



Full wwPDB EM Validation Report ⓘ

Apr 24, 2025 – 10:27 AM EDT

PDB ID : 9BMB / pdb_00009bmb
EMDB ID : EMD-44694
Title : Post-1 motor domain from full-length human dynein-1 bound to microtubules
in 5mM ADP condition
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.60 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.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

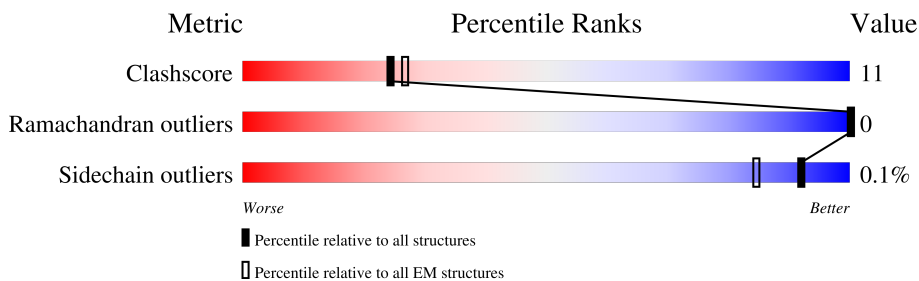
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	4646	<div> <div>9%</div> <div>48%</div> <div>17%</div> <div>35%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 24617 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
			Total	C	N	O	S		
1	A	3043	24503	15606	4234	4541	122	0	0

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



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

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



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

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

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

I2089	L1954	L1811	K1652	L1521	K1441	A1381	VAL	ARG	GLU	ALA	ASN	GLU	ASN	PHE
F2072	E1959	L1815	K1655	L1527	N1442	S1382	ALA	PHE	PHE	LEU	LEU	LEU	PHE	PHE
C2076	F1960	V1816	F1658	V1536	E1443	Y1383	GLU	THR	GLN	GLU	GLU	GLU	GLN	GLN
Q2079	N1961	Q1841	V1661	V1536	I1445	E1384	LEU	PRO	PRO	PRO	PRO	PRO	GLY	LYS
Q2083	R1962	N1942	S1662	D1539	V1446	F1385	Q1327	SER	TRP	ASP	ASP	VAL	VAL	VAL
Y2086	R1966	R1943	S1671	V1540	K1447	Q1387	D1328	THR	THR	GLY	GLY	GLN	ILE	GLY
D2087	T1978	F1944	S1677	Q1541	D1448	R1388	L1329	GLY	TYR	ARG	ARG	TYR	ILE	LEU
F2088	Q1979	F1945	I1676	R1542	V1449	L1389	K1330	ILE	ILE	VAL	VAL	GLY	GLY	LEU
R2091	E1980	Q1855	S1678	R1543	L1450	L1390	G1331	ASN	ASN	THR	THR	ALA	ILE	ILE
L2093	E1984	Q1856	S1679	W1544	L1451	K1391	V1332	GLU	GLU	ASP	GLU	PRO	VAL	GLU
K2094	P1988	L1857	R1679	L1547	V1452	G1392	W1333	GLY	GLY	ASN	GLU	ILE	ARG	GLY
L2097	N1989	I1859	I1692	G1553	E1456	Y1393	S1334	LEU	GLU	SER	GLY	LEU	LEU	LYS
N2102	N1990	A1864	I1698	S1554	M1457	K1394	E1335	ALA	GLN	THR	THR	ALA	GLY	ASP
N2105	Y1990	N1867	I1699	A1555	M1457	K1395	L1336	LYS	GLY	VAL	VAL	LEU	LEU	LEU
R2106	D1991	Y1868	I1700	I1571	L1463	K1396	S1337	ARG	ALA	THR	THR	ARG	ARG	GLU
K2112	K1992	Y1872	W1701	S1572	L1463	N1397	K1338	PHE	ALA	ALA	LYS	LYS	ALA	VAL
E2116	T1993	L1717	L1721	I1576	I1466	M1398	V1339	THR	THR	PHE	THR	LYS	ARG	GLU
E2117	S1994	V1875	V1724	M1579	D1476	N1397	W1340	GLY	GLY	VAL	VAL	VAL	GLY	GLU
R2118	A1995	Q1876	V1724	V1582	I1475	E1402	E1341	LYS	LYS	ILE	VAL	VAL	GLU	THR
G2119	E2000	D1877	F1727	V1587	D1476	L1403	Q1342	ARG	ARG	ASP	ASP	GLN	GLY	ALA
E2120	L2001	T1882	Y1738	L1587	V1477	A1404	Q1345	LYS	LYS	TYR	TYR	LYS	ALA	TYR
A2121	L2002	T1891	Y1738	Y1588	V1478	S1405	M1346	ALA	ALA	GLY	GLY	VAL	ALA	ASP
A2122	N2003	M1892	Y1738	Y1588	V1478	E1406	K1347	LYS	LYS	THR	THR	VAL	LYS	LYS
V2122	V2006	E1897	L1749	M1589	Q1481	E1407	E1348	GLN	GLN	SER	SER	LEU	LEU	THR
D2123	K2007	V1750	V1750	V1591	N1482	L1408	Q1349	VAL	VAL	LEU	LEU	VAL	VAL	GLY
E2124	D2011	E1763	E1763	Q1595	R1485	K1409	P1350	CYS	CYS	PRO	PRO	ASN	ASN	ILE
L2127	N2019	M1769	M1769	R1599	D1486	D1410	W1351	ALA	ALA	ARG	ARG	MET	MET	LEU
A2128	P2020	G1770	G1770	S1600	I1487	R1411	V1352	LYS	LYS	ILE	ILE	ASN	ASN	LEU
E2129	G2021	T1913	G1771	L1601	R1488	H1412	S1353	GLN	GLN	THR	THR	THR	THR	ARG
N2130	ALA	E1914	G1772	L1604	R1488	W1413	V1354	LYS	LYS	ASP	ASP	GLN	GLN	VAL
P2132	GLY	S1915	G1773	L1605	D1491	K1414	Q1355	GLU	GLU	SER	SER	ALA	ALA	LYS
E2133	ARG	A1775	D1774	D1605	N1495	Q1415	P1355	ILE	ILE	TRP	TRP	PRO	PRO	LYS
Q2134	L2035	V1785	A1775	L1607	K1498	L1416	R1357	VAL	VAL	GLN	GLN	ALA	ALA	VAL
L2137	L2039	L1792	L1792	L1611	E1499	M1417	K1357	GLU	GLU	ALA	ALA	VAL	VAL	VAL
I2138	A2040	M1798	L1797	Q1612	H1500	R1418	K1358	GLU	GLU	GLY	GLY	VAL	VAL	ASP
L2149	M2041	Q1799	M1798	R1623	M1507	L1421	L1359	ASP	ASP	ASN	ASN	GLY	GLY	SER
L2160	L2048	Q1800	E1789	S1624	K1508	V1422	R1360	ARG	ARG	ILE	ILE	VAL	VAL	LEU
L2161	V2052	L1803	F1626	F1625	L1509	W1425	Q1361	ALA	ALA	TYR	TYR	HIS	HIS	ASN
Q2169	N2053	L1948	R1627	P1627	S1510	V1426	N1362	LEU	LEU	ARG	ARG	GLY	GLY	LEU
Y2170	L2054	G1947	P1628	F1629	P1511	S1427	L1363	THR	THR	GLY	GLY	THR	THR	GLY
H2171	Y2055	C1949	R1805	F1629	Y1512	E1428	L1364	GLN	GLN	GLY	GLY	GLY	GLY	PRO
E2174	S2056	Q1950	R1806	L1637	V1514	L1429	Q1369	ASP	ASP	LEU	LEU	LEU	LEU	LYS
	L2065	V1951			V1515	L1430	L1370	ASN	ASN	GLY	GLY	GLY	GLY	ASN
	A2066				F1516	L1431	K1371	THR	THR	PHE	PHE	THR	THR	HIS
					E1517	S1372	K1371	GLY	GLY	GLN	GLN	GLY	GLY	GLY
					E1518	Q1433	F1373	THR	THR	GLY	GLY	GLY	GLY	GLY
						I1434	P1374	ASP	ASP	THR	THR	THR	THR	THR
						W1435	R1375	GLN	GLN	GLY	GLY	GLY	GLY	GLY
						D1436	R1376	GLY	GLY	GLY	GLY	GLY	GLY	GLY
						V1437	L1377	GLY	GLY	GLY	GLY	GLY	GLY	GLY
						D1438	R1378	GLY	GLY	GLY	GLY	GLY	GLY	GLY
						L1439	Y1380	GLY	GLY	GLY	GLY	GLY	GLY	GLY
						Q1440		GLY	GLY	GLY	GLY	GLY	GLY	GLY



W4592	P4470	LYS	A4215	S4073	T3928	Q3792	N3700	K3608	L3508	RET
W4593	V4476	LYS	C4216	A4074	Q3931	T3796	F3701	R3611	L3509	ILE
K4594	I4475	THR	D4217	E075	A3932	S3810	L3708	F3614	S3510	ARG
T4596	M4247	THR	M4247	A4087	E3933	S3809	E3720	D3617	LEU	LEU
W4597	I4251	ASP	I4251	V4088	R3937	I3811	D3725	A3618	ALA	ALA
T4598	V4256	SER	V4256	K4089	R3937	I3811	D3725	F3619	SER	SER
S4483	V4256	THR	V4256	S4090	F3944	T3814	R3728	K3620	ILE	ILE
E4599	F4260	SER	F4260	G4091	K3945	L3818	R3728	K3621	ALA	ALA
K4600	F4260	GLY	F4260	R4092	D3946	L3818	L3731	N3622	ARG	ARG
P4608	L4264	ARG	L4264	L4096	A3949	L3824	Q3735	L3627	TYR	TYR
V4609	L4265	PRO	L4265	K4097	K3950	S3828	G3736	R3628	GLU	GLU
L4610	M4266	LYS	M4266	N4098	A3951	S3828	G3736	F3629	TYR	TYR
N4612	F4268	THR	F4268	V4099	D3954	I3835	Q3739	G3630	ALA	ALA
I4619	L4270	THR	L4270	W4105	E3955	V3839	L3740	N3631	VAL	VAL
V4622	E4277	THR	E4277	L4106	F3966	L3846	R3743	P3632	LEU	LEU
A4627	F4282	LYS	F4282	L4113	E3967	L3846	E3746	L3633	ILE	ILE
K4629	K4287	THR	K4287	H4114	Y3972	R3855	E3746	Q3636	SER	SER
E4637	V4288	THR	V4288	S4115	L3973	R3855	E3746	G3637	GLU	GLU
R4638	H4291	THR	H4291	L4116	W3974	I3859	L3750	V3638	ALA	ALA
V4642	W4308	THR	W4308	P4118	S3975	L3863	L3753	E3639	ALA	ALA
E4646	L4312	THR	L4312	R4123	E3976	F3864	N3754	D3642	LYS	LYS
V4528	P4313	THR	P4313	L4124	E3977	V3866	E3755	P3647	ALA	ALA
L4541	T4315	THR	T4315	R4124	E3977	V3866	E3755	N3650	ASP	ASP
E4542	S4319	THR	S4319	T4127	E3977	V3866	E3755	R3651	LEU	LEU
V4543	P4324	THR	P4324	K4133	E3977	V3866	E3755	L3560	ALA	ALA
S4548	L4332	THR	L4332	L4138	E3977	V3866	E3755	W3562	ALA	ALA
Q4549	L4344	THR	L4344	L4139	E3977	V3866	E3755	L3567	VAL	VAL
G4550	K4345	THR	K4345	R4140	E3977	V3866	E3755	E3575	GLU	GLU
A4551	M4346	THR	M4346	F4145	E3977	V3866	E3755	N3576	ALA	ALA
T4552	M4346	THR	M4346	F4145	E3977	V3866	E3755	E3575	ALA	ALA
L4553	M4346	THR	M4346	F4145	E3977	V3866	E3755	N3576	ALA	ALA
D4554	M4346	THR	M4346	F4145	E3977	V3866	E3755	E3575	ALA	ALA
S4557	M4346	THR	M4346	F4145	E3977	V3866	E3755	E3575	ALA	ALA
V4560	M4346	THR	M4346	F4145	E3977	V3866	E3755	E3575	ALA	ALA
K4564	M4346	THR	M4346	F4145	E3977	V3866	E3755	E3575	ALA	ALA
N4571	M4346	THR	M4346	F4145	E3977	V3866	E3755	E3575	ALA	ALA
K4574	M4346	THR	M4346	F4145	E3977	V3866	E3755	E3575	ALA	ALA
L4577	M4346	THR	M4346	F4145	E3977	V3866	E3755	E3575	ALA	ALA
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L4590	M4346	THR	M4346	F4145	E3977	V3866	E3755	E3575	ALA	ALA
R4591	M4346	THR	M4346	F4145	E3977	V3866	E3755	E3575	ALA	ALA
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K3953	K3954	K3955	K3956	K3957	K3958	K3959	K3960	K3961	K3962	K3963
K3964	K3965	K3966	K3967	K3968	K3969	K3970	K3971	K3972	K3973	K3974
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K4096	K4097	K4098	K4099	K4100	K4101	K4102	K4103	K4104	K4105	K4106
K4107	K4108	K4109	K4110	K4111	K4112	K4113	K4114	K4115	K4116	K4117
K4118	K4119	K4120	K4121	K4122	K4123	K4124	K4125	K4126	K4127	K4128
K4129	K4130	K4131	K4132	K4133	K4134	K4135	K4136	K4137	K4138	K4139
K4140	K4141	K4142	K4143	K4144	K4145	K4146	K4147	K4148	K4149	K4150
K4151	K4152	K4153	K4154	K4155	K4156	K4157	K4158	K4159	K4160	K4161
K4162	K4163	K4164	K4165	K4166	K4167	K4168	K4169	K4170	K4171	K4172
K4173	K4174	K4175	K4176	K4177	K4178	K4179	K4180	K4181	K4182	K4183
K4184	K4185	K4186	K4187	K4188	K4189	K4190	K4191	K4192	K4193	K4194
K4195	K4196	K4197	K4198	K4199	K4200	K4201	K4202	K4203	K4204	K4205
K4206	K4207	K4208	K4209	K4210	K4211	K4212	K4213	K4214	K4215	K4216
K4217	K4218	K4219	K4220	K4221	K4222	K4223	K4224	K4225	K4226	K4227
K4228	K4229	K4230	K4231	K4232	K4233	K4234	K4235	K4236	K4237	K4238
K4239	K4240	K4241	K4242	K4243	K4244	K4245	K4246	K4247	K4248	K4249
K4250	K4251	K4252	K4253	K4254	K4255	K4256	K4257	K4258	K4259	K4260
K4261	K4262	K4263	K4264	K4265	K4266	K4267	K4268	K4269	K4270	K4271
K4272	K4273	K4274	K4275	K4276	K4277	K4278	K4279	K4280	K4281	K4282
K4283	K4284	K4285	K4286	K4287	K4288	K4289	K4290	K4291	K4292	K4293
K4294	K4295	K4296	K4297	K4298	K4299	K4300	K4301	K4302	K4303	K4304
K4305	K4306	K4307	K4308	K4309	K4310	K4311	K4312	K4313	K4314	K4315
K4316	K4317	K4318	K4319	K4320	K4321	K4322	K4323	K4324	K4325	K4326
K4327	K4328	K4329	K4330	K4331	K4332	K4333	K4334	K4335	K4336	K4337
K4338	K4339	K4340	K4341	K4342	K4343	K4344	K4345</			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	139709	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.327	Depositor
Minimum map value	-0.840	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1573, 1.1573, 1.1573	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: ADP, ATP, 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	0.26	0/25022	0.49	0/33900

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	24503	0	24574	518	0
2	A	81	0	36	5	0
3	A	31	0	12	1	0
4	A	2	0	0	0	0
All	All	24617	0	24622	518	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 11.

