



Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 01:36 AM UTC

PDB ID : 8OXP / pdb_00008oxp
EMDB ID : EMD-17267
Title : ATM(Q2971A) in complex with Mg AMP-PNP
Authors : Howes, A.C.; Perisic, O.; Williams, R.L.
Deposited on : 2023-05-02
Resolution : 2.60 Å(reported)
Based on initial model : 7SIC

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

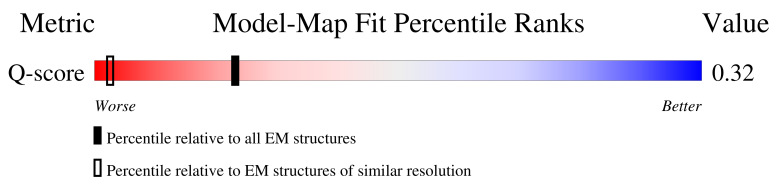
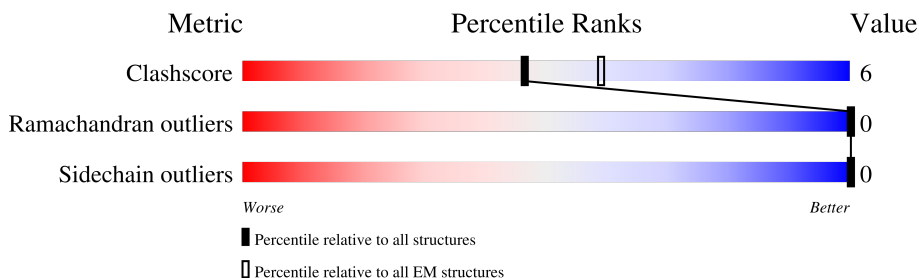
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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	8728 (2.10 - 3.10)

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	3184	17% 72% 15% 13%
1	B	3184	17% 73% 14% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 44460 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 Serine-protein kinase ATM.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2772	Total	C	N	O	S	0	0
			22197	14193	3772	4079	153		
1	B	2772	Total	C	N	O	S	0	0
			22197	14193	3772	4079	153		

There are 258 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-127	MET	-	initiating methionine	UNP Q13315
A	-126	ASP	-	expression tag	UNP Q13315
A	-125	TYR	-	expression tag	UNP Q13315
A	-124	LYS	-	expression tag	UNP Q13315
A	-123	ASP	-	expression tag	UNP Q13315
A	-122	ASP	-	expression tag	UNP Q13315
A	-121	ASP	-	expression tag	UNP Q13315
A	-120	ASP	-	expression tag	UNP Q13315
A	-119	LYS	-	expression tag	UNP Q13315
A	-118	HIS	-	expression tag	UNP Q13315
A	-117	MET	-	expression tag	UNP Q13315
A	-116	GLY	-	expression tag	UNP Q13315
A	-115	VAL	-	expression tag	UNP Q13315
A	-114	GLN	-	expression tag	UNP Q13315
A	-113	VAL	-	expression tag	UNP Q13315
A	-112	GLU	-	expression tag	UNP Q13315
A	-111	THR	-	expression tag	UNP Q13315
A	-110	ILE	-	expression tag	UNP Q13315
A	-109	SER	-	expression tag	UNP Q13315
A	-108	PRO	-	expression tag	UNP Q13315
A	-107	GLY	-	expression tag	UNP Q13315
A	-106	ASP	-	expression tag	UNP Q13315
A	-105	GLY	-	expression tag	UNP Q13315
A	-104	ARG	-	expression tag	UNP Q13315
A	-103	THR	-	expression tag	UNP Q13315
A	-102	PHE	-	expression tag	UNP Q13315

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-101	PRO	-	expression tag	UNP Q13315
A	-100	LYS	-	expression tag	UNP Q13315
A	-99	ARG	-	expression tag	UNP Q13315
A	-98	GLY	-	expression tag	UNP Q13315
A	-97	GLN	-	expression tag	UNP Q13315
A	-96	THR	-	expression tag	UNP Q13315
A	-95	CYS	-	expression tag	UNP Q13315
A	-94	VAL	-	expression tag	UNP Q13315
A	-93	VAL	-	expression tag	UNP Q13315
A	-92	HIS	-	expression tag	UNP Q13315
A	-91	TYR	-	expression tag	UNP Q13315
A	-90	THR	-	expression tag	UNP Q13315
A	-89	GLY	-	expression tag	UNP Q13315
A	-88	MET	-	expression tag	UNP Q13315
A	-87	LEU	-	expression tag	UNP Q13315
A	-86	GLU	-	expression tag	UNP Q13315
A	-85	ASP	-	expression tag	UNP Q13315
A	-84	GLY	-	expression tag	UNP Q13315
A	-83	LYS	-	expression tag	UNP Q13315
A	-82	LYS	-	expression tag	UNP Q13315
A	-81	PHE	-	expression tag	UNP Q13315
A	-80	ASP	-	expression tag	UNP Q13315
A	-79	SER	-	expression tag	UNP Q13315
A	-78	SER	-	expression tag	UNP Q13315
A	-77	ARG	-	expression tag	UNP Q13315
A	-76	ASP	-	expression tag	UNP Q13315
A	-75	ARG	-	expression tag	UNP Q13315
A	-74	ASN	-	expression tag	UNP Q13315
A	-73	LYS	-	expression tag	UNP Q13315
A	-72	PRO	-	expression tag	UNP Q13315
A	-71	PHE	-	expression tag	UNP Q13315
A	-70	LYS	-	expression tag	UNP Q13315
A	-69	PHE	-	expression tag	UNP Q13315
A	-68	MET	-	expression tag	UNP Q13315
A	-67	LEU	-	expression tag	UNP Q13315
A	-66	GLY	-	expression tag	UNP Q13315
A	-65	LYS	-	expression tag	UNP Q13315
A	-64	GLN	-	expression tag	UNP Q13315
A	-63	GLU	-	expression tag	UNP Q13315
A	-62	VAL	-	expression tag	UNP Q13315
A	-61	ILE	-	expression tag	UNP Q13315
A	-60	ARG	-	expression tag	UNP Q13315

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-59	GLY	-	expression tag	UNP Q13315
A	-58	TRP	-	expression tag	UNP Q13315
A	-57	GLU	-	expression tag	UNP Q13315
A	-56	GLU	-	expression tag	UNP Q13315
A	-55	GLY	-	expression tag	UNP Q13315
A	-54	VAL	-	expression tag	UNP Q13315
A	-53	ALA	-	expression tag	UNP Q13315
A	-52	GLN	-	expression tag	UNP Q13315
A	-51	MET	-	expression tag	UNP Q13315
A	-50	SER	-	expression tag	UNP Q13315
A	-49	VAL	-	expression tag	UNP Q13315
A	-48	GLY	-	expression tag	UNP Q13315
A	-47	GLN	-	expression tag	UNP Q13315
A	-46	ARG	-	expression tag	UNP Q13315
A	-45	ALA	-	expression tag	UNP Q13315
A	-44	LYS	-	expression tag	UNP Q13315
A	-43	LEU	-	expression tag	UNP Q13315
A	-42	THR	-	expression tag	UNP Q13315
A	-41	ILE	-	expression tag	UNP Q13315
A	-40	SER	-	expression tag	UNP Q13315
A	-39	PRO	-	expression tag	UNP Q13315
A	-38	ASP	-	expression tag	UNP Q13315
A	-37	TYR	-	expression tag	UNP Q13315
A	-36	ALA	-	expression tag	UNP Q13315
A	-35	TYR	-	expression tag	UNP Q13315
A	-34	GLY	-	expression tag	UNP Q13315
A	-33	ALA	-	expression tag	UNP Q13315
A	-32	THR	-	expression tag	UNP Q13315
A	-31	GLY	-	expression tag	UNP Q13315
A	-30	HIS	-	expression tag	UNP Q13315
A	-29	PRO	-	expression tag	UNP Q13315
A	-28	GLY	-	expression tag	UNP Q13315
A	-27	ILE	-	expression tag	UNP Q13315
A	-26	ILE	-	expression tag	UNP Q13315
A	-25	PRO	-	expression tag	UNP Q13315
A	-24	PRO	-	expression tag	UNP Q13315
A	-23	HIS	-	expression tag	UNP Q13315
A	-22	ALA	-	expression tag	UNP Q13315
A	-21	THR	-	expression tag	UNP Q13315
A	-20	LEU	-	expression tag	UNP Q13315
A	-19	VAL	-	expression tag	UNP Q13315
A	-18	PHE	-	expression tag	UNP Q13315

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	ASP	-	expression tag	UNP Q13315
A	-16	VAL	-	expression tag	UNP Q13315
A	-15	GLU	-	expression tag	UNP Q13315
A	-14	LEU	-	expression tag	UNP Q13315
A	-13	LEU	-	expression tag	UNP Q13315
A	-12	LYS	-	expression tag	UNP Q13315
A	-11	LEU	-	expression tag	UNP Q13315
A	-10	GLU	-	expression tag	UNP Q13315
A	-9	GLY	-	expression tag	UNP Q13315
A	-8	GLY	-	expression tag	UNP Q13315
A	-7	SER	-	expression tag	UNP Q13315
A	-6	ALA	-	expression tag	UNP Q13315
A	-5	GLY	-	expression tag	UNP Q13315
A	-4	SER	-	expression tag	UNP Q13315
A	-3	GLY	-	expression tag	UNP Q13315
A	-2	SER	-	expression tag	UNP Q13315
A	-1	ALA	-	expression tag	UNP Q13315
A	0	SER	-	expression tag	UNP Q13315
A	2971	ALA	GLN	engineered mutation	UNP Q13315
B	-127	MET	-	initiating methionine	UNP Q13315
B	-126	ASP	-	expression tag	UNP Q13315
B	-125	TYR	-	expression tag	UNP Q13315
B	-124	LYS	-	expression tag	UNP Q13315
B	-123	ASP	-	expression tag	UNP Q13315
B	-122	ASP	-	expression tag	UNP Q13315
B	-121	ASP	-	expression tag	UNP Q13315
B	-120	ASP	-	expression tag	UNP Q13315
B	-119	LYS	-	expression tag	UNP Q13315
B	-118	HIS	-	expression tag	UNP Q13315
B	-117	MET	-	expression tag	UNP Q13315
B	-116	GLY	-	expression tag	UNP Q13315
B	-115	VAL	-	expression tag	UNP Q13315
B	-114	GLN	-	expression tag	UNP Q13315
B	-113	VAL	-	expression tag	UNP Q13315
B	-112	GLU	-	expression tag	UNP Q13315
B	-111	THR	-	expression tag	UNP Q13315
B	-110	ILE	-	expression tag	UNP Q13315
B	-109	SER	-	expression tag	UNP Q13315
B	-108	PRO	-	expression tag	UNP Q13315
B	-107	GLY	-	expression tag	UNP Q13315
B	-106	ASP	-	expression tag	UNP Q13315
B	-105	GLY	-	expression tag	UNP Q13315

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-104	ARG	-	expression tag	UNP Q13315
B	-103	THR	-	expression tag	UNP Q13315
B	-102	PHE	-	expression tag	UNP Q13315
B	-101	PRO	-	expression tag	UNP Q13315
B	-100	LYS	-	expression tag	UNP Q13315
B	-99	ARG	-	expression tag	UNP Q13315
B	-98	GLY	-	expression tag	UNP Q13315
B	-97	GLN	-	expression tag	UNP Q13315
B	-96	THR	-	expression tag	UNP Q13315
B	-95	CYS	-	expression tag	UNP Q13315
B	-94	VAL	-	expression tag	UNP Q13315
B	-93	VAL	-	expression tag	UNP Q13315
B	-92	HIS	-	expression tag	UNP Q13315
B	-91	TYR	-	expression tag	UNP Q13315
B	-90	THR	-	expression tag	UNP Q13315
B	-89	GLY	-	expression tag	UNP Q13315
B	-88	MET	-	expression tag	UNP Q13315
B	-87	LEU	-	expression tag	UNP Q13315
B	-86	GLU	-	expression tag	UNP Q13315
B	-85	ASP	-	expression tag	UNP Q13315
B	-84	GLY	-	expression tag	UNP Q13315
B	-83	LYS	-	expression tag	UNP Q13315
B	-82	LYS	-	expression tag	UNP Q13315
B	-81	PHE	-	expression tag	UNP Q13315
B	-80	ASP	-	expression tag	UNP Q13315
B	-79	SER	-	expression tag	UNP Q13315
B	-78	SER	-	expression tag	UNP Q13315
B	-77	ARG	-	expression tag	UNP Q13315
B	-76	ASP	-	expression tag	UNP Q13315
B	-75	ARG	-	expression tag	UNP Q13315
B	-74	ASN	-	expression tag	UNP Q13315
B	-73	LYS	-	expression tag	UNP Q13315
B	-72	PRO	-	expression tag	UNP Q13315
B	-71	PHE	-	expression tag	UNP Q13315
B	-70	LYS	-	expression tag	UNP Q13315
B	-69	PHE	-	expression tag	UNP Q13315
B	-68	MET	-	expression tag	UNP Q13315
B	-67	LEU	-	expression tag	UNP Q13315
B	-66	GLY	-	expression tag	UNP Q13315
B	-65	LYS	-	expression tag	UNP Q13315
B	-64	GLN	-	expression tag	UNP Q13315
B	-63	GLU	-	expression tag	UNP Q13315

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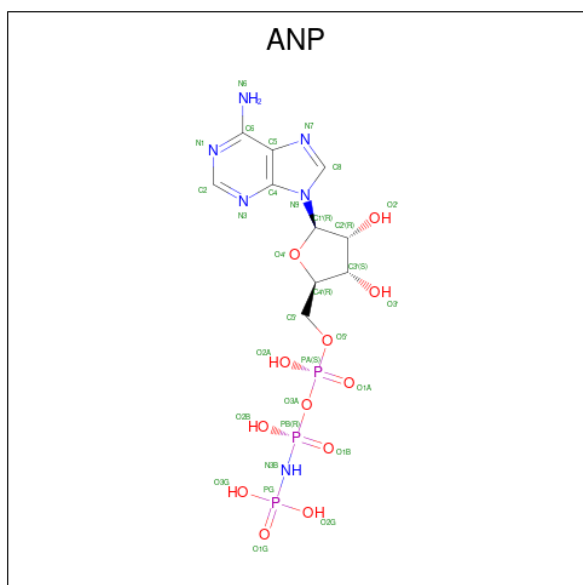
Chain	Residue	Modelled	Actual	Comment	Reference
B	-62	VAL	-	expression tag	UNP Q13315
B	-61	ILE	-	expression tag	UNP Q13315
B	-60	ARG	-	expression tag	UNP Q13315
B	-59	GLY	-	expression tag	UNP Q13315
B	-58	TRP	-	expression tag	UNP Q13315
B	-57	GLU	-	expression tag	UNP Q13315
B	-56	GLU	-	expression tag	UNP Q13315
B	-55	GLY	-	expression tag	UNP Q13315
B	-54	VAL	-	expression tag	UNP Q13315
B	-53	ALA	-	expression tag	UNP Q13315
B	-52	GLN	-	expression tag	UNP Q13315
B	-51	MET	-	expression tag	UNP Q13315
B	-50	SER	-	expression tag	UNP Q13315
B	-49	VAL	-	expression tag	UNP Q13315
B	-48	GLY	-	expression tag	UNP Q13315
B	-47	GLN	-	expression tag	UNP Q13315
B	-46	ARG	-	expression tag	UNP Q13315
B	-45	ALA	-	expression tag	UNP Q13315
B	-44	LYS	-	expression tag	UNP Q13315
B	-43	LEU	-	expression tag	UNP Q13315
B	-42	THR	-	expression tag	UNP Q13315
B	-41	ILE	-	expression tag	UNP Q13315
B	-40	SER	-	expression tag	UNP Q13315
B	-39	PRO	-	expression tag	UNP Q13315
B	-38	ASP	-	expression tag	UNP Q13315
B	-37	TYR	-	expression tag	UNP Q13315
B	-36	ALA	-	expression tag	UNP Q13315
B	-35	TYR	-	expression tag	UNP Q13315
B	-34	GLY	-	expression tag	UNP Q13315
B	-33	ALA	-	expression tag	UNP Q13315
B	-32	THR	-	expression tag	UNP Q13315
B	-31	GLY	-	expression tag	UNP Q13315
B	-30	HIS	-	expression tag	UNP Q13315
B	-29	PRO	-	expression tag	UNP Q13315
B	-28	GLY	-	expression tag	UNP Q13315
B	-27	ILE	-	expression tag	UNP Q13315
B	-26	ILE	-	expression tag	UNP Q13315
B	-25	PRO	-	expression tag	UNP Q13315
B	-24	PRO	-	expression tag	UNP Q13315
B	-23	HIS	-	expression tag	UNP Q13315
B	-22	ALA	-	expression tag	UNP Q13315
B	-21	THR	-	expression tag	UNP Q13315

