



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:15 PM UTC

PDB ID : 9BMA / pdb_00009bma
EMDB ID : EMD-44693
Title : Motor domain from full-length human dynein-1 bound to microtubules in apo condition
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

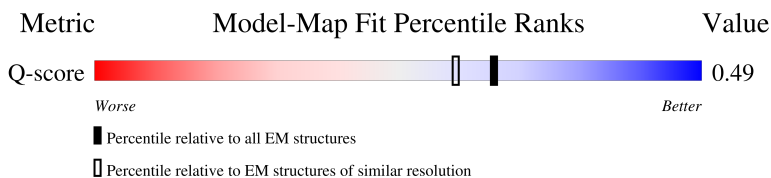
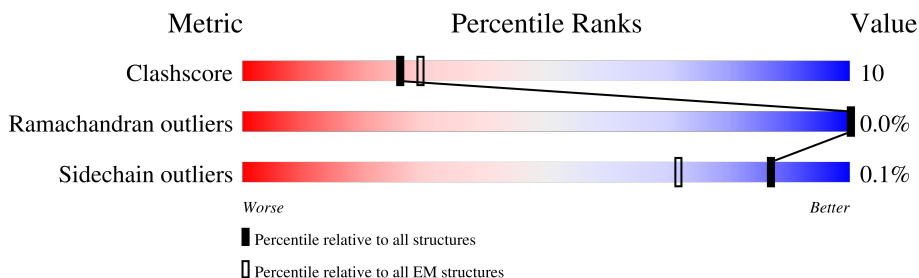
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 24476 atoms, of which 0 are hydrogens and 0 are deuteriums.

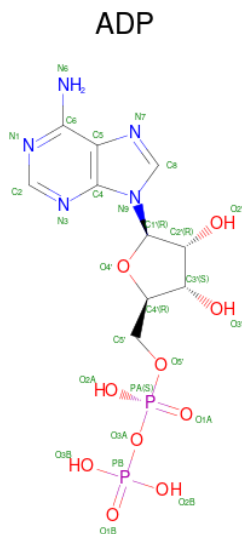
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- 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	3029	24390	15542	4208	4518	122	0	0

- Molecule 2 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 27	C 10	N 5	O 10	P 2	0
3	A	1	Total 27	C 10	N 5	O 10	P 2	0

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

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	

G2119	E2120	A2121	V2122	D2123	E2126	I2127	A2128	E2129	N2130	L2131	P2132	E2133	Q2134	C2142	V2146	P2147	K2148	L2156	L2160	E2174	E2181	M2189	Y2190	G2200	V2204	V2207	L2210	Q2211	Q2212	I2213	Q2214	Q2215	I2216	R2217	H2218	M2221	G2224	S2228	G2229	K2230	S2231	W2234	R2235															
L2002	N2003	L2016	T2017	M2018	N2019	P2020	G2021	TYR	ALA	GLY	ARG	S2026	N2027	L2028	P2029	D2030	N2031	L2032	K2033	K2034	L2035	F2036	L2039	K2043	P2044	D2045	Q2047	Q2051	V2052	M2053	L2054	R2060	L2065	H2068	Y2068	D2087	K2094	L2097	E2106	R2107	I2108	R2113	E2114	K2115	E2116	E2117	R2118											
Q1856	L1857	I1859	T1860	M1861	A1862	Y1868	E1871	D1877	C1888	Y1889	L1890	T1891	M1931	G1932	D1933	E1934	R1943	E1959	F1960	M1961	E1964	E1965	R1966	M1967	L1968	S1972	V1975	I1978	Q1979	E1980	H1985	S1986	M1987	P1988	M1989	Y1990	D1991	K1992	T1993	S1994	A1995	P1996	I1997	E2000	L2001													
S1720	V1724	A1730	T1731	S1732	I1733	D1734	P1735	N1736	Y1738	D1743	L1752	I1756	E1763	G1771	G1772	G1773	D1774	L1792	A1793	D1794	M1798	E1799	Q1800	R1804	R1805	K1806	L1807	E1809	L1825	I1830	E1837	M1838	M1842	R1843	F1846	Q1850	T1851	D1852	L1854	Q1855	E2000	L2001																
K1581	V1582	L1587	V1591	L1601	L1604	L1607	L1619	R1623	R1628	L1637	L1638	I1641	S1644	K1645	F1646	L1650	M1657	I1664	I1665	L1666	N1667	E1668	V1672	I1676	E1683	V1684	M1685	V1690	S1691	E1694	I1698	L1702	E1706	R1707	E1708	Q1850	T1851	D1852	L1854	Q1855	E2000	L2001																
I1466	R1467	E1474	L1475	D1476	L1477	C1484	R1488	G1489	W1490	L1493	H1500	M1507	S1510	D1519	A1520	W1523	F1534	W1537	I1538	V1540	Q1541	R1542	I1543	I1550	F1551	T1552	Q1553	S1554	A1555	D1556	I1557	K1558	H1559	L1560	L1561	V1562	V1563	E1564	I1571	L1576	K1580																	
A1381	S1382	Y1383	E1384	F1385	V1386	Q1387	R1388	L1389	L1390	K1391	G1392	Y1393	M1394	K1395	I1396	M1397	M1398	I1401	L1408	I1414	M1417	L1420	H1421	V1422	V1423	W1424	V1425	V1426	S1427	E1428	L1429	T1430	L1431	Q1432	Q1433	I1434	W1435	D1436	V1437	D1438	L1439	Q1440	K1441	M1442	E1443													
VAL	ALA	LEU	GLU	LEU	Q1327	D1328	L1329	K1330	G1331	V1332	W1333	S1334	E1335	L1336	S1337	K1338	V1339	W1340	E1341	Q1342	I1343	D1344	Q1345	M1346	K1347	E1348	Q1349	P1350	W1351	V1352	S1353	V1354	Q1355	P1356	R1357	K1358	L1359	R1360	Q1361	M1362	L1363	D1364	A1365	L1366	L1367	M1368	Q1369	L1370	K1371	S1372	F1373	P1374	A1375	R1376	L1377	R1378	Q1379	Y1380
TRP	GLU	PHE	GLN	PHE	LYS	THR	LYS	PRO	VAL	THR	GLY	ASN	ARG	PRO	ASN	ILE	GLU	ALA	GLY	GLU	TRP	GLN	ALA	GLY	ASP	ASP	GLN	LYS	ILE	VAL	GLU	GLN	LYS	PHE	GLU	LYS	VAL	GLU	ARG	GLU	ASN	SER	ARG	THR	GLY	THR	THR	GLU	LEU	ASP	GLN							
ARG	PHE	GLN	PHE	THR	LYS	PRO	VAL	THR	GLY	ASN	ARG	PRO	ASN	ILE	GLU	ALA	GLY	GLU	TRP	GLN	ALA	GLY	ASP	ASP	GLN	LYS	ILE	VAL	GLU	GLN	LYS	PHE	GLU	LYS	VAL	GLU	ARG	GLU	ASN	SER	ARG	THR	GLY	THR	THR	GLU	LEU	ASP	GLN									
GLU	LEU	HIS	SER	GLN	ILE	SER	LYS	THR	LYS	SER	GLN	GLY	THR	VAL	ASP	THR	ALA	VAL	VAL	THR	ILE	ASP	PHE	GLY	THR	ILE	GLY	THR	LYS	ASN	ARG	LEU	LYS	THR	GLN	VAL	GLU	ASN	TRP	GLY	GLN	THR	THR	GLU	LEU	ASP	GLN											
ASN	ALA	LEU	THR	MET	GLY	PRO	ARG	GLY	VAL	LEU	GLU	GLY	THR	LYS	VAL	VAL	LYS	LYS	THR	ILE	ASP	PHE	GLY	THR	ILE	GLY	THR	LYS	ASN	ARG	LEU	LYS	THR	GLN	VAL	GLU	ASN	TRP	GLY	GLN	THR	THR	GLU	LEU	ASP	GLN												
PHE	ASN	PHE	GLN	LYS	GLY	VAL	ASP	ILE	GLY	PRO	ARG	GLU	GLY	THR	VAL	THR	LYS	LYS	THR	ILE	ASP	PHE	GLY	THR	ILE	GLY	THR	LYS	ASN	ARG	LEU	LYS	THR	GLN	VAL	GLU	ASN	TRP	GLY	GLN	THR	THR	GLU	LEU	ASP	GLN												



V4604	K4502	Q4425	D4351	E4192	I4071	D3946	E3816	R3705	A3577
V4609	E4503	D4426	E4352	R4195	G4072	L3947	S3817	R3706	I3578
F4613	L4504	V4427	E4353	R4196	S4073	Q3952	L3818	C3712	K3579
L4619	L4511	R4428	ASP	Y4205	A4074	A3953	Y3827	V3716	L3580
T4626	G4512	D4429	LEU	L4212	E4075	D3954	I3835	V3724	R3585
A4627	G4513	L4430	ALA	R4213	A4080	E3955	N3838	L3732	D3591
T4628	P4517	D4432	TYR	S4214	D4081	Q3956	V3839	L3733	P3592
K4629	I4521	D4433	GLU	D4220	K4082	I3959	L3863	Q3739	T3597
E4630	R4525	V4434	THR	D4224	V4088	S3964	V3866	R3743	I3600
P4632	V4528	Q4436	LYS	K4237	R4092	P3966	R3870	Q3744	K3601
F4635	C4438	E4439	THR	G4287	M4095	E3977	A3872	L3745	R3607
V4642	E4439	G4440	ARG	V4288	L4096	N3983	A3871	K3608	I3609
L4643	G4440	R4441	ASP	I4251	K4097	A3995	A3874	T3610	R3611
E4646	E4537	K4442	THR	D4261	M4098	A3995	N3875	L3750	K3621
	E4542	K4443	SER	Q4262	V4099	R4000	L3876	A3752	E3624
		Q4444	ASP	M4266	A4102	V4009	F3883	L3763	R3628
		T4445	GLY	F4278	W4105	N4012	A3884	E3755	F3629
		M4446	ARG	K4287	L4106	M4021	L3887	V3756	P3632
		Y4447	PRO	V4288	M4107	E4022	A3888	K3757	L3633
		L4448	A4375	D4289	Q4108	Q4023	D3902	G3768	L3634
		R4449	W4376	M4291	L4109	L4025	H3907	R3769	D3642
		T4450	M4377	T4294	E4110	D4026	R3910	L3761	P3643
		L4451	R4378	D4298	K4111	L4027	E3913	D3762	X3650
		T4452	T4379	E4301	L4113	I4030	I3914	D3763	R3654
		M4453	L4380	R4302	E4115	V4031	V3915	D3764	R3659
		E4454	H4381	E4303	Q4117	G4032	L3916	T3765	T3663
		L4455	T4382	Q4307	P4118	K4036	S3917	I3767	L3664
		V4456	T4383	W4308	E4129	P4037	A3918	T3768	T3669
		K4457	A4384	E4309	L4138	N4038	G3919	T3769	S3674
		G4458	S4385	L4311	G4142	V4041	S3920	L3770	T3689
		C4459	N4386	D4314	F4145	L4042	T3921	E3771	R3682
		L4460	W4387	T4317	F4146	M4043	P3922	K3774	P3684
		P4461	L4390	R4329	M4157	E4056	Q3925	R3782	D3691
		R4462	I4391	T4333	T4160	D4057	G3926	E3785	L3692
		V4475	Q4393	L4340	S4172	L4058	L3927	I3788	C3693
		T4476	T4401	T4340	E4175	E4061	E3830	D3789	S3694
		Q4477	M4404	S4341	R4176	Q4062	Q3931	I3789	R3695
		W4478	D4407	K4342	E4180	T4064	V3935	Q3792	V3699
		V4479	P4408	M4346	T4189	Q4065	V3936	V3797	N3700
		F4482	F4410			T4066	R3937	I3811	
		S4483	R4411			S4068	L3938	M3815	
		E4484	E4414						
		R4485	E4418						
		T4486	K4418						
		K4487	A4421						
		Q4488							
		T4492							
		A4496							
		A4497							
		S4498							
		Q4499							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136496	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.091	Depositor
Minimum map value	-0.677	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	316.8, 316.8, 316.8	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.21	0/24908	0.34	0/33751

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	24390	0	24462	499	0
2	A	31	0	12	3	0
3	A	54	0	24	3	0
4	A	1	0	0	0	0
All	All	24476	0	24498	500	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 10.

