



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 05:14 PM UTC

PDB ID : 6KIO / pdb_00006kio
EMDB ID : EMD-9996
Title : Complex of yeast cytoplasmic dynein MTBD-High and MT without DTT
Authors : Komori, Y.; Nishida, N.; Shimada, I.; Kikkawa, M.
Deposited on : 2019-07-19
Resolution : 3.94 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

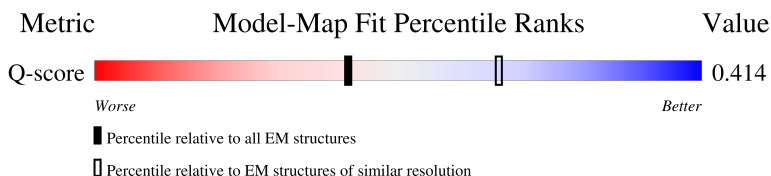
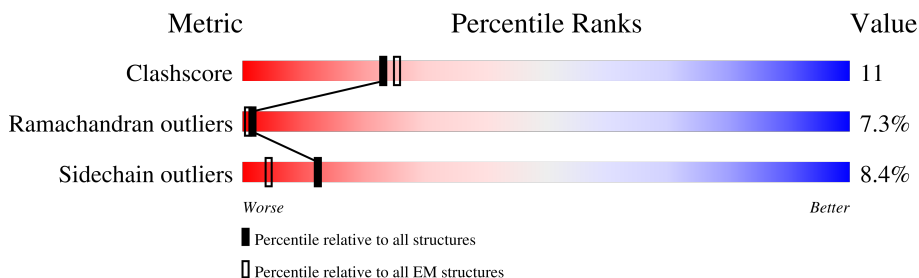
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.94 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	7757 (3.44 - 4.43)

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	b	426	 25% 48% 22% 5%
2	M	130	 38% 72% 26% .
3	a	412	 28% 49% 18% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15091 atoms, of which 7442 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 Tubulin beta chain.

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

- Molecule 2 is a protein called Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	M	130	Total	C	H	N	O	S	0	0
			2132	679	1063	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

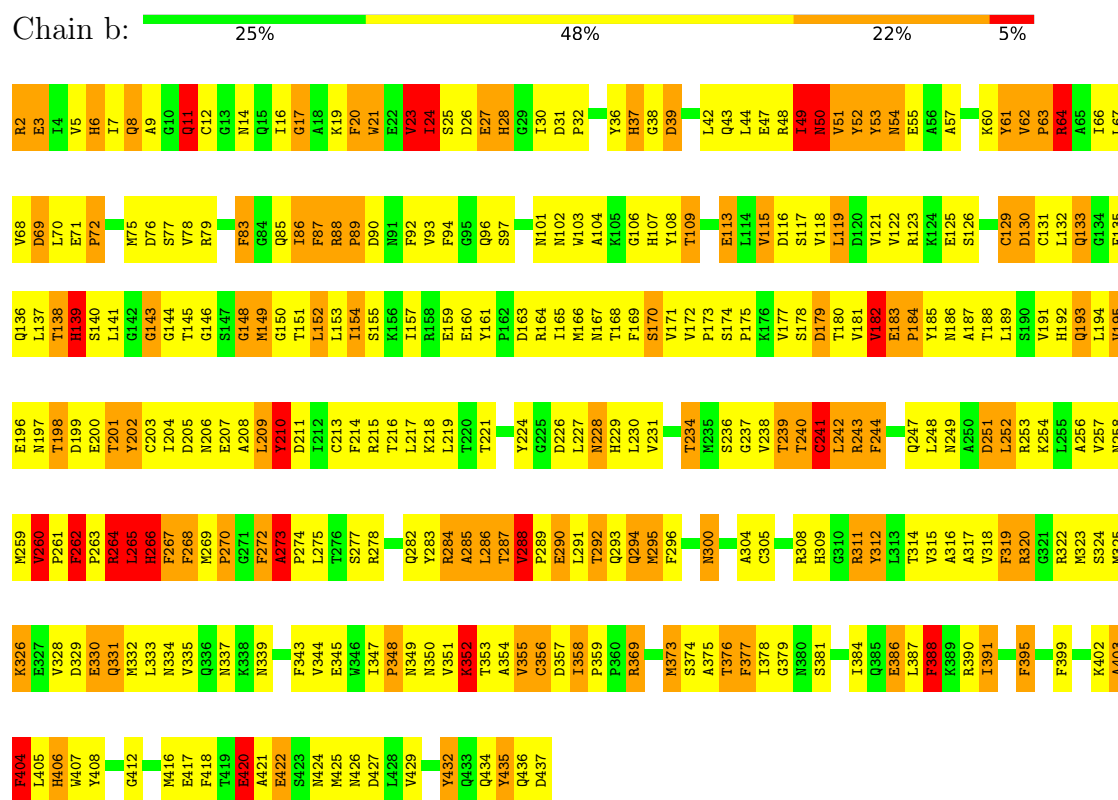
- Molecule 3 is a protein called Tubulin alpha-1A chain.

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

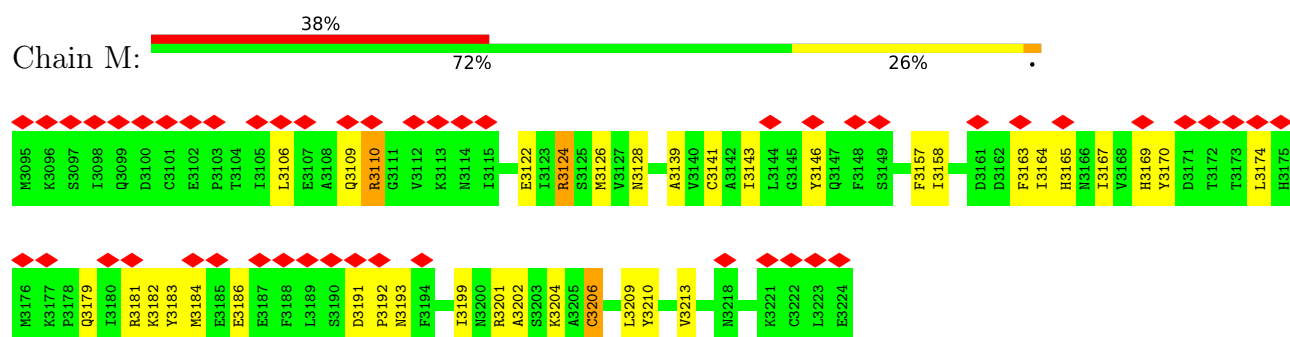
3 Residue-property plots

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

• Molecule 1: Tubulin beta chain

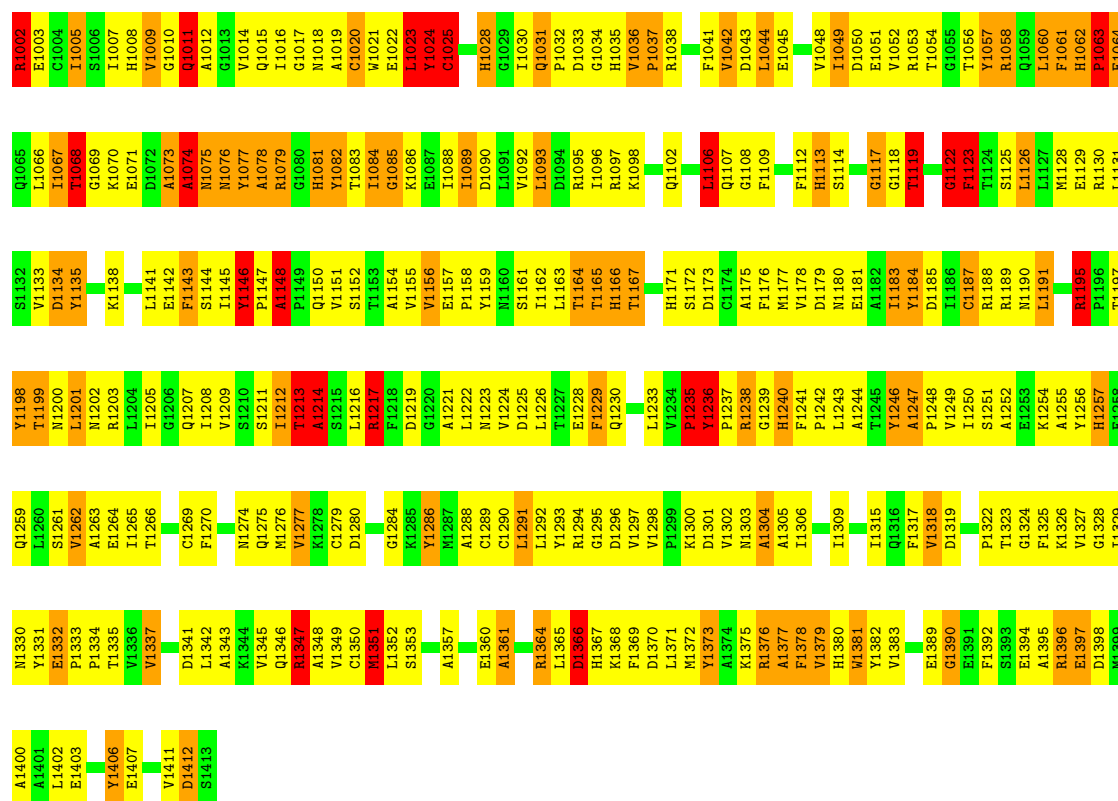


• Molecule 2: Dynein heavy chain, cytoplasmic



• Molecule 3: Tubulin alpha-1A chain

Age Group	Percentage
18-24	28%
25-34	49%
35-44	18%
45-54	6%



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-25.7561°, rise=9.20776 Å, axial sym=C1	Depositor
Number of segments used	58999	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	0.732	Depositor
Minimum map value	-0.159	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.14	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	b	2.75	272/3427 (7.9%)	2.33	181/4642 (3.9%)
2	M	1.26	0/1092	1.82	20/1472 (1.4%)
3	a	2.69	235/3302 (7.1%)	2.33	181/4485 (4.0%)
All	All	2.57	507/7821 (6.5%)	2.27	382/10599 (3.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	b	0	20
2	M	0	5
3	a	0	16
All	All	0	41

