



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 05:00 PM UTC

PDB ID : 7BJP / pdb_00007bjp
EMDB ID : EMD-12194
Title : The cryo-EM structure of vesivirus 2117, an adventitious agent and possible cause of haemorrhagic gastroenteritis in dogs.
Authors : Sutherland, H.; Conley, M.J.; Emmott, E.; Streetley, J.; Goodfellow, I.G.; Bhella, D.
Deposited on : 2021-01-14
Resolution : 3.65 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

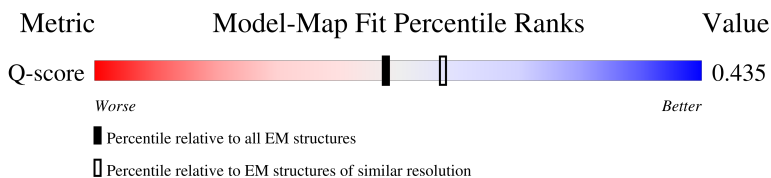
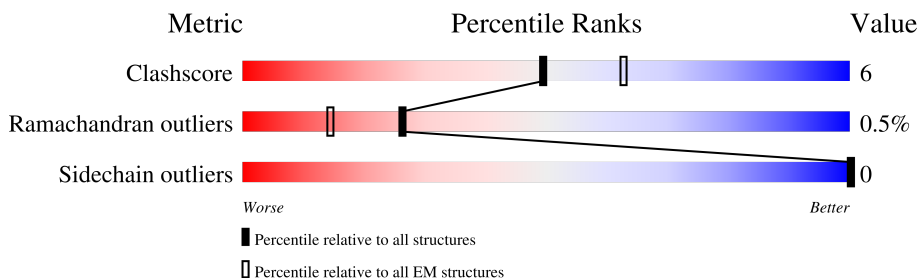
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.65 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11564 (3.15 - 4.15)

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

Mol	Chain	Length	Quality of chain
1	A	533	29% 68% 26% • •
1	B	533	31% 48% 38% 7% 6%
1	C	533	34% 65% 29% • •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23560 atoms, of which 11649 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 Capsid protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	513	Total	C	H	N	O	S	0	0
			7896	2568	3904	663	744	17		
1	B	501	Total	C	H	N	O	S	0	0
			7733	2517	3824	650	725	17		
1	C	516	Total	C	H	N	O	S	0	0
			7931	2577	3921	667	749	17		

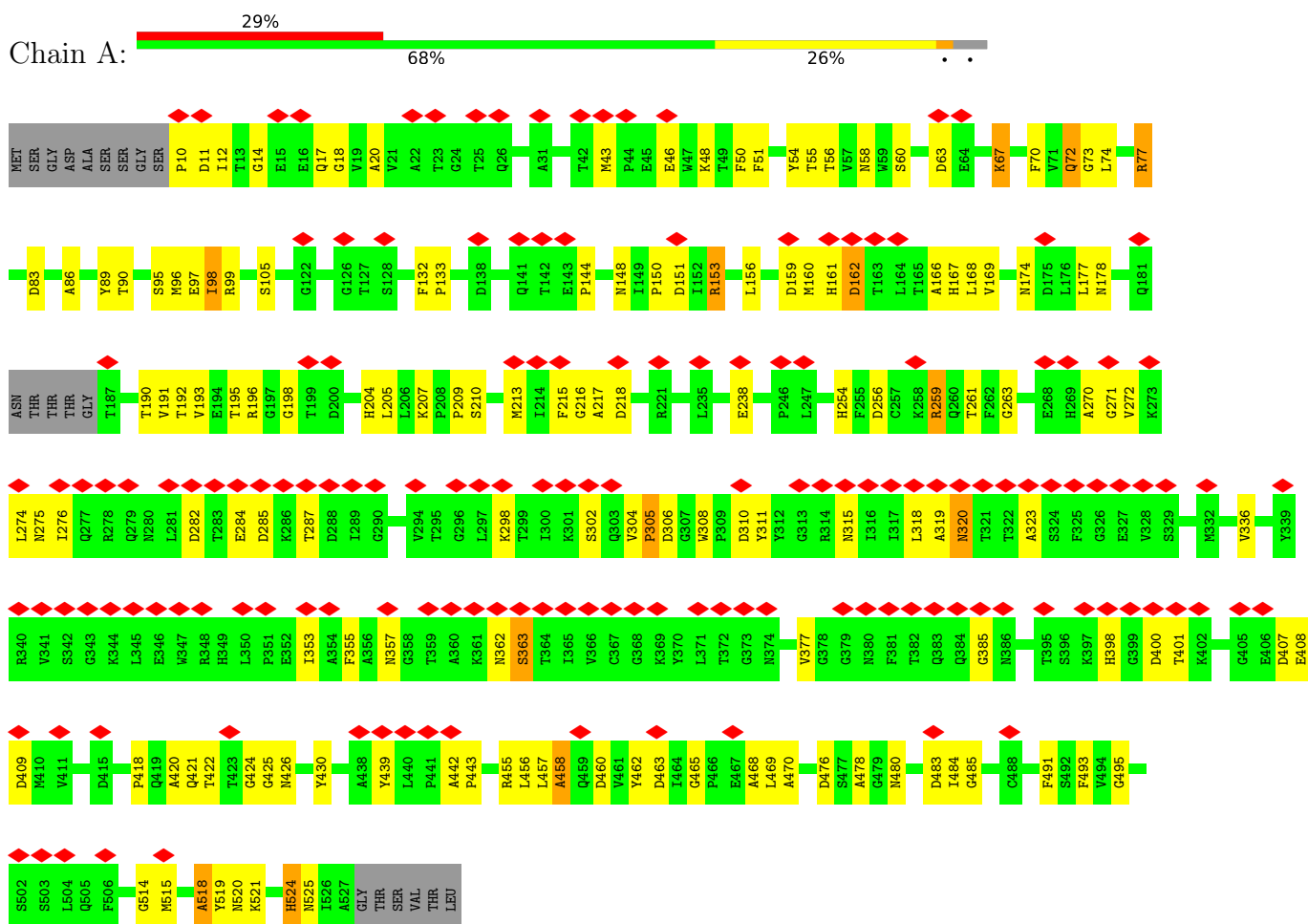
There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q6VCZ3
A	357	ASN	SER	conflict	UNP Q6VCZ3
A	370	TYR	HIS	conflict	UNP Q6VCZ3
A	497	PRO	SER	conflict	UNP Q6VCZ3
A	519	TYR	HIS	conflict	UNP Q6VCZ3
B	1	MET	-	initiating methionine	UNP Q6VCZ3
B	357	ASN	SER	conflict	UNP Q6VCZ3
B	370	TYR	HIS	conflict	UNP Q6VCZ3
B	497	PRO	SER	conflict	UNP Q6VCZ3
B	519	TYR	HIS	conflict	UNP Q6VCZ3
C	1	MET	-	initiating methionine	UNP Q6VCZ3
C	357	ASN	SER	conflict	UNP Q6VCZ3
C	370	TYR	HIS	conflict	UNP Q6VCZ3
C	497	PRO	SER	conflict	UNP Q6VCZ3
C	519	TYR	HIS	conflict	UNP Q6VCZ3

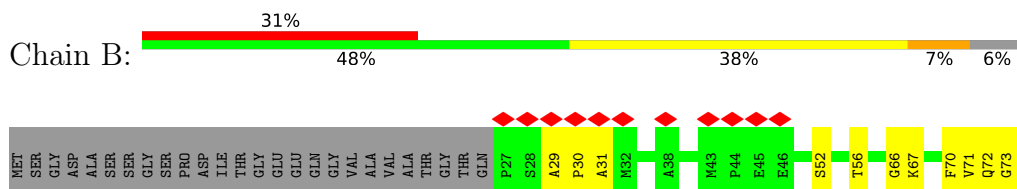
3 Residue-property plots

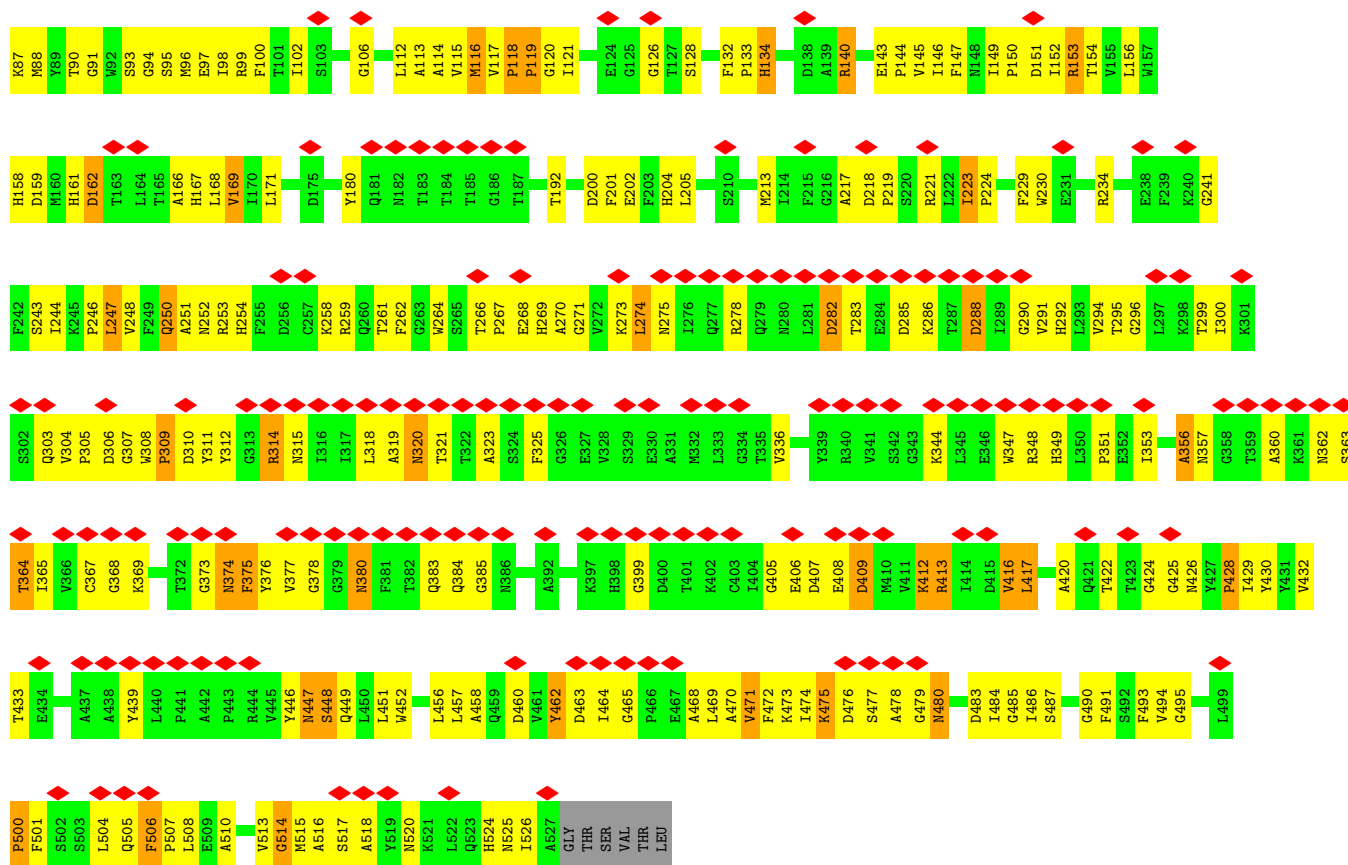
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

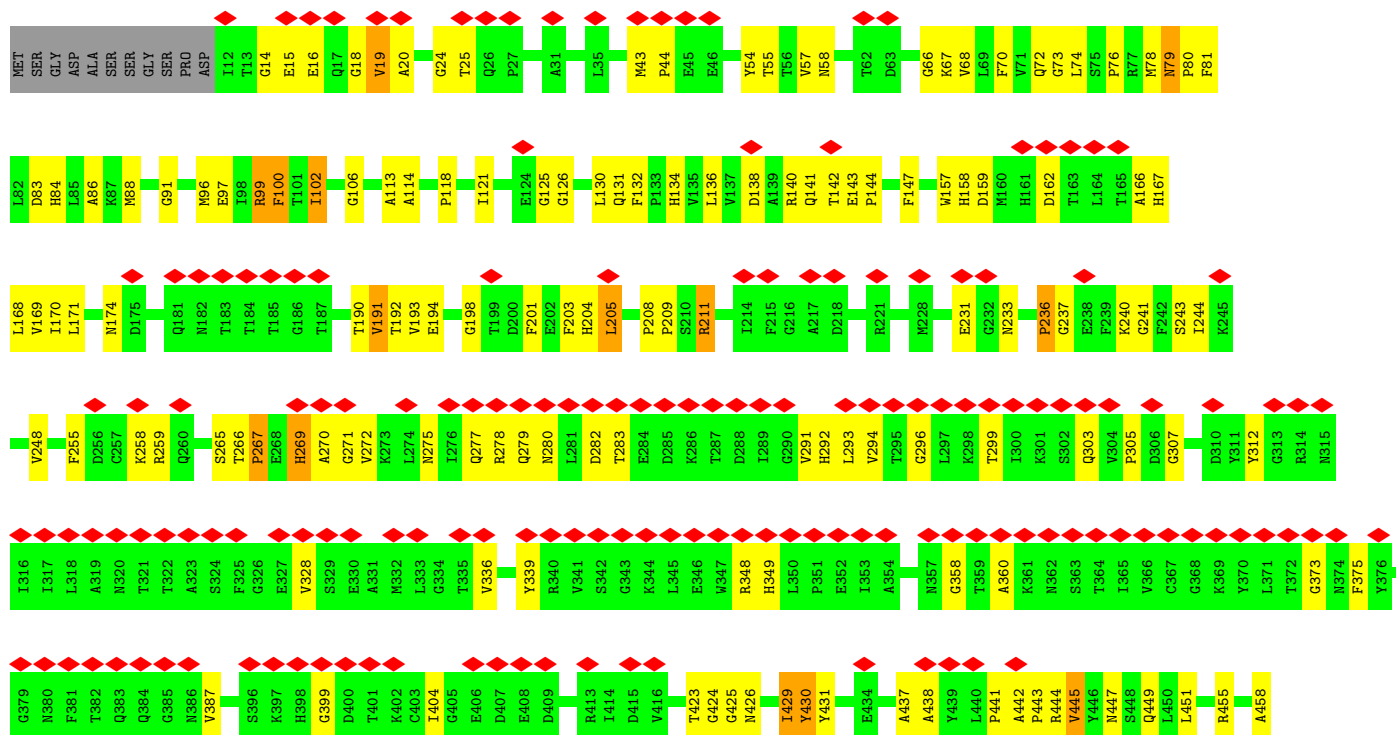


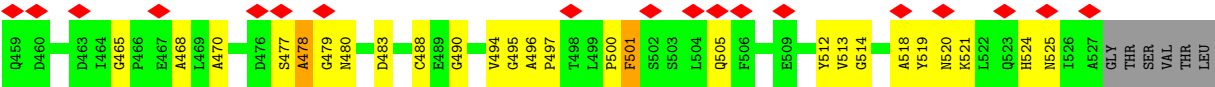
• Molecule 1: Capsid protein





• Molecule 1: Capsid protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	15989	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-64 (8k x 8k)	Depositor
Maximum map value	0.047	Depositor
Minimum map value	-0.027	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	510.976, 510.976, 510.976	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.998, 0.998, 0.998	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	2.00	68/4105 (1.7%)	1.91	132/5594 (2.4%)
1	B	2.58	140/4022 (3.5%)	2.31	246/5482 (4.5%)
1	C	2.20	93/4123 (2.3%)	2.00	143/5621 (2.5%)
All	All	2.27	301/12250 (2.5%)	2.08	521/16697 (3.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	2
All	All	0	7

