



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 10:41 AM UTC

PDB ID : 6R24 / pdb_00006r24
EMDB ID : EMD-4709
Title : The structure of a Ty3 retrotransposon icosahedral capsid
Authors : Dodonova, S.O.; Prinz, S.; Bilanchone, V.; Sandmeyer, S.; Briggs, J.A.G.
Deposited on : 2019-03-15
Resolution : 7.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

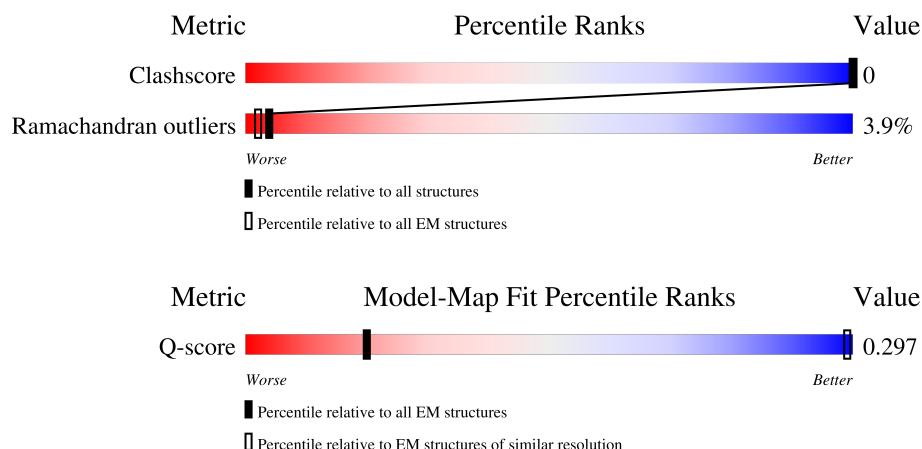
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 7.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	436 (7.00 - 8.00)

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	309	 6% 27% 24% 49%
1	B	309	 25% 24% 50%
1	C	309	 24% 26% 49%
1	D	309	 24% 27% 49%
1	E	309	 26% 25% 49%

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Mol	Chain	Length	Quality of chain
1	F	309	25%24%50%
1	G	309	25%26%49%
1	H	309	25%24%50%
1	I	309	25%26%49%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5676 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.

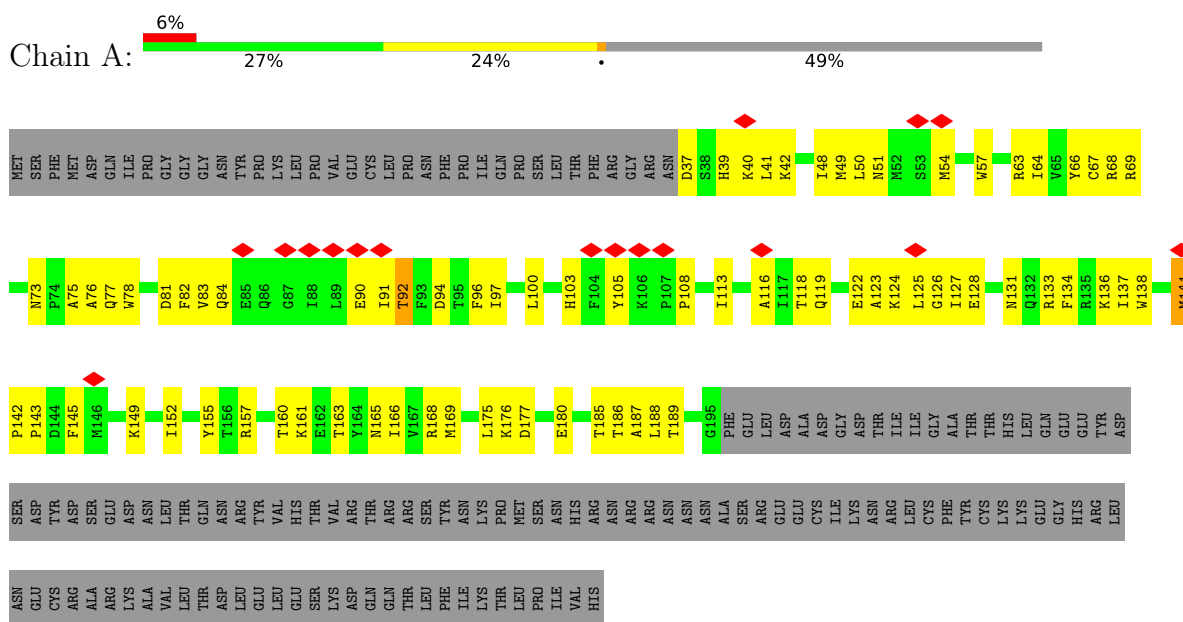
- Molecule 1 is a protein called Transposon Ty3-I Gag-Pol polyprotein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	159	Total 636	C 318	N 159	O 159	0	0
1	B	155	Total 620	C 310	N 155	O 155	0	0
1	C	159	Total 636	C 318	N 159	O 159	0	0
1	D	159	Total 636	C 318	N 159	O 159	0	0
1	E	159	Total 636	C 318	N 159	O 159	0	0
1	F	155	Total 620	C 310	N 155	O 155	0	0
1	G	159	Total 636	C 318	N 159	O 159	0	0
1	H	155	Total 620	C 310	N 155	O 155	0	0
1	I	159	Total 636	C 318	N 159	O 159	0	0

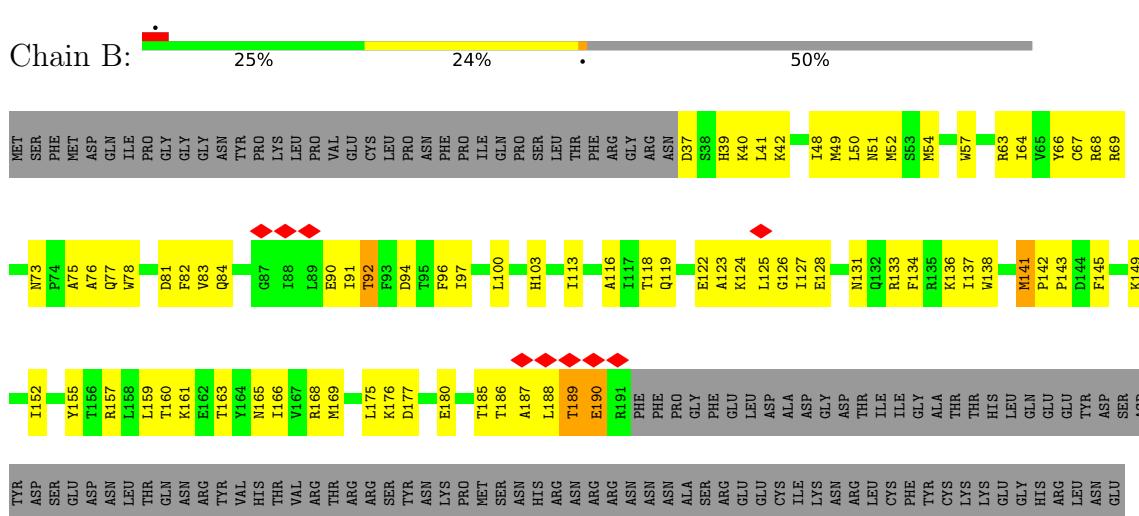
3 Residue-property plots

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

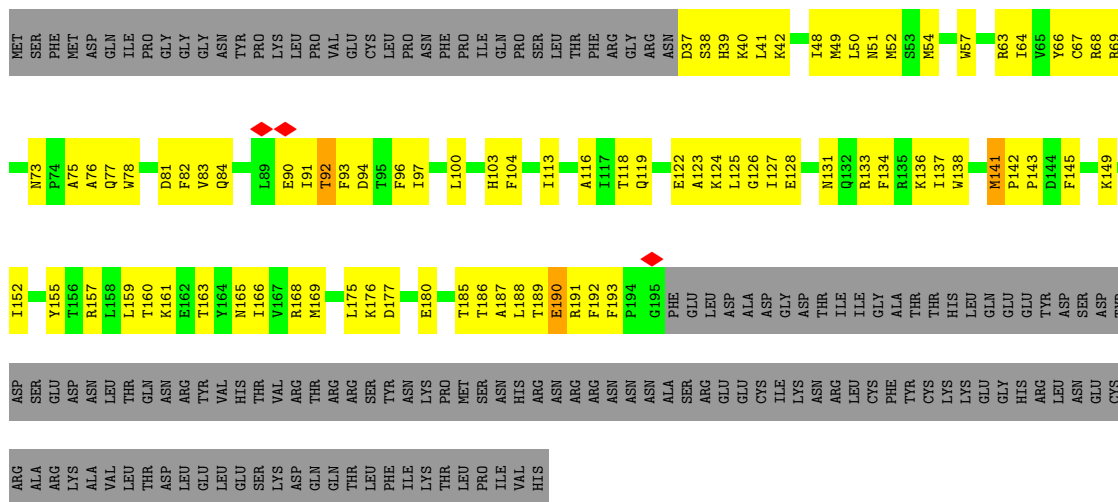
• Molecule 1: Transposon Ty3-I Gag-Pol polyprotein



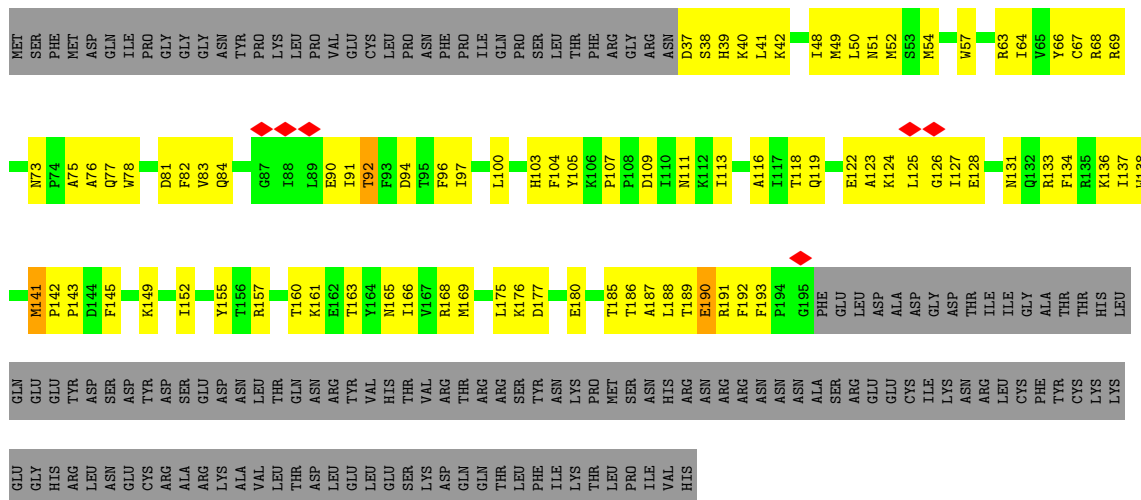
• Molecule 1: Transposon Ty3-I Gag-Pol polyprotein



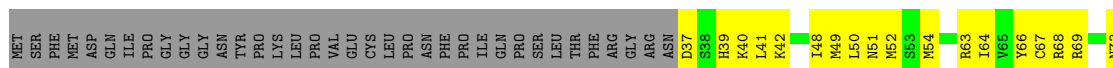
Chain C:



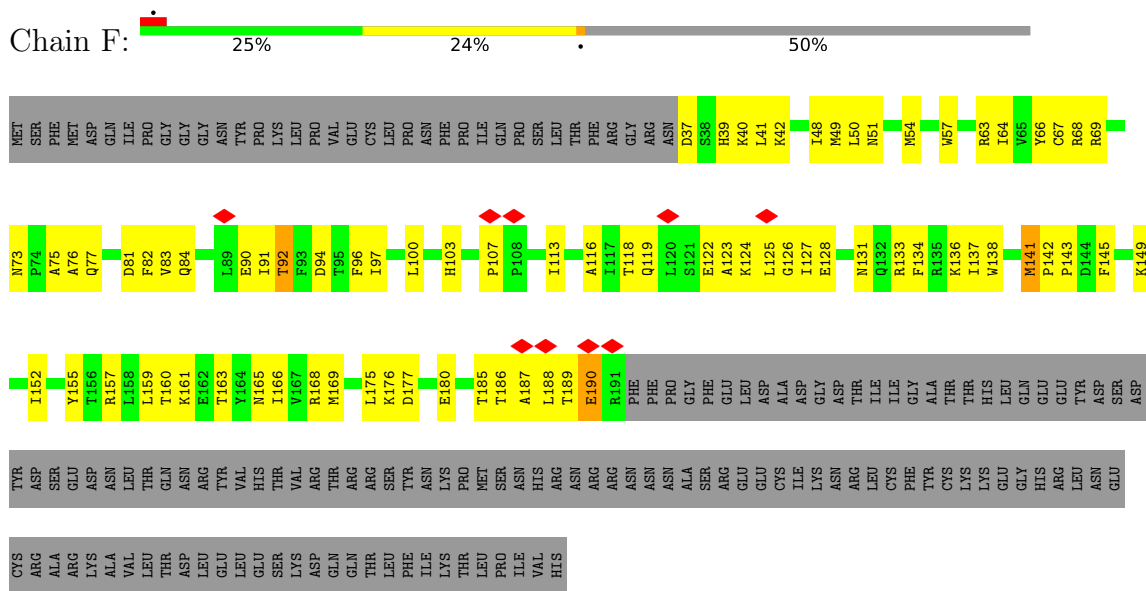
Chain D:



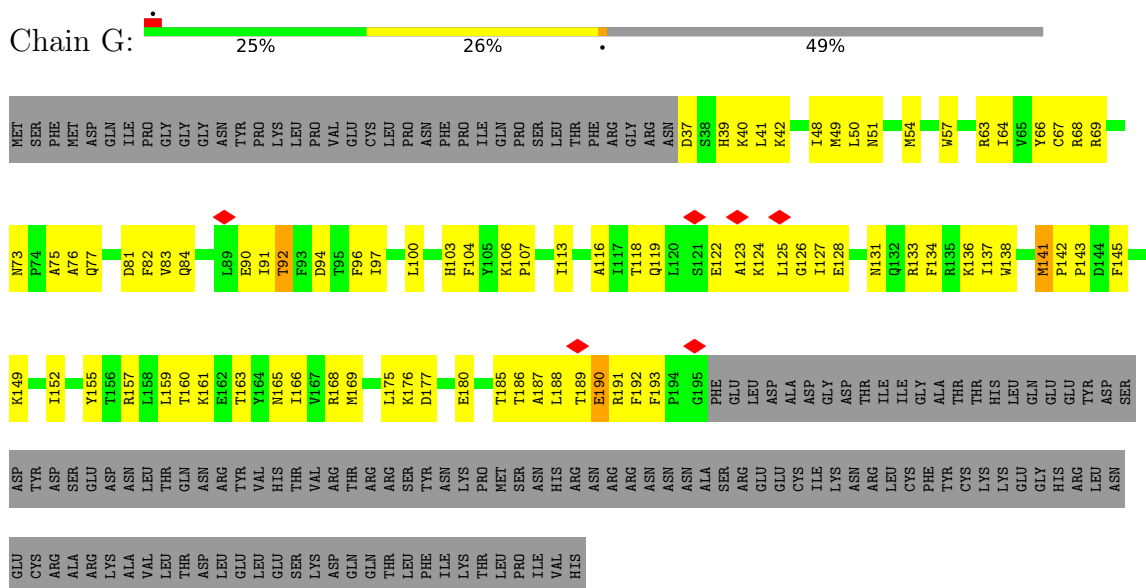
Chain E:



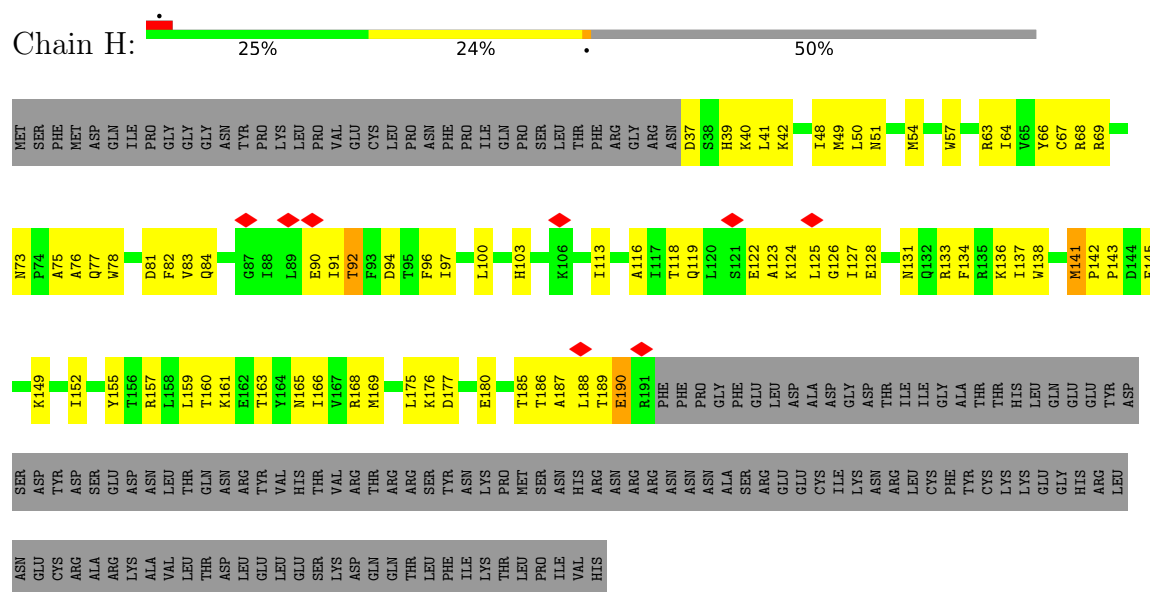
- Molecule 1: Transposon Ty3-I Gag-Pol polyprotein



