



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 12:37 PM UTC

PDB ID : 6GDI / pdb_00006gdi
EMDB ID : EMD-4391
Title : Structure of P-glycoprotein(ABCB1) in the post-hydrolytic state
Authors : Ford, R.C.; Thonghin, N.; Collins, R.F.; Barbieri, A.; Shafi, T.; Siebert, A.
Deposited on : 2018-04-23
Resolution : 7.90 Å(reported)
Based on initial model : 4KSB

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

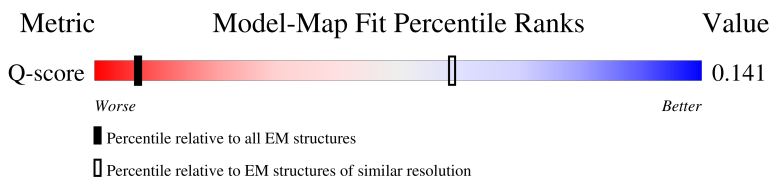
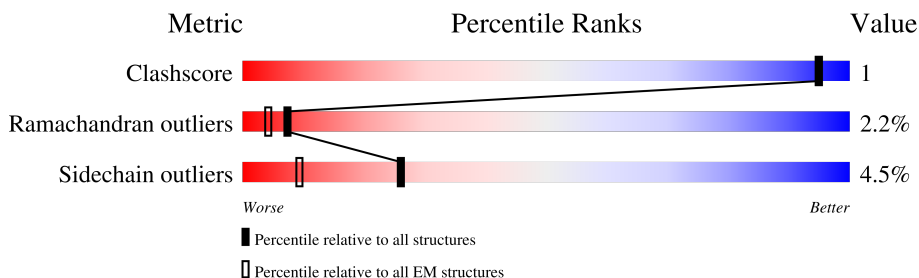
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	366 (7.40 - 8.40)

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	1284	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9171 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 Multidrug resistance protein 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1182	Total	C	N	O	S	0	0
			9171	5895	1552	1686	38		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1277	LEU	-	expression tag	UNP P21447
A	1278	GLU	-	expression tag	UNP P21447
A	1279	HIS	-	expression tag	UNP P21447
A	1280	HIS	-	expression tag	UNP P21447
A	1281	HIS	-	expression tag	UNP P21447
A	1282	HIS	-	expression tag	UNP P21447
A	1283	HIS	-	expression tag	UNP P21447
A	1284	HIS	-	expression tag	UNP P21447



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	135357	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 ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.220	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	165.35999, 165.35999, 165.35999	wwPDB
Map dimensions	156, 156, 156	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.27	332/9339 (3.6%)	2.51	671/12626 (5.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	25

