



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 05:55 AM UTC

PDB ID : 9E11 / pdb_00009e11
EMDB ID : EMD-47380
Title : Dimeric motor domains from phi-like dynein-1 bound to a Lis1 dimer under Lis1 condition
Authors : Yang, J.; Zhang, K.
Deposited on : 2024-10-21
Resolution : 2.86 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

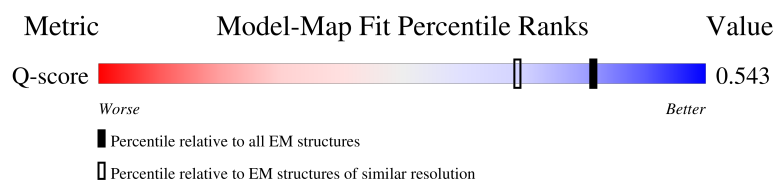
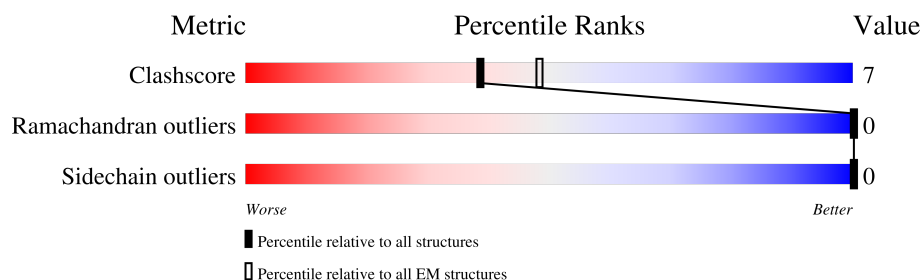
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.86 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	12017 (2.36 - 3.36)

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	<div> <div>7%</div> <div>51%</div> <div>12%</div> <div>37%</div> </div>
1	B	4646	<div> <div>.</div> <div>52%</div> <div>11%</div> <div>37%</div> </div>
2	C	410	<div> <div>.</div> <div>61%</div> <div>18%</div> <div>21%</div> </div>
2	D	410	<div> <div>22%</div> <div>52%</div> <div>26%</div> <div>22%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 52502 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.

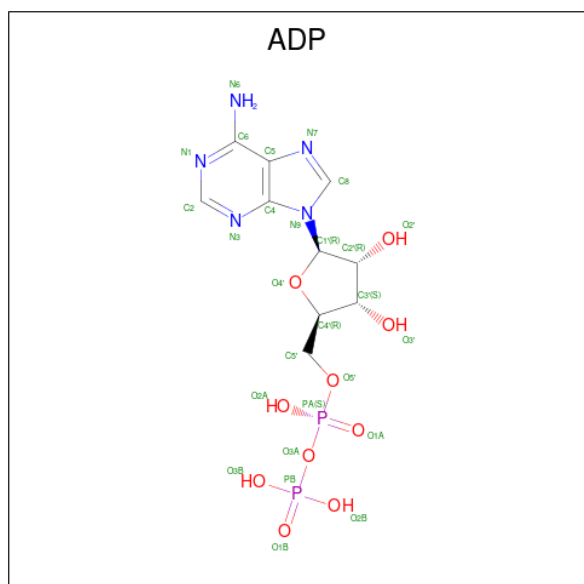
- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

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

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

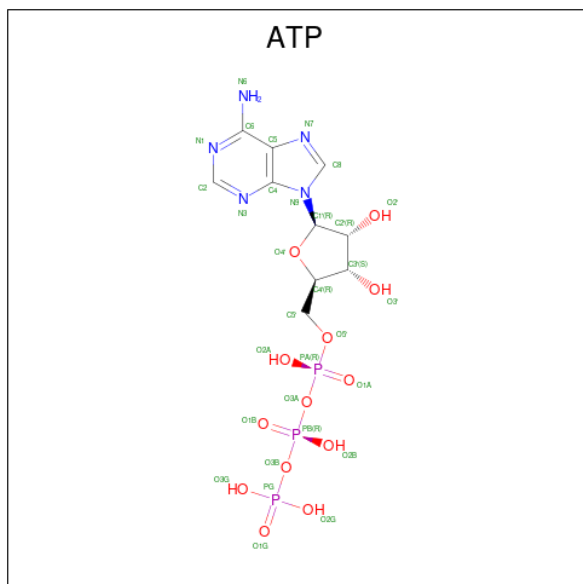
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	322	Total	C	N	O	S	0	0
			2557	1608	452	477	20		
2	D	319	Total	C	N	O	S	0	0
			2531	1593	446	472	20		

- Molecule 3 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
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 4 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
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

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

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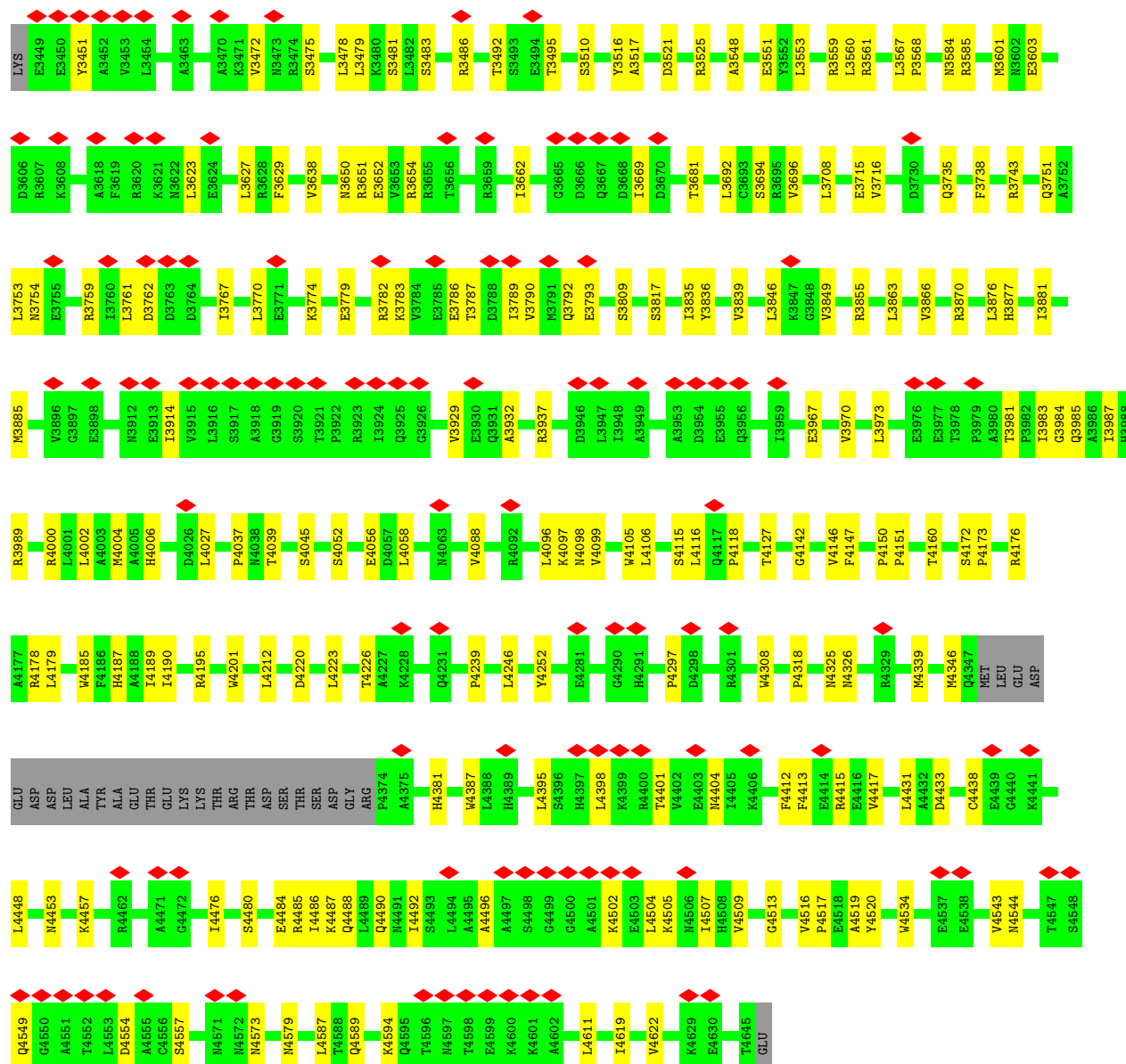
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	B	2	2	2	0