All (500) 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:1462:PHE:HB2	1:A:3628:ARG:HD3	1.51	0.91
1:A:1830:ILE:HD11	1:A:1837:GLU:HB2	1.61	0.81
1:A:1650:LEU:HD21	1:A:1698:ILE:HD11	1.64	0.78
1:A:2481:MET:SD	1:A:2485:GLN:NE2	2.57	0.77
1:A:2346:GLN:HB2	1:A:2726:ARG:HD2	1.69	0.74
1:A:2386:PRO:HG3	1:A:2413:LEU:HD22	1.69	0.72
1:A:1360:ARG:NH1	1:A:1394:MET:SD	2.62	0.72
1:A:3488:ARG:HA	1:A:3491:LYS:HD3	1.68	0.72
1:A:1408:LEU:HD21	1:A:1450:LEU:HD22	1.70	0.72
1:A:2606:PHE:HE1	1:A:2617:VAL:HG11	1.56	0.71
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.72	0.71
1:A:2744:LEU:HD22	1:A:2748:TYR:HE2	1.55	0.70
1:A:3114:ASP:HB2	1:A:3191:ARG:HH12	1.57	0.70
1:A:2053:MET:HE1	1:A:2094:LYS:HA	1.75	0.68
1:A:2598:GLY:HA3	1:A:2795:SER:HB2	1.75	0.68
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.76	0.68
1:A:1507:MET:HE2	1:A:1520:ALA:HB2	1.76	0.67
1:A:4116:LEU:HG	1:A:4118:PRO:HD3	1.76	0.67
1:A:4563:LEU:HD12	1:A:4588:THR:HG21	1.77	0.66
1:A:2200:GLY:HA2	1:A:2373:MET:HE3	1.77	0.66
1:A:1842:MET:HA	1:A:1861:MET:HB2	1.78	0.66
1:A:1478:VAL:HG11	1:A:1488:ARG:HE	1.61	0.66
1:A:4071:ILE:HD11	1:A:4096:LEU:HD22	1.77	0.66
1:A:1431:LEU:O	1:A:1435:TRP:HB2	1.95	0.66
1:A:3921:THR:HA	1:A:3936:VAL:HG21	1.78	0.65
1:A:1394:MET:HE2	1:A:1394:MET:HA	1.79	0.65
1:A:2600:GLY:HA3	1:A:2603:MET:HE2	1.79	0.64
1:A:4042:LEU:HD21	1:A:4138:LEU:HG	1.79	0.64
1:A:3884:ALA:HB1	1:A:4009:VAL:HG11	1.79	0.64
1:A:2882:ILE:HG12	1:A:2883:PRO:HD2	1.79	0.64
1:A:2999:VAL:HG13	1:A:3005:LEU:HD21	1.78	0.64
1:A:1683:GLU:HB3	1:A:1685:MET:HE2	1.79	0.64
1:A:1931:ASN:ND2	1:A:1933:ASP:OD1	2.31	0.64
1:A:2987:ASN:OD1	1:A:3057:GLN:NE2	2.31	0.64
1:A:4630:GLU:HB3	1:A:4635:PHE:HE1	1.63	0.64
1:A:1557:ILE:HA	1:A:1560:LEU:HB2	1.80	0.64
1:A:2028:LEU:HD23	1:A:2033:LYS:HA	1.80	0.63
1:A:1644:SER:OG	1:A:1645:LYS:NZ	2.32	0.63
1:A:2495:VAL:HG11	1:A:2526:LEU:HD21	1.80	0.63
1:A:2020:PRO:HA	1:A:2026:SER:HA	1.80	0.62
1:A:2666:ILE:HG22	1:A:2712:CYS:HB3	1.79	0.62
1:A:3553:LEU:HB2	1:A:3578:ILE:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4287:LYS:HA	1:A:4287:LYS:HE3	1.80	0.62
1:A:4180:TYR:OH	1:A:4220:ASP:OD2	2.16	0.62
1:A:3875:MET:HE1	1:A:3883:PHE:HB2	1.82	0.62
1:A:1537:TRP:CE3	1:A:1601:LEU:HD11	2.35	0.62
1:A:4042:LEU:HD13	1:A:4142:GLY:HA3	1.81	0.61
1:A:3922:PRO:HD2	1:A:3936:VAL:CG2	2.30	0.61
1:A:2500:TRP:CD2	1:A:2580:LEU:HD11	2.36	0.61
1:A:2744:LEU:HD22	1:A:2748:TYR:CE2	2.35	0.61
1:A:3592:PRO:HB3	1:A:3684:PRO:HD3	1.81	0.61
1:A:3782:ARG:HG2	1:A:3782:ARG:HH11	1.64	0.61
1:A:3739:GLN:O	1:A:3743:ARG:HG2	2.01	0.61
1:A:2995:ASP:OD1	1:A:2996:GLU:N	2.33	0.61
1:A:3922:PRO:HD2	1:A:3936:VAL:HG21	1.82	0.61
1:A:4055:VAL:HB	1:A:4095:MET:HE1	1.80	0.61
1:A:1417:MET:HE3	1:A:1424:TRP:O	2.01	0.61
1:A:2224:GLY:O	1:A:2230:LYS:NZ	2.33	0.61
1:A:2536:ASP:OD1	1:A:2576:ARG:NH1	2.34	0.60
1:A:2596:PRO:HB2	1:A:2738:TYR:CE1	2.36	0.60
1:A:3544:ARG:HB3	1:A:3547:ILE:HG12	1.83	0.60
1:A:2307:VAL:HA	1:A:2311:TRP:HE1	1.65	0.60
1:A:3040:GLU:OE1	1:A:3053:TRP:NE1	2.35	0.60
1:A:1964:GLU:HG2	1:A:1967:MET:HB2	1.84	0.60
1:A:3211:THR:O	1:A:3215:VAL:HG22	2.02	0.60
1:A:4036:LYS:HE3	1:A:4036:LYS:HA	1.82	0.60
1:A:4288:VAL:HG21	1:A:4294:ILE:HG12	1.82	0.60
1:A:2414:GLN:NE2	1:A:2418:ASP:OD1	2.29	0.60
1:A:2845:TRP:O	1:A:2849:ASN:ND2	2.32	0.60
1:A:2085:HIS:HB2	1:A:2361:MET:HG2	1.84	0.59
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.37	0.59
1:A:3478:LEU:HD21	1:A:3760:ILE:HG13	1.83	0.59
1:A:3174:ARG:NH1	1:A:3650:ASN:OD1	2.35	0.59
1:A:3886:LEU:HD11	1:A:4346:MET:HG3	1.85	0.59
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.67	0.59
1:A:1430:THR:HG23	1:A:1433:GLN:H	1.67	0.59
1:A:4566:GLN:HG3	1:A:4643:LEU:HG	1.84	0.59
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.84	0.58
1:A:3838:ASN:OD1	1:A:3870:ARG:NH2	2.35	0.58
1:A:2304:ASP:OD1	1:A:2726:ARG:NH2	2.36	0.58
1:A:4088:VAL:HG22	1:A:4118:PRO:HA	1.86	0.58
1:A:3585:ARG:NH1	1:A:3694:SER:O	2.36	0.58
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3521:ASP:OD1	1:A:3521:ASP:N	2.37	0.58
1:A:4116:LEU:HD12	1:A:4117:GLN:H	1.69	0.57
1:A:1356:PRO:HB2	1:A:1401:ILE:HD13	1.85	0.57
1:A:3712:CYS:O	1:A:3716:VAL:HG23	2.05	0.57
1:A:1657:MET:HE1	1:A:1702:LEU:HD13	1.86	0.57
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.86	0.57
1:A:4025:LEU:HD23	1:A:4027:LEU:HB2	1.87	0.57
1:A:2598:GLY:O	3:A:4702:ADP:H5'1	2.05	0.57
1:A:2790:PRO:HB3	1:A:3076:LYS:HG3	1.86	0.57
1:A:3766:ILE:O	1:A:3769:THR:OG1	2.19	0.57
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.87	0.56
1:A:4262:GLN:NE2	1:A:4266:ASN:OD1	2.37	0.56
1:A:4073:SER:OG	1:A:4075:GLU:OE1	2.23	0.56
1:A:2248:GLU:HB2	1:A:2297:LYS:HD3	1.86	0.56
1:A:2126:GLU:O	1:A:2130:ASN:ND2	2.38	0.56
1:A:1850:GLN:HB2	1:A:1856:GLN:HG2	1.87	0.56
1:A:2598:GLY:HA3	1:A:2795:SER:CB	2.35	0.56
1:A:1537:TRP:CH2	1:A:1582:VAL:HG21	2.41	0.56
1:A:1628:ARG:NH2	1:A:1871:GLU:OE1	2.39	0.56
1:A:2230:LYS:HG2	2:A:4701:ATP:O2B	2.06	0.56
1:A:3491:LYS:O	1:A:3495:THR:HG23	2.04	0.56
1:A:4301:ARG:NH1	1:A:4303:GLU:OE1	2.39	0.56
1:A:4342:LYS:O	1:A:4346:MET:HG2	2.06	0.56
1:A:3133:LEU:HD12	1:A:3134:PRO:HD2	1.87	0.55
1:A:4410:PHE:HE1	1:A:4414:GLU:OE1	1.89	0.55
1:A:4430:ASP:HB3	1:A:4451:LEU:HD11	1.88	0.55
1:A:4485:ARG:NH1	1:A:4513:GLY:O	2.39	0.55
1:A:1397:ASN:O	1:A:1401:ILE:HG12	2.07	0.55
1:A:1510:SER:HB2	1:A:3629:PHE:HB3	1.88	0.55
1:A:2551:LYS:HB3	1:A:2575:VAL:HG21	1.88	0.55
1:A:1425:VAL:HB	1:A:1428:GLU:HB2	1.89	0.55
1:A:2538:GLU:HB2	1:A:2548:TRP:CE2	2.42	0.55
1:A:3873:ARG:HG2	1:A:4021:MET:HE1	1.89	0.55
1:A:1691:SER:OG	1:A:1694:GLU:OE2	2.20	0.55
1:A:2562:VAL:HG11	1:A:2755:MET:HB2	1.87	0.55
1:A:4525:ARG:HG2	1:A:4536:LEU:HD22	1.89	0.55
1:A:3917:SER:HB2	1:A:3920:SER:HB3	1.89	0.55
1:A:1731:THR:OG1	1:A:1732:SER:N	2.40	0.54
1:A:2054:LEU:HG	1:A:2097:LEU:HD13	1.89	0.54
1:A:4421:ALA:O	1:A:4425:GLN:HG2	2.08	0.54
1:A:3174:ARG:HD2	1:A:3694:SER:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4601:LYS:HB2	1:A:4604:VAL:HG13	1.89	0.54
1:A:2382:LEU:HD23	1:A:2420:ALA:HB2	1.88	0.54
1:A:2446:ILE:HG13	1:A:2735:TYR:CD1	2.43	0.54
1:A:3551:GLU:OE1	1:A:3732:LEU:HB3	2.08	0.54
1:A:3607:ARG:NH2	1:A:3674:SER:O	2.40	0.54
1:A:2379:LEU:O	1:A:2383:ARG:HG3	2.07	0.54
1:A:1756:ILE:HD13	1:A:1846:PHE:HB2	1.88	0.54
1:A:2467:ARG:NE	1:A:2587:GLU:OE2	2.41	0.54
1:A:1975:VAL:HG11	1:A:2016:ILE:HD11	1.88	0.54
1:A:3133:LEU:HD11	1:A:3141:GLU:HB3	1.89	0.54
1:A:4205:TYR:OH	1:A:4261:ASP:OD2	2.20	0.53
1:A:1426:VAL:HA	1:A:1429:LEU:HD23	1.91	0.53
1:A:1431:LEU:HA	1:A:1434:ILE:HG12	1.89	0.53
1:A:1474:GLU:HG2	1:A:1587:LEU:HD22	1.91	0.53
1:A:2935:LEU:HD22	1:A:3094:PHE:HE1	1.74	0.53
1:A:2963:VAL:HB	1:A:2998:ASN:HB3	1.91	0.53
1:A:4022:GLU:OE1	1:A:4023:GLN:NE2	2.41	0.53
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.91	0.53
1:A:3204:GLY:HA3	1:A:3489:TRP:HZ3	1.74	0.53
1:A:2449:LEU:HD11	1:A:2454:CYS:SG	2.49	0.53
1:A:3130:TYR:CZ	1:A:3132:LYS:HB2	2.43	0.53
1:A:1968:LEU:HD21	1:A:2029:PRO:HG3	1.91	0.53
1:A:2065:LEU:HD11	1:A:2133:GLU:HB3	1.90	0.53
1:A:2667:ASN:ND2	1:A:2713:ASN:O	2.41	0.53
1:A:4172:SER:O	1:A:4176:ARG:NH1	2.41	0.52
1:A:4407:ASP:HB3	1:A:4410:PHE:HB3	1.91	0.52
1:A:4088:VAL:HG21	1:A:4116:LEU:HD21	1.91	0.52
1:A:1446:VAL:O	1:A:1450:LEU:HG	2.09	0.52
1:A:1571:ILE:HD11	1:A:1607:LEU:HB3	1.91	0.52
1:A:1420:LEU:HD13	1:A:1437:VAL:HG11	1.91	0.52
1:A:1537:TRP:HH2	1:A:1582:VAL:HG21	1.73	0.52
1:A:1619:LEU:HD11	1:A:1638:LEU:HG	1.92	0.52
1:A:4192:GLU:OE1	1:A:4195:ARG:NH1	2.39	0.52
1:A:4380:LEU:HD13	1:A:4456:VAL:HG23	1.92	0.52
1:A:2549:GLN:HG2	1:A:2572:LEU:HD13	1.90	0.52
1:A:2715:PRO:HA	1:A:2720:ARG:HB3	1.92	0.52
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.92	0.52
1:A:4041:VAL:HG12	1:A:4043:MET:HG2	1.90	0.52
1:A:1961:ASN:ND2	1:A:2019:ASN:O	2.43	0.52
1:A:3624:GLU:HG2	1:A:3669:ILE:HG21	1.92	0.52
1:A:2087:ASP:HB2	1:A:2356:VAL:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2855:LEU:HD11	1:A:2863:ARG:HG3	1.90	0.51
1:A:1461:GLU:OE1	1:A:3659:ARG:NE	2.43	0.51
1:A:1619:LEU:HD13	1:A:1637:LEU:HD23	1.92	0.51
1:A:1792:LEU:HD22	1:A:1808:LEU:HD22	1.93	0.51
1:A:1891:THR:HG22	1:A:4250:SER:HA	1.92	0.51
1:A:2784:PHE:HB2	1:A:2794:TYR:HE2	1.75	0.51
1:A:4535:SER:OG	1:A:4537:GLU:OE1	2.29	0.51