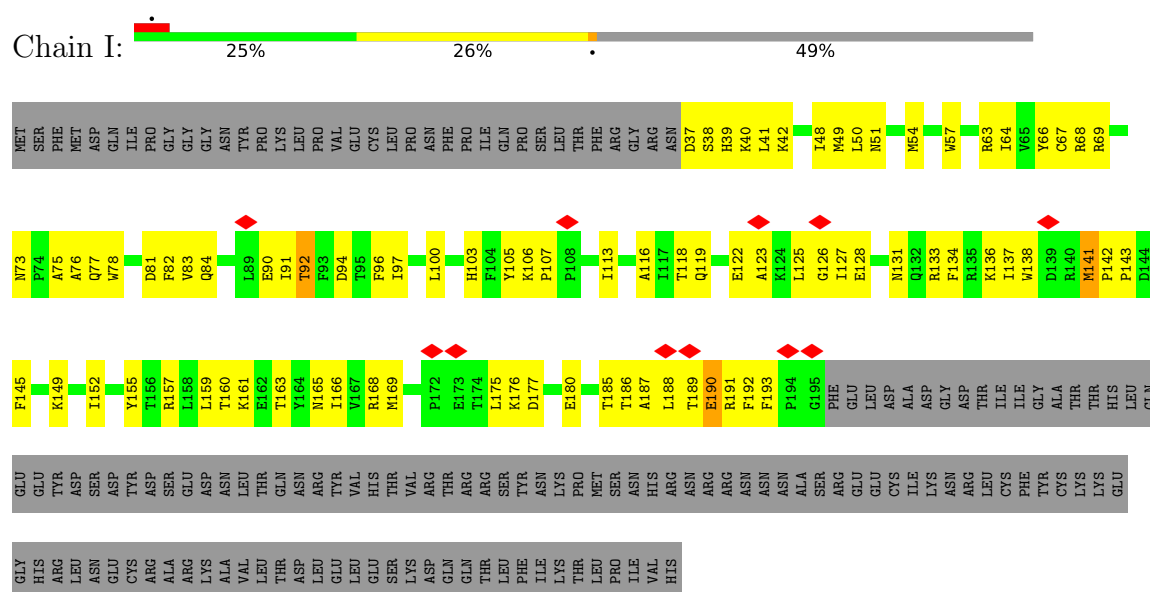
- Molecule 1: Transposon Ty3-I Gag-Pol polyprotein



• Molecule 1: Transposon Ty3-I Gag-Pol polyprotein



• Molecule 1: Transposon Ty3-I Gag-Pol polyprotein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	1236	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.041	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	648.0, 648.0, 648.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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	2.55	38/635 (6.0%)	3.03	85/792 (10.7%)
1	B	2.56	38/619 (6.1%)	3.04	84/772 (10.9%)
1	C	2.58	41/635 (6.5%)	3.13	99/792 (12.5%)
1	D	2.63	41/635 (6.5%)	3.15	97/792 (12.2%)
1	E	2.63	40/635 (6.3%)	3.12	95/792 (12.0%)
1	F	2.63	40/619 (6.5%)	3.07	87/772 (11.3%)
1	G	2.65	40/635 (6.3%)	3.16	97/792 (12.2%)
1	H	2.64	38/619 (6.1%)	3.09	87/772 (11.3%)
1	I	2.63	40/635 (6.3%)	3.12	98/792 (12.4%)
All	All	2.61	356/5667 (6.3%)	3.10	829/7068 (11.7%)

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	B	0	1

All (356) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	187	ALA	C-N	14.99	1.54	1.33
1	I	187	ALA	C-N	14.97	1.54	1.33
1	G	187	ALA	C-N	14.93	1.54	1.33
1	F	187	ALA	C-N	14.91	1.54	1.33
1	E	187	ALA	C-N	14.87	1.54	1.33
1	D	187	ALA	C-N	14.87	1.54	1.33
1	F	128	GLU	CA-C	-7.85	1.42	1.52
1	D	81	ASP	CA-C	-7.83	1.42	1.52
1	I	81	ASP	CA-C	-7.75	1.43	1.52
1	A	81	ASP	CA-C	-7.73	1.43	1.52
1	G	81	ASP	CA-C	-7.68	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	128	GLU	CA-C	-7.67	1.42	1.52
1	E	128	GLU	CA-C	-7.67	1.42	1.52
1	C	81	ASP	CA-C	-7.67	1.43	1.52
1	H	81	ASP	CA-C	-7.65	1.43	1.52
1	B	81	ASP	CA-C	-7.64	1.43	1.52
1	G	128	GLU	CA-C	-7.63	1.42	1.52
1	A	128	GLU	CA-C	-7.61	1.42	1.52
1	I	128	GLU	CA-C	-7.60	1.43	1.52
1	C	128	GLU	CA-C	-7.59	1.43	1.52
1	F	81	ASP	CA-C	-7.58	1.43	1.52
1	I	131	ASN	N-CA	-7.58	1.37	1.46
1	D	128	GLU	CA-C	-7.57	1.43	1.52
1	H	128	GLU	CA-C	-7.53	1.43	1.52
1	E	81	ASP	CA-C	-7.53	1.43	1.52
1	D	131	ASN	N-CA	-7.51	1.37	1.46
1	H	131	ASN	N-CA	-7.50	1.37	1.46
1	F	131	ASN	N-CA	-7.49	1.37	1.46
1	C	131	ASN	N-CA	-7.40	1.37	1.46
1	B	131	ASN	N-CA	-7.40	1.37	1.46
1	E	131	ASN	N-CA	-7.39	1.37	1.46
1	A	131	ASN	N-CA	-7.39	1.37	1.46
1	G	131	ASN	N-CA	-7.35	1.37	1.46
1	H	39	HIS	CA-C	-7.03	1.43	1.52
1	D	39	HIS	CA-C	-6.94	1.44	1.52
1	B	39	HIS	CA-C	-6.92	1.44	1.52
1	F	39	HIS	CA-C	-6.89	1.44	1.52
1	C	39	HIS	CA-C	-6.86	1.44	1.52
1	I	39	HIS	CA-C	-6.86	1.44	1.52
1	A	39	HIS	CA-C	-6.85	1.44	1.52
1	G	39	HIS	CA-C	-6.84	1.44	1.52
1	E	39	HIS	CA-C	-6.77	1.44	1.52
1	A	90	GLU	CA-C	-6.74	1.44	1.52
1	G	90	GLU	CA-C	-6.69	1.44	1.52
1	H	90	GLU	CA-C	-6.68	1.44	1.52
1	F	90	GLU	CA-C	-6.63	1.44	1.52
1	B	90	GLU	CA-C	-6.62	1.44	1.52
1	C	90	GLU	CA-C	-6.61	1.44	1.52
1	A	69	ARG	CA-C	-6.60	1.44	1.52
1	D	90	GLU	CA-C	-6.57	1.44	1.52
1	C	69	ARG	CA-C	-6.56	1.44	1.52
1	E	90	GLU	CA-C	-6.55	1.44	1.52
1	H	69	ARG	CA-C	-6.55	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	83	VAL	C-N	6.54	1.42	1.33
1	A	83	VAL	C-N	6.54	1.42	1.33
1	C	83	VAL	C-N	6.54	1.42	1.33
1	H	83	VAL	C-N	6.54	1.42	1.33
1	E	180	GLU	N-CA	-6.53	1.38	1.46
1	D	69	ARG	CA-C	-6.53	1.44	1.52
1	I	180	GLU	N-CA	-6.53	1.38	1.46
1	E	83	VAL	C-N	6.52	1.42	1.33
1	I	69	ARG	CA-C	-6.52	1.44	1.52
1	B	69	ARG	CA-C	-6.51	1.44	1.52
1	F	69	ARG	CA-C	-6.50	1.44	1.52
1	I	83	VAL	C-N	6.50	1.42	1.33
1	I	90	GLU	CA-C	-6.50	1.44	1.52
1	G	69	ARG	CA-C	-6.48	1.44	1.52
1	D	48	ILE	C-N	6.46	1.42	1.33
1	E	82	PHE	C-N	6.46	1.42	1.33
1	B	82	PHE	C-N	6.45	1.42	1.33
1	C	180	GLU	N-CA	-6.45	1.38	1.46
1	H	180	GLU	N-CA	-6.45	1.38	1.46
1	G	83	VAL	C-N	6.45	1.42	1.33
1	F	180	GLU	N-CA	-6.44	1.38	1.46
1	E	69	ARG	CA-C	-6.44	1.44	1.52
1	E	48	ILE	C-N	6.44	1.42	1.33
1	G	82	PHE	C-N	6.41	1.41	1.33
1	B	180	GLU	N-CA	-6.40	1.38	1.46
1	A	48	ILE	C-N	6.39	1.42	1.33
1	H	82	PHE	C-N	6.39	1.41	1.33
1	C	82	PHE	C-N	6.39	1.41	1.33
1	F	83	VAL	C-N	6.39	1.42	1.33
1	G	180	GLU	N-CA	-6.37	1.38	1.46
1	A	180	GLU	N-CA	-6.36	1.38	1.46
1	D	83	VAL	C-N	6.35	1.42	1.33
1	B	48	ILE	C-N	6.35	1.42	1.33
1	G	48	ILE	C-N	6.35	1.42	1.33
1	D	82	PHE	C-N	6.34	1.41	1.33
1	F	48	ILE	C-N	6.33	1.42	1.33
1	A	82	PHE	C-N	6.33	1.41	1.33
1	C	48	ILE	C-N	6.33	1.42	1.33
1	F	82	PHE	C-N	6.30	1.41	1.33
1	G	51	ASN	C-N	6.30	1.41	1.33
1	F	51	ASN	CA-C	-6.27	1.44	1.52
1	F	100	LEU	N-CA	6.27	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	48	ILE	C-N	6.26	1.41	1.33
1	C	51	ASN	C-N	6.25	1.41	1.33
1	I	82	PHE	C-N	6.25	1.41	1.33
1	D	180	GLU	N-CA	-6.24	1.38	1.46
1	I	48	ILE	C-N	6.24	1.41	1.33
1	G	100	LEU	N-CA	6.23	1.53	1.46
1	D	100	LEU	N-CA	6.23	1.53	1.46
1	E	100	LEU	N-CA	6.20	1.53	1.46
1	D	188	LEU	C-N	6.20	1.40	1.33
1	D	51	ASN	C-N	6.17	1.41	1.33
1	I	100	LEU	N-CA	6.17	1.53	1.46
1	B	100	LEU	N-CA	6.17	1.53	1.46
1	A	51	ASN	C-N	6.16	1.41	1.33
1	I	188	LEU	C-N	6.16	1.40	1.33
1	H	188	LEU	C-N	6.16	1.40	1.33
1	H	100	LEU	N-CA	6.14	1.53	1.46
1	I	51	ASN	C-N	6.14	1.41	1.33
1	E	188	LEU	C-N	6.13	1.40	1.33
1	C	188	LEU	C-N	6.12	1.40	1.33
1	B	51	ASN	CA-C	-6.12	1.45	1.52
1	G	51	ASN	CA-C	-6.12	1.45	1.52
1	H	51	ASN	CA-C	-6.12	1.45	1.52
1	B	51	ASN	C-N	6.12	1.41	1.33
1	C	100	LEU	N-CA	6.11	1.53	1.46
1	D	161	LYS	N-CA	-6.10	1.39	1.46
1	F	51	ASN	C-N	6.09	1.41	1.33
1	A	100	LEU	N-CA	6.09	1.53	1.46
1	D	51	ASN	CA-C	-6.08	1.45	1.52
1	H	51	ASN	C-N	6.08	1.41	1.33
1	E	51	ASN	C-N	6.07	1.41	1.33
1	I	51	ASN	CA-C	-6.07	1.45	1.52
1	C	51	ASN	CA-C	-6.07	1.45	1.52
1	I	161	LYS	N-CA	-6.06	1.39	1.46
1	B	188	LEU	C-N	6.05	1.40	1.33
1	E	161	LYS	N-CA	-6.05	1.39	1.46
1	F	188	LEU	C-N	6.04	1.40	1.33
1	A	51	ASN	CA-C	-6.04	1.45	1.52
1	G	161	LYS	N-CA	-5.99	1.39	1.46
1	E	51	ASN	CA-C	-5.99	1.45	1.52
1	C	161	LYS	N-CA	-5.95	1.39	1.46
1	H	161	LYS	N-CA	-5.95	1.39	1.46
1	G	188	LEU	C-N	5.92	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	LYS	N-CA	-5.91	1.39	1.46
1	F	161	LYS	N-CA	-5.91	1.39	1.46
1	D	113	ILE	N-CA	-5.85	1.39	1.46
1	E	113	ILE	N-CA	-5.85	1.39	1.46
1	B	161	LYS	N-CA	-5.83	1.39	1.46
1	H	152	ILE	C-O	-5.82	1.17	1.24
1	I	152	ILE	C-O	-5.81	1.17	1.24
1	F	76	ALA	C-N	5.80	1.41	1.33
1	E	152	ILE	C-O	-5.77	1.17	1.24
1	D	152	ILE	C-O	-5.77	1.17	1.24
1	A	152	ILE	C-O	-5.76	1.17	1.24
1	H	76	ALA	C-N	5.75	1.41	1.33
1	F	113	ILE	N-CA	-5.75	1.39	1.46
1	G	113	ILE	N-CA	-5.75	1.39	1.46
1	I	177	ASP	N-CA	-5.74	1.39	1.46
1	G	76	ALA	C-N	5.74	1.41	1.33
1	F	152	ILE	C-O	-5.74	1.17	1.24
1	C	152	ILE	C-O	-5.73	1.17	1.24
1	A	76	ALA	C-N	5.73	1.41	1.33
1	H	168	ARG	N-CA	-5.71	1.39	1.46
1	E	177	ASP	N-CA	-5.70	1.39	1.46
1	B	152	ILE	C-O	-5.70	1.17	1.24
1	D	76	ALA	C-N	5.70	1.41	1.33
1	B	113	ILE	N-CA	-5.69	1.40	1.46
1	G	152	ILE	C-O	-5.68	1.17	1.24
1	H	113	ILE	N-CA	-5.67	1.40	1.46
1	B	76	ALA	C-N	5.67	1.41	1.33
1	E	76	ALA	C-N	5.67	1.41	1.33
1	A	113	ILE	N-CA	-5.67	1.40	1.46
1	B	177	ASP	N-CA	-5.67	1.39	1.46
1	A	188	LEU	C-N	5.66	1.40	1.33
1	G	177	ASP	N-CA	-5.66	1.39	1.46
1	H	177	ASP	N-CA	-5.66	1.39	1.46
1	C	113	ILE	N-CA	-5.66	1.40	1.46
1	D	177	ASP	N-CA	-5.66	1.39	1.46
1	I	76	ALA	C-N	5.65	1.41	1.33
1	I	113	ILE	N-CA	-5.64	1.40	1.46
1	C	168	ARG	N-CA	-5.63	1.39	1.46
1	D	138	TRP	CA-C	-5.63	1.45	1.52
1	I	168	ARG	N-CA	-5.62	1.39	1.46
1	F	177	ASP	N-CA	-5.60	1.39	1.46
1	A	168	ARG	N-CA	-5.60	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	138	TRP	CA-C	-5.59	1.45	1.52
1	C	76	ALA	C-N	5.58	1.41	1.33
1	D	168	ARG	N-CA	-5.58	1.39	1.46
1	A	177	ASP	N-CA	-5.58	1.39	1.46
1	F	138	TRP	CA-C	-5.58	1.45	1.52
1	B	168	ARG	N-CA	-5.57	1.39	1.46
1	C	163	THR	C-N	5.56	1.41	1.33
1	H	77	GLN	N-CA	-5.56	1.39	1.46
1	H	138	TRP	CA-C	-5.55	1.45	1.52
1	C	189	THR	C-N	5.55	1.41	1.33
1	C	90	GLU	N-CA	-5.55	1.39	1.46
1	C	177	ASP	N-CA	-5.52	1.39	1.46
1	H	155	TYR	N-CA	-5.52	1.39	1.46
1	E	163	THR	C-N	5.51	1.41	1.33
1	D	155	TYR	N-CA	-5.51	1.39	1.46
1	I	73	ASN	C-N	-5.51	1.26	1.34
1	B	163	THR	C-N	5.50	1.41	1.33
1	F	168	ARG	N-CA	-5.50	1.39	1.46
1	G	168	ARG	N-CA	-5.50	1.39	1.46
1	G	138	TRP	CA-C	-5.50	1.46	1.52
1	E	138	TRP	CA-C	-5.50	1.46	1.52
1	E	168	ARG	N-CA	-5.49	1.39	1.46
1	G	163	THR	C-N	5.48	1.41	1.33
1	A	188	LEU	N-CA	-5.47	1.39	1.46
1	I	189	THR	C-N	5.47	1.41	1.33
1	C	138	TRP	CA-C	-5.46	1.46	1.52
1	F	77	GLN	N-CA	-5.46	1.39	1.46
1	I	63	ARG	N-CA	-5.46	1.39	1.46
1	B	90	GLU	N-CA	-5.45	1.39	1.46
1	C	192	PHE	C-N	5.45	1.39	1.33
1	F	73	ASN	C-N	-5.45	1.26	1.34
1	C	91	ILE	CA-C	-5.44	1.45	1.52
1	F	163	THR	C-N	5.44	1.41	1.33
1	F	90	GLU	N-CA	-5.44	1.39	1.46
1	G	73	ASN	C-N	-5.44	1.26	1.34
1	G	189	THR	C-N	5.44	1.41	1.33
1	A	77	GLN	N-CA	-5.44	1.40	1.46
1	C	155	TYR	N-CA	-5.44	1.39	1.46
1	B	138	TRP	CA-C	-5.43	1.46	1.52
1	E	155	TYR	N-CA	-5.42	1.39	1.46
1	F	189	THR	C-N	5.42	1.41	1.33
1	H	163	THR	C-N	5.42	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	PHE	C-N	5.41	1.41	1.33
1	F	91	ILE	CA-C	-5.41	1.45	1.52
1	I	163	THR	C-N	5.41	1.41	1.33
1	B	77	GLN	N-CA	-5.41	1.40	1.46
1	A	73	ASN	C-N	-5.40	1.26	1.34
1	G	155	TYR	N-CA	-5.40	1.39	1.46
1	B	91	ILE	CA-C	-5.40	1.45	1.52
1	A	163	THR	C-N	5.40	1.41	1.33
1	G	77	GLN	N-CA	-5.40	1.40	1.46
1	F	155	TYR	N-CA	-5.39	1.39	1.46
1	E	189	THR	C-N	5.39	1.41	1.33
1	B	155	TYR	N-CA	-5.38	1.39	1.46
1	F	188	LEU	N-CA	-5.38	1.39	1.46
1	I	155	TYR	N-CA	-5.38	1.39	1.46
1	D	192	PHE	C-N	5.38	1.39	1.33
1	H	189	THR	C-N	5.37	1.41	1.33
1	I	77	GLN	N-CA	-5.37	1.40	1.46
1	E	73	ASN	C-N	-5.37	1.26	1.34
1	C	77	GLN	N-CA	-5.37	1.40	1.46
1	E	91	ILE	CA-C	-5.36	1.45	1.52
1	H	73	ASN	C-N	-5.36	1.26	1.34
1	A	138	TRP	CA-C	-5.35	1.46	1.52
1	E	63	ARG	N-CA	-5.35	1.39	1.46
1	A	155	TYR	N-CA	-5.35	1.39	1.46
1	D	189	THR	C-N	5.34	1.41	1.33
1	I	91	ILE	CA-C	-5.34	1.45	1.52
1	G	192	PHE	C-N	5.34	1.39	1.33
1	G	134	PHE	C-N	5.34	1.41	1.33
1	D	91	ILE	CA-C	-5.34	1.45	1.52
1	E	134	PHE	C-N	5.34	1.41	1.33
1	I	192	PHE	C-N	5.33	1.39	1.33
1	D	73	ASN	C-N	-5.33	1.26	1.34
1	D	77	GLN	N-CA	-5.33	1.40	1.46
1	A	63	ARG	N-CA	-5.33	1.39	1.46
1	E	77	GLN	N-CA	-5.33	1.40	1.46
1	H	63	ARG	N-CA	-5.33	1.39	1.46
1	G	91	ILE	CA-C	-5.33	1.45	1.52
1	E	192	PHE	C-N	5.32	1.39	1.33
1	C	188	LEU	N-CA	-5.32	1.40	1.46
1	C	73	ASN	C-N	-5.32	1.26	1.34
1	H	91	ILE	CA-C	-5.31	1.45	1.52
1	I	90	GLU	N-CA	-5.31	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	63	ARG	N-CA	-5.30	1.39	1.46
1	E	90	GLU	N-CA	-5.29	1.40	1.46
1	F	134	PHE	C-N	5.29	1.40	1.33
1	B	134	PHE	C-N	5.29	1.40	1.33
1	I	188	LEU	N-CA	-5.29	1.39	1.46
1	B	68	ARG	N-CA	-5.29	1.40	1.46
1	B	73	ASN	C-N	-5.29	1.26	1.34
1	I	134	PHE	C-N	5.28	1.40	1.33
1	C	68	ARG	N-CA	-5.28	1.40	1.46
1	H	188	LEU	N-CA	-5.27	1.39	1.46
1	B	188	LEU	N-CA	-5.26	1.40	1.46
1	F	124	LYS	CA-C	-5.26	1.45	1.52
1	B	187	ALA	C-N	5.26	1.40	1.33
1	H	134	PHE	C-N	5.26	1.40	1.33
1	B	127	ILE	CA-C	-5.25	1.46	1.52
1	I	68	ARG	N-CA	-5.25	1.40	1.46
1	H	90	GLU	N-CA	-5.25	1.40	1.46
1	B	63	ARG	N-CA	-5.25	1.40	1.46
1	G	188	LEU	N-CA	-5.25	1.40	1.46
1	A	90	GLU	N-CA	-5.24	1.40	1.46
1	C	63	ARG	N-CA	-5.24	1.40	1.46
1	A	91	ILE	CA-C	-5.24	1.46	1.52
1	H	131	ASN	C-N	5.24	1.41	1.33
1	A	187	ALA	C-N	5.24	1.40	1.33
1	G	90	GLU	N-CA	-5.23	1.40	1.46
1	D	68	ARG	N-CA	-5.23	1.40	1.46
1	F	63	ARG	N-CA	-5.22	1.40	1.46
1	H	68	ARG	N-CA	-5.22	1.40	1.46
1	D	188	LEU	N-CA	-5.21	1.40	1.46
1	G	127	ILE	CA-C	-5.21	1.46	1.52
1	I	127	ILE	CA-C	-5.21	1.46	1.52
1	A	68	ARG	N-CA	-5.21	1.40	1.46
1	C	124	LYS	CA-C	-5.21	1.45	1.52
1	D	90	GLU	N-CA	-5.21	1.40	1.46
1	F	50	LEU	CA-C	-5.20	1.46	1.52
1	F	68	ARG	N-CA	-5.20	1.40	1.46
1	E	127	ILE	CA-C	-5.19	1.46	1.52
1	F	57	TRP	CA-C	-5.19	1.46	1.52
1	C	127	ILE	CA-C	-5.19	1.46	1.52
1	A	127	ILE	CA-C	-5.18	1.46	1.52
1	C	134	PHE	C-N	5.18	1.40	1.33
1	I	50	LEU	CA-C	-5.18	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	127	ILE	CA-C	-5.18	1.46	1.52
1	D	163	THR	C-N	5.18	1.40	1.33
1	I	57	TRP	CA-C	-5.18	1.46	1.52
1	D	57	TRP	CA-C	-5.17	1.46	1.52
1	D	96	PHE	C-N	5.17	1.40	1.33
1	D	134	PHE	C-N	5.17	1.40	1.33
1	A	96	PHE	C-N	5.17	1.40	1.33
1	C	159	LEU	C-N	5.17	1.40	1.33
1	G	68	ARG	N-CA	-5.17	1.40	1.46
1	A	124	LYS	CA-C	-5.17	1.45	1.52
1	D	127	ILE	CA-C	-5.16	1.46	1.52
1	E	131	ASN	C-N	5.16	1.41	1.33
1	D	124	LYS	CA-C	-5.15	1.46	1.52
1	G	57	TRP	CA-C	-5.15	1.46	1.52
1	E	68	ARG	N-CA	-5.15	1.40	1.46
1	C	187	ALA	C-N	5.14	1.40	1.33
1	F	96	PHE	C-N	5.14	1.40	1.33
1	D	63	ARG	N-CA	-5.13	1.40	1.46
1	B	124	LYS	CA-C	-5.12	1.46	1.52
1	B	50	LEU	CA-C	-5.12	1.46	1.52
1	G	159	LEU	C-N	5.11	1.40	1.33
1	A	131	ASN	C-N	5.11	1.40	1.33
1	B	57	TRP	CA-C	-5.10	1.46	1.52
1	G	131	ASN	C-N	5.10	1.40	1.33
1	H	57	TRP	CA-C	-5.10	1.46	1.52
1	C	57	TRP	CA-C	-5.10	1.46	1.52
1	H	124	LYS	CA-C	-5.09	1.46	1.52
1	B	159	LEU	C-N	5.09	1.40	1.33
1	E	96	PHE	C-N	5.08	1.40	1.33
1	E	50	LEU	CA-C	-5.08	1.46	1.52
1	I	131	ASN	C-N	5.07	1.40	1.33
1	C	50	LEU	CA-C	-5.07	1.46	1.52
1	H	159	LEU	C-N	5.07	1.40	1.33
1	A	57	TRP	CA-C	-5.06	1.46	1.52
1	D	52	MET	N-CA	-5.06	1.40	1.46
1	G	124	LYS	CA-C	-5.06	1.46	1.52
1	H	50	LEU	CA-C	-5.05	1.46	1.52
1	D	50	LEU	CA-C	-5.05	1.46	1.52
1	D	131	ASN	C-N	5.05	1.40	1.33
1	I	159	LEU	C-N	5.05	1.40	1.33
1	G	96	PHE	C-N	5.05	1.40	1.33
1	I	96	PHE	C-N	5.05	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	LEU	CA-C	-5.04	1.46	1.52
1	E	52	MET	N-CA	-5.04	1.40	1.46
1	C	52	MET	N-CA	-5.03	1.40	1.46
1	F	159	LEU	C-N	5.01	1.40	1.33
1	E	124	LYS	CA-C	-5.01	1.46	1.52
1	F	131	ASN	C-N	5.00	1.40	1.33
1	B	52	MET	N-CA	-5.00	1.40	1.46
1	C	131	ASN	C-N	5.00	1.40	1.33
1	E	188	LEU	N-CA	-5.00	1.40	1.46

