



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 05:03 AM UTC

PDB ID : 3JAO / pdb_00003jao
EMDB ID : EMD-6312
Title : Ciliary microtubule doublet
Authors : Maheshwari, A.; Obbineni, J.M.; Bui, K.H.; Shibata, K.; Toyoshima, Y.Y.;
Ishikawa, T.
Deposited on : 2015-06-18
Resolution : 23.00 Å(reported)
Based on initial model : 3J6E

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

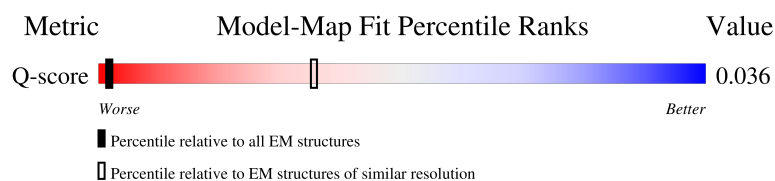
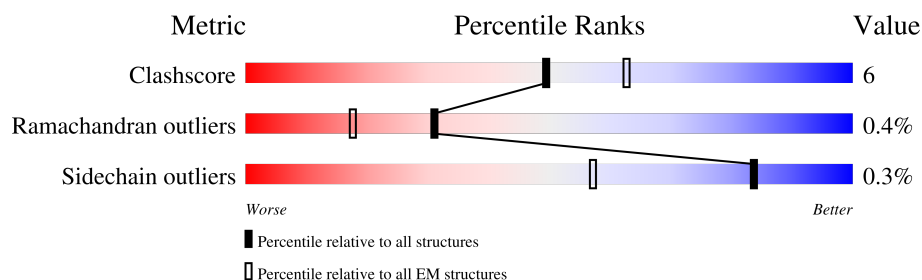
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 23.00 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	17 (22.90 - 23.50)

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	451	8% 72% 19% • 5%
2	B	445	13% 74% 18% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	G2P	B	501	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6774 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.

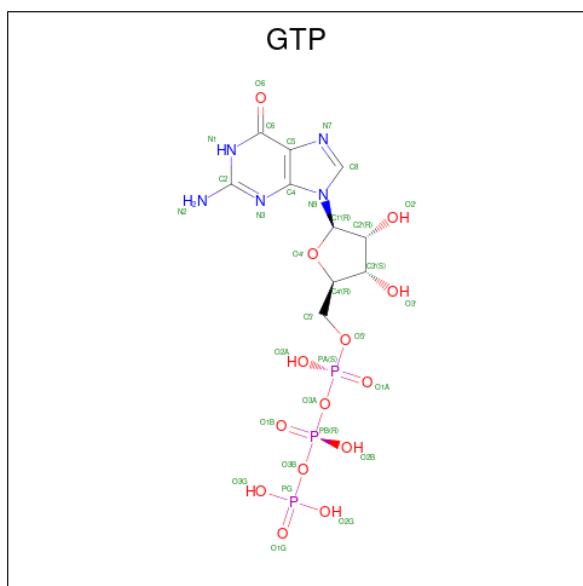
- Molecule 1 is a protein called Tubulin alpha 1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	428	3349	2121	570	637	21	0	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	426	3351	2105	575	646	25	0	0

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

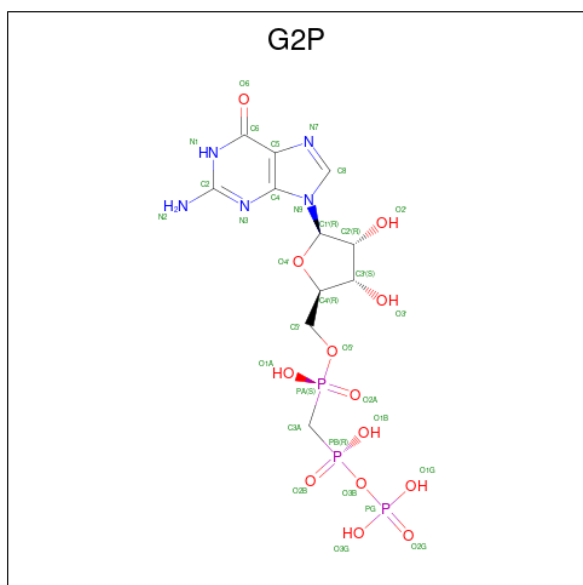


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	32	10	5	14	3	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	

- Molecule 5 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: G2P) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			32	11	5	13	3	

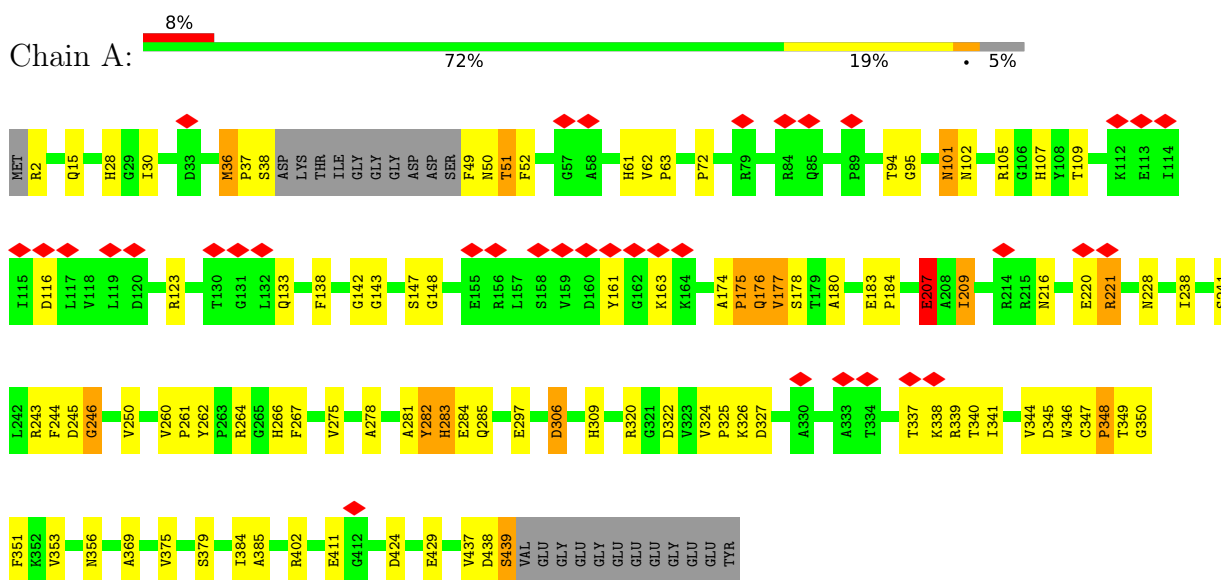
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	4	Total	O	0
			4	4	
6	B	4	Total	O	0
			4	4	

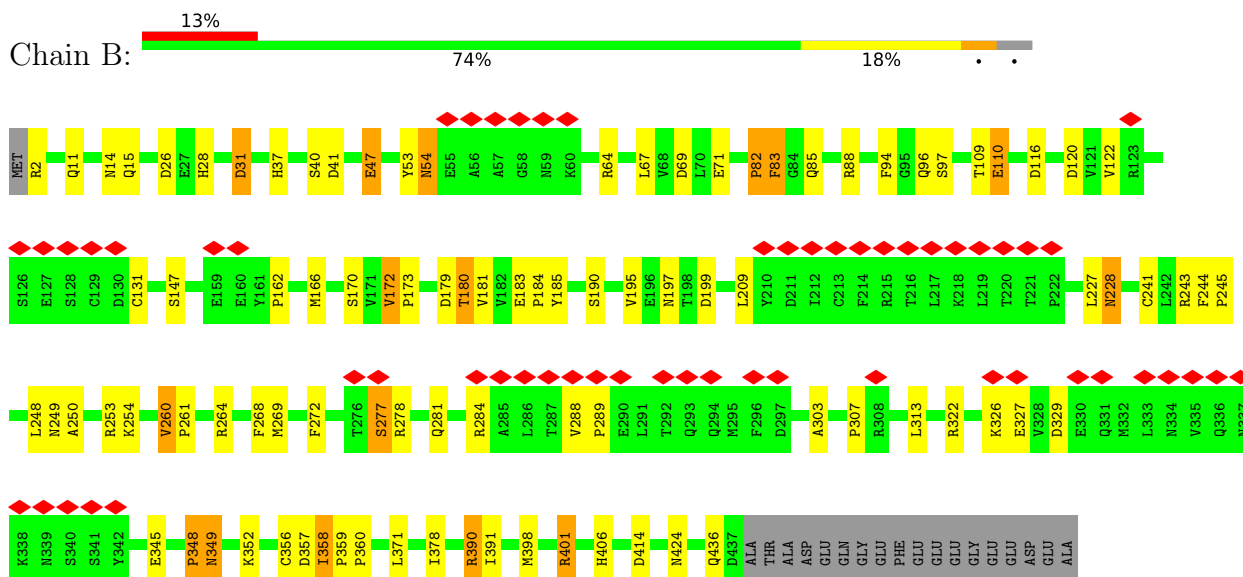
3 Residue-property plots

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 alpha 1A chain



• Molecule 2: Tubulin beta chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of particles used	10700	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	each particle	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	67000	Depositor
Image detector	GENERIC CCD	Depositor
Maximum map value	33.660	Depositor
Minimum map value	-33.726	Depositor
Average map value	0.093	Depositor
Map value standard deviation	2.300	Depositor
Recommended contour level	1.3	Depositor
Map size (Å)	1441.916, 1441.916, 1441.916	wwPDB
Map dimensions	322, 322, 322	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	4.478, 4.478, 4.478	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, G2P, GTP

