



## wwPDB EM Validation Summary Report ⓘ

Mar 21, 2026 – 04:28 PM UTC

PDB ID : 9E0X / pdb\_00009e0x  
EMDB ID : EMD-47373  
Title : Cryo-EM structure of Phi dynein  
Authors : Nguyen, K.H.V.; Kendrick, A.A.; Leschziner, A.E.  
Deposited on : 2024-10-20  
Resolution : 2.70 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](mailto: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>.

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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

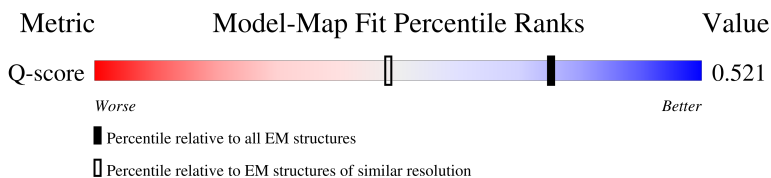
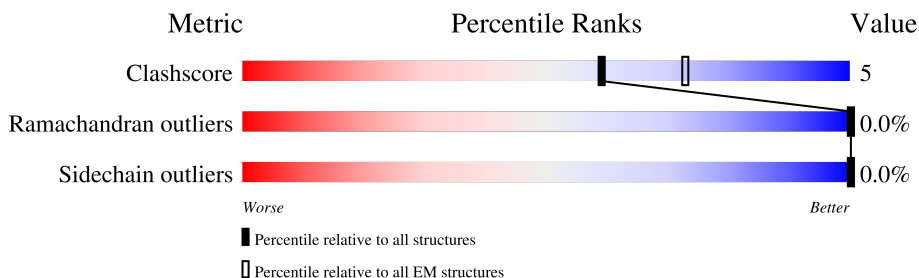
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.70 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	10327 ( 2.20 - 3.20 )

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  $\geq 3$ , 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	4843	<div> <div>22%</div> <div>53%</div> <div>7%</div> <div>40%</div> </div>
1	B	4843	<div> <div>19%</div> <div>52%</div> <div>8%</div> <div>40%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 46234 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	2920	Total 23003	C 14686	N 3978	O 4227	S 112	0	0
1	B	2920	Total 23003	C 14686	N 3978	O 4227	S 112	0	0

There are 396 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-196	GLY	-	expression tag	UNP Q14204
A	-195	ASP	-	expression tag	UNP Q14204
A	-194	TYR	-	expression tag	UNP Q14204
A	-193	ASP	-	expression tag	UNP Q14204
A	-192	ILE	-	expression tag	UNP Q14204
A	-191	PRO	-	expression tag	UNP Q14204
A	-190	THR	-	expression tag	UNP Q14204
A	-189	THR	-	expression tag	UNP Q14204
A	-188	GLU	-	expression tag	UNP Q14204
A	-187	ASN	-	expression tag	UNP Q14204
A	-186	LEU	-	expression tag	UNP Q14204
A	-185	TYR	-	expression tag	UNP Q14204
A	-184	PHE	-	expression tag	UNP Q14204
A	-183	GLN	-	expression tag	UNP Q14204
A	-182	GLY	-	expression tag	UNP Q14204
A	-181	ASP	-	expression tag	UNP Q14204
A	-180	LYS	-	expression tag	UNP Q14204
A	-179	ASP	-	expression tag	UNP Q14204
A	-178	CYS	-	expression tag	UNP Q14204
A	-177	GLU	-	expression tag	UNP Q14204
A	-176	MET	-	expression tag	UNP Q14204
A	-175	LYS	-	expression tag	UNP Q14204
A	-174	ARG	-	expression tag	UNP Q14204
A	-173	THR	-	expression tag	UNP Q14204
A	-172	THR	-	expression tag	UNP Q14204
A	-171	LEU	-	expression tag	UNP Q14204

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-170	ASP	-	expression tag	UNP Q14204
A	-169	SER	-	expression tag	UNP Q14204
A	-168	PRO	-	expression tag	UNP Q14204
A	-167	LEU	-	expression tag	UNP Q14204
A	-166	GLY	-	expression tag	UNP Q14204
A	-165	LYS	-	expression tag	UNP Q14204
A	-164	LEU	-	expression tag	UNP Q14204
A	-163	GLU	-	expression tag	UNP Q14204
A	-162	LEU	-	expression tag	UNP Q14204
A	-161	SER	-	expression tag	UNP Q14204
A	-160	GLY	-	expression tag	UNP Q14204
A	-159	CYS	-	expression tag	UNP Q14204
A	-158	GLU	-	expression tag	UNP Q14204
A	-157	GLN	-	expression tag	UNP Q14204
A	-156	GLY	-	expression tag	UNP Q14204
A	-155	LEU	-	expression tag	UNP Q14204
A	-154	HIS	-	expression tag	UNP Q14204
A	-153	ARG	-	expression tag	UNP Q14204
A	-152	ILE	-	expression tag	UNP Q14204
A	-151	ILE	-	expression tag	UNP Q14204
A	-150	PHE	-	expression tag	UNP Q14204
A	-149	LEU	-	expression tag	UNP Q14204
A	-148	GLY	-	expression tag	UNP Q14204
A	-147	LYS	-	expression tag	UNP Q14204
A	-146	GLY	-	expression tag	UNP Q14204
A	-145	THR	-	expression tag	UNP Q14204
A	-144	SER	-	expression tag	UNP Q14204
A	-143	ALA	-	expression tag	UNP Q14204
A	-142	ALA	-	expression tag	UNP Q14204
A	-141	ASP	-	expression tag	UNP Q14204
A	-140	ALA	-	expression tag	UNP Q14204
A	-139	VAL	-	expression tag	UNP Q14204
A	-138	GLU	-	expression tag	UNP Q14204
A	-137	VAL	-	expression tag	UNP Q14204
A	-136	PRO	-	expression tag	UNP Q14204
A	-135	ALA	-	expression tag	UNP Q14204
A	-134	PRO	-	expression tag	UNP Q14204
A	-133	ALA	-	expression tag	UNP Q14204
A	-132	ALA	-	expression tag	UNP Q14204
A	-131	VAL	-	expression tag	UNP Q14204
A	-130	LEU	-	expression tag	UNP Q14204
A	-129	GLY	-	expression tag	UNP Q14204

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-128	GLY	-	expression tag	UNP Q14204
A	-127	PRO	-	expression tag	UNP Q14204
A	-126	GLU	-	expression tag	UNP Q14204
A	-125	PRO	-	expression tag	UNP Q14204
A	-124	LEU	-	expression tag	UNP Q14204
A	-123	MET	-	expression tag	UNP Q14204
A	-122	GLN	-	expression tag	UNP Q14204
A	-121	ALA	-	expression tag	UNP Q14204
A	-120	THR	-	expression tag	UNP Q14204
A	-119	ALA	-	expression tag	UNP Q14204
A	-118	TRP	-	expression tag	UNP Q14204
A	-117	LEU	-	expression tag	UNP Q14204
A	-116	ASN	-	expression tag	UNP Q14204
A	-115	ALA	-	expression tag	UNP Q14204
A	-114	TYR	-	expression tag	UNP Q14204
A	-113	PHE	-	expression tag	UNP Q14204
A	-112	HIS	-	expression tag	UNP Q14204
A	-111	GLN	-	expression tag	UNP Q14204
A	-110	PRO	-	expression tag	UNP Q14204
A	-109	GLU	-	expression tag	UNP Q14204
A	-108	ALA	-	expression tag	UNP Q14204
A	-107	ILE	-	expression tag	UNP Q14204
A	-106	GLU	-	expression tag	UNP Q14204
A	-105	GLU	-	expression tag	UNP Q14204
A	-104	PHE	-	expression tag	UNP Q14204
A	-103	PRO	-	expression tag	UNP Q14204
A	-102	VAL	-	expression tag	UNP Q14204
A	-101	PRO	-	expression tag	UNP Q14204
A	-100	ALA	-	expression tag	UNP Q14204
A	-99	LEU	-	expression tag	UNP Q14204
A	-98	HIS	-	expression tag	UNP Q14204
A	-97	HIS	-	expression tag	UNP Q14204
A	-96	PRO	-	expression tag	UNP Q14204
A	-95	VAL	-	expression tag	UNP Q14204
A	-94	PHE	-	expression tag	UNP Q14204
A	-93	GLN	-	expression tag	UNP Q14204
A	-92	GLN	-	expression tag	UNP Q14204
A	-91	GLU	-	expression tag	UNP Q14204
A	-90	SER	-	expression tag	UNP Q14204
A	-89	PHE	-	expression tag	UNP Q14204
A	-88	THR	-	expression tag	UNP Q14204
A	-87	ARG	-	expression tag	UNP Q14204

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-86	GLN	-	expression tag	UNP Q14204
A	-85	VAL	-	expression tag	UNP Q14204
A	-84	LEU	-	expression tag	UNP Q14204
A	-83	TRP	-	expression tag	UNP Q14204
A	-82	LYS	-	expression tag	UNP Q14204
A	-81	LEU	-	expression tag	UNP Q14204
A	-80	LEU	-	expression tag	UNP Q14204
A	-79	LYS	-	expression tag	UNP Q14204
A	-78	VAL	-	expression tag	UNP Q14204
A	-77	VAL	-	expression tag	UNP Q14204
A	-76	LYS	-	expression tag	UNP Q14204
A	-75	PHE	-	expression tag	UNP Q14204
A	-74	GLY	-	expression tag	UNP Q14204
A	-73	GLU	-	expression tag	UNP Q14204
A	-72	VAL	-	expression tag	UNP Q14204
A	-71	ILE	-	expression tag	UNP Q14204
A	-70	SER	-	expression tag	UNP Q14204
A	-69	TYR	-	expression tag	UNP Q14204
A	-68	SER	-	expression tag	UNP Q14204
A	-67	HIS	-	expression tag	UNP Q14204
A	-66	LEU	-	expression tag	UNP Q14204
A	-65	ALA	-	expression tag	UNP Q14204
A	-64	ALA	-	expression tag	UNP Q14204
A	-63	LEU	-	expression tag	UNP Q14204
A	-62	ALA	-	expression tag	UNP Q14204
A	-61	GLY	-	expression tag	UNP Q14204
A	-60	ASN	-	expression tag	UNP Q14204
A	-59	PRO	-	expression tag	UNP Q14204
A	-58	ALA	-	expression tag	UNP Q14204
A	-57	ALA	-	expression tag	UNP Q14204
A	-56	THR	-	expression tag	UNP Q14204
A	-55	ALA	-	expression tag	UNP Q14204
A	-54	ALA	-	expression tag	UNP Q14204
A	-53	VAL	-	expression tag	UNP Q14204
A	-52	LYS	-	expression tag	UNP Q14204
A	-51	THR	-	expression tag	UNP Q14204
A	-50	ALA	-	expression tag	UNP Q14204
A	-49	LEU	-	expression tag	UNP Q14204
A	-48	SER	-	expression tag	UNP Q14204
A	-47	GLY	-	expression tag	UNP Q14204
A	-46	ASN	-	expression tag	UNP Q14204
A	-45	PRO	-	expression tag	UNP Q14204

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-44	VAL	-	expression tag	UNP Q14204
A	-43	PRO	-	expression tag	UNP Q14204
A	-42	ILE	-	expression tag	UNP Q14204
A	-41	LEU	-	expression tag	UNP Q14204
A	-40	ILE	-	expression tag	UNP Q14204
A	-39	PRO	-	expression tag	UNP Q14204
A	-38	CYS	-	expression tag	UNP Q14204
A	-37	HIS	-	expression tag	UNP Q14204
A	-36	ARG	-	expression tag	UNP Q14204
A	-35	VAL	-	expression tag	UNP Q14204
A	-34	VAL	-	expression tag	UNP Q14204
A	-33	GLN	-	expression tag	UNP Q14204
A	-32	GLY	-	expression tag	UNP Q14204
A	-31	ASP	-	expression tag	UNP Q14204
A	-30	LEU	-	expression tag	UNP Q14204
A	-29	ASP	-	expression tag	UNP Q14204
A	-28	VAL	-	expression tag	UNP Q14204
A	-27	GLY	-	expression tag	UNP Q14204
A	-26	GLY	-	expression tag	UNP Q14204
A	-25	TYR	-	expression tag	UNP Q14204
A	-24	GLU	-	expression tag	UNP Q14204
A	-23	GLY	-	expression tag	UNP Q14204
A	-22	GLY	-	expression tag	UNP Q14204
A	-21	LEU	-	expression tag	UNP Q14204
A	-20	ALA	-	expression tag	UNP Q14204
A	-19	VAL	-	expression tag	UNP Q14204
A	-18	LYS	-	expression tag	UNP Q14204
A	-17	GLU	-	expression tag	UNP Q14204
A	-16	TRP	-	expression tag	UNP Q14204
A	-15	LEU	-	expression tag	UNP Q14204
A	-14	LEU	-	expression tag	UNP Q14204
A	-13	ALA	-	expression tag	UNP Q14204
A	-12	HIS	-	expression tag	UNP Q14204
A	-11	GLU	-	expression tag	UNP Q14204
A	-10	GLY	-	expression tag	UNP Q14204
A	-9	HIS	-	expression tag	UNP Q14204
A	-8	ARG	-	expression tag	UNP Q14204
A	-7	LEU	-	expression tag	UNP Q14204
A	-6	GLY	-	expression tag	UNP Q14204
A	-5	LYS	-	expression tag	UNP Q14204
A	-4	PRO	-	expression tag	UNP Q14204
A	-3	GLY	-	expression tag	UNP Q14204

