



## Full wwPDB EM Validation 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 Full wwPDB EM Validation 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

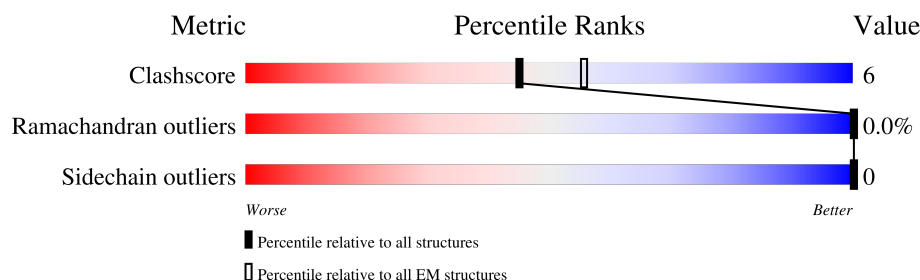
# 1 Overall quality at a glance

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

## 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...*

*Continued from previous page...*

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

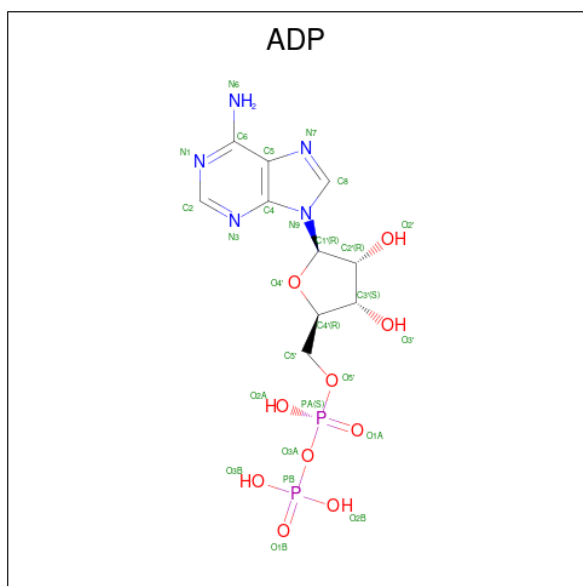
- Molecule 2 is a protein called Platelet-activating factor acetylhydrolase IB subunit beta.

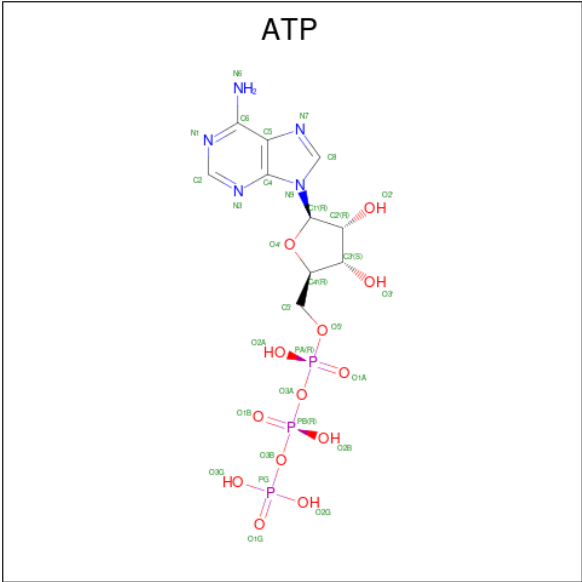
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	320	Total	C	N	O	S	0	0
			2493	1570	437	466	20		
2	C	306	Total	C	N	O	S	0	0
			2372	1497	413	442	20		

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
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	P2613	W2510	LYS	E2248	GLU	GLY	Y1845
SER	Q3248	A3162	G3023	R2889	L2773	D2614	R2511	ASP	G2256	VAL	ASP	F1846
ALA	E3249	R3164	D3024	R2890	F2784	P2617	E2512	GLY	P2256	ASP	ASP	D1847
ASN	A3250	G3165	E3025	E2904	T2785	V2617	E2513	GLY	K2257	GLY	GLY	P1848
PRO	E3251	G3166	K3034	D2906	Q2786	S2623	E2514	GLU	A2258	ILE	GLU	K1849
LEU	K3252	R3167	A3037	N2913	D2787	S2624	G2515	ALA	D2269	A2128	GLU	Q1850
VAL	L3253	V2914	Q3038	E2914	Y2794	P2628	E2516	ALA	E2270	E2129	ILE	T1851
LYS	G3167	L2915	Q3039	V2916	R2797	K2633	R2519	ALA	E2271	E2130	LYS	D1852
LEU	T3168	L2916	E3040	L2920	E2798	T2644	R2520	ALA	E2272	E2131	LEU	Q1856
LEU	K3169	L2917	G3041	L2921	N2799	P2645	T2521	ALA	E2273	E2132	LEU	L1857
GLN	T3172	L2918	L3042	L2925	R2804	N2646	V2524	ALA	E2274	E2133	GLN	M1861
GLN	P3173	L2919	D3045	L2933	R2811	G2647	P2525	ALA	E2275	E2134	GLN	A1862
GLN	R3174	L2920	H3047	L2934	L2650	L2650	P2526	ALA	E2276	E2135	GLN	N1863
GLN	H3175	L2921	E3048	L2935	L2651	L2651	P2527	ALA	E2277	E2136	GLN	V1880
GLN	L3194	L2922	E3049	K2943	L2652	L2652	T2528	ALA	E2278	E2137	GLN	L1881
GLN	T3208	L2923	T3067	V2958	L2653	L2653	A2529	ALA	E2279	E2138	GLN	T1882
GLN	K3209	L2924	S3071	L2961	L2654	L2654	P2530	ALA	E2280	E2139	GLN	F1883
GLN	E3210	L2925	S3072	H2964	L2655	L2655	P2531	ALA	E2281	E2140	GLN	L1884
GLN	T3211	L2926	Q3073	R2965	L2656	L2656	T2532	ALA	E2282	E2141	GLN	Q1894
GLN	V3212	L2927	G3074	R2966	L2657	L2657	L2541	ALA	E2283	E2142	GLN	E1914
GLN	D3213	L2928	L3075	V2967	L2658	L2658	E2544	ALA	E2284	E2143	GLN	L1928
GLN	L3218	L2929	A3080	T2968	L2659	L2659	W2545	ALA	E2285	E2144	GLN	V1929
GLN	R3219	L2930	T3081	G2969	L2660	L2660	S2546	ALA	E2286	E2145	GLN	F1930
GLN	R3220	L2931	L3091	D2973	L2661	L2661	P2553	ALA	E2287	E2146	GLN	N1931
GLN	D3221	L2932	F3094	E2974	L2662	L2662	Q2554	ALA	E2288	E2147	GLN	V1946
GLN	L3222	L2933	W3097	D2975	L2663	L2663	T2555	ALA	E2289	E2148	GLN	Q1950
GLN	R3223	L2934	K3112	R2976	L2664	L2664	E2556	ALA	E2290	E2149	GLN	D2077
GLN	T3224	L2935	M3113	L2977	L2665	L2665	E2557	ALA	E2291	E2150	GLN	R1966
GLN	K3225	L2936	E3116	R2982	L2666	L2666	E2558	ALA	E2292	E2151	GLN	M1967
GLN	S3226	L2937	M3119	E2983	L2667	L2667	E2559	ALA	E2293	E2152	GLN	L1968
GLN	Q3227	L2938	P3123	K2988	L2668	L2668	E2560	ALA	E2294	E2153	GLN	Q1974
GLN	E3228	L2939	D3124	N2998	L2669	L2669	E2561	ALA	E2295	E2154	GLN	E1980
GLN	L3229	L2940	Y3125	V2999	L2670	L2670	E2562	ALA	E2296	E2155	GLN	A1981
GLN	V3231	L2941	K3126	L3000	L2671	L2671	E2563	ALA	E2297	E2156	GLN	E1984
GLN	K3232	L2942	P3127	D3001	L2672	L2672	E2564	ALA	E2298	E2157	GLN	H1985
GLN	A3234	L2943	A3236	D3002	L2673	L2673	E2565	ALA	E2299	E2158	GLN	S1986
GLN	A3235	L2944	A3237	D3003	L2674	L2674	E2566	ALA	E2300	E2159	GLN	N1987
GLN	A3236	L2945	A3238	D3004	L2675	L2675	E2567	ALA	E2301	E2160	GLN	PRO
GLN	A3237	L2946	A3239	D3005	L2676	L2676	E2568	ALA	E2302	E2161	GLN	ASN
GLN	A3238	L2947	A3240	D3006	L2677	L2677	E2569	ALA	E2303	E2162	GLN	TYR
GLN	A3239	L2948	A3241	D3007	L2678	L2678	E2570	ALA	E2304	E2163	GLN	ASP
GLN	A3240	L2949	A3242	D3008	L2679	L2679	E2571	ALA	E2305	E2164	GLN	
GLN	A3241	L2950	A3243	D3009	L2680	L2680	E2572	ALA	E2306	E2165	GLN	
GLN	A3242	L2951	A3244	D3010	L2681	L2681	E2573	ALA	E2307	E2166	GLN	
GLN	A3243	L2952	A3245	D3011	L2682	L2682	E2574	ALA	E2308	E2167	GLN	
GLN	A3244	L2953	A3246	D3012	L2683	L2683	E2575	ALA	E2309	E2168	GLN	
GLN	A3245	L2954	A3247	D3013	L2684	L2684	E2576	ALA	E2310	E2169	GLN	
GLN	A3246	L2955	A3248	D3014	L2685	L2685	E2577	ALA	E2311	E2170	GLN	
GLN	A3247	L2956	A3249	D3015	L2686	L2686	E2578	ALA	E2312	E2171	GLN	
GLN	A3248	L2957	A3250	D3016	L2687	L2687	E2579	ALA	E2313	E2172	GLN	
GLN	A3249	L2958	A3251	D3017	L2688	L2688	E2580	ALA	E2314	E2173	GLN	
GLN	A3250	L2959	A3252	D3018	L2689	L2689	E2581	ALA	E2315	E2174	GLN	
GLN	A3251	L2960	A3253	D3019	L2690	L2690	E2582	ALA	E2316	E2175	GLN	
GLN	A3252	L2961	A3254	D3020	L2691	L2691	E2583	ALA	E2317	E2176	GLN	
GLN	A3253	L2962	A3255	D3021	L2692	L2692	E2584	ALA	E2318	E2177	GLN	
GLN	A3254	L2963	A3256	D3022	L2693	L2693	E2585	ALA	E2319	E2178	GLN	
GLN	A3255	L2964	A3257	D3023	L2694	L2694	E2586	ALA	E2320	E2179	GLN	
GLN	A3256	L2965	A3258	D3024	L2695	L2695	E2587	ALA	E2321	E2180	GLN	
GLN	A3257	L2966	A3259	D3025	L2696	L2696	E2588	ALA	E2322	E2181	GLN	
GLN	A3258	L2967	A3260	D3026	L2697	L2697	E2589	ALA	E2323	E2182	GLN	
GLN	A3259	L2968	A3261	D3027	L2698	L2698	E2590	ALA	E2324	E2183	GLN	
GLN	A3260	L2969	A3262	D3028	L2699	L2699	E2591	ALA	E2325	E2184	GLN	
GLN	A3261	L2970	A3263	D3029	L2700	L2700	E2592	ALA	E2326	E2185	GLN	
GLN	A3262	L2971	A3264	D3030	L2701	L2701	E2593	ALA	E2327	E2186	GLN	
GLN	A3263	L2972	A3265	D3031	L2702	L2702	E2594	ALA	E2328	E2187	GLN	
GLN	A3264	L2973	A3266	D3032	L2703	L2703	E2595	ALA	E2329	E2188	GLN	
GLN	A3265	L2974	A3267	D3033	L2704	L2704	E2596	ALA	E2330	E2189	GLN	
GLN	A3266	L2975	A3268	D3034	L2705	L2705	E2597	ALA	E2331	E2190	GLN	
GLN	A3267	L2976	A3269	D3035	L2706	L2706	E2598	ALA	E2332	E2191	GLN	
GLN	A3268	L2977	A3270	D3036	L2707	L2707	E2599	ALA	E2333	E2192	GLN	
GLN	A3269	L2978	A3271	D3037	L2708	L2708	E2600	ALA	E2334	E2193	GLN	
GLN	A3270	L2979	A3272	D3038	L2709	L2709	E2601	ALA	E2335	E2194	GLN	
GLN	A3271	L2980	A3273	D3039	L2710	L2710	E2602	ALA	E2336	E2195	GLN	
GLN	A3272	L2981	A3274	D3040	L2711	L2711	E2603	ALA	E2337	E2196	GLN	
GLN	A3273	L2982	A3275	D3041	L2712	L2712	E2604	ALA	E2338	E2197	GLN	
GLN	A3274	L2983	A3276	D3042	L2713	L2713	E2605	ALA	E2339	E2198	GLN	
GLN	A3275	L2984	A3277	D3043	L2714	L2714	E2606	ALA	E2340	E2199	GLN	
GLN	A3276	L2985	A3278	D3044	L2715	L2715	E2607	ALA	E2341	E2200	GLN	
GLN	A3277	L2986	A3279	D3045	L2716	L2716	E2608	ALA	E2342	E2201	GLN	
GLN	A3278	L2987	A3280	D3046	L2717	L2717	E2609	ALA	E2343	E2202	GLN	
GLN	A3279	L2988	A3281	D3047	L2718	L2718	E2610	ALA	E2344	E2203	GLN	
GLN	A3280	L2989	A3282	D3048	L2719	L2719	E2611	ALA	E2345	E2204	GLN	
GLN	A3281	L2990	A3283	D3049	L2720	L2720	E2612	ALA	E2346	E2205	GLN	
GLN	A3282	L2991	A3284	D3050	L2721	L2721	E2613	ALA	E2347	E2206	GLN	
GLN	A3283	L2992	A3285	D3051	L2722	L2722	E2614	ALA	E2348	E2207	GLN	
GLN	A3284	L2993	A3286	D3052	L2723	L2723	E2615	ALA	E2349	E2208	GLN	
GLN	A3285	L2994	A3287	D3053	L2724	L2724	E2616	ALA	E2350	E2209	GLN	
GLN	A3286	L2995	A3288	D3054	L2725	L2725	E2617	ALA	E2351	E2210	GLN	
GLN	A3287	L2996	A3289	D3055	L2726	L2726	E2618	ALA	E2352	E2211	GLN	
GLN	A3288	L2997	A3290	D3056	L2727	L2727	E2619	ALA	E2353	E2212	GLN	
GLN	A3289	L2998	A3291	D3057	L2728	L2728	E2620	ALA	E2354	E2213	GLN	
GLN	A3290	L2999	A3292	D3058	L2729	L2729	E2621	ALA	E2355	E2214	GLN	
GLN	A3291	L3000	A3293	D3059	L2730	L2730	E2622	ALA	E2356	E2215	GLN	
GLN	A3292	L3001	A3294	D3060	L2731	L2731	E2623	ALA	E2357	E2216	GLN	
GLN	A3293	L3002	A3295	D3061	L2732	L2732	E2624	ALA	E2358	E2217	GLN	
GLN	A3294	L3003	A3296	D3062	L2733	L2733	E2625	ALA	E2359	E2218	GLN	
GLN	A3295	L3004	A3297	D3063	L2734	L2734	E2626	ALA	E2360	E2219	GLN	
GLN	A3296	L3005	A3298	D3064	L2735	L2735	E2627	ALA	E2361	E2220	GLN	
GLN	A3297	L3006	A3299	D3065	L2736	L2736	E2628	ALA	E2362	E2221	GLN	
GLN	A3298	L3007	A3300	D3066	L2737	L2737	E2629	ALA	E2363	E2222	GLN	
GLN	A3299	L3008	A3301	D3067	L2738	L2738	E2630	ALA	E2364	E2223	GLN	
GLN	A3300	L3009	A3302	D3068	L2739	L2739	E2631	ALA	E2365	E2224	GLN	
GLN	A3301	L3010	A3303	D3069	L2740	L2740	E2632	ALA	E2366	E2225	GLN	
GLN	A3302	L3011	A3304	D3								

SER	ASP	ALA	ILE	ARG	GLU	LYS	LYS	LYS	ASN	TYR	MET	SER	ASN	PRO	SER	TYR	ASN	TYR	ILE	VAL	ASN	ARG	ALA	SER	LEU	ALA	CYS	GLY	PRO	MET	VAL	LYS	TRP	ALA	ILE	ALA	GLN	LEU	ASN	TYR	ALA	ASP	MET	LYS	ARG	VAL	GLU	LYS	LYS	LEU	LEU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
GLU	ASP	ALA	ALA	LYS	ASP	ASN	GLN	GLN	LYS	ALA	ASN	GLU	VAL	GLU	Q3435	M3436	I3437	R3438	D3439	L3440	E3441	S3442	S3443	I3444	A3445	R3446	Y3447	K3448	E3449	Q3450	Y3451	A3452	V3453	L3454	I3455	S3456	E3457	A3458	Q3459	A3460	I3461	K3462	A3463	D3464	L3465	A3466	A3467	V3468	E3469	A3470	K3471	V3472	N3473	R3474	A3477	L3478	L3479	K3480																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
S3481	L3482	S3483	A3484	E3485	R3486	E3487	R3488	R3489	E3490	R3491	T3495	F3496	R3497	N3498	S3510	Y3516	A3517	F3520	D3521	F3524	R3525	D3546	I3547	T3550	L3553	R3557	L3560	A3569	D3570	E3575	S3593	G3594	Q3595	A3596	T3597	E3598	N3601	K3608	T3609	T3610	L3615	D3616	D3617	A3618	F3619	R3620	K3621	E3624	S3625	A3626	L3627	R3628	F3629	N3631	L3634	V3638	E3639	E3652	V3653	R3654	T3655	G3657	R3658	R3659	V3660	L3661	L3664	G3665	D3666	Q3667	D3668	I3669	D3670	R3671	S3679	T3681	R3682	D3683	P3684	T3685	V3686	E3687	S3694	R3705	L3708	C3712	L3713	N3714	E3715	V3716	L3717	K3718	A3719	E3720	R3721	F3722	R3723	V3724	D3725	E3726	R3727	R3728	S3729	D3730	L3731	L3732	R3733	E3737	F3738	Q3739	L3740	R3741	Q3744	L3745	E3746	K3747	Q3751	A3752	L3753	R3754	E3755	V3756	K3757	R3758	R3759	L3760	D3762	D3763	D3764	T3765	I3766	I3767	T3768	T3769	L3770	E3771	N3772	L3773	R3775	E3776	A3777	R3778	V3780	T3781	R3782	K3783	V3784	E3785	E3786	T3787	D3788	L3789	V3790	M3791	Q3792	E3793	V3794	E3795	T3796	V3797	S3798	Q3799	Q3800	L3802	A3807	C3808	S3809	T3814	I3821	R3822	L3824	Y3825	Q3826	Y3827	D3834	G3835	Y3836	H3837	N3838	E3842	N3845	L3846	GLY	V3849	T3850	D3851	H3852	T3853	Q3854	R3855	L3856	K3861	F3868	V3871	A3872	R3873	Q3878	F3883	I3890	K3891	L3892	K3893	G3894	T3895	VAL	G3897	P3898	T3900	Y3901	D3902	A3903	F3905	Q3906	H3907	R3910	G3911	N3912	E3913	I3914	V3915	L3916	S3917	A3918	R3919	S3920	T3921	P3922	R3923	I3924	Q3925	G3926	L3927	T3928	V3929	E3930	Q3931	A3932	R3933	A3934	V3935	V3936	R3937	L3938	S3939	C3940	L3941	P3942	A3943	F3944	K3945	D3946	L3947	I3948	A3949	K3950	V3951	Q3952	K3953	D3954	E3955	Q3956	F3957	Q3958	T3959	S3960	L3961	D3962	S3963	S3964	S3965	P3966	Q3967	Q3968	F3971	Y3972	L3973	V3974	SER	GLU	T3978	F3979	A3980	T3981	P3982	I3983	G3984	Q3985	H3988	R3989	L3992	T3993	F3996	N4004	N4007	T4011	E4015	S4019	E4022	Q4023	P4024	L4025	D4026	H4029	I4030	G4031	G4032	T4033	K4036	P4037	N4038	D4050	D4057	A4060	E4061	Q4062	N4063	T4064	Q4065	S4068	I4071	E4075	N4078	K4082	K4089	S4090	G4091	R4092	W4093	M4095	L4096	K4097	W4098	V4099	E4110	S4115	L4116	Q4117	P4118	H4119	A4120	L4124	F4125	L4126	T4127	K4133	N4137	F4145	S4167	C4170	K4171	S4172	F4173	N4174	E4175	R4176	A4177	R4178	I4190	L4194	W4201	S4202	K4203	E4209	R4213	D4217	T4218	L4223	D4224	D4225	T4226	A4227	K4228	G4229	R4230	Q4231	M4232	I4233	D4236	K4237	T4238	P4239	W4240	S4241	A4242	L4246	M4247	T4275	R4276	S4277	F4278	D4279	S4280	E4281	F4282	K4283	L4284	A4285	C4286	K4287	V4288	D4289	G4290	H4291	K4292	D4293	I4294	Q4295	N4296	P4297	D4298	G4299	I4300	R4301	R4302	E4303	E4304	Q4307	L4311	D4314	T4315	L4321	G4322	P4324	N4325	M4326	R4329	V4330	L4331	D4338	K4342	M4343	L4344	K4345	M4346	M4348	L4349	E4350	ASP	GLU	ASP	ASP	ALA	TYR	ALA	TYR	GLU	GLU	LYS	LYS	THR	THR	THR	ASP	GLY	ARG	PRO	ALA	TRP	ARG	T4379	L4380	H4381	T4382	T4383	A4384	S4385	M4386	W4387	L4388	H4389	L4390	I4391	Q4392	Q4393	T4394	L4395	S4396	H4397	L4398	K4399	R4400	T4401	VAL	E4403	N4404	I4405	K4406	D4407	F4410	R4411	F4412	F4413	E4414	R4415	E4416	V4417	K4418	M4419	G4420	L4421	A4422	K4423	L4424	Q4425	D4426	V4427	R4428	Q4429	D4430	L4431	A4432	D4433	V4434	V4435	Q4436	V4437	C4438	E4439	G4440	K4441	K4442	K4443	R4449	N4453	E4454	K4457	G4458	I4459	L4460	P4461	K4462	S4463	H4466	P4470	A4471	G4472	M4473

