



wwPDB EM Validation Summary Report ⓘ

Aug 4, 2025 – 06:03 PM EDT

PDB ID : 9E10 / pdb_00009e10
EMDB ID : EMD-47379
Title : Dimeric motor domains from phi dynein-1 under Lis1 condition
Authors : Yang, J.; Zhang, K.
Deposited on : 2024-10-21
Resolution : 2.71 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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.dev126
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

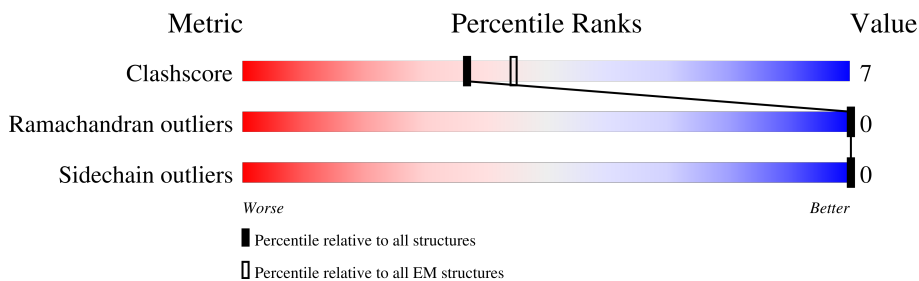
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.71 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 47414 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 ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



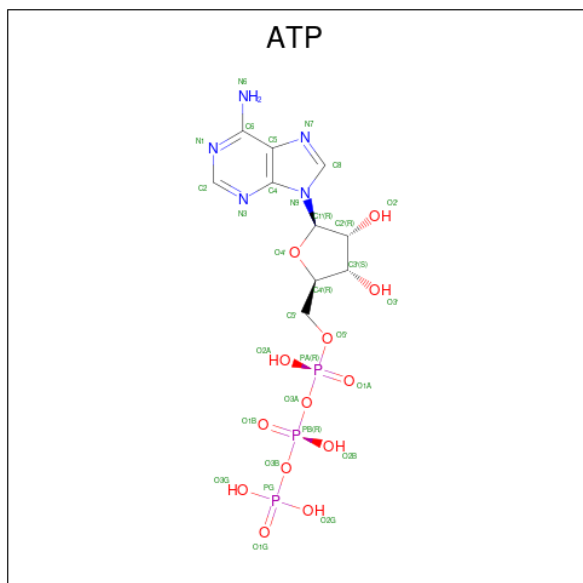
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

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



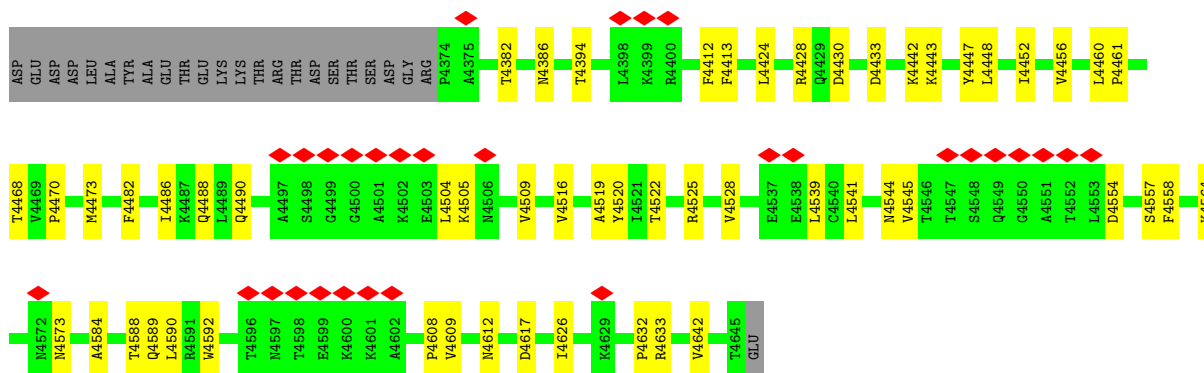
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

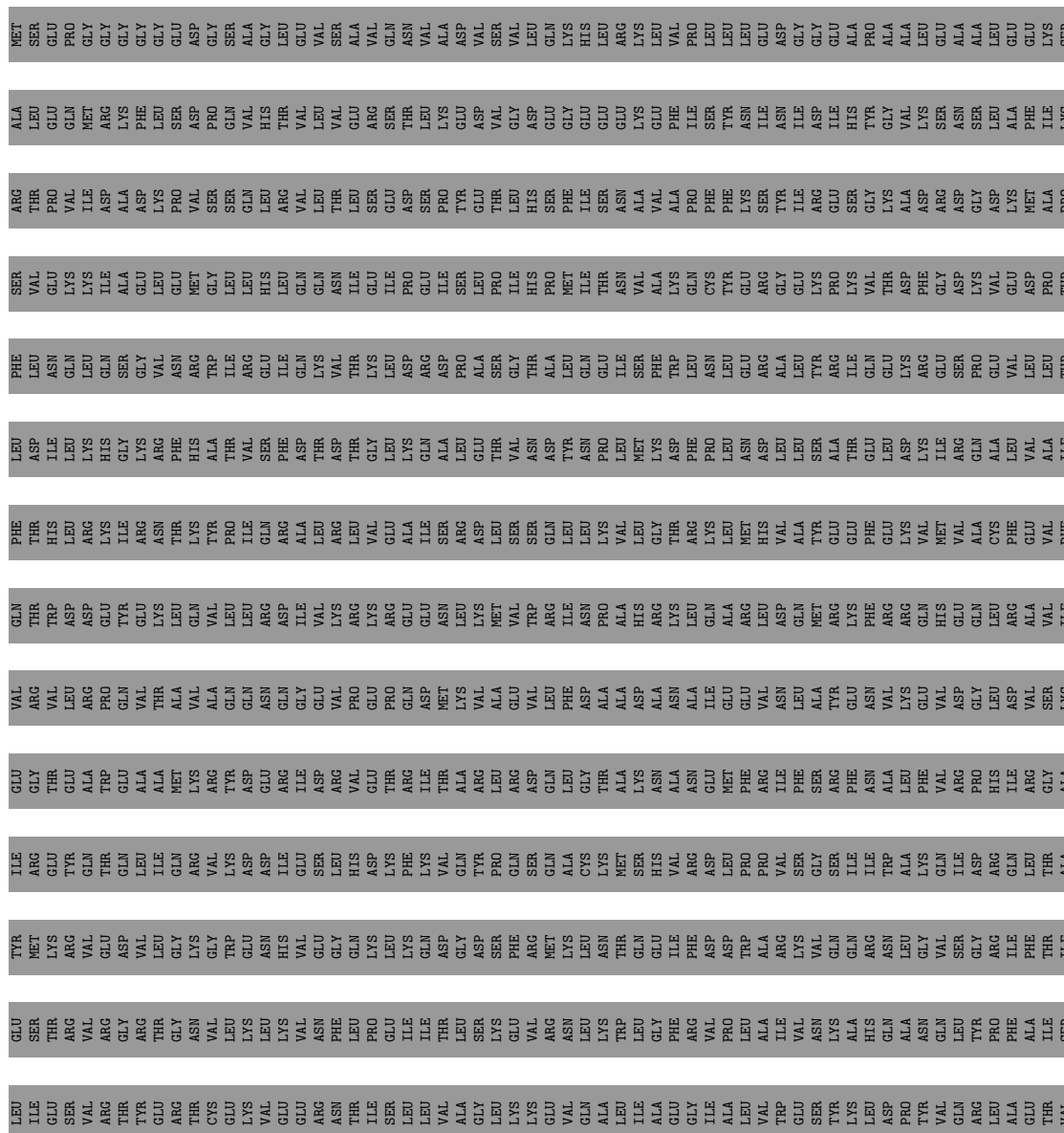
Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Mg	0
			2	2	
4	B	2	Total	Mg	0
			2	2	