All (829) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	191	ARG	CA-C-N	10.23	139.00	122.53
1	D	191	ARG	C-N-CA	10.23	139.00	122.53
1	I	191	ARG	CA-C-N	10.19	138.94	122.53
1	I	191	ARG	C-N-CA	10.19	138.94	122.53
1	E	191	ARG	CA-C-N	10.19	138.93	122.53
1	E	191	ARG	C-N-CA	10.19	138.93	122.53
1	C	191	ARG	CA-C-N	10.18	138.92	122.53
1	C	191	ARG	C-N-CA	10.18	138.92	122.53
1	G	191	ARG	CA-C-N	10.16	138.89	122.53
1	G	191	ARG	C-N-CA	10.16	138.89	122.53
1	C	67	CYS	CA-C-N	10.12	133.85	120.28
1	C	67	CYS	C-N-CA	10.12	133.85	120.28
1	H	67	CYS	CA-C-N	10.12	133.84	120.28
1	H	67	CYS	C-N-CA	10.12	133.84	120.28
1	E	67	CYS	CA-C-N	10.11	133.83	120.28
1	E	67	CYS	C-N-CA	10.11	133.83	120.28
1	G	67	CYS	CA-C-N	10.10	133.81	120.28
1	G	67	CYS	C-N-CA	10.10	133.81	120.28
1	B	67	CYS	CA-C-N	10.08	133.79	120.28
1	B	67	CYS	C-N-CA	10.08	133.79	120.28
1	D	67	CYS	CA-C-N	10.04	133.74	120.28
1	D	67	CYS	C-N-CA	10.04	133.74	120.28
1	I	67	CYS	CA-C-N	10.04	133.73	120.28
1	I	67	CYS	C-N-CA	10.04	133.73	120.28
1	F	67	CYS	CA-C-N	10.03	133.72	120.28
1	F	67	CYS	C-N-CA	10.03	133.72	120.28
1	A	67	CYS	CA-C-N	10.01	133.69	120.28
1	A	67	CYS	C-N-CA	10.01	133.69	120.28
1	I	189	THR	CA-C-N	8.78	138.31	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	189	THR	C-N-CA	8.78	138.31	121.54
1	G	189	THR	CA-C-N	8.76	138.28	121.54
1	G	189	THR	C-N-CA	8.76	138.28	121.54
1	E	189	THR	CA-C-N	8.74	138.24	121.54
1	E	189	THR	C-N-CA	8.74	138.24	121.54
1	C	189	THR	CA-C-N	8.74	138.23	121.54
1	C	189	THR	C-N-CA	8.74	138.23	121.54
1	H	189	THR	CA-C-N	8.73	138.22	121.54
1	H	189	THR	C-N-CA	8.73	138.22	121.54
1	D	37	ASP	CA-C-N	8.72	131.78	120.44
1	D	37	ASP	C-N-CA	8.72	131.78	120.44
1	D	189	THR	CA-C-N	8.71	138.17	121.54
1	D	189	THR	C-N-CA	8.71	138.17	121.54
1	F	189	THR	CA-C-N	8.71	138.17	121.54
1	F	189	THR	C-N-CA	8.71	138.17	121.54
1	C	37	ASP	CA-C-N	8.68	131.73	120.44
1	C	37	ASP	C-N-CA	8.68	131.73	120.44
1	H	37	ASP	CA-C-N	8.68	131.72	120.44
1	H	37	ASP	C-N-CA	8.68	131.72	120.44
1	I	37	ASP	CA-C-N	8.68	131.73	120.44
1	I	37	ASP	C-N-CA	8.68	131.73	120.44
1	B	37	ASP	CA-C-N	8.67	131.71	120.44
1	B	37	ASP	C-N-CA	8.67	131.71	120.44
1	A	37	ASP	CA-C-N	8.65	131.68	120.44
1	A	37	ASP	C-N-CA	8.65	131.68	120.44
1	E	37	ASP	CA-C-N	8.64	131.68	120.44
1	E	37	ASP	C-N-CA	8.64	131.68	120.44
1	G	37	ASP	CA-C-N	8.64	131.67	120.44
1	G	37	ASP	C-N-CA	8.64	131.67	120.44
1	F	37	ASP	CA-C-N	8.59	131.61	120.44
1	F	37	ASP	C-N-CA	8.59	131.61	120.44
1	E	141	MET	O-C-N	-8.34	111.72	121.32
1	B	141	MET	O-C-N	-8.31	111.77	121.32
1	H	141	MET	O-C-N	-8.30	111.77	121.32
1	C	141	MET	O-C-N	-8.30	111.78	121.32
1	A	141	MET	O-C-N	-8.29	111.79	121.32
1	D	141	MET	O-C-N	-8.29	111.79	121.32
1	G	141	MET	O-C-N	-8.28	111.80	121.32
1	I	141	MET	O-C-N	-8.27	111.81	121.32
1	F	141	MET	O-C-N	-8.22	111.87	121.32
1	H	116	ALA	CA-C-N	8.01	130.65	120.56
1	H	116	ALA	C-N-CA	8.01	130.65	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	116	ALA	CA-C-N	8.00	130.65	120.56
1	D	116	ALA	C-N-CA	8.00	130.65	120.56
1	C	116	ALA	CA-C-N	7.98	130.61	120.56
1	C	116	ALA	C-N-CA	7.98	130.61	120.56
1	F	116	ALA	CA-C-N	7.97	130.61	120.56
1	F	116	ALA	C-N-CA	7.97	130.61	120.56
1	E	116	ALA	CA-C-N	7.95	130.57	120.56
1	E	116	ALA	C-N-CA	7.95	130.57	120.56
1	G	116	ALA	CA-C-N	7.94	130.56	120.56
1	G	116	ALA	C-N-CA	7.94	130.56	120.56
1	I	116	ALA	CA-C-N	7.94	130.56	120.56
1	I	116	ALA	C-N-CA	7.94	130.56	120.56
1	A	116	ALA	CA-C-N	7.93	130.56	120.56
1	A	116	ALA	C-N-CA	7.93	130.56	120.56
1	B	116	ALA	CA-C-N	7.92	130.54	120.56
1	B	116	ALA	C-N-CA	7.92	130.54	120.56
1	A	91	ILE	N-CA-C	-7.92	96.05	107.77
1	G	91	ILE	N-CA-C	-7.92	96.05	107.77
1	H	91	ILE	N-CA-C	-7.92	96.05	107.77
1	E	91	ILE	N-CA-C	-7.92	96.05	107.77
1	D	91	ILE	N-CA-C	-7.91	96.07	107.77
1	B	91	ILE	N-CA-C	-7.89	96.09	107.77
1	I	91	ILE	N-CA-C	-7.89	96.10	107.77
1	C	91	ILE	N-CA-C	-7.86	96.14	107.77
1	F	91	ILE	N-CA-C	-7.84	96.17	107.77
1	F	50	LEU	N-CA-C	7.75	119.36	111.07
1	A	50	LEU	N-CA-C	7.75	119.36	111.07
1	D	50	LEU	N-CA-C	7.75	119.36	111.07
1	I	50	LEU	N-CA-C	7.73	119.34	111.07
1	H	97	ILE	CA-C-O	-7.72	112.92	120.95
1	D	97	ILE	CA-C-O	-7.72	112.92	120.95
1	F	97	ILE	CA-C-O	-7.71	112.93	120.95
1	I	97	ILE	CA-C-O	-7.69	112.96	120.95
1	B	50	LEU	N-CA-C	7.67	119.28	111.07
1	F	49	MET	O-C-N	-7.67	114.17	122.07
1	E	50	LEU	N-CA-C	7.64	119.25	111.07
1	B	97	ILE	CA-C-O	-7.63	113.01	120.95
1	D	49	MET	O-C-N	-7.63	114.21	122.07
1	H	50	LEU	N-CA-C	7.62	119.22	111.07
1	G	50	LEU	N-CA-C	7.61	119.21	111.07
1	C	50	LEU	N-CA-C	7.60	119.20	111.07
1	A	97	ILE	CA-C-O	-7.59	113.05	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	193	PHE	N-CA-C	7.58	117.04	108.25
1	E	97	ILE	CA-C-O	-7.58	113.07	120.95
1	C	97	ILE	CA-C-O	-7.57	113.08	120.95
1	C	49	MET	O-C-N	-7.57	114.28	122.07
1	A	49	MET	O-C-N	-7.52	114.32	122.07
1	D	193	PHE	N-CA-C	7.51	116.96	108.25
1	G	49	MET	O-C-N	-7.51	114.34	122.07
1	E	165	ASN	N-CA-C	7.50	119.09	111.07
1	G	189	THR	N-CA-C	-7.49	98.48	109.11
1	G	193	PHE	N-CA-C	7.49	116.94	108.25
1	H	49	MET	O-C-N	-7.49	114.36	122.07
1	G	97	ILE	CA-C-O	-7.47	113.18	120.95
1	B	49	MET	O-C-N	-7.47	114.38	122.07
1	C	189	THR	N-CA-C	-7.47	98.50	109.11
1	C	193	PHE	N-CA-C	7.46	116.90	108.25
1	I	189	THR	N-CA-C	-7.45	98.53	109.11
1	I	193	PHE	N-CA-C	7.44	116.88	108.25
1	B	165	ASN	N-CA-C	7.43	119.02	111.07
1	I	49	MET	O-C-N	-7.42	114.42	122.07
1	D	165	ASN	N-CA-C	7.42	119.00	111.07
1	B	189	THR	N-CA-C	-7.40	98.60	109.11
1	G	165	ASN	N-CA-C	7.39	118.98	111.07
1	H	189	THR	N-CA-C	-7.39	98.61	109.11
1	D	189	THR	N-CA-C	-7.38	98.62	109.11
1	F	189	THR	N-CA-C	-7.38	98.63	109.11
1	E	49	MET	O-C-N	-7.38	114.47	122.07
1	I	165	ASN	N-CA-C	7.37	118.95	111.07
1	E	189	THR	N-CA-C	-7.36	98.66	109.11
1	C	165	ASN	N-CA-C	7.35	118.94	111.07
1	A	165	ASN	N-CA-C	7.33	118.91	111.07
1	F	165	ASN	N-CA-C	7.32	118.90	111.07
1	C	81	ASP	O-C-N	-7.32	114.53	122.07
1	H	165	ASN	N-CA-C	7.31	118.89	111.07
1	D	81	ASP	O-C-N	-7.29	114.56	122.07
1	H	81	ASP	O-C-N	-7.27	114.59	122.07
1	B	81	ASP	O-C-N	-7.26	114.59	122.07
1	A	81	ASP	O-C-N	-7.24	114.61	122.07
1	G	81	ASP	O-C-N	-7.22	114.63	122.07
1	D	119	GLN	CA-C-O	-7.20	112.86	120.63
1	F	81	ASP	O-C-N	-7.18	114.67	122.07
1	A	119	GLN	CA-C-O	-7.16	112.90	120.63
1	H	63	ARG	N-CA-C	7.16	119.16	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	GLN	CA-C-O	-7.16	112.90	120.63
1	I	119	GLN	CA-C-O	-7.15	112.91	120.63
1	H	119	GLN	CA-C-O	-7.13	112.93	120.63
1	C	119	GLN	CA-C-O	-7.13	112.93	120.63
1	F	119	GLN	CA-C-O	-7.13	112.93	120.63
1	E	81	ASP	O-C-N	-7.11	114.74	122.07
1	I	81	ASP	O-C-N	-7.11	114.74	122.07
1	G	137	ILE	N-CA-C	7.11	117.24	110.42
1	D	137	ILE	N-CA-C	7.10	117.24	110.42
1	C	63	ARG	N-CA-C	7.10	119.09	111.36
1	B	137	ILE	N-CA-C	7.09	117.23	110.42
1	G	119	GLN	CA-C-O	-7.09	112.98	120.63
1	E	119	GLN	CA-C-O	-7.08	112.98	120.63
1	F	63	ARG	N-CA-C	7.08	119.08	111.36
1	B	63	ARG	N-CA-C	7.05	119.04	111.36
1	I	63	ARG	N-CA-C	7.04	119.04	111.36
1	F	137	ILE	N-CA-C	7.03	117.16	110.42
1	A	63	ARG	N-CA-C	7.02	119.01	111.36
1	I	137	ILE	N-CA-C	7.00	117.14	110.42
1	C	137	ILE	N-CA-C	7.00	117.14	110.42
1	G	63	ARG	N-CA-C	7.00	118.99	111.36
1	D	109	ASP	N-CA-C	-6.99	97.02	108.41
1	D	63	ARG	N-CA-C	6.99	118.97	111.36
1	E	63	ARG	N-CA-C	6.98	118.97	111.36
1	F	100	LEU	CA-C-N	6.94	129.47	120.44
1	F	100	LEU	C-N-CA	6.94	129.47	120.44
1	A	137	ILE	N-CA-C	6.93	117.08	110.42
1	C	42	LYS	CA-C-O	-6.92	113.55	120.82
1	B	42	LYS	CA-C-O	-6.92	113.55	120.82
1	G	42	LYS	CA-C-O	-6.91	113.56	120.82
1	E	137	ILE	N-CA-C	6.89	117.03	110.42
1	B	100	LEU	CA-C-N	6.88	129.38	120.44
1	B	100	LEU	C-N-CA	6.88	129.38	120.44
1	H	100	LEU	CA-C-N	6.87	129.37	120.44
1	H	100	LEU	C-N-CA	6.87	129.37	120.44
1	E	42	LYS	CA-C-O	-6.87	113.61	120.82
1	H	42	LYS	CA-C-O	-6.85	113.62	120.82
1	H	137	ILE	N-CA-C	6.84	116.99	110.42
1	D	42	LYS	CA-C-O	-6.83	113.64	120.82
1	F	42	LYS	CA-C-O	-6.82	113.66	120.82
1	A	42	LYS	CA-C-O	-6.81	113.67	120.82
1	A	100	LEU	CA-C-N	6.77	129.35	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	LEU	C-N-CA	6.77	129.35	120.28
1	I	100	LEU	CA-C-N	6.75	129.22	120.44
1	I	100	LEU	C-N-CA	6.75	129.22	120.44
1	G	100	LEU	CA-C-N	6.74	129.31	120.28
1	G	100	LEU	C-N-CA	6.74	129.31	120.28
1	C	100	LEU	CA-C-N	6.74	129.31	120.28
1	C	100	LEU	C-N-CA	6.74	129.31	120.28
1	I	42	LYS	CA-C-O	-6.73	113.76	120.82
1	E	100	LEU	CA-C-N	6.71	129.27	120.28
1	E	100	LEU	C-N-CA	6.71	129.27	120.28
1	H	103	HIS	CA-C-O	-6.68	113.80	120.82
1	C	103	HIS	CA-C-O	-6.65	113.84	120.82
1	D	49	MET	CA-C-N	6.65	129.08	120.44
1	D	49	MET	C-N-CA	6.65	129.08	120.44
1	G	103	HIS	CA-C-O	-6.64	113.85	120.82
1	F	103	HIS	CA-C-O	-6.64	113.85	120.82
1	D	100	LEU	CA-C-N	6.62	129.16	120.28
1	D	100	LEU	C-N-CA	6.62	129.16	120.28
1	F	49	MET	CA-C-N	6.62	129.04	120.44
1	F	49	MET	C-N-CA	6.62	129.04	120.44
1	G	49	MET	CA-C-N	6.62	129.04	120.44
1	G	49	MET	C-N-CA	6.62	129.04	120.44
1	F	185	THR	CA-C-O	-6.61	113.89	120.70
1	I	185	THR	CA-C-O	-6.61	113.89	120.70
1	B	103	HIS	CA-C-O	-6.61	113.88	120.82
1	C	49	MET	CA-C-N	6.61	129.03	120.44
1	C	49	MET	C-N-CA	6.61	129.03	120.44
1	I	103	HIS	CA-C-O	-6.60	113.89	120.82
1	D	185	THR	CA-C-O	-6.60	113.90	120.70
1	H	49	MET	CA-C-N	6.59	129.01	120.44
1	H	49	MET	C-N-CA	6.59	129.01	120.44
1	E	49	MET	CA-C-N	6.59	129.00	120.44
1	E	49	MET	C-N-CA	6.59	129.00	120.44
1	E	103	HIS	CA-C-O	-6.58	113.91	120.82
1	I	157	ARG	CA-C-N	6.58	129.76	120.28
1	I	157	ARG	C-N-CA	6.58	129.76	120.28
1	B	122	GLU	N-CA-C	-6.58	103.86	112.41
1	G	185	THR	CA-C-O	-6.58	113.92	120.70
1	B	103	HIS	O-C-N	6.58	128.84	122.07
1	C	185	THR	CA-C-O	-6.57	113.93	120.70
1	C	122	GLU	N-CA-C	-6.57	103.87	112.41
1	A	49	MET	CA-C-N	6.57	128.97	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	MET	C-N-CA	6.57	128.97	120.44
1	B	49	MET	CA-C-N	6.56	128.97	120.44
1	B	49	MET	C-N-CA	6.56	128.97	120.44
1	H	122	GLU	N-CA-C	-6.56	103.88	112.41
1	A	103	HIS	CA-C-O	-6.55	113.94	120.82
1	E	122	GLU	N-CA-C	-6.55	103.90	112.41
1	H	103	HIS	O-C-N	6.55	128.81	122.07
1	D	157	ARG	CA-C-N	6.54	129.69	120.28
1	D	157	ARG	C-N-CA	6.54	129.69	120.28
1	H	185	THR	CA-C-O	-6.54	113.97	120.70
1	I	49	MET	CA-C-N	6.53	128.93	120.44
1	I	49	MET	C-N-CA	6.53	128.93	120.44
1	G	157	ARG	CA-C-N	6.53	129.69	120.28
1	G	157	ARG	C-N-CA	6.53	129.69	120.28
1	B	185	THR	CA-C-O	-6.53	113.97	120.70
1	C	157	ARG	CA-C-N	6.53	129.68	120.28
1	C	157	ARG	C-N-CA	6.53	129.68	120.28
1	F	157	ARG	CA-C-N	6.53	129.68	120.28
1	F	157	ARG	C-N-CA	6.53	129.68	120.28
1	I	122	GLU	N-CA-C	-6.53	103.93	112.41
1	G	122	GLU	N-CA-C	-6.52	103.93	112.41
1	G	103	HIS	CA-C-N	-6.52	112.68	123.04
1	G	103	HIS	C-N-CA	-6.52	112.68	123.04
1	H	157	ARG	CA-C-N	6.52	129.66	120.28
1	H	157	ARG	C-N-CA	6.52	129.66	120.28
1	A	157	ARG	CA-C-N	6.52	129.66	120.28
1	A	157	ARG	C-N-CA	6.52	129.66	120.28
1	A	185	THR	CA-C-O	-6.51	113.99	120.70
1	A	122	GLU	N-CA-C	-6.51	103.95	112.41
1	D	122	GLU	N-CA-C	-6.50	103.96	112.41
1	B	157	ARG	CA-C-N	6.49	129.63	120.28
1	B	157	ARG	C-N-CA	6.49	129.63	120.28
1	F	122	GLU	N-CA-C	-6.47	104.00	112.41
1	E	185	THR	CA-C-O	-6.46	114.05	120.70
1	F	64	ILE	CA-C-N	6.46	130.89	120.30
1	F	64	ILE	C-N-CA	6.46	130.89	120.30
1	E	157	ARG	CA-C-N	6.46	129.58	120.28
1	E	157	ARG	C-N-CA	6.46	129.58	120.28
1	G	107	PRO	CA-C-O	-6.46	115.63	120.73
1	I	64	ILE	CA-C-N	6.42	130.82	120.30
1	I	64	ILE	C-N-CA	6.42	130.82	120.30
1	G	107	PRO	N-CA-C	-6.41	103.72	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	ILE	CA-C-N	6.39	130.78	120.30
1	D	64	ILE	C-N-CA	6.39	130.78	120.30
1	G	64	ILE	CA-C-N	6.39	130.78	120.30
1	G	64	ILE	C-N-CA	6.39	130.78	120.30
1	H	186	THR	CA-C-N	6.39	129.36	120.29
1	H	186	THR	C-N-CA	6.39	129.36	120.29
1	A	64	ILE	CA-C-N	6.38	130.77	120.30
1	A	64	ILE	C-N-CA	6.38	130.77	120.30
1	E	84	GLN	CA-C-N	6.38	129.12	120.38
1	E	84	GLN	C-N-CA	6.38	129.12	120.38
1	H	84	GLN	CA-C-N	6.37	129.11	120.38
1	H	84	GLN	C-N-CA	6.37	129.11	120.38
1	E	64	ILE	CA-C-N	6.37	130.75	120.30
1	E	64	ILE	C-N-CA	6.37	130.75	120.30
1	B	64	ILE	CA-C-N	6.37	130.74	120.30
1	B	64	ILE	C-N-CA	6.37	130.74	120.30
1	G	84	GLN	CA-C-N	6.36	129.10	120.38
1	G	84	GLN	C-N-CA	6.36	129.10	120.38
1	E	186	THR	CA-C-N	6.36	129.32	120.29
1	E	186	THR	C-N-CA	6.36	129.32	120.29
1	D	191	ARG	N-CA-C	6.35	124.33	110.80
1	C	186	THR	CA-C-N	6.35	129.30	120.29
1	C	186	THR	C-N-CA	6.35	129.30	120.29
1	H	64	ILE	CA-C-N	6.34	130.70	120.30
1	H	64	ILE	C-N-CA	6.34	130.70	120.30
1	C	64	ILE	CA-C-N	6.34	130.69	120.30
1	C	64	ILE	C-N-CA	6.34	130.69	120.30
1	F	186	THR	CA-C-N	6.34	129.29	120.29
1	F	186	THR	C-N-CA	6.34	129.29	120.29
1	A	186	THR	CA-C-N	6.33	129.28	120.29
1	A	186	THR	C-N-CA	6.33	129.28	120.29
1	D	84	GLN	CA-C-N	6.32	129.04	120.38
1	D	84	GLN	C-N-CA	6.32	129.04	120.38
1	A	84	GLN	CA-C-N	6.32	129.04	120.38
1	A	84	GLN	C-N-CA	6.32	129.04	120.38
1	C	166	ILE	CA-C-N	6.32	130.67	120.30
1	C	166	ILE	C-N-CA	6.32	130.67	120.30
1	E	191	ARG	N-CA-C	6.32	124.25	110.80
1	I	186	THR	CA-C-N	6.32	129.26	120.29
1	I	186	THR	C-N-CA	6.32	129.26	120.29
1	C	191	ARG	N-CA-C	6.31	124.25	110.80
1	F	84	GLN	CA-C-N	6.31	129.02	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	84	GLN	C-N-CA	6.31	129.02	120.38
1	D	103	HIS	CA-C-O	-6.30	113.87	120.55
1	E	166	ILE	CA-C-N	6.30	130.64	120.30
1	E	166	ILE	C-N-CA	6.30	130.64	120.30
1	F	166	ILE	CA-C-N	6.30	130.64	120.30
1	F	166	ILE	C-N-CA	6.30	130.64	120.30
1	I	191	ARG	N-CA-C	6.30	124.23	110.80
1	B	186	THR	CA-C-N	6.30	129.24	120.29
1	B	186	THR	C-N-CA	6.30	129.24	120.29
1	G	166	ILE	CA-C-N	6.29	130.62	120.30
1	G	166	ILE	C-N-CA	6.29	130.62	120.30
1	A	166	ILE	CA-C-N	6.29	130.62	120.30
1	A	166	ILE	C-N-CA	6.29	130.62	120.30
1	C	84	GLN	CA-C-N	6.29	129.00	120.38
1	C	84	GLN	C-N-CA	6.29	129.00	120.38
1	G	176	LYS	CA-C-O	-6.29	113.88	120.55
1	G	186	THR	CA-C-N	6.29	129.22	120.29
1	G	186	THR	C-N-CA	6.29	129.22	120.29
1	G	191	ARG	N-CA-C	6.29	124.20	110.80
1	D	166	ILE	CA-C-N	6.29	130.61	120.30
1	D	166	ILE	C-N-CA	6.29	130.61	120.30
1	A	176	LYS	CA-C-O	-6.29	113.89	120.55
1	C	123	ALA	CA-C-N	6.28	130.28	121.24
1	C	123	ALA	C-N-CA	6.28	130.28	121.24
1	D	186	THR	CA-C-N	6.28	129.21	120.29
1	D	186	THR	C-N-CA	6.28	129.21	120.29
1	B	84	GLN	CA-C-N	6.28	128.98	120.38
1	B	84	GLN	C-N-CA	6.28	128.98	120.38
1	D	107	PRO	N-CA-C	6.28	118.36	110.70
1	I	166	ILE	CA-C-N	6.28	130.59	120.30
1	I	166	ILE	C-N-CA	6.28	130.59	120.30
1	E	176	LYS	CA-C-O	-6.28	113.90	120.55
1	H	123	ALA	CA-C-N	6.27	130.27	121.24
1	H	123	ALA	C-N-CA	6.27	130.27	121.24
1	B	123	ALA	CA-C-N	6.27	130.27	121.24
1	B	123	ALA	C-N-CA	6.27	130.27	121.24
1	B	166	ILE	CA-C-N	6.27	130.58	120.30
1	B	166	ILE	C-N-CA	6.27	130.58	120.30
1	H	166	ILE	CA-C-N	6.26	130.56	120.30
1	H	166	ILE	C-N-CA	6.26	130.56	120.30
1	D	157	ARG	CA-C-O	6.25	127.17	120.10
1	I	123	ALA	CA-C-N	6.25	130.24	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	123	ALA	C-N-CA	6.25	130.24	121.24
1	G	127	ILE	CA-C-N	6.25	128.65	120.28
1	G	127	ILE	C-N-CA	6.25	128.65	120.28
1	I	84	GLN	CA-C-N	6.25	128.94	120.38
1	I	84	GLN	C-N-CA	6.25	128.94	120.38
1	D	127	ILE	CA-C-N	6.24	128.64	120.28
1	D	127	ILE	C-N-CA	6.24	128.64	120.28
1	C	176	LYS	CA-C-O	-6.24	113.94	120.55
1	B	157	ARG	CA-C-O	6.22	127.12	120.10
1	F	127	ILE	CA-C-N	6.22	128.61	120.28
1	F	127	ILE	C-N-CA	6.22	128.61	120.28
1	E	123	ALA	CA-C-N	6.21	130.19	121.24
1	E	123	ALA	C-N-CA	6.21	130.19	121.24
1	H	94	ASP	CA-C-O	-6.20	113.98	120.55
1	E	127	ILE	CA-C-N	6.20	128.59	120.28
1	E	127	ILE	C-N-CA	6.20	128.59	120.28
1	F	157	ARG	CA-C-O	6.20	127.10	120.10
1	A	127	ILE	CA-C-N	6.19	128.58	120.28
1	A	127	ILE	C-N-CA	6.19	128.58	120.28
1	A	157	ARG	CA-C-O	6.19	127.10	120.10
1	B	176	LYS	CA-C-O	-6.19	113.99	120.55
1	E	157	ARG	CA-C-O	6.19	127.10	120.10
1	G	123	ALA	CA-C-N	6.19	130.16	121.24
1	G	123	ALA	C-N-CA	6.19	130.16	121.24
1	B	127	ILE	CA-C-N	6.19	128.57	120.28
1	B	127	ILE	C-N-CA	6.19	128.57	120.28
1	C	157	ARG	CA-C-O	6.19	127.09	120.10
1	H	190	GLU	CA-C-N	6.18	132.82	121.70
1	H	190	GLU	C-N-CA	6.18	132.82	121.70
1	A	123	ALA	CA-C-N	6.18	130.13	121.24
1	A	123	ALA	C-N-CA	6.18	130.13	121.24
1	D	91	ILE	CA-C-N	6.18	133.34	121.54
1	D	91	ILE	C-N-CA	6.18	133.34	121.54
1	I	176	LYS	CA-C-O	-6.17	114.01	120.55
1	F	91	ILE	CA-C-N	6.15	133.29	121.54
1	F	91	ILE	C-N-CA	6.15	133.29	121.54
1	D	123	ALA	CA-C-N	6.15	130.09	121.24
1	D	123	ALA	C-N-CA	6.15	130.09	121.24
1	F	123	ALA	CA-C-N	6.15	130.09	121.24
1	F	123	ALA	C-N-CA	6.15	130.09	121.24
1	G	91	ILE	CA-C-N	6.14	133.28	121.54
1	G	91	ILE	C-N-CA	6.14	133.28	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	127	ILE	CA-C-N	6.14	128.51	120.28
1	I	127	ILE	C-N-CA	6.14	128.51	120.28
1	C	127	ILE	CA-C-N	6.14	128.51	120.28
1	C	127	ILE	C-N-CA	6.14	128.51	120.28
1	H	91	ILE	CA-C-N	6.13	133.26	121.54
1	H	91	ILE	C-N-CA	6.13	133.26	121.54