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	LEU	-	expression tag	UNP Q14204
A	-1	GLY	-	expression tag	UNP Q14204
A	0	GLY	-	expression tag	UNP Q14204
A	1	SER	-	expression tag	UNP Q14204
B	-196	GLY	-	expression tag	UNP Q14204
B	-195	ASP	-	expression tag	UNP Q14204
B	-194	TYR	-	expression tag	UNP Q14204
B	-193	ASP	-	expression tag	UNP Q14204
B	-192	ILE	-	expression tag	UNP Q14204
B	-191	PRO	-	expression tag	UNP Q14204
B	-190	THR	-	expression tag	UNP Q14204
B	-189	THR	-	expression tag	UNP Q14204
B	-188	GLU	-	expression tag	UNP Q14204
B	-187	ASN	-	expression tag	UNP Q14204
B	-186	LEU	-	expression tag	UNP Q14204
B	-185	TYR	-	expression tag	UNP Q14204
B	-184	PHE	-	expression tag	UNP Q14204
B	-183	GLN	-	expression tag	UNP Q14204
B	-182	GLY	-	expression tag	UNP Q14204
B	-181	ASP	-	expression tag	UNP Q14204
B	-180	LYS	-	expression tag	UNP Q14204
B	-179	ASP	-	expression tag	UNP Q14204
B	-178	CYS	-	expression tag	UNP Q14204
B	-177	GLU	-	expression tag	UNP Q14204
B	-176	MET	-	expression tag	UNP Q14204
B	-175	LYS	-	expression tag	UNP Q14204
B	-174	ARG	-	expression tag	UNP Q14204
B	-173	THR	-	expression tag	UNP Q14204
B	-172	THR	-	expression tag	UNP Q14204
B	-171	LEU	-	expression tag	UNP Q14204
B	-170	ASP	-	expression tag	UNP Q14204
B	-169	SER	-	expression tag	UNP Q14204
B	-168	PRO	-	expression tag	UNP Q14204
B	-167	LEU	-	expression tag	UNP Q14204
B	-166	GLY	-	expression tag	UNP Q14204
B	-165	LYS	-	expression tag	UNP Q14204
B	-164	LEU	-	expression tag	UNP Q14204
B	-163	GLU	-	expression tag	UNP Q14204
B	-162	LEU	-	expression tag	UNP Q14204
B	-161	SER	-	expression tag	UNP Q14204
B	-160	GLY	-	expression tag	UNP Q14204
B	-159	CYS	-	expression tag	UNP Q14204

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-158	GLU	-	expression tag	UNP Q14204
B	-157	GLN	-	expression tag	UNP Q14204
B	-156	GLY	-	expression tag	UNP Q14204
B	-155	LEU	-	expression tag	UNP Q14204
B	-154	HIS	-	expression tag	UNP Q14204
B	-153	ARG	-	expression tag	UNP Q14204
B	-152	ILE	-	expression tag	UNP Q14204
B	-151	ILE	-	expression tag	UNP Q14204
B	-150	PHE	-	expression tag	UNP Q14204
B	-149	LEU	-	expression tag	UNP Q14204
B	-148	GLY	-	expression tag	UNP Q14204
B	-147	LYS	-	expression tag	UNP Q14204
B	-146	GLY	-	expression tag	UNP Q14204
B	-145	THR	-	expression tag	UNP Q14204
B	-144	SER	-	expression tag	UNP Q14204
B	-143	ALA	-	expression tag	UNP Q14204
B	-142	ALA	-	expression tag	UNP Q14204
B	-141	ASP	-	expression tag	UNP Q14204
B	-140	ALA	-	expression tag	UNP Q14204
B	-139	VAL	-	expression tag	UNP Q14204
B	-138	GLU	-	expression tag	UNP Q14204
B	-137	VAL	-	expression tag	UNP Q14204
B	-136	PRO	-	expression tag	UNP Q14204
B	-135	ALA	-	expression tag	UNP Q14204
B	-134	PRO	-	expression tag	UNP Q14204
B	-133	ALA	-	expression tag	UNP Q14204
B	-132	ALA	-	expression tag	UNP Q14204
B	-131	VAL	-	expression tag	UNP Q14204
B	-130	LEU	-	expression tag	UNP Q14204
B	-129	GLY	-	expression tag	UNP Q14204
B	-128	GLY	-	expression tag	UNP Q14204
B	-127	PRO	-	expression tag	UNP Q14204
B	-126	GLU	-	expression tag	UNP Q14204
B	-125	PRO	-	expression tag	UNP Q14204
B	-124	LEU	-	expression tag	UNP Q14204
B	-123	MET	-	expression tag	UNP Q14204
B	-122	GLN	-	expression tag	UNP Q14204
B	-121	ALA	-	expression tag	UNP Q14204
B	-120	THR	-	expression tag	UNP Q14204
B	-119	ALA	-	expression tag	UNP Q14204
B	-118	TRP	-	expression tag	UNP Q14204
B	-117	LEU	-	expression tag	UNP Q14204

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-116	ASN	-	expression tag	UNP Q14204
B	-115	ALA	-	expression tag	UNP Q14204
B	-114	TYR	-	expression tag	UNP Q14204
B	-113	PHE	-	expression tag	UNP Q14204
B	-112	HIS	-	expression tag	UNP Q14204
B	-111	GLN	-	expression tag	UNP Q14204
B	-110	PRO	-	expression tag	UNP Q14204
B	-109	GLU	-	expression tag	UNP Q14204
B	-108	ALA	-	expression tag	UNP Q14204
B	-107	ILE	-	expression tag	UNP Q14204
B	-106	GLU	-	expression tag	UNP Q14204
B	-105	GLU	-	expression tag	UNP Q14204
B	-104	PHE	-	expression tag	UNP Q14204
B	-103	PRO	-	expression tag	UNP Q14204
B	-102	VAL	-	expression tag	UNP Q14204
B	-101	PRO	-	expression tag	UNP Q14204
B	-100	ALA	-	expression tag	UNP Q14204
B	-99	LEU	-	expression tag	UNP Q14204
B	-98	HIS	-	expression tag	UNP Q14204
B	-97	HIS	-	expression tag	UNP Q14204
B	-96	PRO	-	expression tag	UNP Q14204
B	-95	VAL	-	expression tag	UNP Q14204
B	-94	PHE	-	expression tag	UNP Q14204
B	-93	GLN	-	expression tag	UNP Q14204
B	-92	GLN	-	expression tag	UNP Q14204
B	-91	GLU	-	expression tag	UNP Q14204
B	-90	SER	-	expression tag	UNP Q14204
B	-89	PHE	-	expression tag	UNP Q14204
B	-88	THR	-	expression tag	UNP Q14204
B	-87	ARG	-	expression tag	UNP Q14204
B	-86	GLN	-	expression tag	UNP Q14204
B	-85	VAL	-	expression tag	UNP Q14204
B	-84	LEU	-	expression tag	UNP Q14204
B	-83	TRP	-	expression tag	UNP Q14204
B	-82	LYS	-	expression tag	UNP Q14204
B	-81	LEU	-	expression tag	UNP Q14204
B	-80	LEU	-	expression tag	UNP Q14204
B	-79	LYS	-	expression tag	UNP Q14204
B	-78	VAL	-	expression tag	UNP Q14204
B	-77	VAL	-	expression tag	UNP Q14204
B	-76	LYS	-	expression tag	UNP Q14204
B	-75	PHE	-	expression tag	UNP Q14204

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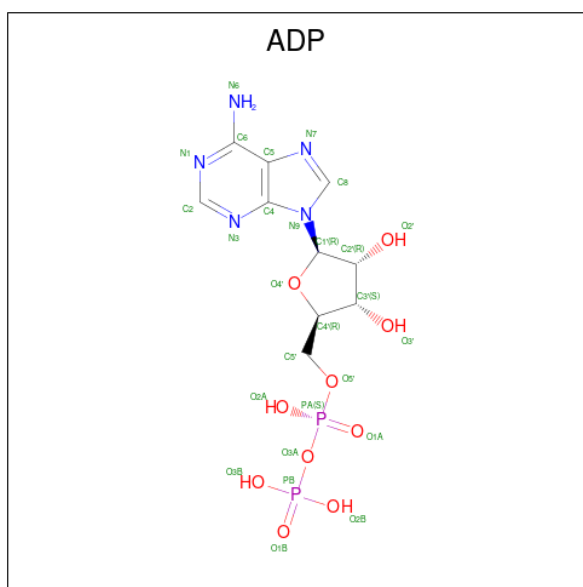
Chain	Residue	Modelled	Actual	Comment	Reference
B	-74	GLY	-	expression tag	UNP Q14204
B	-73	GLU	-	expression tag	UNP Q14204
B	-72	VAL	-	expression tag	UNP Q14204
B	-71	ILE	-	expression tag	UNP Q14204
B	-70	SER	-	expression tag	UNP Q14204
B	-69	TYR	-	expression tag	UNP Q14204
B	-68	SER	-	expression tag	UNP Q14204
B	-67	HIS	-	expression tag	UNP Q14204
B	-66	LEU	-	expression tag	UNP Q14204
B	-65	ALA	-	expression tag	UNP Q14204
B	-64	ALA	-	expression tag	UNP Q14204
B	-63	LEU	-	expression tag	UNP Q14204
B	-62	ALA	-	expression tag	UNP Q14204
B	-61	GLY	-	expression tag	UNP Q14204
B	-60	ASN	-	expression tag	UNP Q14204
B	-59	PRO	-	expression tag	UNP Q14204
B	-58	ALA	-	expression tag	UNP Q14204
B	-57	ALA	-	expression tag	UNP Q14204
B	-56	THR	-	expression tag	UNP Q14204
B	-55	ALA	-	expression tag	UNP Q14204
B	-54	ALA	-	expression tag	UNP Q14204
B	-53	VAL	-	expression tag	UNP Q14204
B	-52	LYS	-	expression tag	UNP Q14204
B	-51	THR	-	expression tag	UNP Q14204
B	-50	ALA	-	expression tag	UNP Q14204
B	-49	LEU	-	expression tag	UNP Q14204
B	-48	SER	-	expression tag	UNP Q14204
B	-47	GLY	-	expression tag	UNP Q14204
B	-46	ASN	-	expression tag	UNP Q14204
B	-45	PRO	-	expression tag	UNP Q14204
B	-44	VAL	-	expression tag	UNP Q14204
B	-43	PRO	-	expression tag	UNP Q14204
B	-42	ILE	-	expression tag	UNP Q14204
B	-41	LEU	-	expression tag	UNP Q14204
B	-40	ILE	-	expression tag	UNP Q14204
B	-39	PRO	-	expression tag	UNP Q14204
B	-38	CYS	-	expression tag	UNP Q14204
B	-37	HIS	-	expression tag	UNP Q14204
B	-36	ARG	-	expression tag	UNP Q14204
B	-35	VAL	-	expression tag	UNP Q14204
B	-34	VAL	-	expression tag	UNP Q14204
B	-33	GLN	-	expression tag	UNP Q14204

*Continued on next page...*

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-32	GLY	-	expression tag	UNP Q14204
B	-31	ASP	-	expression tag	UNP Q14204
B	-30	LEU	-	expression tag	UNP Q14204
B	-29	ASP	-	expression tag	UNP Q14204
B	-28	VAL	-	expression tag	UNP Q14204
B	-27	GLY	-	expression tag	UNP Q14204
B	-26	GLY	-	expression tag	UNP Q14204
B	-25	TYR	-	expression tag	UNP Q14204
B	-24	GLU	-	expression tag	UNP Q14204
B	-23	GLY	-	expression tag	UNP Q14204
B	-22	GLY	-	expression tag	UNP Q14204
B	-21	LEU	-	expression tag	UNP Q14204
B	-20	ALA	-	expression tag	UNP Q14204
B	-19	VAL	-	expression tag	UNP Q14204
B	-18	LYS	-	expression tag	UNP Q14204
B	-17	GLU	-	expression tag	UNP Q14204
B	-16	TRP	-	expression tag	UNP Q14204
B	-15	LEU	-	expression tag	UNP Q14204
B	-14	LEU	-	expression tag	UNP Q14204
B	-13	ALA	-	expression tag	UNP Q14204
B	-12	HIS	-	expression tag	UNP Q14204
B	-11	GLU	-	expression tag	UNP Q14204
B	-10	GLY	-	expression tag	UNP Q14204
B	-9	HIS	-	expression tag	UNP Q14204
B	-8	ARG	-	expression tag	UNP Q14204
B	-7	LEU	-	expression tag	UNP Q14204
B	-6	GLY	-	expression tag	UNP Q14204
B	-5	LYS	-	expression tag	UNP Q14204
B	-4	PRO	-	expression tag	UNP Q14204
B	-3	GLY	-	expression tag	UNP Q14204
B	-2	LEU	-	expression tag	UNP Q14204
B	-1	GLY	-	expression tag	UNP Q14204
B	0	GLY	-	expression tag	UNP Q14204
B	1	SER	-	expression tag	UNP Q14204

- 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).



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

- 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 2	Mg 2	0
4	B	2	Total 2	Mg 2	0



