



Full wwPDB EM Validation Report ⓘ

Jun 30, 2025 – 06:30 PM EDT

PDB ID : 9E0X / pdb_00009e0x
EMDB ID : EMD-47373
Title : Cryo-EM structure of Phi dynein
Authors : Nguyen, K.H.V.; Kendrick, A.A.; Leschziner, A.E.
Deposited on : 2024-10-20
Resolution : 2.70 Å(reported)

This is a Full wwPDB EM Validation 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.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

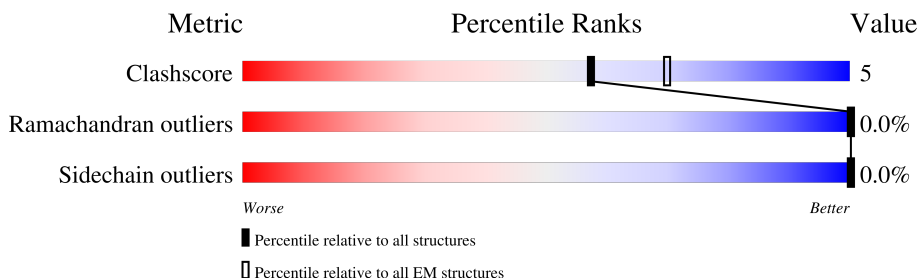
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4843	
1	B	4843	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 46234 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2920	Total 23003	C 14686	N 3978	O 4227	S 112	0	0
1	B	2920	Total 23003	C 14686	N 3978	O 4227	S 112	0	0

There are 396 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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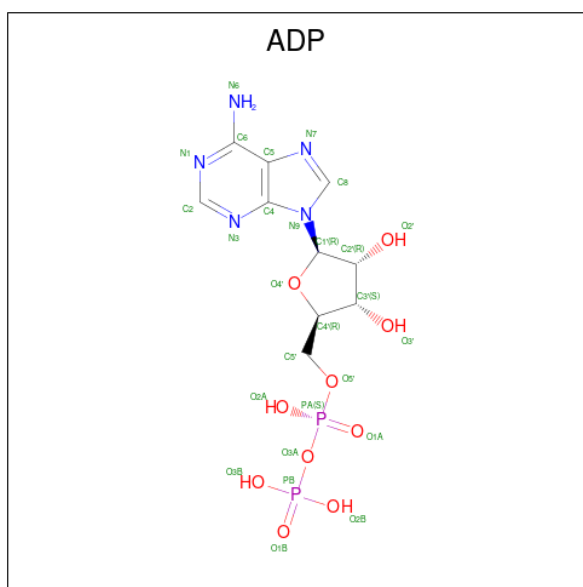
Chain	Residue	Modelled	Actual	Comment	Reference
B	-74	GLY	-	expression tag	UNP Q14204
B	-73	GLU	-	expression tag	UNP Q14204
B	-72	VAL	-	expression tag	UNP Q14204
B	-71	ILE	-	expression tag	UNP Q14204
B	-70	SER	-	expression tag	UNP Q14204
B	-69	TYR	-	expression tag	UNP Q14204
B	-68	SER	-	expression tag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

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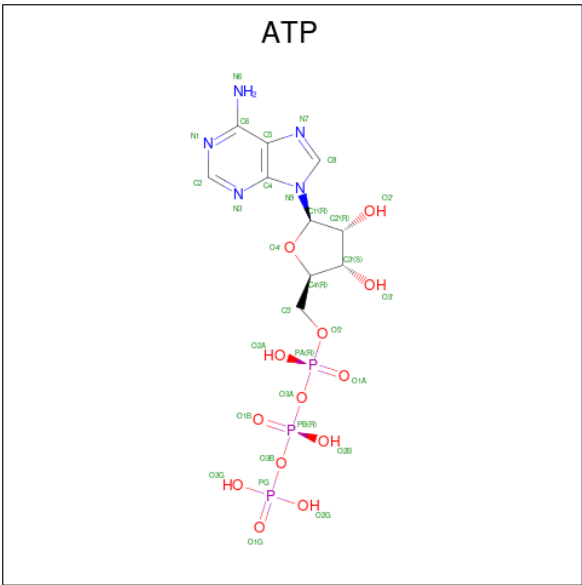
Chain	Residue	Modelled	Actual	Comment	Reference
B	-32	GLY	-	expression tag	UNP Q14204
B	-31	ASP	-	expression tag	UNP Q14204
B	-30	LEU	-	expression tag	UNP Q14204
B	-29	ASP	-	expression tag	UNP Q14204
B	-28	VAL	-	expression tag	UNP Q14204
B	-27	GLY	-	expression tag	UNP Q14204
B	-26	GLY	-	expression tag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

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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

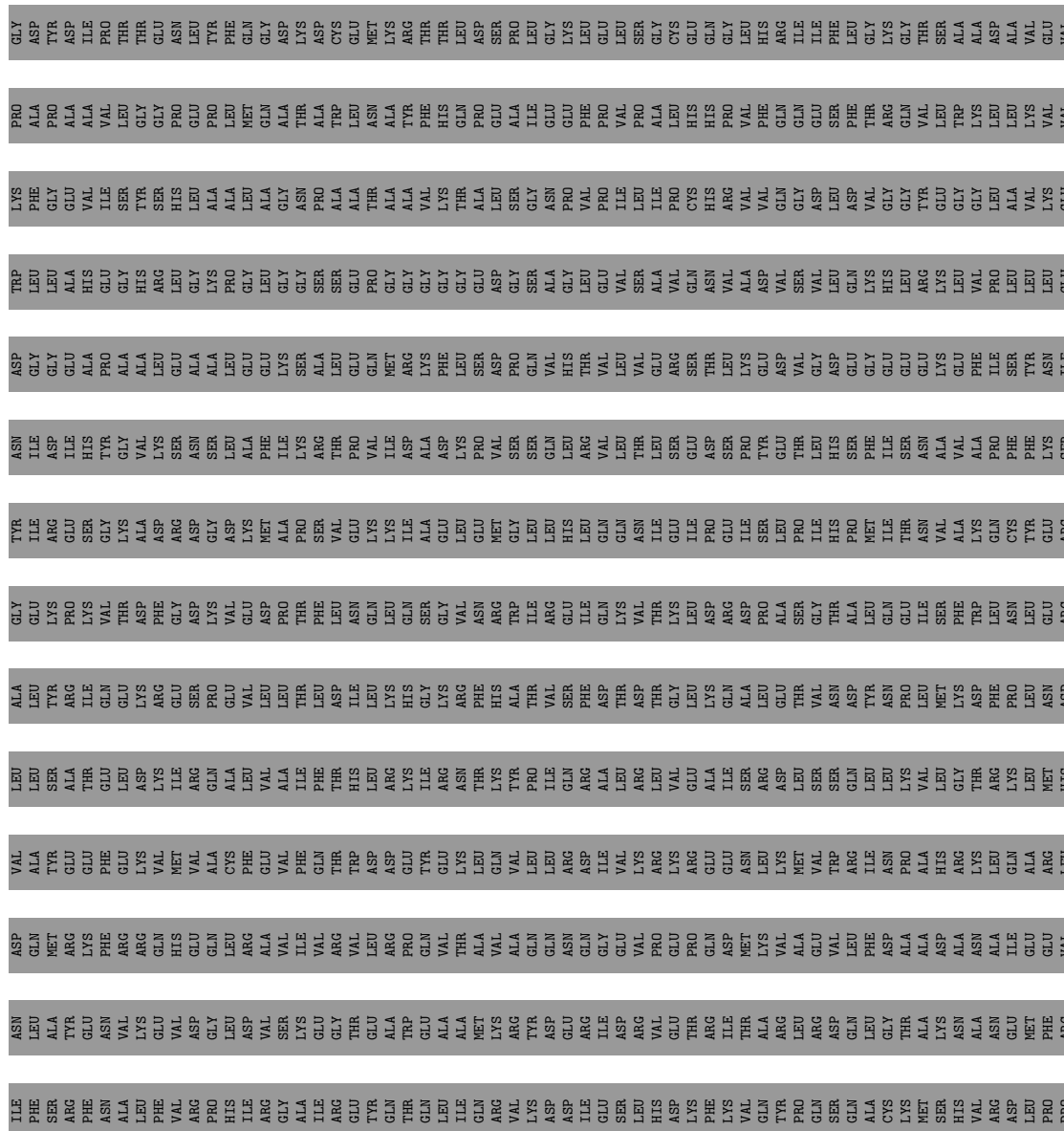
Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Mg	0
			2	2	
4	B	2	Total	Mg	0
			2	2	







- Molecule 1: Cytoplasmic dynein 1 heavy chain 1











4 Experimental information

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.15	0/23476	0.35	0/31857
1	B	0.15	0/23476	0.34	0/31857
All	All	0.15	0/46952	0.35	0/63714

