



Full wwPDB EM Validation Report ⓘ

Apr 24, 2025 – 01:29 PM EDT

PDB ID : 9BMS / pdb_00009bms
EMDB ID : EMD-44709
Title : State-2 of motor domain from full-length human dynein-1 in 5 mM ADP
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.04 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

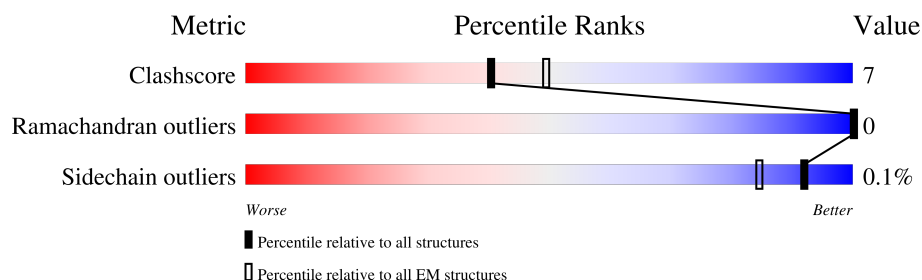
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.04 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	4646	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	A	4705	-	-	X	-
4	MG	A	4706	-	-	X	-

2 Entry composition [i](#)

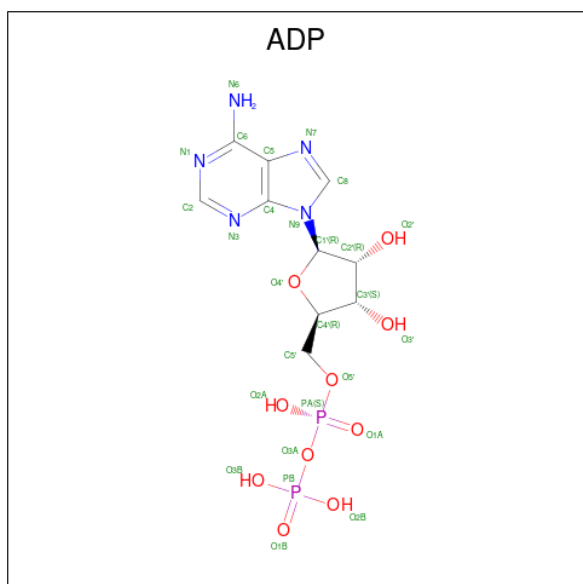
There are 4 unique types of molecules in this entry. The entry contains 23707 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

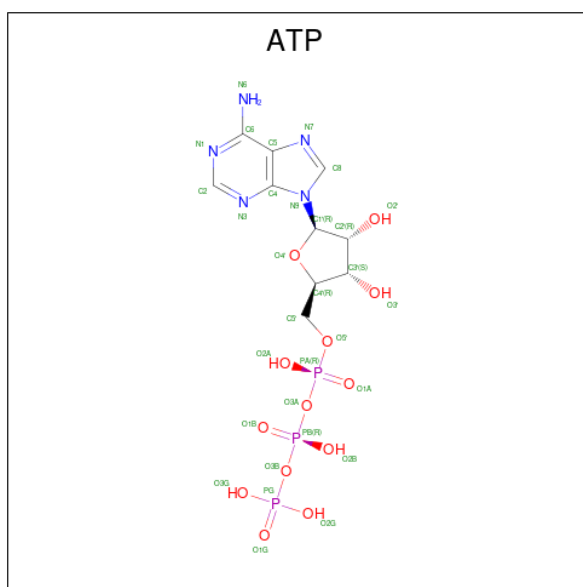
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2937	23593	15028	4070	4378	117	0	0

- 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).



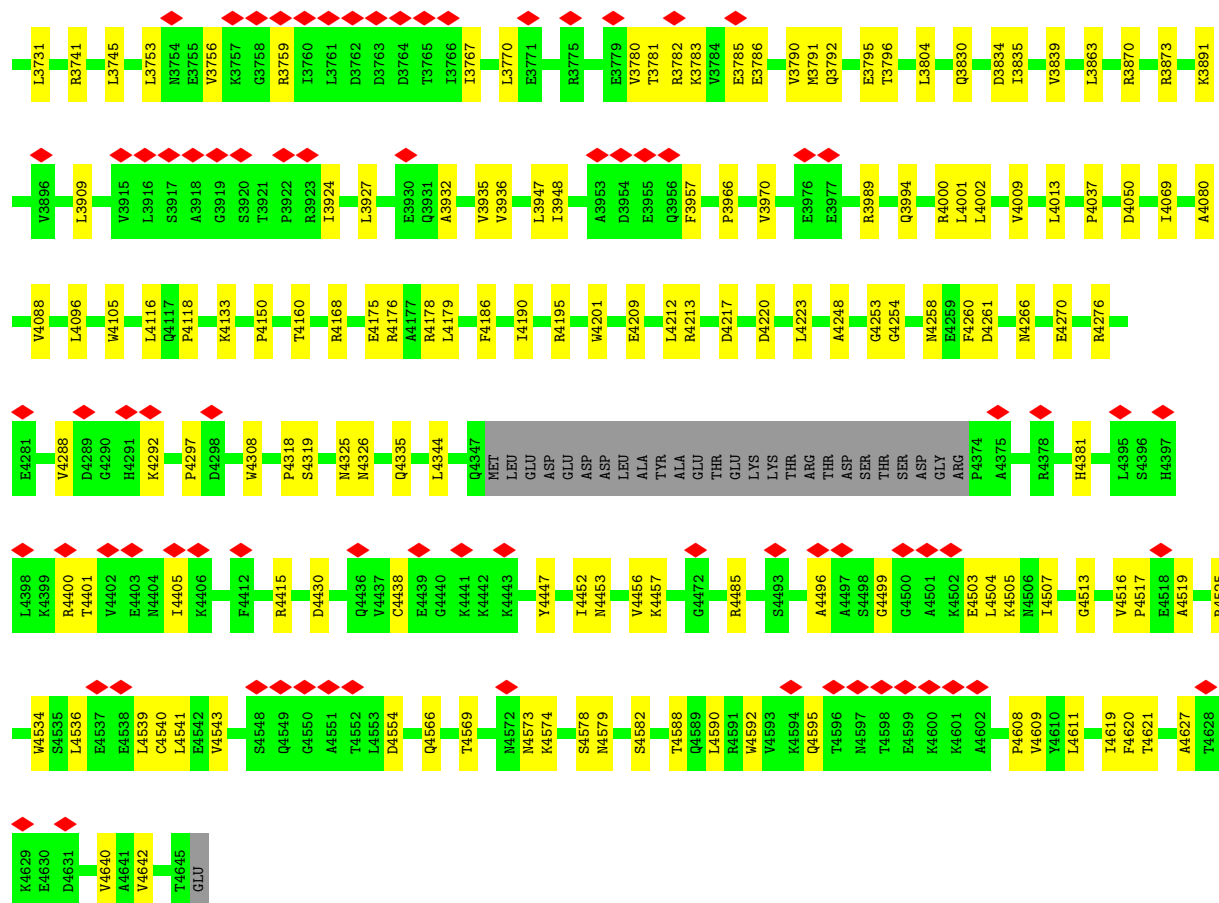
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

- 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

M2012	Q1850	E1622	L1561	I1501	LYS	ALA	VAL	TRP	ARG	GLU	ALA	ASN	GLU	ASN	PHE
T2017	V1853	R1623	P1562	N1502	ASN	SER	ALA	GLU	PHE	PHE	GLN	LEU	LEU	LEU	PHE
G2024	L1854	F1626	V1563	S1503	ALA	THR	GLU	THR	PHE	THR	VAL	THR	ILE	ASP	GLN
D2030	Q1855	P1627	E1564	V1504	ILE	PHE	GLU	PRO	PRO	THR	GLN	MET	GLY	GLY	LYS
R2037	Q1856	R1628	T1565	S1505	VAL	GLN	LEU	VAL	SER	ILE	ARG	PRO	ASN	ASN	GLY
S2038	I1859	F1629	Q1566	A1506	LYS	ARG	ASP	THR	TRP	VAL	LYS	ASP	VAL	GLU	ILE
L2039	N1867	G1633	R1567	M1507	ASP	ARG	LEU	THR	SER	VAL	LYS	ASP	VAL	GLU	VAL
D2045	Y1868	D1634	F1568	K1508	VAL	LEU	LEU	THR	LEU	LEU	LYS	ASP	PRO	TYR	ASP
R2046	K1878	E1635	Q1569	L1509	VAL	GLY	VAL	ARG	ASP	GLU	THR	THR	ASN	ASN	ILE
Q2047	Q1881	D1636	S1570	M1510	VAL	TYR	TRP	PRO	ILE	LEU	ASP	PRO	PRO	VAL	VAL
L2048	T1882	L1638	I1571	P1511	GLN	MET	SER	GLU	ILE	GLU	ASP	GLU	ARG	ARG	GLU
T2049	P1883	E1639	T1572	Y1512	GLY	LYS	GLU	GLU	GLU	GLU	ASN	GLU	ILE	LEU	GLY
L2050	L1884	I1640	E1573	K1513	ASN	ASN	SER	LEU	GLY	SER	THR	TYR	GLY	ALA	ILE
A2050	T1885	N1643	E1574	Y1514	MET	LEU	VAL	ALA	GLY	TRP	THR	ALA	CYS	GLY	ASP
Q2051	D1886	S1644	F1575	K1514	LEU	VAL	TRP	LEU	ALA	GLY	ASP	VAL	ARG	LEU	LEU
V2052	Y1889	K1645	L1576	V1515	ILE	VAL	TRP	LEU	PHE	ALA	THR	VAL	TYR	ARG	GLU
M2053	A1895	F1649	M1579	F1516	E1460	GLU	GLU	THR	THR	GLY	ALA	VAL	LEU	ALA	VAL
E2063	P1904	H1653	K1581	E1517	E1461	LEU	GLN	ILE	ASN	GLY	PHE	GLY	LEU	ALA	VAL
V2064	P1907	I1664	V1582	E1518	F1462	GLU	ILE	THR	ASP	THR	THR	GLY	TRP	TRP	ARG
L2065	T1910	E1668	S1583	D1519	L1463	SER	GLN	GLY	ILE	SER	PRO	VAL	GLN	GLN	THR
A2066	G1911	S1671	K1584	E1524	R1467	ASP	TRP	LYS	ALA	GLU	TYR	VAL	GLY	LEU	GLY
L2067	K1912	I1676	S1585	D1525	E1468	ARG	VAL	ASP	ILE	VAL	LYS	VAL	VAL	LEU	LEU
K2068	T1913	R1679	P1586	K1526	V1469	HIS	TRP	SER	ASP	VAL	GLN	VAL	VAL	LEU	LEU
L2069	V1929	D1693	L1587	L1527	N1470	LYS	VAL	GLN	GLN	GLN	LYS	VAL	VAL	LEU	LEU
T2070	F1930	E1679	V1588	N1528	N1471	LEU	GLN	GLU	ARG	GLN	SER	LEU	ALA	GLY	MET
P2071	F1945	T1693	D1590	R1529	T1472	LEU	MET	CYS	CYS	VAL	VAL	LEU	VAL	GLN	TYR
K2074	V1946	M1699	V1591	T1530	Y1473	LYS	LYS	ALA	ALA	LYS	ASN	PRO	PRO	ASP	ASP
L2080	Q1950	E1700	L1592	M1531	E1474	ARG	LEU	ARG	LEU	LYS	LEU	ARG	ARG	MET	LEU
D2087	D1958	E1709	G1595	A1532	L1475	HIS	GLN	GLN	GLN	LYS	ASP	TRP	TRP	ASP	ASN
E2116	E1959	V1721	I1594	L1533	D1476	VAL	ASN	GLU	LYS	GLN	SER	ALA	ALA	GLN	GLN
E2117	R1962	V1724	Q1595	F1534	L1477	ASN	TRP	ALA	ILE	PHE	TRP	MET	PRO	LYS	LYS
A2121	I1978	E1738	Q1598	D1539	V1478	THR	ASP	LEU	VAL	GLU	THR	ARG	GLN	ALA	VAL
V2122	P1988	G1770	R1599	V1540	N1479	VAL	ALA	GLU	GLN	LYS	LYS	ALA	VAL	VAL	VAL
D2123	N1989	G1771	S1600	Q1541	Y1480	VAL	LEU	THR	GLU	GLU	GLU	SER	SER	SER	ASP
E2126	Y1990	L1601	L1601	R1542	C1484	SER	LEU	LEU	ASP	VAL	VAL	GLY	GLY	HIS	ASP
E2129	K1992	E1602	E1602	R1543	R1485	ILE	LYS	GLY	ARG	GLU	VAL	THR	THR	PRO	ASN
N2130	T1993	R1603	R1603	Y1544	L1486	THR	LEU	THR	VAL	LEU	LEU	GLY	GLY	GLY	LEU
L2131	S1994	L1604	A1605	Y1545	I1487	ASP	GLU	GLY	ALA	ALA	ALA	THR	THR	ASN	ASN
P2132	V2006	A1775	A1605	Y1546	R1488	VAL	LEU	GLU	ARG	LEU	LEU	ASP	GLU	LYS	LYS
E2133	D2011	L1792	D1606	L1547	G1489	ASP	GLN	ARG	LEU	LEU	LEU	ASN	GLU	ASN	PRO
Q2134		L1839	L1607	L1547	Y1490	THR	LEU	THR	GLY	VAL	THR	ASN	THR	GLY	LEU
L2136		R1843	L1608	E1548	Y1492	GLY	VAL	GLY	GLY	LYS	PHE	ARG	GLY	GLY	GLY
L2137		K1849	G1609	Q1549	D1492	ILE	THR	SER	ARG	LYS	GLN	GLY	THR	PRO	THR
L2138			K1610	F1551	L1493	THR	ASP	GLY	THR	LYS	GLN	GLY	GLY	ASN	VAL
			I1611	T1552	F1494	ASP	ALA	ALA	THR	LYS	THR	ASP	GLY	LYS	VAL
			Q1612	G1553	N1495	THR	ARG	SER	THR	LYS	THR	ASP	GLY	LYS	ILE
			K1613	S1554	K1496	VAL	LEU	GLU	ASP	LEU	LEU	ASN	GLY	ASN	PRO
			A1614	A1555	V1497	VAL	LEU	GLU	LEU	LEU	LEU	ASN	GLY	LYS	ILE
			E1617	D1556	K1498	ASP	GLN	ARG	LEU	LEU	LEU	LYS	THR	VAL	VAL
			Y1618	T1557	E1499	GLN	LEU	THR	THR	GLY	THR	TRP	TRP	TRP	HIS
			L1619	K1558	H1500	THR	TYR	VAL	ASP	GLN	GLN	GLN	GLN	GLN	GLN
			E1620	L1560											
			R1621												





