



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 11:41 PM UTC

PDB ID : 9BMW / pdb_00009bmw
EMDB ID : EMD-44713
Title : State-7b-post2 of motor domain from full-length human dynein-1 in 5 mM ADP
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.30 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

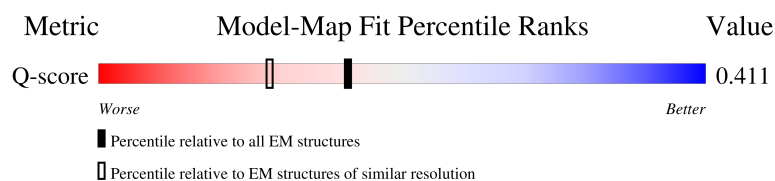
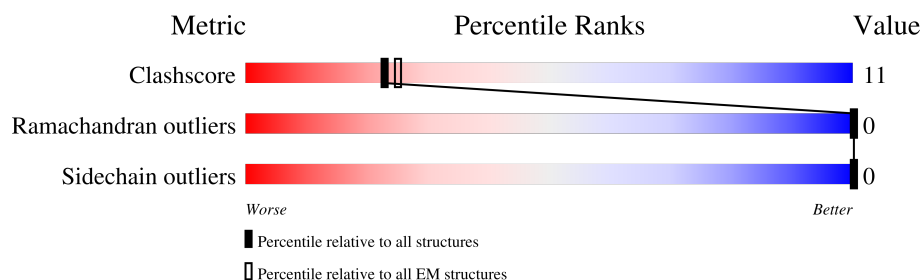
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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](#)

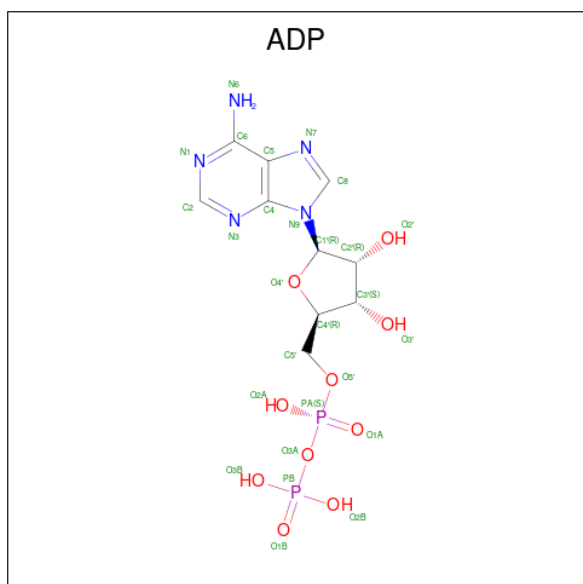
There are 4 unique types of molecules in this entry. The entry contains 24617 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

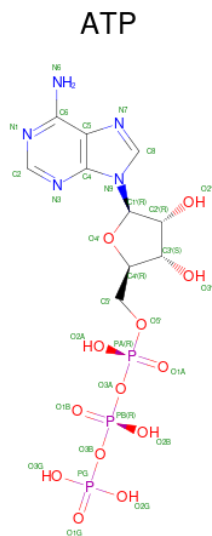
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3043	24503	15606	4234	4541	122	0	0

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



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

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



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

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

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

Y1990	L1811	E1683	S1583	M1507	K1441	VAL	TRP	ARG	GLU	ALA	ASN	GLU	ASN	PHE
D1991	I1812	V1684	K1584	L1508	N1442	ALA	GLU	PHE	LEU	LEU	LYS	LEU	LYS	ASN
K1992	L1815	H1695	M1589	L1509	E1443	GLU	GLU	PHE	THR	THR	GLN	ASP	ASP	PHE
T1993	V1816	L1698	D1590	S1510	A1444	LEU	LEU	GLN	THR	THR	GLN	MET	GLY	GLY
S1994	L1831	I1699	V1591	P1511	I1445	Q1327	VAL	PRO	ASN	PRO	ASN	GLY	VAL	VAL
A1995	N1832	M1698	L1592	V1512	V1446	D1328	THR	TRP	VAL	ASP	GLY	ILE	GLY	GLY
M2018	M1842	E1700	N1593	Y1513	K1447	L1329	GLY	LEU	THR	GLY	ASP	ILE	LEU	ASP
N2019	L1843	W1701	I1594	K1514	D1448	K1330	ASN	TYR	THR	ARG	PRO	ILE	LEU	ASP
G2020	F1844	L1713	G1595	V1515	V1449	G1331	ARG	ASP	GLU	THR	ALA	GLY	GLY	ILE
G2021	Y1845	L1717	G1596	F1516	L1450	V1332	PRO	ASN	LEU	PHE	LEU	VAL	VAL	ILE
THR				E1517	L1451	W1333	GLU	ILE	PRO	ASP	GLY	ARG	ARG	GLY
ALA				E1518	V1452	S1334	GLU	GLY	ILE	ASN	GLY	LEU	LEU	GLY
GLY				D1519	A1453	E1335	ALA	GLY	ALA	SER	GLY	ALA	GLY	GLY
ARG				A1520	Q1454	L1336	GLN	GLY	ASP	THR	GLY	LEU	LEU	ASP
S2026	L1857	L1724	L1604	L1521	G1455	S1337	ALA	GLY	VAL	VAL	ALA	ARG	LEU	LEU
D2030	A1864	E1725	L1607	S1522	E1456	K1338	LEU	PHE	TYR	MET	VAL	ARG	GLY	GLY
K2033	Y1868	I1726	L1607	W1523	M1457	V1339	THR	PHE	LYS	ALA	VAL	LYS	ALA	VAL
L2039	Y1872	G1728	K1610	E1524	A1458	W1340	THR	GLY	THR	PHE	GLY	THR	THR	THR
A2040	Y1872	K1729	I1611	D1525	L1459	E1341	GLY	ILE	SER	ILE	VAL	GLN	GLN	GLN
M2041	V1880	W1741	R1623	K1526	E1460	Q1342	LYS	ARG	GLY	VAL	VAL	GLY	VAL	VAL
D2045	C1888	K1744	S1624	L1527	E1461	I1343	ALA	ARG	ALA	ILE	VAL	VAL	VAL	VAL
I2049	M1892	Y1745	S1625	N1528	F1462	D1344	THR	LYS	THR	ASP	GLY	GLY	GLY	GLY
V2052	E1897	Q1748	F1626	R1529	L1463	Q1345	ILE	SER	THR	ASP	LYS	VAL	VAL	VAL
M2053	G1902	L1749	P1627	W1530	K1464	M1346	THR	ALA	THR	VAL	LYS	VAL	VAL	VAL
L2054	P1907	V1750	V1632	M1531	Q1465	K1347	VAL	ILE	TYR	VAL	VAL	VAL	VAL	VAL
S2056	G1770	M1769	G1633	F1534	E1466	E1348	ASP	GLN	VAL	GLN	ASN	GLN	GLN	GLN
L2065	G1771	G1772	D1634	D1535	R1467	Q1349	GLY	LYS	GLN	GLN	LEU	LEU	LEU	LEU
A2066	L1636	G1772	E1635	W1536	E1468	P1350	LEU	LYS	VAL	VAL	ASN	PRO	ASP	ASP
I2069	L1637	G1773	L1638	W1537	V1469	W1351	LYS	ALA	LYS	ASN	GLY	ARG	MET	MET
G1920	I1641	A1775	I1641	Q1541	Y1473	W1352	LYS	ALA	LYS	ASN	GLY	TYR	ASP	ASP
H1921	K1645	L1778	K1645	R1542	E1474	S1353	LYS	GLY	LYS	VAL	CTR	ILE	ASP	ASP
Q1922	N1646	E1786	N1646	R1543	L1475	V1354	GLY	ILE	GLN	ASP	GLY	GLN	ASP	ASP
V1927	V1647	L1789	V1647	Y1546	D1476	Q1355	PHE	VAL	PHE	TRP	ASN	GLN	ALA	ALA
L1928	L1650	L1789	L1650	L1547	L1477	P1356	LYS	GLN	LYS	TRP	GLN	VAL	VAL	VAL
D1937	F1658	L1792	F1658	I1550	N1482	R1357	GLY	VAL	GLY	GLY	ASN	VAL	VAL	VAL
A1940	V1661	A1793	V1661	F1551	K1483	L1359	THR	ASP	GLY	GLY	ASN	SER	SER	SER
L1948	V1796	V1796	V1661	T1552	R1485	R1360	THR	ARG	VAL	VAL	GLY	GLY	GLY	GLY
W1954	I1665	Q1800	I1665	G1553	L1486	Q1361	ALA	VAL	LEU	LEU	ILE	ILE	ILE	ILE
N1961	E1668	L1804	E1668	S1554	R1488	L1363	VAL	VAL	TYR	ASN	TYR	PRO	PRO	PRO
P1968	L1674	R1804	L1674	L1561	G1489	D1364	GLY	GLY	ARG	ASN	ARG	GLY	GLY	GLY
N1989	G1675	K1807	G1675	L1561	W1490	A1365	THR	THR	GLY	GLY	ASN	GLY	GLY	GLY
R2105	L1676	L1807	L1676	L1561	D1491	L1367	GLY	GLY	VAL	VAL	GLY	GLY	GLY	GLY
R2107	S1677	L1808	S1677	F1568	D1492	N1368	THR	THR	VAL	VAL	ASN	ASN	ASN	ASN
K2110	S1678		S1678	I1571	N1495	Q1369	ASP	ASP	GLY	GLY	LEU	LEU	LEU	LEU
	R1679		R1679	A1577	K1496	L1370	LEU	LEU	ARG	ARG	LEU	LEU	LEU	LEU
				L1578	V1497	K1371	GLY	GLY	THR	THR	GLY	GLY	GLY	GLY
				K1579	K1498	S1372	THR	THR	ARG	ARG	ASP	ASP	ASP	ASP
				M1580	E1499	F1373	GLY	GLY	GLY	GLY	LEU	LEU	LEU	LEU
				K1581	H1500	P1374	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
				V1582	I1501	A1375	THR	THR	THR	THR	ASN	ASN	ASN	ASN
					N1502	R1376	GLY	GLY	GLY	GLY	LYS	LYS	LYS	LYS
					S1505	L1377	GLY	GLY	GLY	GLY	LYS	LYS	LYS	LYS
					A1506	R1378	VAL	VAL	VAL	VAL	ASN	ASN	ASN	ASN
						Q1379	ARG	ARG	ARG	ARG	LYS	LYS	LYS	LYS
						Y1380	THR	THR	THR	THR	TRP	TRP	TRP	TRP
							GLN	ASP	GLN	GLN	GLN	GLN	GLN	GLN





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41042	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	1.144	Depositor
Minimum map value	-0.610	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	329.984, 329.984, 329.984	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0312, 1.0312, 1.0312	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, 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	0.16	0/25022	0.34	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	1409	LYS	CB-CA-C	-5.03	110.39	117.23

