



Full wwPDB EM Validation Report ⓘ

Aug 17, 2026 – 04:16 PM 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

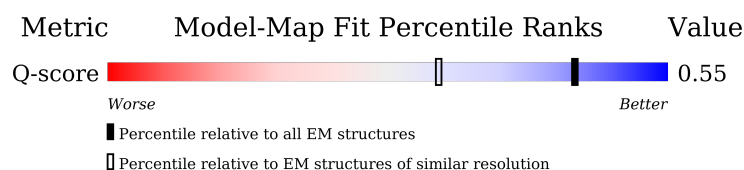
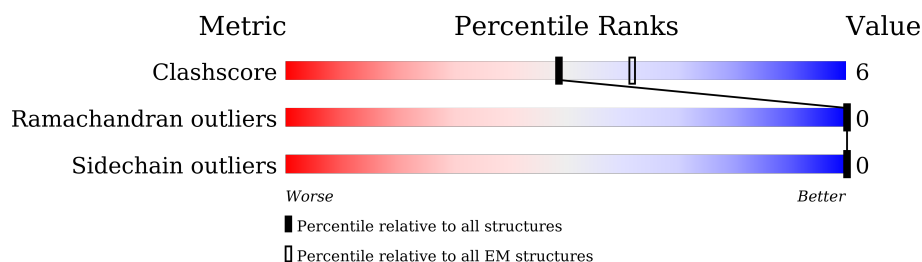
1 Overall quality at a glance

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.

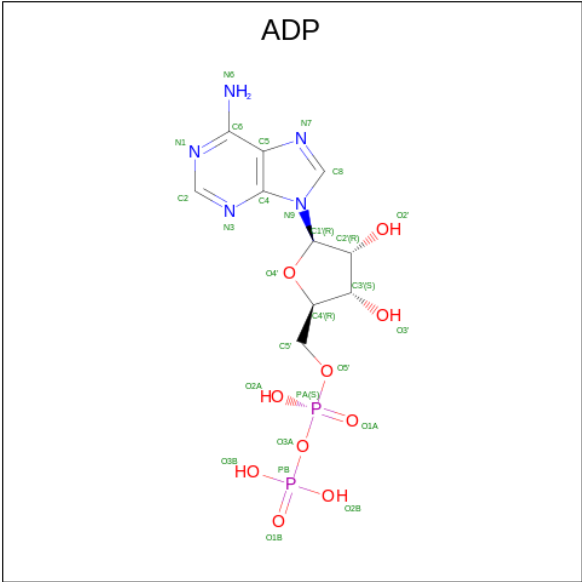
- Molecule 1 is a protein called Dynein heavy chain, cytoplasmic.

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:

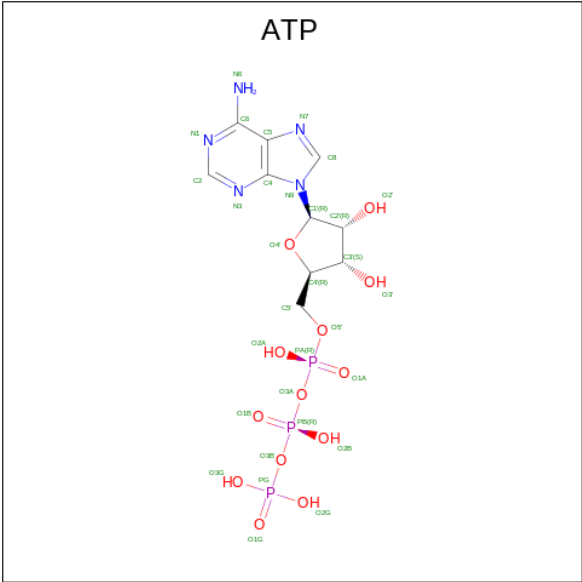
Chain	Residue	Modelled	Actual	Comment	Reference
A	1364	MET	-	initiating methionine	UNP P34036
A	1365	THR	-	expression tag	UNP P34036
A	1366	ARG	-	expression tag	UNP P34036
A	1367	HIS	-	expression tag	UNP P34036
A	1368	HIS	-	expression tag	UNP P34036
A	1369	HIS	-	expression tag	UNP P34036
A	1370	HIS	-	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).

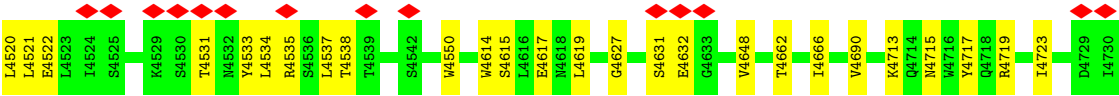


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

- 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	GLY	D3294	H3109	I2950	S2750
Q4195	Q4195	Q4068	A3866	A3771	K3629	GLU	GLY	ILE	ILE	T3295	H3110	L2951	T2751
W4196	W4196	Q4068	A3866	A3771	K3629	TYR	PRO	ALA	ALA	E3296	K3113	Y2952	Q2757
L4197	L4197	I4076	L3867	D3776	L3632	THR	VAL	LEU	VAL	A3297	E3114	Q2961	Q2757
S4435	V4198	I4076	K3868	D3776	L3632	LEU	VAL	GLN	GLN	Q3298	T3115	P2962	R2764
E4437	Q4199	W4079	V3869	R3780	K3640	ILE	TRP	ALA	VAL	V3299	A3116	R2965	F2788
E4438	K4202	I4083	E3870	V3781	E3660	ARG	ALA	ASP	LYS	K3300	Q3117	R2965	F2788
D4439	L4202	E3871	E3871	N3785	N3661	GLU	THR	ILE	ALA	D3301	A3118	K2973	T2804
G4440	N4400	E3872	E3872	V3788	K3666	THR	ALA	ARG	TYR	R2975	N3119	A2974	H2805
E4441	R4093	E3873	E3873	T3789	R3667	GLN	THR	LYS	LYS	L3302	L3120	R2976	R2806
D4442	C3893	C3893	C3893	S3792	R3667	LYS	TYR	ILE	LEU	Q3303	G3121	F2807	F2807
ASP	L3903	L3903	L3903	D3815	R3670	THR	SER	GLU	GLU	S3305	L3121	L2815	L2815
GLN	S3912	S3912	S3912	D3815	Y3671	GLU	ILE	ASN	ALA	D2985	L3123	P2840	P2840
VAL	L3913	L3913	L3913	D3815	D3676	SER	LEU	PHE	PRO	V2986	D3124	R2843	R2843
SER	F3916	F3916	F3916	K3818	A3681	LYS	ASP	ILE	ALA	L2990	S3125	R2843	R2843
LYS	L3917	L3917	L3917	I3819	L3685	V3553	ARG	THR	ILE	L2999	E3128	E2855	E2855
LYS	Q3918	Q3918	Q3918	Q3820	L3685	K3554	LYS	SER	ILE	R3000	L3129	F2864	F2864
GLU	I3919	I3919	I3919	G3821	F3699	N3555	PRO	ILE	ALA	R3003	T3134	R3003	R3003
SER	D3932	D3932	D3932	E3822	L3700	K3556	LEU	ASN	GLN	V3004	S3135	V3004	V3004
SER	R3954	R3954	R3954	F3823	L3712	V3557	GLU	ASP	VAL	F3005	Q3136	F3005	F3005
SER	R3957	R3957	R3957	Q3824	L3712	R3558	VAL	THR	VAL	R3006	V3137	R3006	R3006
SER	R3957	R3957	R3957	V3825	V3723	S3560	GLU	ILE	ILE	A3012	R3138	A3012	A3012
SER	R3957	R3957	R3957	K3826	E3724	I3561	GLN	MET	ALA	V3024	P3162	V3024	V3024
SER	L3960	L3960	L3960	L3830	D3727	A3562	GLU	THR	LYS	M3032	F3188	M3032	M3032
SER	K3964	K3964	K3964	E3831	P3728	L3563	ASN	PRO	LYS	N3043	T3189	N3043	N3043
SER	I3973	I3973	I3973	K3832	N3735	L3564	ALA	ILE	LEU	N3044	D3193	N3044	N3044
SER	K3977	K3977	K3977	L3833	K3740	N3566	ASN	GLU	ASP	N3045	G3213	N3045	N3045
SER	L4011	L4011	L4011	L3834	K3741	L3567	GLU	ILE	ILE	S3048	N3214	S3048	S3048
SER	K4018	K4018	K4018	N3836	G3742	N3568	LYS	THR	LYS	L3058	N3215	L3058	L3058
SER	I4021	I4021	I4021	L3838	G3743	E3570	GLY	GLY	LEU	R3061	R3224	R3061	R3061
SER	R4024	R4024	R4024	S3839	R3744	R3571	ASP	TYR	PRO	A3062	L3231	A3062	A3062
SER	F4030	F4030	F4030	Q3840	I3745	G3572	GLU	LEU	ALA	K3065	I3238	K3065	K3065
SER	K4045	K4045	K4045	L3846	I3747	E3575	VAL	ASP	THR	I3069	A3241	I3069	I3069
SER	D4051	D4051	D4051	L3847	D3755	N3582	THR	PHE	VAL	E3080	R3251	E3080	E3080
SER	Q4052	Q4052	Q4052	D3848	F3756	T3583	LYS	GLY	GLU	N3088	Y3260	N3088	N3088
SER	V4053	V4053	V4053	S3850	S3759	Y3601	SER	VAL	VAL	T3089	I3263	T3089	T3089
SER	G4054	G4054	G4054	V3851	F3760	G3603	ASN	GLU	GLU	L3090	F3264	L3090	L3090
SER	E4055	E4055	E4055	I3852	M3761	F3605	ILE	ALA	CYS	F3100	I3271	F3100	F3100
SER	V4064	V4064	V4064	S3853	L3764	D3606	THR	LEU	LEU	E3101	R3275	E3101	E3101
SER	V4064	V4064	V4064	T3854	F3765	R3610	LYS	MET	GLY	L3108	R3275	L3108	L3108
SER	L3855	L3855	L3855	L3855	T3766	L3613	ARG	ARG	ARG	K3290	K3291	K3290	K3290
SER	E3856	E3856	E3856	E3856	R3767	L3613	LYS	GLY	GLY	L3292	R3293	L3292	L3292
SER	T3857	T3857	T3857	T3857	R3767	L3613	LYS	GLY	GLY	R3293	R3293	R3293	R3293
SER	L3858	L3858	L3858	L3858	R3767	L3613	LYS	GLY	GLY	R3293	R3293	R3293	R3293
SER	K3859	K3859	K3859	K3859	R3767	L3613	LYS	GLY	GLY	R3293	R3293	R3293	R3293
SER	K3860	K3860	K3860	K3860	R3767	L3613	LYS	GLY	GLY	R3293	R3293	R3293	R3293
SER	E3861	E3861	E3861	E3861	R3767	L3613	LYS	GLY	GLY	R3293	R3293	R3293	R3293



