



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 03:34 AM UTC

PDB ID : 5MD1 / pdb_00005md1
EMDB ID : EMD-3469
Title : The structure of the mature HIV-1 CA hexameric lattice with curvature parameters: tilt=5, twist=0
Authors : Mattei, S.; Glass, B.; Hagen, W.J.H.; Kraeusslich, H.-G.; Briggs, J.A.G.
Deposited on : 2016-11-10
Resolution : 8.20 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:

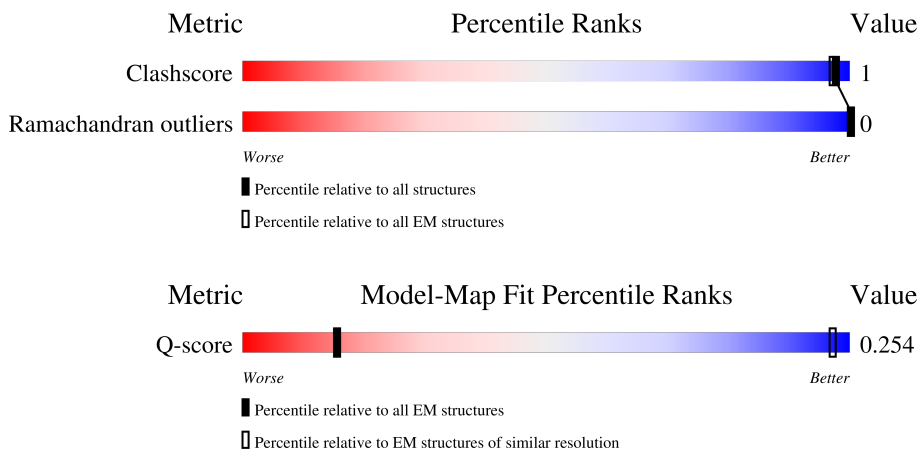
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 8.20 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	-
Q-score	-	25397	337 (7.70 - 8.70)

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	74	12% 73% 27%
1	B	74	12% 70% 30%
1	C	74	16% 74% 26%
1	D	74	20% 70% 30%
1	E	74	42% 72% 28%

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Mol	Chain	Length	Quality of chain
1	F	74	
1	G	74	
1	W	74	
2	H	147	
2	I	147	
2	J	147	
2	a	147	
2	b	147	
2	f	147	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5888 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 Capsid protein p24.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	74	Total	C	N	O	0	0
			295	148	74	73		
1	B	74	Total	C	N	O	0	0
			295	148	74	73		
1	F	74	Total	C	N	O	0	0
			295	148	74	73		
1	W	74	Total	C	N	O	0	0
			295	148	74	73		
1	C	74	Total	C	N	O	0	0
			295	148	74	73		
1	D	74	Total	C	N	O	0	0
			295	148	74	73		
1	E	74	Total	C	N	O	0	0
			295	148	74	73		
1	G	74	Total	C	N	O	0	0
			295	148	74	73		

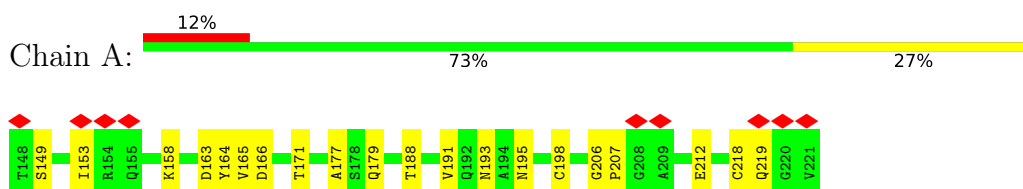
- Molecule 2 is a protein called Capsid protein p24.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	a	147	Total	C	N	O	0	0
			588	294	147	147		
2	b	147	Total	C	N	O	0	0
			588	294	147	147		
2	f	147	Total	C	N	O	0	0
			588	294	147	147		
2	H	147	Total	C	N	O	0	0
			588	294	147	147		
2	I	147	Total	C	N	O	0	0
			588	294	147	147		
2	J	147	Total	C	N	O	0	0
			588	294	147	147		

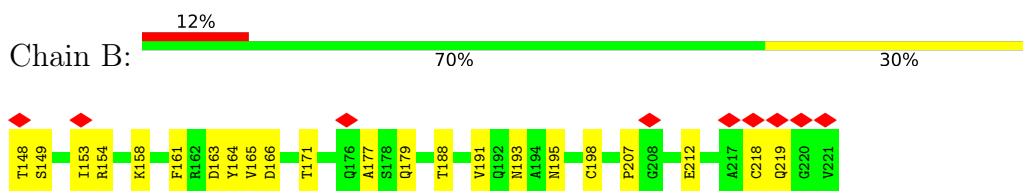
3 Residue-property plots

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.

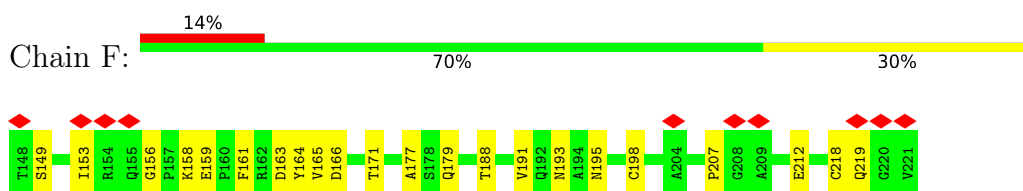
- Molecule 1: Capsid protein p24



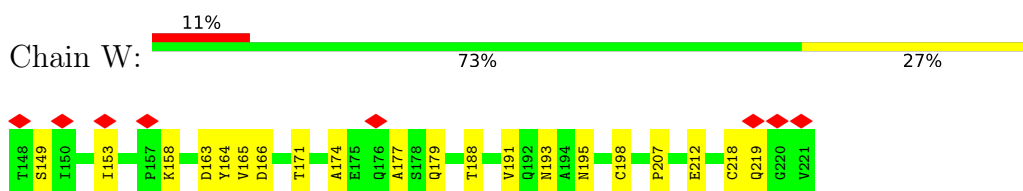
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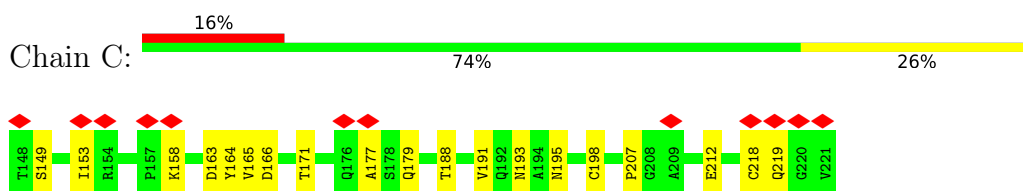
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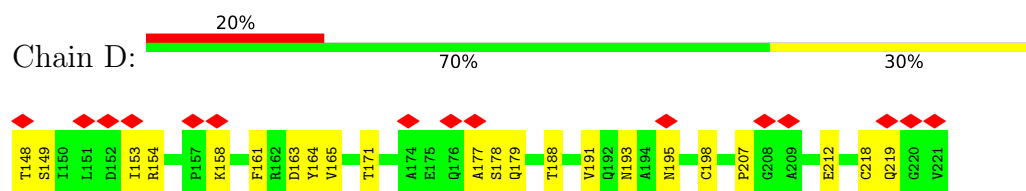
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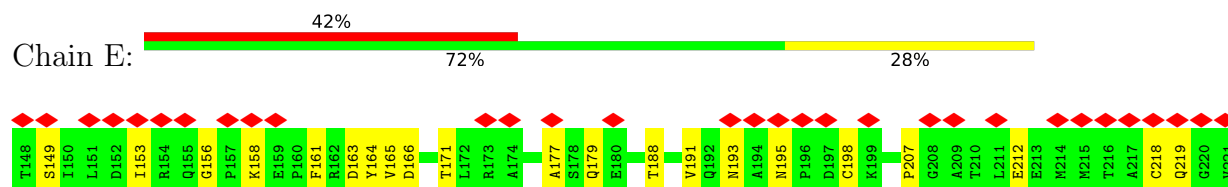
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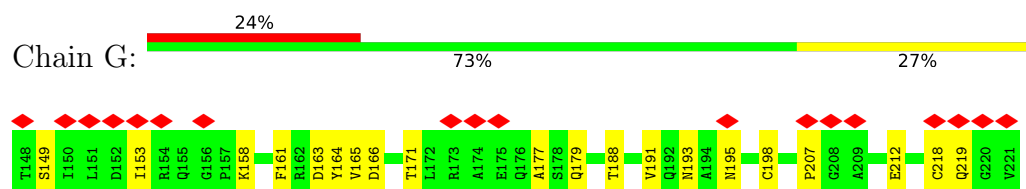
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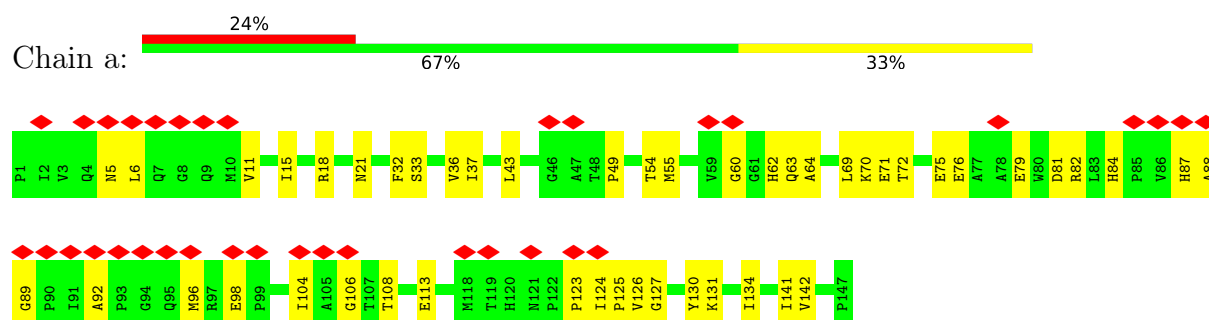
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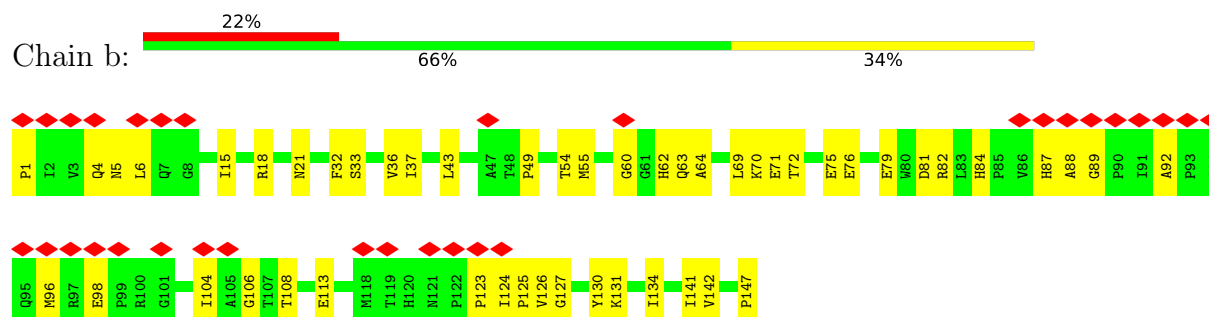
- Molecule 1: Capsid protein p24



