	C	N	O	0	0
			3939	2346	797	796		

- Molecule 2 is a protein called Actin, alpha skeletal muscle.

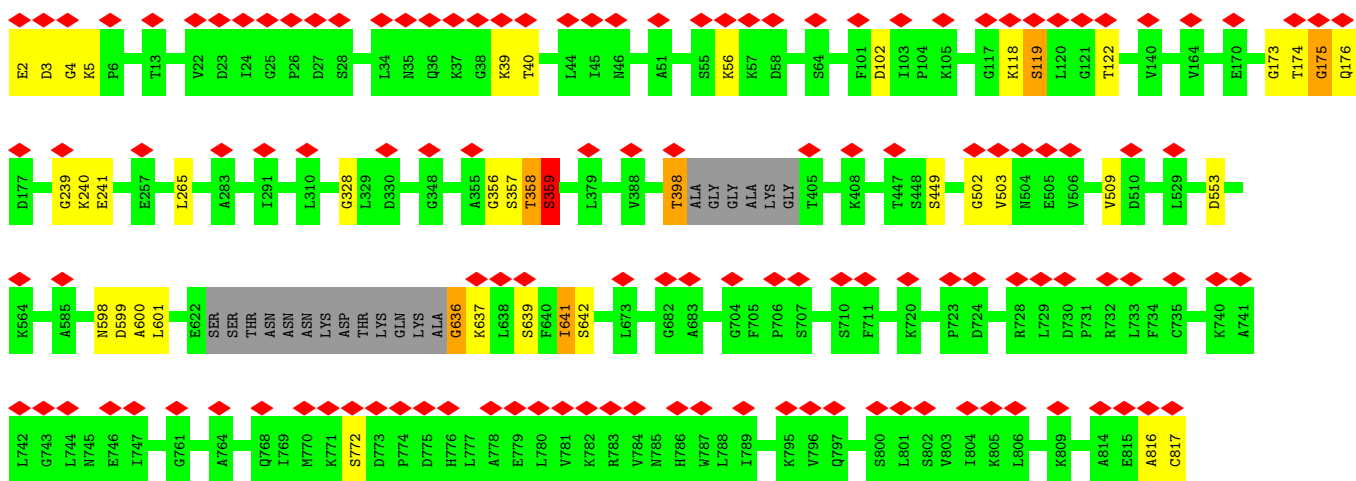
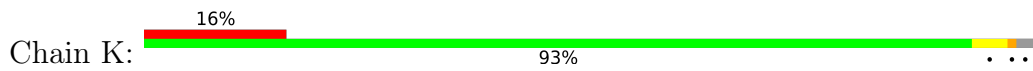
Mol	Chain	Residues	Atoms				AltConf	Trace
2	A	367	Total	C	N	O	0	0
			1806	1073	367	366		
2	B	367	Total	C	N	O	0	0
			1806	1073	367	366		
2	C	367	Total	C	N	O	0	0
			1806	1073	367	366		
2	D	367	Total	C	N	O	0	0
			1806	1073	367	366		
2	E	367	Total	C	N	O	0	0
			1806	1073	367	366		
2	F	367	Total	C	N	O	0	0
			1806	1073	367	366		
2	G	367	Total	C	N	O	0	0
			1806	1073	367	366		
2	H	367	Total	C	N	O	0	0
			1806	1073	367	366		

- Molecule 3 is a protein called Calmodulin.

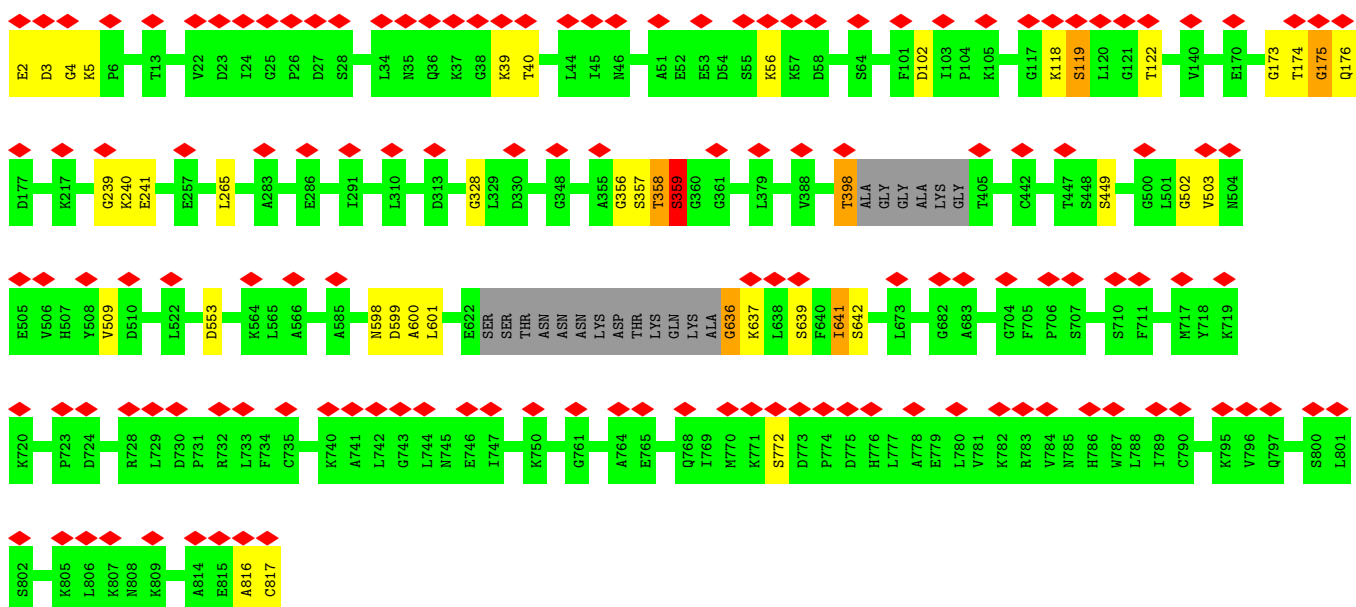
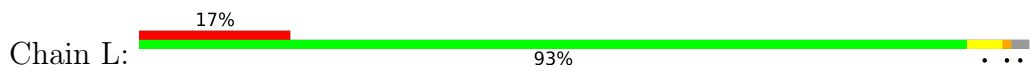
Mol	Chain	Residues	Atoms				AltConf	Trace
3	O	145	Total 713	C 424	N 145	O 144	0	0
3	P	145	Total 713	C 424	N 145	O 144	0	0
3	Q	145	Total 713	C 424	N 145	O 144	0	0
3	R	145	Total 713	C 424	N 145	O 144	0	0
3	S	145	Total 713	C 424	N 145	O 144	0	0
3	T	145	Total 713	C 424	N 145	O 144	0	0



• Molecule 1: Unconventional myosin-VI

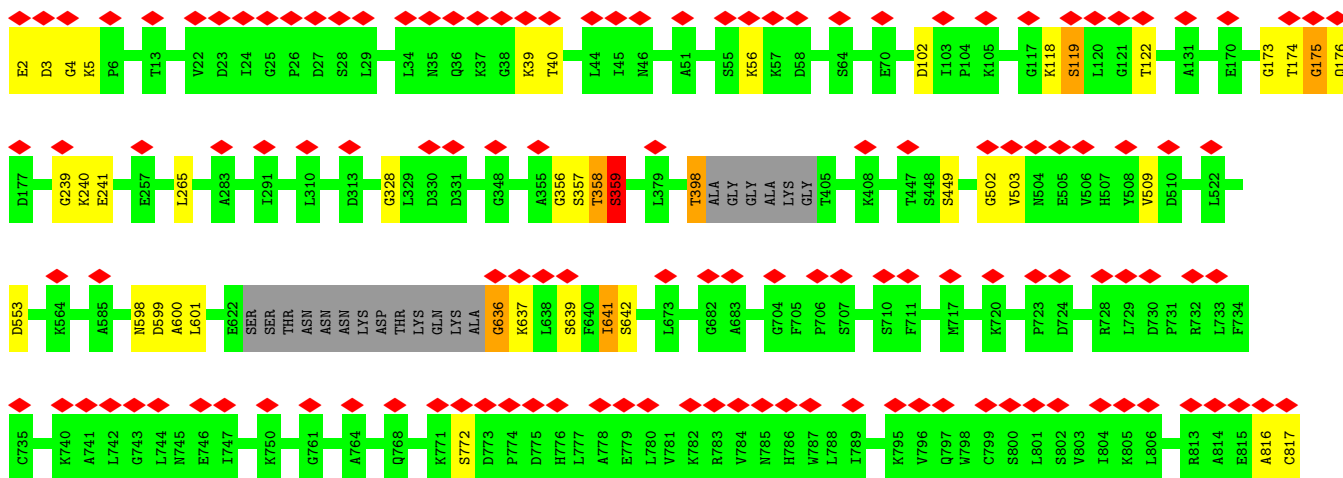


• Molecule 1: Unconventional myosin-VI



• Molecule 1: Unconventional myosin-VI

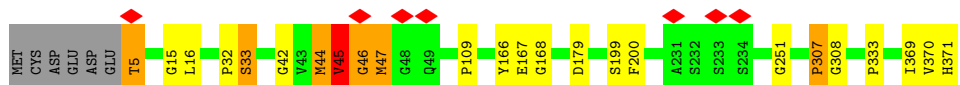
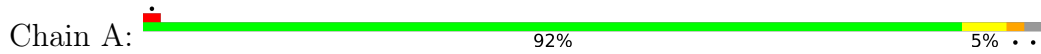




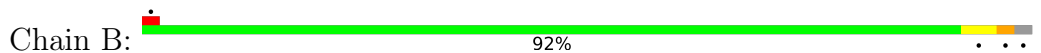
• Molecule 1: Unconventional myosin-VI

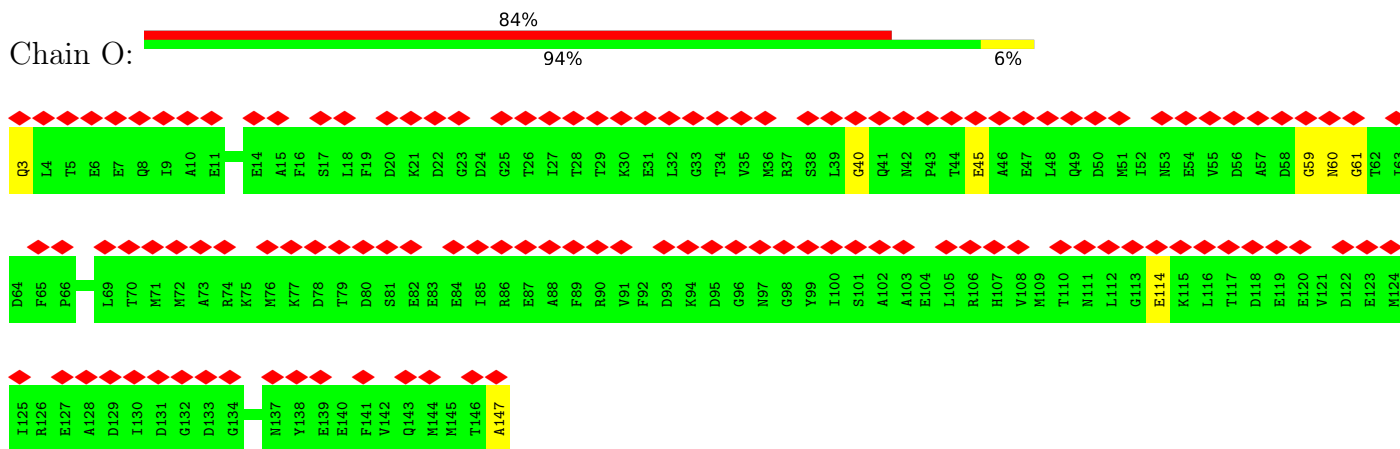


• Molecule 2: Actin, alpha skeletal muscle

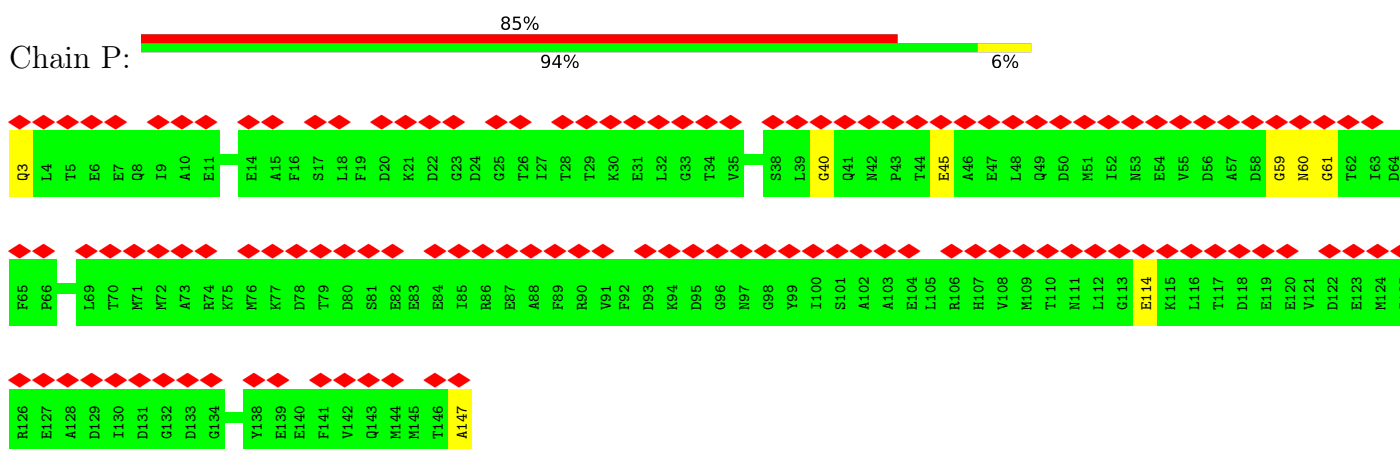


• Molecule 2: Actin, alpha skeletal muscle

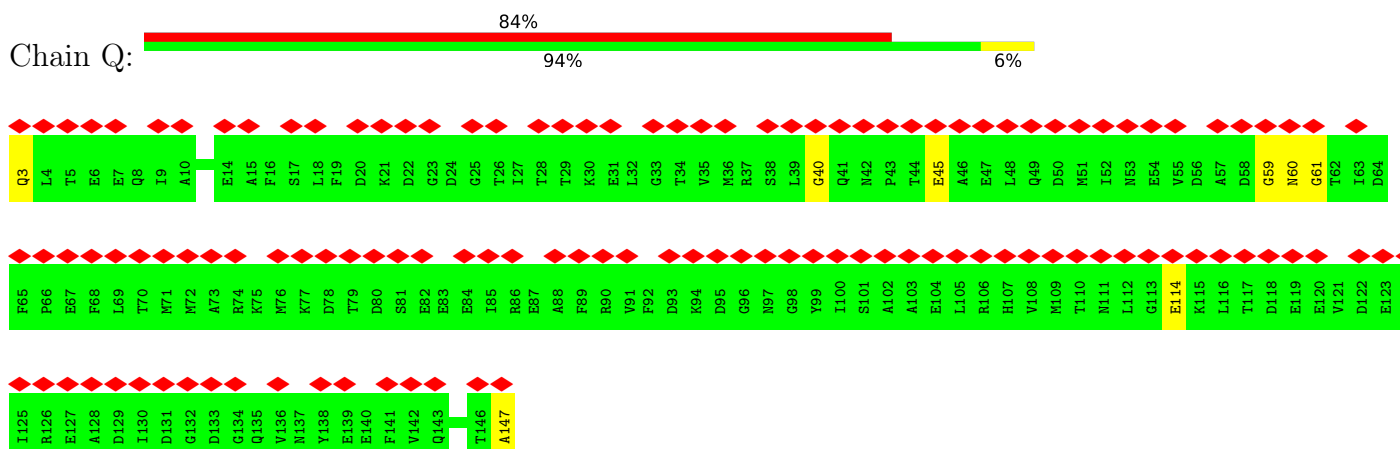




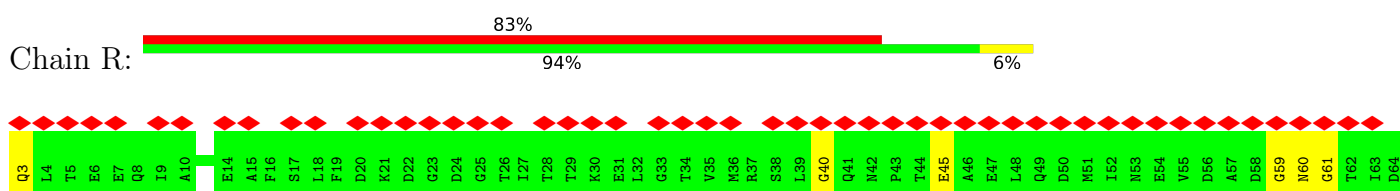
• Molecule 3: Calmodulin

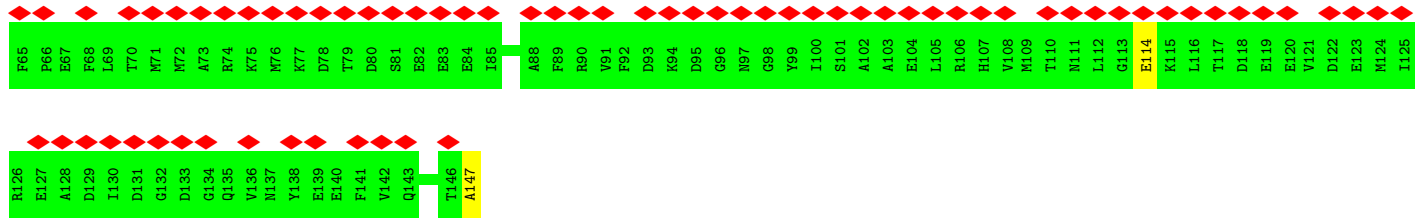


• Molecule 3: Calmodulin

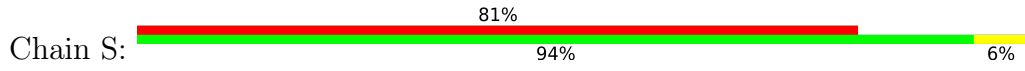


• Molecule 3: Calmodulin

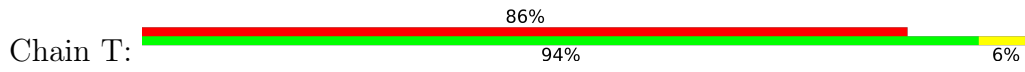




• Molecule 3: Calmodulin



• Molecule 3: Calmodulin



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-166.73°, rise=28.06 Å, axial sym=C1	Depositor
Number of segments used	56116	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI 20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{Å}^2$)	1.5	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	20.608	Depositor
Minimum map value	-9.432	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6.0	Depositor
Map size (Å)	650.24, 650.24, 650.24	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.27, 1.27, 1.27	Depositor

5 Model quality i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	I	2.08	72/3936 (1.8%)	1.65	35/5479 (0.6%)
1	J	2.07	72/3936 (1.8%)	1.65	35/5479 (0.6%)
1	K	2.07	72/3936 (1.8%)	1.65	35/5479 (0.6%)
1	L	2.08	72/3936 (1.8%)	1.65	35/5479 (0.6%)
1	M	2.07	72/3936 (1.8%)	1.65	35/5479 (0.6%)
1	N	2.08	72/3936 (1.8%)	1.65	35/5479 (0.6%)
2	A	2.79	35/1805 (1.9%)	2.15	31/2509 (1.2%)
2	B	2.78	35/1805 (1.9%)	2.15	31/2509 (1.2%)
2	C	2.79	35/1805 (1.9%)	2.15	31/2509 (1.2%)
2	D	2.79	35/1805 (1.9%)	2.15	31/2509 (1.2%)
2	E	2.79	35/1805 (1.9%)	2.15	31/2509 (1.2%)
2	F	2.79	35/1805 (1.9%)	2.15	31/2509 (1.2%)
2	G	2.78	35/1805 (1.9%)	2.15	31/2509 (1.2%)
2	H	2.79	35/1805 (1.9%)	2.15	31/2509 (1.2%)
3	O	1.83	14/712 (2.0%)	1.15	6/989 (0.6%)
3	P	1.83	14/712 (2.0%)	1.15	6/989 (0.6%)
3	Q	1.83	14/712 (2.0%)	1.15	6/989 (0.6%)
3	R	1.83	14/712 (2.0%)	1.15	6/989 (0.6%)
3	S	1.82	14/712 (2.0%)	1.15	6/989 (0.6%)
3	T	1.83	14/712 (2.0%)	1.14	6/989 (0.6%)
All	All	2.32	796/42328 (1.9%)	1.79	494/58880 (0.8%)

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	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	N	0	1
2	A	1	0
2	B	1	0
2	C	1	0
2	D	1	0
2	E	1	0
2	F	1	0
2	G	1	0
2	H	1	0
All	All	8	6

