



## wwPDB EM Validation Summary Report ⓘ

Jun 30, 2025 – 06:28 PM EDT

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](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.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

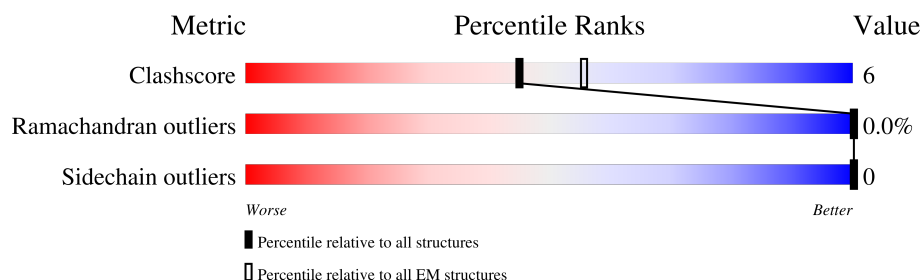
# 1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
1	B	4843	
2	C	411	
2	E	411	

## 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

*Continued on next page...*

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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

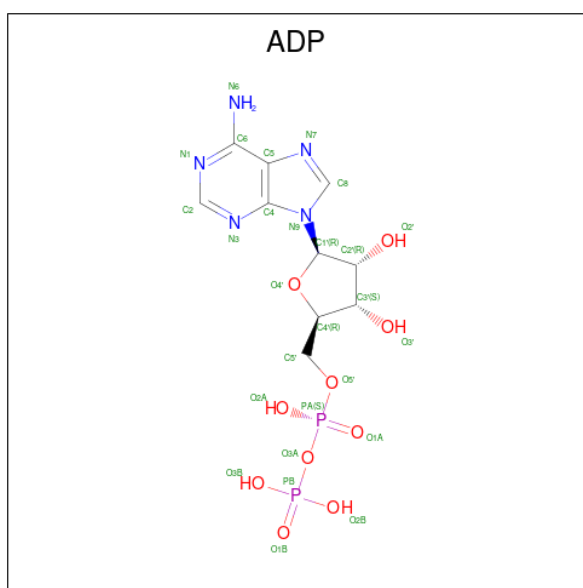
- Molecule 2 is a protein called Platelet-activating factor acetylhydrolase IB subunit beta.

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:

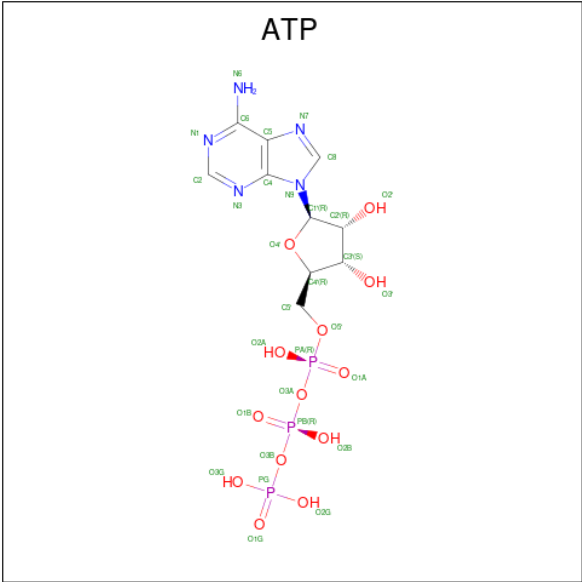
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	GLY	-	expression tag	UNP P43034
E	1	SER	-	expression tag	UNP P43034
C	0	GLY	-	expression tag	UNP P43034
C	1	SER	-	expression tag	UNP P43034

- 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	



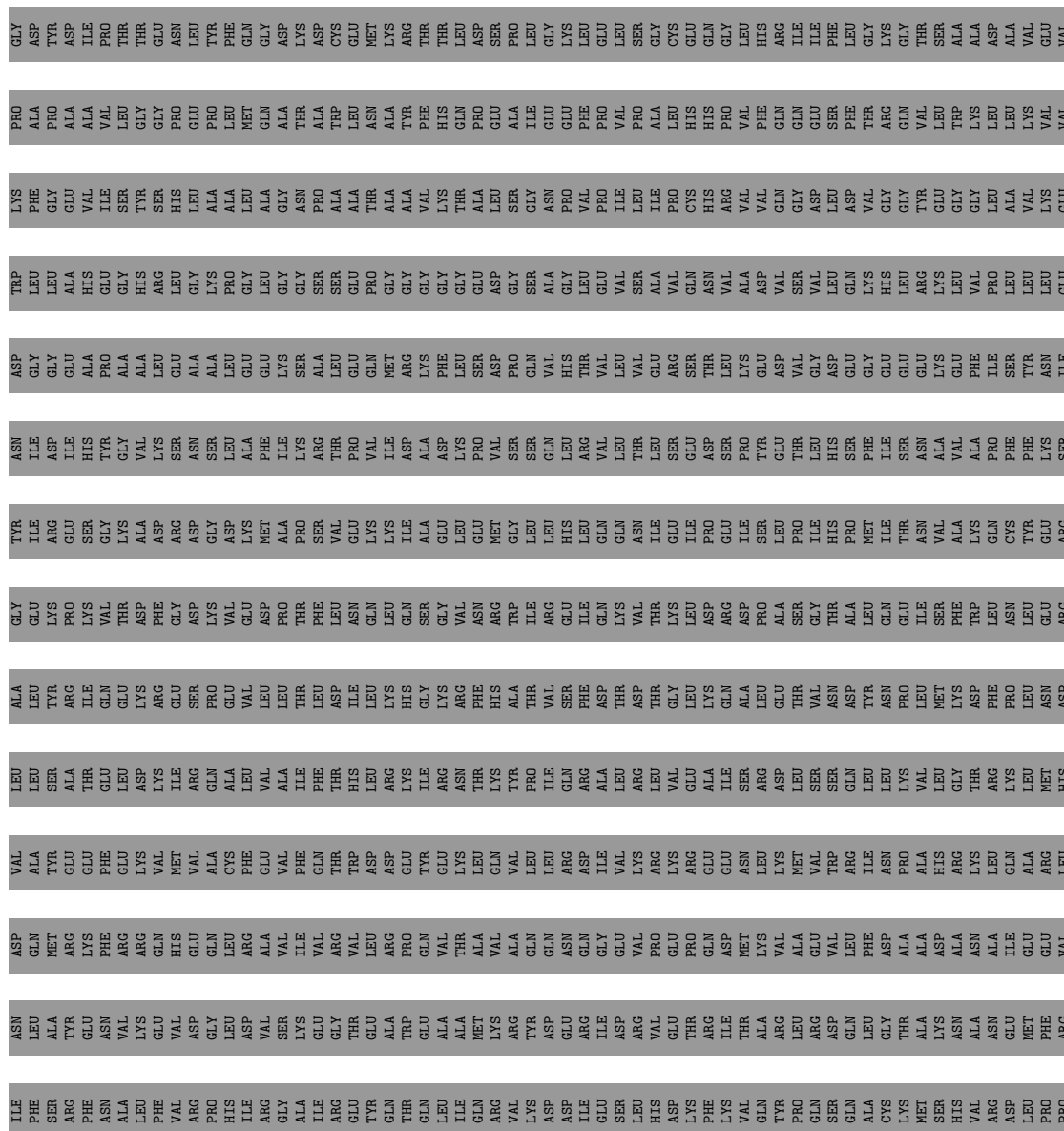




LYS	L3240	D5131	S3002	R2863	L2744	P2590	E2484	GLU	S2231	K2112	LYS	S1835
GLN	K3241	Q3135	G3003	E2864	I2747	L2691	Q2485	ALA	W2234	R2113	THR	F1836
HIS	K3242	P3136	F3004	R2869	N2762	V2592	L2486	ARG	P1996	E2114	SER	E1837
LEU	M3243	P3137	L3005	R2870	N2762	M2603	E2487	ARG	L2238	GLU	ALA	W1838
VAL	V3244	R3140	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
ASN	E3249	R3164	D3024	R2890	F2784	R2614	E2512	GLY	P2256	ASP	ASP	D1847
PRO	A3250	G3165	E3025	E2904	T2785	D2614	E2513	GLY	K2257	GLY	GLY	P1848
PRO	E3251	G3166	K3034	L2905	Q2786	V2617	E2514	GLU	A2258	ILE	GLU	K1849
ALA	K3252	R3167	A3037	D2906	D2787	S2623	E2515	GLU	A2258	ALA	GLU	Q1850
VAL	K3253	V2914	Q3038	N2913	Y2794	S2624	E2516	ALA	D2269	A2128	ILE	T1851
LYS	LYS	E2915	Q3039	E2914	R2797	P2628	R2519	A2409	D2270	E2129	LYS	D1852
LEU	VAL	L2916	E3040	V2915	E2798	K2633	R2520	S2410	P2271	E2130	GLY	Q1856
LEU	ALA	L2916	G3041	L2916	N2799	T2644	R2521	P2411	N2272	N2136	GLY	L1857
GLN	GLN	L2916	L3042	L2920	M2799	P2645	T2522	M2412	T2273	L2137	GLY	M1861
GLN	GLN	L2925	L3042	L2925	R2804	N2646	V2524	M2413	R2274	Q2139	GLY	A1862
GLN	GLN	L2933	D3045	L2933	R2811	G2647	P2525	D2418	L2284	E2143	GLY	M1863
GLN	GLN	L2934	H3047	L2934	L2650	L2650	P2526	T2428	I2288	A2151	GLY	V1880
GLN	GLN	L2935	E3048	L2935	L2655	L2655	P2527	S2429	D2289	E2152	GLY	Q1881
GLN	GLN	K2943	E3049	K2943	E2665	N2667	A2528	M2430	R2298	D2163	GLY	T1882
GLN	GLN	V2958	T3067	V2958	E2667	L2668	A2529	L2437	F2303	D2167	GLY	F1883
GLN	GLN	T2961	S3071	T2961	L2671	L2671	P2530	E2438	V2307	G2168	GLY	L1884
GLN	GLN	H2964	S3072	H2964	W2825	W2825	L2541	Q2442	E2310	Q2169	GLY	Q1894
GLN	GLN	R2965	G3074	R2965	V2679	V2679	T2541	L2443	W2312	Q2170	GLY	E1914
GLN	GLN	K2966	L3075	K2966	Q2834	Q2834	E2544	E2444	E2311	V2168	GLY	L1928
GLN	GLN	T2967	L3075	T2967	D2835	D2835	W2545	H2445	N2316	L2085	GLY	V1929
GLN	GLN	T2968	A3080	T2968	R2836	R2836	W2546	I2446	N2316	A2066	GLY	F1930
GLN	GLN	G2969	T3081	G2969	D2697	D2697	S2546	L2452	D2321	K2068	GLY	N1931
GLN	GLN	D2973	L3091	D2973	K2702	K2702	P2553	L2455	T2326	G2173	GLY	V1946
GLN	GLN	E2974	F3094	E2974	L2703	L2703	Q2554	Q2464	N2329	E2180	GLY	Q1950
GLN	GLN	D2975	F3094	D2975	E2704	E2704	Q2555	V2469	E2331	E2181	GLY	R1966
GLN	GLN	L2976	W3097	L2976	C2712	C2712	E2556	A2470	R2332	K2184	GLY	M1967
GLN	GLN	R2982	K3112	R2982	K2721	K2721	H2560	Q2471	L2335	D2195	GLY	L1968
GLN	GLN	E2988	M3113	E2988	R2729	R2729	A2563	Y2472	S2334	G2196	GLY	Q1974
GLN	GLN	K2989	E3116	K2989	H2730	H2730	V2567	N2475	E2331	E2197	GLY	E1980
GLN	GLN	L2993	N3119	L2993	V2731	V2731	V2568	P2476	R2332	M2202	GLY	A1981
GLN	GLN	N2998	P3123	N2998	V2732	V2732	V2568	D2478	L2335	E2205	GLY	E1984
GLN	GLN	V2999	D3124	V2999	V2733	V2733	V2568	F2479	P2336	E2205	GLY	H1985
GLN	GLN	L3000	Y3125	L3000	Y2735	Y2735	V2582	P2481	E2388	E2212	GLY	S1986
GLN	GLN	D3001	K3126	D3001	D2862	D2862	V2582	Q2482	E2389	Q2216	GLY	N1987
GLN	GLN	K3239	P3127	K3239	D2862	D2862	V2582	Q2482	E2389	I2216	GLY	PRO
GLN	GLN	K3239	V3128	K3239	D2862	D2862	V2582	Q2482	E2389	I2216	GLY	ASN
GLN	GLN	K3239	V3128	K3239	D2862	D2862	V2582	Q2482	E2389	I2216	GLY	TYR
GLN	GLN	K3239	V3128	K3239	D2862	D2862	V2582	Q2482	E2389	I2216	GLY	ASP