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38237	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	1.456	Depositor
Minimum map value	-0.716	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.21	Depositor
Map size (Å)	329.984, 329.984, 329.984	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0312, 1.0312, 1.0312	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, 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	0.26	0/24093	0.48	0/32651

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2091	ARG	Sidechain
1	A	2358	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	23593	0	23659	324	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	81	0	36	2	0
3	A	31	0	12	4	0
4	A	2	0	0	4	0
All	All	23707	0	23707	324	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 7.

All (324) 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:1913:THR:HG1	4:A:4705:MG:MG	0.82	0.87
1:A:3127:PRO:HG3	1:A:3538:GLN:HG2	1.64	0.79
1:A:1959:GLU:HB3	1:A:1962:ARG:HD3	1.71	0.73
1:A:3178:ASP:OD2	1:A:3585:ARG:NE	2.22	0.72
1:A:2149:LEU:HD11	1:A:2157:LEU:HD13	1.72	0.72
1:A:2231:SER:OG	4:A:4706:MG:MG	1.33	0.70
1:A:1904:PRO:HG2	1:A:2017:THR:HG22	1.72	0.70
1:A:3782:ARG:NH1	1:A:3786:GLU:OE1	2.25	0.69
1:A:2760:PRO:HA	1:A:2763:ARG:HG3	1.75	0.68
1:A:3129:VAL:HG21	1:A:3149:PHE:HB2	1.75	0.68
1:A:1504:VAL:HG12	1:A:1508:LYS:HE3	1.77	0.67
1:A:4088:VAL:HG11	1:A:4116:LEU:HD21	1.77	0.67
1:A:3114:ASP:O	1:A:3140:ARG:NH2	2.29	0.65
1:A:3791:MET:O	1:A:3795:GLU:HG2	1.97	0.65
1:A:3499:GLN:O	1:A:3503:ILE:HG13	1.97	0.65
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.79	0.64
1:A:2320:ASP:OD1	1:A:2358:ARG:NE	2.31	0.64
1:A:2970:GLU:OE2	1:A:2970:GLU:N	2.29	0.64
1:A:1503:SER:O	1:A:1507:MET:HG2	1.97	0.64
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.31	0.63
1:A:3207:LYS:NZ	1:A:3756:VAL:O	2.32	0.63
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.81	0.62
1:A:2229:GLY:HA2	3:A:4702:ATP:O2A	2.00	0.62
1:A:3177:LEU:O	1:A:3181:ASN:ND2	2.32	0.62
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.33	0.62
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.28	0.62
1:A:4190:ILE:HD12	1:A:4201:TRP:HZ2	1.65	0.62
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.81	0.61
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	1.81	0.61
1:A:3597:THR:HG23	1:A:3634:LEU:HD21	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4266:ASN:O	1:A:4270:GLU:HG2	2.00	0.61
1:A:2449:LEU:HA	1:A:2453:ARG:HH21	1.65	0.60
1:A:4540:CYS:HB3	1:A:4595:GLN:HG2	1.83	0.60
1:A:1883:PRO:HD2	1:A:2045:ASP:OD2	2.02	0.60
1:A:3581:LYS:HE3	1:A:3582:ARG:HG3	1.82	0.60
1:A:1958:ASP:OD1	1:A:2017:THR:OG1	2.19	0.60
1:A:2316:ASN:O	1:A:2320:ASP:OD1	2.20	0.60
1:A:2621:ASN:OD1	1:A:3014:ASN:ND2	2.35	0.60
1:A:1850:GLN:HB3	1:A:1856:GLN:HG2	1.83	0.60
1:A:1962:ARG:NH2	1:A:2314:ASN:OD1	2.34	0.59
1:A:1913:THR:OG1	4:A:4705:MG:MG	1.42	0.59
1:A:2316:ASN:O	1:A:2320:ASP:CG	2.40	0.59
1:A:4525:ARG:NH2	1:A:4536:LEU:O	2.30	0.59
1:A:1521:LEU:O	1:A:1524:GLU:HG2	2.02	0.59
1:A:1930:PHE:HA	1:A:2326:THR:HG21	1.85	0.59
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.84	0.59
1:A:2172:ARG:NH1	1:A:2205:GLU:OE1	2.36	0.58
1:A:2138:ILE:HD11	1:A:2165:PHE:CG	2.38	0.58
1:A:2590:PRO:HA	1:A:2708:PHE:O	2.03	0.58
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.36	0.58
1:A:4541:LEU:HD11	1:A:4590:LEU:HB3	1.85	0.57
1:A:2138:ILE:HD12	1:A:2161:LEU:HD22	1.86	0.57
1:A:4496:ALA:HB2	1:A:4504:LEU:HD21	1.86	0.57
1:A:2080:LEU:O	1:A:4415:ARG:NH1	2.38	0.57
1:A:3970:VAL:HB	1:A:3989:ARG:HD3	1.87	0.57
1:A:2231:SER:HG	4:A:4706:MG:MG	1.10	0.57
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.86	0.57
1:A:2297:LYS:O	1:A:2338:ASN:ND2	2.36	0.56
1:A:4569:THR:HG23	1:A:4578:SER:HB2	1.87	0.56
1:A:3005:LEU:HD11	1:A:3078:ARG:HH11	1.71	0.56
1:A:4150:PRO:O	1:A:4195:ARG:NH2	2.38	0.56
1:A:1491:ASP:OD1	1:A:1492:ASP:N	2.38	0.56
1:A:3830:GLN:NE2	1:A:3834:ASP:OD1	2.37	0.56
1:A:2818:VAL:O	1:A:2822:ILE:HG12	2.06	0.56
1:A:3214:GLN:HG3	1:A:3759:ARG:HD2	1.87	0.55
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.88	0.55
1:A:2788:THR:HG22	1:A:2789:GLN:HG2	1.88	0.55
1:A:1978:ILE:HG23	1:A:2012:MET:HE1	1.88	0.55
1:A:3459:GLN:HA	1:A:3462:LYS:HD2	1.87	0.55
1:A:3558:GLU:HG3	1:A:3561:ARG:HH12	1.71	0.55
1:A:2773:MET:HG2	1:A:2825:TRP:HE1	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2457:SER:OG	1:A:2732:PRO:HB3	2.07	0.54
1:A:3486:ARG:NH1	1:A:3487:GLU:OE2	2.40	0.54
1:A:2942:GLY:HA2	2:A:4704:ADP:O1A	2.07	0.54
1:A:3932:ALA:O	1:A:3936:VAL:HG23	2.07	0.54
1:A:1671:SER:HB2	1:A:1693:THR:HG23	1.89	0.54
1:A:3559:ARG:O	1:A:3563:GLN:HG2	2.07	0.54
1:A:1512:TYR:O	1:A:1515:VAL:HG12	2.08	0.54
1:A:3655:ARG:HG2	1:A:3660:VAL:HG22	1.90	0.54
1:A:2174:GLU:OE1	1:A:2176:THR:OG1	2.27	0.53
1:A:4566:GLN:O	1:A:4640:VAL:HA	2.09	0.53
1:A:1561:LEU:O	1:A:1565:THR:OG1	2.20	0.53
1:A:2285:ARG:NH1	1:A:2331:GLU:OE2	2.30	0.53
1:A:2049:ILE:O	1:A:2053:MET:HG3	2.08	0.53
1:A:4574:LYS:HB3	1:A:4627:ALA:HB2	1.91	0.53
1:A:2498:ILE:HG23	1:A:2502:LEU:HD22	1.90	0.53
1:A:2557:VAL:O	1:A:2757:ARG:NH2	2.42	0.53
1:A:1623:ARG:NH2	1:A:1634:ASP:OD1	2.40	0.53
1:A:3017:VAL:HB	1:A:3020:LEU:HB2	1.91	0.52
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.91	0.52
1:A:2454:CYS:HB3	1:A:2502:LEU:HD12	1.92	0.52
1:A:2974:GLU:OE1	1:A:2977:ARG:NH1	2.43	0.52
1:A:3154:LEU:HG	1:A:3516:TYR:CD1	2.44	0.52
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.89	0.52
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.42	0.52
1:A:2688:GLU:OE1	1:A:2730:HIS:NE2	2.43	0.52
1:A:2967:TYR:OH	1:A:2975:ASP:OD2	2.24	0.52
1:A:3215:VAL:HG21	1:A:3479:LEU:HD11	1.91	0.52
1:A:1470:TRP:HE1	1:A:1500:HIS:HD1	1.57	0.52
1:A:2623:SER:OG	1:A:3006:GLU:OE1	2.28	0.52
1:A:4096:LEU:HD13	1:A:4105:TRP:HH2	1.75	0.52
1:A:1855:GLN:OE1	1:A:1867:ASN:ND2	2.43	0.52
1:A:2863:ARG:HG2	1:A:2863:ARG:HH11	1.75	0.52
1:A:4485:ARG:HG2	1:A:4513:GLY:HA2	1.92	0.51
1:A:1881:GLN:NE2	1:A:1886:ASP:OD1	2.43	0.51
1:A:2308:ASP:O	1:A:2312:VAL:HG12	2.09	0.51
1:A:2925:ILE:HG21	1:A:2933:LEU:HG	1.91	0.51
1:A:3176:TYR:O	1:A:3180:ILE:HG12	2.11	0.51
1:A:2905:LEU:HD11	1:A:3652:GLU:HB3	1.91	0.51
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	1.93	0.51
1:A:1907:PRO:HG2	1:A:1910:THR:HG21	1.93	0.51
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4525:ARG:HD3	1:A:4536:LEU:HD23	1.92	0.51
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.43	0.51
1:A:2039:LEU:HD12	1:A:4254:GLY:HA2	1.92	0.50
1:A:2452:LEU:HD11	3:A:4702:ATP:H4'	1.92	0.50
1:A:3650:ASN:HD21	1:A:3695:ARG:HH11	1.60	0.50
1:A:2050:ALA:O	1:A:2051:GLN:C	2.48	0.50
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.94	0.50
1:A:1946:VAL:HG22	1:A:2006:VAL:HG21	1.93	0.50
1:A:2784:PHE:HB2	1:A:2794:TYR:HE2	1.76	0.49
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.12	0.49
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.95	0.49
1:A:2030:ASP:HB2	1:A:4050:ASP:HB2	1.94	0.49
1:A:1507:MET:O	1:A:1513:TYR:HB2	2.12	0.49
1:A:1587:LEU:HB3	1:A:1590:ASP:HB2	1.94	0.49
1:A:2257:LYS:NZ	1:A:2308:ASP:OD2	2.45	0.49
1:A:2388:ASP:OD1	1:A:2389:GLU:N	2.46	0.49
1:A:2581:LEU:HD11	1:A:2593:LEU:HD21	1.93	0.49
1:A:2980:LEU:HB3	1:A:3054:PHE:HZ	1.76	0.49
1:A:4503:GLU:O	1:A:4507:ILE:HG23	2.13	0.49
1:A:2972:PHE:HB2	1:A:3004:PHE:HE1	1.77	0.49
1:A:3127:PRO:HG2	1:A:3539:ALA:HB2	1.95	0.49
1:A:3161:LEU:HD23	1:A:3168:THR:HG22	1.95	0.49
1:A:3741:ARG:HD3	1:A:3745:LEU:HG	1.95	0.49
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.95	0.49
1:A:2068:LYS:NZ	1:A:2164:VAL:O	2.43	0.49
1:A:2087:ASP:O	1:A:2148:LYS:NZ	2.45	0.48
1:A:2132:PRO:HB2	1:A:2135:GLU:HB2	1.94	0.48
1:A:2290:SER:HB2	1:A:2295:LEU:HG	1.95	0.48
1:A:2956:LEU:HD22	1:A:2989:LYS:HB3	1.95	0.48
1:A:3100:GLU:OE1	1:A:3132:LYS:NZ	2.45	0.48
1:A:3935:VAL:HG13	1:A:3947:LEU:HD23	1.94	0.48
1:A:1664:ILE:HG22	1:A:1676:ILE:HG22	1.95	0.48
1:A:2354:ALA:O	1:A:2358:ARG:HD2	2.13	0.48
1:A:3927:LEU:HD11	1:A:3957:PHE:HE2	1.77	0.48
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.96	0.48
1:A:4453:ASN:O	1:A:4457:LYS:HG2	2.13	0.48
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.46	0.47
1:A:2972:PHE:HB2	1:A:3004:PHE:CE1	2.49	0.47
1:A:3109:PHE:CD2	1:A:3180:ILE:HG22	2.49	0.47
1:A:3624:GLU:HG3	1:A:3669:ILE:HD13	1.95	0.47
1:A:4176:ARG:NH1	1:A:4220:ASP:OD1	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1619:LEU:HD11	1:A:1638:LEU:HG	1.96	0.47
1:A:3716:VAL:HG21	1:A:3804:LEU:HD23	1.96	0.47
