



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 11:00 PM EDT

PDB ID : 9BMH / pdb_00009bmh
EMDB ID : EMD-44699
Title : State-4 of motor domain from full-length human dynein-1 in 5mM ATPVi
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 2.80 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.dev133
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) : 2.50

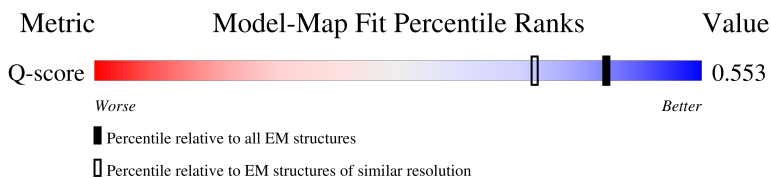
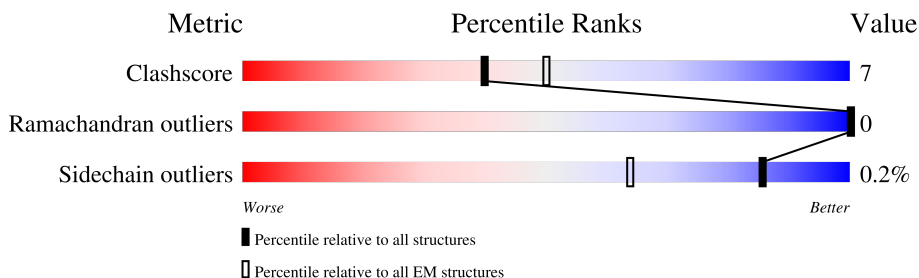
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	11806 (2.30 - 3.30)

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](#)

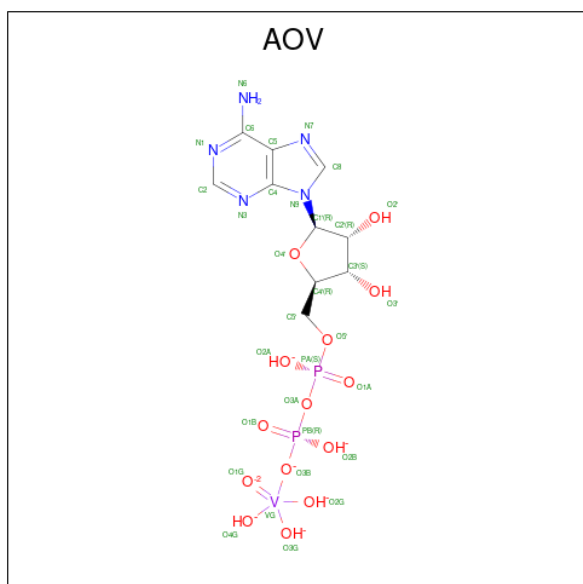
There are 5 unique types of molecules in this entry. The entry contains 23044 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

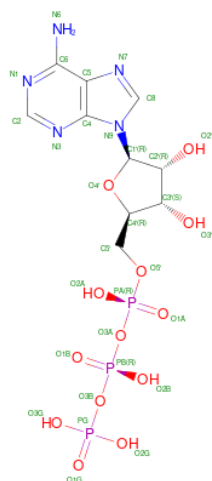
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2859	22925	14595	3960	4257	113	0	0

- Molecule 2 is ADP ORTHOVANADATE (CCD ID: AOV) (formula: $C_{10}H_{17}N_5O_{14}P_2V$) (labeled as "Ligand of Interest" by depositor).



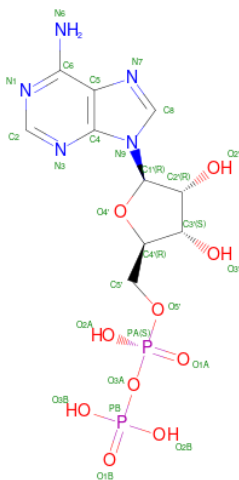
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	V	
2	A	1	32	10	5	14	2	1	0

- 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 ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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



L3876	L3886	L3887	A3888	F3905	F3908	L3909	R3910	L3916	S3917	A3918	G3919	P3922	R3923	I3924	Q3925	V3929	E3933	V3936	R3937	P3942	I3943	K3945	I3948	E3955	Q3956	P3966	V3970	P3971	Y3972	E3976	E3977	T3981	F3982	I3983	G3984	Q3985	A3986	I3987	H3988	R3989	R4000																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
L3732	Q3735	R3741	L3742	R3743	Q3744	L3745	Q3751	E3755	V3756	K3757	Q3758	R3759	I3760	L3761	I3764	I3765	I3766	E3776	R3782	E3785	E3786	I3787	I3788	I3789	V3790	M3791	V3794	E3795	Q3799	L3802	S3809	Q3830	D3834	I3835	Y3836	V3839	L3845	R3855	R3859	L3863	F3868																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
C3573	L3580	R3585	I3600	M3601	D3606	R3611	F3614	D3637	V3638	E3639	P3643	N3650	V3653	R3654	R3655	T3656	Q3657	R3658	R3659	V3660	L3661	G3665	D3666	L3671	T3681	T3685	D3691	S3694	R3695	V3696	T3697	S3699	L3708	V3716	D3723	V3724	R3728	L3731																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
E3449	E3450	Y3451	A3452	V3453	I3454	I3455	S3456	E3457	A3458	Q3459	A3460	I3461	K3462	A3463	D3464	I3465	A3466	A3467	V3468	A3470	K3471	V3472	R3473	R3474	T3475	A3477	L3478	K3480	E3487	E3490	K3491	E3494	T3502	S3510	Y3516	A3517	R3525	Q3542	F3543	L3553	A3556	D3557	F3558	R3559	F3568																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
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R3191	V3203	R3206	D3213	Q3214	T3099	F3109	T3110	M3113	D3114	L3115	D3124	V3129	Y3130	D3131	K3132	L3133	P3134	Q3135	P3136	P3137	R3140	E3141	A3142	I3143	V3148	F3149	Q3152	T3153	L3154	L3161	A3162	K3163	R3167	T3168	T3172	P3173	R3174	H3175	Y3176	L3177	D3178	F3179	I3180	F3187																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
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H4004	S4172	I4340	E4454	E4625
F4008	R4178	L4344	L4460	T4645
N4012	L4179	K4345	P4461	GLU
H4018	H4187	M4346	T4468	
P4037	I4190	Q4347	V4469	
N4038	Q4191	YET	P4470	
T4039	R4195	LEU	M4473	
H4043	R4195	ASP	T4474	
G4048	Y4196	ASP	V4475	
A4051	A4197	ASP	L4489	
E4056	P4198	LEU	S4493	
S4068	W4201	ALA	K4505	
N4085	E4206	ALA	L4511	
V4088	F4207	THR	F4515	
K4089	L4212	LYS	V4516	
S4090	A4215	THR	P4517	
G4091	L4223	ARG	Y4520	
R4092	A4227	ASP	I4521	
L4096	I4233	SER	T4522	
H4100	S4234	ASP	Q4526	
W4105	K4237	GLY	L4536	
L4106	M4247	ARG	L4541	
H4107	S4250	P4374	E4542	
K4111	I4251	H4381	V4543	
L4116	Y4252	L4398	Q4549	
Q4117	G4253	T4401	T4552	
P4118	G4254	I4405	L4553	
T4127	D4257	F4412	D4554	
H4128	F4278	R4415	K4574	
N4137	E4281	M4419	N4579	
L4138	V4288	D4430	T4588	
G4142	D4289	C4438	Q4589	
V4146	H4291	Q4444	L4590	
P4149	I4294	T4445	K4594	
P4150	P4297	N4446	E4599	
T4160	W4308	Y4447	K4600	
K4171	N4326	L4448	D4617	
		R4449	L4618	
		T4450	I4619	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	248329	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.561	Depositor
Minimum map value	-1.593	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1573, 1.1573, 1.1573	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: AOV, MG, ATP, ADP

