



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:11 AM UTC

PDB ID : 9BMS / pdb_00009bms
EMDB ID : EMD-44709
Title : State-2 of motor domain from full-length human dynein-1 in 5 mM ADP
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.04 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
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

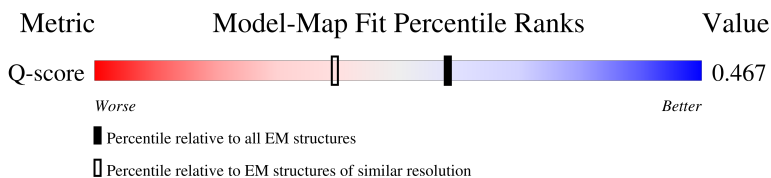
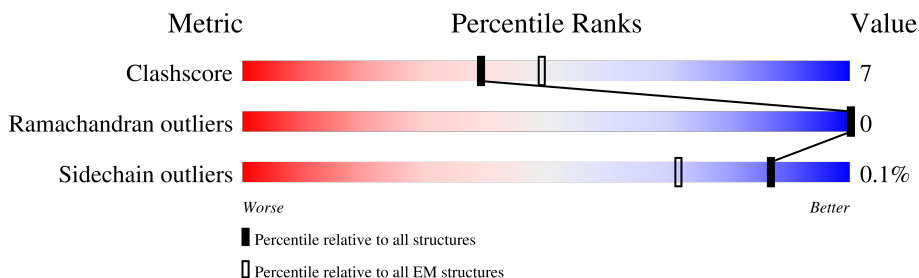
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.04 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	13952 (2.54 - 3.54)

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	4646	

2 Entry composition [i](#)

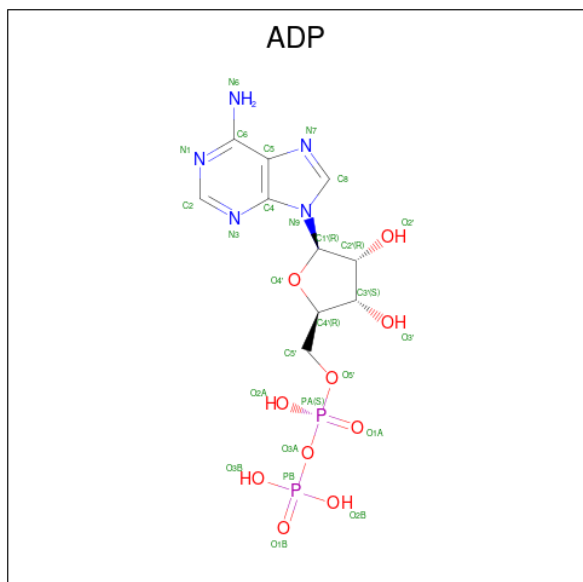
There are 4 unique types of molecules in this entry. The entry contains 23707 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cytoplasmic dynein 1 heavy chain 1.

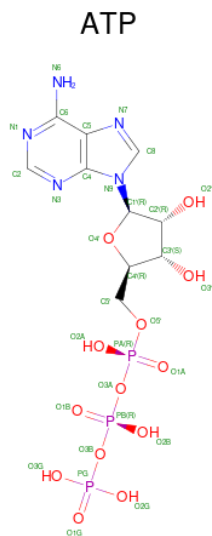
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2937	23593	15028	4070	4378	117	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0
2	A	1	27	10	5	10	2	0
2	A	1	27	10	5	10	2	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total 2	Mg 2	0





GLU	E4542	E4543	S4548	Q4549	Q4550	A4551	T4552	L4553	D4554	Q4566	T4569	N4572	N4573	K4574	S4578	N4579	S4582	T4588	Q4589	L4590	R4591	W4592	V4593	K4594	Q4595	T4596	N4597	T4598	E4599	K4600	K4601	A4602	P4608	V4609	Y4610	L4611	T4619	F4620	T4621	A4627	T4628	K4629	E4630	D4631	V4640	A4641	V4642	T4645		
	F4412	R4415	D4430	Q4436	W4437	C4438	E4439	G4440	K4441	K4442	K4443	Y4447	I4452	N4453	V4456	K4457	G4472	R4485	S4493	A4496	A4497	S4498	G4499	Q4500	A4501	K4502	E4503	L4504	K4505	N4506	I4507	G4513	V4516	P4517	E4518	A4519	R4525	W4534	S4535	L4536	E4537	E4538	L4539	C4540	L4541					
	P4297	D4298	W4308	P4318	M4325	N4326	Q4335	L4344	Q4347	MET	LEU	GLU	ASP	GLU	ASP	ASP	LEU	ALA	TYR	ALA	GLU	THR	GLU	LYS	THR	ARG	THR	ASP	SER	THR	SER	ASP	GLY	ARG	P4374	A4375	R4376	H4381	L4395	S4396	H4397	L4398	K4399	R4400	T4401	V4402	E4403	M4404	I4405	K4406
	M4157	T4160	R4168	E4175	R4176	A4177	R4178	L4179	F4186	T4190	R4195	W4201	Y4205	E4209	L4212	R4213	S4214	A4215	C4216	D4217	D4220	L4223	M4247	A4248	G4253	G4254	M4258	E4259	F4260	D4261	M4266	E4270	R4276	E4281	V4288	D4289	Q4290	H4291	K4292											
	A3953	D3954	E3955	Q3956	F3957	P3966	V3970	E3976	E3977	R3989	Q3994	R4000	L4001	L4002	V4009	L4013	T4020	M4021	L4027	P4037	L4042	M4043	D4050	T4069	A4080	V4088	M4095	L4096	K4097	W4105	L4116	Q4117	P4118	M4128	K4133	P4150														
	R3782	K3783	V3784	E3785	E3786	V3790	K3791	Q3792	E3795	T3796	L3804	Y3825	Q3830	D3834	I3835	Y3839	L3863	R3870	R3873	D3879	K3891	V3896	L3909	V3915	L3916	S3917	A3918	G3919	S3920	T3921	P3922	R3923	I3924	L3927	E3930	Q3931	A3932	V3935	V3936	L3947	I3948									

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38237	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.456	Depositor
Minimum map value	-0.716	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.21	Depositor
Map size ($\text{\AA}$)	329.984, 329.984, 329.984	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0312, 1.0312, 1.0312	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.17	0/24093	0.31	5/32651 (0.0%)

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	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2322	ASN	N-CA-C	-6.76	103.72	112.23
1	A	1885	THR	N-CA-C	-6.65	104.99	113.23
1	A	1883	PRO	N-CA-CB	-5.32	97.65	103.39
1	A	2093	LEU	N-CA-C	-5.25	105.23	111.69
1	A	2321	ASP	N-CA-C	-5.12	105.93	113.61

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2091	ARG	Sidechain
1	A	2358	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	23593	0	23659	339	0
2	A	81	0	36	2	0
3	A	31	0	12	5	0
4	A	2	0	0	2	0
All	All	23707	0	23707	339	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 7.