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	24573	550	0
2	A	81	0	36	4	0
3	A	31	0	12	2	0
4	A	2	0	0	0	0
All	All	24617	0	24621	550	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 (550) 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:1698:ILE:HD13	1:A:1701:TRP:HE1	1.44	0.82
1:A:3601:MET:HE2	1:A:3634:LEU:HD23	1.64	0.79
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.65	0.77
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.66	0.77
1:A:4153:VAL:HG12	1:A:4157:MET:HE2	1.69	0.75
1:A:4326:ASN:HD22	1:A:4581:ILE:HD13	1.49	0.74
1:A:2189:MET:HG3	1:A:2191:LEU:HD23	1.70	0.73
1:A:3756:VAL:HG23	1:A:3760:ILE:HG21	1.73	0.71
1:A:2755:MET:HE1	1:A:2803:VAL:HG13	1.70	0.71
1:A:2943:LYS:NZ	2:A:4704:ADP:O1B	2.23	0.70
1:A:4096:LEU:HD13	1:A:4105:TRP:HH2	1.55	0.70
1:A:1961:ASN:HB3	1:A:2018:MET:HE1	1.74	0.69
1:A:2386:PRO:HA	1:A:2416:GLN:HE22	1.56	0.69
1:A:1769:MET:HE2	1:A:1775:ALA:HA	1.74	0.69
1:A:2785:THR:HG22	1:A:2787:ASP:H	1.58	0.69
1:A:2943:LYS:HG2	1:A:3094:PHE:HE1	1.57	0.69
1:A:3069:ASN:HD21	1:A:3690:PRO:HB2	1.57	0.69
1:A:2413:LEU:HA	1:A:2416:GLN:HE21	1.57	0.68
1:A:1486:LEU:HD23	1:A:1579:MET:HE3	1.76	0.68
1:A:1713:LEU:HD11	1:A:1872:TYR:HB2	1.75	0.68
1:A:4193:ARG:NH2	1:A:4637:GLU:O	2.21	0.68
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.75	0.68
1:A:1880:VAL:HG11	1:A:2049:ILE:HD13	1.74	0.68
1:A:2320:ASP:OD1	1:A:2358:ARG:NE	2.27	0.68
1:A:1332:VAL:HB	1:A:1377:LEU:HD22	1.76	0.67
1:A:2189:MET:HE1	1:A:2239:LYS:HD3	1.77	0.67
1:A:3113:MET:O	1:A:3140:ARG:NH2	2.28	0.67
1:A:2131:LEU:HD12	1:A:2132:PRO:HD2	1.77	0.66
1:A:2956:LEU:HD13	1:A:2989:LYS:HB3	1.75	0.66
1:A:3593:SER:OG	1:A:3595:GLN:OE1	2.13	0.66
1:A:1511:PRO:HG2	1:A:3659:ARG:HE	1.60	0.66
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.27	0.66
1:A:2419:ALA:O	1:A:2423:MET:HG2	1.96	0.66
1:A:3742:LEU:HD11	1:A:3780:VAL:HG21	1.78	0.66
1:A:2053:MET:HE1	1:A:2094:LYS:HE3	1.78	0.65
1:A:3518:GLY:HA3	1:A:3579:MET:HE1	1.77	0.65
1:A:3886:LEU:HD11	1:A:4346:MET:HG3	1.79	0.65
1:A:2922:ILE:HD11	1:A:2935:LEU:HD21	1.78	0.64
1:A:1463:LEU:HA	1:A:1466:ILE:HD12	1.80	0.64
1:A:2923:ASP:OD2	1:A:2954:ASN:ND2	2.23	0.64
1:A:3553:LEU:O	1:A:3582:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1857:LEU:HD22	1:A:1868:TYR:HB2	1.80	0.64
1:A:4631:ASP:O	1:A:4634:SER:OG	2.16	0.64
1:A:2901:TYR:OH	1:A:2909:LEU:N	2.27	0.63
1:A:2248:GLU:OE2	1:A:2248:GLU:N	2.31	0.63
1:A:2834:GLN:HG2	1:A:2843:ARG:HD3	1.81	0.62
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.81	0.62
1:A:3955:GLU:N	1:A:3955:GLU:OE1	2.33	0.62
1:A:2987:ASN:OD1	1:A:3057:GLN:NE2	2.31	0.62
1:A:3151:HIS:ND1	1:A:3516:TYR:OH	2.21	0.62
1:A:3933:GLU:OE2	1:A:3937:ARG:NE	2.33	0.62
1:A:4324:PRO:HB3	1:A:4638:ARG:NH1	2.14	0.62
1:A:1912:LYS:HG2	1:A:2041:MET:HG3	1.81	0.62
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	1.82	0.62
1:A:1661:VAL:HG22	1:A:1676:ILE:HG21	1.82	0.61
1:A:2291:VAL:HG23	1:A:2292:ARG:HG2	1.81	0.61
1:A:1529:ARG:HH21	1:A:1592:LEU:HG	1.64	0.61
1:A:1713:LEU:HD22	1:A:1749:LEU:HD21	1.81	0.61
1:A:3909:LEU:HB3	1:A:4344:LEU:HD13	1.82	0.61
1:A:4071:ILE:HG23	1:A:4077:PHE:HE1	1.65	0.61
1:A:4339:MET:SD	1:A:4343:MET:HE2	2.40	0.61
1:A:4574:LYS:NZ	1:A:4625:GLU:OE1	2.29	0.61
1:A:3828:SER:HB3	1:A:4140:ARG:HG2	1.83	0.60
1:A:4069:ILE:HD13	1:A:4079:GLN:HG2	1.83	0.60
1:A:4511:LEU:HD23	1:A:4560:VAL:HG13	1.83	0.60
1:A:3030:MET:HE1	1:A:3050:LEU:HB2	1.83	0.60
1:A:3078:ARG:HA	1:A:3081:THR:HG22	1.83	0.60
1:A:4629:LYS:HE3	1:A:4629:LYS:HA	1.83	0.60
1:A:4482:PHE:O	1:A:4486:ILE:HG12	2.01	0.60
1:A:1717:LEU:HB2	1:A:1749:LEU:HD12	1.83	0.59
1:A:2448:ASP:OD2	1:A:2725:HIS:NE2	2.35	0.59
1:A:2930:GLN:HB2	1:A:3059:ILE:HG23	1.83	0.59
1:A:1800:GLN:OE1	1:A:1804:ARG:NH1	2.34	0.59
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.83	0.59
1:A:2609:LEU:HD21	1:A:2615:MET:HB2	1.84	0.59
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.35	0.59
1:A:1864:ALA:HB2	1:A:1897:GLU:HB2	1.84	0.59
1:A:1816:VAL:HG11	1:A:2052:VAL:HG22	1.83	0.59
1:A:2112:LYS:HG3	1:A:2122:VAL:HG11	1.84	0.59
1:A:2413:LEU:HD21	1:A:2417:ARG:HH21	1.67	0.59
1:A:2983:SER:HB3	1:A:2990:ILE:HD12	1.84	0.59
1:A:2054:LEU:HG	1:A:2097:LEU:HD22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1490:TRP:CH2	1:A:1537:TRP:HD1	2.21	0.58
1:A:3772:ASN:HA	1:A:3775:ARG:HH11	1.67	0.58
1:A:1928:LEU:HD12	1:A:1948:LEU:HD21	1.86	0.58
1:A:4574:LYS:HG2	1:A:4627:ALA:HB2	1.84	0.58
1:A:1720:SER:HB2	1:A:1745:TYR:CD1	2.38	0.58
1:A:2610:ARG:HG2	1:A:2610:ARG:HH11	1.68	0.57
1:A:2925:ILE:HD12	1:A:3090:VAL:HG11	1.86	0.57
1:A:2970:GLU:N	1:A:2970:GLU:OE1	2.36	0.57
1:A:3910:ARG:NH2	1:A:4348:MET:SD	2.77	0.57
1:A:3914:ILE:H	1:A:3937:ARG:HH12	1.52	0.57
1:A:2346:GLN:HB2	1:A:2726:ARG:HD2	1.86	0.57
1:A:4153:VAL:HG22	1:A:4192:GLU:HG3	1.87	0.57
1:A:2191:LEU:HD12	3:A:4702:ATP:C6	2.40	0.57
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.87	0.57
1:A:2571:THR:H	1:A:2574:THR:HB	1.70	0.57
1:A:2994:MET:HB2	1:A:2998:ASN:HD21	1.70	0.57
1:A:1750:VAL:HG12	1:A:1811:LEU:HD21	1.85	0.57
1:A:1463:LEU:HD13	1:A:1466:ILE:HD12	1.87	0.57
1:A:3074:GLY:O	1:A:3078:ARG:NE	2.35	0.57
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.37	0.57
1:A:3913:GLU:HG3	1:A:4476:ILE:HD13	1.87	0.57
1:A:1487:ILE:HD13	1:A:1537:TRP:HE1	1.70	0.56
1:A:1721:VAL:O	1:A:1725:GLU:HG2	2.05	0.56
1:A:1626:PHE:CE1	1:A:1628:ARG:HB2	2.39	0.56
1:A:2747:ILE:O	1:A:2750:THR:OG1	2.21	0.56
1:A:3055:THR:O	1:A:3059:ILE:HD12	2.06	0.56
1:A:3739:GLN:HA	1:A:3742:LEU:HD12	1.87	0.56
1:A:1539:ASP:OD2	1:A:1543:ARG:NH1	2.35	0.56
1:A:3731:LEU:HD11	1:A:3790:VAL:HG12	1.86	0.56
1:A:2516:GLU:O	1:A:2520:ARG:HG3	2.06	0.56
1:A:2755:MET:SD	1:A:2807:PHE:HB2	2.45	0.56
1:A:4104:GLY:HA2	1:A:4107:MET:HE3	1.86	0.56
1:A:2726:ARG:NH1	3:A:4702:ATP:O3G	2.39	0.56
1:A:4075:GLU:N	1:A:4075:GLU:OE1	2.39	0.56
1:A:2370:SER:H	1:A:2373:MET:HE2	1.71	0.55
1:A:1398:MET:SD	1:A:1399:LEU:HD22	2.47	0.55
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.88	0.55
1:A:3208:ILE:HG23	1:A:3482:LEU:HD12	1.87	0.55
1:A:2413:LEU:HA	1:A:2416:GLN:NE2	2.22	0.55
1:A:4414:GLU:O	1:A:4418:LYS:HG3	2.07	0.55
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2976:LEU:HA	1:A:2979:VAL:HG12	1.89	0.55
1:A:3935:VAL:HG22	1:A:3996:PHE:HE1	1.72	0.55
1:A:2616:GLU:N	1:A:2616:GLU:OE1	2.40	0.55
1:A:1961:ASN:HD21	1:A:2019:ASN:HB3	1.71	0.55
1:A:2102:ASN:OD1	1:A:2105:ARG:NH2	2.35	0.55
1:A:3154:LEU:HD13	1:A:3516:TYR:CD1	2.42	0.55
1:A:3811:ILE:O	1:A:3815:MET:HG3	2.07	0.55
1:A:2449:LEU:HD11	1:A:2454:CYS:SG	2.46	0.54
1:A:2603:MET:HE1	2:A:4703:ADP:C4	2.42	0.54
1:A:1561:LEU:HB3	1:A:1564:GLU:HB2	1.89	0.54
1:A:2146:VAL:HA	1:A:2149:LEU:HD12	1.89	0.54
1:A:3846:LEU:HD21	1:A:3859:ILE:HG13	1.88	0.54
1:A:1623:ARG:NH2	1:A:1634:ASP:OD1	2.41	0.54
1:A:3551:GLU:OE2	1:A:3559:ARG:NH1	2.38	0.54
1:A:2065:LEU:HD11	1:A:2133:GLU:HB3	1.90	0.54
1:A:1571:ILE:HG23	1:A:1604:LEU:HD22	1.89	0.54
1:A:2265:TYR:OH	1:A:2311:TRP:O	2.18	0.54
1:A:3763:ASP:OD2	1:A:3765:THR:OG1	2.25	0.54
1:A:4180:TYR:OH	1:A:4220:ASP:OD2	2.25	0.54
1:A:1744:LYS:C	1:A:1745:TYR:HD2	2.16	0.53
1:A:2290:SER:HB3	1:A:2295:LEU:HG	1.90	0.53
1:A:4547:THR:HG22	1:A:4586:PRO:HG2	1.89	0.53
1:A:2919:VAL:HG13	1:A:2950:VAL:HG22	1.90	0.53
1:A:3486:ARG:O	1:A:3490:GLU:HG2	2.07	0.53
1:A:1843:ARG:NH1	1:A:1845:TYR:OH	2.42	0.53
1:A:1927:VAL:HG22	1:A:1954:TRP:HB2	1.91	0.53
1:A:4619:ILE:HG22	1:A:4620:PHE:HD1	1.73	0.53
1:A:2773:MET:HE2	1:A:2799:MET:SD	2.49	0.53
1:A:3194:LEU:HD22	1:A:3500:MET:HE3	1.91	0.53
1:A:3667:GLN:N	1:A:3667:GLN:OE1	2.41	0.53
1:A:3103:TYR:OH	1:A:3141:GLU:OE1	2.18	0.53
1:A:4448:LEU:O	1:A:4452:ILE:HG12	2.08	0.53
1:A:2603:MET:HE1	2:A:4703:ADP:C5	2.44	0.52
1:A:2936:ILE:HG22	1:A:3070:PRO:HG3	1.90	0.52
1:A:3505:GLY:HA3	1:A:3543:PHE:HB3	1.91	0.52
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.91	0.52
1:A:4564:LYS:HG3	1:A:4646:GLU:HB2	1.90	0.52
1:A:2873:TYR:HE1	1:A:2883:PRO:HD3	1.73	0.52
1:A:3580:LEU:HD21	1:A:3589:ILE:HD11	1.91	0.52
1:A:3755:GLU:OE2	1:A:3759:ARG:NH1	2.42	0.52
1:A:2750:THR:HG22	1:A:2753:ARG:HH22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1571:ILE:HD11	1:A:1607:LEU:HB3	1.91	0.52
1:A:1831:ASP:OD1	1:A:1832:ASN:N	2.41	0.52
1:A:4104:GLY:O	1:A:4108:GLN:HG2	2.09	0.52
1:A:4264:LEU:O	1:A:4267:THR:OG1	2.25	0.52
1:A:2910:VAL:HG22	1:A:3108:GLU:HG2	1.92	0.52
1:A:2393:GLU:HB3	1:A:2397:ARG:HH12	1.75	0.52
1:A:1411:ARG:NH2	1:A:1456:GLU:OE1	2.39	0.51
1:A:4460:LEU:HA	1:A:4475:VAL:HG22	1.91	0.51
1:A:4560:VAL:HB	1:A:4588:THR:HB	1.91	0.51
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.45	0.51
1:A:3723:ASP:O	1:A:3727:LYS:HG3	2.11	0.51
1:A:1336:LEU:HD11	1:A:1386:VAL:HG21	1.93	0.51
1:A:2258:ALA:HB1	1:A:2682:PHE:HD1	1.75	0.51
1:A:2045:ASP:O	1:A:2049:ILE:HG12	2.11	0.51
1:A:2223:VAL:HG12	1:A:2223:VAL:O	2.11	0.51
1:A:2519:ARG:HG3	1:A:2526:LEU:HD12	1.92	0.51
1:A:2838:VAL:HA	1:A:3093:TRP:CD1	2.46	0.51
1:A:4485:ARG:NH1	1:A:4513:GLY:O	2.44	0.51
1:A:2666:ILE:HG22	1:A:2723:LEU:HD21	1.92	0.51
1:A:1546:TYR:O	1:A:1550:ILE:HG12	2.10	0.51
1:A:4202:SER:OG	1:A:4261:ASP:OD2	2.24	0.51
1:A:1476:ASP:HB3	1:A:1488:ARG:NH1	2.26	0.51
1:A:1888:CYS:HB2	1:A:2041:MET:HE1	1.92	0.51
1:A:2039:LEU:HD23	1:A:2041:MET:HE2	1.92	0.51
1:A:2369:LEU:HD12	1:A:2373:MET:HE3	1.93	0.51
1:A:2577:HIS:O	1:A:2581:LEU:HD23	2.11	0.51
1:A:3690:PRO:HA	1:A:3693:CYS:HB2	1.93	0.51
1:A:3947:LEU:O	1:A:3951:VAL:HG23	2.11	0.51
1:A:2651:ALA:HB1	1:A:2705:ARG:HH21	1.76	0.51
1:A:2965:ARG:NH2	1:A:2966:LYS:HD3	2.26	0.51
1:A:2192:THR:HB	1:A:2373:MET:HB3	1.94	0.50
1:A:1466:ILE:HG12	1:A:1500:HIS:CE1	2.45	0.50
1:A:1638:LEU:HD23	1:A:1641:ILE:HD11	1.93	0.50
1:A:2306:ASP:N	1:A:2306:ASP:OD1	2.43	0.50
1:A:2993:ILE:HG12	1:A:3065:VAL:HB	1.93	0.50
1:A:3611:ARG:NH1	1:A:3636:GLN:OE1	2.44	0.50
1:A:2591:LEU:HD12	1:A:2592:VAL:H	1.76	0.50
1:A:1698:ILE:HA	1:A:1701:TRP:NE1	2.27	0.50
1:A:3873:ARG:HH11	1:A:4025:LEU:HD12	1.77	0.50
1:A:4176:ARG:NH2	1:A:4224:ASP:OD1	2.42	0.50
1:A:1632:VAL:HG22	1:A:1636:ASP:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1842:MET:HE3	1:A:1922:GLN:HG2	1.92	0.50
1:A:2327:LEU:HD12	1:A:2331:GLU:HB3	1.94	0.50
1:A:2395:GLN:HB3	1:A:2398:ARG:HH22	1.77	0.50
1:A:3891:LYS:HD2	1:A:4013:LEU:HD23	1.92	0.50
1:A:2778:THR:O	1:A:2782:GLU:HG2	2.12	0.50
1:A:2973:ASP:OD1	1:A:3007:ARG:NE	2.45	0.50
1:A:3801:TYR:CE1	1:A:3856:LEU:HD12	2.47	0.49
1:A:2304:ASP:OD2	1:A:2684:ARG:NH2	2.45	0.49
1:A:2905:LEU:HD11	1:A:2948:ARG:HH21	1.77	0.49
1:A:4445:THR:O	1:A:4449:ARG:HG2	2.11	0.49
1:A:1741:TRP:CH2	1:A:1750:VAL:HG13	2.47	0.49
1:A:2943:LYS:HE2	1:A:3067:THR:HB	1.94	0.49
1:A:3600:ILE:HD11	1:A:3634:LEU:HD22	1.93	0.49
1:A:2329:ASN:OD1	1:A:2330:GLY:N	2.46	0.49
1:A:2589:LYS:HE3	1:A:2732:PRO:HD3	1.95	0.49
1:A:4391:ILE:O	1:A:4428:ARG:NH2	2.45	0.49
1:A:1438:ASP:HB3	1:A:1441:LYS:HB3	1.94	0.49
1:A:1470:TRP:HE1	1:A:1500:HIS:CD2	2.30	0.49
1:A:1547:LEU:HD12	1:A:1551:PHE:HE2	1.76	0.49
1:A:2619:GLY:HA2	1:A:2662:PHE:HB3	1.94	0.49
1:A:3612:THR:HG22	1:A:3619:PHE:HD1	1.78	0.49
1:A:2149:LEU:HD11	1:A:2157:LEU:HD22	1.95	0.49
1:A:4185:TRP:O	1:A:4189:ILE:HG12	2.12	0.49
1:A:4303:GLU:HG2	1:A:4304:GLU:N	2.28	0.49
1:A:1907:PRO:O	1:A:1912:LYS:NZ	2.45	0.49
1:A:4205:TYR:OH	1:A:4261:ASP:OD2	2.23	0.49
1:A:1420:LEU:HD13	1:A:1437:VAL:HG11	1.95	0.49
1:A:1462:PHE:O	1:A:1466:ILE:HG13	2.13	0.49
1:A:2743:SER:O	1:A:2747:ILE:HG22	2.13	0.49
1:A:4445:THR:HG22	1:A:4448:LEU:HB2	1.94	0.49
1:A:3614:PHE:CE1	1:A:3635:VAL:HG11	2.47	0.49
1:A:3028:THR:O	1:A:3031:THR:OG1	2.18	0.48
1:A:3551:GLU:OE1	1:A:3733:LYS:HA	2.12	0.48
1:A:4097:LYS:HA	1:A:4127:THR:HG22	1.95	0.48
1:A:2191:LEU:HD11	1:A:2232:MET:HG2	1.95	0.48
1:A:2684:ARG:HH12	1:A:2726:ARG:NE	2.11	0.48
1:A:2835:ASP:OD1	1:A:2921:ARG:NH1	2.46	0.48
1:A:3708:LEU:HD22	1:A:3809:SER:HA	1.95	0.48
1:A:3824:LEU:HD11	1:A:4144:ILE:HG21	1.94	0.48
1:A:4128:MET:CE	1:A:4134:VAL:HG11	2.43	0.48
1:A:1363:LEU:HD11	1:A:1435:TRP:HH2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1717:LEU:HB2	1:A:1749:LEU:CD1	2.44	0.48
1:A:2325:LEU:HB3	1:A:2333:LEU:HB2	1.96	0.48
1:A:3601:MET:O	1:A:3605:LYS:HG2	2.13	0.48
1:A:2265:TYR:OH	1:A:2315:LEU:HG	2.14	0.48
1:A:4154:LYS:O	1:A:4158:LEU:HD23	2.13	0.48
1:A:1490:TRP:HZ3	1:A:1534:PHE:CD2	2.32	0.48
1:A:2767:GLU:HG2	1:A:2768:PRO:HD3	1.95	0.47
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.47	0.47
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.96	0.47
1:A:4119:HIS:CD2	1:A:4120:ALA:H	2.32	0.47
1:A:3967:GLU:N	1:A:3967:GLU:OE1	2.48	0.47
1:A:1486:LEU:HB3	1:A:1541:GLN:NE2	2.29	0.47
1:A:2444:GLU:HG3	1:A:2510:MET:HE1	1.96	0.47
1:A:2995:ASP:OD1	1:A:2996:GLU:N	2.37	0.47
1:A:3534:HIS:HA	1:A:3537:GLN:HG2	1.97	0.47
1:A:3731:LEU:HD13	1:A:3791:MET:HG2	1.96	0.47
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.96	0.47
1:A:2605:LEU:HD13	1:A:2662:PHE:CE2	2.50	0.47
1:A:1490:TRP:CH2	1:A:1537:TRP:CD1	3.01	0.47
1:A:1582:VAL:HG23	1:A:1591:VAL:HG22	1.96	0.47
1:A:2972:PHE:CE1	1:A:2976:LEU:HD11	2.50	0.47
1:A:4226:THR:HG21	1:A:4239:PRO:HD3	1.97	0.47
1:A:2728:LEU:HA	1:A:2731:VAL:HG22	1.96	0.47
1:A:3027:ALA:O	1:A:3031:THR:HG23	2.14	0.47
1:A:4508:HIS:HE1	1:A:4553:LEU:HD21	1.79	0.47
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.96	0.47
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.47	0.47
1:A:2773:MET:HG3	1:A:2825:TRP:HE1	1.80	0.47
1:A:4324:PRO:HB2	1:A:4326:ASN:OD1	2.13	0.47
1:A:4445:THR:HG23	1:A:4448:LEU:H	1.80	0.47
1:A:2260:SER:OG	1:A:2263:HIS:ND1	2.48	0.47
1:A:2413:LEU:HG	1:A:2417:ARG:HE	1.80	0.47
1:A:2982:ARG:HG2	1:A:2990:ILE:HD11	1.97	0.47
1:A:3192:SER:O	1:A:3196:GLU:OE1	2.33	0.47
1:A:3716:VAL:HG23	1:A:3836:TYR:OH	2.15	0.47
1:A:2422:ILE:HD13	1:A:2487:GLU:HA	1.97	0.46