All (796) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	175	GLY	C-O	-47.03	0.48	1.23
1	N	175	GLY	C-O	-46.98	0.48	1.23
1	J	175	GLY	C-O	-46.97	0.48	1.23
1	K	175	GLY	C-O	-46.96	0.48	1.23
1	I	175	GLY	C-O	-46.93	0.48	1.23
1	M	175	GLY	C-O	-46.93	0.48	1.23
1	I	358	THR	C-O	-43.83	0.40	1.23
1	M	358	THR	C-O	-43.78	0.40	1.23
1	L	358	THR	C-O	-43.78	0.40	1.23
1	N	358	THR	C-O	-43.78	0.40	1.23
1	J	358	THR	C-O	-43.76	0.40	1.23
1	K	358	THR	C-O	-43.75	0.40	1.23
2	F	5	THR	N-CA	-39.36	0.67	1.46
2	C	5	THR	N-CA	-39.35	0.67	1.46
2	A	5	THR	N-CA	-39.32	0.67	1.46
2	E	5	THR	N-CA	-39.32	0.67	1.46
2	H	5	THR	N-CA	-39.31	0.67	1.46
2	B	5	THR	N-CA	-39.30	0.67	1.46
2	G	5	THR	N-CA	-39.30	0.67	1.46
2	D	5	THR	N-CA	-39.28	0.67	1.46
2	C	307	PRO	C-O	-38.55	0.46	1.23
2	A	307	PRO	C-O	-38.55	0.46	1.23
2	D	307	PRO	C-O	-38.55	0.46	1.23
2	E	307	PRO	C-O	-38.55	0.46	1.23
2	B	307	PRO	C-O	-38.54	0.46	1.23
2	G	307	PRO	C-O	-38.54	0.46	1.23
2	F	307	PRO	C-O	-38.53	0.46	1.23
2	H	307	PRO	C-O	-38.53	0.46	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	5	THR	CA-CB	-37.36	0.56	1.53
2	F	5	THR	CA-CB	-37.35	0.56	1.53
2	A	5	THR	CA-CB	-37.35	0.56	1.53
2	H	5	THR	CA-CB	-37.35	0.56	1.53
2	B	5	THR	CA-CB	-37.34	0.56	1.53
2	D	5	THR	CA-CB	-37.34	0.56	1.53
2	E	5	THR	CA-CB	-37.33	0.56	1.53
2	G	5	THR	CA-CB	-37.29	0.56	1.53
2	H	44	MET	C-O	-35.79	0.55	1.23
2	D	44	MET	C-O	-35.79	0.55	1.23
2	B	44	MET	C-O	-35.77	0.55	1.23
2	C	44	MET	C-O	-35.76	0.55	1.23
2	E	44	MET	C-O	-35.77	0.55	1.23
2	F	44	MET	C-O	-35.76	0.55	1.23
2	G	44	MET	C-O	-35.76	0.55	1.23
2	A	44	MET	C-O	-35.75	0.55	1.23
1	N	174	THR	C-O	-33.81	0.59	1.23
1	K	174	THR	C-O	-33.76	0.59	1.23
1	I	174	THR	C-O	-33.75	0.59	1.23
1	L	174	THR	C-O	-33.74	0.59	1.23
1	J	174	THR	C-O	-33.71	0.59	1.23
1	M	174	THR	C-O	-33.70	0.59	1.23
1	K	553	ASP	C-O	-32.80	0.61	1.23
1	I	553	ASP	C-O	-32.80	0.61	1.23
1	L	553	ASP	C-O	-32.76	0.61	1.23
1	M	553	ASP	C-O	-32.76	0.61	1.23
1	N	553	ASP	C-O	-32.76	0.61	1.23
1	J	553	ASP	C-O	-32.73	0.61	1.23
2	C	45	VAL	C-O	-28.86	0.68	1.23
2	F	45	VAL	C-O	-28.84	0.68	1.23
2	G	45	VAL	C-O	-28.83	0.68	1.23
2	A	45	VAL	C-O	-28.82	0.68	1.23
2	E	45	VAL	C-O	-28.82	0.68	1.23
2	H	45	VAL	C-O	-28.82	0.68	1.23
2	B	45	VAL	C-O	-28.82	0.68	1.23
2	D	45	VAL	C-O	-28.80	0.68	1.23
2	C	109	PRO	C-O	-28.67	0.66	1.23
2	E	109	PRO	C-O	-28.66	0.66	1.23
2	H	109	PRO	C-O	-28.65	0.66	1.23
2	B	109	PRO	C-O	-28.62	0.66	1.23
2	A	109	PRO	C-O	-28.62	0.66	1.23
2	G	109	PRO	C-O	-28.62	0.66	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	109	PRO	C-O	-28.61	0.66	1.23
2	F	109	PRO	C-O	-28.60	0.66	1.23
2	C	32	PRO	C-O	-28.40	0.66	1.23
2	E	32	PRO	C-O	-28.39	0.66	1.23
2	D	32	PRO	C-O	-28.39	0.66	1.23
2	F	32	PRO	C-O	-28.37	0.66	1.23
2	G	32	PRO	C-O	-28.37	0.66	1.23
2	A	32	PRO	C-O	-28.36	0.66	1.23
2	H	32	PRO	C-O	-28.36	0.66	1.23
2	B	32	PRO	C-O	-28.32	0.66	1.23
1	M	772	SER	C-O	-27.91	0.70	1.23
1	K	772	SER	C-O	-27.91	0.70	1.23
1	N	772	SER	C-O	-27.91	0.70	1.23
1	L	772	SER	C-O	-27.90	0.70	1.23
1	I	772	SER	C-O	-27.86	0.70	1.23
1	J	772	SER	C-O	-27.84	0.70	1.23
2	C	371	HIS	CA-CB	-25.37	0.98	1.53
2	E	371	HIS	CA-CB	-25.35	0.98	1.53
2	H	371	HIS	CA-CB	-25.35	0.98	1.53
2	D	371	HIS	CA-CB	-25.34	0.98	1.53
2	A	371	HIS	CA-CB	-25.33	0.98	1.53
2	G	371	HIS	CA-CB	-25.31	0.98	1.53
2	F	371	HIS	CA-CB	-25.30	0.98	1.53
2	B	371	HIS	CA-CB	-25.30	0.98	1.53
1	I	357	SER	C-O	-24.66	0.76	1.23
1	N	357	SER	C-O	-24.59	0.76	1.23
1	J	357	SER	C-O	-24.59	0.76	1.23
1	L	357	SER	C-O	-24.58	0.76	1.23
1	M	357	SER	C-O	-24.57	0.76	1.23
1	K	357	SER	C-O	-24.56	0.76	1.23
1	J	398	THR	C-O	-24.18	0.77	1.23
1	I	398	THR	C-O	-24.16	0.77	1.23
1	K	398	THR	C-O	-24.15	0.77	1.23
1	L	398	THR	C-O	-24.15	0.77	1.23
1	N	398	THR	C-O	-24.15	0.77	1.23
1	M	398	THR	C-O	-24.11	0.77	1.23
2	A	44	MET	C-N	-22.85	0.81	1.34
2	G	44	MET	C-N	-22.85	0.81	1.34
2	C	44	MET	C-N	-22.84	0.81	1.34
2	D	44	MET	C-N	-22.84	0.81	1.34
2	B	44	MET	C-N	-22.84	0.81	1.34
2	E	44	MET	C-N	-22.83	0.81	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	44	MET	C-N	-22.83	0.81	1.34
2	F	44	MET	C-N	-22.81	0.81	1.34
1	I	358	THR	C-N	-22.80	0.81	1.34
1	N	358	THR	C-N	-22.79	0.81	1.34
1	M	358	THR	C-N	-22.78	0.81	1.34
1	J	358	THR	C-N	-22.78	0.81	1.34
2	D	307	PRO	C-N	-22.77	0.92	1.33
2	C	307	PRO	C-N	-22.76	0.92	1.33
2	F	307	PRO	C-N	-22.75	0.92	1.33
1	K	358	THR	C-N	-22.74	0.81	1.34
1	L	358	THR	C-N	-22.74	0.81	1.34
2	B	307	PRO	C-N	-22.73	0.92	1.33
2	G	307	PRO	C-N	-22.72	0.92	1.33
2	H	307	PRO	C-N	-22.71	0.92	1.33
2	A	307	PRO	C-N	-22.70	0.92	1.33
2	E	307	PRO	C-N	-22.70	0.92	1.33
3	R	3	GLN	N-CA	-21.97	1.02	1.46
3	P	3	GLN	N-CA	-21.95	1.02	1.46
3	O	3	GLN	N-CA	-21.95	1.02	1.46
3	S	3	GLN	N-CA	-21.93	1.02	1.46
3	T	3	GLN	N-CA	-21.92	1.02	1.46
3	Q	3	GLN	N-CA	-21.92	1.02	1.46
1	L	175	GLY	C-N	-21.89	0.83	1.34
1	M	175	GLY	C-N	-21.89	0.83	1.34
1	J	175	GLY	C-N	-21.88	0.83	1.34
1	I	175	GLY	C-N	-21.88	0.83	1.34
1	N	175	GLY	C-N	-21.88	0.83	1.34
1	K	175	GLY	C-N	-21.86	0.83	1.34
2	G	45	VAL	C-N	-20.83	0.95	1.33
2	D	45	VAL	C-N	-20.80	0.95	1.33
2	E	45	VAL	C-N	-20.80	0.95	1.33
2	C	45	VAL	C-N	-20.78	0.95	1.33
2	F	45	VAL	C-N	-20.78	0.95	1.33
2	H	45	VAL	C-N	-20.77	0.95	1.33
2	A	45	VAL	C-N	-20.77	0.95	1.33
2	B	45	VAL	C-N	-20.74	0.95	1.33
2	H	371	HIS	CA-C	-19.43	1.02	1.52
2	F	371	HIS	CA-C	-19.42	1.02	1.52
2	B	371	HIS	CA-C	-19.42	1.02	1.52
2	A	371	HIS	CA-C	-19.40	1.02	1.52
2	C	371	HIS	CA-C	-19.40	1.02	1.52
2	G	371	HIS	CA-C	-19.40	1.02	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	371	HIS	CA-C	-19.40	1.02	1.52
2	D	371	HIS	CA-C	-19.38	1.02	1.52
3	T	3	GLN	CA-CB	-18.09	1.14	1.53
3	P	3	GLN	CA-CB	-18.09	1.14	1.53
3	O	3	GLN	CA-CB	-18.09	1.14	1.53
3	R	3	GLN	CA-CB	-18.07	1.14	1.53
3	Q	3	GLN	CA-CB	-18.06	1.14	1.53
2	E	370	VAL	C-O	-18.06	0.89	1.23
2	F	370	VAL	C-O	-18.05	0.89	1.23
2	A	370	VAL	C-O	-18.05	0.89	1.23
2	B	370	VAL	C-O	-18.03	0.89	1.23
2	D	370	VAL	C-O	-18.02	0.89	1.23
2	C	370	VAL	C-O	-18.02	0.89	1.23
3	S	3	GLN	CA-CB	-18.01	1.14	1.53
2	H	370	VAL	C-O	-18.00	0.89	1.23
2	G	370	VAL	C-O	-18.00	0.89	1.23
1	K	599	ASP	C-O	-17.32	0.90	1.23
1	N	599	ASP	C-O	-17.32	0.90	1.23
1	L	599	ASP	C-O	-17.31	0.90	1.23
1	I	599	ASP	C-O	-17.29	0.90	1.23
1	J	599	ASP	C-O	-17.25	0.90	1.23
1	M	599	ASP	C-O	-17.22	0.90	1.23
2	A	370	VAL	C-N	-17.19	0.94	1.34
2	C	370	VAL	C-N	-17.18	0.94	1.34
2	E	370	VAL	C-N	-17.17	0.94	1.34
2	D	370	VAL	C-N	-17.17	0.94	1.34
2	B	370	VAL	C-N	-17.17	0.94	1.34
2	G	370	VAL	C-N	-17.15	0.94	1.34
2	H	370	VAL	C-N	-17.15	0.94	1.34
2	F	370	VAL	C-N	-17.14	0.94	1.34
3	T	147	ALA	CA-CB	-16.46	1.17	1.52
3	R	147	ALA	CA-CB	-16.44	1.18	1.52
3	P	147	ALA	CA-CB	-16.43	1.18	1.52
3	O	147	ALA	CA-CB	-16.42	1.18	1.52
3	Q	147	ALA	CA-CB	-16.42	1.18	1.52
3	S	147	ALA	CA-CB	-16.41	1.18	1.52
1	N	119	SER	C-O	-16.39	0.92	1.23
1	J	119	SER	C-O	-16.38	0.92	1.23
1	I	119	SER	C-O	-16.37	0.92	1.23
1	M	119	SER	C-O	-16.35	0.92	1.23
1	K	119	SER	C-O	-16.34	0.92	1.23
1	L	119	SER	C-O	-16.30	0.92	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	359	SER	CA-CB	-16.05	1.28	1.52
1	K	359	SER	CA-CB	-16.05	1.28	1.52
1	L	359	SER	CA-CB	-16.03	1.28	1.52
1	J	359	SER	CA-CB	-16.01	1.28	1.52
1	M	359	SER	CA-CB	-16.00	1.28	1.52
1	I	359	SER	CA-CB	-15.99	1.28	1.52
1	L	553	ASP	C-N	-15.55	0.98	1.34
1	K	553	ASP	C-N	-15.53	0.98	1.34
1	I	553	ASP	C-N	-15.52	0.98	1.34
1	N	553	ASP	C-N	-15.52	0.98	1.34
1	M	553	ASP	C-N	-15.51	0.98	1.34
1	J	553	ASP	C-N	-15.51	0.98	1.34
1	L	174	THR	C-N	-15.40	1.05	1.33
1	N	174	THR	C-N	-15.39	1.05	1.33
1	K	174	THR	C-N	-15.36	1.05	1.33
1	I	174	THR	C-N	-15.36	1.05	1.33
1	M	174	THR	C-N	-15.34	1.05	1.33
1	J	174	THR	C-N	-15.33	1.05	1.33
1	K	636	GLY	N-CA	-14.31	1.24	1.46
1	I	636	GLY	N-CA	-14.29	1.24	1.46
1	N	636	GLY	N-CA	-14.27	1.24	1.46
1	J	636	GLY	N-CA	-14.26	1.24	1.46
1	L	636	GLY	N-CA	-14.25	1.24	1.46
1	M	636	GLY	N-CA	-14.23	1.24	1.46
1	M	119	SER	C-N	-14.21	1.01	1.34
1	N	119	SER	C-N	-14.19	1.01	1.34
1	J	119	SER	C-N	-14.18	1.01	1.34
1	K	119	SER	C-N	-14.16	1.01	1.34
1	I	119	SER	C-N	-14.14	1.01	1.34
1	L	119	SER	C-N	-14.13	1.01	1.34
2	H	32	PRO	C-N	-14.00	1.01	1.34
2	C	32	PRO	C-N	-13.99	1.01	1.34
2	E	32	PRO	C-N	-13.99	1.01	1.34
2	G	32	PRO	C-N	-13.99	1.01	1.34
2	A	32	PRO	C-N	-13.98	1.01	1.34
2	D	32	PRO	C-N	-13.98	1.01	1.34
2	B	32	PRO	C-N	-13.97	1.01	1.34
2	F	32	PRO	C-N	-13.97	1.01	1.34
1	J	118	LYS	C-O	-13.39	0.97	1.23
1	L	118	LYS	C-O	-13.38	0.97	1.23
1	N	118	LYS	C-O	-13.37	0.97	1.23
1	K	118	LYS	C-O	-13.35	0.97	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	118	LYS	C-O	-13.33	0.98	1.23
1	I	118	LYS	C-O	-13.31	0.98	1.23
1	J	56	LYS	C-O	-13.11	0.98	1.23
1	K	56	LYS	C-O	-13.10	0.98	1.23
1	N	56	LYS	C-O	-13.09	0.98	1.23
1	L	56	LYS	C-O	-13.08	0.98	1.23
1	M	56	LYS	C-O	-13.08	0.98	1.23
1	I	56	LYS	C-O	-13.04	0.98	1.23
1	L	4	GLY	C-O	-12.78	1.03	1.23
1	K	4	GLY	C-O	-12.75	1.03	1.23
3	R	114	GLU	C-O	-12.75	0.99	1.23
1	N	4	GLY	C-O	-12.71	1.03	1.23
3	T	114	GLU	C-O	-12.71	0.99	1.23
1	I	4	GLY	C-O	-12.70	1.03	1.23
3	Q	114	GLU	C-O	-12.69	0.99	1.23
3	O	114	GLU	C-O	-12.69	0.99	1.23
3	S	114	GLU	C-O	-12.68	0.99	1.23
1	M	4	GLY	C-O	-12.67	1.03	1.23
3	P	114	GLU	C-O	-12.67	0.99	1.23
1	J	4	GLY	C-O	-12.65	1.03	1.23
2	F	109	PRO	C-N	-12.45	1.05	1.34
2	D	109	PRO	C-N	-12.44	1.05	1.34
2	G	109	PRO	C-N	-12.41	1.05	1.34
2	A	109	PRO	C-N	-12.40	1.05	1.34
2	E	109	PRO	C-N	-12.39	1.05	1.34
2	B	109	PRO	C-N	-12.38	1.05	1.34
2	H	109	PRO	C-N	-12.38	1.05	1.34
2	C	109	PRO	C-N	-12.37	1.05	1.34
2	H	370	VAL	CA-CB	-11.91	1.29	1.54
3	O	45	GLU	C-O	-11.90	1.00	1.23
3	S	45	GLU	C-O	-11.90	1.00	1.23
3	T	45	GLU	C-O	-11.90	1.00	1.23
3	P	45	GLU	C-O	-11.89	1.00	1.23
3	R	45	GLU	C-O	-11.89	1.00	1.23
2	D	370	VAL	CA-CB	-11.89	1.29	1.54
2	B	370	VAL	CA-CB	-11.88	1.29	1.54
3	Q	45	GLU	C-O	-11.87	1.00	1.23
2	G	370	VAL	CA-CB	-11.86	1.29	1.54
2	E	370	VAL	CA-CB	-11.85	1.29	1.54
2	A	370	VAL	CA-CB	-11.84	1.29	1.54
2	C	370	VAL	CA-CB	-11.83	1.29	1.54
2	F	370	VAL	CA-CB	-11.83	1.29	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	357	SER	C-N	-11.35	1.07	1.34
1	K	357	SER	C-N	-11.34	1.07	1.34
1	M	357	SER	C-N	-11.32	1.08	1.34
1	I	357	SER	C-N	-11.32	1.08	1.34
1	J	357	SER	C-N	-11.31	1.08	1.34
1	L	357	SER	C-N	-11.30	1.08	1.34
1	N	816	ALA	C-O	-11.03	1.02	1.23
1	J	816	ALA	C-O	-11.02	1.02	1.23
1	K	816	ALA	C-O	-11.01	1.02	1.23
1	L	816	ALA	C-O	-11.01	1.02	1.23
1	M	816	ALA	C-O	-10.98	1.02	1.23
1	I	816	ALA	C-O	-10.94	1.02	1.23
2	C	369	ILE	C-O	-10.89	1.02	1.23
2	D	369	ILE	C-O	-10.89	1.02	1.23
2	G	369	ILE	C-O	-10.88	1.02	1.23
2	B	369	ILE	C-O	-10.87	1.02	1.23
2	A	369	ILE	C-O	-10.86	1.02	1.23
2	E	369	ILE	C-O	-10.86	1.02	1.23
2	F	369	ILE	C-O	-10.84	1.02	1.23
2	H	369	ILE	C-O	-10.83	1.02	1.23
2	G	5	THR	C-O	-10.49	1.03	1.23
2	A	5	THR	C-O	-10.47	1.03	1.23
2	D	5	THR	C-O	-10.47	1.03	1.23
2	C	5	THR	C-O	-10.45	1.03	1.23
2	F	5	THR	C-O	-10.45	1.03	1.23
1	N	772	SER	C-N	-10.44	1.10	1.34
2	H	5	THR	C-O	-10.44	1.03	1.23
2	E	5	THR	C-O	-10.44	1.03	1.23
1	I	772	SER	C-N	-10.43	1.10	1.34
2	B	5	THR	C-O	-10.42	1.03	1.23
1	J	772	SER	C-N	-10.41	1.10	1.34
1	L	772	SER	C-N	-10.40	1.10	1.34
1	M	772	SER	C-N	-10.40	1.10	1.34
1	K	772	SER	C-N	-10.37	1.10	1.34
1	L	239	GLY	C-O	-10.06	1.07	1.23
1	J	175	GLY	N-CA	-10.04	1.30	1.46
1	N	239	GLY	C-O	-10.03	1.07	1.23
1	J	239	GLY	C-O	-10.03	1.07	1.23
1	I	239	GLY	C-O	-10.02	1.07	1.23
1	M	239	GLY	C-O	-10.01	1.07	1.23
1	K	239	GLY	C-O	-10.01	1.07	1.23
1	M	175	GLY	N-CA	-10.00	1.31	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	175	GLY	N-CA	-10.00	1.31	1.46
1	I	175	GLY	N-CA	-9.98	1.31	1.46
1	N	118	LYS	C-N	-9.97	1.11	1.34
1	I	641	ILE	C-O	-9.96	1.04	1.23
1	M	118	LYS	C-N	-9.96	1.11	1.34
1	K	175	GLY	N-CA	-9.96	1.31	1.46
1	N	175	GLY	N-CA	-9.96	1.31	1.46
1	M	641	ILE	C-O	-9.95	1.04	1.23
1	I	118	LYS	C-N	-9.94	1.11	1.34
1	L	118	LYS	C-N	-9.94	1.11	1.34
1	J	641	ILE	C-O	-9.93	1.04	1.23
1	K	118	LYS	C-N	-9.92	1.11	1.34
1	N	641	ILE	C-O	-9.92	1.04	1.23
1	J	118	LYS	C-N	-9.91	1.11	1.34
1	K	641	ILE	C-O	-9.91	1.04	1.23
1	L	641	ILE	C-O	-9.89	1.04	1.23
1	J	817	CYS	CA-C	-9.44	1.28	1.52
1	N	817	CYS	CA-C	-9.41	1.28	1.52
1	M	817	CYS	CA-C	-9.39	1.28	1.52
1	L	817	CYS	CA-C	-9.38	1.28	1.52
1	I	817	CYS	CA-C	-9.37	1.28	1.52
1	K	817	CYS	CA-C	-9.38	1.28	1.52
3	O	114	GLU	C-N	-9.25	1.12	1.34
3	Q	114	GLU	C-N	-9.25	1.12	1.34
3	P	114	GLU	C-N	-9.24	1.12	1.34
1	L	599	ASP	C-N	-9.23	1.12	1.34
3	R	114	GLU	C-N	-9.22	1.12	1.34
3	T	114	GLU	C-N	-9.21	1.12	1.34
3	S	114	GLU	C-N	-9.21	1.12	1.34
1	M	599	ASP	C-N	-9.20	1.12	1.34
1	J	599	ASP	C-N	-9.20	1.12	1.34
1	N	502	GLY	C-O	-9.19	1.08	1.23
1	J	502	GLY	C-O	-9.18	1.08	1.23
1	N	599	ASP	C-N	-9.18	1.12	1.34
1	K	599	ASP	C-N	-9.18	1.12	1.34
1	K	502	GLY	C-O	-9.18	1.08	1.23
1	I	599	ASP	C-N	-9.17	1.12	1.34
1	L	502	GLY	C-O	-9.17	1.08	1.23
1	I	502	GLY	C-O	-9.14	1.09	1.23
1	M	502	GLY	C-O	-9.12	1.09	1.23
2	G	199	SER	C-O	-9.08	1.06	1.23
2	H	199	SER	C-O	-9.08	1.06	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	199	SER	C-O	-9.08	1.06	1.23
2	D	199	SER	C-O	-9.08	1.06	1.23
2	A	199	SER	C-O	-9.06	1.06	1.23
2	B	199	SER	C-O	-9.06	1.06	1.23
2	C	199	SER	C-O	-9.05	1.06	1.23
2	E	199	SER	C-O	-9.04	1.06	1.23
2	H	47	MET	CA-CB	-8.91	1.34	1.53
2	C	47	MET	CA-CB	-8.89	1.34	1.53
2	G	47	MET	CA-CB	-8.89	1.34	1.53
2	B	47	MET	CA-CB	-8.88	1.34	1.53
2	F	47	MET	CA-CB	-8.88	1.34	1.53
2	A	47	MET	CA-CB	-8.87	1.34	1.53
2	E	47	MET	CA-CB	-8.87	1.34	1.53
2	D	47	MET	CA-CB	-8.85	1.34	1.53
3	Q	45	GLU	C-N	-8.71	1.14	1.34
3	P	45	GLU	C-N	-8.71	1.14	1.34
3	T	45	GLU	C-N	-8.70	1.14	1.34
3	S	45	GLU	C-N	-8.69	1.14	1.34
3	O	45	GLU	C-N	-8.67	1.14	1.34
3	R	45	GLU	C-N	-8.67	1.14	1.34
1	L	358	THR	CA-CB	-8.44	1.31	1.53
1	I	358	THR	CA-CB	-8.43	1.31	1.53
1	M	358	THR	CA-CB	-8.43	1.31	1.53
1	K	358	THR	CA-CB	-8.41	1.31	1.53
1	J	358	THR	CA-CB	-8.40	1.31	1.53
1	N	358	THR	CA-CB	-8.40	1.31	1.53
1	M	816	ALA	C-N	-8.39	1.14	1.34
1	I	816	ALA	C-N	-8.38	1.14	1.34
1	M	4	GLY	C-N	-8.38	1.14	1.34
1	J	816	ALA	C-N	-8.38	1.14	1.34