All (507) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	50	ASN	CA-C	-13.37	1.34	1.52
3	a	1298	VAL	CA-CB	-12.17	1.45	1.54
3	a	1257	HIS	N-CA	-12.07	1.36	1.47
1	b	63	PRO	CA-C	-11.83	1.38	1.52
3	a	1330	ASN	CA-C	-11.80	1.38	1.52
1	b	216	THR	CA-C	-11.32	1.43	1.52
1	b	269	MET	C-N	-11.10	1.19	1.33
1	b	332	MET	CA-C	-10.35	1.39	1.52
3	a	1150	GLN	CA-C	-10.30	1.44	1.52
1	b	234	THR	CA-C	-10.10	1.39	1.52
3	a	1302	VAL	CA-C	-9.97	1.40	1.52
3	a	1200	ASN	CA-C	-9.89	1.41	1.52
1	b	343	PHE	CA-C	-9.68	1.40	1.52
3	a	1097	ARG	CA-C	-9.64	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	1037	PRO	CA-C	-9.63	1.41	1.52
3	a	1154	ALA	CA-C	-9.59	1.41	1.52
3	a	1298	VAL	CA-C	-9.47	1.46	1.52
1	b	288	VAL	CA-C	-9.45	1.43	1.52
1	b	180	THR	CA-C	-9.39	1.41	1.52
1	b	138	THR	CA-C	-9.32	1.41	1.52
3	a	1036	VAL	CA-CB	-9.20	1.42	1.54
1	b	21	TRP	NE1-CE2	-9.09	1.27	1.37
3	a	1014	VAL	CA-CB	-9.09	1.41	1.54
1	b	435	TYR	CA-C	-9.02	1.41	1.53
3	a	1014	VAL	CA-C	-8.84	1.41	1.53
1	b	154	ILE	CA-C	-8.83	1.41	1.52
3	a	1017	GLY	CA-C	-8.79	1.42	1.52
3	a	1041	PHE	CA-C	-8.78	1.42	1.52
1	b	408	TYR	CA-C	-8.77	1.42	1.53
1	b	231	VAL	CA-C	-8.77	1.42	1.52
1	b	248	LEU	CA-C	-8.67	1.41	1.52
1	b	50	ASN	C-N	-8.62	1.22	1.33
3	a	1246	TYR	CA-C	-8.59	1.41	1.52
3	a	1383	VAL	CA-CB	-8.58	1.44	1.54
3	a	1183	ILE	CA-C	-8.57	1.41	1.53
1	b	239	THR	CA-C	-8.55	1.41	1.52
3	a	1250	ILE	CA-C	-8.51	1.41	1.52
3	a	1177	MET	CA-C	-8.49	1.42	1.52
3	a	1256	TYR	CA-C	-8.45	1.43	1.53
3	a	1309	ILE	CA-C	-8.39	1.42	1.52
1	b	62	VAL	CA-CB	-8.36	1.43	1.54
1	b	312	TYR	CA-C	-8.35	1.42	1.52
3	a	1203	ARG	CA-C	-8.31	1.41	1.52
1	b	201	THR	CA-C	-8.29	1.42	1.52
1	b	6	HIS	CB-CG	-8.24	1.38	1.50
3	a	1021	TRP	CA-C	-8.24	1.41	1.52
1	b	102	ASN	N-CA	-8.21	1.36	1.46
3	a	1152	SER	CA-C	-8.18	1.42	1.52
3	a	1372	MET	CA-C	-8.07	1.42	1.52
1	b	17	GLY	CA-C	-8.06	1.42	1.51
3	a	1113	HIS	CA-C	-8.06	1.42	1.52
3	a	1293	TYR	CA-C	-7.99	1.42	1.52
1	b	226	ASP	CA-C	-7.96	1.42	1.52
3	a	1205	ILE	CA-CB	-7.95	1.45	1.54
1	b	209	LEU	N-CA	-7.89	1.36	1.46
3	a	1209	VAL	CA-CB	-7.87	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	1349	VAL	CA-CB	-7.85	1.43	1.54
3	a	1365	LEU	CA-C	-7.84	1.42	1.52
1	b	173	PRO	CA-C	-7.83	1.45	1.52
3	a	1300	LYS	CA-C	-7.83	1.42	1.52
3	a	1229	PHE	CA-C	-7.80	1.42	1.52
3	a	1297	VAL	CA-C	-7.80	1.42	1.52
3	a	1351	MET	CA-C	-7.73	1.42	1.52
3	a	1382	TYR	CA-C	-7.72	1.43	1.52
1	b	52	TYR	C-N	-7.69	1.24	1.33
1	b	161	TYR	CA-C	-7.68	1.44	1.52
3	a	1329	ILE	CA-CB	-7.67	1.44	1.54
1	b	121	VAL	CA-CB	-7.66	1.44	1.54
1	b	137	LEU	CA-C	-7.66	1.43	1.52
1	b	355	VAL	CA-C	-7.62	1.43	1.52
3	a	1190	ASN	CA-C	-7.61	1.42	1.52
3	a	1249	VAL	CA-C	-7.58	1.45	1.53
1	b	168	THR	CA-C	-7.58	1.43	1.52
1	b	123	ARG	CA-C	-7.58	1.42	1.52
3	a	1294	ARG	CA-C	-7.54	1.43	1.52
1	b	136	GLN	CA-C	-7.53	1.43	1.52
1	b	64	ARG	CA-C	-7.53	1.43	1.52
3	a	1042	VAL	CA-CB	-7.50	1.44	1.54
1	b	191	VAL	CA-C	-7.49	1.43	1.52
1	b	189	LEU	CA-C	-7.49	1.42	1.52
3	a	1067	ILE	CA-CB	-7.48	1.44	1.54
1	b	66	ILE	CA-CB	-7.48	1.44	1.54
3	a	1208	ILE	CA-C	-7.48	1.43	1.52
3	a	1348	ALA	CA-C	-7.46	1.43	1.52
1	b	52	TYR	CA-C	-7.46	1.42	1.52
3	a	1109	PHE	CA-C	-7.45	1.43	1.52
3	a	1264	GLU	CA-C	-7.45	1.44	1.53
3	a	1327	VAL	CA-CB	-7.44	1.45	1.54
3	a	1109	PHE	N-CA	-7.42	1.37	1.46
3	a	1233	LEU	CA-C	-7.42	1.43	1.52
3	a	1052	VAL	CA-C	-7.42	1.42	1.52
3	a	1242	PRO	CA-C	-7.41	1.43	1.52
1	b	269	MET	CA-C	-7.40	1.43	1.52
1	b	48	ARG	CA-C	-7.40	1.42	1.52
3	a	1241	PHE	C-N	-7.39	1.24	1.33
1	b	201	THR	CA-CB	-7.39	1.40	1.53
1	b	62	VAL	C-N	-7.38	1.24	1.33
3	a	1335	THR	CA-C	-7.38	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	54	ASN	CA-C	-7.37	1.43	1.52
1	b	328	VAL	CA-C	-7.37	1.43	1.52
3	a	1274	ASN	CA-C	-7.37	1.43	1.53
1	b	219	LEU	CA-C	-7.36	1.43	1.52
3	a	1162	ILE	CA-C	-7.35	1.42	1.52
3	a	1257	HIS	CB-CG	-7.34	1.39	1.50
1	b	345	GLU	CA-C	-7.31	1.42	1.52
1	b	268	PHE	CA-C	-7.29	1.42	1.53
3	a	1024	TYR	CA-C	-7.29	1.43	1.52
1	b	267	PHE	CA-C	-7.29	1.44	1.52
1	b	352	LYS	CA-C	-7.28	1.43	1.53
3	a	1049	ILE	CA-C	-7.28	1.42	1.52
3	a	1063	PRO	CA-C	-7.23	1.42	1.52
3	a	1057	TYR	CA-C	-7.22	1.43	1.52
3	a	1289	CYS	CA-C	-7.20	1.43	1.52
1	b	101	ASN	CA-C	-7.20	1.43	1.52
3	a	1269	CYS	CA-C	-7.20	1.42	1.52
1	b	28	HIS	CA-C	-7.19	1.44	1.53
1	b	67	LEU	CA-C	-7.18	1.43	1.53
1	b	86	ILE	N-CA	-7.18	1.37	1.46
3	a	1325	PHE	CA-C	-7.15	1.45	1.53
1	b	197	ASN	CA-C	-7.15	1.43	1.53
3	a	1090	ASP	CA-C	-7.14	1.43	1.52
3	a	1052	VAL	CA-CB	-7.13	1.45	1.54
1	b	265	LEU	CA-C	-7.11	1.43	1.52
3	a	1297	VAL	CA-CB	-7.11	1.45	1.54
3	a	1173	ASP	CA-C	-7.09	1.44	1.52
3	a	1212	ILE	CA-CB	-7.09	1.44	1.54
1	b	218	LYS	CA-C	-7.08	1.44	1.52
3	a	1054	THR	CA-C	-7.07	1.45	1.52
3	a	1390	GLY	CA-C	-7.05	1.42	1.51
1	b	335	VAL	CA-CB	-7.04	1.46	1.54
1	b	172	VAL	CA-CB	-7.03	1.45	1.54
1	b	253	ARG	N-CA	-7.03	1.38	1.46
3	a	1060	LEU	N-CA	-7.03	1.37	1.46
1	b	28	HIS	N-CA	-7.01	1.40	1.46
3	a	1114	SER	CA-C	-7.00	1.44	1.52
1	b	231	VAL	CA-CB	-6.97	1.46	1.54
3	a	1383	VAL	CA-C	-6.95	1.44	1.52
1	b	274	PRO	CA-C	-6.93	1.45	1.53
1	b	47	GLU	CA-C	-6.92	1.43	1.52
1	b	64	ARG	N-CA	-6.92	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	344	VAL	CA-CB	-6.92	1.47	1.54
3	a	1098	LYS	CA-C	-6.91	1.43	1.52
3	a	1327	VAL	CA-C	-6.90	1.44	1.52
1	b	262	PHE	C-N	-6.89	1.28	1.33
1	b	300	ASN	CA-C	-6.88	1.43	1.52
3	a	1165	THR	CA-C	-6.88	1.44	1.52
1	b	387	LEU	CA-C	-6.85	1.43	1.52
1	b	429	VAL	CA-C	-6.84	1.44	1.52
3	a	1346	GLN	CA-C	-6.83	1.43	1.52
1	b	420	GLU	CA-C	-6.82	1.43	1.52
1	b	86	ILE	CA-CB	-6.82	1.46	1.54
1	b	30	ILE	CA-CB	-6.79	1.46	1.54
1	b	157	ILE	CA-CB	-6.79	1.46	1.54
1	b	198	THR	CA-C	-6.79	1.44	1.52
1	b	286	LEU	CA-C	-6.79	1.43	1.52
3	a	1145	ILE	CA-C	-6.79	1.44	1.52
3	a	1075	ASN	CA-C	-6.77	1.43	1.52
1	b	270	PRO	CA-C	-6.77	1.43	1.52
1	b	24	ILE	CA-CB	-6.76	1.45	1.54
1	b	140	SER	CA-C	-6.76	1.44	1.52
1	b	113	GLU	CA-C	-6.75	1.44	1.52
1	b	376	THR	CA-C	-6.75	1.44	1.52
3	a	1066	LEU	CA-C	-6.74	1.43	1.53
3	a	1050	ASP	CA-C	-6.72	1.44	1.52
3	a	1092	VAL	CA-CB	-6.72	1.47	1.54
1	b	416	MET	CA-C	-6.71	1.43	1.52
3	a	1070	LYS	CA-C	-6.71	1.43	1.52
1	b	353	THR	CA-C	-6.71	1.44	1.52
3	a	1060	LEU	CA-C	-6.70	1.43	1.52
1	b	14	ASN	N-CA	-6.69	1.38	1.46
1	b	291	LEU	CA-C	-6.68	1.44	1.52
1	b	177	VAL	CA-C	-6.67	1.44	1.52
1	b	185	TYR	CA-C	-6.67	1.44	1.52
1	b	292	THR	CA-C	-6.66	1.43	1.52
3	a	1349	VAL	CA-C	-6.64	1.44	1.52
1	b	436	GLN	CA-C	-6.64	1.46	1.53
3	a	1184	TYR	CA-C	-6.63	1.44	1.52
1	b	229	HIS	C-N	-6.63	1.25	1.33
3	a	1329	ILE	CA-C	-6.62	1.44	1.52
1	b	204	ILE	CA-CB	-6.62	1.45	1.53
3	a	1074	ALA	CA-C	-6.62	1.44	1.52
1	b	207	GLU	CA-C	-6.62	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	1068	THR	CA-C	-6.61	1.44	1.52
3	a	1302	VAL	CA-CB	-6.61	1.46	1.54
3	a	1250	ILE	CA-CB	-6.60	1.45	1.54
1	b	63	PRO	C-N	-6.60	1.24	1.33
1	b	208	ALA	CA-C	-6.58	1.43	1.52
3	a	1089	ILE	CA-C	-6.58	1.44	1.52
1	b	240	THR	CA-C	-6.58	1.44	1.52
3	a	1164	THR	CA-C	-6.58	1.43	1.52
3	a	1297	VAL	N-CA	-6.57	1.38	1.46
1	b	83	PHE	CA-C	-6.57	1.44	1.53
1	b	181	VAL	N-CA	-6.55	1.38	1.46
3	a	1156	VAL	CA-CB	-6.55	1.45	1.54
3	a	1352	LEU	CA-C	-6.54	1.44	1.52
1	b	68	VAL	CA-C	-6.54	1.44	1.52
1	b	115	VAL	CA-C	-6.54	1.44	1.52
3	a	1254	LYS	CA-C	-6.54	1.44	1.53
1	b	247	GLN	CA-C	-6.53	1.44	1.52
1	b	379	GLY	CA-C	-6.53	1.47	1.52
3	a	1324	GLY	CA-C	-6.52	1.42	1.51
3	a	1171	HIS	CA-C	-6.51	1.44	1.52
1	b	277	SER	CA-C	-6.51	1.44	1.52
1	b	300	ASN	N-CA	-6.51	1.38	1.46
1	b	131	CYS	N-CA	-6.50	1.38	1.46
1	b	86	ILE	CA-C	-6.49	1.44	1.52
1	b	169	PHE	CA-C	-6.49	1.44	1.53
1	b	295	MET	CA-C	-6.49	1.44	1.52
3	a	1007	ILE	CA-CB	-6.49	1.45	1.53
3	a	1178	VAL	CA-C	-6.48	1.45	1.52
3	a	1241	PHE	CA-C	-6.47	1.45	1.53
1	b	234	THR	CA-CB	-6.46	1.43	1.53
3	a	1375	LYS	CA-C	-6.46	1.44	1.52
1	b	63	PRO	CA-CB	-6.46	1.44	1.53
3	a	1151	VAL	CA-CB	-6.45	1.47	1.54
3	a	1328	GLY	CA-C	-6.45	1.42	1.51
1	b	259	MET	CA-C	-6.45	1.43	1.52
1	b	417	GLU	CA-C	-6.43	1.44	1.52
1	b	196	GLU	CA-C	-6.43	1.44	1.52
1	b	374	SER	CA-C	-6.42	1.44	1.52
1	b	237	GLY	CA-C	-6.42	1.45	1.52
3	a	1119	THR	CA-C	-6.42	1.44	1.52
1	b	256	ALA	N-CA	-6.41	1.38	1.46
3	a	1058	ARG	CA-C	-6.40	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	1045	GLU	C-N	-6.38	1.25	1.33
3	a	1301	ASP	CA-C	-6.37	1.44	1.52
3	a	1208	ILE	CA-CB	-6.36	1.46	1.54
1	b	287	THR	CA-C	-6.35	1.43	1.52
1	b	148	GLY	CA-C	-6.35	1.43	1.51
1	b	184	PRO	C-N	-6.34	1.25	1.33
1	b	71	GLU	C-N	-6.33	1.24	1.33
1	b	347	ILE	CA-C	-6.33	1.47	1.52
1	b	200	GLU	CA-C	-6.32	1.45	1.52
1	b	318	VAL	CA-CB	-6.32	1.44	1.53
1	b	239	THR	CA-CB	-6.32	1.42	1.53
1	b	50	ASN	CA-CB	-6.31	1.42	1.53
3	a	1042	VAL	CA-C	-6.31	1.45	1.52
3	a	1189	ARG	CA-C	-6.31	1.44	1.52
3	a	1333	PRO	CA-C	-6.30	1.46	1.52
1	b	152	LEU	CA-C	-6.30	1.44	1.52
3	a	1261	SER	CA-C	-6.30	1.45	1.52
1	b	171	VAL	CA-C	-6.29	1.44	1.52
3	a	1028	HIS	CA-C	-6.29	1.43	1.52
1	b	199	ASP	CA-C	-6.29	1.44	1.52
3	a	1381	TRP	CA-C	-6.29	1.44	1.52
1	b	256	ALA	CA-C	-6.28	1.45	1.52
3	a	1191	LEU	CA-C	-6.27	1.44	1.52
1	b	243	ARG	CA-C	-6.26	1.42	1.52
1	b	377	PHE	CA-C	-6.25	1.45	1.52
1	b	165	ILE	CA-CB	-6.24	1.46	1.54
1	b	88	ARG	CA-C	-6.24	1.46	1.52
1	b	261	PRO	CA-C	-6.23	1.43	1.52
1	b	21	TRP	CA-C	-6.23	1.44	1.52
3	a	1093	LEU	CA-C	-6.23	1.44	1.52
1	b	79	ARG	CA-C	-6.21	1.44	1.52
1	b	121	VAL	CA-C	-6.21	1.44	1.52
3	a	1207	GLN	N-CA	-6.20	1.38	1.46
3	a	1304	ALA	CA-C	-6.19	1.44	1.52
1	b	404	PHE	CA-C	-6.19	1.43	1.52
3	a	1145	ILE	CA-CB	-6.19	1.46	1.54
3	a	1180	ASN	CA-C	-6.19	1.44	1.52
1	b	166	MET	CA-C	-6.18	1.46	1.53
3	a	1251	SER	CA-C	-6.17	1.44	1.52
3	a	1248	PRO	CA-C	-6.17	1.47	1.53
3	a	1379	VAL	CA-CB	-6.17	1.46	1.54
3	a	1226	LEU	CA-C	-6.14	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	1067	ILE	CA-C	-6.14	1.44	1.52
1	b	388	PHE	CA-C	-6.13	1.44	1.52
1	b	68	VAL	CA-CB	-6.13	1.47	1.54
3	a	1022	GLU	N-CA	-6.12	1.39	1.46
3	a	1248	PRO	N-CD	-6.12	1.39	1.47
3	a	1379	VAL	CA-C	-6.12	1.44	1.52
3	a	1372	MET	N-CA	-6.12	1.39	1.46
3	a	1262	VAL	CA-CB	-6.11	1.46	1.54
1	b	282	GLN	N-CA	-6.09	1.39	1.46
1	b	288	VAL	C-N	-6.09	1.26	1.33
3	a	1280	ASP	C-N	-6.08	1.28	1.33
3	a	1133	VAL	CA-C	-6.07	1.46	1.52
1	b	395	PHE	N-CA	-6.05	1.38	1.46
3	a	1207	GLN	CA-C	-6.03	1.45	1.53
1	b	429	VAL	CA-CB	-6.03	1.46	1.54
1	b	288	VAL	N-CA	-6.03	1.39	1.46
3	a	1155	VAL	N-CA	-6.03	1.40	1.46
1	b	51	VAL	CA-CB	-6.02	1.46	1.54
3	a	1133	VAL	CA-CB	-6.02	1.47	1.54
1	b	329	ASP	CA-C	-6.01	1.44	1.52
1	b	62	VAL	CA-C	-6.00	1.46	1.52
1	b	333	LEU	N-CA	-5.99	1.39	1.46
3	a	1096	ILE	CA-C	-5.98	1.45	1.52
1	b	146	GLY	CA-C	-5.97	1.43	1.51
3	a	1266	THR	CA-C	-5.96	1.44	1.52
3	a	1298	VAL	N-CA	-5.96	1.40	1.46
3	a	1011	GLN	CA-C	-5.95	1.44	1.52
1	b	375	ALA	CA-C	-5.94	1.44	1.52
3	a	1187	CYS	CA-C	-5.94	1.44	1.52
1	b	213	CYS	C-N	-5.94	1.25	1.33
1	b	274	PRO	CA-CB	-5.93	1.47	1.53
3	a	1212	ILE	N-CA	-5.93	1.39	1.46
3	a	1007	ILE	CA-C	-5.92	1.45	1.52
3	a	1240	HIS	CA-C	-5.92	1.45	1.53
3	a	1303	ASN	N-CA	-5.91	1.38	1.46
1	b	339	ASN	CA-C	-5.91	1.45	1.53
3	a	1018	ASN	N-CA	-5.90	1.39	1.46
3	a	1276	MET	CA-C	-5.89	1.45	1.52
3	a	1084	ILE	CA-CB	-5.89	1.46	1.54
3	a	1088	ILE	CA-CB	-5.88	1.46	1.54
1	b	221	THR	CA-C	-5.88	1.46	1.52
1	b	335	VAL	CA-C	-5.88	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	330	GLU	N-CA	-5.88	1.39	1.46
1	b	378	ILE	CA-C	-5.87	1.45	1.52
1	b	171	VAL	CA-CB	-5.86	1.46	1.54
1	b	315	VAL	CA-CB	-5.86	1.46	1.55
1	b	49	ILE	N-CA	-5.86	1.39	1.46
3	a	1235	PRO	CA-C	-5.85	1.44	1.52
1	b	314	THR	CA-C	-5.85	1.45	1.52
3	a	1030	ILE	CA-C	-5.84	1.46	1.52
1	b	25	SER	CA-C	-5.84	1.45	1.52
3	a	1062	HIS	CB-CG	5.83	1.58	1.50
3	a	1061	PHE	CA-C	-5.81	1.45	1.52
1	b	270	PRO	CA-CB	-5.81	1.45	1.53
1	b	24	ILE	CA-C	-5.81	1.45	1.52
1	b	179	ASP	CA-C	-5.81	1.45	1.52
1	b	37	HIS	CA-C	-5.80	1.45	1.53
3	a	1265	ILE	CA-CB	-5.80	1.46	1.54
1	b	230	LEU	N-CA	-5.80	1.39	1.46
1	b	132	LEU	N-CA	-5.80	1.39	1.46
1	b	324	SER	CA-C	-5.80	1.45	1.52
1	b	132	LEU	CA-C	-5.79	1.45	1.52
3	a	1243	LEU	CA-C	-5.78	1.45	1.52
3	a	1398	ASP	CA-C	-5.78	1.45	1.52
1	b	213	CYS	CA-C	-5.78	1.45	1.52
1	b	355	VAL	CA-CB	-5.76	1.46	1.54
1	b	249	ASN	CA-C	-5.76	1.45	1.52
1	b	191	VAL	CA-CB	-5.75	1.47	1.54
1	b	104	ALA	CA-C	-5.75	1.45	1.52
1	b	139	HIS	CA-C	-5.75	1.45	1.52
3	a	1302	VAL	N-CA	-5.75	1.39	1.46
1	b	384	ILE	CA-CB	-5.73	1.46	1.54
3	a	1129	GLU	CA-C	-5.73	1.45	1.52
3	a	1368	LYS	CA-C	-5.73	1.45	1.52
1	b	252	LEU	CA-C	-5.73	1.45	1.52
1	b	194	LEU	CA-C	-5.72	1.45	1.52
1	b	50	ASN	N-CA	-5.71	1.38	1.46
1	b	403	ALA	C-N	-5.71	1.27	1.33
3	a	1249	VAL	CA-CB	-5.70	1.47	1.53
3	a	1021	TRP	NE1-CE2	-5.70	1.31	1.37
1	b	168	THR	CA-CB	-5.70	1.43	1.53
3	a	1131	LEU	CA-C	-5.69	1.45	1.52
1	b	121	VAL	N-CA	-5.69	1.39	1.46
3	a	1331	TYR	N-CA	-5.69	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	432	TYR	CA-C	-5.68	1.44	1.52
1	b	315	VAL	CA-C	-5.68	1.45	1.52
1	b	118	VAL	CA-CB	-5.67	1.46	1.54
3	a	1071	GLU	CA-C	-5.67	1.45	1.52
3	a	1155	VAL	CA-C	-5.67	1.45	1.52
1	b	356	CYS	CA-C	-5.67	1.45	1.53
3	a	1222	LEU	CA-C	-5.66	1.45	1.52
1	b	326	LYS	CA-C	-5.66	1.45	1.53
3	a	1112	PHE	CA-C	-5.66	1.46	1.52
1	b	125	GLU	CA-C	-5.65	1.45	1.52
3	a	1052	VAL	N-CA	-5.65	1.39	1.46
1	b	57	ALA	CA-C	-5.64	1.45	1.52
1	b	425	MET	N-CA	-5.64	1.39	1.46
1	b	243	ARG	N-CA	-5.64	1.40	1.46
1	b	405	LEU	C-N	-5.64	1.26	1.33
1	b	194	LEU	N-CA	-5.63	1.39	1.46
1	b	328	VAL	CA-CB	-5.63	1.46	1.54
3	a	1086	LYS	CA-C	-5.63	1.45	1.52
3	a	1022	GLU	CA-C	-5.62	1.45	1.52
1	b	116	ASP	CA-C	-5.61	1.45	1.52
1	b	133	GLN	N-CA	-5.59	1.39	1.46
1	b	178	SER	CA-C	-5.59	1.45	1.53
1	b	138	THR	CA-CB	-5.57	1.44	1.53
3	a	1154	ALA	C-N	-5.57	1.27	1.33
1	b	30	ILE	CA-C	-5.55	1.46	1.52
1	b	434	GLN	CA-C	-5.54	1.44	1.52
1	b	97	SER	CA-C	-5.53	1.45	1.53
3	a	1172	SER	CA-C	-5.53	1.45	1.52
1	b	8	GLN	CA-CB	-5.52	1.45	1.52
1	b	136	GLN	CA-CB	-5.52	1.45	1.53
3	a	1188	ARG	N-CA	-5.51	1.39	1.46
1	b	126	SER	CA-C	-5.50	1.45	1.52
3	a	1125	SER	CA-C	-5.49	1.45	1.52
3	a	1142	GLU	CA-CB	-5.49	1.45	1.53
3	a	1306	ILE	CA-CB	-5.49	1.46	1.54
3	a	1163	LEU	CA-C	-5.49	1.45	1.52
3	a	1183	ILE	CA-CB	-5.49	1.46	1.54
3	a	1347	ARG	CA-C	-5.49	1.45	1.52
1	b	90	ASP	CA-C	-5.48	1.45	1.52
3	a	1122	GLY	CA-C	-5.48	1.44	1.51
1	b	244	PHE	CA-CB	-5.47	1.45	1.54
1	b	292	THR	CA-CB	-5.47	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	170	SER	CA-C	-5.47	1.46	1.52
3	a	1318	VAL	CA-CB	-5.47	1.48	1.54
3	a	1378	PHE	CA-C	-5.47	1.43	1.52
1	b	85	GLN	C-N	-5.47	1.28	1.34
1	b	202	TYR	CA-C	-5.47	1.46	1.53
1	b	349	ASN	CA-C	-5.46	1.45	1.52
3	a	1301	ASP	N-CA	-5.46	1.39	1.46
3	a	1008	HIS	CA-CB	-5.45	1.46	1.53
1	b	26	ASP	N-CA	-5.45	1.39	1.46
1	b	37	HIS	CB-CG	-5.45	1.42	1.50
3	a	1252	ALA	CA-C	-5.45	1.45	1.52
1	b	23	VAL	CA-CB	-5.43	1.47	1.54
3	a	1135	TYR	CA-C	-5.42	1.45	1.52
1	b	19	LYS	CA-C	-5.39	1.45	1.52
3	a	1331	TYR	CA-C	-5.39	1.45	1.52
3	a	1248	PRO	CA-CB	-5.38	1.47	1.53
3	a	1305	ALA	N-CA	-5.38	1.39	1.46
3	a	1178	VAL	CA-CB	-5.37	1.46	1.54
3	a	1020	CYS	N-CA	-5.37	1.39	1.46
3	a	1255	ALA	N-CA	-5.36	1.39	1.46
3	a	1185	ASP	CA-C	-5.35	1.45	1.52
1	b	5	VAL	CA-CB	-5.34	1.46	1.54
3	a	1015	GLN	CA-C	-5.33	1.45	1.52
1	b	144	GLY	CA-C	-5.33	1.44	1.51
1	b	417	GLU	N-CA	-5.33	1.40	1.46
3	a	1353	SER	CA-C	-5.33	1.46	1.52
1	b	77	SER	CA-C	-5.32	1.45	1.52
3	a	1076	ASN	N-CA	-5.32	1.39	1.46
1	b	249	ASN	N-CA	-5.32	1.39	1.46
1	b	354	ALA	CA-C	-5.32	1.46	1.52
3	a	1049	ILE	CA-CB	-5.30	1.47	1.54
3	a	1394	GLU	CA-C	-5.30	1.45	1.52
1	b	71	GLU	CA-C	-5.29	1.44	1.52
1	b	348	PRO	CA-C	-5.29	1.44	1.52
3	a	1211	SER	CA-C	-5.29	1.45	1.52
3	a	1403	GLU	N-CA	-5.29	1.39	1.46
3	a	1128	MET	CA-C	-5.28	1.45	1.52
1	b	135	PHE	CA-C	-5.28	1.46	1.52
3	a	1337	VAL	CA-C	-5.28	1.46	1.52
1	b	93	VAL	CA-CB	-5.26	1.46	1.53
3	a	1396	ARG	CA-C	-5.26	1.46	1.52
1	b	106	GLY	CA-C	-5.26	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	425	MET	CA-C	-5.26	1.45	1.52
1	b	43	GLN	CA-C	-5.25	1.45	1.52
3	a	1038	ARG	CA-C	-5.25	1.45	1.53
1	b	44	LEU	N-CA	-5.25	1.39	1.46
1	b	193	GLN	CA-C	-5.25	1.45	1.52
1	b	351	VAL	CA-CB	-5.25	1.48	1.54
3	a	1054	THR	CA-CB	-5.24	1.45	1.54
3	a	1009	VAL	CA-C	-5.24	1.46	1.52
1	b	137	LEU	N-CA	-5.23	1.40	1.46
3	a	1134	ASP	CA-C	-5.21	1.45	1.52
1	b	182	VAL	CA-CB	-5.21	1.47	1.54
1	b	288	VAL	CA-CB	-5.21	1.47	1.54
1	b	181	VAL	CA-CB	-5.20	1.48	1.54
1	b	215	ARG	CA-C	-5.20	1.45	1.52
1	b	274	PRO	N-CD	-5.19	1.40	1.47
1	b	347	ILE	CA-CB	-5.19	1.48	1.54
1	b	435	TYR	N-CA	-5.19	1.40	1.46
3	a	1002	ARG	CD-NE	5.18	1.53	1.46
3	a	1226	LEU	N-CA	-5.18	1.40	1.46
1	b	53	TYR	CA-C	-5.18	1.46	1.53
1	b	266	HIS	N-CA	-5.18	1.39	1.46
1	b	78	VAL	CA-C	-5.17	1.44	1.52
1	b	350	ASN	CA-C	-5.17	1.46	1.52
1	b	358	ILE	CA-CB	-5.17	1.47	1.54
3	a	1042	VAL	N-CA	-5.17	1.40	1.46
3	a	1154	ALA	N-CA	-5.17	1.40	1.46
3	a	1167	THR	CA-C	-5.17	1.45	1.52
1	b	402	LYS	CA-C	-5.16	1.44	1.52
3	a	1158	PRO	N-CA	-5.16	1.40	1.47
3	a	1265	ILE	N-CA	-5.16	1.40	1.46
3	a	1350	CYS	CA-C	-5.16	1.46	1.53
1	b	187	ALA	CA-C	-5.15	1.47	1.53
1	b	17	GLY	N-CA	-5.15	1.39	1.45
1	b	20	PHE	CA-C	-5.15	1.45	1.52
1	b	101	ASN	C-N	-5.15	1.26	1.33
1	b	172	VAL	C-N	-5.14	1.29	1.33
1	b	253	ARG	CA-CB	-5.14	1.45	1.53
1	b	387	LEU	N-CA	-5.14	1.39	1.46
1	b	418	PHE	CA-C	-5.13	1.46	1.52
1	b	287	THR	N-CA	-5.13	1.40	1.46
1	b	290	GLU	CA-C	-5.13	1.45	1.52
3	a	1323	THR	CA-C	-5.12	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	185	TYR	N-CA	-5.12	1.40	1.46
1	b	244	PHE	C-N	-5.12	1.26	1.33
3	a	1035	HIS	CB-CG	5.11	1.57	1.50
3	a	1016	ILE	CA-C	-5.11	1.46	1.52
3	a	1106	LEU	CA-C	-5.11	1.46	1.53
1	b	119	LEU	CA-C	-5.10	1.46	1.52
1	b	216	THR	CA-CB	-5.10	1.45	1.53
3	a	1337	VAL	C-N	-5.09	1.27	1.34
1	b	214	PHE	N-CA	-5.08	1.39	1.45
3	a	1102	GLN	N-CA	-5.07	1.40	1.46
1	b	151	THR	CA-C	-5.06	1.45	1.52
1	b	391	ILE	CA-CB	-5.06	1.47	1.54
3	a	1158	PRO	C-N	-5.05	1.27	1.33
3	a	1235	PRO	N-CA	-5.05	1.40	1.47
1	b	150	GLY	CA-C	-5.04	1.45	1.51
1	b	211	ASP	CA-C	-5.04	1.46	1.52
3	a	1067	ILE	N-CA	-5.04	1.40	1.46
1	b	131	CYS	CA-C	-5.03	1.46	1.52
3	a	1108	GLY	CA-C	-5.03	1.47	1.52
3	a	1371	LEU	CA-C	-5.03	1.45	1.52
3	a	1005	ILE	CA-CB	-5.02	1.47	1.54
1	b	89	PRO	C-N	-5.02	1.27	1.34
1	b	263	PRO	CA-C	-5.02	1.47	1.52
3	a	1250	ILE	N-CA	-5.01	1.40	1.46
3	a	1296	ASP	CA-C	-5.01	1.46	1.52
1	b	63	PRO	N-CA	-5.01	1.41	1.47
3	a	1079	ARG	CA-C	-5.01	1.46	1.52
3	a	1159	TYR	CA-C	-5.01	1.46	1.52
3	a	1143	PHE	CA-C	-5.01	1.46	1.52
3	a	1071	GLU	N-CA	-5.00	1.40	1.45
1	b	399	PHE	CA-C	-5.00	1.46	1.52

