



Full wwPDB EM Validation Report ⓘ

Mar 3, 2024 – 08:38 AM EST

PDB ID : 6BNW
EMDB ID : EMD-7117
Title : CryoEM structure of Myosin VI-Actin complex in the ADP state, backbone-averaged with side chains truncated to alanine
Authors : Gurel, P.G.; Alushin, G.M.
Deposited on : 2017-11-17
Resolution : 5.50 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:

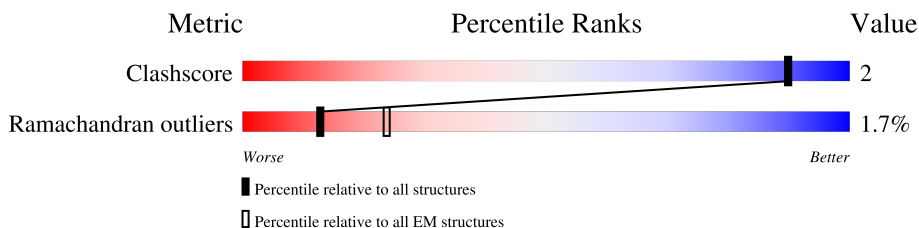
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 5.50 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	
1	J	816	
1	K	816	
1	L	816	
1	M	816	
1	N	816	
2	A	373	
2	B	373	
2	C	373	

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Mol	Chain	Length	Quality of chain
2	D	373	 91% 6% ..
2	E	373	 91% 6% ..
2	F	373	 91% 6% ..
2	G	373	 91% 6% ..
2	H	373	 91% 6% ..

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 37398 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
			Total	C	N	O		
1	I	774	3825	2278	774	773	0	0
1	J	774	3825	2278	774	773	0	0
1	K	774	3825	2278	774	773	0	0
1	L	774	3825	2278	774	773	0	0
1	M	774	3825	2278	774	773	0	0
1	N	774	3825	2278	774	773	0	0

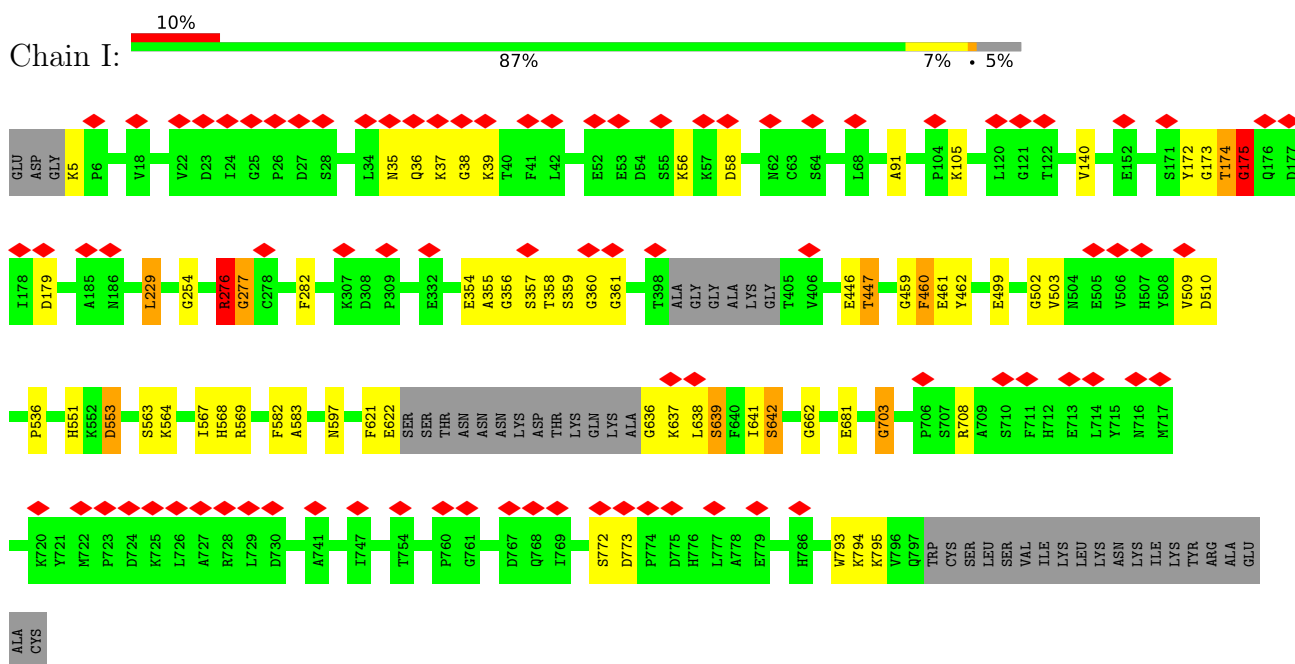
- Molecule 2 is a protein called Actin, alpha skeletal muscle.

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

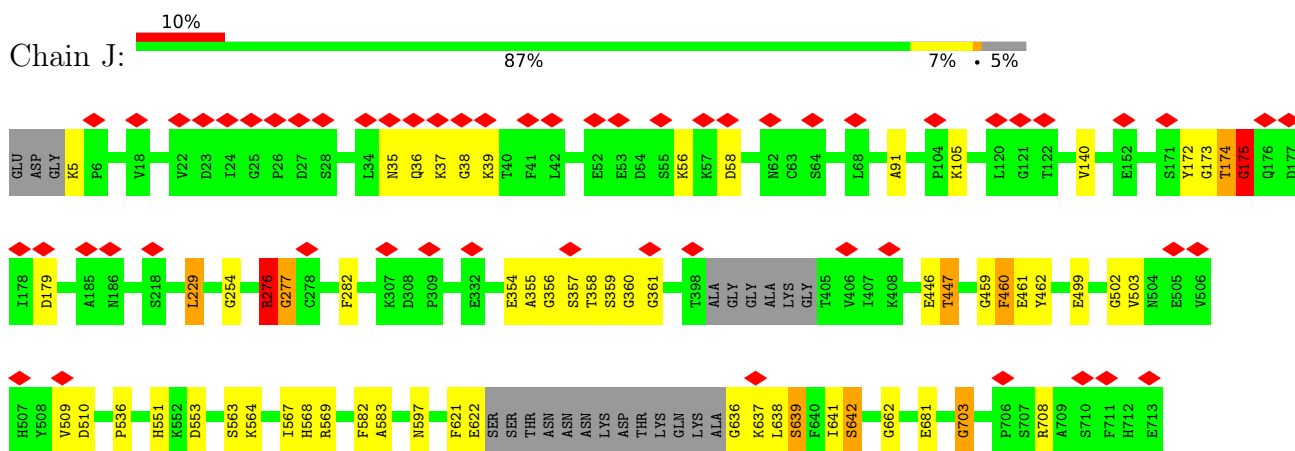
3 Residue-property plots

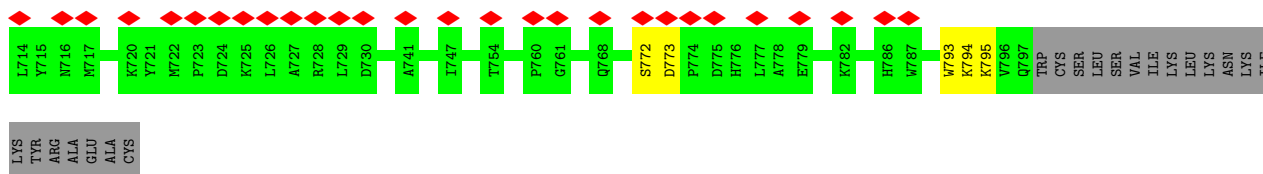
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Unconventional myosin-VI

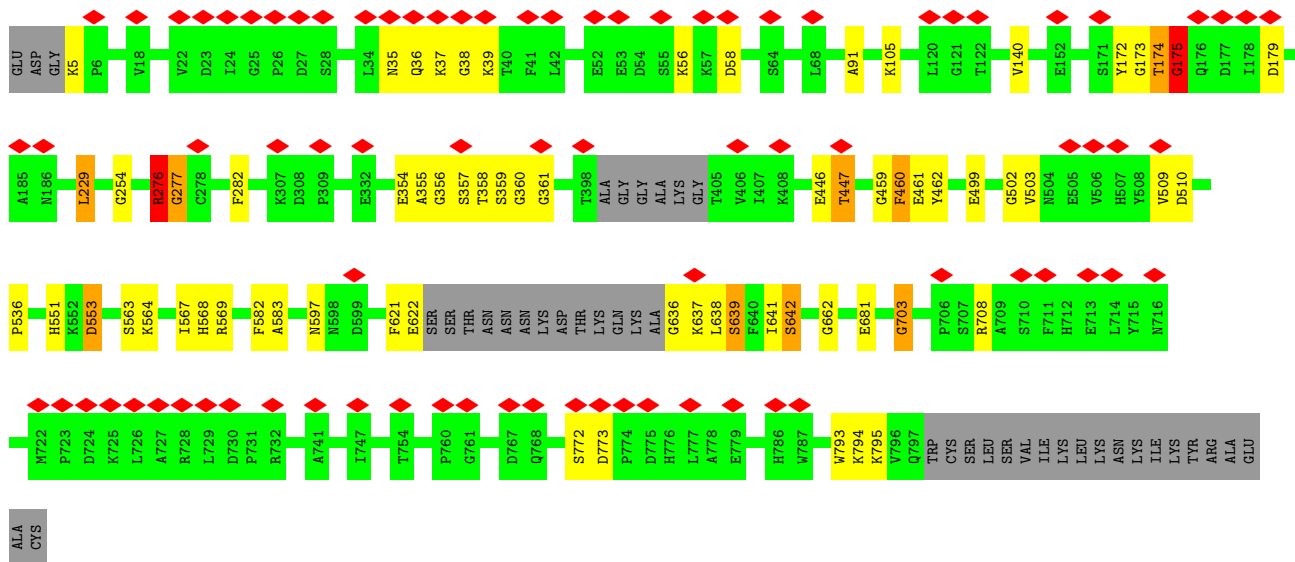
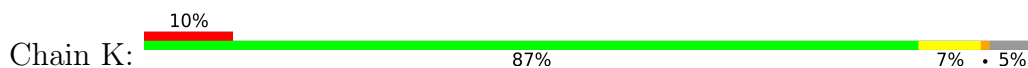


• Molecule 1: Unconventional myosin-VI

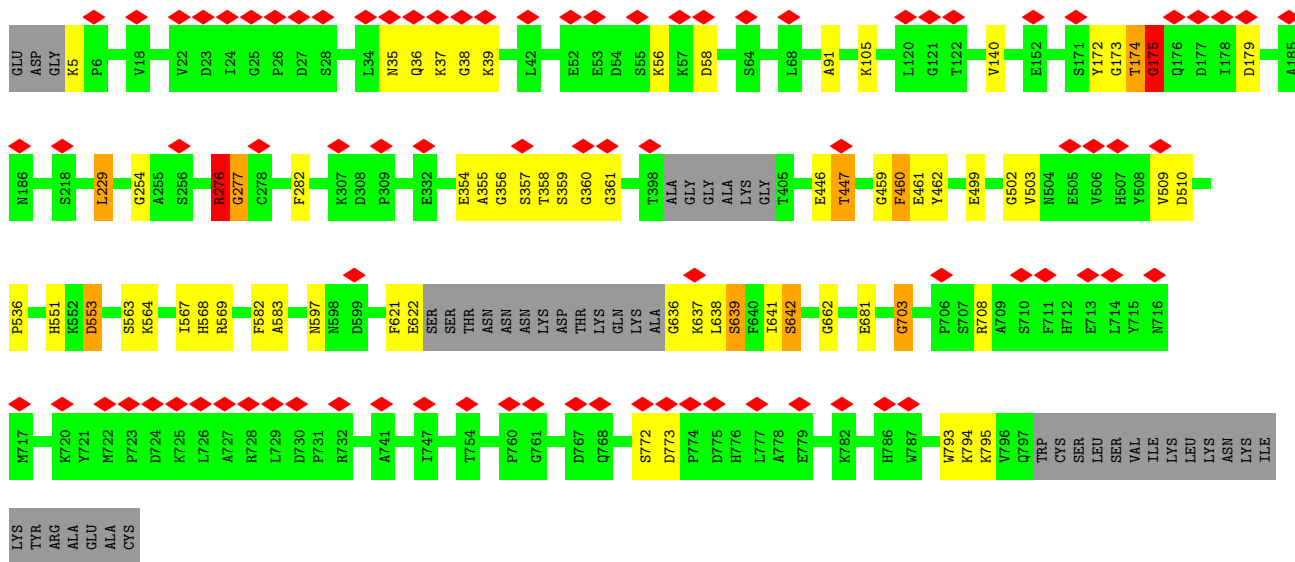
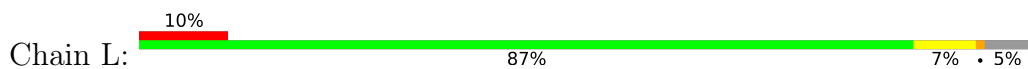




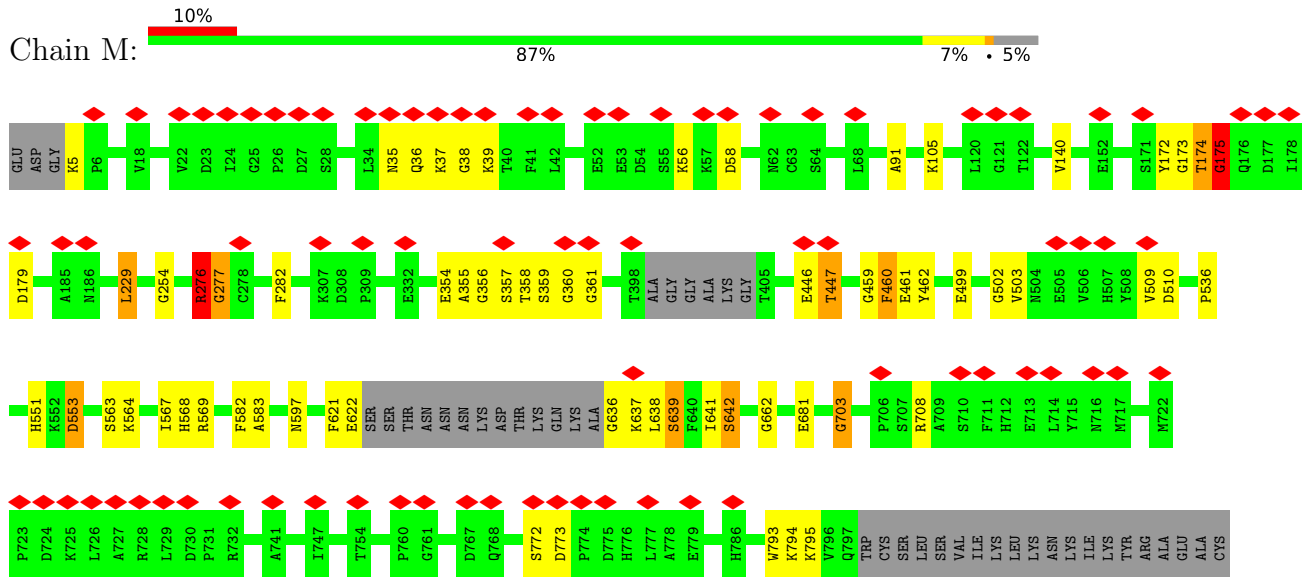
• Molecule 1: Unconventional myosin-VI



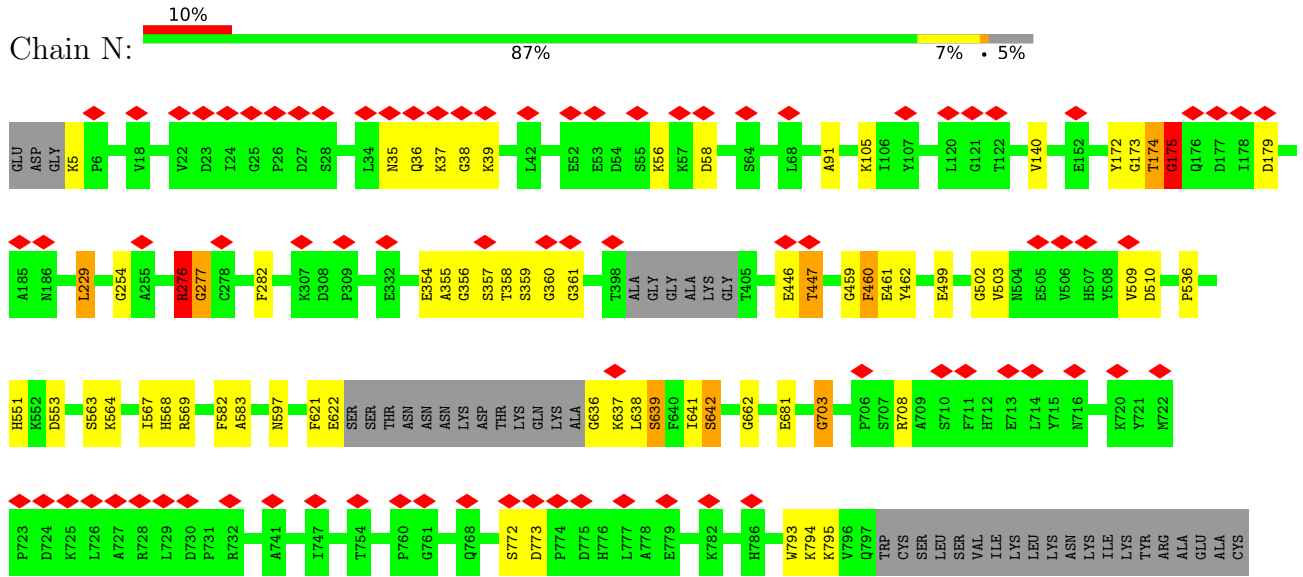
• Molecule 1: Unconventional myosin-VI



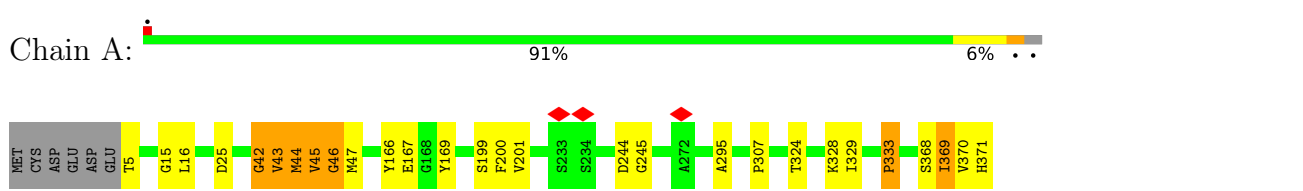
• Molecule 1: Unconventional myosin-VI



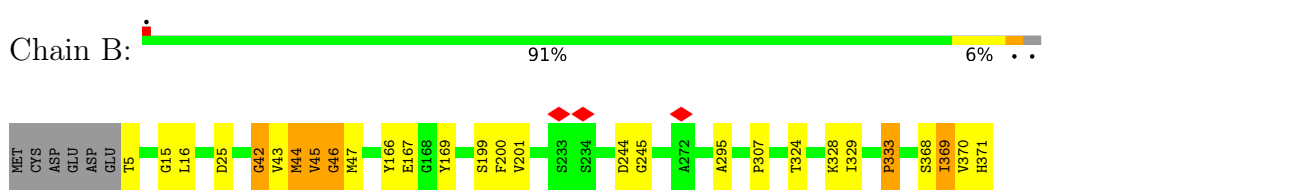
• Molecule 1: Unconventional myosin-VI



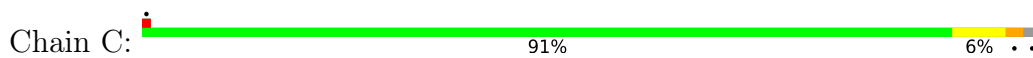
• Molecule 2: Actin, alpha skeletal muscle



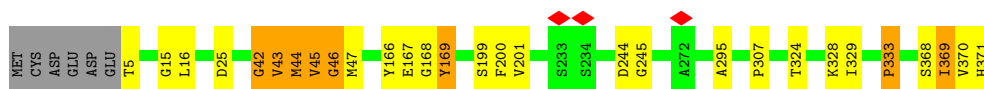
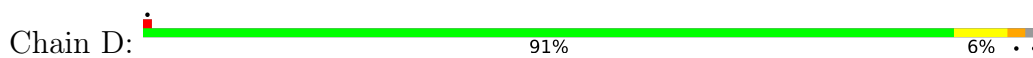
• Molecule 2: Actin, alpha skeletal muscle



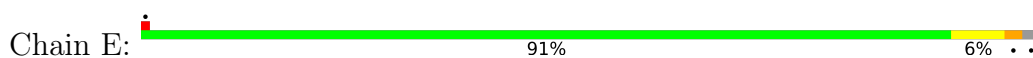
- Molecule 2: Actin, alpha skeletal muscle



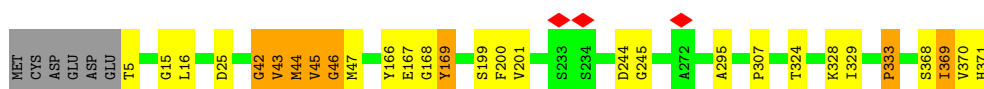
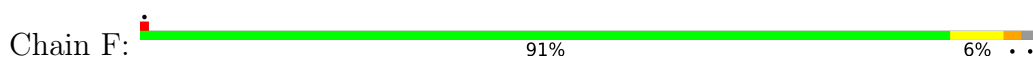
- Molecule 2: Actin, alpha skeletal muscle



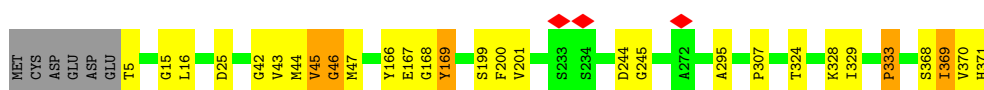
- Molecule 2: Actin, alpha skeletal muscle



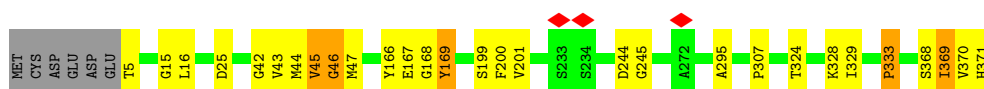
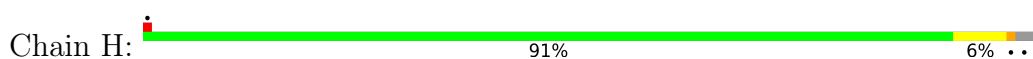
- Molecule 2: Actin, alpha skeletal muscle



- Molecule 2: Actin, alpha skeletal muscle



- Molecule 2: Actin, alpha skeletal muscle



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-166.69°, rise=28.06 Å, axial sym=C1	Depositor
Number of segments used	36114	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	18.043	Depositor
Minimum map value	-7.049	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.8	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	2.89	137/3822 (3.6%)	2.00	81/5320 (1.5%)
1	J	2.89	137/3822 (3.6%)	2.00	80/5320 (1.5%)
1	K	2.89	136/3822 (3.6%)	2.00	81/5320 (1.5%)
1	L	2.89	137/3822 (3.6%)	2.00	81/5320 (1.5%)
1	M	2.89	137/3822 (3.6%)	2.00	81/5320 (1.5%)
1	N	2.89	136/3822 (3.6%)	2.00	81/5320 (1.5%)
2	A	2.22	48/1805 (2.7%)	1.36	22/2509 (0.9%)
2	B	2.22	48/1805 (2.7%)	1.36	22/2509 (0.9%)
2	C	2.22	47/1805 (2.6%)	1.36	22/2509 (0.9%)
2	D	2.22	48/1805 (2.7%)	1.36	22/2509 (0.9%)
2	E	2.22	48/1805 (2.7%)	1.36	22/2509 (0.9%)
2	F	2.22	48/1805 (2.7%)	1.36	22/2509 (0.9%)
2	G	2.21	48/1805 (2.7%)	1.36	22/2509 (0.9%)
2	H	2.22	48/1805 (2.7%)	1.36	22/2509 (0.9%)
All	All	2.65	1203/37372 (3.2%)	1.78	661/51992 (1.3%)