All (332) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	GLN	CA-C	-10.48	1.38	1.52
1	A	1251	GLY	CA-C	-10.28	1.41	1.51
1	A	932	HIS	ND1-CE1	10.26	1.42	1.32
1	A	991	ALA	N-CA	-9.87	1.37	1.46
1	A	141	HIS	ND1-CE1	9.53	1.42	1.32
1	A	997	ALA	N-CA	-9.52	1.35	1.46
1	A	1089	SER	CA-C	-8.84	1.41	1.52
1	A	619	PHE	CA-CB	8.80	1.67	1.53
1	A	1246	LYS	CA-C	-8.71	1.42	1.52
1	A	347	ASN	C-N	8.68	1.44	1.33
1	A	71	PHE	CA-CB	8.50	1.67	1.53
1	A	407	LYS	C-N	8.46	1.43	1.32
1	A	712	PHE	C-N	8.41	1.45	1.33
1	A	492	THR	CA-C	-8.37	1.41	1.52
1	A	81	VAL	CA-C	-8.36	1.42	1.52
1	A	1083	TYR	N-CA	-8.30	1.36	1.46
1	A	458	ASN	C-N	8.25	1.44	1.33
1	A	861	VAL	CA-CB	-8.18	1.50	1.54
1	A	1061	THR	CA-C	-8.14	1.42	1.52
1	A	170	ARG	NE-CZ	8.13	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	ASN	C-N	8.03	1.44	1.33
1	A	689	PRO	C-N	8.01	1.44	1.33
1	A	863	ILE	C-N	7.99	1.43	1.34
1	A	199	GLY	CA-C	-7.91	1.43	1.52
1	A	967	PHE	C-N	7.83	1.43	1.33
1	A	991	ALA	CA-C	7.80	1.62	1.52
1	A	740	PRO	C-N	7.75	1.42	1.33
1	A	1225	VAL	CA-C	-7.73	1.42	1.52
1	A	194	ALA	CA-C	-7.71	1.42	1.52
1	A	912	PHE	CA-C	-7.63	1.42	1.52
1	A	750	LEU	N-CA	-7.58	1.36	1.46
1	A	242	ALA	N-CA	-7.57	1.37	1.46
1	A	133	CYS	N-CA	-7.46	1.38	1.46
1	A	973	VAL	C-N	7.44	1.43	1.33
1	A	755	PHE	CA-C	-7.43	1.45	1.53
1	A	1061	THR	N-CA	-7.42	1.36	1.46
1	A	1230	LEU	CA-C	-7.41	1.44	1.52
1	A	107	MET	N-CA	-7.33	1.37	1.46
1	A	292	ASN	C-N	7.27	1.43	1.33
1	A	463	ARG	NE-CZ	7.27	1.41	1.33
1	A	237	ASP	CA-C	-7.24	1.43	1.52
1	A	715	ILE	C-N	7.22	1.42	1.33
1	A	1197	GLU	CA-C	-7.21	1.46	1.53
1	A	414	LYS	C-N	7.20	1.43	1.33
1	A	517	ASP	C-N	7.19	1.43	1.33
1	A	1230	LEU	N-CA	-7.19	1.37	1.46
1	A	279	GLU	C-N	7.14	1.43	1.34
1	A	1115	GLU	N-CA	-7.13	1.39	1.46
1	A	243	TYR	C-N	7.08	1.43	1.33
1	A	497	GLU	N-CA	-7.01	1.38	1.46
1	A	573	ARG	NE-CZ	6.99	1.40	1.33
1	A	61	GLY	CA-C	6.99	1.60	1.52
1	A	708	VAL	N-CA	6.97	1.55	1.46
1	A	1206	SER	C-N	6.96	1.43	1.33
1	A	79	ALA	CA-C	-6.96	1.44	1.52
1	A	545	PRO	CA-C	-6.93	1.46	1.53
1	A	541	LEU	CA-CB	6.93	1.64	1.53
1	A	201	ILE	C-N	6.91	1.42	1.33
1	A	131	PHE	N-CA	-6.88	1.38	1.46
1	A	390	PHE	N-CA	-6.86	1.37	1.46
1	A	1020	GLN	CA-C	-6.83	1.43	1.53
1	A	311	TRP	NE1-CE2	6.82	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	712	PHE	CA-CB	6.81	1.64	1.53
1	A	724	PHE	CA-CB	6.77	1.64	1.53
1	A	715	ILE	CA-C	-6.76	1.44	1.52
1	A	1078	LEU	C-N	6.76	1.43	1.34
1	A	296	GLY	CA-C	-6.74	1.44	1.52
1	A	1165	VAL	CA-C	-6.71	1.44	1.52
1	A	196	PHE	CA-CB	6.70	1.62	1.53
1	A	400	ARG	NE-CZ	6.70	1.40	1.33
1	A	934	PHE	N-CA	-6.69	1.38	1.46
1	A	751	PHE	CA-CB	6.68	1.63	1.53
1	A	225	ALA	C-N	6.67	1.41	1.34
1	A	1245	GLY	C-N	6.66	1.42	1.33
1	A	197	PHE	N-CA	-6.65	1.38	1.46
1	A	774	GLY	C-N	6.63	1.42	1.34
1	A	111	ALA	CA-C	-6.62	1.44	1.52
1	A	840	GLY	CA-C	-6.62	1.42	1.51
1	A	1239	ILE	C-N	6.62	1.42	1.33
1	A	410	ASN	CA-C	-6.61	1.45	1.52
1	A	905	SER	CA-C	-6.61	1.44	1.52
1	A	617	ILE	CA-CB	-6.60	1.46	1.54
1	A	1211	GLN	CA-CB	6.60	1.63	1.53
1	A	1250	HIS	C-N	6.59	1.41	1.32
1	A	598	ASP	C-N	6.57	1.41	1.33
1	A	1132	ASN	CA-C	-6.56	1.44	1.52
1	A	988	SER	C-N	6.51	1.42	1.33
1	A	1069	GLY	C-N	6.51	1.42	1.33
1	A	863	ILE	CA-CB	-6.49	1.46	1.54
1	A	1045	SER	CA-CB	6.45	1.64	1.54
1	A	1082	PHE	CA-C	-6.44	1.44	1.52
1	A	268	LYS	N-CA	-6.43	1.38	1.46
1	A	611	LEU	CA-C	-6.42	1.44	1.52
1	A	1091	PHE	CA-C	-6.41	1.44	1.52
1	A	887	GLU	C-N	6.40	1.42	1.33
1	A	771	PHE	N-CA	-6.39	1.38	1.46
1	A	849	TYR	CA-CB	6.37	1.62	1.53
1	A	851	TRP	CA-CB	6.37	1.62	1.53
1	A	776	ALA	N-CA	-6.36	1.38	1.46
1	A	328	LEU	CA-C	-6.36	1.44	1.52
1	A	1195	LEU	CA-C	-6.35	1.45	1.52
1	A	685	ASP	CA-CB	6.35	1.61	1.53
1	A	778	GLU	C-N	6.34	1.41	1.33
1	A	829	LEU	CA-CB	6.34	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	HIS	CA-C	6.33	1.60	1.52
1	A	388	LEU	CA-C	-6.33	1.45	1.52
1	A	1100	LEU	N-CA	-6.33	1.38	1.46
1	A	775	LYS	N-CA	-6.32	1.38	1.46
1	A	555	SER	CA-C	-6.31	1.45	1.52
1	A	1203	ASP	CA-C	-6.27	1.44	1.52
1	A	802	ASP	CA-C	-6.27	1.45	1.52
1	A	836	ILE	N-CA	-6.25	1.38	1.46
1	A	1245	GLY	CA-C	-6.24	1.42	1.51
1	A	798	SER	CA-CB	6.24	1.62	1.53
1	A	488	ARG	CA-C	-6.24	1.44	1.52
1	A	304	ALA	C-N	6.24	1.42	1.33
1	A	557	LEU	N-CA	-6.23	1.37	1.45
1	A	582	ALA	N-CA	-6.21	1.38	1.45
1	A	430	SER	N-CA	-6.21	1.38	1.46
1	A	695	ARG	C-N	6.19	1.42	1.33
1	A	1178	GLN	N-CA	6.18	1.53	1.46
1	A	363	LYS	CA-C	-6.17	1.44	1.52
1	A	901	ARG	NE-CZ	6.14	1.39	1.33
1	A	591	ALA	CA-C	-6.14	1.44	1.52
1	A	355	ARG	CD-NE	6.13	1.54	1.46
1	A	578	THR	N-CA	-6.12	1.38	1.45
1	A	234	SER	CA-C	-6.12	1.45	1.52
1	A	501	LYS	N-CA	-6.11	1.38	1.46
1	A	394	HIS	CB-CG	6.11	1.58	1.50
1	A	736	THR	N-CA	-6.10	1.39	1.46
1	A	1212	GLU	CA-CB	6.10	1.62	1.53
1	A	1054	LEU	C-N	6.07	1.41	1.33
1	A	1175	GLY	C-N	6.06	1.42	1.33
1	A	1255	GLN	CA-C	-6.05	1.45	1.52
1	A	56	ALA	C-N	6.05	1.42	1.34
1	A	1184	ARG	N-CA	-6.03	1.39	1.46
1	A	1025	ASN	C-N	6.02	1.41	1.33
1	A	1236	ALA	C-N	6.01	1.41	1.33
1	A	1229	ARG	NE-CZ	6.00	1.39	1.33
1	A	228	TRP	CA-C	-5.98	1.45	1.52
1	A	797	VAL	C-N	5.96	1.42	1.33
1	A	237	ASP	CA-CB	5.95	1.62	1.53
1	A	462	LEU	C-N	5.95	1.41	1.33
1	A	507	ASP	N-CA	-5.93	1.40	1.47
1	A	584	ARG	CA-C	-5.93	1.45	1.52
1	A	144	ARG	CZ-NH2	5.93	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	749	ASN	N-CA	-5.92	1.39	1.46
1	A	816	ASN	CA-CB	5.92	1.62	1.53
1	A	693	PHE	CA-CB	5.91	1.64	1.53
1	A	142	LYS	C-N	5.90	1.41	1.33
1	A	57	ALA	C-N	5.89	1.41	1.33
1	A	932	HIS	CA-CB	5.89	1.62	1.53
1	A	130	SER	CA-CB	5.89	1.62	1.53
1	A	1200	SER	CA-C	-5.88	1.45	1.52
1	A	548	LEU	N-CA	-5.87	1.38	1.46
1	A	777	GLY	N-CA	5.86	1.53	1.45
1	A	245	LYS	N-CA	-5.85	1.39	1.46
1	A	699	LEU	CA-C	-5.85	1.44	1.52
1	A	449	ILE	C-N	5.84	1.39	1.33
1	A	1140	GLU	C-N	5.84	1.40	1.34
1	A	783	ARG	CD-NE	5.83	1.54	1.46
1	A	206	ARG	C-N	5.82	1.42	1.33
1	A	584	ARG	N-CA	5.82	1.53	1.46
1	A	817	ASP	CA-C	5.82	1.60	1.52
1	A	534	ARG	N-CA	5.81	1.53	1.46
1	A	448	SER	N-CA	-5.81	1.39	1.46
1	A	459	VAL	CA-CB	-5.81	1.47	1.54
1	A	897	ILE	N-CA	-5.81	1.38	1.46
1	A	531	GLN	CA-C	-5.80	1.45	1.52
1	A	1133	SER	CA-C	-5.80	1.45	1.52
1	A	529	GLY	CA-C	5.79	1.58	1.52
1	A	221	LEU	C-N	5.76	1.41	1.34
1	A	1027	LEU	C-N	5.76	1.41	1.33
1	A	1076	VAL	CA-C	-5.76	1.45	1.52
1	A	1232	THR	C-N	5.75	1.40	1.33
1	A	227	ILE	C-N	5.75	1.41	1.33
1	A	345	SER	CA-C	5.73	1.60	1.52
1	A	970	VAL	N-CA	-5.73	1.38	1.46
1	A	1093	ASP	CA-C	-5.73	1.45	1.52
1	A	332	PHE	CA-CB	5.72	1.62	1.53
1	A	174	ASP	N-CA	5.71	1.53	1.46
1	A	689	PRO	CA-C	-5.71	1.46	1.52
1	A	1189	GLN	CA-CB	5.71	1.62	1.53
1	A	349	GLU	CA-C	5.71	1.60	1.52
1	A	146	LYS	C-N	5.70	1.41	1.33
1	A	1112	VAL	CA-CB	-5.69	1.46	1.54
1	A	903	VAL	CA-CB	5.68	1.61	1.54
1	A	391	LYS	CA-C	-5.68	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	982	MET	CA-CB	5.67	1.62	1.53
1	A	542	VAL	C-N	5.67	1.41	1.33
1	A	801	ASP	N-CA	5.65	1.53	1.46
1	A	337	GLY	C-N	5.64	1.42	1.33
1	A	945	MET	CA-CB	5.64	1.62	1.53
1	A	1207	GLU	CA-C	-5.64	1.45	1.52
1	A	925	ARG	CD-NE	5.63	1.54	1.46
1	A	1078	LEU	CA-C	-5.61	1.45	1.52
1	A	316	LEU	CA-CB	5.61	1.63	1.53
1	A	794	ARG	NE-CZ	5.61	1.39	1.33
1	A	355	ARG	CA-C	-5.61	1.46	1.52
1	A	936	ILE	C-N	5.61	1.40	1.33
1	A	828	ARG	CA-CB	5.60	1.62	1.53
1	A	617	ILE	CB-CG1	5.60	1.64	1.53
1	A	165	GLY	C-N	5.60	1.42	1.33
1	A	239	GLU	C-N	5.60	1.41	1.33
1	A	282	ARG	CD-NE	5.59	1.54	1.46
1	A	848	ILE	CA-C	-5.58	1.44	1.52
1	A	1036	VAL	CA-CB	-5.58	1.47	1.54
1	A	553	ALA	CA-C	-5.57	1.44	1.52
1	A	1076	VAL	C-N	5.57	1.41	1.33
1	A	825	THR	CA-C	5.56	1.60	1.52
1	A	289	ILE	CA-C	5.56	1.59	1.52
1	A	1208	LYS	C-N	5.56	1.40	1.34
1	A	493	MET	C-N	5.54	1.41	1.33
1	A	787	MET	C-N	5.53	1.40	1.33
1	A	856	LEU	N-CA	-5.53	1.39	1.46
1	A	1231	SER	C-N	-5.52	1.25	1.34
1	A	204	PHE	C-N	5.51	1.41	1.33
1	A	373	SER	N-CA	-5.50	1.39	1.46
1	A	545	PRO	C-O	-5.50	1.16	1.23
1	A	1131	ASP	N-CA	5.50	1.53	1.46
1	A	359	TYR	C-N	5.50	1.41	1.33
1	A	498	LYS	CA-CB	5.49	1.62	1.53
1	A	1215	ASP	N-CA	-5.49	1.39	1.46
1	A	389	GLU	C-O	-5.49	1.17	1.24
1	A	1164	ARG	NE-CZ	5.48	1.39	1.33
1	A	83	ASN	CA-C	-5.47	1.45	1.52
1	A	721	GLN	N-CA	-5.47	1.41	1.46
1	A	889	SER	CA-C	-5.47	1.45	1.52
1	A	492	THR	C-N	5.46	1.41	1.34
1	A	117	ILE	N-CA	5.46	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	730	LYS	C-N	5.45	1.41	1.33
1	A	606	GLY	N-CA	-5.45	1.39	1.45
1	A	956	GLY	CA-C	-5.45	1.46	1.52
1	A	1269	VAL	C-N	5.45	1.41	1.34
1	A	570	ASP	N-CA	5.43	1.52	1.46
1	A	784	LEU	N-CA	-5.43	1.40	1.46
1	A	1128	ALA	CA-C	-5.43	1.46	1.52
1	A	515	GLN	CA-C	-5.42	1.48	1.53
1	A	896	ALA	C-N	5.42	1.40	1.33
1	A	1218	ARG	CA-C	-5.42	1.45	1.52
1	A	941	THR	N-CA	-5.42	1.39	1.46
1	A	1213	ALA	N-CA	-5.42	1.39	1.46
1	A	948	SER	CA-C	-5.42	1.46	1.52
1	A	179	ASN	CA-C	-5.41	1.45	1.52
1	A	454	ILE	C-O	-5.41	1.17	1.24
1	A	568	ALA	C-O	5.41	1.30	1.24
1	A	208	TRP	CA-C	5.40	1.59	1.52
1	A	1219	GLU	CA-CB	5.40	1.60	1.53
1	A	1031	VAL	C-O	-5.40	1.18	1.24
1	A	119	ALA	CA-C	-5.39	1.45	1.52
1	A	601	VAL	CA-C	-5.38	1.46	1.52
1	A	1151	HIS	ND1-CE1	5.37	1.38	1.32
1	A	261	ILE	CA-CB	-5.36	1.48	1.54
1	A	453	ASP	CA-C	-5.36	1.45	1.52
1	A	912	PHE	CA-CB	5.35	1.61	1.53
1	A	1250	HIS	CA-C	-5.35	1.45	1.52
1	A	873	LYS	CA-C	5.35	1.59	1.52
1	A	299	PHE	CA-CB	5.35	1.62	1.53
1	A	750	LEU	C-O	-5.35	1.17	1.24
1	A	1135	VAL	N-CA	-5.34	1.40	1.46
1	A	1198	ALA	CA-C	-5.34	1.45	1.52
1	A	733	GLY	N-CA	-5.34	1.39	1.45
1	A	160	ASP	CA-C	-5.33	1.45	1.52
1	A	1055	GLU	CA-C	-5.33	1.45	1.52
1	A	138	ARG	CD-NE	5.31	1.53	1.46
1	A	1229	ARG	CA-CB	5.31	1.61	1.53
1	A	514	HIS	CA-C	-5.30	1.45	1.52
1	A	449	ILE	CA-CB	5.29	1.60	1.54
1	A	851	TRP	NE1-CE2	5.29	1.43	1.37
1	A	805	ASN	N-CA	5.28	1.52	1.46
1	A	925	ARG	C-N	-5.26	1.26	1.34
1	A	110	TYR	CA-C	-5.25	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1054	LEU	CA-C	-5.24	1.46	1.52
1	A	1202	LEU	CA-C	-5.23	1.46	1.52
1	A	103	LEU	C-O	-5.22	1.18	1.24
1	A	1133	SER	C-N	5.22	1.41	1.33
1	A	478	THR	CA-CB	5.22	1.61	1.53
1	A	492	THR	N-CA	-5.22	1.39	1.45
1	A	768	LEU	N-CA	5.22	1.52	1.46
1	A	1019	THR	N-CA	5.22	1.52	1.46
1	A	805	ASN	C-N	5.21	1.41	1.33
1	A	298	ALA	C-N	5.21	1.41	1.34
1	A	1102	VAL	N-CA	5.21	1.52	1.46
1	A	895	GLU	C-N	5.21	1.40	1.33
1	A	903	VAL	C-N	5.21	1.40	1.33
1	A	100	PHE	C-N	5.21	1.40	1.33
1	A	355	ARG	C-N	5.20	1.40	1.33
1	A	539	ARG	N-CA	-5.20	1.40	1.46
1	A	696	ILE	CA-C	5.20	1.59	1.52
1	A	1199	THR	N-CA	-5.19	1.41	1.46
1	A	408	GLY	C-O	5.19	1.30	1.23
1	A	1184	ARG	CD-NE	5.19	1.53	1.46
1	A	756	LEU	CA-CB	5.18	1.61	1.53
1	A	813	ARG	CZ-NH2	5.18	1.40	1.33
1	A	537	ILE	C-O	5.18	1.29	1.24
1	A	164	VAL	CA-C	5.17	1.59	1.52
1	A	1110	GLY	C-N	5.17	1.41	1.33
1	A	300	LEU	CA-C	5.17	1.59	1.52
1	A	611	LEU	N-CA	-5.17	1.40	1.46
1	A	1218	ARG	CD-NE	5.17	1.53	1.46
1	A	1191	HIS	CG-ND1	5.17	1.44	1.38
1	A	694	TRP	CA-CB	5.16	1.62	1.53
1	A	290	THR	C-N	5.16	1.40	1.33
1	A	730	LYS	C-O	-5.16	1.18	1.24
1	A	939	SER	C-N	5.16	1.41	1.33
1	A	516	PHE	C-N	5.14	1.40	1.33
1	A	751	PHE	N-CA	-5.14	1.40	1.46
1	A	875	LEU	CA-CB	5.14	1.61	1.53
1	A	170	ARG	CA-C	-5.12	1.46	1.52
1	A	350	ALA	C-N	5.12	1.40	1.33
1	A	1178	GLN	CA-C	5.12	1.59	1.52
1	A	244	ALA	N-CA	-5.11	1.40	1.46
1	A	122	LEU	CA-CB	5.11	1.61	1.53
1	A	812	THR	C-N	5.11	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	894	THR	N-CA	-5.10	1.40	1.46
1	A	931	ALA	C-N	5.08	1.40	1.33
1	A	221	LEU	CA-CB	5.08	1.61	1.53
1	A	605	GLN	CA-C	-5.08	1.46	1.52
1	A	1087	ALA	C-N	5.08	1.40	1.33
1	A	917	ALA	CA-C	-5.08	1.46	1.52
1	A	710	GLY	CA-C	-5.07	1.46	1.52
1	A	893	ALA	C-N	5.07	1.40	1.34
1	A	604	GLU	N-CA	-5.06	1.39	1.45
1	A	324	ILE	C-O	-5.05	1.19	1.24
1	A	864	ILE	N-CA	5.05	1.52	1.46
1	A	893	ALA	CA-C	-5.05	1.46	1.52
1	A	1194	LEU	N-CA	-5.05	1.40	1.46
1	A	374	PHE	CA-C	-5.05	1.46	1.52
1	A	41	TYR	CA-CB	5.04	1.61	1.53
1	A	254	LEU	CA-C	-5.04	1.46	1.52
1	A	1048	VAL	C-N	5.01	1.40	1.33
1	A	727	ILE	N-CA	-5.01	1.40	1.46