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	23003	0	22807	196	0
1	B	23003	0	22807	229	0
2	A	81	0	36	1	0
2	B	81	0	36	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
All	All	46234	0	45710	423	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (423) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3712:CYS:HG	1:A:3836:TYR:HH	1.10	0.96
1:B:3712:CYS:HG	1:B:3836:TYR:HH	1.30	0.78
1:B:4052:SER:HA	1:B:4095:MET:HE1	1.69	0.74
1:A:1612:GLN:NE2	1:A:1635:GLU:OE1	2.22	0.73
1:A:2410:SER:HB3	1:A:2413:LEU:HD23	1.72	0.70
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.73	0.68
1:A:4052:SER:HA	1:A:4095:MET:HE1	1.76	0.68
1:B:1933:ASP:OD2	1:B:2314:ASN:ND2	2.28	0.67
1:B:4326:ASN:ND2	1:B:4579:ASN:O	2.28	0.67
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.76	0.66
1:A:2042:THR:HG22	1:A:2043:LYS:HG3	1.78	0.66
1:A:2872:LEU:HD12	1:A:2920:LEU:HD12	1.76	0.65
1:B:2461:MET:HG2	1:B:2583:THR:HG21	1.79	0.65
1:A:3798:SER:O	1:A:3802:LEU:HB2	1.96	0.65
1:B:2346:GLN:HB2	1:B:2726:ARG:HD3	1.80	0.64
1:B:3517:ALA:HB1	1:B:3525:ARG:HG2	1.79	0.63
1:A:4088:VAL:HG13	1:A:4118:PRO:HA	1.80	0.63
1:A:1912:LYS:HG2	1:A:2041:MET:HG3	1.79	0.63
1:A:1623:ARG:NH1	1:A:1632:VAL:O	2.30	0.63
1:A:4043:MET:HB2	1:A:4127:THR:HG22	1.81	0.63
1:A:4066:ILE:HG22	1:A:4093:TRP:HB2	1.80	0.63
1:A:1475:LEU:HG	1:A:1588:VAL:HG22	1.81	0.62
1:B:4286:CYS:HA	1:B:4293:ASP:HA	1.81	0.62
1:B:2453:ARG:NH2	1:B:2505:ASP:OD2	2.32	0.62
1:B:1581:LYS:HE3	1:B:1594:ILE:HD12	1.82	0.62
1:A:1734:ASP:HB3	1:A:1737:THR:HG22	1.81	0.62
1:A:3810:SER:HB3	1:A:3890:ILE:HD12	1.81	0.62
1:A:3639:GLU:OE2	1:A:4111:LYS:NZ	2.31	0.61
1:B:1554:SER:HB2	1:B:1557:ILE:HD11	1.80	0.61
1:A:2346:GLN:HB2	1:A:2726:ARG:HD2	1.82	0.61
1:A:2242:GLU:HG3	1:A:2248:GLU:HA	1.83	0.61
1:B:4611:LEU:HB2	1:B:4619:ILE:HD11	1.83	0.60
1:B:3712:CYS:SG	1:B:3836:TYR:OH	2.49	0.60
1:A:3873:ARG:NH2	1:A:4021:MET:SD	2.63	0.60
1:B:2221:MET:HG2	1:B:2343:PHE:HB2	1.83	0.60
1:B:3638:VAL:HG12	1:B:3681:THR:HB	1.84	0.60
1:A:3483:SER:HA	1:A:3486:ARG:HG2	1.84	0.60
1:B:4042:LEU:HD11	1:B:4144:ILE:HG12	1.83	0.59
1:A:2823:ARG:NH2	1:A:2868:SER:OG	2.36	0.59
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.84	0.59
1:A:1825:LEU:HG	1:A:1830:ILE:HD11	1.84	0.59
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.83	0.59
1:A:1623:ARG:NH2	1:A:1634:ASP:OD1	2.35	0.59
1:B:3966:PRO:HD2	1:B:4000:ARG:HG3	1.85	0.59
1:B:2437:LEU:HD21	1:B:2451:ARG:HG3	1.85	0.58
1:A:3882:THR:HG21	1:A:4342:LYS:HD3	1.85	0.58
1:B:4544:ASN:HA	1:B:4573:ASN:HD21	1.68	0.58
1:A:4239:PRO:HB2	1:A:4242:ALA:HB3	1.86	0.58
1:A:4424:LEU:HD21	1:A:4428:ARG:HH21	1.69	0.58
1:B:4088:VAL:HG13	1:B:4118:PRO:HA	1.84	0.58
1:B:3818:LEU:HB3	1:B:3825:TYR:HE2	1.69	0.58
1:B:3798:SER:O	1:B:3802:LEU:HB2	2.04	0.58
1:B:2181:GLU:HG3	1:B:2244:LEU:HG	1.86	0.57
1:A:2536:ASP:OD1	1:A:2576:ARG:NH1	2.37	0.57
1:A:2304:ASP:OD1	1:A:2726:ARG:NH2	2.36	0.57
1:B:3483:SER:HA	1:B:3486:ARG:HG2	1.86	0.57
1:B:4185:TRP:HD1	1:B:4272:LEU:HD21	1.70	0.57
1:B:2245:GLU:OE1	1:B:2298:ARG:NH2	2.37	0.57
1:B:2562:VAL:HG21	1:B:2755:MET:HB3	1.87	0.57
1:A:3892:LEU:HD21	1:A:3983:ILE:HG21	1.86	0.57
1:B:1965:GLU:HG2	1:B:2026:SER:HB2	1.85	0.57
1:B:4271:ARG:HH21	1:B:4272:LEU:HD13	1.70	0.57
1:B:2717:ASP:O	1:B:4446:ASN:ND2	2.35	0.57
1:B:3499:GLN:HA	1:B:3502:THR:HG22	1.87	0.56
1:B:3236:ALA:HB1	1:B:3451:TYR:HE1	1.69	0.56
1:A:1888:CYS:HB2	1:A:2041:MET:HE1	1.87	0.56
1:B:3243:MET:HE1	1:B:3444:ILE:HG23	1.86	0.56
1:A:3597:THR:HG23	1:A:3634:LEU:HD21	1.87	0.56
1:B:4042:LEU:HB2	1:B:4128:MET:HE1	1.87	0.56
1:A:2181:GLU:HG3	1:A:2244:LEU:HG	1.88	0.56
1:B:4234:SER:HB2	1:B:4237:LYS:HG2	1.87	0.56
1:B:3827:TYR:O	1:B:4140:ARG:NH1	2.38	0.56
1:B:1627:PRO:HB3	1:B:1950:GLN:HB3	1.86	0.55
1:A:2938:VAL:O	1:A:2943:LYS:NZ	2.40	0.55
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.88	0.55
1:A:4470:PRO:HB3	1:A:4612:ASN:HD22	1.71	0.55
1:B:2823:ARG:HH22	1:B:2868:SER:HG	1.55	0.55
1:A:4171:LYS:HD3	1:A:4176:ARG:HH22	1.71	0.55
1:B:2299:GLN:HB2	1:B:2339:VAL:HG22	1.89	0.55
1:A:1530:ILE:HD11	1:A:1588:VAL:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2058:GLY:O	1:A:2104:LYS:NZ	2.32	0.55
1:A:1985:HIS:HA	1:A:1997:ILE:HD13	1.89	0.55
1:B:1933:ASP:OD1	1:B:1962:ARG:NH2	2.40	0.55
1:B:4100:HIS:HB3	1:B:4128:MET:HB2	1.87	0.55
1:B:4287:LYS:O	1:B:4319:SER:OG	2.24	0.55
1:B:1929:VAL:O	1:B:2332:ARG:NH1	2.39	0.54
1:B:1825:LEU:HG	1:B:1830:ILE:HD11	1.89	0.54
1:B:3892:LEU:HD21	1:B:3983:ILE:HG21	1.90	0.54
1:A:4235:PRO:HA	1:A:4238:ILE:HD12	1.88	0.54
1:B:2091:ARG:NH1	1:B:2320:ASP:OD1	2.41	0.54
1:B:3474:ARG:HD3	1:B:3767:ILE:HG21	1.89	0.54
1:B:4434:VAL:HB	1:B:4448:LEU:HD11	1.90	0.54
1:B:4318:PRO:HG2	1:B:4325:ASN:HA	1.89	0.54
1:B:4525:ARG:NH2	1:B:4539:LEU:O	2.38	0.54
1:A:2556:GLU:OE1	1:A:2757:ARG:NH2	2.40	0.54
1:A:3240:LEU:HD21	1:B:3243:MET:HE2	1.90	0.54
1:A:1477:LEU:HB3	1:A:1485:ARG:HB3	1.89	0.53
1:B:2536:ASP:OD1	1:B:2576:ARG:NH1	2.41	0.53
1:B:1766:LEU:HD22	1:B:1830:ILE:HG21	1.90	0.53
1:A:3129:VAL:HG21	1:A:3149:PHE:HB2	1.90	0.53
1:A:3208:ILE:HD11	1:A:3482:LEU:HB3	1.90	0.53
1:B:2335:LEU:HD12	1:B:2336:PRO:HD2	1.90	0.53
1:B:3520:PHE:HB3	1:B:3524:MET:HB3	1.91	0.53
1:A:4222:TRP:HE1	1:A:4246:LEU:HD13	1.72	0.53
1:B:4271:ARG:NH1	1:B:4637:GLU:OE2	2.42	0.53
1:A:3872:ALA:HA	1:A:3875:MET:HG2	1.89	0.52
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.91	0.52
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.43	0.52
1:B:1623:ARG:HD3	1:B:1630:TYR:HA	1.91	0.52
1:B:1861:MET:HG3	1:B:1862:ALA:H	1.74	0.52
1:A:4557:SER:N	1:A:4590:LEU:O	2.42	0.52
1:B:2138:ILE:HD12	1:B:2161:LEU:HD22	1.91	0.52
1:B:3835:ILE:HG12	1:B:3870:ARG:HD2	1.91	0.52
1:B:2837:LEU:O	1:B:2843:ARG:NH1	2.42	0.52
1:B:2581:LEU:HD11	1:B:2593:LEU:HD21	1.92	0.52
1:B:3158:ASN:ND2	1:B:3169:MET:O	2.38	0.52
1:B:4492:ILE:HG23	1:B:4504:LEU:HD11	1.92	0.52
1:A:2552:VAL:HG21	1:A:2570:PRO:HB2	1.92	0.52
1:A:3868:PHE:HA	1:A:3883:PHE:HE2	1.74	0.52
1:B:2943:LYS:HE2	1:B:3067:THR:HG23	1.91	0.52
1:B:3618:ALA:O	1:B:3622:ASN:ND2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2775:GLU:OE1	1:B:2857:HIS:NE2	2.40	0.52
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.92	0.52
1:B:1537:TRP:HE3	1:B:1601:LEU:HD11	1.74	0.52
1:B:3882:THR:HG23	1:B:4343:MET:HE2	1.90	0.52
1:A:1537:TRP:HE3	1:A:1601:LEU:HD11	1.75	0.51
1:A:1792:LEU:HB3	1:A:1812:ILE:HG12	1.91	0.51
1:B:3007:ARG:HD3	1:B:3017:VAL:HG11	1.93	0.51
1:A:3717:LEU:HD11	1:A:3797:VAL:HG11	1.92	0.51
1:A:4099:VAL:HG22	1:A:4128:MET:HB3	1.92	0.51
1:B:1929:VAL:H	1:B:2332:ARG:HH22	1.58	0.51
1:A:4110:GLU:HG3	1:A:4138:LEU:HA	1.91	0.51
1:B:4110:GLU:HG3	1:B:4138:LEU:HA	1.93	0.51
1:B:2925:ILE:HG21	1:B:2933:LEU:HD13	1.91	0.51
1:B:3981:THR:HG22	1:B:3983:ILE:H	1.75	0.51
1:A:3886:LEU:HD11	1:A:4346:MET:HE3	1.92	0.51
1:B:2629:GLU:HG3	1:B:2633:LYS:HE2	1.93	0.51
1:B:4178:ARG:HE	1:B:4296:MET:HE2	1.76	0.51
1:A:4203:LYS:NZ	1:A:4258:ASN:OD1	2.40	0.51
1:B:2798:GLU:OE1	1:B:2801:ARG:NH1	2.43	0.51
1:B:2989:LYS:NZ	1:B:3061:ASN:OD1	2.43	0.51
1:A:3138:SER:OG	1:A:3141:GLU:OE1	2.20	0.51
1:B:3510:SER:HB3	1:B:3553:LEU:HD21	1.93	0.51
1:B:4071:ILE:HG13	1:B:4099:VAL:HG12	1.93	0.50
1:A:3835:ILE:HD11	1:A:3866:VAL:HG12	1.93	0.50
1:B:3983:ILE:O	1:B:3987:ILE:HD12	2.12	0.50
1:B:1958:ASP:HA	1:B:2017:THR:HB	1.92	0.50
1:A:2837:LEU:O	1:A:2843:ARG:NH1	2.44	0.50
1:A:1943:ARG:NH1	1:A:2329:ASN:O	2.44	0.50
1:A:2665:GLU:HB3	1:A:2668:LEU:HD12	1.94	0.50
1:B:2107:ARG:NH2	1:B:2139:GLN:OE1	2.45	0.50
1:B:2433:VAL:HG22	1:B:2498:ILE:HD11	1.93	0.50
1:A:1817:HIS:CE1	1:A:1881:GLN:HG2	2.47	0.50
1:A:4434:VAL:HA	1:A:4437:VAL:HG22	1.94	0.50
1:A:4099:VAL:HG11	1:A:4126:LEU:HB2	1.93	0.50
1:B:3182:HIS:NE2	1:B:3582:ARG:O	2.43	0.50
1:B:3604:TYR:HB2	1:B:3609:ILE:HD11	1.93	0.50
1:B:4099:VAL:HB	1:B:4106:LEU:HD21	1.93	0.50
1:A:1972:SER:HB2	1:A:2032:LEU:HB2	1.94	0.50
1:B:4096:LEU:HD13	1:B:4105:TRP:HH2	1.76	0.50
1:A:4387:TRP:HE1	1:A:4476:ILE:HD13	1.77	0.49
1:B:3811:ILE:HD13	1:B:3890:ILE:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3597:THR:HG23	1:B:3634:LEU:HD21	1.95	0.49
1:A:2603:MET:HE1	2:A:4803:ADP:C5	2.46	0.49
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.94	0.49
1:B:3821:ILE:HD13	1:B:4342:LYS:HD2	1.93	0.49
1:B:3478:LEU:HD13	1:B:3770:LEU:HD13	1.95	0.49
1:B:4511:LEU:HD22	1:B:4517:PRO:HB3	1.94	0.49
1:A:4164:ILE:HD13	1:A:4180:TYR:HD2	1.78	0.49
1:B:3825:TYR:HB2	1:B:3827:TYR:CZ	2.48	0.49
1:A:3236:ALA:HB1	1:A:3451:TYR:HE1	1.78	0.49
1:B:3499:GLN:O	1:B:3503:ILE:HG12	2.12	0.49
1:A:4137:ASN:OD1	1:A:4138:LEU:N	2.46	0.49
1:B:1550:ILE:HD11	1:B:1618:TYR:HE2	1.78	0.49
1:A:1766:LEU:HG	1:A:1830:ILE:HG21	1.94	0.48
1:A:2181:GLU:O	1:A:2185:VAL:HG22	2.13	0.48
1:A:3659:ARG:NE	1:A:3670:ASP:OD1	2.46	0.48
1:A:4379:THR:O	1:A:4382:THR:OG1	2.29	0.48
1:A:2213:ILE:HD12	1:A:2362:VAL:HG22	1.94	0.48
1:A:3721:ARG:HB3	1:A:3724:VAL:HB	1.94	0.48
1:B:3769:THR:O	1:B:3773:LEU:HG	2.14	0.48
1:B:3818:LEU:HB3	1:B:3825:TYR:CE2	2.48	0.48
1:B:3869:ASN:O	1:B:3873:ARG:HG2	2.13	0.48
1:B:4239:PRO:HB2	1:B:4242:ALA:HB3	1.96	0.48
1:A:3124:ASP:N	1:A:3124:ASP:OD2	2.45	0.48
1:A:3207:LYS:NZ	1:A:3758:GLY:O	2.46	0.48
1:A:2671:MET:HG3	1:A:2721:LYS:HD2	1.96	0.48
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.96	0.48
1:A:4156:ASN:ND2	1:A:4191:GLN:OE1	2.46	0.48
1:B:2149:LEU:HD11	1:B:2157:LEU:HD13	1.95	0.48
1:A:3474:ARG:HD3	1:A:3767:ILE:HG21	1.96	0.48
1:B:2508:LEU:HA	1:B:2511:ARG:HG2	1.96	0.48
1:B:3807:ALA:O	1:B:3811:ILE:HG12	2.13	0.48
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.41	0.47
1:B:2441:PHE:HD1	1:B:2449:LEU:HD23	1.79	0.47
1:B:2538:GLU:HB2	1:B:2548:TRP:CE2	2.49	0.47
1:B:3745:LEU:HD13	1:B:3776:GLU:HB2	1.95	0.47
1:A:3990:LEU:HA	1:A:4004:MET:HG2	1.96	0.47
1:B:2964:HIS:ND1	1:B:2965:ARG:O	2.37	0.47
1:B:3749:LEU:HD12	1:B:3773:LEU:HD13	1.96	0.47
1:A:3832:PHE:O	1:A:3835:ILE:HG22	2.13	0.47
1:B:3654:ARG:NH2	1:B:3668:ASP:OD1	2.47	0.47
1:A:2444:GLU:HB3	1:A:2510:MET:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1963:LEU:HB3	1:B:1968:LEU:HD13	1.96	0.47
1:B:2046:ARG:HG2	1:B:2090:LEU:HD13	1.97	0.47
1:A:1907:PRO:O	1:A:1912:LYS:NZ	2.48	0.47
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.47	0.47
1:B:1539:ASP:OD2	1:B:2292:ARG:NH2	2.48	0.47
1:B:2087:ASP:O	1:B:2148:LYS:NZ	2.48	0.47
1:B:2590:PRO:HB2	1:B:2731:VAL:HG12	1.97	0.47
1:B:3609:ILE:HG12	1:B:3632:PRO:HB2	1.97	0.47