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
1	N	0	1
All	All	0	6

All (1203) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	276	ARG	C-O	-42.26	0.43	1.23
1	M	276	ARG	C-O	-42.25	0.43	1.23
1	N	276	ARG	C-O	-42.23	0.43	1.23
1	I	276	ARG	C-O	-42.23	0.43	1.23
1	K	276	ARG	C-O	-42.19	0.43	1.23
1	J	276	ARG	C-O	-42.19	0.43	1.23
1	L	174	THR	C-N	-38.59	0.63	1.33
1	I	174	THR	C-N	-38.58	0.63	1.33
1	K	174	THR	C-N	-38.57	0.63	1.33
1	N	174	THR	C-N	-38.56	0.63	1.33
1	M	174	THR	C-N	-38.54	0.63	1.33
1	J	174	THR	C-N	-38.53	0.63	1.33
1	I	174	THR	C-O	-37.97	0.51	1.23
1	L	174	THR	C-O	-37.96	0.51	1.23
1	M	174	THR	C-O	-37.94	0.51	1.23
1	J	174	THR	C-O	-37.94	0.51	1.23
1	N	174	THR	C-O	-37.92	0.51	1.23
1	K	174	THR	C-O	-37.86	0.51	1.23
1	I	772	SER	C-O	-33.97	0.58	1.23
1	J	772	SER	C-O	-33.97	0.58	1.23
1	M	772	SER	C-O	-33.97	0.58	1.23
1	N	772	SER	C-O	-33.94	0.58	1.23
1	K	772	SER	C-O	-33.93	0.58	1.23
1	L	772	SER	C-O	-33.92	0.58	1.23
1	N	641	ILE	C-O	-32.77	0.61	1.23
1	M	641	ILE	C-O	-32.75	0.61	1.23
1	K	641	ILE	C-O	-32.75	0.61	1.23
1	I	641	ILE	C-O	-32.73	0.61	1.23
1	J	641	ILE	C-O	-32.72	0.61	1.23
1	L	641	ILE	C-O	-32.71	0.61	1.23
1	L	446	GLU	C-O	-31.53	0.63	1.23
1	N	446	GLU	C-O	-31.52	0.63	1.23
1	J	446	GLU	C-O	-31.49	0.63	1.23
1	K	446	GLU	C-O	-31.48	0.63	1.23
1	M	446	GLU	C-O	-31.47	0.63	1.23
1	I	446	GLU	C-O	-31.44	0.63	1.23
1	K	359	SER	C-O	-31.32	0.63	1.23
1	N	359	SER	C-O	-31.30	0.63	1.23
1	J	359	SER	C-O	-31.28	0.64	1.23
1	I	359	SER	C-O	-31.27	0.64	1.23
1	L	359	SER	C-O	-31.27	0.64	1.23
1	M	359	SER	C-O	-31.26	0.64	1.23
1	N	502	GLY	C-O	-30.18	0.75	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	502	GLY	C-O	-30.16	0.75	1.23
1	J	502	GLY	C-O	-30.16	0.75	1.23
1	M	502	GLY	C-O	-30.15	0.75	1.23
1	L	502	GLY	C-O	-30.14	0.75	1.23
1	I	502	GLY	C-O	-30.11	0.75	1.23
1	I	553	ASP	C-O	-29.91	0.66	1.23
1	J	553	ASP	C-O	-29.86	0.66	1.23
1	K	553	ASP	C-O	-29.84	0.66	1.23
1	M	553	ASP	C-O	-29.82	0.66	1.23
1	L	553	ASP	C-O	-29.80	0.66	1.23
1	N	553	ASP	C-O	-29.79	0.66	1.23
2	G	45	VAL	C-O	-29.69	0.67	1.23
2	A	45	VAL	C-O	-29.67	0.67	1.23
2	F	45	VAL	C-O	-29.66	0.67	1.23
2	H	45	VAL	C-O	-29.66	0.67	1.23
2	C	45	VAL	C-O	-29.65	0.67	1.23
2	D	45	VAL	C-O	-29.65	0.67	1.23
2	E	45	VAL	C-O	-29.65	0.67	1.23
2	B	45	VAL	C-O	-29.63	0.67	1.23
1	M	636	GLY	C-O	-29.02	0.77	1.23
1	J	636	GLY	C-O	-28.99	0.77	1.23
1	K	636	GLY	C-O	-28.97	0.77	1.23
1	N	636	GLY	C-O	-28.97	0.77	1.23
1	L	636	GLY	C-O	-28.97	0.77	1.23
1	I	636	GLY	C-O	-28.93	0.77	1.23
1	N	361	GLY	C-O	-27.62	0.79	1.23
1	I	361	GLY	C-O	-27.60	0.79	1.23
1	L	361	GLY	C-O	-27.57	0.79	1.23
1	M	361	GLY	C-O	-27.57	0.79	1.23
1	K	361	GLY	C-O	-27.55	0.79	1.23
1	J	361	GLY	C-O	-27.52	0.79	1.23
1	K	638	LEU	C-O	-27.38	0.71	1.23
1	N	638	LEU	C-O	-27.36	0.71	1.23
1	I	638	LEU	C-O	-27.35	0.71	1.23
1	L	638	LEU	C-O	-27.35	0.71	1.23
1	M	638	LEU	C-O	-27.33	0.71	1.23
1	J	638	LEU	C-O	-27.32	0.71	1.23
1	M	276	ARG	C-N	-25.20	0.87	1.33
1	L	276	ARG	C-N	-25.19	0.87	1.33
1	K	276	ARG	C-N	-25.18	0.87	1.33
1	I	276	ARG	C-N	-25.18	0.87	1.33
1	N	276	ARG	C-N	-25.14	0.87	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	276	ARG	C-N	-25.14	0.87	1.33
2	H	42	GLY	C-O	-24.05	0.85	1.23
2	C	42	GLY	C-O	-24.04	0.85	1.23
2	B	42	GLY	C-O	-24.02	0.85	1.23
2	E	42	GLY	C-O	-24.01	0.85	1.23
2	F	42	GLY	C-O	-24.01	0.85	1.23
2	A	42	GLY	C-O	-24.01	0.85	1.23
2	D	42	GLY	C-O	-23.98	0.85	1.23
2	G	42	GLY	C-O	-23.94	0.85	1.23
2	F	25	ASP	C-O	-23.57	0.78	1.23
2	B	25	ASP	C-O	-23.56	0.78	1.23
2	H	25	ASP	C-O	-23.54	0.78	1.23
2	G	25	ASP	C-O	-23.54	0.78	1.23
2	C	25	ASP	C-O	-23.52	0.78	1.23
2	D	25	ASP	C-O	-23.51	0.78	1.23
2	A	25	ASP	C-O	-23.50	0.78	1.23
2	E	25	ASP	C-O	-23.50	0.78	1.23
1	M	173	GLY	C-O	-22.90	0.87	1.23
1	K	173	GLY	C-O	-22.89	0.87	1.23
1	J	173	GLY	C-O	-22.89	0.87	1.23
1	I	173	GLY	C-O	-22.87	0.87	1.23
1	L	173	GLY	C-O	-22.86	0.87	1.23
1	N	173	GLY	C-O	-22.84	0.87	1.23
1	K	360	GLY	C-O	-21.82	0.88	1.23
1	M	360	GLY	C-O	-21.79	0.88	1.23
1	L	360	GLY	C-O	-21.77	0.88	1.23
1	I	360	GLY	C-O	-21.77	0.88	1.23
1	N	360	GLY	C-O	-21.75	0.88	1.23
1	J	360	GLY	C-O	-21.71	0.89	1.23
1	J	58	ASP	C-O	-21.68	0.82	1.23
1	I	703	GLY	C-O	-21.64	0.89	1.23
1	J	355	ALA	CA-CB	-21.64	1.07	1.52
1	I	58	ASP	C-O	-21.64	0.82	1.23
1	K	355	ALA	CA-CB	-21.63	1.07	1.52
1	L	58	ASP	C-O	-21.63	0.82	1.23
1	K	703	GLY	C-O	-21.62	0.89	1.23
1	N	355	ALA	CA-CB	-21.62	1.07	1.52
1	M	355	ALA	CA-CB	-21.61	1.07	1.52
1	M	703	GLY	C-O	-21.61	0.89	1.23
1	M	58	ASP	C-O	-21.61	0.82	1.23
1	L	703	GLY	C-O	-21.61	0.89	1.23
1	K	58	ASP	C-O	-21.60	0.82	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	355	ALA	CA-CB	-21.59	1.07	1.52
1	J	703	GLY	C-O	-21.59	0.89	1.23
1	N	58	ASP	C-O	-21.59	0.82	1.23
1	N	703	GLY	C-O	-21.59	0.89	1.23
1	L	355	ALA	CA-CB	-21.57	1.07	1.52
2	E	42	GLY	CA-C	-21.48	1.17	1.51
2	F	42	GLY	CA-C	-21.47	1.17	1.51
2	D	42	GLY	CA-C	-21.47	1.17	1.51
2	A	42	GLY	CA-C	-21.47	1.17	1.51
2	G	42	GLY	CA-C	-21.45	1.17	1.51
2	H	42	GLY	CA-C	-21.45	1.17	1.51
2	C	42	GLY	CA-C	-21.42	1.17	1.51
2	B	42	GLY	CA-C	-21.42	1.17	1.51
1	K	356	GLY	N-CA	-21.20	1.14	1.46
1	I	356	GLY	N-CA	-21.10	1.14	1.46
1	K	459	GLY	C-O	-21.10	0.89	1.23
1	M	356	GLY	N-CA	-21.07	1.14	1.46
1	L	356	GLY	N-CA	-21.06	1.14	1.46
1	N	356	GLY	N-CA	-21.05	1.14	1.46
1	J	356	GLY	N-CA	-21.04	1.14	1.46
1	I	459	GLY	C-O	-21.02	0.90	1.23
1	J	459	GLY	C-O	-21.02	0.90	1.23
1	N	459	GLY	C-O	-21.02	0.90	1.23
1	M	459	GLY	C-O	-20.99	0.90	1.23
1	L	459	GLY	C-O	-20.98	0.90	1.23
1	J	359	SER	C-N	-20.18	0.96	1.33
1	I	359	SER	C-N	-20.15	0.96	1.33
1	L	359	SER	C-N	-20.11	0.96	1.33
1	N	359	SER	C-N	-20.11	0.96	1.33
1	K	359	SER	C-N	-20.09	0.96	1.33
1	M	359	SER	C-N	-20.07	0.96	1.33
2	A	43	VAL	CA-CB	-19.74	1.13	1.54
2	E	43	VAL	CA-CB	-19.73	1.13	1.54
2	G	43	VAL	CA-CB	-19.71	1.13	1.54
2	H	43	VAL	CA-CB	-19.70	1.13	1.54
2	B	43	VAL	CA-CB	-19.70	1.13	1.54
2	D	43	VAL	CA-CB	-19.69	1.13	1.54
2	F	43	VAL	CA-CB	-19.68	1.13	1.54
2	C	43	VAL	CA-CB	-19.66	1.13	1.54
1	M	499	GLU	C-O	-19.05	0.87	1.23
1	N	499	GLU	C-O	-19.02	0.87	1.23
1	J	499	GLU	C-O	-19.00	0.87	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	499	GLU	C-O	-19.00	0.87	1.23
1	L	499	GLU	C-O	-18.99	0.87	1.23
1	K	499	GLU	C-O	-18.95	0.87	1.23
1	K	681	GLU	C-O	-18.69	0.87	1.23
1	M	681	GLU	C-O	-18.69	0.87	1.23
1	L	681	GLU	C-O	-18.68	0.87	1.23
1	J	681	GLU	C-O	-18.66	0.88	1.23
1	I	681	GLU	C-O	-18.64	0.88	1.23
1	N	681	GLU	C-O	-18.62	0.88	1.23
2	G	42	GLY	C-N	-18.51	0.91	1.34
2	H	42	GLY	C-N	-18.47	0.91	1.34
2	C	42	GLY	C-N	-18.46	0.91	1.34
2	E	42	GLY	C-N	-18.44	0.91	1.34
2	A	42	GLY	C-N	-18.44	0.91	1.34
2	D	42	GLY	C-N	-18.42	0.91	1.34
1	L	536	PRO	C-O	-18.42	0.86	1.23
2	F	42	GLY	C-N	-18.42	0.91	1.34
2	B	42	GLY	C-N	-18.41	0.91	1.34
1	K	536	PRO	C-O	-18.40	0.86	1.23
1	N	536	PRO	C-O	-18.39	0.86	1.23
1	I	536	PRO	C-O	-18.39	0.86	1.23
1	M	536	PRO	C-O	-18.38	0.86	1.23
1	J	536	PRO	C-O	-18.37	0.86	1.23
2	B	43	VAL	N-CA	-18.34	1.09	1.46
2	H	43	VAL	N-CA	-18.32	1.09	1.46
2	A	43	VAL	N-CA	-18.31	1.09	1.46
2	G	43	VAL	N-CA	-18.31	1.09	1.46
2	D	43	VAL	N-CA	-18.31	1.09	1.46
2	F	43	VAL	N-CA	-18.31	1.09	1.46
2	C	43	VAL	N-CA	-18.30	1.09	1.46
2	E	43	VAL	N-CA	-18.29	1.09	1.46
1	I	38	GLY	C-O	-18.01	0.94	1.23
1	J	38	GLY	C-O	-17.99	0.94	1.23
1	M	38	GLY	C-O	-17.97	0.94	1.23
1	K	38	GLY	C-O	-17.94	0.94	1.23
1	L	38	GLY	C-O	-17.89	0.95	1.23
1	N	38	GLY	C-O	-17.89	0.95	1.23
1	J	175	GLY	N-CA	-17.49	1.19	1.46
1	M	175	GLY	N-CA	-17.47	1.19	1.46
1	I	175	GLY	N-CA	-17.47	1.19	1.46
1	L	175	GLY	N-CA	-17.45	1.19	1.46
1	K	175	GLY	N-CA	-17.44	1.19	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	175	GLY	N-CA	-17.41	1.20	1.46
1	N	641	ILE	C-N	-17.21	0.94	1.34
1	J	641	ILE	C-N	-17.19	0.94	1.34
1	L	641	ILE	C-N	-17.19	0.94	1.34
1	K	641	ILE	C-N	-17.18	0.94	1.34
1	I	641	ILE	C-N	-17.18	0.94	1.34
1	M	641	ILE	C-N	-17.17	0.94	1.34
2	A	43	VAL	C-O	-16.20	0.92	1.23
2	F	43	VAL	C-O	-16.19	0.92	1.23
2	C	43	VAL	C-O	-16.18	0.92	1.23
2	G	43	VAL	C-O	-16.16	0.92	1.23
2	E	43	VAL	C-O	-16.16	0.92	1.23
1	M	172	TYR	C-N	-16.16	1.03	1.33
1	N	172	TYR	C-N	-16.16	1.03	1.33
1	I	172	TYR	C-N	-16.15	1.03	1.33
1	L	172	TYR	C-N	-16.15	1.03	1.33
2	H	43	VAL	C-O	-16.14	0.92	1.23
1	J	172	TYR	C-N	-16.11	1.04	1.33
2	D	43	VAL	C-O	-16.11	0.92	1.23
2	B	43	VAL	C-O	-16.10	0.92	1.23
1	K	172	TYR	C-N	-16.09	1.04	1.33
1	L	361	GLY	N-CA	-16.09	1.22	1.46
1	K	361	GLY	N-CA	-16.08	1.22	1.46
1	J	361	GLY	N-CA	-16.01	1.22	1.46
1	M	361	GLY	N-CA	-16.00	1.22	1.46
1	N	361	GLY	N-CA	-15.96	1.22	1.46
1	I	361	GLY	N-CA	-15.92	1.22	1.46
1	K	360	GLY	CA-C	-15.75	1.26	1.51
1	N	360	GLY	CA-C	-15.73	1.26	1.51
1	I	360	GLY	CA-C	-15.71	1.26	1.51
1	M	360	GLY	CA-C	-15.71	1.26	1.51
1	L	360	GLY	CA-C	-15.68	1.26	1.51
1	J	360	GLY	CA-C	-15.68	1.26	1.51
2	F	5	THR	N-CA	-15.59	1.15	1.46
2	D	5	THR	N-CA	-15.57	1.15	1.46
2	A	5	THR	N-CA	-15.55	1.15	1.46
2	C	5	THR	N-CA	-15.55	1.15	1.46
2	H	5	THR	N-CA	-15.53	1.15	1.46
2	B	5	THR	N-CA	-15.52	1.15	1.46
2	E	5	THR	N-CA	-15.52	1.15	1.46
2	G	5	THR	N-CA	-15.46	1.15	1.46
1	I	38	GLY	CA-C	-15.37	1.27	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	38	GLY	CA-C	-15.35	1.27	1.51
1	K	38	GLY	CA-C	-15.35	1.27	1.51
1	L	38	GLY	CA-C	-15.32	1.27	1.51
1	M	38	GLY	CA-C	-15.30	1.27	1.51
1	J	38	GLY	CA-C	-15.28	1.27	1.51
1	I	662	GLY	C-O	-15.12	0.99	1.23
1	M	662	GLY	C-O	-15.08	0.99	1.23
1	N	662	GLY	C-O	-15.05	0.99	1.23
1	K	662	GLY	C-O	-15.05	0.99	1.23
1	L	662	GLY	C-O	-15.03	0.99	1.23
2	H	333	PRO	C-O	-14.99	0.93	1.23
1	J	662	GLY	C-O	-14.99	0.99	1.23
2	D	333	PRO	C-O	-14.95	0.93	1.23
2	E	333	PRO	C-O	-14.95	0.93	1.23
2	F	333	PRO	C-O	-14.95	0.93	1.23
2	C	333	PRO	C-O	-14.94	0.93	1.23
2	B	333	PRO	C-O	-14.93	0.93	1.23
2	G	333	PRO	C-O	-14.93	0.93	1.23
2	A	333	PRO	C-O	-14.91	0.93	1.23
2	A	307	PRO	C-O	-14.64	0.94	1.23
2	D	307	PRO	C-O	-14.62	0.94	1.23
2	B	307	PRO	C-O	-14.62	0.94	1.23
2	C	307	PRO	C-O	-14.62	0.94	1.23
2	F	307	PRO	C-O	-14.62	0.94	1.23
2	H	307	PRO	C-O	-14.59	0.94	1.23
2	E	307	PRO	C-O	-14.59	0.94	1.23
2	G	307	PRO	C-O	-14.58	0.94	1.23
1	L	499	GLU	C-N	-14.57	1.06	1.33
2	B	43	VAL	C-N	-14.56	1.00	1.34
2	C	43	VAL	C-N	-14.55	1.00	1.34
2	H	43	VAL	C-N	-14.55	1.00	1.34
2	H	5	THR	CA-CB	-14.54	1.15	1.53
1	I	499	GLU	C-N	-14.54	1.06	1.33
1	K	499	GLU	C-N	-14.54	1.06	1.33
1	M	499	GLU	C-N	-14.54	1.06	1.33
2	A	43	VAL	C-N	-14.54	1.00	1.34
2	A	5	THR	CA-CB	-14.53	1.15	1.53
2	F	43	VAL	C-N	-14.53	1.00	1.34
2	D	43	VAL	C-N	-14.53	1.00	1.34
1	J	499	GLU	C-N	-14.52	1.06	1.33
1	N	499	GLU	C-N	-14.52	1.06	1.33
2	D	5	THR	CA-CB	-14.51	1.15	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	43	VAL	C-N	-14.51	1.00	1.34
2	G	5	THR	CA-CB	-14.51	1.15	1.53
2	F	5	THR	CA-CB	-14.50	1.15	1.53
2	B	5	THR	CA-CB	-14.50	1.15	1.53
2	E	5	THR	CA-CB	-14.50	1.15	1.53
2	G	43	VAL	C-N	-14.48	1.00	1.34
2	C	5	THR	CA-CB	-14.48	1.15	1.53
1	M	173	GLY	CA-C	-14.43	1.28	1.51
1	L	173	GLY	CA-C	-14.38	1.28	1.51
1	N	173	GLY	CA-C	-14.35	1.28	1.51
1	J	173	GLY	CA-C	-14.35	1.28	1.51
1	K	173	GLY	CA-C	-14.34	1.28	1.51
1	I	173	GLY	CA-C	-14.33	1.28	1.51
1	I	622	GLU	CA-CB	-14.32	1.22	1.53
1	L	622	GLU	CA-CB	-14.30	1.22	1.53
1	M	622	GLU	CA-CB	-14.30	1.22	1.53
1	J	622	GLU	CA-CB	-14.28	1.22	1.53
1	N	622	GLU	CA-CB	-14.28	1.22	1.53
1	K	622	GLU	CA-CB	-14.25	1.22	1.53
1	I	622	GLU	C-O	-13.89	0.96	1.23
1	J	622	GLU	C-O	-13.87	0.97	1.23
1	M	622	GLU	C-O	-13.87	0.97	1.23
1	N	622	GLU	C-O	-13.86	0.97	1.23
1	K	622	GLU	C-O	-13.85	0.97	1.23
1	L	622	GLU	C-O	-13.81	0.97	1.23
1	M	638	LEU	C-N	-13.76	1.02	1.34
1	I	638	LEU	C-N	-13.76	1.02	1.34
1	J	638	LEU	C-N	-13.74	1.02	1.34
1	K	638	LEU	C-N	-13.74	1.02	1.34
1	N	638	LEU	C-N	-13.74	1.02	1.34
1	L	638	LEU	C-N	-13.73	1.02	1.34
1	J	174	THR	CA-CB	-13.71	1.17	1.53
1	L	174	THR	CA-CB	-13.70	1.17	1.53
1	M	174	THR	CA-CB	-13.68	1.17	1.53
1	N	174	THR	CA-CB	-13.68	1.17	1.53
1	K	174	THR	CA-CB	-13.67	1.17	1.53
1	I	174	THR	CA-CB	-13.66	1.17	1.53
1	M	642	SER	C-O	-13.43	0.97	1.23
1	K	642	SER	C-O	-13.43	0.97	1.23
1	N	642	SER	C-O	-13.43	0.97	1.23
1	J	642	SER	C-O	-13.40	0.97	1.23
1	I	642	SER	C-O	-13.37	0.97	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	642	SER	C-O	-13.33	0.98	1.23
1	L	360	GLY	C-N	-13.32	1.09	1.33
1	J	360	GLY	C-N	-13.32	1.09	1.33
1	M	360	GLY	C-N	-13.31	1.09	1.33
1	M	357	SER	CA-CB	-13.30	1.32	1.52
1	N	360	GLY	C-N	-13.30	1.09	1.33
1	I	357	SER	CA-CB	-13.30	1.33	1.52
1	N	357	SER	CA-CB	-13.30	1.33	1.52
1	I	360	GLY	C-N	-13.29	1.09	1.33
1	N	356	GLY	CA-C	-13.29	1.30	1.51
1	K	360	GLY	C-N	-13.29	1.09	1.33
1	K	357	SER	CA-CB	-13.28	1.33	1.52
1	M	356	GLY	CA-C	-13.28	1.30	1.51
1	J	356	GLY	CA-C	-13.27	1.30	1.51
1	L	356	GLY	CA-C	-13.27	1.30	1.51
1	L	357	SER	CA-CB	-13.26	1.33	1.52
1	J	357	SER	CA-CB	-13.25	1.33	1.52
1	I	356	GLY	CA-C	-13.25	1.30	1.51
1	K	356	GLY	CA-C	-13.22	1.30	1.51
1	N	502	GLY	C-N	-12.84	1.04	1.34
1	M	502	GLY	C-N	-12.82	1.04	1.34
1	I	502	GLY	C-N	-12.82	1.04	1.34
1	J	502	GLY	C-N	-12.81	1.04	1.34
1	L	502	GLY	C-N	-12.81	1.04	1.34
1	K	502	GLY	C-N	-12.79	1.04	1.34
1	M	38	GLY	C-N	-12.67	1.04	1.34
1	L	38	GLY	C-N	-12.66	1.04	1.34
1	I	38	GLY	C-N	-12.65	1.04	1.34
1	J	38	GLY	C-N	-12.65	1.04	1.34
1	N	38	GLY	C-N	-12.64	1.04	1.34
1	N	681	GLU	C-N	-12.62	1.10	1.33
1	I	681	GLU	C-N	-12.62	1.10	1.33
1	K	38	GLY	C-N	-12.62	1.05	1.34
1	K	681	GLU	C-N	-12.58	1.10	1.33
1	L	681	GLU	C-N	-12.58	1.10	1.33
1	J	681	GLU	C-N	-12.56	1.10	1.33
1	M	681	GLU	C-N	-12.53	1.10	1.33
2	A	371	HIS	CA-CB	-12.50	1.26	1.53
2	F	371	HIS	CA-CB	-12.47	1.26	1.53
2	C	371	HIS	CA-CB	-12.47	1.26	1.53
2	G	371	HIS	CA-CB	-12.47	1.26	1.53
2	B	371	HIS	CA-CB	-12.47	1.26	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	371	HIS	CA-CB	-12.46	1.26	1.53
2	H	371	HIS	CA-CB	-12.45	1.26	1.53
2	E	371	HIS	CA-CB	-12.43	1.26	1.53
2	F	45	VAL	CA-CB	-12.41	1.28	1.54
2	C	45	VAL	CA-CB	-12.41	1.28	1.54
2	E	45	VAL	CA-CB	-12.39	1.28	1.54
2	D	45	VAL	CA-CB	-12.38	1.28	1.54
2	G	45	VAL	CA-CB	-12.38	1.28	1.54
2	A	45	VAL	CA-CB	-12.38	1.28	1.54
2	B	45	VAL	CA-CB	-12.37	1.28	1.54
2	H	45	VAL	CA-CB	-12.34	1.28	1.54
2	B	368	SER	C-O	-12.29	0.99	1.23
1	N	708	ARG	C-O	-12.29	1.00	1.23
2	C	368	SER	C-O	-12.28	1.00	1.23
2	A	368	SER	C-O	-12.28	1.00	1.23
1	J	553	ASP	C-N	-12.24	1.05	1.34
2	G	368	SER	C-O	-12.24	1.00	1.23
1	M	708	ARG	C-O	-12.24	1.00	1.23
2	E	368	SER	C-O	-12.24	1.00	1.23
1	L	708	ARG	C-O	-12.24	1.00	1.23
1	K	708	ARG	C-O	-12.23	1.00	1.23
1	L	553	ASP	C-N	-12.23	1.05	1.34
2	F	368	SER	C-O	-12.22	1.00	1.23
1	J	708	ARG	C-O	-12.22	1.00	1.23
1	N	553	ASP	C-N	-12.22	1.05	1.34
2	D	368	SER	C-O	-12.22	1.00	1.23
1	I	708	ARG	C-O	-12.22	1.00	1.23
1	K	553	ASP	C-N	-12.22	1.05	1.34
2	H	368	SER	C-O	-12.20	1.00	1.23
1	I	553	ASP	C-N	-12.19	1.06	1.34
1	M	553	ASP	C-N	-12.18	1.06	1.34
1	L	461	GLU	C-O	-12.11	1.00	1.23
1	N	461	GLU	C-O	-12.08	1.00	1.23
1	M	461	GLU	C-O	-12.06	1.00	1.23
1	I	461	GLU	C-O	-12.05	1.00	1.23
1	K	461	GLU	C-O	-12.04	1.00	1.23
1	J	461	GLU	C-O	-12.04	1.00	1.23
2	D	244	ASP	C-O	-11.85	1.00	1.23
2	A	244	ASP	C-O	-11.81	1.00	1.23
2	E	244	ASP	C-O	-11.81	1.00	1.23
2	G	244	ASP	C-O	-11.81	1.00	1.23
2	B	244	ASP	C-O	-11.80	1.00	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	244	ASP	C-O	-11.80	1.00	1.23
2	H	244	ASP	C-O	-11.80	1.00	1.23
2	C	244	ASP	C-O	-11.80	1.00	1.23
1	J	553	ASP	CA-CB	-11.62	1.28	1.53
1	M	553	ASP	CA-CB	-11.62	1.28	1.53
1	N	553	ASP	CA-CB	-11.59	1.28	1.53
1	K	553	ASP	CA-CB	-11.59	1.28	1.53
1	L	553	ASP	CA-CB	-11.57	1.28	1.53
1	I	553	ASP	CA-CB	-11.56	1.28	1.53
2	H	368	SER	C-N	-11.32	1.08	1.34
2	A	368	SER	C-N	-11.32	1.08	1.34
2	B	368	SER	C-N	-11.32	1.08	1.34
2	E	368	SER	C-N	-11.31	1.08	1.34
2	F	368	SER	C-N	-11.31	1.08	1.34
2	D	368	SER	C-N	-11.31	1.08	1.34
2	H	245	GLY	C-O	-11.28	1.05	1.23
2	G	368	SER	C-N	-11.27	1.08	1.34
2	C	368	SER	C-N	-11.25	1.08	1.34
2	F	245	GLY	C-O	-11.24	1.05	1.23
2	E	245	GLY	C-O	-11.24	1.05	1.23
2	G	245	GLY	C-O	-11.22	1.05	1.23
2	A	245	GLY	C-O	-11.20	1.05	1.23
2	B	245	GLY	C-O	-11.19	1.05	1.23
2	D	245	GLY	C-O	-11.19	1.05	1.23
1	J	39	LYS	CA-CB	-11.17	1.29	1.53
2	C	245	GLY	C-O	-11.17	1.05	1.23
1	L	39	LYS	CA-CB	-11.16	1.29	1.53
1	K	39	LYS	CA-CB	-11.14	1.29	1.53
1	M	355	ALA	CA-C	-11.12	1.24	1.52
1	N	39	LYS	CA-CB	-11.12	1.29	1.53
1	N	355	ALA	CA-C	-11.11	1.24	1.52
1	L	355	ALA	CA-C	-11.11	1.24	1.52
1	I	355	ALA	CA-C	-11.10	1.24	1.52
1	J	355	ALA	CA-C	-11.10	1.24	1.52
1	K	355	ALA	CA-C	-11.09	1.24	1.52
1	M	39	LYS	CA-CB	-11.09	1.29	1.53
1	I	39	LYS	CA-CB	-11.06	1.29	1.53
1	I	56	LYS	C-O	-10.96	1.02	1.23
1	L	56	LYS	C-O	-10.95	1.02	1.23
1	N	56	LYS	C-O	-10.94	1.02	1.23
1	M	56	LYS	C-O	-10.93	1.02	1.23
1	K	56	LYS	C-O	-10.93	1.02	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	56	LYS	C-O	-10.89	1.02	1.23
1	I	636	GLY	C-N	-10.87	1.09	1.34
1	J	636	GLY	C-N	-10.86	1.09	1.34
1	K	174	THR	CA-C	-10.86	1.24	1.52
1	N	636	GLY	C-N	-10.86	1.09	1.34
1	K	58	ASP	C-N	-10.85	1.09	1.34
1	N	58	ASP	C-N	-10.84	1.09	1.34
1	L	636	GLY	C-N	-10.83	1.09	1.34
1	M	636	GLY	C-N	-10.83	1.09	1.34
1	M	58	ASP	C-N	-10.82	1.09	1.34
1	I	58	ASP	C-N	-10.82	1.09	1.34
1	K	636	GLY	C-N	-10.81	1.09	1.34
1	J	58	ASP	C-N	-10.81	1.09	1.34
1	L	58	ASP	C-N	-10.81	1.09	1.34
1	J	174	THR	CA-C	-10.81	1.24	1.52
1	N	174	THR	CA-C	-10.79	1.24	1.52
1	L	174	THR	CA-C	-10.76	1.25	1.52
1	M	174	THR	CA-C	-10.76	1.25	1.52
1	L	172	TYR	C-O	-10.75	1.02	1.23
2	E	46	GLY	CA-C	-10.75	1.34	1.51
1	J	172	TYR	C-O	-10.75	1.02	1.23
1	I	174	THR	CA-C	-10.74	1.25	1.52
2	F	46	GLY	CA-C	-10.74	1.34	1.51
2	H	46	GLY	CA-C	-10.74	1.34	1.51
1	M	172	TYR	C-O	-10.73	1.02	1.23
1	K	172	TYR	C-O	-10.73	1.02	1.23
1	N	172	TYR	C-O	-10.73	1.02	1.23
1	I	172	TYR	C-O	-10.73	1.02	1.23
2	A	46	GLY	CA-C	-10.73	1.34	1.51
2	B	46	GLY	CA-C	-10.73	1.34	1.51
2	G	46	GLY	CA-C	-10.73	1.34	1.51
1	I	355	ALA	C-N	-10.71	1.13	1.33
1	N	551	HIS	C-O	-10.70	1.03	1.23
2	D	46	GLY	CA-C	-10.69	1.34	1.51
1	K	551	HIS	C-O	-10.68	1.03	1.23
1	L	355	ALA	C-N	-10.67	1.13	1.33
2	C	46	GLY	CA-C	-10.67	1.34	1.51
1	I	551	HIS	C-O	-10.64	1.03	1.23
1	J	355	ALA	C-N	-10.64	1.13	1.33
1	M	355	ALA	C-N	-10.64	1.13	1.33
1	N	355	ALA	C-N	-10.64	1.13	1.33
1	L	551	HIS	C-O	-10.64	1.03	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	355	ALA	C-N	-10.63	1.14	1.33
1	K	39	LYS	N-CA	-10.62	1.25	1.46
1	I	39	LYS	N-CA	-10.62	1.25	1.46
1	M	551	HIS	C-O	-10.61	1.03	1.23
1	J	551	HIS	C-O	-10.60	1.03	1.23
1	L	39	LYS	N-CA	-10.59	1.25	1.46
1	J	39	LYS	N-CA	-10.59	1.25	1.46
1	M	39	LYS	N-CA	-10.59	1.25	1.46
1	N	39	LYS	N-CA	-10.58	1.25	1.46
2	H	25	ASP	C-N	-10.50	1.09	1.34
2	B	25	ASP	C-N	-10.50	1.09	1.34
2	D	25	ASP	C-N	-10.48	1.09	1.34
2	A	25	ASP	C-N	-10.47	1.09	1.34
2	C	25	ASP	C-N	-10.47	1.09	1.34
2	E	25	ASP	C-N	-10.47	1.09	1.34
2	G	25	ASP	C-N	-10.46	1.09	1.34
2	F	25	ASP	C-N	-10.44	1.10	1.34
1	J	357	SER	N-CA	-10.26	1.25	1.46
2	B	47	MET	CA-CB	-10.24	1.31	1.53
2	H	47	MET	CA-CB	-10.23	1.31	1.53
1	K	357	SER	N-CA	-10.22	1.25	1.46
2	E	47	MET	CA-CB	-10.22	1.31	1.53
1	L	357	SER	N-CA	-10.20	1.25	1.46
1	I	357	SER	N-CA	-10.19	1.25	1.46
2	D	47	MET	CA-CB	-10.18	1.31	1.53
1	N	357	SER	N-CA	-10.18	1.25	1.46
2	G	47	MET	CA-CB	-10.17	1.31	1.53
1	M	357	SER	N-CA	-10.17	1.26	1.46
2	C	47	MET	CA-CB	-10.16	1.31	1.53
2	F	47	MET	CA-CB	-10.14	1.31	1.53
2	A	47	MET	CA-CB	-10.12	1.31	1.53
1	J	282	PHE	C-O	-10.07	1.04	1.23
1	K	282	PHE	C-O	-10.06	1.04	1.23
1	I	282	PHE	C-O	-10.04	1.04	1.23
1	L	282	PHE	C-O	-10.03	1.04	1.23
1	N	282	PHE	C-O	-10.03	1.04	1.23
1	M	282	PHE	C-O	-10.02	1.04	1.23
1	J	637	LYS	CA-CB	-9.74	1.32	1.53
1	M	637	LYS	CA-CB	-9.74	1.32	1.53
1	I	637	LYS	CA-CB	-9.73	1.32	1.53
1	L	622	GLU	CA-C	-9.71	1.27	1.52
1	N	637	LYS	CA-CB	-9.70	1.32	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	622	GLU	CA-C	-9.69	1.27	1.52
1	I	622	GLU	CA-C	-9.69	1.27	1.52
1	K	637	LYS	CA-CB	-9.69	1.32	1.53
1	L	637	LYS	CA-CB	-9.68	1.32	1.53
2	B	200	PHE	C-O	-9.68	1.04	1.23
1	J	622	GLU	CA-C	-9.67	1.27	1.52
1	K	622	GLU	CA-C	-9.66	1.27	1.52
1	M	622	GLU	CA-C	-9.66	1.27	1.52
2	C	200	PHE	C-O	-9.65	1.05	1.23
2	G	200	PHE	C-O	-9.64	1.05	1.23
2	E	200	PHE	C-O	-9.61	1.05	1.23
2	F	200	PHE	C-O	-9.61	1.05	1.23
2	A	200	PHE	C-O	-9.60	1.05	1.23
2	H	200	PHE	C-O	-9.59	1.05	1.23
2	D	200	PHE	C-O	-9.59	1.05	1.23
2	D	46	GLY	C-O	-9.52	1.08	1.23
2	B	46	GLY	C-O	-9.52	1.08	1.23
2	G	46	GLY	C-O	-9.51	1.08	1.23
2	H	333	PRO	C-N	-9.51	1.12	1.34
2	H	46	GLY	C-O	-9.50	1.08	1.23
2	A	333	PRO	C-N	-9.50	1.12	1.34
2	C	46	GLY	C-O	-9.50	1.08	1.23
2	E	333	PRO	C-N	-9.50	1.12	1.34
2	C	333	PRO	C-N	-9.49	1.12	1.34
2	C	45	VAL	C-N	-9.49	1.16	1.33
2	D	333	PRO	C-N	-9.49	1.12	1.34
2	E	46	GLY	C-O	-9.48	1.08	1.23
2	G	333	PRO	C-N	-9.47	1.12	1.34
2	A	46	GLY	C-O	-9.47	1.08	1.23
2	H	45	VAL	C-N	-9.47	1.16	1.33
2	F	46	GLY	C-O	-9.47	1.08	1.23
2	B	333	PRO	C-N	-9.46	1.12	1.34
2	E	45	VAL	C-N	-9.46	1.16	1.33
2	F	45	VAL	C-N	-9.44	1.16	1.33
2	B	45	VAL	C-N	-9.44	1.16	1.33
2	G	45	VAL	C-N	-9.43	1.16	1.33
2	A	45	VAL	C-N	-9.43	1.16	1.33
2	D	45	VAL	C-N	-9.43	1.16	1.33
2	F	333	PRO	C-N	-9.43	1.12	1.34
1	M	175	GLY	C-O	-9.21	1.08	1.23
1	N	175	GLY	C-O	-9.19	1.08	1.23
1	J	175	GLY	C-O	-9.18	1.08	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	175	GLY	C-O	-9.18	1.08	1.23
1	K	175	GLY	C-O	-9.16	1.08	1.23
1	L	175	GLY	C-O	-9.15	1.09	1.23
1	M	536	PRO	C-N	-9.02	1.13	1.34
1	L	536	PRO	C-N	-8.97	1.13	1.34