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	1.52	49/3426 (1.4%)	1.79	92/4651 (2.0%)
2	B	1.15	9/3426 (0.3%)	1.72	76/4642 (1.6%)
All	All	1.35	58/6852 (0.8%)	1.75	168/9293 (1.8%)

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	THR	CA-C	-17.59	1.32	1.52
1	A	50	ASN	N-CA	-14.47	1.25	1.46
1	A	339	ARG	CA-C	-12.66	1.35	1.53
1	A	340	THR	N-CA	-12.17	1.30	1.46
1	A	283	HIS	CA-C	-11.75	1.36	1.53
1	A	177	VAL	CA-C	-10.55	1.41	1.53
1	A	282	TYR	CA-C	-10.53	1.39	1.52
2	B	249	ASN	CA-C	-10.32	1.42	1.53
1	A	338	LYS	CA-C	-10.30	1.38	1.52
1	A	339	ARG	N-CA	-10.00	1.34	1.45
1	A	36	MET	CA-C	-9.84	1.40	1.52
1	A	284	GLU	N-CA	-9.71	1.34	1.46
1	A	37	PRO	CA-C	-9.10	1.44	1.52
1	A	284	GLU	CA-C	-8.59	1.42	1.52
1	A	51	THR	N-CA	-8.52	1.34	1.46
2	B	436	GLN	CA-C	-8.46	1.41	1.52
1	A	174	ALA	CA-C	-8.43	1.42	1.53
1	A	37	PRO	N-CA	-8.29	1.35	1.48
2	B	82	PRO	CA-C	-8.22	1.42	1.52
1	A	178	SER	CA-C	-8.13	1.43	1.52
1	A	438	ASP	CA-C	-8.01	1.42	1.52
1	A	283	HIS	N-CA	-7.57	1.35	1.46
2	B	96	GLN	CA-C	-7.52	1.44	1.53
1	A	349	THR	N-CA	-7.43	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	THR	CA-C	-7.42	1.42	1.52
1	A	437	VAL	CA-C	-7.40	1.44	1.52
1	A	348	PRO	CA-C	-7.27	1.42	1.52
1	A	281	ALA	CA-C	-7.16	1.42	1.52
1	A	282	TYR	N-CA	-7.08	1.37	1.46
1	A	285	GLN	N-CA	-6.98	1.38	1.46
1	A	351	PHE	N-CA	-6.98	1.37	1.46
1	A	175	PRO	N-CA	-6.98	1.38	1.47
1	A	38	SER	CA-C	-6.96	1.38	1.52
1	A	246	GLY	N-CA	-6.94	1.39	1.45
1	A	178	SER	N-CA	-6.84	1.38	1.46
1	A	243	ARG	CA-C	-6.82	1.43	1.52
1	A	176	GLN	N-CA	-6.72	1.38	1.46
1	A	347	CYS	CA-C	-6.71	1.44	1.52
1	A	244	PHE	CA-C	-6.54	1.44	1.52
1	A	50	ASN	CA-C	-6.53	1.41	1.52
1	A	348	PRO	N-CA	-6.40	1.39	1.47
1	A	282	TYR	C-N	-6.29	1.25	1.33
2	B	180	THR	CA-C	-6.08	1.45	1.52
2	B	250	ALA	N-CA	-5.96	1.38	1.46
1	A	52	PHE	N-CA	-5.90	1.37	1.45
1	A	245	ASP	CA-C	-5.67	1.45	1.52
1	A	266	HIS	N-CA	-5.42	1.40	1.46
1	A	337	THR	CA-C	-5.38	1.45	1.52
1	A	177	VAL	N-CA	-5.34	1.40	1.46
2	B	326	LYS	CA-C	-5.33	1.46	1.52
1	A	285	GLN	CA-C	-5.32	1.46	1.52
2	B	401	ARG	CD-NE	-5.32	1.38	1.46
1	A	244	PHE	N-CA	-5.28	1.39	1.46
1	A	262	TYR	CA-C	-5.27	1.47	1.52
1	A	339	ARG	C-N	-5.25	1.27	1.33
1	A	344	VAL	CA-C	-5.18	1.47	1.52
1	A	283	HIS	C-N	-5.06	1.26	1.33
2	B	349	ASN	CA-C	-5.00	1.47	1.53

