



Full wwPDB EM Validation Report ⓘ

Aug 23, 2026 – 12:16 AM JST

PDB ID : 27PY / pdb_000027py
EMDB ID : EMD-81335
Title : Dictyostelium discoideum cytoplasmic dynein motor domain in the presence of ADP (ADP state 1)
Authors : Shimo-Kon, R.; Tokita, H.; Imai, H.; Maeshima, T.; Kon, T.
Deposited on : 2026-06-09
Resolution : 2.61 Å(reported)
Based on initial model : 3VKG

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 : 1.8.5 (274361), CSD as541be (2020)
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

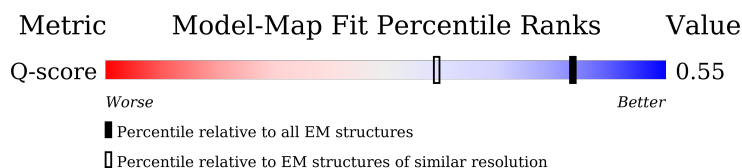
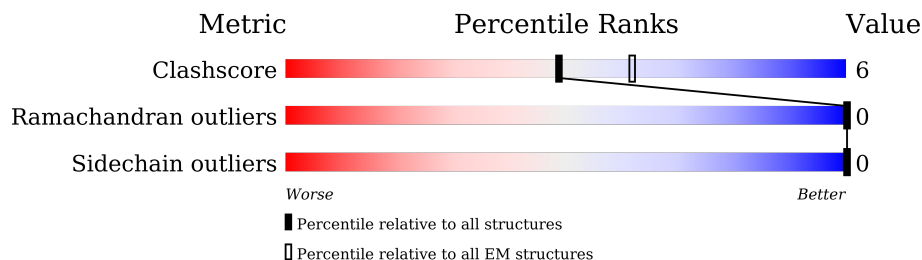
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.61 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	8735 (2.11 - 3.11)

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	3367	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24518 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.

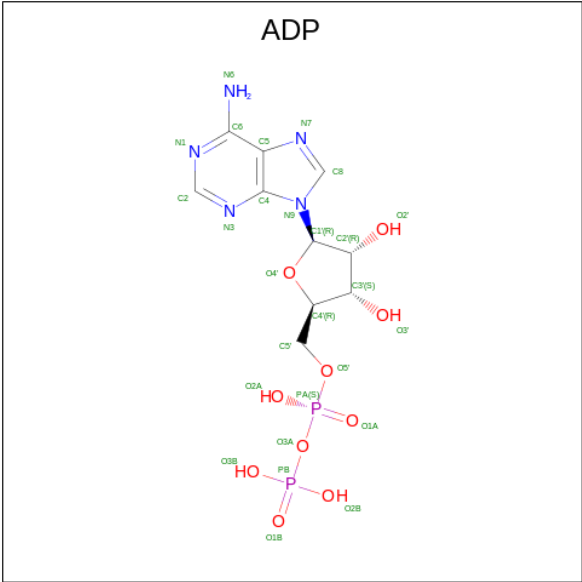
- Molecule 1 is a protein called Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3034	Total	C	N	O	S	0	0
			24405	15575	4154	4578	98		

There are 24 discrepancies between the modelled and reference sequences:

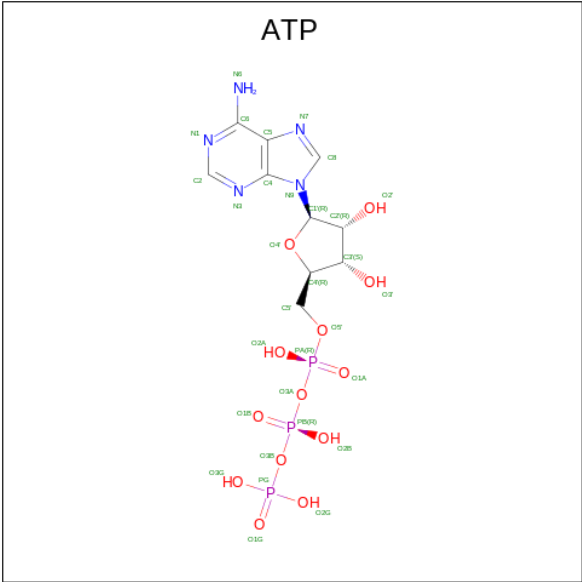
Chain	Residue	Modelled	Actual	Comment	Reference
A	1364	MET	-	initiating methionine	UNP P34036
A	1365	THR	-	expression tag	UNP P34036
A	1366	ARG	-	expression tag	UNP P34036
A	1367	HIS	-	expression tag	UNP P34036
A	1368	HIS	-	expression tag	UNP P34036
A	1369	HIS	-	expression tag	UNP P34036
A	1370	HIS	-	expression tag	UNP P34036
A	1371	HIS	-	expression tag	UNP P34036
A	1372	HIS	-	expression tag	UNP P34036
A	1373	GLY	-	expression tag	UNP P34036
A	1374	GLY	-	expression tag	UNP P34036
A	1375	GLY	-	expression tag	UNP P34036
A	1376	ASP	-	expression tag	UNP P34036
A	1377	TYR	-	expression tag	UNP P34036
A	1378	LYS	-	expression tag	UNP P34036
A	1379	ASP	-	expression tag	UNP P34036
A	1380	ASP	-	expression tag	UNP P34036
A	1381	ASP	-	expression tag	UNP P34036
A	1382	ASP	-	expression tag	UNP P34036
A	1383	LYS	-	expression tag	UNP P34036
A	1384	GLY	-	expression tag	UNP P34036
A	1385	GLY	-	expression tag	UNP P34036
A	1386	GLY	-	expression tag	UNP P34036
A	1387	LYS	-	expression tag	UNP P34036

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

- 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).

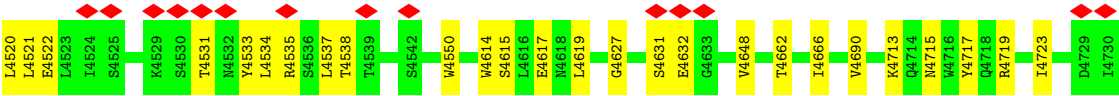


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

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

M4433	P4194	A4065	I3865	D3768	W3617	GLU	CYS	GLY	GLN	D3294	H3109	I2950	S2750
Q4195	Q4195	Q4068	A3866	A3771	K3629	GLU	GLY	LYS	ILE	T3295	H3110	L2951	T2751
W4196	W4196	Q4068	A3866	A3771	K3629	TYR	PRO	LYS	ALA	E3296	K3113	Y2952	Q2757
L4197	L4197	T4076	K3867	D3776	L3632	THR	VAL	LEU	VAL	A3297	E3114	Q2961	R2764
S4435	V4198	T4076	K3868	R3780	K3640	LEU	LYS	TRP	GLN	Q3298	T3115	P2962	F2768
S4436	Q4199	W4079	V3870	V3781	E3660	ILE	ALA	ASP	LYS	V3299	A3116	R2965	F2788
E4437	K4202	N4079	E3871	N3785	N3661	ARG	THR	ILE	ALA	K3300	Q3117	K2973	T2804
E4438	L4083	L4083	E3872	V3788	K3666	GLU	ALA	ARG	TYR	D3301	K3118	A2974	H2805
D4439	R4093	R4093	E3873	T3789	R3667	GLN	THR	LYS	ASP	L3302	N3119	R2975	R2806
C4440	F4101	F4101	C3893	S3792	R3670	LYS	TYR	ILE	GLU	Q3303	K3120	L2976	F2807
E4441	F4115	F4115	L3903	D3815	Y3671	THR	SER	GLU	LYS	S3305	L3121	L2984	L2815
D4442	L4116	L4116	S3912	Q3820	D3676	GLU	ILE	ASN	ALA	L3306	L3123	V2986	P2840
ASP	K4127	K4127	L3913	E3822	D3676	SER	THR	PHE	PRO	A3307	D3124	L2990	R2843
GLN	F3916	F3916	F3916	K3818	A3681	LYS	ARG	ILE	ILE	LYS	S3125	L2999	E2855
VAL	L3917	L3917	L3917	I3819	L3685	V3553	ILE	SER	THR	ASN	E3128	R3000	F2864
SER	L3918	L3918	L3918	Q3821	L3685	K3554	LYS	ILE	ALA	ARG	L3129	R3003	V2872
GLY	I3919	I3919	I3919	G3822	F3699	N3555	LEU	ASN	GLN	LEU	T3134	V3004	F3005
SER	D3932	D3932	D3932	F3823	L3700	K3556	GLU	ASP	ALA	VAL	Q3135	R3006	R2877
SER	R3954	R3954	R3954	Q3824	L3712	V3557	VAL	THR	THR	ASP	Q3136	A3012	W2882
SER	R3957	R3957	R3957	V3825	L3723	R3558	GLU	LYS	THR	GLN	V3137	V3024	D2883
SER	L3960	L3960	L3960	K3826	E3724	S3560	GLN	ILE	ALA	ALA	P3162	M3032	R2884
D4459	L4151	L4151	L3830	L3830	D3727	I3561	GLU	THR	LYS	LYS	F3188	N3043	L2887
D4460	L4151	L4151	E3831	E3831	P3728	A3562	ASN	PRO	LYS	GLN	T3189	N3044	E2888
K4461	K3964	K3964	K3832	K3832	N3735	L3563	ALA	ILE	LEU	LEU	D3193	N3045	A2889
L4285	Q4156	Q4156	S3833	S3833	K3740	L3564	ASN	GLU	ASP	GLN	G3213	S3048	I2890
K4463	Y4157	Y4157	L3834	L3834	K3741	N3566	GLU	ILE	ALA	ILE	N3214	L3058	C2896
A4464	T4161	T4161	L3835	L3835	G3742	L3567	LEU	ILE	LYS	VAL	R3224	L3059	R2903
K4465	L4162	L4162	N3836	N3836	G3742	N3568	LYS	THR	LYS	GLN	L3231	R3061	L2904
L4466	G4163	G4163	L3837	L3837	G3743	E3570	GLN	GLY	PRO	GLN	I3238	A3062	A2909
I4470	E4166	E4166	L3838	L3838	R3744	S3569	ASP	TYR	PRO	ALA	A3241	K3065	K2929
T4471	G4167	G4167	S3839	S3839	I3745	R3571	LYS	GLU	THR	GLN	R3251	I3069	T2950
F4472	F4168	F4168	Q3840	Q3840	L3746	G3572	ILE	GLU	ASP	ALA	Y3260	N3088	D2931
W4473	E4169	E4169	L3747	L3747	D3751	E3575	VAL	ASP	THR	ILE	I3264	T3089	E2932
L4476	L4170	L4170	S3842	S3842	D3755	F3575	ALA	PRO	PRO	LYS	F3263	L3090	H2937
L4477	K4173	K4173	G3843	G3843	F3756	Y3601	THR	PHE	GLY	VAL	I3271	L3090	F2938
K4485	W4184	W4184	N3844	N3844	S3759	I3602	LYS	ASN	VAL	GLU	R3275	F3100	V2941
K4486	L4185	L4185	S3850	S3850	F3760	G3603	ILE	ARG	VAL	GLN	K3290	E3101	R2947
T4487	L4186	L4186	V3851	V3851	M3761	F3605	ALA	ALA	LEU	VAL	L3291	L3108	R2948
T4488	L4187	L4187	I3852	I3852	L3764	F3605	THR	SER	LEU	GLN	R3292	L3108	P2949
Q4489	K4188	K4188	S3853	S3853	T3766	D3606	TYR	LYS	GLY	ASP	K3293	L3108	
N4490	L4189	L4189	T3854	T3854	R3767	R3610	LYS	ALA	ALA	ARG			
L4491	L4190	L4190	L3855	L3855	E3767	L3613				LYS			
F4496	A4193	A4193	E3856	E3856									
L4509			T3857	T3857									
D4516			L3858	L3858									
L4517			K3859	K3859									
A4518			K3860	K3860									
N4519			E3861	E3861									



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	2128136	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF parameters were estimated using Patch CTF estimation in cryoSPARC and further refined by global and local CTF refinement.	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.754	Depositor
Minimum map value	-1.655	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.12	Depositor
Map size ($\text{\AA}$)	261.9, 261.9, 261.9	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.87299997, 0.87299997, 0.87299997	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: ADP, MG, ATP

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	0.11	0/24926	0.28	0/33768

There are no bond length outliers.