All (301) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	478	ALA	CA-CB	-9.21	1.43	1.54
1	C	204	HIS	ND1-CE1	-9.12	1.23	1.32
1	C	167	HIS	CE1-NE2	-9.06	1.23	1.32
1	C	158	HIS	CE1-NE2	-9.00	1.23	1.32
1	B	269	HIS	CE1-NE2	-8.98	1.23	1.32
1	C	134	HIS	ND1-CE1	-8.98	1.23	1.32
1	B	158	HIS	ND1-CE1	-8.96	1.23	1.32
1	B	254	HIS	CE1-NE2	-8.95	1.23	1.32
1	B	349	HIS	CE1-NE2	-8.94	1.23	1.32
1	B	161	HIS	CE1-NE2	-8.93	1.23	1.32
1	C	84	HIS	CE1-NE2	-8.93	1.23	1.32
1	B	524	HIS	CE1-NE2	-8.93	1.23	1.32
1	A	167	HIS	CE1-NE2	-8.92	1.23	1.32
1	B	84	HIS	CE1-NE2	-8.91	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	134	HIS	ND1-CE1	-8.91	1.23	1.32
1	A	524	HIS	CE1-NE2	-8.91	1.23	1.32
1	A	161	HIS	CE1-NE2	-8.86	1.23	1.32
1	B	204	HIS	ND1-CE1	-8.85	1.23	1.32
1	B	167	HIS	ND1-CE1	-8.84	1.23	1.32
1	C	524	HIS	CE1-NE2	-8.84	1.23	1.32
1	C	292	HIS	ND1-CE1	-8.82	1.23	1.32
1	C	269	HIS	CE1-NE2	-8.81	1.23	1.32
1	A	398	HIS	CE1-NE2	-8.77	1.23	1.32
1	B	292	HIS	CE1-NE2	-8.76	1.23	1.32
1	C	84	HIS	CD2-NE2	-8.49	1.28	1.37
1	C	140	ARG	CZ-NH2	-8.43	1.22	1.33
1	C	167	HIS	CD2-NE2	-8.41	1.28	1.37
1	B	349	HIS	CD2-NE2	-8.38	1.28	1.37
1	B	514	GLY	N-CA	-8.36	1.37	1.45
1	C	524	HIS	CD2-NE2	-8.33	1.28	1.37
1	A	167	HIS	CD2-NE2	-8.31	1.28	1.37
1	B	84	HIS	CD2-NE2	-8.30	1.28	1.37
1	C	158	HIS	CD2-NE2	-8.28	1.28	1.37
1	B	524	HIS	CD2-NE2	-8.25	1.28	1.37
1	A	524	HIS	CD2-NE2	-8.25	1.28	1.37
1	B	99	ARG	CZ-NH2	-8.25	1.22	1.33
1	B	153	ARG	CZ-NH2	-8.22	1.22	1.33
1	A	161	HIS	CD2-NE2	-8.21	1.28	1.37
1	C	73	GLY	N-CA	-8.21	1.37	1.44
1	B	269	HIS	CD2-NE2	-8.20	1.28	1.37
1	B	254	HIS	CD2-NE2	-8.19	1.28	1.37
1	B	140	ARG	CZ-NH2	-8.16	1.22	1.33
1	B	161	HIS	CD2-NE2	-8.13	1.28	1.37
1	A	196	ARG	CZ-NH2	-8.13	1.22	1.33
1	A	99	ARG	CZ-NH2	-8.10	1.23	1.33
1	B	253	ARG	CZ-NH2	-8.09	1.23	1.33
1	A	455	ARG	CZ-NH2	-8.08	1.23	1.33
1	C	211	ARG	CZ-NH2	-8.06	1.23	1.33
1	C	114	ALA	CA-CB	-8.05	1.41	1.53
1	B	292	HIS	CD2-NE2	-8.05	1.28	1.37
1	A	153	ARG	CZ-NH2	-8.03	1.23	1.33
1	A	398	HIS	CD2-NE2	-8.02	1.29	1.37
1	C	259	ARG	CZ-NH2	-8.02	1.23	1.33
1	B	77	ARG	CZ-NH2	-7.98	1.23	1.33
1	B	259	ARG	CZ-NH2	-7.96	1.23	1.33
1	C	269	HIS	CD2-NE2	-7.93	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	234	ARG	CZ-NH2	-7.92	1.23	1.33
1	C	455	ARG	CZ-NH2	-7.92	1.23	1.33
1	A	77	ARG	CZ-NH2	-7.85	1.23	1.33
1	B	413	ARG	CZ-NH2	-7.77	1.23	1.33
1	B	271	GLY	N-CA	-7.74	1.36	1.45
1	C	278	ARG	CZ-NH2	-7.74	1.23	1.33
1	A	420	ALA	CA-CB	-7.72	1.42	1.53
1	B	348	ARG	CZ-NH2	-7.72	1.23	1.33
1	B	221	ARG	CZ-NH2	-7.71	1.23	1.33
1	B	278	ARG	CZ-NH2	-7.71	1.23	1.33
1	A	259	ARG	CZ-NH2	-7.71	1.23	1.33
1	C	444	ARG	CZ-NH2	-7.69	1.23	1.33
1	C	259	ARG	CZ-NH1	-7.68	1.22	1.32
1	B	314	ARG	CZ-NH2	-7.64	1.23	1.33
1	C	211	ARG	CZ-NH1	-7.59	1.22	1.32
1	B	113	ALA	CA-CB	-7.57	1.42	1.53
1	C	91	GLY	N-CA	-7.54	1.37	1.45
1	A	270	ALA	CA-CB	-7.54	1.43	1.53
1	B	153	ARG	CZ-NH1	-7.38	1.22	1.32
1	B	516	ALA	CA-CB	-7.36	1.42	1.53
1	B	114	ALA	CA-CB	-7.35	1.41	1.53
1	C	140	ARG	CZ-NH1	-7.27	1.22	1.32
1	C	360	ALA	CA-CB	-7.24	1.43	1.52
1	A	470	ALA	CA-CB	-7.22	1.42	1.52
1	A	177	LEU	C-N	-7.19	1.28	1.33
1	B	478	ALA	CA-CB	-7.17	1.42	1.53
1	C	86	ALA	CA-CB	-7.12	1.42	1.53
1	C	496	ALA	CA-CB	-7.10	1.43	1.54
1	C	20	ALA	CA-CB	-7.08	1.41	1.53
1	B	91	GLY	N-CA	-7.07	1.38	1.45
1	A	455	ARG	CZ-NH1	-7.06	1.22	1.32
1	B	253	ARG	CZ-NH1	-7.05	1.22	1.32
1	C	271	GLY	N-CA	-7.04	1.37	1.45
1	C	458	ALA	CA-CB	-7.04	1.42	1.53
1	A	166	ALA	CA-CB	-7.04	1.42	1.53
1	C	126	GLY	N-CA	-7.03	1.36	1.45
1	B	140	ARG	CZ-NH1	-7.03	1.23	1.32
1	B	259	ARG	CZ-NH1	-6.98	1.23	1.32
1	A	263	GLY	N-CA	-6.97	1.37	1.45
1	A	518	ALA	CA-CB	-6.97	1.42	1.53
1	B	385	GLY	N-CA	-6.96	1.38	1.45
1	A	196	ARG	CZ-NH1	-6.96	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	ARG	CZ-NH1	-6.92	1.23	1.32
1	C	237	GLY	N-CA	-6.92	1.38	1.45
1	B	126	GLY	N-CA	-6.91	1.37	1.45
1	B	470	ALA	CA-CB	-6.91	1.42	1.53
1	B	468	ALA	CA-CB	-6.89	1.42	1.53
1	A	153	ARG	CZ-NH1	-6.89	1.23	1.32
1	C	113	ALA	CA-CB	-6.88	1.41	1.53
1	A	458	ALA	CA-CB	-6.88	1.42	1.53
1	B	77	ARG	CZ-NH1	-6.87	1.23	1.32
1	A	99	ARG	CZ-NH1	-6.84	1.23	1.32
1	C	438	ALA	CA-CB	-6.83	1.42	1.53
1	B	510	ALA	CA-CB	-6.79	1.42	1.53
1	C	455	ARG	CZ-NH1	-6.78	1.23	1.32
1	A	18	GLY	N-CA	-6.76	1.37	1.45
1	B	99	ARG	CZ-NH1	-6.75	1.23	1.32
1	A	217	ALA	CA-CB	-6.73	1.43	1.53
1	C	444	ARG	CZ-NH1	-6.73	1.23	1.32
1	B	314	ARG	CZ-NH1	-6.73	1.23	1.32
1	A	259	ARG	CZ-NH1	-6.71	1.23	1.32
1	B	485	GLY	N-CA	-6.71	1.38	1.46
1	C	442	ALA	CA-CB	-6.71	1.42	1.53
1	B	413	ARG	CZ-NH1	-6.70	1.23	1.32
1	C	500	PRO	CA-CB	-6.69	1.46	1.53
1	B	31	ALA	CA-CB	-6.68	1.43	1.53
1	B	356	ALA	CA-CB	-6.64	1.43	1.53
1	B	234	ARG	CZ-NH1	-6.64	1.23	1.32
1	B	217	ALA	CA-CB	-6.63	1.42	1.53
1	C	278	ARG	CZ-NH1	-6.61	1.23	1.32
1	B	221	ARG	CZ-NH1	-6.59	1.23	1.32
1	B	348	ARG	CZ-NH1	-6.58	1.23	1.32
1	B	278	ARG	CZ-NH1	-6.58	1.23	1.32
1	C	518	ALA	CA-CB	-6.57	1.43	1.53
1	B	29	ALA	CA-CB	-6.56	1.43	1.53
1	B	166	ALA	CA-CB	-6.53	1.42	1.53
1	A	478	ALA	CA-CB	-6.52	1.43	1.53
1	B	518	ALA	CA-CB	-6.47	1.42	1.53
1	B	86	ALA	CA-CB	-6.43	1.42	1.53
1	B	251	ALA	CA-CB	-6.41	1.43	1.53
1	B	117	VAL	N-CA	-6.41	1.41	1.46
1	A	323	ALA	CA-CB	-6.32	1.43	1.53
1	C	270	ALA	CA-CB	-6.31	1.43	1.53
1	A	442	ALA	CA-CB	-6.26	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	428	PRO	CA-CB	-6.26	1.45	1.53
1	B	93	SER	CA-CB	-6.23	1.45	1.53
1	B	259	ARG	CA-CB	-6.21	1.47	1.54
1	B	368	GLY	N-CA	-6.19	1.37	1.45
1	C	106	GLY	N-CA	-6.17	1.37	1.45
1	A	385	GLY	N-CA	-6.14	1.37	1.45
1	A	14	GLY	N-CA	-6.11	1.37	1.45
1	B	420	ALA	CA-CB	-6.11	1.43	1.53
1	A	178	ASN	CA-CB	-6.10	1.46	1.53
1	A	271	GLY	N-CA	-6.10	1.38	1.45
1	B	323	ALA	CA-CB	-6.09	1.43	1.53
1	A	455	ARG	CD-NE	-6.08	1.37	1.46
1	A	485	GLY	CA-C	-6.02	1.48	1.52
1	B	490	GLY	N-CA	-6.00	1.37	1.45
1	B	153	ARG	CD-NE	-5.99	1.37	1.46
1	C	18	GLY	N-CA	-5.98	1.36	1.45
1	B	319	ALA	CA-CB	-5.94	1.43	1.53
1	B	99	ARG	CD-NE	-5.93	1.38	1.46
1	B	303	GLN	C-N	-5.92	1.28	1.33
1	B	106	GLY	N-CA	-5.91	1.37	1.45
1	A	77	ARG	CD-NE	-5.88	1.38	1.46
1	B	270	ALA	CA-CB	-5.87	1.43	1.53
1	A	465	GLY	N-CA	-5.86	1.36	1.44
1	A	153	ARG	CD-NE	-5.84	1.38	1.46
1	B	296	GLY	N-CA	-5.83	1.38	1.45
1	C	125	GLY	N-CA	-5.82	1.37	1.45
1	A	259	ARG	CD-NE	-5.81	1.38	1.46
1	B	465	GLY	N-CA	-5.79	1.36	1.44
1	C	259	ARG	CD-NE	-5.79	1.38	1.46
1	C	201	PHE	CA-CB	-5.78	1.45	1.52
1	B	77	ARG	CD-NE	-5.78	1.38	1.46
1	A	73	GLY	N-CA	-5.78	1.36	1.45
1	B	373	GLY	N-CA	-5.75	1.37	1.45
1	B	234	ARG	CD-NE	-5.75	1.38	1.46
1	B	303	GLN	CA-CB	-5.75	1.47	1.54
1	B	413	ARG	CD-NE	-5.75	1.38	1.46
1	C	204	HIS	CA-CB	-5.74	1.45	1.53
1	A	178	ASN	N-CA	-5.74	1.41	1.46
1	C	514	GLY	N-CA	-5.73	1.37	1.45
1	C	465	GLY	N-CA	-5.72	1.36	1.44
1	C	455	ARG	CD-NE	-5.71	1.38	1.46
1	C	444	ARG	CD-NE	-5.71	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	161	HIS	CA-CB	-5.69	1.46	1.54
1	C	437	ALA	CA-CB	-5.69	1.43	1.53
1	A	196	ARG	CD-NE	-5.69	1.38	1.46
1	C	373	GLY	N-CA	-5.67	1.37	1.45
1	A	514	GLY	N-CA	-5.67	1.37	1.45
1	B	369	LYS	CA-CB	-5.65	1.47	1.54
1	B	254	HIS	CA-CB	-5.63	1.45	1.53
1	C	140	ARG	CD-NE	-5.62	1.38	1.46
1	B	399	GLY	N-CA	-5.59	1.37	1.45
1	A	319	ALA	CA-CB	-5.58	1.43	1.53
1	C	211	ARG	CA-CB	-5.58	1.45	1.53
1	B	348	ARG	CD-NE	-5.56	1.38	1.46
1	B	360	ALA	CA-CB	-5.56	1.43	1.54
1	C	208	PRO	CA-CB	-5.55	1.46	1.54
1	C	72	GLN	C-N	-5.54	1.27	1.33
1	C	241	GLY	N-CA	-5.51	1.37	1.45
1	C	66	GLY	N-CA	-5.49	1.38	1.45
1	B	514	GLY	CA-C	-5.48	1.46	1.52
1	A	99	ARG	CD-NE	-5.47	1.38	1.46
1	B	150	PRO	CA-CB	-5.46	1.46	1.53
1	C	497	PRO	CA-CB	-5.46	1.46	1.53
1	C	305	PRO	CA-CB	-5.46	1.46	1.53
1	C	425	GLY	N-CA	-5.45	1.37	1.45
1	C	424	GLY	N-CA	-5.44	1.37	1.45
1	B	264	TRP	CA-CB	-5.44	1.44	1.54
1	A	418	PRO	CA-CB	-5.44	1.46	1.53
1	C	441	PRO	CA-CB	-5.44	1.46	1.53
1	B	133	PRO	CA-CB	-5.42	1.46	1.53
1	C	296	GLY	N-CA	-5.42	1.38	1.45
1	B	304	VAL	N-CA	-5.42	1.42	1.46
1	C	14	GLY	N-CA	-5.41	1.37	1.45
1	B	144	PRO	CA-CB	-5.39	1.46	1.53
1	C	495	GLY	N-CA	-5.38	1.38	1.45
1	B	221	ARG	CD-NE	-5.36	1.38	1.46
1	A	443	PRO	CA-CB	-5.36	1.46	1.53
1	B	66	GLY	N-CA	-5.35	1.36	1.45
1	B	253	ARG	CD-NE	-5.35	1.38	1.46
1	B	230	TRP	CA-CB	-5.34	1.46	1.52
1	B	219	PRO	CA-CB	-5.33	1.46	1.53
1	C	168	LEU	CA-CB	-5.33	1.46	1.53
1	B	73	GLY	N-CA	-5.32	1.36	1.45
1	B	290	GLY	N-CA	-5.31	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	314	ARG	CD-NE	-5.29	1.38	1.46
1	B	412	LYS	CA-CB	-5.29	1.45	1.53
1	A	60	SER	CA-CB	-5.29	1.45	1.53
1	C	80	PRO	CA-CB	-5.28	1.46	1.53
1	B	94	GLY	N-CA	-5.27	1.37	1.45
1	C	443	PRO	CA-CB	-5.26	1.46	1.53
1	C	211	ARG	CD-NE	-5.26	1.38	1.46
1	A	525	ASN	CA-CB	-5.25	1.46	1.52
1	A	495	GLY	N-CA	-5.25	1.37	1.45
1	A	524	HIS	CA-CB	-5.25	1.45	1.53
1	B	246	PRO	CA-CB	-5.25	1.46	1.53
1	A	10	PRO	N-CD	-5.24	1.40	1.47
1	B	118	PRO	CA-CB	-5.22	1.46	1.54
1	B	259	ARG	CD-NE	-5.22	1.39	1.46
1	B	424	GLY	N-CA	-5.21	1.37	1.45
1	C	280	ASN	N-CA	-5.21	1.41	1.46
1	C	58	ASN	CA-CB	-5.21	1.46	1.53
1	B	306	ASP	CA-CB	-5.20	1.46	1.52
1	B	493	PHE	CA-CB	-5.19	1.45	1.53
1	C	358	GLY	N-CA	-5.18	1.37	1.45
1	A	520	ASN	CA-CB	-5.18	1.45	1.53
1	B	223	ILE	N-CA	-5.18	1.41	1.46
1	A	216	GLY	N-CA	-5.18	1.37	1.45
1	A	259	ARG	CA-CB	-5.17	1.46	1.53
1	B	119	PRO	CA-CB	-5.17	1.46	1.53
1	B	305	PRO	CA-CB	-5.17	1.46	1.53
1	A	424	GLY	N-CA	-5.16	1.37	1.45
1	B	485	GLY	CA-C	-5.16	1.47	1.52
1	B	378	GLY	N-CA	-5.16	1.37	1.45
1	B	479	GLY	N-CA	-5.16	1.37	1.45
1	B	307	GLY	N-CA	-5.16	1.37	1.45
1	C	525	ASN	CA-CB	-5.15	1.46	1.52
1	C	140	ARG	CA-CB	-5.14	1.46	1.53
1	B	224	PRO	CA-CB	-5.14	1.46	1.53
1	A	151	ASP	CA-CB	-5.13	1.46	1.52
1	B	30	PRO	CA-CB	-5.13	1.46	1.53
1	C	399	GLY	N-CA	-5.12	1.38	1.45
1	A	425	GLY	N-CA	-5.12	1.37	1.45
1	A	17	GLN	CD-NE2	-5.12	1.22	1.33
1	A	485	GLY	N-CA	-5.12	1.38	1.45
1	B	140	ARG	CD-NE	-5.12	1.39	1.46
1	C	19	VAL	N-CA	-5.11	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	250	GLN	CA-CB	-5.11	1.45	1.53
1	C	76	PRO	CA-CB	-5.11	1.46	1.53
1	C	303	GLN	CA-CB	-5.11	1.47	1.53
1	B	500	PRO	CA-CB	-5.10	1.46	1.53
1	A	168	LEU	CA-CB	-5.10	1.46	1.53
1	C	237	GLY	CA-C	-5.09	1.46	1.52
1	C	131	GLN	CD-NE2	-5.08	1.22	1.33
1	C	78	MET	C-N	-5.08	1.24	1.33
1	A	72	GLN	CA-CB	-5.08	1.46	1.52
1	B	480	ASN	CG-ND2	-5.07	1.22	1.33
1	B	205	LEU	CA-CB	-5.07	1.46	1.53
1	B	275	ASN	CA-CB	-5.07	1.46	1.53
1	B	202	GLU	N-CA	-5.07	1.40	1.46
1	B	134	HIS	CA-CB	-5.07	1.45	1.53
1	C	141	GLN	CD-NE2	-5.06	1.22	1.33
1	C	280	ASN	CA-CB	-5.06	1.47	1.53
1	B	116	MET	C-N	-5.06	1.28	1.33
1	B	171	LEU	CA-CB	-5.05	1.45	1.53
1	B	67	LYS	C-N	-5.05	1.28	1.33
1	C	307	GLY	N-CA	-5.05	1.37	1.45
1	B	448	SER	CA-CB	-5.05	1.45	1.53
1	B	132	PHE	CA-CB	-5.04	1.46	1.53
1	B	525	ASN	CG-ND2	-5.04	1.22	1.33
1	C	209	PRO	CA-CB	-5.04	1.46	1.53
1	C	447	ASN	CG-ND2	-5.04	1.22	1.33
1	B	426	ASN	CG-ND2	-5.03	1.22	1.33
1	B	278	ARG	CD-NE	-5.03	1.39	1.46
1	B	140	ARG	CA-CB	-5.02	1.46	1.53
1	C	58	ASN	CG-ND2	-5.01	1.22	1.33
1	A	144	PRO	CA-CB	-5.01	1.47	1.53
1	A	150	PRO	CA-CB	-5.01	1.46	1.53
1	B	143	GLU	N-CA	-5.01	1.39	1.45
1	B	473	LYS	CE-NZ	-5.01	1.34	1.49
1	C	447	ASN	CA-CB	-5.01	1.45	1.53
1	C	480	ASN	CA-CB	-5.01	1.45	1.53