1	N	536	PRO	C-N	-8.97	1.13	1.34
1	K	536	PRO	C-N	-8.96	1.13	1.34
1	J	536	PRO	C-N	-8.95	1.13	1.34
1	I	536	PRO	C-N	-8.94	1.13	1.34
1	N	174	THR	N-CA	-8.87	1.28	1.46
1	J	174	THR	N-CA	-8.87	1.28	1.46
1	I	174	THR	N-CA	-8.84	1.28	1.46
1	K	174	THR	N-CA	-8.82	1.28	1.46
1	L	174	THR	N-CA	-8.80	1.28	1.46
1	M	174	THR	N-CA	-8.80	1.28	1.46
1	I	356	GLY	C-O	-8.77	1.09	1.23
1	K	358	THR	N-CA	-8.76	1.28	1.46
1	J	358	THR	N-CA	-8.74	1.28	1.46
1	I	358	THR	N-CA	-8.74	1.28	1.46
1	M	361	GLY	C-N	-8.74	1.14	1.34
1	L	358	THR	N-CA	-8.73	1.28	1.46
1	J	356	GLY	C-O	-8.73	1.09	1.23
1	M	358	THR	N-CA	-8.73	1.28	1.46
1	K	446	GLU	C-N	-8.72	1.14	1.34
1	M	793	TRP	CA-CB	-8.72	1.34	1.53
1	J	793	TRP	CA-CB	-8.72	1.34	1.53
1	K	356	GLY	C-O	-8.71	1.09	1.23
1	N	793	TRP	CA-CB	-8.71	1.34	1.53
1	K	361	GLY	C-N	-8.71	1.14	1.34
1	N	361	GLY	C-N	-8.71	1.14	1.34
1	N	356	GLY	C-O	-8.71	1.09	1.23
1	M	356	GLY	C-O	-8.71	1.09	1.23
1	I	361	GLY	C-N	-8.70	1.14	1.34
1	J	361	GLY	C-N	-8.70	1.14	1.34
1	K	793	TRP	CA-CB	-8.70	1.34	1.53
1	L	361	GLY	C-N	-8.69	1.14	1.34
1	I	793	TRP	CA-CB	-8.69	1.34	1.53
1	L	793	TRP	CA-CB	-8.68	1.34	1.53
1	L	356	GLY	C-O	-8.68	1.09	1.23
1	M	446	GLU	C-N	-8.68	1.14	1.34
1	L	446	GLU	C-N	-8.68	1.14	1.34
1	J	708	ARG	C-N	-8.67	1.14	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	358	THR	N-CA	-8.67	1.29	1.46
1	J	446	GLU	C-N	-8.65	1.14	1.34
1	I	446	GLU	C-N	-8.64	1.14	1.34
1	N	446	GLU	C-N	-8.64	1.14	1.34
1	M	708	ARG	C-N	-8.61	1.14	1.34
1	K	708	ARG	C-N	-8.59	1.14	1.34
1	I	708	ARG	C-N	-8.58	1.14	1.34
1	L	708	ARG	C-N	-8.58	1.14	1.34
1	N	708	ARG	C-N	-8.55	1.14	1.34
1	N	359	SER	N-CA	-8.51	1.29	1.46
1	L	772	SER	CA-CB	-8.50	1.40	1.52
1	M	359	SER	N-CA	-8.49	1.29	1.46
1	K	359	SER	N-CA	-8.49	1.29	1.46
1	J	359	SER	N-CA	-8.48	1.29	1.46
1	N	36	GLN	C-O	-8.47	1.07	1.23
1	L	36	GLN	C-O	-8.47	1.07	1.23
1	J	772	SER	CA-CB	-8.46	1.40	1.52
1	L	359	SER	N-CA	-8.46	1.29	1.46
1	K	36	GLN	C-O	-8.46	1.07	1.23
1	I	359	SER	N-CA	-8.45	1.29	1.46
1	J	36	GLN	C-O	-8.45	1.07	1.23
1	I	772	SER	CA-CB	-8.44	1.40	1.52
1	I	36	GLN	C-O	-8.44	1.07	1.23
1	M	36	GLN	C-O	-8.44	1.07	1.23
1	M	772	SER	CA-CB	-8.43	1.40	1.52
1	N	772	SER	CA-CB	-8.43	1.40	1.52
2	C	47	MET	N-CA	-8.38	1.29	1.46
2	A	47	MET	N-CA	-8.37	1.29	1.46
1	J	461	GLU	C-N	-8.36	1.14	1.34
1	M	461	GLU	C-N	-8.36	1.14	1.34
1	K	637	LYS	CA-C	-8.36	1.31	1.52
1	K	772	SER	CA-CB	-8.36	1.40	1.52
1	N	637	LYS	CA-C	-8.36	1.31	1.52
2	D	47	MET	N-CA	-8.36	1.29	1.46
2	E	47	MET	N-CA	-8.36	1.29	1.46
1	J	637	LYS	CA-C	-8.35	1.31	1.52
1	L	461	GLU	C-N	-8.35	1.14	1.34
1	L	637	LYS	CA-C	-8.35	1.31	1.52
1	M	637	LYS	CA-C	-8.35	1.31	1.52
1	N	461	GLU	C-N	-8.35	1.14	1.34
2	F	47	MET	N-CA	-8.34	1.29	1.46
1	I	637	LYS	CA-C	-8.34	1.31	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	461	GLU	C-N	-8.34	1.14	1.34
1	K	461	GLU	C-N	-8.34	1.14	1.34
2	H	47	MET	N-CA	-8.33	1.29	1.46
1	K	642	SER	CA-CB	-8.32	1.40	1.52
1	M	642	SER	CA-CB	-8.32	1.40	1.52
2	B	47	MET	N-CA	-8.32	1.29	1.46
2	G	47	MET	N-CA	-8.31	1.29	1.46
1	N	642	SER	CA-CB	-8.30	1.40	1.52
1	I	642	SER	CA-CB	-8.28	1.40	1.52
1	L	642	SER	CA-CB	-8.26	1.40	1.52
1	J	642	SER	CA-CB	-8.24	1.40	1.52
2	A	371	HIS	CA-C	-8.20	1.31	1.52
2	D	371	HIS	CA-C	-8.19	1.31	1.52
2	G	371	HIS	CA-C	-8.19	1.31	1.52
2	E	371	HIS	CA-C	-8.19	1.31	1.52
2	H	371	HIS	CA-C	-8.19	1.31	1.52
2	C	371	HIS	CA-C	-8.18	1.31	1.52
2	F	371	HIS	CA-C	-8.17	1.31	1.52
2	B	371	HIS	CA-C	-8.16	1.31	1.52
2	D	329	ILE	C-O	-8.14	1.07	1.23
2	E	329	ILE	C-O	-8.13	1.07	1.23
2	G	329	ILE	C-O	-8.12	1.07	1.23
2	B	329	ILE	C-O	-8.12	1.07	1.23
1	I	229	LEU	C-O	-8.11	1.07	1.23
2	F	329	ILE	C-O	-8.11	1.07	1.23
1	L	356	GLY	C-N	-8.10	1.15	1.34
1	J	229	LEU	C-O	-8.10	1.07	1.23
1	J	356	GLY	C-N	-8.09	1.15	1.34
1	N	356	GLY	C-N	-8.09	1.15	1.34
1	I	356	GLY	C-N	-8.09	1.15	1.34
2	A	329	ILE	C-O	-8.09	1.07	1.23
2	H	329	ILE	C-O	-8.08	1.08	1.23
1	M	356	GLY	C-N	-8.07	1.15	1.34
1	N	229	LEU	C-O	-8.07	1.08	1.23
1	K	229	LEU	C-O	-8.06	1.08	1.23
1	K	356	GLY	C-N	-8.06	1.15	1.34
2	C	329	ILE	C-O	-8.05	1.08	1.23
1	L	229	LEU	C-O	-8.05	1.08	1.23
1	M	229	LEU	C-O	-8.03	1.08	1.23
1	J	564	LYS	CA-CB	-7.96	1.36	1.53
1	K	564	LYS	CA-CB	-7.95	1.36	1.53
1	L	564	LYS	CA-CB	-7.94	1.36	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	564	LYS	CA-CB	-7.93	1.36	1.53
1	M	564	LYS	CA-CB	-7.92	1.36	1.53
1	I	564	LYS	CA-CB	-7.92	1.36	1.53
2	A	166	TYR	C-O	-7.90	1.08	1.23
2	E	45	VAL	N-CA	-7.90	1.30	1.46
2	D	166	TYR	C-O	-7.89	1.08	1.23
2	G	166	TYR	C-O	-7.89	1.08	1.23
2	E	166	TYR	C-O	-7.88	1.08	1.23
2	F	166	TYR	C-O	-7.88	1.08	1.23
2	F	45	VAL	N-CA	-7.88	1.30	1.46
2	C	45	VAL	N-CA	-7.88	1.30	1.46
2	G	45	VAL	N-CA	-7.88	1.30	1.46
2	B	166	TYR	C-O	-7.87	1.08	1.23
2	D	45	VAL	N-CA	-7.86	1.30	1.46
2	B	45	VAL	N-CA	-7.85	1.30	1.46
2	H	166	TYR	C-O	-7.85	1.08	1.23
2	C	166	TYR	C-O	-7.85	1.08	1.23
2	A	45	VAL	N-CA	-7.85	1.30	1.46
1	I	36	GLN	C-N	-7.82	1.16	1.34
1	J	36	GLN	C-N	-7.82	1.16	1.34
1	N	36	GLN	C-N	-7.82	1.16	1.34
1	L	36	GLN	C-N	-7.81	1.16	1.34
1	M	36	GLN	C-N	-7.80	1.16	1.34
2	H	45	VAL	N-CA	-7.79	1.30	1.46
1	K	36	GLN	C-N	-7.79	1.16	1.34
1	J	772	SER	C-N	-7.77	1.16	1.34
2	D	46	GLY	N-CA	-7.77	1.34	1.46
2	B	46	GLY	N-CA	-7.76	1.34	1.46
2	H	46	GLY	N-CA	-7.76	1.34	1.46
1	L	772	SER	C-N	-7.76	1.16	1.34
1	I	772	SER	C-N	-7.76	1.16	1.34
1	L	37	LYS	C-N	-7.75	1.19	1.33
2	E	46	GLY	N-CA	-7.75	1.34	1.46
1	K	772	SER	C-N	-7.75	1.16	1.34
1	K	462	TYR	CA-CB	-7.73	1.36	1.53
1	M	37	LYS	C-N	-7.72	1.19	1.33
1	M	772	SER	C-N	-7.72	1.16	1.34
1	N	772	SER	C-N	-7.72	1.16	1.34
2	G	46	GLY	N-CA	-7.72	1.34	1.46
1	N	462	TYR	CA-CB	-7.72	1.36	1.53
2	A	46	GLY	N-CA	-7.71	1.34	1.46
1	I	37	LYS	C-N	-7.71	1.19	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	46	GLY	N-CA	-7.71	1.34	1.46
1	J	462	TYR	CA-CB	-7.71	1.36	1.53
2	C	46	GLY	N-CA	-7.71	1.34	1.46
1	J	37	LYS	C-N	-7.70	1.19	1.33
1	N	37	LYS	C-N	-7.69	1.19	1.33
1	K	37	LYS	C-N	-7.67	1.19	1.33
1	I	462	TYR	CA-CB	-7.67	1.37	1.53
1	L	462	TYR	CA-CB	-7.67	1.37	1.53
1	M	462	TYR	CA-CB	-7.66	1.37	1.53
1	N	637	LYS	C-O	-7.64	1.08	1.23
1	K	637	LYS	C-O	-7.63	1.08	1.23
1	J	637	LYS	C-O	-7.62	1.08	1.23
1	I	637	LYS	C-O	-7.60	1.08	1.23
1	L	637	LYS	C-O	-7.57	1.08	1.23
1	L	662	GLY	C-N	-7.55	1.16	1.34
1	J	662	GLY	C-N	-7.55	1.16	1.34
1	K	662	GLY	C-N	-7.55	1.16	1.34
1	M	637	LYS	C-O	-7.55	1.09	1.23
1	I	662	GLY	C-N	-7.54	1.16	1.34
1	N	662	GLY	C-N	-7.53	1.16	1.34
1	M	56	LYS	C-N	-7.52	1.16	1.34
1	J	56	LYS	C-N	-7.49	1.16	1.34
1	L	56	LYS	C-N	-7.49	1.16	1.34
1	M	662	GLY	C-N	-7.47	1.16	1.34
1	K	56	LYS	C-N	-7.46	1.16	1.34
1	N	56	LYS	C-N	-7.46	1.17	1.34
2	D	201	VAL	CA-CB	-7.41	1.39	1.54
1	I	56	LYS	C-N	-7.41	1.17	1.34
2	E	371	HIS	N-CA	-7.40	1.31	1.46
2	C	371	HIS	N-CA	-7.38	1.31	1.46
2	H	201	VAL	CA-CB	-7.38	1.39	1.54
2	H	44	MET	CA-CB	-7.37	1.37	1.53
2	F	201	VAL	CA-CB	-7.36	1.39	1.54
2	G	201	VAL	CA-CB	-7.36	1.39	1.54
2	H	371	HIS	N-CA	-7.36	1.31	1.46
2	A	201	VAL	CA-CB	-7.35	1.39	1.54
2	F	371	HIS	N-CA	-7.35	1.31	1.46
2	E	44	MET	CA-CB	-7.35	1.37	1.53
2	B	371	HIS	N-CA	-7.34	1.31	1.46
2	C	201	VAL	CA-CB	-7.34	1.39	1.54
2	G	44	MET	CA-CB	-7.34	1.37	1.53
2	A	371	HIS	N-CA	-7.33	1.31	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	371	HIS	N-CA	-7.33	1.31	1.46
2	D	371	HIS	N-CA	-7.33	1.31	1.46
2	E	201	VAL	CA-CB	-7.33	1.39	1.54
2	F	44	MET	CA-CB	-7.31	1.37	1.53
2	B	201	VAL	CA-CB	-7.31	1.39	1.54
2	A	44	MET	CA-CB	-7.31	1.37	1.53
2	B	44	MET	CA-CB	-7.29	1.38	1.53
2	B	307	PRO	C-N	-7.29	1.20	1.33
2	F	307	PRO	C-N	-7.29	1.20	1.33
2	D	307	PRO	C-N	-7.29	1.20	1.33
2	C	44	MET	CA-CB	-7.28	1.38	1.53
2	D	44	MET	CA-CB	-7.28	1.38	1.53
2	H	307	PRO	C-N	-7.28	1.20	1.33
2	C	307	PRO	C-N	-7.27	1.20	1.33
2	G	307	PRO	C-N	-7.24	1.20	1.33
2	E	307	PRO	C-N	-7.22	1.20	1.33
2	A	307	PRO	C-N	-7.22	1.20	1.33
1	J	447	THR	C-O	-7.21	1.09	1.23
2	E	244	ASP	C-N	-7.19	1.20	1.33
1	K	447	THR	C-O	-7.17	1.09	1.23
1	M	447	THR	C-O	-7.17	1.09	1.23
2	H	244	ASP	C-N	-7.17	1.20	1.33
2	A	244	ASP	C-N	-7.17	1.20	1.33
1	L	447	THR	C-O	-7.16	1.09	1.23
1	N	447	THR	C-O	-7.16	1.09	1.23
2	G	244	ASP	C-N	-7.15	1.20	1.33
1	I	447	THR	C-O	-7.14	1.09	1.23
2	D	244	ASP	C-N	-7.13	1.20	1.33
2	B	244	ASP	C-N	-7.13	1.20	1.33
2	F	244	ASP	C-N	-7.13	1.20	1.33
2	C	244	ASP	C-N	-7.12	1.20	1.33
2	D	369	ILE	C-O	-6.96	1.10	1.23
2	B	369	ILE	C-O	-6.94	1.10	1.23
2	E	369	ILE	C-O	-6.90	1.10	1.23
2	G	369	ILE	C-O	-6.89	1.10	1.23
2	H	369	ILE	C-O	-6.88	1.10	1.23
2	C	369	ILE	C-O	-6.87	1.10	1.23
2	F	369	ILE	C-O	-6.87	1.10	1.23
1	J	361	GLY	CA-C	-6.86	1.40	1.51
1	N	563	SER	CA-CB	-6.85	1.42	1.52
2	A	369	ILE	C-O	-6.84	1.10	1.23
1	J	563	SER	CA-CB	-6.83	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	563	SER	CA-CB	-6.83	1.42	1.52
1	I	361	GLY	CA-C	-6.83	1.41	1.51
1	M	563	SER	CA-CB	-6.82	1.42	1.52
1	L	357	SER	C-O	-6.81	1.10	1.23
1	M	357	SER	C-O	-6.81	1.10	1.23
1	K	563	SER	CA-CB	-6.81	1.42	1.52
1	M	361	GLY	CA-C	-6.81	1.41	1.51
1	I	357	SER	C-O	-6.80	1.10	1.23
1	L	361	GLY	CA-C	-6.80	1.41	1.51
1	J	357	SER	C-O	-6.80	1.10	1.23
1	L	563	SER	CA-CB	-6.80	1.42	1.52
1	N	361	GLY	CA-C	-6.80	1.41	1.51
1	J	175	GLY	C-N	-6.79	1.18	1.34
1	N	357	SER	C-O	-6.78	1.10	1.23
1	N	357	SER	CA-C	-6.78	1.35	1.52
1	K	175	GLY	C-N	-6.77	1.18	1.34
1	K	361	GLY	CA-C	-6.76	1.41	1.51
1	L	5	LYS	N-CA	-6.76	1.32	1.46
1	N	175	GLY	C-N	-6.76	1.18	1.34
1	I	175	GLY	C-N	-6.76	1.18	1.34
1	L	175	GLY	C-N	-6.75	1.18	1.34
1	J	5	LYS	N-CA	-6.75	1.32	1.46
1	M	175	GLY	C-N	-6.75	1.18	1.34
1	I	357	SER	CA-C	-6.74	1.35	1.52
1	K	5	LYS	N-CA	-6.74	1.32	1.46
1	J	357	SER	CA-C	-6.74	1.35	1.52
1	K	357	SER	CA-C	-6.74	1.35	1.52
1	L	357	SER	CA-C	-6.74	1.35	1.52
1	I	5	LYS	N-CA	-6.74	1.32	1.46
1	K	357	SER	C-O	-6.74	1.10	1.23
1	M	357	SER	CA-C	-6.73	1.35	1.52
2	H	200	PHE	CA-CB	-6.72	1.39	1.53
2	C	200	PHE	CA-CB	-6.72	1.39	1.53
2	D	200	PHE	CA-CB	-6.72	1.39	1.53
2	F	200	PHE	CA-CB	-6.71	1.39	1.53
2	G	200	PHE	CA-CB	-6.71	1.39	1.53
2	A	200	PHE	CA-CB	-6.69	1.39	1.53
1	M	5	LYS	N-CA	-6.68	1.32	1.46
2	B	200	PHE	CA-CB	-6.68	1.39	1.53
1	N	5	LYS	N-CA	-6.67	1.33	1.46
2	E	200	PHE	CA-CB	-6.66	1.39	1.53
1	L	703	GLY	CA-C	-6.66	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	703	GLY	CA-C	-6.63	1.41	1.51
1	J	358	THR	C-O	-6.63	1.10	1.23
1	N	358	THR	C-O	-6.61	1.10	1.23
1	J	703	GLY	CA-C	-6.61	1.41	1.51
1	N	703	GLY	CA-C	-6.60	1.41	1.51
1	I	358	THR	C-O	-6.60	1.10	1.23
1	M	703	GLY	CA-C	-6.59	1.41	1.51
1	I	703	GLY	CA-C	-6.57	1.41	1.51
1	L	358	THR	C-O	-6.56	1.10	1.23
1	K	358	THR	C-O	-6.55	1.10	1.23
1	K	358	THR	C-N	-6.55	1.19	1.34
1	K	282	PHE	C-N	-6.54	1.19	1.34
1	K	795	LYS	N-CA	-6.53	1.33	1.46
1	N	795	LYS	N-CA	-6.53	1.33	1.46
1	M	358	THR	C-N	-6.53	1.19	1.34
1	M	358	THR	C-O	-6.52	1.10	1.23
1	J	795	LYS	N-CA	-6.52	1.33	1.46
1	N	282	PHE	C-N	-6.52	1.19	1.34
1	I	282	PHE	C-N	-6.52	1.19	1.34
1	J	358	THR	C-N	-6.52	1.19	1.34
1	M	282	PHE	C-N	-6.52	1.19	1.34
1	N	597	ASN	C-O	-6.52	1.10	1.23
1	I	358	THR	C-N	-6.51	1.19	1.34
1	L	282	PHE	C-N	-6.51	1.19	1.34
1	J	282	PHE	C-N	-6.51	1.19	1.34
1	N	358	THR	C-N	-6.50	1.19	1.34
1	L	358	THR	C-N	-6.49	1.19	1.34
1	L	795	LYS	N-CA	-6.49	1.33	1.46
1	J	597	ASN	C-O	-6.49	1.11	1.23
1	L	597	ASN	C-O	-6.48	1.11	1.23
1	I	597	ASN	C-O	-6.48	1.11	1.23
1	I	795	LYS	N-CA	-6.46	1.33	1.46
1	M	795	LYS	N-CA	-6.46	1.33	1.46
1	K	639	SER	CA-CB	-6.46	1.43	1.52
1	N	639	SER	CA-CB	-6.46	1.43	1.52
1	M	597	ASN	C-O	-6.45	1.11	1.23
1	I	354	GLU	C-O	-6.45	1.11	1.23
1	M	639	SER	CA-CB	-6.45	1.43	1.52
1	L	639	SER	CA-CB	-6.44	1.43	1.52
1	N	354	GLU	C-O	-6.44	1.11	1.23
1	M	354	GLU	C-O	-6.43	1.11	1.23
1	L	642	SER	C-N	-6.43	1.19	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	354	GLU	C-O	-6.42	1.11	1.23
1	K	597	ASN	C-O	-6.42	1.11	1.23
1	N	642	SER	C-N	-6.42	1.19	1.34
1	J	354	GLU	C-O	-6.42	1.11	1.23
1	K	642	SER	C-N	-6.42	1.19	1.34
2	G	369	ILE	CA-CB	-6.42	1.40	1.54
1	I	642	SER	C-N	-6.41	1.19	1.34
2	F	369	ILE	CA-CB	-6.41	1.40	1.54
1	M	642	SER	C-N	-6.40	1.19	1.34
2	A	45	VAL	CA-C	-6.40	1.36	1.52
2	B	369	ILE	CA-CB	-6.40	1.40	1.54
1	L	354	GLU	C-O	-6.40	1.11	1.23
1	J	642	SER	C-N	-6.40	1.19	1.34
2	C	369	ILE	CA-CB	-6.40	1.40	1.54
1	J	639	SER	CA-CB	-6.39	1.43	1.52
2	H	369	ILE	CA-CB	-6.38	1.40	1.54
2	H	45	VAL	CA-C	-6.38	1.36	1.52
2	E	45	VAL	CA-C	-6.38	1.36	1.52
2	C	45	VAL	CA-C	-6.38	1.36	1.52
2	D	369	ILE	CA-CB	-6.37	1.40	1.54
2	D	45	VAL	CA-C	-6.37	1.36	1.52
1	N	5	LYS	CA-CB	-6.37	1.40	1.53
2	F	45	VAL	CA-C	-6.37	1.36	1.52
2	B	45	VAL	CA-C	-6.36	1.36	1.52
1	I	639	SER	CA-CB	-6.36	1.43	1.52
1	L	5	LYS	CA-CB	-6.36	1.40	1.53
2	G	45	VAL	CA-C	-6.35	1.36	1.52
2	A	369	ILE	CA-CB	-6.35	1.40	1.54
1	I	5	LYS	CA-CB	-6.35	1.40	1.53
2	E	369	ILE	CA-CB	-6.34	1.40	1.54
1	J	5	LYS	CA-CB	-6.31	1.40	1.53
1	K	5	LYS	CA-CB	-6.31	1.40	1.53
1	M	5	LYS	CA-CB	-6.31	1.40	1.53
1	I	358	THR	CA-C	-6.29	1.36	1.52
1	L	358	THR	CA-C	-6.28	1.36	1.52
1	K	358	THR	CA-C	-6.27	1.36	1.52
1	M	358	THR	CA-C	-6.26	1.36	1.52
1	M	355	ALA	C-O	-6.26	1.11	1.23
1	N	358	THR	CA-C	-6.26	1.36	1.52
1	M	459	GLY	C-N	-6.25	1.19	1.34
1	J	355	ALA	C-O	-6.25	1.11	1.23
1	J	358	THR	CA-C	-6.25	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	459	GLY	C-N	-6.25	1.19	1.34
1	N	355	ALA	C-O	-6.24	1.11	1.23
1	J	39	LYS	C-O	-6.24	1.11	1.23
1	I	355	ALA	C-O	-6.23	1.11	1.23
1	L	355	ALA	C-O	-6.23	1.11	1.23
1	K	355	ALA	C-O	-6.22	1.11	1.23
1	J	459	GLY	C-N	-6.21	1.19	1.34
1	I	39	LYS	C-O	-6.21	1.11	1.23
1	M	39	LYS	C-O	-6.21	1.11	1.23
1	N	39	LYS	C-O	-6.21	1.11	1.23
1	N	459	GLY	C-N	-6.21	1.19	1.34
1	K	39	LYS	C-O	-6.20	1.11	1.23
1	K	459	GLY	C-N	-6.19	1.19	1.34
1	L	39	LYS	C-O	-6.19	1.11	1.23
1	I	459	GLY	C-N	-6.17	1.19	1.34
1	K	37	LYS	C-O	-6.05	1.11	1.23
1	M	37	LYS	C-O	-6.04	1.11	1.23
1	N	37	LYS	C-O	-6.04	1.11	1.23
1	I	37	LYS	C-O	-6.02	1.11	1.23
1	I	460	PHE	C-N	-6.01	1.20	1.34
1	J	37	LYS	C-O	-6.00	1.11	1.23
1	J	510	ASP	CA-CB	-6.00	1.40	1.53
1	N	460	PHE	C-N	-6.00	1.20	1.34
1	J	460	PHE	C-N	-6.00	1.20	1.34
1	L	37	LYS	C-O	-5.98	1.11	1.23
1	I	510	ASP	CA-CB	-5.97	1.40	1.53
1	M	510	ASP	CA-CB	-5.97	1.40	1.53
1	I	35	ASN	C-O	-5.97	1.12	1.23
1	M	460	PHE	C-N	-5.96	1.20	1.34
1	K	510	ASP	CA-CB	-5.96	1.40	1.53
1	K	460	PHE	C-N	-5.96	1.20	1.34
1	L	510	ASP	CA-CB	-5.95	1.40	1.53
2	E	44	MET	CA-C	-5.95	1.37	1.52
1	L	460	PHE	C-N	-5.95	1.20	1.34
1	K	638	LEU	N-CA	-5.94	1.34	1.46
1	J	35	ASN	C-O	-5.94	1.12	1.23
1	J	638	LEU	N-CA	-5.94	1.34	1.46
1	I	638	LEU	N-CA	-5.93	1.34	1.46
1	M	638	LEU	N-CA	-5.92	1.34	1.46
1	K	460	PHE	C-O	-5.92	1.12	1.23
1	M	35	ASN	C-O	-5.92	1.12	1.23
1	N	638	LEU	N-CA	-5.92	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	447	THR	C-N	-5.92	1.20	1.34
1	M	460	PHE	C-O	-5.92	1.12	1.23
1	N	510	ASP	CA-CB	-5.92	1.41	1.53
1	N	460	PHE	C-O	-5.91	1.12	1.23
1	L	638	LEU	N-CA	-5.91	1.34	1.46
1	L	460	PHE	C-O	-5.91	1.12	1.23
1	L	35	ASN	C-O	-5.90	1.12	1.23
1	N	35	ASN	C-O	-5.90	1.12	1.23
1	N	447	THR	C-N	-5.90	1.20	1.34
1	I	460	PHE	C-O	-5.89	1.12	1.23
2	B	44	MET	CA-C	-5.89	1.37	1.52
2	C	44	MET	CA-C	-5.88	1.37	1.52
2	D	44	MET	CA-C	-5.88	1.37	1.52
1	J	460	PHE	C-O	-5.88	1.12	1.23
2	G	44	MET	CA-C	-5.88	1.37	1.52
1	M	447	THR	C-N	-5.88	1.20	1.34
2	F	44	MET	CA-C	-5.88	1.37	1.52
1	I	447	THR	C-N	-5.87	1.20	1.34
1	K	35	ASN	C-O	-5.87	1.12	1.23
1	L	621	PHE	C-O	-5.87	1.12	1.23
1	K	621	PHE	C-O	-5.87	1.12	1.23
2	A	44	MET	CA-C	-5.87	1.37	1.52
2	H	44	MET	CA-C	-5.87	1.37	1.52
1	N	621	PHE	C-O	-5.86	1.12	1.23
1	L	447	THR	C-N	-5.85	1.20	1.34
1	J	447	THR	C-N	-5.85	1.20	1.34
1	N	568	HIS	N-CA	-5.84	1.34	1.46
1	I	568	HIS	N-CA	-5.84	1.34	1.46
1	J	621	PHE	C-O	-5.83	1.12	1.23
1	J	568	HIS	N-CA	-5.83	1.34	1.46
1	K	568	HIS	N-CA	-5.83	1.34	1.46
1	I	621	PHE	C-O	-5.82	1.12	1.23
1	M	621	PHE	C-O	-5.82	1.12	1.23
1	L	568	HIS	N-CA	-5.82	1.34	1.46
1	M	568	HIS	N-CA	-5.80	1.34	1.46
1	L	795	LYS	CA-CB	-5.76	1.41	1.53
1	I	795	LYS	CA-CB	-5.75	1.41	1.53
1	K	795	LYS	CA-CB	-5.75	1.41	1.53
1	N	795	LYS	CA-CB	-5.74	1.41	1.53
1	M	795	LYS	CA-CB	-5.74	1.41	1.53
1	J	795	LYS	CA-CB	-5.73	1.41	1.53
1	K	567	ILE	CA-CB	-5.69	1.41	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	169	TYR	C-O	-5.68	1.12	1.23
1	M	567	ILE	CA-CB	-5.68	1.41	1.54
1	N	567	ILE	CA-CB	-5.68	1.41	1.54
1	L	509	VAL	CA-CB	-5.67	1.42	1.54
1	M	509	VAL	CA-CB	-5.67	1.42	1.54
1	I	509	VAL	CA-CB	-5.67	1.42	1.54
2	E	169	TYR	C-O	-5.67	1.12	1.23
1	L	567	ILE	CA-CB	-5.67	1.41	1.54
1	K	509	VAL	CA-CB	-5.66	1.42	1.54
1	J	509	VAL	CA-CB	-5.66	1.42	1.54
1	J	567	ILE	CA-CB	-5.65	1.41	1.54
1	I	567	ILE	CA-CB	-5.65	1.41	1.54
2	D	169	TYR	C-O	-5.65	1.12	1.23
2	C	169	TYR	C-O	-5.65	1.12	1.23
1	N	509	VAL	CA-CB	-5.64	1.42	1.54
2	G	169	TYR	C-O	-5.64	1.12	1.23
2	F	169	TYR	C-O	-5.63	1.12	1.23
1	M	510	ASP	C-O	-5.63	1.12	1.23
1	K	510	ASP	C-O	-5.62	1.12	1.23
2	A	169	TYR	C-O	-5.62	1.12	1.23
2	H	169	TYR	C-O	-5.62	1.12	1.23
1	J	510	ASP	C-O	-5.62	1.12	1.23
2	A	200	PHE	C-N	-5.62	1.21	1.34
1	L	510	ASP	C-O	-5.61	1.12	1.23
2	D	200	PHE	C-N	-5.61	1.21	1.34
1	I	510	ASP	C-O	-5.61	1.12	1.23
1	N	510	ASP	C-O	-5.60	1.12	1.23
2	H	200	PHE	C-N	-5.60	1.21	1.34
2	E	200	PHE	C-N	-5.59	1.21	1.34
2	G	200	PHE	C-N	-5.59	1.21	1.34
2	F	200	PHE	C-N	-5.59	1.21	1.34
1	K	254	GLY	C-O	-5.58	1.14	1.23
2	C	200	PHE	C-N	-5.57	1.21	1.34
1	M	772	SER	CA-C	-5.57	1.38	1.52
2	B	200	PHE	C-N	-5.57	1.21	1.34
1	J	254	GLY	C-O	-5.56	1.14	1.23
1	L	254	GLY	C-O	-5.56	1.14	1.23
1	M	254	GLY	C-O	-5.56	1.14	1.23
1	I	254	GLY	C-O	-5.55	1.14	1.23
1	K	772	SER	CA-C	-5.54	1.38	1.52
1	N	772	SER	CA-C	-5.53	1.38	1.52
1	I	772	SER	CA-C	-5.53	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	772	SER	CA-C	-5.52	1.38	1.52
1	J	772	SER	CA-C	-5.51	1.38	1.52
1	N	254	GLY	C-O	-5.50	1.14	1.23
1	N	794	LYS	N-CA	-5.44	1.35	1.46
2	B	370	VAL	C-O	-5.42	1.13	1.23
1	J	794	LYS	N-CA	-5.42	1.35	1.46
2	D	370	VAL	C-O	-5.40	1.13	1.23
2	A	370	VAL	C-O	-5.40	1.13	1.23
1	I	794	LYS	N-CA	-5.39	1.35	1.46
2	F	370	VAL	C-O	-5.39	1.13	1.23
1	L	175	GLY	CA-C	-5.39	1.43	1.51
1	M	794	LYS	N-CA	-5.38	1.35	1.46
2	E	370	VAL	C-O	-5.38	1.13	1.23
1	L	794	LYS	N-CA	-5.38	1.35	1.46
2	H	370	VAL	C-O	-5.38	1.13	1.23
2	C	370	VAL	C-O	-5.37	1.13	1.23
1	K	794	LYS	N-CA	-5.37	1.35	1.46
2	G	370	VAL	C-O	-5.36	1.13	1.23
1	L	229	LEU	C-N	-5.36	1.21	1.34
1	N	175	GLY	CA-C	-5.35	1.43	1.51
1	M	175	GLY	CA-C	-5.35	1.43	1.51
1	K	229	LEU	C-N	-5.34	1.21	1.34
1	I	175	GLY	CA-C	-5.34	1.43	1.51
1	K	175	GLY	CA-C	-5.32	1.43	1.51
1	N	229	LEU	C-N	-5.32	1.21	1.34
1	M	229	LEU	C-N	-5.32	1.21	1.34
1	N	795	LYS	C-O	-5.31	1.13	1.23
1	I	229	LEU	C-N	-5.31	1.21	1.34
1	I	795	LYS	C-O	-5.30	1.13	1.23
1	J	175	GLY	CA-C	-5.30	1.43	1.51
1	J	229	LEU	C-N	-5.29	1.21	1.34
1	L	795	LYS	C-O	-5.28	1.13	1.23
1	L	583	ALA	C-O	-5.27	1.13	1.23
1	J	569	ARG	CA-CB	-5.26	1.42	1.53
1	M	795	LYS	C-O	-5.26	1.13	1.23
1	K	795	LYS	C-O	-5.25	1.13	1.23
1	I	583	ALA	C-O	-5.25	1.13	1.23
1	J	795	LYS	C-O	-5.25	1.13	1.23
1	M	583	ALA	C-O	-5.25	1.13	1.23
1	L	569	ARG	CA-CB	-5.24	1.42	1.53
1	M	569	ARG	CA-CB	-5.24	1.42	1.53
1	N	569	ARG	CA-CB	-5.24	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	569	ARG	CA-CB	-5.23	1.42	1.53
1	K	569	ARG	CA-CB	-5.23	1.42	1.53
1	K	583	ALA	C-O	-5.23	1.13	1.23
1	J	583	ALA	C-O	-5.23	1.13	1.23
1	N	583	ALA	C-O	-5.22	1.13	1.23
2	H	199	SER	CA-CB	-5.21	1.45	1.52
1	M	91	ALA	C-O	-5.21	1.13	1.23
1	J	91	ALA	C-O	-5.21	1.13	1.23
2	F	199	SER	CA-CB	-5.20	1.45	1.52
1	L	91	ALA	C-O	-5.19	1.13	1.23
1	K	91	ALA	C-O	-5.19	1.13	1.23
2	D	324	THR	C-O	-5.18	1.13	1.23
1	I	91	ALA	C-O	-5.17	1.13	1.23
2	E	324	THR	C-O	-5.16	1.13	1.23
1	N	91	ALA	C-O	-5.15	1.13	1.23
1	K	569	ARG	N-CA	-5.15	1.36	1.46
2	B	324	THR	C-O	-5.15	1.13	1.23
2	C	324	THR	C-O	-5.15	1.13	1.23
2	H	324	THR	C-O	-5.14	1.13	1.23
1	M	582	PHE	C-O	-5.14	1.13	1.23
2	E	199	SER	CA-CB	-5.13	1.45	1.52
2	G	324	THR	C-O	-5.13	1.13	1.23
2	A	199	SER	CA-CB	-5.13	1.45	1.52
1	N	569	ARG	N-CA	-5.12	1.36	1.46
2	F	324	THR	C-O	-5.12	1.13	1.23
1	J	569	ARG	N-CA	-5.12	1.36	1.46
2	G	199	SER	CA-CB	-5.12	1.45	1.52
1	J	582	PHE	C-O	-5.12	1.13	1.23
1	M	569	ARG	N-CA	-5.12	1.36	1.46
2	D	199	SER	CA-CB	-5.11	1.45	1.52
2	C	199	SER	CA-CB	-5.11	1.45	1.52
1	I	582	PHE	C-O	-5.10	1.13	1.23
2	A	324	THR	C-O	-5.10	1.13	1.23
1	I	173	GLY	C-N	-5.10	1.22	1.34
2	B	199	SER	CA-CB	-5.10	1.45	1.52
1	M	563	SER	C-O	-5.10	1.13	1.23
1	I	553	ASP	N-CA	-5.09	1.36	1.46
1	I	563	SER	C-O	-5.09	1.13	1.23
1	N	563	SER	C-O	-5.09	1.13	1.23
1	K	582	PHE	C-O	-5.09	1.13	1.23
1	K	597	ASN	C-N	-5.08	1.22	1.34
1	L	569	ARG	N-CA	-5.08	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	582	PHE	C-O	-5.08	1.13	1.23
1	N	582	PHE	C-O	-5.08	1.13	1.23
1	N	173	GLY	C-N	-5.08	1.22	1.34
1	L	553	ASP	N-CA	-5.07	1.36	1.46
1	N	553	ASP	N-CA	-5.06	1.36	1.46
1	K	563	SER	C-O	-5.06	1.13	1.23
1	M	553	ASP	N-CA	-5.06	1.36	1.46
2	B	370	VAL	C-N	-5.05	1.22	1.34
1	J	563	SER	C-O	-5.05	1.13	1.23
1	M	173	GLY	C-N	-5.04	1.22	1.34
1	I	569	ARG	N-CA	-5.04	1.36	1.46
1	J	597	ASN	C-N	-5.04	1.22	1.34
1	L	173	GLY	C-N	-5.03	1.22	1.34
1	K	173	GLY	C-N	-5.03	1.22	1.34
1	L	563	SER	C-O	-5.03	1.13	1.23
1	I	597	ASN	C-N	-5.03	1.22	1.34
2	G	370	VAL	C-N	-5.03	1.22	1.34
1	M	597	ASN	C-N	-5.03	1.22	1.34
2	F	370	VAL	C-N	-5.03	1.22	1.34
1	J	173	GLY	C-N	-5.02	1.22	1.34
1	J	553	ASP	N-CA	-5.02	1.36	1.46
2	A	370	VAL	C-N	-5.02	1.22	1.34
2	D	370	VAL	C-N	-5.02	1.22	1.34
2	H	370	VAL	C-N	-5.01	1.22	1.34
1	L	597	ASN	C-N	-5.01	1.22	1.34
2	E	370	VAL	C-N	-5.00	1.22	1.34

