



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 04:55 AM UTC

PDB ID : 3J4S / pdb_00003j4s
EMDB ID : EMD-5762
Title : Helical Model of TubZ-Bt four-stranded filament
Authors : Montabana, E.A.; Agard, D.A.
Deposited on : 2013-10-03
Resolution : 6.80 Å(reported)
Based on initial models : 2XKB, 2XKA

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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

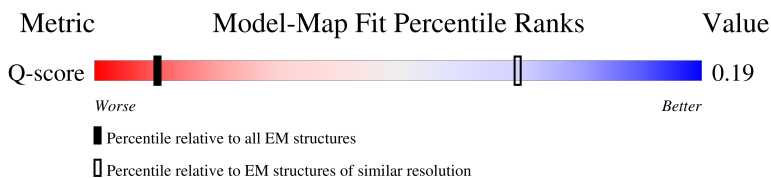
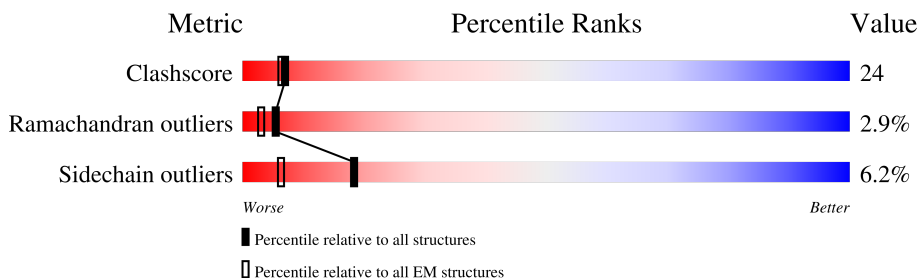
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.80 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	479 (6.40 - 7.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	484	

2 Entry composition [i](#)

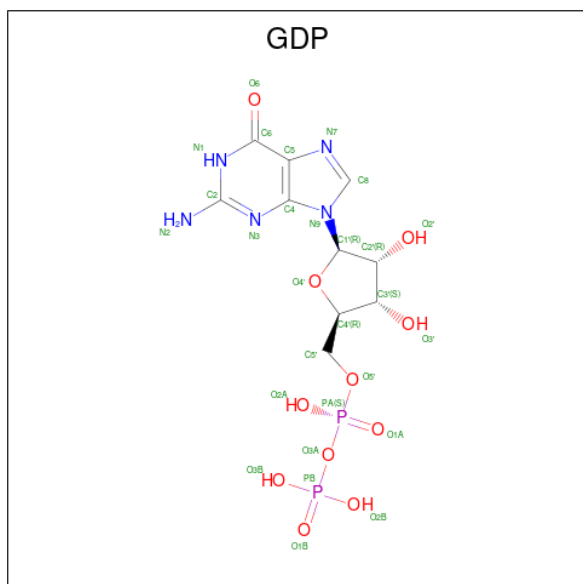
There are 2 unique types of molecules in this entry. The entry contains 3305 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called FtsZ/tubulin-related protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	414	3277	2061	564	639	13	0	0

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

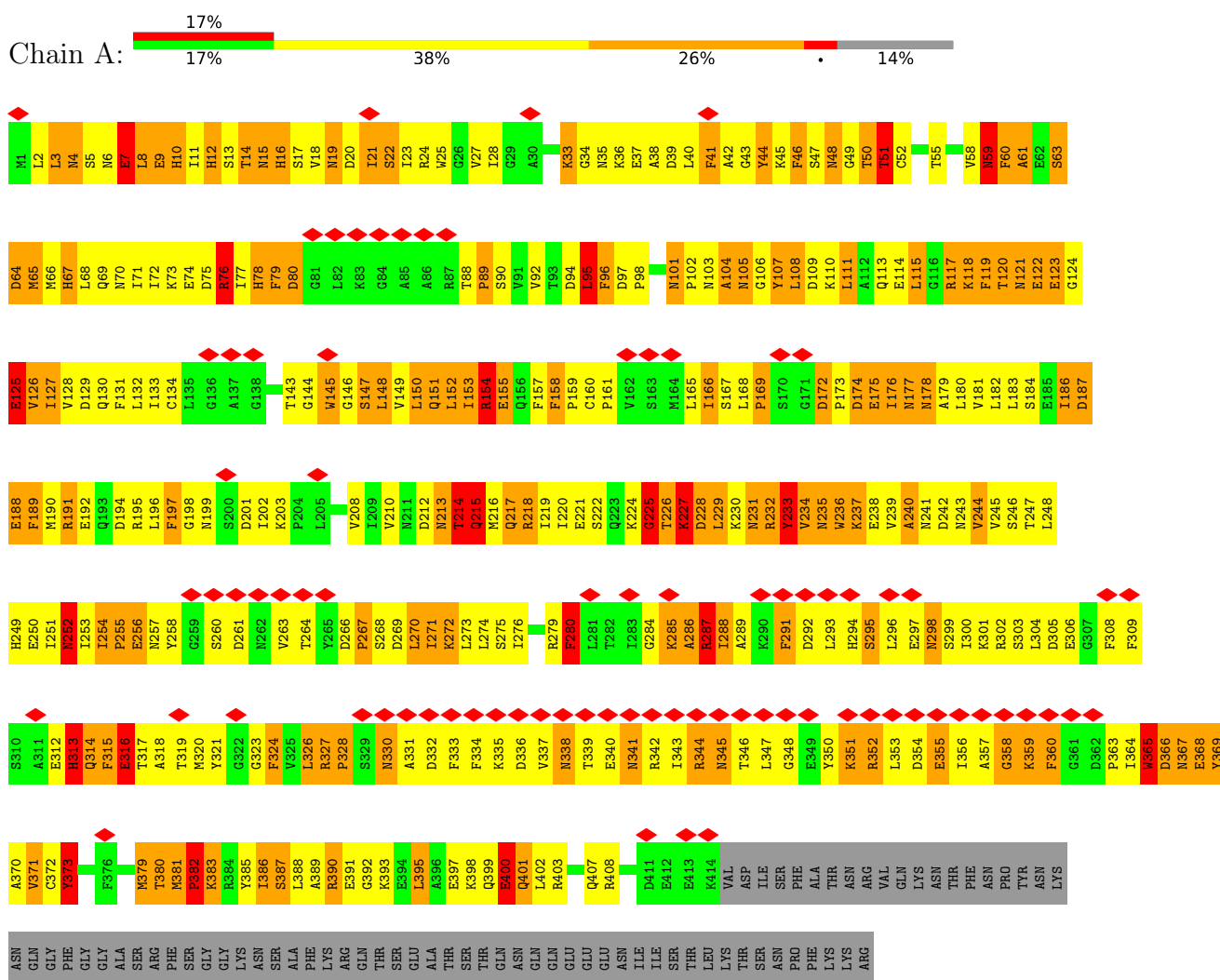


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	28	10	5	11	2	0

3 Residue-property plots

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

- Molecule 1: FtsZ/tubulin-related protein



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=31.78843°, rise=43.54512 Å, axial sym=C4	Depositor
Number of segments used	Not provided	
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Whole Micrograph	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{Å}^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	62000	Depositor
Image detector	TVIPS TEMCAM-F816 (8k x 8k)	Depositor
Maximum map value	0.096	Depositor
Minimum map value	-0.082	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0155	Depositor
Map size (Å)	240.64, 240.64, 240.64	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.94, 0.94, 0.94	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP

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	2.91	383/3339 (11.5%)	2.25	180/4511 (4.0%)

