



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 10:47 AM UTC

PDB ID : 6KIQ / pdb_00006kiq
EMDB ID : EMD-9997
Title : Complex of yeast cytoplasmic dynein MTBD-High and MT with DTT
Authors : Komori, Y.; Nishida, N.; Shimada, I.; Kikkawa, M.
Deposited on : 2019-07-19
Resolution : 3.62 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

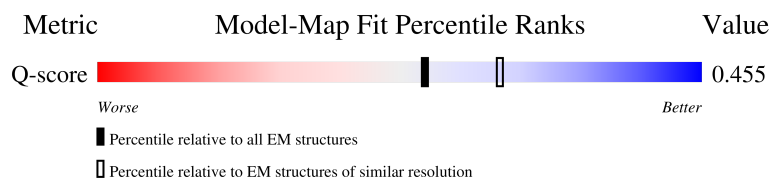
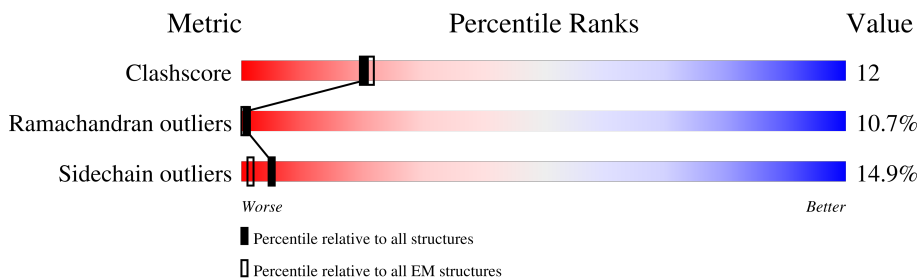
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.62 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	11773 (3.12 - 4.12)

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	412	
2	b	426	
3	M	130	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15093 atoms, of which 7444 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 Alpha tubulin.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	a	412	Total	C	H	N	O	S	0	0
			6375	2043	3147	551	614	20		

- Molecule 2 is a protein called Tubulin beta chain.

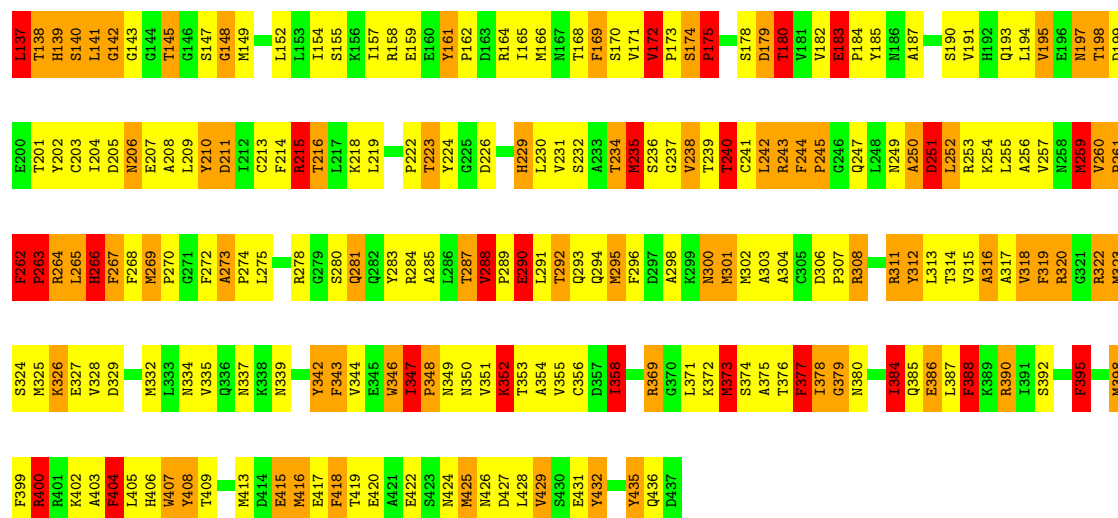
Mol	Chain	Residues	Atoms						AltConf	Trace
2	b	426	Total	C	H	N	O	S	0	0
			6584	2105	3232	575	647	25		

- Molecule 3 is a protein called Dynein heavy chain, cytoplasmic.

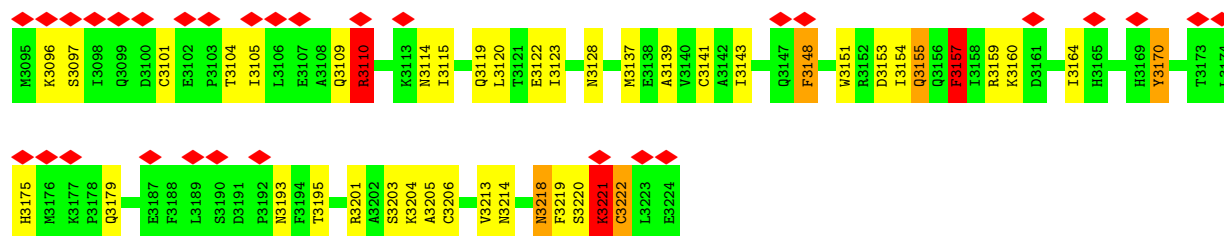
Mol	Chain	Residues	Atoms						AltConf	Trace
3	M	130	Total	C	H	N	O	S	0	0
			2134	679	1065	184	197	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	3101	CYS	ILE	engineered mutation	UNP P36022
M	3222	CYS	VAL	engineered mutation	UNP P36022



• Molecule 3: Dynein heavy chain, cytoplasmic



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-25.7519°, rise=9.2219 Å, axial sym=C1	Depositor
Number of segments used	32666	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{Å}^2$)	54.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.898	Depositor
Minimum map value	-0.367	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.125	Depositor
Map size (Å)	237.6, 237.6, 237.6	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	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	2.71	249/3302 (7.5%)	2.55	255/4485 (5.7%)
2	b	2.63	239/3427 (7.0%)	2.46	239/4642 (5.1%)
3	M	1.32	3/1092 (0.3%)	1.92	33/1472 (2.2%)
All	All	2.52	491/7821 (6.3%)	2.43	527/10599 (5.0%)

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	46
2	b	0	33
3	M	0	4
All	All	0	83