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	228	ASN	CA-CB-CG	-11.58	101.02	112.60
1	A	338	LYS	CA-C-N	-10.85	103.89	122.67
1	A	338	LYS	C-N-CA	-10.85	103.89	122.67
1	A	283	HIS	CA-C-N	-10.62	103.42	121.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	HIS	C-N-CA	-10.62	103.42	121.89
1	A	228	ASN	CA-CB-CG	-9.91	102.69	112.60
1	A	177	VAL	CB-CA-C	-9.76	100.69	111.23
1	A	339	ARG	N-CA-C	9.74	124.87	110.46
1	A	350	GLY	CA-C-N	-9.40	109.89	123.05
1	A	350	GLY	C-N-CA	-9.40	109.89	123.05
1	A	339	ARG	O-C-N	9.27	133.59	122.84
2	B	26	ASP	CA-CB-CG	-9.04	103.56	112.60
2	B	37	HIS	CA-C-N	-8.98	114.44	122.43
2	B	37	HIS	C-N-CA	-8.98	114.44	122.43
2	B	249	ASN	CA-CB-CG	8.83	121.43	112.60
1	A	281	ALA	CA-C-N	-8.67	108.56	120.87
1	A	281	ALA	C-N-CA	-8.67	108.56	120.87
1	A	339	ARG	CA-C-O	8.34	132.48	121.89
2	B	436	GLN	CA-C-N	-8.29	106.78	121.70
2	B	436	GLN	C-N-CA	-8.29	106.78	121.70
2	B	116	ASP	CA-CB-CG	-8.28	104.33	112.60
2	B	88	ARG	NE-CZ-NH1	8.12	129.62	121.50
2	B	197	ASN	N-CA-C	8.11	122.89	112.92
2	B	249	ASN	N-CA-C	8.00	121.02	111.02
1	A	264	ARG	N-CA-C	7.75	122.73	113.28
1	A	28	HIS	CA-CB-CG	-7.68	106.12	113.80
1	A	177	VAL	CA-C-N	-7.60	111.14	122.39
1	A	177	VAL	C-N-CA	-7.60	111.14	122.39
1	A	402	ARG	NE-CZ-NH2	7.39	125.85	119.20
2	B	424	ASN	CA-CB-CG	-7.39	105.21	112.60
2	B	69	ASP	CA-CB-CG	7.36	119.96	112.60
2	B	172	VAL	N-CA-C	7.35	115.18	107.76
2	B	348	PRO	N-CA-C	-7.27	99.78	111.19
2	B	401	ARG	NE-CZ-NH1	7.20	128.70	121.50
1	A	348	PRO	CA-C-N	-7.17	111.77	122.39
1	A	348	PRO	C-N-CA	-7.17	111.77	122.39
1	A	282	TYR	N-CA-C	-7.16	99.69	110.28
2	B	120	ASP	CA-CB-CG	-7.04	105.56	112.60
1	A	61	HIS	CA-CB-CG	-6.97	106.83	113.80
2	B	358	ILE	N-CA-C	6.96	115.67	107.73
1	A	105	ARG	NE-CZ-NH2	-6.96	112.94	119.20
1	A	37	PRO	CA-C-N	-6.91	109.27	121.70
1	A	37	PRO	C-N-CA	-6.91	109.27	121.70
1	A	284	GLU	CA-C-N	-6.83	113.37	123.00
1	A	284	GLU	C-N-CA	-6.83	113.37	123.00
1	A	177	VAL	N-CA-C	6.75	118.17	107.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	249	ASN	CB-CG-ND2	6.69	126.44	116.40
2	B	401	ARG	NE-CZ-NH2	-6.68	113.18	119.20
1	A	50	ASN	CA-C-N	-6.62	110.02	121.66
1	A	50	ASN	C-N-CA	-6.62	110.02	121.66
1	A	244	PHE	CA-C-N	-6.52	112.94	122.65
1	A	244	PHE	C-N-CA	-6.52	112.94	122.65
2	B	322	ARG	N-CA-C	6.45	120.11	108.17
2	B	96	GLN	N-CA-C	6.38	121.29	109.56
2	B	249	ASN	CA-C-N	-6.37	109.69	120.58
2	B	249	ASN	C-N-CA	-6.37	109.69	120.58
1	A	283	HIS	N-CA-C	6.36	120.33	112.58
2	B	14	ASN	CA-CB-CG	-6.34	106.25	112.60
2	B	166	MET	CA-C-N	-6.31	112.68	122.59
2	B	166	MET	C-N-CA	-6.31	112.68	122.59
1	A	109	THR	N-CA-C	6.30	118.95	111.33
1	A	50	ASN	N-CA-C	6.25	120.58	113.15
2	B	53	TYR	N-CA-C	6.24	119.36	109.50
1	A	375	VAL	N-CA-C	6.23	117.09	108.12
1	A	283	HIS	CB-CA-C	-6.22	101.75	111.39
1	A	176	GLN	CA-C-N	-6.21	113.20	122.01
1	A	176	GLN	C-N-CA	-6.21	113.20	122.01
2	B	83	PHE	CB-CA-C	6.16	119.34	110.04
1	A	228	ASN	OD1-CG-ND2	6.15	128.75	122.60
1	A	337	THR	N-CA-C	6.15	120.95	112.90
1	A	37	PRO	CA-N-CD	6.10	120.54	112.00
2	B	28	HIS	CA-CB-CG	-6.06	107.74	113.80
1	A	379	SER	N-CA-C	6.06	119.11	108.75
1	A	37	PRO	N-CA-C	6.05	123.64	112.33
1	A	142	GLY	CA-C-N	-6.04	113.62	121.96
1	A	142	GLY	C-N-CA	-6.04	113.62	121.96
1	A	161	TYR	CA-CB-CG	-6.03	103.05	113.90
1	A	282	TYR	O-C-N	6.03	130.24	122.89
2	B	401	ARG	CD-NE-CZ	-5.94	116.08	124.40
1	A	250	VAL	N-CA-C	5.90	117.16	107.24
2	B	378	ILE	CA-C-N	-5.88	116.90	122.66
2	B	378	ILE	C-N-CA	-5.88	116.90	122.66
2	B	71	GLU	CA-C-N	5.85	125.99	119.32
2	B	71	GLU	C-N-CA	5.85	125.99	119.32
2	B	277	SER	CA-C-N	5.85	128.93	120.38
2	B	277	SER	C-N-CA	5.85	128.93	120.38
1	A	327	ASP	CA-CB-CG	-5.84	106.76	112.60
1	A	61	HIS	CA-C-N	-5.83	118.26	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	HIS	C-N-CA	-5.83	118.26	123.33
1	A	285	GLN	CA-C-N	-5.82	114.97	123.00
1	A	285	GLN	C-N-CA	-5.82	114.97	123.00
2	B	253	ARG	NE-CZ-NH1	5.81	127.31	121.50
1	A	243	ARG	CA-C-N	-5.74	113.21	121.42
1	A	243	ARG	C-N-CA	-5.74	113.21	121.42
1	A	37	PRO	N-CA-CB	-5.74	98.28	102.35
1	A	322	ASP	N-CA-C	5.71	118.46	108.52
2	B	243	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	A	123	ARG	NE-CZ-NH2	-5.69	114.08	119.20
2	B	272	PHE	N-CA-C	5.69	118.48	108.75
1	A	250	VAL	CB-CA-C	-5.68	103.97	110.73
2	B	88	ARG	CA-C-N	5.65	126.03	119.47
2	B	88	ARG	C-N-CA	5.65	126.03	119.47
1	A	101	ASN	CB-CA-C	-5.65	103.87	111.89
2	B	54	ASN	CA-C-N	-5.64	114.68	122.30
2	B	54	ASN	C-N-CA	-5.64	114.68	122.30
1	A	306	ASP	CA-C-N	5.63	125.30	119.56
1	A	306	ASP	C-N-CA	5.63	125.30	119.56
2	B	199	ASP	CA-CB-CG	-5.61	106.99	112.60
1	A	320	ARG	NH1-CZ-NH2	-5.57	112.06	119.30
2	B	329	ASP	CA-CB-CG	-5.57	107.03	112.60
1	A	353	VAL	N-CA-C	5.56	115.86	107.75
1	A	28	HIS	N-CA-C	5.55	120.76	112.94
2	B	243	ARG	NH1-CZ-NH2	-5.53	112.11	119.30
1	A	267	PHE	N-CA-C	5.49	118.57	109.79
1	A	102	ASN	CA-CB-CG	5.44	118.04	112.60
1	A	175	PRO	CA-C-N	-5.43	112.08	120.88
1	A	175	PRO	C-N-CA	-5.43	112.08	120.88
2	B	88	ARG	CD-NE-CZ	5.39	131.94	124.40
1	A	320	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	A	209	ILE	CB-CA-C	-5.36	104.90	112.14
1	A	424	ASP	CA-CB-CG	5.33	117.93	112.60
2	B	110	GLU	N-CA-C	5.32	116.76	111.07
2	B	357	ASP	N-CA-C	5.30	119.74	113.16
1	A	138	PHE	CA-CB-CG	-5.29	108.51	113.80
1	A	163	LYS	N-CA-C	5.29	119.35	113.01
2	B	345	GLU	N-CA-C	5.25	119.17	112.87
1	A	439	SER	N-CA-C	5.23	125.64	111.00
2	B	391	ILE	N-CA-C	5.23	115.44	110.53
1	A	411	GLU	CA-CB-CG	5.22	124.54	114.10
1	A	221	ARG	N-CA-C	5.22	119.34	108.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	390	ARG	NE-CZ-NH2	5.22	123.89	119.20
2	B	436	GLN	O-C-N	5.21	127.51	122.09
2	B	248	LEU	N-CA-C	5.17	117.87	109.24
1	A	116	ASP	CA-CB-CG	-5.16	107.44	112.60
1	A	221	ARG	NE-CZ-NH1	-5.16	116.34	121.50
2	B	47	GLU	N-CA-C	5.15	121.77	110.80
2	B	94	PHE	N-CA-C	5.14	116.65	108.79
1	A	51	THR	CA-C-N	-5.13	114.11	122.26
1	A	51	THR	C-N-CA	-5.13	114.11	122.26
1	A	107	HIS	CA-C-N	-5.13	111.75	121.54
1	A	107	HIS	C-N-CA	-5.13	111.75	121.54
2	B	264	ARG	CA-C-N	-5.13	115.18	123.23
2	B	264	ARG	C-N-CA	-5.13	115.18	123.23
2	B	185	TYR	CA-CB-CG	5.12	123.12	113.90
2	B	268	PHE	N-CA-C	5.12	117.91	109.72
2	B	406	HIS	CA-CB-CG	5.10	118.90	113.80
1	A	297	GLU	CA-C-N	5.10	125.39	119.47
1	A	297	GLU	C-N-CA	5.10	125.39	119.47
2	B	162	PRO	CA-C-N	-5.10	114.50	122.65
2	B	162	PRO	C-N-CA	-5.10	114.50	122.65
2	B	260	VAL	CA-C-N	5.09	124.78	119.64
2	B	260	VAL	C-N-CA	5.09	124.78	119.64
2	B	401	ARG	CB-CG-CD	-5.09	99.59	111.30
1	A	209	ILE	CA-CB-CG2	-5.08	101.86	110.50
1	A	351	PHE	CB-CA-C	-5.08	101.87	110.19
2	B	122	VAL	CB-CA-C	-5.07	105.39	111.88
2	B	31	ASP	CA-C-N	5.07	124.79	119.82
2	B	31	ASP	C-N-CA	5.07	124.79	119.82
2	B	179	ASP	CA-C-N	-5.06	114.73	122.87
2	B	179	ASP	C-N-CA	-5.06	114.73	122.87
2	B	88	ARG	NE-CZ-NH2	-5.05	114.65	119.20
2	B	313	LEU	N-CA-C	-5.05	105.97	112.68
1	A	72	PRO	N-CA-C	5.04	121.27	113.75
2	B	414	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	309	HIS	CA-CB-CG	-5.04	108.76	113.80
2	B	170	SER	N-CA-C	5.03	116.89	108.99
1	A	207	GLU	CA-CB-CG	-5.02	104.06	114.10
1	A	345	ASP	N-CA-C	5.01	118.16	111.75

There are no chirality outliers.

There are no planarity outliers.

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	3349	0	3254	37	0
2	B	3351	0	3229	41	0
3	A	32	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	32	0	13	4	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
All	All	6774	0	6508	76	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 6.