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.43	0.51
1:A:4488:GLN:O	1:A:4492:ILE:HG22	2.11	0.51
1:A:1431:LEU:HD11	1:A:1435:TRP:CD2	2.46	0.51
1:A:3915:VAL:HG21	1:A:4386:ASN:ND2	2.26	0.51
1:A:4307:GLN:O	1:A:4311:LEU:HG	2.10	0.51
1:A:3935:VAL:HG13	1:A:3947:LEU:HD23	1.93	0.51
1:A:3601:MET:HE3	1:A:3601:MET:HA	1.93	0.51
1:A:1637:LEU:O	1:A:1641:ILE:HG13	2.11	0.51
1:A:1720:SER:O	1:A:1724:VAL:HG23	2.11	0.51
1:A:4482:PHE:HE1	1:A:4486:ILE:HD11	1.75	0.51
1:A:2320:ASP:OD1	1:A:2358:ARG:NE	2.44	0.50
1:A:2065:LEU:HD21	1:A:2134:GLN:HG2	1.93	0.50
1:A:2775:GLU:O	1:A:2779:MET:HG3	2.11	0.50
1:A:4569:THR:HG22	1:A:4583:THR:HG21	1.92	0.50
1:A:2444:GLU:HG2	1:A:2510:MET:HG3	1.94	0.50
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.93	0.50
1:A:4108:GLN:O	1:A:4112:LYS:HG3	2.12	0.50
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	1.93	0.50
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.94	0.50
1:A:4626:ILE:HD12	1:A:4630:GLU:O	2.10	0.50
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.93	0.50
1:A:3766:ILE:O	1:A:3770:LEU:HD12	2.12	0.50
1:A:1978:ILE:HD11	1:A:2001:LEU:HD11	1.94	0.50
1:A:2190:TYR:O	1:A:2377:ASN:ND2	2.44	0.50
1:A:3576:ASN:ND2	1:A:3700:ASN:O	2.43	0.50
1:A:3767:ILE:HA	1:A:3770:LEU:HD13	1.94	0.50
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.94	0.50
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.92	0.50
1:A:2774:VAL:HG22	1:A:2799:MET:HE1	1.94	0.49
1:A:3817:SER:C	1:A:4346:MET:HE1	2.37	0.49
1:A:2031:ASN:OD1	1:A:2031:ASN:N	2.43	0.49
1:A:2290:SER:HA	1:A:2294:GLU:HG2	1.94	0.49
1:A:2308:ASP:OD1	1:A:2311:TRP:HD1	1.95	0.49
1:A:2509:LYS:O	1:A:2513:GLU:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1431:LEU:HD11	1:A:1435:TRP:CE2	2.48	0.49
1:A:2307:VAL:HG13	1:A:2312:VAL:HG11	1.93	0.49
1:A:4528:VAL:HG21	1:A:4592:TRP:HB2	1.93	0.49
1:A:2366:GLU:OE2	1:A:2451:ARG:NH2	2.46	0.49
1:A:4408:PRO:HA	1:A:4411:ARG:HE	1.77	0.49
1:A:4446:ASN:HA	1:A:4449:ARG:HD2	1.92	0.49
1:A:3705:ARG:NH1	1:A:4353:ASP:OD2	2.46	0.49
1:A:4026:ASP:O	1:A:4030:ILE:HG13	2.13	0.49
1:A:4433:ASP:HB3	1:A:4448:LEU:HD11	1.95	0.49
1:A:2127:ILE:O	1:A:2131:LEU:HG	2.12	0.49
1:A:2982:ARG:NH2	1:A:2988:GLU:OE2	2.43	0.49
1:A:2473:ASN:OD1	1:A:2481:MET:N	2.45	0.49
1:A:2503:SER:HB2	1:A:2511:ARG:HG2	1.94	0.49
1:A:2827:HIS:CE1	1:A:2831:ARG:HH11	2.31	0.49
1:A:3008:MET:HE3	1:A:3008:MET:HA	1.95	0.49
1:A:1843:ARG:HH21	1:A:1862:ALA:H	1.59	0.49
1:A:1467:ARG:NH2	1:A:1519:ASP:OD2	2.45	0.48
1:A:1557:ILE:HD11	1:A:1561:LEU:HD12	1.95	0.48
1:A:1628:ARG:NE	1:A:1706:GLU:OE2	2.41	0.48
1:A:2615:MET:HE1	1:A:2707:GLN:OE1	2.13	0.48
1:A:2595:GLY:O	1:A:2714:PRO:HD3	2.13	0.48
1:A:2964:HIS:HA	1:A:3643:PRO:HG2	1.95	0.48
1:A:3551:GLU:OE2	1:A:3559:ARG:NH1	2.45	0.48
1:A:3592:PRO:O	1:A:3682:ARG:NH1	2.46	0.48
1:A:1360:ARG:HA	1:A:1394:MET:HE1	1.95	0.48
1:A:2212:GLN:O	1:A:2216:ILE:HG12	2.12	0.48
1:A:3767:ILE:O	1:A:3771:GLU:HG2	2.12	0.48
1:A:4542:GLU:HB2	1:A:4591:ARG:HG2	1.95	0.48
1:A:2956:LEU:HD23	1:A:2991:ALA:HB2	1.96	0.48
1:A:1466:ILE:HD12	1:A:1500:HIS:ND1	2.29	0.48
1:A:2229:GLY:N	2:A:4701:ATP:O1A	2.46	0.48
1:A:3486:ARG:O	1:A:3490:GLU:HG2	2.14	0.48
1:A:4475:VAL:O	1:A:4479:VAL:HG12	2.13	0.48
1:A:2302:VAL:HG22	1:A:2342:MET:HE2	1.96	0.48
1:A:3175:HIS:CE1	1:A:3585:ARG:HH12	2.32	0.48
1:A:1493:LEU:HD21	1:A:1534:PHE:CD2	2.49	0.48
1:A:1664:ILE:HG22	1:A:1676:ILE:HG22	1.96	0.48
1:A:1891:THR:HG21	1:A:2039:LEU:HD13	1.96	0.48
1:A:2148:LYS:HB2	1:A:2361:MET:HB3	1.95	0.48
1:A:2940:GLY:HA3	1:A:3174:ARG:HG3	1.96	0.48
1:A:3568:PRO:HG2	1:A:3573:CYS:SG	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2740:GLY:O	1:A:2744:LEU:HG	2.14	0.47
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.49	0.47
1:A:3127:PRO:HD3	1:A:3538:GLN:HG2	1.96	0.47
1:A:3654:ARG:HH21	1:A:3663:THR:HG22	1.79	0.47
1:A:1933:ASP:OD1	1:A:1933:ASP:N	2.48	0.47
1:A:2969:GLY:HA2	1:A:3004:PHE:HE1	1.79	0.47
1:A:3835:ILE:HG12	1:A:3870:ARG:HG3	1.96	0.47
1:A:1347:LYS:HB2	1:A:1432:GLY:HA2	1.96	0.47
1:A:1507:MET:HB2	1:A:3629:PHE:CE1	2.49	0.47
1:A:1961:ASN:ND2	1:A:2019:ASN:H	2.12	0.47
1:A:1861:MET:HE2	1:A:1890:LEU:HA	1.95	0.47
1:A:2534:ILE:HD12	1:A:2534:ILE:H	1.80	0.47
1:A:4492:ILE:HD11	1:A:4504:LEU:HG	1.97	0.47
1:A:1484:CYS:HB3	1:A:1576:LEU:HD22	1.96	0.47
1:A:2481:MET:SD	1:A:2485:GLN:HG2	2.55	0.47
1:A:2581:LEU:HG	1:A:2591:LEU:HD21	1.97	0.47
1:A:2759:ILE:HG23	1:A:2815:THR:HA	1.97	0.47
1:A:2774:VAL:CG2	1:A:2799:MET:HE1	2.44	0.47
1:A:3104:GLN:O	1:A:3108:GLU:HG2	2.14	0.47
1:A:3591:ASP:N	1:A:3591:ASP:OD1	2.47	0.47
1:A:3818:LEU:HD12	1:A:4346:MET:HE2	1.96	0.47
1:A:1667:ASN:HB2	1:A:1672:VAL:HG22	1.97	0.47
1:A:2728:LEU:HA	1:A:2731:VAL:HG22	1.97	0.47
1:A:3926:GLY:O	1:A:3927:LEU:HD23	2.15	0.47
1:A:1477:LEU:HD11	1:A:1582:VAL:HG12	1.97	0.47
1:A:2623:SER:OG	1:A:2624:SER:N	2.48	0.47
1:A:2992:PHE:HE1	1:A:2994:MET:HG3	1.80	0.47
1:A:4409:LEU:HD11	1:A:4558:PHE:HE2	1.80	0.47
1:A:1447:LYS:HD3	1:A:1447:LYS:HA	1.77	0.46
1:A:2418:ASP:O	1:A:2422:ILE:HG12	2.16	0.46
1:A:2602:THR:HG22	1:A:2662:PHE:CZ	2.50	0.46
1:A:2934:LEU:HD11	1:A:3068:MET:HE3	1.97	0.46
1:A:3143:ILE:HD13	1:A:3541:ILE:HD13	1.97	0.46
1:A:4626:ILE:HD13	1:A:4632:PRO:HG3	1.96	0.46
1:A:1551:PHE:HB3	1:A:1558:LYS:HZ2	1.79	0.46
1:A:1647:VAL:HA	1:A:1650:LEU:HD13	1.98	0.46
1:A:1684:VAL:HG12	1:A:1684:VAL:O	2.15	0.46
1:A:1752:LEU:HD11	1:A:1868:TYR:CZ	2.50	0.46
1:A:2271:ASN:O	1:A:2272:THR:OG1	2.32	0.46
1:A:2279:LEU:HD21	1:A:2693:TYR:CD2	2.50	0.46
1:A:2703:LEU:HD23	1:A:2706:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2937:GLY:C	1:A:3070:PRO:HD3	2.41	0.46
1:A:3540:ASN:O	1:A:3540:ASN:ND2	2.47	0.46
1:A:2609:LEU:HD13	1:A:2617:VAL:HG22	1.97	0.46
1:A:3743:ARG:O	1:A:3747:LYS:HD3	2.16	0.46
1:A:2629:GLU:O	1:A:2633:LYS:HG2	2.16	0.46
1:A:1571:ILE:HG23	1:A:1604:LEU:HD22	1.97	0.46
1:A:2325:LEU:HB3	1:A:2333:LEU:HB2	1.97	0.46
1:A:2123:ASP:O	1:A:2127:ILE:HG13	2.16	0.46
1:A:2602:THR:HG22	1:A:2662:PHE:HZ	1.80	0.46
1:A:2979:VAL:HG21	1:A:2992:PHE:CE2	2.51	0.46
1:A:1665:ILE:HD12	1:A:1685:MET:HE1	1.98	0.46
1:A:2189:MET:HE1	1:A:2235:ARG:HH12	1.81	0.46
1:A:3077:ASP:O	1:A:3081:THR:HG22	2.16	0.46
1:A:3483:SER:O	1:A:3487:GLU:HG2	2.16	0.46
1:A:1582:VAL:HG22	1:A:1591:VAL:HG22	1.98	0.46
1:A:2127:ILE:HA	1:A:2130:ASN:HD21	1.81	0.46
1:A:4071:ILE:HG13	1:A:4099:VAL:HG12	1.97	0.46
1:A:2348:LEU:HD13	1:A:2356:VAL:HG22	1.99	0.45
1:A:4387:TRP:HZ3	1:A:4455:LEU:HD13	1.81	0.45
1:A:2028:LEU:HD21	1:A:2036:PHE:HB2	1.98	0.45
1:A:2204:VAL:HA	1:A:2207:VAL:HG12	1.98	0.45
1:A:2843:ARG:NH2	1:A:3093:TRP:O	2.49	0.45
1:A:4176:ARG:NH2	1:A:4224:ASP:OD1	2.40	0.45
1:A:1346:MET:HE1	1:A:1362:ASN:HB2	1.97	0.45
1:A:1738:TYR:HE2	1:A:1792:LEU:HD21	1.81	0.45
1:A:2228:SER:OG	1:A:2364:PHE:HB3	2.17	0.45
1:A:3888:ALA:O	1:A:4012:ASN:ND2	2.49	0.45
1:A:1374:PRO:HD2	1:A:1377:LEU:HD12	1.99	0.45
1:A:2748:TYR:HE1	1:A:2800:THR:HG22	1.82	0.45
1:A:2935:LEU:O	1:A:3067:THR:HA	2.16	0.45
1:A:3611:ARG:HG3	1:A:3634:LEU:HD23	1.99	0.45
1:A:4095:MET:HE3	1:A:4097:LYS:NZ	2.32	0.45
1:A:1466:ILE:HD12	1:A:1500:HIS:CE1	2.51	0.45
1:A:1805:ARG:O	1:A:1809:GLU:HG3	2.17	0.45
1:A:4534:TRP:CG	1:A:4594:LYS:HZ3	2.34	0.45
1:A:1877:ASP:N	1:A:1877:ASP:OD1	2.49	0.45
1:A:1997:ILE:H	1:A:1997:ILE:HD12	1.82	0.45
1:A:1623:ARG:CZ	1:A:1943:ARG:HD2	2.47	0.45
1:A:3938:LEU:HD13	1:A:3995:ALA:HB2	1.99	0.45
1:A:1336:LEU:HD11	1:A:1386:VAL:HG21	1.99	0.45
1:A:2571:THR:HG23	1:A:2574:THR:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2762:LEU:HD22	1:A:2821:LEU:HD22	1.99	0.45
1:A:2837:LEU:HD13	1:A:2842:GLU:HB3	1.99	0.45
1:A:3691:ASP:O	1:A:3695:ARG:HG3	2.17	0.45
1:A:2510:MET:SD	1:A:2510:MET:N	2.90	0.44
1:A:2569:VAL:HG11	1:A:2747:ILE:HA	1.99	0.44
1:A:2979:VAL:HG21	1:A:2992:PHE:HE2	1.83	0.44
1:A:2995:ASP:O	1:A:2999:VAL:HG23	2.18	0.44
1:A:1743:ASP:OD1	1:A:1804:ARG:NE	2.50	0.44
1:A:2901:TYR:OH	1:A:2909:LEU:N	2.50	0.44
1:A:1554:SER:O	1:A:1557:ILE:HG22	2.18	0.44
1:A:2030:ASP:HA	1:A:2033:LYS:HB2	1.99	0.44
1:A:2452:LEU:HD23	1:A:2452:LEU:HA	1.64	0.44
1:A:2795:SER:HB2	1:A:2796:PRO:HD2	1.99	0.44
1:A:2828:GLU:OE1	1:A:2924:ARG:NH1	2.51	0.44
1:A:2923:ASP:O	1:A:2927:ARG:HG2	2.18	0.44
1:A:3010:THR:HB	1:A:3017:VAL:HG12	2.00	0.44
1:A:1980:GLU:HG3	1:A:2035:LEU:HD11	1.99	0.44
1:A:2377:ASN:O	1:A:2381:ARG:HG3	2.17	0.44