All (521) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	MET	CA-C-N	11.01	130.51	122.59
1	B	116	MET	C-N-CA	11.01	130.51	122.59
1	B	309	PRO	CA-C-N	10.01	135.52	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	309	PRO	C-N-CA	10.01	135.52	120.31
1	B	484	ILE	CA-C-N	9.83	129.51	122.33
1	B	484	ILE	C-N-CA	9.83	129.51	122.33
1	A	476	ASP	CA-CB-CG	8.25	120.85	112.60
1	B	505	GLN	CA-C-N	8.25	130.40	120.09
1	B	505	GLN	C-N-CA	8.25	130.40	120.09
1	C	132	PHE	CA-CB-CG	8.00	121.80	113.80
1	B	147	PHE	CA-CB-CG	7.66	121.46	113.80
1	C	255	PHE	CA-CB-CG	7.64	121.44	113.80
1	C	203	PHE	CA-CB-CG	7.63	121.43	113.80
1	C	147	PHE	CA-CB-CG	7.54	121.34	113.80
1	B	132	PHE	CA-CB-CG	7.52	121.32	113.80
1	B	501	PHE	CA-CB-CG	7.45	121.25	113.80
1	C	138	ASP	CA-CB-CG	7.35	119.95	112.60
1	C	520	ASN	CA-CB-CG	7.31	119.91	112.60
1	B	347	TRP	CA-C-N	7.20	133.82	121.29
1	B	347	TRP	C-N-CA	7.20	133.82	121.29
1	C	83	ASP	CA-CB-CG	7.17	119.77	112.60
1	B	158	HIS	CA-CB-CG	7.17	120.97	113.80
1	B	269	HIS	CA-CB-CG	7.16	120.96	113.80
1	B	480	ASN	CA-CB-CG	7.16	119.76	112.60
1	C	70	PHE	CA-CB-CG	7.15	120.95	113.80
1	A	362	ASN	CA-CB-CG	7.14	119.74	112.60
1	A	58	ASN	CA-CB-CG	7.09	119.69	112.60
1	B	460	ASP	CA-CB-CG	7.06	119.66	112.60
1	B	385	GLY	N-CA-C	7.05	120.06	110.69
1	A	70	PHE	CA-CB-CG	7.03	120.83	113.80
1	C	190	THR	CA-C-N	7.02	131.15	122.37
1	C	190	THR	C-N-CA	7.02	131.15	122.37
1	A	11	ASP	CA-CB-CG	6.99	119.59	112.60
1	A	51	PHE	CA-CB-CG	6.95	120.75	113.80
1	C	480	ASN	CA-CB-CG	6.94	119.54	112.60
1	B	303	GLN	CA-C-N	6.93	127.31	122.60
1	B	303	GLN	C-N-CA	6.93	127.31	122.60
1	A	285	ASP	CA-CB-CG	6.90	119.50	112.60
1	B	167	HIS	CA-CB-CG	6.89	120.69	113.80
1	C	158	HIS	CA-CB-CG	6.88	120.68	113.80
1	B	493	PHE	CA-CB-CG	6.87	120.67	113.80
1	B	525	ASN	CA-CB-CG	6.86	119.46	112.60
1	B	463	ASP	CA-CB-CG	6.85	119.45	112.60
1	A	178	ASN	CA-CB-CG	6.84	119.44	112.60
1	A	463	ASP	CA-CB-CG	6.83	119.43	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	PHE	CA-CB-CG	6.83	120.63	113.80
1	A	83	ASP	CA-CB-CG	6.82	119.42	112.60
1	B	472	PHE	CA-CB-CG	6.78	120.58	113.80
1	B	84	HIS	CA-CB-CG	6.78	120.58	113.80
1	B	162	ASP	CA-CB-CG	6.76	119.36	112.60
1	B	475	LYS	CA-CB-CG	6.76	127.61	114.10
1	B	380	ASN	CA-CB-CG	6.73	119.33	112.60
1	B	310	ASP	CA-CB-CG	6.72	119.32	112.60
1	A	304	VAL	N-CA-C	6.71	123.39	108.88
1	A	483	ASP	CA-CB-CG	6.71	119.31	112.60
1	C	231	GLU	CA-C-N	6.71	127.38	120.60
1	C	231	GLU	C-N-CA	6.71	127.38	120.60
1	C	159	ASP	CA-CB-CG	6.70	119.30	112.60
1	C	236	PRO	CA-C-N	6.69	130.15	120.91
1	C	236	PRO	C-N-CA	6.69	130.15	120.91
1	C	525	ASN	CA-CB-CG	6.69	119.29	112.60
1	A	282	ASP	CA-CB-CG	6.69	119.29	112.60
1	C	100	PHE	CA-CB-CG	6.69	120.49	113.80
1	A	151	ASP	CA-CB-CG	6.67	119.27	112.60
1	B	151	ASP	CA-CB-CG	6.66	119.26	112.60
1	B	374	ASN	CA-CB-CG	6.66	119.26	112.60
1	B	290	GLY	CA-C-N	6.66	131.44	123.19
1	B	290	GLY	C-N-CA	6.66	131.44	123.19
1	A	493	PHE	CA-CB-CG	6.65	120.45	113.80
1	B	201	PHE	CA-CB-CG	6.64	120.44	113.80
1	C	84	HIS	CA-CB-CG	6.62	120.42	113.80
1	A	460	ASP	CA-CB-CG	6.62	119.22	112.60
1	C	58	ASN	CA-CB-CG	6.60	119.20	112.60
1	C	479	GLY	N-CA-C	6.60	123.50	114.92
1	A	161	HIS	CA-CB-CG	6.59	120.39	113.80
1	C	162	ASP	CA-CB-CG	6.59	119.19	112.60
1	B	70	PHE	CA-CB-CG	6.58	120.38	113.80
1	B	473	LYS	CA-CB-CG	6.58	127.26	114.10
1	B	97	GLU	CA-C-N	6.57	131.84	123.10
1	B	97	GLU	C-N-CA	6.57	131.84	123.10
1	C	167	HIS	CA-CB-CG	6.57	120.37	113.80
1	C	275	ASN	CA-CB-CG	6.57	119.17	112.60
1	A	162	ASP	CA-CB-CG	6.56	119.16	112.60
1	A	256	ASP	CA-CB-CG	6.55	119.15	112.60
1	B	315	ASN	CA-CB-CG	6.52	119.12	112.60
1	B	100	PHE	CA-CB-CG	6.50	120.30	113.80
1	B	357	ASN	CA-CB-CG	6.50	119.10	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	ARG	CA-C-N	6.50	130.71	121.42
1	B	99	ARG	C-N-CA	6.50	130.71	121.42
1	C	483	ASP	CA-CB-CG	6.50	119.10	112.60
1	A	97	GLU	CA-C-N	6.49	131.55	123.12
1	A	97	GLU	C-N-CA	6.49	131.55	123.12
1	B	83	ASP	CA-CB-CG	6.49	119.09	112.60
1	A	409	ASP	CA-CB-CG	6.47	119.07	112.60
1	B	474	ILE	CA-C-N	6.47	132.31	122.93
1	B	474	ILE	C-N-CA	6.47	132.31	122.93
1	A	400	ASP	CA-CB-CG	6.47	119.07	112.60
1	B	320	ASN	CA-CB-CG	6.45	119.05	112.60
1	C	501	PHE	CA-CB-CG	6.45	120.25	113.80
1	C	447	ASN	CA-CB-CG	6.45	119.05	112.60
1	B	218	ASP	CA-CB-CG	6.45	119.05	112.60
1	B	299	THR	CA-C-N	6.43	129.94	120.74
1	B	299	THR	C-N-CA	6.43	129.94	120.74
1	A	167	HIS	CA-CB-CG	6.42	120.22	113.80
1	A	174	ASN	CA-CB-CG	6.42	119.02	112.60
1	A	320	ASN	CA-CB-CG	6.42	119.02	112.60
1	C	280	ASN	CA-CB-CG	6.41	119.01	112.60
1	A	310	ASP	CA-CB-CG	6.40	119.00	112.60
1	B	409	ASP	CA-CB-CG	6.39	119.00	112.60
1	C	79	ASN	CA-CB-CG	6.39	118.99	112.60
1	B	483	ASP	CA-C-N	6.38	130.97	122.93
1	B	483	ASP	C-N-CA	6.38	130.97	122.93
1	B	520	ASN	CA-CB-CG	6.38	118.98	112.60
1	B	491	PHE	CA-CB-CG	6.38	120.18	113.80
1	A	491	PHE	CA-CB-CG	6.37	120.17	113.80
1	B	229	PHE	CA-CB-CG	6.35	120.15	113.80
1	B	426	ASN	CA-CB-CG	6.34	118.94	112.60
1	A	407	ASP	CA-CB-CG	6.33	118.94	112.60
1	A	470	ALA	CA-C-N	6.33	130.40	121.66
1	A	470	ALA	C-N-CA	6.33	130.40	121.66
1	A	315	ASN	CA-CB-CG	6.30	118.90	112.60
1	B	275	ASN	CA-CB-CG	6.30	118.90	112.60
1	A	63	ASP	CA-CB-CG	6.29	118.89	112.60
1	A	426	ASN	CA-CB-CG	6.29	118.89	112.60
1	C	328	VAL	N-CA-C	6.28	118.70	108.97
1	B	407	ASP	CA-CB-CG	6.27	118.87	112.60
1	C	81	PHE	CA-CB-CG	6.26	120.06	113.80
1	B	146	ILE	CA-C-N	6.23	131.32	122.72
1	B	146	ILE	C-N-CA	6.23	131.32	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	513	VAL	CA-C-N	6.23	129.57	121.23
1	B	513	VAL	C-N-CA	6.23	129.57	121.23
1	C	375	PHE	CA-CB-CG	6.22	120.02	113.80
1	C	192	THR	CA-C-N	6.17	130.85	123.19
1	C	192	THR	C-N-CA	6.17	130.85	123.19
1	B	200	ASP	CA-CB-CG	6.16	118.76	112.60
1	C	271	GLY	CA-C-N	6.16	130.78	122.90
1	C	271	GLY	C-N-CA	6.16	130.78	122.90
1	C	292	HIS	CA-CB-CG	6.15	119.95	113.80
1	B	87	LYS	CA-C-N	6.15	131.89	122.29
1	B	87	LYS	C-N-CA	6.15	131.89	122.29
1	A	254	HIS	CA-CB-CG	-6.14	107.66	113.80
1	B	288	ASP	CA-CB-CG	6.14	118.74	112.60
1	B	506	PHE	CA-CB-CG	6.14	119.94	113.80
1	C	102	ILE	N-CA-CB	6.14	118.15	110.05
1	B	485	GLY	CA-C-N	6.13	130.66	122.93
1	B	485	GLY	C-N-CA	6.13	130.66	122.93
1	C	243	SER	CA-C-N	6.12	130.27	122.37
1	C	243	SER	C-N-CA	6.12	130.27	122.37
1	A	190	THR	CA-C-N	6.11	131.15	123.14
1	A	190	THR	C-N-CA	6.11	131.15	123.14
1	B	204	HIS	CA-CB-CG	6.11	119.91	113.80
1	C	265	SER	CA-C-N	6.11	129.95	120.60
1	C	265	SER	C-N-CA	6.11	129.95	120.60
1	C	429	ILE	CA-C-N	6.10	131.59	123.05
1	C	429	ILE	C-N-CA	6.10	131.59	123.05
1	A	218	ASP	CA-CB-CG	6.10	118.70	112.60
1	C	169	VAL	CA-C-N	6.10	130.92	122.93
1	C	169	VAL	C-N-CA	6.10	130.92	122.93
1	B	204	HIS	N-CA-C	6.09	120.48	112.13
1	A	271	GLY	CA-C-N	6.09	131.03	123.12
1	A	271	GLY	C-N-CA	6.09	131.03	123.12
1	C	205	LEU	CA-C-N	6.08	129.34	120.71
1	C	205	LEU	C-N-CA	6.08	129.34	120.71
1	B	144	PRO	CA-C-N	6.07	130.71	123.19
1	B	144	PRO	C-N-CA	6.07	130.71	123.19
1	B	493	PHE	CA-C-N	6.06	131.30	122.69
1	B	493	PHE	C-N-CA	6.06	131.30	122.69
1	A	148	ASN	CA-CB-CG	6.06	118.66	112.60
1	A	525	ASN	CA-CB-CG	6.06	118.66	112.60
1	B	56	THR	CA-C-N	6.05	130.98	123.12
1	B	56	THR	C-N-CA	6.05	130.98	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	134	HIS	CA-C-N	6.04	130.78	121.71
1	B	134	HIS	C-N-CA	6.04	130.78	121.71
1	B	243	SER	CA-C-N	6.04	131.05	123.14
1	B	243	SER	C-N-CA	6.04	131.05	123.14
1	B	306	ASP	CA-CB-CG	6.04	118.64	112.60
1	B	169	VAL	CA-C-N	6.03	130.43	122.95
1	B	169	VAL	C-N-CA	6.03	130.43	122.95
1	B	252	ASN	CA-CB-CG	6.03	118.63	112.60
1	B	367	CYS	CA-C-N	6.00	129.07	120.56
1	B	367	CYS	C-N-CA	6.00	129.07	120.56
1	B	275	ASN	CA-C-N	5.98	129.96	122.43
1	B	275	ASN	C-N-CA	5.98	129.96	122.43
1	B	259	ARG	CD-NE-CZ	5.97	132.76	124.40
1	A	50	PHE	CA-C-N	5.97	130.92	122.09
1	A	50	PHE	C-N-CA	5.97	130.92	122.09
1	B	491	PHE	CA-C-N	5.94	130.34	121.72
1	B	491	PHE	C-N-CA	5.94	130.34	121.72
1	C	272	VAL	CA-C-N	5.93	130.87	122.09
1	C	272	VAL	C-N-CA	5.93	130.87	122.09
1	B	416	VAL	CA-C-N	5.92	131.07	121.83
1	B	416	VAL	C-N-CA	5.92	131.07	121.83
1	B	282	ASP	CA-CB-CG	5.92	118.52	112.60
1	B	278	ARG	CD-NE-CZ	5.92	132.68	124.40
1	A	305	PRO	N-CA-CB	5.92	108.58	103.31
1	C	136	LEU	CA-C-N	5.90	131.35	122.91
1	C	136	LEU	C-N-CA	5.90	131.35	122.91
1	A	484	ILE	CA-C-N	5.88	128.20	122.73
1	A	484	ILE	C-N-CA	5.88	128.20	122.73
1	C	278	ARG	CD-NE-CZ	5.88	132.62	124.40
1	B	286	LYS	CA-C-N	5.87	131.15	121.99
1	B	286	LYS	C-N-CA	5.87	131.15	121.99
1	C	426	ASN	CA-CB-CG	5.87	118.47	112.60
1	B	374	ASN	CA-C-N	5.87	130.82	122.72
1	B	374	ASN	C-N-CA	5.87	130.82	122.72
1	C	201	PHE	CA-CB-CG	5.87	119.67	113.80
1	A	20	ALA	CA-C-N	5.86	130.81	123.14
1	A	20	ALA	C-N-CA	5.86	130.81	123.14
1	C	358	GLY	CA-C-N	5.85	130.20	122.30
1	C	358	GLY	C-N-CA	5.85	130.20	122.30
1	B	159	ASP	CA-CB-CG	5.85	118.45	112.60
1	B	383	GLN	CA-C-N	5.85	129.87	121.50
1	B	383	GLN	C-N-CA	5.85	129.87	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	VAL	CA-C-N	5.85	131.07	123.11
1	B	145	VAL	C-N-CA	5.85	131.07	123.11
1	A	99	ARG	CD-NE-CZ	5.84	132.58	124.40
1	A	193	VAL	CA-C-N	5.83	131.22	122.99
1	A	193	VAL	C-N-CA	5.83	131.22	122.99
1	B	504	LEU	CA-C-N	5.83	131.34	122.65
1	B	504	LEU	C-N-CA	5.83	131.34	122.65
1	A	70	PHE	CA-C-N	5.82	130.69	123.12
1	A	70	PHE	C-N-CA	5.82	130.69	123.12
1	C	293	LEU	CA-C-N	5.81	131.06	122.99
1	C	293	LEU	C-N-CA	5.81	131.06	122.99
1	B	349	HIS	CA-CB-CG	5.80	119.61	113.80
1	B	150	PRO	CA-C-N	5.80	130.13	122.06
1	B	150	PRO	C-N-CA	5.80	130.13	122.06
1	B	376	TYR	CA-C-N	5.80	131.22	122.98
1	B	376	TYR	C-N-CA	5.80	131.22	122.98
1	A	355	PHE	CA-CB-CG	5.80	119.60	113.80
1	C	525	ASN	CA-C-N	5.80	131.21	122.98
1	C	525	ASN	C-N-CA	5.80	131.21	122.98
1	C	113	ALA	CA-C-N	5.79	131.17	123.00
1	C	113	ALA	C-N-CA	5.79	131.17	123.00
1	C	67	LYS	CA-C-N	5.77	129.70	122.43
1	C	67	LYS	C-N-CA	5.77	129.70	122.43
1	C	495	GLY	N-CA-C	5.76	121.13	114.16
1	A	177	LEU	CA-C-N	5.75	129.19	122.52
1	A	177	LEU	C-N-CA	5.75	129.19	122.52
1	A	238	GLU	CA-C-N	5.74	128.86	120.71
1	A	238	GLU	C-N-CA	5.74	128.86	120.71
1	B	67	LYS	N-CA-CB	5.74	118.37	109.48
1	B	384	GLN	N-CA-CB	5.73	118.84	109.95
1	A	357	ASN	CA-CB-CG	5.72	118.32	112.60
1	C	349	HIS	CA-CB-CG	5.71	119.51	113.80
1	B	88	MET	CA-CB-CG	5.70	125.51	114.10
1	B	368	GLY	N-CA-C	5.70	118.84	110.80
1	A	153	ARG	CD-NE-CZ	5.70	132.38	124.40
1	B	120	GLY	CA-C-N	5.68	129.47	122.37
1	B	120	GLY	C-N-CA	5.68	129.47	122.37
1	B	70	PHE	CA-C-N	5.67	130.42	123.10
1	B	70	PHE	C-N-CA	5.67	130.42	123.10
1	B	412	LYS	CA-C-N	5.67	131.15	122.93
1	B	412	LYS	C-N-CA	5.67	131.15	122.93
1	A	11	ASP	CA-C-N	5.66	128.09	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	ASP	C-N-CA	5.66	128.09	120.50
1	A	357	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	C	141	GLN	N-CA-CB	5.64	118.58	110.06