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	LEU	-	expression tag	UNP Q13315
B	-19	VAL	-	expression tag	UNP Q13315
B	-18	PHE	-	expression tag	UNP Q13315
B	-17	ASP	-	expression tag	UNP Q13315
B	-16	VAL	-	expression tag	UNP Q13315
B	-15	GLU	-	expression tag	UNP Q13315
B	-14	LEU	-	expression tag	UNP Q13315
B	-13	LEU	-	expression tag	UNP Q13315
B	-12	LYS	-	expression tag	UNP Q13315
B	-11	LEU	-	expression tag	UNP Q13315
B	-10	GLU	-	expression tag	UNP Q13315
B	-9	GLY	-	expression tag	UNP Q13315
B	-8	GLY	-	expression tag	UNP Q13315
B	-7	SER	-	expression tag	UNP Q13315
B	-6	ALA	-	expression tag	UNP Q13315
B	-5	GLY	-	expression tag	UNP Q13315
B	-4	SER	-	expression tag	UNP Q13315
B	-3	GLY	-	expression tag	UNP Q13315
B	-2	SER	-	expression tag	UNP Q13315
B	-1	ALA	-	expression tag	UNP Q13315
B	0	SER	-	expression tag	UNP Q13315
B	2971	ALA	GLN	engineered mutation	UNP Q13315

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	B	1	Total	C	N	O	P	0
			31	10	6	12	3	

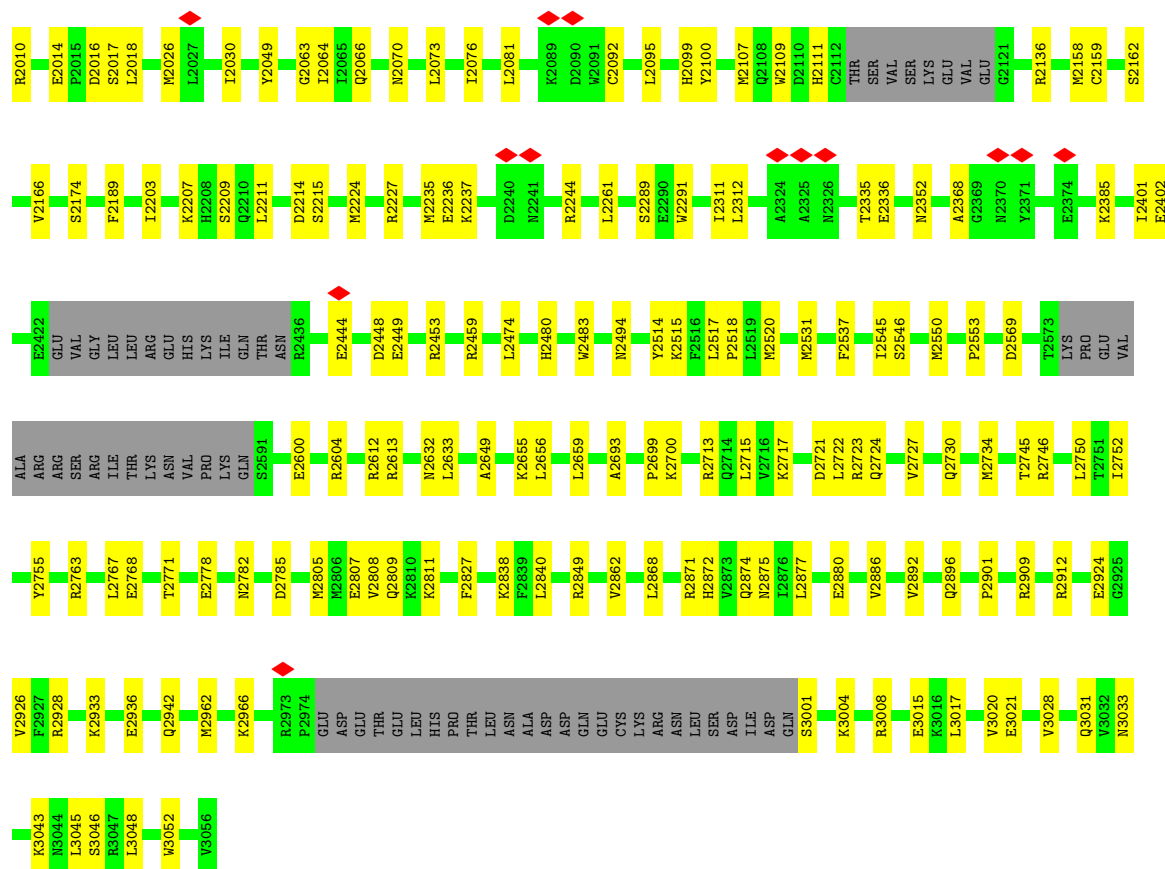
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	
3	B	1	Total	Mg	0
			1	1	

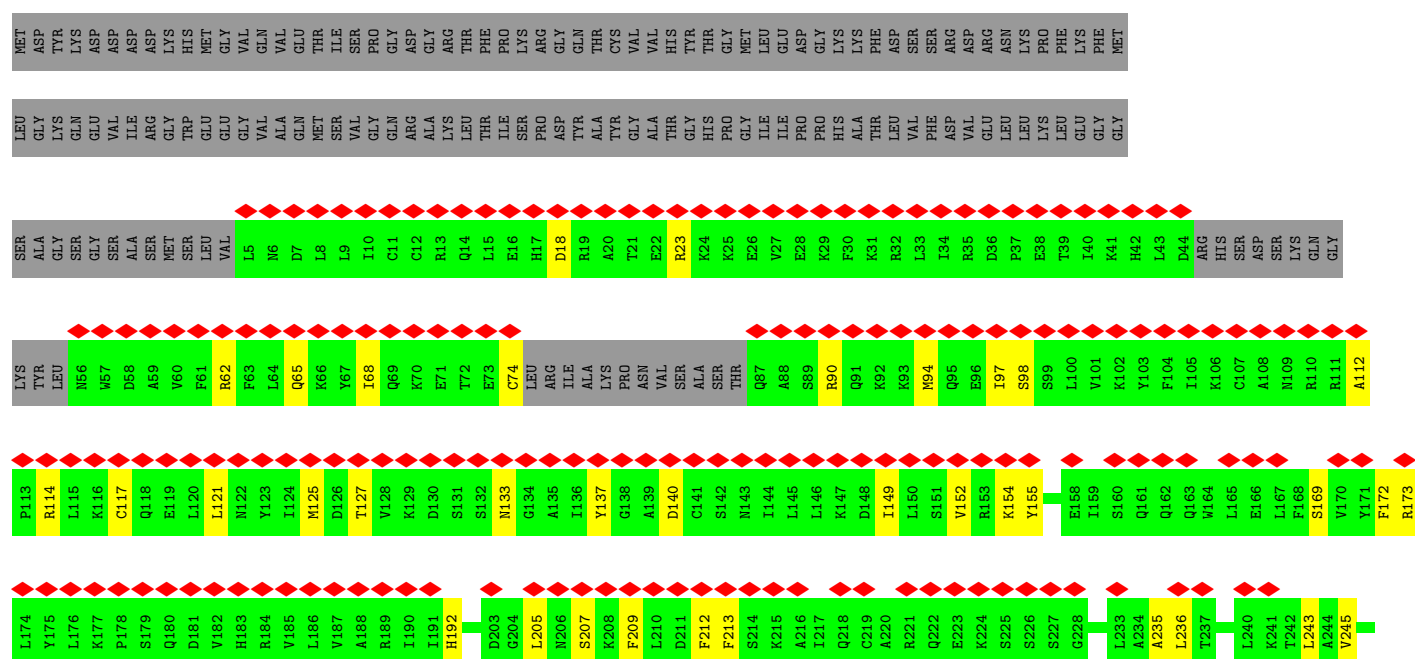
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	
4	B	1	Total	Zn	0
			1	1	

THR	C1899	C1900	L1901	R1918	R1921	P1922	F1932	W1933	L1939	A1949	E1959	I1960	Y1961	A1962	S1974	LEU	ALA	PHE	GLU	GLU	GLY	SER	GLN	SER	T1984	L1989	T1997	L2001	L2006																										
Q1640	K1656	P1680	T1685	S1689	K1610	K1706	W1710	I1713	M1714	L1715	L1718	L1737	T1745	K1754	M1755	P1766	V1777	D1781	I1796	P1797	L1798	G1818	C1821	E1822	I1823	L1824	M1830	L1845	Q1852	R1859	C1873	L1874	R1875	H1876	PHE	SER	GLN																		
R1479	F1491	L1497	L1498	S1499	K1510	L1524	L1527	Q1531	V1532	E1533	L1541	L1542	K1543	Y1544	V1546	I1547	D1548	D1551	N1552	I1559	K1560	D1563	H1568	R1575	Q1578	I1581	K1582	L1606	T1609	D1616	Q1620	H1624	M1628	V1629	D1630	R1633																			
L1351	P1354	ALA	ASN	SER	SER	ALA	ALA	SER	GLN	SER	THR	ASP	LEU	CYS	ASP	PHE	SER	GLY	D1371	L1372	H1380	T1389	Y1392	I1393	K1398	K1402	P1412	D1413	K1417	L1418	L1419	A1426	K1434	R1437	I1438	T1441	L1449	L1450	K1451	K1454	V1464	L1472	I1476												
Q1225	D1226	T1227	Y1228	N1230	L1231	L1255	H1258	L1259	R1262	S1263	H1264	F1265	D1266	E1267	N1273	F1287	P1288	K1289	I1290	L1291	V1292	N1293	I1294	L1295	A1299	T1303	R1304	D1305	S1306	G1307	Q1310	Q1311	A1315	L1322	E1325	H1326	L1327	F1336	N1339	L1340	P1341	E1342	I1343	T1350											
S1092	I1093	Q1098	D1099	T1100	K1101	GLY	ASP	SER	SER	ARG	LEU	L1108	K1109	A1110	L1111	Q1116	A1127	M1131	R1132	E1133	M1134	SER	HIS	ALA	GLU	ASN	PRO	E1142	L1155	T1156	L1157	L1176	V1180	K1181	E1182	E1186	L1189	L1194	E1195	K1196	V1197	L1206	D1215	N1223	L1224										
D965	L970	V976	Q984	D985	V986	H996	V997	K998	K999	N1000	L1001	G1002	Q1003	S1004	N1005	M1006	D1007	S1008	E1009	N1010	T1011	R1012	D1013	A1014	Q1015	F1018	I1035	F1036	M1040	A1041	L1042	L1046	N1062	V1063	M1064	G1065	K1066	D1067	F1074	H1082	Q1083	H1084	V1085	M1087	A1090	E1091									
L895	L896	F897	L898	D899	N900	L901	K902	L906	T909	T910	A911	Q912	T913	N914	V916	S917	F918	R919	A920	A921	D922	Y923	A924	R925	K926	L927	L928	N929	L930	I931	D932	S933	S934	T935	L936	E937	P938	T939	K940	L942	H943	L944	H945	N946	G956	E957	E958	Y959	P960	L961	P962	N963	E964		
S759	I760	K764	N765	K766	T767	N768	E769	E770	F771	R772	I773	G774	S775	L776	R777	N778	M779	M780	Q781	T784	R785	C786	L787	S788	N789	C790	T791	K792	L804	R805	L806	L807	T808	S809	K810	L811	M812	N813	D814	D817	L818	C819	K820	S821	L822	A823	R824	F825	I826	LYS	PRO	PHE	ASP	ARG	
GLN	SER	SER	ILE	G679	F680	S681	V682	K683	Q684	N685	D691	R692	C693	L694	E699	Q700	L701	L702	N703	N704	Y705	S706	S707	E708	I709	T710	N711	R717	L721	L722	V723	G724	G733	V734	I735	A736	E737	E738	E739	K742	S743	E744	L745	L746	Q747	K748	A749	K750	M753	G757	E758				
N602	F603	P604	H605	L606	V607	L608	E609	I611	L612	L615	T616	M617	K618	M624	Q628	S629	V630	P631	G632	C633	GLU	HIS	GLY	ILE	GLN	LYS	ASP	GLN	LYS	GLU	LEU	S644	F645	S646	E647	V648	F652	T655	T656	F657	D661	T664	ILE	VAL	ARG	GLU	CYS	ILE	GLY	LYS	HIS				
L526	F527	T528	G529	S530	A531	C532	R533	P534	S535	A538	T543	L544	A545	S549	I550	V551	P552	G553	T554	VAL	LYS	MET	GLY	ILE	GLU	LYS	ASN	MET	CYS	GLU	VAL	ASN	ARG	SER	F570	S571	Y583	Q584	L585	GLU	GLY	ASP	LEU	GLU	ASN	SER	T593	E594	V595	P596	F597	I598	L599	H600	S601



• Molecule 1: Serine-protein kinase ATM





LYS	ARG	ASN	LEU	SER	ASP	ILE	ASP	GLN	S3001	L3010	M3011	R3012	E3015	K3018	G3019	V3020	E3021	V3028	Q3031	V3032	N3033	Q3037	L3045	L3048	W3055	V3056																					
R2849	V2862	I2865	L2866	G2867	L2868	R2871	H2872	V2873	Q2874	N2875	E2880	G2897	L2900	P2901	R2912	E2924	G2925	V2926	F2927	R2928	K2933	E2936	Q2942	V2951	L2952	L2953	R2973	P2974	GLU	ASP	GLU	THR	GLU	LEU	HIS	PRO	THR	LEU	ASN	ALA	ASP	GLN	CYS				
L2680	A2693	P2699	K2700	R2713	Q2714	L2715	V2716	K2717	G2718	R2719	D2720	D2721	L2722	R2723	Q2724	Q2730	V2731	M2734	C2735	N2736	T2743	E2744	T2745	R2746	L2750	T2751	I2752	V2755	R2763	L2767	E2768	T2771	E2778	N2782	D2785	M2805	V2808	K2811	F2827	K2838							
N2494	E2499	M2503	Y2514	K2515	L2517	P2518	L2519	M2520	Y2521	Q2522	L2523	A2524	T2529	K2530	M2531	M2532	F2537	M2550	T2573	LYS	PRO	GLU	VAL	ALA	ARG	ARG	SER	ARG	ILE	THR	LYS	ASN	VAL	PRO	LYS	GLN	S2591	I2609	L2633	A2649	K2655	L2656	L2659	V2663			
W2239	D2240	W2241	R2244	L2261	S2289	E2290	W2291	L2307	A2324	A2325	E2336	E2374	K2385	I2401	E2402	S2408	E2422	GLU	VAL	GLY	LEU	LEU	ARG	GLU	HIS	ILE	GLN	THR	ASN	R2436	E2444	D2448	E2449	R2453	R2459	L2474	H2480	W2483	V2484								
Y2086	K2089	D2090	W2091	C2092	L2095	W2109	C2112	THR	SER	VAL	SER	LYS	GLU	VAL	GLU	L2132	V2152	E2156	C2159	S2162	V2166	S2174	I2185	F2189	S2209	Q2210	L2211	D2214	M2224	R2227	T2228	V2229	I2230	I2233	L2234	M2235	E2236	K2237	E2238								
R1875	H1876	PHE	SER	GLN	THR	SER	ARG	THR	THR	PRO	ALA	ASN	LEU	ASP	SER	GLU	SER	GLU	GLU	HIS	PHE	PHE	ARG	C1899	C1900	L1901	A1949	E1959	S1974	LEU	ALA	ALA	GLU	GLU	GLY	SER	T1984	S1988	K1992	E2014	P2015	D2016	S2017	L2027	I2030	L2073	I2076
R1633	Q1640	L1647	K1656	P1680	T1685	Q1689	K1706	W1710	T1711	L1718	V1729	P1737	K1738	N1739	P1766	V1777	D1781	I1796	P1797	L1798	I1806	Q1818	C1821	E1822	I1823	L1824	Q1825	L1826	M1830	C1838	L1845	I1849	Q1852	C1873	L1874												
L1497	L1498	S1499	K1510	I1520	L1524	L1527	Q1531	V1532	E1533	V1538	L1541	L1542	K1543	Y1544	L1545	V1546	I1547	D1548	D1551	N1552	T1559	K1560	D1563	P1564	H1568	R1575	I1576	T1577	Q1578	I1581	K1582	I1594	S1601	L1606	T1609	D1616	Q1620	M1628									
SER	THR	ASP	LEU	CYS	ASP	PHE	SER	SER	GLY	D1371	L1372	P1376	H1377	P1378	P1379	H1380	T1389	Y1392	I1393	K1398	K1402	P1412	D1413	S1414	K1417	I1418	L1419	K1435	I1438	I1441	L1444	F1445	V1446	L1449	L1457	V1464	L1472	I1473	I1476	R1479	F1491						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	1207435	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	39.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.475	Depositor
Minimum map value	-0.192	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	330.4, 330.4, 330.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, ZN, 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	0.08	0/22611	0.24	0/30548
1	B	0.09	0/22611	0.25	0/30548
All	All	0.08	0/45222	0.24	0/61096

