



wwPDB EM Validation Summary Report ⓘ

May 2, 2026 – 01:24 PM EDT

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.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

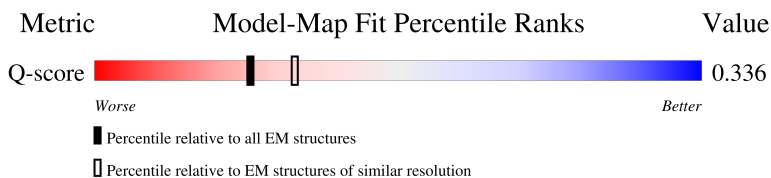
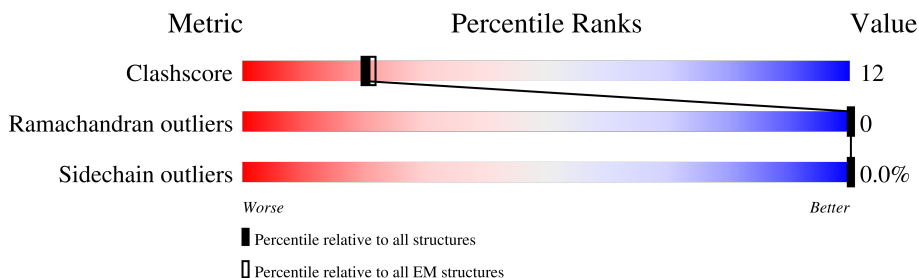
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



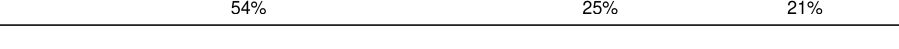

The reported resolution of this entry is 3.93 Å.

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.





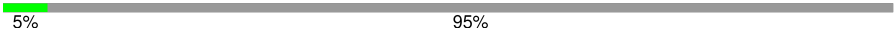
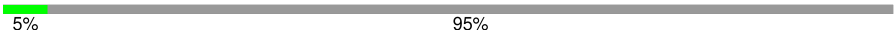


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7811 (3.43 - 4.43)

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	 45% 21% 34%
1	B	4646	 49% 17% 34%
2	C	410	 54% 25% 21%
2	D	410	 48% 29% 24%

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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

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		

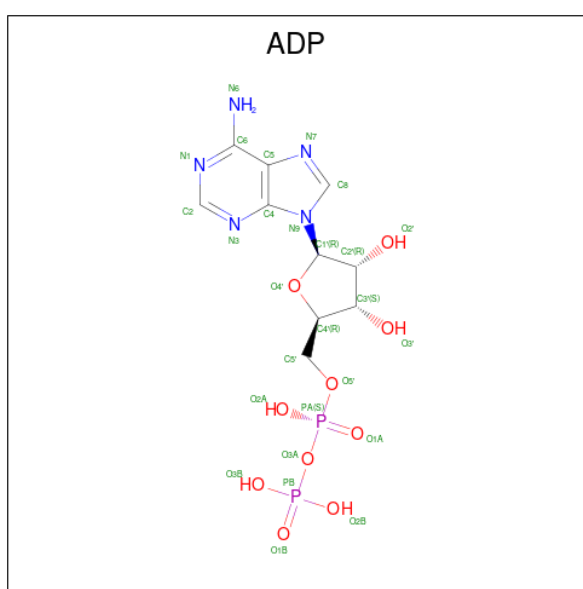
- Molecule 4 is a protein called Dynactin subunit 1.

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:

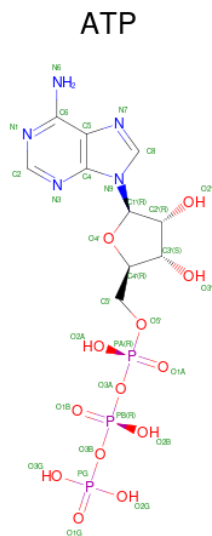
Chain	Residue	Modelled	Actual	Comment	Reference
I	1279	LEU	-	expression tag	UNP A0A287B8J2
I	1280	ILE	-	expression tag	UNP A0A287B8J2
I	1281	SER	-	expression tag	UNP A0A287B8J2
J	1279	LEU	-	expression tag	UNP A0A287B8J2
J	1280	ILE	-	expression tag	UNP A0A287B8J2
J	1281	SER	-	expression tag	UNP A0A287B8J2

- 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

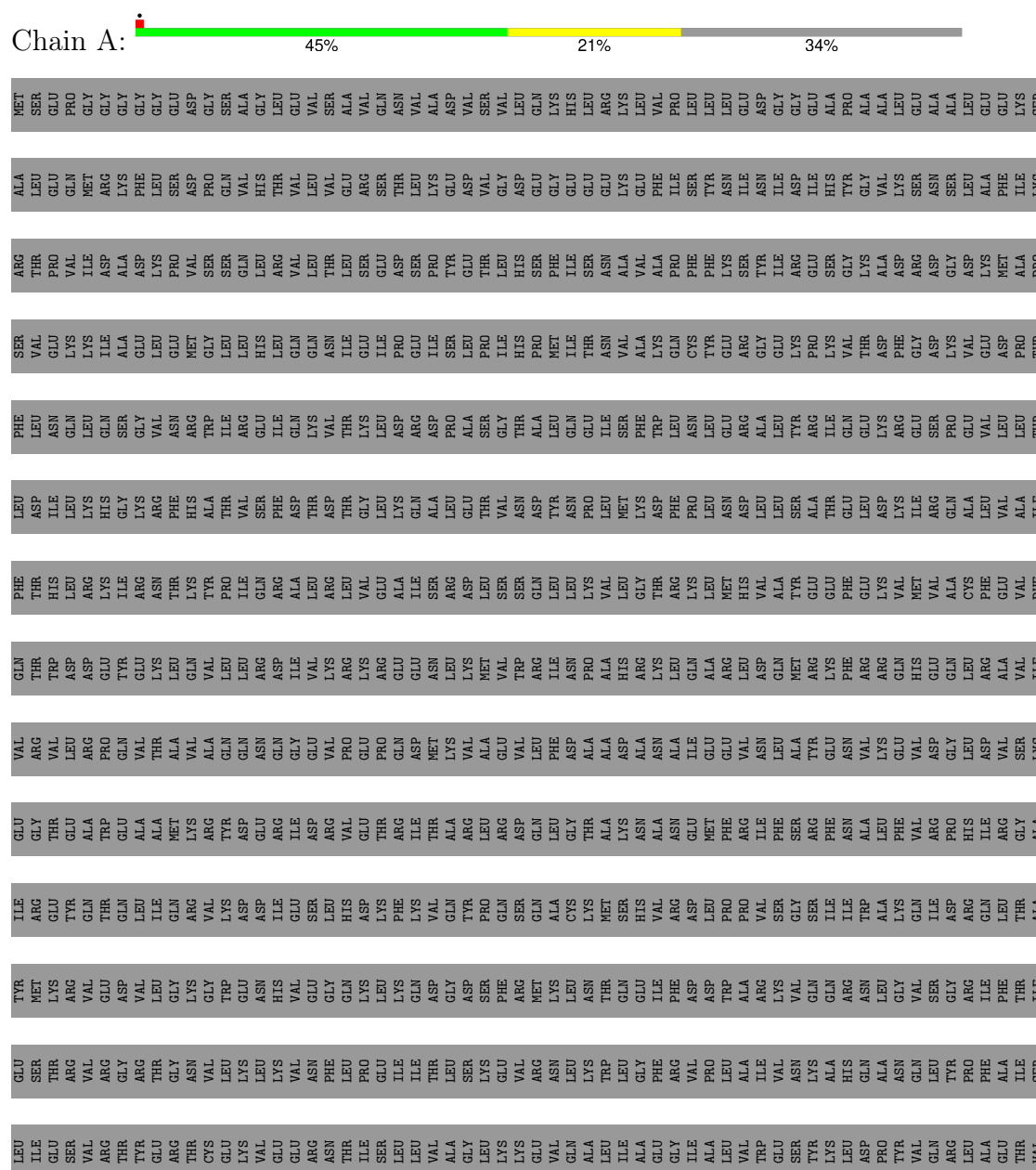
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

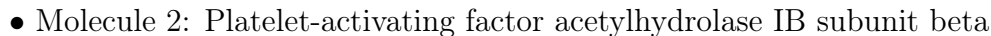






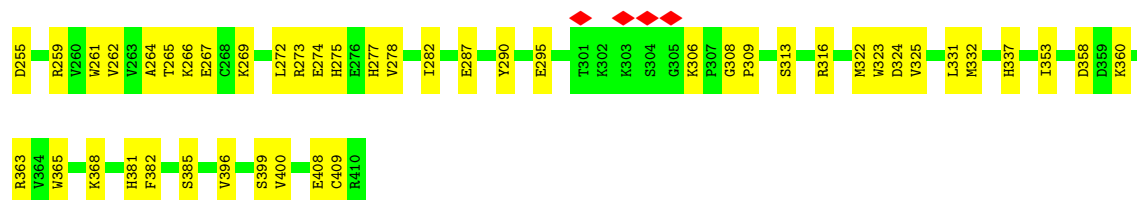
Y1393	VAL	THR	TRP	ARG	GLU	ALA	GLN	ALA	ASN	PHE	LEU	ILE	LEU	GLY	THR	ASP	LEU
M1394	ALA	GLU	LYS	PHE	GLN	LEU	LEU	LEU	LYS	LEU	LEU	THR	LEU	ASP	HIS	ASP	LEU
K1395	GLU	THR	THR	PHE	GLN	GLU	THR	THR	ASP	GLN	GLN	GLN	GLN	GLN	ASP	GLN	GLN
L1399	GLU	LYS	LYS	PRO	PRO	LEU	ILE	ILE	MET	ARG	THR	THR	THR	THR	GLU	PRO	VAL
L1403	GLN	VAL	VAL	SER	SER	ILE	ARG	ARG	ILE	GLU	GLU	VAL	VAL	VAL	GLN	GLN	GLN
K1404	ASP	THR	THR	TRP	LYS	THR	LYS	LYS	PRO	ASP	ASP	THR	THR	THR	TYR	TYR	THR
S1405	LEU	GLY	GLY	LEU	ASN	LEU	ARG	ALA	GLY	GLY	GLY	THR	THR	THR	GLY	ALA	THR
L1408	GLY	LEU	LEU	ILE	ILE	LEU	GLN	GLY	VAL	VAL	VAL	CYS	GLY	GLY	VAL	VAL	GLN
K1409	VAL	TRP	PRO	ASN	ASN	LEU	ASN	ALA	LEU	ILE	ILE	GLY	GLY	GLY	TRP	TRP	THR
D1410	SER	GLU	GLU	ILE	ILE	GLU	GLU	ASP	GLU	GLU	GLU	LYS	LYS	ASP	ASP	ASP	VAL
R1411	GLU	GLN	GLU	GLY	GLY	GLU	SER	ASN	LEU	GLU	GLU	GLY	GLY	GLY	ASN	ASN	GLN
H1412	LEU	LEU	ALA	GLY	ALA	ALA	ALA	ALA	GLY	ILE	ILE	GLU	GLU	GLU	ARG	ARG	THR
W1413	SER	LEU	LEU	GLY	GLY	VAL	SER	THR	THR	THR	THR	CYS	GLY	VAL	VAL	VAL	GLN
R1419	LYS	VAL	ALA	THR	LYS	ALA	GLY	GLY	LEU	ASP	ASP	ARG	ASN	ASN	ARG	VAL	THR
W1424	TRP	LEU	LEU	GLY	LYS	VAL	THR	THR	ARG	GLU	GLU	THR	THR	THR	PRO	PRO	THR
V1425	GLU	THR	THR	PHE	GLY	ALA	ALA	ALA	VAL	VAL	VAL	ILE	ILE	ILE	LYS	LYS	GLY
V1426	GLN	ILE	ILE	ASN	PHE	GLY	SER	THR	THR	THR	THR	SER	SER	SER	ARG	VAL	VAL
S1427	ASP	THR	THR	ASP	THR	THR	THR	THR	THR	THR	THR	LEU	LEU	LEU	ILE	ILE	GLU
E1428	ASP	GLY	GLY	ILE	ILE	ILE	VAL	VAL	VAL	VAL	VAL	LEU	LEU	LEU	ILE	ILE	GLU
T1429	GLY	LYS	LYS	ARG	MET	ASP	VAL	VAL	VAL	VAL	VAL	VAL	VAL	THR	THR	MET	ASN
T1430	MET	GLN	LYS	ARG	ARG	ALA	VAL	VAL	GLU	GLU	GLU	ALA	ALA	THR	THR	LYS	ALA
L1431	GLY	GLY	PHE	ARG	GLY	VAL	VAL	VAL	VAL	VAL	VAL	PHE	PHE	VAL	VAL	VAL	LEU
Q1349	LYS	LEU	ARG	ASP	LYS	GLY	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
P1350	GLU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
W1351	ASP	LEU	LYS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
V1352	THR	ASP	ASP	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
S1353	ASP	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN
V1354	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
Q1355	LYS	VAL	LYS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
P1356	CYS	ALA	CYS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
H1357	ALA	ALA	ALA	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
K1358	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
L1359	LYS	LYS	LYS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
M1362	GLU	GLY	GLY	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
L1363	LEU	LEU	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
D1364	LYS	GLN	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
A1365	GLU	GLU	GLU	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
L1370	ASP	THR	THR	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
K1371	THR	THR	THR	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
A1375	GLY	GLY	GLY	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
E1460	LEU	LEU	LEU	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER
E1461	LEU	LEU	LEU	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
F1462	GLY	THR	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
L1463	SER	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
K1464	ASP	GLU	GLU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
W1470	GLU	GLU	GLU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
Q1387	LEU	LEU	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
V1478	ARG	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
L1389	GLN	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
L1390	GLN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
C1484	GLN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR



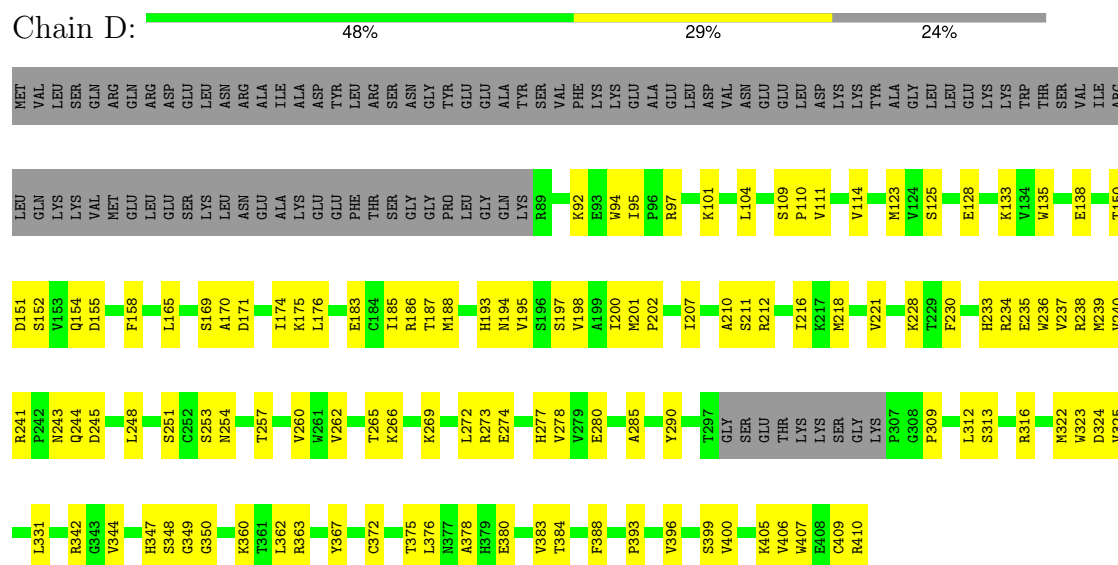


Response	Percentage
A lot	54%
Some	25%
Not much	21%

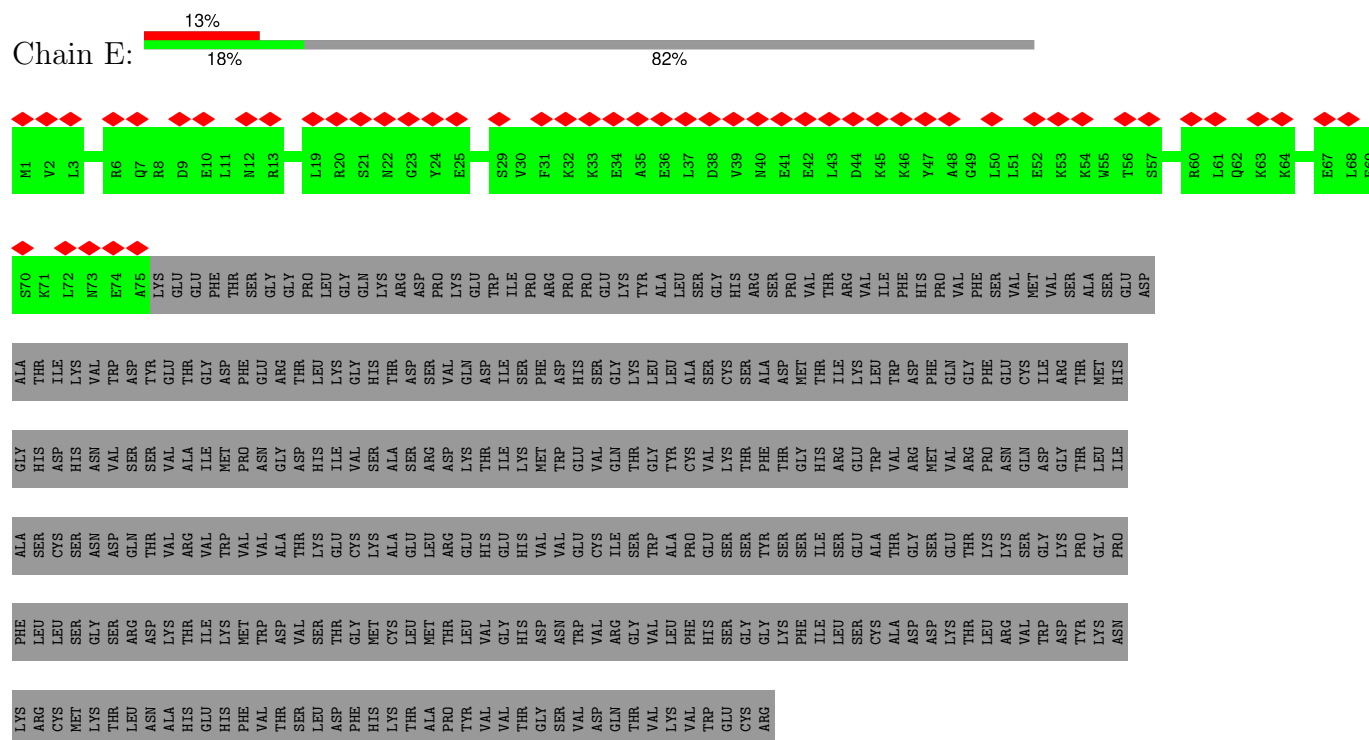




• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta



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

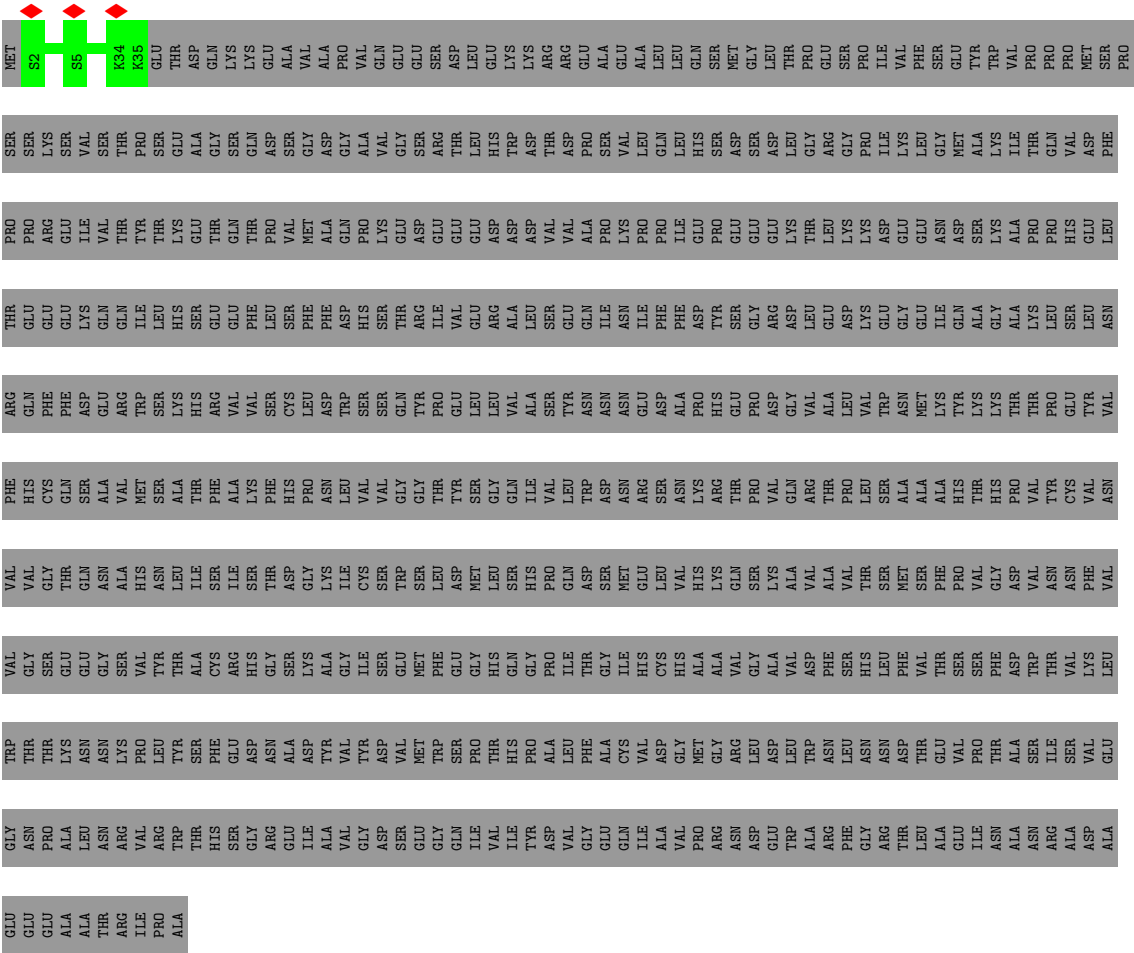


• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta

GLU
GLU
GLU
ALA
ALA
THR
ARG
ILE
PRO
ALA

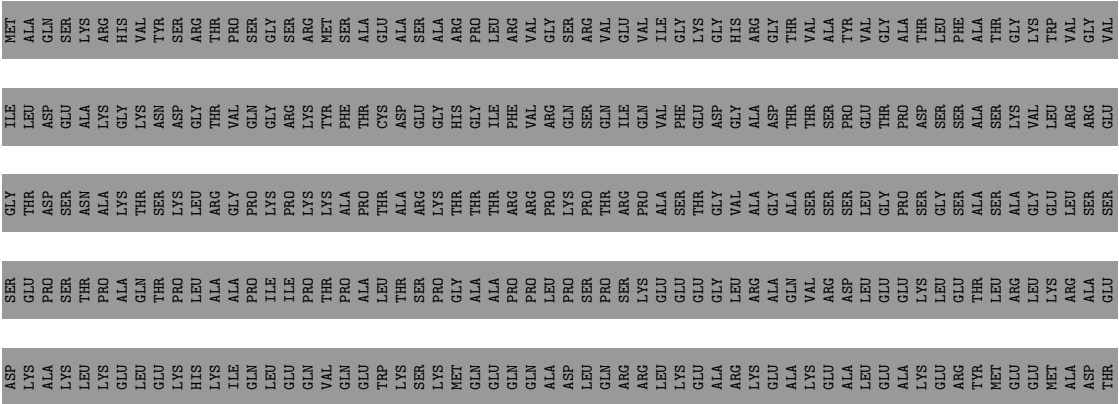
• Molecule 3: Cytoplasmic dynein 1 intermediate chain 2