All (382) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	37	HIS	CA-CB-CG	-14.50	99.30	113.80
1	b	343	PHE	CA-CB-CG	-14.30	99.50	113.80
2	M	3193	ASN	CA-CB-CG	-13.94	98.67	112.60
3	a	1200	ASN	CA-CB-CG	-13.70	98.90	112.60
3	a	1112	PHE	CA-CB-CG	-12.43	101.37	113.80
1	b	226	ASP	CA-CB-CG	-12.33	100.27	112.60
1	b	197	ASN	CA-CB-CG	-11.96	100.64	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	1343	ALA	N-CA-C	11.80	127.18	113.02
1	b	49	ILE	CA-C-N	11.06	142.67	121.54
1	b	49	ILE	C-N-CA	11.06	142.67	121.54
3	a	1176	PHE	CA-CB-CG	-11.02	102.78	113.80
3	a	1229	PHE	CA-CB-CG	-10.74	103.06	113.80
2	M	3109	GLN	N-CA-C	10.51	123.72	111.11
1	b	337	ASN	CA-CB-CG	-10.40	102.19	112.60
3	a	1270	PHE	CA-CB-CG	-10.28	103.52	113.80
1	b	296	PHE	CA-CB-CG	-10.19	103.61	113.80
1	b	249	ASN	CA-CB-CG	-10.08	102.52	112.60
3	a	1041	PHE	CA-CB-CG	-10.01	103.79	113.80
1	b	214	PHE	N-CA-CB	-9.99	95.97	110.65
1	b	309	HIS	CA-CB-CG	-9.95	103.85	113.80
3	a	1257	HIS	CA-CB-CG	-9.83	103.97	113.80
1	b	169	PHE	CA-CB-CG	-9.72	104.08	113.80
1	b	87	PHE	CA-CB-CG	-9.57	104.22	113.80
3	a	1412	ASP	CA-CB-CG	9.48	122.08	112.60
3	a	1241	PHE	CA-CB-CG	-9.44	104.36	113.80
1	b	244	PHE	CA-CB-CG	-9.43	104.38	113.80
3	a	1090	ASP	CA-CB-CG	-9.39	103.21	112.60
3	a	1247	ALA	O-C-N	-9.29	110.64	121.32
1	b	262	PHE	CA-CB-CG	-9.28	104.53	113.80
3	a	1031	GLN	O-C-N	-9.22	110.72	121.32
1	b	130	ASP	CA-CB-CG	9.20	121.80	112.60
1	b	240	THR	N-CA-CB	9.19	126.02	110.49
3	a	1330	ASN	CA-CB-CG	-9.08	103.52	112.60
3	a	1303	ASN	CA-CB-CG	-9.05	103.55	112.60
1	b	14	ASN	CA-CB-CG	-8.94	103.67	112.60
3	a	1146	TYR	CB-CA-C	8.85	122.44	108.91
1	b	50	ASN	CA-CB-CG	-8.84	103.76	112.60
1	b	334	ASN	CA-CB-CG	-8.80	103.80	112.60
3	a	1195	ARG	O-C-N	-8.79	111.22	121.32
1	b	167	ASN	CA-CB-CG	-8.76	103.84	112.60
1	b	51	VAL	N-CA-C	8.74	127.53	109.34
1	b	8	GLN	N-CA-C	8.74	122.72	109.62
3	a	1370	ASP	CA-CB-CG	-8.71	103.89	112.60
3	a	1228	GLU	CB-CG-CD	8.70	127.38	112.60
3	a	1317	PHE	CA-CB-CG	-8.67	105.13	113.80
3	a	1155	VAL	N-CA-C	-8.62	104.77	113.47
1	b	326	LYS	N-CA-C	-8.61	99.64	112.04
3	a	1367	HIS	CA-CB-CG	-8.58	105.22	113.80
3	a	1012	ALA	N-CA-C	8.58	120.32	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	317	ALA	N-CA-C	8.50	122.84	108.23
3	a	1341	ASP	CA-CB-CG	-8.49	104.11	112.60
3	a	1143	PHE	CA-CB-CG	-8.47	105.33	113.80
1	b	273	ALA	O-C-N	-8.43	111.62	121.32
1	b	135	PHE	CA-CB-CG	-8.38	105.42	113.80
1	b	300	ASN	CA-CB-CG	-8.37	104.23	112.60
1	b	406	HIS	CA-CB-CG	-8.27	105.53	113.80
1	b	77	SER	N-CA-C	-8.12	103.89	113.88
2	M	3179	GLN	CA-C-N	8.12	133.61	120.30
2	M	3179	GLN	C-N-CA	8.12	133.61	120.30
3	a	1402	LEU	N-CA-C	-8.10	103.61	113.97
3	a	1219	ASP	CA-CB-CG	-8.07	104.53	112.60
1	b	252	LEU	N-CA-C	8.02	127.88	110.80
1	b	399	PHE	CA-CB-CG	-8.00	105.81	113.80
1	b	6	HIS	N-CA-CB	-7.98	98.31	110.04
3	a	1366	ASP	CA-CB-CG	7.89	120.49	112.60
3	a	1057	TYR	N-CA-CB	7.86	123.78	110.49
1	b	426	ASN	CA-CB-CG	-7.82	104.78	112.60
2	M	3106	LEU	N-CA-C	-7.81	103.88	113.41
3	a	1199	THR	N-CA-C	7.81	122.25	112.87
1	b	318	VAL	N-CA-C	7.81	117.88	106.55
3	a	1256	TYR	CA-CB-CG	-7.80	99.85	113.90
1	b	6	HIS	N-CA-C	7.79	120.94	110.35
3	a	1247	ALA	N-CA-C	7.78	127.01	109.81
3	a	1398	ASP	CA-CB-CG	-7.78	104.82	112.60
3	a	1061	PHE	CA-CB-CG	-7.75	106.05	113.80
3	a	1274	ASN	CA-CB-CG	-7.75	104.85	112.60
3	a	1392	PHE	CA-CB-CG	-7.74	106.06	113.80
3	a	1053	ARG	N-CA-C	-7.68	103.91	113.28
3	a	1050	ASP	CA-CB-CG	-7.65	104.95	112.60
3	a	1016	ILE	CB-CA-C	-7.63	101.84	112.14
3	a	1032	PRO	CA-C-N	7.62	136.10	121.54
3	a	1032	PRO	C-N-CA	7.62	136.10	121.54
3	a	1349	VAL	CB-CA-C	-7.62	101.67	110.73
3	a	1257	HIS	N-CA-C	-7.59	102.58	113.21
1	b	9	ALA	N-CA-C	7.58	121.33	109.96
3	a	1185	ASP	CA-CB-CG	-7.58	105.02	112.60
3	a	1142	GLU	N-CA-C	7.47	121.10	109.07
3	a	1259	GLN	N-CA-C	-7.37	95.10	110.80
1	b	76	ASP	CA-CB-CG	-7.35	105.25	112.60
3	a	1134	ASP	CA-CB-CG	-7.33	105.27	112.60
3	a	1198	TYR	O-C-N	-7.26	114.42	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	1010	GLY	N-CA-C	7.22	120.38	112.29
3	a	1070	LYS	N-CA-C	-7.15	104.18	114.12
1	b	133	GLN	N-CA-C	7.14	118.96	111.03
3	a	1036	VAL	N-CA-CB	-7.14	101.21	111.21
1	b	200	GLU	CB-CA-C	-7.12	100.37	110.34
3	a	1328	GLY	CA-C-N	-7.11	113.88	123.12
3	a	1328	GLY	C-N-CA	-7.11	113.88	123.12
1	b	136	GLN	CB-CG-CD	-7.10	100.53	112.60
3	a	1097	ARG	N-CA-C	-7.05	105.22	114.31
3	a	1036	VAL	CA-C-N	7.03	127.98	120.11
3	a	1036	VAL	C-N-CA	7.03	127.98	120.11
1	b	54	ASN	N-CA-C	-7.01	97.99	108.99
3	a	1364	ARG	CB-CA-C	-6.99	96.89	110.46
1	b	432	TYR	CA-CB-CG	-6.98	101.33	113.90
1	b	388	PHE	CA-CB-CG	-6.98	106.82	113.80
3	a	1221	ALA	N-CA-C	6.96	119.72	111.71
1	b	206	ASN	CA-CB-CG	-6.96	105.64	112.60
1	b	405	LEU	N-CA-CB	-6.93	99.62	110.30
1	b	5	VAL	N-CA-C	6.92	119.16	107.18
3	a	1062	HIS	CA-C-N	6.91	128.48	119.84
3	a	1062	HIS	C-N-CA	6.91	128.48	119.84
1	b	283	TYR	CB-CG-CD1	6.91	131.16	120.80
1	b	436	GLN	N-CA-C	-6.90	102.24	111.96
1	b	90	ASP	CA-CB-CG	-6.89	105.70	112.60
1	b	217	LEU	N-CA-C	-6.89	100.28	110.48
3	a	1180	ASN	CA-CB-CG	-6.87	105.73	112.60
1	b	38	GLY	CA-C-N	6.86	129.35	120.44
1	b	38	GLY	C-N-CA	6.86	129.35	120.44
1	b	166	MET	CB-CA-C	-6.84	102.38	111.82
1	b	316	ALA	O-C-N	-6.81	114.42	123.14
1	b	231	VAL	N-CA-CB	6.81	118.07	110.51
3	a	1030	ILE	N-CA-CB	6.81	118.38	110.82
1	b	27	GLU	N-CA-CB	-6.81	100.70	110.57
3	a	1291	LEU	N-CA-C	6.80	119.51	108.63
1	b	203	CYS	N-CA-C	6.79	119.64	109.25
3	a	1031	GLN	CA-C-O	-6.75	110.91	120.16
1	b	236	SER	CA-C-N	6.74	127.46	119.98
1	b	236	SER	C-N-CA	6.74	127.46	119.98
3	a	1062	HIS	CB-CA-C	6.74	116.84	110.17
3	a	1275	GLN	CA-C-O	-6.73	113.36	120.63
1	b	288	VAL	N-CA-CB	6.72	120.62	111.21
3	a	1188	ARG	N-CA-C	-6.72	102.36	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	239	THR	CA-C-O	-6.70	110.92	120.51
1	b	437	ASP	CA-CB-CG	-6.69	105.91	112.60
3	a	1008	HIS	CA-CB-CG	-6.69	107.11	113.80
1	b	283	TYR	CB-CG-CD2	-6.69	110.77	120.80
3	a	1395	ALA	N-CA-C	-6.68	105.17	113.38
3	a	1060	LEU	N-CA-C	6.68	119.39	111.71
3	a	1023	LEU	CA-C-N	6.67	134.29	121.54
3	a	1023	LEU	C-N-CA	6.67	134.29	121.54
3	a	1142	GLU	O-C-N	-6.62	115.47	123.29
3	a	1403	GLU	N-CA-C	-6.61	104.69	112.89
1	b	51	VAL	CA-C-N	6.61	132.29	121.99
1	b	51	VAL	C-N-CA	6.61	132.29	121.99
1	b	418	PHE	CA-CB-CG	-6.59	107.20	113.80
3	a	1217	ARG	NE-CZ-NH2	-6.57	113.29	119.20
1	b	231	VAL	CB-CA-C	-6.56	103.48	111.88
1	b	275	LEU	N-CA-CB	-6.56	99.58	110.47
1	b	319	PHE	CA-CB-CG	-6.56	107.24	113.80
1	b	129	CYS	N-CA-C	6.55	117.23	108.38
3	a	1051	GLU	CB-CG-CD	-6.54	101.48	112.60
2	M	3110	ARG	CA-C-N	6.54	127.24	119.98
2	M	3110	ARG	C-N-CA	6.54	127.24	119.98
3	a	1302	VAL	CB-CA-C	-6.53	103.46	112.02
3	a	1297	VAL	N-CA-C	-6.52	99.75	108.35
3	a	1244	ALA	O-C-N	-6.50	115.78	123.06
3	a	1247	ALA	CA-C-O	-6.45	111.32	120.16
1	b	422	GLU	N-CA-C	6.43	118.86	111.02
1	b	240	THR	CB-CA-C	-6.37	97.74	110.42
1	b	62	VAL	CA-C-N	6.37	126.74	119.93
1	b	62	VAL	C-N-CA	6.37	126.74	119.93
1	b	350	ASN	CA-CB-CG	-6.36	106.24	112.60
3	a	1236	TYR	N-CA-C	-6.36	95.76	109.81
1	b	149	MET	CG-SD-CE	-6.35	86.93	100.90
3	a	1035	HIS	CA-CB-CG	6.34	120.14	113.80
2	M	3164	ILE	CB-CA-C	-6.33	103.75	112.24
1	b	282	GLN	N-CA-C	6.32	117.84	111.07
1	b	318	VAL	N-CA-CB	-6.31	105.94	112.06
3	a	1020	CYS	N-CA-CB	-6.28	100.89	110.12
3	a	1244	ALA	N-CA-C	6.28	120.30	110.32
1	b	191	VAL	N-CA-C	6.27	117.02	110.62
3	a	1269	CYS	CA-CB-SG	-6.27	99.98	114.40
1	b	8	GLN	N-CA-CB	-6.26	102.89	110.53
3	a	1073	ALA	N-CA-C	6.26	117.77	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	1349	VAL	O-C-N	-6.24	116.98	123.03
3	a	1165	THR	N-CA-C	6.23	117.87	111.14
3	a	1044	LEU	N-CA-C	6.23	118.15	111.36
1	b	349	ASN	CA-CB-CG	-6.22	106.38	112.60
3	a	1229	PHE	CB-CA-C	-6.22	98.04	110.42
2	M	3206	CYS	N-CA-C	6.21	117.85	111.14
1	b	318	VAL	O-C-N	-6.18	115.50	122.36
1	b	273	ALA	N-CA-C	6.16	123.43	109.81
1	b	71	GLU	CB-CA-C	-6.15	104.91	110.44
1	b	435	TYR	N-CA-C	-6.15	103.20	111.87
3	a	1208	ILE	CB-CA-C	-6.14	103.99	112.04
1	b	323	MET	N-CA-C	6.14	116.54	107.88
3	a	1373	TYR	CA-CB-CG	-6.14	102.85	113.90
3	a	1402	LEU	CA-C-O	6.12	125.51	118.97
3	a	1276	MET	CG-SD-CE	-6.11	87.46	100.90
3	a	1202	ASN	CA-CB-CG	-6.10	106.50	112.60
1	b	381	SER	N-CA-C	6.10	119.51	110.48
3	a	1209	VAL	N-CA-C	6.10	116.88	110.72
1	b	11	GLN	CB-CG-CD	6.08	122.93	112.60
2	M	3143	ILE	N-CA-C	6.07	116.81	110.62
1	b	5	VAL	CA-C-N	6.06	129.90	120.75
1	b	5	VAL	C-N-CA	6.06	129.90	120.75
3	a	1298	VAL	N-CA-CB	-6.05	105.95	112.37
1	b	2	ARG	NE-CZ-NH2	-6.03	113.78	119.20
1	b	258	ASN	CA-CB-CG	-6.01	106.59	112.60
3	a	1280	ASP	O-C-N	-6.01	115.54	121.19
3	a	1342	LEU	N-CA-C	6.01	118.05	110.24
1	b	47	GLU	CA-C-N	-6.00	112.64	122.54
1	b	47	GLU	C-N-CA	-6.00	112.64	122.54
3	a	1035	HIS	CA-C-N	5.98	133.19	122.13
3	a	1035	HIS	C-N-CA	5.98	133.19	122.13
2	M	3181	ARG	NE-CZ-NH1	5.97	127.47	121.50
1	b	358	ILE	O-C-N	-5.96	114.31	121.10
3	a	1036	VAL	N-CA-C	5.96	121.75	108.88
1	b	133	GLN	CB-CG-CD	-5.95	102.48	112.60
3	a	1142	GLU	CB-CG-CD	-5.93	102.51	112.60
3	a	1330	ASN	N-CA-C	-5.93	101.42	110.14
1	b	153	LEU	N-CA-C	5.93	118.50	111.33
3	a	1025	CYS	N-CA-C	5.92	118.50	111.33
3	a	1286	TYR	CA-CB-CG	-5.92	103.24	113.90
3	a	1019	ALA	CA-C-O	5.89	126.96	120.90
3	a	1319	ASP	N-CA-C	5.87	118.15	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	1082	TYR	CA-C-N	5.83	132.68	121.54
3	a	1082	TYR	C-N-CA	5.83	132.68	121.54
3	a	1296	ASP	CA-CB-CG	-5.82	106.78	112.60
1	b	231	VAL	CA-CB-CG2	-5.81	100.52	110.40
3	a	1161	SER	O-C-N	-5.81	115.45	122.48
1	b	395	PHE	CA-CB-CG	-5.80	108.00	113.80
3	a	1024	TYR	CB-CA-C	5.80	121.96	110.42
1	b	186	ASN	CA-CB-CG	-5.78	106.82	112.60
2	M	3141	CYS	N-CA-CB	5.77	118.61	110.12
1	b	31	ASP	CA-CB-CG	-5.77	106.83	112.60
1	b	152	LEU	N-CA-C	-5.77	104.36	111.40
3	a	1214	ALA	CA-C-N	5.77	128.29	120.38
3	a	1214	ALA	C-N-CA	5.77	128.29	120.38
3	a	1257	HIS	CB-CG-CD2	-5.77	123.70	131.20
1	b	129	CYS	CA-C-N	5.77	134.39	121.76
1	b	129	CYS	C-N-CA	5.77	134.39	121.76
2	M	3167	ILE	N-CA-C	5.77	116.50	110.62
1	b	159	GLU	N-CA-C	-5.75	106.61	113.97
1	b	314	THR	N-CA-C	-5.75	100.33	109.07
3	a	1223	ASN	CA-CB-CG	-5.75	106.85	112.60
1	b	26	ASP	CA-CB-CG	-5.73	106.87	112.60
1	b	242	LEU	N-CA-C	5.72	119.74	112.87
1	b	108	TYR	N-CA-C	-5.70	98.65	110.80
1	b	213	CYS	CA-C-O	5.69	125.63	119.15
1	b	417	GLU	N-CA-C	-5.69	105.08	111.28
1	b	229	HIS	CA-CB-CG	-5.68	108.12	113.80
1	b	315	VAL	CA-C-O	-5.67	115.35	121.19
1	b	264	ARG	NE-CZ-NH1	5.65	127.15	121.50
3	a	1028	HIS	CA-CB-CG	-5.65	108.15	113.80
1	b	260	VAL	N-CA-CB	-5.64	103.31	111.21
3	a	1002	ARG	NE-CZ-NH1	5.64	127.14	121.50
3	a	1092	VAL	N-CA-C	5.64	116.09	110.23
3	a	1063	PRO	N-CA-C	5.63	124.08	112.47
1	b	39	ASP	N-CA-C	5.63	117.09	111.07
3	a	1275	GLN	N-CA-C	5.62	118.14	111.33
3	a	1213	THR	CA-C-N	5.62	132.28	121.54
3	a	1213	THR	C-N-CA	5.62	132.28	121.54
3	a	1229	PHE	N-CA-CB	5.62	119.98	110.49
1	b	229	HIS	N-CA-C	5.61	118.12	111.33
3	a	1008	HIS	N-CA-C	5.60	117.43	108.41
1	b	311	ARG	N-CA-C	-5.59	100.92	109.65
3	a	1166	HIS	CA-CB-CG	-5.58	108.22	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	1042	VAL	CA-C-O	-5.57	114.15	120.67
3	a	1289	CYS	CA-CB-SG	-5.57	101.59	114.40
3	a	1011	GLN	OE1-CD-NE2	-5.56	117.04	122.60
2	M	3128	ASN	CA-CB-CG	-5.54	107.06	112.60
1	b	374	SER	CA-C-O	-5.54	115.25	121.40
3	a	1300	LYS	CA-C-N	5.54	127.97	120.38
3	a	1300	LYS	C-N-CA	5.54	127.97	120.38
1	b	61	TYR	O-C-N	-5.54	116.46	123.05
3	a	1069	GLY	N-CA-C	-5.54	104.13	112.89
1	b	412	GLY	CA-C-O	5.53	124.94	118.96
1	b	251	ASP	N-CA-C	5.53	117.65	109.69
3	a	1098	LYS	N-CA-C	-5.52	105.28	112.23
1	b	349	ASN	N-CA-C	-5.51	100.03	109.24
3	a	1043	ASP	N-CA-CB	5.51	120.00	111.24
3	a	1343	ALA	N-CA-CB	-5.51	102.48	110.47
3	a	1389	GLU	CA-C-O	5.49	126.14	119.49
3	a	1002	ARG	CB-CG-CD	5.49	123.93	111.30
3	a	1295	GLY	O-C-N	-5.48	118.19	122.90
3	a	1349	VAL	N-CA-C	5.47	116.43	107.24
1	b	244	PHE	O-C-N	-5.47	116.20	121.94
1	b	403	ALA	O-C-N	-5.46	115.33	122.59
3	a	1298	VAL	CA-C-O	-5.46	116.13	119.51
1	b	69	ASP	CA-CB-CG	-5.45	107.15	112.60
1	b	408	TYR	N-CA-C	-5.44	103.23	111.56
1	b	8	GLN	O-C-N	-5.44	115.91	122.71
1	b	282	GLN	CB-CG-CD	-5.44	103.36	112.60
3	a	1256	TYR	CA-C-O	5.43	128.27	122.13
1	b	217	LEU	CA-C-N	-5.43	115.16	122.86
1	b	217	LEU	C-N-CA	-5.43	115.16	122.86
2	M	3141	CYS	CB-CA-C	-5.42	101.79	110.79
3	a	1081	HIS	CA-CB-CG	-5.42	108.39	113.80
1	b	265	LEU	N-CA-C	5.41	122.32	110.80
1	b	79	ARG	N-CA-C	-5.41	106.69	113.28
1	b	92	PHE	CA-CB-CG	-5.38	108.42	113.80
1	b	248	LEU	N-CA-C	-5.38	99.33	110.80
2	M	3186	GLU	N-CA-C	5.38	118.63	111.75
3	a	1113	HIS	N-CA-C	-5.36	101.15	109.14
3	a	1034	GLY	O-C-N	-5.35	116.82	122.97
1	b	314	THR	O-C-N	-5.35	117.15	123.25
2	M	3146	TYR	N-CA-C	-5.35	105.98	112.88
3	a	1256	TYR	CA-C-N	5.35	128.33	119.35
3	a	1256	TYR	C-N-CA	5.35	128.33	119.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	92	PHE	N-CA-C	5.34	117.17	108.63
1	b	7	ILE	O-C-N	-5.31	118.19	122.97
3	a	1406	TYR	CA-CB-CG	-5.29	104.37	113.90
3	a	1235	PRO	N-CA-C	-5.29	101.57	112.47
1	b	16	ILE	CB-CA-C	-5.29	105.00	112.14
1	b	62	VAL	O-C-N	-5.29	115.07	121.10
3	a	1107	GLN	N-CA-C	5.28	121.27	114.56
1	b	247	GLN	CB-CA-C	-5.28	100.46	109.65
1	b	214	PHE	N-CA-C	-5.28	106.86	113.72
1	b	109	THR	N-CA-C	5.27	122.03	110.80
1	b	282	GLN	N-CA-CB	-5.27	102.36	110.01
1	b	377	PHE	CA-C-O	-5.27	114.67	120.36
1	b	149	MET	N-CA-C	5.27	117.93	111.82
1	b	102	ASN	N-CA-CB	-5.26	101.91	110.59
1	b	358	ILE	N-CA-C	5.25	120.22	108.88
1	b	48	ARG	CG-CD-NE	-5.24	100.48	112.00
2	M	3213	VAL	N-CA-CB	5.23	116.67	110.55
3	a	1325	PHE	CA-CB-CG	-5.23	108.57	113.80
3	a	1397	GLU	N-CA-C	5.23	117.66	111.33
3	a	1007	ILE	N-CA-C	5.23	115.59	107.28
1	b	60	LYS	CG-CD-CE	5.22	123.32	111.30
1	b	206	ASN	N-CA-C	5.22	121.92	110.80
3	a	1051	GLU	N-CA-C	5.21	117.70	111.71
2	M	3170	TYR	CA-C-N	5.21	129.07	121.31
2	M	3170	TYR	C-N-CA	5.21	129.07	121.31
3	a	1199	THR	O-C-N	-5.21	115.50	122.43
1	b	42	LEU	N-CA-CB	-5.21	101.69	110.49
3	a	1350	CYS	O-C-N	-5.21	116.28	122.63
1	b	160	GLU	CA-C-N	-5.20	117.53	122.37
1	b	160	GLU	C-N-CA	-5.20	117.53	122.37
3	a	1031	GLN	CB-CG-CD	5.20	121.45	112.60
1	b	264	ARG	N-CA-CB	5.20	118.45	110.60
1	b	53	TYR	CA-CB-CG	-5.20	104.54	113.90
3	a	1005	ILE	N-CA-C	5.19	120.14	109.34
3	a	1152	SER	N-CA-C	-5.19	100.84	108.79
3	a	1148	ALA	N-CA-C	5.18	121.27	109.81
1	b	28	HIS	N-CA-C	-5.18	104.65	112.99
1	b	408	TYR	CA-CB-CG	-5.16	104.61	113.90
1	b	264	ARG	CA-C-N	5.16	131.39	121.54
1	b	264	ARG	C-N-CA	5.16	131.39	121.54
3	a	1175	ALA	N-CA-C	5.14	117.09	107.99
3	a	1045	GLU	CA-C-N	5.14	124.59	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	1045	GLU	C-N-CA	5.14	124.59	119.24
3	a	1123	PHE	CA-CB-CG	-5.14	108.66	113.80
3	a	1217	ARG	NE-CZ-NH1	5.14	126.64	121.50
1	b	210	TYR	CA-CB-CG	-5.13	104.67	113.90
1	b	432	TYR	N-CA-C	5.13	119.01	112.34
1	b	429	VAL	CA-CB-CG2	-5.12	101.69	110.40
3	a	1107	GLN	N-CA-CB	-5.11	104.20	111.00
1	b	228	ASN	OD1-CG-ND2	-5.11	117.49	122.60
3	a	1249	VAL	CB-CA-C	-5.11	105.29	111.88
1	b	229	HIS	CB-CA-C	-5.10	102.00	110.68
1	b	243	ARG	CA-CB-CG	-5.10	103.90	114.10
3	a	1346	GLN	CB-CG-CD	-5.10	103.93	112.60
3	a	1361	ALA	O-C-N	-5.10	115.81	122.59
1	b	11	GLN	CA-CB-CG	5.10	124.29	114.10
3	a	1118	GLY	N-CA-C	5.09	118.41	112.50
1	b	315	VAL	O-C-N	-5.09	117.40	123.00
3	a	1326	LYS	CA-C-N	-5.09	115.92	122.99
3	a	1326	LYS	C-N-CA	-5.09	115.92	122.99
1	b	181	VAL	CA-C-N	-5.08	113.34	121.02
1	b	181	VAL	C-N-CA	-5.08	113.34	121.02
1	b	154	ILE	CB-CA-C	-5.08	105.20	112.22
1	b	241	CYS	CA-CB-SG	-5.08	102.72	114.40
1	b	316	ALA	N-CA-C	5.08	117.24	107.44
1	b	180	THR	N-CA-CB	5.07	119.27	111.56
3	a	1319	ASP	CB-CA-C	-5.07	102.70	110.81
1	b	208	ALA	N-CA-C	-5.07	105.94	111.82
3	a	1377	ALA	O-C-N	-5.07	115.85	122.59
1	b	247	GLN	N-CA-C	-5.06	107.16	113.38
1	b	319	PHE	CB-CA-C	-5.04	99.73	109.76
3	a	1107	GLN	O-C-N	-5.04	116.76	122.10
3	a	1207	GLN	N-CA-C	-5.03	103.86	111.56
1	b	320	ARG	N-CA-C	5.03	116.80	107.60
1	b	379	GLY	O-C-N	-5.02	118.25	123.48
3	a	1238	ARG	NE-CZ-NH2	-5.01	114.69	119.20
3	a	1257	HIS	N-CA-CB	-5.01	102.08	110.65
3	a	1304	ALA	N-CA-C	-5.01	100.13	110.80
3	a	1332	GLU	N-CA-C	5.01	120.88	109.81
3	a	1284	GLY	N-CA-C	-5.00	105.72	112.57
1	b	7	ILE	N-CA-C	5.00	115.83	107.18