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	22197	0	22381	285	0
1	B	22197	0	22381	268	0
2	A	31	0	13	0	0
2	B	31	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	44460	0	44788	547	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 (547) 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:2514:TYR:HA	1:B:2517:LEU:HD23	1.65	0.78
1:A:2514:TYR:HA	1:A:2517:LEU:HD23	1.66	0.77
1:A:942:LEU:HG	1:A:946:MET:HE1	1.66	0.76
1:B:942:LEU:HG	1:B:946:MET:HE1	1.66	0.76
1:B:941:SER:O	1:B:945:HIS:ND1	2.22	0.71
1:B:940:LYS:HE2	1:B:942:LEU:HB3	1.73	0.71
1:B:818:ILE:HG22	1:B:900:MET:HE1	1.72	0.71
1:A:1818:GLY:O	1:A:1852:GLN:NE2	2.24	0.70
1:B:1341:PRO:HG2	1:B:1417:LYS:HD2	1.73	0.70
1:B:1685:THR:HG23	1:B:2166:VAL:HG21	1.74	0.69
1:B:1739:ASN:HB3	1:B:1826:LEU:HD13	1.74	0.69
1:A:1685:THR:HG23	1:A:2166:VAL:HG21	1.75	0.68
1:A:940:LYS:HE2	1:A:942:LEU:HB3	1.75	0.68
1:B:3045:LEU:HA	1:B:3048:LEU:HD12	1.76	0.68
1:A:3045:LEU:HA	1:A:3048:LEU:HD12	1.76	0.68
1:A:1546:VAL:HG13	1:A:1559:ILE:HD11	1.75	0.68
1:B:2719:ARG:HA	1:B:2763:ARG:HE	1.58	0.67
1:A:2656:LEU:HD13	1:A:2659:LEU:HD11	1.76	0.67
1:B:1818:GLY:O	1:B:1852:GLN:NE2	2.25	0.67
1:A:349:MET:HG2	1:A:415:ILE:HG12	1.77	0.66
1:B:2649:ALA:O	1:B:2655:LYS:NZ	2.29	0.66
1:B:412:TRP:HA	1:B:415:ILE:HD12	1.78	0.66
1:B:2656:LEU:HD13	1:B:2659:LEU:HD11	1.76	0.66
1:A:412:TRP:HA	1:A:415:ILE:HD12	1.78	0.66
1:A:2136:ARG:NH1	1:A:2236:GLU:OE2	2.30	0.65
1:A:1294:ILE:HG23	1:A:1315:ALA:HB1	1.79	0.65
1:A:2649:ALA:O	1:A:2655:LYS:NZ	2.29	0.65
1:B:349:MET:HG2	1:B:415:ILE:HG12	1.77	0.65
1:A:2569:ASP:HB3	1:A:2763:ARG:HH21	1.62	0.65
1:B:2942:GLN:HE22	1:B:3018:LYS:HG3	1.62	0.64
1:B:2752:ILE:HD11	1:B:2862:VAL:HG21	1.80	0.64
1:A:2480:HIS:HB3	1:A:2483:TRP:HD1	1.63	0.64
1:B:1294:ILE:HG23	1:B:1315:ALA:HB1	1.79	0.64
1:A:722:LEU:HD22	1:A:749:ALA:HB2	1.79	0.64
1:A:1875:ARG:O	1:A:1876:HIS:ND1	2.31	0.64
1:B:722:LEU:HD22	1:B:749:ALA:HB2	1.79	0.64
1:B:1729:VAL:HG13	1:B:1830:MET:HE1	1.80	0.63
1:A:280:ILE:HG23	1:A:348:LEU:HD22	1.81	0.63
1:B:2897:GLY:HA2	1:B:2900:LEU:HD23	1.79	0.63
1:B:1546:VAL:HG13	1:B:1559:ILE:HD11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:805:ARG:NH1	1:B:915:THR:O	2.32	0.62
1:B:2717:LYS:HD2	1:B:2722:LEU:HD21	1.79	0.62
1:B:1419:LEU:HD11	1:B:1464:VAL:HG23	1.80	0.62
1:B:1875:ARG:O	1:B:1876:HIS:ND1	2.31	0.62
1:B:2289:SER:HG	1:B:2291:TRP:CD1	2.18	0.62
1:A:2752:ILE:HD11	1:A:2862:VAL:HG21	1.81	0.62
1:A:805:ARG:NH1	1:A:915:THR:O	2.32	0.62
1:A:2100:TYR:HE1	1:A:2111:HIS:HE1	1.48	0.62
1:B:169:SER:OG	1:B:173:ARG:NH1	2.33	0.62
1:B:329:ARG:NH2	1:B:407:PHE:O	2.33	0.62
1:A:169:SER:OG	1:A:173:ARG:NH1	2.33	0.61
1:B:2448:ASP:OD1	1:B:2449:GLU:N	2.33	0.61
1:A:1419:LEU:HD11	1:A:1464:VAL:HG23	1.81	0.61
1:B:280:ILE:HG23	1:B:348:LEU:HD22	1.81	0.61
1:B:1524:LEU:HD22	1:B:1538:VAL:HG23	1.81	0.61
1:A:2448:ASP:OD1	1:A:2449:GLU:N	2.33	0.61
1:A:1341:PRO:HG2	1:A:1417:LYS:HD2	1.82	0.61
1:A:329:ARG:NH2	1:A:407:PHE:O	2.33	0.61
1:B:1351:LEU:HB3	1:B:1441:ILE:HG22	1.83	0.61
1:A:896:LEU:HG	1:A:900:MET:HE1	1.82	0.61
1:B:1377:ASN:OD1	1:B:1379:PRO:HD2	2.01	0.60
1:B:1876:HIS:CE1	1:B:1900:CYS:H	2.20	0.60
1:B:825:PHE:O	1:B:940:LYS:NZ	2.34	0.60
1:B:1988:SER:OG	1:B:1992:LYS:NZ	2.34	0.60
1:B:248:ARG:HD2	1:B:652:PHE:CE1	2.37	0.59
1:B:2474:LEU:O	1:B:2515:LYS:NZ	2.35	0.59
1:A:248:ARG:HD2	1:A:652:PHE:CE1	2.37	0.59
1:A:2214:ASP:OD1	1:A:2746:ARG:NH1	2.36	0.59
1:B:617:MET:HA	1:B:682:VAL:HA	1.84	0.59
1:B:602:ASN:OD1	1:B:717:ARG:NH1	2.36	0.59
1:A:1876:HIS:CE1	1:A:1900:CYS:H	2.20	0.59
1:B:2531:MET:HE1	1:B:2537:PHE:HB3	1.84	0.58
1:A:2531:MET:HE1	1:A:2537:PHE:HB3	1.84	0.58
1:B:1412:PRO:HB2	1:B:1766:PRO:HA	1.85	0.58
1:A:2553:PRO:HG3	1:A:2613:ARG:NH1	2.18	0.58
1:B:205:LEU:HD12	1:B:209:PHE:HD2	1.68	0.58
1:B:1288:PRO:HA	1:B:1343:ILE:HG22	1.84	0.58
1:A:2474:LEU:O	1:A:2515:LYS:NZ	2.37	0.58
1:A:602:ASN:OD1	1:A:717:ARG:NH1	2.36	0.58
1:A:2896:GLN:HB3	1:A:2962:MET:HG2	1.84	0.58
1:B:1110:ALA:HB3	1:B:1372:LEU:HD21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1543:LYS:HG2	1:B:1547:ILE:HD12	1.85	0.58
1:B:1594:ILE:HG23	1:B:1647:LEU:HD12	1.84	0.58
1:A:205:LEU:HD12	1:A:209:PHE:HD2	1.68	0.57
1:A:1543:LYS:HG2	1:A:1547:ILE:HD12	1.86	0.57
1:B:938:PRO:HB3	1:B:976:VAL:HG22	1.86	0.57
1:B:2928:ARG:NH1	1:B:3033:ASN:OD1	2.37	0.57
1:A:1110:ALA:HB3	1:A:1372:LEU:HD21	1.86	0.57
1:A:2289:SER:HG	1:A:2291:TRP:CD1	2.22	0.57
1:B:2871:ARG:NH2	1:B:2875:ASN:O	2.37	0.57
1:A:2612:ARG:NH1	1:A:2613:ARG:HH21	2.03	0.57
1:B:898:LEU:HD21	1:B:945:HIS:HB3	1.86	0.57
1:A:747:GLN:OE1	1:A:750:LYS:NZ	2.38	0.57
1:A:2632:ASN:OD1	1:A:2763:ARG:NH2	2.36	0.57
1:B:747:GLN:OE1	1:B:750:LYS:NZ	2.38	0.57
1:A:941:SER:O	1:A:945:HIS:ND1	2.38	0.57
1:A:2871:ARG:NH2	1:A:2875:ASN:O	2.38	0.56
1:A:825:PHE:O	1:A:940:LYS:NZ	2.38	0.56
1:A:956:GLY:O	1:A:1000:ASN:ND2	2.30	0.56
1:A:2066:GLN:NE2	1:A:2070:ASN:OD1	2.37	0.56
1:B:925:ARG:HG2	1:B:929:MET:HE1	1.87	0.56
1:B:2531:MET:HE1	1:B:2537:PHE:H	1.70	0.56
1:B:956:GLY:O	1:B:1000:ASN:ND2	2.30	0.56
1:B:1223:ASN:OD1	1:B:1262:ARG:NH2	2.38	0.56
1:B:1446:VAL:HG11	1:B:1497:LEU:HD21	1.86	0.56
1:B:1499:SER:HA	1:B:1541:LEU:HD13	1.86	0.56
1:A:1098:GLN:HG3	1:A:1100:THR:HG23	1.88	0.56
1:A:773:ILE:HG21	1:A:892:LYS:HB3	1.87	0.56
1:B:609:GLU:HG2	1:B:724:GLY:HA3	1.88	0.56
1:B:957:GLU:HB2	1:B:999:LYS:HD3	1.87	0.56
1:A:609:GLU:HG2	1:A:724:GLY:HA3	1.88	0.56
1:A:617:MET:HA	1:A:682:VAL:HA	1.89	0.55
1:A:1656:LYS:NZ	1:A:2159:CYS:O	2.38	0.55
1:A:2693:ALA:HB3	1:A:2699:PRO:HG2	1.88	0.55
1:B:2827:PHE:O	1:B:2912:ARG:NH1	2.34	0.55
1:A:925:ARG:HG2	1:A:929:MET:HE1	1.88	0.55
1:A:1351:LEU:HB3	1:A:1441:ILE:HG22	1.89	0.55
1:B:1476:ILE:O	1:B:1479:ARG:NH1	2.38	0.55
1:A:2827:PHE:O	1:A:2912:ARG:NH1	2.34	0.55
1:A:2928:ARG:NH1	1:A:3033:ASN:OD1	2.37	0.55
1:B:1438:ILE:HA	1:B:1441:ILE:HG12	1.89	0.55
1:A:1223:ASN:OD1	1:A:1262:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2092:CYS:SG	1:B:2095:LEU:HD23	2.46	0.55
1:A:599:LEU:O	1:A:717:ARG:NE	2.39	0.55
1:B:2550:MET:HE1	1:B:2609:ILE:HA	1.88	0.55
1:A:1544:TYR:HA	1:A:1548:ASP:HB2	1.89	0.55
1:A:1680:PRO:O	1:A:2215:SER:OG	2.24	0.55
1:B:1098:GLN:HG3	1:B:1100:THR:HG23	1.88	0.55
1:A:1083:HIS:CE1	1:A:1087:MET:HE3	2.41	0.55
1:B:2480:HIS:HB3	1:B:2483:TRP:HD1	1.72	0.55
1:A:812:MET:SD	1:A:918:PHE:HB2	2.47	0.54
1:A:127:THR:O	1:A:133:ASN:ND2	2.40	0.54
1:A:938:PRO:HB3	1:A:976:VAL:HG22	1.88	0.54
1:B:127:THR:O	1:B:133:ASN:ND2	2.40	0.54
1:B:599:LEU:O	1:B:717:ARG:NE	2.39	0.54
1:B:655:THR:HA	1:B:1087:MET:HE1	1.89	0.54
1:B:734:VAL:HG12	1:B:735:ILE:HG13	1.88	0.54
1:B:812:MET:SD	1:B:918:PHE:HB2	2.47	0.54
1:B:2808:VAL:HG23	1:B:2811:LYS:HD2	1.90	0.54
1:B:1568:HIS:H	1:B:1575:ARG:NH2	2.06	0.54
1:B:2693:ALA:HB3	1:B:2699:PRO:HG2	1.89	0.54
1:A:2633:LEU:HB3	1:A:2700:LYS:HE2	1.89	0.54
1:A:1472:LEU:HD21	1:A:1497:LEU:HD23	1.89	0.54
1:B:2091:TRP:CZ2	1:B:2095:LEU:HB3	2.43	0.54
1:B:2336:GLU:OE2	1:B:2385:LYS:NZ	2.41	0.54
1:A:734:VAL:HG12	1:A:735:ILE:HG13	1.89	0.54
1:B:1310:GLN:HE21	1:B:1311:GLN:NE2	2.06	0.53
1:A:1310:GLN:HE21	1:A:1311:GLN:NE2	2.06	0.53
1:B:943:HIS:HA	1:B:946:MET:HE2	1.90	0.53
1:A:1830:MET:HE3	1:A:1830:MET:O	2.08	0.53
1:B:1875:ARG:HD2	1:B:1899:CYS:HB2	1.91	0.53
1:A:957:GLU:HB2	1:A:999:LYS:HD3	1.91	0.53
1:A:1568:HIS:H	1:A:1575:ARG:NH2	2.07	0.53
1:A:1231:LEU:HD11	1:A:1255:LEU:HD22	1.91	0.53
1:A:1875:ARG:HD2	1:A:1899:CYS:HB2	1.91	0.53
1:A:2203:ILE:HG22	1:A:2207:LYS:HE2	1.90	0.53
1:B:1718:LEU:HB3	1:B:1737:LEU:HD21	1.90	0.53
1:A:1082:HIS:HB3	1:A:1085:VAL:HG23	1.91	0.53
1:A:1438:ILE:HA	1:A:1441:ILE:HG12	1.90	0.53
1:A:2073:LEU:HD22	1:A:2076:ILE:HD12	1.89	0.53
1:B:2014:GLU:OE1	1:B:2017:SER:N	2.39	0.53
1:A:2612:ARG:HH12	1:A:2613:ARG:HH21	1.56	0.53
1:A:2715:LEU:HD23	1:A:2767:LEU:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2868:LEU:HG	1:A:2871:ARG:HD3	1.91	0.53
1:B:98:SER:OG	1:B:140:ASP:OD2	2.26	0.53
1:B:617:MET:SD	1:B:623:ALA:HB2	2.49	0.53
1:A:98:SER:OG	1:A:140:ASP:OD2	2.26	0.53
1:A:780:MET:HG2	1:A:900:MET:HA	1.91	0.53
1:A:1560:LYS:HG3	1:A:1582:LYS:HA	1.91	0.53
1:B:2745:THR:HG22	1:B:2750:LEU:HD12	1.91	0.53
1:B:466:GLN:OE1	1:B:484:TRP:NE1	2.38	0.52
1:B:2715:LEU:HD23	1:B:2767:LEU:HD11	1.90	0.52
1:A:530:SER:HA	1:A:533:ARG:HH22	1.74	0.52
1:B:1578:GLN:HA	1:B:1581:ILE:HG22	1.91	0.52
1:A:611:ILE:HA	1:A:624:MET:HE1	1.91	0.52
1:A:2235:MET:O	1:A:2244:ARG:NH2	2.42	0.52
1:B:2713:ARG:HD3	1:B:2771:THR:HG22	1.90	0.52
1:B:2073:LEU:HD22	1:B:2076:ILE:HD12	1.91	0.52
1:A:2713:ARG:HD3	1:A:2771:THR:HG22	1.91	0.52
1:B:2633:LEU:HB3	1:B:2700:LYS:HE2	1.91	0.52
1:A:1551:ASP:OD1	1:A:1551:ASP:N	2.42	0.52
1:B:2214:ASP:OD1	1:B:2746:ARG:NH1	2.42	0.52
1:A:2838:LYS:HE2	1:A:2880:GLU:HG2	1.92	0.52
1:A:1288:PRO:HA	1:A:1343:ILE:HG22	1.92	0.52
1:A:1340:LEU:HD23	1:A:1341:PRO:HD3	1.91	0.52
1:B:1547:ILE:HG12	1:B:1577:THR:HG21	1.91	0.51
1:B:2484:VAL:HG13	1:B:2519:LEU:HD21	1.92	0.51
1:B:1291:LEU:HD12	1:B:1343:ILE:HG21	1.93	0.51
1:B:2518:PRO:HB2	1:B:2734:MET:HE1	1.93	0.51
1:B:1544:TYR:HA	1:B:1548:ASP:HB2	1.92	0.51
1:A:245:VAL:HG12	1:A:1083:HIS:HB3	1.92	0.51
1:B:2402:GLU:OE2	1:B:2459:ARG:NE	2.34	0.51
1:B:2185:ILE:HG13	1:B:2230:ILE:HD12	1.92	0.51
1:B:1706:LYS:HE3	1:B:1710:TRP:HE1	1.75	0.51
1:B:1215:ASP:OD1	1:B:1258:HIS:NE2	2.32	0.51
1:B:2868:LEU:HG	1:B:2871:ARG:HD3	1.93	0.51
1:A:2026:MET:HE3	1:B:2307:LEU:HD13	1.92	0.50
1:A:112:ALA:H	1:A:114:ARG:NH1	2.09	0.50
1:A:1087:MET:HA	1:A:1090:ALA:HB3	1.94	0.50
1:A:2401:ILE:HG21	1:A:2459:ARG:HB2	1.92	0.50
1:A:2892:VAL:HG22	1:A:2962:MET:HE1	1.93	0.50
1:B:112:ALA:H	1:B:114:ARG:NH1	2.09	0.50
1:A:2546:SER:O	1:A:2550:MET:HG2	2.12	0.50
1:B:780:MET:HG2	1:B:900:MET:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1551:ASP:OD1	1:B:1551:ASP:N	2.42	0.50
1:B:1082:HIS:HB3	1:B:1085:VAL:HG23	1.94	0.50
1:B:1063:VAL:HG13	1:B:1064:MET:SD	2.52	0.50
1:B:1231:LEU:HD11	1:B:1255:LEU:HD22	1.94	0.50
1:A:466:GLN:OE1	1:A:484:TRP:NE1	2.39	0.49
1:A:1182:GLU:OE2	1:A:1229:TYR:OH	2.30	0.49
1:B:753:MET:HE1	1:B:808:THR:HG23	1.94	0.49
1:B:1472:LEU:HD11	1:B:1497:LEU:HD22	1.94	0.49
1:B:530:SER:HA	1:B:533:ARG:HH22	1.77	0.49
1:B:2730:GLN:O	1:B:2734:MET:HG2	2.11	0.49
1:A:1426:ALA:HB2	1:A:1438:ILE:HG21	1.95	0.49
1:A:1195:GLU:HG2	1:A:1206:LEU:HD22	1.95	0.49
1:A:1859:ARG:NE	1:A:1933:TRP:O	2.42	0.49
1:A:1706:LYS:HE3	1:A:1710:TRP:HE1	1.76	0.49
1:A:1063:VAL:HG13	1:A:1064:MET:SD	2.52	0.49
1:B:1195:GLU:HG2	1:B:1206:LEU:HD22	1.95	0.49
1:B:1351:LEU:HD12	1:B:1444:LEU:HD22	1.94	0.49
1:B:2152:VAL:O	1:B:2156:GLU:HG3	2.13	0.49
1:B:2719:ARG:HG3	1:B:2763:ARG:HH21	1.78	0.49
1:A:192:HIS:HA	1:A:235:ALA:HB2	1.95	0.49
1:A:1680:PRO:HG3	1:A:2174:SER:HB2	1.94	0.49
1:B:773:ILE:HG21	1:B:892:LYS:HB3	1.94	0.49
1:B:1182:GLU:OE2	1:B:1229:TYR:OH	2.30	0.49
1:A:18:ASP:O	1:A:23:ARG:NH1	2.46	0.49
1:A:2014:GLU:OE1	1:A:2017:SER:N	2.44	0.49
1:B:2401:ILE:HG21	1:B:2459:ARG:HB2	1.95	0.49
1:A:1322:LEU:HA	1:A:1327:LEU:HD12	1.95	0.49
1:A:2189:PHE:CE1	1:A:2237:LYS:HD3	2.48	0.49
1:A:2531:MET:HE1	1:A:2537:PHE:H	1.78	0.49
1:B:1322:LEU:HA	1:B:1327:LEU:HD12	1.95	0.49
1:B:1339:ASN:HB2	1:B:1342:GLU:OE1	2.13	0.49
1:A:94:MET:CE	1:A:137:TYR:HB2	2.43	0.48
1:A:655:THR:HA	1:A:1087:MET:HE1	1.94	0.48
1:A:970:LEU:HD11	1:A:997:VAL:HG11	1.95	0.48
1:A:1412:PRO:HB2	1:A:1766:PRO:HA	1.95	0.48
1:B:1949:ALA:HB1	1:B:2162:SER:HB2	1.96	0.48
1:B:2189:PHE:CE1	1:B:2237:LYS:HD3	2.48	0.48
1:A:284:GLN:NE2	1:A:351:ASP:OD2	2.45	0.48
1:A:434:PRO:HA	1:A:437:MET:HE2	1.94	0.48
1:A:1959:GLU:OE2	1:A:2849:ARG:NH1	2.44	0.48
1:B:94:MET:CE	1:B:137:TYR:HB2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:MET:HE1	1:A:808:THR:HG23	1.94	0.48
1:A:2942:GLN:HA	1:A:3017:LEU:HD13	1.96	0.48
1:B:18:ASP:O	1:B:23:ARG:NH1	2.46	0.48
1:B:970:LEU:HD11	1:B:997:VAL:HG11	1.96	0.48
1:B:2229:VAL:O	1:B:2233:ILE:HG12	2.12	0.48
1:A:1295:LEU:HD13	1:A:1393:ILE:HD11	1.95	0.48
1:A:2722:LEU:HD13	1:A:2767:LEU:HD23	1.95	0.48
1:B:2838:LYS:HE2	1:B:2880:GLU:HG2	1.94	0.48
1:B:192:HIS:HA	1:B:235:ALA:HB2	1.95	0.48
1:A:2924:GLU:OE2	1:A:2928:ARG:NH2	2.44	0.48
1:B:780:MET:HE3	1:B:900:MET:HB3	1.95	0.48
1:B:1824:LEU:HD13	1:B:1845:LEU:HD23	1.96	0.48
1:B:2924:GLU:OE2	1:B:2928:ARG:NH2	2.44	0.48
1:A:943:HIS:HA	1:A:946:MET:HE2	1.96	0.48
1:A:3015:GLU:HB2	1:A:3020:VAL:HB	1.95	0.48
1:B:1560:LYS:HG3	1:B:1582:LYS:HA	1.95	0.48
1:A:2158:MET:HA	1:A:2158:MET:HE2	1.96	0.48
1:A:2402:GLU:OE2	1:A:2459:ARG:NE	2.39	0.48
1:A:2721:ASP:OD2	1:A:2724:GLN:NE2	2.43	0.48
1:B:1340:LEU:HD12	1:B:1343:ILE:HD11	1.94	0.48
1:A:1087:MET:O	1:A:1091:GLU:N	2.35	0.48
1:A:2444:GLU:OE1	1:B:2901:PRO:HB3	2.13	0.48
1:B:1376:PRO:HG2	1:B:1380:HIS:CD2	2.49	0.48
1:B:1796:ILE:HG23	1:B:1798:LEU:HD23	1.96	0.47
1:B:2778:GLU:O	1:B:2782:ASN:HB2	2.14	0.47
1:A:706:SER:N	1:A:710:THR:OG1	2.47	0.47
1:B:1295:LEU:HD13	1:B:1393:ILE:HD11	1.95	0.47
1:B:1491:PHE:HZ	1:B:1527:LEU:HD22	1.79	0.47
1:A:2745:THR:HG22	1:A:2750:LEU:HD12	1.95	0.47
1:B:1680:PRO:HG3	1:B:2174:SER:HB2	1.96	0.47
1:A:1215:ASP:OD1	1:A:1258:HIS:NE2	2.40	0.47
1:A:2224:MET:HE2	1:A:2261:LEU:HD22	1.96	0.47
1:B:2520:MET:HE3	1:B:2524:ALA:HB2	1.96	0.47
1:B:3012:ARG:NH1	1:B:3015:GLU:OE2	2.45	0.47