1:A:3177:LEU:CD1	3:A:4703:ADP:H1'	2.47	0.44
1:A:1667:ASN:OD1	1:A:1668:GLU:N	2.48	0.44
1:A:2644:THR:OG1	1:A:2647:GLY:O	2.31	0.44
1:A:2156:LEU:O	1:A:2160:LEU:HG	2.17	0.44
1:A:2434:THR:O	1:A:2438:GLU:HG2	2.18	0.44
1:A:1972:SER:OG	1:A:2031:ASN:ND2	2.51	0.44
1:A:2800:THR:HG21	3:A:4702:ADP:O2'	2.18	0.44
1:A:2813:LEU:HD13	1:A:2816:LEU:HD21	2.00	0.44
1:A:3753:LEU:O	1:A:3756:VAL:HG22	2.18	0.44
1:A:1794:ASP:OD2	1:A:2060:ARG:NH1	2.51	0.44
1:A:3959:ILE:HD12	1:A:3959:ILE:H	1.82	0.44
1:A:3113:MET:SD	1:A:3184:ALA:HA	2.58	0.44
1:A:3550:THR:HA	1:A:3578:ILE:HD12	1.99	0.44
1:A:3597:THR:O	1:A:3601:MET:HG2	2.18	0.44
1:A:4038:ASN:OD1	1:A:4038:ASN:N	2.51	0.44
1:A:2231:SER:HA	1:A:2234:TRP:NE1	2.33	0.43
1:A:2959:TYR:HE1	1:A:2961:ILE:HG22	1.83	0.43
1:A:4401:THR:OG1	1:A:4404:ASN:ND2	2.51	0.43
1:A:1798:MET:HE2	1:A:1800:GLN:HE22	1.83	0.43
1:A:1690:VAL:HG23	1:A:1708:GLU:HG3	1.99	0.43
1:A:4214:SER:HB2	1:A:4251:ILE:HG23	2.00	0.43
1:A:4574:LYS:HB3	1:A:4627:ALA:HB2	2.01	0.43
1:A:1825:LEU:HD22	1:A:1830:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2115:LYS:HE2	1:A:2127:ILE:HD11	2.00	0.43
1:A:2323:LYS:HB3	1:A:2335:LEU:HB3	2.00	0.43
1:A:2482:GLN:HG3	1:A:2483:ILE:N	2.34	0.43
1:A:2839:GLU:HG2	1:A:2841:GLU:H	1.84	0.43
1:A:3008:MET:HE1	1:A:3011:LEU:HD23	2.00	0.43
1:A:2765:TYR:C	1:A:2768:PRO:HD2	2.44	0.43
1:A:4108:GLN:HB3	1:A:4112:LYS:NZ	2.33	0.43
1:A:4451:LEU:HD23	1:A:4455:LEU:HG	2.00	0.43
1:A:4511:LEU:HD23	1:A:4511:LEU:HA	1.76	0.43
2:A:4701:ATP:O2A	2:A:4701:ATP:H4'	2.19	0.43
1:A:3201:LEU:O	1:A:3205:LEU:HD23	2.18	0.43
1:A:3724:VAL:HG21	1:A:3797:VAL:HG11	2.01	0.43
1:A:4175:GLU:HG3	1:A:4278:PHE:HE2	1.83	0.43
1:A:1763:GLU:OE1	1:A:1838:TRP:NE1	2.47	0.43
1:A:2283:VAL:O	1:A:2287:ILE:HG12	2.18	0.43
1:A:2767:GLU:HB3	1:A:2768:PRO:HD3	2.01	0.43
1:A:3547:ILE:HD13	1:A:3547:ILE:HA	1.90	0.43
1:A:3907:HIS:NE2	1:A:3938:LEU:HA	2.34	0.43
1:A:4534:TRP:CD1	1:A:4594:LYS:HZ3	2.36	0.43
1:A:1539:ASP:O	1:A:1543:ARG:HG3	2.19	0.43
1:A:1550:ILE:HG23	1:A:1638:LEU:HD13	2.01	0.43
1:A:3876:LEU:HD23	1:A:4146:VAL:HG11	2.01	0.43
1:A:4378:ARG:O	1:A:4382:THR:HG23	2.18	0.43
1:A:1359:LEU:HD11	1:A:1435:TRP:CH2	2.54	0.42
1:A:2018:MET:HE2	1:A:2018:MET:HB3	1.83	0.42
1:A:2218:HIS:HA	1:A:2340:ARG:HH11	1.83	0.42
1:A:2412:MET:HG3	1:A:2470:ALA:HB2	2.00	0.42
1:A:3498:ASN:O	1:A:3501:SER:OG	2.26	0.42
1:A:4102:ALA:HB1	1:A:4105:TRP:HB3	2.00	0.42
1:A:1859:ILE:HD11	1:A:1868:TYR:HD1	1.83	0.42
1:A:2572:LEU:O	1:A:2575:VAL:HG12	2.19	0.42
1:A:3205:LEU:HD21	1:A:3489:TRP:HB3	2.01	0.42
1:A:3621:LYS:HD3	1:A:3621:LYS:HA	1.80	0.42
1:A:3756:VAL:HB	1:A:3759:ARG:HB2	2.01	0.42
1:A:4106:LEU:HB3	1:A:4138:LEU:HD22	2.00	0.42
1:A:4189:ILE:HD13	1:A:4189:ILE:HA	1.87	0.42
1:A:1475:LEU:HD12	1:A:1591:VAL:HG21	2.01	0.42
1:A:1490:TRP:HE1	1:A:1541:GLN:NE2	2.18	0.42
1:A:2472:TYR:CD1	1:A:2541:ILE:HG21	2.55	0.42
1:A:2495:VAL:HG13	1:A:2518:ILE:HG21	2.00	0.42
1:A:2609:LEU:HD23	1:A:2609:LEU:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1332:VAL:HB	1:A:1377:LEU:HD22	2.02	0.42
1:A:1580:LYS:HA	1:A:1580:LYS:HD2	1.80	0.42
1:A:2538:GLU:OE1	1:A:2546:SER:OG	2.37	0.42
1:A:2943:LYS:HG2	1:A:3094:PHE:CZ	2.53	0.42
1:A:2964:HIS:ND1	1:A:2965:ARG:O	2.53	0.42
1:A:3175:HIS:HB3	1:A:3516:TYR:CE1	2.54	0.42
1:A:1463:LEU:HD23	1:A:1463:LEU:HA	1.86	0.42
1:A:1562:PRO:O	1:A:1564:GLU:N	2.43	0.42
1:A:2108:ILE:HG12	1:A:2131:LEU:HD11	2.00	0.42
1:A:2641:TYR:CE2	1:A:2694:ARG:HD3	2.55	0.42
1:A:3115:LEU:HB2	1:A:3140:ARG:HD3	2.01	0.42
1:A:3788:ASP:C	1:A:3792:GLN:HE21	2.28	0.42
1:A:4117:GLN:OE1	1:A:4117:GLN:HA	2.19	0.42
1:A:2142:CYS:O	1:A:2146:VAL:HB	2.20	0.42
1:A:3931:GLN:O	1:A:3935:VAL:HG23	2.19	0.42
1:A:2268:LEU:HB3	1:A:2275:TRP:HE3	1.85	0.42
1:A:3624:GLU:HG3	1:A:3664:LEU:HD23	2.02	0.42
1:A:2529:ALA:HB2	1:A:2537:TYR:OH	2.20	0.42
1:A:3140:ARG:O	1:A:3144:VAL:HG23	2.20	0.42
1:A:1350:PRO:O	1:A:1354:VAL:HG23	2.19	0.42
1:A:2210:LEU:O	1:A:2214:THR:HG23	2.20	0.42
1:A:4483:SER:O	1:A:4487:LYS:HG3	2.19	0.42
1:A:4587:LEU:HA	1:A:4587:LEU:HD12	1.80	0.42
1:A:2287:ILE:HD12	1:A:2336:PRO:HG2	2.02	0.41
1:A:1959:GLU:OE1	1:A:2019:ASN:HB2	2.20	0.41
1:A:2527:PRO:HD3	1:A:2545:TRP:CE2	2.54	0.41
1:A:2960:GLN:HG2	1:A:2993:ILE:HB	2.02	0.41
1:A:3472:VAL:O	1:A:3476:THR:HG23	2.21	0.41
1:A:3811:ILE:O	1:A:3815:MET:HG3	2.20	0.41
1:A:4043:MET:HE2	1:A:4147:PHE:HE2	1.85	0.41
1:A:4517:PRO:HG2	1:A:4619:ILE:HD12	2.02	0.41
1:A:4517:PRO:O	1:A:4521:ILE:HG12	2.20	0.41
1:A:1985:HIS:CD2	1:A:1997:ILE:HD13	2.55	0.41
1:A:2387:LEU:HD22	1:A:2467:ARG:NH2	2.36	0.41
1:A:4485:ARG:HG2	1:A:4513:GLY:O	2.20	0.41
1:A:1853:VAL:HG23	1:A:1854:LEU:HD23	2.02	0.41
1:A:2345:VAL:HG11	1:A:2348:LEU:HD21	2.02	0.41
1:A:2904:GLU:HB3	1:A:2905:LEU:H	1.64	0.41
1:A:3866:VAL:O	1:A:3870:ARG:HG2	2.20	0.41
1:A:4066:ILE:HD11	1:A:4095:MET:HB2	2.01	0.41
1:A:1756:ILE:HD11	1:A:1857:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2047:GLN:O	1:A:2051:GLN:HG3	2.20	0.41
1:A:2511:ARG:HD3	1:A:2535:ILE:HD13	2.02	0.41
1:A:3609:ILE:HB	1:A:3632:PRO:HG2	2.02	0.41
1:A:1628:ARG:HE	1:A:1706:GLU:CD	2.29	0.41
1:A:2054:LEU:HD21	1:A:2097:LEU:HD22	2.02	0.41
1:A:2445:HIS:NE2	1:A:2449:LEU:HD22	2.35	0.41
1:A:3910:ARG:HB3	1:A:3913:GLU:OE1	2.20	0.41
1:A:4027:LEU:HG	1:A:4058:LEU:HD22	2.02	0.41
1:A:4065:GLN:HB3	1:A:4092:ARG:HD3	2.02	0.41
1:A:4289:ASP:OD1	1:A:4317:THR:OG1	2.28	0.41
1:A:4414:GLU:O	1:A:4418:LYS:HG3	2.21	0.41
1:A:2288:ILE:HD12	1:A:2333:LEU:HD22	2.02	0.41
1:A:2382:LEU:O	1:A:2416:GLN:NE2	2.50	0.41
1:A:3789:ILE:H	1:A:3789:ILE:HG13	1.71	0.41
1:A:3983:ILE:HD12	1:A:3983:ILE:HA	1.83	0.41
1:A:1398:MET:HA	1:A:1401:ILE:HG12	2.02	0.41
1:A:2499:LEU:O	1:A:2503:SER:OG	2.32	0.41
1:A:2758:LEU:HD11	1:A:2807:PHE:CE1	2.56	0.41
1:A:2897:LEU:HD23	1:A:2897:LEU:HA	1.88	0.41
1:A:2934:LEU:HD11	1:A:3068:MET:CE	2.51	0.41
1:A:3579:MET:HE3	1:A:3699:VAL:HG22	2.02	0.41
1:A:3827:TYR:CZ	1:A:3871:VAL:HG13	2.55	0.41
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	2.02	0.41
1:A:4410:PHE:HA	1:A:4504:LEU:HD23	2.03	0.41
1:A:4613:PHE:CD1	1:A:4613:PHE:C	2.99	0.41
1:A:1684:VAL:O	1:A:1685:MET:C	2.63	0.41
1:A:1463:LEU:HD13	1:A:1519:ASP:CG	2.45	0.40
1:A:2614:ASP:OD1	1:A:2614:ASP:N	2.52	0.40
1:A:3048:GLU:HG3	1:A:3052:LYS:HE2	2.03	0.40
1:A:3194:LEU:HD13	1:A:3500:MET:SD	2.61	0.40
1:A:4157:MET:CE	1:A:4309:VAL:HG22	2.51	0.40
1:A:4450:THR:O	1:A:4454:GLU:HG2	2.21	0.40
1:A:1702:LEU:HD23	1:A:1702:LEU:HA	1.84	0.40
1:A:2465:ALA:O	1:A:2469:VAL:HG23	2.22	0.40
1:A:4329:ARG:O	1:A:4333:THR:HG22	2.20	0.40
1:A:1519:ASP:OD1	1:A:1523:TRP:HD1	2.04	0.40
1:A:2579:ALA:O	1:A:2583:THR:HG23	2.21	0.40
1:A:2595:GLY:HA2	1:A:2735:TYR:CE1	2.56	0.40
1:A:2939:SER:O	1:A:3172:THR:HB	2.22	0.40
1:A:2445:HIS:CE1	1:A:2449:LEU:HD22	2.57	0.40
1:A:3116:GLU:HA	1:A:3116:GLU:OE2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3788:ASP:OD1	1:A:3788:ASP:N	2.53	0.40
1:A:1424:TRP:NE1	1:A:1433:GLN:HB3	2.36	0.40
1:A:2509:LYS:HB2	1:A:2509:LYS:HE2	1.80	0.40
1:A:2548:TRP:HZ3	1:A:2551:LYS:HD2	1.87	0.40
1:A:2623:SER:O	1:A:2626:THR:HG22	2.21	0.40
1:A:3562:TRP:HB3	1:A:3567:LEU:HD22	2.02	0.40
1:A:3642:ASP:OD1	1:A:3642:ASP:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3019/4646 (65%)	2950 (98%)	68 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2741	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2696/4125 (65%)	2692 (100%)	4 (0%)	88	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1888	CYS
1	A	2626	THR
1	A	2998	ASN
1	A	4340	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1387	GLN
1	A	1454	GLN
1	A	1528	ASN
1	A	1755	GLN
1	A	1790	ASN
1	A	2005	GLN
1	A	2109	GLN
1	A	2130	ASN
1	A	2218	HIS
1	A	2377	ASN
1	A	2430	ASN
1	A	2439	HIS
1	A	2491	GLN
1	A	2667	ASN
1	A	2713	ASN
1	A	2827	HIS
1	A	3087	ASN
1	A	3498	ASN
1	A	3735	GLN
1	A	4012	ASN
1	A	4065	GLN
1	A	4100	HIS
1	A	4156	ASN
1	A	4325	ASN
1	A	4386	ASN
1	A	4446	ASN
1	A	4453	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	ATP	A	4701	4	32,33,33	0.52	0	48,52,52	0.59	0
3	ADP	A	4702	-	28,29,29	0.47	0	43,45,45	0.56	0
3	ADP	A	4703	-	28,29,29	0.47	0	43,45,45	0.50	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	ATP	A	4701	4	-	1/22/38/38	0/3/3/3
3	ADP	A	4702	-	-	1/16/32/32	0/3/3/3
3	ADP	A	4703	-	-	0/16/32/32	0/3/3/3