1	H	176	LYS	CA-C-O	-6.13	114.05	120.55
1	H	157	ARG	CA-C-O	6.13	127.03	120.10
1	C	91	ILE	CA-C-N	6.13	133.24	121.54
1	C	91	ILE	C-N-CA	6.13	133.24	121.54
1	D	176	LYS	CA-C-O	-6.12	114.06	120.55
1	B	91	ILE	CA-C-N	6.12	133.24	121.54
1	B	91	ILE	C-N-CA	6.12	133.24	121.54
1	F	176	LYS	CA-C-O	-6.12	114.06	120.55
1	F	190	GLU	CA-C-N	6.12	132.72	121.70
1	F	190	GLU	C-N-CA	6.12	132.72	121.70
1	D	94	ASP	CA-C-O	-6.12	114.06	120.55
1	H	127	ILE	CA-C-N	6.12	128.48	120.28
1	H	127	ILE	C-N-CA	6.12	128.48	120.28
1	G	104	PHE	CA-C-N	-6.12	114.14	123.07
1	G	104	PHE	C-N-CA	-6.12	114.14	123.07
1	I	157	ARG	CA-C-O	6.11	127.01	120.10
1	F	107	PRO	N-CA-C	-6.11	103.24	110.70
1	E	91	ILE	CA-C-N	6.10	133.19	121.54
1	E	91	ILE	C-N-CA	6.10	133.19	121.54
1	A	91	ILE	CA-C-N	6.09	133.17	121.54
1	A	91	ILE	C-N-CA	6.09	133.17	121.54
1	I	91	ILE	CA-C-N	6.09	133.17	121.54
1	I	91	ILE	C-N-CA	6.09	133.17	121.54
1	G	157	ARG	CA-C-O	6.07	126.96	120.10
1	D	123	ALA	N-CA-C	-6.06	105.37	112.89
1	C	123	ALA	N-CA-C	-6.05	105.38	112.89
1	B	123	ALA	N-CA-C	-6.05	105.39	112.89
1	G	40	LYS	CA-C-N	6.05	128.30	120.44
1	G	40	LYS	C-N-CA	6.05	128.30	120.44
1	F	40	LYS	CA-C-N	6.03	128.27	120.44
1	F	40	LYS	C-N-CA	6.03	128.27	120.44
1	F	94	ASP	CA-C-O	-6.02	114.17	120.55
1	G	94	ASP	CA-C-O	-6.02	114.17	120.55
1	C	193	PHE	CA-C-N	6.02	127.37	119.84
1	C	193	PHE	C-N-CA	6.02	127.37	119.84
1	G	123	ALA	N-CA-C	-6.02	105.42	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ASP	CA-C-O	-6.02	114.17	120.55
1	E	123	ALA	N-CA-C	-6.01	105.43	112.89
1	H	123	ALA	N-CA-C	-6.01	105.44	112.89
1	B	94	ASP	CA-C-O	-6.01	114.18	120.55
1	H	66	TYR	CA-C-N	6.01	128.33	120.28
1	H	66	TYR	C-N-CA	6.01	128.33	120.28
1	I	193	PHE	CA-C-N	6.01	127.35	119.84
1	I	193	PHE	C-N-CA	6.01	127.35	119.84
1	C	94	ASP	CA-C-O	-6.00	114.19	120.55
1	G	169	MET	O-C-N	-6.00	115.31	122.63
1	I	123	ALA	N-CA-C	-5.99	105.46	112.89
1	H	142	PRO	CA-C-O	-5.99	111.88	120.56
1	E	94	ASP	CA-C-O	-5.99	114.20	120.55
1	D	193	PHE	CA-C-N	5.98	127.32	119.84
1	D	193	PHE	C-N-CA	5.98	127.32	119.84
1	D	66	TYR	CA-C-N	5.98	128.29	120.28
1	D	66	TYR	C-N-CA	5.98	128.29	120.28
1	F	169	MET	O-C-N	-5.98	115.34	122.63
1	I	94	ASP	CA-C-O	-5.98	114.22	120.55
1	A	123	ALA	N-CA-C	-5.97	105.48	112.89
1	B	40	LYS	CA-C-N	5.97	128.20	120.44
1	B	40	LYS	C-N-CA	5.97	128.20	120.44
1	D	142	PRO	CA-C-O	-5.97	111.91	120.56
1	F	123	ALA	N-CA-C	-5.97	105.49	112.89
1	H	40	LYS	CA-C-N	5.96	128.19	120.44
1	H	40	LYS	C-N-CA	5.96	128.19	120.44
1	E	169	MET	O-C-N	-5.96	115.36	122.63
1	G	142	PRO	CA-C-O	-5.96	111.92	120.56
1	B	169	MET	O-C-N	-5.96	115.36	122.63
1	H	169	MET	O-C-N	-5.95	115.37	122.63
1	I	169	MET	O-C-N	-5.95	115.37	122.63
1	D	104	PHE	CA-C-N	5.95	128.18	120.44
1	D	104	PHE	C-N-CA	5.95	128.18	120.44
1	E	40	LYS	CA-C-N	5.95	128.18	120.44
1	E	40	LYS	C-N-CA	5.95	128.18	120.44
1	A	66	TYR	CA-C-N	5.95	128.25	120.28
1	A	66	TYR	C-N-CA	5.95	128.25	120.28
1	C	169	MET	O-C-N	-5.95	115.37	122.63
1	E	193	PHE	CA-C-N	5.95	127.27	119.84
1	E	193	PHE	C-N-CA	5.95	127.27	119.84
1	G	193	PHE	CA-C-N	5.95	127.28	119.84
1	G	193	PHE	C-N-CA	5.95	127.28	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	40	LYS	CA-C-N	5.95	128.17	120.44
1	I	40	LYS	C-N-CA	5.95	128.17	120.44
1	D	169	MET	O-C-N	-5.95	115.38	122.63
1	D	40	LYS	CA-C-N	5.94	128.16	120.44
1	D	40	LYS	C-N-CA	5.94	128.16	120.44
1	I	142	PRO	CA-C-O	-5.94	111.95	120.56
1	A	169	MET	O-C-N	-5.94	115.39	122.63
1	F	142	PRO	CA-C-O	-5.93	111.95	120.56
1	C	40	LYS	CA-C-N	5.93	128.15	120.44
1	C	40	LYS	C-N-CA	5.93	128.15	120.44
1	B	142	PRO	CA-C-O	-5.93	111.96	120.56
1	E	66	TYR	CA-C-N	5.93	128.22	120.28
1	E	66	TYR	C-N-CA	5.93	128.22	120.28
1	A	40	LYS	CA-C-N	5.92	128.13	120.44
1	A	40	LYS	C-N-CA	5.92	128.13	120.44
1	I	66	TYR	CA-C-N	5.92	128.21	120.28
1	I	66	TYR	C-N-CA	5.92	128.21	120.28
1	B	66	TYR	CA-C-N	5.91	128.21	120.28
1	B	66	TYR	C-N-CA	5.91	128.21	120.28
1	C	142	PRO	CA-C-O	-5.90	112.00	120.56
1	G	190	GLU	CA-C-N	5.89	132.79	121.54
1	G	190	GLU	C-N-CA	5.89	132.79	121.54
1	A	142	PRO	CA-C-O	-5.89	112.02	120.56
1	G	66	TYR	CA-C-N	5.88	128.17	120.28
1	G	66	TYR	C-N-CA	5.88	128.17	120.28
1	C	66	TYR	CA-C-N	5.88	128.16	120.28
1	C	66	TYR	C-N-CA	5.88	128.16	120.28
1	C	190	GLU	CA-C-N	5.88	132.76	121.54
1	C	190	GLU	C-N-CA	5.88	132.76	121.54
1	I	190	GLU	CA-C-N	5.88	132.76	121.54
1	I	190	GLU	C-N-CA	5.88	132.76	121.54
1	D	190	GLU	CA-C-N	5.86	132.73	121.54
1	D	190	GLU	C-N-CA	5.86	132.73	121.54
1	E	142	PRO	CA-C-O	-5.86	112.06	120.56
1	F	66	TYR	CA-C-N	5.84	128.10	120.28
1	F	66	TYR	C-N-CA	5.84	128.10	120.28
1	A	108	PRO	CA-C-N	5.84	130.60	120.68
1	A	108	PRO	C-N-CA	5.84	130.60	120.68
1	E	190	GLU	CA-C-N	5.83	132.67	121.54
1	E	190	GLU	C-N-CA	5.83	132.67	121.54
1	D	92	THR	CA-C-N	5.81	127.99	120.44
1	D	92	THR	C-N-CA	5.81	127.99	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	92	THR	CA-C-N	5.81	127.99	120.44
1	F	92	THR	C-N-CA	5.81	127.99	120.44
1	C	92	THR	CA-C-N	5.80	127.98	120.44
1	C	92	THR	C-N-CA	5.80	127.98	120.44
1	I	136	LYS	CA-C-O	5.78	126.66	120.70
1	A	92	THR	CA-C-N	5.78	127.95	120.44
1	A	92	THR	C-N-CA	5.78	127.95	120.44
1	G	54	MET	N-CA-C	5.78	117.25	111.07
1	D	54	MET	N-CA-C	5.77	117.25	111.07
1	H	92	THR	CA-C-N	5.77	127.94	120.44
1	H	92	THR	C-N-CA	5.77	127.94	120.44
1	H	136	LYS	CA-C-O	5.76	126.63	120.70
1	D	136	LYS	CA-C-O	5.75	126.63	120.70
1	I	92	THR	CA-C-N	5.75	127.91	120.44
1	I	92	THR	C-N-CA	5.75	127.91	120.44
1	E	54	MET	N-CA-C	5.74	117.22	111.07
1	E	92	THR	CA-C-N	5.74	127.91	120.44
1	E	92	THR	C-N-CA	5.74	127.91	120.44
1	G	136	LYS	CA-C-O	5.74	126.61	120.70
1	B	92	THR	CA-C-N	5.73	127.89	120.44
1	B	92	THR	C-N-CA	5.73	127.89	120.44
1	B	54	MET	N-CA-C	5.73	117.20	111.07
1	E	160	THR	CA-C-O	-5.73	115.47	121.55
1	I	54	MET	N-CA-C	5.72	117.19	111.07
1	A	136	LYS	CA-C-O	5.72	126.59	120.70
1	I	163	THR	CA-C-N	5.71	127.94	120.28
1	I	163	THR	C-N-CA	5.71	127.94	120.28
1	D	163	THR	CA-C-N	5.71	127.93	120.28
1	D	163	THR	C-N-CA	5.71	127.93	120.28
1	G	92	THR	CA-C-N	5.71	127.86	120.44
1	G	92	THR	C-N-CA	5.71	127.86	120.44
1	C	136	LYS	CA-C-O	5.69	126.56	120.70
1	B	136	LYS	CA-C-O	5.69	126.56	120.70
1	F	103	HIS	O-C-N	5.69	127.93	122.07
1	H	54	MET	N-CA-C	5.68	117.15	111.07
1	E	163	THR	CA-C-N	5.68	127.89	120.28
1	E	163	THR	C-N-CA	5.68	127.89	120.28
1	F	54	MET	N-CA-C	5.68	117.15	111.07
1	A	54	MET	N-CA-C	5.68	117.14	111.07
1	C	54	MET	N-CA-C	5.67	117.14	111.07
1	F	163	THR	CA-C-N	5.67	127.88	120.28
1	F	163	THR	C-N-CA	5.67	127.88	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	163	THR	CA-C-N	5.67	127.87	120.28
1	G	163	THR	C-N-CA	5.67	127.87	120.28
1	F	160	THR	CA-C-O	-5.66	115.56	121.55
1	C	163	THR	CA-C-N	5.65	127.85	120.28
1	C	163	THR	C-N-CA	5.65	127.85	120.28
1	B	190	GLU	CA-C-N	5.65	131.86	121.70
1	B	190	GLU	C-N-CA	5.65	131.86	121.70
1	B	163	THR	CA-C-N	5.64	127.84	120.28
1	B	163	THR	C-N-CA	5.64	127.84	120.28
1	E	136	LYS	CA-C-O	5.64	126.51	120.70
1	E	103	HIS	CA-C-N	-5.64	114.04	122.39
1	E	103	HIS	C-N-CA	-5.64	114.04	122.39
1	H	163	THR	CA-C-N	5.64	127.84	120.28
1	H	163	THR	C-N-CA	5.64	127.84	120.28
1	F	136	LYS	CA-C-O	5.63	126.50	120.70
1	A	163	THR	CA-C-N	5.63	127.82	120.28
1	A	163	THR	C-N-CA	5.63	127.82	120.28
1	F	149	LYS	CA-C-N	5.62	127.81	120.28
1	F	149	LYS	C-N-CA	5.62	127.81	120.28
1	B	160	THR	CA-C-O	-5.61	115.60	121.55
1	C	104	PHE	CA-C-N	-5.61	113.63	121.99
1	C	104	PHE	C-N-CA	-5.61	113.63	121.99
1	I	160	THR	CA-C-O	-5.59	115.62	121.55
1	A	160	THR	CA-C-O	-5.59	115.63	121.55
1	C	160	THR	CA-C-O	-5.59	115.63	121.55
1	I	149	LYS	CA-C-N	5.58	127.76	120.28
1	I	149	LYS	C-N-CA	5.58	127.76	120.28
1	C	161	LYS	CA-C-N	5.58	127.76	120.28
1	C	161	LYS	C-N-CA	5.58	127.76	120.28
1	A	149	LYS	CA-C-N	5.58	127.75	120.28
1	A	149	LYS	C-N-CA	5.58	127.75	120.28
1	D	161	LYS	CA-C-N	5.58	127.69	120.44
1	D	161	LYS	C-N-CA	5.58	127.69	120.44
1	A	161	LYS	CA-C-N	5.58	127.75	120.28
1	A	161	LYS	C-N-CA	5.58	127.75	120.28
1	D	149	LYS	CA-C-N	5.57	127.74	120.28
1	D	149	LYS	C-N-CA	5.57	127.74	120.28
1	C	149	LYS	CA-C-N	5.56	127.73	120.28
1	C	149	LYS	C-N-CA	5.56	127.73	120.28
1	D	105	TYR	N-CA-C	5.56	117.02	111.07
1	G	160	THR	CA-C-O	-5.56	115.66	121.55
1	H	149	LYS	CA-C-N	5.55	127.72	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	149	LYS	C-N-CA	5.55	127.72	120.28
1	H	160	THR	CA-C-O	-5.55	115.67	121.55
1	I	161	LYS	CA-C-N	5.54	127.71	120.28
1	I	161	LYS	C-N-CA	5.54	127.71	120.28
1	B	161	LYS	CA-C-N	5.54	127.70	120.28
1	B	161	LYS	C-N-CA	5.54	127.70	120.28
1	G	149	LYS	CA-C-N	5.51	127.67	120.28
1	G	149	LYS	C-N-CA	5.51	127.67	120.28
1	E	149	LYS	CA-C-N	5.51	127.66	120.28
1	E	149	LYS	C-N-CA	5.51	127.66	120.28
1	B	126	GLY	CA-C-N	5.50	128.00	120.46
1	B	126	GLY	C-N-CA	5.50	128.00	120.46
1	H	126	GLY	CA-C-N	5.50	128.00	120.46
1	H	126	GLY	C-N-CA	5.50	128.00	120.46
1	G	161	LYS	CA-C-N	5.50	127.64	120.28
1	G	161	LYS	C-N-CA	5.50	127.64	120.28
1	B	149	LYS	CA-C-N	5.50	127.64	120.28
1	B	149	LYS	C-N-CA	5.50	127.64	120.28
1	I	103	HIS	O-C-N	5.50	127.73	122.07
1	C	133	ARG	CA-C-N	5.49	128.08	120.29
1	C	133	ARG	C-N-CA	5.49	128.08	120.29
1	E	161	LYS	CA-C-N	5.47	127.61	120.28
1	E	161	LYS	C-N-CA	5.47	127.61	120.28
1	D	160	THR	CA-C-O	-5.46	115.76	121.55
1	H	82	PHE	CA-C-N	5.46	127.44	120.56
1	H	82	PHE	C-N-CA	5.46	127.44	120.56
1	F	161	LYS	CA-C-N	5.46	127.60	120.28
1	F	161	LYS	C-N-CA	5.46	127.60	120.28
1	E	126	GLY	CA-C-N	5.46	127.94	120.46
1	E	126	GLY	C-N-CA	5.46	127.94	120.46
1	F	41	LEU	O-C-N	-5.46	116.45	122.07
1	F	126	GLY	CA-C-N	5.45	127.93	120.46
1	F	126	GLY	C-N-CA	5.45	127.93	120.46
1	C	126	GLY	CA-C-N	5.44	127.91	120.46
1	C	126	GLY	C-N-CA	5.44	127.91	120.46
1	A	126	GLY	CA-C-N	5.44	127.91	120.46
1	A	126	GLY	C-N-CA	5.44	127.91	120.46
1	I	82	PHE	CA-C-N	5.43	127.41	120.56
1	I	82	PHE	C-N-CA	5.43	127.41	120.56
1	A	133	ARG	CA-C-N	5.43	128.00	120.29
1	A	133	ARG	C-N-CA	5.43	128.00	120.29
1	G	106	LYS	N-CA-C	-5.42	103.31	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	175	LEU	CA-C-N	5.41	127.53	120.28
1	F	175	LEU	C-N-CA	5.41	127.53	120.28
1	G	175	LEU	CA-C-N	5.41	127.53	120.28
1	G	175	LEU	C-N-CA	5.41	127.53	120.28
1	C	118	THR	CA-C-N	5.41	127.79	120.38
1	C	118	THR	C-N-CA	5.41	127.79	120.38
1	D	141	MET	N-CA-C	5.40	121.75	109.81
1	G	82	PHE	CA-C-N	5.40	127.36	120.56
1	G	82	PHE	C-N-CA	5.40	127.36	120.56
1	G	126	GLY	CA-C-N	5.40	127.85	120.46
1	G	126	GLY	C-N-CA	5.40	127.85	120.46
1	A	82	PHE	CA-C-N	5.39	127.36	120.56
1	A	82	PHE	C-N-CA	5.39	127.36	120.56
1	E	41	LEU	O-C-N	-5.39	116.51	122.07
1	G	141	MET	N-CA-C	5.39	121.73	109.81
1	B	118	THR	CA-C-N	5.39	127.77	120.38
1	B	118	THR	C-N-CA	5.39	127.77	120.38
1	C	141	MET	N-CA-C	5.39	121.72	109.81
1	H	118	THR	CA-C-N	5.39	127.76	120.38
1	H	118	THR	C-N-CA	5.39	127.76	120.38
1	I	118	THR	CA-C-N	5.39	127.76	120.38
1	I	118	THR	C-N-CA	5.39	127.76	120.38
1	I	126	GLY	CA-C-N	5.39	127.84	120.46
1	I	126	GLY	C-N-CA	5.39	127.84	120.46
1	I	175	LEU	CA-C-N	5.39	127.50	120.28
1	I	175	LEU	C-N-CA	5.39	127.50	120.28
1	H	41	LEU	O-C-N	-5.38	116.52	122.07
1	H	161	LYS	CA-C-N	5.38	127.50	120.28
1	H	161	LYS	C-N-CA	5.38	127.50	120.28
1	D	118	THR	CA-C-N	5.38	127.75	120.38
1	D	118	THR	C-N-CA	5.38	127.75	120.38
1	B	41	LEU	O-C-N	-5.38	116.53	122.07
1	F	118	THR	CA-C-N	5.38	127.75	120.38
1	F	118	THR	C-N-CA	5.38	127.75	120.38
1	B	141	MET	N-CA-C	5.38	121.69	109.81
1	C	82	PHE	CA-C-N	5.38	127.33	120.56
1	C	82	PHE	C-N-CA	5.38	127.33	120.56
1	A	118	THR	CA-C-N	5.38	127.74	120.38
1	A	118	THR	C-N-CA	5.38	127.74	120.38
1	B	175	LEU	CA-C-N	5.38	127.48	120.28
1	B	175	LEU	C-N-CA	5.38	127.48	120.28
1	D	82	PHE	CA-C-N	5.38	127.33	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	82	PHE	C-N-CA	5.38	127.33	120.56
1	E	141	MET	N-CA-C	5.37	121.68	109.81
1	H	133	ARG	CA-C-N	5.37	127.92	120.29
1	H	133	ARG	C-N-CA	5.37	127.92	120.29
1	G	133	ARG	CA-C-N	5.37	127.91	120.29
1	G	133	ARG	C-N-CA	5.37	127.91	120.29
1	B	133	ARG	CA-C-N	5.36	127.91	120.29
1	B	133	ARG	C-N-CA	5.36	127.91	120.29
1	C	175	LEU	CA-C-N	5.36	127.47	120.28
1	C	175	LEU	C-N-CA	5.36	127.47	120.28
1	D	133	ARG	CA-C-N	5.36	127.91	120.29
1	D	133	ARG	C-N-CA	5.36	127.91	120.29
1	H	175	LEU	CA-C-N	5.36	127.47	120.28
1	H	175	LEU	C-N-CA	5.36	127.47	120.28
1	I	133	ARG	CA-C-N	5.36	127.91	120.29
1	I	133	ARG	C-N-CA	5.36	127.91	120.29
1	F	82	PHE	CA-C-N	5.36	127.32	120.56
1	F	82	PHE	C-N-CA	5.36	127.32	120.56
1	I	141	MET	N-CA-C	5.36	121.66	109.81
1	G	118	THR	CA-C-N	5.36	127.72	120.38
1	G	118	THR	C-N-CA	5.36	127.72	120.38
1	F	141	MET	N-CA-C	5.36	121.65	109.81
1	H	141	MET	N-CA-C	5.36	121.65	109.81
1	A	175	LEU	CA-C-N	5.35	127.45	120.28
1	A	175	LEU	C-N-CA	5.35	127.45	120.28
1	F	133	ARG	CA-C-N	5.35	127.89	120.29
1	F	133	ARG	C-N-CA	5.35	127.89	120.29
1	D	175	LEU	CA-C-N	5.35	127.45	120.28
1	D	175	LEU	C-N-CA	5.35	127.45	120.28
1	A	141	MET	N-CA-C	5.35	121.63	109.81
1	E	133	ARG	CA-C-N	5.35	127.89	120.29
1	E	133	ARG	C-N-CA	5.35	127.89	120.29
1	B	82	PHE	CA-C-N	5.35	127.30	120.56
1	B	82	PHE	C-N-CA	5.35	127.30	120.56
1	C	75	ALA	CA-C-N	5.35	127.45	120.28
1	C	75	ALA	C-N-CA	5.35	127.45	120.28
1	E	118	THR	CA-C-N	5.35	127.71	120.38
1	E	118	THR	C-N-CA	5.35	127.71	120.38
1	I	41	LEU	O-C-N	-5.34	116.57	122.07
1	E	175	LEU	CA-C-N	5.34	127.43	120.28
1	E	175	LEU	C-N-CA	5.34	127.43	120.28
1	D	41	LEU	O-C-N	-5.33	116.58	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	ALA	CA-C-N	5.33	127.42	120.28
1	B	75	ALA	C-N-CA	5.33	127.42	120.28
1	C	41	LEU	O-C-N	-5.33	116.58	122.07
1	F	75	ALA	CA-C-N	5.33	127.42	120.28
1	F	75	ALA	C-N-CA	5.33	127.42	120.28
1	A	75	ALA	CA-C-N	5.33	127.42	120.28
1	A	75	ALA	C-N-CA	5.33	127.42	120.28
1	D	126	GLY	CA-C-N	5.31	127.73	120.46
1	D	126	GLY	C-N-CA	5.31	127.73	120.46
1	E	82	PHE	CA-C-N	5.31	127.25	120.56
1	E	82	PHE	C-N-CA	5.31	127.25	120.56
1	G	41	LEU	O-C-N	-5.30	116.61	122.07
1	G	75	ALA	CA-C-N	5.30	127.38	120.28
1	G	75	ALA	C-N-CA	5.30	127.38	120.28
1	I	75	ALA	CA-C-N	5.28	127.36	120.28
1	I	75	ALA	C-N-CA	5.28	127.36	120.28
1	A	41	LEU	O-C-N	-5.27	116.64	122.07
1	E	75	ALA	CA-C-N	5.27	127.34	120.28
1	E	75	ALA	C-N-CA	5.27	127.34	120.28
1	H	75	ALA	CA-C-N	5.26	127.33	120.28
1	H	75	ALA	C-N-CA	5.26	127.33	120.28
1	I	128	GLU	N-CA-C	5.25	117.00	111.28
1	I	105	TYR	N-CA-C	-5.25	105.46	111.07
1	I	107	PRO	N-CA-C	-5.22	104.33	110.70
1	D	75	ALA	CA-C-N	5.22	127.27	120.28
1	D	75	ALA	C-N-CA	5.22	127.27	120.28
1	F	128	GLU	N-CA-C	5.21	116.96	111.28
1	G	137	ILE	O-C-N	5.19	127.00	121.91
1	A	78	TRP	O-C-N	5.18	127.41	122.07
1	B	128	GLU	N-CA-C	5.18	116.92	111.28
1	E	110	ILE	CA-C-N	5.18	127.74	120.28
1	E	110	ILE	C-N-CA	5.18	127.74	120.28
1	D	128	GLU	N-CA-C	5.17	116.92	111.28
1	G	128	GLU	N-CA-C	5.16	116.91	111.28
1	C	103	HIS	CA-C-N	-5.15	111.71	121.54
1	C	103	HIS	C-N-CA	-5.15	111.71	121.54
1	H	128	GLU	N-CA-C	5.14	116.89	111.28
1	H	137	ILE	O-C-N	5.14	126.95	121.91
1	A	105	TYR	CA-C-N	5.13	133.44	124.01
1	A	105	TYR	C-N-CA	5.13	133.44	124.01
1	C	128	GLU	N-CA-C	5.13	116.87	111.28
1	F	137	ILE	O-C-N	5.13	126.93	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	96	PHE	N-CA-C	5.12	116.86	111.28
1	I	96	PHE	N-CA-C	5.12	116.86	111.28
1	I	137	ILE	O-C-N	5.12	126.93	121.91
1	E	134	PHE	O-C-N	5.11	127.98	122.15
1	B	78	TRP	O-C-N	5.11	127.33	122.07
1	C	96	PHE	N-CA-C	5.11	116.84	111.28
1	E	128	GLU	N-CA-C	5.10	116.84	111.28
1	F	96	PHE	N-CA-C	5.10	116.84	111.28
1	G	134	PHE	O-C-N	5.10	127.97	122.15
1	B	137	ILE	O-C-N	5.10	126.91	121.91
1	I	78	TRP	O-C-N	5.09	127.32	122.07
1	C	137	ILE	O-C-N	5.09	126.90	121.91
1	D	134	PHE	O-C-N	5.09	127.95	122.15
1	D	78	TRP	O-C-N	5.09	127.31	122.07
1	E	96	PHE	N-CA-C	5.09	116.83	111.28
1	I	134	PHE	O-C-N	5.08	127.94	122.15
1	C	134	PHE	O-C-N	5.07	127.93	122.15
1	A	128	GLU	N-CA-C	5.07	116.80	111.28
1	B	96	PHE	N-CA-C	5.06	116.79	111.28
1	D	96	PHE	N-CA-C	5.05	116.79	111.28
1	C	78	TRP	O-C-N	5.05	127.28	122.07
1	A	189	THR	N-CA-C	-5.05	98.64	107.73
1	A	137	ILE	O-C-N	5.04	126.85	121.91
1	I	51	ASN	CA-C-N	5.04	126.99	120.44
1	I	51	ASN	C-N-CA	5.04	126.99	120.44
1	B	134	PHE	O-C-N	5.03	127.89	122.15
1	E	92	THR	CA-C-O	5.03	127.70	120.51
1	C	93	PHE	N-CA-C	-5.03	105.69	111.07
1	A	96	PHE	N-CA-C	5.02	116.75	111.28
1	C	92	THR	CA-C-O	5.02	127.69	120.51
1	H	51	ASN	CA-C-N	5.02	126.97	120.44
1	H	51	ASN	C-N-CA	5.02	126.97	120.44
1	C	38	SER	CA-C-N	5.02	126.96	120.44
1	C	38	SER	C-N-CA	5.02	126.96	120.44
1	A	134	PHE	O-C-N	5.01	127.87	122.15
1	E	137	ILE	O-C-N	5.01	126.83	121.91
1	H	78	TRP	O-C-N	5.01	127.23	122.07
1	F	134	PHE	O-C-N	5.01	127.86	122.15
1	D	38	SER	CA-C-N	5.00	126.95	120.44
1	D	38	SER	C-N-CA	5.00	126.95	120.44
1	F	67	CYS	N-CA-C	5.00	116.73	111.28
1	H	96	PHE	N-CA-C	5.00	116.73	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	38	SER	CA-C-N	5.00	126.94	120.44
1	I	38	SER	C-N-CA	5.00	126.94	120.44