All (491) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	63	PRO	CA-C	-12.10	1.38	1.52
1	a	1024	TYR	CA-C	-11.86	1.36	1.52
2	b	269	MET	C-N	-11.58	1.18	1.33
1	a	1350	CYS	CA-C	-11.10	1.39	1.53
2	b	288	VAL	CA-C	-11.00	1.41	1.52
1	a	1241	PHE	C-N	-10.80	1.20	1.33
1	a	1327	VAL	CA-C	-10.14	1.40	1.52
1	a	1207	GLN	CA-C	-9.99	1.42	1.53
2	b	49	ILE	CA-CB	-9.95	1.43	1.54
2	b	346	TRP	CA-C	-9.94	1.44	1.52
2	b	168	THR	CA-C	-9.92	1.40	1.52
2	b	377	PHE	CA-C	-9.79	1.41	1.52
1	a	1302	VAL	CA-C	-9.77	1.40	1.52
1	a	1280	ASP	C-N	-9.73	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	379	GLY	CA-C	-9.56	1.43	1.52
2	b	62	VAL	CA-CB	-9.54	1.42	1.54
1	a	1330	ASN	CA-C	-9.49	1.41	1.52
1	a	1262	VAL	CA-CB	-9.48	1.41	1.54
1	a	1294	ARG	CA-C	-9.46	1.40	1.52
1	a	1293	TYR	CA-C	-9.45	1.40	1.52
2	b	137	LEU	CA-C	-9.42	1.41	1.52
1	a	1276	MET	CA-C	-9.40	1.42	1.53
2	b	17	GLY	CA-C	-9.40	1.41	1.51
2	b	356	CYS	CA-C	-9.39	1.40	1.52
1	a	1200	ASN	CA-C	-9.35	1.42	1.52
1	a	1037	PRO	CA-C	-9.33	1.41	1.52
2	b	21	TRP	NE1-CE2	-9.33	1.27	1.37
1	a	1171	HIS	CA-C	-9.09	1.40	1.52
1	a	1245	THR	CA-C	-9.08	1.41	1.52
2	b	312	TYR	CA-C	-9.04	1.41	1.52
1	a	1233	LEU	CA-C	-9.03	1.41	1.52
1	a	1042	VAL	CA-C	-8.97	1.42	1.52
1	a	1269	CYS	CA-C	-8.89	1.40	1.52
1	a	1154	ALA	CA-C	-8.86	1.42	1.52
1	a	1235	PRO	CA-C	-8.85	1.39	1.52
1	a	1113	HIS	CA-C	-8.79	1.41	1.52
2	b	291	LEU	CA-C	-8.79	1.41	1.52
2	b	374	SER	CA-C	-8.76	1.41	1.52
1	a	1376	ARG	CA-C	-8.72	1.41	1.52
2	b	123	ARG	CA-C	-8.70	1.40	1.52
1	a	1014	VAL	CA-CB	-8.61	1.42	1.54
1	a	1068	THR	CA-C	-8.59	1.42	1.52
1	a	1041	PHE	CA-C	-8.57	1.42	1.52
1	a	1346	GLN	CA-C	-8.56	1.41	1.52
1	a	1045	GLU	C-N	-8.54	1.22	1.33
1	a	1242	PRO	CA-C	-8.50	1.42	1.52
1	a	1111	VAL	CA-C	-8.47	1.41	1.52
2	b	139	HIS	CA-C	-8.47	1.42	1.52
1	a	1348	ALA	CA-C	-8.45	1.42	1.52
2	b	54	ASN	CA-C	-8.45	1.42	1.52
2	b	136	GLN	CA-C	-8.45	1.42	1.52
1	a	1203	ARG	CA-C	-8.43	1.41	1.52
1	a	1331	TYR	CA-C	-8.42	1.44	1.53
2	b	255	LEU	CA-C	-8.40	1.41	1.52
1	a	1365	LEU	CA-C	-8.37	1.41	1.52
1	a	1349	VAL	CA-CB	-8.34	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1352	LEU	CA-C	-8.31	1.42	1.52
2	b	6	HIS	CB-CG	-8.28	1.38	1.50
1	a	1042	VAL	CA-CB	-8.25	1.44	1.54
1	a	1326	LYS	CA-C	-8.23	1.42	1.52
2	b	102	ASN	N-CA	-8.21	1.36	1.46
1	a	1017	GLY	CA-C	-8.15	1.43	1.52
1	a	1247	ALA	CA-C	-8.13	1.42	1.52
1	a	1142	GLU	CA-C	-8.12	1.42	1.52
2	b	260	VAL	C-N	-8.10	1.27	1.33
1	a	1241	PHE	CA-C	-8.09	1.43	1.52
2	b	140	SER	CA-C	-8.06	1.42	1.52
2	b	68	VAL	CA-CB	-8.05	1.44	1.54
2	b	319	PHE	CA-C	-8.02	1.42	1.53
2	b	49	ILE	CA-C	-7.93	1.43	1.52
1	a	1251	SER	CA-C	-7.92	1.42	1.53
2	b	247	GLN	CA-C	-7.90	1.42	1.52
1	a	1354	ASN	CA-C	-7.89	1.43	1.52
1	a	1351	MET	CA-C	-7.88	1.43	1.52
2	b	404	PHE	CA-C	-7.88	1.42	1.52
1	a	1302	VAL	CA-CB	-7.88	1.45	1.54
2	b	351	VAL	CA-CB	-7.85	1.46	1.54
2	b	281	GLN	CA-C	-7.84	1.44	1.53
1	a	1146	TYR	CA-C	-7.83	1.44	1.52
1	a	1302	VAL	N-CA	-7.81	1.37	1.46
2	b	231	VAL	CA-CB	-7.77	1.45	1.54
2	b	353	THR	CA-C	-7.77	1.42	1.52
1	a	1353	SER	CA-C	-7.75	1.43	1.52
1	a	1036	VAL	CA-CB	-7.75	1.44	1.54
2	b	180	THR	CA-C	-7.73	1.42	1.52
2	b	316	ALA	CA-C	-7.73	1.44	1.53
2	b	234	THR	CA-C	-7.72	1.42	1.52
2	b	55	GLU	CA-C	-7.71	1.43	1.52
1	a	1205	ILE	CA-CB	-7.69	1.45	1.54
1	a	1265	ILE	CA-C	-7.68	1.42	1.52
2	b	288	VAL	N-CA	-7.68	1.37	1.46
1	a	1243	LEU	CA-C	-7.67	1.43	1.52
1	a	1234	VAL	CA-C	-7.66	1.44	1.52
2	b	216	THR	CA-C	-7.65	1.45	1.52
2	b	60	LYS	CA-C	-7.64	1.43	1.52
2	b	231	VAL	CA-C	-7.61	1.43	1.52
2	b	64	ARG	N-CA	-7.53	1.37	1.46
2	b	101	ASN	CA-C	-7.53	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1368	LYS	CA-C	-7.48	1.42	1.52
1	a	1021	TRP	CA-C	-7.46	1.42	1.52
1	a	1229	PHE	CA-C	-7.46	1.42	1.52
1	a	1022	GLU	CA-C	-7.42	1.43	1.52
1	a	1221	ALA	CA-C	-7.42	1.42	1.52
2	b	198	THR	CA-C	-7.42	1.43	1.52
1	a	1052	VAL	CA-C	-7.41	1.43	1.52
1	a	1076	ASN	N-CA	-7.41	1.37	1.46
2	b	261	PRO	CA-C	-7.41	1.45	1.52
1	a	1328	GLY	CA-C	-7.41	1.41	1.51
1	a	1162	ILE	CA-CB	-7.40	1.46	1.54
1	a	1190	ASN	CA-C	-7.39	1.42	1.52
1	a	1066	LEU	CA-C	-7.37	1.42	1.53
2	b	48	ARG	CA-C	-7.36	1.43	1.52
1	a	1173	ASP	CA-C	-7.36	1.43	1.52
2	b	260	VAL	CA-CB	-7.35	1.44	1.54
1	a	1347	ARG	CA-C	-7.33	1.43	1.52
2	b	50	ASN	CA-C	-7.33	1.43	1.52
2	b	197	ASN	CA-C	-7.33	1.43	1.52
2	b	125	GLU	CA-C	-7.33	1.42	1.52
2	b	183	GLU	CA-C	-7.32	1.43	1.52
1	a	1067	ILE	CA-C	-7.31	1.43	1.52
2	b	376	THR	CA-C	-7.31	1.43	1.52
1	a	1309	ILE	CA-C	-7.29	1.44	1.52
2	b	64	ARG	CA-C	-7.29	1.43	1.52
2	b	63	PRO	C-N	-7.29	1.23	1.33
1	a	1297	VAL	CA-C	-7.29	1.43	1.52
2	b	8	GLN	CA-C	-7.28	1.45	1.53
1	a	1250	ILE	CA-C	-7.27	1.44	1.52
1	a	1246	TYR	CA-C	-7.26	1.43	1.52
1	a	1337	VAL	CA-C	-7.23	1.45	1.52
2	b	62	VAL	C-N	-7.23	1.24	1.33
2	b	157	ILE	CA-CB	-7.22	1.46	1.54
1	a	1265	ILE	CA-CB	-7.19	1.44	1.54
2	b	121	VAL	CA-CB	-7.18	1.45	1.54
1	a	1070	LYS	CA-C	-7.16	1.43	1.52
1	a	1297	VAL	CA-CB	-7.16	1.45	1.54
2	b	183	GLU	C-N	-7.16	1.25	1.33
2	b	209	LEU	N-CA	-7.12	1.37	1.46
1	a	1362	TRP	CA-C	-7.12	1.43	1.52
2	b	375	ALA	CA-C	-7.11	1.43	1.52
1	a	1183	ILE	CA-C	-7.09	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1111	VAL	CA-CB	-7.07	1.45	1.54
1	a	1383	VAL	CA-C	-7.07	1.44	1.52
2	b	256	ALA	CA-C	-7.06	1.44	1.52
2	b	154	ILE	CA-CB	-7.04	1.45	1.54
1	a	1109	PHE	N-CA	-7.00	1.38	1.46
2	b	51	VAL	CA-CB	-7.00	1.45	1.54
2	b	292	THR	CA-C	-6.99	1.43	1.52
1	a	1109	PHE	CA-C	-6.96	1.44	1.52
1	a	1150	GLN	CA-C	-6.96	1.45	1.52
1	a	1120	GLY	CA-C	-6.95	1.42	1.51
1	a	1165	THR	CA-C	-6.92	1.43	1.52
1	a	1063	PRO	CA-C	-6.92	1.42	1.52
2	b	303	ALA	CA-C	-6.91	1.44	1.52
2	b	429	VAL	CA-CB	-6.88	1.45	1.54
1	a	1264	GLU	CA-C	-6.88	1.44	1.53
1	a	1098	LYS	CA-C	-6.86	1.43	1.52
2	b	218	LYS	CA-C	-6.84	1.42	1.53
2	b	355	VAL	CA-C	-6.83	1.44	1.52
1	a	1274	ASN	CA-C	-6.83	1.43	1.52
1	a	1095	ARG	CA-C	-6.82	1.44	1.52
2	b	14	ASN	N-CA	-6.82	1.38	1.46
2	b	403	ALA	N-CA	-6.81	1.38	1.46
1	a	1067	ILE	CA-CB	-6.81	1.45	1.54
1	a	1208	ILE	CA-CB	-6.81	1.46	1.54
1	a	1016	ILE	CA-C	-6.80	1.44	1.52
2	b	41	ASP	CA-C	-6.80	1.43	1.52
2	b	138	THR	CA-C	-6.78	1.44	1.52
1	a	1011	GLN	CA-C	-6.76	1.43	1.52
1	a	1060	LEU	N-CA	-6.76	1.38	1.46
2	b	47	GLU	CA-C	-6.74	1.43	1.52
1	a	1234	VAL	CA-CB	-6.73	1.45	1.54
1	a	1241	PHE	N-CA	-6.72	1.39	1.46
2	b	429	VAL	CA-C	-6.72	1.44	1.52
2	b	63	PRO	CA-CB	-6.71	1.44	1.53
1	a	1009	VAL	CA-C	-6.70	1.44	1.52
2	b	59	ASN	CA-C	-6.70	1.45	1.53
2	b	83	PHE	CA-C	-6.69	1.43	1.53
2	b	349	ASN	N-CA	-6.68	1.37	1.46
1	a	1090	ASP	CA-C	-6.68	1.43	1.52
1	a	1382	TYR	CA-C	-6.67	1.45	1.52
2	b	191	VAL	CA-CB	-6.67	1.46	1.54
1	a	1383	VAL	CA-CB	-6.65	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1131	LEU	CA-C	-6.63	1.44	1.52
1	a	1172	SER	CA-C	-6.63	1.44	1.52
1	a	1335	THR	CA-C	-6.63	1.45	1.52
2	b	399	PHE	CA-C	-6.62	1.44	1.52
1	a	1208	ILE	CA-C	-6.60	1.44	1.52
1	a	1261	SER	CA-C	-6.59	1.44	1.52
2	b	335	VAL	CA-CB	-6.59	1.46	1.54
2	b	215	ARG	CA-C	-6.58	1.43	1.52
1	a	1248	PRO	CA-C	-6.58	1.46	1.52
2	b	86	ILE	CA-C	-6.57	1.44	1.52
2	b	269	MET	CA-C	-6.57	1.44	1.52
2	b	354	ALA	CA-C	-6.56	1.44	1.52
1	a	1157	GLU	C-N	-6.55	1.25	1.33
2	b	116	ASP	CA-C	-6.55	1.44	1.52
2	b	226	ASP	CA-C	-6.53	1.44	1.52
2	b	89	PRO	CA-C	-6.53	1.40	1.52
2	b	52	TYR	CA-C	-6.52	1.44	1.52
2	b	417	GLU	CA-C	-6.50	1.44	1.52
2	b	52	TYR	C-N	-6.48	1.24	1.33
1	a	1402	LEU	CA-C	-6.47	1.44	1.52
1	a	1056	THR	CA-C	-6.47	1.44	1.52
2	b	24	ILE	CA-CB	-6.47	1.45	1.54
1	a	1325	PHE	CA-C	-6.46	1.44	1.53
2	b	283	TYR	C-N	6.46	1.42	1.33
2	b	237	GLY	CA-C	-6.45	1.44	1.52
1	a	1329	ILE	CA-CB	-6.45	1.46	1.54
2	b	352	LYS	CA-C	-6.45	1.44	1.53
2	b	25	SER	CA-C	-6.42	1.44	1.52
2	b	339	ASN	CA-C	-6.41	1.44	1.53
2	b	21	TRP	CA-C	-6.41	1.43	1.52
2	b	161	TYR	CA-C	-6.40	1.45	1.52
2	b	187	ALA	CA-C	-6.40	1.46	1.53
1	a	1248	PRO	N-CD	-6.37	1.38	1.47
2	b	166	MET	CA-C	-6.36	1.46	1.53
2	b	49	ILE	N-CA	-6.35	1.39	1.46
2	b	376	THR	CA-CB	-6.34	1.42	1.53
2	b	353	THR	CA-CB	-6.33	1.42	1.53
2	b	259	MET	CA-C	-6.32	1.46	1.53
2	b	287	THR	CA-C	-6.32	1.44	1.52
2	b	417	GLU	N-CA	-6.31	1.38	1.46
2	b	350	ASN	CA-C	-6.31	1.44	1.52
1	a	1183	ILE	CA-CB	-6.31	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	274	PRO	N-CD	-6.31	1.39	1.47
1	a	1204	LEU	N-CA	-6.30	1.39	1.46
2	b	243	ARG	CA-CB	-6.30	1.45	1.53
2	b	152	LEU	CA-C	-6.28	1.44	1.52
1	a	1156	VAL	CA-CB	-6.27	1.46	1.54
1	a	1277	VAL	CA-C	-6.27	1.44	1.52
1	a	1324	GLY	CA-C	-6.26	1.43	1.51
2	b	20	PHE	CA-C	-6.26	1.44	1.52
2	b	327	GLU	CA-C	-6.25	1.44	1.52
2	b	432	TYR	CA-C	-6.24	1.43	1.52
1	a	1292	LEU	CA-CB	-6.23	1.44	1.53
1	a	1250	ILE	CA-CB	-6.23	1.44	1.54
1	a	1266	THR	CA-C	-6.21	1.44	1.52
2	b	252	LEU	CA-C	-6.21	1.44	1.52
2	b	219	LEU	CA-C	-6.19	1.45	1.52
1	a	1045	GLU	CA-C	-6.18	1.45	1.52
2	b	115	VAL	CA-C	-6.16	1.45	1.52
1	a	1306	ILE	CA-CB	-6.16	1.45	1.54
1	a	1092	VAL	CA-CB	-6.15	1.47	1.54
2	b	71	GLU	CA-C	-6.14	1.45	1.52
1	a	1141	LEU	CA-C	-6.14	1.45	1.52
2	b	207	GLU	CA-C	-6.14	1.44	1.52
1	a	1097	ARG	CA-C	-6.13	1.44	1.52
1	a	1113	HIS	CB-CG	-6.12	1.41	1.50
2	b	24	ILE	CA-C	-6.11	1.45	1.52
1	a	1060	LEU	CA-C	-6.11	1.44	1.52
2	b	92	PHE	CA-C	-6.10	1.44	1.52
1	a	1349	VAL	CA-C	-6.09	1.45	1.52
2	b	320	ARG	CA-C	-6.09	1.46	1.53
1	a	1006	SER	CA-C	-6.08	1.44	1.52
2	b	346	TRP	N-CA	-6.08	1.41	1.47
2	b	313	LEU	CA-C	-6.07	1.45	1.52
1	a	1209	VAL	CA-CB	-6.06	1.46	1.54
1	a	1057	TYR	CA-C	-6.05	1.44	1.52
1	a	1245	THR	CA-CB	-6.05	1.41	1.54
1	a	1248	PRO	N-CA	-6.04	1.41	1.47
1	a	1406	TYR	CA-C	-6.03	1.44	1.52
3	M	3154	ILE	CA-CB	-6.03	1.46	1.54
1	a	1025	CYS	N-CA	-6.02	1.39	1.46
2	b	267	PHE	N-CA	-6.01	1.38	1.46
1	a	1048	VAL	CA-C	-6.01	1.45	1.52
2	b	182	VAL	CA-CB	-6.01	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	323	MET	CA-C	-5.99	1.44	1.52
2	b	18	ALA	N-CA	-5.98	1.38	1.46
1	a	1316	GLN	CA-C	-5.97	1.45	1.52
1	a	1145	ILE	CA-C	-5.95	1.45	1.52
1	a	1299	PRO	CA-C	-5.95	1.44	1.52
2	b	199	ASP	CA-C	-5.94	1.44	1.52
2	b	135	PHE	CA-C	-5.94	1.45	1.52
1	a	1315	ILE	CA-C	-5.94	1.46	1.52
1	a	1114	SER	CA-C	-5.93	1.45	1.52
1	a	1064	GLU	N-CA	-5.93	1.38	1.46
1	a	1142	GLU	CA-CB	-5.93	1.45	1.53
1	a	1257	HIS	N-CA	-5.93	1.38	1.46
2	b	148	GLY	CA-C	-5.93	1.43	1.51
1	a	1222	LEU	CA-C	-5.93	1.44	1.52
2	b	201	THR	CA-C	-5.93	1.45	1.52
1	a	1014	VAL	CA-C	-5.92	1.45	1.53
1	a	1017	GLY	C-N	-5.91	1.26	1.34
2	b	295	MET	CA-C	-5.91	1.44	1.52
2	b	63	PRO	N-CA	-5.91	1.40	1.47
1	a	1241	PHE	C-O	-5.90	1.20	1.25
1	a	1293	TYR	C-N	-5.89	1.26	1.33
2	b	407	TRP	CA-CB	5.89	1.63	1.53
2	b	329	ASP	CA-C	-5.89	1.44	1.52
2	b	28	HIS	CA-C	-5.88	1.44	1.52
1	a	1046	PRO	CA-CB	-5.88	1.44	1.53
1	a	1053	ARG	CA-C	-5.88	1.44	1.52
2	b	302	MET	N-CA	-5.86	1.38	1.46
1	a	1350	CYS	C-N	-5.86	1.25	1.33
2	b	324	SER	CA-C	-5.86	1.45	1.52
1	a	1122	GLY	CA-C	-5.85	1.43	1.51
2	b	211	ASP	CA-C	-5.85	1.45	1.52
1	a	1231	THR	CA-CB	-5.84	1.44	1.53
2	b	256	ALA	N-CA	-5.84	1.39	1.46
2	b	191	VAL	CA-C	-5.83	1.45	1.52
2	b	413	MET	CA-C	-5.83	1.45	1.52
1	a	1395	ALA	CA-C	-5.80	1.45	1.52
2	b	347	ILE	N-CA	-5.79	1.41	1.46
2	b	326	LYS	CA-C	-5.79	1.45	1.53
1	a	1274	ASN	N-CA	-5.79	1.39	1.46
1	a	1154	ALA	N-CA	-5.78	1.39	1.46
1	a	1379	VAL	N-CA	-5.77	1.39	1.46
1	a	1084	ILE	CA-CB	-5.77	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	409	THR	CA-C	-5.76	1.45	1.52
1	a	1294	ARG	N-CA	-5.76	1.39	1.46
2	b	209	LEU	CA-C	-5.76	1.45	1.52
2	b	328	VAL	CA-C	-5.76	1.45	1.52
1	a	1167	THR	CA-C	-5.76	1.44	1.52
1	a	1133	VAL	CA-CB	-5.75	1.46	1.54
1	a	1018	ASN	N-CA	-5.75	1.39	1.46
2	b	17	GLY	C-N	-5.75	1.26	1.34
1	a	1112	PHE	CA-C	-5.74	1.45	1.53
2	b	314	THR	CA-C	-5.74	1.45	1.52
2	b	292	THR	CA-CB	-5.73	1.43	1.53
2	b	266	HIS	CA-C	-5.71	1.45	1.52
2	b	273	ALA	CA-C	-5.70	1.45	1.52
2	b	54	ASN	N-CA	-5.70	1.38	1.45
2	b	261	PRO	N-CA	-5.70	1.40	1.47
2	b	267	PHE	CA-C	-5.70	1.45	1.52
2	b	138	THR	CA-CB	-5.69	1.43	1.53
2	b	388	PHE	CA-C	-5.69	1.44	1.52
2	b	168	THR	CA-CB	-5.69	1.43	1.53
2	b	205	ASP	CA-C	-5.68	1.45	1.52
2	b	171	VAL	CA-CB	-5.67	1.46	1.54
1	a	1329	ILE	CA-C	-5.67	1.46	1.52
1	a	1394	GLU	CA-C	-5.67	1.44	1.52
1	a	1089	ILE	CA-C	-5.67	1.45	1.52
1	a	1021	TRP	NE1-CE2	-5.66	1.31	1.37
2	b	266	HIS	N-CA	-5.66	1.38	1.46
1	a	1075	ASN	CA-C	-5.66	1.45	1.52
2	b	236	SER	CA-C	-5.65	1.45	1.52
1	a	1240	HIS	N-CA	-5.64	1.39	1.46
1	a	1210	SER	CA-C	-5.63	1.45	1.52
2	b	154	ILE	CA-C	-5.63	1.45	1.52
1	a	1220	GLY	CA-C	-5.62	1.44	1.51
2	b	40	SER	CA-C	-5.62	1.45	1.52
2	b	72	PRO	CA-C	-5.62	1.44	1.52
2	b	278	ARG	CA-C	-5.61	1.45	1.52
2	b	120	ASP	CA-C	-5.61	1.45	1.52
3	M	3206	CYS	CA-C	-5.61	1.45	1.52
2	b	214	PHE	CA-C	-5.61	1.45	1.52
1	a	1180	ASN	N-CA	-5.60	1.39	1.46
2	b	62	VAL	N-CA	-5.59	1.40	1.46
2	b	67	LEU	CA-C	-5.58	1.45	1.53
1	a	1226	LEU	CA-C	-5.58	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	386	GLU	CA-C	-5.58	1.45	1.52
1	a	1203	ARG	C-N	-5.58	1.26	1.33
2	b	68	VAL	CA-C	-5.58	1.46	1.52
2	b	5	VAL	CA-CB	-5.57	1.46	1.54
1	a	1212	ILE	CA-CB	-5.57	1.46	1.54
1	a	1038	ARG	CA-C	-5.56	1.44	1.52
1	a	1162	ILE	CA-C	-5.56	1.46	1.52
2	b	155	SER	CA-C	-5.56	1.44	1.52
2	b	335	VAL	CA-C	-5.56	1.45	1.52
1	a	1298	VAL	CA-CB	-5.56	1.47	1.54
2	b	141	LEU	N-CA	-5.55	1.39	1.46
1	a	1063	PRO	C-N	-5.54	1.26	1.34
1	a	1158	PRO	C-N	-5.54	1.26	1.33
2	b	347	ILE	CA-CB	-5.54	1.49	1.55
1	a	1391	GLU	CA-C	-5.52	1.45	1.52
2	b	94	PHE	CA-C	-5.52	1.45	1.53
1	a	1078	ALA	CA-C	-5.52	1.45	1.52
1	a	1306	ILE	CA-C	-5.51	1.44	1.52
2	b	165	ILE	CA-CB	-5.50	1.47	1.54
1	a	1213	THR	CA-CB	-5.49	1.44	1.53
1	a	1073	ALA	CA-C	-5.47	1.45	1.52
1	a	1372	MET	CA-C	-5.47	1.46	1.52
1	a	1019	ALA	CA-C	-5.47	1.46	1.52
1	a	1342	LEU	CA-C	-5.47	1.46	1.52
1	a	1309	ILE	CA-CB	-5.46	1.48	1.54
1	a	1255	ALA	CA-C	-5.45	1.45	1.52
2	b	270	PRO	CA-C	-5.45	1.45	1.52
2	b	268	PHE	CA-C	-5.44	1.45	1.53
2	b	408	TYR	CA-C	-5.44	1.46	1.53
2	b	7	ILE	CA-C	-5.43	1.46	1.52
2	b	238	VAL	CA-CB	-5.43	1.47	1.54
2	b	342	TYR	CA-C	-5.42	1.46	1.52
1	a	1059	GLN	CA-C	-5.41	1.45	1.52
2	b	170	SER	CA-C	-5.41	1.46	1.52
2	b	376	THR	C-N	-5.38	1.26	1.33
2	b	61	TYR	CA-C	-5.38	1.46	1.52
2	b	387	LEU	N-CA	-5.38	1.39	1.46
2	b	373	MET	CA-C	-5.38	1.45	1.52
2	b	55	GLU	N-CA	-5.37	1.39	1.46
1	a	1301	ASP	CA-C	-5.37	1.45	1.52
2	b	280	SER	CA-C	-5.37	1.44	1.52
2	b	238	VAL	CA-C	-5.37	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1214	ALA	CA-C	-5.37	1.45	1.52
2	b	169	PHE	CA-C	-5.37	1.46	1.53
1	a	1061	PHE	CA-C	-5.36	1.46	1.52
1	a	1366	ASP	N-CA	-5.36	1.40	1.46
1	a	1204	LEU	CA-C	-5.36	1.46	1.52
2	b	201	THR	CA-CB	-5.35	1.43	1.53
2	b	405	LEU	N-CA	-5.35	1.39	1.46
1	a	1049	ILE	CA-C	-5.34	1.45	1.52
1	a	1358	ILE	CA-CB	-5.34	1.47	1.54
2	b	243	ARG	CA-C	-5.34	1.44	1.52
1	a	1212	ILE	C-N	-5.34	1.26	1.33
2	b	66	ILE	CA-CB	-5.34	1.47	1.54
2	b	332	MET	CA-C	-5.34	1.45	1.52
2	b	355	VAL	CA-CB	-5.33	1.46	1.54
2	b	90	ASP	N-CA	-5.33	1.39	1.46
1	a	1036	VAL	CA-C	-5.33	1.47	1.52
2	b	328	VAL	CA-CB	-5.33	1.47	1.54
2	b	204	ILE	CA-CB	-5.32	1.48	1.54
2	b	42	LEU	N-CA	-5.32	1.39	1.46
1	a	1166	HIS	N-CA	-5.32	1.39	1.46
1	a	1387	MET	CA-C	-5.31	1.46	1.52
2	b	101	ASN	C-N	-5.31	1.26	1.33
2	b	272	PHE	CA-C	-5.30	1.46	1.53
2	b	315	VAL	CA-CB	-5.30	1.47	1.55
1	a	1326	LYS	N-CA	-5.30	1.40	1.46
1	a	1297	VAL	N-CA	-5.29	1.40	1.46
2	b	159	GLU	CA-C	-5.29	1.45	1.52
1	a	1008	HIS	CA-CB	-5.29	1.46	1.53
1	a	1315	ILE	CA-CB	-5.28	1.47	1.53
1	a	1145	ILE	CA-CB	-5.28	1.48	1.54
1	a	1226	LEU	N-CA	-5.28	1.40	1.46
2	b	56	ALA	CA-C	-5.28	1.46	1.52
2	b	314	THR	C-N	-5.27	1.27	1.33
2	b	348	PRO	CA-C	-5.27	1.45	1.52
1	a	1155	VAL	CA-C	-5.25	1.46	1.52
2	b	229	HIS	CB-CG	-5.25	1.42	1.50
1	a	1392	PHE	CA-C	-5.24	1.45	1.52
2	b	165	ILE	N-CA	-5.24	1.39	1.46
1	a	1222	LEU	N-CA	-5.24	1.39	1.46
1	a	1104	THR	CA-C	-5.24	1.46	1.52
1	a	1185	ASP	CA-C	-5.24	1.46	1.52
1	a	1348	ALA	C-O	-5.23	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	3195	THR	CA-C	-5.23	1.46	1.52
2	b	26	ASP	N-CA	-5.23	1.39	1.46
2	b	112	ALA	CA-C	-5.23	1.45	1.52
1	a	1128	MET	CA-C	-5.22	1.45	1.52
1	a	1283	HIS	CA-C	-5.22	1.45	1.52
2	b	86	ILE	N-CA	-5.22	1.39	1.46
1	a	1242	PRO	N-CD	-5.21	1.40	1.47
2	b	120	ASP	N-CA	-5.21	1.40	1.46
1	a	1403	GLU	CA-C	-5.21	1.45	1.52
2	b	425	MET	CA-C	-5.21	1.45	1.52
2	b	74	THR	CA-C	-5.20	1.45	1.52
2	b	124	LYS	N-CA	-5.20	1.39	1.46
1	a	1265	ILE	N-CA	-5.20	1.40	1.46
1	a	1157	GLU	CA-C	-5.19	1.46	1.52
2	b	273	ALA	C-N	-5.19	1.21	1.33
2	b	283	TYR	N-CA	-5.19	1.40	1.46
1	a	1073	ALA	N-CA	-5.19	1.39	1.46
1	a	1186	ILE	CA-CB	-5.18	1.47	1.54
2	b	270	PRO	CA-CB	-5.18	1.46	1.53
2	b	93	VAL	CA-CB	-5.17	1.46	1.53
1	a	1125	SER	CA-C	-5.17	1.45	1.52
1	a	1024	TYR	C-N	-5.16	1.27	1.33
2	b	190	SER	CA-C	-5.16	1.45	1.52
1	a	1059	GLN	C-N	-5.16	1.27	1.33
1	a	1061	PHE	N-CA	-5.15	1.39	1.45
2	b	375	ALA	N-CA	-5.15	1.39	1.46
1	a	1378	PHE	C-N	-5.15	1.27	1.33
2	b	198	THR	CA-CB	-5.14	1.45	1.53
1	a	1221	ALA	C-N	-5.14	1.26	1.33
1	a	1366	ASP	CA-C	-5.14	1.46	1.52
2	b	347	ILE	CA-C	-5.13	1.48	1.52
2	b	86	ILE	CA-CB	-5.13	1.47	1.54
1	a	1390	GLY	CA-C	-5.12	1.44	1.51
1	a	1209	VAL	CA-C	-5.11	1.46	1.52
1	a	1052	VAL	CA-CB	-5.11	1.47	1.54
2	b	328	VAL	N-CA	-5.10	1.40	1.46
1	a	1240	HIS	CA-C	-5.10	1.46	1.52
1	a	1303	ASN	N-CA	-5.10	1.39	1.46
1	a	1373	TYR	CA-C	-5.10	1.46	1.52
1	a	1326	LYS	C-N	-5.09	1.28	1.33
2	b	37	HIS	CA-C	-5.09	1.46	1.53
2	b	376	THR	C-O	-5.09	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	244	PHE	N-CA	-5.09	1.42	1.46
2	b	352	LYS	C-N	-5.09	1.26	1.33
1	a	1349	VAL	N-CA	-5.08	1.40	1.46
1	a	1399	MET	N-CA	-5.08	1.40	1.46
2	b	395	PHE	CA-C	-5.07	1.46	1.52
2	b	194	LEU	CA-C	-5.06	1.46	1.52
1	a	1260	LEU	N-CA	-5.06	1.40	1.46
1	a	1282	ARG	CA-C	-5.05	1.46	1.52
1	a	1164	THR	CA-CB	-5.05	1.45	1.53
1	a	1207	GLN	CA-CB	-5.04	1.46	1.53
1	a	1375	LYS	CA-C	-5.04	1.46	1.52
1	a	1120	GLY	C-N	-5.03	1.27	1.33
1	a	1007	ILE	CA-CB	-5.02	1.47	1.53
1	a	1299	PRO	CA-CB	-5.01	1.46	1.53
1	a	1300	LYS	CA-C	-5.00	1.46	1.52