All (518) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3618:ALA:O	1:A:3621:LYS:HB3	1.61	0.98
1:A:1698:ILE:HD13	1:A:1701:TRP:HE1	1.48	0.79
1:A:2593:LEU:HD12	1:A:2605:LEU:HD12	1.67	0.75
1:A:1857:LEU:HD22	1:A:1868:TYR:HB2	1.69	0.74
1:A:1978:ILE:HD11	1:A:2001:LEU:HD11	1.70	0.74
1:A:3659:ARG:HE	1:A:3661:LEU:HD11	1.52	0.74
1:A:3481:SER:HB2	1:A:3770:LEU:HD11	1.70	0.74
1:A:3103:TYR:OH	1:A:3141:GLU:OE1	2.06	0.73
1:A:1407:ALA:HA	1:A:1457:MET:HE3	1.71	0.73
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.70	0.73
1:A:2834:GLN:HA	1:A:2837:LEU:HD13	1.69	0.72
1:A:2593:LEU:HD23	1:A:2734:VAL:HB	1.72	0.71
1:A:3928:THR:OG1	1:A:3931:GLN:OE1	2.09	0.71
1:A:4193:ARG:NH2	1:A:4637:GLU:O	2.24	0.70
1:A:4574:LYS:HB3	1:A:4627:ALA:HB2	1.74	0.70
1:A:3576:ASN:ND2	1:A:3700:ASN:O	2.26	0.69
1:A:2112:LYS:HG3	1:A:2122:VAL:HG11	1.73	0.69
1:A:2290:SER:HB3	1:A:2295:LEU:HD23	1.74	0.68
1:A:1912:LYS:HG2	1:A:2041:MET:HG3	1.76	0.67
1:A:1332:VAL:HB	1:A:1377:LEU:HD22	1.76	0.66
1:A:3576:ASN:HA	1:A:3579:MET:HG3	1.78	0.66
1:A:2943:LYS:HE2	1:A:3067:THR:HB	1.77	0.66
1:A:2999:VAL:HG13	1:A:3005:LEU:HD21	1.77	0.65
1:A:3113:MET:O	1:A:3140:ARG:NH2	2.30	0.65
1:A:3622:ASN:HB3	1:A:3633:LEU:HD11	1.78	0.65
1:A:3763:ASP:OD2	1:A:3765:THR:OG1	2.14	0.65
1:A:4113:LEU:HD13	1:A:4116:LEU:HD13	1.78	0.65
1:A:1499:GLU:HA	1:A:3621:LYS:HE2	1.77	0.65
1:A:4595:GLN:NE2	1:A:4596:THR:O	2.29	0.65
1:A:3553:LEU:O	1:A:3582:ARG:NH1	2.30	0.65
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.77	0.65
1:A:1406:GLU:HG3	1:A:3658:GLY:HA3	1.79	0.64
1:A:3601:MET:HE1	1:A:3611:ARG:HE	1.63	0.64
1:A:2933:LEU:HB3	1:A:3065:VAL:HG22	1.79	0.64
1:A:3546:ASP:O	1:A:3735:GLN:NE2	2.22	0.64
1:A:1798:MET:HG2	1:A:2124:GLU:HG3	1.81	0.63
1:A:2897:LEU:HD21	1:A:2909:LEU:HB2	1.80	0.63
1:A:2901:TYR:OH	1:A:2909:LEU:N	2.28	0.63
1:A:2453:ARG:NH1	1:A:2505:ASP:OD2	2.29	0.63
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.80	0.62
1:A:2620:LEU:HD12	1:A:2630:LEU:HD21	1.81	0.62
1:A:3074:GLY:O	1:A:3078:ARG:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2581:LEU:HD13	1:A:2591:LEU:HD13	1.81	0.62
1:A:2221:MET:HE1	1:A:2348:LEU:HD21	1.82	0.62
1:A:1979:GLN:HB3	1:A:2035:LEU:HD13	1.81	0.62
1:A:2830:LEU:HD22	1:A:2850:ILE:HD13	1.79	0.62
1:A:4031:VAL:O	1:A:4123:ARG:NH1	2.33	0.62
1:A:1939:GLN:N	1:A:1939:GLN:OE1	2.33	0.61
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.33	0.61
1:A:2790:PRO:HB3	1:A:3076:LYS:HE2	1.83	0.61
1:A:1959:GLU:OE2	1:A:2019:ASN:ND2	2.31	0.61
1:A:3204:GLY:HA2	1:A:3750:LEU:HD21	1.83	0.61
1:A:1800:GLN:OE1	1:A:1804:ARG:NH1	2.34	0.60
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.82	0.60
1:A:2387:LEU:HD21	1:A:2463:HIS:HB3	1.83	0.60
1:A:2684:ARG:HH12	1:A:2726:ARG:HE	1.49	0.60
1:A:2874:SER:HB3	1:A:2920:LEU:HD21	1.82	0.60
1:A:2671:MET:HB2	1:A:2675:GLY:HA2	1.83	0.60
1:A:3914:ILE:H	1:A:3937:ARG:HH12	1.49	0.60
1:A:2644:THR:OG1	1:A:2647:GLY:O	2.20	0.59
1:A:2536:ASP:OD1	1:A:2576:ARG:NH1	2.35	0.59
1:A:3044:LEU:HD22	1:A:3049:GLU:HG2	1.82	0.59
1:A:3508:LEU:HD23	1:A:3536:LEU:HD21	1.83	0.59
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.85	0.59
1:A:1415:GLN:O	1:A:1419:ARG:HG2	2.02	0.59
1:A:2910:VAL:N	2:A:4704:ADP:N1	2.44	0.59
1:A:2660:VAL:HG22	1:A:2707:GLN:HB2	1.84	0.59
1:A:2324:LEU:HD21	1:A:2332:ARG:HD3	1.84	0.58
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.83	0.58
1:A:2413:LEU:HA	1:A:2416:GLN:HE21	1.67	0.58
1:A:4511:LEU:HD23	1:A:4560:VAL:HG13	1.86	0.58
1:A:2939:SER:OG	1:A:3069:ASN:OD1	2.20	0.58
1:A:4042:LEU:HD11	1:A:4138:LEU:HG	1.86	0.58
1:A:2419:ALA:O	1:A:2423:MET:HG2	2.03	0.58
1:A:2965:ARG:HD3	1:A:2966:LYS:H	1.69	0.58
1:A:4445:THR:O	1:A:4449:ARG:N	2.31	0.58
1:A:2983:SER:HB3	1:A:2990:ILE:HD12	1.85	0.58
1:A:3756:VAL:HG13	1:A:3757:LYS:H	1.68	0.57
1:A:2131:LEU:HD12	1:A:2132:PRO:HD2	1.86	0.57
1:A:2643:ARG:NH1	1:A:2644:THR:O	2.37	0.57
1:A:3511:ALA:HA	1:A:3514:ILE:HG22	1.85	0.57
1:A:4445:THR:H	1:A:4448:LEU:HB2	1.69	0.57
1:A:1403:LEU:HD23	1:A:1450:LEU:HD21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2963:VAL:HB	1:A:2998:ASN:HB3	1.86	0.57
1:A:3736:GLY:O	1:A:3740:LEU:N	2.32	0.57
1:A:3755:GLU:OE2	1:A:3759:ARG:NH1	2.37	0.57
1:A:1652:LYS:O	1:A:1655:LYS:NZ	2.38	0.57
1:A:1678:SER:HB2	1:A:1872:TYR:HE2	1.69	0.57
1:A:3130:TYR:CZ	1:A:3132:LYS:HB2	2.39	0.57
1:A:1579:MET:HA	1:A:1582:VAL:HG12	1.86	0.57
1:A:1510:SER:O	1:A:1512:TYR:N	2.37	0.57
1:A:3489:TRP:NE1	1:A:3746:GLU:OE1	2.37	0.57
1:A:3739:GLN:O	1:A:3743:ARG:HD3	2.05	0.57
1:A:2083:GLN:HB2	1:A:2086:TYR:CD2	2.40	0.56
1:A:2297:LYS:O	1:A:2338:ASN:ND2	2.38	0.56
1:A:2465:ALA:HB2	1:A:2493:TYR:CE2	2.39	0.56
1:A:4460:LEU:HA	1:A:4475:VAL:HG22	1.86	0.56
1:A:2584:TRP:HB2	1:A:2591:LEU:HD12	1.86	0.56
1:A:1440:GLN:HA	1:A:1443:GLU:HG3	1.86	0.56
1:A:2325:LEU:HB3	1:A:2333:LEU:HB2	1.87	0.56
1:A:3835:ILE:HG23	1:A:3866:VAL:HG12	1.87	0.56
1:A:2325:LEU:HD23	1:A:2333:LEU:HD12	1.87	0.56
1:A:1351:TRP:H	1:A:1430:THR:HA	1.70	0.56
1:A:3525:ARG:NH1	1:A:3576:ASN:OD1	2.38	0.56
1:A:3767:ILE:O	1:A:3771:GLU:HG3	2.05	0.56
1:A:1498:LYS:HA	1:A:1501:ILE:HG12	1.88	0.56
1:A:1336:LEU:HD11	1:A:1386:VAL:HG21	1.88	0.56
1:A:1429:LEU:HD11	1:A:1434:ILE:HD11	1.86	0.56
1:A:1511:PRO:O	1:A:1514:LYS:HG2	2.06	0.56
1:A:2925:ILE:HD12	1:A:3090:VAL:HG11	1.86	0.56
1:A:1882:THR:HA	1:A:2048:LEU:HD23	1.88	0.55
1:A:2925:ILE:HG21	1:A:2933:LEU:HD13	1.87	0.55
1:A:3008:MET:HE2	1:A:3064:VAL:HG11	1.88	0.55
1:A:1625:SER:OG	1:A:1699:ASN:OD1	2.20	0.55
1:A:3154:LEU:HD22	1:A:3171:ILE:HG12	1.88	0.55
1:A:2039:LEU:HD23	1:A:2040:ALA:N	2.21	0.55
1:A:2308:ASP:HB2	1:A:2674:TYR:HD2	1.71	0.55
1:A:2666:ILE:HB	1:A:2712:CYS:SG	2.46	0.55
1:A:3043:MET:HA	1:A:3043:MET:HE2	1.87	0.55
1:A:3178:ASP:OD1	1:A:3585:ARG:NE	2.39	0.55
1:A:3761:LEU:HD22	1:A:3764:ASP:OD1	2.07	0.55
1:A:1927:VAL:HG22	1:A:1954:TRP:HB2	1.87	0.55
1:A:2491:GLN:HB3	1:A:2524:VAL:HG21	1.88	0.55
1:A:4564:LYS:HG3	1:A:4646:GLU:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2386:PRO:HG3	1:A:2413:LEU:HD21	1.89	0.55
1:A:2838:VAL:HG13	1:A:3093:TRP:CZ2	2.43	0.54
1:A:1959:GLU:OE1	1:A:1962:ARG:NH1	2.40	0.54
1:A:2174:GLU:HB2	1:A:2179:ARG:HH21	1.71	0.54
1:A:3096:ASP:OD2	1:A:3097:TRP:N	2.40	0.54
1:A:3661:LEU:HD23	1:A:3668:ASP:HB2	1.90	0.54
1:A:1405:SER:HB2	1:A:3658:GLY:HA2	1.89	0.54
1:A:3143:ILE:HD13	1:A:3541:ILE:HD13	1.88	0.54
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.88	0.54
1:A:2987:ASN:OD1	1:A:3057:GLN:NE2	2.28	0.54
1:A:3499:GLN:HA	1:A:3502:THR:HG22	1.89	0.54
1:A:1661:VAL:HG22	1:A:1676:ILE:HG21	1.88	0.54
1:A:1717:LEU:HB2	1:A:1749:LEU:HD22	1.90	0.54
1:A:2393:GLU:O	1:A:2397:ARG:NH1	2.40	0.54
1:A:3486:ARG:O	1:A:3490:GLU:HG2	2.08	0.53
1:A:3913:GLU:HG3	1:A:4476:ILE:HG21	1.90	0.53
1:A:2291:VAL:HG23	1:A:2292:ARG:HG2	1.89	0.53
1:A:2577:HIS:CE1	1:A:2736:VAL:HG22	2.44	0.53
1:A:2102:ASN:OD1	1:A:2105:ARG:NH2	2.37	0.53
1:A:3973:LEU:HB2	1:A:3992:LEU:HD11	1.90	0.53
1:A:2448:ASP:OD2	1:A:2725:HIS:NE2	2.41	0.53
1:A:2519:ARG:HH21	1:A:2534:ILE:HD11	1.73	0.53
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.91	0.53
1:A:3481:SER:HB2	1:A:3770:LEU:CD1	2.38	0.53
1:A:3909:LEU:HB3	1:A:4344:LEU:HD13	1.90	0.52
1:A:2585:LEU:HD21	1:A:2709:VAL:HG21	1.92	0.52
1:A:2744:LEU:HA	1:A:2747:ILE:HG22	1.91	0.52
1:A:2386:PRO:HA	1:A:2416:GLN:HE22	1.74	0.52
1:A:2784:PHE:HB3	1:A:2792:TYR:CD1	2.44	0.52
1:A:1626:PHE:HB2	1:A:1699:ASN:ND2	2.24	0.52
1:A:1816:VAL:HG11	1:A:2052:VAL:HG22	1.92	0.52
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.92	0.52
1:A:2464:GLN:HG3	1:A:2583:THR:HG23	1.91	0.52
1:A:2558:GLU:HA	1:A:2757:ARG:HH21	1.75	0.52
1:A:2789:GLN:HB2	1:A:2792:TYR:HE2	1.75	0.52
1:A:2461:MET:HG2	1:A:2493:TYR:HE2	1.75	0.52
1:A:3207:LYS:NZ	1:A:3210:GLU:OE1	2.42	0.52
1:A:3514:ILE:HD11	1:A:3582:ARG:HB2	1.92	0.52
1:A:1539:ASP:OD1	1:A:1542:ARG:NH2	2.43	0.52
1:A:2762:LEU:HD21	1:A:2821:LEU:HD22	1.91	0.52
1:A:2962:LYS:HD2	1:A:3647:PRO:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3731:LEU:HD21	1:A:3791:MET:HG2	1.92	0.52
1:A:4398:LEU:HG	1:A:4417:VAL:HG21	1.92	0.52
1:A:1536:VAL:HG12	1:A:1601:LEU:HG	1.91	0.52
1:A:2465:ALA:HB2	1:A:2493:TYR:CD2	2.44	0.52
1:A:2686:MET:HE2	1:A:2703:LEU:HD11	1.91	0.51
1:A:4324:PRO:HB3	1:A:4638:ARG:HH11	1.74	0.51