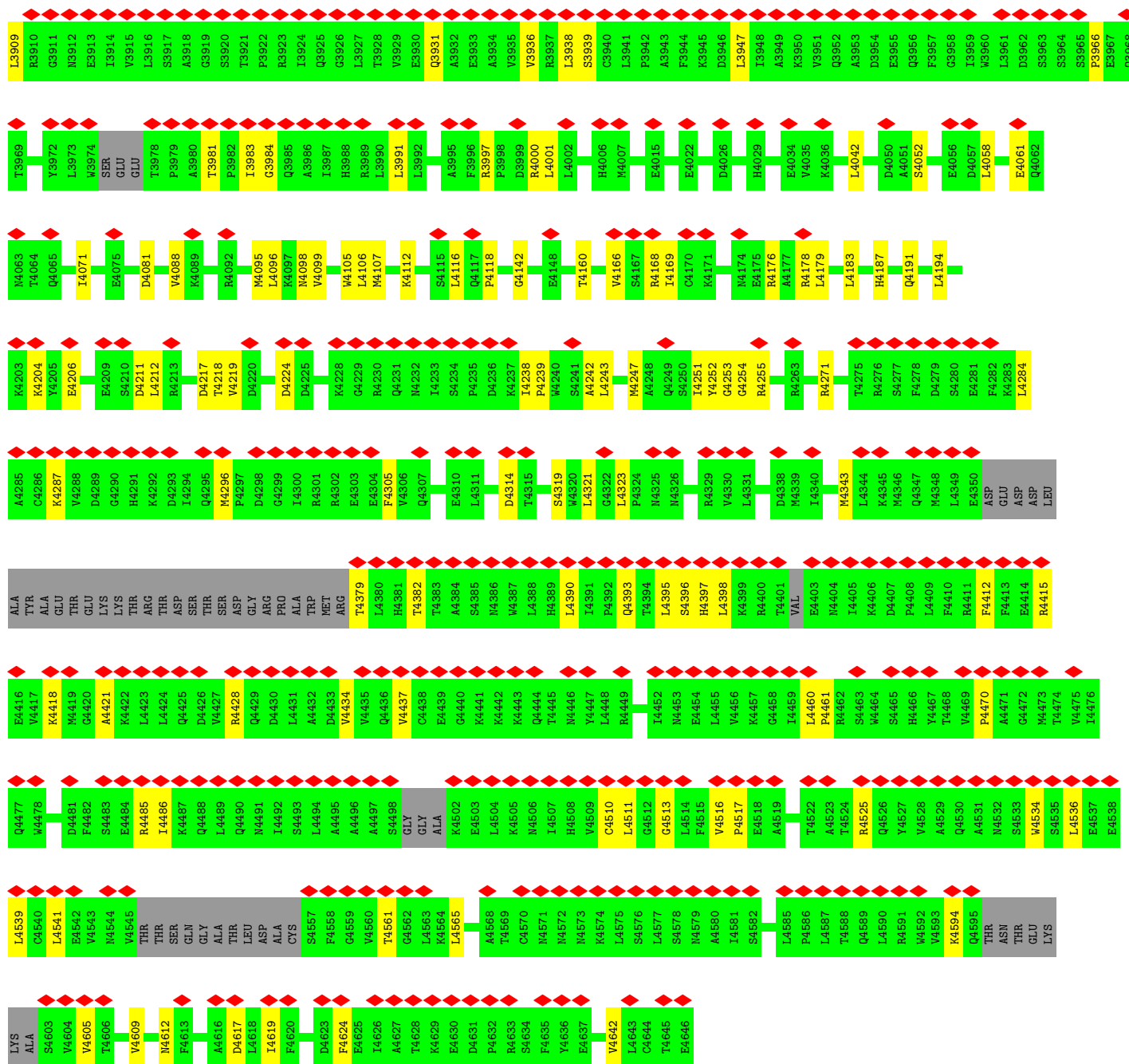




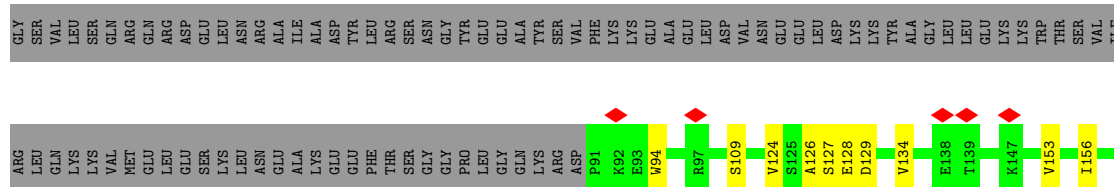


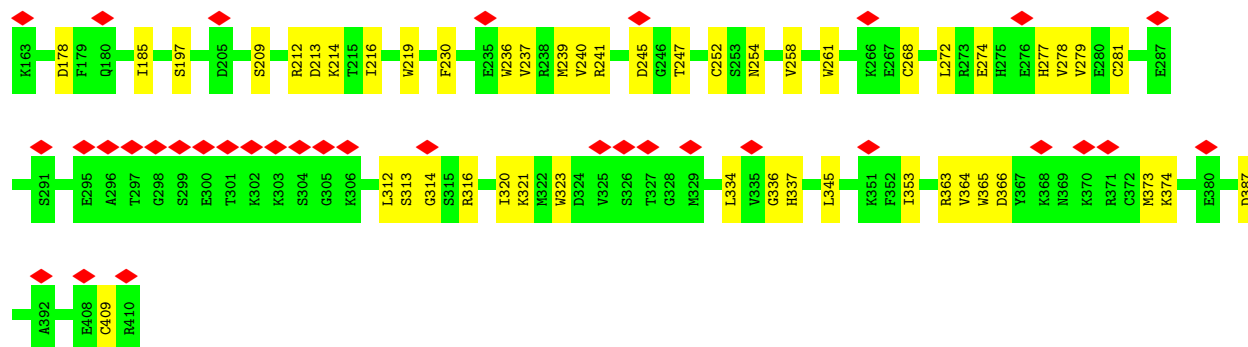




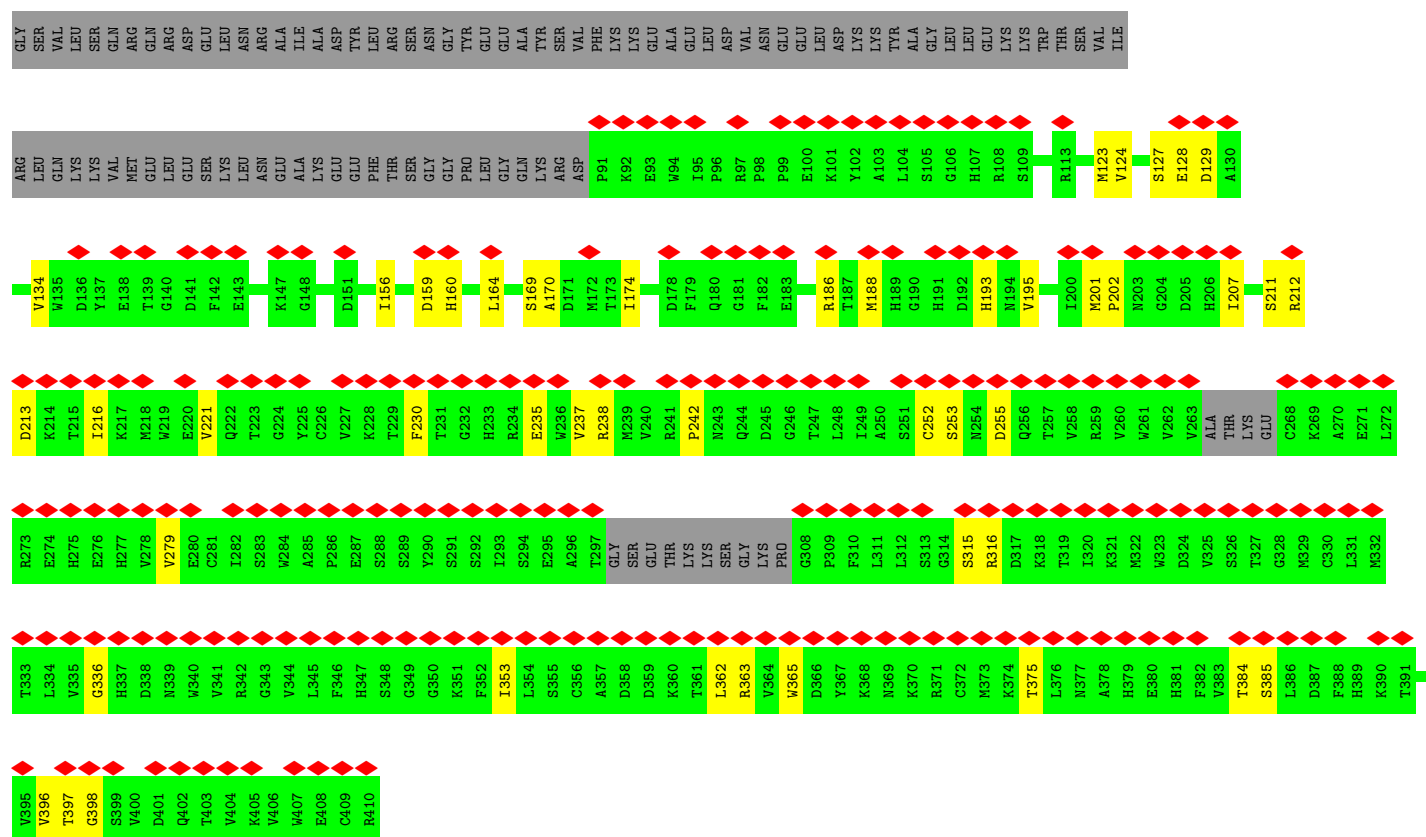


• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta





• 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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (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
1:A:4179:LEU:HD11	1:A:4238:ILE:HD11	1.73	0.70
1:A:4052:SER:HA	1:A:4095:MET:HE1	1.74	0.70
1:B:2965:ARG:HH12	1:B:3615:LEU:HA	1.57	0.68
2:C:201:MET:HE3	2:C:202:PRO:HD2	1.75	0.67
1:A:2307:VAL:HG13	1:A:2312:VAL:HG21	1.74	0.67
1:B:1717:LEU:HD11	1:B:1752:LEU:HD22	1.77	0.67
2:E:320:ILE:HB	2:E:334:LEU:HB2	1.77	0.67
2:C:123:MET:HE3	2:C:396:VAL:HG21	1.76	0.66
1:B:3981:THR:HG23	1:B:3984:GLY:H	1.60	0.66
1:A:4206:GLU:O	1:A:4255:ARG:NH1	2.30	0.65
2:E:258:VAL:HG22	2:E:279:VAL:HG11	1.78	0.65
2:E:254:ASN:HA	2:E:278:VAL:HG13	1.80	0.64
1:B:3731:LEU:HD21	1:B:3790:VAL:HG22	1.80	0.64
1:A:3584:ASN:O	1:A:3651:ARG:NH2	2.31	0.63
1:A:1933:ASP:OD1	1:A:1962:ARG:NH1	2.31	0.63
1:A:3839:VAL:O	1:A:3843:ASN:ND2	2.31	0.63
1:A:3981:THR:HG23	1:A:3984:GLY:H	1.63	0.63
1:B:2221:MET:HG2	1:B:2343:PHE:HB2	1.80	0.62
1:B:3712:CYS:SG	1:B:3836:TYR:OH	2.57	0.62
1:A:3232:LYS:HD2	1:A:3454:LEU:HD22	1.80	0.62
1:A:2245:GLU:OE1	1:A:2298:ARG:NH2	2.33	0.61
1:B:1931:ASN:ND2	1:B:2316:ASN:OD1	2.34	0.61
1:B:3483:SER:HA	1:B:3486:ARG:HG2	1.82	0.61
1:B:3681:THR:HG22	1:B:3683:ASP:H	1.65	0.61
1:A:4525:ARG:NH1	1:A:4536:LEU:O	2.33	0.61
1:B:2028:LEU:HB2	1:B:2033:LYS:HE3	1.82	0.61
1:A:1539:ASP:OD2	1:A:2292:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3455:ILE:O	1:B:3459:GLN:NE2	2.33	0.61
1:A:1882:THR:HG22	1:A:1884:LEU:H	1.66	0.60
1:B:3801:TYR:HE1	1:B:3856:LEU:HD21	1.66	0.60
1:A:2996:GLU:HB3	1:A:3068:MET:HB3	1.83	0.60
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.81	0.60
1:B:2816:LEU:HD12	1:B:2817:PRO:HD2	1.83	0.60
1:B:3225:LYS:NZ	1:B:3464:ASP:OD2	2.33	0.60
1:A:3158:ASN:ND2	1:A:3169:MET:O	2.34	0.60
1:B:4424:LEU:HD12	1:B:4486:ILE:HD12	1.84	0.60
1:A:2492:ARG:NH1	1:A:2543:GLY:O	2.34	0.60
1:A:4284:LEU:HG	1:A:4296:MET:HB2	1.84	0.60
1:B:3922:PRO:HD2	1:B:3932:ALA:HB1	1.84	0.60
1:B:3941:LEU:HD12	1:B:3942:PRO:HD2	1.84	0.59
2:C:124:VAL:HG12	2:C:134:VAL:HG22	1.85	0.59
1:B:2172:ARG:NH1	1:B:2205:GLU:OE2	2.35	0.59
1:B:3212:VAL:HG22	1:B:3479:LEU:HD21	1.85	0.59
1:A:3604:TYR:HB2	1:A:3609:ILE:HD11	1.84	0.59
1:B:4346:MET:HA	1:B:4349:LEU:HD12	1.84	0.59
1:A:2861:ILE:O	1:A:2863:ARG:NH1	2.35	0.59
1:B:2472:TYR:HB2	1:B:2541:ILE:HD11	1.85	0.58
1:B:4481:ASP:OD2	1:B:4485:ARG:NH1	2.36	0.58
1:A:2272:THR:HG23	1:A:2274:GLU:HG2	1.85	0.58
1:B:3113:MET:O	1:B:3140:ARG:NH2	2.36	0.58
1:B:2413:LEU:HG	1:B:2417:ARG:HE	1.68	0.58
1:B:2469:VAL:HG13	1:B:2481:MET:HG2	1.84	0.58
1:A:1540:VAL:HG11	1:A:1601:LEU:HD12	1.85	0.58
1:A:1661:VAL:HG13	1:A:1676:ILE:HG23	1.85	0.58
1:A:2060:ARG:HH12	1:A:2130:ASN:HA	1.67	0.58
1:A:2278:GLY:O	1:A:2282:HIS:HB3	2.04	0.58
1:B:2665:GLU:HB3	1:B:2668:LEU:HD12	1.86	0.58
1:B:2887:GLU:OE2	1:B:2890:ARG:NH1	2.37	0.58
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.85	0.58
1:A:1734:ASP:HB2	1:A:1737:THR:HG22	1.85	0.57
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	1.86	0.57
1:A:3013:ALA:HA	1:A:3088:ARG:HG3	1.85	0.57
1:A:1550:ILE:HD11	1:A:1618:TYR:HE2	1.70	0.57
1:B:1734:ASP:HB3	1:B:1737:THR:HG22	1.86	0.57
1:A:3219:ARG:HH22	1:A:3472:VAL:HG21	1.69	0.57
1:A:2060:ARG:NH2	1:A:2129:GLU:O	2.34	0.57
1:B:1836:PHE:HA	1:B:1839:LEU:HB2	1.86	0.57
1:B:3158:ASN:ND2	1:B:3169:MET:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3172:THR:HG22	1:B:3174:ARG:H	1.70	0.57
1:A:2558:GLU:OE2	1:A:2561:LYS:NZ	2.37	0.57
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.87	0.57
1:B:2063:GLU:OE2	1:B:2067:ASN:ND2	2.38	0.56
1:A:2304:ASP:OD1	1:A:2726:ARG:NH2	2.39	0.56
1:A:4187:HIS:ND1	1:A:4252:TYR:OH	2.36	0.56
1:A:4395:LEU:O	1:A:4428:ARG:NH1	2.39	0.56
1:B:3721:ARG:NH1	1:B:3801:TYR:OH	2.39	0.56
1:B:1946:VAL:HG22	1:B:2006:VAL:HG21	1.88	0.56
1:A:1746:GLN:HB2	1:A:1749:LEU:HD23	1.86	0.56
1:A:2831:ARG:NH2	1:A:2917:ASP:OD1	2.39	0.56
1:B:2245:GLU:OE1	1:B:2298:ARG:NH2	2.39	0.56
1:B:3126:MET:HE2	1:B:3137:PRO:HG3	1.87	0.56
2:C:186:ARG:NH1	2:C:221:VAL:O	2.39	0.56
1:A:4510:CYS:HB3	1:A:4561:THR:HG23	1.88	0.56
1:A:1524:GLU:OE2	1:A:1528:ASN:ND2	2.38	0.56
1:A:3597:THR:HG23	1:A:3634:LEU:HD21	1.87	0.56
1:B:2969:GLY:HA2	1:B:3004:PHE:HE1	1.71	0.56
1:B:4385:SER:O	1:B:4389:HIS:ND1	2.39	0.55
1:A:2503:SER:HB3	1:A:2514:LEU:HD23	1.86	0.55
1:A:2694:ARG:NH2	1:A:2697:ASP:OD2	2.39	0.55
1:A:1680:GLU:N	1:A:1680:GLU:OE1	2.39	0.55
1:A:4088:VAL:HG13	1:A:4118:PRO:HA	1.89	0.55
1:B:2107:ARG:NH2	1:B:2139:GLN:OE1	2.40	0.55
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.89	0.55
1:B:2102:ASN:OD1	1:B:2105:ARG:NH2	2.39	0.55
2:C:216:ILE:HB	2:C:230:PHE:HB2	1.89	0.55
1:A:1743:ASP:OD2	1:A:1804:ARG:NH1	2.39	0.55
1:A:2068:LYS:HB3	1:A:2165:PHE:HE1	1.71	0.55
1:A:4176:ARG:NH2	1:A:4224:ASP:OD1	2.37	0.55
1:A:4178:ARG:HD2	1:A:4305:PHE:HZ	1.72	0.55
1:A:3174:ARG:NH1	1:A:3650:ASN:OD1	2.40	0.55
1:B:3593:SER:HB2	1:B:3595:GLN:HG2	1.88	0.55
1:A:3110:THR:O	1:A:3140:ARG:NH2	2.40	0.55
1:B:4395:LEU:O	1:B:4428:ARG:NH1	2.40	0.55
2:C:127:SER:OG	2:C:128:GLU:N	2.40	0.55
1:A:2968:THR:HG22	1:A:2970:GLU:H	1.71	0.55
1:B:1639:GLU:OE2	1:B:1652:LYS:NZ	2.40	0.55
1:A:2075:LEU:O	1:A:2079:GLN:HB2	2.07	0.55
1:A:2906:ASP:OD2	1:A:3655:ARG:NH1	2.41	0.54
1:A:3222:LEU:HD12	1:A:3465:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2666:ILE:HG22	1:B:2712:CYS:HB3	1.89	0.54
1:A:3654:ARG:HG2	1:A:3656:THR:HG23	1.90	0.54
1:A:3776:GLU:O	1:A:3779:GLU:HG3	2.07	0.54
2:C:159:ASP:HB2	2:C:164:LEU:HB3	1.89	0.54
1:B:1862:ALA:O	1:B:1894:GLN:NE2	2.40	0.54
1:B:2065:LEU:HD22	1:B:2137:LEU:HD12	1.89	0.54
2:C:336:GLY:O	2:C:363:ARG:NH1	2.40	0.54
1:B:2563:ALA:HB3	1:B:2804:ARG:HD3	1.90	0.54
1:B:3219:ARG:HD3	1:B:3222:LEU:HD21	1.89	0.54
2:C:211:SER:OG	2:C:213:ASP:OD1	2.26	0.54
1:B:2773:MET:HG2	1:B:2825:TRP:HE1	1.71	0.54
1:A:1633:GLY:N	1:A:2331:GLU:OE1	2.41	0.54
1:A:4211:ASP:OD2	1:A:4255:ARG:NH1	2.41	0.54
1:B:1882:THR:HG22	1:B:1884:LEU:H	1.74	0.53
1:B:3822:HIS:O	1:B:3822:HIS:ND1	2.42	0.53
1:B:4544:ASN:HA	1:B:4573:ASN:HD21	1.74	0.53
2:C:188:MET:HE1	2:C:207:ILE:HD12	1.90	0.53
1:B:2335:LEU:HD12	1:B:2336:PRO:HD2	1.90	0.53
2:E:126:ALA:HB1	2:E:153:VAL:HG13	1.90	0.53
1:A:4398:LEU:HD12	1:A:4486:ILE:HD11	1.89	0.53
1:B:1968:LEU:HD21	1:B:2028:LEU:HD23	1.91	0.53
1:B:2849:ASN:HA	1:B:2852:THR:HG22	1.90	0.53
2:E:245:ASP:OD1	2:E:247:THR:OG1	2.25	0.53
1:A:1636:ASP:OD1	1:A:1653:HIS:NE2	2.41	0.53
1:B:2925:ILE:HG21	1:B:2933:LEU:HG	1.91	0.53
1:A:2099:SER:OG	1:A:2140:SER:OG	2.25	0.53
1:A:3444:ILE:O	1:A:3448:LYS:HG3	2.09	0.53
1:A:3749:LEU:HD12	1:A:3773:LEU:HD23	1.90	0.53
2:E:336:GLY:O	2:E:363:ARG:NH1	2.42	0.53
1:A:2943:LYS:HG2	1:A:3094:PHE:HD2	1.73	0.53
1:B:2511:ARG:HD3	1:B:2535:ILE:HD13	1.90	0.53
1:B:2582:TYR:HD1	1:B:2612:LEU:HD11	1.74	0.53
1:A:1917:LYS:NZ	1:A:2322:ASN:OD1	2.38	0.53
1:B:1741:TRP:CH2	1:B:1750:VAL:HG23	2.44	0.53
1:A:1737:THR:HA	1:A:1740:THR:HG22	1.90	0.53
1:A:1786:GLU:OE2	1:A:1819:ARG:NH1	2.42	0.53
1:B:4437:VAL:HA	1:B:4442:LYS:HB3	1.91	0.52
1:A:2448:ASP:O	1:A:2453:ARG:NH2	2.34	0.52
1:A:2886:GLN:OE1	1:A:2890:ARG:NH2	2.43	0.52
1:A:2987:ASN:OD1	1:A:3057:GLN:NE2	2.42	0.52
1:A:2642:ARG:NH2	1:A:2704:GLU:OE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2601:LYS:HB3	1:A:2736:VAL:HG21	1.90	0.52
1:A:4470:PRO:HA	1:A:4612:ASN:HD22	1.75	0.52
1:B:3517:ALA:HB1	1:B:3525:ARG:HG2	1.92	0.52
1:A:1529:ARG:HE	1:A:1592:LEU:HD21	1.74	0.52
1:B:2623:SER:OG	1:B:3081:THR:O	2.19	0.52
2:C:252:CYS:HB2	2:C:279:VAL:HG13	1.90	0.52
2:E:124:VAL:HG23	2:E:156:ILE:HD12	1.92	0.51
2:C:363:ARG:HG2	2:C:375:THR:HG22	1.93	0.51
1:A:2983:SER:O	1:A:3061:ASN:ND2	2.38	0.51
1:B:1537:TRP:HE3	1:B:1601:LEU:HD11	1.74	0.51
1:B:3814:THR:HG21	1:B:3890:ILE:HD11	1.92	0.51
1:A:2132:PRO:HB2	1:A:2135:GLU:HB3	1.92	0.51
2:E:127:SER:OG	2:E:129:ASP:OD1	2.21	0.51
1:A:1478:VAL:HG21	1:A:1488:ARG:HH12	1.76	0.51
1:A:1836:PHE:HA	1:A:1839:LEU:HB2	1.93	0.51
1:B:1720:SER:O	1:B:1724:VAL:HG23	2.10	0.51
1:B:3071:SER:O	1:B:3075:LEU:HB2	2.11	0.51
1:A:1795:SER:OG	1:A:1800:GLN:NE2	2.43	0.51
1:A:2957:SER:HB2	1:A:2990:ILE:HD13	1.91	0.51
1:B:1558:LYS:HA	1:B:1565:THR:HG21	1.92	0.51
1:B:3497:LYS:O	1:B:3497:LYS:NZ	2.32	0.51
1:A:1625:SER:OG	1:A:1699:ASN:ND2	2.43	0.51
1:A:3217:GLU:HA	1:A:3220:ARG:HG2	1.92	0.51
1:A:4088:VAL:HG21	1:A:4116:LEU:HD11	1.93	0.51
1:B:2053:MET:HE1	1:B:2094:LYS:HG3	1.91	0.51
2:C:124:VAL:HG23	2:C:156:ILE:HD12	1.93	0.51
2:C:353:ILE:HB	2:C:365:TRP:HB2	1.91	0.51
1:B:4417:VAL:HG23	1:B:4489:LEU:HD12	1.92	0.51
1:A:1775:ALA:O	1:A:1779:HIS:ND1	2.37	0.51
1:A:4412:PHE:HE1	1:A:4516:VAL:HG23	1.76	0.51
1:B:1698:ILE:HA	1:B:1701:TRP:CD1	2.46	0.51
1:B:4434:VAL:HA	1:B:4437:VAL:HG12	1.93	0.50
1:A:1961:ASN:HB3	1:A:2018:MET:HE3	1.92	0.50
1:B:3738:PHE:HB3	1:B:3783:LYS:HE2	1.93	0.50
1:B:3821:ILE:HD13	1:B:4342:LYS:HE3	1.93	0.50
1:A:1469:VAL:HG11	1:A:1496:LYS:HE2	1.94	0.50
1:B:2628:PRO:HD3	1:B:2679:VAL:HG22	1.93	0.50
2:E:209:SER:OG	2:E:219:TRP:NE1	2.40	0.50
1:B:2256:PRO:HG3	1:B:2303:PHE:HD1	1.76	0.50
1:B:2568:VAL:HG22	1:B:2603:MET:HE3	1.93	0.50
1:B:2889:LEU:HD22	1:B:2916:LEU:HG	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2981:ARG:NH2	1:A:3025:GLU:OE1	2.39	0.50
1:B:4414:GLU:HA	1:B:4417:VAL:HG12	1.94	0.50
1:A:2308:ASP:N	1:A:2308:ASP:OD1	2.43	0.50
1:A:2354:ALA:O	1:A:2358:ARG:NH1	2.37	0.50
1:B:1724:VAL:HG21	1:B:1753:SER:HB3	1.94	0.50
1:B:2091:ARG:NH2	3:B:4706:ADP:O3A	2.44	0.50
1:B:3116:GLU:OE2	1:B:3140:ARG:NH1	2.45	0.50
1:A:2412:MET:HE1	1:A:2467:ARG:HD3	1.93	0.50
1:A:2980:LEU:HD22	1:A:3058:VAL:HG21	1.92	0.50
1:A:3499:GLN:HA	1:A:3502:THR:HG22	1.93	0.50