All (527) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1231	THR	N-CA-C	14.37	126.97	111.03
2	b	318	VAL	N-CA-CB	-14.35	97.93	112.28
2	b	37	HIS	CA-CB-CG	-14.10	99.70	113.80
1	a	1176	PHE	CA-CB-CG	-12.79	101.01	113.80
1	a	1270	PHE	CA-CB-CG	-12.33	101.47	113.80
2	b	318	VAL	O-C-N	-11.57	112.24	121.96
2	b	318	VAL	N-CA-C	11.51	118.53	106.21
2	b	6	HIS	N-CA-C	11.14	125.50	110.35
1	a	1200	ASN	CA-CB-CG	-11.14	101.46	112.60
2	b	300	ASN	CA-CB-CG	-10.69	101.91	112.60
2	b	337	ASN	CA-CB-CG	-10.64	101.95	112.60
2	b	273	ALA	O-C-N	-10.44	109.31	121.32
1	a	1367	HIS	N-CA-C	10.31	123.60	111.02
2	b	407	TRP	N-CA-CB	10.28	128.38	110.39
2	b	231	VAL	N-CA-CB	10.23	121.87	110.51
2	b	349	ASN	CA-CB-CG	-10.08	102.52	112.60
2	b	347	ILE	N-CA-C	-10.06	96.37	108.45
2	b	54	ASN	CA-CB-CG	-9.72	102.88	112.60
2	b	26	ASP	CA-CB-CG	-9.66	102.94	112.60
2	b	226	ASP	CA-CB-CG	-9.48	103.12	112.60
2	b	77	SER	N-CA-C	-9.43	102.29	113.88
2	b	407	TRP	CA-CB-CG	9.38	131.42	113.60
1	a	1215	SER	CB-CA-C	-9.31	94.85	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1378	PHE	CA-CB-CG	-9.29	104.51	113.80
1	a	1097	ARG	N-CA-C	-9.28	102.34	114.31
2	b	317	ALA	N-CA-C	9.18	124.14	107.99
1	a	1040	VAL	O-C-N	-9.16	112.67	123.02
2	b	206	ASN	CA-CB-CG	-9.13	103.47	112.60
2	b	62	VAL	N-CA-C	9.10	118.78	108.05
1	a	1015	GLN	N-CA-C	-9.05	101.50	111.36
1	a	1387	MET	N-CA-C	-9.05	94.49	108.42
3	M	3110	ARG	CA-C-N	8.99	129.95	119.98
3	M	3110	ARG	C-N-CA	8.99	129.95	119.98
2	b	240	THR	N-CA-CB	8.96	125.64	110.49
1	a	1392	PHE	CA-CB-CG	-8.94	104.86	113.80
1	a	1214	ALA	CA-C-N	8.93	132.61	120.38
1	a	1214	ALA	C-N-CA	8.93	132.61	120.38
1	a	1335	THR	CA-C-N	8.90	135.22	123.11
1	a	1335	THR	C-N-CA	8.90	135.22	123.11
1	a	1053	ARG	N-CA-C	-8.88	102.22	113.23
1	a	1244	ALA	O-C-N	-8.87	113.13	123.06
1	a	1366	ASP	CA-CB-CG	8.86	121.46	112.60
1	a	1314	THR	CA-C-N	8.85	134.45	121.18
1	a	1314	THR	C-N-CA	8.85	134.45	121.18
1	a	1215	SER	N-CA-CB	-8.72	96.98	110.06
2	b	247	GLN	N-CA-C	-8.71	92.25	110.80
1	a	1247	ALA	CA-C-O	-8.71	108.23	120.16
1	a	1303	ASN	CA-CB-CG	-8.68	103.92	112.60
1	a	1137	LYS	N-CA-C	8.65	120.32	111.07
1	a	1364	ARG	CB-CA-C	-8.60	93.78	110.46
1	a	1199	THR	N-CA-C	8.60	123.19	112.87
1	a	1402	LEU	N-CA-C	-8.58	102.98	113.97
1	a	1112	PHE	CA-CB-CG	-8.58	105.22	113.80
1	a	1366	ASP	N-CA-C	-8.56	101.89	111.14
1	a	1229	PHE	CA-CB-CG	-8.48	105.32	113.80
1	a	1330	ASN	CA-CB-CG	-8.47	104.13	112.60
2	b	14	ASN	CA-CB-CG	-8.43	104.17	112.60
1	a	1038	ARG	N-CA-C	-8.42	100.11	110.88
1	a	1254	LYS	N-CA-C	-8.36	102.10	112.88
2	b	193	GLN	N-CA-C	8.34	121.30	111.71
2	b	102	ASN	N-CA-CB	-8.32	97.71	110.77
1	a	1062	HIS	N-CA-C	-8.31	99.34	109.72
1	a	1395	ALA	N-CA-C	-8.18	103.08	113.72
1	a	1095	ARG	N-CA-CB	8.18	122.27	110.16
3	M	3193	ASN	CA-CB-CG	-8.15	104.44	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	398	MET	N-CA-C	-8.15	103.86	113.88
1	a	1367	HIS	CA-CB-CG	-8.08	105.72	113.80
2	b	319	PHE	CA-CB-CG	-8.08	105.72	113.80
3	M	3153	ASP	CA-CB-CG	-8.03	104.57	112.60
1	a	1020	CYS	N-CA-CB	-7.99	98.38	110.12
2	b	140	SER	N-CA-CB	7.95	124.66	110.83
1	a	1222	LEU	N-CA-C	-7.90	93.96	110.80
1	a	1061	PHE	N-CA-C	-7.86	96.64	108.99
2	b	39	ASP	CA-CB-CG	-7.84	104.76	112.60
2	b	244	PHE	CA-CB-CG	-7.79	106.01	113.80
1	a	1328	GLY	CA-C-N	-7.78	113.55	123.19
1	a	1328	GLY	C-N-CA	-7.78	113.55	123.19
1	a	1353	SER	O-C-N	-7.75	115.79	123.46
2	b	54	ASN	N-CA-C	-7.71	96.88	108.99
2	b	62	VAL	N-CA-CB	-7.70	101.44	111.21
3	M	3213	VAL	N-CA-CB	7.68	120.40	110.57
1	a	1295	GLY	O-C-N	-7.67	116.30	122.90
1	a	1350	CYS	CB-CA-C	-7.67	98.87	111.68
2	b	235	MET	N-CA-C	7.66	122.20	113.01
2	b	407	TRP	N-CA-C	-7.65	103.83	113.01
1	a	1155	VAL	N-CA-C	-7.64	105.40	112.43
3	M	3109	GLN	N-CA-C	7.63	120.27	111.11
3	M	3219	PHE	CA-CB-CG	-7.61	106.19	113.80
1	a	1011	GLN	N-CA-CB	7.55	122.56	109.72
2	b	203	CYS	N-CA-C	7.54	120.79	109.25
1	a	1092	VAL	N-CA-CB	7.52	118.52	110.62
1	a	1248	PRO	CB-CA-C	-7.52	105.56	111.87
1	a	1290	CYS	O-C-N	-7.52	111.74	122.87
1	a	1298	VAL	CA-C-N	7.50	129.22	119.84
1	a	1298	VAL	C-N-CA	7.50	129.22	119.84
2	b	169	PHE	CA-CB-CG	-7.48	106.32	113.80
3	M	3155	GLN	CB-CG-CD	7.44	125.25	112.60
2	b	83	PHE	CA-CB-CG	-7.44	106.36	113.80
2	b	432	TYR	N-CA-C	7.39	121.94	112.34
1	a	1214	ALA	N-CA-CB	7.38	122.96	110.49
1	a	1327	VAL	N-CA-C	-7.38	98.62	108.06
2	b	355	VAL	CB-CA-C	-7.37	102.01	110.41
1	a	1300	LYS	N-CA-CB	-7.37	99.26	110.16
1	a	1173	ASP	CA-CB-CG	-7.37	105.23	112.60
1	a	1141	LEU	CB-CA-C	-7.34	99.04	110.78
2	b	378	ILE	O-C-N	-7.30	113.75	122.66
1	a	1108	GLY	O-C-N	-7.29	116.92	123.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1208	ILE	N-CA-CB	7.28	119.57	110.47
2	b	179	ASP	CA-CB-CG	-7.25	105.35	112.60
1	a	1079	ARG	CA-C-N	7.24	129.42	120.22
1	a	1079	ARG	C-N-CA	7.24	129.42	120.22
1	a	1292	LEU	O-C-N	-7.23	114.82	123.13
1	a	1098	LYS	N-CA-C	-7.21	103.46	112.90
2	b	234	THR	N-CA-CB	7.20	120.82	110.16
3	M	3221	LYS	CA-C-N	7.19	130.63	120.28
3	M	3221	LYS	C-N-CA	7.19	130.63	120.28
1	a	1008	HIS	N-CA-C	7.17	119.96	108.41
1	a	1209	VAL	N-CA-C	7.17	117.96	110.72
1	a	1057	TYR	N-CA-CB	7.17	122.61	110.49
1	a	1289	CYS	O-C-N	-7.16	114.43	123.24
1	a	1007	ILE	N-CA-CB	-7.13	103.53	112.15
2	b	28	HIS	N-CA-C	-7.12	102.01	110.41
2	b	343	PHE	CA-CB-CG	-7.11	106.69	113.80
2	b	202	TYR	N-CA-C	7.11	121.62	107.62
2	b	329	ASP	CA-CB-CG	-7.11	105.50	112.60
2	b	262	PHE	N-CA-C	-7.06	94.22	109.81
1	a	1119	THR	N-CA-C	7.06	118.97	111.28
1	a	1341	ASP	CA-CB-CG	-7.04	105.56	112.60
1	a	1370	ASP	CA-CB-CG	-7.01	105.58	112.60
1	a	1291	LEU	N-CA-C	6.99	119.82	108.63
2	b	429	VAL	N-CA-CB	6.97	121.04	110.58
2	b	8	GLN	N-CA-C	6.96	120.06	109.62
1	a	1215	SER	CA-C-N	6.95	129.60	120.28
1	a	1215	SER	C-N-CA	6.95	129.60	120.28
2	b	136	GLN	CB-CG-CD	-6.94	100.80	112.60
1	a	1005	ILE	N-CA-CB	-6.94	99.79	111.23
2	b	232	SER	N-CA-C	6.92	120.61	111.75
1	a	1036	VAL	N-CA-CB	-6.92	101.53	111.21
2	b	202	TYR	CB-CG-CD2	-6.92	110.43	120.80
1	a	1079	ARG	N-CA-CB	-6.91	99.64	109.94
1	a	1161	SER	N-CA-C	-6.91	105.01	113.50
1	a	1234	VAL	CA-C-N	-6.91	111.21	119.84
1	a	1234	VAL	C-N-CA	-6.91	111.21	119.84
1	a	1267	ASN	CA-CB-CG	-6.91	105.69	112.60
2	b	62	VAL	O-C-N	-6.88	115.35	121.61
2	b	269	MET	O-C-N	-6.88	113.41	121.32
2	b	312	TYR	N-CA-C	-6.87	98.99	109.85
1	a	1333	PRO	CA-C-O	-6.85	110.63	120.56
3	M	3151	TRP	N-CA-C	6.84	118.73	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	6	HIS	CB-CG-CD2	-6.83	122.32	131.20
1	a	1326	LYS	N-CA-C	-6.82	98.26	107.88
1	a	1216	LEU	N-CA-C	-6.81	103.85	111.28
2	b	379	GLY	O-C-N	-6.80	116.55	123.35
2	b	349	ASN	N-CA-C	-6.79	98.40	108.79
2	b	236	SER	N-CA-C	-6.79	103.67	112.23
2	b	436	GLN	N-CA-C	-6.78	104.75	113.16
1	a	1349	VAL	N-CA-C	6.75	123.38	109.34
1	a	1180	ASN	CA-CB-CG	-6.74	105.86	112.60
2	b	101	ASN	CA-CB-CG	6.72	119.33	112.60
1	a	1218	PHE	CB-CA-C	-6.72	97.95	109.65
2	b	273	ALA	N-CA-C	6.71	124.63	109.81
2	b	296	PHE	CA-CB-CG	-6.71	107.09	113.80
2	b	266	HIS	CA-CB-CG	-6.70	107.10	113.80
2	b	320	ARG	N-CA-C	6.70	119.85	107.60
1	a	1336	VAL	CB-CA-C	-6.67	101.91	111.19
1	a	1347	ARG	CB-CA-C	-6.67	97.15	110.42
2	b	83	PHE	N-CA-C	-6.65	100.43	109.54
1	a	1247	ALA	O-C-N	-6.64	113.68	121.32
1	a	1183	ILE	N-CA-C	-6.64	102.99	112.35
2	b	198	THR	N-CA-C	-6.63	98.64	108.79
1	a	1376	ARG	N-CA-CB	6.61	121.66	110.49
2	b	284	ARG	N-CA-CB	6.59	121.62	110.49
2	b	16	ILE	CA-C-N	6.57	127.41	119.99
2	b	16	ILE	C-N-CA	6.57	127.41	119.99
1	a	1227	THR	N-CA-C	6.56	118.98	111.11
2	b	149	MET	N-CA-C	6.56	119.25	111.71
2	b	308	ARG	N-CA-CB	-6.56	99.41	110.49
1	a	1060	LEU	N-CA-CB	-6.55	101.09	110.79
2	b	161	TYR	CA-CB-CG	-6.55	102.12	113.90
1	a	1179	ASP	CA-C-N	6.53	129.35	120.54
1	a	1179	ASP	C-N-CA	6.53	129.35	120.54
1	a	1352	LEU	CA-C-O	-6.52	113.83	121.46
1	a	1215	SER	N-CA-C	6.52	119.22	111.33
2	b	406	HIS	N-CA-C	6.52	120.33	112.38
2	b	244	PHE	CA-C-O	-6.51	114.37	120.94
1	a	1190	ASN	CA-CB-CG	-6.51	106.09	112.60
1	a	1321	CYS	N-CA-C	-6.50	100.15	110.10
1	a	1008	HIS	O-C-N	-6.50	115.13	122.93
2	b	418	PHE	CA-CB-CG	-6.48	107.32	113.80
1	a	1142	GLU	CB-CG-CD	-6.45	101.64	112.60
2	b	15	GLN	N-CA-C	6.45	122.01	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1174	CYS	CB-CA-C	6.43	119.63	110.24
1	a	1349	VAL	N-CA-CB	-6.43	100.61	111.23
3	M	3097	SER	N-CA-C	6.43	119.10	110.35
1	a	1018	ASN	CA-CB-CG	-6.43	106.17	112.60
2	b	275	LEU	CB-CA-C	-6.43	100.03	110.77
2	b	273	ALA	CA-C-O	-6.42	111.37	120.16
1	a	1225	ASP	CA-CB-CG	-6.38	106.22	112.60
2	b	135	PHE	CA-CB-CG	-6.38	107.42	113.80
2	b	63	PRO	N-CA-C	6.38	121.65	111.26
1	a	1353	SER	CB-CA-C	-6.37	99.73	110.43
1	a	1378	PHE	N-CA-C	6.37	124.37	110.80
2	b	384	ILE	O-C-N	-6.36	114.62	122.57
2	b	339	ASN	CA-CB-CG	-6.34	106.26	112.60
2	b	213	CYS	CA-C-N	-6.33	112.19	122.26
2	b	213	CYS	C-N-CA	-6.33	112.19	122.26
1	a	1180	ASN	CB-CA-C	6.33	120.94	110.81
2	b	139	HIS	CA-C-O	-6.32	114.18	121.26
2	b	205	ASP	CA-CB-CG	-6.32	106.28	112.60
3	M	3096	LYS	CA-C-N	6.32	130.29	120.75
3	M	3096	LYS	C-N-CA	6.32	130.29	120.75
2	b	142	GLY	N-CA-C	6.32	115.96	110.21
3	M	3205	ALA	N-CA-C	6.32	120.30	112.47
2	b	202	TYR	CB-CA-C	-6.31	100.36	111.22
1	a	1366	ASP	CB-CA-C	6.31	120.88	110.90
2	b	358	ILE	O-C-N	-6.31	113.91	121.10
1	a	1195	ARG	O-C-N	-6.29	114.09	121.32
1	a	1301	ASP	CA-C-O	6.28	127.42	120.63
2	b	88	ARG	N-CA-CB	6.28	120.62	109.94
2	b	139	HIS	CA-CB-CG	6.28	120.08	113.80
1	a	1393	SER	N-CA-CB	-6.28	100.64	110.06
2	b	91	ASN	N-CA-C	6.28	119.11	111.82
2	b	50	ASN	CB-CA-C	-6.28	97.93	110.42
1	a	1116	GLY	CA-C-N	6.27	133.69	121.41
1	a	1116	GLY	C-N-CA	6.27	133.69	121.41
1	a	1194	GLU	CA-C-O	6.27	126.17	119.34
1	a	1317	PHE	CA-CB-CG	-6.24	107.56	113.80
2	b	374	SER	N-CA-CB	-6.23	101.52	111.62
1	a	1166	HIS	CA-CB-CG	-6.23	107.57	113.80
1	a	1042	VAL	CA-C-O	-6.23	113.38	120.67
2	b	56	ALA	CA-C-N	6.22	130.14	120.75
2	b	56	ALA	C-N-CA	6.22	130.14	120.75
1	a	1024	TYR	N-CA-CB	6.21	120.98	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	350	ASN	CA-CB-CG	-6.20	106.40	112.60
1	a	1292	LEU	N-CA-C	6.18	118.79	108.96
2	b	432	TYR	CA-CB-CG	-6.16	102.82	113.90
2	b	307	PRO	CA-C-N	6.15	133.28	121.54
2	b	307	PRO	C-N-CA	6.15	133.28	121.54
1	a	1202	ASN	OD1-CG-ND2	-6.14	116.46	122.60
1	a	1007	ILE	O-C-N	-6.13	115.18	122.66
1	a	1039	ALA	N-CA-C	6.12	117.19	108.74
1	a	1365	LEU	N-CA-C	-6.12	105.97	113.50
2	b	152	LEU	CB-CA-C	-6.11	100.53	110.79
2	b	355	VAL	O-C-N	-6.11	117.47	122.97
1	a	1291	LEU	O-C-N	-6.10	114.18	122.48
1	a	1068	THR	CB-CA-C	-6.10	96.03	109.56
2	b	175	PRO	N-CA-CB	-6.09	96.85	103.25
1	a	1046	PRO	N-CA-C	6.08	123.64	113.78
1	a	1319	ASP	CB-CA-C	-6.08	101.34	110.88
1	a	1062	HIS	CA-CB-CG	6.06	119.86	113.80
1	a	1094	ASP	N-CA-C	6.06	123.71	110.80
1	a	1043	ASP	O-C-N	-6.05	116.70	123.48
2	b	165	ILE	N-CA-CB	-6.05	101.24	111.23
2	b	315	VAL	O-C-N	-6.05	116.34	123.00
2	b	174	SER	CA-C-N	6.05	127.40	119.84
2	b	174	SER	C-N-CA	6.05	127.40	119.84
2	b	208	ALA	N-CA-C	-6.04	104.61	112.23
1	a	1112	PHE	CB-CA-C	-6.04	101.08	111.23
1	a	1239	GLY	CA-C-N	6.04	133.08	121.54
1	a	1239	GLY	C-N-CA	6.04	133.08	121.54
2	b	6	HIS	O-C-N	-6.03	115.39	122.81
2	b	284	ARG	NE-CZ-NH1	6.03	127.53	121.50
1	a	1095	ARG	CB-CA-C	-6.01	100.64	110.85