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	9

All (383) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	ASN	CA-C	-13.63	1.35	1.52
1	A	341	ASN	CA-C	-13.27	1.36	1.52
1	A	258	TYR	CA-C	-11.76	1.38	1.52
1	A	119	PHE	CA-C	-11.03	1.38	1.52
1	A	233	TYR	CA-C	-10.95	1.43	1.52
1	A	395	LEU	CA-C	-10.72	1.42	1.52
1	A	8	LEU	CA-C	-10.47	1.39	1.52
1	A	7	GLU	CA-C	-10.26	1.39	1.52
1	A	114	GLU	CA-C	-10.10	1.38	1.52
1	A	180	LEU	CA-C	-9.94	1.40	1.52
1	A	269	ASP	CA-C	-9.93	1.40	1.52
1	A	298	ASN	CA-C	-9.86	1.40	1.52
1	A	188	GLU	CA-C	-9.85	1.40	1.52
1	A	275	SER	CA-C	-9.55	1.43	1.53
1	A	279	ARG	CA-C	-9.51	1.40	1.52
1	A	19	ASN	N-CA	-9.44	1.37	1.46
1	A	388	LEU	CA-C	-9.38	1.41	1.52
1	A	111	LEU	CA-C	-9.26	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	328	PRO	CA-C	-9.25	1.40	1.52
1	A	257	ASN	CA-C	-9.21	1.40	1.52
1	A	120	THR	CA-C	-8.94	1.41	1.52
1	A	105	ASN	CA-C	-8.94	1.40	1.52
1	A	243	ASN	CA-C	-8.92	1.41	1.52
1	A	177	ASN	CA-C	-8.91	1.41	1.52
1	A	50	THR	CA-C	-8.89	1.42	1.52
1	A	387	SER	CA-C	-8.88	1.40	1.52
1	A	343	ILE	CA-C	-8.79	1.41	1.52
1	A	247	THR	CA-C	-8.78	1.41	1.52
1	A	365	TRP	CA-C	-8.77	1.42	1.53
1	A	130	GLN	CA-C	-8.75	1.41	1.52
1	A	386	ILE	N-CA	-8.75	1.36	1.46
1	A	7	GLU	N-CA	-8.74	1.35	1.46
1	A	12	HIS	CA-C	-8.70	1.40	1.52
1	A	215	GLN	CA-C	-8.70	1.41	1.52
1	A	302	ARG	CA-C	-8.69	1.41	1.52
1	A	94	ASP	CA-C	-8.67	1.41	1.52
1	A	301	LYS	CA-C	-8.60	1.41	1.52
1	A	10	HIS	CA-C	-8.59	1.41	1.52
1	A	250	GLU	CA-C	-8.57	1.42	1.52
1	A	15	ASN	CA-C	-8.55	1.42	1.52
1	A	358	GLY	CA-C	-8.53	1.43	1.52
1	A	233	TYR	N-CA	-8.49	1.39	1.47
1	A	175	GLU	CA-C	-8.46	1.41	1.52
1	A	401	GLN	CA-C	-8.44	1.42	1.52
1	A	72	ILE	CA-C	-8.43	1.42	1.52
1	A	79	PHE	CA-C	-8.40	1.42	1.52
1	A	254	ILE	CA-CB	-8.34	1.49	1.54
1	A	69	GLN	CA-C	-8.30	1.42	1.52
1	A	23	ILE	CA-C	-8.28	1.42	1.52
1	A	300	ILE	CA-C	-8.14	1.43	1.52
1	A	9	GLU	N-CA	-8.11	1.36	1.46
1	A	217	GLN	CA-C	-8.07	1.42	1.52
1	A	174	ASP	CA-C	-8.05	1.42	1.52
1	A	391	GLU	CA-C	-8.04	1.42	1.52
1	A	5	SER	CA-C	-8.04	1.42	1.52
1	A	249	HIS	N-CA	-8.01	1.36	1.46
1	A	47	SER	CA-C	-7.98	1.44	1.53
1	A	244	VAL	CA-C	-7.98	1.43	1.52
1	A	342	ARG	N-CA	-7.95	1.36	1.46
1	A	222	SER	CA-C	-7.95	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	364	ILE	N-CA	-7.91	1.37	1.46
1	A	242	ASP	CA-C	-7.90	1.42	1.52
1	A	121	ASN	CA-C	-7.88	1.42	1.52
1	A	237	LYS	CA-C	-7.86	1.42	1.52
1	A	220	ILE	CA-C	-7.79	1.42	1.52
1	A	245	VAL	CA-C	-7.77	1.43	1.52
1	A	186	ILE	CA-C	-7.75	1.43	1.52
1	A	190	MET	CA-C	-7.75	1.42	1.52
1	A	5	SER	N-CA	-7.74	1.36	1.46
1	A	197	PHE	CA-C	-7.71	1.42	1.53
1	A	9	GLU	CA-C	-7.69	1.43	1.52
1	A	335	LYS	CA-C	-7.69	1.42	1.52
1	A	238	GLU	CA-C	-7.68	1.42	1.52
1	A	273	LEU	CA-C	-7.68	1.42	1.52
1	A	14	THR	CA-C	-7.67	1.44	1.52
1	A	270	LEU	CA-C	-7.65	1.42	1.52
1	A	339	THR	N-CA	-7.63	1.37	1.46
1	A	334	PHE	CA-C	-7.62	1.42	1.52
1	A	153	ILE	CA-C	-7.60	1.43	1.52
1	A	6	ASN	CA-C	-7.60	1.42	1.52
1	A	246	SER	CA-C	-7.58	1.43	1.52
1	A	179	ALA	N-CA	-7.58	1.37	1.46
1	A	345	ASN	CA-C	-7.50	1.43	1.52
1	A	342	ARG	CA-C	-7.48	1.43	1.52
1	A	327	ARG	N-CA	-7.46	1.37	1.45
1	A	305	ASP	CA-C	-7.44	1.42	1.52
1	A	51	THR	CA-C	-7.40	1.42	1.52
1	A	11	ILE	N-CA	-7.37	1.38	1.46
1	A	292	ASP	CA-C	-7.36	1.43	1.52
1	A	78	HIS	CA-C	-7.32	1.43	1.52
1	A	183	LEU	CA-C	-7.30	1.43	1.52
1	A	327	ARG	CA-C	-7.27	1.43	1.52
1	A	109	ASP	CA-C	-7.27	1.43	1.52
1	A	241	ASN	N-CA	-7.26	1.37	1.46
1	A	302	ARG	N-CA	-7.25	1.37	1.46
1	A	390	ARG	CA-C	-7.25	1.42	1.52
1	A	244	VAL	N-CA	-7.24	1.38	1.46
1	A	220	ILE	N-CA	-7.21	1.37	1.46
1	A	61	ALA	CA-C	-7.18	1.43	1.52
1	A	18	VAL	CA-C	-7.16	1.43	1.52
1	A	178	ASN	CA-C	-7.15	1.43	1.52
1	A	133	ILE	CA-CB	-7.13	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	288	ILE	N-CA	-7.12	1.37	1.46
1	A	107	TYR	CA-C	-7.12	1.43	1.52
1	A	244	VAL	CA-CB	-7.11	1.46	1.54
1	A	11	ILE	CA-C	-7.10	1.44	1.52
1	A	248	LEU	CA-C	-7.09	1.43	1.52
1	A	272	LYS	CA-C	-7.08	1.43	1.52
1	A	240	ALA	CA-C	-7.07	1.43	1.52
1	A	16	HIS	N-CA	-7.06	1.40	1.46
1	A	363	PRO	CA-C	-7.06	1.43	1.52
1	A	303	SER	CA-C	-7.03	1.43	1.52
1	A	218	ARG	CA-C	-7.02	1.44	1.52
1	A	88	THR	C-N	-7.02	1.26	1.34
1	A	58	VAL	CA-C	-7.01	1.44	1.52
1	A	189	PHE	N-CA	-7.01	1.37	1.46
1	A	131	PHE	CA-C	-7.00	1.43	1.52
1	A	52	CYS	N-CA	-6.98	1.37	1.46
1	A	115	LEU	N-CA	-6.97	1.38	1.46
1	A	341	ASN	N-CA	-6.96	1.38	1.46
1	A	391	GLU	N-CA	-6.95	1.37	1.46
1	A	268	SER	CA-C	-6.93	1.43	1.52
1	A	77	ILE	CA-C	-6.90	1.44	1.52
1	A	254	ILE	CA-C	-6.90	1.46	1.52
1	A	299	SER	CA-C	-6.88	1.43	1.52
1	A	296	LEU	CA-C	-6.87	1.44	1.52
1	A	221	GLU	CA-C	-6.85	1.43	1.52
1	A	19	ASN	CA-C	-6.83	1.44	1.53
1	A	181	VAL	CA-C	-6.82	1.43	1.52
1	A	106	GLY	CA-C	-6.80	1.44	1.52
1	A	182	LEU	N-CA	-6.79	1.38	1.46
1	A	40	LEU	CA-C	-6.77	1.44	1.52
1	A	150	LEU	CA-C	-6.75	1.44	1.52
1	A	326	LEU	CA-C	-6.75	1.44	1.52
1	A	340	GLU	CA-C	-6.74	1.44	1.52
1	A	273	LEU	N-CA	-6.73	1.38	1.46
1	A	13	SER	CA-C	-6.72	1.43	1.52
1	A	166	ILE	CA-C	-6.72	1.44	1.52
1	A	280	PHE	CA-C	-6.70	1.44	1.52
1	A	60	PHE	CA-C	-6.68	1.44	1.52
1	A	71	ILE	CA-C	-6.66	1.44	1.52
1	A	359	LYS	CA-C	-6.66	1.44	1.53
1	A	33	LYS	N-CA	-6.65	1.38	1.46
1	A	296	LEU	N-CA	-6.65	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	366	ASP	CA-C	-6.65	1.42	1.52
1	A	4	ASN	CA-C	-6.63	1.43	1.52
1	A	70	ASN	CA-C	-6.63	1.43	1.52
1	A	249	HIS	CA-C	-6.63	1.44	1.52
1	A	11	ILE	CA-CB	-6.62	1.46	1.54
1	A	235	ASN	N-CA	-6.61	1.38	1.46
1	A	105	ASN	N-CA	-6.58	1.37	1.46
1	A	96	PHE	CA-C	-6.57	1.44	1.52
1	A	256	GLU	N-CA	-6.57	1.37	1.46
1	A	250	GLU	N-CA	-6.56	1.38	1.46
1	A	113	GLN	CA-C	-6.56	1.44	1.52
1	A	165	LEU	CA-C	-6.56	1.44	1.52
1	A	248	LEU	N-CA	-6.55	1.38	1.46
1	A	291	PHE	CA-C	-6.55	1.44	1.53
1	A	216	MET	CA-C	-6.54	1.44	1.52
1	A	236	TRP	N-CA	-6.54	1.38	1.46
1	A	134	CYS	CA-C	-6.52	1.44	1.52
1	A	148	LEU	CA-C	-6.51	1.44	1.52
1	A	300	ILE	N-CA	-6.51	1.39	1.46
1	A	27	VAL	CA-C	-6.50	1.44	1.52
1	A	191	ARG	CA-C	-6.48	1.44	1.52
1	A	149	VAL	CA-C	-6.47	1.45	1.52
1	A	149	VAL	CA-CB	-6.46	1.46	1.54
1	A	306	GLU	N-CA	-6.46	1.37	1.46
1	A	403	ARG	N-CA	-6.44	1.38	1.46
1	A	191	ARG	N-CA	-6.43	1.38	1.46
1	A	202	ILE	CA-C	-6.41	1.45	1.52
1	A	383	LYS	CA-C	-6.41	1.43	1.52
1	A	37	GLU	CA-C	-6.40	1.44	1.52
1	A	400	GLU	CA-C	-6.39	1.44	1.52
1	A	274	LEU	CA-C	-6.38	1.43	1.52
1	A	35	ASN	CA-C	-6.38	1.44	1.52
1	A	245	VAL	N-CA	-6.38	1.39	1.46
1	A	226	THR	CA-C	-6.38	1.44	1.52
1	A	36	LYS	N-CA	-6.37	1.38	1.46
1	A	288	ILE	CA-C	-6.37	1.44	1.52
1	A	271	ILE	CA-C	-6.36	1.45	1.52
1	A	147	SER	CA-C	-6.33	1.44	1.52
1	A	34	GLY	CA-C	-6.33	1.45	1.52
1	A	251	ILE	CA-C	-6.30	1.43	1.52
1	A	241	ASN	CA-C	-6.29	1.44	1.52
1	A	46	PHE	CA-C	-6.29	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	295	SER	CA-C	-6.29	1.43	1.52
1	A	270	LEU	N-CA	-6.28	1.38	1.46
1	A	402	LEU	CA-C	-6.28	1.44	1.52