1:A:2517:TYR:O	1:A:2521:ILE:HG12	2.15	0.46
1:A:2623:SER:HB3	1:A:3006:GLU:OE1	2.15	0.46
1:A:1892:MET:SD	1:A:1902:GLY:HA3	2.55	0.46
1:A:2882:ILE:HG13	1:A:2883:PRO:HD2	1.97	0.46
1:A:3870:ARG:NH2	1:A:4034:GLU:OE1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4434:VAL:HA	1:A:4437:VAL:HG12	1.97	0.46
1:A:2305:GLY:O	1:A:2345:VAL:HG12	2.15	0.46
1:A:2464:GLN:NE2	1:A:2468:ASN:OD1	2.48	0.46
1:A:2593:LEU:HD13	1:A:2605:LEU:HD12	1.97	0.46
1:A:2935:LEU:HD22	1:A:3094:PHE:CZ	2.50	0.46
1:A:4306:VAL:HA	1:A:4309:VAL:HG12	1.96	0.46
1:A:2072:PHE:HE2	1:A:2141:VAL:HG11	1.81	0.46
1:A:2211:TYR:HB2	1:A:2237:LEU:HD11	1.97	0.46
1:A:3536:LEU:HD23	1:A:3541:ILE:HG21	1.97	0.46
1:A:3756:VAL:HG13	1:A:3756:VAL:O	2.15	0.46
1:A:3967:GLU:HG2	1:A:4007:MET:CE	2.45	0.46
1:A:1363:LEU:HD11	1:A:1435:TRP:CH2	2.50	0.46
1:A:2370:SER:N	1:A:2373:MET:HE2	2.30	0.46
1:A:4271:ARG:HH11	1:A:4271:ARG:HG2	1.81	0.46
1:A:2033:LYS:NZ	1:A:4206:GLU:OE2	2.35	0.46
1:A:3474:ARG:HE	1:A:3764:ASP:HB3	1.80	0.46
1:A:3614:PHE:CE2	1:A:3641:TYR:HA	2.51	0.46
1:A:4112:LYS:O	1:A:4116:LEU:HG	2.15	0.46
1:A:1526:LYS:O	1:A:1530:ILE:HG22	2.15	0.46
1:A:1658:PHE:HB2	1:A:1661:VAL:HB	1.97	0.46
1:A:1937:ASP:OD2	1:A:1940:ALA:HB3	2.16	0.46
1:A:2741:PRO:O	1:A:2745:THR:HG23	2.16	0.46
1:A:3562:TRP:HZ2	1:A:3581:LYS:HD3	1.80	0.46
1:A:3999:ASP:OD1	1:A:4000:ARG:N	2.48	0.46
1:A:1355:GLN:HG3	1:A:1358:LYS:H	1.80	0.46
1:A:1793:ALA:HA	1:A:1796:VAL:HG12	1.98	0.46
1:A:3482:LEU:O	1:A:3485:GLU:HG3	2.16	0.46
1:A:1724:VAL:HA	1:A:1727:PHE:HB2	1.98	0.46
1:A:2096:VAL:HG11	1:A:2141:VAL:HG22	1.98	0.46
1:A:2936:ILE:HG21	1:A:3093:TRP:CZ3	2.50	0.45
1:A:2972:PHE:CZ	1:A:3008:MET:HE3	2.51	0.45
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	1.97	0.45
1:A:1920:GLY:HA3	1:A:1927:VAL:HG21	1.97	0.45
1:A:2221:MET:HE1	1:A:2348:LEU:HD21	1.98	0.45
1:A:2797:ARG:HH12	1:A:3088:ARG:HH12	1.63	0.45
1:A:3215:VAL:HG11	1:A:3478:LEU:HD23	1.99	0.45
1:A:4182:LEU:HD21	1:A:4296:MET:HE1	1.98	0.45
1:A:2591:LEU:HD13	1:A:2732:PRO:HG2	1.99	0.45
1:A:3689:PRO:HB2	1:A:3691:ASP:OD1	2.17	0.45
1:A:1409:LYS:HB3	1:A:1410:ASP:H	1.58	0.45
1:A:2189:MET:HG3	1:A:2191:LEU:CD2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2224:GLY:H	1:A:2230:LYS:HD3	1.80	0.45
1:A:4084:ILE:O	1:A:4088:VAL:HG23	2.17	0.45
1:A:1720:SER:HB2	1:A:1745:TYR:CE1	2.50	0.45
1:A:1720:SER:HB2	1:A:1745:TYR:HD1	1.81	0.45
1:A:2826:ALA:O	1:A:2830:LEU:HD23	2.17	0.45
1:A:3108:GLU:HG3	1:A:3109:PHE:HD1	1.82	0.45
1:A:1374:PRO:HD2	1:A:1377:LEU:HD12	1.98	0.45
1:A:2382:LEU:HD23	1:A:2420:ALA:HB2	1.99	0.45
1:A:2790:PRO:HG2	1:A:3075:LEU:HD23	1.98	0.45
1:A:4020:ILE:HG23	1:A:4021:MET:HE3	1.99	0.45
1:A:4482:PHE:CE2	1:A:4486:ILE:HD11	2.50	0.45
1:A:1356:PRO:HB3	1:A:1401:ILE:HG12	1.98	0.45
1:A:2684:ARG:NH1	1:A:2726:ARG:HB3	2.31	0.45
1:A:4442:LYS:HE2	1:A:4442:LYS:HB3	1.82	0.45
1:A:1665:ILE:HD11	1:A:1683:GLU:HB2	1.99	0.45
1:A:1792:LEU:HD12	1:A:1815:LEU:HD12	1.99	0.45
1:A:1792:LEU:HD22	1:A:1808:LEU:HD22	1.99	0.45
1:A:1568:PHE:HB2	1:A:1611:ILE:CD1	2.46	0.45
1:A:1698:ILE:HD13	1:A:1701:TRP:NE1	2.23	0.45
1:A:2686:MET:HE2	1:A:2686:MET:HB3	1.62	0.45
1:A:1665:ILE:O	1:A:1674:LEU:N	2.49	0.45
1:A:2953:MET:HE2	1:A:2953:MET:HB3	1.86	0.45
1:A:3073:GLU:HG2	1:A:3074:GLY:N	2.31	0.45
1:A:3563:GLN:HE22	1:A:3569:ALA:HB2	1.82	0.45
1:A:1397:ASN:O	1:A:1401:ILE:HG13	2.18	0.44
1:A:2110:LYS:HA	1:A:2113:ARG:NH2	2.33	0.44
1:A:2517:TYR:CE1	1:A:2521:ILE:HD13	2.53	0.44
1:A:3488:ARG:HH22	1:A:3773:LEU:HD21	1.81	0.44
1:A:3705:ARG:HG2	1:A:3813:PHE:CD2	2.52	0.44
1:A:2979:VAL:HG13	1:A:2980:LEU:HD12	2.00	0.44
1:A:3567:LEU:HD12	1:A:3568:PRO:HD2	1.98	0.44
1:A:2651:ALA:HB1	1:A:2705:ARG:NH2	2.32	0.44
1:A:2393:GLU:O	1:A:2397:ARG:NH1	2.51	0.44
1:A:2994:MET:O	1:A:3067:THR:OG1	2.26	0.44
1:A:3705:ARG:HA	1:A:3813:PHE:HE2	1.82	0.44
1:A:3913:GLU:N	1:A:3913:GLU:OE1	2.51	0.44
1:A:2683:ILE:HA	1:A:2686:MET:HE2	1.99	0.44
1:A:2827:HIS:CG	1:A:2873:TYR:HD2	2.36	0.44
1:A:3534:HIS:O	1:A:3537:GLN:HG2	2.17	0.44
1:A:4489:LEU:HD23	1:A:4492:ILE:HD12	2.00	0.44
1:A:1725:GLU:O	1:A:1729:LYS:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2123:ASP:O	1:A:2127:ILE:HG13	2.18	0.44
1:A:2273:ARG:HA	1:A:2273:ARG:NE	2.32	0.44
1:A:4601:LYS:HB2	1:A:4604:VAL:HG23	1.99	0.44
1:A:1647:VAL:HA	1:A:1650:LEU:HD13	1.99	0.44
1:A:3028:THR:O	1:A:3032:GLN:OE1	2.35	0.44
1:A:3780:VAL:O	1:A:3784:VAL:HG23	2.17	0.44
1:A:1676:ILE:HB	1:A:1684:VAL:HG22	1.99	0.44
1:A:2715:PRO:HA	1:A:2720:ARG:HB2	2.00	0.44
1:A:2784:PHE:HB3	1:A:2792:TYR:CD2	2.53	0.44
1:A:3123:PRO:HB3	1:A:3540:ASN:OD1	2.18	0.44
1:A:3654:ARG:HH21	1:A:3661:LEU:HG	1.82	0.44
1:A:4025:LEU:HD22	1:A:4027:LEU:HD22	2.00	0.44
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	2.00	0.44
1:A:1695:HIS:HB3	1:A:1700:GLU:HG2	2.00	0.43
1:A:1917:LYS:HG2	1:A:1921:HIS:CD2	2.53	0.43
1:A:2324:LEU:HD23	1:A:2334:SER:HA	2.00	0.43
1:A:1748:GLN:NE2	1:A:1868:TYR:OH	2.39	0.43
1:A:2605:LEU:HD13	1:A:2662:PHE:HE2	1.82	0.43
1:A:2737:ASP:OD1	1:A:2738:TYR:N	2.48	0.43
1:A:3048:GLU:O	1:A:3052:LYS:HG2	2.18	0.43
1:A:3113:MET:HE2	1:A:3115:LEU:HD11	1.99	0.43
1:A:4260:PHE:CE2	1:A:4608:PRO:HB3	2.53	0.43
1:A:1440:GLN:HA	1:A:1443:GLU:HG3	2.01	0.43
1:A:4128:MET:HE1	1:A:4134:VAL:HG11	1.99	0.43
1:A:2460:SER:OG	1:A:2589:LYS:HD2	2.19	0.43
1:A:2464:GLN:HG2	1:A:2583:THR:HG23	2.01	0.43
1:A:3661:LEU:HD12	1:A:3668:ASP:HB3	2.00	0.43
1:A:1678:SER:OG	1:A:1679:ARG:N	2.51	0.43
1:A:1786:GLU:OE1	1:A:1786:GLU:HA	2.18	0.43
1:A:2396:ARG:O	1:A:2399:LYS:HG2	2.18	0.43
1:A:2802:TRP:O	1:A:2806:ILE:HG12	2.18	0.43
1:A:4398:LEU:HG	1:A:4417:VAL:HG21	2.00	0.43
1:A:1880:VAL:HG23	1:A:2052:VAL:HG11	2.01	0.43
1:A:2889:LEU:HG	1:A:2916:LEU:HD11	2.00	0.43
1:A:3600:ILE:HD11	1:A:3634:LEU:HD13	2.00	0.43
1:A:2049:ILE:HG21	1:A:2090:LEU:HD11	2.00	0.43
1:A:2242:GLU:HG3	1:A:2248:GLU:HA	2.00	0.43
1:A:2658:TRP:CE2	1:A:2705:ARG:HG2	2.54	0.43
1:A:3555:ASN:HB2	1:A:3558:GLU:OE1	2.18	0.43
1:A:1547:LEU:HD12	1:A:1551:PHE:CE2	2.54	0.43
1:A:2156:LEU:O	1:A:2160:LEU:HD13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2755:MET:CE	1:A:2803:VAL:HG13	2.45	0.43
1:A:3817:SER:C	1:A:4346:MET:HE1	2.43	0.43
1:A:1393:TYR:HA	1:A:1396:ILE:HG12	2.01	0.43
1:A:1405:SER:OG	1:A:1406:GLU:N	2.52	0.43
1:A:1812:ILE:HG21	1:A:2056:SER:HA	2.01	0.43
1:A:3103:TYR:CE2	1:A:3107:LYS:HD2	2.54	0.43
1:A:3146:SER:O	1:A:3150:VAL:HG23	2.18	0.43
1:A:4332:LEU:HD23	1:A:4332:LEU:HA	1.89	0.43
1:A:2072:PHE:CE2	1:A:2141:VAL:HG11	2.54	0.43
1:A:2683:ILE:O	1:A:2687:VAL:HG22	2.19	0.43
1:A:2972:PHE:HZ	1:A:3008:MET:HE3	1.84	0.43
1:A:3736:GLY:O	1:A:3740:LEU:N	2.43	0.43
1:A:3865:GLN:NE2	1:A:3869:ASN:OD1	2.51	0.43
1:A:2218:HIS:HA	1:A:2340:ARG:HD3	2.01	0.42
1:A:2395:GLN:HB3	1:A:2398:ARG:NH2	2.34	0.42
1:A:3924:ILE:HD12	1:A:3952:GLN:NE2	2.34	0.42
1:A:4031:VAL:O	1:A:4123:ARG:NH1	2.52	0.42
1:A:4423:LEU:HD13	1:A:4466:HIS:HD2	1.84	0.42
1:A:4577:LEU:HD13	1:A:4638:ARG:HD2	1.99	0.42
1:A:2079:GLN:HB2	1:A:2160:LEU:HD21	2.01	0.42
1:A:2206:LYS:HD3	1:A:2206:LYS:HA	1.86	0.42
1:A:2581:LEU:HD13	1:A:2591:LEU:CD2	2.48	0.42
1:A:2972:PHE:CZ	1:A:3004:PHE:HB3	2.53	0.42
1:A:3191:ARG:NE	1:A:3500:MET:HE2	2.34	0.42
1:A:3802:LEU:N	1:A:3803:PRO:HD2	2.35	0.42
1:A:3873:ARG:HD3	1:A:4025:LEU:HG	2.01	0.42
1:A:4560:VAL:N	1:A:4588:THR:O	2.52	0.42
1:A:1463:LEU:O	1:A:1467:ARG:NE	2.48	0.42
1:A:2660:VAL:HG22	1:A:2707:GLN:HB2	2.02	0.42
1:A:3069:ASN:ND2	1:A:3690:PRO:HB2	2.29	0.42
1:A:3079:ALA:HB2	1:A:3086:PHE:CE2	2.54	0.42
1:A:3722:PRO:O	1:A:3725:ASP:N	2.52	0.42
1:A:3909:LEU:HD12	1:A:4344:LEU:HB2	2.00	0.42
1:A:4183:LEU:HD11	1:A:4215:ALA:HB1	2.02	0.42
1:A:2522:THR:OG1	1:A:2524:VAL:HG12	2.19	0.42
1:A:4084:ILE:HD11	1:A:4096:LEU:HD11	2.00	0.42
1:A:2206:LYS:NZ	1:A:2363:TRP:O	2.41	0.42
1:A:2992:PHE:HD2	1:A:3064:VAL:HG13	1.83	0.42
1:A:3576:ASN:ND2	1:A:3700:ASN:O	2.37	0.42
1:A:4423:LEU:HD13	1:A:4466:HIS:CD2	2.54	0.42
1:A:1769:MET:HE1	1:A:1778:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1792:LEU:HD23	1:A:1792:LEU:HA	1.87	0.42
1:A:2257:LYS:O	1:A:2678:ARG:HG3	2.20	0.42
1:A:2263:HIS:HD2	1:A:2695:THR:HB	1.85	0.42
1:A:3620:ARG:O	1:A:3624:GLU:HG2	2.19	0.42
1:A:1601:LEU:HD12	1:A:1601:LEU:HA	1.92	0.42
1:A:1789:LEU:HD23	1:A:1789:LEU:HA	1.85	0.42
1:A:2220:LEU:HD11	1:A:2342:MET:HE2	2.02	0.42
1:A:2443:LEU:HD23	1:A:2510:MET:HG2	2.02	0.42
1:A:2667:ASN:OD1	1:A:2712:CYS:HB3	2.20	0.42
1:A:2828:GLU:OE2	1:A:2924:ARG:NH2	2.53	0.42
1:A:2944:THR:O	1:A:2948:ARG:HG3	2.20	0.42
1:A:3172:THR:HG21	1:A:3694:SER:HB2	2.01	0.42
1:A:3502:THR:HB	1:A:3543:PHE:HA	2.02	0.42
1:A:4594:LYS:HE3	1:A:4594:LYS:HB2	1.93	0.42
1:A:2630:LEU:HA	1:A:2633:LYS:HD2	2.01	0.42
1:A:3815:MET:O	1:A:3818:LEU:HB2	2.19	0.42
1:A:4033:THR:HG22	1:A:4034:GLU:N	2.35	0.42
1:A:4448:LEU:HD12	1:A:4448:LEU:HA	1.81	0.42
1:A:1351:TRP:CH2	1:A:1400:VAL:HG13	2.55	0.41
1:A:2406:GLU:HG2	1:A:2409:ALA:HB2	2.02	0.41
1:A:2440:ALA:HB3	1:A:2502:LEU:HD12	2.02	0.41
1:A:2446:ILE:HD11	1:A:2714:PRO:HG3	2.01	0.41
1:A:2789:GLN:HG3	1:A:2838:VAL:HG21	2.02	0.41
1:A:3150:VAL:HG13	1:A:3532:TRP:CE2	2.55	0.41
1:A:3638:VAL:HG23	1:A:3679:LEU:HD22	2.02	0.41
1:A:3767:ILE:HG13	1:A:3771:GLU:OE2	2.20	0.41
1:A:3100:GLU:HA	1:A:3130:TYR:CE1	2.55	0.41
1:A:3510:SER:OG	1:A:3553:LEU:HD11	2.20	0.41
1:A:1469:VAL:O	1:A:1473:TYR:HB2	2.20	0.41
1:A:1607:LEU:HA	1:A:1610:LYS:HD2	2.02	0.41
1:A:1803:LEU:HG	1:A:1807:LYS:HE3	2.02	0.41
1:A:2065:LEU:HD21	1:A:2134:GLN:HG2	2.01	0.41
1:A:2445:HIS:NE2	1:A:2449:LEU:HD22	2.35	0.41
1:A:2836:ARG:HB2	1:A:3091:LEU:HD11	2.01	0.41
1:A:3589:ILE:N	1:A:3679:LEU:O	2.42	0.41
1:A:4432:ALA:O	1:A:4436:GLN:HG2	2.20	0.41
1:A:2458:LEU:O	1:A:2462:LEU:HG	2.21	0.41
1:A:2898:LYS:HE2	1:A:2898:LYS:HA	2.02	0.41
1:A:3122:VAL:HG21	1:A:3136:PRO:HB2	2.01	0.41
1:A:3781:THR:HG22	1:A:3785:GLU:OE1	2.19	0.41
1:A:2268:LEU:H	1:A:2268:LEU:HD23	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2845:TRP:CE2	1:A:2849:ASN:ND2	2.88	0.41
1:A:3607:ARG:O	1:A:3632:PRO:HD2	2.20	0.41
1:A:3766:ILE:HD12	1:A:3766:ILE:HA	1.92	0.41
1:A:4055:VAL:HB	1:A:4095:MET:HE1	2.01	0.41
1:A:4269:LEU:HD23	1:A:4269:LEU:HA	1.90	0.41
1:A:1638:LEU:HA	1:A:1641:ILE:HG12	2.03	0.41
1:A:2135:GLU:O	1:A:2138:ILE:HG22	2.21	0.41
1:A:2203:TRP:CH2	1:A:2236:VAL:HG11	2.55	0.41
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.55	0.41
1:A:2472:TYR:HE1	1:A:2481:MET:HB2	1.85	0.41
1:A:3759:ARG:H	1:A:3759:ARG:HG3	1.64	0.41
1:A:4243:LEU:O	1:A:4247:MET:HG3	2.21	0.41
1:A:1350:PRO:O	1:A:1354:VAL:HG23	2.21	0.41
1:A:4482:PHE:HE2	1:A:4486:ILE:HD11	1.86	0.41
1:A:1466:ILE:HG23	1:A:1500:HIS:NE2	2.36	0.41
1:A:1538:ILE:HG13	1:A:1539:ASP:N	2.35	0.41
1:A:1579:MET:HA	1:A:1582:VAL:HG12	2.03	0.41
1:A:1625:SER:CB	1:A:1699:ASN:HD21	2.32	0.41
1:A:2200:GLY:O	1:A:2204:VAL:HG23	2.21	0.41
1:A:2306:ASP:OD2	1:A:2676:THR:OG1	2.31	0.41
1:A:2446:ILE:HD11	1:A:2714:PRO:HB3	2.02	0.41
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.56	0.41
1:A:3186:LEU:HD23	1:A:3186:LEU:HA	1.87	0.41
1:A:3508:LEU:HD13	1:A:3536:LEU:HD21	2.03	0.41
1:A:3510:SER:O	1:A:3514:ILE:HG12	2.21	0.41
1:A:3767:ILE:HA	1:A:3770:LEU:HG	2.03	0.41
1:A:3846:LEU:HB3	1:A:3855:ARG:NH1	2.36	0.41
1:A:3916:LEU:HD23	1:A:3916:LEU:HA	1.91	0.41
1:A:1390:LEU:HD23	1:A:1390:LEU:HA	1.90	0.41
1:A:1477:LEU:HB3	1:A:1485:ARG:HG3	2.03	0.41
1:A:2972:PHE:HE1	1:A:2976:LEU:HD11	1.86	0.41
1:A:3597:THR:O	1:A:3601:MET:HG2	2.21	0.41
1:A:3641:TYR:CD2	1:A:3692:LEU:HD12	2.56	0.41
1:A:3792:GLN:O	1:A:3796:THR:HG23	2.20	0.41
1:A:4037:PRO:HB2	1:A:4118:PRO:HB2	2.02	0.41
1:A:4324:PRO:HB3	1:A:4638:ARG:HH12	1.83	0.41
1:A:1508:LYS:HG3	1:A:1513:TYR:CZ	2.55	0.40
1:A:1880:VAL:HG12	2:A:4701:ADP:N1	2.35	0.40
1:A:2138:ILE:HG13	1:A:2161:LEU:HD11	2.03	0.40
1:A:4495:ALA:HB1	1:A:4503:GLU:HG3	2.03	0.40
1:A:1665:ILE:HG22	1:A:1674:LEU:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1849:LYS:HE2	1:A:1849:LYS:HB3	1.93	0.40
1:A:2030:ASP:OD2	1:A:4131:ASN:ND2	2.55	0.40
1:A:2072:PHE:CZ	1:A:2161:LEU:HD13	2.57	0.40
1:A:2086:TYR:CZ	1:A:2149:LEU:HD23	2.56	0.40
1:A:2491:GLN:HB3	1:A:2524:VAL:HG21	2.02	0.40
1:A:2090:LEU:O	1:A:2094:LYS:HG3	2.21	0.40
1:A:2577:HIS:HE1	1:A:2736:VAL:HA	1.87	0.40
1:A:2922:ILE:HG22	1:A:2950:VAL:HG11	2.04	0.40
1:A:1477:LEU:HB3	1:A:1485:ARG:CG	2.52	0.40
1:A:1678:SER:HB2	1:A:1872:TYR:OH	2.21	0.40
1:A:3506:ASP:OD1	1:A:3544:ARG:HG3	2.22	0.40
1:A:4087:ALA:HB1	1:A:4092:ARG:O	2.21	0.40
1:A:1451:LEU:HD12	1:A:3656:THR:HG21	2.04	0.40
1:A:2962:LYS:CE	1:A:3665:GLY:H	2.35	0.40
1:A:3835:ILE:O	1:A:3839:VAL:HG23	2.22	0.40
1:A:4086:THR:HA	1:A:4089:LYS:NZ	2.37	0.40
1:A:4247:MET:HE2	1:A:4247:MET:HB3	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3035/4646 (65%)	2967 (98%)	68 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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 (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1421	HIS
1	A	1440	GLN
1	A	1500	HIS
1	A	1593	ASN
1	A	1755	GLN
1	A	1850	GLN
1	A	1876	GLN
1	A	1894	GLN
1	A	1931	ASN
1	A	2130	ASN
1	A	2209	GLN
1	A	2217	ASN
1	A	2416	GLN
1	A	2577	HIS
1	A	2588	HIS
1	A	2621	ASN
1	A	2637	HIS
1	A	2685	GLN
1	A	2913	ASN
1	A	3197	GLN
1	A	3820	GLN
1	A	3845	ASN
1	A	4114	HIS
1	A	4506	ASN
1	A	4508	HIS
1	A	4573	ASN
1	A	4579	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 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$
3	ATP	A	4702	4	32,33,33	0.37	0	48,52,52	0.28	0
2	ADP	A	4701	-	28,29,29	1.39	5 (17%)	43,45,45	1.81	10 (23%)
2	ADP	A	4703	-	28,29,29	1.42	4 (14%)	43,45,45	1.91	8 (18%)
2	ADP	A	4704	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	4702	4	-	3/22/38/38	0/3/3/3
2	ADP	A	4701	-	-	3/16/32/32	0/3/3/3
2	ADP	A	4703	-	-	7/16/32/32	0/3/3/3
2	ADP	A	4704	-	-	4/16/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4703	ADP	C5-C4	4.92	1.47	1.39

