



wwPDB EM Validation Summary Report ⓘ

Jan 20, 2026 – 01:08 PM EST

PDB ID : 9YNC / pdb_00009ync
EMDB ID : EMD-73173
Title : Motor domains of phi-like human dynein-1 bound to dynactin-p150glued and LIS1
Authors : Yang, J.; Rao, Q.; Chai, P.; Zhang, K.
Deposited on : 2025-10-10
Resolution : 3.93 Å(reported)

This is a wwPDB EM Validation Summary 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.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.47

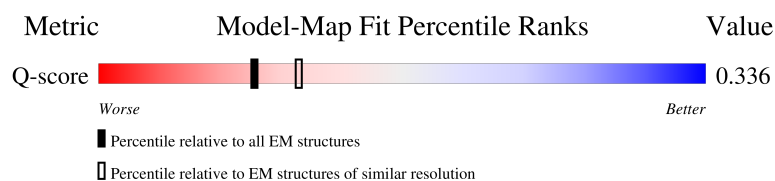
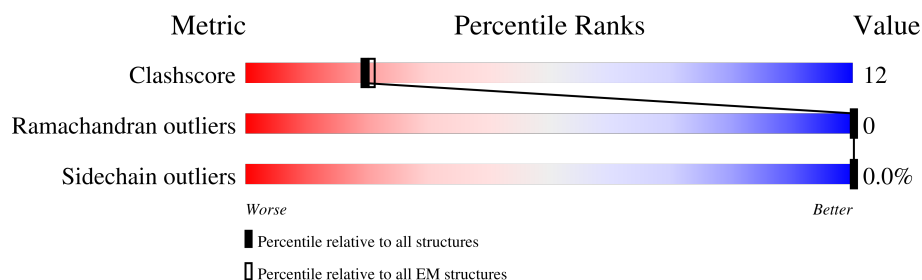
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





The reported resolution of this entry is 3.93 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.





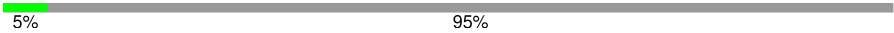
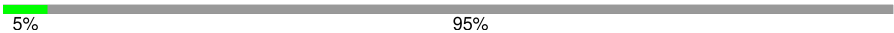


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	7811 (3.43 - 4.43)

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	
1	B	4646	
2	C	410	
2	D	410	

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Mol	Chain	Length	Quality of chain
2	E	410	 13% 18%82%
2	F	410	 8% 18%82%
3	G	638	 5%95%
3	H	638	 5%95%
4	I	1281	 10%90%
4	J	1281	 9%91%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 56882 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
1	A	3064	Total	C	N	O	S	0	0
			24650	15707	4259	4563	121		
1	B	3065	Total	C	N	O	S	0	0
			24658	15711	4260	4566	121		

- Molecule 2 is a protein called Platelet-activating factor acetylhydrolase IB subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	322	Total	C	N	O	S	0	0
			2557	1608	452	477	20		
2	D	313	Total	C	N	O	S	0	0
			2494	1571	440	463	20		
2	E	75	Total	C	N	O		0	0
			373	223	75	75			
2	F	75	Total	C	N	O		0	0
			373	223	75	75			

- Molecule 3 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	34	Total	C	N	O	0	0
			170	102	34	34		
3	H	34	Total	C	N	O	0	0
			170	102	34	34		

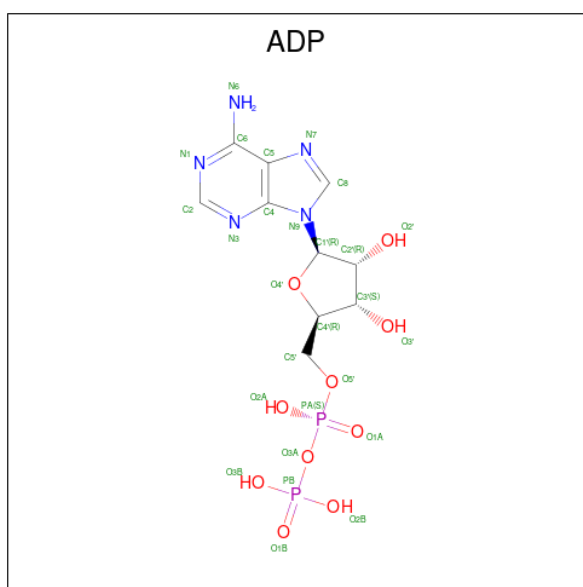
- Molecule 4 is a protein called Dynactin subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	122	Total	C	N	O	0	0
			607	363	122	122		
4	J	120	Total	C	N	O	1	0
			602	360	121	121		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1279	LEU	-	expression tag	UNP A0A287B8J2
I	1280	ILE	-	expression tag	UNP A0A287B8J2
I	1281	SER	-	expression tag	UNP A0A287B8J2
J	1279	LEU	-	expression tag	UNP A0A287B8J2
J	1280	ILE	-	expression tag	UNP A0A287B8J2
J	1281	SER	-	expression tag	UNP A0A287B8J2

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



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

- Molecule 6 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
6	A	1	Total 31	C 10	N 5	O 13	P 3	0
6	B	1	Total 31	C 10	N 5	O 13	P 3	0

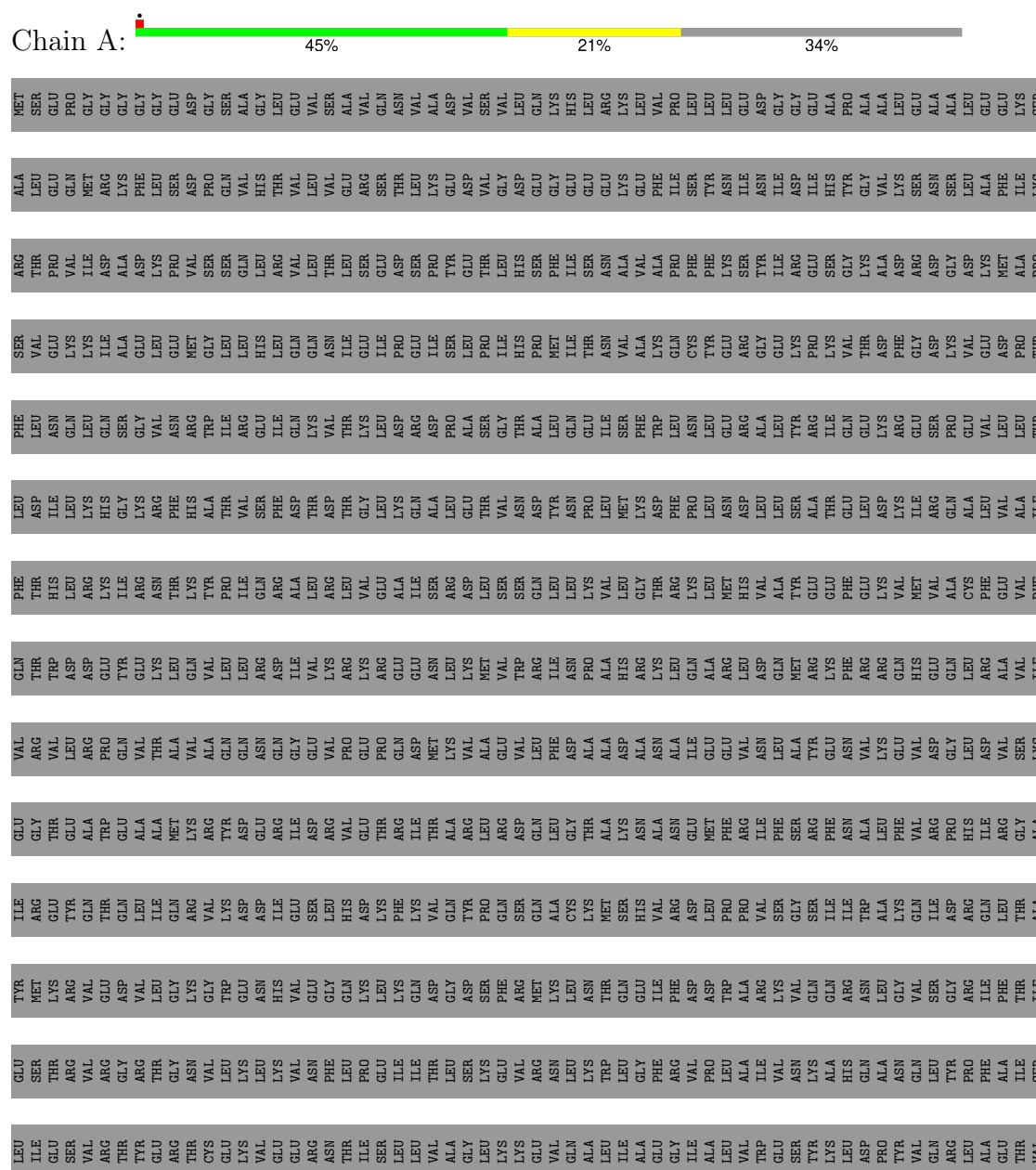
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
7	A	2	Total Mg 2 2	0
7	B	2	Total Mg 2 2	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Cytoplasmic dynein 1 heavy chain 1