There are no chirality outliers.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	3110	ARG	Sidechain
2	M	3124	ARG	Sidechain
2	M	3157	PHE	Sidechain
2	M	3183	TYR	Sidechain
2	M	3210	TYR	Sidechain
3	a	1002	ARG	Sidechain
3	a	1024	TYR	Sidechain
3	a	1079	ARG	Sidechain
3	a	1095	ARG	Sidechain
3	a	1123	PHE	Sidechain
3	a	1130	ARG	Sidechain
3	a	1146	TYR	Sidechain
3	a	1184	TYR	Sidechain
3	a	1195	ARG	Sidechain
3	a	1198	TYR	Sidechain
3	a	1236	TYR	Sidechain
3	a	1257	HIS	Sidechain
3	a	1286	TYR	Sidechain
3	a	1347	ARG	Sidechain
3	a	1364	ARG	Sidechain
3	a	1373	TYR	Sidechain
1	b	139	HIS	Sidechain
1	b	20	PHE	Sidechain
1	b	202	TYR	Sidechain
1	b	210	TYR	Sidechain
1	b	224	TYR	Sidechain
1	b	244	PHE	Sidechain
1	b	262	PHE	Sidechain
1	b	264	ARG	Sidechain
1	b	272	PHE	Sidechain
1	b	28	HIS	Sidechain
1	b	311	ARG	Sidechain
1	b	312	TYR	Sidechain
1	b	322	ARG	Sidechain
1	b	369	ARG	Sidechain
1	b	388	PHE	Sidechain
1	b	404	PHE	Sidechain
1	b	432	TYR	Sidechain
1	b	435	TYR	Sidechain
1	b	49	ILE	Mainchain
1	b	64	ARG	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	b	3352	3232	3229	89	0
2	M	1069	1063	1060	11	0
3	a	3228	3147	3144	75	0
All	All	7649	7442	7433	168	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 11.