1:A:1914:GLU:HG3	2:A:4701:ADP:H3'	1.91	0.51
1:A:2623:SER:HA	1:A:2668:LEU:HB3	1.91	0.51
1:A:2258:ALA:HB1	1:A:2682:PHE:HD1	1.74	0.51
1:A:1452:VAL:HA	1:A:1512:TYR:CE1	2.46	0.51
1:A:1864:ALA:HB2	1:A:1897:GLU:HB2	1.92	0.51
1:A:1946:VAL:HG13	1:A:2006:VAL:HG21	1.93	0.51
1:A:3026:TYR:O	1:A:3030:MET:HG2	2.11	0.51
1:A:2309:PRO:HA	1:A:2312:VAL:HG12	1.92	0.51
1:A:2354:ALA:HB1	1:A:2358:ARG:HH21	1.75	0.51
1:A:2797:ARG:HA	1:A:2800:THR:HG22	1.93	0.51
1:A:2831:ARG:HH21	1:A:2921:ARG:HH21	1.58	0.51
1:A:3113:MET:SD	1:A:3184:ALA:HA	2.51	0.51
1:A:2965:ARG:HE	1:A:2965:ARG:HA	1.76	0.51
1:A:3650:ASN:OD1	1:A:3695:ARG:NH1	2.43	0.51
1:A:4183:LEU:HD11	1:A:4215:ALA:HB1	1.93	0.51
1:A:4541:LEU:HD11	1:A:4590:LEU:HB3	1.93	0.51
1:A:2265:TYR:CZ	1:A:2314:ASN:HB2	2.46	0.51
1:A:2527:PRO:HD3	1:A:2545:TRP:CE2	2.45	0.51
1:A:3865:GLN:NE2	1:A:3869:ASN:OD1	2.44	0.51
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.76	0.51
1:A:1451:LEU:HG	1:A:3673:PRO:HG2	1.93	0.51
1:A:3596:ALA:HB2	1:A:3701:PHE:CD2	2.46	0.51
1:A:1626:PHE:HB2	1:A:1699:ASN:HD22	1.76	0.50
1:A:1466:ILE:HD11	1:A:1527:LEU:HD11	1.91	0.50
1:A:1501:ILE:HG22	1:A:1527:LEU:HB3	1.93	0.50
1:A:1582:VAL:HG23	1:A:1591:VAL:HG22	1.92	0.50
1:A:2569:VAL:HB	1:A:2747:ILE:HD12	1.93	0.50
1:A:2789:GLN:HB2	1:A:2792:TYR:CE2	2.47	0.50
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.93	0.50
1:A:2315:LEU:HA	1:A:2318:VAL:HG12	1.93	0.50
1:A:3967:GLU:HB2	1:A:4004:MET:HE2	1.94	0.50
1:A:4031:VAL:HG21	1:A:4058:LEU:HD21	1.93	0.50
1:A:3780:VAL:O	1:A:3784:VAL:HG23	2.11	0.50
1:A:4423:LEU:HD13	1:A:4466:HIS:CD2	2.47	0.50
1:A:2843:ARG:HH21	1:A:3093:TRP:HD1	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3910:ARG:NE	1:A:4344:LEU:HD11	2.27	0.49
1:A:2503:SER:HB3	1:A:2514:LEU:HD22	1.93	0.49
1:A:2623:SER:OG	1:A:3006:GLU:OE1	2.28	0.49
1:A:2646:ASN:OD1	1:A:2647:GLY:N	2.45	0.49
1:A:2296:GLN:N	1:A:2296:GLN:OE1	2.45	0.49
1:A:2961:ILE:HD13	1:A:2975:ASP:CG	2.33	0.49
1:A:3886:LEU:HD11	1:A:4346:MET:HG3	1.93	0.49
1:A:2995:ASP:OD1	1:A:3067:THR:OG1	2.28	0.49
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	1.94	0.49
1:A:1785:VAL:HG13	1:A:1815:LEU:HD12	1.95	0.49
1:A:3017:VAL:O	1:A:3020:LEU:HD22	2.12	0.49
1:A:3561:ARG:NH2	1:A:3603:GLU:OE2	2.46	0.49
1:A:3576:ASN:HB2	1:A:3701:PHE:HE1	1.77	0.49
1:A:2346:GLN:HB2	1:A:2726:ARG:HD2	1.94	0.49
1:A:3162:ALA:HB2	1:A:3168:THR:HG21	1.94	0.49
1:A:3620:ARG:HH21	1:A:3665:GLY:HA3	1.78	0.49
1:A:1469:VAL:HG21	1:A:1500:HIS:HE1	1.78	0.49
1:A:2254:ILE:HG23	1:A:2279:LEU:HD23	1.94	0.49
1:A:4050:ASP:OD1	1:A:4051:ALA:N	2.45	0.49
1:A:1812:ILE:HG21	1:A:2056:SER:HA	1.95	0.49
1:A:2720:ARG:NH2	1:A:3083:PRO:HG3	2.27	0.49
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	1.93	0.49
1:A:3594:GLY:HA3	1:A:3682:ARG:HH12	1.78	0.48
1:A:3828:SER:HB3	1:A:4140:ARG:HG2	1.94	0.48
1:A:4277:SER:HA	1:A:4282:PHE:CG	2.48	0.48
1:A:4596:THR:HG23	1:A:4598:THR:H	1.78	0.48
1:A:2242:GLU:HG3	1:A:2248:GLU:HA	1.95	0.48
1:A:2584:TRP:HE3	1:A:2591:LEU:HG	1.78	0.48
1:A:4087:ALA:O	1:A:4091:GLY:N	2.45	0.48
1:A:3525:ARG:HH22	1:A:3576:ASN:HD21	1.61	0.48
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.95	0.48
1:A:1806:ARG:NH2	1:A:1877:ASP:OD1	2.42	0.48
1:A:2083:GLN:HB2	1:A:2086:TYR:HD2	1.78	0.48
1:A:4391:ILE:O	1:A:4428:ARG:NH2	2.47	0.48
1:A:2635:PHE:CZ	1:A:2650:LEU:HD22	2.48	0.48
1:A:3021:PHE:CD2	1:A:3029:LEU:HD22	2.48	0.48
1:A:3846:LEU:HD21	1:A:3859:ILE:HG13	1.96	0.48
1:A:2506:SER:OG	1:A:2507:ARG:N	2.46	0.48
1:A:3549:ARG:NH2	1:A:3575:GLU:OE2	2.38	0.48
1:A:3590:ILE:HD11	1:A:3700:ASN:ND2	2.28	0.48
1:A:1388:ARG:HA	1:A:1391:LYS:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1547:LEU:HD11	1:A:1612:GLN:HB2	1.94	0.48
1:A:1571:ILE:HG23	1:A:1604:LEU:HD22	1.96	0.48
1:A:1349:GLN:O	1:A:1430:THR:OG1	2.31	0.48
1:A:2203:TRP:CH2	1:A:2236:VAL:HG11	2.49	0.48
1:A:2631:LEU:O	1:A:2635:PHE:HB2	2.13	0.48
1:A:3756:VAL:HG13	1:A:3757:LYS:N	2.29	0.48
1:A:1920:GLY:HA3	1:A:1927:VAL:HG21	1.96	0.48
1:A:4247:MET:HA	1:A:4251:ILE:HB	1.94	0.48
1:A:1626:PHE:CE2	1:A:1628:ARG:HB2	2.49	0.47
1:A:1891:THR:HB	1:A:2039:LEU:HD12	1.96	0.47
1:A:2395:GLN:HB3	1:A:2398:ARG:HH22	1.79	0.47
1:A:1844:PHE:CD2	1:A:1859:ILE:HG12	2.49	0.47
1:A:3788:ASP:N	1:A:3788:ASP:OD1	2.47	0.47
1:A:1466:ILE:HG13	1:A:1500:HIS:ND1	2.28	0.47
1:A:1509:LEU:HB2	1:A:3608:LYS:NZ	2.30	0.47
1:A:2275:TRP:NE1	1:A:2277:ASP:OD1	2.47	0.47
1:A:3591:ASP:N	1:A:3591:ASP:OD1	2.47	0.47
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.49	0.47
1:A:2396:ARG:NH1	1:A:2406:GLU:OE2	2.48	0.47
1:A:2599:SER:OG	1:A:2737:ASP:O	2.32	0.47
1:A:2729:ARG:HE	1:A:2730:HIS:CD2	2.33	0.47
1:A:1356:PRO:HB3	1:A:1401:ILE:HG12	1.97	0.47
1:A:1571:ILE:HG21	1:A:1608:LEU:HG	1.97	0.47
1:A:2514:LEU:O	1:A:2518:ILE:HG12	2.15	0.47
1:A:2224:GLY:H	1:A:2230:LYS:HD3	1.79	0.47
1:A:1403:LEU:HD21	1:A:1446:VAL:HG13	1.96	0.46
1:A:2915:VAL:HG21	2:A:4704:ADP:HN61	1.80	0.46
1:A:3873:ARG:NH1	1:A:4025:LEU:HB3	2.30	0.46
1:A:4313:PRO:HB2	1:A:4315:THR:HG22	1.97	0.46
1:A:1374:PRO:HD2	1:A:1377:LEU:HD12	1.98	0.46
1:A:2912:PHE:CE1	1:A:2915:VAL:HG23	2.50	0.46
1:A:3009:ASN:HD21	1:A:3083:PRO:HD2	1.79	0.46
1:A:3190:LYS:HE3	1:A:3552:TYR:CE2	2.51	0.46
1:A:1599:ARG:HA	1:A:1599:ARG:NE	2.29	0.46
1:A:1892:MET:SD	1:A:1902:GLY:HA3	2.55	0.46
1:A:2591:LEU:HD23	1:A:2592:VAL:N	2.30	0.46
1:A:2683:ILE:HA	1:A:2686:MET:HG2	1.97	0.46
1:A:2921:ARG:O	1:A:2925:ILE:HG12	2.16	0.46
1:A:3211:THR:HG21	1:A:3753:LEU:HD21	1.96	0.46
1:A:3562:TRP:HZ2	1:A:3581:LYS:HD3	1.81	0.46
1:A:1477:LEU:HB3	1:A:1485:ARG:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2666:ILE:O	1:A:2669:PRO:HD2	2.15	0.46
1:A:4485:ARG:NH1	1:A:4513:GLY:O	2.48	0.46
1:A:1855:GLN:HG3	1:A:1867:ASN:HD21	1.81	0.46
1:A:2335:LEU:HD23	1:A:2336:PRO:O	2.16	0.46
1:A:2755:MET:SD	1:A:2807:PHE:HB2	2.56	0.46
1:A:2831:ARG:HB3	1:A:2924:ARG:NH2	2.31	0.46
1:A:2094:LYS:HE2	1:A:2094:LYS:HB3	1.78	0.46
1:A:3202:ASN:O	1:A:3206:ARG:HG3	2.15	0.46
1:A:3627:LEU:HD21	1:A:3662:ILE:HG21	1.98	0.46
1:A:3990:LEU:HA	1:A:4004:MET:HG2	1.97	0.46
1:A:1396:ILE:O	1:A:1400:VAL:HG23	2.16	0.46
1:A:2382:LEU:HD23	1:A:2420:ALA:HB2	1.98	0.46
1:A:3720:GLU:OE1	1:A:3855:ARG:HD3	2.15	0.46
1:A:3756:VAL:HG23	1:A:3760:ILE:HB	1.98	0.46
1:A:1408:LEU:HD12	1:A:1413:TRP:CE3	2.51	0.46
1:A:1587:LEU:HD23	1:A:1589:MET:H	1.81	0.46
1:A:2492:ARG:HD2	1:A:2545:TRP:CE2	2.51	0.46
1:A:3008:MET:HG2	1:A:3066:PHE:HZ	1.80	0.46
1:A:2488:ARG:O	1:A:2492:ARG:HG2	2.16	0.45
1:A:2652:PRO:HD2	1:A:2705:ARG:HH11	1.80	0.45
1:A:4042:LEU:HD12	1:A:4139:LEU:HD23	1.98	0.45
1:A:1507:MET:HG3	1:A:3629:PHE:CE1	2.52	0.45
1:A:2791:HIS:CD2	1:A:3091:LEU:HD11	2.52	0.45
1:A:2999:VAL:HG12	1:A:3078:ARG:NH1	2.30	0.45
1:A:3175:HIS:CE1	1:A:3585:ARG:HH12	2.35	0.45
1:A:2205:GLU:O	1:A:2209:GLN:HG3	2.17	0.45
1:A:2054:LEU:HD21	1:A:2097:LEU:HD12	1.99	0.45
1:A:2065:LEU:HD22	1:A:2137:LEU:HD23	1.98	0.45
1:A:3639:GLU:HB3	1:A:3686:VAL:HG21	1.98	0.45
1:A:2323:LYS:HB3	1:A:2335:LEU:HB3	1.99	0.45
1:A:3811:ILE:HD11	1:A:3864:PHE:CE1	2.52	0.45
1:A:3946:ASP:O	1:A:3950:LYS:HG2	2.16	0.45
1:A:3814:THR:O	1:A:3818:LEU:HG	2.16	0.45
1:A:4096:LEU:HD13	1:A:4105:TRP:HH2	1.82	0.45
1:A:2065:LEU:HD23	1:A:2065:LEU:HA	1.83	0.45
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.98	0.45
1:A:3611:ARG:HH11	1:A:3636:GLN:HE22	1.64	0.45
1:A:4040:PRO:HB3	1:A:4124:LEU:HD23	1.97	0.45
1:A:1406:GLU:H	1:A:3658:GLY:HA3	1.82	0.45
1:A:2076:CYS:HB3	1:A:2088:PHE:CZ	2.51	0.45
1:A:2481:MET:SD	1:A:2481:MET:N	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3725:ASP:OD1	1:A:3728:ARG:NH2	2.50	0.45
1:A:4577:LEU:HD22	1:A:4638:ARG:HD2	1.99	0.45
1:A:2304:ASP:OD1	1:A:2726:ARG:NH2	2.50	0.45
1:A:2412:MET:O	1:A:2416:GLN:HG2	2.17	0.45
1:A:4393:GLN:OE1	1:A:4393:GLN:N	2.37	0.45
1:A:1724:VAL:HA	1:A:1727:PHE:HB2	1.99	0.44
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	2.00	0.44
1:A:2666:ILE:HG22	1:A:2723:LEU:HD21	1.97	0.44
1:A:2845:TRP:O	1:A:2848:GLU:HG3	2.17	0.44
1:A:4038:ASN:HB3	1:A:4118:PRO:HG3	2.00	0.44
1:A:1431:LEU:HD21	1:A:1435:TRP:CZ2	2.52	0.44
1:A:2406:GLU:HG2	1:A:2409:ALA:HB2	2.00	0.44
1:A:2093:LEU:O	1:A:2097:LEU:HD23	2.17	0.44
1:A:4088:VAL:HG23	1:A:4118:PRO:HA	2.00	0.44
1:A:2224:GLY:N	1:A:2230:LYS:HD3	2.33	0.44
1:A:2798:GLU:OE1	1:A:2836:ARG:NH2	2.50	0.44