All (671) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	739	GLY	CA-C-N	11.33	132.05	120.38
1	A	739	GLY	C-N-CA	11.33	132.05	120.38
1	A	1233	ILE	N-CA-C	-10.48	102.84	112.90
1	A	371	ILE	N-CA-C	-10.44	102.50	112.83
1	A	941	THR	CA-C-O	-9.81	110.15	120.55
1	A	139	GLN	N-CA-C	9.76	121.68	111.14
1	A	110	TYR	CA-C-N	9.53	133.05	120.28
1	A	110	TYR	C-N-CA	9.53	133.05	120.28
1	A	276	ASN	CA-CB-CG	-9.43	103.17	112.60
1	A	391	LYS	CA-C-N	9.19	135.11	122.34
1	A	391	LYS	C-N-CA	9.19	135.11	122.34
1	A	310	PHE	CA-C-N	9.17	132.36	120.44
1	A	310	PHE	C-N-CA	9.17	132.36	120.44
1	A	162	HIS	CE1-NE2-CD2	-9.10	99.90	109.00
1	A	58	ILE	O-C-N	9.07	131.28	121.94
1	A	908	ARG	NE-CZ-NH2	9.06	127.36	119.20
1	A	95	ASP	CA-CB-CG	9.00	121.60	112.60
1	A	119	ALA	CA-C-N	8.97	129.89	119.94
1	A	119	ALA	C-N-CA	8.97	129.89	119.94
1	A	456	THR	N-CA-C	-8.93	100.24	114.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ILE	CA-C-O	-8.92	111.71	121.17
1	A	878	GLN	CA-C-O	-8.90	110.36	120.24
1	A	811	THR	CA-C-N	8.84	132.13	120.28
1	A	811	THR	C-N-CA	8.84	132.13	120.28
1	A	852	GLN	N-CA-C	-8.74	100.29	112.45
1	A	613	ARG	NE-CZ-NH2	-8.72	111.36	119.20
1	A	205	THR	O-C-N	8.70	131.34	122.12
1	A	324	ILE	N-CA-C	-8.65	103.30	113.42
1	A	1020	GLN	CA-C-N	8.64	129.57	119.98
1	A	1020	GLN	C-N-CA	8.64	129.57	119.98
1	A	113	TYR	N-CA-C	-8.62	98.37	111.56
1	A	737	ASN	N-CA-C	8.55	122.10	110.55
1	A	695	ARG	NE-CZ-NH2	8.55	126.89	119.20
1	A	938	PHE	CA-C-N	8.51	131.50	120.44
1	A	938	PHE	C-N-CA	8.51	131.50	120.44
1	A	1161	TYR	N-CA-C	8.43	122.67	112.38
1	A	695	ARG	NE-CZ-NH1	-8.42	113.08	121.50
1	A	1023	LYS	CA-C-O	-8.39	111.80	119.86
1	A	210	LEU	CA-C-N	8.39	131.34	120.44
1	A	210	LEU	C-N-CA	8.39	131.34	120.44
1	A	206	ARG	N-CA-C	-8.38	103.06	113.28
1	A	1261	GLY	CA-C-N	8.37	131.39	120.60
1	A	1261	GLY	C-N-CA	8.37	131.39	120.60
1	A	558	ASP	CA-CB-CG	-8.31	104.29	112.60
1	A	155	GLU	CA-C-N	8.26	132.18	120.53
1	A	155	GLU	C-N-CA	8.26	132.18	120.53
1	A	593	VAL	N-CA-C	-8.22	96.28	108.45
1	A	991	ALA	CA-C-N	8.21	127.89	119.19
1	A	991	ALA	C-N-CA	8.21	127.89	119.19
1	A	162	HIS	ND1-CE1-NE2	8.17	116.57	108.40
1	A	1028	GLU	N-CA-C	-8.16	102.27	112.72
1	A	984	VAL	CA-C-N	8.13	128.97	119.94
1	A	984	VAL	C-N-CA	8.13	128.97	119.94
1	A	358	ALA	CA-C-N	8.10	132.62	120.31
1	A	358	ALA	C-N-CA	8.10	132.62	120.31
1	A	917	ALA	CA-C-O	-8.06	112.35	120.82
1	A	740	PRO	CA-C-O	-8.01	108.95	120.56
1	A	1092	LEU	N-CA-C	-7.92	103.42	113.72
1	A	424	ASN	N-CA-C	-7.92	103.20	113.17
1	A	510	MET	N-CA-CB	7.91	121.55	110.07
1	A	816	ASN	CA-C-N	7.91	130.72	120.44
1	A	816	ASN	C-N-CA	7.91	130.72	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1228	HIS	CA-CB-CG	7.87	121.67	113.80
1	A	991	ALA	O-C-N	-7.84	113.50	120.48
1	A	513	PRO	O-C-N	7.79	131.47	122.98
1	A	598	ASP	N-CA-C	-7.78	103.37	113.17
1	A	595	ALA	CA-C-N	7.75	129.08	121.57
1	A	595	ALA	C-N-CA	7.75	129.08	121.57
1	A	100	PHE	CA-C-N	7.72	130.47	120.44
1	A	100	PHE	C-N-CA	7.72	130.47	120.44
1	A	709	VAL	N-CA-C	-7.71	101.11	111.44
1	A	490	ASP	CA-CB-CG	7.70	120.30	112.60
1	A	1198	ALA	N-CA-C	-7.68	102.97	112.88
1	A	1158	PRO	CA-C-O	-7.67	112.69	121.36
1	A	491	VAL	CA-CB-CG1	7.65	123.40	110.40
1	A	687	ASP	CA-CB-CG	7.64	120.24	112.60
1	A	295	MET	CA-C-N	7.63	128.26	119.94
1	A	295	MET	C-N-CA	7.63	128.26	119.94
1	A	725	SER	N-CA-C	7.61	120.46	111.71
1	A	497	GLU	N-CA-C	7.60	119.20	111.07
1	A	414	LYS	N-CA-CB	7.55	121.96	110.70
1	A	182	ILE	O-C-N	7.54	128.88	122.09
1	A	884	LYS	CA-C-N	7.54	130.24	120.44
1	A	884	LYS	C-N-CA	7.54	130.24	120.44
1	A	81	VAL	O-C-N	7.51	129.27	121.91
1	A	93	GLU	CA-C-N	7.51	130.34	120.28
1	A	93	GLU	C-N-CA	7.51	130.34	120.28
1	A	98	ALA	N-CA-C	7.49	119.22	111.14
1	A	356	GLY	O-C-N	7.47	129.36	122.19
1	A	885	GLU	CA-C-O	7.45	128.65	120.82
1	A	341	VAL	CA-C-N	7.45	129.68	120.22
1	A	341	VAL	C-N-CA	7.45	129.68	120.22
1	A	1014	ILE	N-CA-C	-7.43	97.70	108.11
1	A	889	SER	CA-C-N	7.42	129.65	120.22
1	A	889	SER	C-N-CA	7.42	129.65	120.22
1	A	300	LEU	CA-C-N	7.39	130.92	120.28
1	A	300	LEU	C-N-CA	7.39	130.92	120.28
1	A	325	GLY	CA-C-N	7.38	130.67	120.63
1	A	325	GLY	C-N-CA	7.38	130.67	120.63
1	A	592	ASP	CA-CB-CG	7.38	119.98	112.60
1	A	1210	VAL	CA-C-N	7.37	130.47	120.38
1	A	1210	VAL	C-N-CA	7.37	130.47	120.38
1	A	816	ASN	CA-C-O	-7.36	113.09	120.82
1	A	696	ILE	CA-C-N	7.35	130.87	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	696	ILE	C-N-CA	7.35	130.87	120.28
1	A	213	VAL	CA-C-O	-7.35	113.38	121.17
1	A	607	ASN	CA-C-N	7.34	130.45	120.54
1	A	607	ASN	C-N-CA	7.34	130.45	120.54
1	A	1184	ARG	CD-NE-CZ	-7.34	114.13	124.40
1	A	515	GLN	OE1-CD-NE2	7.33	129.93	122.60
1	A	848	ILE	O-C-N	-7.33	114.01	122.07
1	A	1191	HIS	CA-CB-CG	7.32	121.11	113.80
1	A	115	THR	CA-C-N	7.31	128.09	119.98
1	A	115	THR	C-N-CA	7.31	128.09	119.98
1	A	156	ILE	N-CA-C	7.31	118.95	110.62
1	A	709	VAL	CA-C-N	7.30	128.04	119.94
1	A	709	VAL	C-N-CA	7.30	128.04	119.94
1	A	205	THR	CA-C-O	-7.29	112.83	120.55
1	A	239	GLU	N-CA-CB	7.29	120.83	110.12
1	A	312	TYR	CB-CG-CD1	-7.24	109.94	120.80
1	A	63	ALA	CA-C-N	7.21	129.92	120.26
1	A	63	ALA	C-N-CA	7.21	129.92	120.26
1	A	567	ALA	CA-C-O	7.18	128.35	120.82
1	A	1130	GLY	O-C-N	-7.17	116.82	122.99
1	A	460	ARG	CA-C-N	7.16	130.46	120.29
1	A	460	ARG	C-N-CA	7.16	130.46	120.29
1	A	132	TRP	CA-CB-CG	7.16	127.20	113.60
1	A	864	ILE	O-C-N	7.16	129.10	121.87
1	A	854	THR	N-CA-C	-7.15	103.42	111.07
1	A	1253	HIS	CB-CG-CD2	-7.14	121.92	131.20
1	A	588	VAL	N-CA-C	-7.12	103.32	113.07
1	A	326	GLN	OE1-CD-NE2	7.10	129.70	122.60
1	A	173	ASP	CA-C-N	7.08	130.34	120.29
1	A	173	ASP	C-N-CA	7.08	130.34	120.29
1	A	1075	VAL	CB-CA-C	-7.04	102.87	111.88
1	A	114	TYR	CA-C-N	7.02	129.99	120.44
1	A	114	TYR	C-N-CA	7.02	129.99	120.44
1	A	206	ARG	N-CA-CB	7.00	121.45	110.46
1	A	622	VAL	N-CA-CB	6.99	118.24	110.62
1	A	466	ILE	CA-C-N	6.99	128.86	121.45
1	A	466	ILE	C-N-CA	6.99	128.86	121.45
1	A	353	ASN	N-CA-C	6.96	119.72	111.71
1	A	401	LYS	N-CA-C	-6.96	103.90	112.88
1	A	1186	LEU	CA-C-N	6.95	129.45	120.56
1	A	1186	LEU	C-N-CA	6.95	129.45	120.56
1	A	921	GLN	OE1-CD-NE2	6.94	129.54	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1236	ALA	CA-C-N	6.94	129.58	120.28
1	A	1236	ALA	C-N-CA	6.94	129.58	120.28
1	A	745	ARG	CA-C-N	6.94	129.91	120.54
1	A	745	ARG	C-N-CA	6.94	129.91	120.54
1	A	612	MET	CA-C-N	6.93	129.57	120.28
1	A	612	MET	C-N-CA	6.93	129.57	120.28
1	A	1003	HIS	N-CA-C	-6.93	103.65	111.07
1	A	114	TYR	N-CA-CB	6.92	120.44	110.06
1	A	1237	ASP	CB-CA-C	-6.91	99.31	110.79
1	A	1091	PHE	CA-C-O	-6.91	113.03	121.11
1	A	256	ALA	CA-C-N	6.89	130.25	120.53
1	A	256	ALA	C-N-CA	6.89	130.25	120.53
1	A	775	LYS	N-CA-C	6.88	119.62	111.71
1	A	753	LEU	CA-C-N	6.88	130.76	120.31
1	A	753	LEU	C-N-CA	6.88	130.76	120.31
1	A	1220	GLY	N-CA-C	-6.87	104.74	115.67
1	A	114	TYR	O-C-N	-6.87	114.84	122.12
1	A	860	ILE	CA-C-N	6.86	127.02	120.43
1	A	860	ILE	C-N-CA	6.86	127.02	120.43
1	A	253	VAL	CA-C-N	6.86	130.74	120.31
1	A	253	VAL	C-N-CA	6.86	130.74	120.31
1	A	1104	TRP	CE2-CD2-CE3	6.83	125.63	118.80
1	A	1063	ALA	O-C-N	-6.83	115.07	122.85
1	A	538	ALA	CA-C-N	6.83	129.43	120.28
1	A	538	ALA	C-N-CA	6.83	129.43	120.28
1	A	1013	GLU	N-CA-C	-6.80	105.52	113.88
1	A	1073	SER	CA-C-N	6.80	129.39	120.28
1	A	1073	SER	C-N-CA	6.80	129.39	120.28
1	A	145	GLN	CA-C-N	6.78	132.18	120.58
1	A	145	GLN	C-N-CA	6.78	132.18	120.58
1	A	198	GLY	CA-C-N	6.77	127.32	119.94
1	A	198	GLY	C-N-CA	6.77	127.32	119.94
1	A	1082	PHE	CA-CB-CG	-6.77	107.03	113.80
1	A	1101	ASN	CA-CB-CG	6.77	119.37	112.60
1	A	228	TRP	CB-CG-CD2	6.76	136.27	126.80
1	A	413	VAL	N-CA-C	-6.75	98.39	108.12
1	A	163	ASP	CB-CA-C	-6.73	99.91	110.74
1	A	819	ALA	CA-C-N	6.72	129.58	120.44
1	A	819	ALA	C-N-CA	6.72	129.58	120.44
1	A	258	ARG	CD-NE-CZ	-6.71	115.00	124.40
1	A	408	GLY	N-CA-C	-6.71	101.07	111.00
1	A	1228	HIS	N-CA-C	-6.70	104.73	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1003	HIS	CE1-NE2-CD2	-6.69	102.31	109.00
1	A	608	HIS	CA-C-N	6.66	129.20	120.28
1	A	608	HIS	C-N-CA	6.66	129.20	120.28
1	A	861	VAL	CB-CA-C	-6.66	107.38	113.70
1	A	508	PHE	CA-CB-CG	6.65	120.45	113.80
1	A	1191	HIS	N-CA-C	-6.62	105.11	113.72
1	A	1074	THR	CA-C-N	6.62	129.14	120.60
1	A	1074	THR	C-N-CA	6.62	129.14	120.60
1	A	380	LYS	O-C-N	-6.62	116.39	121.55
1	A	1085	PRO	CB-CA-C	6.61	120.00	111.21
1	A	109	THR	CA-C-N	6.60	129.45	120.54
1	A	109	THR	C-N-CA	6.60	129.45	120.54
1	A	1197	GLU	N-CA-C	6.60	118.63	110.91
1	A	279	GLU	CA-C-N	6.57	129.74	120.28
1	A	279	GLU	C-N-CA	6.57	129.74	120.28
1	A	312	TYR	CB-CG-CD2	6.57	130.65	120.80
1	A	1084	ASP	CA-C-O	-6.57	113.34	120.17
1	A	979	PHE	CA-C-N	6.56	128.56	120.22
1	A	979	PHE	C-N-CA	6.56	128.56	120.22
1	A	354	ALA	CA-C-O	6.56	127.37	120.42
1	A	915	MET	CA-C-N	6.56	129.07	120.28
1	A	915	MET	C-N-CA	6.56	129.07	120.28
1	A	728	PHE	N-CA-C	6.56	118.43	111.28
1	A	504	ASN	CA-CB-CG	6.55	119.15	112.60
1	A	516	PHE	CA-C-N	6.55	133.83	122.56
1	A	516	PHE	C-N-CA	6.55	133.83	122.56
1	A	932	HIS	CA-C-N	6.53	128.92	120.56
1	A	932	HIS	C-N-CA	6.53	128.92	120.56
1	A	1183	ALA	CA-C-N	6.53	129.56	120.29
1	A	1183	ALA	C-N-CA	6.53	129.56	120.29
1	A	983	ALA	CA-C-N	6.52	129.01	120.60
1	A	983	ALA	C-N-CA	6.52	129.01	120.60
1	A	67	MET	N-CA-C	6.52	118.38	111.28
1	A	278	GLU	CA-C-O	-6.50	113.66	120.55
1	A	983	ALA	O-C-N	6.50	129.05	122.03
1	A	258	ARG	NE-CZ-NH2	-6.50	113.35	119.20
1	A	885	GLU	CA-C-N	6.50	131.57	120.72
1	A	885	GLU	C-N-CA	6.50	131.57	120.72
1	A	530	GLY	CA-C-N	6.50	130.18	120.31
1	A	530	GLY	C-N-CA	6.50	130.18	120.31
1	A	755	PHE	CA-CB-CG	6.46	120.26	113.80
1	A	84	VAL	CA-C-N	6.46	129.46	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	VAL	C-N-CA	6.46	129.46	120.29
1	A	317	VAL	CB-CA-C	-6.45	106.22	111.71
1	A	959	LEU	CA-C-N	6.45	129.29	120.46
1	A	959	LEU	C-N-CA	6.45	129.29	120.46
1	A	764	ILE	CA-C-N	6.44	129.56	120.28
1	A	764	ILE	C-N-CA	6.44	129.56	120.28
1	A	66	LEU	N-CA-CB	6.42	119.56	110.12
1	A	1083	TYR	CA-C-N	6.42	129.32	120.39
1	A	1083	TYR	C-N-CA	6.42	129.32	120.39
1	A	1251	GLY	CA-C-N	6.41	130.25	120.82
1	A	1251	GLY	C-N-CA	6.41	130.25	120.82
1	A	1116	PRO	N-CA-C	-6.41	100.21	112.01
1	A	717	ASN	CA-CB-CG	6.41	119.01	112.60
1	A	594	ILE	N-CA-C	-6.39	99.28	108.48
1	A	458	ASN	CA-CB-CG	6.39	118.99	112.60
1	A	1206	SER	CA-C-O	6.38	127.52	120.63
1	A	303	TYR	CB-CA-C	-6.35	100.25	110.79
1	A	453	ASP	CA-CB-CG	6.34	118.94	112.60
1	A	765	THR	CA-C-N	6.33	129.28	120.29
1	A	765	THR	C-N-CA	6.33	129.28	120.29
1	A	362	PHE	CA-C-N	6.33	128.76	120.28
1	A	362	PHE	C-N-CA	6.33	128.76	120.28
1	A	431	THR	CA-C-N	6.31	128.73	120.28
1	A	431	THR	C-N-CA	6.31	128.73	120.28
1	A	721	GLN	O-C-N	-6.30	114.87	120.48
1	A	1101	ASN	OD1-CG-ND2	6.29	128.90	122.60
1	A	531	GLN	CA-C-O	6.29	127.20	119.97
1	A	701	SER	N-CA-C	6.27	118.92	111.71
1	A	383	ASN	CA-C-N	6.25	130.18	122.37
1	A	383	ASN	C-N-CA	6.25	130.18	122.37
1	A	986	GLN	CA-C-O	-6.24	113.80	120.42
1	A	843	ILE	N-CA-CB	6.24	117.85	110.55
1	A	1143	ARG	NE-CZ-NH1	6.24	127.73	121.50
1	A	576	ARG	O-C-N	-6.23	115.14	122.81
1	A	1184	ARG	CA-C-N	6.23	128.54	120.44
1	A	1184	ARG	C-N-CA	6.23	128.54	120.44
1	A	759	GLY	CA-C-N	6.23	129.64	120.74
1	A	759	GLY	C-N-CA	6.23	129.64	120.74
1	A	53	GLY	CA-C-O	-6.22	114.28	121.00
1	A	1174	GLY	O-C-N	6.21	128.16	122.19
1	A	253	VAL	CA-C-O	-6.21	114.59	121.17
1	A	334	VAL	CA-C-N	6.21	129.10	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	VAL	C-N-CA	6.21	129.10	120.29
1	A	927	ALA	N-CA-CB	6.21	119.24	110.12
1	A	711	ILE	CA-C-N	6.20	129.20	120.28
1	A	711	ILE	C-N-CA	6.20	129.20	120.28
1	A	812	THR	CA-C-N	6.20	128.49	120.44
1	A	812	THR	C-N-CA	6.20	128.49	120.44
1	A	1097	ILE	CA-C-N	6.19	128.87	120.38
1	A	1097	ILE	C-N-CA	6.19	128.87	120.38
1	A	723	ALA	CA-C-N	6.18	128.88	120.54
1	A	723	ALA	C-N-CA	6.18	128.88	120.54
1	A	494	ASP	CB-CA-C	-6.17	100.55	110.79
1	A	876	SER	CA-C-N	6.16	126.82	119.98
1	A	876	SER	C-N-CA	6.16	126.82	119.98
1	A	1191	HIS	CA-C-N	6.15	131.71	122.98
1	A	1191	HIS	C-N-CA	6.15	131.71	122.98
1	A	1069	GLY	O-C-N	-6.13	117.08	122.90
1	A	606	GLY	CA-C-O	-6.13	114.42	121.47
1	A	937	THR	CA-C-N	6.12	128.49	120.28
1	A	937	THR	C-N-CA	6.12	128.49	120.28
1	A	1019	THR	N-CA-C	-6.12	107.65	114.62
1	A	707	PHE	N-CA-CB	6.11	120.82	110.49
1	A	441	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	117	ILE	N-CA-C	-6.08	104.37	111.00
1	A	162	HIS	CA-CB-CG	-6.08	107.72	113.80
1	A	604	GLU	CB-CA-C	-6.07	98.27	109.37
1	A	1077	GLN	N-CA-C	6.06	117.97	111.36
1	A	923	PRO	CA-C-N	6.06	128.31	120.44
1	A	923	PRO	C-N-CA	6.06	128.31	120.44
1	A	290	THR	CA-CB-OG1	6.05	118.67	109.60
1	A	745	ARG	CB-CG-CD	6.05	125.20	111.30
1	A	1164	ARG	N-CA-C	-6.05	98.78	109.06
1	A	1234	GLN	N-CA-C	-6.05	105.83	112.72
1	A	1253	HIS	CB-CG-ND1	6.05	131.77	122.70
1	A	78	PHE	O-C-N	-6.04	115.15	122.22
1	A	1116	PRO	CA-C-O	-6.03	114.60	122.19
1	A	228	TRP	CB-CG-CD1	-6.00	117.90	126.90
1	A	522	GLU	CB-CG-CD	-6.00	102.40	112.60
1	A	775	LYS	CA-C-N	5.99	128.23	120.44
1	A	775	LYS	C-N-CA	5.99	128.23	120.44
1	A	1201	ALA	CA-C-N	5.98	132.16	122.29
1	A	1201	ALA	C-N-CA	5.98	132.16	122.29
1	A	530	GLY	O-C-N	-5.98	116.39	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ILE	N-CA-C	-5.97	104.51	110.30
1	A	685	ASP	N-CA-C	-5.97	99.00	108.73
1	A	482	GLU	N-CA-CB	5.96	118.98	110.16
1	A	351	PHE	CA-CB-CG	5.95	119.75	113.80
1	A	1157	LEU	CA-C-N	5.93	125.95	119.90
1	A	1157	LEU	C-N-CA	5.93	125.95	119.90
1	A	38	MET	CA-C-O	-5.93	114.14	120.42
1	A	268	LYS	CA-C-N	5.92	129.32	120.31
1	A	268	LYS	C-N-CA	5.92	129.32	120.31
1	A	308	LEU	CA-C-N	5.92	128.21	120.28
1	A	308	LEU	C-N-CA	5.92	128.21	120.28
1	A	227	ILE	CB-CA-C	-5.92	102.68	112.26
1	A	335	LEU	CA-C-N	5.92	129.82	120.47
1	A	335	LEU	C-N-CA	5.92	129.82	120.47
1	A	207	GLY	O-C-N	5.91	130.39	122.70
1	A	541	LEU	N-CA-CB	5.91	118.91	110.16
1	A	132	TRP	O-C-N	-5.90	115.31	122.22
1	A	269	GLU	CA-C-N	5.90	128.50	120.54
1	A	269	GLU	C-N-CA	5.90	128.50	120.54
1	A	60	HIS	ND1-CE1-NE2	5.90	114.30	108.40
1	A	938	PHE	CA-CB-CG	5.89	119.69	113.80
1	A	897	ILE	N-CA-C	5.88	118.44	111.09