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: 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	0.11	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
3	ATP	A	5002	4	29,33,33	0.68	0	44,52,52	0.61	0
2	ADP	A	5001	-	27,29,29	0.62	0	42,45,45	0.58	0
2	ADP	A	5005	-	27,29,29	0.52	0	42,45,45	0.49	0
2	ADP	A	5004	-	27,29,29	0.61	0	42,45,45	0.60	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
3	ATP	A	5002	4	-	2/22/38/38	0/3/3/3
2	ADP	A	5001	-	-	2/16/32/32	0/3/3/3
2	ADP	A	5005	-	-	1/16/32/32	0/3/3/3
2	ADP	A	5004	-	-	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'

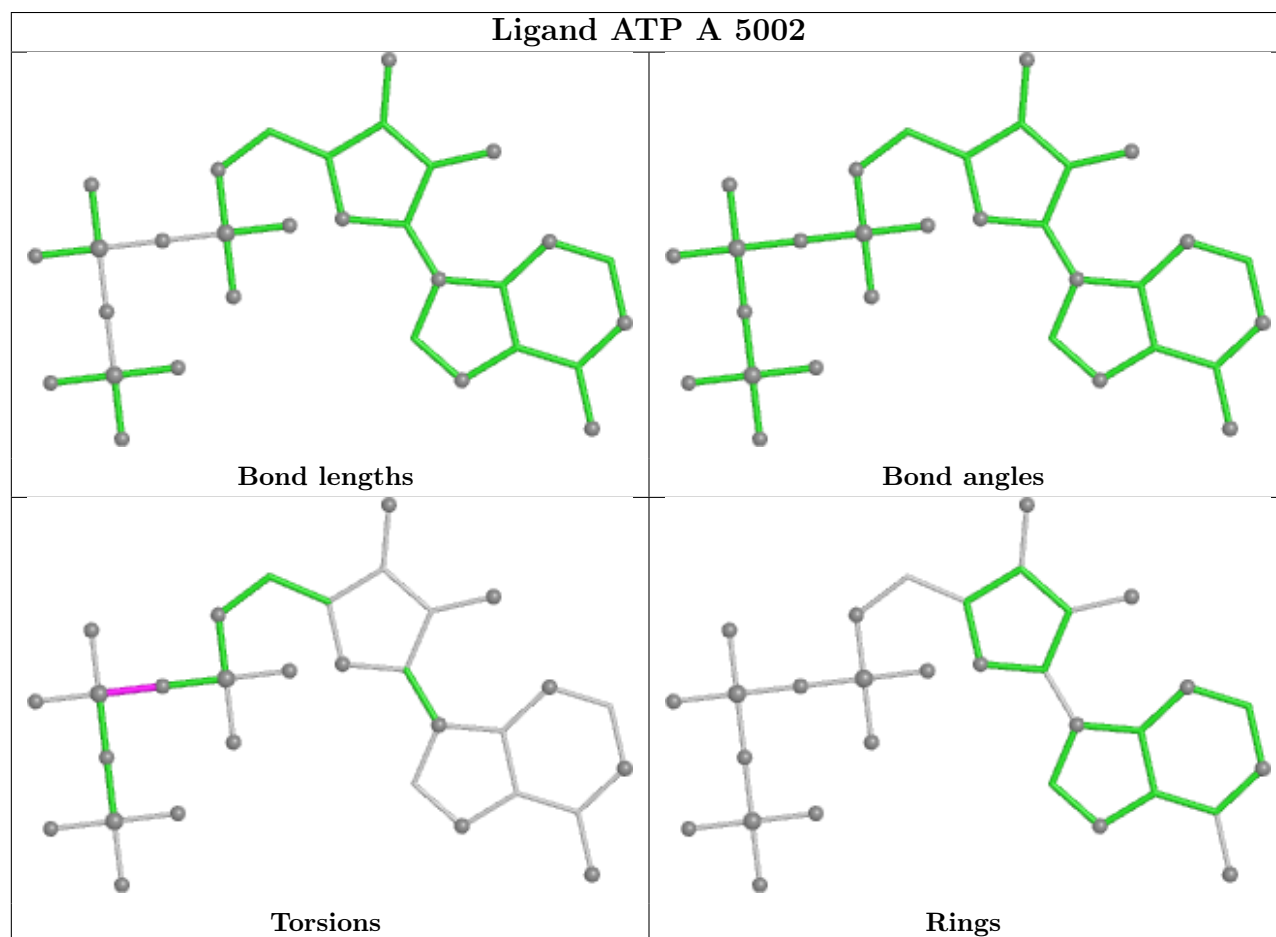
There are no ring outliers.

