



## Full wwPDB EM Validation Report ⓘ

May 5, 2025 – 10:16 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

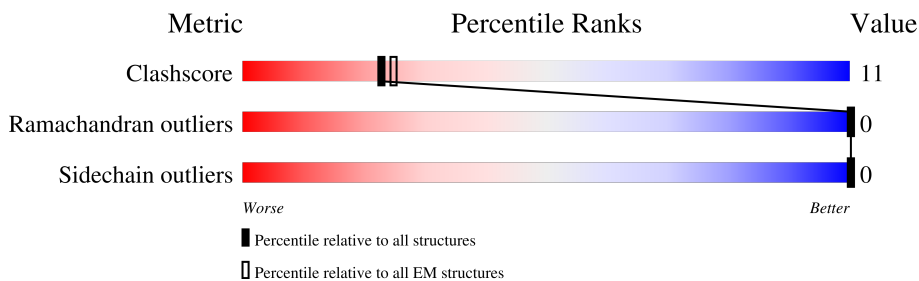
# 1 Overall quality at a glance

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4646	<div> <div>9%</div> <div>48%</div> <div>18%</div> <div>35%</div> </div>

## 2 Entry composition [i](#)

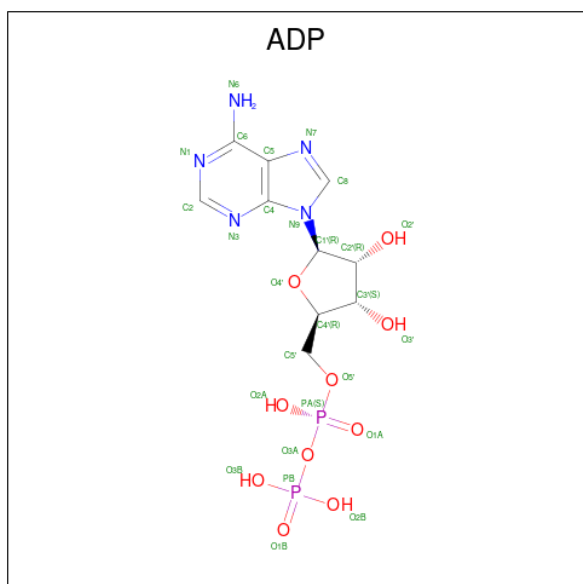
There are 4 unique types of molecules in this entry. The entry contains 24617 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

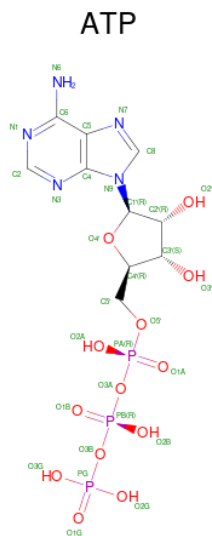
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3043	24503	15606	4234	4541	122	0	0

- 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 31	C 10	N 5	O 13	P 3	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	2	Total	Mg	0
			2	2	



L2065	A2066	I2069	F2072	C2076	Q2079	Q2083	Y2086	D2087	F2088	R2091	A2092	L2093	K2094	L2097	N2102	R2105	K2112	E2116	E2117	R2118	G2119	E2120	A2121	V2122	D2123	E2124	I2127	A2128	E2129	N2130	L2131	P2132	E2133	Q2134	L2137	I2138	M2145	L2149	L2160	L2161	Q2169																		
Q1960	V1951	W1954	E1959	F1960	N1961	R1962	R1966	I1978	Q1979	E1980	E1984	P1988	N1989	Y1990	D1991	K1992	T1993	S1994	A1995	E2000	L2001	L2002	N2003	V2006	K2007	D2011	N2019	P2020	G2021	TYR	ALA	GLY	ARG	S2026	L2035	L2039	A2040	M2041	L2048	V2052	M2053	L2054	Y2055	S2056															
R1806	L1811	I1812	L1815	V1816	Q1841	M1842	R1843	F1844	Y1845	Q1855	Q1856	L1857	S1858	I1859	A1864	N1867	Y1868	Y1872	V1875	Q1876	D1877	T1882	C1888	T1891	M1892	E1897	G1902	K1912	T1913	E1914	G1920	R1925	F1926	V1927	E1934	Q1939	V1946	G1947	L1948	C1949																			
K1652	K1655	K1656	M1657	F1658	V1661	S1662	S1671	I1676	S1677	S1678	R1679	I1692	I1698	N1699	E1700	W1701	L1702	L1717	V1721	V1724	F1727	Y1738	L1749	V1750	E1763	M1769	G1770	G1771	G1772	G1773	D1774	A1775	V1785	L1792	L1797	M1798	E1799	Q1800	L1803	R1804	R1805																		
L1521	L1527	V1536	D1539	Q1541	R1542	R1543	W1544	L1547	G1553	S1554	A1555	I1571	S1572	L1576	M1579	V1582	L1587	Y1588	M1589	D1590	V1591	Q1595	R1599	S1600	L1601	L1604	A1605	D1606	L1607	L1608	I1611	Q1612	R1623	S1624	F1625	F1626	P1627	R1628	F1629	L1637																			
K1441	N1442	E1443	A1444	I1445	V1446	K1447	D1448	V1449	L1450	L1451	V1452	A1453	F1456	M1457	L1463	I1466	R1467	E1468	V1469	L1475	D1476	L1477	V1478	Q1481	N1482	R1485	L1486	I1487	R1488	D1491	N1495	K1498	E1499	H1500	I1501	S1505	A1506	M1507	K1508	L1509	S1510	P1511	Y1512	Y1513	K1514	V1515	F1516	E1517	E1518										
A1381	S1382	Y1383	E1384	F1385	V1386	Q1387	R1388	L1389	L1390	K1391	G1392	Y1393	M1394	K1395	I1396	N1397	M1398	L1399	V1400	I1401	E1402	L1403	K1404	S1405	E1406	A1407	L1408	K1409	D1410	R1411	H1412	W1413	K1414	Q1415	L1416	M1417	K1418	R1419	L1420	H1421	V1422	N1423	W1424	V1425	V1426	S1427	E1428	L1429	T1430	L1431	G1432	Q1433	I1434	W1435	D1436	V1437	D1438	L1439	Q1440
VAL	ALA	LEU	GLU	LEU	Q1327	D1328	L1329	K1330	G1331	V1332	W1333	S1334	E1335	L1336	S1337	K1338	V1339	W1340	E1341	Q1342	I1343	D1344	Q1345	K1347	E1348	Q1349	F1350	W1351	V1352	S1353	V1354	Q1355	P1356	R1357	K1358	L1359	R1360	Q1361	N1362	L1363	D1364	A1365	L1366	L1367	N1368	Q1369	L1370	K1371	S1372	F1373	P1374	A1375	R1376	L1377	R1378	Q1379	Y1380		
TRP	GLU	PHE	GLN	PHE	PRO	PRO	TRP	VAL	THR	GLY	ASN	TYR	ILE	GLN	ARG	PRO	ASN	ILE	GLU	GLY	ALA	LEU	GLN	GLY	ASP	ALA	ALA	ASN	LEU	LYS	GLN	MET	LYS	ILE	VAL	GLU	GLU	THR	THR	ASP	ARG	ALA	V1436	V1437	D1438	L1439	Q1440												
ARG	PHE	GLN	PHE	GLN	PRO	PRO	TRP	VAL	THR	GLY	ASN	TYR	ILE	GLN	ARG	PRO	ASN	ILE	GLU	GLY	ALA	LEU	GLN	GLY	ASP	ALA	ALA	ASN	LEU	LYS	GLN	MET	LYS	ILE	VAL	GLU	GLU	THR	THR	ASP	ARG	ALA	V1436	V1437	D1438	L1439	Q1440												
GLU	PHE	HIS	GLN	THR	GLN	ILE	SER	LYS	SER	LYS	GLN	GLN	SER	VAL	ASP	THR	ALA	THR	ALA	VAL	ILE	THR	PHE	GLN	GLY	ASP	ALA	ASN	ILE	VAL	GLU	GLU	THR	THR	ASP	ARG	ALA	V1436	V1437	D1438	L1439	Q1440																	
ASN	ALA	LEU	VAL	THR	ILE	MET	ARG	LYS	ARG	PRO	ASN	THR	PHE	LYS	VAL	VAL	LYS	VAL	ILE	VAL	ILE	THR	PHE	GLN	GLY	ASP	ALA	ASN	ILE	VAL	GLU	GLU	THR	THR	ASP	ARG	ALA	V1436	V1437	D1438	L1439	Q1440																	
ASN	LYS	LEU	ASP	GLN	MET	GLY	ILE	GLU	VAL	ILE	GLU	ARG	LEU	ARG	GLY	LEU	ARG	GLY	LEU	GLU	VAL	ILE	THR	PHE	GLN	GLY	ASP	ALA	ASN	ILE	VAL	GLU	GLU	THR	THR	ASP	ARG	ALA	V1436	V1437	D1438	L1439	Q1440																
PHE	ASN	PHE	GLN	LYS	VAL	VAL	ASP	ILE	VAL	ILE	GLU	ARG	LEU	GLY	LEU	GLU	VAL	THR	ALA	VAL	ILE	THR	PHE	GLN	GLY	ASP	ALA	ASN	ILE	VAL	GLU	GLU	THR	THR	ASP	ARG	ALA	V1436	V1437	D1438	L1439	Q1440																	