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	0.23	1/23409 (0.0%)	0.39	11/31728 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	SER	CA-CB	-5.41	1.45	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2020	PRO	N-CA-CB	-10.12	94.55	103.35
1	A	2320	ASP	CB-CA-C	-9.59	102.42	114.40
1	A	1883	PRO	N-CA-CB	-6.92	95.98	103.25
1	A	1886	ASP	N-CA-C	-6.67	104.78	113.12
1	A	1885	THR	N-CA-C	-6.60	105.19	113.18
1	A	2020	PRO	N-CA-C	6.41	121.40	111.21
1	A	2319	LEU	N-CA-CB	-6.40	101.73	110.56
1	A	1879	LEU	N-CA-CB	-6.37	100.04	110.43
1	A	1885	THR	CA-CB-OG1	-5.56	101.27	109.60
1	A	1912	LYS	N-CA-CB	-5.11	102.65	110.07
1	A	2321	ASP	N-CA-C	-5.10	106.75	113.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	22925	0	22997	326	0
2	A	32	0	12	3	0
3	A	31	0	12	2	0
4	A	54	0	24	1	0
5	A	2	0	0	0	0
All	All	23044	0	23045	326	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 (326) 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:2753:ARG:HA	1:A:2763:ARG:HH22	1.30	0.95
1:A:1882:THR:HG22	1:A:2048:LEU:HD23	1.66	0.77
1:A:3799:GLN:HA	1:A:3802:LEU:HD23	1.66	0.76
1:A:2688:GLU:OE1	1:A:2730:HIS:NE2	2.18	0.75
1:A:3639:GLU:OE2	1:A:4111:LYS:NZ	2.16	0.71
1:A:4541:LEU:HD11	1:A:4590:LEU:HB3	1.73	0.70
1:A:1797:LEU:HD11	1:A:2060:ARG:HH21	1.56	0.69
1:A:2149:LEU:HD11	1:A:2157:LEU:HD13	1.73	0.69
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.76	0.68
1:A:2564:ALA:HB3	1:A:2567:VAL:HG23	1.76	0.68
1:A:4470:PRO:HD2	1:A:4473:MET:HE3	1.75	0.68
1:A:3113:MET:HE2	1:A:3115:LEU:HD21	1.75	0.67
1:A:3970:VAL:HB	1:A:3989:ARG:HD3	1.76	0.67
1:A:3178:ASP:OD2	1:A:3585:ARG:NE	2.28	0.67
1:A:3972:TYR:OH	1:A:3976:GLU:OE1	2.13	0.66
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.77	0.66
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.79	0.65
1:A:2987:ASN:OD1	1:A:3057:GLN:NE2	2.27	0.65
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.28	0.65
1:A:3129:VAL:HG21	1:A:3149:PHE:HB2	1.78	0.65
1:A:3981:THR:HG23	1:A:3984:GLY:H	1.61	0.65
1:A:1984:GLU:HG3	1:A:1997:ILE:HD12	1.79	0.64
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.80	0.64
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.79	0.64
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.30	0.63
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3735:GLN:NE2	1:A:3788:ASP:OD1	2.29	0.62
1:A:1661:VAL:HG22	1:A:1676:ILE:HD12	1.81	0.62
1:A:2557:VAL:O	1:A:2757:ARG:NH2	2.33	0.62
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.33	0.62
1:A:1543:ARG:HA	1:A:1546:TYR:CE1	2.34	0.61
1:A:3068:MET:HE1	1:A:3078:ARG:HG3	1.82	0.61
1:A:1907:PRO:HD3	1:A:2042:THR:HG22	1.83	0.61
1:A:4227:ALA:HB2	1:A:4233:ILE:HD12	1.84	0.60
1:A:2087:ASP:O	1:A:2148:LYS:NZ	2.35	0.59
1:A:2967:TYR:OH	1:A:2975:ASP:OD2	2.15	0.59
1:A:4574:LYS:NZ	1:A:4625:GLU:OE2	2.32	0.59
1:A:1640:ILE:HG23	1:A:1650:LEU:HD21	1.83	0.59
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.85	0.58
1:A:3109:PHE:HD2	1:A:3180:ILE:HG22	1.67	0.58
1:A:3830:GLN:NE2	1:A:3834:ASP:OD1	2.37	0.58
1:A:1932:CYS:HB2	1:A:1959:GLU:O	2.04	0.58
1:A:3174:ARG:NH1	1:A:3650:ASN:OD1	2.38	0.57
1:A:2320:ASP:OD1	1:A:2358:ARG:NE	2.37	0.57
1:A:2581:LEU:HD11	1:A:2593:LEU:HD21	1.85	0.57
1:A:3886:LEU:HD12	1:A:4346:MET:HE3	1.86	0.57
1:A:4430:ASP:OD2	1:A:4447:TYR:OH	2.23	0.57
1:A:2290:SER:HB2	1:A:2295:LEU:HG	1.86	0.57
1:A:1563:VAL:HG22	1:A:1567:ARG:HE	1.68	0.56
1:A:2623:SER:OG	1:A:3006:GLU:OE1	2.23	0.56
1:A:3745:LEU:HD11	1:A:3776:GLU:HG3	1.87	0.56
1:A:1900:LEU:HD11	1:A:2037:ARG:HG2	1.86	0.56
1:A:3115:LEU:HD13	1:A:3143:ILE:HG21	1.88	0.56
1:A:1546:TYR:OH	1:A:1612:GLN:OE1	2.21	0.56
1:A:3650:ASN:HD21	1:A:3695:ARG:HH11	1.54	0.56
1:A:4288:VAL:HG11	1:A:4294:ILE:HG12	1.88	0.56
1:A:2220:LEU:HB2	1:A:2342:MET:HG2	1.88	0.56
1:A:2220:LEU:HD12	1:A:2342:MET:HG2	1.88	0.56
1:A:2557:VAL:HG23	1:A:2750:THR:HG22	1.88	0.56
1:A:3728:ARG:HB2	1:A:3794:VAL:HG11	1.87	0.56
1:A:2065:LEU:HD11	1:A:2133:GLU:HB3	1.88	0.55
1:A:2894:LYS:HG3	1:A:2911:LEU:HD12	1.88	0.55
1:A:3723:ASP:OD1	1:A:3724:VAL:N	2.39	0.55
1:A:3110:THR:O	1:A:3140:ARG:NH1	2.39	0.55
1:A:3028:THR:O	1:A:3032:GLN:HG3	2.07	0.55
1:A:3585:ARG:HB2	1:A:3697:THR:HG23	1.87	0.55
1:A:2949:PHE:CZ	1:A:2953:MET:HE3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2037:ARG:HH21	1:A:4250:SER:HB3	1.72	0.55
1:A:3040:GLU:OE1	1:A:3053:TRP:NE1	2.34	0.54
1:A:4191:GLN:NE2	1:A:4207:PHE:O	2.36	0.54
1:A:2369:LEU:HD12	1:A:2373:MET:HE2	1.88	0.54
1:A:2536:ASP:OD1	1:A:2576:ARG:NH1	2.40	0.54
1:A:2751:PHE:HB3	1:A:2803:VAL:HG11	1.89	0.54
1:A:2969:GLY:HA2	1:A:3004:PHE:HE1	1.72	0.54
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.07	0.54
1:A:2558:GLU:OE1	1:A:2560:HIS:NE2	2.41	0.54
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.40	0.54
1:A:1735:PRO:O	1:A:1739:ILE:HG12	2.07	0.54
1:A:4190:ILE:HD12	1:A:4201:TRP:HZ2	1.72	0.54
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.89	0.53
1:A:4543:VAL:HG13	1:A:4588:THR:HG23	1.89	0.53
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.36	0.53
1:A:3989:ARG:HB2	1:A:4004:MET:HE2	1.89	0.53
1:A:4450:THR:O	1:A:4454:GLU:HG3	2.07	0.53
1:A:3916:LEU:HD11	1:A:3937:ARG:HG3	1.90	0.53
1:A:2211:TYR:HB2	1:A:2237:LEU:HD11	1.91	0.53
1:A:1795:SER:O	1:A:1800:GLN:NE2	2.34	0.53
1:A:2353:LEU:HG	1:A:2353:LEU:O	2.07	0.53
1:A:2382:LEU:HD23	1:A:2420:ALA:HB2	1.91	0.52
1:A:1853:VAL:HG13	1:A:1854:LEU:HD22	1.90	0.52
1:A:2826:ALA:HB2	1:A:2867:MET:HE1	1.91	0.52
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.91	0.52
1:A:2225:PRO:HB2	1:A:2366:GLU:HG3	1.91	0.52
1:A:2956:LEU:HD23	1:A:2989:LYS:HB3	1.91	0.52
1:A:2257:LYS:NZ	1:A:2308:ASP:OD2	2.36	0.52
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.91	0.52
1:A:1684:VAL:HG12	1:A:1746:GLN:NE2	2.25	0.52
1:A:4171:LYS:HG2	1:A:4172:SER:H	1.74	0.52
1:A:4297:PRO:HG3	1:A:4308:TRP:CG	2.45	0.51
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.91	0.51
1:A:1941:MET:HE2	1:A:1960:PHE:HE1	1.76	0.51
1:A:2075:LEU:HD22	1:A:4522:THR:HG23	1.92	0.51
1:A:2964:HIS:HA	1:A:3643:PRO:HD2	1.93	0.51
1:A:4088:VAL:HG11	1:A:4116:LEU:HD21	1.91	0.51
1:A:4137:ASN:OD1	1:A:4138:LEU:N	2.44	0.51
1:A:4489:LEU:HD11	1:A:4515:PHE:HE1	1.74	0.51
1:A:2753:ARG:HA	1:A:2763:ARG:NH2	2.13	0.51
1:A:3109:PHE:CD2	1:A:3180:ILE:HG22	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.92	0.51
1:A:2313:GLU:OE2	1:A:2352:THR:OG1	2.29	0.51
1:A:2885:ASP:HB3	1:A:2888:GLU:OE1	2.10	0.51
1:A:4107:MET:O	1:A:4111:LYS:HG2	2.11	0.51
1:A:3795:GLU:O	1:A:3799:GLN:HG2	2.10	0.51
1:A:2313:GLU:OE1	1:A:2316:ASN:ND2	2.43	0.51
1:A:3985:GLN:O	1:A:3989:ARG:HG3	2.11	0.51
1:A:2221:MET:SD	1:A:2361:MET:HE1	2.51	0.50
1:A:3130:TYR:CZ	1:A:3132:LYS:HB2	2.47	0.50
1:A:3187:PHE:CE2	1:A:3191:ARG:HD2	2.47	0.50
1:A:2818:VAL:O	1:A:2822:ILE:HG12	2.11	0.50
1:A:2963:VAL:HG13	1:A:3000:LEU:HD11	1.93	0.50
1:A:3759:ARG:HH21	1:A:3761:LEU:HB2	1.77	0.50
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.94	0.50
1:A:1698:ILE:HD12	1:A:1701:TRP:NE1	2.27	0.50
1:A:2327:LEU:HD12	1:A:2331:GLU:HB3	1.93	0.50
1:A:2564:ALA:HB3	1:A:2567:VAL:CG2	2.41	0.49
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	1.94	0.49
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.94	0.49
1:A:3888:ALA:HB1	1:A:4012:ASN:HD22	1.78	0.49
1:A:1550:ILE:O	1:A:1554:SER:OG	2.30	0.49
1:A:1914:GLU:HG3	2:A:4701:AOV:H2'	1.93	0.49
1:A:2374:ILE:HD13	1:A:2452:LEU:HD21	1.95	0.49
1:A:3650:ASN:HD21	1:A:3695:ARG:NH1	2.09	0.49
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.93	0.49
1:A:1543:ARG:HB3	1:A:1608:LEU:HD12	1.94	0.49
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.94	0.49
1:A:2827:HIS:CE1	1:A:2831:ARG:HH11	2.31	0.48
1:A:4090:SER:OG	1:A:4092:ARG:HG3	2.13	0.48
1:A:2598:GLY:HA3	1:A:2795:SER:HB2	1.96	0.48
1:A:3728:ARG:O	1:A:3732:LEU:HG	2.14	0.48
1:A:2572:LEU:O	1:A:2575:VAL:HG22	2.13	0.48
1:A:3655:ARG:HG2	1:A:3660:VAL:HG22	1.95	0.48
1:A:4043:MET:HB2	1:A:4127:THR:HA	1.95	0.48
1:A:4526:GLN:HA	1:A:4536:LEU:HD21	1.95	0.48
1:A:1879:LEU:HD11	1:A:1914:GLU:HB3	1.94	0.48
1:A:2548:TRP:CD1	1:A:2576:ARG:HG2	2.48	0.48
1:A:2792:TYR:OH	1:A:2842:GLU:OE1	2.29	0.48
1:A:1907:PRO:HG2	1:A:1910:THR:HG21	1.95	0.48
1:A:1946:VAL:HG22	1:A:2006:VAL:HG21	1.95	0.48
1:A:3732:LEU:HD23	1:A:3791:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2229:GLY:HA2	3:A:4702:ATP:O2A	2.14	0.47
1:A:2091:ARG:NH1	2:A:4701:AOV:O1G	2.38	0.47
1:A:3006:GLU:O	1:A:3010:THR:HG23	2.15	0.47
1:A:3149:PHE:O	1:A:3153:THR:HG23	2.14	0.47
1:A:4117:GLN:HG2	1:A:4117:GLN:O	2.13	0.47
1:A:3176:TYR:O	1:A:3180:ILE:HG12	2.14	0.47
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.49	0.47
1:A:2232:MET:HG3	3:A:4702:ATP:C8	2.50	0.47
1:A:3716:VAL:HB	1:A:3836:TYR:OH	2.14	0.47