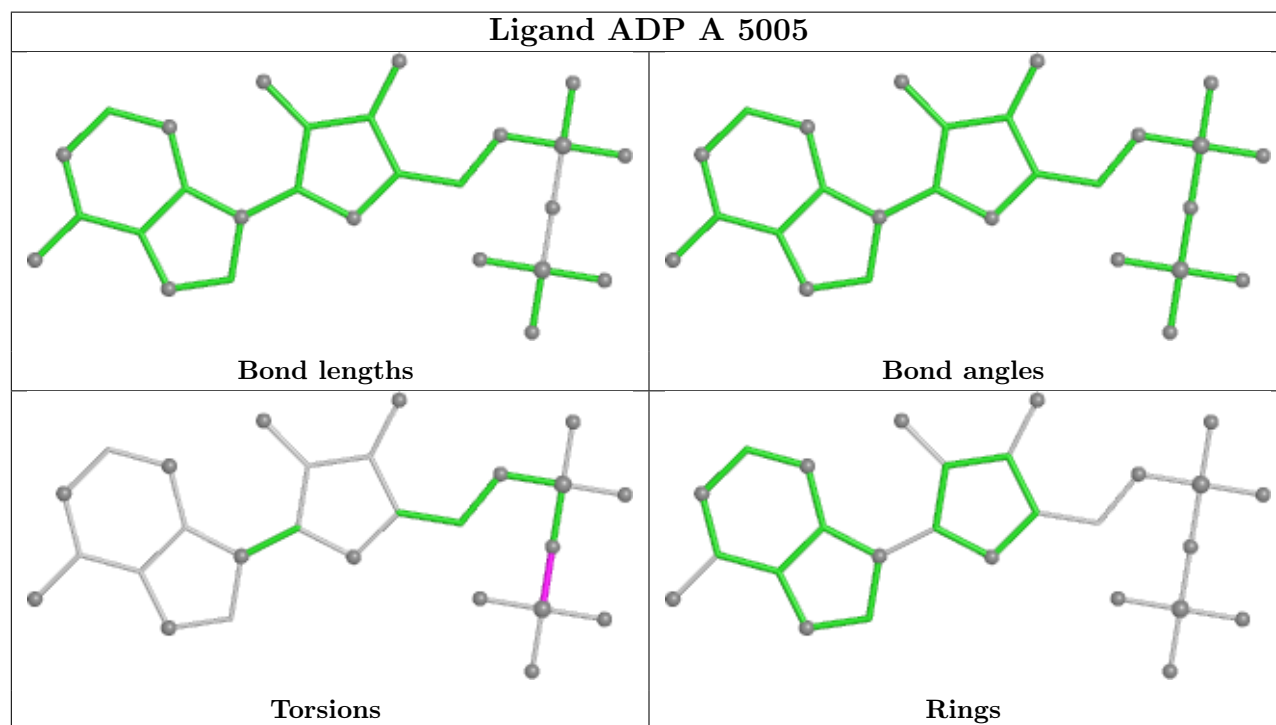
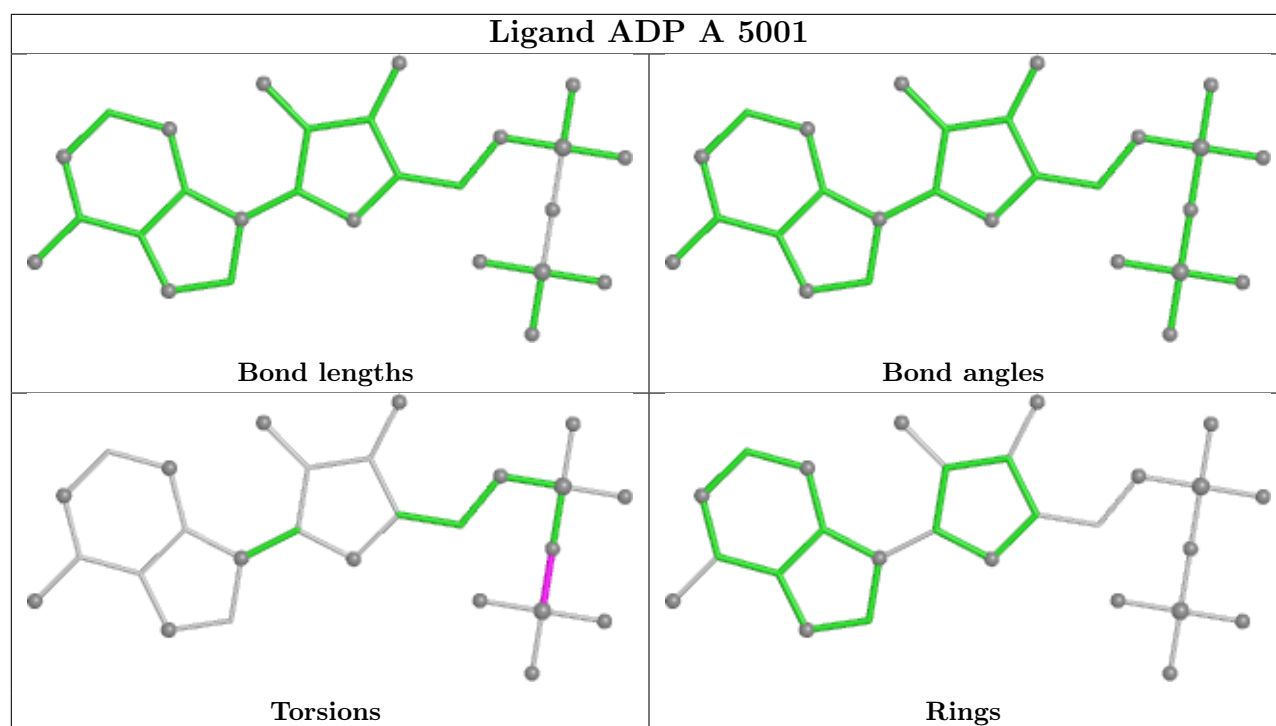
3 monomers are involved in 4 short contacts:

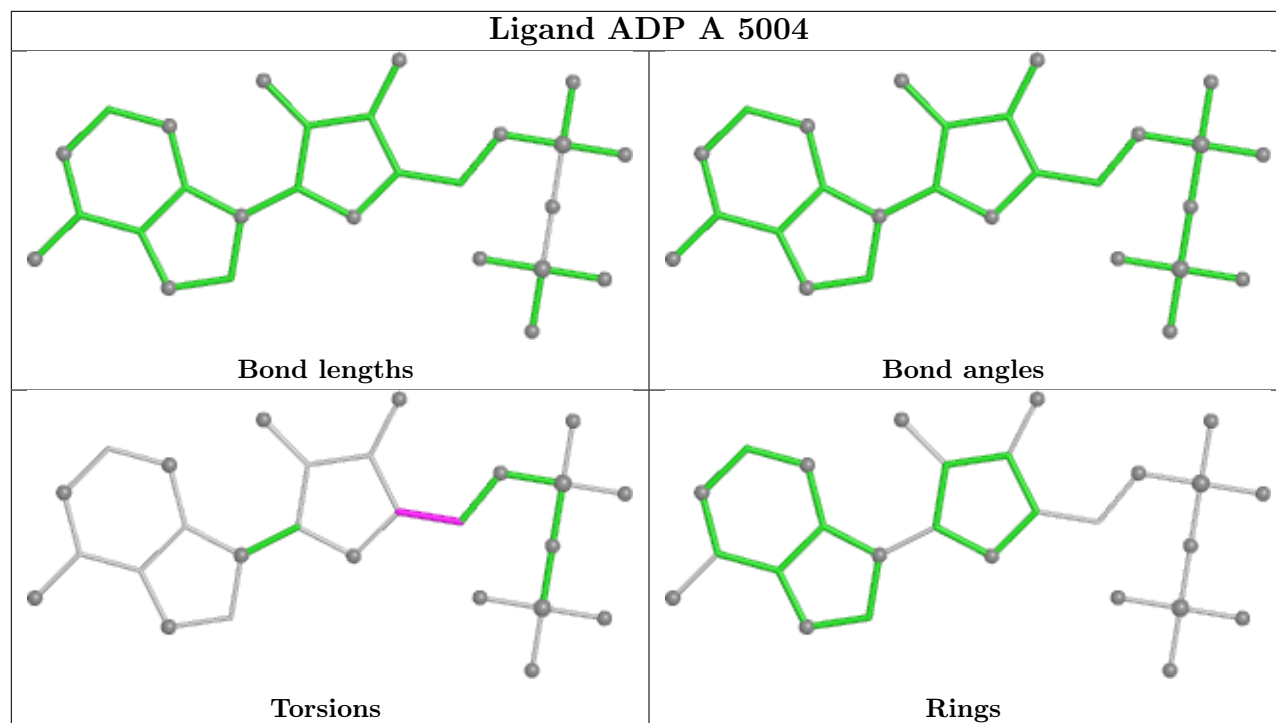
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5001	ADP	2	0
2	A	5005	ADP	1	0
2	A	5004	ADP	1	0

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.

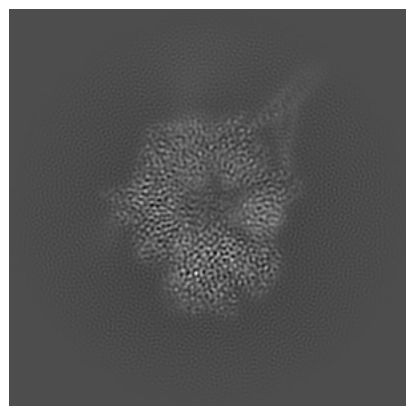
6 Map visualisation [i](#)

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.