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	189	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	636	0	158	0	0
1	B	620	0	153	0	0
1	C	636	0	158	0	0
1	D	636	0	158	0	0
1	E	636	0	158	0	0
1	F	620	0	153	0	0
1	G	636	0	158	0	0
1	H	620	0	153	0	0
1	I	636	0	158	0	0
All	All	5676	0	1407	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	157/309 (51%)	143 (91%)	9 (6%)	5 (3%)	3	21
1	B	153/309 (50%)	140 (92%)	7 (5%)	6 (4%)	2	19
1	C	157/309 (51%)	141 (90%)	10 (6%)	6 (4%)	2	19
1	D	157/309 (51%)	140 (89%)	10 (6%)	7 (4%)	2	17
1	E	157/309 (51%)	141 (90%)	10 (6%)	6 (4%)	2	19
1	F	153/309 (50%)	139 (91%)	8 (5%)	6 (4%)	2	19
1	G	157/309 (51%)	141 (90%)	10 (6%)	6 (4%)	2	19
1	H	153/309 (50%)	139 (91%)	8 (5%)	6 (4%)	2	19
1	I	157/309 (51%)	139 (88%)	11 (7%)	7 (4%)	2	17
All	All	1401/2781 (50%)	1263 (90%)	83 (6%)	55 (4%)	4	19