A2040	E1837	H1701	D1590	L1509	LYS	ALA	VAL	TRP	ARG	GLU	ALA	ASN	GLU	LEU	ARG	GLU	ASN	PHE
R2046	W1836	L1702	V1591	S1510	ASN	SER	ALA	GLU	PHE	PHE	GLN	GLN	THR	LEU	THR	LEU	LEU	ASN
Q2047	L1839	E1706	Q1595	K1514	GLU	THR	GLU	LYS	THR	THR	VAL	VAL	GLN	ILE	ARG	ILE	ASP	PHE
Q2051	R1843	K1707	G1596	V1515	ILE	PHE	GLU	LYS	PRO	PRO	VAL	VAL	LEU	VAL	ILE	ILE	GLY	LYS
L2054	Q1850	E1708	V1597	F1516	VAL	GLN	GLN	VAL	SER	TRP	ASP	LYS	SER	ARG	PRO	VAL	GLY	VAL
R2060	T1851	M1709	Q1598	E1517	LYS	ARG	ASP	GLN	TRP	TRP	ASP	PRO	ASP	ILE	ASP	GLN	GLY	LYS
E2063	D1852	R1710	Q1599	E1518	ASP	GLN	VAL	VAL	TRP	TRP	VAL	VAL	GLY	VAL	VAL	LEU	LEU	ASP
A2066	Q1856	T1711	E1602	D1519	LEU	LEU	GLY	GLY	ARG	ILE	TRP	TRP	ASN	ASN	ASN	GLY	GLY	ILE
I2069	Y1872	L1717	D1606	L1520	VAL	THR	THR	THR	PRO	ILE	GLU	GLU	LEU	LEU	LEU	PRO	VAL	ILE
V2070	D1877	V1721	L1607	S1522	GLN	MET	SER	GLU	GLU	GLU	SER	GLU	GLU	GLU	GLU	ARG	VAL	GLU
P2071	K1878	V1724	L1608	W1523	GLY	LYS	GLU	ALA	ALA	ALA	GLY	GLY	GLN	GLN	GLN	ILE	LEU	LYS
F2072	L1879	E1725	G1609	E1524	ILE	ILE	SER	LEU	LEU	LEU	SER	SER	SER	SER	THR	THR	ALA	ILE
V2073	K1879	D1726	K1610	D1525	ASN	ASN	LEU	GLN	GLN	GLN	GLY	GLY	GLY	GLY	THR	THR	GLY	ASP
K2074	V1880	T1727	I1611	K1526	LEU	VAL	VAL	ALA	ALA	ALA	GLY	GLY	GLY	GLY	VAL	VAL	LEU	LEU
L2080	Q1881	G1728	Q1612	L1527	VAL	VAL	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	LYS	LYS	ARG	GLU
L2090	C1888	K1729	E1617	L1533	ILE	ILE	GLU	THR	PHE	PHE	VAL	MET	MET	VAL	VAL	VAL	ALA	VAL
R2091	A1895	A1730	R1623	F1534	GLU	GLU	GLN	ILE	ASN	ASN	GLN	GLY	GLY	GLY	THR	THR	GLY	THR
V2096	L1896	D1734	P1627	W1537	SER	SER	GLY	GLY	ILE	ILE	ASP	GLY	GLY	GLY	VAL	VAL	VAL	GLY
L2097	E1897	P1735	D1632	D1539	GLU	GLU	MET	LYS	ARG	ARG	MET	ASP	ASP	ASP	VAL	VAL	VAL	THR
E2106	A1898	K1736	G1633	R1543	ALA	ALA	LYS	TRP	LYS	LYS	GLN	GLY	GLY	GLY	ILE	ILE	GLY	THR
R2110	R1918	T1739	D1634	Y1546	ASP	ASP	PRO	TRP	LYS	LYS	GLN	GLY	GLY	GLY	THR	THR	THR	GLY
R2113	N1931	I1740	E1635	L1547	LYS	LYS	GLN	TRP	ASP	ASP	GLN	GLY	GLY	GLY	ASP	ASP	ALA	ALA
E2114	V1946	W1741	D1636	E1548	THR	THR	GLN	VAL	VAL	VAL	VAL	THR	THR	THR	VAL	VAL	GLN	THR
E2116	Q1950	L1749	I1640	S1554	LEU	LEU	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	THR
R2117	R1962	V1750	I1641	D1555	ARG	ARG	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	THR
E2118	E1984	I1756	K1649	T1557	LYS	LYS	LEU	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	THR
G2119	N1987	E1760	H1653	H1558	HIS	HIS	LEU	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	THR
E2120	P1988	G1770	F1654	L1560	ASN	ASN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	THR
A2121	N1989	G1771	K1655	E1564	VAL	VAL	LEU	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	THR
V2122	Y1990	G1772	K1656	T1565	TRP	TRP	LEU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	THR
D2123	D1991	G1773	I1665	Q1569	VAL	VAL	LEU	ASP	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	THR
E2124	K1992	D1774	E1668	S1572	GLU	GLU	LEU	LEU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	THR
G2125	T1993	S1795	D1669	T1573	LEU	LEU	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR
E2126	S1994	Q1800	N1670	L1576	LYS	LYS	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	THR
E2129	A1995	L1811	S1671	A1577	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
R2130	E2000	E1814	R1679	L1578	GLY	GLY	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	THR
L2131	V2006	E1814	E1683	M1579	ILE	ILE	PHE	PRO	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	THR
E2133	V2006	H1817	K1687	K1580	TRP	TRP	ALA	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
Q2134	M2012	D1831	T1693	K1581	ASP	ASP	VAL	VAL	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	THR
I2138	R2037	S1835	T1698	S1583	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	THR
L2149	L2039	F1836	E1700	L1587	M1507	M1507	K1508	K1508	K1508	K1508	K1508	K1508	K1508	K1508	K1508	K1508	K1508	THR

S5483	L2157	D2304	L2413	K2551	R2729	R2863	L3012	V3148	D3238	SER	GLU	LYS	S5483
R3486	L2161	G2305	T2423	Q2554	H2730	E2864	A3013	F3149	K3239	ILE	ILE	LEU	R3486
E3490	D2162	D2306	M2423	V2562	V2731	S2868	N3014	G3019	L3240	LYS	ASP	ASP	E3490
K3491	D2163	V2307	N2430	A2563	P2732	L2877	G3019	T3153	K3241	GLN	ALA	ALA	K3491
E3494	V2164	D2308	V2433	A2564	V2733	S2878	D3024	L3154	K3242	HIS	ARG	ARG	E3494
T3495	F2165	N2314	V2437	P2565	V2734	R2879	C3033	A3157	VAL	LEU	GLU	GLU	T3495
M3500	R2172	N2316	H2445	D2573	Y2738	D2880	Q3038	L3161	GLN	ASP	GLN	ASP	M3500
S3501	Q2173	D2320	L2446	D2576	L2756	V2884	K3039	A3162	VAL	GLN	ASP	GLN	S3501
T3502	E2174	L2315	M2447	D2577	R2757	D2885	E3040	K3163	ALA	GLU	ALA	ALA	T3502
D3506	L2175	L2324	H2448	R2576	L2758	K2894	M3043	T3168	GLU	GLU	GLU	GLU	D3506
S3510	T2176	E2331	L2449	L2581	P2768	A2895	L3044	T3172	LYS	LYS	PRO	LYS	S3510
Y3516	E2180	R2332	T2450	L2581	L2769	R2896	D3045	F3173	LYS	ALA	ALA	ALA	Y3516
A3517	E2181	M2342	R2451	V2584	M2773	K2898	S3046	R3175	VAL	ALA	VAL	VAL	A3517
D3521	C2186	F2343	R2452	P2590	F2784	V2899	H3047	H3175	MET	LYS	VAL	VAL	D3521
M3524	K2189	Q2346	C2454	P2592	Y2792	E2902	E3048	D3178	GLN	LEU	GLN	GLN	M3524
R3525	Y2190	T2355	S2457	V2592	I2793	E2903	E3049	H3182	ILE	LEU	ILE	ILE	R3525
W3532	L2191	V2356	H2462	L2593	Y2794	L2905	F3054	R3191	GLN	GLN	GLN	GLN	W3532
Q3542	E2205	S2357	L2463	P2596	S2795	L2911	R3060	S3192	GLU	GLN	GLN	GLN	Q3542
D3546	L2208	M2361	R2467	G2598	R2801	L2934	F3066	E3193	GLY	GLY	GLY	GLY	D3546
I3547	Y2211	T2371	Y2472	G2598	W2802	L2934	T3067	L3194	GLU	GLU	GLU	GLU	I3547
L3553	Q2215	I2374	N2475	G2619	R2804	K2943	M3068	G3204	THR	THR	THR	THR	L3553
D3557	L2220	I2385	D2478	T2626	E2811	A2951	E3073	T3208	ASP	ASP	ASP	ASP	D3557
E3558	M2221	P2386	F2479	K2633	E2814	L2956	D3077	K3209	LYS	LYS	LYS	LYS	E3558
R3559	V2222	L2387	P2480	F2635	T2815	K2962	R3088	E3210	GLN	GLN	GLN	GLN	R3559
W3562	G2224	E2388	M2481	R2643	E2819	R2963	F3094	T3211	MET	MET	MET	MET	W3562
Q3563	Q2227	GLY	Q2482	T2644	E2822	R2964	T3099	V3212	VAL	VAL	VAL	VAL	Q3563
L3567	S2231	ASP	I2483	N2646	R2823	R2965	E3100	E3216	GLU	GLU	GLU	GLU	L3567
R3582	M2232	GLU	L2486	P2645	W2825	E2970	D3114	L3218	ASP	ASP	ASP	ASP	R3582
F3583	A2233	ALA	E2487	L2650	L2824	L2980	L3115	R3219	ILE	ILE	ILE	ILE	F3583
N3584	W2234	ARG	V2495	Q2654	W2825	K2989	E3116	E3217	GLN	GLN	GLN	GLN	N3584
R3585	L2244	ARG	T2498	T2644	E2829	V2998	D3124	L3218	VAL	VAL	VAL	VAL	R3585
T3597	K2267	ARG	T2507	N2646	R2836	V2998	Y3125	E3218	PRO	PRO	PRO	PRO	T3597
R3611	W2271	LYS	L2508	L2650	L2837	V2998	M3126	R3220	ALA	ALA	ALA	ALA	R3611
L3615	T2275	GLU	K2509	Q2654	E2840	V2998	V3129	R3221	ILE	ILE	ILE	ILE	L3615
L3627	T2276	GLU	L2526	F2662	E2842	V2998	Y3130	D3221	THR	THR	THR	THR	L3627
L3634	D2277	GLY	T2276	F2662	E2842	V2998	D3131	Q3227	VAL	VAL	VAL	VAL	L3634
Q3636	R2285	GLU	W2531	P2669	R2843	V2998	K3132	E3228	ASN	ASN	ASN	ASN	Q3636
	S2290	ALA	T2534	V2709	R2844	L3000	L3133	E3229	ALA	ALA	ALA	ALA	
	L2295	ALA	E2538	P2714	R2861	D3001	F3004	R3231	VAL	VAL	VAL	VAL	
									LYS	LYS	LYS	LYS	

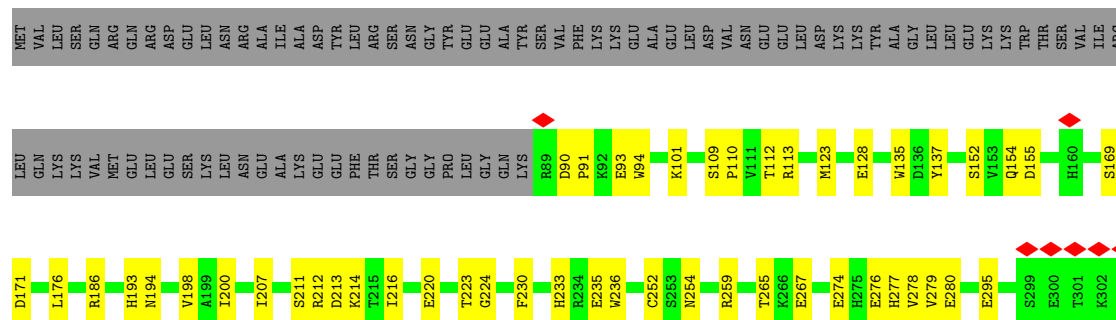


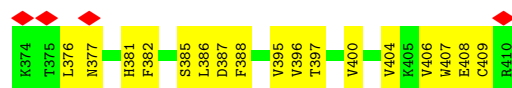




- Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta

Chain C: 61% 18% 21%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	215049	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	2.214	Depositor
Minimum map value	-1.179	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1573, 1.1573, 1.1573	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.11	0/24093	0.27	0/32651
1	B	0.12	0/24093	0.27	0/32651
2	C	0.13	0/2624	0.31	0/3555
2	D	0.13	0/2597	0.34	0/3518
All	All	0.12	0/53407	0.28	0/72375