1	B	253	ARG	CA-C-N	5.64	130.27	122.77
1	B	253	ARG	C-N-CA	5.64	130.27	122.77
1	C	144	PRO	CA-C-N	5.63	130.59	123.10
1	C	144	PRO	C-N-CA	5.63	130.59	123.10
1	C	157	TRP	CA-C-N	5.62	129.76	120.94
1	C	157	TRP	C-N-CA	5.62	129.76	120.94
1	B	292	HIS	CA-CB-CG	5.62	119.42	113.80
1	B	112	LEU	CA-C-N	5.61	130.38	122.09
1	B	112	LEU	C-N-CA	5.61	130.38	122.09
1	B	294	VAL	CA-C-N	5.61	130.89	122.99
1	B	294	VAL	C-N-CA	5.61	130.89	122.99
1	C	99	ARG	CA-C-N	5.60	130.38	122.09
1	C	99	ARG	C-N-CA	5.60	130.38	122.09
1	B	460	ASP	CA-C-N	5.60	130.58	121.62
1	B	460	ASP	C-N-CA	5.60	130.58	121.62
1	B	254	HIS	CA-CB-CG	5.59	119.39	113.80
1	B	364	THR	CA-C-N	5.59	130.32	123.17
1	B	364	THR	C-N-CA	5.59	130.32	123.17
1	A	304	VAL	CA-CB-CG2	5.58	119.89	110.40
1	B	300	ILE	CA-C-N	5.58	131.02	122.93
1	B	300	ILE	C-N-CA	5.58	131.02	122.93
1	B	151	ASP	N-CA-CB	5.58	116.60	110.35
1	A	96	MET	CA-C-N	5.57	130.04	122.19
1	A	96	MET	C-N-CA	5.57	130.04	122.19
1	B	425	GLY	CA-C-N	5.57	130.68	123.00
1	B	425	GLY	C-N-CA	5.57	130.68	123.00
1	B	154	THR	CA-C-N	5.56	131.01	122.68
1	B	154	THR	C-N-CA	5.56	131.01	122.68
1	B	295	THR	CA-C-N	5.54	126.13	119.98
1	B	295	THR	C-N-CA	5.54	126.13	119.98
1	C	451	LEU	N-CA-CB	5.52	118.34	110.06
1	B	408	GLU	CA-C-N	5.52	129.43	120.60
1	B	408	GLU	C-N-CA	5.52	129.43	120.60
1	B	473	LYS	CA-C-N	5.52	130.16	122.93
1	B	473	LYS	C-N-CA	5.52	130.16	122.93
1	A	254	HIS	CB-CG-CD2	-5.51	124.04	131.20
1	C	204	HIS	CE1-NE2-CD2	-5.49	103.51	109.00
1	B	114	ALA	CA-C-N	5.49	130.40	123.10
1	B	114	ALA	C-N-CA	5.49	130.40	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	GLN	CA-C-N	5.48	128.47	120.91
1	B	384	GLN	C-N-CA	5.48	128.47	120.91
1	C	134	HIS	CE1-NE2-CD2	-5.48	103.52	109.00
1	A	520	ASN	CA-CB-CG	5.47	118.07	112.60
1	A	151	ASP	N-CA-CB	5.46	117.19	110.53
1	B	517	SER	N-CA-CB	5.46	118.14	109.51
1	A	425	GLY	CA-C-N	5.45	130.67	122.99
1	A	425	GLY	C-N-CA	5.45	130.67	122.99
1	A	514	GLY	N-CA-C	5.45	118.66	111.52
1	B	285	ASP	CA-C-N	5.45	128.98	120.75
1	B	285	ASP	C-N-CA	5.45	128.98	120.75
1	C	67	LYS	N-CA-CB	5.45	117.93	109.48
1	A	192	THR	CA-C-N	5.45	130.28	123.14
1	A	192	THR	C-N-CA	5.45	130.28	123.14
1	A	276	ILE	CA-C-N	5.44	129.86	122.19
1	A	276	ILE	C-N-CA	5.44	129.86	122.19
1	A	55	THR	CA-C-N	5.43	130.75	122.65
1	A	55	THR	C-N-CA	5.43	130.75	122.65
1	B	406	GLU	CA-C-N	5.43	130.21	122.72
1	B	406	GLU	C-N-CA	5.43	130.21	122.72
1	A	259	ARG	CD-NE-CZ	5.43	132.00	124.40
1	B	369	LYS	CA-CB-CG	5.43	124.96	114.10
1	A	169	VAL	CA-C-N	5.42	129.26	122.48
1	A	169	VAL	C-N-CA	5.42	129.26	122.48
1	A	216	GLY	CA-C-N	5.42	131.06	122.60
1	A	216	GLY	C-N-CA	5.42	131.06	122.60
1	A	132	PHE	CB-CA-C	5.42	117.86	108.91
1	B	134	HIS	CE1-NE2-CD2	-5.42	103.58	109.00
1	B	367	CYS	N-CA-CB	5.42	118.01	110.26
1	B	158	HIS	CE1-NE2-CD2	-5.41	103.59	109.00
1	B	204	HIS	CE1-NE2-CD2	-5.41	103.59	109.00
1	C	114	ALA	CA-C-N	5.40	131.28	122.69
1	C	114	ALA	C-N-CA	5.40	131.28	122.69
1	B	253	ARG	CD-NE-CZ	5.40	131.96	124.40
1	B	422	THR	CA-C-N	5.40	130.26	122.16
1	B	422	THR	C-N-CA	5.40	130.26	122.16
1	C	277	GLN	CA-C-N	5.40	128.05	120.28
1	C	277	GLN	C-N-CA	5.40	128.05	120.28
1	B	167	HIS	CE1-NE2-CD2	-5.39	103.61	109.00
1	B	113	ALA	CA-C-N	5.39	130.52	122.86
1	B	113	ALA	C-N-CA	5.39	130.52	122.86
1	C	521	LYS	N-CA-CB	5.39	117.93	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	PHE	N-CA-CB	5.39	117.88	109.85
1	B	363	SER	CA-C-N	5.39	130.94	122.21
1	B	363	SER	C-N-CA	5.39	130.94	122.21
1	A	83	ASP	N-CA-CB	5.39	117.82	110.01
1	C	292	HIS	CE1-NE2-CD2	-5.38	103.61	109.00
1	C	294	VAL	CA-C-N	5.37	130.57	123.05
1	C	294	VAL	C-N-CA	5.37	130.57	123.05
1	A	455	ARG	N-CA-CB	5.37	117.75	109.91
1	B	67	LYS	CA-C-N	5.37	129.64	122.01
1	B	67	LYS	C-N-CA	5.37	129.64	122.01
1	C	166	ALA	CA-C-N	5.37	130.57	123.00
1	C	166	ALA	C-N-CA	5.37	130.57	123.00
1	A	12	ILE	CA-C-N	5.36	130.33	122.77
1	A	12	ILE	C-N-CA	5.36	130.33	122.77
1	B	271	GLY	CA-C-N	5.35	130.08	123.12
1	B	271	GLY	C-N-CA	5.35	130.08	123.12
1	C	299	THR	CA-C-N	5.35	128.39	120.74
1	C	299	THR	C-N-CA	5.35	128.39	120.74
1	A	401	THR	CA-C-N	5.35	129.73	122.19
1	A	401	THR	C-N-CA	5.35	129.73	122.19
1	B	514	GLY	N-CA-C	5.34	118.27	110.63
1	B	167	HIS	CA-C-N	5.34	130.53	123.00
1	B	167	HIS	C-N-CA	5.34	130.53	123.00
1	A	105	SER	N-CA-CB	5.34	118.17	109.69
1	C	505	GLN	N-CA-CB	5.33	117.85	110.17
1	A	271	GLY	N-CA-C	5.33	119.63	112.17
1	B	192	THR	CA-C-N	5.33	129.80	123.19
1	B	192	THR	C-N-CA	5.33	129.80	123.19
1	C	174	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	A	77	ARG	CB-CG-CD	5.32	123.54	111.30
1	B	515	MET	CA-C-N	5.32	129.96	122.09
1	B	515	MET	C-N-CA	5.32	129.96	122.09
1	C	512	TYR	CA-C-N	5.32	129.43	121.77
1	C	512	TYR	C-N-CA	5.32	129.43	121.77
1	C	468	ALA	CA-C-N	5.31	130.48	122.99
1	C	468	ALA	C-N-CA	5.31	130.48	122.99
1	B	407	ASP	CA-C-N	5.31	127.39	120.28
1	B	407	ASP	C-N-CA	5.31	127.39	120.28
1	A	150	PRO	CA-C-N	5.30	129.90	122.05
1	A	150	PRO	C-N-CA	5.30	129.90	122.05
1	A	95	SER	CA-C-N	5.29	130.89	122.74
1	A	95	SER	C-N-CA	5.29	130.89	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	GLY	CA-C-N	5.29	129.39	121.72
1	C	73	GLY	C-N-CA	5.29	129.39	121.72
1	C	237	GLY	N-CA-C	5.29	117.72	110.69
1	A	191	VAL	CA-C-N	5.29	130.59	122.93
1	A	191	VAL	C-N-CA	5.29	130.59	122.93
1	A	285	ASP	CA-C-N	5.29	131.70	122.82
1	A	285	ASP	C-N-CA	5.29	131.70	122.82
1	B	102	ILE	N-CA-CB	5.28	117.52	111.39
1	C	430	TYR	CA-CB-CG	5.27	123.39	113.90
1	C	20	ALA	CA-C-N	5.27	130.05	121.62
1	C	20	ALA	C-N-CA	5.27	130.05	121.62
1	C	488	CYS	N-CA-CB	5.27	117.96	110.06
1	B	273	LYS	CA-C-N	5.26	131.66	122.81
1	B	273	LYS	C-N-CA	5.26	131.66	122.81
1	A	421	GLN	CA-CB-CG	5.26	124.62	114.10
1	B	447	ASN	CA-C-N	5.26	127.28	120.44
1	B	447	ASN	C-N-CA	5.26	127.28	120.44
1	C	204	HIS	ND1-CG-CD2	-5.26	100.84	106.10
1	C	16	GLU	CA-C-N	5.25	129.08	120.63
1	C	16	GLU	C-N-CA	5.25	129.08	120.63
1	C	88	MET	CA-CB-CG	5.24	124.57	114.10
1	A	468	ALA	CA-C-N	5.23	131.20	122.73
1	A	468	ALA	C-N-CA	5.23	131.20	122.73
1	C	134	HIS	N-CA-C	5.23	116.55	107.93
1	C	279	GLN	N-CA-CB	5.23	117.85	109.28
1	A	74	LEU	N-CA-CB	5.22	117.57	109.48
1	C	470	ALA	CA-C-N	5.22	129.58	122.90
1	C	470	ALA	C-N-CA	5.22	129.58	122.90
1	B	88	MET	CA-C-N	5.22	130.66	122.21
1	B	88	MET	C-N-CA	5.22	130.66	122.21
1	B	151	ASP	CA-C-N	5.21	128.99	121.18
1	B	151	ASP	C-N-CA	5.21	128.99	121.18
1	C	57	VAL	CA-C-N	5.21	129.69	122.77
1	C	57	VAL	C-N-CA	5.21	129.69	122.77
1	C	204	HIS	CG-CD2-NE2	5.20	112.40	107.20
1	C	431	TYR	CA-C-N	5.20	129.48	122.93
1	C	431	TYR	C-N-CA	5.20	129.48	122.93
1	B	229	PHE	CA-C-N	5.20	130.05	122.41
1	B	229	PHE	C-N-CA	5.20	130.05	122.41
1	B	167	HIS	CG-CD2-NE2	5.19	112.39	107.20
1	C	134	HIS	CG-CD2-NE2	5.19	112.39	107.20
1	B	134	HIS	CG-CD2-NE2	5.19	112.39	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	78	MET	CA-C-N	5.19	128.46	121.20
1	C	78	MET	C-N-CA	5.19	128.46	121.20
1	C	292	HIS	ND1-CG-CD2	-5.18	100.92	106.10
1	C	15	GLU	CA-C-N	5.18	127.67	120.63
1	C	15	GLU	C-N-CA	5.18	127.67	120.63
1	B	204	HIS	CG-CD2-NE2	5.18	112.38	107.20
1	B	250	GLN	CB-CG-CD	5.18	121.40	112.60
1	C	292	HIS	CG-CD2-NE2	5.18	112.38	107.20
1	A	385	GLY	N-CA-C	5.17	118.13	110.63
1	C	79	ASN	N-CA-CB	5.17	117.96	109.90
1	B	296	GLY	N-CA-C	5.16	118.92	112.73
1	B	449	GLN	CA-CB-CG	5.15	124.41	114.10
1	B	507	PRO	CA-C-N	5.15	128.53	120.75
1	B	507	PRO	C-N-CA	5.15	128.53	120.75
1	B	471	VAL	CA-C-N	5.15	131.46	122.81
1	B	471	VAL	C-N-CA	5.15	131.46	122.81
1	A	363	SER	CA-C-N	5.14	128.78	121.42
1	A	363	SER	C-N-CA	5.14	128.78	121.42
1	B	462	TYR	CA-C-N	5.14	128.83	120.60
1	B	462	TYR	C-N-CA	5.14	128.83	120.60
1	A	480	ASN	CA-CB-CG	5.14	117.74	112.60
1	C	204	HIS	CA-CB-CG	5.14	118.94	113.80
1	B	417	LEU	N-CA-CB	5.13	117.50	110.01
1	A	217	ALA	CA-C-N	5.12	129.47	121.17
1	A	217	ALA	C-N-CA	5.12	129.47	121.17
1	B	115	VAL	CA-C-N	5.12	129.21	122.30
1	B	115	VAL	C-N-CA	5.12	129.21	122.30
1	B	152	ILE	N-CA-CB	5.12	116.50	110.82
1	B	224	PRO	CA-C-N	5.11	128.08	120.31
1	B	224	PRO	C-N-CA	5.11	128.08	120.31
1	B	167	HIS	ND1-CG-CD2	-5.11	100.99	106.10
1	A	462	TYR	CA-C-N	5.11	130.97	122.54
1	A	462	TYR	C-N-CA	5.11	130.97	122.54
1	A	408	GLU	CA-C-N	5.11	127.38	120.38
1	A	408	GLU	C-N-CA	5.11	127.38	120.38
1	A	67	LYS	N-CA-CB	5.11	117.58	109.51
1	A	439	TYR	CA-C-N	5.11	130.36	123.46
1	A	439	TYR	C-N-CA	5.11	130.36	123.46
1	B	96	MET	CA-C-N	5.11	130.60	122.94
1	B	96	MET	C-N-CA	5.11	130.60	122.94
1	B	158	HIS	CG-CD2-NE2	5.11	112.31	107.20
1	B	252	ASN	N-CA-CB	5.10	117.80	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	267	PRO	CA-C-N	5.10	127.42	120.54
1	C	267	PRO	C-N-CA	5.10	127.42	120.54
1	C	170	ILE	CA-C-N	5.10	131.30	122.64
1	C	170	ILE	C-N-CA	5.10	131.30	122.64
1	C	134	HIS	ND1-CG-CD2	-5.09	101.01	106.10
1	B	52	SER	CA-C-N	5.09	127.94	120.71
1	B	52	SER	C-N-CA	5.09	127.94	120.71
1	B	282	ASP	N-CA-CB	5.09	117.54	110.26
1	B	469	LEU	CA-C-N	5.08	128.07	120.95
1	B	469	LEU	C-N-CA	5.08	128.07	120.95
1	B	204	HIS	ND1-CG-CD2	-5.08	101.02	106.10
1	B	291	VAL	CA-C-N	5.08	130.17	123.00
1	B	291	VAL	C-N-CA	5.08	130.17	123.00
1	C	445	VAL	CA-C-N	5.08	130.22	122.65
1	C	445	VAL	C-N-CA	5.08	130.22	122.65
1	B	128	SER	N-CA-CB	5.08	117.44	110.07
1	C	16	GLU	CA-CB-CG	5.08	124.26	114.10
1	C	201	PHE	N-CA-CB	5.08	117.92	110.35
1	B	168	LEU	CA-C-N	5.07	129.84	123.10
1	B	168	LEU	C-N-CA	5.07	129.84	123.10
1	A	515	MET	CA-C-N	5.07	130.94	122.73
1	A	515	MET	C-N-CA	5.07	130.94	122.73
1	B	95	SER	CA-C-N	5.07	130.42	122.21
1	B	95	SER	C-N-CA	5.07	130.42	122.21
1	B	274	LEU	CA-C-N	5.07	129.51	122.77
1	B	274	LEU	C-N-CA	5.07	129.51	122.77
1	B	134	HIS	ND1-CG-CD2	-5.07	101.03	106.10
1	B	375	PHE	CA-CB-CG	5.07	118.87	113.80
1	A	275	ASN	CA-CB-CG	5.06	117.66	112.60
1	C	278	ARG	CG-CD-NE	5.06	123.14	112.00
1	B	247	LEU	CA-C-N	5.06	129.69	121.95
1	B	247	LEU	C-N-CA	5.06	129.69	121.95
1	A	521	LYS	CA-CB-CG	5.06	124.21	114.10
1	B	158	HIS	ND1-CG-CD2	-5.05	101.05	106.10
1	C	67	LYS	CG-CD-CE	5.05	122.92	111.30
1	B	487	SER	CA-C-N	5.04	127.00	120.44
1	B	487	SER	C-N-CA	5.04	127.00	120.44
1	A	56	THR	CA-C-N	5.04	129.94	122.94
1	A	56	THR	C-N-CA	5.04	129.94	122.94
1	B	83	ASP	N-CA-CB	5.03	117.52	110.12
1	B	452	TRP	N-CA-CB	5.03	117.47	109.82
1	C	191	VAL	N-CA-CB	5.03	116.74	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	519	TYR	CA-C-N	5.03	127.92	120.82
1	C	519	TYR	C-N-CA	5.03	127.92	120.82
1	B	98	ILE	CA-C-N	5.03	130.58	123.14
1	B	98	ILE	C-N-CA	5.03	130.58	123.14
1	B	374	ASN	N-CA-CB	5.02	117.42	110.04
1	C	455	ARG	N-CA-CB	5.02	117.29	110.01
1	A	284	GLU	CA-C-N	5.01	128.70	120.63
1	A	284	GLU	C-N-CA	5.01	128.70	120.63
1	A	98	ILE	CA-C-N	5.01	130.23	123.11
1	A	98	ILE	C-N-CA	5.01	130.23	123.11
1	C	296	GLY	CA-C-N	5.01	127.41	120.29
1	C	296	GLY	C-N-CA	5.01	127.41	120.29
1	A	298	LYS	CA-C-N	5.00	129.76	121.86
1	A	298	LYS	C-N-CA	5.00	129.76	121.86