1:A:4470:PRO:HG3	1:A:4612:ASN:HD22	1.83	0.44
1:A:3627:LEU:HD11	1:A:3662:ILE:HG21	1.99	0.44
1:A:3824:LEU:HD11	1:A:4044:CYS:SG	2.58	0.44
1:A:2890:ARG:O	1:A:2894:LYS:HG2	2.18	0.44
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.99	0.44
1:A:1678:SER:OG	1:A:1679:ARG:N	2.50	0.44
1:A:1911:GLY:O	1:A:1915:SER:OG	2.29	0.44
1:A:2054:LEU:HD23	1:A:2054:LEU:HA	1.80	0.44
1:A:3945:LYS:HB2	1:A:3945:LYS:HE2	1.75	0.44
1:A:2307:VAL:HA	1:A:2311:TRP:CZ2	2.53	0.44
1:A:2684:ARG:HH11	1:A:2726:ARG:HB3	1.83	0.44
1:A:2793:ILE:O	1:A:2793:ILE:HG13	2.17	0.44
1:A:2823:ARG:HH12	1:A:2868:SER:HB3	1.83	0.44
1:A:3562:TRP:HB3	1:A:3567:LEU:HD22	1.99	0.44
1:A:4097:LYS:HA	1:A:4127:THR:OG1	2.17	0.44
1:A:4413:PHE:HD2	1:A:4504:LEU:HD13	1.83	0.44
1:A:1425:VAL:HB	1:A:1428:GLU:HB2	2.00	0.43
1:A:2222:MET:HG2	1:A:2364:PHE:HE1	1.81	0.43
1:A:2609:LEU:HD22	1:A:2617:VAL:HG23	1.99	0.43
1:A:3496:PHE:HE1	1:A:3743:ARG:NH2	2.15	0.43
1:A:3654:ARG:NH2	1:A:3661:LEU:HD22	2.33	0.43
1:A:4543:VAL:HG21	1:A:4622:VAL:HG12	2.00	0.43
1:A:2464:GLN:HG3	1:A:2583:THR:HA	1.98	0.43
1:A:2837:LEU:HD23	1:A:2842:GLU:CB	2.48	0.43
1:A:1539:ASP:HB3	1:A:1543:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1571:ILE:HD11	1:A:1607:LEU:HD12	1.99	0.43
1:A:1607:LEU:O	1:A:1611:ILE:HG12	2.18	0.43
1:A:2285:ARG:HA	1:A:2288:ILE:HG22	2.00	0.43
1:A:2605:LEU:HD11	1:A:2709:VAL:HG12	1.99	0.43
1:A:2818:VAL:O	1:A:2822:ILE:HG12	2.17	0.43
1:A:3097:TRP:HE3	1:A:3102:LEU:HD23	1.83	0.43
1:A:3175:HIS:CG	1:A:3585:ARG:HH12	2.36	0.43
1:A:1803:LEU:HD11	1:A:1875:VAL:HG21	2.00	0.43
1:A:2169:GLN:OE1	1:A:2171:HIS:NE2	2.50	0.43
1:A:1391:LYS:O	1:A:1395:LYS:HG2	2.18	0.43
1:A:1486:LEU:HB3	1:A:1541:GLN:NE2	2.34	0.43
1:A:1661:VAL:HG13	1:A:1676:ILE:HG23	2.00	0.43
1:A:1671:SER:O	1:A:1692:ILE:HG22	2.19	0.43
1:A:2943:LYS:HG2	1:A:3094:PHE:CZ	2.53	0.43
1:A:2976:LEU:HA	1:A:2979:VAL:HG12	2.00	0.43
1:A:1391:LYS:HE2	1:A:1391:LYS:HB3	1.82	0.43
1:A:1475:LEU:HD13	1:A:1487:ILE:HD13	2.01	0.43
1:A:1750:VAL:HG12	1:A:1811:LEU:HD21	2.00	0.43
1:A:2762:LEU:HD12	1:A:2765:TYR:CD2	2.53	0.43
1:A:3792:GLN:O	1:A:3796:THR:HG23	2.19	0.43
1:A:2478:ASP:OD1	1:A:2479:PHE:N	2.52	0.43
1:A:1463:LEU:O	1:A:1466:ILE:HG22	2.19	0.43
1:A:2138:ILE:HG13	1:A:2161:LEU:HD21	2.00	0.43
1:A:3614:PHE:HE2	1:A:3642:ASP:H	1.66	0.43
1:A:4480:SER:O	1:A:4483:SER:OG	2.22	0.43
1:A:1738:TYR:HE2	1:A:1792:LEU:HD21	1.84	0.42
1:A:2965:ARG:O	1:A:2966:LYS:HG3	2.19	0.42
1:A:2826:ALA:O	1:A:2830:LEU:HD23	2.19	0.42
1:A:2972:PHE:HD1	1:A:3004:PHE:CD1	2.37	0.42
1:A:4027:LEU:O	1:A:4031:VAL:HG22	2.19	0.42
1:A:1393:TYR:HA	1:A:1396:ILE:HG12	2.01	0.42
1:A:1925:ARG:HG2	1:A:1954:TRP:CD1	2.54	0.42
1:A:2123:ASP:O	1:A:2127:ILE:HG13	2.20	0.42
1:A:2499:LEU:HD21	1:A:2515:GLY:HA2	2.01	0.42
1:A:3597:THR:O	1:A:3601:MET:HG3	2.19	0.42
1:A:3944:PHE:CE1	1:A:3974:TRP:HB3	2.54	0.42
1:A:1769:MET:HE2	1:A:1775:ALA:HA	2.02	0.42
1:A:2834:GLN:HE21	1:A:2843:ARG:HB3	1.84	0.42
1:A:3044:LEU:HD13	1:A:3049:GLU:HG3	2.01	0.42
1:A:4288:VAL:O	1:A:4319:SER:OG	2.27	0.42
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2211:TYR:O	1:A:2214:THR:OG1	2.34	0.42
1:A:2484:GLU:O	1:A:2487:GLU:HG3	2.19	0.42
1:A:3122:VAL:HG11	1:A:3136:PRO:HB2	2.01	0.42
1:A:3872:ALA:O	1:A:3880:HIS:NE2	2.52	0.42
1:A:4205:TYR:HE2	1:A:4256:VAL:HA	1.84	0.42
1:A:4393:GLN:HG2	1:A:4394:THR:HG22	2.00	0.42
1:A:3608:LYS:HE2	1:A:3631:ASN:HB3	2.02	0.42
1:A:2265:TYR:OH	1:A:2315:LEU:HG	2.20	0.42
1:A:2522:THR:HG21	1:A:2526:LEU:HD11	2.02	0.42
1:A:2596:PRO:O	1:A:2601:LYS:NZ	2.53	0.42
1:A:3743:ARG:HA	1:A:3746:GLU:HG2	2.01	0.42
1:A:4189:ILE:O	1:A:4193:ARG:N	2.52	0.42
1:A:2091:ARG:NH2	2:A:4701:ADP:O3'	2.52	0.42
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	2.01	0.42
1:A:2534:ILE:HD12	1:A:2534:ILE:H	1.85	0.42
1:A:3916:LEU:HD12	1:A:3933:GLU:HG3	2.02	0.42
1:A:4174:ASN:N	1:A:4174:ASN:OD1	2.52	0.42
1:A:1662:SER:HB2	1:A:1679:ARG:HG3	2.01	0.42
1:A:3510:SER:HB3	1:A:3553:LEU:HD11	2.01	0.42
1:A:1544:TRP:HE1	1:A:1572:SER:HA	1.85	0.42
1:A:2065:LEU:HD21	1:A:2134:GLN:HG2	2.02	0.42
1:A:2079:GLN:HB2	1:A:2160:LEU:HD11	2.02	0.42
1:A:2461:MET:HG2	1:A:2493:TYR:CE2	2.54	0.42
1:A:4496:ALA:HB2	1:A:4504:LEU:HD21	2.01	0.42
1:A:1495:ASN:HA	1:A:1498:LYS:NZ	2.35	0.41
1:A:1658:PHE:HB2	1:A:1661:VAL:HB	2.02	0.41
1:A:2606:PHE:CE1	1:A:2617:VAL:HG21	2.55	0.41
1:A:2976:LEU:O	1:A:2980:LEU:HD23	2.20	0.41
1:A:4489:LEU:HA	1:A:4492:ILE:HG22	2.00	0.41
1:A:1949:CYS:HB3	1:A:2007:LYS:O	2.20	0.41
1:A:1980:GLU:O	1:A:1984:GLU:HG2	2.20	0.41
1:A:2308:ASP:OD1	1:A:2311:TRP:NE1	2.53	0.41
1:A:2718:PRO:HB2	1:A:3080:ALA:HB2	2.02	0.41
1:A:3772:ASN:HA	1:A:3775:ARG:HE	1.85	0.41
1:A:4269:LEU:HD23	1:A:4269:LEU:HA	1.90	0.41
1:A:1412:HIS:CE1	1:A:1453:ALA:HA	2.55	0.41
1:A:1499:GLU:HG2	1:A:3621:LYS:HD2	2.02	0.41
1:A:1623:ARG:HE	1:A:1637:LEU:HD22	1.85	0.41
1:A:1797:LEU:HD21	1:A:2128:ALA:HB2	2.01	0.41
1:A:1855:GLN:HG3	1:A:1867:ASN:ND2	2.35	0.41
1:A:3551:GLU:OE2	1:A:3559:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4332:LEU:HD23	1:A:4332:LEU:HA	1.87	0.41
1:A:2182:LEU:HD11	1:A:2207:VAL:HG11	2.02	0.41
1:A:2446:ILE:HG22	1:A:2505:ASP:HB3	2.02	0.41
1:A:3872:ALA:HA	1:A:3875:MET:HE2	2.02	0.41
1:A:4260:PHE:CE2	1:A:4608:PRO:HB3	2.55	0.41
1:A:4554:ASP:N	1:A:4557:SER:OG	2.52	0.41
1:A:2220:LEU:O	1:A:2342:MET:HA	2.20	0.41
1:A:2275:TRP:CZ2	1:A:2327:LEU:HD12	2.56	0.41
1:A:2395:GLN:HB3	1:A:2398:ARG:NH2	2.35	0.41
1:A:3197:GLN:HG2	1:A:3496:PHE:CZ	2.56	0.41
1:A:3596:ALA:HB2	1:A:3701:PHE:CE2	2.55	0.41
1:A:4628:THR:C	1:A:4629:LYS:HD2	2.41	0.41
1:A:1397:ASN:O	1:A:1401:ILE:HG13	2.21	0.41
1:A:2227:GLY:H	3:A:4702:ATP:PG	2.44	0.41
1:A:2387:LEU:HD23	1:A:2467:ARG:NH2	2.36	0.41
1:A:2839:GLU:HB2	1:A:2842:GLU:OE1	2.20	0.41
1:A:3782:ARG:O	1:A:3786:GLU:HG2	2.20	0.41
1:A:4423:LEU:HD13	1:A:4466:HIS:HD2	1.86	0.41
1:A:1486:LEU:HA	1:A:1579:MET:HE2	2.03	0.41
1:A:2253:ILE:HG21	1:A:2689:HIS:CE1	2.56	0.41
1:A:4594:LYS:HE3	1:A:4594:LYS:HB2	1.97	0.41
1:A:1509:LEU:HB2	1:A:3608:LYS:HZ1	1.86	0.41
1:A:1626:PHE:HB3	1:A:1629:PHE:CD2	2.56	0.41
1:A:1841:GLN:O	1:A:1843:ARG:HG3	2.21	0.41
1:A:1947:GLY:O	1:A:1951:VAL:HG12	2.21	0.41
1:A:2072:PHE:CZ	1:A:2161:LEU:HD13	2.56	0.41
1:A:2231:SER:HA	1:A:2234:TRP:NE1	2.36	0.41
1:A:2704:GLU:O	1:A:2706:ILE:HG12	2.21	0.41
1:A:2987:ASN:OD1	1:A:3061:ASN:ND2	2.54	0.41
1:A:4156:ASN:ND2	1:A:4188:ALA:HA	2.35	0.41
1:A:4308:TRP:CH2	1:A:4312:LEU:HD21	2.56	0.41
1:A:4482:PHE:CE2	1:A:4486:ILE:HG13	2.56	0.41
1:A:1407:ALA:O	1:A:1453:ALA:HB1	2.21	0.41
1:A:2086:TYR:OH	1:A:2149:LEU:HD13	2.22	0.41
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	2.03	0.41
1:A:2775:GLU:O	1:A:2778:THR:OG1	2.29	0.41
1:A:2784:PHE:HB3	1:A:2792:TYR:HD1	1.84	0.41
1:A:3009:ASN:HD21	1:A:3083:PRO:CD	2.33	0.41
1:A:3601:MET:HE1	1:A:3611:ARG:NE	2.35	0.41
1:A:3766:ILE:HD12	1:A:3766:ILE:HA	1.91	0.41
1:A:4264:LEU:O	1:A:4267:THR:OG1	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4266:ASN:O	1:A:4270:GLU:HG2	2.21	0.41
1:A:3150:VAL:HG22	1:A:3532:TRP:CD1	2.56	0.40
1:A:3652:GLU:O	1:A:3652:GLU:HG3	2.21	0.40
1:A:3972:TYR:O	1:A:3973:LEU:HD23	2.21	0.40
1:A:4194:LEU:HD11	1:A:4204:LYS:HA	2.03	0.40
1:A:1445:ILE:O	1:A:1449:VAL:HG23	2.22	0.40
1:A:3178:ASP:OD2	1:A:3182:HIS:ND1	2.54	0.40
1:A:2069:ILE:HD12	1:A:2069:ILE:HA	1.95	0.40
1:A:2584:TRP:CZ3	1:A:2732:PRO:HB2	2.56	0.40
1:A:1763:GLU:OE2	1:A:1845:TYR:OH	2.32	0.40
1:A:1961:ASN:ND2	1:A:2019:ASN:H	2.19	0.40
1:A:2220:LEU:HD11	1:A:2342:MET:SD	2.62	0.40
1:A:2797:ARG:HH12	1:A:3088:ARG:HH12	1.69	0.40
1:A:2982:ARG:HE	1:A:2988:GLU:CD	2.25	0.40
1:A:3008:MET:CE	1:A:3064:VAL:HG11	2.51	0.40
1:A:3016:GLU:N	1:A:3016:GLU:OE2	2.55	0.40
1:A:3474:ARG:HB3	1:A:3764:ASP:HB3	2.04	0.40
1:A:4324:PRO:HD3	1:A:4638:ARG:HG3	2.02	0.40
1:A:1414:LYS:HB2	1:A:1414:LYS:HE2	1.79	0.40
1:A:1424:TRP:NE1	1:A:1433:GLN:HB3	2.36	0.40
1:A:1478:VAL:HG21	1:A:1488:ARG:NH2	2.36	0.40
1:A:2281:THR:HG21	1:A:2327:LEU:HD11	2.02	0.40
1:A:2747:ILE:HD11	2:A:4703:ADP:N1	2.36	0.40
1:A:2965:ARG:HA	1:A:2965:ARG:NE	2.36	0.40
1:A:3169:MET:HB3	1:A:3693:CYS:SG	2.61	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	3035/4646 (65%)	2952 (97%)	83 (3%)	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	2706/4125 (66%)	2704 (100%)	2 (0%)	92 97