1	a	1189	ARG	CA-C-N	-6.00	113.11	123.25
1	a	1189	ARG	C-N-CA	-6.00	113.11	123.25
1	a	1198	TYR	N-CA-C	-6.00	104.07	111.33
2	b	44	LEU	N-CA-CB	-6.00	101.26	110.44
1	a	1275	GLN	CB-CG-CD	-6.00	102.41	112.60
1	a	1233	LEU	N-CA-CB	5.99	118.99	110.67
1	a	1349	VAL	O-C-N	-5.98	115.09	122.57
1	a	1198	TYR	O-C-N	-5.98	115.78	122.12
2	b	315	VAL	CA-C-O	-5.98	115.03	121.19
2	b	16	ILE	CA-C-O	5.97	127.16	120.95
2	b	202	TYR	CB-CG-CD1	5.97	129.75	120.80
2	b	306	ASP	N-CA-C	-5.96	102.27	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1311	THR	CB-CA-C	-5.96	101.86	111.28
1	a	1026	LEU	N-CA-C	5.96	117.77	111.28
2	b	201	THR	O-C-N	-5.94	116.36	123.31
1	a	1241	PHE	CA-CB-CG	-5.94	107.86	113.80
1	a	1274	ASN	N-CA-C	-5.94	104.25	112.03
2	b	374	SER	CA-C-O	-5.90	114.90	121.51
2	b	214	PHE	N-CA-C	-5.90	106.06	113.72
1	a	1269	CYS	CA-CB-SG	-5.89	100.84	114.40
2	b	202	TYR	O-C-N	-5.89	115.35	123.01
1	a	1096	ILE	O-C-N	-5.89	115.21	122.57
1	a	1352	LEU	N-CA-C	-5.89	100.55	109.85
1	a	1370	ASP	CB-CA-C	-5.88	101.57	110.92
2	b	313	LEU	N-CA-C	-5.88	106.15	113.55
1	a	1100	ALA	CA-C-O	5.87	126.99	120.82
1	a	1079	ARG	CD-NE-CZ	-5.87	116.18	124.40
3	M	3139	ALA	N-CA-C	5.86	117.67	111.28
3	M	3170	TYR	N-CA-C	5.85	117.45	110.19
2	b	375	ALA	N-CA-CB	-5.85	100.60	110.49
2	b	224	TYR	CB-CA-C	5.85	120.06	110.88
2	b	166	MET	CB-CA-C	-5.84	104.05	111.70
2	b	87	PHE	CA-CB-CG	-5.84	107.96	113.80
2	b	343	PHE	N-CA-CB	-5.84	102.04	110.56
2	b	346	TRP	N-CA-C	-5.83	105.05	113.21
2	b	232	SER	O-C-N	-5.83	115.56	122.20
2	b	210	TYR	CA-C-N	5.82	132.65	121.54
2	b	210	TYR	C-N-CA	5.82	132.65	121.54
2	b	253	ARG	CB-CA-C	5.82	119.92	110.96
1	a	1188	ARG	N-CA-C	-5.81	103.68	112.04
1	a	1246	TYR	N-CA-C	-5.80	100.93	109.81
2	b	122	VAL	O-C-N	-5.80	115.44	122.06
1	a	1094	ASP	O-C-N	-5.80	114.88	122.59
2	b	369	ARG	N-CA-C	5.80	123.15	110.80
2	b	16	ILE	N-CA-CB	-5.80	102.66	110.54
2	b	407	TRP	CB-CG-CD2	5.79	134.91	126.80
2	b	234	THR	CA-CB-OG1	5.79	118.29	109.60
1	a	1350	CYS	O-C-N	-5.78	115.58	122.63
2	b	224	TYR	N-CA-C	-5.78	104.89	111.07
2	b	260	VAL	N-CA-CB	-5.77	103.13	111.21
2	b	7	ILE	CB-CA-C	-5.77	103.83	110.41
2	b	87	PHE	CA-C-O	-5.76	115.19	121.87
1	a	1137	LYS	N-CA-CB	-5.76	101.66	110.01
2	b	191	VAL	N-CA-C	5.75	116.48	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1350	CYS	N-CA-C	5.74	118.70	107.57
1	a	1202	ASN	CB-CG-OD1	5.74	132.28	120.80
2	b	380	ASN	O-C-N	-5.74	114.96	122.59
2	b	86	ILE	N-CA-C	5.73	121.27	109.34
1	a	1207	GLN	N-CA-C	-5.73	103.88	111.96
1	a	1079	ARG	NE-CZ-NH1	5.73	127.23	121.50
2	b	123	ARG	NE-CZ-NH1	5.72	127.22	121.50
1	a	1240	HIS	N-CA-C	5.71	122.97	110.80
2	b	197	ASN	CA-CB-CG	-5.71	106.89	112.60
1	a	1348	ALA	N-CA-CB	-5.71	102.13	111.66
2	b	6	HIS	CB-CA-C	-5.71	99.41	109.62
2	b	290	GLU	CB-CG-CD	-5.71	102.90	112.60
1	a	1109	PHE	N-CA-CB	-5.70	101.64	110.65
1	a	1203	ARG	CB-CA-C	-5.70	100.09	110.63
2	b	291	LEU	N-CA-C	-5.69	105.16	111.36
1	a	1260	LEU	O-C-N	-5.68	116.11	122.93
2	b	354	ALA	CA-C-O	-5.68	114.46	121.11
1	a	1380	HIS	N-CA-C	5.68	119.31	112.38
1	a	1043	ASP	CA-CB-CG	-5.68	106.92	112.60
1	a	1354	ASN	CA-C-O	-5.68	114.29	120.36
2	b	283	TYR	CA-C-N	5.68	132.38	121.54
2	b	283	TYR	C-N-CA	5.68	132.38	121.54
2	b	316	ALA	O-C-N	-5.67	115.34	123.06
1	a	1158	PRO	N-CA-C	5.67	122.96	113.78
2	b	377	PHE	CA-C-O	-5.67	114.24	120.36
3	M	3143	ILE	N-CA-C	5.67	116.40	110.62
2	b	58	GLY	N-CA-C	-5.66	101.32	110.95
2	b	232	SER	CB-CA-C	-5.66	99.48	110.46
1	a	1025	CYS	N-CA-C	5.65	118.16	111.33
1	a	1329	ILE	O-C-N	-5.64	117.25	123.18
2	b	426	ASN	CA-CB-CG	-5.63	106.97	112.60
3	M	3157	PHE	N-CA-C	5.63	117.11	110.97
3	M	3148	PHE	CA-CB-CG	-5.63	108.17	113.80
2	b	242	LEU	O-C-N	-5.63	115.11	122.59
2	b	4	ILE	CB-CA-C	-5.63	103.47	111.40
1	a	1336	VAL	N-CA-CB	-5.62	104.59	111.67
2	b	380	ASN	OD1-CG-ND2	-5.62	116.98	122.60
2	b	79	ARG	N-CA-C	-5.61	106.43	113.28
2	b	262	PHE	CA-C-O	-5.59	112.50	120.16
2	b	93	VAL	N-CA-CB	-5.58	106.08	111.89
2	b	314	THR	O-C-N	-5.58	116.89	123.25
1	a	1018	ASN	N-CA-C	5.57	118.12	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1113	HIS	CA-C-O	-5.57	115.11	121.40
1	a	1300	LYS	CB-CA-C	-5.57	101.38	110.85
3	M	3222	CYS	N-CA-C	5.57	118.11	111.71
1	a	1108	GLY	N-CA-C	5.57	118.09	110.69
2	b	326	LYS	N-CA-C	-5.57	104.03	112.04
2	b	420	GLU	CA-C-N	5.55	128.51	120.79
2	b	420	GLU	C-N-CA	5.55	128.51	120.79
1	a	1022	GLU	N-CA-CB	5.54	118.01	109.98
1	a	1248	PRO	N-CA-CB	5.54	106.02	102.92
2	b	71	GLU	CA-C-O	-5.54	112.58	120.16
2	b	251	ASP	N-CA-CB	5.53	119.83	110.49
1	a	1087	GLU	N-CA-C	5.52	122.56	110.80
2	b	92	PHE	CB-CA-C	-5.52	102.05	110.88
1	a	1218	PHE	CA-CB-CG	-5.51	108.29	113.80
1	a	1232	ASN	CB-CA-C	-5.49	99.03	109.95
1	a	1231	THR	CA-CB-CG2	-5.49	101.17	110.50
1	a	1262	VAL	N-CA-C	5.48	120.75	109.34
2	b	6	HIS	N-CA-CB	-5.48	101.98	110.04
1	a	1198	TYR	CA-CB-CG	5.46	123.73	113.90
2	b	375	ALA	CB-CA-C	-5.46	99.55	110.42
2	b	101	ASN	CB-CA-C	5.46	119.57	111.88
2	b	351	VAL	O-C-N	-5.46	116.85	122.63
1	a	1092	VAL	CB-CA-C	-5.45	104.72	111.70
2	b	252	LEU	CA-C-N	-5.44	113.46	120.65
2	b	252	LEU	C-N-CA	-5.44	113.46	120.65
1	a	1249	VAL	O-C-N	-5.44	116.86	122.14
1	a	1300	LYS	CA-C-N	5.44	127.83	120.38
1	a	1300	LYS	C-N-CA	5.44	127.83	120.38
1	a	1302	VAL	N-CA-C	-5.43	105.42	110.53
1	a	1160	ASN	O-C-N	-5.43	115.15	122.43
1	a	1393	SER	O-C-N	-5.43	116.37	122.12
3	M	3128	ASN	CA-CB-CG	-5.43	107.17	112.60
2	b	404	PHE	CA-CB-CG	-5.42	108.38	113.80
1	a	1062	HIS	N-CA-CB	5.42	118.34	110.32
1	a	1350	CYS	CA-CB-SG	-5.41	101.95	114.40
2	b	260	VAL	O-C-N	-5.40	114.95	121.10
1	a	1262	VAL	O-C-N	-5.39	115.83	122.57
3	M	3157	PHE	CA-CB-CG	-5.39	108.41	113.80
2	b	229	HIS	CA-CB-CG	-5.39	108.41	113.80
1	a	1126	LEU	N-CA-CB	-5.38	102.06	110.44
1	a	1405	ASP	CA-CB-CG	-5.37	107.23	112.60
1	a	1032	PRO	CA-C-N	5.36	131.79	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1032	PRO	C-N-CA	5.36	131.79	121.54
2	b	229	HIS	N-CA-C	5.36	117.82	111.33
1	a	1167	THR	CA-CB-CG2	5.36	119.61	110.50
2	b	62	VAL	CA-C-O	5.36	122.67	119.19
2	b	223	THR	O-C-N	-5.36	115.47	122.59
2	b	73	GLY	CA-C-N	5.34	131.74	121.54
2	b	73	GLY	C-N-CA	5.34	131.74	121.54
2	b	435	TYR	N-CA-C	-5.33	105.48	112.41
1	a	1123	PHE	CA-CB-CG	-5.33	108.47	113.80
1	a	1111	VAL	CB-CA-C	-5.33	103.91	111.21
2	b	116	ASP	CA-CB-CG	-5.32	107.28	112.60
2	b	178	SER	CB-CA-C	-5.32	101.02	109.80
1	a	1285	LYS	O-C-N	-5.32	117.16	123.22
1	a	1009	VAL	CA-CB-CG2	5.31	119.43	110.40
1	a	1403	GLU	N-CA-CB	5.31	118.73	110.44
1	a	1052	VAL	N-CA-C	-5.30	105.26	113.16
1	a	1296	ASP	CB-CA-C	-5.30	102.81	111.50
2	b	157	ILE	N-CA-C	5.30	115.51	110.42
2	b	264	ARG	CA-C-N	5.30	131.66	121.54
2	b	264	ARG	C-N-CA	5.30	131.66	121.54
2	b	290	GLU	N-CA-CB	5.29	118.45	110.30
2	b	295	MET	N-CA-C	5.28	122.05	110.80
3	M	3179	GLN	N-CA-C	-5.28	106.51	113.17
2	b	203	CYS	CB-CA-C	-5.28	101.63	110.29
2	b	48	ARG	NE-CZ-NH2	-5.28	114.45	119.20
2	b	97	SER	CB-CA-C	-5.28	102.60	110.88
2	b	122	VAL	N-CA-C	5.27	119.48	111.89
1	a	1098	LYS	N-CA-CB	5.27	118.24	110.33
2	b	152	LEU	N-CA-C	-5.27	104.97	111.40
2	b	205	ASP	CB-CA-C	-5.27	100.16	109.70
1	a	1306	ILE	CB-CA-C	-5.26	103.58	112.16
2	b	108	TYR	CA-CB-CG	-5.26	104.42	113.90
2	b	422	GLU	N-CA-C	5.26	117.44	111.02
1	a	1400	ALA	CA-C-O	5.26	126.53	120.90
2	b	392	SER	N-CA-CB	5.25	118.44	110.14
2	b	244	PHE	CA-C-N	5.25	126.40	119.84
2	b	244	PHE	C-N-CA	5.25	126.40	119.84
1	a	1062	HIS	CE1-NE2-CD2	-5.24	103.76	109.00
2	b	222	PRO	CA-C-N	5.24	131.54	121.54
2	b	222	PRO	C-N-CA	5.24	131.54	121.54
2	b	132	LEU	N-CA-CB	-5.24	101.64	110.49
2	b	322	ARG	N-CA-C	5.24	117.90	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1165	THR	N-CA-CB	5.23	117.90	110.16
2	b	138	THR	O-C-N	-5.23	116.56	123.21
2	b	204	ILE	CB-CA-C	-5.23	102.86	110.81
2	b	94	PHE	CB-CA-C	-5.23	100.68	109.83
1	a	1353	SER	CA-C-N	-5.22	115.82	122.77
1	a	1353	SER	C-N-CA	-5.22	115.82	122.77
2	b	301	MET	CB-CA-C	-5.22	101.24	109.80
2	b	337	ASN	CB-CA-C	-5.21	100.11	109.24
1	a	1204	LEU	CA-C-O	-5.21	115.54	120.90
1	a	1289	CYS	CA-CB-SG	-5.21	102.42	114.40
2	b	175	PRO	N-CA-C	5.20	123.18	112.47
2	b	376	THR	N-CA-C	5.20	117.97	110.28
2	b	405	LEU	CA-C-O	5.20	125.92	119.79
1	a	1315	ILE	N-CA-CB	-5.20	105.05	110.82
2	b	108	TYR	N-CA-C	-5.20	99.73	110.80
1	a	1036	VAL	CA-C-N	5.18	125.92	120.11
1	a	1036	VAL	C-N-CA	5.18	125.92	120.11
1	a	1063	PRO	CB-CA-C	-5.18	103.01	111.56
2	b	416	MET	CA-C-N	5.18	127.22	120.28
2	b	416	MET	C-N-CA	5.18	127.22	120.28
2	b	215	ARG	CB-CA-C	-5.18	100.31	109.02
1	a	1263	ALA	N-CA-C	5.17	121.82	110.80
1	a	1199	THR	O-C-N	-5.17	115.55	122.43
1	a	1256	TYR	CA-CB-CG	-5.17	104.59	113.90
1	a	1277	VAL	N-CA-CB	5.17	119.75	111.23
1	a	1160	ASN	CA-C-N	-5.16	112.99	121.92
1	a	1160	ASN	C-N-CA	-5.16	112.99	121.92
2	b	417	GLU	CA-CB-CG	-5.16	103.78	114.10
1	a	1190	ASN	N-CA-C	-5.16	103.92	111.30
2	b	103	TRP	O-C-N	-5.16	116.66	122.12
1	a	1290	CYS	N-CA-C	5.15	118.62	107.49
1	a	1198	TYR	CB-CG-CD1	5.15	128.53	120.80
2	b	293	GLN	N-CA-CB	5.15	117.43	109.91
1	a	1387	MET	O-C-N	-5.15	118.37	123.46
1	a	1185	ASP	CB-CA-C	-5.14	102.58	110.81
2	b	431	GLU	CB-CA-C	-5.14	102.30	110.84
2	b	206	ASN	CA-C-N	-5.14	113.03	121.92
2	b	206	ASN	C-N-CA	-5.14	113.03	121.92
1	a	1264	GLU	CB-CA-C	-5.14	101.42	111.03
2	b	259	MET	CG-SD-CE	-5.14	89.60	100.90
1	a	1351	MET	CG-SD-CE	-5.13	89.60	100.90
1	a	1285	LYS	CB-CA-C	5.13	118.22	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	147	SER	O-C-N	-5.13	116.30	122.15
1	a	1165	THR	CA-CB-OG1	5.13	117.30	109.60
2	b	387	LEU	N-CA-CB	-5.13	101.83	110.49
1	a	1142	GLU	O-C-N	-5.12	117.48	123.27
2	b	385	GLN	CA-C-N	5.12	131.32	121.54
2	b	385	GLN	C-N-CA	5.12	131.32	121.54
1	a	1331	TYR	N-CA-CB	5.12	117.31	109.94
3	M	3218	ASN	N-CA-CB	-5.11	101.64	110.32
1	a	1276	MET	CB-CA-C	-5.11	103.33	111.86
1	a	1208	ILE	N-CA-C	5.10	116.43	110.62
3	M	3104	THR	N-CA-C	-5.10	106.57	112.89
2	b	101	ASN	N-CA-CB	-5.09	104.04	110.45
2	b	3	GLU	CB-CG-CD	5.09	121.25	112.60
3	M	3214	ASN	CA-CB-CG	5.08	117.69	112.60
1	a	1042	VAL	CA-CB-CG2	-5.08	101.77	110.40
1	a	1160	ASN	CA-CB-CG	-5.08	107.53	112.60
1	a	1298	VAL	CA-C-O	-5.07	115.93	119.38
1	a	1095	ARG	CG-CD-NE	-5.07	100.85	112.00
1	a	1138	LYS	N-CA-C	5.07	116.47	110.19
1	a	1197	THR	O-C-N	-5.07	115.85	122.59
2	b	235	MET	CG-SD-CE	-5.06	89.76	100.90
2	b	9	ALA	N-CA-C	5.06	117.55	109.96
3	M	3179	GLN	CA-C-N	5.05	128.45	120.47
3	M	3179	GLN	C-N-CA	5.05	128.45	120.47
1	a	1337	VAL	CA-C-O	-5.05	113.18	119.95
1	a	1408	GLU	CB-CA-C	-5.05	102.41	110.79
3	M	3160	LYS	N-CA-C	5.05	116.80	110.24
1	a	1005	ILE	CA-CB-CG2	5.04	119.08	110.50
1	a	1230	GLN	N-CA-C	5.04	121.52	110.80
2	b	249	ASN	CB-CA-C	-5.03	103.02	110.62
2	b	28	HIS	CA-CB-CG	5.03	118.83	113.80
2	b	376	THR	O-C-N	-5.03	116.75	122.89
1	a	1297	VAL	CA-C-O	-5.03	115.11	120.39
1	a	1333	PRO	CA-C-N	5.02	126.12	119.84
1	a	1333	PRO	C-N-CA	5.02	126.12	119.84
3	M	3123	ILE	CB-CA-C	-5.02	105.36	112.14
3	M	3139	ALA	O-C-N	-5.02	116.80	122.12
1	a	1245	THR	O-C-N	-5.01	117.45	123.27
2	b	413	MET	N-CA-C	-5.01	101.58	109.50
2	b	123	ARG	N-CA-CB	5.00	117.72	110.26
2	b	245	PRO	O-C-N	-5.00	115.89	122.64
3	M	3214	ASN	N-CA-CB	-5.00	101.62	109.78