1:B:3825:TYR:OH	1:B:4342:LYS:NZ	2.48	0.47
1:B:4222:TRP:HE1	1:B:4246:LEU:HD12	1.80	0.47
1:A:2964:HIS:ND1	1:A:2965:ARG:O	2.38	0.47
1:B:1508:LYS:HG2	1:B:1513:TYR:CZ	2.50	0.47
1:B:1628:ARG:NH2	1:B:1706:GLU:OE2	2.46	0.47
1:A:1792:LEU:HD13	1:A:1812:ILE:HA	1.96	0.47
1:B:1671:SER:HA	1:B:1692:ILE:HB	1.96	0.47
1:B:3071:SER:O	1:B:3075:LEU:HB2	2.14	0.47
1:B:3851:ASP:HB2	1:B:3854:GLN:HG2	1.97	0.47
1:A:2922:ILE:HG12	1:A:2933:LEU:HD21	1.96	0.47
1:B:3544:ARG:HH21	1:B:3547:ILE:HD13	1.80	0.47
1:B:4065:GLN:HB3	1:B:4092:ARG:HH21	1.79	0.46
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	1.98	0.46
1:B:1609:GLY:O	1:B:1613:LYS:HG2	2.15	0.46
1:B:2464:GLN:HG2	1:B:2583:THR:HG23	1.97	0.46
1:B:1490:TRP:HZ3	1:B:1534:PHE:HB3	1.79	0.46
1:B:2784:PHE:HB2	1:B:2794:TYR:HE2	1.80	0.46
1:B:4489:LEU:HD11	1:B:4515:PHE:HE2	1.81	0.46
1:A:4487:LYS:HB2	1:A:4487:LYS:HE3	1.75	0.46
1:B:2370:SER:O	1:B:2374:ILE:HD12	2.15	0.46
1:B:3815:MET:HA	1:B:3818:LEU:HD12	1.97	0.46
1:B:3731:LEU:HD21	1:B:3786:GLU:HG3	1.97	0.46
1:A:3232:LYS:NZ	1:A:3457:GLU:OE1	2.43	0.46
1:A:3869:ASN:O	1:A:3873:ARG:HG2	2.15	0.46
1:B:3126:MET:HG3	1:B:3128:VAL:HG23	1.98	0.46
1:B:2226:SER:HB2	1:B:2726:ARG:HD2	1.98	0.46
1:B:3717:LEU:HD11	1:B:3797:VAL:HG11	1.97	0.46
1:A:2943:LYS:HE2	1:A:3067:THR:HG23	1.97	0.46
1:B:1469:VAL:O	1:B:1473:TYR:HB2	2.16	0.46
1:B:2444:GLU:HG2	1:B:2510:MET:HE1	1.98	0.46
1:B:4575:LEU:HD11	1:B:4624:PHE:HD2	1.81	0.46
1:A:3194:LEU:HD11	1:A:3499:GLN:HG3	1.98	0.46
1:A:4042:LEU:HD12	1:A:4144:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4164:ILE:HD13	1:B:4180:TYR:HD2	1.81	0.46
1:B:2454:CYS:HB3	1:B:2502:LEU:HD12	1.98	0.45
1:B:3990:LEU:HA	1:B:4004:MET:HG2	1.98	0.45
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.98	0.45
1:A:3609:ILE:HG12	1:A:3632:PRO:HB2	1.98	0.45
1:B:3530:THR:HG22	1:B:3534:HIS:CE1	2.52	0.45
1:A:2799:MET:HB3	1:A:2799:MET:HE3	1.80	0.45
1:B:4379:THR:O	1:B:4382:THR:OG1	2.33	0.45
1:A:4511:LEU:HD12	1:A:4563:LEU:HD21	1.99	0.45
1:B:2552:VAL:HG21	1:B:2570:PRO:HB2	1.98	0.45
1:A:1795:SER:HB2	1:A:1808:LEU:HD21	1.97	0.45
1:B:4434:VAL:HA	1:B:4437:VAL:HG22	1.99	0.45
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.99	0.45
1:B:2623:SER:OG	1:B:2624:SER:N	2.50	0.45
1:B:2755:MET:HE1	1:B:2810:LEU:HD12	1.97	0.45
1:B:1665:ILE:HD11	1:B:1683:GLU:HB2	1.97	0.45
1:A:1613:LYS:NZ	1:A:2274:GLU:OE2	2.45	0.45
1:A:1861:MET:HB3	1:A:1864:ALA:HB3	1.98	0.45
1:B:4160:THR:HG23	1:B:4212:LEU:HD21	1.97	0.45
1:A:2623:SER:OG	1:A:2624:SER:N	2.50	0.45
1:A:3946:ASP:OD1	1:A:3946:ASP:N	2.45	0.45
1:A:3581:LYS:HG3	1:A:3582:ARG:HG3	1.99	0.45
1:B:2987:ASN:OD1	1:B:3060:ARG:NH2	2.50	0.45
1:B:4066:ILE:HD11	1:B:4095:MET:HB2	1.98	0.45
1:A:4100:HIS:HB2	1:A:4131:ASN:HD22	1.80	0.44
1:B:1717:LEU:HA	1:B:1749:LEU:HD11	1.98	0.44
1:A:3134:PRO:HG2	1:A:3141:GLU:HG2	1.99	0.44
1:B:2365:SER:OG	1:B:2367:ASP:OD1	2.30	0.44
1:B:3099:THR:HG23	1:B:3148:VAL:HG11	1.98	0.44
1:B:3873:ARG:NH1	1:B:4025:LEU:HD23	2.32	0.44
1:A:1998:THR:HG22	1:A:2007:LYS:HA	1.99	0.44
1:A:2571:THR:H	1:A:2574:THR:HB	1.82	0.44
1:B:1981:ALA:HB2	1:B:1999:CYS:HB3	1.99	0.44
1:A:1766:LEU:HD23	1:A:1833:ALA:HA	1.99	0.44
1:A:2784:PHE:HB2	1:A:2794:TYR:HE2	1.83	0.44
1:B:1742:ILE:HG23	1:B:1807:LYS:HD2	2.00	0.44
1:B:3826:GLN:HG3	1:B:4136:VAL:HG13	1.99	0.44
1:A:2923:ASP:OD2	1:A:2927:ARG:NH1	2.51	0.44
1:A:3776:GLU:O	1:A:3780:VAL:HG23	2.17	0.44
1:B:2813:LEU:HD23	1:B:2816:LEU:HG	1.99	0.44
1:B:3811:ILE:HG22	1:B:3815:MET:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1673:VAL:HB	1:A:1690:VAL:HG22	2.00	0.44
1:A:1699:ASN:OD1	1:A:1700:GLU:N	2.51	0.44
1:A:1720:SER:O	1:A:1724:VAL:HG23	2.17	0.44
1:A:2697:ASP:OD1	1:A:2697:ASP:N	2.48	0.44
1:A:3110:THR:HG21	1:A:3143:ILE:HD11	1.99	0.44
1:B:1594:ILE:HG13	1:B:1597:VAL:HG21	2.00	0.44
1:A:1687:LYS:HG3	1:A:1715:LYS:HD2	1.99	0.44
1:A:2505:ASP:HB3	1:A:2733:VAL:HG13	2.00	0.44
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.52	0.44
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.99	0.44
1:A:3884:ALA:HB1	1:A:4009:VAL:HG11	1.98	0.44
1:A:1667:ASN:HB2	1:A:1672:VAL:HB	2.00	0.44
1:A:4607:LEU:N	1:A:4622:VAL:O	2.44	0.44
1:B:2716:THR:HG23	1:B:4445:THR:HA	1.99	0.44
1:A:3745:LEU:HD11	1:A:3776:GLU:HB3	2.01	0.43
1:B:1466:ILE:HG23	1:B:1500:HIS:HD2	1.82	0.43
1:B:2773:MET:HB3	1:B:2799:MET:HE1	2.00	0.43
1:A:3448:LYS:HE3	1:B:3240:LEU:HD13	1.99	0.43
1:B:3175:HIS:CD2	1:B:3585:ARG:HH22	2.36	0.43
1:A:1835:SER:OG	1:A:1837:GLU:OE1	2.34	0.43
1:A:2667:ASN:ND2	1:A:2713:ASN:O	2.50	0.43
1:A:2808:GLU:HA	1:A:2811:ARG:HE	1.83	0.43
1:B:1888:CYS:HA	1:B:2039:LEU:HD22	2.00	0.43
1:A:1490:TRP:CH2	1:A:1537:TRP:HD1	2.36	0.43
1:A:1508:LYS:HG2	1:A:1513:TYR:CZ	2.53	0.43
1:A:1861:MET:HG3	1:A:1862:ALA:H	1.83	0.43
1:A:2967:TYR:OH	1:A:2975:ASP:OD2	2.29	0.43
1:B:2623:SER:H	1:B:2626:THR:HG1	1.63	0.43
1:B:3735:GLN:HG2	1:B:3783:LYS:HE2	1.99	0.43
1:A:2323:LYS:HB3	1:A:2335:LEU:HB3	2.00	0.43
1:B:3550:THR:O	1:B:3554:SER:OG	2.31	0.43
1:B:4171:LYS:HD3	1:B:4176:ARG:HH22	1.83	0.43
1:A:1867:ASN:O	1:A:1925:ARG:NH1	2.44	0.43
1:B:2657:LYS:O	1:B:2705:ARG:NH1	2.49	0.43
1:A:1752:LEU:HA	1:A:1755:GLN:HE21	1.82	0.43
1:A:2299:GLN:HB2	1:A:2339:VAL:HG22	2.00	0.43
1:A:2447:MET:HB3	1:A:2728:LEU:HD21	2.01	0.43
1:B:1547:LEU:HD23	1:B:1547:LEU:HA	1.87	0.43
1:B:2354:ALA:O	1:B:2358:ARG:HD3	2.19	0.43
1:B:2295:LEU:HD23	1:B:2295:LEU:HA	1.91	0.43
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2452:LEU:HB3	1:A:2729:ARG:HG3	2.01	0.43
1:B:3172:THR:HG21	1:B:3694:SER:HB3	2.01	0.43
1:A:1959:GLU:N	1:A:2017:THR:O	2.52	0.43
1:A:2996:GLU:HB3	1:A:3068:MET:HB3	2.01	0.43
1:B:2085:HIS:HB2	1:B:2361:MET:HE2	2.01	0.43
1:B:3791:MET:HA	1:B:3794:VAL:HG12	1.99	0.43
1:B:4168:ARG:NH2	1:B:4217:ASP:OD1	2.50	0.43
1:B:3770:LEU:HD23	1:B:3773:LEU:HD12	2.01	0.42
1:B:1601:LEU:HD23	1:B:1601:LEU:HA	1.83	0.42
1:B:1619:LEU:HD23	1:B:1619:LEU:HA	1.86	0.42
1:A:1574:GLU:OE1	1:A:1603:ARG:NH1	2.52	0.42
1:A:1930:PHE:HA	1:A:2326:THR:HG21	2.00	0.42
1:B:4460:LEU:HD21	1:B:4478:TRP:CG	2.54	0.42
1:A:2039:LEU:HD12	1:A:4254:GLY:HA2	2.02	0.42
1:B:2527:PRO:HD3	1:B:2545:TRP:CD1	2.54	0.42
1:B:2804:ARG:HD2	1:B:2804:ARG:HA	1.85	0.42
1:B:3822:HIS:O	1:B:3822:HIS:ND1	2.52	0.42
1:B:4609:VAL:HG22	1:B:4642:VAL:HB	2.01	0.42
1:A:3182:HIS:NE2	1:A:3582:ARG:O	2.43	0.42
1:A:3222:LEU:HD12	1:A:3465:LEU:HD23	2.00	0.42
1:A:4002:LEU:O	1:A:4006:HIS:ND1	2.49	0.42
1:B:2257:LYS:HG3	1:B:2306:ASP:HB2	2.00	0.42
1:B:4385:SER:O	1:B:4389:HIS:ND1	2.52	0.42
1:B:1728:GLY:O	1:B:1784:ASN:ND2	2.52	0.42
1:A:1540:VAL:HG21	1:A:1601:LEU:HD22	2.00	0.42
1:B:1688:THR:OG1	1:B:1708:GLU:OE1	2.37	0.42
1:A:2917:ASP:OD2	1:A:2921:ARG:NH2	2.50	0.42
1:B:1587:LEU:HB2	1:B:1590:ASP:HB2	2.02	0.42
1:B:2996:GLU:HB2	1:B:3078:ARG:HH22	1.85	0.42
1:B:3691:ASP:OD1	1:B:3692:LEU:N	2.53	0.42
1:A:2033:LYS:HB2	1:A:2033:LYS:HE3	1.84	0.42
1:B:2697:ASP:N	1:B:2697:ASP:OD1	2.53	0.42
1:B:3717:LEU:HD23	1:B:3717:LEU:HA	1.94	0.42
1:A:2103:VAL:HG23	1:A:2136:ILE:HG23	2.01	0.42
1:B:2449:LEU:HD12	1:B:2453:ARG:HH21	1.85	0.42
1:B:2556:GLU:HB3	1:B:2757:ARG:HH22	1.84	0.42
1:B:3819:LYS:HD2	1:B:3826:GLN:HE22	1.85	0.42
1:B:4223:LEU:HA	1:B:4226:THR:HG22	2.02	0.42
1:A:2356:VAL:HG13	1:A:2361:MET:HE3	2.01	0.41
1:A:3825:TYR:HB2	1:A:3827:TYR:CZ	2.54	0.41
1:B:4460:LEU:HD21	1:B:4478:TRP:CD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2149:LEU:HD11	1:A:2157:LEU:HD22	2.01	0.41
1:A:1946:VAL:HB	1:A:2006:VAL:HG21	2.01	0.41
1:A:2813:LEU:HD21	1:A:2816:LEU:HD13	2.02	0.41
1:B:3175:HIS:HB3	1:B:3516:TYR:HE1	1.84	0.41
1:A:2065:LEU:HD22	1:A:2137:LEU:HD22	2.03	0.41
1:A:2073:PHE:HZ	1:A:2096:VAL:HG21	1.85	0.41
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	2.01	0.41
1:B:2529:ALA:HA	1:B:2530:PRO:HD3	1.95	0.41
1:B:1795:SER:O	1:B:1800:GLN:NE2	2.52	0.41
1:B:2974:GLU:OE1	1:B:2977:ARG:NH1	2.53	0.41
1:A:2600:GLY:HA3	1:A:2603:MET:HE2	2.03	0.41
1:A:2925:ILE:HG21	1:A:2933:LEU:HD13	2.02	0.41
1:B:1708:GLU:OE2	1:B:1712:THR:OG1	2.39	0.41
1:B:2948:ARG:HG2	1:B:2958:VAL:HG11	2.01	0.41
1:B:4288:VAL:HG12	1:B:4290:GLY:H	1.86	0.41
1:A:1490:TRP:CZ2	1:A:1537:TRP:HD1	2.39	0.41
1:A:2265:TYR:OH	1:A:2311:TRP:O	2.25	0.41
1:B:2178:LEU:HA	1:B:2244:LEU:HD11	2.02	0.41
1:B:3167:ARG:HH21	1:B:3685:THR:HB	1.85	0.41
1:A:2256:PRO:HG3	1:A:2303:PHE:HD1	1.84	0.41
1:A:3586:TYR:HA	1:A:3587:PRO:HD3	1.92	0.41
1:A:4385:SER:O	1:A:4389:HIS:ND1	2.54	0.41
1:B:1638:LEU:HD23	1:B:1638:LEU:HA	1.82	0.41
1:B:1937:ASP:OD1	1:B:1938:PHE:N	2.53	0.41
1:B:3154:LEU:HG	1:B:3516:TYR:CD1	2.56	0.41
1:A:3150:VAL:HG22	1:A:3532:TRP:CD1	2.56	0.41
1:A:3604:TYR:HB2	1:A:3609:ILE:HD11	2.01	0.41
1:A:3873:ARG:HH11	1:A:4025:LEU:HD23	1.86	0.41
1:B:2517:TYR:CE1	1:B:2521:ILE:HD12	2.56	0.41
1:B:2532:ILE:HA	1:B:2533:PRO:HD3	1.91	0.41
1:A:1601:LEU:HA	1:A:1601:LEU:HD23	1.81	0.41
1:A:4165:PRO:HG2	1:A:4168:ARG:HB3	2.01	0.41
1:B:1747:ALA:HA	1:B:1807:LYS:HG3	2.02	0.41
1:B:1972:SER:HB2	1:B:2032:LEU:HB2	2.02	0.41
1:B:2446:ILE:HD11	1:B:2735:TYR:CG	2.56	0.41
1:A:1891:THR:HG21	1:A:2039:LEU:HB2	2.03	0.40
1:A:2223:VAL:HG13	1:A:2363:TRP:HE3	1.86	0.40
1:A:2498:ILE:O	1:A:2502:LEU:HB2	2.21	0.40
1:A:2834:GLN:HE21	1:A:2843:ARG:HB3	1.85	0.40
1:A:3175:HIS:HB3	1:A:3516:TYR:HE1	1.86	0.40
1:B:2443:LEU:HB3	1:B:2510:MET:SD	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1466:ILE:HG12	1:B:1500:HIS:CD2	2.55	0.40
1:B:2755:MET:HE1	1:B:2806:ILE:HG22	2.04	0.40
1:B:3708:LEU:HD23	1:B:3809:SER:HA	2.02	0.40
1:A:2518:ILE:O	1:A:2522:THR:HG22	2.21	0.40
1:B:1626:PHE:HB3	1:B:1629:PHE:CD2	2.57	0.40
1:B:1879:LEU:HD11	1:B:1914:GLU:HB3	2.03	0.40
1:B:2065:LEU:HD22	1:B:2137:LEU:HD22	2.03	0.40
1:B:2386:PRO:HB3	1:B:2413:LEU:HB2	2.03	0.40
1:B:2495:VAL:HG21	1:B:2524:VAL:HG11	2.03	0.40
1:A:1619:LEU:HD21	1:A:1638:LEU:HD23	2.03	0.40
1:B:2426:TYR:OH	1:B:2491:GLN:NE2	2.54	0.40
1:B:4152:GLY:HA2	1:B:4316:GLN:NE2	2.36	0.40
1:A:1723:GLU:HA	1:A:1726:ILE:HG12	2.03	0.40
1:A:2206:LYS:HA	1:A:2206:LYS:HD2	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2892/4843 (60%)	2806 (97%)	85 (3%)	1 (0%)	100	100
1	B	2892/4843 (60%)	2819 (98%)	72 (2%)	1 (0%)	100	100
All	All	5784/9686 (60%)	5625 (97%)	157 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2472/4279 (58%)	2472 (100%)	0	100	100
1	B	2472/4279 (58%)	2470 (100%)	2 (0%)	92	98
All	All	4944/8558 (58%)	4942 (100%)	2 (0%)	100	100

