



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 09:05 AM UTC

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

This is a 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:

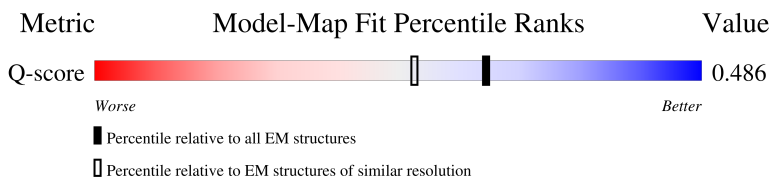
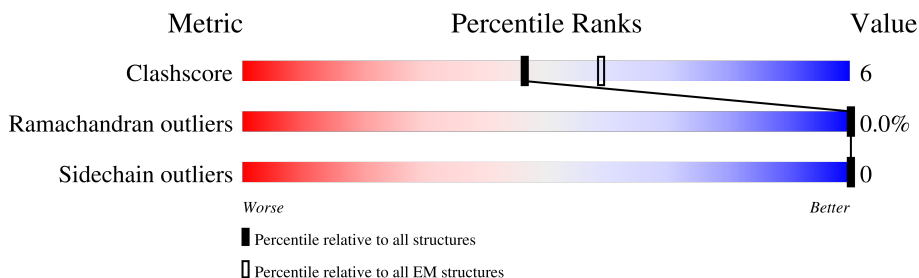
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	A	4843	29% 50% 10% 40%
1	B	4843	18% 51% 9% 40%
2	C	411	54% 63% 11% 26%
2	E	411	10% 64% 14% 22%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 51122 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	2920	Total	C	N	O	S	0	0
			23025	14699	3982	4232	112		
1	A	2920	Total	C	N	O	S	0	0
			23004	14686	3978	4228	112		

There are 396 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

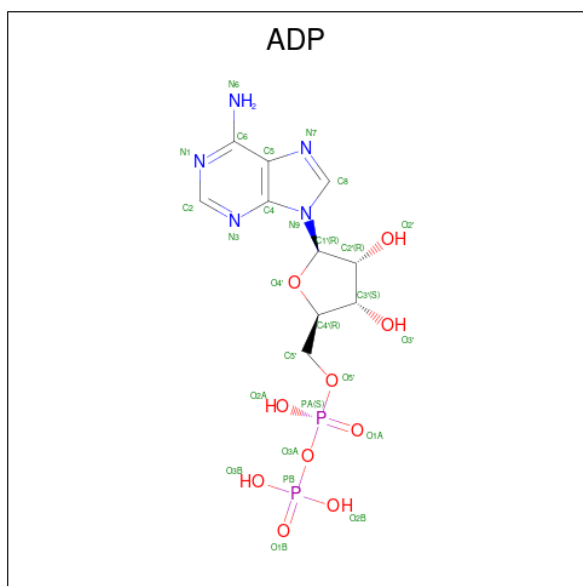
- Molecule 2 is a protein called Platelet-activating factor acetylhydrolase IB subunit beta.

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

There are 4 discrepancies between the modelled and reference sequences:

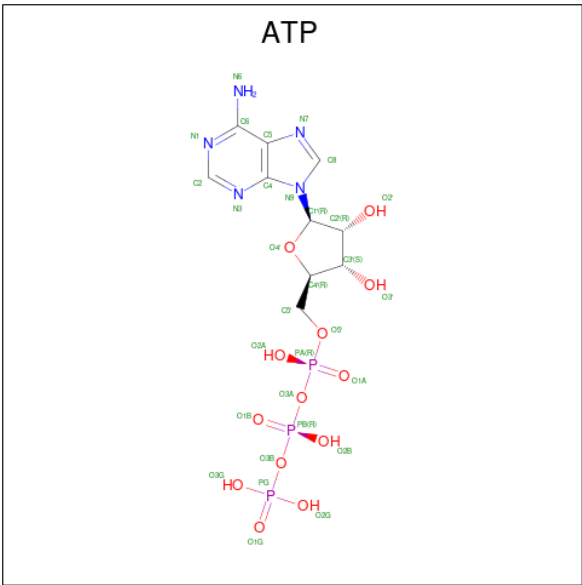
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	GLY	-	expression tag	UNP P43034
E	1	SER	-	expression tag	UNP P43034
C	0	GLY	-	expression tag	UNP P43034
C	1	SER	-	expression tag	UNP P43034

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



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

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



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

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

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



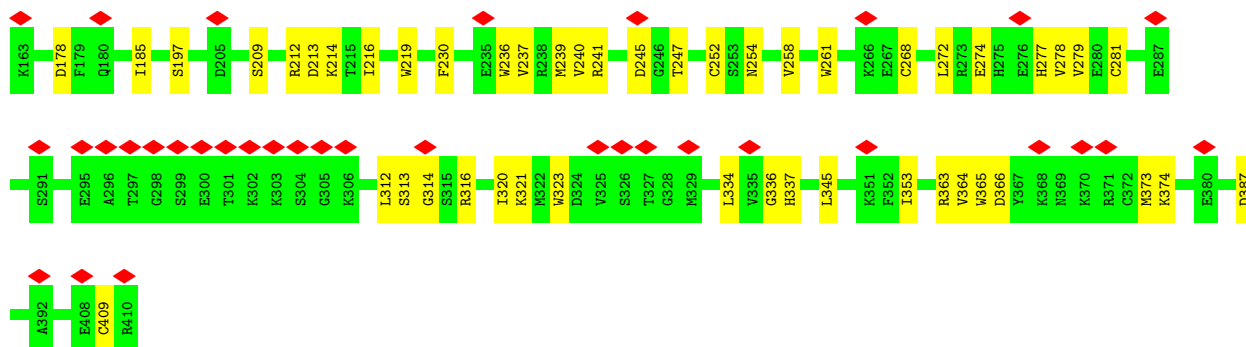
LYS	L3240	D5131	S3002	R2863	L2744	P2590	E2484	GLU	S2231	K2112	LYS	S1835
GLN	K3241	Q3135	G3003	E2864	I2747	L2691	Q2485	ALA	W2234	R2113	THR	F1836
HIS	K3242	P3136	F3004	R2869	N2762	V2592	L2486	ARG	P1996	E2114	SER	E1837
LEU	M3243	P3137	L3005	R2870	N2762	M2603	E2487	ARG	L2238	GLU	ALA	W1838
VAL	V3244	R3140	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	R2510	LYS	E2248	GLU	GLY	Y1845
SER	Q3248	A3162	G3023	R2889	L2773	D2614	R2511	ASP	G2249	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	E2515	ALA	D2269	A2128	GLU	Q1850
VAL	L3253	Q3038	Q3038	E2914	Y2794	P2628	E2516	ALA	E2270	E2129	ILE	T1851
LYS	L3254	R3039	E3040	V2915	R2797	K2633	R2519	ALA	E2271	E2130	LYS	D1852
LEU	L3255	L3041	L3042	L2920	E2798	T2644	R2520	LYS	E2272	E2131	GLY	Q1856
LEU	L3256	G3042	E3043	L2925	N2799	P2645	R2521	GLY	E2273	E2132	GLY	L1857
GLN	L3257	L3043	E3044	L2930	R2804	N2646	T2522	GLY	E2274	E2133	GLY	M1861
GLN	L3258	D3045	E3045	L2935	R2811	G2647	V2524	GLY	E2275	E2134	GLY	A1862
GLN	L3259	S3046	H3047	L2936	L2650	L2655	P2525	GLY	E2276	E2135	GLY	M1863
GLN	L3260	E3048	E3049	K2943	L2656	E2665	P2526	GLY	E2277	E2136	GLY	V1880
GLN	L3261	T3067	T3067	V2958	N2667	E2666	P2530	GLY	E2278	E2137	GLY	L2048
GLN	L3262	S3071	S3071	T2961	L2668	N2667	N2531	GLY	E2279	E2138	GLY	T1881
GLN	L3263	S3072	S3072	H2964	M2671	E2671	T2535	GLY	E2280	E2139	GLY	T1882
GLN	L3264	Q3214	Q3214	R2965	V2679	V2679	S2540	GLY	E2281	E2140	GLY	F1883
GLN	L3265	V3215	G3073	R2966	Q2834	Q2834	T2541	GLY	E2282	E2141	GLY	L1884
GLN	L3266	E3216	L3075	K2967	D2835	D2835	E2544	GLY	E2283	E2142	GLY	Q1894
GLN	L3267	E3217	L3076	T2968	P2882	P2882	W2545	GLY	E2284	E2143	GLY	E1914
GLN	L3268	L3218	A3080	G2969	D2697	D2697	S2546	GLY	E2285	E2144	GLY	L1928
GLN	L3269	R3219	T3081	D2973	K2702	K2702	P2553	GLY	E2286	E2145	GLY	V2064
GLN	L3270	R3220	L3091	E2974	L2703	L2703	Q2554	GLY	E2287	E2146	GLY	L2065
GLN	L3271	D3221	F3094	D2975	E2704	E2704	T2555	GLY	E2288	E2147	GLY	F1929
GLN	L3272	L3222	W3097	R2976	R2844	R2844	E2556	GLY	E2289	E2148	GLY	A2066
GLN	L3273	R3223	W3097	R2977	D2847	D2847	E2557	GLY	E2290	E2149	GLY	N2067
GLN	L3274	T3224	K3112	R2982	N2849	N2849	H2560	GLY	E2291	E2150	GLY	V1946
GLN	L3275	K3225	M3113	E2988	T2852	T2852	A2563	GLY	E2292	E2151	GLY	Q1950
GLN	L3276	S3226	E3116	K2989	L2855	L2855	D2566	GLY	E2293	E2152	GLY	E1966
GLN	L3277	Q3227	N3119	K2990	N2860	N2860	V2567	GLY	E2294	E2153	GLY	M1967
GLN	L3278	E3228	P3123	L2999	I2861	I2861	V2568	GLY	E2295	E2154	GLY	L1968
GLN	L3279	L3229	D3124	N2998	D2862	D2862	Y2582	GLY	E2296	E2155	GLY	Q1974
GLN	L3280	V3231	K3232	N2999	L2862	L2862	V2583	GLY	E2297	E2156	GLY	E1980
GLN	L3281	N3232	Y3125	D3000	D2862	D2862	E2584	GLY	E2298	E2157	GLY	A1981
GLN	L3282	A3234	M3126	D3001	D2862	D2862	E2585	GLY	E2299	E2158	GLY	E1984
GLN	L3283	A3235	P3127	D3001	D2862	D2862	E2586	GLY	E2300	E2159	GLY	H1985
GLN	L3284	A3236	N3237	D3001	D2862	D2862	E2587	GLY	E2301	E2160	GLY	S1986
GLN	L3285	D3238	K3239	D3001	D2862	D2862	E2587	GLY	E2302	E2161	GLY	N1987
GLN	L3286			D3001	D2862	D2862	E2587	GLY	E2303	E2162	GLY	PRO
GLN	L3287			D3001	D2862	D2862	E2587	GLY	E2304	E2163	GLY	ASN
GLN	L3288			D3001	D2862	D2862	E2587	GLY	E2305	E2164	GLY	TYR
GLN	L3289			D3001	D2862	D2862	E2587	GLY	E2306	E2165	GLY	ASP
GLN	L3290			D3001	D2862	D2862	E2587	GLY	E2307	E2166	GLY	
GLN	L3291			D3001	D2862	D2862	E2587	GLY	E2308	E2167	GLY	
GLN	L3292			D3001	D2862	D2862	E2587	GLY	E2309	E2168	GLY	
GLN	L3293			D3001	D2862	D2862	E2587	GLY	E2310	E2169	GLY	
GLN	L3294			D3001	D2862	D2862	E2587	GLY	E2311	E2170	GLY	
GLN	L3295			D3001	D2862	D2862	E2587	GLY	E2312	E2171	GLY	
GLN	L3296			D3001	D2862	D2862	E2587	GLY	E2313	E2172	GLY	
GLN	L3297			D3001	D2862	D2862	E2587	GLY	E2314	E2173	GLY	
GLN	L3298			D3001	D2862	D2862	E2587	GLY	E2315	E2174	GLY	
GLN	L3299			D3001	D2862	D2862	E2587	GLY	E2316	E2175	GLY	
GLN	L3300			D3001	D2862	D2862	E2587	GLY	E2317	E2176	GLY	
GLN	L3301			D3001	D2862	D2862	E2587	GLY	E2318	E2177	GLY	
GLN	L3302			D3001	D2862	D2862	E2587	GLY	E2319	E2178	GLY	
GLN	L3303			D3001	D2862	D2862	E2587	GLY	E2320	E2179	GLY	
GLN	L3304			D3001	D2862	D2862	E2587	GLY	E2321	E2180	GLY	
GLN	L3305			D3001	D2862	D2862	E2587	GLY	E2322	E2181	GLY	
GLN	L3306			D3001	D2862	D2862	E2587	GLY	E2323	E2182	GLY	
GLN	L3307			D3001	D2862	D2862	E2587	GLY	E2324	E2183	GLY	
GLN	L3308			D3001	D2862	D2862	E2587	GLY	E2325	E2184	GLY	
GLN	L3309			D3001	D2862	D2862	E2587	GLY	E2326	E2185	GLY	
GLN	L3310			D3001	D2862	D2862	E2587	GLY	E2327	E2186	GLY	
GLN	L3311			D3001	D2862	D2862	E2587	GLY	E2328	E2187	GLY	
GLN	L3312			D3001	D2862	D2862	E2587	GLY	E2329	E2188	GLY	
GLN	L3313			D3001	D2862	D2862	E2587	GLY	E2330	E2189	GLY	
GLN	L3314			D3001	D2862	D2862	E2587	GLY	E2331	E2190	GLY	
GLN	L3315			D3001	D2862	D2862	E2587	GLY	E2332	E2191	GLY	
GLN	L3316			D3001	D2862	D2862	E2587	GLY	E2333	E2192	GLY	
GLN	L3317			D3001	D2862	D2862	E2587	GLY	E2334	E2193	GLY	
GLN	L3318			D3001	D2862	D2862	E2587	GLY	E2335	E2194	GLY	
GLN	L3319			D3001	D2862	D2862	E2587	GLY	E2336	E2195	GLY	
GLN	L3320			D3001	D2862	D2862	E2587	GLY	E2337	E2196	GLY	
GLN	L3321			D3001	D2862	D2862	E2587	GLY	E2338	E2197	GLY	
GLN	L3322			D3001	D2862	D2862	E2587	GLY	E2339	E2198	GLY	
GLN	L3323			D3001	D2862	D2862	E2587	GLY	E2340	E2199	GLY	
GLN	L3324			D3001	D2862	D2862	E2587	GLY	E2341	E2200	GLY	
GLN	L3325			D3001	D2862	D2862	E2587	GLY	E2342	E2201	GLY	
GLN	L3326			D3001	D2862	D2862	E2587	GLY	E2343	E2202	GLY	
GLN	L3327			D3001	D2862	D2862	E2587	GLY	E2344	E2203	GLY	
GLN	L3328			D3001	D2862	D2862	E2587	GLY	E2345	E2204	GLY	
GLN	L3329			D3001	D2862	D2862	E2587	GLY	E2346	E2205	GLY	
GLN	L3330			D3001	D2862	D2862	E2587	GLY	E2347	E2206	GLY	
GLN	L3331			D3001	D2862	D2862	E2587	GLY	E2348	E2207	GLY	
GLN	L3332			D3001	D2862	D2862	E2587	GLY	E2349	E2208	GLY	
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GLN	L3335			D3001	D2862	D2862	E2587	GLY	E2352	E2211	GLY	
GLN	L3336			D3001	D2862	D2862	E2587	GLY	E2353	E2212	GLY	
GLN	L3337			D3001	D2862	D2862	E2587	GLY	E2354	E2213	GLY	
GLN	L3338			D3001	D2862	D2862	E2587	GLY	E2355	E2214	GLY	
GLN	L3339			D3001	D2862	D2862	E2587	GLY	E2356	E2215	GLY	
GLN	L3340			D3001	D2862	D2862	E2587	GLY	E2357	E2216	GLY	
GLN	L3341			D3001	D2862	D2862	E2587	GLY	E2358	E2217	GLY	
GLN	L3342			D3001	D2862	D2862	E2587	GLY	E2359	E2218	GLY	
GLN	L3343			D3001	D2862	D2862	E2587	GLY	E2360	E2219	GLY	
GLN	L3344			D3001	D2862	D2862	E2587	GLY	E2361	E2220	GLY	
GLN	L3345			D3001	D2862	D2862	E2587	GLY	E2362	E2221	GLY	
GLN	L3346			D3001	D2862	D2862	E2587	GLY	E2363	E2222	GLY	
GLN	L3347			D3001	D2862	D2862	E2587	GLY	E2364	E2223	GLY	
GLN	L3348			D3001	D2862	D2862	E2587	GLY	E2365	E2224	GLY	
GLN	L3349			D3001	D2862	D2862	E2587	GLY	E2366	E2225	GLY	
GLN	L3350			D3001	D2862	D2862	E2587	GLY	E2367	E2226	GLY	
GLN	L3351			D3001	D2862	D2862	E2587	GLY	E2368	E2227	GLY	
GLN	L3352			D3001	D2862	D2862	E2587	GLY	E2369	E2228	GLY	
GLN	L3353			D3001	D2862	D2862	E2587	GLY	E2370	E2229	GLY	
GLN	L3354			D3001	D2862	D2862	E2587	GLY	E2371	E2230	GLY	
GLN	L3355			D3001	D2862	D2862	E2587	GLY				