L4553	C4438	M4343	M4174	L4042	E3913	R3782	T3681	E3490	GLN
D4554	E4439	L4344	M4043	M4043	I3914	R3783	R3682	K3491	LYS
S4557	C4440	M4346	C4044	D4050	V3915	V3784	V3686	F3496	ALA
V4560	K4441	Q4347	A4051	A4051	L3916	E3785	V3686	F3496	ASN
K4564	K4442	M4348	A4188	V4055	S3917	E3786	C3693	Q3499	VAL
N4571	K4443	L4349	L4189	E4056	A3918	T3787	S3694	T3502	GLU
K4574	Q4444	GLU	R4193	D4057	Q3919	D3788	R3695	R3607	GLU
K4574	T4445	ASP	L4194	D4058	S3920	M3791	N3700	R3608	MET
L4577	M4446	ASP	K4204	L4058	R3923	Q3792	F3701	R3611	ILE
I4581	L4448	ALA	Y4205	E4061	T3796	T3796	L3708	F3614	ASP
L4590	P4461	TYR	D4211	S4073	S3809	S3809	E3720	D3617	GLU
V4592	P4462	ALA	L4212	A4074	I3810	I3810	D3725	I3514	ALA
V4593	H4466	GLU	A4215	E4075	E3932	E3932	F3619	F3520	SER
K4594	P4470	LYS	D4217	A4087	E3933	T3814	R3728	M3524	ILE
Q4595	V4475	THR	L4243	V4088	R3937	S3817	L3731	R3525	ALA
T4596	V4476	ARG	M4247	K4089	F3944	L3818	Q3735	W3532	VAL
N4597	I4476	THR	M4251	S4090	K3945	L3824	G3736	L3536	ALA
T4598	S4480	ASP	I4251	G4091	D3946	S3828	Q3739	I3541	TYR
E4599	F4481	SER	R4255	R4092	A3949	L3835	L3740	D3546	ILE
K4600	F4482	THR	V4256	M4095	K3950	V3839	R3743	R3549	SER
P4608	S4483	GLY	F4260	K4097	D3954	L3846	E3746	T3550	GLU
V4609	E4484	ARG	L4264	V4099	E3955	R3855	L3750	Y3551	ALA
L4611	R4485	PRO	L4265	W4105	P3966	R3855	L3753	Y3552	ILE
N4612	I4486	A4375	L4266	L4106	E3967	I3859	N3753	L3553	LYS
I4619	L4489	R4378	F4267	L4113	Y3972	L3863	E3754	D3557	ALA
V4622	I4492	H4381	F4268	H4114	L3973	F3864	N3755	E3558	ASP
A4627	A4496	T4391	S4277	S4115	W3974	Q3865	V3756	R3559	LEU
T4628	C4499	Q4392	F4282	L4116	S3975	V3866	K3757	L3560	ALA
K4629	Q4500	Q4393	F4287	Q4117	E3976	R3869	R3759	R3561	ALA
E4637	A4501	T4394	K4287	L4123	E3977	R3870	L3761	W3562	VAL
R4638	K4502	L4398	R4291	L4124	L3991	A3872	D3762	L3567	GLU
V4642	E4503	K4399	W4308	L4127	L3992	R3873	D3763	E3575	V3472
E4646	L4504	E4403	V4309	T4127	R4000	G3874	D3764	N3576	R3473
	L4511	N4404	V4309	K4133	M4004	M3875	T3765	M3579	S3475
	Q4512	F4413	L4312	L4138	M4021	H3880	T3766	L3580	T3476
	Q4513	V4417	P4313	L4139	L4025	L3886	I3767	K3581	A3477
	V4528	L4423	D4314	R4140	D4026	G3897	L3661	R3582	
	L4541	L4423	T4315	F4145	L4027	D3802	I3662	R3585	R3480
	E4542	P4524	P4524	N4156	T4030	R3910	G3665	I3590	S3481
	V4543	L4332	L4332	M4157	V4031		D3666	D3591	L3482
	S4548	Q4429	Q4436	T4160	L4038		D3667	G3594	S3483
	Q4549	Q4436	V4437	R4168	T4039		D3668	Q3585	A3484
	C4550				P4040		P3673	E3485	R3486
	A4551							A3596	
	T4552								K3489

## 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 ( $\text{\AA}$ )	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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, MG, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.15	0/25022	0.32	1/33900 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1410	ASP	N-CA-C	-5.01	108.19	114.56

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	539	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	539	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 (539) 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:2039:LEU:HD22	1:A:2041:MET:HE2	1.67	0.77
1:A:1407:ALA:HA	1:A:1457:MET:HE3	1.66	0.77
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: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:2473:ASN:HB2	1:A:2481:MET:HE1	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:2221:MET:HE1	1:A:2348:LEU:HD21	1.72	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:1888:CYS:HB2	1:A:2041:MET:HE1	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:2581:LEU:HD13	1:A:2591:LEU:HD13	1.81	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:2444:GLU:H	1:A:2510:MET:HE1	1.64	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:3043:MET:HA	1:A:3043:MET:HE2	1.84	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:2769:LEU:HG	1:A:2773:MET:HE3	1.85	0.58
1:A:2387:LEU:HB2	1:A:2412:MET:HE2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:3008:MET:HE1	1:A:3064:VAL:HG11	1.86	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:4043:MET:HE3	1:A:4127:THR:HG22	1.88	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:3871:VAL:HG12	1:A:3875:MET:HE2	1.88	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:3601:MET:HE2	1:A:3634:LEU:HD23	1.88	0.55
1:A:1625:SER:OG	1:A:1699:ASN:OD1	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:2386:PRO:HG3	1:A:2413:LEU:HD21	1.89	0.55
1:A:2686:MET:HE2	1:A:2708:PHE:HZ	1.71	0.54
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:2961:ILE:HD13	1:A:2975:ASP:CG	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:3731:LEU:HD21	1:A:3791:MET:HG2	1.92	0.52
1:A:3967:GLU:HB2	1:A:4004:MET:HE2	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: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:3008:MET:HE3	1:A:3012:LEU:HG	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3601:MET:HE1	1:A:3611:ARG:HE	1.75	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: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:4480:SER:O	1:A:4483:SER:OG	2.22	0.50
1:A:2843:ARG:HH21	1:A:3093:TRP:HD1	1.60	0.49
1:A:3030:MET:HE3	1:A:3050:LEU:HD11	1.93	0.49
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: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:1343:ILE:HA	1:A:1346:MET:HE2	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:3008:MET:HE2	1:A:3066:PHE:CZ	2.48	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:2265:TYR:OH	1:A:2311:TRP:O	2.20	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:3817:SER:HB2	1:A:4346:MET:HE1	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2224:GLY:H	1:A:2230:LYS:HD3	1.79	0.47
1:A:4043:MET:HE1	1:A:4055:VAL:HG21	1.96	0.47
1:A:1403:LEU:HD21	1:A:1446:VAL:HG13	1.96	0.46
1:A:1657:MET:HE1	1:A:1702:LEU:HD21	1.97	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:2145:MET:HE2	1:A:2145:MET:HB2	1.81	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
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:4628:THR:C	1:A:4629:LYS:HD2	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4042:LEU:HD12	1:A:4139:LEU:HD23	1.98	0.45
1:A:4343:MET:HE3	1:A:4343:MET:HB2	1.62	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:2982:ARG:HE	1:A:2988:GLU:CD	2.25	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
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:3880:HIS:CE1	1:A:4021:MET:HE2	2.52	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:1769:MET:HE2	1:A:1775:ALA:HA	2.00	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:2686:MET:HE2	1:A:2708:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:1678:SER:OG	1:A:1679:ARG:N	2.50	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:3618:ALA:C	1:A:3621:LYS:HB3	2.40	0.43
1:A:4211:ASP:CG	1:A:4255:ARG:HH12	2.27	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:1991:ASP:CG	1:A:1993:THR:HG1	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:4611:LEU:HB2	1:A:4619:ILE:HD11	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1486:LEU:HA	1:A:1579:MET:HE2	2.02	0.41
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:4157:MET:HE3	1:A:4309:VAL:HG22	2.02	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4423:LEU:HD13	1:A:4466:HIS:HD2	1.86	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: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:3766:ILE:HD12	1:A:3766:ILE:HA	1.91	0.41
1:A:4243:LEU:O	1:A:4247:MET:HE3	2.20	0.41
1:A:4264:LEU:O	1:A:4267:THR:OG1	2.32	0.41
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:4095:MET:HE2	1:A:4127:THR:HG21	2.01	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:3016:GLU:N	1:A:3016:GLU:OE2	2.55	0.40
1:A:3038:GLN:HG2	1:A:3043:MET:HE1	2.04	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	3035/4646 (65%)	2952 (97%)	83 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	2706/4125 (66%)	2706 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1397	ASN
1	A	1479	ASN
1	A	1495	ASN
1	A	1566	GLN
1	A	1755	GLN
1	A	1784	ASN
1	A	1876	GLN
1	A	1894	GLN
1	A	1922	GLN
1	A	1931	ASN
1	A	2282	HIS
1	A	2299	GLN
1	A	2377	ASN
1	A	2414	GLN
1	A	2416	GLN
1	A	2475	ASN
1	A	2667	ASN
1	A	2677	GLN
1	A	2698	GLN
1	A	2886	GLN
1	A	2932	HIS
1	A	3009	ASN
1	A	3061	ASN
1	A	3063	HIS
1	A	3087	ASN
1	A	3202	ASN
1	A	3523	GLN
1	A	3535	HIS
1	A	3709	GLN
1	A	3822	HIS
1	A	3845	ASN
1	A	3865	GLN
1	A	3869	ASN
1	A	3956	GLN
1	A	4156	ASN
1	A	4262	GLN
1	A	4291	HIS
1	A	4397	HIS
1	A	4526	GLN
1	A	4571	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	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%)
2	ADP	A	4703	-	24,29,29	0.87	0	29,45,45	1.24	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	4704	-	-	2/12/32/32	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
2	ADP	A	4703	-	-	5/12/32/32	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