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	311	TYR	Sidechain
1	A	430	TYR	Sidechain
1	B	180	TYR	Sidechain
1	B	312	TYR	Sidechain
1	B	439	TYR	Sidechain
1	C	339	TYR	Sidechain
1	C	348	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3992	3904	3901	38	0
1	B	3909	3824	3824	57	0
1	C	4010	3921	3920	43	0
All	All	11911	11649	11645	134	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 6.

All (134) 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:C:336:VAL:HG13	1:C:387:VAL:HG13	1.50	0.92
1:A:287:THR:O	1:A:320:ASN:N	2.11	0.84
1:B:336:VAL:HG22	1:B:353:ILE:HD12	1.62	0.82
1:A:318:LEU:HD12	1:A:318:LEU:O	1.82	0.78
1:B:314:ARG:NH1	1:B:409:ASP:O	2.16	0.77
1:A:48:LYS:NZ	1:A:198:GLY:O	2.20	0.75
1:C:99:ARG:NH2	1:C:194:GLU:OE2	2.20	0.74
1:C:336:VAL:HG13	1:C:387:VAL:CG1	2.20	0.72
1:C:283:THR:HG22	1:C:283:THR:O	1.91	0.70
1:A:159:ASP:N	1:A:162:ASP:OD2	2.27	0.67
1:B:336:VAL:HG22	1:B:353:ILE:CD1	2.25	0.66
1:B:374:ASN:OD1	1:B:375:PHE:N	2.28	0.66
1:A:519:TYR:HB2	1:B:258:LYS:HE2	1.78	0.65
1:B:118:PRO:HG2	1:B:121:ILE:HD13	1.79	0.64
1:B:433:THR:HG22	1:B:447:ASN:HD21	1.61	0.63
1:B:356:ALA:HB1	1:B:365:ILE:HG21	1.81	0.63
1:A:353:ILE:HG23	1:A:377:VAL:HB	1.81	0.62
1:B:77:ARG:NH2	1:B:83:ASP:OD1	2.32	0.62
1:B:476:ASP:HB3	1:B:508:LEU:HD23	1.82	0.61
1:B:247:LEU:HD12	1:B:248:VAL:H	1.65	0.61
1:B:353:ILE:HG23	1:B:377:VAL:HG13	1.82	0.60
1:B:476:ASP:OD1	1:B:477:SER:N	2.33	0.59
1:B:153:ARG:NH1	1:B:156:LEU:O	2.35	0.59
1:B:282:ASP:OD1	1:B:283:THR:N	2.36	0.59
1:C:449:GLN:NE2	1:C:490:GLY:O	2.34	0.59
1:C:68:VAL:HG22	1:C:171:LEU:HG	1.86	0.58
1:C:244:ILE:HD13	1:C:429:ILE:HG22	1.84	0.58
1:B:457:LEU:HD23	1:B:462:TYR:CD2	2.39	0.58
1:C:429:ILE:HG21	1:C:494:VAL:HG23	1.85	0.57
1:A:336:VAL:HG21	1:A:353:ILE:HG13	1.87	0.56
1:A:54:TYR:OH	1:A:72:GLN:NE2	2.39	0.56
1:C:404:ILE:HB	1:C:445:VAL:HG23	1.88	0.56
1:A:204:HIS:O	1:A:205:LEU:C	2.51	0.54
1:B:248:VAL:HG23	1:B:430:TYR:CZ	2.43	0.54
1:B:262:PHE:CD2	1:B:416:VAL:HG13	2.43	0.54
1:A:77:ARG:NH2	1:A:160:MET:O	2.41	0.53
1:A:422:THR:O	1:A:422:THR:HG23	2.08	0.53
1:C:211:ARG:HH11	1:C:211:ARG:HG3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LYS:NZ	1:A:524:HIS:O	2.37	0.53
1:A:209:PRO:O	1:A:210:SER:OG	2.24	0.53
1:C:99:ARG:NE	1:C:194:GLU:OE2	2.43	0.52
1:B:244:ILE:HD12	1:B:428:PRO:O	2.10	0.52
1:A:456:LEU:O	1:A:457:LEU:HB2	2.11	0.51
1:B:432:VAL:HG12	1:B:446:TYR:HD1	1.74	0.51
1:C:54:TYR:CD2	1:C:55:THR:HG22	2.46	0.51
1:C:233:ASN:C	1:C:233:ASN:OD1	2.53	0.51
1:A:89:TYR:CD2	1:A:204:HIS:O	2.63	0.51
1:A:86:ALA:HB1	1:A:160:MET:HE1	1.93	0.50
1:A:336:VAL:HG22	1:A:353:ILE:HD12	1.94	0.50
1:B:456:LEU:O	1:B:457:LEU:HB2	2.12	0.50
1:B:476:ASP:OD1	1:B:480:ASN:HB2	2.12	0.50
1:C:423:THR:O	1:C:423:THR:HG23	2.10	0.49
1:A:207:LYS:HZ2	1:A:213:MET:HE2	1.76	0.49
1:A:86:ALA:HB1	1:A:160:MET:CE	2.42	0.49
1:B:149:ILE:O	1:B:149:ILE:HG23	2.11	0.49
1:C:130:LEU:HD12	1:C:171:LEU:HD22	1.93	0.49
1:C:258:LYS:O	1:C:258:LYS:HG3	2.13	0.49
1:C:244:ILE:HD11	1:C:501:PHE:CZ	2.48	0.48
1:A:261:THR:HG23	1:A:261:THR:O	2.12	0.48
1:B:250:GLN:OE1	1:B:448:SER:OG	2.29	0.48
1:B:471:VAL:HG22	1:B:514:GLY:O	2.14	0.48
1:A:207:LYS:NZ	1:A:213:MET:HE2	2.29	0.48
1:C:248:VAL:HG13	1:C:430:TYR:CE1	2.49	0.47
1:C:99:ARG:CZ	1:C:194:GLU:OE2	2.61	0.47
1:A:469:LEU:HD13	1:A:518:ALA:HB2	1.96	0.47
1:B:288:ASP:OD1	1:B:320:ASN:N	2.47	0.47
1:B:318:LEU:O	1:B:321:THR:OG1	2.26	0.47
1:B:476:ASP:O	1:B:477:SER:OG	2.19	0.47
1:B:241:GLY:C	1:B:432:VAL:HG22	2.39	0.47
1:B:506:PHE:O	1:B:508:LEU:N	2.42	0.47
1:C:24:GLY:O	1:C:25:THR:OG1	2.31	0.47
1:C:477:SER:O	1:C:478:ALA:HB3	2.15	0.47
1:B:121:ILE:HD12	1:B:121:ILE:N	2.30	0.46
1:C:283:THR:O	1:C:283:THR:CG2	2.62	0.46
1:A:318:LEU:HD11	1:A:363:SER:O	2.15	0.46
1:C:102:ILE:H	1:C:102:ILE:HD12	1.81	0.46
1:B:162:ASP:C	1:B:162:ASP:OD1	2.59	0.46
1:C:236:PRO:HG3	1:C:269:HIS:CD2	2.51	0.46
1:C:240:LYS:HG3	1:C:240:LYS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ARG:HH11	1:B:140:ARG:HG2	1.81	0.45
1:A:153:ARG:NH2	1:A:156:LEU:O	2.50	0.45
1:B:72:GLN:HA	1:B:72:GLN:OE1	2.17	0.45
1:B:475:LYS:O	1:B:508:LEU:HA	2.17	0.45
1:C:266:THR:OG1	1:C:267:PRO:HD2	2.17	0.45
1:A:209:PRO:O	1:A:210:SER:CB	2.64	0.45
1:B:266:THR:OG1	1:B:268:GLU:OE1	2.29	0.44
1:B:119:PRO:HD2	1:C:205:LEU:HD22	2.00	0.44
1:A:287:THR:HG22	1:A:320:ASN:H	1.82	0.44
1:A:336:VAL:CG2	1:A:353:ILE:HG13	2.46	0.44
1:B:362:ASN:OD1	1:B:364:THR:OG1	2.28	0.44
1:B:267:PRO:O	1:B:451:LEU:HD11	2.17	0.44
1:C:244:ILE:HD11	1:C:501:PHE:HZ	1.82	0.44
1:C:513:VAL:O	1:C:513:VAL:HG12	2.17	0.44
1:A:98:ILE:HD13	1:A:195:THR:HG22	2.00	0.44
1:A:287:THR:O	1:A:287:THR:HG22	2.18	0.44
1:A:469:LEU:HD13	1:A:518:ALA:CB	2.48	0.44
1:B:413:ARG:HD2	1:B:417:LEU:HD22	2.00	0.44
1:B:311:TYR:CE1	1:B:405:GLY:HA2	2.53	0.44
1:B:344:LYS:O	1:B:344:LYS:HG3	2.17	0.44
1:B:432:VAL:HG12	1:B:446:TYR:CD1	2.52	0.44
1:C:43:MET:HG2	1:C:44:PRO:HD2	2.00	0.44
1:A:519:TYR:CD2	1:A:519:TYR:N	2.84	0.43
1:B:309:PRO:O	1:B:412:LYS:NZ	2.51	0.43
1:C:429:ILE:HG21	1:C:494:VAL:CG2	2.49	0.43
1:B:456:LEU:C	1:B:458:ALA:H	2.26	0.43
1:C:74:LEU:HD12	1:C:96:MET:HG2	2.01	0.43
1:A:272:VAL:HG23	1:A:306:ASP:O	2.19	0.42
1:B:274:LEU:HD11	1:B:308:TRP:HZ3	1.84	0.42
1:B:223:ILE:HD11	1:B:486:ILE:HD11	2.00	0.42
1:C:19:VAL:HG22	1:C:19:VAL:O	2.19	0.42
1:B:116:MET:SD	1:B:116:MET:O	2.77	0.42
1:C:142:THR:OG1	1:C:143:GLU:N	2.51	0.42
1:C:244:ILE:CD1	1:C:429:ILE:HG22	2.48	0.42
1:A:205:LEU:HD13	1:C:118:PRO:HB3	2.02	0.42
1:B:134:HIS:O	1:B:134:HIS:ND1	2.52	0.42
1:A:259:ARG:NH2	1:A:458:ALA:O	2.49	0.42
1:C:102:ILE:HG13	1:C:191:VAL:HG22	2.02	0.41
1:A:43:MET:N	1:A:46:GLU:OE2	2.40	0.41
1:C:79:ASN:OD1	1:C:79:ASN:C	2.63	0.41
1:B:494:VAL:CG1	1:B:495:GLY:N	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ASP:N	1:C:282:ASP:OD1	2.52	0.41
1:B:244:ILE:HD13	1:B:429:ILE:HG22	2.03	0.41
1:C:100:PHE:CE1	1:C:193:VAL:HG22	2.55	0.41
1:C:97:GLU:HG2	1:C:198:GLY:HA2	2.03	0.41
1:B:71:VAL:HG22	1:B:169:VAL:HG12	2.02	0.41
1:B:90:THR:HA	1:B:213:MET:HE3	2.02	0.41
1:B:261:THR:O	1:B:261:THR:HG23	2.20	0.41
1:C:282:ASP:CB	1:C:291:VAL:H	2.33	0.41
1:B:500:PRO:HD2	1:B:526:ILE:HD11	2.02	0.41
1:B:140:ARG:HG2	1:B:140:ARG:NH1	2.36	0.41
1:A:90:THR:HG22	1:C:121:ILE:HD11	2.04	0.40
1:A:305:PRO:HD2	1:A:308:TRP:HE1	1.86	0.40
1:B:258:LYS:HG3	1:B:258:LYS:O	2.21	0.40
1:A:274:LEU:C	1:A:274:LEU:HD12	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	509/533 (96%)	456 (90%)	51 (10%)	2 (0%)	30	58
1	B	499/533 (94%)	425 (85%)	70 (14%)	4 (1%)	16	45
1	C	514/533 (96%)	452 (88%)	61 (12%)	1 (0%)	43	70
All	All	1522/1599 (95%)	1333 (88%)	182 (12%)	7 (0%)	26	55