1	J	4	GLY	C-N	-8.36	1.14	1.34
2	G	33	SER	C-O	-8.36	1.07	1.23
2	H	33	SER	C-O	-8.36	1.07	1.23
1	K	816	ALA	C-N	-8.36	1.14	1.34
1	N	816	ALA	C-N	-8.35	1.14	1.34
2	C	33	SER	C-O	-8.35	1.07	1.23
1	L	816	ALA	C-N	-8.35	1.14	1.34
1	N	4	GLY	C-N	-8.34	1.14	1.34
2	A	33	SER	C-O	-8.34	1.07	1.23
2	D	33	SER	C-O	-8.34	1.07	1.23
2	B	33	SER	C-O	-8.34	1.07	1.23
1	L	4	GLY	C-N	-8.32	1.15	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	4	GLY	C-N	-8.32	1.15	1.34
1	I	4	GLY	C-N	-8.32	1.15	1.34
2	E	33	SER	C-O	-8.31	1.07	1.23
2	F	33	SER	C-O	-8.29	1.07	1.23
2	D	179	ASP	C-O	-8.28	1.07	1.23
2	E	179	ASP	C-O	-8.26	1.07	1.23
2	G	179	ASP	C-O	-8.24	1.07	1.23
2	A	179	ASP	C-O	-8.24	1.07	1.23
2	C	179	ASP	C-O	-8.24	1.07	1.23
2	B	179	ASP	C-O	-8.24	1.07	1.23
2	H	179	ASP	C-O	-8.23	1.07	1.23
2	G	45	VAL	CA-CB	-8.22	1.37	1.54
2	F	179	ASP	C-O	-8.21	1.07	1.23
2	A	45	VAL	CA-CB	-8.20	1.37	1.54
1	L	359	SER	N-CA	-8.20	1.29	1.46
2	D	45	VAL	CA-CB	-8.19	1.37	1.54
2	F	45	VAL	CA-CB	-8.19	1.37	1.54
2	C	45	VAL	CA-CB	-8.18	1.37	1.54
1	K	359	SER	N-CA	-8.18	1.29	1.46
1	I	4	GLY	N-CA	-8.17	1.33	1.46
2	H	45	VAL	CA-CB	-8.17	1.37	1.54
1	J	2	GLU	CA-CB	-8.16	1.35	1.53
2	B	45	VAL	CA-CB	-8.16	1.37	1.54
2	E	45	VAL	CA-CB	-8.15	1.37	1.54
1	K	4	GLY	N-CA	-8.14	1.33	1.46
1	I	359	SER	N-CA	-8.14	1.30	1.46
1	M	359	SER	N-CA	-8.14	1.30	1.46
1	N	359	SER	N-CA	-8.14	1.30	1.46
1	K	2	GLU	CA-CB	-8.12	1.36	1.53
1	J	4	GLY	N-CA	-8.12	1.33	1.46
1	M	2	GLU	CA-CB	-8.12	1.36	1.53
1	L	4	GLY	N-CA	-8.11	1.33	1.46
1	K	358	THR	CA-C	-8.11	1.31	1.52
1	N	2	GLU	CA-CB	-8.11	1.36	1.53
1	J	359	SER	N-CA	-8.10	1.30	1.46
1	I	122	THR	C-O	-8.09	1.07	1.23
1	L	2	GLU	CA-CB	-8.09	1.36	1.53
1	M	4	GLY	N-CA	-8.09	1.33	1.46
1	L	122	THR	C-O	-8.09	1.07	1.23
1	I	2	GLU	CA-CB	-8.09	1.36	1.53
1	I	358	THR	CA-C	-8.09	1.31	1.52
1	J	358	THR	CA-C	-8.08	1.31	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	358	THR	CA-C	-8.07	1.31	1.52
1	K	122	THR	C-O	-8.07	1.08	1.23
1	L	358	THR	CA-C	-8.07	1.31	1.52
1	N	4	GLY	N-CA	-8.06	1.33	1.46
1	N	122	THR	C-O	-8.06	1.08	1.23
1	N	358	THR	CA-C	-8.06	1.32	1.52
1	I	509	VAL	CA-CB	-8.05	1.37	1.54
1	J	122	THR	C-O	-8.05	1.08	1.23
1	M	122	THR	C-O	-8.03	1.08	1.23
1	M	509	VAL	CA-CB	-8.03	1.37	1.54
1	K	509	VAL	CA-CB	-8.02	1.38	1.54
1	L	509	VAL	CA-CB	-7.98	1.38	1.54
1	J	509	VAL	CA-CB	-7.95	1.38	1.54
1	N	509	VAL	CA-CB	-7.92	1.38	1.54
3	Q	60	ASN	CA-CB	-7.88	1.32	1.53
3	T	60	ASN	CA-CB	-7.87	1.32	1.53
3	S	60	ASN	CA-CB	-7.86	1.32	1.53
3	O	60	ASN	CA-CB	-7.86	1.32	1.53
3	R	60	ASN	CA-CB	-7.84	1.32	1.53
3	P	60	ASN	CA-CB	-7.84	1.32	1.53
2	F	369	ILE	C-N	-7.84	1.16	1.34
2	D	369	ILE	C-N	-7.83	1.16	1.34
2	H	369	ILE	C-N	-7.82	1.16	1.34
2	E	369	ILE	C-N	-7.82	1.16	1.34
2	C	369	ILE	C-N	-7.81	1.16	1.34
2	A	369	ILE	C-N	-7.80	1.16	1.34
2	G	369	ILE	C-N	-7.80	1.16	1.34
2	B	369	ILE	C-N	-7.79	1.16	1.34
1	M	173	GLY	C-O	-7.76	1.11	1.23
1	J	173	GLY	C-O	-7.76	1.11	1.23
1	I	173	GLY	C-O	-7.76	1.11	1.23
1	N	173	GLY	C-O	-7.71	1.11	1.23
1	I	174	THR	CA-CB	-7.71	1.33	1.53
1	L	173	GLY	C-O	-7.69	1.11	1.23
1	L	174	THR	CA-CB	-7.68	1.33	1.53
1	K	173	GLY	C-O	-7.68	1.11	1.23
1	K	174	THR	CA-CB	-7.68	1.33	1.53
1	J	356	GLY	C-O	-7.68	1.11	1.23
1	M	174	THR	CA-CB	-7.67	1.33	1.53
1	N	174	THR	CA-CB	-7.67	1.33	1.53
3	P	147	ALA	CA-C	-7.66	1.33	1.52
1	J	174	THR	CA-CB	-7.65	1.33	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	356	GLY	C-O	-7.65	1.11	1.23
1	L	356	GLY	C-O	-7.64	1.11	1.23
3	Q	147	ALA	CA-C	-7.64	1.33	1.52
1	M	356	GLY	C-O	-7.63	1.11	1.23
3	O	147	ALA	CA-C	-7.63	1.33	1.52
3	S	147	ALA	CA-C	-7.63	1.33	1.52
1	K	356	GLY	C-O	-7.62	1.11	1.23
3	R	147	ALA	CA-C	-7.62	1.33	1.52
3	T	147	ALA	CA-C	-7.61	1.33	1.52
1	I	356	GLY	C-O	-7.59	1.11	1.23
1	I	39	LYS	C-O	-7.53	1.09	1.23
1	M	39	LYS	C-O	-7.52	1.09	1.23
1	L	39	LYS	C-O	-7.51	1.09	1.23
1	K	39	LYS	C-O	-7.49	1.09	1.23
1	K	641	ILE	C-N	-7.49	1.16	1.34
1	L	641	ILE	C-N	-7.48	1.16	1.34
1	N	641	ILE	C-N	-7.48	1.16	1.34
1	N	39	LYS	C-O	-7.48	1.09	1.23
1	M	641	ILE	C-N	-7.47	1.16	1.34
1	J	641	ILE	C-N	-7.46	1.16	1.34
1	J	39	LYS	C-O	-7.46	1.09	1.23
1	I	641	ILE	C-N	-7.45	1.17	1.34
1	L	3	ASP	N-CA	-7.33	1.31	1.46
1	L	357	SER	CA-CB	-7.28	1.42	1.52
1	M	3	ASP	N-CA	-7.27	1.31	1.46
1	I	601	LEU	C-O	-7.27	1.09	1.23
1	I	3	ASP	N-CA	-7.26	1.31	1.46
1	K	357	SER	CA-CB	-7.26	1.42	1.52
1	N	3	ASP	N-CA	-7.26	1.31	1.46
1	K	3	ASP	N-CA	-7.25	1.31	1.46
1	M	601	LEU	C-O	-7.24	1.09	1.23
1	K	601	LEU	C-O	-7.24	1.09	1.23
1	J	3	ASP	N-CA	-7.21	1.31	1.46
1	M	357	SER	CA-CB	-7.21	1.42	1.52
1	J	601	LEU	C-O	-7.20	1.09	1.23
1	N	601	LEU	C-O	-7.20	1.09	1.23
1	L	601	LEU	C-O	-7.19	1.09	1.23
1	I	357	SER	CA-CB	-7.18	1.42	1.52
1	N	357	SER	CA-CB	-7.18	1.42	1.52
1	J	357	SER	CA-CB	-7.17	1.42	1.52
1	J	509	VAL	C-O	-7.11	1.09	1.23
1	M	509	VAL	C-O	-7.10	1.09	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	509	VAL	C-O	-7.10	1.09	1.23
1	N	509	VAL	C-O	-7.07	1.09	1.23
1	L	509	VAL	C-O	-7.06	1.09	1.23
1	I	509	VAL	C-O	-7.05	1.09	1.23
1	N	642	SER	C-O	-7.04	1.09	1.23
1	L	642	SER	C-O	-7.03	1.10	1.23
1	I	642	SER	C-O	-7.02	1.10	1.23
1	M	642	SER	C-O	-7.02	1.10	1.23
1	J	642	SER	C-O	-7.02	1.10	1.23
1	K	642	SER	C-O	-7.00	1.10	1.23
2	H	371	HIS	N-CA	-6.88	1.32	1.46
2	F	371	HIS	N-CA	-6.86	1.32	1.46
2	E	371	HIS	N-CA	-6.86	1.32	1.46
2	D	371	HIS	N-CA	-6.85	1.32	1.46
2	G	371	HIS	N-CA	-6.85	1.32	1.46
1	I	2	GLU	N-CA	-6.85	1.32	1.46
1	N	2	GLU	N-CA	-6.84	1.32	1.46
1	M	2	GLU	N-CA	-6.84	1.32	1.46
1	I	174	THR	CA-C	-6.84	1.35	1.52
2	B	371	HIS	N-CA	-6.83	1.32	1.46
1	J	174	THR	CA-C	-6.83	1.35	1.52
1	L	2	GLU	N-CA	-6.82	1.32	1.46
1	L	553	ASP	CA-CB	-6.82	1.39	1.53
1	K	2	GLU	N-CA	-6.81	1.32	1.46
1	M	553	ASP	CA-CB	-6.81	1.39	1.53
2	A	371	HIS	N-CA	-6.81	1.32	1.46
1	K	174	THR	CA-C	-6.80	1.35	1.52
1	J	2	GLU	N-CA	-6.80	1.32	1.46
1	I	553	ASP	CA-CB	-6.79	1.39	1.53
1	M	174	THR	CA-C	-6.79	1.35	1.52
1	K	553	ASP	CA-CB	-6.78	1.39	1.53
1	N	174	THR	CA-C	-6.78	1.35	1.52
2	C	371	HIS	N-CA	-6.78	1.32	1.46
1	J	553	ASP	CA-CB	-6.77	1.39	1.53
1	L	174	THR	CA-C	-6.77	1.35	1.52
1	N	553	ASP	CA-CB	-6.76	1.39	1.53
1	M	240	LYS	C-O	-6.72	1.10	1.23
1	I	240	LYS	C-O	-6.71	1.10	1.23
1	K	240	LYS	C-O	-6.67	1.10	1.23
1	N	240	LYS	C-O	-6.67	1.10	1.23
1	J	240	LYS	C-O	-6.67	1.10	1.23
1	L	240	LYS	C-O	-6.65	1.10	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	598	ASN	C-O	-6.65	1.10	1.23
1	L	598	ASN	C-O	-6.64	1.10	1.23
1	I	598	ASN	C-O	-6.63	1.10	1.23
3	O	59	GLY	CA-C	-6.60	1.41	1.51
3	R	59	GLY	CA-C	-6.60	1.41	1.51
3	Q	59	GLY	CA-C	-6.59	1.41	1.51
1	K	598	ASN	C-O	-6.59	1.10	1.23
3	S	59	GLY	CA-C	-6.59	1.41	1.51
1	M	598	ASN	C-O	-6.59	1.10	1.23
1	N	598	ASN	C-O	-6.58	1.10	1.23
2	B	166	TYR	C-O	-6.55	1.10	1.23
3	T	59	GLY	CA-C	-6.54	1.41	1.51
2	A	166	TYR	C-O	-6.53	1.10	1.23
2	H	166	TYR	C-O	-6.52	1.10	1.23
2	D	166	TYR	C-O	-6.52	1.10	1.23
2	E	166	TYR	C-O	-6.50	1.10	1.23
3	P	59	GLY	CA-C	-6.50	1.41	1.51
2	F	166	TYR	C-O	-6.50	1.11	1.23
2	C	166	TYR	C-O	-6.49	1.11	1.23
2	G	166	TYR	C-O	-6.49	1.11	1.23
2	E	47	MET	N-CA	-6.39	1.33	1.46
2	C	47	MET	N-CA	-6.38	1.33	1.46
2	D	47	MET	N-CA	-6.38	1.33	1.46
2	A	47	MET	N-CA	-6.37	1.33	1.46
1	L	56	LYS	C-N	-6.37	1.19	1.34
2	G	47	MET	N-CA	-6.37	1.33	1.46
2	B	47	MET	N-CA	-6.36	1.33	1.46
2	H	47	MET	N-CA	-6.35	1.33	1.46
1	K	56	LYS	C-N	-6.34	1.19	1.34
2	F	47	MET	N-CA	-6.34	1.33	1.46
1	N	56	LYS	C-N	-6.34	1.19	1.34
1	I	56	LYS	C-N	-6.33	1.19	1.34
1	J	56	LYS	C-N	-6.30	1.19	1.34
1	M	56	LYS	C-N	-6.29	1.19	1.34
3	S	3	GLN	C-O	-6.25	1.11	1.23
3	R	3	GLN	C-O	-6.25	1.11	1.23
1	K	241	GLU	N-CA	-6.25	1.33	1.46
1	L	241	GLU	N-CA	-6.25	1.33	1.46
3	P	3	GLN	C-O	-6.24	1.11	1.23
1	I	241	GLU	N-CA	-6.24	1.33	1.46
1	M	241	GLU	N-CA	-6.24	1.33	1.46
1	N	241	GLU	N-CA	-6.24	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	3	GLN	C-O	-6.23	1.11	1.23
2	F	179	ASP	C-N	-6.22	1.19	1.34
2	B	179	ASP	C-N	-6.22	1.19	1.34
2	A	199	SER	C-N	-6.22	1.19	1.34
2	C	179	ASP	C-N	-6.21	1.19	1.34
2	A	179	ASP	C-N	-6.21	1.19	1.34
2	D	179	ASP	C-N	-6.21	1.19	1.34
1	J	241	GLU	N-CA	-6.20	1.33	1.46
2	E	179	ASP	C-N	-6.20	1.19	1.34
2	G	179	ASP	C-N	-6.20	1.19	1.34
3	Q	3	GLN	C-O	-6.20	1.11	1.23
2	D	199	SER	C-N	-6.20	1.19	1.34
2	G	199	SER	C-N	-6.20	1.19	1.34
2	B	199	SER	C-N	-6.19	1.19	1.34
2	H	179	ASP	C-N	-6.18	1.19	1.34
2	H	199	SER	C-N	-6.18	1.19	1.34
3	O	3	GLN	C-O	-6.18	1.11	1.23
2	C	199	SER	C-N	-6.16	1.19	1.34
2	E	199	SER	C-N	-6.16	1.19	1.34
2	F	199	SER	C-N	-6.15	1.19	1.34
2	H	200	PHE	C-O	-6.15	1.11	1.23
2	A	200	PHE	C-O	-6.14	1.11	1.23
2	D	200	PHE	C-O	-6.12	1.11	1.23
2	H	46	GLY	C-O	-6.12	1.13	1.23
2	F	200	PHE	C-O	-6.11	1.11	1.23
2	G	200	PHE	C-O	-6.10	1.11	1.23
2	F	46	GLY	C-O	-6.10	1.13	1.23
2	C	46	GLY	C-O	-6.10	1.13	1.23
2	E	46	GLY	C-O	-6.09	1.14	1.23
2	C	200	PHE	C-O	-6.08	1.11	1.23
2	E	200	PHE	C-O	-6.08	1.11	1.23
1	M	2	GLU	CA-C	-6.08	1.37	1.52
2	D	46	GLY	C-O	-6.08	1.14	1.23
1	I	2	GLU	CA-C	-6.07	1.37	1.52
1	K	2	GLU	CA-C	-6.07	1.37	1.52
1	L	2	GLU	CA-C	-6.07	1.37	1.52
2	A	46	GLY	C-O	-6.06	1.14	1.23
2	B	200	PHE	C-O	-6.06	1.11	1.23
1	N	2	GLU	CA-C	-6.05	1.37	1.52
2	G	46	GLY	C-O	-6.04	1.14	1.23
2	B	46	GLY	C-O	-6.03	1.14	1.23
1	J	2	GLU	CA-C	-6.00	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	168	GLY	C-O	-5.87	1.14	1.23
2	C	168	GLY	C-O	-5.86	1.14	1.23
1	M	4	GLY	CA-C	-5.85	1.42	1.51
2	A	168	GLY	C-O	-5.85	1.14	1.23
1	I	4	GLY	CA-C	-5.85	1.42	1.51
2	E	168	GLY	C-O	-5.84	1.14	1.23
2	F	168	GLY	C-O	-5.84	1.14	1.23
1	N	4	GLY	CA-C	-5.84	1.42	1.51
2	B	168	GLY	C-O	-5.84	1.14	1.23
2	D	168	GLY	C-O	-5.83	1.14	1.23
1	K	4	GLY	CA-C	-5.83	1.42	1.51
2	H	168	GLY	C-O	-5.83	1.14	1.23
1	L	4	GLY	CA-C	-5.83	1.42	1.51
1	J	4	GLY	CA-C	-5.83	1.42	1.51
1	J	639	SER	C-O	-5.77	1.12	1.23
1	N	265	LEU	C-O	-5.77	1.12	1.23
1	I	265	LEU	C-O	-5.77	1.12	1.23
1	K	265	LEU	C-O	-5.76	1.12	1.23
1	L	265	LEU	C-O	-5.76	1.12	1.23
1	M	265	LEU	C-O	-5.74	1.12	1.23
1	J	265	LEU	C-O	-5.74	1.12	1.23
1	K	639	SER	C-O	-5.73	1.12	1.23
1	I	639	SER	C-O	-5.72	1.12	1.23
1	N	817	CYS	CA-CB	-5.72	1.41	1.53
1	L	639	SER	C-O	-5.71	1.12	1.23
1	I	817	CYS	CA-CB	-5.70	1.41	1.53
1	N	639	SER	C-O	-5.69	1.12	1.23
1	M	639	SER	C-O	-5.69	1.12	1.23
1	L	817	CYS	CA-CB	-5.68	1.41	1.53
1	K	817	CYS	CA-CB	-5.67	1.41	1.53
1	M	817	CYS	CA-CB	-5.67	1.41	1.53
1	J	817	CYS	CA-CB	-5.67	1.41	1.53
1	L	503	VAL	CA-CB	-5.64	1.43	1.54
1	N	503	VAL	CA-CB	-5.60	1.43	1.54
1	K	398	THR	CA-CB	-5.59	1.38	1.53
1	K	503	VAL	CA-CB	-5.58	1.43	1.54
1	J	503	VAL	CA-CB	-5.58	1.43	1.54
1	M	503	VAL	CA-CB	-5.57	1.43	1.54
1	L	398	THR	CA-CB	-5.57	1.38	1.53
3	P	60	ASN	N-CA	-5.57	1.35	1.46
3	R	60	ASN	N-CA	-5.57	1.35	1.46
3	T	60	ASN	N-CA	-5.56	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	398	THR	CA-CB	-5.55	1.39	1.53
1	N	398	THR	CA-CB	-5.55	1.39	1.53
3	Q	60	ASN	N-CA	-5.55	1.35	1.46
2	A	46	GLY	CA-C	-5.54	1.43	1.51
1	I	503	VAL	CA-CB	-5.54	1.43	1.54
3	S	60	ASN	N-CA	-5.54	1.35	1.46
1	J	398	THR	CA-CB	-5.53	1.39	1.53
1	I	398	THR	CA-CB	-5.53	1.39	1.53
2	C	46	GLY	CA-C	-5.52	1.43	1.51
2	D	46	GLY	CA-C	-5.51	1.43	1.51
2	E	46	GLY	CA-C	-5.50	1.43	1.51
2	F	46	GLY	CA-C	-5.50	1.43	1.51
3	O	60	ASN	N-CA	-5.49	1.35	1.46
2	B	46	GLY	CA-C	-5.49	1.43	1.51
2	H	46	GLY	CA-C	-5.47	1.43	1.51
2	G	46	GLY	CA-C	-5.47	1.43	1.51
1	N	601	LEU	C-N	-5.46	1.21	1.34
1	J	601	LEU	C-N	-5.46	1.21	1.34
1	K	601	LEU	C-N	-5.46	1.21	1.34
1	L	601	LEU	C-N	-5.45	1.21	1.34
1	M	601	LEU	C-N	-5.44	1.21	1.34
1	I	601	LEU	C-N	-5.44	1.21	1.34
3	Q	61	GLY	N-CA	-5.35	1.38	1.46
3	R	40	GLY	C-O	-5.34	1.15	1.23
3	T	61	GLY	N-CA	-5.34	1.38	1.46
3	P	61	GLY	N-CA	-5.33	1.38	1.46
3	O	40	GLY	C-O	-5.33	1.15	1.23
3	S	61	GLY	N-CA	-5.33	1.38	1.46
3	R	61	GLY	N-CA	-5.31	1.38	1.46
1	N	102	ASP	C-O	-5.29	1.13	1.23
2	C	370	VAL	CA-C	-5.29	1.39	1.52
1	M	102	ASP	C-O	-5.28	1.13	1.23
3	O	61	GLY	N-CA	-5.28	1.38	1.46
3	T	40	GLY	C-O	-5.27	1.15	1.23
2	F	370	VAL	CA-C	-5.27	1.39	1.52
3	S	40	GLY	C-O	-5.26	1.15	1.23
2	G	370	VAL	CA-C	-5.26	1.39	1.52
2	H	370	VAL	CA-C	-5.26	1.39	1.52
3	P	40	GLY	C-O	-5.26	1.15	1.23
3	Q	40	GLY	C-O	-5.26	1.15	1.23
1	K	641	ILE	CA-CB	-5.26	1.42	1.54
1	L	240	LYS	CA-C	-5.26	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	240	LYS	CA-C	-5.26	1.39	1.52
1	K	5	LYS	CA-CB	-5.25	1.42	1.53
1	L	641	ILE	CA-CB	-5.25	1.42	1.54
1	I	102	ASP	C-O	-5.25	1.13	1.23
1	K	102	ASP	C-O	-5.25	1.13	1.23
2	A	370	VAL	CA-C	-5.24	1.39	1.52
1	J	240	LYS	CA-C	-5.24	1.39	1.52
2	D	370	VAL	CA-C	-5.24	1.39	1.52
1	L	102	ASP	C-O	-5.24	1.13	1.23
2	B	370	VAL	CA-C	-5.24	1.39	1.52
1	I	240	LYS	CA-C	-5.24	1.39	1.52
1	M	240	LYS	CA-C	-5.24	1.39	1.52
2	E	370	VAL	CA-C	-5.24	1.39	1.52
1	N	240	LYS	CA-C	-5.22	1.39	1.52
1	N	398	THR	CA-C	-5.22	1.39	1.52
1	J	641	ILE	CA-CB	-5.21	1.42	1.54
1	N	5	LYS	CA-CB	-5.21	1.42	1.53
1	M	398	THR	CA-C	-5.21	1.39	1.52
1	L	398	THR	CA-C	-5.21	1.39	1.52
1	J	5	LYS	CA-CB	-5.21	1.42	1.53
1	L	5	LYS	CA-CB	-5.21	1.42	1.53
1	M	5	LYS	CA-CB	-5.21	1.42	1.53
1	M	641	ILE	CA-CB	-5.21	1.42	1.54
1	N	641	ILE	CA-CB	-5.21	1.42	1.54
1	J	102	ASP	C-O	-5.20	1.13	1.23
1	I	398	THR	CA-C	-5.20	1.39	1.52
1	J	398	THR	CA-C	-5.20	1.39	1.52
1	I	5	LYS	CA-CB	-5.19	1.42	1.53
1	K	398	THR	CA-C	-5.18	1.39	1.52
1	I	641	ILE	CA-CB	-5.17	1.43	1.54
1	K	3	ASP	CA-C	-5.15	1.39	1.52
1	J	3	ASP	CA-C	-5.15	1.39	1.52
1	L	3	ASP	CA-C	-5.14	1.39	1.52
1	M	3	ASP	CA-C	-5.14	1.39	1.52
1	N	3	ASP	CA-C	-5.14	1.39	1.52
1	M	642	SER	C-N	-5.11	1.22	1.34
1	I	600	ALA	C-O	-5.10	1.13	1.23
1	K	642	SER	C-N	-5.10	1.22	1.34
1	J	642	SER	C-N	-5.09	1.22	1.34
1	L	642	SER	C-N	-5.09	1.22	1.34
1	I	642	SER	C-N	-5.08	1.22	1.34
1	I	3	ASP	CA-C	-5.08	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	600	ALA	C-O	-5.07	1.13	1.23
1	N	600	ALA	C-O	-5.07	1.13	1.23
1	M	600	ALA	C-O	-5.07	1.13	1.23
1	N	642	SER	C-N	-5.06	1.22	1.34
1	I	3	ASP	CA-CB	-5.05	1.42	1.53
1	J	3	ASP	CA-CB	-5.05	1.42	1.53
1	N	3	ASP	CA-CB	-5.05	1.42	1.53
1	K	600	ALA	C-O	-5.04	1.13	1.23
1	L	3	ASP	CA-CB	-5.04	1.42	1.53
1	M	3	ASP	CA-CB	-5.04	1.42	1.53
1	L	600	ALA	C-O	-5.01	1.13	1.23
1	K	3	ASP	CA-CB	-5.01	1.43	1.53