1	A	388	LEU	N-CA	-6.27	1.38	1.46
1	A	179	ALA	CA-C	-6.27	1.44	1.52
1	A	149	VAL	N-CA	-6.25	1.39	1.46
1	A	188	GLU	N-CA	-6.24	1.39	1.46
1	A	216	MET	N-CA	-6.24	1.38	1.46
1	A	16	HIS	CA-C	-6.24	1.45	1.53
1	A	379	MET	CA-C	-6.24	1.44	1.53
1	A	236	TRP	CA-C	-6.23	1.45	1.52
1	A	127	ILE	CA-CB	-6.23	1.46	1.54
1	A	301	LYS	N-CA	-6.22	1.38	1.46
1	A	276	ILE	N-CA	-6.22	1.39	1.46
1	A	104	ALA	CA-C	-6.22	1.43	1.52
1	A	271	ILE	N-CA	-6.21	1.39	1.46
1	A	161	PRO	CA-C	-6.20	1.46	1.52
1	A	287	ARG	CA-C	-6.16	1.44	1.52
1	A	118	LYS	N-CA	-6.16	1.37	1.46
1	A	247	THR	N-CA	-6.16	1.39	1.46
1	A	350	TYR	CA-C	-6.16	1.44	1.52
1	A	276	ILE	CA-CB	-6.14	1.49	1.53
1	A	373	TYR	CA-C	-6.14	1.45	1.52
1	A	189	PHE	CA-C	-6.12	1.44	1.52
1	A	364	ILE	CA-C	-6.12	1.44	1.52
1	A	201	ASP	CA-C	-6.12	1.45	1.52
1	A	299	SER	N-CA	-6.11	1.38	1.46
1	A	33	LYS	CA-C	-6.11	1.44	1.52
1	A	111	LEU	N-CA	-6.11	1.38	1.46
1	A	132	LEU	CA-C	-6.10	1.45	1.52
1	A	146	GLY	CA-C	-6.09	1.45	1.51
1	A	152	LEU	CA-C	-6.09	1.44	1.52
1	A	158	PHE	CA-C	-6.08	1.45	1.52
1	A	219	ILE	CA-C	-6.05	1.44	1.52
1	A	312	GLU	CA-C	-6.04	1.45	1.53
1	A	132	LEU	N-CA	-6.03	1.39	1.46
1	A	133	ILE	CA-C	-6.00	1.45	1.52
1	A	67	HIS	CA-C	-6.00	1.43	1.52
1	A	380	THR	CA-C	-5.99	1.45	1.52
1	A	399	GLN	CA-C	-5.97	1.44	1.52
1	A	59	ASN	CA-C	-5.96	1.45	1.52
1	A	344	ARG	CA-C	-5.95	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	VAL	CA-C	-5.93	1.45	1.52
1	A	2	LEU	CA-C	-5.92	1.45	1.52
1	A	240	ALA	N-CA	-5.92	1.39	1.46
1	A	108	LEU	CA-C	-5.92	1.44	1.52
1	A	208	VAL	CA-C	-5.92	1.45	1.52
1	A	14	THR	N-CA	-5.92	1.38	1.46
1	A	345	ASN	N-CA	-5.89	1.39	1.46
1	A	27	VAL	N-CA	-5.89	1.39	1.46
1	A	38	ALA	N-CA	-5.89	1.39	1.46
1	A	235	ASN	CA-C	-5.87	1.45	1.52
1	A	225	GLY	CA-C	-5.87	1.43	1.51
1	A	59	ASN	N-CA	-5.85	1.39	1.46
1	A	280	PHE	N-CA	-5.84	1.38	1.46
1	A	113	GLN	N-CA	-5.81	1.39	1.46
1	A	151	GLN	N-CA	-5.79	1.39	1.46
1	A	125	GLU	CA-C	-5.78	1.45	1.52
1	A	166	ILE	N-CA	-5.78	1.39	1.46
1	A	315	PHE	CA-C	-5.77	1.45	1.52
1	A	371	VAL	CA-CB	-5.77	1.47	1.54
1	A	24	ARG	N-CA	-5.76	1.39	1.46
1	A	157	PHE	CA-C	-5.76	1.44	1.52
1	A	293	LEU	CA-C	-5.75	1.45	1.52
1	A	121	ASN	N-CA	-5.73	1.38	1.46
1	A	213	ASN	N-CA	-5.72	1.39	1.46
1	A	122	GLU	CA-C	-5.70	1.45	1.52
1	A	182	LEU	CA-C	-5.70	1.45	1.52
1	A	22	SER	N-CA	-5.70	1.39	1.46
1	A	386	ILE	CA-CB	-5.69	1.47	1.54
1	A	203	LYS	CA-C	-5.69	1.45	1.52
1	A	24	ARG	CA-C	-5.68	1.45	1.52
1	A	231	ASN	CA-C	-5.68	1.45	1.52
1	A	324	PHE	CA-C	-5.67	1.45	1.52
1	A	336	ASP	N-CA	-5.67	1.38	1.46
1	A	222	SER	N-CA	-5.65	1.39	1.46
1	A	367	ASN	CA-C	-5.65	1.45	1.53
1	A	144	GLY	CA-C	-5.64	1.46	1.52
1	A	373	TYR	N-CA	-5.63	1.39	1.46
1	A	23	ILE	CA-CB	-5.63	1.47	1.54
1	A	370	ALA	CA-C	-5.62	1.45	1.52
1	A	304	LEU	CA-C	-5.62	1.45	1.52
1	A	226	THR	CA-CB	-5.61	1.44	1.53
1	A	258	TYR	N-CA	-5.61	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	TRP	N-CA	-5.60	1.39	1.46
1	A	397	GLU	CA-C	-5.60	1.45	1.52
1	A	52	CYS	CA-C	-5.59	1.45	1.52
1	A	367	ASN	CA-CB	-5.59	1.45	1.53
1	A	385	TYR	CA-C	-5.59	1.45	1.52
1	A	386	ILE	CA-C	-5.58	1.46	1.52
1	A	118	LYS	CA-C	-5.58	1.45	1.52
1	A	218	ARG	N-CA	-5.57	1.39	1.46
1	A	391	GLU	CA-CB	-5.57	1.44	1.53
1	A	123	GLU	CA-C	-5.56	1.45	1.52
1	A	13	SER	N-CA	-5.56	1.38	1.46
1	A	313	HIS	N-CA	-5.55	1.39	1.45
1	A	175	GLU	N-CA	-5.54	1.39	1.46
1	A	344	ARG	N-CA	-5.54	1.39	1.46
1	A	285	LYS	CA-C	-5.54	1.46	1.52
1	A	117	ARG	CA-C	-5.52	1.45	1.52
1	A	25	TRP	CA-C	-5.51	1.45	1.52
1	A	366	ASP	N-CA	-5.51	1.38	1.46
1	A	245	VAL	CA-CB	-5.50	1.47	1.54
1	A	55	THR	N-CA	-5.47	1.39	1.46
1	A	151	GLN	CA-C	-5.47	1.46	1.52
1	A	214	THR	CA-C	-5.47	1.45	1.52
1	A	167	SER	CA-C	-5.47	1.46	1.52
1	A	395	LEU	N-CA	-5.47	1.39	1.46
1	A	183	LEU	N-CA	-5.46	1.39	1.46
1	A	72	ILE	N-CA	-5.45	1.38	1.46
1	A	252	ASN	CA-C	-5.45	1.46	1.52
1	A	110	LYS	CA-C	-5.45	1.45	1.52
1	A	187	ASP	N-CA	-5.45	1.39	1.46
1	A	231	ASN	N-CA	-5.44	1.39	1.46
1	A	286	ALA	CA-C	-5.44	1.46	1.52
1	A	122	GLU	N-CA	-5.44	1.39	1.46
1	A	176	ILE	CA-C	-5.44	1.45	1.52
1	A	333	PHE	N-CA	-5.43	1.39	1.46
1	A	232	ARG	N-CA	-5.42	1.39	1.46
1	A	256	GLU	CA-C	-5.42	1.45	1.52
1	A	365	TRP	NE1-CE2	-5.40	1.31	1.37
1	A	372	CYS	CA-C	-5.40	1.46	1.52
1	A	297	GLU	CA-C	-5.38	1.45	1.52
1	A	38	ALA	CA-C	-5.38	1.45	1.52
1	A	197	PHE	N-CA	-5.38	1.38	1.46
1	A	68	LEU	CA-C	-5.38	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	274	LEU	N-CA	-5.37	1.39	1.46
1	A	95	LEU	N-CA	-5.37	1.39	1.46
1	A	215	GLN	N-CA	-5.36	1.39	1.46
1	A	95	LEU	CA-C	-5.36	1.45	1.52
1	A	393	LYS	CA-C	-5.35	1.45	1.52
1	A	397	GLU	N-CA	-5.35	1.39	1.46
1	A	346	THR	CA-C	-5.35	1.46	1.52
1	A	227	LYS	N-CA	-5.34	1.39	1.46
1	A	153	ILE	CA-CB	-5.34	1.47	1.54
1	A	21	ILE	CA-C	-5.34	1.45	1.53
1	A	238	GLU	N-CA	-5.34	1.39	1.46
1	A	127	ILE	CA-C	-5.33	1.46	1.52
1	A	269	ASP	N-CA	-5.33	1.40	1.46
1	A	8	LEU	N-CA	-5.32	1.39	1.46
1	A	147	SER	N-CA	-5.31	1.40	1.46
1	A	314	GLN	N-CA	-5.31	1.39	1.46
1	A	88	THR	CA-C	-5.31	1.46	1.52
1	A	18	VAL	N-CA	-5.30	1.39	1.46
1	A	252	ASN	N-CA	-5.30	1.40	1.46
1	A	243	ASN	C-N	-5.30	1.27	1.33
1	A	367	ASN	N-CA	-5.30	1.39	1.45
1	A	239	VAL	N-CA	-5.29	1.39	1.46
1	A	186	ILE	N-CA	-5.29	1.40	1.46
1	A	154	ARG	CA-C	-5.28	1.46	1.52
1	A	272	LYS	N-CA	-5.28	1.40	1.46
1	A	49	GLY	CA-C	-5.26	1.44	1.51
1	A	192	GLU	CA-C	-5.25	1.46	1.52
1	A	339	THR	CA-C	-5.25	1.45	1.52
1	A	353	LEU	CA-C	-5.24	1.45	1.52
1	A	346	THR	N-CA	-5.23	1.40	1.46
1	A	229	LEU	CA-C	-5.23	1.45	1.52
1	A	380	THR	CA-CB	-5.23	1.45	1.53
1	A	184	SER	N-CA	-5.22	1.40	1.46
1	A	44	TYR	CA-C	-5.21	1.46	1.52
1	A	332	ASP	CA-C	-5.20	1.45	1.52
1	A	28	ILE	CA-C	-5.20	1.46	1.52
1	A	251	ILE	CA-CB	-5.18	1.47	1.54
1	A	393	LYS	N-CA	-5.18	1.39	1.46
1	A	382	PRO	CA-C	-5.17	1.45	1.52
1	A	90	SER	CA-C	-5.17	1.45	1.52
1	A	117	ARG	N-CA	-5.16	1.40	1.46
1	A	17	SER	CA-C	-5.16	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	316	GLU	N-CA	-5.16	1.39	1.46
1	A	133	ILE	N-CA	-5.16	1.40	1.46
1	A	294	HIS	CA-C	-5.16	1.46	1.52
1	A	368	GLU	N-CA	-5.16	1.40	1.46
1	A	408	ARG	CA-C	-5.16	1.46	1.52
1	A	264	THR	N-CA	-5.14	1.40	1.46
1	A	337	VAL	N-CA	-5.13	1.39	1.46
1	A	166	ILE	CA-CB	-5.13	1.48	1.54
1	A	35	ASN	N-CA	-5.12	1.40	1.46
1	A	92	VAL	CA-C	-5.12	1.46	1.52
1	A	355	GLU	CA-C	-5.12	1.45	1.52
1	A	249	HIS	CB-CG	-5.11	1.43	1.50
1	A	129	ASP	CA-C	-5.11	1.47	1.52
1	A	195	ARG	CA-C	-5.11	1.45	1.52
1	A	72	ILE	CA-CB	-5.11	1.47	1.54
1	A	343	ILE	N-CA	-5.10	1.40	1.46
1	A	181	VAL	N-CA	-5.07	1.40	1.46
1	A	356	ILE	CA-C	-5.07	1.47	1.52
1	A	314	GLN	CA-C	-5.06	1.46	1.53
1	A	390	ARG	C-N	-5.06	1.27	1.33
1	A	369	TYR	N-CA	-5.05	1.40	1.46
1	A	347	LEU	CA-C	-5.05	1.45	1.52
1	A	187	ASP	CA-C	-5.05	1.46	1.52
1	A	194	ASP	CA-C	-5.04	1.46	1.52
1	A	76	ARG	CA-C	-5.04	1.46	1.53
1	A	12	HIS	N-CA	-5.04	1.39	1.46
1	A	255	PRO	CA-C	-5.03	1.43	1.52
1	A	226	THR	N-CA	-5.02	1.39	1.46
1	A	36	LYS	CA-C	-5.02	1.46	1.52