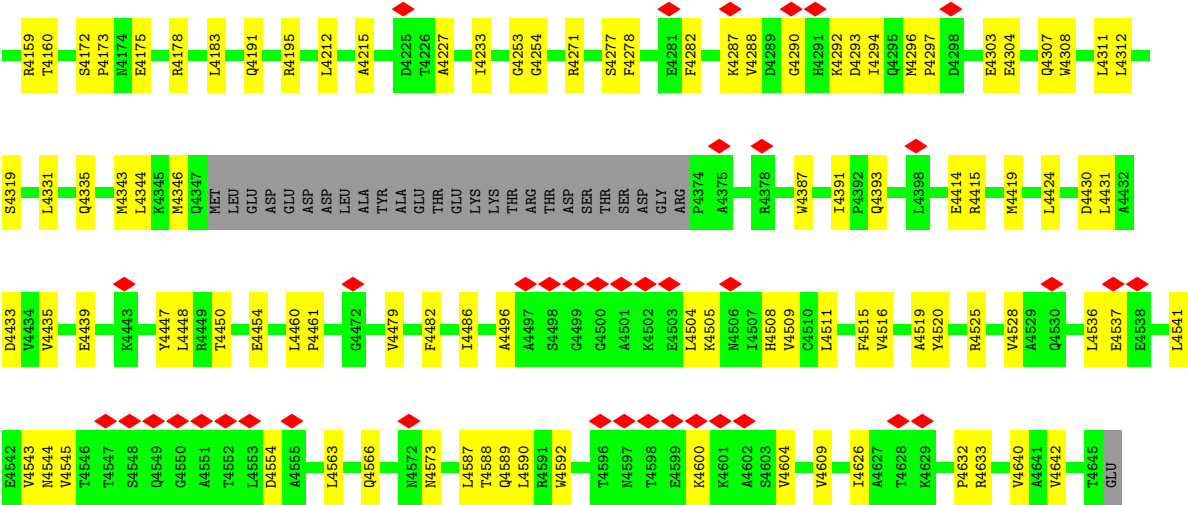


- Molecule 1: Cytoplasmic dynein 1 heavy chain 1





A3986	D3902	D3762	R3569	S3456	ALA	GLN	LYS	ASP	T3099	G2937	N2752	P2525	ASP
I3987	L3909	D3763	Q3563	E3457	ILE	ILE	SER	GLY	E3100	K2943	M2755	A2529	GLY
H3988		D3764	Q3563	A3458	GLN	ARG	LYS	GLY	Q3104	A2951	T2770	P2530	GLY
R3989			Q3563	A3459	LEU	SER	ASP	GLY	T3110	L2956	F2784	N2531	ALA
L3990			Q3563	A3460	ASN	ILE	LEU	ALA	S3111	L2956	F2784	D2536	ALA
F3996			Q3563	A3461	TYR	ILE	LEU	ALA	S3112	L2956	F2784	D2536	ALA
M4004			Q3563	A3462	ALA	ASP	ASP	ASP	M3113	L2956	F2784	D2536	ALA
M4007			Q3563	A3463	ASP	ASP	ASP	ASP	M3114	L2956	F2784	D2536	ALA
T4011			Q3563	A3464	LEU	LEU	LEU	LEU	M3115	L2956	F2784	D2536	ALA
M4012			Q3563	A3465	LYS	PRO	PRO	PRO	E3116	L2956	F2784	D2536	ALA
L4013			Q3563	A3466	ARG	ILE	ILE	ILE	D3227	L2956	F2784	D2536	ALA
F4017			Q3563	A3467	VAL	PRO	PRO	PRO	E3228	L2956	F2784	D2536	ALA
M4018			Q3563	A3468	GLU	THR	THR	THR	L3229	L2956	F2784	D2536	ALA
S4019			Q3563	A3469	LEU	ILE	ILE	ILE	E3230	L2956	F2784	D2536	ALA
L4020			Q3563	A3470	ARG	VAL	VAL	VAL	E3231	L2956	F2784	D2536	ALA
M4021			Q3563	A3471	ASN	ASN	ASN	ASN	E3232	L2956	F2784	D2536	ALA
P4037			Q3563	A3472	GLU	GLU	GLU	GLU	E3233	L2956	F2784	D2536	ALA
Y4049			Q3563	A3473	LEU	LEU	LEU	LEU	E3234	L2956	F2784	D2536	ALA
Q4065			Q3563	A3474	GLN	GLN	GLN	GLN	E3235	L2956	F2784	D2536	ALA
K4082			Q3563	A3475	LYS	LYS	LYS	LYS	E3236	L2956	F2784	D2536	ALA
T4086			Q3563	A3476	ASP	ASP	ASP	ASP	E3237	L2956	F2784	D2536	ALA
A4087			Q3563	A3477	ASP	ASP	ASP	ASP	E3238	L2956	F2784	D2536	ALA
V4088			Q3563	A3478	ASP	ASP	ASP	ASP	E3239	L2956	F2784	D2536	ALA
R4092			Q3563	A3479	ASP	ASP	ASP	ASP	E3240	L2956	F2784	D2536	ALA
M4095			Q3563	A3480	ASN	ASN	ASN	ASN	E3241	L2956	F2784	D2536	ALA
L4096			Q3563	A3481	GLN	GLN	GLN	GLN	E3242	L2956	F2784	D2536	ALA
K4097			Q3563	A3482	LYS	LYS	LYS	LYS	E3243	L2956	F2784	D2536	ALA
W4105			Q3563	A3483	LYS	LYS	LYS	LYS	E3244	L2956	F2784	D2536	ALA
M4107			Q3563	A3484	LYS	LYS	LYS	LYS	E3245	L2956	F2784	D2536	ALA
L4116			Q3563	A3485	LYS	LYS	LYS	LYS	E3246	L2956	F2784	D2536	ALA
Q4117			Q3563	A3486	LYS	LYS	LYS	LYS	E3247	L2956	F2784	D2536	ALA
P4118			Q3563	A3487	LYS	LYS	LYS	LYS	E3248	L2956	F2784	D2536	ALA
N4131			Q3563	A3488	LYS	LYS	LYS	LYS	E3249	L2956	F2784	D2536	ALA
P4132			Q3563	A3489	LYS	LYS	LYS	LYS	E3250	L2956	F2784	D2536	ALA
K4133			Q3563	A3490	LYS	LYS	LYS	LYS	E3251	L2956	F2784	D2536	ALA
V4135			Q3563	A3491	LYS	LYS	LYS	LYS	E3252	L2956	F2784	D2536	ALA
N4137			Q3563	A3492	LYS	LYS	LYS	LYS	E3253	L2956	F2784	D2536	ALA
L4138			Q3563	A3493	LYS	LYS	LYS	LYS	E3254	L2956	F2784	D2536	ALA
P4150			Q3563	A3494	LYS	LYS	LYS	LYS	E3255	L2956	F2784	D2536	ALA
N4156			Q3563	A3495	LYS	LYS	LYS	LYS	E3256	L2956	F2784	D2536	ALA
			Q3563	A3496	LYS	LYS	LYS	LYS	E3257	L2956	F2784	D2536	ALA
			Q3563	A3497	LYS	LYS	LYS	LYS	E3258	L2956	F2784	D2536	ALA
			Q3563	A3498	LYS	LYS	LYS	LYS	E3259	L2956	F2784	D2536	ALA
			Q3563	A3499	LYS	LYS	LYS	LYS	E3260	L2956	F2784	D2536	ALA
			Q3563	A3500	LYS	LYS	LYS	LYS	E3261	L2956	F2784	D2536	ALA
			Q3563	A3501	LYS	LYS	LYS	LYS	E3262	L2956	F2784	D2536	ALA
			Q3563	A3502	LYS	LYS	LYS	LYS	E3263	L2956	F2784	D2536	ALA
			Q3563	A3503	LYS	LYS	LYS	LYS	E3264	L2956	F2784	D2536	ALA
			Q3563	A3504	LYS	LYS	LYS	LYS	E3265	L2956	F2784	D2536	ALA
			Q3563	A3505	LYS	LYS	LYS	LYS	E3266	L2956	F2784	D2536	ALA
			Q3563	A3506	LYS	LYS	LYS	LYS	E3267	L2956	F2784	D2536	ALA
			Q3563	A3507	LYS	LYS	LYS	LYS	E3268	L2956	F2784	D2536	ALA
			Q3563	A3508	LYS	LYS	LYS	LYS	E3269	L2956	F2784	D2536	ALA
			Q3563	A3509	LYS	LYS	LYS	LYS	E3270	L2956	F2784	D2536	ALA
			Q3563	A3510	LYS	LYS	LYS	LYS	E3271	L2956	F2784	D2536	ALA
			Q3563	A3511	LYS	LYS	LYS	LYS	E3272	L2956	F2784	D2536	ALA
			Q3563	A3512	LYS	LYS	LYS	LYS	E3273	L2956	F2784	D2536	ALA
			Q3563	A3513	LYS	LYS	LYS	LYS	E3274	L2956	F2784	D2536	ALA
			Q3563	A3514	LYS	LYS	LYS	LYS	E3275	L2956	F2784	D2536	ALA
			Q3563	A3515	LYS	LYS	LYS	LYS	E3276	L2956	F2784	D2536	ALA
			Q3563	A3516	LYS	LYS	LYS	LYS	E3277	L2956	F2784	D2536	ALA
			Q3563	A3517	LYS	LYS	LYS	LYS	E3278	L2956	F2784	D2536	ALA
			Q3563	A3518	LYS	LYS	LYS	LYS	E3279	L2956	F2784	D2536	ALA
			Q3563	A3519	LYS	LYS	LYS	LYS	E3280	L2956	F2784	D2536	ALA
			Q3563	A3520	LYS	LYS	LYS	LYS	E3281	L2956	F2784	D2536	ALA
			Q3563	A3521	LYS	LYS	LYS	LYS	E3282	L2956	F2784	D2536	ALA
			Q3563	A3522	LYS	LYS	LYS	LYS	E3283	L2956	F2784	D2536	ALA
			Q3563	A3523	LYS	LYS	LYS	LYS	E3284	L2956	F2784	D2536	ALA
			Q3563	A3524	LYS	LYS	LYS	LYS	E3285	L2956	F2784	D2536	ALA
			Q3563	A3525	LYS	LYS	LYS	LYS	E3286	L2956	F2784	D2536	ALA
			Q3563	A3526	LYS	LYS	LYS	LYS	E3287	L2956	F2784	D2536	ALA
			Q3563	A3527	LYS	LYS	LYS	LYS	E3288	L2956	F2784	D2536	ALA
			Q3563	A3528	LYS	LYS	LYS	LYS	E3289	L2956	F2784	D2536	ALA
			Q3563	A3529	LYS	LYS	LYS	LYS	E3290	L2956	F2784	D2536	ALA
			Q3563	A3530	LYS	LYS	LYS	LYS	E3291	L2956	F2784	D2536	ALA
			Q3563	A3531	LYS	LYS	LYS	LYS	E3292	L2956	F2784	D2536	ALA
			Q3563	A3532	LYS	LYS	LYS	LYS	E3293	L2956	F2784	D2536	ALA
			Q3563	A3533	LYS	LYS	LYS	LYS	E3294	L2956	F2784	D2536	ALA
			Q3563	A3534	LYS	LYS	LYS	LYS	E3295	L2956	F2784	D2536	ALA
			Q3563	A3535	LYS	LYS	LYS	LYS	E3296	L2956	F2784	D2536	ALA
			Q3563	A3536	LYS	LYS	LYS	LYS	E3297	L2956	F2784	D2536	ALA
			Q3563	A3537	LYS	LYS	LYS	LYS	E3298	L2956	F2784	D2536	ALA
			Q3563	A3538	LYS	LYS	LYS	LYS	E3299	L2956	F2784	D2536	ALA
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			Q3563	A3543	LYS	LYS	LYS	LYS	E3304	L2956	F2784	D2536	ALA
			Q3563	A3544	LYS	LYS	LYS	LYS	E3305	L2956	F2784	D2536	ALA
			Q3563	A3545	LYS	LYS	LYS	LYS	E3306	L2956	F2784	D2536	ALA
			Q3563	A3546	LYS	LYS	LYS	LYS	E3307	L2956	F2784	D2536	ALA
			Q3563	A3547	LYS	LYS	LYS	LYS	E3308	L2956	F2784	D2536	ALA
			Q3563	A3548	LYS	LYS	LYS	LYS	E3309	L2956	F2784	D2536	ALA
			Q3563	A3549	LYS	LYS	LYS	LYS	E3310	L2956	F2784	D2536	ALA
			Q3563	A3550	LYS	LYS	LYS	LYS	E3311	L2956	F2784	D2536	ALA
			Q3563	A3551	LYS	LYS	LYS	LYS	E3312	L2956	F2784	D2536	ALA
			Q3563	A3552	LYS	LYS	LYS	LYS	E3313	L2956	F2784	D2536	ALA
			Q3563	A3553	LYS	LYS	LYS	LYS	E3314	L2956	F2784	D2536	ALA
			Q3563	A3554	LYS	LYS	LYS	LYS	E3315	L2956	F2784	D2536	ALA
			Q3563	A3555	LYS	LYS	LYS	LYS	E3316	L2956	F2784	D2536	ALA
			Q3563	A3556	LYS	LYS	LYS	LYS	E3317	L2956	F2784	D2536	ALA
			Q3563	A3557	LYS	LYS	LYS	LYS	E3318	L2956	F2784	D2536	ALA
			Q3563	A3558	LYS	LYS	LYS	LYS	E3319	L2956	F2784	D2536	ALA
			Q3563	A3559	LYS	LYS	LYS	LYS	E3320	L2956	F2784	D2536	ALA
			Q3563	A3560	LYS	LYS	LYS	LYS	E3321	L2956	F2784	D2536	ALA
			Q3563	A3561	LYS	LYS	LYS	LYS	E3322	L2956	F2784	D2536	ALA
			Q3563	A3562	LYS	LYS	LYS	LYS	E3323	L2956	F2784	D2536	ALA
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			Q3563	A3566	LYS	LYS	LYS	LYS	E3327	L2956	F2784	D2536	ALA
			Q3563	A3567	LYS	LYS	LYS	LYS	E3328	L2956	F2784	D2536	ALA
			Q3563	A3568	LYS	LYS	LYS	LYS	E3329	L2956	F2784	D25	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	160539	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)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.763	Depositor
Minimum map value	-1.378	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.058	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, 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	0.13	0/24093	0.29	0/32651
1	B	0.13	0/24093	0.30	0/32651
All	All	0.13	0/48186	0.29	0/65302