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4704	ADP	C5-C4	4.63	1.47	1.39
2	A	4701	ADP	C5-C4	4.56	1.47	1.39
2	A	4703	ADP	C5-C6	2.73	1.48	1.41
2	A	4704	ADP	C5-C6	2.57	1.48	1.41
2	A	4701	ADP	C5-C6	2.49	1.47	1.41
2	A	4701	ADP	C5-N7	-2.40	1.34	1.39
2	A	4704	ADP	C5-N7	-2.39	1.34	1.39
2	A	4703	ADP	C5-N7	-2.38	1.34	1.39
2	A	4704	ADP	C8-N7	2.30	1.36	1.31
2	A	4701	ADP	C8-N7	2.22	1.36	1.31
2	A	4703	ADP	C8-N7	2.21	1.35	1.31
2	A	4701	ADP	C4-N9	-2.13	1.33	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	C5-C4-N3	-6.44	117.84	126.72
2	A	4704	ADP	C5-C4-N3	-5.65	118.93	126.72
2	A	4701	ADP	C5-C4-N3	-5.50	119.14	126.72
2	A	4703	ADP	N3-C4-N9	5.14	135.91	127.17
2	A	4704	ADP	N3-C4-N9	4.52	134.85	127.17
2	A	4701	ADP	N3-C4-N9	4.47	134.76	127.17
2	A	4703	ADP	C2-N3-C4	3.95	121.49	111.83
2	A	4704	ADP	C2-N3-C4	3.62	120.67	111.83
2	A	4701	ADP	C2-N3-C4	3.59	120.59	111.83
2	A	4701	ADP	N3-C2-N1	-3.39	123.45	128.58
2	A	4704	ADP	C4-C5-N7	-3.34	106.77	110.58
2	A	4703	ADP	C4-C5-N7	-3.33	106.78	110.58
2	A	4704	ADP	N3-C2-N1	-3.28	123.61	128.58
2	A	4703	ADP	N3-C2-N1	-3.25	123.67	128.58
2	A	4701	ADP	C4-C5-N7	-3.22	106.90	110.58
2	A	4703	ADP	C3'-C2'-C1'	2.87	106.89	101.46
2	A	4701	ADP	C4-N9-C8	2.83	108.71	105.74
2	A	4704	ADP	C4-N9-C8	2.72	108.59	105.74
2	A	4703	ADP	C5-N7-C8	2.45	107.29	103.45
2	A	4704	ADP	C5-N7-C8	2.44	107.29	103.45
2	A	4704	ADP	C3'-C2'-C1'	2.36	105.93	101.46
2	A	4701	ADP	C5-N7-C8	2.35	107.14	103.45
2	A	4701	ADP	C3'-C2'-C1'	2.20	105.62	101.46
2	A	4703	ADP	C4-N9-C8	2.14	107.98	105.74
2	A	4701	ADP	C2-N1-C6	2.12	122.21	118.73
2	A	4704	ADP	C6-C5-N7	2.03	136.00	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	ADP	C6-C5-N7	2.00	135.95	132.09