- Molecule 1: Cytoplasmic dynein 1 heavy chain 1

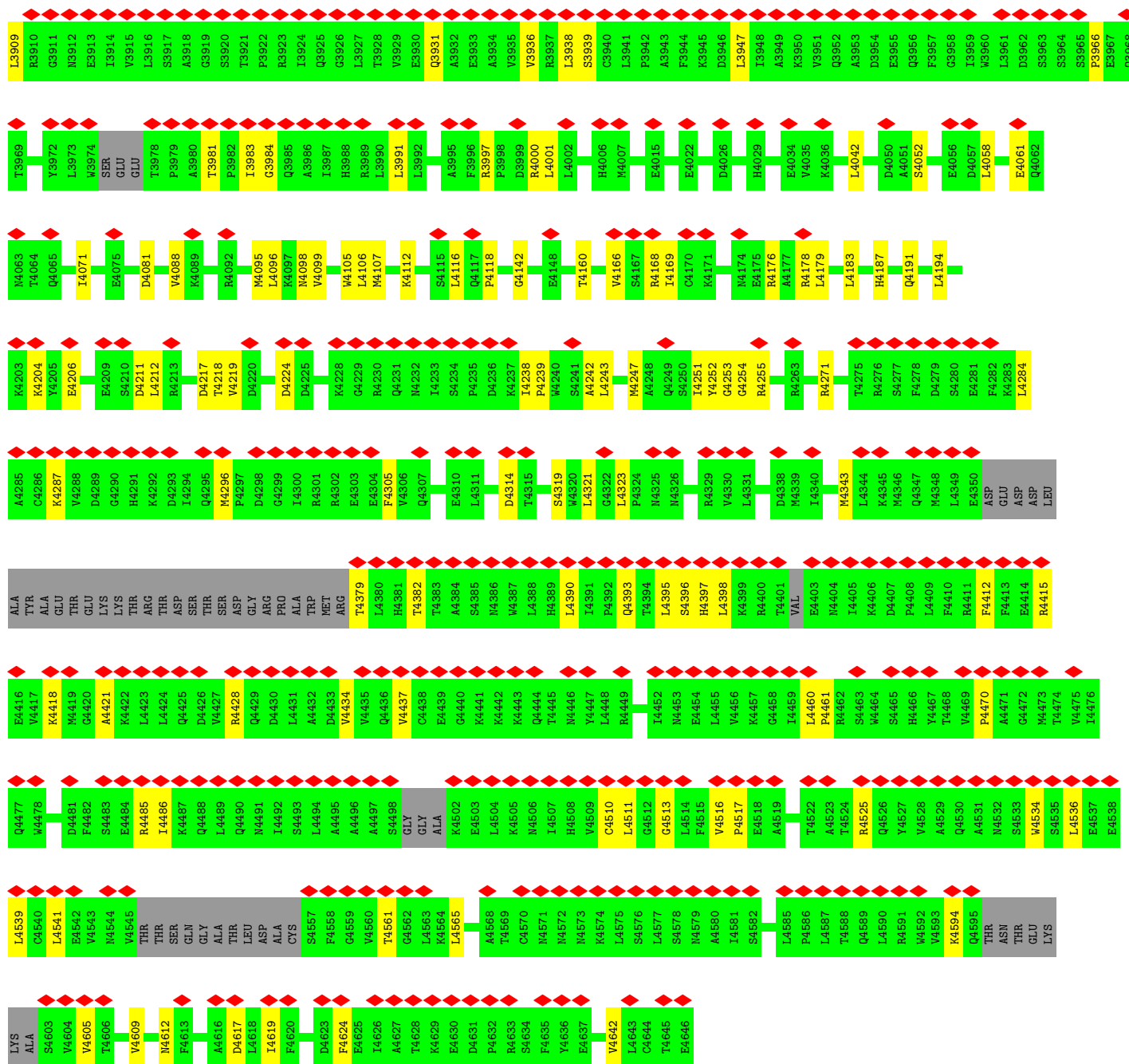




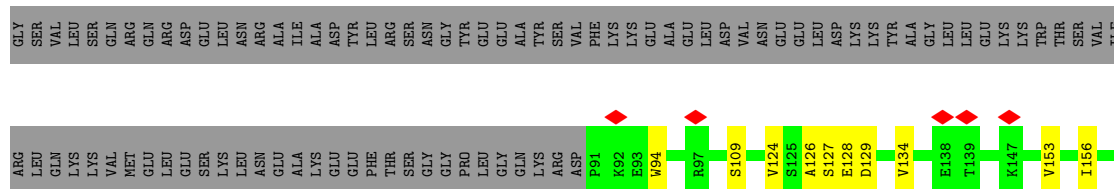
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E1799	Q1800	R1804	R1805	R1806	K1807	L1808	E1809	T1813	E1814	R1819	D1820	V1821	T1822	R1823	S1824	L1825	I1826	K1827	S1828	K1829	I1830	D1831	N1832	A1833	K1834	S1835	F1836	E1837	W1838	L1839	Y1845	F1846	D1847	P1848	K1849	Q1850	T1851	D1852	V1853	L1854	Q1855	Q1856	L1857	S1858	N1863	A1864	K1865	Y1868	V1875	Q1876	D1877	K1878				
L1879	V1880	T1881	P1882	P1883	L1884	T1885	D1886	R1887	C1888	M1892	R1899	P1904	E1914	K1917	D1933	E1934	Q1939	A1940	M1941	Q1950	V1951	G1952	D1958	M1961	R1962	L1963	E1964	E1965	R1966	E1980	R1983	E1984	H1985	S1986	N1987	PRO	ASN	TYR	ASP	LYS	THR	SER	ALA	P1996	I1997	K2004										
Q2005	V2006	K2007	D2011	T2016	T2017	M2018	Y2022	A2023	N2031	K2043	P2044	D2045	R2046	Q2047	L2048	A2050	R2060	T2061	A2062	E2063	V2064	L2065	A2066	N2067	K2068	L2069	S2070	P2071	F2072	F2073	K2074	L2075	C2076	D2077	E2078	Q2079	L2080	S2081	D2087	S2095	V2096	L2097	V2098	S2099	N2102											
V2103	K2104	R2105	E2106	R2107	I2108	Q2109	K2110	I2111	K2112	R2113	E2114	LYS	GLU	GLU	ARG	GLY	GLU	ALA	VAL	ASP	GLU	GLY	ILE	A2128	E2129	N2130	L2131	P2132	E2133	Q2134	E2135	I2136	L2137	I2138	Q2139	S2140	A2151	E2152	D2153	I2154	L2157	F2158	S2159	L2160	L2161	S2162	D2163	V2164	F2165	P2166	G2167	V2168	Q2169	I2170	H2171	R2172
G2173	E2174	M2175	T2176	A2177	L2178	R2179	E2180	E2181	L2182	K2183	K2184	Q2187	L2187	L2188	M2189	G2194	D2195	G2196	E2197	E2198	V2199	V2204	Y2211	I2216	N2217	H2218	W2221	G2227	S2228	S2231	W2234	L2237	L2238	K2239	E2242	R2243	L2244	E2245	E2248	G2249	D2255	P2256	K2257	D2262	D2269											
P2270	N2271	T2272	R2273	E2274	T2275	D2276	D2277	G2278	H2282	L2283	R2285	K2286	L2287	L2288	D2289	R2292	G2293	E2294	L2295	Q2296	K2297	R2298	D2304	G2305	D2306	V2307	D2308	P2309	E2310	W2311	G2312	N2316	D2320	D2321	N2322	K2323	L2324	N2329	G2330	E2331	R2332	L2333	S2334	L2335	P2336	F2343	E2344	V2345	Y2346	D2347	T2348	L2348				
K2349	A2354	T2355	V2356	S2357	R2358	M2361	S2365	L2379	L2382	T2385	P2386	L2387	D2388	E2389	D2389	R2292	G2293	E2294	L2295	Q2296	K2297	R2298	D2304	G2305	D2306	V2307	D2308	P2309	E2310	W2311	G2312	N2316	D2320	D2321	N2322	K2323	L2324	N2329	G2330	E2331	R2332	L2333	S2334	L2335	P2336	F2343	E2344	V2345	Y2426	T2427	T2428	S2429				
N2430	G2431	L2432	K2435	E2438	F2441	Q2442	L2443	E2444	H2445	L2446	M2447	D2448	L2452	R2453	M2461	A2465	C2466	N2467	R2468	V2469	A2470	Q2471	T2472	N2473	A2474	N2475	H2476	P2477	D2478	F2479	P2480	M2481	Q2482	L2483	E2484	Q2485	L2486	E2487	R2488	Q2491	R2492	V2495	Y2496	A2497	L2498	S2503	G2504	D2505	S2506	R2507						
L2508	K2509	M2510	R2511	A2512	E2513	L2514	G2515	E2516	Y2517	L2518	R2519	R2520	L2521	T2522	T2523	V2524	P2525	L2526	P2527	T2528	A2529	P2530	N2531	L2532	P2533	L2534	L2535	V2539	S2540	L2541	S2542	G2543	E2544	W2545	Q2549	A2550	K2551	P2552	Q2554	L2555	E2556	V2557	E2558	T2559	H2560	K2561	V2562	A2563	A2564	P2565	D2566	V2567	T2571	L2572	D2573	
T2574	H2577	E2578	L2581	Y2582	T2583	P2590	L2591	V2592	P2596	P2597	G2598	K2601	T2602	V2603	F2606	L2609	R2610	A2611	L2612	P2613	D2614	M2615	E2616	V2617	V2618	Q2619	F2622	S2623	F2635	D2636	H2637	Y2641	R2642	R2643	T2644	P2645	N2646	G2647	L2650	V2653	Q2654	L2655	G2656	T2657	L2661											
E2665	L2668	P2669	D2670	Q2677	L2680	R2694	D2697	E2704	G2710	G2719	R2720	K2721	R2726	R2729	H2730	V2731	V2736	G2740	P2741	A2742	S2743	L2744	T2745	Q2746	G2749	T2750	F2751	N2752	R2753	A2754	M2755	L2756	R2757	L2758	L2759	P2760	S2761	L2762	R2763	T2764	L2765	D2766	E2767	P2768	A2772											
E2782	E2783	D2787	D2788	D2789	D2790	D2791	S2795	R2801	R2804	G2805	E2808	A2809	L2810	R2811	L2812	L2813	E2814	T2815	L2816	P2817	V2818	E2819	G2820	E2828	R2831	R2836	E2839	D2840	E2841	R2844	D2847	E2848	D2851	L2855	K2856	L2857	P2858	P2859	N2860	L2861	D2862	R2863	K2864	K2865	A2866											