All (494) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	175	GLY	O-C-N	-48.44	45.20	122.70
1	L	175	GLY	O-C-N	-48.40	45.26	122.70
1	J	175	GLY	O-C-N	-48.39	45.27	122.70
1	N	175	GLY	O-C-N	-48.39	45.27	122.70
1	I	175	GLY	O-C-N	-48.38	45.29	122.70
1	M	175	GLY	O-C-N	-48.36	45.33	122.70
1	K	358	THR	O-C-N	-45.95	49.17	122.70
1	J	358	THR	O-C-N	-45.94	49.19	122.70
1	N	358	THR	O-C-N	-45.94	49.20	122.70
1	L	358	THR	O-C-N	-45.89	49.28	122.70
1	I	358	THR	O-C-N	-45.89	49.28	122.70
1	M	358	THR	O-C-N	-45.87	49.31	122.70
2	B	44	MET	O-C-N	-43.90	52.46	122.70
2	F	44	MET	O-C-N	-43.90	52.46	122.70
2	C	44	MET	O-C-N	-43.89	52.48	122.70
2	D	44	MET	O-C-N	-43.89	52.48	122.70
2	A	44	MET	O-C-N	-43.88	52.49	122.70
2	H	44	MET	O-C-N	-43.87	52.50	122.70
2	G	44	MET	O-C-N	-43.87	52.52	122.70
2	E	44	MET	O-C-N	-43.85	52.54	122.70
2	F	307	PRO	O-C-N	-40.41	54.51	123.20
2	A	307	PRO	O-C-N	-40.38	54.55	123.20
2	G	307	PRO	O-C-N	-40.36	54.58	123.20
2	E	307	PRO	O-C-N	-40.36	54.59	123.20
2	H	307	PRO	O-C-N	-40.36	54.59	123.20
2	B	307	PRO	O-C-N	-40.32	54.66	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	307	PRO	O-C-N	-40.32	54.66	123.20
2	C	307	PRO	O-C-N	-40.30	54.69	123.20
1	M	553	ASP	O-C-N	-24.18	84.01	122.70
1	J	553	ASP	O-C-N	-24.17	84.03	122.70
1	L	553	ASP	O-C-N	-24.16	84.04	122.70
1	K	553	ASP	O-C-N	-24.16	84.05	122.70
1	N	553	ASP	O-C-N	-24.16	84.05	122.70
1	I	553	ASP	O-C-N	-24.13	84.09	122.70
2	A	45	VAL	O-C-N	-23.97	82.44	123.20
2	B	45	VAL	O-C-N	-23.96	82.46	123.20
2	D	45	VAL	O-C-N	-23.96	82.46	123.20
2	E	45	VAL	O-C-N	-23.95	82.48	123.20
2	C	45	VAL	O-C-N	-23.93	82.52	123.20
2	G	45	VAL	O-C-N	-23.93	82.52	123.20
2	H	45	VAL	O-C-N	-23.93	82.52	123.20
2	F	45	VAL	O-C-N	-23.91	82.55	123.20
2	C	307	PRO	CA-C-N	23.02	162.24	116.20
2	E	307	PRO	CA-C-N	23.02	162.24	116.20
2	F	307	PRO	CA-C-N	23.01	162.23	116.20
2	B	307	PRO	CA-C-N	23.01	162.22	116.20
2	A	307	PRO	CA-C-N	23.00	162.21	116.20
2	D	307	PRO	CA-C-N	23.00	162.20	116.20
2	H	307	PRO	CA-C-N	23.00	162.20	116.20
2	G	307	PRO	CA-C-N	22.99	162.18	116.20
2	C	32	PRO	O-C-N	-21.11	88.93	122.70
2	H	32	PRO	O-C-N	-21.10	88.94	122.70
2	G	32	PRO	O-C-N	-21.10	88.94	122.70
2	F	32	PRO	O-C-N	-21.08	88.97	122.70
2	D	32	PRO	O-C-N	-21.07	88.98	122.70
2	A	32	PRO	O-C-N	-21.07	88.99	122.70
2	B	32	PRO	O-C-N	-21.06	89.00	122.70
2	E	32	PRO	O-C-N	-21.03	89.05	122.70
2	B	5	THR	N-CA-CB	-20.83	70.72	110.30
2	H	5	THR	N-CA-CB	-20.83	70.72	110.30
2	G	5	THR	N-CA-CB	-20.83	70.73	110.30
2	F	5	THR	N-CA-CB	-20.82	70.75	110.30
2	D	5	THR	N-CA-CB	-20.82	70.75	110.30
2	E	5	THR	N-CA-CB	-20.80	70.79	110.30
2	C	5	THR	N-CA-CB	-20.77	70.83	110.30
2	A	5	THR	N-CA-CB	-20.76	70.86	110.30
1	I	175	GLY	CA-C-N	20.17	161.58	117.20
1	N	175	GLY	CA-C-N	20.15	161.52	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	175	GLY	CA-C-N	20.14	161.52	117.20
1	J	175	GLY	CA-C-N	20.14	161.51	117.20
1	K	175	GLY	CA-C-N	20.12	161.47	117.20
1	L	175	GLY	CA-C-N	20.10	161.43	117.20
1	M	358	THR	CA-C-N	20.05	161.32	117.20
1	K	358	THR	CA-C-N	20.05	161.31	117.20
1	I	358	THR	CA-C-N	20.05	161.31	117.20
1	N	358	THR	CA-C-N	20.05	161.30	117.20
1	J	358	THR	CA-C-N	20.04	161.28	117.20
1	L	358	THR	CA-C-N	20.02	161.24	117.20
2	G	109	PRO	O-C-N	-19.28	91.85	122.70
2	H	109	PRO	O-C-N	-19.27	91.87	122.70
2	F	109	PRO	O-C-N	-19.22	91.95	122.70
2	B	109	PRO	O-C-N	-19.22	91.95	122.70
2	A	109	PRO	O-C-N	-19.21	91.96	122.70
2	D	109	PRO	O-C-N	-19.18	92.01	122.70
2	E	109	PRO	O-C-N	-19.17	92.03	122.70
2	C	109	PRO	O-C-N	-19.17	92.03	122.70
2	F	307	PRO	C-N-CA	18.66	161.48	122.30
2	E	307	PRO	C-N-CA	18.64	161.45	122.30
2	B	307	PRO	C-N-CA	18.64	161.44	122.30
2	G	307	PRO	C-N-CA	18.63	161.43	122.30
2	D	307	PRO	C-N-CA	18.62	161.41	122.30
2	A	307	PRO	C-N-CA	18.62	161.41	122.30
2	C	307	PRO	C-N-CA	18.62	161.40	122.30
2	H	307	PRO	C-N-CA	18.60	161.36	122.30
2	C	44	MET	CA-C-N	18.39	157.66	117.20
2	A	44	MET	CA-C-N	18.37	157.61	117.20
2	D	44	MET	CA-C-N	18.36	157.59	117.20
2	B	44	MET	CA-C-N	18.36	157.58	117.20
2	H	44	MET	CA-C-N	18.35	157.57	117.20
2	E	44	MET	CA-C-N	18.35	157.57	117.20
2	F	44	MET	CA-C-N	18.34	157.56	117.20
2	G	44	MET	CA-C-N	18.34	157.55	117.20
1	K	175	GLY	CA-C-O	18.18	153.32	120.60
1	L	175	GLY	CA-C-O	18.17	153.30	120.60
1	J	175	GLY	CA-C-O	18.11	153.21	120.60
1	N	175	GLY	CA-C-O	18.11	153.19	120.60
1	M	175	GLY	CA-C-O	18.08	153.14	120.60
1	I	175	GLY	CA-C-O	18.07	153.13	120.60
1	M	175	GLY	C-N-CA	17.83	166.27	121.70
1	N	175	GLY	C-N-CA	17.83	166.26	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	175	GLY	C-N-CA	17.82	166.25	121.70
1	K	175	GLY	C-N-CA	17.80	166.21	121.70
1	J	175	GLY	C-N-CA	17.80	166.19	121.70
1	L	175	GLY	C-N-CA	17.77	166.13	121.70
1	M	358	THR	C-N-CA	17.55	165.57	121.70
1	N	358	THR	C-N-CA	17.55	165.57	121.70
1	I	358	THR	C-N-CA	17.55	165.56	121.70
1	J	358	THR	C-N-CA	17.55	165.56	121.70
1	K	358	THR	C-N-CA	17.55	165.56	121.70
1	L	358	THR	C-N-CA	17.51	165.48	121.70
1	K	174	THR	O-C-N	-16.09	95.85	123.20
1	I	174	THR	O-C-N	-16.07	95.88	123.20
1	M	174	THR	O-C-N	-16.07	95.89	123.20
1	L	174	THR	O-C-N	-16.06	95.90	123.20
1	J	174	THR	O-C-N	-16.04	95.93	123.20
1	N	174	THR	O-C-N	-15.97	96.04	123.20
1	J	772	SER	O-C-N	-15.57	97.79	122.70
2	A	44	MET	C-N-CA	15.57	160.62	121.70
2	C	44	MET	C-N-CA	15.57	160.62	121.70
2	B	44	MET	C-N-CA	15.56	160.61	121.70
2	E	44	MET	C-N-CA	15.56	160.60	121.70
1	K	772	SER	O-C-N	-15.55	97.82	122.70
2	H	44	MET	C-N-CA	15.55	160.57	121.70
2	D	44	MET	C-N-CA	15.54	160.56	121.70
1	L	772	SER	O-C-N	-15.54	97.84	122.70
2	F	44	MET	C-N-CA	15.54	160.54	121.70
2	G	44	MET	C-N-CA	15.53	160.51	121.70
1	I	772	SER	O-C-N	-15.51	97.89	122.70
1	M	772	SER	O-C-N	-15.51	97.89	122.70
1	N	772	SER	O-C-N	-15.49	97.92	122.70
1	J	174	THR	CA-C-N	14.74	145.67	116.20
1	K	174	THR	CA-C-N	14.72	145.63	116.20
1	M	174	THR	CA-C-N	14.71	145.62	116.20
1	I	174	THR	CA-C-N	14.70	145.59	116.20
1	L	174	THR	CA-C-N	14.69	145.57	116.20
1	N	174	THR	CA-C-N	14.68	145.55	116.20
1	K	119	SER	O-C-N	-14.20	99.99	122.70
2	F	44	MET	CA-C-O	14.18	149.88	120.10
2	B	44	MET	CA-C-O	14.18	149.87	120.10
1	L	119	SER	O-C-N	-14.17	100.03	122.70
2	G	44	MET	CA-C-O	14.17	149.86	120.10
2	D	44	MET	CA-C-O	14.16	149.85	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	44	MET	CA-C-O	14.16	149.84	120.10
2	A	44	MET	CA-C-O	14.15	149.82	120.10
2	E	44	MET	CA-C-O	14.15	149.81	120.10
2	C	44	MET	CA-C-O	14.13	149.77	120.10
1	I	119	SER	O-C-N	-14.11	100.13	122.70
1	M	119	SER	O-C-N	-14.07	100.19	122.70
1	J	119	SER	O-C-N	-14.06	100.20	122.70
1	N	119	SER	O-C-N	-14.06	100.21	122.70
1	J	358	THR	CA-C-O	13.99	149.47	120.10
1	K	358	THR	CA-C-O	13.98	149.46	120.10
1	N	358	THR	CA-C-O	13.97	149.44	120.10
1	L	358	THR	CA-C-O	13.97	149.43	120.10
1	I	358	THR	CA-C-O	13.93	149.36	120.10
1	M	358	THR	CA-C-O	13.91	149.32	120.10
1	K	357	SER	O-C-N	-13.84	100.55	122.70
1	J	357	SER	O-C-N	-13.84	100.56	122.70
1	M	357	SER	O-C-N	-13.83	100.57	122.70
1	L	357	SER	O-C-N	-13.82	100.58	122.70
1	N	357	SER	O-C-N	-13.82	100.59	122.70
1	I	357	SER	O-C-N	-13.76	100.68	122.70
1	J	553	ASP	CA-C-N	13.41	146.70	117.20
1	M	553	ASP	CA-C-N	13.39	146.66	117.20
1	N	553	ASP	CA-C-N	13.38	146.64	117.20
1	L	553	ASP	CA-C-N	13.37	146.62	117.20
1	K	553	ASP	CA-C-N	13.36	146.59	117.20
1	I	553	ASP	CA-C-N	13.34	146.55	117.20
2	F	370	VAL	O-C-N	-13.02	101.86	122.70
2	G	370	VAL	O-C-N	-13.02	101.87	122.70
2	C	370	VAL	O-C-N	-12.99	101.92	122.70
2	D	370	VAL	O-C-N	-12.99	101.92	122.70
2	B	370	VAL	O-C-N	-12.98	101.92	122.70
2	H	370	VAL	O-C-N	-12.98	101.93	122.70
2	E	370	VAL	O-C-N	-12.97	101.95	122.70
2	A	370	VAL	O-C-N	-12.95	101.98	122.70
2	B	5	THR	N-CA-C	12.82	145.63	111.00
2	F	5	THR	N-CA-C	12.81	145.57	111.00
2	G	5	THR	N-CA-C	12.80	145.56	111.00
2	E	5	THR	N-CA-C	12.80	145.55	111.00
2	D	5	THR	N-CA-C	12.78	145.50	111.00
2	H	5	THR	N-CA-C	12.78	145.50	111.00
2	A	5	THR	N-CA-C	12.76	145.45	111.00
2	C	5	THR	N-CA-C	12.76	145.44	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	174	THR	C-N-CA	12.71	148.99	122.30
1	K	174	THR	C-N-CA	12.71	148.99	122.30
1	L	174	THR	C-N-CA	12.70	148.97	122.30
1	M	174	THR	C-N-CA	12.69	148.94	122.30
1	I	174	THR	C-N-CA	12.67	148.91	122.30
1	N	174	THR	C-N-CA	12.66	148.88	122.30
2	G	45	VAL	CA-C-N	12.62	141.44	116.20
2	A	45	VAL	CA-C-N	12.61	141.42	116.20
2	B	45	VAL	CA-C-N	12.61	141.42	116.20
2	E	45	VAL	CA-C-N	12.61	141.42	116.20
2	D	45	VAL	CA-C-N	12.60	141.39	116.20
2	H	45	VAL	CA-C-N	12.60	141.39	116.20
2	F	45	VAL	CA-C-N	12.58	141.35	116.20
2	C	45	VAL	CA-C-N	12.57	141.35	116.20
1	M	553	ASP	C-N-CA	12.38	152.66	121.70
1	K	553	ASP	C-N-CA	12.38	152.65	121.70
1	N	553	ASP	C-N-CA	12.38	152.65	121.70
1	J	553	ASP	C-N-CA	12.38	152.64	121.70
1	L	553	ASP	C-N-CA	12.37	152.63	121.70
1	I	553	ASP	C-N-CA	12.34	152.55	121.70
2	G	109	PRO	CA-C-N	12.33	144.32	117.20
2	H	109	PRO	CA-C-N	12.33	144.32	117.20
2	F	109	PRO	CA-C-N	12.32	144.31	117.20
2	A	109	PRO	CA-C-N	12.32	144.30	117.20
2	B	109	PRO	CA-C-N	12.32	144.30	117.20
2	E	109	PRO	CA-C-N	12.30	144.26	117.20
2	D	109	PRO	CA-C-N	12.30	144.26	117.20
2	C	109	PRO	CA-C-N	12.27	144.20	117.20
2	G	32	PRO	CA-C-N	12.06	143.73	117.20
2	C	32	PRO	CA-C-N	12.06	143.73	117.20
2	H	32	PRO	CA-C-N	12.06	143.73	117.20
2	B	32	PRO	CA-C-N	12.05	143.72	117.20
2	F	32	PRO	CA-C-N	12.05	143.70	117.20
2	A	32	PRO	CA-C-N	12.04	143.69	117.20
2	D	32	PRO	CA-C-N	12.04	143.69	117.20
2	E	32	PRO	CA-C-N	12.04	143.69	117.20
2	A	45	VAL	C-N-CA	11.86	147.20	122.30
2	B	45	VAL	C-N-CA	11.86	147.20	122.30
2	G	45	VAL	C-N-CA	11.84	147.17	122.30
2	D	45	VAL	C-N-CA	11.84	147.15	122.30
2	E	45	VAL	C-N-CA	11.83	147.15	122.30
2	H	45	VAL	C-N-CA	11.83	147.14	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	45	VAL	C-N-CA	11.79	147.05	122.30
2	F	45	VAL	C-N-CA	11.78	147.03	122.30
1	K	599	ASP	O-C-N	-11.75	103.90	122.70
1	I	599	ASP	O-C-N	-11.75	103.90	122.70
1	J	599	ASP	O-C-N	-11.71	103.96	122.70
1	L	599	ASP	O-C-N	-11.69	104.00	122.70
1	M	599	ASP	O-C-N	-11.69	104.00	122.70
1	N	599	ASP	O-C-N	-11.66	104.04	122.70
2	H	32	PRO	C-N-CA	11.34	150.06	121.70