All (76) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:ASN:HD21	5:B:501:G2P:H1	1.13	0.97
1:A:341:ILE:HG13	1:A:341:ILE:O	1.67	0.92
2:B:401:ARG:N	2:B:401:ARG:HD3	2.07	0.69
2:B:85:GLN:H	2:B:85:GLN:CD	2.03	0.67
1:A:439:SER:O	1:A:439:SER:OG	2.05	0.66
1:A:177:VAL:HG23	1:A:207:GLU:OE1	1.95	0.66
1:A:147:SER:OG	1:A:148:GLY:N	2.26	0.65
2:B:401:ARG:N	2:B:401:ARG:CD	2.56	0.65
1:A:30:ILE:HG12	1:A:36:MET:SD	2.41	0.61
1:A:207:GLU:N	1:A:207:GLU:OE2	2.35	0.60
2:B:228:ASN:ND2	5:B:501:G2P:H1	1.93	0.59
2:B:390:ARG:NE	2:B:390:ARG:HA	2.18	0.59
1:A:2:ARG:HA	1:A:133:GLN:HG3	1.84	0.58
2:B:85:GLN:CD	2:B:85:GLN:N	2.64	0.56
1:A:246:GLY:HA3	1:A:356:ASN:HA	1.89	0.55
2:B:277:SER:OG	2:B:278:ARG:N	2.41	0.53
1:A:341:ILE:O	1:A:341:ILE:CG1	2.43	0.53
2:B:269:MET:SD	2:B:307:PRO:HG3	2.48	0.53
1:A:346:TRP:CD1	1:A:346:TRP:H	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:N	2:B:131:CYS:O	2.43	0.51
1:A:143:GLY:O	1:A:147:SER:OG	2.28	0.51
2:B:288:VAL:HB	2:B:327:GLU:HG2	1.91	0.51
2:B:360:PRO:HG2	2:B:371:LEU:HB2	1.93	0.51
1:A:180:ALA:HB3	1:A:183:GLU:HG3	1.94	0.50
1:A:326:LYS:HD2	1:A:326:LYS:C	2.37	0.50
2:B:195:VAL:HG22	2:B:195:VAL:O	2.12	0.50
1:A:282:TYR:O	1:A:283:HIS:HB2	2.11	0.50
1:A:15:GLN:OE1	1:A:15:GLN:HA	2.13	0.49
2:B:181:VAL:O	2:B:398:MET:SD	2.71	0.48
1:A:346:TRP:CD1	1:A:346:TRP:N	2.78	0.48
2:B:348:PRO:O	2:B:349:ASN:HB2	2.14	0.48
2:B:390:ARG:HA	2:B:390:ARG:HE	1.80	0.47
2:B:31:ASP:OD1	2:B:31:ASP:C	2.58	0.47
1:A:306:ASP:OD1	1:A:306:ASP:C	2.56	0.46
2:B:40:SER:OG	2:B:41:ASP:N	2.46	0.46
1:A:220:GLU:OE2	1:A:221:ARG:NH1	2.49	0.46
1:A:49:PHE:C	1:A:51:THR:N	2.73	0.46
1:A:241:SER:O	1:A:356:ASN:ND2	2.48	0.46
2:B:180:THR:HG23	2:B:183:GLU:HB2	1.98	0.45
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.98	0.45
2:B:401:ARG:HA	2:B:401:ARG:HD2	1.61	0.45
1:A:238:ILE:O	1:A:238:ILE:HG22	2.16	0.45
1:A:216:ASN:HB3	1:A:275:VAL:O	2.16	0.45
2:B:67:LEU:HD12	2:B:67:LEU:N	2.31	0.45
1:A:260:VAL:HA	1:A:261:PRO:HD2	1.87	0.44
2:B:54:ASN:OD1	2:B:64:ARG:NH1	2.50	0.44
1:A:49:PHE:C	1:A:51:THR:H	2.24	0.44
2:B:269:MET:O	2:B:269:MET:HG2	2.18	0.44
1:A:385:ALA:HB1	1:A:429:GLU:HG3	1.98	0.44
2:B:183:GLU:N	2:B:184:PRO:CD	2.80	0.44
1:A:101:ASN:OD1	2:B:254:LYS:NZ	2.48	0.44
1:A:209:ILE:O	1:A:209:ILE:HG22	2.16	0.44
2:B:209:LEU:HB3	2:B:227:LEU:HD22	2.00	0.43
1:A:62:VAL:HA	1:A:63:PRO:HD3	1.88	0.43
1:A:175:PRO:O	2:B:349:ASN:ND2	2.51	0.43
2:B:281:GLN:HA	2:B:284:ARG:HG2	2.01	0.43
2:B:15:GLN:NE2	5:B:501:G2P:O6	2.52	0.42
2:B:269:MET:HG3	2:B:303:ALA:HB3	2.01	0.42
2:B:241:CYS:SG	2:B:356:CYS:HB3	2.59	0.42
2:B:358:ILE:HA	2:B:359:PRO:HD2	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:SER:HB2	2:B:190:SER:HB3	2.02	0.42
1:A:183:GLU:N	1:A:184:PRO:CD	2.83	0.42
1:A:49:PHE:HD1	1:A:49:PHE:HA	1.72	0.42
1:A:238:ILE:O	1:A:238:ILE:CG2	2.67	0.41
2:B:109:THR:OG1	2:B:110:GLU:N	2.53	0.41
2:B:172:VAL:HA	2:B:173:PRO:HD3	1.82	0.41
1:A:94:THR:OG1	1:A:95:GLY:N	2.53	0.41
2:B:82:PRO:O	2:B:83:PHE:HB2	2.20	0.41
2:B:244:PHE:HA	2:B:245:PRO:HD3	1.91	0.41
1:A:324:VAL:HA	1:A:325:PRO:HD3	1.93	0.41
1:A:384:ILE:O	1:A:384:ILE:HG12	2.21	0.41
2:B:11:GLN:HB3	5:B:501:G2P:O1A	2.21	0.41
1:A:176:GLN:HB3	1:A:207:GLU:HG2	2.03	0.40
2:B:288:VAL:N	2:B:289:PRO:CD	2.83	0.40
2:B:260:VAL:HA	2:B:261:PRO:HD2	1.87	0.40
2:B:401:ARG:N	2:B:401:ARG:HD2	2.29	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	424/451 (94%)	405 (96%)	18 (4%)	1 (0%)	43	78
2	B	424/445 (95%)	411 (97%)	11 (3%)	2 (0%)	24	63
All	All	848/896 (95%)	816 (96%)	29 (3%)	3 (0%)	31	67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	348	PRO
2	B	97	SER

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Mol	Chain	Res	Type
2	B	47	GLU

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	360/377 (96%)	359 (100%)	1 (0%)	86	86
2	B	367/381 (96%)	366 (100%)	1 (0%)	86	86
All	All	727/758 (96%)	725 (100%)	2 (0%)	84	86

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	GLU
2	B	352	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	107	HIS
1	A	216	ASN
2	B	11	GLN
2	B	15	GLN
2	B	192	HIS
2	B	247	GLN
2	B	309	HIS
2	B	385	GLN
2	B	433	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
3	GTP	A	501	4	33,34,34	1.89	3 (9%)	50,54,54	0.97	4 (8%)
5	G2P	B	501	4	30,34,34	3.91	25 (83%)	46,54,54	3.05	22 (47%)

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
3	GTP	A	501	4	-	3/22/38/38	0/3/3/3
5	G2P	B	501	4	-	6/19/38/38	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	G2P	O3'-C3'	7.64	1.61	1.43
5	B	501	G2P	C2-N2	7.17	1.51	1.34
5	B	501	G2P	PA-O1A	-6.14	1.41	1.56
3	A	501	GTP	PA-O3A	-5.92	1.53	1.59
5	B	501	G2P	C2-N3	5.89	1.47	1.33
5	B	501	G2P	O2'-C2'	-5.82	1.28	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	GTP	PB-O3A	-5.74	1.53	1.59
3	A	501	GTP	PB-O3B	5.29	1.65	1.59
5	B	501	G2P	C4-N9	-5.00	1.25	1.38
5	B	501	G2P	PA-O2A	4.66	1.62	1.51
5	B	501	G2P	C4-N3	4.56	1.44	1.34
5	B	501	G2P	O5'-C5'	-4.49	1.27	1.44
5	B	501	G2P	C2-N1	4.23	1.47	1.37
5	B	501	G2P	PB-O2B	4.07	1.61	1.51
5	B	501	G2P	C8-N9	-4.01	1.28	1.37
5	B	501	G2P	PG-O3G	-3.48	1.41	1.54
5	B	501	G2P	C2'-C1'	3.47	1.64	1.53
5	B	501	G2P	C3'-C4'	3.23	1.61	1.53
5	B	501	G2P	PB-O1B	2.84	1.63	1.56
5	B	501	G2P	O6-C6	-2.80	1.18	1.23
5	B	501	G2P	C1'-N9	-2.77	1.39	1.47
5	B	501	G2P	O4'-C4'	2.75	1.51	1.45
5	B	501	G2P	C8-N7	-2.69	1.25	1.32
5	B	501	G2P	PG-O1G	2.41	1.63	1.54
5	B	501	G2P	C2'-C3'	-2.31	1.47	1.53
5	B	501	G2P	C5-C6	2.29	1.53	1.44
5	B	501	G2P	C5-C4	2.19	1.44	1.38
5	B	501	G2P	PB-O3B	2.15	1.60	1.58