1:A:2892:TYR:HE2	1:A:2953:MET:HE1	1.80	0.47
1:A:2492:ARG:HG2	1:A:2545:TRP:NE1	2.30	0.47
1:A:3239:LYS:HB3	1:A:3451:TYR:CD1	2.49	0.47
1:A:3727:LYS:O	1:A:3731:LEU:HD13	2.14	0.47
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.97	0.47
1:A:4179:LEU:HD12	1:A:4223:LEU:HD22	1.96	0.47
1:A:4499:GLY:HA3	1:A:4503:GLU:HG3	1.97	0.47
1:A:1882:THR:HG22	1:A:2048:LEU:HD23	1.97	0.47
1:A:3471:LYS:HG3	1:A:3474:ARG:HH21	1.80	0.47
1:A:3741:ARG:HD3	1:A:3741:ARG:O	2.15	0.47
1:A:3514:ILE:HD11	1:A:3553:LEU:HD22	1.97	0.47
1:A:2751:PHE:HB3	1:A:2803:VAL:HG11	1.97	0.46
1:A:4517:PRO:HG2	1:A:4619:ILE:HD12	1.97	0.46
1:A:1895:ALA:HB2	1:A:2037:ARG:HB2	1.97	0.46
1:A:2063:GLU:O	1:A:2067:ASN:ND2	2.48	0.46
1:A:2912:PHE:CE2	1:A:2914:GLU:HB2	2.50	0.46
1:A:4400:ARG:HD2	1:A:4405:ILE:HD11	1.97	0.46
1:A:3753:LEU:HD21	1:A:3770:LEU:HD11	1.96	0.46
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	1.96	0.46
1:A:3721:ARG:HE	1:A:3724:VAL:HG21	1.80	0.46
1:A:2452:LEU:HD13	1:A:2729:ARG:HE	1.80	0.46
1:A:1606:ASP:O	1:A:1610:LYS:HG3	2.16	0.46
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.98	0.46
1:A:1508:LYS:NZ	1:A:1524:GLU:OE1	2.28	0.46
1:A:1853:VAL:HA	1:A:1856:GLN:HG3	1.98	0.46
1:A:2912:PHE:HE2	1:A:2914:GLU:HB2	1.80	0.46
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.16	0.46
1:A:3013:ALA:HA	1:A:3088:ARG:HG3	1.98	0.45
1:A:2134:GLN:O	1:A:2138:ILE:HG12	2.16	0.45
1:A:3627:LEU:HD12	1:A:3664:LEU:HD22	1.97	0.45
1:A:2224:GLY:O	1:A:2346:GLN:HA	2.15	0.45
1:A:3133:LEU:HD11	1:A:3141:GLU:HB3	1.97	0.45
1:A:2776:PHE:HZ	1:A:2846:THR:HG23	1.82	0.45
1:A:3154:LEU:HD21	1:A:3532:TRP:HZ2	1.81	0.45
1:A:2892:TYR:CE2	1:A:2953:MET:HE1	2.51	0.45
1:A:2894:LYS:O	1:A:2898:LYS:HG3	2.16	0.45
1:A:3150:VAL:O	1:A:3154:LEU:HD23	2.17	0.45
1:A:3211:THR:O	1:A:3215:VAL:HG13	2.17	0.45
1:A:1878:LYS:HB3	1:A:1878:LYS:HE3	1.61	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3891:LYS:HD2	1:A:4013:LEU:HD23	1.98	0.45
1:A:2665:GLU:HB3	1:A:2668:LEU:HD12	1.98	0.45
1:A:3588:LEU:HD11	1:A:3638:VAL:HG11	1.98	0.45
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.99	0.45
1:A:4186:PHE:O	1:A:4190:ILE:HG12	2.17	0.44
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.53	0.44
1:A:3239:LYS:HB3	1:A:3451:TYR:CE1	2.52	0.44
1:A:3873:ARG:HD3	1:A:3873:ARG:HA	1.83	0.44
1:A:3731:LEU:HD21	1:A:3790:VAL:HG12	1.99	0.44
1:A:3783:LYS:O	1:A:3786:GLU:HG2	2.17	0.44
1:A:4209:GLU:O	1:A:4213:ARG:HG3	2.17	0.44
1:A:1699:ASN:OD1	1:A:1700:GLU:N	2.50	0.44
1:A:1907:PRO:HG2	1:A:1910:THR:CG2	2.48	0.44
1:A:3644:VAL:HG22	1:A:3664:LEU:HD12	1.99	0.44
1:A:3780:VAL:HA	1:A:3783:LYS:HD2	2.00	0.44
1:A:2211:TYR:O	1:A:2214:THR:OG1	2.30	0.44
1:A:3478:LEU:HD11	1:A:3767:ILE:HG23	2.00	0.44
1:A:1598:GLN:O	1:A:1602:GLU:HG3	2.18	0.44
1:A:3229:LEU:HD11	1:A:3462:LYS:HG3	1.99	0.44
1:A:3457:GLU:O	1:A:3461:ILE:HG12	2.17	0.44
1:A:4175:GLU:OE1	1:A:4175:GLU:N	2.50	0.44
1:A:4516:VAL:HG12	1:A:4519:ALA:H	1.83	0.44
1:A:2245:GLU:OE1	1:A:2298:ARG:NH2	2.43	0.44
1:A:2275:TRP:NE1	1:A:2277:ASP:OD1	2.43	0.44
1:A:2694:ARG:O	1:A:2698:GLN:N	2.51	0.44
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.99	0.44
1:A:2671:MET:HG2	1:A:2675:GLY:HA2	1.99	0.44
1:A:3127:PRO:O	1:A:3145:ASN:ND2	2.51	0.44
1:A:3477:ALA:O	1:A:3480:LYS:HG3	2.18	0.44
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	1.99	0.44
1:A:2694:ARG:HG3	1:A:2701:VAL:HG21	2.00	0.43
1:A:3039:LYS:HB3	1:A:3039:LYS:HE3	1.74	0.43
1:A:3692:LEU:O	1:A:3696:VAL:HG22	2.18	0.43
1:A:3792:GLN:O	1:A:3796:THR:HG23	2.19	0.43
1:A:3924:ILE:HG12	1:A:3948:ILE:HG23	1.99	0.43
1:A:4069:ILE:HD13	1:A:4080:ALA:HA	1.99	0.43
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.51	0.43
1:A:1885:THR:O	1:A:1889:TYR:CD1	2.70	0.43
1:A:2773:MET:HG2	1:A:2825:TRP:NE1	2.33	0.43
1:A:4430:ASP:OD2	1:A:4447:TYR:OH	2.36	0.43
1:A:2413:LEU:HD12	1:A:2413:LEU:HA	1.89	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.53	0.43
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	1.99	0.43
1:A:4566:GLN:OE1	1:A:4582:SER:OG	2.26	0.43
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.53	0.43
1:A:3781:THR:O	1:A:3785:GLU:OE1	2.36	0.43
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.51	0.43
1:A:3741:ARG:HG3	1:A:3780:VAL:HG21	2.01	0.43
1:A:2369:LEU:HD21	3:A:4702:ATP:O4'	2.18	0.43
1:A:3568:PRO:HG2	1:A:3573:CYS:SG	2.59	0.43
1:A:2065:LEU:HD22	1:A:2137:LEU:HD22	2.01	0.43
1:A:2074:LYS:HE2	1:A:2074:LYS:HB3	1.75	0.43
1:A:2571:THR:H	1:A:2574:THR:HB	1.84	0.43
1:A:3238:ASP:HA	1:A:3241:LYS:HD2	2.00	0.43
1:A:1547:LEU:HD12	1:A:1608:LEU:HD22	2.01	0.43
1:A:2012:MET:HE3	1:A:2012:MET:HB3	1.93	0.43
1:A:4452:ILE:O	1:A:4456:VAL:HG23	2.19	0.42
1:A:2901:TYR:CZ	1:A:2908:PRO:HA	2.54	0.42
1:A:3024:ASP:N	1:A:3024:ASP:OD1	2.51	0.42
1:A:3114:ASP:O	1:A:3116:GLU:HG2	2.19	0.42
1:A:3148:VAL:O	1:A:3152:GLN:HG3	2.20	0.42
1:A:3741:ARG:HH11	1:A:3745:LEU:HD21	1.84	0.42
1:A:3482:LEU:HD11	1:A:3770:LEU:HD13	2.00	0.42
1:A:4002:LEU:HD11	1:A:4335:GLN:HB3	2.01	0.42
1:A:1626:PHE:HB3	1:A:1629:PHE:CD2	2.54	0.42
1:A:4288:VAL:HG21	1:A:4292:LYS:HE2	2.01	0.42
1:A:4525:ARG:HG3	1:A:4592:TRP:CZ3	2.55	0.42
1:A:2867:MET:HB3	1:A:2869:ARG:HH21	1.85	0.42
1:A:3659:ARG:HE	1:A:3661:LEU:HD21	1.84	0.42
1:A:1477:LEU:HB3	1:A:1485:ARG:HB3	2.01	0.42
1:A:1547:LEU:HD23	1:A:1547:LEU:HA	1.89	0.42
1:A:2387:LEU:N	1:A:2416:GLN:OE1	2.47	0.42
1:A:2633:LYS:HD2	1:A:3019:GLY:HA3	2.02	0.42
1:A:3010:THR:HG21	1:A:3018:PRO:HD3	2.01	0.42
1:A:3207:LYS:HD3	1:A:3207:LYS:HA	1.84	0.42
1:A:3546:ASP:OD1	1:A:3546:ASP:N	2.52	0.42
1:A:1521:LEU:HD23	1:A:1521:LEU:HA	1.91	0.42
1:A:1738:TYR:HE2	1:A:1792:LEU:HD21	1.85	0.42
1:A:1945:PHE:HB3	1:A:1978:ILE:HD11	2.01	0.42
1:A:3786:GLU:O	1:A:3790:VAL:HG23	2.20	0.42
1:A:1619:LEU:HD21	1:A:1638:LEU:HD23	2.01	0.41
1:A:1859:ILE:HD11	1:A:1868:TYR:HD1	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2374:ILE:HD13	1:A:2452:LEU:HD21	2.01	0.41
1:A:2697:ASP:OD1	1:A:2697:ASP:N	2.53	0.41
1:A:3558:GLU:OE2	1:A:3581:LYS:HD3	2.19	0.41
1:A:1543:ARG:HA	1:A:1546:TYR:CE2	2.55	0.41
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.55	0.41
1:A:4297:PRO:HG3	1:A:4308:TRP:CD2	2.55	0.41
1:A:2307:VAL:HA	1:A:2311:TRP:HE1	1.84	0.41
1:A:2688:GLU:HB2	1:A:2730:HIS:CE1	2.54	0.41
1:A:2945:THR:OG1	2:A:4704:ADP:O1A	2.26	0.41
1:A:4190:ILE:HD12	1:A:4201:TRP:CZ2	2.50	0.41
1:A:1538:ILE:HG23	1:A:1539:ASP:H	1.86	0.41
1:A:2490:ILE:HD13	1:A:2490:ILE:HA	1.93	0.41
1:A:3115:LEU:HD22	1:A:3143:ILE:HG13	2.03	0.41
1:A:2231:SER:HB2	3:A:4702:ATP:O1A	2.21	0.41
1:A:2615:MET:SD	1:A:2707:GLN:NE2	2.93	0.41
1:A:3909:LEU:HB3	1:A:4344:LEU:HD13	2.02	0.41
1:A:4248:ALA:O	1:A:4253:GLY:HA3	2.21	0.41
1:A:4288:VAL:O	1:A:4319:SER:OG	2.27	0.41
1:A:4401:THR:O	1:A:4405:ILE:HG12	2.20	0.41
1:A:4276:ARG:HA	1:A:4276:ARG:HE	1.84	0.41
1:A:4260:PHE:CE2	1:A:4608:PRO:HB3	2.56	0.41
1:A:1493:LEU:HD21	1:A:1534:PHE:CD2	2.55	0.41
1:A:1884:LEU:HG	1:A:1884:LEU:O	2.20	0.41
1:A:1912:LYS:HB2	1:A:1912:LYS:HE3	1.57	0.41
1:A:1929:VAL:H	1:A:2332:ARG:HH21	1.69	0.41
1:A:2268:LEU:HD12	1:A:2268:LEU:HA	1.94	0.41
1:A:3731:LEU:HD21	1:A:3790:VAL:CG1	2.51	0.41
1:A:4258:ASN:HB3	1:A:4261:ASP:HB2	2.02	0.41
1:A:4260:PHE:HZ	1:A:4621:THR:HG22	1.86	0.41
1:A:4543:VAL:HG13	1:A:4588:THR:HG23	2.02	0.41
1:A:1640:ILE:HD11	1:A:1653:HIS:HB3	2.03	0.41
1:A:2413:LEU:O	1:A:2417:ARG:HG3	2.21	0.41
1:A:3003:GLY:O	1:A:3007:ARG:HG3	2.21	0.41
1:A:1459:LEU:HD23	1:A:1507:MET:HB3	2.03	0.40
1:A:4619:ILE:HG22	1:A:4620:PHE:HD1	1.86	0.40
1:A:2446:ILE:HD12	1:A:2446:ILE:HA	1.93	0.40
1:A:2548:TRP:CD1	1:A:2576:ARG:HG2	2.56	0.40
1:A:2629:GLU:OE1	1:A:2633:LYS:HE3	2.21	0.40
1:A:3182:HIS:NE2	1:A:3582:ARG:O	2.46	0.40
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	2.03	0.40
1:A:4133:LYS:HB2	1:A:4133:LYS:HE2	1.81	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3225:LYS:HZ1	1:A:3464:ASP:HB3	1.86	0.40
1:A:2668:LEU:HD23	1:A:2668:LEU:HA	1.96	0.40
1:A:2894:LYS:HG3	1:A:2911:LEU:HD12	2.03	0.40
1:A:3028:THR:O	1:A:3032:GLN:HG3	2.21	0.40
1:A:3835:ILE:HG12	1:A:3870:ARG:HD2	2.04	0.40
1:A:4534:TRP:HE3	1:A:4539:LEU:HD21	1.86	0.40
1:A:3994:GLN:HB2	1:A:4001:LEU:HD13	2.02	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	2929/4646 (63%)	2879 (98%)	50 (2%)	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	2605/4125 (63%)	2602 (100%)	3 (0%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2047	GLN
1	A	3480	LYS
1	A	4573	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1855	GLN
1	A	1867	ASN