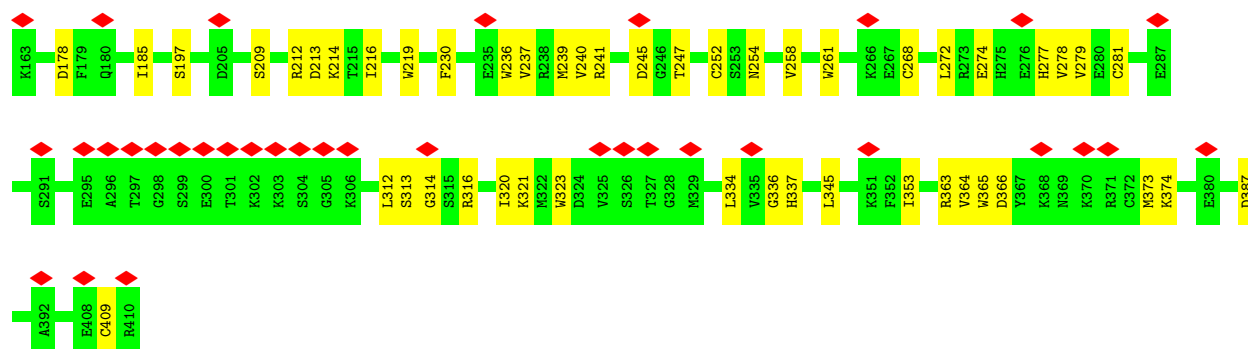




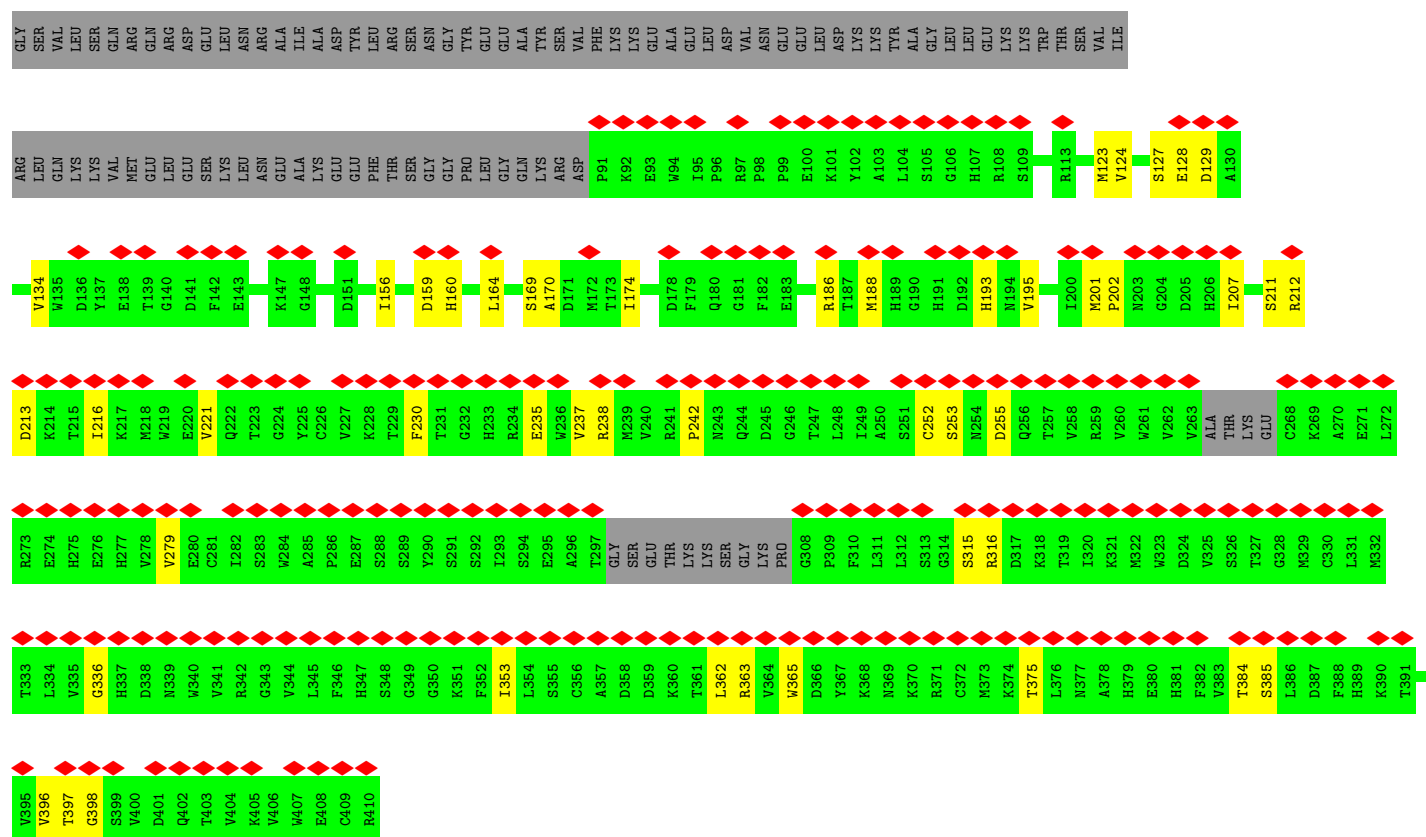


• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta





• 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: MG, ADP, ATP

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

*Continued on next page...*

*Continued from previous page...*

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	24,29,29	0.88	0	29,45,45	1.21	2 (6%)
3	ADP	B	4701	-	24,29,29	0.83	0	29,45,45	1.19	2 (6%)
3	ADP	A	4703	-	24,29,29	0.87	0	29,45,45	1.18	2 (6%)
4	ATP	A	4701	-	28,33,33	0.77	0	34,52,52	0.62	1 (2%)
3	ADP	A	4702	-	24,29,29	0.88	0	29,45,45	1.23	2 (6%)
3	ADP	B	4705	-	24,29,29	0.83	0	29,45,45	1.29	2 (6%)
4	ATP	B	4702	5	28,33,33	0.80	0	34,52,52	0.65	1 (2%)
3	ADP	B	4706	5	24,29,29	0.87	0	29,45,45	1.23	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	4706	5	-	2/12/32/32	0/3/3/3
3	ADP	B	4701	-	-	3/12/32/32	0/3/3/3
3	ADP	A	4703	-	-	0/12/32/32	0/3/3/3
4	ATP	A	4701	-	-	2/18/38/38	0/3/3/3
3	ADP	A	4702	-	-	2/12/32/32	0/3/3/3
3	ADP	B	4705	-	-	0/12/32/32	0/3/3/3
4	ATP	B	4702	5	-	3/18/38/38	0/3/3/3
3	ADP	B	4706	5	-	6/12/32/32	0/3/3/3

There are no bond length outliers.

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



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4705	ADP	N3-C2-N1	-4.09	123.12	128.67
3	A	4702	ADP	N3-C2-N1	-3.91	123.37	128.67
3	B	4706	ADP	N3-C2-N1	-3.75	123.58	128.67
3	A	4706	ADP	N3-C2-N1	-3.67	123.69	128.67
3	B	4701	ADP	N3-C2-N1	-3.64	123.73	128.67

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

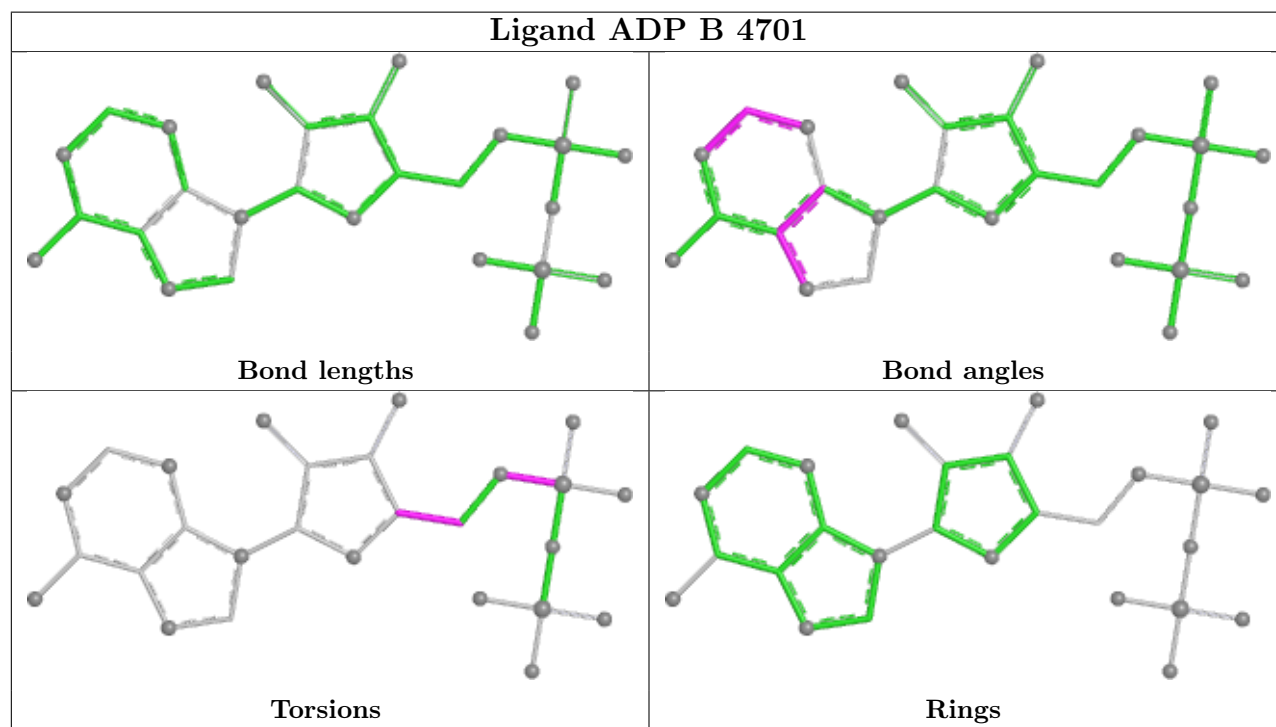
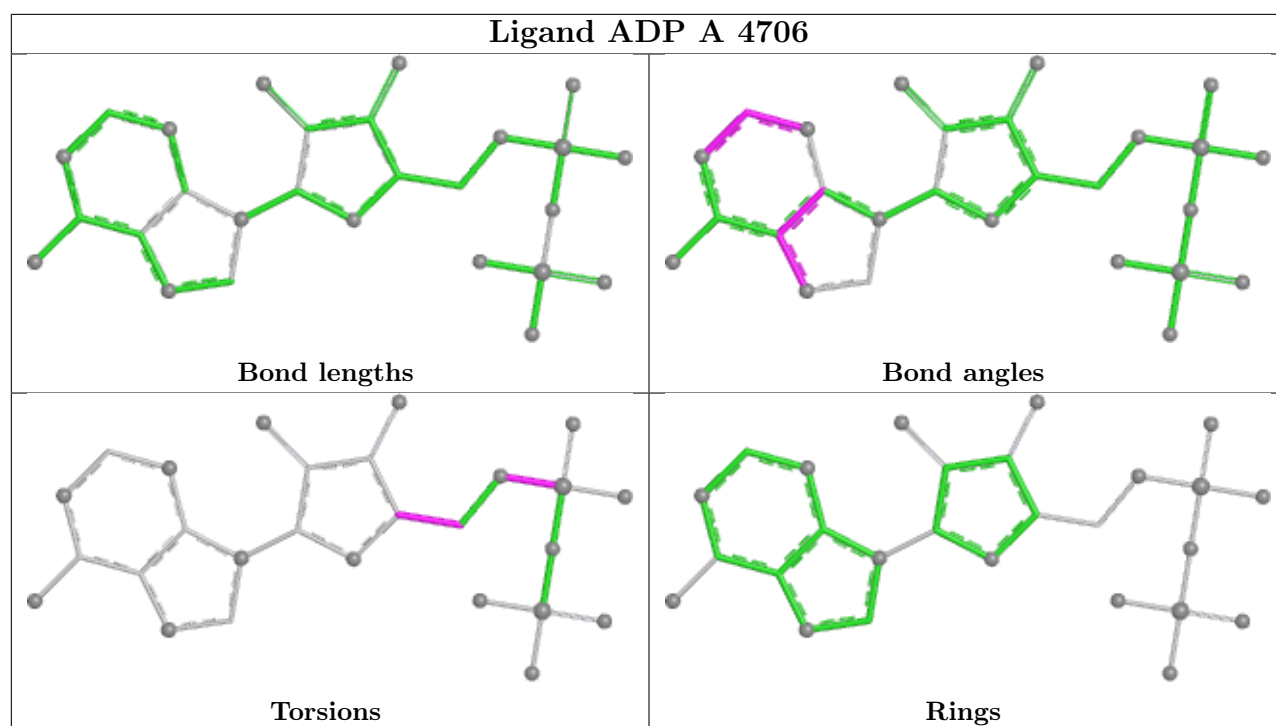
Mol	Chain	Res	Type	Atoms
3	B	4706	ADP	PA-O3A-PB-O3B
3	B	4706	ADP	C5'-O5'-PA-O1A
3	A	4706	ADP	C5'-O5'-PA-O1A
4	B	4702	ATP	C3'-C4'-C5'-O5'
4	B	4702	ATP	O4'-C4'-C5'-O5'