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

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1736	ASN
1	A	1748	GLN
1	A	1755	GLN
1	A	1817	HIS
1	A	1863	ASN
1	A	1894	GLN
1	A	1922	GLN
1	A	1950	GLN
1	A	1976	GLN
1	A	1985	HIS
1	A	2005	GLN
1	A	2314	ASN
1	A	2464	GLN
1	A	2485	GLN
1	A	2646	ASN
1	A	2827	HIS
1	A	2886	GLN
1	A	2960	GLN
1	A	2998	ASN
1	A	3092	ASN

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Mol	Chain	Res	Type
1	A	3158	ASN
1	A	3622	ASN
1	A	3667	GLN
1	A	3792	GLN
1	A	3800	GLN
1	A	3830	GLN
1	A	3843	ASN
1	A	3865	GLN
1	A	4023	GLN
1	A	4063	ASN
1	A	4156	ASN
1	A	4436	GLN
1	A	4453	ASN
1	A	4566	GLN
1	B	1500	HIS
1	B	1598	GLN
1	B	1670	ASN
1	B	1736	ASN
1	B	1818	GLN
1	B	2215	GLN
1	B	2485	GLN
1	B	2621	ASN
1	B	3014	ASN
1	B	3057	GLN
1	B	3069	ASN
1	B	3152	GLN
1	B	3498	ASN
1	B	3526	GLN
1	B	3535	HIS
1	B	3667	GLN
1	B	3830	GLN
1	B	4023	GLN
1	B	4078	ASN
1	B	4098	ASN
1	B	4436	GLN
1	B	4488	GLN
1	B	4506	ASN
1	B	4508	HIS
1	B	4526	GLN
1	B	4566	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	A	4801	4	24,29,29	0.86	0	29,45,45	1.24	2 (6%)
2	ADP	B	4803	-	24,29,29	0.92	0	29,45,45	1.20	2 (6%)
2	ADP	B	4804	-	24,29,29	0.89	0	29,45,45	1.18	2 (6%)
2	ADP	A	4803	-	24,29,29	0.92	1 (4%)	29,45,45	1.21	2 (6%)
2	ADP	A	4804	-	24,29,29	0.88	0	29,45,45	1.19	2 (6%)
3	ATP	B	4802	4	28,33,33	0.67	0	34,52,52	0.61	1 (2%)
2	ADP	B	4801	4	24,29,29	0.87	0	29,45,45	1.23	2 (6%)
3	ATP	A	4802	4	28,33,33	0.66	0	34,52,52	0.61	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	4801	4	-	1/12/32/32	0/3/3/3
2	ADP	B	4803	-	-	2/12/32/32	0/3/3/3
2	ADP	B	4804	-	-	2/12/32/32	0/3/3/3
2	ADP	A	4803	-	-	1/12/32/32	0/3/3/3
2	ADP	A	4804	-	-	3/12/32/32	0/3/3/3
3	ATP	B	4802	4	-	2/18/38/38	0/3/3/3
2	ADP	B	4801	4	-	3/12/32/32	0/3/3/3
3	ATP	A	4802	4	-	3/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4803	ADP	O4'-C1'	2.10	1.43	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4801	ADP	N3-C2-N1	-3.92	123.35	128.67
2	A	4803	ADP	N3-C2-N1	-3.84	123.46	128.67
2	B	4803	ADP	N3-C2-N1	-3.76	123.57	128.67
2	B	4801	ADP	N3-C2-N1	-3.72	123.62	128.67
2	A	4804	ADP	N3-C2-N1	-3.69	123.67	128.67
2	B	4804	ADP	N3-C2-N1	-3.60	123.79	128.67
2	B	4801	ADP	C4-C5-N7	-2.62	106.56	109.34
2	B	4804	ADP	C4-C5-N7	-2.60	106.59	109.34
2	A	4804	ADP	C4-C5-N7	-2.54	106.65	109.34
2	A	4801	ADP	C4-C5-N7	-2.52	106.67	109.34
2	B	4803	ADP	C4-C5-N7	-2.42	106.78	109.34
2	A	4803	ADP	C4-C5-N7	-2.39	106.81	109.34
3	B	4802	ATP	C5-C6-N6	2.33	123.86	120.31
3	A	4802	ATP	C5-C6-N6	2.30	123.82	120.31

There are no chirality outliers.

All (17) torsion outliers are listed below:

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

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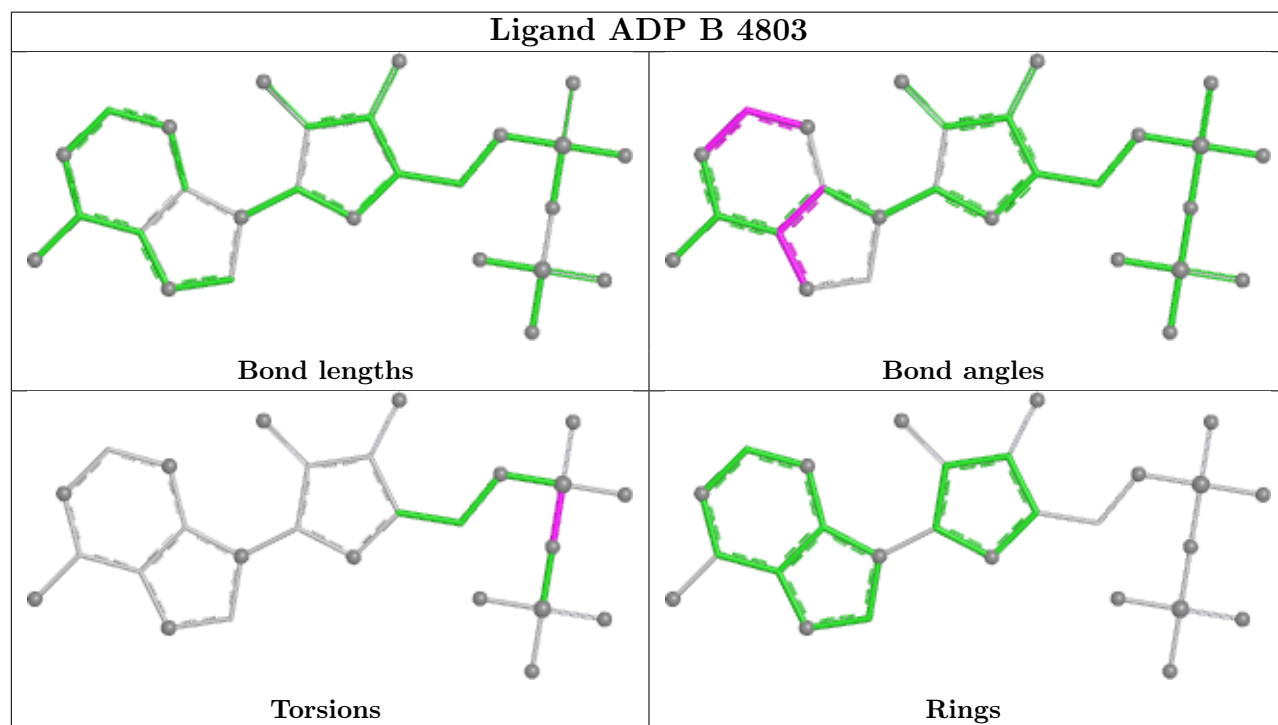
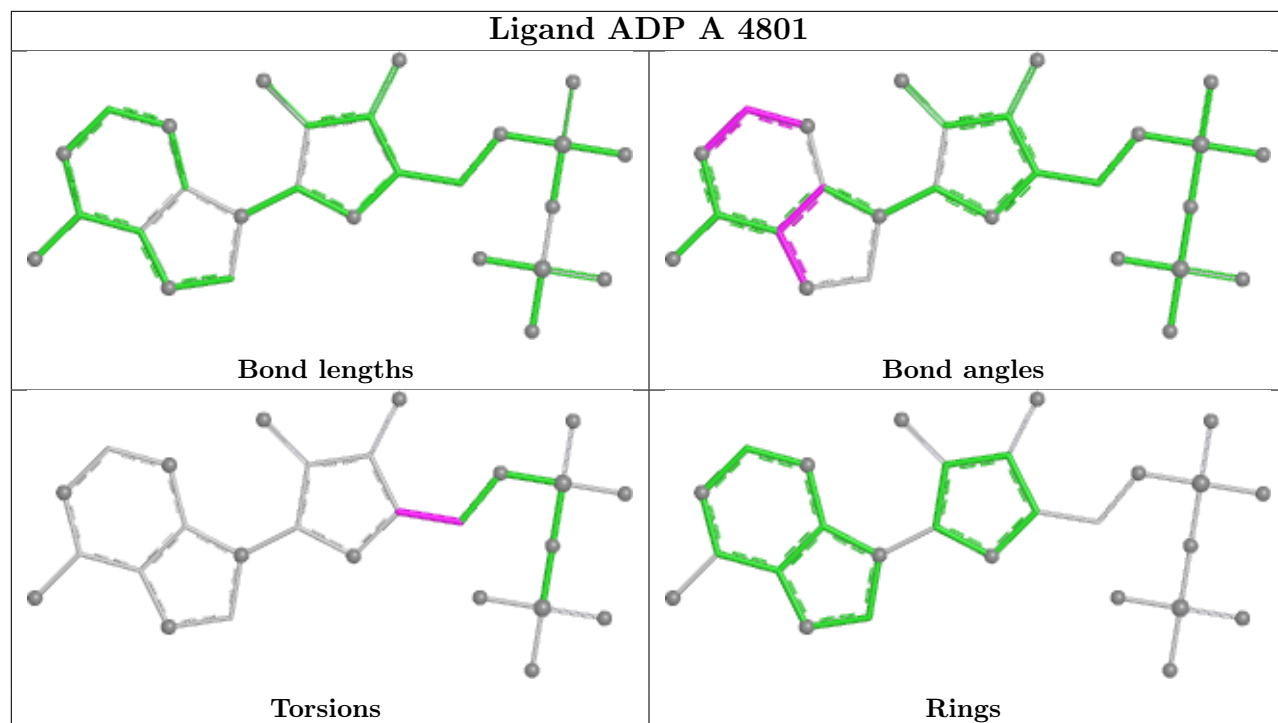
Mol	Chain	Res	Type	Atoms
2	B	4801	ADP	O4'-C4'-C5'-O5'
2	A	4801	ADP	O4'-C4'-C5'-O5'
2	B	4803	ADP	PB-O3A-PA-O2A
3	A	4802	ATP	PB-O3A-PA-O1A
2	A	4804	ADP	C5'-O5'-PA-O1A
2	A	4803	ADP	PB-O3A-PA-O2A
3	A	4802	ATP	PG-O3B-PB-O2B
3	B	4802	ATP	PG-O3B-PB-O1B
3	B	4802	ATP	PG-O3B-PB-O2B
2	B	4801	ADP	C3'-C4'-C5'-O5'
2	B	4803	ADP	PB-O3A-PA-O1A
3	A	4802	ATP	PB-O3A-PA-O2A