1:A:427:LEU:O	1:A:469:ARG:NH2	2.35	0.47
1:A:700:GLN:NE2	1:A:704:ASN:OD1	2.47	0.47
1:A:898:LEU:HD21	1:A:945:HIS:HB3	1.97	0.47
1:A:1413:ASP:OD1	1:A:1413:ASP:N	2.46	0.47
1:A:1796:ILE:HG23	1:A:1798:LEU:HD23	1.96	0.47
1:A:2352:ASN:HB3	1:B:3037:GLN:NE2	2.29	0.47
1:B:700:GLN:NE2	1:B:704:ASN:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2449:GLU:OE1	1:A:2453:ARG:NH2	2.36	0.47
1:A:3021:GLU:OE2	1:A:3031:GLN:NE2	2.44	0.47
1:B:1628:MET:HE2	1:B:2211:LEU:HD13	1.97	0.47
1:A:1628:MET:HE2	1:A:2211:LEU:HD13	1.97	0.47
1:A:2209:SER:HG	1:A:2227:ARG:HH12	1.61	0.47
1:A:2962:MET:SD	1:A:2966:LYS:HD2	2.54	0.47
1:A:1259:LEU:HB3	1:A:1264:HIS:HB2	1.96	0.47
1:A:1640:GLN:O	1:A:1689:GLN:NE2	2.48	0.47
1:A:2520:MET:HE1	1:A:2545:ILE:HG23	1.97	0.47
1:B:284:GLN:NE2	1:B:351:ASP:OD2	2.46	0.47
1:B:1473:ILE:HD11	1:B:1520:ILE:HG22	1.96	0.47
1:A:2311:ILE:HD11	1:B:2027:LEU:HD11	1.97	0.46
1:B:1821:CYS:SG	1:B:1823:ILE:HG12	2.54	0.46
1:A:1491:PHE:HZ	1:A:1527:LEU:HD22	1.80	0.46
1:A:1339:ASN:HB2	1:A:1342:GLU:OE1	2.14	0.46
1:A:2335:THR:HG21	1:A:2368:ALA:HB2	1.97	0.46
1:A:2778:GLU:O	1:A:2782:ASN:HB2	2.15	0.46
1:B:706:SER:N	1:B:710:THR:OG1	2.47	0.46
1:A:207:SER:HB2	1:A:243:LEU:HD21	1.97	0.46
1:A:2336:GLU:OE2	1:A:2385:LYS:NZ	2.39	0.46
1:B:448:HIS:CE1	1:B:497:SER:HG	2.29	0.46
1:B:1711:THR:HG22	1:B:1823:ILE:HG21	1.97	0.46
1:A:2550:MET:HE1	1:A:2612:ARG:HD3	1.97	0.46
1:B:1413:ASP:OD1	1:B:1413:ASP:N	2.47	0.46
1:B:1640:GLN:O	1:B:1689:GLN:NE2	2.48	0.46
1:B:2936:GLU:HG3	1:B:3028:VAL:HG11	1.97	0.46
1:A:448:HIS:CE1	1:A:497:SER:HG	2.30	0.46
1:A:1499:SER:HA	1:A:1541:LEU:HD13	1.96	0.46
1:A:2081:LEU:HD13	1:A:2099:HIS:HD1	1.81	0.46
1:B:1457:LEU:HD22	1:B:1464:VAL:HG11	1.98	0.46
1:B:1606:LEU:HD23	1:B:1609:THR:HG23	1.98	0.46
1:A:1451:LYS:O	1:A:1454:LYS:NZ	2.42	0.46
1:A:1578:GLN:HA	1:A:1581:ILE:HG22	1.97	0.45
1:A:2936:GLU:HG3	1:A:3028:VAL:HG11	1.98	0.45
1:B:1336:PHE:HZ	1:B:1393:ILE:HG23	1.80	0.45
1:B:1568:HIS:H	1:B:1575:ARG:HH22	1.64	0.45
1:B:2522:GLN:HG2	1:B:2951:VAL:HG12	1.98	0.45
1:A:2808:VAL:HG23	1:A:2811:LYS:HD2	1.98	0.45
1:A:604:PRO:HB2	1:A:607:VAL:HG21	1.97	0.45
1:B:1656:LYS:NZ	1:B:2159:CYS:O	2.34	0.45
1:A:1949:ALA:HB1	1:A:2162:SER:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:PHE:CE2	1:B:212:PHE:HB3	2.52	0.45
1:B:1040:MET:SD	1:B:1085:VAL:HG22	2.57	0.45
1:B:1435:LYS:HA	1:B:1438:ILE:HG12	1.98	0.45
1:B:773:ILE:HG12	1:B:896:LEU:HD22	1.99	0.45
1:B:1389:THR:O	1:B:1393:ILE:HG12	2.16	0.45
1:B:2224:MET:HE2	1:B:2261:LEU:HD22	1.99	0.45
1:A:1921:ARG:HA	1:A:1933:TRP:CZ2	2.51	0.45
1:B:3021:GLU:OE2	1:B:3031:GLN:NE2	2.46	0.45
1:A:172:PHE:CE2	1:A:212:PHE:HB3	2.52	0.45
1:A:1821:CYS:SG	1:A:1823:ILE:HG12	2.57	0.45
1:B:323:ILE:O	1:B:329:ARG:NH1	2.50	0.45
1:B:604:PRO:HB2	1:B:607:VAL:HG21	1.97	0.45
1:B:2755:TYR:HB2	1:B:2768:GLU:HB3	1.98	0.45
1:A:543:THR:HB	1:A:611:ILE:HD11	1.99	0.45
1:A:648:VAL:HG12	1:A:652:PHE:CE2	2.52	0.45
1:A:1568:HIS:H	1:A:1575:ARG:HH22	1.64	0.45
1:A:2459:ARG:NH2	1:A:2494:ASN:OD1	2.50	0.45
1:B:2721:ASP:OD2	1:B:2724:GLN:NE2	2.47	0.45
1:A:1291:LEU:HD12	1:A:1343:ILE:HG21	1.99	0.44
1:A:1434:LYS:O	1:A:1437:ARG:HG2	2.16	0.44
1:B:1633:ARG:HG2	1:B:1633:ARG:HH11	1.82	0.44
1:A:1718:LEU:HB3	1:A:1737:LEU:HD21	1.99	0.44
1:A:2755:TYR:HB2	1:A:2768:GLU:HB3	1.98	0.44
1:B:207:SER:HB2	1:B:243:LEU:HD21	1.98	0.44
1:A:1336:PHE:HZ	1:A:1393:ILE:HG23	1.82	0.44
1:A:2901:PRO:HB3	1:B:2444:GLU:OE1	2.17	0.44
1:B:648:VAL:HG12	1:B:652:PHE:CE2	2.52	0.44
1:B:1564:PRO:HA	1:B:1578:GLN:OE1	2.17	0.44
1:B:2736:ASN:OD1	1:B:2752:ILE:N	2.45	0.44
1:A:266:TRP:CG	1:A:318:LEU:HD21	2.52	0.44
1:A:323:ILE:O	1:A:329:ARG:NH1	2.50	0.44
1:B:2953:LEU:HD12	1:B:3010:LEU:HG	1.99	0.44
1:A:117:CYS:HB2	1:A:155:TYR:CD1	2.53	0.44
1:A:749:ALA:HB1	1:A:806:LEU:HD11	2.00	0.44
1:A:1745:THR:OG1	1:A:1822:GLU:OE2	2.28	0.44
1:B:266:TRP:CG	1:B:318:LEU:HD21	2.52	0.44
1:A:1476:ILE:O	1:A:1479:ARG:NH1	2.44	0.44
1:B:495:ILE:HG21	1:B:526:LEU:HD21	1.99	0.44
1:A:1389:THR:O	1:A:1393:ILE:HG12	2.17	0.44
1:A:1176:LEU:O	1:A:1180:VAL:HG23	2.19	0.43
1:B:117:CYS:HB2	1:B:155:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ILE:HA	1:B:155:TYR:HD2	1.83	0.43
1:B:996:HIS:O	1:B:999:LYS:HG2	2.18	0.43
1:B:1194:LEU:HA	1:B:1197:VAL:HG12	2.00	0.43
1:A:403:SER:HB2	1:A:409:LEU:HD13	2.01	0.43
1:A:775:SER:O	1:A:779:MET:HG2	2.18	0.43
1:A:1510:LYS:HG2	1:A:1552:ASN:HD21	1.81	0.43
1:B:595:VAL:HG13	1:B:600:HIS:HB2	2.00	0.43
1:B:749:ALA:HB1	1:B:806:LEU:HD11	2.00	0.43
1:B:1080:ASP:O	1:B:1086:ARG:NE	2.52	0.43
1:B:1176:LEU:O	1:B:1180:VAL:HG23	2.18	0.43
1:A:2600:GLU:OE2	1:A:2604:ARG:NH2	2.51	0.43
1:B:527:PHE:HE1	1:B:538:ALA:HB1	1.82	0.43
1:A:213:PHE:CG	1:A:236:LEU:HD13	2.53	0.43
1:A:1961:TYR:CE2	1:A:2001:LEU:HD12	2.54	0.43
1:B:431:GLU:C	1:B:434:PRO:HD2	2.43	0.43
1:A:1873:CYS:HA	1:A:1901:LEU:HD13	2.01	0.43
1:A:1918:ARG:HG2	1:A:2840:LEU:HD13	2.01	0.43
1:A:2092:CYS:SG	1:A:2095:LEU:HD23	2.58	0.43
1:A:3004:LYS:HD2	1:A:3008:ARG:HH21	1.83	0.43
1:A:1036:PHE:CD2	1:A:1040:MET:HE1	2.54	0.43
1:A:2730:GLN:O	1:A:2734:MET:HG2	2.19	0.43
1:B:2722:LEU:HD13	1:B:2767:LEU:HD23	2.00	0.43
1:A:2872:HIS:CE1	1:A:2874:GLN:HB2	2.54	0.43
1:B:74:CYS:O	1:B:90:ARG:NH1	2.45	0.43
1:B:213:PHE:CG	1:B:236:LEU:HD13	2.53	0.43
1:B:403:SER:HB2	1:B:409:LEU:HD13	2.01	0.43
1:B:661:ASP:O	1:B:664:THR:OG1	2.33	0.43
1:B:775:SER:O	1:B:779:MET:HG2	2.19	0.43
1:B:1873:CYS:HA	1:B:1901:LEU:HD13	2.01	0.43
1:A:996:HIS:O	1:A:999:LYS:HG2	2.18	0.43
1:B:248:ARG:HD2	1:B:652:PHE:CD1	2.54	0.43
1:B:1287:PHE:HD1	1:B:1290:ILE:HD11	1.84	0.43
1:B:2459:ARG:NH2	1:B:2494:ASN:OD1	2.51	0.43
1:B:3015:GLU:HB2	1:B:3020:VAL:HB	1.99	0.43
1:A:405:ASN:OD1	1:A:405:ASN:N	2.52	0.43
1:A:2312:LEU:HD12	1:A:2312:LEU:HA	1.88	0.43
1:B:1093:ILE:HG21	1:B:1157:LEU:HD12	2.01	0.43
1:B:2109:TRP:HH2	1:B:2132:LEU:HD13	1.84	0.43
1:B:405:ASN:OD1	1:B:405:ASN:N	2.52	0.42
1:B:1510:LYS:HG2	1:B:1552:ASN:HD21	1.83	0.42
1:B:2731:VAL:HG11	1:B:2866:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1194:LEU:HA	1:A:1197:VAL:HG12	2.00	0.42
1:A:1266:ASP:OD1	1:A:1267:GLU:N	2.52	0.42
1:A:1630:ASP:OD1	1:A:1633:ARG:NH2	2.46	0.42
1:B:2942:GLN:NE2	1:B:3018:LYS:HG3	2.30	0.42
1:A:68:ILE:HD12	1:A:97:ILE:HD12	2.01	0.42
1:A:1299:ALA:HB2	1:A:1392:TYR:HB2	2.02	0.42
1:A:2107:MET:HG2	1:A:2109:TRP:CZ2	2.54	0.42
1:B:814:ASP:O	1:B:818:ILE:HG13	2.20	0.42
1:B:1531:GLN:OE1	1:B:1533:GLU:HB3	2.18	0.42
1:A:248:ARG:HD2	1:A:652:PHE:CD1	2.55	0.42
1:A:657:PHE:CZ	1:A:1155:LEU:HB3	2.54	0.42
1:A:1111:LEU:H	1:A:1116:GLN:HE21	1.67	0.42
1:A:1859:ARG:NH2	1:A:1932:PHE:O	2.45	0.42
1:A:1922:PRO:HD3	1:A:1933:TRP:CH2	2.55	0.42
1:A:2717:LYS:HD3	1:A:2722:LEU:HD21	2.01	0.42
1:B:748:LYS:HA	1:B:748:LYS:HD3	1.88	0.42
1:B:1398:LYS:H	1:B:1398:LYS:HG2	1.69	0.42
1:B:2872:HIS:CE1	1:B:2874:GLN:HB2	2.54	0.42
1:A:1754:LYS:HG3	1:A:1755:MET:HE2	2.02	0.42
1:B:2529:THR:O	1:B:2532:MET:HG2	2.20	0.42
1:A:431:GLU:C	1:A:434:PRO:HD2	2.44	0.42
1:A:804:LEU:HD13	1:A:911:ALA:HA	2.01	0.42
1:A:1350:THR:HB	1:A:1380:HIS:HA	2.00	0.42
1:A:2006:LEU:O	1:A:2010:ARG:HG3	2.19	0.42
1:A:2933:LYS:HA	1:A:2933:LYS:HD3	1.85	0.42
1:B:62:ARG:HA	1:B:65:GLN:HB2	2.01	0.42
1:B:68:ILE:HD12	1:B:97:ILE:HD12	2.01	0.42
1:A:102:LYS:HZ1	1:A:106:LYS:HD3	1.82	0.42
1:A:595:VAL:HG13	1:A:600:HIS:HB2	2.01	0.42
1:A:753:MET:HE2	1:A:807:LEU:HA	2.02	0.42
1:A:814:ASP:O	1:A:818:ILE:HG13	2.20	0.42
1:A:1127:ALA:O	1:A:1131:MET:HG2	2.20	0.42
1:A:2010:ARG:HG2	1:A:2018:LEU:HD11	2.02	0.42
1:B:657:PHE:CZ	1:B:1155:LEU:HB3	2.54	0.42
1:B:1777:VAL:HG21	1:B:1822:GLU:HB2	2.02	0.42
1:A:618:LYS:HG2	1:A:683:HIS:CD2	2.55	0.42
1:A:1989:LEU:HD22	1:A:2001:LEU:HD13	2.02	0.42
1:A:2723:ARG:O	1:A:2727:VAL:HG23	2.19	0.42
1:B:349:MET:HE3	1:B:353:CYS:SG	2.60	0.42
1:B:753:MET:HE2	1:B:807:LEU:HA	2.02	0.42
1:B:1449:LEU:HD22	1:B:1457:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2209:SER:HG	1:B:2227:ARG:HH12	1.64	0.42
1:B:2235:MET:O	1:B:2244:ARG:NH2	2.53	0.42
1:A:149:ILE:HA	1:A:155:TYR:HD2	1.83	0.42
1:A:495:ILE:HG21	1:A:526:LEU:HD21	2.00	0.42
1:A:1093:ILE:HG21	1:A:1157:LEU:HD12	2.01	0.42
1:A:2517:LEU:N	1:A:2518:PRO:HD2	2.35	0.42
1:A:2909:ARG:HG3	1:A:3052:TRP:CZ2	2.55	0.42
1:B:1036:PHE:CD2	1:B:1040:MET:HE1	2.55	0.42
1:B:1959:GLU:OE2	1:B:2849:ARG:NH1	2.44	0.42
1:A:928:LEU:HD11	1:A:965:ASP:CG	2.45	0.41
1:A:1531:GLN:OE1	1:A:1533:GLU:HB3	2.20	0.41
1:A:1606:LEU:HD23	1:A:1609:THR:HG23	2.02	0.41
1:A:1777:VAL:HG21	1:A:1822:GLU:HB2	2.02	0.41
1:A:2016:ASP:HB3	1:A:2926:VAL:HA	2.02	0.41
1:B:611:ILE:HA	1:B:624:MET:HE1	2.01	0.41
1:B:2663:VAL:HG21	1:B:2680:LEU:HD13	2.02	0.41
1:B:2865:ILE:HD13	1:B:2865:ILE:HA	1.92	0.41
1:B:2933:LYS:HA	1:B:2933:LYS:HD3	1.85	0.41
1:A:984:GLN:HB3	1:A:1035:ILE:HG12	2.02	0.41
1:A:1046:LEU:HD22	1:A:1074:PHE:HD1	1.84	0.41
1:A:1289:LYS:O	1:A:1293:ASN:ND2	2.52	0.41
1:A:1524:LEU:HD23	1:A:1527:LEU:HD12	2.02	0.41
1:A:3001:SER:HB3	1:A:3004:LYS:HG2	2.01	0.41
1:B:245:VAL:HG12	1:B:1083:HIS:HB3	2.02	0.41
1:B:928:LEU:HD11	1:B:965:ASP:CG	2.45	0.41
1:B:1299:ALA:HB2	1:B:1392:TYR:HB2	2.01	0.41
1:B:1449:LEU:HD23	1:B:1449:LEU:HA	1.91	0.41
1:A:250:ARG:HA	1:A:250:ARG:HD2	1.84	0.41
1:A:2807:GLU:O	1:A:2811:LYS:NZ	2.53	0.41
1:A:3008:ARG:HH12	1:B:2408:SER:CB	2.33	0.41
1:B:940:LYS:HD3	1:B:943:HIS:CD2	2.55	0.41
1:B:2743:THR:HG22	1:B:2746:ARG:HH12	1.85	0.41
1:A:62:ARG:HA	1:A:65:GLN:HB2	2.02	0.41
1:A:1001:LEU:HD21	1:A:1015:GLN:HA	2.01	0.41
1:A:1287:PHE:HD1	1:A:1290:ILE:HD11	1.85	0.41
1:A:1962:ALA:HB2	1:A:2001:LEU:HD11	2.01	0.41
1:B:790:CYS:SG	1:B:792:LYS:HG2	2.60	0.41
1:B:1046:LEU:HD22	1:B:1074:PHE:HD1	1.85	0.41
1:B:2449:GLU:OE1	1:B:2453:ARG:NH2	2.38	0.41
1:B:2499:GLU:O	1:B:2503:MET:HG3	2.21	0.41
1:A:790:CYS:SG	1:A:792:LYS:HG2	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2877:LEU:HB2	1:A:2886:VAL:HB	2.03	0.41
1:A:74:CYS:O	1:A:90:ARG:NH1	2.45	0.41
1:A:121:LEU:O	1:A:125:MET:HG2	2.20	0.41
1:A:784:THR:HG23	1:A:906:LEU:HD12	2.03	0.41
1:A:1040:MET:SD	1:A:1085:VAL:HG22	2.60	0.41
1:A:1715:LEU:HD22	1:A:1737:LEU:HD13	2.02	0.41
1:A:1961:TYR:CD2	1:A:2001:LEU:HD12	2.55	0.41
1:A:2782:ASN:ND2	1:A:2785:ASP:OD1	2.54	0.41
1:B:427:LEU:O	1:B:469:ARG:NH2	2.34	0.41
1:B:804:LEU:HD13	1:B:911:ALA:HA	2.02	0.41
1:B:1289:LYS:O	1:B:1293:ASN:ND2	2.52	0.41
1:A:409:LEU:HD23	1:A:451:ARG:HD3	2.03	0.41
1:A:1449:LEU:HD23	1:A:1449:LEU:HA	1.90	0.41
1:B:784:THR:HG23	1:B:906:LEU:HD12	2.03	0.41
1:B:984:GLN:HB3	1:B:1035:ILE:HG12	2.02	0.41
1:A:1620:GLN:O	1:A:1624:HIS:HB2	2.21	0.41
1:B:1075:THR:O	1:B:1126:LYS:HG2	2.20	0.41
1:B:1158:ILE:HG21	1:B:1176:LEU:HB2	2.03	0.41
1:B:1186:GLU:HB2	1:B:1189:LEU:HB2	2.02	0.41
1:B:2805:MET:HG3	1:B:3055:TRP:CZ3	2.56	0.41
1:B:812:MET:HB2	1:B:923:ILE:HD11	2.03	0.41
1:B:1111:LEU:H	1:B:1116:GLN:HE21	1.67	0.41
1:B:2016:ASP:HB3	1:B:2926:VAL:HA	2.02	0.41
1:B:2030:ILE:HD12	1:B:2030:ILE:H	1.86	0.41
1:A:1824:LEU:HD13	1:A:1845:LEU:HD23	2.02	0.41
1:A:2805:MET:O	1:A:2809:GLN:HG2	2.21	0.41
1:B:1001:LEU:HD21	1:B:1015:GLN:HA	2.01	0.41
1:A:3043:LYS:O	1:A:3046:SER:OG	2.40	0.40
1:A:152:VAL:HG12	1:A:154:LYS:H	1.86	0.40
1:A:897:PHE:HA	1:A:900:MET:SD	2.61	0.40
1:A:923:ILE:O	1:A:927:LEU:HG	2.20	0.40
1:A:1186:GLU:HB2	1:A:1189:LEU:HB2	2.03	0.40
1:B:152:VAL:HG12	1:B:154:LYS:H	1.86	0.40
1:B:1706:LYS:HE3	1:B:1710:TRP:NE1	2.36	0.40
1:A:743:SER:O	1:A:747:GLN:HG2	2.22	0.40
1:A:812:MET:HB2	1:A:923:ILE:HD11	2.04	0.40
1:A:897:PHE:HE2	1:A:946:MET:HE3	1.87	0.40
1:A:1939:LEU:HD23	1:A:1997:THR:HG21	2.03	0.40
1:B:1266:ASP:OD1	1:B:1267:GLU:N	2.54	0.40
1:B:1845:LEU:O	1:B:1849:ILE:HG12	2.21	0.40
1:A:190:ILE:O	1:A:194:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:MET:HE3	1:A:353:CYS:SG	2.60	0.40
1:A:753:MET:O	1:A:757:GLY:N	2.55	0.40
1:A:1291:LEU:O	1:A:1295:LEU:HB2	2.22	0.40
1:B:2782:ASN:ND2	1:B:2785:ASP:OD1	2.54	0.40
1:A:1616:ASP:O	1:A:1620:GLN:HG2	2.21	0.40
1:A:1713:ILE:HG22	1:A:1714:MET:HE2	2.02	0.40
1:A:2030:ILE:H	1:A:2030:ILE:HD12	1.87	0.40
1:A:2049:TYR:CZ	1:A:2063:GLY:HA3	2.56	0.40
1:A:2049:TYR:HB3	1:A:2064:ILE:HG13	2.04	0.40
1:B:121:LEU:O	1:B:125:MET:HG2	2.21	0.40
1:B:1082:HIS:HD2	1:B:1084:GLN:HB3	1.86	0.40
1:B:1341:PRO:HG3	1:B:1414:SER:HB2	2.03	0.40
1:B:1472:LEU:HD11	1:B:1497:LEU:CD2	2.51	0.40
1:B:1616:ASP:O	1:B:1620:GLN:HG2	2.21	0.40
1:B:1806:ILE:HG13	1:B:1838:CYS:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	2734/3184 (86%)	2684 (98%)	50 (2%)	0	100	100
1	B	2734/3184 (86%)	2687 (98%)	47 (2%)	0	100	100
All	All	5468/6368 (86%)	5371 (98%)	97 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2467/2883 (86%)	2467 (100%)	0	100	100
1	B	2467/2883 (86%)	2467 (100%)	0	100	100
All	All	4934/5766 (86%)	4934 (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 (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
1	A	246	ASN
1	A	445	GLN
1	A	700	GLN
1	A	893	GLN
1	A	975	ASN
1	A	1117	GLN
1	A	1128	GLN
1	A	1310	GLN
1	A	1352	HIS
1	A	1578	GLN
1	A	1596	HIS
1	A	1906	GLN
1	A	1946	GLN
1	A	2066	GLN
1	A	2111	HIS
1	A	2206	GLN
1	A	2280	GLN
1	A	2658	ASN
1	A	2684	GLN
1	A	2714	GLN
1	A	2802	GLN
1	A	2874	GLN
1	A	3014	GLN
1	B	118	GLN
1	B	201	GLN
1	B	246	ASN
1	B	445	GLN
1	B	700	GLN