1:A:1671:SER:HB2	1:A:1693:THR:HG23	1.97	0.47
1:A:3886:LEU:CD1	1:A:4346:MET:HE3	2.45	0.47
1:A:2075:LEU:HD13	1:A:4536:LEU:HD13	1.97	0.47
1:A:2245:GLU:OE1	1:A:2298:ARG:NH2	2.40	0.47
1:A:4460:LEU:HA	1:A:4475:VAL:HG22	1.97	0.46
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.97	0.46
1:A:2457:SER:OG	1:A:2732:PRO:HB3	2.15	0.46
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	1.97	0.46
1:A:4043:MET:HE3	1:A:4051:ALA:HB1	1.98	0.46
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	1.98	0.46
1:A:3735:GLN:NE2	1:A:3787:THR:HG23	2.30	0.46
1:A:1578:LEU:O	1:A:1582:VAL:HG12	2.15	0.46
1:A:1711:VAL:O	1:A:1715:LYS:HG2	2.16	0.46
1:A:2028:LEU:HG	1:A:2032:LEU:HD23	1.98	0.46
1:A:2571:THR:HG22	1:A:2746:GLN:NE2	2.31	0.46
1:A:2948:ARG:HG2	1:A:2958:VAL:HG11	1.97	0.46
1:A:2188:GLU:OE2	1:A:2243:ARG:NH2	2.48	0.46
1:A:4197:ALA:HB3	1:A:4198:PRO:HD3	1.98	0.46
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.48	0.46
1:A:3557:ASP:OD1	1:A:3743:ARG:NH1	2.49	0.46
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.98	0.46
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.98	0.46
1:A:2965:ARG:HH22	1:A:3614:PHE:HB3	1.81	0.46
1:A:1800:GLN:OE1	1:A:1804:ARG:NE	2.49	0.45
1:A:2452:LEU:HD23	1:A:2452:LEU:HA	1.80	0.45
1:A:3846:LEU:HD22	1:A:3855:ARG:HG2	1.98	0.45
1:A:1844:PHE:HE1	1:A:1859:ILE:HG23	1.81	0.45
1:A:2132:PRO:HB2	1:A:2135:GLU:HB3	1.97	0.45
1:A:2596:PRO:HB2	1:A:2738:TYR:CZ	2.51	0.45
1:A:3048:GLU:O	1:A:3052:LYS:HG2	2.16	0.45
1:A:2018:MET:HB2	1:A:2018:MET:HE3	1.44	0.45
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3167:ARG:NH1	1:A:3685:THR:HA	2.32	0.45
1:A:3653:VAL:HG11	1:A:3671:LEU:HD22	1.98	0.45
1:A:3876:LEU:HD23	1:A:4146:VAL:HG11	1.97	0.45
1:A:1661:VAL:HG13	1:A:1676:ILE:HB	1.98	0.45
1:A:1929:VAL:H	1:A:2332:ARG:HH22	1.64	0.45
1:A:3154:LEU:HG	1:A:3516:TYR:CD1	2.51	0.45
1:A:3741:ARG:HA	1:A:3741:ARG:HD2	1.65	0.45
1:A:4085:ASN:O	1:A:4089:LYS:NZ	2.37	0.45
1:A:1904:PRO:HG2	1:A:2017:THR:HG22	1.98	0.45
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.49	0.45
1:A:2572:LEU:O	1:A:2576:ARG:HG3	2.16	0.45
1:A:3230:GLU:HA	1:A:3233:ASN:HD21	1.81	0.45
1:A:2320:ASP:HB3	1:A:2321:ASP:H	1.40	0.45
1:A:3731:LEU:HD11	1:A:3790:VAL:HG12	1.99	0.45
1:A:3785:GLU:O	1:A:3789:ILE:HG13	2.17	0.45
1:A:3948:ILE:HD12	1:A:3948:ILE:H	1.82	0.45
1:A:4178:ARG:HD3	1:A:4278:PHE:CD2	2.52	0.45
1:A:2776:PHE:HZ	1:A:2846:THR:HG23	1.82	0.44
1:A:2962:LYS:HG3	1:A:3665:GLY:HA2	1.98	0.44
1:A:3601:MET:CE	1:A:3611:ARG:HB2	2.47	0.44
1:A:4468:THR:HG21	1:A:4617:ASP:OD1	2.16	0.44
1:A:2257:LYS:HE3	1:A:2676:THR:HG21	1.98	0.44
1:A:3024:ASP:O	1:A:3028:THR:HG23	2.17	0.44
1:A:1652:LYS:HG3	1:A:1653:HIS:CD2	2.52	0.44
1:A:1852:ASP:O	1:A:1856:GLN:NE2	2.50	0.44
1:A:4179:LEU:HD12	1:A:4223:LEU:HD22	1.99	0.44
1:A:1878:LYS:HB3	1:A:1878:LYS:HE3	1.41	0.44
1:A:2797:ARG:O	1:A:2801:ARG:HG3	2.18	0.44
1:A:2909:LEU:HA	4:A:4704:ADP:C2	2.51	0.44
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.52	0.44
1:A:2453:ARG:HD3	1:A:2728:LEU:O	2.18	0.43
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.52	0.43
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	2.00	0.43
1:A:2457:SER:HB2	1:A:2501:SER:HB3	2.00	0.43
1:A:3203:VAL:O	1:A:3206:ARG:HG2	2.18	0.43
1:A:4106:LEU:HD23	1:A:4106:LEU:HA	1.89	0.43
1:A:1560:LEU:O	1:A:1561:LEU:HD23	2.19	0.43
1:A:1929:VAL:HG13	1:A:1958:ASP:OD2	2.19	0.43
1:A:3161:LEU:HB2	1:A:3168:THR:HG22	2.01	0.43
1:A:2820:GLY:O	1:A:2824:ILE:HG13	2.18	0.43
1:A:1561:LEU:HD21	1:A:1618:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1859:ILE:HD11	1:A:1868:TYR:HD1	1.84	0.43
1:A:2308:ASP:O	1:A:2312:VAL:HG12	2.19	0.43
1:A:3751:GLN:O	1:A:3755:GLU:HG2	2.17	0.43
1:A:4594:LYS:HE3	1:A:4594:LYS:HB3	1.93	0.43
1:A:1834:LYS:HD3	1:A:1834:LYS:HA	1.78	0.43
1:A:1887:ARG:NH2	1:A:4253:GLY:O	2.51	0.43
1:A:3924:ILE:HD12	1:A:3924:ILE:H	1.83	0.43
1:A:4297:PRO:HG3	1:A:4308:TRP:CD2	2.54	0.43
1:A:3922:PRO:HD2	1:A:3936:VAL:HG11	2.00	0.43
1:A:2905:LEU:HD21	1:A:2948:ARG:CZ	2.49	0.43
1:A:3024:ASP:OD1	1:A:3025:GLU:N	2.52	0.43
1:A:4043:MET:HB2	1:A:4127:THR:HG22	1.99	0.43
1:A:4048:GLY:HA3	1:A:4206:GLU:OE1	2.19	0.43
1:A:3214:GLN:HG3	1:A:3759:ARG:CZ	2.49	0.42
1:A:1547:LEU:HD23	1:A:1547:LEU:HA	1.81	0.42
1:A:3910:ARG:NH1	1:A:4344:LEU:HD11	2.34	0.42
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.54	0.42
1:A:3491:LYS:HA	1:A:3491:LYS:HD3	1.77	0.42
1:A:4100:HIS:HB3	1:A:4128:MET:HB2	2.01	0.42
1:A:2552:VAL:HG22	1:A:2575:VAL:HG11	2.02	0.42
1:A:3215:VAL:HG21	1:A:3479:LEU:HD11	2.00	0.42
1:A:4149:PRO:HA	1:A:4150:PRO:HD3	1.96	0.42
1:A:4448:LEU:HD23	1:A:4448:LEU:HA	1.91	0.42
1:A:2163:ASP:OD2	1:A:4526:GLN:HG3	2.20	0.42
1:A:2224:GLY:O	1:A:2346:GLN:HA	2.19	0.42
1:A:1739:ILE:HG23	1:A:1804:ARG:HD2	2.02	0.42
1:A:1945:PHE:HB3	1:A:1978:ILE:HD11	2.01	0.42
1:A:3614:PHE:HD2	1:A:3637:ASP:O	2.02	0.42
1:A:3983:ILE:O	1:A:3987:ILE:HG13	2.19	0.42
1:A:1783:SER:O	1:A:1787:VAL:HG13	2.20	0.42
1:A:1907:PRO:HD2	1:A:2042:THR:HA	2.02	0.42
1:A:2449:LEU:HD11	1:A:2454:CYS:SG	2.60	0.42
1:A:2758:LEU:HD11	1:A:2807:PHE:CE1	2.54	0.42
1:A:2949:PHE:CE2	1:A:2953:MET:HE3	2.54	0.42
1:A:3868:PHE:CZ	1:A:4018:MET:HG2	2.55	0.42
1:A:4150:PRO:O	1:A:4195:ARG:NH2	2.52	0.42
1:A:2040:ALA:HB1	1:A:4257:ASP:HB3	2.02	0.42
1:A:2422:ILE:HD13	1:A:2487:GLU:HA	2.02	0.42
1:A:2968:THR:HG23	1:A:2970:GLU:HG2	2.00	0.42
1:A:3502:THR:HG22	1:A:3542:GLN:HB3	2.02	0.42
1:A:2622:PHE:HB2	1:A:2665:GLU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1797:LEU:HD11	1:A:2060:ARG:NH2	2.31	0.41
1:A:3886:LEU:HD23	1:A:3886:LEU:HA	1.89	0.41
1:A:1895:ALA:HB2	1:A:2037:ARG:HB2	2.02	0.41
1:A:2031:ASN:HA	1:A:2034:LYS:HE3	2.01	0.41
1:A:2039:LEU:HD12	1:A:4254:GLY:HA2	2.02	0.41
1:A:2221:MET:CG	1:A:2343:PHE:HB2	2.49	0.41
1:A:4444:GLN:HG2	1:A:4449:ARG:HG3	2.02	0.41
1:A:2042:THR:HG21	1:A:4257:ASP:HB2	2.02	0.41
1:A:3659:ARG:HE	1:A:3661:LEU:HD21	1.85	0.41
1:A:4056:GLU:OE1	1:A:4068:SER:OG	2.31	0.41
1:A:2716:THR:HB	1:A:4445:THR:HB	2.02	0.41
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	2.01	0.41
1:A:3556:ALA:HB3	1:A:3743:ARG:NH1	2.36	0.41
1:A:3908:PHE:CZ	1:A:4340:ILE:HD11	2.55	0.41
1:A:3929:VAL:HG12	1:A:3933:GLU:OE2	2.20	0.41
1:A:4415:ARG:HG2	1:A:4419:MET:HE2	2.03	0.41
1:A:3017:VAL:HB	1:A:3020:LEU:HB2	2.01	0.41
1:A:4096:LEU:HD13	1:A:4105:TRP:HH2	1.86	0.41
1:A:4215:ALA:HB1	1:A:4247:MET:HE2	2.02	0.41
1:A:4288:VAL:HG23	1:A:4289:ASP:OD1	2.21	0.41
1:A:2065:LEU:HD21	1:A:2134:GLN:HG2	2.02	0.41
1:A:2864:GLU:O	1:A:2868:SER:OG	2.31	0.41
1:A:4234:SER:HB3	1:A:4237:LYS:HG2	2.03	0.41
1:A:2049:ILE:O	1:A:2053:MET:HG3	2.21	0.41
1:A:2965:ARG:NH1	1:A:3614:PHE:O	2.48	0.41
1:A:3230:GLU:HA	1:A:3233:ASN:ND2	2.35	0.41
1:A:3568:PRO:HG2	1:A:3573:CYS:SG	2.61	0.41
1:A:3942:PRO:HA	1:A:3945:LYS:HG3	2.02	0.41
1:A:3606:ASP:N	1:A:3606:ASP:OD1	2.54	0.41
1:A:3728:ARG:NH1	1:A:3732:LEU:HD11	2.36	0.41
1:A:4039:THR:HG23	1:A:4142:GLY:HA2	2.03	0.41
1:A:1571:ILE:HD13	1:A:1608:LEU:HD22	2.03	0.41
1:A:1957:PHE:HB2	1:A:2016:ILE:HG22	2.03	0.41
1:A:2758:LEU:HD13	1:A:2811:ARG:HA	2.03	0.41
1:A:2898:LYS:O	1:A:2902:GLU:HG3	2.21	0.41
1:A:4187:HIS:ND1	1:A:4252:TYR:OH	2.46	0.41
1:A:3148:VAL:O	1:A:3152:GLN:HG3	2.21	0.40
1:A:3556:ALA:HA	1:A:3559:ARG:HB2	2.02	0.40
1:A:2951:ALA:HB1	1:A:2956:LEU:HB2	2.02	0.40
1:A:2984:GLY:HA2	1:A:3057:GLN:HB3	2.04	0.40
1:A:1912:LYS:NZ	2:A:4701:AOV:O4G	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2570:PRO:O	1:A:2746:GLN:NE2	2.54	0.40
1:A:3502:THR:HB	1:A:3543:PHE:HA	2.04	0.40
1:A:4401:THR:O	1:A:4405:ILE:HG12	2.22	0.40
1:A:1762:VAL:HG13	1:A:1778:LEU:HD11	2.04	0.40
1:A:1860:GLN:HG2	1:A:1865:LYS:HG2	2.03	0.40
1:A:2142:CYS:O	1:A:2146:VAL:HB	2.21	0.40
1:A:3133:LEU:HD11	1:A:3141:GLU:HB3	2.02	0.40
1:A:3905:PHE:HZ	1:A:4008:PHE:CZ	2.40	0.40
1:A:4398:LEU:HD21	1:A:4493:SER:HA	2.03	0.40
1:A:4511:LEU:HD23	1:A:4511:LEU:HA	1.93	0.40
1:A:4517:PRO:HG2	1:A:4619:ILE:HD12	2.02	0.40
1:A:1580:LYS:HD3	1:A:1580:LYS:HA	1.91	0.40
1:A:2773:MET:HE2	1:A:2773:MET:HB3	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2851/4646 (61%)	2803 (98%)	48 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	2532/4125 (61%)	2527 (100%)	5 (0%)	87 96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1878	LYS
1	A	1879	LEU
1	A	1883	PRO
1	A	2094	LYS
1	A	2355	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1598	GLN
1	A	1779	HIS
1	A	1817	HIS
1	A	1855	GLN
1	A	1894	GLN
1	A	1922	GLN
1	A	2051	GLN
1	A	2079	GLN
1	A	2263	HIS
1	A	2439	HIS
1	A	2637	HIS
1	A	2698	GLN
1	A	2827	HIS
1	A	2860	ASN
1	A	2918	HIS
1	A	2954	ASN
1	A	2960	GLN
1	A	3063	HIS
1	A	3523	GLN
1	A	3563	GLN
1	A	3744	GLN
1	A	3799	GLN
1	A	3820	GLN
1	A	3877	HIS
1	A	4029	HIS
1	A	4098	ASN
1	A	4114	HIS
1	A	4295	GLN