All (661) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	276	ARG	O-C-N	-54.86	29.93	123.20
1	K	276	ARG	O-C-N	-54.84	29.98	123.20
1	M	276	ARG	O-C-N	-54.83	29.99	123.20
1	J	276	ARG	O-C-N	-54.81	30.02	123.20
1	I	276	ARG	O-C-N	-54.77	30.10	123.20
1	L	276	ARG	O-C-N	-54.75	30.12	123.20
1	K	174	THR	O-C-N	-44.83	46.98	123.20
1	J	174	THR	O-C-N	-44.81	47.03	123.20
1	N	174	THR	O-C-N	-44.80	47.04	123.20
1	I	174	THR	O-C-N	-44.78	47.07	123.20
1	M	174	THR	O-C-N	-44.78	47.08	123.20
1	L	174	THR	O-C-N	-44.71	47.19	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	641	ILE	O-C-N	-27.71	78.37	122.70
1	N	641	ILE	O-C-N	-27.69	78.40	122.70
1	K	641	ILE	O-C-N	-27.68	78.41	122.70
1	J	641	ILE	O-C-N	-27.67	78.43	122.70
1	M	641	ILE	O-C-N	-27.67	78.43	122.70
1	L	641	ILE	O-C-N	-27.62	78.51	122.70
1	J	276	ARG	CA-C-N	27.43	171.06	116.20
1	M	276	ARG	CA-C-N	27.43	171.05	116.20
1	K	276	ARG	CA-C-N	27.38	170.96	116.20
1	L	276	ARG	CA-C-N	27.37	170.95	116.20
1	I	276	ARG	CA-C-N	27.36	170.92	116.20
1	N	276	ARG	CA-C-N	27.36	170.92	116.20
1	I	359	SER	O-C-N	-23.16	83.82	123.20
1	M	359	SER	O-C-N	-23.16	83.83	123.20
1	N	359	SER	O-C-N	-23.15	83.84	123.20
1	L	359	SER	O-C-N	-23.14	83.87	123.20
1	K	359	SER	O-C-N	-23.13	83.88	123.20
1	J	359	SER	O-C-N	-23.11	83.90	123.20
1	J	276	ARG	C-N-CA	22.85	170.28	122.30
1	M	276	ARG	C-N-CA	22.82	170.23	122.30
1	N	276	ARG	C-N-CA	22.81	170.20	122.30
1	L	276	ARG	C-N-CA	22.78	170.14	122.30
1	I	276	ARG	C-N-CA	22.76	170.10	122.30
1	K	276	ARG	C-N-CA	22.75	170.08	122.30
1	K	174	THR	CA-C-N	21.64	159.48	116.20
1	J	174	THR	CA-C-N	21.53	159.26	116.20
1	N	174	THR	CA-C-N	21.53	159.26	116.20
1	I	174	THR	CA-C-N	21.53	159.25	116.20
1	M	174	THR	CA-C-N	21.50	159.21	116.20
1	L	174	THR	CA-C-N	21.48	159.17	116.20
1	I	356	GLY	N-CA-C	19.34	161.46	113.10
1	L	356	GLY	N-CA-C	19.30	161.36	113.10
1	K	356	GLY	N-CA-C	19.30	161.34	113.10
1	M	356	GLY	N-CA-C	19.29	161.32	113.10
1	J	356	GLY	N-CA-C	19.28	161.30	113.10
1	N	356	GLY	N-CA-C	19.27	161.28	113.10
1	N	553	ASP	O-C-N	-18.96	92.37	122.70
1	K	553	ASP	O-C-N	-18.95	92.38	122.70
1	N	638	LEU	O-C-N	-18.92	92.44	122.70
1	L	553	ASP	O-C-N	-18.91	92.45	122.70
1	M	553	ASP	O-C-N	-18.90	92.46	122.70
1	I	553	ASP	O-C-N	-18.89	92.48	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	638	LEU	O-C-N	-18.89	92.48	122.70
1	J	638	LEU	O-C-N	-18.87	92.51	122.70
1	J	553	ASP	O-C-N	-18.84	92.55	122.70
1	M	638	LEU	O-C-N	-18.81	92.60	122.70
1	I	638	LEU	O-C-N	-18.81	92.61	122.70
1	K	638	LEU	O-C-N	-18.80	92.62	122.70
1	N	276	ARG	CA-C-O	18.59	159.14	120.10
1	K	276	ARG	CA-C-O	18.55	159.07	120.10
1	I	276	ARG	CA-C-O	18.51	158.98	120.10
1	M	276	ARG	CA-C-O	18.50	158.96	120.10
1	L	276	ARG	CA-C-O	18.49	158.93	120.10
1	J	276	ARG	CA-C-O	18.48	158.92	120.10
1	K	174	THR	C-N-CA	17.32	158.67	122.30
1	M	174	THR	C-N-CA	17.23	158.47	122.30
1	J	174	THR	C-N-CA	17.22	158.47	122.30
1	N	174	THR	C-N-CA	17.22	158.47	122.30
1	I	174	THR	C-N-CA	17.20	158.43	122.30
1	L	174	THR	C-N-CA	17.20	158.41	122.30
1	K	502	GLY	O-C-N	-17.06	95.40	122.70
1	L	502	GLY	O-C-N	-17.06	95.41	122.70
1	M	502	GLY	O-C-N	-17.05	95.43	122.70
1	J	502	GLY	O-C-N	-17.03	95.45	122.70
1	N	502	GLY	O-C-N	-17.01	95.48	122.70
1	I	502	GLY	O-C-N	-17.01	95.48	122.70
1	M	174	THR	CA-C-O	15.99	153.67	120.10
1	N	174	THR	CA-C-O	15.98	153.66	120.10
1	J	174	THR	CA-C-O	15.98	153.66	120.10
1	I	174	THR	CA-C-O	15.97	153.63	120.10
1	L	174	THR	CA-C-O	15.95	153.59	120.10
1	K	174	THR	CA-C-O	15.90	153.50	120.10
2	E	25	ASP	O-C-N	-15.48	97.92	122.70
2	F	25	ASP	O-C-N	-15.46	97.96	122.70
2	B	25	ASP	O-C-N	-15.46	97.97	122.70
2	G	25	ASP	O-C-N	-15.46	97.97	122.70
2	A	25	ASP	O-C-N	-15.44	97.99	122.70
2	H	25	ASP	O-C-N	-15.43	98.01	122.70
2	C	25	ASP	O-C-N	-15.42	98.03	122.70
2	D	25	ASP	O-C-N	-15.42	98.03	122.70
2	G	43	VAL	O-C-N	-15.24	98.31	122.70
2	D	43	VAL	O-C-N	-15.24	98.32	122.70
2	H	43	VAL	O-C-N	-15.22	98.34	122.70
2	B	43	VAL	O-C-N	-15.22	98.35	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	43	VAL	O-C-N	-15.21	98.37	122.70
2	E	43	VAL	O-C-N	-15.19	98.40	122.70
2	F	43	VAL	O-C-N	-15.19	98.40	122.70
2	C	43	VAL	O-C-N	-15.12	98.52	122.70
1	N	58	ASP	O-C-N	-14.47	99.55	122.70
1	J	58	ASP	O-C-N	-14.47	99.56	122.70
1	M	58	ASP	O-C-N	-14.46	99.56	122.70
1	K	58	ASP	O-C-N	-14.46	99.57	122.70
1	L	58	ASP	O-C-N	-14.45	99.58	122.70
1	I	58	ASP	O-C-N	-14.43	99.61	122.70
1	K	641	ILE	CA-C-N	14.33	148.72	117.20
1	N	641	ILE	CA-C-N	14.33	148.73	117.20
1	I	641	ILE	CA-C-N	14.32	148.71	117.20
1	L	641	ILE	CA-C-N	14.30	148.66	117.20
1	M	641	ILE	CA-C-N	14.30	148.66	117.20
1	J	641	ILE	CA-C-N	14.29	148.64	117.20
1	K	636	GLY	O-C-N	-14.14	100.07	122.70
1	N	636	GLY	O-C-N	-14.14	100.07	122.70
1	I	636	GLY	O-C-N	-14.12	100.10	122.70
1	M	636	GLY	O-C-N	-14.12	100.10	122.70
1	J	636	GLY	O-C-N	-14.12	100.11	122.70
1	L	636	GLY	O-C-N	-14.10	100.15	122.70
1	K	446	GLU	O-C-N	-14.09	100.15	122.70
1	M	446	GLU	O-C-N	-14.08	100.17	122.70
1	I	446	GLU	O-C-N	-14.07	100.18	122.70
1	J	446	GLU	O-C-N	-14.04	100.23	122.70
1	N	446	GLU	O-C-N	-14.02	100.27	122.70
1	L	446	GLU	O-C-N	-14.01	100.29	122.70
1	N	499	GLU	O-C-N	-13.70	99.92	123.20
1	K	499	GLU	O-C-N	-13.68	99.94	123.20
1	L	499	GLU	O-C-N	-13.66	99.97	123.20
1	M	499	GLU	O-C-N	-13.66	99.97	123.20
1	J	499	GLU	O-C-N	-13.64	100.00	123.20
1	I	499	GLU	O-C-N	-13.64	100.01	123.20
1	I	359	SER	CA-C-N	13.63	143.46	116.20
1	J	359	SER	CA-C-N	13.62	143.45	116.20
1	M	359	SER	CA-C-N	13.62	143.45	116.20
1	L	359	SER	CA-C-N	13.61	143.41	116.20
1	N	359	SER	CA-C-N	13.59	143.38	116.20
1	K	359	SER	CA-C-N	13.58	143.36	116.20
1	K	772	SER	CA-C-N	13.41	146.71	117.20
1	M	772	SER	CA-C-N	13.41	146.71	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	772	SER	CA-C-N	13.41	146.70	117.20
1	N	772	SER	CA-C-N	13.40	146.69	117.20
1	J	772	SER	CA-C-N	13.39	146.65	117.20
1	I	772	SER	CA-C-N	13.38	146.64	117.20
2	H	45	VAL	CA-C-N	13.05	142.31	116.20
2	A	45	VAL	CA-C-N	13.02	142.24	116.20
2	C	45	VAL	CA-C-N	13.02	142.24	116.20
1	L	772	SER	O-C-N	-13.02	101.88	122.70
2	F	45	VAL	CA-C-N	13.01	142.22	116.20
1	M	772	SER	O-C-N	-13.01	101.89	122.70
2	B	45	VAL	CA-C-N	13.00	142.19	116.20
2	D	45	VAL	CA-C-N	13.00	142.19	116.20
2	E	45	VAL	CA-C-N	13.00	142.19	116.20
2	G	45	VAL	CA-C-N	12.97	142.15	116.20
1	K	772	SER	O-C-N	-12.97	101.94	122.70
1	N	772	SER	O-C-N	-12.97	101.95	122.70
1	I	772	SER	O-C-N	-12.94	102.00	122.70
1	L	772	SER	C-N-CA	12.92	154.00	121.70
1	K	772	SER	C-N-CA	12.91	153.98	121.70
1	J	772	SER	C-N-CA	12.91	153.97	121.70
1	M	772	SER	C-N-CA	12.91	153.97	121.70
1	I	772	SER	C-N-CA	12.90	153.96	121.70
1	N	772	SER	C-N-CA	12.90	153.96	121.70
1	J	772	SER	O-C-N	-12.88	102.09	122.70
1	I	359	SER	C-N-CA	12.83	149.23	122.30
1	N	359	SER	C-N-CA	12.82	149.22	122.30
1	J	359	SER	C-N-CA	12.80	149.19	122.30
1	K	359	SER	C-N-CA	12.80	149.18	122.30
1	M	359	SER	C-N-CA	12.80	149.17	122.30
1	L	359	SER	C-N-CA	12.79	149.16	122.30
1	K	446	GLU	CA-C-N	12.73	145.21	117.20
1	I	446	GLU	CA-C-N	12.73	145.20	117.20
1	N	446	GLU	CA-C-N	12.72	145.18	117.20
1	M	446	GLU	CA-C-N	12.70	145.15	117.20
1	N	641	ILE	C-N-CA	12.70	153.45	121.70
1	I	641	ILE	C-N-CA	12.69	153.43	121.70
1	J	446	GLU	CA-C-N	12.69	145.11	117.20
1	K	641	ILE	C-N-CA	12.68	153.40	121.70
1	L	446	GLU	CA-C-N	12.68	145.09	117.20
1	J	641	ILE	C-N-CA	12.67	153.39	121.70
1	L	641	ILE	C-N-CA	12.64	153.30	121.70
1	M	641	ILE	C-N-CA	12.64	153.30	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	681	GLU	O-C-N	-12.56	101.84	123.20
1	N	681	GLU	O-C-N	-12.53	101.89	123.20
1	K	681	GLU	O-C-N	-12.52	101.91	123.20
1	L	681	GLU	O-C-N	-12.52	101.92	123.20
1	I	681	GLU	O-C-N	-12.51	101.93	123.20
1	M	681	GLU	O-C-N	-12.50	101.95	123.20
1	N	553	ASP	CA-C-N	12.42	144.53	117.20
1	L	553	ASP	CA-C-N	12.41	144.51	117.20
1	M	553	ASP	CA-C-N	12.40	144.48	117.20
1	K	553	ASP	CA-C-N	12.40	144.47	117.20
1	J	553	ASP	CA-C-N	12.39	144.46	117.20
1	I	553	ASP	CA-C-N	12.37	144.42	117.20
2	C	45	VAL	C-N-CA	12.23	147.98	122.30
2	H	45	VAL	C-N-CA	12.22	147.97	122.30
2	A	45	VAL	C-N-CA	12.20	147.93	122.30
2	D	45	VAL	C-N-CA	12.19	147.90	122.30
2	G	45	VAL	C-N-CA	12.19	147.90	122.30
2	F	45	VAL	C-N-CA	12.18	147.88	122.30
2	E	45	VAL	C-N-CA	12.18	147.88	122.30
2	B	45	VAL	C-N-CA	12.15	147.82	122.30
1	I	446	GLU	C-N-CA	11.28	149.90	121.70
1	K	446	GLU	C-N-CA	11.28	149.91	121.70
1	N	446	GLU	C-N-CA	11.26	149.84	121.70
1	M	446	GLU	C-N-CA	11.24	149.81	121.70
1	J	446	GLU	C-N-CA	11.24	149.80	121.70
1	L	446	GLU	C-N-CA	11.24	149.79	121.70
1	L	361	GLY	O-C-N	-11.08	104.97	122.70
1	J	361	GLY	O-C-N	-11.05	105.02	122.70
1	I	361	GLY	O-C-N	-11.03	105.05	122.70
1	M	638	LEU	CA-C-N	11.03	141.46	117.20
1	M	361	GLY	O-C-N	-11.02	105.07	122.70
1	N	638	LEU	CA-C-N	11.01	141.43	117.20
1	K	361	GLY	O-C-N	-11.01	105.08	122.70
1	J	638	LEU	CA-C-N	11.00	141.39	117.20
1	N	361	GLY	O-C-N	-10.99	105.11	122.70
1	L	638	LEU	CA-C-N	10.98	141.36	117.20
1	I	638	LEU	CA-C-N	10.98	141.35	117.20
1	K	638	LEU	CA-C-N	10.96	141.32	117.20
2	A	45	VAL	O-C-N	-10.84	104.78	123.20
1	L	536	PRO	O-C-N	-10.83	105.38	122.70
1	K	536	PRO	O-C-N	-10.82	105.39	122.70
1	J	536	PRO	O-C-N	-10.80	105.41	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	536	PRO	O-C-N	-10.80	105.42	122.70
2	E	45	VAL	O-C-N	-10.80	104.84	123.20
2	F	45	VAL	O-C-N	-10.78	104.87	123.20
1	I	536	PRO	O-C-N	-10.78	105.45	122.70
2	D	45	VAL	O-C-N	-10.78	104.87	123.20
1	M	536	PRO	O-C-N	-10.78	105.45	122.70
2	H	45	VAL	O-C-N	-10.78	104.88	123.20
2	C	45	VAL	O-C-N	-10.76	104.91	123.20
2	G	45	VAL	O-C-N	-10.76	104.91	123.20
2	B	45	VAL	O-C-N	-10.73	104.96	123.20
2	E	25	ASP	CA-C-N	10.08	139.38	117.20
2	B	25	ASP	CA-C-N	10.07	139.36	117.20
2	D	25	ASP	CA-C-N	10.06	139.33	117.20
2	C	25	ASP	CA-C-N	10.05	139.32	117.20
2	F	25	ASP	CA-C-N	10.05	139.30	117.20
2	A	25	ASP	CA-C-N	10.04	139.29	117.20
2	G	25	ASP	CA-C-N	10.04	139.28	117.20
2	H	25	ASP	CA-C-N	10.02	139.25	117.20
2	D	368	SER	O-C-N	-9.93	106.82	122.70
2	G	368	SER	O-C-N	-9.93	106.82	122.70
2	B	368	SER	O-C-N	-9.92	106.82	122.70
2	C	368	SER	O-C-N	-9.91	106.84	122.70
2	A	368	SER	O-C-N	-9.89	106.88	122.70
2	F	368	SER	O-C-N	-9.88	106.89	122.70
2	E	368	SER	O-C-N	-9.88	106.90	122.70
2	H	368	SER	O-C-N	-9.88	106.90	122.70
1	I	553	ASP	C-N-CA	9.68	145.90	121.70
1	N	553	ASP	C-N-CA	9.68	145.89	121.70
1	K	553	ASP	C-N-CA	9.67	145.88	121.70
1	L	553	ASP	C-N-CA	9.66	145.86	121.70
1	J	553	ASP	C-N-CA	9.65	145.83	121.70
1	M	553	ASP	C-N-CA	9.64	145.80	121.70
1	N	638	LEU	C-N-CA	9.57	145.63	121.70
1	M	638	LEU	C-N-CA	9.56	145.60	121.70
1	L	638	LEU	C-N-CA	9.55	145.58	121.70
1	J	638	LEU	C-N-CA	9.54	145.55	121.70
1	K	638	LEU	C-N-CA	9.53	145.53	121.70
1	I	638	LEU	C-N-CA	9.52	145.50	121.70
2	F	333	PRO	O-C-N	-9.35	107.74	122.70
2	D	333	PRO	O-C-N	-9.29	107.83	122.70
2	B	333	PRO	O-C-N	-9.29	107.84	122.70
2	G	333	PRO	O-C-N	-9.26	107.89	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	708	ARG	O-C-N	-9.26	107.89	122.70
2	A	333	PRO	O-C-N	-9.25	107.90	122.70
2	C	333	PRO	O-C-N	-9.24	107.91	122.70
1	L	708	ARG	O-C-N	-9.22	107.95	122.70
1	M	708	ARG	O-C-N	-9.22	107.95	122.70
2	E	333	PRO	O-C-N	-9.22	107.95	122.70
1	I	708	ARG	O-C-N	-9.21	107.95	122.70
1	K	502	GLY	C-N-CA	9.21	144.74	121.70
1	L	502	GLY	C-N-CA	9.21	144.74	121.70
2	H	333	PRO	O-C-N	-9.21	107.95	122.70
1	J	502	GLY	C-N-CA	9.21	144.73	121.70
1	N	708	ARG	O-C-N	-9.21	107.96	122.70
1	L	502	GLY	CA-C-N	9.21	137.46	117.20
1	M	502	GLY	C-N-CA	9.20	144.71	121.70
1	I	502	GLY	C-N-CA	9.20	144.70	121.70
1	N	502	GLY	C-N-CA	9.19	144.68	121.70
1	J	708	ARG	O-C-N	-9.19	108.00	122.70
1	I	502	GLY	CA-C-N	9.19	137.41	117.20
1	J	502	GLY	CA-C-N	9.18	137.40	117.20
1	K	502	GLY	CA-C-N	9.18	137.39	117.20
1	M	502	GLY	CA-C-N	9.17	137.38	117.20
1	N	502	GLY	CA-C-N	9.14	137.31	117.20
1	J	172	TYR	O-C-N	-9.14	107.66	123.20
1	K	172	TYR	O-C-N	-9.13	107.67	123.20
1	I	172	TYR	O-C-N	-9.11	107.71	123.20
1	L	172	TYR	O-C-N	-9.09	107.75	123.20
1	M	172	TYR	O-C-N	-9.09	107.76	123.20
1	N	172	TYR	O-C-N	-9.08	107.77	123.20
1	J	662	GLY	O-C-N	-8.93	108.42	122.70
1	N	662	GLY	O-C-N	-8.93	108.42	122.70
1	K	662	GLY	O-C-N	-8.89	108.47	122.70
1	L	662	GLY	O-C-N	-8.88	108.50	122.70
1	I	662	GLY	O-C-N	-8.85	108.55	122.70
1	M	662	GLY	O-C-N	-8.83	108.57	122.70
1	K	58	ASP	CA-C-N	8.68	136.31	117.20
1	N	636	GLY	CA-C-N	8.67	136.28	117.20
1	I	636	GLY	CA-C-N	8.67	136.27	117.20
1	N	58	ASP	CA-C-N	8.66	136.26	117.20
1	M	58	ASP	CA-C-N	8.65	136.24	117.20
1	I	58	ASP	CA-C-N	8.64	136.21	117.20
1	K	636	GLY	CA-C-N	8.64	136.20	117.20
1	L	636	GLY	CA-C-N	8.63	136.19	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	636	GLY	CA-C-N	8.63	136.19	117.20
1	J	58	ASP	CA-C-N	8.63	136.18	117.20
1	J	636	GLY	CA-C-N	8.63	136.18	117.20
1	L	58	ASP	CA-C-N	8.62	136.16	117.20
1	N	636	GLY	C-N-CA	8.41	142.72	121.70
1	I	636	GLY	C-N-CA	8.39	142.67	121.70
1	K	636	GLY	C-N-CA	8.39	142.66	121.70
1	J	636	GLY	C-N-CA	8.38	142.64	121.70
1	L	636	GLY	C-N-CA	8.37	142.62	121.70
1	M	636	GLY	C-N-CA	8.35	142.58	121.70
2	G	307	PRO	CA-C-N	8.15	132.50	116.20
2	H	307	PRO	CA-C-N	8.14	132.48	116.20
2	D	307	PRO	CA-C-N	8.14	132.48	116.20
2	C	307	PRO	CA-C-N	8.14	132.47	116.20
2	F	307	PRO	CA-C-N	8.13	132.47	116.20
2	E	307	PRO	CA-C-N	8.12	132.45	116.20
2	B	307	PRO	CA-C-N	8.12	132.44	116.20
2	A	307	PRO	CA-C-N	8.12	132.43	116.20
2	G	307	PRO	O-C-N	-8.10	109.43	123.20
1	M	459	GLY	O-C-N	-8.09	109.76	122.70
2	F	307	PRO	O-C-N	-8.09	109.45	123.20
2	H	307	PRO	O-C-N	-8.08	109.46	123.20
1	J	361	GLY	CA-C-N	8.08	134.98	117.20
2	A	307	PRO	O-C-N	-8.08	109.47	123.20
2	D	307	PRO	O-C-N	-8.08	109.46	123.20
2	E	307	PRO	O-C-N	-8.08	109.46	123.20
1	L	361	GLY	CA-C-N	8.07	134.96	117.20
1	J	459	GLY	O-C-N	-8.06	109.80	122.70
1	I	459	GLY	O-C-N	-8.06	109.81	122.70
1	K	361	GLY	CA-C-N	8.05	134.91	117.20
1	K	459	GLY	O-C-N	-8.05	109.82	122.70
1	N	459	GLY	O-C-N	-8.05	109.82	122.70
2	C	307	PRO	O-C-N	-8.05	109.52	123.20
1	M	361	GLY	CA-C-N	8.04	134.90	117.20
1	N	681	GLU	CA-C-N	8.04	132.28	116.20
1	I	681	GLU	CA-C-N	8.03	132.26	116.20
1	L	499	GLU	CA-C-N	8.03	132.26	116.20
1	M	499	GLU	CA-C-N	8.03	132.26	116.20
2	B	307	PRO	O-C-N	-8.03	109.55	123.20
1	L	459	GLY	O-C-N	-8.02	109.87	122.70
1	L	681	GLU	CA-C-N	8.01	132.22	116.20
1	N	361	GLY	CA-C-N	8.01	134.83	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	499	GLU	CA-C-N	8.01	132.22	116.20
1	N	499	GLU	CA-C-N	8.01	132.22	116.20
1	J	681	GLU	CA-C-N	8.01	132.21	116.20
1	I	361	GLY	CA-C-N	8.00	134.81	117.20
1	K	681	GLU	CA-C-N	8.00	132.20	116.20
1	I	499	GLU	CA-C-N	8.00	132.19	116.20
1	J	499	GLU	CA-C-N	7.99	132.19	116.20
1	M	681	GLU	CA-C-N	7.99	132.17	116.20
1	L	361	GLY	C-N-CA	7.88	141.39	121.70
1	J	361	GLY	C-N-CA	7.87	141.38	121.70
1	M	361	GLY	C-N-CA	7.87	141.36	121.70
1	K	361	GLY	C-N-CA	7.85	141.34	121.70
1	N	361	GLY	C-N-CA	7.85	141.32	121.70
1	I	361	GLY	C-N-CA	7.85	141.31	121.70
1	L	355	ALA	CB-CA-C	-7.80	98.39	110.10
1	K	355	ALA	CB-CA-C	-7.80	98.40	110.10
1	I	355	ALA	CB-CA-C	-7.80	98.40	110.10
2	B	25	ASP	C-N-CA	7.78	141.14	121.70
1	N	355	ALA	CB-CA-C	-7.77	98.44	110.10
2	E	25	ASP	C-N-CA	7.77	141.12	121.70
2	A	25	ASP	C-N-CA	7.76	141.10	121.70
1	K	622	GLU	CB-CA-C	-7.76	94.88	110.40
2	G	25	ASP	C-N-CA	7.76	141.09	121.70
2	D	25	ASP	C-N-CA	7.75	141.07	121.70
1	N	622	GLU	CB-CA-C	-7.74	94.91	110.40
2	F	25	ASP	C-N-CA	7.74	141.06	121.70
1	J	355	ALA	CB-CA-C	-7.73	98.50	110.10
2	C	25	ASP	C-N-CA	7.73	141.04	121.70
1	M	355	ALA	CB-CA-C	-7.73	98.50	110.10
2	H	25	ASP	C-N-CA	7.72	141.00	121.70
1	M	622	GLU	CB-CA-C	-7.71	94.99	110.40
1	I	622	GLU	CB-CA-C	-7.70	94.99	110.40
1	L	622	GLU	CB-CA-C	-7.70	95.00	110.40
1	J	622	GLU	CB-CA-C	-7.68	95.03	110.40
1	K	461	GLU	O-C-N	-7.65	110.47	122.70
1	J	461	GLU	O-C-N	-7.63	110.50	122.70
1	N	461	GLU	O-C-N	-7.62	110.51	122.70
1	I	461	GLU	O-C-N	-7.61	110.52	122.70
1	N	56	LYS	O-C-N	-7.60	110.54	122.70
1	M	703	GLY	C-N-CA	7.60	138.25	122.30
1	J	703	GLY	C-N-CA	7.59	138.25	122.30
1	J	703	GLY	CA-C-N	7.59	131.38	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	703	GLY	C-N-CA	7.59	138.24	122.30
1	N	703	GLY	CA-C-N	7.58	131.37	116.20
1	N	703	GLY	C-N-CA	7.58	138.23	122.30
1	L	703	GLY	CA-C-N	7.58	131.36	116.20
1	M	703	GLY	CA-C-N	7.58	131.36	116.20
1	L	461	GLU	O-C-N	-7.58	110.57	122.70
1	M	461	GLU	O-C-N	-7.58	110.57	122.70
1	L	703	GLY	C-N-CA	7.58	138.21	122.30
1	L	56	LYS	O-C-N	-7.57	110.58	122.70
1	I	56	LYS	O-C-N	-7.57	110.58	122.70
1	K	703	GLY	CA-C-N	7.57	131.34	116.20
1	J	56	LYS	O-C-N	-7.57	110.59	122.70
1	I	703	GLY	C-N-CA	7.56	138.19	122.30
1	I	703	GLY	CA-C-N	7.56	131.32	116.20
1	K	56	LYS	O-C-N	-7.55	110.62	122.70
1	M	56	LYS	O-C-N	-7.54	110.64	122.70
1	L	361	GLY	N-CA-C	7.37	131.52	113.10
1	J	361	GLY	N-CA-C	7.36	131.50	113.10
1	M	361	GLY	N-CA-C	7.35	131.48	113.10
1	K	361	GLY	N-CA-C	7.33	131.43	113.10
1	N	361	GLY	N-CA-C	7.33	131.42	113.10
1	I	361	GLY	N-CA-C	7.33	131.42	113.10
1	N	681	GLU	C-N-CA	7.25	137.51	122.30
1	L	681	GLU	C-N-CA	7.24	137.51	122.30
1	J	681	GLU	C-N-CA	7.24	137.49	122.30
1	I	681	GLU	C-N-CA	7.23	137.48	122.30
1	L	536	PRO	CA-C-N	7.21	133.07	117.20
1	J	536	PRO	CA-C-N	7.21	133.07	117.20
1	K	681	GLU	C-N-CA	7.21	137.45	122.30
1	M	536	PRO	CA-C-N	7.21	133.07	117.20
1	N	536	PRO	CA-C-N	7.21	133.05	117.20
1	K	536	PRO	CA-C-N	7.20	133.05	117.20
1	M	681	GLU	C-N-CA	7.20	137.42	122.30
1	I	536	PRO	CA-C-N	7.19	133.02	117.20
2	H	244	ASP	O-C-N	-7.19	110.98	123.20
2	D	244	ASP	O-C-N	-7.15	111.04	123.20
2	B	244	ASP	O-C-N	-7.15	111.04	123.20
2	F	244	ASP	O-C-N	-7.14	111.06	123.20
2	A	244	ASP	O-C-N	-7.13	111.08	123.20
2	E	244	ASP	O-C-N	-7.12	111.09	123.20
2	G	244	ASP	O-C-N	-7.12	111.10	123.20
2	C	244	ASP	O-C-N	-7.12	111.10	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	642	SER	O-C-N	-7.08	111.37	122.70
1	I	622	GLU	CA-C-O	7.07	134.95	120.10
1	K	622	GLU	CA-C-O	7.07	134.95	120.10
1	L	642	SER	O-C-N	-7.07	111.39	122.70
1	I	642	SER	O-C-N	-7.07	111.39	122.70
1	M	622	GLU	CA-C-O	7.04	134.88	120.10
1	M	642	SER	O-C-N	-7.03	111.45	122.70
1	N	622	GLU	CA-C-O	7.03	134.87	120.10
1	J	622	GLU	CA-C-O	7.03	134.86	120.10
1	L	622	GLU	CA-C-O	7.03	134.86	120.10
1	N	642	SER	O-C-N	-7.02	111.47	122.70
1	K	642	SER	O-C-N	-6.98	111.53	122.70
1	L	282	PHE	O-C-N	-6.97	111.54	122.70
1	N	282	PHE	O-C-N	-6.97	111.55	122.70
1	M	282	PHE	O-C-N	-6.96	111.56	122.70
1	I	282	PHE	O-C-N	-6.93	111.61	122.70
1	K	282	PHE	O-C-N	-6.91	111.64	122.70
1	J	282	PHE	O-C-N	-6.91	111.65	122.70
1	K	58	ASP	C-N-CA	6.89	138.93	121.70
1	N	58	ASP	C-N-CA	6.88	138.90	121.70
1	M	58	ASP	C-N-CA	6.88	138.89	121.70
1	J	58	ASP	C-N-CA	6.88	138.89	121.70
1	I	58	ASP	C-N-CA	6.87	138.88	121.70
1	M	536	PRO	C-N-CA	6.84	138.81	121.70
1	L	58	ASP	C-N-CA	6.84	138.81	121.70
1	L	536	PRO	C-N-CA	6.84	138.81	121.70
1	N	536	PRO	C-N-CA	6.84	138.79	121.70
1	J	536	PRO	C-N-CA	6.83	138.78	121.70
1	K	536	PRO	C-N-CA	6.83	138.78	121.70
1	I	536	PRO	C-N-CA	6.83	138.77	121.70
1	L	499	GLU	C-N-CA	6.56	136.09	122.30
1	N	499	GLU	C-N-CA	6.56	136.07	122.30
1	K	499	GLU	C-N-CA	6.55	136.05	122.30
1	M	499	GLU	C-N-CA	6.54	136.04	122.30
1	I	499	GLU	C-N-CA	6.54	136.04	122.30
1	J	499	GLU	C-N-CA	6.54	136.03	122.30
1	M	36	GLN	O-C-N	-6.49	112.32	122.70
1	J	36	GLN	O-C-N	-6.48	112.33	122.70
1	K	36	GLN	O-C-N	-6.47	112.34	122.70
1	L	36	GLN	O-C-N	-6.47	112.35	122.70
1	I	36	GLN	O-C-N	-6.47	112.36	122.70
1	N	36	GLN	O-C-N	-6.46	112.36	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	42	GLY	O-C-N	-6.39	112.48	122.70
2	C	42	GLY	O-C-N	-6.36	112.52	122.70
2	G	42	GLY	O-C-N	-6.36	112.52	122.70
2	H	42	GLY	O-C-N	-6.36	112.53	122.70
2	A	42	GLY	O-C-N	-6.35	112.53	122.70
2	D	42	GLY	O-C-N	-6.35	112.54	122.70
2	B	42	GLY	O-C-N	-6.35	112.55	122.70
2	E	42	GLY	O-C-N	-6.33	112.56	122.70
1	J	459	GLY	C-N-CA	6.28	137.40	121.70
1	N	459	GLY	C-N-CA	6.26	137.36	121.70
1	L	459	GLY	C-N-CA	6.26	137.34	121.70
1	M	459	GLY	C-N-CA	6.25	137.32	121.70
1	N	459	GLY	CA-C-N	6.25	130.95	117.20
1	I	459	GLY	C-N-CA	6.25	137.31	121.70
1	J	459	GLY	CA-C-N	6.24	130.93	117.20
1	N	173	GLY	C-N-CA	6.24	137.29	121.70
1	K	459	GLY	C-N-CA	6.24	137.29	121.70
1	L	459	GLY	CA-C-N	6.23	130.91	117.20
1	M	459	GLY	CA-C-N	6.23	130.90	117.20
1	K	173	GLY	C-N-CA	6.22	137.26	121.70
1	I	459	GLY	CA-C-N	6.22	130.89	117.20
1	I	173	GLY	C-N-CA	6.22	137.25	121.70
1	J	173	GLY	C-N-CA	6.22	137.24	121.70
1	N	229	LEU	O-C-N	-6.21	112.77	122.70
1	M	173	GLY	C-N-CA	6.20	137.19	121.70
1	K	459	GLY	CA-C-N	6.19	130.83	117.20
1	L	173	GLY	C-N-CA	6.19	137.17	121.70
1	J	172	TYR	CA-C-O	6.17	133.06	120.10
1	J	229	LEU	O-C-N	-6.17	112.83	122.70
1	K	229	LEU	O-C-N	-6.17	112.83	122.70
1	M	229	LEU	O-C-N	-6.17	112.83	122.70
1	I	229	LEU	O-C-N	-6.17	112.84	122.70
1	L	229	LEU	O-C-N	-6.16	112.84	122.70
1	I	172	TYR	CA-C-O	6.15	133.01	120.10
1	K	172	TYR	CA-C-O	6.14	133.00	120.10
1	L	172	TYR	CA-C-O	6.13	132.98	120.10
1	N	172	TYR	CA-C-O	6.13	132.97	120.10
1	M	172	TYR	CA-C-O	6.12	132.96	120.10
1	I	641	ILE	CA-C-O	6.10	132.90	120.10
1	J	641	ILE	CA-C-O	6.10	132.91	120.10
1	M	641	ILE	CA-C-O	6.09	132.89	120.10
1	N	641	ILE	CA-C-O	6.07	132.85	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	641	ILE	CA-C-O	6.07	132.85	120.10
2	D	43	VAL	CA-C-N	6.06	130.54	117.20
2	H	43	VAL	CA-C-N	6.06	130.53	117.20
1	L	641	ILE	CA-C-O	6.06	132.82	120.10
2	B	43	VAL	CA-C-N	6.05	130.52	117.20
2	F	43	VAL	CA-C-N	6.03	130.47	117.20
2	C	43	VAL	CA-C-N	6.03	130.47	117.20
2	E	43	VAL	CA-C-N	6.03	130.47	117.20
2	A	43	VAL	CA-C-N	6.03	130.46	117.20
2	G	43	VAL	CA-C-N	6.00	130.40	117.20
1	M	597	ASN	O-C-N	-5.94	113.19	122.70
1	K	597	ASN	O-C-N	-5.93	113.20	122.70
1	L	622	GLU	N-CA-C	5.93	127.02	111.00
1	N	597	ASN	O-C-N	-5.93	113.21	122.70
2	F	333	PRO	C-N-CA	5.93	136.53	121.70
1	I	597	ASN	O-C-N	-5.93	113.21	122.70
1	J	622	GLU	N-CA-C	5.93	127.00	111.00
2	C	333	PRO	C-N-CA	5.93	136.52	121.70
2	D	333	PRO	C-N-CA	5.93	136.52	121.70
2	B	333	PRO	C-N-CA	5.92	136.51	121.70
1	N	622	GLU	N-CA-C	5.92	126.99	111.00
2	E	333	PRO	C-N-CA	5.92	136.50	121.70
2	A	333	PRO	C-N-CA	5.92	136.50	121.70
1	I	622	GLU	N-CA-C	5.91	126.96	111.00
2	G	333	PRO	C-N-CA	5.91	136.49	121.70
1	N	359	SER	CA-C-O	5.91	132.51	120.10
1	L	173	GLY	N-CA-C	5.91	127.87	113.10
1	M	173	GLY	N-CA-C	5.91	127.86	113.10
1	N	173	GLY	N-CA-C	5.91	127.86	113.10
1	K	173	GLY	N-CA-C	5.90	127.86	113.10
1	K	359	SER	CA-C-O	5.90	132.50	120.10
1	L	597	ASN	O-C-N	-5.90	113.26	122.70
1	K	622	GLU	N-CA-C	5.90	126.93	111.00
1	M	622	GLU	N-CA-C	5.90	126.93	111.00
1	J	173	GLY	N-CA-C	5.90	127.84	113.10
1	J	597	ASN	O-C-N	-5.90	113.26	122.70
2	H	333	PRO	C-N-CA	5.90	136.44	121.70
1	L	359	SER	CA-C-O	5.89	132.47	120.10
1	I	359	SER	CA-C-O	5.89	132.46	120.10
1	M	359	SER	CA-C-O	5.89	132.46	120.10
1	I	173	GLY	N-CA-C	5.88	127.81	113.10
1	J	359	SER	CA-C-O	5.86	132.40	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	173	GLY	CA-C-N	5.83	130.03	117.20
1	K	173	GLY	CA-C-N	5.82	129.99	117.20
1	J	173	GLY	CA-C-N	5.81	129.98	117.20
1	I	173	GLY	CA-C-N	5.80	129.95	117.20
1	M	173	GLY	CA-C-N	5.80	129.95	117.20
1	L	173	GLY	CA-C-N	5.79	129.95	117.20
1	N	447	THR	O-C-N	-5.76	113.48	122.70
1	L	447	THR	O-C-N	-5.76	113.49	122.70
1	I	447	THR	O-C-N	-5.75	113.51	122.70
1	K	447	THR	O-C-N	-5.75	113.51	122.70
1	M	447	THR	O-C-N	-5.74	113.51	122.70
1	J	447	THR	O-C-N	-5.73	113.53	122.70
2	D	15	GLY	C-N-CA	5.63	135.77	121.70
1	J	637	LYS	C-N-CA	5.63	135.77	121.70
2	B	15	GLY	C-N-CA	5.63	135.77	121.70
2	A	15	GLY	C-N-CA	5.62	135.76	121.70
1	L	460	PHE	O-C-N	-5.62	113.70	122.70
2	H	15	GLY	C-N-CA	5.62	135.75	121.70
1	N	460	PHE	O-C-N	-5.62	113.71	122.70
1	N	637	LYS	C-N-CA	5.62	135.75	121.70
1	K	460	PHE	O-C-N	-5.62	113.71	122.70
1	K	637	LYS	C-N-CA	5.62	135.75	121.70
1	J	460	PHE	O-C-N	-5.61	113.72	122.70
2	C	15	GLY	C-N-CA	5.61	135.73	121.70
2	G	15	GLY	C-N-CA	5.61	135.71	121.70
2	F	15	GLY	C-N-CA	5.60	135.71	121.70
1	L	637	LYS	C-N-CA	5.60	135.70	121.70
2	E	15	GLY	C-N-CA	5.60	135.70	121.70
1	I	637	LYS	C-N-CA	5.59	135.69	121.70
1	M	637	LYS	C-N-CA	5.59	135.69	121.70
1	N	38	GLY	O-C-N	-5.59	113.75	122.70
1	J	703	GLY	O-C-N	-5.59	113.70	123.20
1	K	38	GLY	O-C-N	-5.57	113.78	122.70
1	L	703	GLY	O-C-N	-5.57	113.73	123.20
1	M	460	PHE	O-C-N	-5.56	113.80	122.70
1	M	703	GLY	O-C-N	-5.56	113.75	123.20
1	M	38	GLY	O-C-N	-5.54	113.83	122.70
1	I	460	PHE	O-C-N	-5.54	113.83	122.70
2	B	245	GLY	O-C-N	-5.54	113.83	122.70
1	L	38	GLY	O-C-N	-5.53	113.86	122.70
1	J	38	GLY	O-C-N	-5.53	113.86	122.70
1	K	703	GLY	O-C-N	-5.53	113.81	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	703	GLY	O-C-N	-5.52	113.82	123.20
2	D	245	GLY	O-C-N	-5.52	113.87	122.70
1	N	703	GLY	O-C-N	-5.52	113.82	123.20
2	C	245	GLY	O-C-N	-5.51	113.88	122.70
2	H	245	GLY	O-C-N	-5.51	113.88	122.70
2	F	245	GLY	O-C-N	-5.51	113.89	122.70
1	I	38	GLY	O-C-N	-5.50	113.89	122.70
2	A	245	GLY	O-C-N	-5.50	113.89	122.70
2	E	245	GLY	O-C-N	-5.50	113.90	122.70
2	G	245	GLY	O-C-N	-5.50	113.90	122.70
2	F	329	ILE	O-C-N	-5.38	114.09	122.70
2	H	329	ILE	O-C-N	-5.36	114.13	122.70
2	A	329	ILE	O-C-N	-5.34	114.16	122.70
2	D	329	ILE	O-C-N	-5.33	114.17	122.70
2	G	43	VAL	CA-C-O	5.33	131.29	120.10
2	E	329	ILE	O-C-N	-5.32	114.19	122.70
1	L	355	ALA	N-CA-C	5.32	125.35	111.00
1	I	355	ALA	N-CA-C	5.31	125.35	111.00
2	G	329	ILE	O-C-N	-5.30	114.21	122.70
2	C	329	ILE	O-C-N	-5.29	114.24	122.70
1	K	355	ALA	N-CA-C	5.28	125.26	111.00
1	N	355	ALA	N-CA-C	5.28	125.26	111.00
2	B	329	ILE	O-C-N	-5.28	114.25	122.70
1	J	355	ALA	N-CA-C	5.28	125.24	111.00
2	A	43	VAL	CA-C-O	5.27	131.17	120.10
2	D	43	VAL	CA-C-O	5.25	131.14	120.10
1	M	355	ALA	N-CA-C	5.25	125.18	111.00
2	B	43	VAL	CA-C-O	5.25	131.13	120.10
2	E	43	VAL	CA-C-O	5.25	131.13	120.10
2	F	43	VAL	CA-C-O	5.25	131.13	120.10
2	H	43	VAL	CA-C-O	5.25	131.12	120.10
2	F	333	PRO	CA-C-N	5.21	128.67	117.20
2	C	43	VAL	CA-C-O	5.20	131.01	120.10
2	C	333	PRO	CA-C-N	5.20	128.63	117.20
2	E	333	PRO	CA-C-N	5.19	128.62	117.20
2	D	333	PRO	CA-C-N	5.19	128.61	117.20
2	B	333	PRO	CA-C-N	5.18	128.61	117.20
2	G	333	PRO	CA-C-N	5.18	128.60	117.20
2	A	333	PRO	CA-C-N	5.18	128.60	117.20
2	H	333	PRO	CA-C-N	5.16	128.56	117.20
2	F	307	PRO	C-N-CA	5.14	133.09	122.30
2	G	307	PRO	C-N-CA	5.13	133.08	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	307	PRO	C-N-CA	5.13	133.06	122.30
2	D	42	GLY	N-CA-C	5.12	125.90	113.10
2	E	307	PRO	C-N-CA	5.12	133.05	122.30
2	H	307	PRO	C-N-CA	5.12	133.04	122.30
2	D	307	PRO	C-N-CA	5.11	133.02	122.30
2	B	307	PRO	C-N-CA	5.11	133.02	122.30
2	E	42	GLY	N-CA-C	5.10	125.86	113.10
2	H	42	GLY	N-CA-C	5.10	125.85	113.10
2	C	42	GLY	N-CA-C	5.10	125.84	113.10
2	B	42	GLY	N-CA-C	5.09	125.83	113.10
2	A	307	PRO	C-N-CA	5.09	132.99	122.30
2	G	42	GLY	N-CA-C	5.09	125.82	113.10
2	A	42	GLY	N-CA-C	5.08	125.79	113.10
2	F	42	GLY	N-CA-C	5.08	125.80	113.10
1	I	38	GLY	N-CA-C	5.03	125.67	113.10
1	K	38	GLY	N-CA-C	5.02	125.65	113.10
1	M	38	GLY	N-CA-C	5.02	125.65	113.10
1	L	38	GLY	N-CA-C	5.01	125.63	113.10
1	N	38	GLY	N-CA-C	5.01	125.63	113.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	179	ASP	Peptide
1	J	179	ASP	Peptide
1	K	179	ASP	Peptide
1	L	179	ASP	Peptide
1	M	179	ASP	Peptide
1	N	179	ASP	Peptide