1	A	135	ALA	CA-C-N	5.88	128.64	120.29
1	A	135	ALA	C-N-CA	5.88	128.64	120.29
1	A	143	ILE	N-CA-C	-5.87	104.78	110.42
1	A	1075	VAL	CA-CB-CG1	5.85	120.35	110.40
1	A	789	PHE	CA-C-O	5.84	126.75	120.20
1	A	1124	ALA	CA-C-N	5.84	129.19	120.31
1	A	1124	ALA	C-N-CA	5.84	129.19	120.31
1	A	450	ASP	CA-C-N	5.84	126.42	120.00
1	A	450	ASP	C-N-CA	5.84	126.42	120.00
1	A	162	HIS	CG-CD2-NE2	5.83	113.03	107.20
1	A	258	ARG	CG-CD-NE	-5.82	99.19	112.00
1	A	945	MET	CA-C-N	5.82	128.07	120.28
1	A	945	MET	C-N-CA	5.82	128.07	120.28
1	A	1104	TRP	CD2-CE2-CZ2	-5.82	116.58	122.40
1	A	708	VAL	N-CA-C	-5.81	106.07	113.22
1	A	865	ALA	CB-CA-C	-5.81	101.72	110.90
1	A	1114	GLN	CA-C-N	5.81	129.90	122.64
1	A	1114	GLN	C-N-CA	5.81	129.90	122.64
1	A	831	VAL	CA-CB-CG2	-5.80	100.53	110.40
1	A	434	GLN	O-C-N	5.80	128.76	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	480	ILE	N-CA-C	5.80	118.34	111.09
1	A	958	TYR	CA-C-N	5.80	128.32	120.38
1	A	958	TYR	C-N-CA	5.80	128.32	120.38
1	A	402	GLU	O-C-N	-5.79	116.99	123.48
1	A	480	ILE	CA-C-O	5.78	126.72	120.47
1	A	364	ILE	CA-C-N	5.78	128.34	120.77
1	A	364	ILE	C-N-CA	5.78	128.34	120.77
1	A	405	ILE	CA-CB-CG1	5.78	120.23	110.40
1	A	928	MET	CA-C-N	5.78	128.50	120.29
1	A	928	MET	C-N-CA	5.78	128.50	120.29
1	A	691	ALA	CA-C-N	5.77	129.04	120.90
1	A	691	ALA	C-N-CA	5.77	129.04	120.90
1	A	267	LYS	CA-C-N	5.77	130.35	120.71
1	A	267	LYS	C-N-CA	5.77	130.35	120.71
1	A	81	VAL	CA-C-N	5.76	127.34	120.14
1	A	81	VAL	C-N-CA	5.76	127.34	120.14
1	A	1253	HIS	ND1-CE1-NE2	5.75	114.16	108.40
1	A	1193	LEU	N-CA-C	-5.75	100.81	109.95
1	A	908	ARG	CA-C-N	5.74	128.23	120.65
1	A	908	ARG	C-N-CA	5.74	128.23	120.65
1	A	1126	ASN	CA-CB-CG	-5.74	106.86	112.60
1	A	878	GLN	O-C-N	5.74	129.69	122.23
1	A	133	CYS	N-CA-C	5.73	119.73	111.02
1	A	1090	VAL	N-CA-C	-5.73	99.92	108.46
1	A	93	GLU	N-CA-C	-5.73	102.80	111.34
1	A	70	ILE	N-CA-C	5.72	116.46	110.62
1	A	549	LEU	N-CA-C	-5.72	99.08	108.41
1	A	610	GLU	N-CA-C	5.72	117.52	111.28
1	A	1225	VAL	O-C-N	-5.72	117.13	123.20
1	A	463	ARG	NE-CZ-NH1	5.72	127.22	121.50
1	A	1153	PHE	N-CA-C	5.71	118.45	111.82
1	A	289	ILE	N-CA-C	5.71	116.17	110.23
1	A	142	LYS	CA-C-N	5.70	127.75	120.56
1	A	142	LYS	C-N-CA	5.70	127.75	120.56
1	A	686	GLU	CA-C-N	5.70	132.43	121.54
1	A	686	GLU	C-N-CA	5.70	132.43	121.54
1	A	986	GLN	O-C-N	5.70	128.65	122.15
1	A	362	PHE	CA-CB-CG	-5.69	108.11	113.80
1	A	1244	ASN	N-CA-CB	5.69	120.12	111.70
1	A	726	VAL	CA-C-N	5.69	127.73	120.56
1	A	726	VAL	C-N-CA	5.69	127.73	120.56
1	A	153	ASN	CA-C-O	-5.68	112.42	119.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	613	ARG	NE-CZ-NH1	5.68	127.18	121.50
1	A	816	ASN	OD1-CG-ND2	5.68	128.28	122.60
1	A	689	PRO	N-CA-C	5.68	117.63	110.70
1	A	153	ASN	N-CA-C	-5.68	106.36	113.28
1	A	598	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	157	GLY	N-CA-C	5.67	119.75	112.83
1	A	692	SER	N-CA-C	5.67	118.23	110.24
1	A	1161	TYR	CA-CB-CG	-5.66	103.70	113.90
1	A	471	GLN	OE1-CD-NE2	5.66	128.26	122.60
1	A	951	ALA	N-CA-C	5.66	118.22	111.71
1	A	150	ALA	CA-C-O	-5.66	113.47	119.97
1	A	132	TRP	CA-C-N	5.64	129.16	122.44
1	A	132	TRP	C-N-CA	5.64	129.16	122.44
1	A	576	ARG	N-CA-CB	5.64	118.33	110.04
1	A	1129	TYR	CA-C-N	5.64	127.41	120.92
1	A	1129	TYR	C-N-CA	5.64	127.41	120.92
1	A	223	LEU	N-CA-C	-5.64	105.05	111.14
1	A	287	LYS	N-CA-C	5.64	117.43	111.28
1	A	1119	PHE	N-CA-C	-5.63	101.41	110.14
1	A	37	THR	CA-C-N	5.63	128.28	120.29
1	A	37	THR	C-N-CA	5.63	128.28	120.29
1	A	883	LYS	CG-CD-CE	5.63	124.24	111.30
1	A	930	LYS	CA-C-N	5.62	127.75	120.44
1	A	930	LYS	C-N-CA	5.62	127.75	120.44
1	A	1025	ASN	N-CA-C	-5.62	106.41	113.72
1	A	887	GLU	N-CA-CB	5.62	118.12	109.91
1	A	182	ILE	CA-C-O	-5.61	113.77	119.89
1	A	926	ASN	CA-CB-CG	5.61	118.21	112.60
1	A	974	PHE	CA-CB-CG	5.61	119.41	113.80
1	A	788	VAL	N-CA-CB	5.61	117.37	110.64
1	A	608	HIS	CG-CD2-NE2	5.60	112.80	107.20
1	A	966	THR	CA-CB-OG1	5.60	118.00	109.60
1	A	182	ILE	CA-C-N	5.60	129.69	121.96
1	A	182	ILE	C-N-CA	5.60	129.69	121.96
1	A	356	GLY	CA-C-O	-5.60	114.99	120.75
1	A	347	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	811	THR	N-CA-C	5.59	117.37	111.28
1	A	889	SER	N-CA-C	5.59	117.45	111.36
1	A	934	PHE	CA-C-N	5.58	126.14	120.00
1	A	934	PHE	C-N-CA	5.58	126.14	120.00
1	A	788	VAL	N-CA-C	-5.58	105.67	110.74
1	A	1026	MET	N-CA-C	-5.58	106.36	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	514	HIS	N-CA-CB	5.57	119.90	110.49
1	A	352	ALA	O-C-N	5.57	127.81	122.07
1	A	376	LYS	CA-C-N	5.57	132.17	121.54
1	A	376	LYS	C-N-CA	5.57	132.17	121.54
1	A	1196	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	193	MET	N-CA-C	5.55	118.09	111.71
1	A	360	GLU	CB-CG-CD	-5.55	103.17	112.60
1	A	852	GLN	CA-C-O	5.54	126.76	120.00
1	A	578	THR	CA-C-O	5.54	127.66	121.40
1	A	58	ILE	CA-C-O	-5.52	115.39	121.29
1	A	1239	ILE	N-CA-CB	5.51	117.61	110.99
1	A	1225	VAL	CA-C-O	5.51	126.12	120.39
1	A	1163	THR	CA-CB-OG1	5.50	117.86	109.60
1	A	597	PHE	CG-CD2-CE2	-5.50	111.34	120.70
1	A	785	ARG	CA-C-N	5.50	128.10	120.63
1	A	785	ARG	C-N-CA	5.50	128.10	120.63
1	A	585	LEU	N-CA-C	-5.49	106.09	112.89
1	A	1091	PHE	CA-CB-CG	-5.49	108.31	113.80
1	A	333	SER	N-CA-CB	5.48	118.78	110.28
1	A	1131	ASP	CA-CB-CG	-5.48	107.12	112.60
1	A	1015	ASP	N-CA-C	-5.48	99.13	110.80
1	A	732	VAL	CA-C-N	5.47	126.02	119.94
1	A	732	VAL	C-N-CA	5.47	126.02	119.94
1	A	239	GLU	CA-C-O	5.47	126.35	120.55
1	A	410	ASN	OD1-CG-ND2	5.47	128.07	122.60
1	A	531	GLN	O-C-N	-5.47	115.54	122.27
1	A	396	SER	CA-C-N	5.47	128.65	120.83
1	A	396	SER	C-N-CA	5.47	128.65	120.83
1	A	741	PRO	CA-C-N	5.46	131.97	121.54
1	A	741	PRO	C-N-CA	5.46	131.97	121.54
1	A	892	ILE	CA-C-N	5.46	127.87	120.44
1	A	892	ILE	C-N-CA	5.46	127.87	120.44
1	A	528	SER	CA-C-N	5.45	126.03	119.98
1	A	528	SER	C-N-CA	5.45	126.03	119.98
1	A	596	GLY	CA-C-O	-5.45	116.38	121.18
1	A	933	VAL	CA-C-O	-5.45	115.00	121.05
1	A	1058	LYS	N-CA-C	5.45	118.25	110.24
1	A	354	ALA	CA-C-N	5.45	127.84	120.65
1	A	354	ALA	C-N-CA	5.45	127.84	120.65
1	A	1252	THR	CA-C-O	-5.44	115.56	121.44
1	A	1096	GLU	CA-C-N	5.44	127.91	120.46
1	A	1096	GLU	C-N-CA	5.44	127.91	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	LEU	N-CA-CB	5.43	117.94	110.07
1	A	428	GLY	N-CA-C	-5.42	100.34	113.18
1	A	1098	LYS	O-C-N	-5.42	116.38	122.12
1	A	953	PHE	CA-C-N	5.40	128.30	120.79
1	A	953	PHE	C-N-CA	5.40	128.30	120.79
1	A	1157	LEU	CA-C-O	-5.40	114.95	119.76
1	A	438	ARG	N-CA-C	-5.39	106.29	112.92
1	A	1081	ARG	CA-C-N	5.39	127.95	120.29
1	A	1081	ARG	C-N-CA	5.39	127.95	120.29
1	A	1052	LEU	CA-C-O	5.38	126.25	120.38
1	A	758	LEU	CA-C-N	5.38	126.07	119.99
1	A	758	LEU	C-N-CA	5.38	126.07	119.99
1	A	88	SER	CA-C-N	5.37	129.80	122.34
1	A	88	SER	C-N-CA	5.37	129.80	122.34
1	A	1255	GLN	N-CA-CB	-5.37	102.29	110.07
1	A	818	ALA	O-C-N	-5.36	115.94	122.22
1	A	372	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	460	ARG	NE-CZ-NH2	-5.36	114.38	119.20
1	A	959	LEU	O-C-N	5.36	127.80	122.12
1	A	440	TYR	N-CA-C	-5.36	101.22	109.52
1	A	230	LYS	N-CA-C	5.35	117.19	111.36
1	A	302	ILE	N-CA-C	5.35	115.56	110.53
1	A	1017	TYR	CA-C-N	5.35	131.75	121.54
1	A	1017	TYR	C-N-CA	5.35	131.75	121.54
1	A	332	PHE	N-CA-C	-5.34	105.54	111.36
1	A	581	ILE	N-CA-C	-5.34	99.95	107.75
1	A	618	TYR	N-CA-CB	-5.34	102.27	110.01
1	A	822	LYS	CA-C-N	5.34	127.00	120.22
1	A	822	LYS	C-N-CA	5.34	127.00	120.22
1	A	871	GLU	O-C-N	5.34	127.86	122.09
1	A	980	GLY	CA-C-N	5.33	129.70	120.58
1	A	980	GLY	C-N-CA	5.33	129.70	120.58
1	A	899	ASN	CA-CB-CG	-5.32	107.28	112.60
1	A	1217	ALA	CA-C-O	5.32	126.06	120.42
1	A	834	GLN	CB-CG-CD	5.31	121.63	112.60
1	A	736	THR	N-CA-C	5.31	116.92	111.03
1	A	143	ILE	CA-C-N	5.31	127.39	120.28
1	A	143	ILE	C-N-CA	5.31	127.39	120.28
1	A	186	ILE	CA-C-O	5.30	126.47	120.95
1	A	395	PHE	CB-CA-C	-5.30	100.46	110.16
1	A	983	ALA	CA-C-O	-5.29	115.45	120.90
1	A	197	PHE	CA-CB-CG	-5.29	108.51	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	GLY	CA-C-N	5.29	127.36	120.28
1	A	247	GLY	C-N-CA	5.29	127.36	120.28
1	A	529	GLY	N-CA-C	5.29	119.07	112.73
1	A	224	SER	O-C-N	5.28	127.72	122.12
1	A	816	ASN	N-CA-C	5.28	116.72	111.07
1	A	298	ALA	CB-CA-C	-5.27	102.60	110.88
1	A	132	TRP	CD2-CE2-CZ2	-5.27	117.13	122.40
1	A	520	VAL	CA-CB-CG2	-5.27	101.45	110.40
1	A	686	GLU	N-CA-C	-5.26	99.86	108.76
1	A	239	GLU	CA-C-N	5.26	127.33	120.28
1	A	239	GLU	C-N-CA	5.26	127.33	120.28
1	A	1244	ASN	CA-CB-CG	-5.25	107.35	112.60
1	A	900	PHE	CA-C-O	5.25	125.99	119.79
1	A	979	PHE	N-CA-CB	5.25	118.42	110.28
1	A	614	GLU	CA-C-N	5.25	130.02	122.35
1	A	614	GLU	C-N-CA	5.25	130.02	122.35
1	A	571	LYS	N-CA-C	5.25	119.31	113.01
1	A	805	ASN	N-CA-C	-5.25	106.19	112.59
1	A	851	TRP	N-CA-C	5.24	120.85	113.56
1	A	61	GLY	O-C-N	5.24	127.79	122.24
1	A	244	ALA	CA-C-N	5.24	127.25	120.44
1	A	244	ALA	C-N-CA	5.24	127.25	120.44
1	A	733	GLY	CA-C-O	-5.24	115.35	121.00
1	A	1151	HIS	ND1-CE1-NE2	5.23	113.63	108.40
1	A	785	ARG	N-CA-C	5.22	117.72	111.71
1	A	795	GLN	O-C-N	-5.22	116.38	122.96
1	A	224	SER	CA-C-O	-5.22	115.02	120.55
1	A	916	TYR	CA-C-N	5.22	127.23	120.44
1	A	916	TYR	C-N-CA	5.22	127.23	120.44
1	A	364	ILE	CA-C-O	-5.22	115.12	120.71
1	A	825	THR	CA-C-N	5.21	126.84	120.22
1	A	825	THR	C-N-CA	5.21	126.84	120.22
1	A	292	ASN	O-C-N	-5.21	116.59	122.12
1	A	1071	GLY	N-CA-C	-5.21	108.50	115.32
1	A	1178	GLN	N-CA-C	-5.21	105.61	111.28
1	A	344	ALA	CA-C-N	5.20	127.45	120.58
1	A	344	ALA	C-N-CA	5.20	127.45	120.58
1	A	823	GLY	CA-C-N	5.20	127.20	120.44
1	A	823	GLY	C-N-CA	5.20	127.20	120.44
1	A	1080	GLU	CA-C-N	5.20	130.23	122.74
1	A	1080	GLU	C-N-CA	5.20	130.23	122.74
1	A	140	ILE	O-C-N	5.20	126.91	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	THR	N-CA-CB	5.20	117.76	110.12
1	A	762	SER	CA-C-N	5.19	127.24	120.28
1	A	762	SER	C-N-CA	5.19	127.24	120.28
1	A	164	VAL	N-CA-C	5.19	120.13	109.34
1	A	49	TYR	CA-C-N	5.19	127.66	120.29
1	A	49	TYR	C-N-CA	5.19	127.66	120.29
1	A	702	THR	CA-CB-OG1	5.19	117.38	109.60
1	A	766	PHE	CA-C-O	5.19	125.92	120.42
1	A	278	GLU	O-C-N	5.19	127.62	122.12
1	A	143	ILE	O-C-N	-5.18	116.83	121.91
1	A	180	GLU	CA-C-O	5.18	125.93	119.97
1	A	1051	GLY	CA-C-O	-5.18	111.56	120.57
1	A	878	GLN	CA-C-N	5.18	127.22	120.28
1	A	878	GLN	C-N-CA	5.18	127.22	120.28
1	A	394	HIS	ND1-CG-CD2	5.17	111.27	106.10
1	A	1239	ILE	N-CA-C	-5.17	100.96	108.36
1	A	879	ALA	CA-C-N	5.17	127.16	120.44
1	A	879	ALA	C-N-CA	5.17	127.16	120.44
1	A	127	ILE	CA-C-O	-5.16	115.32	121.05
1	A	1056	VAL	CA-CB-CG2	5.16	119.17	110.40
1	A	147	PHE	O-C-N	5.15	127.38	122.07
1	A	1009	GLU	CA-C-O	-5.15	114.28	120.10
1	A	469	VAL	N-CA-C	-5.14	99.10	107.28
1	A	350	ALA	N-CA-C	-5.14	105.76	111.36
1	A	747	ASN	CA-C-N	5.14	127.12	120.44
1	A	747	ASN	C-N-CA	5.14	127.12	120.44
1	A	320	LYS	CG-CD-CE	5.14	123.11	111.30
1	A	469	VAL	CA-C-O	5.14	126.13	120.48
1	A	865	ALA	CA-C-N	5.13	127.49	120.46
1	A	865	ALA	C-N-CA	5.13	127.49	120.46
1	A	96	LYS	N-CA-C	-5.13	106.28	112.54
1	A	441	ASP	O-C-N	-5.13	115.34	121.39
1	A	842	GLY	CA-C-N	5.13	127.02	120.56
1	A	842	GLY	C-N-CA	5.13	127.02	120.56
1	A	296	GLY	O-C-N	-5.12	117.28	122.19
1	A	312	TYR	N-CA-CB	5.12	118.74	110.40
1	A	1199	THR	CA-C-O	5.11	124.12	118.65
1	A	379	HIS	CG-CD2-NE2	5.11	112.31	107.20
1	A	62	VAL	O-C-N	5.11	127.09	121.83
1	A	623	MET	CA-C-N	5.11	127.54	120.29
1	A	623	MET	C-N-CA	5.11	127.54	120.29
1	A	894	THR	CA-C-O	-5.10	114.33	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	608	HIS	CE1-NE2-CD2	-5.10	103.90	109.00
1	A	1107	ALA	CA-C-O	5.10	125.32	119.35
1	A	819	ALA	O-C-N	5.10	127.96	122.15
1	A	350	ALA	CA-C-N	5.10	127.37	120.44
1	A	350	ALA	C-N-CA	5.10	127.37	120.44
1	A	699	LEU	CA-C-N	5.09	127.38	120.65
1	A	699	LEU	C-N-CA	5.09	127.38	120.65
1	A	818	ALA	CA-C-N	5.09	127.52	120.29
1	A	818	ALA	C-N-CA	5.09	127.52	120.29
1	A	611	LEU	CA-C-O	-5.09	115.46	120.70
1	A	912	PHE	CA-C-O	-5.08	115.16	120.55
1	A	1217	ALA	N-CA-C	-5.08	105.82	111.36
1	A	193	MET	CG-SD-CE	5.08	112.08	100.90
1	A	1265	SER	CA-C-N	5.08	127.09	120.28
1	A	1265	SER	C-N-CA	5.08	127.09	120.28
1	A	206	ARG	CA-C-O	-5.08	113.14	119.18
1	A	1144	ALA	O-C-N	5.07	127.29	122.07
1	A	488	ARG	CA-C-N	-5.07	114.54	122.65
1	A	488	ARG	C-N-CA	-5.07	114.54	122.65
1	A	577	THR	N-CA-C	-5.07	102.19	110.20
1	A	705	PRO	N-CA-CB	5.07	108.57	103.25
1	A	138	ARG	N-CA-C	-5.07	105.94	111.82
1	A	351	PHE	CA-C-N	5.06	127.02	120.44
1	A	351	PHE	C-N-CA	5.06	127.02	120.44
1	A	717	ASN	CA-C-N	5.06	125.56	119.94
1	A	717	ASN	C-N-CA	5.06	125.56	119.94
1	A	862	PRO	CA-C-N	5.06	126.94	120.56
1	A	862	PRO	C-N-CA	5.06	126.94	120.56
1	A	779	ILE	N-CA-CB	5.06	119.93	110.77
1	A	1074	THR	N-CA-CB	5.06	117.56	110.12
1	A	544	ASN	CA-CB-CG	5.05	117.65	112.60
1	A	1071	GLY	CA-C-N	5.05	131.19	121.54
1	A	1071	GLY	C-N-CA	5.05	131.19	121.54
1	A	232	LEU	CA-C-N	5.05	127.05	120.28
1	A	232	LEU	C-N-CA	5.05	127.05	120.28
1	A	1239	ILE	CA-C-N	-5.05	116.53	123.14
1	A	1239	ILE	C-N-CA	-5.05	116.53	123.14
1	A	718	GLY	CA-C-N	5.04	129.77	120.79
1	A	718	GLY	C-N-CA	5.04	129.77	120.79
1	A	930	LYS	CG-CD-CE	5.04	122.90	111.30
1	A	1009	GLU	O-C-N	5.04	128.12	122.22
1	A	730	LYS	N-CA-C	-5.04	105.87	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	770	GLY	N-CA-C	5.04	119.84	113.24
1	A	1027	LEU	N-CA-C	-5.04	101.42	109.23
1	A	219	PRO	CA-C-N	5.03	126.89	120.56
1	A	219	PRO	C-N-CA	5.03	126.89	120.56
1	A	562	GLU	CB-CA-C	-5.03	102.99	110.88
1	A	405	ILE	CA-C-O	5.03	124.54	119.97
1	A	484	ILE	CA-C-N	5.02	128.64	120.60
1	A	484	ILE	C-N-CA	5.02	128.64	120.60
1	A	761	ILE	CA-C-N	5.02	127.01	120.28
1	A	761	ILE	C-N-CA	5.02	127.01	120.28
1	A	1003	HIS	CG-CD2-NE2	5.02	112.22	107.20
1	A	549	LEU	O-C-N	-5.02	117.45	123.27
1	A	752	SER	CA-C-N	5.01	127.00	120.28
1	A	752	SER	C-N-CA	5.01	127.00	120.28
1	A	190	PHE	CA-C-N	5.01	126.95	120.44
1	A	190	PHE	C-N-CA	5.01	126.95	120.44
1	A	1009	GLU	CB-CA-C	-5.01	101.36	110.63
1	A	123	ILE	CA-C-O	5.01	126.48	121.17
1	A	464	GLU	N-CA-C	5.00	117.62	111.82
1	A	583	HIS	CA-CB-CG	-5.00	108.80	113.80
1	A	893	ALA	O-C-N	-5.00	116.69	122.09