There are no bond angle outliers.

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	24405	0	24447	286	0
2	A	81	0	36	4	0
3	A	31	0	12	0	0
4	A	1	0	0	0	0
All	All	24518	0	24495	286	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (286) 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:2642:ALA:HB3	1:A:2884:ARG:HG3	1.63	0.80
1:A:1972:PRO:HG2	1:A:2076:THR:HG22	1.64	0.79
1:A:1558:TRP:HH2	1:A:1605:TRP:HD1	1.30	0.78
1:A:3271:ILE:HG12	1:A:3592:VAL:HG11	1.69	0.74
1:A:3559:ARG:HD2	1:A:3847:ASP:HA	1.70	0.72
1:A:4387:THR:HG22	1:A:4388:THR:H	1.56	0.69
1:A:1828:ASP:OD1	1:A:1906:TRP:NE1	2.28	0.66
1:A:1558:TRP:CH2	1:A:1605:TRP:HD1	2.12	0.66
1:A:2139:LEU:HD23	1:A:2214:LEU:HD22	1.75	0.66
1:A:4032:LYS:HZ2	1:A:4065:ALA:HB1	1.59	0.65
1:A:2376:LEU:HD11	1:A:2384:ARG:HB3	1.79	0.65
1:A:3238:ILE:HD11	1:A:3617:TRP:HZ2	1.61	0.65
1:A:2840:PRO:HA	1:A:2843:ARG:HG3	1.79	0.65
1:A:2975:ARG:HG3	1:A:3032:MET:HE3	1.79	0.65
1:A:2764:ARG:HD2	1:A:2806:ARG:HG2	1.79	0.64
1:A:2855:GLU:OE1	1:A:2937:HIS:NE2	2.27	0.63
1:A:1558:TRP:HH2	1:A:1605:TRP:CD1	2.15	0.63
1:A:1739:THR:HG23	1:A:1740:THR:HG23	1.81	0.63
1:A:4161:ALA:HB2	1:A:4188:LYS:HE3	1.80	0.63
1:A:1423:ILE:HB	1:A:1426:LYS:HG3	1.80	0.63
1:A:3058:LEU:HD11	1:A:3069:ILE:HG21	1.81	0.63
1:A:3291:LYS:HD2	1:A:3835:LEU:HB2	1.80	0.62
1:A:1477:LYS:NZ	1:A:1528:GLU:OE1	2.33	0.62
1:A:4190:ILE:HB	1:A:4219:SER:HB2	1.82	0.61
1:A:3741:LYS:HG3	1:A:3742:GLY:H	1.66	0.61
1:A:1452:ASP:O	1:A:1456:ASN:ND2	2.34	0.61
1:A:2105:ARG:HG2	1:A:2149:LEU:HD21	1.84	0.60
1:A:4520:LEU:HD11	1:A:4538:THR:HG22	1.84	0.60
1:A:3723:VAL:HG21	1:A:3764:LEU:HB3	1.83	0.59
1:A:4509:LEU:HD11	1:A:4550:TRP:HB2	1.84	0.59
1:A:2721:LYS:HD2	1:A:2731:ARG:HH12	1.68	0.59
1:A:2582:GLY:HA2	1:A:2585:MET:HE3	1.84	0.58
1:A:3724:GLU:OE2	1:A:3766:THR:OG1	2.18	0.58
1:A:4194:PRO:HB3	1:A:4224:ALA:HB1	1.86	0.58
1:A:3676:ASP:OD2	1:A:3681:ALA:N	2.34	0.57
1:A:3957:ARG:HG2	1:A:4116:LEU:HD11	1.85	0.57
1:A:4648:VAL:HG23	1:A:4662:THR:HG21	1.85	0.57
1:A:2903:ARG:NH1	1:A:2947:LYS:O	2.33	0.57
1:A:4615:SER:OG	1:A:4617:GLU:OE1	2.17	0.57
1:A:2128:ILE:HD12	1:A:2131:LEU:HD23	1.85	0.57
1:A:1408:TRP:HA	1:A:1411:ILE:HG22	1.87	0.57
1:A:1719:GLN:O	1:A:1723:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2027:GLU:OE2	1:A:2030:ARG:NH1	2.39	0.56
1:A:3670:ARG:NH1	1:A:3781:VAL:O	2.39	0.56
1:A:1459:LYS:HA	1:A:1462:LEU:HD12	1.88	0.56
1:A:3832:LYS:HA	1:A:3835:LEU:HG	1.88	0.56
1:A:1639:ILE:HG23	1:A:1672:LEU:HD22	1.88	0.55
1:A:2651:VAL:O	1:A:2655:ARG:HG3	2.06	0.55
1:A:4434:GLN:NE2	1:A:4438:GLU:OE1	2.37	0.55
1:A:1516:GLU:HB3	1:A:3741:LYS:HE2	1.89	0.55
1:A:2570:THR:HG21	1:A:2603:THR:HG21	1.88	0.55
1:A:2598:GLN:NE2	1:A:2606:PRO:O	2.40	0.55
1:A:1720:LYS:HA	1:A:1723:ARG:HH21	1.72	0.55
1:A:1578:SER:HB2	1:A:1579:PRO:HD3	1.89	0.55
1:A:3260:TYR:O	1:A:3264:ILE:HG12	2.07	0.55
1:A:4473:TRP:HD1	1:A:4476:LEU:HD12	1.71	0.55
1:A:3912:SER:HB3	1:A:4231:ARG:HG2	1.89	0.54
1:A:1483:ILE:HG22	1:A:1487:ARG:HG2	1.90	0.54
1:A:3238:ILE:HG13	1:A:3601:TYR:CG	2.43	0.54
1:A:4064:VAL:O	1:A:4068:GLN:HG2	2.08	0.54
1:A:1494:ILE:HA	1:A:1497:LEU:HD23	1.90	0.54
1:A:2642:ALA:O	1:A:2884:ARG:NH1	2.40	0.54
1:A:3088:ASN:HD21	1:A:3162:PRO:HD2	1.71	0.54
1:A:1863:VAL:O	1:A:1872:ARG:NH2	2.33	0.53
1:A:2283:THR:OG1	1:A:2396:GLU:OE2	2.25	0.53
1:A:3136:GLN:O	1:A:3137:VAL:HB	2.07	0.53
1:A:1534:VAL:HG22	1:A:1568:HIS:CE1	2.43	0.53
1:A:2125:ALA:HA	1:A:2128:ILE:HG22	1.90	0.53
1:A:2375:LYS:HB3	1:A:2387:LEU:HB3	1.89	0.53
1:A:2113:LEU:HD11	1:A:2156:LEU:HD22	1.91	0.53
1:A:4535:ARG:O	1:A:4538:THR:OG1	2.22	0.52
1:A:3685:LEU:HD12	1:A:3765:PHE:HZ	1.74	0.52
1:A:1532:LYS:HD2	1:A:1535:ARG:HH12	1.74	0.52
1:A:3918:ASP:OD2	1:A:4127:LYS:NZ	2.33	0.52
1:A:4470:ILE:HG21	1:A:4521:LEU:HB2	1.91	0.52
1:A:2113:LEU:HA	1:A:2116:GLN:HB2	1.91	0.52
1:A:4021:ILE:HA	1:A:4024:ARG:HG2	1.92	0.52
1:A:2126:GLY:O	1:A:4617:GLU:HG2	2.10	0.52
1:A:3024:VAL:HG11	2:A:5005:ADP:H3'	1.92	0.51
1:A:4473:TRP:O	1:A:4477:LEU:N	2.44	0.51
1:A:2063:LYS:HD2	1:A:2065:ILE:HD11	1.92	0.51
1:A:3629:LYS:HB3	1:A:3632:LEU:HB2	1.91	0.51
1:A:4136:SER:HB3	1:A:4140:TYR:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2152:LEU:O	1:A:2156:LEU:HG	2.11	0.50
1:A:2176:ASP:OD1	1:A:2177:ALA:N	2.44	0.50
1:A:2259:ILE:HG23	1:A:2289:TYR:HB2	1.92	0.50
1:A:3822:GLU:O	1:A:3826:LYS:HG3	2.10	0.50
1:A:1512:ASN:HA	1:A:1515:ARG:HE	1.76	0.50
1:A:2415:TRP:CD1	1:A:2417:SER:HG	2.30	0.50
1:A:2751:THR:HG22	1:A:2757:GLN:HG3	1.92	0.50
1:A:4473:TRP:HA	1:A:4476:LEU:HB2	1.93	0.50
1:A:4247:ASN:ND2	1:A:4282:GLN:OE1	2.36	0.50
1:A:2036:LEU:HD21	1:A:2088:PRO:HG3	1.93	0.50
1:A:2641:VAL:HG12	1:A:2883:ASP:HB3	1.93	0.50
1:A:3606:ASP:O	1:A:3610:ARG:HG3	2.12	0.50
1:A:1615:LEU:HD22	1:A:1619:PHE:HE2	1.77	0.49
1:A:4477:LEU:HD11	1:A:4517:LEU:HD12	1.93	0.49
1:A:2093:LYS:HE2	1:A:4299:ASN:HB2	1.95	0.49
1:A:3768:ASP:HB3	1:A:3771:ALA:HB2	1.94	0.49
1:A:2616:SER:HB3	1:A:2627:TRP:CE2	2.47	0.49
1:A:3598:PHE:HZ	1:A:3660:GLU:HB3	1.78	0.49
1:A:1538:TRP:HB2	1:A:1591:TRP:CZ2	2.47	0.49
1:A:2283:THR:HA	1:A:2286:TRP:NE1	2.27	0.49
1:A:4331:TRP:CD1	1:A:4366:PRO:HD3	2.48	0.49
1:A:2647:VAL:HG21	1:A:2686:SER:HB3	1.95	0.49
1:A:1513:ILE:O	1:A:1517:VAL:HG23	2.13	0.48
1:A:4531:THR:O	1:A:4534:LEU:N	2.46	0.48
1:A:4537:LEU:HD11	1:A:4550:TRP:CZ3	2.48	0.48
1:A:4487:THR:OG1	1:A:4488:THR:N	2.45	0.48
1:A:3193:ASP:O	1:A:3275:ARG:NH1	2.40	0.48
1:A:3251:ARG:NH2	1:A:3604:PHE:O	2.40	0.48
1:A:3241:ALA:HB2	1:A:3613:LEU:HD21	1.95	0.48
1:A:1585:GLU:O	1:A:1589:ASN:ND2	2.46	0.48
1:A:2446:GLN:HA	1:A:2449:ARG:HH11	1.79	0.48
1:A:1928:HIS:CD2	1:A:1933:THR:HG22	2.49	0.48
1:A:2929:LYS:HA	1:A:2932:GLU:HG2	1.95	0.48
1:A:2327:TRP:NE1	1:A:2329:ASP:OD1	2.44	0.48
1:A:3189:THR:O	1:A:3224:ARG:NH1	2.46	0.47
1:A:2441:PRO:HA	1:A:2444:LYS:HD2	1.96	0.47
1:A:1982:GLU:HG3	2:A:5001:ADP:H2'	1.96	0.47
1:A:3048:SER:OG	1:A:3080:GLU:OE1	2.28	0.47
1:A:3004:VAL:HG11	1:A:3012:ALA:HB2	1.97	0.47
1:A:3188:PHE:HB3	1:A:3264:ILE:HG21	1.96	0.47
1:A:4466:LEU:O	1:A:4470:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2931:ASP:OD1	1:A:2948:ARG:NH1	2.45	0.47
1:A:3776:ASP:O	1:A:3780:ARG:HG3	2.15	0.47
1:A:4631:SER:O	1:A:4632:GLU:HB2	2.15	0.47
1:A:2640:LYS:HB3	1:A:2646:VAL:HG21	1.97	0.47
1:A:1782:ALA:HB1	1:A:1921:VAL:HG22	1.97	0.46
1:A:3557:VAL:O	1:A:3561:ILE:HG23	2.15	0.46
1:A:4195:GLN:O	1:A:4199:GLN:NE2	2.45	0.46
1:A:4249:LEU:O	1:A:4253:ILE:HG13	2.16	0.46
1:A:4534:LEU:O	1:A:4538:THR:HG23	2.16	0.46
1:A:2163:LYS:HB2	1:A:2194:VAL:HG11	1.98	0.46
1:A:2764:ARG:CZ	1:A:2806:ARG:HD3	2.45	0.46
1:A:1527:LEU:HD22	1:A:1575:MET:HG2	1.98	0.46
1:A:3000:ARG:O	1:A:3003:ARG:HG2	2.15	0.46
1:A:3062:ALA:HB3	1:A:3137:VAL:HG22	1.97	0.46
1:A:3746:LEU:HA	1:A:3756:PHE:H	1.80	0.46
1:A:4344:GLY:O	1:A:4353:MET:HE1	2.15	0.46
1:A:4429:ASP:HB3	1:A:4433:MET:HE2	1.96	0.46
1:A:3231:LEU:HG	1:A:3263:PHE:CE2	2.50	0.46
1:A:3746:LEU:HA	1:A:3755:ASP:HA	1.98	0.46