Chain H: 5% 95%



• Molecule 4: Dynactin subunit 1

Chain I: 10% 90%







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

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	0.12	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

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%)	86	86
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
5	ADP	A	4703	-	28,29,29	1.41	4 (14%)	43,45,45	1.87	8 (18%)
5	ADP	B	4704	-	28,29,29	1.41	4 (14%)	43,45,45	1.83	9 (20%)
5	ADP	B	4703	-	28,29,29	1.41	4 (14%)	43,45,45	1.92	8 (18%)
6	ATP	A	4702	7	32,33,33	0.29	0	48,52,52	0.29	0
5	ADP	A	4701	7	28,29,29	1.44	4 (14%)	43,45,45	1.77	8 (18%)
6	ATP	B	4702	7	32,33,33	0.37	0	48,52,52	0.30	0
5	ADP	B	4701	7	28,29,29	1.40	4 (14%)	43,45,45	1.83	8 (18%)
5	ADP	A	4704	-	28,29,29	1.40	4 (14%)	43,45,45	1.82	9 (20%)

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
5	ADP	A	4703	-	-	0/16/32/32	0/3/3/3
5	ADP	B	4704	-	-	2/16/32/32	0/3/3/3
5	ADP	B	4703	-	-	2/16/32/32	0/3/3/3
6	ATP	A	4702	7	-	7/22/38/38	0/3/3/3
5	ADP	A	4701	7	-	0/16/32/32	0/3/3/3
6	ATP	B	4702	7	-	5/22/38/38	0/3/3/3
5	ADP	B	4701	7	-	2/16/32/32	0/3/3/3
5	ADP	A	4704	-	-	1/16/32/32	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)
5	A	4701	ADP	C5-C4	4.90	1.47	1.39
5	A	4703	ADP	C5-C4	4.75	1.47	1.39
5	B	4703	ADP	C5-C4	4.75	1.47	1.39
5	A	4704	ADP	C5-C4	4.73	1.47	1.39
5	B	4704	ADP	C5-C4	4.72	1.47	1.39

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	4703	ADP	C5-C4-N3	-6.52	117.74	126.72
5	A	4703	ADP	C5-C4-N3	-6.10	118.32	126.72
5	A	4704	ADP	C5-C4-N3	-5.92	118.56	126.72
5	B	4701	ADP	C5-C4-N3	-5.90	118.59	126.72
5	B	4704	ADP	C5-C4-N3	-5.87	118.64	126.72

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

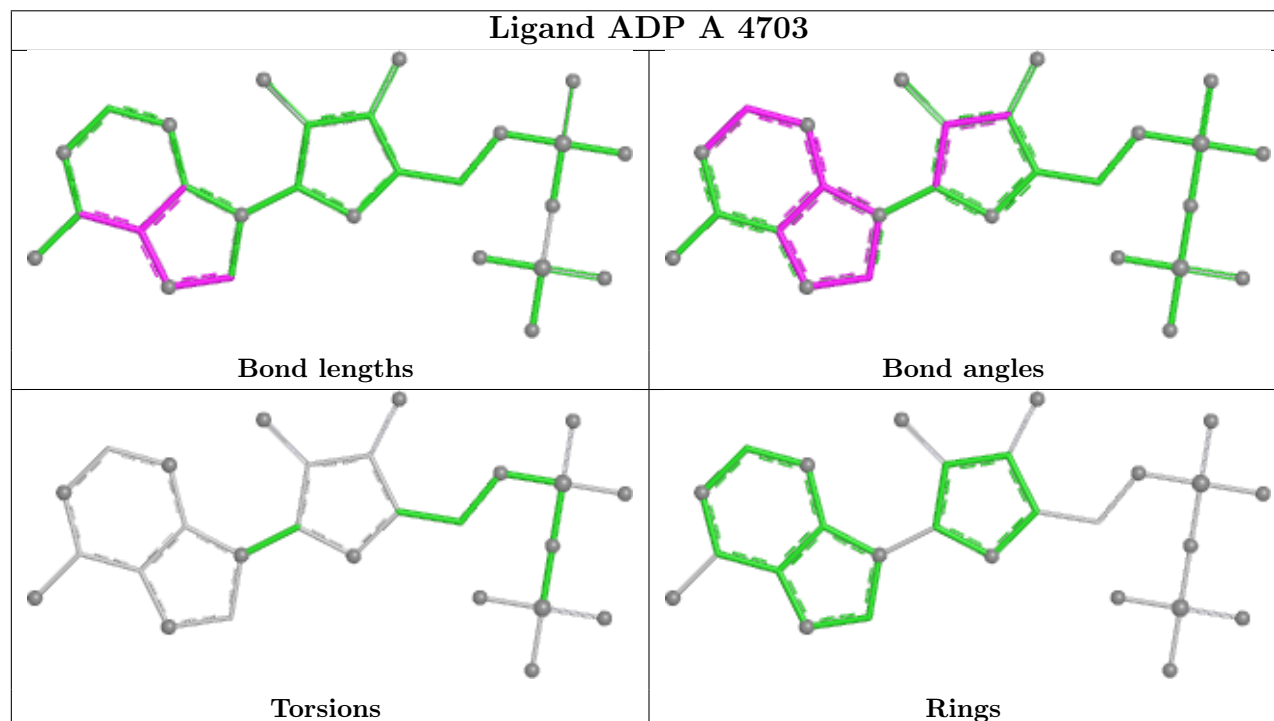
Mol	Chain	Res	Type	Atoms
5	B	4701	ADP	C5'-O5'-PA-O2A
5	B	4701	ADP	C5'-O5'-PA-O3A
6	A	4702	ATP	C5'-O5'-PA-O1A
6	A	4702	ATP	C5'-O5'-PA-O2A
6	A	4702	ATP	C5'-O5'-PA-O3A

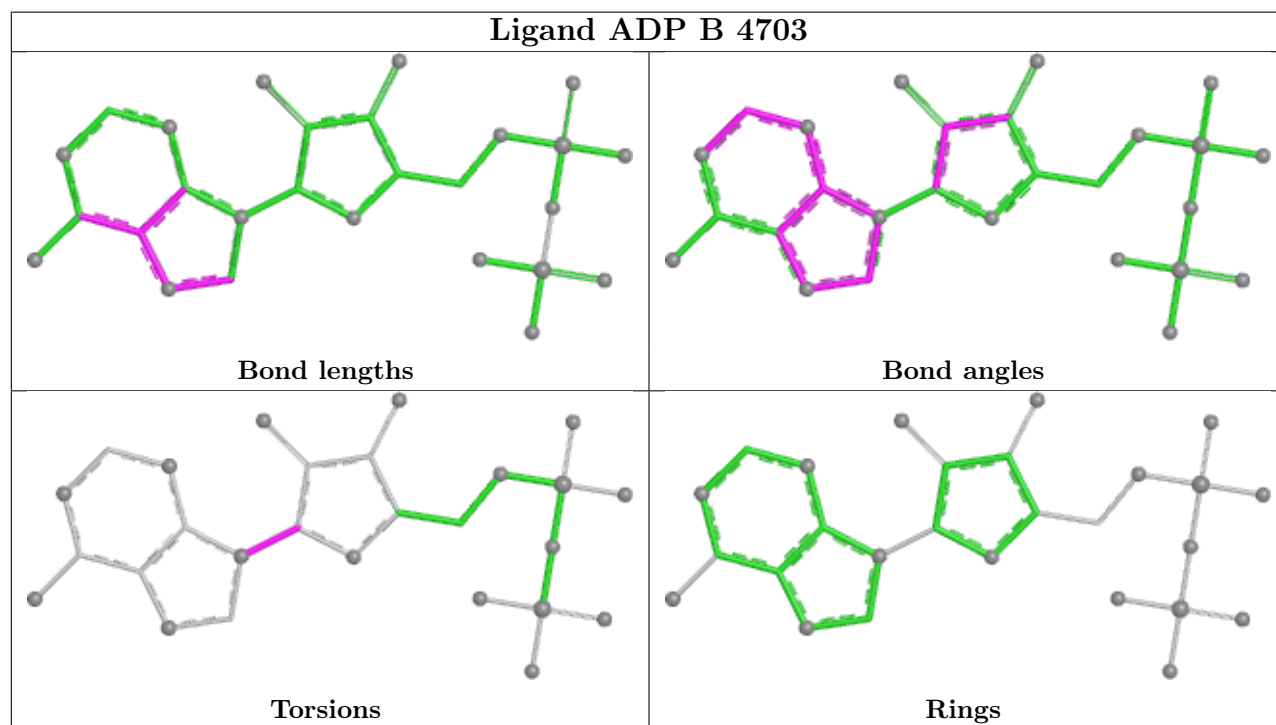
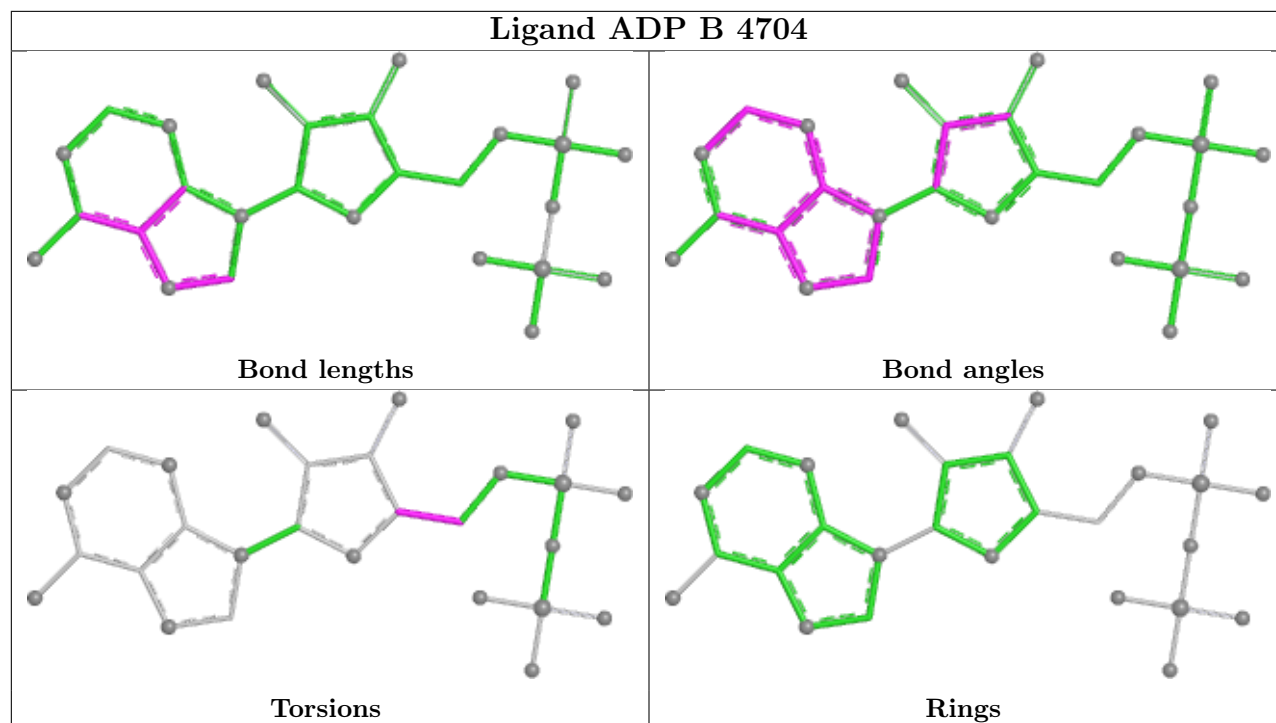
There are no ring outliers.