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

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	23658	333	0
1	B	23593	0	23657	368	0
2	A	81	0	36	3	0
2	B	81	0	36	2	0
3	A	31	0	12	0	0
3	B	31	0	12	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
All	All	47414	0	47411	700	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 700 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:2320:ASP:OD1	1:A:2321:ASP:N	2.12	0.83
1:B:2320:ASP:OD1	1:B:2321:ASP:N	2.13	0.80
1:B:3970:VAL:HB	1:B:3989:ARG:HD3	1.65	0.78
1:B:2452:LEU:HD13	1:B:2729:ARG:HH21	1.52	0.73
1:B:2492:ARG:HE	1:B:2525:PRO:HG2	1.54	0.73

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%)	2881 (98%)	48 (2%)	0	100	100
1	B	2929/4646 (63%)	2889 (99%)	40 (1%)	0	100	100
All	All	5858/9292 (63%)	5770 (98%)	88 (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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	2605/4125 (63%)	2605 (100%)	0	100	100
All	All	5210/8250 (63%)	5210 (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 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2430	ASN
1	B	3499	GLN
1	B	2464	GLN
1	B	2834	GLN
1	B	3535	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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
2	ADP	B	4701	4	24,29,29	0.89	0	29,45,45	1.22	2 (6%)
3	ATP	B	4702	4	28,33,33	0.68	0	34,52,52	0.59	1 (2%)
3	ATP	A	4702	4	28,33,33	0.68	0	34,52,52	0.59	1 (2%)
2	ADP	A	4701	4	24,29,29	0.88	0	29,45,45	1.23	2 (6%)
2	ADP	B	4703	-	24,29,29	0.87	0	29,45,45	1.23	2 (6%)
2	ADP	A	4703	-	24,29,29	0.88	0	29,45,45	1.23	2 (6%)
2	ADP	A	4704	-	24,29,29	0.88	0	29,45,45	1.19	2 (6%)
2	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
2	ADP	B	4701	4	-	4/12/32/32	0/3/3/3
3	ATP	B	4702	4	-	4/18/38/38	0/3/3/3
3	ATP	A	4702	4	-	4/18/38/38	0/3/3/3
2	ADP	A	4701	4	-	3/12/32/32	0/3/3/3
2	ADP	B	4703	-	-	1/12/32/32	0/3/3/3
2	ADP	A	4703	-	-	0/12/32/32	0/3/3/3
2	ADP	A	4704	-	-	3/12/32/32	0/3/3/3
2	ADP	B	4704	-	-	3/12/32/32	0/3/3/3

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4703	ADP	N3-C2-N1	-3.79	123.52	128.67
2	A	4703	ADP	N3-C2-N1	-3.78	123.54	128.67
2	A	4701	ADP	N3-C2-N1	-3.76	123.57	128.67
2	B	4701	ADP	N3-C2-N1	-3.74	123.59	128.67
2	A	4704	ADP	N3-C2-N1	-3.65	123.72	128.67

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

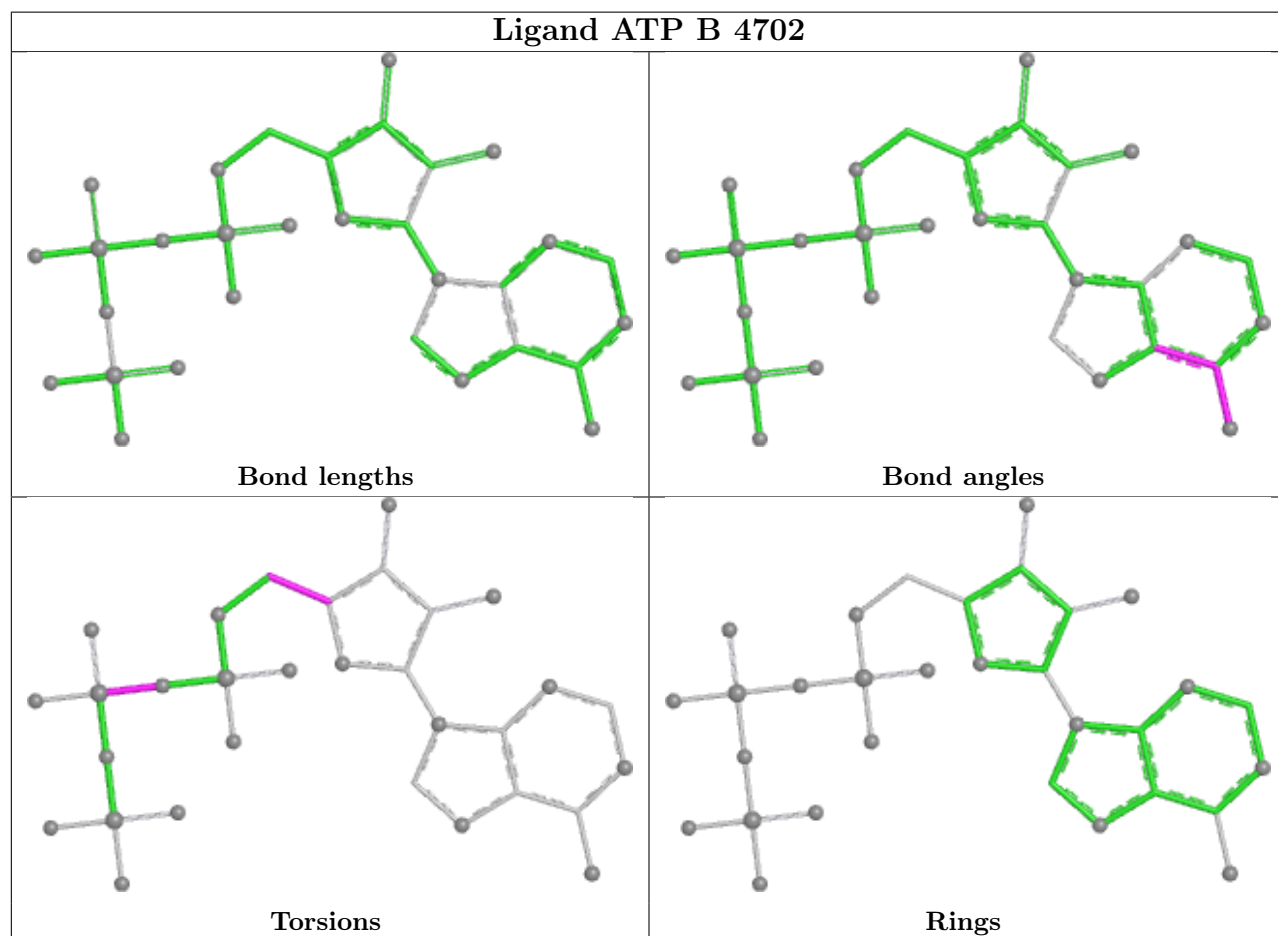
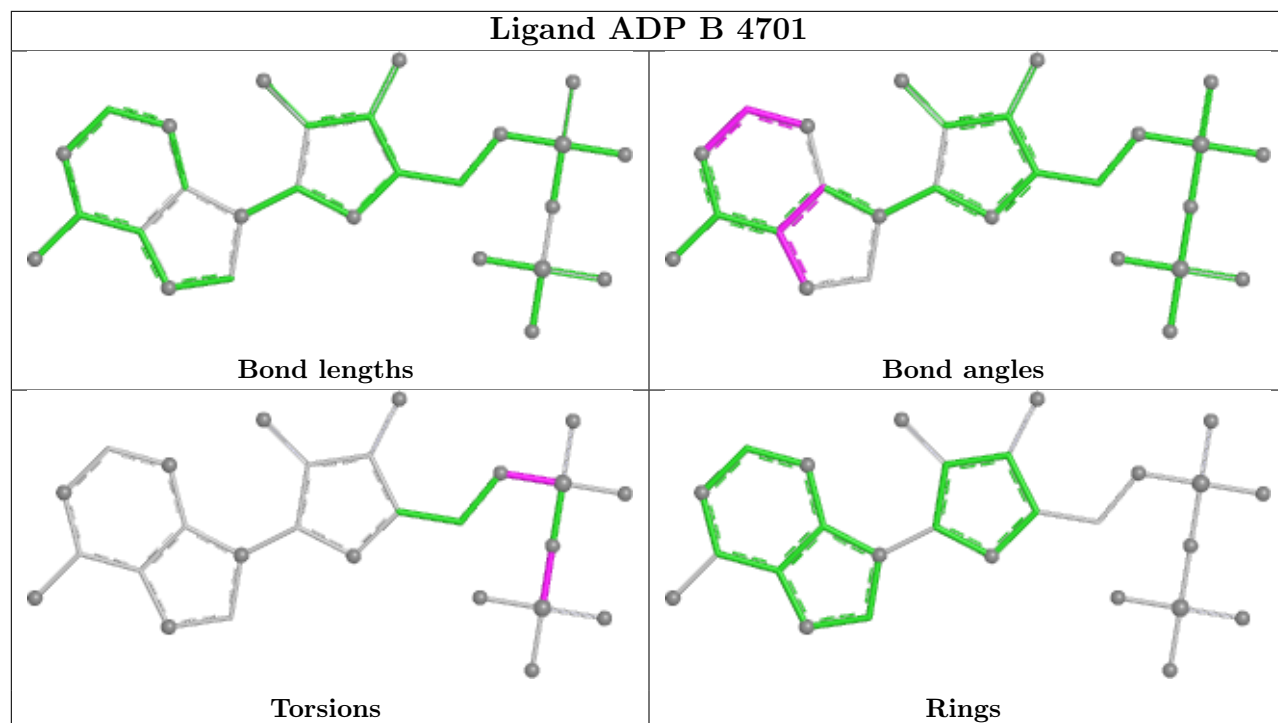
Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O1A
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O1A
2	B	4701	ADP	C5'-O5'-PA-O1A