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	GLU	N-CA-C	-15.41	91.95	110.44
1	A	338	ASN	CA-CB-CG	-15.13	97.47	112.60
1	A	197	PHE	CA-CB-CG	-13.47	100.33	113.80
1	A	119	PHE	CA-CB-CG	-13.12	100.68	113.80
1	A	331	ALA	CA-C-N	13.02	138.22	120.38
1	A	331	ALA	C-N-CA	13.02	138.22	120.38
1	A	96	PHE	CA-CB-CG	-12.89	100.91	113.80
1	A	157	PHE	CA-CB-CG	-12.74	101.06	113.80
1	A	257	ASN	CA-CB-CG	-11.64	100.96	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	PHE	CA-CB-CG	-10.99	102.81	113.80
1	A	360	PHE	CA-CB-CG	-10.58	103.22	113.80
1	A	79	PHE	CA-CB-CG	-10.01	103.80	113.80
1	A	291	PHE	CA-CB-CG	-9.96	103.84	113.80
1	A	391	GLU	N-CA-CB	-9.90	95.50	110.16
1	A	365	TRP	N-CA-C	-9.75	95.61	108.19
1	A	244	VAL	N-CA-CB	-9.73	100.01	110.62
1	A	12	HIS	CA-CB-CG	-9.35	104.45	113.80
1	A	160	CYS	N-CA-CB	9.34	120.36	109.72
1	A	341	ASN	CA-CB-CG	-9.26	103.34	112.60
1	A	336	ASP	CA-CB-CG	-9.22	103.38	112.60
1	A	227	LYS	N-CA-C	-9.07	101.64	112.89
1	A	189	PHE	CA-CB-CG	-8.98	104.82	113.80
1	A	158	PHE	CA-CB-CG	-8.93	104.87	113.80
1	A	80	ASP	CA-CB-CG	-8.90	103.70	112.60
1	A	88	THR	N-CA-C	-8.85	98.89	110.39
1	A	113	GLN	CB-CG-CD	-8.79	97.66	112.60
1	A	123	GLU	N-CA-C	-8.66	102.72	113.38
1	A	366	ASP	N-CA-C	-8.64	99.82	110.88
1	A	59	ASN	CA-CB-CG	-8.31	104.29	112.60
1	A	172	ASP	CA-CB-CG	-8.29	104.31	112.60
1	A	258	TYR	CA-CB-CG	-8.21	99.12	113.90
1	A	174	ASP	CA-CB-CG	-8.19	104.41	112.60
1	A	197	PHE	N-CA-C	-7.87	97.37	109.65
1	A	226	THR	N-CA-C	-7.87	102.76	113.30
1	A	190	MET	CB-CA-C	-7.69	98.03	110.79
1	A	298	ASN	CA-CB-CG	-7.65	104.95	112.60
1	A	104	ALA	CA-C-N	7.61	131.88	120.31
1	A	104	ALA	C-N-CA	7.61	131.88	120.31
1	A	19	ASN	N-CA-C	-7.61	100.74	112.99
1	A	75	ASP	CA-CB-CG	-7.60	105.00	112.60
1	A	336	ASP	CA-C-N	7.47	132.56	120.30
1	A	336	ASP	C-N-CA	7.47	132.56	120.30
1	A	19	ASN	CA-CB-CG	-7.38	105.22	112.60
1	A	243	ASN	CA-CB-CG	-7.38	105.22	112.60
1	A	228	ASP	CA-CB-CG	7.26	119.86	112.60
1	A	121	ASN	CA-CB-CG	-7.21	105.39	112.60
1	A	350	TYR	CA-CB-CG	-7.16	101.01	113.90
1	A	334	PHE	CA-CB-CG	-7.15	106.65	113.80
1	A	94	ASP	CB-CA-C	-7.08	98.82	110.85
1	A	338	ASN	O-C-N	7.01	129.29	122.07
1	A	25	TRP	CA-CB-CG	-7.01	100.29	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	GLY	N-CA-C	-6.99	99.27	112.27
1	A	124	GLY	N-CA-C	-6.88	106.46	115.47
1	A	407	GLN	CB-CG-CD	-6.77	101.09	112.60
1	A	89	PRO	N-CA-C	-6.75	105.16	114.27
1	A	305	ASP	CA-CB-CG	-6.74	105.86	112.60
1	A	121	ASN	N-CA-C	-6.72	96.48	110.80
1	A	391	GLU	CB-CG-CD	-6.70	101.21	112.60
1	A	294	HIS	N-CA-C	-6.69	103.92	111.14
1	A	104	ALA	CA-C-O	6.65	128.37	120.92
1	A	17	SER	N-CA-C	-6.63	104.33	112.88
1	A	196	LEU	N-CA-C	-6.63	105.34	113.50
1	A	355	GLU	N-CA-C	-6.60	104.94	114.12
1	A	101	ASN	CA-CB-CG	-6.57	106.03	112.60
1	A	131	PHE	CA-CB-CG	-6.52	107.28	113.80
1	A	309	PHE	N-CA-C	-6.51	105.38	113.38
1	A	333	PHE	N-CA-CB	-6.48	98.52	110.18
1	A	341	ASN	N-CA-C	-6.48	104.14	111.14
1	A	109	ASP	CA-CB-CG	-6.46	106.14	112.60
1	A	266	ASP	CA-CB-CG	-6.46	106.14	112.60
1	A	243	ASN	CB-CA-C	-6.44	100.77	110.88
1	A	65	MET	N-CA-C	-6.42	103.04	113.19
1	A	330	ASN	CA-CB-CG	-6.41	106.19	112.60
1	A	369	TYR	N-CA-C	-6.40	98.41	108.14
1	A	230	LYS	CA-C-N	6.38	128.83	120.28
1	A	230	LYS	C-N-CA	6.38	128.83	120.28
1	A	177	ASN	CB-CA-C	-6.32	100.91	110.90
1	A	97	ASP	CA-C-N	6.30	125.80	119.24
1	A	97	ASP	C-N-CA	6.30	125.80	119.24
1	A	105	ASN	CA-CB-CG	-6.30	106.30	112.60
1	A	5	SER	CA-C-N	6.29	129.00	120.38
1	A	5	SER	C-N-CA	6.29	129.00	120.38
1	A	258	TYR	O-C-N	6.29	131.32	123.15
1	A	401	GLN	N-CA-C	-6.26	104.37	111.07
1	A	233	TYR	CA-CB-CG	-6.24	102.68	113.90
1	A	407	GLN	N-CA-C	-6.23	104.38	112.23
1	A	252	ASN	N-CA-C	-6.22	104.42	111.14
1	A	214	THR	CA-C-N	6.20	128.58	120.28
1	A	214	THR	C-N-CA	6.20	128.58	120.28
1	A	315	PHE	N-CA-C	6.15	117.98	111.28
1	A	373	TYR	CA-CB-CG	-6.12	102.89	113.90
1	A	385	TYR	CA-C-O	6.11	127.02	120.55
1	A	21	ILE	CB-CA-C	-6.09	102.85	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	PHE	CA-CB-CG	-6.09	107.71	113.80
1	A	28	ILE	N-CA-C	-6.08	99.59	108.11
1	A	314	GLN	N-CA-CB	-6.05	100.41	110.39
1	A	340	GLU	CA-C-O	6.04	126.95	120.55
1	A	195	ARG	N-CA-C	-6.01	105.95	113.28
1	A	115	LEU	N-CA-CB	-5.99	101.33	110.01
1	A	249	HIS	CA-CB-CG	-5.97	107.83	113.80
1	A	275	SER	CA-C-N	5.97	124.00	120.24
1	A	275	SER	C-N-CA	5.97	124.00	120.24
1	A	44	TYR	CA-CB-CG	-5.97	103.16	113.90
1	A	5	SER	N-CA-C	-5.96	99.34	108.76
1	A	288	ILE	N-CA-C	-5.95	96.96	109.34
1	A	260	SER	N-CA-C	-5.91	100.59	108.74
1	A	237	LYS	CB-CA-C	-5.90	100.65	110.68
1	A	6	ASN	CA-C-O	5.87	126.97	120.63
1	A	313	HIS	CA-C-N	5.85	130.98	122.85
1	A	313	HIS	C-N-CA	5.85	130.98	122.85
1	A	395	LEU	N-CA-C	-5.84	105.17	112.93
1	A	212	ASP	N-CA-CB	5.83	119.93	110.42
1	A	70	ASN	CA-CB-CG	-5.79	106.81	112.60
1	A	351	LYS	N-CA-C	-5.77	98.50	110.80
1	A	352	ARG	CA-C-N	5.76	128.78	120.38
1	A	352	ARG	C-N-CA	5.76	128.78	120.38
1	A	332	ASP	CA-CB-CG	-5.74	106.86	112.60
1	A	261	ASP	N-CA-C	-5.72	105.50	112.88
1	A	248	LEU	CA-C-O	5.71	126.81	120.82
1	A	63	SER	CA-C-N	5.69	132.41	121.54
1	A	63	SER	C-N-CA	5.69	132.41	121.54
1	A	52	CYS	CB-CA-C	5.67	121.70	110.42
1	A	51	THR	N-CA-CB	5.67	120.07	110.49
1	A	296	LEU	N-CA-C	-5.66	105.02	111.07
1	A	308	PHE	N-CA-C	-5.65	106.51	113.41
1	A	13	SER	N-CA-C	-5.65	105.89	112.89
1	A	92	VAL	CA-C-N	5.62	128.59	120.38
1	A	92	VAL	C-N-CA	5.62	128.59	120.38
1	A	174	ASP	CB-CA-C	-5.59	102.07	110.90
1	A	332	ASP	CA-C-O	5.58	126.66	120.63
1	A	274	LEU	CA-C-N	-5.57	113.79	122.42
1	A	274	LEU	C-N-CA	-5.57	113.79	122.42
1	A	97	ASP	N-CA-C	-5.56	99.86	109.15
1	A	199	ASN	CA-CB-CG	-5.55	107.05	112.60
1	A	331	ALA	CA-C-O	5.53	128.43	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	ASN	N-CA-C	-5.51	105.28	111.28
1	A	94	ASP	CA-CB-CG	-5.49	107.11	112.60
1	A	103	ASN	CA-C-N	5.49	129.05	120.82
1	A	103	ASN	C-N-CA	5.49	129.05	120.82
1	A	212	ASP	CA-C-O	5.48	126.23	120.36
1	A	49	GLY	CA-C-N	-5.46	115.47	123.00
1	A	49	GLY	C-N-CA	-5.46	115.47	123.00
1	A	3	LEU	N-CA-C	-5.45	102.45	110.52
1	A	6	ASN	CB-CA-C	-5.44	101.44	110.68
1	A	47	SER	N-CA-C	-5.41	103.83	110.65
1	A	76	ARG	CD-NE-CZ	-5.38	116.86	124.40
1	A	60	PHE	CA-CB-CG	-5.37	108.43	113.80
1	A	168	LEU	CB-CA-C	-5.37	102.70	109.31
1	A	276	ILE	CA-C-O	-5.37	114.28	118.85
1	A	52	CYS	CA-CB-SG	-5.37	102.05	114.40
1	A	126	VAL	N-CA-C	-5.37	101.91	109.21
1	A	43	GLY	N-CA-C	-5.36	108.77	114.67
1	A	15	ASN	CA-CB-CG	-5.36	107.24	112.60
1	A	146	GLY	CA-C-O	5.35	126.56	121.05
1	A	152	LEU	N-CA-C	5.35	118.60	111.75
1	A	10	HIS	N-CA-C	-5.32	105.48	111.28
1	A	145	TRP	CB-CG-CD2	-5.29	119.39	126.80
1	A	41	PHE	CA-C-N	5.25	127.84	120.28
1	A	41	PHE	C-N-CA	5.25	127.84	120.28
1	A	240	ALA	CA-C-O	5.24	126.33	120.82
1	A	16	HIS	N-CA-C	-5.24	104.56	112.99
1	A	256	GLU	N-CA-C	-5.23	105.64	112.23
1	A	335	LYS	N-CA-C	-5.23	105.66	111.36
1	A	317	THR	N-CA-C	-5.21	106.70	113.16
1	A	145	TRP	CB-CG-CD1	5.18	134.68	126.90
1	A	233	TYR	N-CA-C	-5.18	105.96	113.21
1	A	237	LYS	N-CA-CB	5.17	117.82	110.06
1	A	400	GLU	N-CA-C	-5.16	105.65	111.28
1	A	217	GLN	CA-CB-CG	-5.14	103.82	114.10
1	A	217	GLN	CB-CG-CD	-5.13	103.87	112.60
1	A	365	TRP	N-CA-CB	5.11	118.83	110.55
1	A	120	THR	N-CA-C	-5.11	102.00	109.81
1	A	230	LYS	N-CA-C	-5.11	107.05	113.28
1	A	266	ASP	CA-C-N	5.07	124.52	119.24
1	A	266	ASP	C-N-CA	5.07	124.52	119.24
1	A	160	CYS	CB-CA-C	-5.03	102.42	109.96
1	A	258	TYR	N-CA-C	-5.03	101.73	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	LYS	N-CA-C	5.01	117.12	111.11
1	A	177	ASN	CA-CB-CG	-5.01	107.59	112.60
1	A	379	MET	CG-SD-CE	-5.00	89.90	100.90