2	D	32	PRO	C-N-CA	11.32	150.01	121.70
2	A	32	PRO	C-N-CA	11.32	149.99	121.70
2	C	32	PRO	C-N-CA	11.32	149.99	121.70
2	G	32	PRO	C-N-CA	11.32	149.99	121.70
2	F	32	PRO	C-N-CA	11.31	149.98	121.70
2	B	32	PRO	C-N-CA	11.31	149.97	121.70
2	E	32	PRO	C-N-CA	11.30	149.94	121.70
1	J	772	SER	C-N-CA	11.03	149.28	121.70
1	K	772	SER	C-N-CA	10.99	149.18	121.70
1	I	772	SER	C-N-CA	10.98	149.16	121.70
1	N	772	SER	C-N-CA	10.98	149.16	121.70
1	L	772	SER	C-N-CA	10.97	149.14	121.70
1	M	772	SER	C-N-CA	10.97	149.12	121.70
2	G	109	PRO	C-N-CA	10.86	148.84	121.70
2	B	109	PRO	C-N-CA	10.85	148.83	121.70
2	F	109	PRO	C-N-CA	10.85	148.82	121.70
2	H	109	PRO	C-N-CA	10.84	148.80	121.70
2	A	109	PRO	C-N-CA	10.84	148.79	121.70
1	J	772	SER	CA-C-N	10.84	141.04	117.20
2	D	109	PRO	C-N-CA	10.84	148.79	121.70
2	E	109	PRO	C-N-CA	10.81	148.74	121.70
2	C	109	PRO	C-N-CA	10.81	148.73	121.70
1	I	772	SER	CA-C-N	10.80	140.96	117.20
1	K	772	SER	CA-C-N	10.79	140.94	117.20
1	N	772	SER	CA-C-N	10.79	140.94	117.20
1	M	772	SER	CA-C-N	10.77	140.89	117.20
1	L	772	SER	CA-C-N	10.76	140.87	117.20
1	I	118	LYS	O-C-N	-10.21	106.37	122.70
1	J	118	LYS	O-C-N	-10.20	106.37	122.70
1	K	118	LYS	O-C-N	-10.19	106.39	122.70
1	M	118	LYS	O-C-N	-10.15	106.46	122.70
1	N	118	LYS	O-C-N	-10.15	106.47	122.70
1	L	118	LYS	O-C-N	-10.14	106.48	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	307	PRO	CA-C-O	9.61	143.26	120.20
2	A	307	PRO	CA-C-O	9.60	143.23	120.20
2	G	307	PRO	CA-C-O	9.59	143.23	120.20
2	H	307	PRO	CA-C-O	9.58	143.20	120.20
2	E	307	PRO	CA-C-O	9.57	143.17	120.20
2	D	307	PRO	CA-C-O	9.55	143.13	120.20
2	B	307	PRO	CA-C-O	9.55	143.12	120.20
2	C	307	PRO	CA-C-O	9.53	143.06	120.20
3	Q	114	GLU	O-C-N	-9.47	107.54	122.70
3	O	114	GLU	O-C-N	-9.46	107.56	122.70
3	R	114	GLU	O-C-N	-9.45	107.58	122.70
3	S	114	GLU	O-C-N	-9.45	107.58	122.70
3	P	114	GLU	O-C-N	-9.45	107.58	122.70
3	T	114	GLU	O-C-N	-9.42	107.63	122.70
3	S	45	GLU	O-C-N	-9.35	107.74	122.70
3	R	45	GLU	O-C-N	-9.33	107.78	122.70
3	O	45	GLU	O-C-N	-9.32	107.78	122.70
3	P	45	GLU	O-C-N	-9.32	107.79	122.70
3	T	45	GLU	O-C-N	-9.29	107.84	122.70
3	Q	45	GLU	O-C-N	-9.28	107.86	122.70
3	O	3	GLN	N-CA-CB	-8.97	94.44	110.60
3	S	3	GLN	N-CA-CB	-8.97	94.46	110.60
3	T	3	GLN	N-CA-CB	-8.95	94.50	110.60
3	R	3	GLN	N-CA-CB	-8.94	94.51	110.60
3	P	3	GLN	N-CA-CB	-8.92	94.54	110.60
3	Q	3	GLN	N-CA-CB	-8.90	94.58	110.60
1	K	357	SER	CA-C-N	8.52	135.95	117.20
1	N	357	SER	CA-C-N	8.51	135.91	117.20
1	J	357	SER	CA-C-N	8.50	135.89	117.20
1	L	357	SER	CA-C-N	8.50	135.89	117.20
1	M	357	SER	CA-C-N	8.49	135.87	117.20
1	I	357	SER	CA-C-N	8.48	135.85	117.20
2	H	369	ILE	O-C-N	-8.33	109.38	122.70
2	B	369	ILE	O-C-N	-8.32	109.39	122.70
2	G	369	ILE	O-C-N	-8.32	109.39	122.70
2	A	369	ILE	O-C-N	-8.31	109.41	122.70
2	C	369	ILE	O-C-N	-8.31	109.41	122.70
2	F	369	ILE	O-C-N	-8.30	109.43	122.70
2	E	369	ILE	O-C-N	-8.28	109.45	122.70
2	D	369	ILE	O-C-N	-8.26	109.48	122.70
2	E	371	HIS	N-CA-CB	8.14	125.25	110.60
2	H	5	THR	CB-CA-C	8.14	133.57	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5	THR	CB-CA-C	8.13	133.56	111.60
2	E	5	THR	CB-CA-C	8.13	133.55	111.60
2	G	5	THR	CB-CA-C	8.12	133.53	111.60
2	C	5	THR	CB-CA-C	8.12	133.52	111.60
2	D	5	THR	CB-CA-C	8.11	133.51	111.60
1	J	357	SER	C-N-CA	8.11	141.97	121.70
1	N	357	SER	C-N-CA	8.11	141.97	121.70
2	F	371	HIS	N-CA-CB	8.10	125.19	110.60
1	K	357	SER	C-N-CA	8.10	141.96	121.70
2	A	5	THR	CB-CA-C	8.10	133.46	111.60
2	H	371	HIS	N-CA-CB	8.10	125.18	110.60
2	C	371	HIS	N-CA-CB	8.10	125.17	110.60
1	I	357	SER	C-N-CA	8.09	141.92	121.70
2	A	371	HIS	N-CA-CB	8.09	125.16	110.60
2	G	371	HIS	N-CA-CB	8.09	125.16	110.60
2	B	371	HIS	N-CA-CB	8.09	125.15	110.60
1	L	357	SER	C-N-CA	8.08	141.91	121.70
1	M	357	SER	C-N-CA	8.08	141.90	121.70
2	F	5	THR	CB-CA-C	8.08	133.41	111.60
2	D	371	HIS	N-CA-CB	8.07	125.13	110.60
1	I	398	THR	CA-C-O	7.99	136.88	120.10
1	K	398	THR	CA-C-O	7.99	136.88	120.10
1	N	398	THR	CA-C-O	7.99	136.88	120.10
1	L	398	THR	CA-C-O	7.97	136.84	120.10
1	M	398	THR	CA-C-O	7.97	136.84	120.10
1	J	398	THR	CA-C-O	7.96	136.82	120.10
2	D	45	VAL	CA-C-O	7.64	136.14	120.10
2	A	45	VAL	CA-C-O	7.63	136.13	120.10
2	C	45	VAL	CA-C-O	7.63	136.13	120.10
2	B	45	VAL	CA-C-O	7.63	136.11	120.10
2	F	45	VAL	CA-C-O	7.62	136.10	120.10
2	E	45	VAL	CA-C-O	7.62	136.10	120.10
2	H	45	VAL	CA-C-O	7.61	136.08	120.10
3	T	3	GLN	CB-CA-C	7.60	125.59	110.40
2	G	45	VAL	CA-C-O	7.59	136.03	120.10
3	P	3	GLN	CB-CA-C	7.58	125.56	110.40
3	O	3	GLN	CB-CA-C	7.57	125.53	110.40
3	S	3	GLN	CB-CA-C	7.56	125.52	110.40
3	R	3	GLN	CB-CA-C	7.54	125.48	110.40
1	N	56	LYS	O-C-N	-7.53	110.65	122.70
3	Q	3	GLN	CB-CA-C	7.53	125.45	110.40
1	J	56	LYS	O-C-N	-7.52	110.67	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	56	LYS	O-C-N	-7.50	110.70	122.70
1	M	56	LYS	O-C-N	-7.48	110.72	122.70
1	I	56	LYS	O-C-N	-7.48	110.73	122.70
1	K	56	LYS	O-C-N	-7.46	110.77	122.70
1	L	641	ILE	O-C-N	-7.43	110.82	122.70
1	K	641	ILE	O-C-N	-7.42	110.83	122.70
1	M	641	ILE	O-C-N	-7.41	110.84	122.70
1	I	641	ILE	O-C-N	-7.40	110.86	122.70
1	J	641	ILE	O-C-N	-7.40	110.86	122.70
1	N	641	ILE	O-C-N	-7.37	110.91	122.70
1	I	816	ALA	O-C-N	-7.33	110.97	122.70
1	K	816	ALA	O-C-N	-7.31	111.00	122.70
1	M	816	ALA	O-C-N	-7.30	111.02	122.70
1	L	816	ALA	O-C-N	-7.29	111.03	122.70
1	N	816	ALA	O-C-N	-7.28	111.06	122.70
1	J	816	ALA	O-C-N	-7.27	111.07	122.70
3	S	147	ALA	CB-CA-C	-7.24	99.24	110.10
3	R	147	ALA	CB-CA-C	-7.22	99.26	110.10
3	Q	147	ALA	CB-CA-C	-7.21	99.29	110.10
3	O	147	ALA	CB-CA-C	-7.18	99.33	110.10
3	T	147	ALA	CB-CA-C	-7.17	99.34	110.10
3	P	147	ALA	CB-CA-C	-7.17	99.34	110.10
3	S	147	ALA	N-CA-C	6.59	128.80	111.00
3	P	147	ALA	N-CA-C	6.58	128.77	111.00
1	J	599	ASP	CA-C-N	6.58	131.68	117.20
3	Q	147	ALA	N-CA-C	6.58	128.76	111.00
1	K	599	ASP	CA-C-N	6.57	131.65	117.20
3	R	147	ALA	N-CA-C	6.57	128.73	111.00
1	M	599	ASP	CA-C-N	6.55	131.62	117.20
3	O	147	ALA	N-CA-C	6.55	128.69	111.00
1	I	599	ASP	CA-C-N	6.55	131.61	117.20
1	L	599	ASP	CA-C-N	6.54	131.60	117.20
3	T	147	ALA	N-CA-C	6.54	128.65	111.00
1	N	599	ASP	CA-C-N	6.51	131.51	117.20
2	E	199	SER	O-C-N	-6.33	112.58	122.70
2	D	199	SER	O-C-N	-6.31	112.60	122.70
2	C	199	SER	O-C-N	-6.31	112.61	122.70
2	F	199	SER	O-C-N	-6.30	112.61	122.70
2	B	199	SER	O-C-N	-6.29	112.63	122.70
2	G	199	SER	O-C-N	-6.29	112.64	122.70
2	H	199	SER	O-C-N	-6.29	112.64	122.70
2	C	179	ASP	O-C-N	-6.28	112.66	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	179	ASP	O-C-N	-6.28	112.66	122.70
2	A	179	ASP	O-C-N	-6.27	112.67	122.70
2	A	199	SER	O-C-N	-6.27	112.67	122.70
2	G	179	ASP	O-C-N	-6.27	112.67	122.70
2	F	179	ASP	O-C-N	-6.26	112.68	122.70
2	B	179	ASP	O-C-N	-6.25	112.69	122.70
2	E	179	ASP	O-C-N	-6.24	112.71	122.70
2	D	179	ASP	O-C-N	-6.22	112.75	122.70
2	D	371	HIS	CB-CA-C	-6.04	98.31	110.40
2	E	371	HIS	CB-CA-C	-6.01	98.37	110.40
2	G	371	HIS	CB-CA-C	-6.01	98.38	110.40
2	B	371	HIS	CB-CA-C	-5.99	98.41	110.40
2	H	371	HIS	CB-CA-C	-5.99	98.41	110.40
2	F	371	HIS	CB-CA-C	-5.99	98.42	110.40
2	A	371	HIS	CB-CA-C	-5.98	98.43	110.40
2	C	371	HIS	CB-CA-C	-5.96	98.48	110.40
1	I	4	GLY	O-C-N	-5.90	113.26	122.70
1	J	4	GLY	O-C-N	-5.89	113.28	122.70
1	N	4	GLY	O-C-N	-5.89	113.28	122.70
1	M	4	GLY	O-C-N	-5.87	113.31	122.70
1	K	4	GLY	O-C-N	-5.86	113.32	122.70
1	L	4	GLY	O-C-N	-5.85	113.34	122.70
1	N	601	LEU	O-C-N	-5.67	113.63	122.70
1	L	601	LEU	O-C-N	-5.64	113.68	122.70
1	M	601	LEU	O-C-N	-5.64	113.68	122.70
1	J	601	LEU	O-C-N	-5.62	113.70	122.70
1	I	601	LEU	O-C-N	-5.62	113.71	122.70
1	K	601	LEU	O-C-N	-5.62	113.71	122.70
2	F	33	SER	O-C-N	-5.51	113.89	122.70
2	A	33	SER	O-C-N	-5.51	113.89	122.70
2	E	33	SER	O-C-N	-5.50	113.91	122.70
2	D	33	SER	O-C-N	-5.49	113.91	122.70
1	J	39	LYS	C-N-CA	5.47	135.38	121.70
1	N	39	LYS	C-N-CA	5.47	135.37	121.70
1	M	39	LYS	C-N-CA	5.47	135.37	121.70
2	H	33	SER	O-C-N	-5.47	113.95	122.70
1	K	39	LYS	C-N-CA	5.46	135.36	121.70
2	G	33	SER	O-C-N	-5.46	113.96	122.70
1	L	39	LYS	C-N-CA	5.45	135.32	121.70
2	C	33	SER	O-C-N	-5.45	113.98	122.70
1	I	39	LYS	C-N-CA	5.44	135.30	121.70
1	L	119	SER	CA-C-N	5.43	129.15	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	119	SER	CA-C-N	5.42	129.12	117.20
2	B	33	SER	O-C-N	-5.40	114.06	122.70
1	M	119	SER	CA-C-N	5.39	129.06	117.20
1	I	119	SER	CA-C-N	5.38	129.04	117.20
1	N	119	SER	CA-C-N	5.38	129.04	117.20
1	J	119	SER	CA-C-N	5.36	128.99	117.20
1	N	642	SER	O-C-N	-5.32	114.19	122.70
1	J	642	SER	O-C-N	-5.32	114.20	122.70
1	I	642	SER	O-C-N	-5.30	114.21	122.70
1	L	642	SER	O-C-N	-5.30	114.22	122.70
1	K	642	SER	O-C-N	-5.27	114.26	122.70
1	M	642	SER	O-C-N	-5.27	114.27	122.70
2	G	370	VAL	CA-C-O	5.22	131.06	120.10
2	D	370	VAL	CA-C-O	5.20	131.02	120.10
2	B	370	VAL	CA-C-O	5.19	131.00	120.10
2	F	370	VAL	CA-C-O	5.19	131.00	120.10
2	C	370	VAL	CA-C-O	5.19	131.00	120.10
2	A	370	VAL	CA-C-O	5.18	130.98	120.10
1	J	599	ASP	C-N-CA	5.17	134.62	121.70
2	E	370	VAL	CA-C-O	5.17	130.95	120.10
2	H	370	VAL	CA-C-O	5.16	130.94	120.10
2	F	15	GLY	C-N-CA	5.15	134.57	121.70
2	A	15	GLY	C-N-CA	5.14	134.55	121.70
2	E	5	THR	O-C-N	-5.14	114.48	122.70
2	E	15	GLY	C-N-CA	5.14	134.55	121.70
1	K	599	ASP	C-N-CA	5.14	134.54	121.70
1	I	599	ASP	C-N-CA	5.14	134.54	121.70
2	B	15	GLY	C-N-CA	5.14	134.54	121.70
2	D	15	GLY	C-N-CA	5.13	134.53	121.70
1	L	599	ASP	C-N-CA	5.13	134.53	121.70
1	M	599	ASP	C-N-CA	5.12	134.51	121.70
2	B	5	THR	O-C-N	-5.12	114.50	122.70
2	C	15	GLY	C-N-CA	5.12	134.50	121.70
2	G	15	GLY	C-N-CA	5.12	134.50	121.70
2	D	5	THR	O-C-N	-5.12	114.51	122.70
2	H	15	GLY	C-N-CA	5.12	134.49	121.70
2	G	5	THR	O-C-N	-5.11	114.52	122.70
2	F	5	THR	O-C-N	-5.11	114.53	122.70
2	H	5	THR	O-C-N	-5.10	114.53	122.70
1	N	599	ASP	C-N-CA	5.10	134.45	121.70
2	C	5	THR	O-C-N	-5.09	114.55	122.70
1	K	119	SER	CA-C-O	5.07	130.75	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5	THR	O-C-N	-5.06	114.60	122.70
1	I	119	SER	CA-C-O	5.04	130.69	120.10
1	L	119	SER	CA-C-O	5.04	130.68	120.10
1	J	119	SER	CA-C-O	5.03	130.66	120.10
1	N	119	SER	CA-C-O	5.01	130.62	120.10
1	M	119	SER	CA-C-O	5.00	130.60	120.10