All (168) 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)
3:a:1141:LEU:HD23	3:a:1141:LEU:H	1.51	0.76
3:a:1011:GLN:HG2	3:a:1117:GLY:HA3	1.70	0.73
1:b:6:HIS:CD2	1:b:21:TRP:HE1	2.15	0.65
1:b:139:HIS:C	1:b:139:HIS:CD2	2.73	0.65
1:b:205:ASP:CG	1:b:304:ALA:H	2.06	0.63
1:b:264:ARG:O	1:b:266:HIS:CD2	2.53	0.61
1:b:262:PHE:HA	3:a:1376:ARG:HH22	1.64	0.61
1:b:406:HIS:CD2	1:b:407:TRP:N	2.71	0.59
1:b:358:ILE:HD12	1:b:359:PRO:HD2	1.84	0.58
3:a:1011:GLN:CG	3:a:1117:GLY:HA3	2.32	0.58
3:a:1064:GLU:H	3:a:1064:GLU:CD	2.10	0.58
3:a:1049:ILE:HD12	3:a:1068:THR:HG22	1.85	0.58
2:M:3201:ARG:CZ	3:a:1390:GLY:HA2	2.32	0.58
2:M:3174:LEU:HD23	2:M:3174:LEU:H	1.68	0.57
1:b:198:THR:O	1:b:265:LEU:HD13	2.04	0.57
1:b:163:ASP:CG	1:b:164:ARG:HH21	2.13	0.57
3:a:1238:ARG:O	3:a:1240:HIS:CD2	2.58	0.56
3:a:1084:ILE:HG23	3:a:1085:GLY:H	1.70	0.56
3:a:1217:ARG:HA	3:a:1217:ARG:HE	1.71	0.55
2:M:3139:ALA:HB1	2:M:3184:MET:HE1	1.89	0.55
3:a:1141:LEU:H	3:a:1141:LEU:CD2	2.20	0.55
3:a:1081:HIS:CE1	3:a:1126:LEU:HB3	2.42	0.55
1:b:55:GLU:HG2	1:b:61:TYR:CD2	2.42	0.54
1:b:352:LYS:O	1:b:352:LYS:HD3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:377:PHE:C	1:b:377:PHE:CD2	2.85	0.54
1:b:192:HIS:CD2	1:b:193:GLN:NE2	2.76	0.54
1:b:290:GLU:H	1:b:290:GLU:CD	2.14	0.54
1:b:32:PRO:HA	1:b:83:PHE:CE2	2.43	0.53
3:a:1224:VAL:HG22	3:a:1225:ASP:H	1.74	0.53
3:a:1002:ARG:HD2	3:a:1003:GLU:HG2	1.89	0.53
3:a:1238:ARG:HB2	3:a:1240:HIS:NE2	2.23	0.53
1:b:3:GLU:OE2	1:b:50:ASN:HB3	2.08	0.53
3:a:1290:CYS:SG	3:a:1292:LEU:HD21	2.49	0.53
2:M:3158:ILE:HG22	2:M:3163:PHE:CE1	2.44	0.52
3:a:1366:ASP:CG	3:a:1396:ARG:HH22	2.17	0.52
1:b:264:ARG:C	1:b:266:HIS:CD2	2.87	0.52
3:a:1081:HIS:CD2	3:a:1081:HIS:C	2.88	0.52
3:a:1113:HIS:CD2	3:a:1113:HIS:C	2.87	0.52
3:a:1077:TYR:CD1	3:a:1122:GLY:HA2	2.44	0.52
3:a:1238:ARG:O	3:a:1240:HIS:CG	2.63	0.51
1:b:52:TYR:C	1:b:53:TYR:CD1	2.89	0.51
1:b:88:ARG:NE	1:b:88:ARG:HA	2.25	0.51
1:b:242:LEU:C	1:b:243:ARG:HD3	2.36	0.50
1:b:241:CYS:SG	1:b:320:ARG:HD2	2.51	0.50
3:a:1291:LEU:HD12	3:a:1291:LEU:N	2.25	0.50
1:b:62:VAL:HG23	1:b:62:VAL:O	2.10	0.50
1:b:257:VAL:HG12	1:b:257:VAL:O	2.12	0.50
1:b:129:CYS:SG	1:b:130:ASP:N	2.85	0.49
3:a:1240:HIS:CG	3:a:1406:TYR:OH	2.65	0.49
1:b:51:VAL:O	1:b:51:VAL:HG12	2.12	0.49
1:b:251:ASP:H	1:b:254:LYS:HD3	1.78	0.49
1:b:53:TYR:C	1:b:54:ASN:HD22	2.21	0.48
3:a:1235:PRO:O	3:a:1236:TYR:CD1	2.66	0.48
3:a:1143:PHE:CD1	3:a:1143:PHE:N	2.79	0.48
1:b:54:ASN:HD21	1:b:64:ARG:NH1	2.12	0.48
1:b:272:PHE:CD2	1:b:273:ALA:N	2.81	0.48
1:b:149:MET:SD	1:b:149:MET:C	2.97	0.47
1:b:388:PHE:CD2	1:b:388:PHE:N	2.78	0.47
1:b:138:THR:O	1:b:139:HIS:HB3	2.13	0.47
3:a:1049:ILE:HD12	3:a:1068:THR:CG2	2.44	0.47
3:a:1077:TYR:CE1	3:a:1122:GLY:HA2	2.49	0.47
3:a:1011:GLN:CG	3:a:1117:GLY:CA	2.92	0.47
3:a:1369:PHE:C	3:a:1369:PHE:CD2	2.92	0.47
3:a:1376:ARG:O	3:a:1379:VAL:HG23	2.14	0.47
1:b:141:LEU:HD13	1:b:170:SER:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:55:GLU:HG2	1:b:61:TYR:CE2	2.49	0.47
1:b:107:HIS:CD2	1:b:152:LEU:HB2	2.49	0.47
3:a:1061:PHE:N	3:a:1061:PHE:CD1	2.82	0.47
3:a:1351:MET:C	3:a:1351:MET:SD	2.97	0.47
1:b:242:LEU:HD13	1:b:251:ASP:CA	2.45	0.47
3:a:1279:CYS:SG	3:a:1357:ALA:HB1	2.55	0.47
3:a:1031:GLN:C	3:a:1033:ASP:H	2.23	0.46
3:a:1146:TYR:C	3:a:1146:TYR:CD1	2.92	0.46
3:a:1217:ARG:HA	3:a:1217:ARG:NE	2.30	0.46
3:a:1073:ALA:O	3:a:1074:ALA:HB3	2.15	0.46
1:b:287:THR:O	1:b:288:VAL:CB	2.63	0.46
1:b:319:PHE:CD1	1:b:319:PHE:N	2.84	0.46
1:b:376:THR:HG22	1:b:377:PHE:N	2.31	0.46
3:a:1246:TYR:C	3:a:1246:TYR:CD2	2.93	0.46
1:b:293:GLN:HA	1:b:293:GLN:OE1	2.15	0.46
1:b:88:ARG:HA	1:b:88:ARG:HE	1.80	0.45
1:b:183:GLU:CB	1:b:184:PRO:CD	2.95	0.45
1:b:420:GLU:HA	1:b:420:GLU:OE1	2.16	0.45
1:b:182:VAL:O	1:b:183:GLU:C	2.59	0.45
3:a:1067:ILE:HD12	3:a:1067:ILE:N	2.32	0.45
1:b:330:GLU:O	1:b:331:GLN:C	2.59	0.45
1:b:8:GLN:NE2	1:b:17:GLY:HA3	2.31	0.45
3:a:1113:HIS:CE1	3:a:1144:SER:HB3	2.51	0.45
3:a:1020:CYS:O	3:a:1024:TYR:HB2	2.16	0.45
1:b:272:PHE:CG	1:b:273:ALA:N	2.84	0.45
1:b:305:CYS:SG	1:b:386:GLU:HB2	2.57	0.45
1:b:325:MET:N	1:b:325:MET:SD	2.90	0.45
3:a:1291:LEU:HD12	3:a:1291:LEU:H	1.82	0.45
3:a:1093:LEU:HD23	3:a:1093:LEU:HA	1.86	0.45
1:b:103:TRP:CZ2	1:b:107:HIS:CG	3.05	0.44
1:b:139:HIS:CD2	1:b:139:HIS:O	2.69	0.44
1:b:87:PHE:CD1	1:b:87:PHE:N	2.86	0.44
1:b:257:VAL:HG13	3:a:1381:TRP:CG	2.53	0.44
1:b:188:THR:HG22	1:b:421:ALA:HB1	1.99	0.44
1:b:260:VAL:HG13	3:a:1381:TRP:HE1	1.82	0.44
3:a:1397:GLU:O	3:a:1400:ALA:HB3	2.17	0.44
3:a:1201:LEU:HD23	3:a:1201:LEU:N	2.32	0.44
3:a:1058:ARG:HH11	3:a:1058:ARG:HG2	1.81	0.44
3:a:1217:ARG:NE	3:a:1217:ARG:CA	2.80	0.44
1:b:284:ARG:O	1:b:285:ALA:HB2	2.18	0.44
3:a:1024:TYR:O	3:a:1025:CYS:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:11:GLN:HE22	1:b:143:GLY:HA3	1.81	0.44
1:b:356:CYS:SG	1:b:357:ASP:N	2.91	0.44
1:b:154:ILE:CG1	1:b:155:SER:N	2.81	0.43
3:a:1042:VAL:HG11	3:a:1123:PHE:CE1	2.53	0.43
3:a:1197:THR:OG1	3:a:1199:THR:HG22	2.18	0.43
3:a:1146:TYR:CG	3:a:1147:PRO:HD2	2.53	0.43
1:b:11:GLN:HE22	1:b:143:GLY:CA	2.32	0.43
1:b:51:VAL:O	1:b:51:VAL:CG1	2.67	0.43
1:b:227:LEU:O	1:b:228:ASN:C	2.61	0.43
1:b:404:PHE:CD1	1:b:404:PHE:N	2.87	0.43
3:a:1166:HIS:CG	3:a:1167:THR:N	2.85	0.43
1:b:234:THR:HG21	1:b:270:PRO:HB3	2.01	0.43
1:b:69:ASP:HB3	1:b:75:MET:HE3	2.00	0.42
2:M:3126:MET:HE2	3:a:1380:HIS:HA	2.01	0.42
2:M:3199:ILE:O	2:M:3202:ALA:HB3	2.19	0.42
3:a:1183:ILE:O	3:a:1187:CYS:SG	2.77	0.42
1:b:11:GLN:OE1	1:b:143:GLY:HA3	2.18	0.42
1:b:404:PHE:HA	1:b:406:HIS:CE1	2.54	0.42
3:a:1134:ASP:HB3	3:a:1135:TYR:CE1	2.55	0.42
3:a:1378:PHE:N	3:a:1378:PHE:CD1	2.86	0.42
1:b:205:ASP:OD2	1:b:304:ALA:HB3	2.19	0.42
1:b:406:HIS:CD2	1:b:407:TRP:CD1	3.08	0.42
1:b:23:VAL:HG12	1:b:24:ILE:N	2.34	0.42
3:a:1106:LEU:HD11	3:a:1138:LYS:HE3	2.00	0.42
3:a:1164:THR:O	3:a:1164:THR:HG22	2.19	0.42
3:a:1023:LEU:HD13	3:a:1023:LEU:C	2.45	0.42
2:M:3165:HIS:O	2:M:3169:HIS:CG	2.73	0.42
1:b:103:TRP:CH2	1:b:107:HIS:CG	3.08	0.42
1:b:209:LEU:O	1:b:210:TYR:C	2.61	0.42
1:b:352:LYS:HD3	1:b:352:LYS:C	2.45	0.42
1:b:32:PRO:HA	1:b:83:PHE:CD2	2.55	0.41
1:b:103:TRP:CD1	1:b:148:GLY:HA2	2.55	0.41
3:a:1134:ASP:C	3:a:1135:TYR:CG	2.98	0.41
3:a:1213:THR:O	3:a:1214:ALA:C	2.63	0.41
3:a:1291:LEU:H	3:a:1291:LEU:CD1	2.33	0.41
1:b:201:THR:HB	1:b:267:PHE:CD2	2.55	0.41
1:b:390:ARG:O	1:b:391:ILE:C	2.61	0.41
2:M:3191:ASP:HA	2:M:3192:PRO:HD3	1.93	0.41
3:a:1044:LEU:HG	3:a:1119:THR:HG21	2.02	0.41
1:b:287:THR:OG1	1:b:289:PRO:HD2	2.21	0.41
1:b:355:VAL:HG12	1:b:356:CYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:3124:ARG:HA	2:M:3158:ILE:HD12	2.03	0.41
3:a:1036:VAL:HG12	3:a:1037:PRO:O	2.20	0.41
1:b:2:ARG:O	1:b:133:GLN:HB2	2.20	0.41
1:b:287:THR:O	1:b:288:VAL:HG23	2.21	0.41
3:a:1028:HIS:CD2	3:a:1028:HIS:N	2.87	0.41
3:a:1076:ASN:O	3:a:1076:ASN:CG	2.64	0.41
3:a:1376:ARG:O	3:a:1376:ARG:HG2	2.20	0.41
1:b:406:HIS:CG	1:b:407:TRP:N	2.89	0.41
1:b:70:LEU:O	1:b:72:PRO:HD3	2.21	0.41
2:M:3201:ARG:NE	3:a:1390:GLY:HA2	2.36	0.41
1:b:36:TYR:O	1:b:37:HIS:CD2	2.74	0.41
1:b:103:TRP:NE1	1:b:148:GLY:HA2	2.36	0.41
1:b:243:ARG:HD3	1:b:243:ARG:N	2.35	0.40
3:a:1216:LEU:HG	3:a:1217:ARG:HH22	1.86	0.40
1:b:262:PHE:CD2	3:a:1376:ARG:NH1	2.90	0.40
3:a:1238:ARG:HB2	3:a:1240:HIS:CD2	2.57	0.40
1:b:209:LEU:HD12	1:b:209:LEU:HA	1.83	0.40
1:b:268:PHE:CD2	1:b:268:PHE:N	2.85	0.40
2:M:3182:LYS:HA	2:M:3182:LYS:HE2	2.03	0.40
3:a:1077:TYR:O	3:a:1078:ALA:C	2.64	0.40
3:a:1148:ALA:HB1	3:a:1181:GLU:OE1	2.22	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	b	424/426 (100%)	304 (72%)	88 (21%)	32 (8%)	1	13
2	M	128/130 (98%)	112 (88%)	16 (12%)	0	100	100
3	a	410/412 (100%)	297 (72%)	75 (18%)	38 (9%)	0	10
All	All	962/968 (99%)	713 (74%)	179 (19%)	70 (7%)	1	13