- Molecule 2: Capsid protein p24

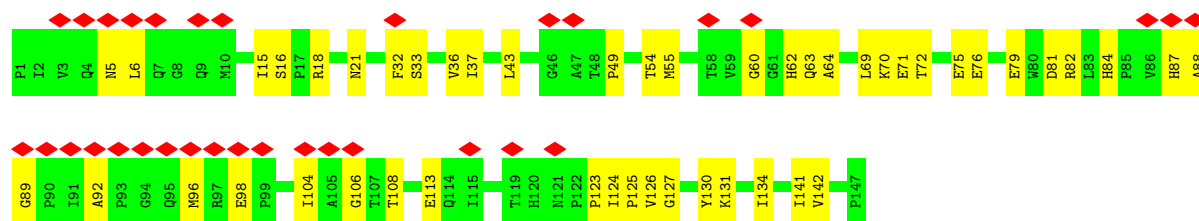


- Molecule 2: Capsid protein p24

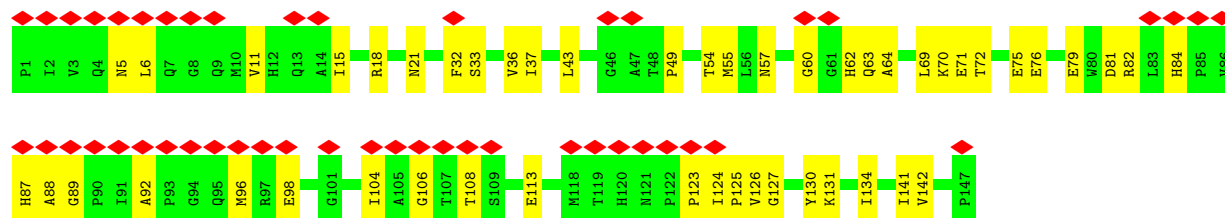


- Molecule 2: Capsid protein p24

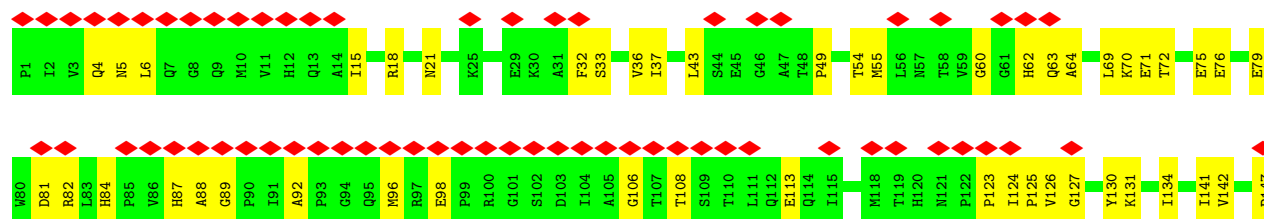
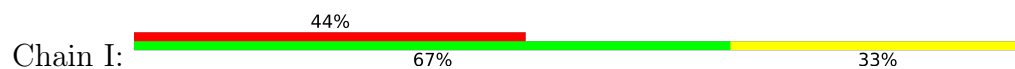




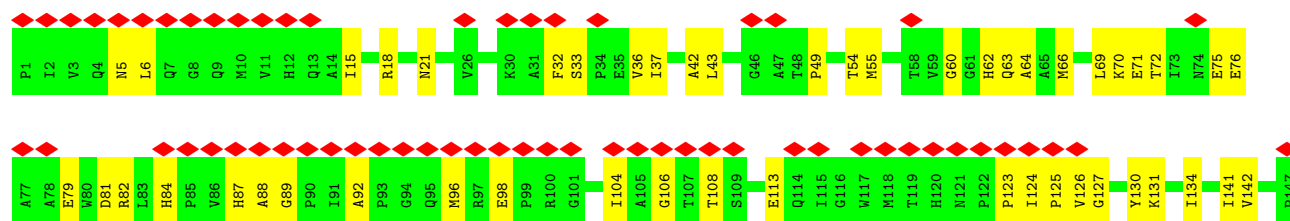
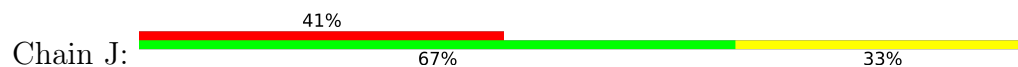
- Molecule 2: Capsid protein p24



- Molecule 2: Capsid protein p24



- Molecule 2: Capsid protein p24



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	16208	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; CTF correction was performed using the ctfphaseflip program in IMOD prior to backprojection.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.2	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	6500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.588	Depositor
Minimum map value	-0.352	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	284.8, 284.8, 284.8	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.78, 1.78, 1.78	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	2.30	11/294 (3.7%)	2.76	21/366 (5.7%)
1	B	2.30	12/294 (4.1%)	2.76	21/366 (5.7%)
1	C	2.30	11/294 (3.7%)	2.76	20/366 (5.5%)
1	D	2.29	11/294 (3.7%)	2.76	22/366 (6.0%)
1	E	2.29	12/294 (4.1%)	2.76	21/366 (5.7%)
1	F	2.29	11/294 (3.7%)	2.75	22/366 (6.0%)
1	G	2.31	12/294 (4.1%)	2.76	20/366 (5.5%)
1	W	2.31	12/294 (4.1%)	2.76	20/366 (5.5%)
2	H	2.40	21/587 (3.6%)	2.83	57/732 (7.8%)
2	I	2.40	18/587 (3.1%)	2.82	58/732 (7.9%)
2	J	2.41	21/587 (3.6%)	2.84	56/732 (7.7%)
2	a	2.40	20/587 (3.4%)	2.83	57/732 (7.8%)
2	b	2.40	20/587 (3.4%)	2.82	58/732 (7.9%)
2	f	2.40	19/587 (3.2%)	2.84	58/732 (7.9%)
All	All	2.36	211/5874 (3.6%)	2.80	511/7320 (7.0%)

All (211) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	a	60	GLY	CA-C	-11.55	1.41	1.52
2	J	60	GLY	CA-C	-11.53	1.41	1.52
2	H	60	GLY	CA-C	-11.51	1.41	1.52
2	f	60	GLY	CA-C	-11.51	1.41	1.52
2	b	60	GLY	CA-C	-11.49	1.41	1.52
2	I	60	GLY	CA-C	-11.41	1.41	1.52
1	W	188	THR	CA-C	-8.10	1.44	1.53
1	G	188	THR	CA-C	-8.10	1.44	1.53
1	B	188	THR	CA-C	-8.01	1.44	1.53
1	D	188	THR	CA-C	-8.00	1.44	1.53
1	C	188	THR	CA-C	-7.93	1.44	1.53
1	F	188	THR	CA-C	-7.92	1.44	1.53
1	A	188	THR	CA-C	-7.91	1.45	1.53
1	E	188	THR	CA-C	-7.89	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	127	GLY	N-CA	7.80	1.55	1.45
2	b	127	GLY	N-CA	7.75	1.55	1.45
2	H	127	GLY	N-CA	7.71	1.55	1.45
2	a	127	GLY	N-CA	7.70	1.55	1.45
2	J	127	GLY	N-CA	7.68	1.55	1.45
2	f	127	GLY	N-CA	7.65	1.55	1.45
2	H	113	GLU	N-CA	-7.27	1.37	1.46
2	f	113	GLU	N-CA	-7.27	1.37	1.46
2	a	113	GLU	N-CA	-7.27	1.37	1.46
2	J	113	GLU	N-CA	-7.25	1.37	1.46
2	I	113	GLU	N-CA	-7.19	1.37	1.46
1	G	191	VAL	N-CA	-7.18	1.37	1.46
1	W	191	VAL	N-CA	-7.17	1.37	1.46
2	b	113	GLU	N-CA	-7.16	1.37	1.46
2	f	49	PRO	CA-C	-7.16	1.41	1.52
1	A	191	VAL	N-CA	-7.15	1.37	1.46
1	C	191	VAL	N-CA	-7.15	1.37	1.46
1	D	191	VAL	N-CA	-7.11	1.37	1.46
2	H	49	PRO	CA-C	-7.08	1.41	1.52
1	B	191	VAL	N-CA	-7.08	1.37	1.46
2	a	49	PRO	CA-C	-7.05	1.41	1.52
2	J	49	PRO	CA-C	-7.05	1.41	1.52
2	b	49	PRO	CA-C	-7.02	1.42	1.52
2	I	49	PRO	CA-C	-7.01	1.42	1.52
1	E	191	VAL	N-CA	-6.94	1.38	1.46
1	F	191	VAL	N-CA	-6.92	1.38	1.46
1	W	207	PRO	N-CA	-6.33	1.41	1.46
1	B	193	ASN	C-N	6.29	1.42	1.33
1	D	153	ILE	C-N	6.29	1.41	1.33
1	G	207	PRO	N-CA	-6.29	1.41	1.46
2	I	18	ARG	C-N	6.28	1.41	1.33
1	A	207	PRO	N-CA	-6.28	1.41	1.46
1	G	193	ASN	C-N	6.28	1.42	1.33
1	B	153	ILE	C-N	6.27	1.41	1.33
1	C	163	ASP	CA-C	6.26	1.61	1.52
2	H	18	ARG	C-N	6.24	1.41	1.33
1	F	153	ILE	C-N	6.24	1.41	1.33
1	W	193	ASN	C-N	6.24	1.41	1.33
1	E	153	ILE	C-N	6.23	1.41	1.33
1	A	163	ASP	CA-C	6.23	1.61	1.52
1	G	153	ILE	C-N	6.23	1.41	1.33
1	C	207	PRO	N-CA	-6.22	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	193	ASN	C-N	6.20	1.41	1.33
1	W	153	ILE	C-N	6.19	1.41	1.33
2	b	18	ARG	C-N	6.19	1.41	1.33
1	A	153	ILE	C-N	6.17	1.41	1.33
1	C	193	ASN	C-N	6.17	1.41	1.33
1	A	193	ASN	C-N	6.15	1.41	1.33
2	a	18	ARG	C-N	6.15	1.41	1.33
2	J	18	ARG	C-N	6.13	1.41	1.33
1	B	163	ASP	CA-C	6.13	1.61	1.52
2	f	18	ARG	C-N	6.12	1.41	1.33
1	F	163	ASP	CA-C	6.12	1.61	1.52
1	C	153	ILE	C-N	6.11	1.41	1.33
1	E	163	ASP	CA-C	6.10	1.60	1.52
1	G	163	ASP	CA-C	6.10	1.60	1.52
1	D	207	PRO	N-CA	-6.09	1.41	1.46
1	F	193	ASN	C-N	6.08	1.41	1.33
1	W	163	ASP	CA-C	6.05	1.60	1.52
1	E	207	PRO	N-CA	-6.05	1.41	1.46
1	E	193	ASN	C-N	6.05	1.41	1.33
1	B	207	PRO	N-CA	-6.05	1.41	1.46
1	D	163	ASP	CA-C	6.02	1.60	1.52
1	F	207	PRO	N-CA	-5.97	1.41	1.46
2	H	108	THR	CA-C	-5.83	1.44	1.52
2	f	108	THR	CA-C	-5.82	1.44	1.52
2	a	108	THR	CA-C	-5.82	1.44	1.52
2	I	108	THR	CA-C	-5.81	1.45	1.52
2	J	108	THR	CA-C	-5.81	1.45	1.52
1	G	177	ALA	N-CA	5.78	1.53	1.46
1	W	177	ALA	N-CA	5.75	1.53	1.46
2	I	63	GLN	CA-C	-5.74	1.44	1.52
2	b	108	THR	CA-C	-5.74	1.45	1.52
2	a	96	MET	CA-C	5.74	1.59	1.52
1	D	177	ALA	N-CA	5.73	1.53	1.46
2	b	63	GLN	CA-C	-5.73	1.44	1.52
1	B	177	ALA	N-CA	5.73	1.53	1.46
2	J	63	GLN	CA-C	-5.69	1.44	1.52
1	E	177	ALA	N-CA	5.68	1.53	1.46
2	H	63	GLN	CA-C	-5.68	1.44	1.52
2	H	96	MET	CA-C	5.66	1.59	1.52
2	f	63	GLN	CA-C	-5.66	1.44	1.52
1	F	177	ALA	N-CA	5.65	1.53	1.46
2	a	63	GLN	CA-C	-5.65	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	108	THR	N-CA	5.65	1.53	1.46
2	f	96	MET	CA-C	5.65	1.59	1.52
2	I	108	THR	N-CA	5.65	1.53	1.46
2	J	96	MET	CA-C	5.65	1.59	1.52
2	H	108	THR	N-CA	5.64	1.53	1.46
2	b	72	THR	C-N	5.63	1.41	1.33
2	I	72	THR	C-N	5.63	1.41	1.33
2	a	108	THR	N-CA	5.63	1.53	1.46
2	b	108	THR	N-CA	5.62	1.53	1.46
2	I	96	MET	CA-C	5.62	1.59	1.52
2	f	108	THR	N-CA	5.61	1.53	1.46
2	b	96	MET	CA-C	5.60	1.59	1.52
2	f	72	THR	C-N	5.59	1.41	1.33
1	C	177	ALA	N-CA	5.58	1.53	1.46
2	I	125	PRO	CA-C	-5.58	1.48	1.53
2	J	72	THR	C-N	5.57	1.41	1.33
1	A	177	ALA	N-CA	5.56	1.53	1.46
2	H	125	PRO	CA-C	-5.55	1.48	1.53
2	a	125	PRO	CA-C	-5.52	1.48	1.53
2	a	72	THR	C-N	5.52	1.40	1.33
2	J	125	PRO	CA-C	-5.51	1.48	1.53
2	b	125	PRO	CA-C	-5.50	1.48	1.53
2	H	72	THR	C-N	5.49	1.40	1.33
2	f	125	PRO	CA-C	-5.45	1.48	1.53
2	I	69	LEU	N-CA	-5.38	1.39	1.46
2	I	131	LYS	N-CA	-5.37	1.40	1.46
2	b	131	LYS	N-CA	-5.36	1.40	1.46
2	J	6	LEU	N-CA	-5.35	1.39	1.46
2	f	6	LEU	N-CA	-5.34	1.39	1.46
2	f	69	LEU	N-CA	-5.33	1.40	1.46
2	H	6	LEU	N-CA	-5.33	1.39	1.46
2	f	131	LYS	N-CA	-5.32	1.40	1.46
1	W	191	VAL	C-O	-5.32	1.17	1.24
2	J	131	LYS	N-CA	-5.31	1.40	1.46
2	a	131	LYS	N-CA	-5.30	1.40	1.46
2	H	131	LYS	N-CA	-5.30	1.40	1.46
1	F	191	VAL	C-O	-5.30	1.17	1.24
1	G	191	VAL	C-O	-5.30	1.17	1.24
2	I	98	GLU	C-N	5.30	1.40	1.33
2	b	69	LEU	N-CA	-5.30	1.40	1.46
2	J	69	LEU	N-CA	-5.30	1.40	1.46
1	B	191	VAL	C-O	-5.29	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	81	ASP	N-CA	-5.29	1.40	1.46
2	a	6	LEU	N-CA	-5.28	1.39	1.46
1	W	166	ASP	C-O	-5.27	1.18	1.24
2	b	98	GLU	C-N	5.27	1.39	1.33
1	C	191	VAL	C-O	-5.26	1.17	1.24
2	a	69	LEU	N-CA	-5.26	1.40	1.46
1	G	166	ASP	C-O	-5.25	1.18	1.24
2	H	98	GLU	C-N	5.24	1.39	1.33
2	a	98	GLU	C-N	5.24	1.39	1.33
2	I	81	ASP	N-CA	-5.24	1.40	1.46
1	W	158	LYS	C-N	5.24	1.42	1.33
2	f	98	GLU	C-N	5.24	1.39	1.33
2	H	69	LEU	N-CA	-5.24	1.40	1.46
2	J	98	GLU	C-N	5.23	1.39	1.33
1	D	191	VAL	C-O	-5.23	1.18	1.24
1	G	158	LYS	C-N	5.21	1.42	1.33
1	A	191	VAL	C-O	-5.20	1.18	1.24
1	E	191	VAL	C-O	-5.20	1.18	1.24
1	D	158	LYS	C-N	5.20	1.41	1.33
2	H	104	ILE	CA-C	-5.20	1.46	1.52
2	I	6	LEU	N-CA	-5.18	1.40	1.46
2	b	6	LEU	N-CA	-5.17	1.40	1.46
1	A	158	LYS	C-N	5.17	1.41	1.33
1	C	158	LYS	C-N	5.17	1.41	1.33
2	f	32	PHE	C-N	5.16	1.40	1.33
2	I	79	GLU	C-N	5.16	1.40	1.33
2	f	79	GLU	C-N	5.16	1.40	1.33
2	b	79	GLU	C-N	5.16	1.40	1.33
2	J	79	GLU	C-N	5.15	1.40	1.33
1	B	158	LYS	C-N	5.14	1.41	1.33
1	D	161	PHE	CA-C	-5.14	1.46	1.52
2	a	79	GLU	C-N	5.13	1.40	1.33
1	E	158	LYS	C-N	5.12	1.41	1.33
1	F	158	LYS	C-N	5.12	1.41	1.33
2	a	104	ILE	CA-C	-5.11	1.46	1.52
2	H	32	PHE	C-N	5.11	1.40	1.33
2	H	81	ASP	N-CA	-5.11	1.40	1.46
2	a	81	ASP	N-CA	-5.11	1.40	1.46
2	J	32	PHE	C-N	5.11	1.40	1.33
2	J	104	ILE	CA-C	-5.11	1.46	1.52
1	B	161	PHE	CA-C	-5.11	1.46	1.52
2	f	81	ASP	N-CA	-5.11	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	166	ASP	C-O	-5.10	1.18	1.24
2	H	79	GLU	C-N	5.10	1.40	1.33
2	I	32	PHE	C-N	5.09	1.40	1.33
1	E	166	ASP	C-O	-5.09	1.18	1.24
2	a	32	PHE	C-N	5.07	1.40	1.33
2	f	104	ILE	CA-C	-5.07	1.46	1.52
1	G	191	VAL	CA-C	-5.07	1.46	1.52
2	J	81	ASP	N-CA	-5.07	1.40	1.46
1	C	191	VAL	CA-C	-5.07	1.46	1.52
1	B	166	ASP	C-O	-5.06	1.18	1.24
1	A	191	VAL	CA-C	-5.06	1.46	1.52
1	D	191	VAL	CA-C	-5.05	1.46	1.52
2	b	1	PRO	N-CA	5.04	1.54	1.47
2	b	32	PHE	C-N	5.04	1.40	1.33
1	F	161	PHE	CA-C	-5.04	1.46	1.52
1	W	191	VAL	CA-C	-5.04	1.46	1.52
2	b	104	ILE	CA-C	-5.04	1.46	1.52
1	A	166	ASP	C-O	-5.03	1.18	1.24
1	E	161	PHE	CA-C	-5.03	1.46	1.52
1	B	191	VAL	CA-C	-5.02	1.46	1.52
1	W	174	ALA	N-CA	5.02	1.52	1.46
1	F	166	ASP	C-O	-5.02	1.18	1.24
2	a	11	VAL	CA-C	-5.02	1.46	1.52
2	H	11	VAL	CA-C	-5.02	1.46	1.52
2	J	98	GLU	CA-C	5.01	1.58	1.53
2	H	57	ASN	CA-C	-5.01	1.46	1.52
2	J	42	ALA	C-O	5.01	1.29	1.24
1	E	191	VAL	CA-C	-5.00	1.46	1.52
1	G	161	PHE	CA-C	-5.00	1.46	1.52