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	G2P	O4'-C4'-C3'	-7.77	89.73	105.15
5	B	501	G2P	C2-N3-C4	6.21	123.00	112.30
5	B	501	G2P	N1-C2-N3	-5.89	112.54	123.32
5	B	501	G2P	N2-C2-N3	5.62	130.64	119.67
5	B	501	G2P	N9-C4-N3	5.47	136.89	125.95
5	B	501	G2P	O1B-PB-O2B	5.03	126.34	109.95
5	B	501	G2P	O1A-PA-C3A	4.61	125.81	106.73
5	B	501	G2P	O2'-C2'-C3'	-4.54	97.27	111.82
5	B	501	G2P	C3'-C2'-C1'	-4.20	93.51	101.46
5	B	501	G2P	C5-C4-N3	-4.15	121.78	128.39
5	B	501	G2P	C4'-O4'-C1'	3.78	117.81	109.47
5	B	501	G2P	C8-N9-C4	3.70	112.96	106.03
5	B	501	G2P	O4'-C1'-C2'	-3.57	98.97	106.62
5	B	501	G2P	O2A-PA-C3A	-3.26	100.46	109.05
5	B	501	G2P	O2'-C2'-C1'	3.03	120.55	110.10
5	B	501	G2P	O6-C6-C5	-2.65	119.53	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	GTP	O2G-PG-O3B	2.63	113.47	104.64
3	A	501	GTP	O3A-PB-O1B	-2.42	103.41	110.70
5	B	501	G2P	C5-C4-N9	-2.42	101.33	105.66
5	B	501	G2P	O3'-C3'-C2'	2.30	119.18	111.82
5	B	501	G2P	C1'-N9-C4	-2.22	119.93	126.49
3	A	501	GTP	O2B-PB-O3A	2.16	113.12	107.27
5	B	501	G2P	O6-C6-N1	2.16	124.18	120.11
3	A	501	GTP	O5'-C5'-C4'	2.11	116.19	108.99
5	B	501	G2P	O4'-C4'-C5'	2.09	116.02	109.33
5	B	501	G2P	O3'-C3'-C4'	2.07	117.02	111.08

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	501	G2P	PB-O3B-PG-O3G
5	B	501	G2P	C5'-O5'-PA-O2A
3	A	501	GTP	C3'-C4'-C5'-O5'
3	A	501	GTP	O4'-C4'-C5'-O5'
5	B	501	G2P	C3'-C4'-C5'-O5'
5	B	501	G2P	C5'-O5'-PA-O1A
5	B	501	G2P	PB-O3B-PG-O1G
3	A	501	GTP	PG-O3B-PB-O1B
5	B	501	G2P	C5'-O5'-PA-C3A

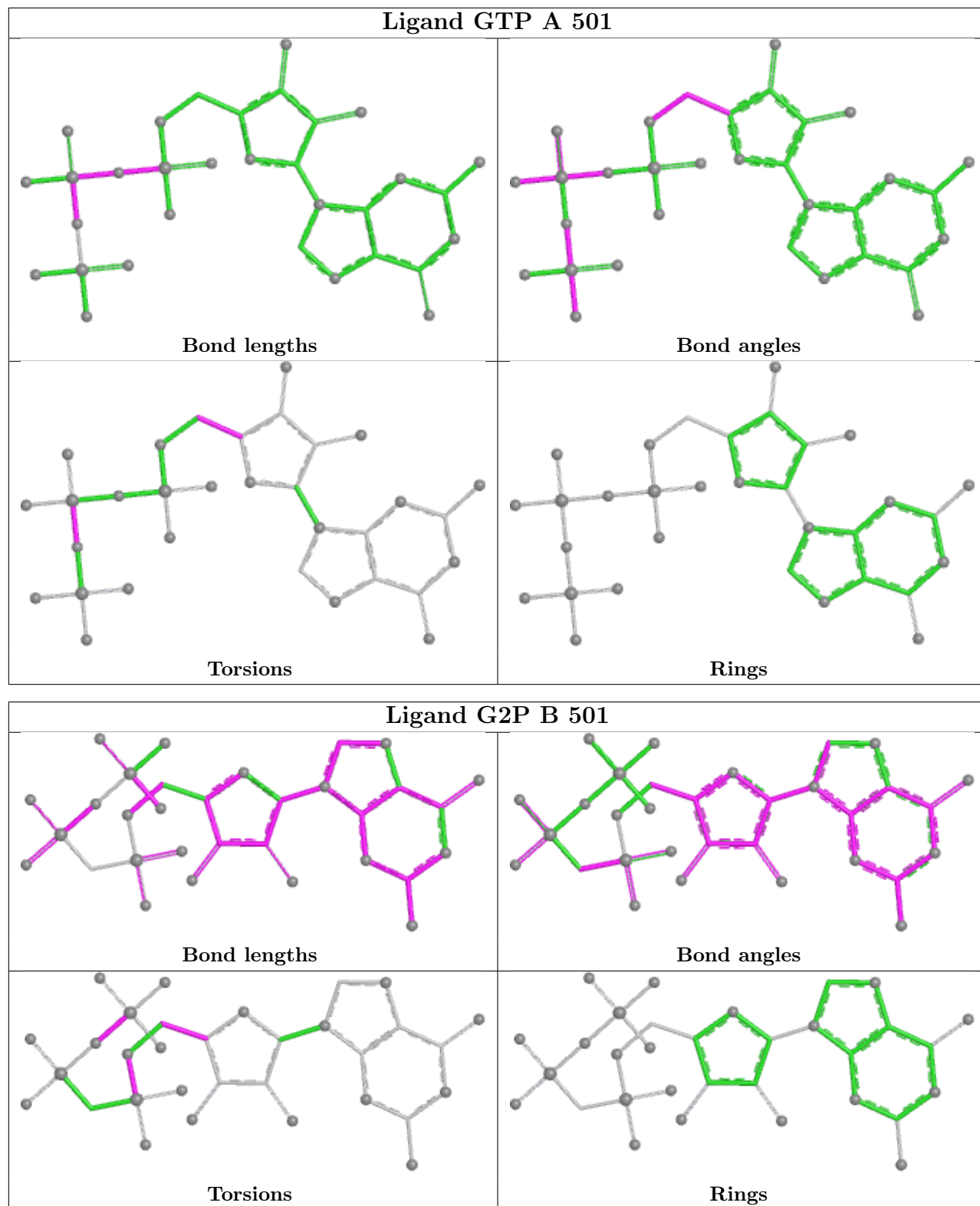
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	G2P	4	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

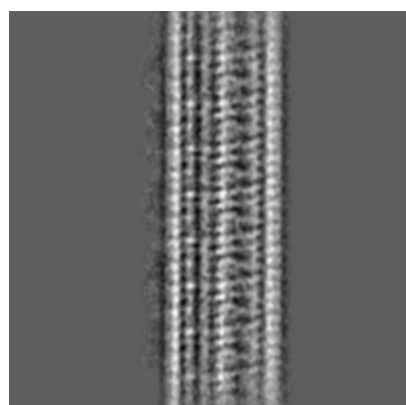
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6312. These allow visual inspection of the internal detail of the map and identification of artifacts.