5.3.3 RNA [i](#)

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	$\# Z > 2$
2	ADP	A	4703	-	24,29,29	0.93	1 (4%)	29,45,45	0.79	1 (3%)
2	ADP	A	4701	4	24,29,29	0.80	1 (4%)	29,45,45	0.74	1 (3%)
2	ADP	A	4704	-	24,29,29	0.79	0	29,45,45	0.92	2 (6%)
3	ATP	A	4702	4	28,33,33	0.85	1 (3%)	34,52,52	0.87	1 (2%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4702	ATP	C1'-N9	-2.12	1.44	1.49
2	A	4703	ADP	C8-N7	-2.04	1.31	1.34
2	A	4701	ADP	C8-N7	-2.02	1.31	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	C5-C6-N6	2.49	124.11	120.31
2	A	4704	ADP	C5-C6-N6	2.28	123.78	120.31
2	A	4704	ADP	C4'-O4'-C1'	-2.25	107.86	109.92
2	A	4701	ADP	C5-C6-N6	2.24	123.72	120.31
3	A	4702	ATP	C5-C6-N6	2.24	123.72	120.31

There are no chirality outliers.

All (11) torsion outliers are listed below:

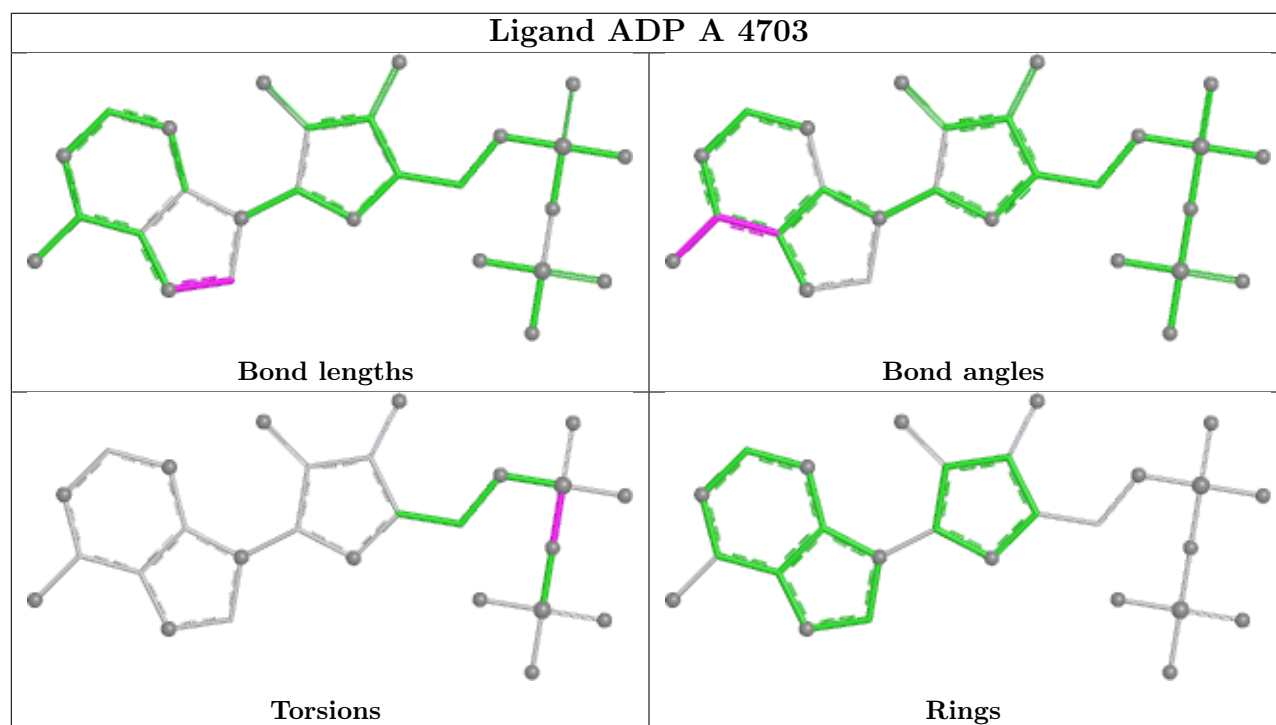
Mol	Chain	Res	Type	Atoms
2	A	4704	ADP	C5'-O5'-PA-O1A
3	A	4702	ATP	O4'-C4'-C5'-O5'
2	A	4704	ADP	O4'-C4'-C5'-O5'
2	A	4704	ADP	C3'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'
2	A	4703	ADP	PB-O3A-PA-O2A
2	A	4704	ADP	PB-O3A-PA-O2A
2	A	4704	ADP	PB-O3A-PA-O1A
3	A	4702	ATP	PA-O3A-PB-O1B
3	A	4702	ATP	PA-O3A-PB-O2B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