1:A:3779:GLU:HA	1:A:3782:ARG:HG2	1.94	0.50
1:B:3225:LYS:HB3	1:B:3465:LEU:HD21	1.93	0.50
1:A:4194:LEU:O	1:A:4204:LYS:NZ	2.44	0.50
1:B:4271:ARG:NH1	1:B:4284:LEU:O	2.44	0.50
1:B:2437:LEU:HD11	1:B:2455:LEU:HD11	1.92	0.49
1:B:3172:THR:HG21	1:B:3694:SER:HB2	1.93	0.49
1:B:3935:VAL:HG13	1:B:3947:LEU:HD23	1.93	0.49
1:A:1623:ARG:HD3	1:A:1630:TYR:HA	1.94	0.49
1:A:2275:TRP:NE1	1:A:2277:ASP:OD1	2.43	0.49
1:B:2964:HIS:ND1	1:B:2965:ARG:O	2.45	0.49
1:A:2571:THR:H	1:A:2574:THR:HG1	1.60	0.49
1:A:4239:PRO:HB2	1:A:4242:ALA:HB3	1.94	0.49
1:B:3510:SER:HB3	1:B:3553:LEU:HD21	1.95	0.49
2:E:345:LEU:HD11	2:E:387:ASP:HA	1.95	0.49
1:B:2841:GLU:OE1	1:B:2844:ARG:NH2	2.43	0.49
1:B:3629:PHE:HZ	1:A:3661:LEU:HD11	1.78	0.49
2:C:169:SER:OG	2:C:170:ALA:N	2.46	0.49
1:A:3660:VAL:HG12	1:A:3671:LEU:HB3	1.94	0.49
1:B:1914:GLU:HG3	3:B:4706:ADP:H2'	1.95	0.49
1:A:1847:ASP:N	1:A:1847:ASP:OD1	2.45	0.49
1:A:4183:LEU:HD11	1:A:4219:VAL:HG21	1.93	0.49
1:A:1698:ILE:HA	1:A:1701:TRP:CD1	2.47	0.49
1:B:2609:LEU:HD23	1:B:2617:VAL:HG22	1.95	0.49
1:B:2967:TYR:OH	1:B:2975:ASP:OD2	2.30	0.49
1:B:4172:SER:O	1:B:4176:ARG:NH2	2.45	0.49
1:A:1530:ILE:HB	1:A:1592:LEU:HD12	1.95	0.49
1:A:2495:VAL:HA	1:A:2498:ILE:HG22	1.95	0.49
1:B:1894:GLN:HG3	1:B:4246:LEU:HD11	1.95	0.48
1:A:2031:ASN:OD1	1:A:4098:ASN:ND2	2.35	0.48
1:A:3723:ASP:N	1:A:3723:ASP:OD1	2.45	0.48
1:B:1550:ILE:O	1:B:1554:SER:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2356:VAL:HG13	1:A:2361:MET:HE3	1.94	0.48
1:A:2609:LEU:HD13	1:A:2617:VAL:HG22	1.95	0.48
1:A:2964:HIS:ND1	1:A:2965:ARG:O	2.45	0.48
1:B:2834:GLN:NE2	1:B:2847:ASP:OD1	2.47	0.48
1:B:4384:ALA:O	1:B:4388:LEU:HB2	2.12	0.48
1:A:3639:GLU:OE2	1:A:3681:THR:OG1	2.25	0.48
1:A:4617:ASP:OD1	1:A:4617:ASP:N	2.44	0.48
1:B:1571:ILE:HG21	1:B:1607:LEU:HD13	1.94	0.48
1:B:2671:MET:HB2	1:B:2721:LYS:HD3	1.95	0.48
1:B:1525:ASP:O	1:B:1529:ARG:HG3	2.14	0.48
1:B:2499:LEU:HD23	1:B:2514:LEU:HD23	1.95	0.48
1:B:3175:HIS:HB3	1:B:3516:TYR:HE1	1.78	0.48
1:B:3222:LEU:HD23	1:B:3472:VAL:HG21	1.95	0.48
1:A:2527:PRO:HD3	1:A:2545:TRP:CD1	2.49	0.48
1:B:1491:ASP:OD1	1:B:1491:ASP:N	2.47	0.48
1:B:1729:LYS:HD2	1:B:1729:LYS:HA	1.63	0.48
1:B:2872:LEU:HD22	1:B:2920:LEU:HD12	1.95	0.48
1:A:2228:SER:OG	1:A:2365:SER:O	2.30	0.48
1:A:4081:ASP:OD1	1:A:4112:LYS:NZ	2.46	0.48
1:A:3175:HIS:HB3	1:A:3516:TYR:HE1	1.79	0.48
1:A:3225:LYS:HE2	1:A:3464:ASP:HB3	1.96	0.47
1:A:3742:LEU:HD11	1:A:3780:VAL:HG11	1.96	0.47
2:E:337:HIS:CE1	2:E:363:ARG:HG3	2.49	0.47
1:A:4166:VAL:HA	1:A:4169:ILE:HG22	1.95	0.47
1:A:4517:PRO:HB2	1:A:4619:ILE:HG21	1.96	0.47
1:B:2889:LEU:HD11	1:B:2920:LEU:HD21	1.95	0.47
1:B:3162:ALA:HB2	1:B:3168:THR:HG21	1.96	0.47
1:B:4178:ARG:HE	1:B:4296:MET:HE2	1.79	0.47
1:A:1888:CYS:O	1:A:1892:MET:HG2	2.15	0.47
1:A:2791:HIS:NE2	1:A:2836:ARG:O	2.46	0.47
1:A:2635:PHE:HE1	1:A:2661:LEU:HD11	1.79	0.47
1:B:2836:ARG:HG3	1:B:3091:LEU:HD23	1.97	0.47
1:A:3189:GLU:OE1	1:A:3582:ARG:NH2	2.46	0.47
1:B:1756:ILE:HD11	1:B:1857:LEU:HD13	1.97	0.47
1:B:1861:MET:HG3	1:B:1862:ALA:H	1.79	0.47
1:B:2485:GLN:HA	1:B:2488:ARG:HG2	1.97	0.47
1:B:3683:ASP:OD2	1:B:4137:ASN:ND2	2.48	0.47
1:A:2453:ARG:NH1	1:A:2505:ASP:OD2	2.44	0.47
1:A:2592:VAL:HG22	1:A:2710:GLY:HA3	1.96	0.47
1:A:2622:PHE:HB2	1:A:2665:GLU:HB2	1.96	0.47
1:B:4202:SER:OG	1:B:4261:ASP:OD2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:109:SER:HB3	2:E:128:GLU:HB2	1.97	0.47
1:A:2623:SER:HB3	1:A:3009:ASN:HD22	1.79	0.47
1:A:3016:GLU:HG3	1:A:3051:TYR:HE2	1.79	0.47
1:A:3591:ASP:N	1:A:3591:ASP:OD1	2.48	0.47
1:A:3209:LYS:HA	1:A:3209:LYS:HD2	1.74	0.47
1:B:3776:GLU:O	1:B:3779:GLU:HG3	2.14	0.47
1:A:2275:TRP:HB2	1:A:2329:ASN:HD21	1.80	0.47
1:A:4485:ARG:NH1	1:A:4513:GLY:O	2.48	0.47
1:B:1625:SER:OG	1:B:1699:ASN:ND2	2.48	0.47
1:B:1756:ILE:HD13	1:B:1846:PHE:HB2	1.97	0.47
1:B:1782:LEU:HD12	1:B:1822:THR:HG22	1.97	0.47
1:B:2231:SER:HA	1:B:2234:TRP:CD1	2.49	0.47
1:B:2667:ASN:OD1	1:B:2712:CYS:HB2	2.15	0.47
1:B:2961:ILE:HD11	1:B:2998:ASN:HB3	1.96	0.47
1:A:2977:ARG:NH1	1:A:3020:LEU:O	2.40	0.47
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.97	0.47
1:A:3715:GLU:HB3	1:A:3836:TYR:HE2	1.80	0.47
1:A:3938:LEU:HD11	1:A:3991:LEU:HB3	1.97	0.47
1:B:2424:GLN:HE21	1:B:2428:THR:HB	1.79	0.46
1:B:4524:THR:HG23	1:B:4558:PHE:CE1	2.50	0.46
1:B:2787:ASP:N	1:B:2787:ASP:OD1	2.48	0.46
1:B:4457:LYS:HB2	1:B:4457:LYS:HE3	1.80	0.46
2:C:362:LEU:HD11	2:C:397:THR:HG21	1.97	0.46
1:A:3798:SER:O	1:A:3802:LEU:HB2	2.15	0.46
1:B:2650:LEU:N	1:B:2702:LYS:O	2.49	0.46
1:A:1619:LEU:HD11	1:A:1638:LEU:HG	1.97	0.46
1:A:4398:LEU:HD22	1:A:4421:ALA:HB2	1.96	0.46
1:B:2958:VAL:HG13	1:B:2993:ILE:HD12	1.97	0.46
1:B:3550:THR:HG22	1:B:3575:GLU:HG3	1.96	0.46
1:B:4218:THR:HG21	1:B:4251:ILE:HD11	1.97	0.46
2:C:235:GLU:N	2:C:255:ASP:OD2	2.49	0.46
1:A:2231:SER:OG	1:A:2344:GLU:OE1	2.33	0.46
1:B:2797:ARG:HG2	3:B:4705:ADP:H4'	1.98	0.46
1:A:1491:ASP:N	1:A:1491:ASP:OD1	2.48	0.46
1:A:2288:ILE:HD11	1:A:2336:PRO:HD3	1.98	0.46
1:A:3738:PHE:HD2	1:A:3783:LYS:HE2	1.80	0.46
1:B:1850:GLN:HG3	1:B:1852:ASP:H	1.80	0.46
1:A:2740:GLY:O	1:A:2744:LEU:HB2	2.15	0.46
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.49	0.46
1:B:4569:THR:HB	1:B:4583:THR:HG21	1.97	0.46
2:E:261:TRP:HB3	2:E:268:CYS:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4321:LEU:HD12	1:A:4323:LEU:HD12	1.98	0.46
1:B:2623:SER:OG	1:B:2624:SER:N	2.48	0.46
1:B:3827:TYR:CZ	1:B:3871:VAL:HG13	2.51	0.46
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.50	0.46
1:B:3097:TRP:CD2	1:B:3173:PRO:HB3	2.51	0.46
1:B:3708:LEU:HD23	1:B:3809:SER:HA	1.98	0.46
1:A:2316:ASN:O	1:A:2320:ASP:HB2	2.16	0.46
1:A:2387:LEU:HD23	1:A:2467:ARG:HH21	1.80	0.46
1:A:3966:PRO:HG2	1:A:3997:ARG:HD3	1.96	0.46
1:A:4379:THR:O	1:A:4382:THR:OG1	2.32	0.46
1:B:2522:THR:HG22	1:B:2524:VAL:HG23	1.98	0.46
1:A:2485:GLN:NE2	1:A:2541:ILE:O	2.49	0.46
1:B:4460:LEU:HD12	1:B:4461:PRO:HD2	1.96	0.45
2:E:124:VAL:HG12	2:E:134:VAL:HG22	1.98	0.45
1:A:3451:TYR:CZ	1:A:3455:ILE:HD11	2.51	0.45
1:A:4565:LEU:HD23	1:A:4642:VAL:HG22	1.97	0.45
1:A:4187:HIS:HD1	1:A:4252:TYR:HH	1.60	0.45
2:E:313:SER:HA	2:E:321:LYS:H	1.81	0.45
2:E:214:LYS:HA	2:E:237:VAL:HG23	1.98	0.45
1:A:1805:ARG:O	1:A:1809:GLU:HG2	2.16	0.45
1:A:2943:LYS:HD2	1:A:3067:THR:HG23	1.97	0.45
1:B:1627:PRO:HB3	1:B:1950:GLN:HB3	1.99	0.45
1:B:1880:VAL:HG11	1:B:2049:ILE:HA	1.98	0.45
1:B:3208:ILE:HD11	1:B:3753:LEU:HD21	1.98	0.45
1:A:1804:ARG:O	1:A:1808:LEU:HG	2.16	0.45
1:B:3521:ASP:OD1	1:B:3521:ASP:N	2.44	0.45
2:E:197:SER:HB3	2:E:239:MET:HA	1.97	0.45
2:C:127:SER:OG	2:C:129:ASP:OD1	2.23	0.45
1:A:2518:ILE:HA	1:A:2521:ILE:HG22	1.98	0.45
1:A:3748:SER:HA	1:A:3751:GLN:HG2	1.99	0.45
1:A:4534:TRP:HB3	1:A:4594:LYS:HE3	1.97	0.45
1:B:1835:SER:OG	1:B:1837:GLU:OE1	2.35	0.45
1:B:4430:ASP:O	1:B:4434:VAL:HG23	2.16	0.45
1:A:2644:THR:OG1	1:A:2647:GLY:O	2.26	0.45
1:A:4287:LYS:O	1:A:4319:SER:OG	2.30	0.45
1:B:4239:PRO:HB2	1:B:4242:ALA:HB3	1.98	0.45
1:B:1604:LEU:HD12	1:B:1607:LEU:HD11	1.99	0.45
2:E:94:TRP:HB2	2:E:409:CYS:HB3	1.99	0.45
2:E:274:GLU:HB2	2:E:323:TRP:HH2	1.82	0.45
2:C:315:SER:OG	2:C:316:ARG:N	2.50	0.45
1:A:2221:MET:HB3	1:A:2343:PHE:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3776:GLU:O	1:A:3780:VAL:HG23	2.16	0.45
1:B:2202:MET:HE3	1:B:2202:MET:HB2	1.89	0.45
2:E:212:ARG:HG2	2:E:236:TRP:CD2	2.52	0.45
1:A:1822:THR:O	1:A:1826:ILE:HG12	2.17	0.45
1:B:4094:VAL:HG13	1:B:4124:LEU:HD13	1.98	0.44
2:E:277:HIS:CE1	2:E:316:ARG:HD2	2.52	0.44
1:A:2419:ALA:O	1:A:2423:MET:HG2	2.17	0.44
1:A:2596:PRO:O	1:A:2601:LYS:NZ	2.49	0.44
1:A:2665:GLU:HB3	1:A:2668:LEU:HD12	1.99	0.44
1:A:2697:ASP:OD1	1:A:2697:ASP:N	2.48	0.44
1:B:1930:PHE:HA	1:B:2326:THR:HG21	1.99	0.44
1:B:3520:PHE:HB3	1:B:3524:MET:HB3	1.98	0.44
1:A:1941:MET:HE2	1:A:1941:MET:HB2	1.81	0.44
1:A:2897:LEU:HD12	1:A:2911:LEU:HD21	1.99	0.44
1:B:2540:SER:OG	1:B:2544:GLU:O	2.30	0.44
1:B:2977:ARG:NH1	1:B:3020:LEU:O	2.48	0.44
1:B:4557:SER:HB3	1:B:4591:ARG:HG2	2.00	0.44
1:A:2533:PRO:HB2	1:A:2535:ILE:HG12	1.99	0.44
1:A:3683:ASP:OD1	1:A:3683:ASP:N	2.51	0.44
1:A:3936:VAL:O	1:A:3939:SER:OG	2.34	0.44
1:A:4218:THR:HG21	1:A:4251:ILE:HD11	1.99	0.44
1:B:2799:MET:HE3	1:B:2799:MET:HB3	1.91	0.44
2:E:240:VAL:O	2:E:241:ARG:NH1	2.50	0.44
2:E:364:VAL:HB	2:E:374:LYS:HB3	1.99	0.44
1:A:4187:HIS:NE2	1:A:4191:GLN:OE1	2.50	0.44
2:C:159:ASP:OD1	2:C:160:HIS:N	2.49	0.44
2:C:193:HIS:ND1	2:C:212:ARG:HD2	2.33	0.44
1:A:1561:LEU:HB3	1:A:1564:GLU:HB2	1.99	0.44
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.98	0.44
1:B:2103:VAL:HG23	1:B:2136:ILE:HG23	2.00	0.44
1:B:4194:LEU:HA	1:B:4201:TRP:HD1	1.82	0.44
1:A:1852:ASP:HB3	1:A:1855:GLN:HB2	2.00	0.44
1:A:1887:ARG:NH2	1:A:4253:GLY:O	2.51	0.44
1:A:4106:LEU:HD23	1:A:4106:LEU:HA	1.86	0.44
2:C:237:VAL:HA	2:C:253:SER:HA	2.00	0.44
1:A:2492:ARG:HH21	1:A:2525:PRO:HB2	1.83	0.44
1:A:2763:ARG:HD2	1:A:2763:ARG:HA	1.78	0.44
1:B:2982:ARG:NH1	1:B:2988:GLU:OE2	2.51	0.44
1:B:4030:ILE:HG21	1:B:4145:PHE:HZ	1.83	0.44
1:A:2257:LYS:HA	1:A:2257:LYS:HD2	1.83	0.44
1:A:2324:LEU:HD11	1:A:2332:ARG:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1958:ASP:HA	1:A:2017:THR:HB	1.99	0.44
1:A:3581:LYS:HE3	1:A:3582:ARG:HG2	2.00	0.44
1:B:1727:PHE:HB3	1:B:1733:ILE:HD11	2.00	0.43
1:B:2307:VAL:HG13	1:B:2312:VAL:HG11	2.00	0.43
1:B:2446:ILE:HG13	1:B:2735:TYR:CD1	2.53	0.43
1:B:2633:LYS:HB2	1:B:2633:LYS:HE3	1.78	0.43
1:B:2904:GLU:O	1:B:3654:ARG:NE	2.36	0.43
1:B:1738:TYR:O	1:B:1742:ILE:HG12	2.18	0.43
1:B:3478:LEU:HG	1:B:3482:LEU:HD13	2.00	0.43
1:B:4099:VAL:HG11	1:B:4126:LEU:HD23	1.98	0.43
1:A:4096:LEU:HD13	1:A:4105:TRP:HH2	1.82	0.43
1:B:3163:LYS:HE3	1:B:3163:LYS:HB3	1.90	0.43
2:C:385:SER:O	2:C:398:GLY:N	2.46	0.43
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	2.00	0.43
1:A:2677:GLN:HB2	1:A:2680:ILE:HB	2.00	0.43