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Mol	Chain	Res	Type
1	B	975	ASN
1	B	1076	GLN
1	B	1117	GLN
1	B	1128	GLN
1	B	1230	ASN
1	B	1310	GLN
1	B	1352	HIS
1	B	1380	HIS
1	B	1416	GLN
1	B	1847	HIS
1	B	1906	GLN
1	B	2066	GLN
1	B	2075	HIS
1	B	2125	HIS
1	B	2280	GLN
1	B	2314	GLN
1	B	2658	ASN
1	B	2684	GLN
1	B	2730	GLN
1	B	2802	GLN
1	B	2874	GLN
1	B	2942	GLN
1	B	3014	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ANP	A	3101	-	33,33,33	0.94	4 (12%)	45,52,52	0.59	0
2	ANP	B	3101	-	33,33,33	0.93	4 (12%)	45,52,52	0.58	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ANP	A	3101	-	-	1/18/38/38	0/3/3/3
2	ANP	B	3101	-	-	1/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3101	ANP	PG-O1G	2.55	1.50	1.46
2	B	3101	ANP	PG-O1G	2.55	1.50	1.46
2	A	3101	ANP	PG-N3B	2.43	1.69	1.63
2	B	3101	ANP	PG-N3B	2.43	1.69	1.63
2	B	3101	ANP	PB-O1B	2.42	1.49	1.46
2	A	3101	ANP	PB-O1B	2.41	1.49	1.46
2	B	3101	ANP	PB-O3A	-2.31	1.56	1.59
2	A	3101	ANP	PB-O3A	-2.30	1.56	1.59