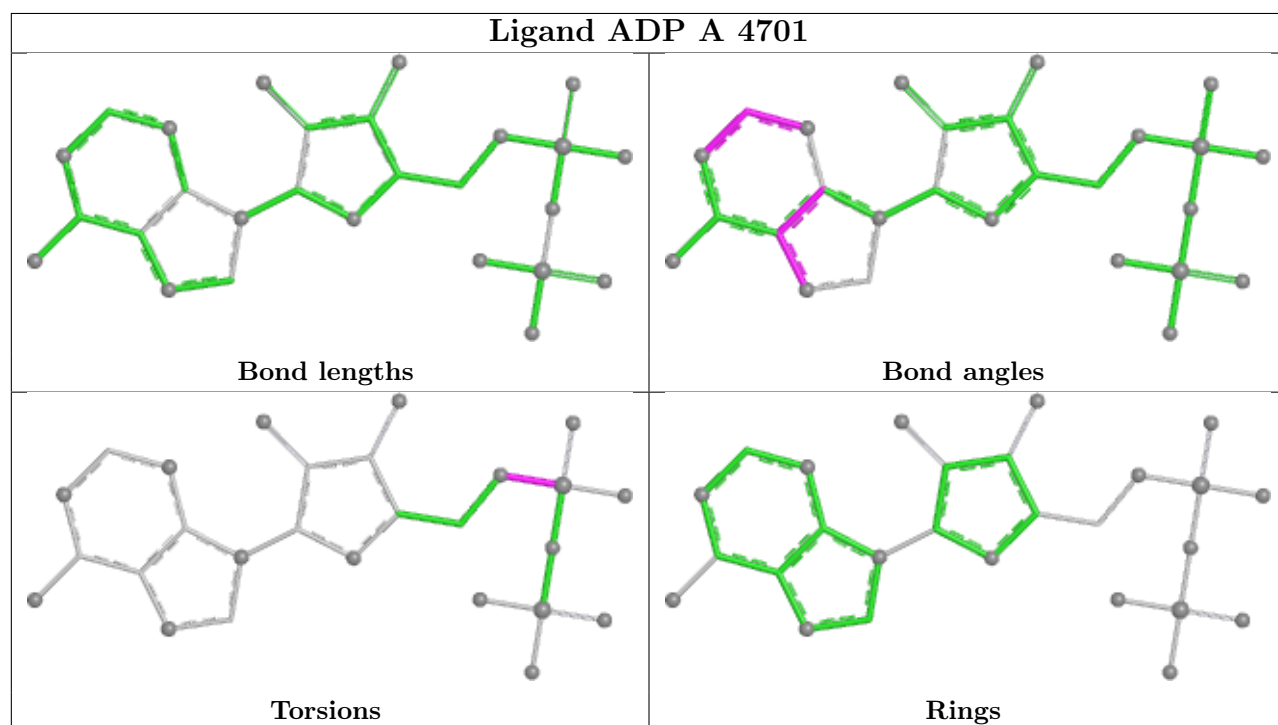
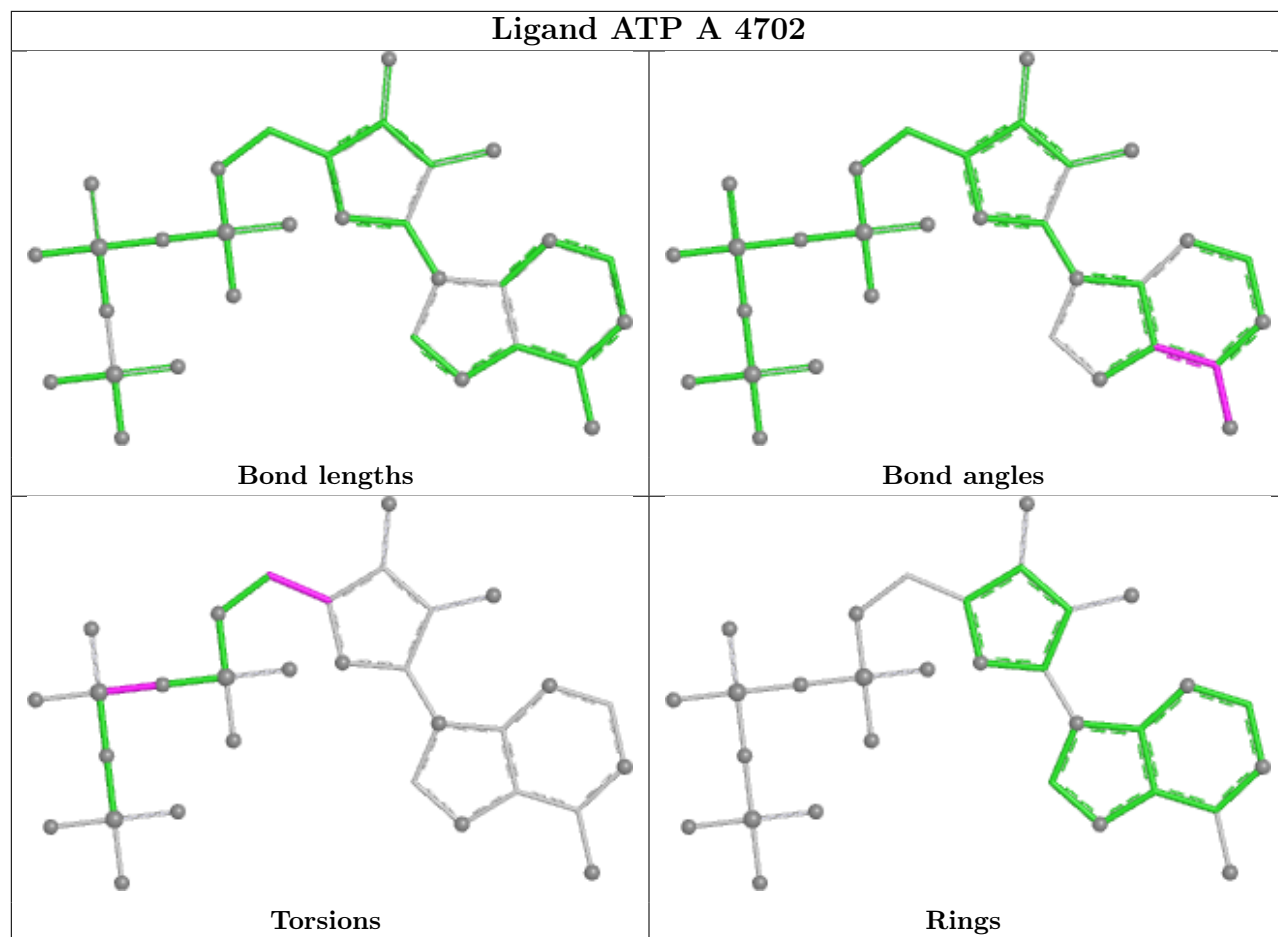
There are no ring outliers.

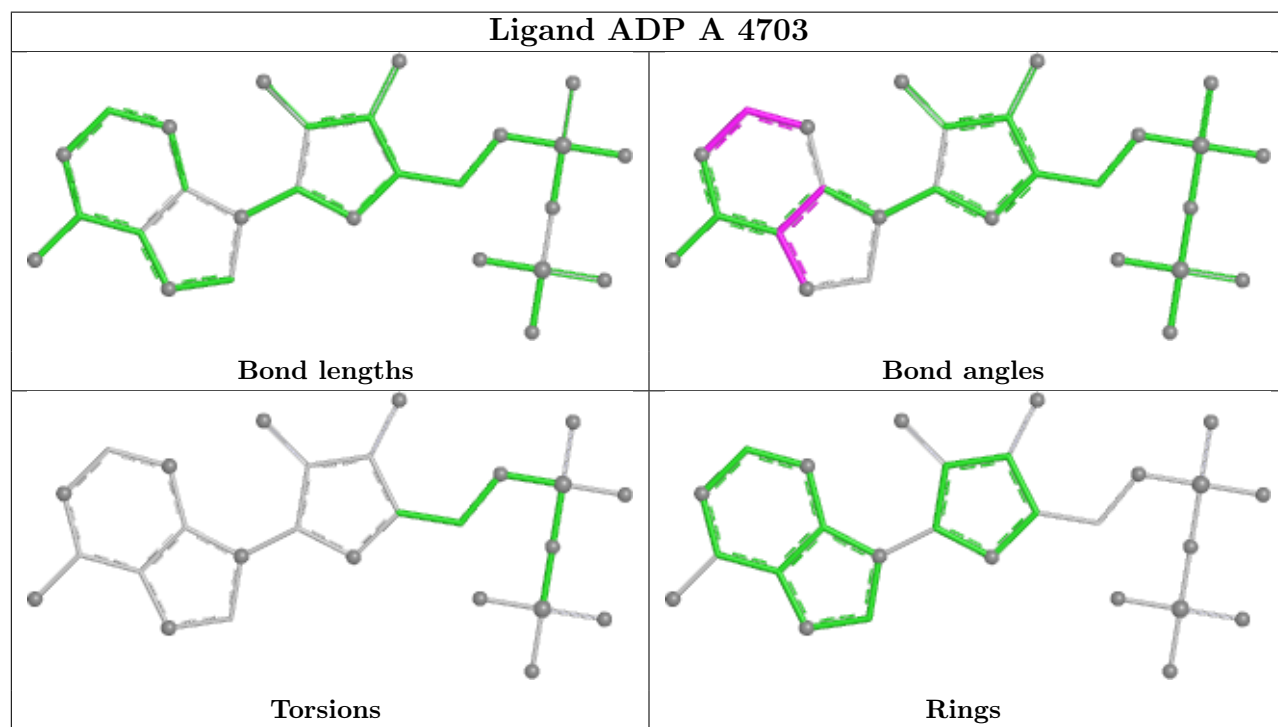
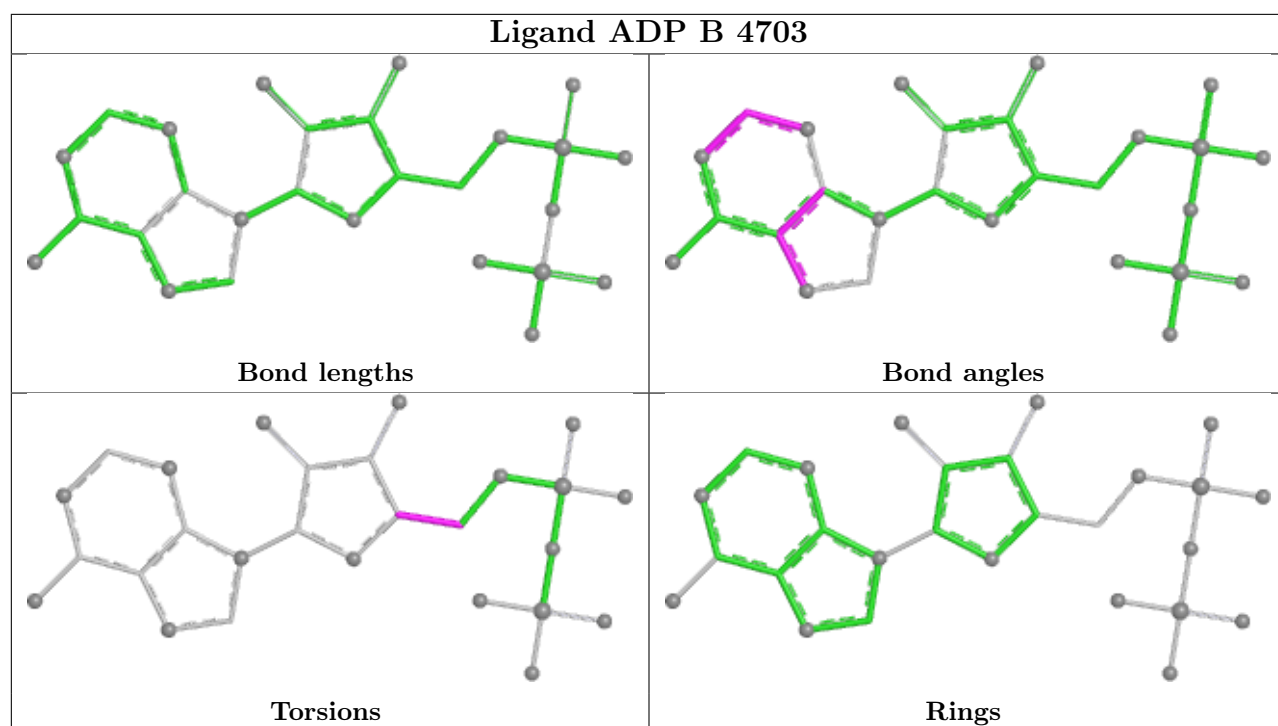
4 monomers are involved in 6 short contacts:

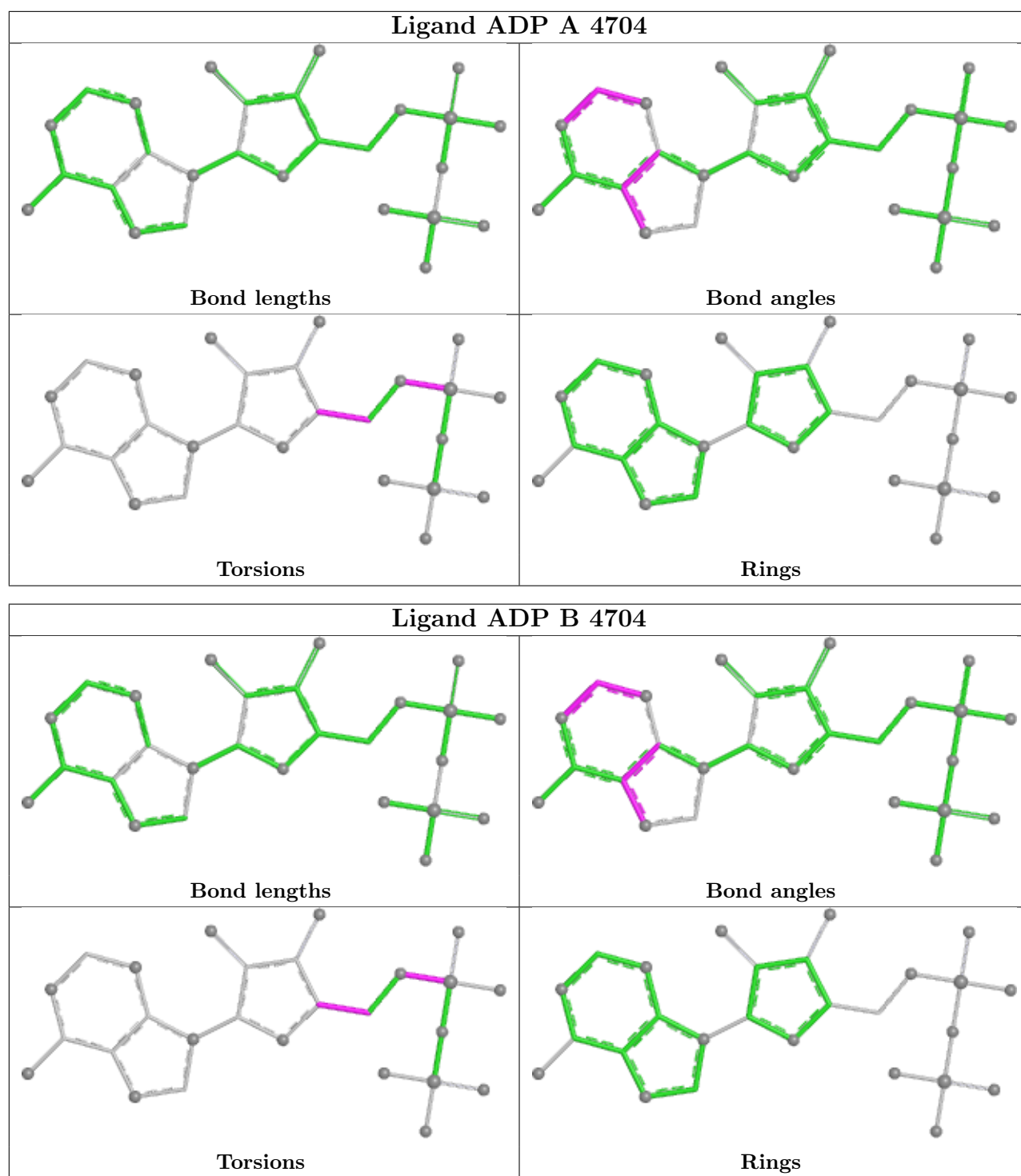
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4701	ADP	1	0
3	B	4702	ATP	1	0
2	A	4701	ADP	3	0
2	B	4703	ADP	1	0

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.

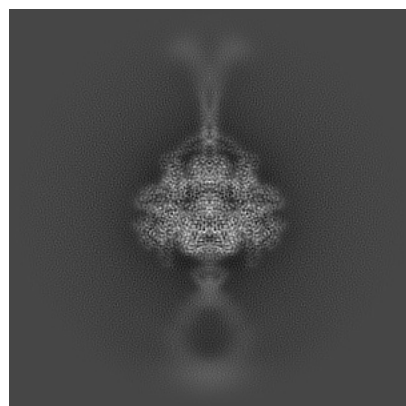
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47379. These allow visual inspection of the internal detail of the map and identification of artifacts.

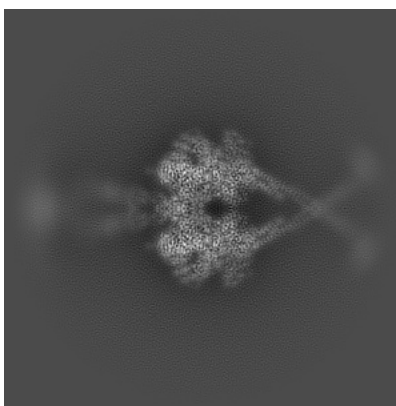
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

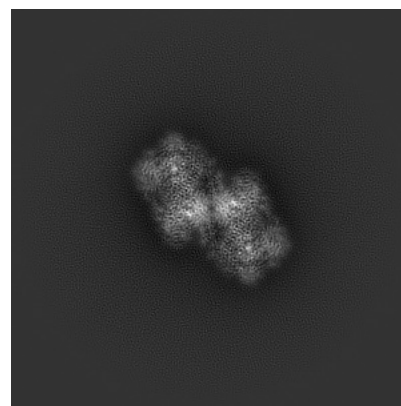
6.1.1 Primary map



X

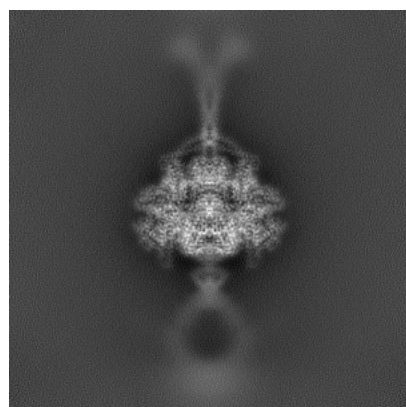


Y

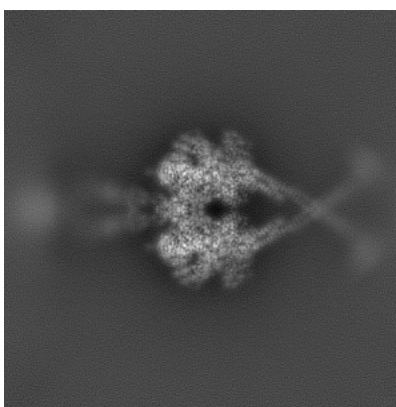


Z

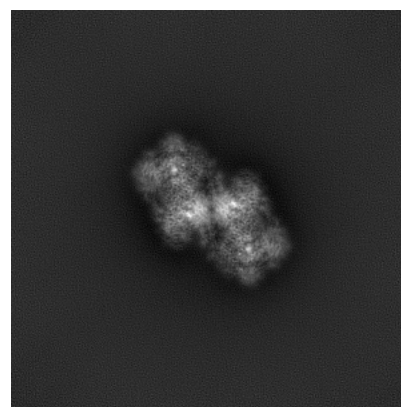
6.1.2 Raw map



X



Y

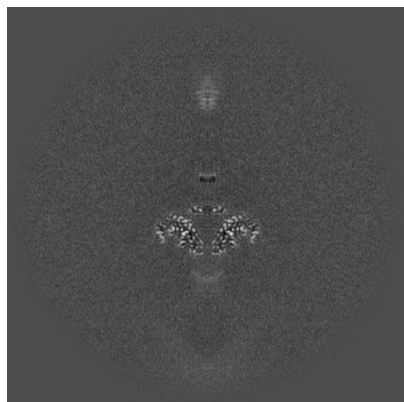


Z

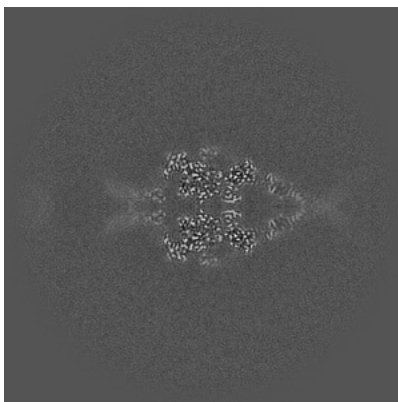
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

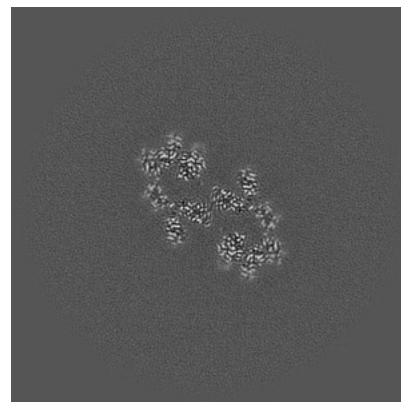
6.2.1 Primary map



X Index: 192

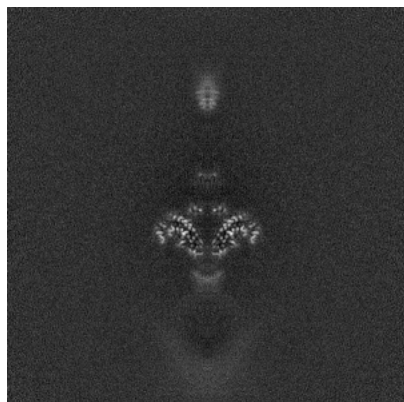


Y Index: 192

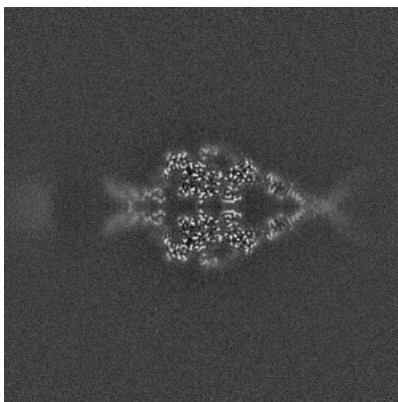


Z Index: 192

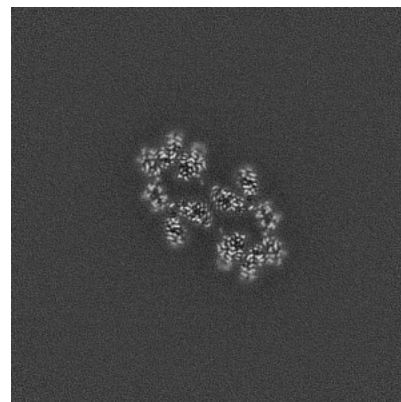
6.2.2 Raw map



X Index: 192



Y Index: 192

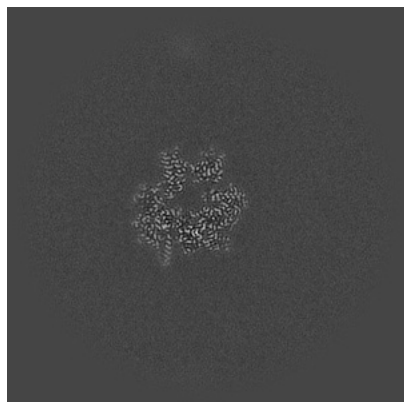


Z Index: 192

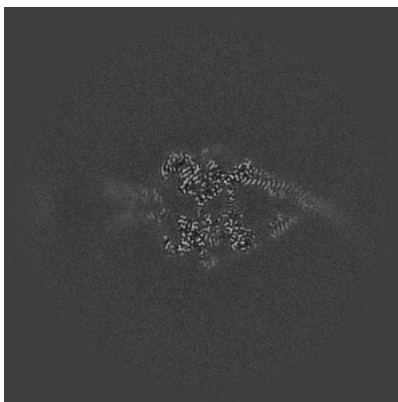
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