1:A:4198:VAL:O	1:A:4202:LYS:HG2	2.15	0.46
1:A:1820:GLN:HB3	1:A:1912:TYR:CD1	2.50	0.46
1:A:2337:ARG:HH12	1:A:2383:GLU:CD	2.23	0.46
1:A:3134:THR:O	1:A:3138:ARG:HB2	2.16	0.46
1:A:4491:ILE:HD13	1:A:4496:PHE:HE2	1.81	0.46
1:A:4147:ASP:OD1	1:A:4157:TYR:OH	2.23	0.46
1:A:2361:PRO:HA	1:A:2364:VAL:HG22	1.98	0.45
1:A:4030:PHE:HD1	1:A:4033:LEU:HD22	1.81	0.45
1:A:4387:THR:O	1:A:4391:HIS:ND1	2.48	0.45
1:A:1817:LEU:HD11	1:A:1936:TYR:CZ	2.52	0.45
1:A:3570:GLU:HB2	1:A:3855:LEU:HD11	1.98	0.45
1:A:1523:GLY:O	1:A:1527:LEU:HG	2.15	0.45
1:A:1985:LYS:HD2	1:A:1997:VAL:HG21	1.96	0.45
1:A:2949:PRO:HG3	1:A:2965:ARG:NE	2.32	0.45
1:A:3661:ASN:ND2	1:A:3785:ASN:O	2.49	0.45
1:A:3815:ASP:O	1:A:3819:ILE:HG12	2.17	0.45
1:A:4055:GLU:HG3	1:A:4093:ARG:CZ	2.47	0.45
1:A:3823:PHE:HB3	1:A:3865:ILE:HD11	1.97	0.45
1:A:2447:GLN:O	1:A:2451:GLU:HG2	2.17	0.45
1:A:2525:ILE:HB	1:A:2815:LEU:HD12	1.98	0.45
1:A:2623:ASN:OD1	1:A:2624:TRP:N	2.50	0.45
1:A:2745:GLU:HB3	1:A:2748:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1423:ILE:HD12	1:A:1426:LYS:HE3	1.97	0.45
1:A:1559:ASP:OD1	1:A:1559:ASP:N	2.49	0.45
1:A:3568:ASN:O	1:A:3571:ARG:HG3	2.17	0.45
1:A:2721:LYS:HE3	1:A:2721:LYS:HB2	1.85	0.45
1:A:3602:ILE:HG23	1:A:3610:ARG:HG2	1.98	0.45
1:A:4132:LEU:HD12	1:A:4132:LEU:H	1.82	0.45
1:A:1594:ARG:HE	1:A:1660:LEU:HD23	1.81	0.45
1:A:3558:ASP:O	1:A:3561:ILE:HG12	2.17	0.45
1:A:2764:ARG:CD	1:A:2806:ARG:HG2	2.47	0.44
1:A:2951:LEU:HD22	1:A:2999:LEU:HD12	1.99	0.44
1:A:1538:TRP:HB2	1:A:1591:TRP:HZ2	1.82	0.44
1:A:2579:TRP:HZ2	1:A:2655:ARG:HD2	1.82	0.44
1:A:3303:GLN:OE1	1:A:3561:ILE:HG22	2.17	0.44
1:A:3555:ASN:OD1	1:A:3556:LYS:N	2.49	0.44
1:A:4018:LYS:HA	1:A:4021:ILE:HG12	2.00	0.44
1:A:1982:GLU:HG2	2:A:5001:ADP:O1A	2.17	0.44
1:A:1519:THR:HG21	1:A:3741:LYS:HE3	2.00	0.44
1:A:3960:LEU:O	1:A:3964:LYS:HG3	2.18	0.44
1:A:1430:SER:O	1:A:1434:THR:HG23	2.18	0.44
1:A:1521:ALA:O	1:A:1525:ILE:HG12	2.17	0.44
1:A:2877:ARG:NH2	2:A:5004:ADP:O3B	2.50	0.44
1:A:3582:ASN:OD1	1:A:3583:THR:N	2.50	0.44
1:A:1468:ILE:HD11	1:A:1503:TRP:HE1	1.83	0.44
1:A:2133:LYS:NZ	1:A:2137:GLU:OE2	2.33	0.44
1:A:2705:THR:HB	1:A:2749:PRO:HG3	2.00	0.44
1:A:1883:VAL:HG11	1:A:2111:VAL:HG22	2.00	0.44
1:A:2200:ASN:HA	1:A:2204:ILE:HG12	1.99	0.44
1:A:2247:ARG:HH12	1:A:2287:GLU:HB3	1.82	0.44
1:A:1548:TYR:HB2	1:A:1554:LEU:HD13	1.99	0.44
1:A:1797:VAL:HG23	1:A:1854:MET:HE1	1.99	0.44
1:A:2339:ILE:HA	1:A:2346:GLU:HG3	2.00	0.44
1:A:4146:VAL:HG21	1:A:4186:LEU:HD11	1.99	0.44
1:A:2961:GLN:HB2	1:A:2962:PRO:HD2	1.99	0.43
1:A:3735:ASN:OD1	1:A:3780:ARG:NH1	2.51	0.43
1:A:3903:LEU:HD23	1:A:4433:MET:SD	2.58	0.43
1:A:1486:LYS:HD2	1:A:1486:LYS:N	2.33	0.43
1:A:2719:GLU:OE2	1:A:2731:ARG:NH2	2.52	0.43
1:A:2890:ILE:HA	1:A:2893:MET:HE2	1.99	0.43
1:A:3640:LYS:HB3	1:A:3640:LYS:HE3	1.87	0.43
1:A:3893:CYS:HB3	1:A:3916:PHE:HZ	1.83	0.43
1:A:4715:ASN:O	1:A:4719:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1918:GLN:HB3	1:A:1924:LYS:HG2	2.00	0.43
1:A:4162:ILE:HB	1:A:4168:PHE:HE1	1.83	0.43
1:A:2349:LYS:O	1:A:2390:ASN:ND2	2.46	0.43
1:A:2976:LEU:HD11	1:A:2990:LEU:HD21	2.00	0.43
1:A:2669:PRO:HA	1:A:2788:PHE:O	2.18	0.43
1:A:2804:THR:HG23	1:A:2807:PHE:H	1.84	0.43
1:A:3061:ARG:O	1:A:3065:LYS:HB2	2.19	0.43
1:A:3869:VAL:HA	1:A:3872:THR:HG22	1.98	0.43
1:A:4079:ASN:O	1:A:4083:ILE:HG13	2.19	0.43
1:A:1935:TYR:O	1:A:1993:ARG:NH1	2.41	0.43
1:A:2882:TRP:CZ2	1:A:2909:ALA:HB2	2.53	0.43
1:A:3919:ILE:HD11	1:A:3954:ARG:HG2	1.99	0.43
1:A:3973:ILE:O	1:A:3977:LYS:HG3	2.19	0.43
1:A:2265:ILE:HG22	1:A:2272:VAL:HG22	2.01	0.43
1:A:2046:ILE:HD11	1:A:2059:LEU:HD21	2.01	0.42
1:A:2376:LEU:HD21	1:A:2384:ARG:HD2	2.01	0.42
1:A:3559:ARG:NH1	1:A:3849:ASP:OD1	2.51	0.42
1:A:3815:ASP:OD1	1:A:3818:LYS:HE3	2.19	0.42
1:A:3832:LYS:HD2	1:A:3835:LEU:HD11	2.01	0.42
1:A:4535:ARG:HA	1:A:4538:THR:HG23	2.01	0.42
1:A:4614:TRP:NE1	1:A:4619:LEU:HD21	2.34	0.42
1:A:1694:PHE:CE2	1:A:1696:ARG:HB2	2.55	0.42
1:A:3712:LEU:HD11	1:A:3747:ILE:HG21	2.02	0.42
1:A:4011:LEU:HD11	1:A:4045:LYS:HA	2.01	0.42
1:A:2056:GLU:OE1	1:A:2064:ASN:ND2	2.52	0.42
1:A:4283:GLU:OE1	1:A:4286:ARG:NH1	2.46	0.42
1:A:1493:ILE:HG13	1:A:1493:ILE:O	2.18	0.42
1:A:2938:PHE:O	1:A:2941:VAL:HG12	2.20	0.42
1:A:2952:TYR:CE2	1:A:2962:PRO:HD3	2.55	0.42
1:A:3299:VAL:O	1:A:3303:GLN:HG2	2.20	0.42
1:A:1791:HIS:O	1:A:1795:VAL:HG23	2.20	0.42
1:A:2239:LYS:O	1:A:2243:ILE:HG12	2.20	0.42
1:A:2275:VAL:HG13	1:A:2397:VAL:HG23	2.01	0.42
1:A:3043:ASN:HA	1:A:3728:PRO:HG2	2.02	0.42
1:A:3059:LEU:HD21	1:A:3090:LEU:HD11	2.02	0.42
1:A:4313:TRP:HB3	1:A:4330:PRO:HG2	2.00	0.42
1:A:4336:THR:O	1:A:4340:SER:OG	2.27	0.42
1:A:3789:THR:H	1:A:3792:SER:HB3	1.85	0.42
1:A:1586:GLU:HA	1:A:1589:ASN:HD21	1.85	0.41
1:A:2973:LYS:HG3	1:A:2990:LEU:HD12	2.02	0.41
1:A:1431:LEU:HD21	1:A:1462:LEU:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3666:LYS:HG3	1:A:3667:ARG:HG2	2.01	0.41
1:A:4193:ALA:O	1:A:4197:LEU:HG	2.20	0.41
1:A:3100:PHE:CG	1:A:3108:LEU:HD22	2.55	0.41
1:A:3788:VAL:HG21	1:A:3913:LEU:HD22	2.02	0.41
1:A:1879:ILE:O	1:A:1883:VAL:HG23	2.20	0.41
1:A:4142:ALA:HB3	1:A:4218:THR:HG23	2.01	0.41
1:A:1459:LYS:O	1:A:1463:LYS:HG2	2.21	0.41
1:A:1908:TYR:CE2	1:A:1958:LEU:HD22	2.55	0.41
1:A:2113:LEU:O	1:A:2118:PHE:HB2	2.21	0.41
1:A:4076:ILE:HG23	1:A:4101:PHE:HE1	1.86	0.41
1:A:2145:TYR:OH	1:A:2211:ASP:OD2	2.31	0.41
1:A:2512:VAL:HG13	1:A:2577:LEU:HD21	2.03	0.41
1:A:2864:PHE:HB3	1:A:2872:TYR:CD2	2.55	0.41
1:A:3671:TYR:HE1	1:A:3761:MET:HA	1.85	0.41
1:A:4713:LYS:HD2	1:A:4717:TYR:CE1	2.56	0.41
1:A:1519:THR:HA	1:A:1522:GLN:OE1	2.21	0.41
1:A:2889:ALA:HB3	1:A:2904:LEU:HD21	2.03	0.41
1:A:3699:PHE:HE2	1:A:3723:VAL:HG13	1.86	0.41
1:A:4024:ARG:HD3	1:A:4034:VAL:HG21	2.02	0.41
1:A:4516:ASP:OD2	1:A:4533:TYR:OH	2.28	0.41
1:A:4690:VAL:HG22	1:A:4723:ILE:HB	2.03	0.41
1:A:2417:SER:O	1:A:2420:ILE:HG12	2.21	0.41
1:A:2893:MET:HE3	1:A:2896:CYS:HB2	2.03	0.41
1:A:1532:LYS:HD2	1:A:1535:ARG:NH1	2.36	0.40
1:A:2641:VAL:HG21	1:A:2887:LEU:HD13	2.02	0.40
1:A:4183:THR:OG1	1:A:4184:TRP:N	2.53	0.40
1:A:4519:ASN:HA	1:A:4522:GLU:HG2	2.02	0.40
1:A:4627:GLY:N	1:A:4666:ILE:O	2.48	0.40
1:A:1400:VAL:HG23	1:A:1402:VAL:H	1.86	0.40
1:A:1642:GLU:CD	1:A:1671:ARG:HH12	2.29	0.40
1:A:2112:MET:C	1:A:2114:TYR:H	2.29	0.40
1:A:4228:ASN:O	1:A:4232:MET:HG2	2.21	0.40
1:A:4487:THR:H	1:A:4490:ASN:HD21	1.69	0.40
1:A:2101:ILE:HG13	1:A:4348:ASP:HB2	2.03	0.40
1:A:4282:GLN:O	1:A:4285:LEU:HB2	2.20	0.40
1:A:2703:SER:HA	1:A:2749:PRO:HA	2.03	0.40
1:A:2984:LEU:HG	1:A:2986:VAL:HG22	2.04	0.40
1:A:3006:ARG:HE	1:A:3006:ARG:HB2	1.72	0.40
1:A:4162:ILE:HB	1:A:4168:PHE:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3024/3367 (90%)	2963 (98%)	61 (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	2733/3028 (90%)	2733 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1510	ASN
1	A	1627	GLN
1	A	1719	GLN
1	A	1731	ASN
1	A	1790	GLN
1	A	1813	GLN
1	A	1844	GLN
1	A	1891	GLN
1	A	1909	HIS
1	A	2018	GLN
1	A	2047	GLN