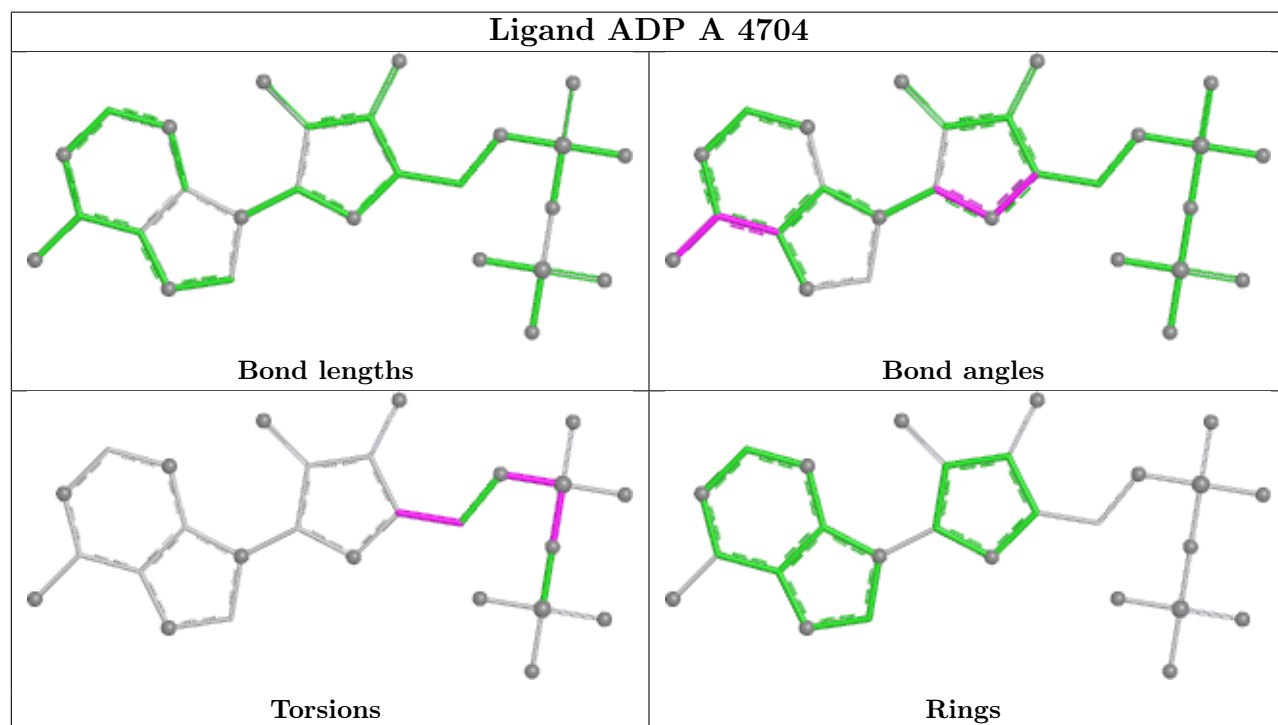
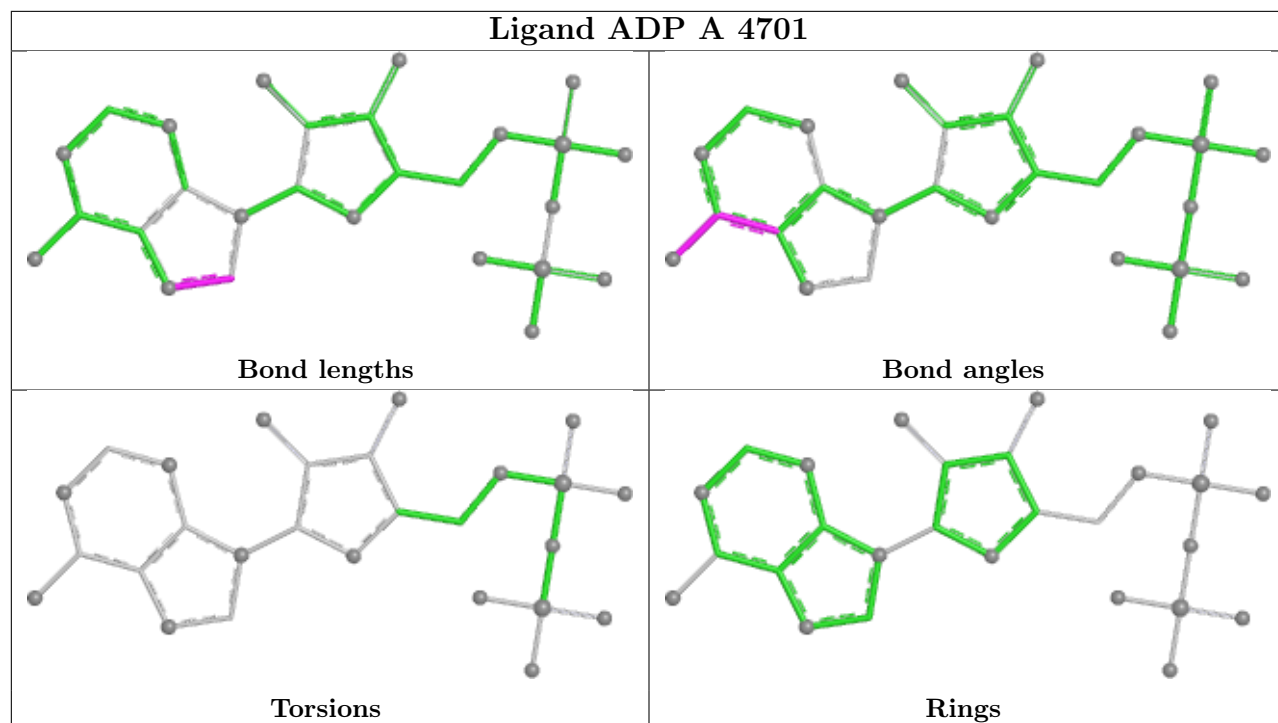
There are no ring outliers.

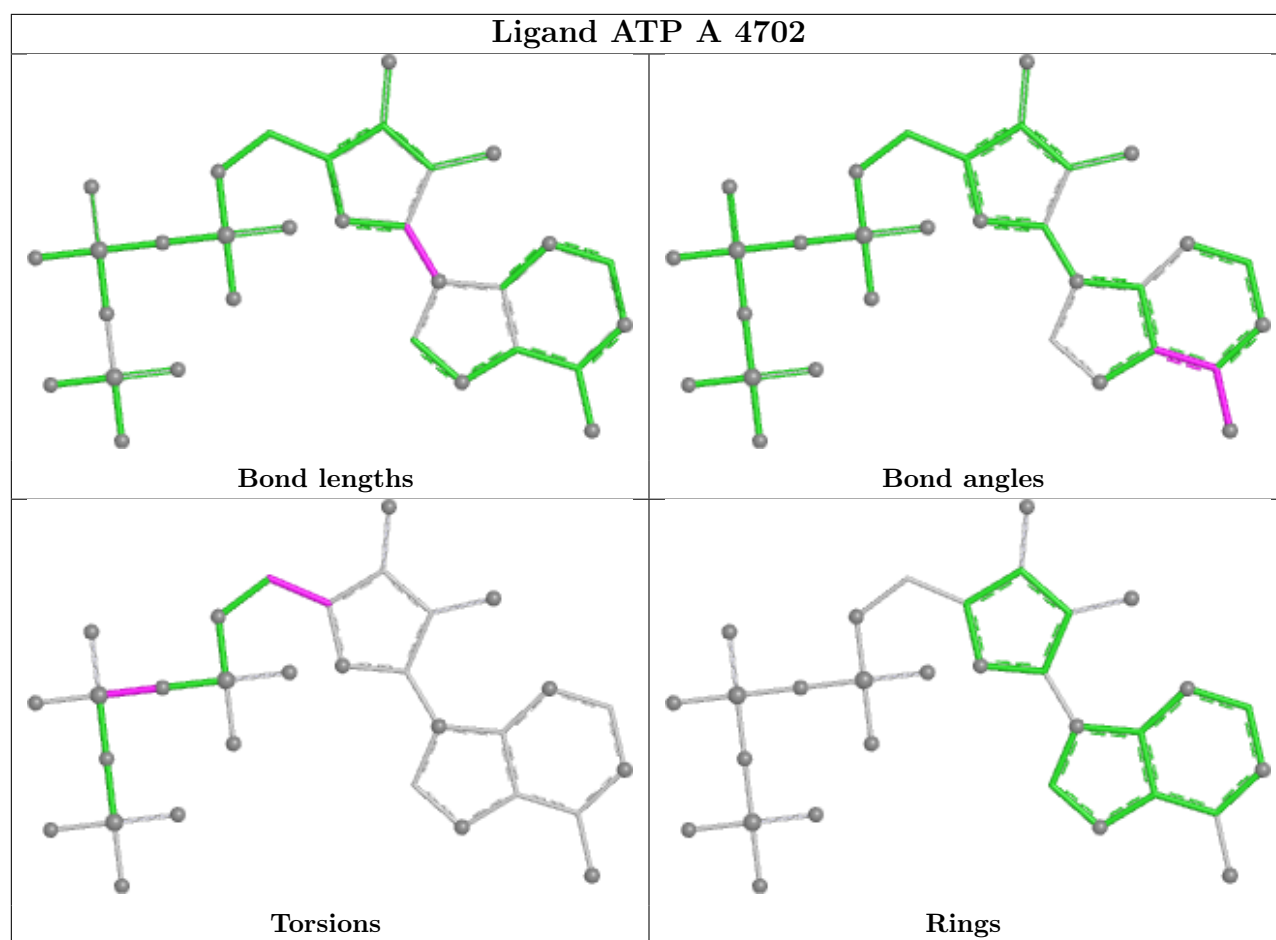
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4704	ADP	2	0
3	A	4702	ATP	4	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.

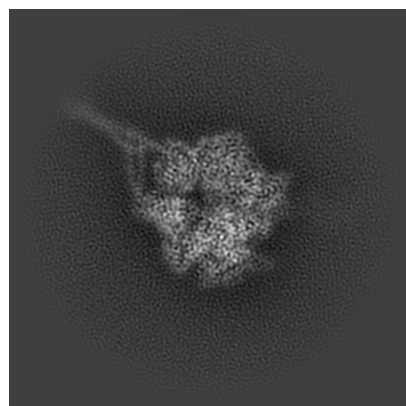
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44709. These allow visual inspection of the internal detail of the map and identification of artifacts.