SER	ASP	ALA	ILE	ARG	GLU	LYS	MET	LYS	LYS	ASN	TYR	MET	SER	ASN	PRO	SER	TYR	ASN	TYR	ILE	VAL	ARG	ALA	SER	LEU	ALA	CYS	GLY	PRO	MET	VAL	LYS	TRP	ALA	ILE	ALA	GLN	LEU	ASN	TYR	ALA	ASP	MET	LYS	ARG	VAL	GLU	PRO	LEU	LEU	ARG	ASN	ASN	GLU	LEU	GLN	LYS	LYS	LEU			
GLU	ASP	ALA	ASP	LYS	ASP	ASN	GLN	GLN	LYS	ALA	ASN	GLU	VAL	GLU	Q3435	M3436	I3437	R3438	D3439	L3440	E3441	S3442	I3444	A3445	R3446	Y3447	K3448	E3449	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	K3491	T3495	F3496	K3497	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	R3655	T3656	G3657	R3658	R3659	V3660	L3661	L3664	G3665	D3666	Q3667	D3668	I3669	D3670	R3671	S3679	T3681	R3682	D3683	P3684	V3685	E3687	S3694	R3705	L3708	C3712	L3713	N3714	E3715	V3716																
L3717	K3718	A3719	E3720	R3721	F3722	D3723	V3724	D3725	E3726	K3727	R3728	S3729	D3730	L3731	L3732	K3733	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	K3774	R3775	E3776	A3777	R3778	V3780									
T3781	R3782	K3783	V3784	E3785	E3786	T3787	D3788	L3789	V3790	K3791	Q3792	E3793	V3794	E3795	T3796	V3797	S3798	Q3800	L3801	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	L3890	K3891	L3892	K3893	G3894	T3895	VAL	G3897	P3899	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	P3971	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	V4031	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	T4251	D4261	R4271	T4275	R4276	S4277	F4278	D4279	S4280	E4281	F4282	K4283	L4284	A4285	C4286	K4287	V4288	D4289	G4290	H4291	K4292	D4293	L4294	Q4295	M4296	P4297	D4298	G4299	I4300	R4301	R4302	E4303	E4304	Q4307	L4311	D4314	T4315	L4321	G4322	P4324	M4325	N4326	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	NET	ARG	T4379	L4380	H4381	T4382	T4383	A4384	S4385	M4386	W4387	L4388	L4389	L4390	I4391	Q4392	Q4393	T4394	L4395	S4396	H4397	L4398	K4399	R4400	T4401	VAL									
E4403	N4404	I4405	K4406	Q4407	F4410	R4411	F4412	F4413	E4414	R4415	E4416	V4417	K4418	M4419	G4420	L4421	K4422	L4423	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									

