



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 09:04 AM UTC

PDB ID : 9DZY / pdb_00009dzy
EMDB ID : EMD-47342
Title : Cryo-EM structure of Pre-Chi dynein bound to Lis1
Authors : Nguyen, K.H.V.; Kendrick, A.A.; Leschziner, A.E.
Deposited on : 2024-10-17
Resolution : 3.10 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

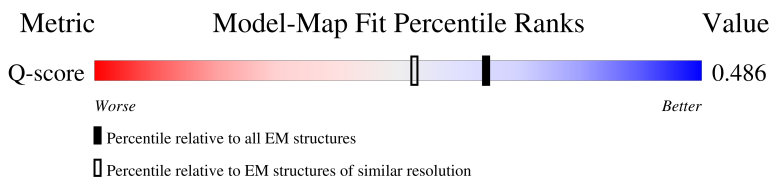
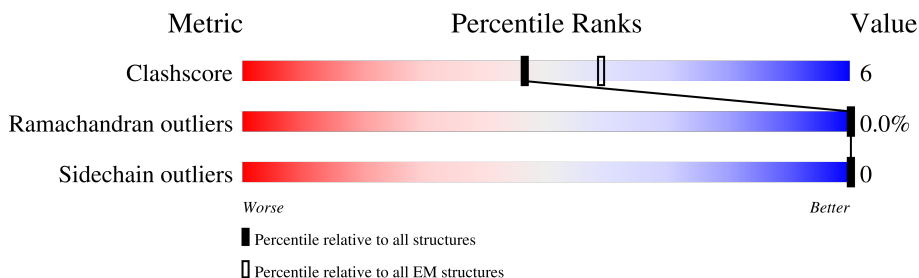
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	4843	29% 50% 10% 40%
1	B	4843	18% 51% 9% 40%
2	C	411	54% 63% 11% 26%
2	E	411	10% 64% 14% 22%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 51122 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	B	2920	Total	C	N	O	S	0	0
			23025	14699	3982	4232	112		
1	A	2920	Total	C	N	O	S	0	0
			23004	14686	3978	4228	112		

There are 396 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

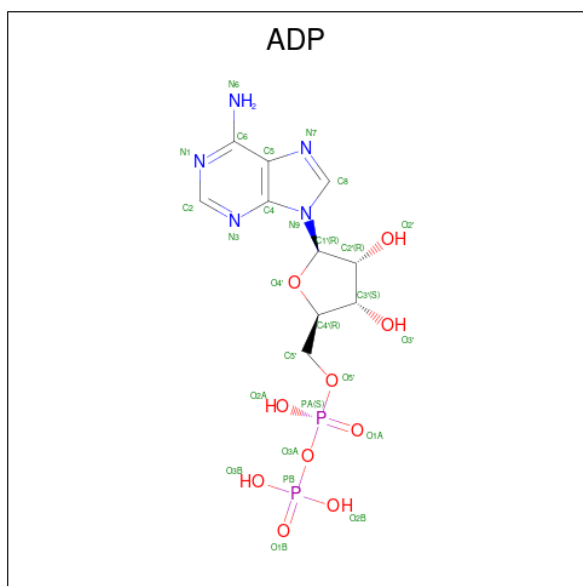
- Molecule 2 is a protein called Platelet-activating factor acetylhydrolase IB subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	320	Total	C	N	O	S	0	0
			2493	1570	437	466	20		
2	C	306	Total	C	N	O	S	0	0
			2372	1497	413	442	20		

There are 4 discrepancies between the modelled and reference sequences:

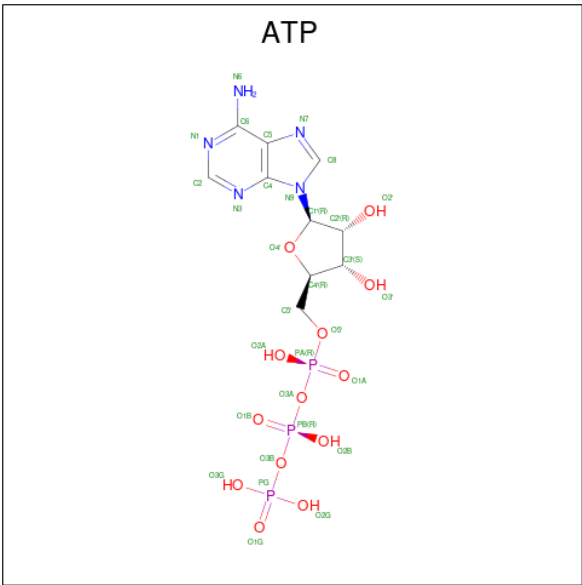
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	GLY	-	expression tag	UNP P43034
E	1	SER	-	expression tag	UNP P43034
C	0	GLY	-	expression tag	UNP P43034
C	1	SER	-	expression tag	UNP P43034

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

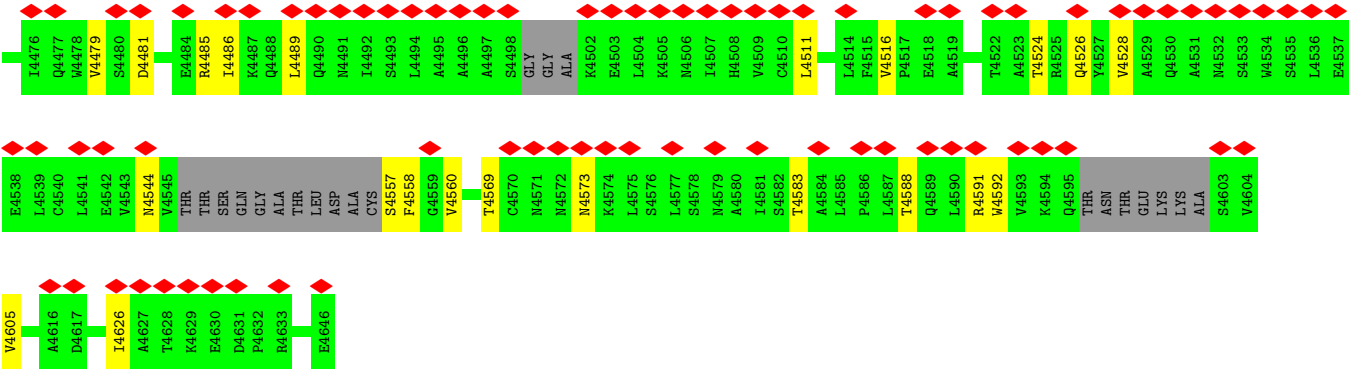
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

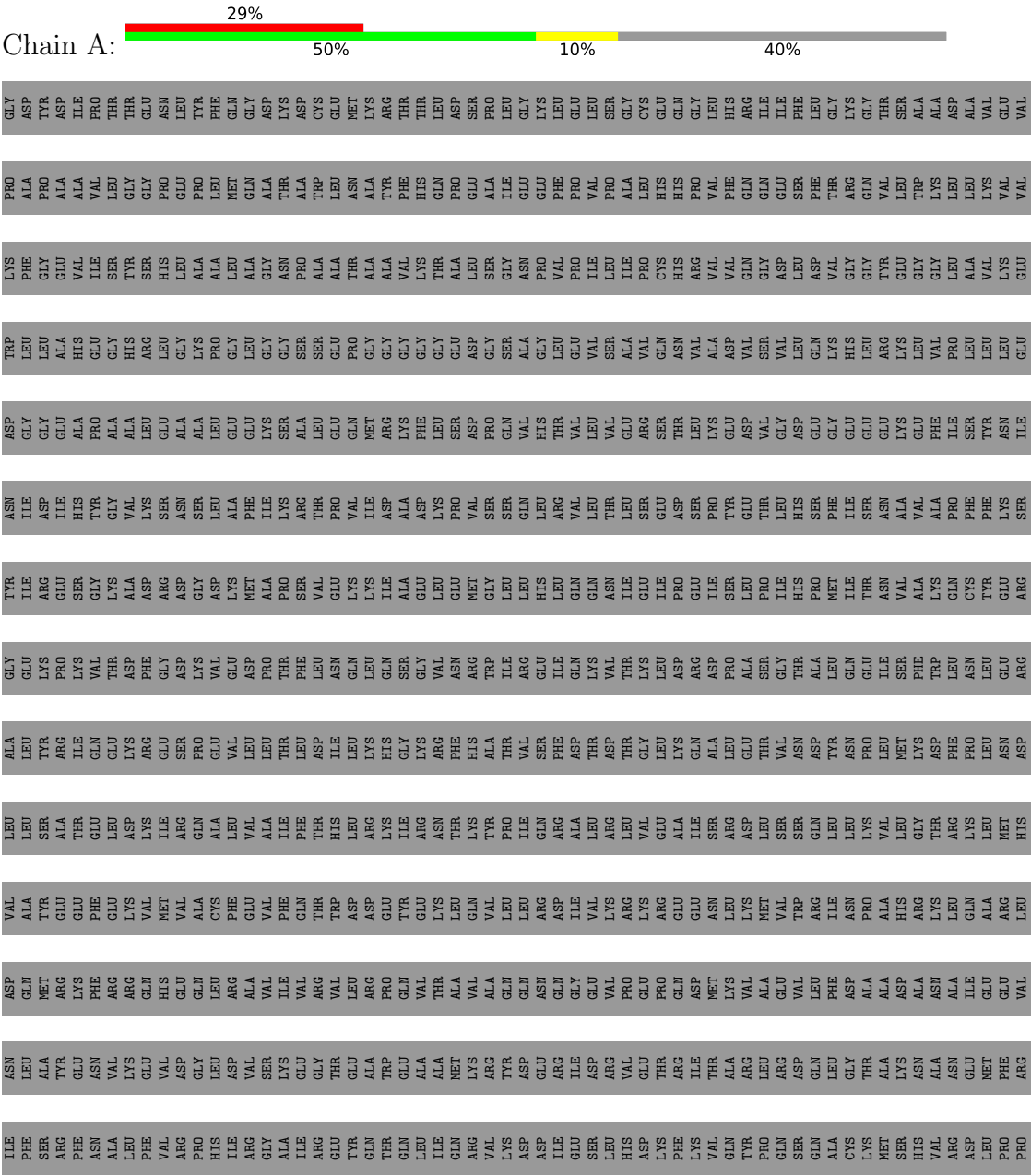
I1733	D1734	F1735	N1736	Y1737	Y1738	W1741	I1742	D1743	V1750	V1751	L1752	S1753	I1756	N1761	V1762	E1763	S1768	MET	GLY	GLY	GLY	ASP	A1775	A1776	F1777	L1782	E1786	N1790	D1794	S1795	M1798	E1799	Q1800	L1811	T1822	L1825	I1826	S1828	K1829	I1830	D1831	N1832	A1833	K1834																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
E1622	S1625	F1626	P1627	D1634	E1639	K1645	N1646	K1649	K1652	N1667	E1668	D1669	L1674	G1675	R1679	K1687	I1692	T1693	E1694	H1695	P1696	K1697	I1698	M1699	E1700	W1701	L1704	V1705	E1706	K1707	E1708	L1717	A1718	E1719	S1720	E1723	V1724	E1725	I1726	F1727	G1728	K1729	A1730	T1731	S1732																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
H1559	L1560	L1561	P1562	V1563	E1564	T1565	Q1566	R1567	F1568	Q1569	S1570	I1571	S1572	T1573	E1574	F1575	L1576	A1577	L1578	M1579	K1580	K1581	V1582	S1583	K1584	S1585	P1586	L1587	V1588	M1589	D1590	V1591	L1592	N1593	I1594	Q1595	G1596	V1597	Q1598	R1599	S1600	L1601	E1602	R1603	L1604	A1605	D1606	L1607	L1608	G1609	K1610	K1613	E1617	Y1618	L1619	E1620	R1621																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
R1485	L1486	I1487	R1488	G1489	W1490	D1491	D1492	N1495	K1496	V1497	K1498	E1499	H1500	I1501	N1502	S1503	V1504	S1505	A1506	M1507	K1508	L1509	S1510	P1511	Y1512	Y1513	K1514	V1515	F1516	E1517	E1518	D1519	A1520	L1521	S1522	W1523	E1524	D1525	K1526	R1529	I1530	M1531	W1537	I1538	D1539	E1548	G1549	I1550	G1553	S1554	A1555	D1556	I1557	K1558																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
TRP	VAL	VAL	SER	GLU	THR	LEU	GLY	GLN	TRP	ASP	VAL	LEU	GLN	LYS	GLU	THR	GLY	THR	GLY	GLY	LYS	VAL	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY

LYS	L3240	D5131	S3002	R2863	L2744	P2590	E2484	GLU	S2231	K2112	LYS	S1835
GLN	K3241	Q3135	G3003	E2864	I2747	L2691	Q2485	ALA	W2234	R2113	THR	F1836
HIS	K3242	P3136	F3004	R2869	N2762	V2592	L2486	ARG	P1996	E2114	SER	E1837
LEU	M3243	P3137	L3005	R2870	N2762	M2603	E2487	ARG	L2238	GLU	ALA	W1838
VAL	V3244	R3140	E3016	I2871	L2758	L2609	R2488	ARG	L2244	GLU	VAL	L1839
GLU	K3245	L3154	L3020	L2872	L2762	R2610	L2499	LYS	E2245	ARG	GLY	R1843
VAL	D3246	N3158	F3021	E2887	R2763	A2611	R2507	GLY	G2249	GLU	GLY	F1844
ARG	Q3247	N3166	E3022	E2888	L2769	L2612	R2510	LYS	E2248	GLU	GLY	Y1845
SER	Q3248	A3162	G3023	R2889	L2773	P2613	R2511	ASP	G2249	VAL	ASP	F1846
ALA	E3249	R3164	D3024	R2890	F2784	R2614	E2512	GLY	P2256	ASP	ASP	D1847
ASN	A3250	G3165	E3025	E2904	T2785	V2617	E2513	GLY	K2257	GLY	GLY	P1848
PRO	E3251	G3166	K3034	D2906	Q2786	S2623	E2514	GLU	A2258	ILE	GLU	K1849
LEU	K3252	R3167	A3037	N2913	D2787	S2624	E2515	ALA	D2269	A2128	GLU	Q1850
VAL	K3253	V2914	Q3038	E2914	Y2794	P2628	E2516	ALA	P2270	E2129	ILE	T1851
LYS	L3254	L2915	K3039	V2915	R2797	K2633	R2519	ALA	N2271	E2130	LYS	D1852
LEU	L3255	L2916	G3040	L2916	E2798	T2644	R2520	LYS	T2272	L2136	LEU	Q1856
GLN	L3256	L2917	G3041	L2917	N2799	P2645	R2521	GLY	R2273	L2137	GLY	L1857
LEU	L3257	L2918	L3042	L2918	N2804	N2646	T2522	GLY	E2274	Q2139	GLY	M1861
GLN	L3258	L2919	D3045	L2919	R2811	G2647	T2523	GLY	L2284	E2143	GLY	A1862
LEU	L3259	L2920	S3046	L2920	L2650	L2655	P2525	GLY	I2288	A2151	GLY	N1863
GLN	L3260	L2921	H3047	L2921	L2656	E2665	P2526	GLY	D2289	E2152	GLY	V1880
LEU	L3261	L2922	E3048	L2922	L2667	E2666	P2527	GLY	R2298	E2163	GLY	L2048
GLN	L3262	L2923	E3049	L2923	N2687	N2687	A2528	GLY	F2303	D2167	GLY	Q1881
LEU	L3263	L2924	T3067	L2924	L2688	L2688	E2529	GLY	V2307	G2168	GLY	T1882
GLN	L3264	L2925	S3071	L2925	E2671	E2671	E2530	GLY	E2310	Q2169	GLY	F1883
LEU	L3265	L2926	S3072	L2926	N2671	N2671	E2531	GLY	W2312	Y2170	GLY	L1884
GLN	L3266	L2927	G3073	L2927	V2679	V2679	T2541	GLY	N2316	R2172	GLY	Q1894
LEU	L3267	L2928	L3075	L2928	Q2834	Q2834	E2544	GLY	D2321	G2173	GLY	E1914
GLN	L3268	L2929	A3080	L2929	R2836	R2836	W2545	GLY	T2326	E2180	GLY	L1928
LEU	L3269	L2930	T3081	L2930	E2839	E2839	W2546	GLY	N2329	E2181	GLY	V2064
GLN	L3270	L2931	L3091	L2931	D2840	D2840	P2553	GLY	E2330	D2195	GLY	L2065
LEU	L3271	L2932	F3094	L2932	E2841	E2841	Q2554	GLY	G2331	G2196	GLY	A2066
GLN	L3272	L2933	L3097	L2933	R2844	R2844	T2555	GLY	R2332	E2197	GLY	N2067
LEU	L3273	L2934	W3097	L2934	D2847	D2847	E2556	GLY	L2333	M2202	GLY	K2068
GLN	L3274	L2935	K3112	L2935	N2849	N2849	H2560	GLY	P2336	E2205	GLY	I2069
LEU	L3275	L2936	E3116	L2936	T2852	T2852	A2563	GLY	F2343	E2206	GLY	V2070
GLN	L3276	L2937	N3119	L2937	L2855	L2855	D2566	GLY	E2388	E2207	GLY	D2077
LEU	L3277	L2938	P3123	L2938	N2860	N2860	V2567	GLY	E2389	E2208	GLY	R1966
GLN	L3278	L2939	D3124	L2939	I2861	I2861	W2568	GLY	GLY	Q2109	GLY	M1967
LEU	L3279	L2940	Y3125	L2940	D2862	D2862	Y2582	GLY	ASP	I2216	GLY	L1968
GLN	L3280	L2941	M3126	L2941			K2585	GLY		W2221	GLY	Q1974
LEU	L3281	L2942	P3127	L2942			W2586	GLY			GLY	E1980
GLN	L3282	L2943	V3128	L2943			E2587	GLY			GLY	A1981
LEU	L3283	L2944	K3239	L2944				GLY			GLY	E1984
GLN	L3284	L2945		L2945				GLY			GLY	H1985
LEU	L3285	L2946		L2946				GLY			GLY	S1986
GLN	L3286	L2947		L2947				GLY			GLY	N1987
LEU	L3287	L2948		L2948				GLY			GLY	PRO
GLN	L3288	L2949		L2949				GLY			GLY	ASN
LEU	L3289	L2950		L2950				GLY			GLY	TYR
GLN	L3290	L2951		L2951				GLY			GLY	ASP
LEU	L3291	L2952		L2952				GLY			GLY	
GLN	L3292	L2953		L2953				GLY			GLY	
LEU	L3293	L2954		L2954				GLY			GLY	
GLN	L3294	L2955		L2955				GLY			GLY	
LEU	L3295	L2956		L2956				GLY			GLY	
GLN	L3296	L2957		L2957				GLY			GLY	
LEU	L3297	L2958		L2958				GLY			GLY	
GLN	L3298	L2959		L2959				GLY			GLY	
LEU	L3299	L2960		L2960				GLY			GLY	
GLN	L3300	L2961		L2961				GLY			GLY	
LEU	L3301	L2962		L2962				GLY			GLY	
GLN	L3302	L2963		L2963				GLY			GLY	
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GLN	L3304	L2965		L2965				GLY			GLY	
LEU	L3305	L2966		L2966				GLY			GLY	
GLN	L3306	L2967		L2967				GLY			GLY	
LEU	L3307	L2968		L2968				GLY			GLY	
GLN	L3308	L2969		L2969				GLY			GLY	
LEU	L3309	L2970		L2970				GLY			GLY	
GLN	L3310	L2971		L2971				GLY			GLY	
LEU	L3311	L2972		L2972				GLY			GLY	
GLN	L3312	L2973		L2973				GLY			GLY	
LEU	L3313	L2974		L2974				GLY			GLY	
GLN	L3314	L2975		L2975				GLY			GLY	
LEU	L3315	L2976		L2976				GLY			GLY	
GLN	L3316	L2977		L2977				GLY			GLY	
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GLN	L3318	L2979		L2979				GLY			GLY	
LEU	L3319	L2980		L2980				GLY			GLY	
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GLN	L3322	L2983		L2983				GLY			GLY	
LEU	L3323	L2984		L2984				GLY			GLY	
GLN	L3324	L2985		L2985				GLY			GLY	
LEU	L3325	L2986		L2986				GLY			GLY	
GLN	L3326	L2987		L2987				GLY			GLY	
LEU	L3327	L2988		L2988				GLY			GLY	
GLN	L3328	L2989		L2989				GLY			GLY	
LEU	L3329	L2990		L2990				GLY			GLY	
GLN	L3330	L2991		L2991				GLY			GLY	
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LEU	L3343	L3004		L3004				GLY			GLY	
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GLN	L3350	L3011		L3011				GLY			GLY	
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LEU	L3369	L3030		L3030				GLY			GLY	
GLN	L3370	L3031		L3031				GLY			GLY	
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GLN	L3372	L3033		L3033				GLY			GLY	
LEU	L3373	L3034		L3034				GLY			GLY	
GLN	L3374	L3035		L3035				GLY				

SER	ASP	ALA	ILE	ARG	GLU	LYS	MET	LYS	LYS	ASN	TYR	MET	SER	ASN	PRO	SER	TYR	ASN	TYR	ILE	VAL	ARG	ALA	SER	LEU	ALA	CYS	GLY	PRO	MET	VAL	LYS	TRP	ALA	ILE	ALA	GLN	LEU	ASN	TYR	ALA	ASP	MET	LYS	ARG	VAL	GLU	PRO	LEU	LEU	ARG	ASN	ASN	GLU	LEU	GLN	LYS	LEU																																																																																																																																																																																																																																																																																																																																																																																																																																																									
GLU	ASP	ALA	ASP	LYS	ASP	ASN	GLN	GLN	LYS	ALA	ASN	GLU	VAL	GLU	Q3435	M3436	I3437	R3438	D3439	L3440	E3441	A3442	S3443	I3444	A3445	R3446	Y3447	K3448	E3449	E3450	Y3451	A3452	V3453	L3454	I3455	S3456	E3457	A3458	Q3459	A3460	I3461	K3462	A3463	D3464	L3465	A3466	A3467	V3468	E3469	A3470	K3471	V3472	N3473	R3474	A3477	L3478	L3479	K3480																																																																																																																																																																																																																																																																																																																																																																																																																																																									
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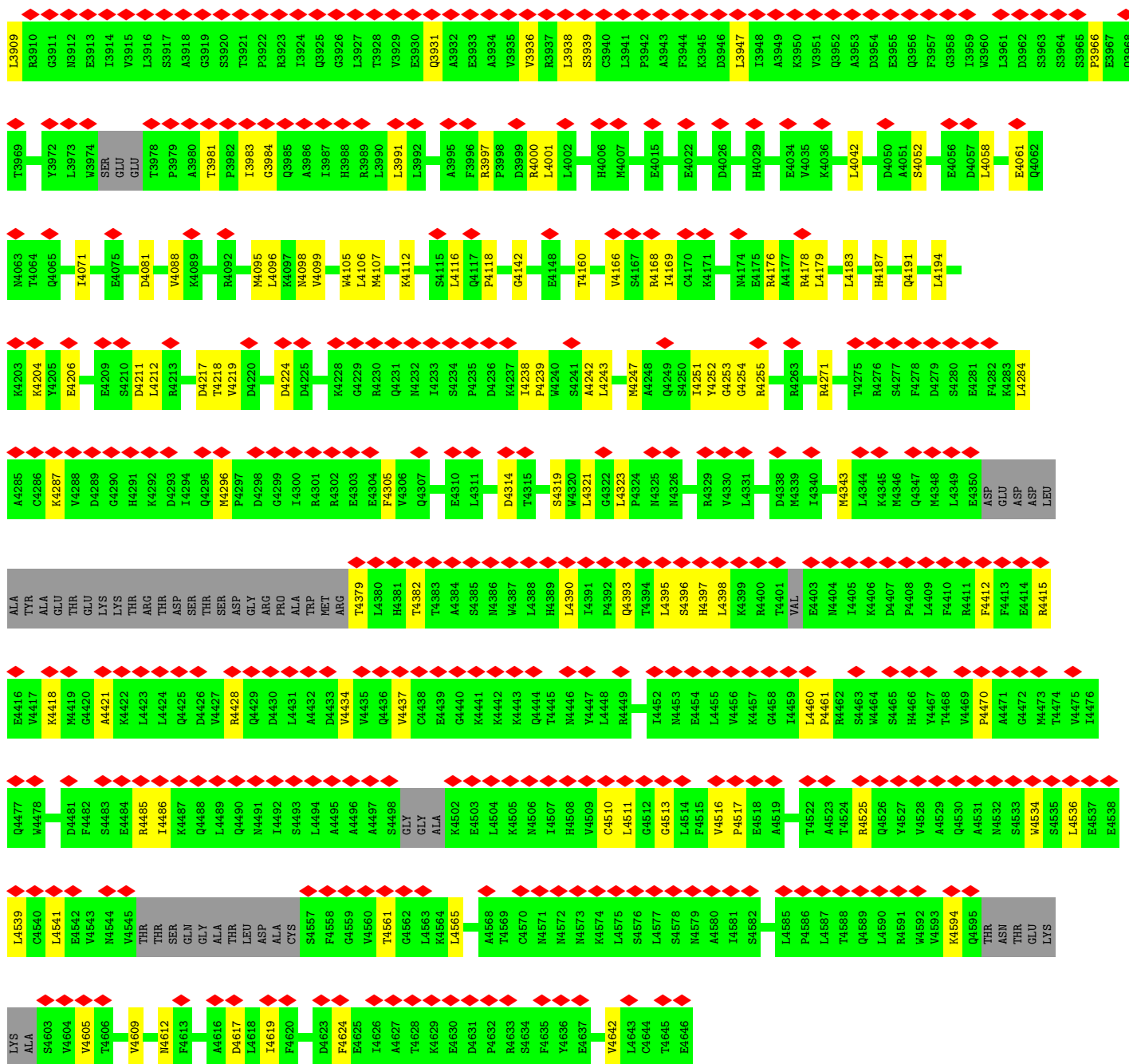
● Molecule 1: Cytoplasmic dynein 1 heavy chain 1