There are no bond length outliers.

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	4701	ATP	C4'-C5'-O5'-PA
3	A	4702	ADP	C2'-C1'-N9-C8

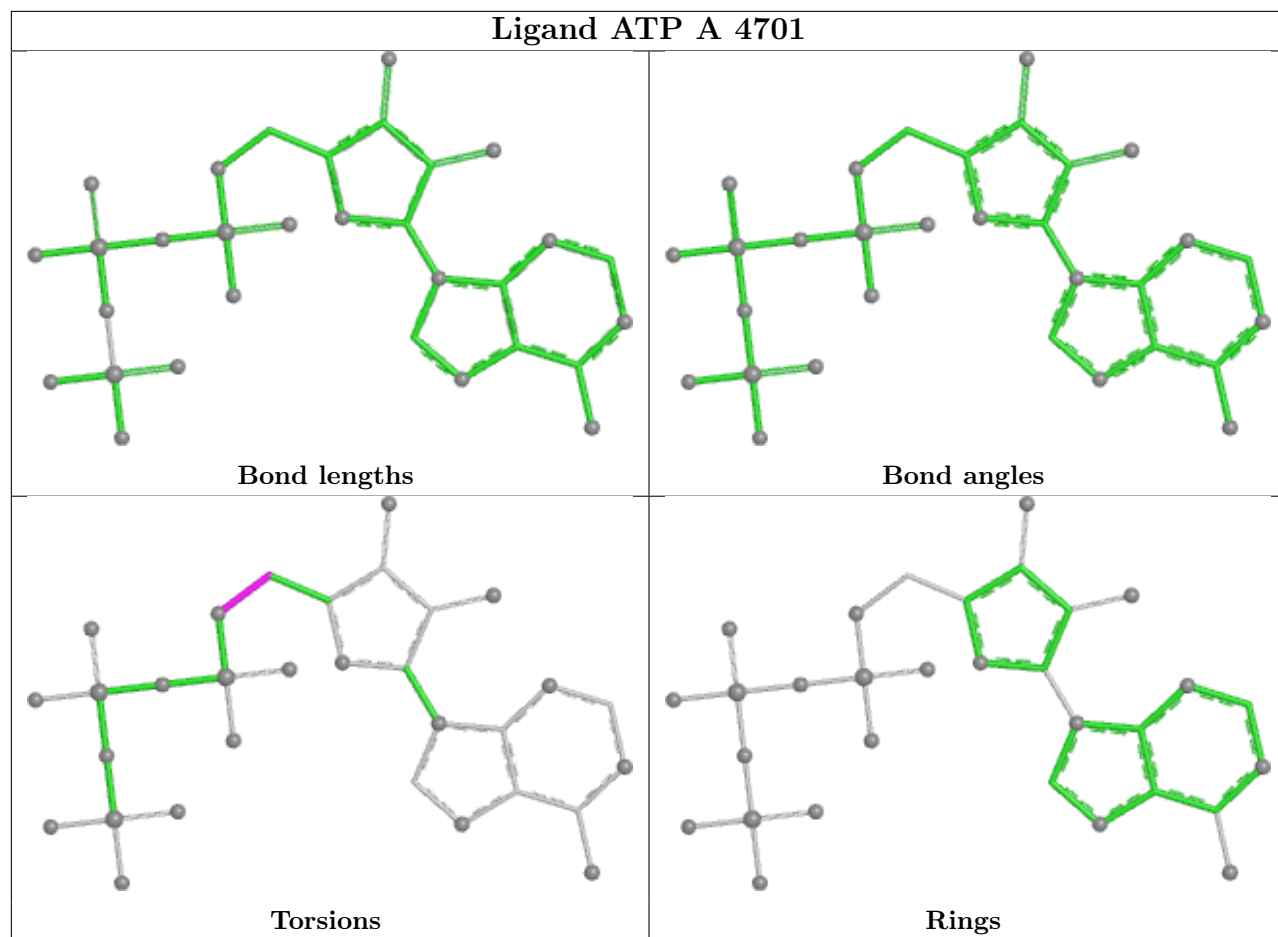
There are no ring outliers.

3 monomers are involved in 6 short contacts:

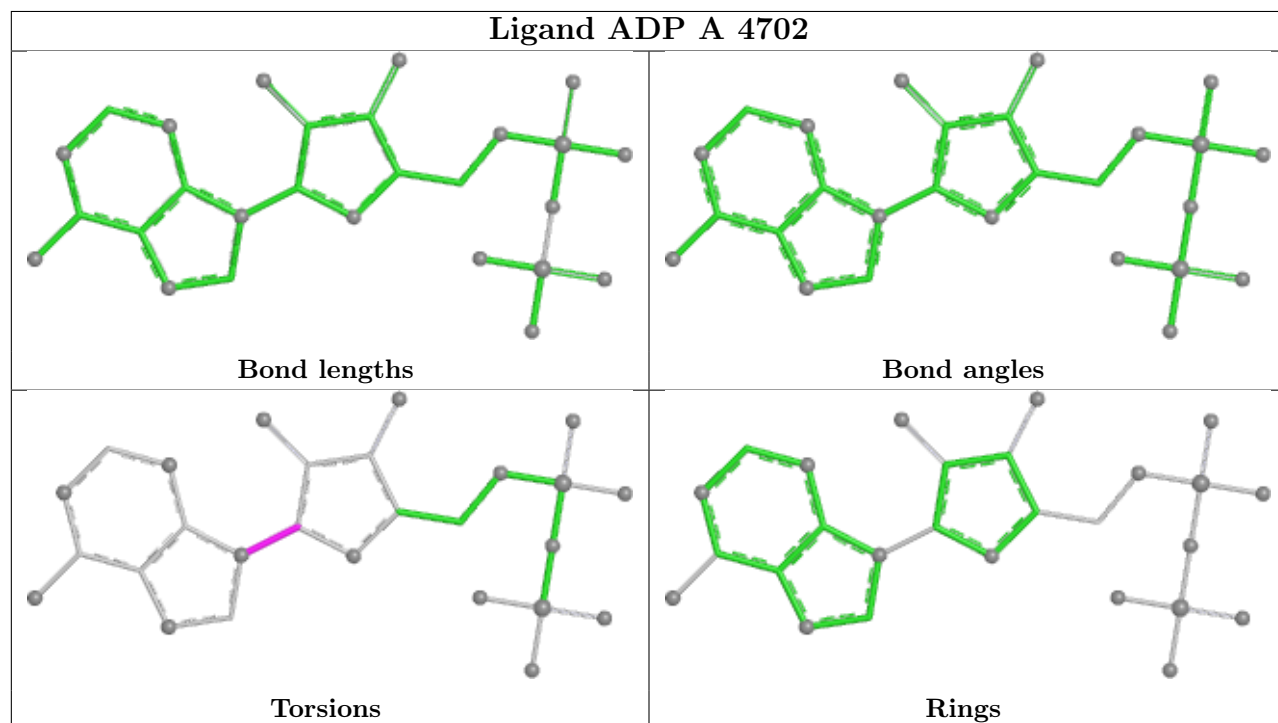
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ATP	3	0
3	A	4702	ADP	2	0
3	A	4703	ADP	1	0