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	23593	0	23659	340	0
1	B	23593	0	23657	305	0
2	C	2557	0	2487	48	0
2	D	2531	0	2463	77	0
3	A	81	0	36	0	0
3	B	81	0	36	2	0
4	A	31	0	12	2	0
4	B	31	0	12	0	0
5	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	2	0	0	0	0
All	All	52502	0	52362	767	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 767 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:4296:MET:HE3	1:A:4297:PRO:HD2	1.53	0.91
1:B:1490:TRP:HH2	1:B:1537:TRP:HD1	1.24	0.86
1:A:1565:THR:HG22	1:A:1569:GLN:HE22	1.43	0.84
1:A:2221:MET:HG3	1:A:2343:PHE:HB2	1.59	0.84
1:B:2495:VAL:HG21	1:B:2524:VAL:HG21	1.65	0.79

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	2929/4646 (63%)	2879 (98%)	50 (2%)	0	100	100
1	B	2929/4646 (63%)	2868 (98%)	61 (2%)	0	100	100
2	C	320/410 (78%)	310 (97%)	10 (3%)	0	100	100
2	D	317/410 (77%)	305 (96%)	12 (4%)	0	100	100
All	All	6495/10112 (64%)	6362 (98%)	133 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2605/4125 (63%)	2605 (100%)	0	100	100
1	B	2605/4125 (63%)	2605 (100%)	0	100	100
2	C	287/364 (79%)	287 (100%)	0	100	100
2	D	284/364 (78%)	284 (100%)	0	100	100
All	All	5781/8978 (64%)	5781 (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. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3526	GLN
2	D	381	HIS
1	B	3744	GLN
1	B	4191	GLN
1	A	3952	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

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
4	ATP	B	4702	5	32,33,33	0.37	0	48,52,52	0.27	0
3	ADP	A	4703	-	28,29,29	1.40	4 (14%)	43,45,45	1.86	8 (18%)
3	ADP	B	4703	-	28,29,29	1.41	4 (14%)	43,45,45	1.87	8 (18%)
3	ADP	B	4704	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	9 (20%)
3	ADP	A	4704	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	9 (20%)
4	ATP	A	4702	5	32,33,33	0.34	0	48,52,52	0.29	0
3	ADP	A	4701	5	28,29,29	1.39	4 (14%)	43,45,45	1.83	9 (20%)
3	ADP	B	4701	5	28,29,29	1.40	4 (14%)	43,45,45	1.83	8 (18%)

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
4	ATP	B	4702	5	-	4/22/38/38	0/3/3/3
3	ADP	A	4703	-	-	2/16/32/32	0/3/3/3
3	ADP	B	4703	-	-	1/16/32/32	0/3/3/3
3	ADP	B	4704	-	-	1/16/32/32	0/3/3/3
3	ADP	A	4704	-	-	3/16/32/32	0/3/3/3
4	ATP	A	4702	5	-	3/22/38/38	0/3/3/3
3	ADP	A	4701	5	-	2/16/32/32	0/3/3/3
3	ADP	B	4701	5	-	4/16/32/32	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	4703	ADP	C5-C4	4.73	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4703	ADP	C5-C4	4.72	1.47	1.39
3	A	4704	ADP	C5-C4	4.69	1.47	1.39
3	A	4701	ADP	C5-C4	4.60	1.47	1.39
3	B	4701	ADP	C5-C4	4.60	1.47	1.39

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4703	ADP	C5-C4-N3	-6.12	118.29	126.72
3	A	4703	ADP	C5-C4-N3	-6.04	118.40	126.72
3	A	4704	ADP	C5-C4-N3	-5.86	118.65	126.72
3	B	4704	ADP	C5-C4-N3	-5.86	118.65	126.72
3	B	4701	ADP	C5-C4-N3	-5.79	118.74	126.72

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4703	ADP	C5'-O5'-PA-O1A
3	A	4704	ADP	C5'-O5'-PA-O1A
3	B	4701	ADP	C5'-O5'-PA-O1A
3	B	4701	ADP	C5'-O5'-PA-O3A
4	B	4702	ATP	O4'-C4'-C5'-O5'

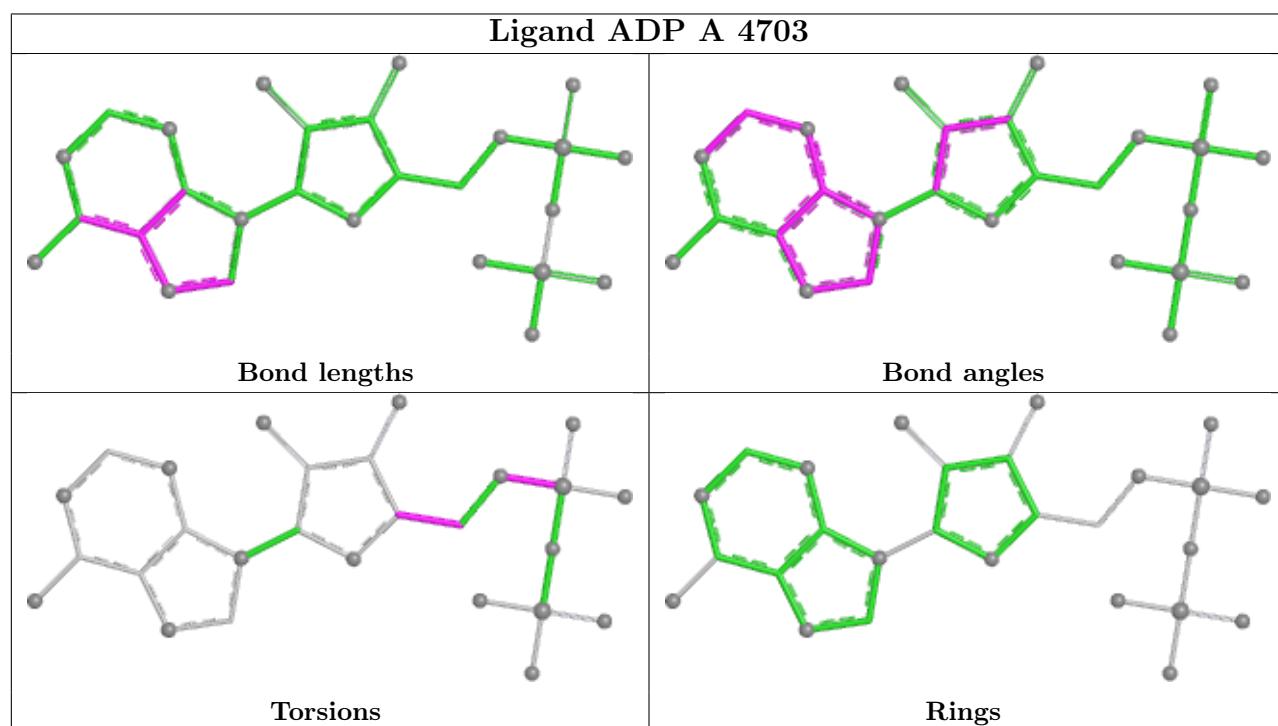
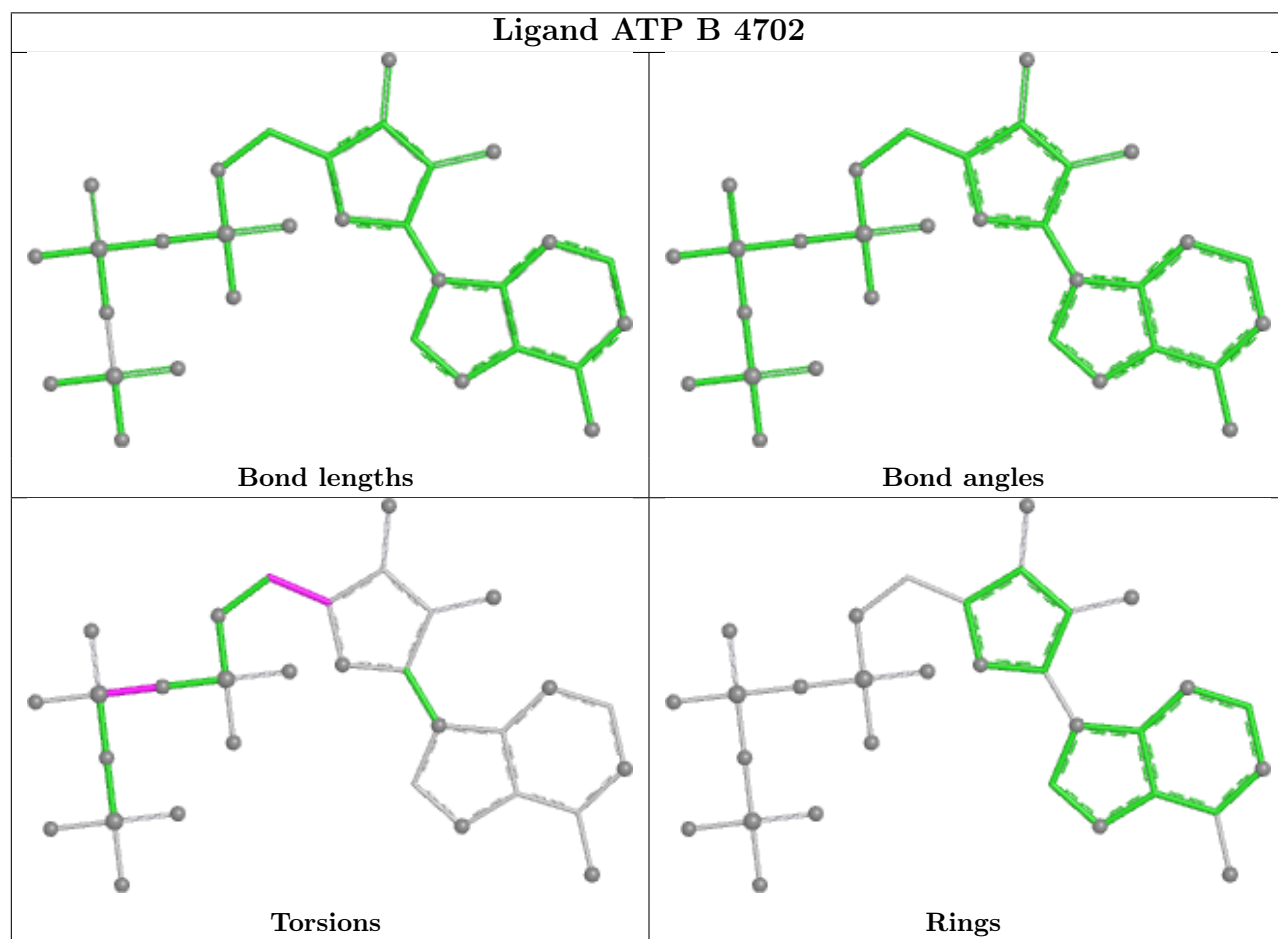
There are no ring outliers.