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	b	50	ASN
1	b	174	SER
1	b	183	GLU
1	b	240	THR
1	b	252	LEU
1	b	265	LEU
1	b	285	ALA
1	b	286	LEU
1	b	288	VAL
1	b	294	GLN
3	a	1057	TYR
3	a	1082	TYR
3	a	1083	THR
3	a	1214	ALA
3	a	1229	PHE
3	a	1235	PRO
3	a	1377	ALA
1	b	23	VAL
1	b	24	ILE
1	b	96	GLN
1	b	109	THR
1	b	238	VAL
1	b	284	ARG
1	b	295	MET
3	a	1085	GLY
3	a	1117	GLY
3	a	1191	LEU
3	a	1213	THR
3	a	1239	GLY
3	a	1263	ALA
3	a	1288	ALA
3	a	1332	GLU
3	a	1360	GLU
3	a	1361	ALA
1	b	3	GLU
1	b	239	THR
1	b	266	HIS
1	b	273	ALA
1	b	369	ARG
1	b	386	GLU
1	b	403	ALA
3	a	1074	ALA

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Mol	Chain	Res	Type
3	a	1212	ILE
3	a	1304	ALA
3	a	1347	ARG
1	b	143	GLY
1	b	308	ARG
1	b	395	PHE
3	a	1024	TYR
3	a	1077	TYR
3	a	1078	ALA
3	a	1123	PHE
3	a	1262	VAL
1	b	195	VAL
1	b	373	MET
3	a	1063	PRO
3	a	1122	GLY
3	a	1237	PRO
3	a	1247	ALA
1	b	424	ASN
3	a	1195	ARG
3	a	1089	ILE
3	a	1157	GLU
1	b	175	PRO
1	b	348	PRO
3	a	1277	VAL
3	a	1322	PRO
3	a	1148	ALA
3	a	1411	VAL
3	a	1345	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	b	367/367 (100%)	335 (91%)	32 (9%)	9	33
2	M	120/120 (100%)	116 (97%)	4 (3%)	33	56
3	a	347/347 (100%)	313 (90%)	34 (10%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	834/834 (100%)	764 (92%)	70 (8%)	12	34

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	11	GLN
1	b	12	CYS
1	b	27	GLU
1	b	39	ASP
1	b	49	ILE
1	b	63	PRO
1	b	72	PRO
1	b	86	ILE
1	b	89	PRO
1	b	94	PHE
1	b	113	GLU
1	b	115	VAL
1	b	117	SER
1	b	119	LEU
1	b	122	VAL
1	b	145	THR
1	b	179	ASP
1	b	182	VAL
1	b	195	VAL
1	b	241	CYS
1	b	260	VAL
1	b	278	ARG
1	b	292	THR
1	b	294	GLN
1	b	300	ASN
1	b	326	LYS
1	b	331	GLN
1	b	352	LYS
1	b	373	MET
1	b	420	GLU
1	b	422	GLU
1	b	427	ASP
2	M	3122	GLU
2	M	3204	LYS
2	M	3206	CYS
2	M	3209	LEU
3	a	1002	ARG

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Mol	Chain	Res	Type
3	a	1005	ILE
3	a	1009	VAL
3	a	1011	GLN
3	a	1023	LEU
3	a	1025	CYS
3	a	1048	VAL
3	a	1056	THR
3	a	1060	LEU
3	a	1062	HIS
3	a	1063	PRO
3	a	1064	GLU
3	a	1068	THR
3	a	1075	ASN
3	a	1106	LEU
3	a	1119	THR
3	a	1126	LEU
3	a	1146	TYR
3	a	1156	VAL
3	a	1165	THR
3	a	1179	ASP
3	a	1201	LEU
3	a	1217	ARG
3	a	1230	GLN
3	a	1277	VAL
3	a	1315	ILE
3	a	1318	VAL
3	a	1334	PRO
3	a	1337	VAL
3	a	1351	MET
3	a	1366	ASP
3	a	1376	ARG
3	a	1407	GLU
3	a	1412	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	b	54	ASN
1	b	101	ASN
1	b	139	HIS
1	b	193	GLN
1	b	294	GLN

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Mol	Chain	Res	Type
1	b	334	ASN
1	b	385	GLN
1	b	406	HIS
1	b	433	GLN
1	b	436	GLN
2	M	3114	ASN
3	a	1018	ASN
3	a	1028	HIS
3	a	1075	ASN
3	a	1113	HIS
3	a	1150	GLN
3	a	1230	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	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	1.19

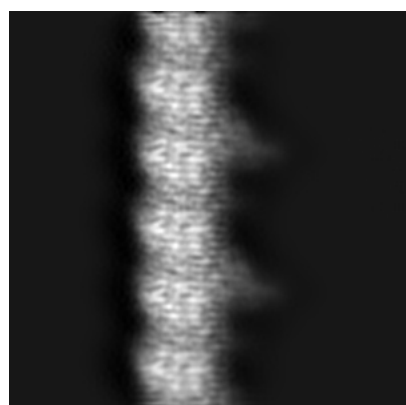
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9996. These allow visual inspection of the internal detail of the map and identification of artifacts.