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	ARG	Sidechain
1	A	197	PHE	Sidechain
1	A	233	TYR	Sidechain
1	A	280	PHE	Sidechain
1	A	287	ARG	Sidechain
1	A	313	HIS	Mainchain
1	A	315	PHE	Sidechain
1	A	373	TYR	Sidechain
1	A	76	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	A	3277	0	3204	157	0
2	A	28	0	12	2	0
All	All	3305	0	3216	157	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 24.

All (157) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:HIS:CE1	1:A:379:MET:HB3	2.08	0.88
1:A:316:GLU:H	1:A:316:GLU:CD	1.94	0.74
1:A:96:PHE:C	1:A:104:ALA:HB1	2.18	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:TRP:CD2	1:A:367:ASN:HB2	2.28	0.69
1:A:108:LEU:HA	1:A:111:LEU:HD12	1.74	0.68
1:A:101:ASN:O	1:A:104:ALA:HB2	1.95	0.67
1:A:365:TRP:CE2	1:A:367:ASN:HB3	2.30	0.66
1:A:225:GLY:HA2	1:A:231:ASN:HD22	1.59	0.66
1:A:22:SER:H	1:A:252:ASN:HD21	1.44	0.65
1:A:313:HIS:CE1	1:A:380:THR:C	2.76	0.64
1:A:326:LEU:HG	1:A:365:TRP:CD2	2.33	0.64
1:A:392:GLY:HA2	1:A:395:LEU:HD12	1.81	0.62
1:A:21:ILE:HB	1:A:252:ASN:HD21	1.63	0.62
1:A:22:SER:H	1:A:252:ASN:ND2	1.97	0.61
1:A:287:ARG:HD3	1:A:288:ILE:H	1.65	0.61
1:A:105:ASN:HA	1:A:108:LEU:HD12	1.83	0.60
1:A:188:GLU:HA	1:A:191:ARG:HH11	1.66	0.59
1:A:215:GLN:HA	1:A:218:ARG:HH21	1.67	0.59
1:A:7:GLU:H	1:A:7:GLU:CD	2.10	0.59
1:A:313:HIS:HE1	1:A:380:THR:C	2.11	0.58
1:A:188:GLU:CD	1:A:188:GLU:C	2.71	0.58
1:A:280:PHE:CD1	1:A:380:THR:HA	2.39	0.57
1:A:188:GLU:HA	1:A:191:ARG:HE	1.70	0.57
1:A:326:LEU:HG	1:A:365:TRP:CE2	2.38	0.56
1:A:352:ARG:HB2	1:A:355:GLU:CD	2.31	0.56
1:A:365:TRP:CD1	1:A:367:ASN:H	2.23	0.56
1:A:313:HIS:CE1	1:A:381:MET:O	2.60	0.55
1:A:365:TRP:CE2	1:A:367:ASN:CB	2.89	0.55
1:A:66:MET:HG3	1:A:67:HIS:CD2	2.41	0.55
1:A:14:THR:C	1:A:16:HIS:CE1	2.85	0.55
1:A:95:LEU:O	1:A:104:ALA:HA	2.06	0.55
1:A:46:PHE:H	1:A:50:THR:H	1.56	0.54
1:A:66:MET:SD	1:A:67:HIS:CG	3.01	0.53
1:A:74:GLU:H	1:A:74:GLU:CD	2.17	0.53
1:A:59:ASN:O	1:A:78:HIS:HA	2.09	0.53
1:A:285:LYS:HG3	1:A:371:VAL:HG11	1.90	0.52
1:A:327:ARG:C	1:A:365:TRP:CD1	2.87	0.52
1:A:252:ASN:C	1:A:252:ASN:HD22	2.18	0.52
1:A:60:PHE:CE2	1:A:79:PHE:O	2.64	0.51
1:A:121:ASN:OD1	1:A:127:ILE:HG21	2.11	0.51
1:A:214:THR:HA	1:A:217:GLN:OE1	2.11	0.51
1:A:231:ASN:C	1:A:233:TYR:H	2.20	0.50
1:A:98:PRO:HG3	1:A:105:ASN:HD21	1.76	0.50
1:A:338:ASN:HA	1:A:341:ASN:ND2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ASN:CG	1:A:368:GLU:H	2.19	0.50
1:A:215:GLN:CA	1:A:218:ARG:HH21	2.23	0.50
1:A:359:LYS:HG2	1:A:360:PHE:H	1.77	0.49
1:A:9:GLU:CD	1:A:9:GLU:C	2.80	0.49
1:A:313:HIS:HA	1:A:382:PRO:HA	1.93	0.49
1:A:324:PHE:HA	1:A:360:PHE:CE2	2.47	0.49
1:A:236:TRP:CD2	1:A:237:LYS:N	2.80	0.49
1:A:287:ARG:HD3	1:A:288:ILE:N	2.28	0.49
1:A:400:GLU:CD	1:A:400:GLU:C	2.80	0.49
1:A:61:ALA:HA	1:A:80:ASP:OD2	2.12	0.49
1:A:151:GLN:HG3	1:A:154:ARG:HH21	1.76	0.49
1:A:314:GLN:HE21	1:A:383:LYS:CG	2.25	0.49
1:A:126:VAL:HG12	1:A:128:VAL:H	1.77	0.49
1:A:46:PHE:HB2	1:A:48:ASN:OD1	2.13	0.49
1:A:316:GLU:CD	1:A:316:GLU:N	2.67	0.48
1:A:381:MET:SD	1:A:382:PRO:O	2.71	0.48
1:A:33:LYS:HA	2:A:900:GDP:C6	2.48	0.48
1:A:236:TRP:CE2	1:A:237:LYS:HG3	2.49	0.48
1:A:254:ILE:N	1:A:255:PRO:HD2	2.29	0.48
1:A:236:TRP:CZ2	1:A:237:LYS:HG2	2.49	0.47
1:A:46:PHE:H	1:A:50:THR:N	2.12	0.47
1:A:8:LEU:O	1:A:12:HIS:CG	2.67	0.47
1:A:235:ASN:HD21	1:A:236:TRP:CD1	2.32	0.47
1:A:253:ILE:O	1:A:256:GLU:HB3	2.14	0.47
1:A:323:GLY:C	1:A:360:PHE:CE1	2.93	0.47
1:A:386:ILE:O	1:A:389:ALA:HB3	2.15	0.47
1:A:229:LEU:HA	1:A:232:ARG:CZ	2.45	0.47
1:A:326:LEU:HD11	1:A:365:TRP:HB3	1.97	0.47
1:A:21:ILE:CB	1:A:252:ASN:HD21	2.28	0.47
1:A:123:GLU:C	1:A:125:GLU:H	2.23	0.47
1:A:286:ALA:O	1:A:371:VAL:HA	2.14	0.47
1:A:314:GLN:HE21	1:A:383:LYS:HG2	1.78	0.47
1:A:10:HIS:CD2	1:A:365:TRP:CE3	3.04	0.46
1:A:73:LYS:HA	1:A:76:ARG:HD2	1.98	0.46
1:A:236:TRP:CG	1:A:237:LYS:N	2.84	0.46
1:A:398:LYS:HA	1:A:401:GLN:CD	2.40	0.46
1:A:15:ASN:C	1:A:16:HIS:CG	2.93	0.46
1:A:120:THR:HA	1:A:125:GLU:O	2.15	0.46
1:A:267:PRO:O	1:A:271:ILE:HG12	2.15	0.46
1:A:295:SER:HA	1:A:298:ASN:OD1	2.15	0.46
1:A:234:VAL:HG22	1:A:235:ASN:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:TRP:CE3	1:A:367:ASN:HB2	2.51	0.46
1:A:102:PRO:C	1:A:104:ALA:H	2.22	0.46
1:A:118:LYS:HG3	1:A:119:PHE:CE2	2.51	0.46
1:A:152:LEU:HA	1:A:155:GLU:HB2	1.98	0.46
1:A:314:GLN:HE22	1:A:381:MET:HE1	1.81	0.46
1:A:39:ASP:O	1:A:42:ALA:HB3	2.16	0.45
1:A:365:TRP:CD2	1:A:367:ASN:CB	2.97	0.45
1:A:41:PHE:HA	1:A:44:TYR:CE2	2.51	0.45
1:A:66:MET:SD	1:A:66:MET:C	3.00	0.45
1:A:45:LYS:HA	1:A:51:THR:HA	2.00	0.44
1:A:224:LYS:HZ2	1:A:227:LYS:N	2.15	0.44
1:A:153:ILE:HA	1:A:158:PHE:HB2	1.99	0.44
1:A:327:ARG:HA	1:A:328:PRO:HD3	1.86	0.44
1:A:45:LYS:HG2	1:A:51:THR:HA	2.00	0.44
1:A:175:GLU:HA	1:A:178:ASN:OD1	2.17	0.44
1:A:151:GLN:HA	1:A:154:ARG:HE	1.83	0.44
1:A:104:ALA:HB3	1:A:105:ASN:OD1	2.18	0.44
1:A:10:HIS:CG	1:A:367:ASN:HD22	2.35	0.44
1:A:60:PHE:O	1:A:78:HIS:HB2	2.18	0.43
1:A:123:GLU:HB2	1:A:125:GLU:CD	2.43	0.43
1:A:188:GLU:CA	1:A:191:ARG:HH11	2.31	0.43
1:A:224:LYS:HG3	1:A:227:LYS:HG2	2.00	0.43
1:A:328:PRO:HD3	1:A:365:TRP:HE1	1.83	0.43
1:A:368:GLU:OE1	1:A:369:TYR:CE1	2.71	0.43
1:A:14:THR:O	1:A:16:HIS:CE1	2.72	0.43
1:A:174:ASP:HA	1:A:177:ASN:OD1	2.18	0.43
1:A:235:ASN:ND2	1:A:236:TRP:CD1	2.87	0.43
1:A:320:MET:HA	1:A:357:ALA:O	2.18	0.43
1:A:348:GLY:HA2	1:A:352:ARG:HA	2.00	0.43
1:A:145:TRP:HA	1:A:148:LEU:HB2	2.01	0.43
1:A:284:GLY:O	1:A:373:TYR:HA	2.18	0.42
1:A:341:ASN:O	1:A:344:ARG:HB3	2.18	0.42
1:A:46:PHE:CB	1:A:48:ASN:OD1	2.67	0.42
1:A:117:ARG:HH22	1:A:118:LYS:HD3	1.84	0.42
1:A:280:PHE:CE1	1:A:380:THR:HA	2.55	0.42
1:A:46:PHE:N	1:A:50:THR:O	2.51	0.42
1:A:115:LEU:O	1:A:119:PHE:CD1	2.73	0.42
1:A:287:ARG:HD2	1:A:289:ALA:HB2	2.01	0.42
1:A:341:ASN:O	1:A:345:ASN:CG	2.62	0.42
1:A:240:ALA:O	1:A:244:VAL:HG23	2.20	0.42
1:A:368:GLU:H	1:A:368:GLU:CD	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:MET:SD	1:A:67:HIS:CD2	3.13	0.42
1:A:63:SER:C	1:A:65:MET:H	2.27	0.42
1:A:19:ASN:HA	1:A:46:PHE:HB3	2.02	0.42
1:A:123:GLU:N	1:A:123:GLU:CD	2.77	0.42
1:A:166:ILE:O	1:A:210:VAL:HA	2.20	0.42
1:A:387:SER:HA	1:A:390:ARG:HE	1.85	0.41
1:A:330:ASN:H	1:A:330:ASN:ND2	2.16	0.41
1:A:387:SER:N	1:A:390:ARG:HH11	2.18	0.41
1:A:226:THR:HA	1:A:232:ARG:HE	1.84	0.41
1:A:387:SER:HA	1:A:390:ARG:NE	2.35	0.41
1:A:186:ILE:O	1:A:189:PHE:HB3	2.21	0.41
1:A:89:PRO:HB3	1:A:143:THR:HB	2.03	0.41
1:A:289:ALA:C	1:A:291:PHE:CZ	2.98	0.41
1:A:46:PHE:CD1	1:A:50:THR:O	2.74	0.41
1:A:263:VAL:HG11	1:A:360:PHE:O	2.21	0.41
1:A:313:HIS:HE1	1:A:380:THR:N	2.18	0.41
1:A:107:TYR:O	1:A:111:LEU:HG	2.21	0.41
1:A:367:ASN:OD1	1:A:369:TYR:CE2	2.74	0.41
1:A:60:PHE:O	1:A:79:PHE:O	2.39	0.41
1:A:169:PRO:HA	1:A:213:ASN:ND2	2.35	0.41
1:A:226:THR:HA	1:A:232:ARG:HH21	1.86	0.41
1:A:267:PRO:O	1:A:270:LEU:HB3	2.21	0.40
1:A:318:ALA:N	1:A:379:MET:HG2	2.36	0.40
1:A:365:TRP:HB2	1:A:366:ASP:H	1.68	0.40
1:A:321:TYR:CG	1:A:358:GLY:HA3	2.56	0.40
1:A:147:SER:HA	1:A:150:LEU:HD12	2.04	0.40
1:A:173:PRO:HA	1:A:176:ILE:HD12	2.03	0.40
1:A:188:GLU:HA	1:A:191:ARG:NH1	2.35	0.40
1:A:236:TRP:O	1:A:237:LYS:C	2.64	0.40
1:A:252:ASN:ND2	1:A:252:ASN:C	2.80	0.40
1:A:33:LYS:HB2	2:A:900:GDP:C8	2.57	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	412/484 (85%)	368 (89%)	32 (8%)	12 (3%)	3	23