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

Mol	Chain	Res	Type
1	A	2671	MET
1	A	2966	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1495	ASN
1	A	2416	GLN
1	A	3038	GLN
1	A	3535	HIS
1	A	3865	GLN
1	A	3869	ASN

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, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	A	4704	-	24,29,29	0.84	0	29,45,45	1.24	2 (6%)
2	ADP	A	4703	-	24,29,29	0.87	0	29,45,45	1.24	2 (6%)
2	ADP	A	4701	4	24,29,29	0.89	0	29,45,45	1.20	2 (6%)
3	ATP	A	4702	4	28,33,33	0.72	0	34,52,52	0.59	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	4704	-	-	2/12/32/32	0/3/3/3
2	ADP	A	4703	-	-	5/12/32/32	0/3/3/3
2	ADP	A	4701	4	-	3/12/32/32	0/3/3/3
3	ATP	A	4702	4	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	N3-C2-N1	-3.76	123.57	128.67
2	A	4701	ADP	N3-C2-N1	-3.72	123.62	128.67
2	A	4704	ADP	N3-C2-N1	-3.59	123.80	128.67
2	A	4704	ADP	C4-C5-N7	-2.55	106.64	109.34
2	A	4703	ADP	C4-C5-N7	-2.40	106.81	109.34
3	A	4702	ATP	C5-C6-N6	2.35	123.89	120.31
2	A	4701	ADP	C4-C5-N7	-2.23	106.98	109.34

There are no chirality outliers.

All (14) torsion outliers are listed below:

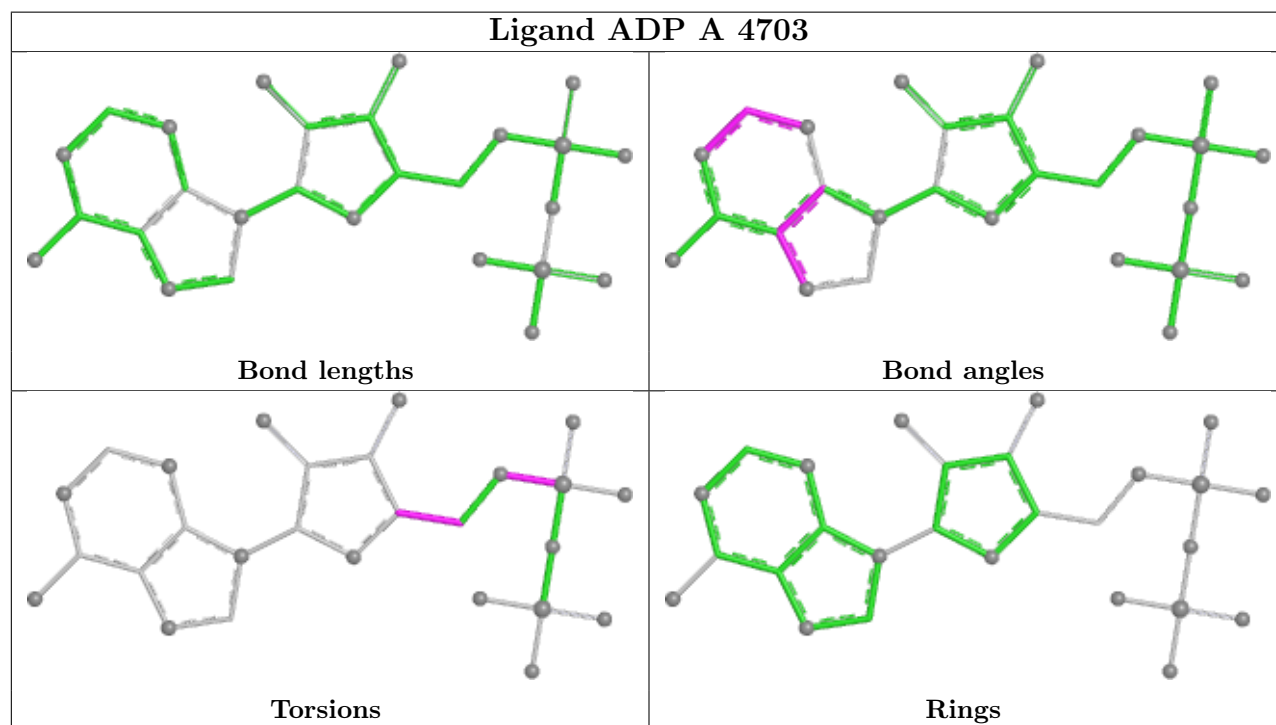
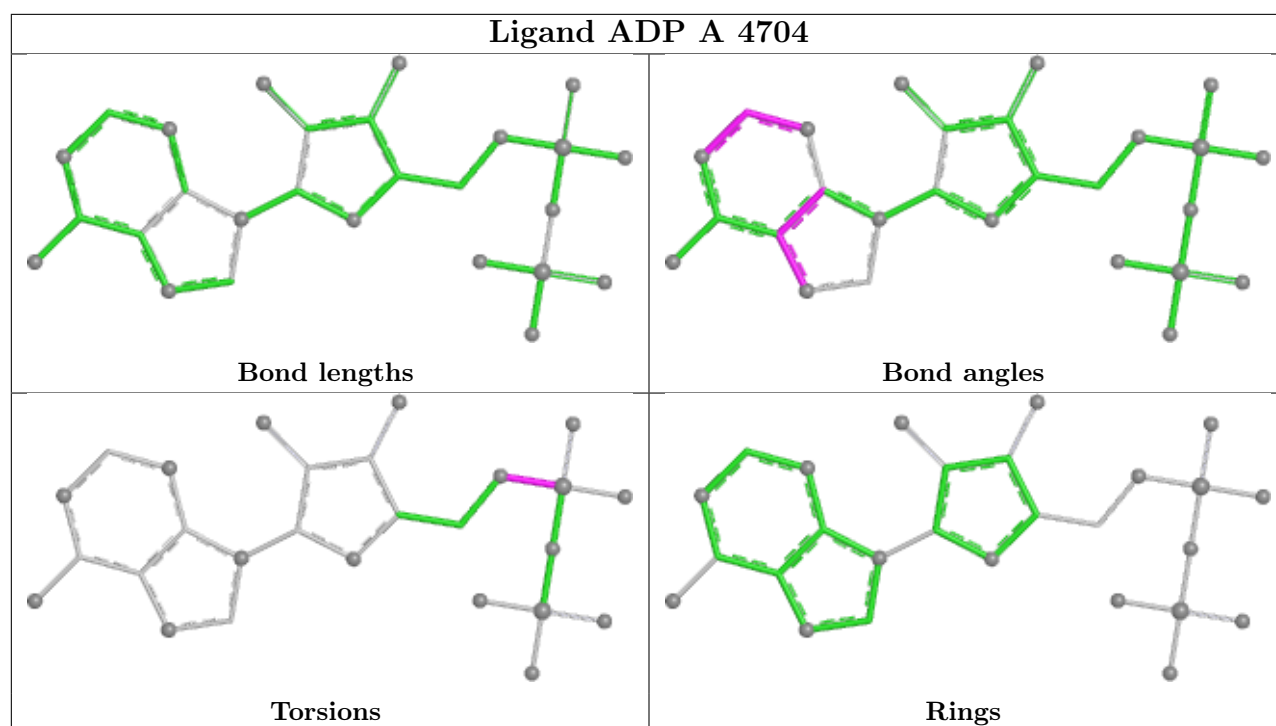
Mol	Chain	Res	Type	Atoms
2	A	4703	ADP	C5'-O5'-PA-O1A
2	A	4703	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A
2	A	4703	ADP	O4'-C4'-C5'-O5'
3	A	4702	ATP	PB-O3B-PG-O1G
2	A	4703	ADP	C3'-C4'-C5'-O5'
3	A	4702	ATP	PB-O3B-PG-O3G
3	A	4702	ATP	PA-O3A-PB-O1B
2	A	4703	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	O4'-C4'-C5'-O5'
2	A	4701	ADP	PB-O3A-PA-O2A
2	A	4701	ADP	PB-O3A-PA-O1A
3	A	4702	ATP	PA-O3A-PB-O2B

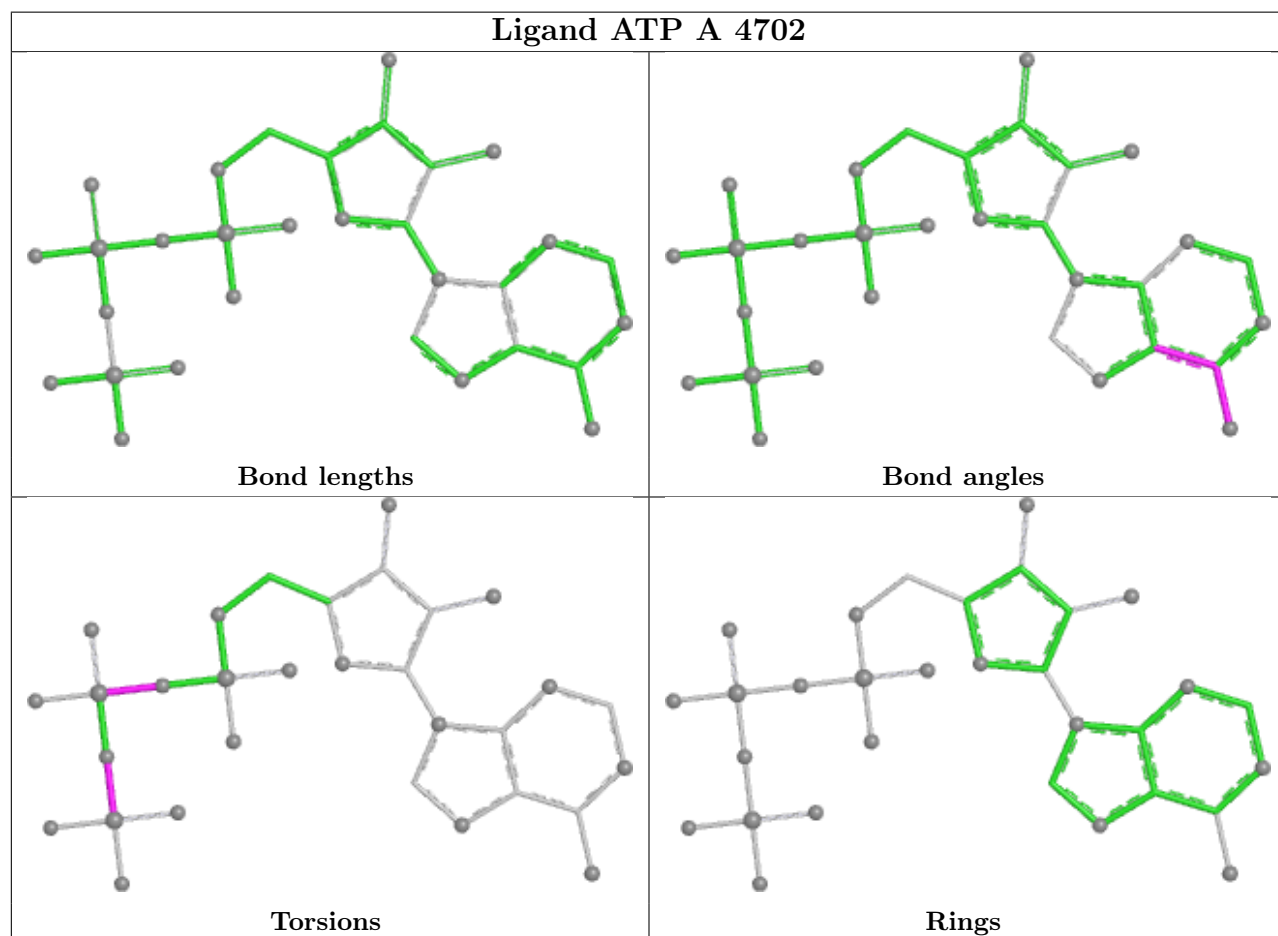
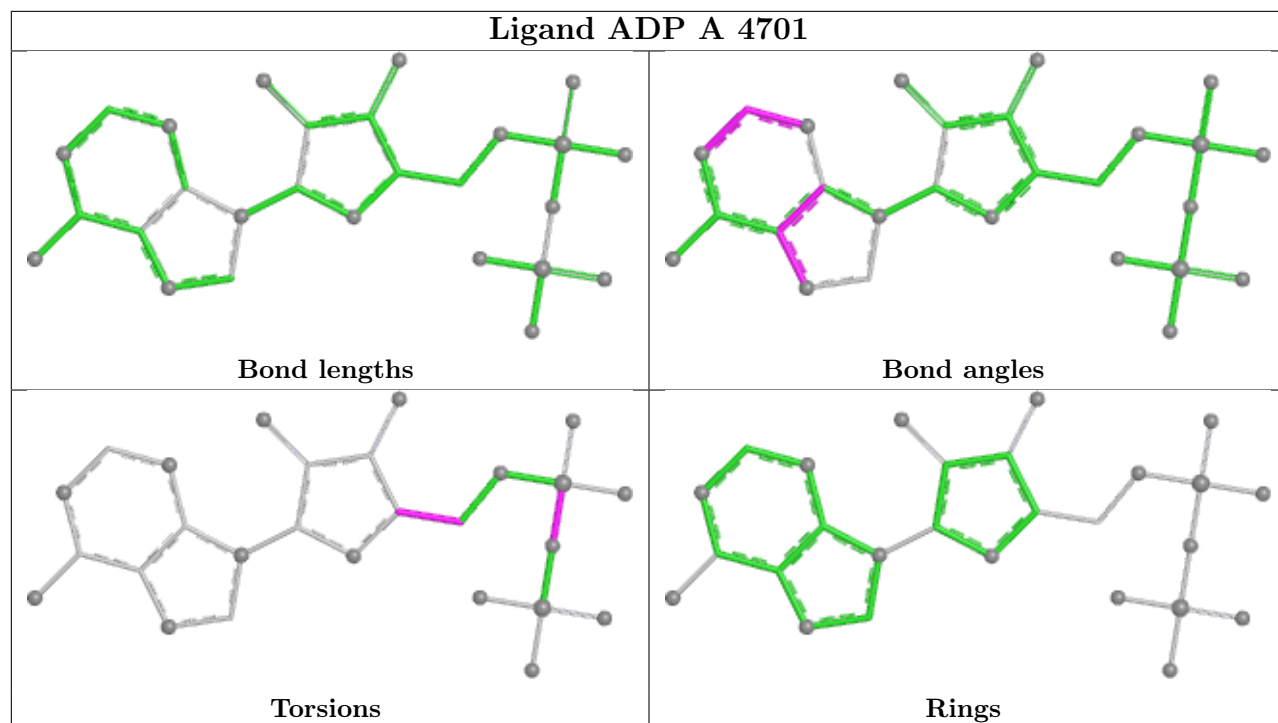
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4704	ADP	2	0
2	A	4703	ADP	1	0
2	A	4701	ADP	2	0
3	A	4702	ATP	1	0