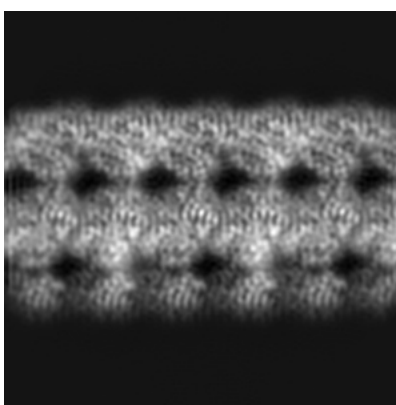
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

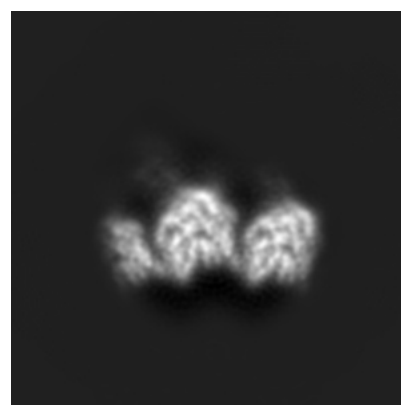
6.1.1 Primary map



X



Y

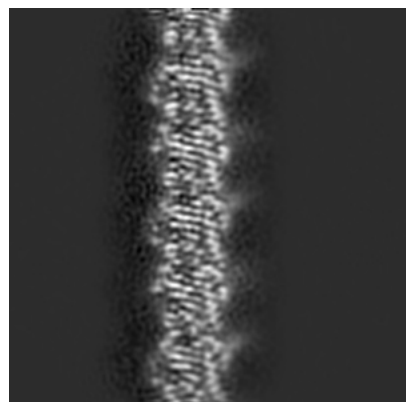


Z

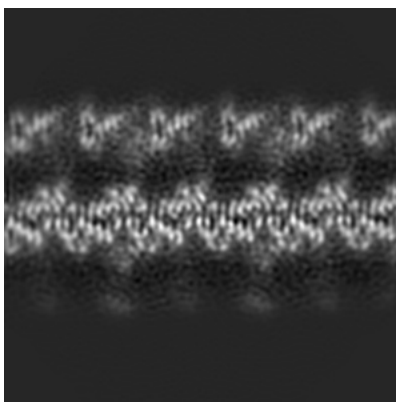
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

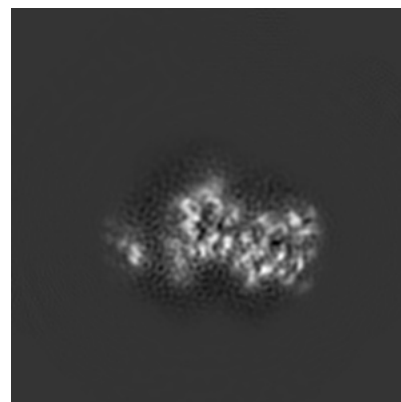
6.2.1 Primary map



X Index: 90



Y Index: 90

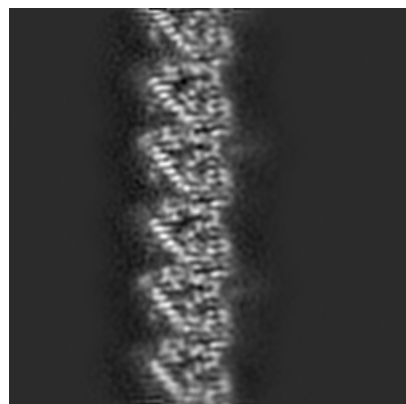


Z Index: 90

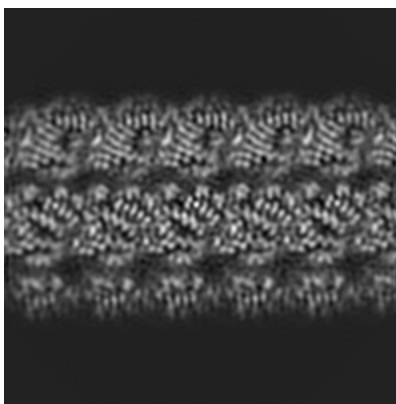
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

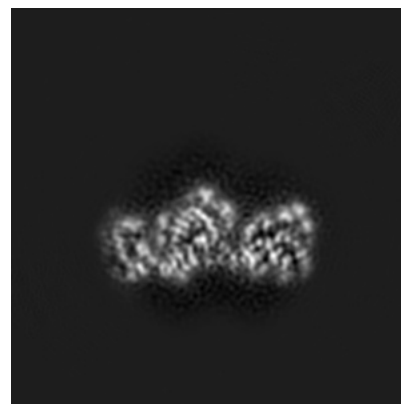
6.3.1 Primary map



X Index: 81



Y Index: 75

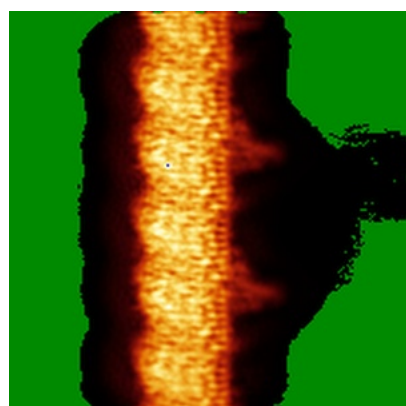


Z Index: 81

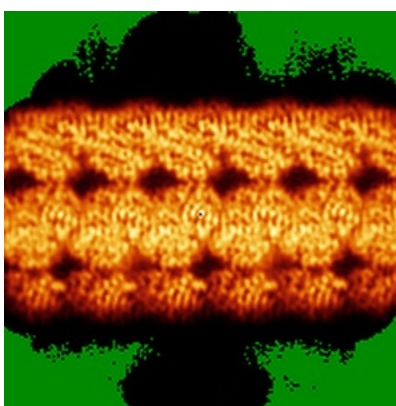
The images above show the largest variance slices of the map in three orthogonal directions.

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

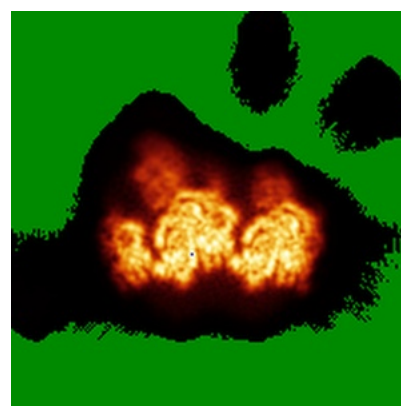
6.4.1 Primary map



X



Y

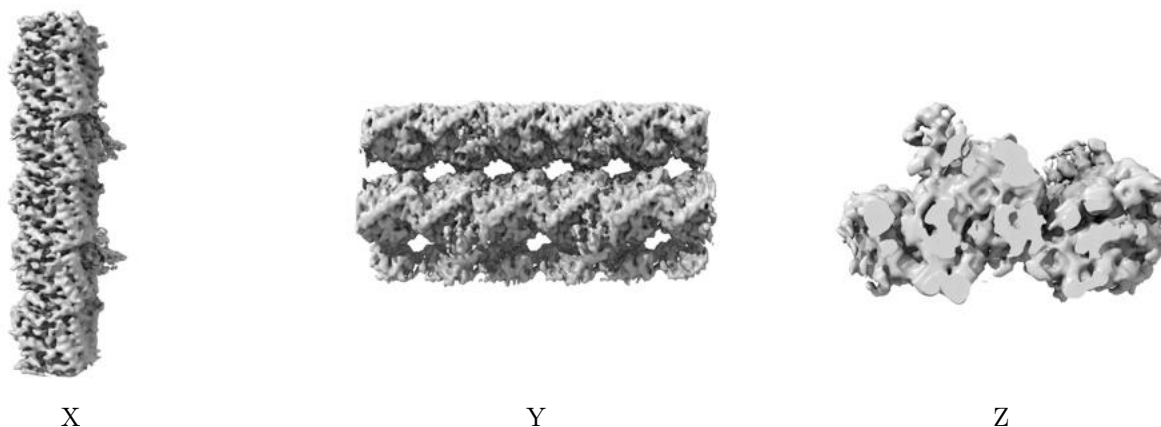


Z

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 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

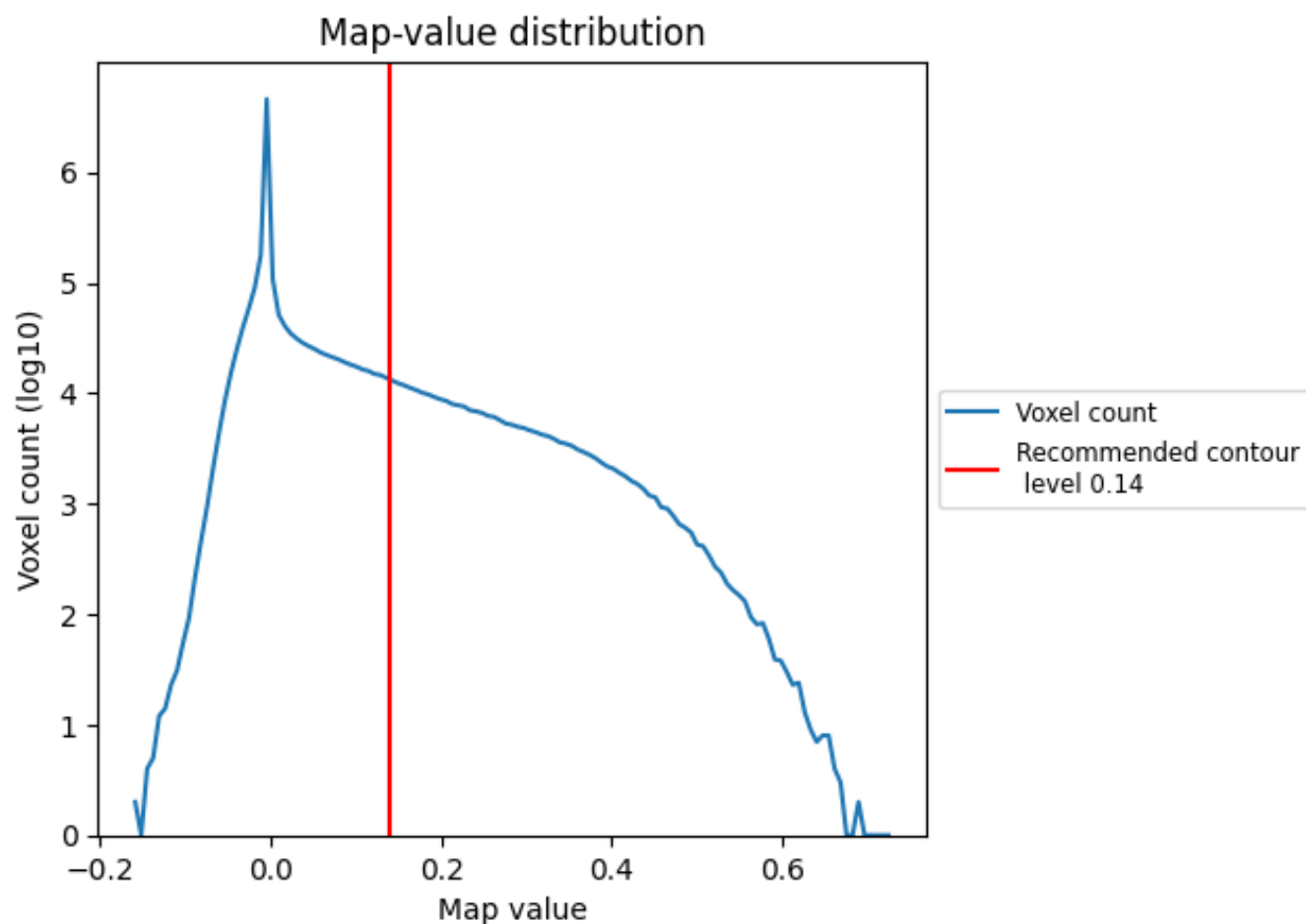
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

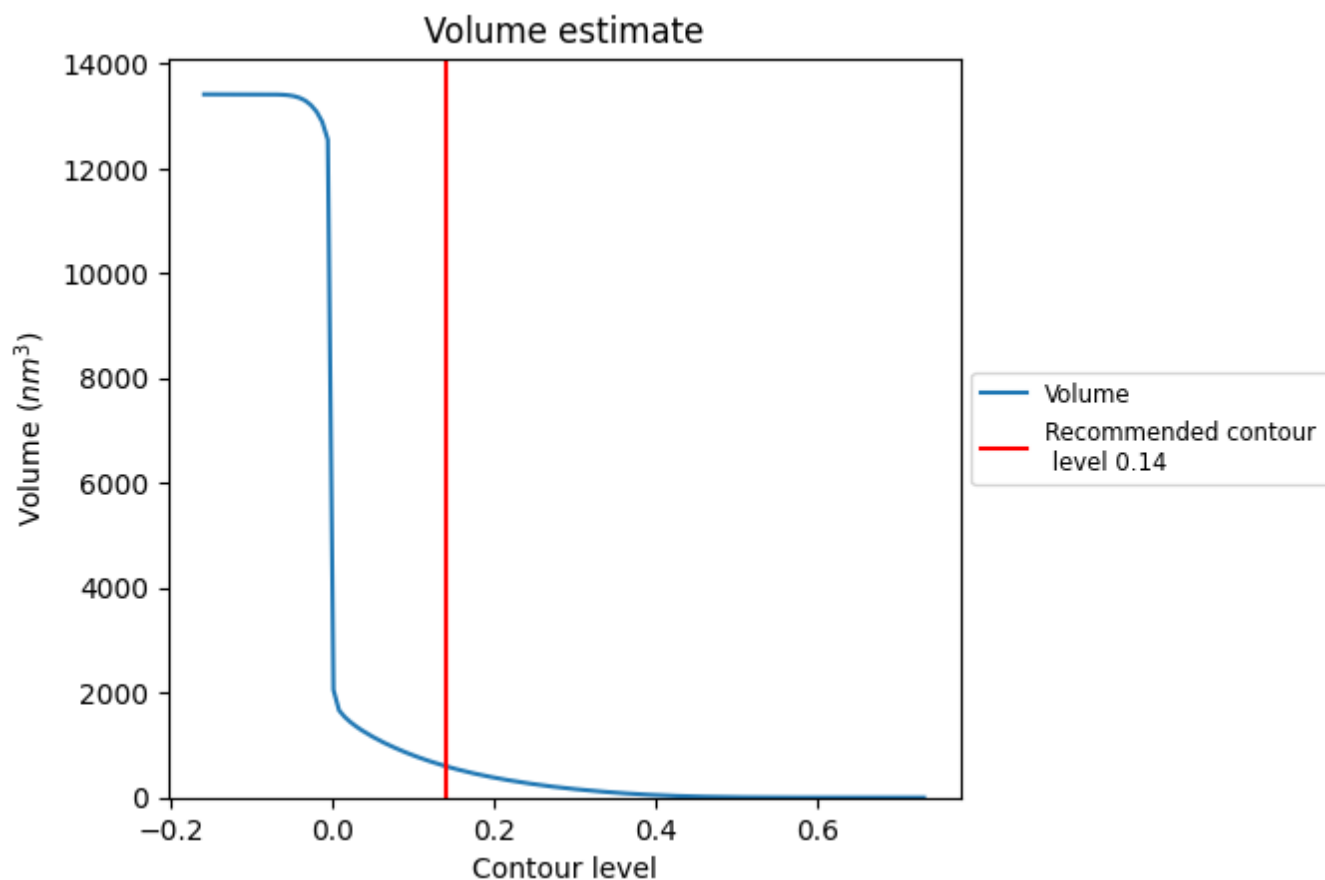
This section contains the results of statistical analysis of the map.