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1138	TYR	Sidechain
1	A	1161	TYR	Sidechain
1	A	1184	ARG	Sidechain
1	A	1218	ARG	Sidechain
1	A	126	TYR	Sidechain
1	A	1263	TYR	Sidechain
1	A	204	PHE	Sidechain
1	A	243	TYR	Sidechain
1	A	322	TYR	Sidechain
1	A	359	TYR	Sidechain
1	A	40	ARG	Sidechain
1	A	438	ARG	Sidechain
1	A	49	TYR	Sidechain
1	A	516	PHE	Sidechain
1	A	539	ARG	Sidechain
1	A	589	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	597	PHE	Sidechain
1	A	619	PHE	Sidechain
1	A	813	ARG	Sidechain
1	A	828	ARG	Sidechain
1	A	900	PHE	Sidechain
1	A	916	TYR	Sidechain
1	A	947	PHE	Sidechain
1	A	955	PHE	Sidechain
1	A	990	PHE	Sidechain

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	9171	0	9344	20	0
All	All	9171	0	9344	20	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 (20) 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:A:1164:ARG:HE	1:A:1164:ARG:HA	1.60	0.66
1:A:609:ASP:CB	1:A:613:ARG:HH21	2.24	0.50
1:A:1181:ALA:HA	1:A:1184:ARG:HE	1.78	0.49
1:A:1223:CYS:O	1:A:1224:ILE:HD13	2.12	0.49
1:A:132:TRP:HA	1:A:183:GLY:HA2	1.98	0.46
1:A:64:LEU:HB2	1:A:65:PRO:HD3	1.98	0.46
1:A:384:ILE:HD13	1:A:384:ILE:HA	1.82	0.44
1:A:594:ILE:HD13	1:A:608:HIS:N	2.34	0.43
1:A:1164:ARG:HE	1:A:1164:ARG:CA	2.28	0.43
1:A:471:GLN:CD	1:A:471:GLN:H	2.26	0.42
1:A:594:ILE:HD12	1:A:594:ILE:N	2.34	0.42
1:A:475:LEU:H	1:A:901:ARG:NH2	2.17	0.42
1:A:963:GLN:HB2	1:A:964:LEU:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:ASP:HB3	1:A:613:ARG:HH21	1.85	0.41
1:A:189:PHE:CD1	1:A:348:ILE:HD11	2.55	0.41
1:A:609:ASP:HB2	1:A:613:ARG:HH21	1.85	0.41
1:A:465:ILE:HG22	1:A:465:ILE:O	2.21	0.40
1:A:273:TYR:CE2	1:A:277:LEU:HD11	2.56	0.40
1:A:1154:ILE:HG21	1:A:1161:TYR:CE1	2.56	0.40
1:A:758:LEU:HD13	1:A:758:LEU:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1178/1284 (92%)	1073 (91%)	79 (7%)	26 (2%)	5	29