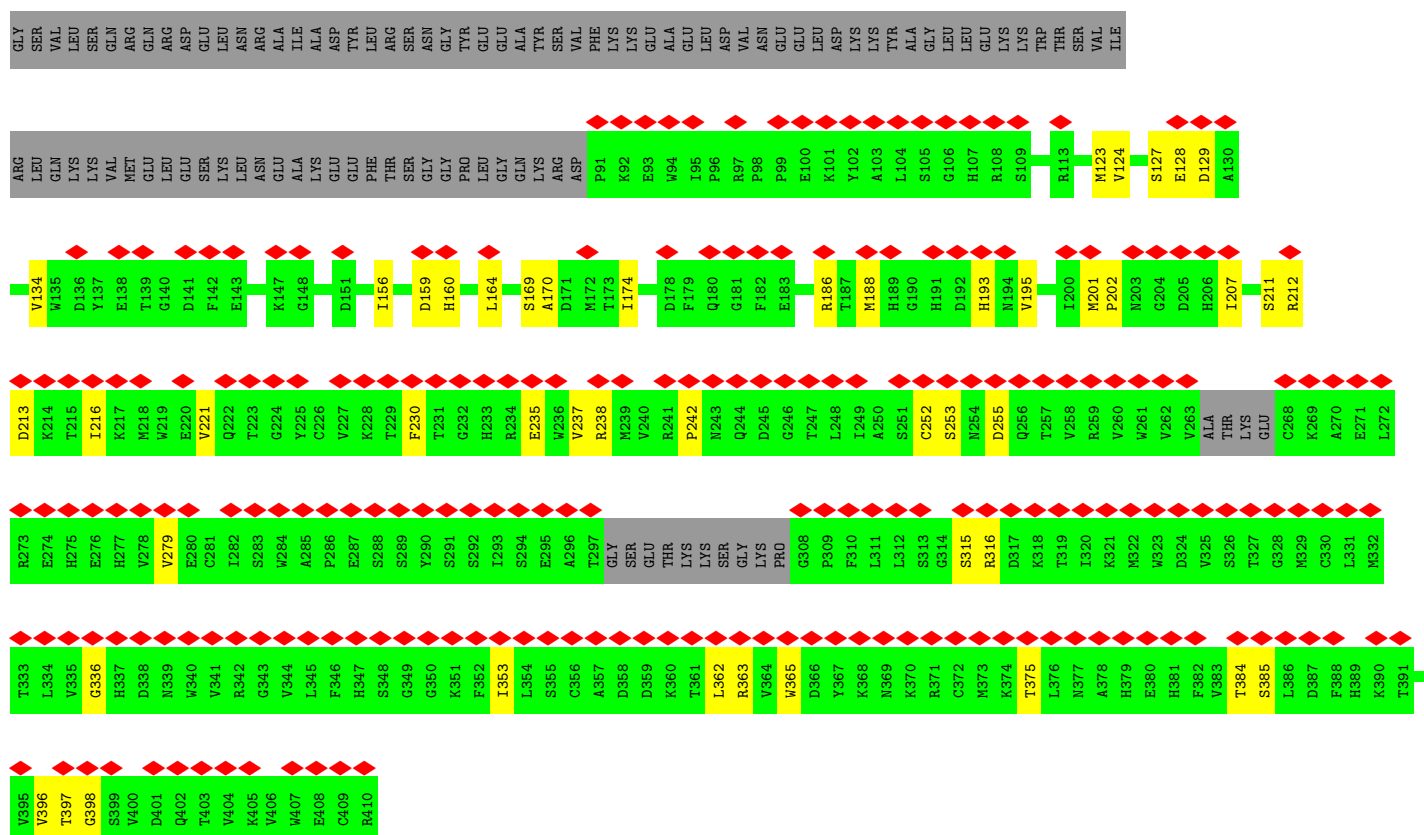


E2782	E2783	D2787	D2788	D2789	D2790	D2791	S2795	R2801	R2804	G2805	E2808	A2809	L2810	R2811	L2812	L2813	E2814	T2815	L2816	P2817	V2818	E2819	G2820	E2828	R2831	R2836	E2839	D2840	E2841	R2844	D2847	E2848	D2851	L2855	K2856	L2857	P2858	P2859	N2860	L2861	D2862	R2863	K2864	K2865	A2866											
E2665	L2668	P2669	D2670	Q2677	L2680	R2694	D2697	E2704	G2710	G2719	R2720	K2721	R2726	R2729	H2730	V2731	V2736	G2740	P2741	A2742	S2743	L2744	T2745	Q2746	G2749	T2750	T2751	N2752	R2753	A2754	M2755	L2756	R2757	L2758	L2759	P2760	S2761	L2762	R2763	T2764	L2765	D2766	E2767	P2768	A2772											
T2874	H2877	E2878	L2881	V2882	T2883	P2890	L2891	V2892	P2896	P2897	G2898	K2901	T2902	M2903	F2906	L2909	R2910	A2911	L2912	P2913	D2914	M2915	E2916	V2917	V2918	F2922	S2923	F2935	D2936	H2937	Y2941	R2942	R2943	T2944	P2945	N2946	G2947	L2950	V2953	P2958	L2959	H2960	K2961	G2965	K2967	L2961										
L2508	K2509	M2510	R2511	A2512	E2513	L2514	G2515	E2516	Y2517	L2518	R2519	R2520	L2521	T2522	T2523	V2524	P2525	L2526	P2527	T2528	A2529	P2530	N2531	L2532	P2533	L2534	L2535	V2539	S2540	L2541	S2542	G2543	E2544	W2545	Q2549	A2550	K2551	P2552	Q2554	L2555	E2556	V2557	E2558	T2559	H2560	K2561	V2562	L2563	A2564	P2565	D2566	V2567	T2571	D2572	L2573	
K2349	A2354	T2355	V2356	S2357	R2358	M2361	S2365	L2379	L2382	T2385	P2386	L2387	D2388	E2389	D2389	R2292	G2293	E2294	L2295	Q2296	K2297	R2298	D2304	G2305	D2306	V2307	L2308	P2309	E2310	W2311	G2312	N2316	D2320	D2321	N2322	K2323	L2324	N2329	G2330	E2331	R2332	L2333	S2334	L2335	P2336	F2343	E2344	V2345	Y2426	T2427	T2428	S2429				
N2430	G2431	L2432	K2435	E2438	F2441	Q2442	L2443	E2444	H2445	L2446	M2447	D2448	L2452	R2453	M2461	A2465	C2466	N2467	R2468	V2469	A2470	Q2471	T2472	N2473	A2474	N2475	H2476	P2477	D2478	F2479	P2480	M2481	Q2482	L2483	E2484	Q2485	L2486	E2487	R2488	Q2491	R2492	V2495	Y2496	F2427	L2498	S2503	G2504	D2505	S2506	R2507						
L2508	K2509	M2510	R2511	A2512	E2513	L2514	G2515	E2516	Y2517	L2518	R2519	R2520	L2521	T2522	T2523	V2524	P2525	L2526	P2527	T2528	A2529	P2530	N2531	L2532	P2533	L2534	L2535	V2539	S2540	L2541	S2542	G2543	E2544	W2545	Q2549	A2550	K2551	P2552	Q2554	L2555	E2556	V2557	E2558	T2559	H2560	K2561	V2562	L2563	A2564	P2565	D2566	V2567	T2571	D2572	L2573	
T2874	H2877	E2878	L2881	V2882	T2883	P2890	L2891	V2892	P2896	P2897	G2898	K2901	T2902	M2903	F2906	L2909	R2910	A2911	L2912	P2913	D2914	M2915	E2916	V2917	V2918	F2922	S2923	F2935	D2936	H2837	Y2841	R2842	R2843	T2844	P2845	N2846	G2847	L2850	V2853	P2858	L2859	H2860	K2861	G2865	K2867	L2861										
E2665	L2668	P2669	D2670	Q2677	L2680	R2694	D2697	E2704	G2710	G2719	R2720	K2721	R2726	R2729	H2730	V2731	V2736	G2740	P2741	A2742	S2743	L2744	T2745	Q2746	G2749	T2750	T2751	N2752	R2753	A2754	M2755	L2756	R2757	L2758	L2759	P2760	S2761	L2762	R2763	T2764	L2765	D2766	E2767	P2768	A2772											
E2782	E2783	D2787	D2788	D2789	D2790	D2791	S2795	R2801	R2804	G2805	E2808	A2809	L2810	R2811	L2812	L2813	E2814	T2815	L2816	P2817	V2818	E2819	G2820	E2828	R2831	R2836	E2839	D2840	E2841	R2844	D2847	E2848	D2851	L2855	K2856	L2857	P2858	P2859	N2860	L2861	D2862	R2863	K2864	K2865	A2866											
P1735	H1736	T1737	Y1738	L1739	T1740	D1743	K1744	Y1745	Q1746	A1747	Q1748	L1749	L1752	S1753	A1757	W1758	S1759	E1760	H1761	V1762	E1763	T1764	A1765	L1766	S1767	S1768	MET	GLY	GLY	GLY	GLY	ASP	A1775	A1776	P1777	L1778	H1779	S1780	V1781	L1782	S1783	H1784	V1785	E1786	V1787	T1788	L1789	N1790	V1791	L1792	A1793	D1794	S1795	V1796	L1797	H1798
E1799	Q1800	R1804	R1805	R1806	K1807	L1808	E1809	T1813	E1814	R1819	D1820	V1821	T1822	R1823	S1824	L1825	L1826	K1827	S1828	K1829	L1830	D1831	N1832	A1833	K1834	S1835	F1836	E1837	W1838	L1839	Y1845	F1846	D1847	P1848	K1849	Q1850	T1851	D1852	V1853	L1854	Q1855	Q1856	L1857	S1858	N1863	A1864	K1865	Y1868	V1875	Q1876	D1877	K1878				
L1879	V1880	Q1881	T1882	L1884	T1885	D1886	C1888	M1892	R1899	P1904	E1914	K1917	D1933	E1934	Q1939	K1940	M1941	Q1950	V1951	G1952	D1958	N1961	R1962	L1963	E1964	E1965	R1966	E1980	R1983	E1984	H1985	S1986	N1987	PRO	ASN	TYR	ASP	LYS	THR	SER	ALA	P1996	I1997	K2004												
Q2005	V2006	K2007	D2011	T2016	T2017	M2018	Y2022	A2023	N2031	K2043	P2044	D2045	R2046	Q2047	L2048	A2050	R2060	T2061	A2062	E2063	V2064	L2065	A2066	N2067	K2068	L2069	V2070	P2071	F2072	F2073	K2074	L2075	C2076	D2077	E2078	Q2079	L2080	S2081	D2087	S2095	V2096	L2097	V2098	S2099	N2102											
V2103	K2104	R2105	E2106	R2107	I2108	Q2109	K2110	I2111	K2112	R2113	E2114	LYS	GLU	GLU	ARG	GLY	GLU	ALA	VAL	ASP	GLU	GLY	ILE	A2128	E2129	N2130	L2131	P2132	E2133	Q2134	E2135	I2136	L2137	I2138	Q2139	S2140	A2151	E2152	D2153	I2154	L2157	F2158	S2159	L2160	L2161	S2162	D2163	V2164	F2165	P2166	G2167	V2168	Q2169	I2170	H2171	R2172
G2173	E2174	M2175	T2176	A2177	L2178	R2179	E2180	E2181	L2182	K2183	K2184	Q2187	L2188	M2189	G2194	D2195	G2196	E2197	E2198	V2199	V2204	Y2211	I2216	N2217	H2218	W2221	G2227	S2228	S2231	W2234	L2237	L2238	K2239	E2242	R2243	L2244	E2245	E2248	G2249	D2255	P2256	K2257	D2262	D2269												
P2270	N2271	T2272	R2273	E2274	T2275	D2276	D2277	G2278	H2282	L2283	R2285	K2286	L2287	L2288	D2289	R2292	G2293	E2294	L2295	Q2296	K2297	R2298	D2304	G2305	D2306	V2307	L2308	P2309	E2310	W2311	G2312	N2316	D2320	D2321	N2322	K2323	L2324	N2329	G2330	E2331	R2332	L2333	S2334	L2335	P2336	F2343	E2344	V2345	Y2346	D2347	L2348					
K2349	A2354	T2355	V2356	S2357	R2358	M2361	S2365	L2379	L2382	T2385	P2386	L2387	D2388	E2389	D2389	R2292	G2293	E2294	L2295	Q2296	K2297	R2298	D2304	G2305	D2306	V2307	L2308	P2309	E2310	W2311	G2312	N2316	D2320	D2321	N2322	K2323	L2324	N2329	G2330	E2331	R2332	L2333	S2334	L2335	P2336	F2343	E2344	V2345	Y2426	T2427	T2428	S2429				
N2430	G2431	L2432	K2435	E2438	F2441	Q2442	L2443	E2444	H2445	L2446	M2447	D2448	L2452	R2453	M2461	A2465	C2466	N2467	R2468	V2469	A2470	Q2471	T2472	N2473	A2474	N2475	H2476	P2477	D2478	F2479	P2480	M2481	Q2482	L2483	E2484	Q2485	L2486	E2487	R2488	Q2491	R2492	V2495	Y2496	F2427	L2498	S2503	G2504	D2505	S2506	R2507						
L2508	K2509	M2510	R2511	A2512	E2513	L2514	G2515	E2516	Y2517	L2518	R2519	R2520	L2521	T2522	T2523	V2524	P2525	L2526	P2527	T2528	A2529	P2530	N2531	L2532	P2533	L2534	L2535	V2539	S2540	L2541	S2542	G2543	E2544	W2545	Q2549	A2550	K2551	P2552	Q2554	L2555	E2556	V2557	E2558	T2559	H2560	K2561	V2562	L2563	A2564	P2565	D2566	V2567	T2571	D2572	L2573	
T2574	H2577	E2578	L2581	Y2582	T2583	P2590	L2591	V2592	P2596	P2597	G2598	K2601	T2602	V2603	F2606	L2609	R2610	A2611	L2612	P2613	D2614	M2615	E2616	V2617	V2618	Q2619	F2622	S2623	F2635	D2636	H2637	Y2641	R2642	R2643	T2644	P2645	N2646	G2647	L2650	V2653	Q2654	L2655	G2656	T2657	L2661											
E2665	L2668	P2669	D2670	Q2677	L2680	R2694	D2697	E2704	G2710	G2719	R2720	K2721	R2726	R2729	H2730	V2731	V2736	G2740	P2741	A2742	S2743	L2744	T2745	Q2746	G2749	T2750	T2751	N2752	R2753	A2754	M2755	L2756	R2757	L2758	L2759	P2760	S2761	L2762	R2763	T2764	L2765	D2766	E2767	P2768	A2772											
E2782	E2783	D2787	D2788	D2789	D2790	D2791	S2795	R2801	R2804	G2805	E2808	A2809	L2810	R2811	L2812	L2813	E2814	T2815	L2816	P2817	V2818	E2819	G2820	E2828	R2831	R2836	E2839	D2840	E2841	R2844	D2847	E2848	D2851	L2855	K2856	L2857	P2858	P2859	N2860	L2861	D2862	R2863	K2864	K2865	A2866											





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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66880	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	610	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.934	Depositor
Minimum map value	-0.503	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.224	Depositor
Map size (Å)	329.12, 329.12, 329.12	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.935, 0.935, 0.935	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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

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

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

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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

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

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	4706	5	-	2/16/32/32	0/3/3/3
4	ATP	B	4702	5	-	3/22/38/38	0/3/3/3
3	ADP	A	4702	-	-	3/16/32/32	0/3/3/3
4	ATP	A	4701	-	-	2/22/38/38	0/3/3/3
3	ADP	B	4706	5	-	6/16/32/32	0/3/3/3
3	ADP	B	4705	-	-	3/16/32/32	0/3/3/3
3	ADP	A	4703	-	-	0/16/32/32	0/3/3/3
3	ADP	B	4701	-	-	3/16/32/32	0/3/3/3

All (27) bond length outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4703	ADP	C5-C4	4.66	1.47	1.39
3	B	4705	ADP	C5-C4	4.56	1.47	1.39
3	A	4706	ADP	C5-C4	4.49	1.47	1.39
3	B	4701	ADP	C5-C4	4.48	1.47	1.39
3	B	4706	ADP	C5-C4	4.39	1.46	1.39
3	A	4703	ADP	C5-C6	2.66	1.48	1.41
3	A	4702	ADP	C5-C6	2.64	1.48	1.41
3	A	4706	ADP	C5-C6	2.57	1.48	1.41
3	B	4706	ADP	C5-C6	2.54	1.48	1.41
3	B	4701	ADP	C5-N7	-2.51	1.34	1.39
3	B	4701	ADP	C5-C6	2.50	1.48	1.41
3	B	4705	ADP	C5-N7	-2.48	1.34	1.39
3	B	4706	ADP	C5-N7	-2.41	1.34	1.39
3	A	4706	ADP	C5-N7	-2.40	1.34	1.39
3	A	4703	ADP	C5-N7	-2.37	1.34	1.39
3	A	4702	ADP	C5-N7	-2.32	1.34	1.39
3	B	4705	ADP	C5-C6	2.30	1.47	1.41
3	B	4705	ADP	C8-N7	2.27	1.36	1.31
3	A	4702	ADP	C8-N7	2.25	1.36	1.31
3	A	4703	ADP	C8-N7	2.24	1.36	1.31
3	B	4706	ADP	C8-N7	2.23	1.36	1.31
3	B	4705	ADP	C4-N9	-2.22	1.33	1.37
3	B	4701	ADP	C8-N7	2.21	1.35	1.31
3	A	4706	ADP	C8-N7	2.20	1.35	1.31
3	B	4701	ADP	C4-N9	-2.18	1.33	1.37
3	B	4706	ADP	C4-N9	-2.03	1.33	1.37

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4702	ADP	C5-C4-N3	-6.63	117.59	126.72
3	A	4703	ADP	C5-C4-N3	-5.84	118.68	126.72
3	A	4706	ADP	C5-C4-N3	-5.80	118.73	126.72
3	B	4706	ADP	C5-C4-N3	-5.64	118.94	126.72
3	B	4701	ADP	C5-C4-N3	-5.60	119.00	126.72
3	A	4702	ADP	N3-C4-N9	5.30	136.18	127.17
3	B	4705	ADP	C5-C4-N3	-5.24	119.50	126.72
3	A	4703	ADP	N3-C4-N9	4.67	135.11	127.17
3	A	4706	ADP	N3-C4-N9	4.66	135.10	127.17
3	B	4706	ADP	N3-C4-N9	4.48	134.78	127.17
3	B	4701	ADP	N3-C4-N9	4.44	134.71	127.17
3	B	4705	ADP	N3-C4-N9	4.37	134.59	127.17

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4702	ADP	C2-N3-C4	4.11	121.88	111.83
3	A	4706	ADP	C2-N3-C4	3.67	120.79	111.83
3	B	4706	ADP	C2-N3-C4	3.65	120.74	111.83
3	A	4703	ADP	C2-N3-C4	3.62	120.68	111.83
3	B	4705	ADP	N3-C2-N1	-3.61	123.12	128.58
3	B	4701	ADP	C2-N3-C4	3.58	120.57	111.83
3	B	4705	ADP	C2-N3-C4	3.50	120.38	111.83
3	B	4701	ADP	C4-C5-N7	-3.46	106.63	110.58
3	A	4702	ADP	N3-C2-N1	-3.45	123.37	128.58
3	B	4706	ADP	C4-C5-N7	-3.44	106.65	110.58
3	A	4703	ADP	C4-C5-N7	-3.38	106.72	110.58
3	A	4706	ADP	C4-C5-N7	-3.38	106.72	110.58
3	A	4702	ADP	C4-C5-N7	-3.34	106.77	110.58
3	B	4706	ADP	N3-C2-N1	-3.31	123.58	128.58
3	A	4706	ADP	N3-C2-N1	-3.23	123.69	128.58
3	B	4701	ADP	N3-C2-N1	-3.20	123.73	128.58
3	A	4703	ADP	N3-C2-N1	-3.09	123.90	128.58
3	B	4705	ADP	C4-C5-N7	-3.03	107.12	110.58
3	B	4705	ADP	C4-N9-C8	3.01	108.90	105.74
3	B	4701	ADP	C4-N9-C8	2.79	108.67	105.74
3	A	4706	ADP	C4-N9-C8	2.79	108.66	105.74
3	B	4706	ADP	C4-N9-C8	2.77	108.65	105.74
3	A	4703	ADP	C4-N9-C8	2.64	108.51	105.74
3	A	4702	ADP	C3'-C2'-C1'	2.63	106.43	101.46
3	A	4703	ADP	C3'-C2'-C1'	2.57	106.33	101.46
3	B	4705	ADP	C2-N1-C6	2.52	122.87	118.73
3	A	4706	ADP	C5-N7-C8	2.51	107.39	103.45
3	A	4702	ADP	C5-N7-C8	2.51	107.39	103.45
3	B	4706	ADP	C5-N7-C8	2.50	107.37	103.45
3	B	4701	ADP	C5-N7-C8	2.47	107.34	103.45
3	A	4703	ADP	C5-N7-C8	2.40	107.22	103.45
3	B	4701	ADP	C3'-C2'-C1'	2.33	105.87	101.46
3	B	4705	ADP	C5-N7-C8	2.28	107.03	103.45
3	A	4702	ADP	C4-N9-C8	2.24	108.09	105.74
3	B	4706	ADP	C6-C5-N7	2.11	136.15	132.09
3	B	4705	ADP	C2'-C1'-N9	-2.08	108.13	113.30
3	B	4705	ADP	N9-C8-N7	-2.04	111.04	113.94
3	B	4706	ADP	N9-C8-N7	-2.04	111.05	113.94
3	B	4701	ADP	C6-C5-N7	2.03	136.01	132.09
3	A	4706	ADP	N9-C8-N7	-2.03	111.06	113.94
3	B	4701	ADP	N9-C8-N7	-2.01	111.08	113.94