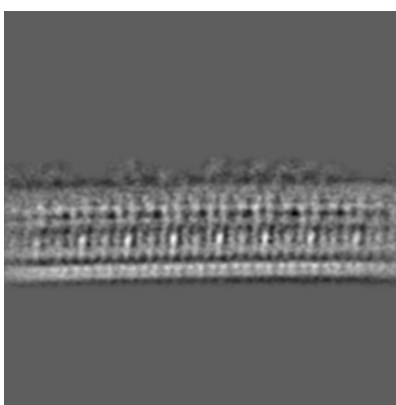
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

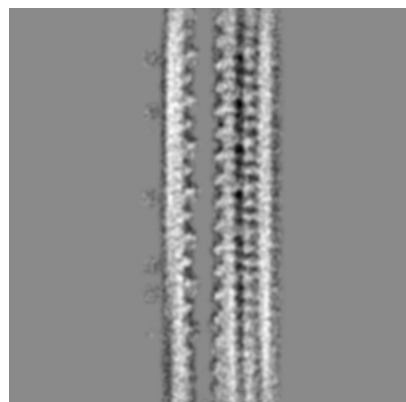


Z

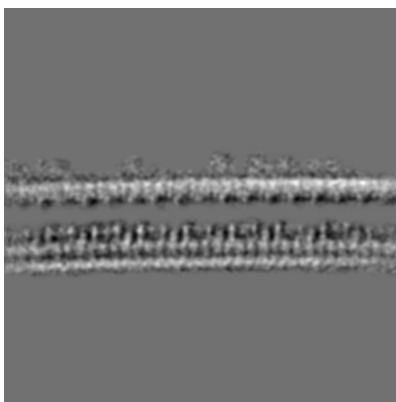
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 161



Y Index: 161

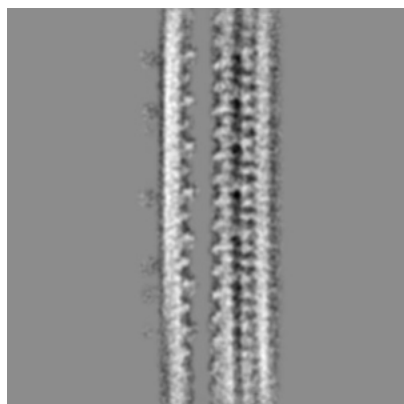


Z Index: 161

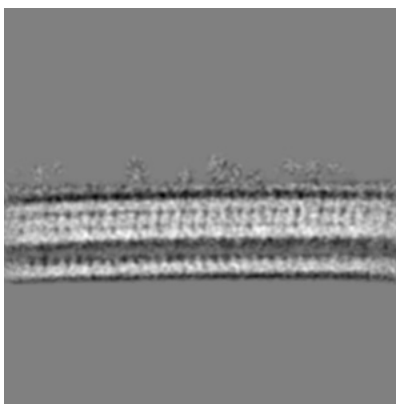
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 160



Y Index: 176

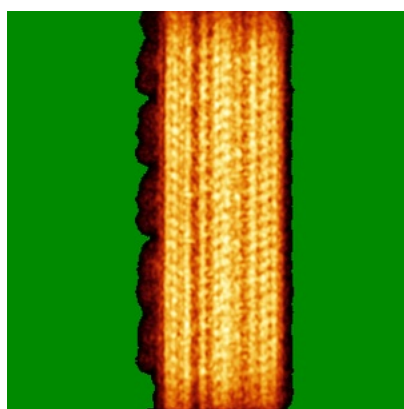


Z Index: 99

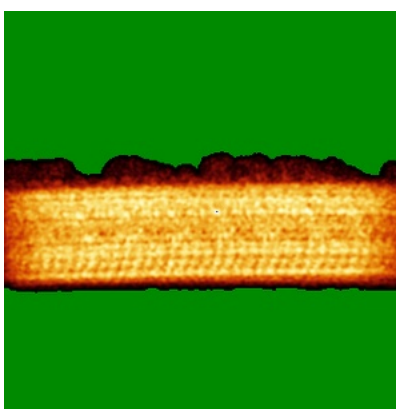
The images above show the largest variance slices of the map in three orthogonal directions.

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

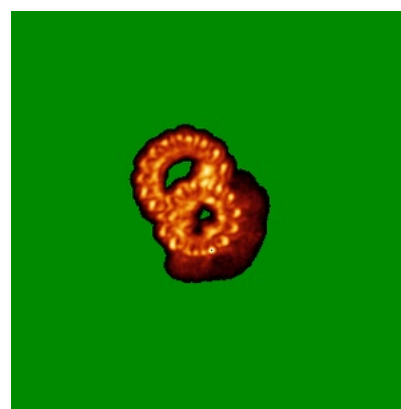
6.4.1 Primary map



X



Y

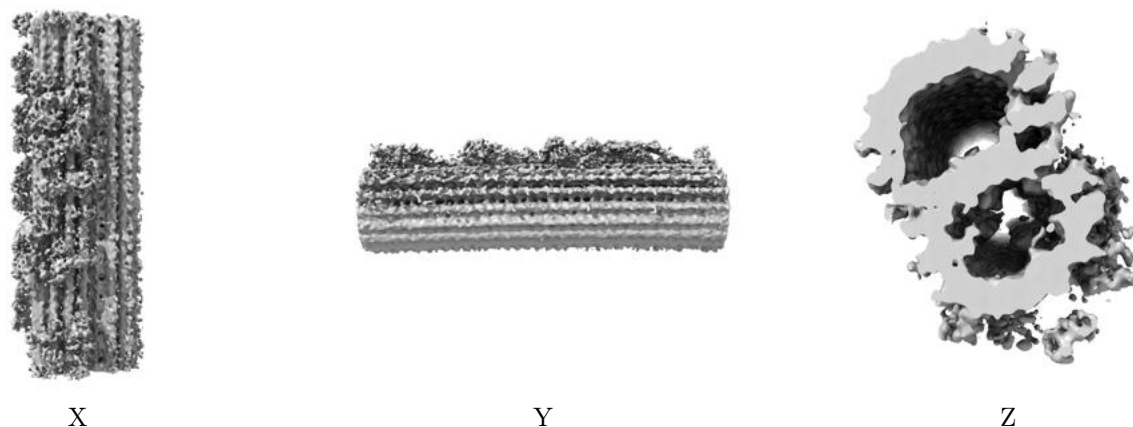


Z

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

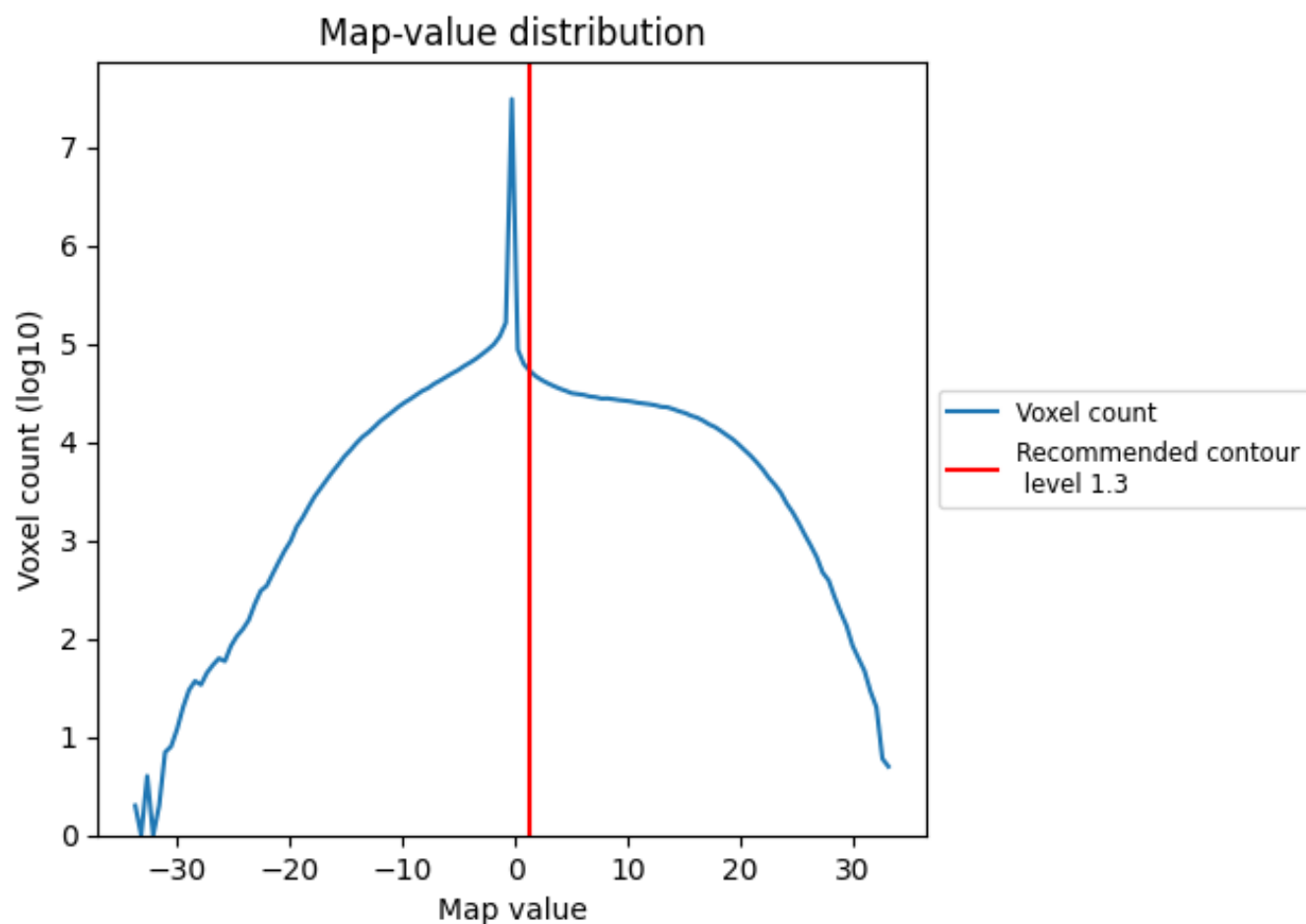
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