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	3825	0	1650	11	0
1	J	3825	0	1650	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	3825	0	1650	11	0
1	L	3825	0	1650	11	0
1	M	3825	0	1650	11	0
1	N	3825	0	1650	10	0
2	A	1806	0	817	4	0
2	B	1806	0	817	3	0
2	C	1806	0	817	7	0
2	D	1806	0	817	6	0
2	E	1806	0	817	8	0
2	F	1806	0	817	7	0
2	G	1806	0	817	5	0
2	H	1806	0	817	4	0
All	All	37398	0	16436	90	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (90) 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:J:174:THR:C	1:J:175:GLY:CA	1.80	1.50
1:L:174:THR:C	1:L:175:GLY:CA	1.80	1.50
1:I:174:THR:C	1:I:175:GLY:CA	1.80	1.48
1:K:174:THR:C	1:K:175:GLY:CA	1.80	1.48
1:N:174:THR:C	1:N:175:GLY:CA	1.80	1.48
1:M:174:THR:C	1:M:175:GLY:CA	1.80	1.45
1:N:174:THR:CA	1:N:175:GLY:N	1.85	1.40
1:L:174:THR:CA	1:L:175:GLY:N	1.85	1.40
1:M:174:THR:CA	1:M:175:GLY:N	1.85	1.39
1:J:174:THR:CA	1:J:175:GLY:N	1.85	1.39
1:K:174:THR:CA	1:K:175:GLY:N	1.85	1.39
1:I:174:THR:O	1:I:174:THR:CA	1.72	1.38
1:I:174:THR:CA	1:I:175:GLY:N	1.85	1.38
1:K:174:THR:CA	1:K:174:THR:O	1.71	1.38
1:M:174:THR:CA	1:M:174:THR:O	1.72	1.38
1:N:174:THR:CA	1:N:174:THR:O	1.71	1.34
1:L:174:THR:CA	1:L:174:THR:O	1.71	1.33
1:J:174:THR:CA	1:J:174:THR:O	1.71	1.32
1:J:276:ARG:O	1:J:276:ARG:CA	1.89	1.21
1:L:276:ARG:O	1:L:276:ARG:CA	1.88	1.21
1:N:276:ARG:O	1:N:276:ARG:CA	1.89	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:276:ARG:O	1:I:276:ARG:CA	1.89	1.19
1:M:276:ARG:O	1:M:276:ARG:CA	1.88	1.19
1:K:276:ARG:O	1:K:276:ARG:CA	1.89	1.18
1:M:276:ARG:O	1:M:277:GLY:CA	1.92	1.17
1:I:276:ARG:O	1:I:277:GLY:CA	1.92	1.16
1:K:276:ARG:O	1:K:277:GLY:CA	1.92	1.16
1:N:276:ARG:O	1:N:277:GLY:CA	1.92	1.16
1:J:276:ARG:O	1:J:277:GLY:CA	1.92	1.15
1:L:276:ARG:O	1:L:277:GLY:CA	1.92	1.14
1:M:174:THR:CB	1:M:175:GLY:N	2.24	1.01
1:K:174:THR:CB	1:K:175:GLY:N	2.24	1.01
1:I:174:THR:CB	1:I:175:GLY:N	2.24	1.00
1:L:174:THR:CB	1:L:175:GLY:N	2.24	1.00
1:N:174:THR:CB	1:N:175:GLY:N	2.24	0.99
1:J:174:THR:CB	1:J:175:GLY:N	2.24	0.99
2:C:44:MET:N	2:E:168:GLY:O	2.07	0.88
2:D:44:MET:N	2:F:168:GLY:O	2.08	0.85
2:A:44:MET:N	2:C:168:GLY:O	2.09	0.85
2:F:44:MET:N	2:H:168:GLY:O	2.13	0.82
2:E:44:MET:N	2:G:168:GLY:O	2.20	0.74
2:B:44:MET:N	2:D:168:GLY:O	2.24	0.70
1:L:276:ARG:O	1:L:277:GLY:N	0.55	0.69
1:I:276:ARG:O	1:I:277:GLY:N	0.55	0.69
1:J:276:ARG:O	1:J:277:GLY:N	0.55	0.68
1:M:276:ARG:O	1:M:277:GLY:N	0.55	0.68
1:N:276:ARG:O	1:N:277:GLY:N	0.55	0.68
1:K:276:ARG:O	1:K:277:GLY:N	0.55	0.67
2:C:42:GLY:HA2	2:E:169:TYR:HA	1.77	0.67
2:E:42:GLY:HA2	2:G:169:TYR:HA	1.83	0.61
1:M:276:ARG:O	1:M:276:ARG:C	0.43	0.59
1:I:276:ARG:O	1:I:276:ARG:C	0.43	0.59
1:K:276:ARG:O	1:K:276:ARG:C	0.43	0.59
2:D:42:GLY:HA2	2:F:169:TYR:HA	1.85	0.58
1:N:276:ARG:O	1:N:276:ARG:C	0.43	0.58
1:L:276:ARG:O	1:L:276:ARG:C	0.43	0.58
1:J:276:ARG:O	1:J:276:ARG:C	0.43	0.56
2:A:42:GLY:HA2	2:C:169:TYR:HA	1.88	0.55
2:C:43:VAL:N	2:E:169:TYR:HA	2.25	0.52
1:M:553:ASP:O	1:M:553:ASP:CB	2.26	0.50
1:K:553:ASP:O	1:K:553:ASP:CB	2.26	0.50
2:E:43:VAL:N	2:G:168:GLY:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:42:GLY:HA2	2:H:169:TYR:HA	1.94	0.49
1:I:553:ASP:O	1:I:553:ASP:CB	2.26	0.49
2:B:42:GLY:HA2	2:D:169:TYR:HA	1.94	0.49
2:G:295:ALA:HA	2:G:328:LYS:H	1.77	0.49
2:D:295:ALA:HA	2:D:328:LYS:H	1.78	0.49
2:F:295:ALA:HA	2:F:328:LYS:H	1.77	0.49
2:B:295:ALA:HA	2:B:328:LYS:H	1.78	0.48
2:C:295:ALA:HA	2:C:328:LYS:H	1.77	0.48
1:L:553:ASP:O	1:L:553:ASP:CB	2.26	0.48
2:A:295:ALA:HA	2:A:328:LYS:H	1.77	0.48
2:D:43:VAL:N	2:F:169:TYR:HA	2.29	0.48
2:E:295:ALA:HA	2:E:328:LYS:H	1.78	0.48
2:H:295:ALA:HA	2:H:328:LYS:H	1.78	0.48
2:A:43:VAL:N	2:C:169:TYR:HA	2.31	0.46
1:K:174:THR:C	1:K:175:GLY:N	0.63	0.46
1:L:174:THR:C	1:L:175:GLY:N	0.63	0.46
1:N:174:THR:C	1:N:175:GLY:N	0.63	0.45
1:I:174:THR:C	1:I:175:GLY:N	0.63	0.44
1:I:174:THR:C	1:I:174:THR:O	0.51	0.44
1:J:174:THR:C	1:J:175:GLY:N	0.63	0.44
1:M:174:THR:C	1:M:174:THR:O	0.51	0.44
1:N:174:THR:C	1:N:174:THR:O	0.51	0.44
2:F:43:VAL:N	2:H:169:TYR:HA	2.32	0.44
1:M:174:THR:C	1:M:175:GLY:N	0.63	0.43
2:E:43:VAL:N	2:G:169:TYR:HA	2.33	0.43
1:J:174:THR:C	1:J:174:THR:O	0.51	0.43
1:K:174:THR:C	1:K:174:THR:O	0.51	0.41
1:L:174:THR:C	1:L:174:THR:O	0.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	768/816 (94%)	705 (92%)	50 (6%)	13 (2%)	9	41
1	J	768/816 (94%)	705 (92%)	50 (6%)	13 (2%)	9	41
1	K	768/816 (94%)	705 (92%)	50 (6%)	13 (2%)	9	41
1	L	768/816 (94%)	705 (92%)	50 (6%)	13 (2%)	9	41
1	M	768/816 (94%)	705 (92%)	50 (6%)	13 (2%)	9	41
1	N	768/816 (94%)	705 (92%)	50 (6%)	13 (2%)	9	41
2	A	365/373 (98%)	335 (92%)	24 (7%)	6 (2%)	9	43
2	B	365/373 (98%)	335 (92%)	24 (7%)	6 (2%)	9	43
2	C	365/373 (98%)	335 (92%)	24 (7%)	6 (2%)	9	43
2	D	365/373 (98%)	335 (92%)	24 (7%)	6 (2%)	9	43
2	E	365/373 (98%)	335 (92%)	24 (7%)	6 (2%)	9	43
2	F	365/373 (98%)	335 (92%)	24 (7%)	6 (2%)	9	43
2	G	365/373 (98%)	335 (92%)	24 (7%)	6 (2%)	9	43
2	H	365/373 (98%)	335 (92%)	24 (7%)	6 (2%)	9	43
All	All	7528/7880 (96%)	6910 (92%)	492 (6%)	126 (2%)	13	41