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





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

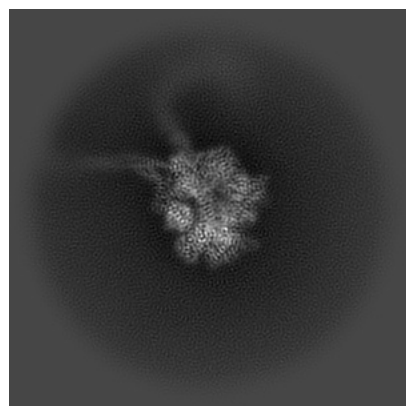
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44694. These allow visual inspection of the internal detail of the map and identification of artifacts.

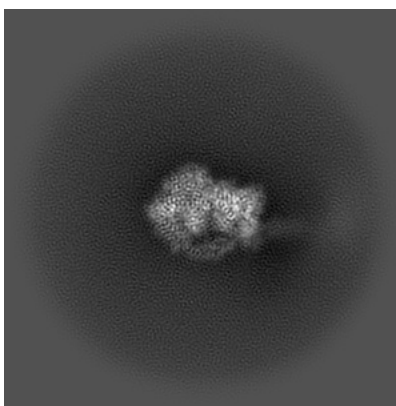
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

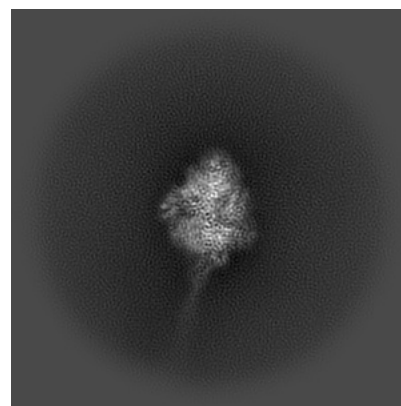
6.1.1 Primary map



X

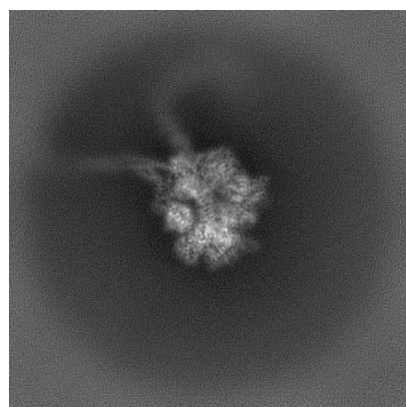


Y

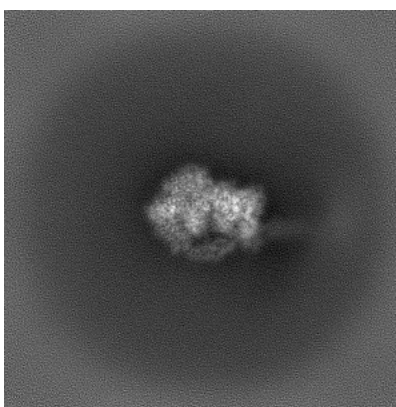


Z

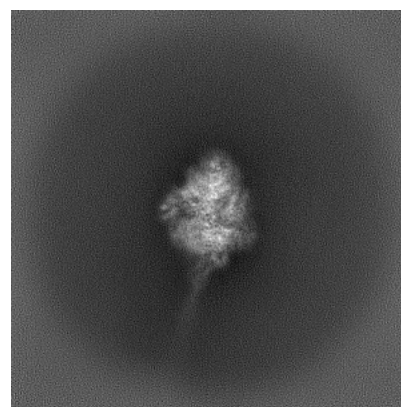
6.1.2 Raw map



X



Y

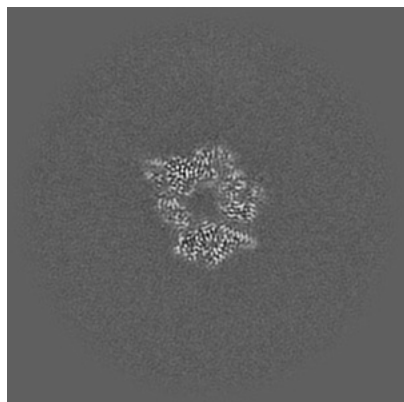


Z

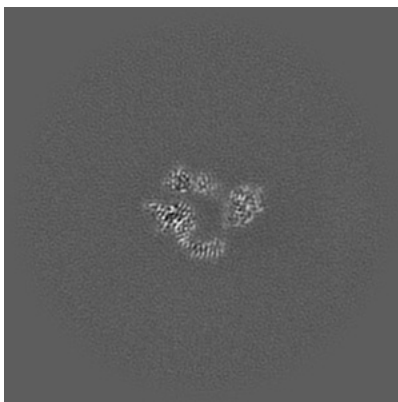
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

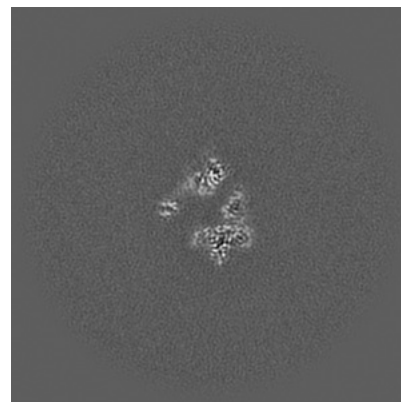
6.2.1 Primary map



X Index: 192



Y Index: 192

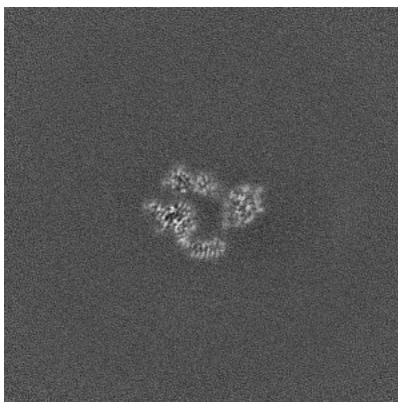


Z Index: 192

6.2.2 Raw map



X Index: 192



Y Index: 192

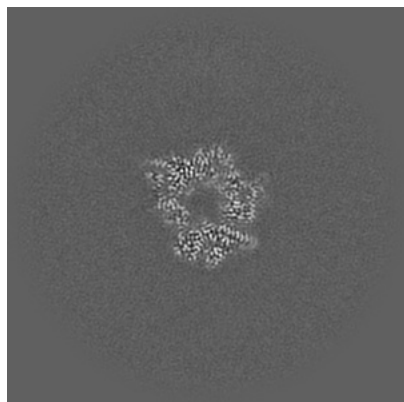


Z Index: 192

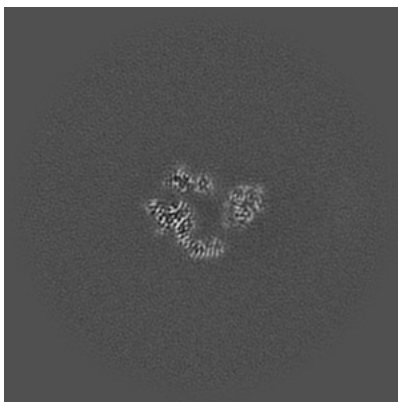
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

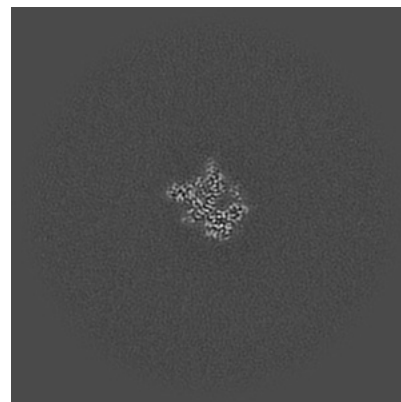
6.3.1 Primary map



X Index: 193

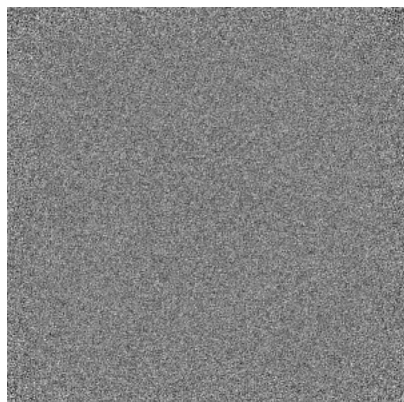


Y Index: 193

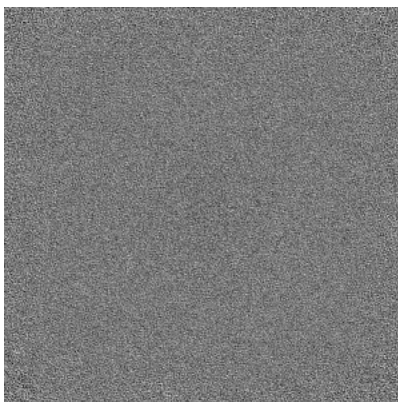


Z Index: 162

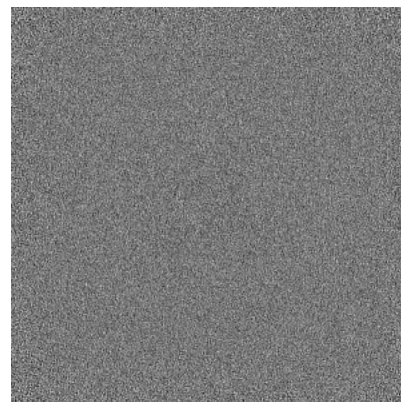
6.3.2 Raw map



X Index: 0



Y Index: 0

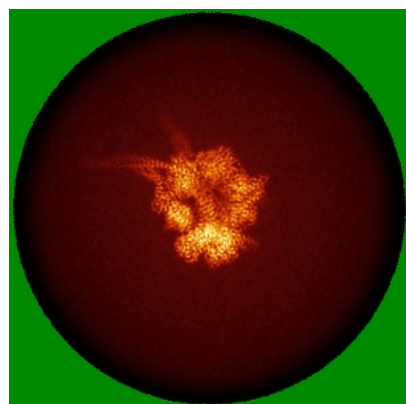


Z Index: 0

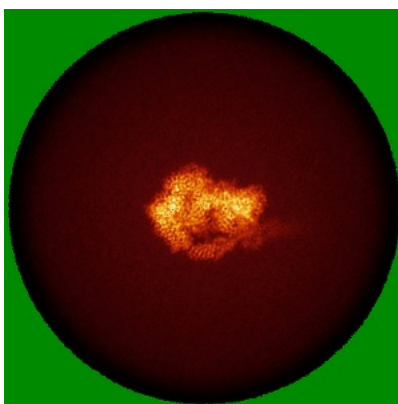
The images above show the largest variance slices of the map in three orthogonal directions.

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

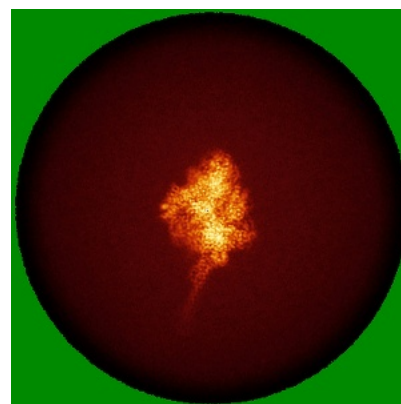
6.4.1 Primary map



X

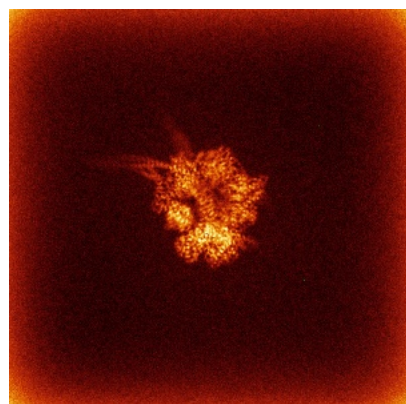


Y

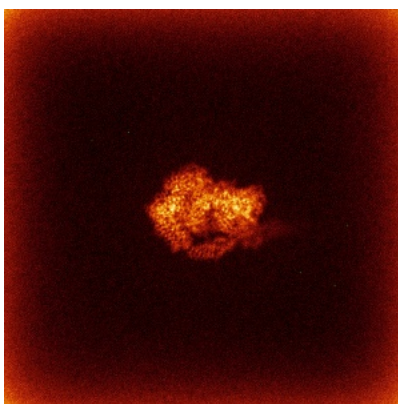


Z

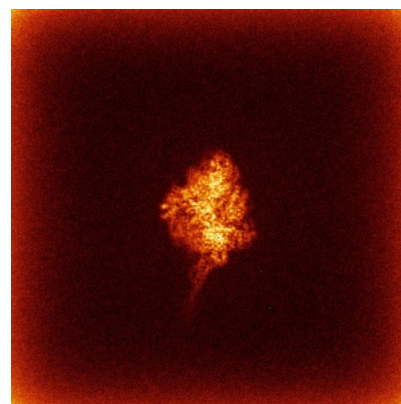
6.4.2 Raw map



X



Y

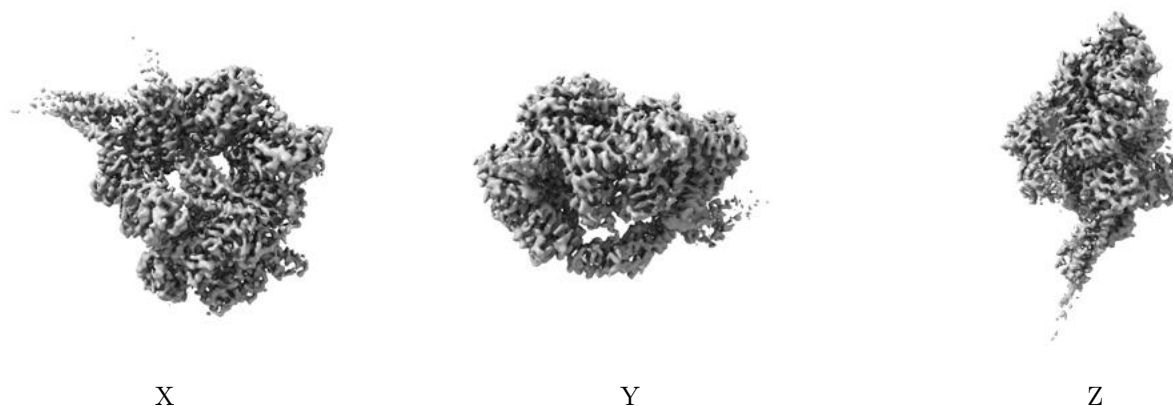


Z

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.