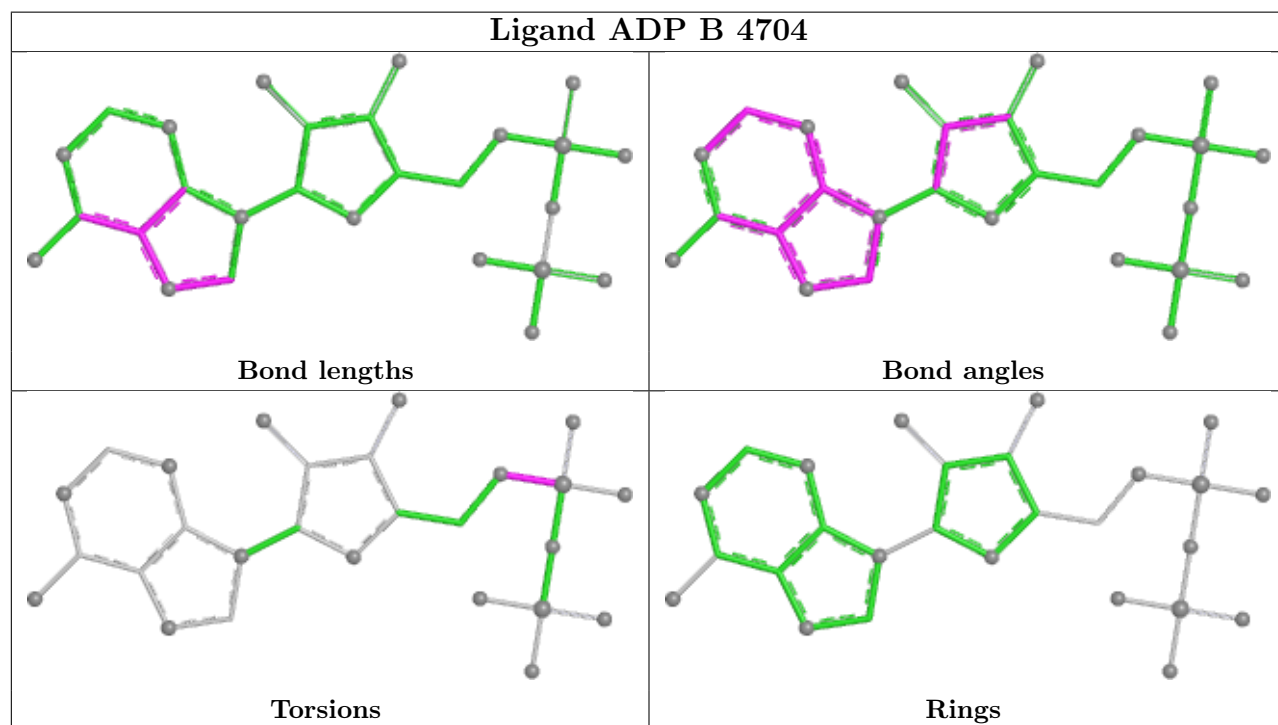
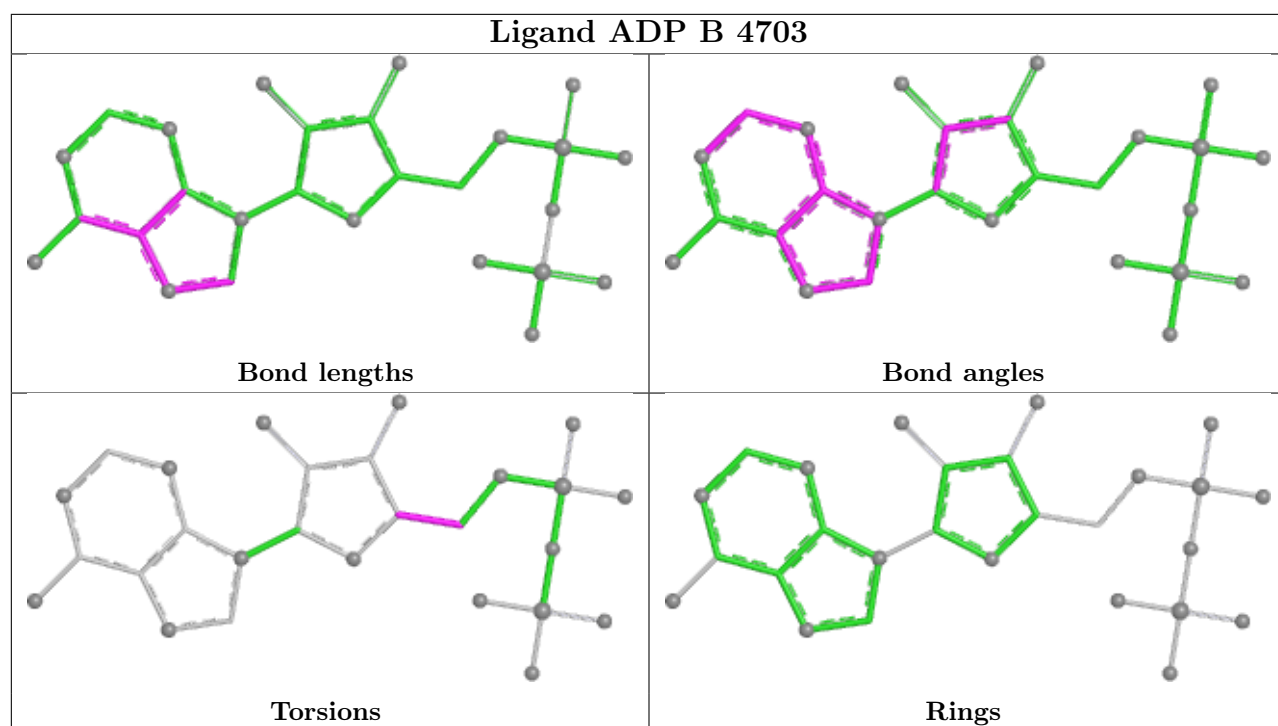
3 monomers are involved in 4 short contacts:

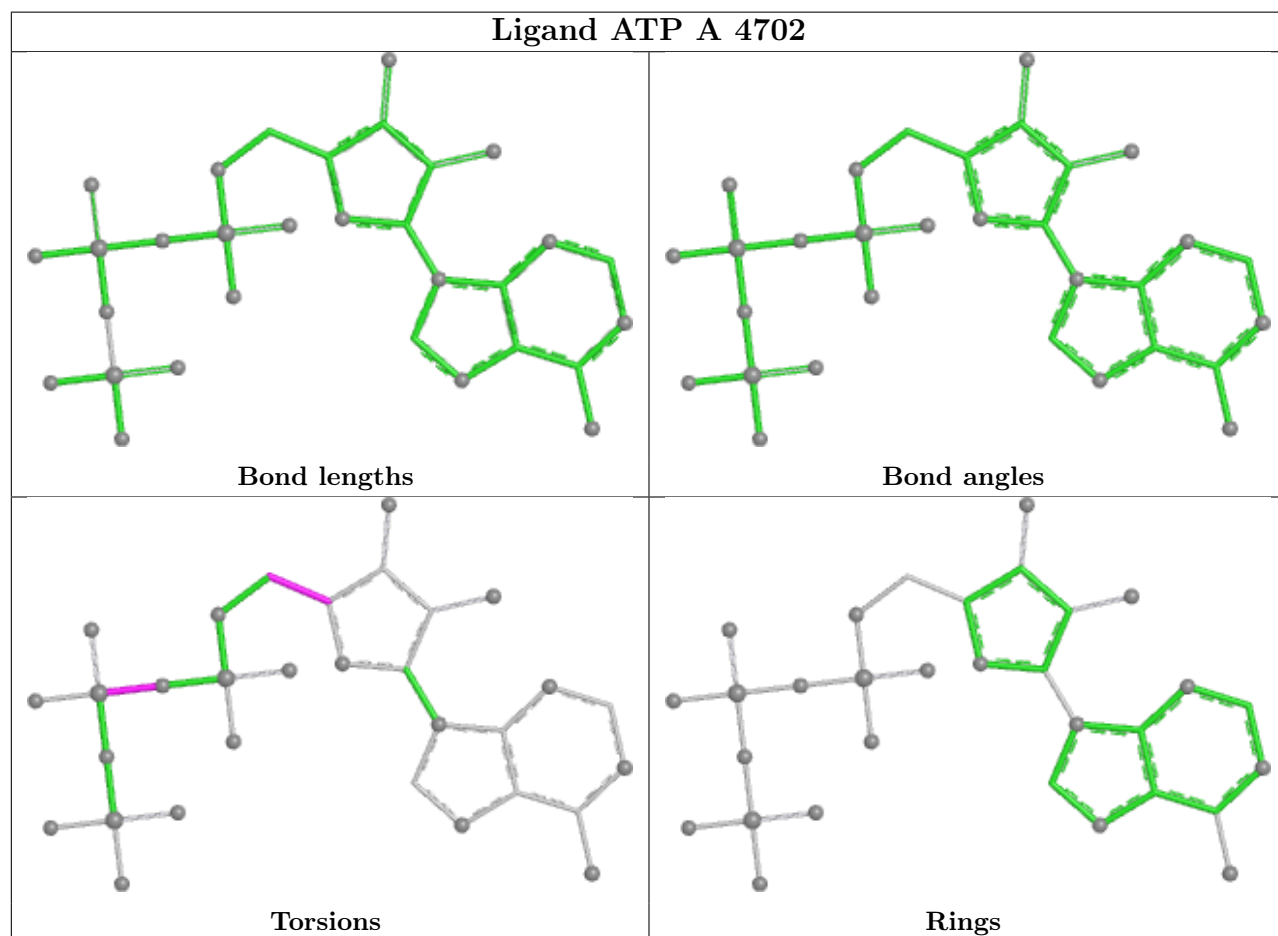
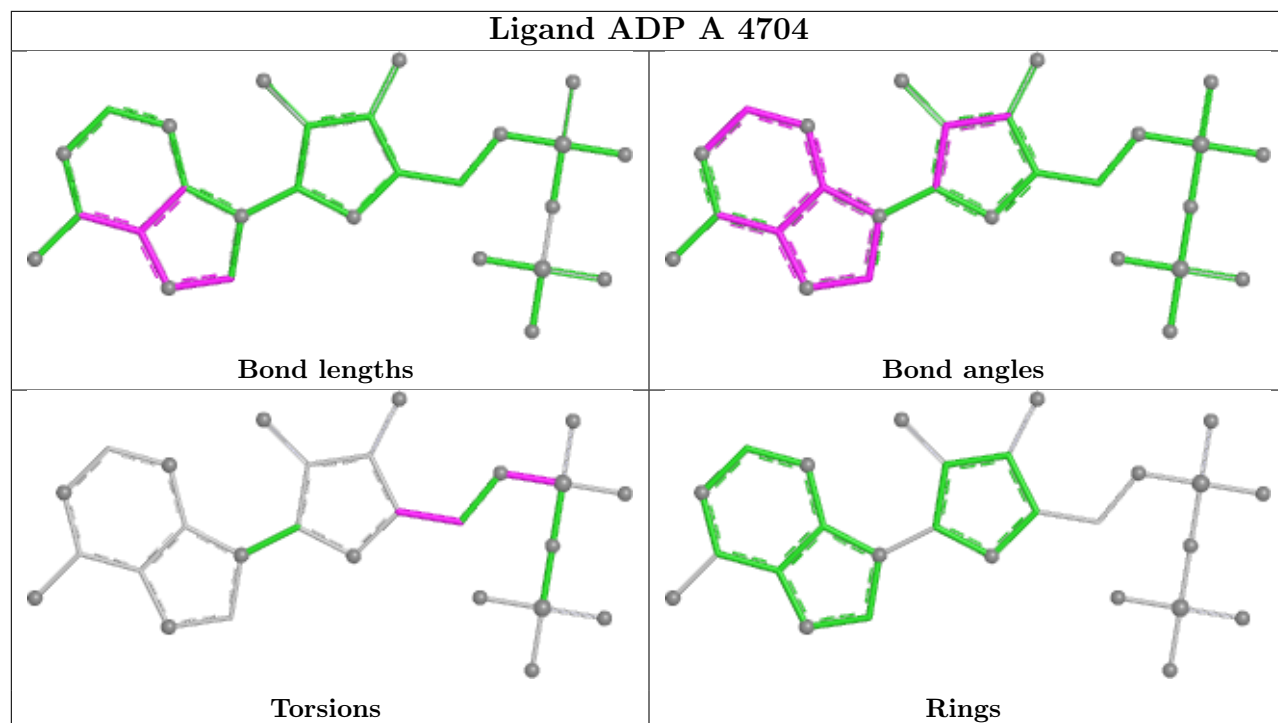
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	4704	ADP	1	0
4	A	4702	ATP	2	0
3	B	4701	ADP	1	0