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	277	GLY
1	I	460	PHE
1	I	503	VAL
1	I	639	SER
1	I	642	SER
1	J	277	GLY
1	J	460	PHE
1	J	503	VAL
1	J	639	SER
1	J	642	SER
1	K	277	GLY
1	K	460	PHE
1	K	503	VAL
1	K	639	SER
1	K	642	SER
1	L	277	GLY
1	L	460	PHE
1	L	503	VAL
1	L	639	SER

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Mol	Chain	Res	Type
1	L	642	SER
1	M	277	GLY
1	M	460	PHE
1	M	503	VAL
1	M	639	SER
1	M	642	SER
1	N	277	GLY
1	N	460	PHE
1	N	503	VAL
1	N	639	SER
1	N	642	SER
2	A	45	VAL
2	A	46	GLY
2	A	167	GLU
2	A	369	ILE
2	B	45	VAL
2	B	46	GLY
2	B	167	GLU
2	B	369	ILE
2	C	45	VAL
2	C	46	GLY
2	C	167	GLU
2	C	369	ILE
2	D	45	VAL
2	D	46	GLY
2	D	167	GLU
2	D	369	ILE
2	E	45	VAL
2	E	46	GLY
2	E	167	GLU
2	E	369	ILE
2	F	45	VAL
2	F	46	GLY
2	F	167	GLU
2	F	369	ILE
2	G	45	VAL
2	G	46	GLY
2	G	167	GLU
2	G	369	ILE
2	H	45	VAL
2	H	46	GLY
2	H	167	GLU

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Mol	Chain	Res	Type
2	H	369	ILE
1	I	105	LYS
1	I	447	THR
1	I	703	GLY
1	J	105	LYS
1	J	447	THR
1	J	703	GLY
1	K	105	LYS
1	K	447	THR
1	K	703	GLY
1	L	105	LYS
1	L	447	THR
1	L	703	GLY
1	M	105	LYS
1	M	447	THR
1	M	703	GLY
1	N	105	LYS
1	N	447	THR
1	N	703	GLY
2	A	16	LEU
2	B	16	LEU
2	C	16	LEU
2	D	16	LEU
2	E	16	LEU
2	F	16	LEU
2	G	16	LEU
2	H	16	LEU
1	I	229	LEU
1	I	276	ARG
1	I	773	ASP
1	J	229	LEU
1	J	276	ARG
1	J	773	ASP
1	K	229	LEU
1	K	276	ARG
1	K	773	ASP
1	L	229	LEU
1	L	276	ARG
1	L	773	ASP
1	M	229	LEU
1	M	276	ARG
1	M	773	ASP

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Mol	Chain	Res	Type
1	N	229	LEU
1	N	276	ARG
1	N	773	ASP
1	I	140	VAL
1	J	140	VAL
1	K	140	VAL
1	L	140	VAL
1	M	140	VAL
1	N	140	VAL
1	M	175	GLY
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
1	I	175	GLY
1	J	175	GLY
1	K	175	GLY
1	L	175	GLY
1	N	175	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	K	33
1	I	32
1	J	32
1	L	32
1	M	32
1	N	32
2	A	8
2	B	8
2	C	8
2	D	8
2	E	8
2	F	8
2	G	8
2	H	8

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	460:PHE	C	461:GLU	N	1.20
1	J	460:PHE	C	461:GLU	N	1.20
1	K	447:THR	C	448:SER	N	1.20
1	K	460:PHE	C	461:GLU	N	1.20
1	L	460:PHE	C	461:GLU	N	1.20
1	M	460:PHE	C	461:GLU	N	1.20
1	N	460:PHE	C	461:GLU	N	1.20
1	A	244:ASP	C	245:GLY	N	1.20
1	A	307:PRO	C	308:GLY	N	1.20
1	B	244:ASP	C	245:GLY	N	1.20
1	C	244:ASP	C	245:GLY	N	1.20
1	C	307:PRO	C	308:GLY	N	1.20

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	244:ASP	C	245:GLY	N	1.20
1	E	244:ASP	C	245:GLY	N	1.20
1	E	307:PRO	C	308:GLY	N	1.20
1	F	244:ASP	C	245:GLY	N	1.20
1	G	244:ASP	C	245:GLY	N	1.20
1	G	307:PRO	C	308:GLY	N	1.20
1	H	244:ASP	C	245:GLY	N	1.20
1	H	307:PRO	C	308:GLY	N	1.20
1	I	37:LYS	C	38:GLY	N	1.19
1	I	282:PHE	C	283:ALA	N	1.19
1	I	358:THR	C	359:SER	N	1.19
1	I	459:GLY	C	460:PHE	N	1.19
1	I	642:SER	C	643:VAL	N	1.19
1	J	37:LYS	C	38:GLY	N	1.19
1	J	282:PHE	C	283:ALA	N	1.19
1	J	358:THR	C	359:SER	N	1.19
1	J	459:GLY	C	460:PHE	N	1.19
1	J	642:SER	C	643:VAL	N	1.19
1	K	37:LYS	C	38:GLY	N	1.19
1	K	282:PHE	C	283:ALA	N	1.19
1	K	358:THR	C	359:SER	N	1.19
1	K	459:GLY	C	460:PHE	N	1.19
1	K	642:SER	C	643:VAL	N	1.19
1	L	37:LYS	C	38:GLY	N	1.19
1	L	282:PHE	C	283:ALA	N	1.19
1	L	358:THR	C	359:SER	N	1.19
1	L	459:GLY	C	460:PHE	N	1.19
1	L	642:SER	C	643:VAL	N	1.19
1	M	37:LYS	C	38:GLY	N	1.19
1	M	282:PHE	C	283:ALA	N	1.19
1	M	358:THR	C	359:SER	N	1.19
1	M	459:GLY	C	460:PHE	N	1.19
1	M	642:SER	C	643:VAL	N	1.19
1	N	37:LYS	C	38:GLY	N	1.19
1	N	282:PHE	C	283:ALA	N	1.19
1	N	358:THR	C	359:SER	N	1.19
1	N	459:GLY	C	460:PHE	N	1.19
1	N	642:SER	C	643:VAL	N	1.19
1	B	307:PRO	C	308:GLY	N	1.19
1	D	307:PRO	C	308:GLY	N	1.19
1	F	307:PRO	C	308:GLY	N	1.19
1	I	175:GLY	C	176:GLN	N	1.18

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	175:GLY	C	176:GLN	N	1.18
1	K	175:GLY	C	176:GLN	N	1.18
1	L	175:GLY	C	176:GLN	N	1.18
1	M	175:GLY	C	176:GLN	N	1.18
1	N	175:GLY	C	176:GLN	N	1.18
1	I	56:LYS	C	57:LYS	N	1.17
1	I	36:GLN	C	37:LYS	N	1.16
1	I	662:GLY	C	663:ALA	N	1.16
1	I	772:SER	C	773:ASP	N	1.16
1	J	36:GLN	C	37:LYS	N	1.16
1	J	56:LYS	C	57:LYS	N	1.16
1	J	662:GLY	C	663:ALA	N	1.16
1	J	772:SER	C	773:ASP	N	1.16
1	K	36:GLN	C	37:LYS	N	1.16
1	K	56:LYS	C	57:LYS	N	1.16
1	K	662:GLY	C	663:ALA	N	1.16
1	K	772:SER	C	773:ASP	N	1.16
1	L	36:GLN	C	37:LYS	N	1.16
1	L	56:LYS	C	57:LYS	N	1.16
1	L	662:GLY	C	663:ALA	N	1.16
1	L	772:SER	C	773:ASP	N	1.16
1	M	36:GLN	C	37:LYS	N	1.16
1	M	56:LYS	C	57:LYS	N	1.16
1	M	662:GLY	C	663:ALA	N	1.16
1	M	772:SER	C	773:ASP	N	1.16
1	N	36:GLN	C	37:LYS	N	1.16
1	N	56:LYS	C	57:LYS	N	1.16
1	N	662:GLY	C	663:ALA	N	1.16
1	N	772:SER	C	773:ASP	N	1.16
1	A	45:VAL	C	46:GLY	N	1.16
1	B	45:VAL	C	46:GLY	N	1.16
1	C	45:VAL	C	46:GLY	N	1.16
1	D	45:VAL	C	46:GLY	N	1.16
1	E	45:VAL	C	46:GLY	N	1.16
1	F	45:VAL	C	46:GLY	N	1.16
1	G	45:VAL	C	46:GLY	N	1.16
1	H	45:VAL	C	46:GLY	N	1.16
1	I	356:GLY	C	357:SER	N	1.15
1	J	356:GLY	C	357:SER	N	1.15
1	K	356:GLY	C	357:SER	N	1.15
1	L	356:GLY	C	357:SER	N	1.15
1	M	356:GLY	C	357:SER	N	1.15