1:A:3691:ASP:HB2	1:A:3695:ARG:HH21	1.83	0.43
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	2.00	0.43
1:B:2585:LEU:HD13	1:B:2609:LEU:HD13	2.00	0.43
1:B:4528:VAL:HG11	1:B:4592:TRP:CD1	2.54	0.43
1:A:1686:PHE:HA	1:A:1712:THR:HG21	2.01	0.43
1:A:3154:LEU:HD22	1:A:3516:TYR:CG	2.54	0.43
1:A:3822:HIS:O	1:A:3822:HIS:ND1	2.52	0.43
1:A:4418:LYS:HA	1:A:4418:LYS:HD3	1.72	0.43
1:B:4412:PHE:HE1	1:B:4516:VAL:HG23	1.84	0.43
1:A:1829:LYS:HA	1:A:1829:LYS:HD2	1.81	0.43
1:A:2831:ARG:HD3	1:A:2831:ARG:HA	1.74	0.43
1:A:4396:SER:O	1:A:4397:HIS:ND1	2.51	0.43
1:B:1981:ALA:HB2	1:B:1999:CYS:HB3	2.00	0.43
2:C:201:MET:HE1	2:C:242:PRO:HB3	2.01	0.43
1:A:2346:GLN:HB2	1:A:2726:ARG:HD2	2.01	0.43
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	2.01	0.43
1:B:1985:HIS:HA	1:B:1997:ILE:HD13	2.00	0.43
1:B:2452:LEU:HD23	1:B:2452:LEU:HA	1.84	0.43
1:B:3873:ARG:HD3	1:B:3873:ARG:HA	1.81	0.43
2:C:216:ILE:HD11	2:C:237:VAL:HG11	2.00	0.43
2:C:238:ARG:HA	2:C:238:ARG:HD2	1.85	0.43
1:A:1504:VAL:HA	1:A:1507:MET:HE2	2.01	0.43
1:B:2181:GLU:HG3	1:B:2244:LEU:HG	2.00	0.43
1:B:4560:VAL:O	1:B:4588:THR:OG1	2.36	0.43
1:A:1899:ARG:HG3	1:A:1983:ARG:HG2	2.01	0.43
1:A:2138:ILE:HG23	1:A:2161:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2719:GLY:O	1:A:2721:LYS:NZ	2.41	0.43
1:A:3873:ARG:HD3	1:A:3873:ARG:HA	1.81	0.43
1:B:2444:GLU:HG2	1:B:2510:MET:HE3	2.00	0.43
1:A:1517:GLU:O	1:A:1521:LEU:HG	2.19	0.43
1:A:1914:GLU:HG3	3:A:4706:ADP:H2'	2.00	0.43
1:A:2065:LEU:HD22	1:A:2137:LEU:HD22	2.00	0.43
1:A:2239:LYS:HD2	1:A:2239:LYS:HA	1.74	0.43
1:A:2347:ASP:OD1	1:A:2347:ASP:N	2.52	0.43
1:A:4434:VAL:HA	1:A:4437:VAL:HG12	2.00	0.43
1:B:1609:GLY:O	1:B:1613:LYS:HG3	2.19	0.43
1:B:2079:GLN:NE2	1:B:4526:GLN:OE1	2.47	0.43
1:B:2258:ALA:HB1	1:B:2682:PHE:HD1	1.84	0.43
1:B:2284:LEU:HD12	1:B:2284:LEU:HA	1.86	0.43
1:B:3194:LEU:HG	1:B:3496:PHE:HD1	1.84	0.43
1:B:4068:SER:HA	1:B:4095:MET:HB3	2.01	0.43
1:B:4321:LEU:HD12	1:B:4323:LEU:HD12	2.00	0.43
1:A:1879:LEU:HD11	1:A:1914:GLU:HB3	2.01	0.43
1:A:2726:ARG:NH1	4:A:4701:ATP:O3G	2.52	0.43
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	2.00	0.43
1:B:1596:GLY:H	1:B:1599:ARG:HH21	1.66	0.42
1:B:4391:ILE:HD12	1:B:4479:VAL:HG11	2.01	0.42
1:B:1795:SER:O	1:B:1800:GLN:NE2	2.45	0.42
1:B:2943:LYS:HG2	1:B:3094:PHE:HD2	1.85	0.42
1:B:3123:PRO:HG2	1:B:3126:MET:HB2	2.01	0.42
2:E:279:VAL:HG13	2:E:314:GLY:O	2.19	0.42
1:A:3662:ILE:HG12	1:A:3671:LEU:HB2	2.00	0.42
1:B:2066:ALA:HA	1:B:2069:ILE:HG22	2.00	0.42
2:E:366:ASP:HB2	2:E:373:MET:HG2	2.01	0.42
1:A:2379:LEU:HD13	1:A:2424:GLN:HG2	2.02	0.42
1:A:4042:LEU:HG	1:A:4142:GLY:HA3	2.01	0.42
1:A:4314:ASP:N	1:A:4314:ASP:OD1	2.51	0.42
1:A:4541:LEU:HD12	1:A:4541:LEU:HA	1.90	0.42
1:B:1811:LEU:HD23	1:B:1811:LEU:HA	1.88	0.42
1:B:2752:ASN:HD21	1:B:2773:MET:HE2	1.83	0.42
1:B:2758:LEU:HD13	1:B:2811:ARG:HA	2.01	0.42
1:B:3638:VAL:HG21	1:B:3679:LEU:HD23	2.00	0.42
1:A:1904:PRO:HD2	1:A:2016:ILE:O	2.20	0.42
1:A:3208:ILE:HG21	1:A:3486:ARG:HE	1.84	0.42
1:A:3459:GLN:HA	1:A:3462:LYS:HB2	2.01	0.42
1:B:2047:GLN:HA	1:B:2070:VAL:HG21	2.00	0.42
1:B:2238:LEU:HD11	1:B:2249:GLY:HA3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2644:THR:OG1	1:B:2647:GLY:O	2.28	0.42
1:A:2194:GLY:H	1:A:2204:VAL:HG21	1.84	0.42
1:A:3738:PHE:CD2	1:A:3783:LYS:HE2	2.55	0.42
1:B:2603:MET:HE1	3:B:4705:ADP:C6	2.55	0.42
1:B:2762:LEU:HD13	1:B:2821:LEU:HD22	2.02	0.42
1:B:3822:HIS:O	1:B:3824:LEU:N	2.53	0.42
1:B:4388:LEU:O	1:B:4392:PRO:HD3	2.18	0.42
1:A:2828:GLU:OE2	1:A:2924:ARG:NH2	2.52	0.42
1:B:1478:VAL:O	1:B:1486:LEU:N	2.53	0.42
1:B:3482:LEU:HA	1:B:3485:GLU:HG3	2.01	0.42
1:B:3892:LEU:HD13	1:B:3983:ILE:HG21	2.01	0.42
1:B:4007:MET:O	1:B:4011:THR:HG23	2.20	0.42
1:A:1766:LEU:HD22	1:A:1778:LEU:HD21	2.01	0.42
1:A:2050:ALA:HA	1:A:2097:LEU:HD21	2.02	0.42
1:A:3840:LEU:HD23	1:A:3840:LEU:HA	1.90	0.42
1:A:3892:LEU:HD11	1:A:3983:ILE:HG21	2.02	0.42
1:A:3904:GLU:HB2	1:A:3991:LEU:HD11	2.02	0.42
1:A:3947:LEU:HD23	1:A:3947:LEU:HA	1.88	0.42
1:B:2989:LYS:HB2	1:B:2989:LYS:HE3	1.75	0.42
1:B:3868:PHE:HA	1:B:3883:PHE:HE2	1.85	0.42
1:B:4071:ILE:HD11	1:B:4096:LEU:HD22	2.01	0.42
1:B:4097:LYS:HA	1:B:4127:THR:HB	2.02	0.42
1:A:1688:THR:HA	1:A:1689:PRO:HD3	1.91	0.42
1:A:2285:ARG:HG3	1:A:2333:LEU:HD21	2.01	0.42
1:B:3723:ASP:OD1	1:B:3723:ASP:N	2.50	0.42
1:B:4511:LEU:HD12	1:B:4511:LEU:HA	1.88	0.42
2:E:252:CYS:HB2	2:E:279:VAL:HG12	2.01	0.42
1:A:4390:LEU:O	1:A:4393:GLN:NE2	2.44	0.42
1:B:2784:PHE:HB2	1:B:2794:TYR:HE2	1.84	0.42
1:B:2890:ARG:NH2	1:B:2913:ASN:OD1	2.52	0.42
1:B:3154:LEU:HA	1:B:3154:LEU:HD12	1.72	0.42
1:A:2103:VAL:HG23	1:A:2136:ILE:HG13	2.02	0.42
1:A:2670:ASP:N	1:A:2670:ASP:OD1	2.53	0.42
1:A:4412:PHE:HD1	1:A:4415:ARG:HH21	1.67	0.42
1:A:4605:VAL:O	1:A:4624:PHE:N	2.51	0.41
1:B:1574:GLU:OE1	1:B:1603:ARG:NH2	2.46	0.41
1:B:2744:LEU:HA	1:B:2747:ILE:HG22	2.01	0.41
1:A:1686:PHE:HD1	1:A:1712:THR:HG21	1.85	0.41
1:A:3487:GLU:O	1:A:3491:LYS:NZ	2.43	0.41
1:A:3774:LYS:HA	1:A:3774:LYS:HD3	1.72	0.41
1:B:1488:ARG:HD3	1:B:1488:ARG:HA	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2592:VAL:HB	1:B:2733:VAL:HG22	2.02	0.41
1:B:3167:ARG:HH12	1:B:3685:THR:HB	1.86	0.41
1:B:3451:TYR:O	1:B:3455:ILE:HG12	2.21	0.41
1:B:3895:THR:HG23	1:B:3898:GLU:HB2	2.03	0.41
1:B:4089:LYS:HD2	1:B:4089:LYS:HA	1.81	0.41
1:A:4071:ILE:HG13	1:A:4099:VAL:HG12	2.03	0.41
1:B:1928:LEU:HD23	1:B:2332:ARG:CZ	2.51	0.41
1:B:2590:PRO:HB2	1:B:2731:VAL:HG12	2.02	0.41
1:B:3721:ARG:HH12	1:B:3800:GLN:HG2	1.86	0.41
2:C:213:ASP:OD1	2:C:213:ASP:N	2.53	0.41
1:A:1613:LYS:HB3	1:A:1613:LYS:HE2	1.88	0.41
1:A:2577:HIS:O	1:A:2581:LEU:HG	2.19	0.41
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	2.03	0.41
1:A:3717:LEU:HD23	1:A:3717:LEU:HA	1.94	0.41
1:B:1697:LYS:HD2	1:B:1697:LYS:HA	1.88	0.41
1:B:3239:LYS:HE2	1:B:3451:TYR:HB2	2.03	0.41
2:C:279:VAL:HA	2:C:315:SER:HB2	2.02	0.41
1:A:3882:THR:HG23	1:A:4343:MET:HG3	2.02	0.41
1:A:4107:MET:HE2	1:A:4107:MET:HB3	1.85	0.41
1:B:2513:GLU:O	1:B:2516:GLU:HG3	2.20	0.41
1:B:2587:GLU:OE2	1:B:2587:GLU:N	2.53	0.41
1:B:3741:ARG:HD2	1:B:3741:ARG:HA	1.76	0.41
1:B:3825:TYR:HB2	1:B:3827:TYR:CZ	2.55	0.41
1:B:4605:VAL:HG21	1:B:4626:ILE:HD13	2.01	0.41
1:A:2218:HIS:NE2	1:A:2335:LEU:HD23	2.35	0.41
1:A:2452:LEU:HD12	1:A:2729:ARG:HH21	1.85	0.41
1:A:2680:ILE:HD13	1:A:2680:ILE:HA	1.88	0.41
1:B:2212:GLN:O	1:B:2216:ILE:HG12	2.20	0.41
1:A:1477:LEU:HB3	1:A:1485:ARG:HG2	2.01	0.41
1:A:2876:TRP:HH2	1:A:2919:VAL:HG12	1.86	0.41
1:A:2901:TYR:CZ	1:A:2908:PRO:HA	2.55	0.41
1:A:3075:LEU:HD23	1:A:3075:LEU:HA	1.94	0.41
1:A:3213:ASP:O	1:A:3216:GLU:HG3	2.21	0.41
1:A:4058:LEU:HA	1:A:4061:GLU:HG2	2.02	0.41
1:B:1479:ASN:HD21	1:B:1482:ASN:HA	1.86	0.41
2:E:216:ILE:HB	2:E:230:PHE:HB2	2.02	0.41
2:E:272:LEU:HD13	2:E:323:TRP:CG	2.55	0.41
1:A:3792:GLN:O	1:A:3795:GLU:HG3	2.21	0.41
1:A:4243:LEU:O	1:A:4247:MET:HG3	2.21	0.41
1:B:2288:ILE:HD12	1:B:2333:LEU:HD23	2.03	0.41
1:B:2452:LEU:HD13	1:B:2729:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2769:LEU:O	1:B:2773:MET:HG3	2.21	0.41
1:B:2785:THR:OG1	1:B:2787:ASP:OD1	2.33	0.41
1:B:3597:THR:HG23	1:B:3634:LEU:HD21	2.03	0.41
1:B:3878:GLN:H	1:B:3878:GLN:HG2	1.68	0.41
1:B:3950:LYS:NZ	1:B:3973:LEU:O	2.54	0.41
1:B:4223:LEU:HA	1:B:4226:THR:HG22	2.01	0.41
2:E:178:ASP:HB2	2:E:185:ILE:HD11	2.03	0.41
2:E:272:LEU:HD13	2:E:323:TRP:CD2	2.56	0.41
2:E:312:LEU:HD21	2:E:353:ILE:HG23	2.02	0.41
1:A:1963:LEU:O	1:A:1964:GLU:HG2	2.20	0.41
1:A:3232:LYS:HD3	1:A:3232:LYS:HA	1.82	0.41
1:B:3240:LEU:HD12	1:B:3240:LEU:HA	1.87	0.41
1:B:4411:ARG:O	1:B:4414:GLU:HG3	2.21	0.41
2:E:213:ASP:OD1	2:E:213:ASP:N	2.53	0.41
1:A:1470:TRP:HZ2	1:A:1497:VAL:HG22	1.86	0.41
1:A:1857:LEU:HD23	1:A:1868:TYR:HB2	2.02	0.41
1:A:2211:TYR:HB2	1:A:2237:LEU:HD11	2.02	0.41
1:A:2453:ARG:HB2	1:A:2729:ARG:HA	2.03	0.41
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	2.03	0.41
1:A:3909:LEU:HD21	1:A:4343:MET:HE2	2.01	0.41
1:B:2452:LEU:HD13	1:B:2729:ARG:HD2	2.03	0.40
1:B:2935:LEU:HD12	1:B:3067:THR:HG22	2.02	0.40
1:B:4240:TRP:HH2	1:B:4277:SER:HA	1.87	0.40
1:A:1677:SER:HA	1:A:1683:GLU:HG2	2.03	0.40
1:A:3485:GLU:OE2	1:A:3489:TRP:NE1	2.54	0.40
1:B:1825:LEU:HD12	1:B:1830:ILE:HG13	2.02	0.40
1:B:1843:ARG:HG3	1:B:1845:TYR:HE1	1.86	0.40
1:A:1492:ASP:OD1	1:A:1492:ASP:N	2.52	0.40
1:A:1550:ILE:HD11	1:A:1618:TYR:CE2	2.51	0.40
1:A:2598:GLY:HA3	1:A:2795:SER:HB2	2.03	0.40
1:A:3835:ILE:HG23	1:A:3866:VAL:HG12	2.03	0.40
1:A:4001:LEU:HD12	1:A:4001:LEU:HA	1.89	0.40
1:A:4511:LEU:HD22	1:A:4517:PRO:HB3	2.03	0.40
1:A:4539:LEU:HD23	1:A:4539:LEU:HA	1.91	0.40
1:B:2499:LEU:HD23	1:B:2499:LEU:HA	1.93	0.40
1:B:4247:MET:HA	1:B:4251:ILE:HD12	2.04	0.40
2:C:174:ILE:HD11	2:C:195:VAL:HG11	2.02	0.40
1:A:2284:LEU:HD12	1:A:2284:LEU:HA	1.91	0.40
1:A:2419:ALA:HA	1:A:2422:ILE:HG12	2.03	0.40
1:A:3219:ARG:HH21	1:A:3222:LEU:HD22	1.86	0.40
1:A:3807:ALA:O	1:A:3811:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3931:GLN:H	1:A:3931:GLN:HG2	1.70	0.40
1:B:3776:GLU:O	1:B:3780:VAL:HG23	2.21	0.40
1:B:4190:ILE:HD12	1:B:4201:TRP:HZ2	1.86	0.40
1:A:2039:LEU:HD12	1:A:4254:GLY:HA2	2.02	0.40
1:B:1974:GLN:H	1:B:1974:GLN:HG2	1.74	0.40
1:B:2521:ILE:HG13	1:B:2522:THR:N	2.36	0.40
2:C:384:THR:OG1	2:C:398:GLY:O	2.34	0.40
1:A:2976:LEU:HD12	1:A:2976:LEU:HA	1.87	0.40
1:A:4271:ARG:HA	1:A:4271:ARG:HD2	2.00	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%)	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. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1541	GLN
1	B	1593	ASN
1	B	1643	ASN
1	B	1695	HIS
1	B	1790	ASN
1	B	1856	GLN
1	B	2067	ASN
1	B	2263	HIS
1	B	2464	GLN
1	B	2471	GLN
1	B	2646	ASN
1	B	2707	GLN
1	B	2752	ASN
1	B	3069	ASN
1	B	3145	ASN
1	B	3237	ASN
1	B	3459	GLN
1	B	3526	GLN
1	B	3602	ASN
1	B	3744	GLN
1	B	3837	HIS
1	B	3852	HIS
1	B	4266	ASN
1	B	4326	ASN
1	B	4429	GLN
1	B	4477	GLN