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	5	THR	CA
2	B	5	THR	CA
2	C	5	THR	CA
2	D	5	THR	CA
2	E	5	THR	CA
2	F	5	THR	CA
2	G	5	THR	CA
2	H	5	THR	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	636	GLY	Peptide
1	J	636	GLY	Peptide
1	K	636	GLY	Peptide
1	L	636	GLY	Peptide
1	M	636	GLY	Peptide
1	N	636	GLY	Peptide

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	I	3939	0	1724	20	0
1	J	3939	0	1724	20	0
1	K	3939	0	1724	20	0
1	L	3939	0	1724	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	3939	0	1724	20	0
1	N	3939	0	1724	20	0
2	A	1806	0	817	21	0
2	B	1806	0	817	20	0
2	C	1806	0	817	21	0
2	D	1806	0	817	20	0
2	E	1806	0	817	21	0
2	F	1806	0	817	21	0
2	G	1806	0	817	21	0
2	H	1806	0	817	21	0
3	O	713	0	326	0	0
3	P	713	0	326	0	0
3	Q	713	0	326	0	0
3	R	713	0	326	0	0
3	S	713	0	326	0	0
3	T	713	0	326	0	0
All	All	42360	0	18836	283	0

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

All (283) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:358:THR:O	1:I:358:THR:CA	1.67	1.43
1:N:358:THR:O	1:N:358:THR:CA	1.67	1.42
1:K:358:THR:O	1:K:358:THR:CA	1.67	1.42
2:B:5:THR:CB	2:B:5:THR:C	1.89	1.41
1:L:358:THR:O	1:L:358:THR:CA	1.67	1.40
1:J:358:THR:O	1:J:358:THR:CA	1.67	1.39
2:D:5:THR:CB	2:D:5:THR:C	1.89	1.39
1:M:358:THR:O	1:M:358:THR:CA	1.67	1.39
2:A:5:THR:CB	2:A:5:THR:C	1.89	1.39
2:C:5:THR:CB	2:C:5:THR:C	1.89	1.38
2:H:5:THR:CB	2:H:5:THR:C	1.89	1.37
2:F:5:THR:CB	2:F:5:THR:C	1.89	1.37
2:E:5:THR:CB	2:E:5:THR:C	1.89	1.36
2:G:5:THR:CB	2:G:5:THR:C	1.89	1.36
2:C:44:MET:O	2:C:45:VAL:CA	1.79	1.30
2:F:44:MET:O	2:F:45:VAL:CA	1.79	1.30
2:H:44:MET:O	2:H:45:VAL:CA	1.79	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:MET:O	2:D:45:VAL:CA	1.79	1.30
2:G:44:MET:O	2:G:45:VAL:CA	1.79	1.29
2:B:44:MET:O	2:B:45:VAL:CA	1.79	1.29
2:A:44:MET:O	2:A:45:VAL:CA	1.79	1.29
1:I:358:THR:O	1:I:359:SER:CA	1.81	1.28
1:M:358:THR:O	1:M:359:SER:CA	1.81	1.27
1:N:358:THR:O	1:N:359:SER:CA	1.81	1.27
2:E:44:MET:O	2:E:45:VAL:CA	1.79	1.27
1:L:358:THR:O	1:L:359:SER:CA	1.81	1.27
1:J:358:THR:O	1:J:359:SER:CA	1.81	1.26
1:K:358:THR:O	1:K:359:SER:CA	1.81	1.25
2:C:307:PRO:O	2:C:307:PRO:CA	1.86	1.24
2:A:307:PRO:O	2:A:307:PRO:CA	1.86	1.24
2:E:307:PRO:O	2:E:307:PRO:CA	1.86	1.23
2:F:307:PRO:O	2:F:307:PRO:CA	1.86	1.23
2:D:307:PRO:O	2:D:307:PRO:CA	1.86	1.22
2:B:307:PRO:O	2:B:307:PRO:CA	1.86	1.22
2:G:307:PRO:O	2:G:307:PRO:CA	1.86	1.22
2:H:307:PRO:O	2:H:307:PRO:CA	1.86	1.22
1:J:175:GLY:O	1:J:176:GLN:CA	1.88	1.21
1:I:358:THR:C	1:I:359:SER:CA	2.09	1.21
1:N:358:THR:C	1:N:359:SER:CA	2.09	1.21
1:M:175:GLY:O	1:M:175:GLY:CA	1.89	1.21
1:N:175:GLY:O	1:N:176:GLN:CA	1.88	1.21
1:I:175:GLY:O	1:I:175:GLY:CA	1.89	1.20
1:L:175:GLY:O	1:L:176:GLN:CA	1.88	1.20
1:K:358:THR:C	1:K:359:SER:CA	2.09	1.20
1:L:358:THR:C	1:L:359:SER:CA	2.09	1.20
1:L:175:GLY:O	1:L:175:GLY:CA	1.89	1.20
1:N:175:GLY:O	1:N:175:GLY:CA	1.89	1.20
1:M:175:GLY:O	1:M:176:GLN:CA	1.88	1.20
1:K:175:GLY:O	1:K:176:GLN:CA	1.88	1.20
1:I:175:GLY:O	1:I:176:GLN:CA	1.88	1.19
1:J:175:GLY:O	1:J:175:GLY:CA	1.89	1.19
1:K:175:GLY:O	1:K:175:GLY:CA	1.89	1.19
1:M:358:THR:C	1:M:359:SER:CA	2.09	1.19
1:J:358:THR:C	1:J:359:SER:CA	2.09	1.18
2:G:5:THR:N	2:G:5:THR:HA	1.49	1.16
2:D:44:MET:O	2:D:44:MET:CA	1.95	1.15
1:J:358:THR:CA	1:J:359:SER:N	2.10	1.14
1:L:358:THR:CA	1:L:359:SER:N	2.10	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:44:MET:O	2:A:44:MET:CA	1.95	1.14
2:D:5:THR:N	2:D:5:THR:HA	1.49	1.14
2:G:44:MET:O	2:G:44:MET:CA	1.95	1.14
1:K:358:THR:CA	1:K:359:SER:N	2.10	1.14
1:I:358:THR:CA	1:I:359:SER:N	2.10	1.13
1:M:358:THR:CA	1:M:359:SER:N	2.10	1.13
2:B:44:MET:O	2:B:44:MET:CA	1.95	1.13
2:H:44:MET:O	2:H:44:MET:CA	1.95	1.13
2:H:44:MET:C	2:H:45:VAL:CA	2.17	1.13
2:A:5:THR:N	2:A:5:THR:HA	1.49	1.13
2:A:44:MET:C	2:A:45:VAL:CA	2.17	1.13
2:E:44:MET:O	2:E:44:MET:CA	1.95	1.13
2:F:44:MET:C	2:F:45:VAL:CA	2.17	1.13
2:C:44:MET:C	2:C:45:VAL:CA	2.17	1.13
2:F:5:THR:N	2:F:5:THR:HA	1.49	1.13
2:C:5:THR:N	2:C:5:THR:HA	1.49	1.13
2:C:44:MET:O	2:C:44:MET:CA	1.95	1.13
2:D:44:MET:C	2:D:45:VAL:CA	2.17	1.13
2:E:44:MET:C	2:E:45:VAL:CA	2.17	1.13
2:F:44:MET:O	2:F:44:MET:CA	1.95	1.12
1:N:358:THR:CA	1:N:359:SER:N	2.10	1.12
2:B:44:MET:C	2:B:45:VAL:CA	2.17	1.12
2:G:44:MET:C	2:G:45:VAL:CA	2.17	1.12
2:E:5:THR:N	2:E:5:THR:HA	1.49	1.10
2:D:5:THR:C	2:D:5:THR:N	2.05	1.10
2:B:5:THR:C	2:B:5:THR:N	2.05	1.09
2:F:5:THR:C	2:F:5:THR:N	2.05	1.09
2:E:5:THR:C	2:E:5:THR:N	2.05	1.09
2:G:5:THR:C	2:G:5:THR:N	2.05	1.08
2:C:5:THR:C	2:C:5:THR:N	2.05	1.08
2:B:5:THR:N	2:B:5:THR:HA	1.49	1.08
1:J:398:THR:O	1:J:398:THR:CA	2.02	1.08
1:N:398:THR:O	1:N:398:THR:CA	2.02	1.08
2:B:307:PRO:O	2:B:308:GLY:CA	2.02	1.08
2:E:307:PRO:O	2:E:308:GLY:CA	2.02	1.08
2:H:307:PRO:O	2:H:308:GLY:CA	2.02	1.08
1:I:398:THR:O	1:I:398:THR:CA	2.02	1.07
1:M:398:THR:O	1:M:398:THR:CA	2.02	1.07
2:A:5:THR:C	2:A:5:THR:N	2.05	1.07
2:D:307:PRO:O	2:D:308:GLY:CA	2.02	1.07
2:G:307:PRO:O	2:G:308:GLY:CA	2.02	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:5:THR:N	2:H:5:THR:HA	1.49	1.07
1:K:398:THR:O	1:K:398:THR:CA	2.02	1.07
2:C:307:PRO:O	2:C:308:GLY:CA	2.02	1.07
2:A:307:PRO:O	2:A:308:GLY:CA	2.02	1.07
2:H:5:THR:C	2:H:5:THR:N	2.05	1.07
1:L:398:THR:O	1:L:398:THR:CA	2.02	1.06
2:F:307:PRO:O	2:F:308:GLY:CA	2.02	1.06
1:J:175:GLY:C	1:J:176:GLN:CA	2.25	1.05
1:N:175:GLY:C	1:N:176:GLN:CA	2.25	1.04
1:I:175:GLY:C	1:I:176:GLN:CA	2.25	1.04
1:L:175:GLY:C	1:L:176:GLN:CA	2.25	1.04
1:M:175:GLY:C	1:M:176:GLN:CA	2.25	1.04
1:K:175:GLY:C	1:K:176:GLN:CA	2.25	1.03
2:D:44:MET:CA	2:D:45:VAL:N	2.22	1.02
2:E:44:MET:CA	2:E:45:VAL:N	2.22	1.02
2:B:44:MET:CA	2:B:45:VAL:N	2.22	1.01
2:G:44:MET:CA	2:G:45:VAL:N	2.22	1.01
2:C:44:MET:CA	2:C:45:VAL:N	2.22	1.01
2:F:44:MET:CA	2:F:45:VAL:N	2.22	1.01
2:A:44:MET:CA	2:A:45:VAL:N	2.22	1.00
2:H:44:MET:CA	2:H:45:VAL:N	2.22	1.00
1:L:175:GLY:CA	1:L:176:GLN:N	2.26	0.99
1:M:175:GLY:CA	1:M:176:GLN:N	2.26	0.99
1:K:175:GLY:CA	1:K:176:GLN:N	2.26	0.99
1:J:175:GLY:CA	1:J:176:GLN:N	2.26	0.99
1:N:175:GLY:CA	1:N:176:GLN:N	2.26	0.98
1:I:175:GLY:CA	1:I:176:GLN:N	2.26	0.98
2:F:5:THR:CB	2:F:5:THR:HA	1.46	0.97
2:H:5:THR:CB	2:H:5:THR:HA	1.46	0.97
1:K:398:THR:O	1:K:398:THR:C	0.77	0.97
1:J:398:THR:O	1:J:398:THR:C	0.77	0.97
1:M:398:THR:O	1:M:398:THR:C	0.77	0.97
2:D:5:THR:CB	2:D:5:THR:HA	1.46	0.97
1:N:398:THR:O	1:N:398:THR:C	0.77	0.96
1:I:398:THR:O	1:I:398:THR:C	0.77	0.96
1:L:398:THR:O	1:L:398:THR:C	0.77	0.96
2:G:5:THR:CB	2:G:5:THR:HA	1.46	0.96
2:B:5:THR:CB	2:B:5:THR:HA	1.46	0.95
2:E:5:THR:CB	2:E:5:THR:HA	1.46	0.95
2:A:5:THR:CB	2:A:5:THR:HA	1.46	0.95
2:C:5:THR:CB	2:C:5:THR:HA	1.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:307:PRO:O	2:D:308:GLY:N	0.75	0.90
2:C:307:PRO:O	2:C:308:GLY:N	0.75	0.90
2:A:307:PRO:O	2:A:308:GLY:N	0.75	0.90
2:G:307:PRO:O	2:G:308:GLY:N	0.75	0.90
2:E:307:PRO:O	2:E:308:GLY:N	0.75	0.90
2:H:307:PRO:O	2:H:308:GLY:N	0.75	0.90
2:B:307:PRO:O	2:B:308:GLY:N	0.75	0.89
2:F:307:PRO:O	2:F:308:GLY:N	0.75	0.89
1:J:175:GLY:C	1:J:176:GLN:N	0.83	0.89
1:K:175:GLY:C	1:K:176:GLN:N	0.83	0.88
1:M:175:GLY:C	1:M:176:GLN:N	0.83	0.88
1:L:175:GLY:C	1:L:176:GLN:N	0.83	0.88
1:I:175:GLY:C	1:I:176:GLN:N	0.83	0.88
2:A:5:THR:CB	2:A:5:THR:N	0.72	0.87
2:G:5:THR:CB	2:G:5:THR:N	0.72	0.87
2:E:5:THR:CB	2:E:5:THR:N	0.72	0.87
1:N:175:GLY:C	1:N:176:GLN:N	0.83	0.87
2:C:5:THR:CB	2:C:5:THR:N	0.72	0.87
2:D:5:THR:CB	2:D:5:THR:N	0.72	0.86
2:B:5:THR:CB	2:B:5:THR:N	0.72	0.86
2:F:5:THR:CB	2:F:5:THR:N	0.72	0.86
2:H:5:THR:CB	2:H:5:THR:N	0.72	0.86
2:D:44:MET:C	2:D:45:VAL:N	0.81	0.86
2:C:44:MET:C	2:C:45:VAL:N	0.81	0.86
2:F:44:MET:C	2:F:45:VAL:N	0.81	0.86
2:A:44:MET:C	2:A:45:VAL:N	0.81	0.86
2:B:44:MET:C	2:B:45:VAL:N	0.81	0.86
1:N:358:THR:O	1:N:358:THR:CB	2.24	0.85
2:E:44:MET:C	2:E:45:VAL:N	0.81	0.85
2:H:44:MET:C	2:H:45:VAL:N	0.81	0.85
1:J:358:THR:O	1:J:358:THR:CB	2.24	0.85
1:K:358:THR:O	1:K:358:THR:CB	2.24	0.84
1:I:358:THR:O	1:I:358:THR:CB	2.24	0.84
2:G:44:MET:C	2:G:45:VAL:N	0.81	0.84
1:M:358:THR:O	1:M:358:THR:CB	2.24	0.84
1:M:358:THR:C	1:M:359:SER:N	0.81	0.83
1:L:358:THR:O	1:L:358:THR:CB	2.24	0.83
1:L:358:THR:C	1:L:359:SER:N	0.81	0.83
2:G:5:THR:N	2:G:5:THR:CA	0.67	0.82
2:C:5:THR:N	2:C:5:THR:CA	0.67	0.82
2:B:5:THR:N	2:B:5:THR:CA	0.67	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:5:THR:N	2:F:5:THR:CA	0.67	0.82
1:N:358:THR:C	1:N:359:SER:N	0.81	0.82
2:A:5:THR:N	2:A:5:THR:CA	0.67	0.82
2:D:5:THR:N	2:D:5:THR:CA	0.67	0.82
2:E:5:THR:N	2:E:5:THR:CA	0.67	0.82
2:H:5:THR:N	2:H:5:THR:CA	0.67	0.82
1:L:358:THR:O	1:L:359:SER:CB	2.29	0.81
1:N:358:THR:O	1:N:359:SER:CB	2.29	0.81
1:J:358:THR:O	1:J:359:SER:CB	2.29	0.81
1:K:358:THR:O	1:K:359:SER:CB	2.29	0.81
1:M:358:THR:O	1:M:359:SER:CB	2.29	0.81
1:K:358:THR:C	1:K:359:SER:N	0.81	0.81
1:I:358:THR:O	1:I:359:SER:CB	2.29	0.81
1:I:358:THR:C	1:I:359:SER:N	0.81	0.80
1:J:358:THR:C	1:J:359:SER:N	0.81	0.80
2:E:44:MET:O	2:E:45:VAL:N	0.65	0.80
2:G:44:MET:O	2:G:45:VAL:N	0.65	0.80
2:C:44:MET:O	2:C:45:VAL:N	0.65	0.79
2:A:44:MET:O	2:A:45:VAL:N	0.65	0.79
2:B:44:MET:O	2:B:45:VAL:N	0.65	0.79
2:D:44:MET:O	2:D:45:VAL:N	0.65	0.79
2:F:44:MET:O	2:F:45:VAL:N	0.65	0.79
2:H:44:MET:O	2:H:45:VAL:N	0.65	0.79
1:J:358:THR:O	1:J:359:SER:N	0.63	0.78
1:N:358:THR:O	1:N:359:SER:N	0.63	0.78
1:M:358:THR:O	1:M:359:SER:N	0.63	0.77
1:I:358:THR:O	1:I:359:SER:N	0.63	0.77
1:L:358:THR:O	1:L:359:SER:N	0.63	0.77
1:K:358:THR:O	1:K:359:SER:N	0.63	0.76
1:N:175:GLY:O	1:N:176:GLN:N	0.60	0.75
1:M:175:GLY:O	1:M:176:GLN:N	0.60	0.75
2:A:44:MET:O	2:A:44:MET:C	0.55	0.75
1:K:175:GLY:O	1:K:176:GLN:N	0.60	0.74
2:B:44:MET:O	2:B:44:MET:C	0.55	0.74
2:G:44:MET:O	2:G:44:MET:C	0.55	0.74
1:J:175:GLY:O	1:J:176:GLN:N	0.60	0.74
1:L:175:GLY:O	1:L:176:GLN:N	0.60	0.74
1:I:175:GLY:O	1:I:176:GLN:N	0.60	0.74
2:D:44:MET:O	2:D:44:MET:C	0.55	0.74
2:F:44:MET:O	2:F:44:MET:C	0.55	0.74
2:C:44:MET:O	2:C:44:MET:C	0.55	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:44:MET:O	2:H:44:MET:C	0.55	0.73
2:E:44:MET:O	2:E:44:MET:C	0.55	0.73
1:M:175:GLY:O	1:M:175:GLY:C	0.48	0.67
1:N:175:GLY:O	1:N:175:GLY:C	0.48	0.66
1:I:175:GLY:O	1:I:175:GLY:C	0.48	0.66
2:F:307:PRO:O	2:F:307:PRO:C	0.46	0.66
1:J:175:GLY:O	1:J:175:GLY:C	0.48	0.66
2:G:307:PRO:O	2:G:307:PRO:C	0.46	0.66
2:G:44:MET:O	2:G:45:VAL:CB	2.44	0.65
2:E:307:PRO:O	2:E:307:PRO:C	0.46	0.65
2:D:307:PRO:O	2:D:307:PRO:C	0.46	0.65
1:L:175:GLY:O	1:L:175:GLY:C	0.48	0.65
1:K:175:GLY:O	1:K:175:GLY:C	0.48	0.65
2:H:307:PRO:O	2:H:307:PRO:C	0.46	0.65
2:B:44:MET:O	2:B:45:VAL:CB	2.44	0.65
2:C:307:PRO:O	2:C:307:PRO:C	0.46	0.64
2:E:44:MET:O	2:E:45:VAL:CB	2.44	0.64
2:B:307:PRO:O	2:B:307:PRO:C	0.46	0.64
2:A:307:PRO:O	2:A:307:PRO:C	0.46	0.64
1:N:358:THR:C	1:N:359:SER:CB	2.66	0.64
1:M:358:THR:C	1:M:359:SER:CB	2.66	0.63
1:I:358:THR:C	1:I:359:SER:CB	2.66	0.62
1:J:358:THR:C	1:J:359:SER:CB	2.66	0.62
2:H:44:MET:O	2:H:45:VAL:CB	2.44	0.60
2:A:44:MET:O	2:A:45:VAL:CB	2.44	0.60
2:F:44:MET:O	2:F:45:VAL:CB	2.44	0.60
1:K:358:THR:C	1:K:359:SER:CB	2.66	0.59
1:N:398:THR:O	1:N:398:THR:CB	2.51	0.59
2:E:46:GLY:N	2:E:47:MET:HA	2.18	0.59
2:A:46:GLY:N	2:A:47:MET:HA	2.18	0.59
2:C:46:GLY:N	2:C:47:MET:HA	2.18	0.59
1:L:358:THR:C	1:L:359:SER:CB	2.66	0.59
1:J:398:THR:O	1:J:398:THR:CB	2.51	0.59
2:G:46:GLY:N	2:G:47:MET:HA	2.18	0.59
2:D:44:MET:O	2:D:45:VAL:CB	2.44	0.59
1:M:398:THR:O	1:M:398:THR:CB	2.51	0.58
2:C:44:MET:O	2:C:45:VAL:CB	2.44	0.58
2:D:46:GLY:N	2:D:47:MET:HA	2.18	0.58
2:H:46:GLY:N	2:H:47:MET:HA	2.18	0.58
1:I:398:THR:O	1:I:398:THR:CB	2.51	0.58
2:B:46:GLY:N	2:B:47:MET:HA	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:398:THR:O	1:L:398:THR:CB	2.51	0.57
2:F:46:GLY:N	2:F:47:MET:HA	2.18	0.57
1:K:398:THR:O	1:K:398:THR:CB	2.51	0.57
1:N:358:THR:O	1:N:358:THR:C	0.40	0.57
1:K:358:THR:O	1:K:358:THR:C	0.40	0.56
1:L:358:THR:O	1:L:358:THR:C	0.40	0.56
1:J:358:THR:O	1:J:358:THR:C	0.40	0.56
2:F:42:GLY:HA2	2:H:169:TYR:HA	1.87	0.56
2:E:5:THR:CB	2:E:5:THR:CA	0.56	0.56
2:G:5:THR:CB	2:G:5:THR:CA	0.56	0.56
2:B:5:THR:CB	2:B:5:THR:CA	0.56	0.56
2:C:5:THR:CB	2:C:5:THR:CA	0.56	0.56
2:D:5:THR:CB	2:D:5:THR:CA	0.56	0.56
2:F:5:THR:CB	2:F:5:THR:CA	0.56	0.56
2:H:5:THR:CB	2:H:5:THR:CA	0.56	0.56
1:M:358:THR:O	1:M:358:THR:C	0.40	0.56
2:A:5:THR:CB	2:A:5:THR:CA	0.56	0.56
1:I:358:THR:O	1:I:358:THR:C	0.40	0.55
2:A:42:GLY:HA2	2:C:169:TYR:HA	1.91	0.53
2:E:42:GLY:HA2	2:G:169:TYR:HA	1.92	0.51

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	I	791/816 (97%)	752 (95%)	32 (4%)	7 (1%)	17 56
1	J	791/816 (97%)	752 (95%)	32 (4%)	7 (1%)	17 56
1	K	791/816 (97%)	752 (95%)	32 (4%)	7 (1%)	17 56
1	L	791/816 (97%)	752 (95%)	32 (4%)	7 (1%)	17 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	791/816 (97%)	752 (95%)	32 (4%)	7 (1%)	17	56
1	N	791/816 (97%)	752 (95%)	32 (4%)	7 (1%)	17	56
2	A	365/373 (98%)	338 (93%)	21 (6%)	6 (2%)	9	45
2	B	365/373 (98%)	338 (93%)	21 (6%)	6 (2%)	9	45
2	C	365/373 (98%)	338 (93%)	21 (6%)	6 (2%)	9	45
2	D	365/373 (98%)	338 (93%)	21 (6%)	6 (2%)	9	45
2	E	365/373 (98%)	338 (93%)	21 (6%)	6 (2%)	9	45
2	F	365/373 (98%)	338 (93%)	21 (6%)	6 (2%)	9	45
2	G	365/373 (98%)	338 (93%)	21 (6%)	6 (2%)	9	45
2	H	365/373 (98%)	338 (93%)	21 (6%)	6 (2%)	9	45
3	O	143/145 (99%)	143 (100%)	0	0	100	100
3	P	143/145 (99%)	143 (100%)	0	0	100	100
3	Q	143/145 (99%)	143 (100%)	0	0	100	100
3	R	143/145 (99%)	143 (100%)	0	0	100	100
3	S	143/145 (99%)	143 (100%)	0	0	100	100
3	T	143/145 (99%)	143 (100%)	0	0	100	100
All	All	8524/8750 (97%)	8074 (95%)	360 (4%)	90 (1%)	18	52

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	359	SER
1	I	641	ILE
1	J	359	SER
1	J	641	ILE
1	K	359	SER
1	K	641	ILE
1	L	359	SER
1	L	641	ILE
1	M	359	SER
1	M	641	ILE
1	N	359	SER
1	N	641	ILE
2	A	33	SER
2	B	33	SER
2	C	33	SER

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Mol	Chain	Res	Type
2	D	33	SER
2	E	33	SER
2	F	33	SER
2	G	33	SER
2	H	33	SER
1	I	40	THR
1	J	40	THR
1	K	40	THR
1	L	40	THR
1	M	40	THR
1	N	40	THR
2	A	16	LEU
2	A	45	VAL
2	A	167	GLU
2	B	16	LEU
2	B	45	VAL
2	B	167	GLU
2	C	16	LEU
2	C	45	VAL
2	C	167	GLU
2	D	16	LEU
2	D	45	VAL
2	D	167	GLU
2	E	16	LEU
2	E	45	VAL
2	E	167	GLU
2	F	16	LEU
2	F	45	VAL
2	F	167	GLU
2	G	16	LEU
2	G	45	VAL
2	G	167	GLU
2	H	16	LEU
2	H	45	VAL
2	H	167	GLU
1	I	637	LYS
1	J	637	LYS
1	K	637	LYS
1	L	637	LYS
1	M	637	LYS
1	N	637	LYS
1	I	119	SER

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Mol	Chain	Res	Type
1	I	328	GLY
1	I	449	SER
1	J	119	SER
1	J	328	GLY
1	J	449	SER
1	K	119	SER
1	K	328	GLY
1	K	449	SER
1	L	119	SER
1	L	328	GLY
1	L	449	SER
1	M	119	SER
1	M	328	GLY
1	M	449	SER
1	N	119	SER
1	N	328	GLY
1	N	449	SER
2	A	333	PRO
2	B	333	PRO
2	C	333	PRO
2	D	333	PRO
2	E	333	PRO
2	F	333	PRO
2	G	333	PRO
2	H	333	PRO
2	A	251	GLY
2	B	251	GLY
2	C	251	GLY
2	D	251	GLY
2	E	251	GLY
2	F	251	GLY
2	G	251	GLY
2	H	251	GLY

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	13
1	J	13
1	K	13
1	L	13
1	M	13
1	N	13
2	A	9
2	B	9
2	C	9
2	D	9
2	E	9
2	F	9
2	G	9
2	H	9
3	O	2
3	P	2
3	Q	2
3	R	2
3	S	2
3	T	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	56:LYS	C	57:LYS	N	1.19
1	J	56:LYS	C	57:LYS	N	1.19
1	K	56:LYS	C	57:LYS	N	1.19
1	L	56:LYS	C	57:LYS	N	1.19
1	M	56:LYS	C	57:LYS	N	1.19
1	N	56:LYS	C	57:LYS	N	1.19
1	A	179:ASP	C	180:LEU	N	1.19
1	A	199:SER	C	200:PHE	N	1.19
1	B	179:ASP	C	180:LEU	N	1.19
1	B	199:SER	C	200:PHE	N	1.19
1	C	179:ASP	C	180:LEU	N	1.19
1	C	199:SER	C	200:PHE	N	1.19
1	D	179:ASP	C	180:LEU	N	1.19
1	D	199:SER	C	200:PHE	N	1.19
1	E	179:ASP	C	180:LEU	N	1.19
1	E	199:SER	C	200:PHE	N	1.19
1	F	179:ASP	C	180:LEU	N	1.19
1	F	199:SER	C	200:PHE	N	1.19
1	G	179:ASP	C	180:LEU	N	1.19
1	G	199:SER	C	200:PHE	N	1.19
1	H	179:ASP	C	180:LEU	N	1.19
1	H	199:SER	C	200:PHE	N	1.19
1	I	641:ILE	C	642:SER	N	1.16
1	J	641:ILE	C	642:SER	N	1.16
1	K	641:ILE	C	642:SER	N	1.16
1	L	641:ILE	C	642:SER	N	1.16
1	M	641:ILE	C	642:SER	N	1.16
1	N	641:ILE	C	642:SER	N	1.16
1	A	369:ILE	C	370:VAL	N	1.16
1	B	369:ILE	C	370:VAL	N	1.16
1	C	369:ILE	C	370:VAL	N	1.16
1	D	369:ILE	C	370:VAL	N	1.16
1	E	369:ILE	C	370:VAL	N	1.16
1	F	369:ILE	C	370:VAL	N	1.16
1	G	369:ILE	C	370:VAL	N	1.16
1	H	369:ILE	C	370:VAL	N	1.16
1	I	4:GLY	C	5:LYS	N	1.14
1	I	816:ALA	C	817:CYS	N	1.14
1	J	4:GLY	C	5:LYS	N	1.14
1	J	816:ALA	C	817:CYS	N	1.14
1	K	4:GLY	C	5:LYS	N	1.14
1	K	816:ALA	C	817:CYS	N	1.14

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	4:GLY	C	5:LYS	N	1.14
1	L	816:ALA	C	817:CYS	N	1.14
1	M	4:GLY	C	5:LYS	N	1.14
1	M	816:ALA	C	817:CYS	N	1.14
1	N	4:GLY	C	5:LYS	N	1.14
1	N	816:ALA	C	817:CYS	N	1.14
1	O	45:GLU	C	46:ALA	N	1.14
1	P	45:GLU	C	46:ALA	N	1.14
1	Q	45:GLU	C	46:ALA	N	1.14
1	R	45:GLU	C	46:ALA	N	1.14
1	S	45:GLU	C	46:ALA	N	1.14
1	T	45:GLU	C	46:ALA	N	1.14
1	I	599:ASP	C	600:ALA	N	1.13
1	J	599:ASP	C	600:ALA	N	1.12
1	K	599:ASP	C	600:ALA	N	1.12
1	L	599:ASP	C	600:ALA	N	1.12
1	M	599:ASP	C	600:ALA	N	1.12
1	N	599:ASP	C	600:ALA	N	1.12
1	O	114:GLU	C	115:LYS	N	1.12
1	P	114:GLU	C	115:LYS	N	1.12
1	Q	114:GLU	C	115:LYS	N	1.12
1	R	114:GLU	C	115:LYS	N	1.12
1	S	114:GLU	C	115:LYS	N	1.12
1	T	114:GLU	C	115:LYS	N	1.12
1	I	118:LYS	C	119:SER	N	1.11
1	J	118:LYS	C	119:SER	N	1.11
1	K	118:LYS	C	119:SER	N	1.11
1	L	118:LYS	C	119:SER	N	1.11
1	M	118:LYS	C	119:SER	N	1.11
1	N	118:LYS	C	119:SER	N	1.11
1	I	772:SER	C	773:ASP	N	1.10
1	J	772:SER	C	773:ASP	N	1.10
1	K	772:SER	C	773:ASP	N	1.10
1	L	772:SER	C	773:ASP	N	1.10
1	M	772:SER	C	773:ASP	N	1.10
1	N	772:SER	C	773:ASP	N	1.10
1	I	357:SER	C	358:THR	N	1.08
1	J	357:SER	C	358:THR	N	1.08
1	K	357:SER	C	358:THR	N	1.08
1	L	357:SER	C	358:THR	N	1.08
1	M	357:SER	C	358:THR	N	1.08
1	N	357:SER	C	358:THR	N	1.08

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	174:THR	C	175:GLY	N	1.05
1	J	174:THR	C	175:GLY	N	1.05
1	K	174:THR	C	175:GLY	N	1.05
1	L	174:THR	C	175:GLY	N	1.05
1	M	174:THR	C	175:GLY	N	1.05
1	N	174:THR	C	175:GLY	N	1.05
1	A	109:PRO	C	110:LEU	N	1.05
1	B	109:PRO	C	110:LEU	N	1.05
1	C	109:PRO	C	110:LEU	N	1.05
1	D	109:PRO	C	110:LEU	N	1.05
1	E	109:PRO	C	110:LEU	N	1.05
1	F	109:PRO	C	110:LEU	N	1.05
1	G	109:PRO	C	110:LEU	N	1.05
1	H	109:PRO	C	110:LEU	N	1.05
1	I	119:SER	C	120:LEU	N	1.01
1	J	119:SER	C	120:LEU	N	1.01
1	K	119:SER	C	120:LEU	N	1.01
1	L	119:SER	C	120:LEU	N	1.01
1	M	119:SER	C	120:LEU	N	1.01
1	N	119:SER	C	120:LEU	N	1.01
1	A	32:PRO	C	33:SER	N	1.01
1	B	32:PRO	C	33:SER	N	1.01
1	C	32:PRO	C	33:SER	N	1.01
1	D	32:PRO	C	33:SER	N	1.01
1	E	32:PRO	C	33:SER	N	1.01
1	F	32:PRO	C	33:SER	N	1.01
1	G	32:PRO	C	33:SER	N	1.01
1	H	32:PRO	C	33:SER	N	1.01
1	I	553:ASP	C	554:HIS	N	0.98
1	J	553:ASP	C	554:HIS	N	0.98
1	K	553:ASP	C	554:HIS	N	0.98
1	L	553:ASP	C	554:HIS	N	0.98
1	M	553:ASP	C	554:HIS	N	0.98
1	N	553:ASP	C	554:HIS	N	0.98
1	A	45:VAL	C	46:GLY	N	0.95
1	B	45:VAL	C	46:GLY	N	0.95
1	C	45:VAL	C	46:GLY	N	0.95
1	D	45:VAL	C	46:GLY	N	0.95
1	E	45:VAL	C	46:GLY	N	0.95
1	F	45:VAL	C	46:GLY	N	0.95
1	G	45:VAL	C	46:GLY	N	0.95
1	H	45:VAL	C	46:GLY	N	0.95