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Mol	Chain	Res	Type
1	A	2428	GLN
1	A	2700	ASN
1	A	2907	HIS
1	A	2961	GLN
1	A	3088	ASN
1	A	3282	GLN
1	A	3607	GLN
1	A	3925	ASN
1	A	4073	GLN
1	A	4154	HIS
1	A	4234	ASN
1	A	4240	ASN
1	A	4483	GLN
1	A	4622	HIS
1	A	4638	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 5 ligands modelled in this entry, 1 is 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	5004	-	27,29,29	0.61	0	42,45,45	0.60	0
2	ADP	A	5001	-	27,29,29	0.62	0	42,45,45	0.58	0
3	ATP	A	5002	4	29,33,33	0.68	0	44,52,52	0.61	0
2	ADP	A	5005	-	27,29,29	0.52	0	42,45,45	0.49	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	5004	-	-	1/16/32/32	0/3/3/3
2	ADP	A	5001	-	-	2/16/32/32	0/3/3/3
3	ATP	A	5002	4	-	2/22/38/38	0/3/3/3
2	ADP	A	5005	-	-	1/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5002	ATP	PA-O3A-PB-O1B
2	A	5001	ADP	PA-O3A-PB-O3B
3	A	5002	ATP	PA-O3A-PB-O2B
2	A	5001	ADP	PA-O3A-PB-O2B
2	A	5005	ADP	PA-O3A-PB-O3B
2	A	5004	ADP	O4'-C4'-C5'-O5'

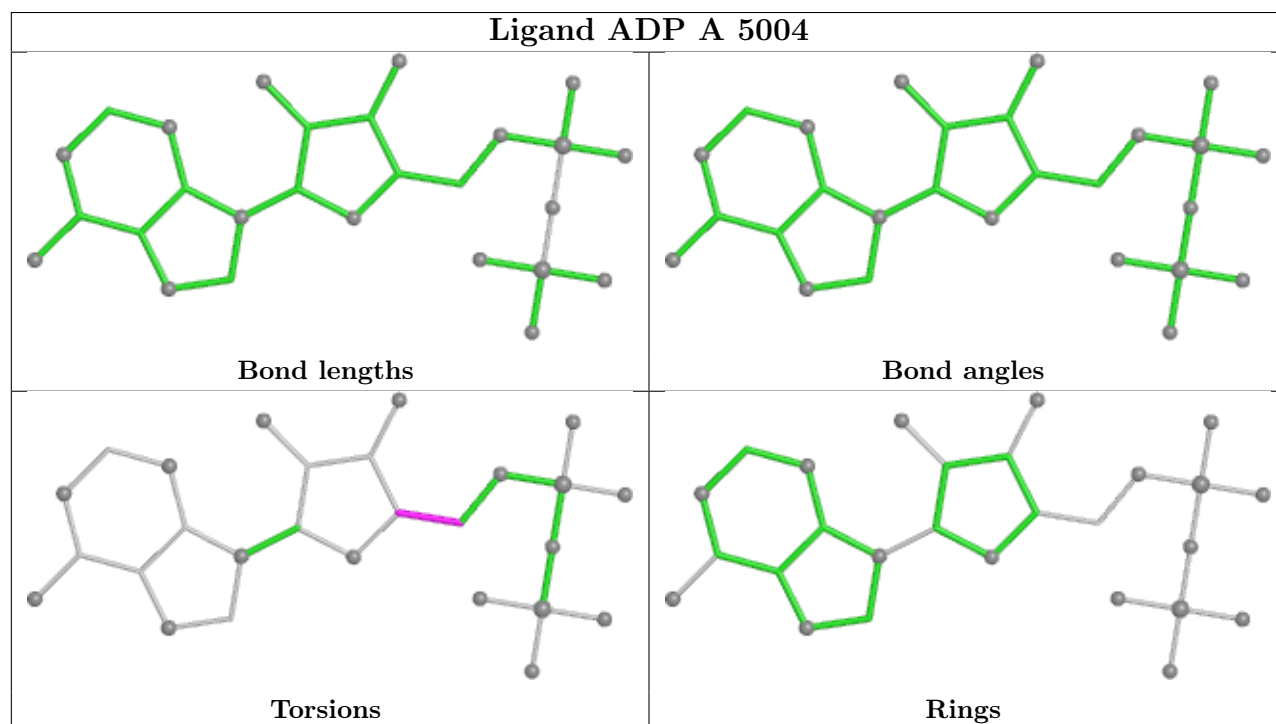
There are no ring outliers.

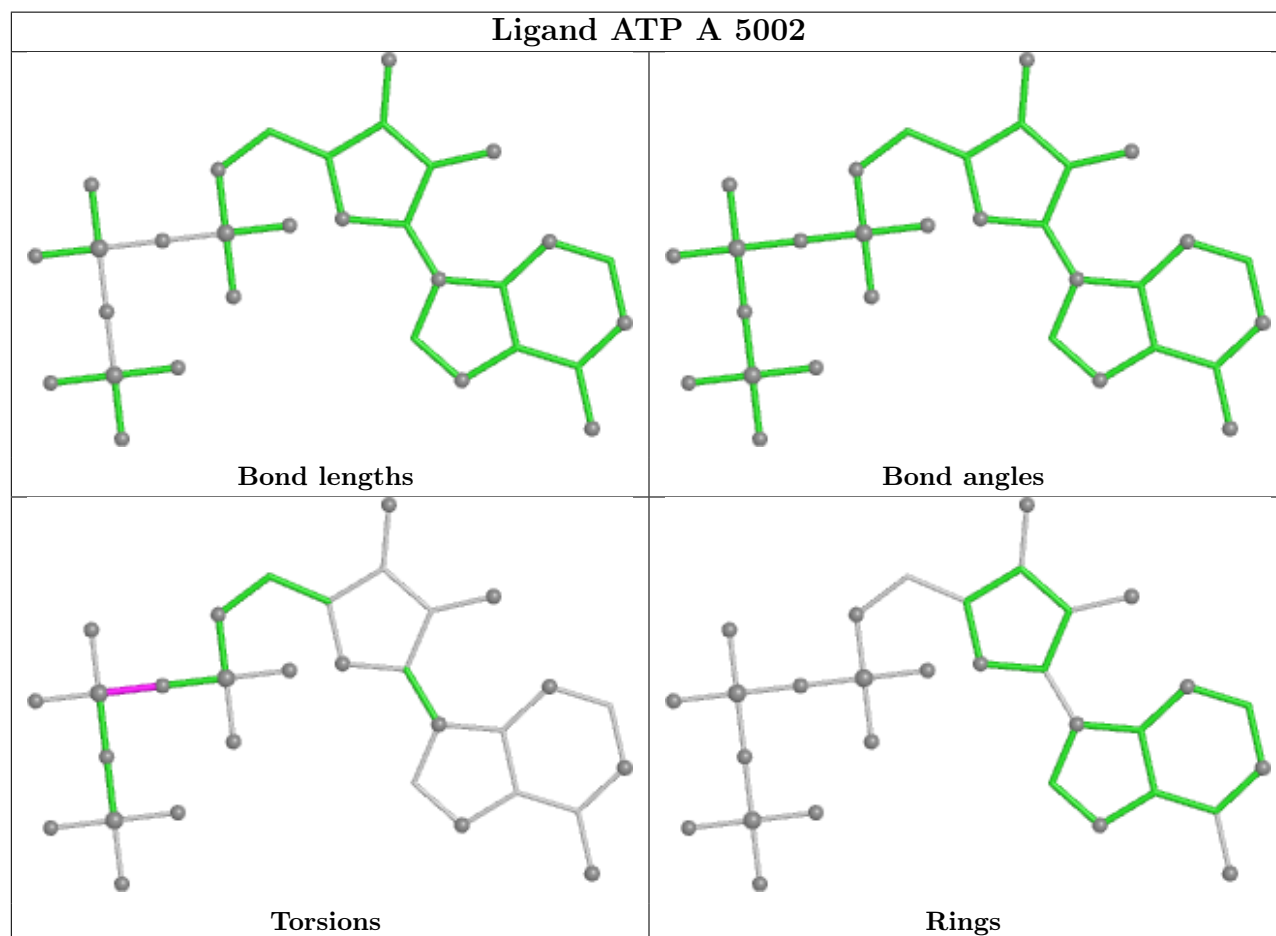
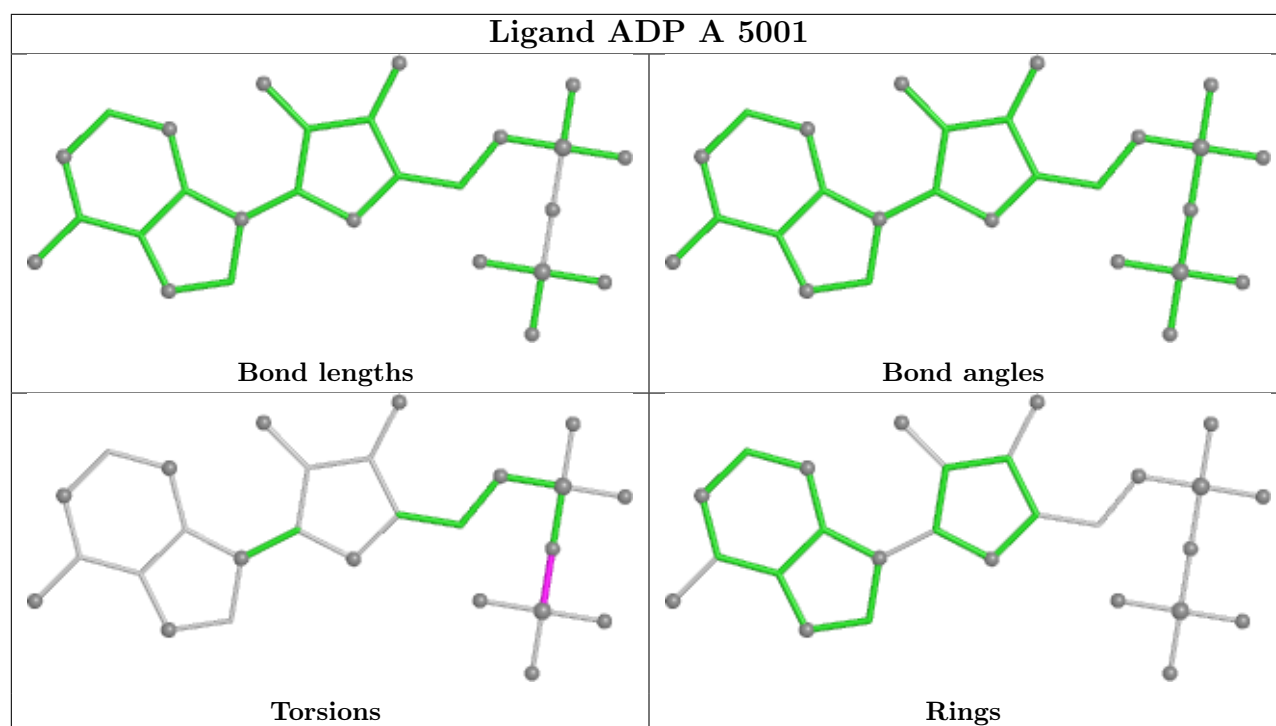
3 monomers are involved in 4 short contacts:

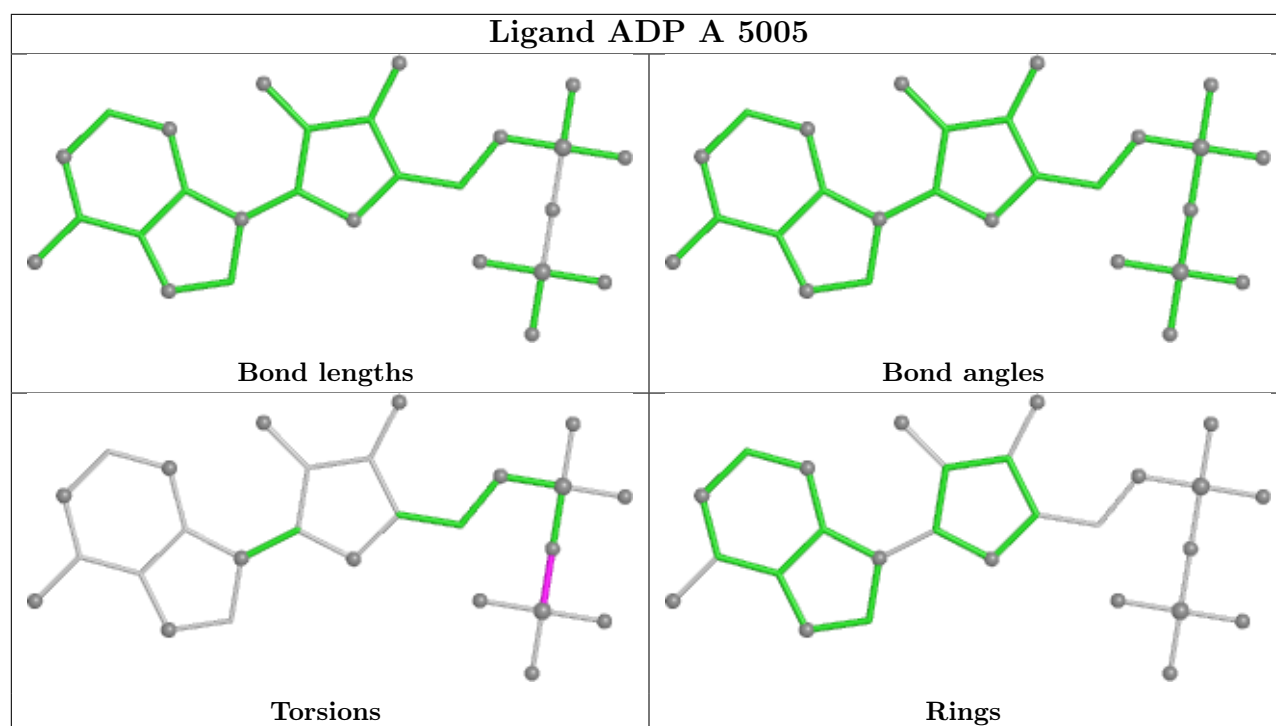
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5004	ADP	1	0
2	A	5001	ADP	2	0
2	A	5005	ADP	1	0

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.

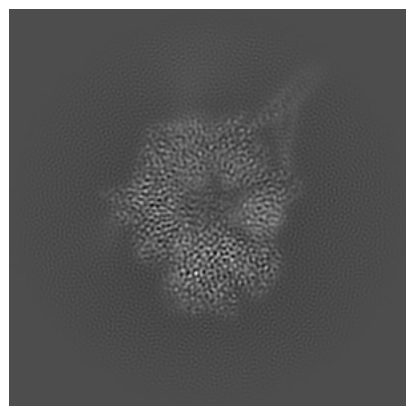
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-81335. These allow visual inspection of the internal detail of the map and identification of artifacts.

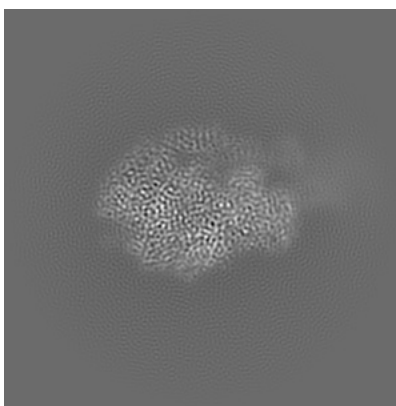
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

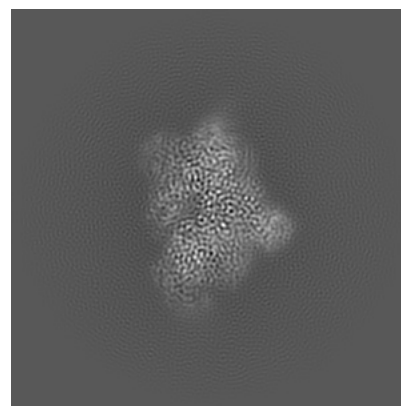
6.1.1 Primary map



X

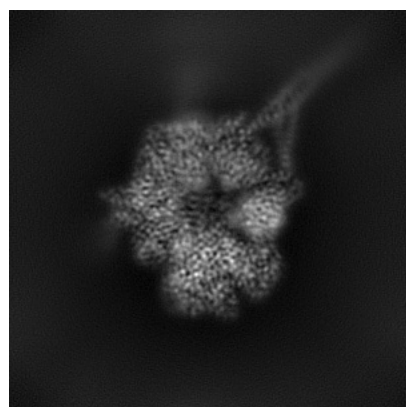


Y

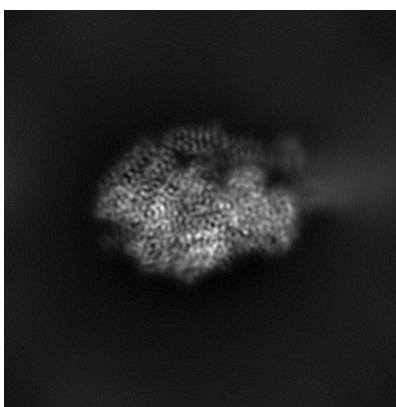


Z

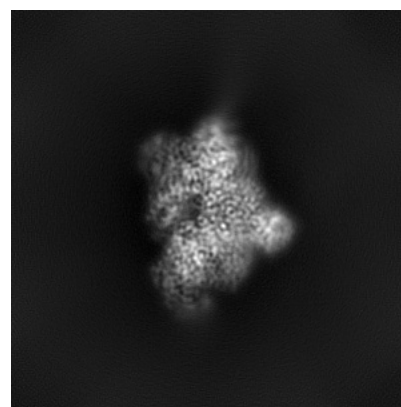
6.1.2 Raw map



X



Y

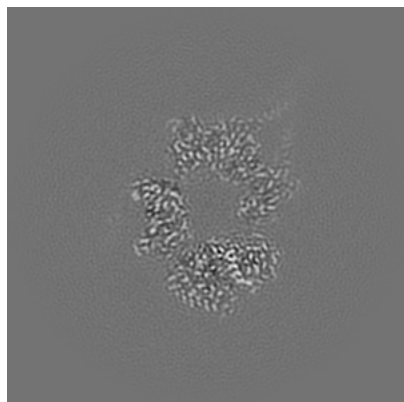


Z

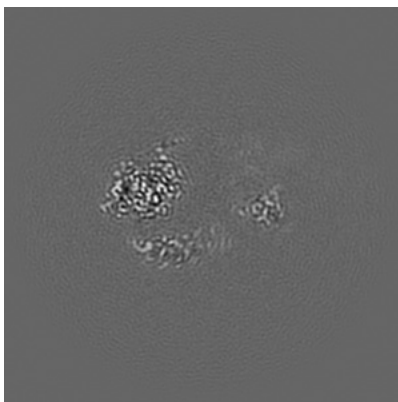
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