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	SER
1	A	321	GLU
1	A	455	ARG
1	A	514	HIS
1	A	707	PHE
1	A	1012	PRO
1	A	90	ASN
1	A	687	ASP
1	A	705	PRO
1	A	1018	SER
1	A	1093	ASP
1	A	1227	ALA
1	A	377	SER
1	A	382	ASP

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Mol	Chain	Res	Type
1	A	404	GLN
1	A	600	GLY
1	A	800	PHE
1	A	1231	SER
1	A	36	LEU
1	A	525	ALA
1	A	797	VAL
1	A	969	ASN
1	A	1010	LYS
1	A	1046	ILE
1	A	379	HIS
1	A	1022	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	976/1065 (92%)	932 (96%)	44 (4%)	24 46

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	95	ASP
1	A	129	VAL
1	A	156	ILE
1	A	185	LYS
1	A	210	LEU
1	A	211	THR
1	A	228	TRP
1	A	240	LEU
1	A	259	THR
1	A	260	VAL
1	A	267	LYS
1	A	320	LYS
1	A	326	GLN

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Mol	Chain	Res	Type
1	A	370	SER
1	A	380	LYS
1	A	383	ASN
1	A	414	LYS
1	A	424	ASN
1	A	429	LYS
1	A	471	GLN
1	A	475	LEU
1	A	498	LYS
1	A	516	PHE
1	A	574	GLU
1	A	585	LEU
1	A	594	ILE
1	A	597	PHE
1	A	744	GLN
1	A	775	LYS
1	A	778	GLU
1	A	779	ILE
1	A	781	THR
1	A	812	THR
1	A	841	THR
1	A	845	ILE
1	A	936	ILE
1	A	998	THR
1	A	1050	GLN
1	A	1056	VAL
1	A	1061	THR
1	A	1095	LYS
1	A	1164	ARG
1	A	1248	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	90	ASN
1	A	128	GLN
1	A	145	GLN
1	A	149	HIS
1	A	274	ASN
1	A	292	ASN
1	A	343	GLN

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Mol	Chain	Res	Type
1	A	379	HIS
1	A	385	GLN
1	A	410	ASN
1	A	424	ASN
1	A	458	ASN
1	A	531	GLN
1	A	747	ASN
1	A	769	GLN
1	A	852	GLN
1	A	969	ASN
1	A	1020	GLN
1	A	1032	GLN
1	A	1050	GLN
1	A	1099	GLN
1	A	1103	GLN
1	A	1149	ASN
1	A	1152	GLN
1	A	1171	GLN
1	A	1176	GLN
1	A	1189	GLN
1	A	1259	GLN

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.

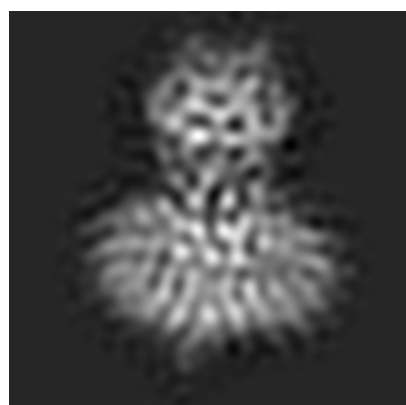
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4391. These allow visual inspection of the internal detail of the map and identification of artifacts.

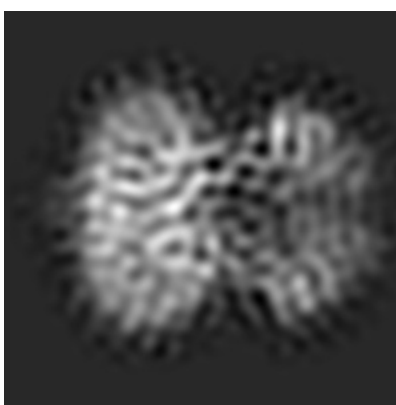
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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](#)

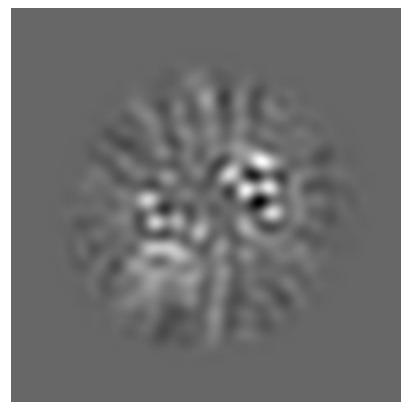
6.2.1 Primary map



X Index: 78



Y Index: 78



Z Index: 78

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: 99



Y Index: 85



Z Index: 106

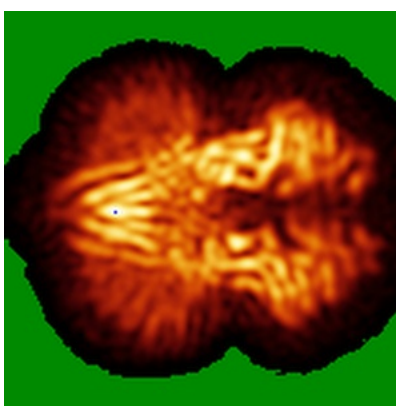
The images above show the largest variance slices of the map in three orthogonal directions.