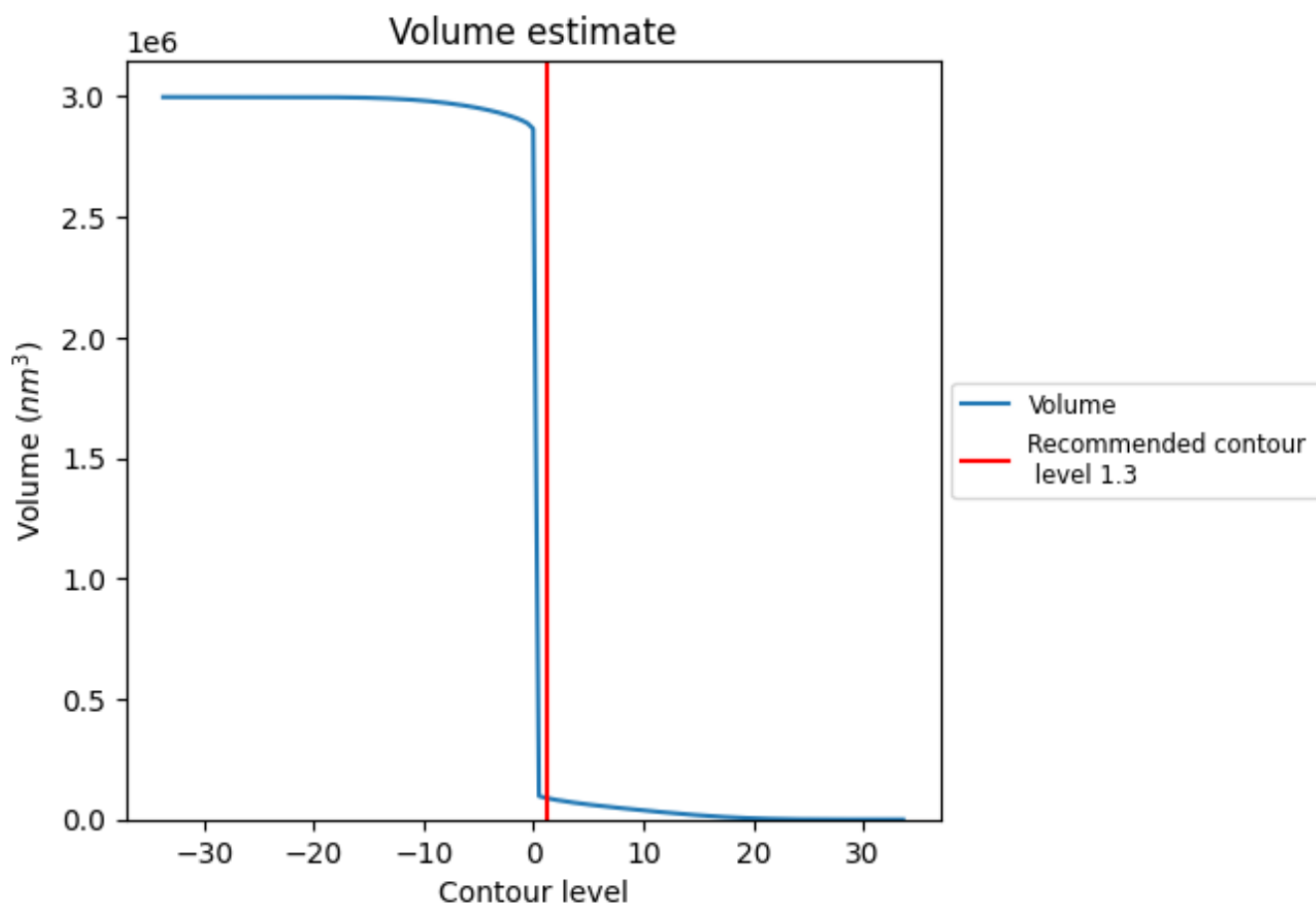
This section contains the results of statistical analysis of the map.

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.

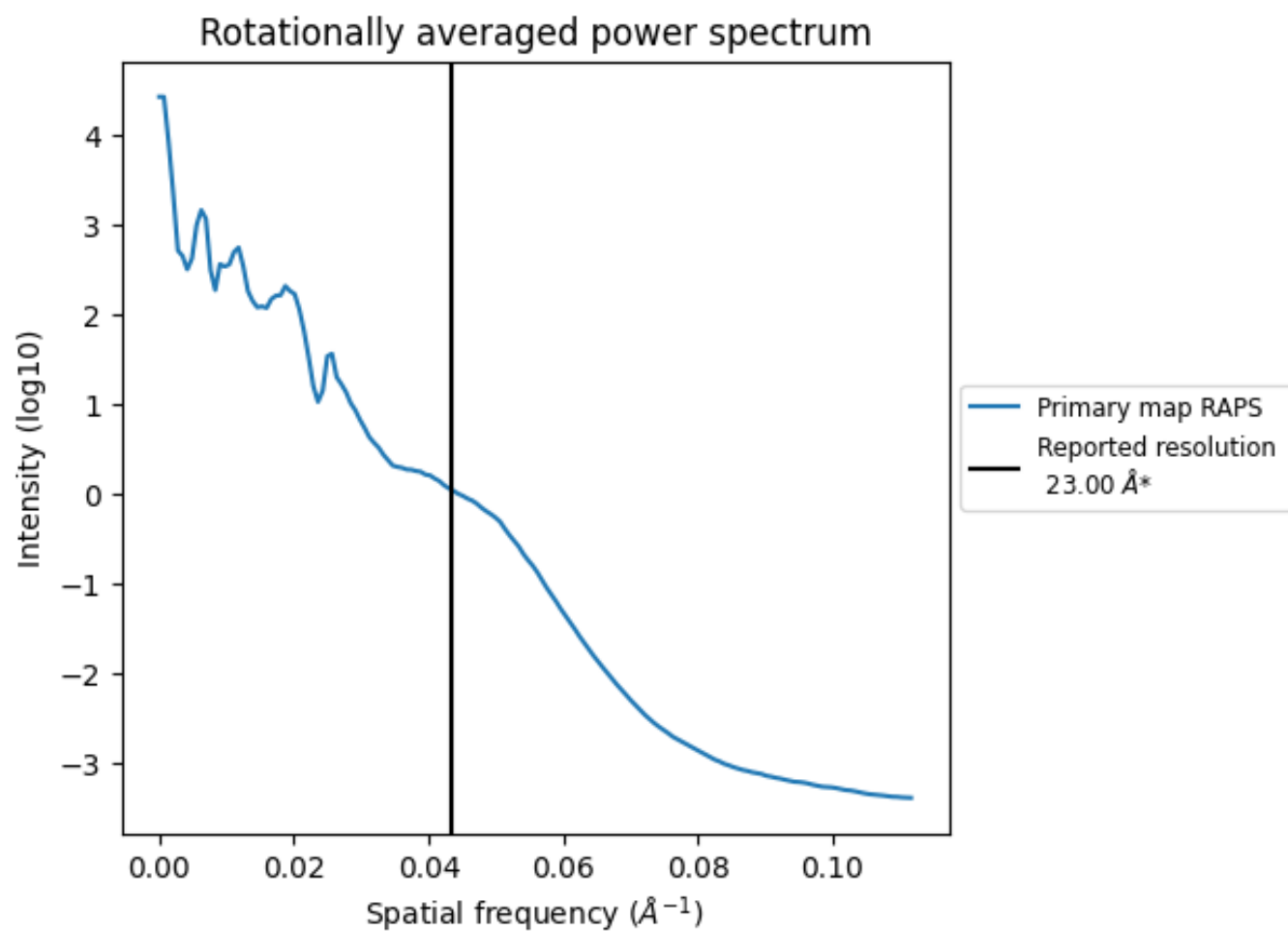
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 88141 nm³; this corresponds to an approximate mass of 79620 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 0.043 Å⁻¹