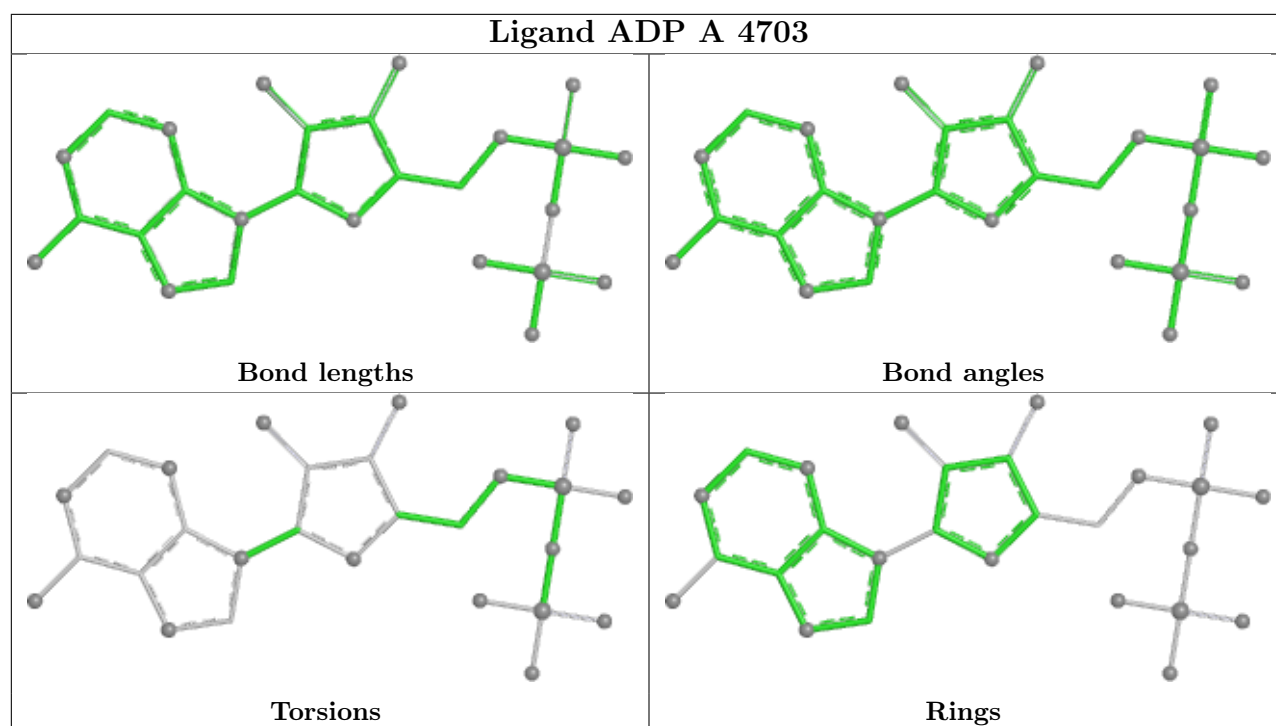
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand ATP A 4701



Ligand ADP A 4702





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.

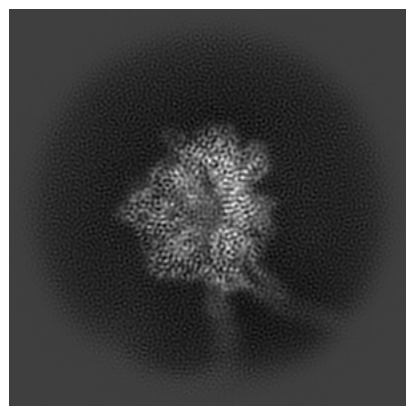
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44693. These allow visual inspection of the internal detail of the map and identification of artifacts.

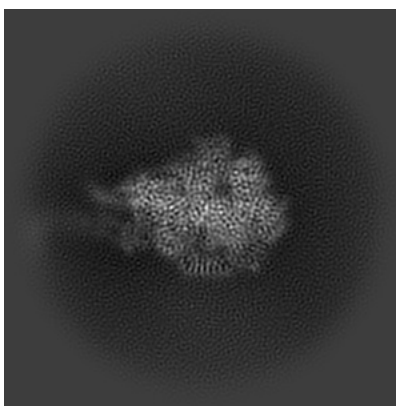
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

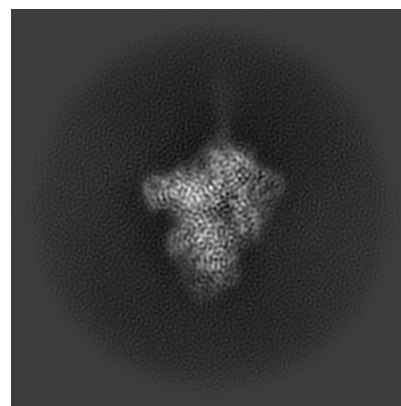
6.1.1 Primary map



X

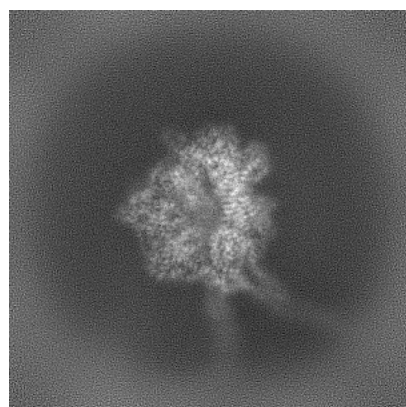


Y

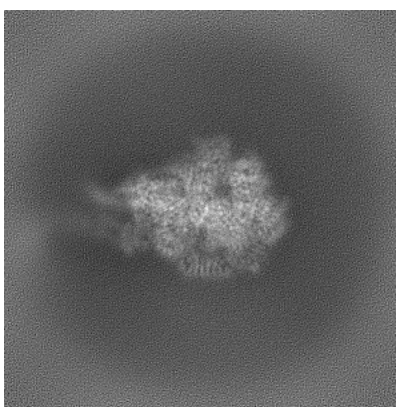


Z

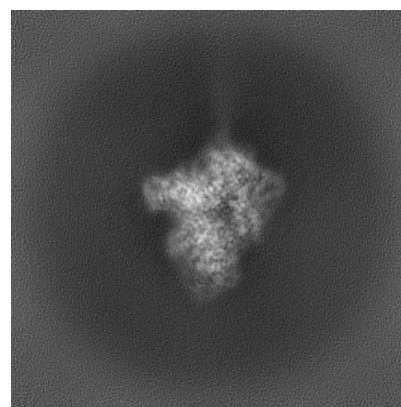
6.1.2 Raw map



X



Y

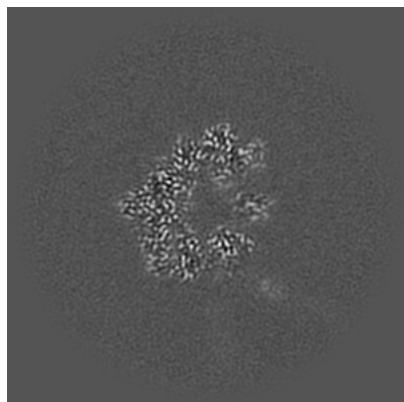


Z

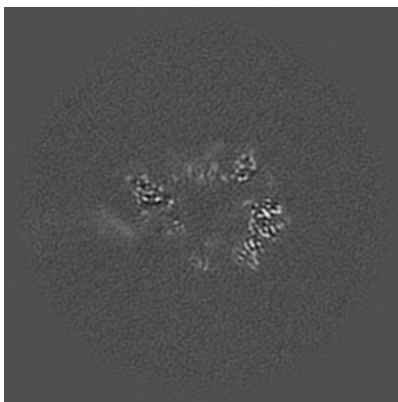
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

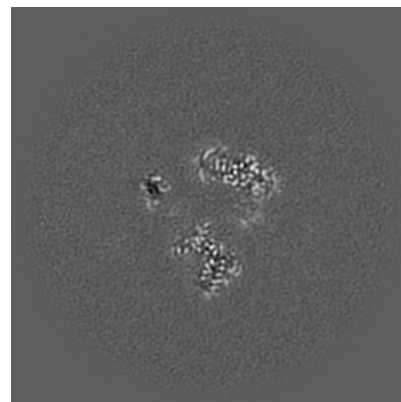
6.2.1 Primary map



X Index: 192

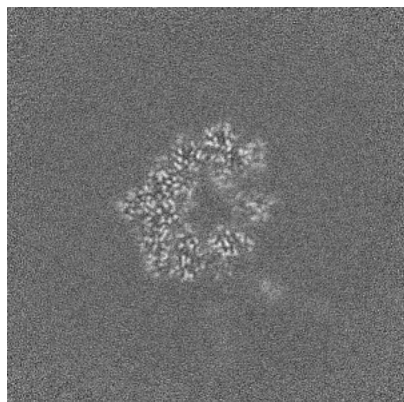


Y Index: 192

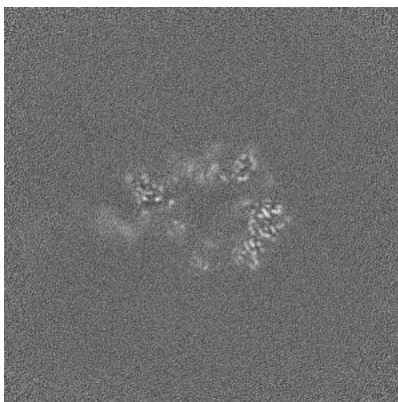


Z Index: 192

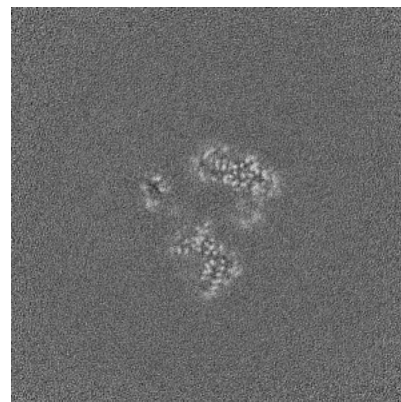
6.2.2 Raw map



X Index: 192



Y Index: 192

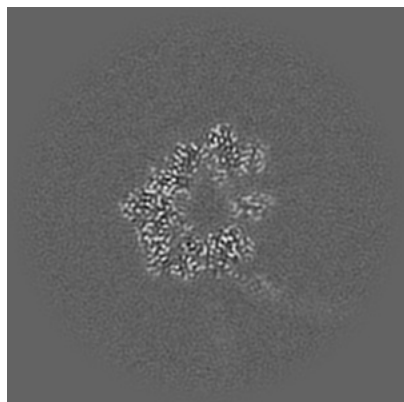


Z Index: 192

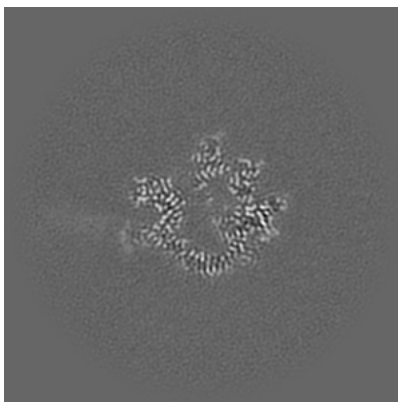
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

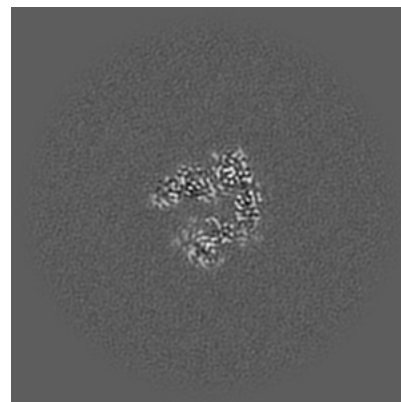
6.3.1 Primary map



X Index: 194

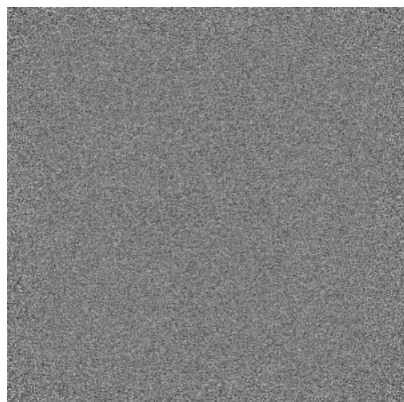


Y Index: 213

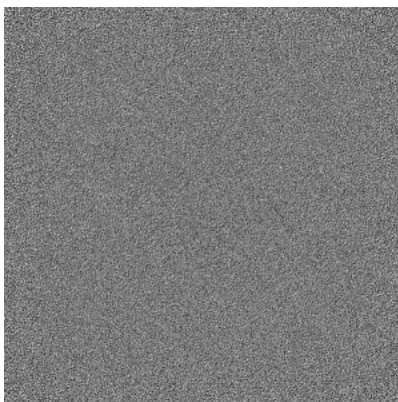


Z Index: 226

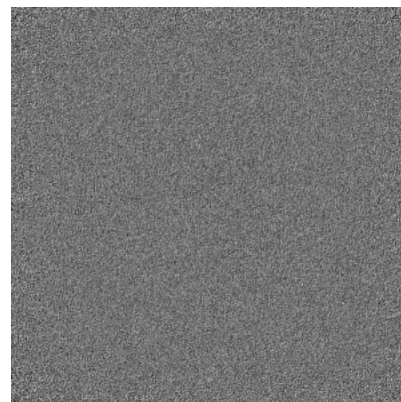
6.3.2 Raw map



X Index: 0



Y Index: 0

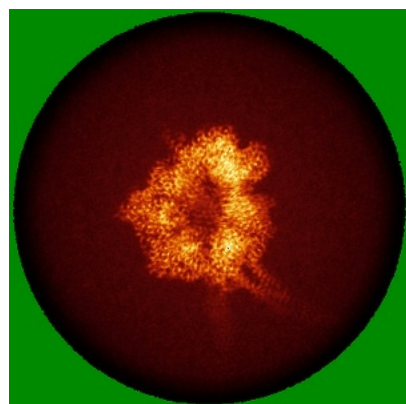


Z Index: 0

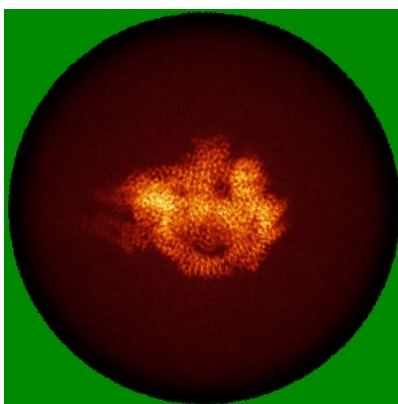
The images above show the largest variance slices of the map in three orthogonal directions.