There are no bond angle outliers.

There are no chirality outliers.

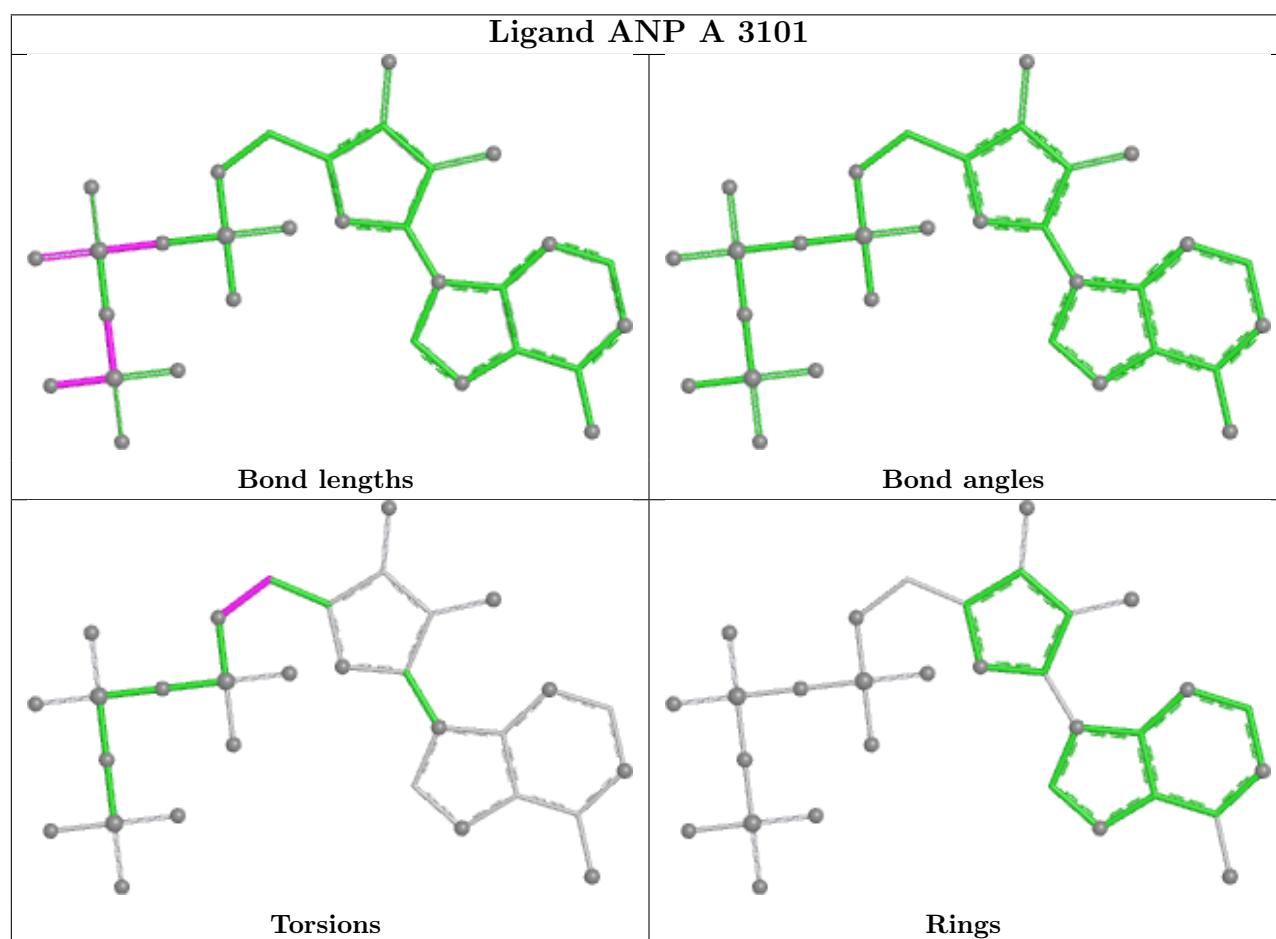
All (2) torsion outliers are listed below:

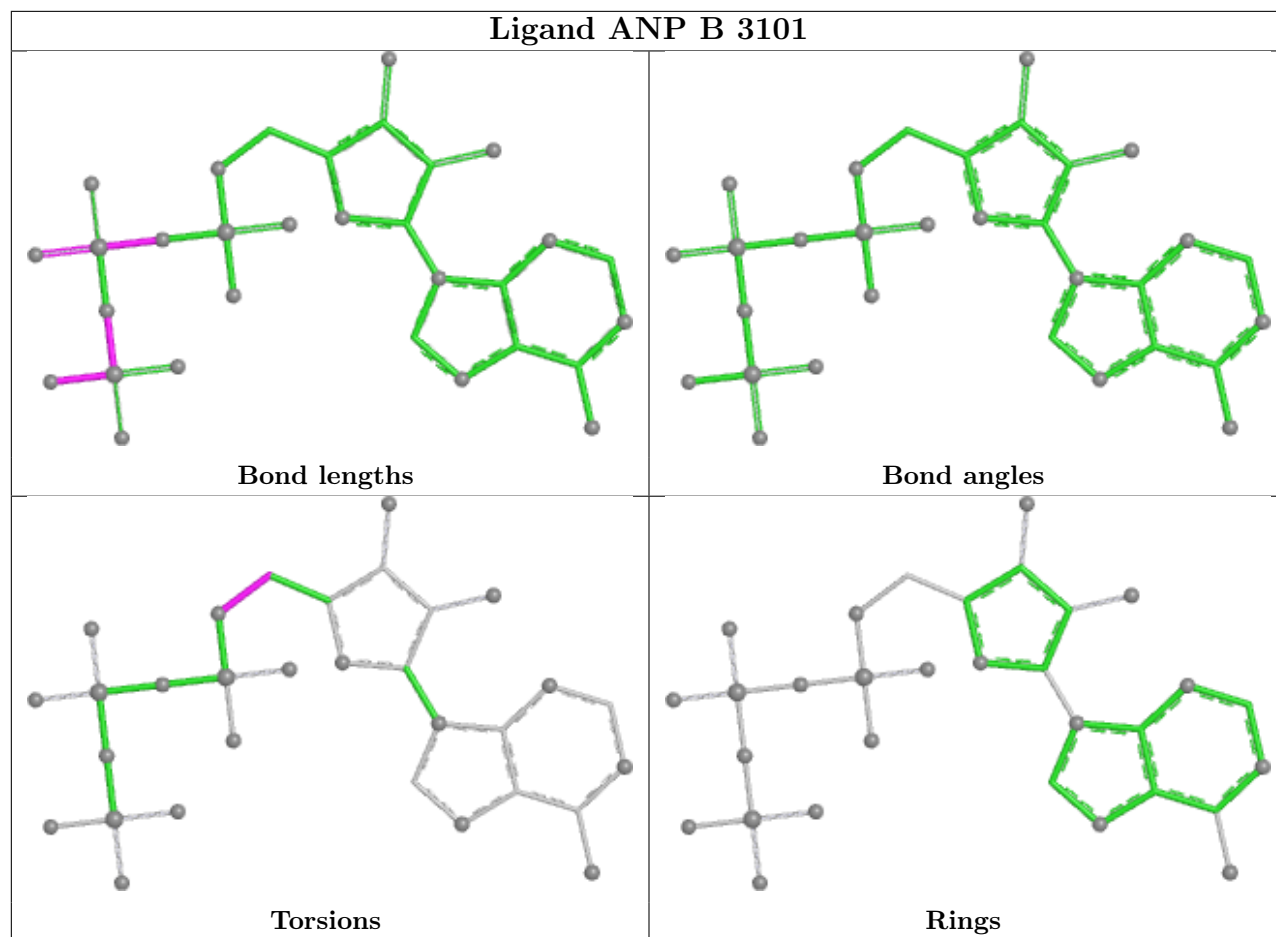
Mol	Chain	Res	Type	Atoms
2	A	3101	ANP	C4'-C5'-O5'-PA
2	B	3101	ANP	C4'-C5'-O5'-PA

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

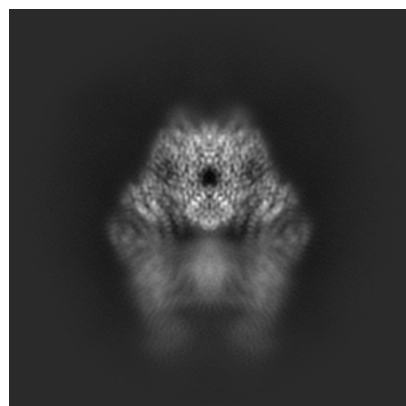
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17267. These allow visual inspection of the internal detail of the map and identification of artifacts.

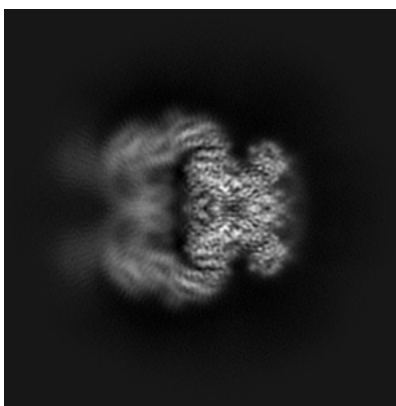
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

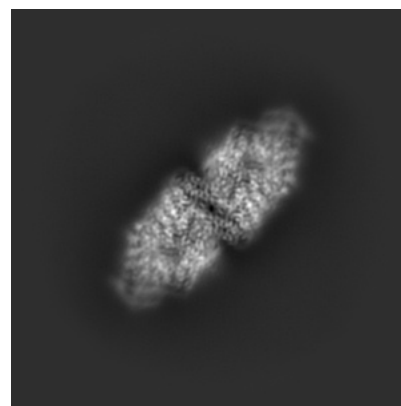
6.1.1 Primary map



X

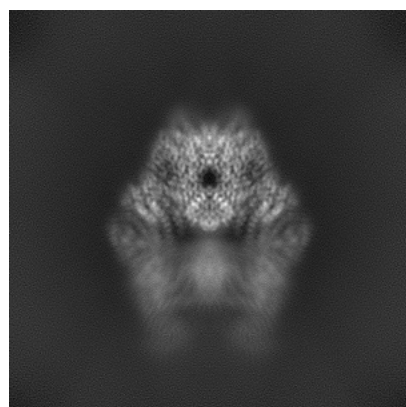


Y

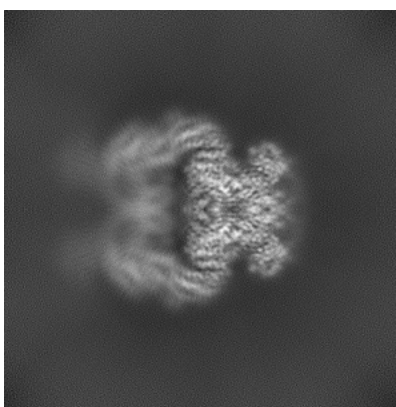


Z

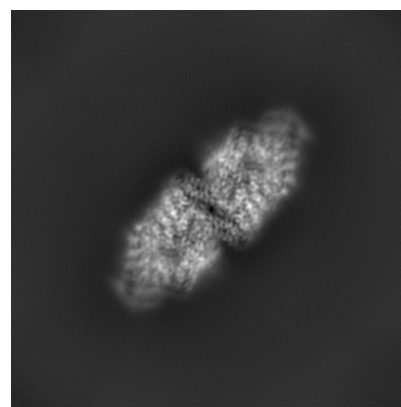
6.1.2 Raw map



X



Y

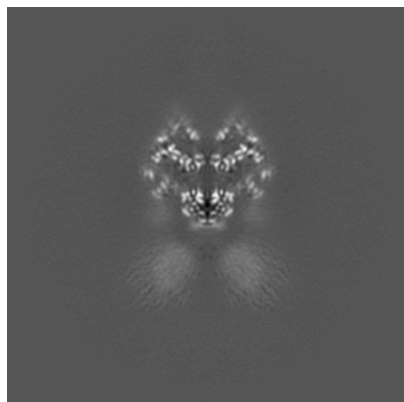


Z

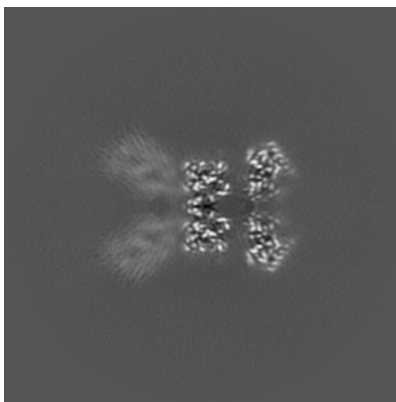
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

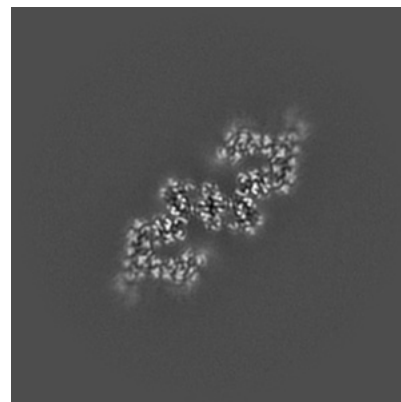
6.2.1 Primary map



X Index: 200

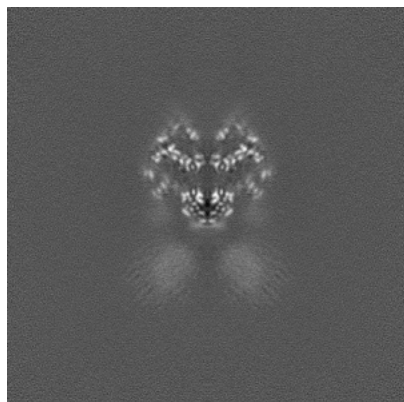


Y Index: 200

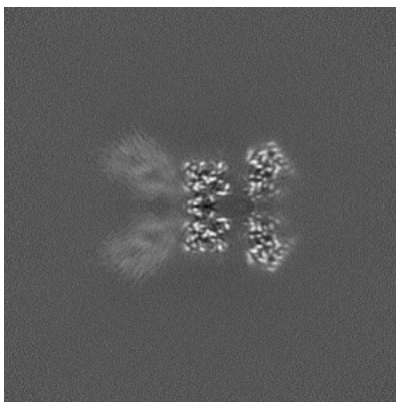


Z Index: 200

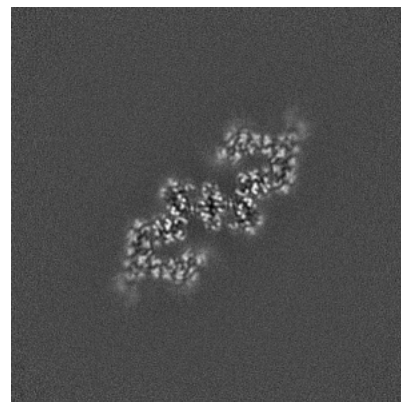
6.2.2 Raw map



X Index: 200



Y Index: 200

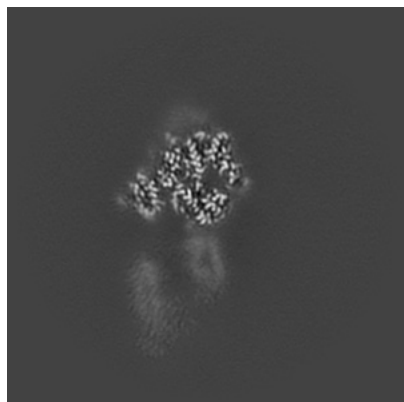


Z Index: 200

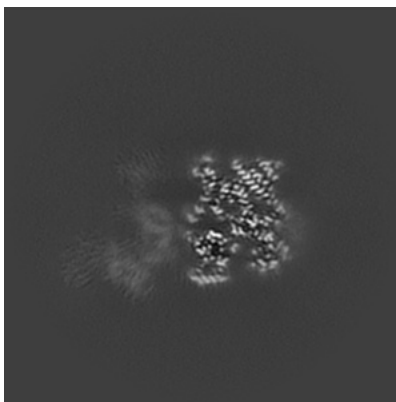
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