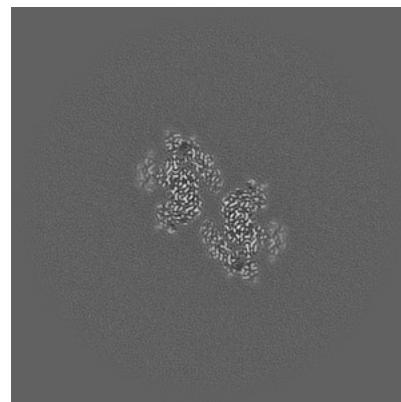
6.3.1 Primary map



X Index: 227

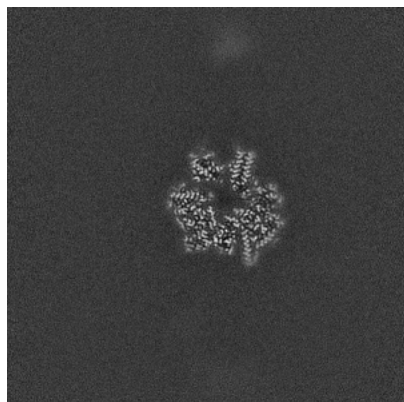


Y Index: 195

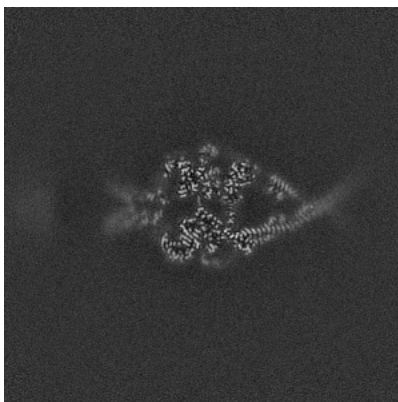


Z Index: 173

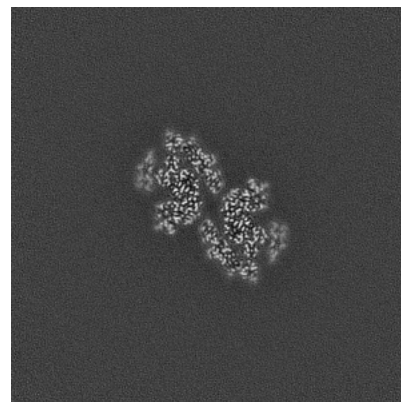
6.3.2 Raw map



X Index: 156



Y Index: 189

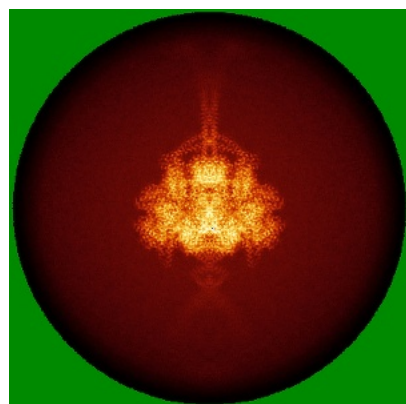


Z Index: 172

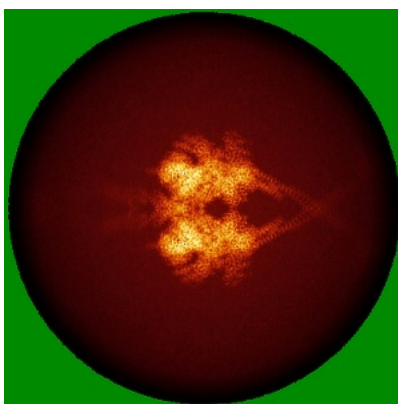
The images above show the largest variance slices of the map in three orthogonal directions.

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

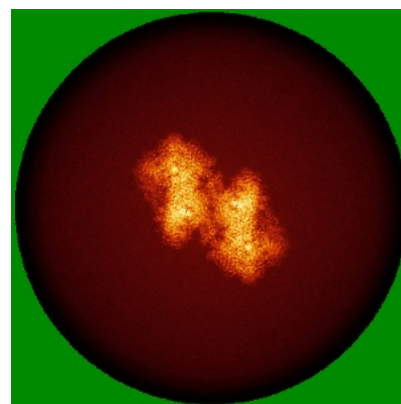
6.4.1 Primary map



X

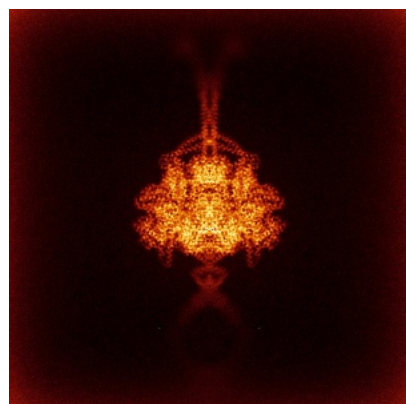


Y

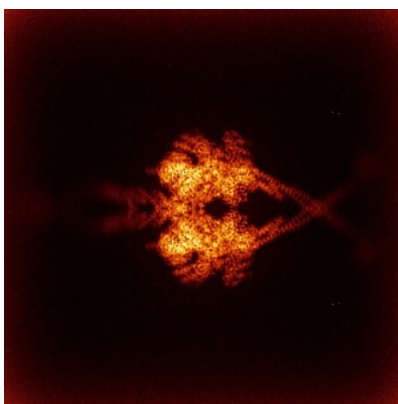


Z

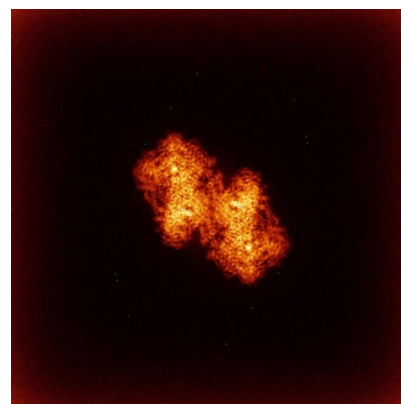
6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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.

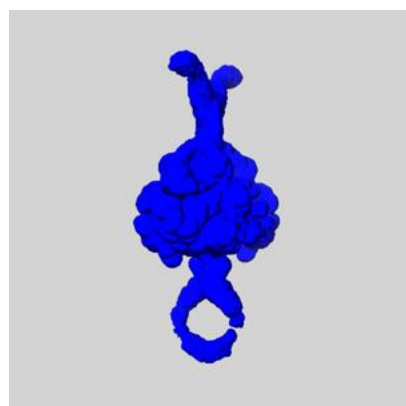
6.6 Mask visualisation [i](#)

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

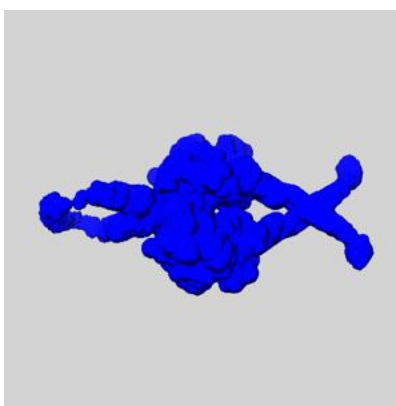
A mask typically either:

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

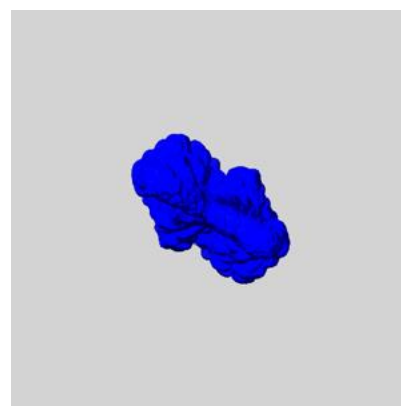
6.6.1 emd_47379_msk_1.map [i](#)