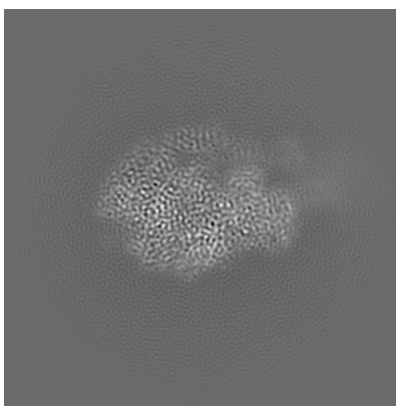
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

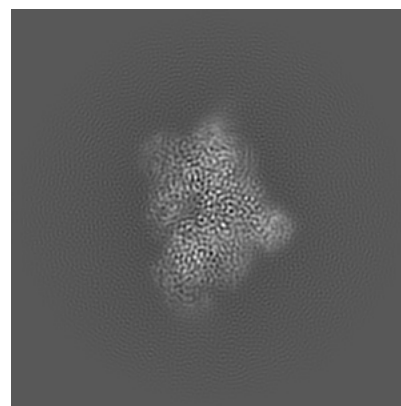
6.1.1 Primary map



X

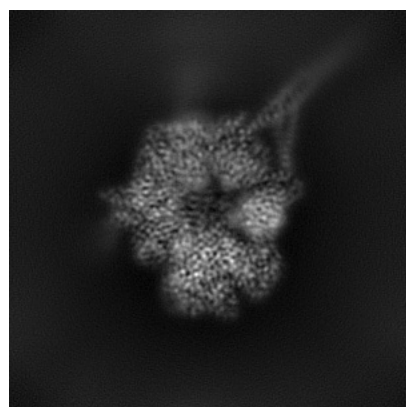


Y

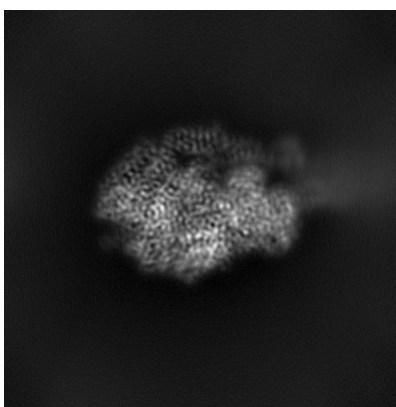


Z

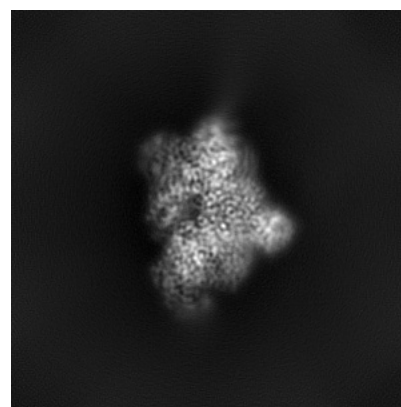
6.1.2 Raw map



X



Y

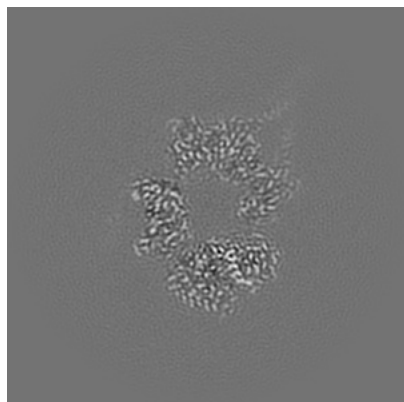


Z

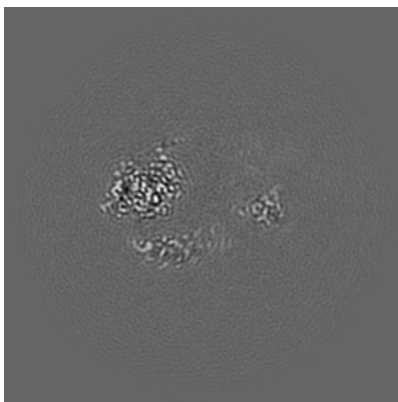
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

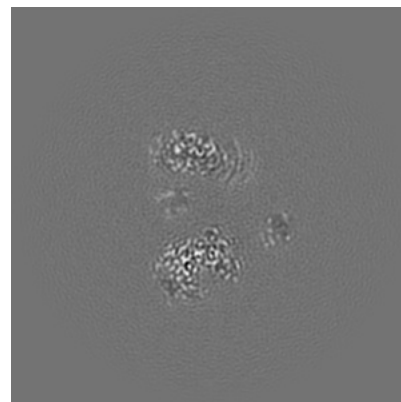
6.2.1 Primary map



X Index: 150

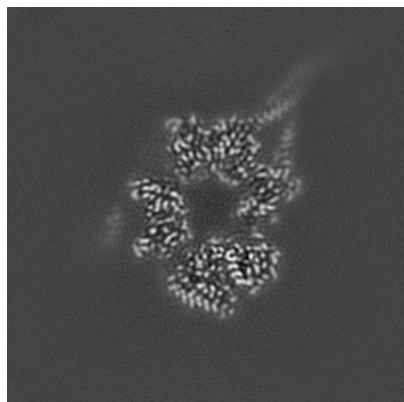


Y Index: 150

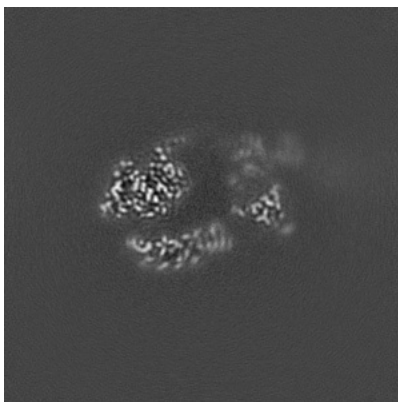


Z Index: 150

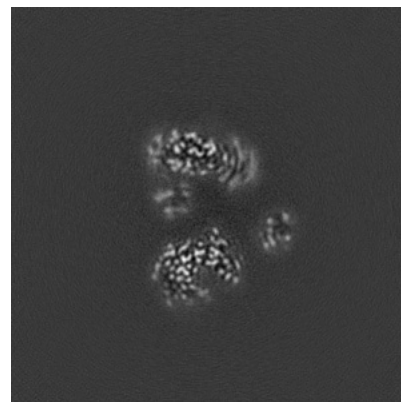
6.2.2 Raw map



X Index: 150



Y Index: 150

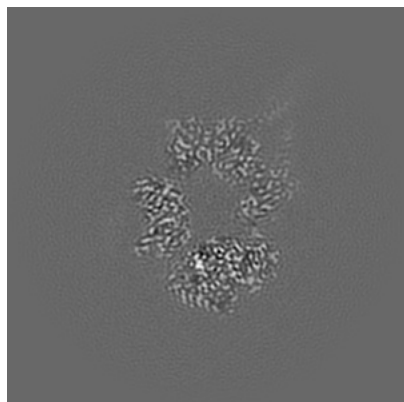


Z Index: 150

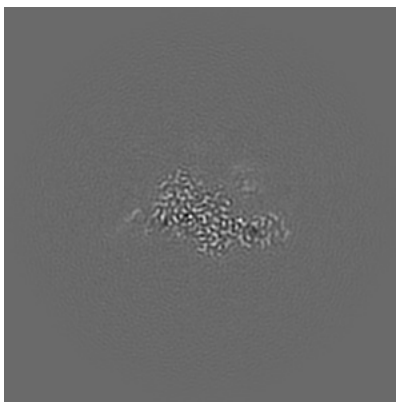
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