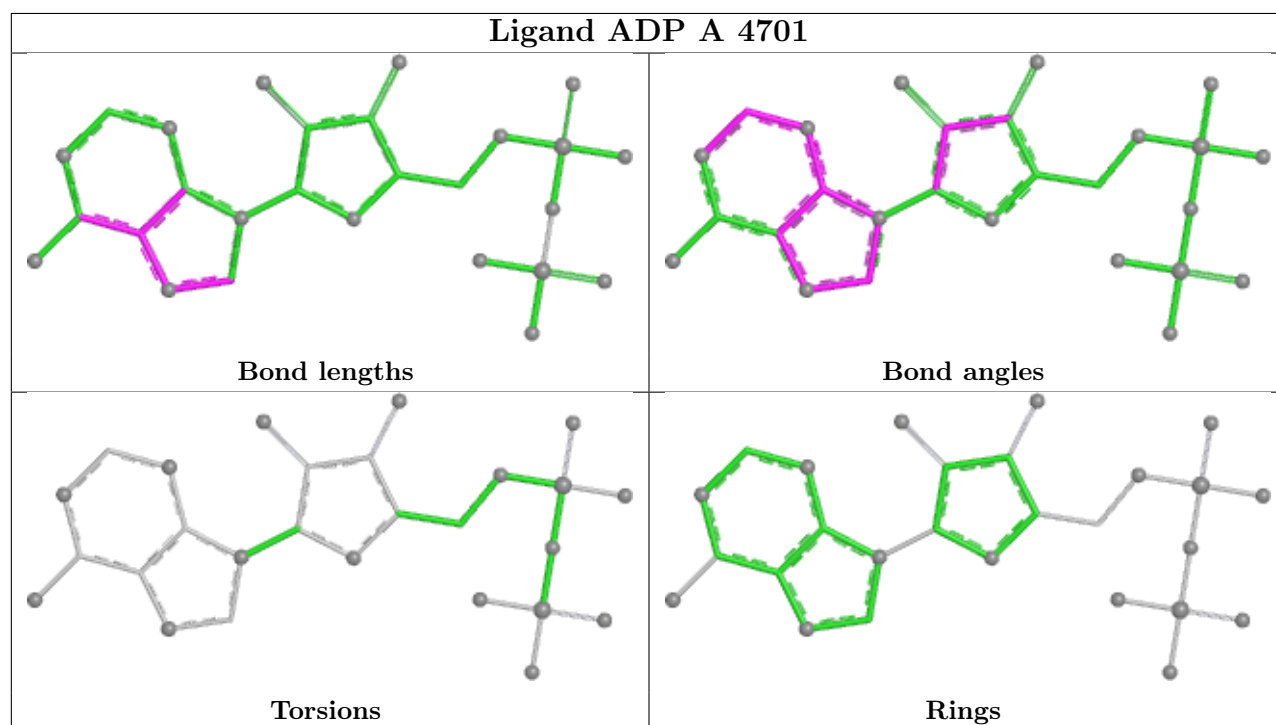
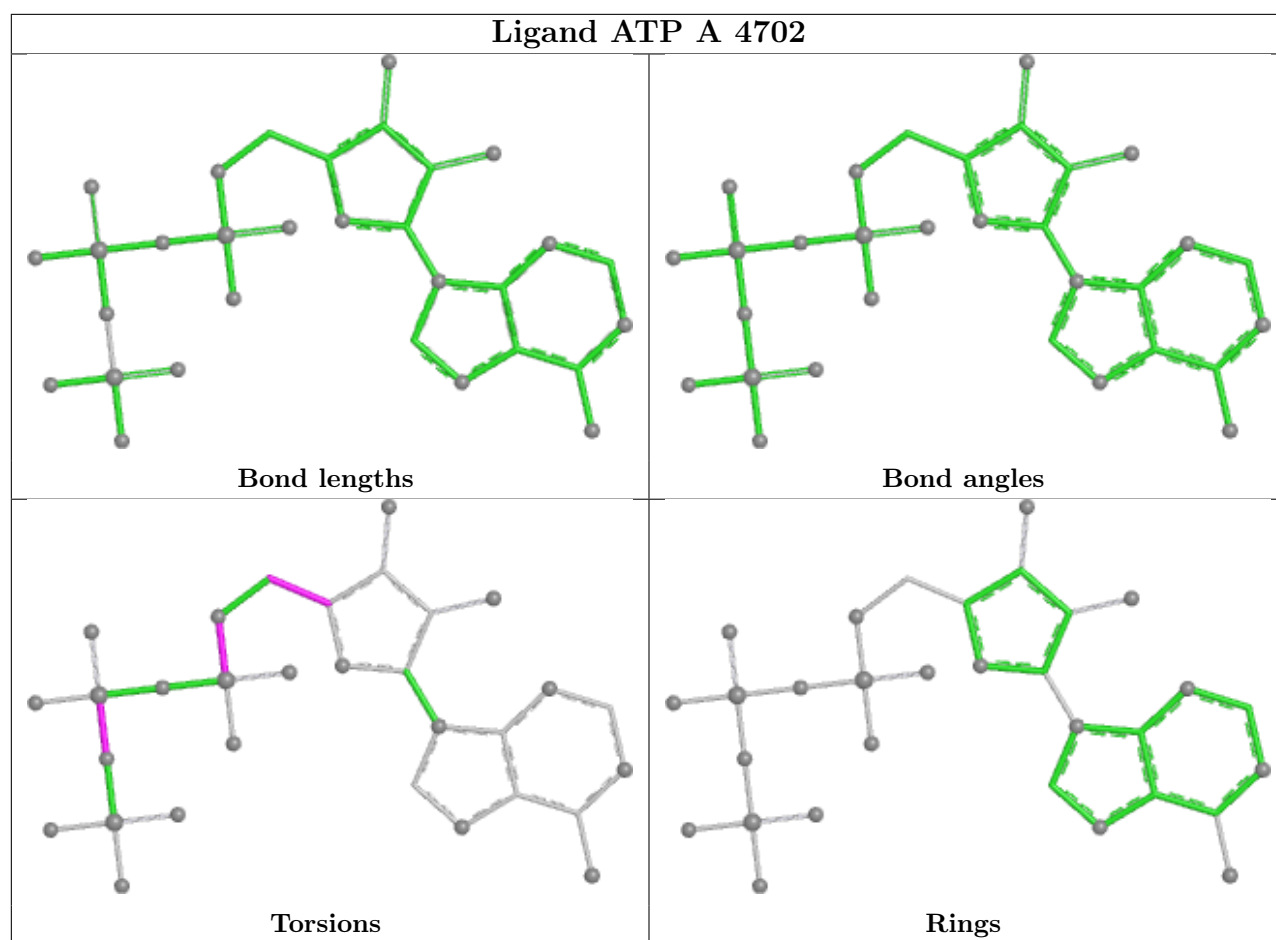
8 monomers are involved in 29 short contacts:

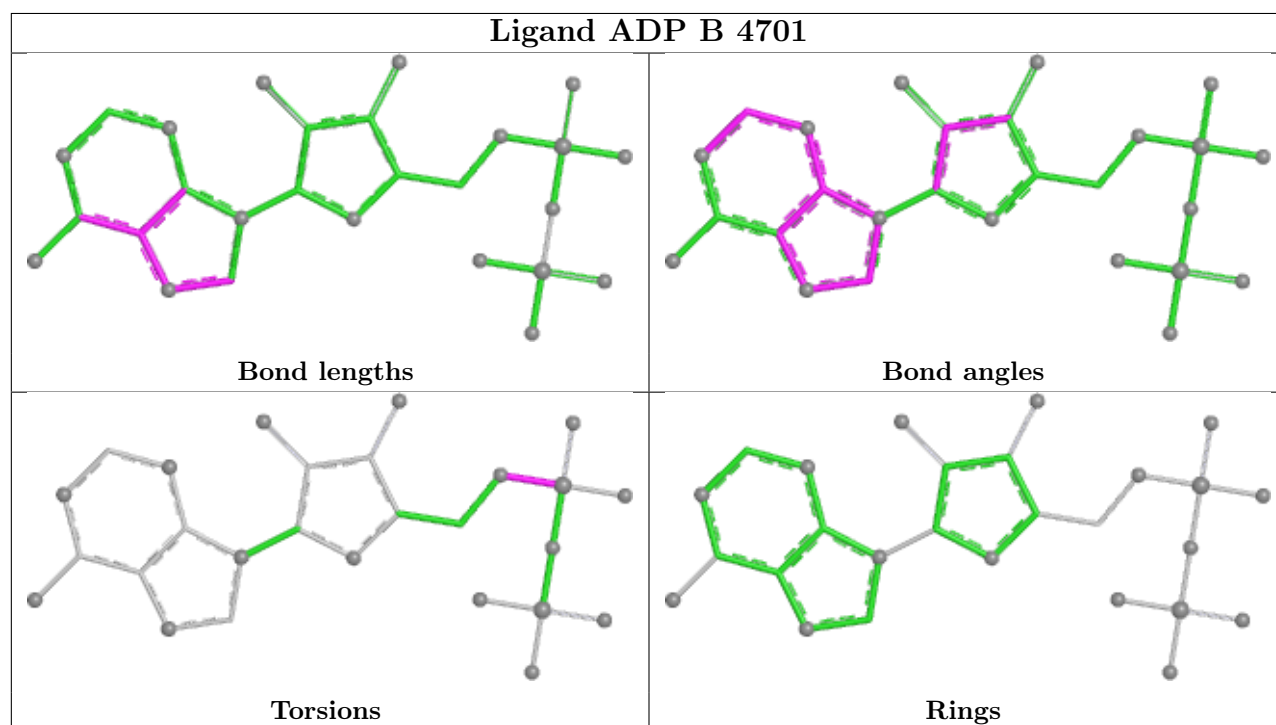
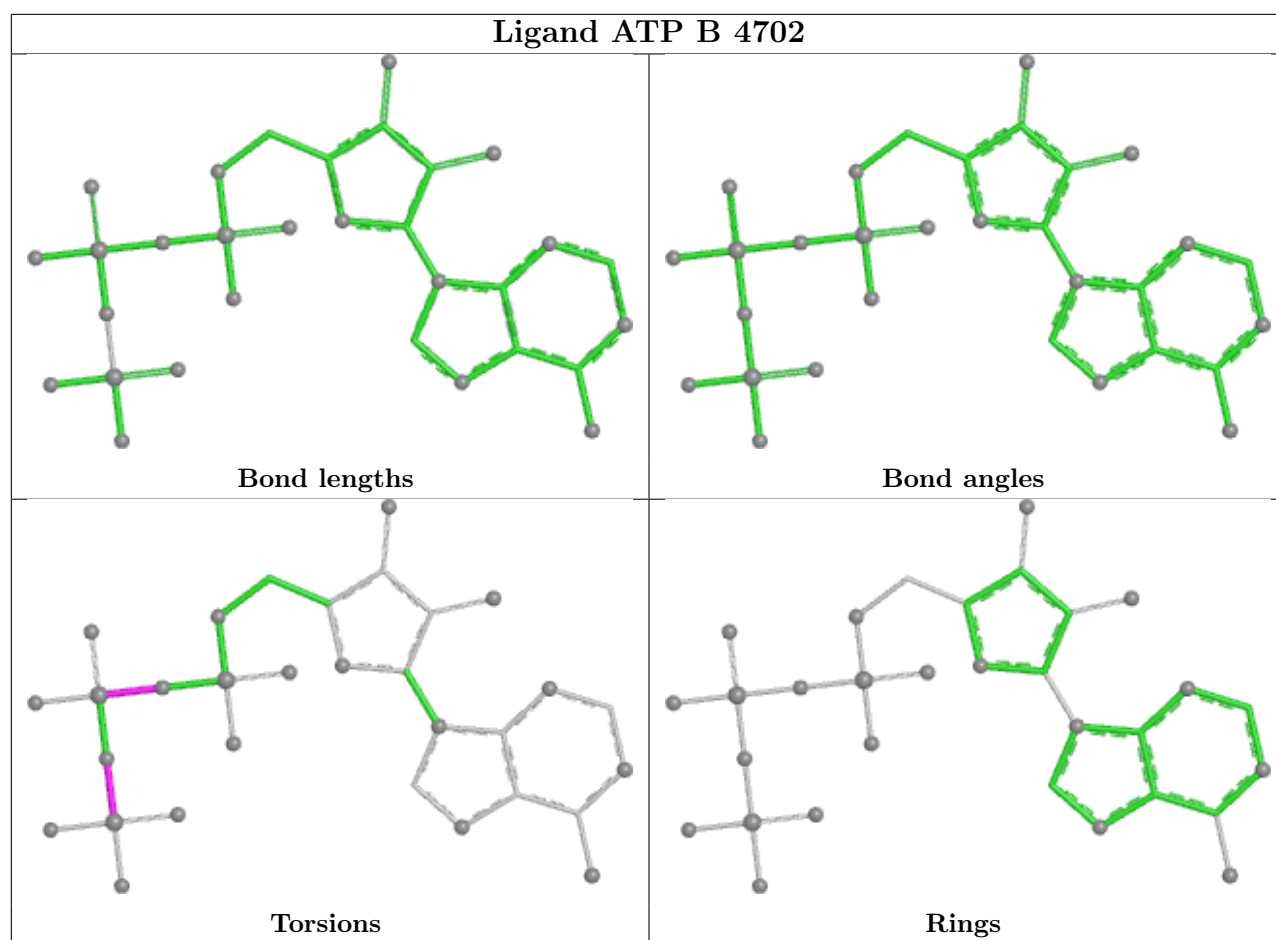
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	4703	ADP	3	0
5	B	4704	ADP	2	0
5	B	4703	ADP	3	0
6	A	4702	ATP	4	0
5	A	4701	ADP	3	0
6	B	4702	ATP	6	0
5	B	4701	ADP	5	0
5	A	4704	ADP	3	0