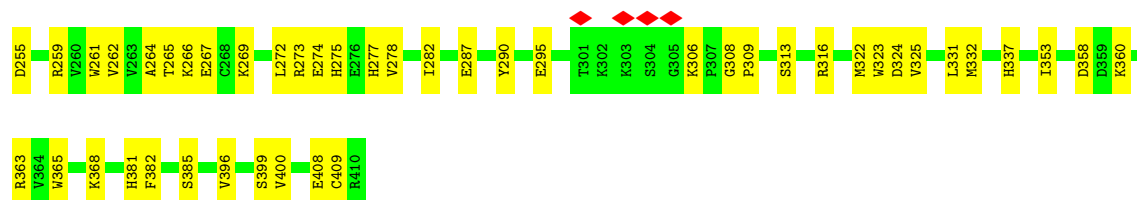




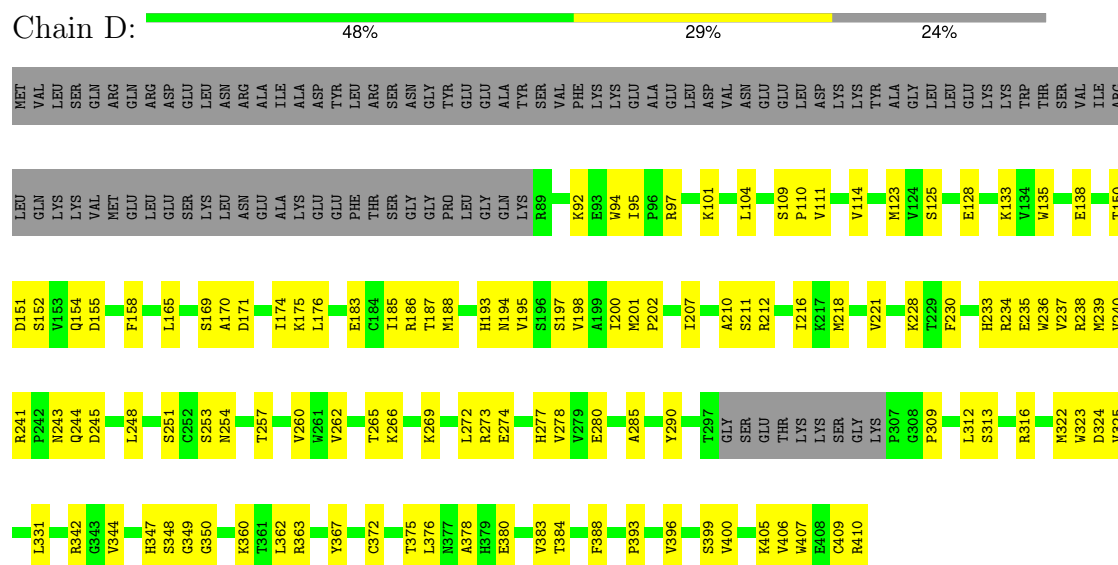




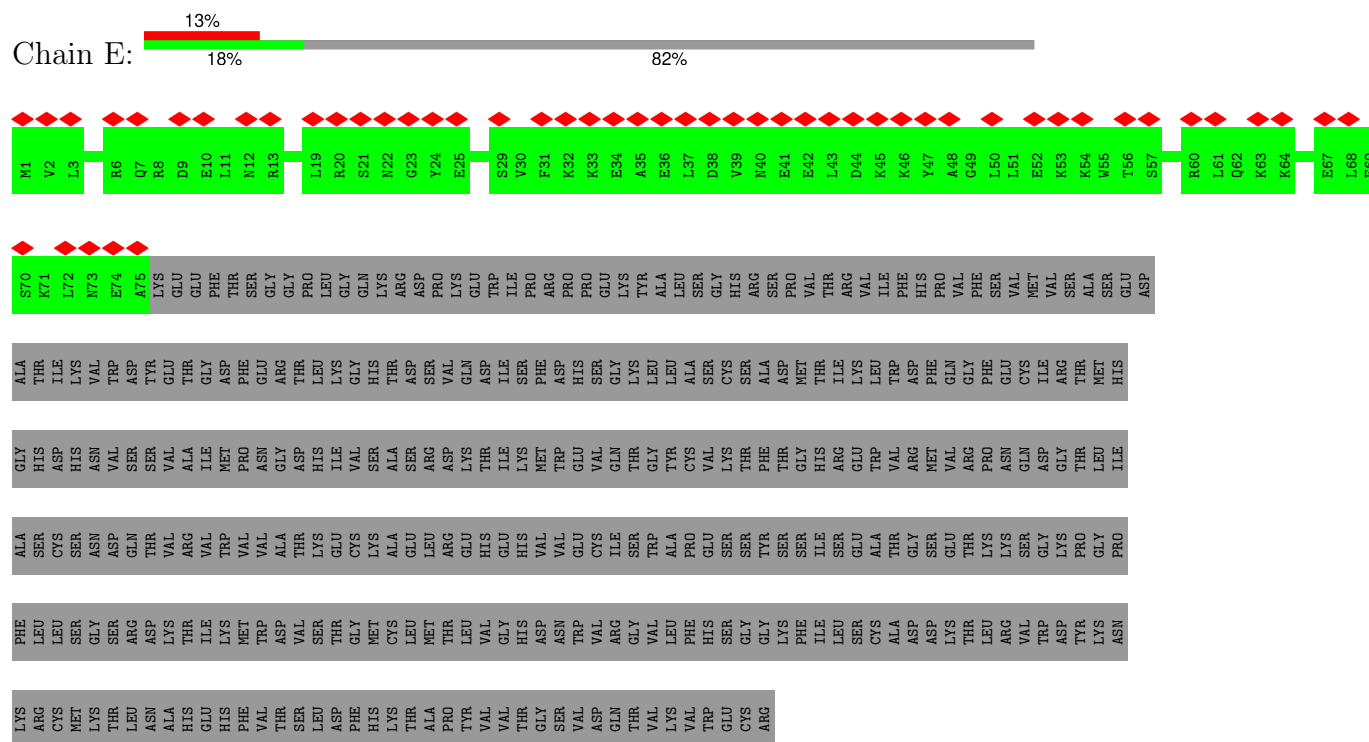
LYS	Q3214	T3081	L2993	Q2834	E2688	W2545	W2545	ASP	V2307	E2188	S2303	S1903	V1724	L1485
VAL	V3216	R3088	M2994	E2839	R2694	W2548	W2548	GLU	D2308	M2189	S2038	S1903	E1725	R1488
PRO	E3216	C3089	E2996	E2842	D2697	W2562	W2562	GLU	E2310	Y2190	T2042	T1910	F1727	R1603
ALA	E3217	F3094	V2999	R2843	K2702	W2563	W2563	ALA	W2311	T2192	K2043	G1911	K1729	L1604
VAL	R3219	G3095	G3003	L2885	Q2707	W2564	W2564	ALA	E2313	E2197	Q2047	E1914	S1753	D1606
ILE	R3220	D3096	F3004	L2861	V2708	P2565	P2565	ALA	M2322	W2203	R2060	S1915	S1756	L1608
GLU	R3223	W3097	L3006	L2862	V2709	W2566	W2566	ALA	T2326	K2206	E2063	K1917	I1756	G1609
ASN	Q3227	T3110	E3006	L2872	N2713	D2573	D2573	ALA	W2329	L2210	A2066	V1929	L1766	I1611
ALA	E3228	S3111	R3007	L2863	P2714	R2576	R2576	ALA	R2332	Y2211	R2067	F1930	M1769	Q1612
VAL	L3229	K3112	M3008	L2862	R2720	T2583	T2583	ALA	L2333	I2213	R2068	D1933	M1798	Y1513
LYS	E3230	W3113	L3012	L2872	R2726	W2584	W2584	ALA	L2344	T2214	P2071	F1936	V1785	E1517
SER	V3231	D3114	A3013	L2872	R2726	L2585	L2585	ALA	W2345	Q2215	S2081	Q1938	V1789	D1518
ILE	N3233	D3124	V3017	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	F1938	V1789	I1519
LYS	N3233	Y3125	V3017	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	A1520
GLN	K3239	V3129	L3020	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	L1521
HIS	M3243	Y3130	D3024	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	S1522
LEU	V3244	D3131	E2903	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	L1527
VAL	K3245	K3132	E3025	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	I1530
VAL	L3246	L3133	L2905	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	D1535
ARG	Q3247	P3134	T3028	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	I1538
SER	Q3248	Q3135	T3028	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	R1543
MET	E3249	P3136	T3028	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	Y1546
LYS	K3252	P3137	T3028	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	L1547
LYS	LYS	R3140	Q3032	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	I1550
PRO	LYS	E3141	Q3033	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	S1554
ALA	VAL	V3144	Q3036	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	K1558
VAL	SER	F3149	Q3038	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	L1561
LYS	GLN	V3150	K3039	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	E1564
LEU	ILE	L3154	L3042	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	T1565
LEU	GLN	T3172	M3043	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	Q1569
SER	GLN	P3173	S3046	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	T1573
ILE	LEU	R3174	H3047	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	L1576
CYS	HIS	H3175	E3048	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	M1579
LEU	LYS	V3176	E3049	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	E1584
LEU	GLN	L3177	L3050	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	T1585
LEU	GLN	D3178	Y3051	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	M1685
GLY	GLU	F3178	K3052	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	T1688
ILE	VAL	H3182	F3054	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	Q1850
SER	ALA	Q3197	R3060	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	T1573
THR	ASP	Q3198	R3060	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	L1576
ASP	LYS	P3199	V3065	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	M1699
THR	GLN	R3200	V3065	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	M1699
LYS	MET	L3201	S3072	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	E1700
GLN	SER	E3073	E3073	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	W1701
ILE	VAL	K3207	E3073	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	L1702
ARG	LYS	T3208	K3076	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	M1589
SER	GLU	L3211	R3077	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	E1708
ILE	ASP	T3211	D3077	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	M1593
ILE	LEU	T3211	R3077	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	R1599
MET	ASP	T3211	R3077	L2872	R2726	L2585	L2585	ALA	R2345	I2216	S2081	Q1938	V1789	S1600



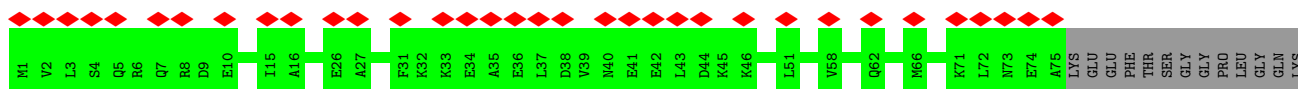
• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta



• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta



• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta

[illegible]

Chain G: 5% 95%

[illegible]





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90591	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)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.483	Depositor
Minimum map value	-0.187	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.08	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: ATP, ADP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.12	0/25169	0.32	0/34101
1	B	0.12	0/25177	0.30	0/34112
2	C	0.12	0/2624	0.39	0/3555
2	D	0.10	0/2560	0.31	0/3470
2	E	0.06	0/372	0.20	0/518
2	F	0.06	0/372	0.17	0/518
3	G	0.05	0/169	0.14	0/235
3	H	0.05	0/169	0.13	0/235
4	I	0.21	0/606	0.30	0/845
4	J	0.35	0/601	0.44	0/838
All	All	0.12	0/57819	0.32	0/78427

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	24650	0	24762	653	0
1	B	24658	0	24766	577	0
2	C	2557	0	2487	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2494	0	2419	89	0
2	E	373	0	172	0	0
2	F	373	0	172	0	0
3	G	170	0	73	1	0
3	H	170	0	73	0	0
4	I	607	0	285	0	0
4	J	602	0	282	0	0
5	A	81	0	36	9	0
5	B	81	0	36	10	0
6	A	31	0	12	4	0
6	B	31	0	12	6	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
All	All	56882	0	55587	1380	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 12.

The worst 5 of 1380 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:275:HIS:HE2	2:C:313:SER:HG	1.16	0.93
1:A:1892:MET:HE1	1:A:1902:GLY:HA3	1.53	0.90
1:A:2096:VAL:HG22	1:A:2144:THR:HG21	1.53	0.90
1:A:2633:LYS:HZ3	1:A:3019:GLY:H	1.20	0.88
1:A:4473:MET:HE1	1:A:4478:TRP:HB2	1.58	0.84

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	3056/4646 (66%)	2984 (98%)	72 (2%)	0	100	100
1	B	3057/4646 (66%)	2974 (97%)	83 (3%)	0	100	100
2	C	320/410 (78%)	301 (94%)	19 (6%)	0	100	100
2	D	309/410 (75%)	294 (95%)	15 (5%)	0	100	100
2	E	73/410 (18%)	73 (100%)	0	0	100	100
2	F	73/410 (18%)	73 (100%)	0	0	100	100
3	G	32/638 (5%)	32 (100%)	0	0	100	100
3	H	32/638 (5%)	32 (100%)	0	0	100	100
4	I	120/1281 (9%)	120 (100%)	0	0	100	100
4	J	119/1281 (9%)	119 (100%)	0	0	100	100
All	All	7191/14770 (49%)	7002 (97%)	189 (3%)	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	2720/4125 (66%)	2720 (100%)	0	100	100
1	B	2721/4125 (66%)	2721 (100%)	0	100	100
2	C	287/364 (79%)	286 (100%)	1 (0%)	91	91
2	D	280/364 (77%)	280 (100%)	0	100	100
All	All	6008/8978 (67%)	6007 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	222	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2549	GLN
1	B	3061	ASN
1	B	3877	HIS
1	A	2707	GLN
1	A	2685	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
6	ATP	A	4702	7	28,33,33	0.63	0	34,52,52	0.60	1 (2%)
5	ADP	B	4703	-	24,29,29	0.90	1 (4%)	29,45,45	1.22	2 (6%)
5	ADP	B	4701	7	24,29,29	0.89	0	29,45,45	1.23	3 (10%)
5	ADP	A	4704	-	24,29,29	0.89	0	29,45,45	1.19	2 (6%)
6	ATP	B	4702	7	28,33,33	0.70	0	34,52,52	0.60	1 (2%)
5	ADP	A	4701	7	24,29,29	0.93	1 (4%)	29,45,45	1.17	3 (10%)
5	ADP	A	4703	-	24,29,29	0.88	0	29,45,45	1.27	3 (10%)
5	ADP	B	4704	-	24,29,29	0.88	0	29,45,45	1.19	2 (6%)