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Mol	Chain	Res	Type
1	A	4326	ASN
1	A	4429	GLN
1	A	4490	GLN
1	A	4508	HIS
1	A	4530	GLN
1	A	4566	GLN
1	A	4579	ASN

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	AOV	A	4701	5	32,34,34	4.97	7 (21%)	42,56,56	2.36	12 (28%)
4	ADP	A	4704	-	28,29,29	0.48	0	43,45,45	0.49	0
4	ADP	A	4703	-	28,29,29	0.47	0	43,45,45	0.48	0
3	ATP	A	4702	5	32,33,33	0.74	0	48,52,52	0.64	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	AOV	A	4701	5	-	2/16/39/39	0/3/3/3
4	ADP	A	4704	-	-	0/16/32/32	0/3/3/3
4	ADP	A	4703	-	-	1/16/32/32	0/3/3/3
3	ATP	A	4702	5	-	6/22/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4701	AOV	O1G-VG	26.61	2.08	1.61
2	A	4701	AOV	C5-C4	3.59	1.45	1.39
2	A	4701	AOV	PA-O3A	-3.53	1.55	1.59
2	A	4701	AOV	C8-N9	-3.45	1.31	1.37
2	A	4701	AOV	C5-N7	-2.98	1.33	1.39
2	A	4701	AOV	C5-C6	2.39	1.47	1.41
2	A	4701	AOV	C4-N9	-2.10	1.33	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	AOV	C5-C4-N3	-7.20	116.80	126.72
2	A	4701	AOV	N3-C4-N9	5.31	136.19	127.17
2	A	4701	AOV	C4-C5-N7	-5.00	104.86	110.58
2	A	4701	AOV	C2-N3-C4	4.54	122.91	111.83
2	A	4701	AOV	N3-C2-N1	-4.07	122.42	128.58
2	A	4701	AOV	C5-N7-C8	3.59	109.09	103.45
2	A	4701	AOV	O2B-PB-O3A	3.57	116.94	107.27
2	A	4701	AOV	C2'-C1'-N9	-3.15	105.47	113.30
2	A	4701	AOV	C4-N9-C8	2.99	108.88	105.74
2	A	4701	AOV	C6-C5-N7	2.83	137.54	132.09
2	A	4701	AOV	N9-C8-N7	-2.67	110.15	113.94
2	A	4701	AOV	O3A-PB-O1B	-2.31	103.75	110.70

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4702	ATP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'

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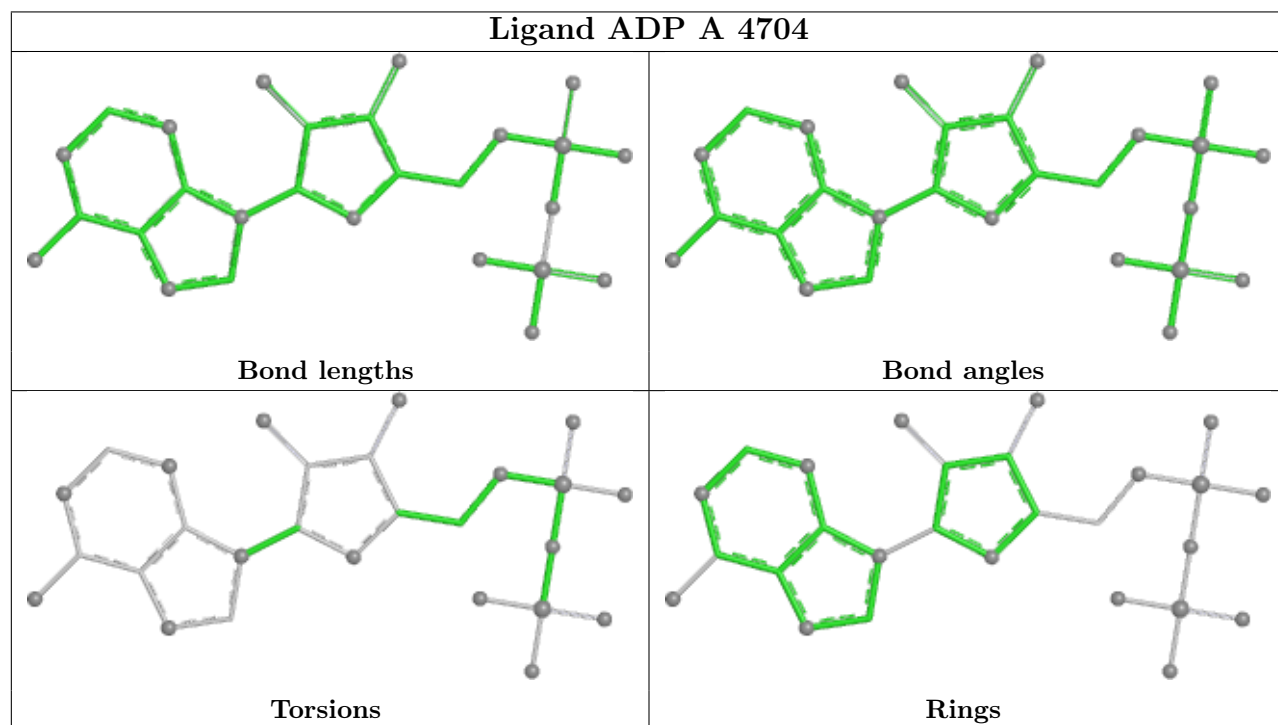
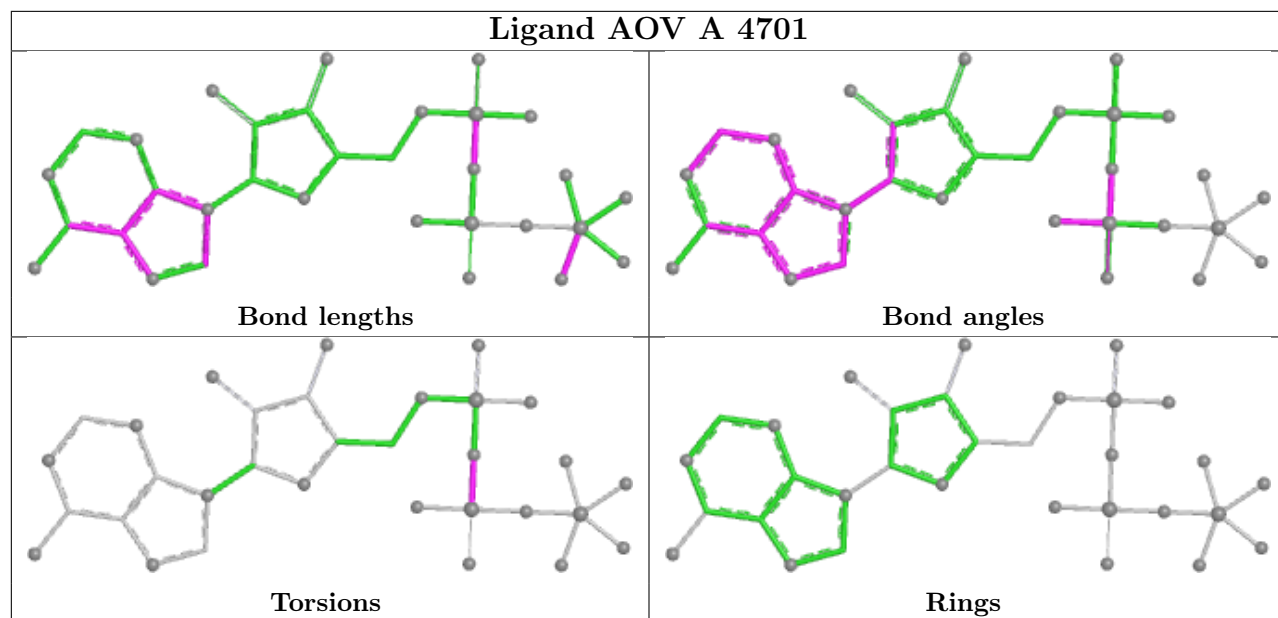
Mol	Chain	Res	Type	Atoms
2	A	4701	AOV	PA-O3A-PB-O2B
3	A	4702	ATP	PA-O3A-PB-O2B
2	A	4701	AOV	PA-O3A-PB-O1B
3	A	4702	ATP	PG-O3B-PB-O2B
4	A	4703	ADP	C2'-C1'-N9-C8
3	A	4702	ATP	PG-O3B-PB-O1B
3	A	4702	ATP	PA-O3A-PB-O1B