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

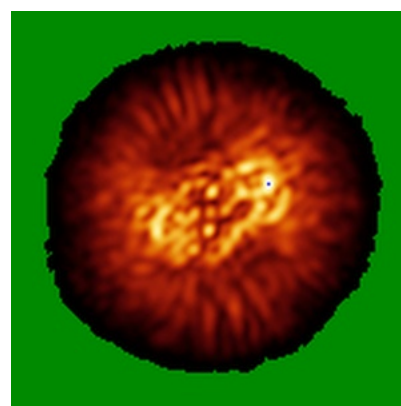
6.4.1 Primary map



X



Y

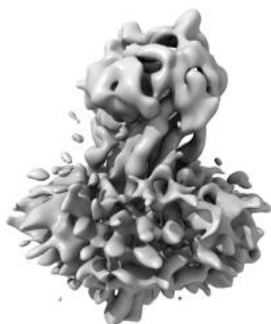


Z

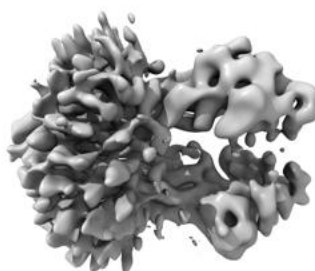
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

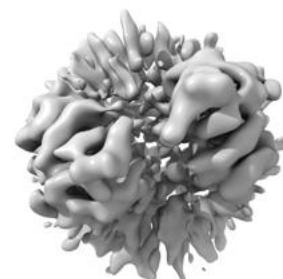
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

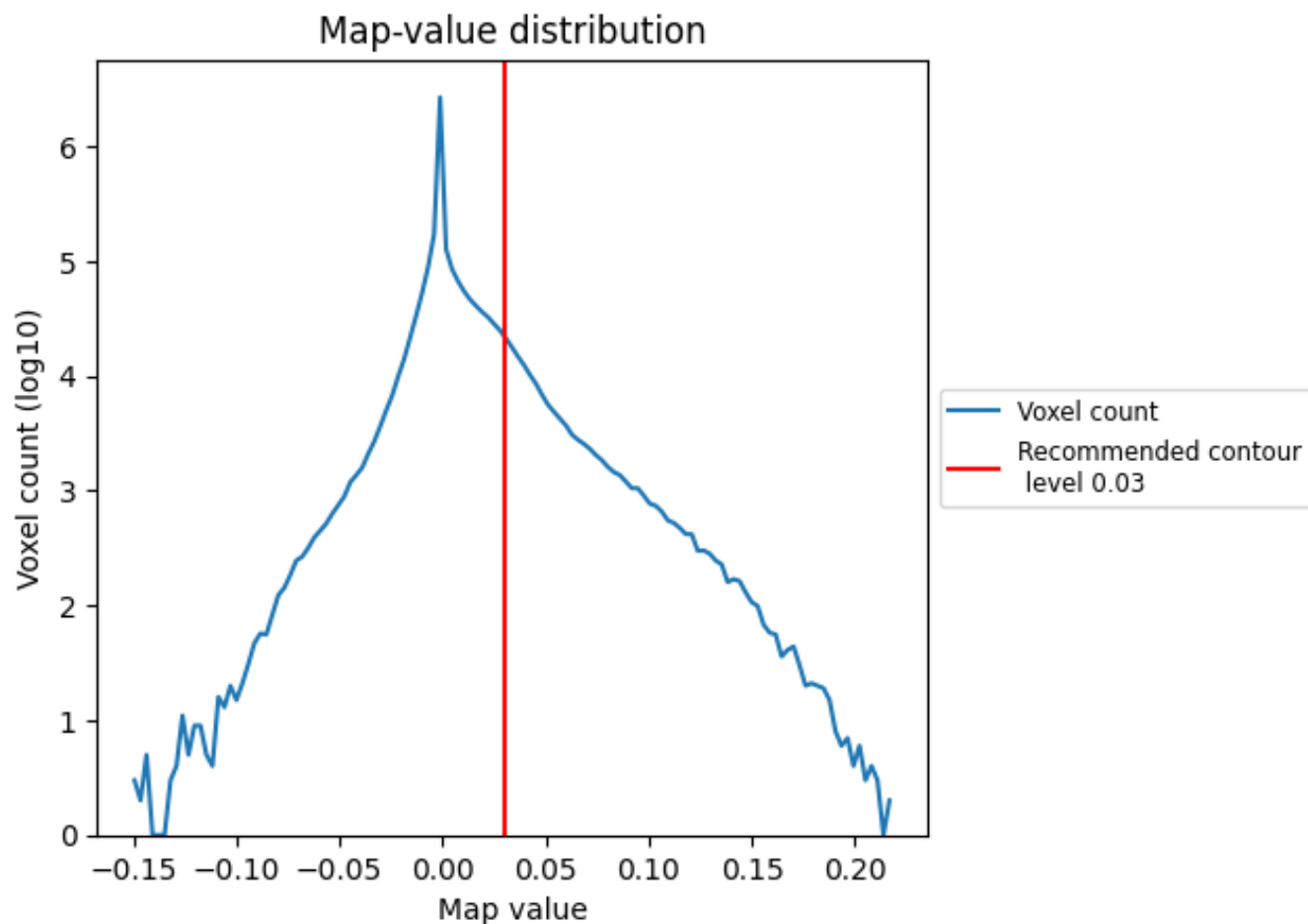
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

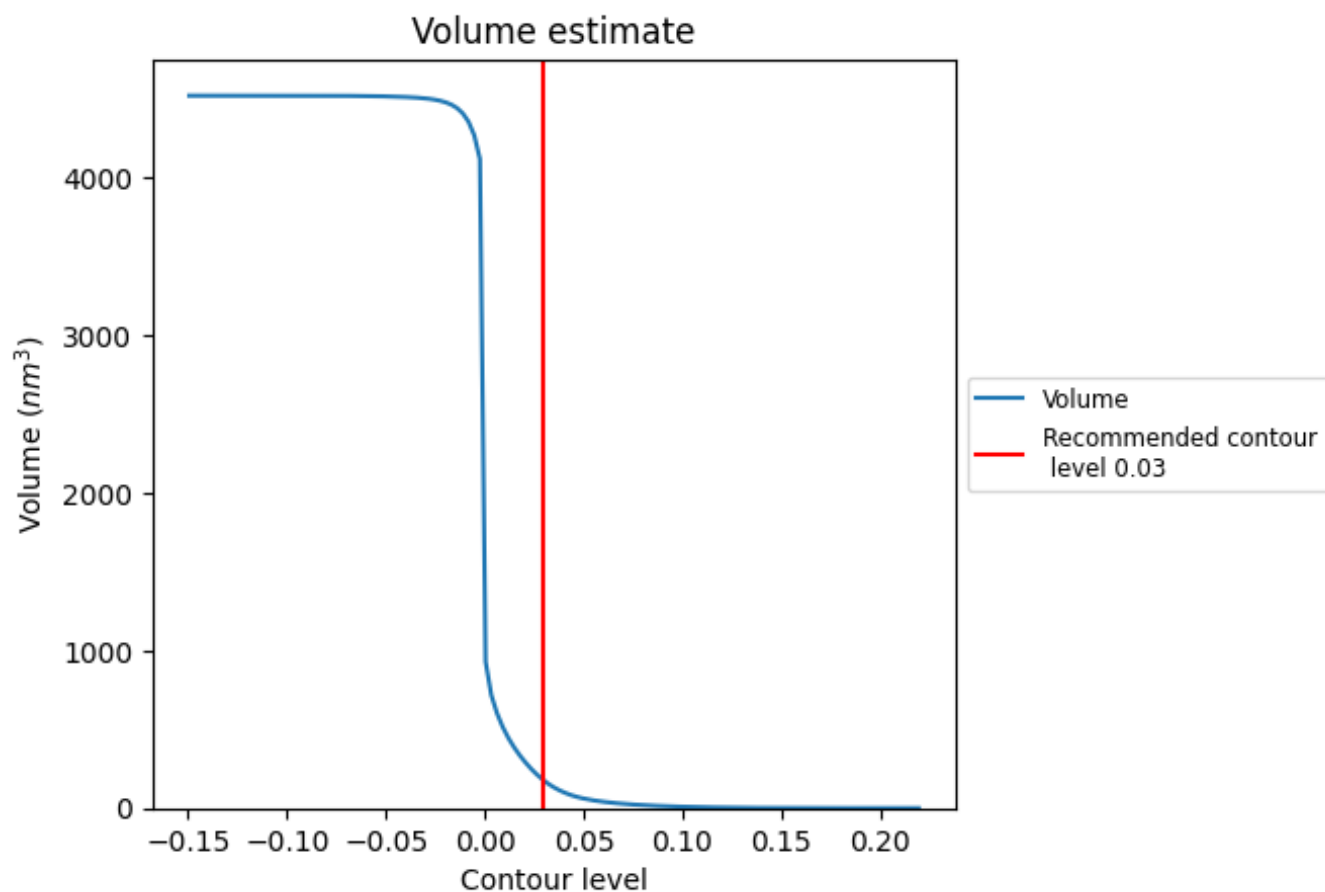
This section contains the results of statistical analysis of the map.

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.

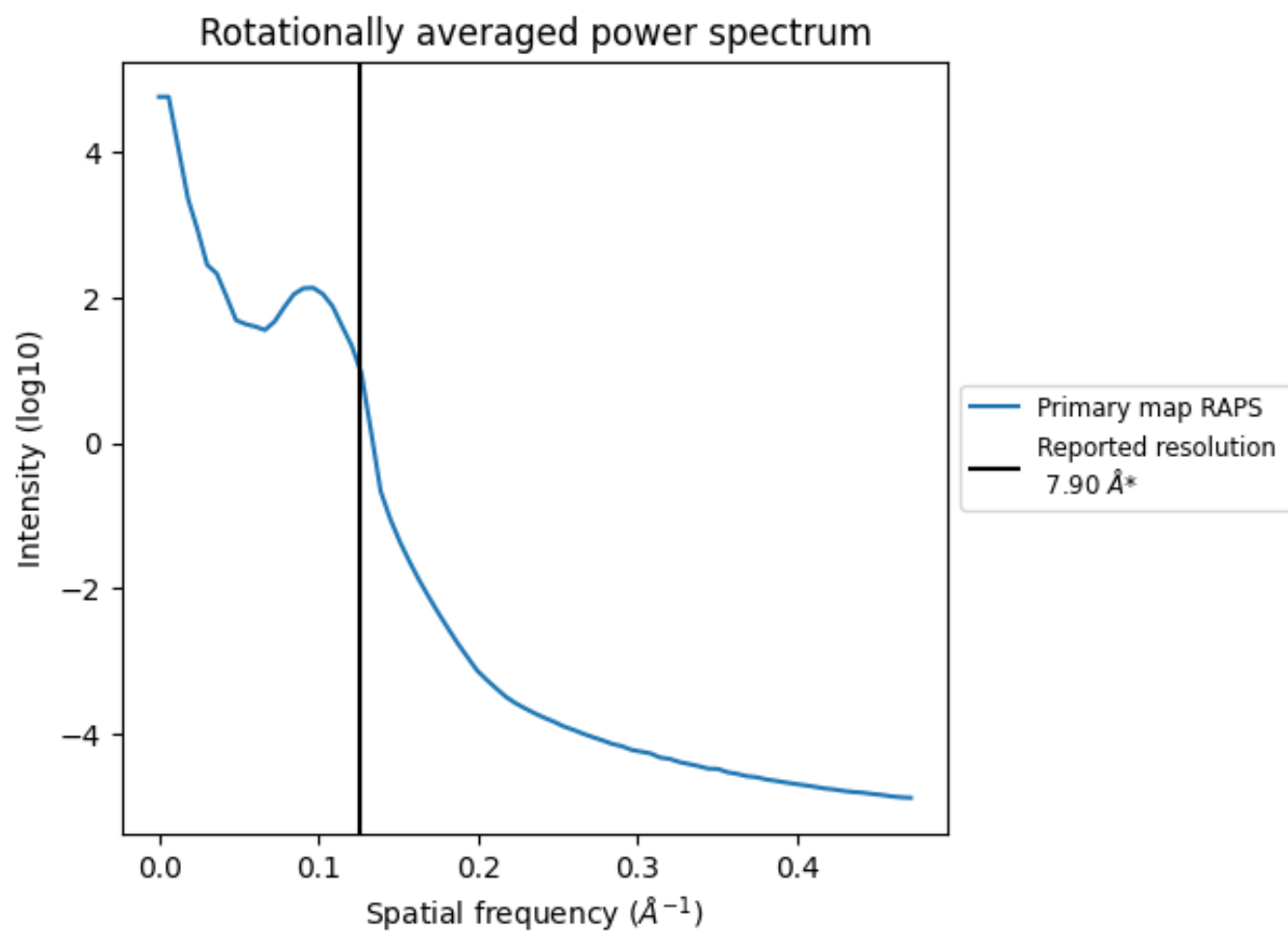
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 176 nm^3 ; this corresponds to an approximate mass of 159 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 ⓘ