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	351	PRO
1	B	325	PHE
1	A	302	SER

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Mol	Chain	Res	Type
1	B	380	ASN
1	C	312	TYR
1	A	133	PRO
1	B	464	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/445 (97%)	430 (100%)	0	100	100
1	B	422/445 (95%)	422 (100%)	0	100	100
1	C	432/445 (97%)	432 (100%)	0	100	100
All	All	1284/1335 (96%)	1284 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	131	GLN
1	A	161	HIS
1	A	260	GLN
1	A	380	ASN
1	A	426	ASN
1	B	174	ASN
1	C	269	HIS
1	C	320	ASN
1	C	357	ASN
1	C	386	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

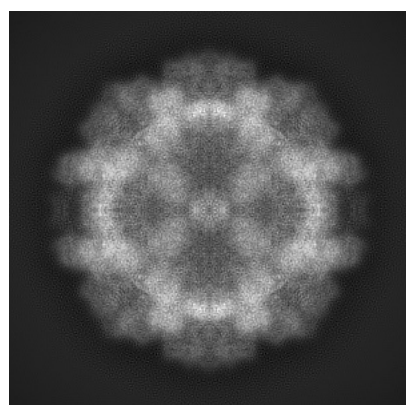
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12194. These allow visual inspection of the internal detail of the map and identification of artifacts.

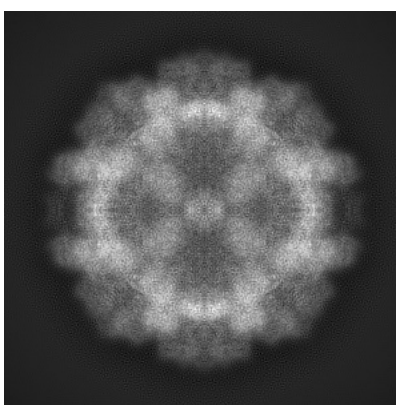
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

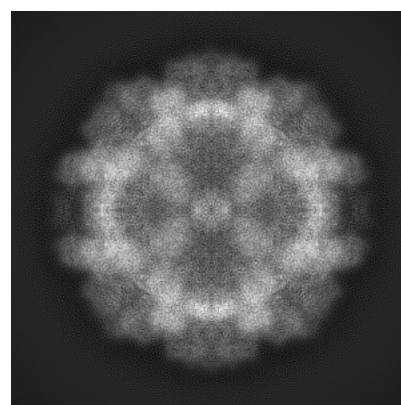
6.1.1 Primary map



X



Y

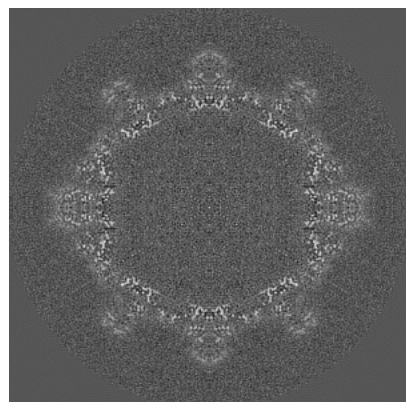


Z

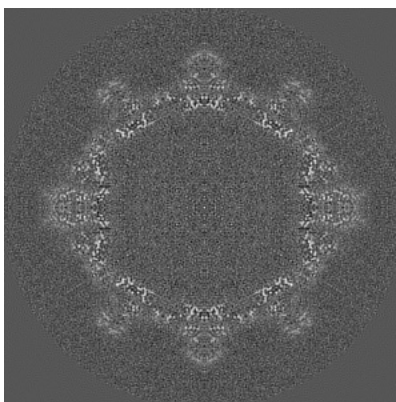
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

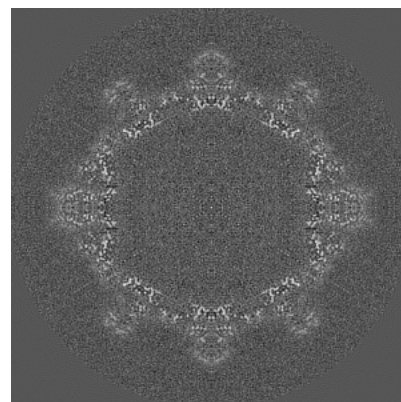
6.2.1 Primary map



X Index: 256



Y Index: 256

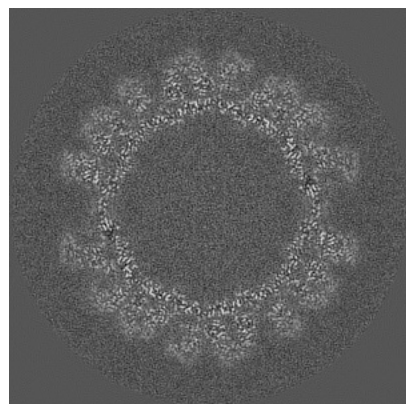


Z Index: 256

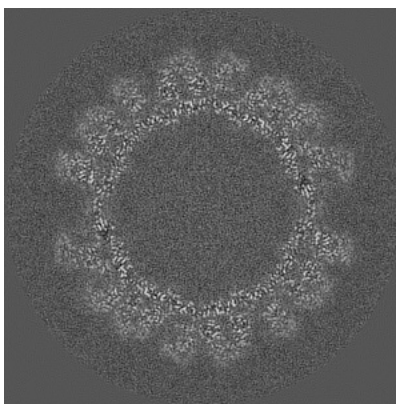
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