All (511) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	GLN	CA-C-N	9.38	132.85	120.28
1	A	179	GLN	C-N-CA	9.38	132.85	120.28
1	W	179	GLN	CA-C-N	9.38	132.85	120.28
1	W	179	GLN	C-N-CA	9.38	132.85	120.28
1	C	179	GLN	CA-C-N	9.36	132.82	120.28
1	C	179	GLN	C-N-CA	9.36	132.82	120.28
1	G	179	GLN	CA-C-N	9.36	132.82	120.28
1	G	179	GLN	C-N-CA	9.36	132.82	120.28
1	F	179	GLN	CA-C-N	9.29	132.73	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	179	GLN	C-N-CA	9.29	132.73	120.28
1	E	179	GLN	CA-C-N	9.29	132.73	120.28
1	E	179	GLN	C-N-CA	9.29	132.73	120.28
1	B	179	GLN	CA-C-N	9.29	132.72	120.28
1	B	179	GLN	C-N-CA	9.29	132.72	120.28
1	D	179	GLN	CA-C-N	9.29	132.72	120.28
1	D	179	GLN	C-N-CA	9.29	132.72	120.28
2	J	89	GLY	CA-C-N	8.03	128.05	119.78
2	J	89	GLY	C-N-CA	8.03	128.05	119.78
2	f	89	GLY	CA-C-N	8.02	128.04	119.78
2	f	89	GLY	C-N-CA	8.02	128.04	119.78
2	H	37	ILE	CA-C-N	7.69	127.58	119.05
2	H	37	ILE	C-N-CA	7.69	127.58	119.05
2	J	37	ILE	CA-C-N	7.64	127.53	119.05
2	J	37	ILE	C-N-CA	7.64	127.53	119.05
2	a	37	ILE	CA-C-N	7.64	127.53	119.05
2	a	37	ILE	C-N-CA	7.64	127.53	119.05
2	f	37	ILE	CA-C-N	7.58	127.47	119.05
2	f	37	ILE	C-N-CA	7.58	127.47	119.05
2	I	37	ILE	CA-C-N	7.55	127.43	119.05
2	I	37	ILE	C-N-CA	7.55	127.43	119.05
2	b	37	ILE	CA-C-N	7.54	127.42	119.05
2	b	37	ILE	C-N-CA	7.54	127.42	119.05
2	a	89	GLY	CA-C-N	7.54	127.98	119.92
2	a	89	GLY	C-N-CA	7.54	127.98	119.92
2	H	89	GLY	CA-C-N	7.51	127.95	119.92
2	H	89	GLY	C-N-CA	7.51	127.95	119.92
2	I	89	GLY	CA-C-N	7.46	127.90	119.92
2	I	89	GLY	C-N-CA	7.46	127.90	119.92
2	b	89	GLY	CA-C-N	7.45	127.90	119.92
2	b	89	GLY	C-N-CA	7.45	127.90	119.92
1	E	164	TYR	N-CA-C	7.45	119.40	111.28
1	F	164	TYR	N-CA-C	7.44	119.39	111.28
1	W	164	TYR	N-CA-C	7.43	119.38	111.28
1	C	164	TYR	N-CA-C	7.43	119.38	111.28
1	G	164	TYR	N-CA-C	7.42	119.36	111.28
1	A	164	TYR	N-CA-C	7.38	119.33	111.28
1	B	164	TYR	N-CA-C	7.38	119.33	111.28
1	D	164	TYR	N-CA-C	7.38	119.32	111.28
2	I	130	TYR	CA-C-N	7.24	129.85	120.44
2	I	130	TYR	C-N-CA	7.24	129.85	120.44
2	a	130	TYR	CA-C-N	7.22	129.82	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	130	TYR	C-N-CA	7.22	129.82	120.44
2	b	130	TYR	CA-C-N	7.21	129.82	120.44
2	b	130	TYR	C-N-CA	7.21	129.82	120.44
1	E	219	GLN	N-CA-C	7.20	119.12	111.28
2	H	130	TYR	CA-C-N	7.19	129.79	120.44
2	H	130	TYR	C-N-CA	7.19	129.79	120.44
1	F	219	GLN	N-CA-C	7.19	119.12	111.28
1	W	219	GLN	N-CA-C	7.14	119.07	111.28
2	f	130	TYR	CA-C-N	7.14	129.73	120.44
2	f	130	TYR	C-N-CA	7.14	129.73	120.44
2	J	130	TYR	CA-C-N	7.14	129.72	120.44
2	J	130	TYR	C-N-CA	7.14	129.72	120.44
1	G	219	GLN	N-CA-C	7.13	119.06	111.28
1	B	219	GLN	N-CA-C	7.10	119.02	111.28
1	C	219	GLN	N-CA-C	7.10	119.02	111.28
1	D	219	GLN	N-CA-C	7.09	119.01	111.28
1	A	219	GLN	N-CA-C	7.08	118.99	111.28
2	I	6	LEU	CA-C-N	7.04	130.42	120.28
2	I	6	LEU	C-N-CA	7.04	130.42	120.28
2	J	82	ARG	CA-C-N	7.02	130.26	120.29
2	J	82	ARG	C-N-CA	7.02	130.26	120.29
2	a	6	LEU	CA-C-N	7.01	130.38	120.28
2	a	6	LEU	C-N-CA	7.01	130.38	120.28
2	b	6	LEU	CA-C-N	7.00	130.36	120.28
2	b	6	LEU	C-N-CA	7.00	130.36	120.28
2	H	6	LEU	CA-C-N	7.00	130.36	120.28
2	H	6	LEU	C-N-CA	7.00	130.36	120.28
2	f	82	ARG	CA-C-N	6.99	130.21	120.29
2	f	82	ARG	C-N-CA	6.99	130.21	120.29
1	C	218	CYS	O-C-N	-6.98	113.44	122.37
1	B	218	CYS	O-C-N	-6.97	113.45	122.37
1	A	218	CYS	O-C-N	-6.95	113.47	122.37
2	b	82	ARG	CA-C-N	6.95	130.16	120.29
2	b	82	ARG	C-N-CA	6.95	130.16	120.29
2	H	82	ARG	CA-C-N	6.94	130.15	120.29
2	H	82	ARG	C-N-CA	6.94	130.15	120.29
2	J	6	LEU	CA-C-N	6.93	130.26	120.28
2	J	6	LEU	C-N-CA	6.93	130.26	120.28
2	I	82	ARG	CA-C-N	6.93	130.13	120.29
2	I	82	ARG	C-N-CA	6.93	130.13	120.29
1	D	218	CYS	O-C-N	-6.92	113.51	122.37
2	a	82	ARG	CA-C-N	6.92	130.12	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	82	ARG	C-N-CA	6.92	130.12	120.29
2	f	6	LEU	CA-C-N	6.91	130.24	120.28
2	f	6	LEU	C-N-CA	6.91	130.24	120.28
1	W	218	CYS	O-C-N	-6.91	113.53	122.37
1	G	218	CYS	O-C-N	-6.88	113.56	122.37
1	E	218	CYS	O-C-N	-6.85	113.60	122.37
1	F	218	CYS	O-C-N	-6.83	113.62	122.37
2	J	55	MET	CA-C-N	6.77	129.91	120.29
2	J	55	MET	C-N-CA	6.77	129.91	120.29
2	I	55	MET	CA-C-N	6.76	129.89	120.29
2	I	55	MET	C-N-CA	6.76	129.89	120.29
2	H	55	MET	CA-C-N	6.76	129.88	120.29
2	H	55	MET	C-N-CA	6.76	129.88	120.29
2	f	55	MET	CA-C-N	6.75	129.88	120.29
2	f	55	MET	C-N-CA	6.75	129.88	120.29
2	a	55	MET	CA-C-N	6.74	129.87	120.29
2	a	55	MET	C-N-CA	6.74	129.87	120.29
2	b	55	MET	CA-C-N	6.73	129.84	120.29
2	b	55	MET	C-N-CA	6.73	129.84	120.29
1	A	218	CYS	CA-C-O	6.71	127.85	119.59
1	C	218	CYS	CA-C-O	6.69	127.82	119.59
1	C	212	GLU	O-C-N	-6.67	115.20	122.07
1	D	218	CYS	CA-C-O	6.67	127.79	119.59
1	B	218	CYS	CA-C-O	6.65	127.77	119.59
1	A	212	GLU	O-C-N	-6.63	115.24	122.07
1	W	218	CYS	CA-C-O	6.62	127.74	119.59
1	E	218	CYS	CA-C-O	6.62	127.74	119.59
1	G	218	CYS	CA-C-O	6.61	127.72	119.59
1	D	212	GLU	O-C-N	-6.61	115.27	122.07
1	B	212	GLU	O-C-N	-6.60	115.27	122.07
2	J	123	PRO	CA-C-N	-6.59	117.60	123.33
2	J	123	PRO	C-N-CA	-6.59	117.60	123.33
1	F	218	CYS	CA-C-O	6.57	127.67	119.59
1	G	212	GLU	O-C-N	-6.56	115.31	122.07
2	f	123	PRO	CA-C-N	-6.56	117.62	123.33
2	f	123	PRO	C-N-CA	-6.56	117.62	123.33
1	W	212	GLU	O-C-N	-6.55	115.32	122.07
2	H	123	PRO	CA-C-N	-6.55	117.63	123.33
2	H	123	PRO	C-N-CA	-6.55	117.63	123.33
1	F	212	GLU	O-C-N	-6.54	115.33	122.07
2	a	123	PRO	CA-C-N	-6.54	117.64	123.33
2	a	123	PRO	C-N-CA	-6.54	117.64	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	158	LYS	CA-C-O	6.52	127.07	119.32
1	G	191	VAL	N-CA-C	6.50	117.29	110.72
1	E	212	GLU	O-C-N	-6.49	115.39	122.07
1	W	191	VAL	N-CA-C	6.48	117.26	110.72
1	E	158	LYS	CA-C-O	6.44	126.98	119.32
1	W	158	LYS	CA-C-O	6.43	126.97	119.32
1	D	191	VAL	N-CA-C	6.43	117.22	110.72
1	G	158	LYS	CA-C-O	6.43	126.97	119.32
1	B	158	LYS	CA-C-O	6.43	126.97	119.32
1	B	191	VAL	N-CA-C	6.42	117.21	110.72
1	F	158	LYS	CA-C-O	6.42	126.97	119.32
1	C	158	LYS	CA-C-O	6.42	126.96	119.32
2	I	123	PRO	CA-C-N	-6.42	117.75	123.33
2	I	123	PRO	C-N-CA	-6.42	117.75	123.33
1	C	191	VAL	N-CA-C	6.41	117.20	110.72
1	A	158	LYS	CA-C-O	6.41	126.95	119.32
2	b	123	PRO	CA-C-N	-6.41	117.76	123.33
2	b	123	PRO	C-N-CA	-6.41	117.76	123.33
1	A	191	VAL	N-CA-C	6.38	117.17	110.72
1	E	191	VAL	N-CA-C	6.30	117.09	110.72
1	F	191	VAL	N-CA-C	6.30	117.08	110.72
2	a	15	ILE	O-C-N	-6.28	114.86	122.59
2	H	15	ILE	O-C-N	-6.28	114.87	122.59
2	f	15	ILE	O-C-N	-6.26	114.89	122.59
2	J	15	ILE	O-C-N	-6.23	114.92	122.59
2	I	15	ILE	O-C-N	-6.20	114.97	122.59
2	b	15	ILE	O-C-N	-6.16	115.01	122.59
2	H	125	PRO	CA-C-N	6.15	130.19	120.47
2	H	125	PRO	C-N-CA	6.15	130.19	120.47
2	I	125	PRO	CA-C-N	6.15	130.18	120.47
2	I	125	PRO	C-N-CA	6.15	130.18	120.47
2	b	125	PRO	CA-C-N	6.14	130.18	120.47
2	b	125	PRO	C-N-CA	6.14	130.18	120.47
2	a	36	VAL	O-C-N	-6.14	115.91	121.87
2	J	36	VAL	O-C-N	-6.14	115.92	121.87
2	a	125	PRO	CA-C-N	6.13	130.16	120.47
2	a	125	PRO	C-N-CA	6.13	130.16	120.47
2	f	125	PRO	CA-C-N	6.13	130.16	120.47
2	f	125	PRO	C-N-CA	6.13	130.16	120.47
2	J	125	PRO	CA-C-N	6.13	130.16	120.47
2	J	125	PRO	C-N-CA	6.13	130.16	120.47
2	f	36	VAL	O-C-N	-6.09	115.96	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	THR	CA-C-N	6.08	128.43	120.28
1	B	171	THR	C-N-CA	6.08	128.43	120.28
2	I	36	VAL	O-C-N	-6.07	115.98	121.87
1	G	171	THR	CA-C-N	6.06	128.41	120.28
1	G	171	THR	C-N-CA	6.06	128.41	120.28
1	D	171	THR	CA-C-N	6.06	128.40	120.28
1	D	171	THR	C-N-CA	6.06	128.40	120.28
2	f	88	ALA	N-CA-C	6.05	119.04	109.96
2	J	88	ALA	N-CA-C	6.05	119.03	109.96
2	I	88	ALA	N-CA-C	6.05	119.03	109.96
1	W	171	THR	CA-C-N	6.04	128.38	120.28
1	W	171	THR	C-N-CA	6.04	128.38	120.28
2	a	88	ALA	N-CA-C	6.04	119.01	109.96
2	b	88	ALA	N-CA-C	6.04	119.02	109.96
2	b	21	ASN	O-C-N	-6.03	115.73	122.12
1	E	171	THR	CA-C-N	6.03	128.36	120.28
1	E	171	THR	C-N-CA	6.03	128.36	120.28
2	H	88	ALA	N-CA-C	6.03	119.01	109.96
2	H	36	VAL	O-C-N	-6.02	116.03	121.87
2	b	36	VAL	O-C-N	-6.02	116.03	121.87
1	E	191	VAL	CA-C-N	6.00	128.32	120.28
1	E	191	VAL	C-N-CA	6.00	128.32	120.28
1	F	191	VAL	CA-C-N	6.00	128.32	120.28
1	F	191	VAL	C-N-CA	6.00	128.32	120.28
1	A	171	THR	CA-C-N	6.00	128.31	120.28
1	A	171	THR	C-N-CA	6.00	128.31	120.28
2	J	21	ASN	O-C-N	-5.99	115.77	122.12
1	F	171	THR	CA-C-N	5.99	128.31	120.28
1	F	171	THR	C-N-CA	5.99	128.31	120.28
2	f	21	ASN	O-C-N	-5.99	115.78	122.12
2	I	21	ASN	O-C-N	-5.98	115.78	122.12
1	B	191	VAL	CA-C-N	5.98	128.29	120.28
1	B	191	VAL	C-N-CA	5.98	128.29	120.28
1	C	195	ASN	CA-C-N	5.98	125.46	119.24
1	C	195	ASN	C-N-CA	5.98	125.46	119.24
1	C	191	VAL	CA-C-N	5.97	128.28	120.28
1	C	191	VAL	C-N-CA	5.97	128.28	120.28
1	A	191	VAL	CA-C-N	5.97	128.28	120.28
1	A	191	VAL	C-N-CA	5.97	128.28	120.28
1	D	195	ASN	CA-C-N	5.96	125.44	119.24
1	D	195	ASN	C-N-CA	5.96	125.44	119.24
1	D	191	VAL	CA-C-N	5.96	128.26	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	191	VAL	C-N-CA	5.96	128.26	120.28
1	C	171	THR	CA-C-N	5.96	128.26	120.28
1	C	171	THR	C-N-CA	5.96	128.26	120.28
1	B	195	ASN	CA-C-N	5.95	125.43	119.24
1	B	195	ASN	C-N-CA	5.95	125.43	119.24
1	F	195	ASN	CA-C-N	5.94	125.42	119.24
1	F	195	ASN	C-N-CA	5.94	125.42	119.24
2	b	55	MET	O-C-N	-5.94	115.95	122.07
2	a	21	ASN	O-C-N	-5.93	115.83	122.12
1	E	195	ASN	CA-C-N	5.93	125.41	119.24
1	E	195	ASN	C-N-CA	5.93	125.41	119.24
1	A	195	ASN	CA-C-N	5.92	125.40	119.24
1	A	195	ASN	C-N-CA	5.92	125.40	119.24
2	J	55	MET	O-C-N	-5.92	115.97	122.07
1	G	191	VAL	CA-C-N	5.92	128.21	120.28
1	G	191	VAL	C-N-CA	5.92	128.21	120.28
2	I	55	MET	O-C-N	-5.92	115.97	122.07
2	f	55	MET	O-C-N	-5.91	115.98	122.07
2	H	21	ASN	O-C-N	-5.91	115.86	122.12
1	W	191	VAL	CA-C-N	5.90	128.18	120.28
1	W	191	VAL	C-N-CA	5.90	128.18	120.28
2	J	92	ALA	CA-C-O	-5.87	113.91	120.25
2	a	55	MET	O-C-N	-5.87	116.03	122.07
2	H	55	MET	O-C-N	-5.87	116.03	122.07
1	G	195	ASN	CA-C-N	5.86	125.34	119.24
1	G	195	ASN	C-N-CA	5.86	125.34	119.24
2	I	92	ALA	CA-C-O	-5.86	113.93	120.25
2	J	81	ASP	N-CA-C	5.86	117.66	111.28
1	W	195	ASN	CA-C-N	5.85	125.33	119.24
1	W	195	ASN	C-N-CA	5.85	125.33	119.24
2	f	106	GLY	CA-C-N	5.85	128.05	120.44
2	f	106	GLY	C-N-CA	5.85	128.05	120.44
2	a	92	ALA	CA-C-O	-5.84	113.94	120.25
2	f	81	ASP	N-CA-C	5.84	117.64	111.28
2	J	106	GLY	CA-C-N	5.84	128.03	120.44
2	J	106	GLY	C-N-CA	5.84	128.03	120.44
2	b	92	ALA	CA-C-O	-5.83	113.95	120.25
2	f	92	ALA	CA-C-O	-5.83	113.95	120.25
1	G	165	VAL	CA-C-O	5.83	127.03	120.85
2	a	81	ASP	N-CA-C	5.82	117.63	111.28