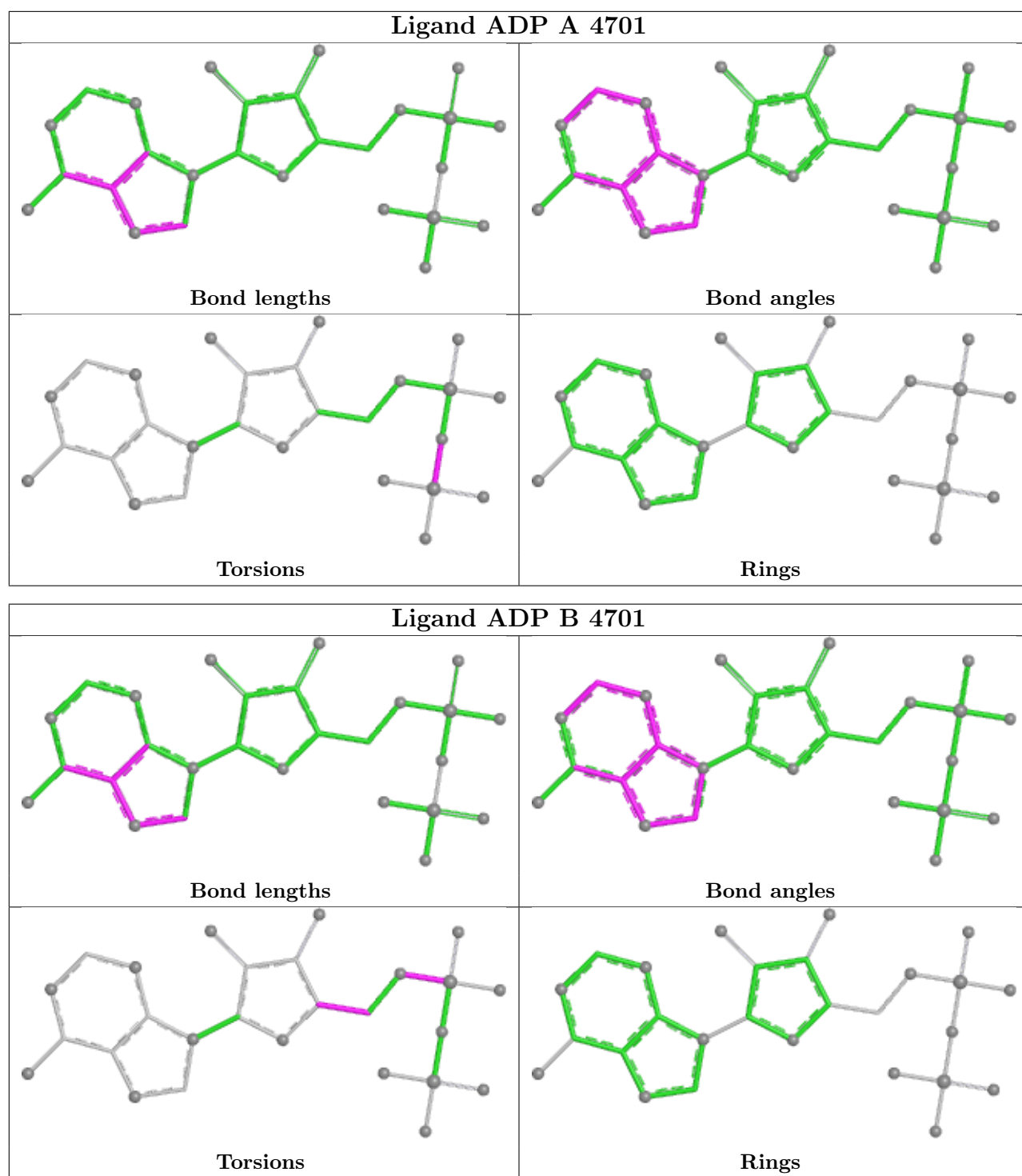
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

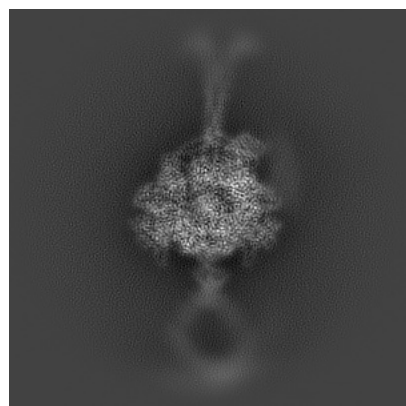
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47380. These allow visual inspection of the internal detail of the map and identification of artifacts.

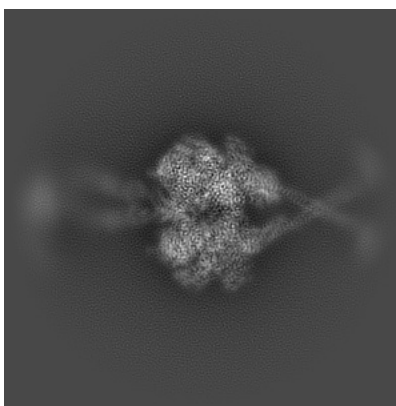
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

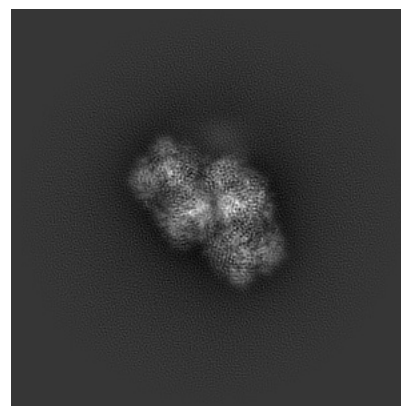
6.1.1 Primary map



X

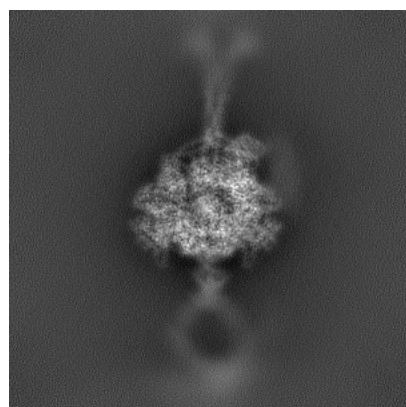


Y

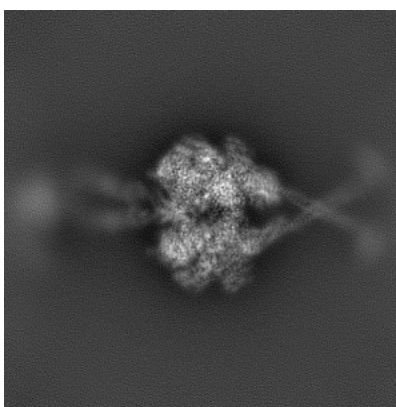


Z

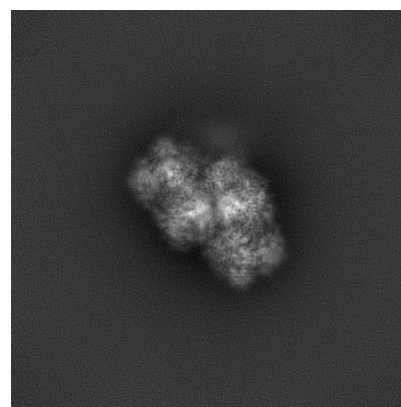
6.1.2 Raw map



X



Y



Z

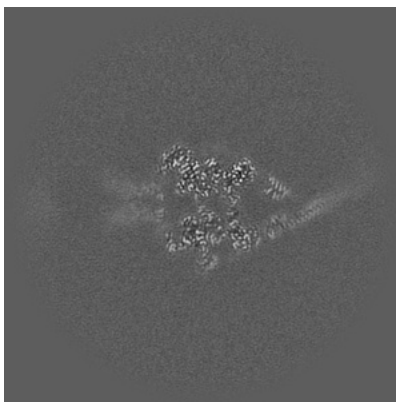
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