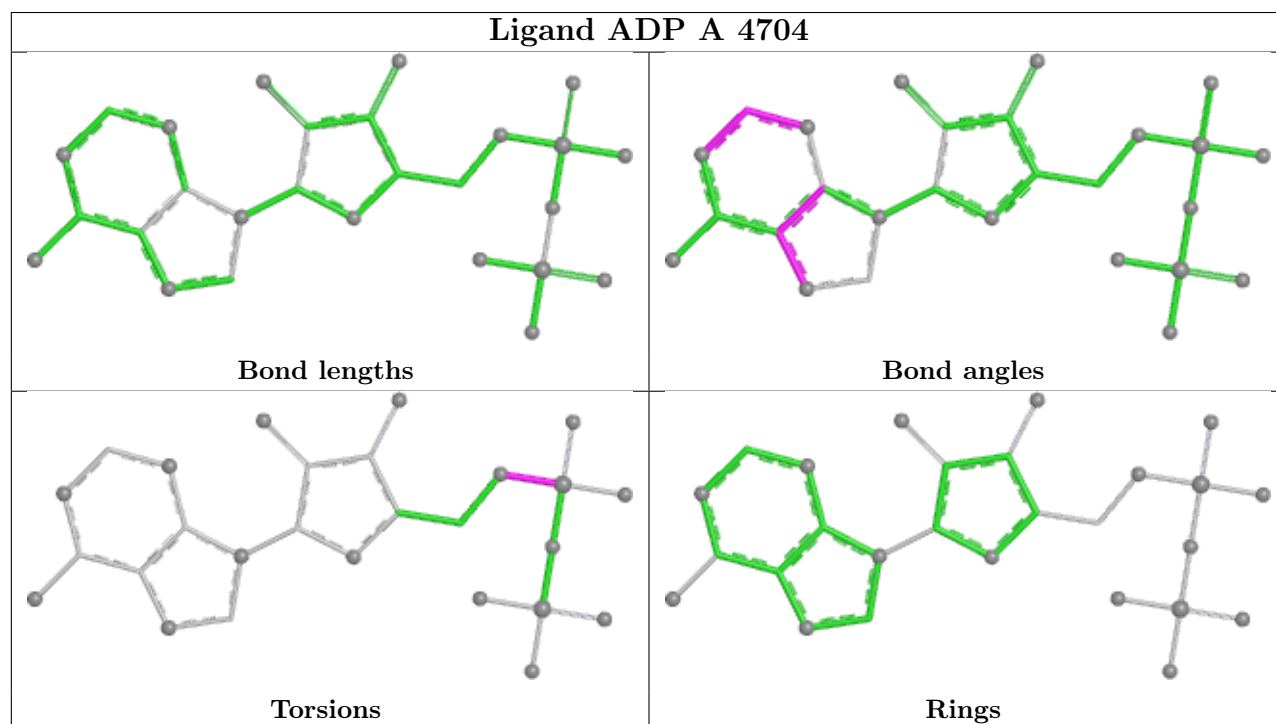
There are no ring outliers.

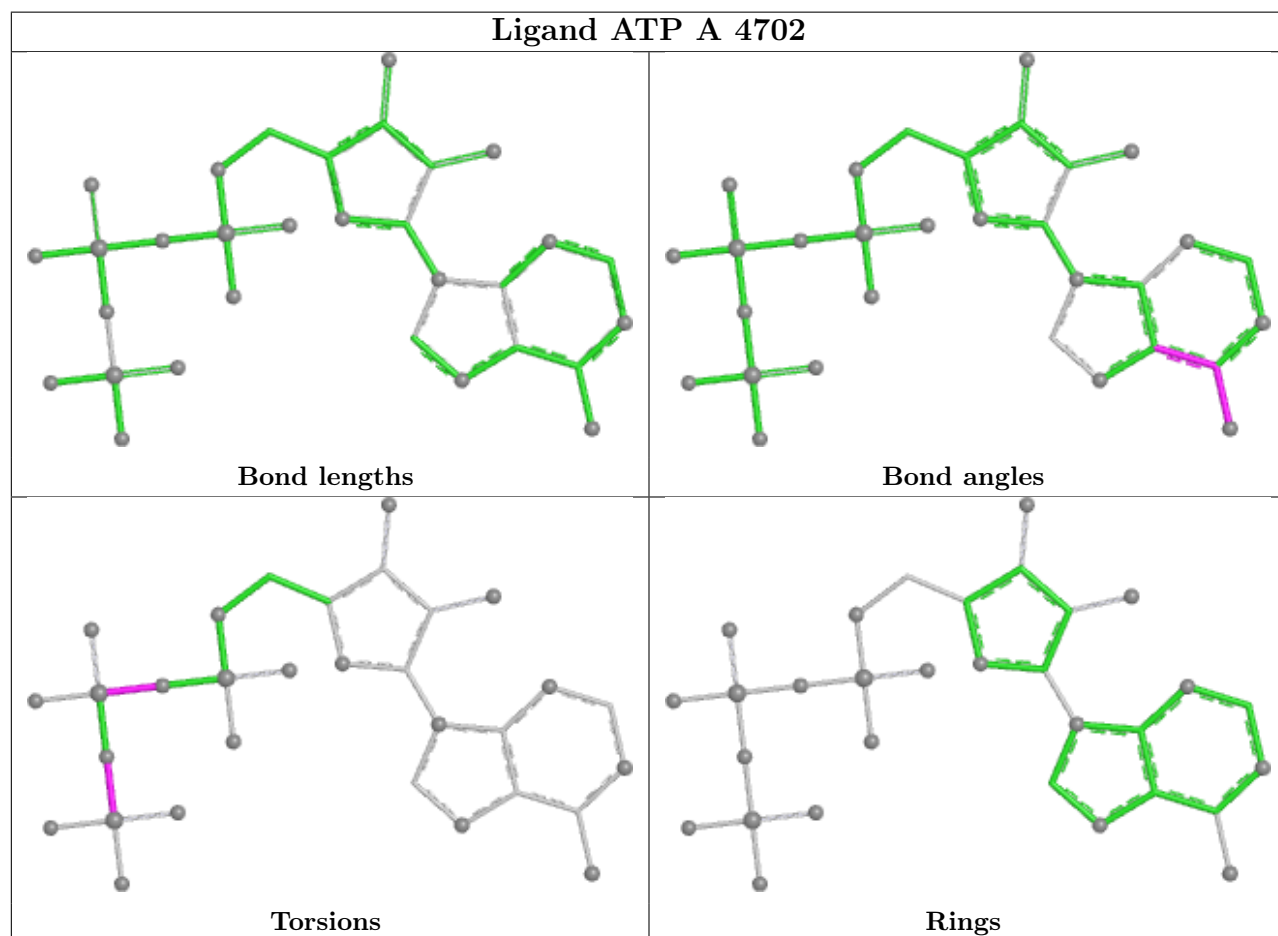
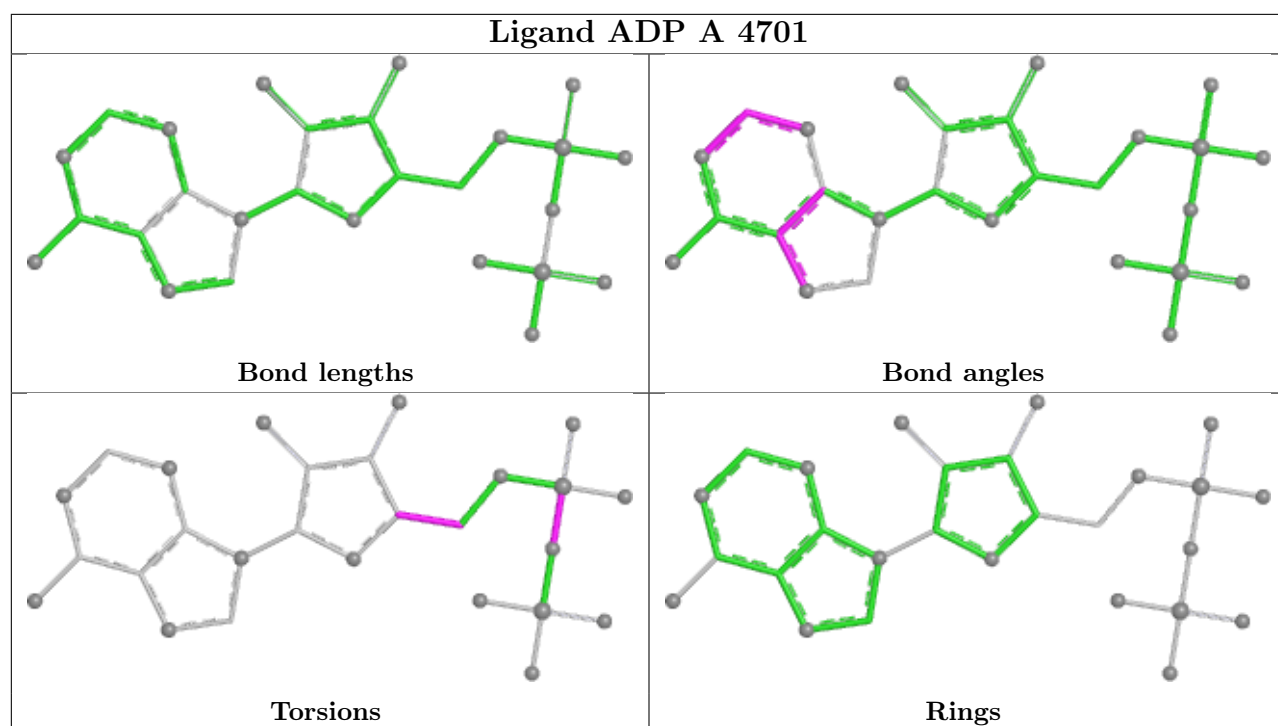
4 monomers are involved in 6 short contacts:

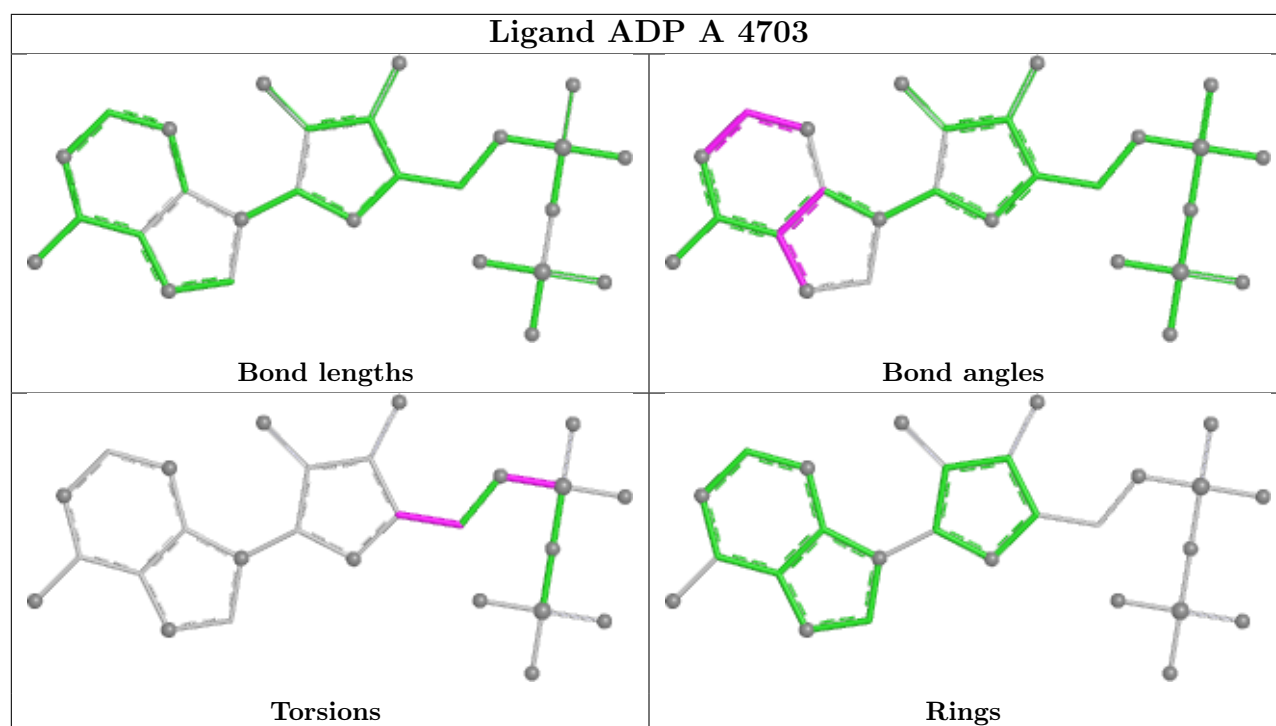
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4704	ADP	2	0
2	A	4701	ADP	2	0
3	A	4702	ATP	1	0
2	A	4703	ADP	1	0

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.







## 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.

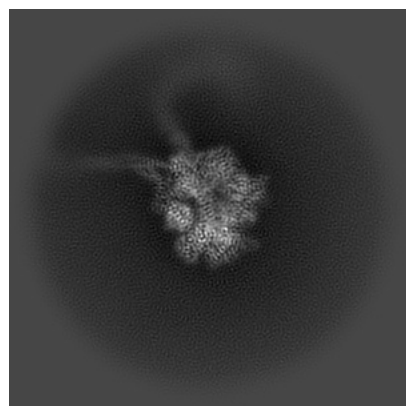
## 6 Map visualisation [i](#)

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

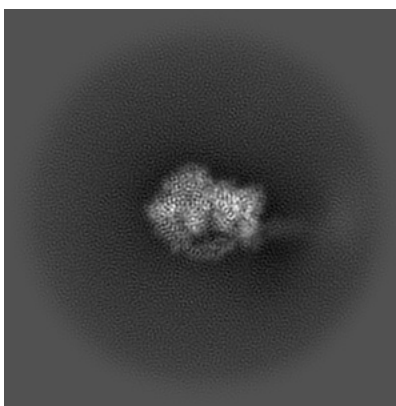
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

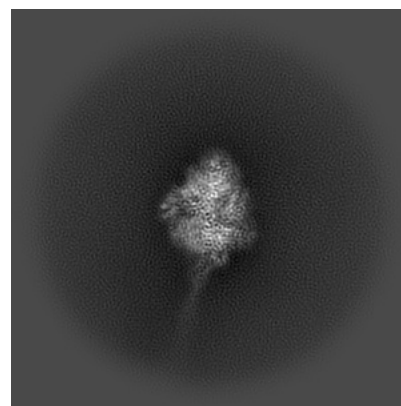
#### 6.1.1 Primary map



X

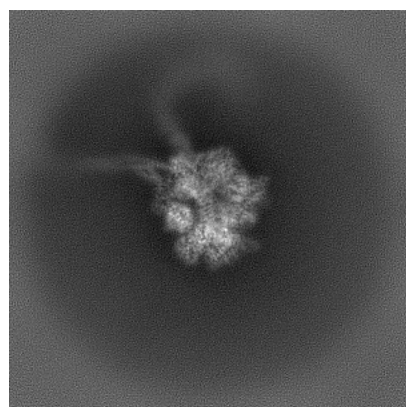


Y

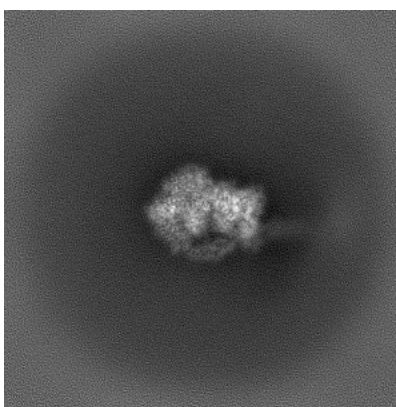


Z

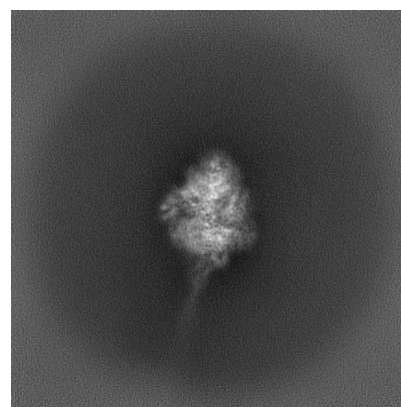
#### 6.1.2 Raw map



X



Y

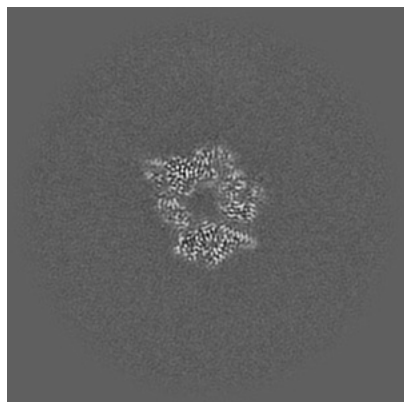


Z

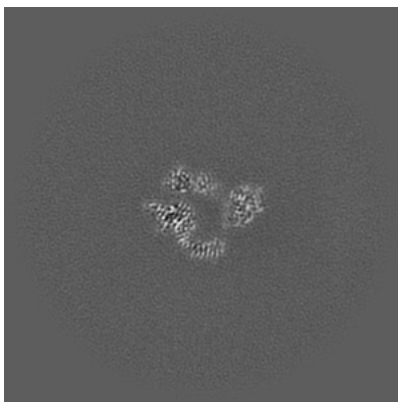
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