There are no chirality outliers.

All (83) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	3110	ARG	Sidechain
3	M	3157	PHE	Sidechain
3	M	3201	ARG	Sidechain
3	M	3203	SER	Peptide
1	a	1002	ARG	Peptide
1	a	1003	GLU	Peptide
1	a	1008	HIS	Sidechain
1	a	1024	TYR	Sidechain
1	a	1037	PRO	Peptide
1	a	1038	ARG	Sidechain
1	a	1041	PHE	Sidechain
1	a	1057	TYR	Sidechain
1	a	1058	ARG	Sidechain
1	a	1059	GLN	Peptide
1	a	1074	ALA	Peptide
1	a	1079	ARG	Sidechain
1	a	1082	TYR	Sidechain
1	a	1097	ARG	Sidechain
1	a	1112	PHE	Sidechain
1	a	1119	THR	Peptide
1	a	1120	GLY	Peptide
1	a	1123	PHE	Sidechain
1	a	1135	TYR	Sidechain
1	a	1145	ILE	Peptide
1	a	1161	SER	Mainchain
1	a	1184	TYR	Sidechain
1	a	1195	ARG	Sidechain
1	a	1198	TYR	Sidechain
1	a	1203	ARG	Sidechain
1	a	1217	ARG	Sidechain
1	a	1229	PHE	Sidechain
1	a	1230	GLN	Peptide
1	a	1236	TYR	Sidechain
1	a	1238	ARG	Sidechain
1	a	1240	HIS	Peptide
1	a	1242	PRO	Peptide
1	a	1244	ALA	Mainchain
1	a	1246	TYR	Sidechain
1	a	1247	ALA	Peptide
1	a	1253	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	a	1256	TYR	Sidechain
1	a	1294	ARG	Sidechain
1	a	1313	ARG	Sidechain
1	a	1323	THR	Peptide
1	a	1335	THR	Peptide
1	a	1364	ARG	Sidechain
1	a	1378	PHE	Sidechain
1	a	1396	ARG	Sidechain
1	a	1406	TYR	Sidechain
1	a	1410	GLY	Peptide
2	b	100	GLY	Peptide
2	b	107	HIS	Peptide
2	b	129	CYS	Peptide
2	b	161	TYR	Sidechain
2	b	179	ASP	Peptide
2	b	185	TYR	Sidechain
2	b	2	ARG	Sidechain
2	b	210	TYR	Sidechain
2	b	215	ARG	Sidechain
2	b	216	THR	Peptide
2	b	259	MET	Peptide
2	b	28	HIS	Sidechain
2	b	311	ARG	Sidechain
2	b	312	TYR	Sidechain
2	b	347	ILE	Peptide
2	b	37	HIS	Sidechain
2	b	388	PHE	Sidechain
2	b	390	ARG	Sidechain
2	b	395	PHE	Sidechain
2	b	4	ILE	Peptide
2	b	400	ARG	Sidechain
2	b	402	LYS	Peptide
2	b	404	PHE	Sidechain,Peptide
2	b	408	TYR	Sidechain
2	b	415	GLU	Peptide
2	b	416	MET	Mainchain
2	b	418	PHE	Sidechain
2	b	432	TYR	Sidechain
2	b	435	TYR	Sidechain
2	b	64	ARG	Sidechain
2	b	79	ARG	Sidechain
2	b	92	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	3228	3147	3144	102	0
2	b	3352	3232	3229	88	0
3	M	1069	1065	1062	7	0
All	All	7649	7444	7435	186	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 12.