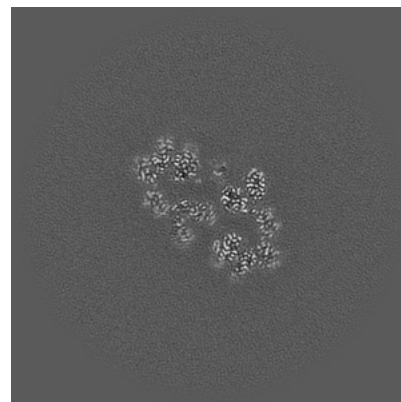
6.2.1 Primary map



X Index: 192



Y Index: 192

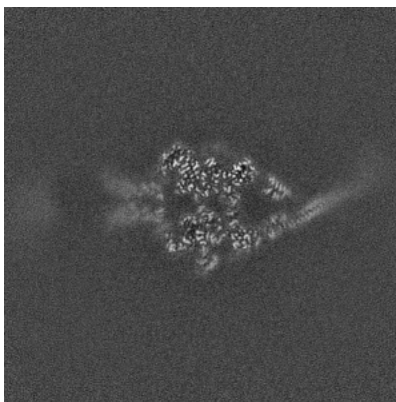


Z Index: 192

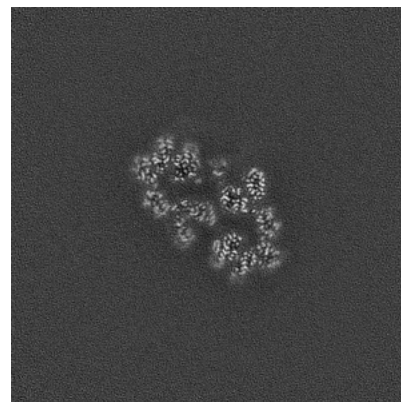
6.2.2 Raw map



X Index: 192



Y Index: 192

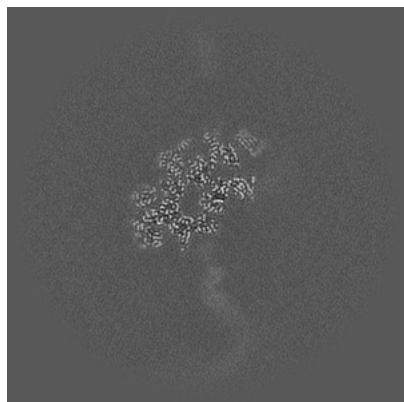


Z Index: 192

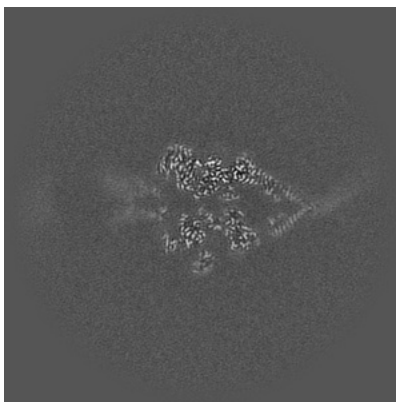
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

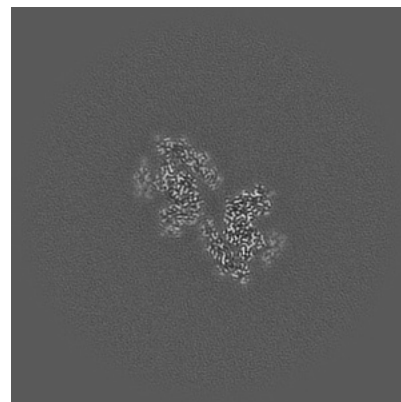
6.3.1 Primary map



X Index: 215

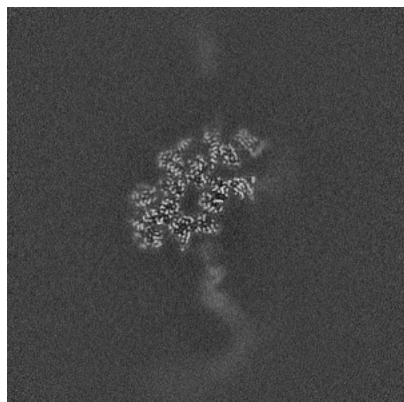


Y Index: 196

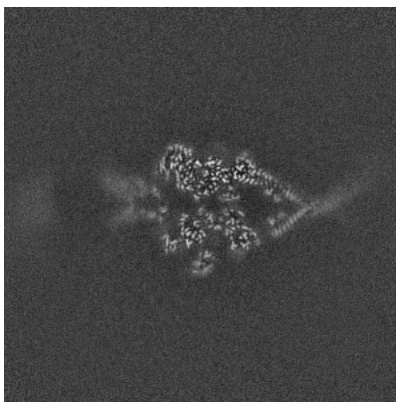


Z Index: 173

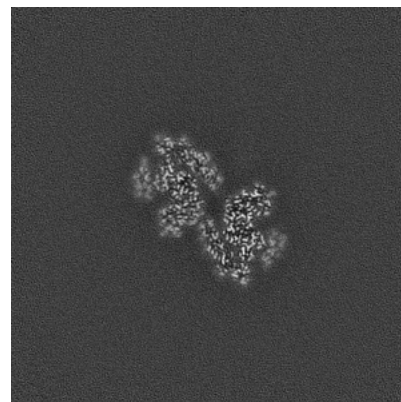
6.3.2 Raw map



X Index: 215



Y Index: 196

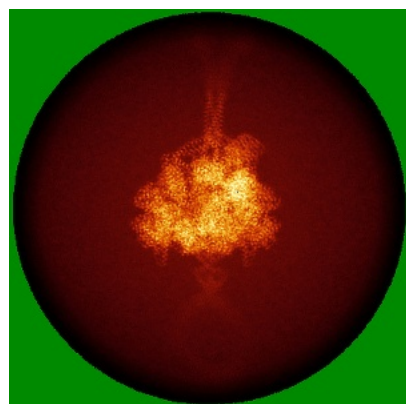


Z Index: 173

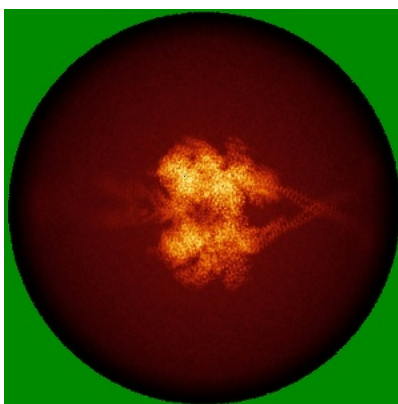
The images above show the largest variance slices of the map in three orthogonal directions.

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

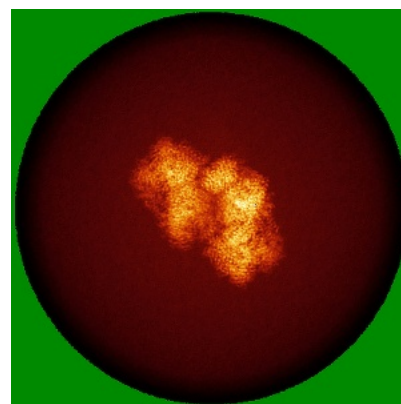
6.4.1 Primary map



X

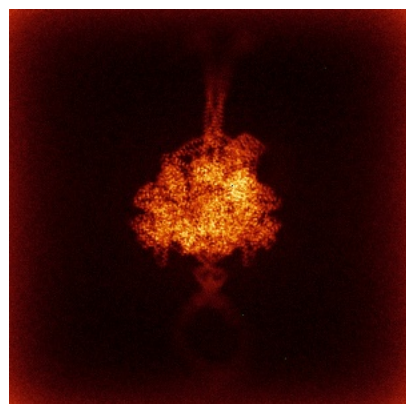


Y

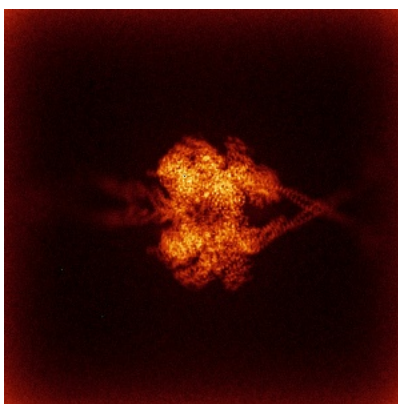


Z

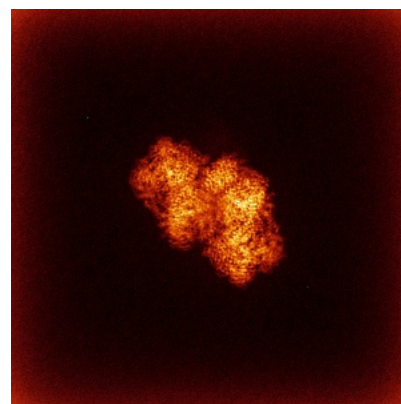
6.4.2 Raw map



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](#)

This section was not generated.

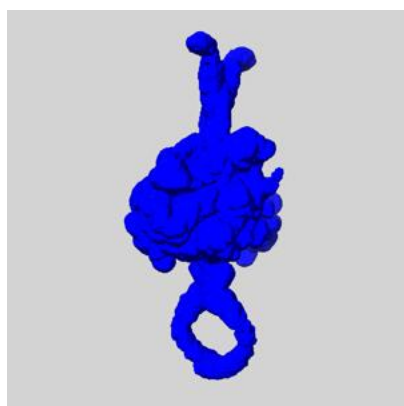
6.6 Mask visualisation [i](#)

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

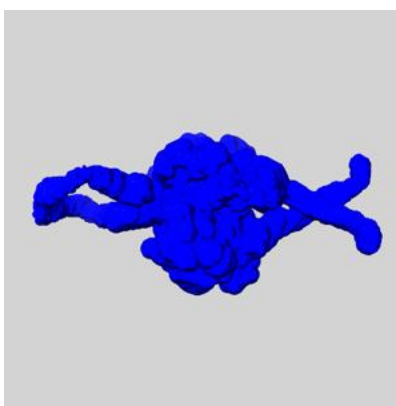
A mask typically either:

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

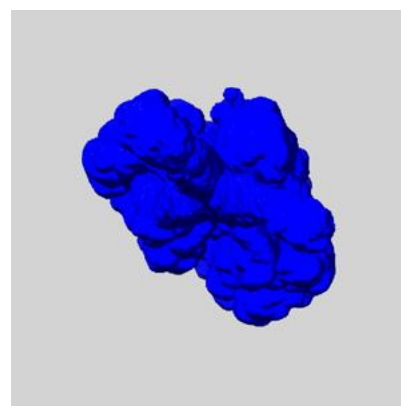
6.6.1 emd_47380_msk_1.map [i](#)