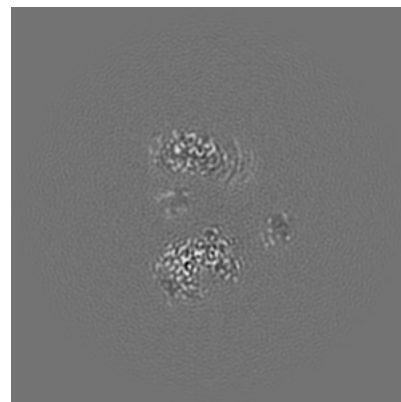
6.2.1 Primary map



X Index: 150

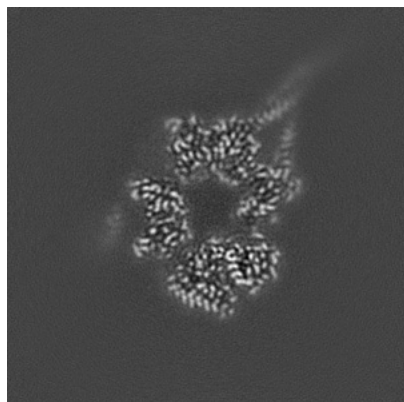


Y Index: 150

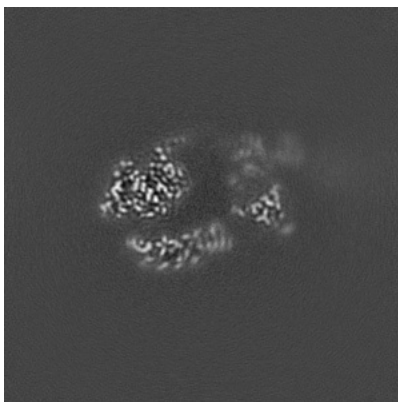


Z Index: 150

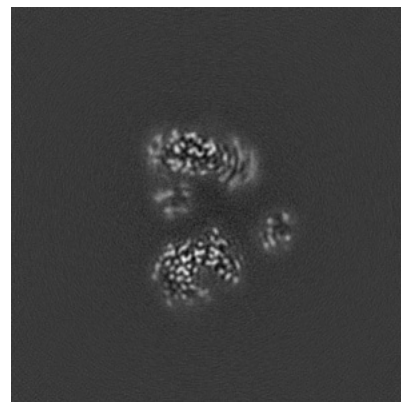
6.2.2 Raw map



X Index: 150



Y Index: 150

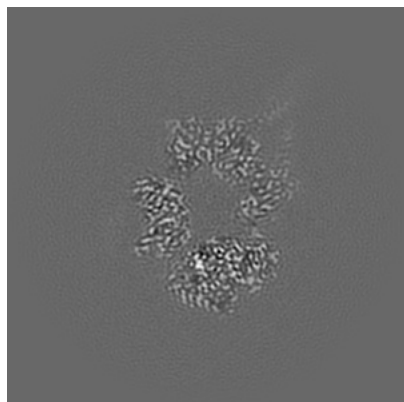


Z Index: 150

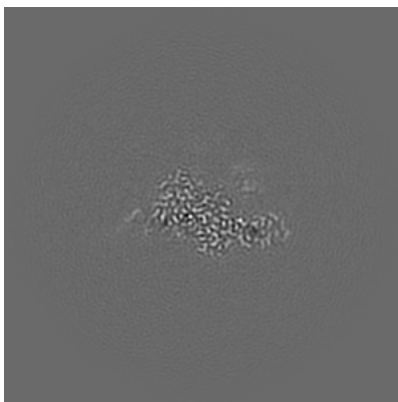
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

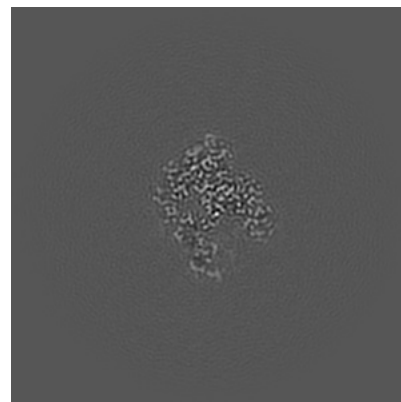
6.3.1 Primary map



X Index: 151

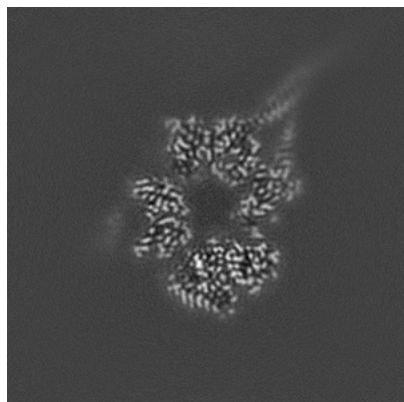


Y Index: 115

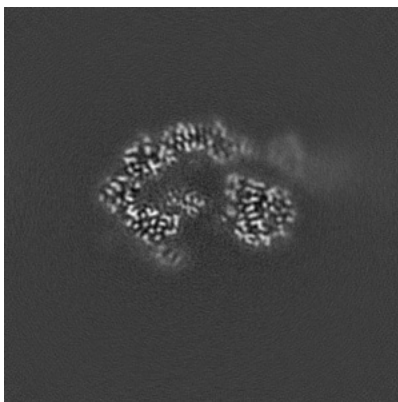


Z Index: 114

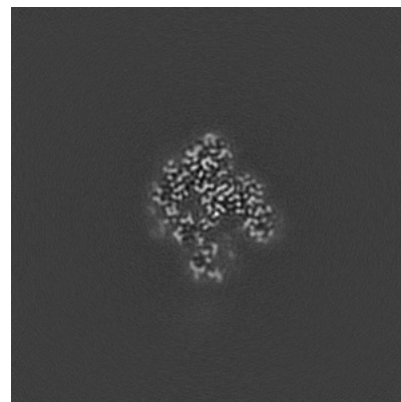
6.3.2 Raw map



X Index: 151



Y Index: 134

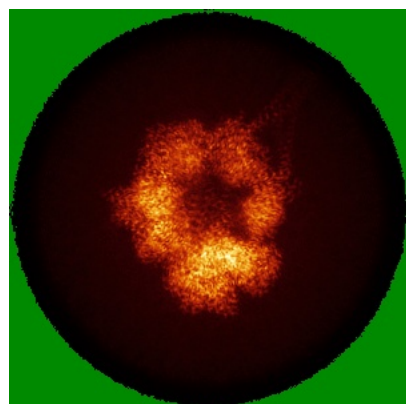


Z Index: 114

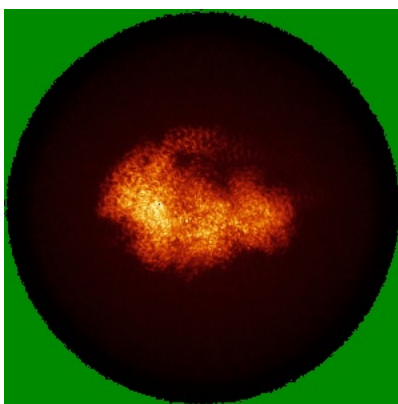
The images above show the largest variance slices of the map in three orthogonal directions.

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

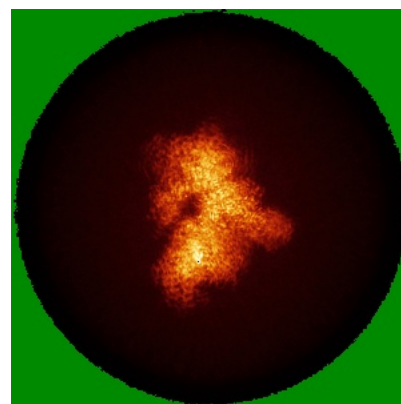
6.4.1 Primary map



X

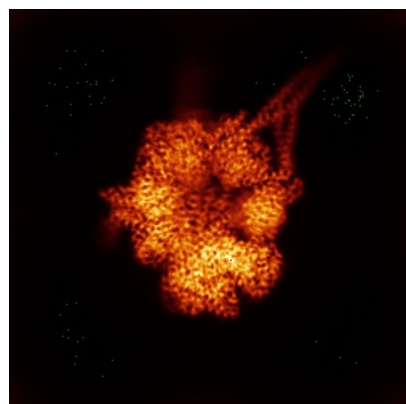


Y

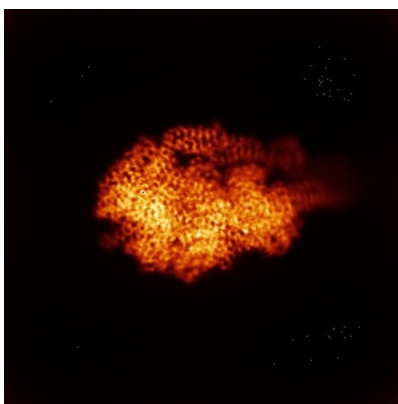


Z

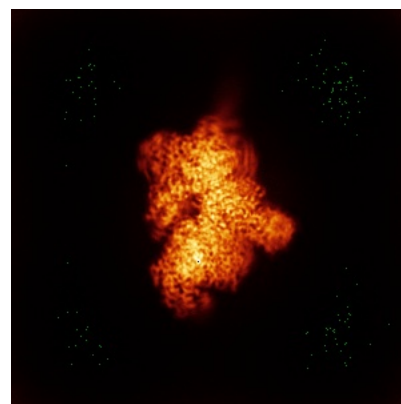
6.4.2 Raw map



X



Y

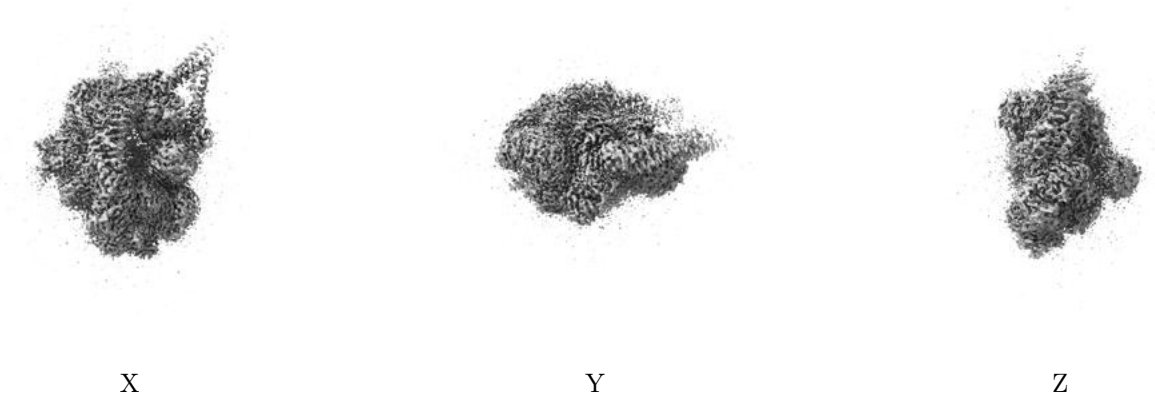


Z

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.

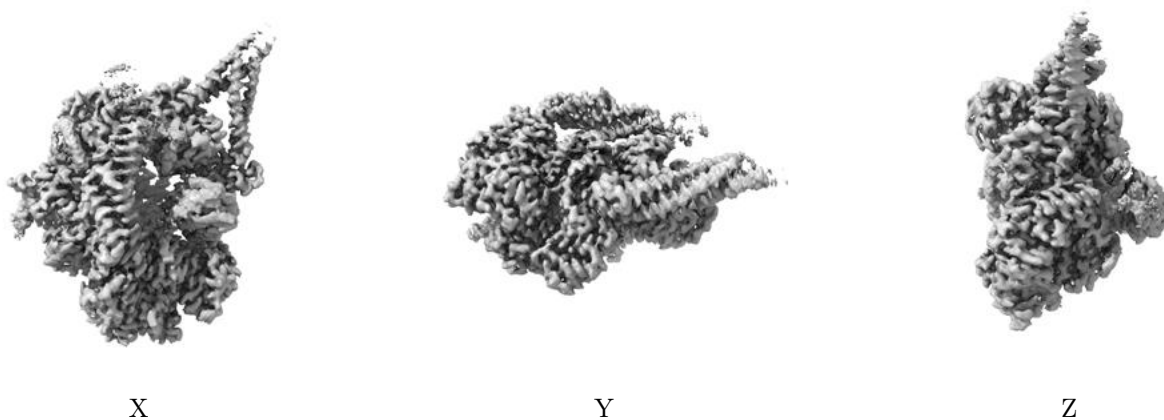
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