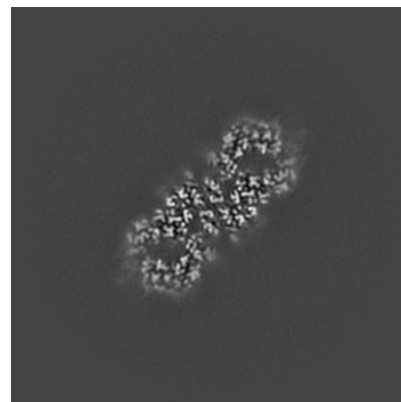
6.3.1 Primary map



X Index: 171

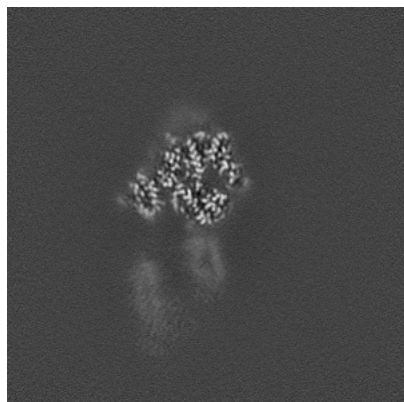


Y Index: 182

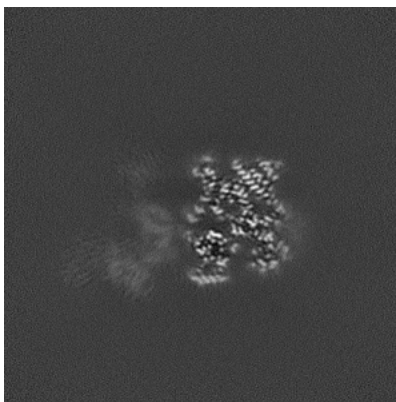


Z Index: 211

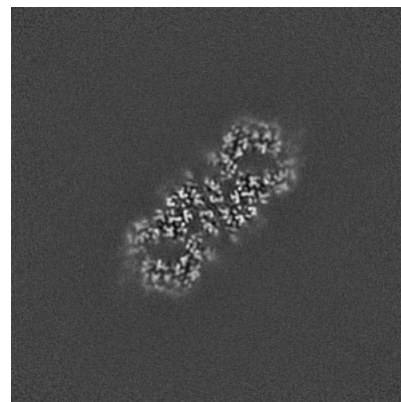
6.3.2 Raw map



X Index: 171



Y Index: 182

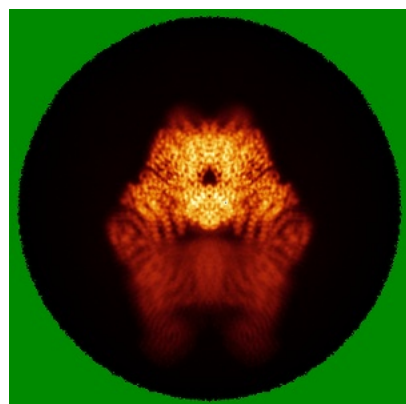


Z Index: 211

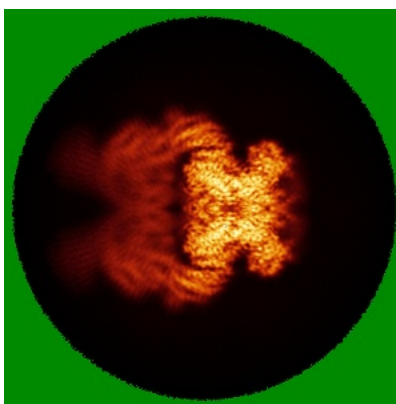
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

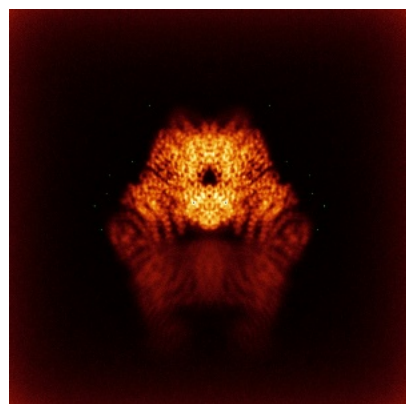


Y

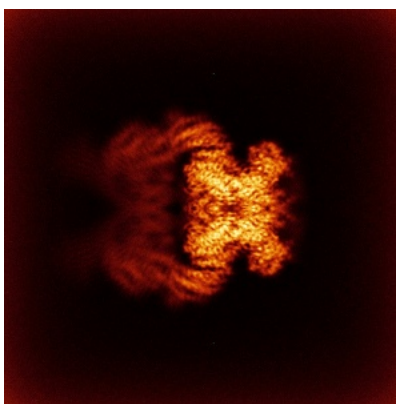


Z

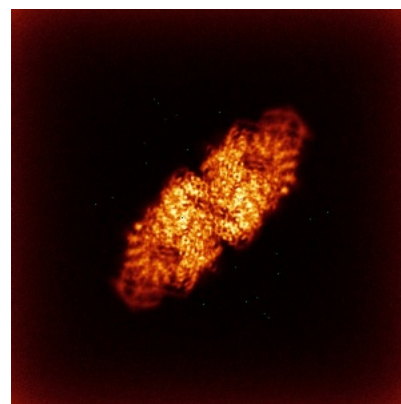
6.4.2 Raw map



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](#)

This section was not generated.

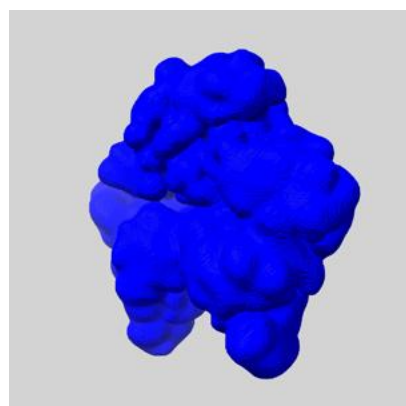
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

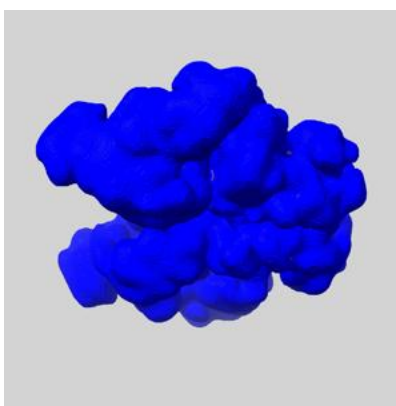
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

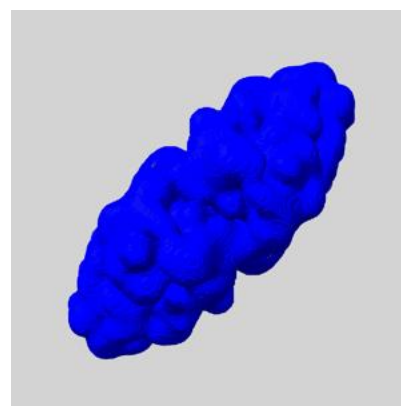
6.6.1 emd_17267_msk_1.map [i](#)



X



Y

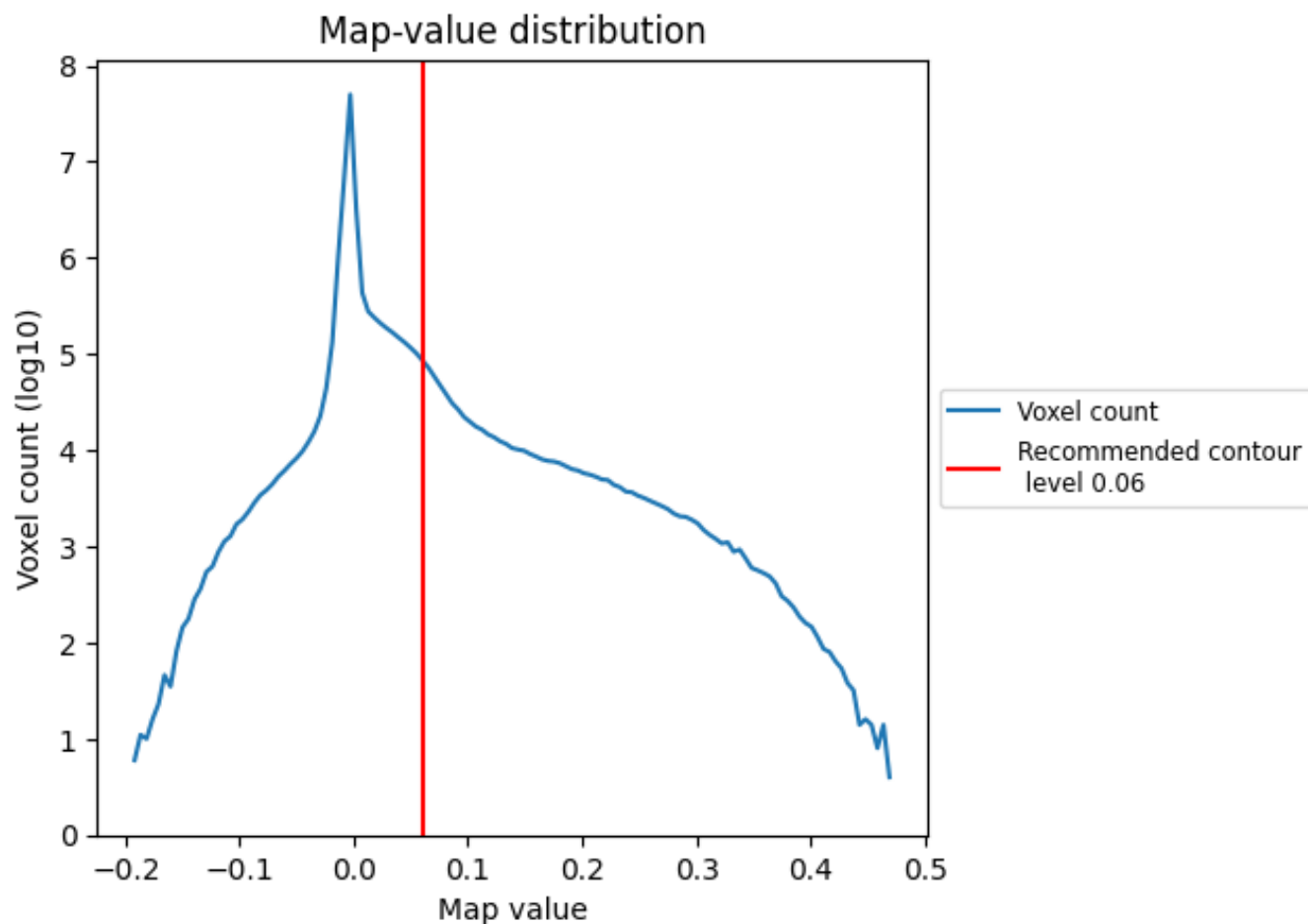


Z

7 Map analysis [i](#)

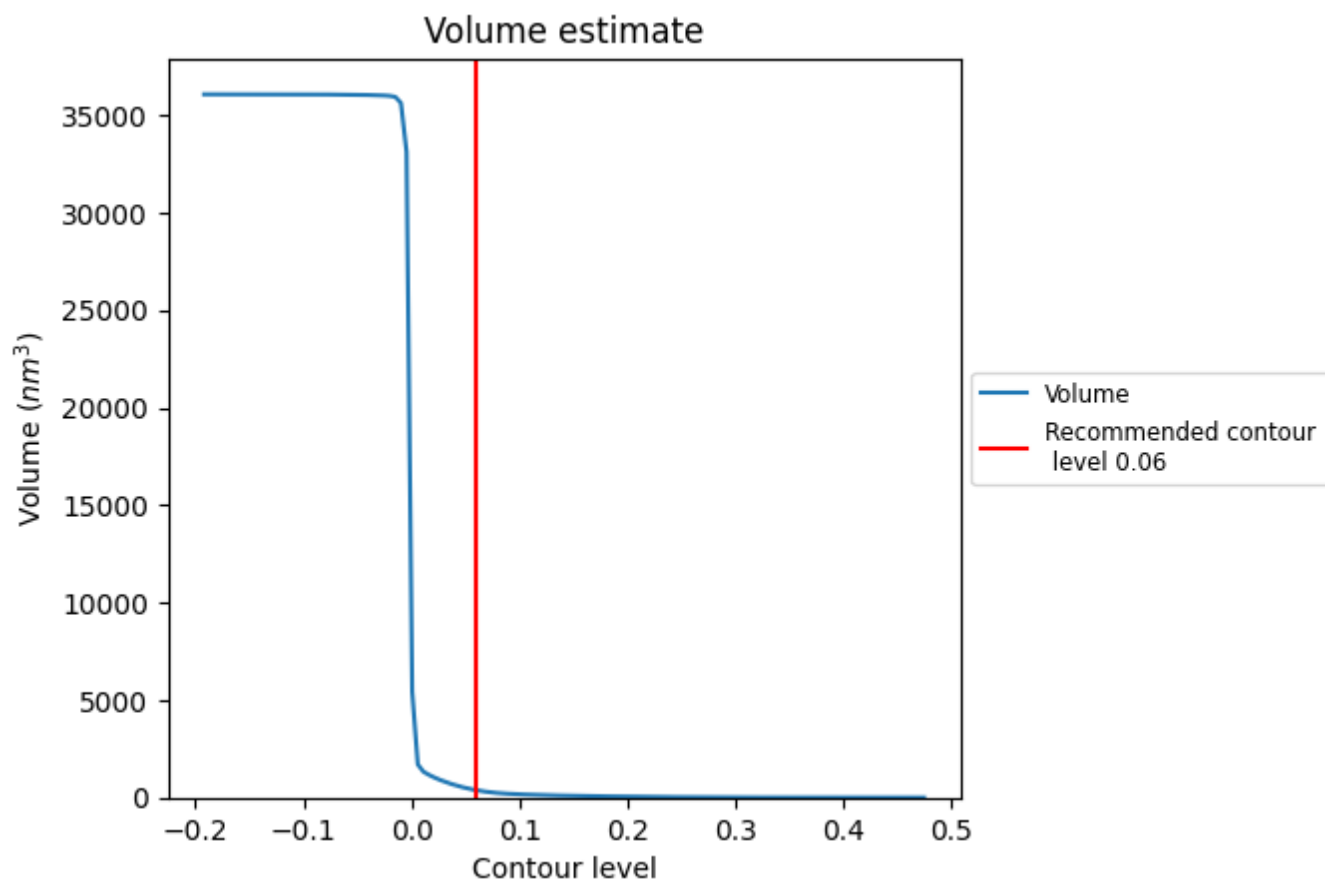
This section contains the results of statistical analysis of the map.

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.