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Mol	Chain	Res	Type
2	E	160	HIS
1	A	1471	ASN
1	A	1651	GLN
1	A	1931	ASN
1	A	2079	GLN
1	A	2083	GLN
1	A	2085	HIS
1	A	2346	GLN
1	A	2377	ASN
1	A	2677	GLN
1	A	2960	GLN
1	A	3009	ASN
1	A	3014	ASN
1	A	3237	ASN
1	A	3523	GLN
1	A	3526	GLN
1	A	3527	ASN
1	A	3535	HIS
1	A	3595	GLN
1	A	3622	ASN
1	A	3877	HIS
1	A	4012	ASN
1	A	4156	ASN
1	A	4386	ASN
1	A	4389	HIS

### 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
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.

All (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
3	A	4703	ADP	N3-C2-N1	-3.51	123.90	128.67
3	B	4701	ADP	C4-C5-N7	-2.56	106.63	109.34
3	B	4706	ADP	C4-C5-N7	-2.54	106.65	109.34
3	A	4703	ADP	C4-C5-N7	-2.48	106.72	109.34
3	A	4706	ADP	C4-C5-N7	-2.48	106.72	109.34
3	A	4702	ADP	C4-C5-N7	-2.43	106.77	109.34
4	A	4701	ATP	C5-C6-N6	2.30	123.81	120.31
4	B	4702	ATP	C5-C6-N6	2.29	123.79	120.31
3	B	4705	ADP	C4-C5-N7	-2.10	107.12	109.34

There are no chirality outliers.

All (18) torsion outliers are listed below:

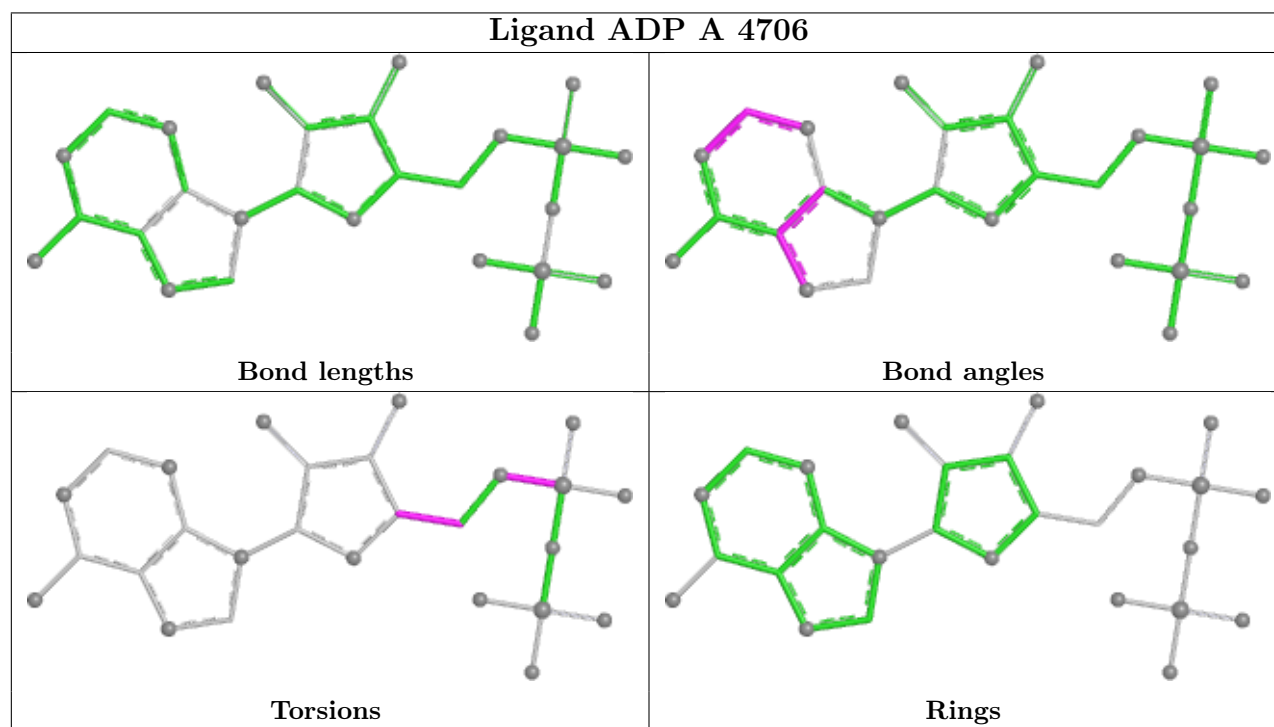
Mol	Chain	Res	Type	Atoms
3	B	4706	ADP	PA-O3A-PB-O3B
3	B	4706	ADP	C5'-O5'-PA-O1A
3	A	4706	ADP	C5'-O5'-PA-O1A
4	B	4702	ATP	C3'-C4'-C5'-O5'
4	B	4702	ATP	O4'-C4'-C5'-O5'
3	B	4701	ADP	C3'-C4'-C5'-O5'
3	B	4701	ADP	O4'-C4'-C5'-O5'
4	A	4701	ATP	PA-O3A-PB-O1B
3	B	4706	ADP	O4'-C4'-C5'-O5'
3	A	4706	ADP	O4'-C4'-C5'-O5'
3	B	4701	ADP	C5'-O5'-PA-O1A
3	B	4706	ADP	C5'-O5'-PA-O2A
3	B	4706	ADP	C5'-O5'-PA-O3A
3	B	4706	ADP	PA-O3A-PB-O1B
3	A	4702	ADP	PB-O3A-PA-O2A
4	B	4702	ATP	PG-O3B-PB-O2B
4	A	4701	ATP	PA-O3A-PB-O2B
3	A	4702	ADP	O4'-C4'-C5'-O5'

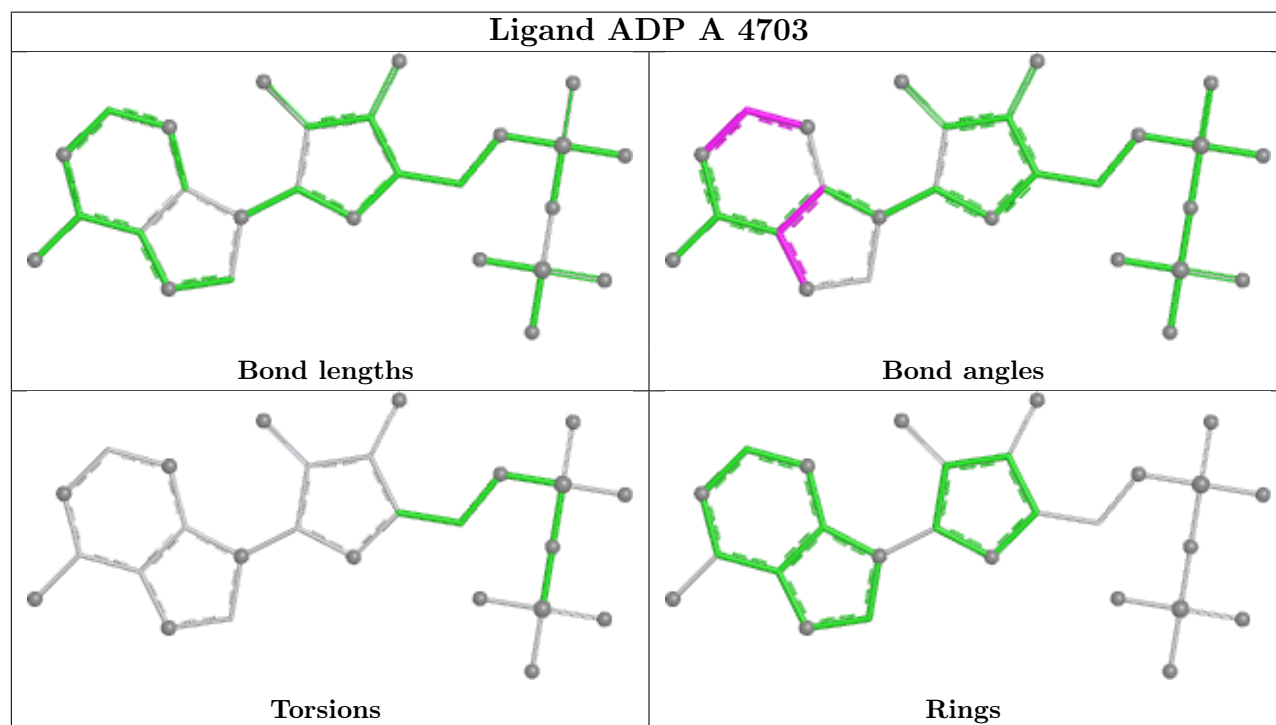
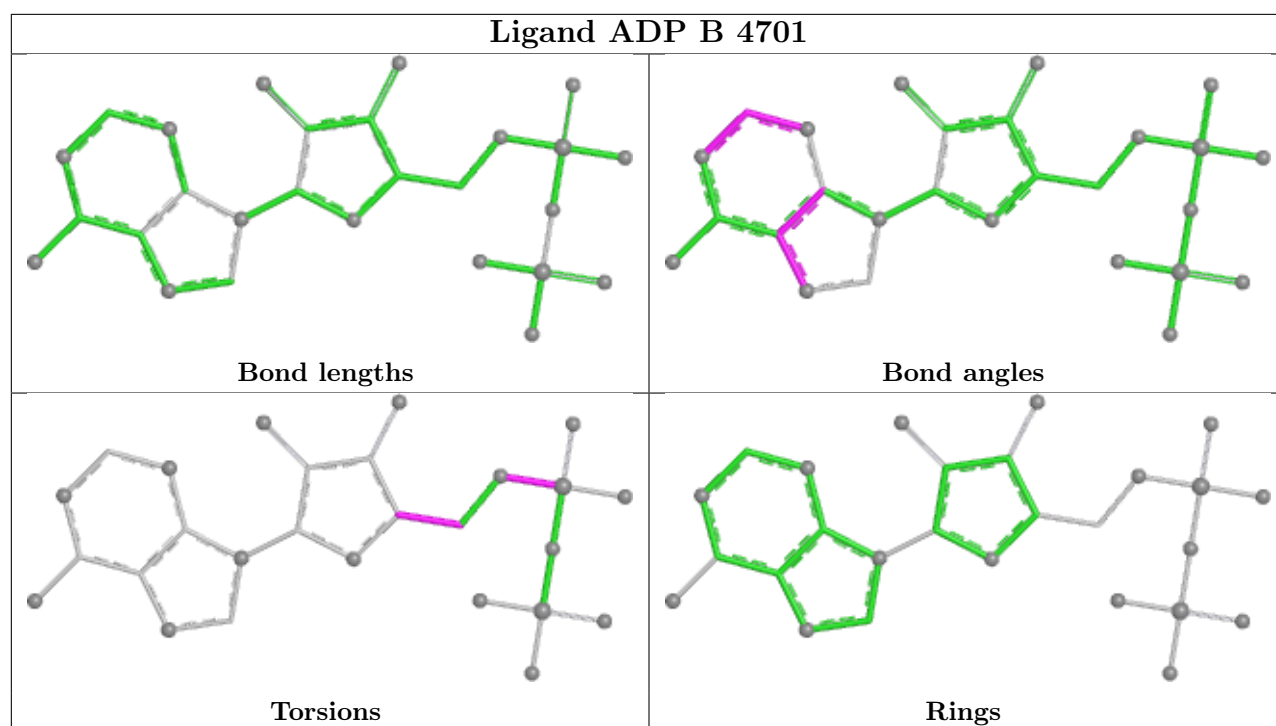
There are no ring outliers.