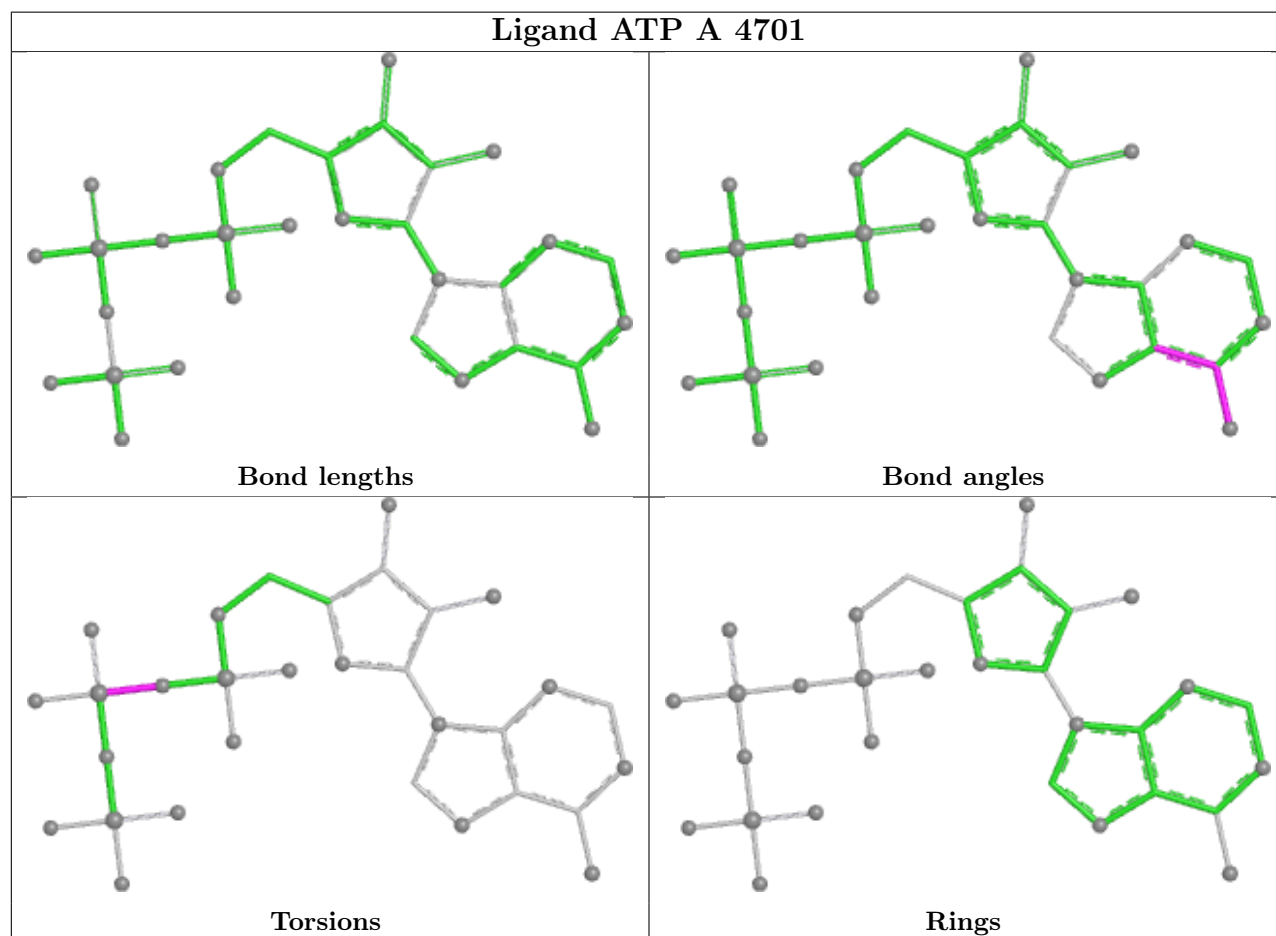
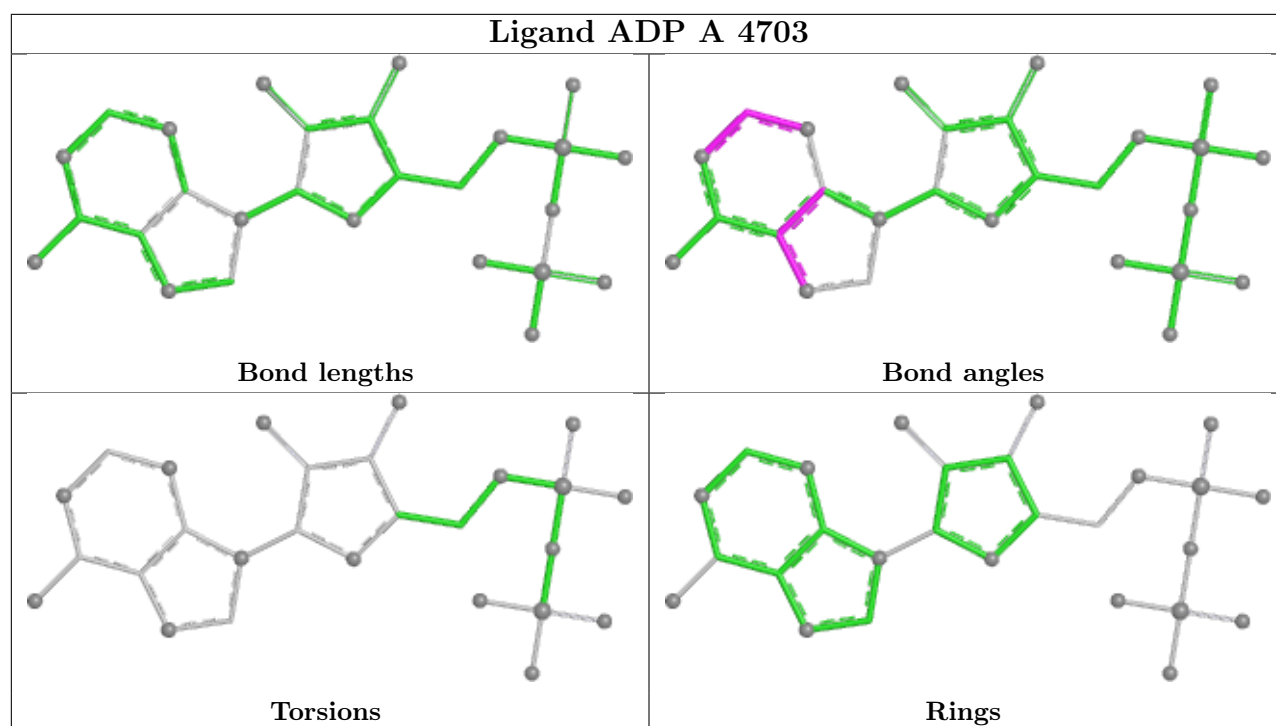
There are no ring outliers.

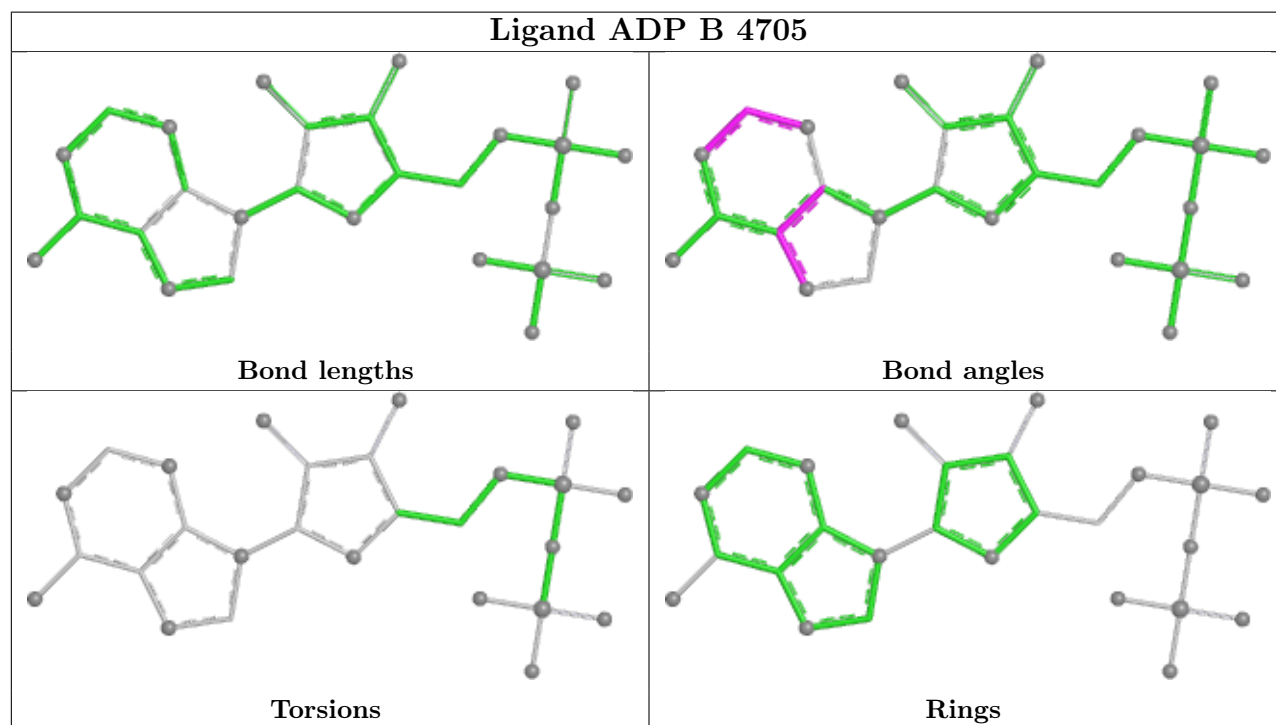
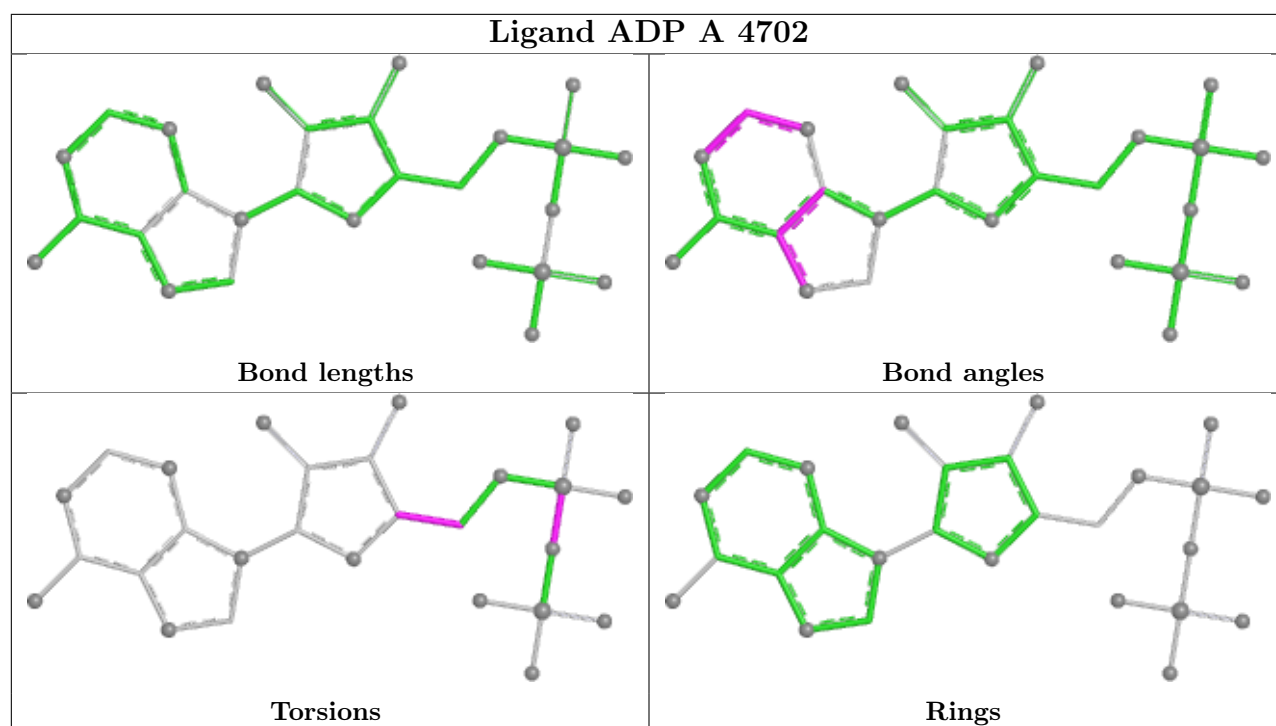
4 monomers are involved in 6 short contacts:

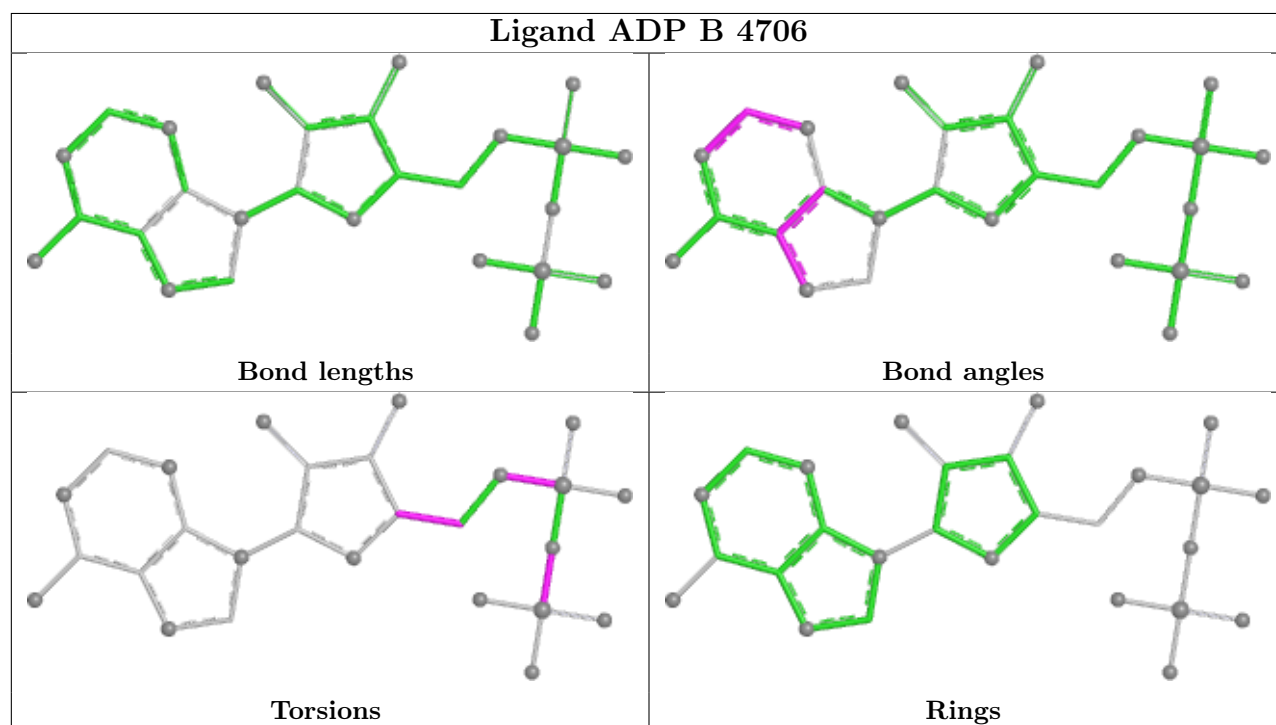
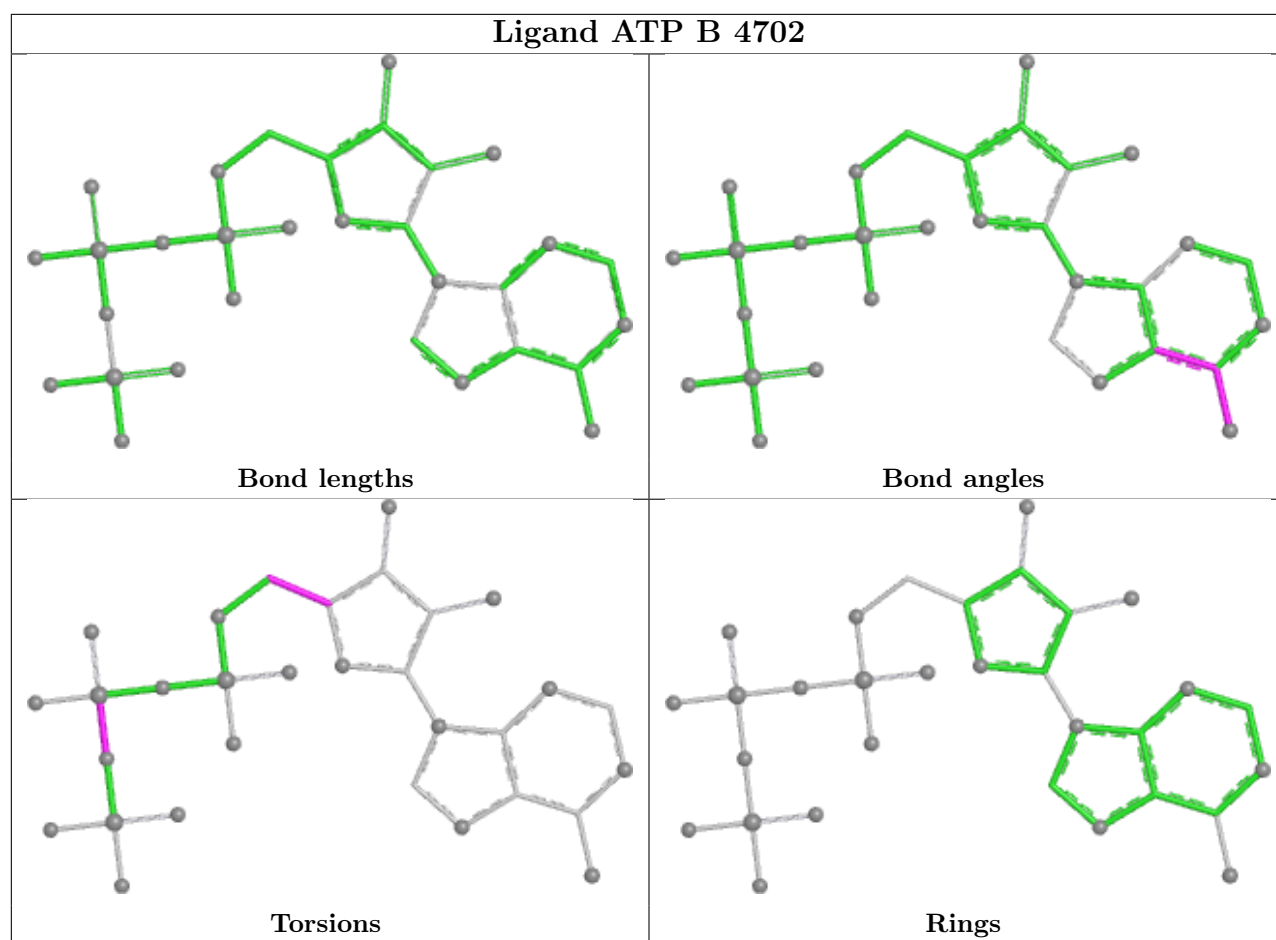
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4706	ADP	1	0
4	A	4701	ATP	1	0
3	B	4705	ADP	2	0
3	B	4706	ADP	2	0

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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

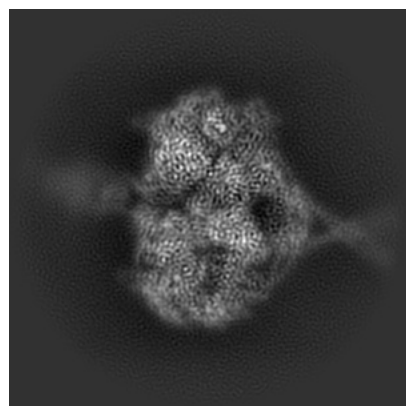
## 6 Map visualisation [i](#)

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

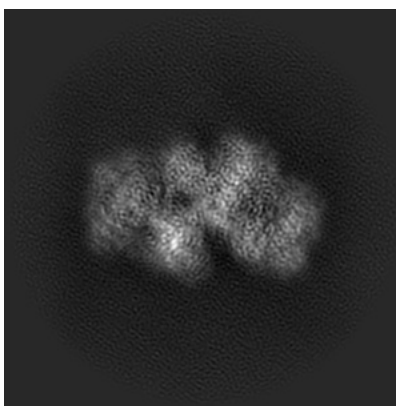
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