X



Y

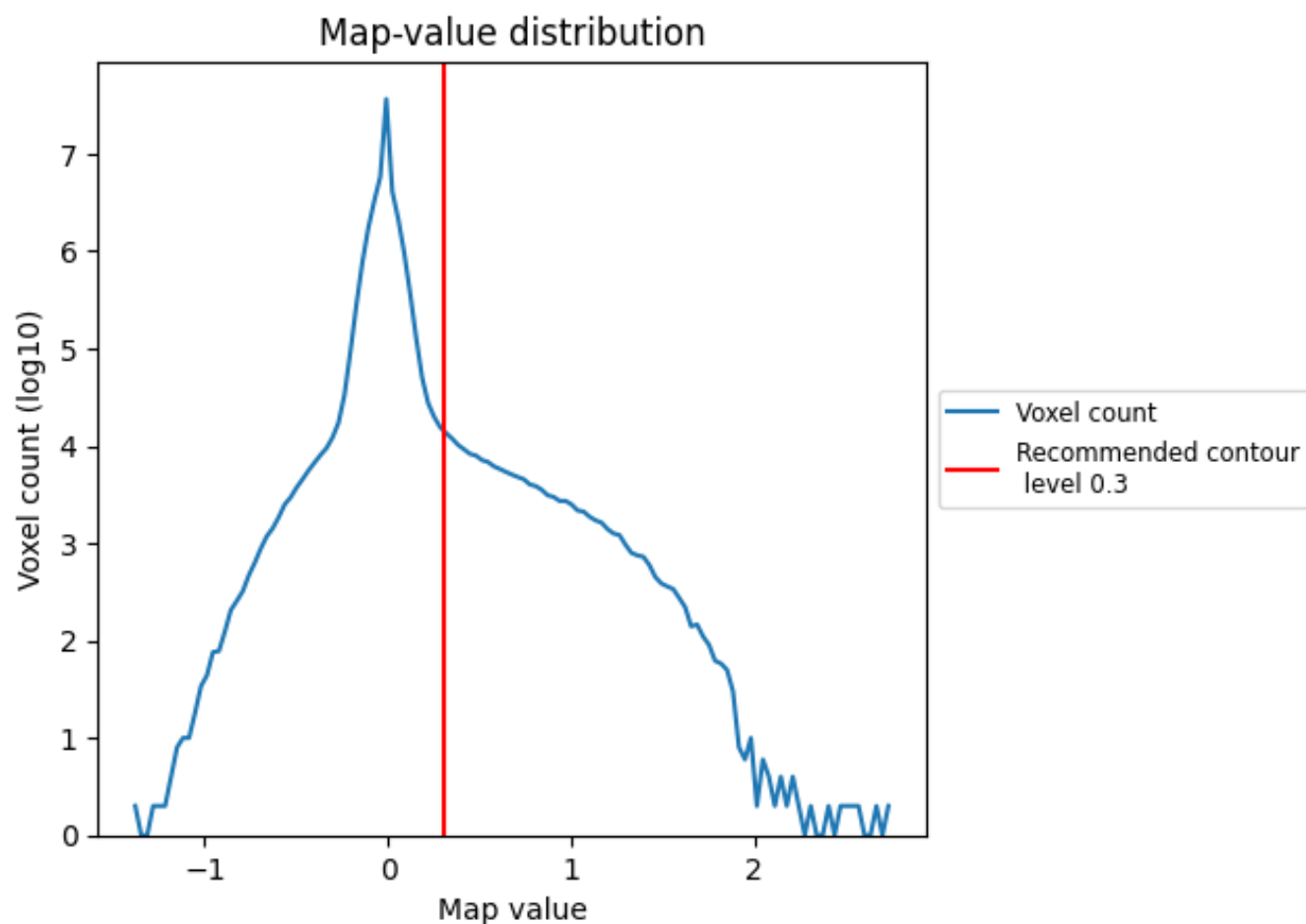


Z

7 Map analysis [i](#)

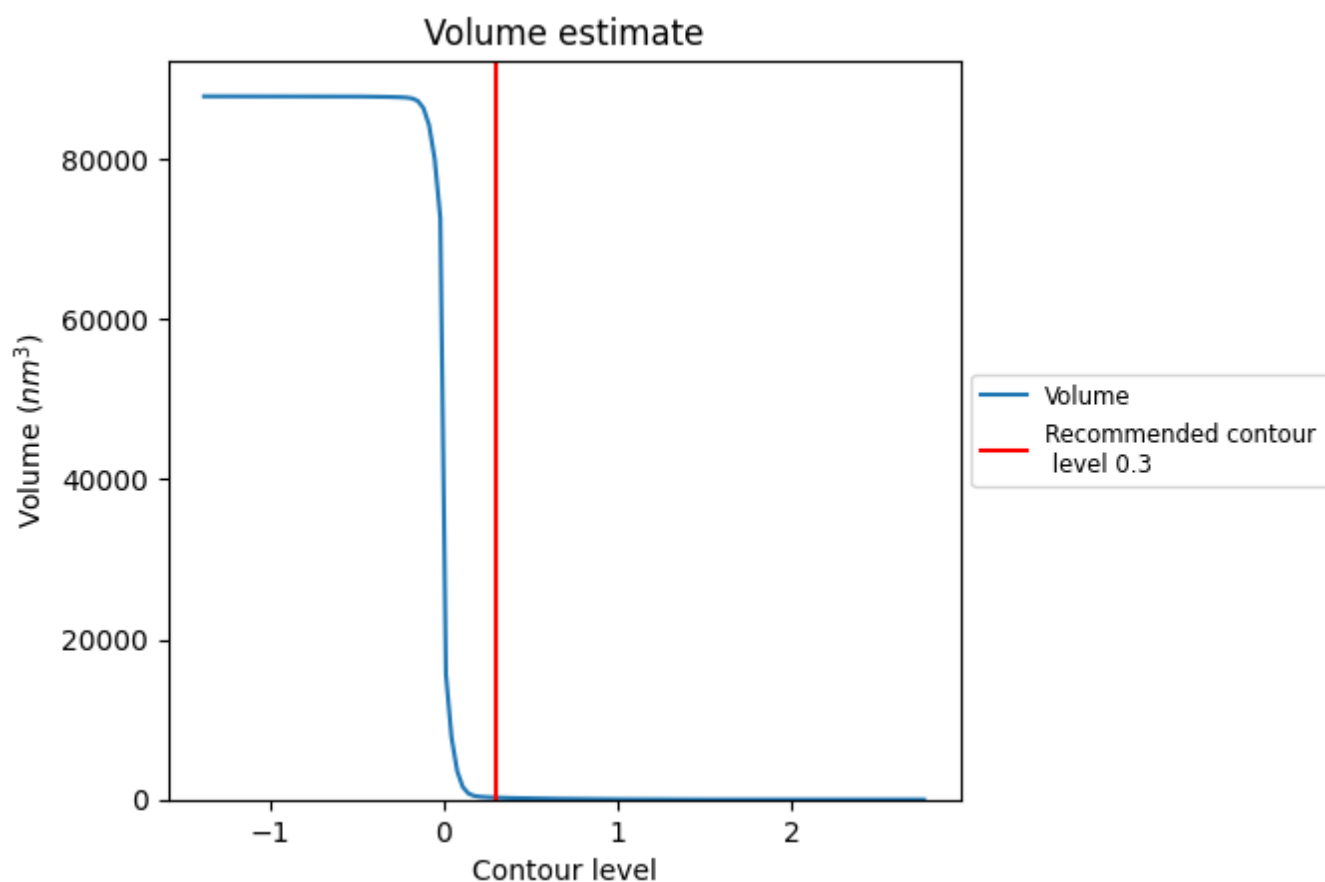
This section contains the results of statistical analysis of the map.

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.

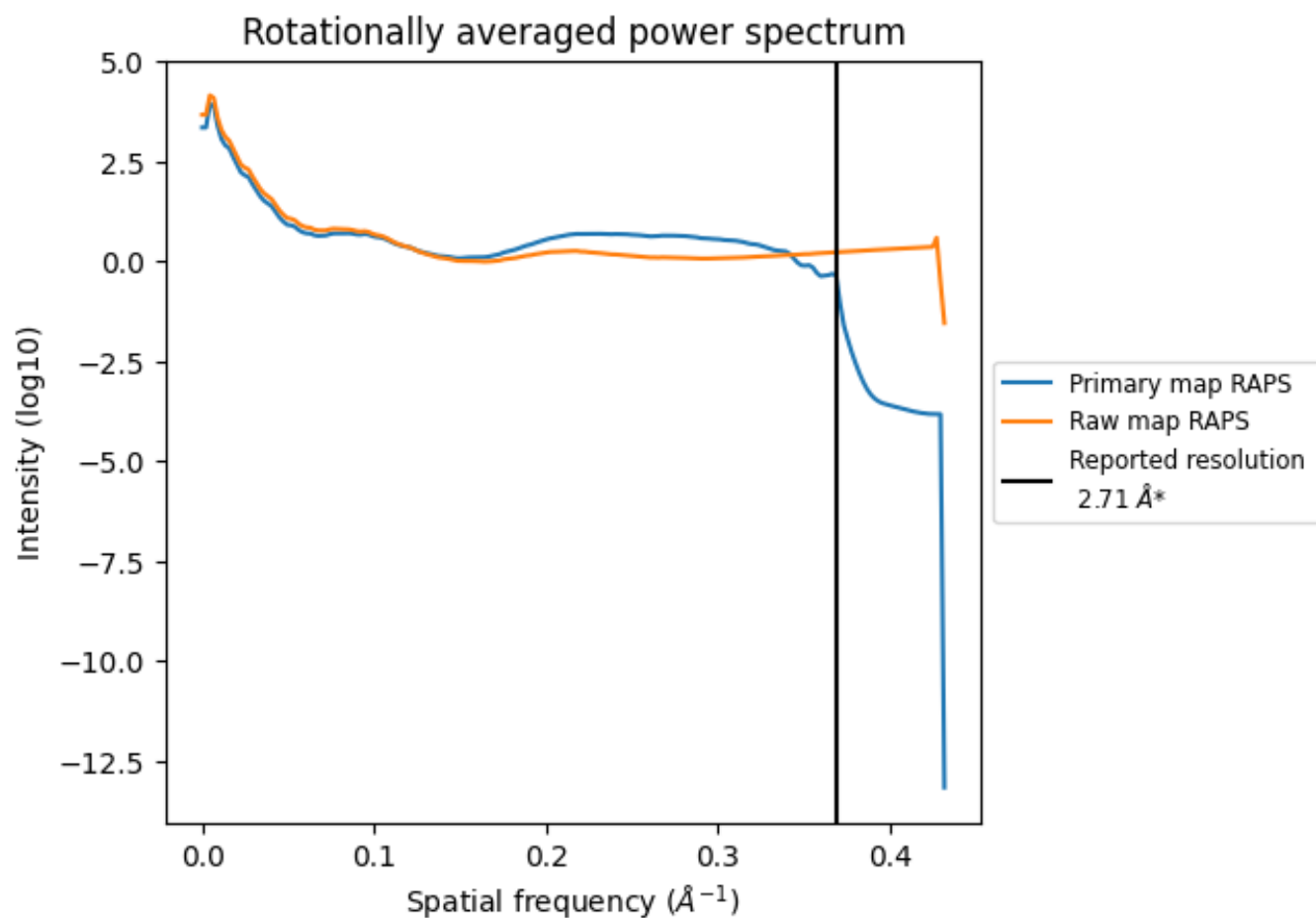
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 249 nm³; this corresponds to an approximate mass of 225 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 ⓘ