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

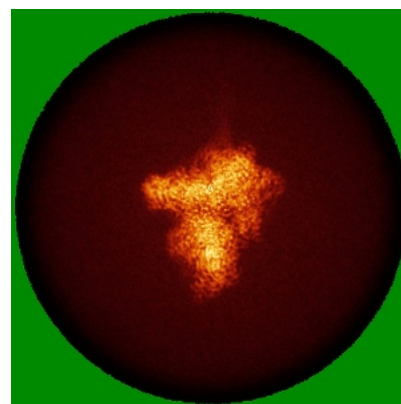
6.4.1 Primary map



X

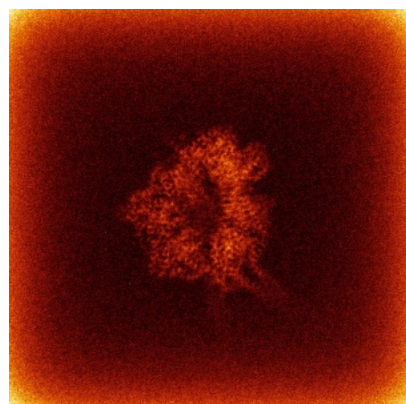


Y

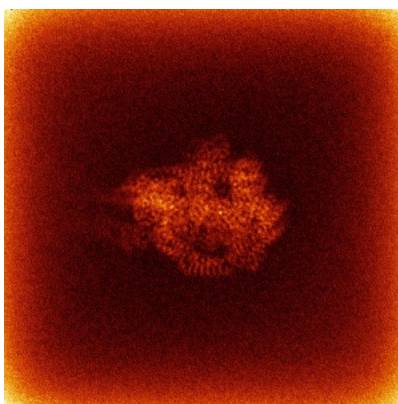


Z

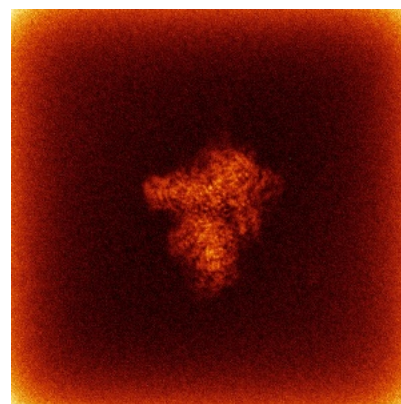
6.4.2 Raw map



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](#)

This section was not generated.

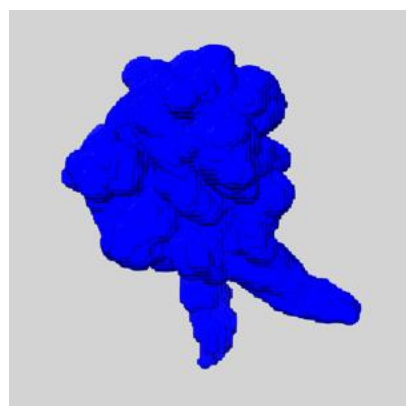
6.6 Mask visualisation [i](#)

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

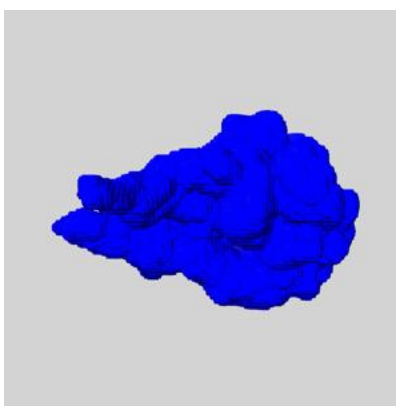
A mask typically either:

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

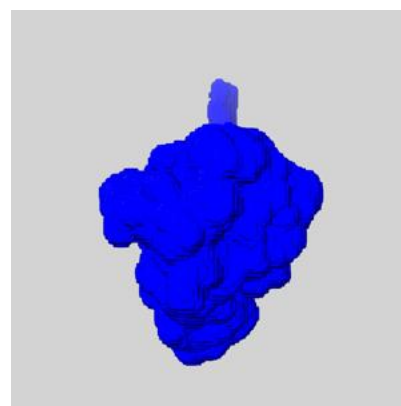
6.6.1 emd_44693_msk_1.map [i](#)



X



Y

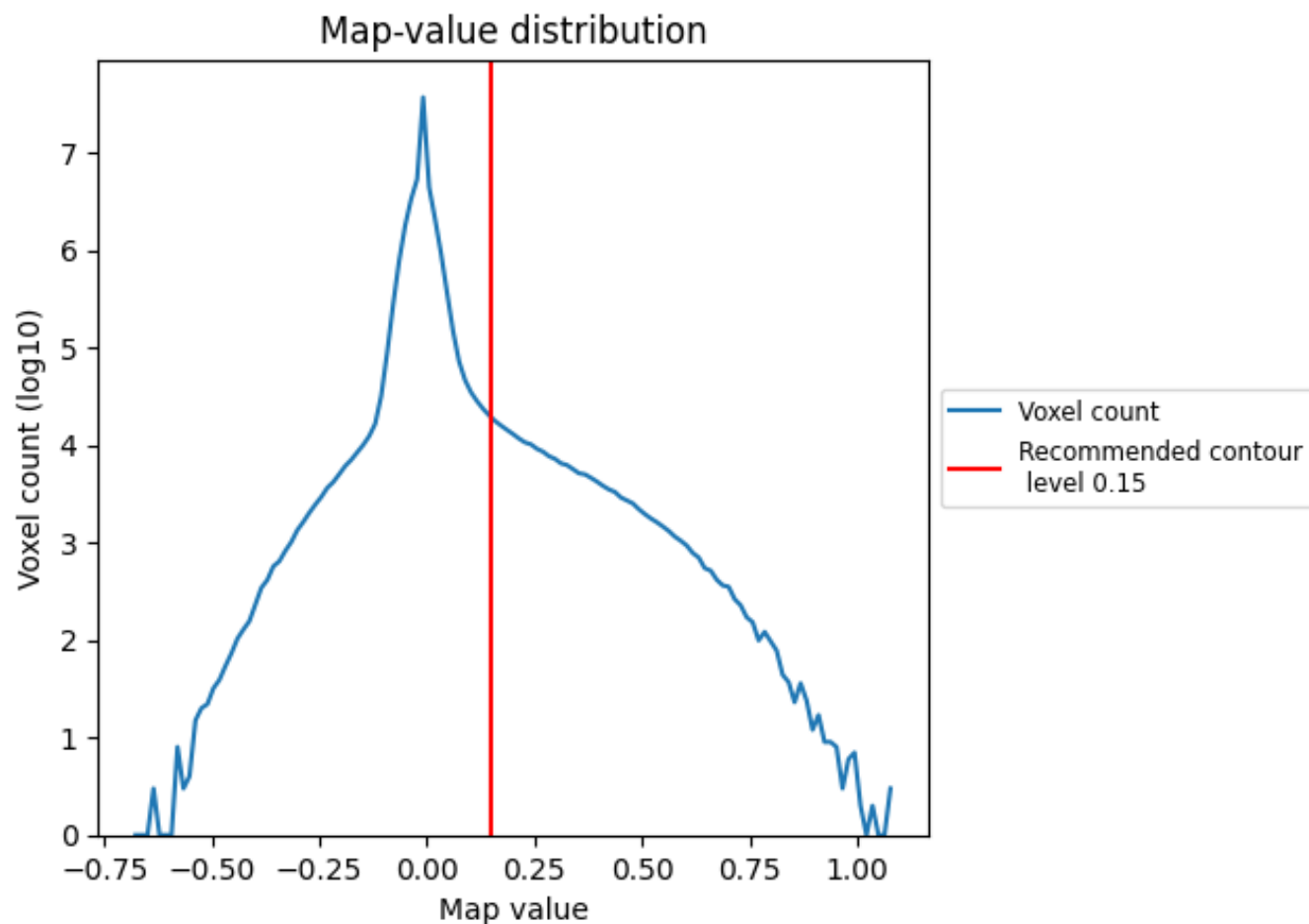


Z

7 Map analysis [i](#)

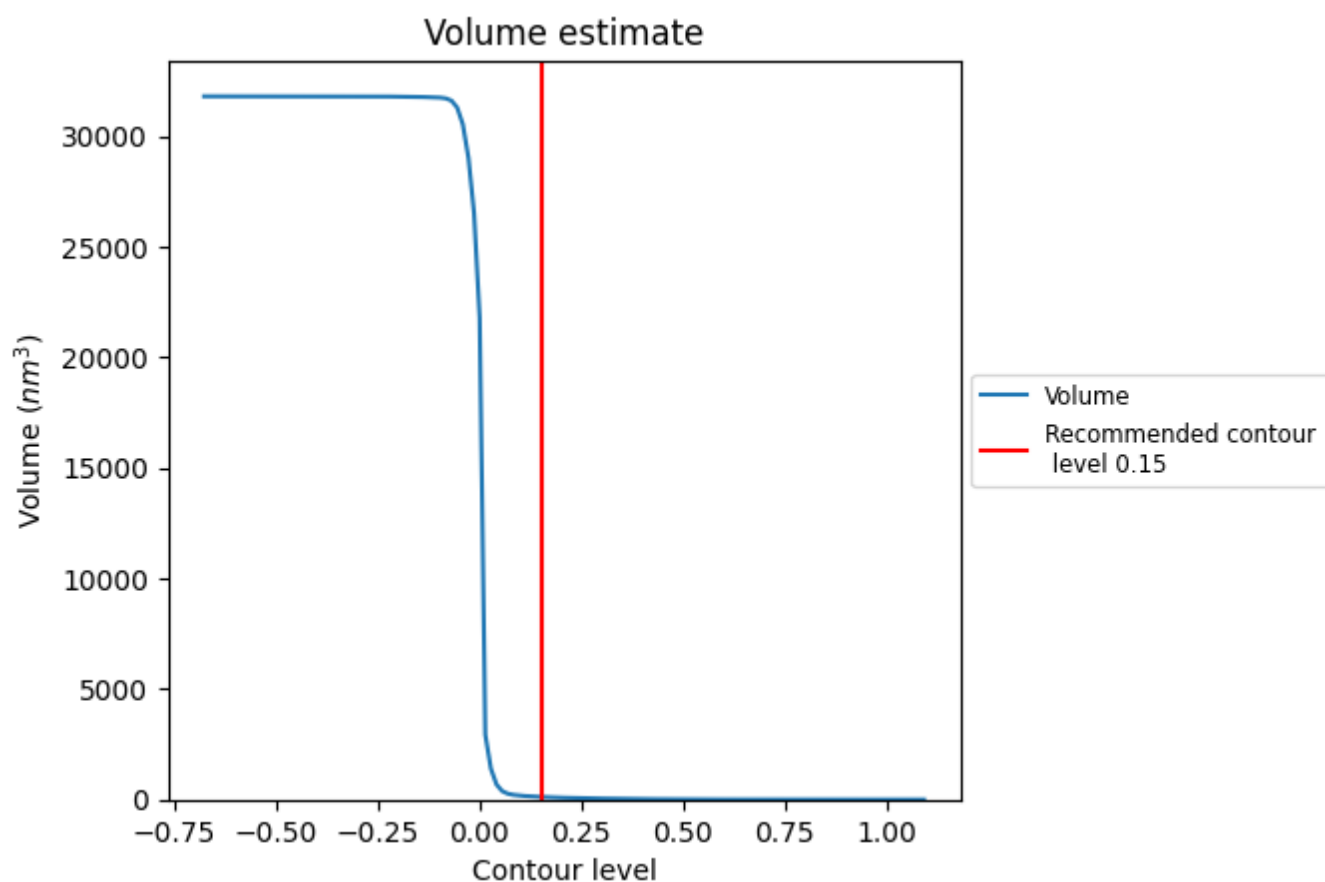
This section contains the results of statistical analysis of the map.

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.