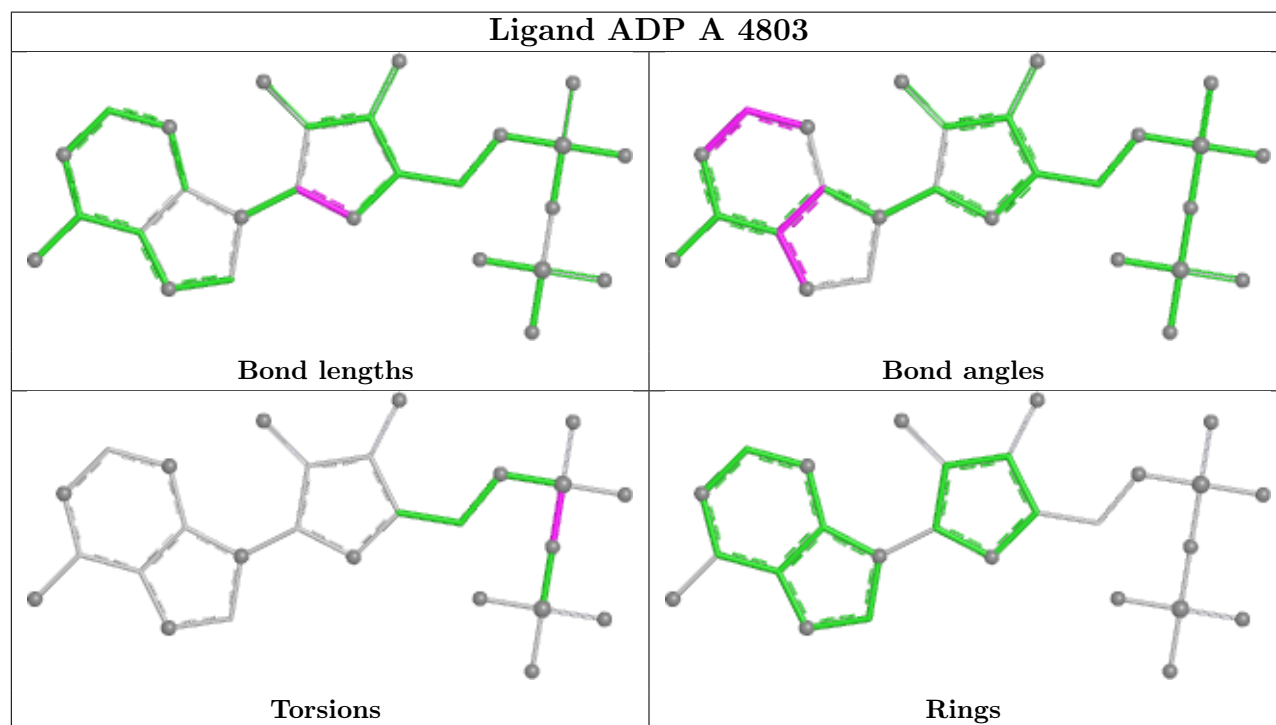
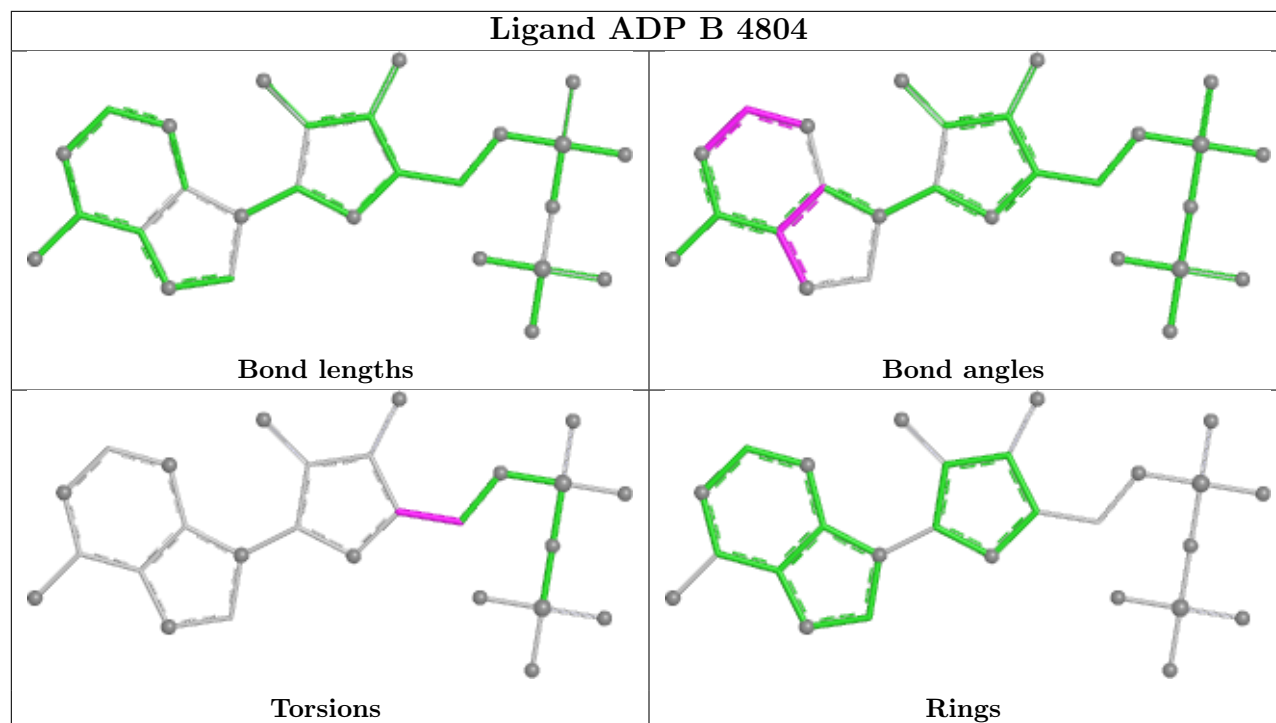
There are no ring outliers.

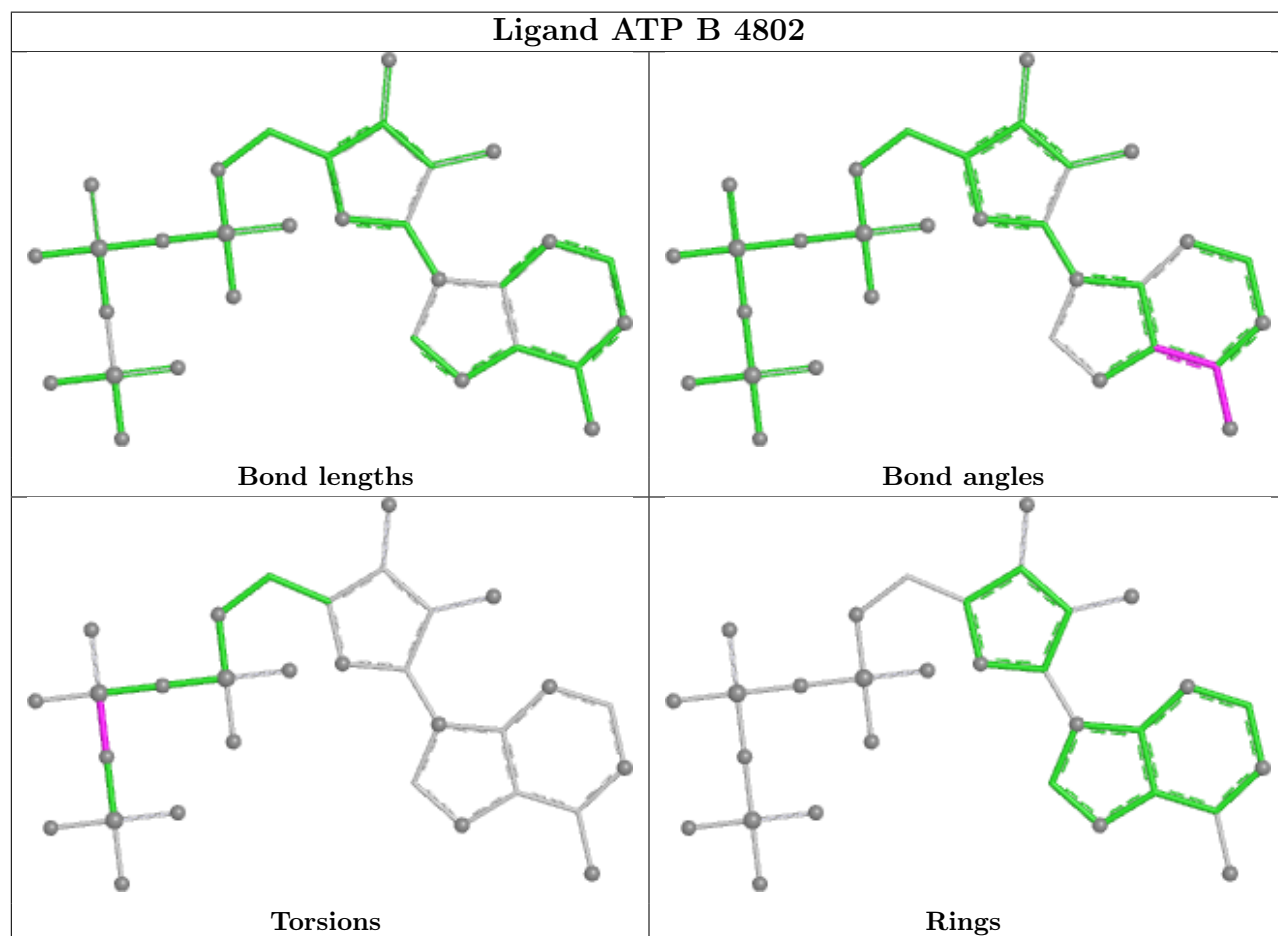
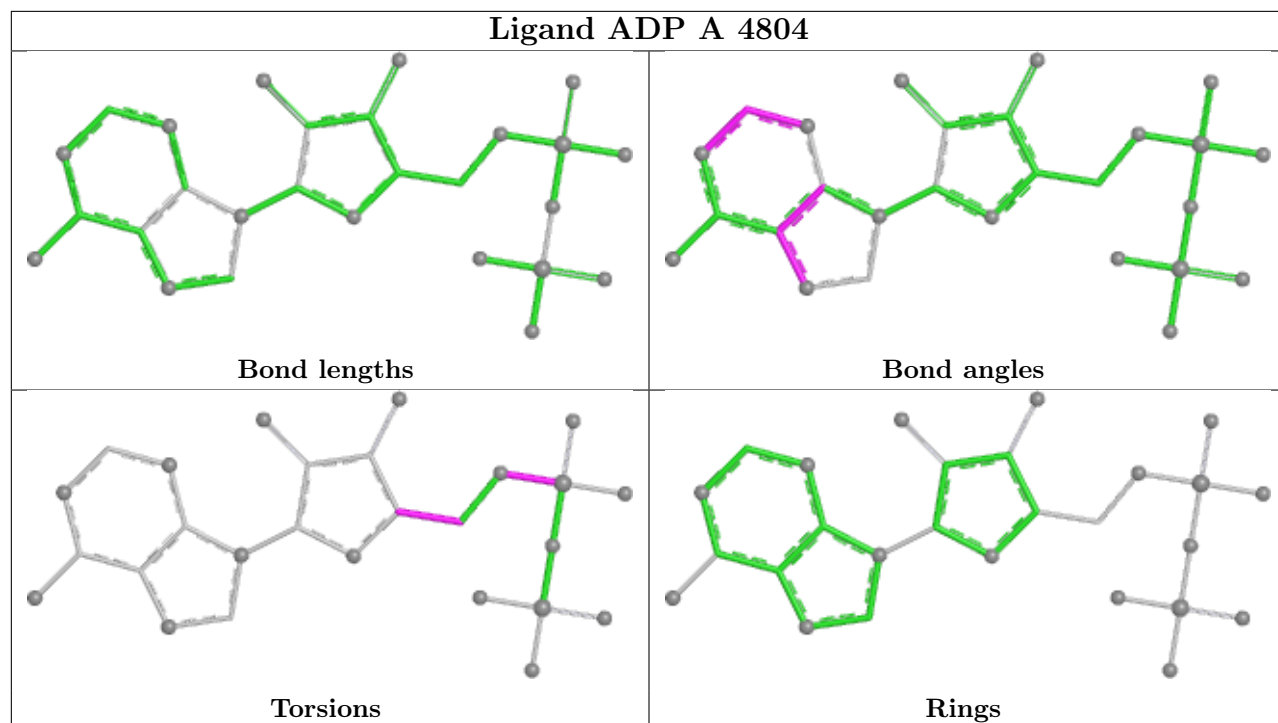
1 monomer is involved in 1 short contact:

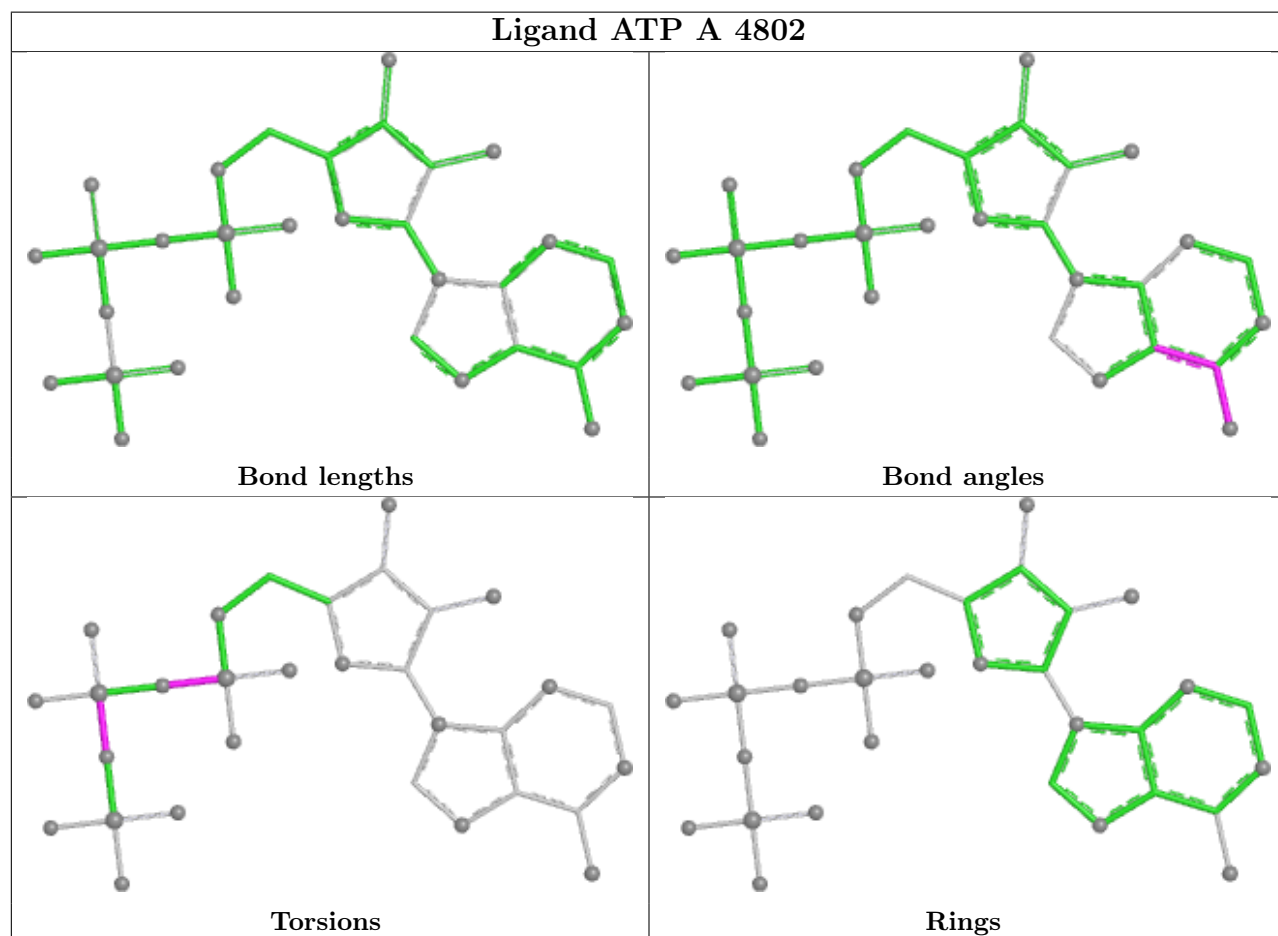
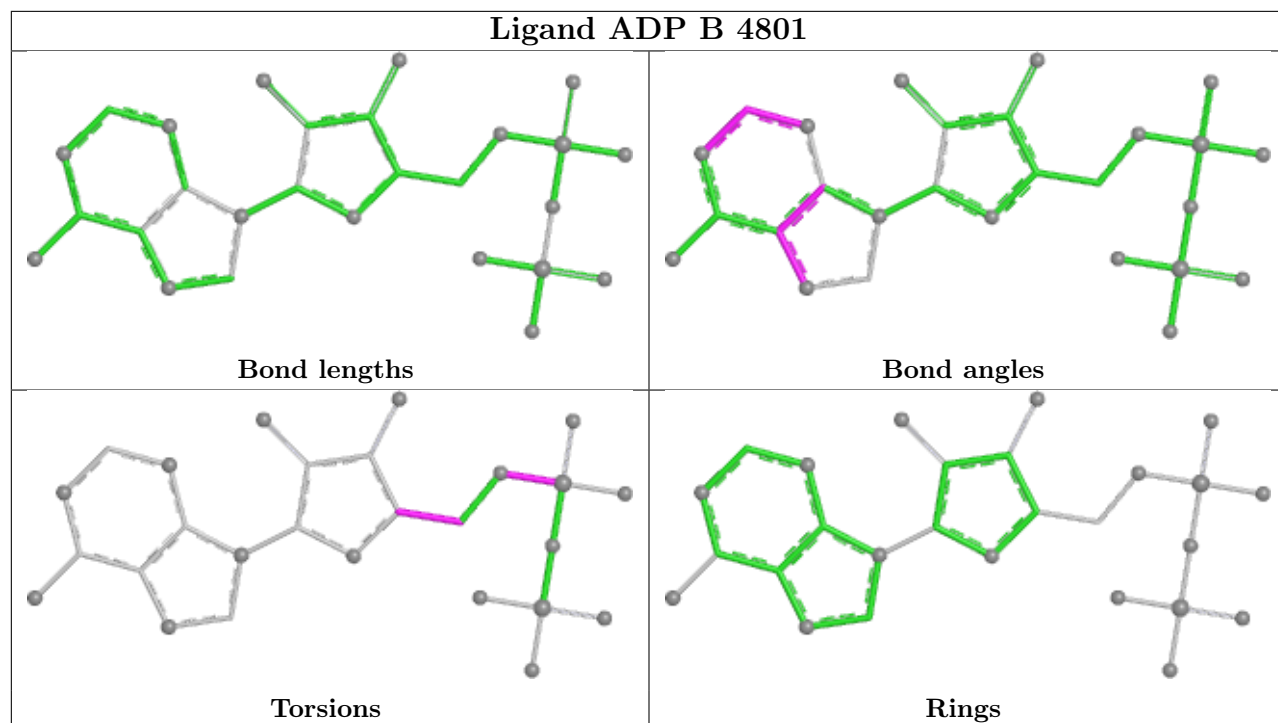
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4803	ADP	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