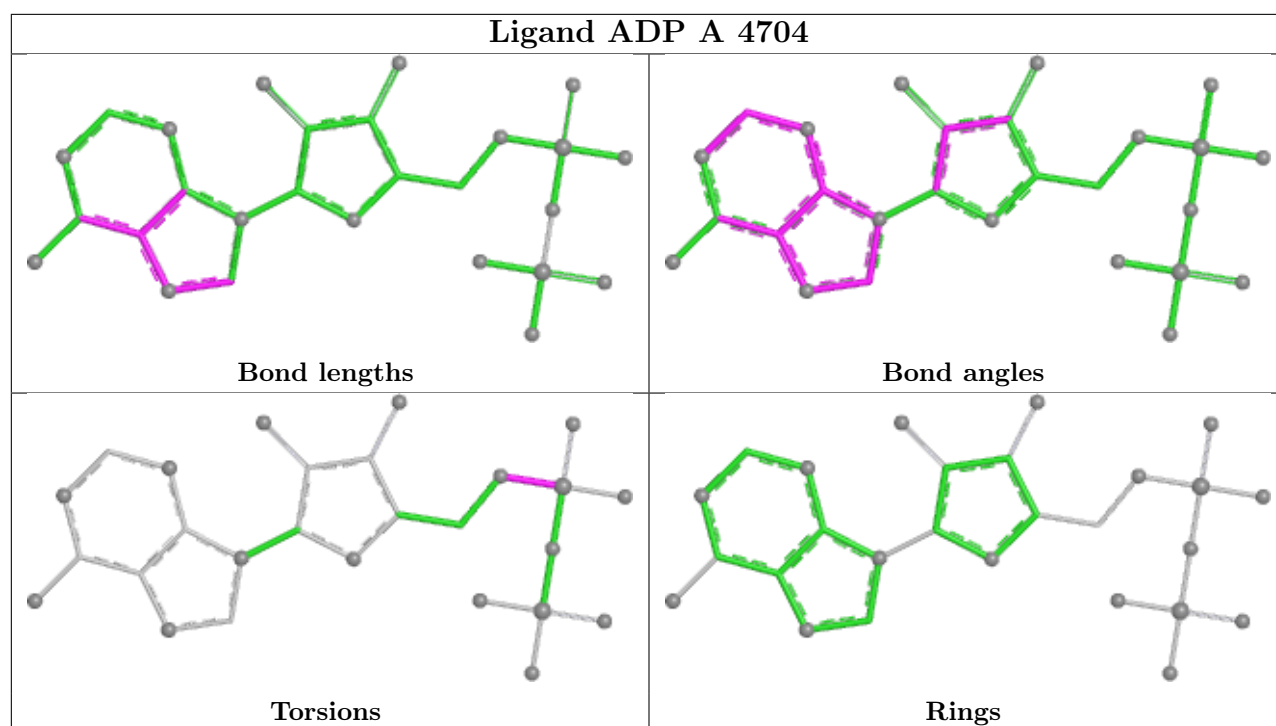
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

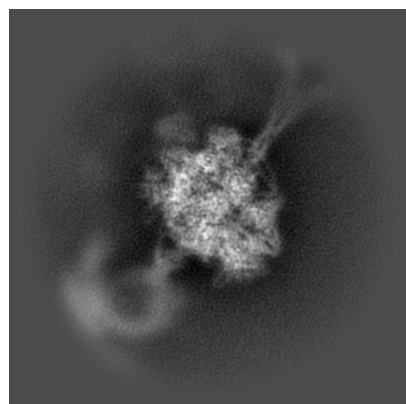
6 Map visualisation [i](#)

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

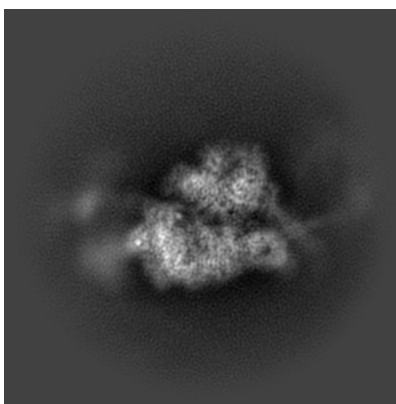
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

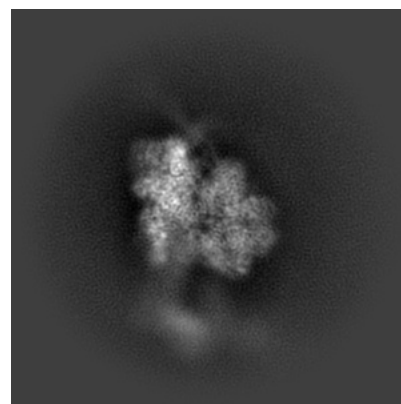
6.1.1 Primary map



X

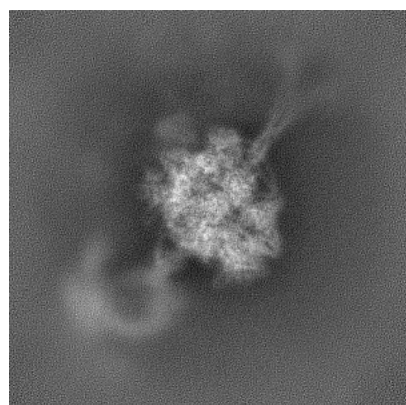


Y

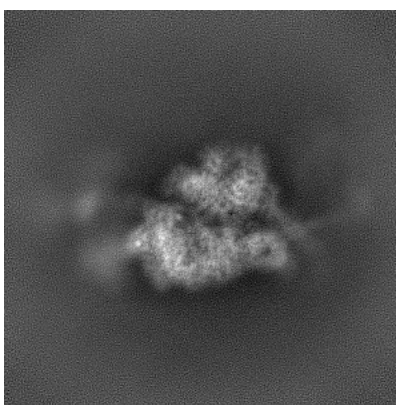


Z

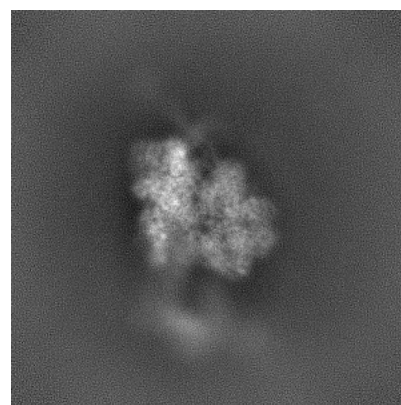
6.1.2 Raw map



X



Y

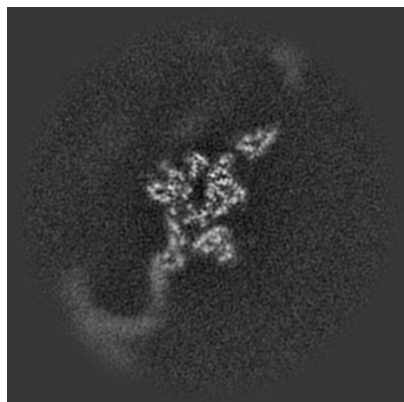


Z

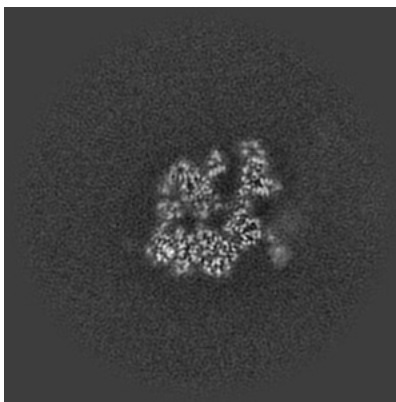
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

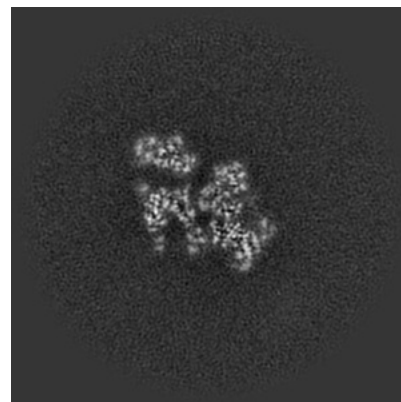
6.2.1 Primary map



X Index: 192

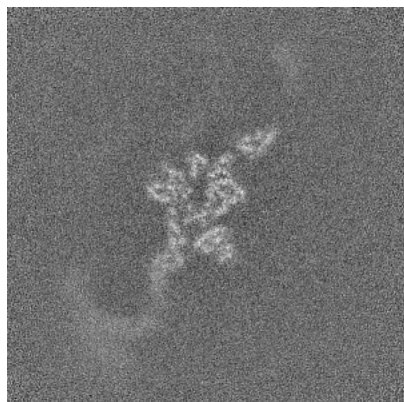


Y Index: 192

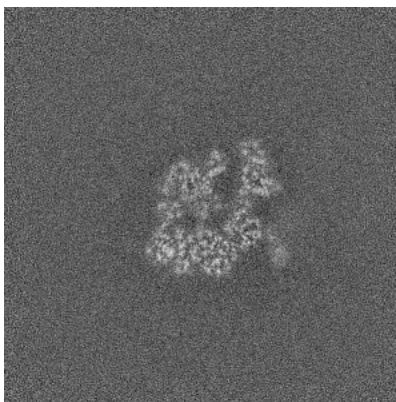


Z Index: 192

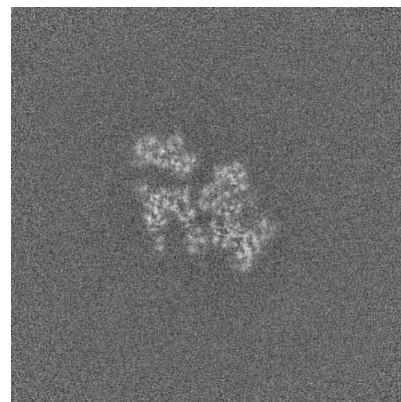
6.2.2 Raw map



X Index: 192



Y Index: 192

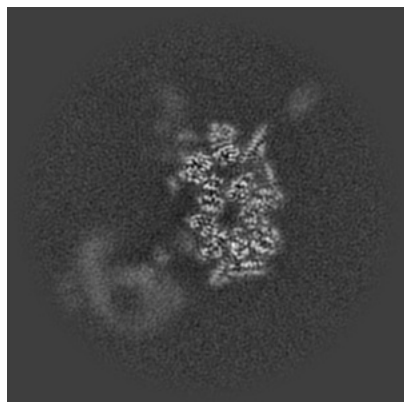


Z Index: 192

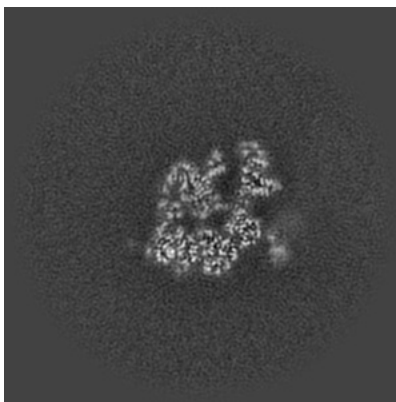
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