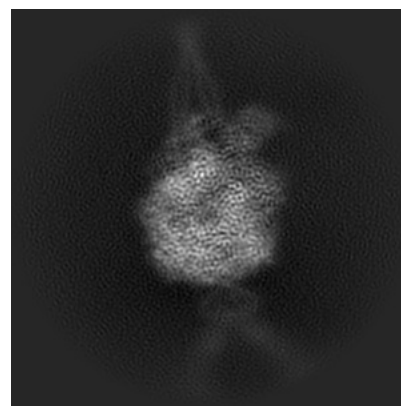
#### 6.1.1 Primary map



X

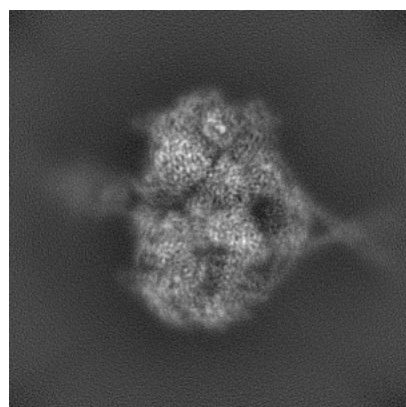


Y

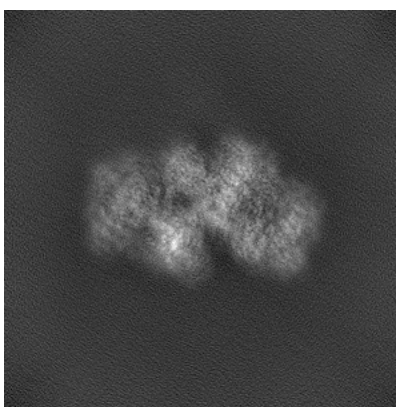


Z

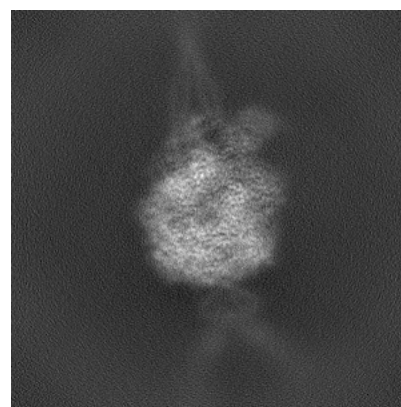
#### 6.1.2 Raw map



X



Y



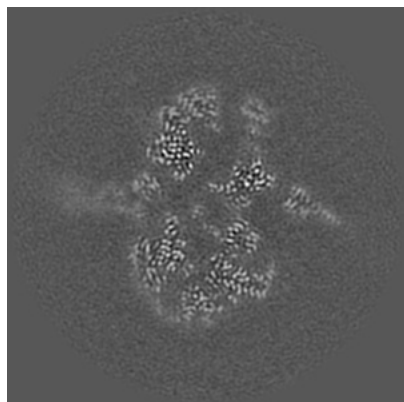
Z

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

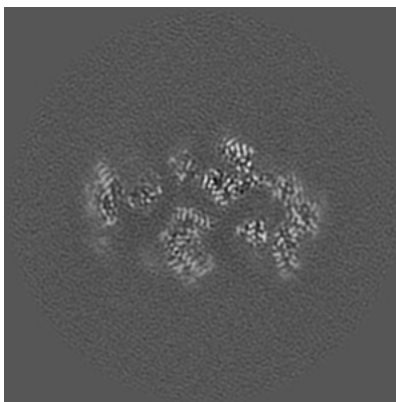


## 6.2 Central slices [i](#)

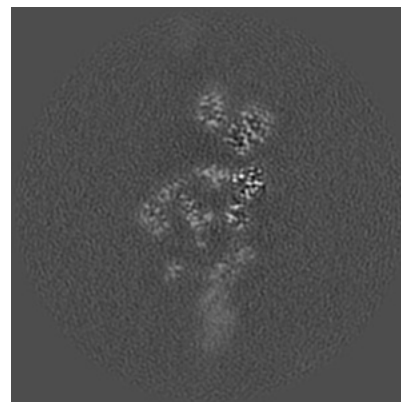
### 6.2.1 Primary map



X Index: 176

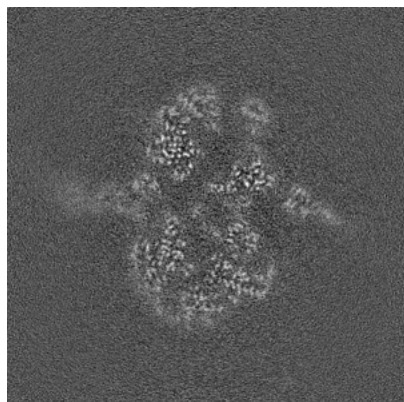


Y Index: 176

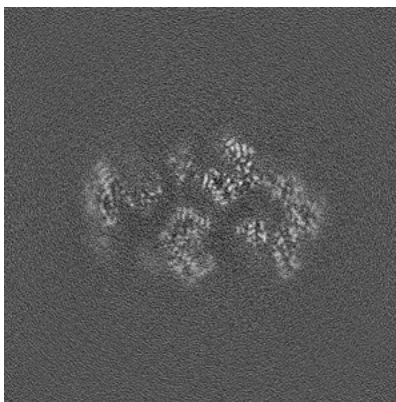


Z Index: 176

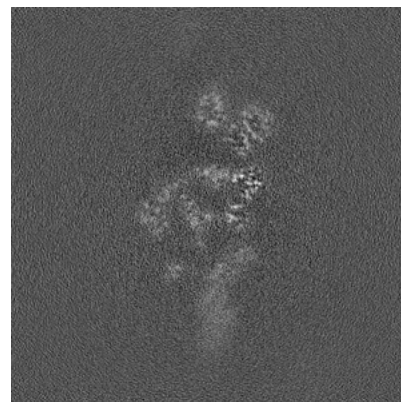
### 6.2.2 Raw map



X Index: 176



Y Index: 176

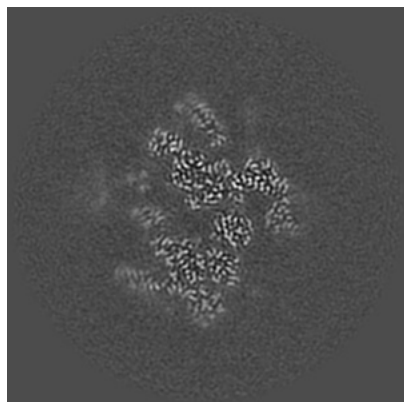


Z Index: 176

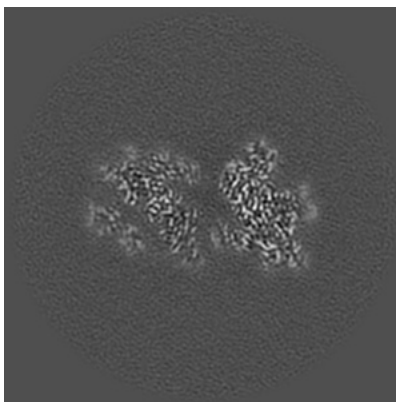
The images above show central slices of the map in three orthogonal directions.

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

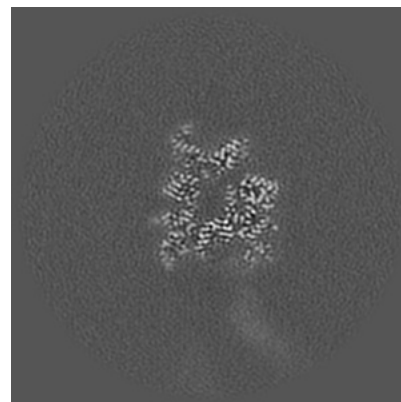
### 6.3.1 Primary map



X Index: 192

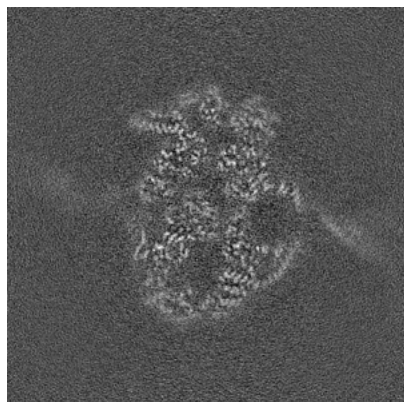


Y Index: 151

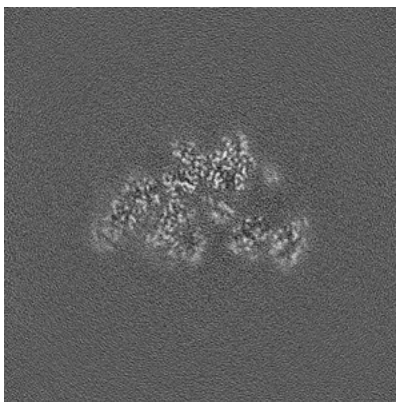


Z Index: 212

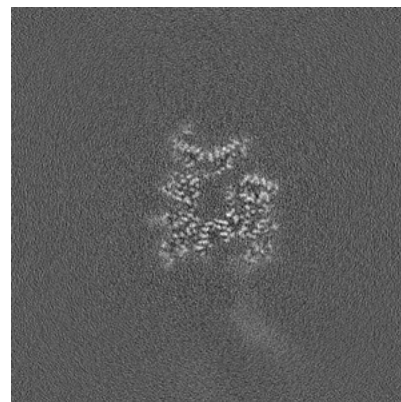
### 6.3.2 Raw map



X Index: 164



Y Index: 195

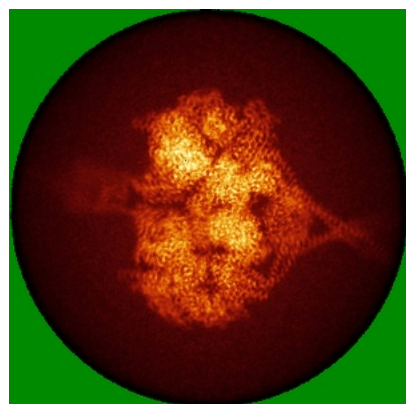


Z Index: 213

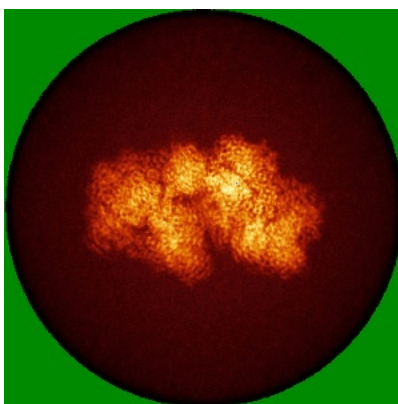
The images above show the largest variance slices of the map in three orthogonal directions.

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

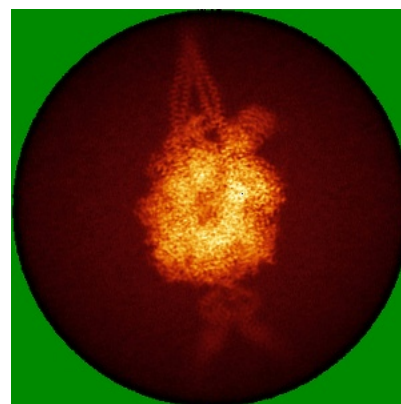
### 6.4.1 Primary map



X

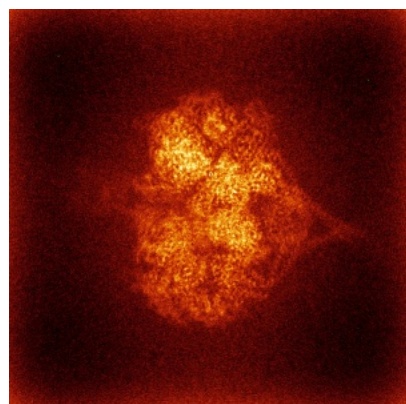


Y

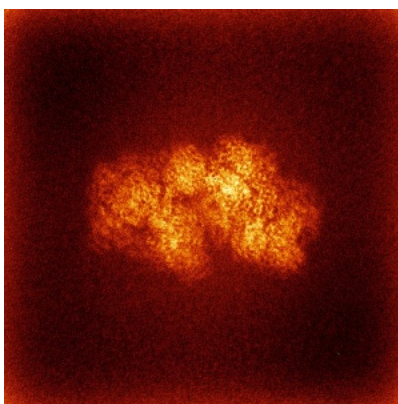


Z

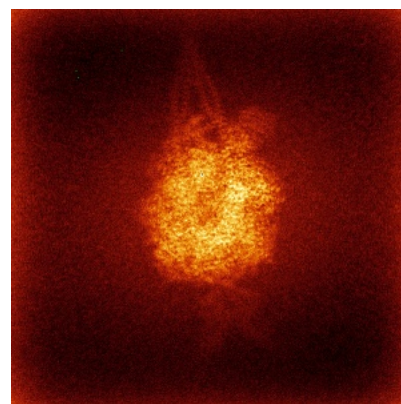
### 6.4.2 Raw map



X



Y



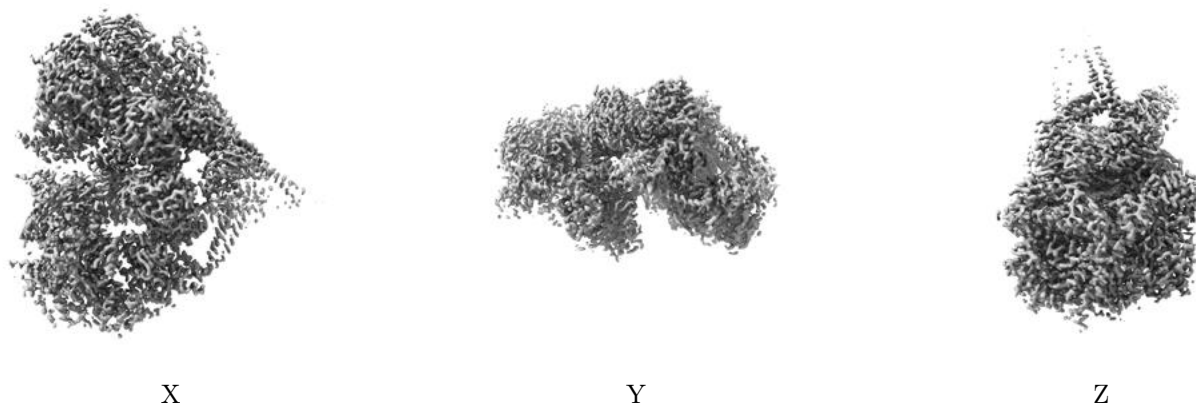
Z

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.



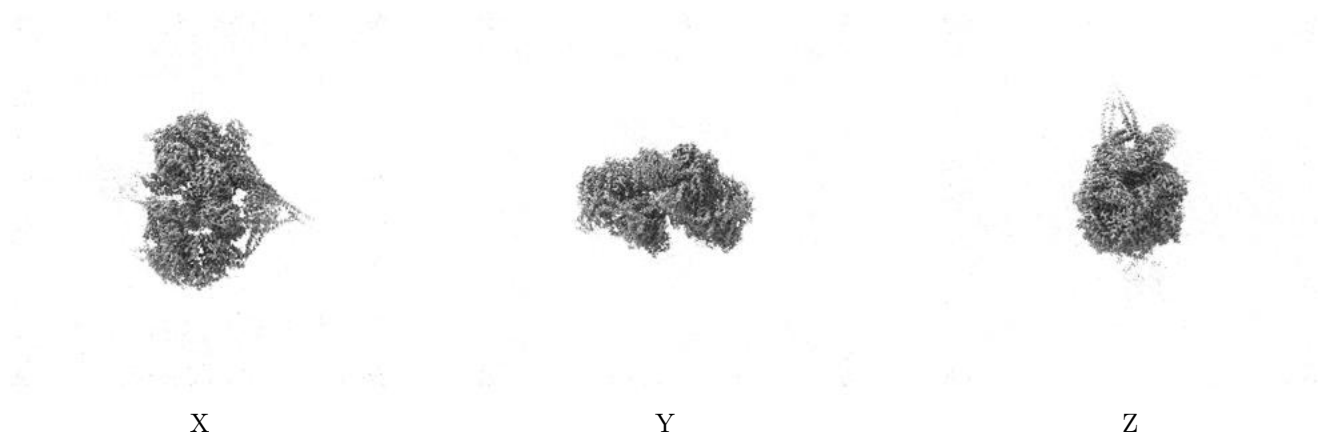
## 6.5 Orthogonal surface views [i](#)