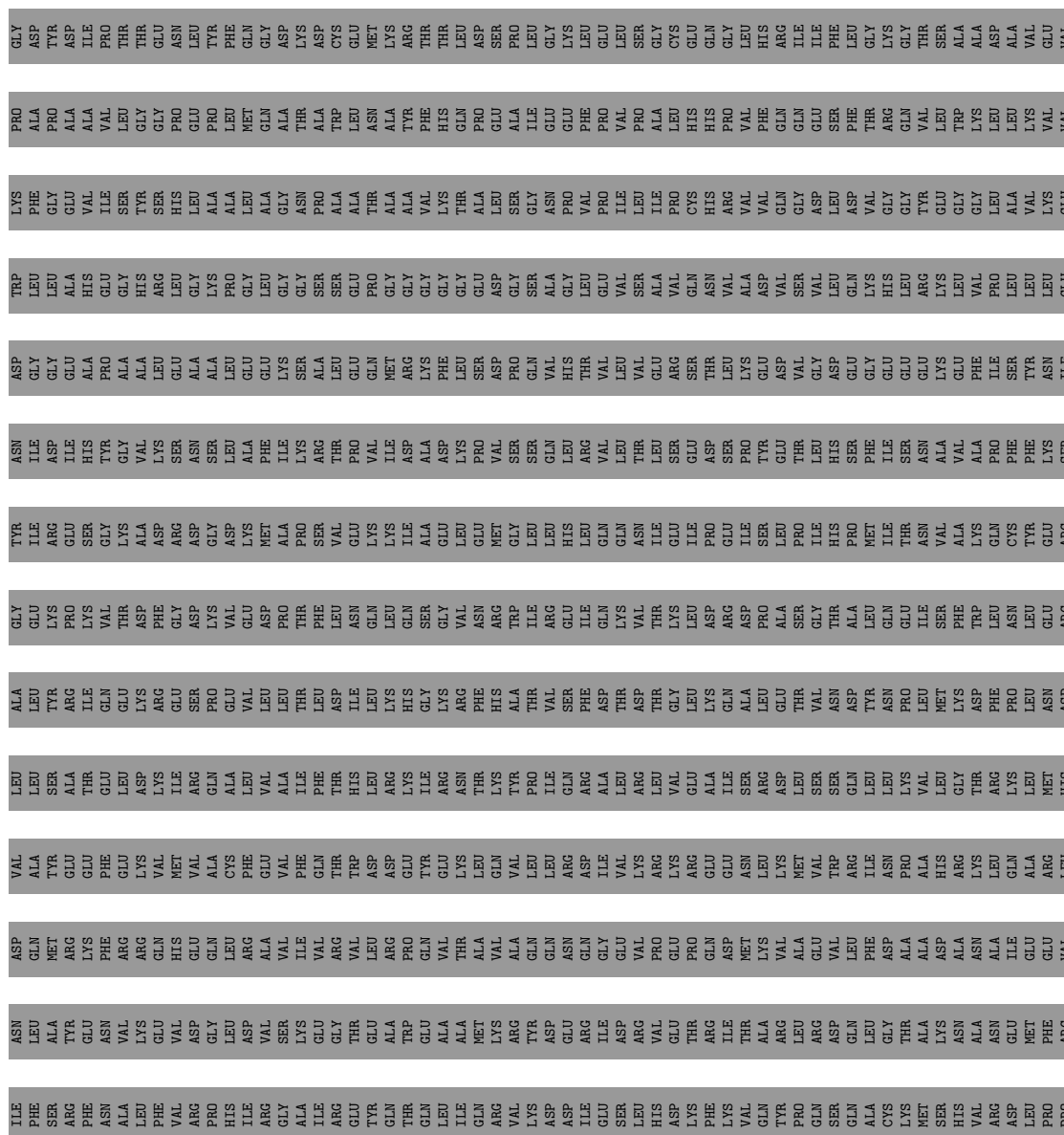






D4430	L4431	A4432	D4433	V4434	V4435	Q4436	V4437	C4438	D4439	G4440	K4441	K4442	K4443	Q4444	V4447	L4448	I4452	I4453	E4454	L4455	V4456	K4457	C4458	L4459	L4460	P4461	R4462	S4463	V4464	S4465	K4466	V4467	T4468	V4469	P4470	A4471	C4472	M4473	V4474	I4476	Q4477	S4480	D4481	F4482	S4483	E4484	R4485	T4486	K4487	Q4488	L4489	Q4490	I4491	T4492	S4493				
SER	ASP	GLY	ARG	PRO	ALA	TRP	MET	ARG	T4379	L4380	H4381	T4382	T4383	A4384	S4385	M4386	V4387	L4388	H4389	L4390	I4391	P4392	Q4393	T4394	L4395	S4396	H4397	L4398	K4399	R4400	T4401	VAL	E4403	N4404	I4405	K4406	D4407	P4408	L4409	F4410	R4411	F4412	F4413	E4414	R4415	E4416	V4417	K4418	M4419	G4420	A4421	K4422	L4423	L4424	Q4425	D4426	V4427	R4428	Q4429
D4225	T4226	A4227	K4228	C4229	R4230	Q4231	M4232	I4233	S4234	P4235	D4236	K4237	I4238	P4239	W4240	S4241	A4242	L4243	L4245	Q4254	D4257	M4258	R4263	M4266	E4270	R4271	T4274	T4275	R4276	S4277	F4278	D4279	S4280	E4281	F4282	K4283	L4284	A4285	C4286	K4287	V4288	D4289	G4290	K4291	K4292	D4293	T4294	Q4295	M4296	P4297	D4298	Q4299							
I4300	R4301	R4302	E4303	E4304	F4305	V4306	Q4307	W4308	V4309	E4310	L4311	L4312	F4313	D4314	T4315	Q4316	T4317	P4318	N4325	M4326	A4327	E4328	R4329	V4330	L4331	D4338	M4339	I4340	S4341	K4342	M4343	L4344	K4345	Q4347	M4348	L4349	E4350	ASP	GLU	ASP	LEU	ALA	ALA	GLU	THR	GLU	LYS	THR	ARG	THR	ASP	SER	THR						
N4137	L4138	I4144	F4151	K4154	A4155	M4156	L4157	L4158	R4159	T4160	F4161	S4162	S4163	I4164	P4165	V4166	S4167	I4169	C4170	K4171	S4172	P4173	M4174	E4175	R4176	A4177	R4178	L4179	Y4180	Q4191	R4195	Y4196	A4197	K4203	K4204	Y4205	E4206	E4209	S4210	D4211	L4212	R4213	D4217	T4218	V4219	D4220	T4221	V4222	L4223	D4224									
G4032	T4033	P4037	L4042	M4043	D4050	A4051	S4052	G4053	H4054	D4057	L4058	A4059	A4060	E4061	Q4062	M4063	T4064	Q4065	I4066	E4075	V4088	K4089	R4092	W4093	A4094	M4095	V4099	H4100	L4106	M4107	Q4108	L4109	E4110	K4111	S4115	L4116	Q4117	P4118	C4121	L4126	T4127	M4128	M4131	P4132	K4133														
S3965	P3966	E3967	Q3968	T3969	V3970	P3971	Y3972	L3973	W3974	SER	GLU	GLU	T3978	P3979	A3980	T3981	P3982	I3983	Q3984	Q3985	A3986	T3987	H3988	P3989	L3990	L3991	L3992	I3993	Q3994	E3993	A3995	F3996	R3997	L4002	A4003	M4004	A4005	H4006	M4007	F4008	V4009	S4010	G4014	F4015	S4016	S4019	I4020	M4021	E4022	Q4023	P4024	L4025	D4026	L4027	T4028	H4029			
F3905	Q3906	H3907	F3908	L3909	R3910	G3911	R3912	E3913	L3914	V3915	L3916	S3917	A3918	G3919	H3920	S3920	T3921	P3922	R3923	I3924	Q3925	G3926	L3927	T3928	V3929	E3930	Q3931	A3932	E3933	A3934	V3935	V3936	R3937	L3938	S3939	C3940	L3941	P3942	A3943	F3944	K3945	D3946	L3947	K3948	A3949	K3950	V3951	Q3952	E3953	D3954	E3955	Q3956	F3957	G3958	T3959	W3960	D3962	S3963	
Y3836	H3837	N3838	Y3841	E3842	P3844	N3845	L3846	LYS	GLY	V3849	T3850	D3851	H3852	S3853	Q3854	R3855	L3856	S3857	I3858	T3859	T3860	K3861	D3862	L3863	V3866	F3867	N3868	N3869	A3872	R3873	G3874	M3875	T3882	F3883	A3884	M3885	L3886	R3889	I3890	K3891	L3892	G3894	T3895	VAL	G3897	E3898	P3899	T3900	Y3901	D3902	A3903	E3904							
D3666	Q3667	D3668	T3669	D3670	T3681	E3687	D3691	L3692	C3712	E3715	V3716	L3717	K3718	A3719	E3720	R3721	P3722	D3723	V3724	D3725	S3726	K3727	R3728	S3729	D3730	L3731	L3732	R3733	L3734	E3737	L3740	R3741	L3742	R3743	Q3744	L3745	E3746	K3747	S3748	L3749	L3750	Q3751	A3752	L3753	N3754	E3755	V3756	K3757	G3758	R3759	I3760								
T3495	F3496	T3497	N3498	Q3499	M3500	S3501	S3510	Y3516	A3517	F3520	M3524	R3525	W3532	S3533	H3534	R3544	T3545	D3546	I3547	L3553	S3554	N3555	A3556	D3557	R3561	K3581	R3582	Y3586	P3587	T3597	K3471	Y3604	I3609	D3617	P3632	L3633	L3634	V3638	E3639	T3656	G3657	G3658	R3659																
Q3435	K3436	T3437	R3438	D3439	L3440	E3441	A3442	S3443	T3444	A3445	R3446	T3447	K3448	E3449	E3450	Y3451	A3452	V3453	L3454	T3455	S3456	E3457	A3458	Q3459	A3460	T3461	K3462	A3463	D3464	L3465	A3466	V3467	E3468	E3469	A3470	V3472	N3473	R3474	S3475	T3476	A3477	L3478	L3479	K3480	S3481	L3482	S3483	A3484	E3485	R3486	E3487	R3488	W3489	E3490	K3491	T3492	S3493	F3494	

- Molecule 1: Cytoplasmic dynein 1 heavy chain 1

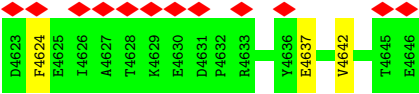


F1777	L1866	T1573	R1488	TRP	ASP	LEU	VAL	GLU	GLY	HIS	TYR	GLN	VAL	ALA	TRP	GLU	TRP	ILE	ARG	VAL
L1778	M1667	E1574	G1489	VAL	ALA	LEU	VAL	GLU	GLY	GLN	GLN	VAL	VAL	GLY	VAL	GLY	GLY	VAL	LYS	GLY
H1779	E1868	F1575	W1490	SER	LEU	THR	SER	ASP	VAL	VAL	VAL	ILE	VAL	LEU	GLN	LYS	TYR	ASN	VAL	SER
N1784	D1669	L1576	D1491	GLU	ASN	THR	GLU	ARG	GLY	LEU	HIS	TYR	LEU	ASN	GLN	LEU	ASP	HIS	ASN	GLY
S1671	M1670	A1577	D1492	THR	LEU	GLY	THR	VAL	TYR	LYS	TYR	GLU	ARG	GLY	ASN	PRO	ASP	GLN	ASN	ALA
D1794	E1683	L1578	M1495	LEU	LYS	LEU	GLY	GLU	ARG	PHE	GLY	GLU	ASN	GLY	ASN	LEU	PRO	PHE	ARG	ALA
S1795	M1579	M1579	K1496	GLY	SER	LEU	GLY	SER	ASN	GLY	LEU	THR	GLY	GLY	GLN	TYR	TYR	ILE	ILE	LYS
M1798	T1688	K1581	V1497	GLN	PHE	GLY	THR	ARG	GLY	GLN	MET	THR	GLY	GLY	GLN	VAL	VAL	PHE	GLY	VAL
E1799	T1688	V1582	K1498	ASP	ALA	SER	THR	ASP	LEU	GLY	SER	GLU	ASN	GLY	ASN	LEU	ALA	PRO	GLY	GLY
Q1800	I1692	S1583	H1500	VAL	LEU	GLU	LEU	LEU	LEU	SER	SER	LYS	ASN	VAL	LYS	PRO	ALA	ILE	ILE	ARG
K1807	T1693	K1594	S1505	ASP	ARG	ARG	LEU	THR	GLU	LYS	THR	TYR	VAL	VAL	VAL	ILE	ILE	THR	THR	THR
D1820	E1694	P1586	A1506	GLN	GLN	VAL	GLN	THR	GLY	GLN	GLN	ARG	GLY	GLY	GLN	THR	VAL	VAL	VAL	VAL
L1825	H1695	L1587	M1507	LYS	ALA	VAL	ALA	GLU	PHE	GLY	GLY	ALA	LEU	LEU	ASN	ASN	LYS	ASN	ASN	ASN
I1826	K1697	V1588	K1508	GLU	TYR	LEU	GLY	LYS	GLN	HIS	SER	PHE	VAL	VAL	LEU	THR	PHE	THR	THR	THR
K1827	E1700	M1589	L1509	THR	PHE	GLU	THR	THR	PHE	SER	THR	GLY	VAL	VAL	THR	GLY	GLY	ARG	ARG	ARG
S1828	E1706	D1590	S1510	VAL	VAL	LEU	GLY	LYS	PRO	ILE	ILE	GLY	GLN	GLN	GLN	GLY	GLY	VAL	VAL	VAL
K1829	K1707	L1592	P1511	GLN	GLN	LEU	ASP	VAL	SER	SER	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
I1830	E1708	N1593	Y1512	ASP	ARG	LEU	GLY	THR	TRP	LYS	LYS	ALA	ALA	ALA	VAL	ASP	ASP	THR	THR	THR
D1831	T1712	I1594	Y1513	LEU	LEU	LYS	GLY	GLY	GLY	GLN	GLN	ASN	ASN	ASN	GLY	GLY	GLY	GLY	GLY	GLY
N1832	L1717	G1596	F1516	THR	TYR	SER	GLU	ILE	ILE	THR	THR	ASP	ASP	ASP	PRO	PRO	PRO	PRO	PRO	PRO
D1847	E1725	Q1598	E1517	LYS	LYS	GLU	GLU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
K1848	I1726	R1599	E1518	ILE	ILE	LEU	ALA	ALA	GLY	HIS	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
K1849	I1726	S1600	Q1454	ASN	ASN	SER	LEU	LEU	GLY	SER	TYR	TYR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
Q1850	F1727	L1601	G1455	MET	LEU	VAL	VAL	ALA	GLY	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
T1851	G1728	L1851	E1461	GLY	ALA	MET	LYS	PHE	ARG	ALA	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
D1852	K1606	D1606	F1462	VAL	VAL	THR	THR	THR	PHE	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
M1861	K1607	L1607	L1463	ILE	ILE	GLY	GLN	ILE	ASN	SER	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
A1862	L1607	L1608	L1464	GLY	GLY	THR	THR	TYR	ASN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
K1865	I1538	G1609	L1465	LYS	LYS	ASP	ASP	ILE	ILE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
D1877	S1732	S1732	E1480	SER	SER	GLN	GLY	GLY	GLY	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
K1878	I1733	I1733	E1481	GLY	ALA	MET	LYS	PHE	ARG	ALA	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
L1879	P1735	P1735	F1462	ALA	ALA	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
C1888	M1736	M1736	L1466	THR	THR	LYS	LYS	THR	ARG	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
E1914	I1742	I1742	I1550	VAL	VAL	GLY	GLY	GLY	LYS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
V1929	A1747	A1747	G1553	LYS	LYS	GLN	GLN	ARG	ASP	PHE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
D1933	Q1748	Q1748	S1554	ASP	ASP	PRO	PRO	LEU	SER	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
D1937	L1749	L1749	A1555	HIS	TRP	SER	VAL	ASP	ILE	ILE	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
F1938	E1763	E1763	D1556	LYS	LYS	VAL	VAL	ARG	LYS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
Q1950	L1766	L1766	I1557	THR	THR	ARG	ARG	LEU	LYS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
D1958	S1767	S1767	F1629	LEU	LEU	THR	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
R1962	S1768	S1768	Y1630	HIS	HIS	GLN	GLN	MET	GLY	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
E1964	NET	NET	L1638	VAL	VAL	ASN	ASN	LYS	LYS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	GLY	GLY	Y1479	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
	GLY	GLY	Y1480	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
	GLY	GLY	Q1481	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
	ASP	ASP	N1482	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
	A1775	A1775	C1483	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	A1776	A1776	R1485	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
			L1486	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
			I1487	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
				LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU



[illegible]





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	161043	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	55	Depositor
Minimum defocus (nm)	610	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.420	Depositor
Minimum map value	-1.263	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.064	Depositor
Recommended contour level	0.406	Depositor
Map size (Å)	329.12, 329.12, 329.12	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.935, 0.935, 0.935	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, 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	0.15	0/23476	0.35	0/31857
1	B	0.15	0/23476	0.34	0/31857
All	All	0.15	0/46952	0.35	0/63714

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	23003	0	22807	196	0
1	B	23003	0	22807	229	0
2	A	81	0	36	1	0
2	B	81	0	36	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
All	All	46234	0	45710	423	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 5.