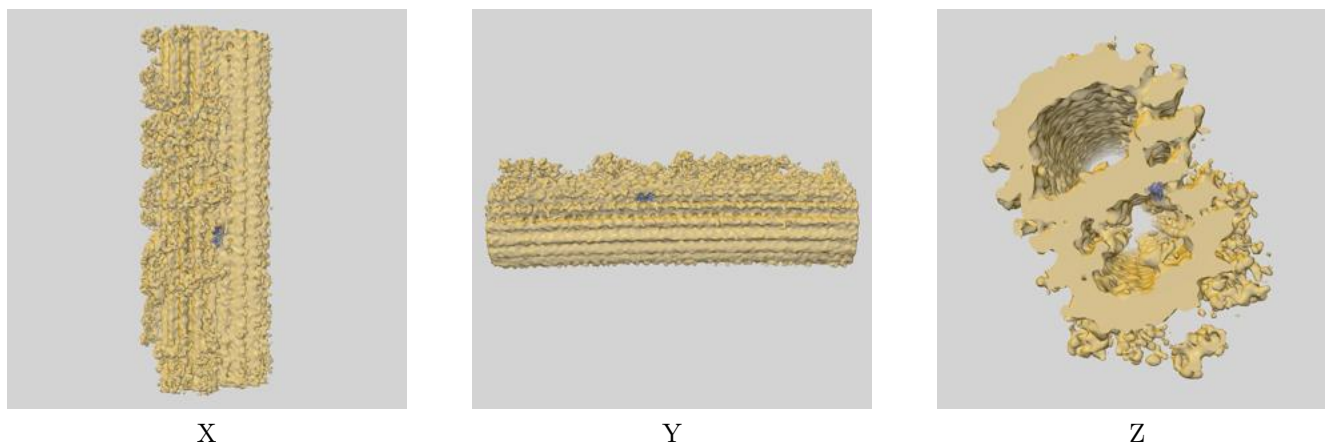
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

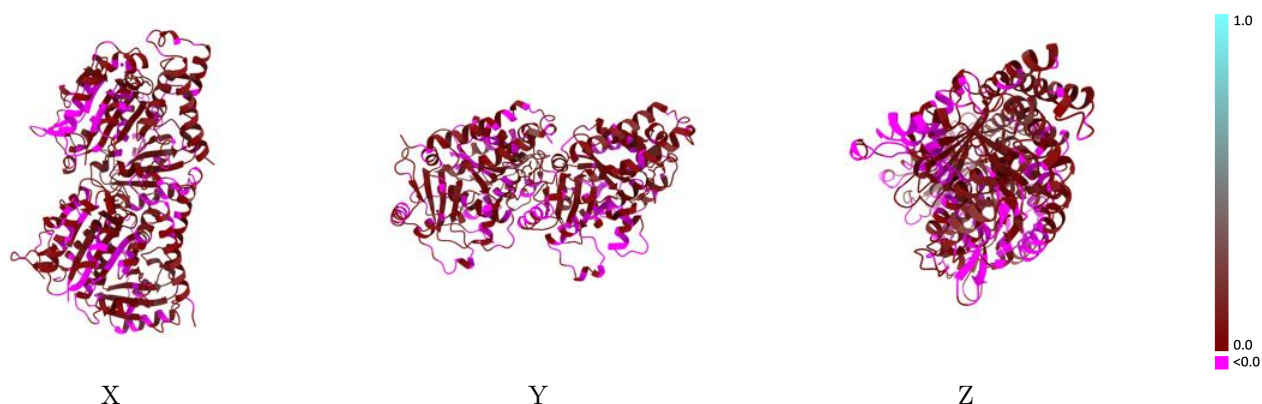
This section contains information regarding the fit between EMDB map EMD-6312 and PDB model 3JAO. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



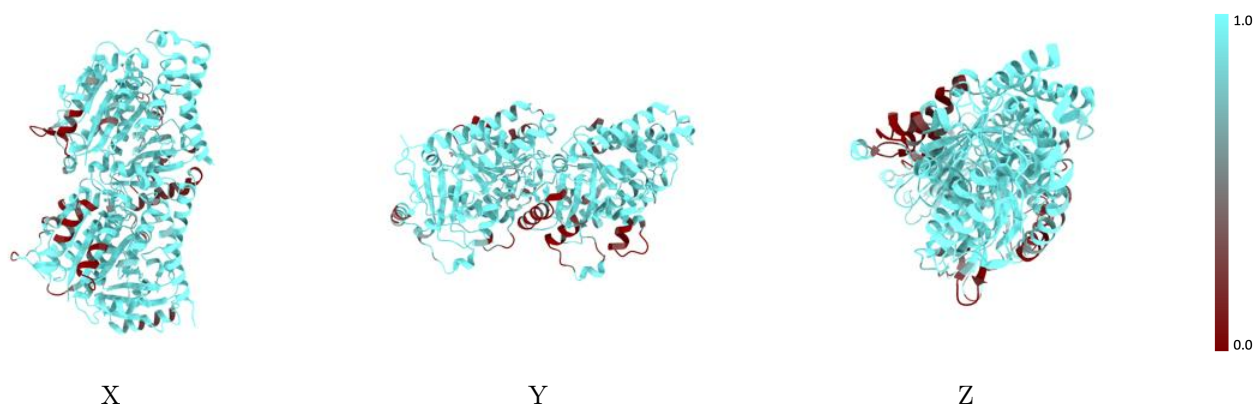
The images above show the 3D surface view of the map at the recommended contour level 1.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



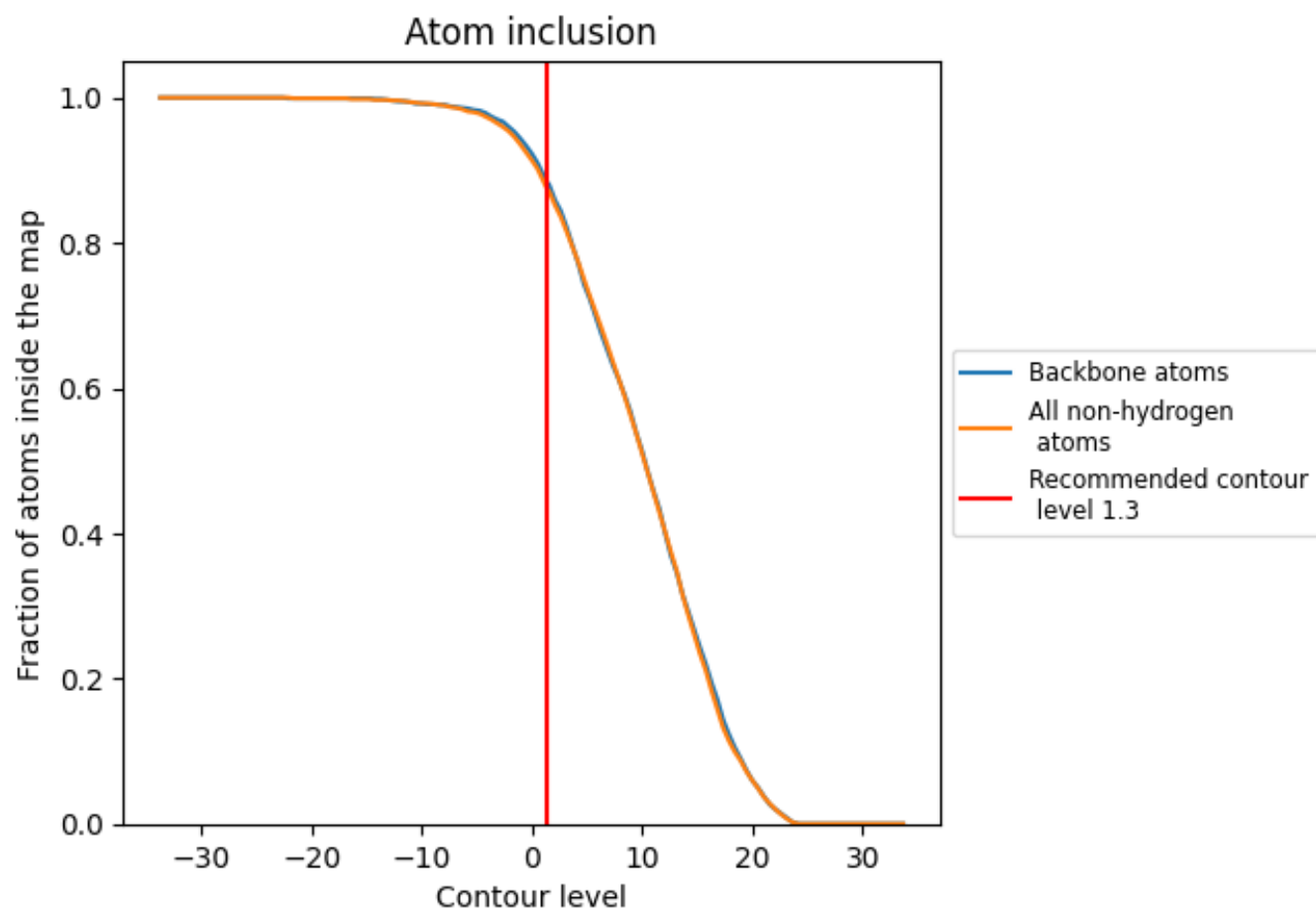
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (1.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8760	0.0360
A	0.9010	0.0390
B	0.8520	0.0330