### 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.

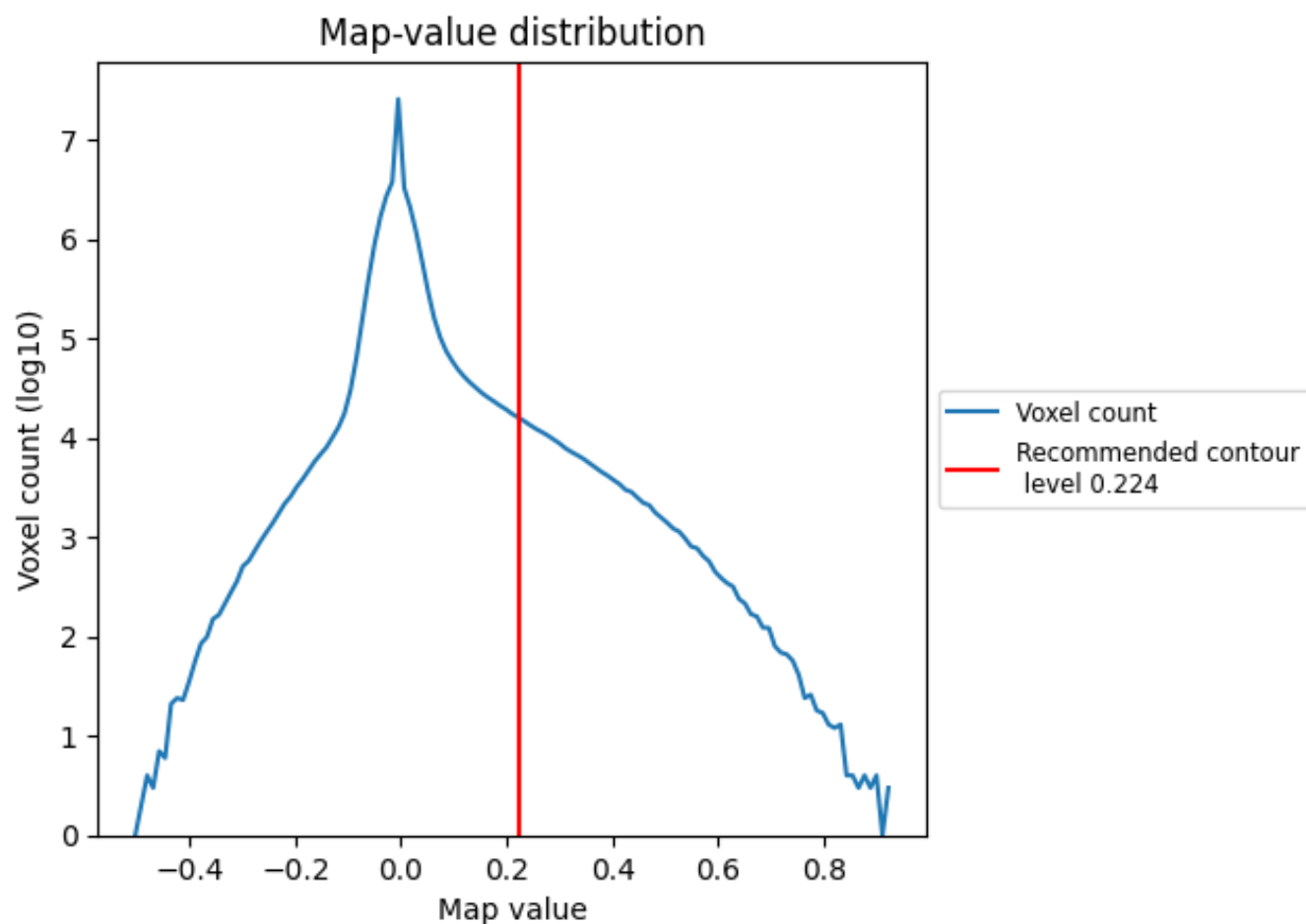
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

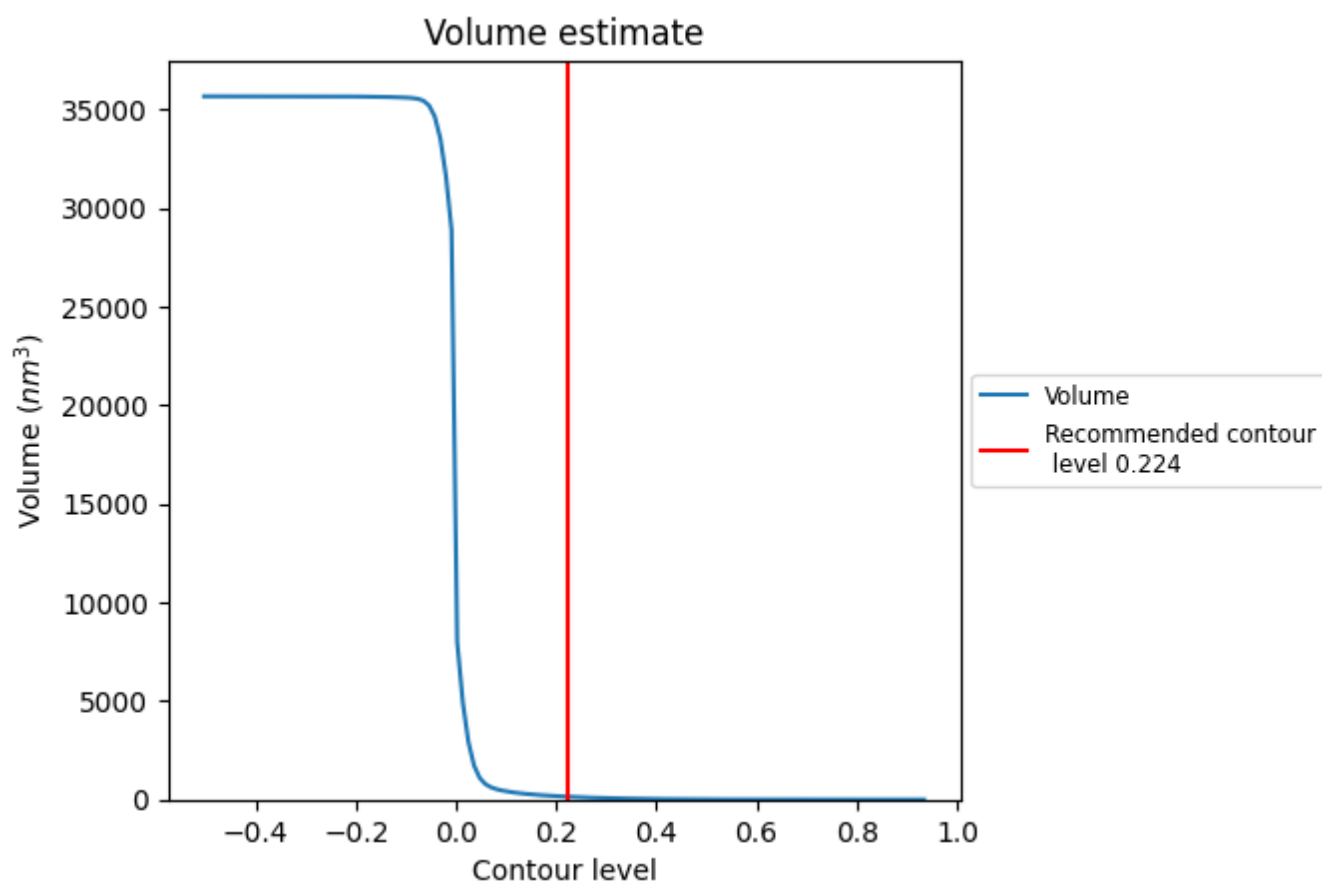
This section contains the results of statistical analysis of the map.

### 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.

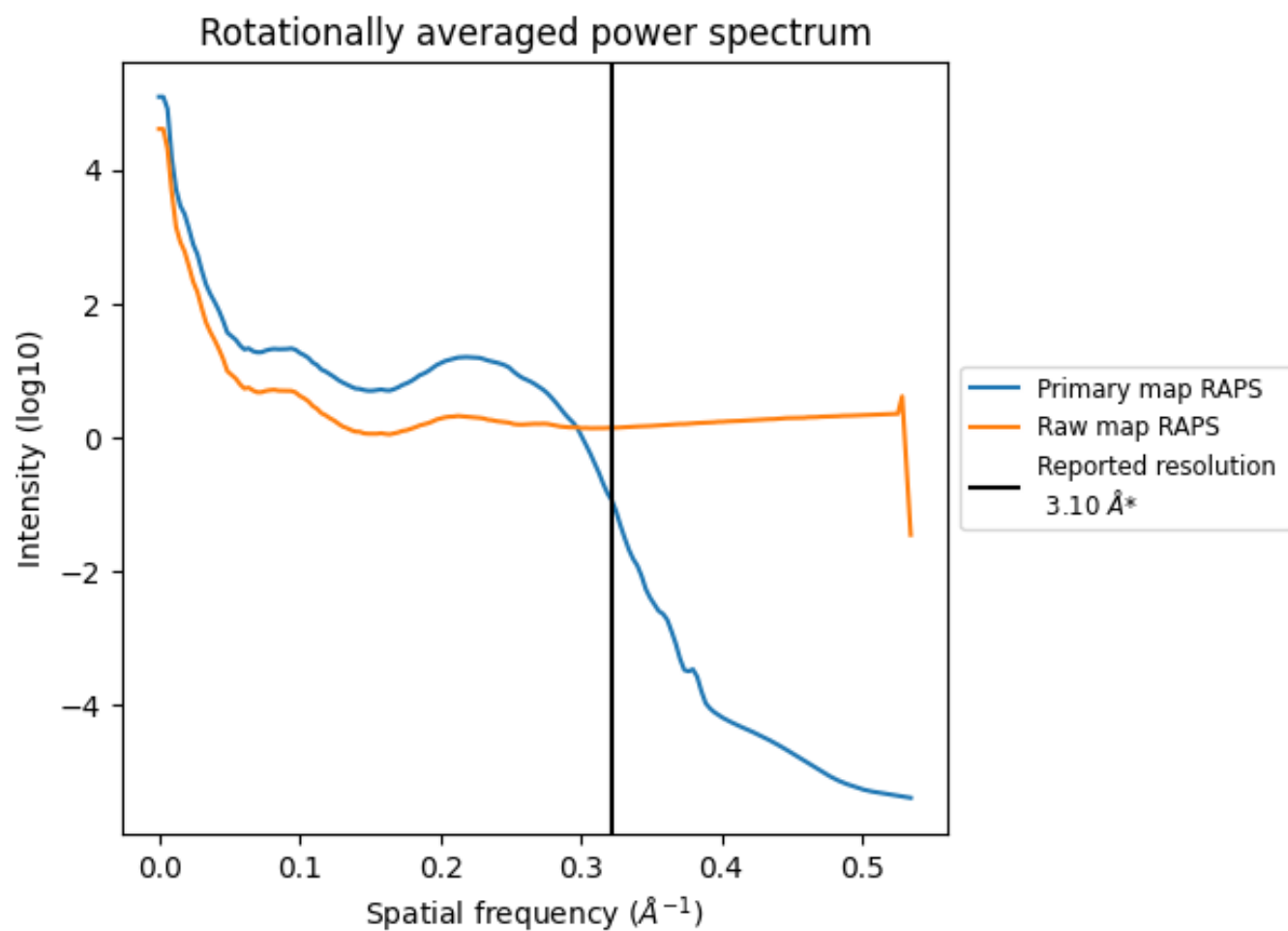
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 142 nm<sup>3</sup>; 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](#)