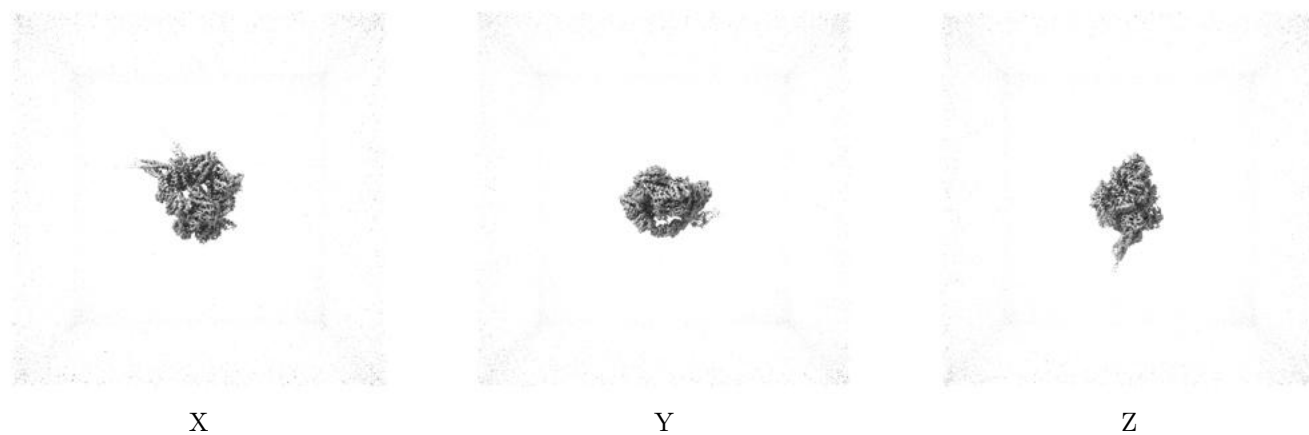
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

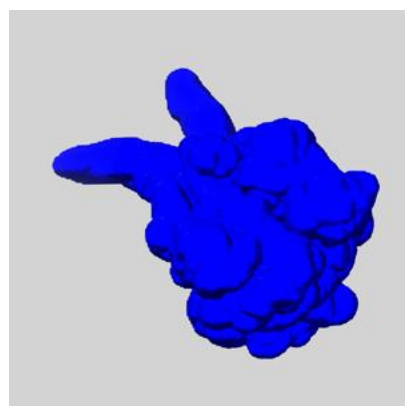
6.6 Mask visualisation [i](#)

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

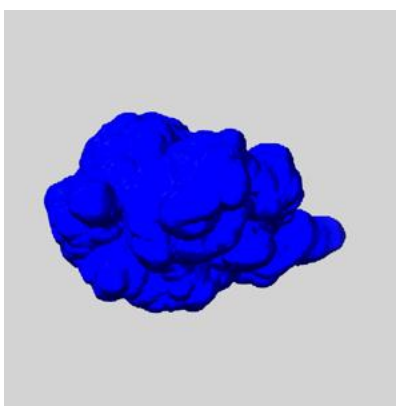
A mask typically either:

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

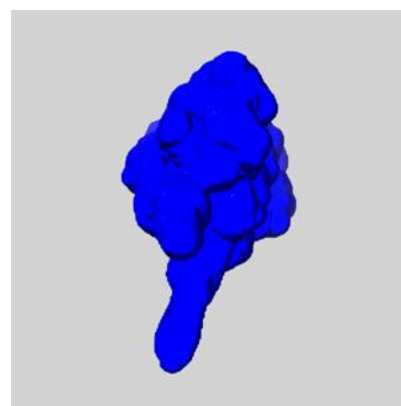
6.6.1 emd_44694_msk_1.map [i](#)



X



Y

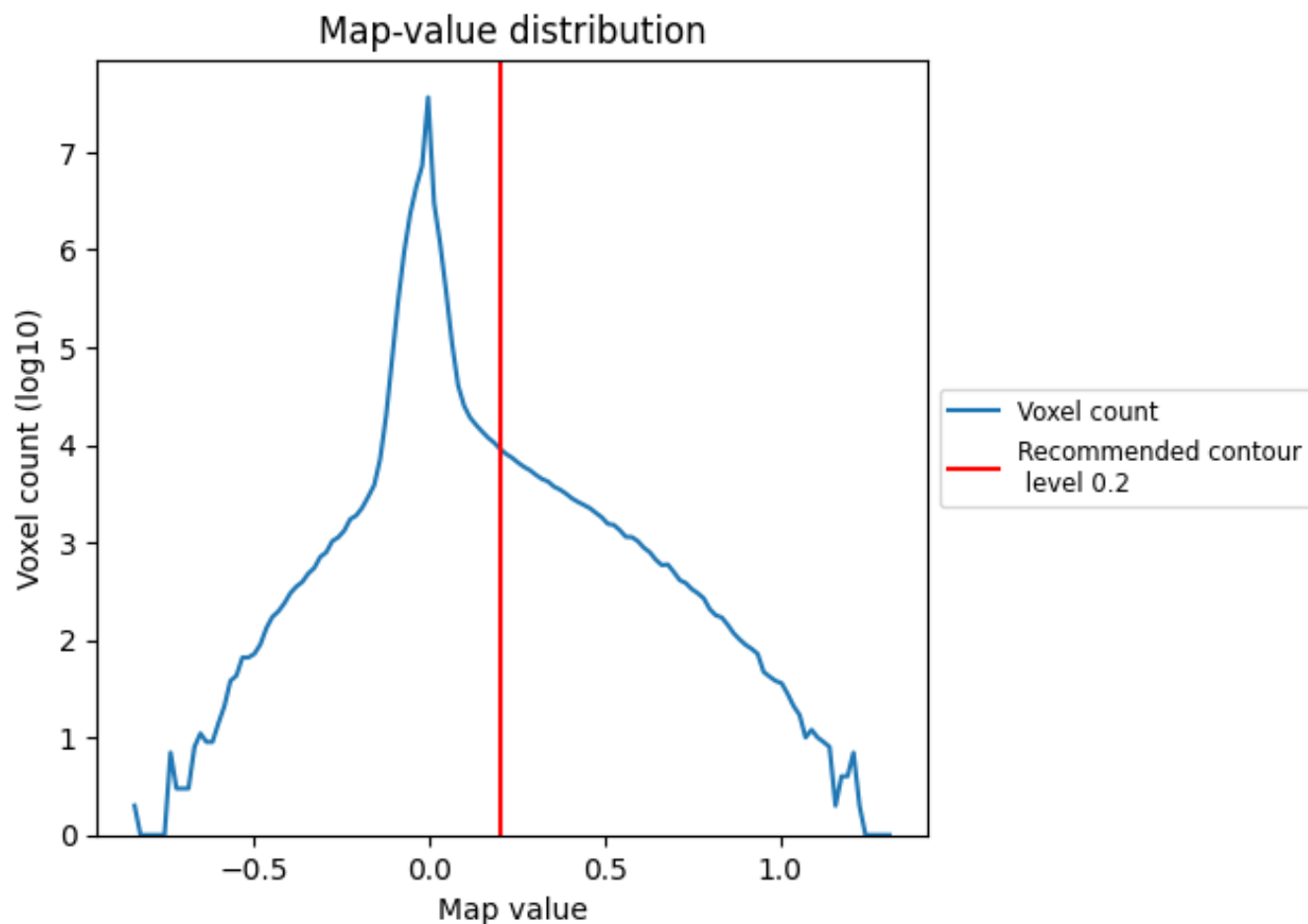


Z

7 Map analysis [i](#)

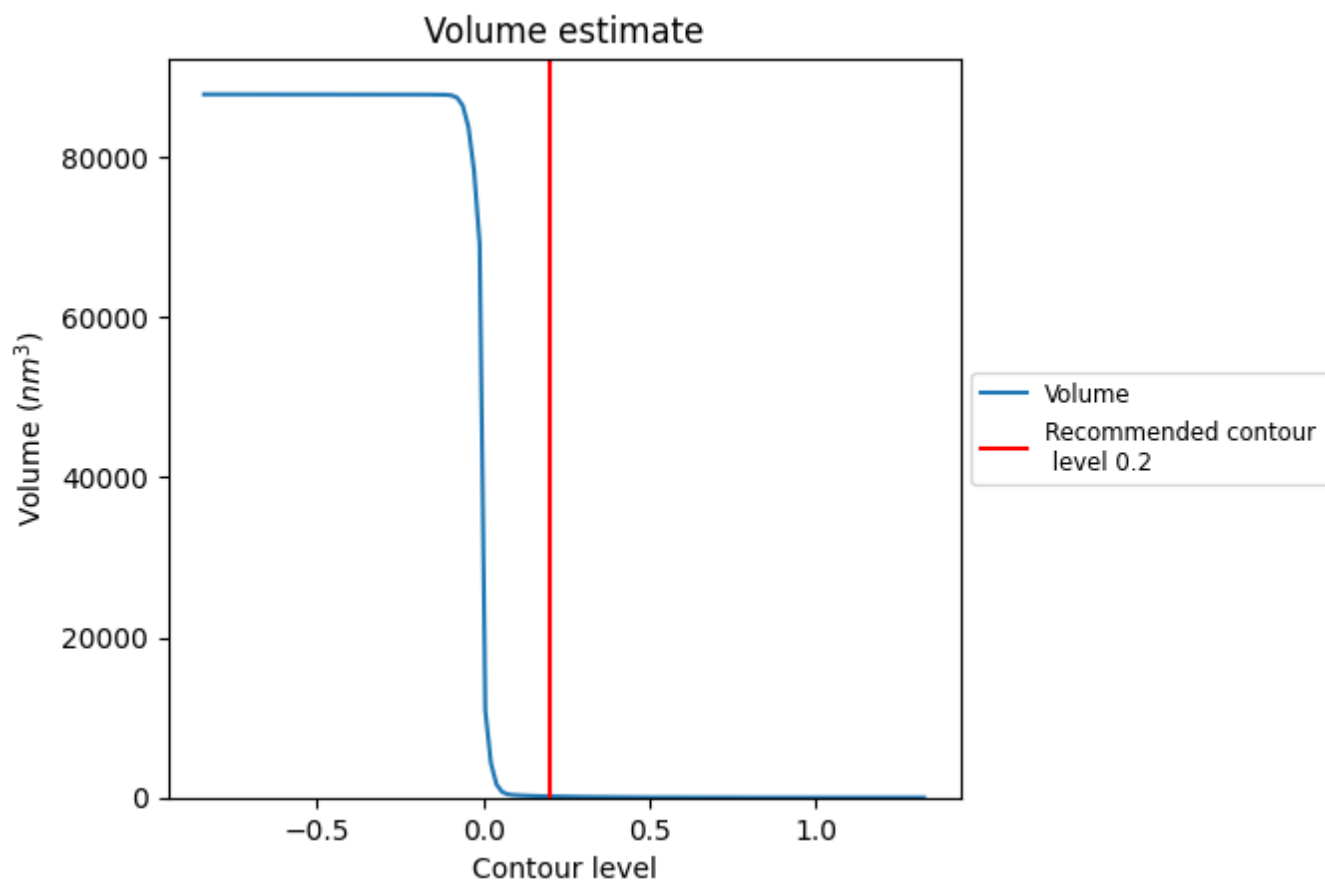
This section contains the results of statistical analysis of the map.

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.