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	4706	ADP	PA-O3A-PB-O3B
3	B	4706	ADP	C5'-O5'-PA-O1A
3	A	4706	ADP	C5'-O5'-PA-O1A
4	B	4702	ATP	C3'-C4'-C5'-O5'
4	B	4702	ATP	O4'-C4'-C5'-O5'
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	B	4705	ADP	O4'-C1'-N9-C4
3	B	4705	ADP	O4'-C1'-N9-C8
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	B	4705	ADP	C2'-C1'-N9-C8
3	A	4702	ADP	C2'-C1'-N9-C8
3	A	4702	ADP	O4'-C4'-C5'-O5'

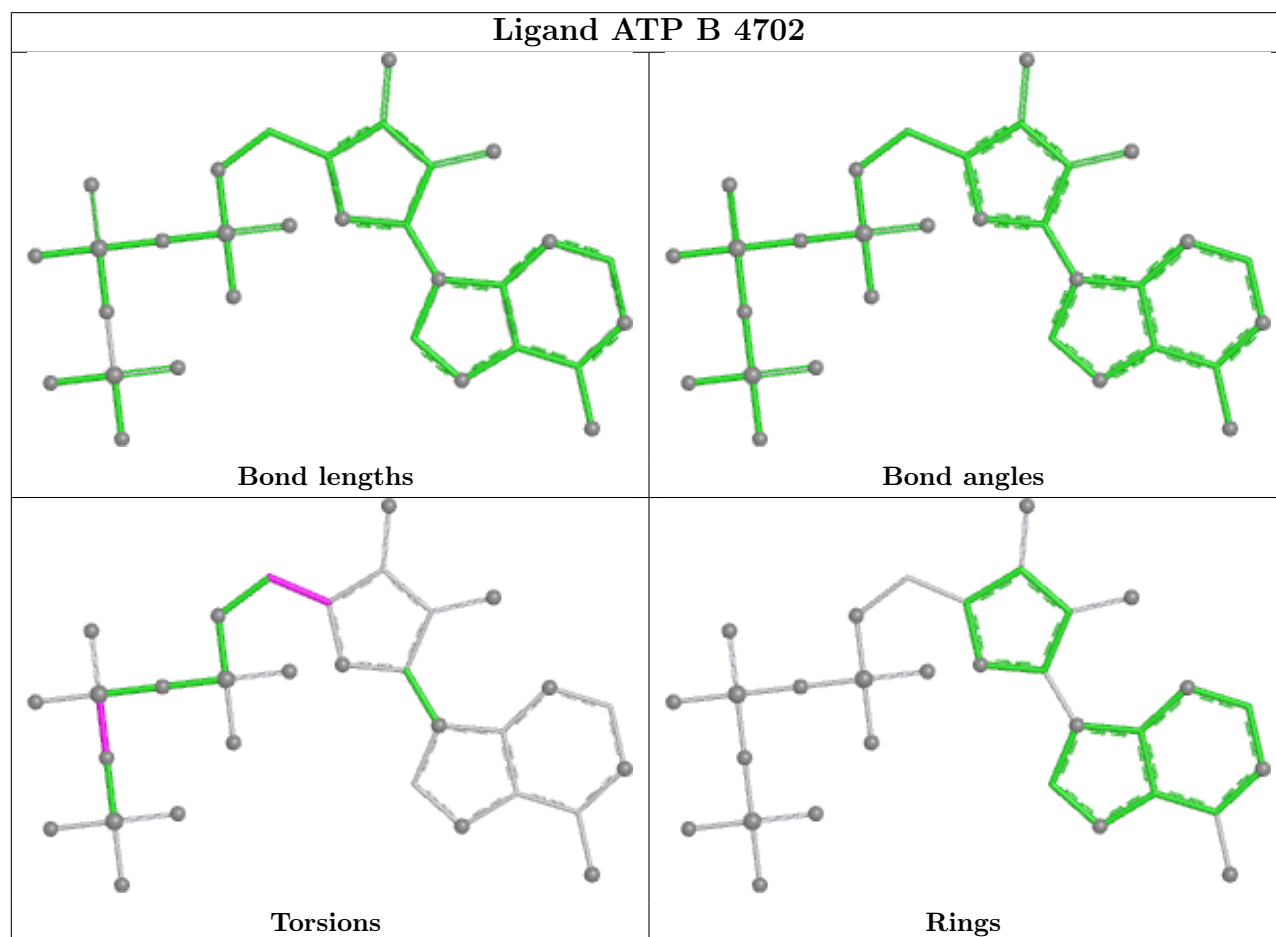
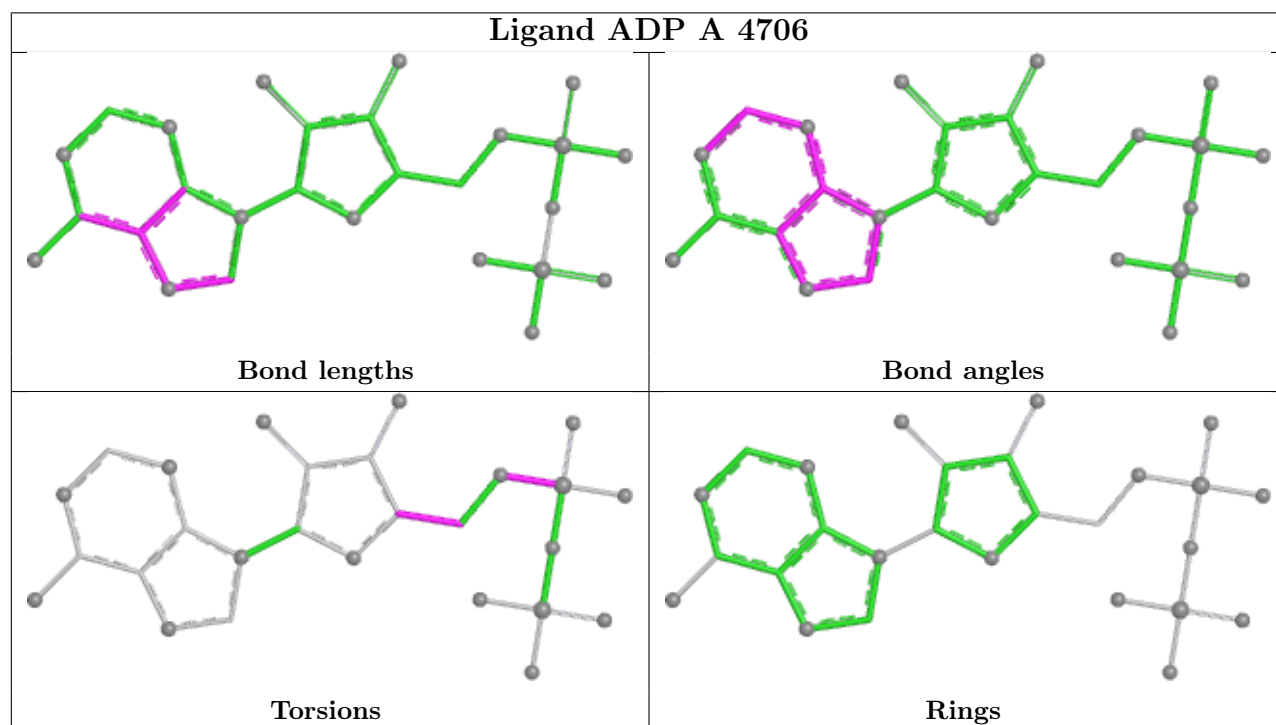
There are no ring outliers.

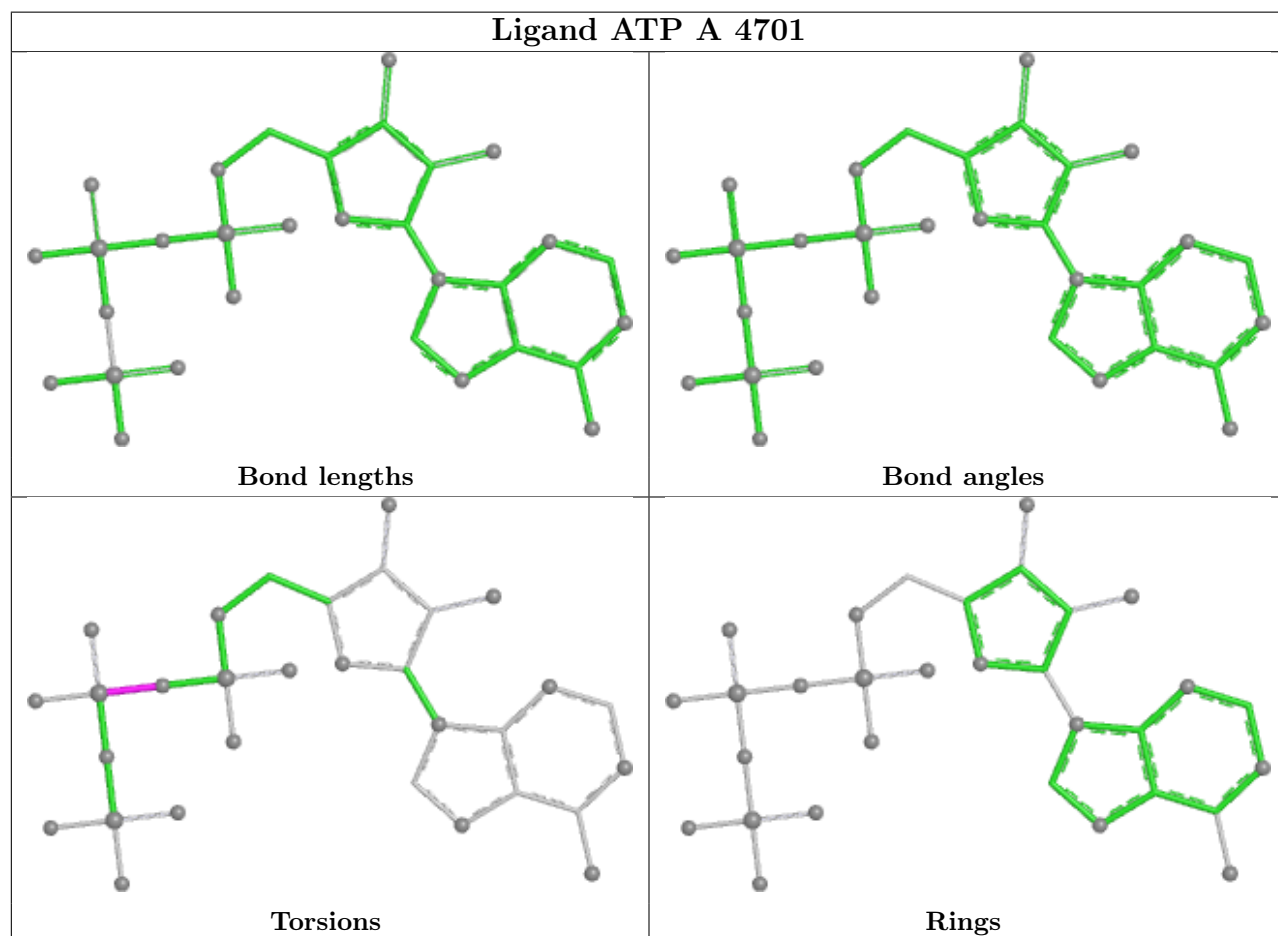
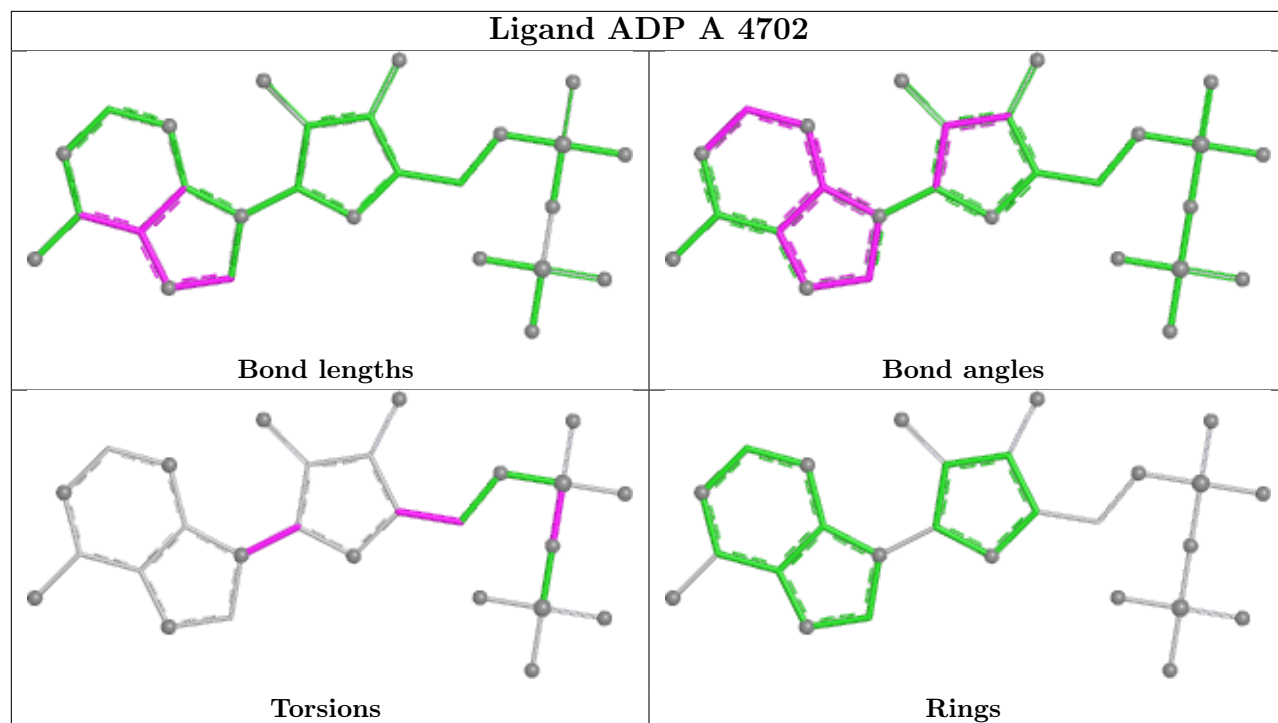
4 monomers are involved in 6 short contacts:

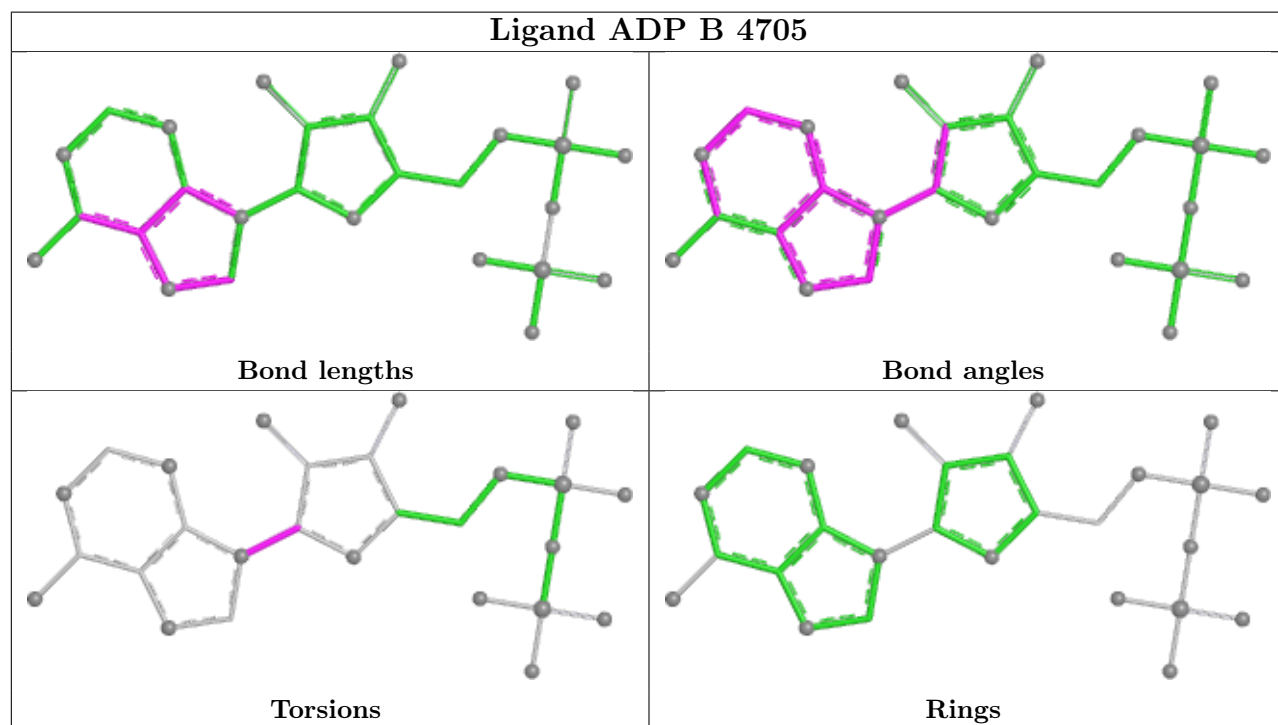
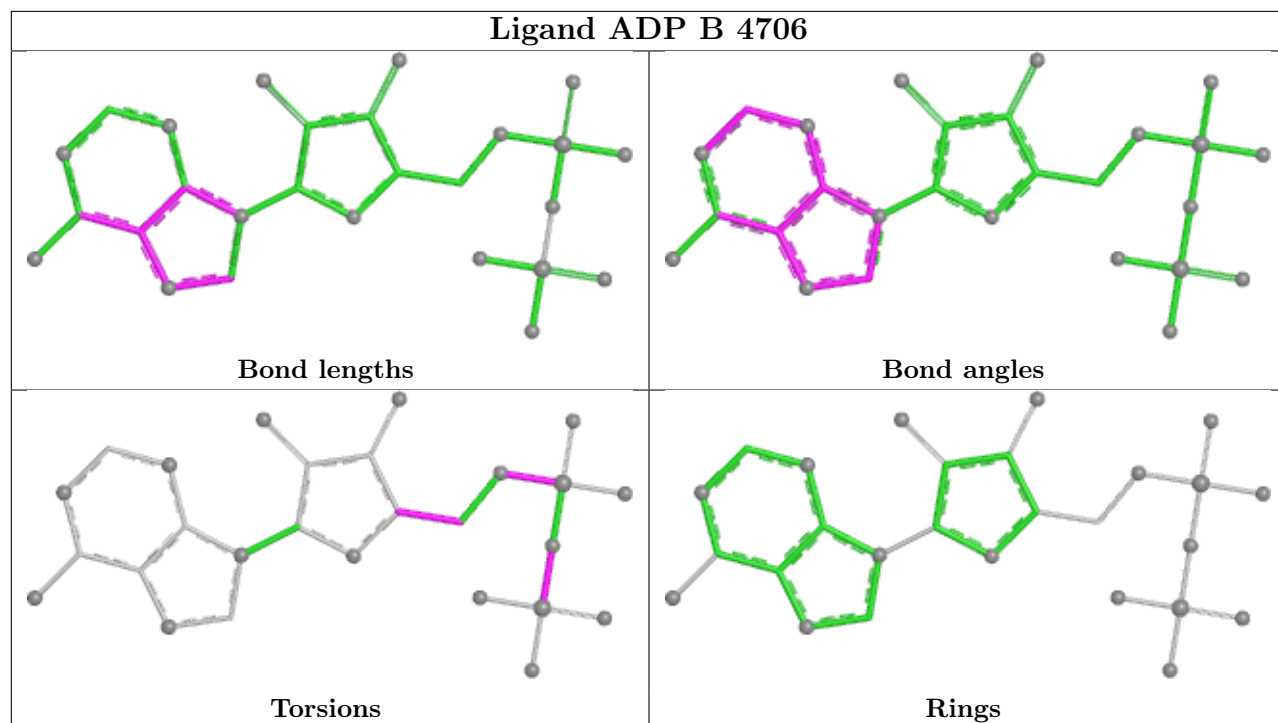
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4706	ADP	1	0
4	A	4701	ATP	1	0
3	B	4706	ADP	2	0
3	B	4705	ADP	2	0

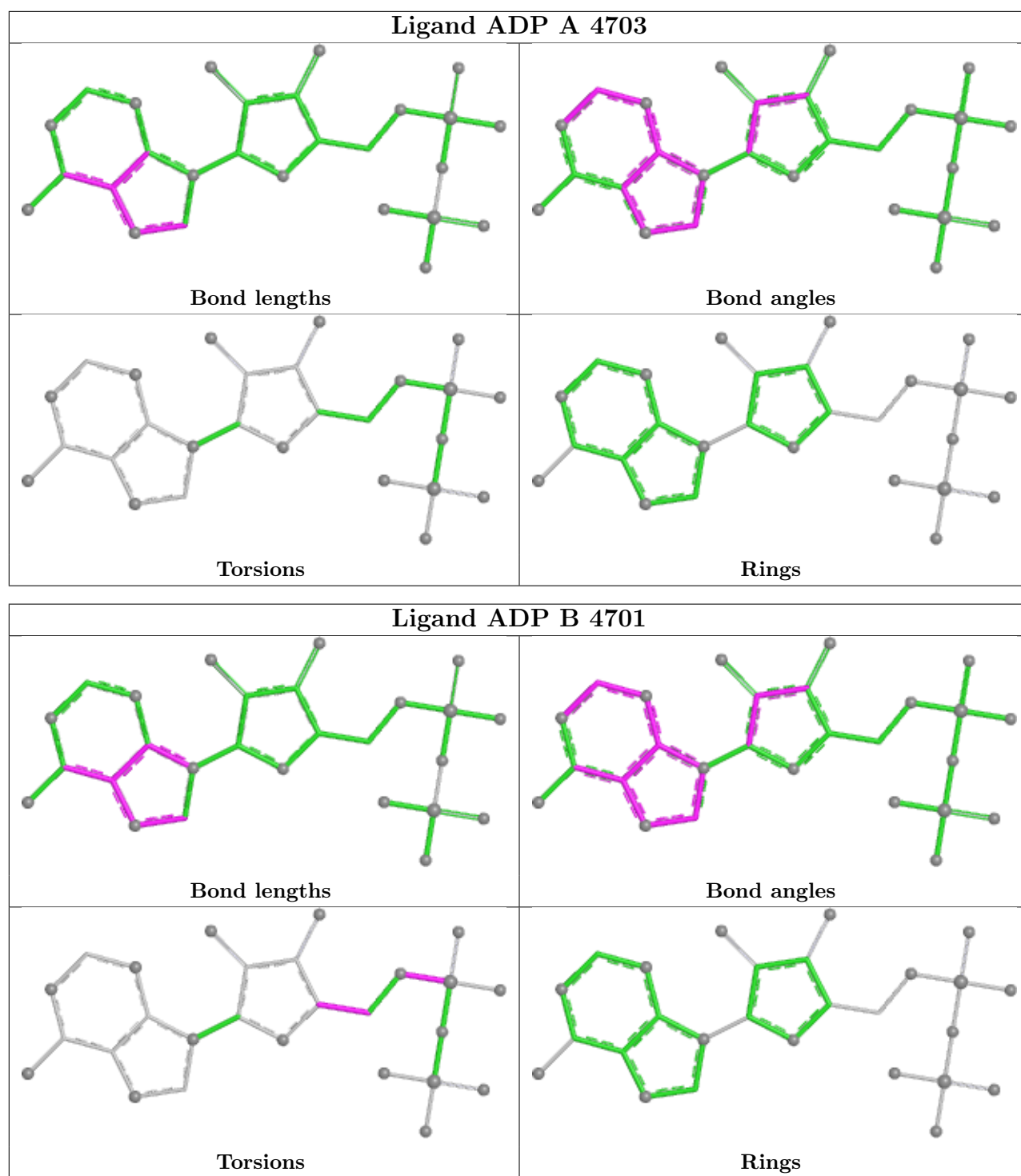
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

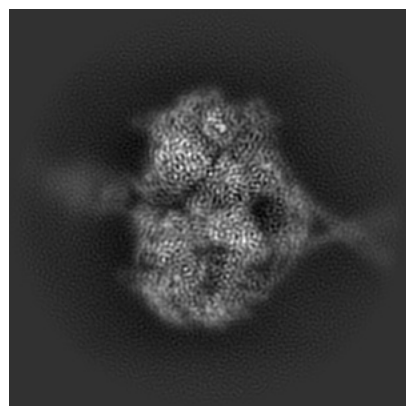
6 Map visualisation [i](#)

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

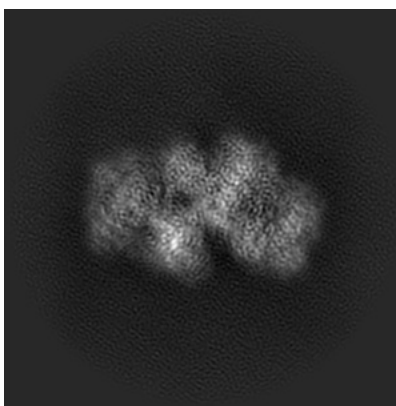
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