There are no chirality outliers.

All (17) 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-O2A
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	4704	ADP	C3'-C4'-C5'-O5'
2	A	4704	ADP	O4'-C4'-C5'-O5'
3	A	4702	ATP	O4'-C4'-C5'-O5'
2	A	4701	ADP	PB-O3A-PA-O1A
2	A	4703	ADP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'
2	A	4703	ADP	C2'-C1'-N9-C4
2	A	4703	ADP	C3'-C4'-C5'-O5'
2	A	4703	ADP	C2'-C1'-N9-C8
2	A	4701	ADP	PB-O3A-PA-O2A
2	A	4701	ADP	O4'-C4'-C5'-O5'
3	A	4702	ATP	PA-O3A-PB-O2B

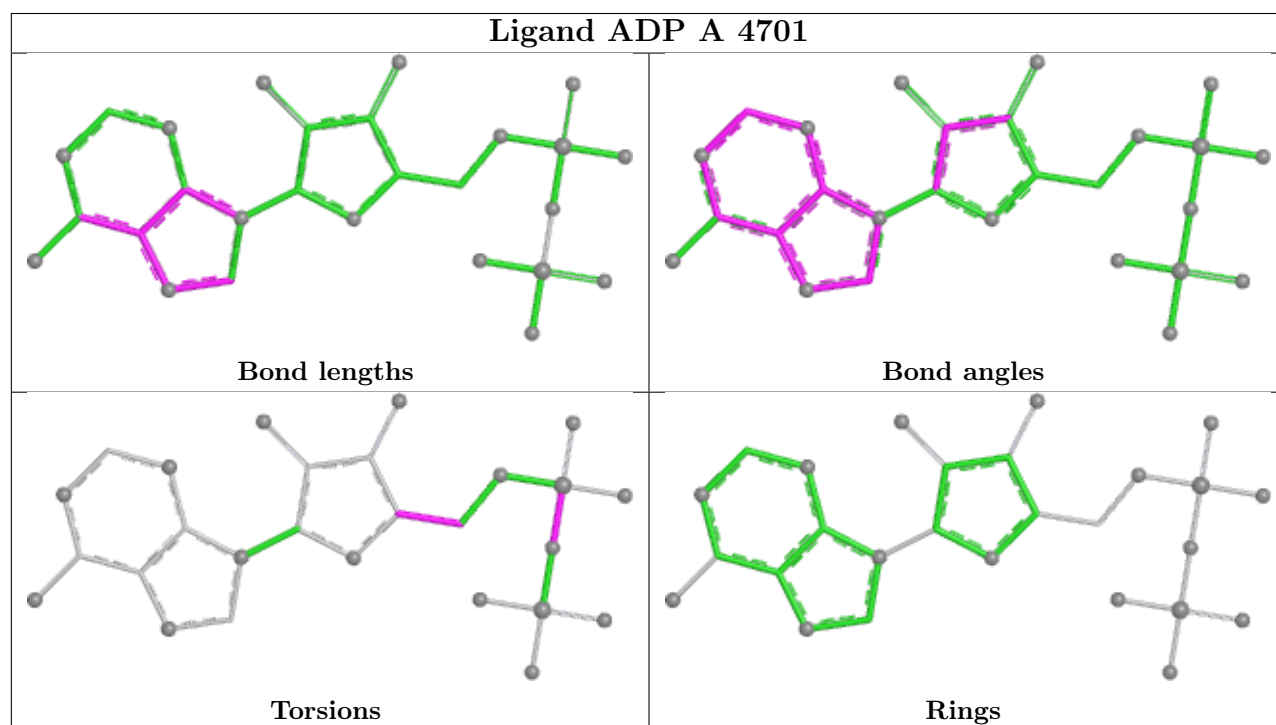
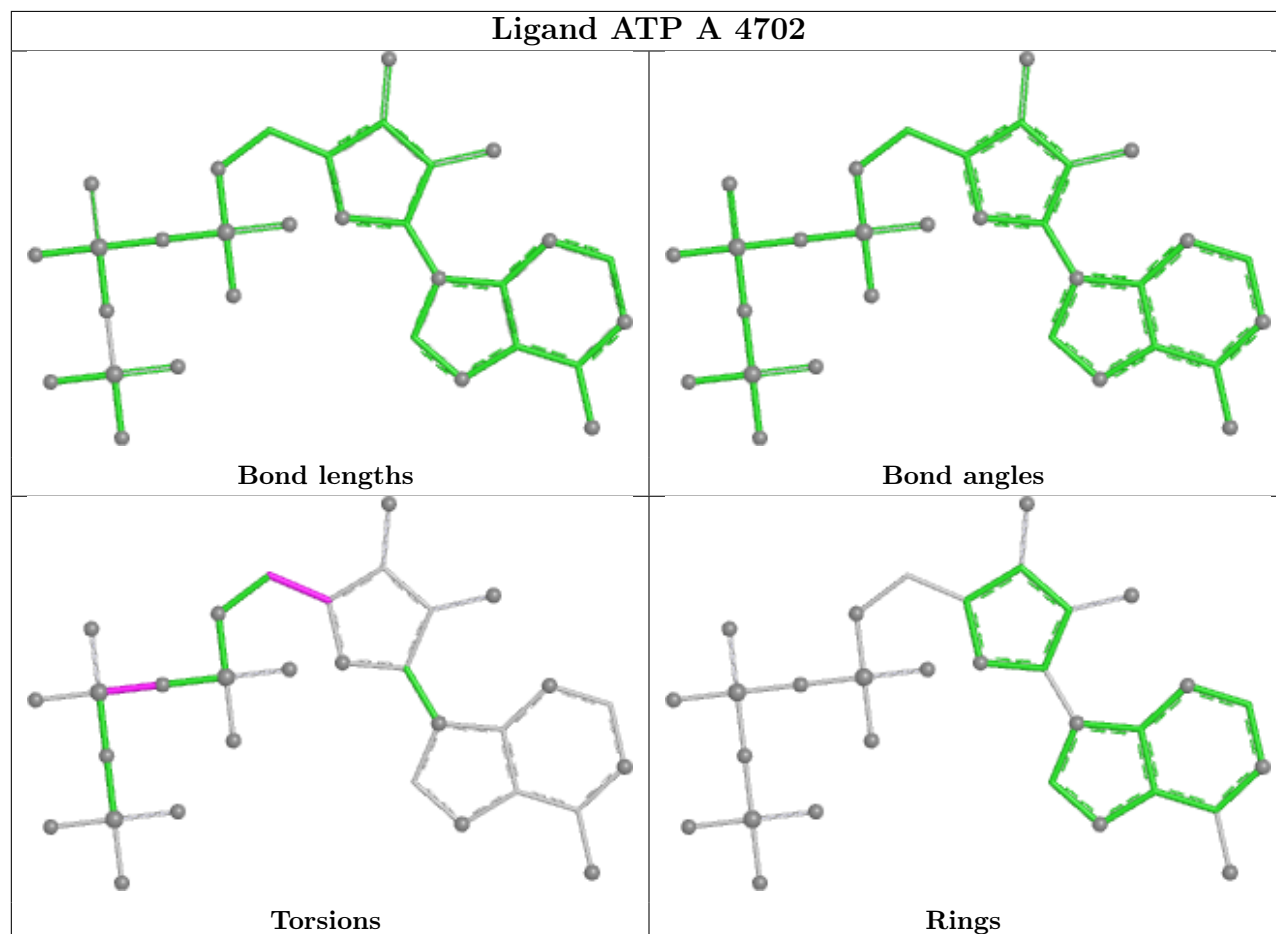
There are no ring outliers.