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
6	ATP	A	4702	7	-	7/18/38/38	0/3/3/3
5	ADP	B	4703	-	-	0/12/32/32	0/3/3/3
5	ADP	B	4701	7	-	2/12/32/32	0/3/3/3
5	ADP	A	4704	-	-	1/12/32/32	0/3/3/3
6	ATP	B	4702	7	-	5/18/38/38	0/3/3/3
5	ADP	A	4701	7	-	0/12/32/32	0/3/3/3
5	ADP	A	4703	-	-	0/12/32/32	0/3/3/3
5	ADP	B	4704	-	-	2/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	4701	ADP	C2-N3	2.18	1.35	1.32
5	B	4703	ADP	O4'-C1'	2.13	1.43	1.40

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	4704	ADP	N3-C2-N1	-3.71	123.63	128.67
5	B	4703	ADP	N3-C2-N1	-3.68	123.67	128.67
5	A	4704	ADP	N3-C2-N1	-3.67	123.70	128.67
5	A	4703	ADP	N3-C2-N1	-3.64	123.74	128.67
5	B	4701	ADP	N3-C2-N1	-3.51	123.90	128.67

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

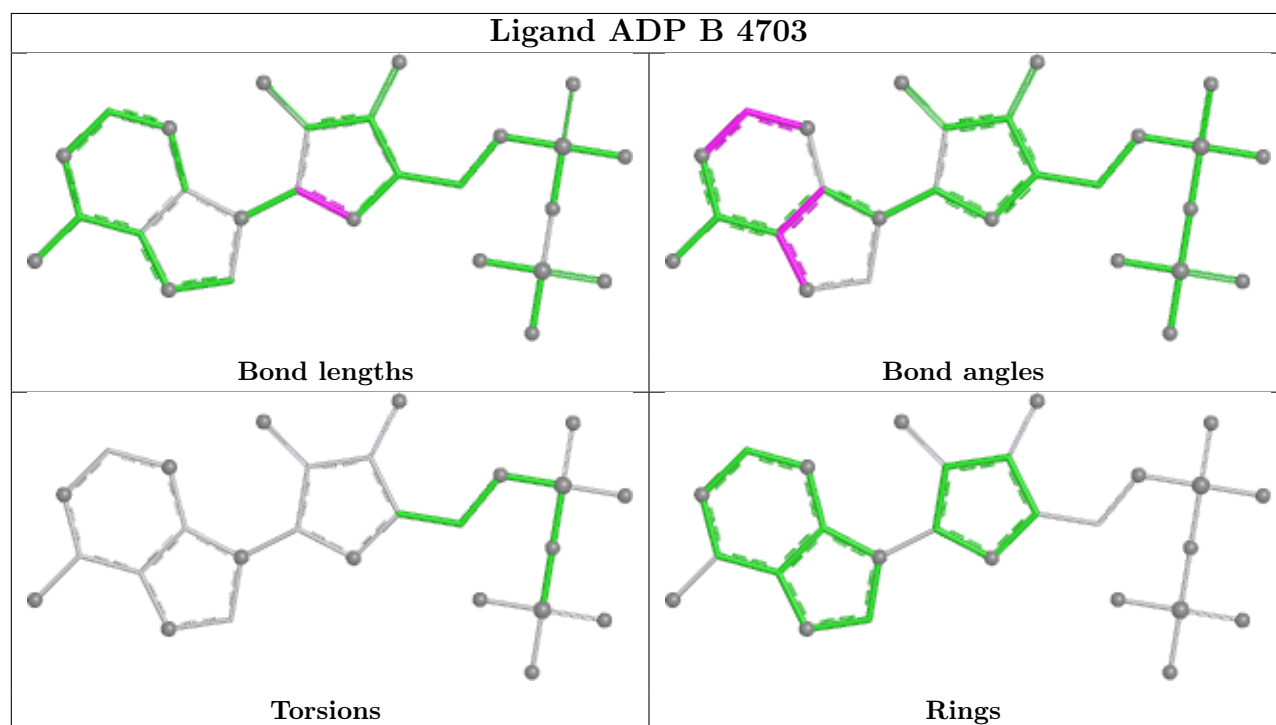
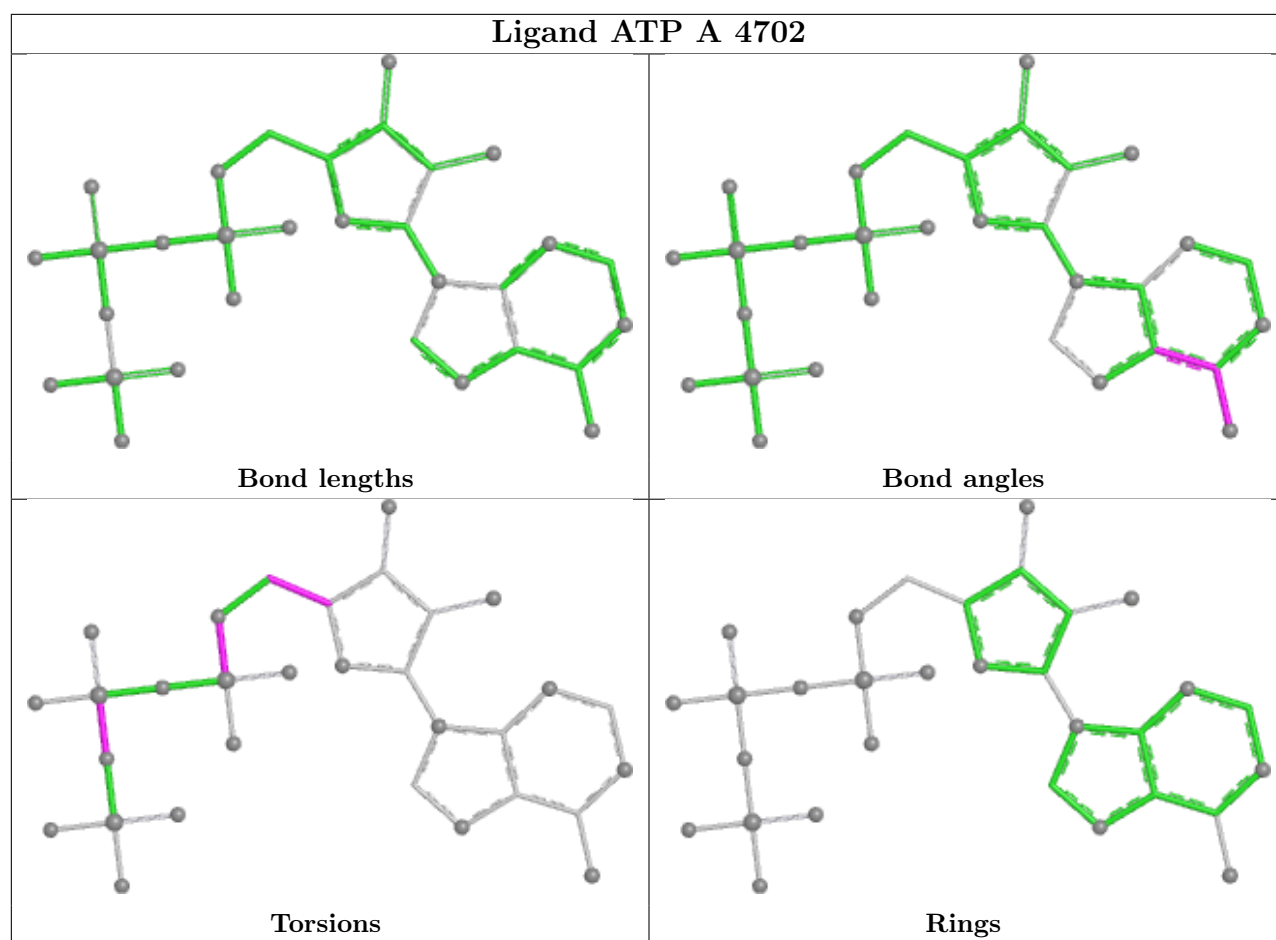
Mol	Chain	Res	Type	Atoms
5	B	4701	ADP	C5'-O5'-PA-O2A
5	B	4701	ADP	C5'-O5'-PA-O3A
6	A	4702	ATP	C5'-O5'-PA-O1A
6	A	4702	ATP	C5'-O5'-PA-O2A
6	A	4702	ATP	C5'-O5'-PA-O3A

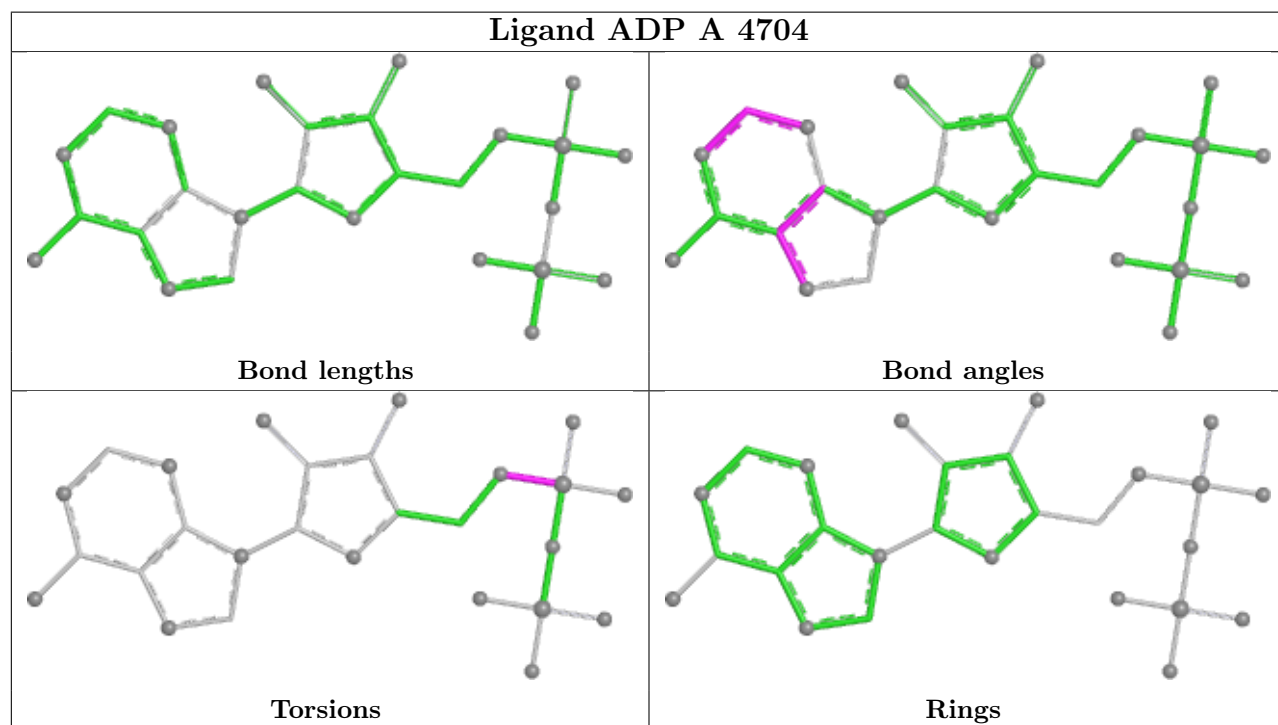
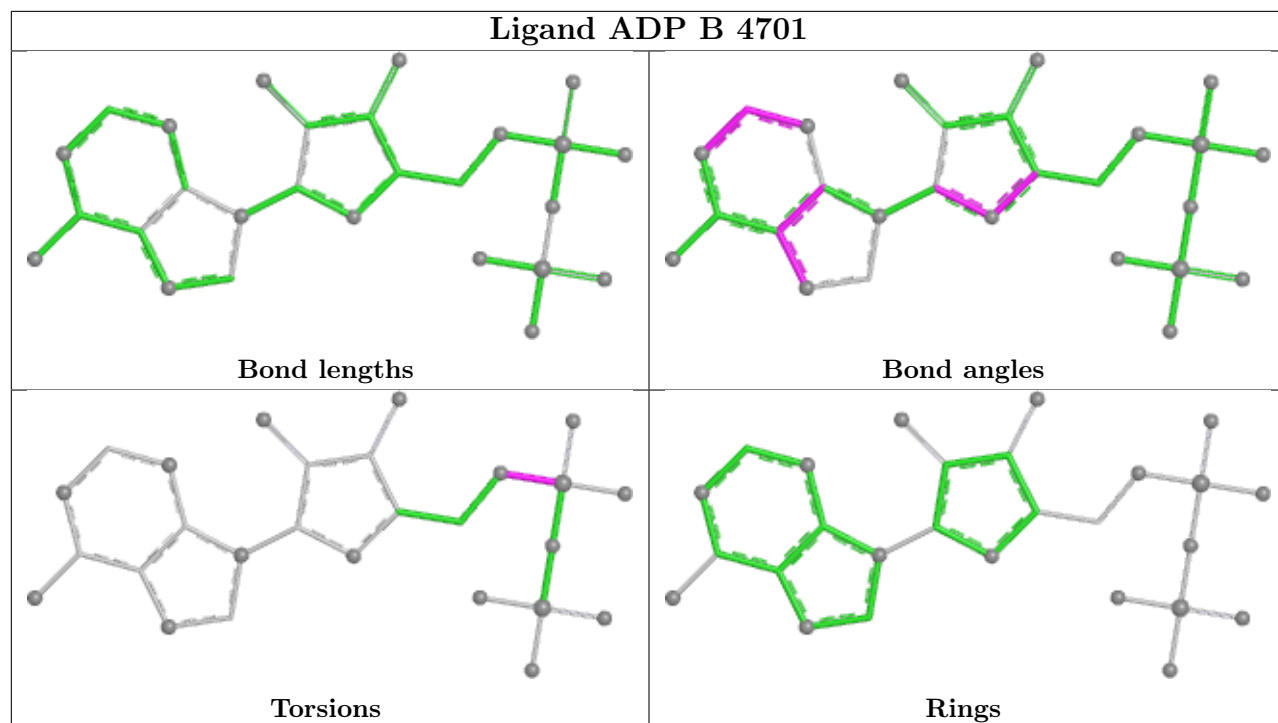
There are no ring outliers.