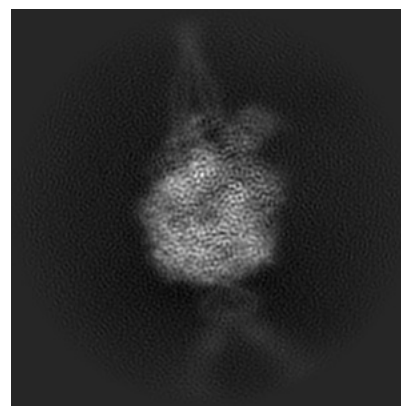
6.1.1 Primary map



X

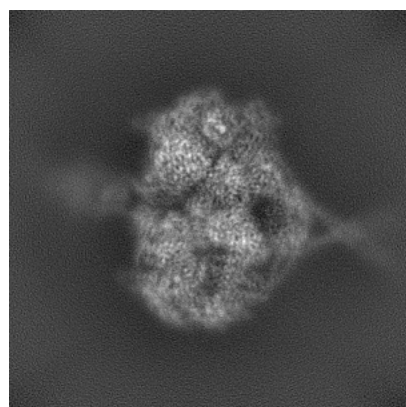


Y

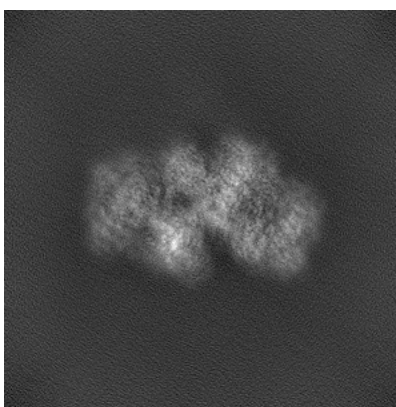


Z

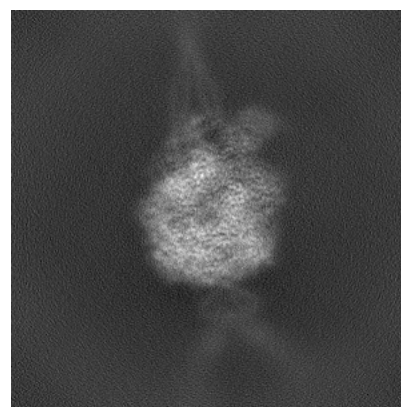
6.1.2 Raw map



X



Y

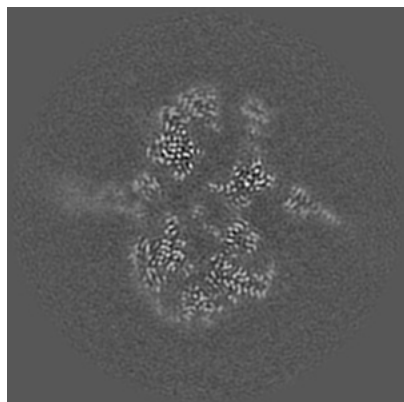


Z

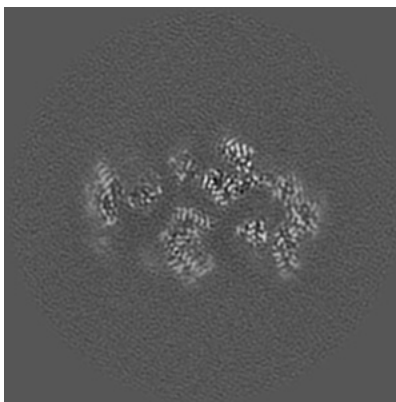
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

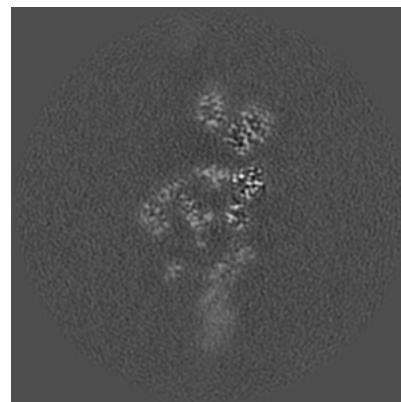
6.2.1 Primary map



X Index: 176

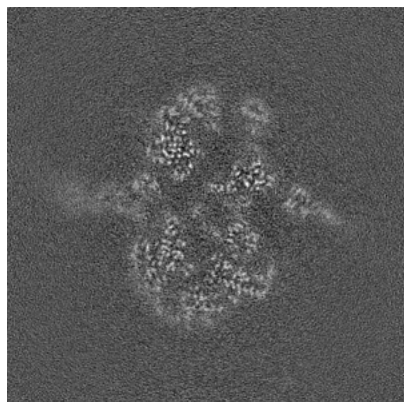


Y Index: 176

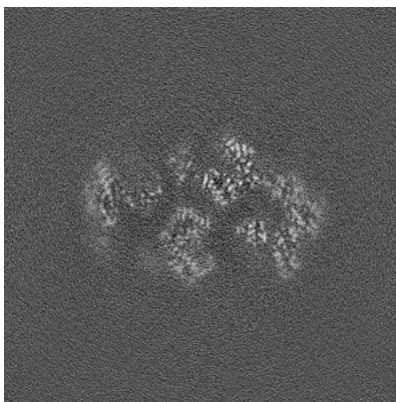


Z Index: 176

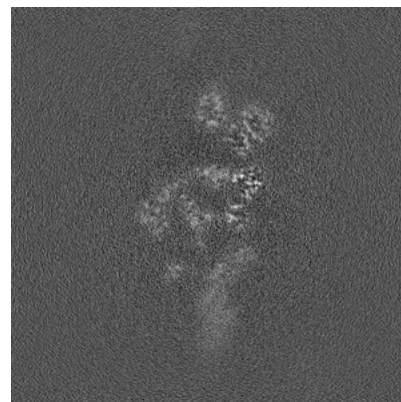
6.2.2 Raw map



X Index: 176



Y Index: 176

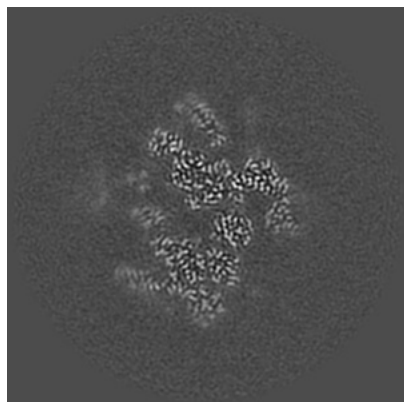


Z Index: 176

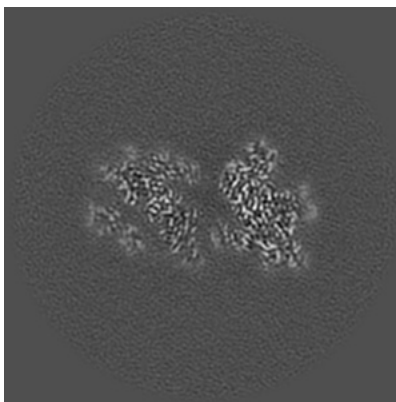
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

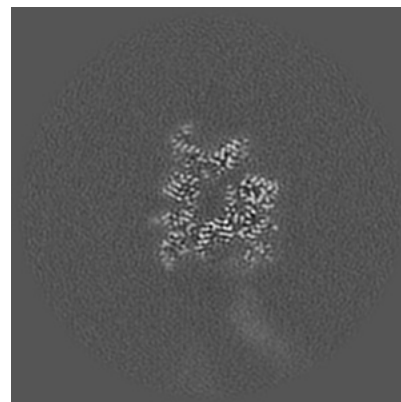
6.3.1 Primary map



X Index: 192

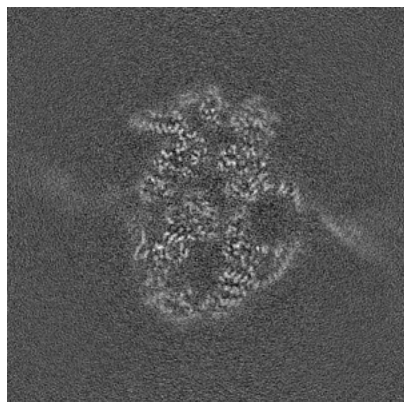


Y Index: 151

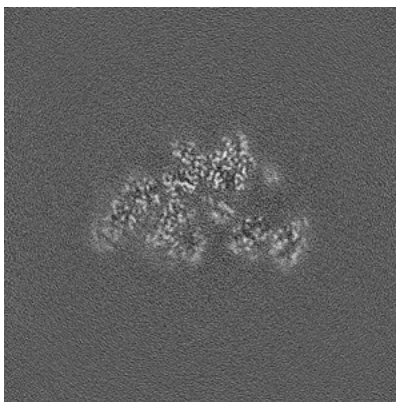


Z Index: 212

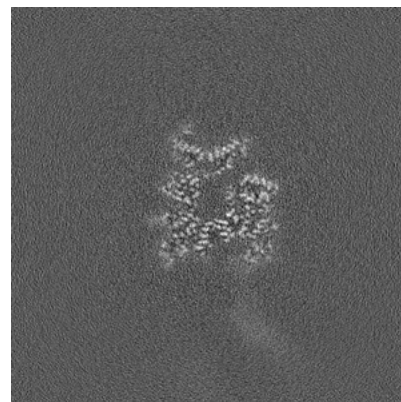
6.3.2 Raw map



X Index: 164



Y Index: 195

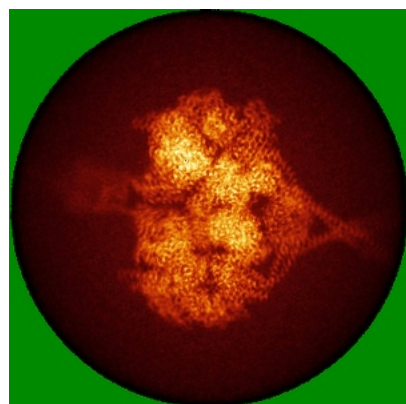


Z Index: 213

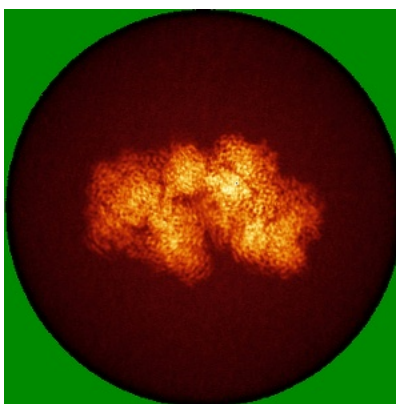
The images above show the largest variance slices of the map in three orthogonal directions.