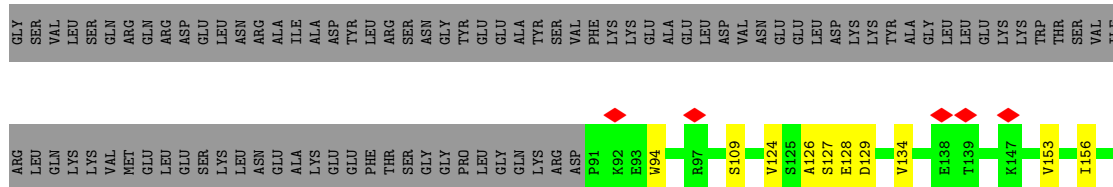


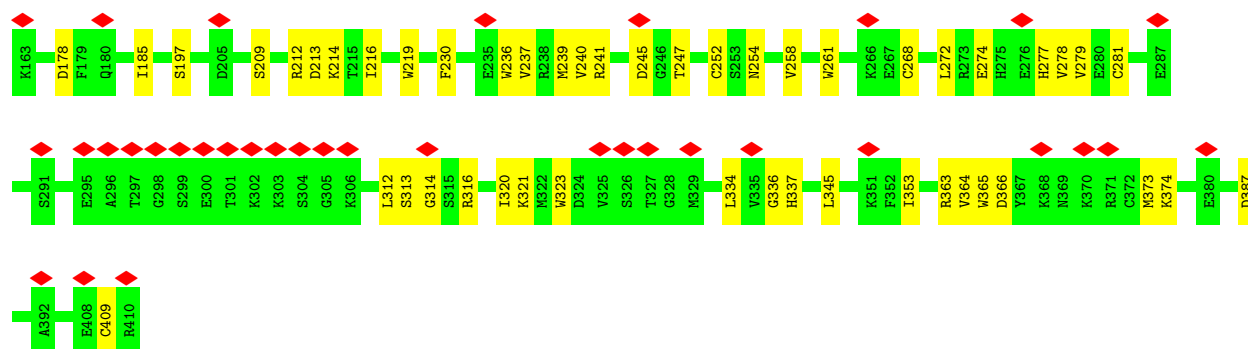
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R3741	L3742	R3743	Q3744	L3745	E3746	K3747	S3748	L3749	L3750	Q3751	A3752	L3753	H3754	E3755	V3756	K3757	Q3758	R3759	L3760	L3761	D3762	D3763	D3764	T3765	L3766	L3767	T3768	T3769	L3770	E3771	H3772	L3773	K3774	R3775	E3776	A3777	E3778	E3779	V3780	T3781	R3782	K3783	V3784	E3785	R3786	T3787	D3788	L3789	V3790	H3791	Q3792	E3793	V3794	E3795	T3796	V3797	S3798	Q3799	Q3800								
T3656	G3657	G3658	R3659	V3660	L3661	I3662	T3663	L3664	G3665	D3666	Q3667	D3668	L3669	D3670	L3671	S3674	T3681	R3682	D3683	E3687	D3691	R3695	R3705	L3708	N3714	E3715	V3716	L3717	K3718	A3719	E3720	P3722	V3724	D3725	E3726	K3727	R3728	S3729	L3730	L3731	L3732	K3733	L3734	Q3735	Q3736	E3737	Q3738	Q3739	L3740																		
R3525	Q3538	A3539	I3540	I3541	Q3542	F3543	Q3549	A3560	I3561	K3562	A3563	D3564	L3565	A3566	A3567	V3568	A3569	A3570	K3571	V3572	N3573	R3574	S3575	N3584	D3591	Q3594	Q3595	A3596	Y3604	K3605	D3606	R3607	V3608	L3609	R3620	R3628	L3634	E3639	N3650	R3651	E3652	V3653	R3654	R3655																							
V3453	L3454	I3455	S3456	N3457	A3458	Q3459	A3460	I3461	K3462	A3463	D3464	L3465	A3466	A3467	V3468	A3469	A3470	K3471	V3472	N3473	R3474	S3475	T3476	A3477	L3478	L3479	K3480	S3481	L3482	S3483	A3484	E3485	R3486	E3487	W3488	E3490	K3491	T3492	S3493	E3494	T3495	F3496	K3497	N3498	Q3499	M3500	S3501	T3502	D3506	S3510	Y3516	A3517	D3521														
VAL	LYS	TRP	ALA	ILE	GLN	LEU	TYR	ALA	MET	LEU	LYS	VAL	PRO	THR	ILE	ASN	ARG	GLU	GLN	LYS	LEU	ASP	ALA	LEU	ASP	ASP	GLN	GLN	ALA	ASN	TYR	MET	ASN	PRO	ALA	VAL	TYR	ASN	R3435	M3436	I3437	R3438	D3439	L3440	E3441	A3442	S3443	I3444	A3445	R3446	V3447	K3448	E3449	S3450	Y3451	A3452											
THR	ASP	TRP	LYS	MET	GLN	SER	ILE	ARG	GLU	LYS	ASP	VAL	ASN	PHE	PRO	VAL	THR	ILE	VAL	ASN	GLN	PHE	ASN	ALA	GLU	GLY	ILE	ILE	ARG	GLU	ASP	ASP	ILE	ARG	GLU	VAL	ASN	TYR	ASN	GLU	VAL	Q3435	M3436	I3437	R3438	D3439	L3440	E3441	A3442	S3443	I3444	A3445	R3446	V3447	K3448	E3449	S3450	Y3451	A3452								
ASP	LYS	GLN	MET	SER	VAL	LYS	GLU	ASN	ASP	LYS	VAL	GLU	PRO	ILE	ALA	VAL	THR	ILE	VAL	ASN	GLN	PHE	ASN	ALA	GLU	GLY	ILE	ILE	ARG	GLU	ASP	ASP	ILE	ARG	GLU	VAL	ASN	TYR	MET	ASN	PRO	ALA	VAL	Q3435	M3436	I3437	R3438	D3439	L3440	E3441	A3442	S3443	I3444	A3445	R3446	V3447	K3448	E3449	S3450	Y3451	A3452						
D3213	Q3214	V3215	E3216	E3217	L3218	R3219	R3220	D3221	L3222	R3223	I3224	K3225	S3226	Q3227	E3228	L3229	E3230	V3231	K3232	N3233	A3234	A3235	A3236	N3237	D3238	L3239	L3240	SER	L3241	K3242	M3243	V3244	D3245	K3246	Q3247	Q3248	E3249	A3250	E3251	K3252	K3253	LYS	VAL	MET	SER	GLN	GLU	ILE	THR																		
H2867	S2868	R2869	I2876	L2877	S2878	D2879	D2880	Y2881	I2882	D2885	Q2886	E2887	E2888	L2889	R2890	D2891	A2895	R2896	L2897	K2898	Y2901	E2902	E2903	E2904	L2905	D2906	V2907	F2908	L2909	F3004	V2910	L2911	F2912	N2913	E2914	D2917	H2918	Y2919	D2923	R2924	R2927	Q2928	P2929	Q2930	K2943	W2952	S2957	I2961	K2962																		

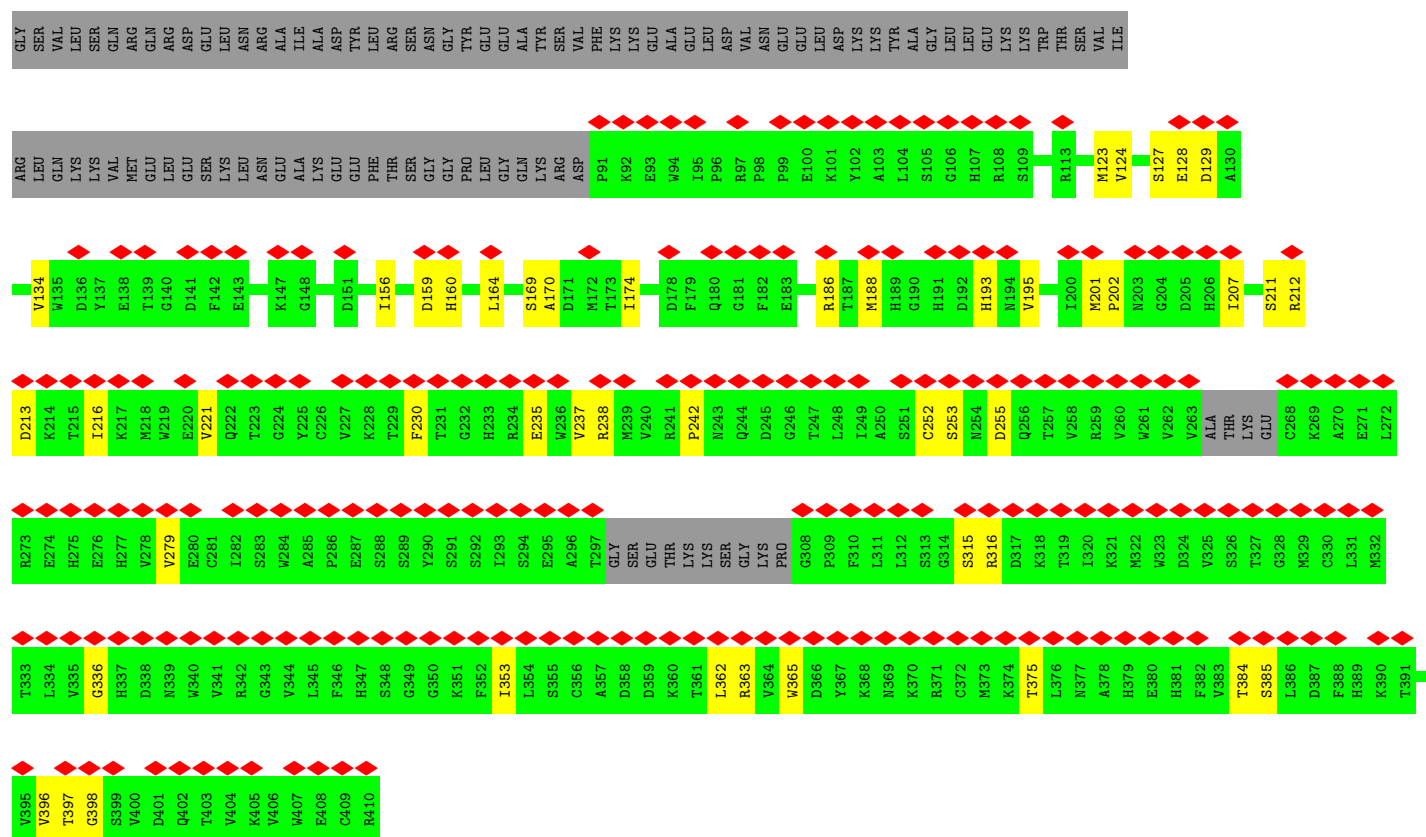


• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta





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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66880	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	0.934	Depositor
Minimum map value	-0.503	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.224	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/23477	0.34	0/31858
1	B	0.18	0/23499	0.35	0/31886
2	C	0.13	0/2436	0.33	0/3313
2	E	0.21	0/2560	0.43	0/3476
All	All	0.17	0/51972	0.35	0/70533

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	23004	0	22809	292	0
1	B	23025	0	22837	259	0
2	C	2372	0	2224	30	0
2	E	2493	0	2372	35	0
3	A	81	0	36	1	0
3	B	81	0	36	4	0
4	A	31	0	12	1	0
4	B	31	0	12	0	0
5	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	2	0	0	0	0
All	All	51122	0	50338	615	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 6.

The worst 5 of 615 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:B:3455:ILE:HG22	1:B:3459:GLN:HE22	1.52	0.74
2:E:313:SER:HB2	2:E:320:ILE:HG23	1.72	0.71
2:E:353:ILE:HB	2:E:365:TRP:HB2	1.71	0.71
2:E:281:CYS:H	2:E:314:GLY:HA2	1.56	0.71
1:A:3731:LEU:HD21	1:A:3790:VAL:HG22	1.73	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%)	2801 (97%)	91 (3%)	0	100	100
1	B	2892/4843 (60%)	2790 (96%)	101 (4%)	1 (0%)	100	100
2	C	300/411 (73%)	283 (94%)	17 (6%)	0	100	100
2	E	318/411 (77%)	295 (93%)	23 (7%)	0	100	100
All	All	6402/10508 (61%)	6169 (96%)	232 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	2473/4279 (58%)	2473 (100%)	0	100	100
1	B	2477/4279 (58%)	2477 (100%)	0	100	100
2	C	257/364 (71%)	257 (100%)	0	100	100
2	E	272/364 (75%)	272 (100%)	0	100	100
All	All	5479/9286 (59%)	5479 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1651	GLN
1	A	2677	GLN
1	A	4386	ASN
1	A	1931	ASN
1	A	2085	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	A	4706	5	28,29,29	1.39	4 (14%)	43,45,45	1.83	8 (18%)
4	ATP	B	4702	5	32,33,33	0.53	0	48,52,52	0.37	0
3	ADP	A	4702	-	28,29,29	1.39	4 (14%)	43,45,45	1.95	8 (18%)
4	ATP	A	4701	-	32,33,33	0.48	0	48,52,52	0.36	0
3	ADP	B	4706	5	28,29,29	1.39	5 (17%)	43,45,45	1.82	9 (20%)
3	ADP	B	4705	-	28,29,29	1.38	5 (17%)	43,45,45	1.82	10 (23%)
3	ADP	A	4703	-	28,29,29	1.41	4 (14%)	43,45,45	1.83	8 (18%)
3	ADP	B	4701	-	28,29,29	1.39	5 (17%)	43,45,45	1.81	10 (23%)