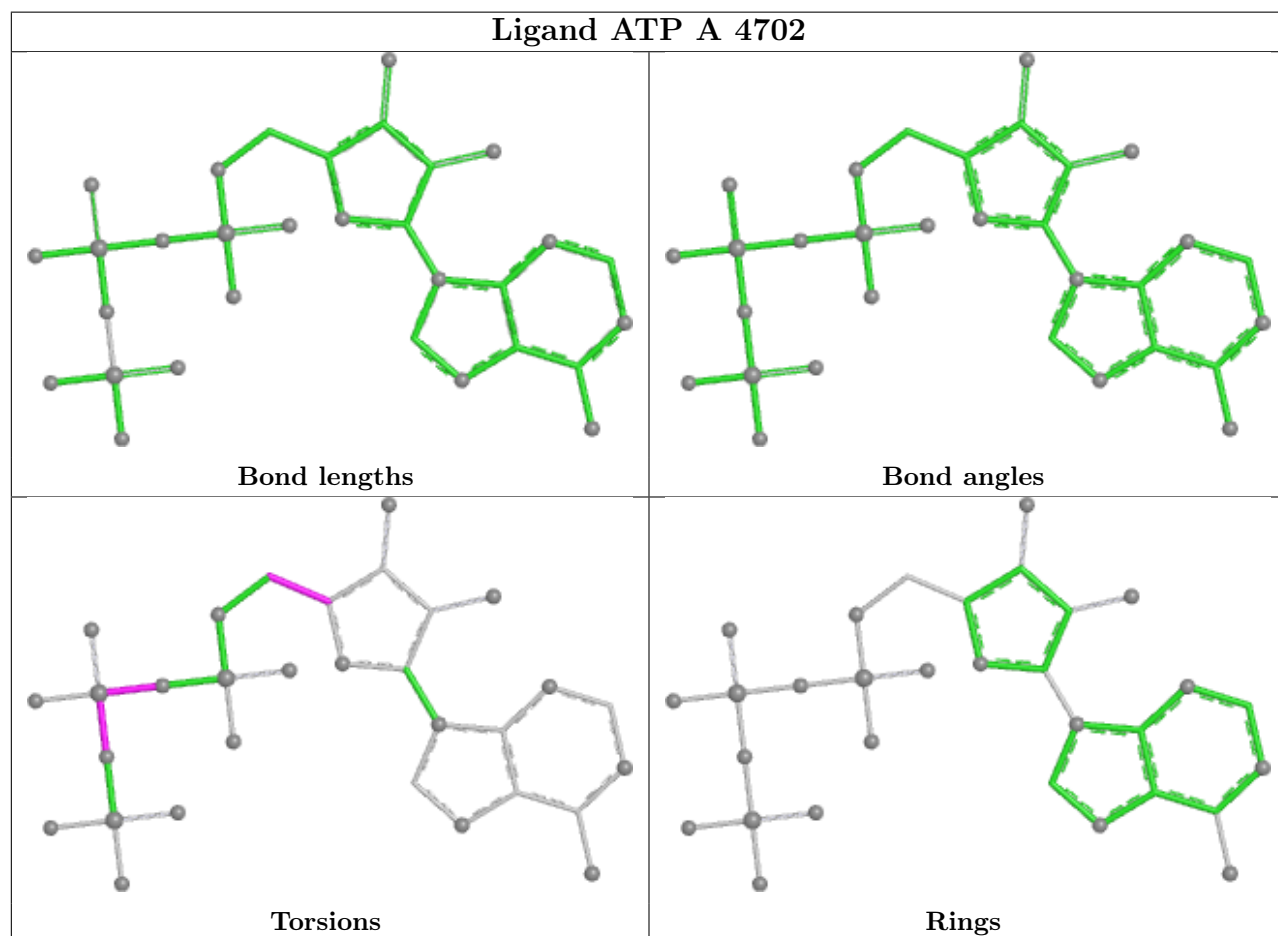
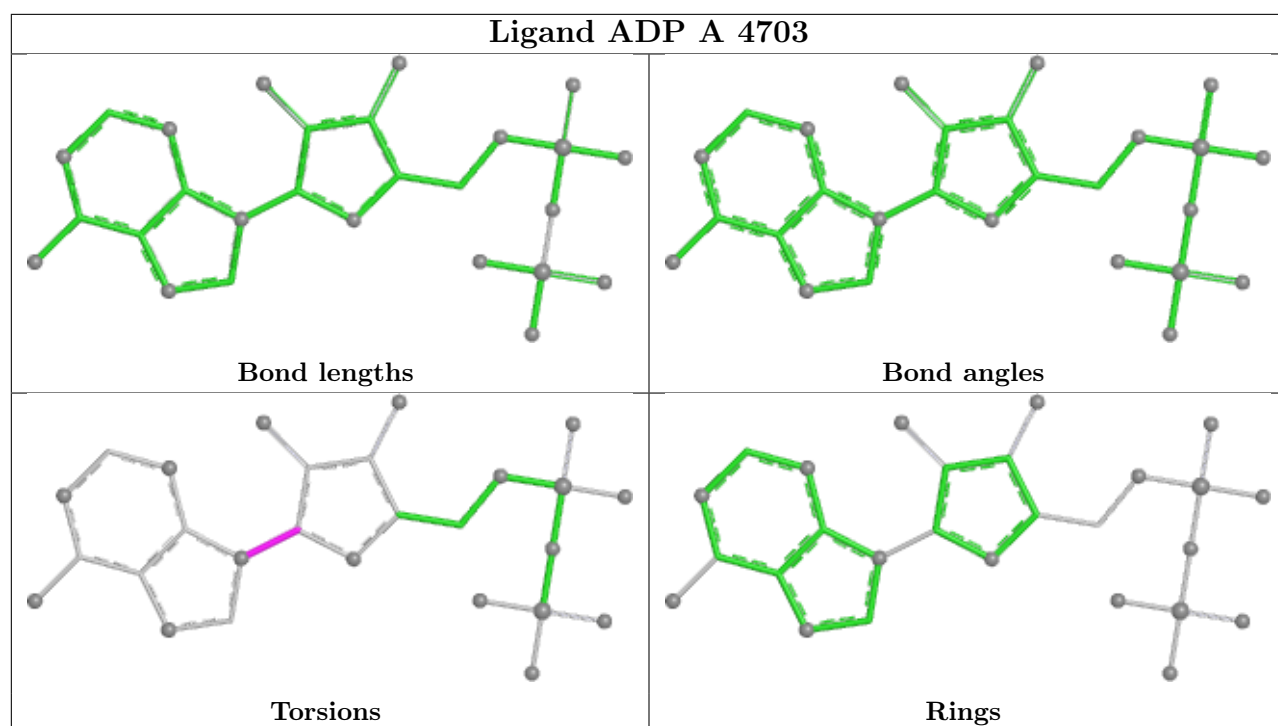
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	AOV	3	0
4	A	4704	ADP	1	0
3	A	4702	ATP	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.

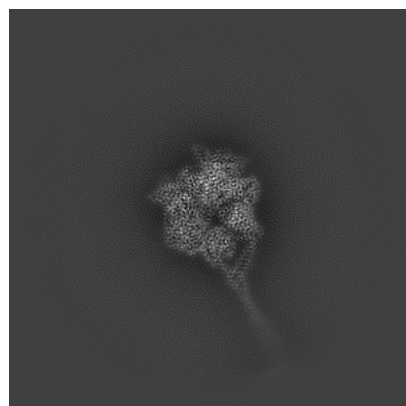
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44699. These allow visual inspection of the internal detail of the map and identification of artifacts.

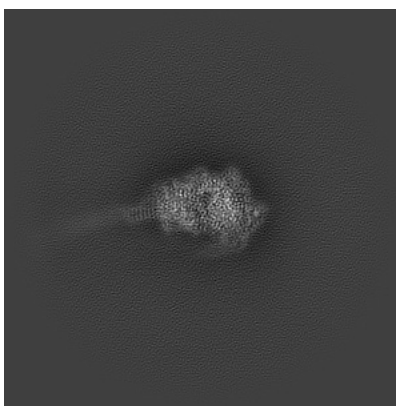
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

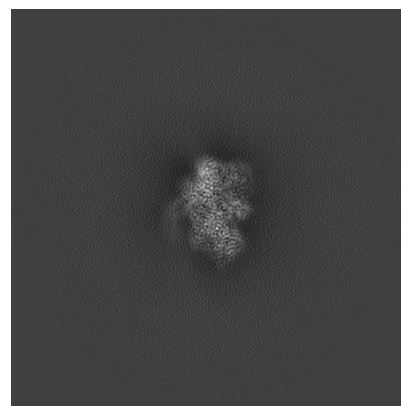
6.1.1 Primary map



X

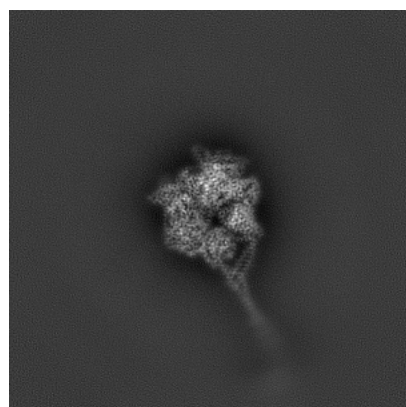


Y

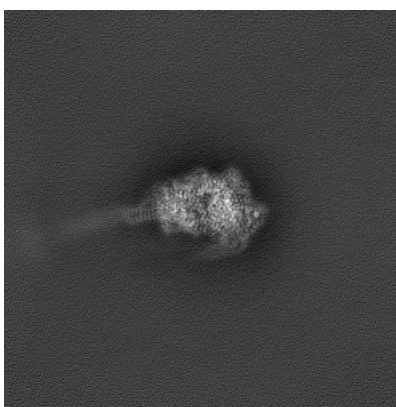


Z

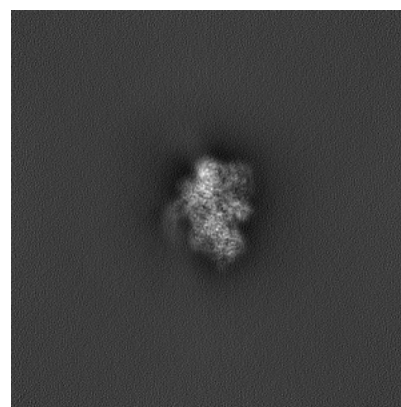
6.1.2 Raw map



X



Y

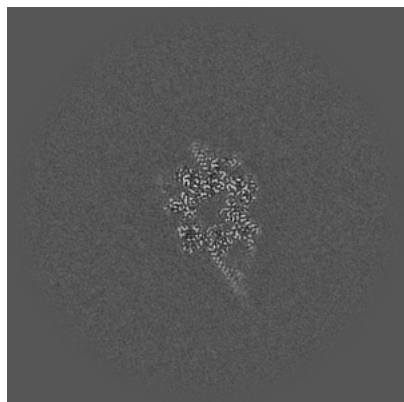


Z

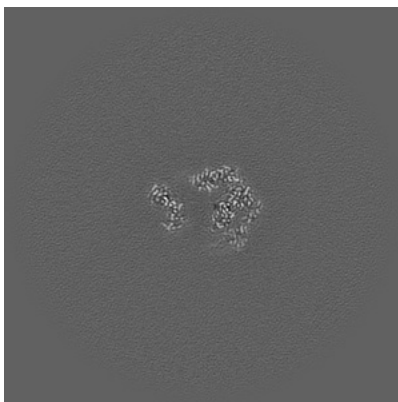
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

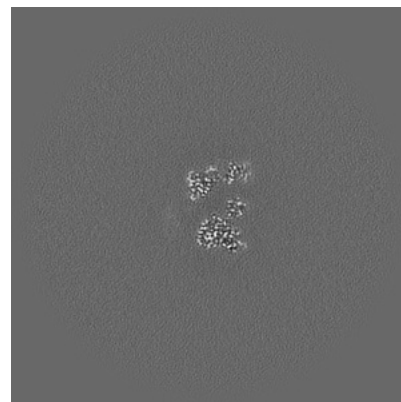
6.2.1 Primary map



X Index: 192

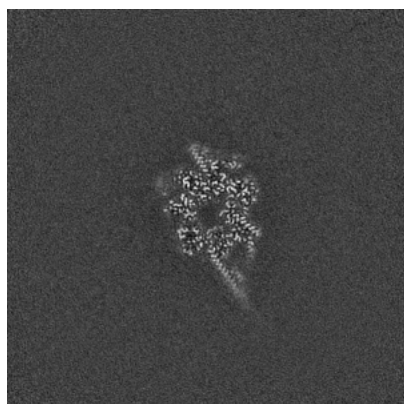


Y Index: 192

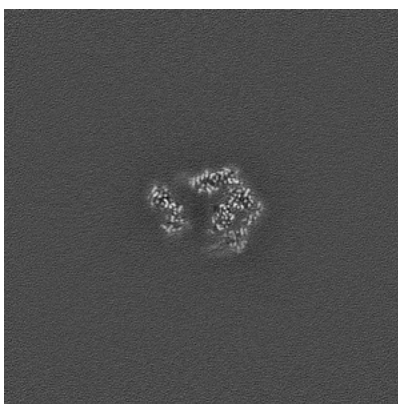


Z Index: 192

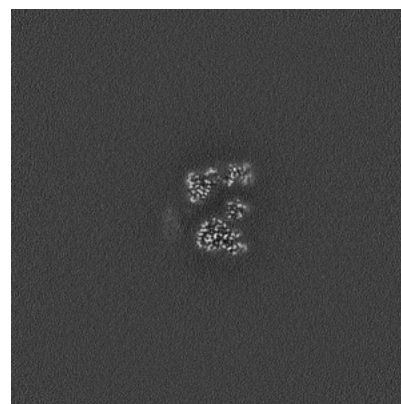
6.2.2 Raw map



X Index: 192



Y Index: 192

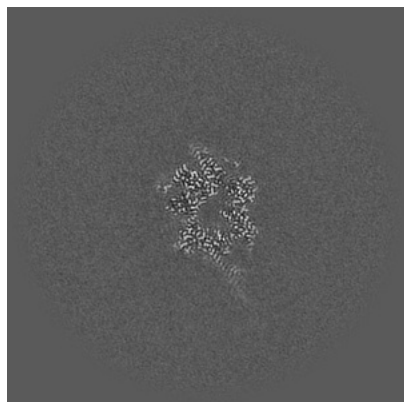


Z Index: 192

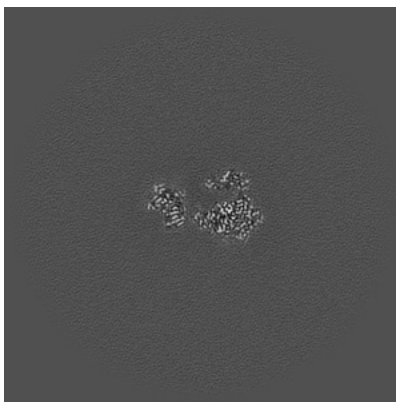
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