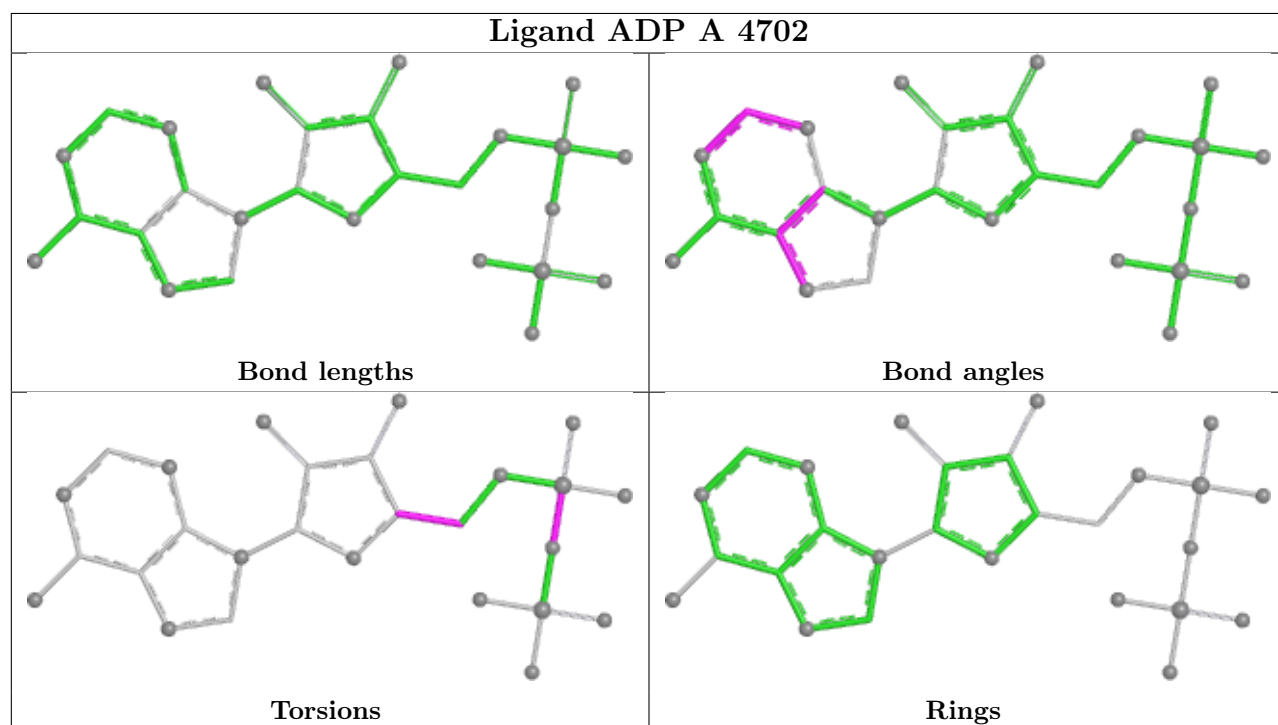
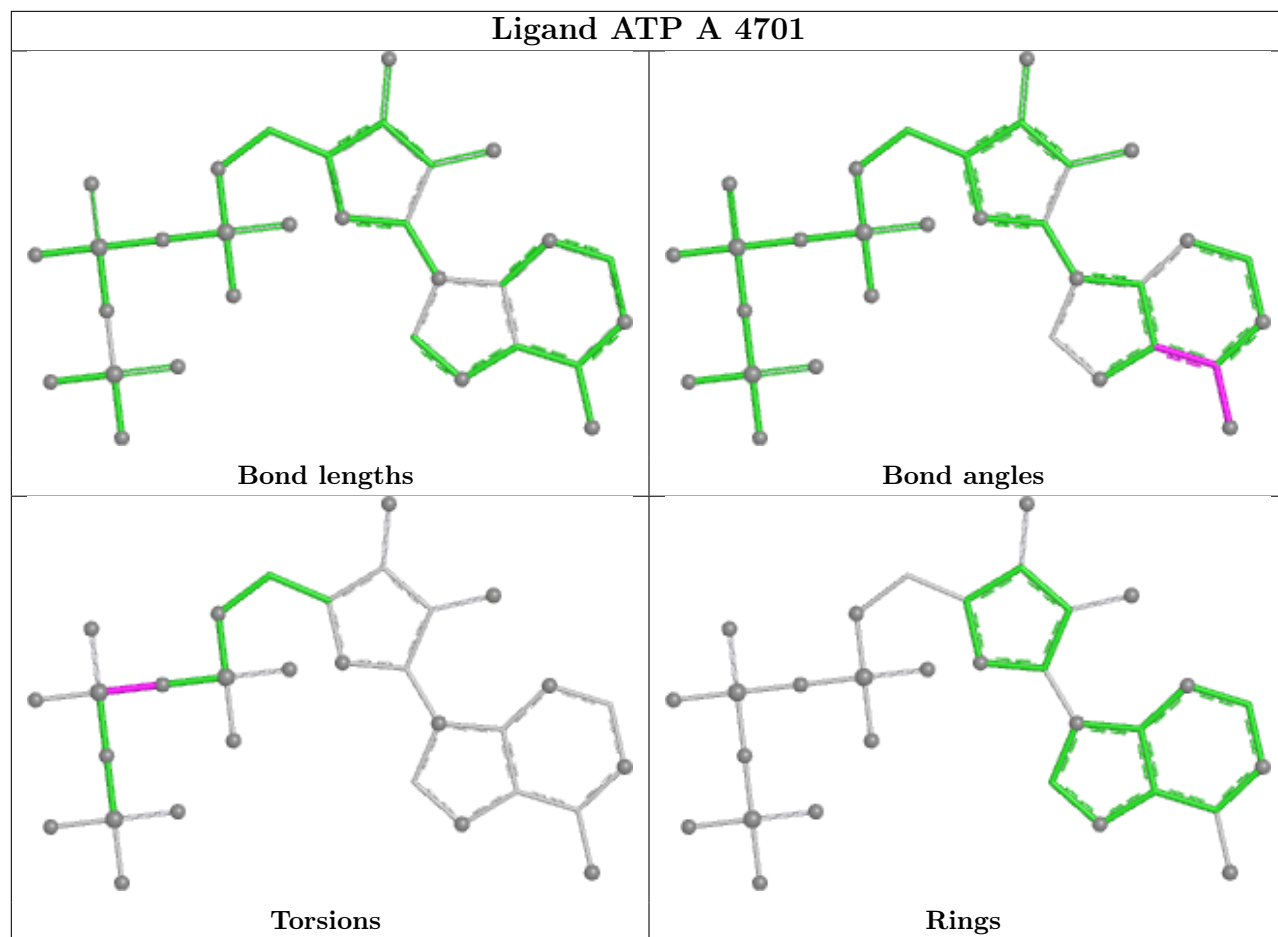
4 monomers are involved in 6 short contacts:

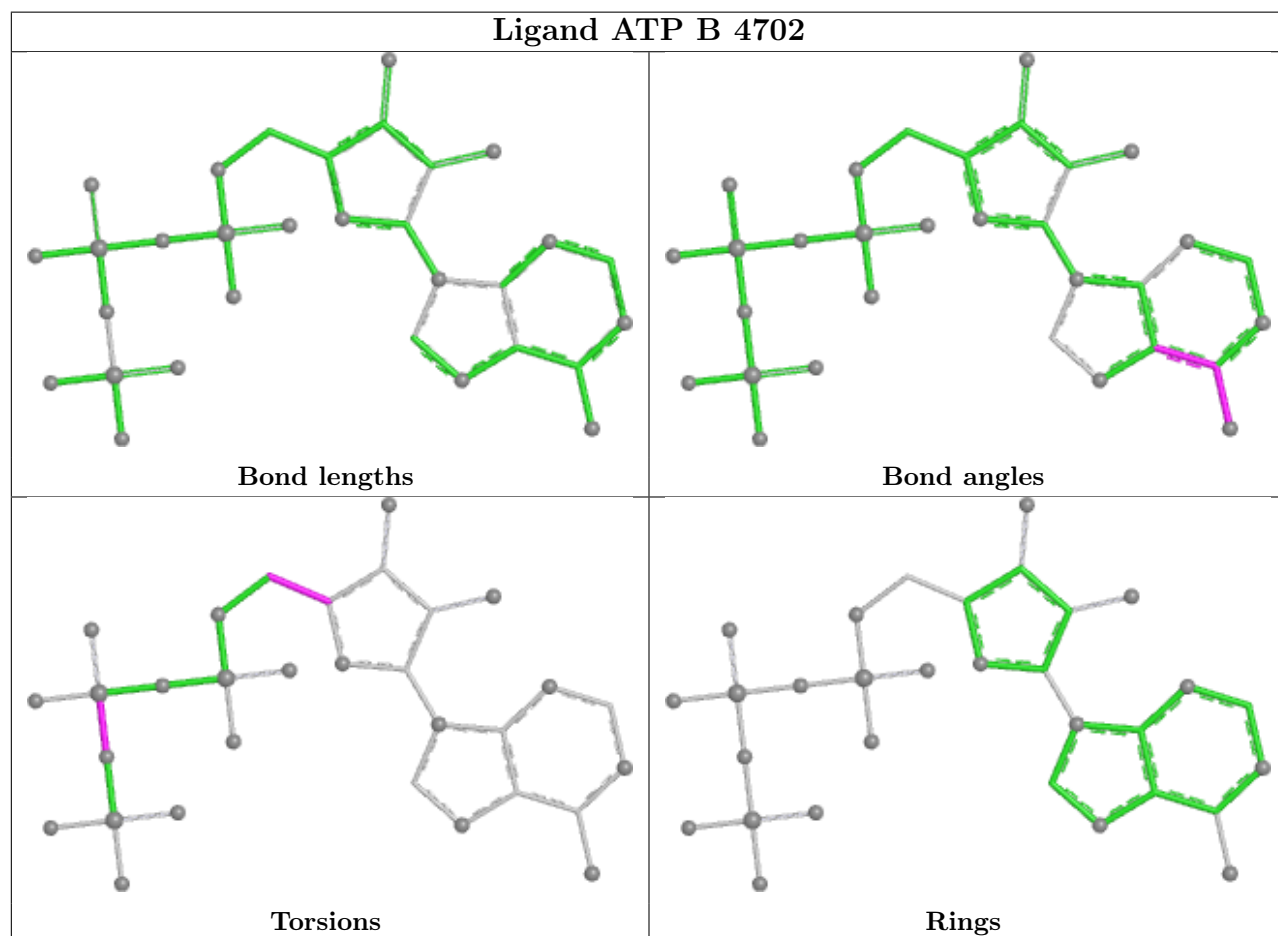
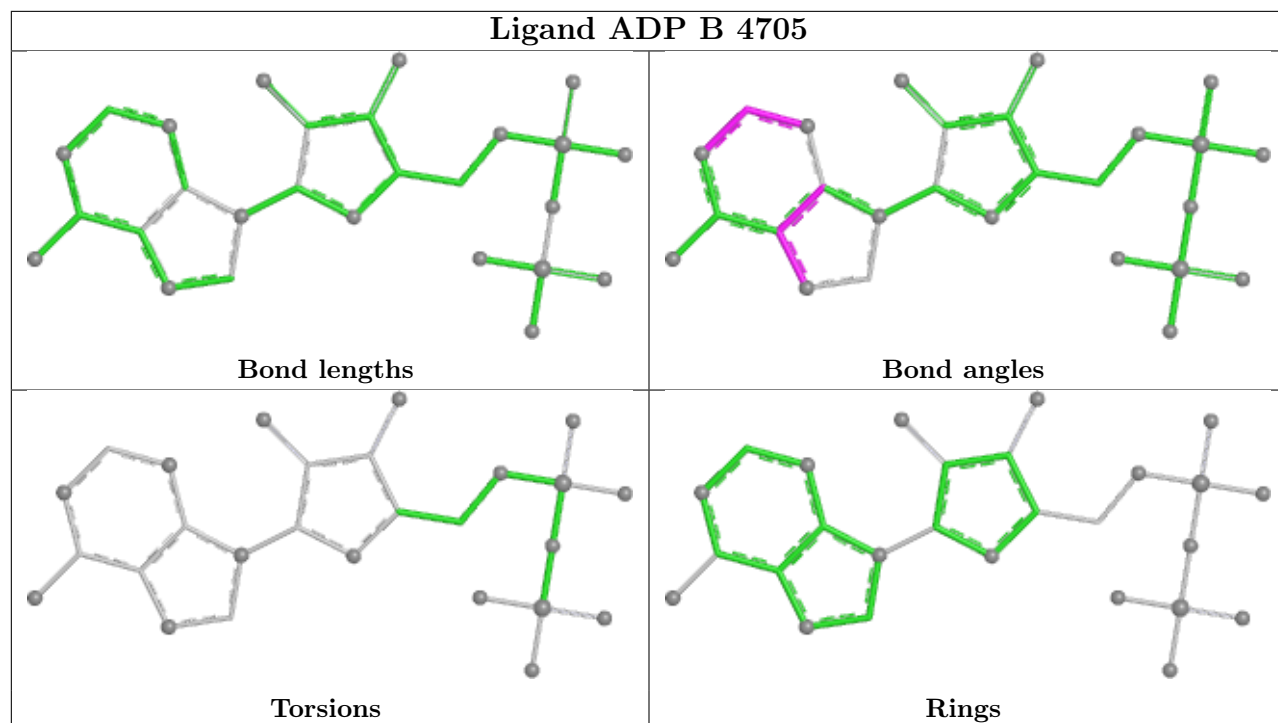
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4706	ADP	1	0
4	A	4701	ATP	1	0
3	B	4705	ADP	2	0
3	B	4706	ADP	2	0

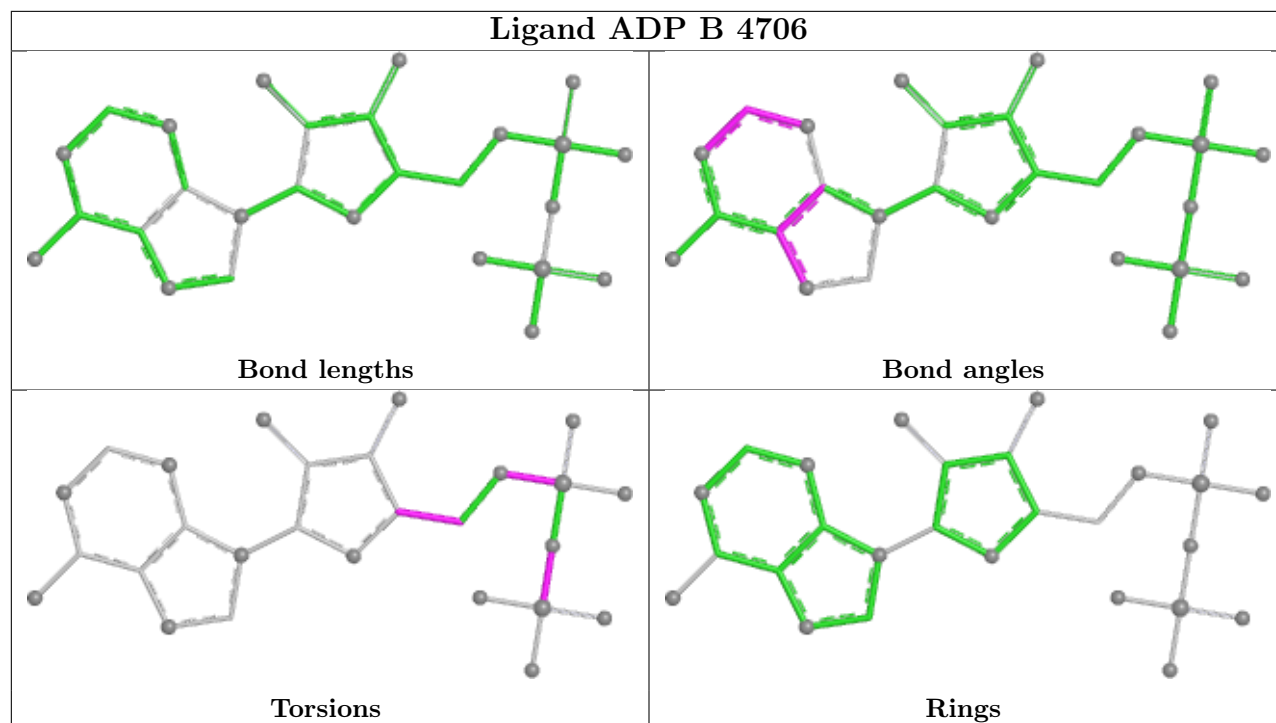
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

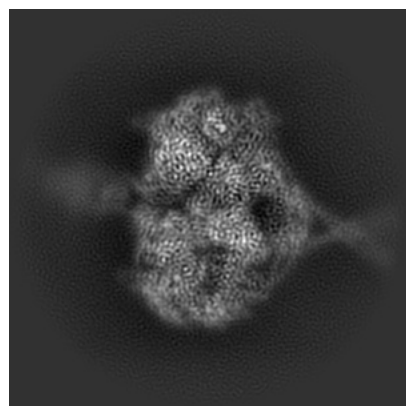
## 6 Map visualisation [i](#)

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.