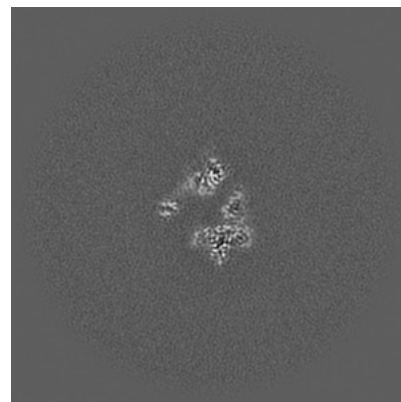
### 6.2.1 Primary map



X Index: 192

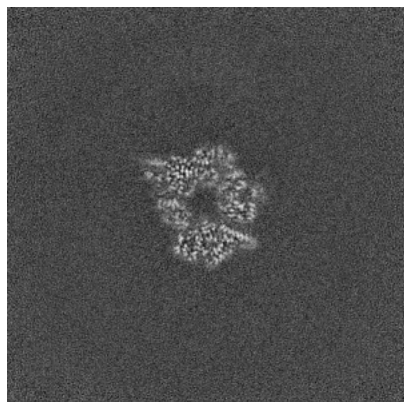


Y Index: 192

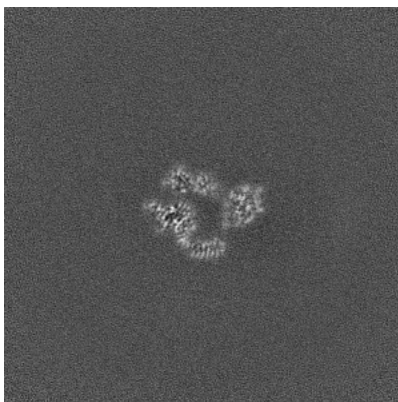


Z Index: 192

### 6.2.2 Raw map



X Index: 192



Y Index: 192

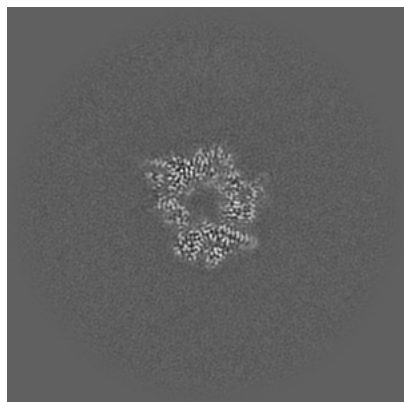


Z Index: 192

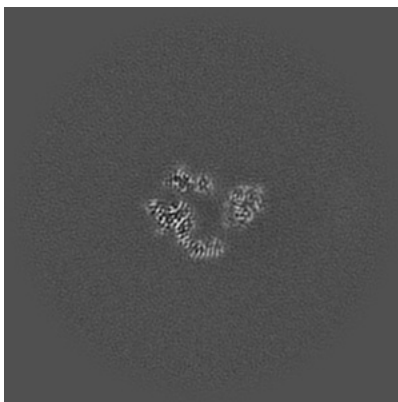
The images above show central slices of the map in three orthogonal directions.

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

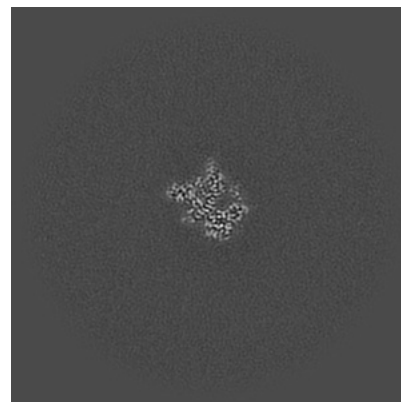
### 6.3.1 Primary map



X Index: 193

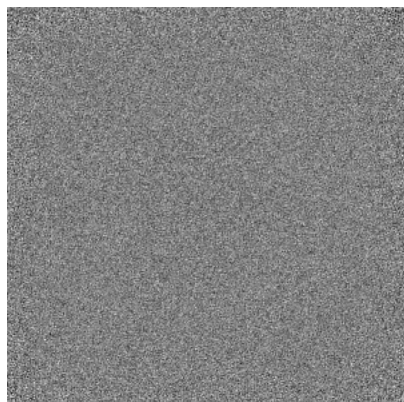


Y Index: 193

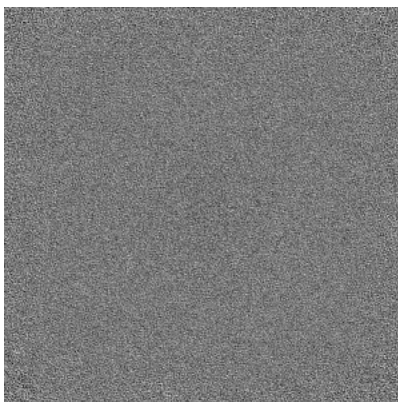


Z Index: 162

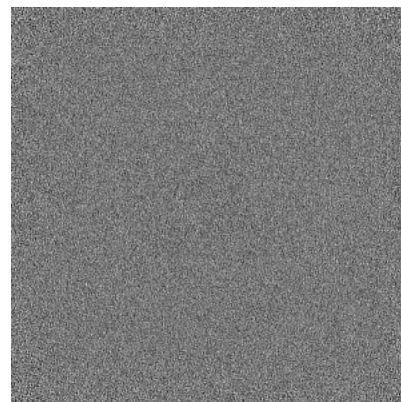
### 6.3.2 Raw map



X Index: 0



Y Index: 0

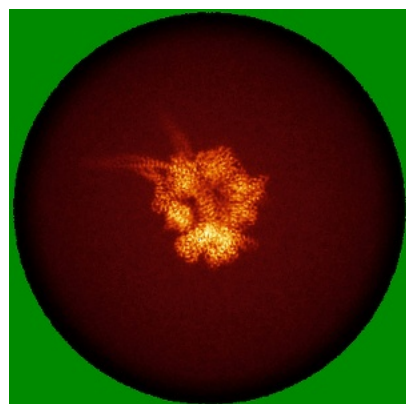


Z Index: 0

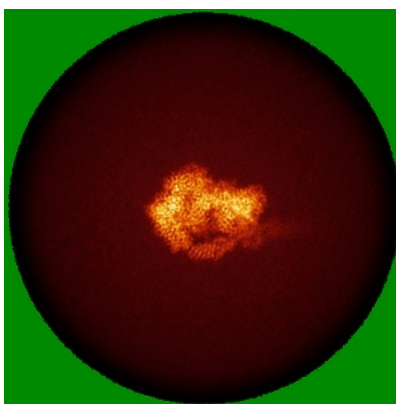
The images above show the largest variance slices of the map in three orthogonal directions.

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

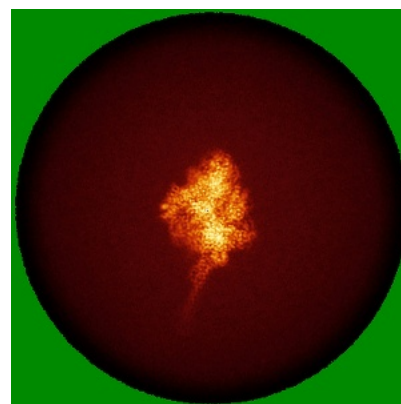
### 6.4.1 Primary map



X

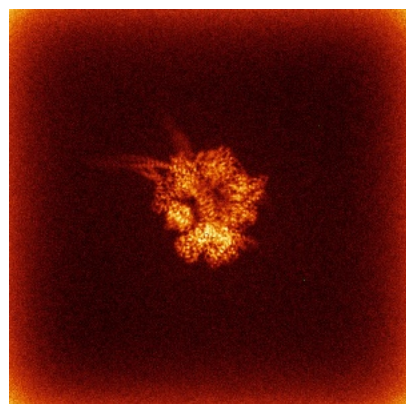


Y

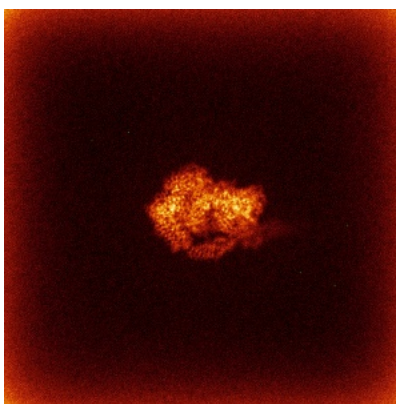


Z

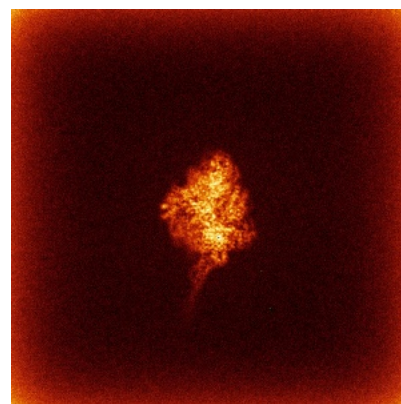
### 6.4.2 Raw map



X



Y

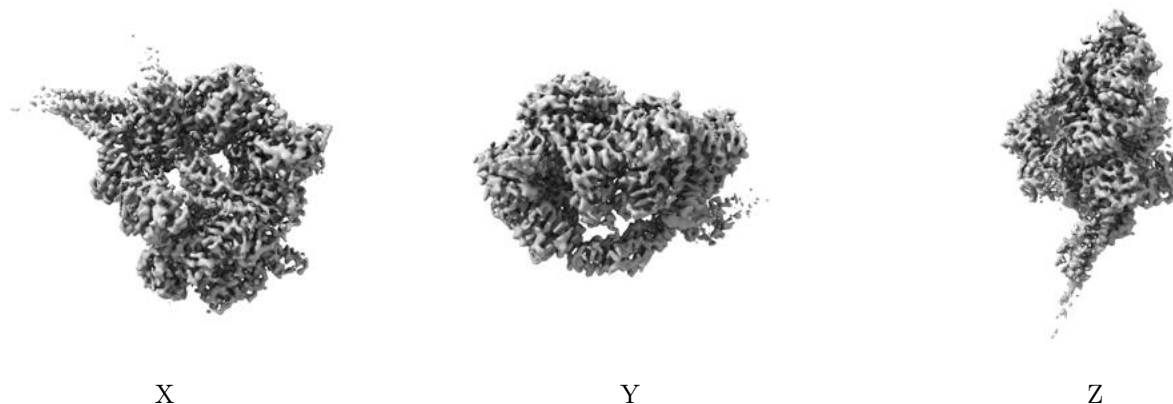


Z

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.