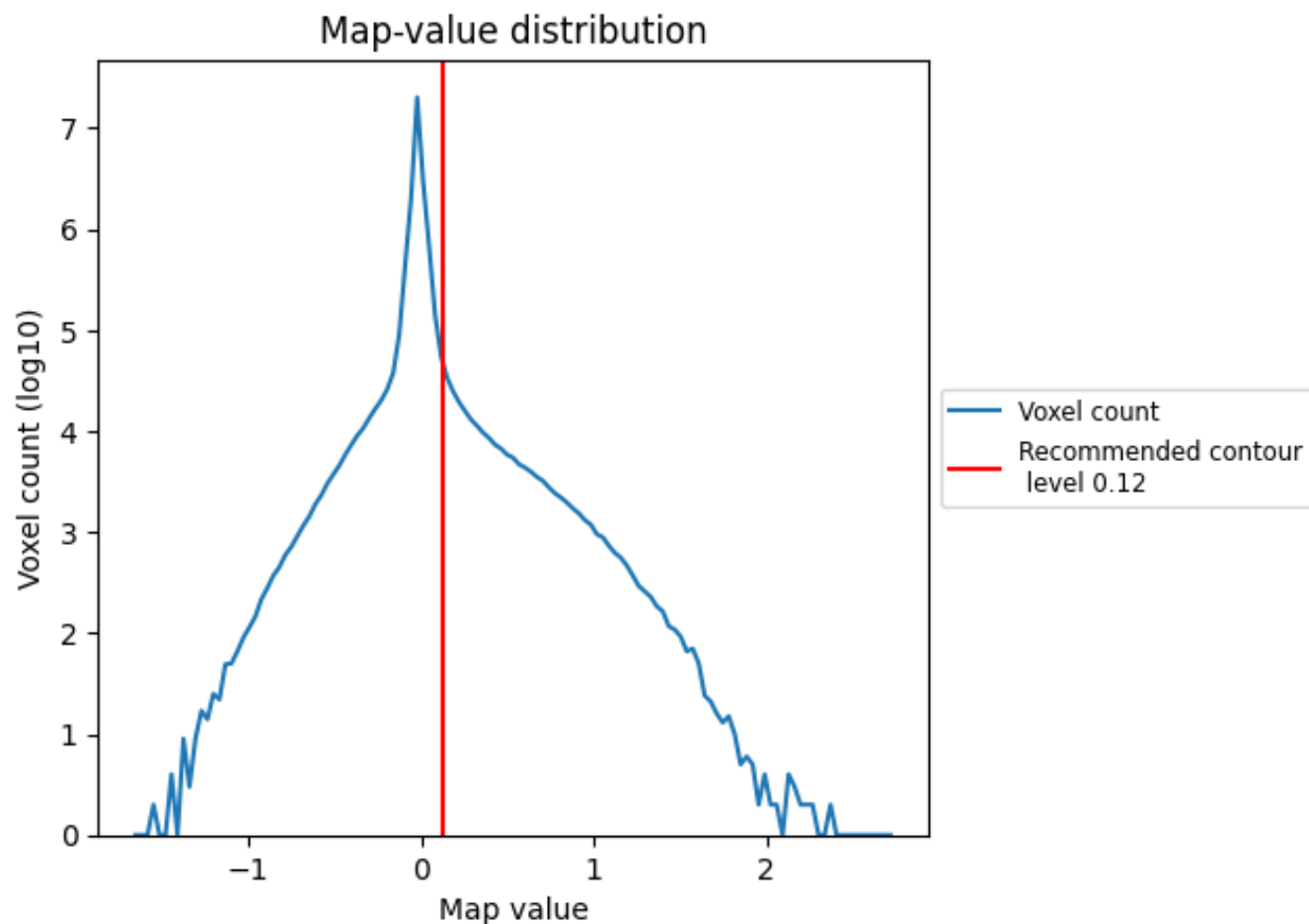
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

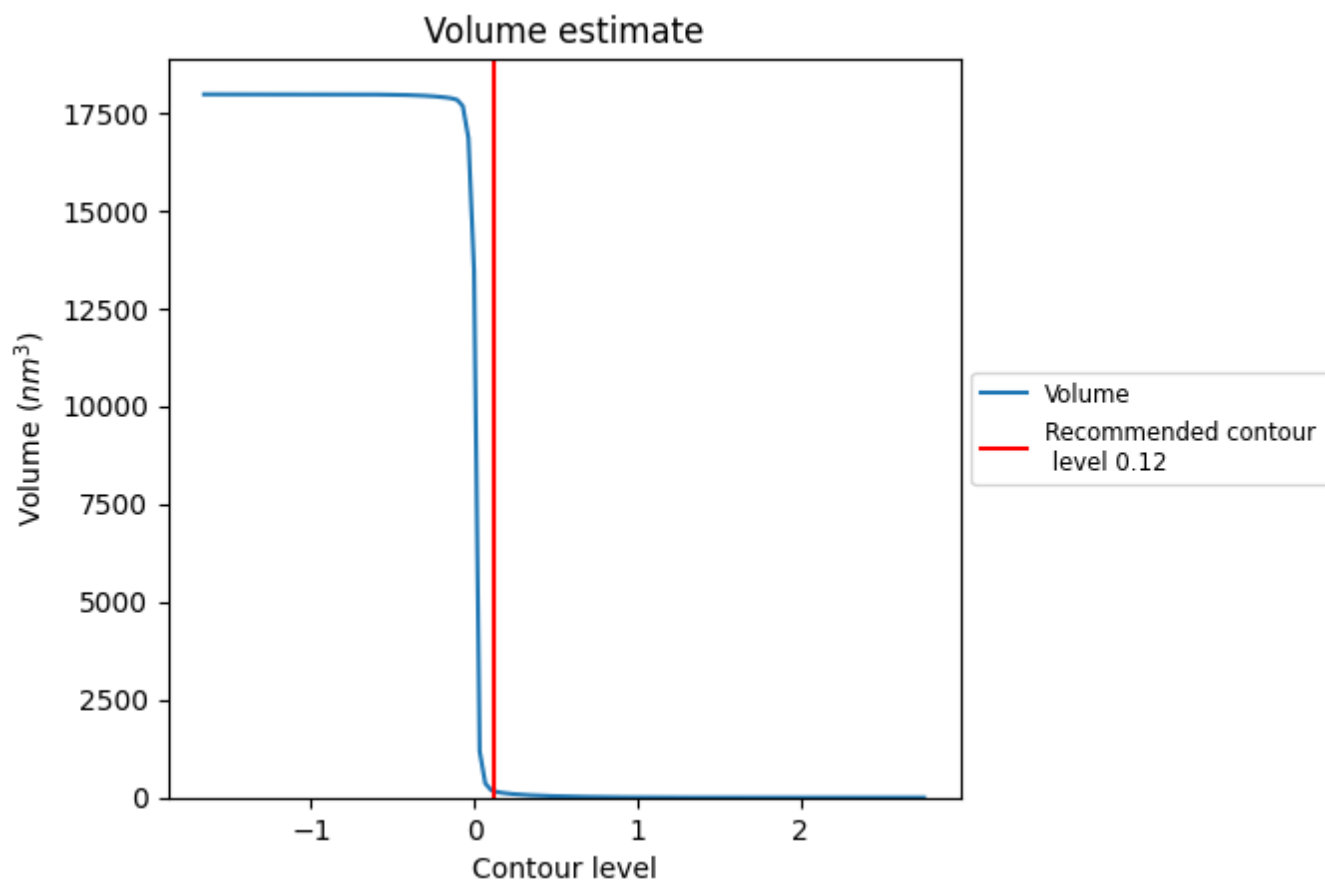
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

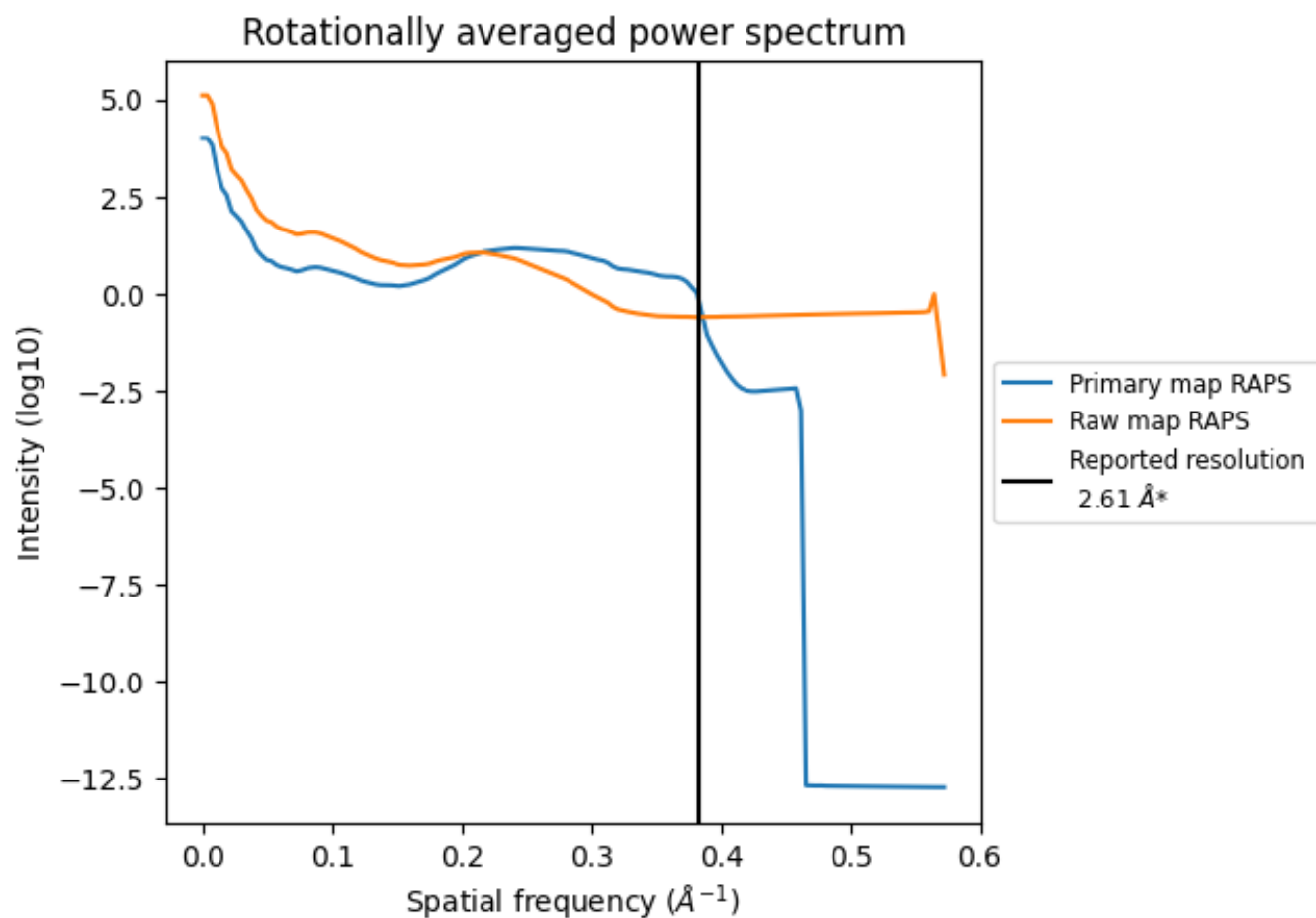
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 170 nm³; this corresponds to an approximate mass of 154 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 ⓘ