All (339) 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:3127:PRO:HG3	1:A:3538:GLN:HG2	1.64	0.79
1:A:1959:GLU:HB3	1:A:1962:ARG:HD3	1.71	0.73
1:A:3178:ASP:OD2	1:A:3585:ARG:NE	2.22	0.72
1:A:2149:LEU:HD11	1:A:2157:LEU:HD13	1.72	0.72
1:A:1470:TRP:HB3	1:A:1589:MET:HE2	1.72	0.71
1:A:2231:SER:OG	4:A:4706:MG:MG	1.33	0.70
1:A:1904:PRO:HG2	1:A:2017:THR:HG22	1.72	0.70
1:A:3782:ARG:NH1	1:A:3786:GLU:OE1	2.25	0.69
1:A:2760:PRO:HA	1:A:2763:ARG:HG3	1.75	0.68
1:A:3129:VAL:HG21	1:A:3149:PHE:HB2	1.75	0.68
1:A:1504:VAL:HG12	1:A:1508:LYS:HE3	1.77	0.67
1:A:4088:VAL:HG11	1:A:4116:LEU:HD21	1.77	0.67
1:A:3114:ASP:O	1:A:3140:ARG:NH2	2.29	0.65
1:A:3791:MET:O	1:A:3795:GLU:HG2	1.97	0.65
1:A:3499:GLN:O	1:A:3503:ILE:HG13	1.97	0.65
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.79	0.64
1:A:2320:ASP:OD1	1:A:2358:ARG:NE	2.31	0.64
1:A:2970:GLU:OE2	1:A:2970:GLU:N	2.29	0.64
1:A:2316:ASN:O	1:A:2320:ASP:CG	2.40	0.64
1:A:1503:SER:O	1:A:1507:MET:HG2	1.97	0.64
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.31	0.63
1:A:3207:LYS:NZ	1:A:3756:VAL:O	2.32	0.63
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2229:GLY:HA2	3:A:4702:ATP:O2A	2.00	0.62
1:A:3177:LEU:O	1:A:3181:ASN:ND2	2.32	0.62
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.33	0.62
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.28	0.62
1:A:4190:ILE:HD12	1:A:4201:TRP:HZ2	1.65	0.62
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.81	0.61
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	1.81	0.61
1:A:3597:THR:HG23	1:A:3634:LEU:HD21	1.81	0.61
1:A:4266:ASN:O	1:A:4270:GLU:HG2	2.00	0.61
1:A:2449:LEU:HA	1:A:2453:ARG:HH21	1.65	0.60
1:A:4540:CYS:HB3	1:A:4595:GLN:HG2	1.83	0.60
1:A:1883:PRO:HD2	1:A:2045:ASP:OD2	2.02	0.60
1:A:3581:LYS:HE3	1:A:3582:ARG:HG3	1.82	0.60
1:A:2316:ASN:O	1:A:2320:ASP:OD1	2.20	0.60
1:A:2621:ASN:OD1	1:A:3014:ASN:ND2	2.35	0.60
1:A:1850:GLN:HB3	1:A:1856:GLN:HG2	1.83	0.60
1:A:1962:ARG:NH2	1:A:2314:ASN:OD1	2.34	0.59
1:A:1913:THR:OG1	4:A:4705:MG:MG	1.42	0.59
1:A:4525:ARG:NH2	1:A:4536:LEU:O	2.30	0.59
1:A:1521:LEU:O	1:A:1524:GLU:HG2	2.02	0.59
1:A:1930:PHE:HA	1:A:2326:THR:HG21	1.85	0.59
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.84	0.59
1:A:2172:ARG:NH1	1:A:2205:GLU:OE1	2.36	0.58
1:A:2138:ILE:HD11	1:A:2165:PHE:CG	2.38	0.58
1:A:2590:PRO:HA	1:A:2708:PHE:O	2.03	0.58
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.36	0.58
1:A:4541:LEU:HD11	1:A:4590:LEU:HB3	1.85	0.57
1:A:2138:ILE:HD12	1:A:2161:LEU:HD22	1.86	0.57
1:A:4496:ALA:HB2	1:A:4504:LEU:HD21	1.86	0.57
1:A:2080:LEU:O	1:A:4415:ARG:NH1	2.38	0.57
1:A:3970:VAL:HB	1:A:3989:ARG:HD3	1.87	0.57
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.86	0.57
1:A:2297:LYS:O	1:A:2338:ASN:ND2	2.36	0.56
1:A:4569:THR:HG23	1:A:4578:SER:HB2	1.87	0.56
1:A:4027:LEU:HD11	1:A:4043:MET:HE1	1.86	0.56
1:A:3005:LEU:HD11	1:A:3078:ARG:HH11	1.71	0.56
1:A:4150:PRO:O	1:A:4195:ARG:NH2	2.38	0.56
1:A:1491:ASP:OD1	1:A:1492:ASP:N	2.38	0.56
1:A:3830:GLN:NE2	1:A:3834:ASP:OD1	2.37	0.56
1:A:2818:VAL:O	1:A:2822:ILE:HG12	2.06	0.56
1:A:3214:GLN:HG3	1:A:3759:ARG:HD2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.88	0.55
1:A:2050:ALA:O	1:A:2051:GLN:C	2.48	0.55
1:A:2788:THR:HG22	1:A:2789:GLN:HG2	1.88	0.55
1:A:3459:GLN:HA	1:A:3462:LYS:HD2	1.87	0.55
1:A:3558:GLU:HG3	1:A:3561:ARG:HH12	1.71	0.55
1:A:2773:MET:HG2	1:A:2825:TRP:HE1	1.72	0.55
1:A:2457:SER:OG	1:A:2732:PRO:HB3	2.07	0.54
1:A:3486:ARG:NH1	1:A:3487:GLU:OE2	2.40	0.54
1:A:2942:GLY:HA2	2:A:4704:ADP:O1A	2.07	0.54
1:A:3932:ALA:O	1:A:3936:VAL:HG23	2.07	0.54
1:A:1671:SER:HB2	1:A:1693:THR:HG23	1.89	0.54
1:A:3559:ARG:O	1:A:3563:GLN:HG2	2.07	0.54
1:A:1512:TYR:O	1:A:1515:VAL:HG12	2.08	0.54
1:A:1958:ASP:OD1	1:A:2017:THR:OG1	2.19	0.54
1:A:3655:ARG:HG2	1:A:3660:VAL:HG22	1.90	0.54
1:A:4042:LEU:HD22	1:A:4128:MET:HE1	1.90	0.54
1:A:2174:GLU:OE1	1:A:2176:THR:OG1	2.27	0.53
1:A:4566:GLN:O	1:A:4640:VAL:HA	2.09	0.53
1:A:1561:LEU:O	1:A:1565:THR:OG1	2.20	0.53
1:A:4020:ILE:HG23	1:A:4021:MET:HE2	1.91	0.53
1:A:2285:ARG:NH1	1:A:2331:GLU:OE2	2.30	0.53
1:A:2049:ILE:O	1:A:2053:MET:HG3	2.08	0.53
1:A:4574:LYS:HB3	1:A:4627:ALA:HB2	1.91	0.53
1:A:2498:ILE:HG23	1:A:2502:LEU:HD22	1.90	0.53
1:A:2557:VAL:O	1:A:2757:ARG:NH2	2.42	0.53
1:A:1623:ARG:NH2	1:A:1634:ASP:OD1	2.40	0.53
1:A:3017:VAL:HB	1:A:3020:LEU:HB2	1.91	0.52
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.91	0.52
1:A:2454:CYS:HB3	1:A:2502:LEU:HD12	1.92	0.52
1:A:2974:GLU:OE1	1:A:2977:ARG:NH1	2.43	0.52
1:A:3154:LEU:HG	1:A:3516:TYR:CD1	2.44	0.52
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.89	0.52
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.42	0.52
1:A:2688:GLU:OE1	1:A:2730:HIS:NE2	2.43	0.52
1:A:2967:TYR:OH	1:A:2975:ASP:OD2	2.24	0.52
1:A:3215:VAL:HG21	1:A:3479:LEU:HD11	1.91	0.52
1:A:2623:SER:OG	1:A:3006:GLU:OE1	2.28	0.52
1:A:4096:LEU:HD13	1:A:4105:TRP:HH2	1.75	0.52
1:A:1855:GLN:OE1	1:A:1867:ASN:ND2	2.43	0.52
1:A:2863:ARG:HG2	1:A:2863:ARG:HH11	1.75	0.52
1:A:4485:ARG:HG2	1:A:4513:GLY:HA2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1881:GLN:NE2	1:A:1886:ASP:OD1	2.43	0.51
1:A:2308:ASP:O	1:A:2312:VAL:HG12	2.09	0.51
1:A:2925:ILE:HG21	1:A:2933:LEU:HG	1.91	0.51
1:A:3176:TYR:O	1:A:3180:ILE:HG12	2.11	0.51
1:A:2905:LEU:HD11	1:A:3652:GLU:HB3	1.91	0.51
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	1.93	0.51
1:A:1907:PRO:HG2	1:A:1910:THR:HG21	1.93	0.51
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.93	0.51
1:A:4525:ARG:HD3	1:A:4536:LEU:HD23	1.92	0.51
1:A:4095:MET:HE3	1:A:4097:LYS:HE2	1.92	0.51
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.43	0.51
1:A:2039:LEU:HD12	1:A:4254:GLY:HA2	1.92	0.50
1:A:2452:LEU:HD11	3:A:4702:ATP:H4'	1.92	0.50
1:A:3650:ASN:HD21	1:A:3695:ARG:HH11	1.60	0.50
1:A:2175:MET:HE3	1:A:2208:LEU:HD22	1.91	0.50
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.94	0.50
1:A:1946:VAL:HG22	1:A:2006:VAL:HG21	1.93	0.50
1:A:2211:TYR:O	1:A:2214:THR:OG1	2.30	0.50
1:A:2784:PHE:HB2	1:A:2794:TYR:HE2	1.76	0.49
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.12	0.49
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.95	0.49
1:A:2030:ASP:HB2	1:A:4050:ASP:HB2	1.94	0.49
1:A:1507:MET:O	1:A:1513:TYR:HB2	2.12	0.49
1:A:1587:LEU:HB3	1:A:1590:ASP:HB2	1.94	0.49
1:A:2388:ASP:OD1	1:A:2389:GLU:N	2.46	0.49
1:A:2581:LEU:HD11	1:A:2593:LEU:HD21	1.93	0.49
1:A:2980:LEU:HB3	1:A:3054:PHE:HZ	1.76	0.49
1:A:4503:GLU:O	1:A:4507:ILE:HG23	2.13	0.49
1:A:2972:PHE:HB2	1:A:3004:PHE:HE1	1.77	0.49
1:A:3127:PRO:HG2	1:A:3539:ALA:HB2	1.95	0.49
1:A:3161:LEU:HD23	1:A:3168:THR:HG22	1.95	0.49
1:A:3741:ARG:HD3	1:A:3745:LEU:HG	1.95	0.49
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.95	0.49
1:A:2068:LYS:NZ	1:A:2164:VAL:O	2.43	0.49
1:A:2087:ASP:O	1:A:2148:LYS:NZ	2.45	0.48
1:A:2132:PRO:HB2	1:A:2135:GLU:HB2	1.94	0.48
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.46	0.48
1:A:2290:SER:HB2	1:A:2295:LEU:HG	1.95	0.48
1:A:2956:LEU:HD22	1:A:2989:LYS:HB3	1.95	0.48
1:A:3100:GLU:OE1	1:A:3132:LYS:NZ	2.45	0.48
1:A:3935:VAL:HG13	1:A:3947:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1664:ILE:HG22	1:A:1676:ILE:HG22	1.95	0.48
1:A:1674:LEU:HB3	1:A:1685:MET:HE1	1.96	0.48
1:A:2354:ALA:O	1:A:2358:ARG:HD2	2.13	0.48
1:A:3927:LEU:HD11	1:A:3957:PHE:HE2	1.77	0.48
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.96	0.48
1:A:1978:ILE:HG23	1:A:2012:MET:HE1	1.95	0.48
1:A:4453:ASN:O	1:A:4457:LYS:HG2	2.13	0.48
1:A:2972:PHE:HB2	1:A:3004:PHE:CE1	2.49	0.47
1:A:3109:PHE:CD2	1:A:3180:ILE:HG22	2.49	0.47
1:A:3624:GLU:HG3	1:A:3669:ILE:HD13	1.95	0.47
1:A:4176:ARG:NH1	1:A:4220:ASP:OD1	2.47	0.47
1:A:1619:LEU:HD11	1:A:1638:LEU:HG	1.96	0.47
1:A:3716:VAL:HG21	1:A:3804:LEU:HD23	1.96	0.47
1:A:2373:MET:HE2	3:A:4702:ATP:C6	2.50	0.47
1:A:2492:ARG:HG2	1:A:2545:TRP:NE1	2.30	0.47
1:A:3239:LYS:HB3	1:A:3451:TYR:CD1	2.49	0.47
1:A:3727:LYS:O	1:A:3731:LEU:HD13	2.14	0.47
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.97	0.47
1:A:4179:LEU:HD12	1:A:4223:LEU:HD22	1.96	0.47
1:A:4499:GLY:HA3	1:A:4503:GLU:HG3	1.97	0.47
1:A:1882:THR:HG22	1:A:2048:LEU:HD23	1.97	0.47
1:A:3471:LYS:HG3	1:A:3474:ARG:HH21	1.80	0.47
1:A:3741:ARG:HD3	1:A:3741:ARG:O	2.15	0.47
1:A:3514:ILE:HD11	1:A:3553:LEU:HD22	1.97	0.47
1:A:2751:PHE:HB3	1:A:2803:VAL:HG11	1.97	0.46
1:A:4517:PRO:HG2	1:A:4619:ILE:HD12	1.97	0.46
1:A:1895:ALA:HB2	1:A:2037:ARG:HB2	1.97	0.46