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	356:GLY	C	357:SER	N	1.15
1	I	361:GLY	C	362:CYS	N	1.14
1	I	446:GLU	C	447:THR	N	1.14
1	I	461:GLU	C	462:TYR	N	1.14
1	I	708:ARG	C	709:ALA	N	1.14
1	J	361:GLY	C	362:CYS	N	1.14
1	J	446:GLU	C	447:THR	N	1.14
1	J	461:GLU	C	462:TYR	N	1.14
1	J	708:ARG	C	709:ALA	N	1.14
1	K	361:GLY	C	362:CYS	N	1.14
1	K	446:GLU	C	447:THR	N	1.14
1	K	461:GLU	C	462:TYR	N	1.14
1	K	708:ARG	C	709:ALA	N	1.14
1	L	361:GLY	C	362:CYS	N	1.14
1	L	446:GLU	C	447:THR	N	1.14
1	L	461:GLU	C	462:TYR	N	1.14
1	L	708:ARG	C	709:ALA	N	1.14
1	M	361:GLY	C	362:CYS	N	1.14
1	M	446:GLU	C	447:THR	N	1.14
1	M	461:GLU	C	462:TYR	N	1.14
1	M	708:ARG	C	709:ALA	N	1.14
1	N	361:GLY	C	362:CYS	N	1.14
1	N	446:GLU	C	447:THR	N	1.14
1	N	461:GLU	C	462:TYR	N	1.14
1	N	708:ARG	C	709:ALA	N	1.14
1	I	355:ALA	C	356:GLY	N	1.13
1	I	536:PRO	C	537:GLN	N	1.13
1	J	355:ALA	C	356:GLY	N	1.13
1	J	536:PRO	C	537:GLN	N	1.13
1	K	355:ALA	C	356:GLY	N	1.13
1	K	536:PRO	C	537:GLN	N	1.13
1	L	355:ALA	C	356:GLY	N	1.13
1	L	536:PRO	C	537:GLN	N	1.13
1	M	355:ALA	C	356:GLY	N	1.13
1	M	536:PRO	C	537:GLN	N	1.13
1	N	355:ALA	C	356:GLY	N	1.13
1	N	536:PRO	C	537:GLN	N	1.13
1	A	333:PRO	C	334:GLU	N	1.12
1	B	333:PRO	C	334:GLU	N	1.12
1	C	333:PRO	C	334:GLU	N	1.12
1	D	333:PRO	C	334:GLU	N	1.12
1	E	333:PRO	C	334:GLU	N	1.12

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	333:PRO	C	334:GLU	N	1.12
1	G	333:PRO	C	334:GLU	N	1.12
1	H	333:PRO	C	334:GLU	N	1.12
1	I	681:GLU	C	682:GLY	N	1.10
1	J	681:GLU	C	682:GLY	N	1.10
1	K	681:GLU	C	682:GLY	N	1.10
1	L	681:GLU	C	682:GLY	N	1.10
1	M	681:GLU	C	682:GLY	N	1.10
1	N	681:GLU	C	682:GLY	N	1.10
1	A	25:ASP	C	26:ALA	N	1.10
1	C	25:ASP	C	26:ALA	N	1.10
1	E	25:ASP	C	26:ALA	N	1.10
1	F	25:ASP	C	26:ALA	N	1.10
1	G	25:ASP	C	26:ALA	N	1.10
1	I	58:ASP	C	59:VAL	N	1.09
1	I	360:GLY	C	361:GLY	N	1.09
1	I	636:GLY	C	637:LYS	N	1.09
1	J	58:ASP	C	59:VAL	N	1.09
1	J	360:GLY	C	361:GLY	N	1.09
1	J	636:GLY	C	637:LYS	N	1.09
1	K	58:ASP	C	59:VAL	N	1.09
1	K	360:GLY	C	361:GLY	N	1.09
1	K	636:GLY	C	637:LYS	N	1.09
1	L	58:ASP	C	59:VAL	N	1.09
1	L	360:GLY	C	361:GLY	N	1.09
1	L	636:GLY	C	637:LYS	N	1.09
1	M	58:ASP	C	59:VAL	N	1.09
1	M	360:GLY	C	361:GLY	N	1.09
1	M	636:GLY	C	637:LYS	N	1.09
1	N	58:ASP	C	59:VAL	N	1.09
1	N	360:GLY	C	361:GLY	N	1.09
1	N	636:GLY	C	637:LYS	N	1.09
1	B	25:ASP	C	26:ALA	N	1.09
1	D	25:ASP	C	26:ALA	N	1.09
1	H	25:ASP	C	26:ALA	N	1.09
1	A	368:SER	C	369:ILE	N	1.08
1	B	368:SER	C	369:ILE	N	1.08
1	C	368:SER	C	369:ILE	N	1.08
1	D	368:SER	C	369:ILE	N	1.08
1	E	368:SER	C	369:ILE	N	1.08
1	F	368:SER	C	369:ILE	N	1.08
1	G	368:SER	C	369:ILE	N	1.08

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	368:SER	C	369:ILE	N	1.08
1	I	499:GLU	C	500:GLY	N	1.06
1	I	553:ASP	C	554:HIS	N	1.06
1	J	499:GLU	C	500:GLY	N	1.06
1	K	499:GLU	C	500:GLY	N	1.06
1	K	553:ASP	C	554:HIS	N	1.06
1	L	499:GLU	C	500:GLY	N	1.06
1	M	499:GLU	C	500:GLY	N	1.06
1	M	553:ASP	C	554:HIS	N	1.06
1	N	499:GLU	C	500:GLY	N	1.06
1	J	38:GLY	C	39:LYS	N	1.05
1	J	553:ASP	C	554:HIS	N	1.05
1	K	38:GLY	C	39:LYS	N	1.05
1	L	553:ASP	C	554:HIS	N	1.05
1	N	38:GLY	C	39:LYS	N	1.05
1	N	553:ASP	C	554:HIS	N	1.05
1	I	38:GLY	C	39:LYS	N	1.04
1	I	172:TYR	C	173:GLY	N	1.04
1	I	502:GLY	C	503:VAL	N	1.04
1	J	172:TYR	C	173:GLY	N	1.04
1	J	502:GLY	C	503:VAL	N	1.04
1	K	172:TYR	C	173:GLY	N	1.04
1	K	502:GLY	C	503:VAL	N	1.04
1	L	38:GLY	C	39:LYS	N	1.04
1	L	172:TYR	C	173:GLY	N	1.04
1	L	502:GLY	C	503:VAL	N	1.04
1	M	38:GLY	C	39:LYS	N	1.04
1	M	172:TYR	C	173:GLY	N	1.04
1	M	502:GLY	C	503:VAL	N	1.04
1	N	172:TYR	C	173:GLY	N	1.04
1	N	502:GLY	C	503:VAL	N	1.04
1	I	638:LEU	C	639:SER	N	1.02
1	J	638:LEU	C	639:SER	N	1.02
1	K	638:LEU	C	639:SER	N	1.02
1	L	638:LEU	C	639:SER	N	1.02
1	M	638:LEU	C	639:SER	N	1.02
1	N	638:LEU	C	639:SER	N	1.02
1	A	43:VAL	C	44:MET	N	1.00
1	B	43:VAL	C	44:MET	N	1.00
1	C	43:VAL	C	44:MET	N	1.00
1	D	43:VAL	C	44:MET	N	1.00
1	E	43:VAL	C	44:MET	N	1.00

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	43:VAL	C	44:MET	N	1.00
1	G	43:VAL	C	44:MET	N	1.00
1	H	43:VAL	C	44:MET	N	1.00
1	I	359:SER	C	360:GLY	N	0.96
1	J	359:SER	C	360:GLY	N	0.96
1	K	359:SER	C	360:GLY	N	0.96
1	L	359:SER	C	360:GLY	N	0.96
1	M	359:SER	C	360:GLY	N	0.96
1	N	359:SER	C	360:GLY	N	0.96
1	I	641:ILE	C	642:SER	N	0.94
1	J	641:ILE	C	642:SER	N	0.94
1	K	641:ILE	C	642:SER	N	0.94
1	L	641:ILE	C	642:SER	N	0.94
1	M	641:ILE	C	642:SER	N	0.94
1	N	641:ILE	C	642:SER	N	0.94
1	A	42:GLY	C	43:VAL	N	0.91
1	B	42:GLY	C	43:VAL	N	0.91
1	C	42:GLY	C	43:VAL	N	0.91
1	D	42:GLY	C	43:VAL	N	0.91
1	E	42:GLY	C	43:VAL	N	0.91
1	F	42:GLY	C	43:VAL	N	0.91
1	G	42:GLY	C	43:VAL	N	0.91
1	H	42:GLY	C	43:VAL	N	0.91
1	I	276:ARG	C	277:GLY	N	0.87
1	J	276:ARG	C	277:GLY	N	0.87
1	K	276:ARG	C	277:GLY	N	0.87
1	L	276:ARG	C	277:GLY	N	0.87
1	M	276:ARG	C	277:GLY	N	0.87
1	N	276:ARG	C	277:GLY	N	0.87
1	I	174:THR	C	175:GLY	N	0.63
1	J	174:THR	C	175:GLY	N	0.63
1	K	174:THR	C	175:GLY	N	0.63
1	L	174:THR	C	175:GLY	N	0.63
1	M	174:THR	C	175:GLY	N	0.63
1	N	174:THR	C	175:GLY	N	0.63

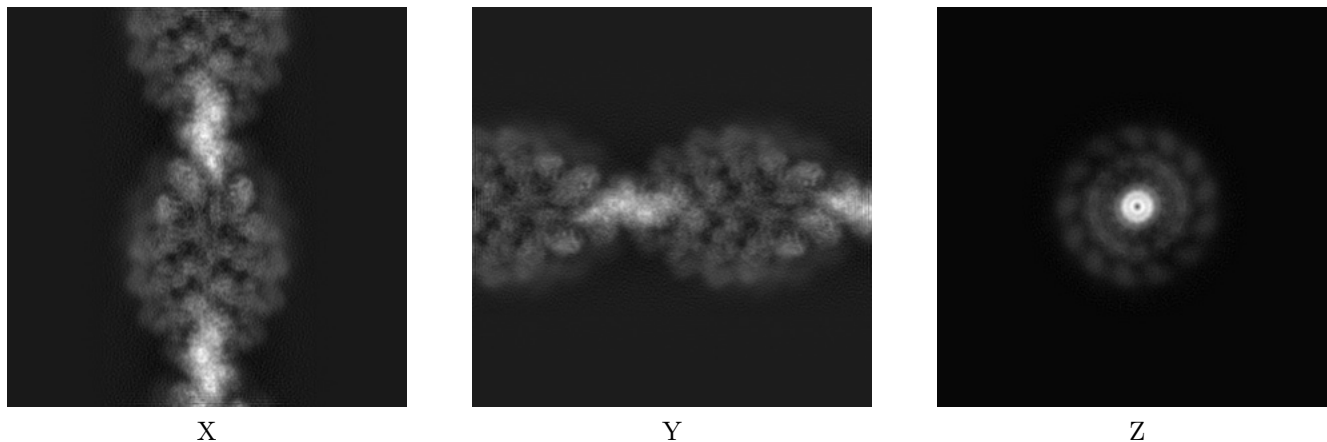
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7117. These allow visual inspection of the internal detail of the map and identification of artifacts.

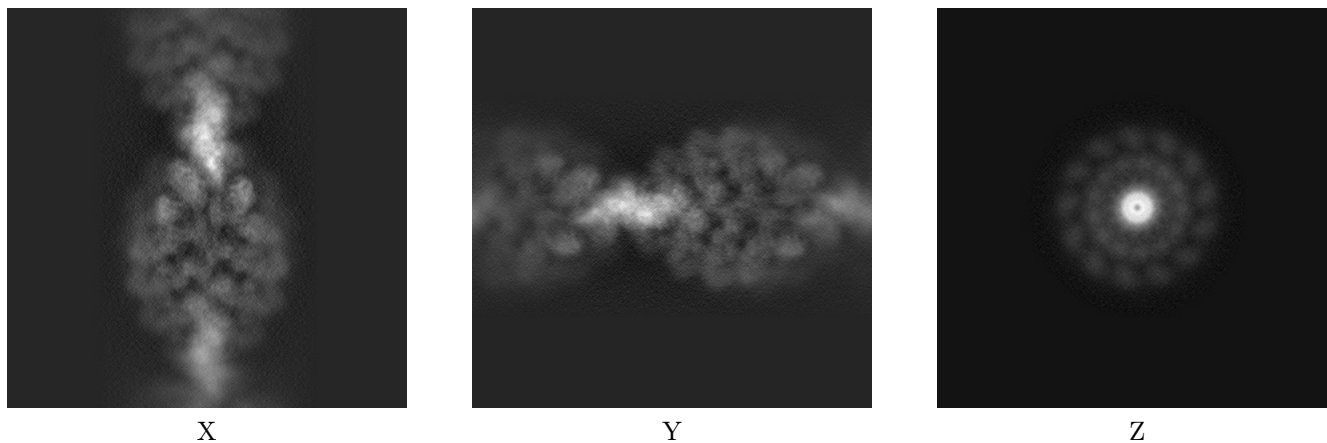
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



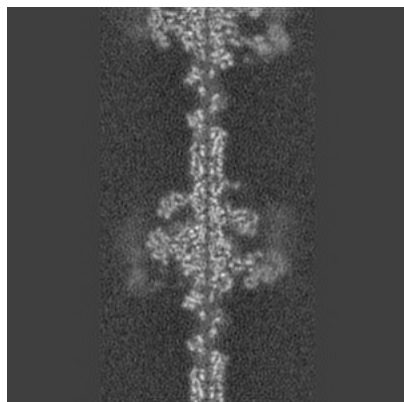
6.1.2 Raw map



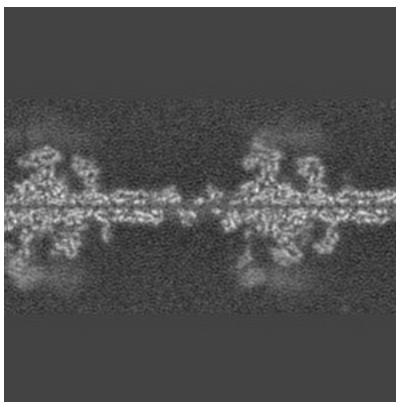
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

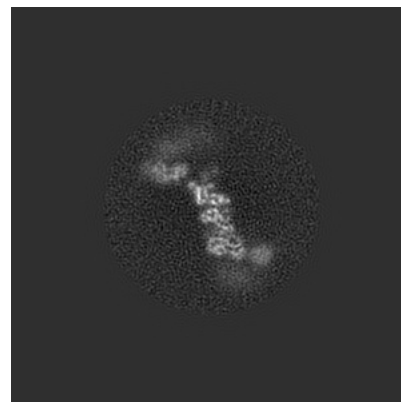
6.2.1 Primary map



X Index: 256

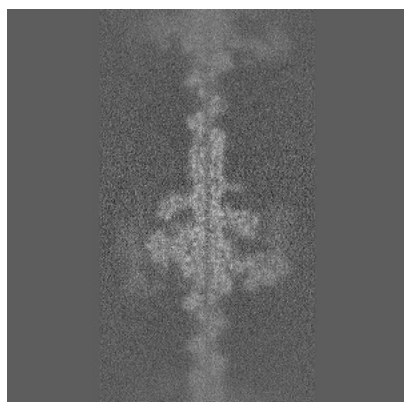


Y Index: 256

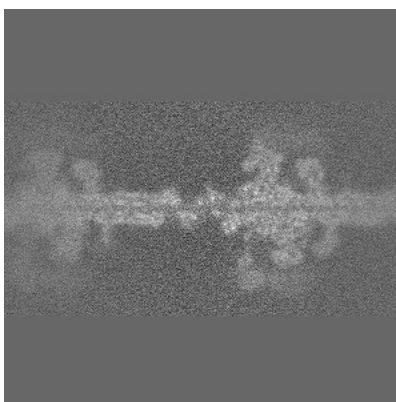


Z Index: 256

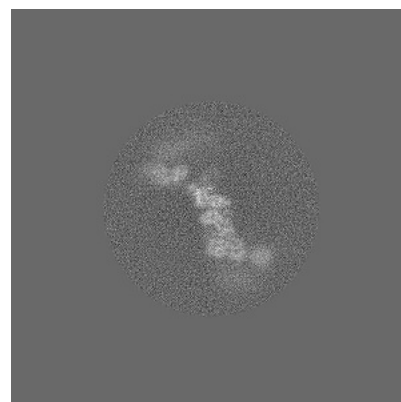
6.2.2 Raw map



X Index: 256



Y Index: 256

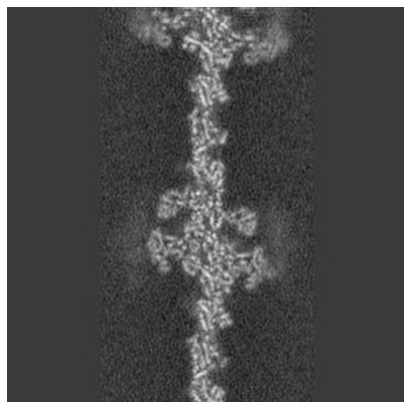


Z Index: 256

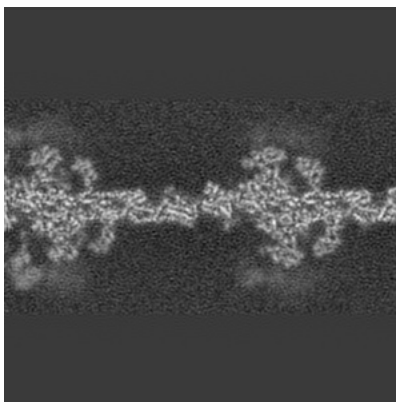
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

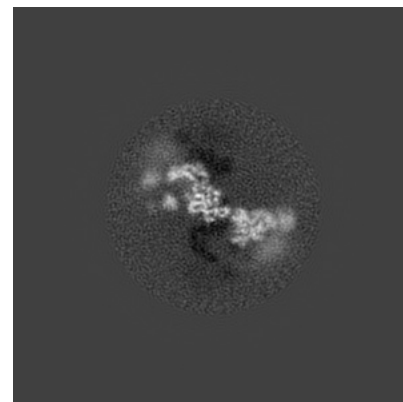
6.3.1 Primary map



X Index: 262

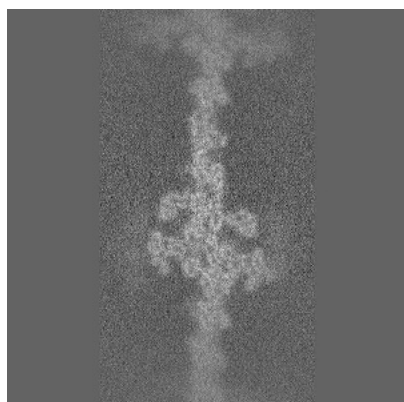


Y Index: 251

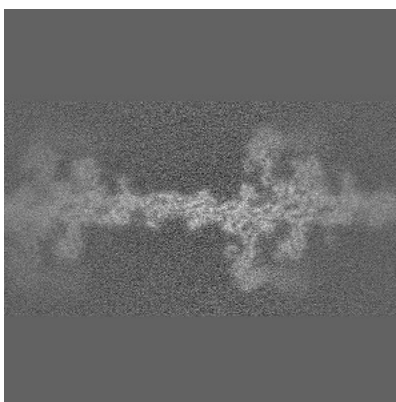


Z Index: 1

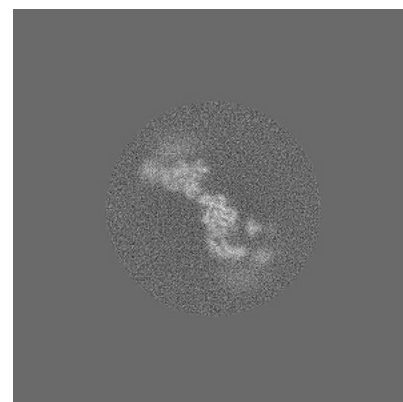
6.3.2 Raw map



X Index: 262



Y Index: 263

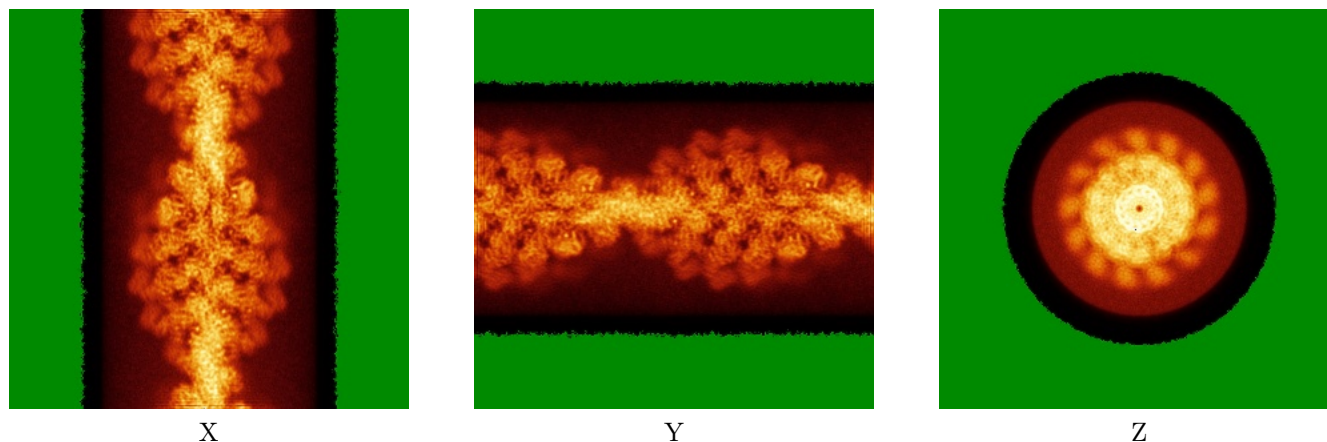


Z Index: 266

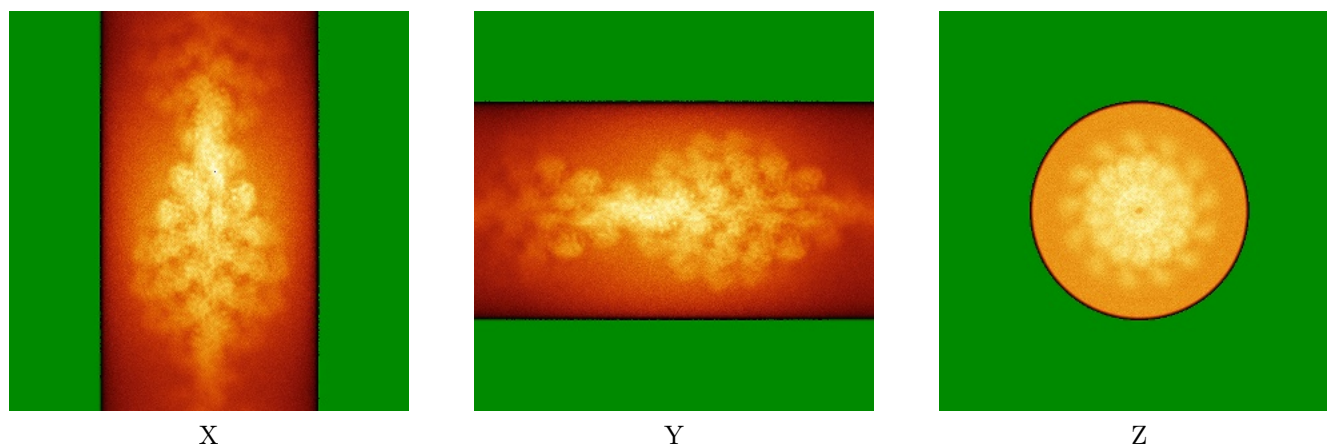
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



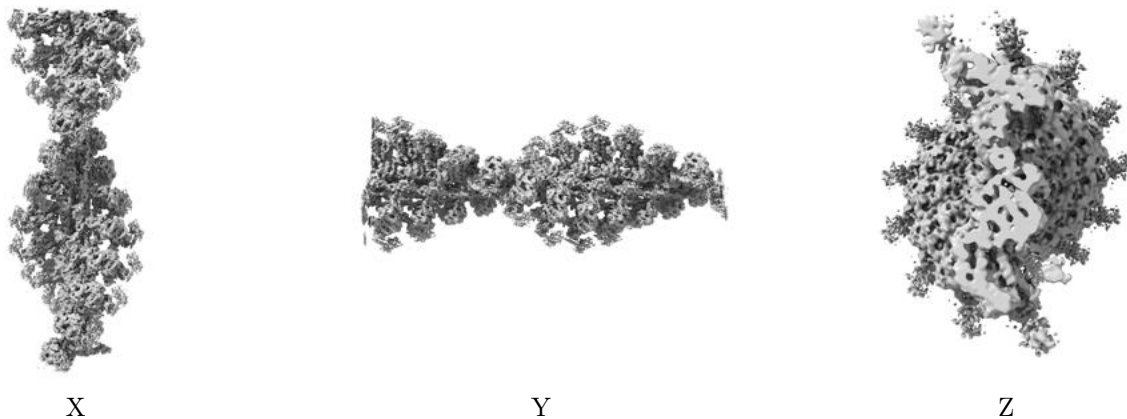
6.4.2 Raw map



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.

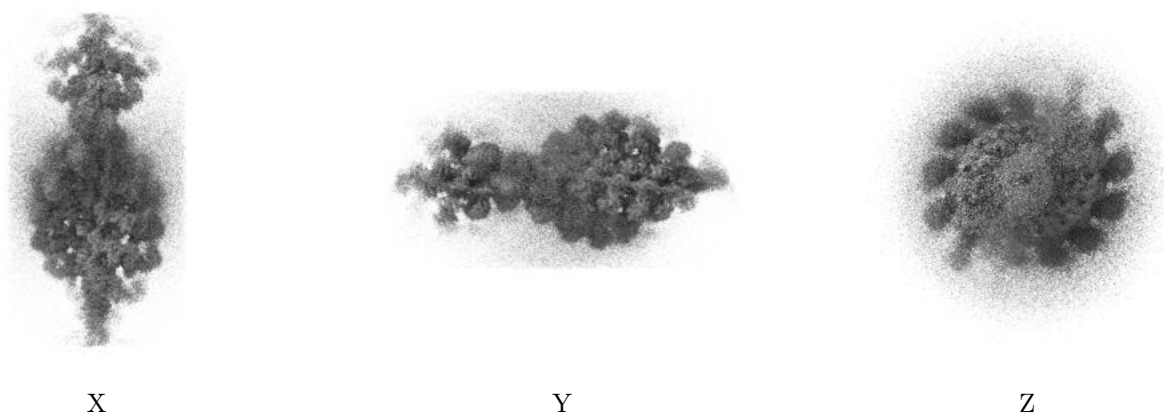
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.8. 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.