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	48	ASN
1	A	51	THR
1	A	351	LYS
1	A	64	ASP
1	A	122	GLU
1	A	159	PRO
1	A	381	MET
1	A	169	PRO
1	A	172	ASP
1	A	382	PRO
1	A	225	GLY

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	357/418 (85%)	335 (94%)	22 (6%)	16	38

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	7	GLU
1	A	20	ASP
1	A	59	ASN
1	A	64	ASP
1	A	95	LEU
1	A	125	GLU

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Mol	Chain	Res	Type
1	A	155	GLU
1	A	187	ASP
1	A	214	THR
1	A	215	GLN
1	A	227	LYS
1	A	228	ASP
1	A	234	VAL
1	A	252	ASN
1	A	267	PRO
1	A	272	LYS
1	A	316	GLU
1	A	319	THR
1	A	354	ASP
1	A	365	TRP
1	A	400	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	231	ASN
1	A	252	ASN
1	A	314	GLN
1	A	330	ASN
1	A	407	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	GDP	A	900	-	29,30,30	1.43	4 (13%)	45,47,47	0.94	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	A	900	-	-	0/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	GDP	C1'-N9	-3.58	1.37	1.47
2	A	900	GDP	C4-N9	-2.65	1.31	1.38
2	A	900	GDP	C5-N7	-2.63	1.33	1.39
2	A	900	GDP	C2'-C1'	-2.60	1.45	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	GDP	O6-C6-N1	2.91	125.59	120.11

There are no chirality outliers.

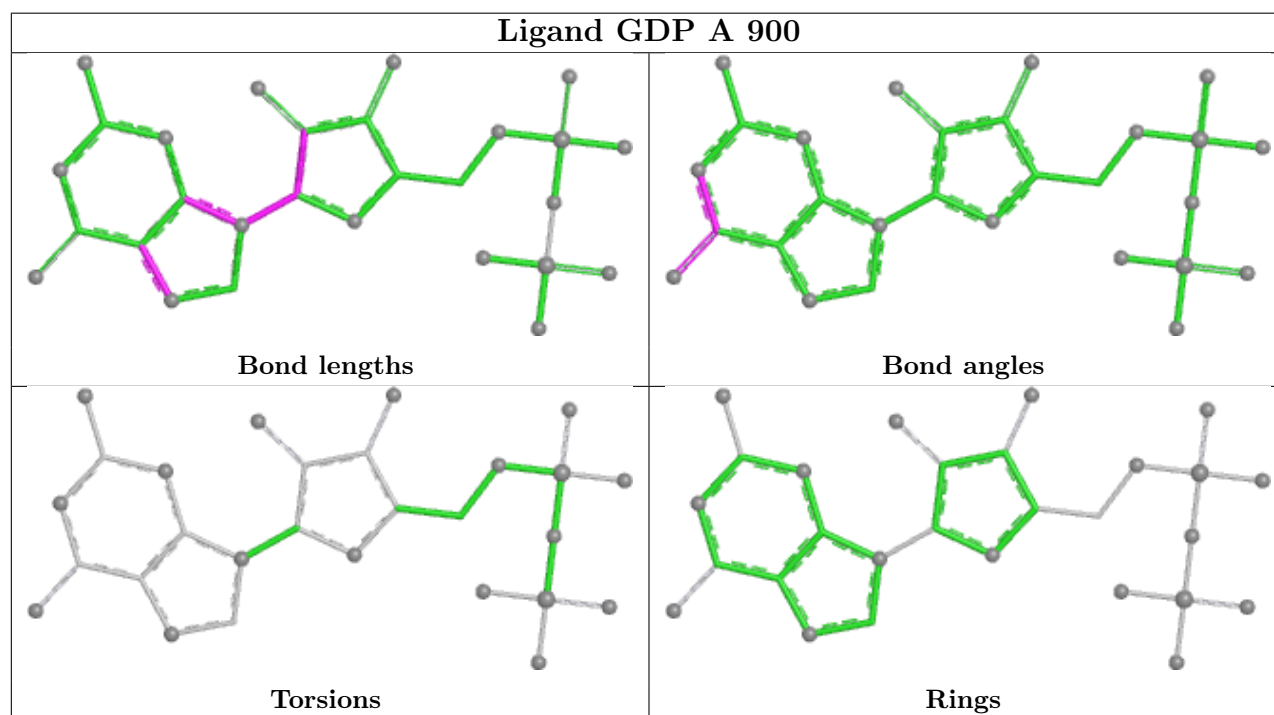
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	GDP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

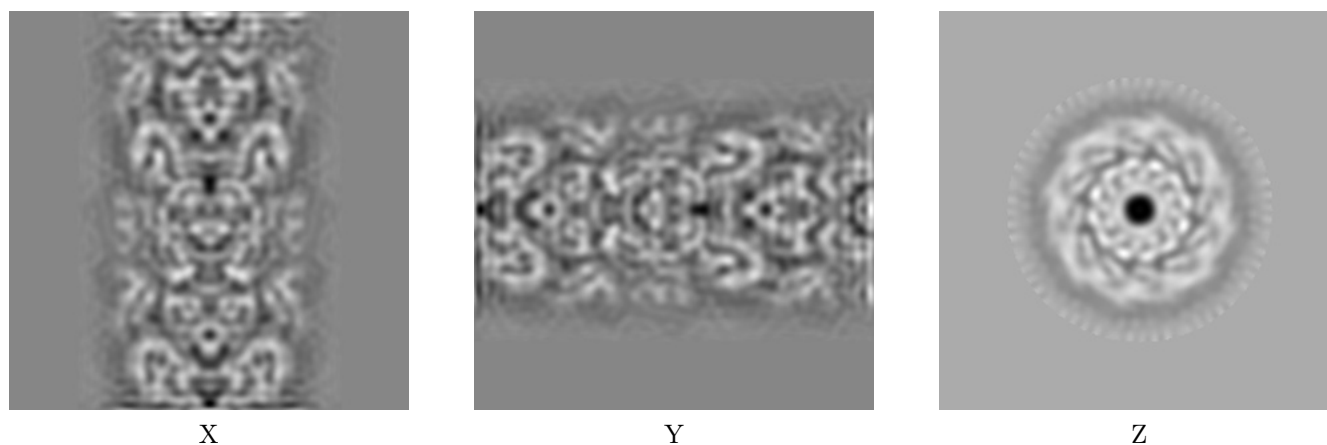
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5762. 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](#)

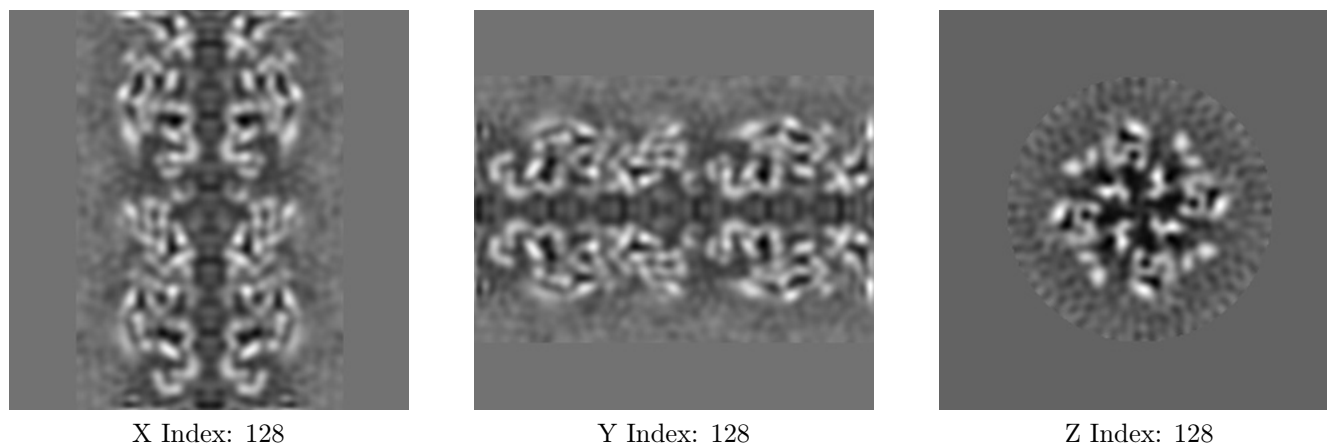
6.1.1 Primary map



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

6.2 Central slices [i](#)

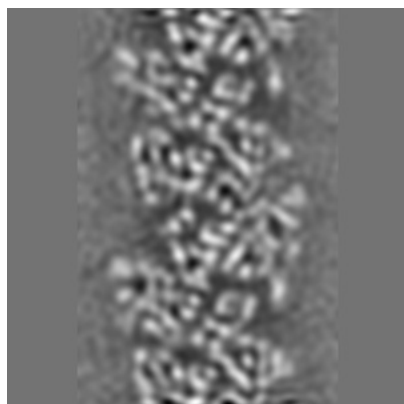
6.2.1 Primary map



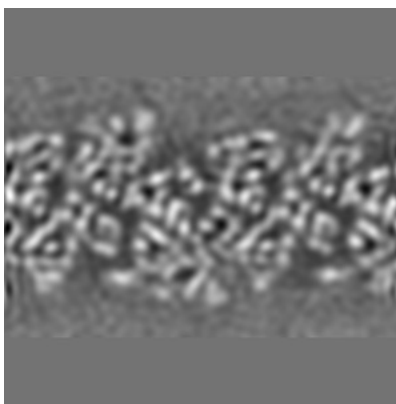
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 110



Y Index: 110

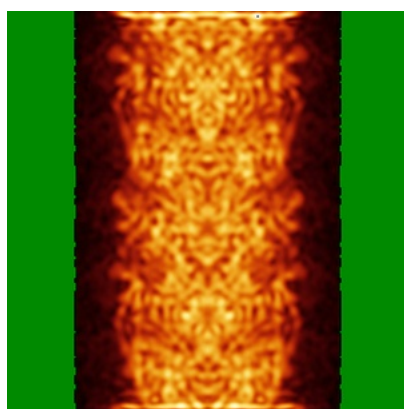


Z Index: 253

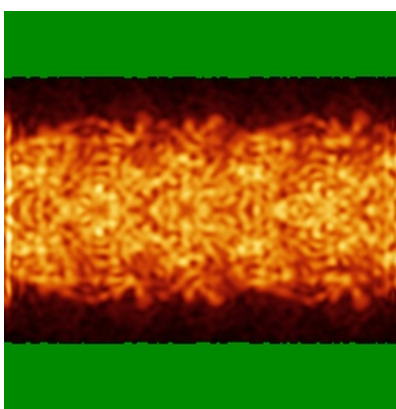
The images above show the largest variance slices of the map in three orthogonal directions.