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	THR
1	A	141	MET
1	B	92	THR
1	B	141	MET
1	B	190	GLU
1	C	92	THR
1	C	141	MET
1	C	190	GLU
1	D	92	THR
1	D	141	MET
1	D	190	GLU
1	E	92	THR
1	E	141	MET
1	E	190	GLU
1	F	92	THR
1	F	141	MET
1	F	190	GLU
1	G	92	THR
1	G	141	MET
1	G	190	GLU
1	H	92	THR
1	H	141	MET
1	H	190	GLU

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Mol	Chain	Res	Type
1	I	92	THR
1	I	106	LYS
1	I	141	MET
1	I	190	GLU
1	A	145	PHE
1	B	145	PHE
1	C	145	PHE
1	D	145	PHE
1	E	145	PHE
1	F	145	PHE
1	G	145	PHE
1	H	145	PHE
1	I	145	PHE
1	A	125	LEU
1	B	125	LEU
1	C	125	LEU
1	D	125	LEU
1	E	125	LEU
1	F	125	LEU
1	G	125	LEU
1	H	125	LEU
1	I	125	LEU
1	D	111	ASN
1	A	143	PRO
1	B	143	PRO
1	C	143	PRO
1	D	143	PRO
1	E	143	PRO
1	F	143	PRO
1	G	143	PRO
1	H	143	PRO
1	I	143	PRO

5.3.2 Protein sidechains ⓘ

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

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.