2	H	92	ALA	CA-C-O	-5.80	113.98	120.25
2	b	106	GLY	CA-C-N	5.80	127.98	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	106	GLY	C-N-CA	5.80	127.98	120.44
2	b	81	ASP	N-CA-C	5.80	117.60	111.28
1	W	149	SER	O-C-N	-5.77	116.27	122.85
2	H	81	ASP	N-CA-C	5.77	117.57	111.28
1	W	165	VAL	CA-C-O	5.77	126.96	120.85
2	I	81	ASP	N-CA-C	5.77	117.57	111.28
2	I	106	GLY	CA-C-N	5.77	127.94	120.44
2	I	106	GLY	C-N-CA	5.77	127.94	120.44
2	b	142	VAL	CA-C-N	5.74	127.97	120.28
2	b	142	VAL	C-N-CA	5.74	127.97	120.28
2	f	142	VAL	CA-C-N	5.74	127.97	120.28
2	f	142	VAL	C-N-CA	5.74	127.97	120.28
1	E	165	VAL	CA-C-O	5.73	126.92	120.85
1	G	149	SER	O-C-N	-5.72	116.32	122.85
2	H	76	GLU	CA-C-N	5.72	128.42	120.29
2	H	76	GLU	C-N-CA	5.72	128.42	120.29
2	I	142	VAL	CA-C-N	5.72	127.95	120.28
2	I	142	VAL	C-N-CA	5.72	127.95	120.28
2	I	76	GLU	CA-C-N	5.72	128.41	120.29
2	I	76	GLU	C-N-CA	5.72	128.41	120.29
2	J	142	VAL	CA-C-N	5.72	127.94	120.28
2	J	142	VAL	C-N-CA	5.72	127.94	120.28
2	a	142	VAL	CA-C-N	5.71	127.94	120.28
2	a	142	VAL	C-N-CA	5.71	127.94	120.28
2	a	76	GLU	CA-C-N	5.71	128.40	120.29
2	a	76	GLU	C-N-CA	5.71	128.40	120.29
2	f	76	GLU	CA-C-N	5.70	128.38	120.29
2	f	76	GLU	C-N-CA	5.70	128.38	120.29
2	J	76	GLU	CA-C-N	5.69	128.37	120.29
2	J	76	GLU	C-N-CA	5.69	128.37	120.29
1	C	165	VAL	CA-C-O	5.68	126.88	120.85
1	F	165	VAL	CA-C-O	5.68	126.87	120.85
2	H	106	GLY	CA-C-N	5.68	127.83	120.44
2	H	106	GLY	C-N-CA	5.68	127.83	120.44
1	A	165	VAL	CA-C-O	5.68	126.87	120.85
2	a	106	GLY	CA-C-N	5.67	127.82	120.44
2	a	106	GLY	C-N-CA	5.67	127.82	120.44
2	b	76	GLU	CA-C-N	5.67	128.35	120.29
2	b	76	GLU	C-N-CA	5.67	128.35	120.29
1	C	149	SER	O-C-N	-5.66	116.40	122.85
1	D	149	SER	O-C-N	-5.65	116.40	122.85
2	H	142	VAL	CA-C-N	5.65	127.86	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	142	VAL	C-N-CA	5.65	127.86	120.28
1	F	149	SER	O-C-N	-5.65	116.41	122.85
1	E	149	SER	O-C-N	-5.64	116.42	122.85
2	I	84	HIS	CA-C-O	-5.63	115.09	119.99
1	A	149	SER	O-C-N	-5.63	116.44	122.85
2	b	84	HIS	CA-C-O	-5.63	115.09	119.99
1	B	149	SER	O-C-N	-5.62	116.44	122.85
2	f	84	HIS	CA-C-O	-5.62	115.10	119.99
2	J	84	HIS	CA-C-O	-5.60	115.12	119.99
2	H	84	HIS	CA-C-O	-5.60	115.12	119.99
1	E	153	ILE	CA-C-O	5.59	127.34	120.74
2	H	134	ILE	CA-C-O	5.59	127.09	121.17
2	a	33	SER	CA-C-N	5.58	125.25	119.56
2	a	33	SER	C-N-CA	5.58	125.25	119.56
2	J	62	HIS	O-C-N	-5.58	116.00	122.86
1	F	153	ILE	CA-C-O	5.55	127.29	120.74
2	H	33	SER	CA-C-N	5.55	125.22	119.56
2	H	33	SER	C-N-CA	5.55	125.22	119.56
1	W	153	ILE	CA-C-O	5.55	127.29	120.74
1	D	153	ILE	CA-C-O	5.55	127.29	120.74
1	G	153	ILE	CA-C-O	5.54	127.28	120.74
2	a	84	HIS	CA-C-O	-5.54	115.17	119.99
1	C	153	ILE	CA-C-O	5.53	127.27	120.74
1	A	153	ILE	CA-C-O	5.53	127.27	120.74
1	B	153	ILE	CA-C-O	5.53	127.26	120.74
2	a	134	ILE	CA-C-O	5.53	127.03	121.17
1	B	165	VAL	CA-C-O	5.50	126.68	120.85
2	b	124	ILE	O-C-N	-5.49	115.56	121.11
1	D	165	VAL	CA-C-O	5.49	126.67	120.85
2	I	124	ILE	O-C-N	-5.46	115.59	121.11
2	f	134	ILE	CA-C-O	5.46	126.95	121.17
2	b	134	ILE	CA-C-O	5.46	126.95	121.17
2	I	134	ILE	CA-C-O	5.43	126.93	121.17
2	J	5	ASN	O-C-N	-5.40	116.69	122.85
2	a	33	SER	O-C-N	-5.40	115.73	121.30
2	b	33	SER	CA-C-N	5.40	125.07	119.56
2	b	33	SER	C-N-CA	5.40	125.07	119.56
2	I	33	SER	CA-C-N	5.40	125.07	119.56
2	I	33	SER	C-N-CA	5.40	125.07	119.56
2	f	126	VAL	CA-C-N	5.39	125.92	119.94
2	f	126	VAL	C-N-CA	5.39	125.92	119.94
2	J	134	ILE	CA-C-O	5.39	126.89	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	54	THR	CA-C-N	5.38	127.44	120.44
2	a	54	THR	C-N-CA	5.38	127.44	120.44
2	f	16	SER	N-CA-C	5.38	116.61	109.93
2	f	33	SER	CA-C-N	5.38	125.05	119.56
2	f	33	SER	C-N-CA	5.38	125.05	119.56
2	f	5	ASN	O-C-N	-5.38	116.72	122.85
2	f	64	ALA	CA-C-O	5.38	126.12	120.42
2	I	54	THR	CA-C-N	5.37	127.42	120.44
2	I	54	THR	C-N-CA	5.37	127.42	120.44
2	b	54	THR	CA-C-N	5.37	127.42	120.44
2	b	54	THR	C-N-CA	5.37	127.42	120.44
2	H	54	THR	CA-C-N	5.36	127.41	120.44
2	H	54	THR	C-N-CA	5.36	127.41	120.44
2	J	33	SER	CA-C-N	5.36	125.03	119.56
2	J	33	SER	C-N-CA	5.36	125.03	119.56
2	b	126	VAL	CA-C-N	5.36	125.89	119.94
2	b	126	VAL	C-N-CA	5.36	125.89	119.94
2	J	124	ILE	O-C-N	-5.36	115.70	121.11
2	J	126	VAL	CA-C-N	5.35	125.88	119.94
2	J	126	VAL	C-N-CA	5.35	125.88	119.94
2	f	54	THR	CA-C-N	5.35	127.40	120.44
2	f	54	THR	C-N-CA	5.35	127.40	120.44
2	H	33	SER	O-C-N	-5.35	115.79	121.30
1	C	198	CYS	N-CA-C	5.35	118.02	111.82
2	J	64	ALA	CA-C-O	5.34	126.08	120.42
2	b	75	GLU	N-CA-C	5.34	116.79	111.07
2	J	54	THR	CA-C-N	5.34	127.39	120.44
2	J	54	THR	C-N-CA	5.34	127.39	120.44
1	E	195	ASN	O-C-N	-5.33	115.95	121.60
2	I	126	VAL	CA-C-N	5.33	125.85	119.94
2	I	126	VAL	C-N-CA	5.33	125.85	119.94
2	a	5	ASN	O-C-N	-5.33	116.78	122.85
1	C	195	ASN	O-C-N	-5.33	115.95	121.60
1	F	195	ASN	O-C-N	-5.32	115.97	121.60
1	A	198	CYS	N-CA-C	5.31	117.98	111.82
2	f	62	HIS	O-C-N	-5.31	115.97	122.55
2	I	75	GLU	N-CA-C	5.31	116.75	111.07
1	E	198	CYS	N-CA-C	5.30	117.97	111.82
2	f	33	SER	O-C-N	-5.30	115.84	121.30
2	H	126	VAL	CA-C-N	5.29	125.82	119.94
2	H	126	VAL	C-N-CA	5.29	125.82	119.94
2	a	64	ALA	CA-C-O	5.29	126.03	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	33	SER	O-C-N	-5.29	115.85	121.30
1	B	198	CYS	N-CA-C	5.29	117.95	111.82
2	f	124	ILE	O-C-N	-5.29	115.77	121.11
2	H	5	ASN	O-C-N	-5.29	116.82	122.85
1	A	195	ASN	O-C-N	-5.29	116.00	121.60
2	H	62	HIS	O-C-N	-5.29	116.00	122.55
1	F	198	CYS	N-CA-C	5.28	117.95	111.82
1	D	198	CYS	N-CA-C	5.28	117.95	111.82
2	H	64	ALA	CA-C-O	5.28	126.02	120.42
2	I	142	VAL	CA-C-O	-5.28	115.78	121.27
2	J	33	SER	O-C-N	-5.28	115.87	121.30
2	a	126	VAL	CA-C-N	5.27	125.79	119.94
2	a	126	VAL	C-N-CA	5.27	125.79	119.94
2	b	142	VAL	CA-C-O	-5.27	115.79	121.27
2	H	124	ILE	O-C-N	-5.27	115.79	121.11
2	a	124	ILE	O-C-N	-5.26	115.80	121.11
2	I	5	ASN	O-C-N	-5.26	116.86	122.85
2	a	62	HIS	O-C-N	-5.25	116.03	122.55
2	H	75	GLU	N-CA-C	5.25	116.69	111.07
1	B	195	ASN	O-C-N	-5.25	116.03	121.60
2	a	75	GLU	N-CA-C	5.25	116.69	111.07
2	H	142	VAL	CA-C-O	-5.25	115.81	121.27
1	D	195	ASN	O-C-N	-5.25	116.04	121.60
1	W	198	CYS	N-CA-C	5.23	117.89	111.82
2	I	33	SER	O-C-N	-5.23	115.91	121.30
2	I	62	HIS	O-C-N	-5.23	116.06	122.55
2	J	142	VAL	CA-C-O	-5.23	115.83	121.27
2	f	142	VAL	CA-C-O	-5.23	115.83	121.27
2	a	142	VAL	CA-C-O	-5.23	115.83	121.27
2	f	98	GLU	CA-C-O	-5.23	114.60	120.25
2	b	62	HIS	O-C-N	-5.23	116.07	122.55
2	J	43	LEU	N-CA-C	-5.23	106.86	113.18
2	b	5	ASN	O-C-N	-5.22	116.89	122.85
2	H	64	ALA	CA-C-N	5.21	127.69	120.29
2	H	64	ALA	C-N-CA	5.21	127.69	120.29
2	I	141	ILE	CA-C-N	5.21	127.33	120.60
2	I	141	ILE	C-N-CA	5.21	127.33	120.60
2	I	43	LEU	N-CA-C	-5.21	106.87	113.18
2	I	64	ALA	CA-C-O	5.21	125.94	120.42
1	G	198	CYS	N-CA-C	5.21	117.86	111.82
2	H	70	LYS	O-C-N	5.21	127.44	122.07
2	H	98	GLU	CA-C-O	-5.21	114.62	120.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	98	GLU	CA-C-O	-5.21	114.63	120.25
2	b	141	ILE	CA-C-N	5.21	127.31	120.60
2	b	141	ILE	C-N-CA	5.21	127.31	120.60
2	b	64	ALA	CA-C-O	5.20	125.94	120.42
2	f	43	LEU	N-CA-C	-5.20	106.89	113.18
2	f	64	ALA	CA-C-N	5.20	127.67	120.29
2	f	64	ALA	C-N-CA	5.20	127.67	120.29
2	a	6	LEU	N-CA-C	5.20	117.62	111.33
2	b	6	LEU	N-CA-C	5.20	117.62	111.33
2	J	75	GLU	N-CA-C	5.20	116.63	111.07
2	H	6	LEU	N-CA-C	5.19	117.61	111.33
2	b	98	GLU	CA-C-O	-5.19	114.65	120.25
2	H	141	ILE	CA-C-N	5.19	127.29	120.60
2	H	141	ILE	C-N-CA	5.19	127.29	120.60
2	f	70	LYS	O-C-N	5.19	127.41	122.07
2	I	6	LEU	N-CA-C	5.19	117.61	111.33
2	f	141	ILE	CA-C-N	5.19	127.29	120.60
2	f	141	ILE	C-N-CA	5.19	127.29	120.60
2	a	98	GLU	CA-C-O	-5.18	114.65	120.25
2	f	75	GLU	N-CA-C	5.18	116.62	111.07
2	a	141	ILE	CA-C-N	5.18	127.28	120.60
2	a	141	ILE	C-N-CA	5.18	127.28	120.60
2	J	64	ALA	CA-C-N	5.18	127.65	120.29
2	J	64	ALA	C-N-CA	5.18	127.65	120.29
2	J	70	LYS	O-C-N	5.18	127.41	122.07
2	a	64	ALA	CA-C-N	5.18	127.64	120.29
2	a	64	ALA	C-N-CA	5.18	127.64	120.29
1	W	195	ASN	O-C-N	-5.18	116.11	121.60
2	f	6	LEU	N-CA-C	5.17	117.59	111.33
1	G	195	ASN	O-C-N	-5.17	116.12	121.60
2	J	141	ILE	CA-C-N	5.17	127.27	120.60
2	J	141	ILE	C-N-CA	5.17	127.27	120.60
2	I	98	GLU	CA-C-O	-5.16	114.68	120.25
2	H	33	SER	N-CA-C	5.16	116.19	109.64
2	a	70	LYS	O-C-N	5.15	127.38	122.07
2	b	71	GLU	CA-C-N	5.15	127.14	120.44
2	b	71	GLU	C-N-CA	5.15	127.14	120.44
2	I	71	GLU	CA-C-N	5.15	127.13	120.44
2	I	71	GLU	C-N-CA	5.15	127.13	120.44
2	J	6	LEU	N-CA-C	5.15	117.56	111.33
2	b	43	LEU	N-CA-C	-5.14	106.95	113.18
2	b	33	SER	N-CA-C	5.14	116.17	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	43	LEU	N-CA-C	-5.13	106.97	113.18
2	a	33	SER	N-CA-C	5.11	116.14	109.64
2	J	71	GLU	CA-C-N	5.11	127.09	120.44
2	J	71	GLU	C-N-CA	5.11	127.09	120.44
2	I	33	SER	N-CA-C	5.11	116.13	109.64
2	a	43	LEU	N-CA-C	-5.11	107.00	113.18
2	f	71	GLU	CA-C-N	5.11	127.08	120.44
2	f	71	GLU	C-N-CA	5.11	127.08	120.44
2	b	4	GLN	CA-C-O	-5.10	114.72	120.43
2	H	98	GLU	O-C-N	5.10	127.14	121.43
1	F	156	GLY	O-C-N	-5.09	116.67	121.77
2	f	87	HIS	N-CA-C	5.09	117.98	110.59
2	J	87	HIS	N-CA-C	5.09	117.97	110.59
2	I	4	GLN	CA-C-O	-5.08	114.74	120.43
2	I	64	ALA	CA-C-N	5.07	127.49	120.29
2	I	64	ALA	C-N-CA	5.07	127.49	120.29
2	b	64	ALA	CA-C-N	5.07	127.49	120.29
2	b	64	ALA	C-N-CA	5.07	127.49	120.29
2	I	87	HIS	N-CA-C	5.07	117.93	110.59
2	b	70	LYS	O-C-N	5.06	127.28	122.07
2	b	87	HIS	N-CA-C	5.06	117.93	110.59
2	I	70	LYS	O-C-N	5.06	127.28	122.07
2	H	71	GLU	CA-C-N	5.06	127.02	120.44
2	H	71	GLU	C-N-CA	5.06	127.02	120.44
2	a	87	HIS	N-CA-C	5.05	117.92	110.59
1	E	156	GLY	O-C-N	-5.05	116.72	121.77
2	I	98	GLU	O-C-N	5.05	127.08	121.43
1	B	154	ARG	CA-C-O	-5.04	115.34	120.99
1	D	154	ARG	CA-C-O	-5.04	115.34	120.99
2	a	71	GLU	CA-C-N	5.04	126.99	120.44
2	a	71	GLU	C-N-CA	5.04	126.99	120.44
2	b	98	GLU	O-C-N	5.04	127.08	121.43
2	H	87	HIS	N-CA-C	5.04	117.89	110.59
2	f	33	SER	N-CA-C	5.02	116.02	109.64
1	F	159	GLU	CA-C-O	-5.01	115.60	119.46
1	A	206	GLY	O-C-N	-5.01	116.76	121.77
2	a	98	GLU	O-C-N	5.01	127.04	121.43
2	f	76	GLU	O-C-N	-5.01	116.81	122.12
2	J	66	MET	O-C-N	5.01	127.43	122.12
1	D	178	SER	O-C-N	-5.00	116.42	122.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	295	0	77	0	0
1	B	295	0	77	2	0
1	C	295	0	77	0	0
1	D	295	0	77	2	0
1	E	295	0	77	0	0
1	F	295	0	77	0	0
1	G	295	0	77	0	0
1	W	295	0	77	0	0
2	H	588	0	156	0	0
2	I	588	0	156	2	0
2	J	588	0	156	0	0
2	a	588	0	156	0	0
2	b	588	0	156	2	0
2	f	588	0	156	0	0
All	All	5888	0	1552	4	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 1.