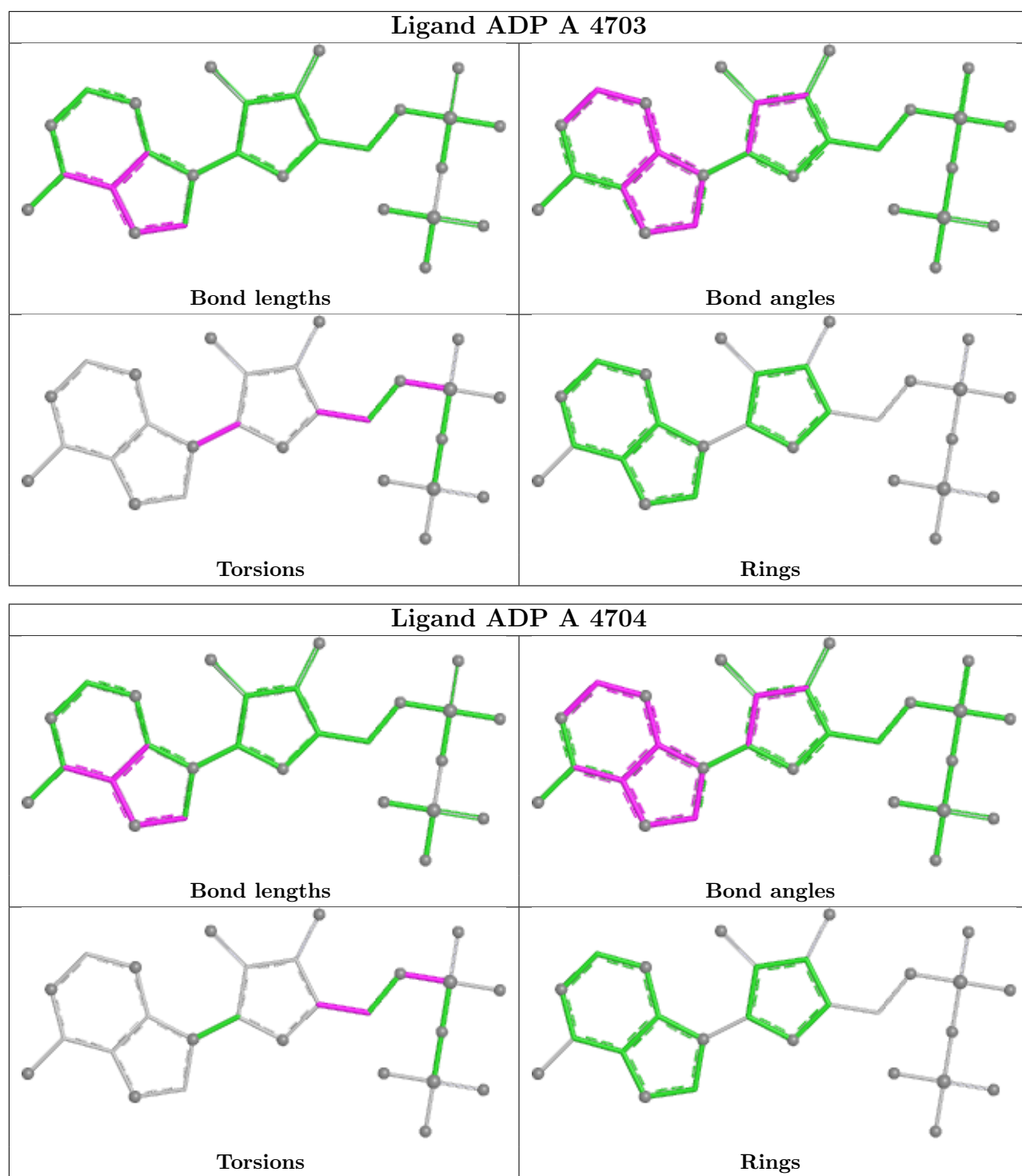
4 monomers are involved in 6 short contacts:

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

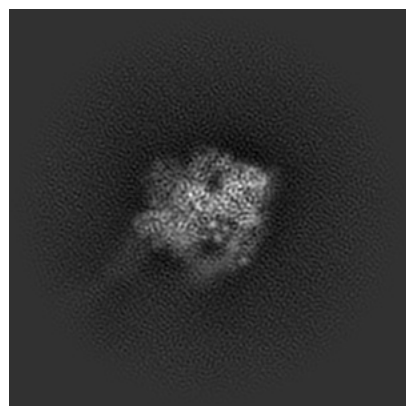
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44713. These allow visual inspection of the internal detail of the map and identification of artifacts.

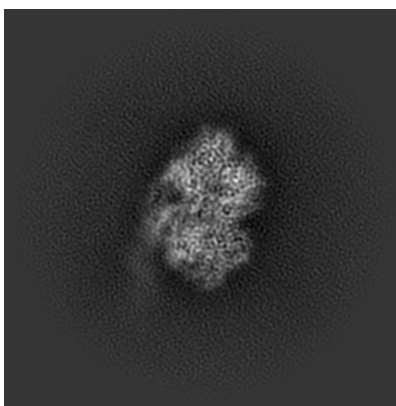
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

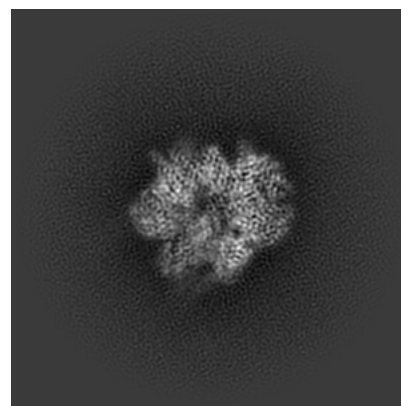
6.1.1 Primary map



X

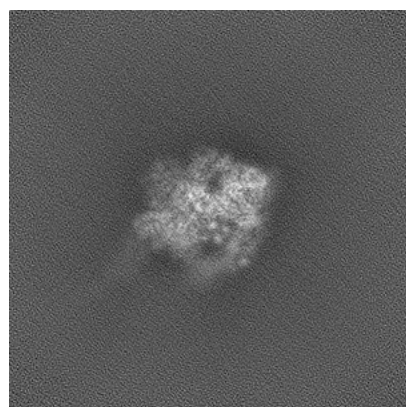


Y

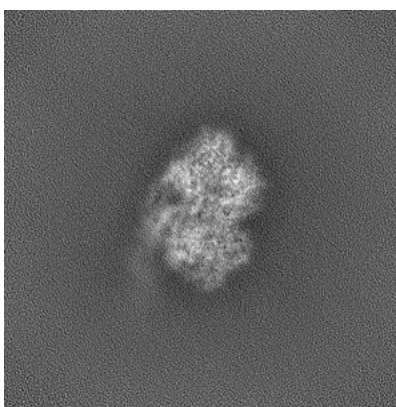


Z

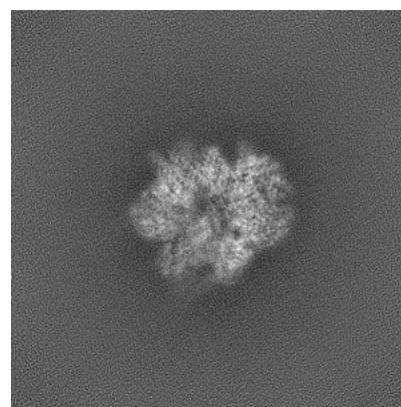
6.1.2 Raw map



X



Y

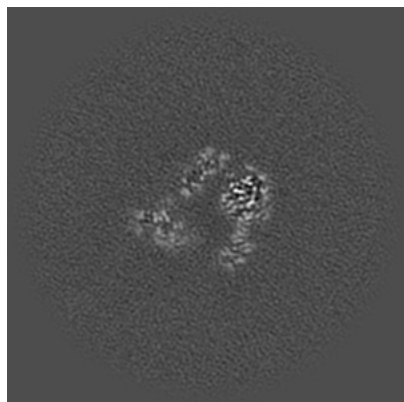


Z

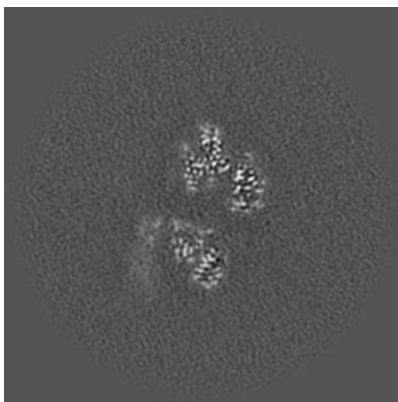
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

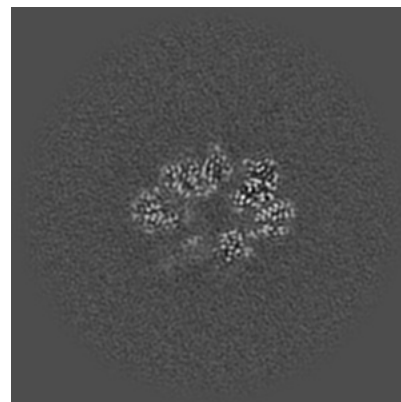
6.2.1 Primary map



X Index: 160

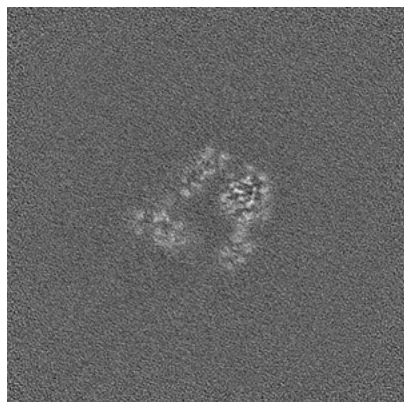


Y Index: 160

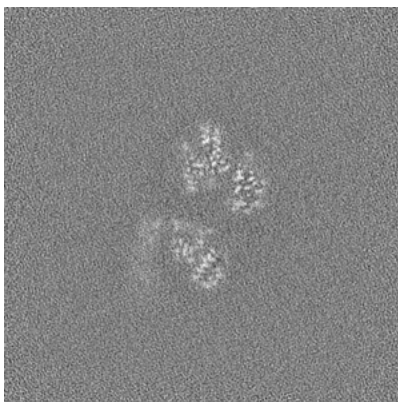


Z Index: 160

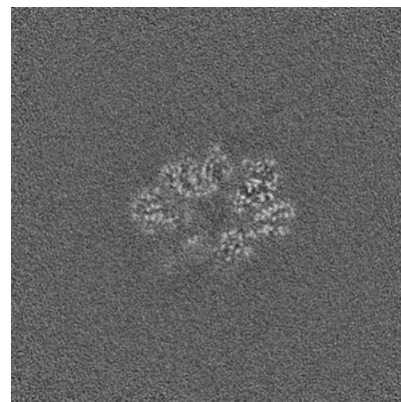
6.2.2 Raw map



X Index: 160



Y Index: 160

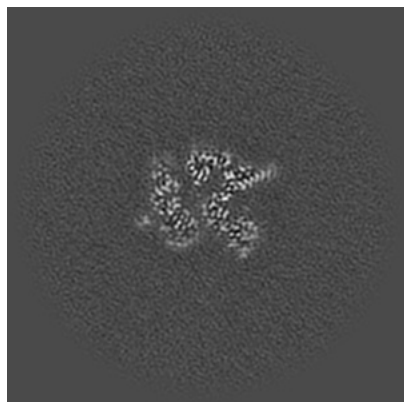


Z Index: 160

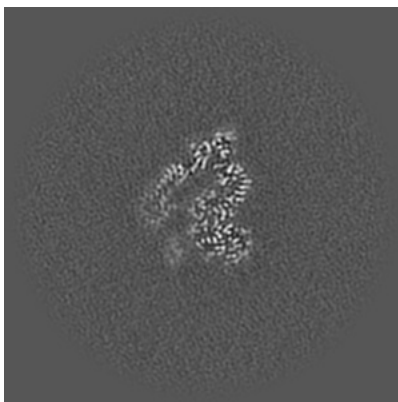
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

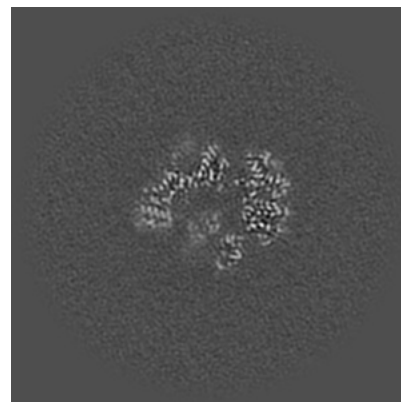
6.3.1 Primary map



X Index: 183

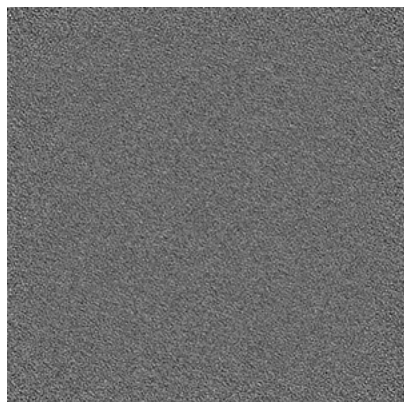


Y Index: 181

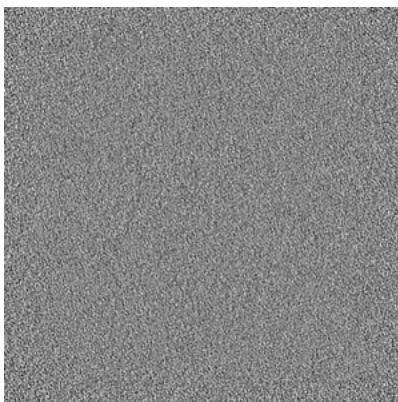


Z Index: 172

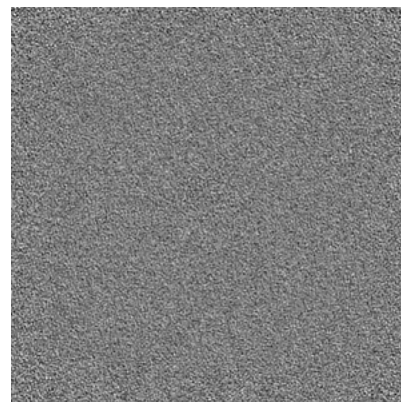
6.3.2 Raw map



X Index: 0



Y Index: 0

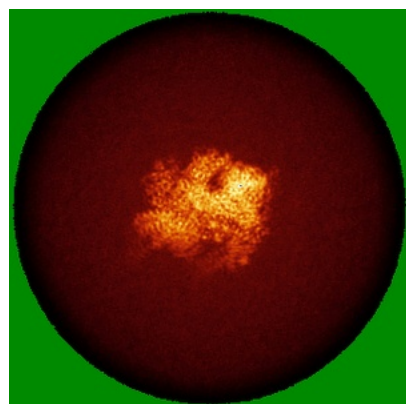


Z Index: 0

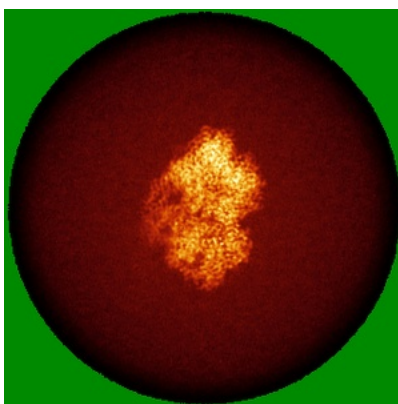
The images above show the largest variance slices of the map in three orthogonal directions.