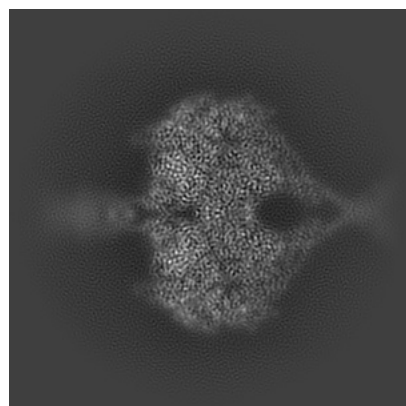
6 Map visualisation [i](#)

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

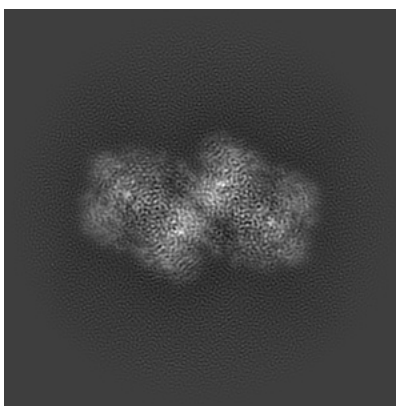
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

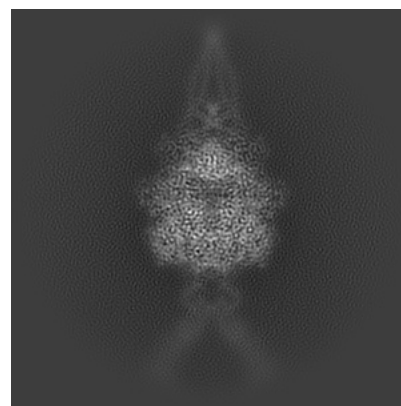
6.1.1 Primary map



X

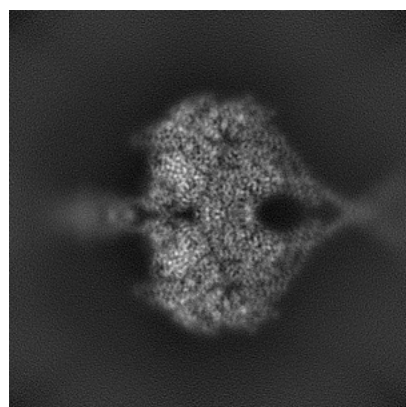


Y

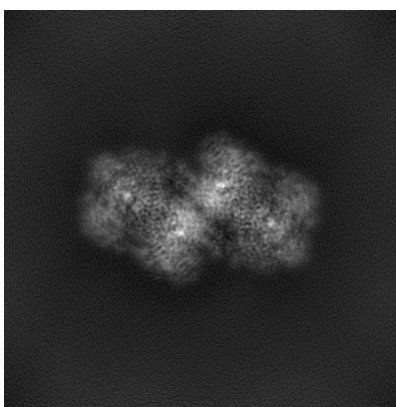


Z

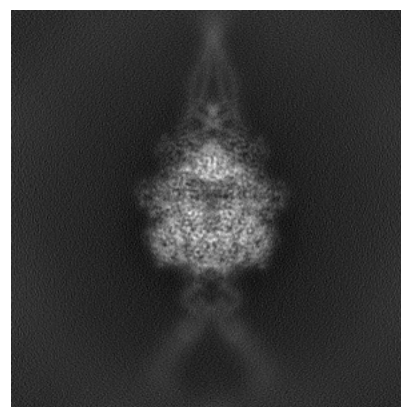
6.1.2 Raw map



X



Y

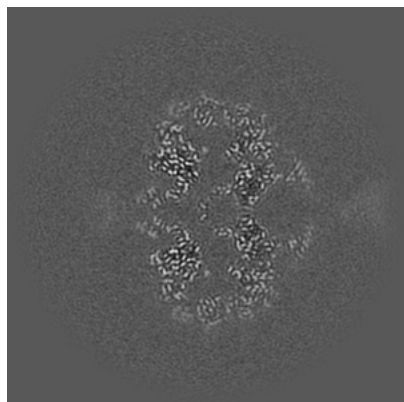


Z

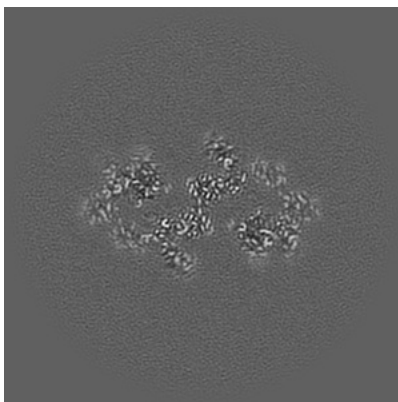
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

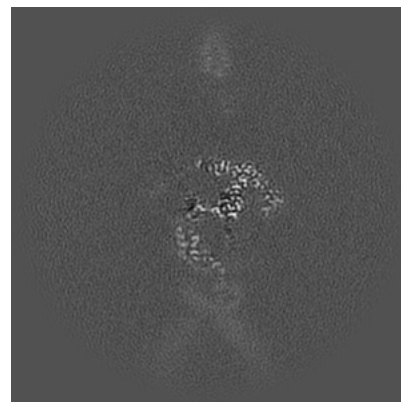
6.2.1 Primary map



X Index: 176

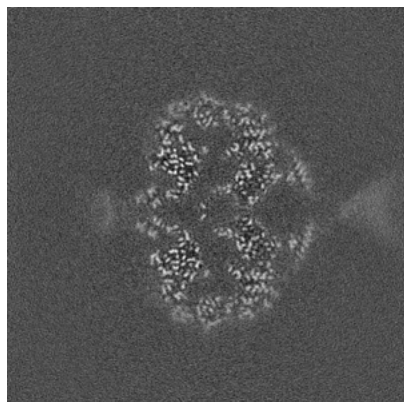


Y Index: 176

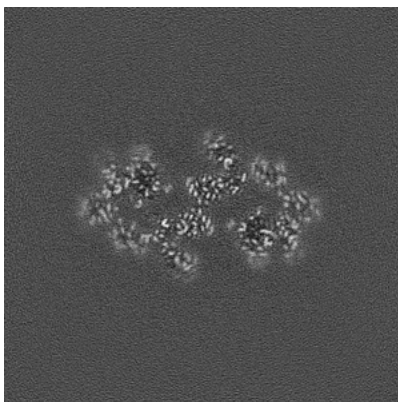


Z Index: 176

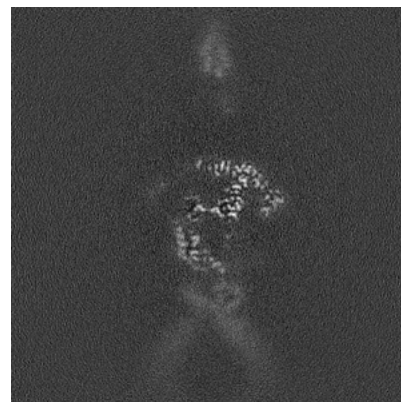
6.2.2 Raw map



X Index: 176



Y Index: 176

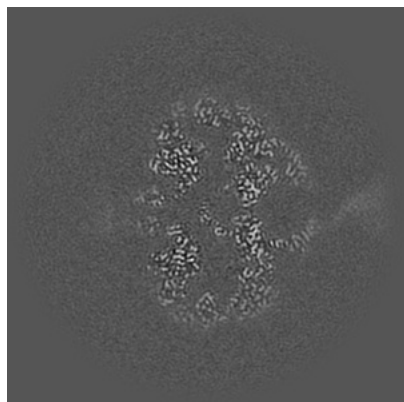


Z Index: 176

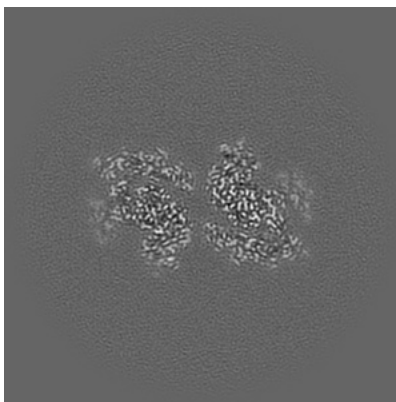
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

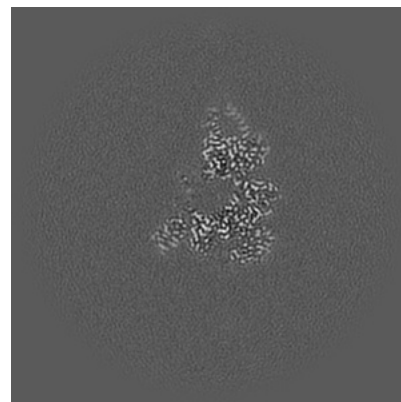
6.3.1 Primary map



X Index: 174

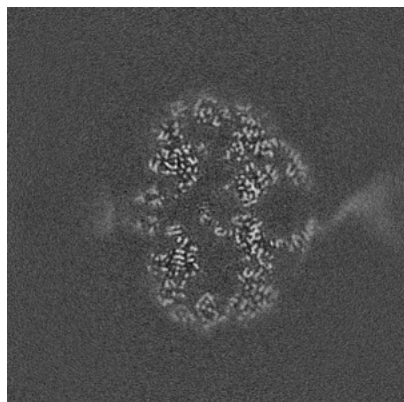


Y Index: 153

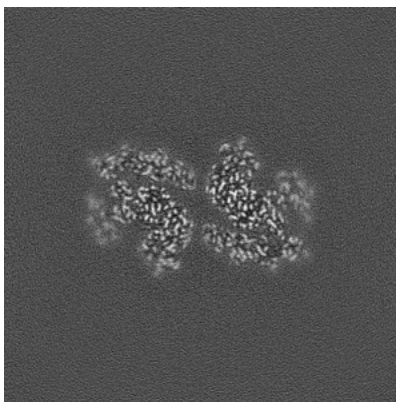


Z Index: 203

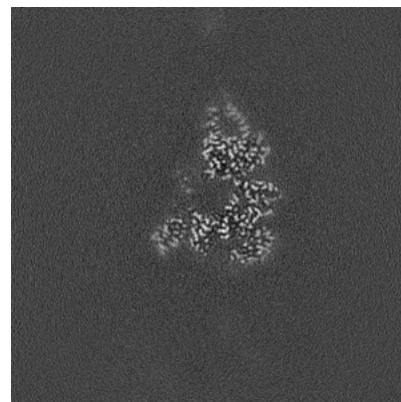
6.3.2 Raw map



X Index: 174



Y Index: 154

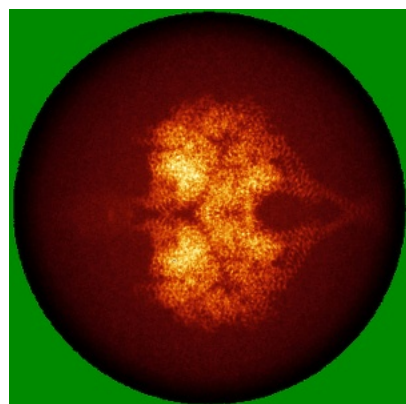


Z Index: 203

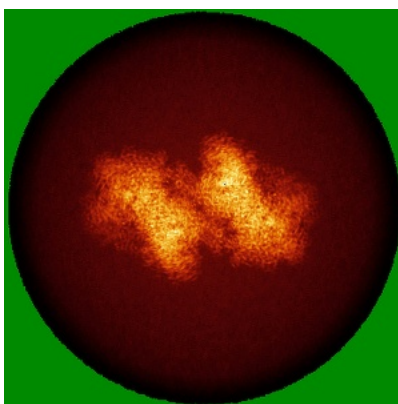
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