All (4) 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:D:148:THR:N	2:I:147:PRO:C	1.88	1.30
1:B:148:THR:N	2:b:147:PRO:C	1.88	1.28
1:B:148:THR:CA	2:b:147:PRO:C	2.75	0.59
1:D:148:THR:CA	2:I:147:PRO:C	2.75	0.57

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	72/74 (97%)	70 (97%)	2 (3%)	0	100	100
1	B	72/74 (97%)	70 (97%)	2 (3%)	0	100	100
1	C	72/74 (97%)	70 (97%)	2 (3%)	0	100	100
1	D	72/74 (97%)	70 (97%)	2 (3%)	0	100	100
1	E	72/74 (97%)	70 (97%)	2 (3%)	0	100	100
1	F	72/74 (97%)	70 (97%)	2 (3%)	0	100	100
1	G	72/74 (97%)	70 (97%)	2 (3%)	0	100	100
1	W	72/74 (97%)	70 (97%)	2 (3%)	0	100	100
2	H	145/147 (99%)	142 (98%)	3 (2%)	0	100	100
2	I	145/147 (99%)	142 (98%)	3 (2%)	0	100	100
2	J	145/147 (99%)	142 (98%)	3 (2%)	0	100	100
2	a	145/147 (99%)	141 (97%)	4 (3%)	0	100	100
2	b	145/147 (99%)	142 (98%)	3 (2%)	0	100	100
2	f	145/147 (99%)	142 (98%)	3 (2%)	0	100	100
All	All	1446/1474 (98%)	1411 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