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

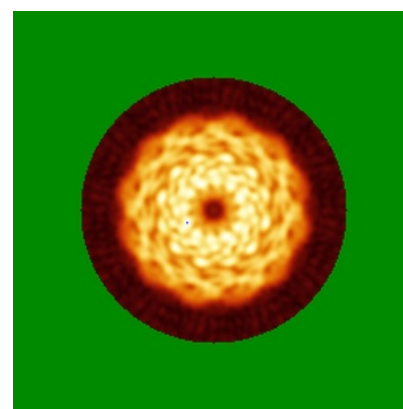
6.4.1 Primary map



X



Y

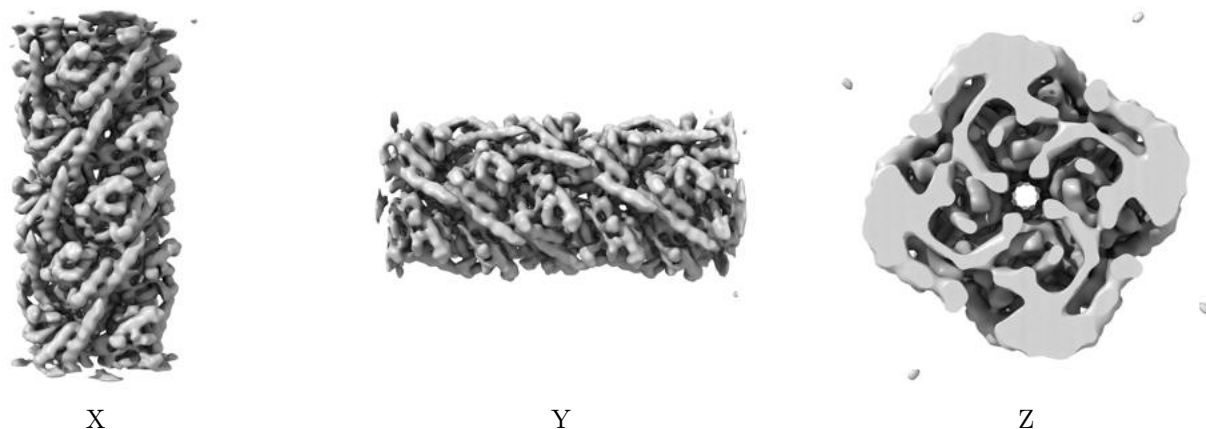


Z

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 0.0155. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

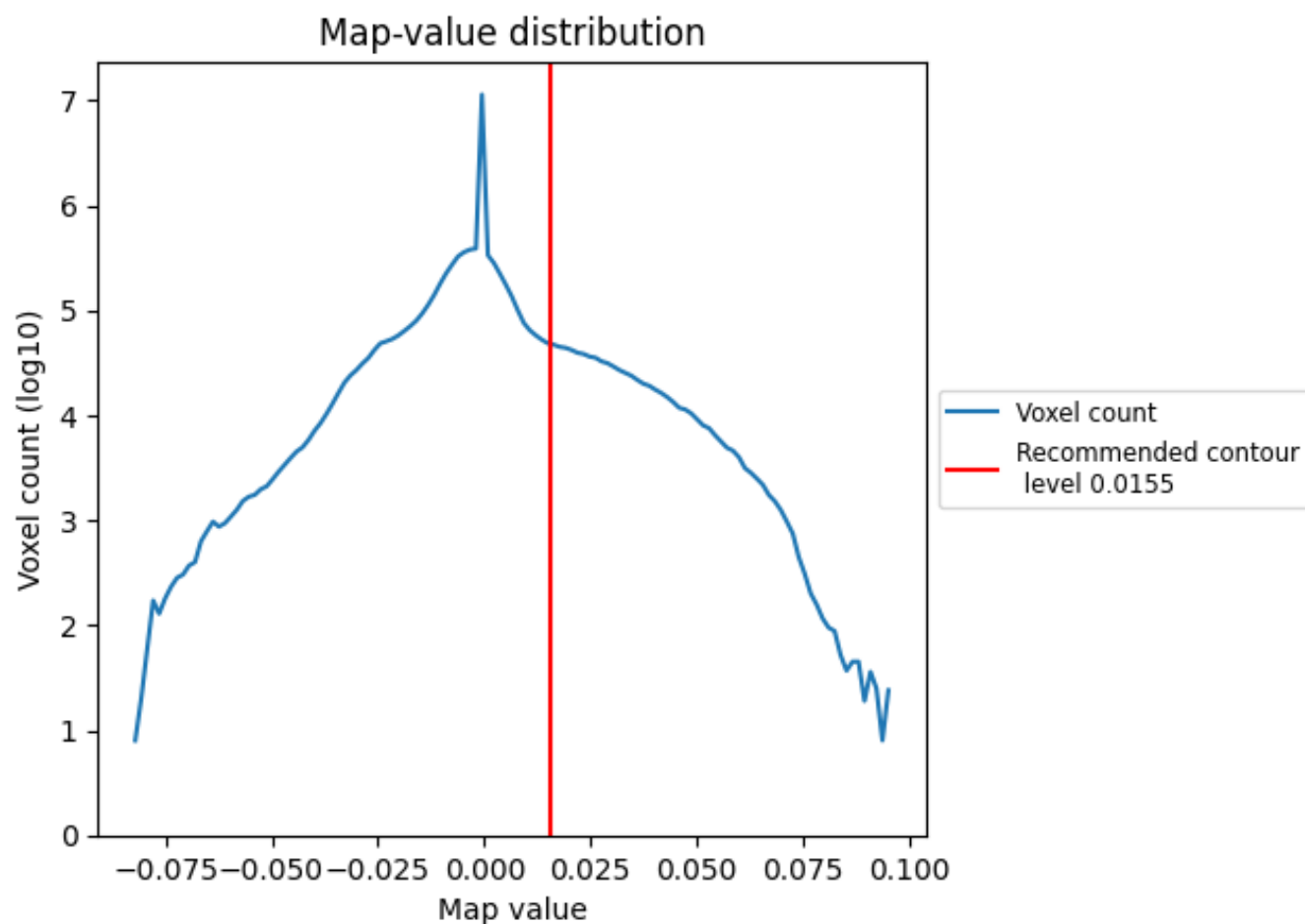
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

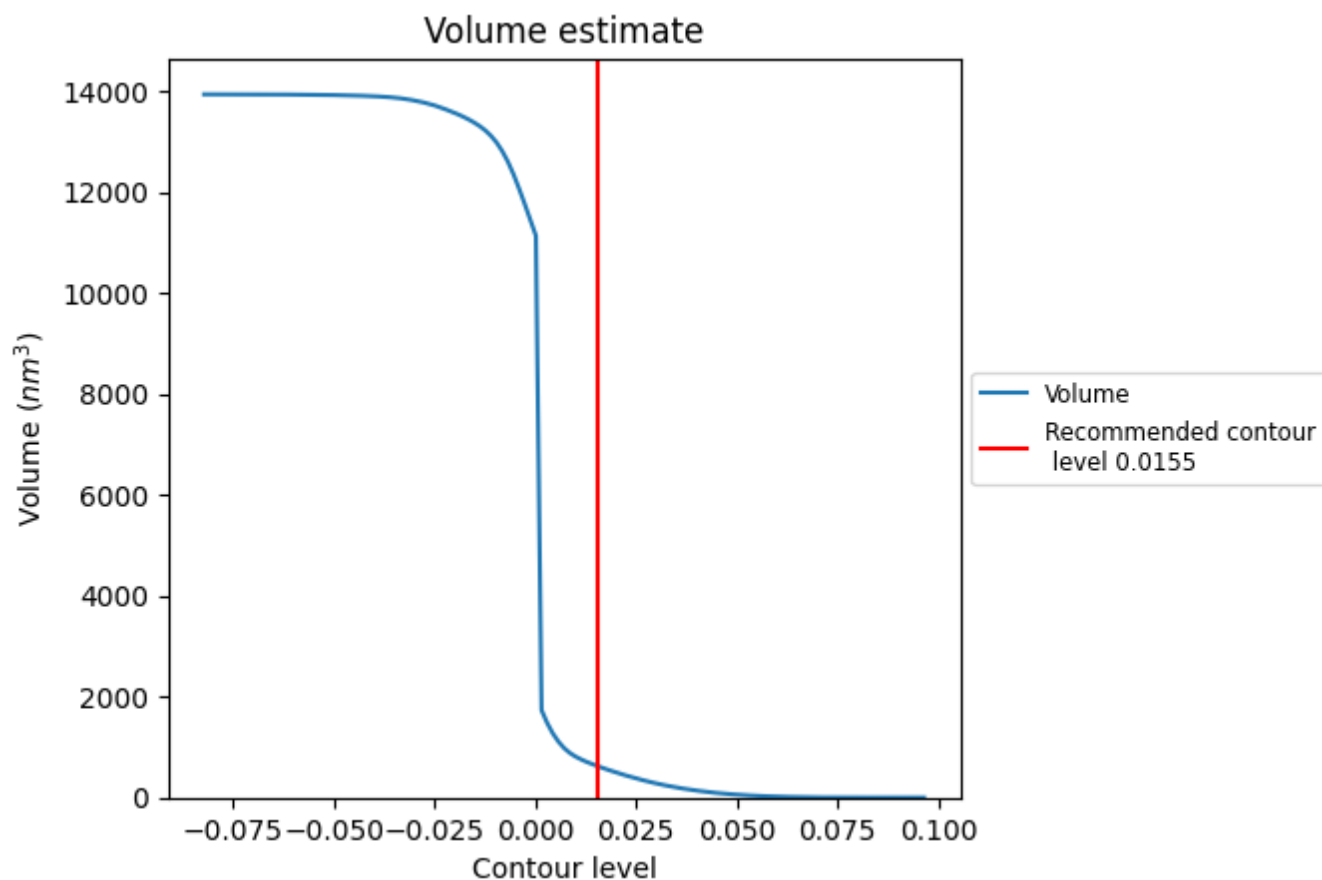
This section contains the results of statistical analysis of the map.

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.