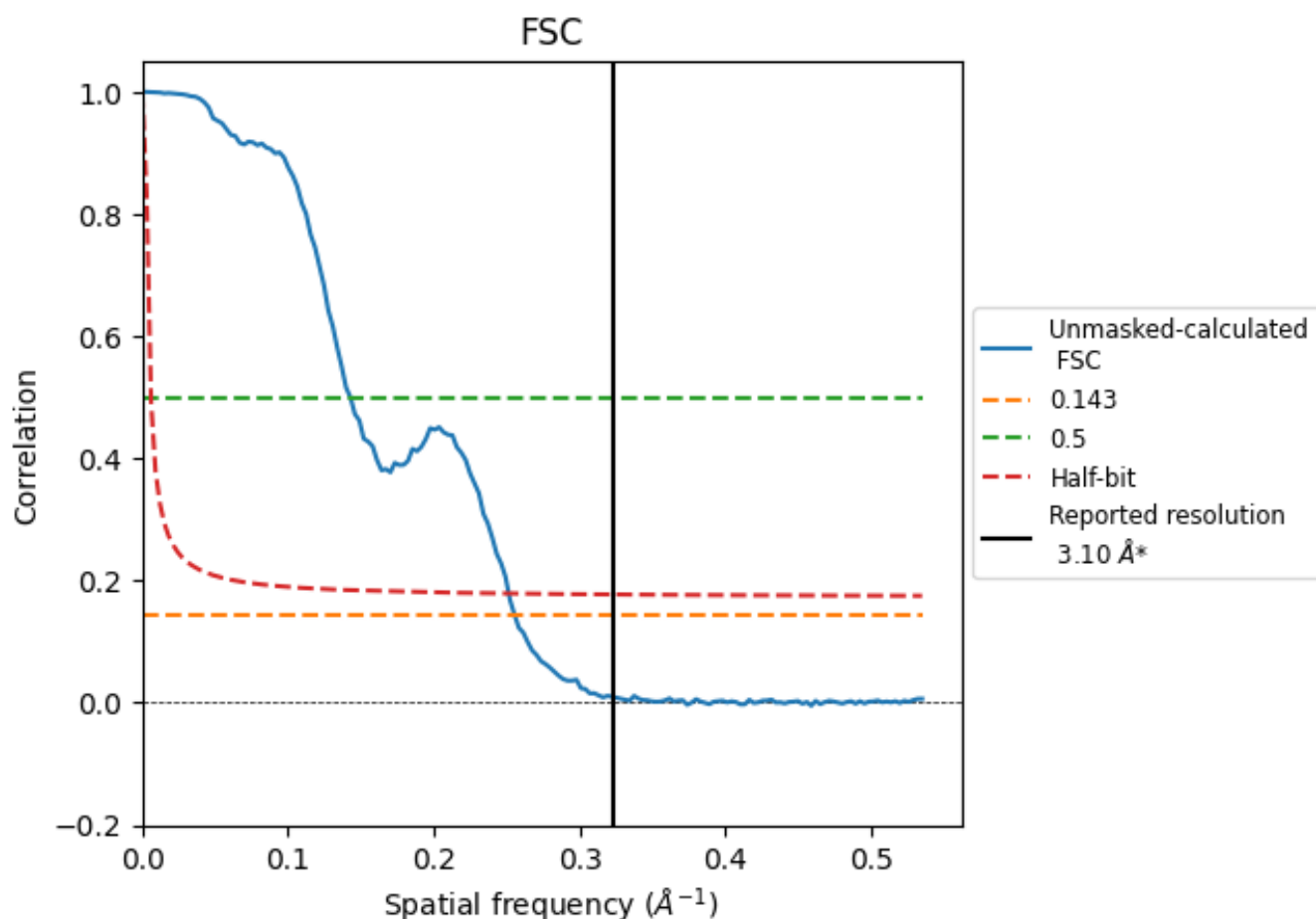


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 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<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

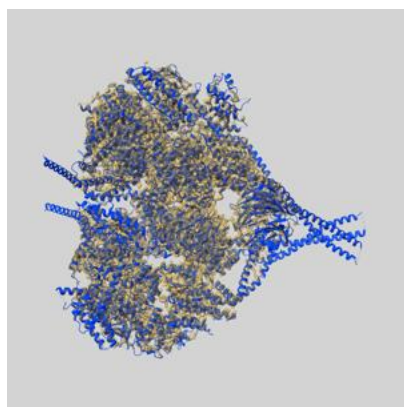
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.92	7.00	3.98

\*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 %

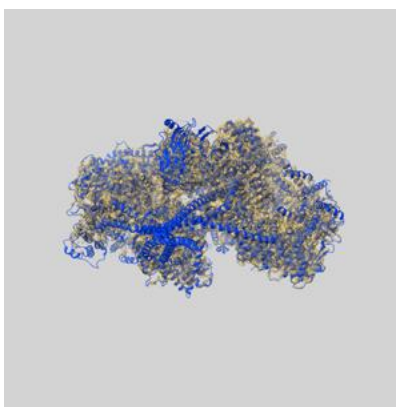
## 9 Map-model fit [i](#)

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.

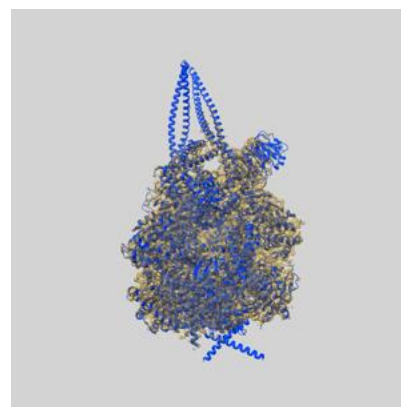
### 9.1 Map-model overlay [i](#)



X



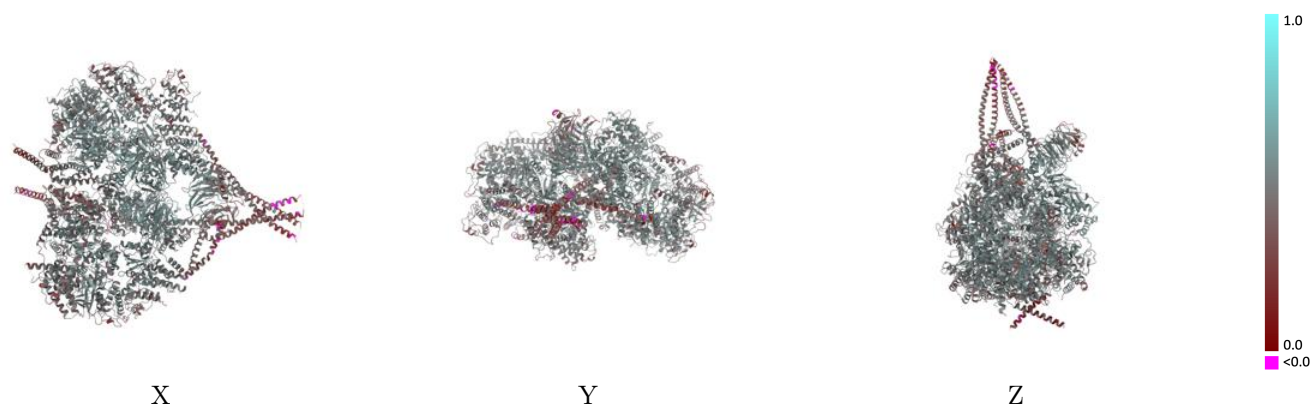
Y



Z

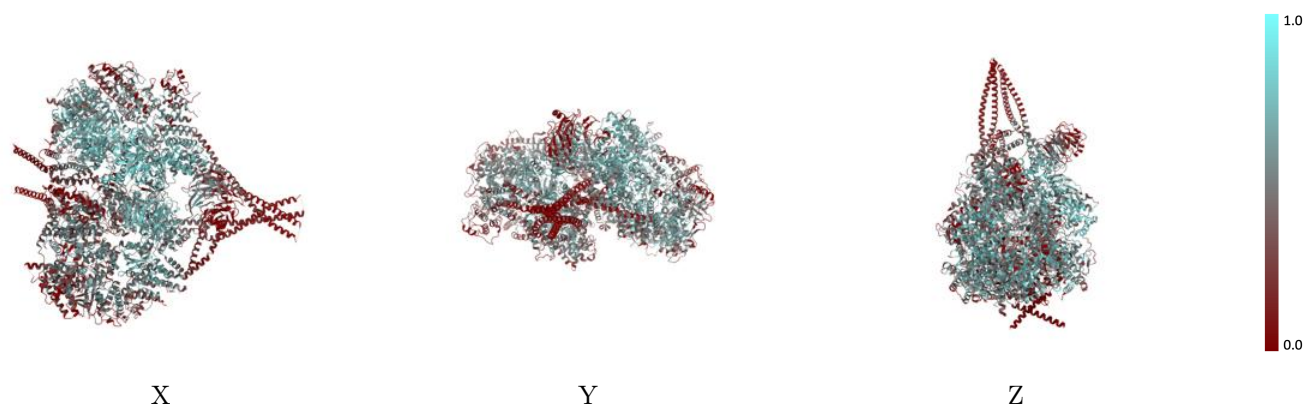
The images above show the 3D surface view of the map at the recommended contour level 0.224 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



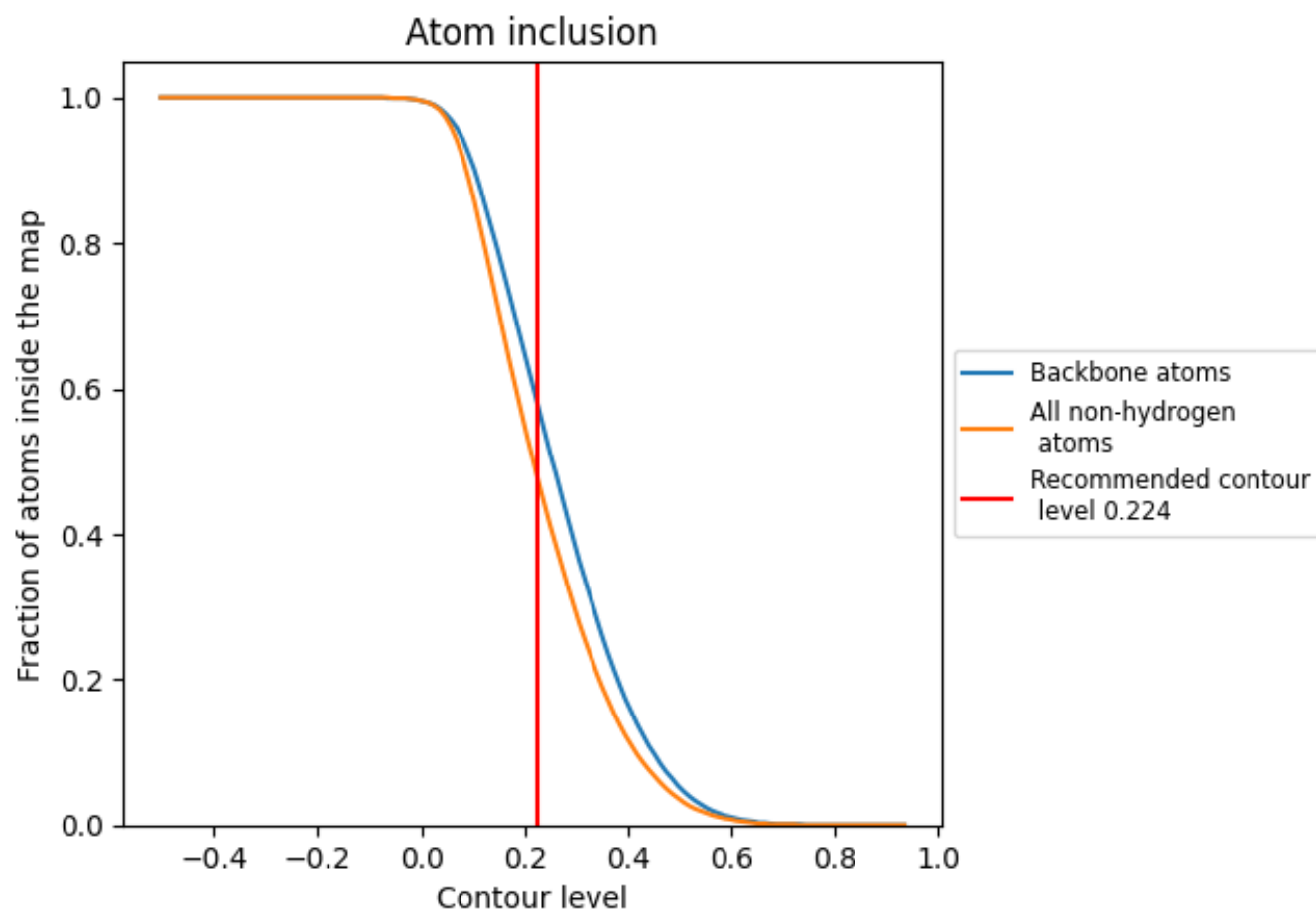
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div></div> 0.4800	<div></div> 0.4860
A	<div></div> 0.4150	<div></div> 0.4710
B	<div></div> 0.5470	<div></div> 0.4980
C	<div></div> 0.2550	<div></div> 0.4600
E	<div></div> 0.6630	<div></div> 0.5360