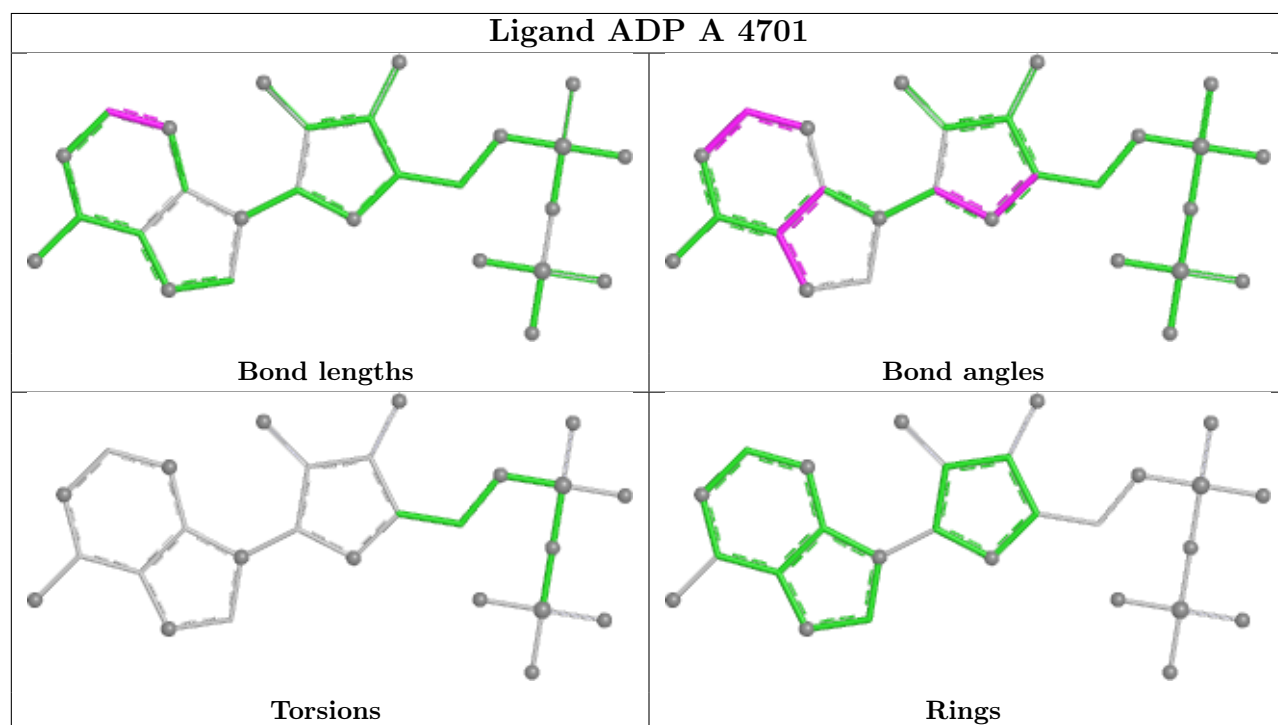
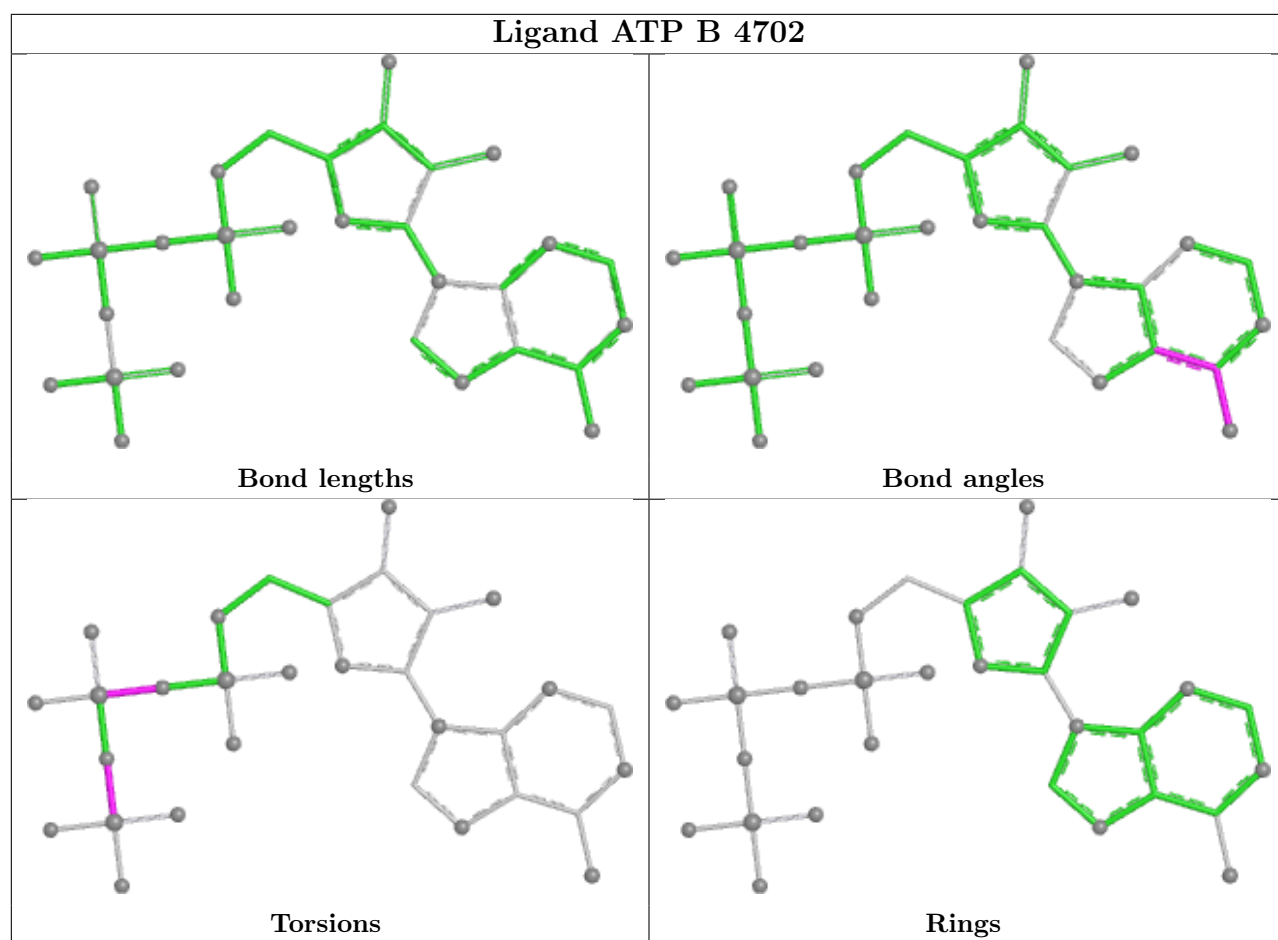
8 monomers are involved in 29 short contacts:

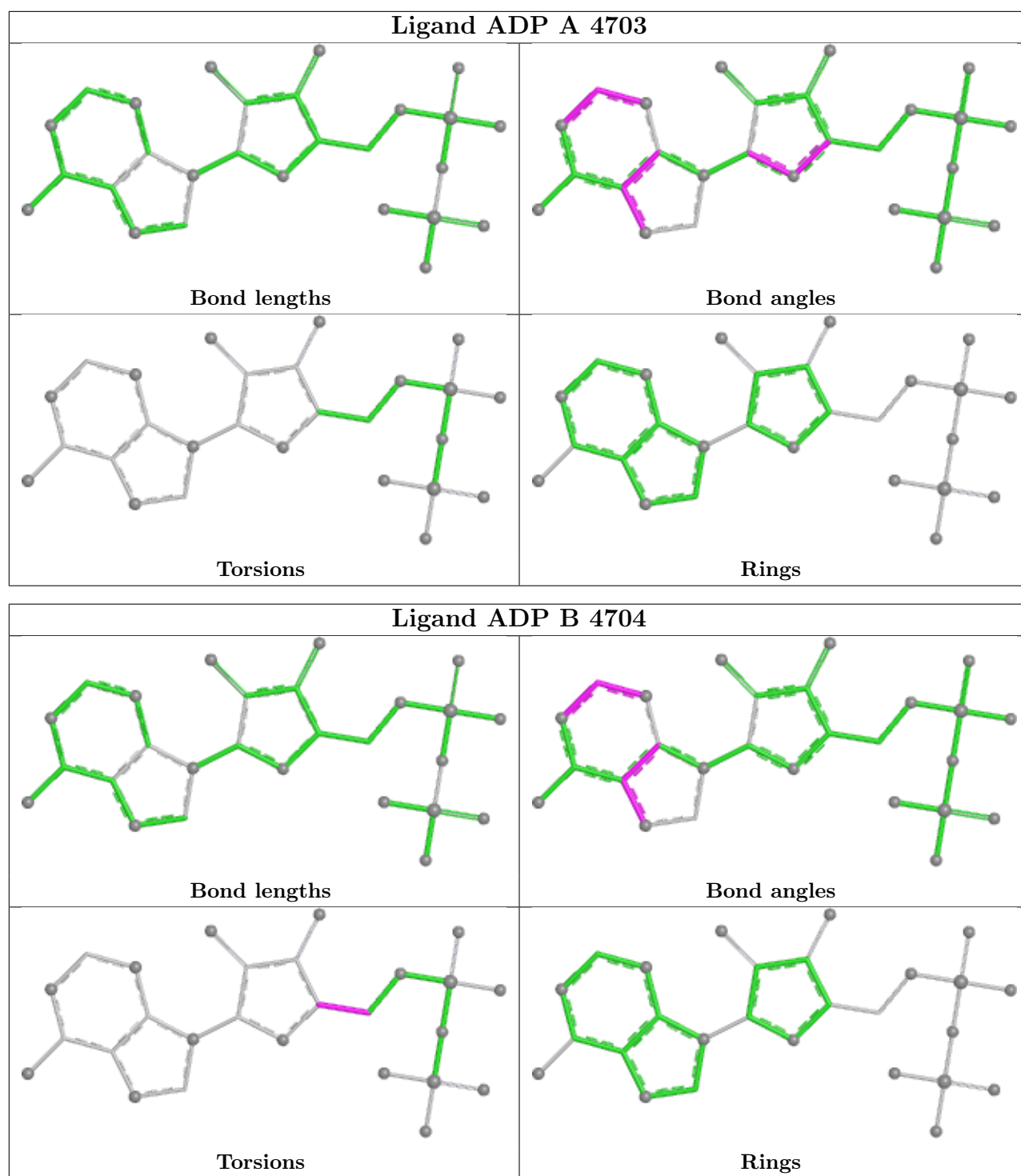
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	4702	ATP	4	0
5	B	4703	ADP	3	0
5	B	4701	ADP	5	0
5	A	4704	ADP	3	0
6	B	4702	ATP	6	0
5	A	4701	ADP	3	0
5	A	4703	ADP	3	0
5	B	4704	ADP	2	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