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

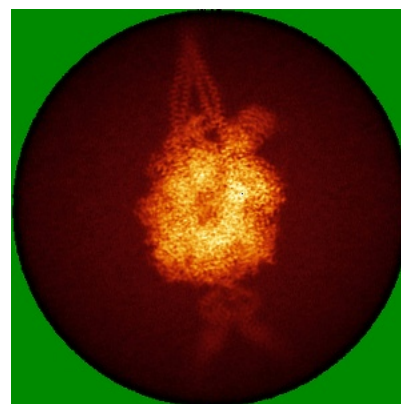
6.4.1 Primary map



X

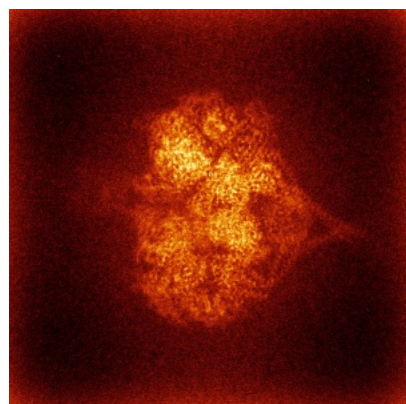


Y

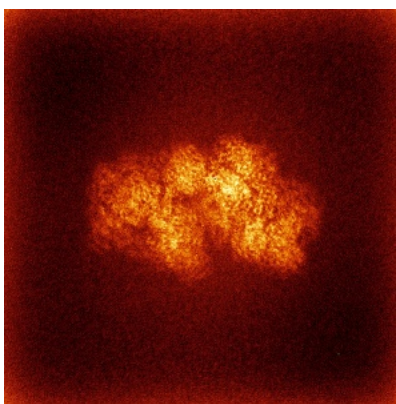


Z

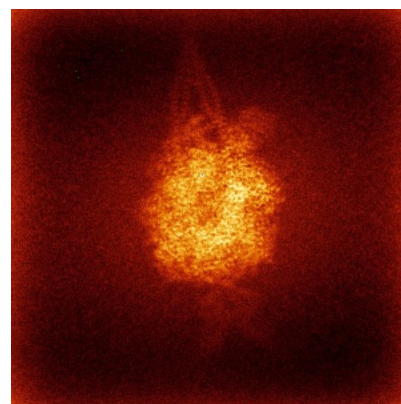
6.4.2 Raw map



X



Y

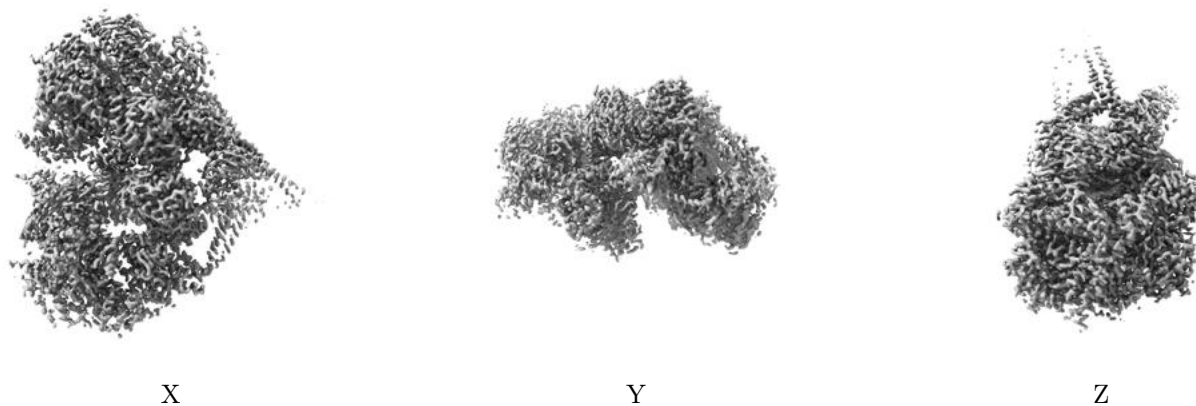


Z

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

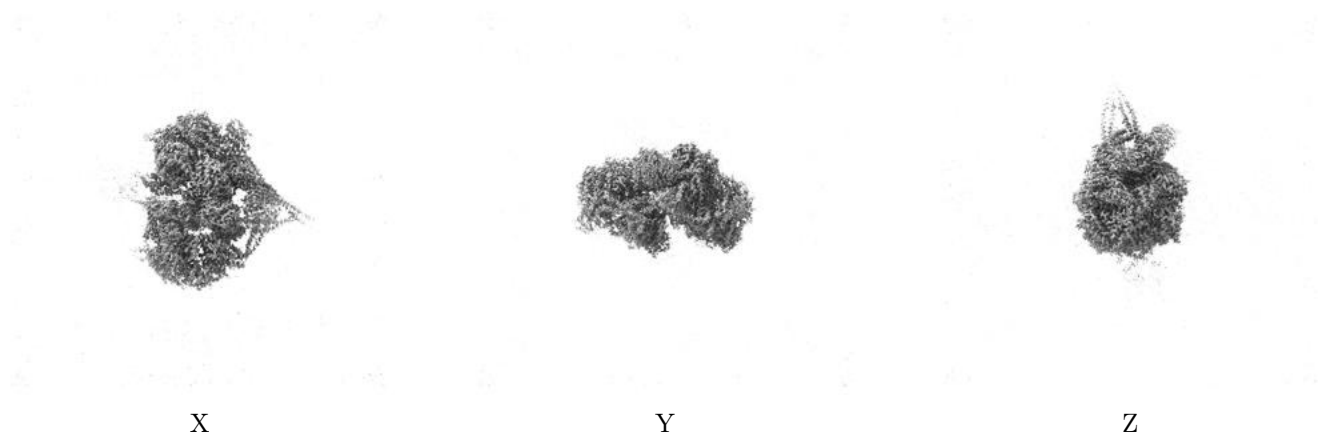
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.224. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

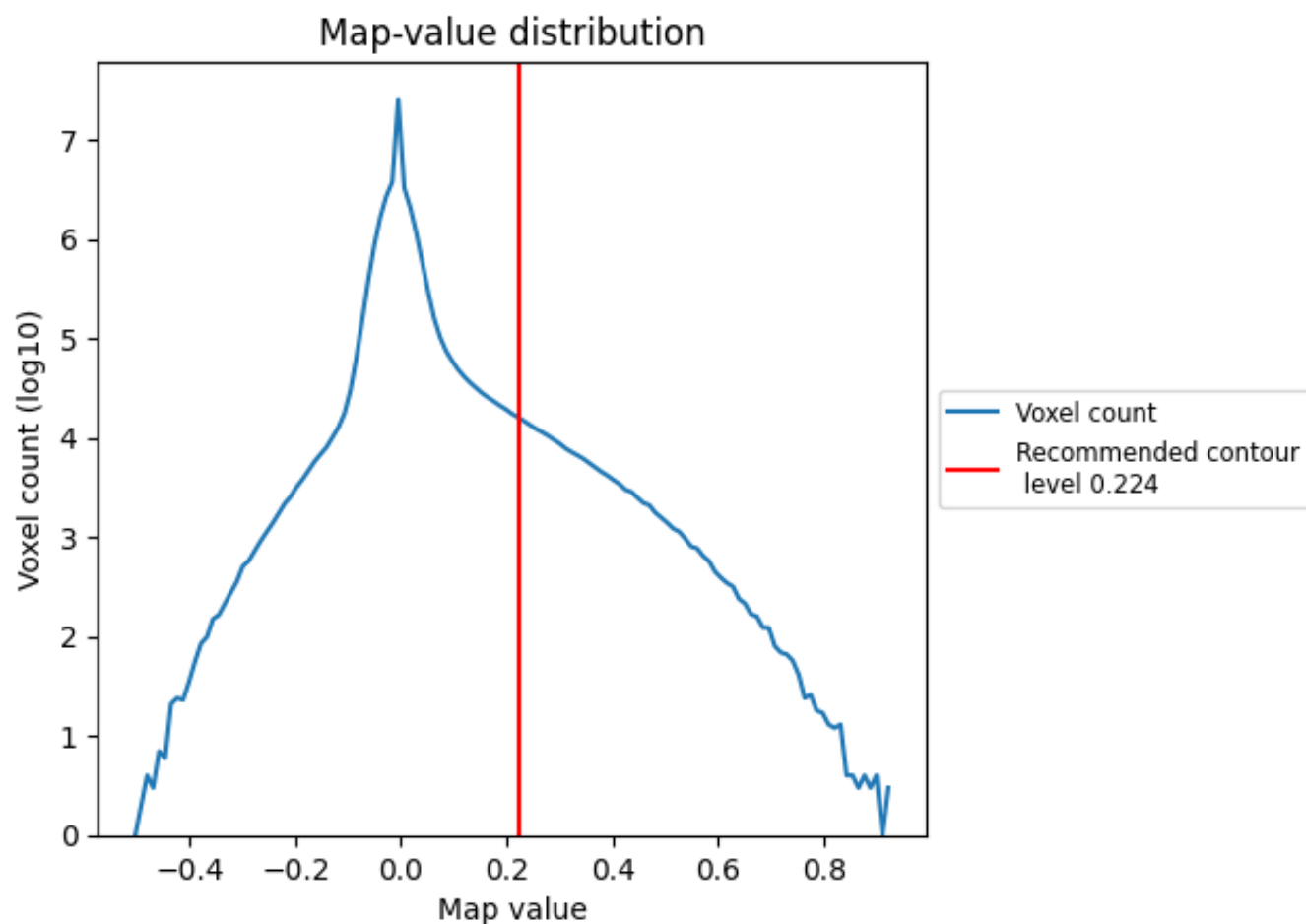
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

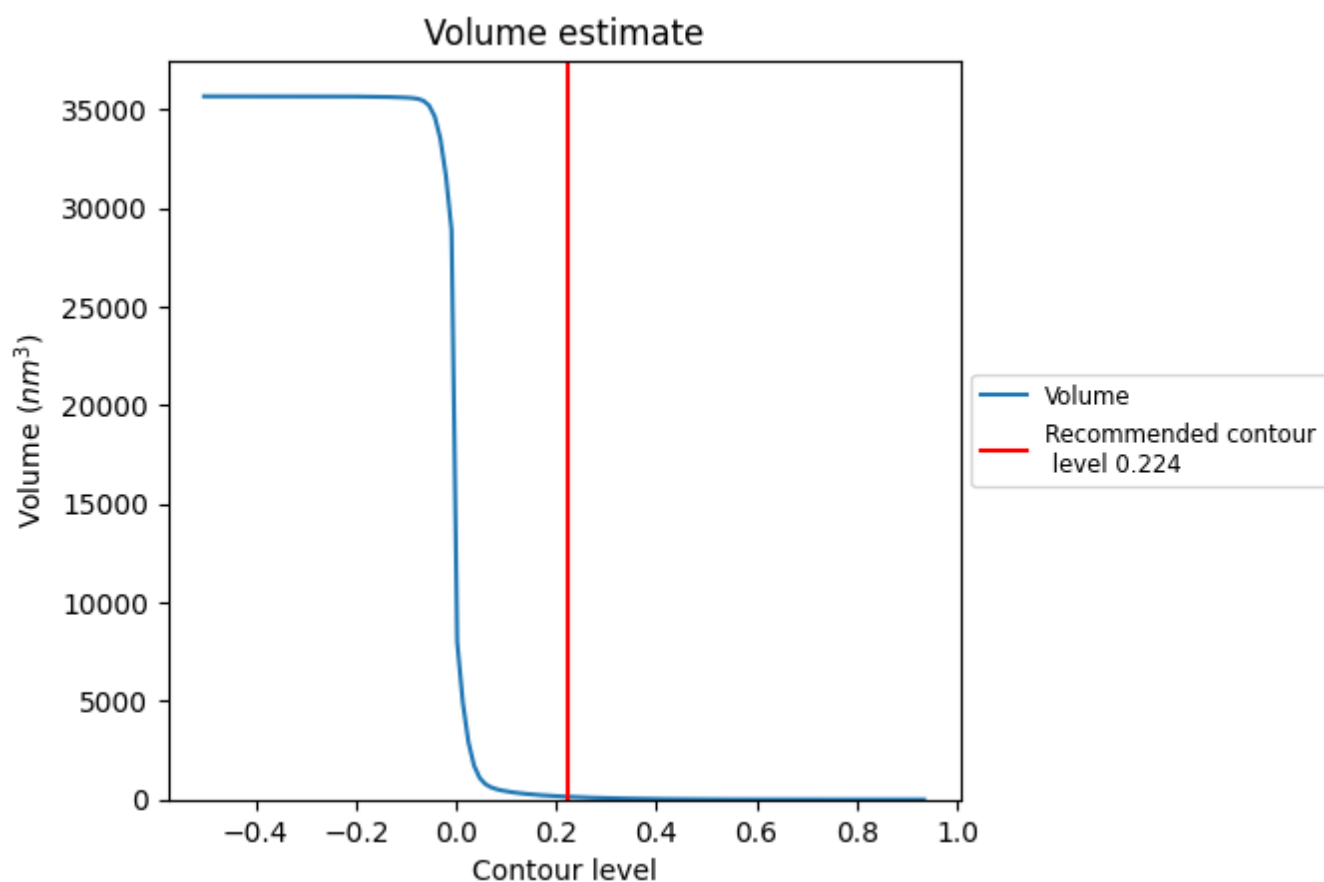
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

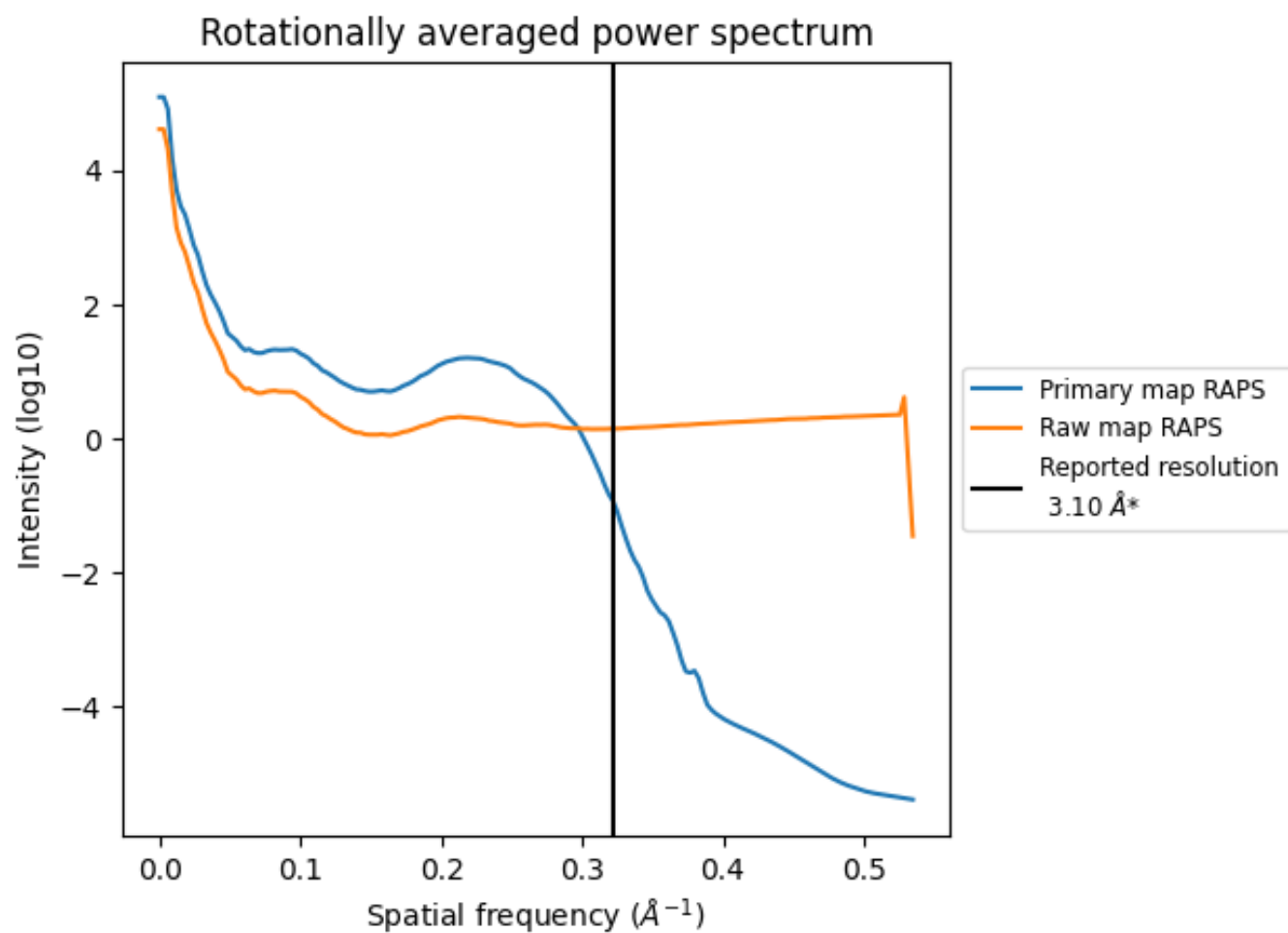
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 142 nm³; this corresponds to an approximate mass of 128 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