1:A:2063:GLU:O	1:A:2067:ASN:ND2	2.48	0.46
1:A:2912:PHE:CE2	1:A:2914:GLU:HB2	2.50	0.46
1:A:4400:ARG:HD2	1:A:4405:ILE:HD11	1.97	0.46
1:A:2257:LYS:NZ	1:A:2308:ASP:OD2	2.45	0.46
1:A:3753:LEU:HD21	1:A:3770:LEU:HD11	1.96	0.46
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	1.96	0.46
1:A:3721:ARG:HE	1:A:3724:VAL:HG21	1.80	0.46
1:A:4215:ALA:HB1	1:A:4247:MET:HE2	1.97	0.46
1:A:2452:LEU:HD13	1:A:2729:ARG:HE	1.80	0.46
1:A:1606:ASP:O	1:A:1610:LYS:HG3	2.16	0.46
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.98	0.46
1:A:1508:LYS:NZ	1:A:1524:GLU:OE1	2.28	0.46
1:A:1853:VAL:HA	1:A:1856:GLN:HG3	1.98	0.46
1:A:2912:PHE:HE2	1:A:2914:GLU:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.16	0.46
1:A:3013:ALA:HA	1:A:3088:ARG:HG3	1.98	0.45
1:A:2134:GLN:O	1:A:2138:ILE:HG12	2.16	0.45
1:A:3627:LEU:HD12	1:A:3664:LEU:HD22	1.97	0.45
1:A:2224:GLY:O	1:A:2346:GLN:HA	2.15	0.45
1:A:2892:TYR:HE2	1:A:2953:MET:HE1	1.80	0.45
1:A:3133:LEU:HD11	1:A:3141:GLU:HB3	1.97	0.45
1:A:1550:ILE:O	1:A:1554:SER:OG	2.35	0.45
1:A:2776:PHE:HZ	1:A:2846:THR:HG23	1.82	0.45
1:A:3154:LEU:HD21	1:A:3532:TRP:HZ2	1.81	0.45
1:A:3825:TYR:OH	1:A:3879:ASP:OD2	2.27	0.45
1:A:2894:LYS:O	1:A:2898:LYS:HG3	2.16	0.45
1:A:3150:VAL:O	1:A:3154:LEU:HD23	2.17	0.45
1:A:3211:THR:O	1:A:3215:VAL:HG13	2.17	0.45
1:A:1878:LYS:HB3	1:A:1878:LYS:HE3	1.61	0.45
1:A:3225:LYS:HZ1	1:A:3464:ASP:HB3	1.81	0.45
1:A:3891:LYS:HD2	1:A:4013:LEU:HD23	1.98	0.45
1:A:2665:GLU:HB3	1:A:2668:LEU:HD12	1.98	0.45
1:A:3588:LEU:HD11	1:A:3638:VAL:HG11	1.98	0.45
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.99	0.45
1:A:4186:PHE:O	1:A:4190:ILE:HG12	2.17	0.44
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.53	0.44
1:A:3239:LYS:HB3	1:A:3451:TYR:CE1	2.52	0.44
1:A:3873:ARG:HD3	1:A:3873:ARG:HA	1.83	0.44
1:A:2220:LEU:HD22	1:A:2342:MET:HE2	1.99	0.44
1:A:3731:LEU:HD21	1:A:3790:VAL:HG12	1.99	0.44
1:A:3783:LYS:O	1:A:3786:GLU:HG2	2.17	0.44
1:A:4205:TYR:OH	1:A:4261:ASP:OD2	2.33	0.44
1:A:4209:GLU:O	1:A:4213:ARG:HG3	2.17	0.44
1:A:1699:ASN:OD1	1:A:1700:GLU:N	2.50	0.44
1:A:1907:PRO:HG2	1:A:1910:THR:CG2	2.48	0.44
1:A:3644:VAL:HG22	1:A:3664:LEU:HD12	1.99	0.44
1:A:3780:VAL:HA	1:A:3783:LYS:HD2	2.00	0.44
1:A:3478:LEU:HD11	1:A:3767:ILE:HG23	2.00	0.44
1:A:1598:GLN:O	1:A:1602:GLU:HG3	2.18	0.44
1:A:3229:LEU:HD11	1:A:3462:LYS:HG3	1.99	0.44
1:A:3457:GLU:O	1:A:3461:ILE:HG12	2.17	0.44
1:A:4157:MET:HE2	1:A:4157:MET:HB3	1.87	0.44
1:A:4175:GLU:OE1	1:A:4175:GLU:N	2.50	0.44
1:A:4516:VAL:HG12	1:A:4519:ALA:H	1.83	0.44
1:A:2245:GLU:OE1	1:A:2298:ARG:NH2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2275:TRP:NE1	1:A:2277:ASP:OD1	2.43	0.44
1:A:2694:ARG:O	1:A:2698:GLN:N	2.51	0.44
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.99	0.44
1:A:2671:MET:HG2	1:A:2675:GLY:HA2	1.99	0.44
1:A:3127:PRO:O	1:A:3145:ASN:ND2	2.51	0.44
1:A:3477:ALA:O	1:A:3480:LYS:HG3	2.18	0.44
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	1.99	0.44
1:A:1969:SER:O	1:A:1972:SER:OG	2.33	0.43
1:A:2694:ARG:HG3	1:A:2701:VAL:HG21	2.00	0.43
1:A:3039:LYS:HB3	1:A:3039:LYS:HE3	1.74	0.43
1:A:3692:LEU:O	1:A:3696:VAL:HG22	2.18	0.43
1:A:3792:GLN:O	1:A:3796:THR:HG23	2.19	0.43
1:A:3924:ILE:HG12	1:A:3948:ILE:HG23	1.99	0.43
1:A:4069:ILE:HD13	1:A:4080:ALA:HA	1.99	0.43
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.51	0.43
1:A:1885:THR:O	1:A:1889:TYR:CD1	2.70	0.43
1:A:2773:MET:HG2	1:A:2825:TRP:NE1	2.33	0.43
1:A:2413:LEU:HD12	1:A:2413:LEU:HA	1.89	0.43
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.53	0.43
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	1.99	0.43
1:A:4566:GLN:OE1	1:A:4582:SER:OG	2.26	0.43
1:A:1906:GLY:C	1:A:1907:PRO:O	2.59	0.43
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.53	0.43
1:A:3781:THR:O	1:A:3785:GLU:OE1	2.36	0.43
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.51	0.43
1:A:3741:ARG:HG3	1:A:3780:VAL:HG21	2.01	0.43
1:A:2369:LEU:HD21	3:A:4702:ATP:O4'	2.18	0.43
1:A:3568:PRO:HG2	1:A:3573:CYS:SG	2.59	0.43
1:A:2065:LEU:HD22	1:A:2137:LEU:HD22	2.01	0.43
1:A:2074:LYS:HE2	1:A:2074:LYS:HB3	1.75	0.43
1:A:2571:THR:H	1:A:2574:THR:HB	1.84	0.43
1:A:3238:ASP:HA	1:A:3241:LYS:HD2	2.00	0.43
1:A:1547:LEU:HD12	1:A:1608:LEU:HD22	2.01	0.43
1:A:4452:ILE:O	1:A:4456:VAL:HG23	2.19	0.42
1:A:2265:TYR:O	1:A:2281:THR:OG1	2.34	0.42
1:A:2901:TYR:CZ	1:A:2908:PRO:HA	2.54	0.42
1:A:3024:ASP:N	1:A:3024:ASP:OD1	2.51	0.42
1:A:3114:ASP:O	1:A:3116:GLU:HG2	2.19	0.42
1:A:3148:VAL:O	1:A:3152:GLN:HG3	2.20	0.42
1:A:3741:ARG:HH11	1:A:3745:LEU:HD21	1.84	0.42
1:A:3482:LEU:HD11	1:A:3770:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4002:LEU:HD11	1:A:4335:GLN:HB3	2.01	0.42
1:A:1626:PHE:HB3	1:A:1629:PHE:CD2	2.54	0.42
1:A:4288:VAL:HG21	1:A:4292:LYS:HE2	2.01	0.42
1:A:4525:ARG:HG3	1:A:4592:TRP:CZ3	2.55	0.42
1:A:2867:MET:HB3	1:A:2869:ARG:HH21	1.85	0.42
1:A:3659:ARG:HE	1:A:3661:LEU:HD21	1.84	0.42
1:A:1477:LEU:HB3	1:A:1485:ARG:HB3	2.01	0.42
1:A:1547:LEU:HD23	1:A:1547:LEU:HA	1.89	0.42
1:A:2387:LEU:N	1:A:2416:GLN:OE1	2.47	0.42
1:A:2633:LYS:HD2	1:A:3019:GLY:HA3	2.02	0.42
1:A:3010:THR:HG21	1:A:3018:PRO:HD3	2.01	0.42
1:A:3207:LYS:HD3	1:A:3207:LYS:HA	1.84	0.42
1:A:3546:ASP:OD1	1:A:3546:ASP:N	2.52	0.42
1:A:1521:LEU:HD23	1:A:1521:LEU:HA	1.91	0.42
1:A:1738:TYR:HE2	1:A:1792:LEU:HD21	1.85	0.42
1:A:1945:PHE:HB3	1:A:1978:ILE:HD11	2.01	0.42
1:A:3786:GLU:O	1:A:3790:VAL:HG23	2.20	0.42
1:A:1619:LEU:HD21	1:A:1638:LEU:HD23	2.01	0.41
1:A:1859:ILE:HD11	1:A:1868:TYR:HD1	1.84	0.41
1:A:2374:ILE:HD13	1:A:2452:LEU:HD21	2.01	0.41
1:A:2697:ASP:OD1	1:A:2697:ASP:N	2.53	0.41
1:A:3558:GLU:OE2	1:A:3581:LYS:HD3	2.19	0.41
1:A:1543:ARG:HA	1:A:1546:TYR:CE2	2.55	0.41
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.55	0.41
1:A:4297:PRO:HG3	1:A:4308:TRP:CD2	2.55	0.41
1:A:2307:VAL:HA	1:A:2311:TRP:HE1	1.84	0.41
1:A:2688:GLU:HB2	1:A:2730:HIS:CE1	2.54	0.41
1:A:2945:THR:OG1	2:A:4704:ADP:O1A	2.26	0.41
1:A:4190:ILE:HD12	1:A:4201:TRP:CZ2	2.50	0.41
1:A:1538:ILE:HG23	1:A:1539:ASP:H	1.86	0.41
1:A:2490:ILE:HD13	1:A:2490:ILE:HA	1.93	0.41
1:A:3115:LEU:HD22	1:A:3143:ILE:HG13	2.03	0.41
1:A:2231:SER:HB2	3:A:4702:ATP:O1A	2.21	0.41
1:A:2615:MET:SD	1:A:2707:GLN:NE2	2.93	0.41
1:A:3909:LEU:HB3	1:A:4344:LEU:HD13	2.02	0.41
1:A:4248:ALA:O	1:A:4253:GLY:HA3	2.21	0.41
1:A:4401:THR:O	1:A:4405:ILE:HG12	2.20	0.41
1:A:4276:ARG:HA	1:A:4276:ARG:HE	1.84	0.41
1:A:2012:MET:HB3	1:A:2012:MET:HE3	1.63	0.41
1:A:4260:PHE:CE2	1:A:4608:PRO:HB3	2.56	0.41
1:A:1493:LEU:HD21	1:A:1534:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1884:LEU:HG	1:A:1884:LEU:O	2.20	0.41
1:A:2896:ARG:HG3	1:A:2953:MET:HE3	2.02	0.41
1:A:4430:ASP:OD2	1:A:4447:TYR:OH	2.36	0.41
1:A:1912:LYS:HB2	1:A:1912:LYS:HE3	1.57	0.41
1:A:1929:VAL:H	1:A:2332:ARG:HH21	1.69	0.41
1:A:2268:LEU:HD12	1:A:2268:LEU:HA	1.94	0.41
1:A:3731:LEU:HD21	1:A:3790:VAL:CG1	2.51	0.41
1:A:4258:ASN:HB3	1:A:4261:ASP:HB2	2.02	0.41
1:A:4260:PHE:HZ	1:A:4621:THR:HG22	1.86	0.41
1:A:4543:VAL:HG13	1:A:4588:THR:HG23	2.02	0.41
1:A:1640:ILE:HD11	1:A:1653:HIS:HB3	2.03	0.41
1:A:2413:LEU:O	1:A:2417:ARG:HG3	2.21	0.41
1:A:3003:GLY:O	1:A:3007:ARG:HG3	2.21	0.41
1:A:3199:MET:HE3	1:A:3200:HIS:CE1	2.56	0.41
1:A:1459:LEU:HD23	1:A:1507:MET:HB3	2.03	0.40
1:A:4619:ILE:HG22	1:A:4620:PHE:HD1	1.86	0.40
1:A:2446:ILE:HD12	1:A:2446:ILE:HA	1.93	0.40
1:A:2548:TRP:CD1	1:A:2576:ARG:HG2	2.56	0.40
1:A:2629:GLU:OE1	1:A:2633:LYS:HE3	2.21	0.40
1:A:3182:HIS:NE2	1:A:3582:ARG:O	2.46	0.40
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	2.03	0.40
1:A:4133:LYS:HB2	1:A:4133:LYS:HE2	1.81	0.40
1:A:2668:LEU:HD23	1:A:2668:LEU:HA	1.96	0.40
1:A:2894:LYS:HG3	1:A:2911:LEU:HD12	2.03	0.40
1:A:3028:THR:O	1:A:3032:GLN:HG3	2.21	0.40
1:A:3835:ILE:HG12	1:A:3870:ARG:HD2	2.04	0.40
1:A:4534:TRP:HE3	1:A:4539:LEU:HD21	1.86	0.40
1:A:3113:MET:HE1	1:A:3183:TYR:CD2	2.56	0.40
1:A:3994:GLN:HB2	1:A:4001:LEU:HD13	2.02	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	2929/4646 (63%)	2879 (98%)	50 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	2605/4125 (63%)	2602 (100%)	3 (0%)	88	91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1878	LYS
1	A	2047	GLN
1	A	4573	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1465	GLN
1	A	1598	GLN
1	A	1643	ASN
1	A	1855	GLN
1	A	1867	ASN
1	A	1894	GLN
1	A	2057	GLN
1	A	2134	GLN
1	A	2217	ASN
1	A	2263	HIS
1	A	2464	GLN
1	A	2713	ASN
1	A	2960	GLN
1	A	3009	ASN
1	A	3152	GLN