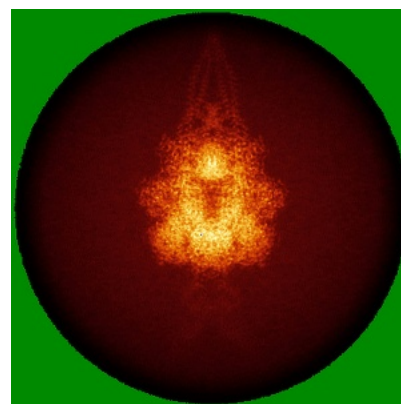
6.4.1 Primary map



X

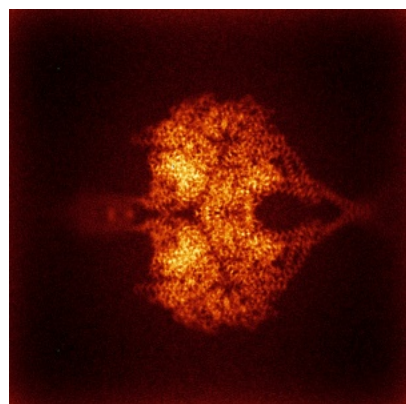


Y

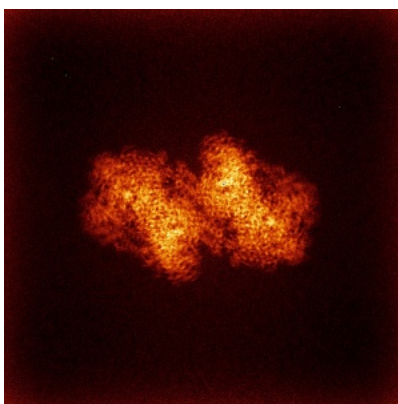


Z

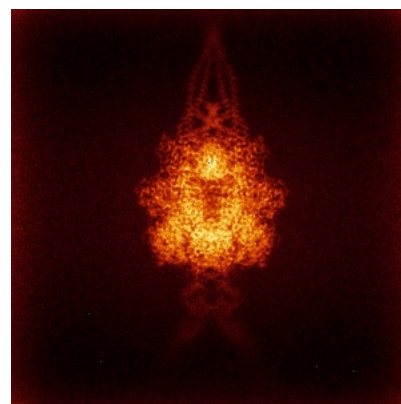
6.4.2 Raw map



X



Y

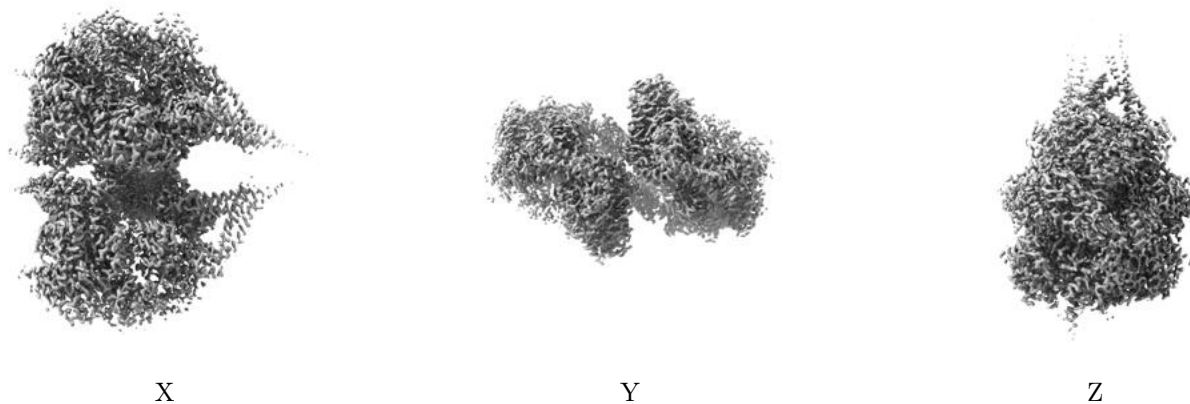


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

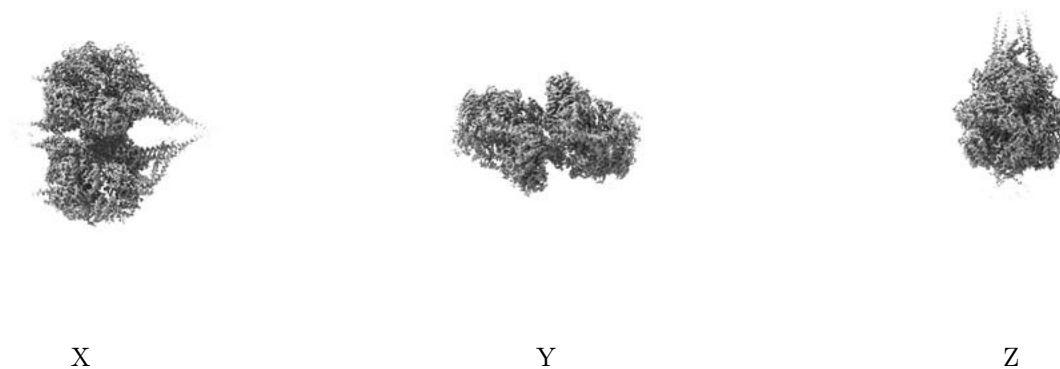
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

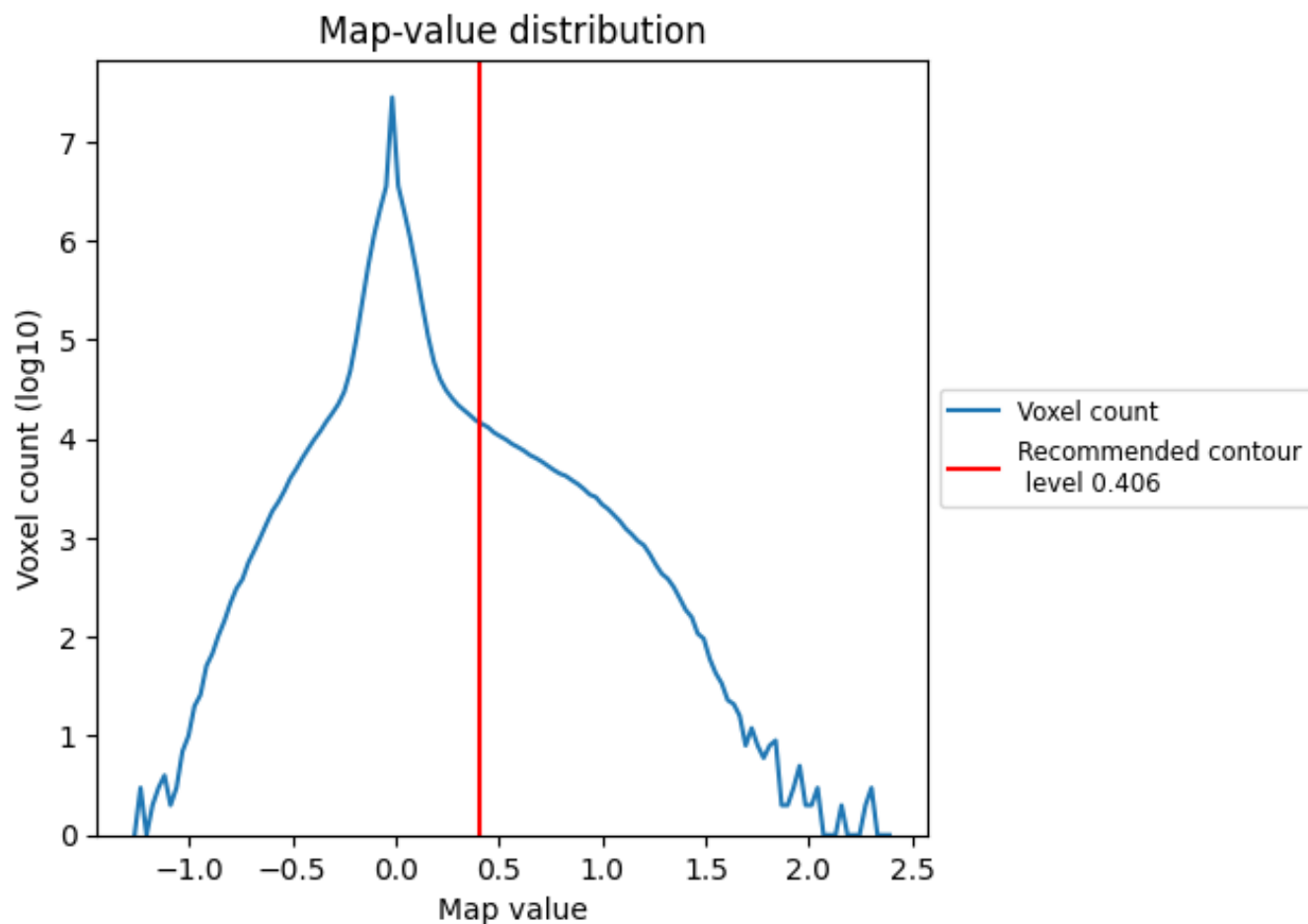
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

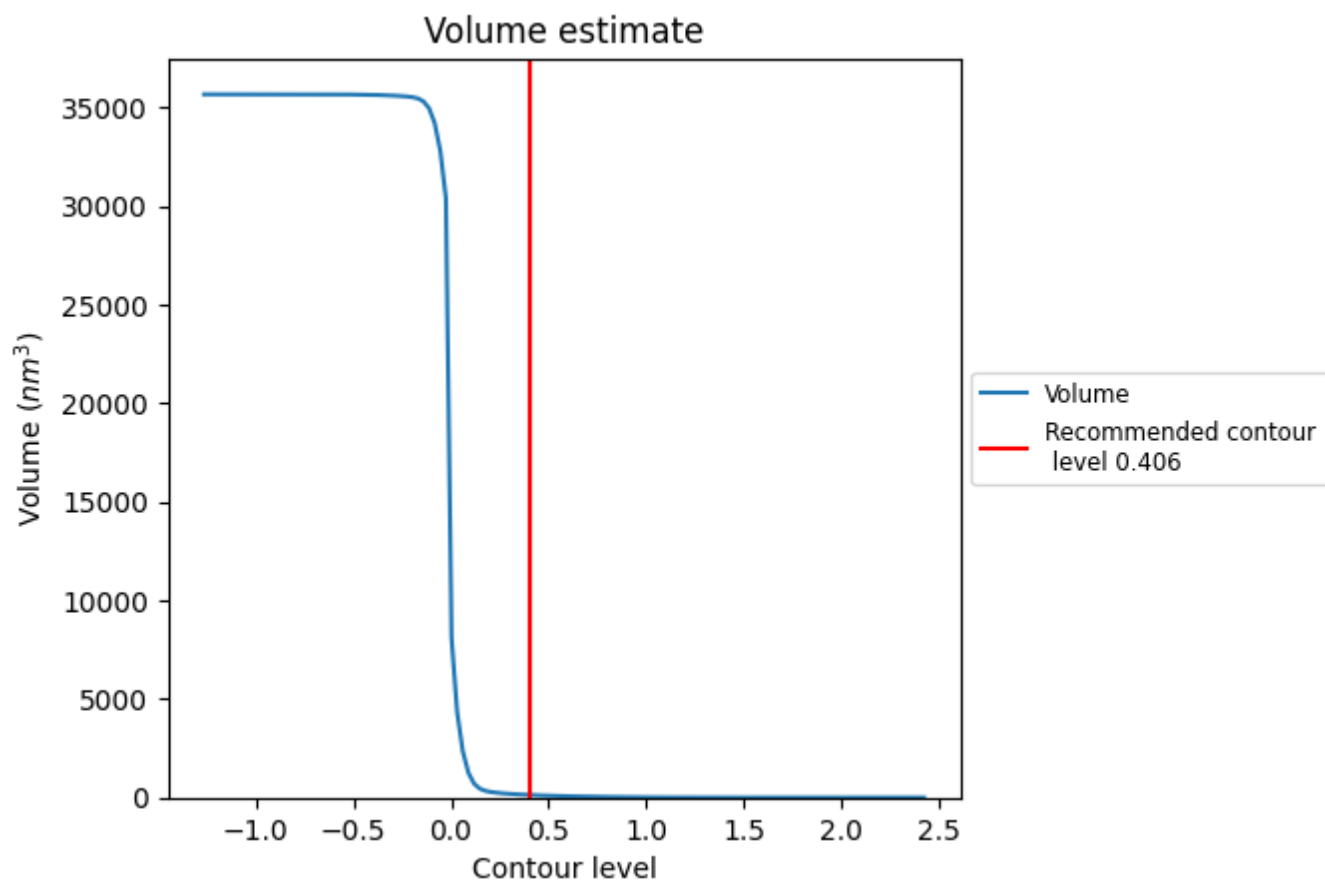
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

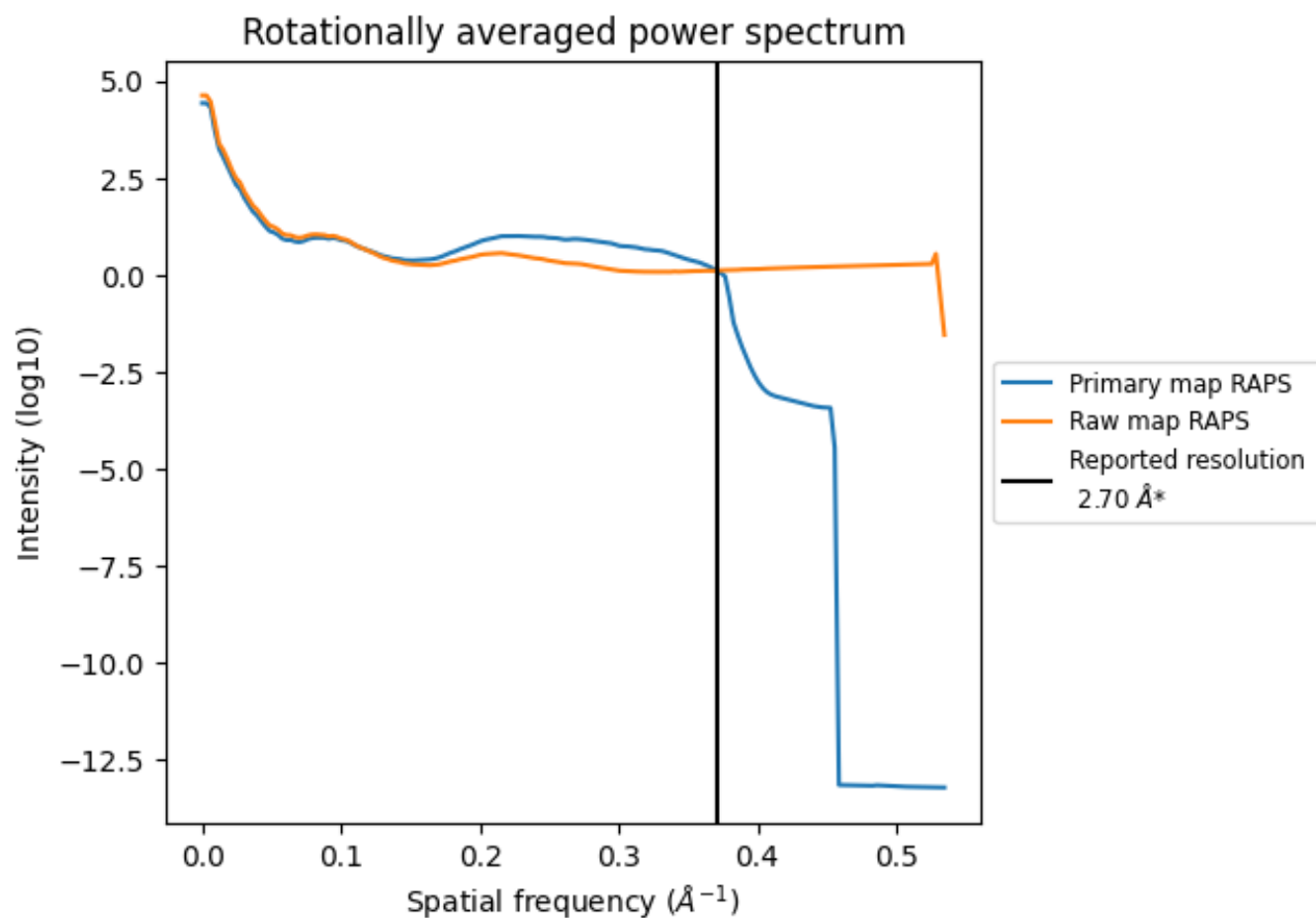
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 130 nm³; this corresponds to an approximate mass of 117 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