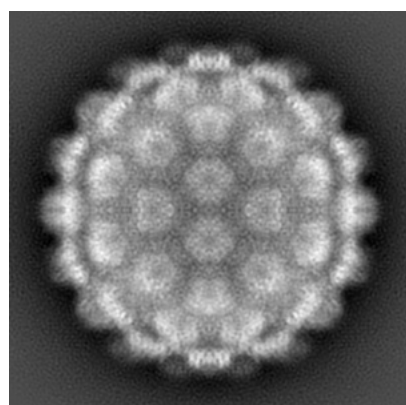
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4709. These allow visual inspection of the internal detail of the map and identification of artifacts.

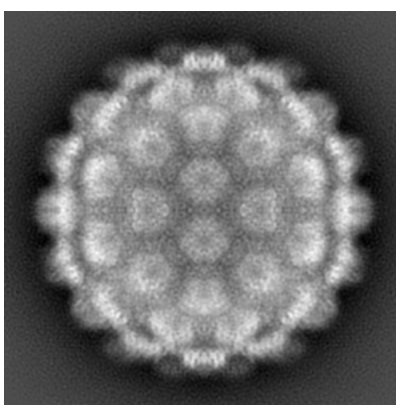
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

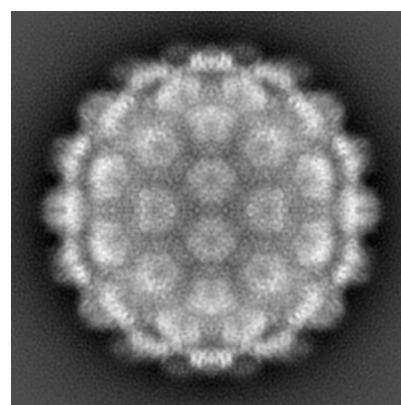
6.1.1 Primary map



X



Y

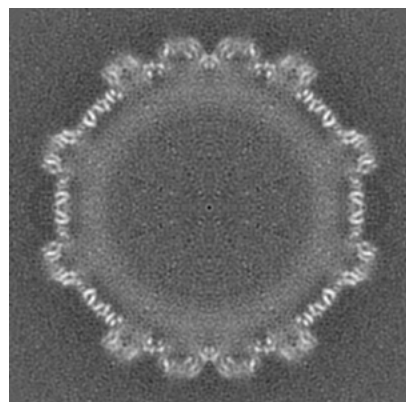


Z

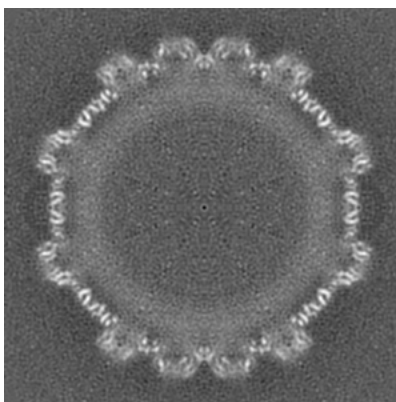
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

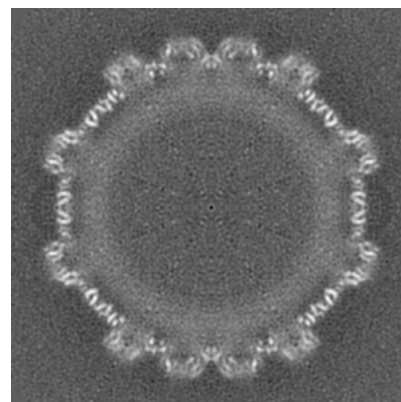
6.2.1 Primary map



X Index: 300



Y Index: 300

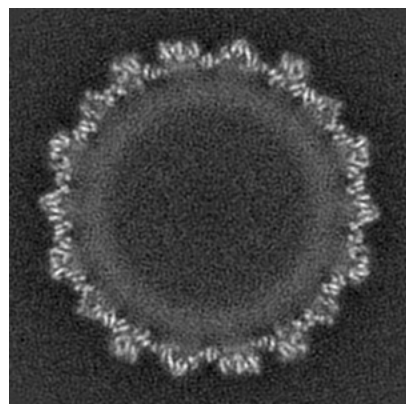


Z Index: 300

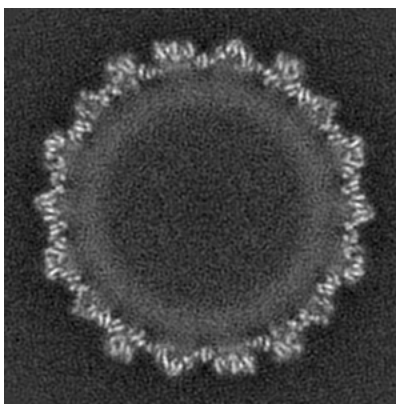
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

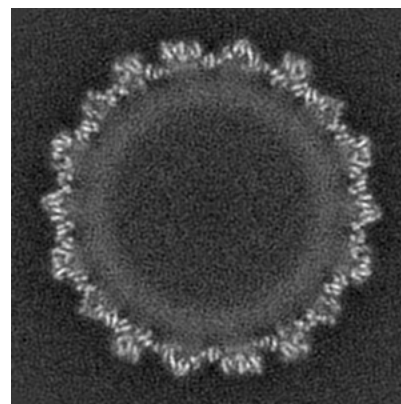
6.3.1 Primary map



X Index: 281



Y Index: 281

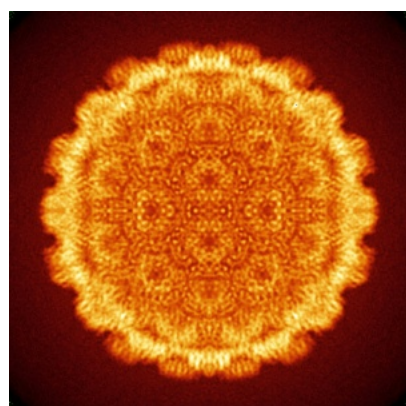


Z Index: 281

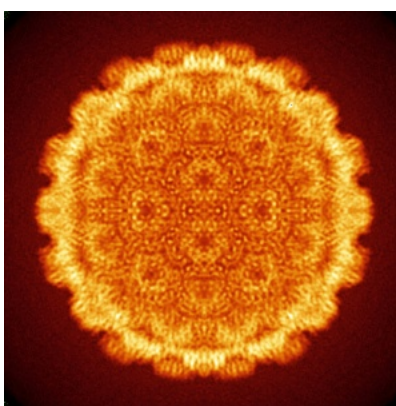
The images above show the largest variance slices of the map in three orthogonal directions.

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

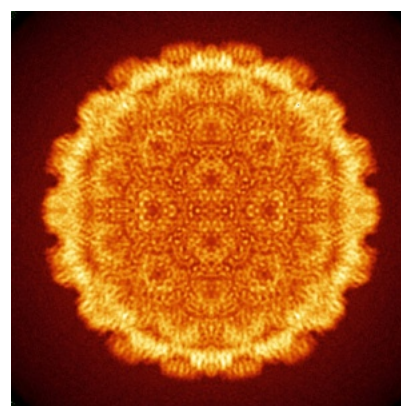
6.4.1 Primary map



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

This section was not generated.

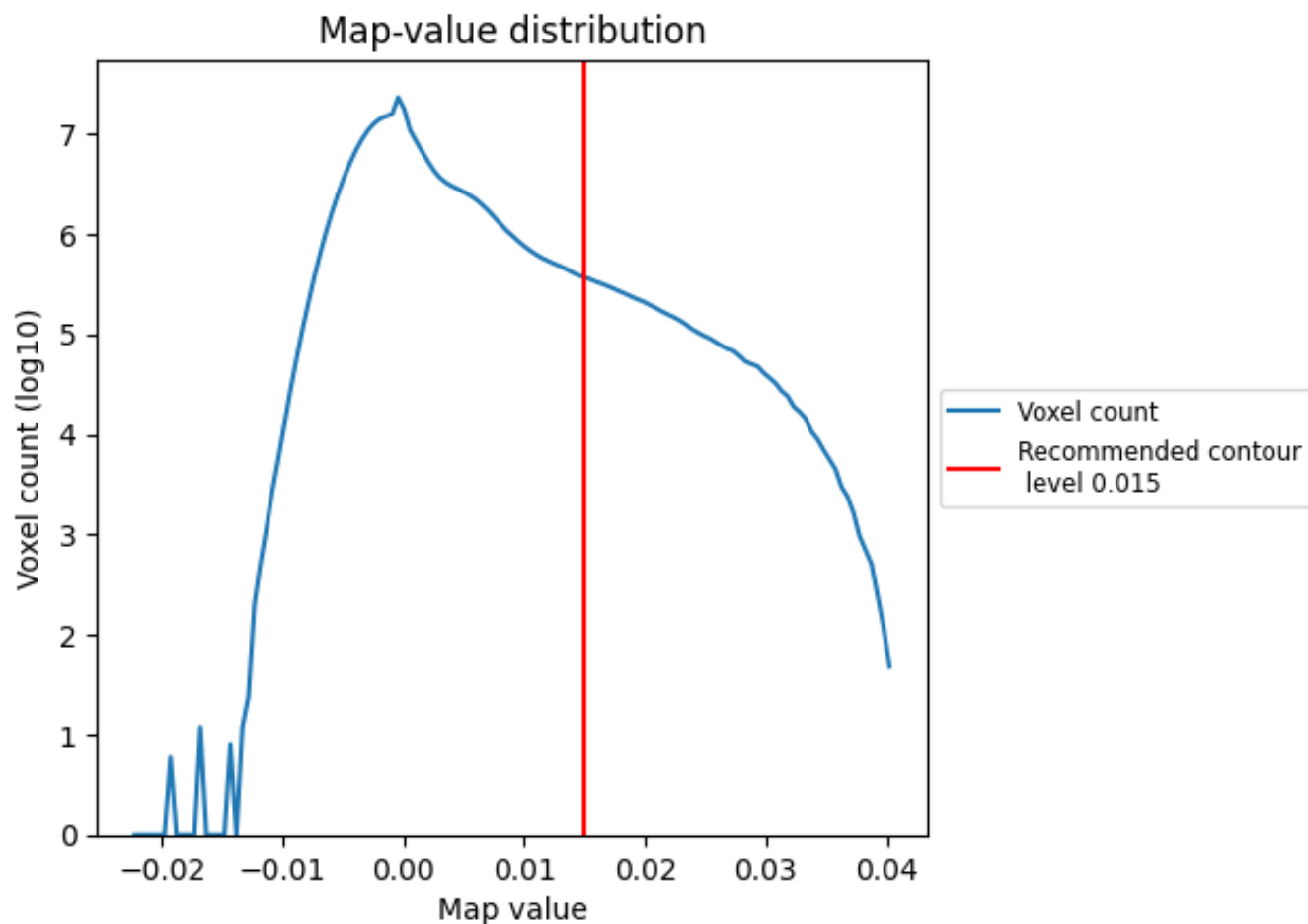
6.6 Mask visualisation

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

7 Map analysis [i](#)

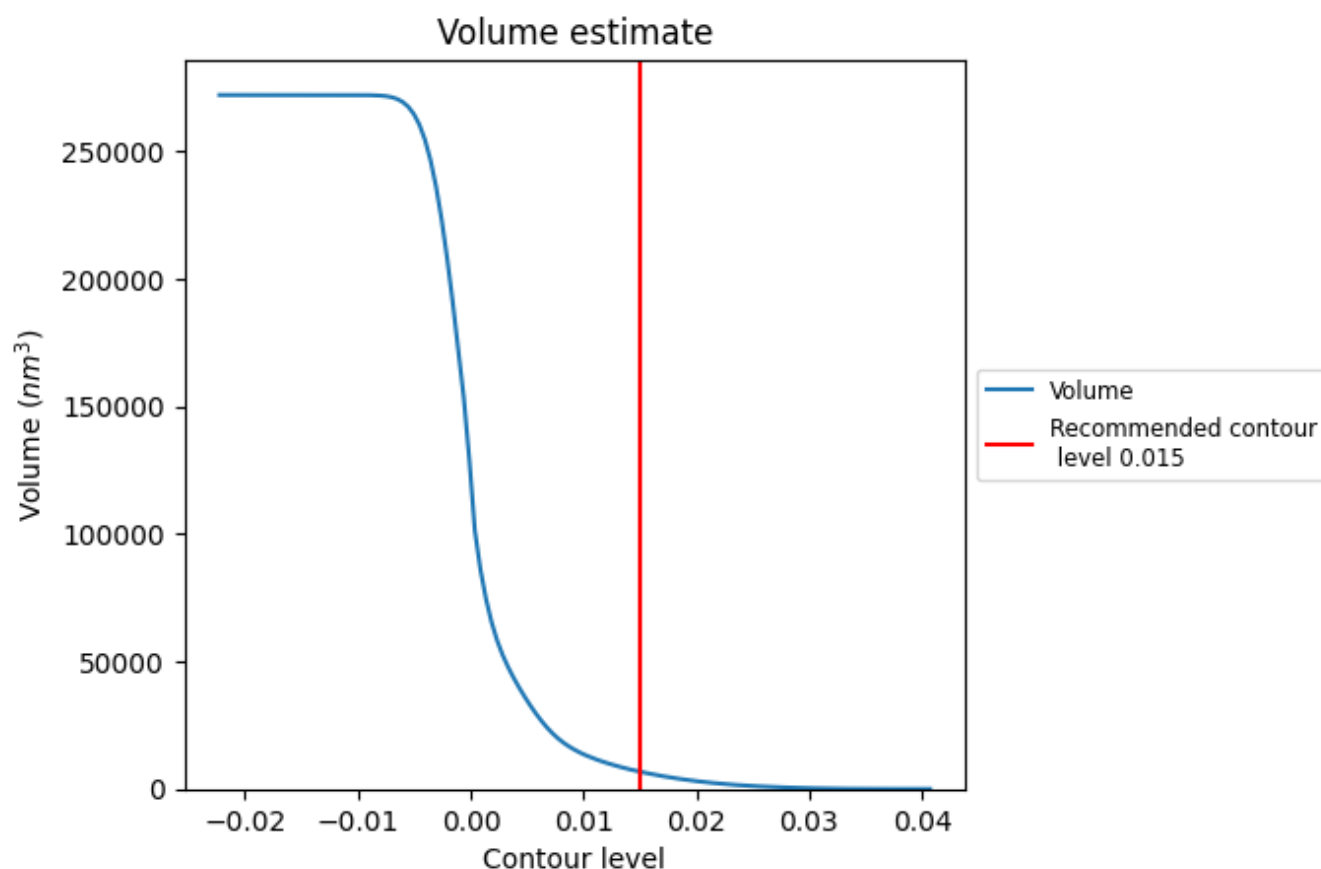
This section contains the results of statistical analysis of the map.

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.