X



Y

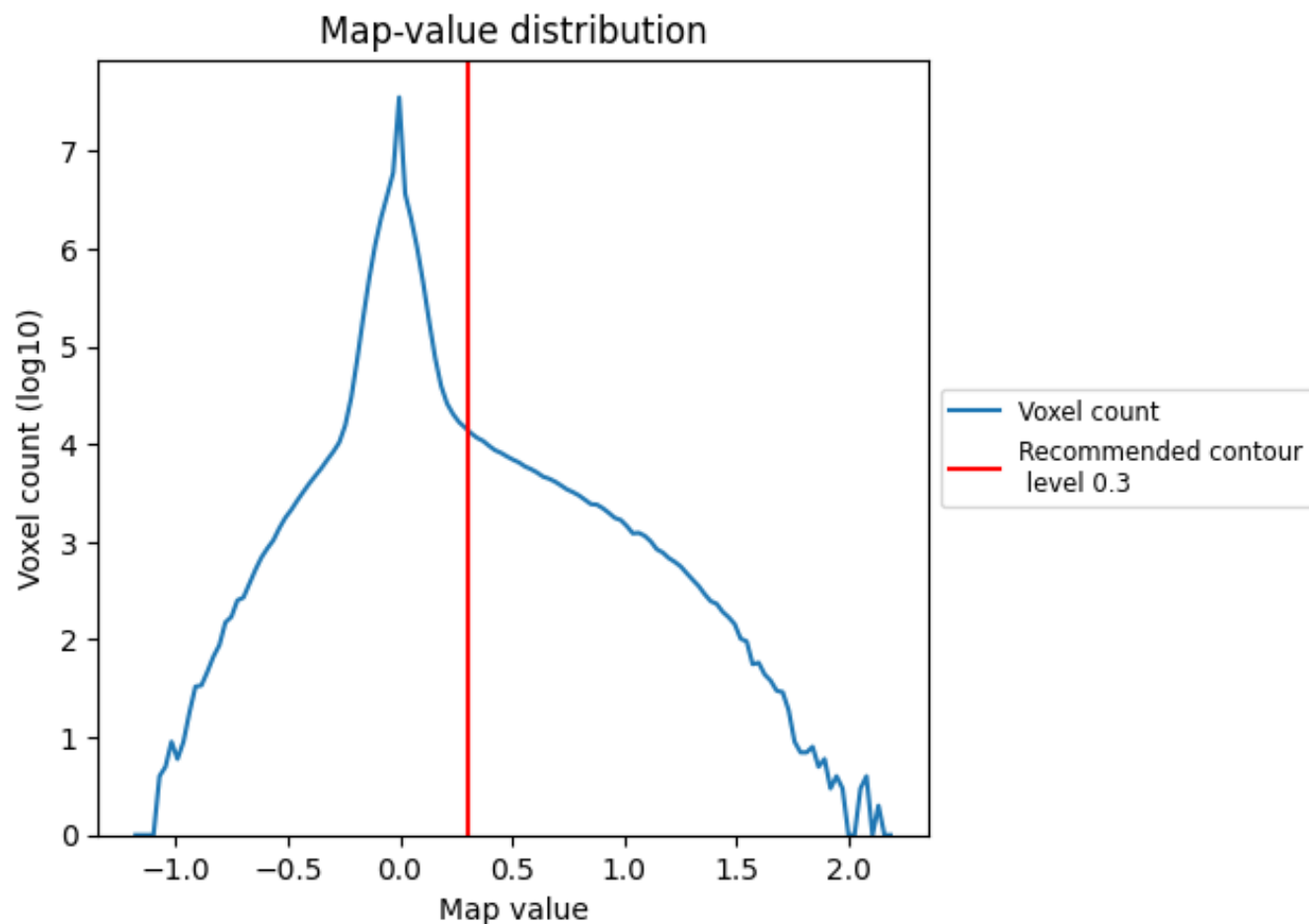


Z

7 Map analysis [i](#)

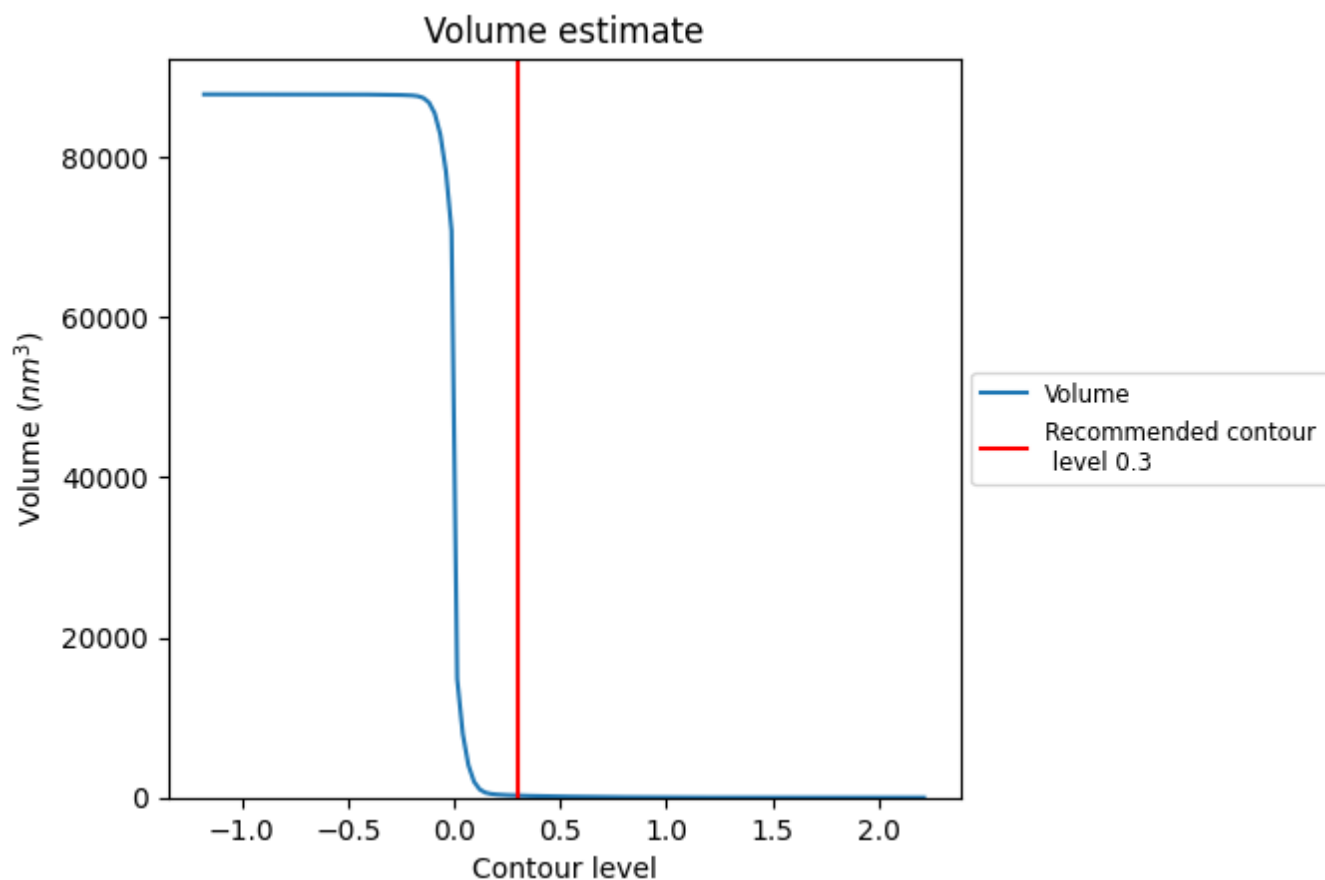
This section contains the results of statistical analysis of the map.

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.

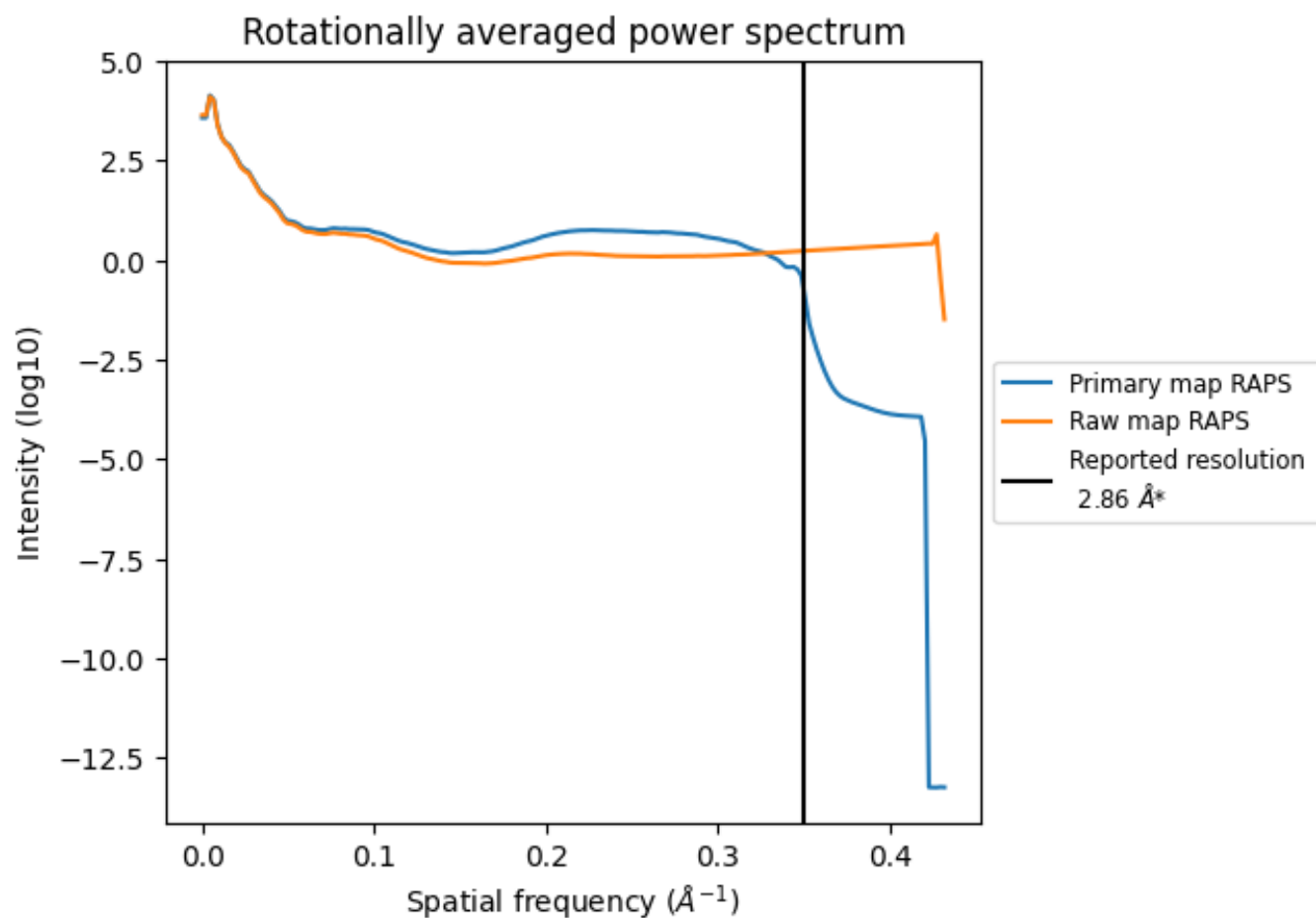
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 253 nm³; this corresponds to an approximate mass of 228 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 ⓘ