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	370:VAL	C	371:HIS	N	0.94
1	B	370:VAL	C	371:HIS	N	0.94
1	C	370:VAL	C	371:HIS	N	0.94
1	D	370:VAL	C	371:HIS	N	0.94
1	E	370:VAL	C	371:HIS	N	0.94
1	F	370:VAL	C	371:HIS	N	0.94
1	G	370:VAL	C	371:HIS	N	0.94
1	H	370:VAL	C	371:HIS	N	0.94
1	A	307:PRO	C	308:GLY	N	0.92
1	B	307:PRO	C	308:GLY	N	0.92
1	C	307:PRO	C	308:GLY	N	0.92
1	D	307:PRO	C	308:GLY	N	0.92
1	E	307:PRO	C	308:GLY	N	0.92
1	F	307:PRO	C	308:GLY	N	0.92
1	G	307:PRO	C	308:GLY	N	0.92
1	H	307:PRO	C	308:GLY	N	0.92
1	I	175:GLY	C	176:GLN	N	0.83
1	J	175:GLY	C	176:GLN	N	0.83
1	K	175:GLY	C	176:GLN	N	0.83
1	L	175:GLY	C	176:GLN	N	0.83
1	M	175:GLY	C	176:GLN	N	0.83
1	N	175:GLY	C	176:GLN	N	0.83
1	I	358:THR	C	359:SER	N	0.81
1	J	358:THR	C	359:SER	N	0.81
1	K	358:THR	C	359:SER	N	0.81
1	L	358:THR	C	359:SER	N	0.81
1	M	358:THR	C	359:SER	N	0.81
1	N	358:THR	C	359:SER	N	0.81
1	A	44:MET	C	45:VAL	N	0.81
1	B	44:MET	C	45:VAL	N	0.81
1	C	44:MET	C	45:VAL	N	0.81
1	D	44:MET	C	45:VAL	N	0.81
1	E	44:MET	C	45:VAL	N	0.81
1	F	44:MET	C	45:VAL	N	0.81
1	G	44:MET	C	45:VAL	N	0.81
1	H	44:MET	C	45:VAL	N	0.81

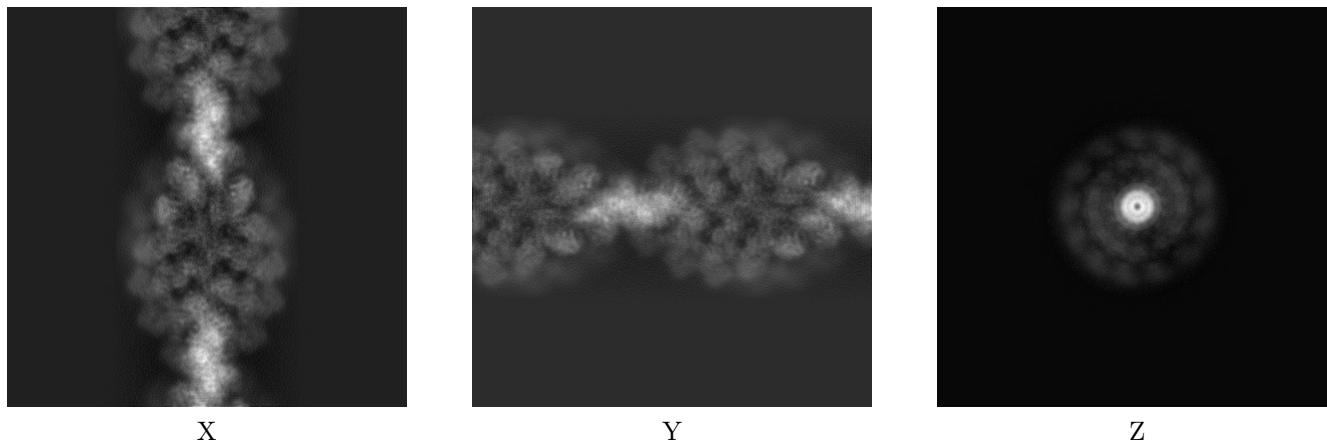
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7116. These allow visual inspection of the internal detail of the map and identification of artifacts.

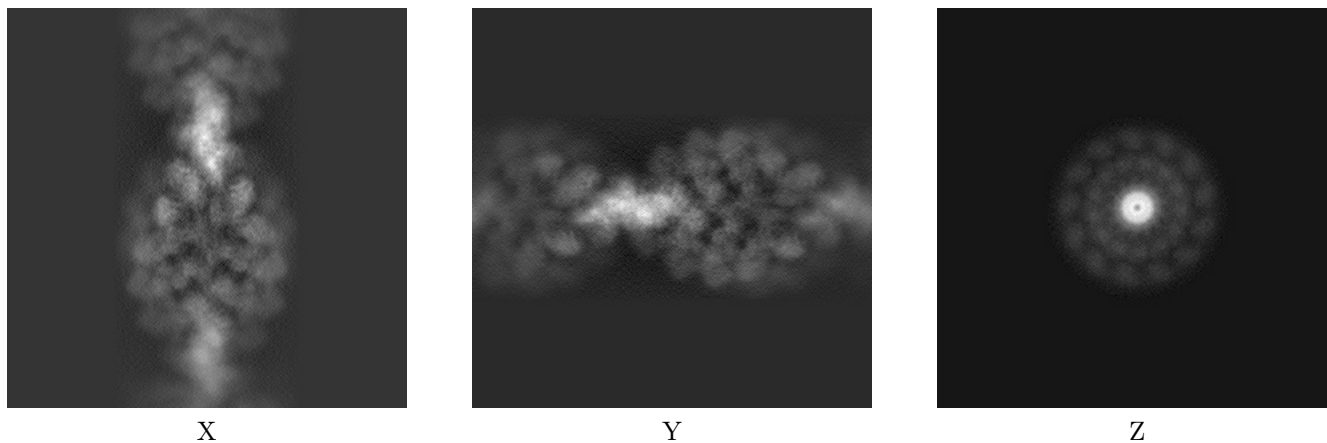
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



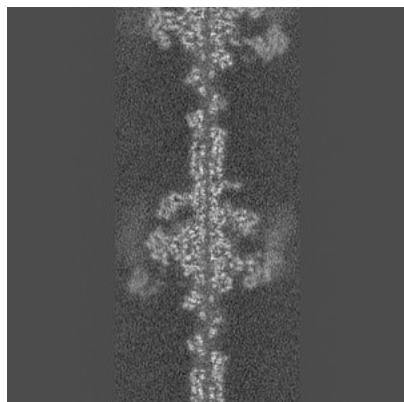
6.1.2 Raw map



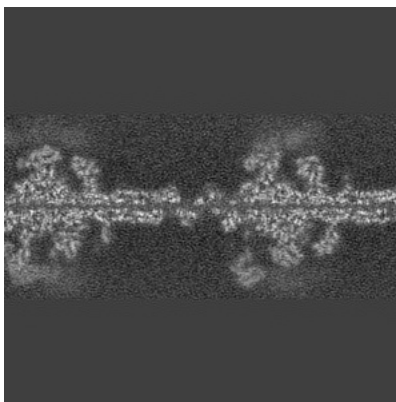
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 256

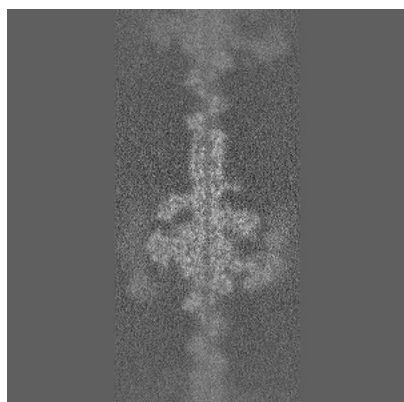


Y Index: 256

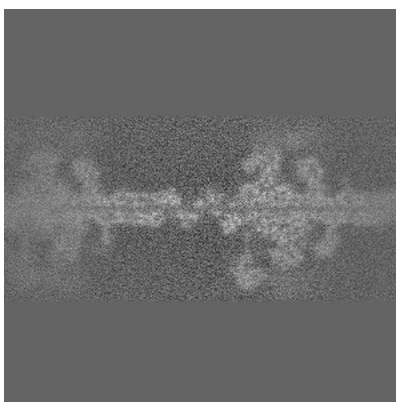


Z Index: 256

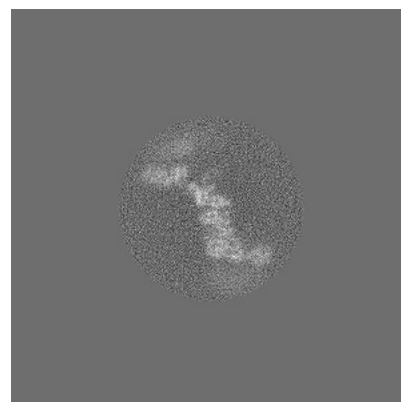
6.2.2 Raw map



X Index: 256



Y Index: 256

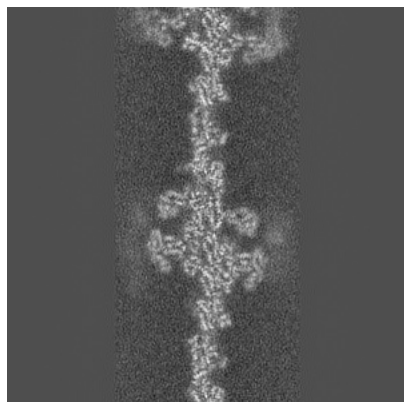


Z Index: 256

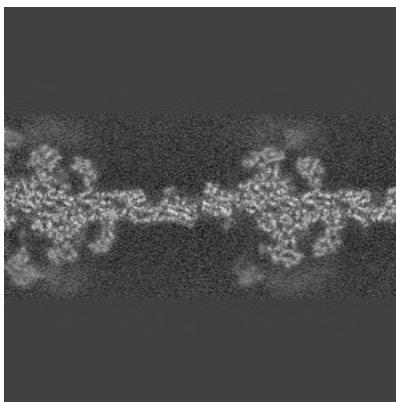
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

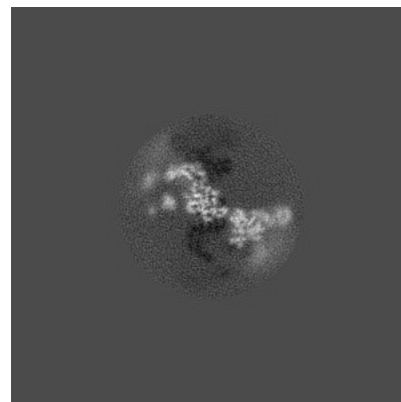
6.3.1 Primary map



X Index: 262

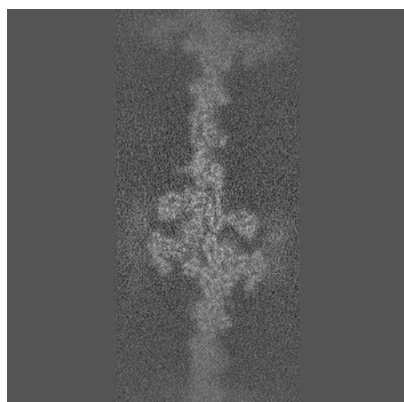


Y Index: 251

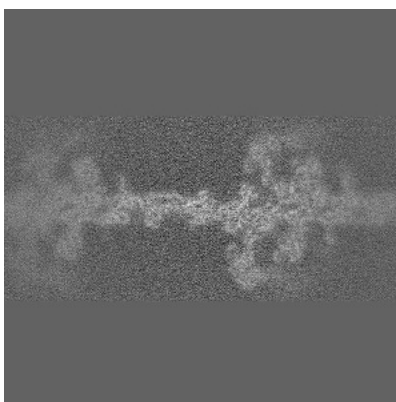


Z Index: 1

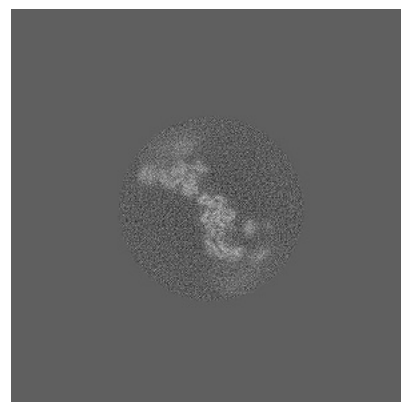
6.3.2 Raw map



X Index: 263



Y Index: 262

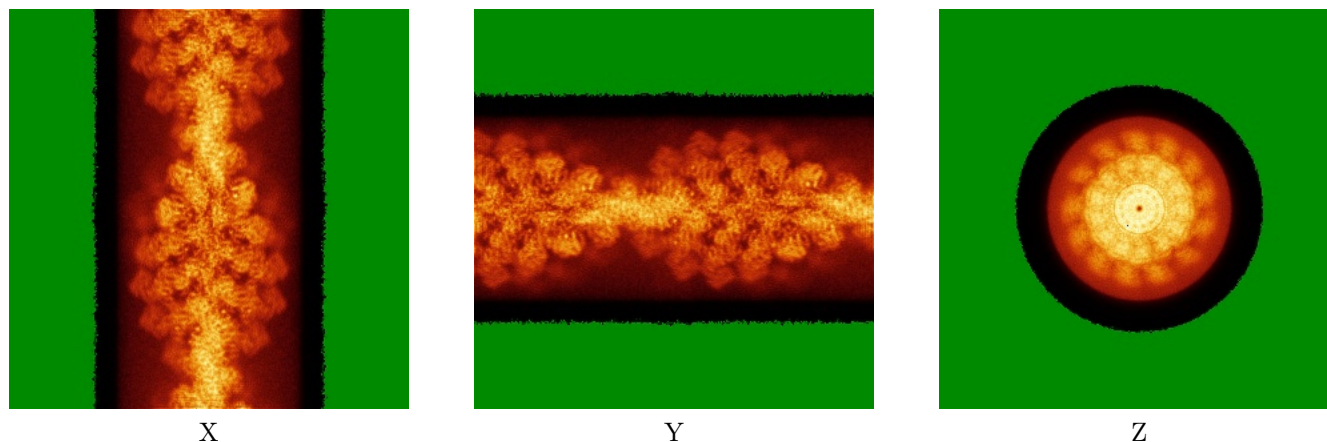


Z Index: 265

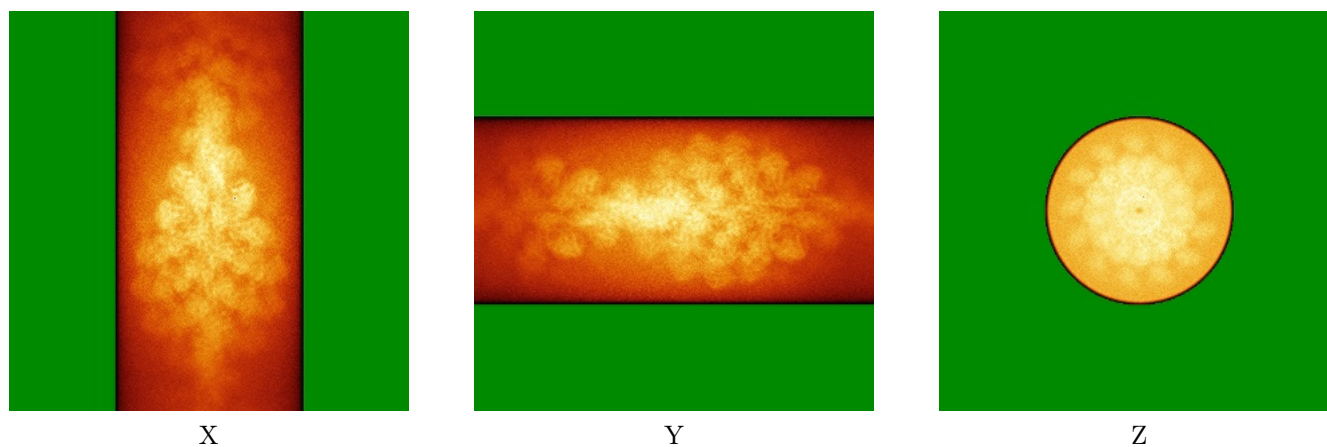
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



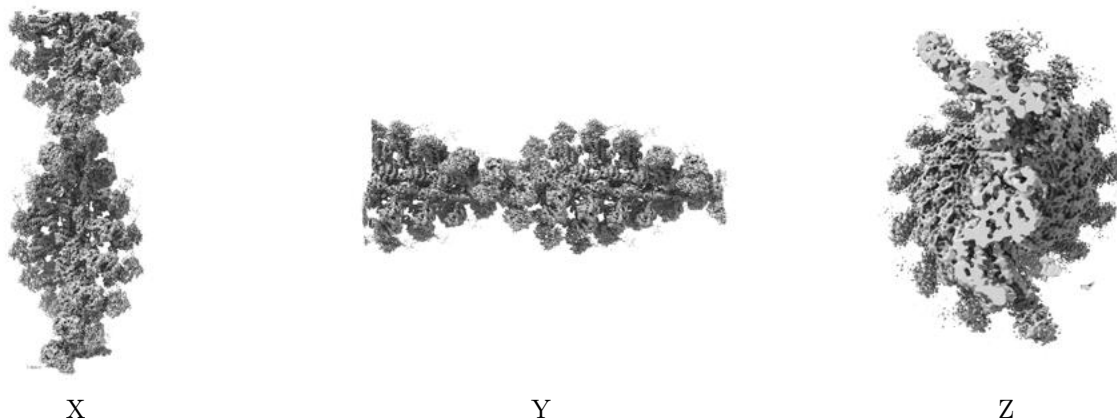
6.4.2 Raw map



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

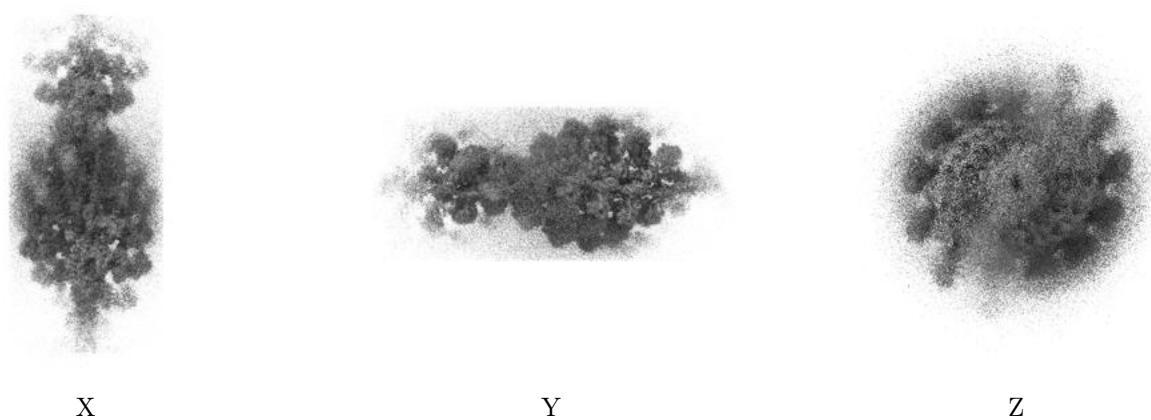
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.0. 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 shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

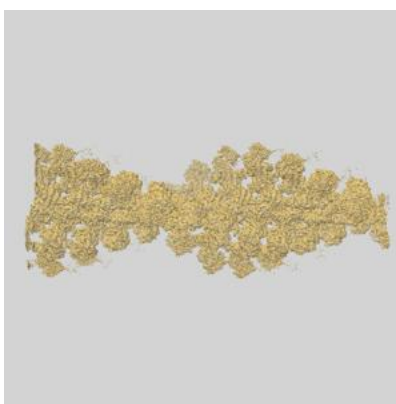
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

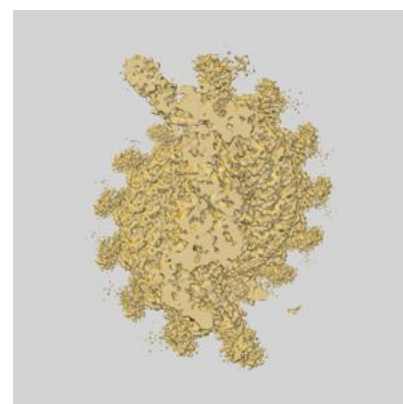
6.6.1 emd_7116_msk_2.map [i](#)



X



Y

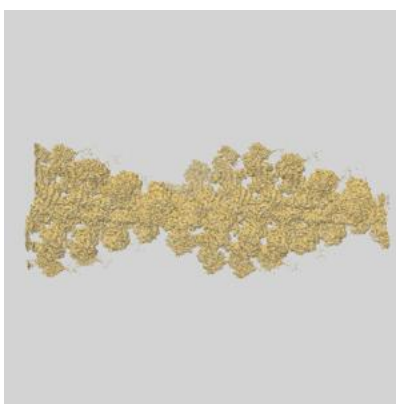


Z

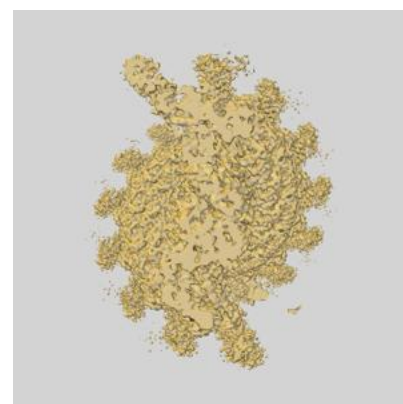
6.6.2 emd_7116_msk_1.map [i](#)