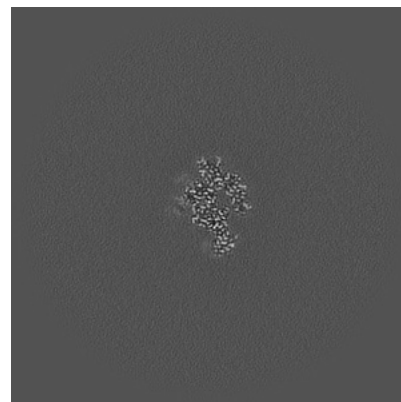
6.3.1 Primary map



X Index: 194

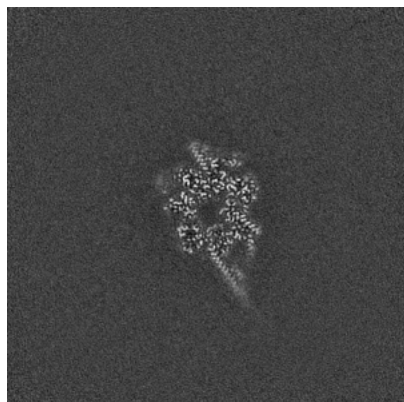


Y Index: 201



Z Index: 213

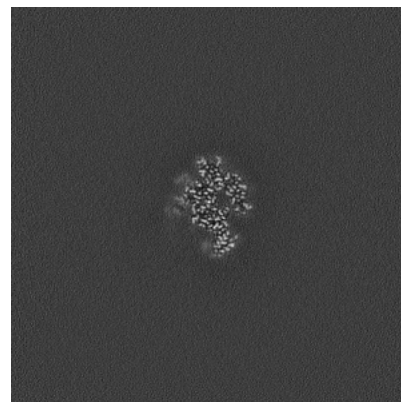
6.3.2 Raw map



X Index: 192



Y Index: 197

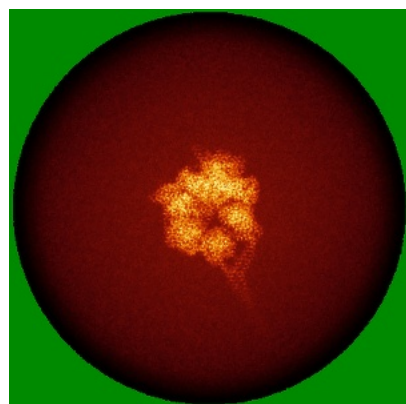


Z Index: 213

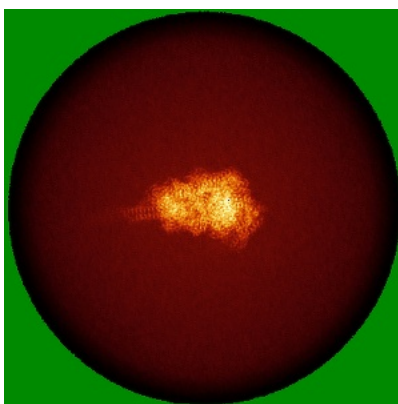
The images above show the largest variance slices of the map in three orthogonal directions.

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

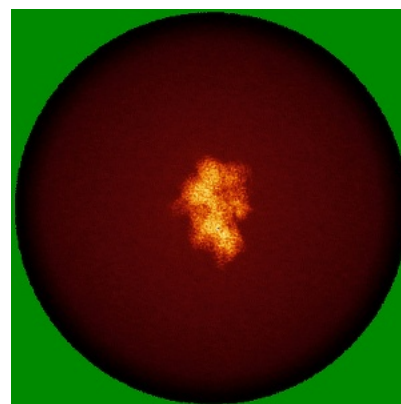
6.4.1 Primary map



X

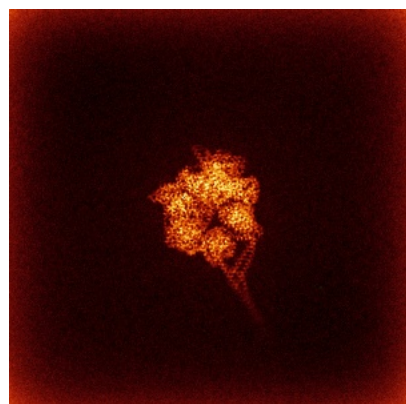


Y

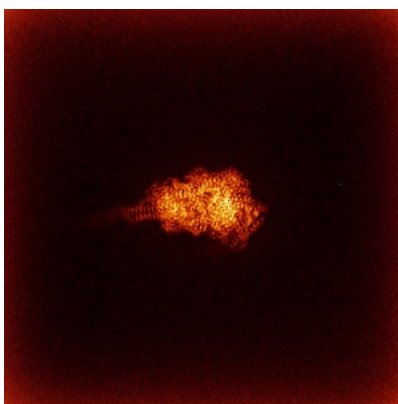


Z

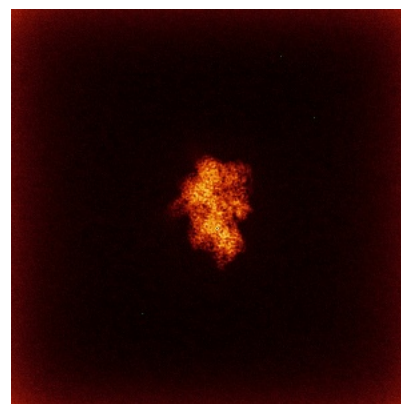
6.4.2 Raw map



X



Y

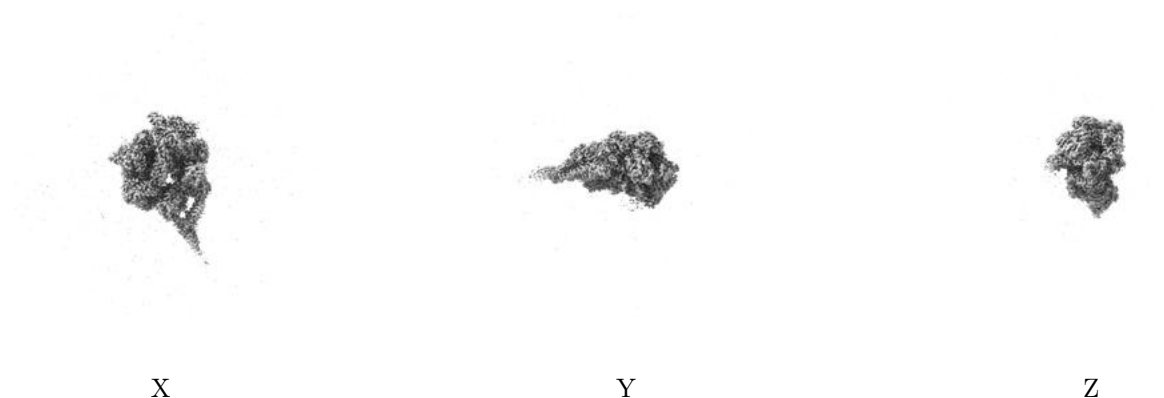


Z

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.

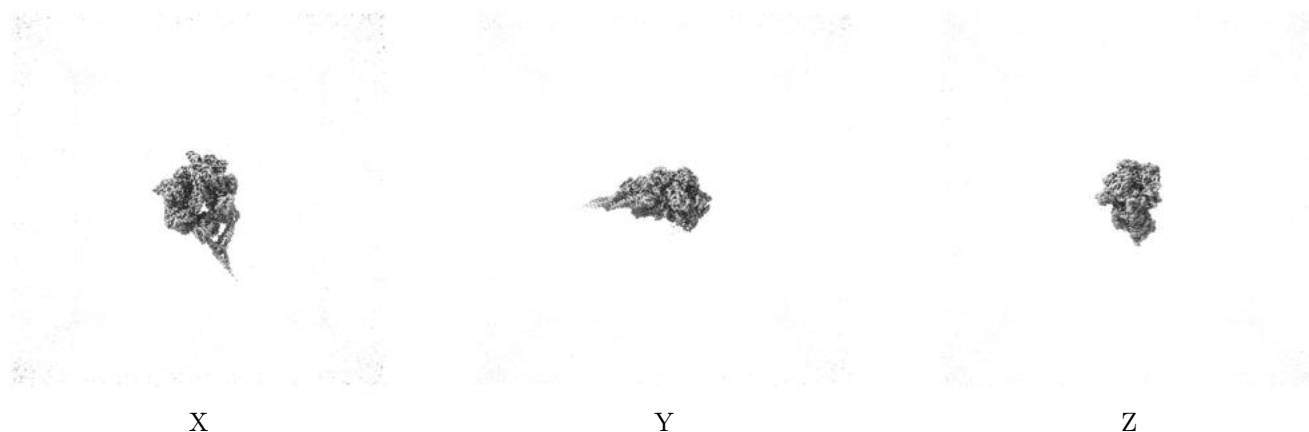
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

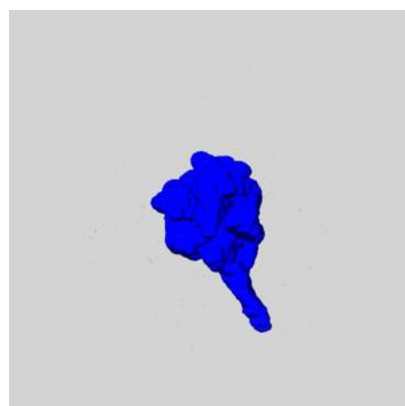
6.6 Mask visualisation [i](#)

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

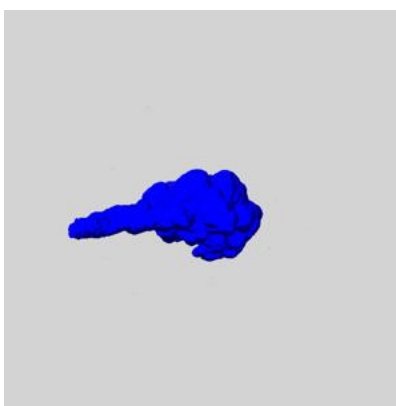
A mask typically either:

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

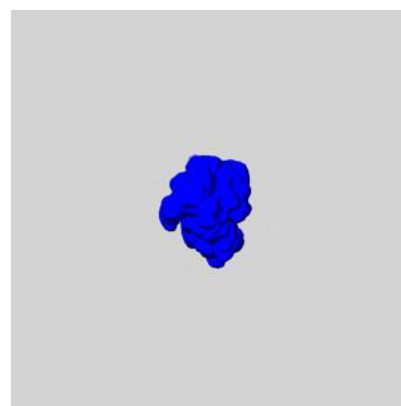
6.6.1 emd_44699_msk_1.map [i](#)



X



Y

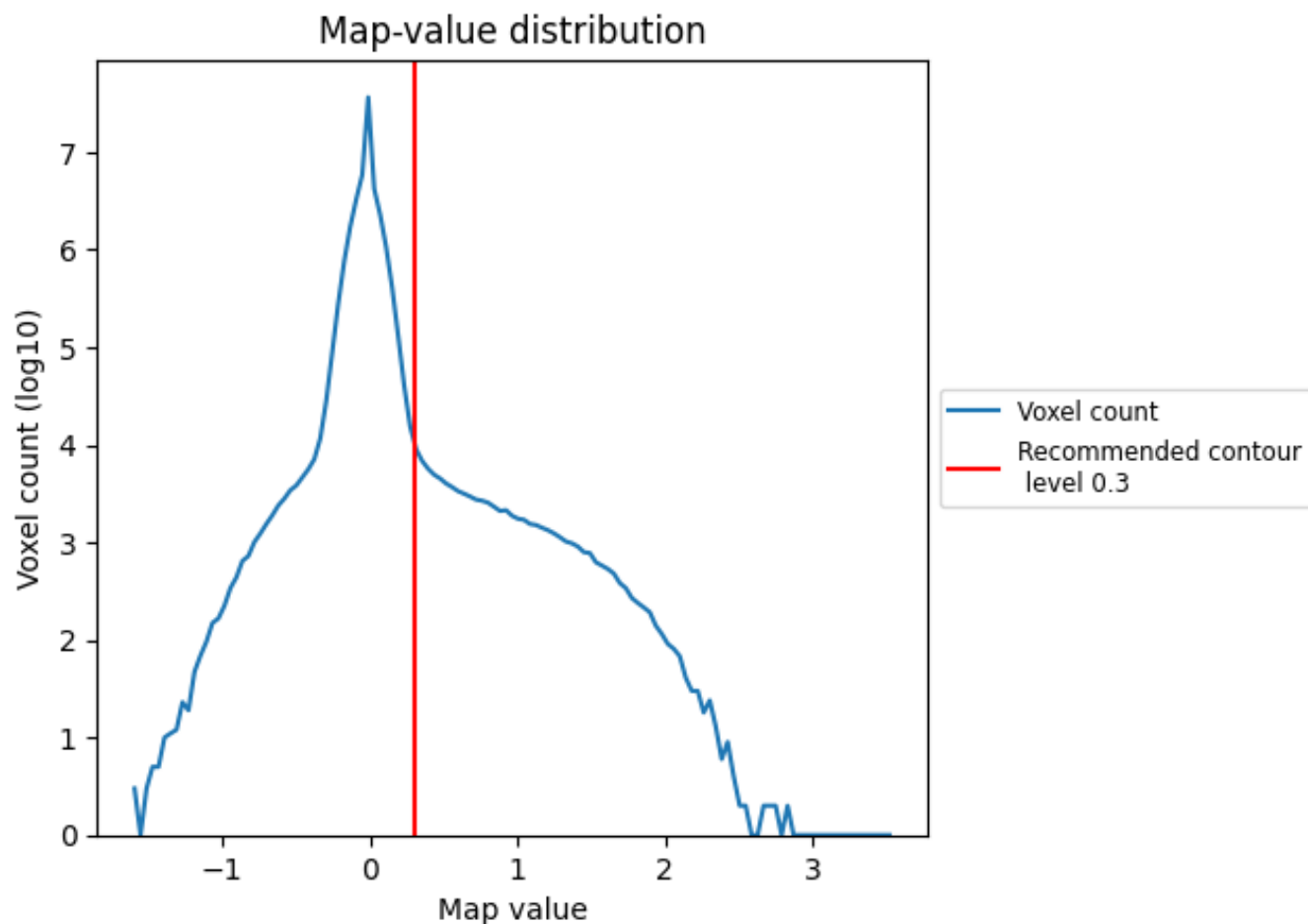


Z

7 Map analysis [i](#)

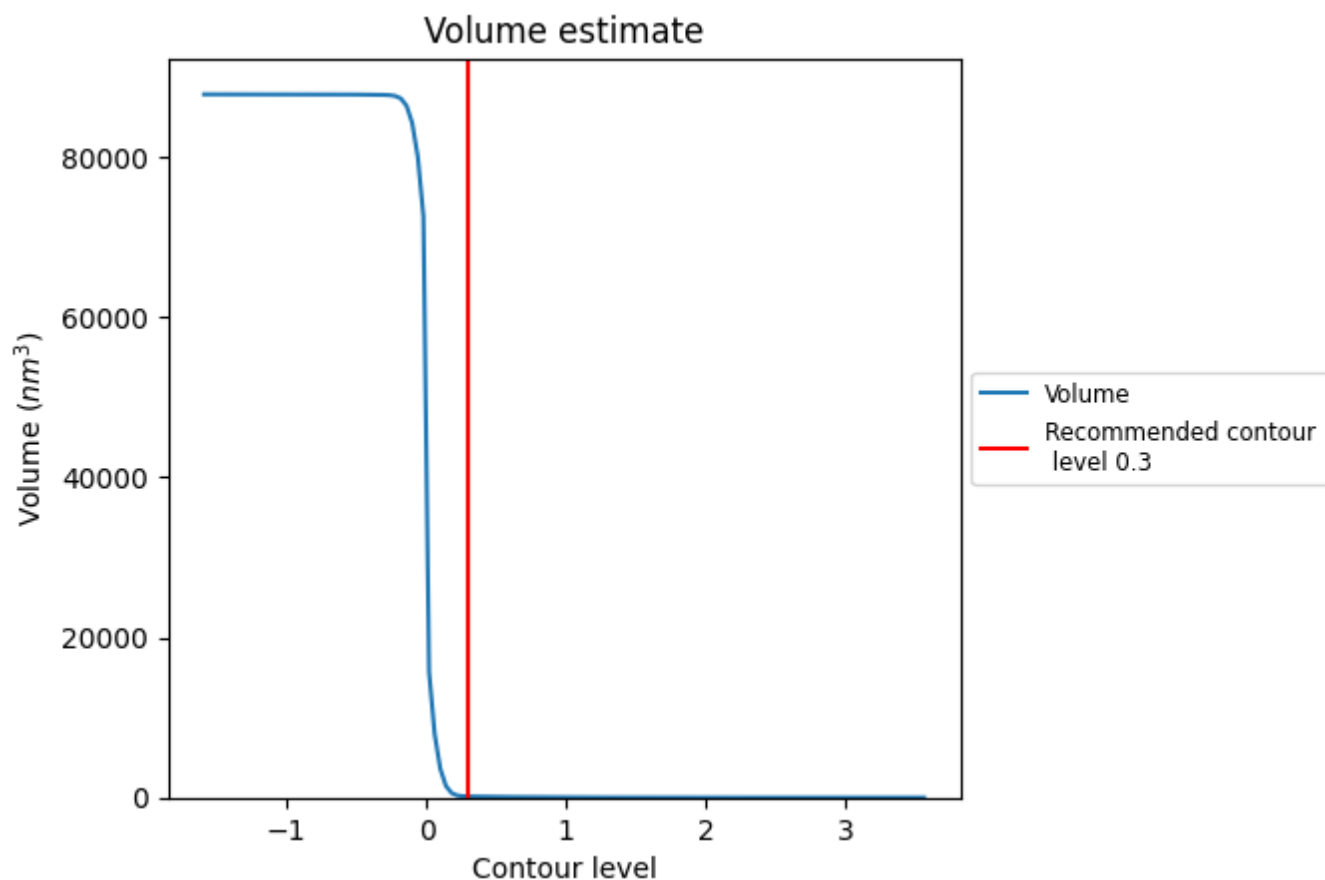
This section contains the results of statistical analysis of the map.

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.

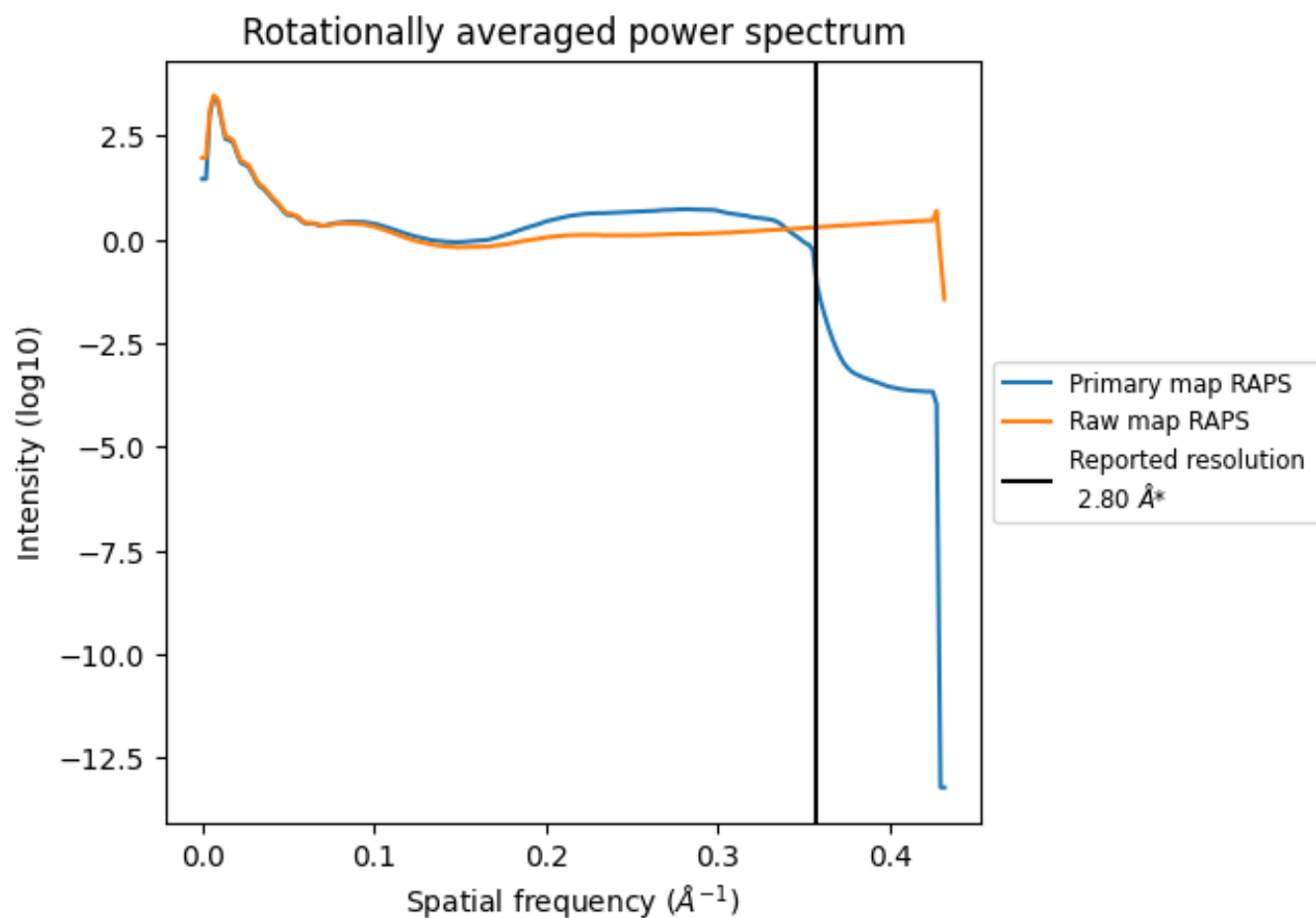
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 138 nm³; this corresponds to an approximate mass of 125 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 ⓘ