The worst 5 of 423 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:3712:CYS:HG	1:A:3836:TYR:HH	1.10	0.96
1:B:3712:CYS:HG	1:B:3836:TYR:HH	1.30	0.78
1:B:4052:SER:HA	1:B:4095:MET:HE1	1.69	0.74
1:A:1612:GLN:NE2	1:A:1635:GLU:OE1	2.22	0.73
1:A:2410:SER:HB3	1:A:2413:LEU:HD23	1.72	0.70

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	2892/4843 (60%)	2806 (97%)	85 (3%)	1 (0%)	100	100
1	B	2892/4843 (60%)	2819 (98%)	72 (2%)	1 (0%)	100	100
All	All	5784/9686 (60%)	5625 (97%)	157 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2871	ILE
1	B	2871	ILE

### 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	2472/4279 (58%)	2472 (100%)	0	100	100
1	B	2472/4279 (58%)	2470 (100%)	2 (0%)	88	96
All	All	4944/8558 (58%)	4942 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2850	ILE
1	B	4189	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4023	GLN
1	B	4488	GLN
1	B	1598	GLN
1	B	4436	GLN
1	B	4566	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
2	ADP	B	4801	4	28,29,29	1.40	4 (14%)	43,45,45	1.83	8 (18%)
2	ADP	B	4803	-	28,29,29	1.41	4 (14%)	43,45,45	1.89	8 (18%)
2	ADP	A	4801	4	28,29,29	1.40	5 (17%)	43,45,45	1.82	11 (25%)
2	ADP	A	4804	-	28,29,29	1.41	4 (14%)	43,45,45	1.85	9 (20%)
3	ATP	A	4802	4	32,33,33	0.34	0	48,52,52	0.35	0
3	ATP	B	4802	4	32,33,33	0.36	0	48,52,52	0.36	0
2	ADP	A	4803	-	28,29,29	1.41	4 (14%)	43,45,45	1.92	8 (18%)
2	ADP	B	4804	-	28,29,29	1.41	4 (14%)	43,45,45	1.83	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
2	ADP	B	4801	4	-	3/16/32/32	0/3/3/3
2	ADP	B	4803	-	-	2/16/32/32	0/3/3/3
2	ADP	A	4801	4	-	1/16/32/32	0/3/3/3
2	ADP	A	4804	-	-	3/16/32/32	0/3/3/3
3	ATP	A	4802	4	-	3/22/38/38	0/3/3/3
3	ATP	B	4802	4	-	2/22/38/38	0/3/3/3
2	ADP	A	4803	-	-	1/16/32/32	0/3/3/3
2	ADP	B	4804	-	-	2/16/32/32	0/3/3/3

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4803	ADP	C5-C4	4.74	1.47	1.39
2	B	4803	ADP	C5-C4	4.69	1.47	1.39
2	A	4801	ADP	C5-C4	4.68	1.47	1.39
2	B	4804	ADP	C5-C4	4.67	1.47	1.39
2	A	4804	ADP	C5-C4	4.66	1.47	1.39

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4803	ADP	C5-C4-N3	-6.55	117.70	126.72
2	B	4803	ADP	C5-C4-N3	-6.30	118.05	126.72
2	B	4804	ADP	C5-C4-N3	-5.97	118.49	126.72
2	A	4804	ADP	C5-C4-N3	-5.88	118.63	126.72
2	B	4801	ADP	C5-C4-N3	-5.83	118.68	126.72

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4801	ADP	C5'-O5'-PA-O3A
2	A	4804	ADP	O4'-C4'-C5'-O5'
2	A	4804	ADP	C3'-C4'-C5'-O5'
2	B	4804	ADP	O4'-C4'-C5'-O5'
2	B	4804	ADP	C3'-C4'-C5'-O5'

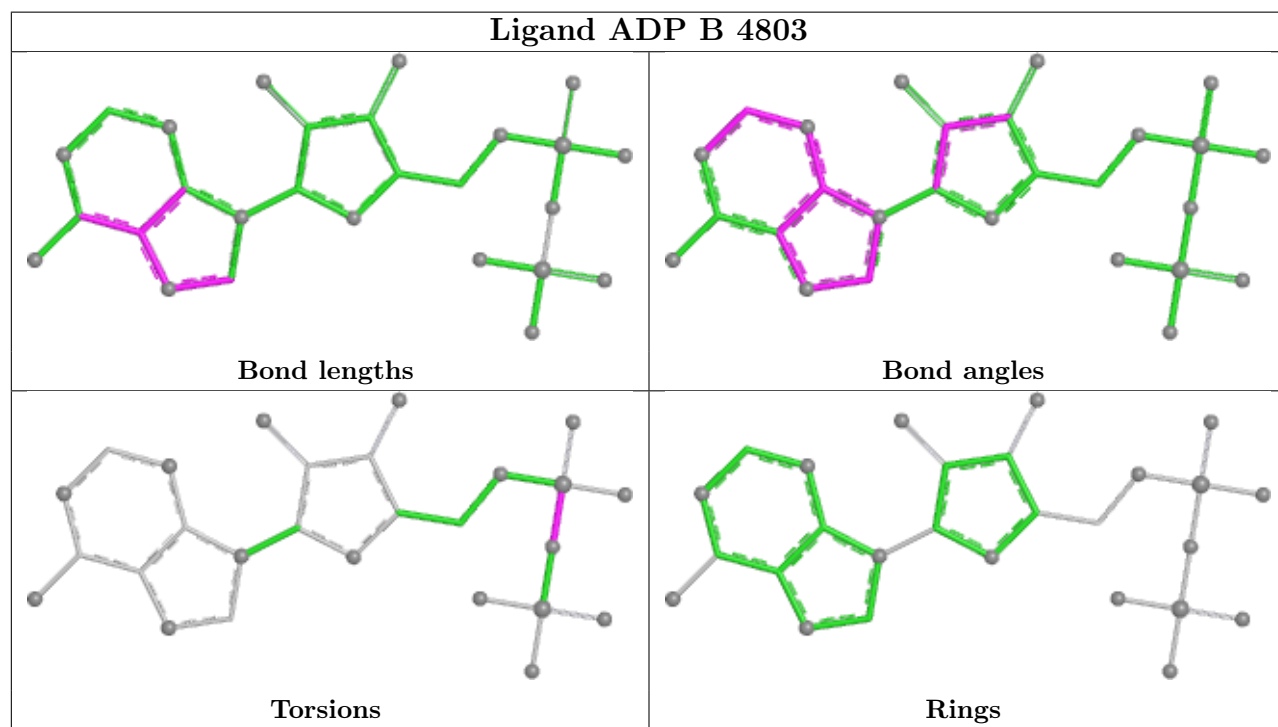
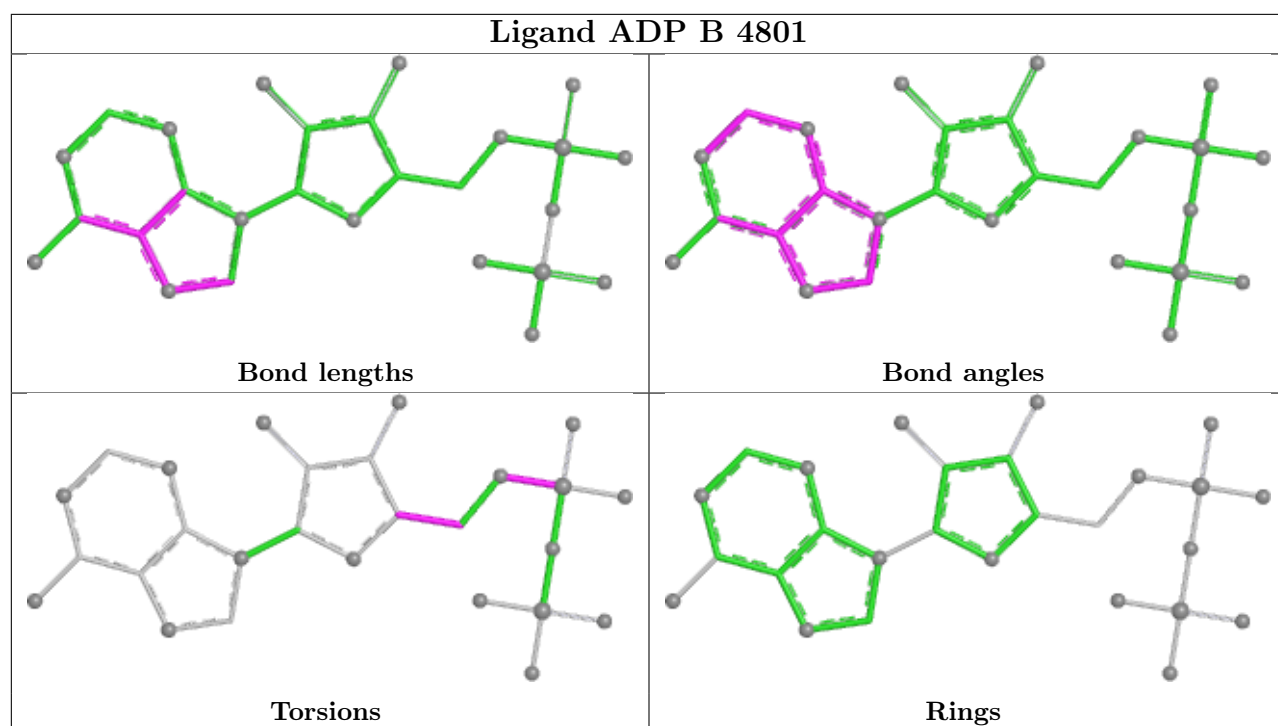
There are no ring outliers.

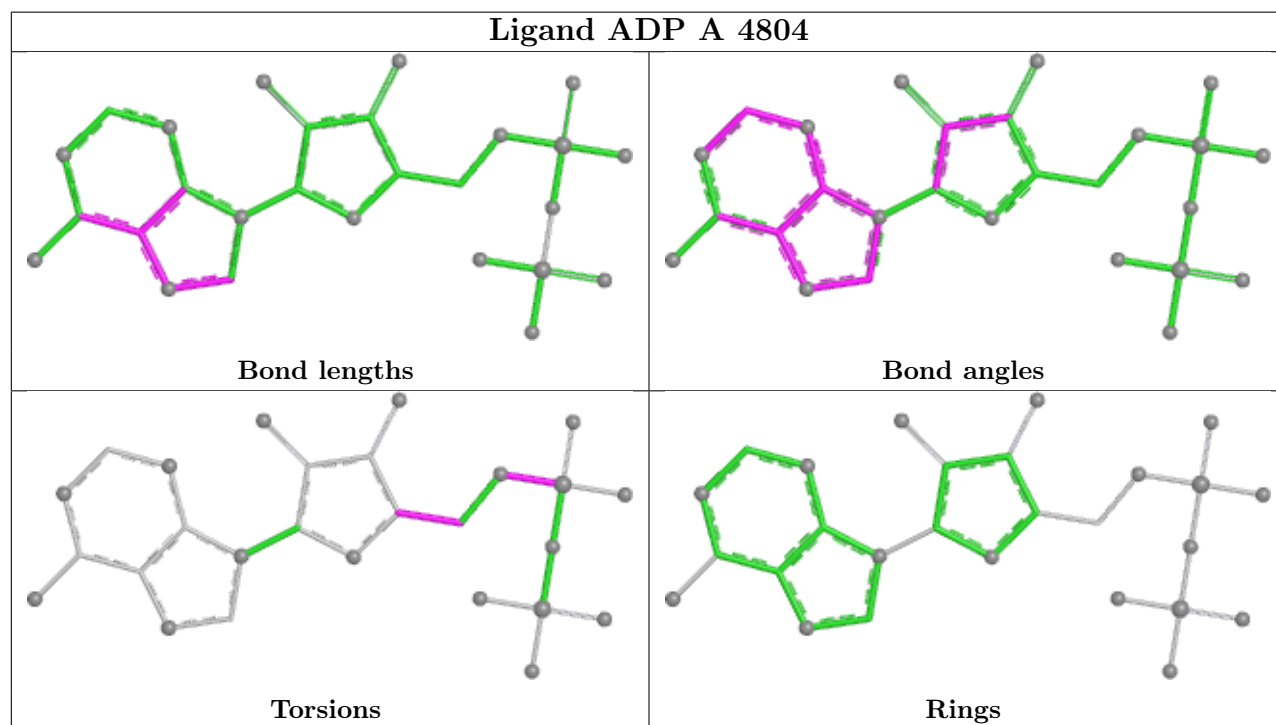
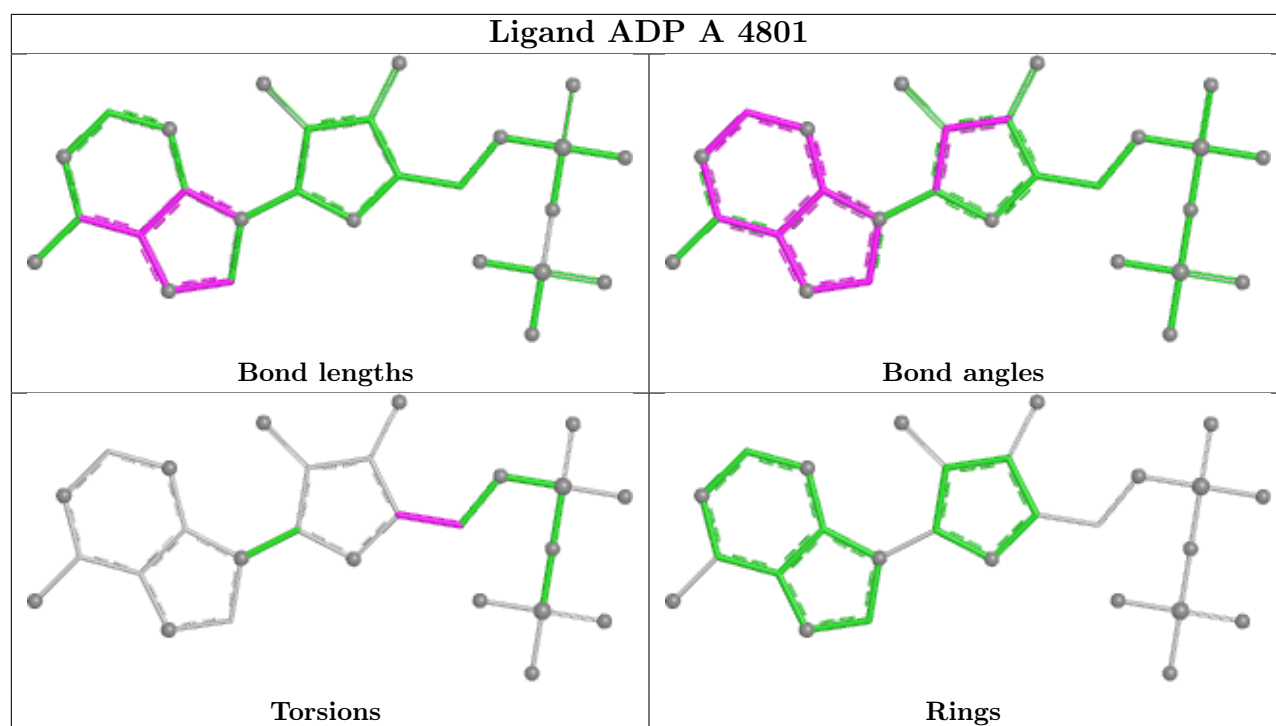
1 monomer is involved in 1 short contact:

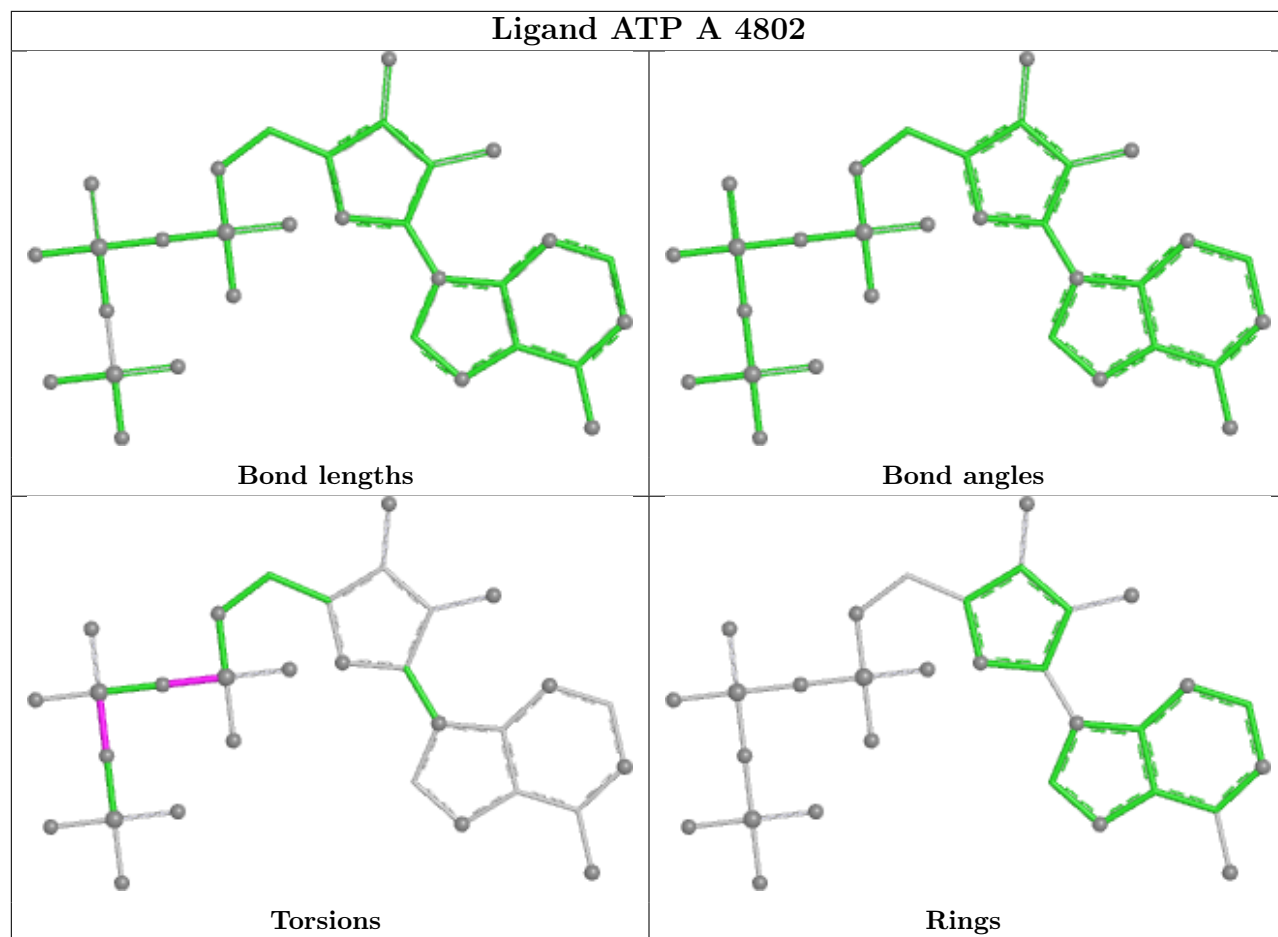
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4803	ADP	1	0

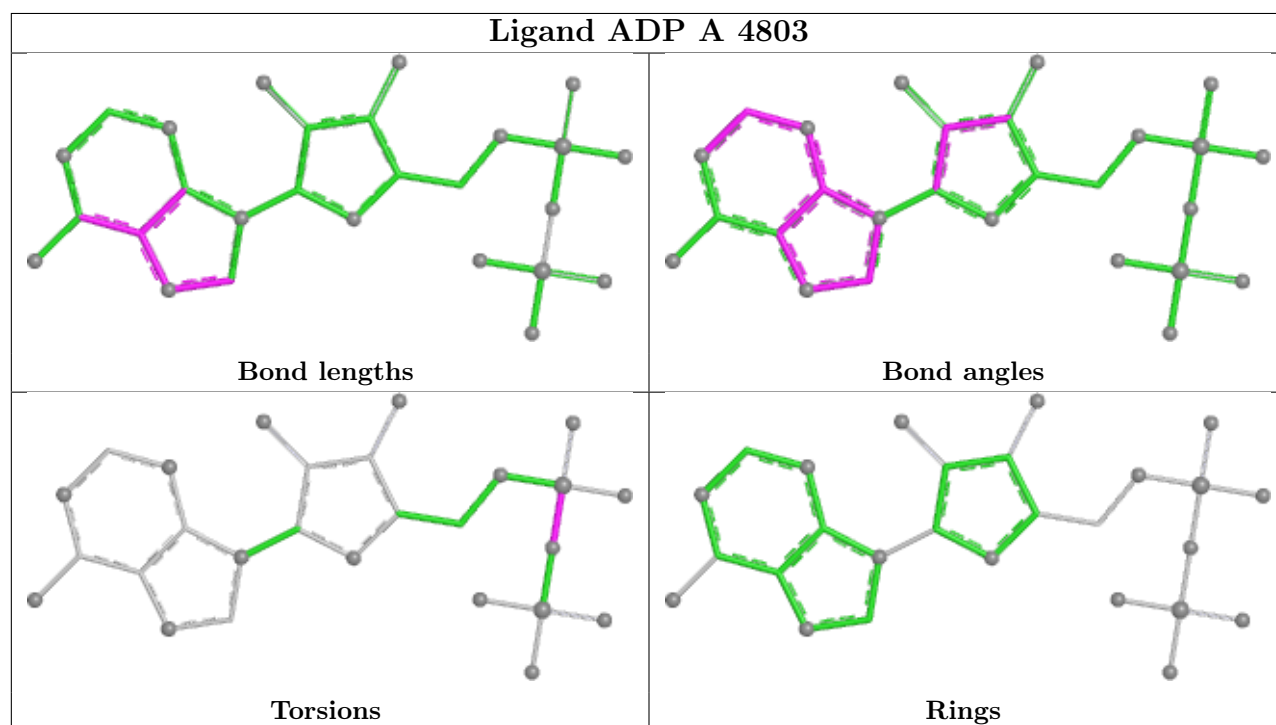
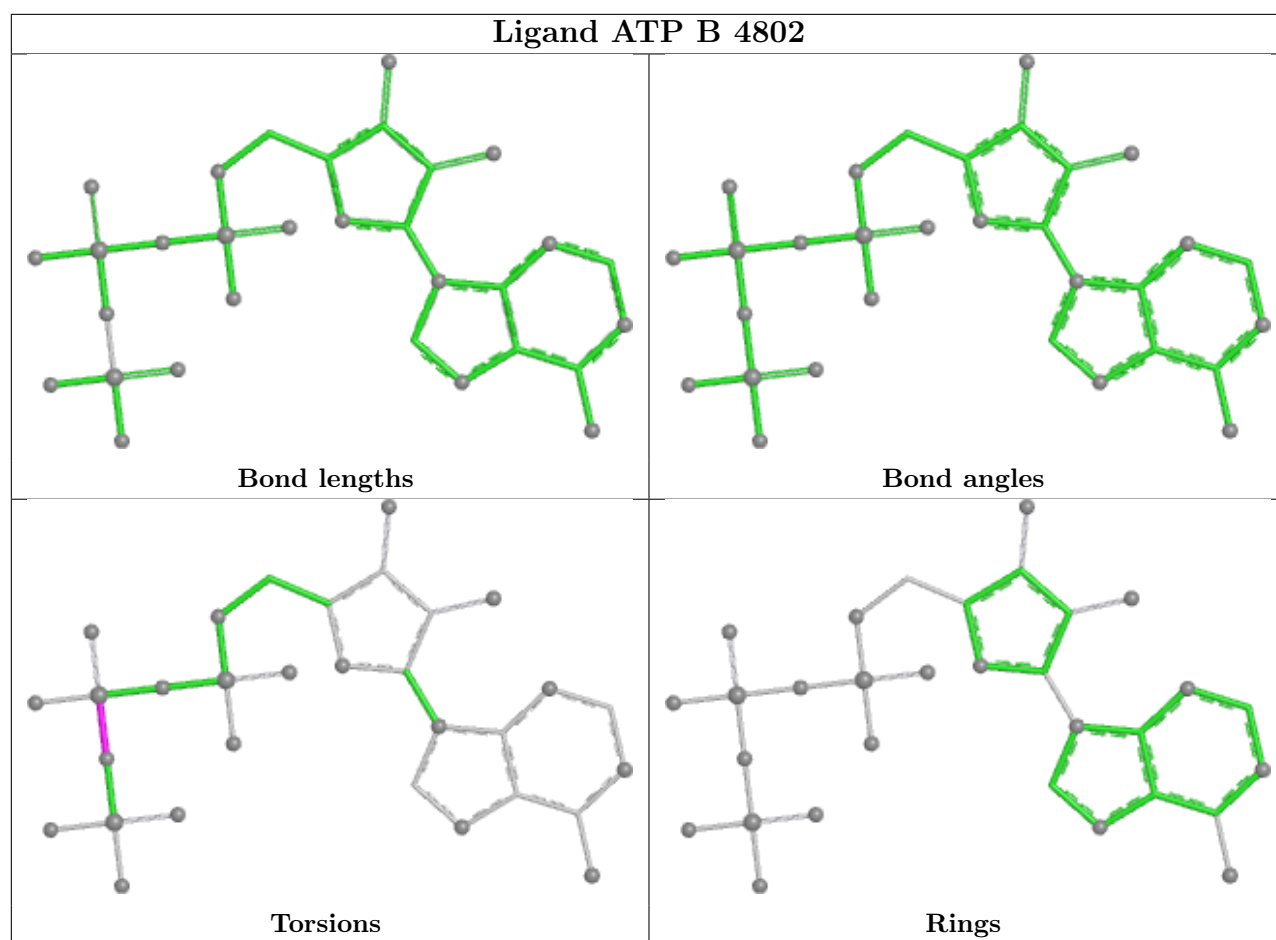
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

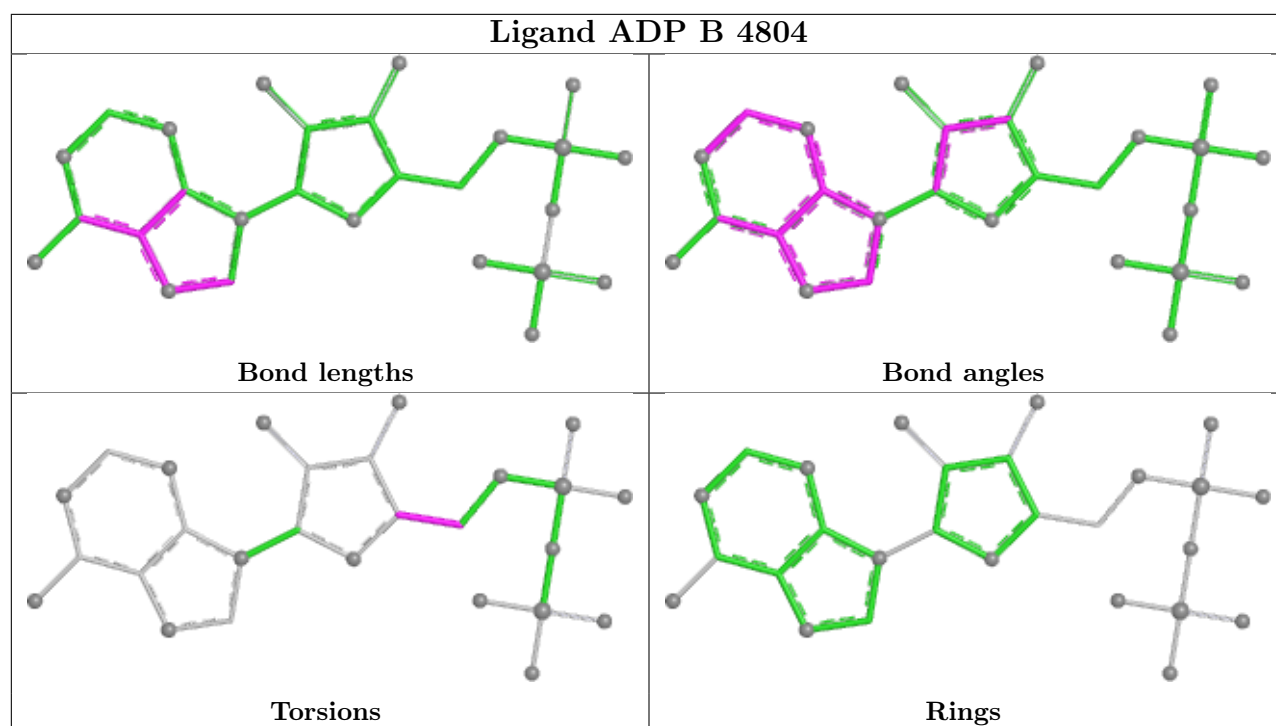












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

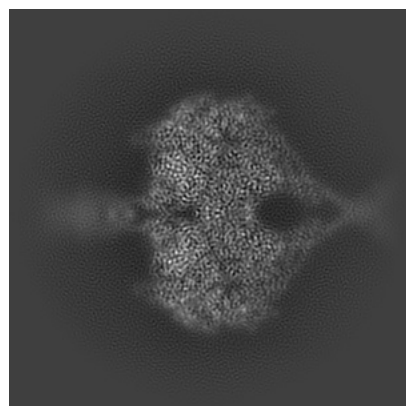
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47373. These allow visual inspection of the internal detail of the map and identification of artifacts.