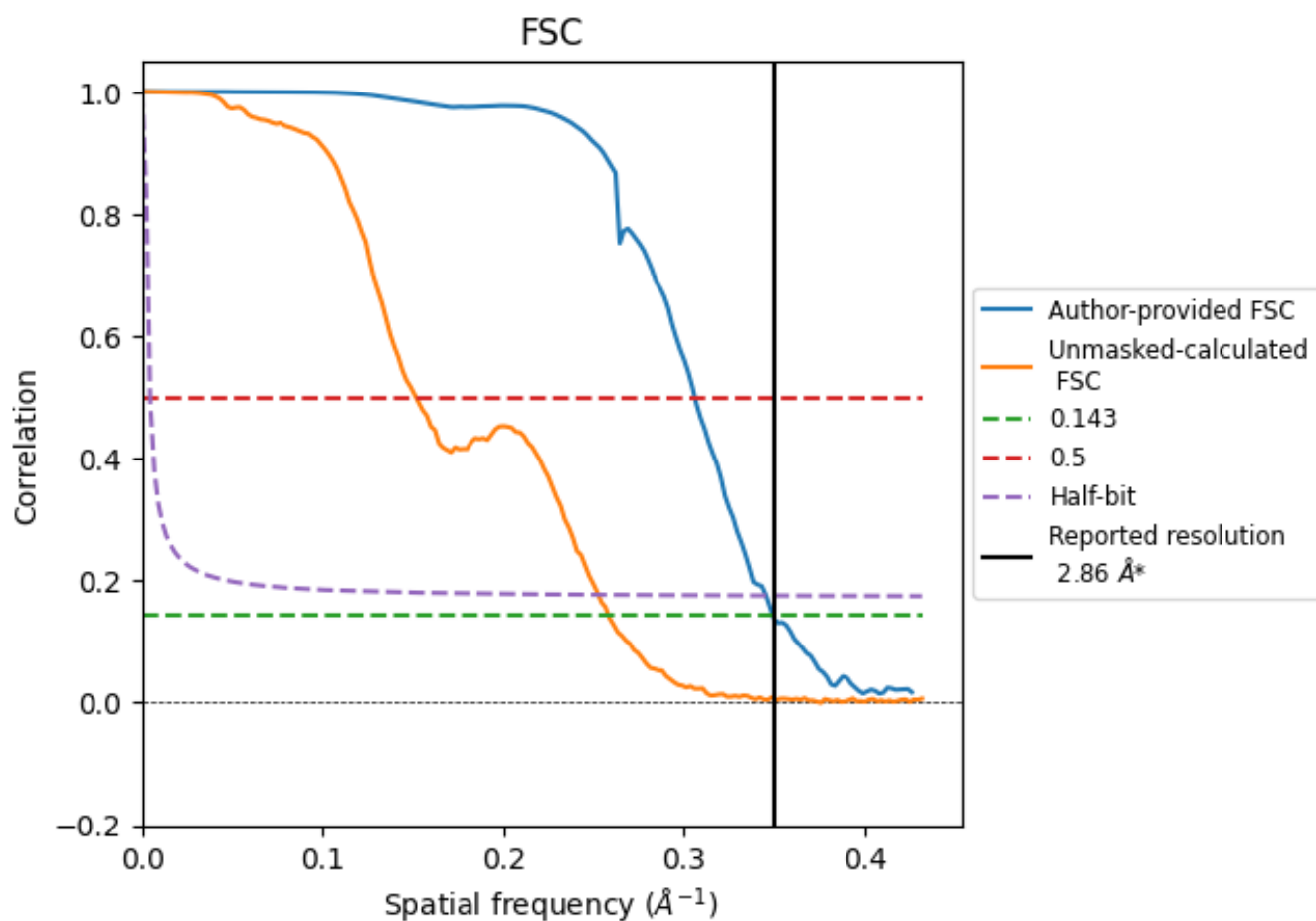


*Reported resolution corresponds to spatial frequency of 0.350 Å⁻¹

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 0.350 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	2.86	3.27	2.89
Unmasked-calculated*	3.87	6.60	3.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 2.86 by more than 10 %

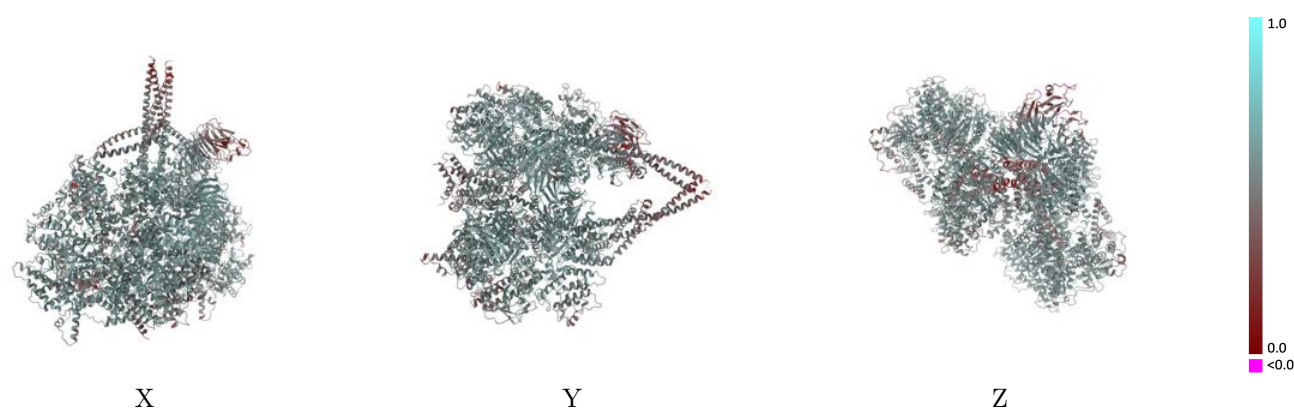
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47380 and PDB model 9E11. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

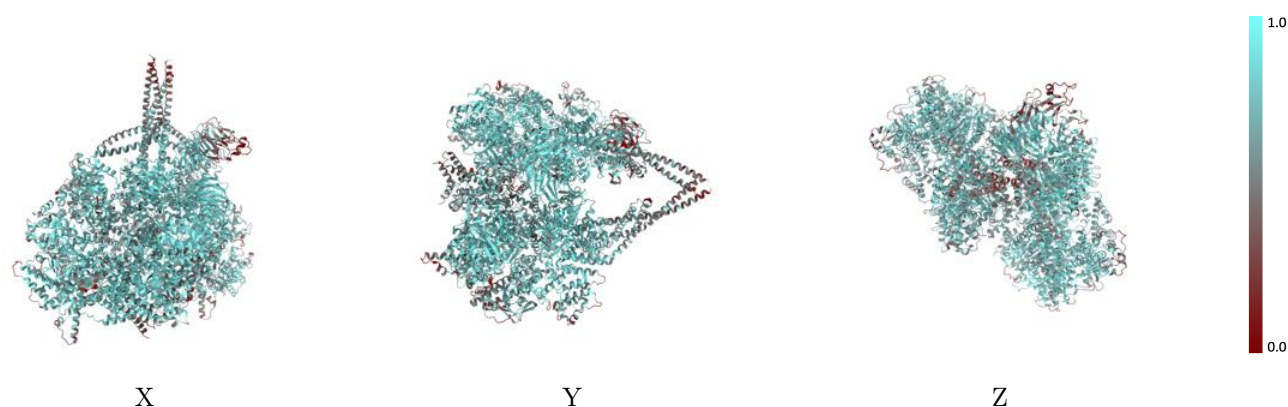
This section was not generated.

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



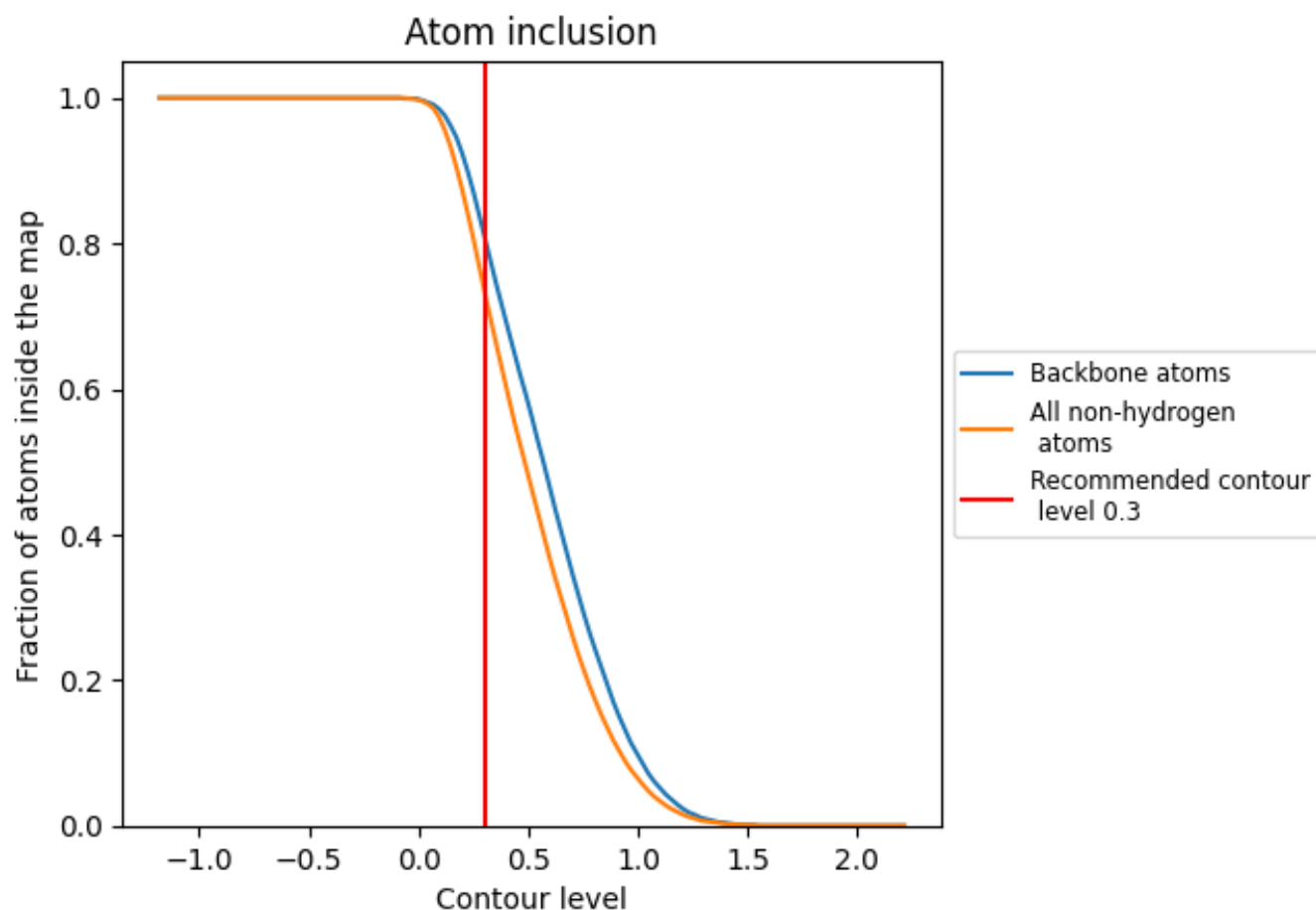
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7360	<div></div> 0.5430
A	<div></div> 0.7130	<div></div> 0.5370
B	<div></div> 0.7660	<div></div> 0.5550
C	<div></div> 0.8490	<div></div> 0.5900
D	<div></div> 0.5620	<div></div> 0.4470