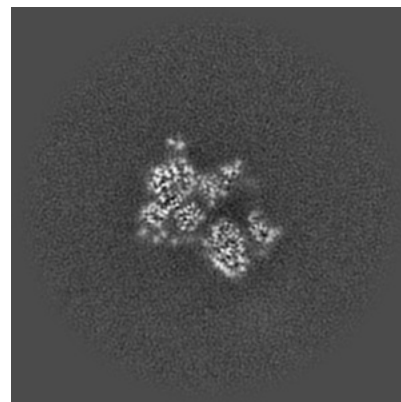
6.3.1 Primary map



X Index: 157

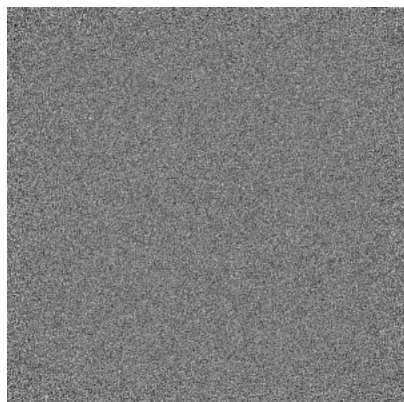


Y Index: 193

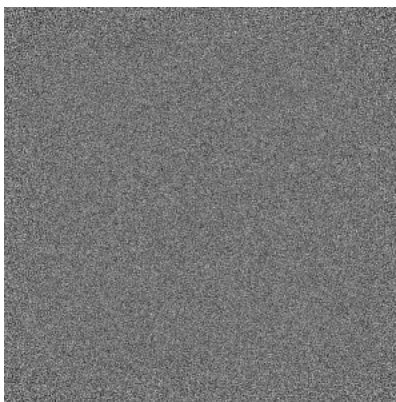


Z Index: 214

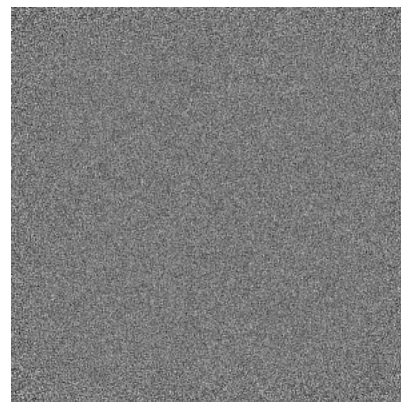
6.3.2 Raw map



X Index: 0



Y Index: 0

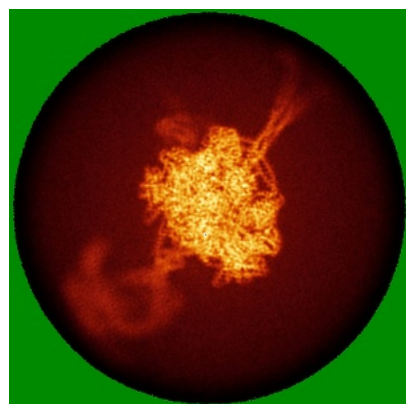


Z Index: 0

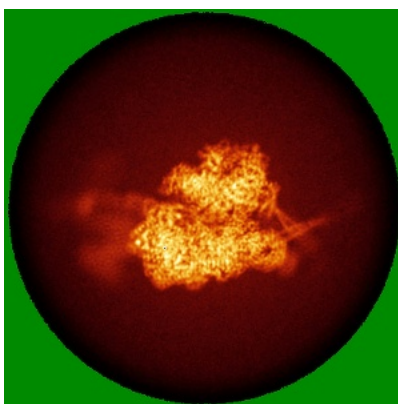
The images above show the largest variance slices of the map in three orthogonal directions.

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

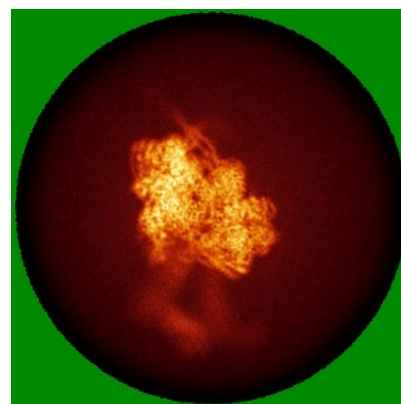
6.4.1 Primary map



X

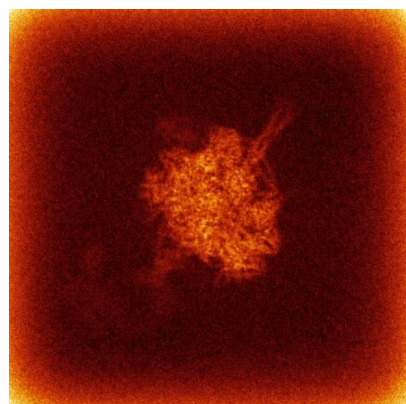


Y

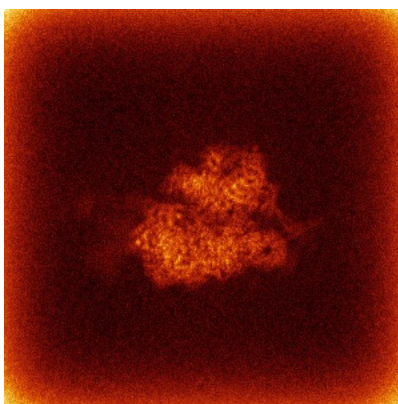


Z

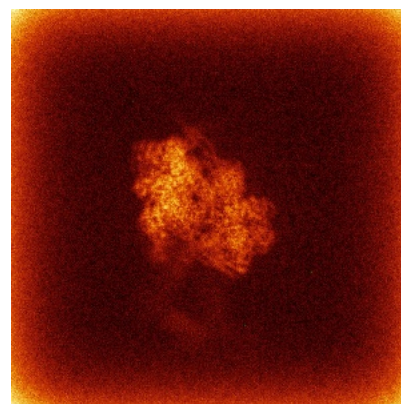
6.4.2 Raw map



X



Y

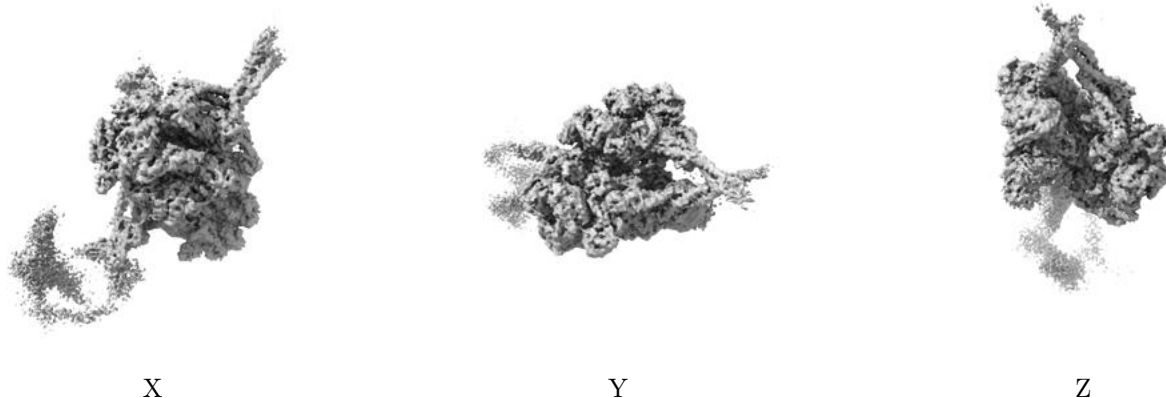


Z

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.

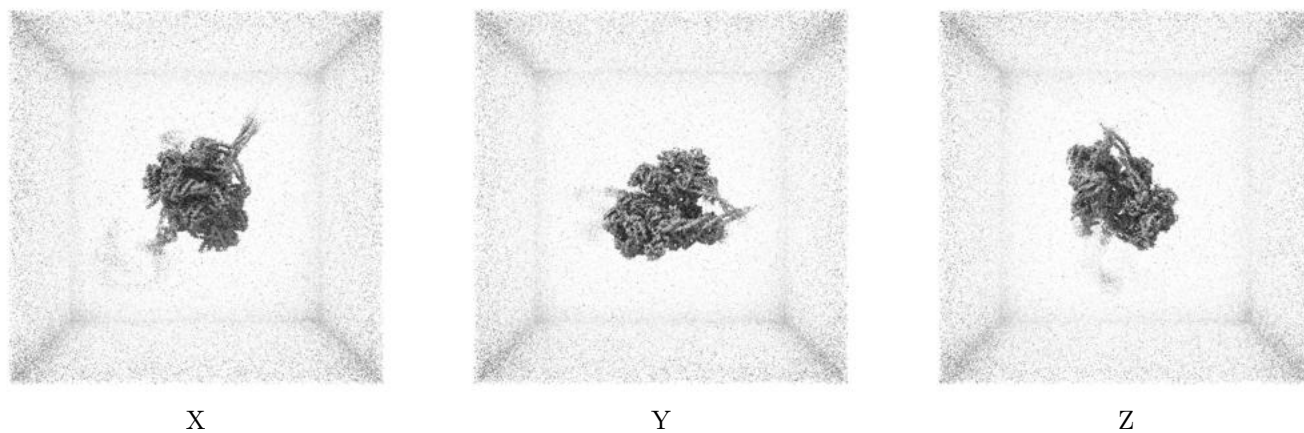
6.5 Orthogonal surface views [i](#)

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.

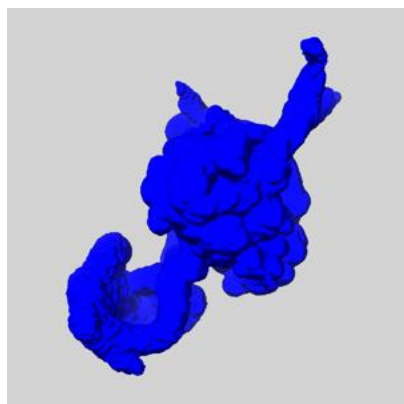
6.6 Mask visualisation [i](#)

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

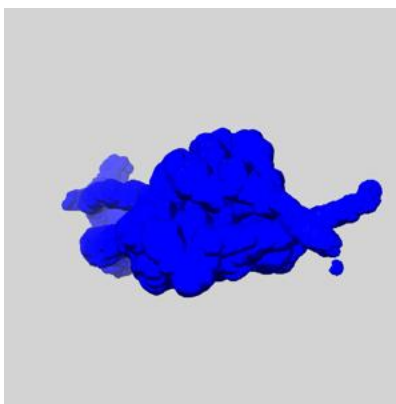
A mask typically either:

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

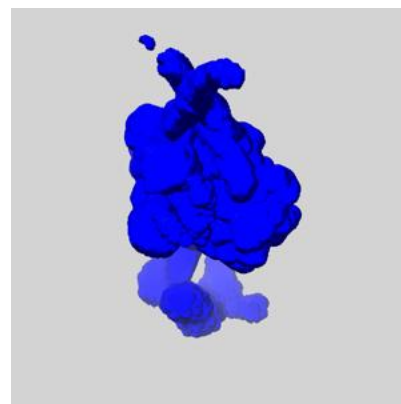
6.6.1 emd_73173_msk_1.map [i](#)