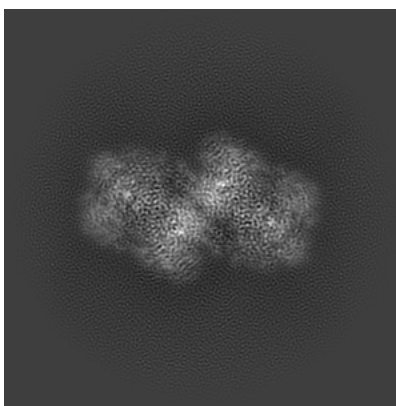
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

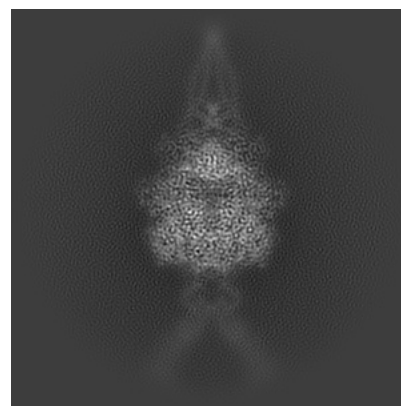
#### 6.1.1 Primary map



X

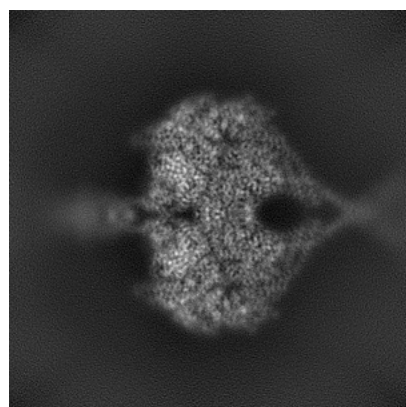


Y

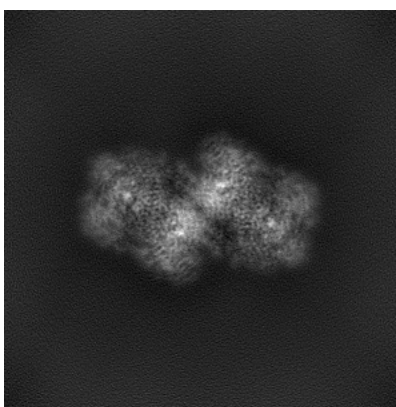


Z

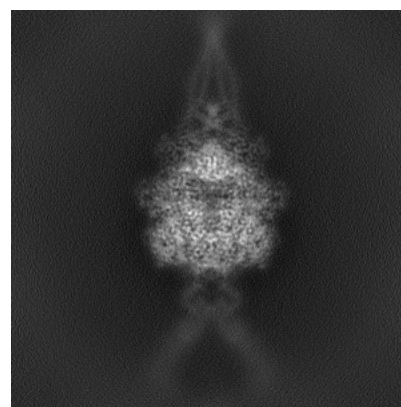
#### 6.1.2 Raw map



X



Y

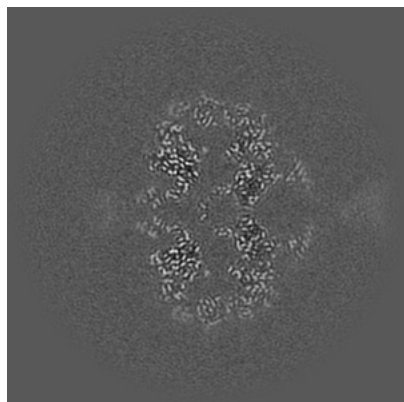


Z

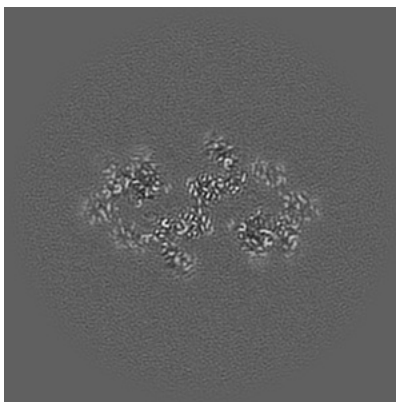
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

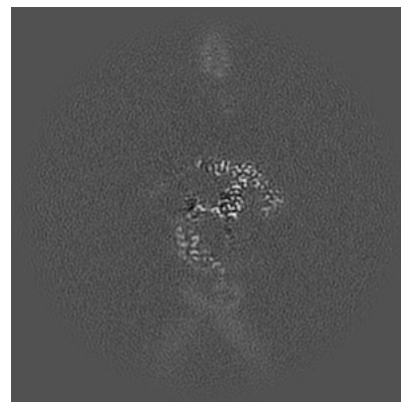
### 6.2.1 Primary map



X Index: 176

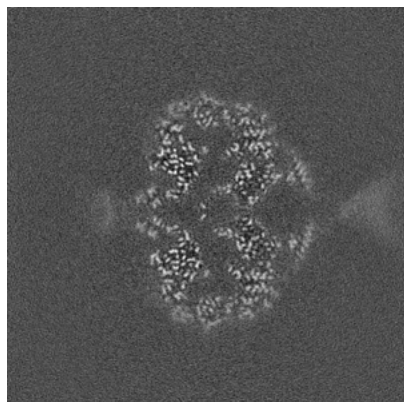


Y Index: 176

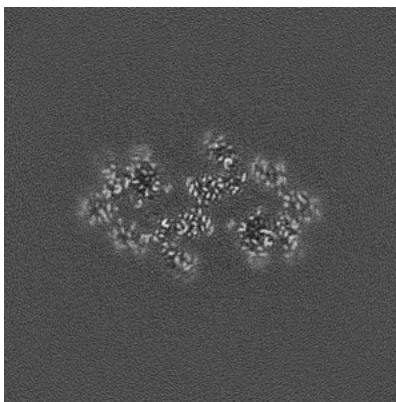


Z Index: 176

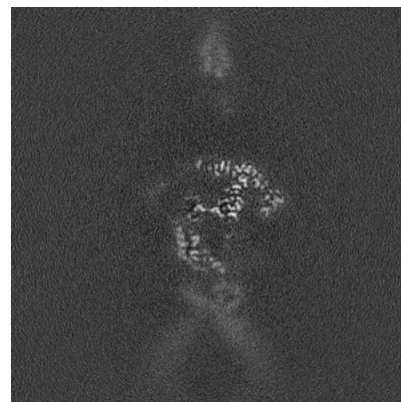
### 6.2.2 Raw map



X Index: 176



Y Index: 176



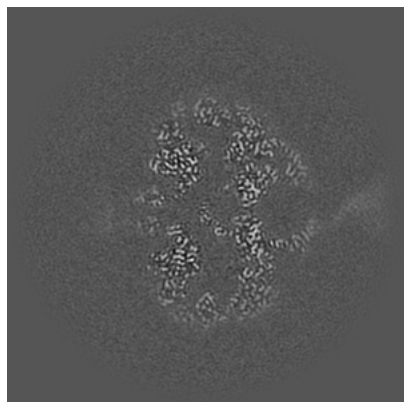
Z Index: 176

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

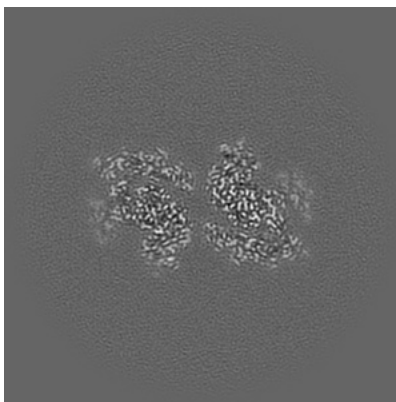


## 6.3 Largest variance slices [i](#)

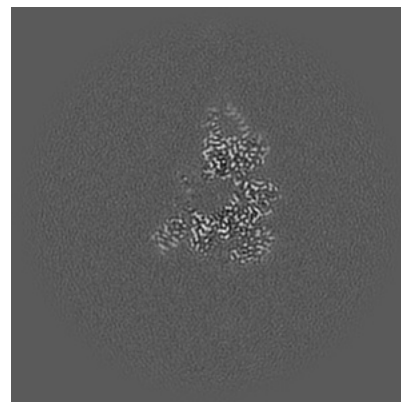
### 6.3.1 Primary map



X Index: 174

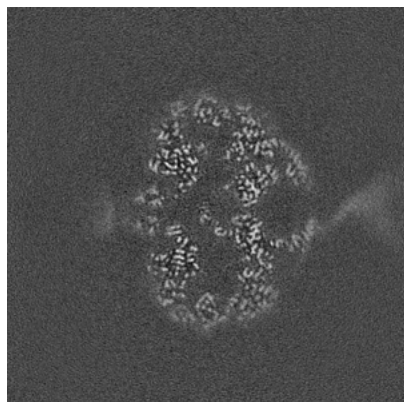


Y Index: 153

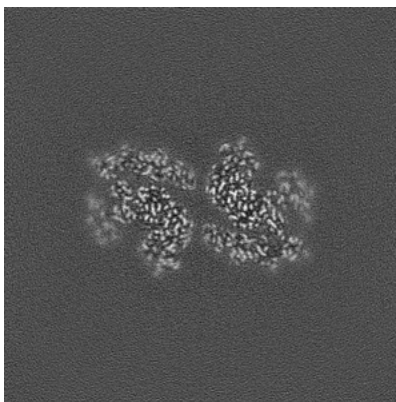


Z Index: 203

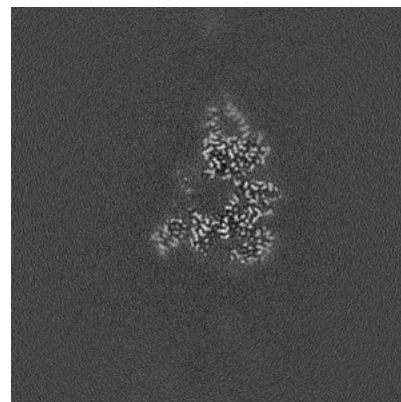
### 6.3.2 Raw map



X Index: 174



Y Index: 154

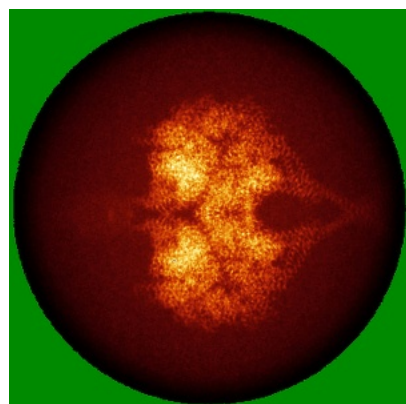


Z Index: 203

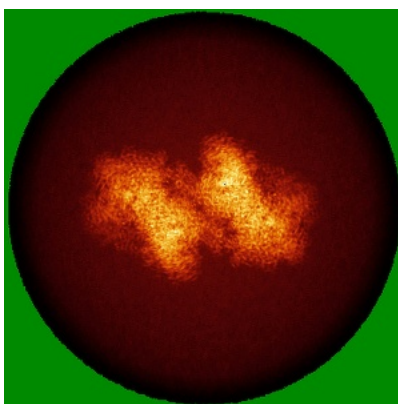
The images above show the largest variance slices of the map in three orthogonal directions.