All (186) 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)
2:b:242:LEU:HD13	2:b:251:ASP:HA	1.39	1.01
1:a:1111:VAL:HG21	1:a:1128:MET:SD	2.27	0.75
1:a:1128:MET:HA	1:a:1128:MET:HE2	1.67	0.75
2:b:6:HIS:CD2	2:b:21:TRP:HE1	2.06	0.73
2:b:301:MET:HA	2:b:301:MET:HE2	1.71	0.70
1:a:1380:HIS:HE1	2:b:260:VAL:HG23	1.56	0.70
1:a:1380:HIS:CE1	2:b:260:VAL:HG23	2.27	0.69
1:a:1238:ARG:O	1:a:1240:HIS:CD2	2.50	0.65
2:b:103:TRP:CH2	2:b:107:HIS:CD2	2.86	0.64
1:a:1077:TYR:CE1	1:a:1122:GLY:HA2	2.33	0.63
1:a:1216:LEU:HD11	1:a:1224:VAL:H	1.64	0.62
1:a:1257:HIS:CG	1:a:1257:HIS:O	2.52	0.61
2:b:197:ASN:ND2	3:M:3159:ARG:HH21	1.98	0.61
1:a:1290:CYS:SG	1:a:1292:LEU:HD11	2.42	0.60
1:a:1151:VAL:HG12	1:a:1151:VAL:O	2.00	0.60
1:a:1235:PRO:O	1:a:1236:TYR:CG	2.56	0.58
1:a:1077:TYR:CD1	1:a:1122:GLY:HA2	2.38	0.57
1:a:1348:ALA:C	1:a:1349:VAL:HG23	2.29	0.57
1:a:1125:SER:HA	1:a:1167:THR:HG21	1.86	0.57
1:a:1270:PHE:CD2	1:a:1315:ILE:HD12	2.39	0.57
2:b:287:THR:H	2:b:290:GLU:CD	2.13	0.56
2:b:12:CYS:SG	2:b:140:SER:HB3	2.45	0.56
1:a:1143:PHE:CE2	1:a:1209:VAL:CG2	2.89	0.56
2:b:259:MET:HE1	2:b:316:ALA:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:229:HIS:C	2:b:229:HIS:CD2	2.83	0.56
1:a:1291:LEU:HD12	1:a:1291:LEU:N	2.23	0.54
2:b:425:MET:C	2:b:425:MET:SD	2.91	0.54
2:b:242:LEU:HD13	2:b:251:ASP:CA	2.27	0.54
2:b:70:LEU:H	2:b:145:THR:HG21	1.73	0.54
1:a:1170:GLU:O	1:a:1171:HIS:CG	2.61	0.54
2:b:264:ARG:O	2:b:266:HIS:CD2	2.61	0.54
1:a:1011:GLN:OE1	1:a:1117:GLY:HA3	2.09	0.53
1:a:1113:HIS:CD2	1:a:1113:HIS:C	2.85	0.53
1:a:1201:LEU:HD23	1:a:1201:LEU:N	2.23	0.53
2:b:62:VAL:HG23	2:b:62:VAL:O	2.09	0.53
1:a:1381:TRP:CE2	2:b:257:VAL:HA	2.43	0.53
2:b:388:PHE:HB2	2:b:429:VAL:HG21	1.90	0.52
1:a:1008:HIS:CD2	1:a:1112:PHE:CD1	2.98	0.52
2:b:195:VAL:HG23	2:b:267:PHE:CZ	2.44	0.52
1:a:1084:ILE:HG23	1:a:1085:GLY:H	1.75	0.52
1:a:1302:VAL:HG12	1:a:1306:ILE:HD11	1.91	0.52
1:a:1381:TRP:CZ2	2:b:257:VAL:HA	2.45	0.52
2:b:6:HIS:CD2	2:b:21:TRP:NE1	2.77	0.52
1:a:1147:PRO:HG2	1:a:1365:LEU:HD21	1.91	0.51
2:b:260:VAL:HG23	2:b:260:VAL:O	2.10	0.51
2:b:183:GLU:CB	2:b:184:PRO:CD	2.87	0.51
1:a:1077:TYR:CD1	1:a:1122:GLY:CA	2.94	0.51
1:a:1235:PRO:O	1:a:1236:TYR:CD1	2.63	0.51
2:b:75:MET:HA	2:b:78:VAL:HG12	1.92	0.51
2:b:261:PRO:O	2:b:262:PHE:CG	2.63	0.51
1:a:1324:GLY:O	1:a:1325:PHE:CD1	2.64	0.50
1:a:1216:LEU:HD21	1:a:1224:VAL:O	2.11	0.50
2:b:87:PHE:CD1	2:b:87:PHE:N	2.80	0.50
2:b:180:THR:HG22	2:b:183:GLU:H	1.77	0.50
1:a:1143:PHE:CD1	1:a:1143:PHE:N	2.80	0.49
1:a:1260:LEU:HA	1:a:1264:GLU:OE1	2.12	0.49
1:a:1283:HIS:C	1:a:1283:HIS:CD2	2.89	0.49
1:a:1045:GLU:HB2	1:a:1073:ALA:HB2	1.94	0.49
2:b:12:CYS:SG	2:b:13:GLY:N	2.85	0.49
1:a:1004:CYS:SG	1:a:1108:GLY:O	2.70	0.49
1:a:1183:ILE:HG21	1:a:1201:LEU:HD22	1.94	0.49
1:a:1348:ALA:C	1:a:1349:VAL:CG2	2.85	0.49
1:a:1032:PRO:HA	1:a:1060:LEU:HD22	1.93	0.48
2:b:12:CYS:SG	2:b:140:SER:CB	3.01	0.48
1:a:1008:HIS:HD2	1:a:1112:PHE:CD1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1287:MET:O	1:a:1288:ALA:HB2	2.14	0.48
1:a:1189:ARG:HB2	1:a:1190:ASN:OD1	2.13	0.48
1:a:1183:ILE:CG2	1:a:1201:LEU:HD22	2.45	0.47
2:b:6:HIS:CD2	2:b:21:TRP:CZ2	3.02	0.47
2:b:137:LEU:HD12	2:b:138:THR:N	2.30	0.47
1:a:1285:LYS:H	1:a:1356:THR:HG22	1.80	0.47
1:a:1282:ARG:CZ	1:a:1283:HIS:CE1	2.98	0.47
2:b:48:ARG:O	2:b:49:ILE:C	2.57	0.47
1:a:1285:LYS:H	1:a:1356:THR:CG2	2.28	0.47
1:a:1293:TYR:CD1	1:a:1293:TYR:N	2.82	0.47
2:b:288:VAL:H	2:b:289:PRO:HD2	1.79	0.47
2:b:400:ARG:HE	2:b:400:ARG:CA	2.28	0.47
2:b:264:ARG:C	2:b:266:HIS:CD2	2.92	0.47
2:b:269:MET:CE	2:b:301:MET:SD	3.03	0.46
1:a:1346:GLN:C	1:a:1347:ARG:HG2	2.40	0.46
2:b:63:PRO:HD2	2:b:86:ILE:HG23	1.97	0.46
2:b:172:VAL:HG13	2:b:173:PRO:HD2	1.97	0.46
1:a:1369:PHE:C	1:a:1369:PHE:CD2	2.94	0.46
2:b:103:TRP:NE1	2:b:148:GLY:HA2	2.31	0.46
1:a:1238:ARG:C	1:a:1240:HIS:H	2.24	0.46
1:a:1291:LEU:N	1:a:1291:LEU:CD1	2.79	0.46
1:a:1236:TYR:HB3	1:a:1237:PRO:CD	2.45	0.46
2:b:265:LEU:O	2:b:265:LEU:HD12	2.15	0.46
1:a:1147:PRO:CG	1:a:1365:LEU:HD21	2.46	0.46
1:a:1290:CYS:SG	1:a:1290:CYS:O	2.74	0.45
2:b:377:PHE:C	2:b:377:PHE:CD2	2.93	0.45
2:b:388:PHE:N	2:b:388:PHE:CD2	2.80	0.45
1:a:1040:VAL:C	1:a:1041:PHE:CD1	2.95	0.45
2:b:169:PHE:CE2	2:b:235:MET:SD	3.10	0.45
2:b:175:PRO:HB3	2:b:390:ARG:CZ	2.47	0.45
3:M:3157:PHE:CD2	3:M:3157:PHE:C	2.95	0.45
1:a:1042:VAL:HG11	1:a:1123:PHE:CZ	2.51	0.45
1:a:1059:GLN:HA	1:a:1059:GLN:OE1	2.17	0.45
2:b:6:HIS:CD2	2:b:21:TRP:HZ2	2.35	0.45
1:a:1042:VAL:HG11	1:a:1123:PHE:CE1	2.52	0.45
2:b:300:ASN:O	2:b:301:MET:HE2	2.17	0.45
2:b:288:VAL:H	2:b:289:PRO:CD	2.31	0.44
1:a:1376:ARG:HB2	3:M:3204:LYS:CE	2.47	0.44
3:M:3220:SER:C	3:M:3222:CYS:H	2.25	0.44
1:a:1143:PHE:CE2	1:a:1209:VAL:HG22	2.53	0.44
1:a:1399:MET:SD	1:a:1399:MET:C	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:2:ARG:N	2:b:3:GLU:CD	2.75	0.44
2:b:261:PRO:O	2:b:262:PHE:CD1	2.70	0.44
2:b:319:PHE:CD1	2:b:319:PHE:N	2.85	0.44
1:a:1225:ASP:O	1:a:1228:GLU:HB2	2.18	0.44
1:a:1077:TYR:O	1:a:1078:ALA:C	2.60	0.44
2:b:241:CYS:SG	2:b:320:ARG:HD2	2.57	0.44
1:a:1073:ALA:O	1:a:1074:ALA:HB3	2.18	0.44
2:b:125:GLU:OE1	2:b:125:GLU:HA	2.17	0.44
2:b:352:LYS:HD3	2:b:352:LYS:C	2.43	0.44
1:a:1011:GLN:CD	1:a:1118:GLY:H	2.25	0.44
2:b:69:ASP:HB3	2:b:75:MET:HE3	2.00	0.44
2:b:137:LEU:HD12	2:b:137:LEU:C	2.42	0.44
1:a:1217:ARG:N	1:a:1217:ARG:HE	2.16	0.43
2:b:262:PHE:HB3	2:b:263:PRO:HD3	2.00	0.43
2:b:140:SER:CB	2:b:142:GLY:H	2.31	0.43
2:b:377:PHE:CE2	2:b:379:GLY:HA3	2.53	0.43
3:M:3137:MET:HA	3:M:3137:MET:HE2	2.00	0.43
1:a:1375:LYS:HG3	2:b:346:TRP:CE3	2.53	0.43
2:b:198:THR:O	2:b:265:LEU:HD13	2.18	0.43
2:b:206:ASN:ND2	2:b:206:ASN:H	2.16	0.43
2:b:20:PHE:CE2	2:b:24:ILE:CG1	3.02	0.43
2:b:372:LYS:O	2:b:373:MET:HE2	2.19	0.43
2:b:377:PHE:C	2:b:378:ILE:HD12	2.44	0.42
2:b:290:GLU:CD	2:b:290:GLU:H	2.27	0.42
1:a:1351:MET:C	1:a:1351:MET:SD	3.01	0.42
1:a:1376:ARG:O	1:a:1379:VAL:HG23	2.18	0.42
2:b:250:ALA:O	2:b:251:ASP:HB3	2.20	0.42
1:a:1380:HIS:HB3	3:M:3122:GLU:CD	2.44	0.42
2:b:250:ALA:C	2:b:254:LYS:HD2	2.44	0.42
1:a:1108:GLY:HA3	1:a:1139:SER:O	2.18	0.42
2:b:52:TYR:C	2:b:53:TYR:CD1	2.98	0.42
1:a:1122:GLY:O	1:a:1123:PHE:C	2.60	0.42
1:a:1243:LEU:C	1:a:1243:LEU:HD12	2.44	0.42
2:b:2:ARG:HA	2:b:131:CYS:O	2.20	0.42
1:a:1162:ILE:HG22	1:a:1162:ILE:O	2.20	0.42
1:a:1178:VAL:HG12	1:a:1179:ASP:N	2.35	0.42
1:a:1315:ILE:H	1:a:1315:ILE:HG22	1.44	0.42
2:b:10:GLY:HA2	2:b:145:THR:OG1	2.19	0.42
1:a:1229:PHE:N	1:a:1229:PHE:CD2	2.82	0.42
2:b:265:LEU:HD12	2:b:265:LEU:C	2.45	0.42
1:a:1033:ASP:HA	1:a:1060:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1367:HIS:CD2	1:a:1367:HIS:C	2.97	0.42
1:a:1265:ILE:HG13	1:a:1349:VAL:HG21	2.02	0.42
1:a:1380:HIS:HE1	2:b:260:VAL:O	2.01	0.42
2:b:103:TRP:CD1	2:b:148:GLY:HA2	2.55	0.42
2:b:211:ASP:CG	2:b:215:ARG:HH21	2.28	0.42
1:a:1076:ASN:HB2	1:a:1382:TYR:CE2	2.55	0.41
1:a:1191:LEU:HD21	1:a:1341:ASP:O	2.20	0.41
2:b:48:ARG:HA	2:b:48:ARG:HD3	1.75	0.41
2:b:301:MET:HE2	2:b:301:MET:CA	2.46	0.41
1:a:1062:HIS:O	1:a:1064:GLU:N	2.53	0.41
1:a:1376:ARG:NH2	2:b:262:PHE:HA	2.35	0.41
1:a:1077:TYR:CD2	1:a:1078:ALA:N	2.88	0.41
1:a:1261:SER:H	1:a:1264:GLU:CD	2.29	0.41
1:a:1089:ILE:HD11	1:a:1126:LEU:HD23	2.02	0.41
1:a:1089:ILE:HG22	1:a:1090:ASP:N	2.36	0.41
1:a:1376:ARG:O	1:a:1377:ALA:C	2.64	0.41
2:b:318:VAL:O	2:b:318:VAL:HG12	2.19	0.41
2:b:378:ILE:O	2:b:378:ILE:HG22	2.21	0.41
1:a:1016:ILE:O	1:a:1020:CYS:HB3	2.20	0.41
2:b:311:ARG:HA	2:b:342:TYR:O	2.21	0.41
1:a:1049:ILE:HD12	1:a:1068:THR:HG22	2.03	0.41
1:a:1375:LYS:HG3	2:b:346:TRP:CZ3	2.56	0.41
2:b:244:PHE:CD1	2:b:358:ILE:HG21	2.56	0.41
2:b:384:ILE:O	2:b:384:ILE:CG2	2.68	0.41
1:a:1264:GLU:O	1:a:1267:ASN:N	2.54	0.41
1:a:1382:TYR:O	1:a:1383:VAL:C	2.62	0.41
1:a:1271:GLU:C	1:a:1273:ALA:H	2.29	0.40
2:b:251:ASP:O	2:b:254:LYS:N	2.54	0.40
1:a:1131:LEU:HD23	1:a:1131:LEU:HA	1.81	0.40
1:a:1166:HIS:CD2	1:a:1166:HIS:O	2.73	0.40
2:b:11:GLN:HG2	2:b:15:GLN:OE1	2.22	0.40
2:b:70:LEU:H	2:b:145:THR:CG2	2.34	0.40
1:a:1072:ASP:OD2	1:a:1079:ARG:NH2	2.54	0.40
2:b:243:ARG:HG3	2:b:243:ARG:HH11	1.86	0.40
3:M:3101:CYS:SG	3:M:3221:LYS:HB2	2.61	0.40
1:a:1389:GLU:HG2	1:a:1390:GLY:N	2.35	0.40
1:a:1076:ASN:O	1:a:1076:ASN:CG	2.64	0.40
1:a:1302:VAL:HG12	1:a:1306:ILE:CD1	2.51	0.40
2:b:36:TYR:CD2	2:b:36:TYR:C	2.98	0.40

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	410/412 (100%)	284 (69%)	74 (18%)	52 (13%)	0	3
2	b	424/426 (100%)	288 (68%)	88 (21%)	48 (11%)	0	4
3	M	128/130 (98%)	108 (84%)	17 (13%)	3 (2%)	5	27
All	All	962/968 (99%)	680 (71%)	179 (19%)	103 (11%)	1	4

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	1031	GLN
1	a	1057	TYR
1	a	1082	TYR
1	a	1083	THR
1	a	1117	GLY
1	a	1148	ALA
1	a	1214	ALA
1	a	1235	PRO
1	a	1236	TYR
1	a	1240	HIS
1	a	1247	ALA
1	a	1258	GLU
1	a	1277	VAL
1	a	1322	PRO
1	a	1361	ALA
1	a	1377	ALA
1	a	1378	PHE
2	b	23	VAL
2	b	72	PRO
2	b	183	GLU
2	b	239	THR
2	b	240	THR
2	b	251	ASP
2	b	252	LEU

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Mol	Chain	Res	Type
2	b	262	PHE
2	b	263	PRO
2	b	265	LEU
2	b	273	ALA
2	b	288	VAL
2	b	294	GLN
2	b	371	LEU
1	a	1085	GLY
1	a	1151	VAL
1	a	1191	LEU
1	a	1219	ASP
1	a	1229	PHE
1	a	1230	GLN
1	a	1263	ALA
1	a	1288	ALA
1	a	1360	GLU
1	a	1376	ARG
2	b	24	ILE
2	b	50	ASN
2	b	81	GLY
2	b	86	ILE
2	b	130	ASP
2	b	143	GLY
2	b	238	VAL
2	b	245	PRO
2	b	285	ALA
2	b	295	MET
2	b	298	ALA
2	b	348	PRO
2	b	373	MET
3	M	3221	LYS
1	a	1077	TYR
1	a	1171	HIS
1	a	1212	ILE
1	a	1213	THR
1	a	1221	ALA
1	a	1222	LEU
1	a	1279	CYS
1	a	1304	ALA
1	a	1347	ARG
2	b	31	ASP
2	b	107	HIS

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Mol	Chain	Res	Type
2	b	141	LEU
2	b	223	THR
2	b	250	ALA
2	b	304	ALA
2	b	369	ARG
2	b	386	GLU
3	M	3148	PHE
1	a	1024	TYR
1	a	1033	ASP
1	a	1078	ALA
1	a	1123	PHE
1	a	1192	ASP
1	a	1237	PRO
1	a	1239	GLY
1	a	1280	ASP
2	b	145	THR
2	b	308	ARG
2	b	344	VAL
2	b	404	PHE
3	M	3175	HIS
1	a	1332	GLU
2	b	82	PRO
2	b	172	VAL
2	b	180	THR
2	b	266	HIS
2	b	395	PHE
2	b	400	ARG
1	a	1262	VAL
2	b	384	ILE
2	b	424	ASN
1	a	1089	ILE
1	a	1122	GLY
1	a	1220	GLY
1	a	1358	ILE
2	b	71	GLU
1	a	1034	GLY
1	a	1411	VAL