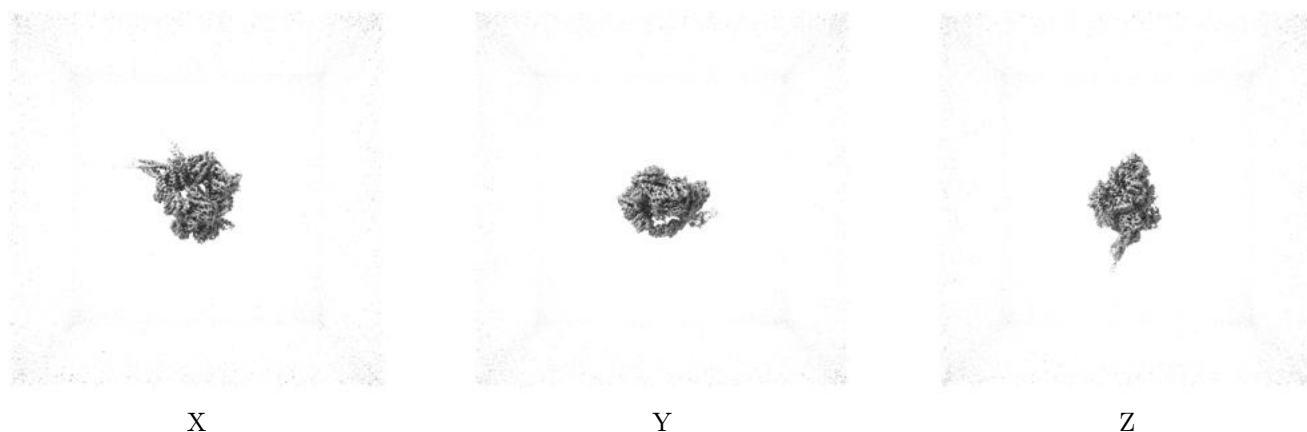
## 6.5 Orthogonal surface views [i](#)

### 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.

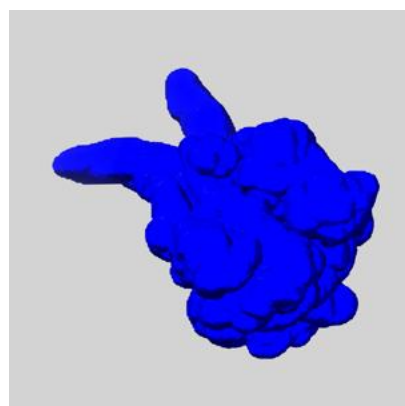
## 6.6 Mask visualisation [i](#)

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

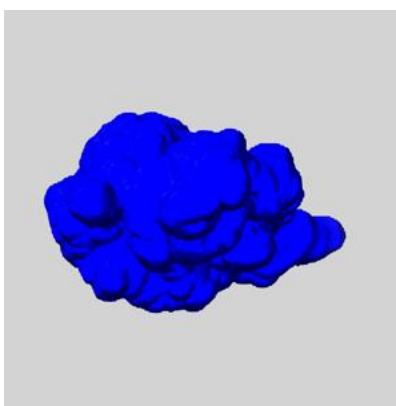
A mask typically either:

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

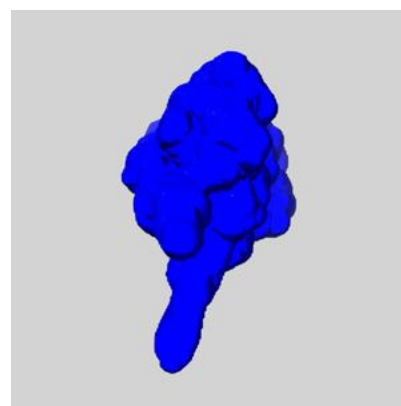
### 6.6.1 emd\_44694\_msk\_1.map [i](#)