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Mol	Chain	Res	Type
1	A	3200	HIS
1	A	3233	ASN
1	A	3237	ASN
1	A	3499	GLN
1	A	3526	GLN
1	A	3602	ASN
1	A	3622	ASN
1	A	3709	GLN
1	A	3711	GLN
1	A	3744	GLN
1	A	3820	GLN
1	A	3838	ASN
1	A	3877	HIS
1	A	3968	GLN
1	A	4012	ASN
1	A	4098	ASN
1	A	4114	HIS
1	A	4156	ASN
1	A	4231	GLN
1	A	4249	GLN
1	A	4295	GLN
1	A	4307	GLN
1	A	4429	GLN
1	A	4477	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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
2	ADP	A	4704	-	28,29,29	0.53	0	43,45,45	0.58	0
2	ADP	A	4701	4	28,29,29	0.53	0	43,45,45	0.52	0
2	ADP	A	4703	-	28,29,29	0.69	0	43,45,45	0.48	0
3	ATP	A	4702	4	32,33,33	0.62	0	48,52,52	0.68	0

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	ADP	A	4704	-	-	5/16/32/32	0/3/3/3
2	ADP	A	4701	4	-	0/16/32/32	0/3/3/3
2	ADP	A	4703	-	-	2/16/32/32	0/3/3/3
3	ATP	A	4702	4	-	4/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

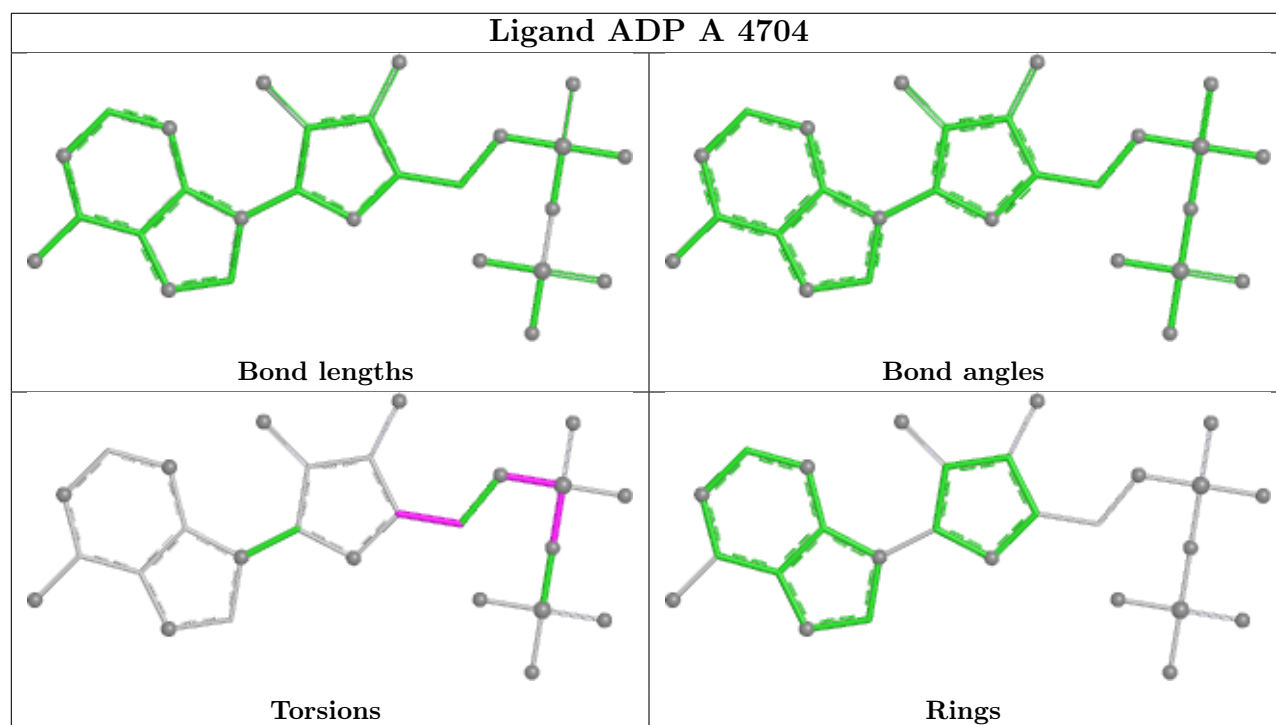
Mol	Chain	Res	Type	Atoms
2	A	4704	ADP	C5'-O5'-PA-O1A
3	A	4702	ATP	O4'-C4'-C5'-O5'
2	A	4704	ADP	O4'-C4'-C5'-O5'
2	A	4704	ADP	C3'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'
2	A	4703	ADP	PB-O3A-PA-O2A
2	A	4704	ADP	PB-O3A-PA-O2A
2	A	4704	ADP	PB-O3A-PA-O1A
3	A	4702	ATP	PA-O3A-PB-O1B
3	A	4702	ATP	PA-O3A-PB-O2B
2	A	4703	ADP	PB-O3A-PA-O1A

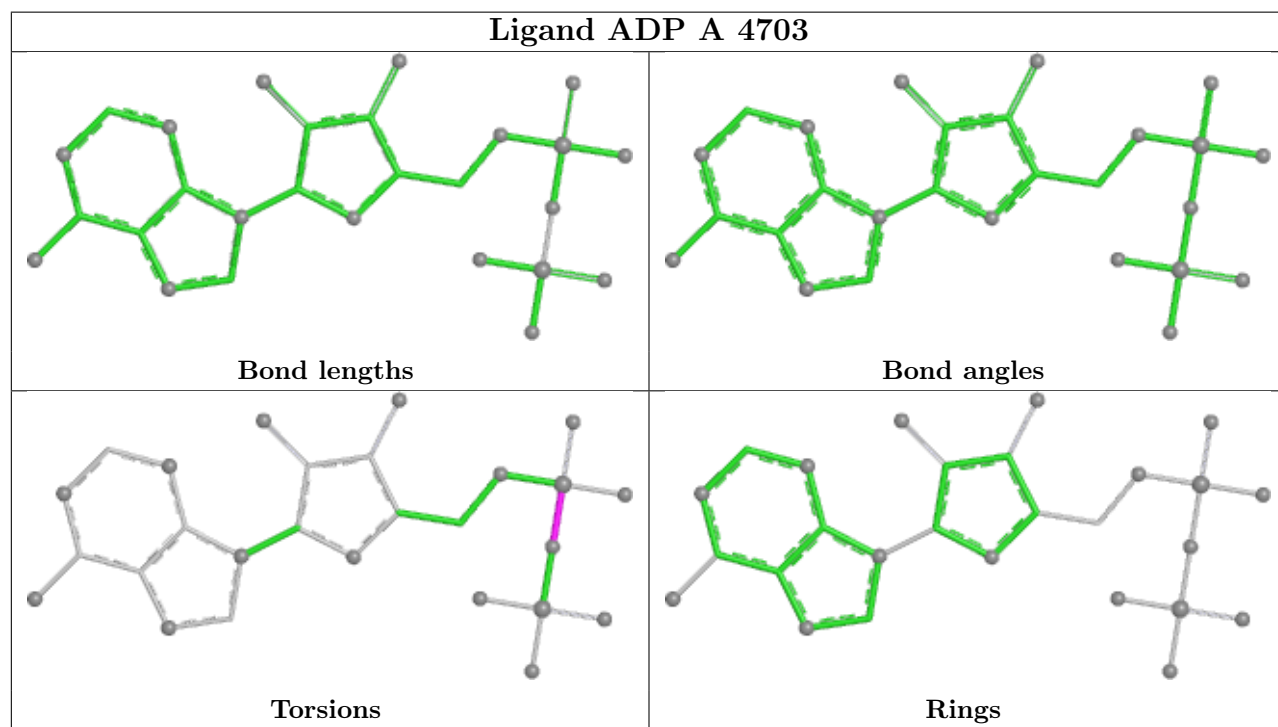
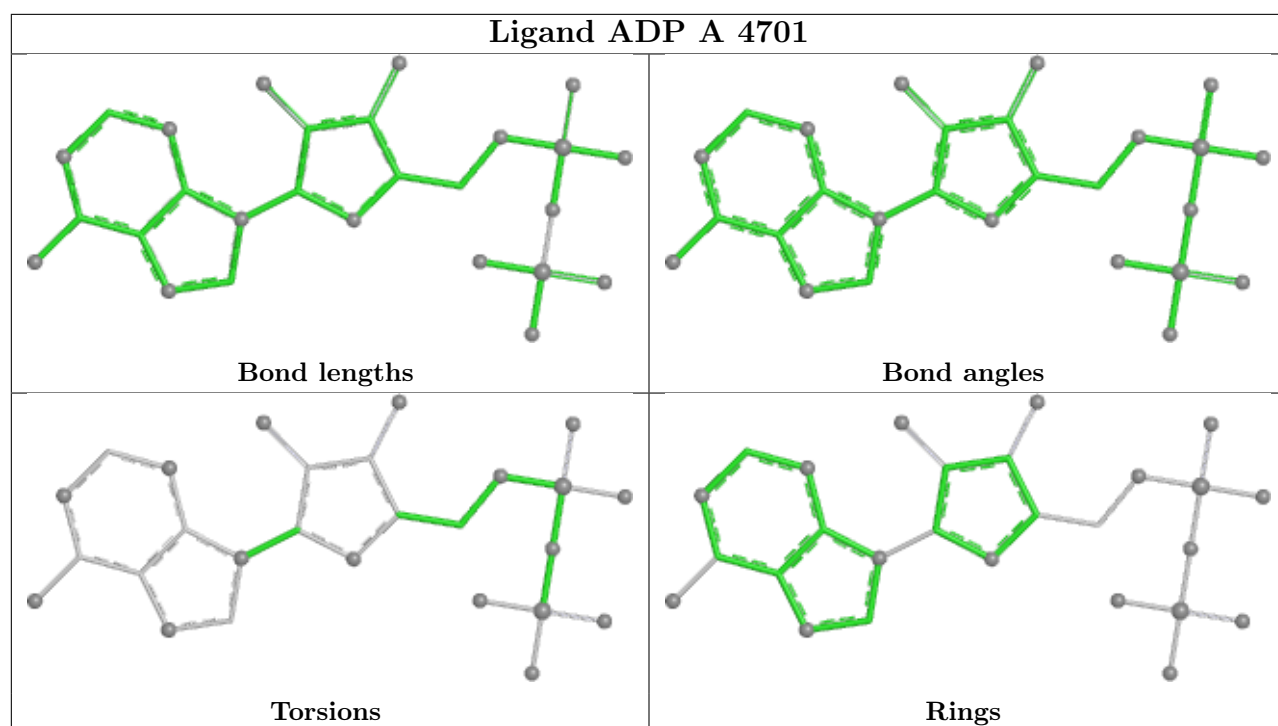
There are no ring outliers.