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
3	ADP	A	4706	5	-	2/16/32/32	0/3/3/3
4	ATP	B	4702	5	-	3/22/38/38	0/3/3/3
3	ADP	A	4702	-	-	3/16/32/32	0/3/3/3
4	ATP	A	4701	-	-	2/22/38/38	0/3/3/3
3	ADP	B	4706	5	-	6/16/32/32	0/3/3/3
3	ADP	B	4705	-	-	3/16/32/32	0/3/3/3
3	ADP	A	4703	-	-	0/16/32/32	0/3/3/3
3	ADP	B	4701	-	-	3/16/32/32	0/3/3/3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4702	ADP	C5-C4	4.70	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4703	ADP	C5-C4	4.66	1.47	1.39
3	B	4705	ADP	C5-C4	4.56	1.47	1.39
3	A	4706	ADP	C5-C4	4.49	1.47	1.39
3	B	4701	ADP	C5-C4	4.48	1.47	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4702	ADP	C5-C4-N3	-6.63	117.59	126.72
3	A	4703	ADP	C5-C4-N3	-5.84	118.68	126.72
3	A	4706	ADP	C5-C4-N3	-5.80	118.73	126.72
3	B	4706	ADP	C5-C4-N3	-5.64	118.94	126.72
3	B	4701	ADP	C5-C4-N3	-5.60	119.00	126.72

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	4706	ADP	PA-O3A-PB-O3B
3	B	4706	ADP	C5'-O5'-PA-O1A
3	A	4706	ADP	C5'-O5'-PA-O1A
4	B	4702	ATP	C3'-C4'-C5'-O5'
4	B	4702	ATP	O4'-C4'-C5'-O5'

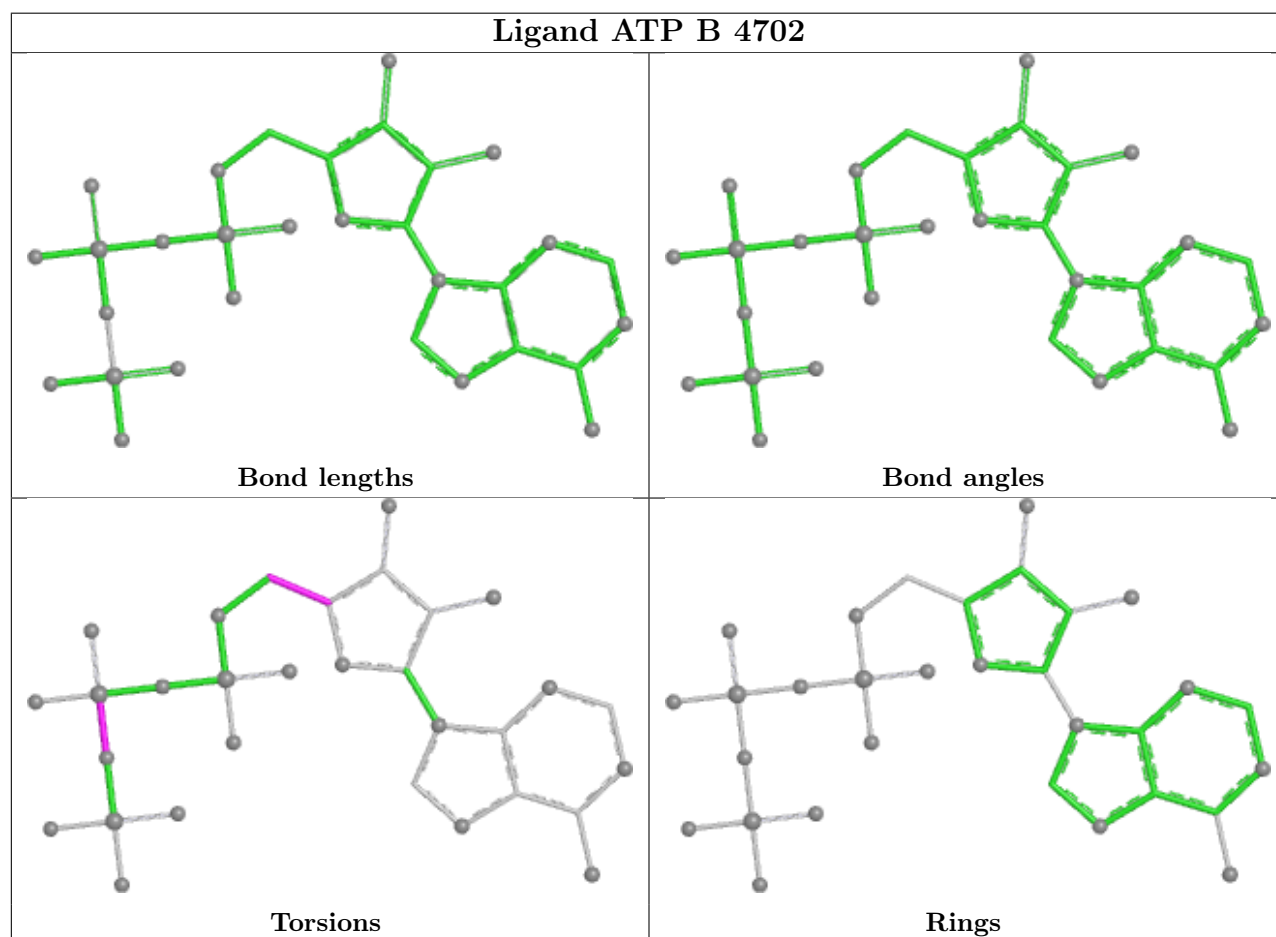
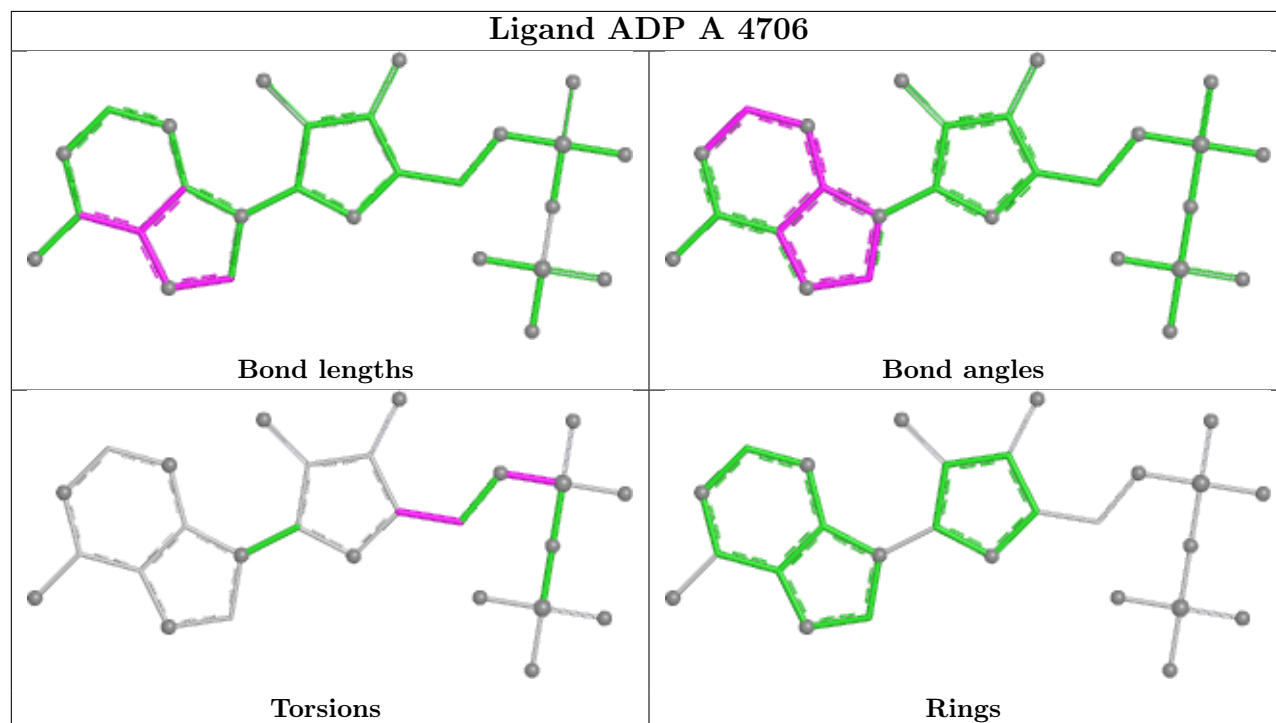
There are no ring outliers.

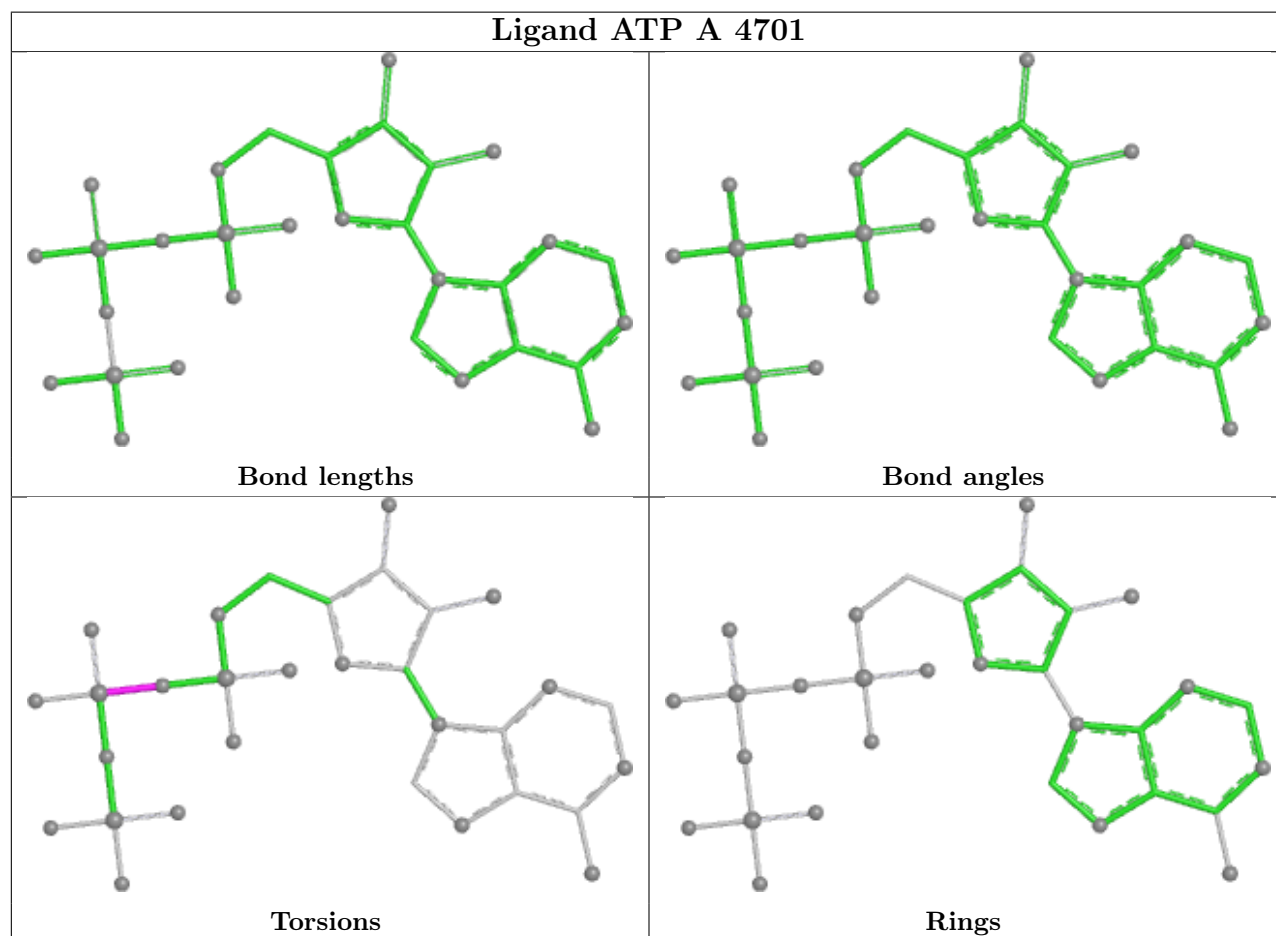
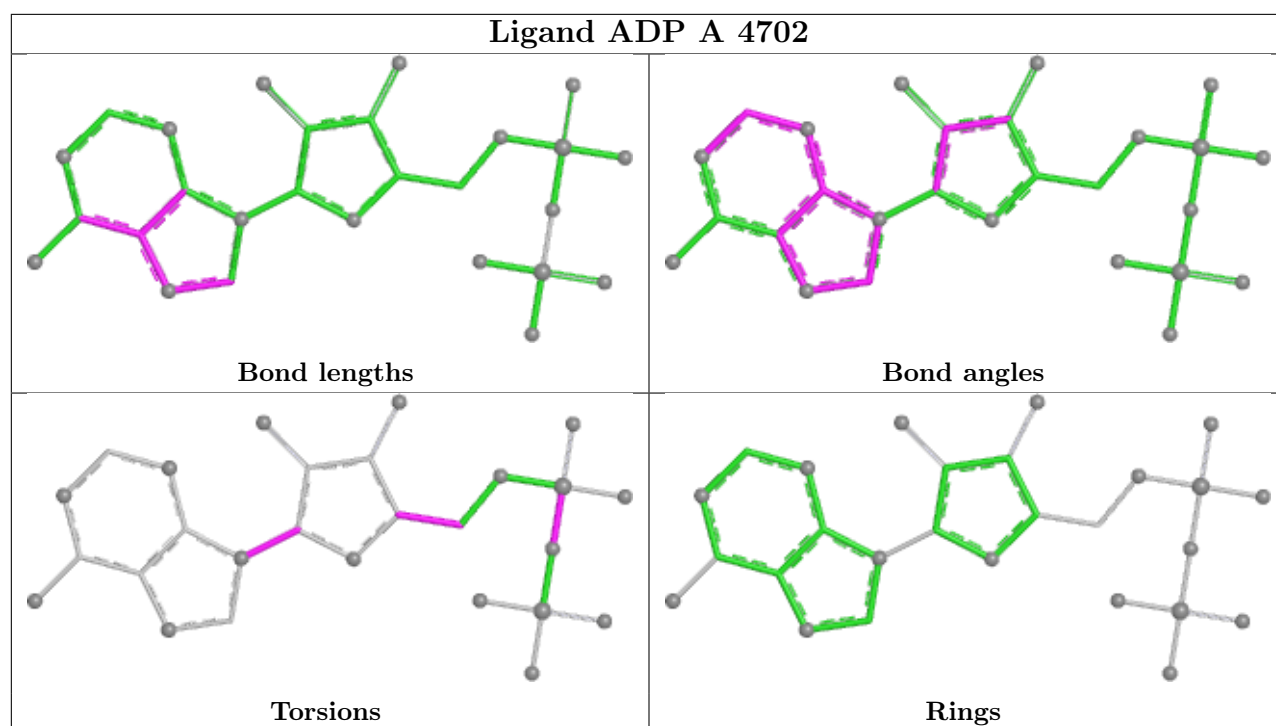
4 monomers are involved in 6 short contacts:

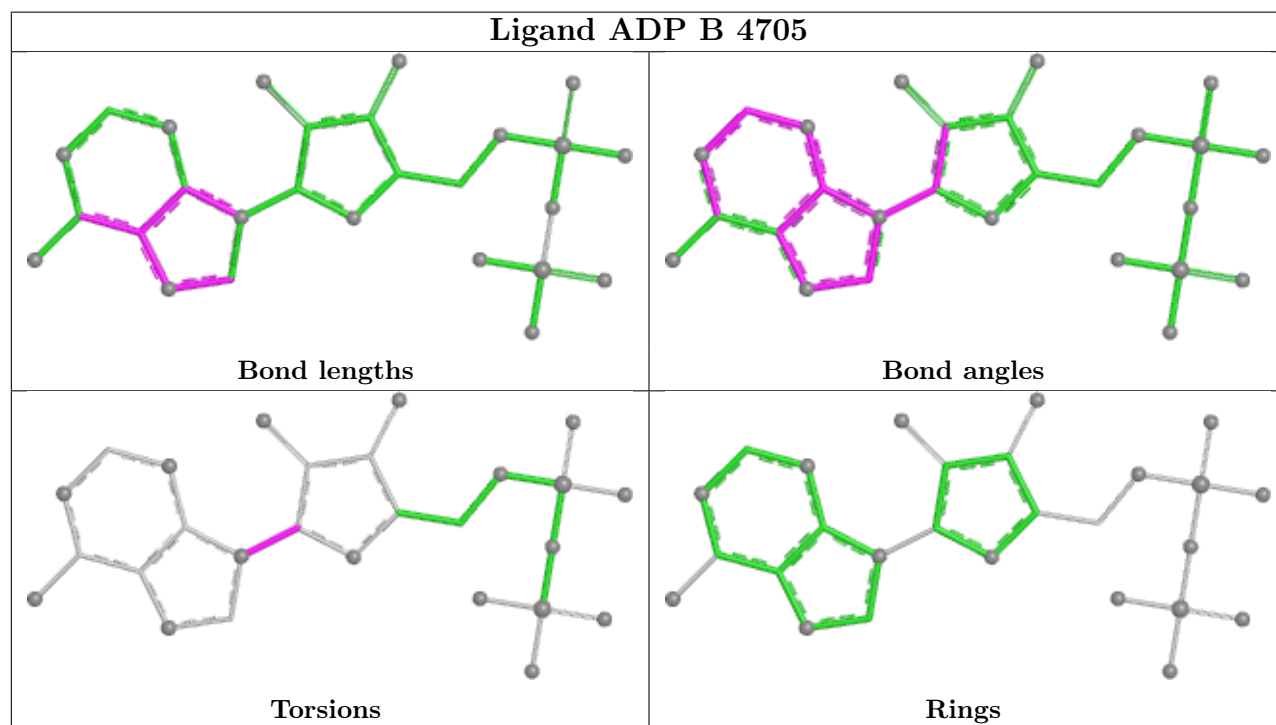
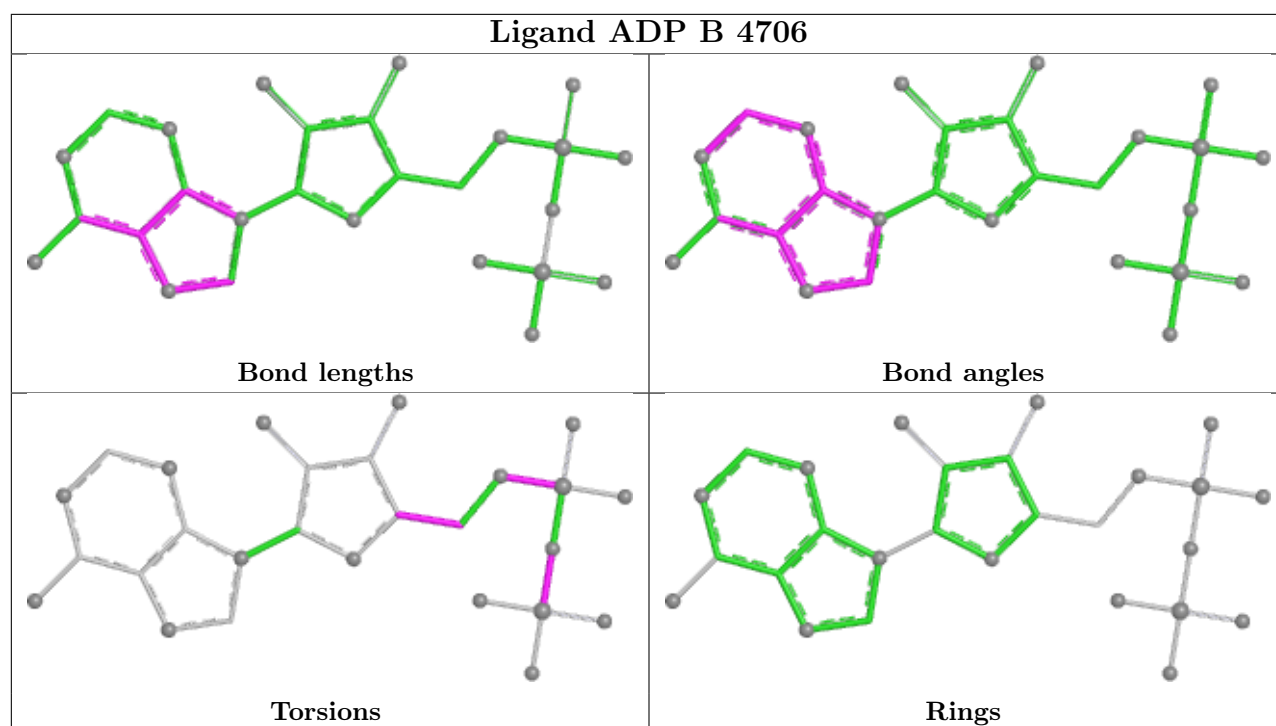
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4706	ADP	1	0
4	A	4701	ATP	1	0
3	B	4706	ADP	2	0
3	B	4705	ADP	2	0

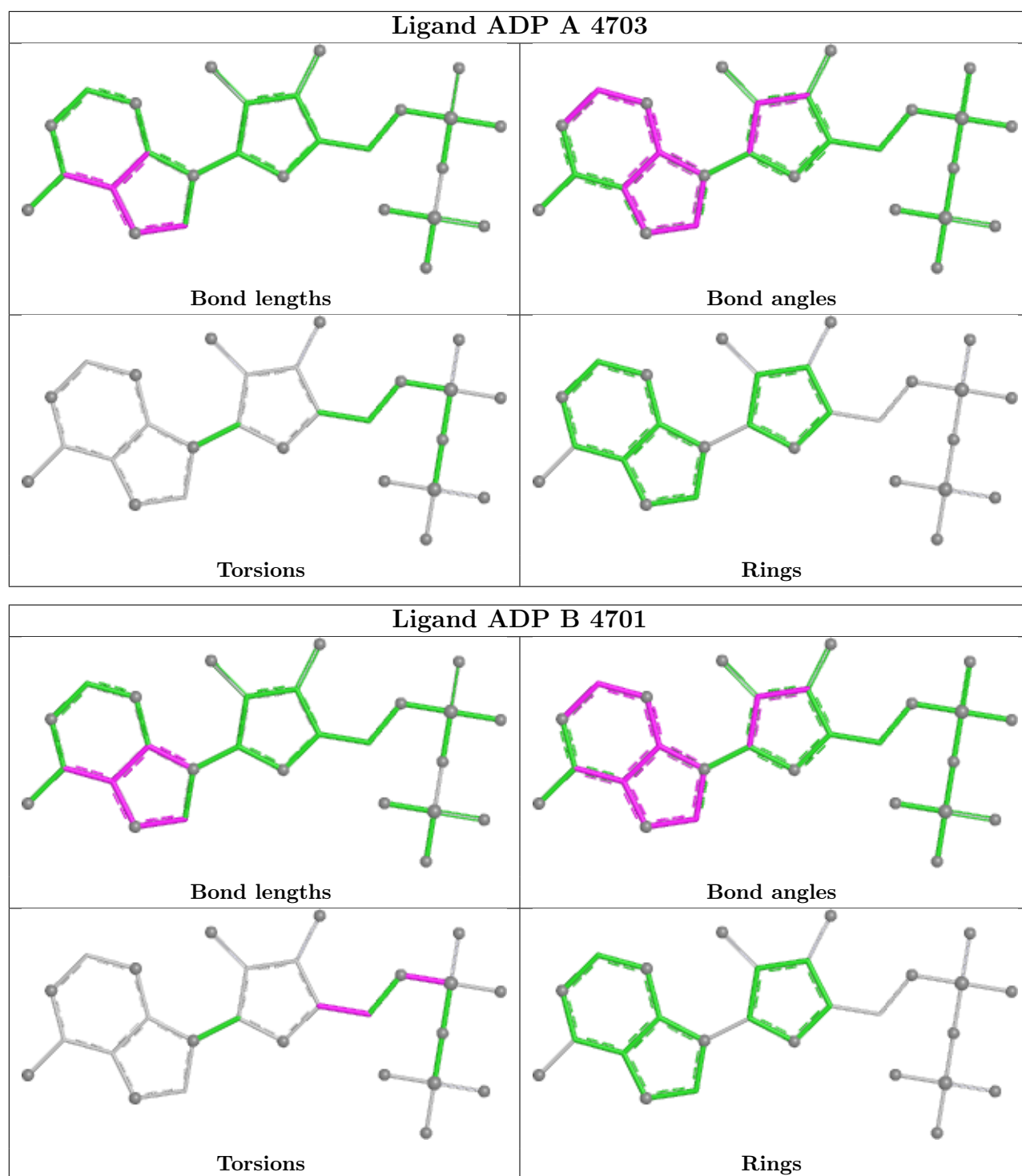
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

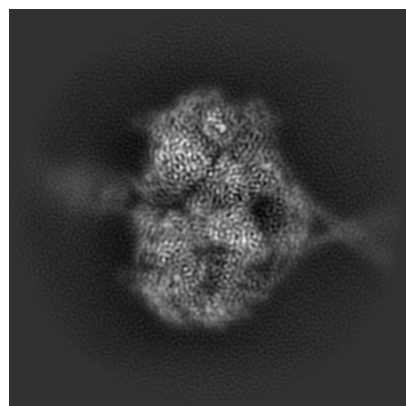
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47342. These allow visual inspection of the internal detail of the map and identification of artifacts.