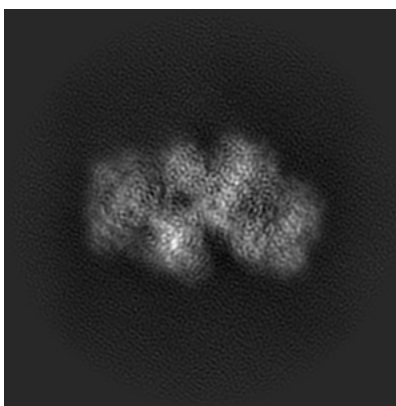
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

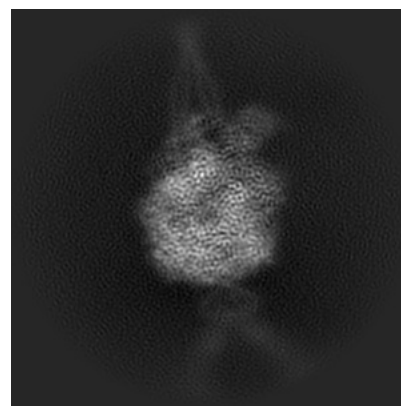
#### 6.1.1 Primary map



X

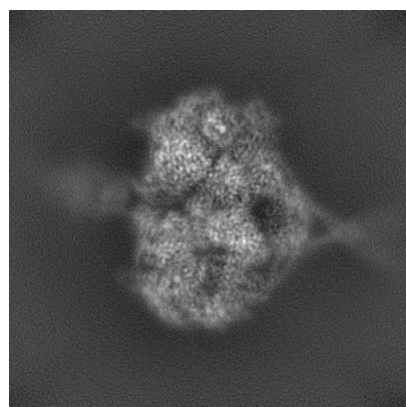


Y

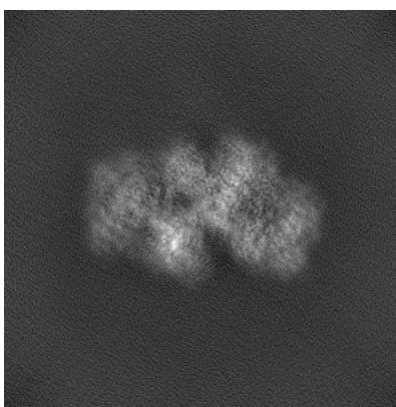


Z

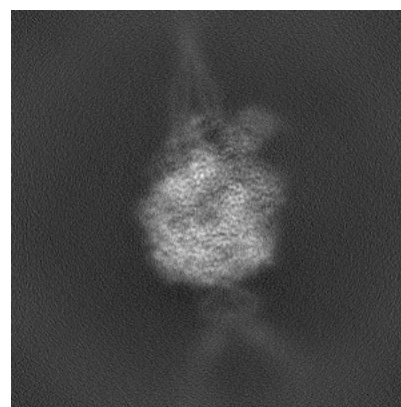
#### 6.1.2 Raw map



X



Y



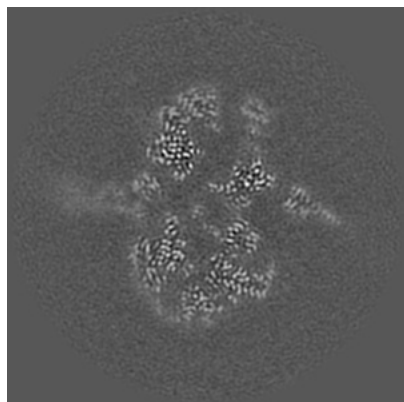
Z

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

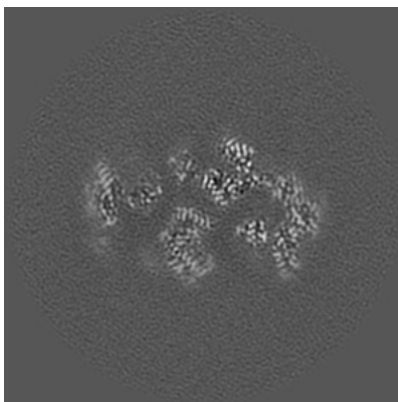


## 6.2 Central slices [i](#)

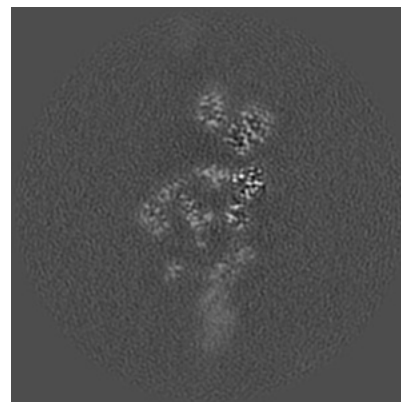
### 6.2.1 Primary map



X Index: 176

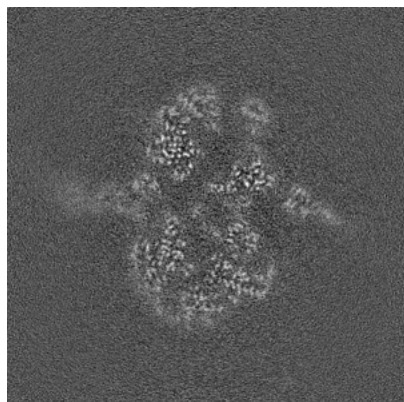


Y Index: 176

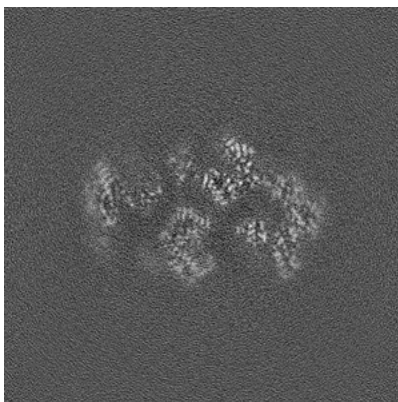


Z Index: 176

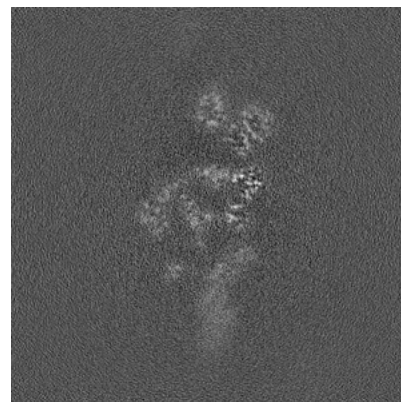
### 6.2.2 Raw map



X Index: 176



Y Index: 176

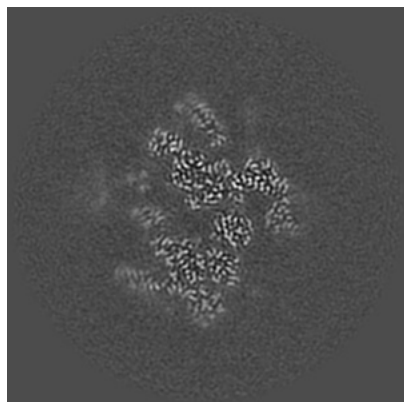


Z Index: 176

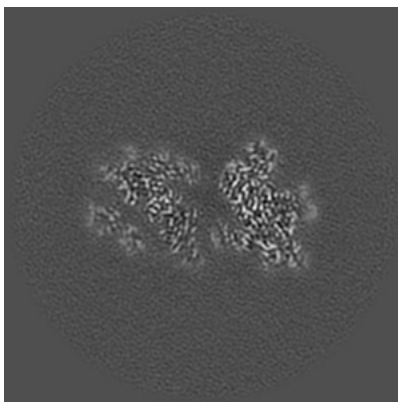
The images above show central slices of the map in three orthogonal directions.

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

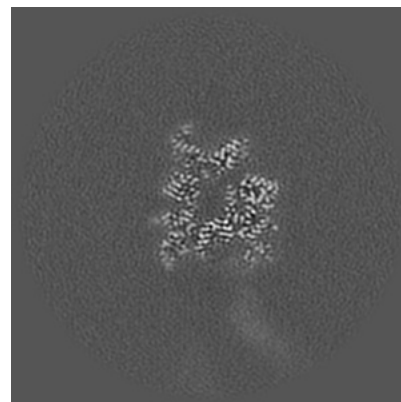
### 6.3.1 Primary map



X Index: 192

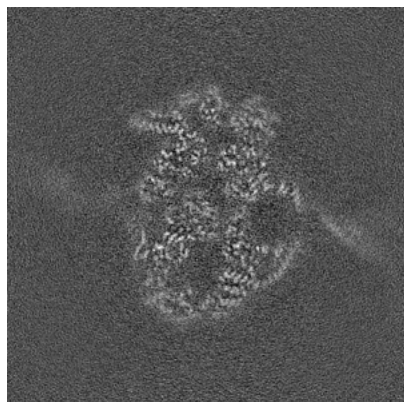


Y Index: 151

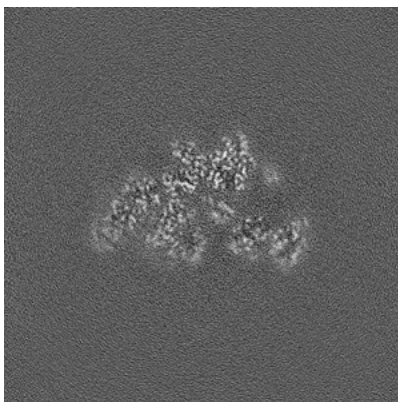


Z Index: 212

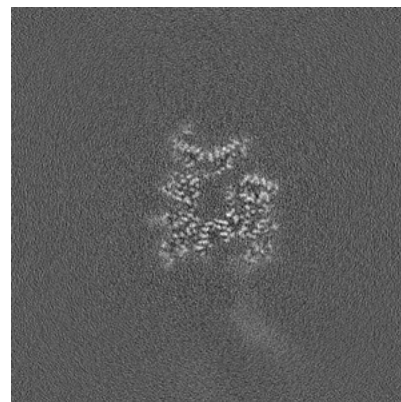
### 6.3.2 Raw map



X Index: 164



Y Index: 195

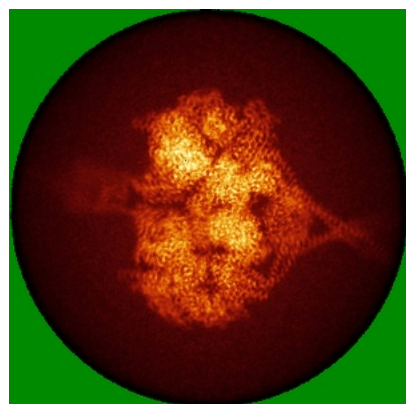


Z Index: 213

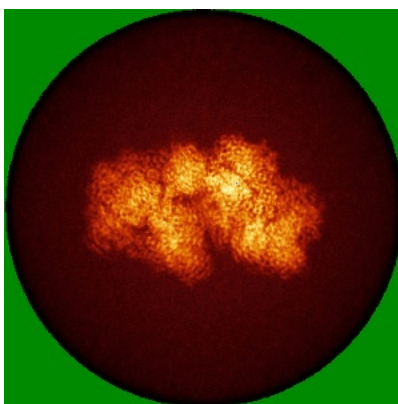
The images above show the largest variance slices of the map in three orthogonal directions.

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

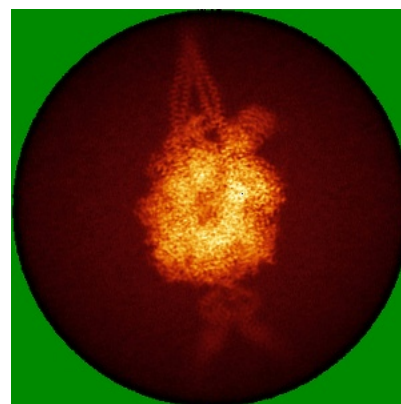
### 6.4.1 Primary map



X

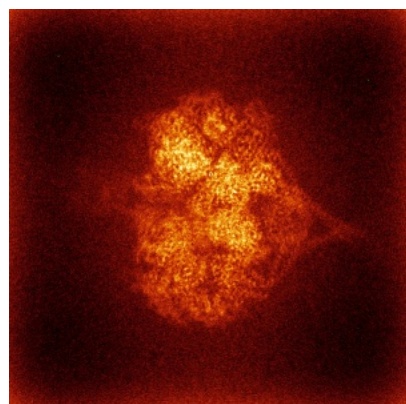


Y

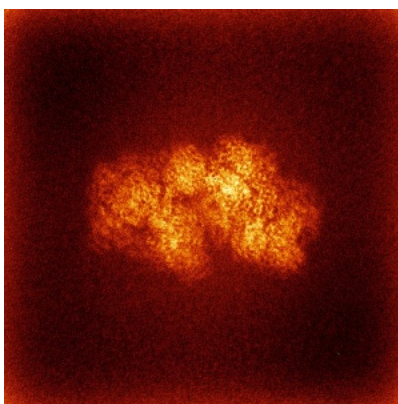


Z

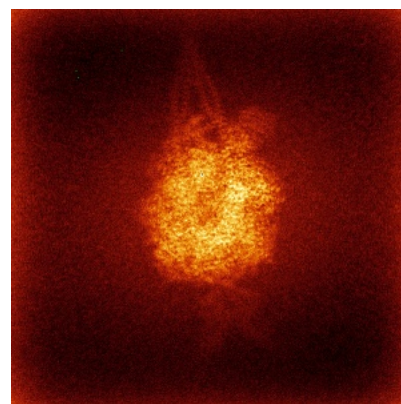
### 6.4.2 Raw map



X



Y



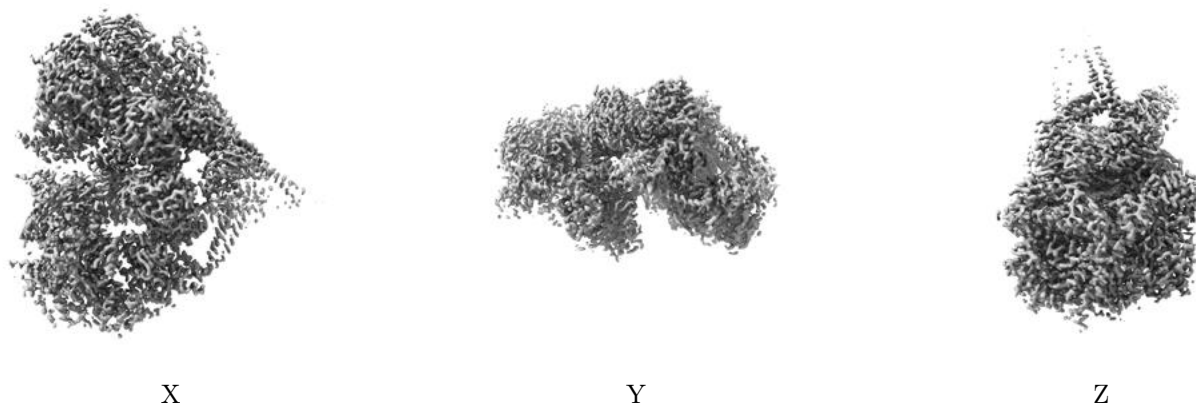
Z

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.



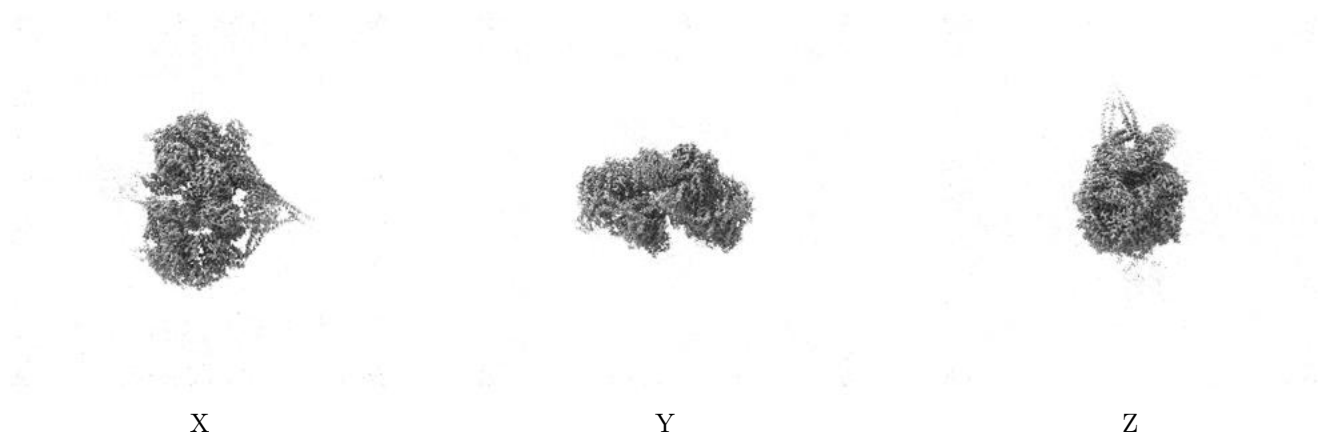
## 6.5 Orthogonal surface views [i](#)

### 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.

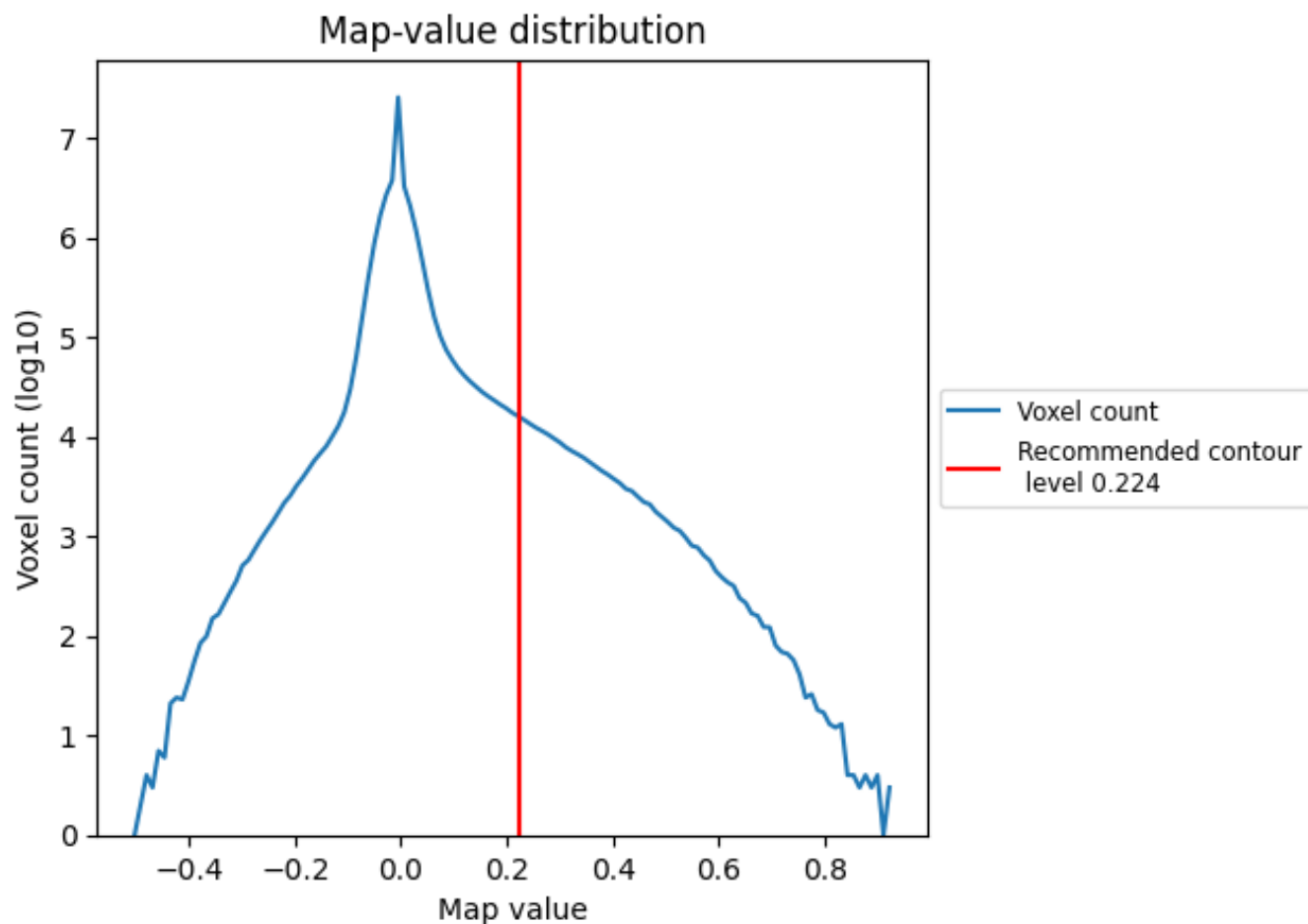
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

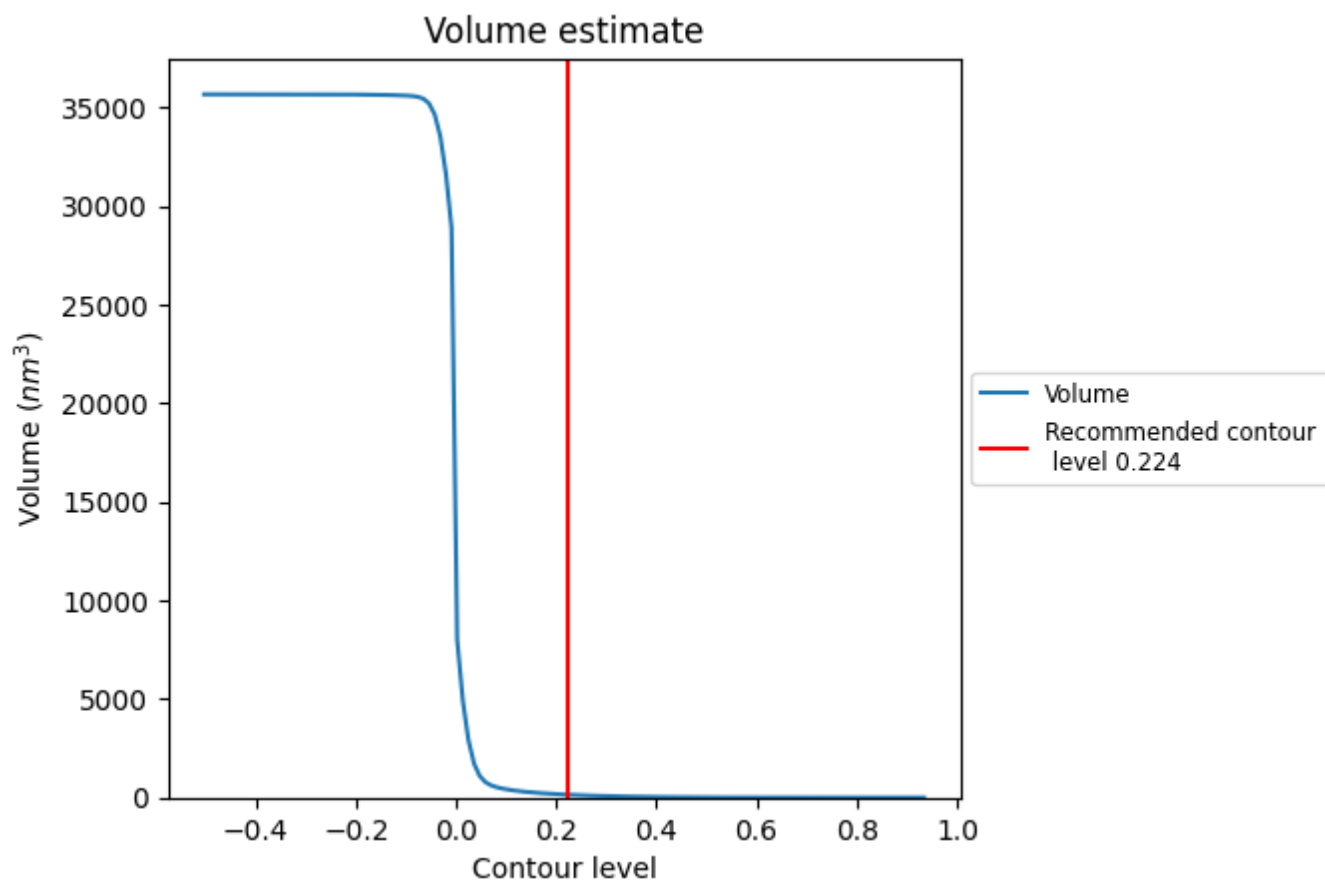
This section contains the results of statistical analysis of the map.