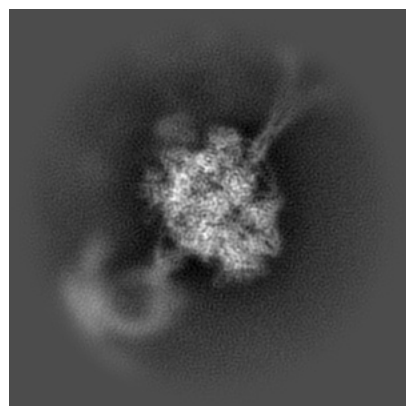
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73173. These allow visual inspection of the internal detail of the map and identification of artifacts.

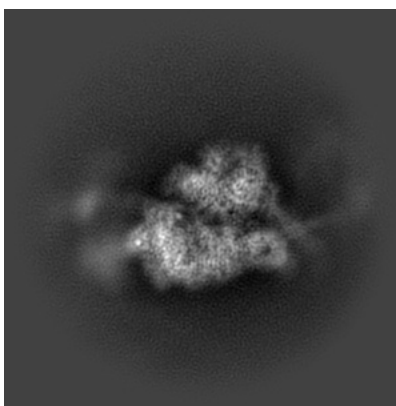
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

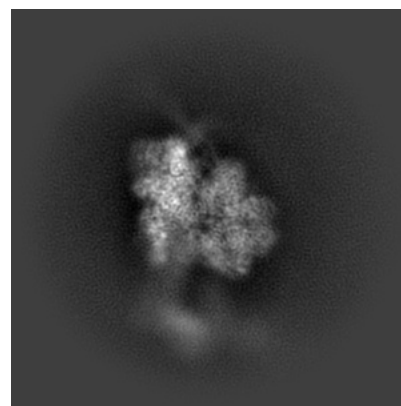
6.1.1 Primary map



X

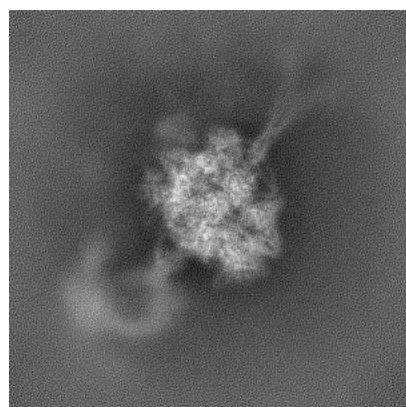


Y

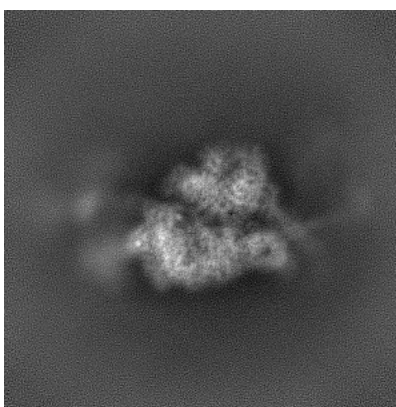


Z

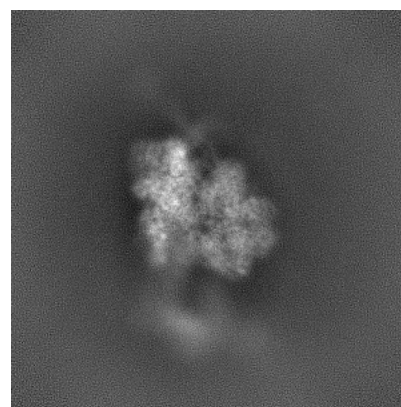
6.1.2 Raw map



X



Y

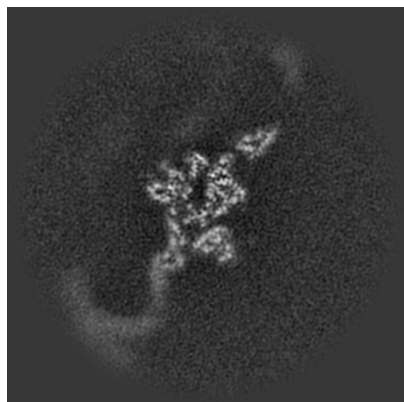


Z

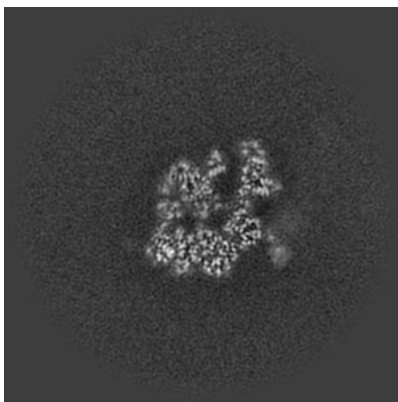
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

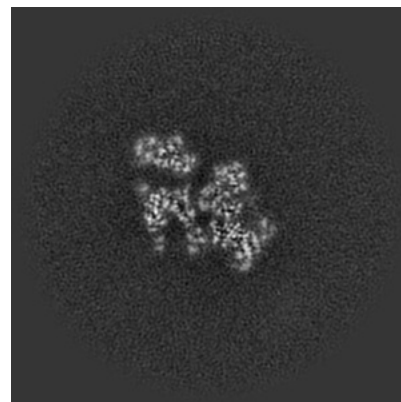
6.2.1 Primary map



X Index: 192

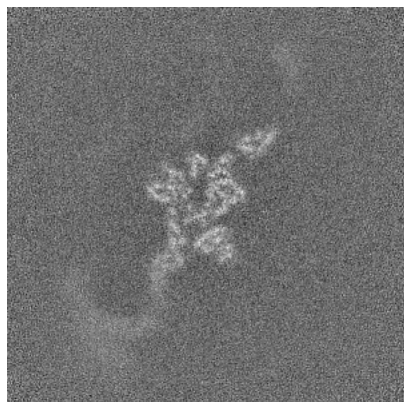


Y Index: 192

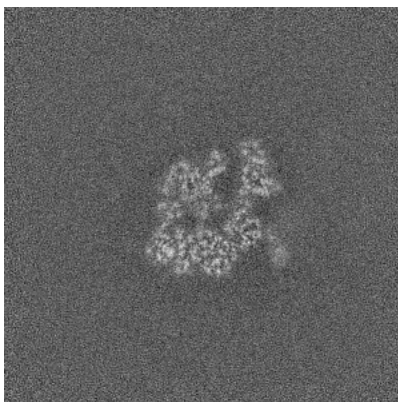


Z Index: 192

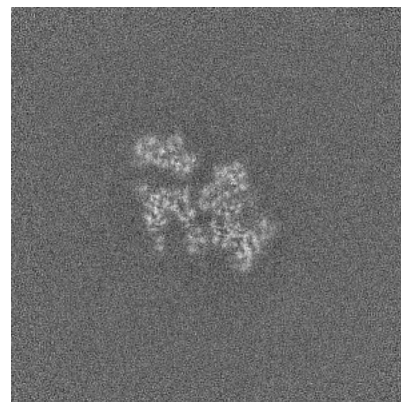
6.2.2 Raw map



X Index: 192



Y Index: 192

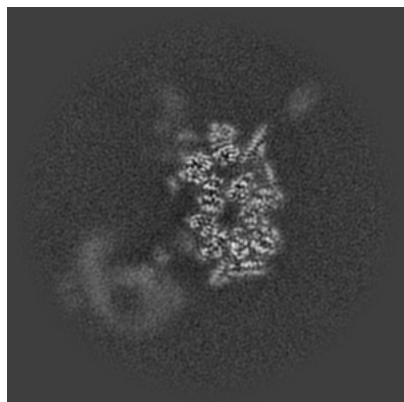


Z Index: 192

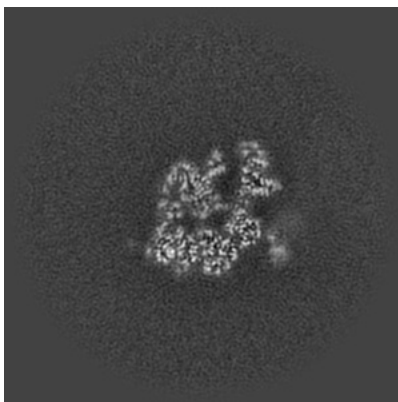
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