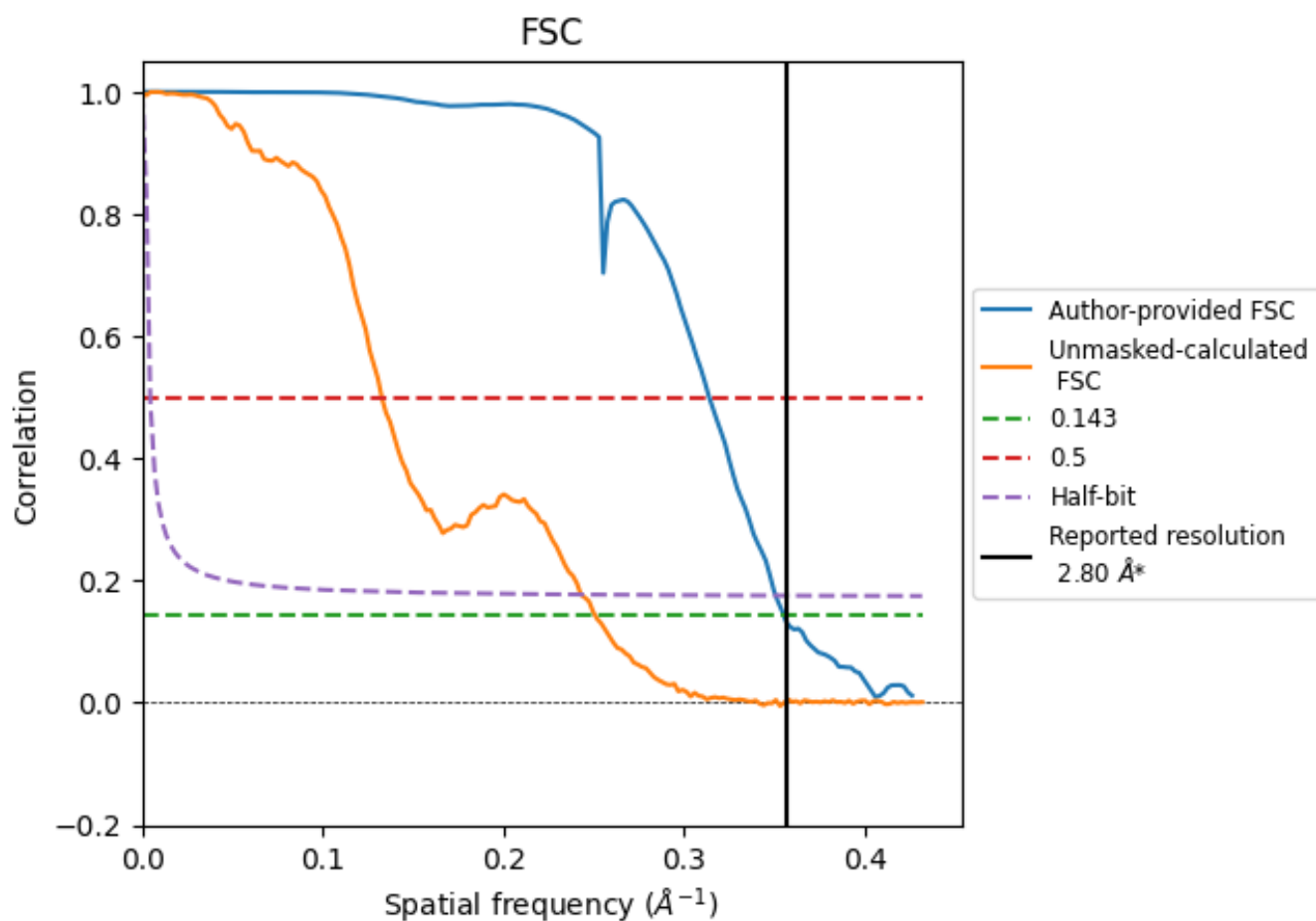


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.81	3.18	2.85
Unmasked-calculated*	3.99	7.54	4.12

*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 3.99 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

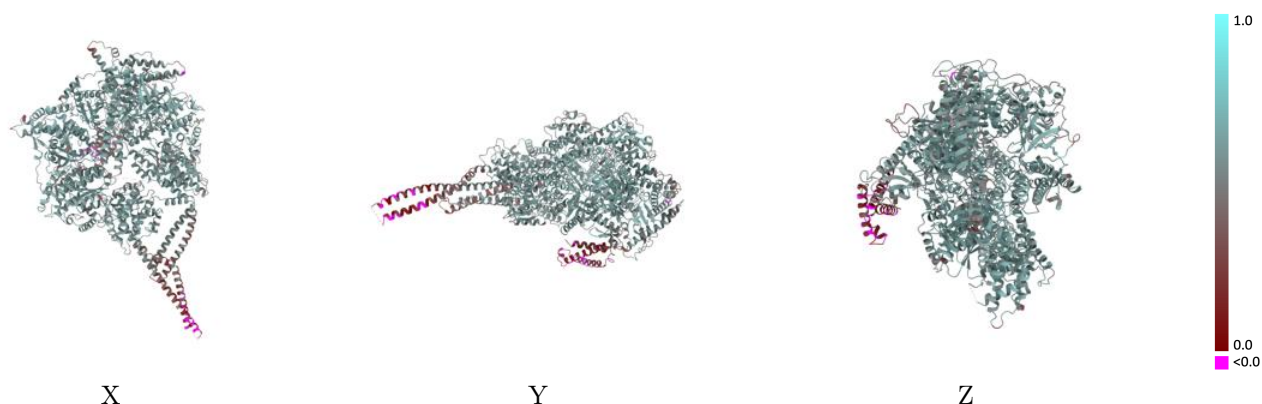
This section contains information regarding the fit between EMDB map EMD-44699 and PDB model 9BMH. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



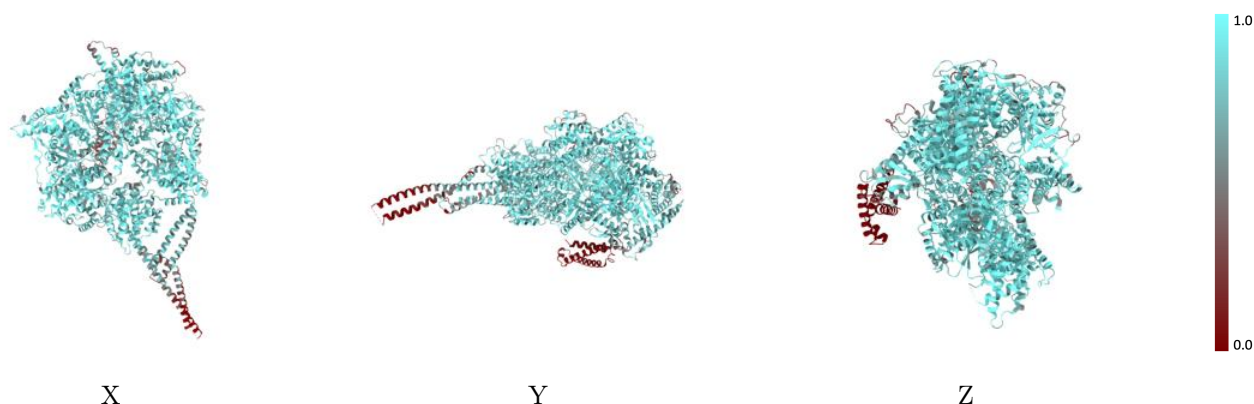
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



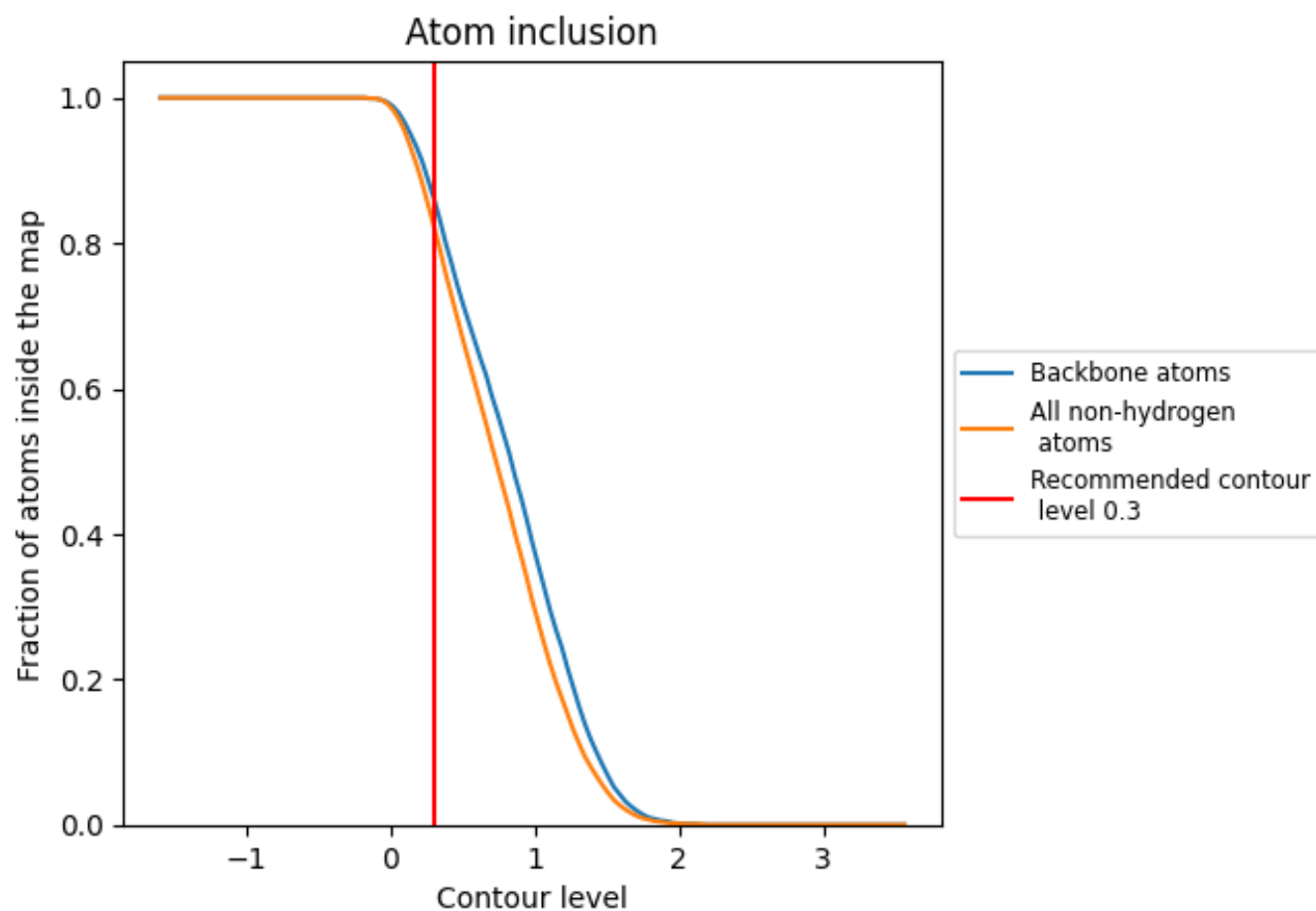
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 82% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8240	0.5530
A	0.8240	0.5530