### 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.

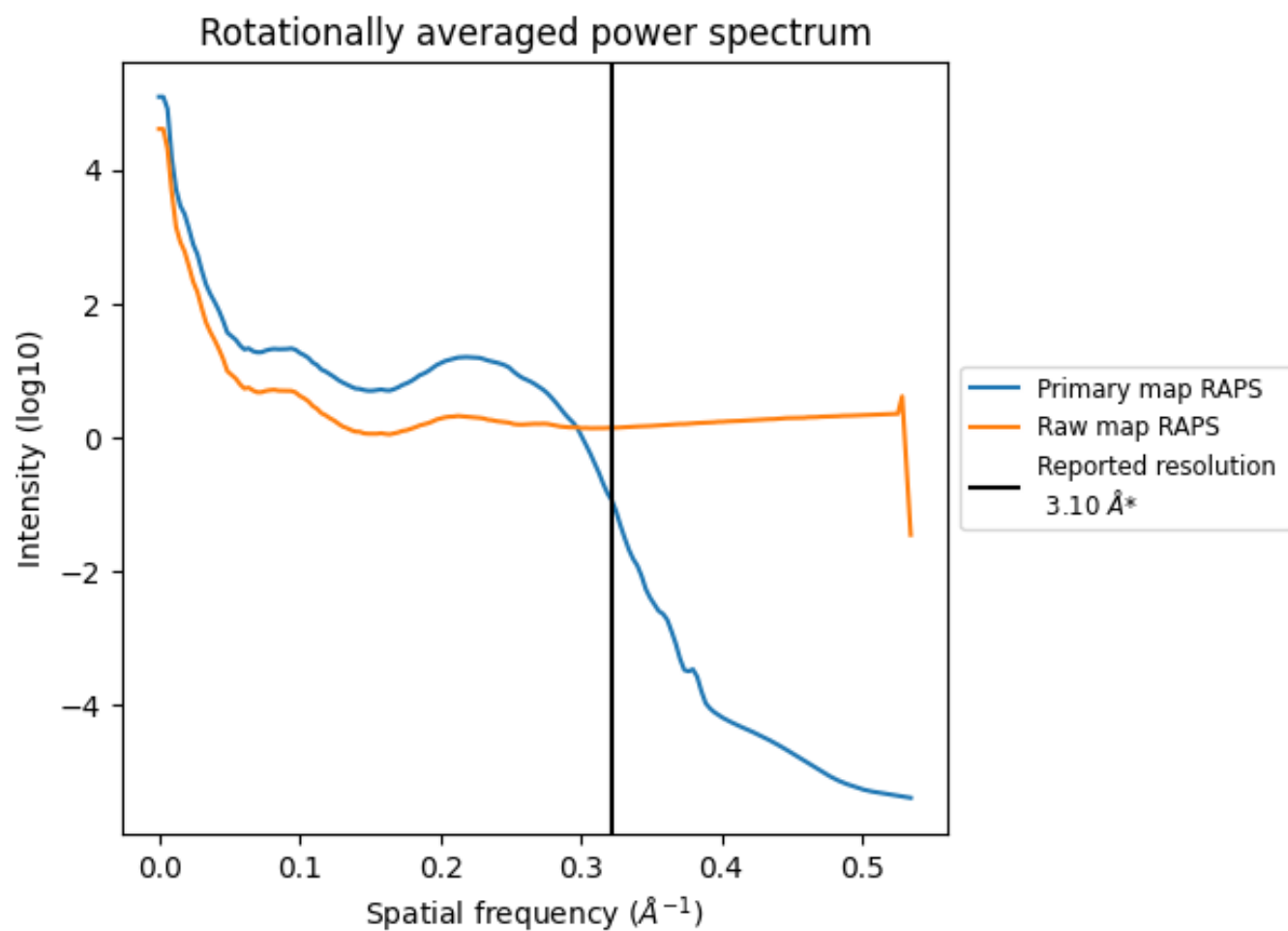
## 7.2 Volume estimate [i](#)



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](#)

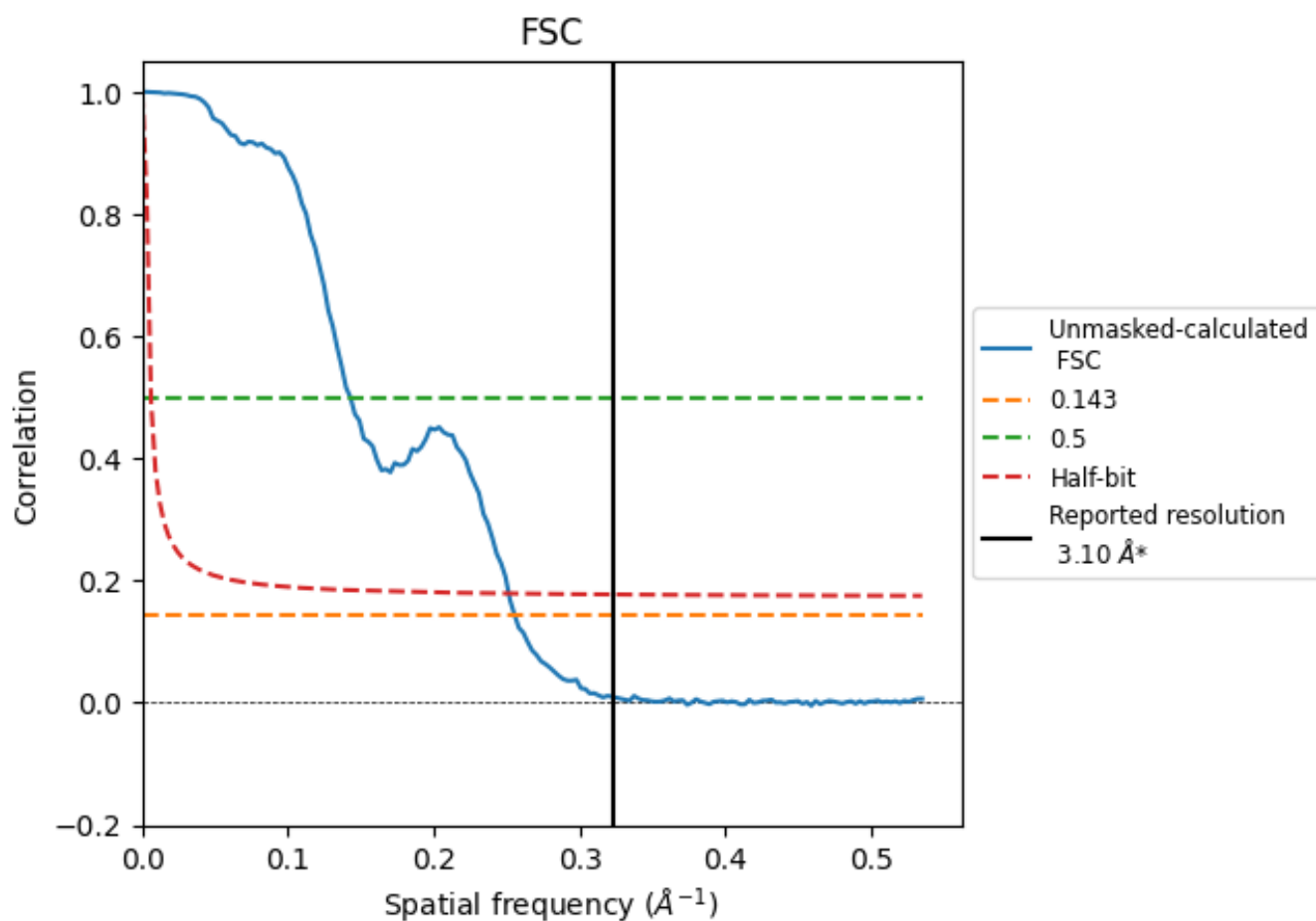


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 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  $0.323 \text{ \AA}^{-1}$



## 8.2 Resolution estimates [i](#)

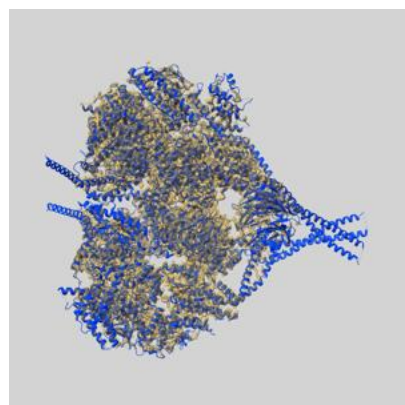
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.92	7.00	3.98

\*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 %

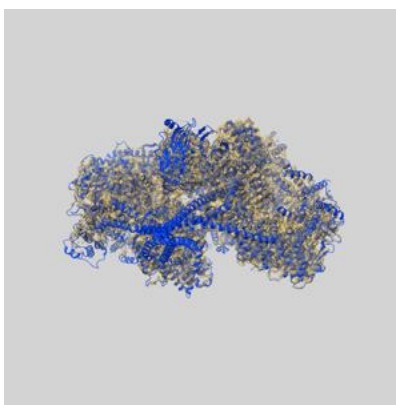
## 9 Map-model fit [i](#)

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.

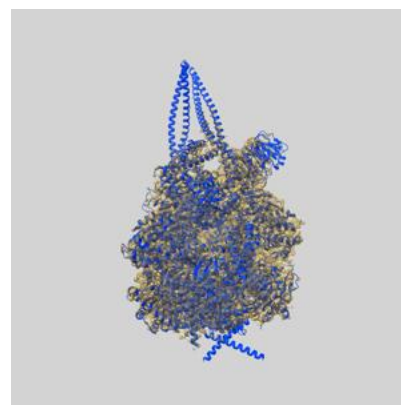
### 9.1 Map-model overlay [i](#)



X



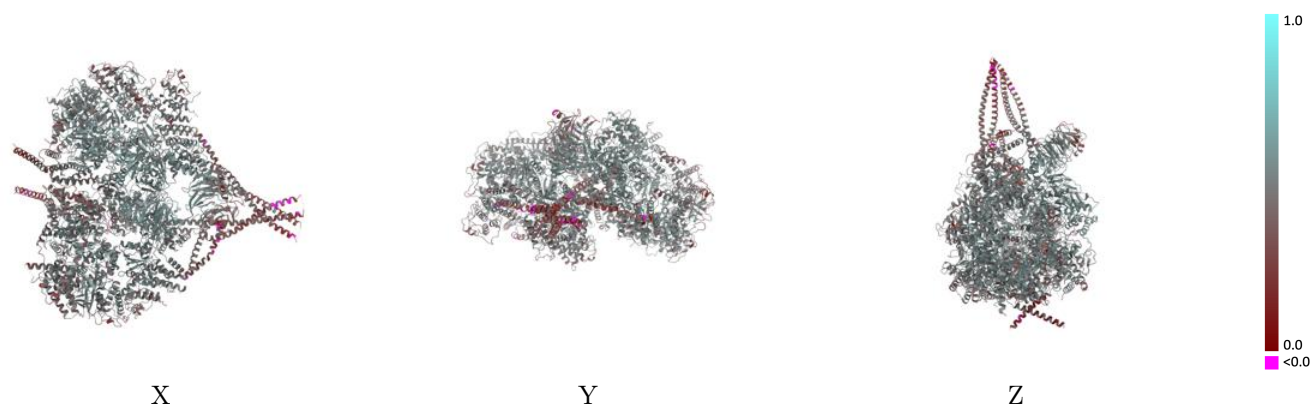
Y



Z

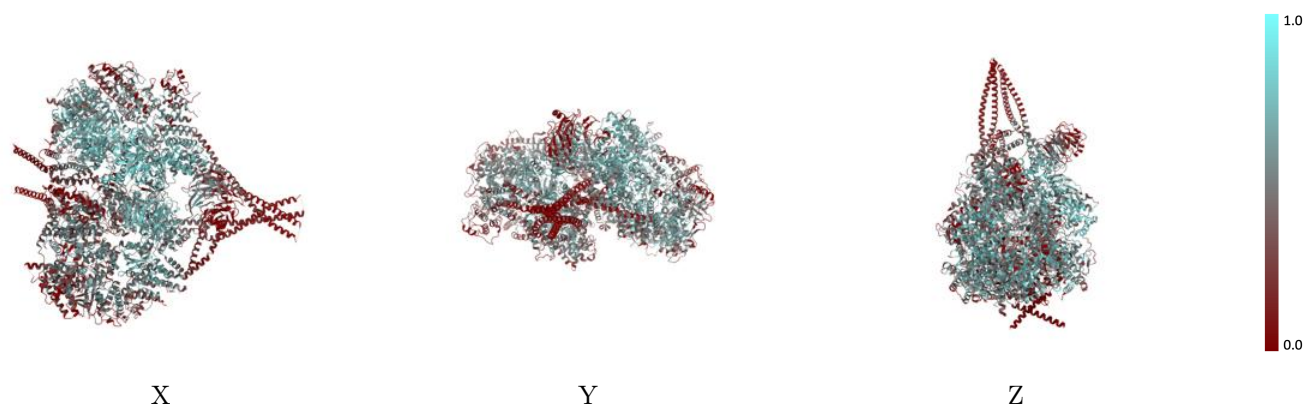
The images above show the 3D surface view of the map at the recommended contour level 0.224 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



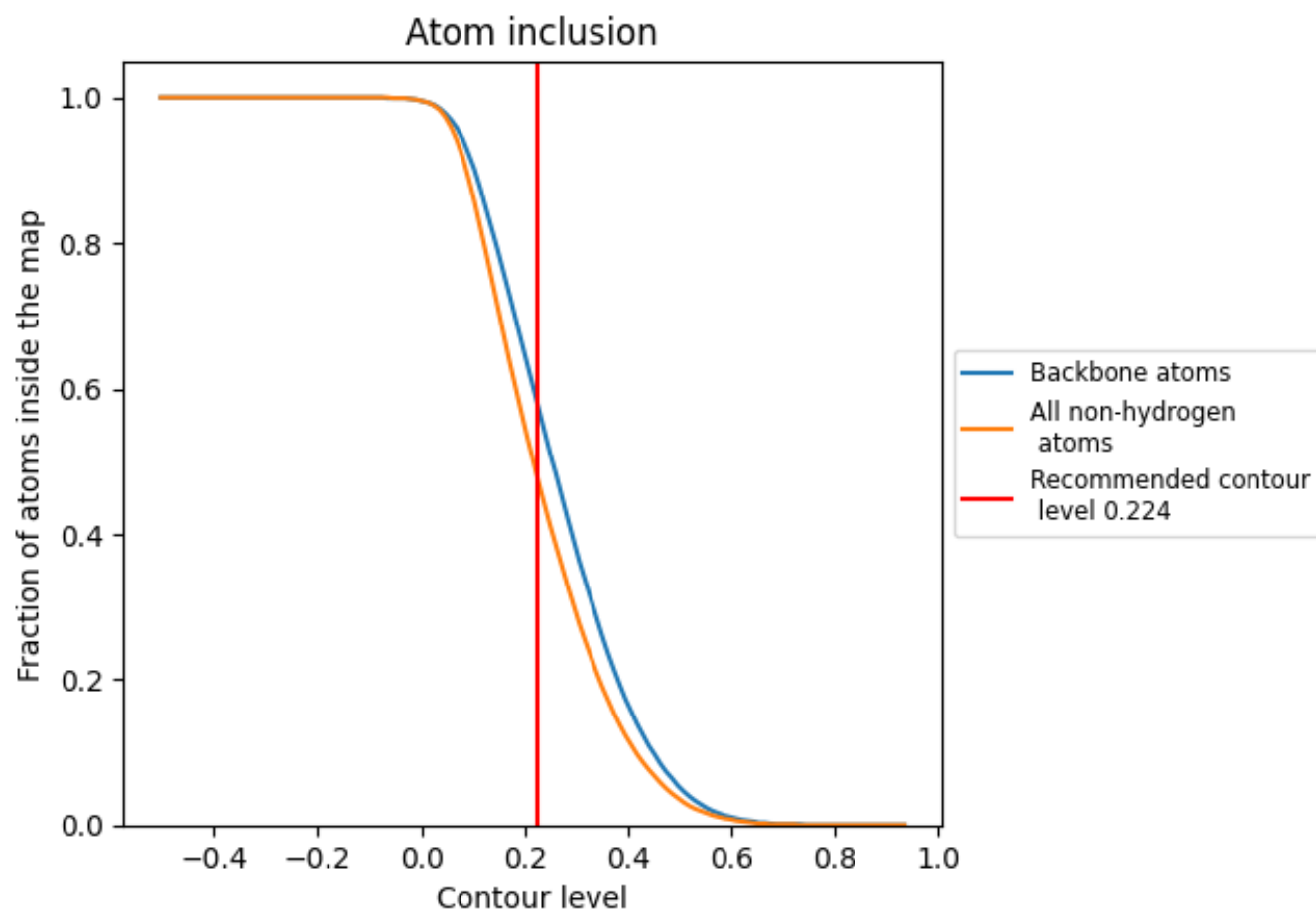
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