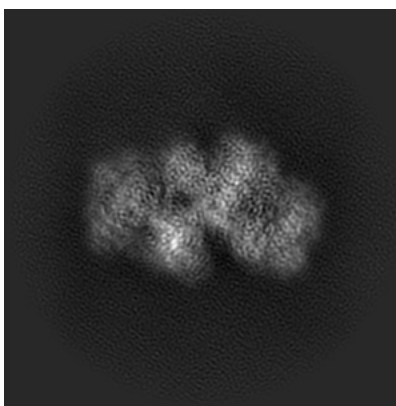
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

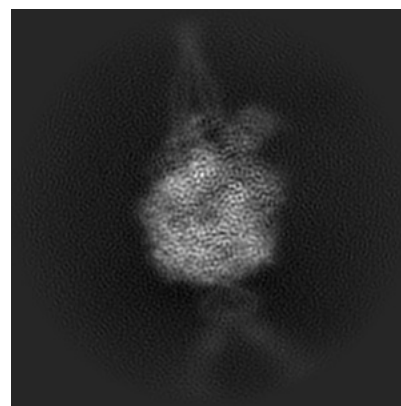
6.1.1 Primary map



X

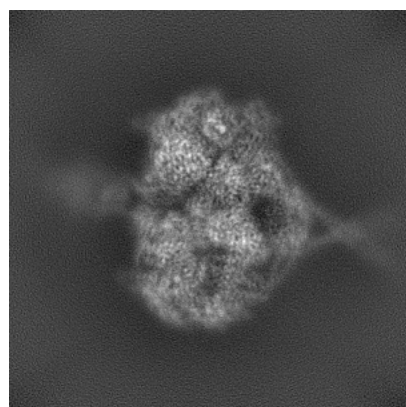


Y

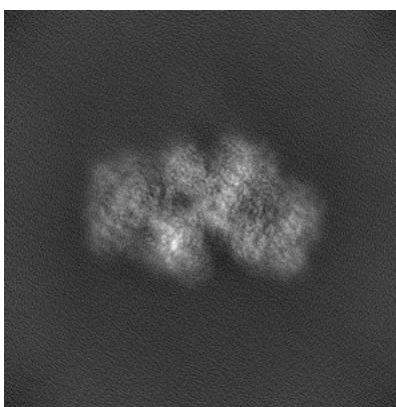


Z

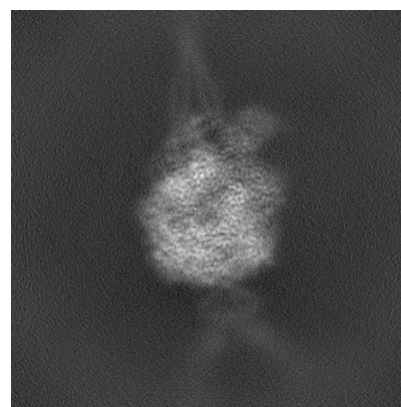
6.1.2 Raw map



X



Y

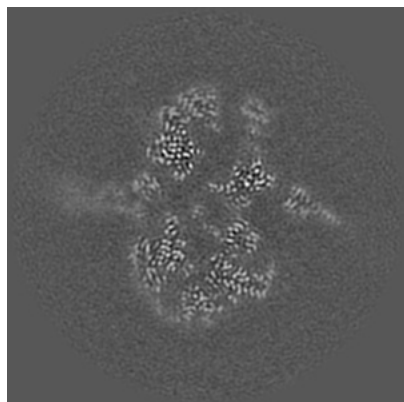


Z

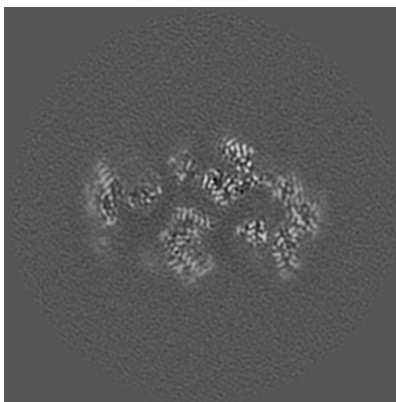
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

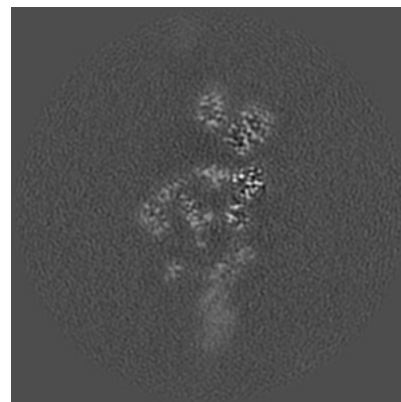
6.2.1 Primary map



X Index: 176

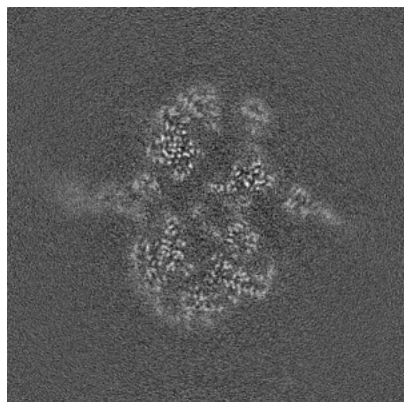


Y Index: 176

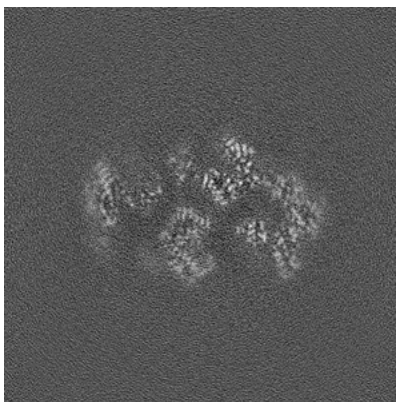


Z Index: 176

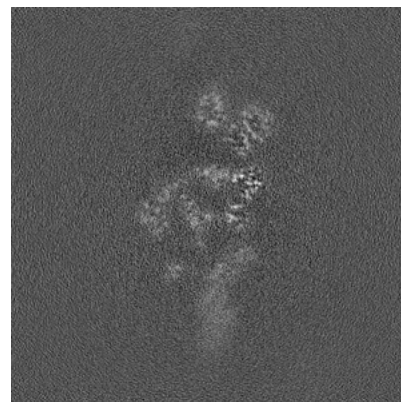
6.2.2 Raw map



X Index: 176



Y Index: 176

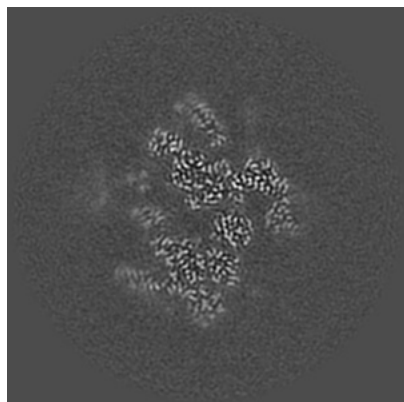


Z Index: 176

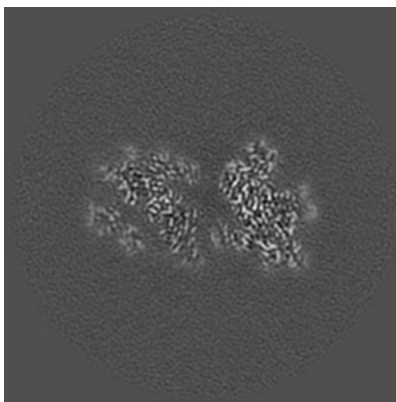
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

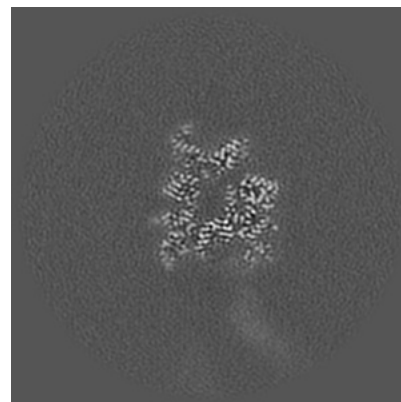
6.3.1 Primary map



X Index: 192

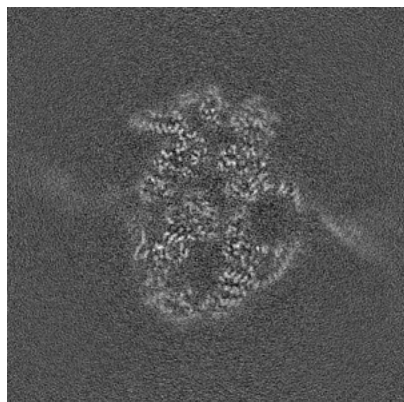


Y Index: 151

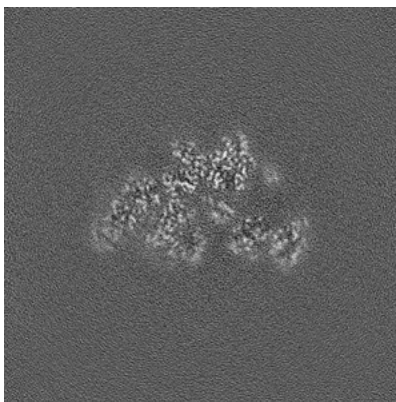


Z Index: 212

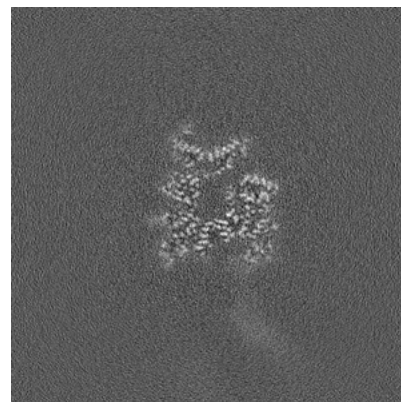
6.3.2 Raw map



X Index: 164



Y Index: 195

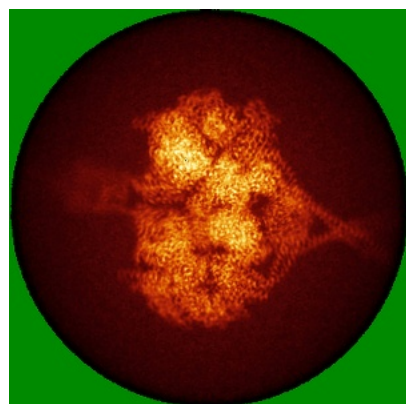


Z Index: 213

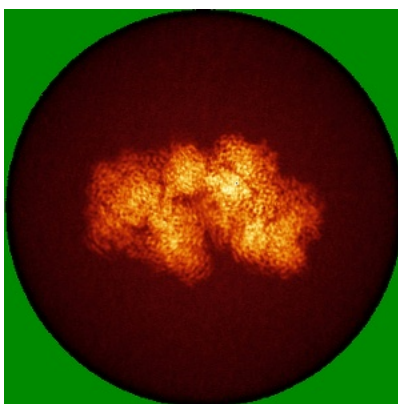
The images above show the largest variance slices of the map in three orthogonal directions.

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

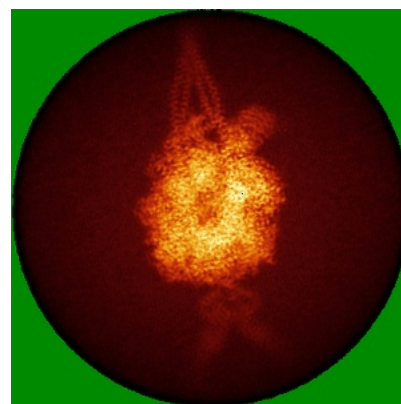
6.4.1 Primary map



X

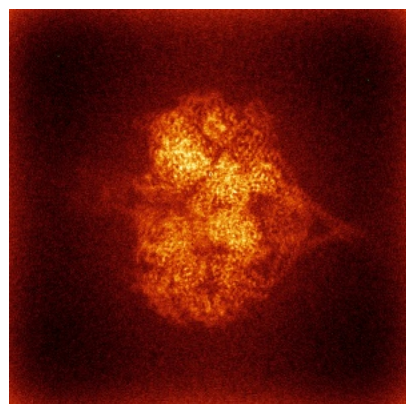


Y

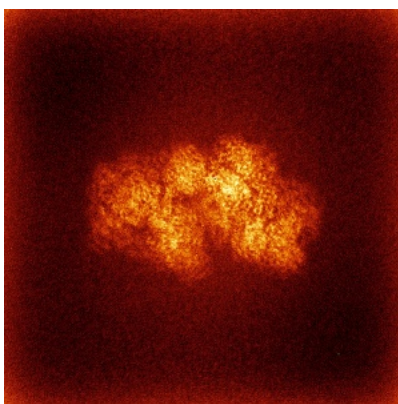


Z

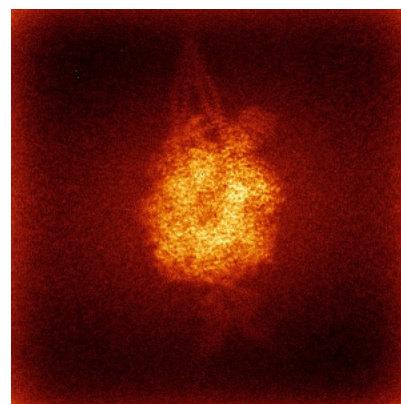
6.4.2 Raw map



X



Y

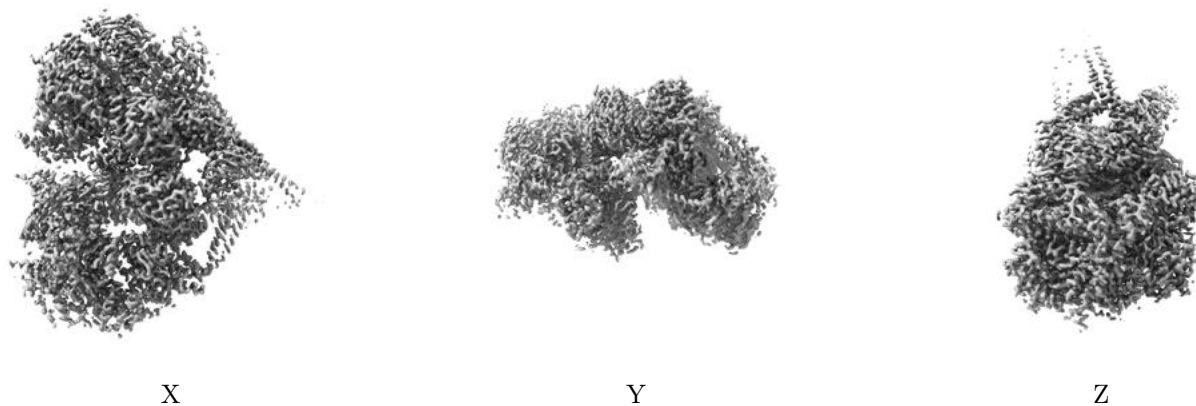


Z

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.