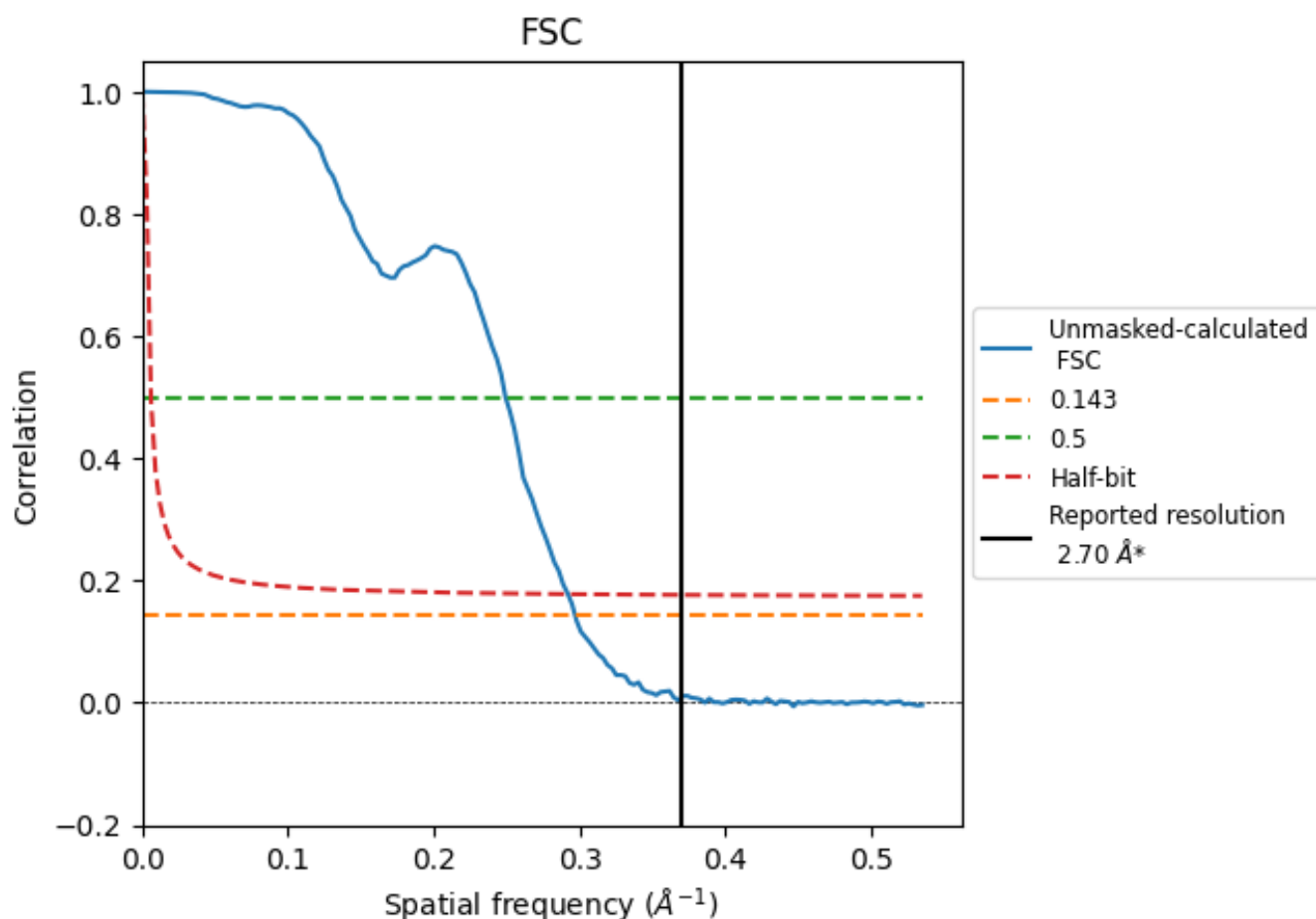


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

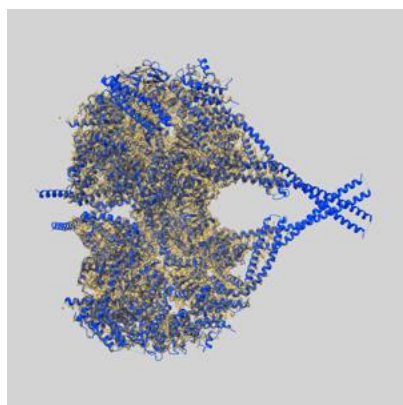
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.37	4.01	3.43

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

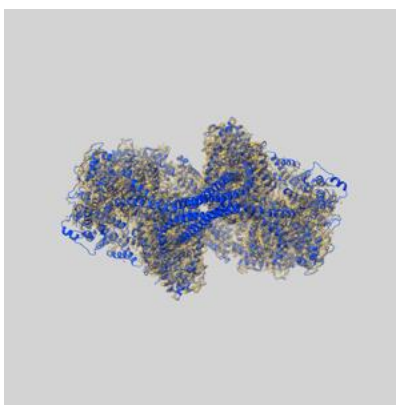
9 Map-model fit [i](#)

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

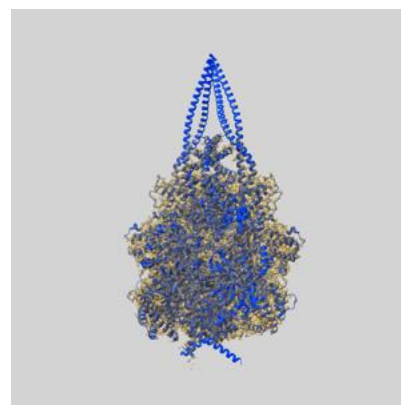
9.1 Map-model overlay [i](#)



X



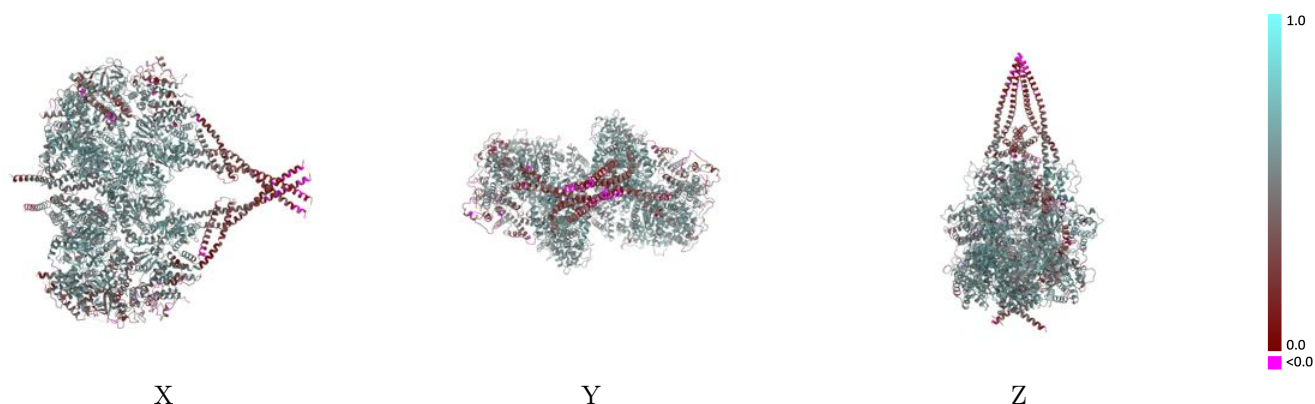
Y



Z

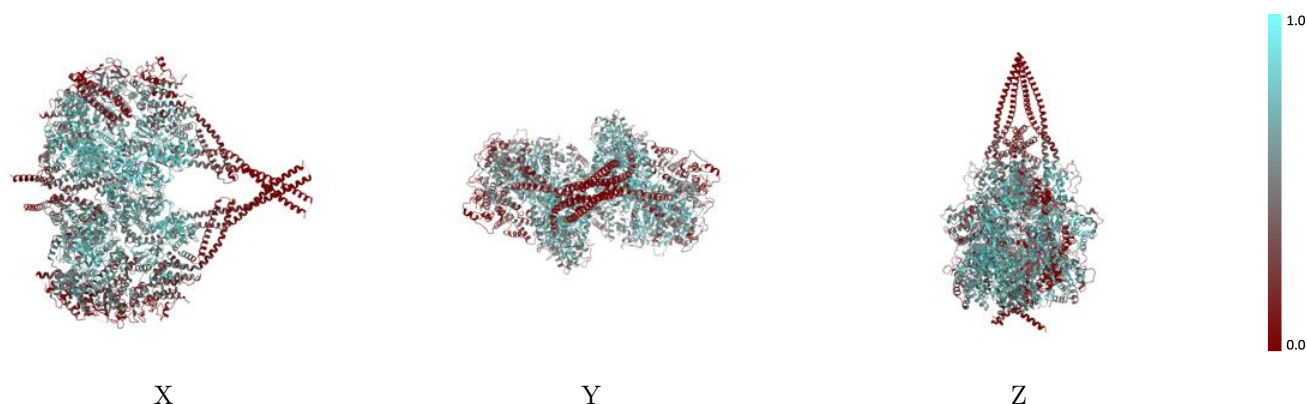
The images above show the 3D surface view of the map at the recommended contour level 0.406 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



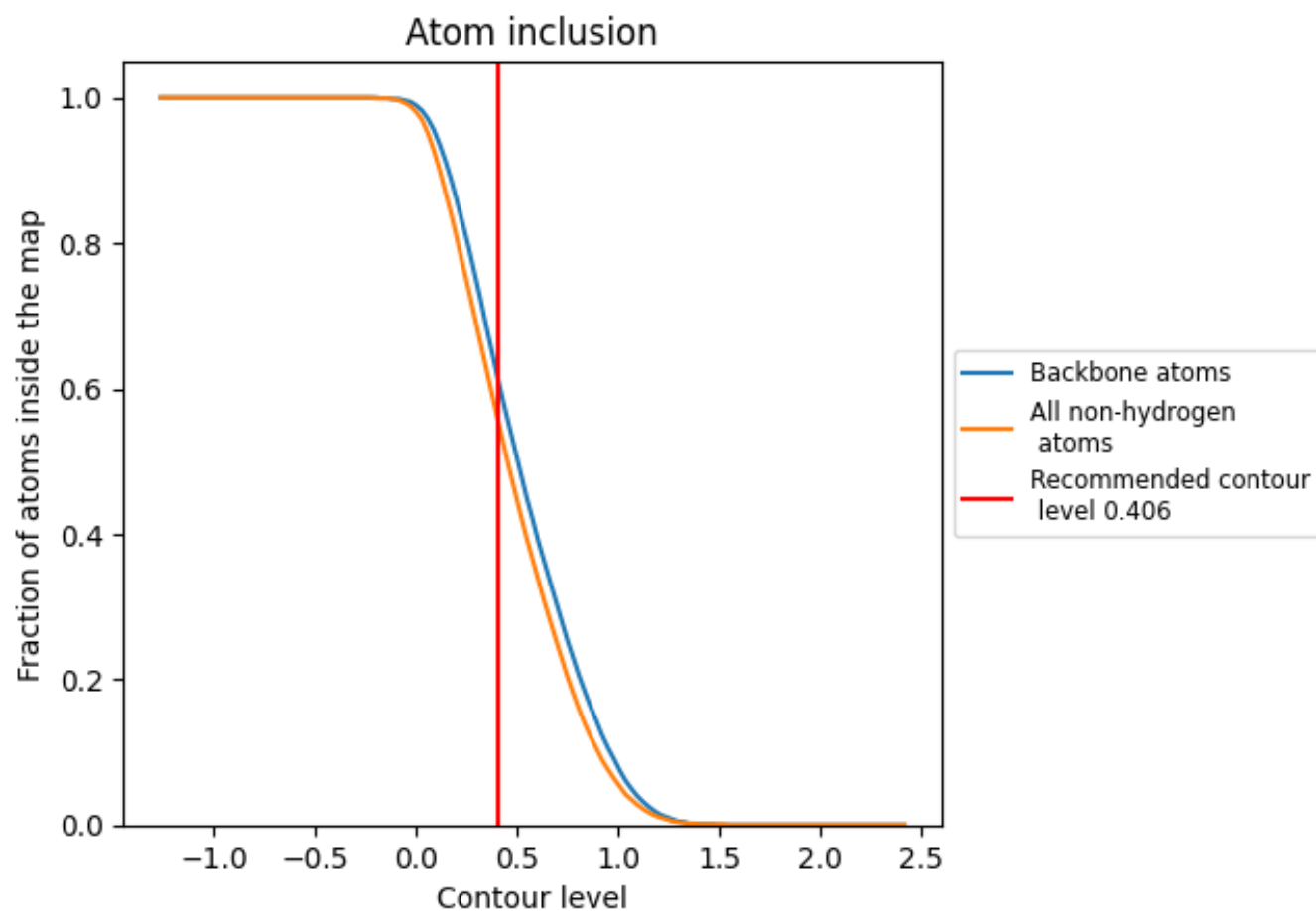
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.406).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.406) and Q-score for the entire model and for each chain.

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