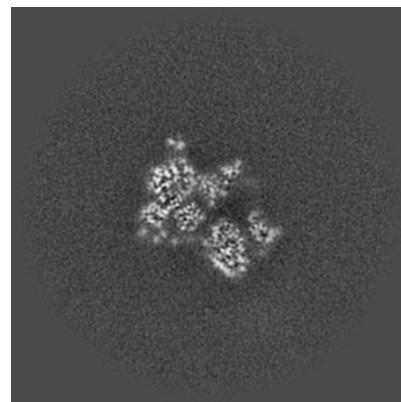
6.3.1 Primary map



X Index: 157

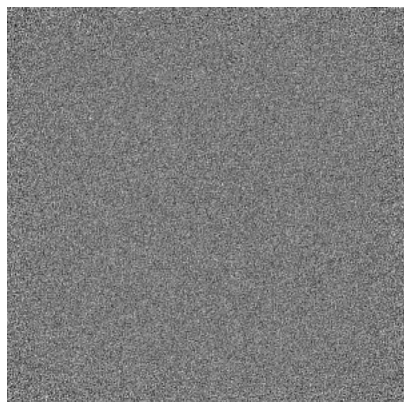


Y Index: 193

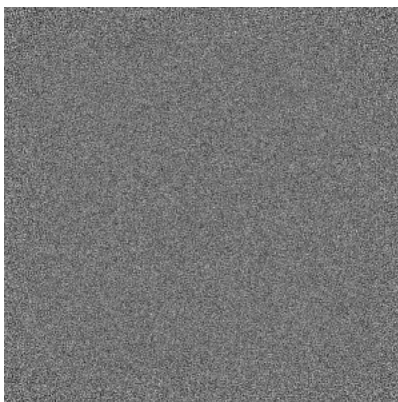


Z Index: 214

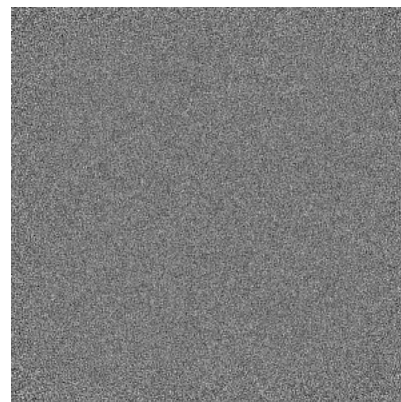
6.3.2 Raw map



X Index: 0



Y Index: 0

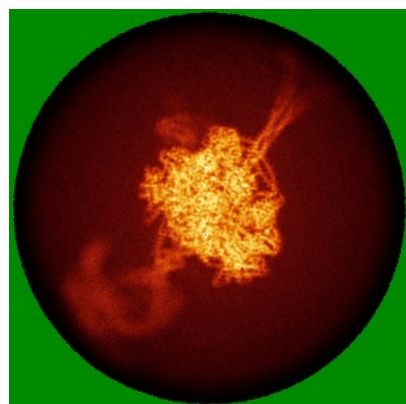


Z Index: 0

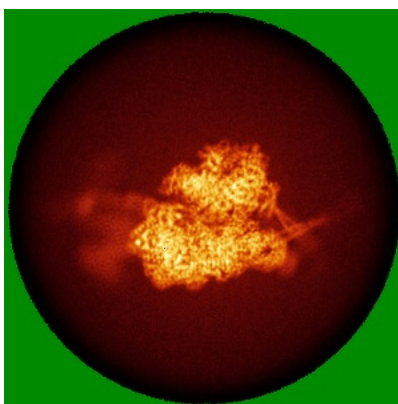
The images above show the largest variance slices of the map in three orthogonal directions.

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

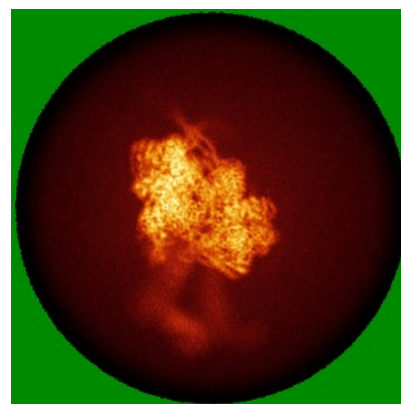
6.4.1 Primary map



X

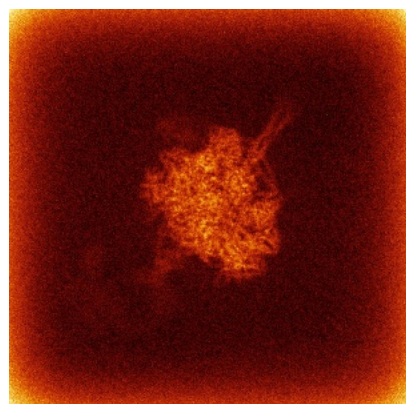


Y

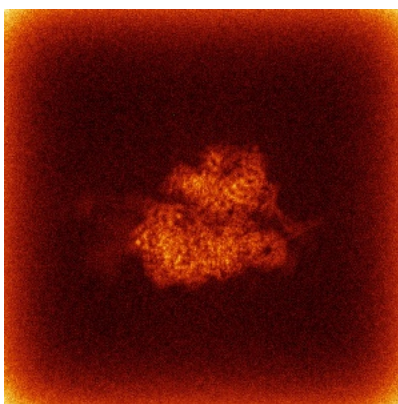


Z

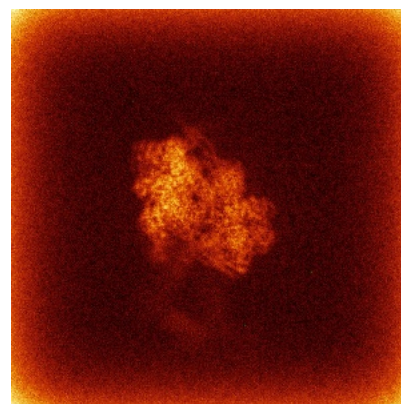
6.4.2 Raw map



X



Y

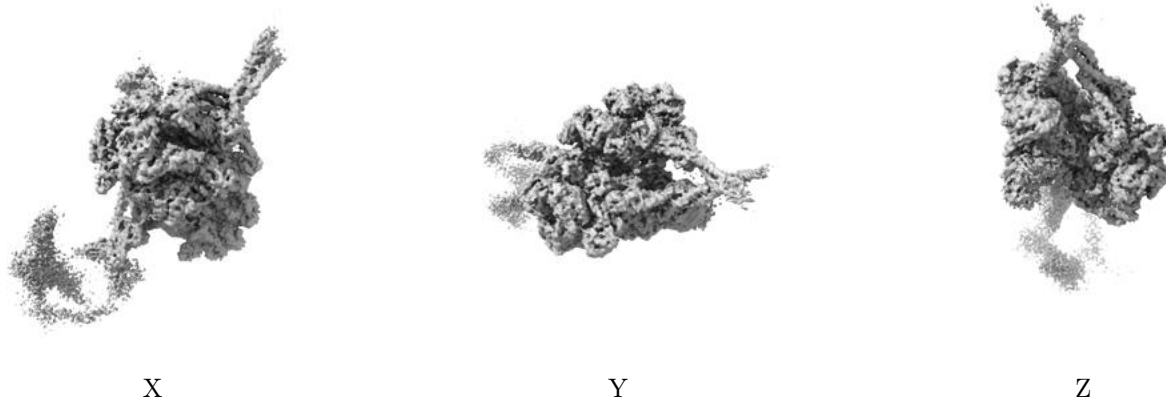


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

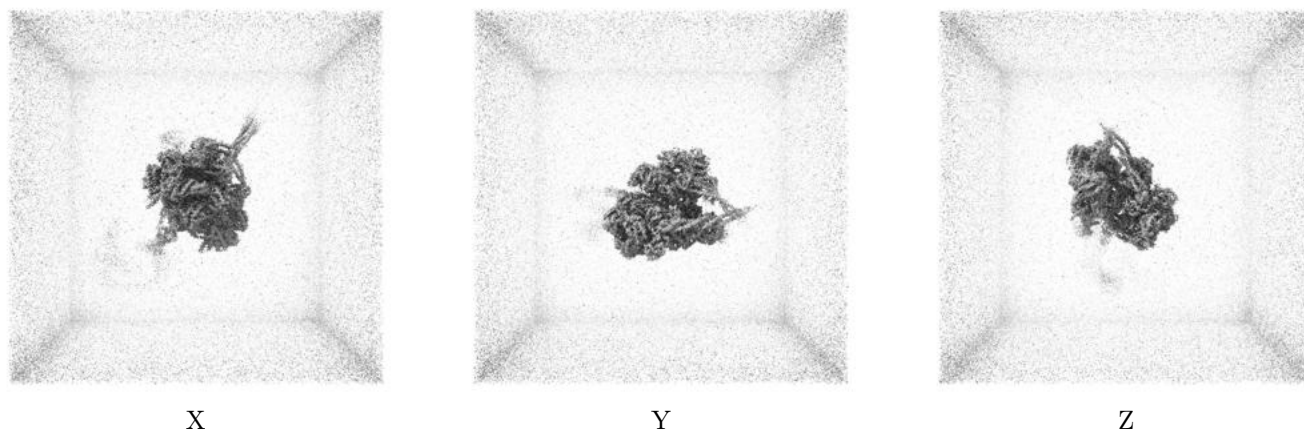
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

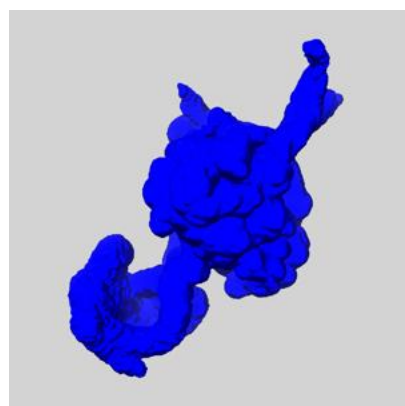
6.6 Mask visualisation [i](#)

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

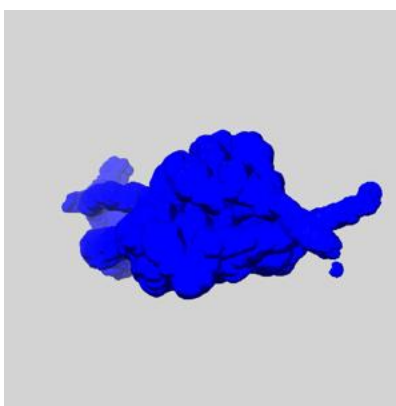
A mask typically either:

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

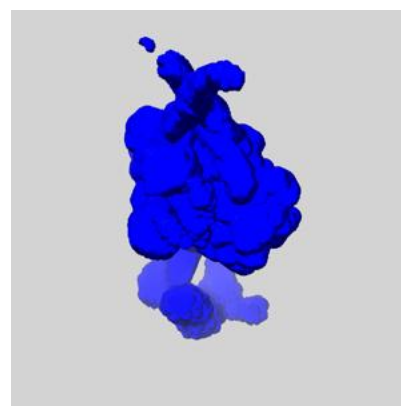
6.6.1 emd_73173_msk_1.map [i](#)