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.

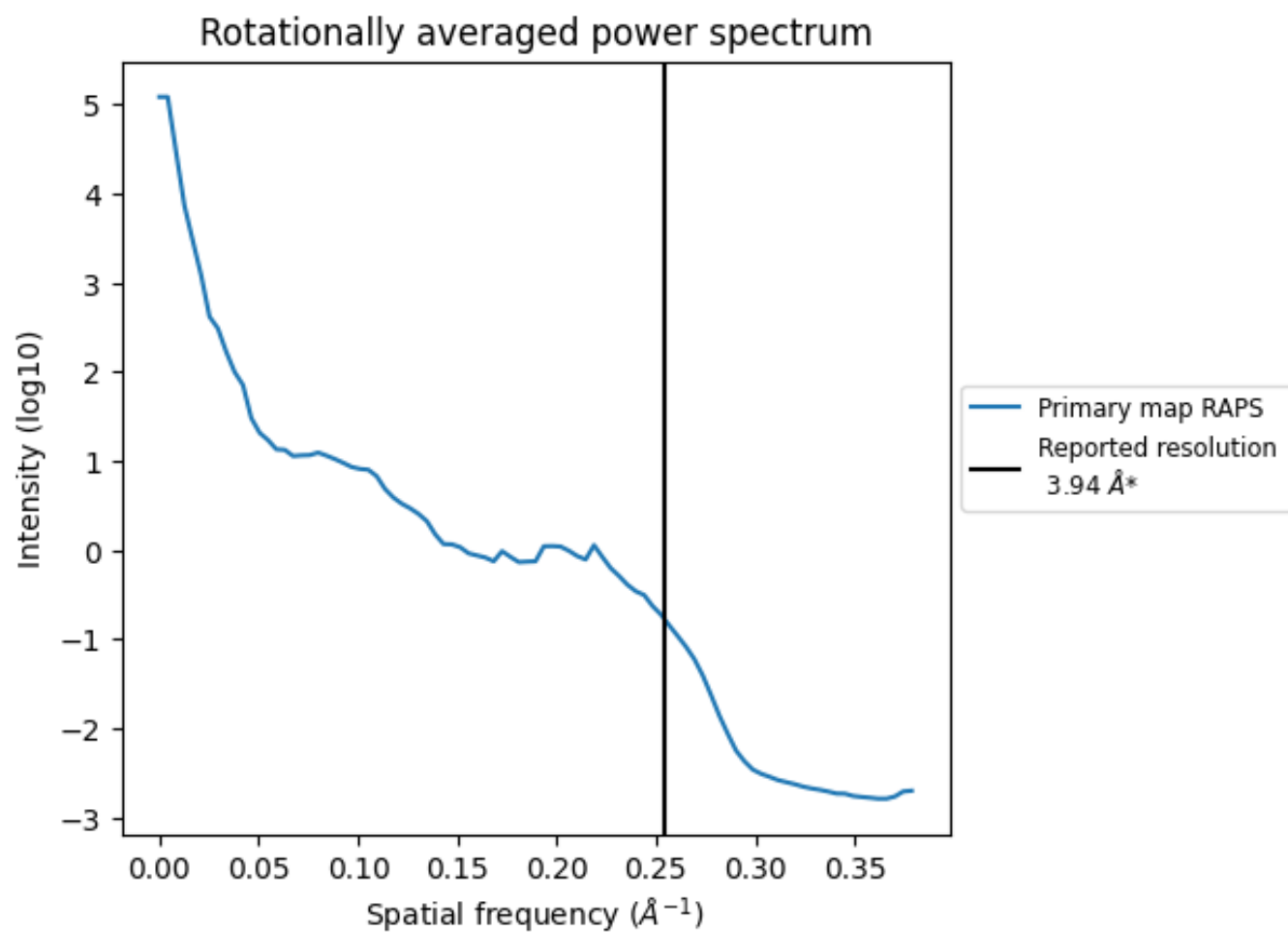
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 599 nm³; this corresponds to an approximate mass of 541 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 0.254 Å⁻¹

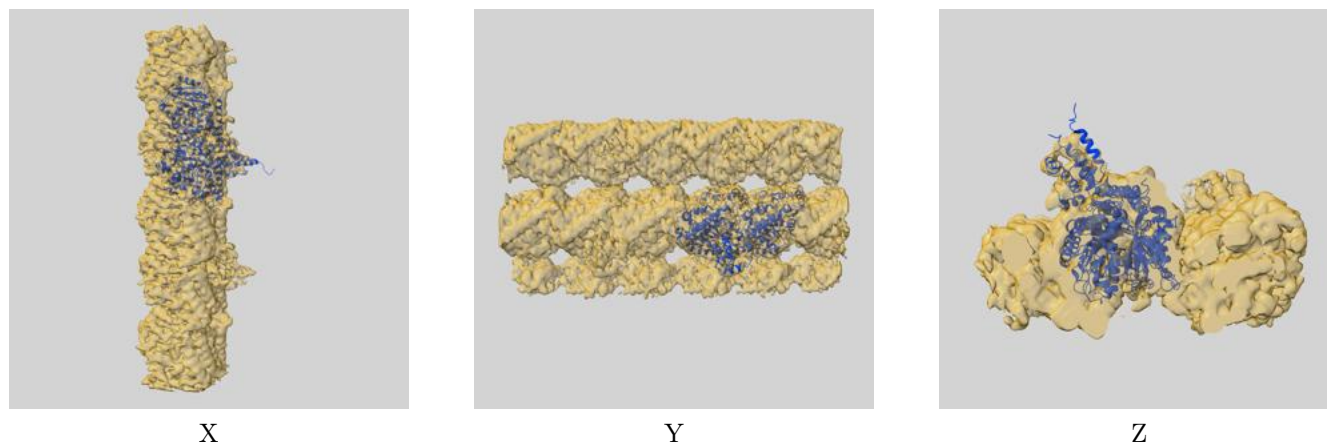
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

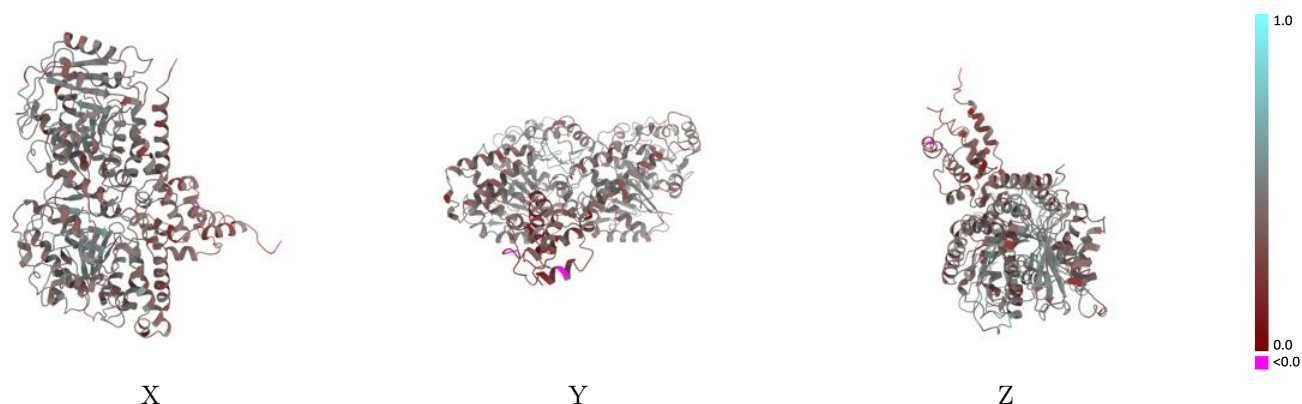
This section contains information regarding the fit between EMDB map EMD-9996 and PDB model 6KIO. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



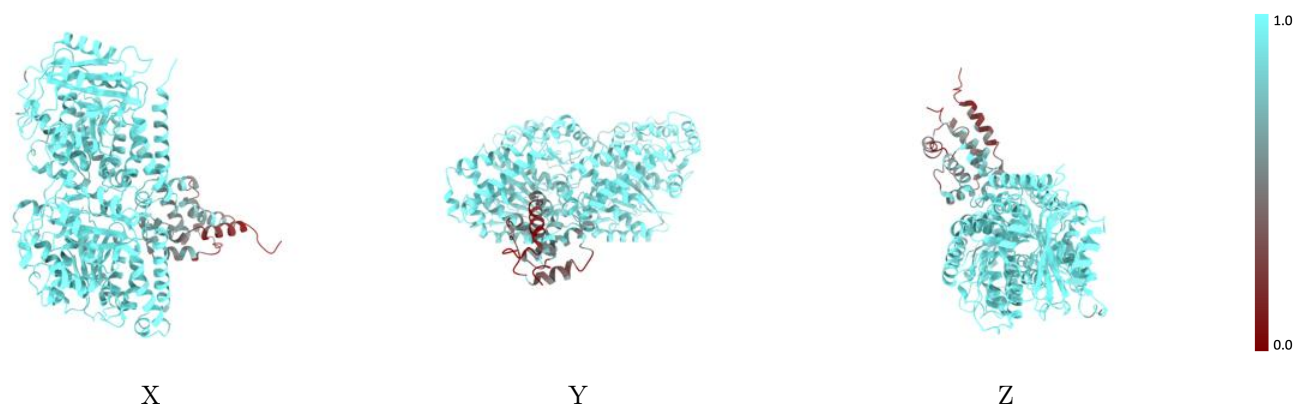
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



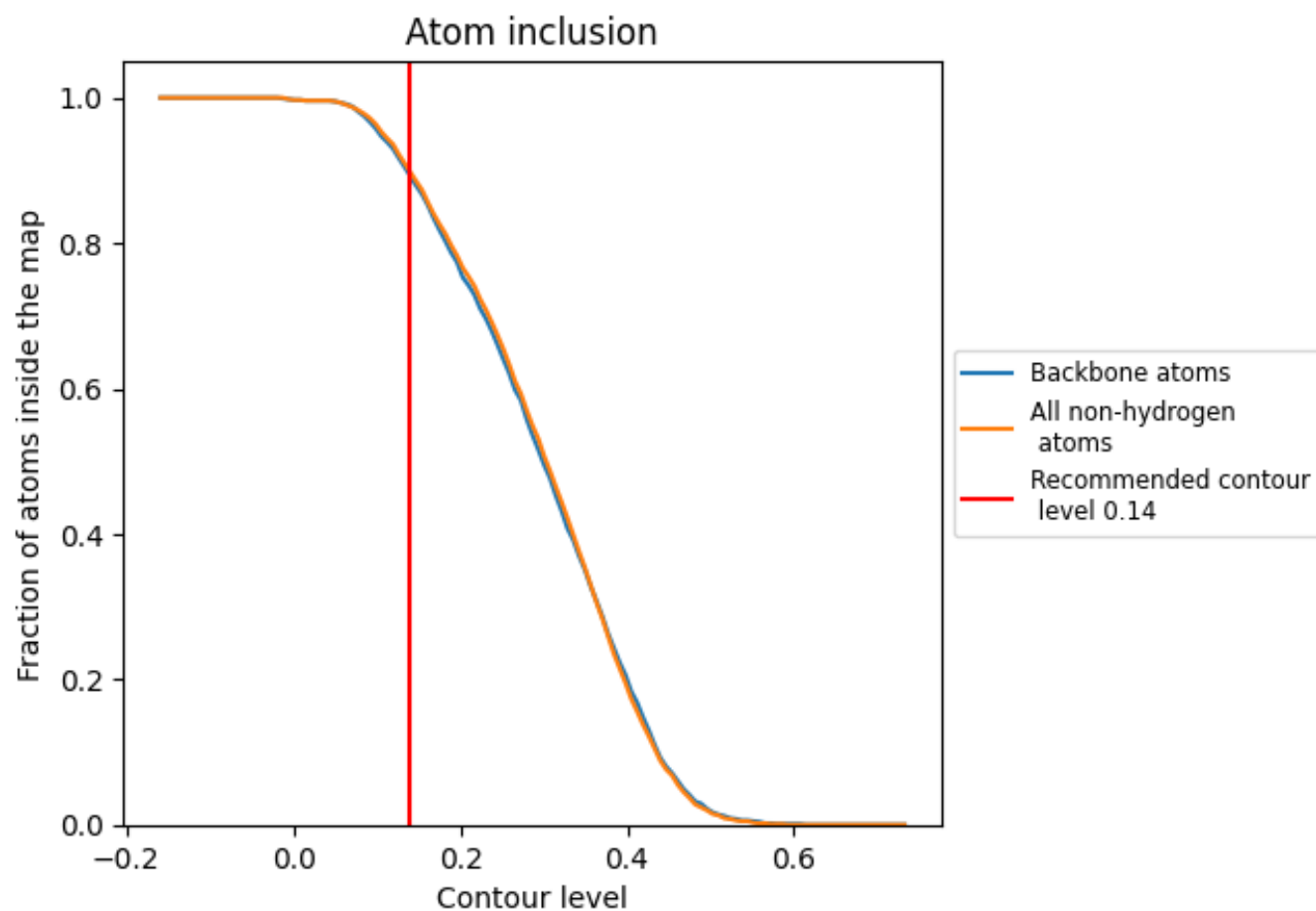
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.14).

9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 90% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8980	0.4140
M	0.4860	0.2800
a	0.9670	0.4320
b	0.9770	0.4400