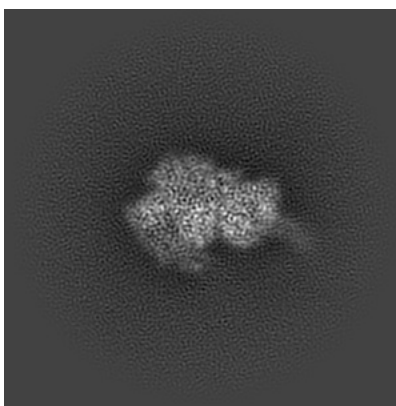
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

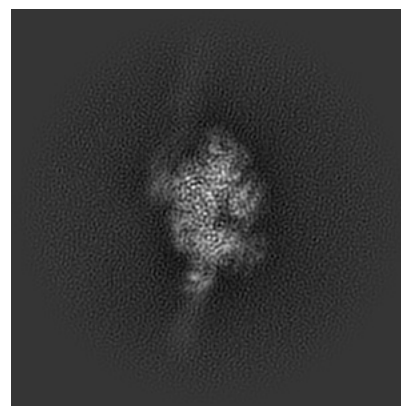
6.1.1 Primary map



X

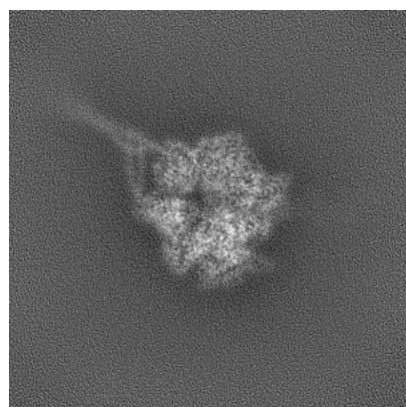


Y

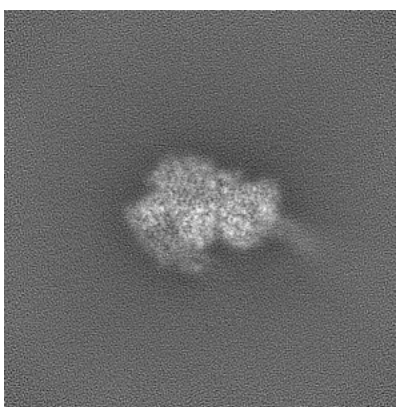


Z

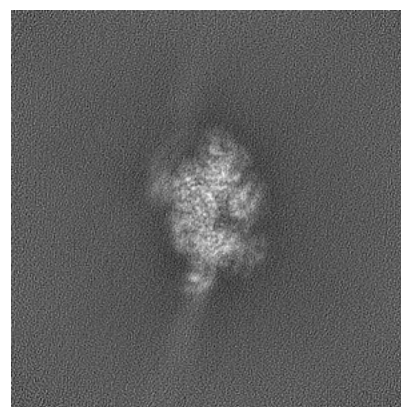
6.1.2 Raw map



X



Y

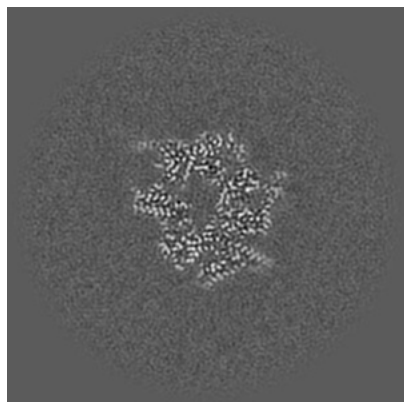


Z

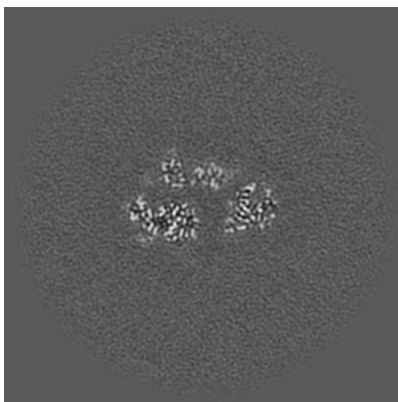
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

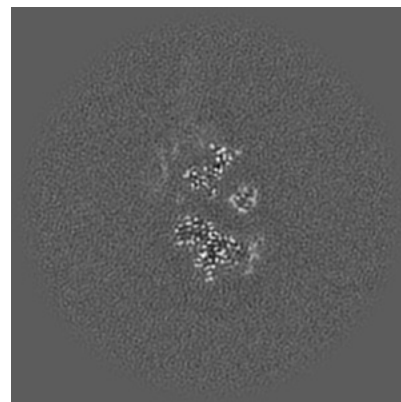
6.2.1 Primary map



X Index: 160

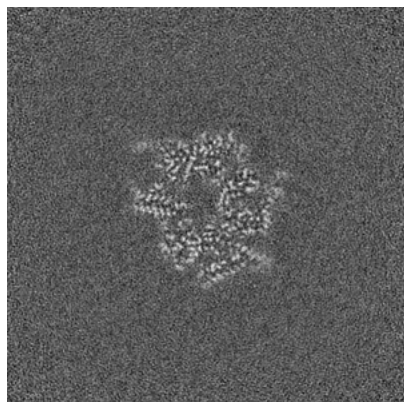


Y Index: 160

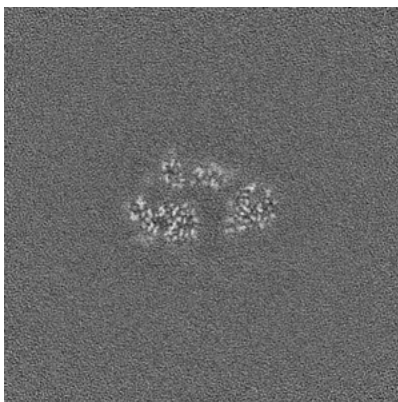


Z Index: 160

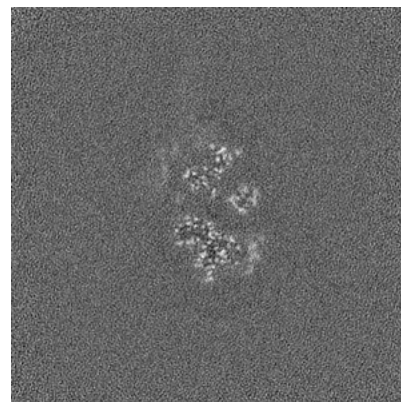
6.2.2 Raw map



X Index: 160



Y Index: 160

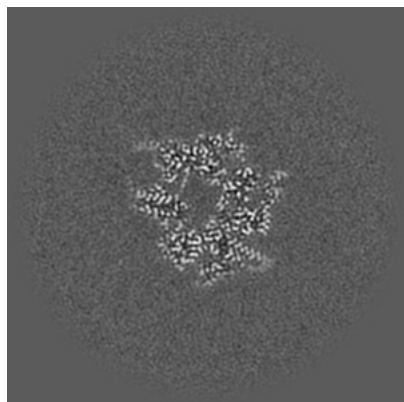


Z Index: 160

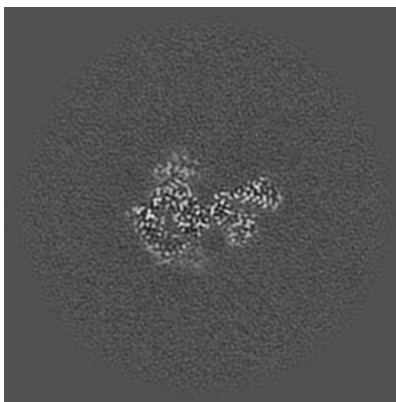
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

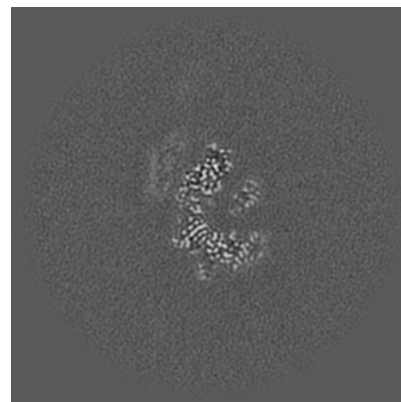
6.3.1 Primary map



X Index: 161

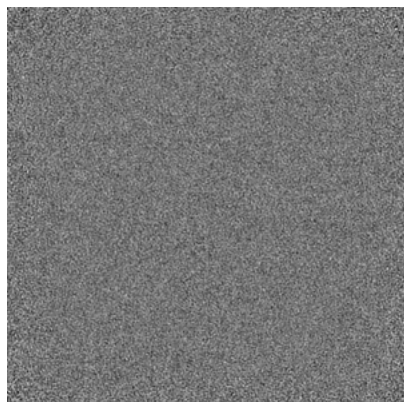


Y Index: 177

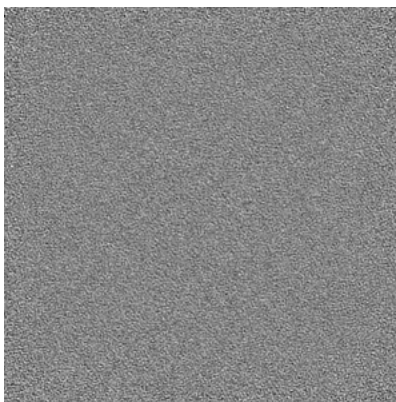


Z Index: 153

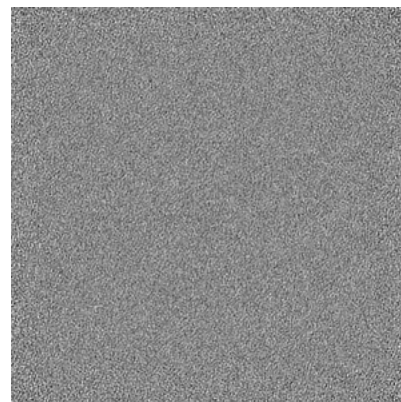
6.3.2 Raw map



X Index: 0



Y Index: 0

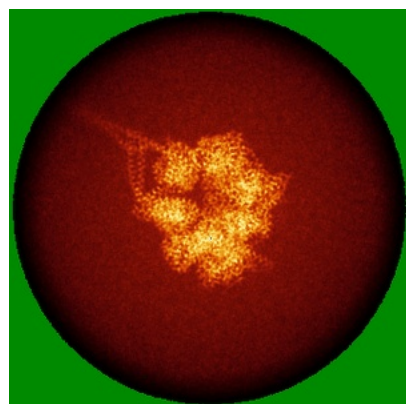


Z Index: 0

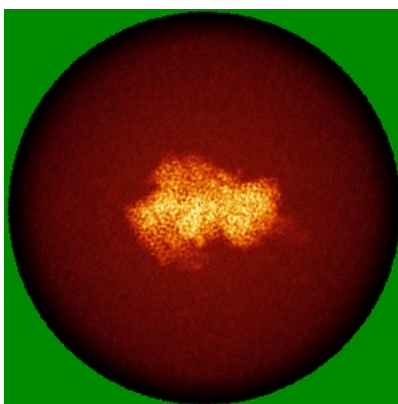
The images above show the largest variance slices of the map in three orthogonal directions.