X



Y

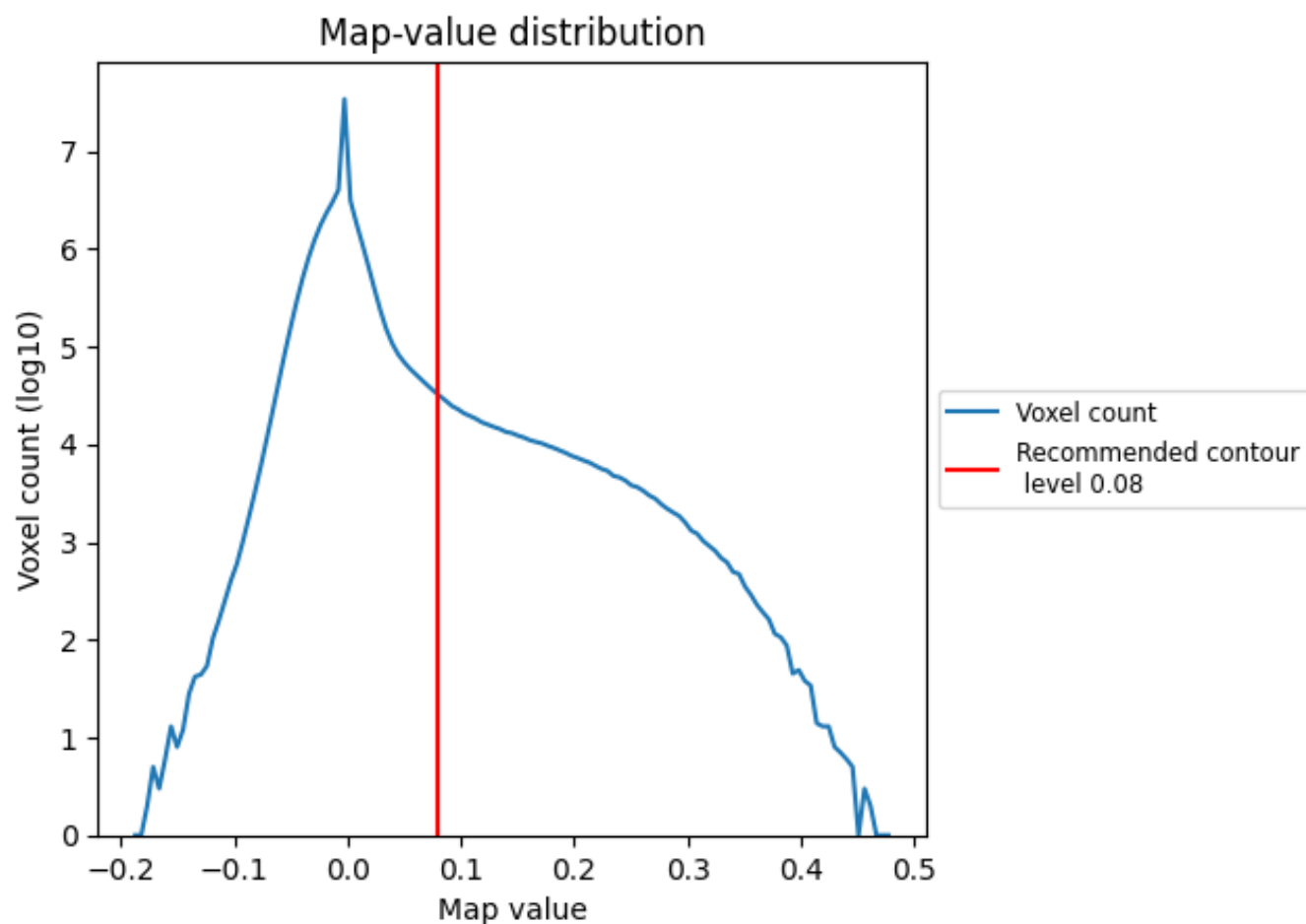


Z

7 Map analysis [i](#)

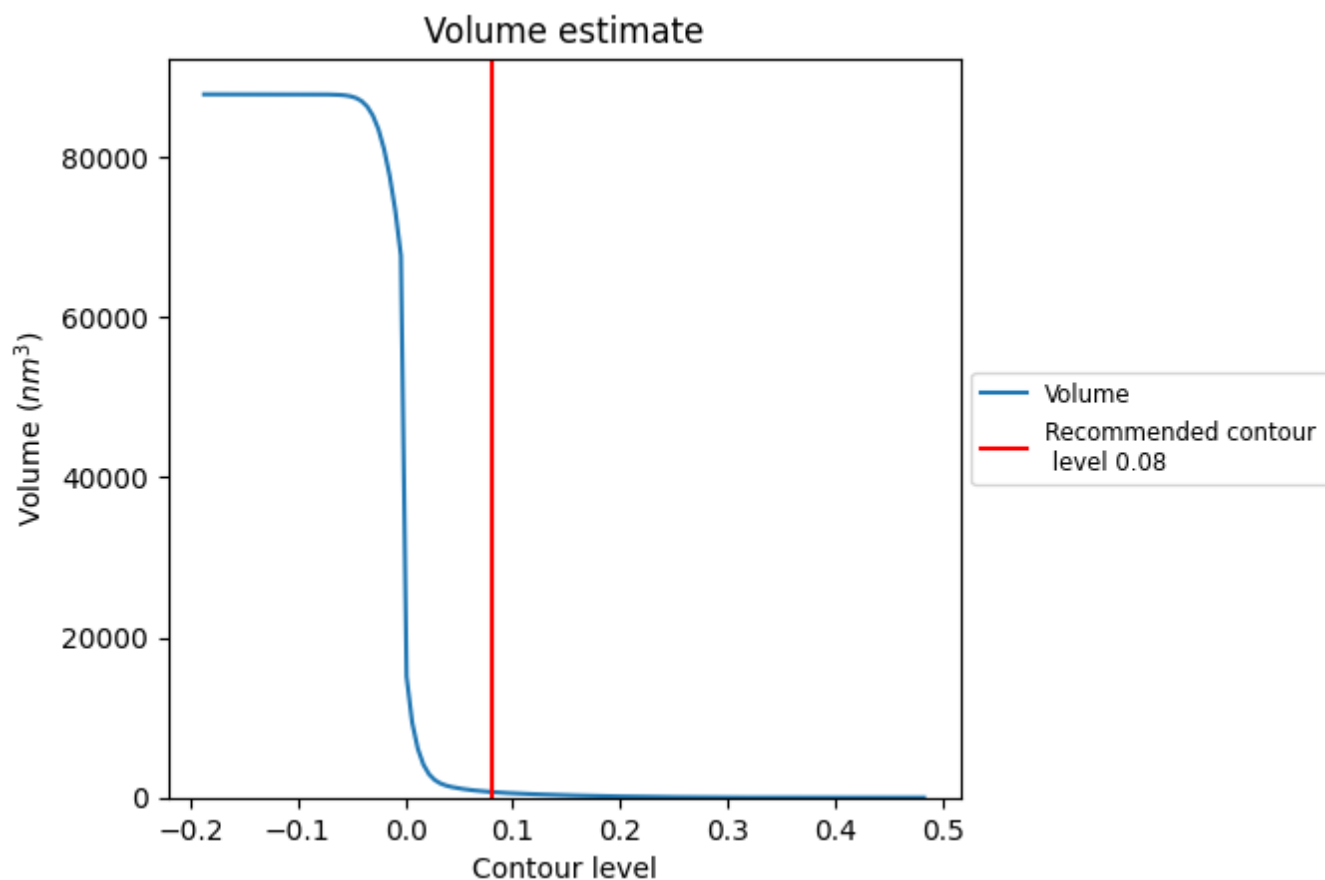
This section contains the results of statistical analysis of the map.

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.

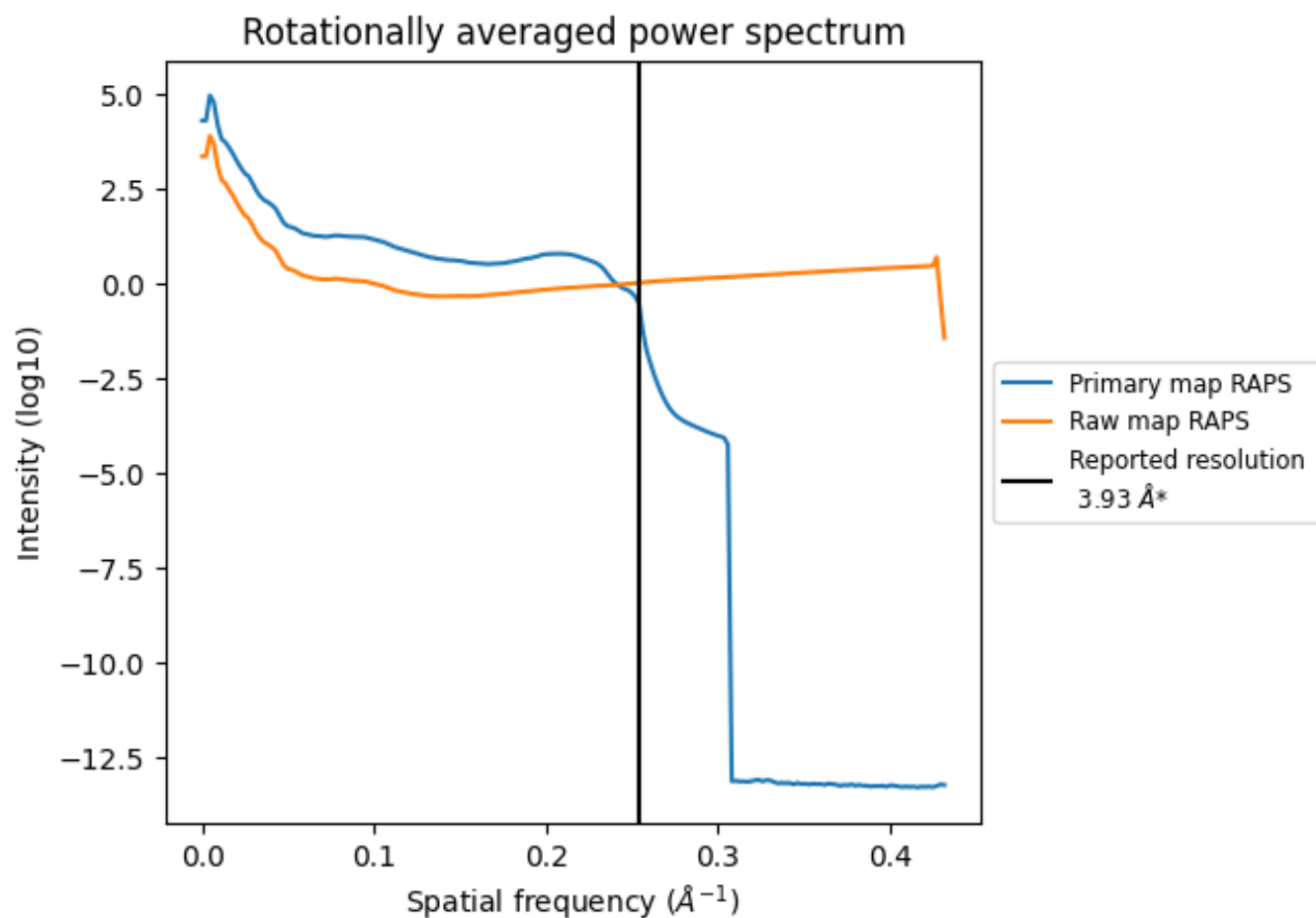
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 698 nm³; this corresponds to an approximate mass of 631 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 ⓘ