X



Y

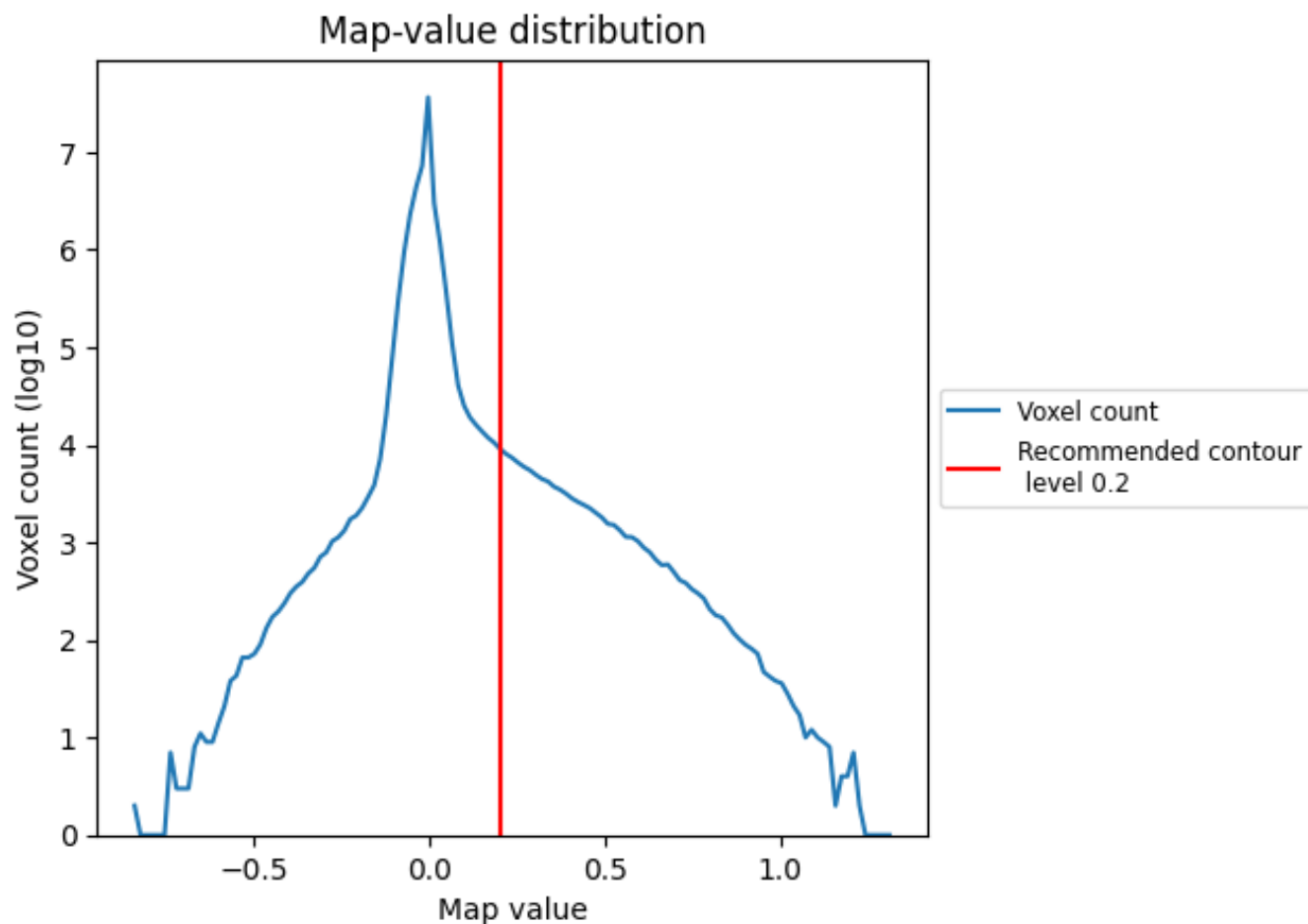


Z

## 7 Map analysis [i](#)

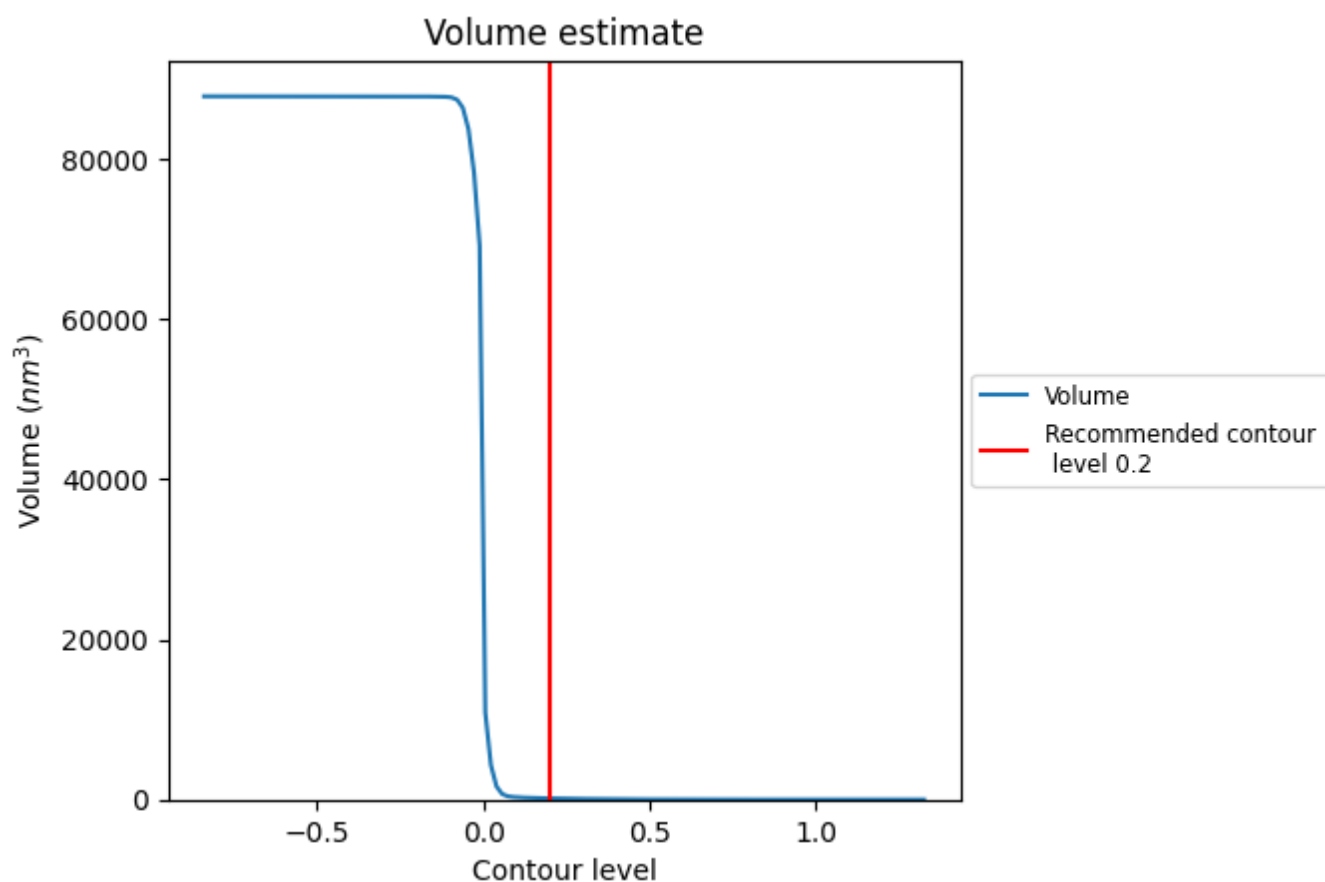
This section contains the results of statistical analysis of the map.

### 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.

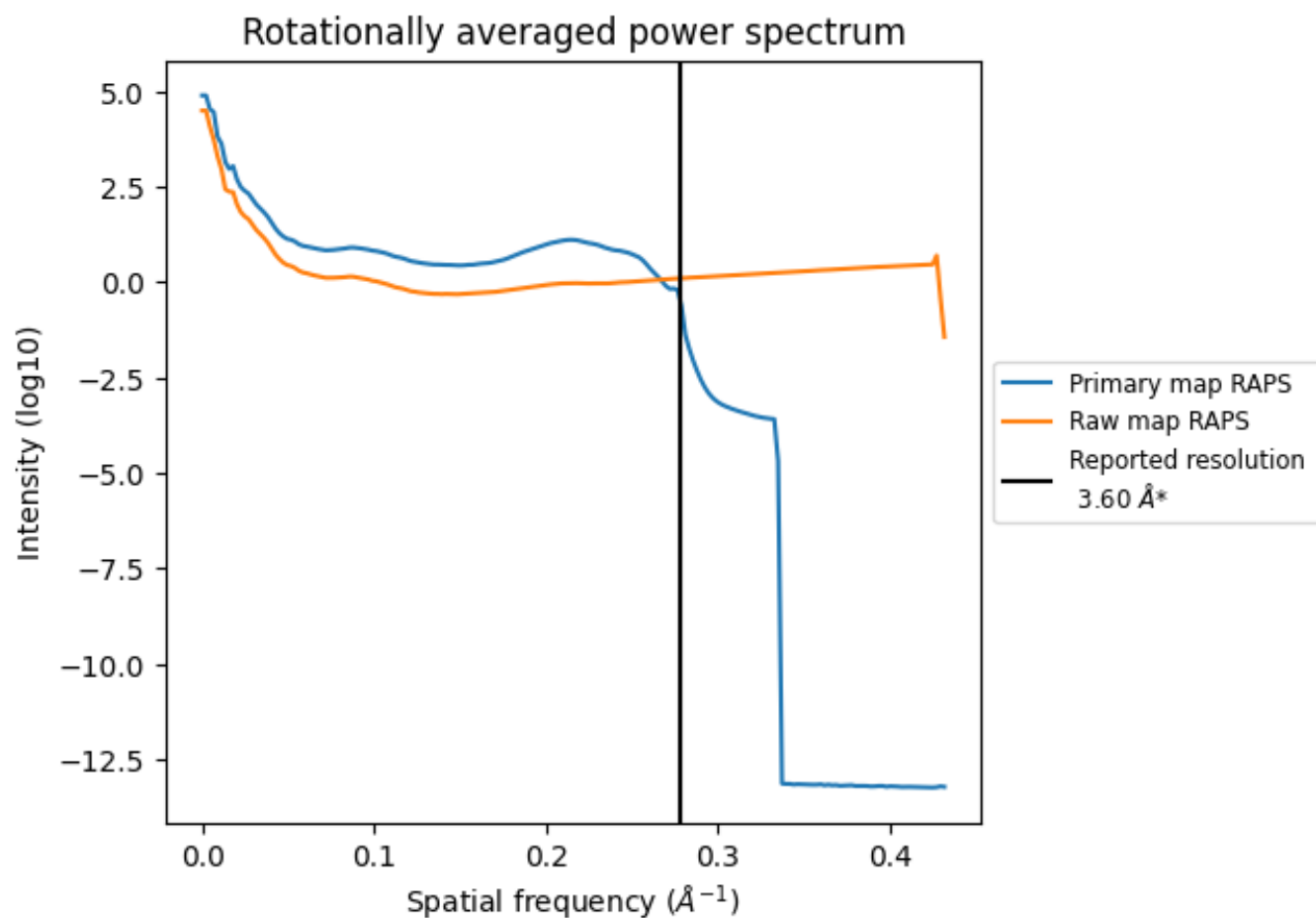
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 149 nm<sup>3</sup>; 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 ⓘ

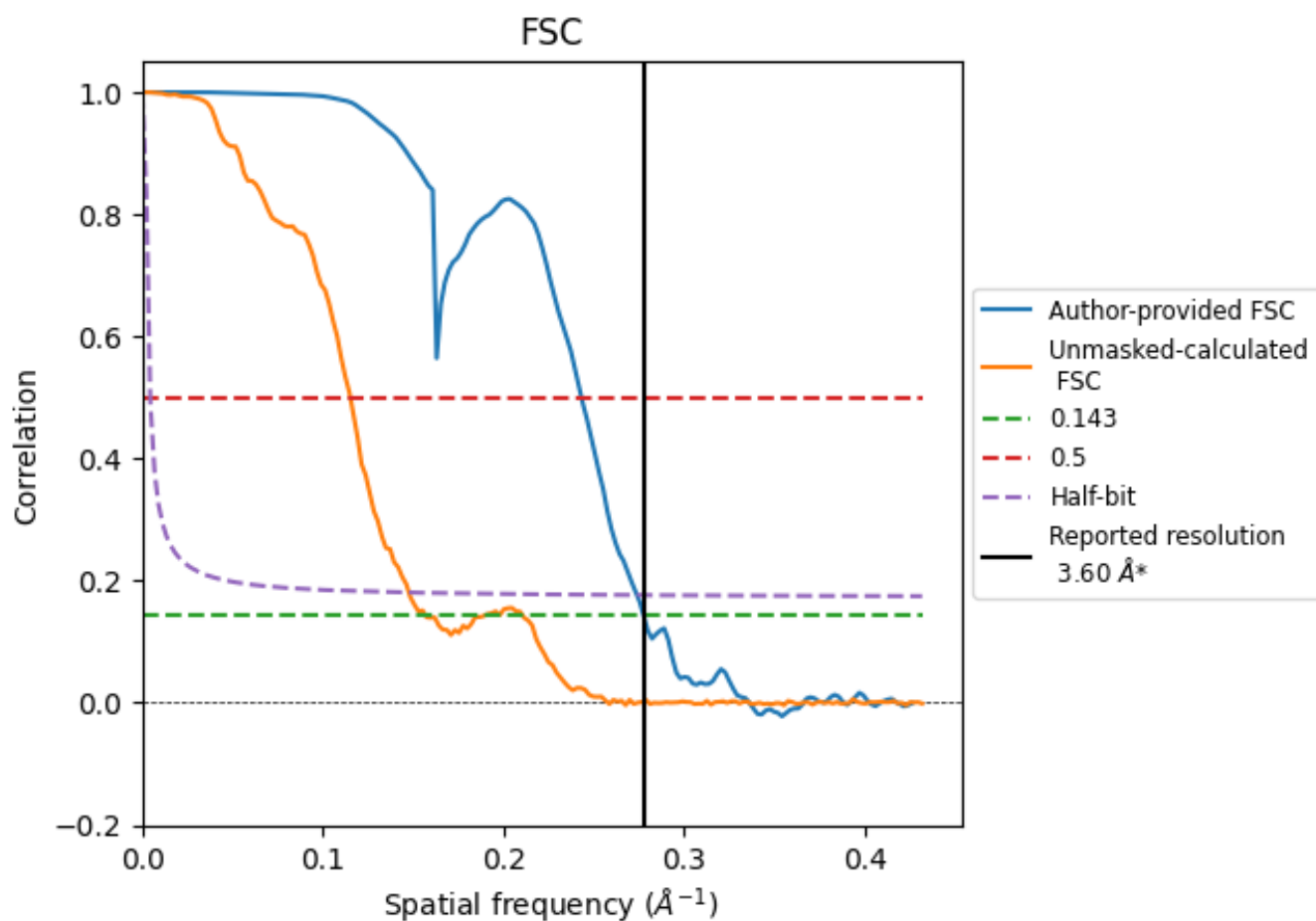


\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.278  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