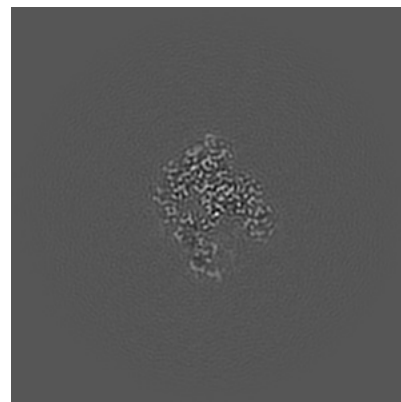
6.3.1 Primary map



X Index: 151

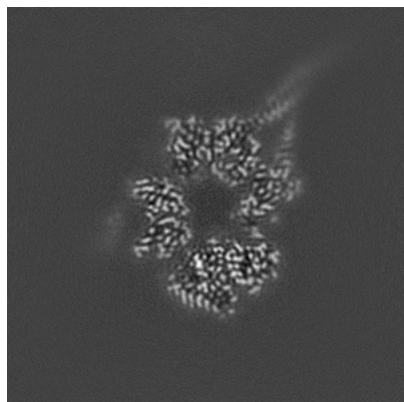


Y Index: 115

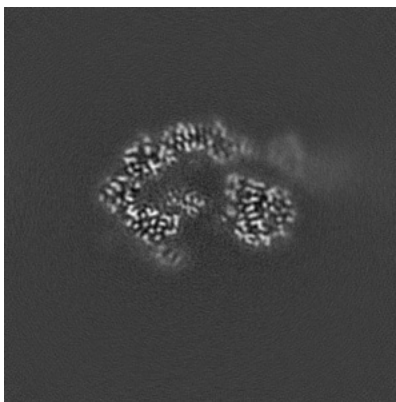


Z Index: 114

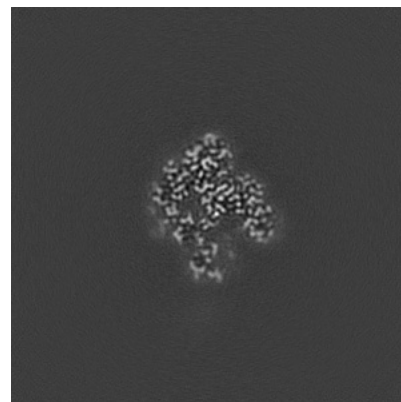
6.3.2 Raw map



X Index: 151



Y Index: 134

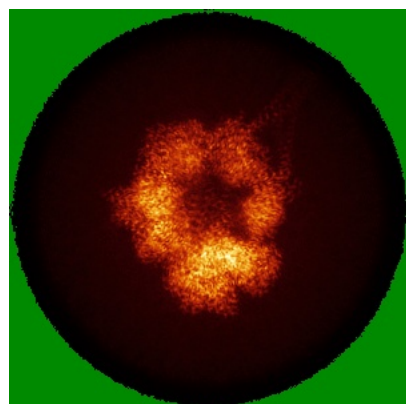


Z Index: 114

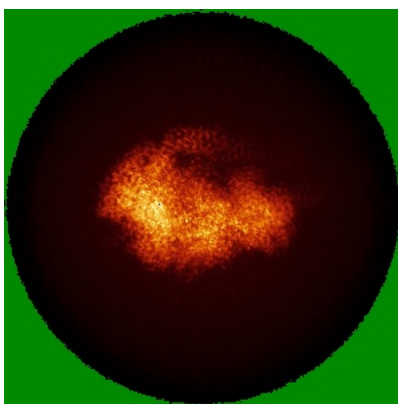
The images above show the largest variance slices of the map in three orthogonal directions.

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

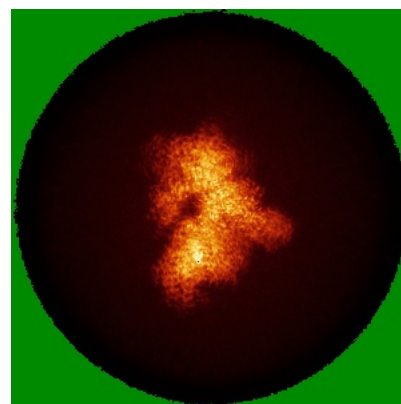
6.4.1 Primary map



X

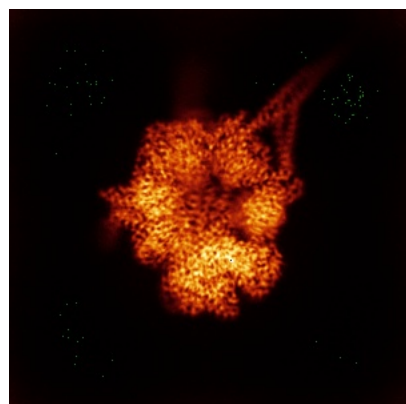


Y

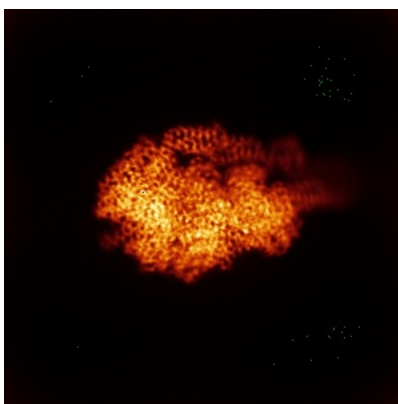


Z

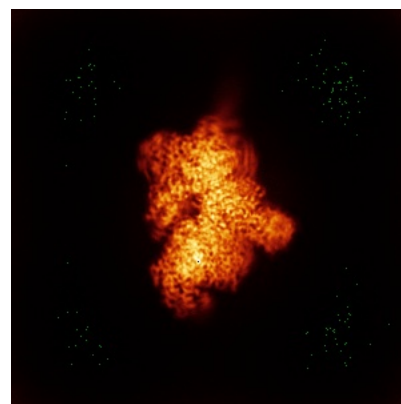
6.4.2 Raw map



X



Y

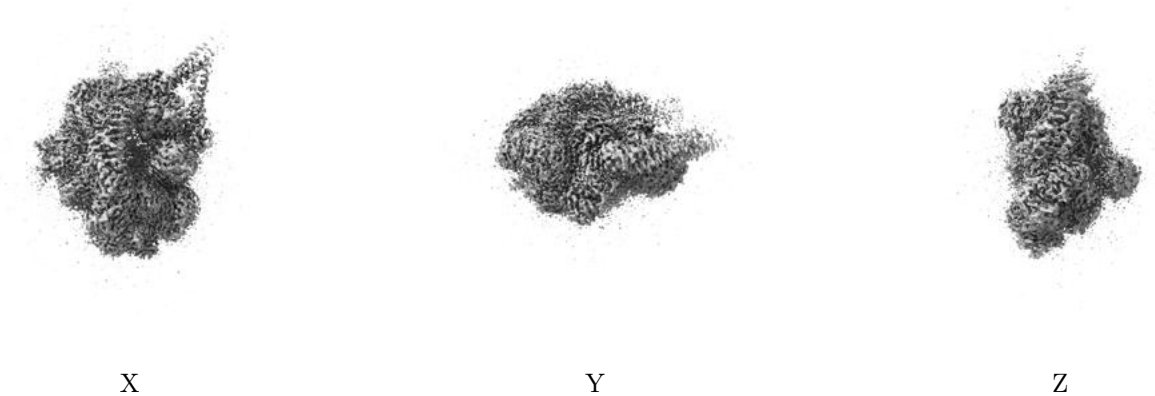


Z

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.

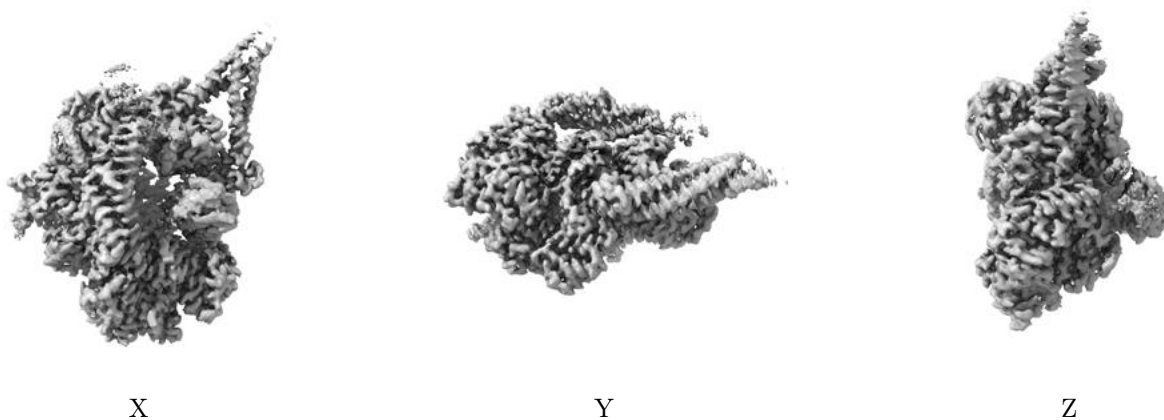
6.5 Orthogonal surface views [i](#)

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.