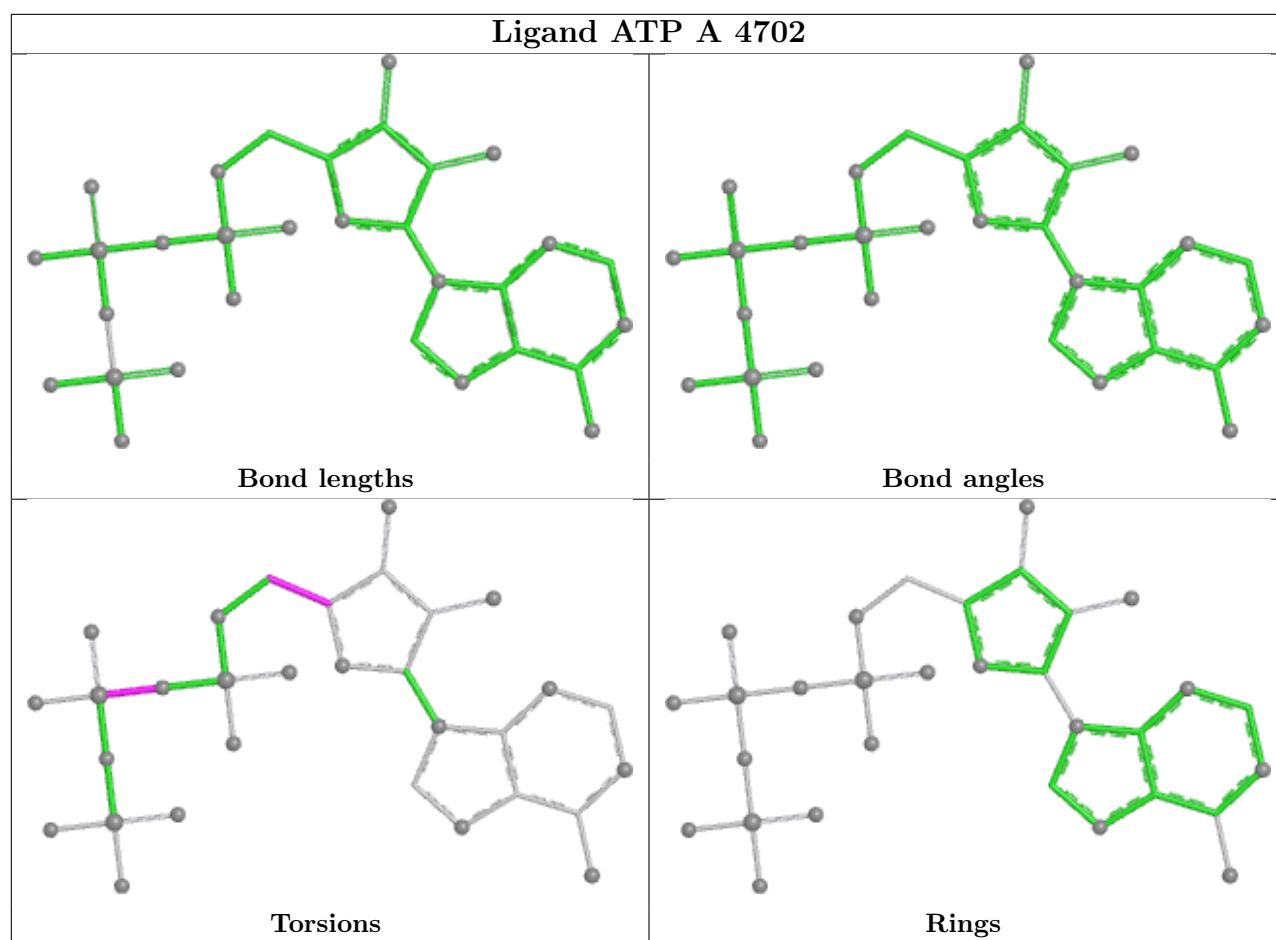
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4704	ADP	2	0
3	A	4702	ATP	5	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.

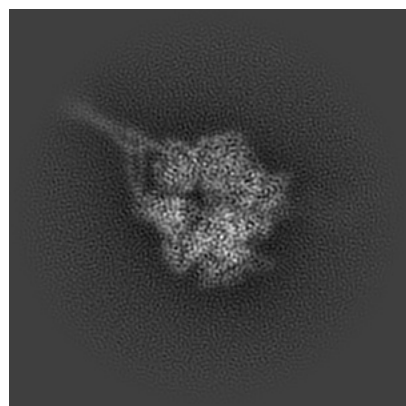
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44709. These allow visual inspection of the internal detail of the map and identification of artifacts.

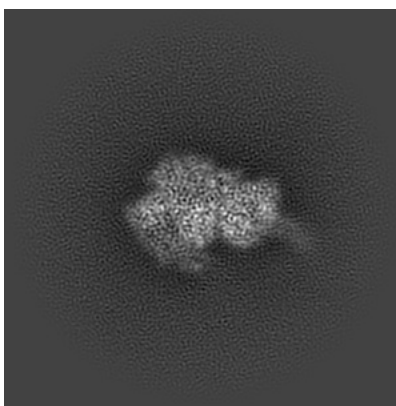
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

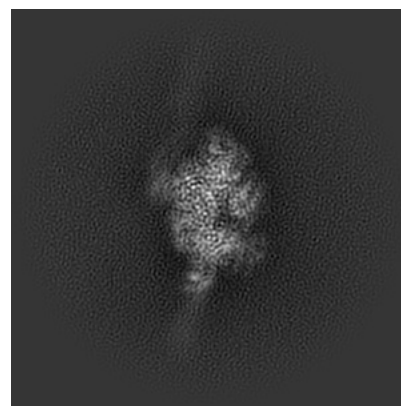
6.1.1 Primary map



X

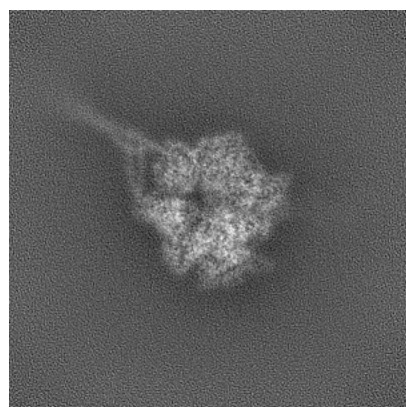


Y

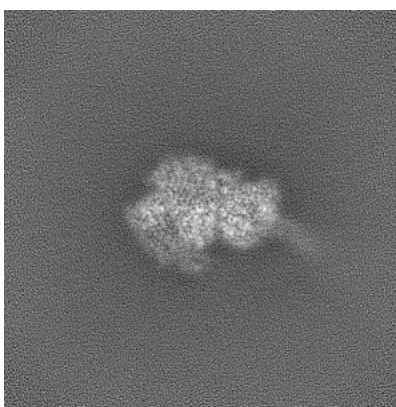


Z

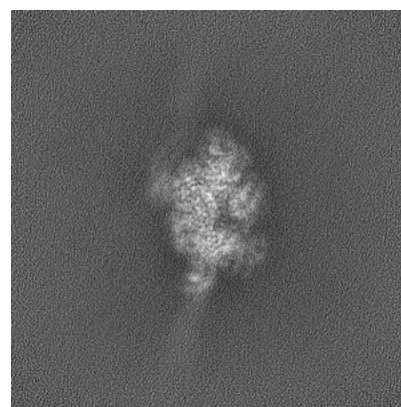
6.1.2 Raw map



X



Y

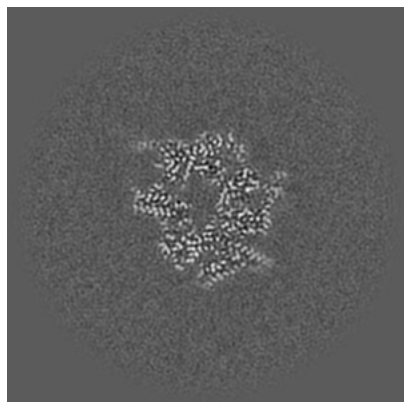


Z

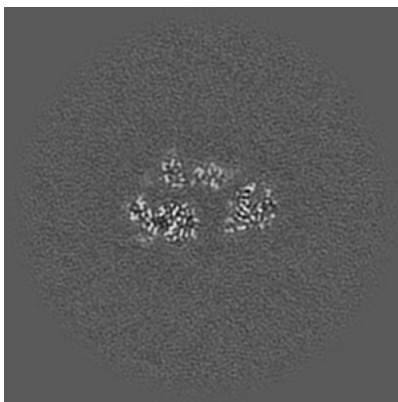
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

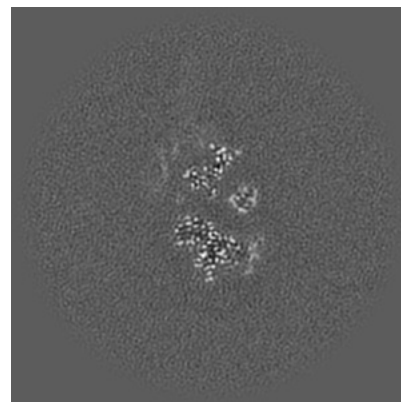
6.2.1 Primary map



X Index: 160

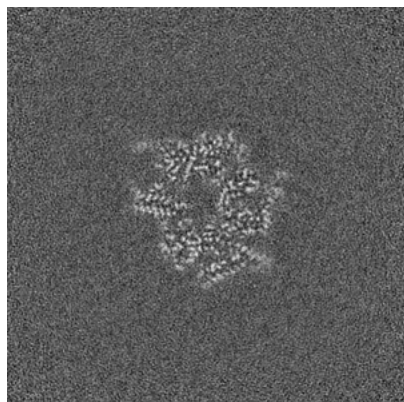


Y Index: 160

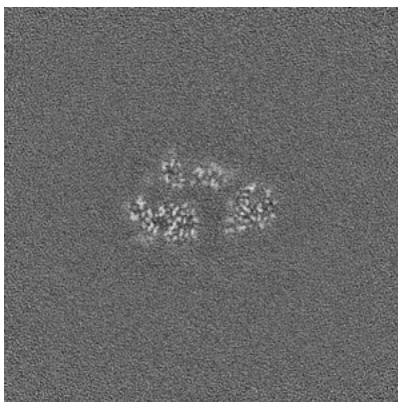


Z Index: 160

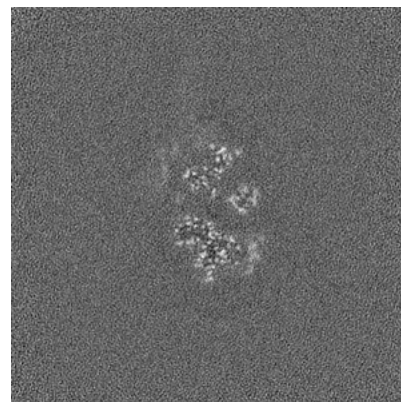
6.2.2 Raw map



X Index: 160



Y Index: 160

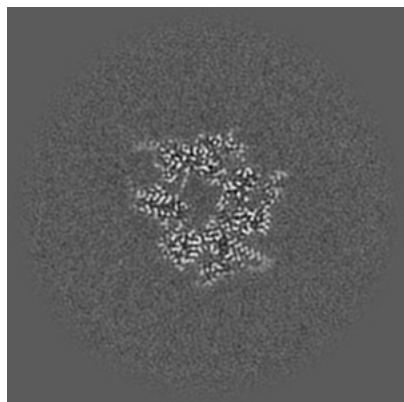


Z Index: 160

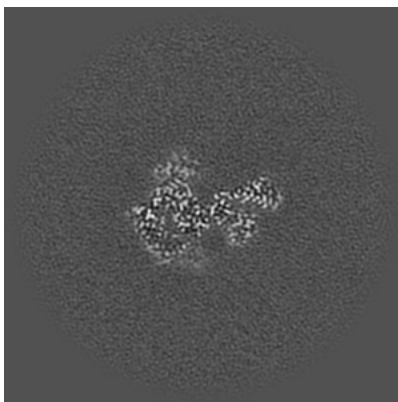
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