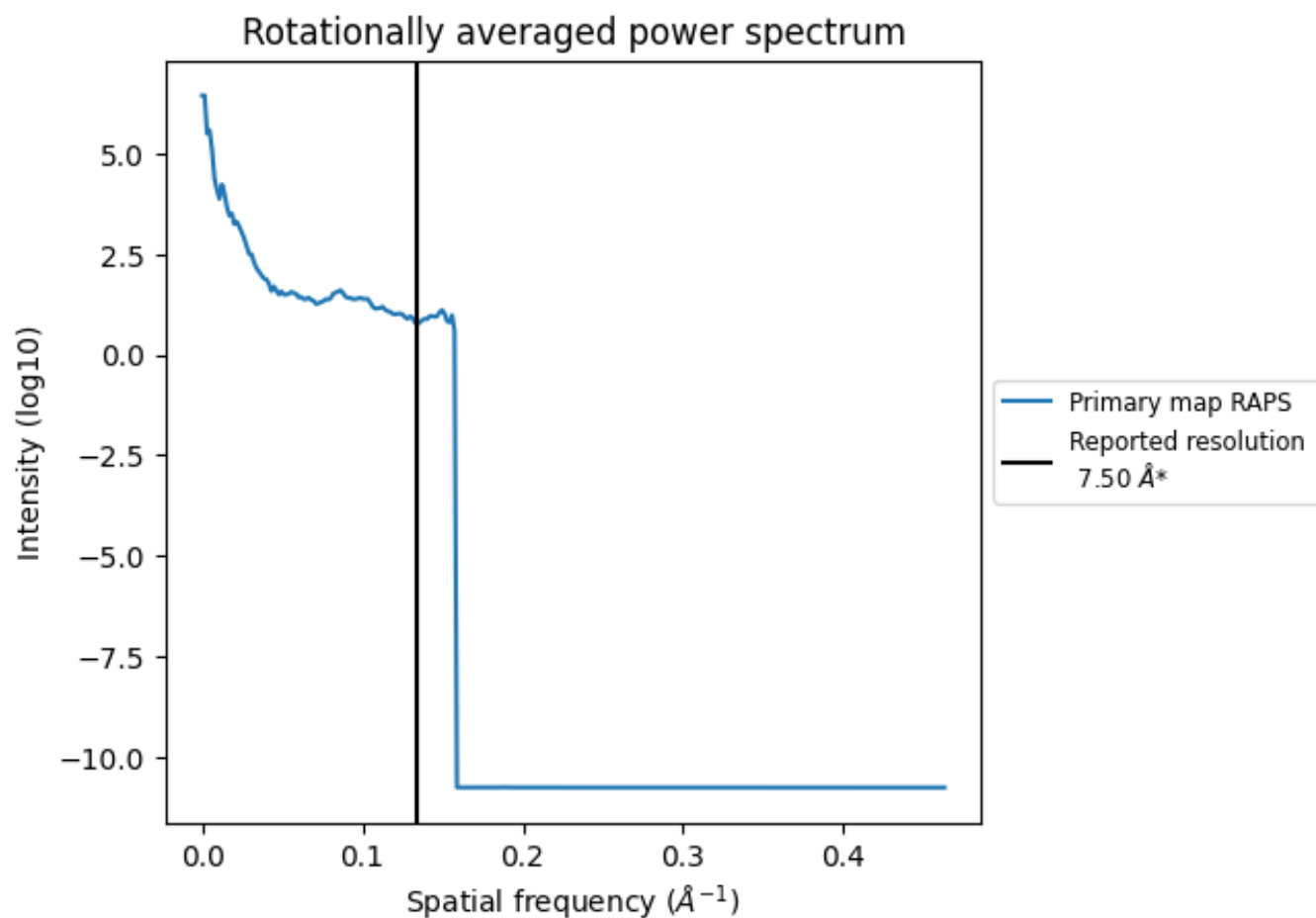
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6781 nm³; this corresponds to an approximate mass of 6125 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 ⓘ

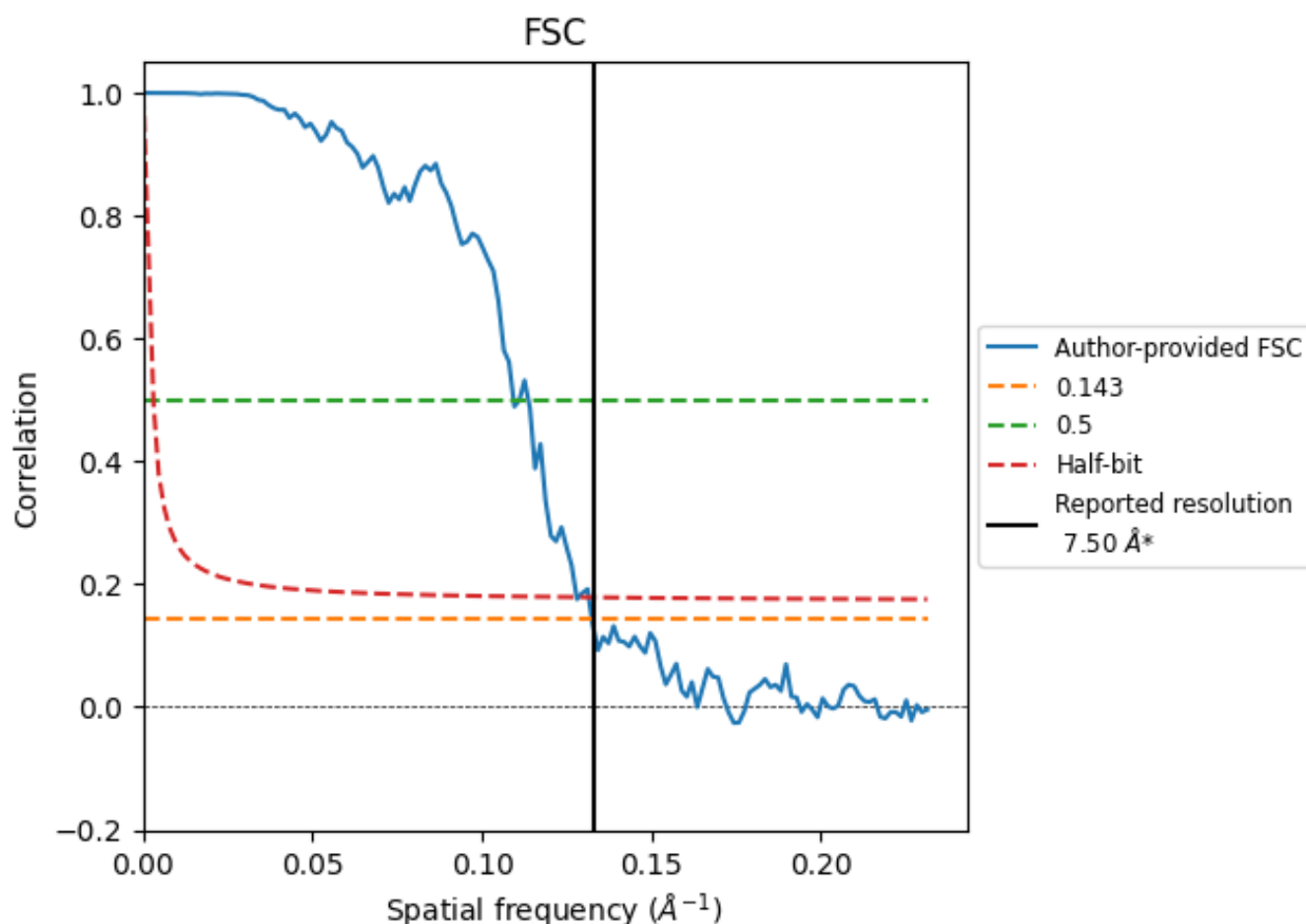


*Reported resolution corresponds to spatial frequency of 0.133 Å⁻¹

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 0.133 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.50	-	-
Author-provided FSC curve	7.55	9.15	7.81
Unmasked-calculated*	-	-	-

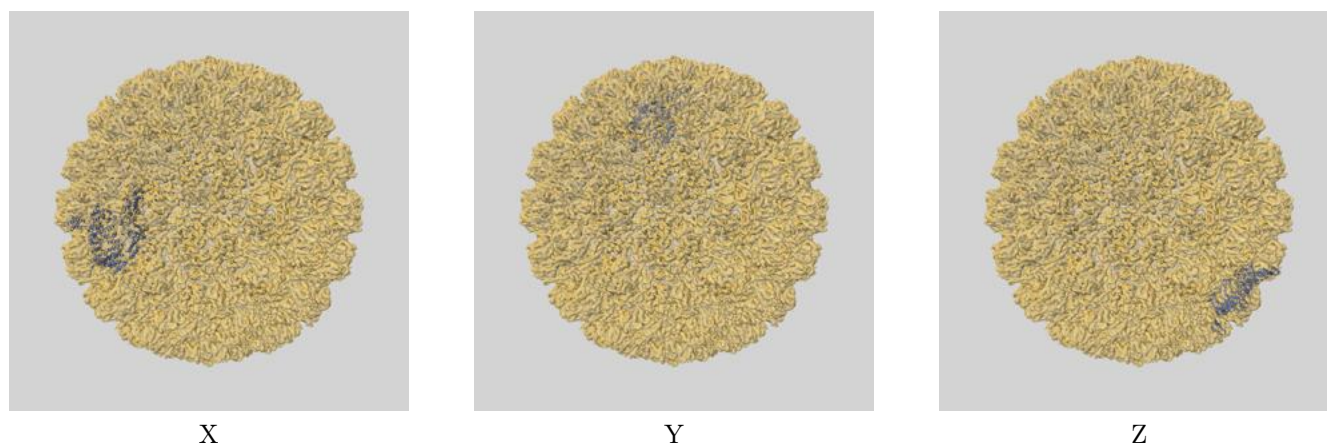
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

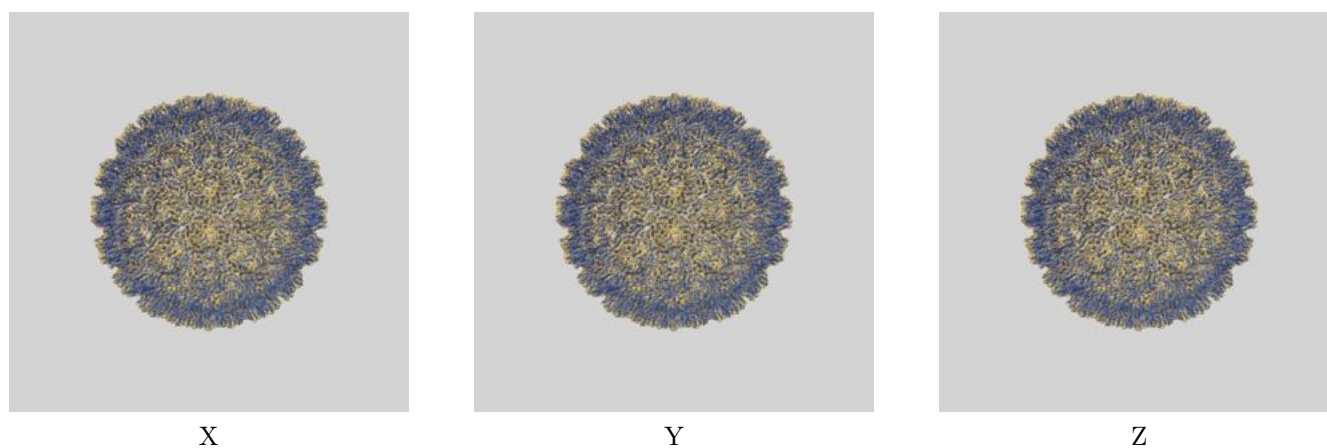
This section contains information regarding the fit between EMDB map EMD-4709 and PDB model 6R24. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

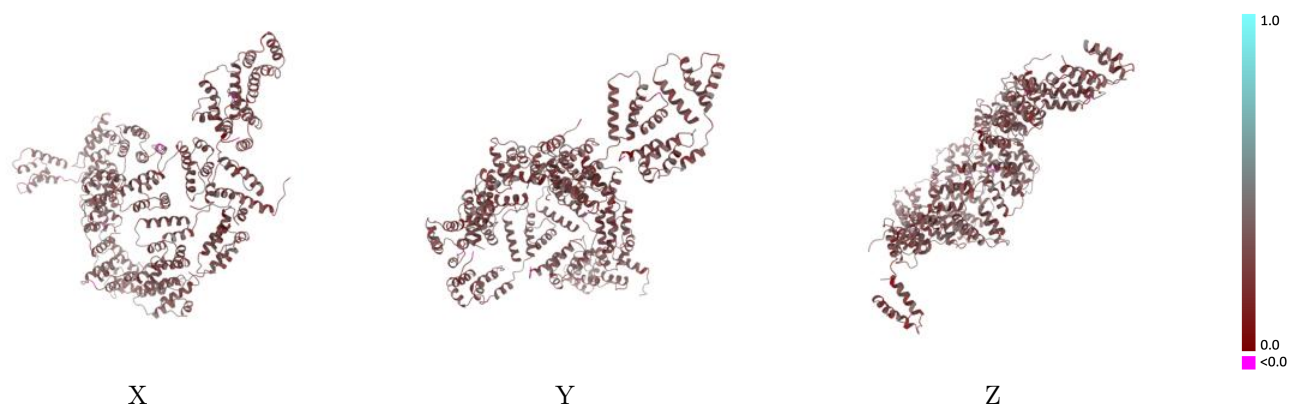


9.1.2 Map-model assembly overlay [i](#)



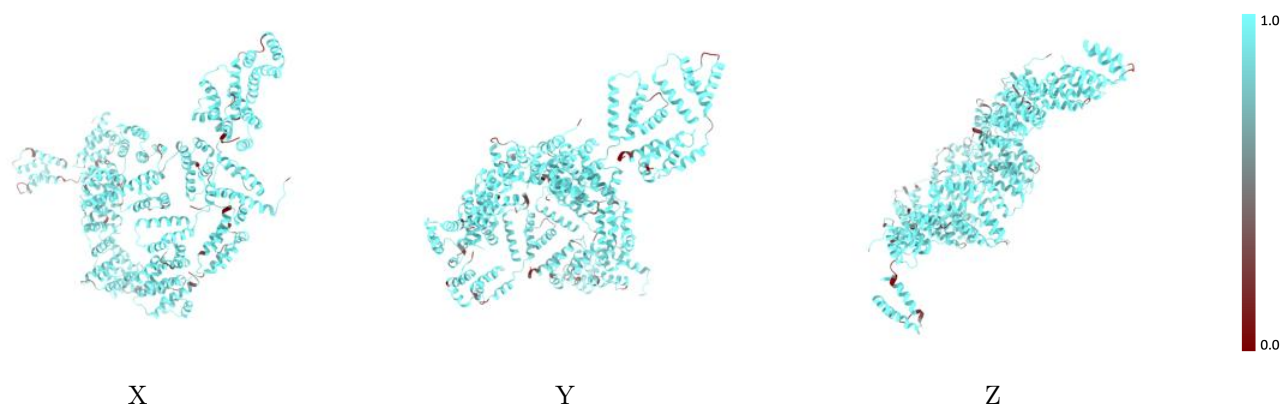
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



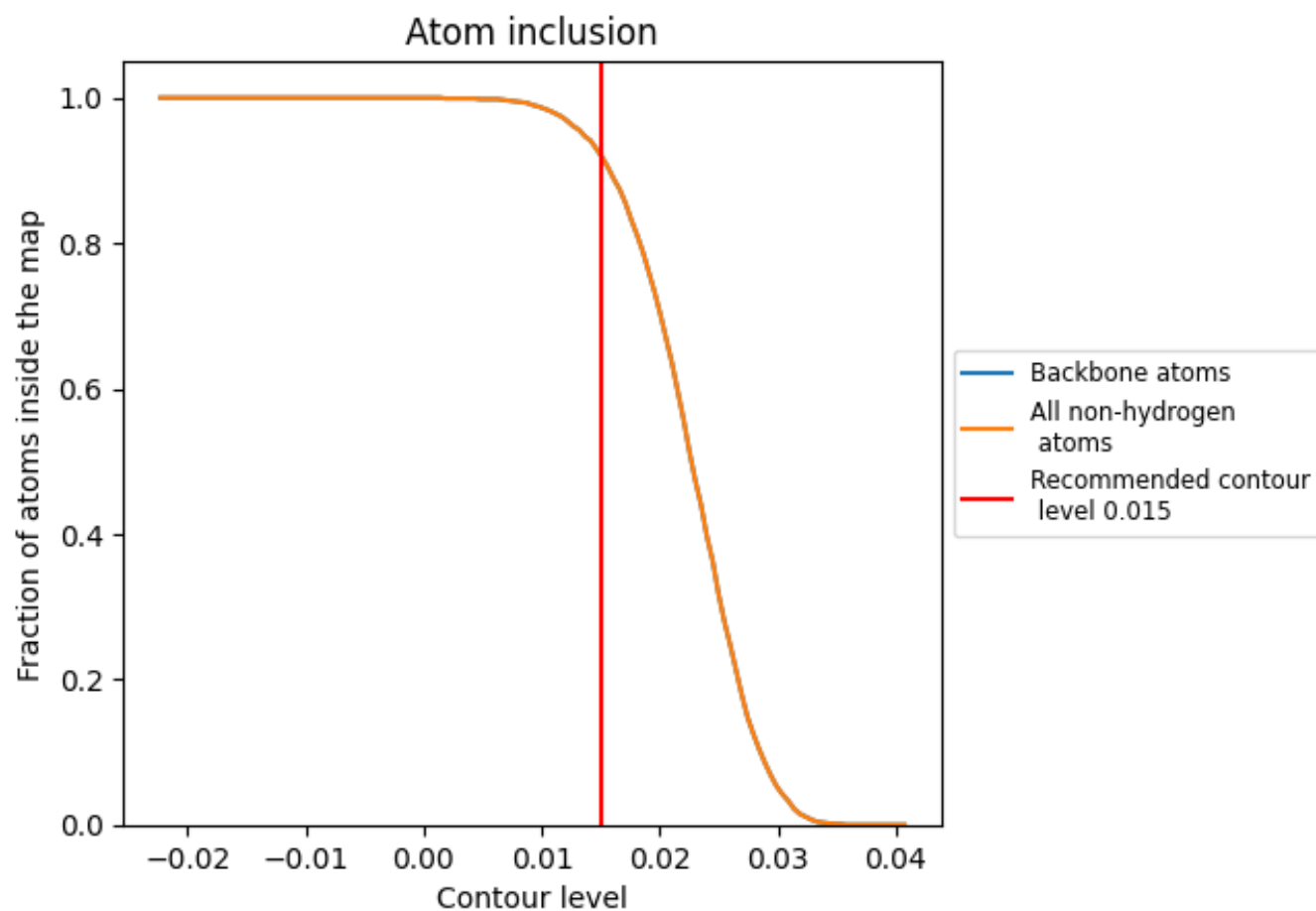
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9210	0.2970
A	0.8570	0.2860
B	0.9180	0.2970
C	0.9580	0.3040
D	0.9320	0.2980
E	0.9350	0.2890
F	0.9210	0.3020
G	0.9370	0.2990
H	0.9210	0.2970
I	0.9120	0.3020

1.0

0.0

<0.0