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

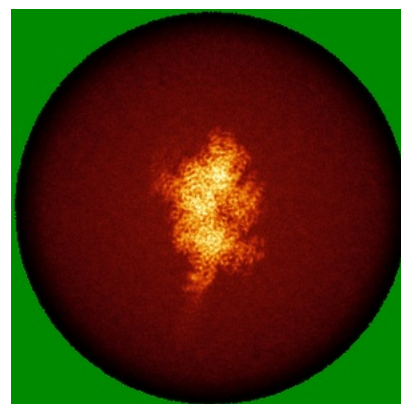
6.4.1 Primary map



X

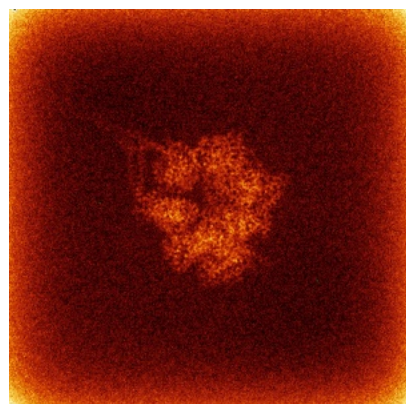


Y

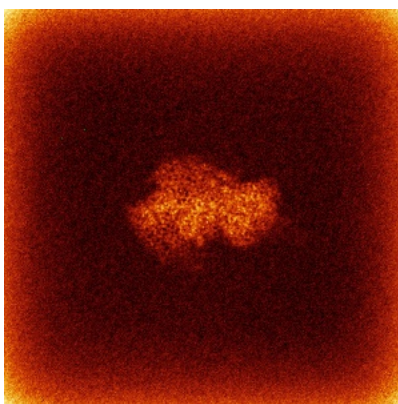


Z

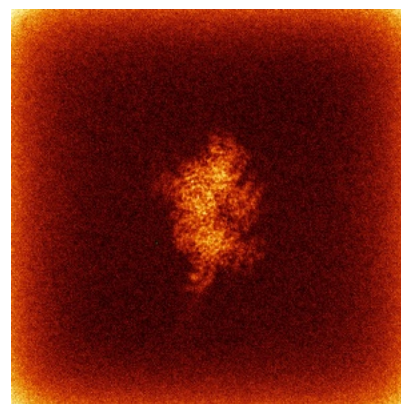
6.4.2 Raw map



X



Y

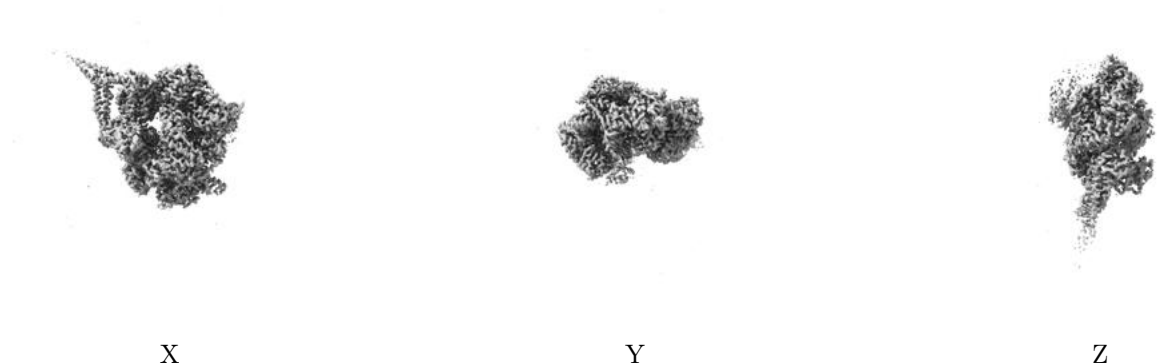


Z

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.

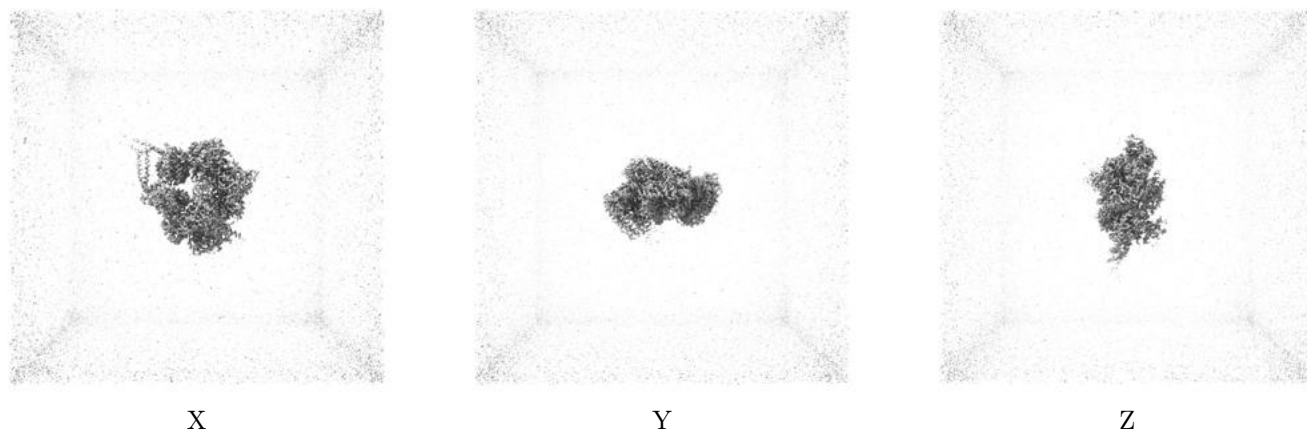
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.21. 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.

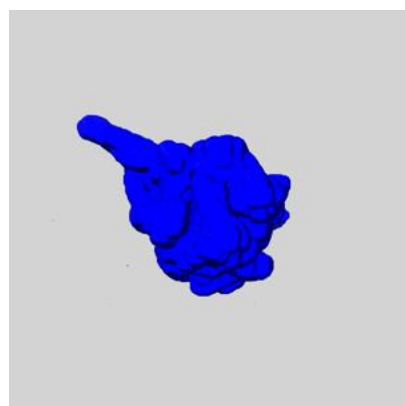
6.6 Mask visualisation [i](#)

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

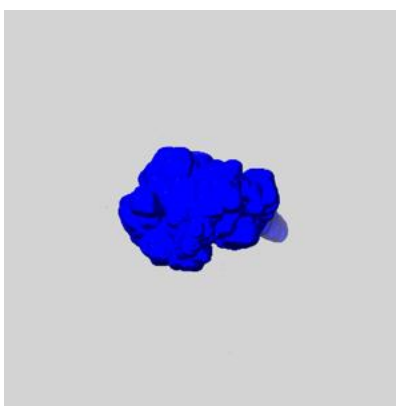
A mask typically either:

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

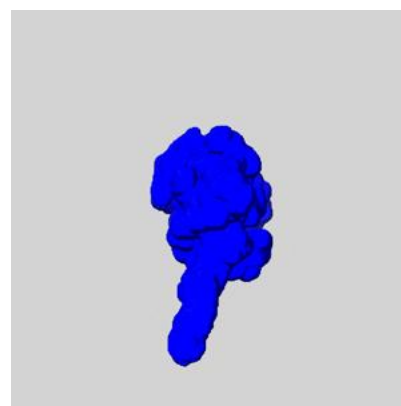
6.6.1 emd_44709_msk_1.map [i](#)



X



Y

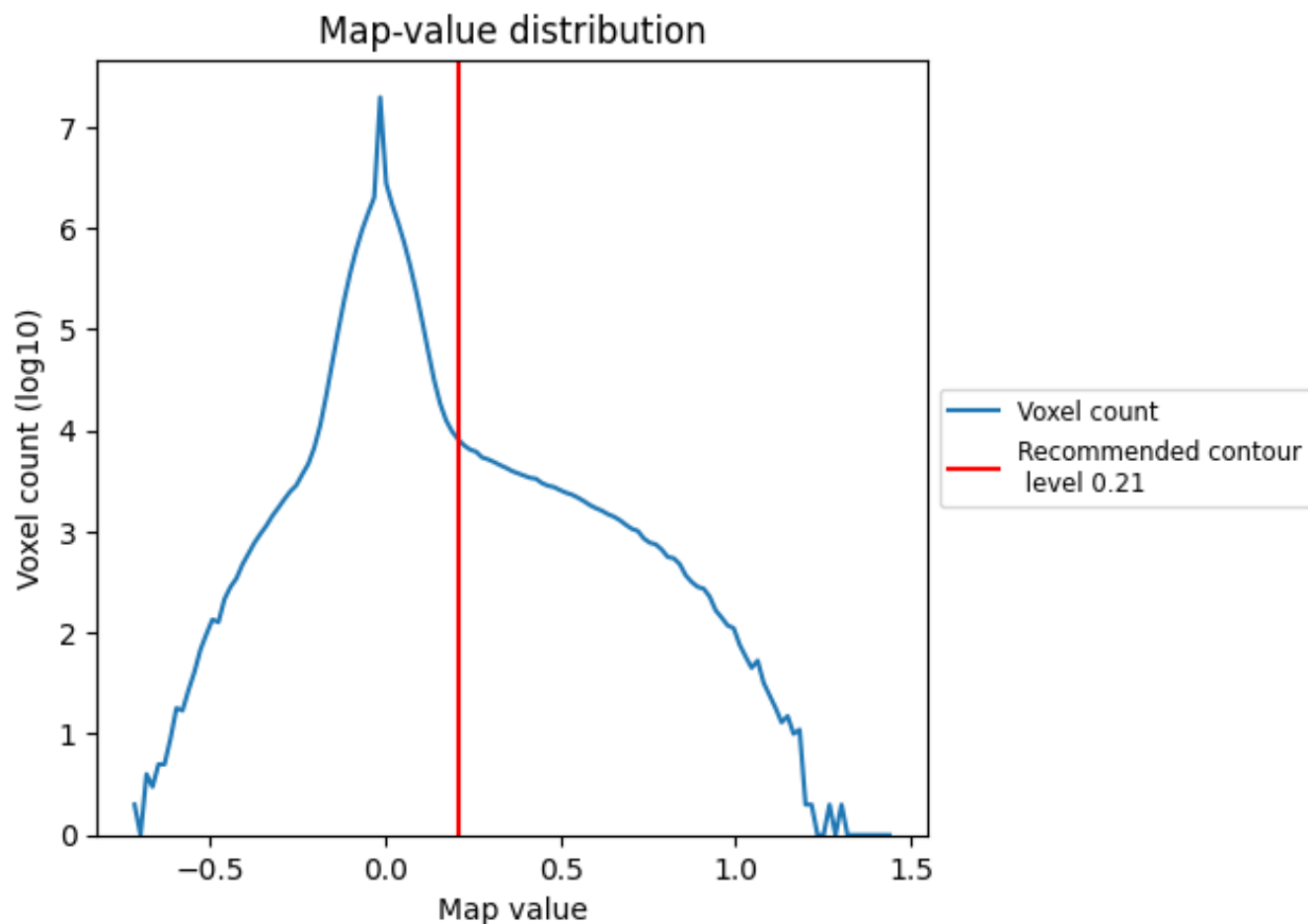


Z

7 Map analysis [i](#)

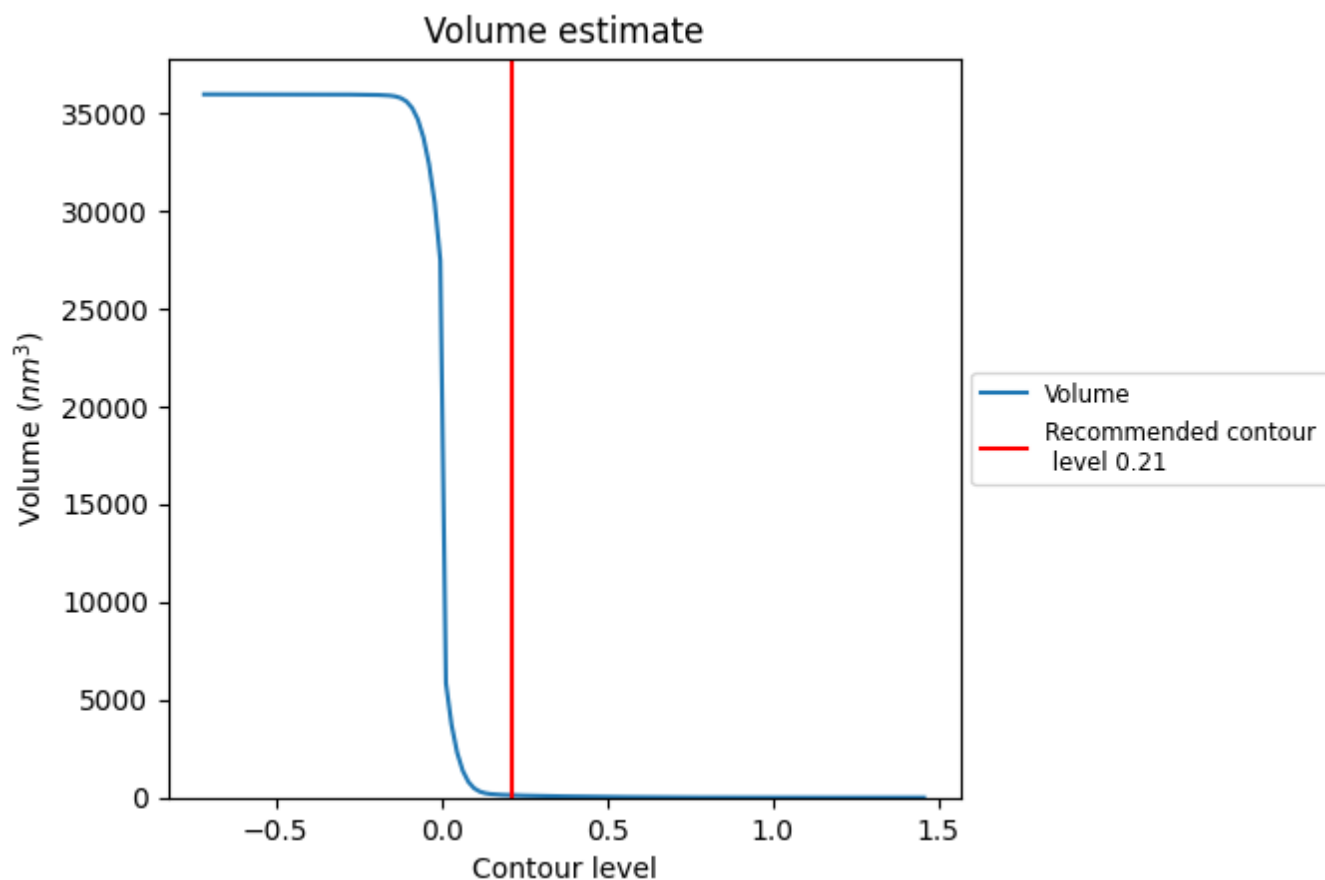
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