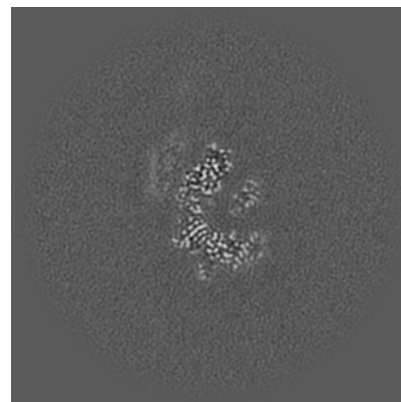
6.3.1 Primary map



X Index: 161

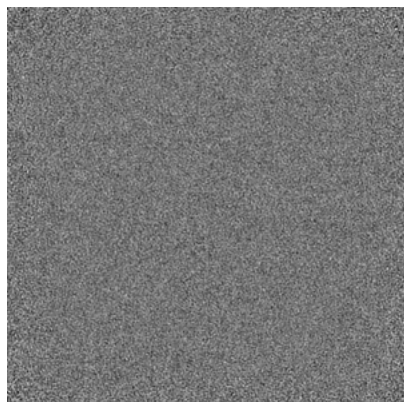


Y Index: 177

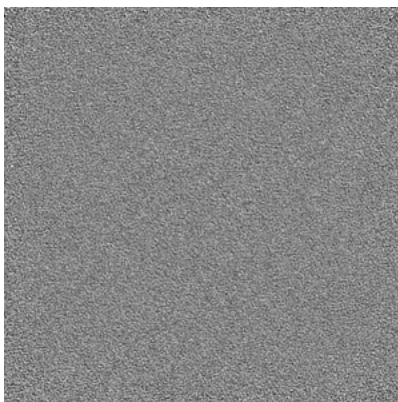


Z Index: 153

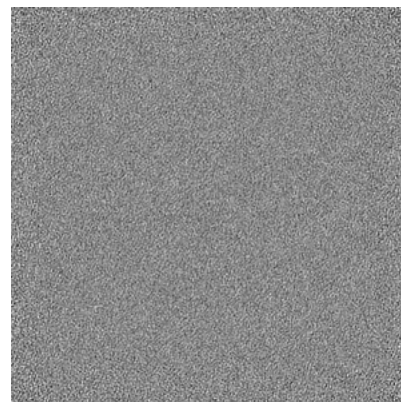
6.3.2 Raw map



X Index: 0



Y Index: 0

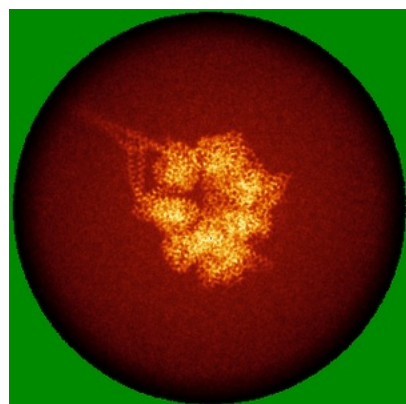


Z Index: 0

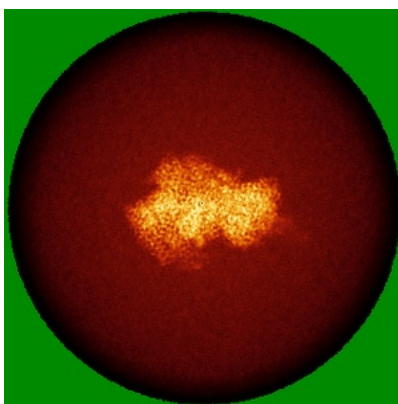
The images above show the largest variance slices of the map in three orthogonal directions.

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

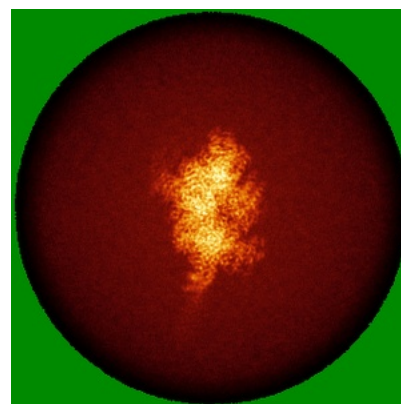
6.4.1 Primary map



X

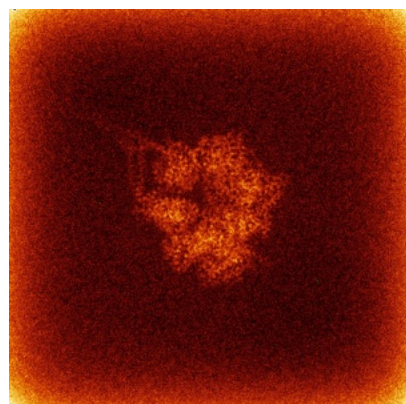


Y

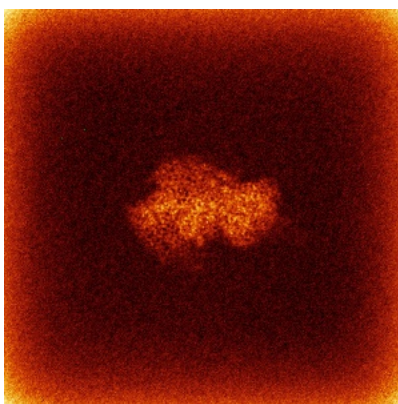


Z

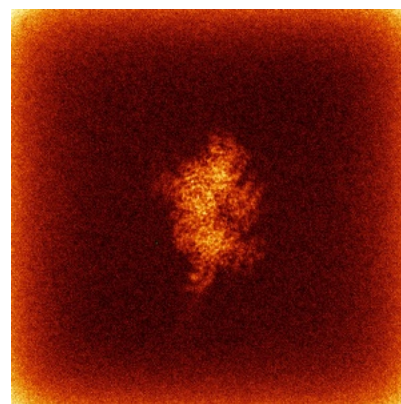
6.4.2 Raw map



X



Y

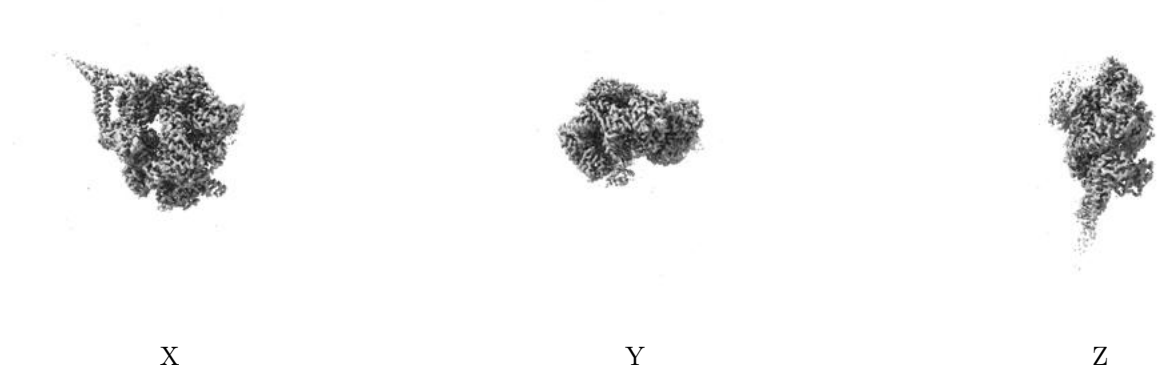


Z

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.

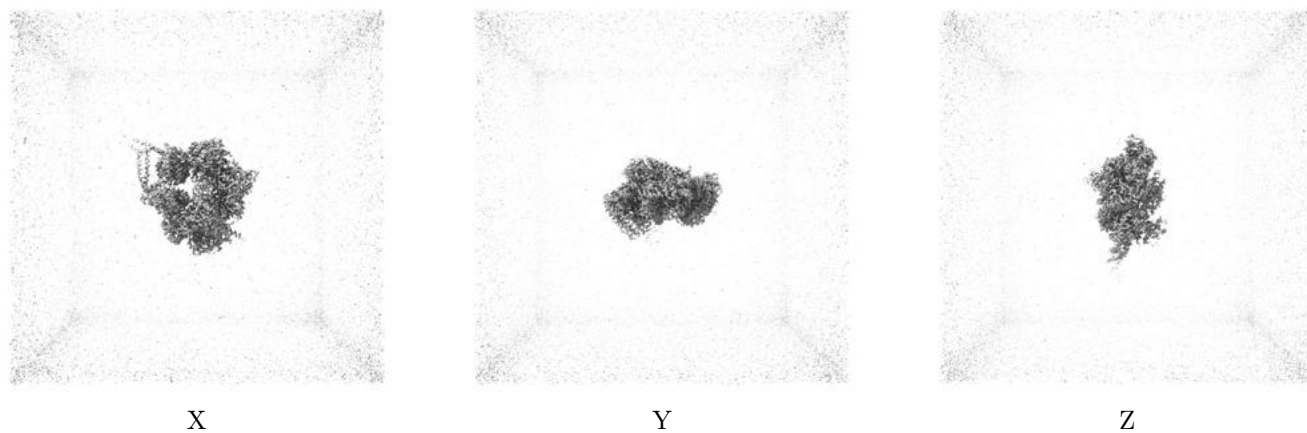
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.21. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

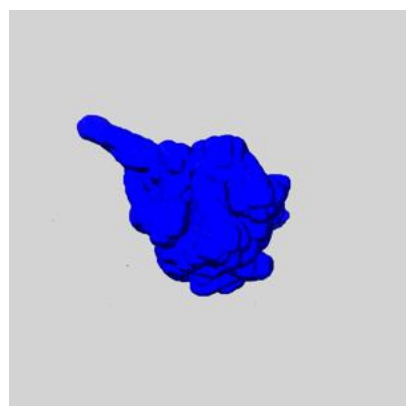
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

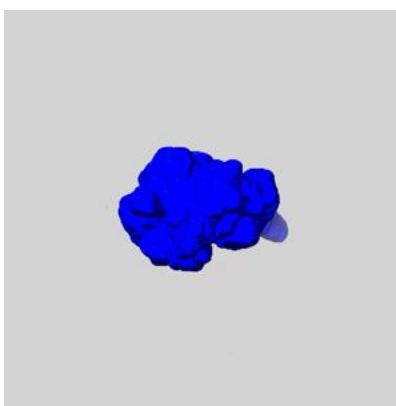
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

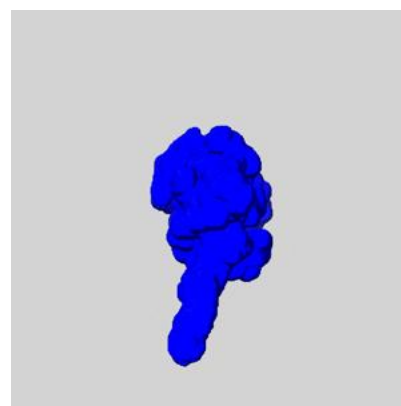
6.6.1 emd_44709_msk_1.map [i](#)