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	347/347 (100%)	283 (82%)	64 (18%)	1	10
2	b	367/367 (100%)	318 (87%)	49 (13%)	4	18
3	M	120/120 (100%)	109 (91%)	11 (9%)	8	31
All	All	834/834 (100%)	710 (85%)	124 (15%)	5	15

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	1003	GLU
1	a	1009	VAL
1	a	1011	GLN
1	a	1015	GLN
1	a	1021	TRP
1	a	1036	VAL
1	a	1037	PRO
1	a	1038	ARG
1	a	1040	VAL
1	a	1045	GLU
1	a	1046	PRO
1	a	1047	THR
1	a	1048	VAL
1	a	1049	ILE
1	a	1062	HIS
1	a	1063	PRO
1	a	1065	GLN
1	a	1068	THR
1	a	1088	ILE
1	a	1124	THR
1	a	1125	SER
1	a	1128	MET
1	a	1129	GLU
1	a	1133	VAL
1	a	1152	SER
1	a	1158	PRO
1	a	1166	HIS
1	a	1167	THR
1	a	1168	THR
1	a	1174	CYS

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Mol	Chain	Res	Type
1	a	1179	ASP
1	a	1187	CYS
1	a	1191	LEU
1	a	1197	THR
1	a	1204	LEU
1	a	1208	ILE
1	a	1217	ARG
1	a	1222	LEU
1	a	1230	GLN
1	a	1234	VAL
1	a	1249	VAL
1	a	1259	GLN
1	a	1274	ASN
1	a	1277	VAL
1	a	1292	LEU
1	a	1315	ILE
1	a	1323	THR
1	a	1326	LYS
1	a	1327	VAL
1	a	1334	PRO
1	a	1335	THR
1	a	1337	VAL
1	a	1345	VAL
1	a	1351	MET
1	a	1352	LEU
1	a	1355	THR
1	a	1362	TRP
1	a	1365	LEU
1	a	1366	ASP
1	a	1376	ARG
1	a	1379	VAL
1	a	1402	LEU
1	a	1403	GLU
1	a	1406	TYR
2	b	6	HIS
2	b	16	ILE
2	b	63	PRO
2	b	66	ILE
2	b	67	LEU
2	b	71	GLU
2	b	83	PHE
2	b	86	ILE

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Mol	Chain	Res	Type
2	b	89	PRO
2	b	94	PHE
2	b	105	LYS
2	b	118	VAL
2	b	122	VAL
2	b	137	LEU
2	b	139	HIS
2	b	158	ARG
2	b	162	PRO
2	b	164	ARG
2	b	172	VAL
2	b	174	SER
2	b	175	PRO
2	b	195	VAL
2	b	230	LEU
2	b	234	THR
2	b	235	MET
2	b	240	THR
2	b	251	ASP
2	b	263	PRO
2	b	281	GLN
2	b	290	GLU
2	b	292	THR
2	b	322	ARG
2	b	323	MET
2	b	325	MET
2	b	326	LYS
2	b	334	ASN
2	b	343	PHE
2	b	347	ILE
2	b	352	LYS
2	b	358	ILE
2	b	377	PHE
2	b	384	ILE
2	b	398	MET
2	b	404	PHE
2	b	407	TRP
2	b	415	GLU
2	b	419	THR
2	b	427	ASP
2	b	428	LEU
3	M	3105	ILE

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Mol	Chain	Res	Type
3	M	3110	ARG
3	M	3114	ASN
3	M	3115	ILE
3	M	3119	GLN
3	M	3120	LEU
3	M	3141	CYS
3	M	3155	GLN
3	M	3164	ILE
3	M	3170	TYR
3	M	3218	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	1008	HIS
1	a	1028	HIS
1	a	1166	HIS
1	a	1180	ASN
1	a	1200	ASN
1	a	1202	ASN
1	a	1240	HIS
1	a	1283	HIS
1	a	1367	HIS
1	a	1380	HIS
2	b	6	HIS
2	b	8	GLN
2	b	14	ASN
2	b	101	ASN
2	b	206	ASN
2	b	229	HIS
2	b	247	GLN
2	b	334	ASN
2	b	394	GLN
3	M	3166	ASN
3	M	3169	HIS

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	b	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	269:MET	C	270:PRO	N	1.18

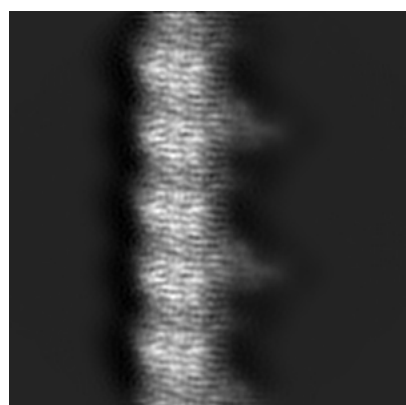
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9997. These allow visual inspection of the internal detail of the map and identification of artifacts.

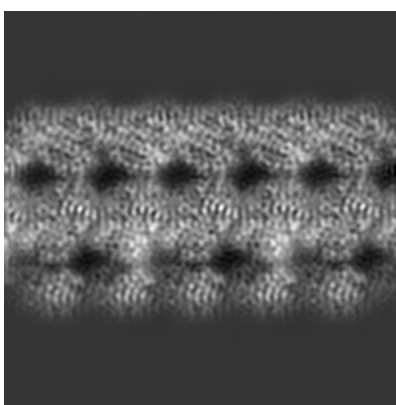
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

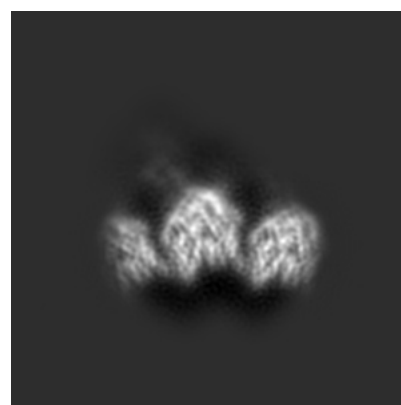
6.1.1 Primary map



X



Y

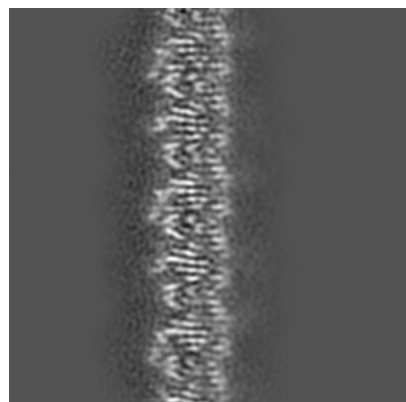


Z

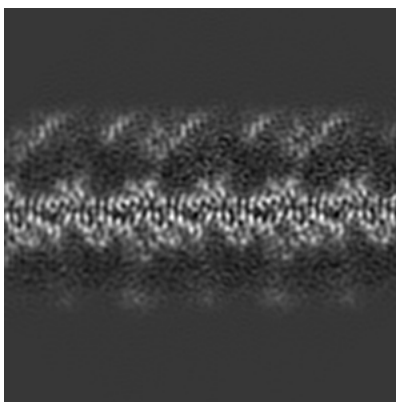
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

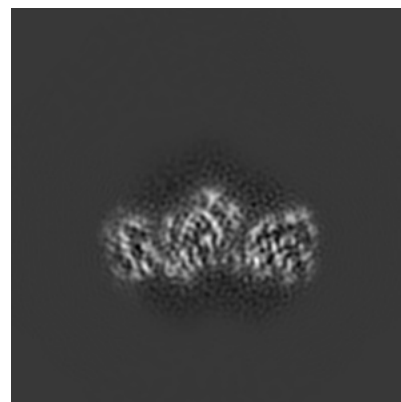
6.2.1 Primary map



X Index: 90



Y Index: 90

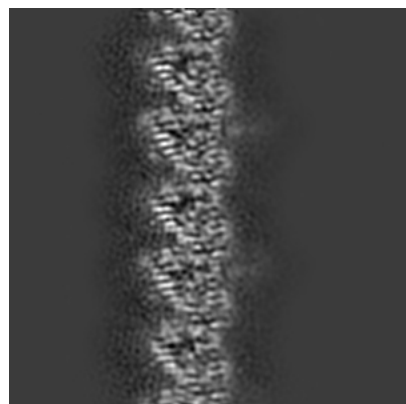


Z Index: 90

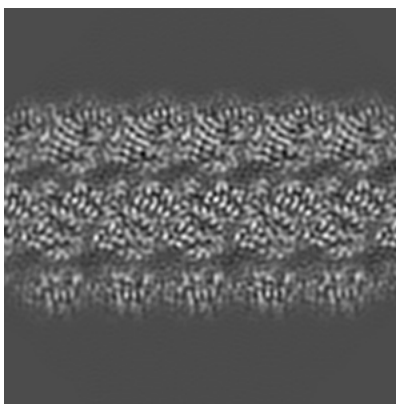
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

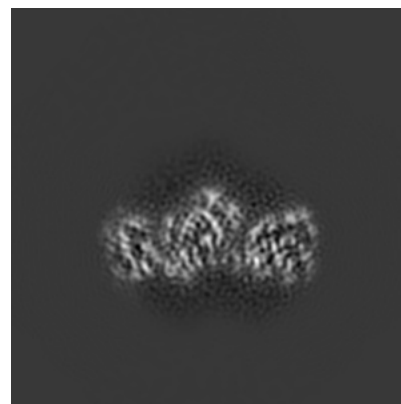
6.3.1 Primary map



X Index: 83



Y Index: 75

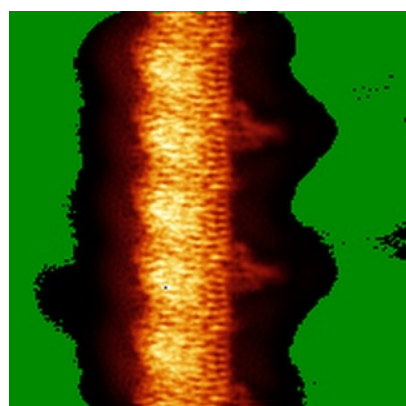


Z Index: 90

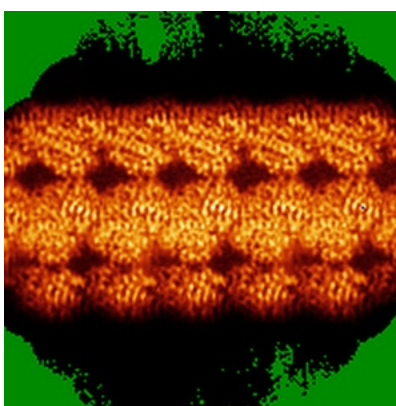
The images above show the largest variance slices of the map in three orthogonal directions.

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

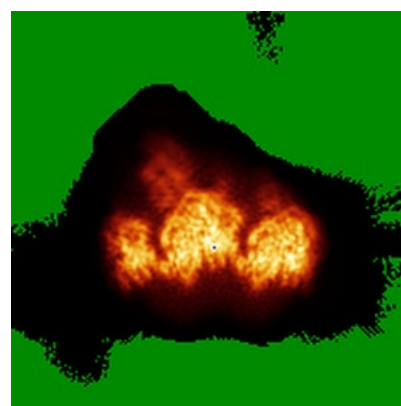
6.4.1 Primary map



X



Y

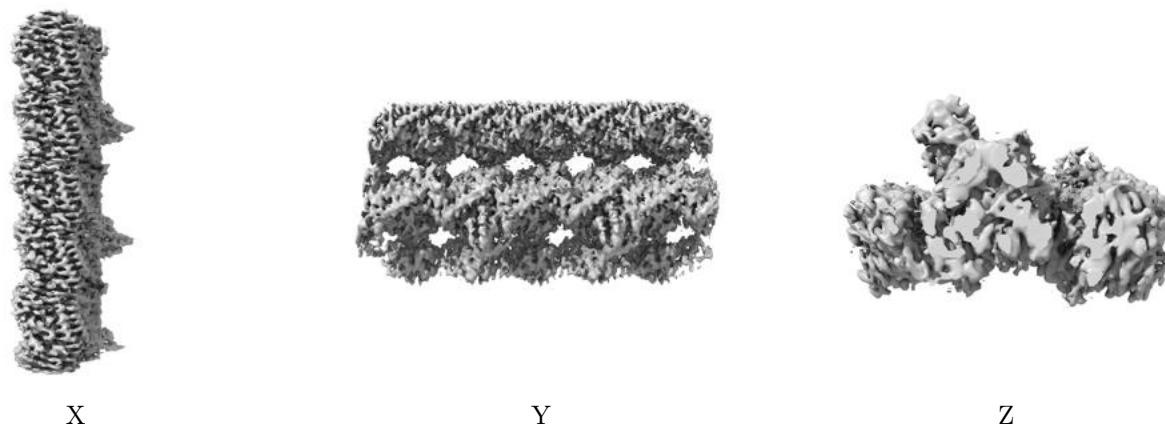


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

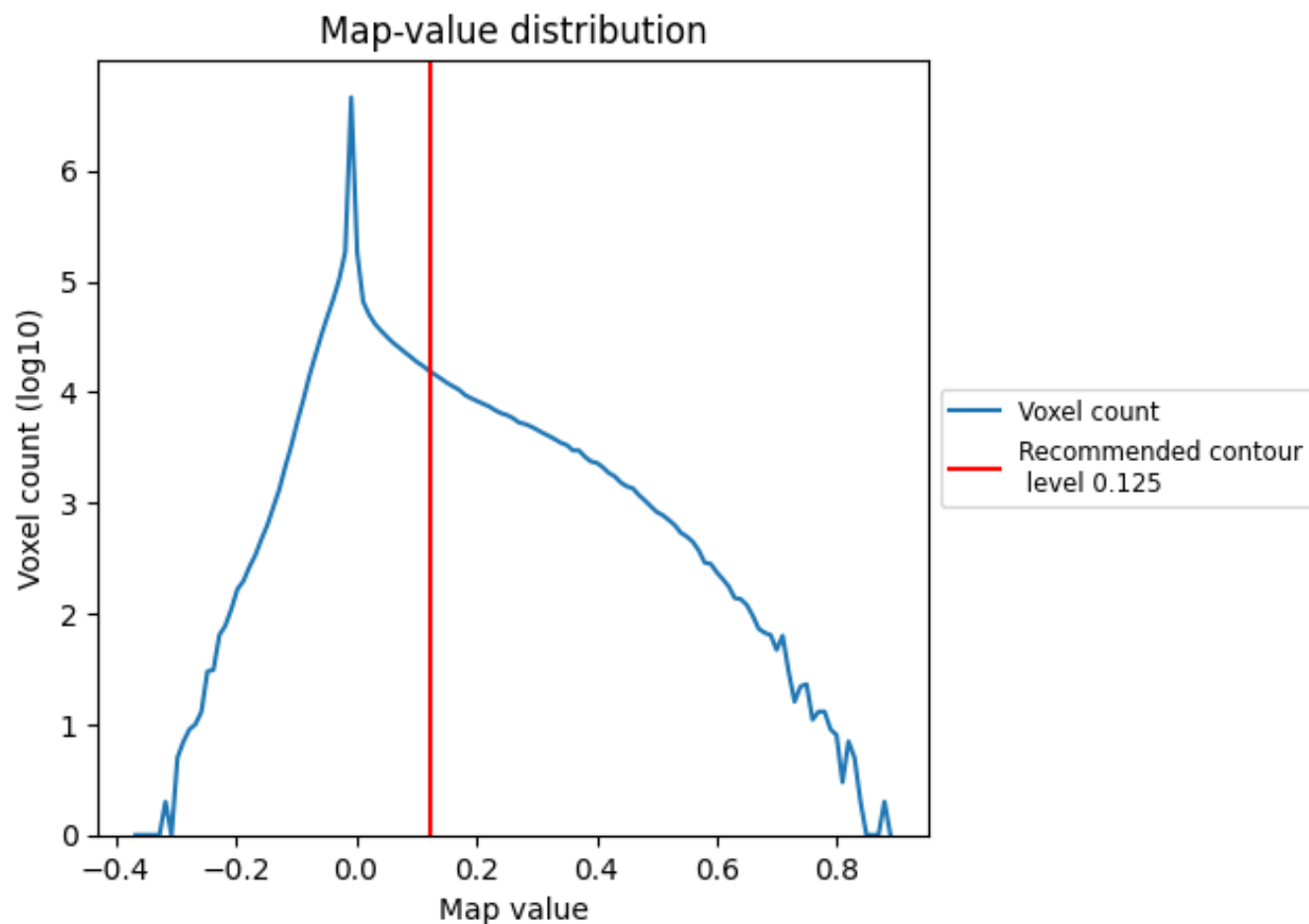
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