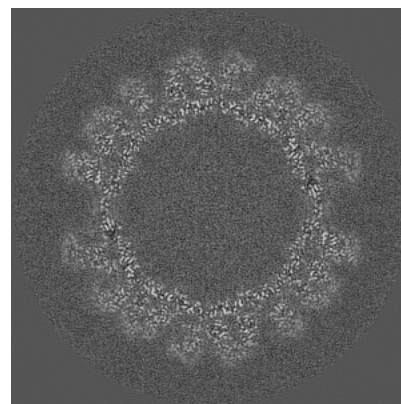
6.3.1 Primary map



X Index: 211



Y Index: 211

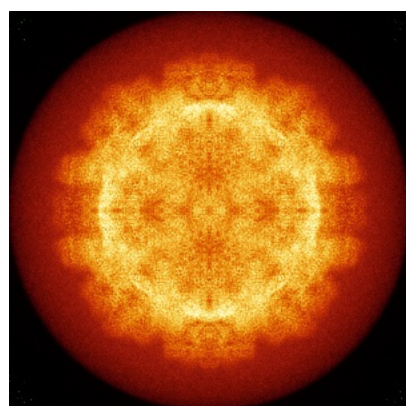


Z Index: 211

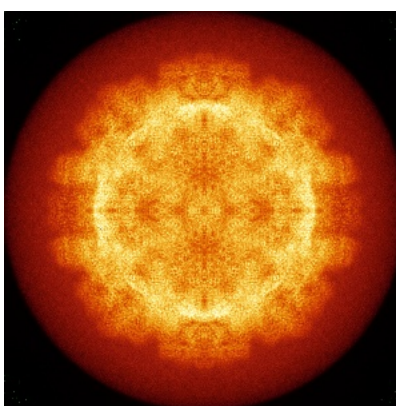
The images above show the largest variance slices of the map in three orthogonal directions.

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

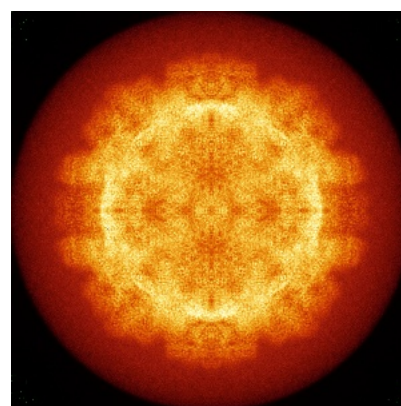
6.4.1 Primary map



X



Y

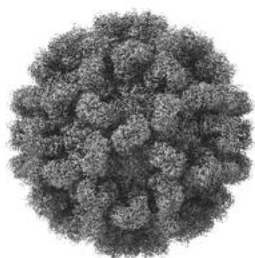


Z

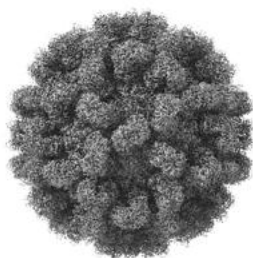
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

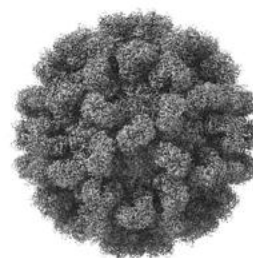
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

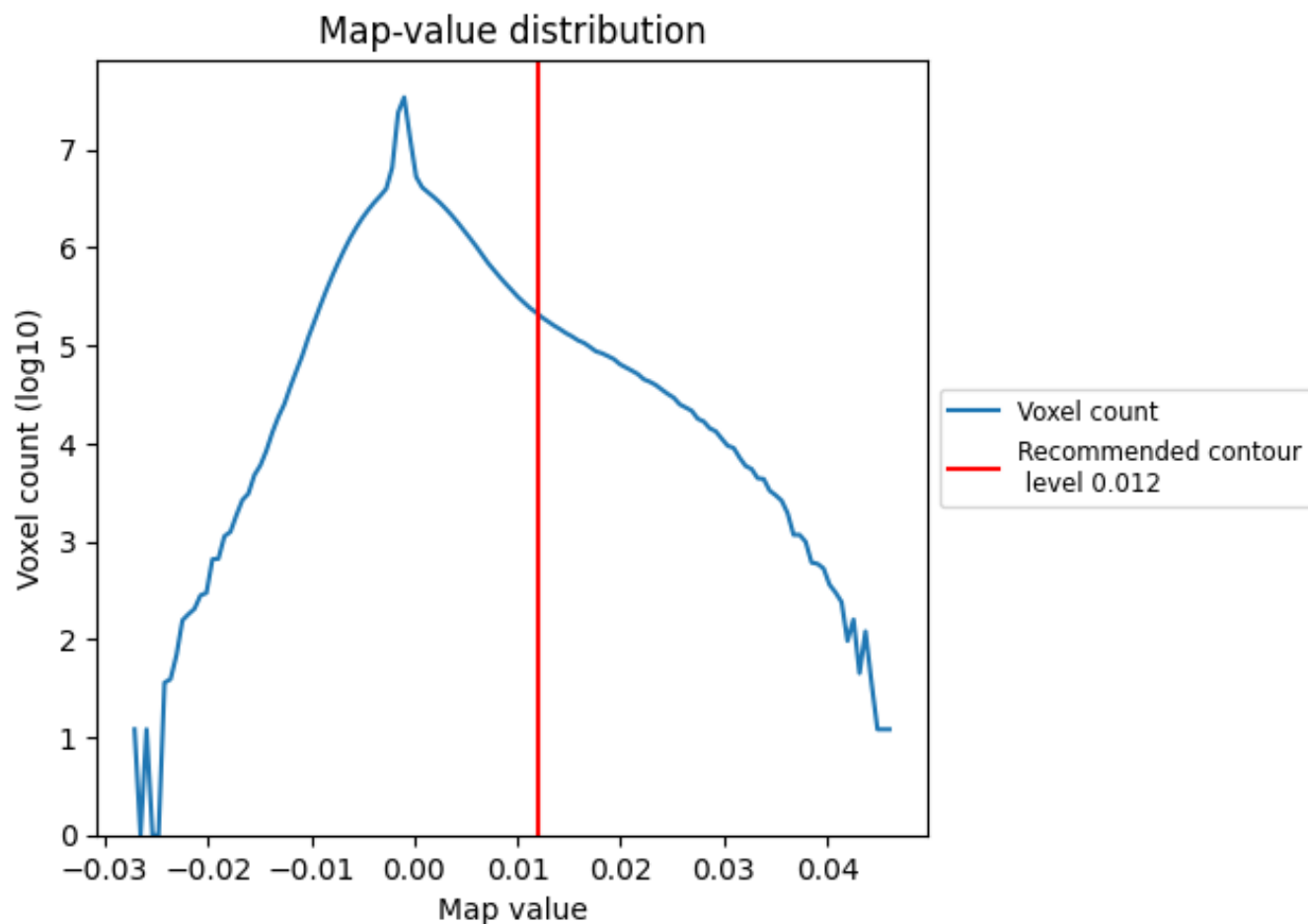
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

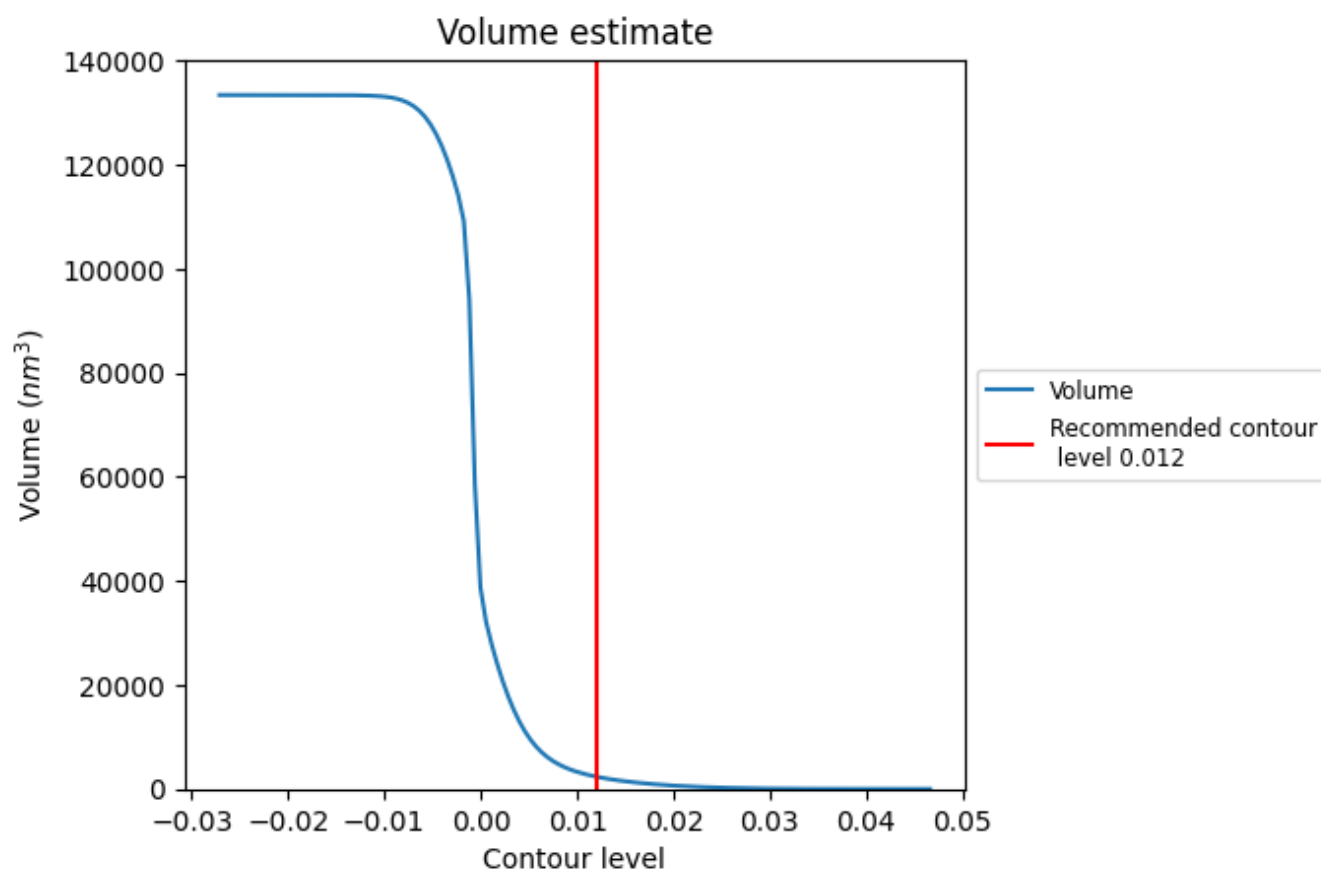
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

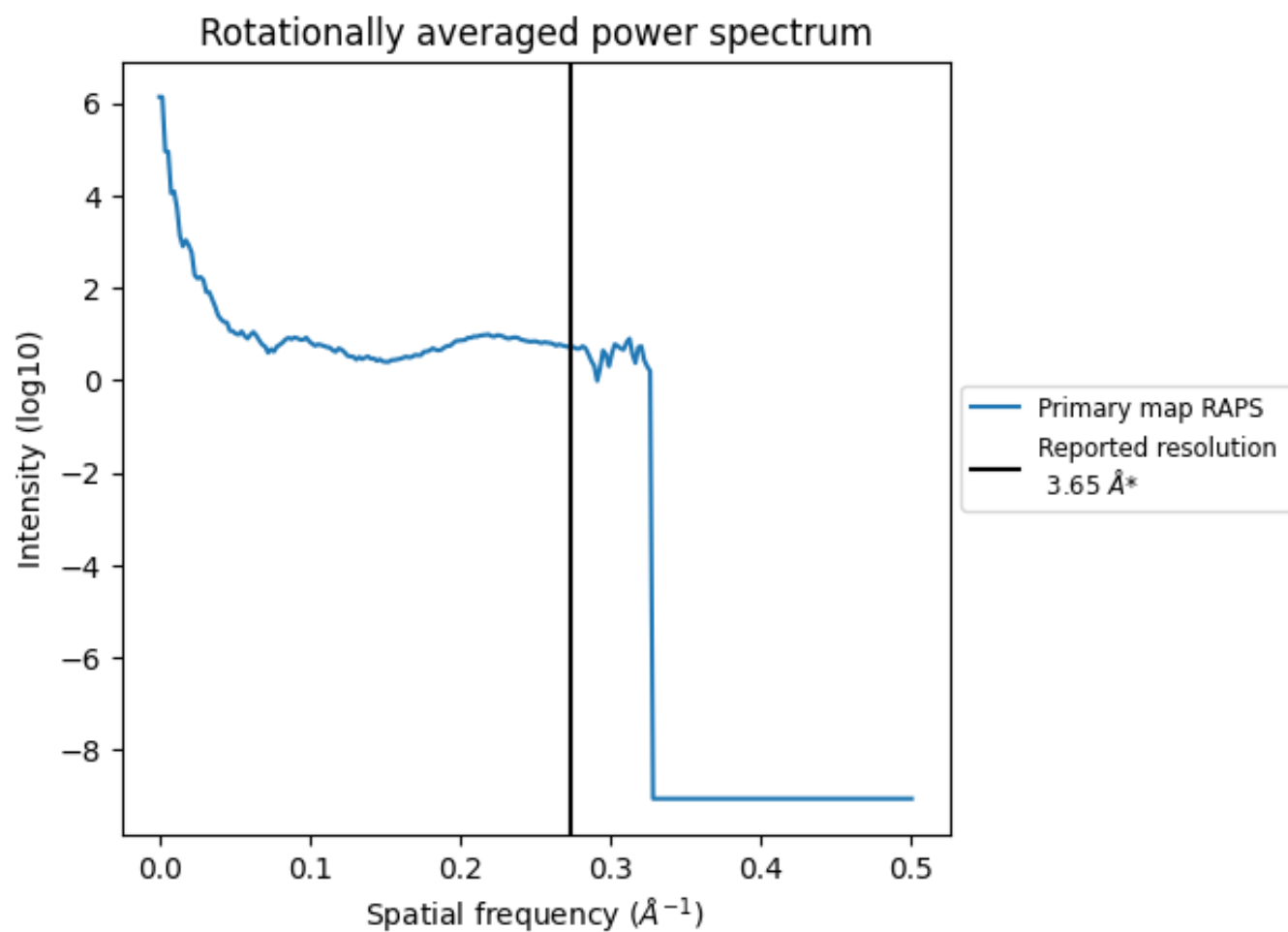
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2356 nm³; this corresponds to an approximate mass of 2128 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