X



Y

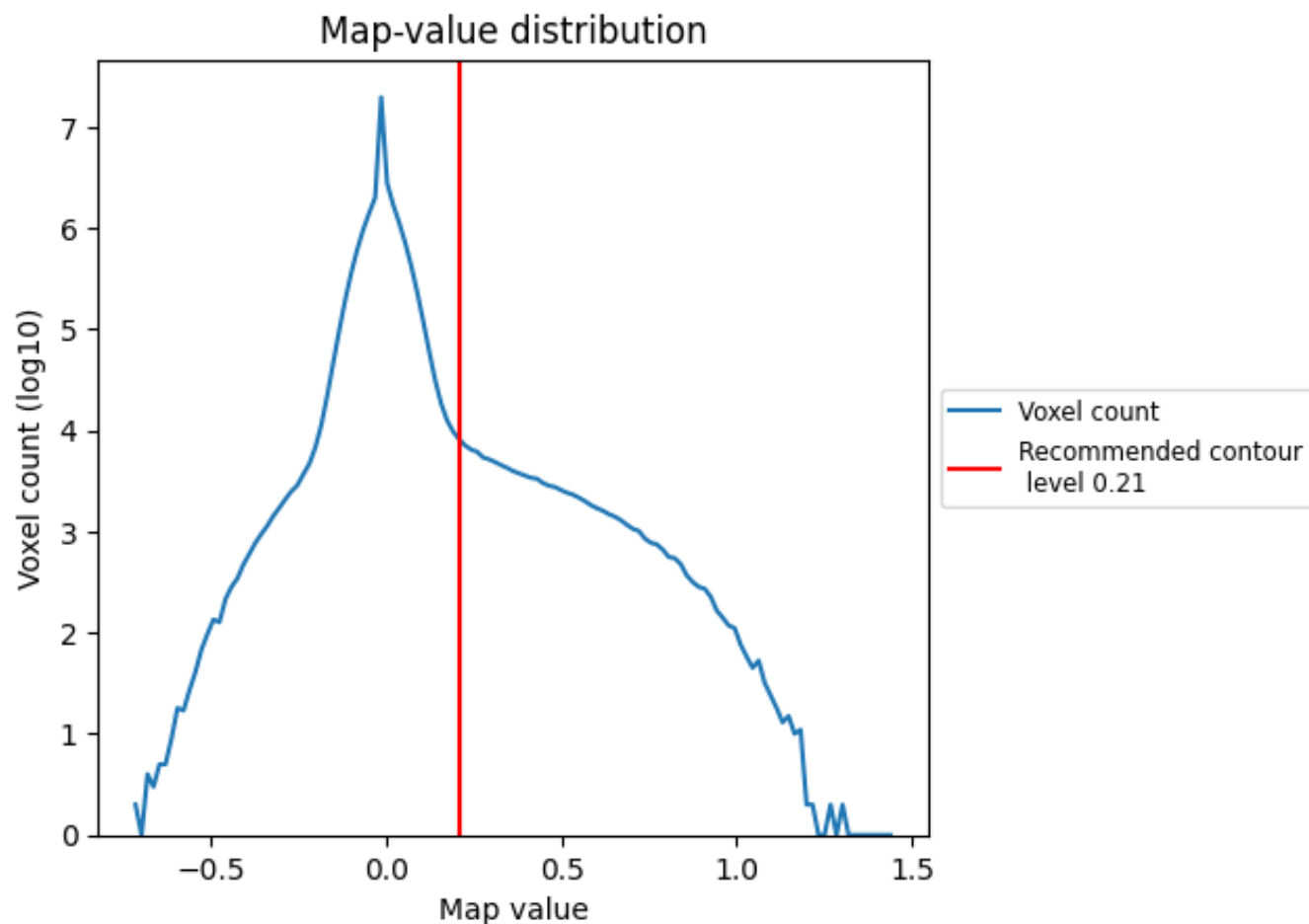


Z

7 Map analysis [i](#)

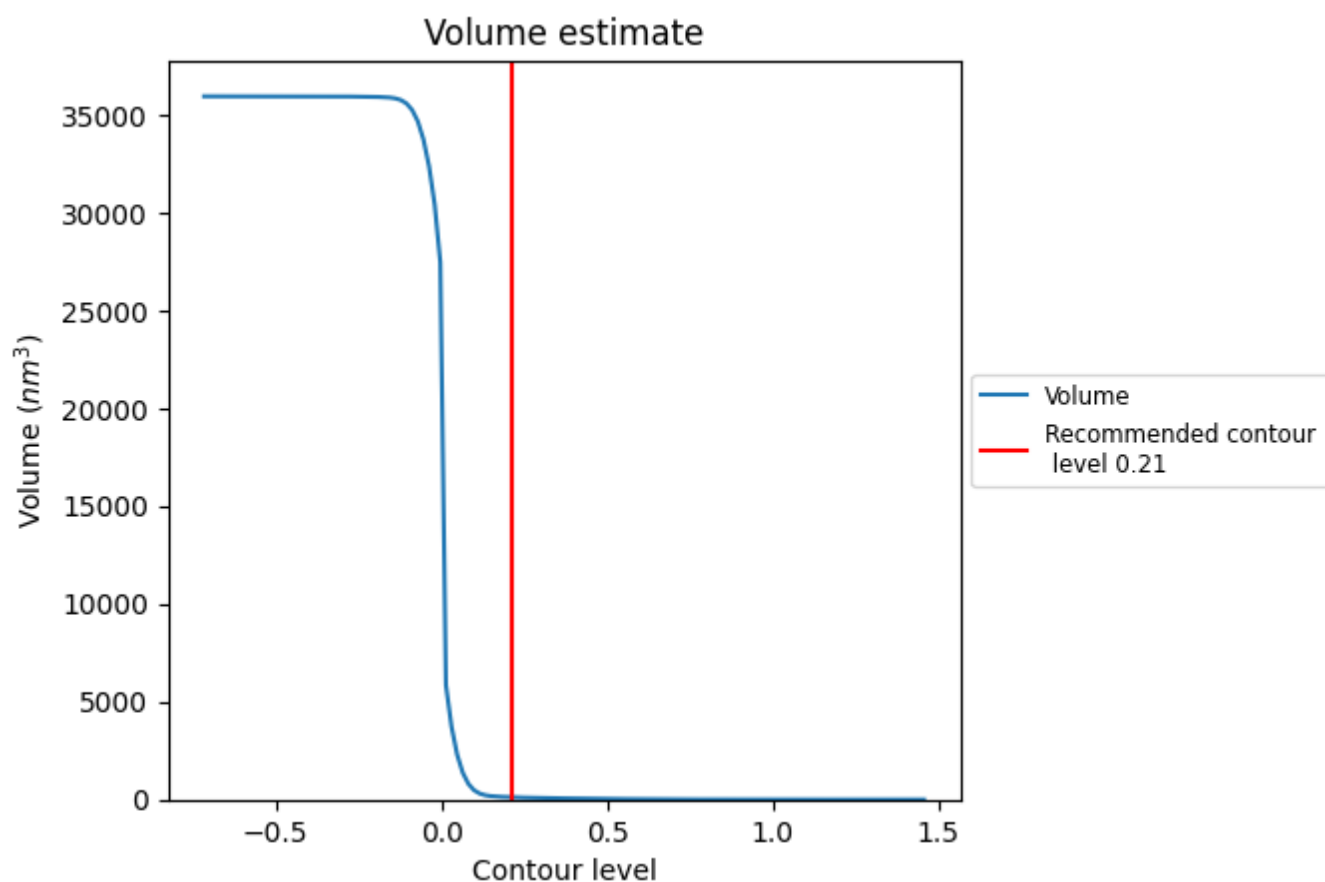
This section contains the results of statistical analysis of the map.

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.

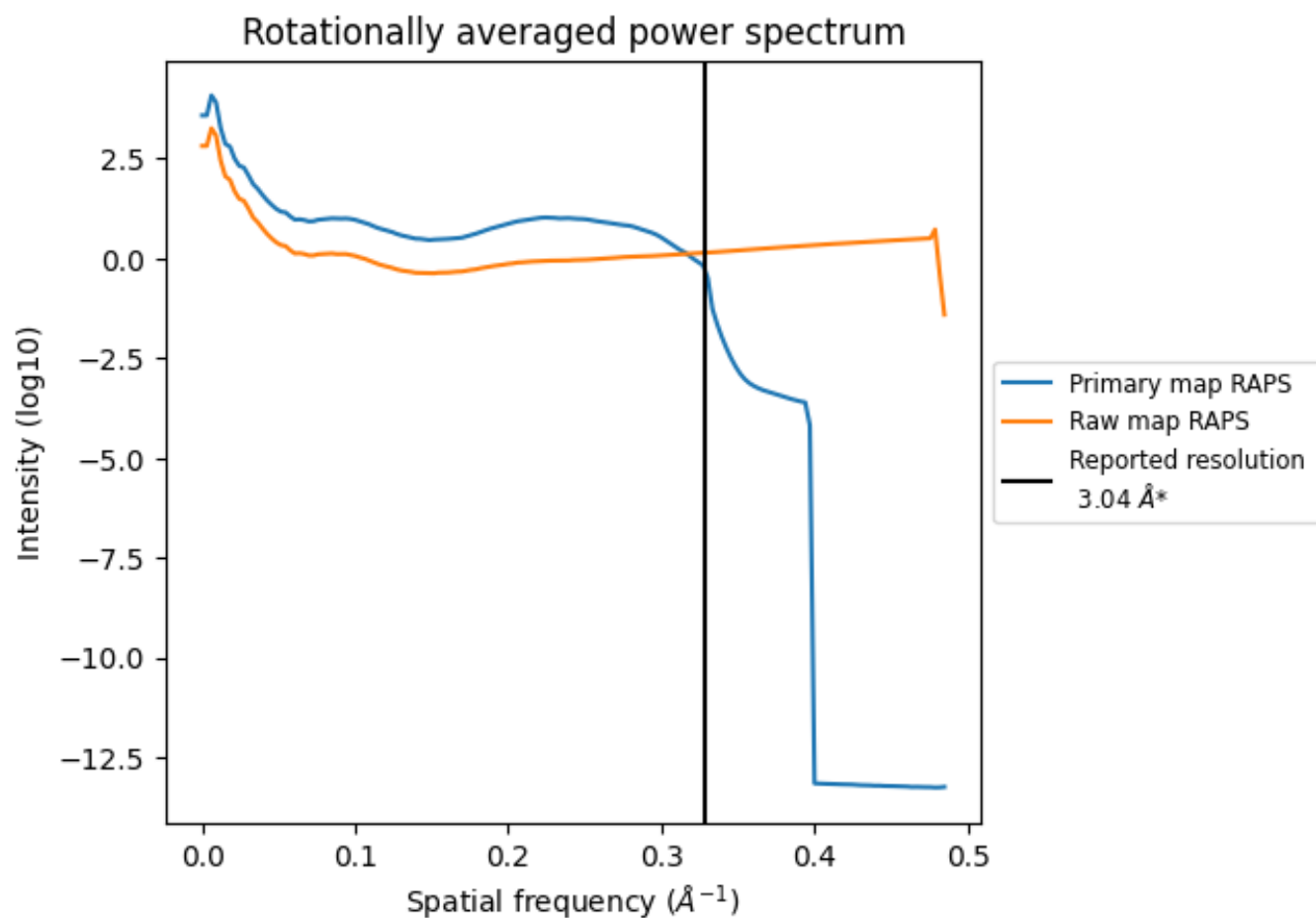
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 119 nm³; this corresponds to an approximate mass of 108 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 ⓘ