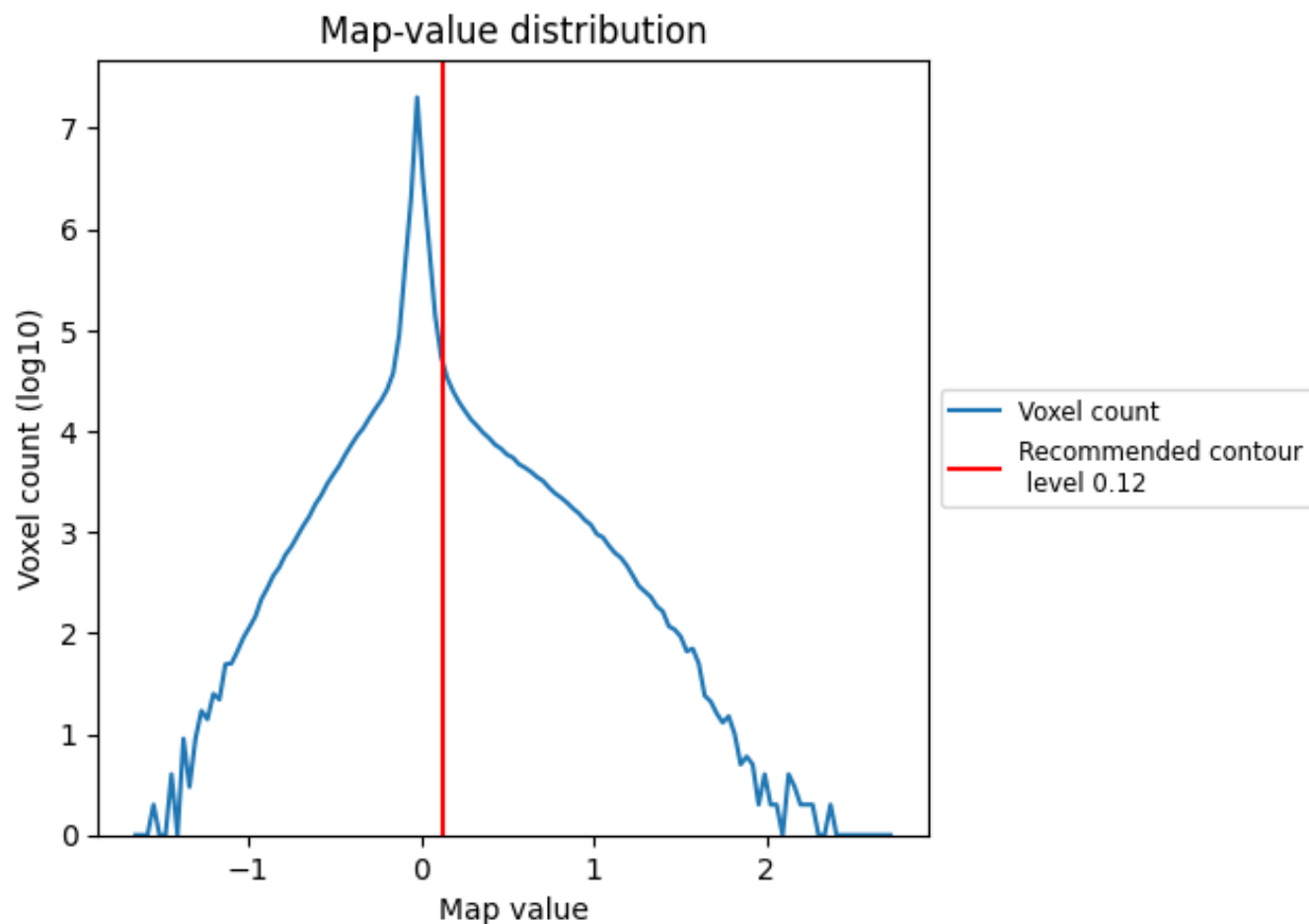
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

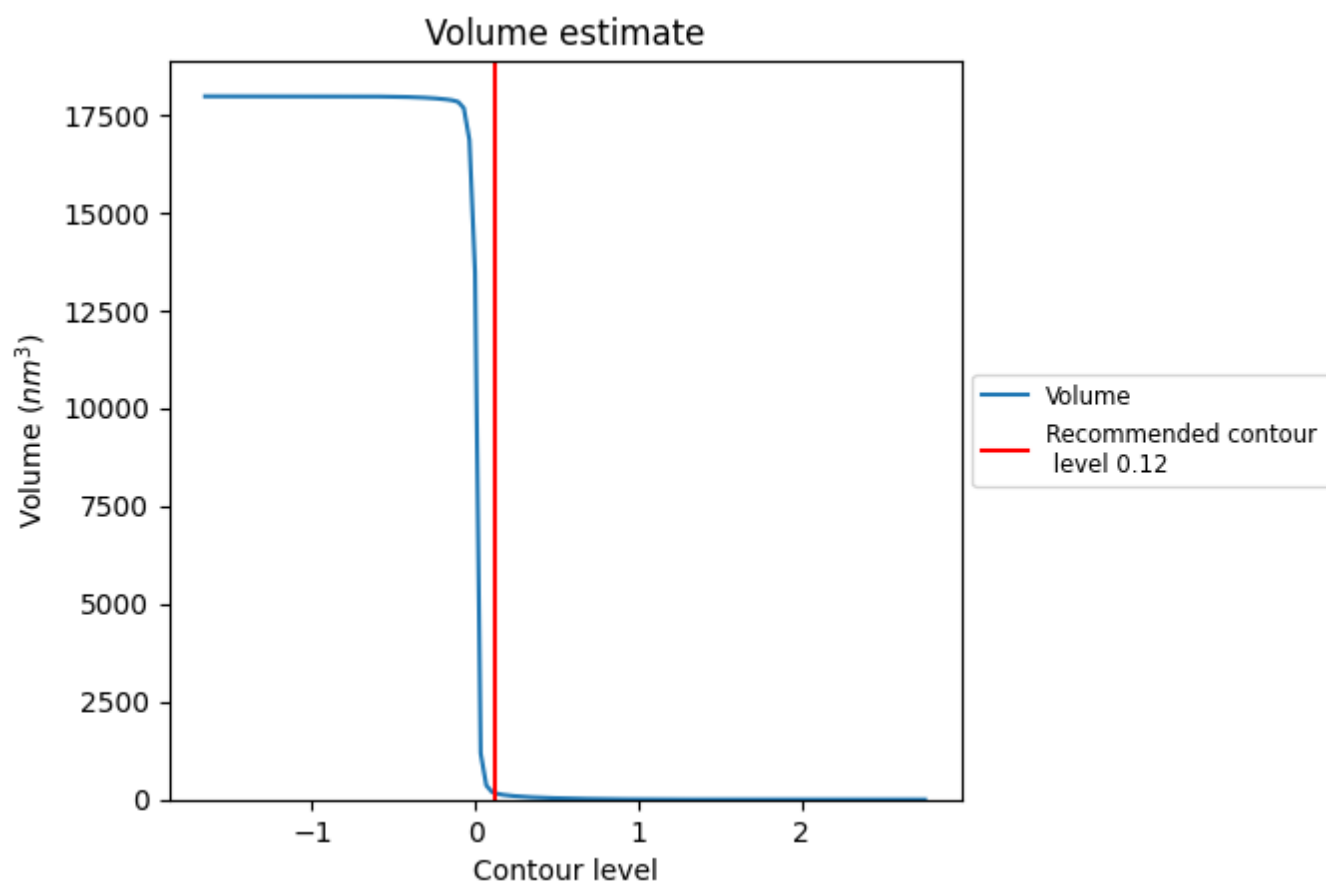
This section contains the results of statistical analysis of the map.

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.