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

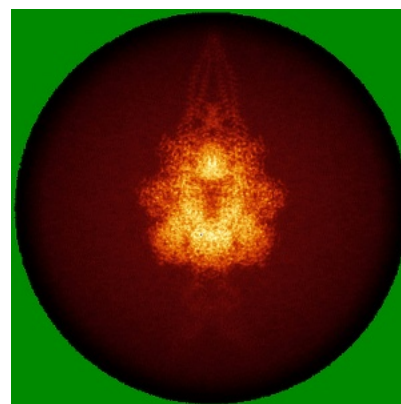
### 6.4.1 Primary map



X

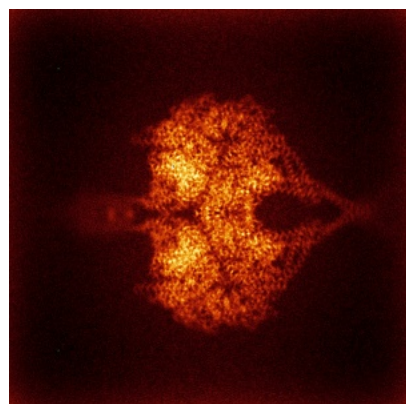


Y

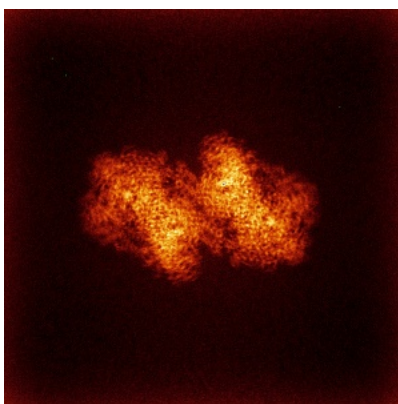


Z

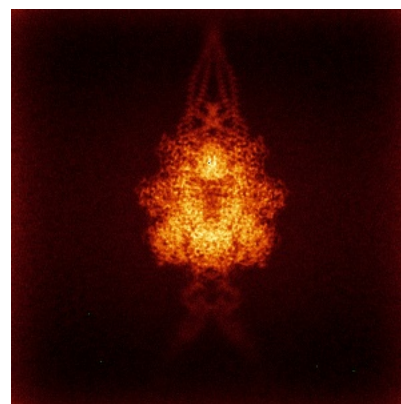
### 6.4.2 Raw map



X



Y

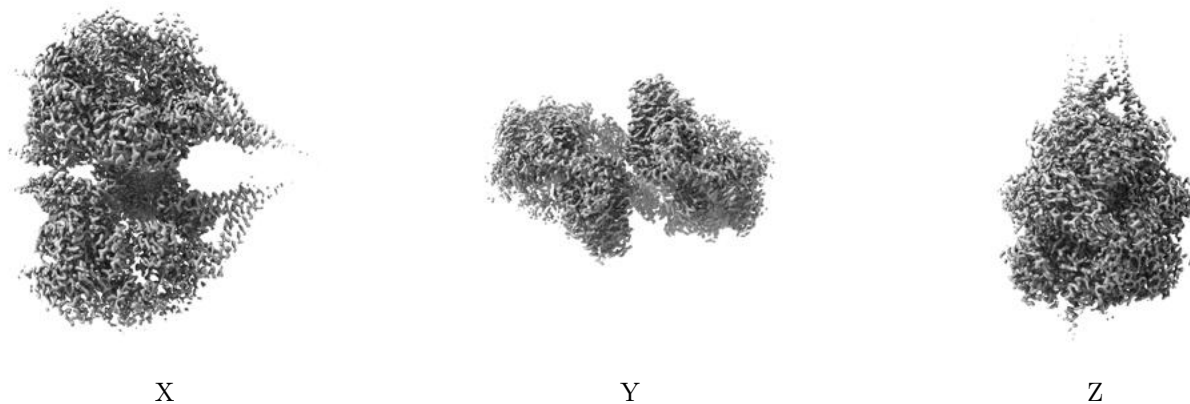


Z

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.

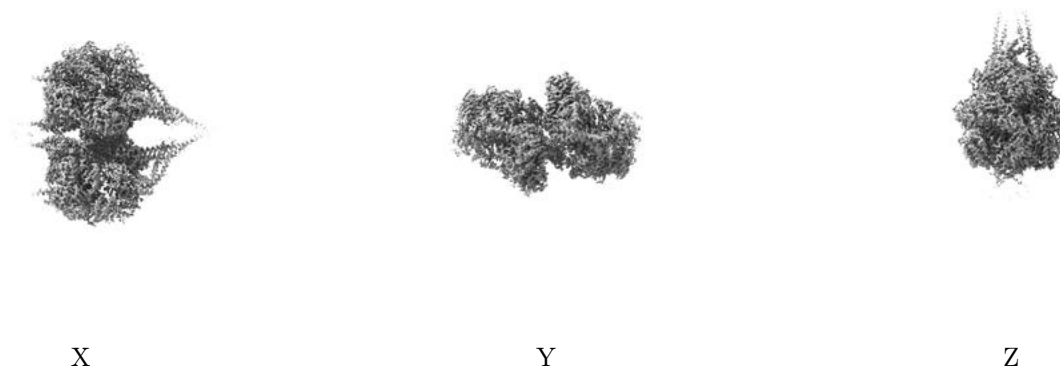
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.406. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

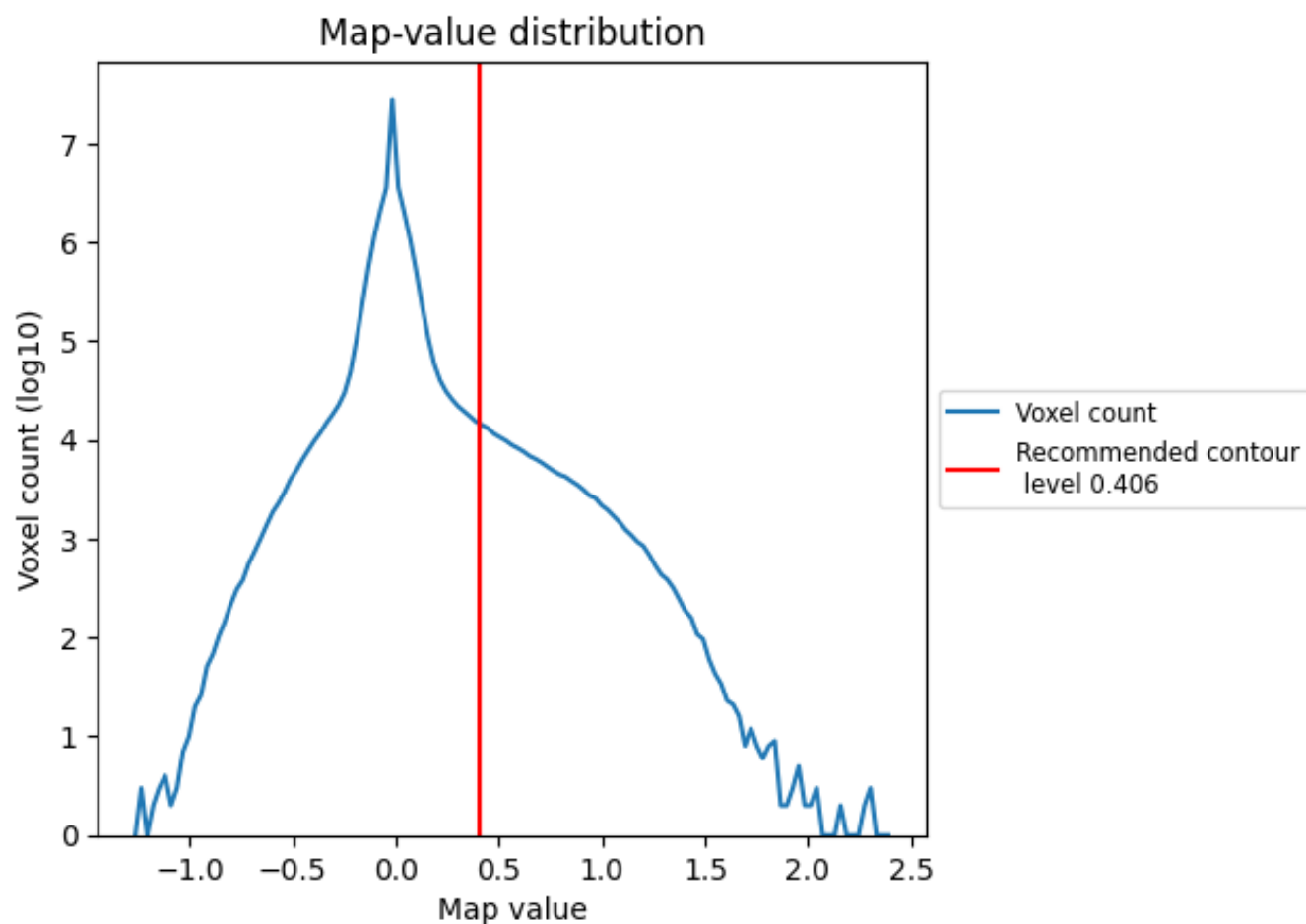
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

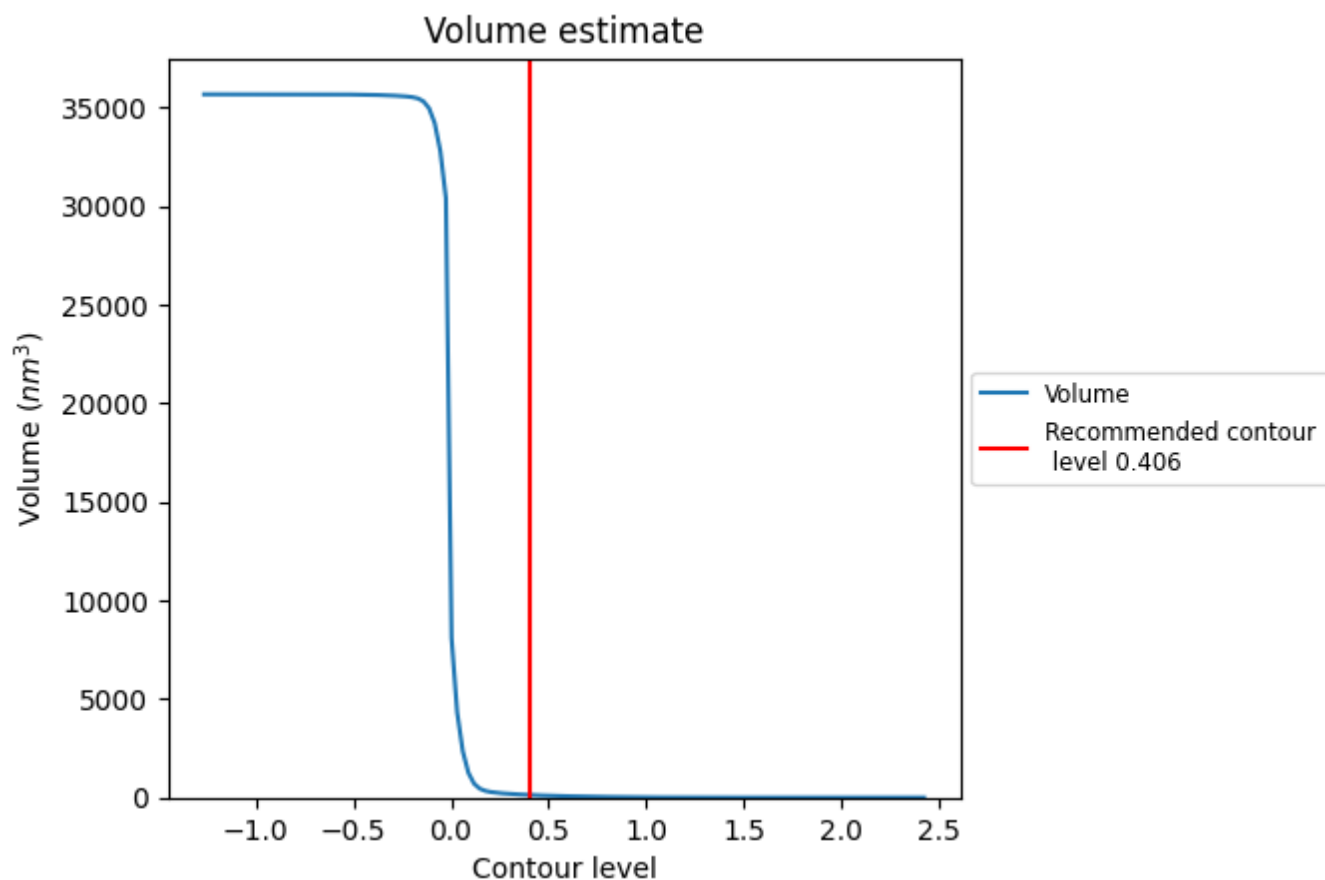
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

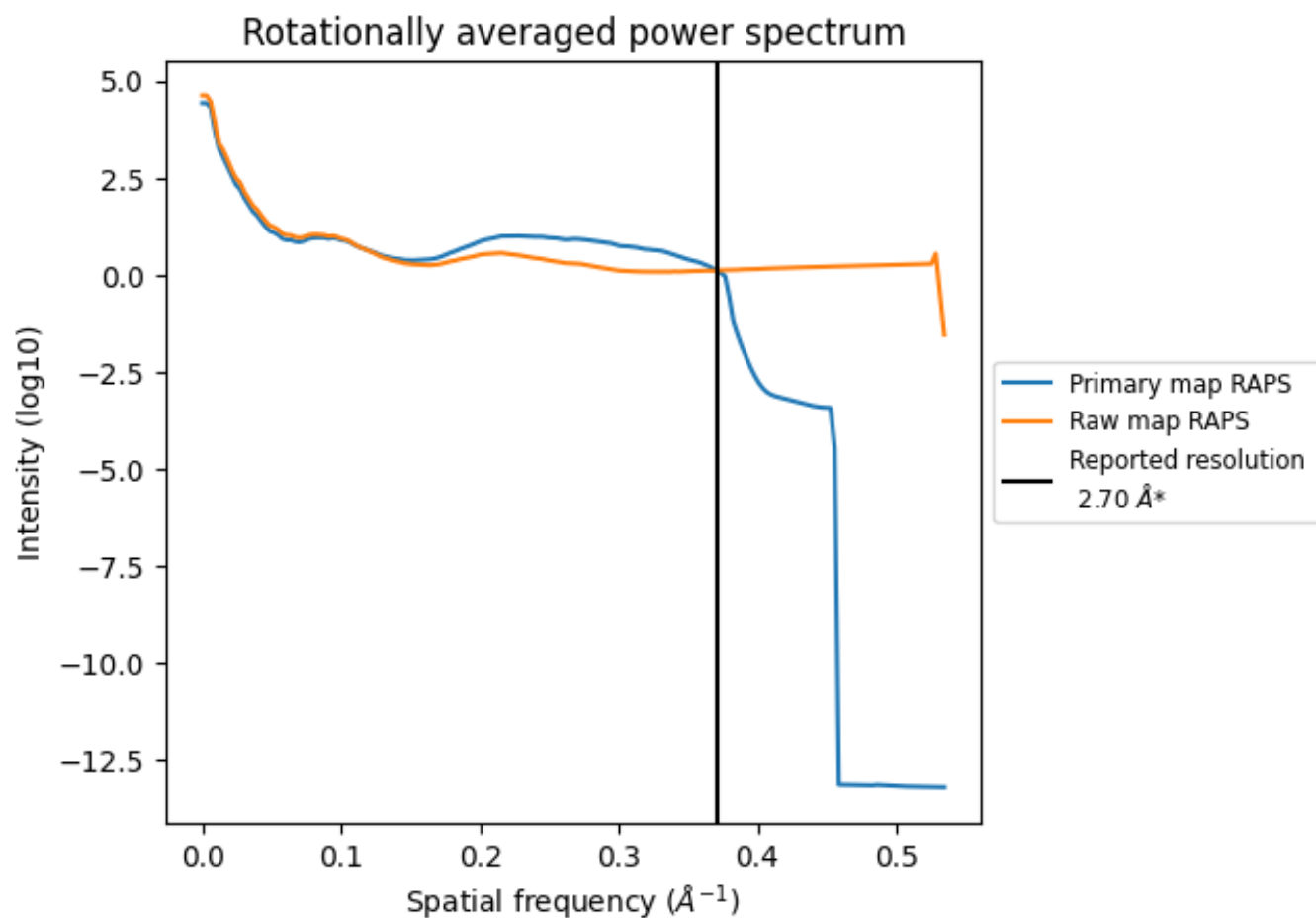
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 130 nm<sup>3</sup>; this corresponds to an approximate mass of 117 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 ⓘ