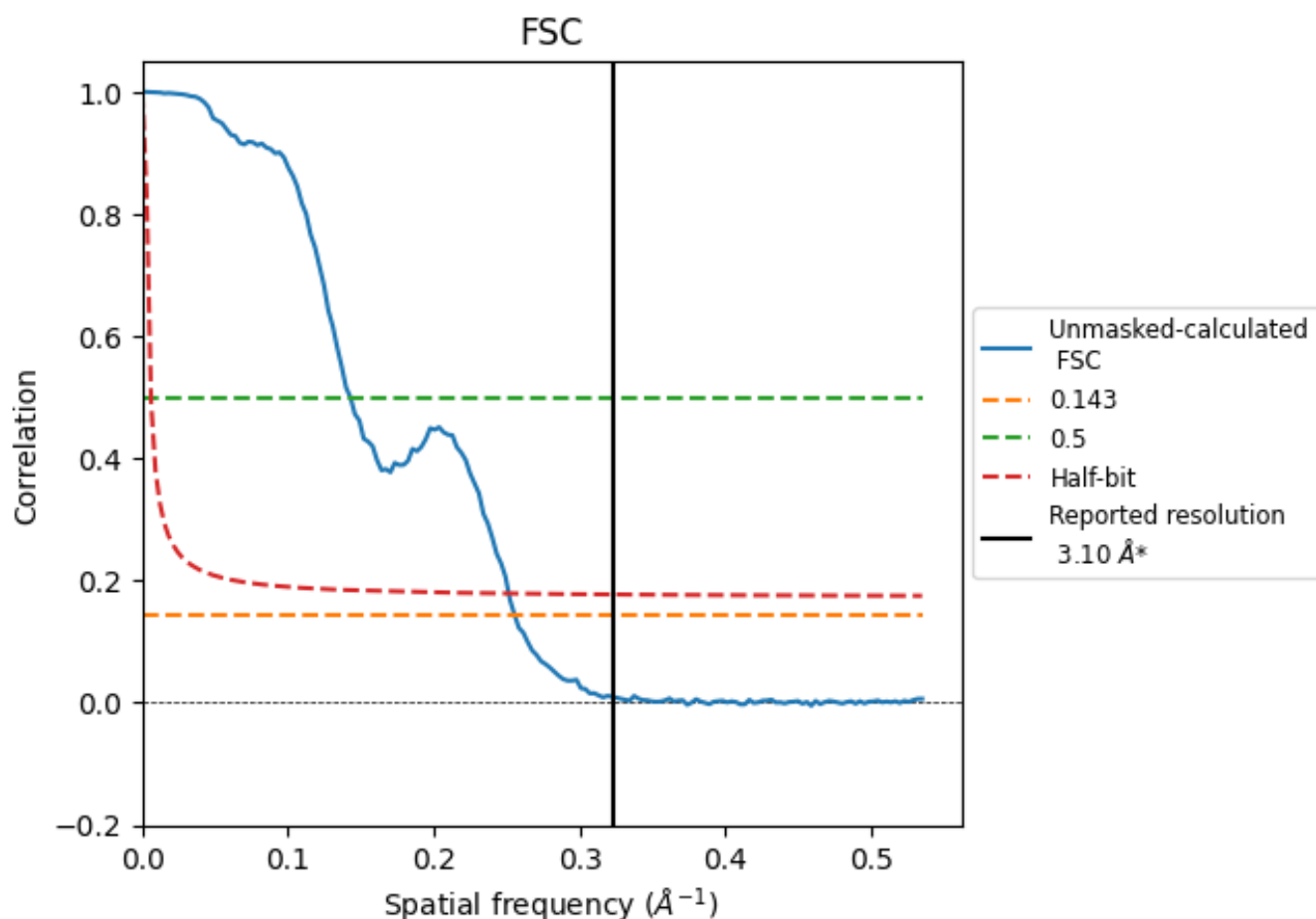


*Reported resolution corresponds to spatial frequency of $0.323 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

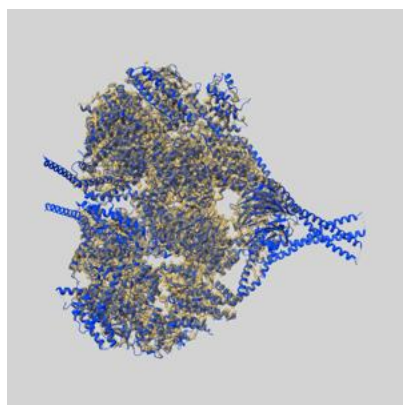
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.92	7.00	3.98

*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 %

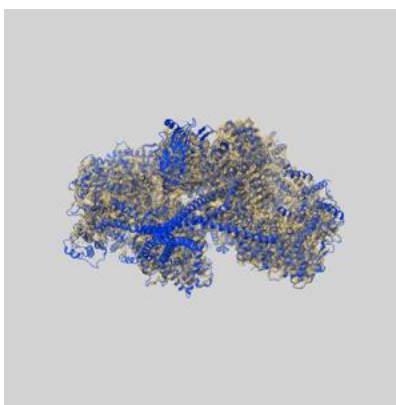
9 Map-model fit [i](#)

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.

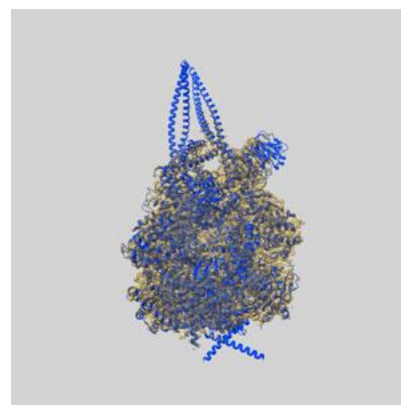
9.1 Map-model overlay [i](#)



X



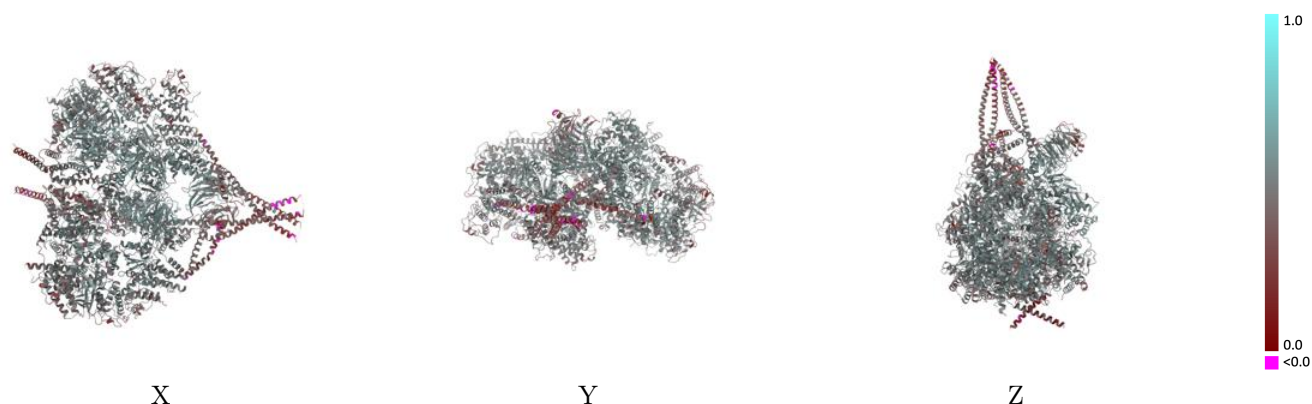
Y



Z

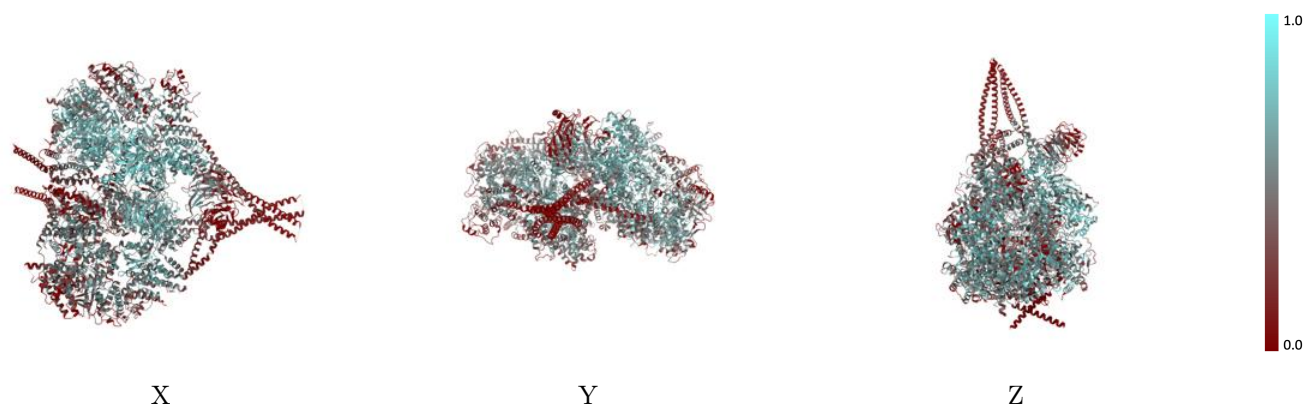
The images above show the 3D surface view of the map at the recommended contour level 0.224 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



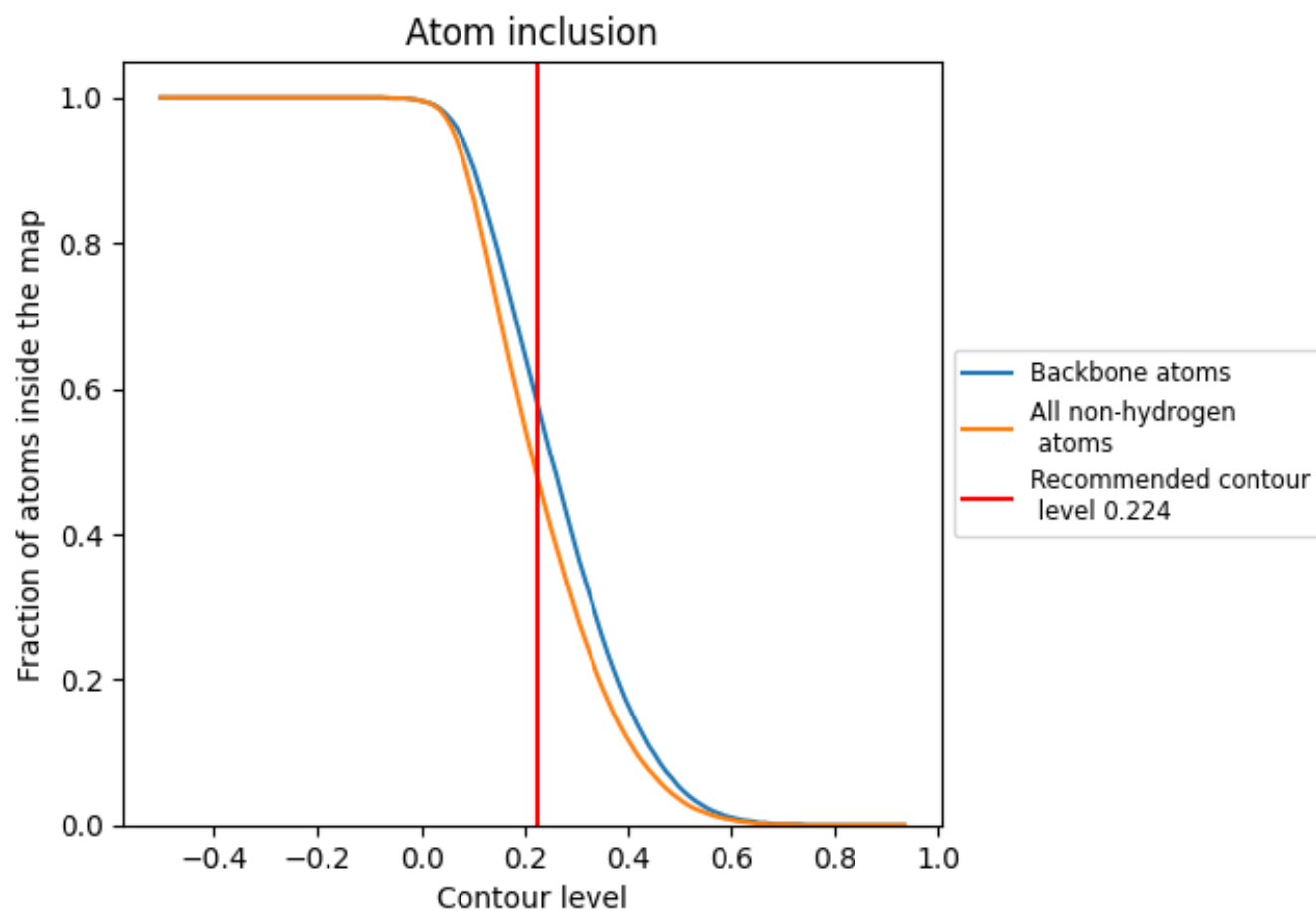
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.224).

9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.224) and Q-score for the entire model and for each chain.

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