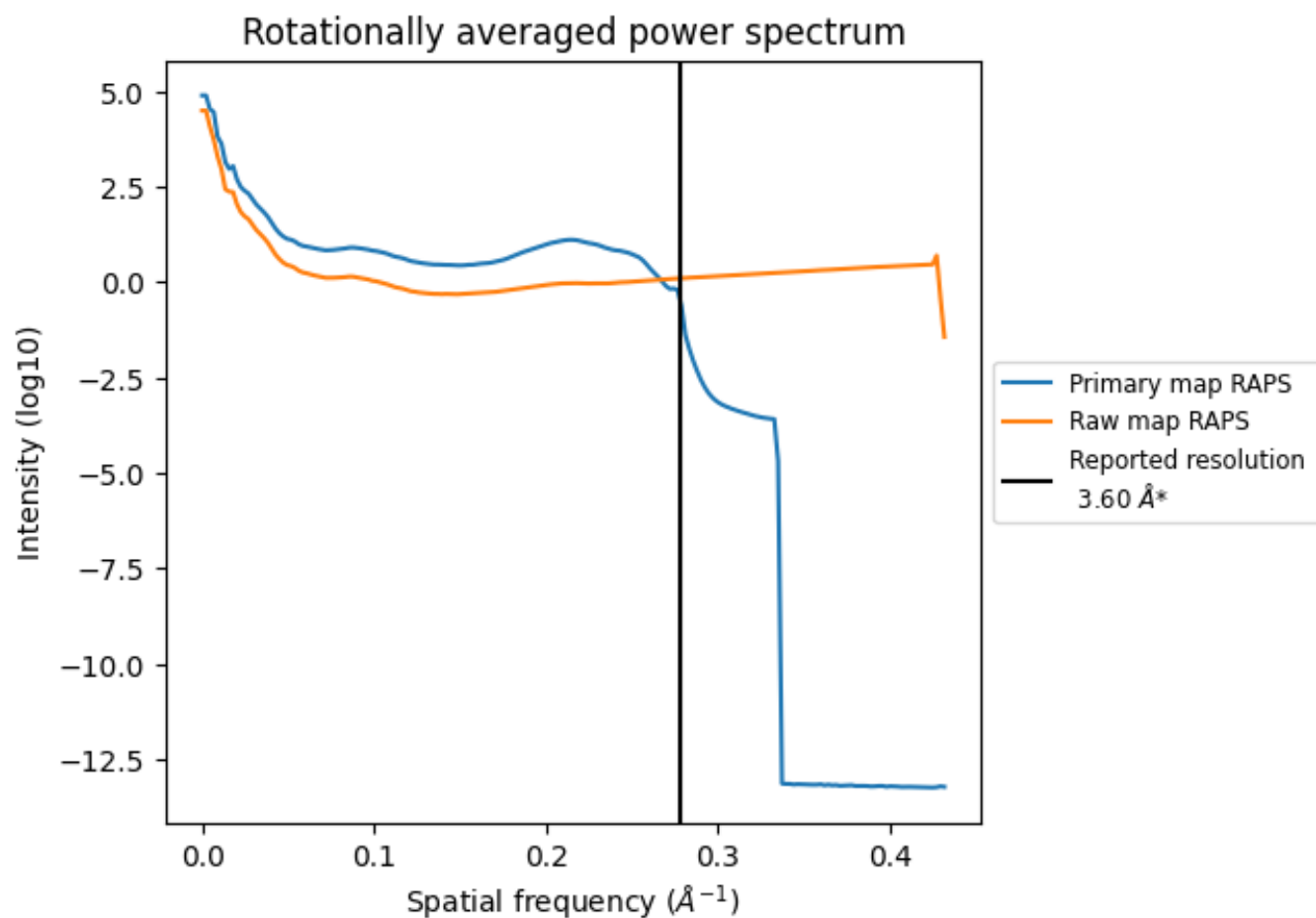
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 149 nm^3 ; this corresponds to an approximate mass of 134 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 ⓘ

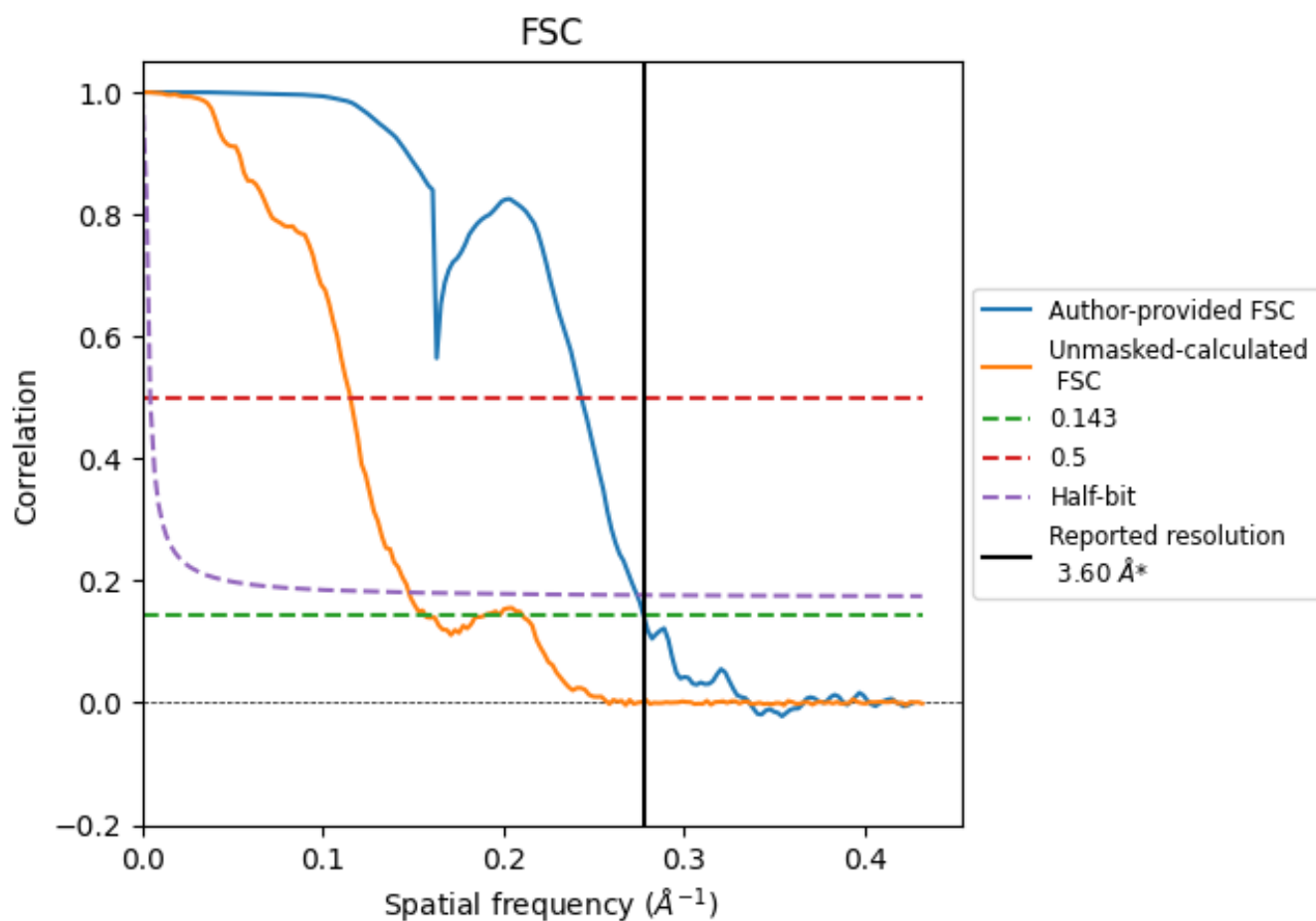


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 \AA^{-1}

8.2 Resolution estimates

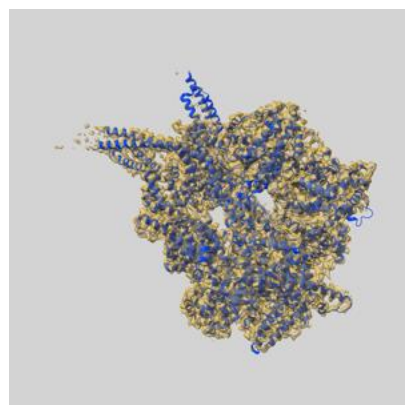
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.11	3.65
Unmasked-calculated*	6.37	8.67	6.77

*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 6.37 differs from the reported value 3.6 by more than 10 %

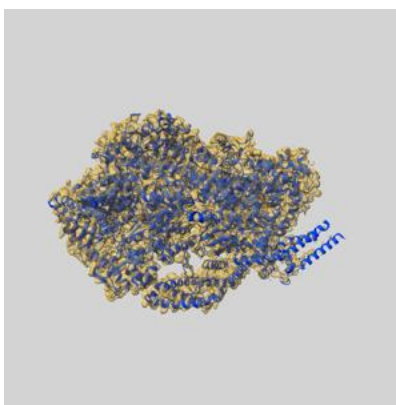
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44694 and PDB model 9BMB. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

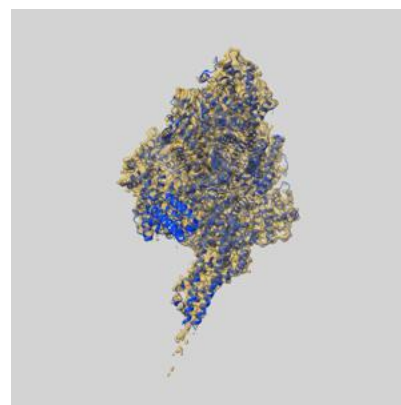
9.1 Map-model overlay [i](#)



X



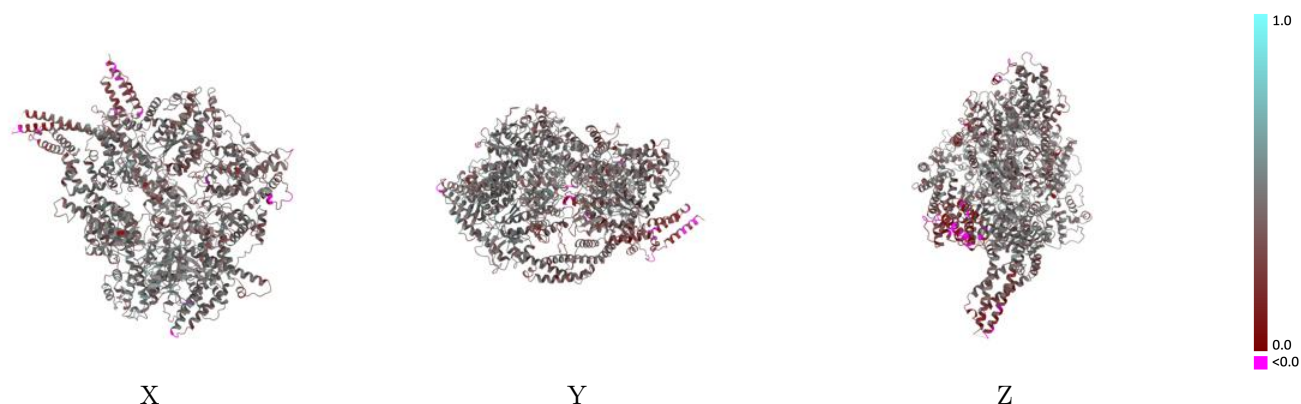
Y



Z

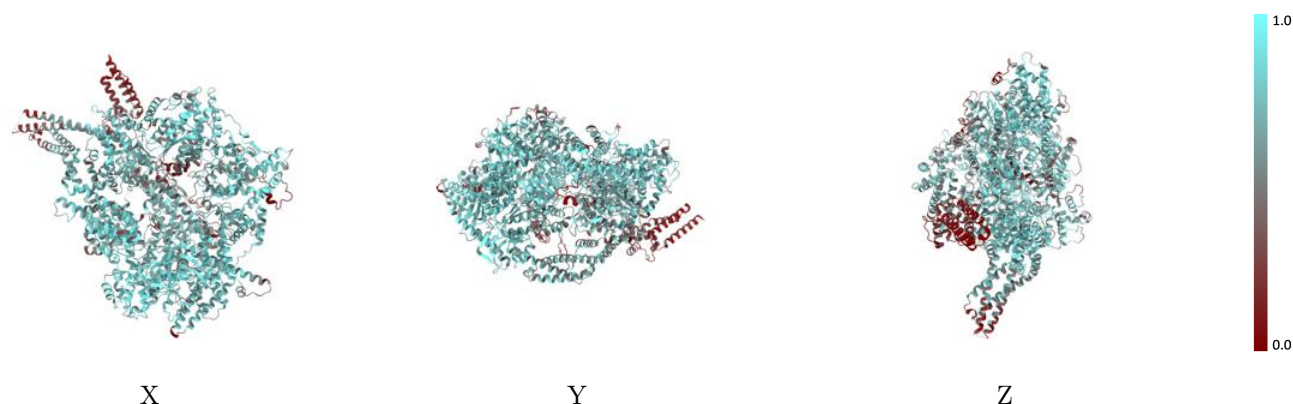
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



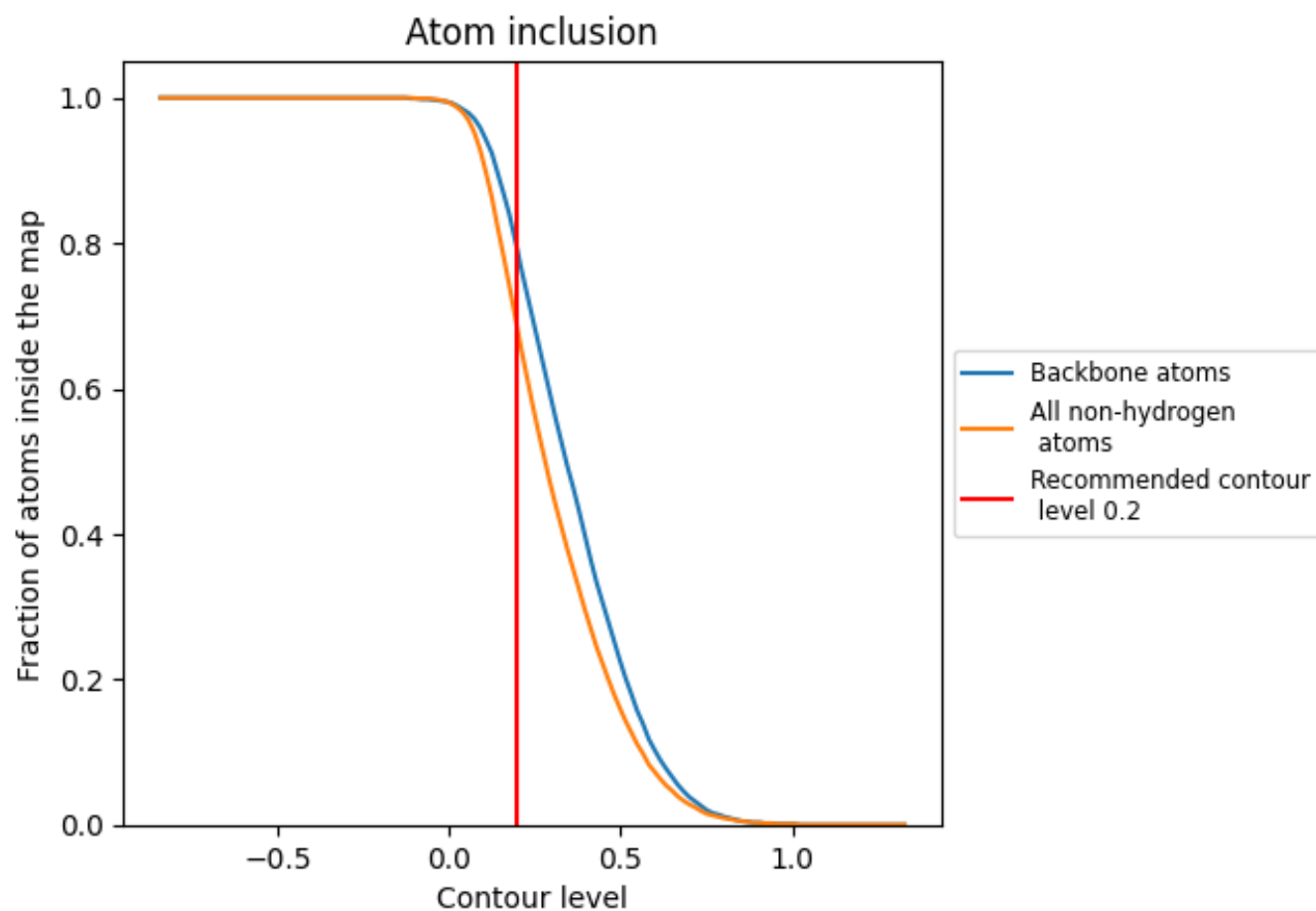
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 68% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6810	<div></div> 0.4140
A	<div></div> 0.6810	<div></div> 0.4140