X



Y

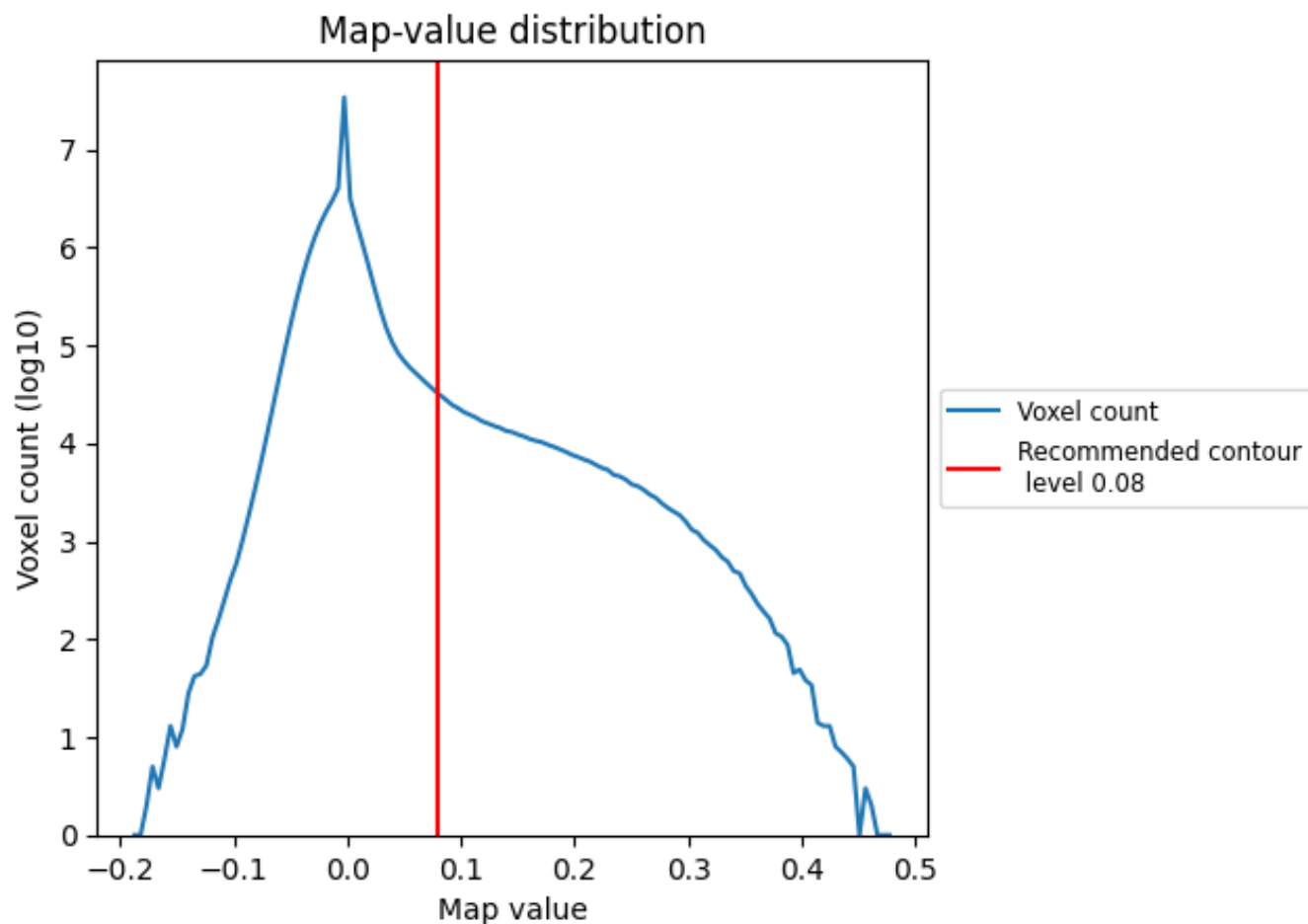


Z

7 Map analysis [i](#)

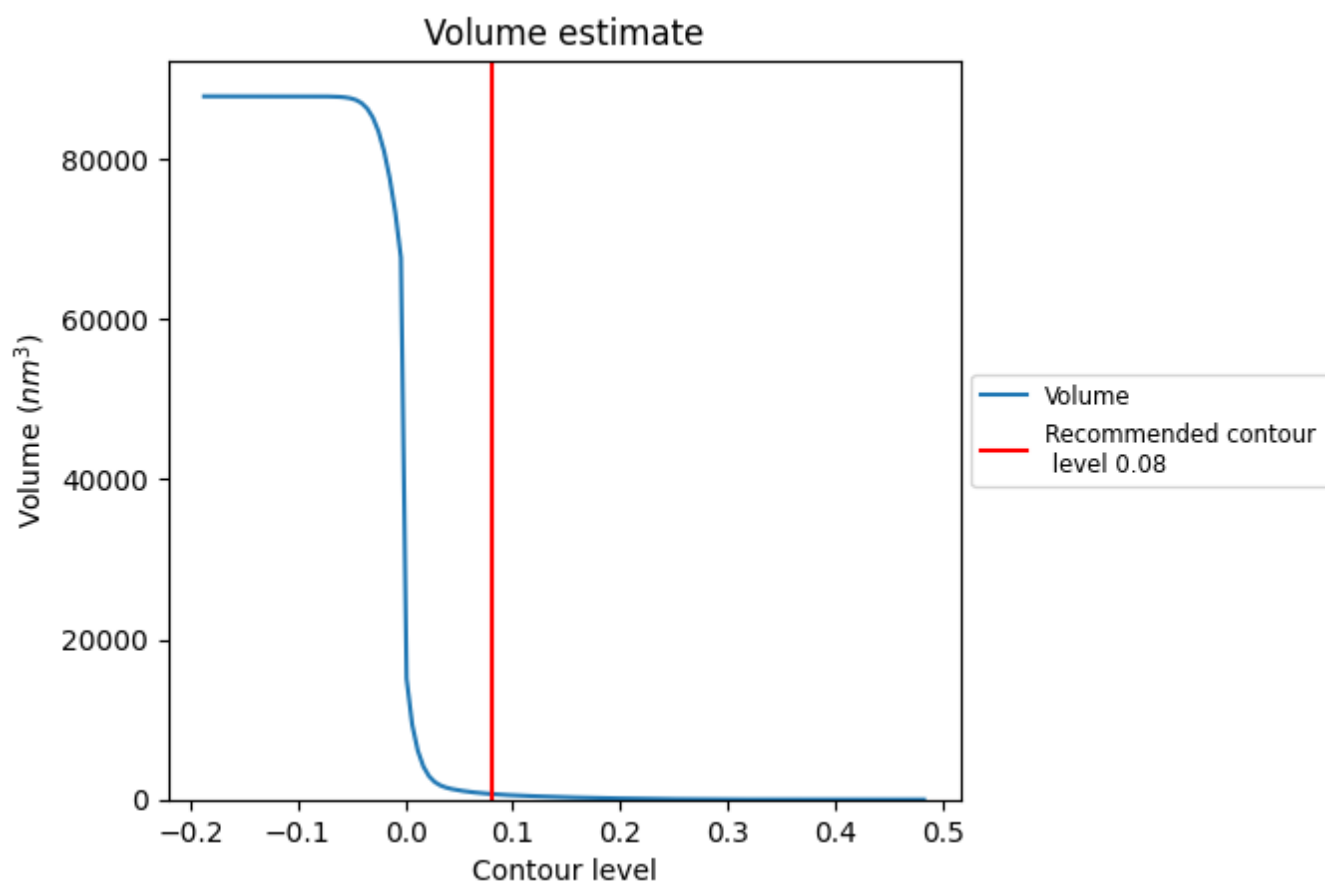
This section contains the results of statistical analysis of the map.

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.

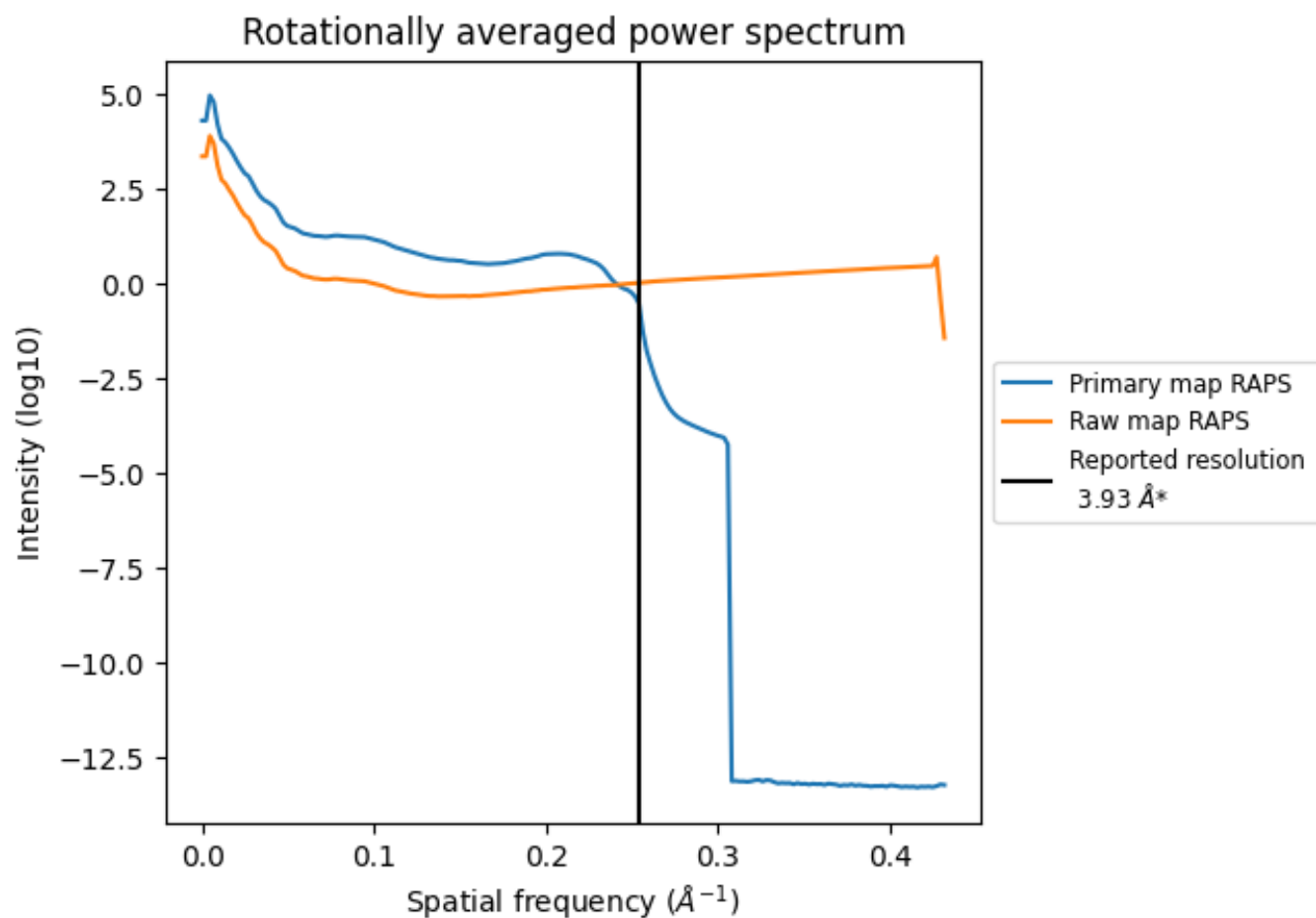
7.2 Volume estimate [i](#)