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

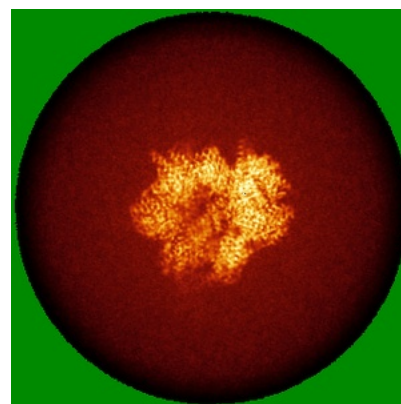
6.4.1 Primary map



X

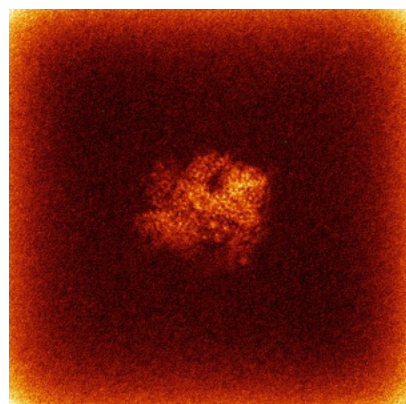


Y

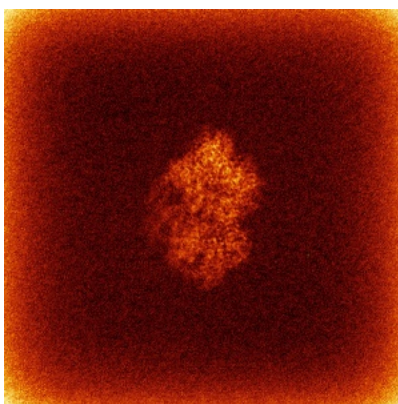


Z

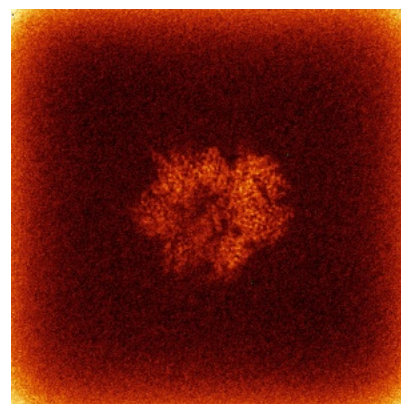
6.4.2 Raw map



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](#)

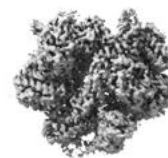
6.5.1 Primary map



X



Y



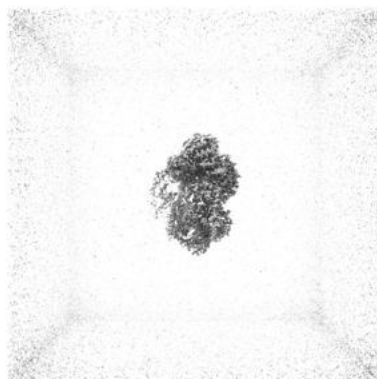
Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

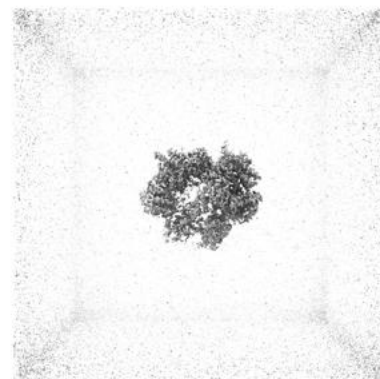
6.5.2 Raw map



X



Y



Z

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.

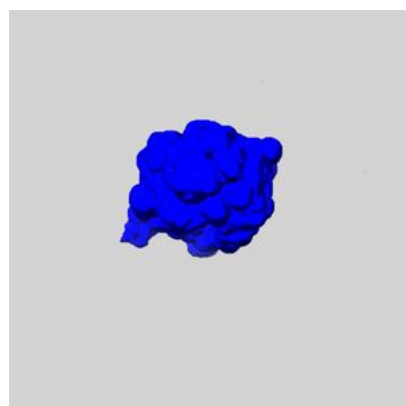
6.6 Mask visualisation [i](#)

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

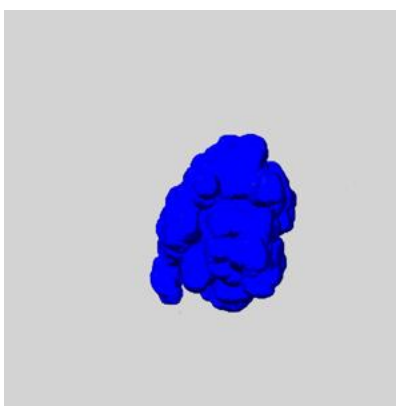
A mask typically either:

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

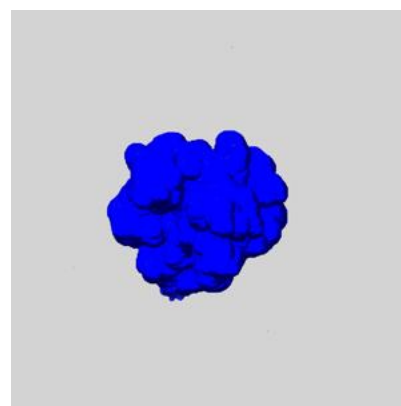
6.6.1 emd_44713_msk_1.map [i](#)



X



Y

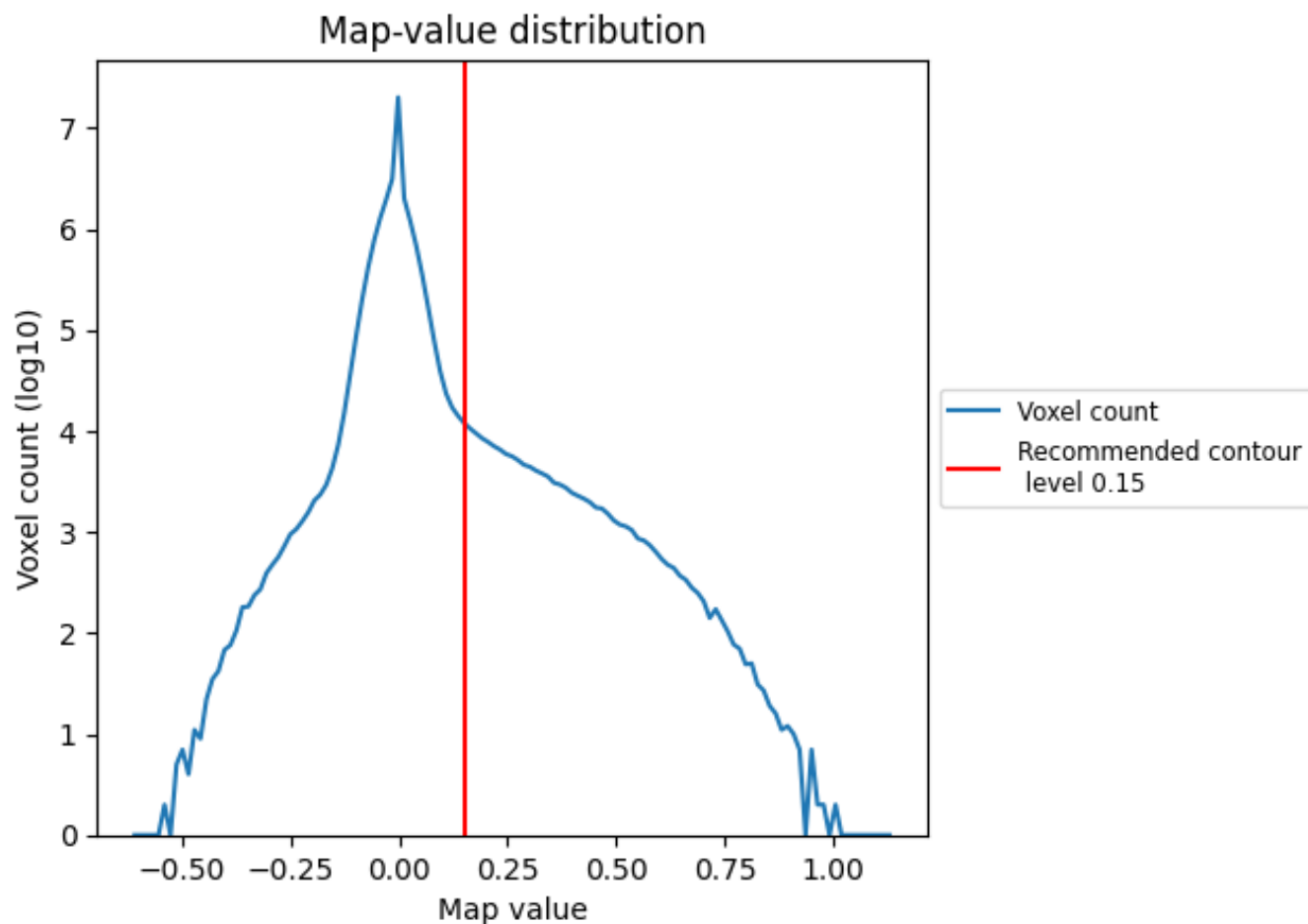


Z

7 Map analysis [i](#)

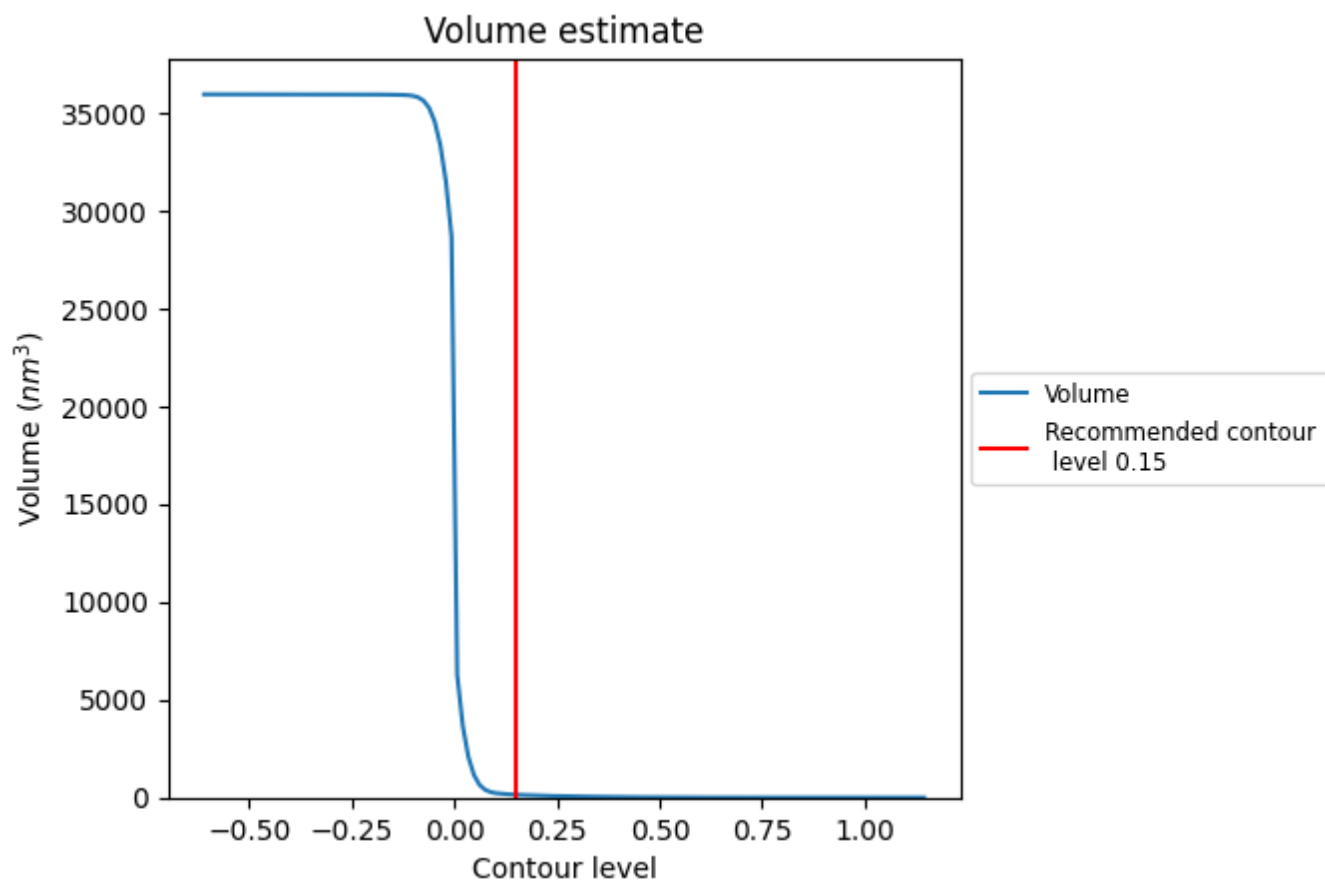
This section contains the results of statistical analysis of the map.

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.

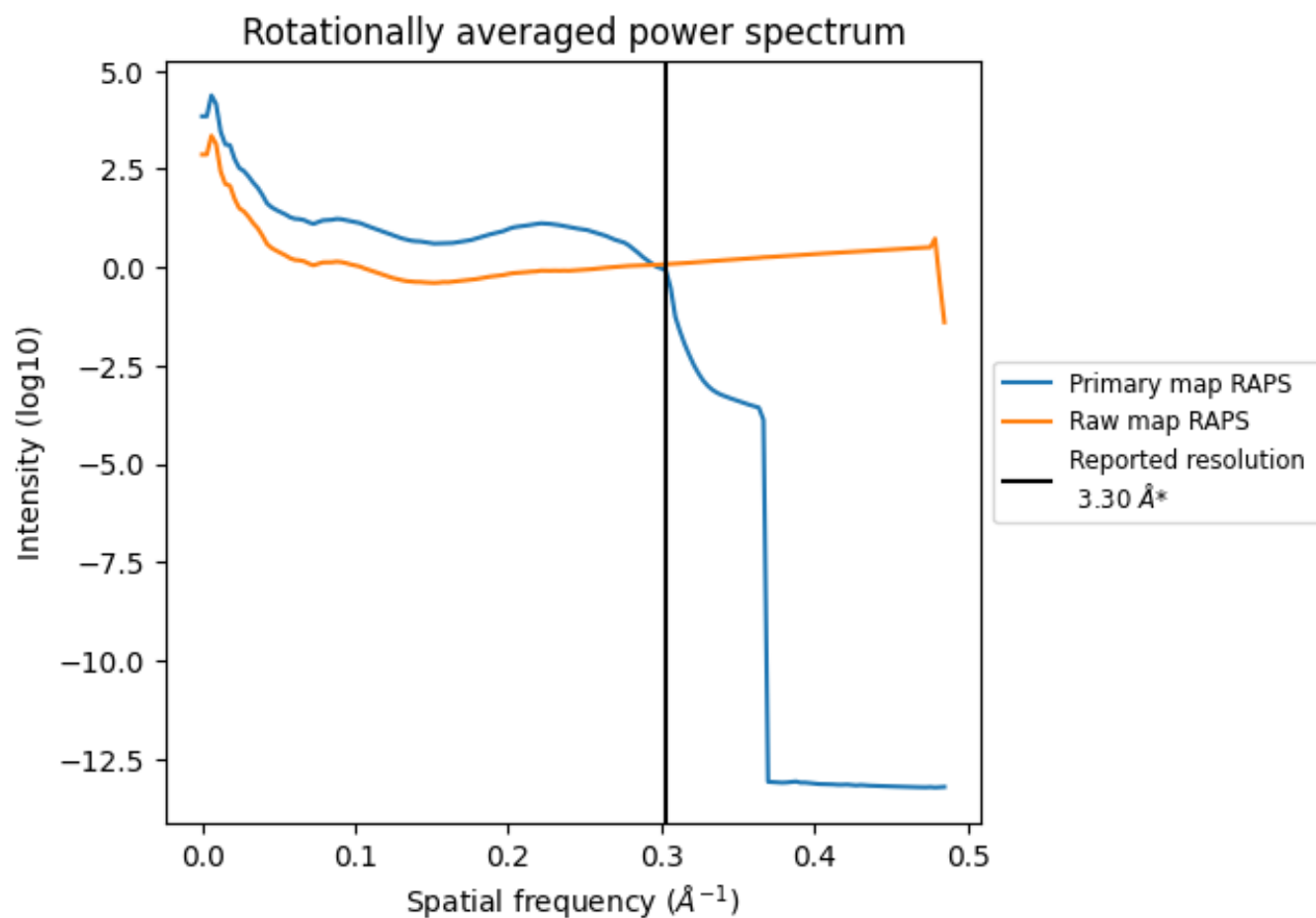
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 146 nm³; this corresponds to an approximate mass of 132 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 ⓘ