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 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.

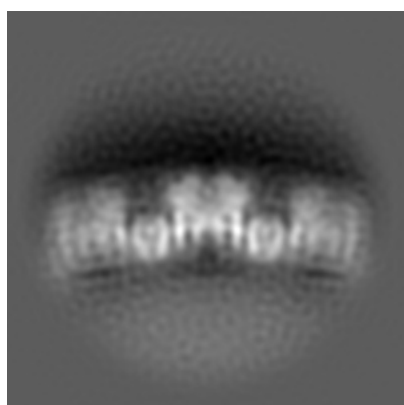
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3469. These allow visual inspection of the internal detail of the map and identification of artifacts.

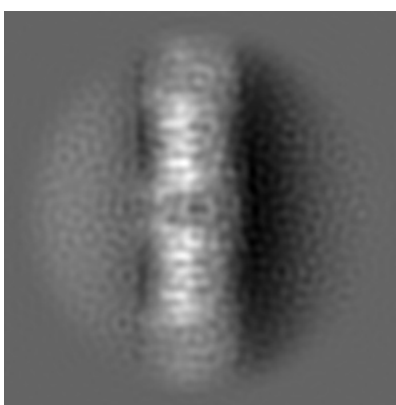
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

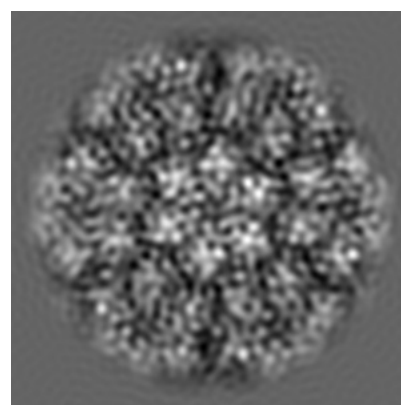
6.1.1 Primary map



X



Y

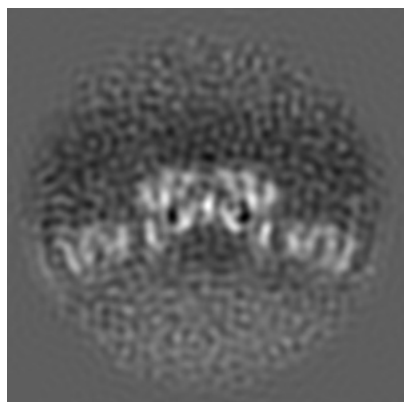


Z

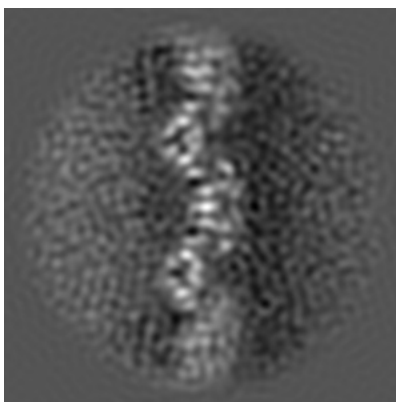
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

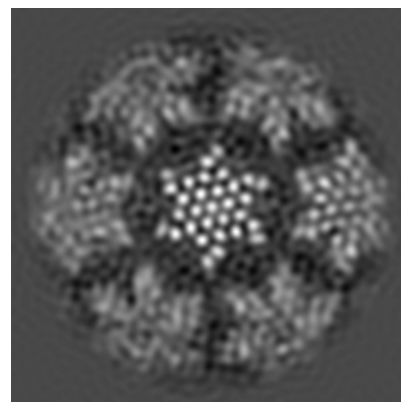
6.2.1 Primary map



X Index: 80



Y Index: 80

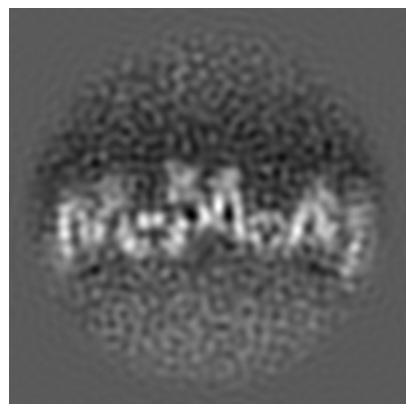


Z Index: 80

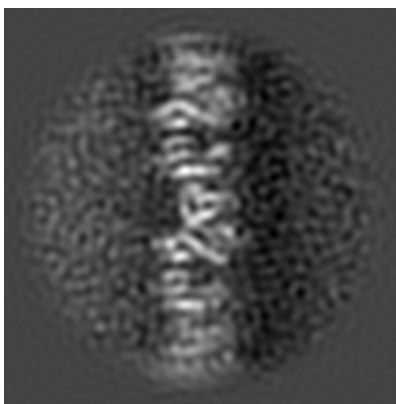
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

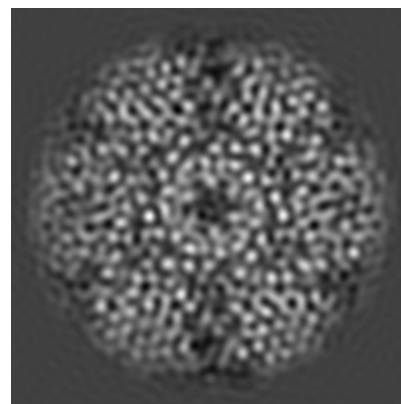
6.3.1 Primary map



X Index: 93



Y Index: 92

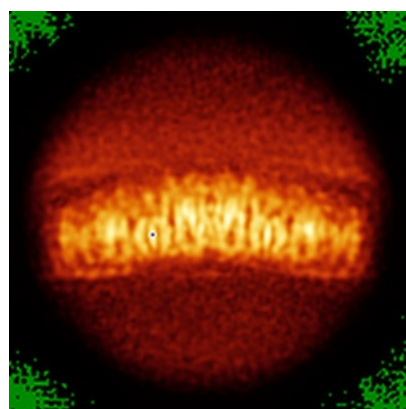


Z Index: 72

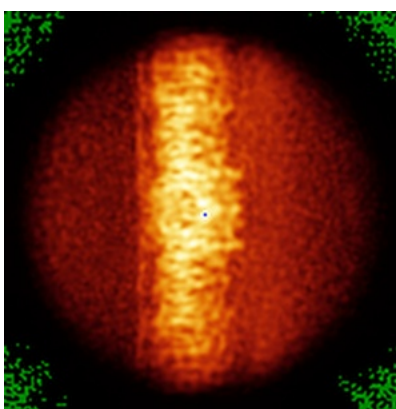
The images above show the largest variance slices of the map in three orthogonal directions.