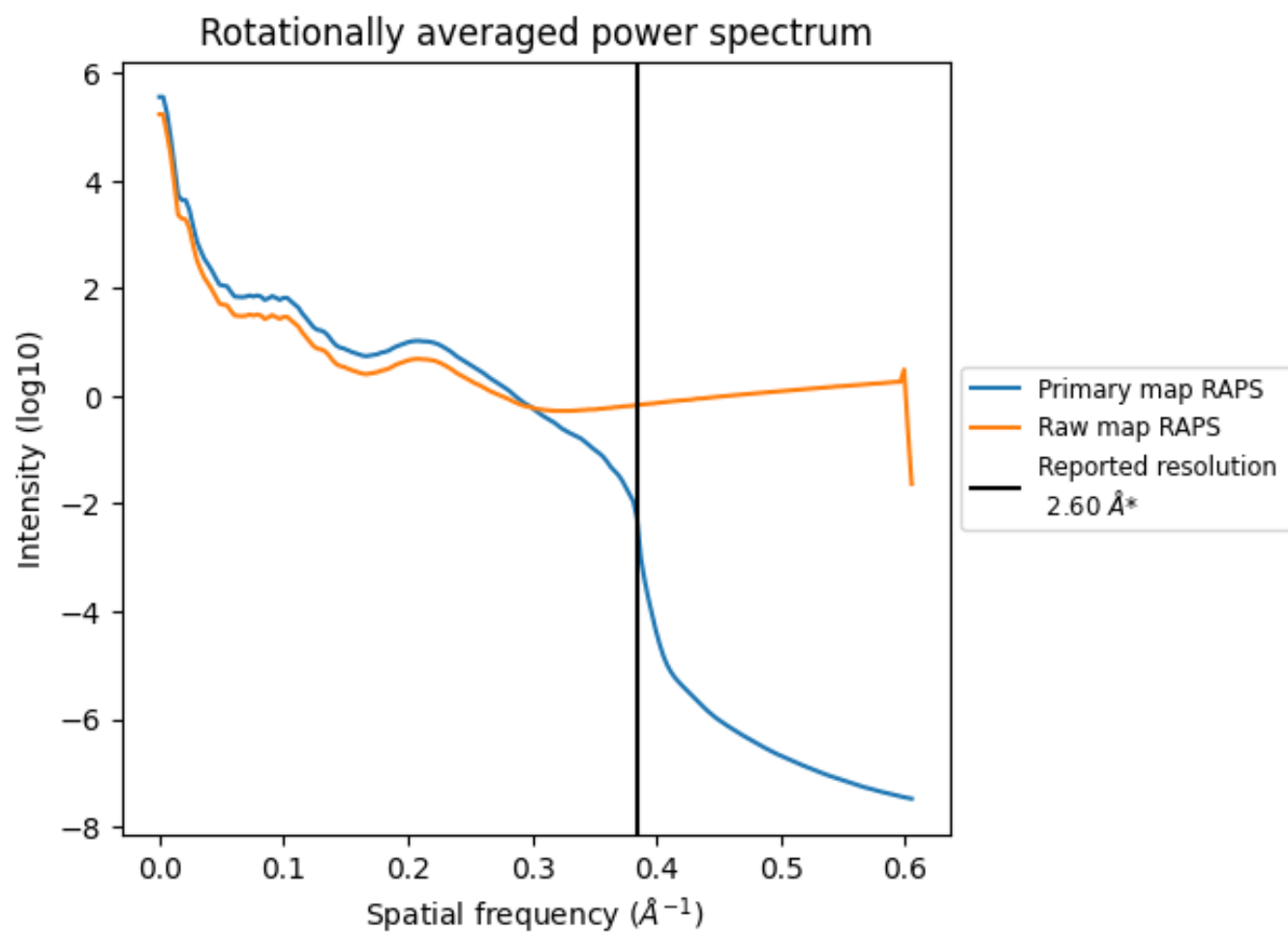
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 378 nm^3 ; this corresponds to an approximate mass of 342 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 ⓘ

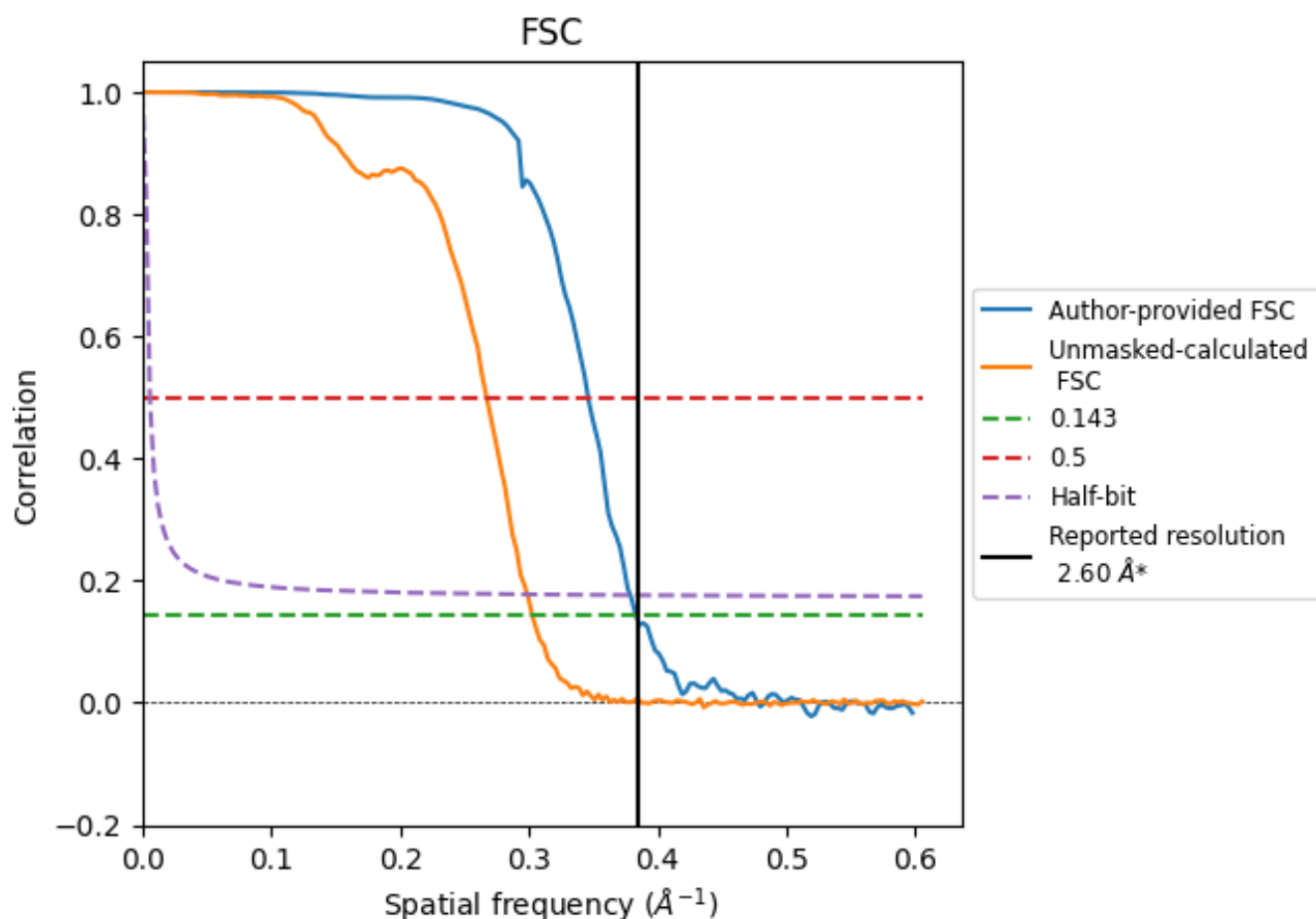


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.385 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

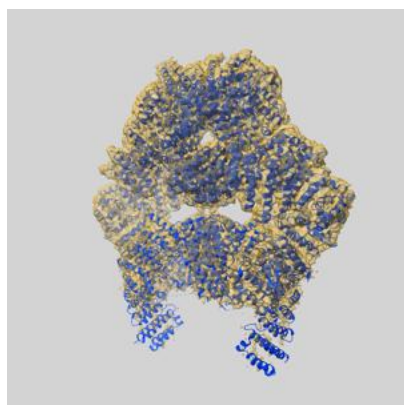
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.61	2.89	2.64
Unmasked-calculated*	3.30	3.74	3.35

*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 3.30 differs from the reported value 2.6 by more than 10 %

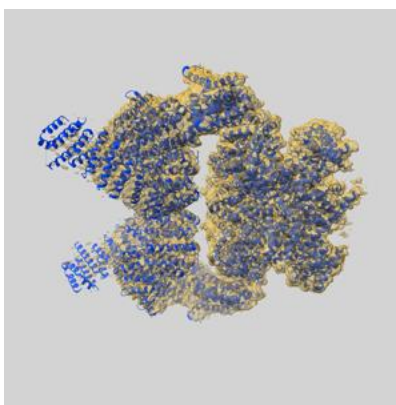
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17267 and PDB model 8OXP. Per-residue inclusion information can be found in section 3 on page 11.

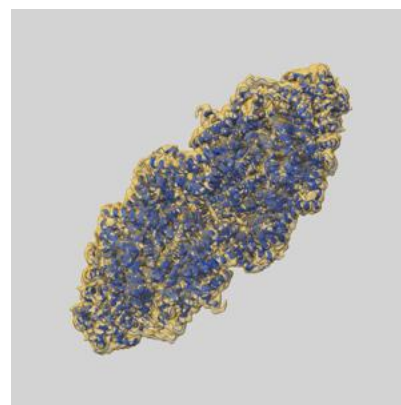
9.1 Map-model overlay [i](#)



X



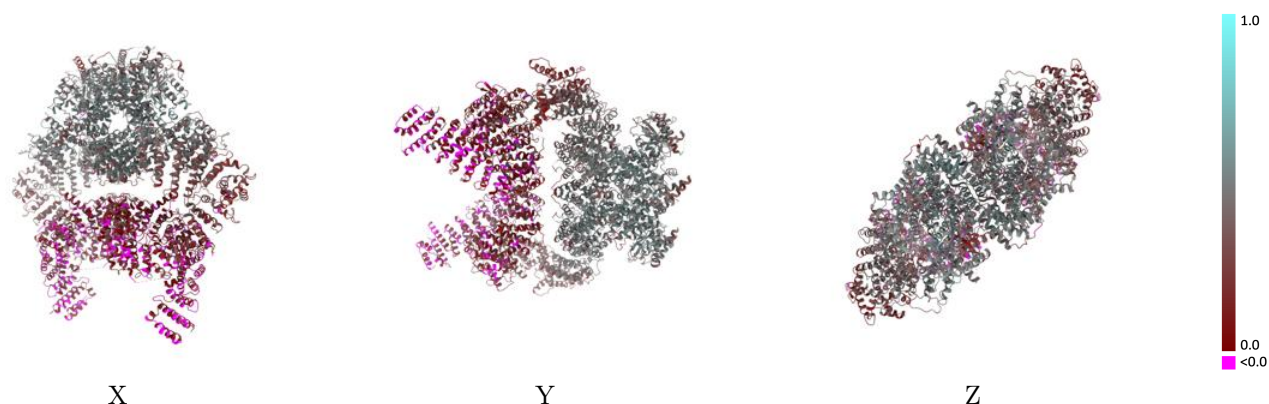
Y



Z

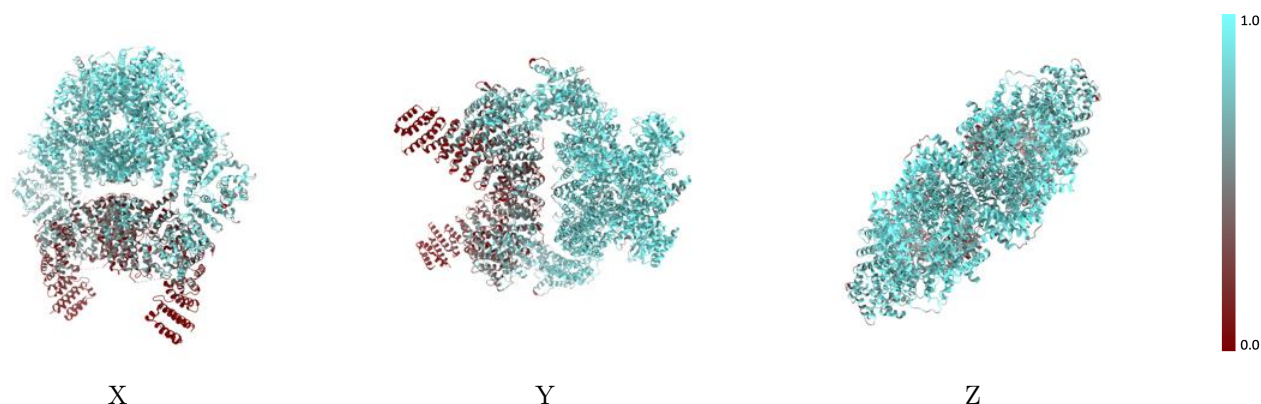
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



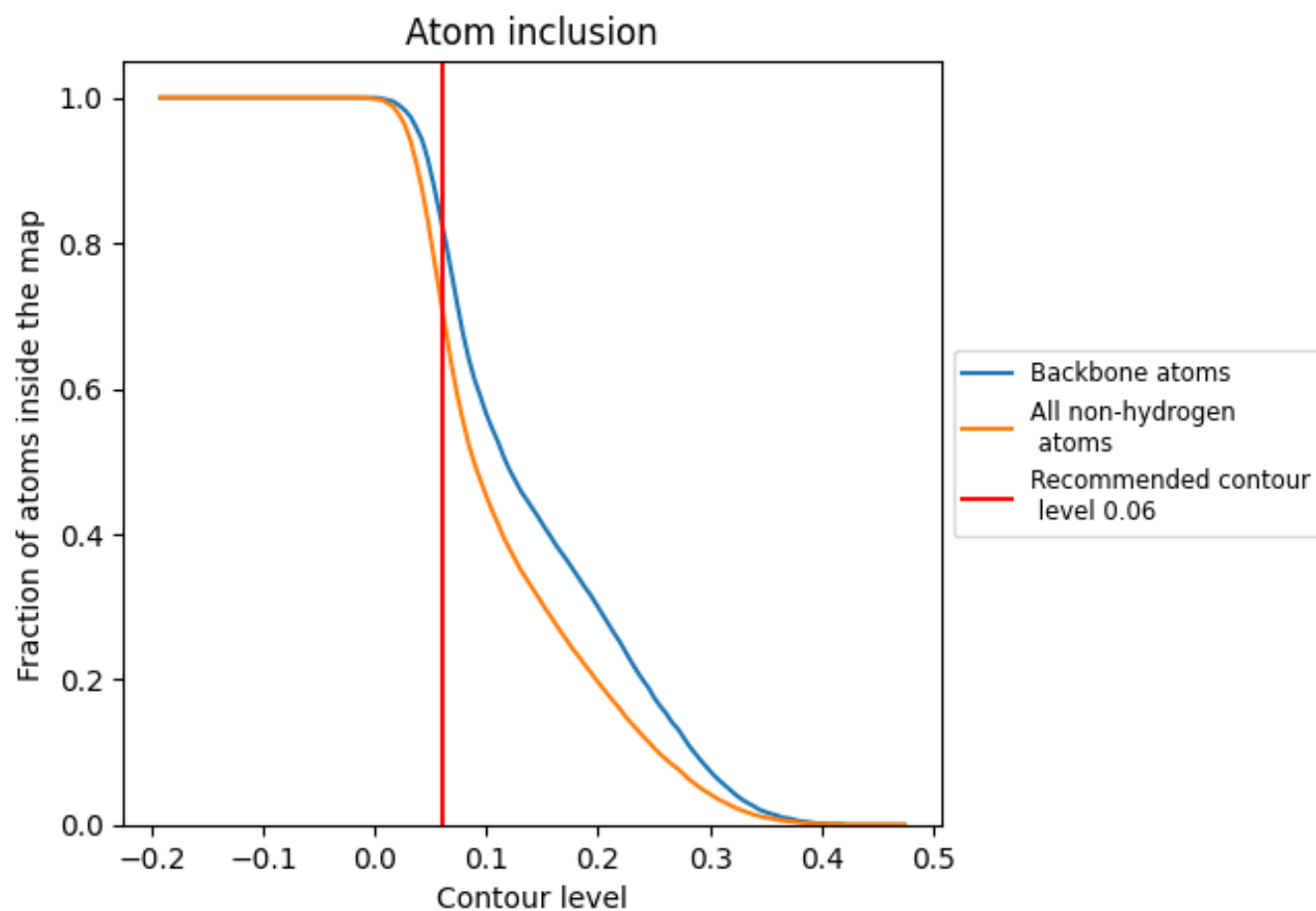
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 71% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7110	0.3200
A	0.7140	0.3250
B	0.7090	0.3140