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 ⓘ

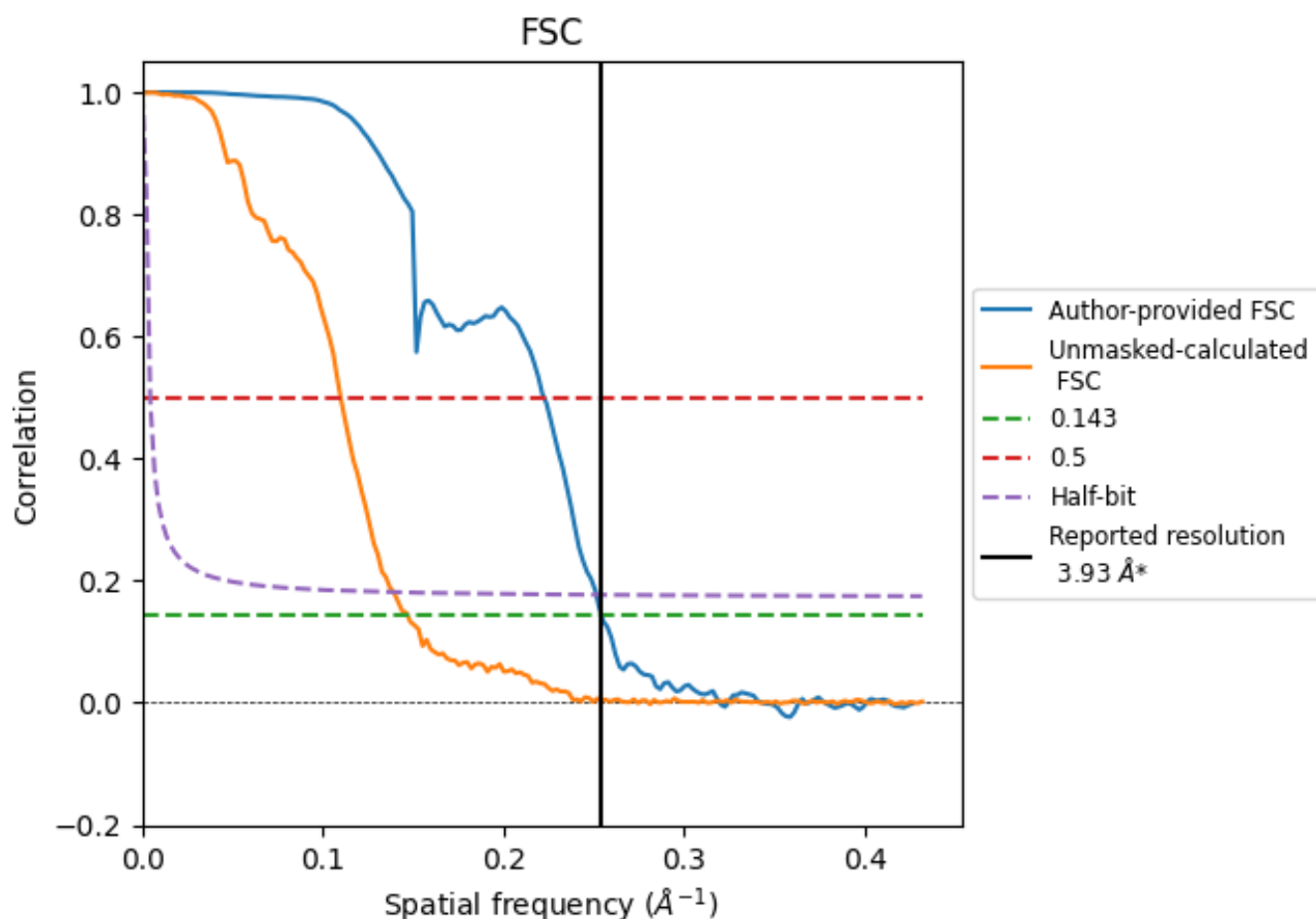


*Reported resolution corresponds to spatial frequency of 0.254 Å⁻¹

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](#)

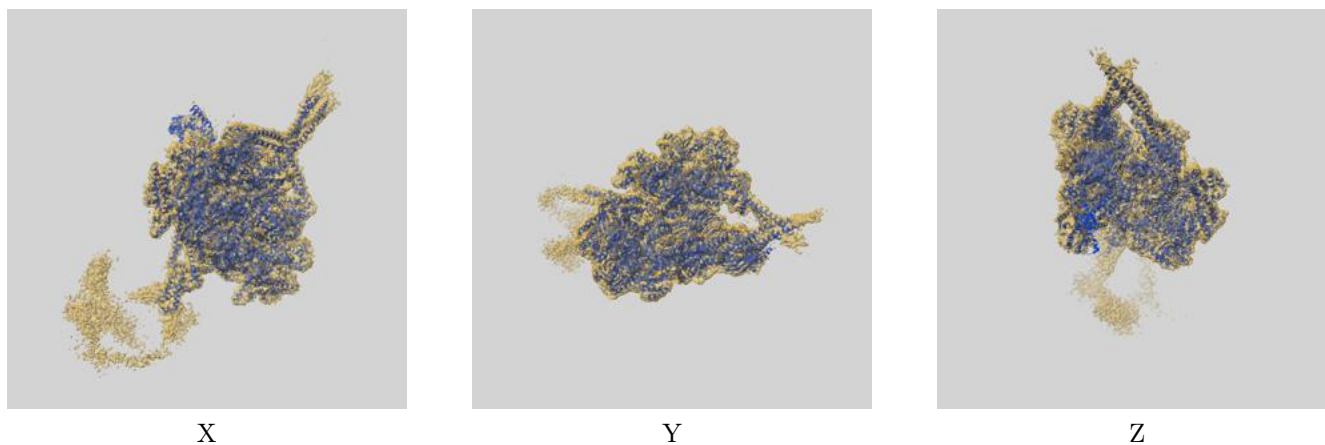
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.93	-	-
Author-provided FSC curve	3.93	4.49	3.98
Unmasked-calculated*	6.81	9.10	7.18

*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](#)

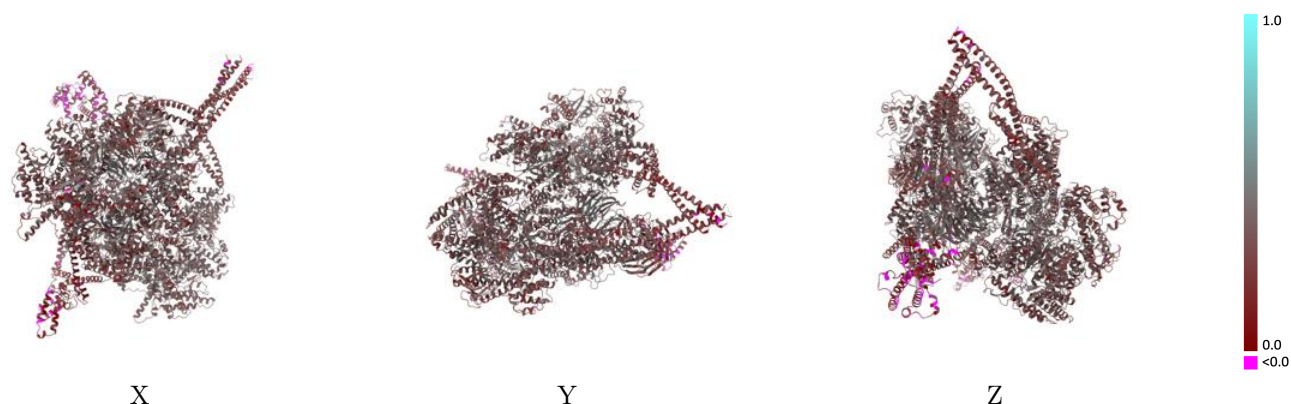
This section contains information regarding the fit between EMDB map EMD-73173 and PDB model 9YNC. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



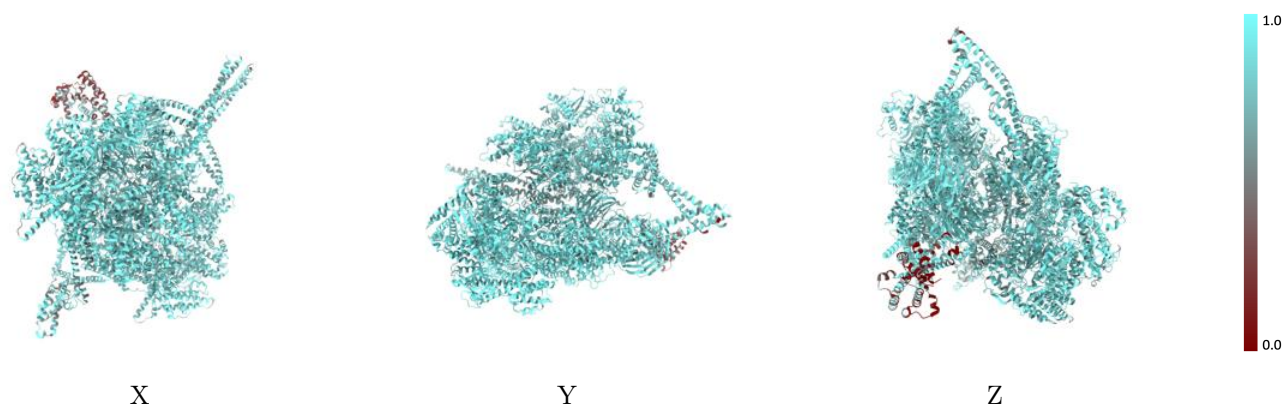
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



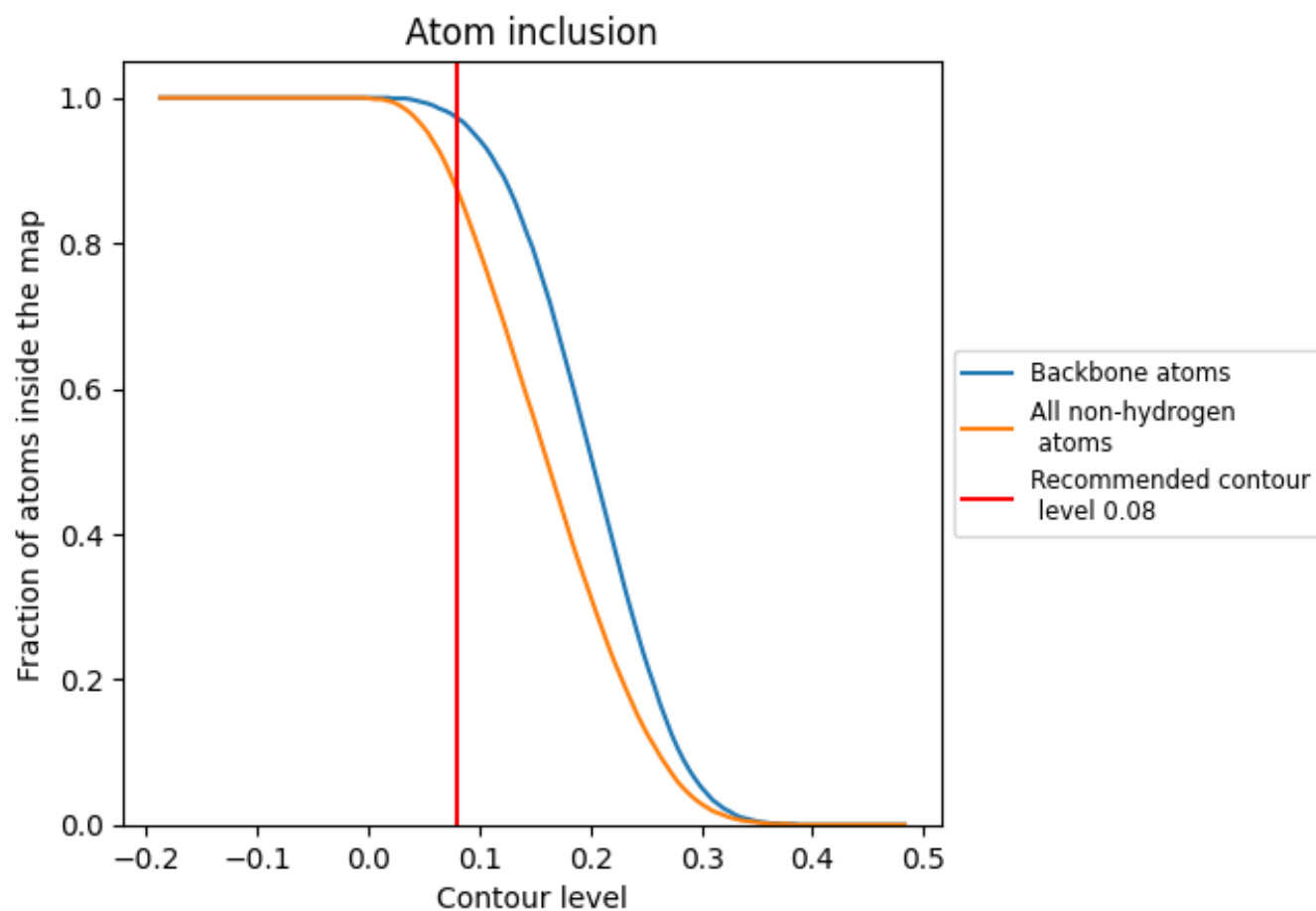
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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