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

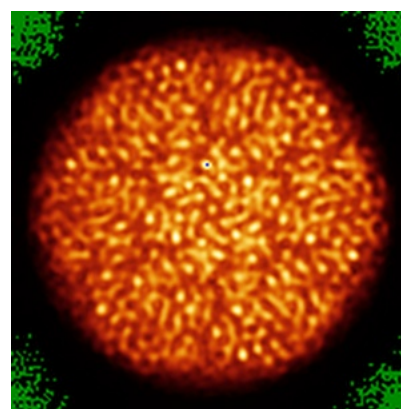
6.4.1 Primary map



X



Y

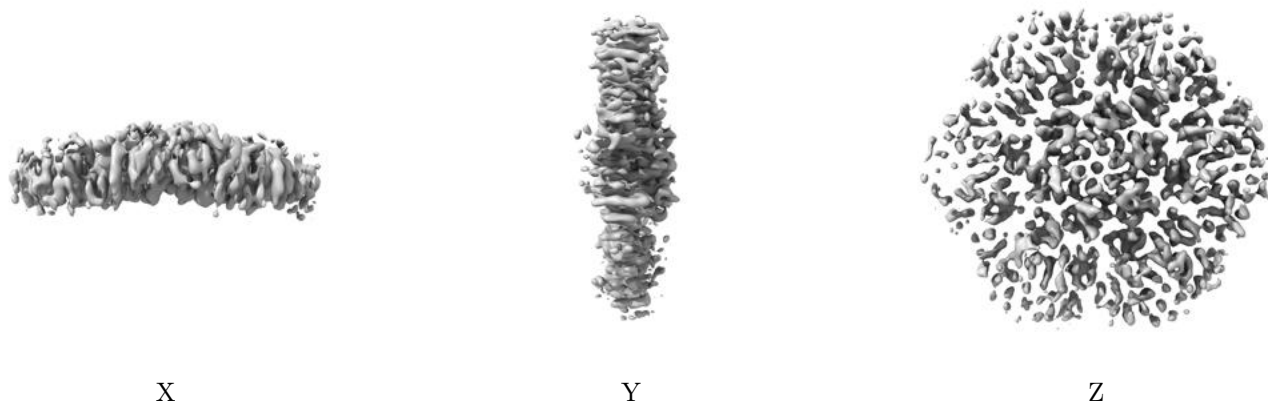


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

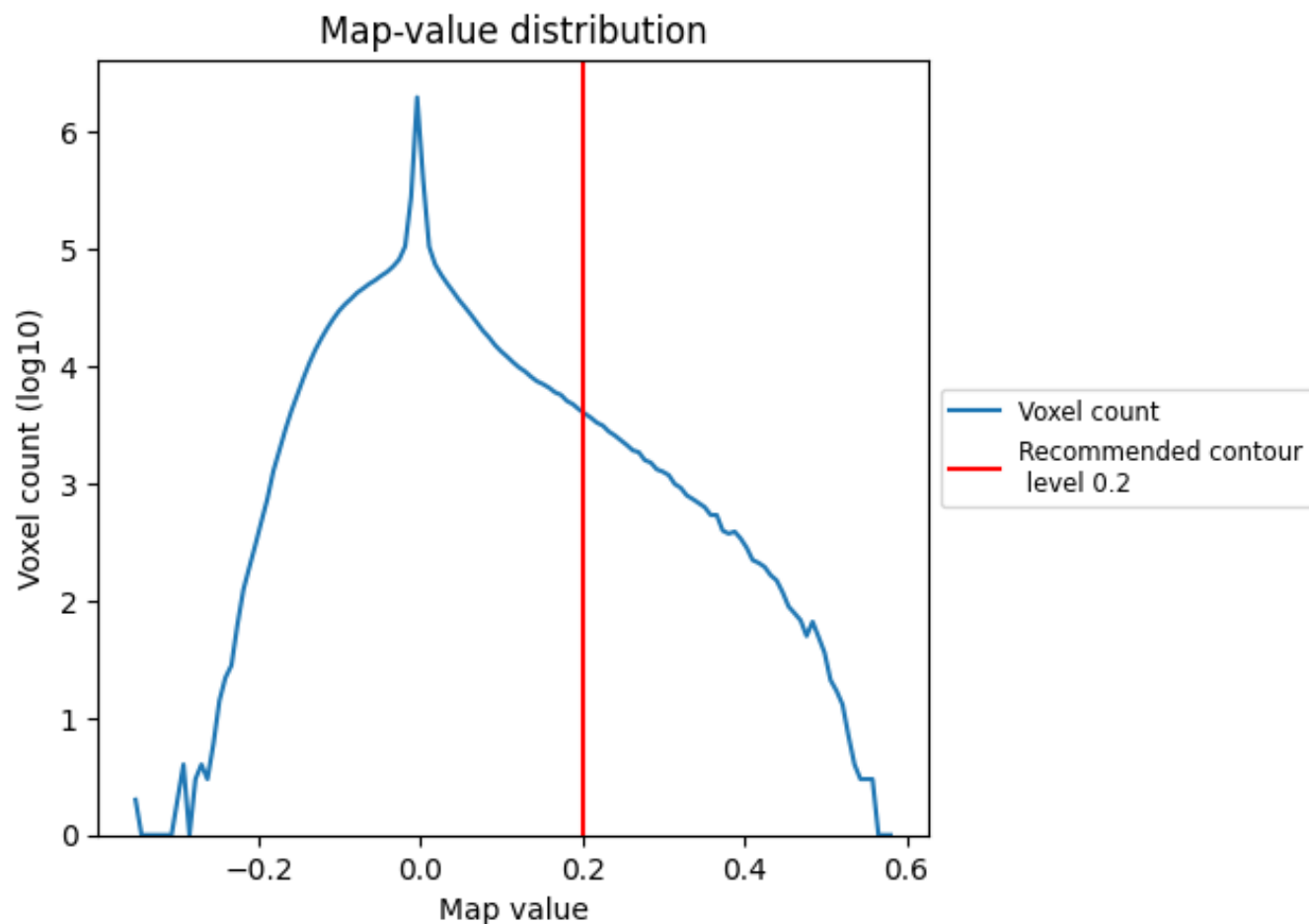
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

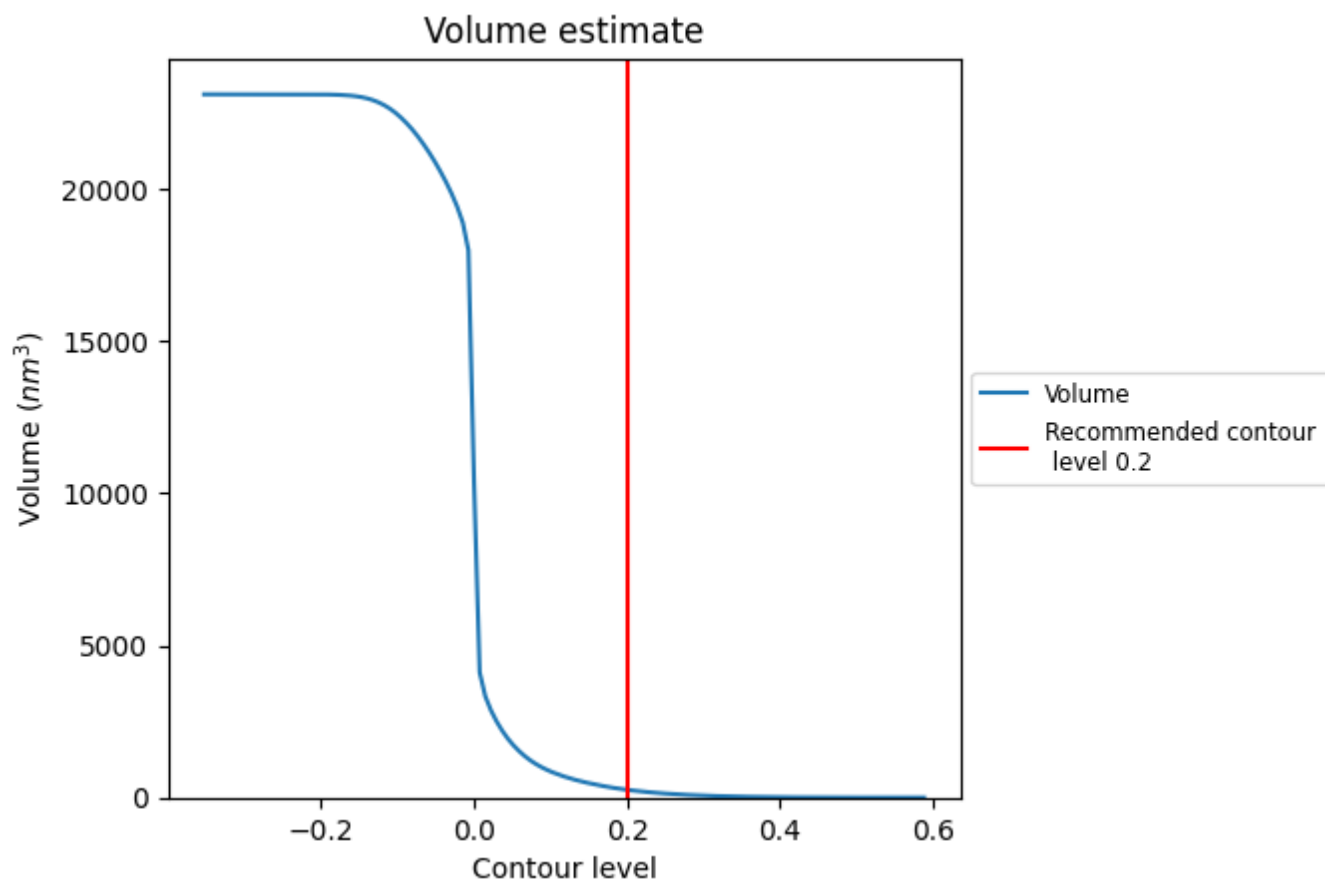
This section contains the results of statistical analysis of the map.

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.