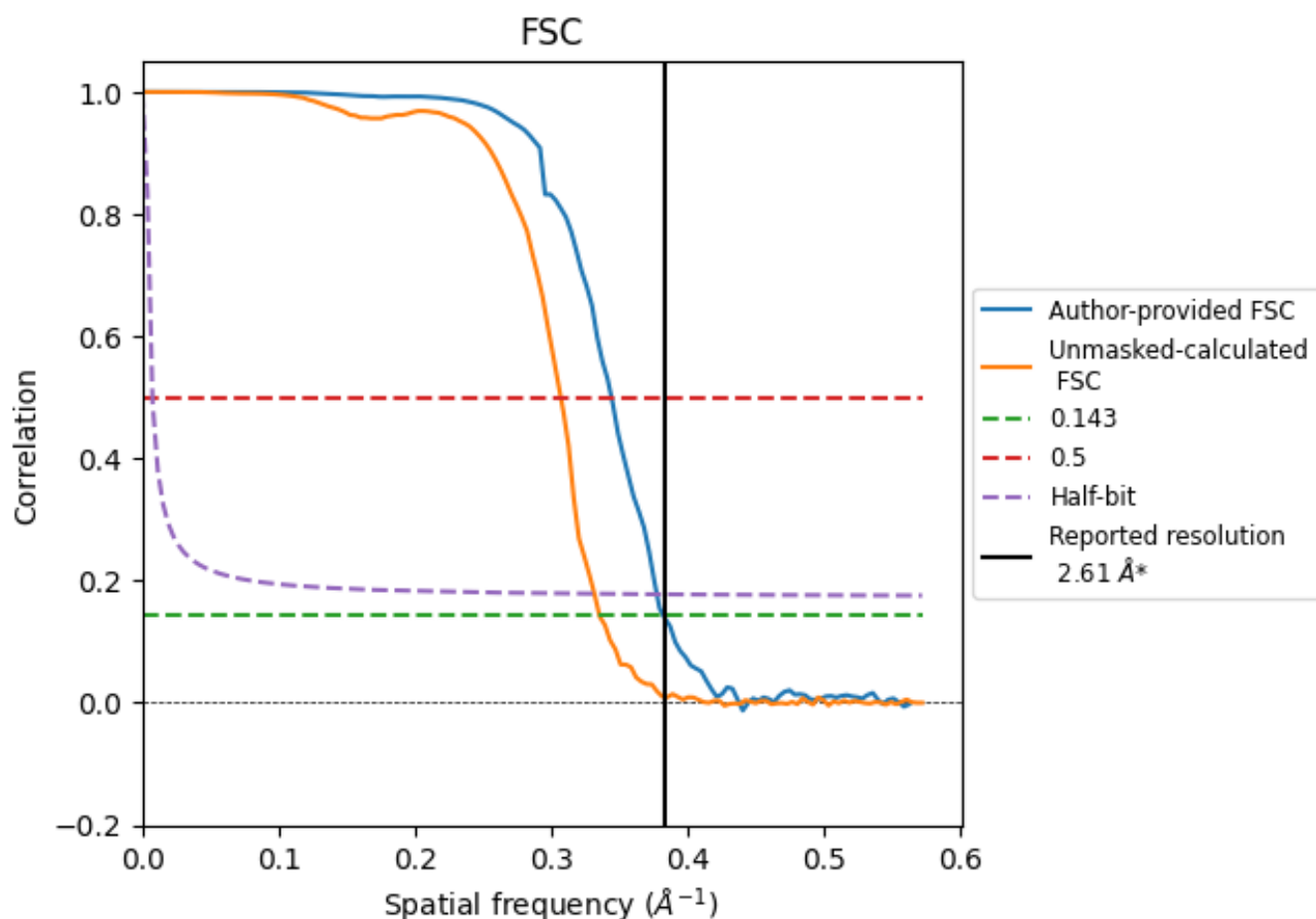


*Reported resolution corresponds to spatial frequency of 0.383 $\text{\AA}^{-1}$

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 0.383 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

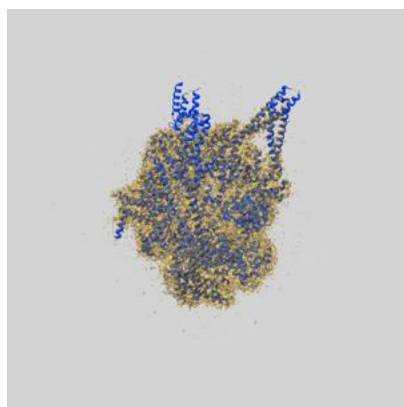
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.61	-	-
Author-provided FSC curve	2.61	2.90	2.65
Unmasked-calculated*	2.98	3.25	3.01

*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 2.98 differs from the reported value 2.61 by more than 10 %

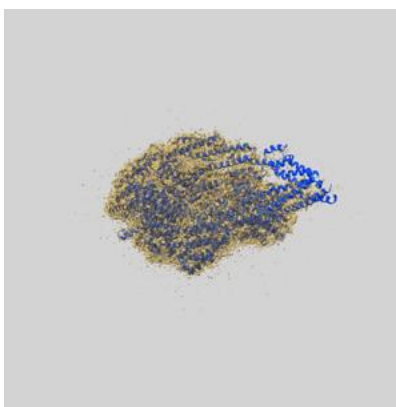
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-81335 and PDB model 27PY. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

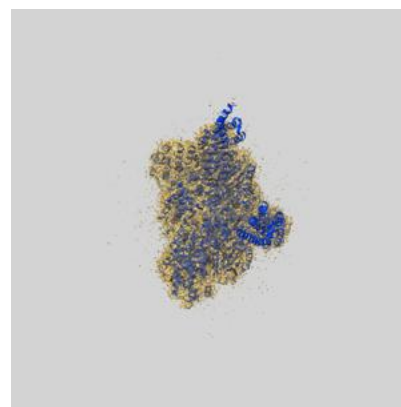
9.1 Map-model overlay [i](#)



X



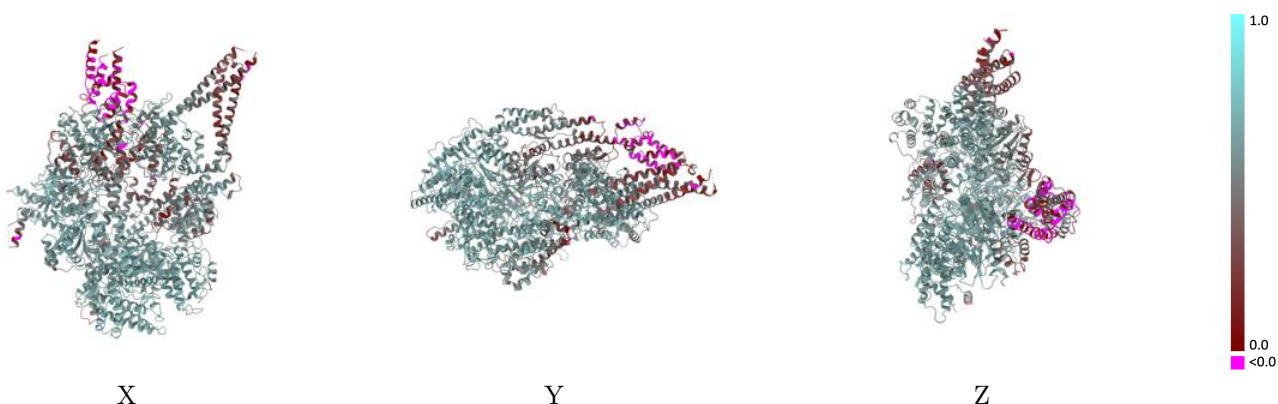
Y



Z

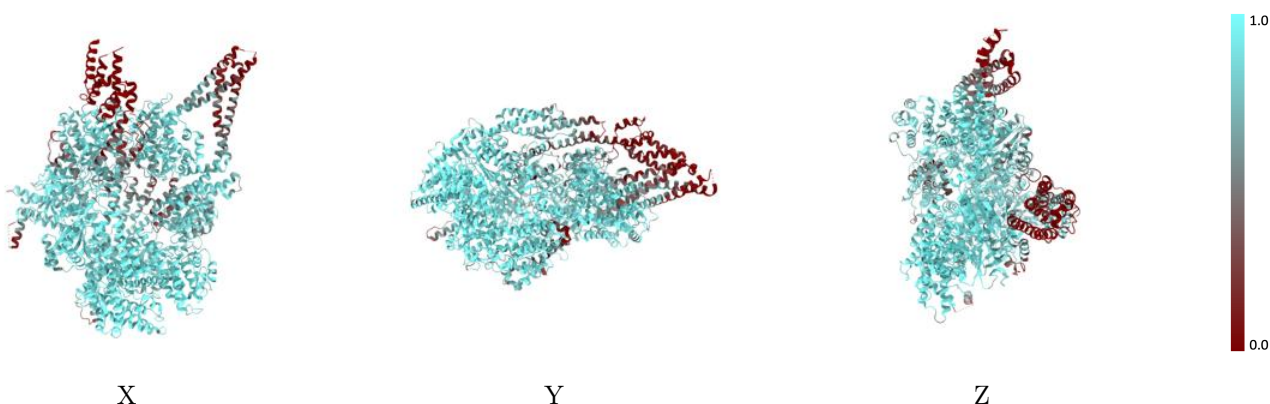
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



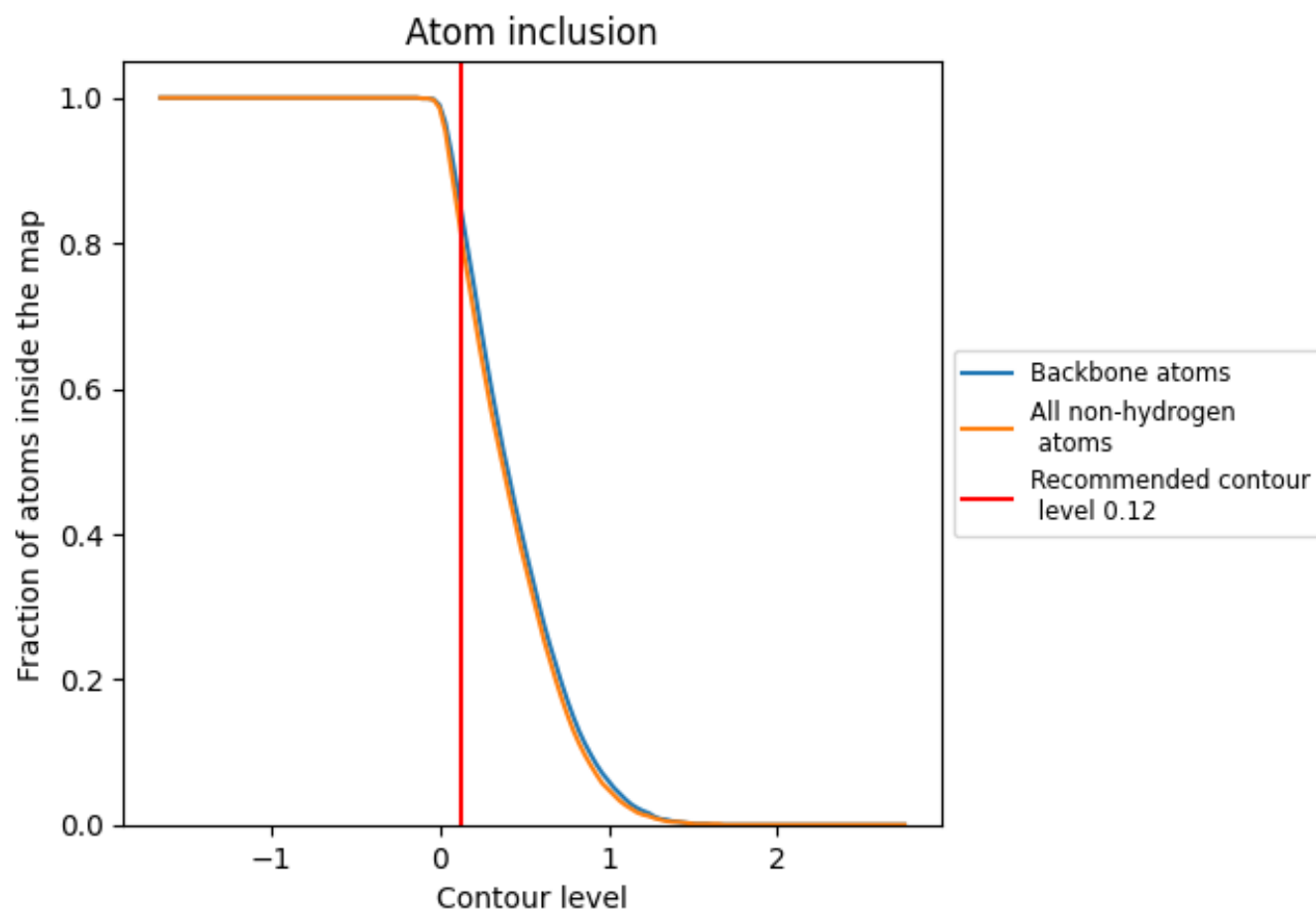
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8220	0.5500
A	0.8220	0.5500