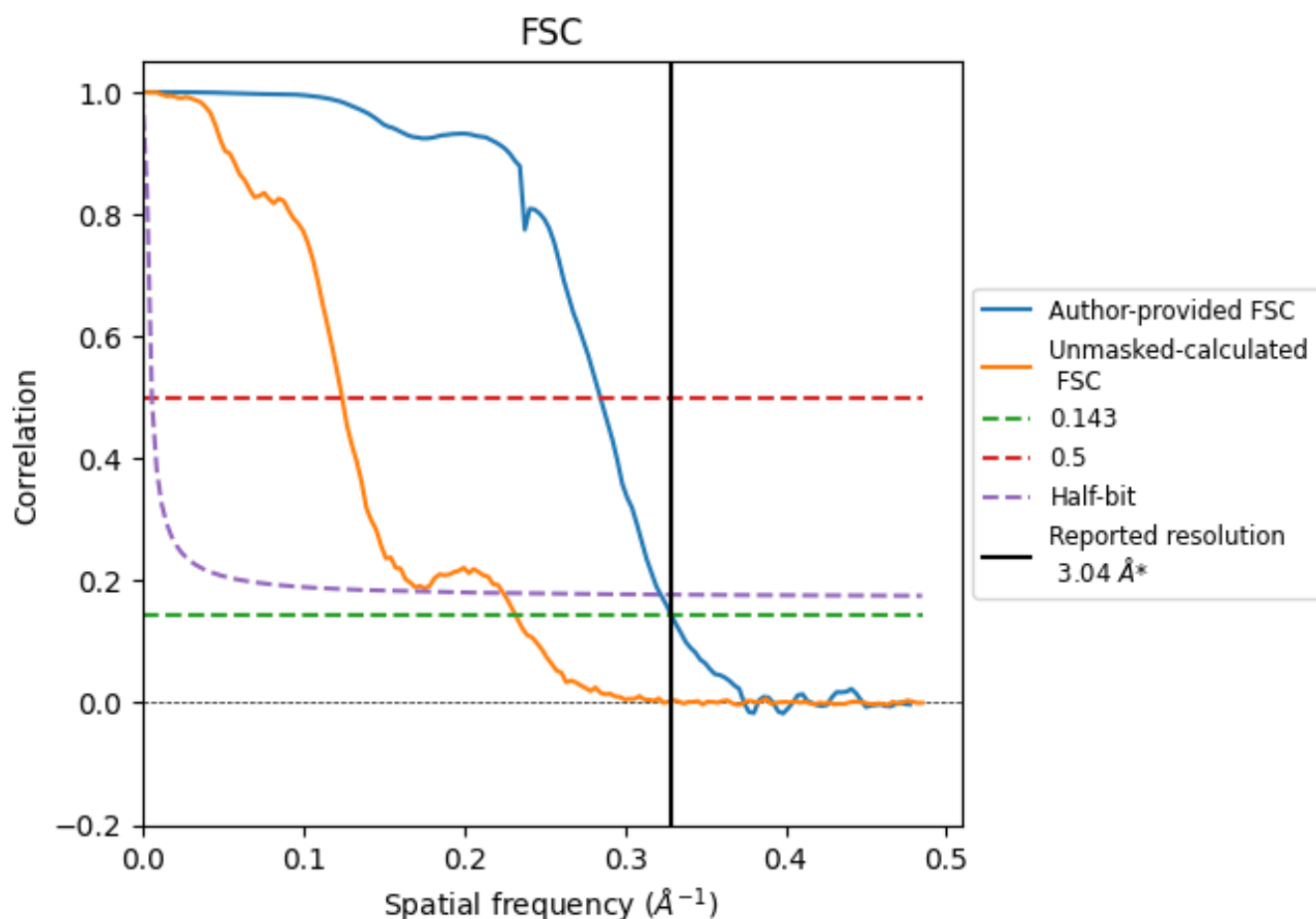


*Reported resolution corresponds to spatial frequency of 0.329 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.329 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

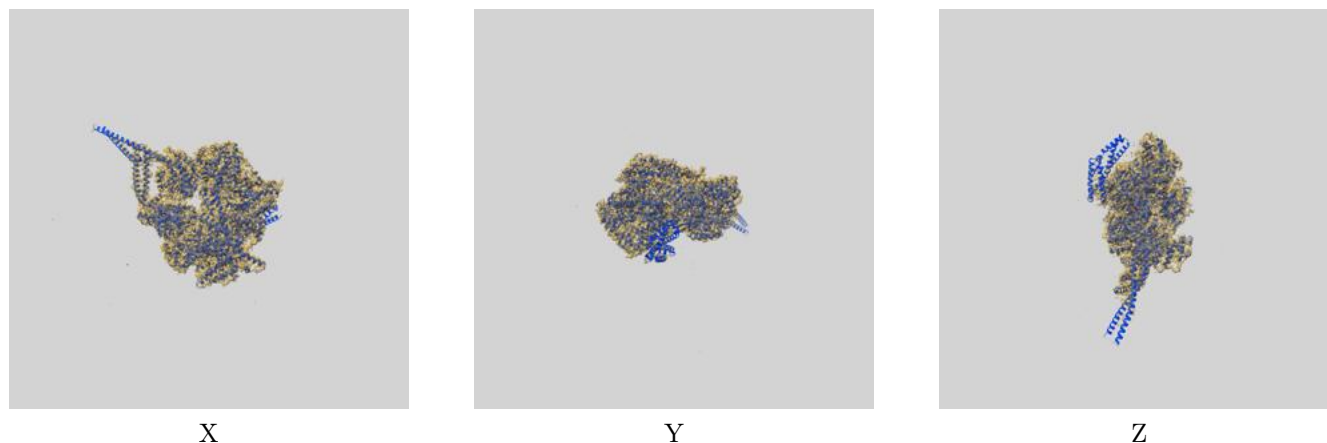
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.04	3.51	3.10
Unmasked-calculated*	4.31	8.05	4.46

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.31 differs from the reported value 3.04 by more than 10 %

9 Map-model fit [i](#)

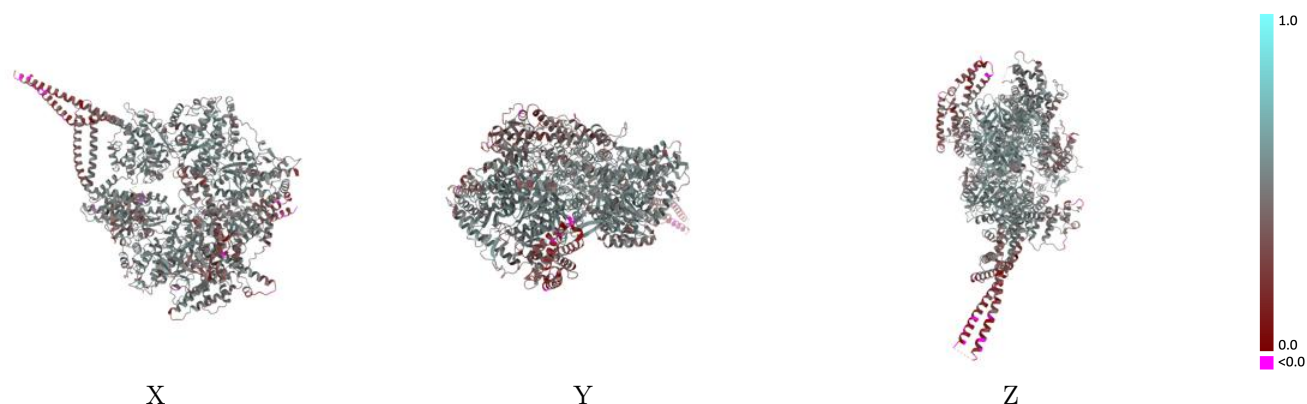
This section contains information regarding the fit between EMDB map EMD-44709 and PDB model 9BMS. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



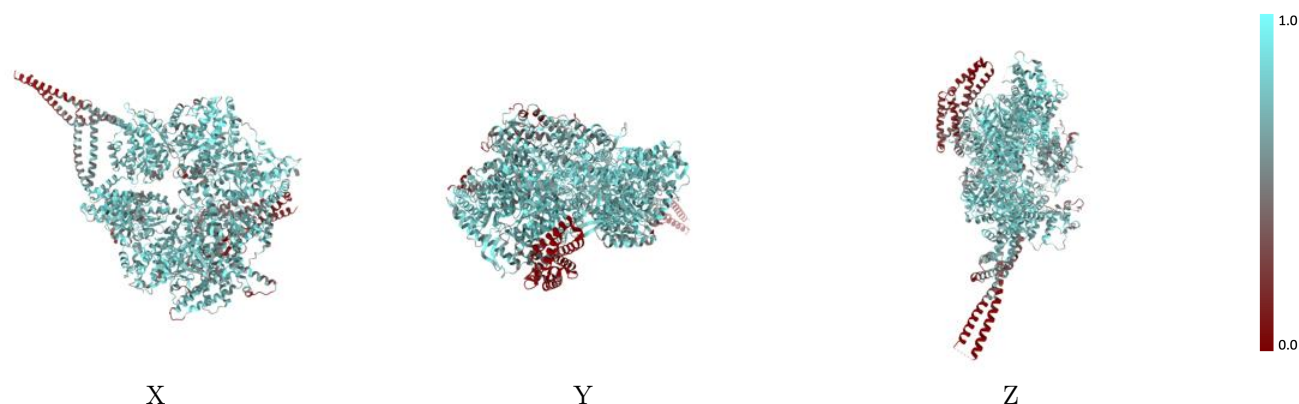
The images above show the 3D surface view of the map at the recommended contour level 0.21 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



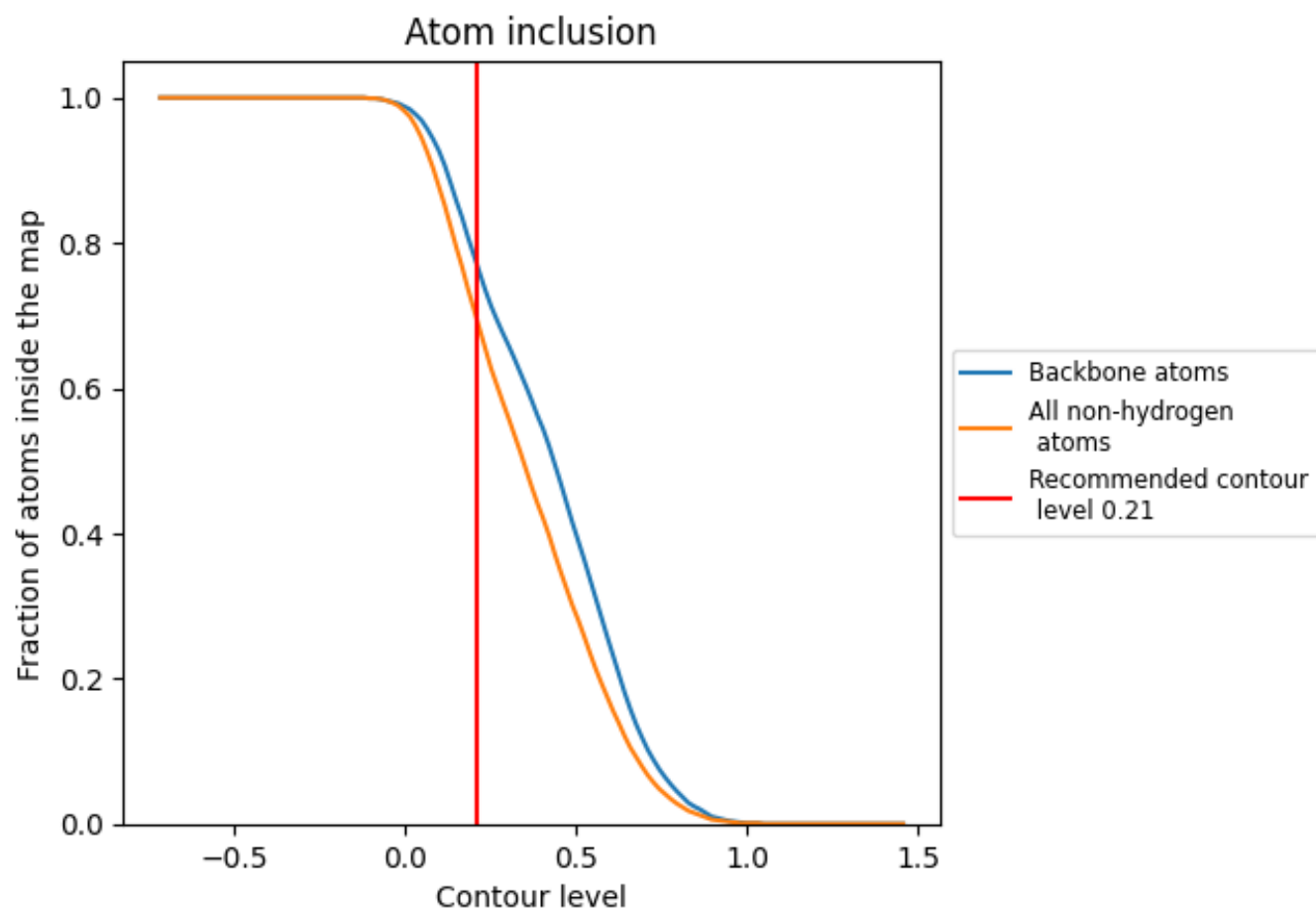
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.21).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 69% 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 (0.21) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6940	0.4670
A	0.6940	0.4670