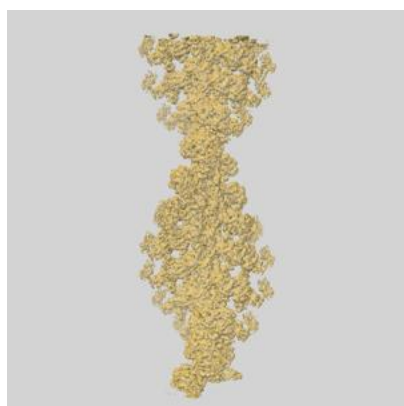
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

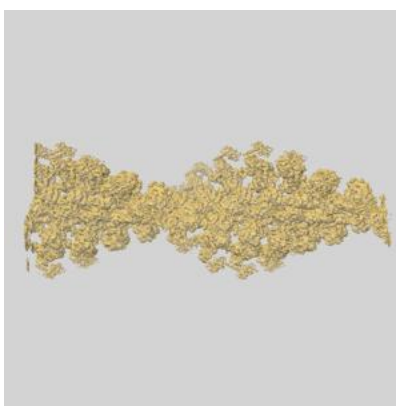
A mask typically either:

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

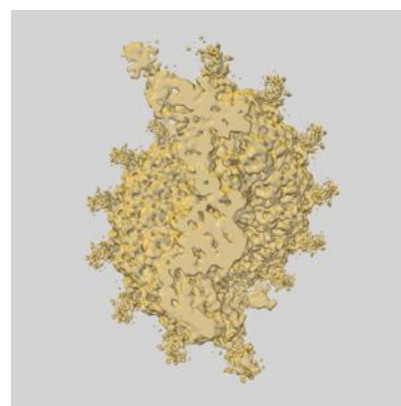
6.6.1 emd_7117_msk_2.map [i](#)



X

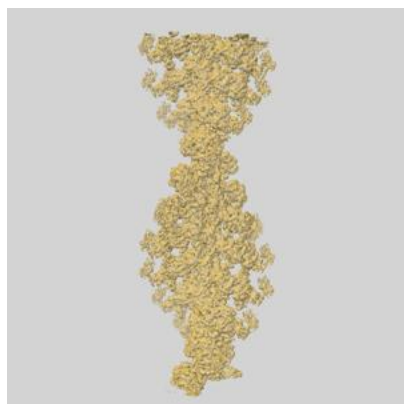


Y

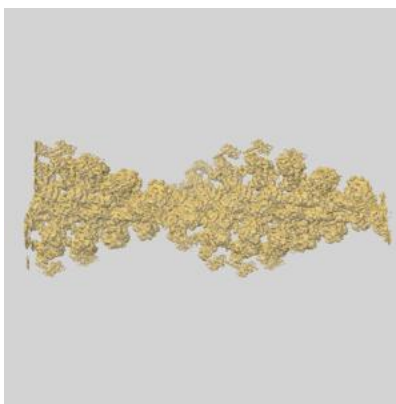


Z

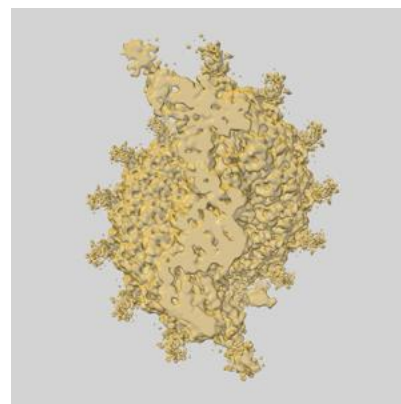
6.6.2 emd_7117_msk_1.map [i](#)



X



Y

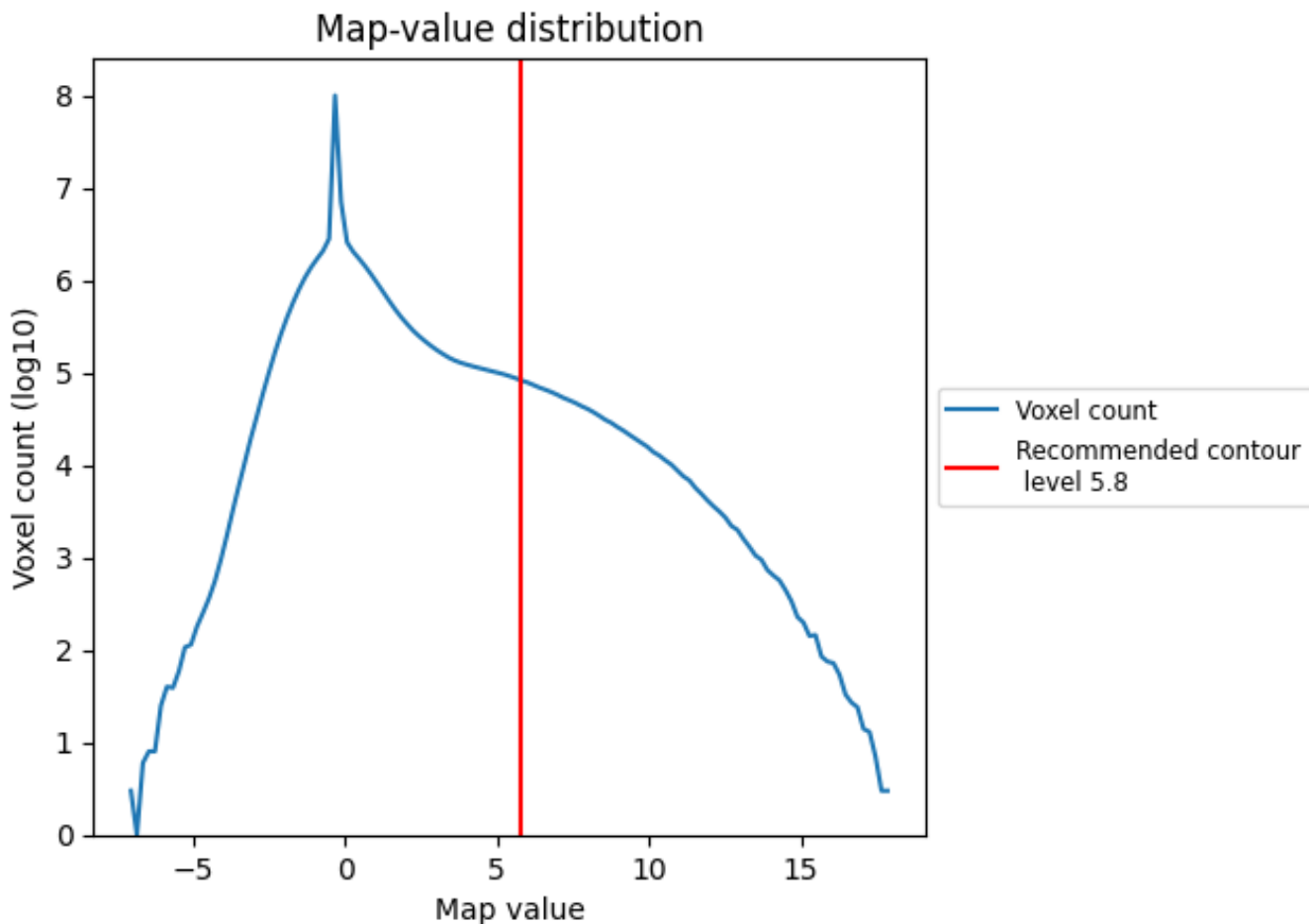


Z

7 Map analysis [i](#)

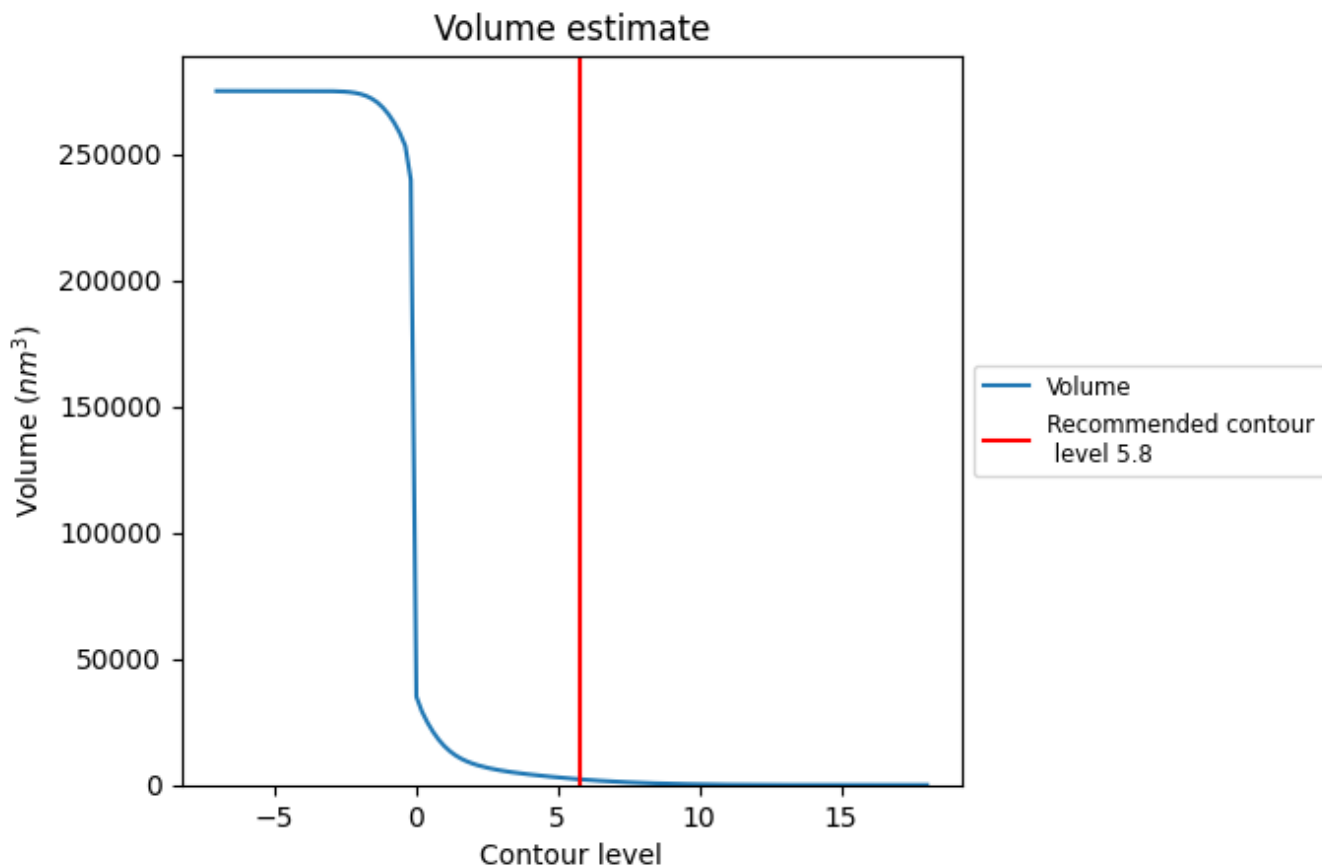
This section contains the results of statistical analysis of the map.

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.

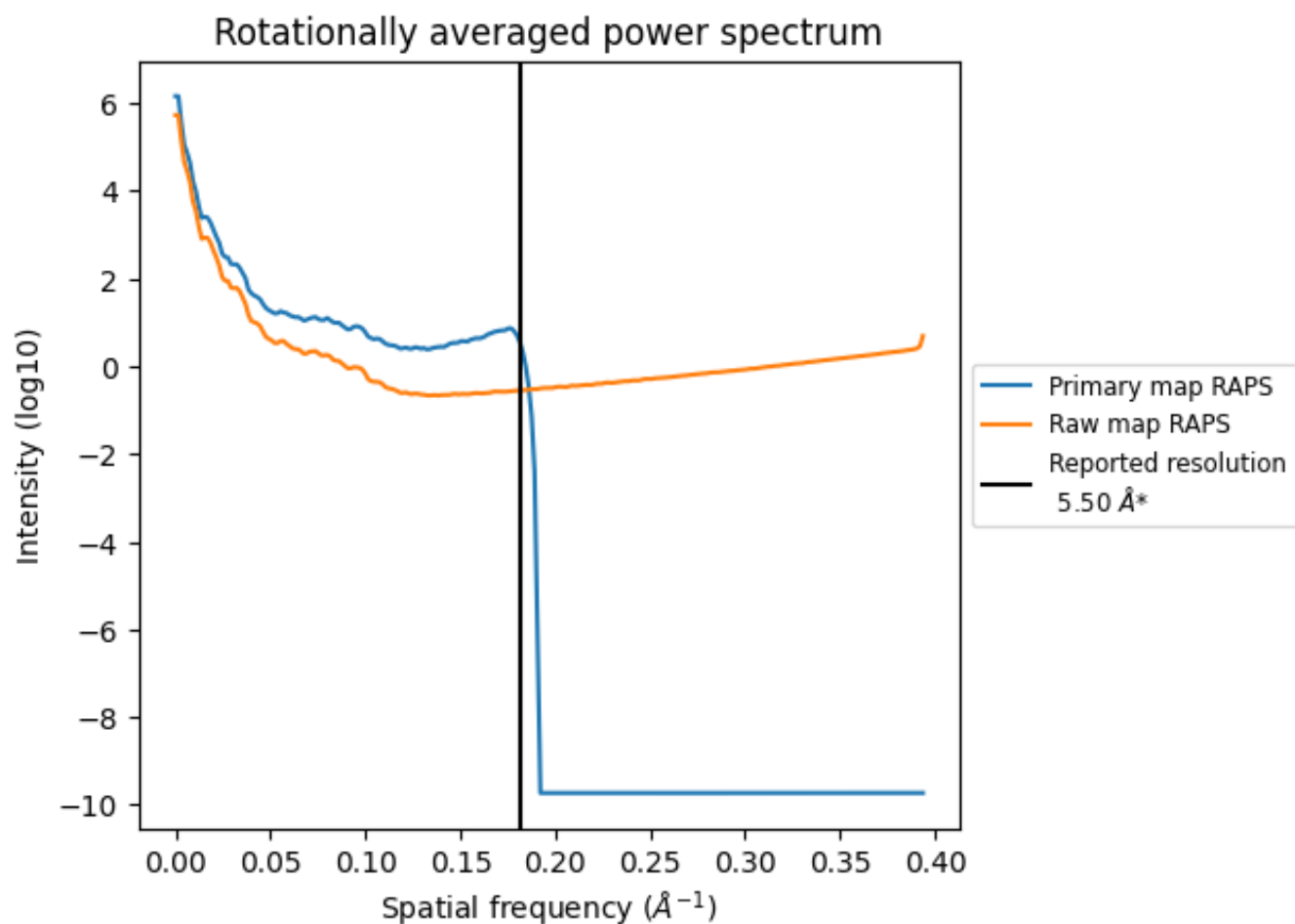
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2222 nm^3 ; this corresponds to an approximate mass of 2007 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

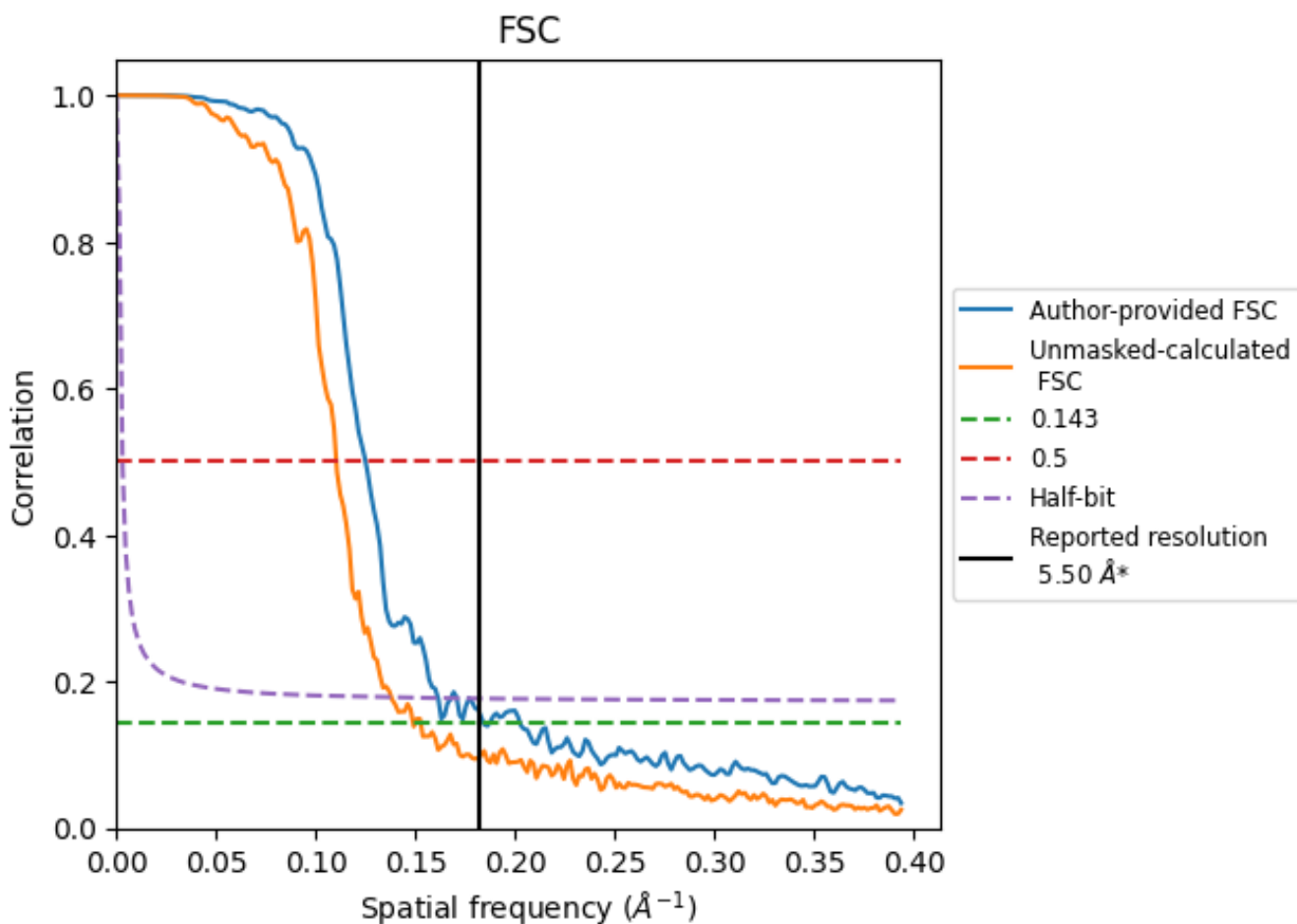


*Reported resolution corresponds to spatial frequency of 0.182 Å⁻¹

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 0.182 Å⁻¹

8.2 Resolution estimates [i](#)

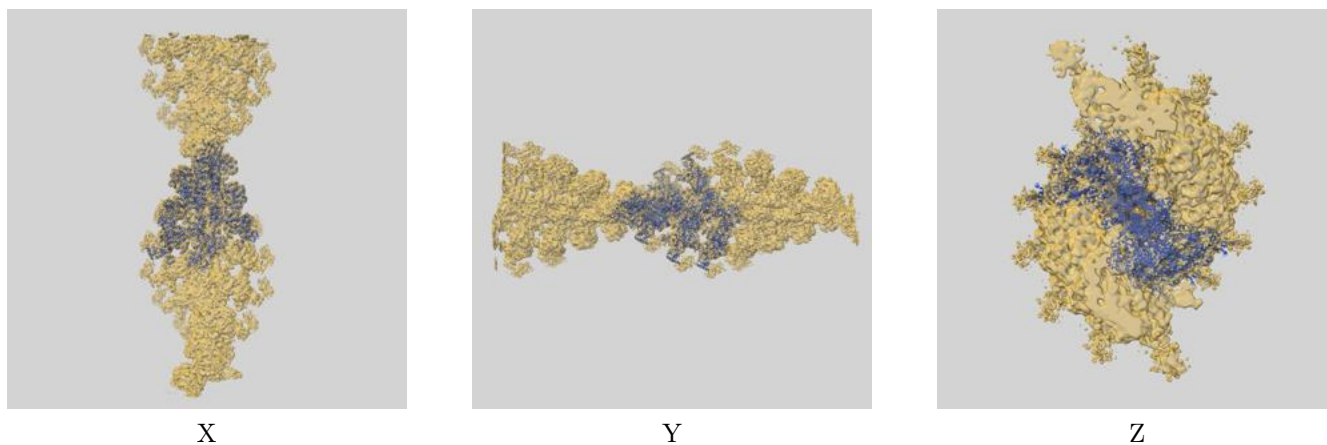
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.50	-	-
Author-provided FSC curve	5.43	8.00	6.20
Unmasked-calculated*	6.72	9.07	7.25

*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 6.72 differs from the reported value 5.5 by more than 10 %

9 Map-model fit [i](#)

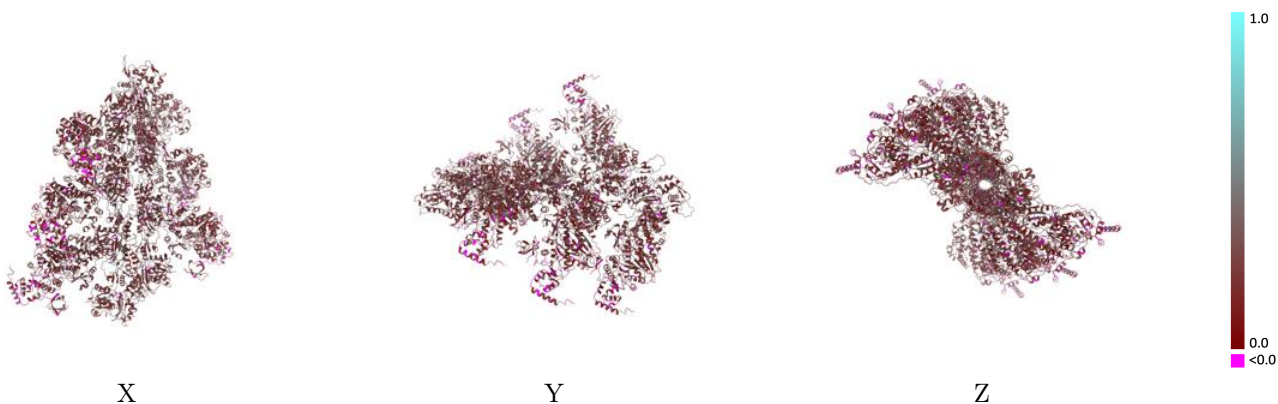
This section contains information regarding the fit between EMDB map EMD-7117 and PDB model 6BNW. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



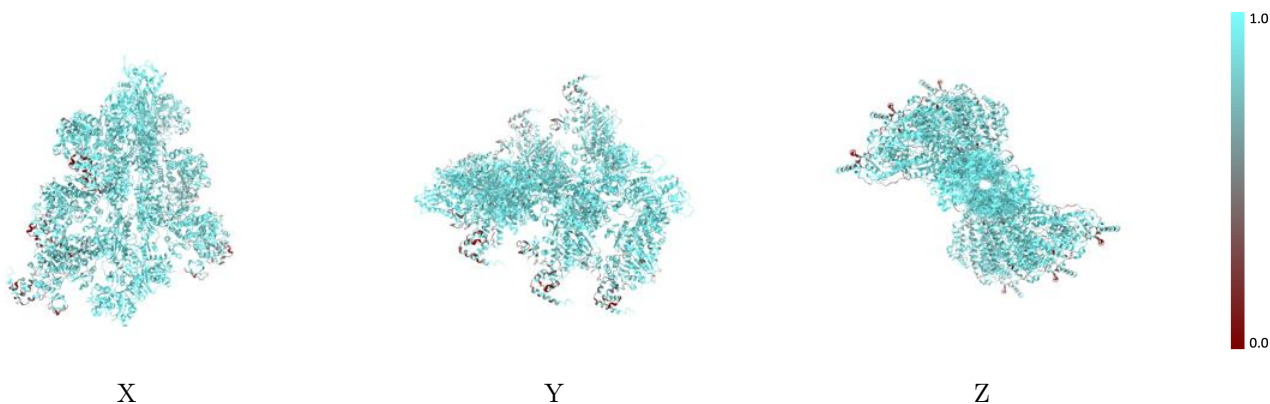
The images above show the 3D surface view of the map at the recommended contour level 5.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



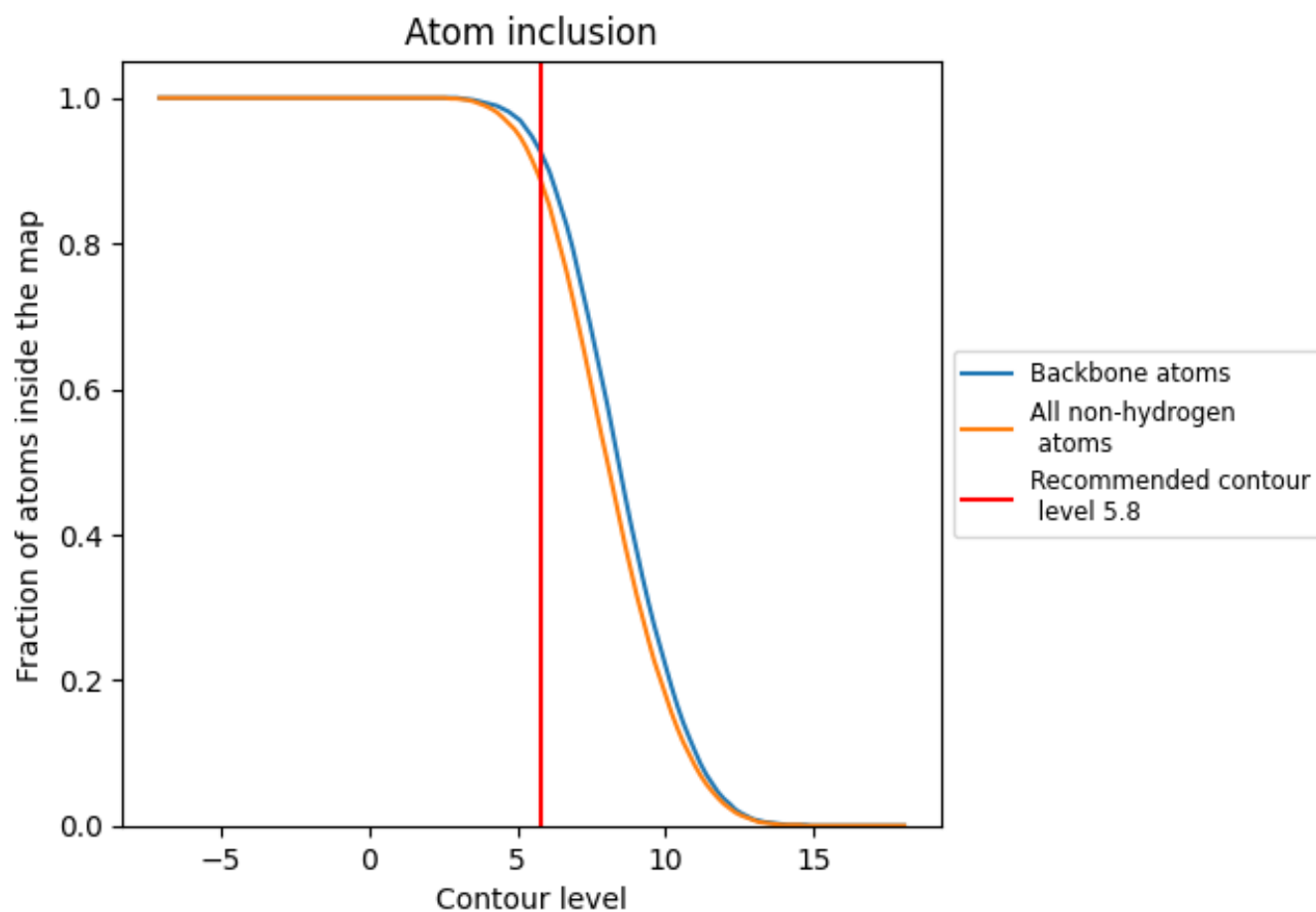
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.8).































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (5.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8860	 0.2500
A	 0.9750	 0.2800
B	 0.9730	 0.2790
C	 0.9710	 0.2780
D	 0.9700	 0.2780
E	 0.9720	 0.2780
F	 0.9700	 0.2800
G	 0.9750	 0.2800
H	 0.9770	 0.2800
I	 0.8310	 0.2330
J	 0.8330	 0.2330
K	 0.8340	 0.2310
L	 0.8310	 0.2320
M	 0.8330	 0.2330
N	 0.8310	 0.2330