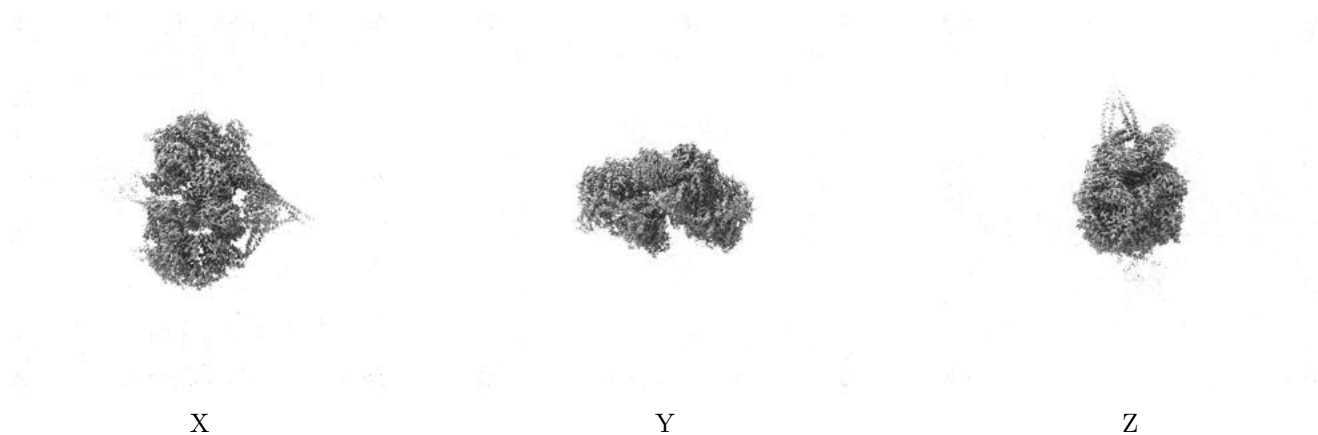
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.224. 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.

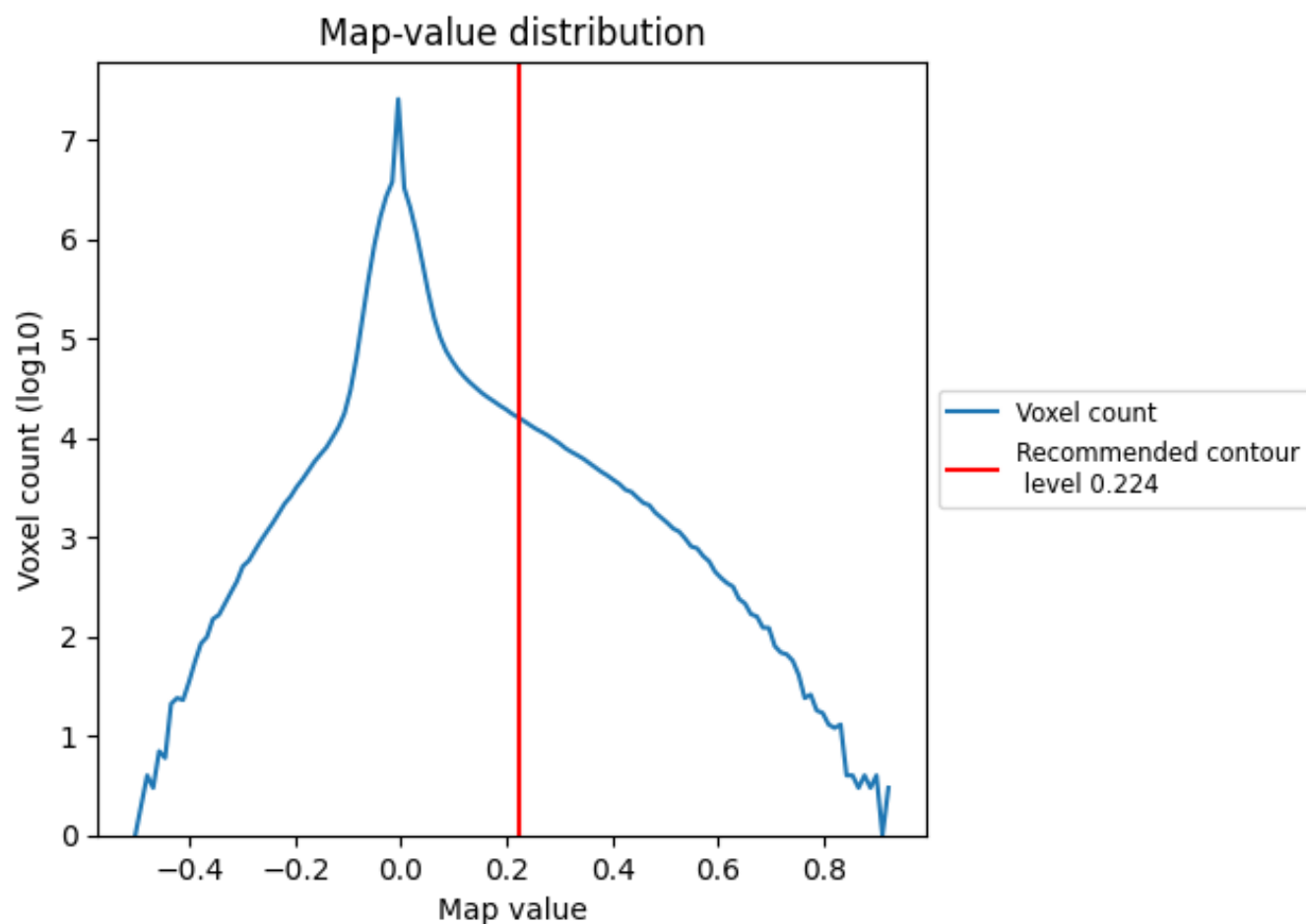
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

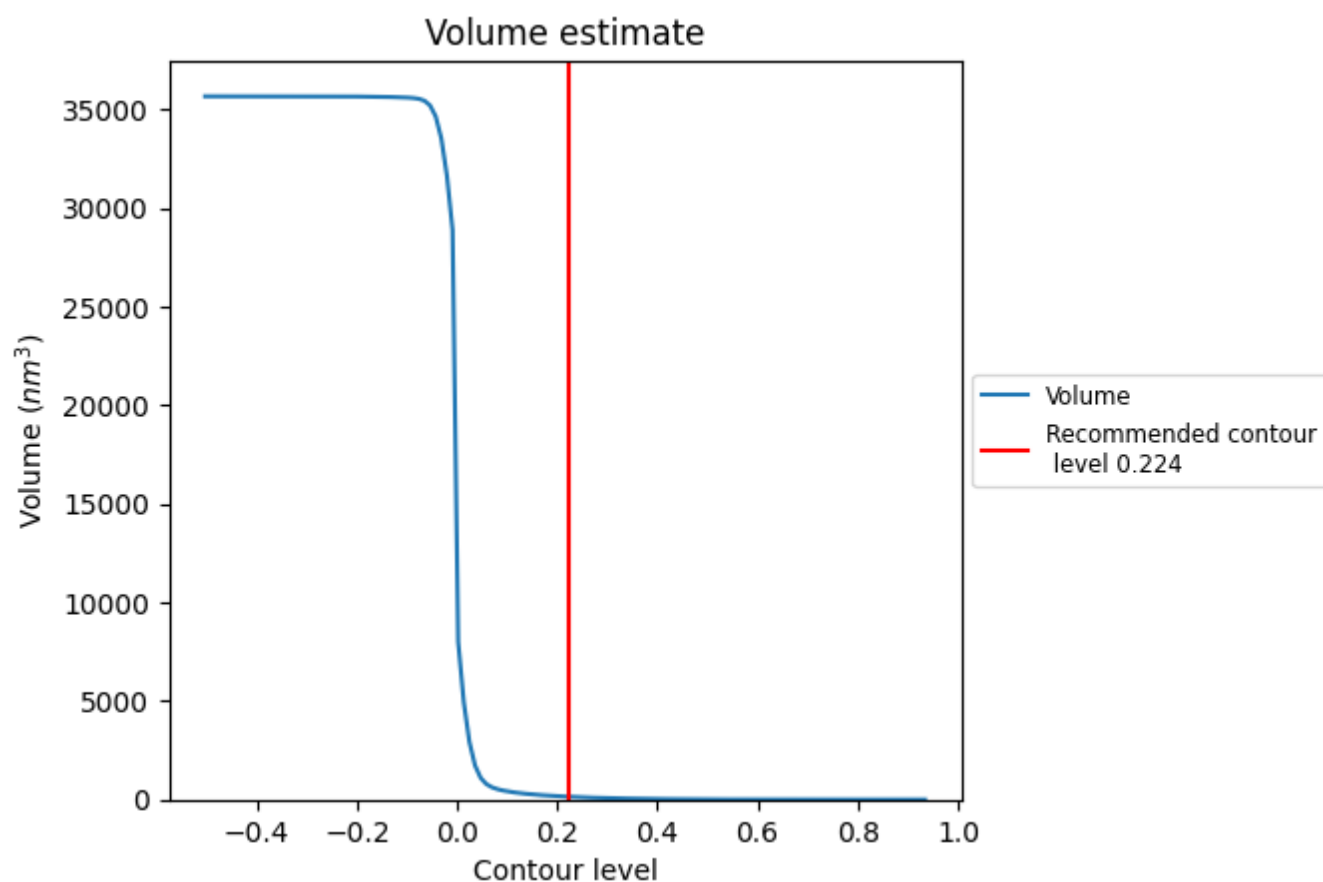
This section contains the results of statistical analysis of the map.

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.

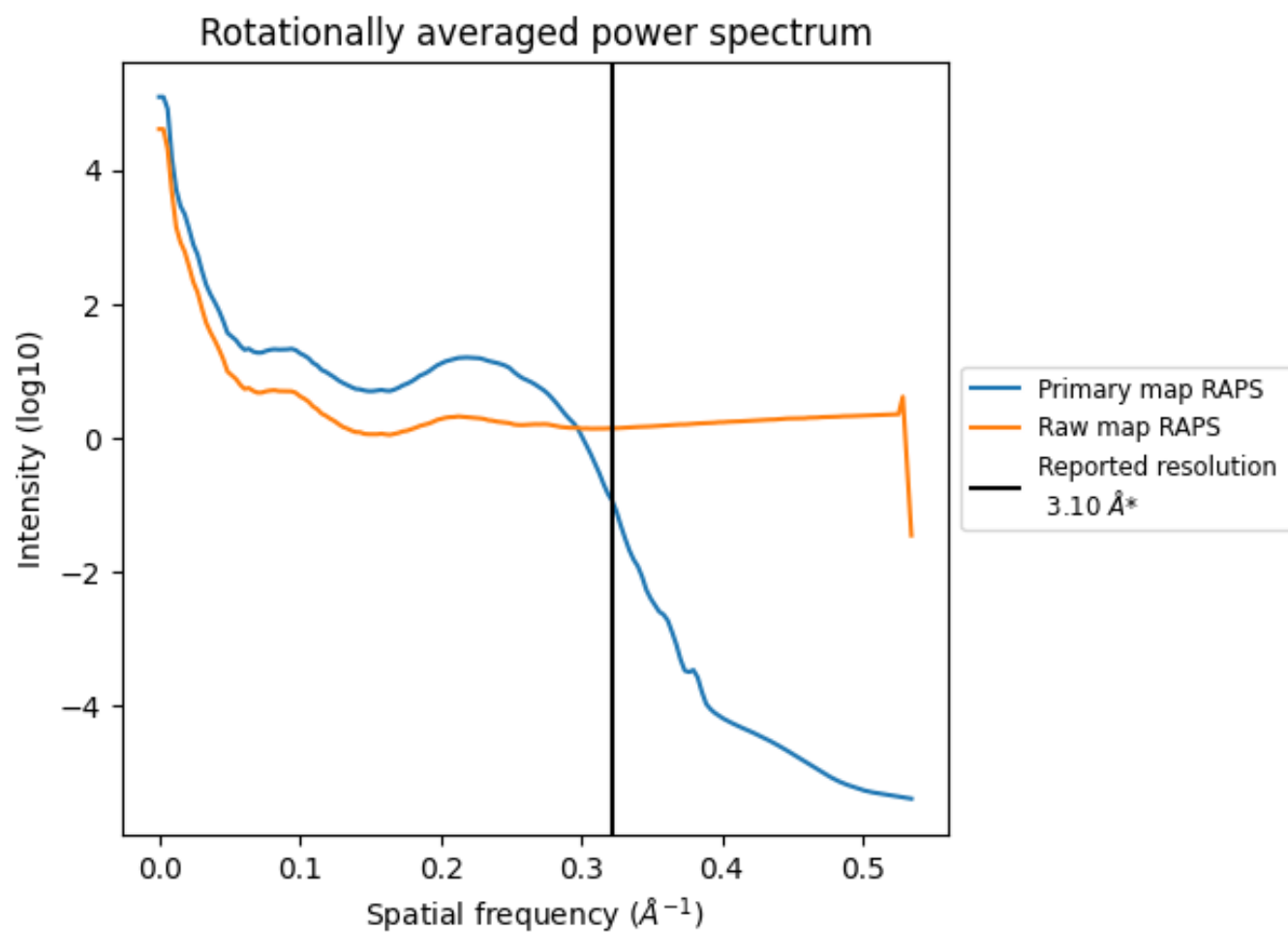
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 142 nm³; this corresponds to an approximate mass of 128 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 [i](#)