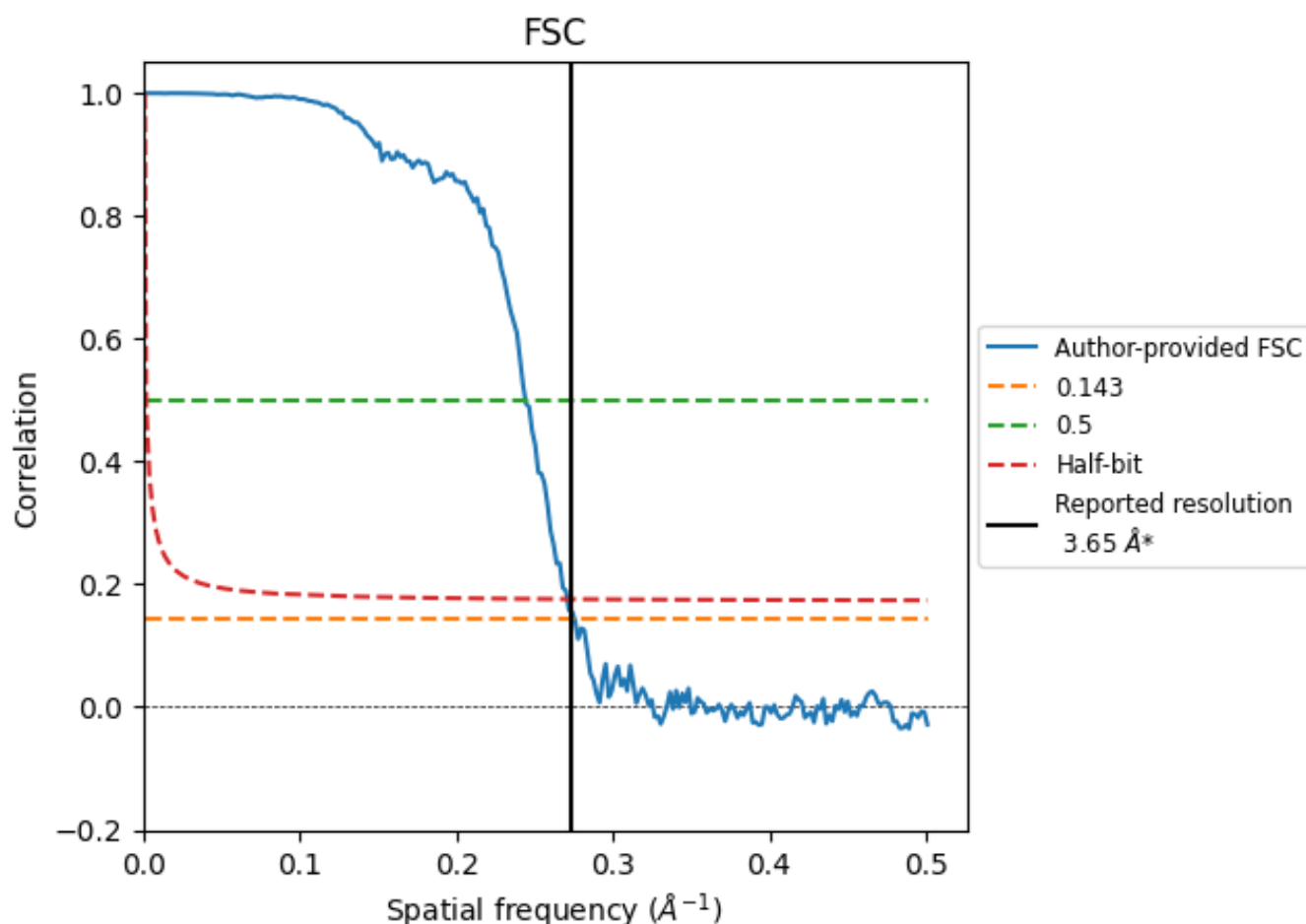


*Reported resolution corresponds to spatial frequency of 0.274 Å⁻¹

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 0.274 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.65	-	-
Author-provided FSC curve	3.63	4.09	3.69
Unmasked-calculated*	-	-	-

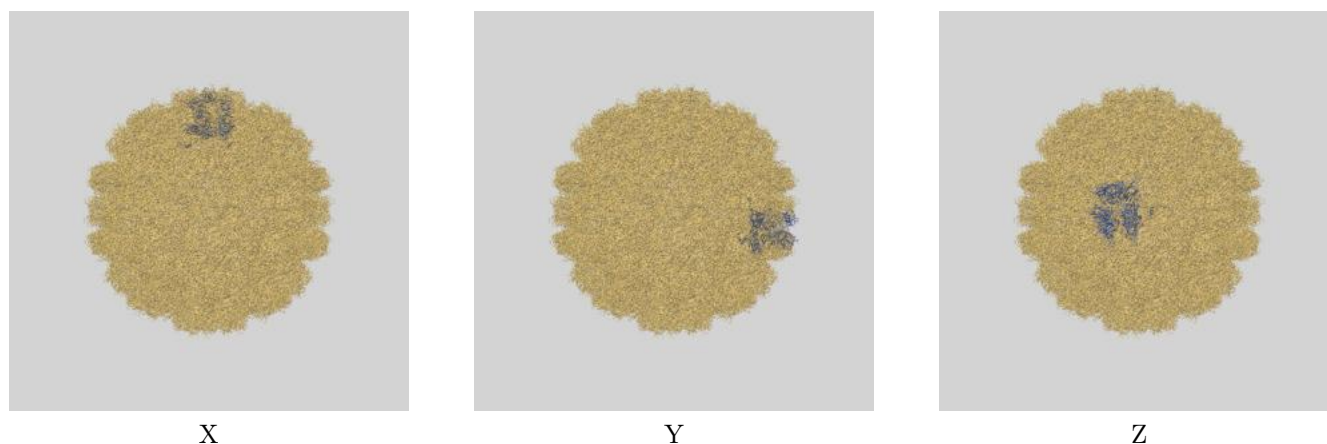
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

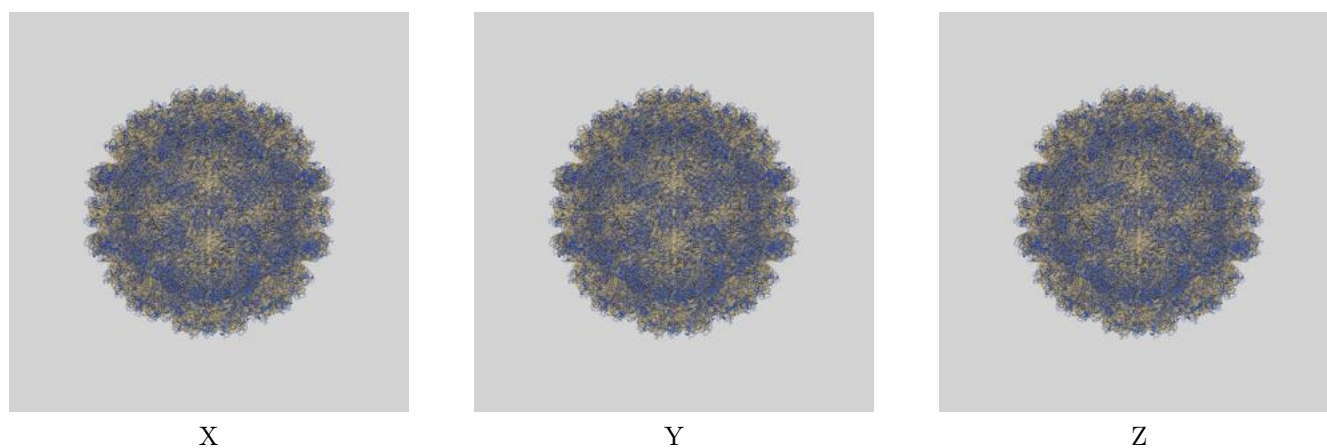
This section contains information regarding the fit between EMDB map EMD-12194 and PDB model 7BJP. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

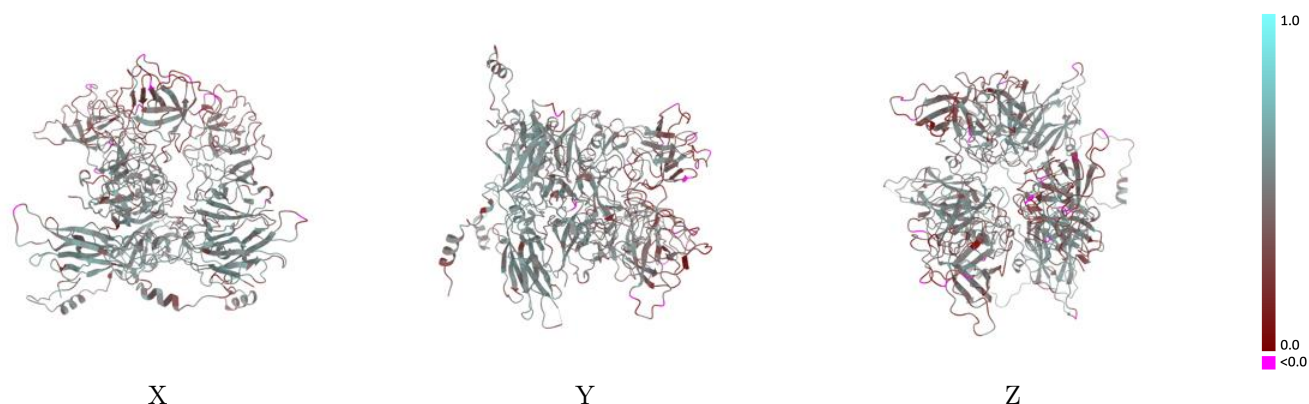


9.1.2 Map-model assembly overlay [i](#)



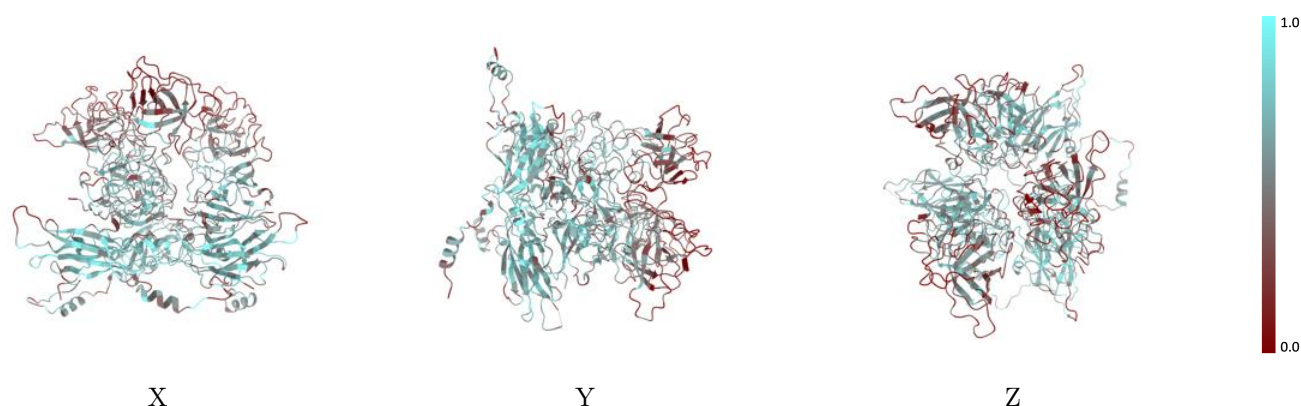
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



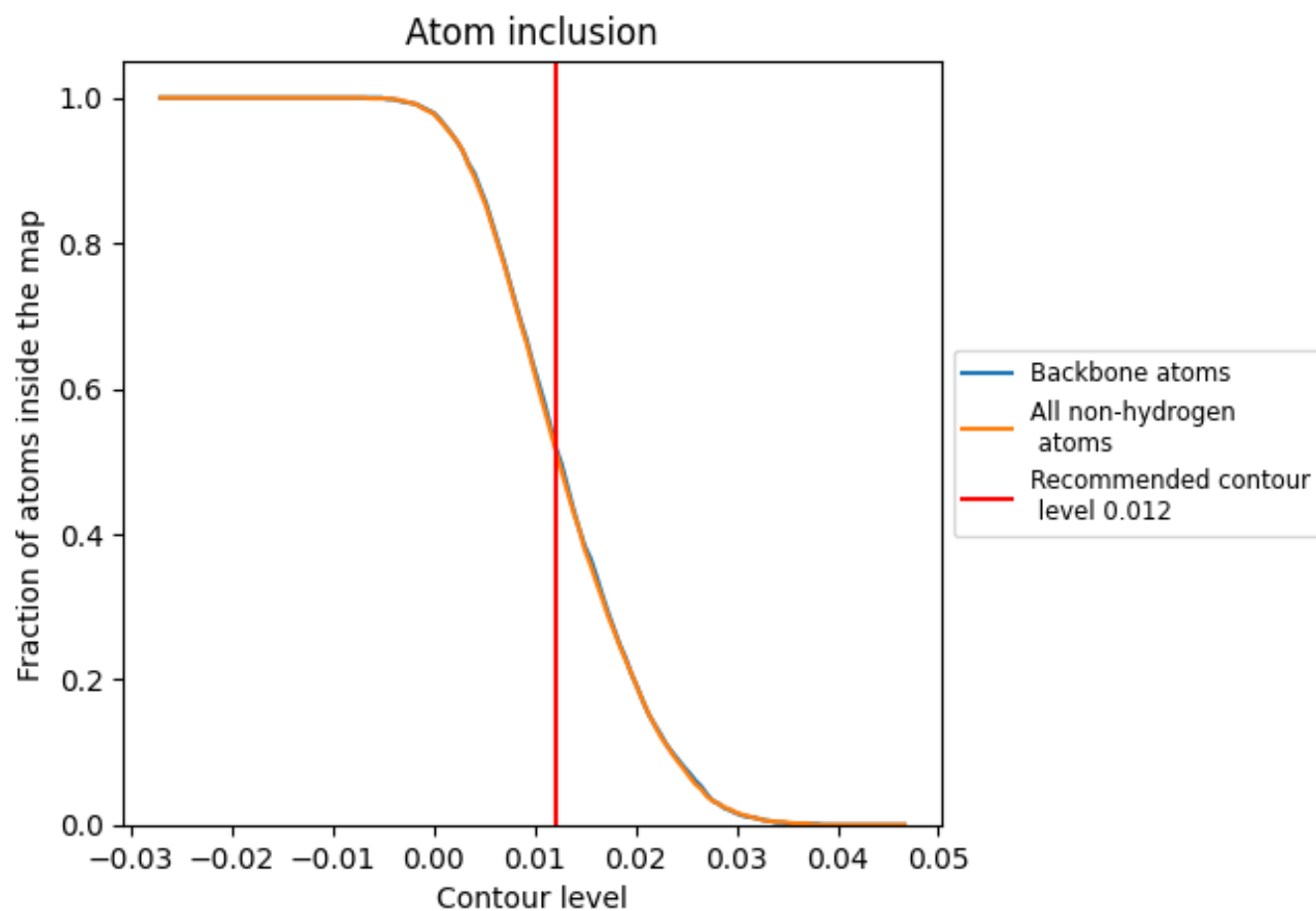
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5180	0.4350
A	0.5310	0.4390
B	0.5260	0.4440
C	0.5050	0.4240