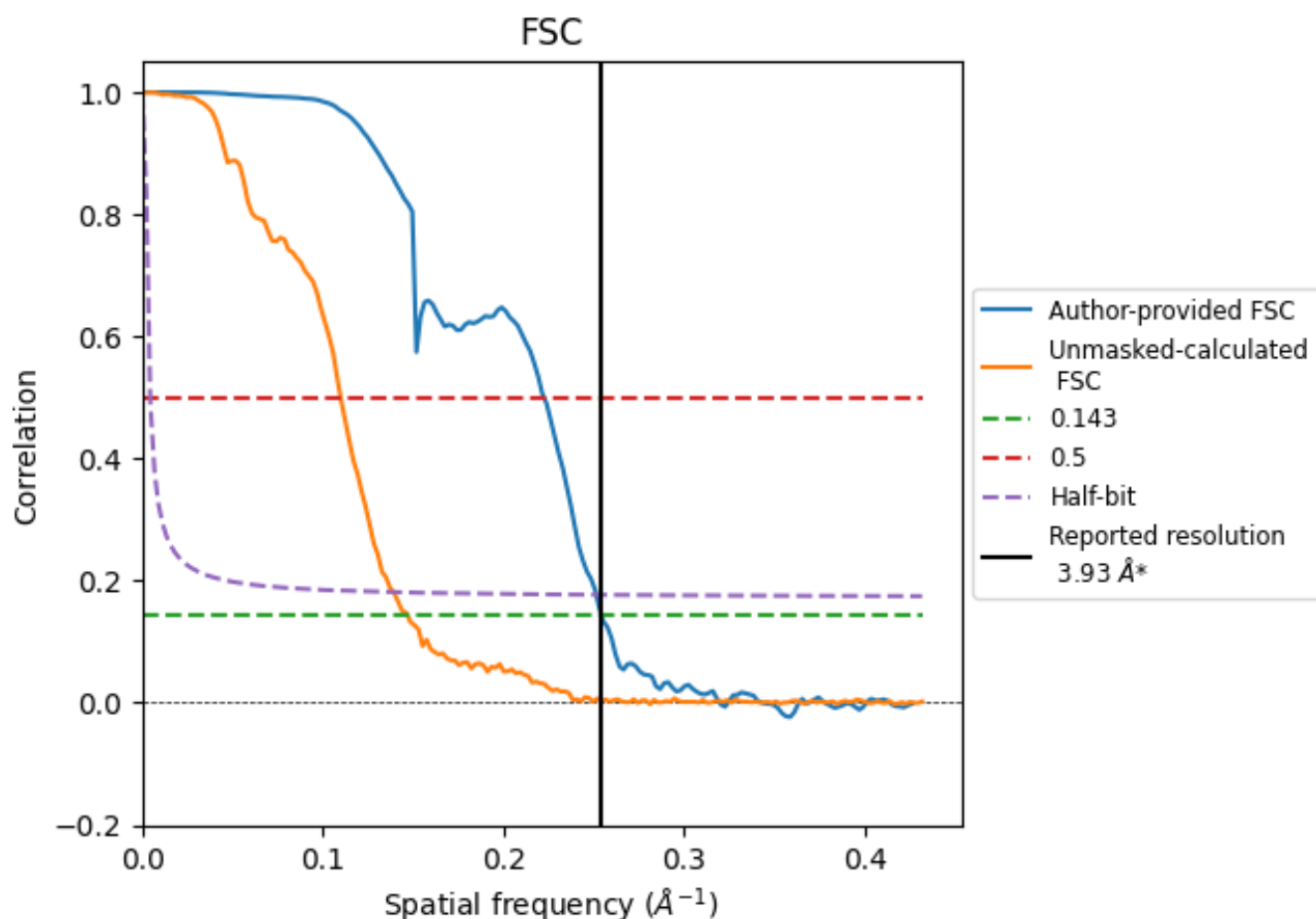


*Reported resolution corresponds to spatial frequency of 0.254 Å⁻¹

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 0.254 \AA^{-1}

8.2 Resolution estimates [i](#)

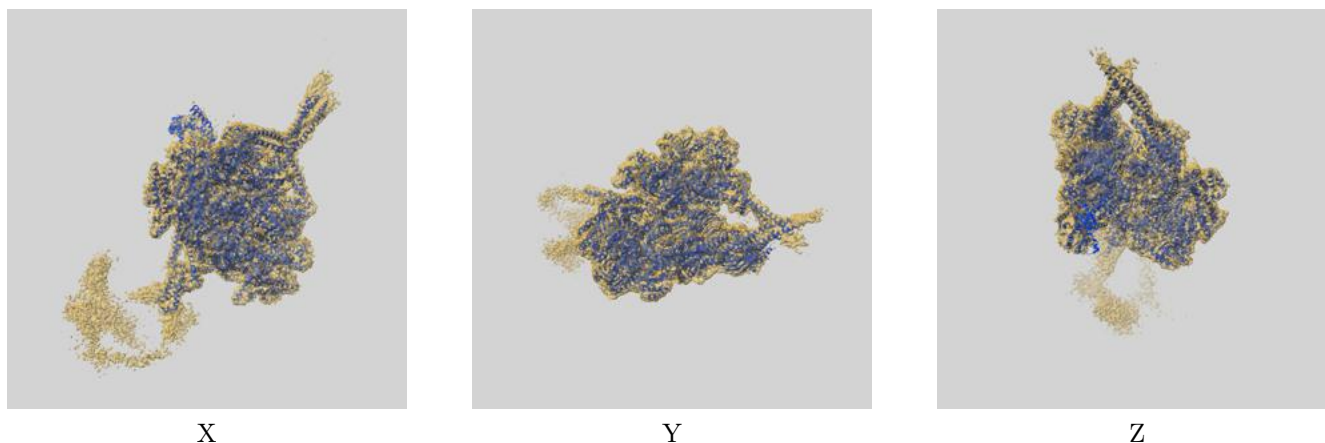
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.93	-	-
Author-provided FSC curve	3.93	4.49	3.98
Unmasked-calculated*	6.81	9.10	7.18

*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 6.81 differs from the reported value 3.93 by more than 10 %

9 Map-model fit [i](#)

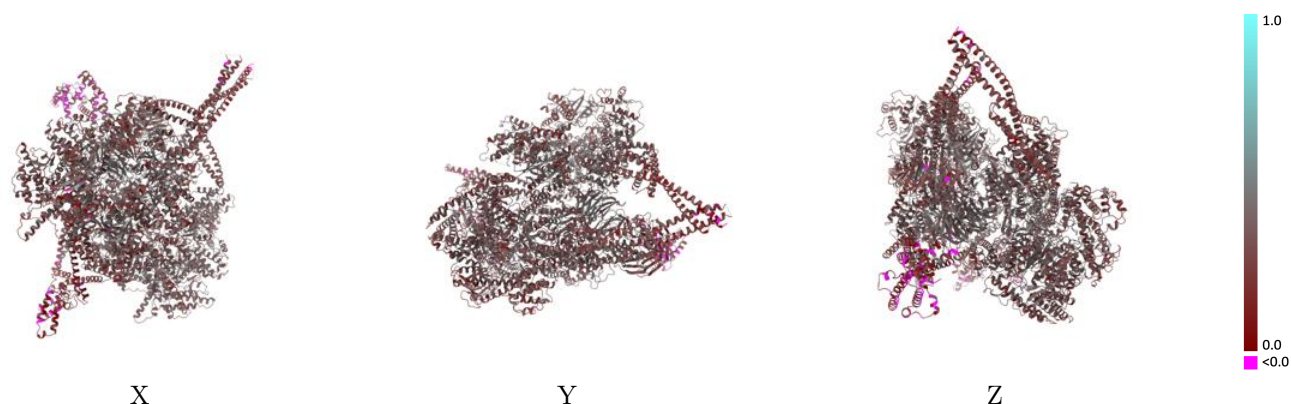
This section contains information regarding the fit between EMDB map EMD-73173 and PDB model 9YNC. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



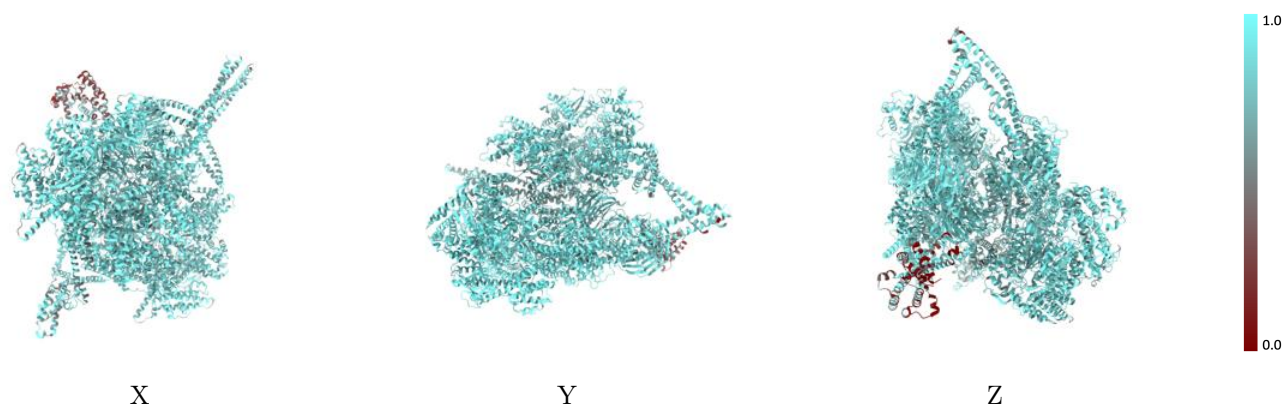
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



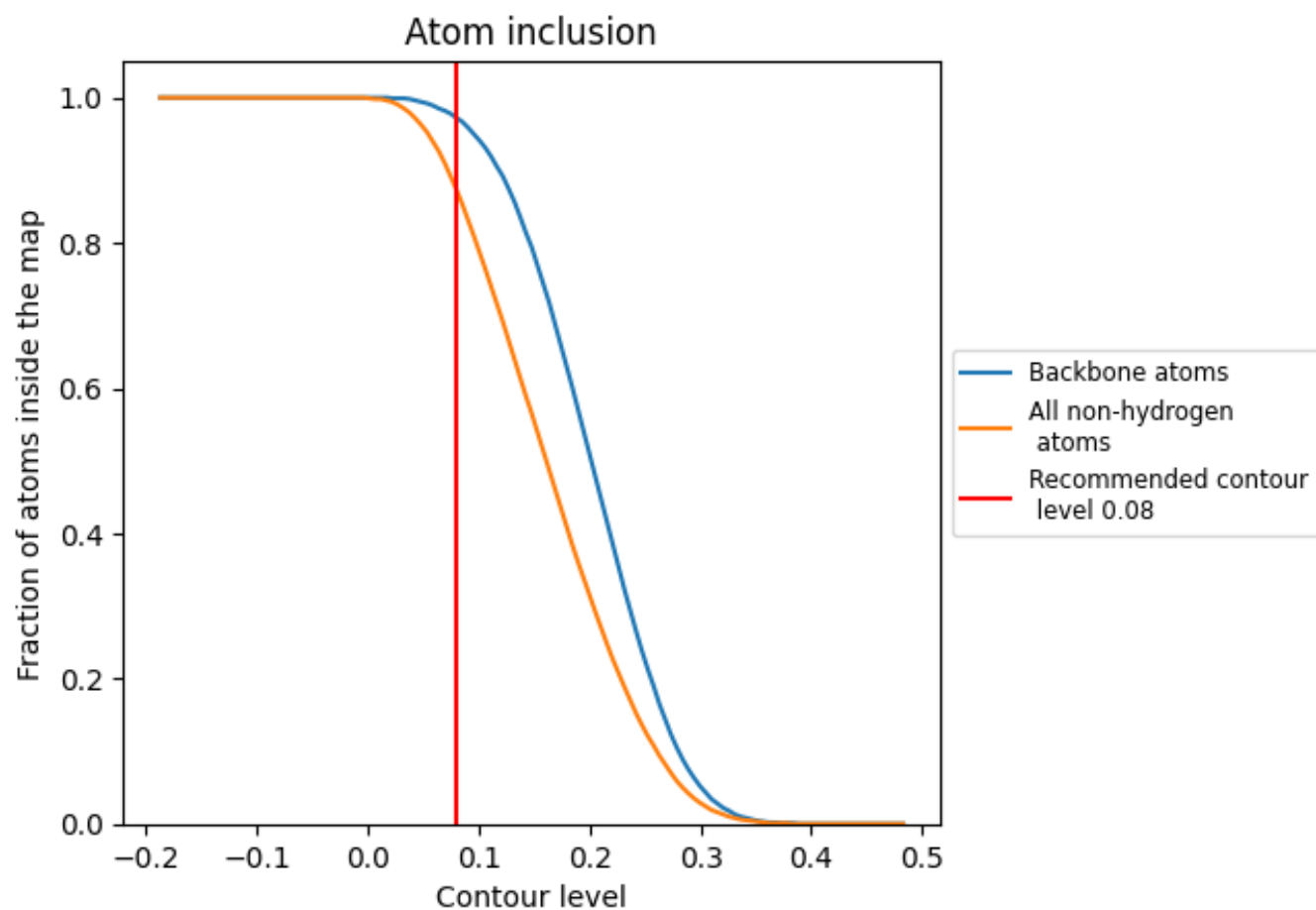
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 87% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8730	<div></div> 0.3360
A	<div></div> 0.8620	<div></div> 0.3330
B	<div></div> 0.8990	<div></div> 0.3430
C	<div></div> 0.8750	<div></div> 0.3970
D	<div></div> 0.9010	<div></div> 0.3220
E	<div></div> 0.3240	<div></div> 0.1010
F	<div></div> 0.5500	<div></div> 0.1330
G	<div></div> 0.8760	<div></div> 0.2920
H	<div></div> 0.8470	<div></div> 0.3090
I	<div></div> 0.7760	<div></div> 0.2370
J	<div></div> 0.8280	<div></div> 0.2870

1.0

0.0

<0.0