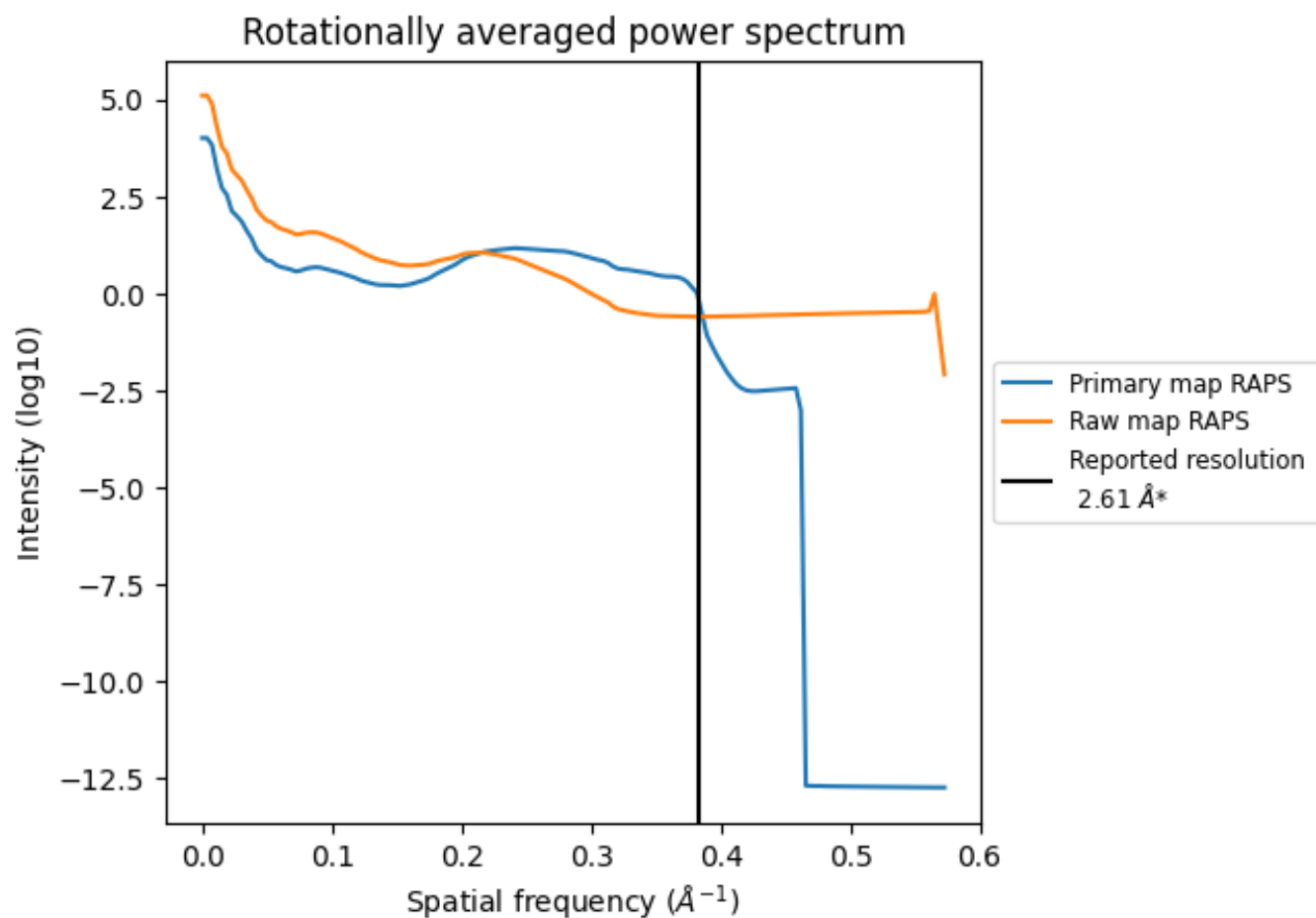
7.2 Volume estimate [i](#)



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 ⓘ

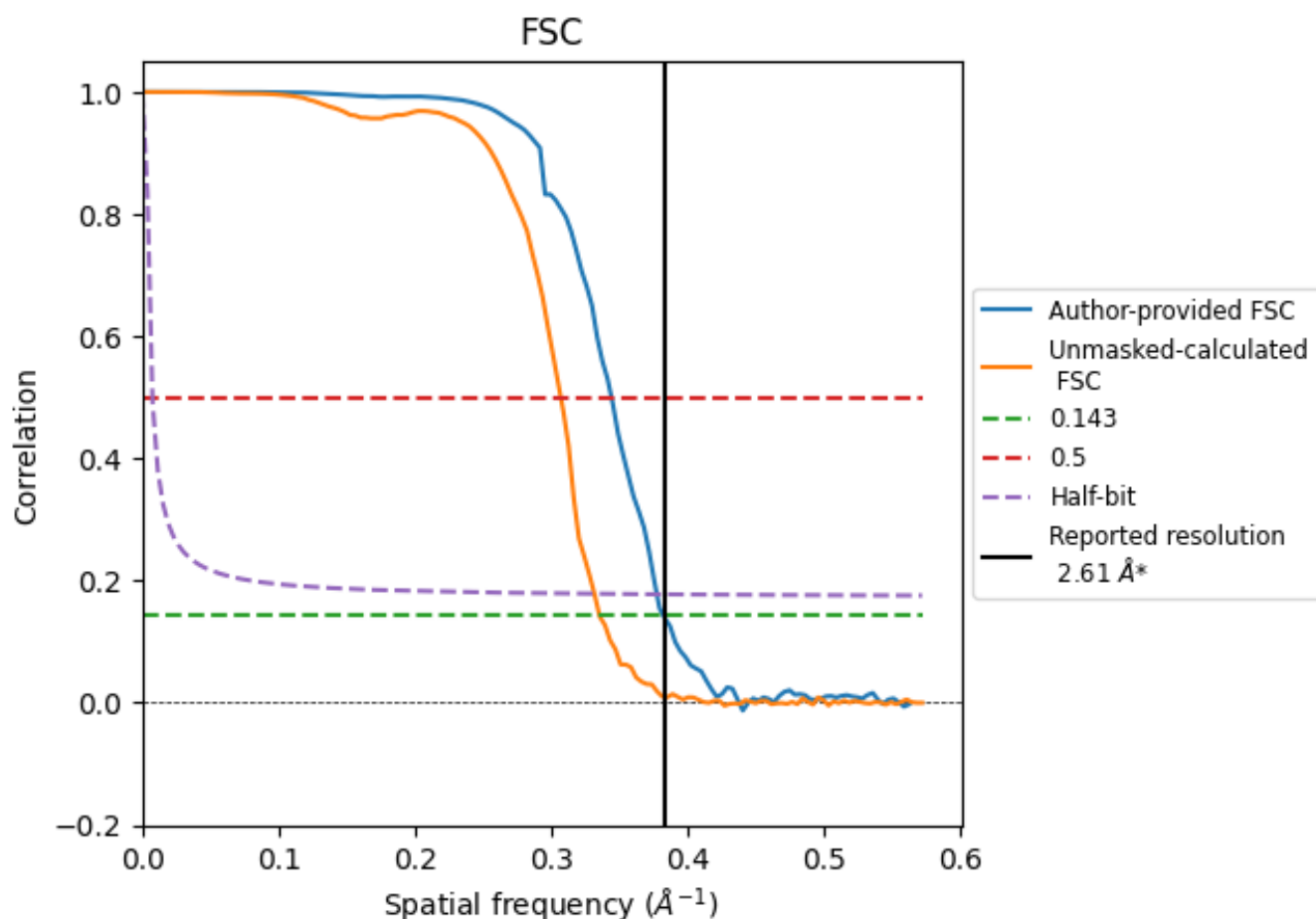


*Reported resolution corresponds to spatial frequency of 0.383 $\text{\AA}^{-1}$

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](#)

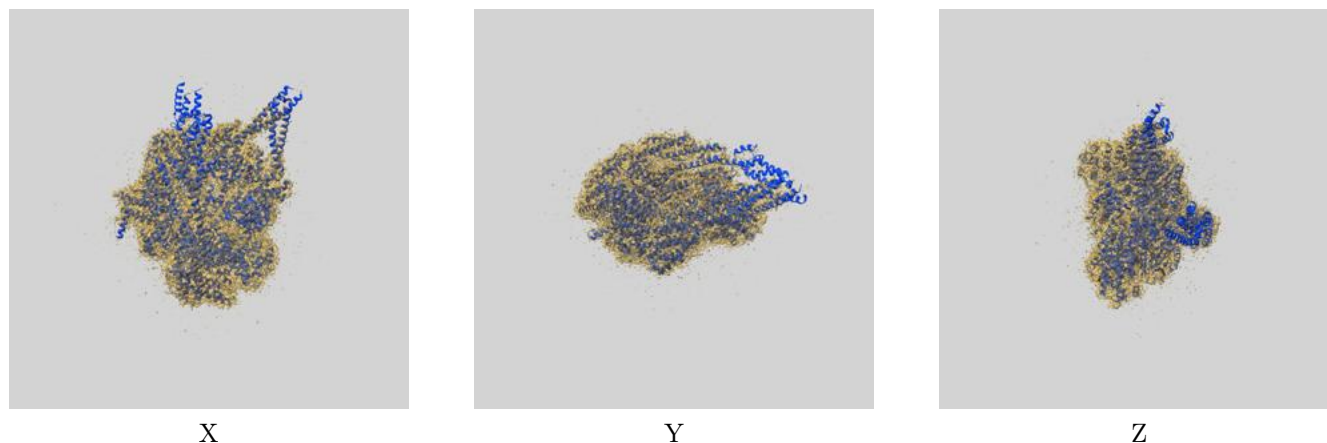
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.61	-	-
Author-provided FSC curve	2.61	2.90	2.65
Unmasked-calculated*	2.98	3.25	3.01