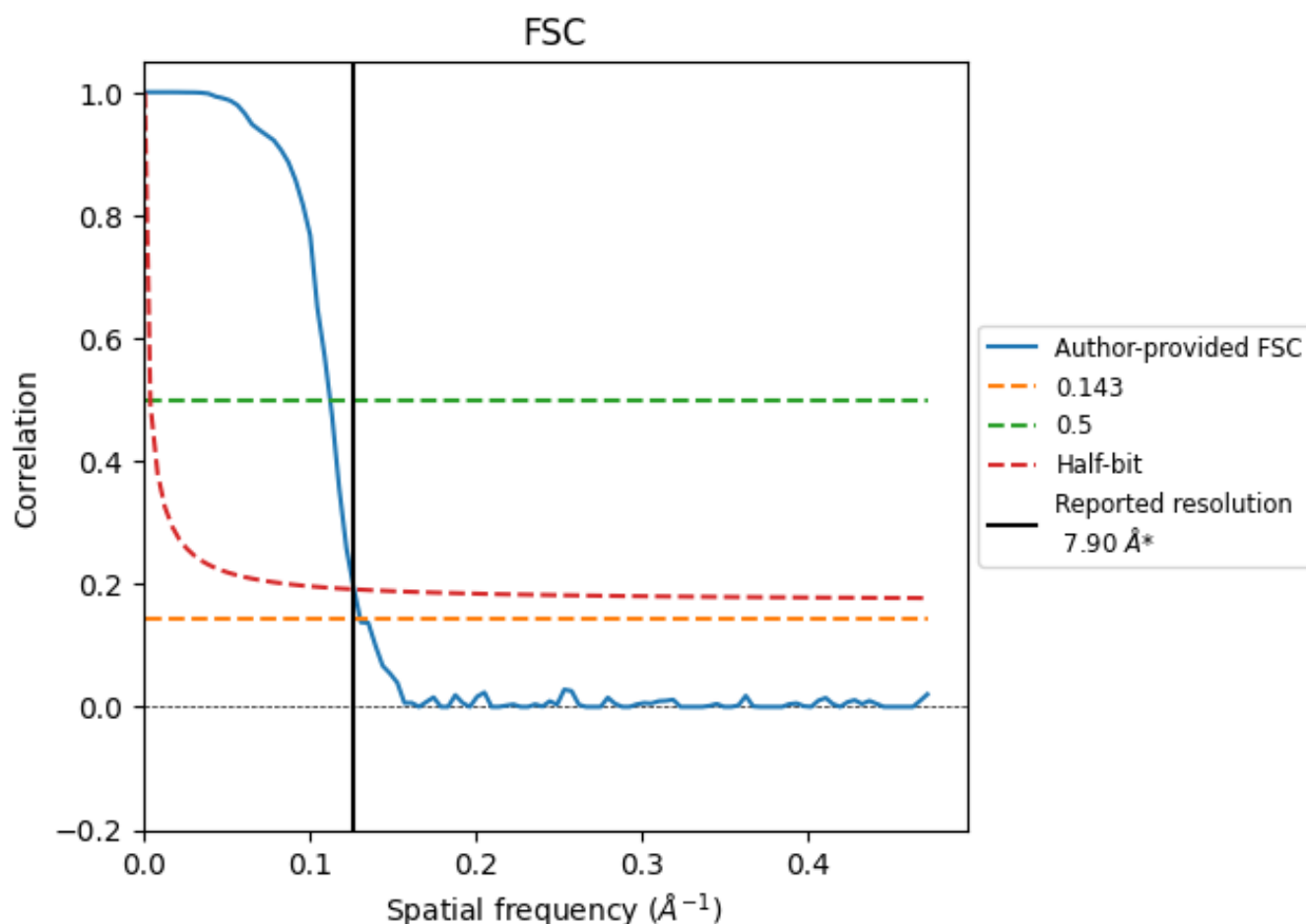


*Reported resolution corresponds to spatial frequency of 0.127 $\text{\AA}^{-1}$

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 0.127 Å⁻¹

8.2 Resolution estimates [i](#)

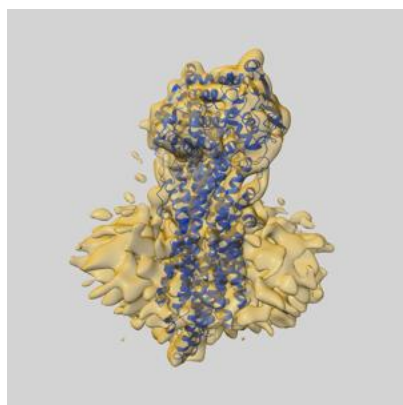
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.90	-	-
Author-provided FSC curve	7.66	8.90	7.89
Unmasked-calculated*	-	-	-

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

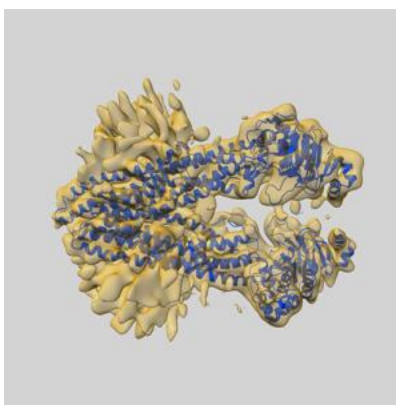
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4391 and PDB model 6GDI. Per-residue inclusion information can be found in section [3](#) on page [4](#).

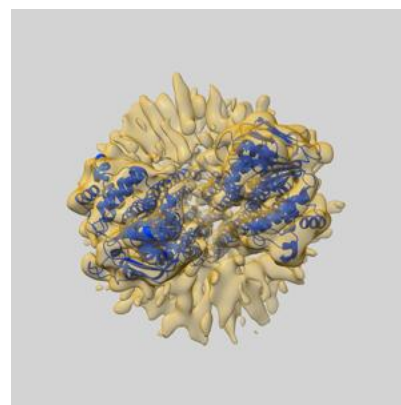
9.1 Map-model overlay [i](#)



X



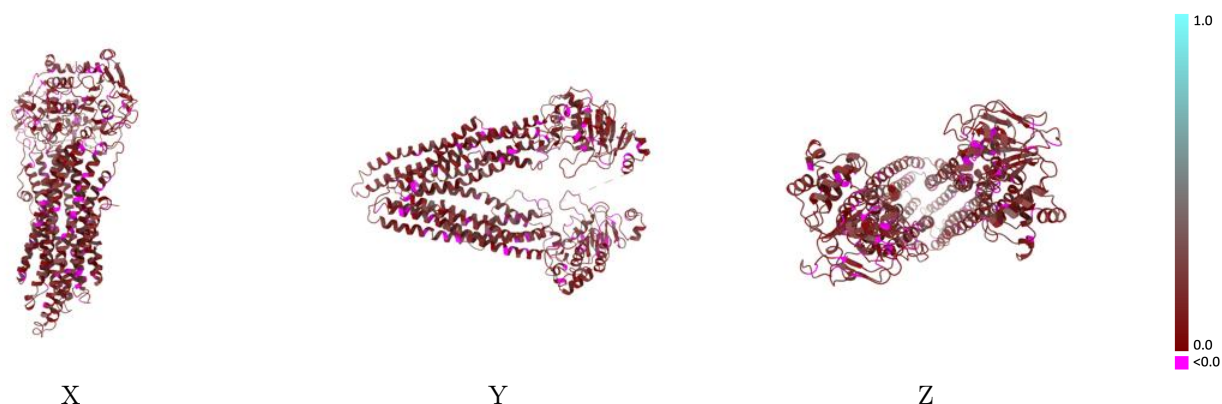
Y



Z

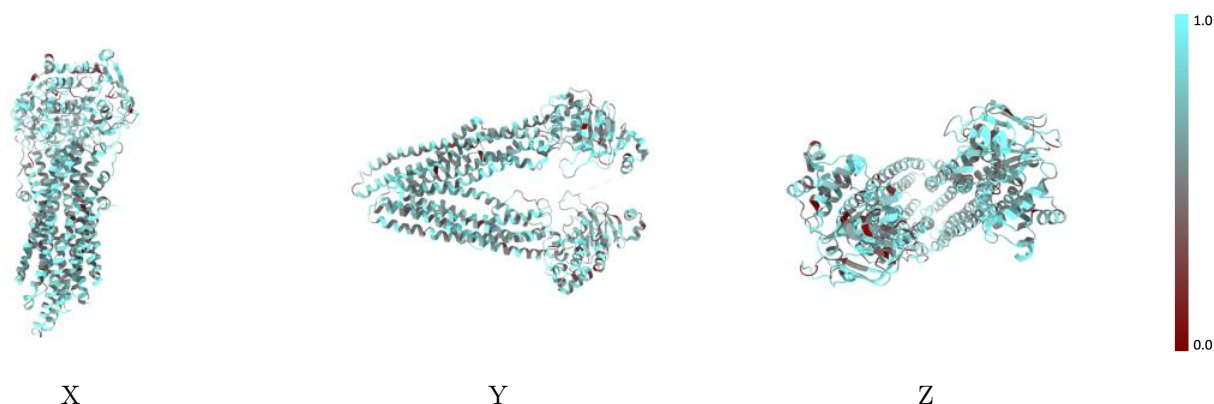
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



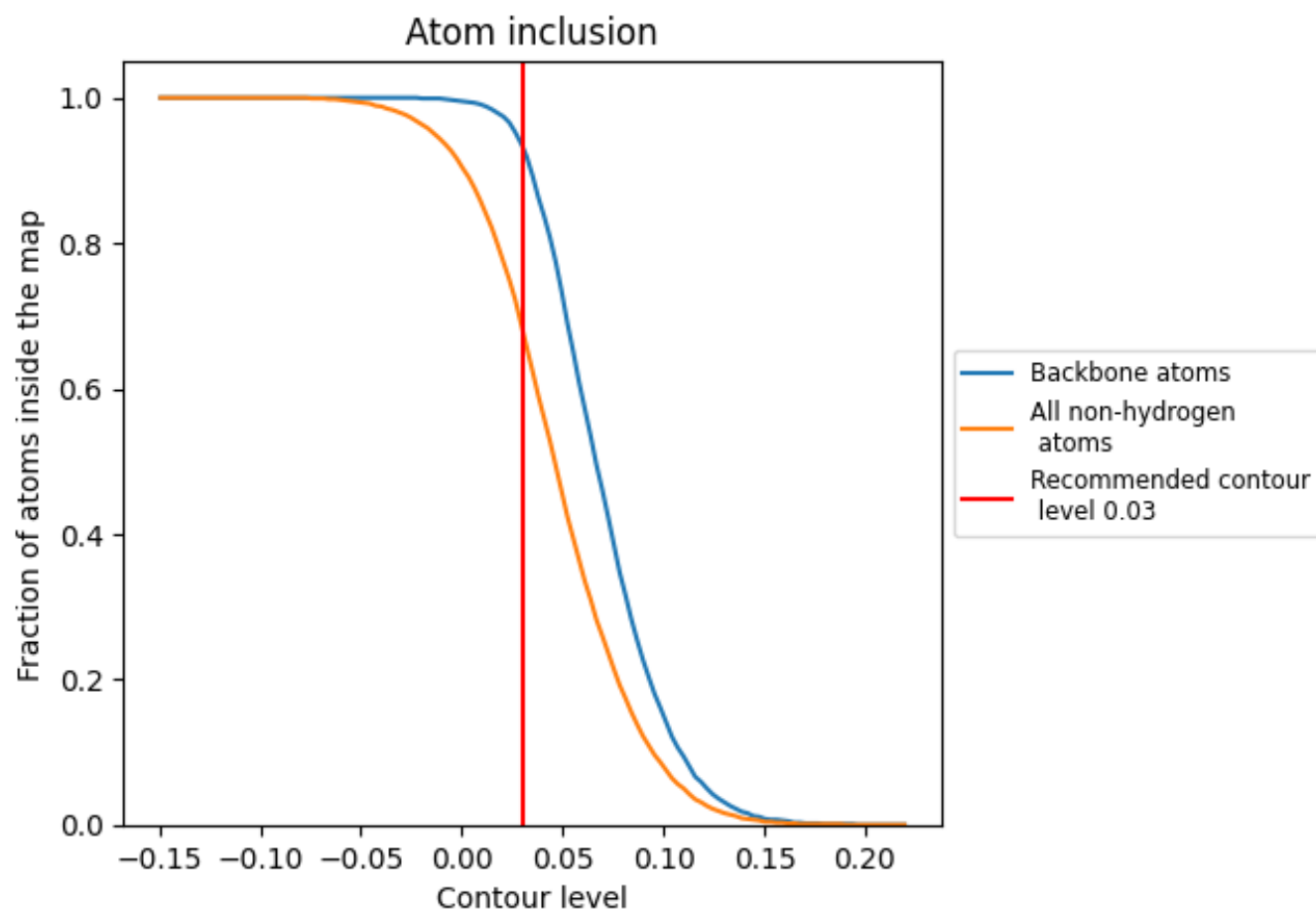
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 68% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6830	0.1410
A	0.6830	0.1410