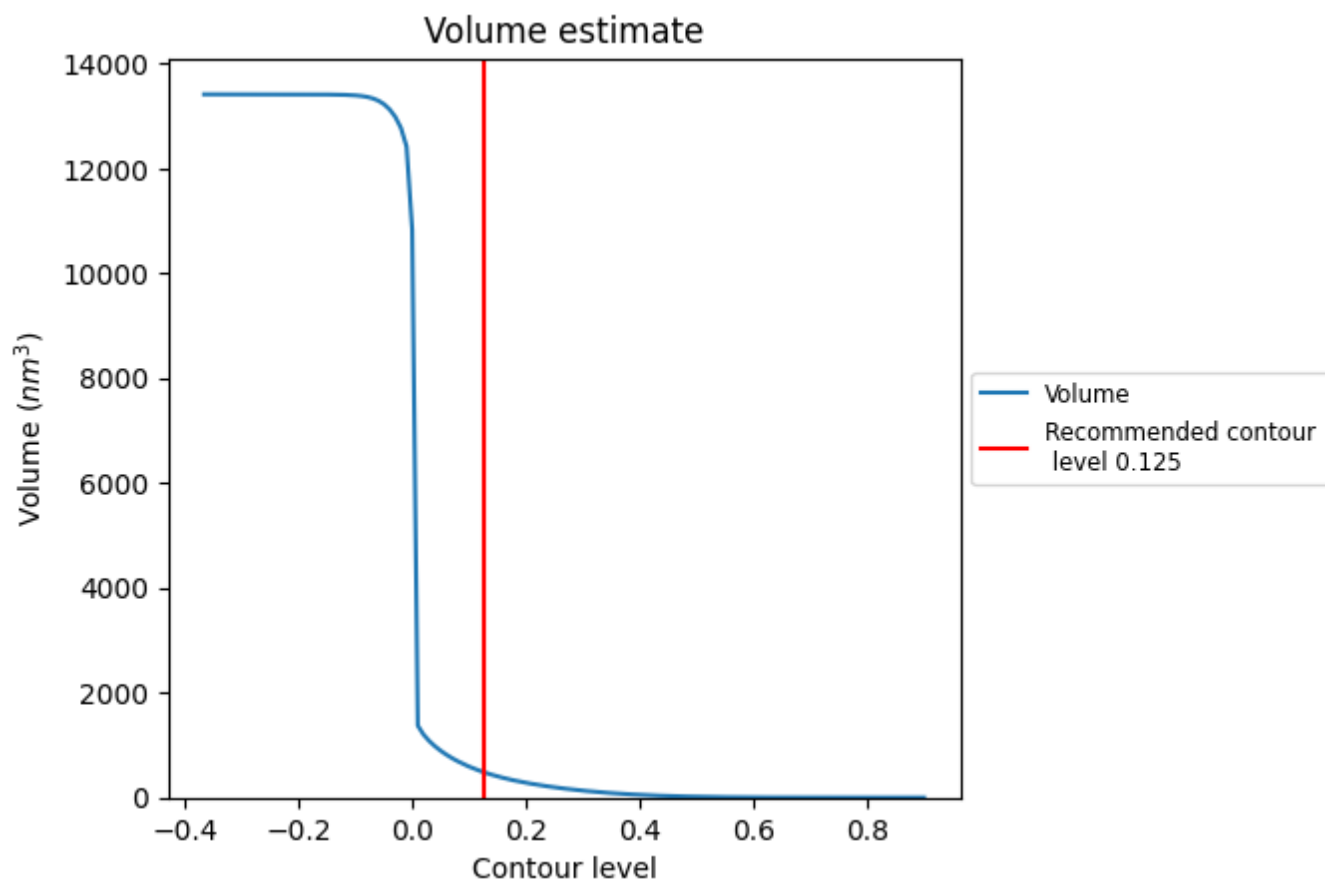
This section contains the results of statistical analysis of the map.

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.

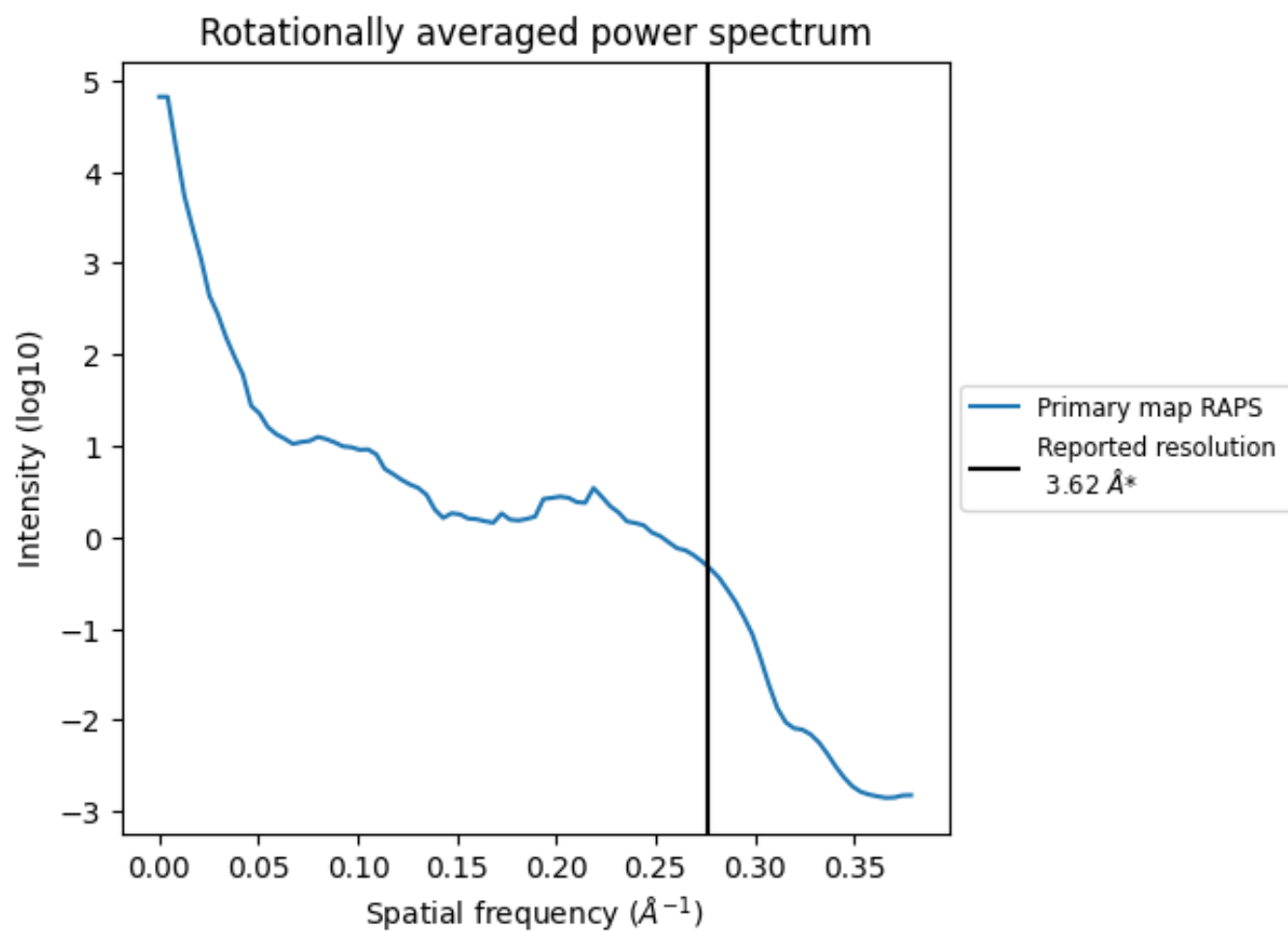
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 484 nm³; this corresponds to an approximate mass of 437 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 0.276 $\text{\AA}^{-1}$

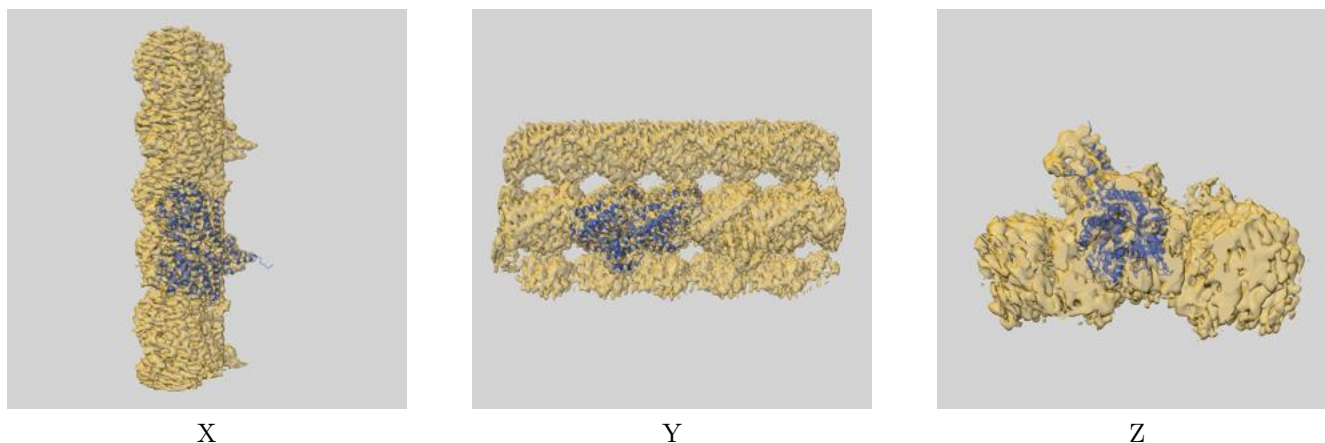
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

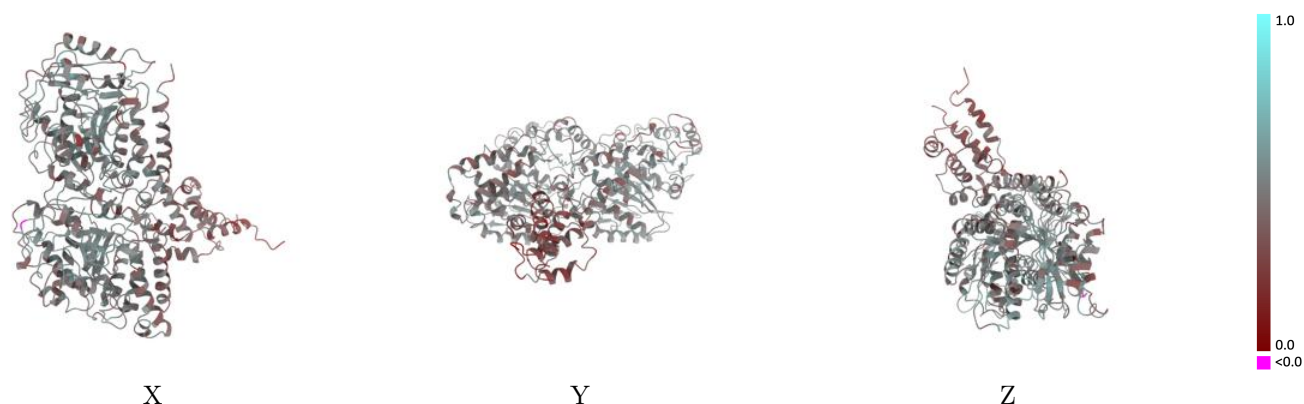
This section contains information regarding the fit between EMDB map EMD-9997 and PDB model 6KIQ. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



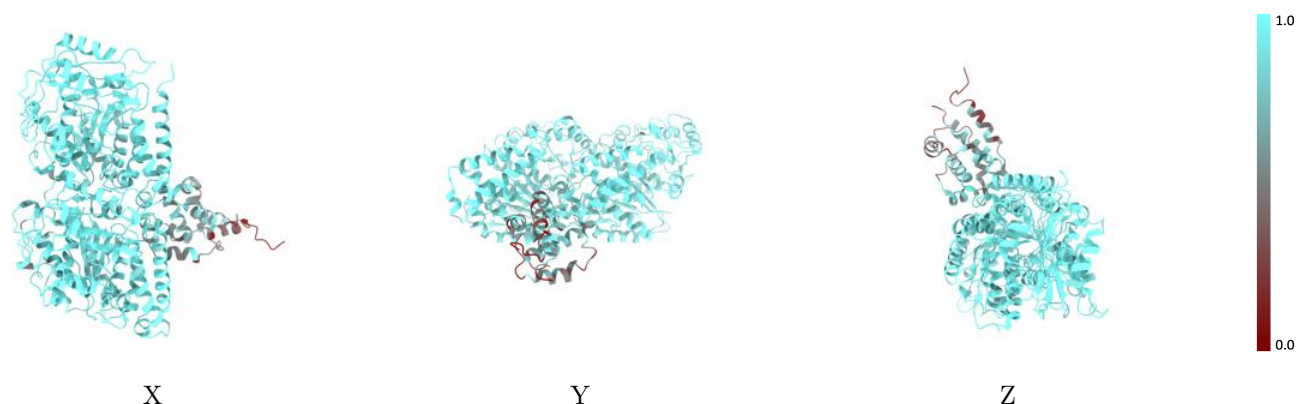
The images above show the 3D surface view of the map at the recommended contour level 0.125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



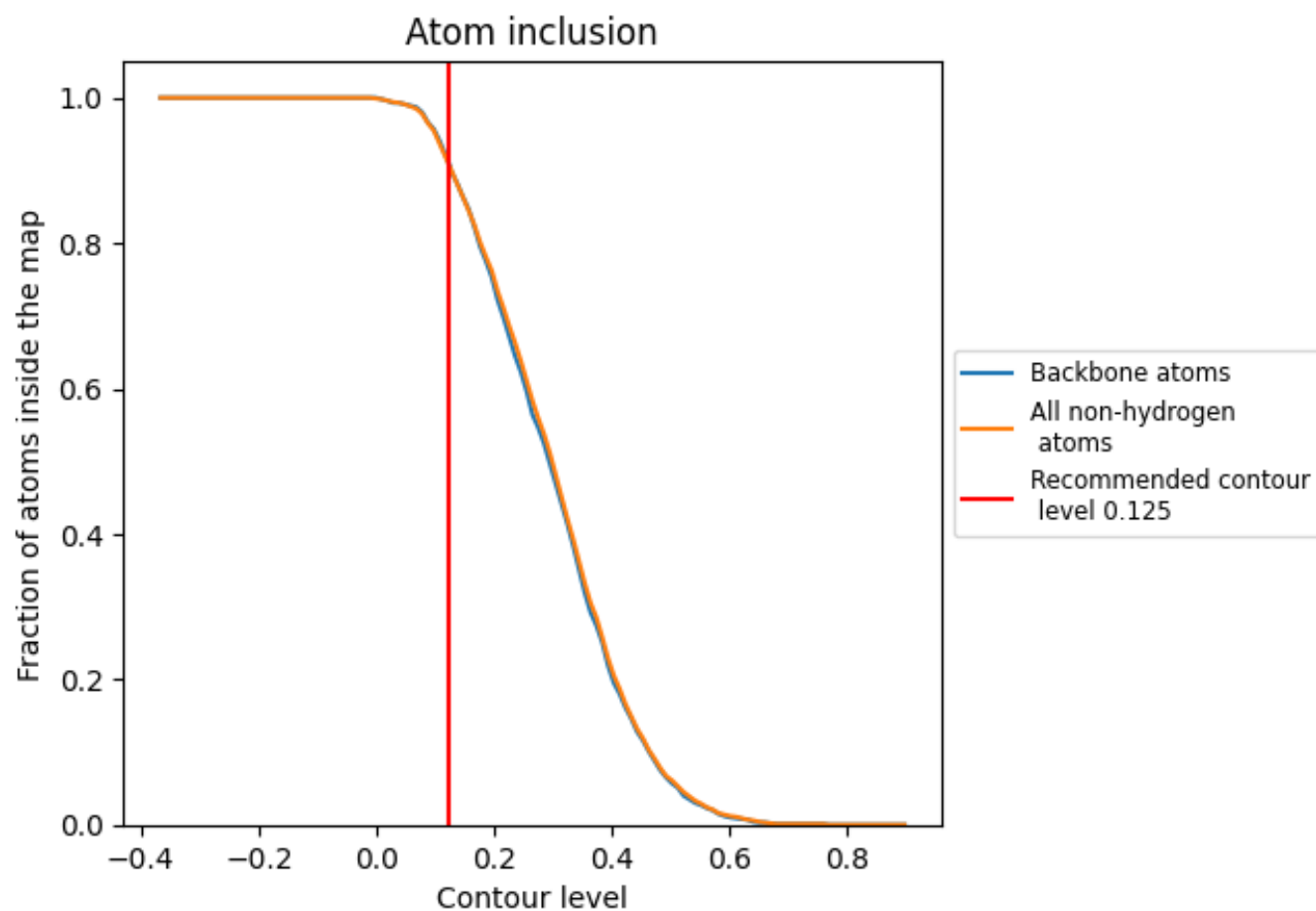
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.125).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 91% 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 (0.125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9060	0.4550
M	0.5810	0.3210
a	0.9660	0.4790
b	0.9660	0.4730