*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](#)

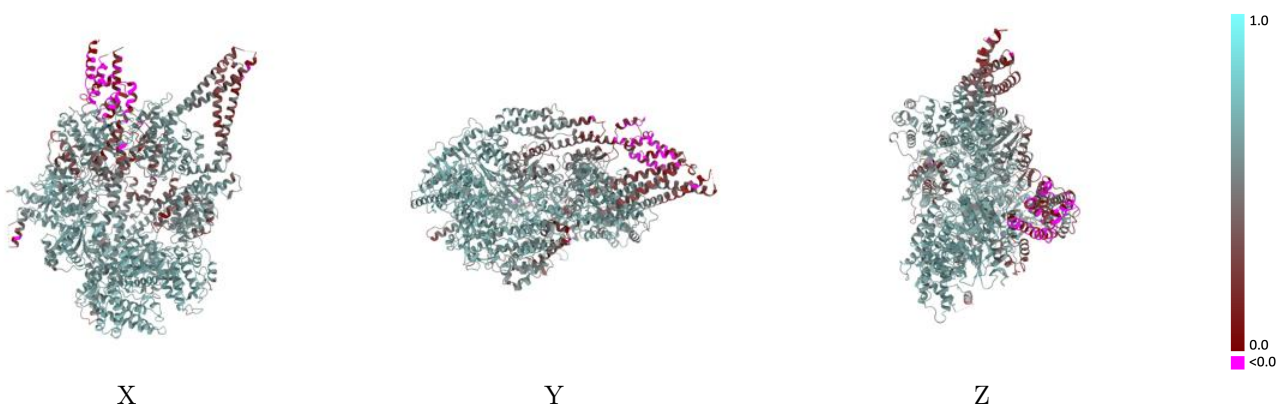
This section contains information regarding the fit between EMDB map EMD-81335 and PDB model 27PY. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



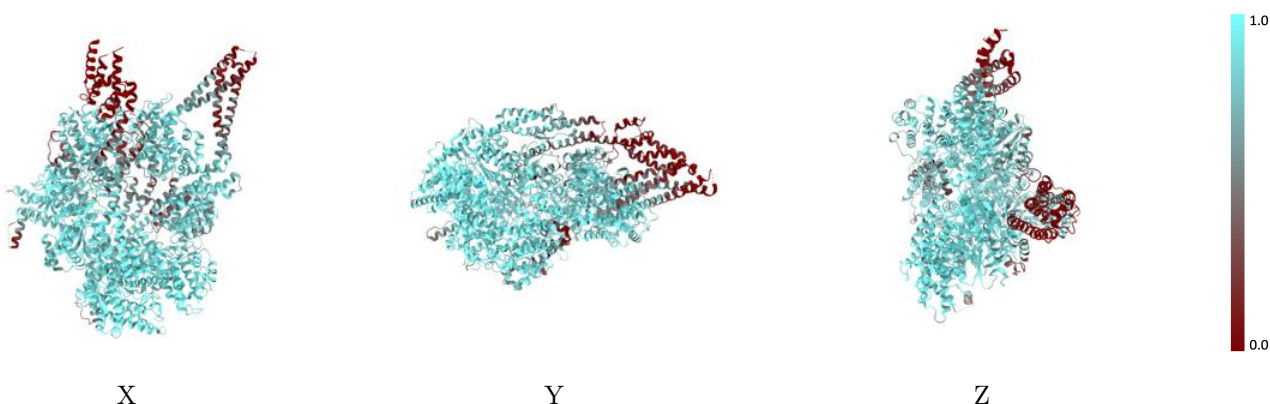
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



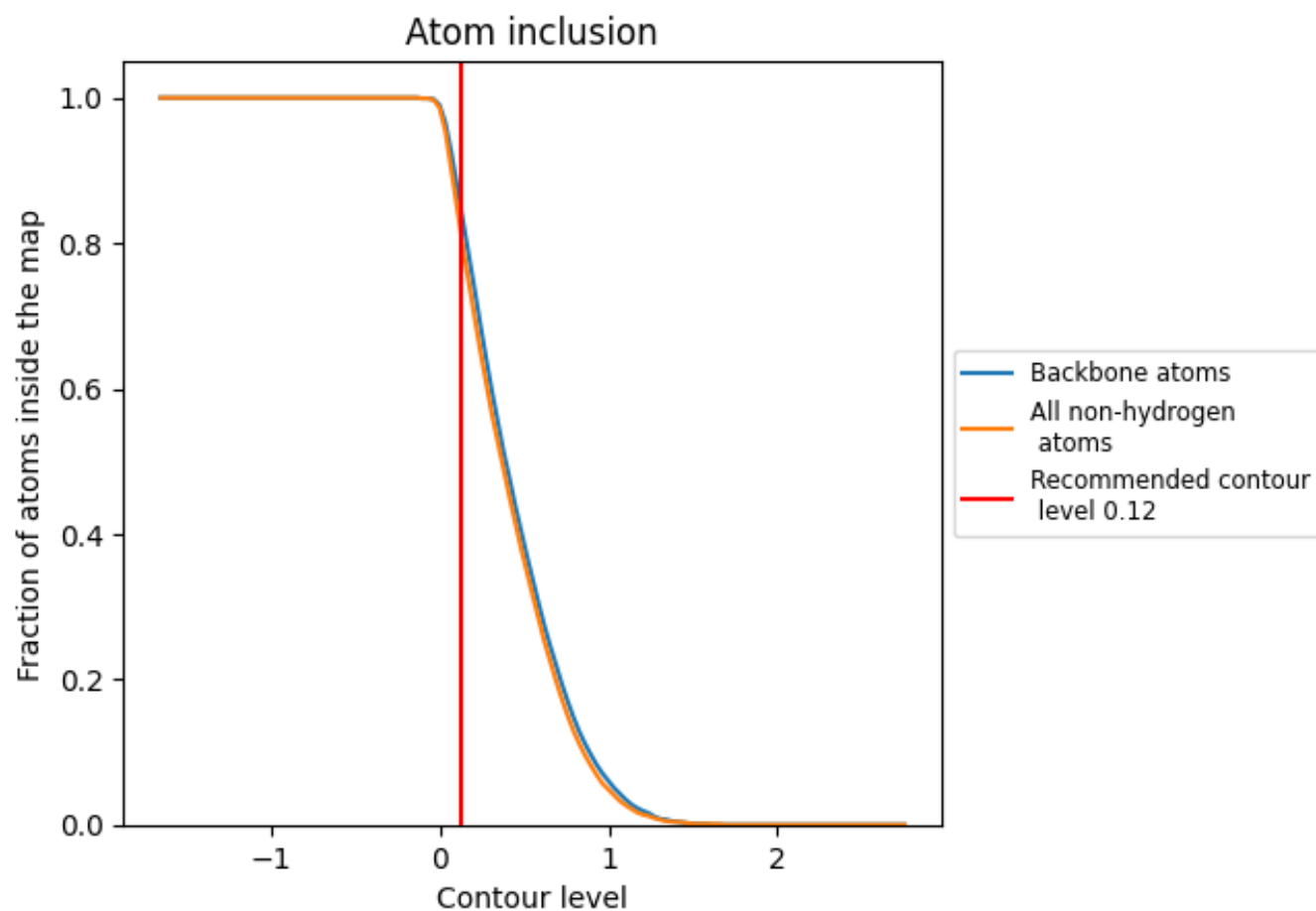
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