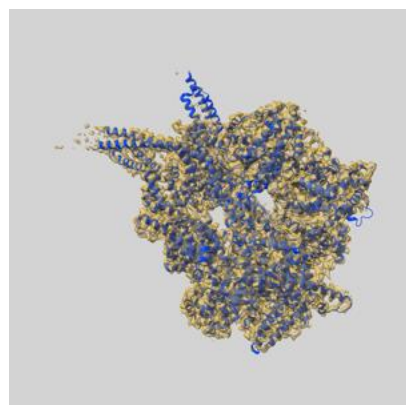
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.11	3.65
Unmasked-calculated*	6.37	8.67	6.77

\*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 %

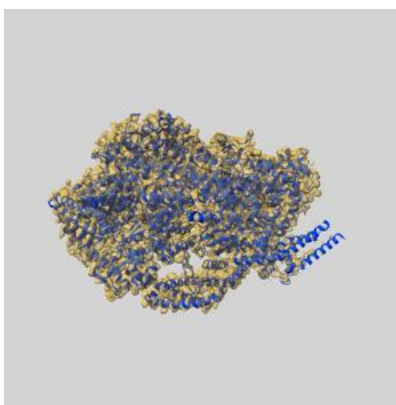
## 9 Map-model fit [i](#)

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](#).

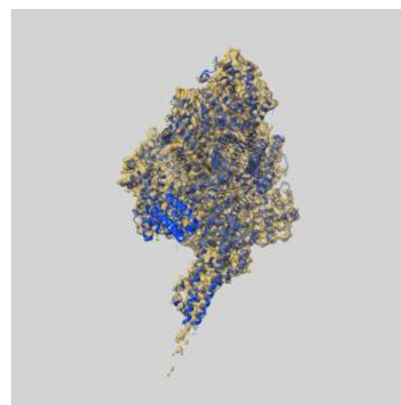
### 9.1 Map-model overlay [i](#)



X



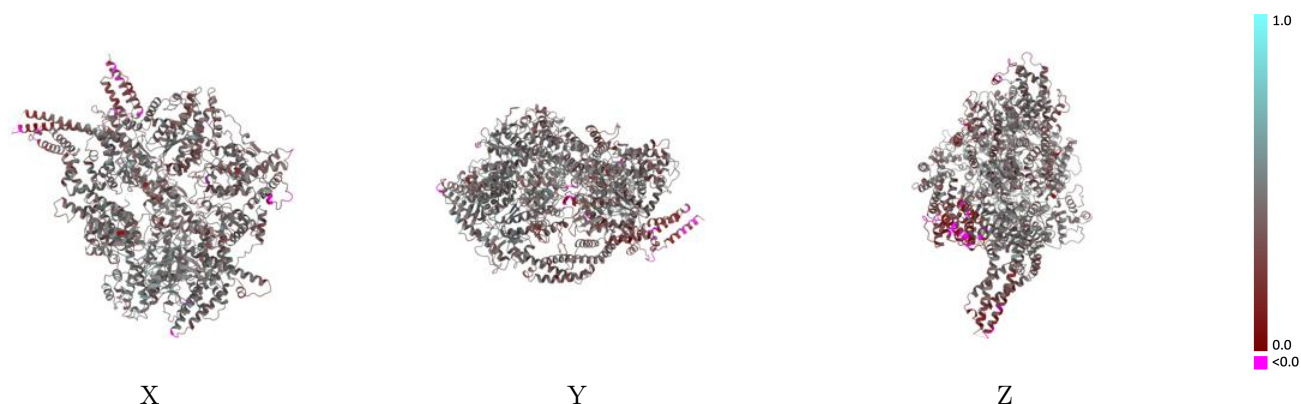
Y



Z

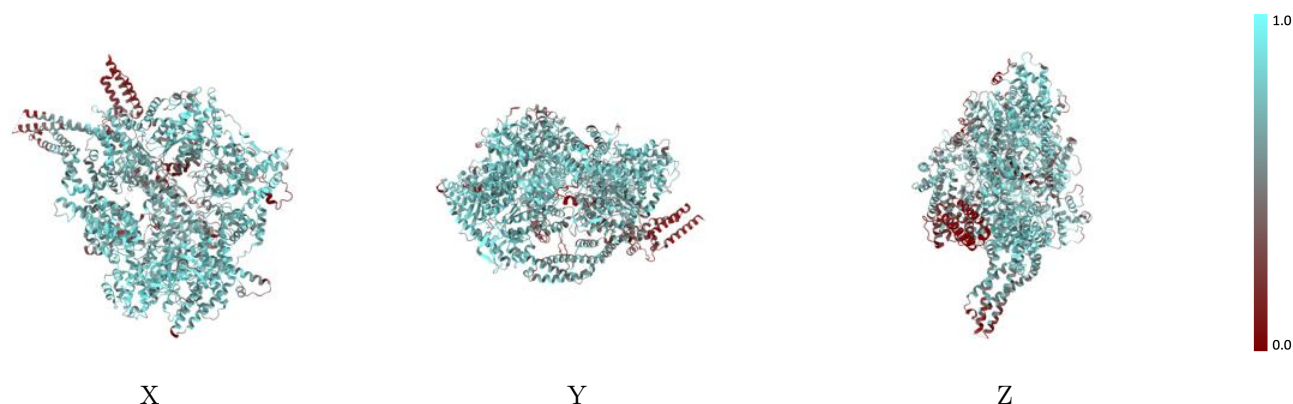
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



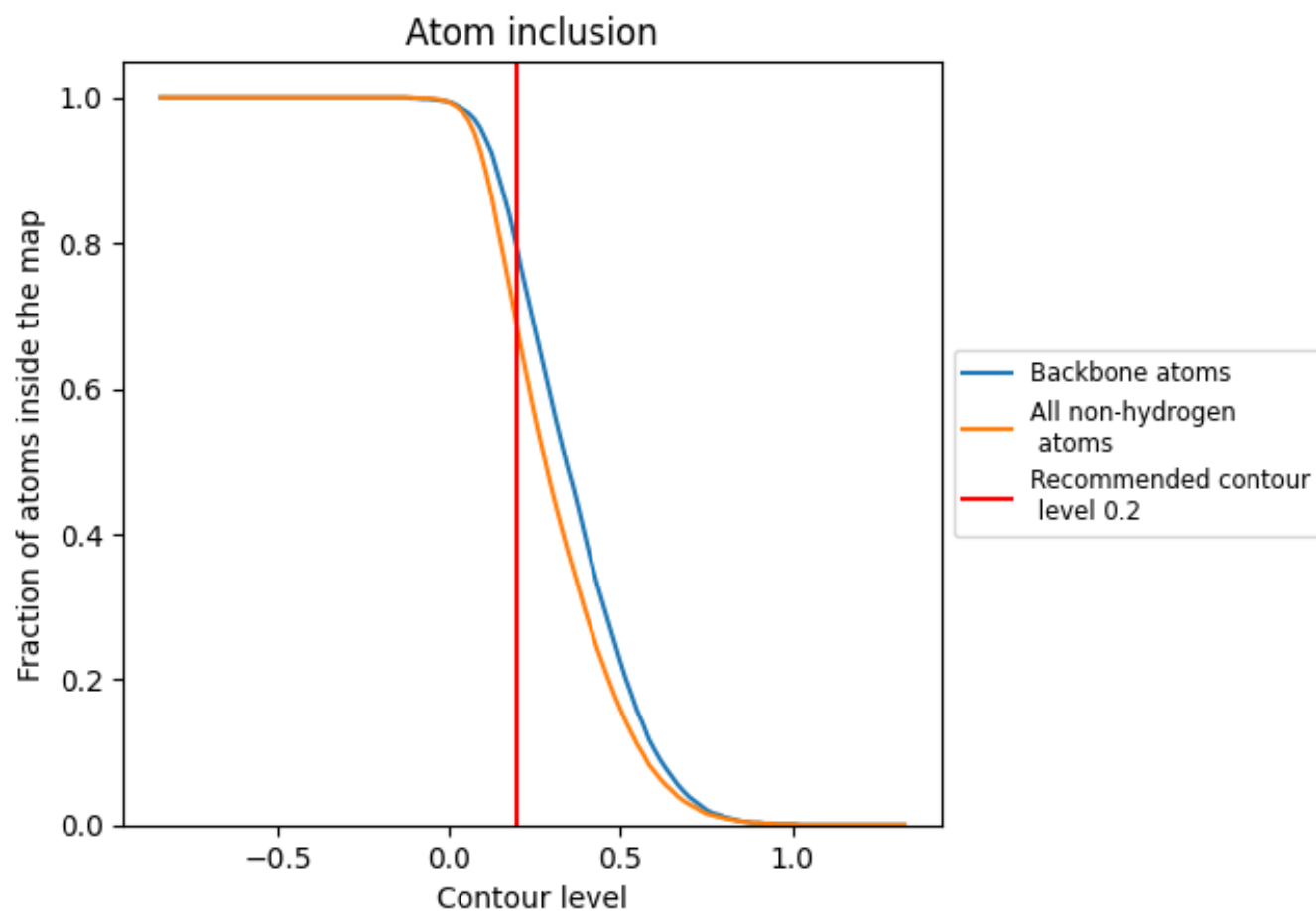
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