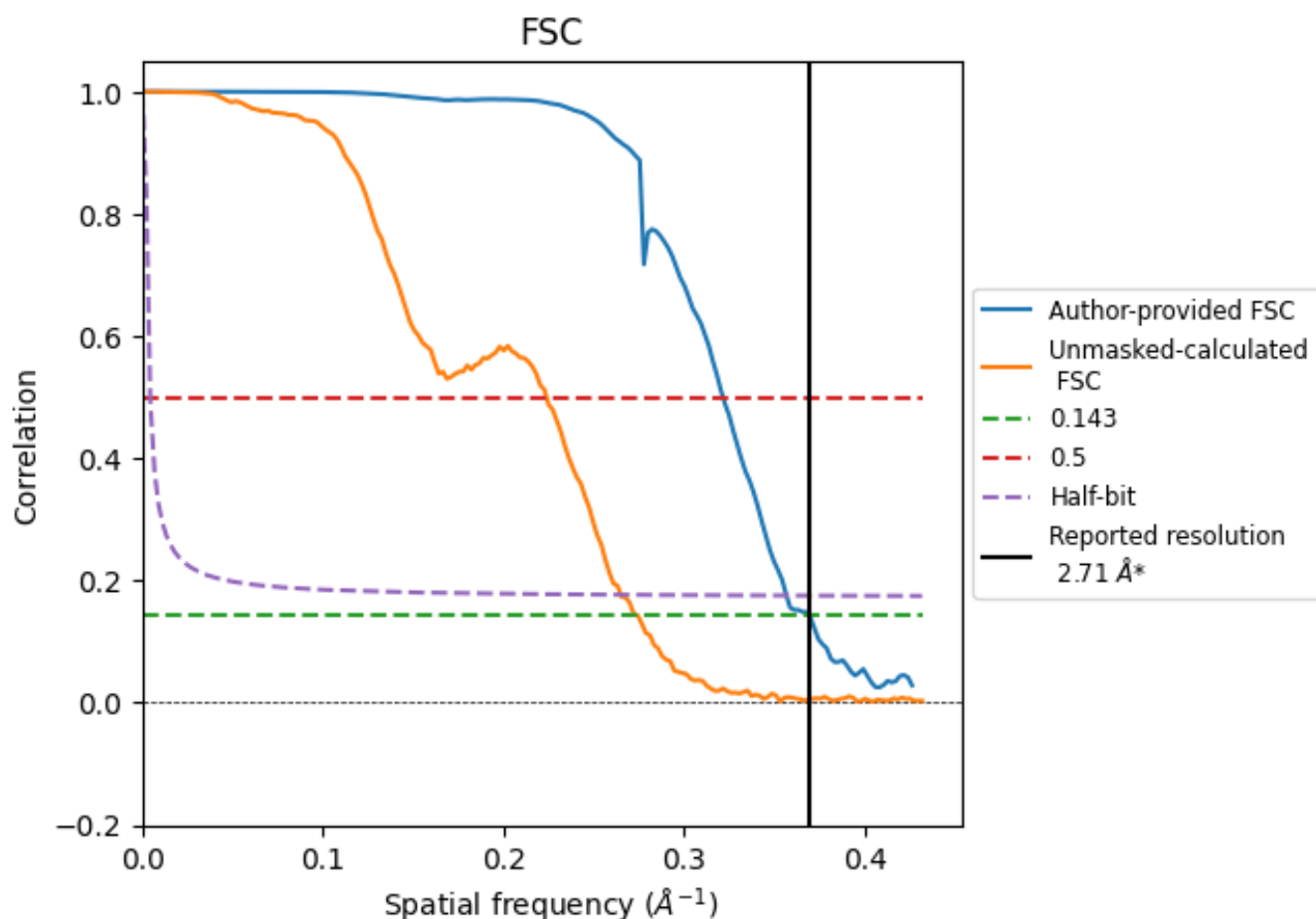


*Reported resolution corresponds to spatial frequency of 0.369 Å⁻¹

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 0.369 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.71	-	-
Author-provided FSC curve	2.71	3.11	2.80
Unmasked-calculated*	3.65	4.47	3.77

*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 3.65 differs from the reported value 2.71 by more than 10 %

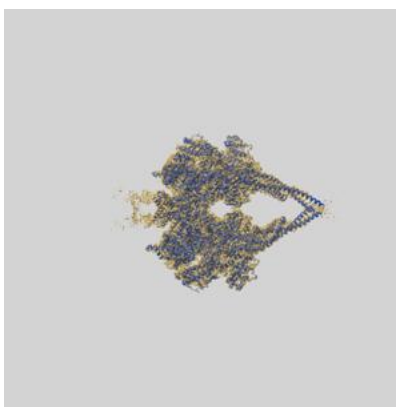
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47379 and PDB model 9E10. Per-residue inclusion information can be found in section [3](#) on page [5](#).

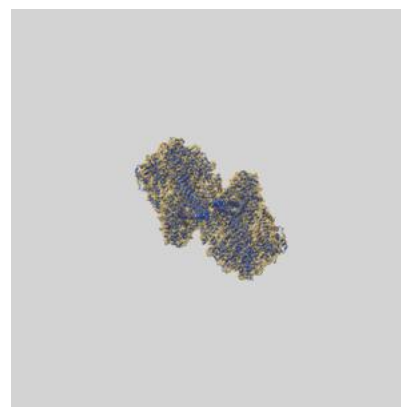
9.1 Map-model overlay [i](#)



X



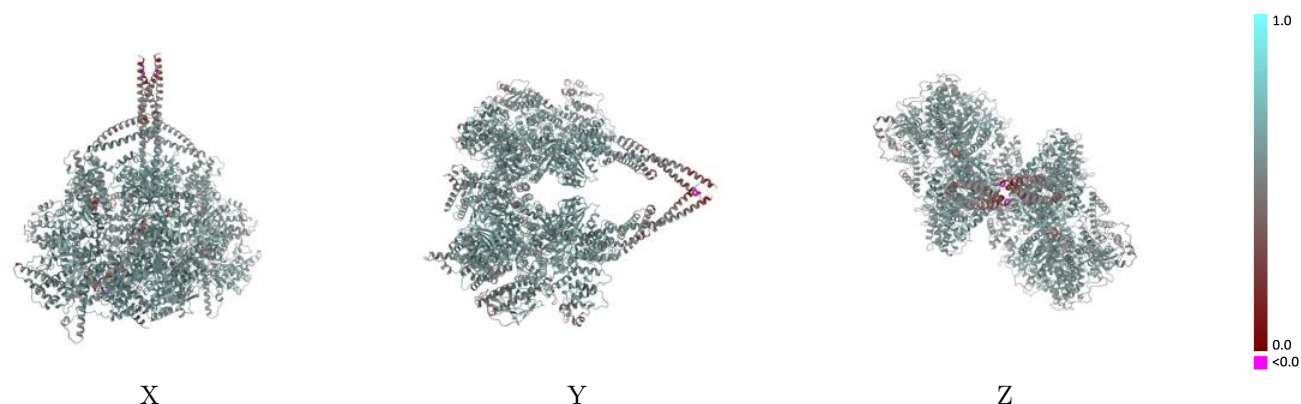
Y



Z

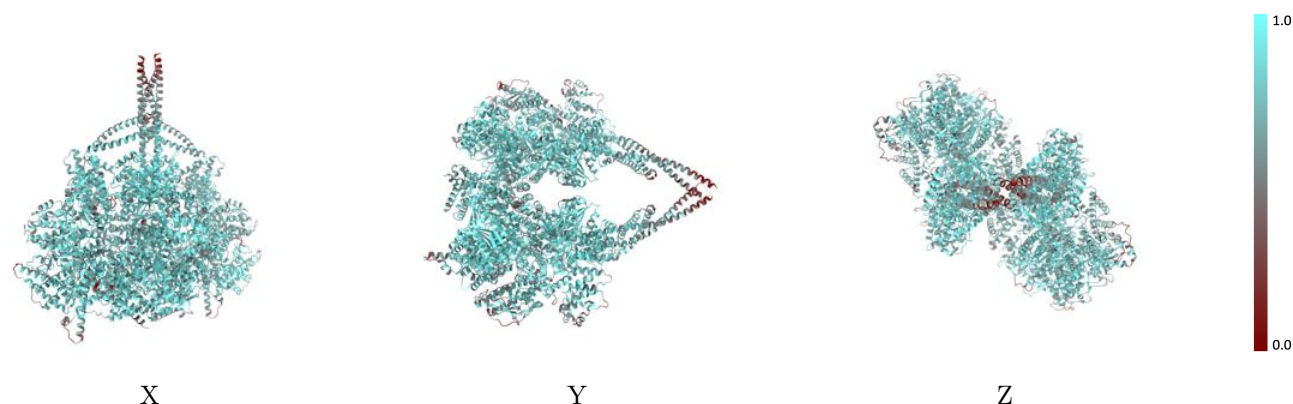
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



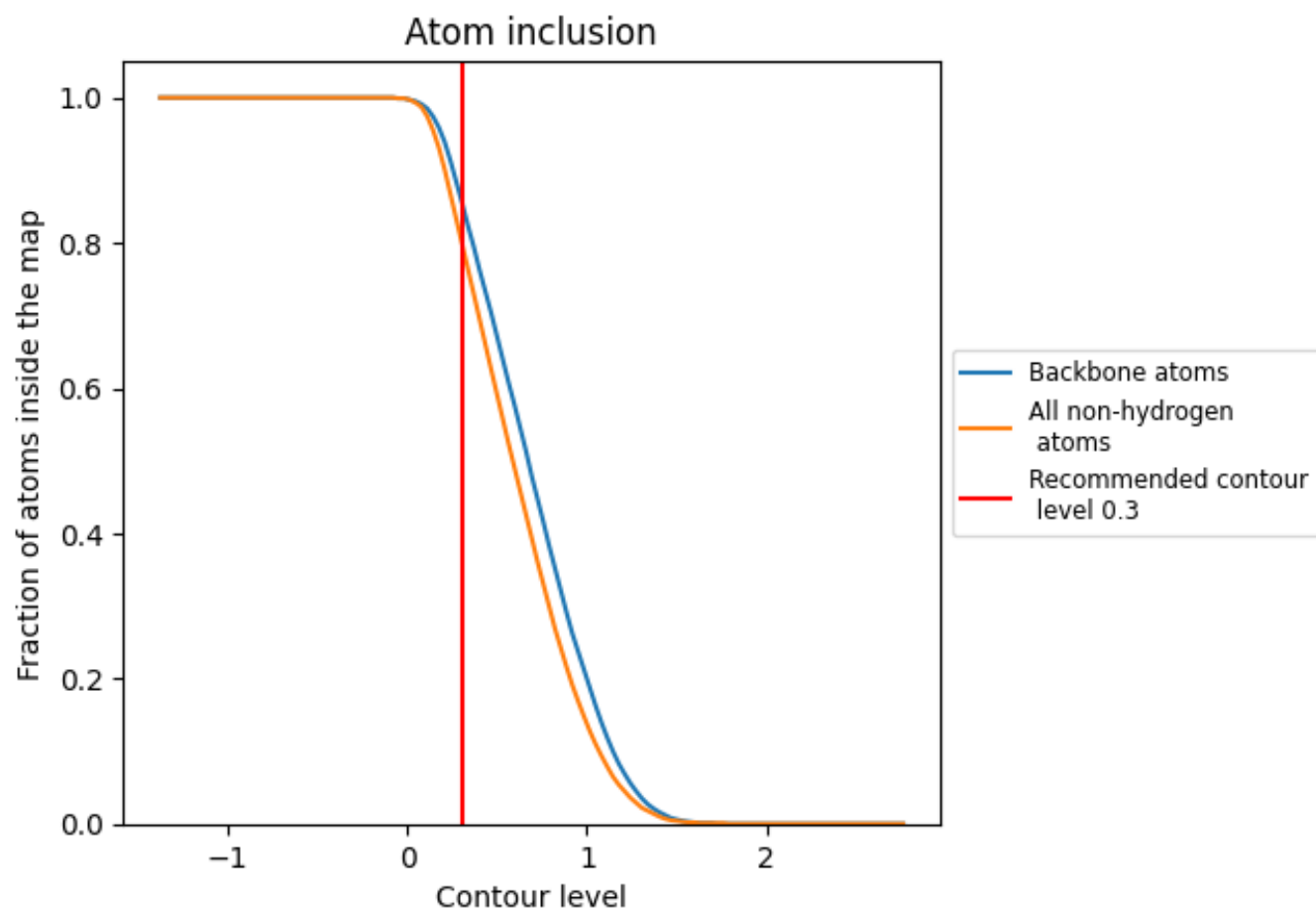
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 80% 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> 0.8040	<div></div> 0.5700
A	<div></div> 0.8050	<div></div> 0.5710
B	<div></div> 0.8040	<div></div> 0.5700