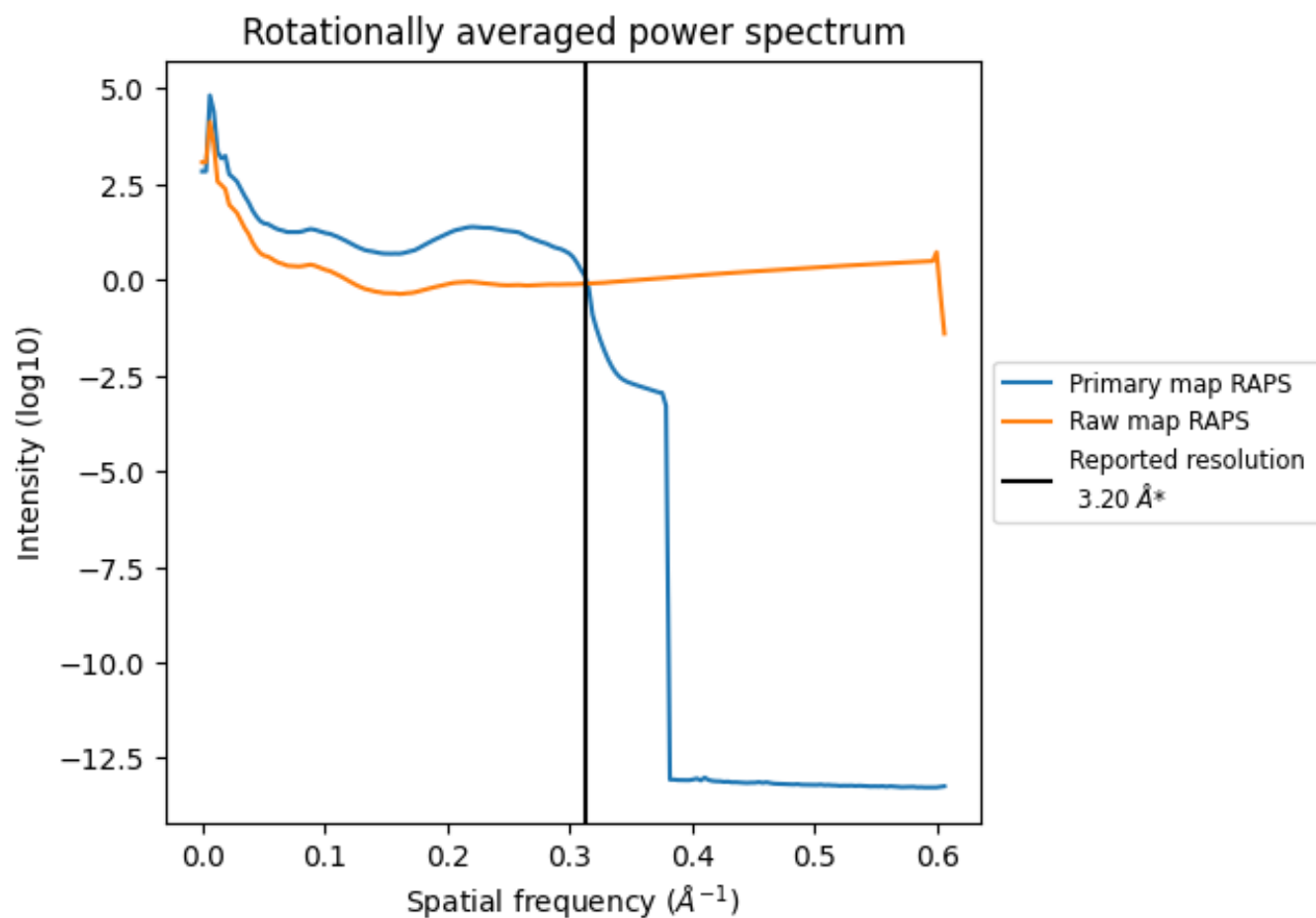
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 119 nm³; this corresponds to an approximate mass of 107 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 ⓘ

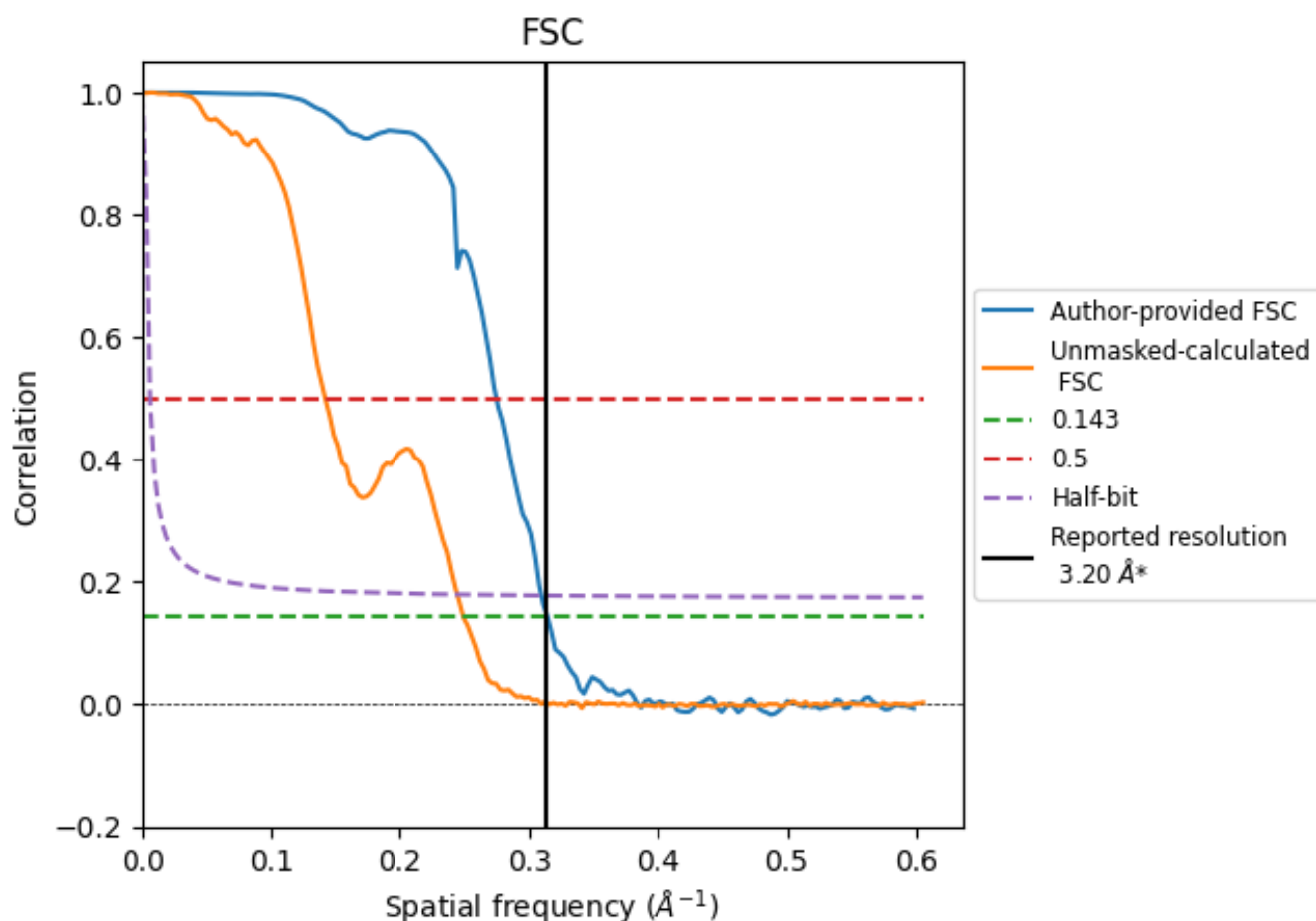


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.64	3.23
Unmasked-calculated*	4.01	7.06	4.09

*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 4.01 differs from the reported value 3.2 by more than 10 %

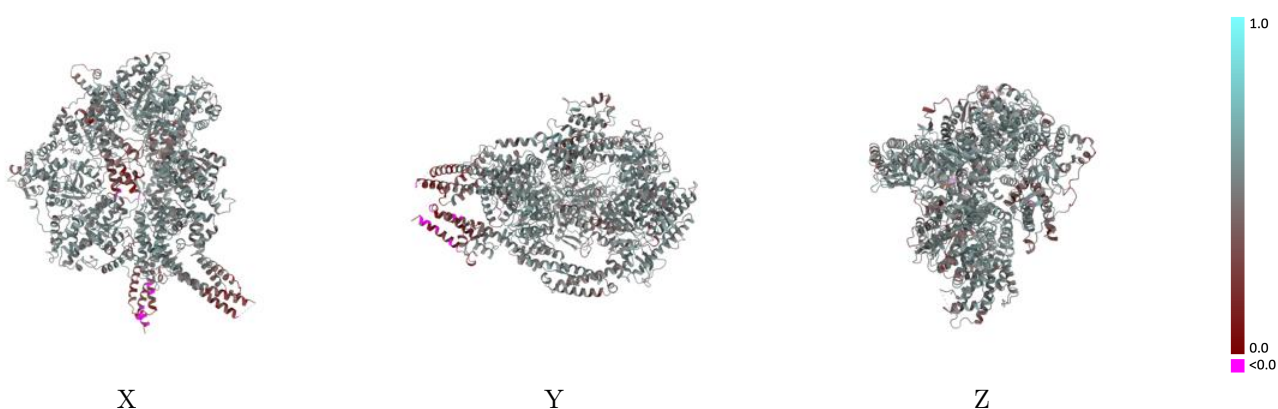
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44693 and PDB model 9BMA. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)

This section was not generated.

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

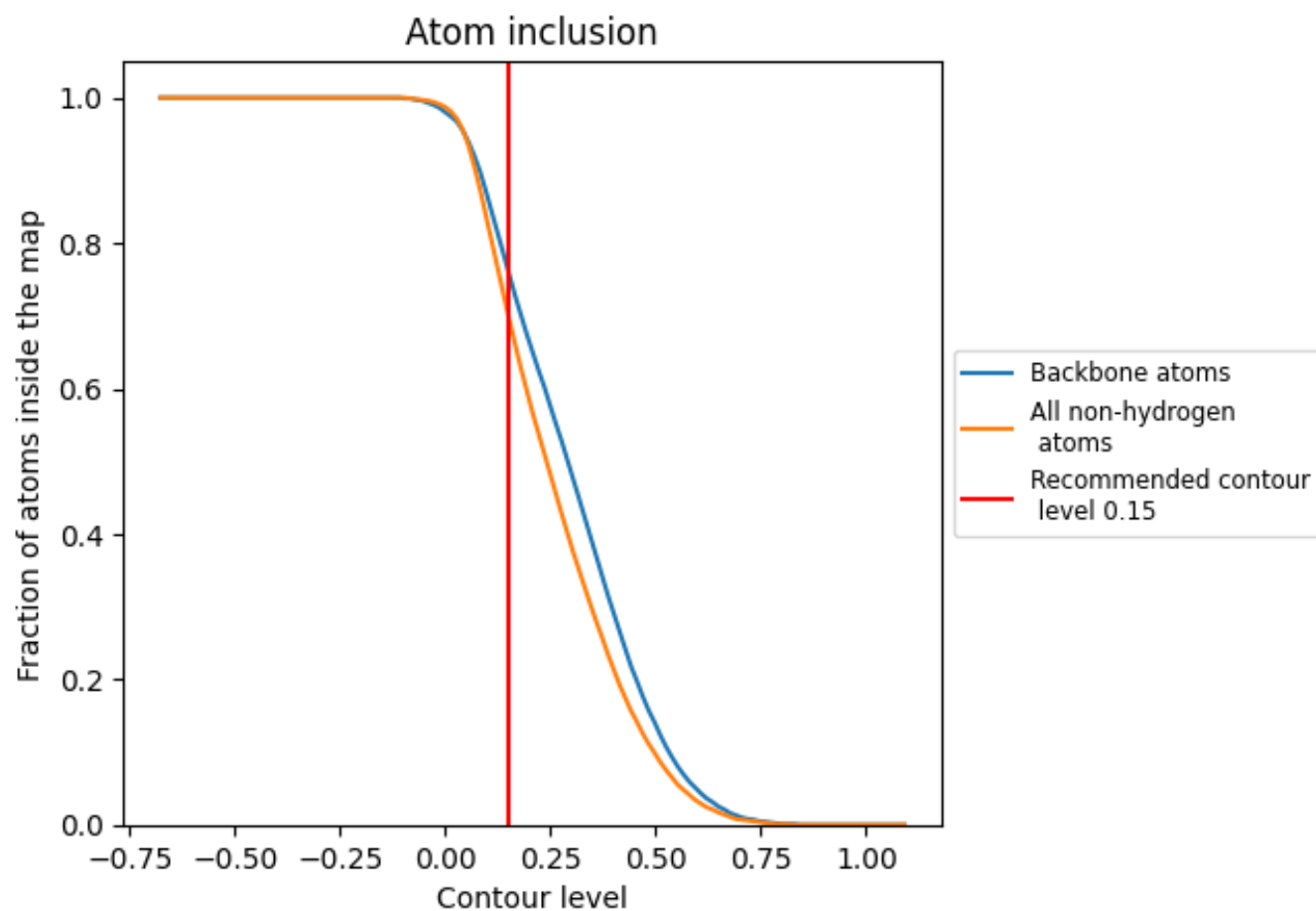


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 70% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6990	0.4900
A	0.7000	0.4900