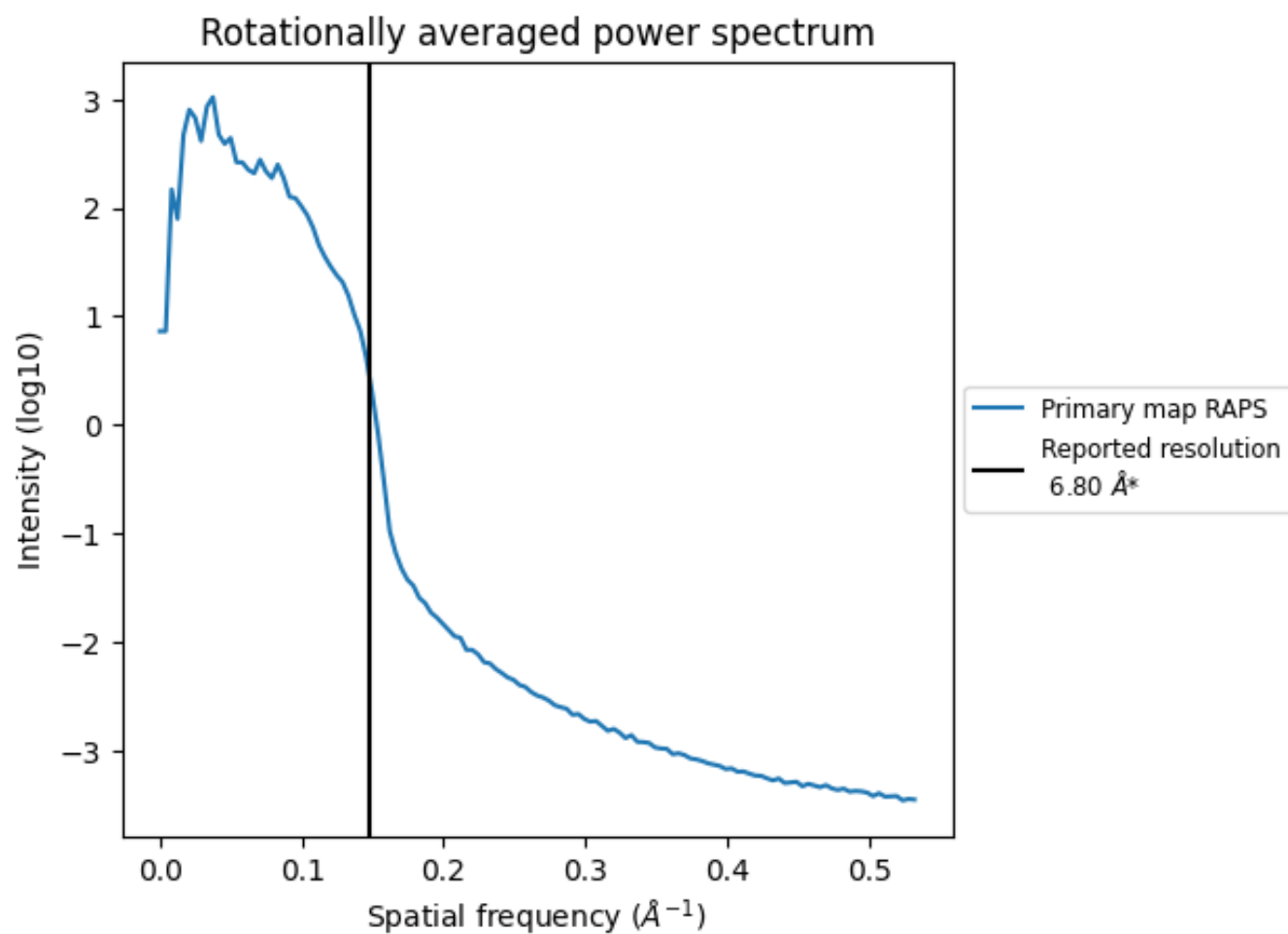
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 622 nm³; this corresponds to an approximate mass of 562 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 0.147 Å⁻¹

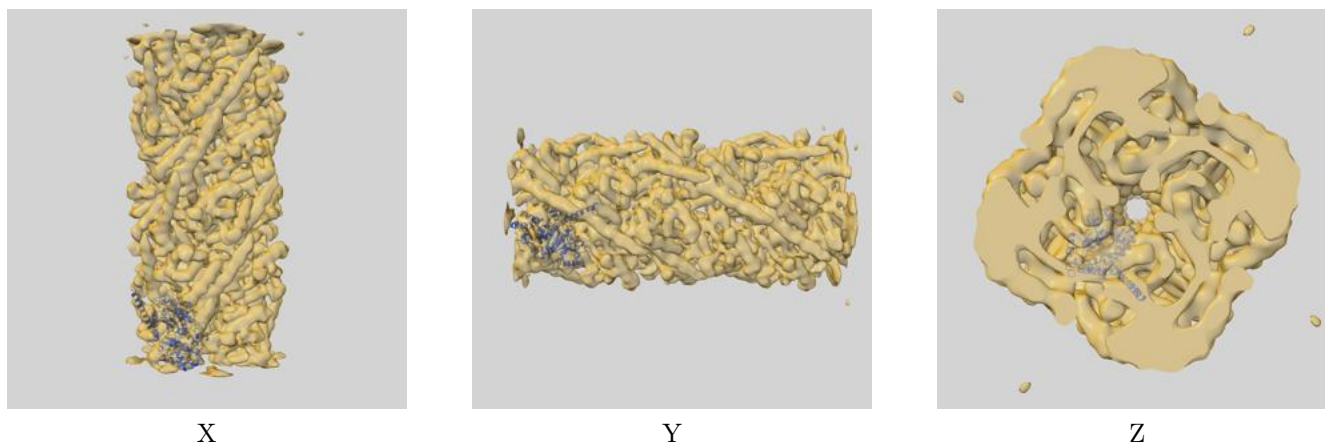
8 Fourier-Shell correlation

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-5762 and PDB model 3J4S. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



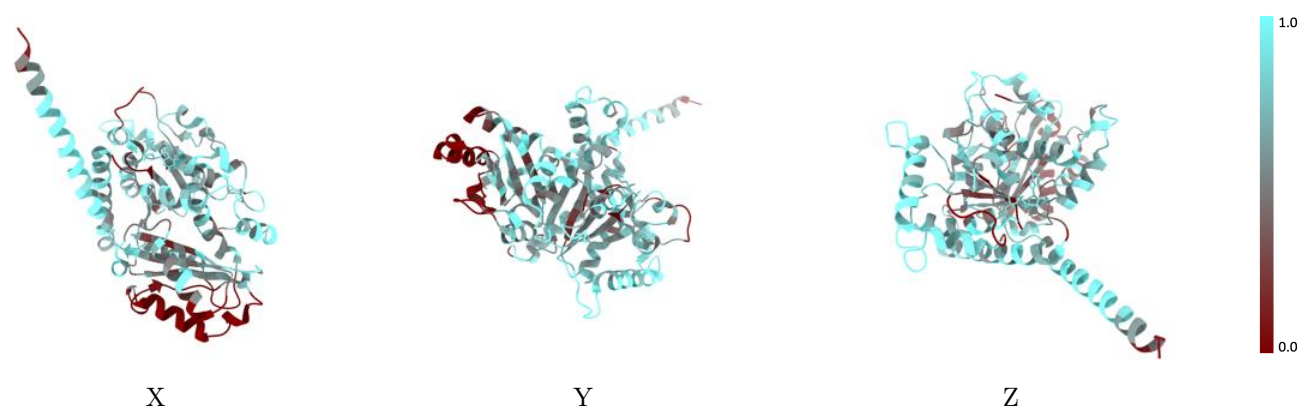
The images above show the 3D surface view of the map at the recommended contour level 0.0155 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



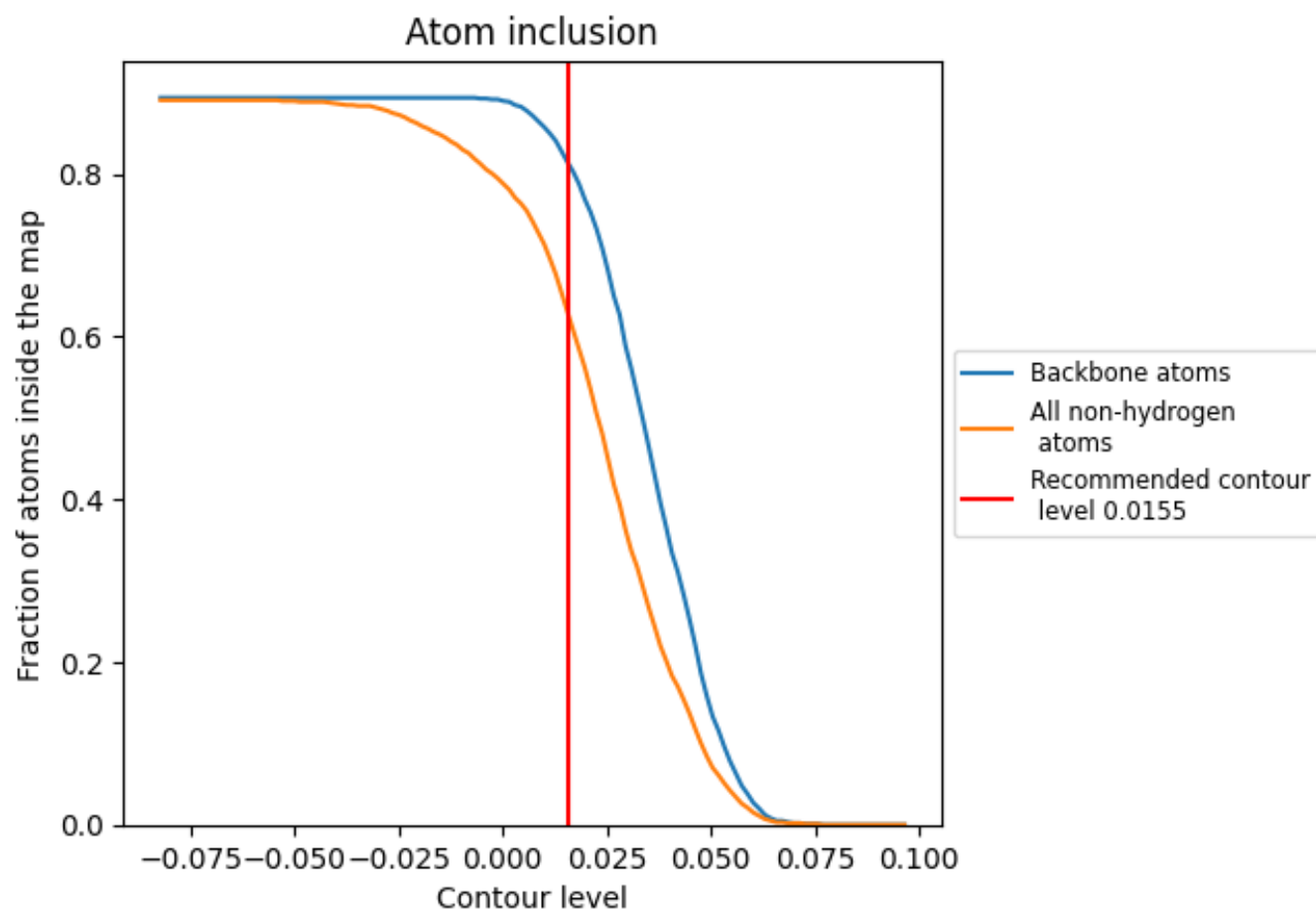
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0155).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 63% 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 (0.0155) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6320	0.1900
A	0.6320	0.1900