X



Y

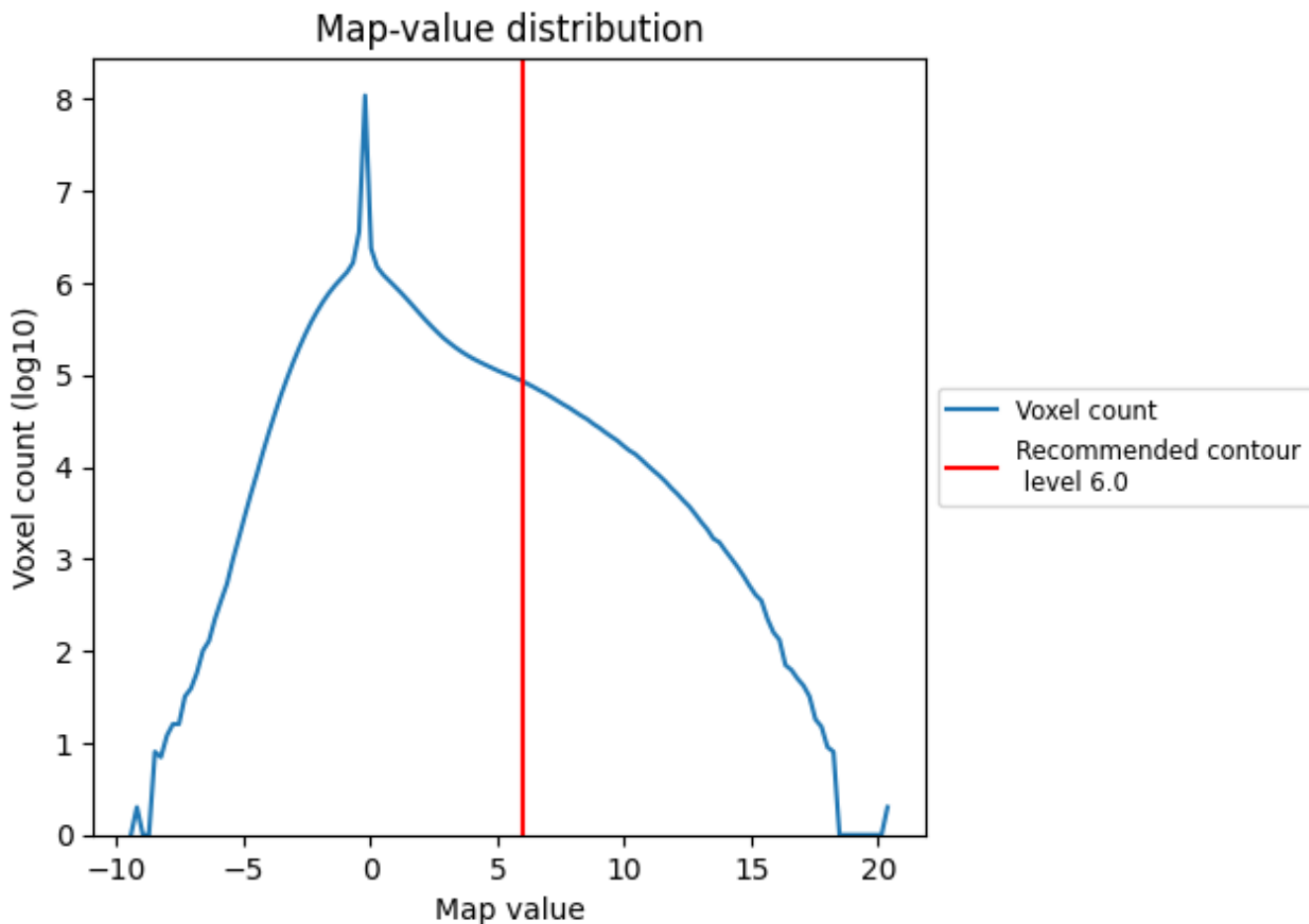


Z

7 Map analysis [i](#)

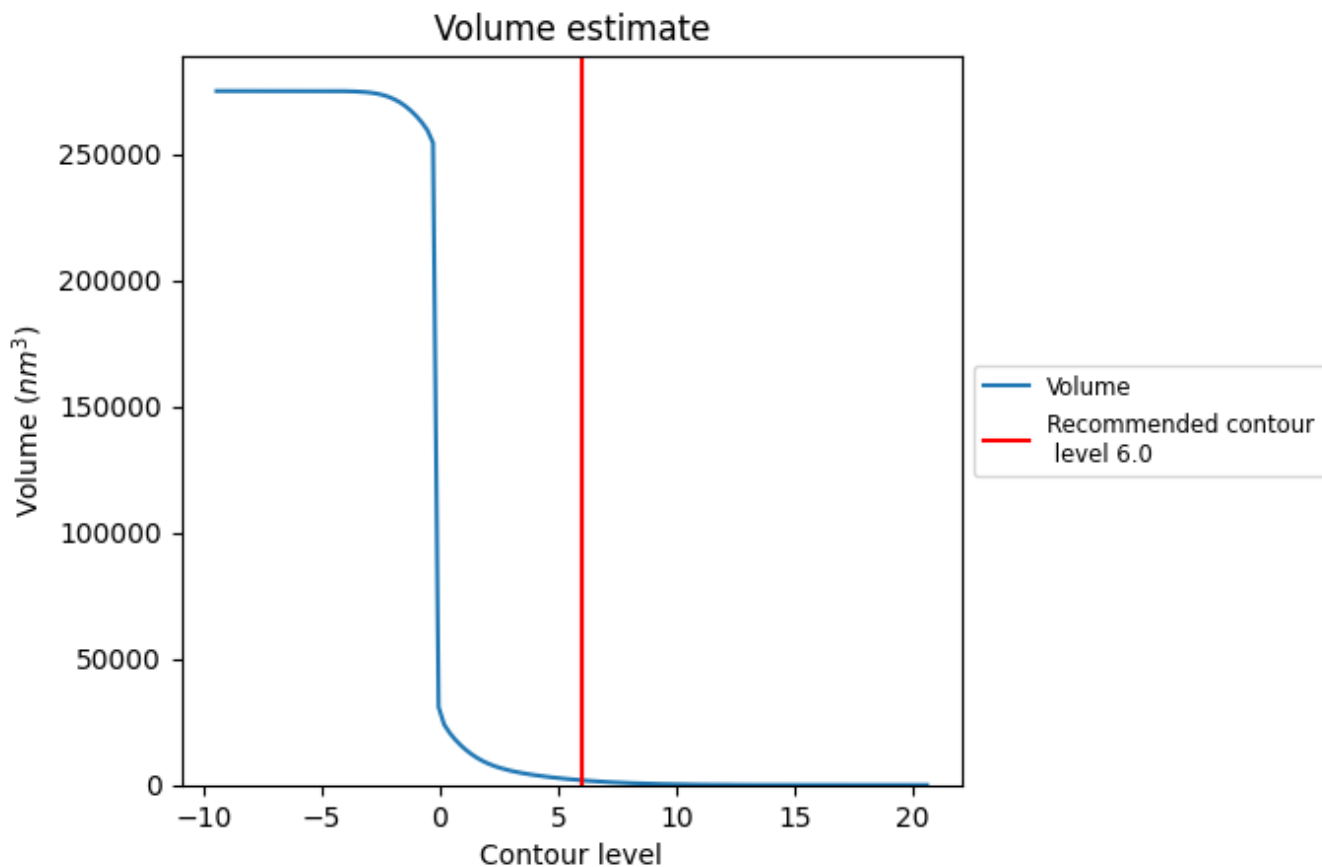
This section contains the results of statistical analysis of the map.

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.

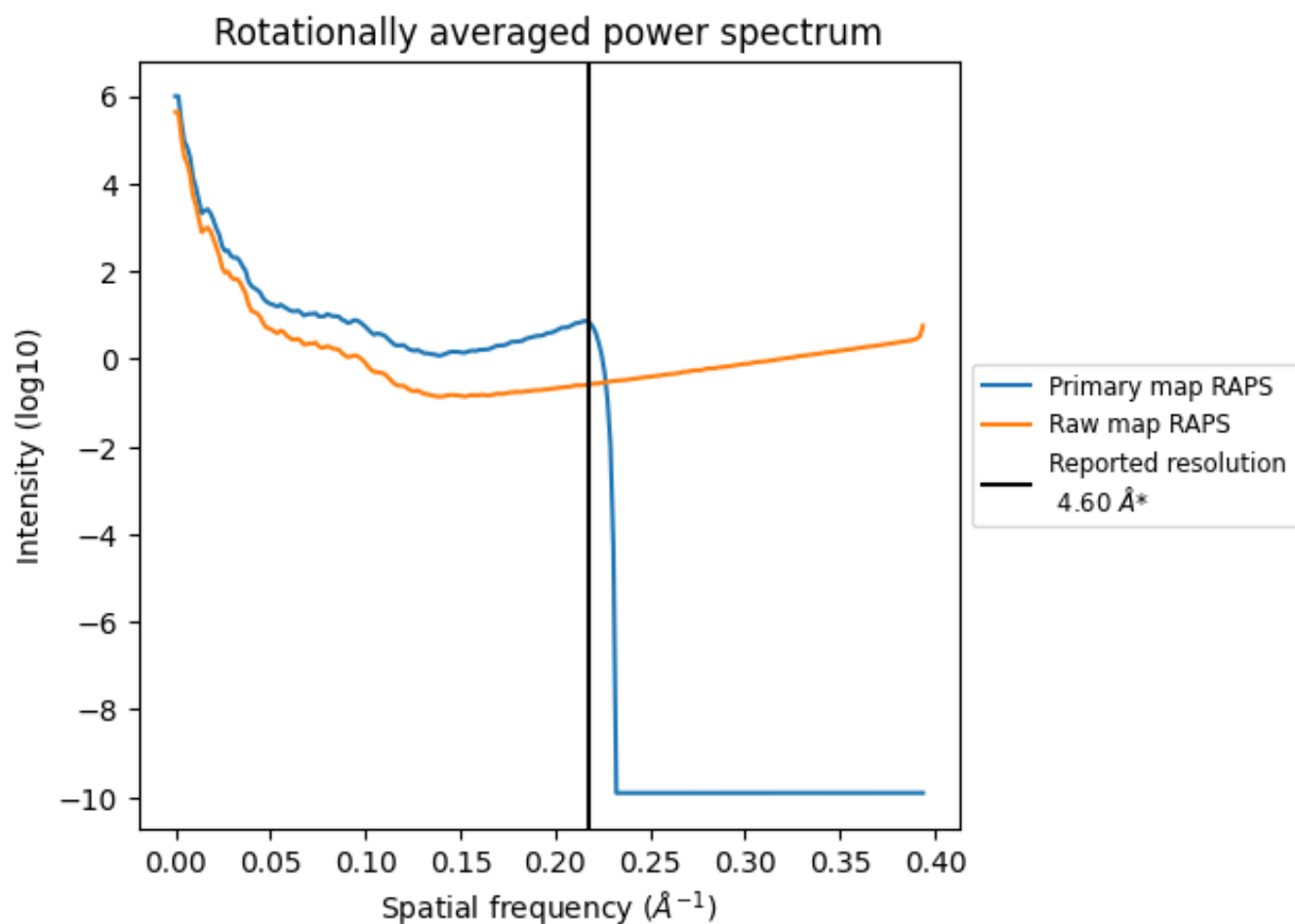
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1866 nm^3 ; this corresponds to an approximate mass of 1686 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

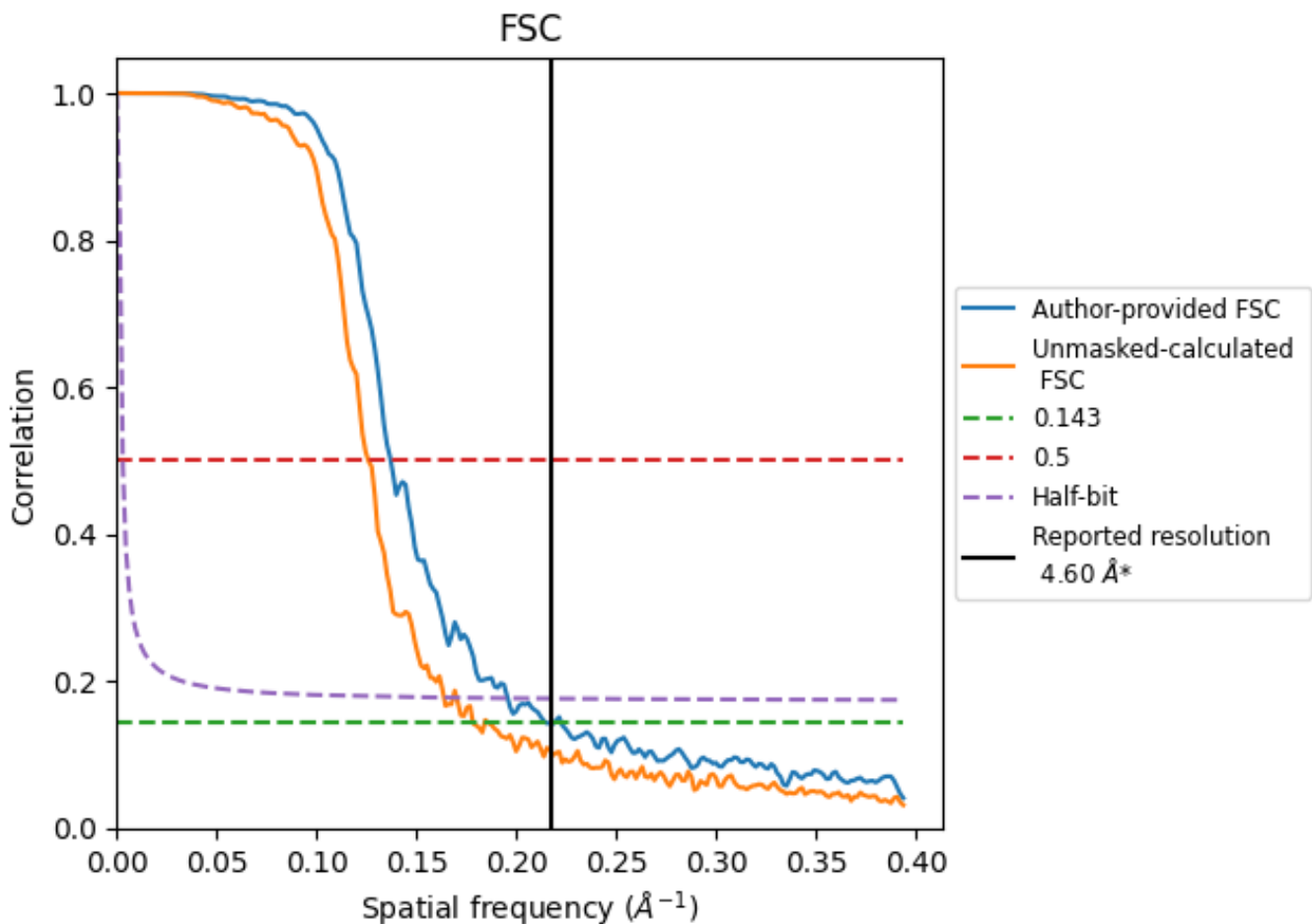


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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 0.217 Å⁻¹

8.2 Resolution estimates [i](#)

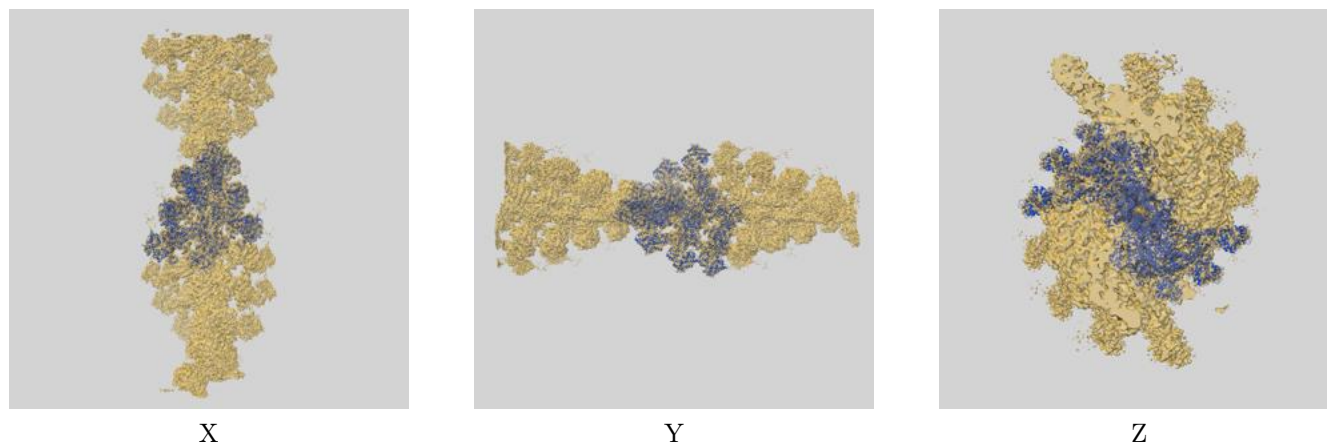
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.66	7.29	5.11
Unmasked-calculated*	5.61	7.94	6.11

*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 5.61 differs from the reported value 4.6 by more than 10 %

9 Map-model fit [i](#)

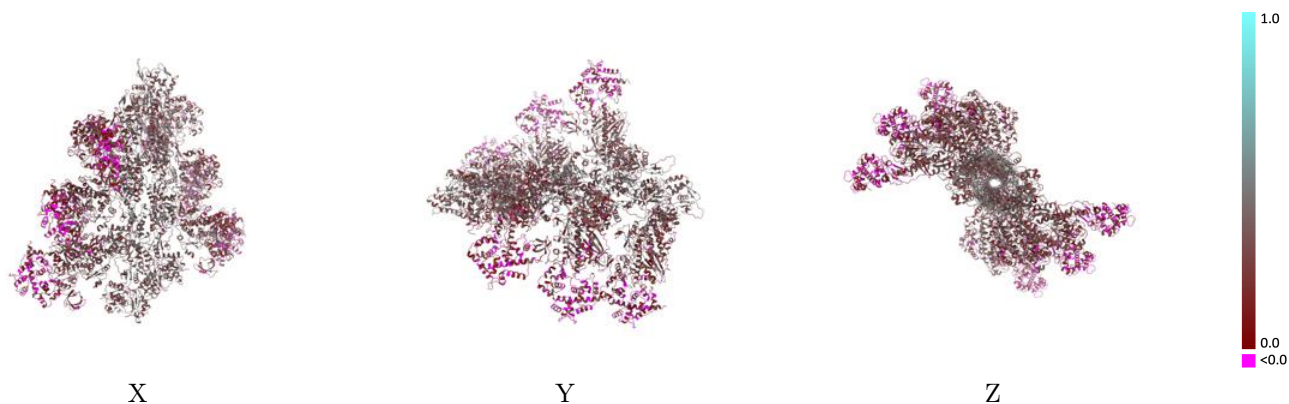
This section contains information regarding the fit between EMDB map EMD-7116 and PDB model 6BNV. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



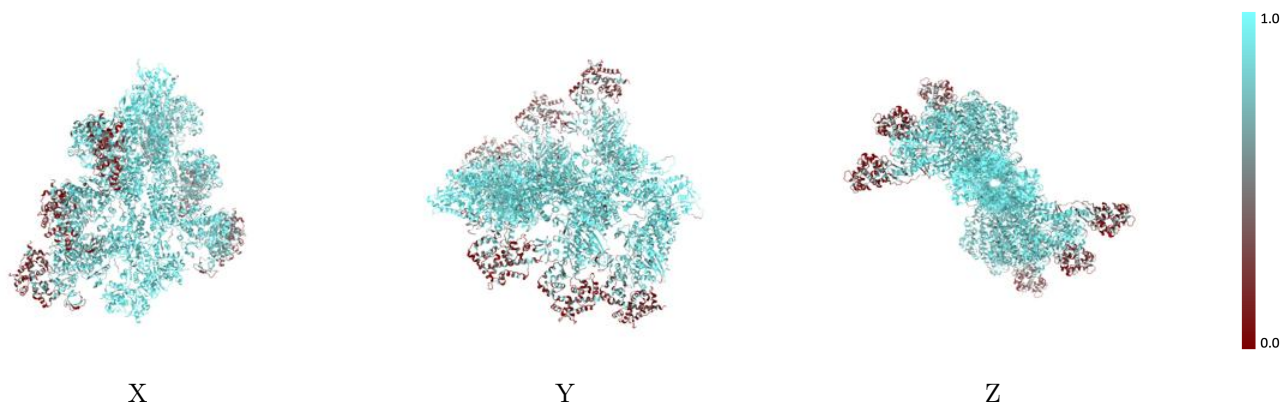
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



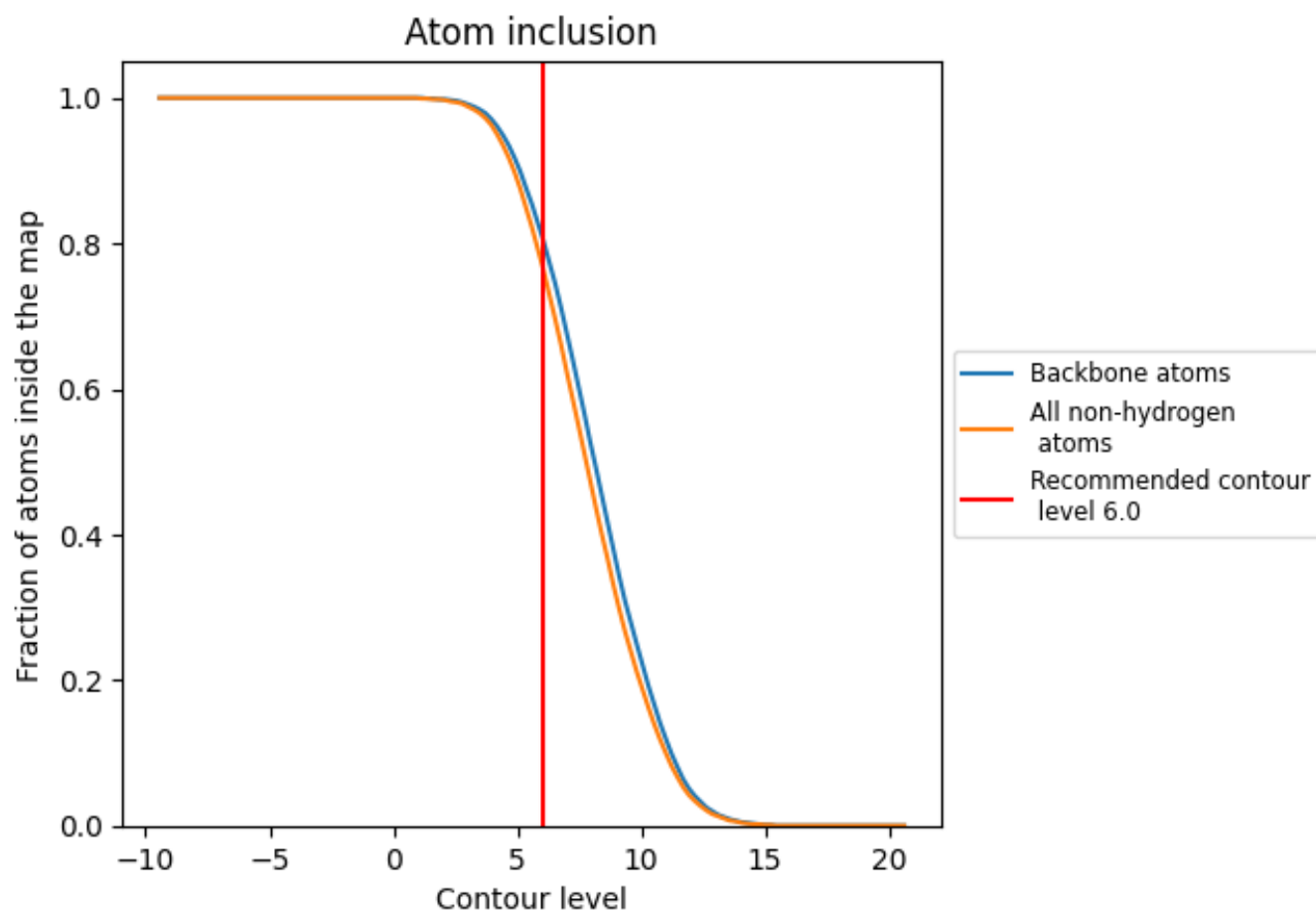
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.0).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 77% 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 (6.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7710	 0.2710
A	 0.9520	 0.3590
B	 0.9500	 0.3640
C	 0.9510	 0.3630
D	 0.9500	 0.3610
E	 0.9470	 0.3610
F	 0.9500	 0.3610
G	 0.9510	 0.3640
H	 0.9500	 0.3630
I	 0.7590	 0.2460
J	 0.7590	 0.2470
K	 0.7630	 0.2430
L	 0.7620	 0.2460
M	 0.7640	 0.2490
N	 0.7590	 0.2520
O	 0.2100	 0.0920
P	 0.2240	 0.0850
Q	 0.2380	 0.0870
R	 0.2220	 0.0910
S	 0.2220	 0.1050
T	 0.2150	 0.0940