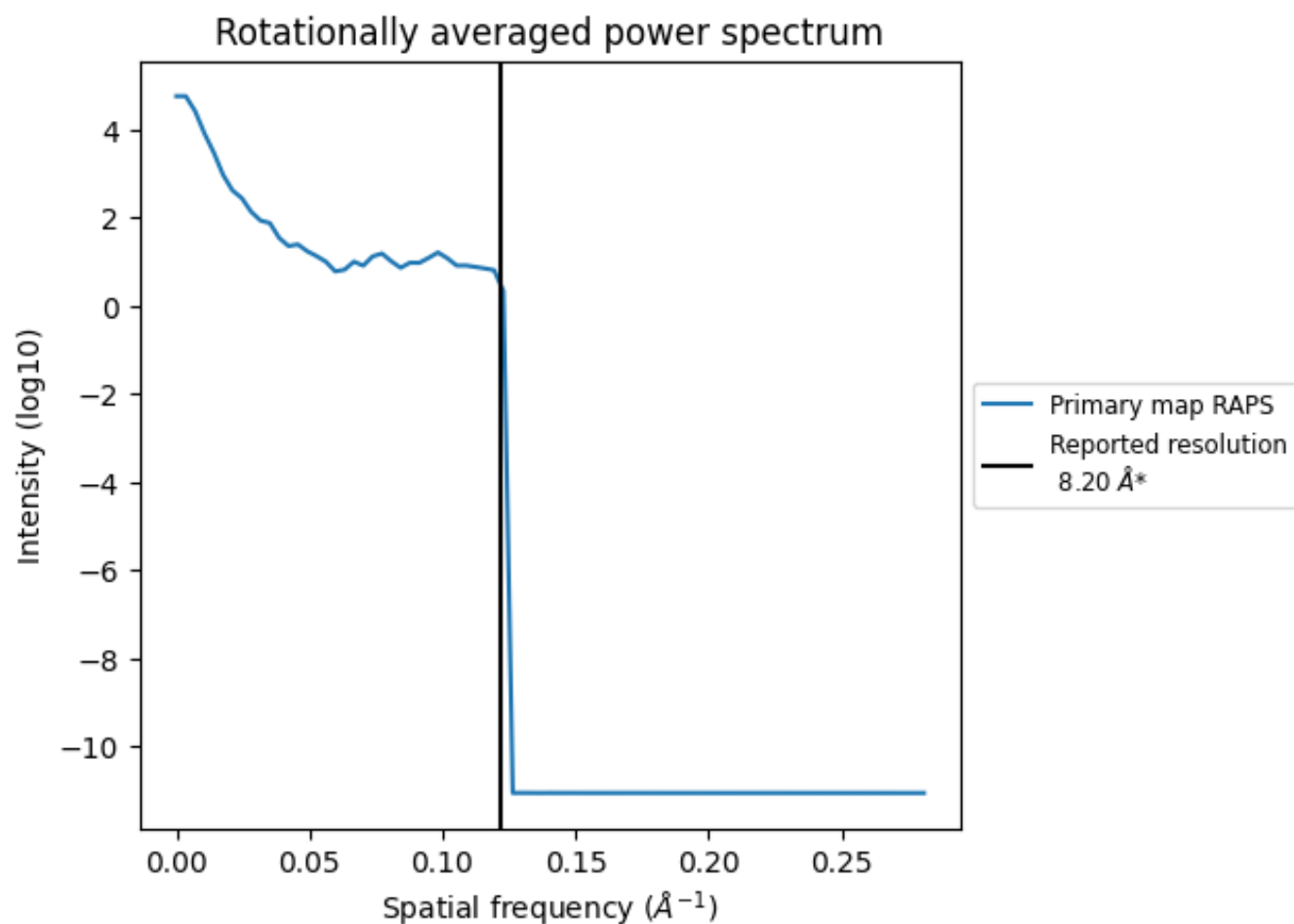
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 255 nm³; this corresponds to an approximate mass of 231 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 0.122 Å⁻¹

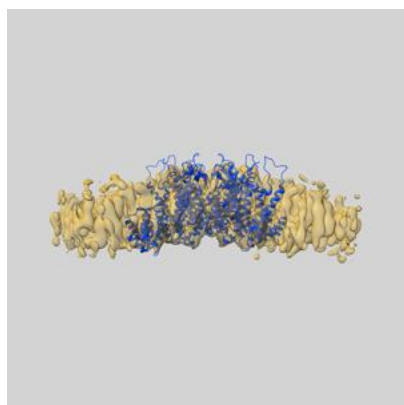
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

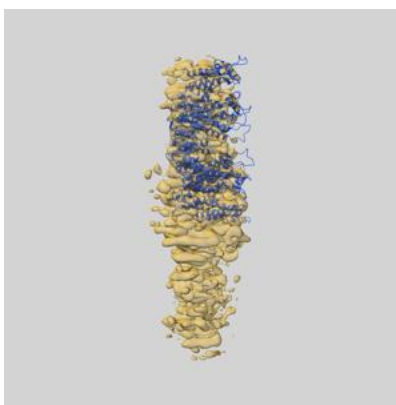
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3469 and PDB model 5MD1. Per-residue inclusion information can be found in section 3 on page 5.

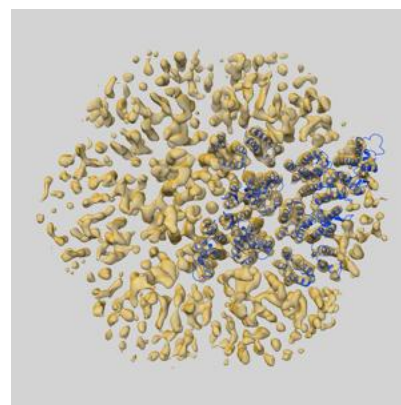
9.1 Map-model overlay [i](#)



X



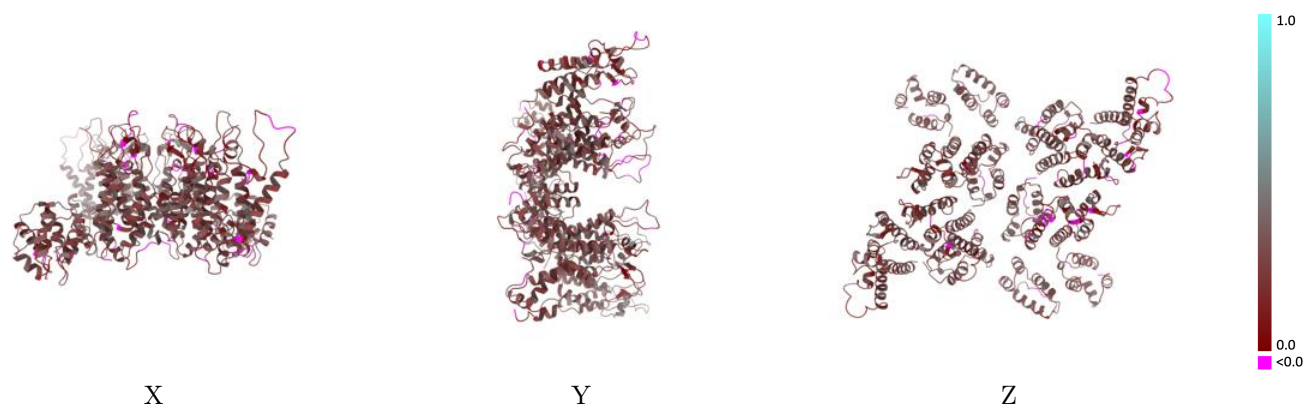
Y



Z

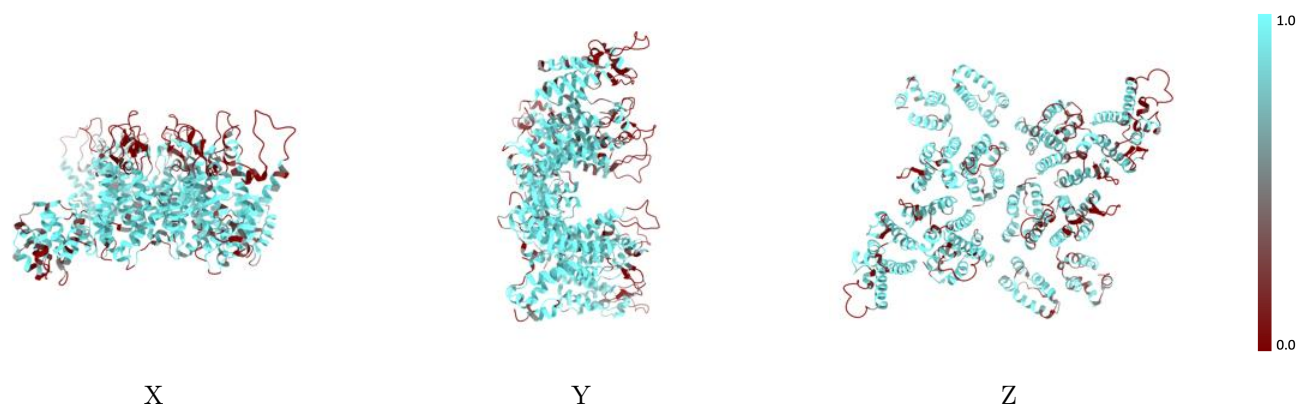
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



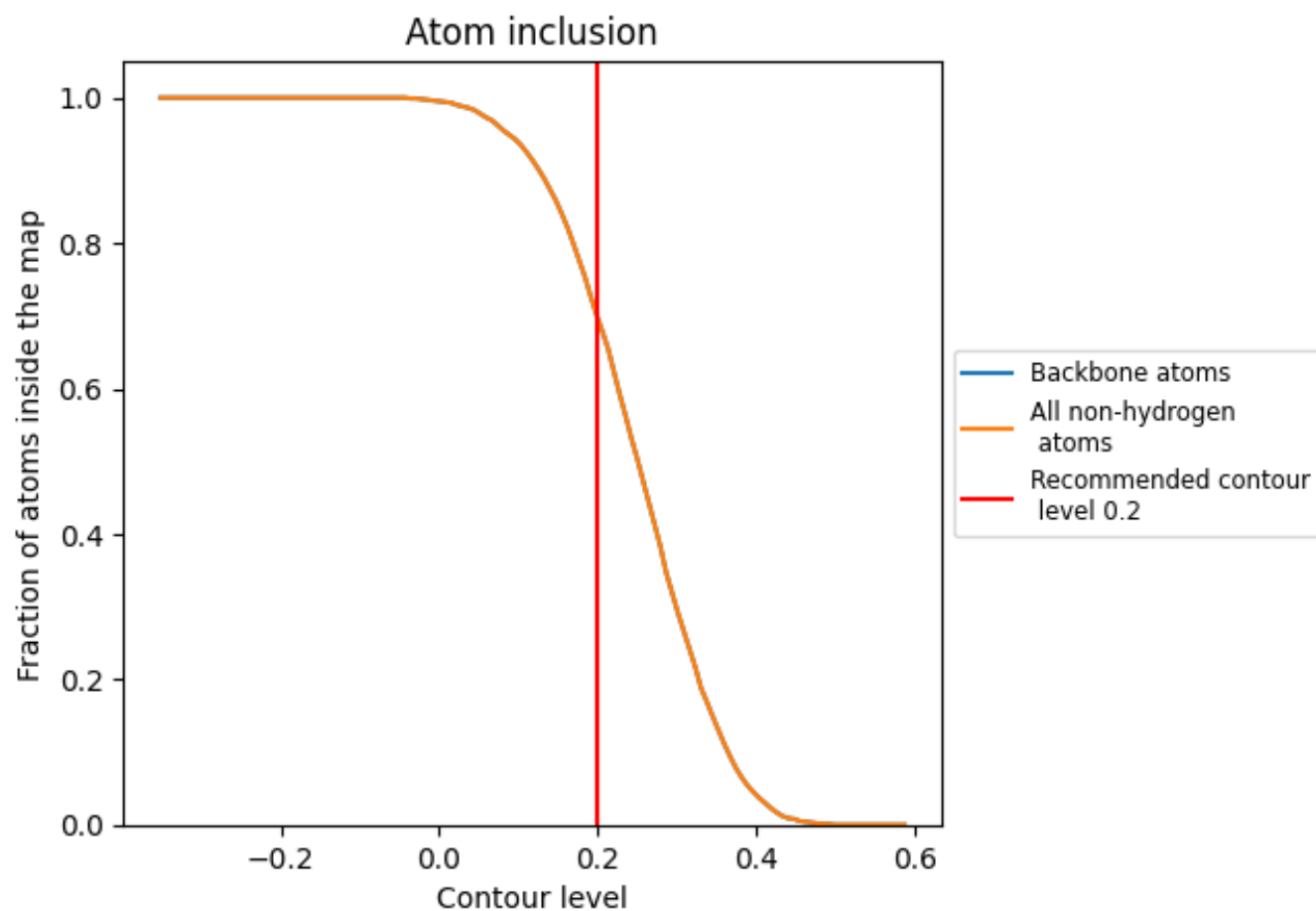
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 70% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6970	 0.2540
A	 0.8370	 0.2690
B	 0.8610	 0.2810
C	 0.8170	 0.2590
D	 0.7460	 0.2630
E	 0.5320	 0.2470
F	 0.8340	 0.2670
G	 0.7050	 0.2520
H	 0.6140	 0.2460
I	 0.5240	 0.2110
J	 0.5460	 0.2200
W	 0.8410	 0.2770
a	 0.7230	 0.2710
b	 0.7450	 0.2740
f	 0.7330	 0.2610