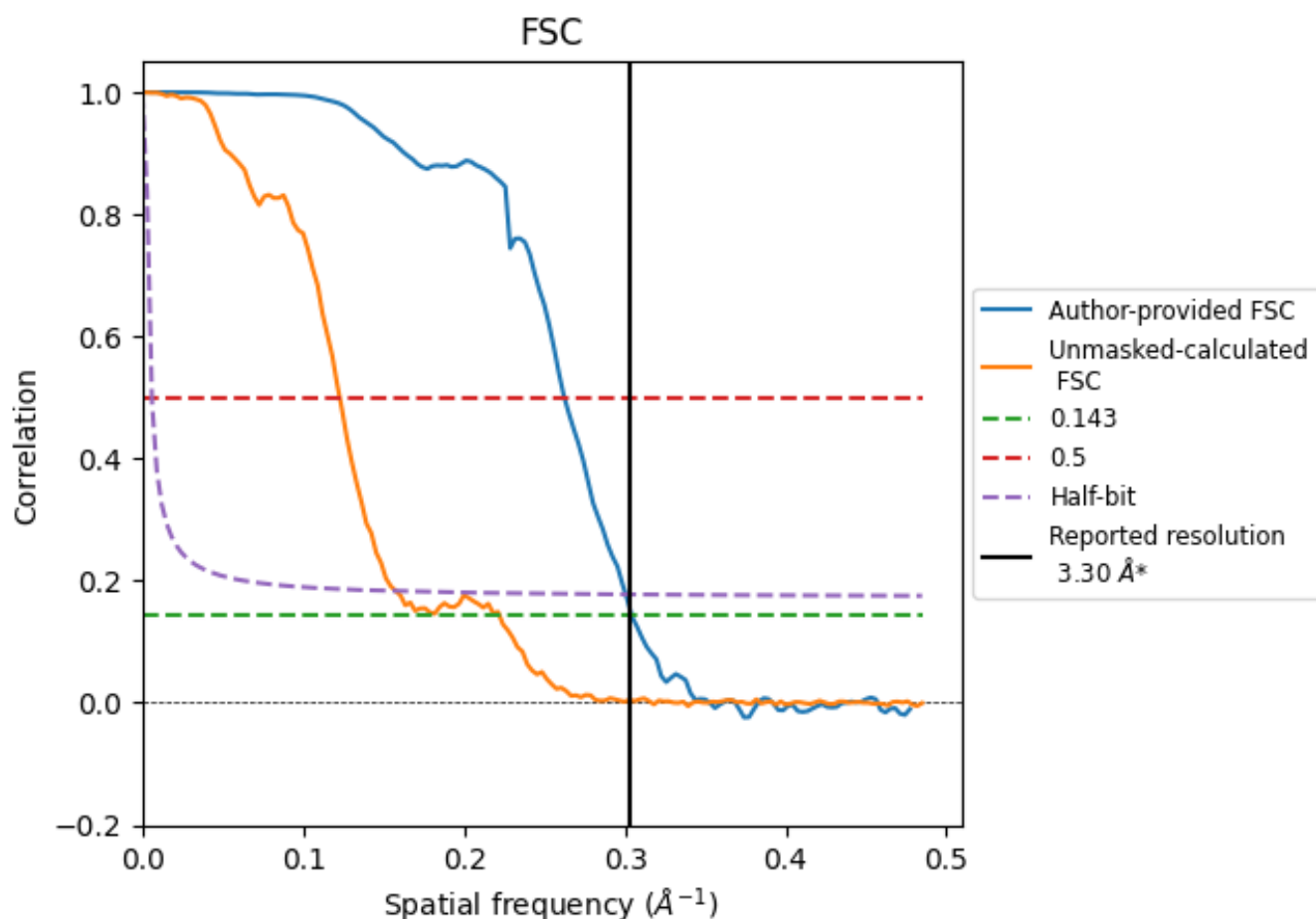


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

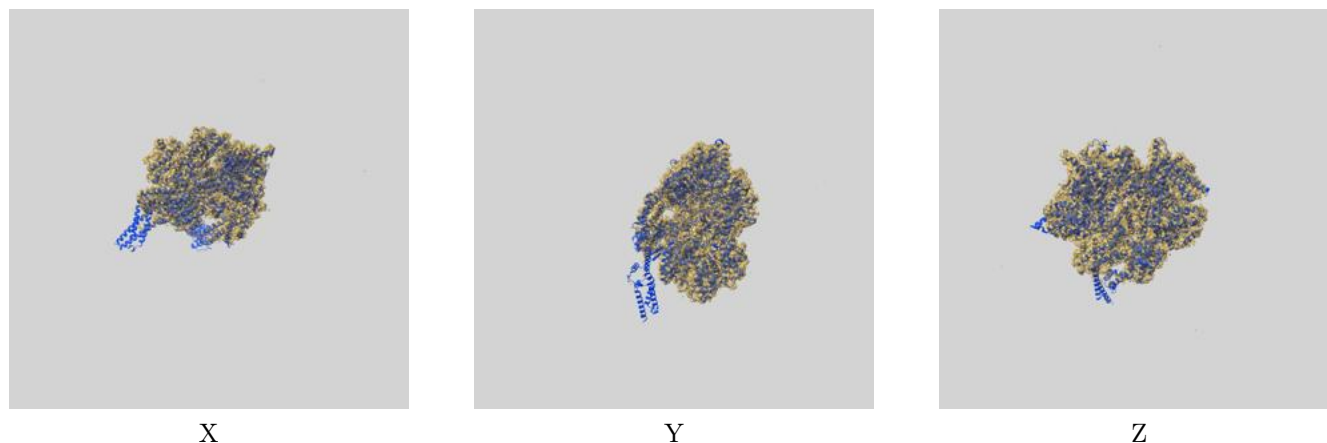
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.81	3.33
Unmasked-calculated*	4.50	8.14	6.34

*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 4.50 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

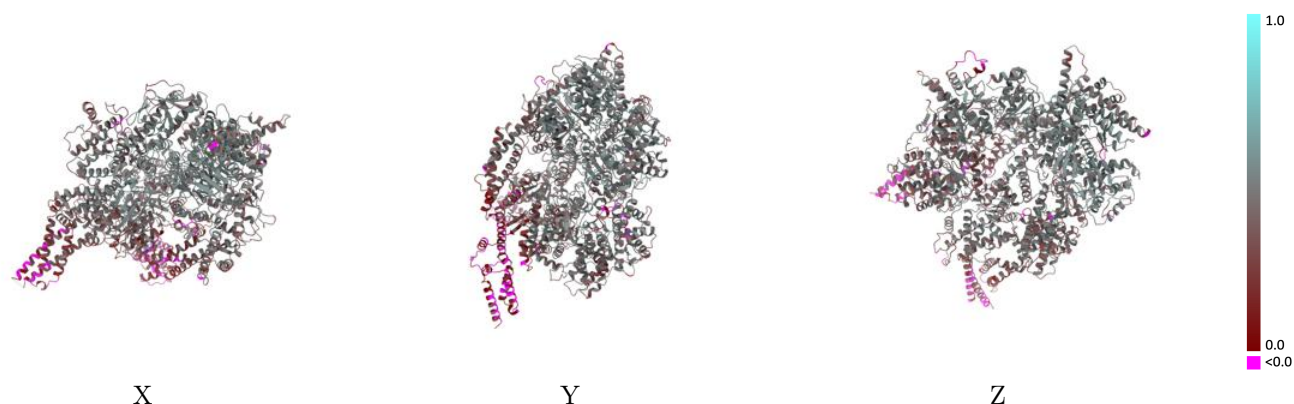
This section contains information regarding the fit between EMDB map EMD-44713 and PDB model 9BMW. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



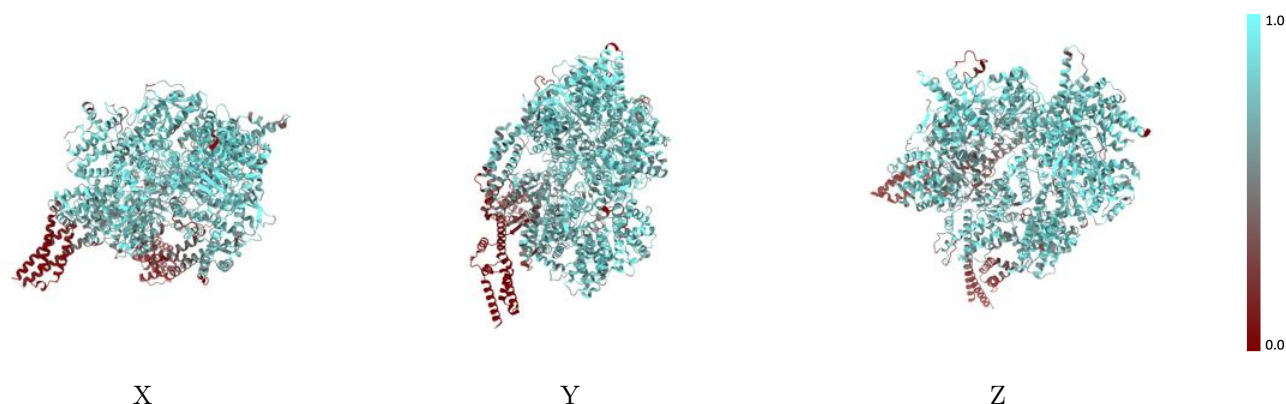
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



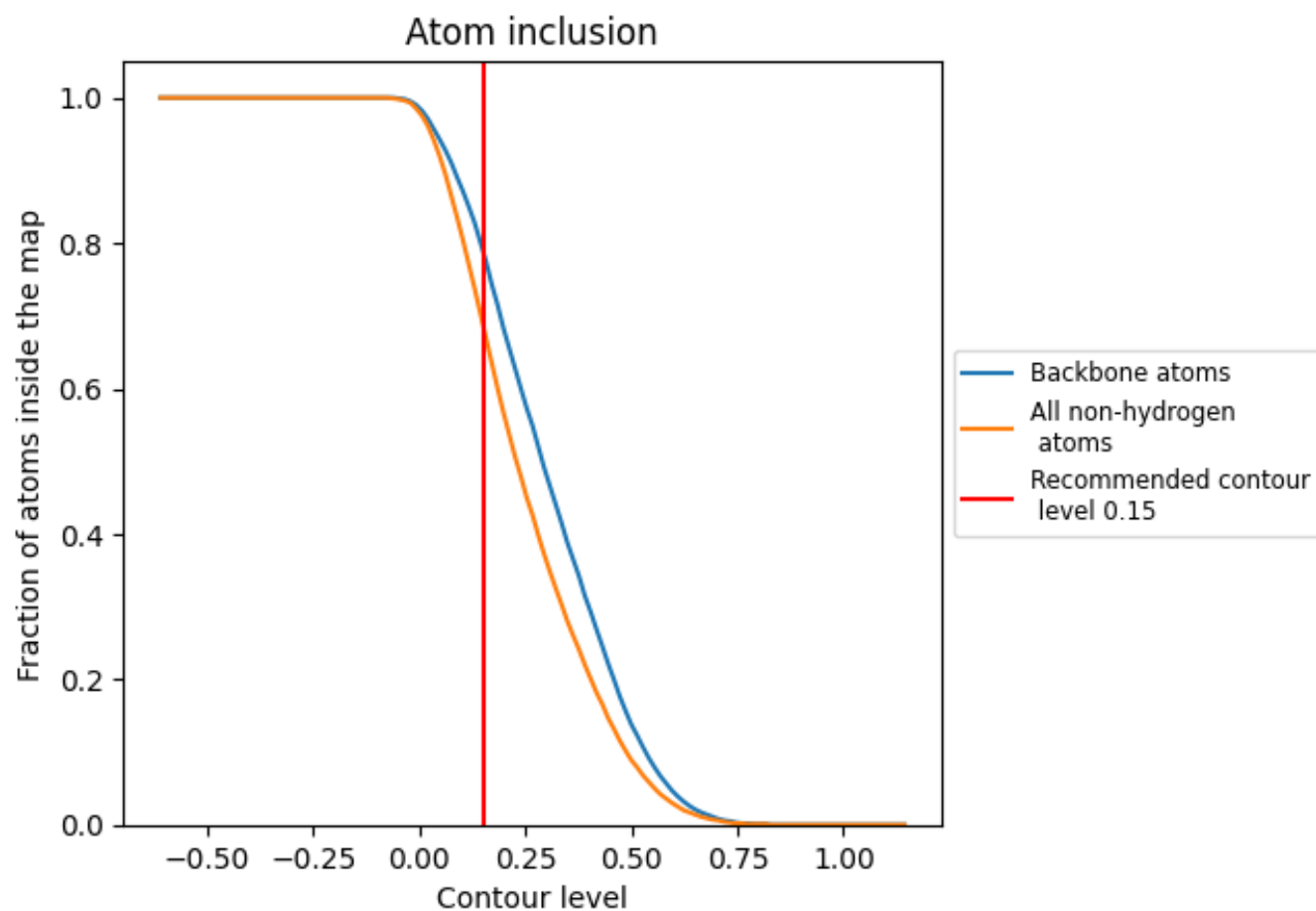
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 69% 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	<div></div> 0.6880	<div></div> 0.4110
A	<div></div> 0.6880	<div></div> 0.4110