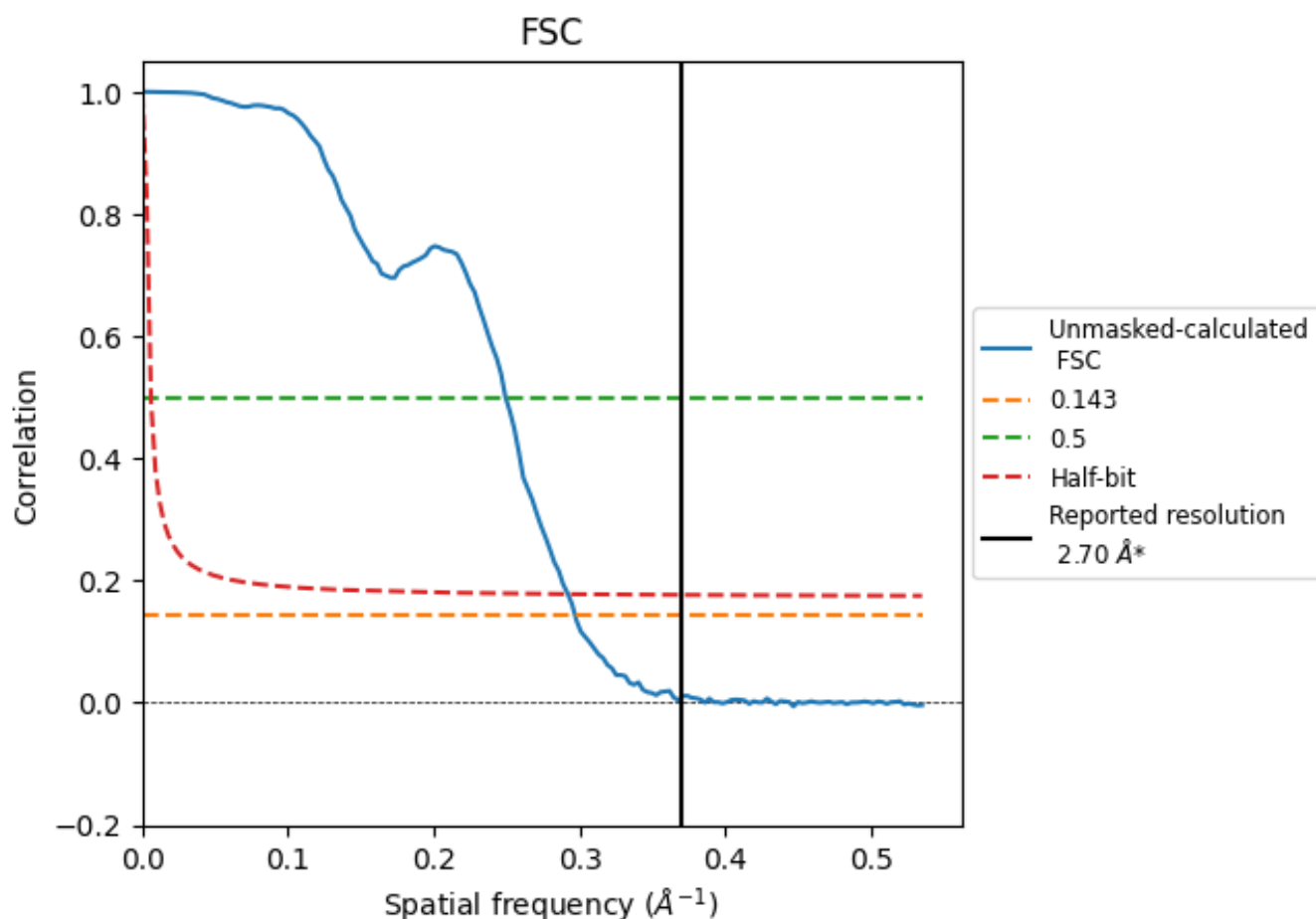


\*Reported resolution corresponds to spatial frequency of 0.370  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.370 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.37	4.01	3.43

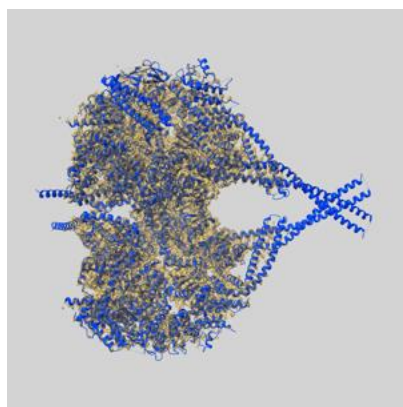
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.37 differs from the reported value 2.7 by more than 10 %



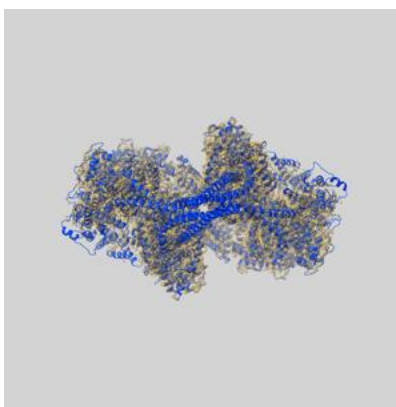
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47373 and PDB model 9E0X. Per-residue inclusion information can be found in section [3](#) on page [15](#).

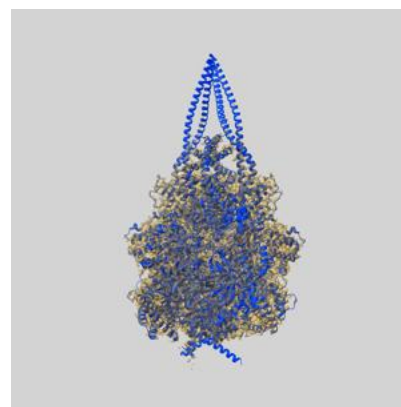
### 9.1 Map-model overlay [i](#)



X



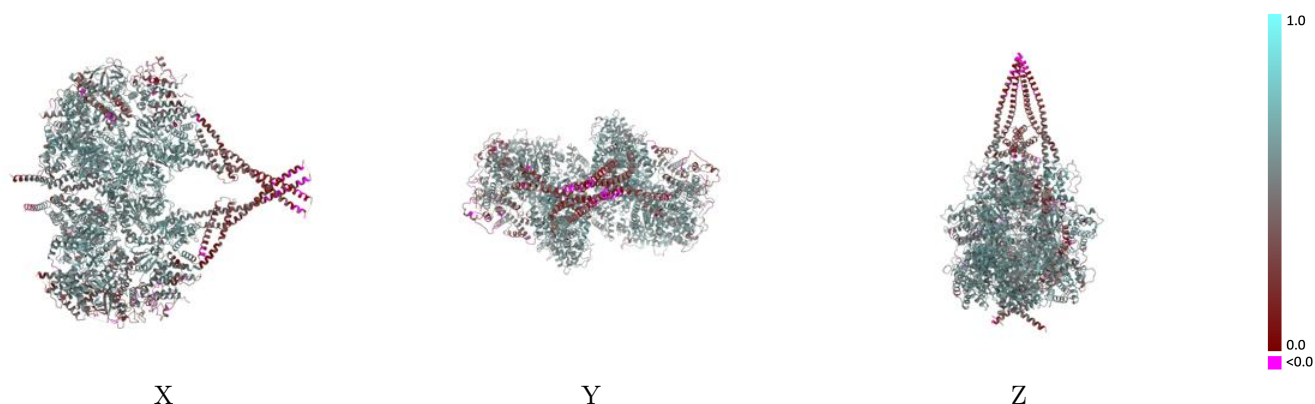
Y



Z

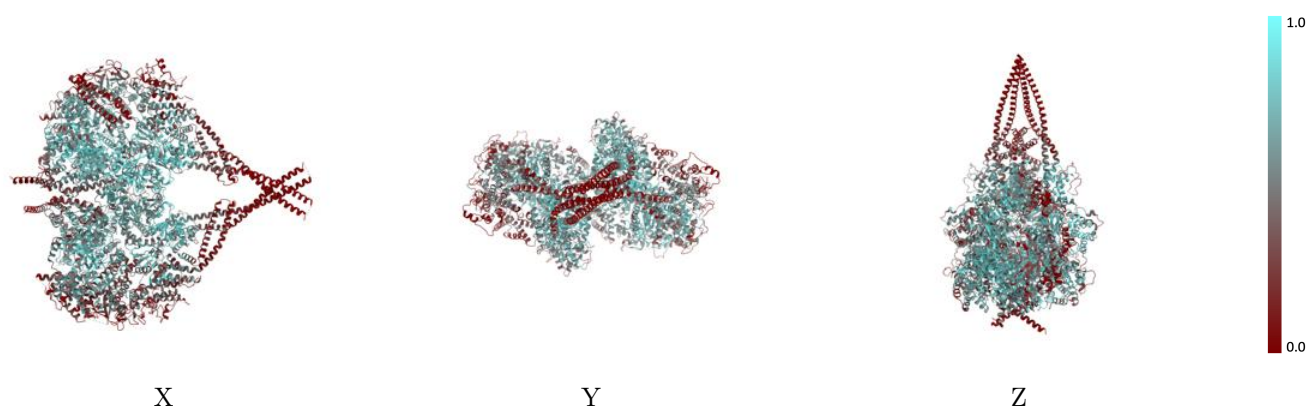
The images above show the 3D surface view of the map at the recommended contour level 0.406 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



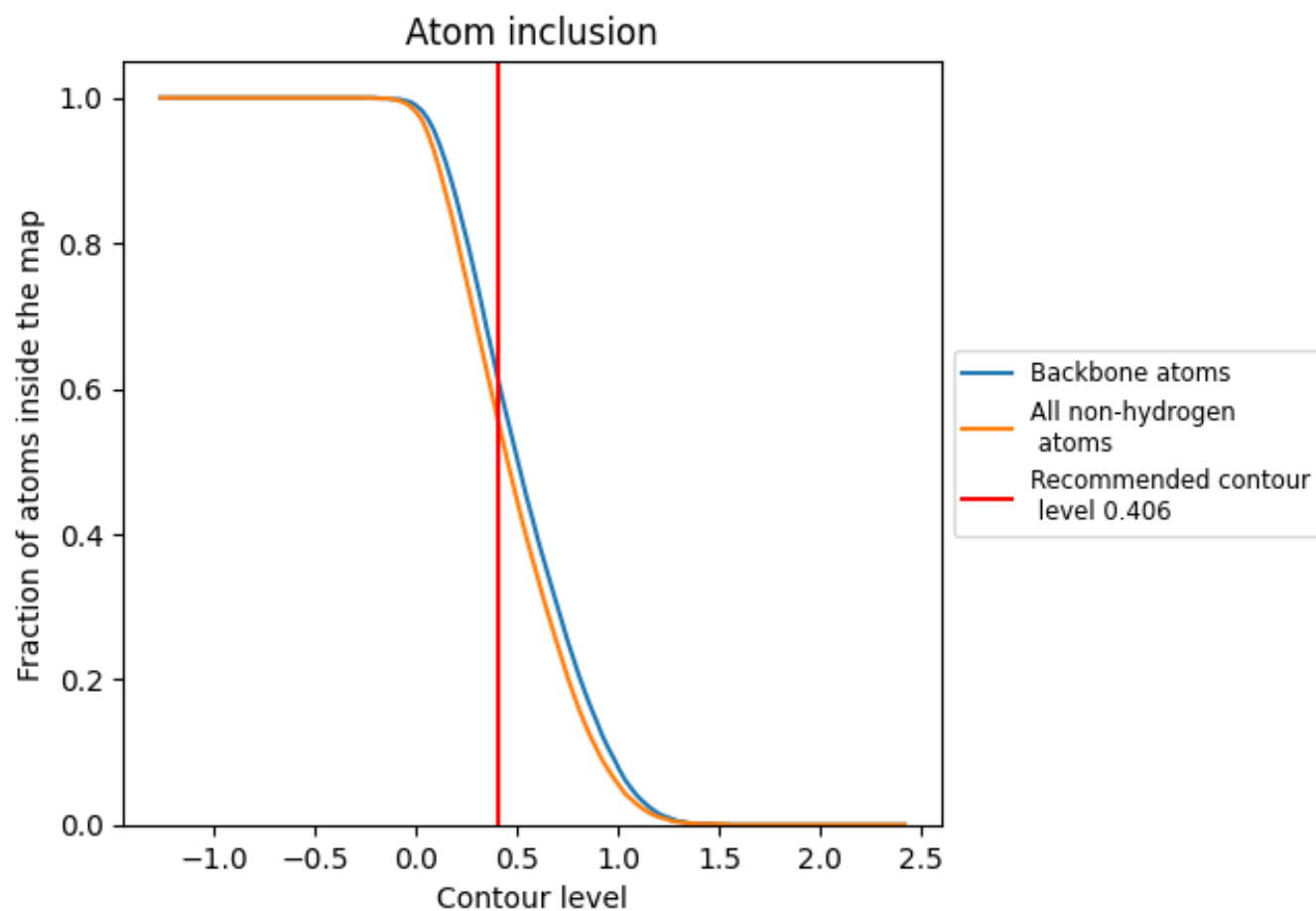
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.406).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 56% 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 (0.406) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5580	<div></div> 0.5210
A	<div></div> 0.5330	<div></div> 0.5070
B	<div></div> 0.5820	<div></div> 0.5340