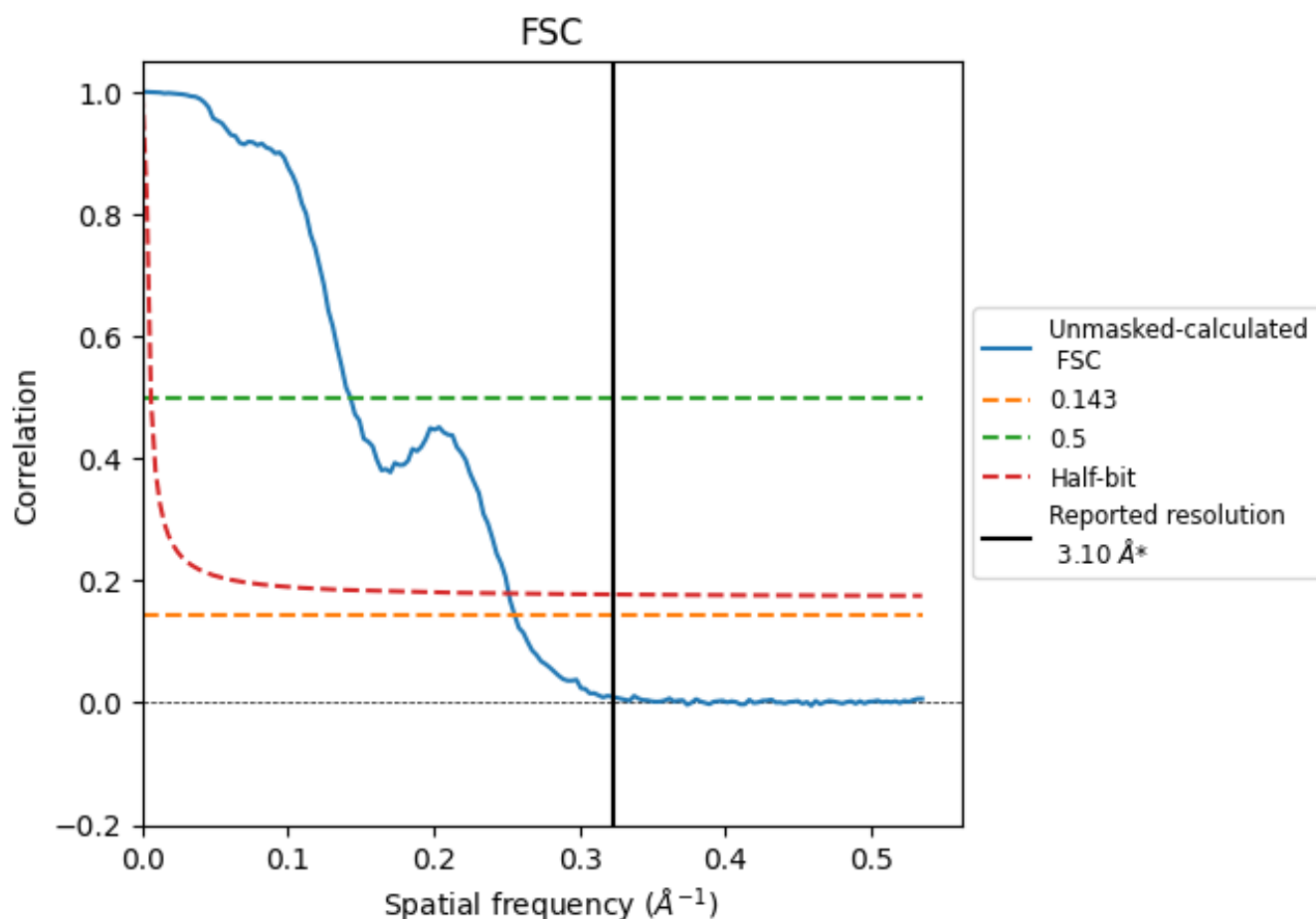


*Reported resolution corresponds to spatial frequency of $0.323 \text{ \AA}^{-1}$

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

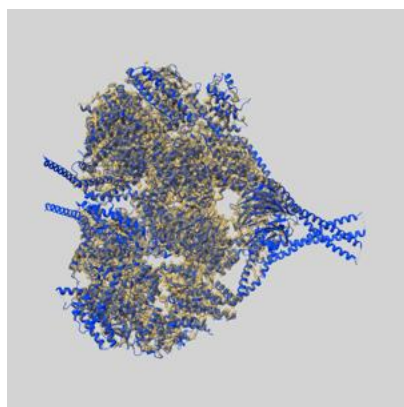
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.92	7.00	3.98

*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 3.92 differs from the reported value 3.1 by more than 10 %

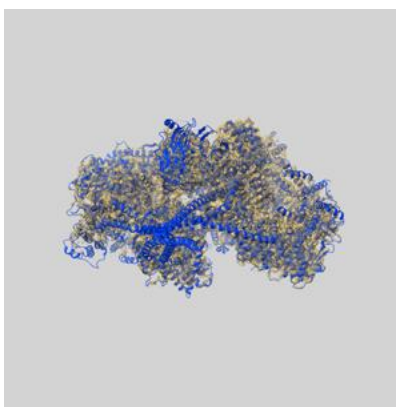
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47342 and PDB model 9DZY. Per-residue inclusion information can be found in section 3 on page 15.

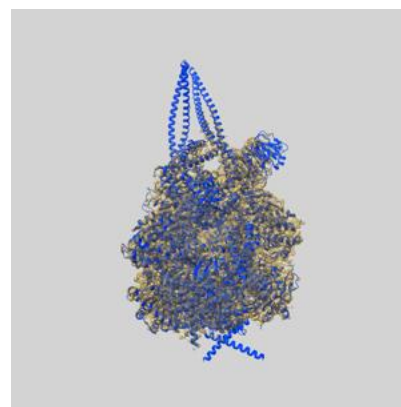
9.1 Map-model overlay [i](#)



X



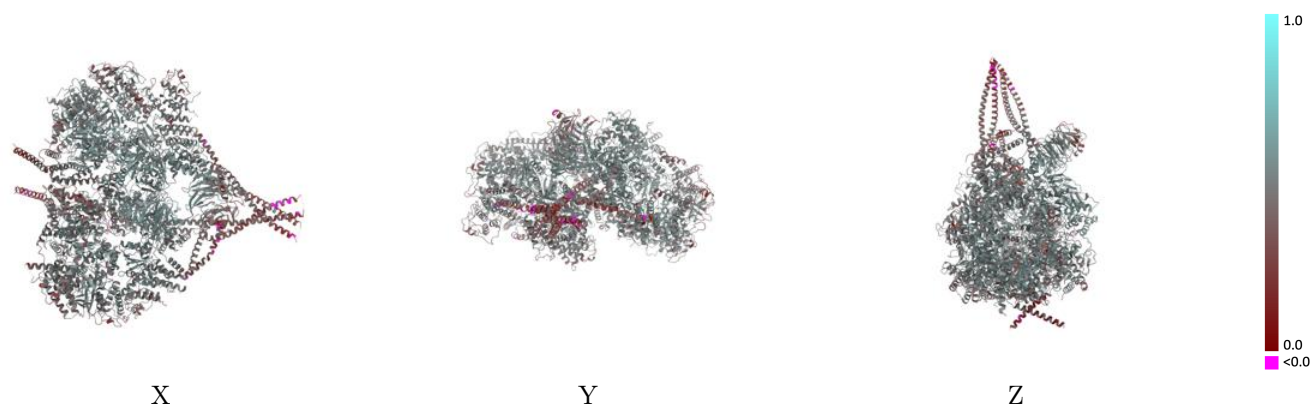
Y



Z

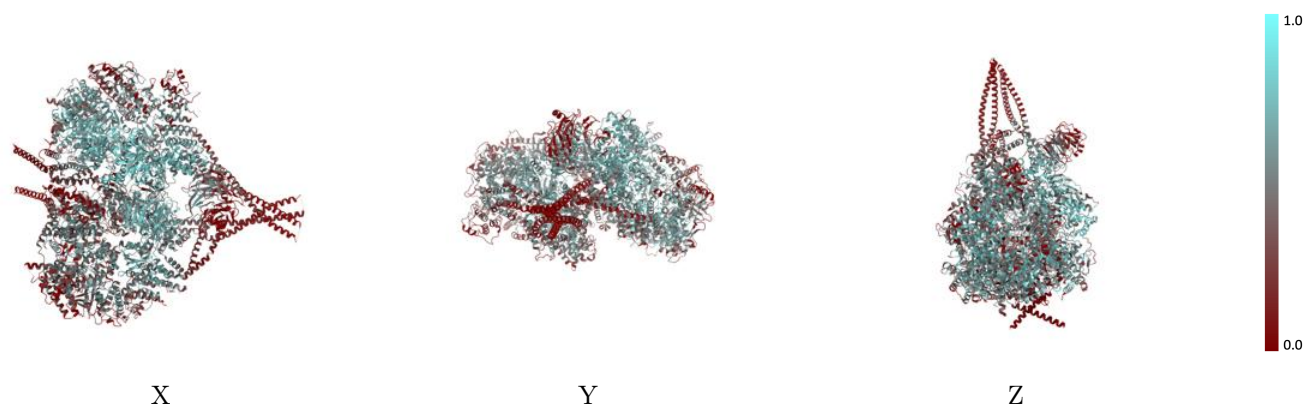
The images above show the 3D surface view of the map at the recommended contour level 0.224 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



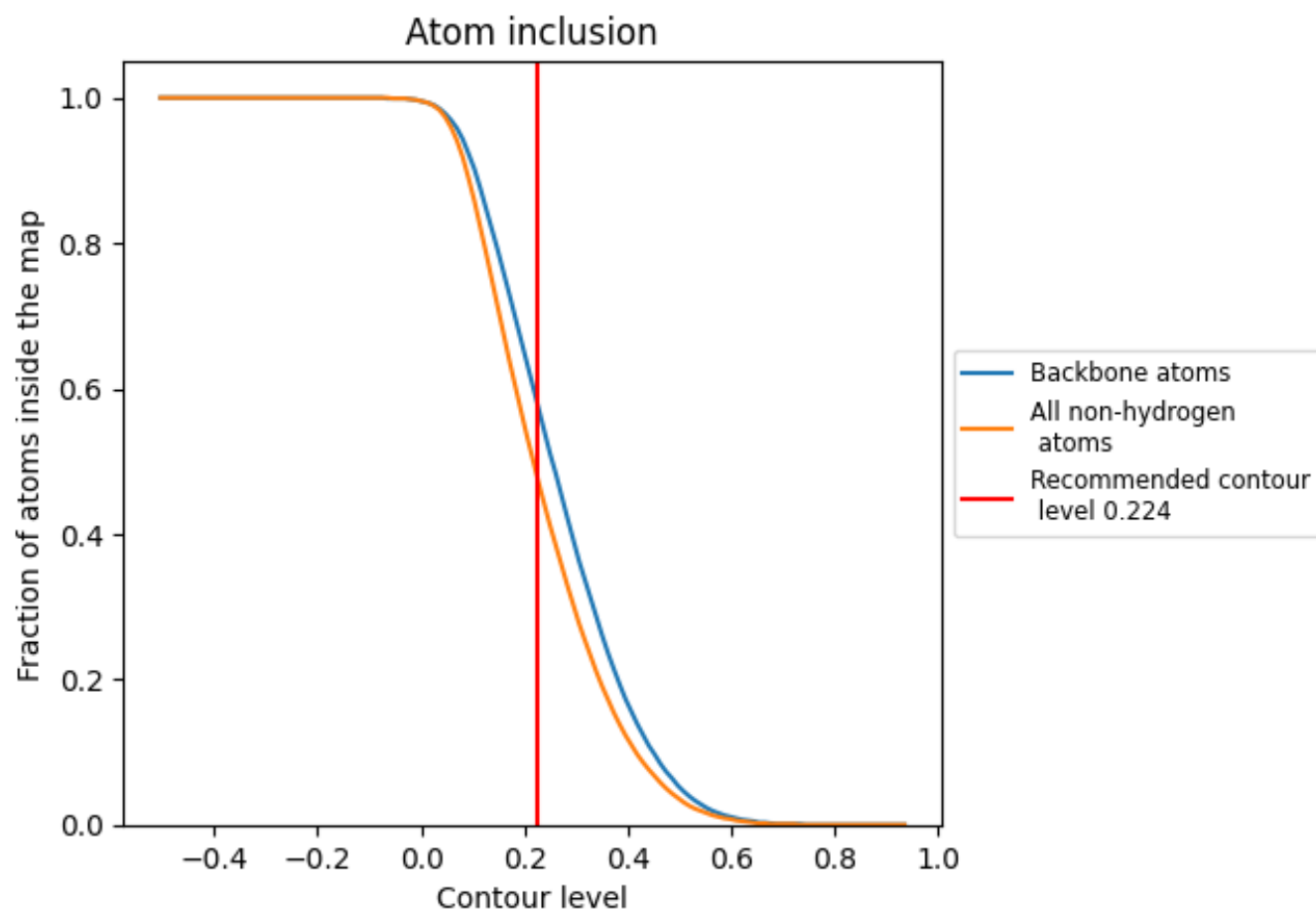
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.224).

9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 48% 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 (0.224) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4800	0.4860
A	0.4150	0.4710
B	0.5470	0.4980
C	0.2550	0.4600
E	0.6630	0.5360