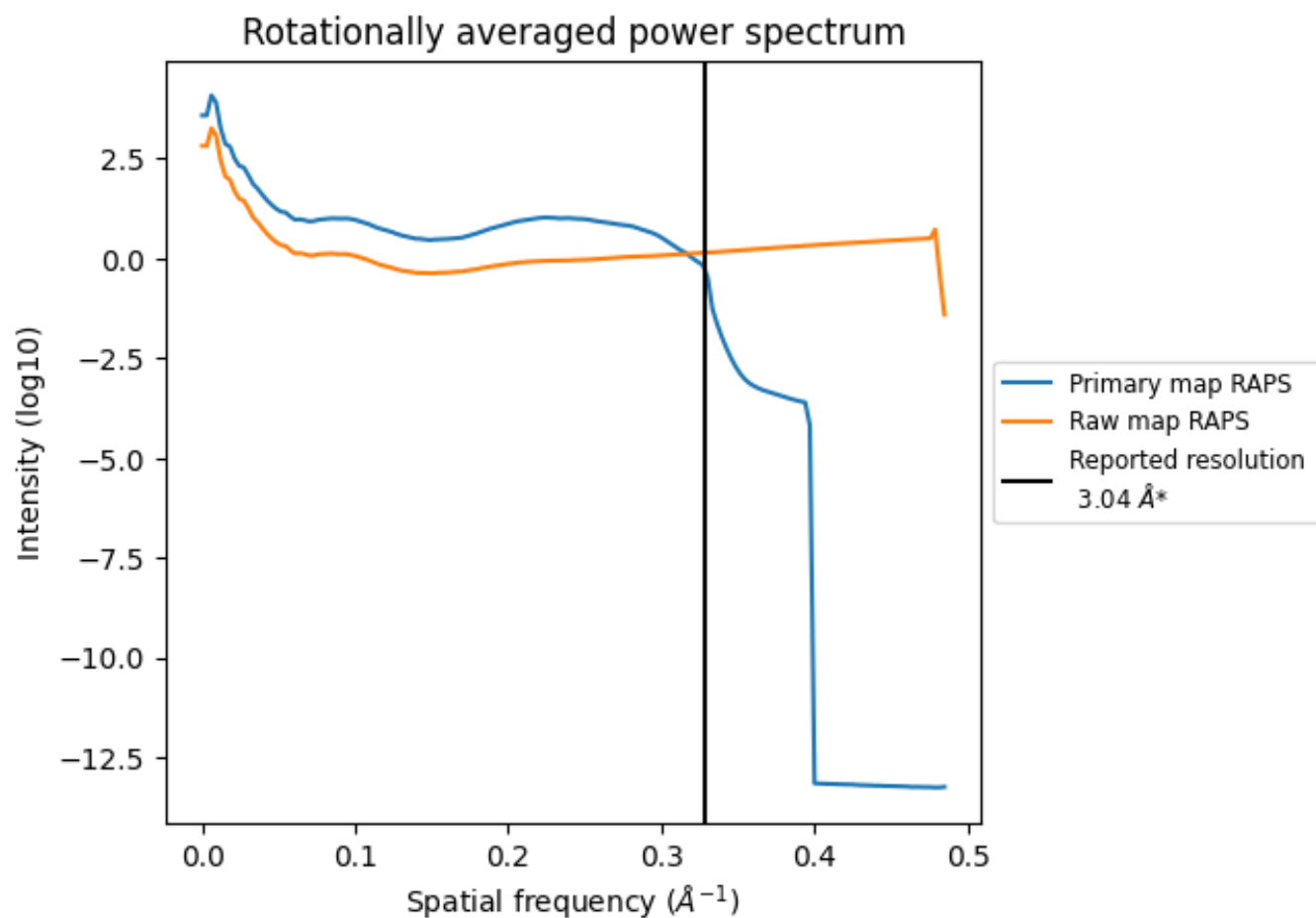
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 119 nm³; this corresponds to an approximate mass of 108 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 ⓘ

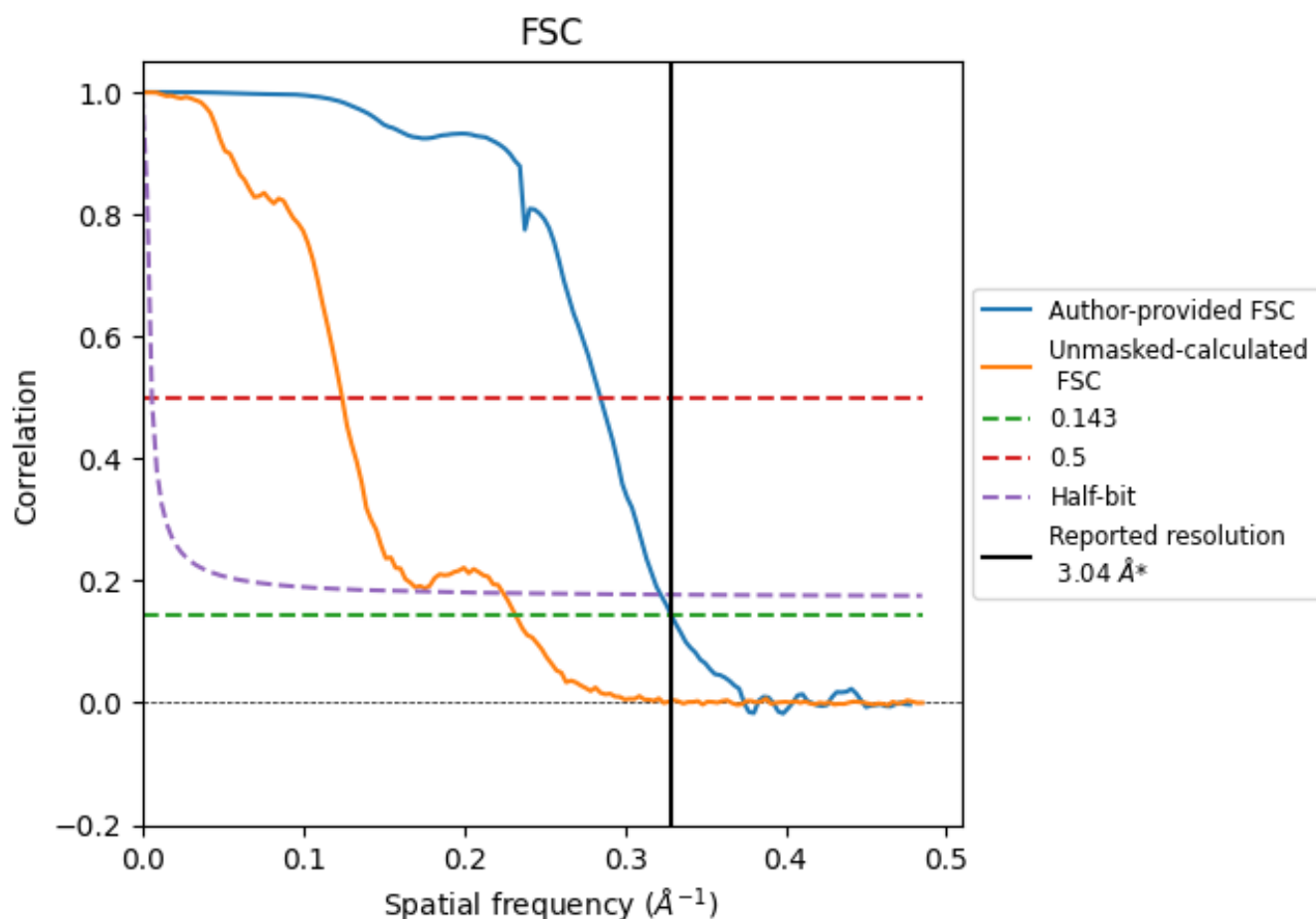


*Reported resolution corresponds to spatial frequency of 0.329 Å⁻¹

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 0.329 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

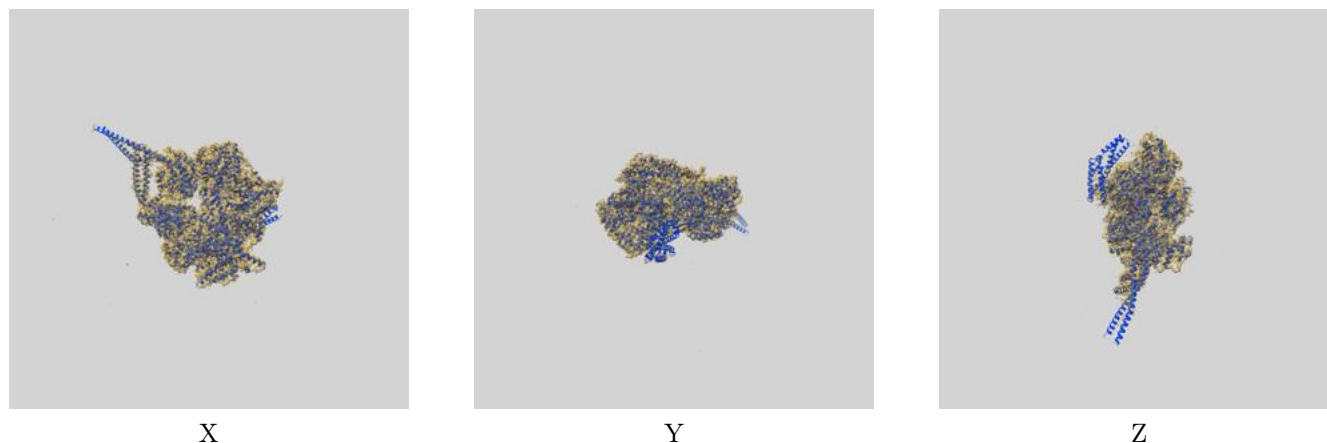
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.04	3.51	3.10
Unmasked-calculated*	4.31	8.05	4.46

*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 4.31 differs from the reported value 3.04 by more than 10 %

9 Map-model fit [i](#)

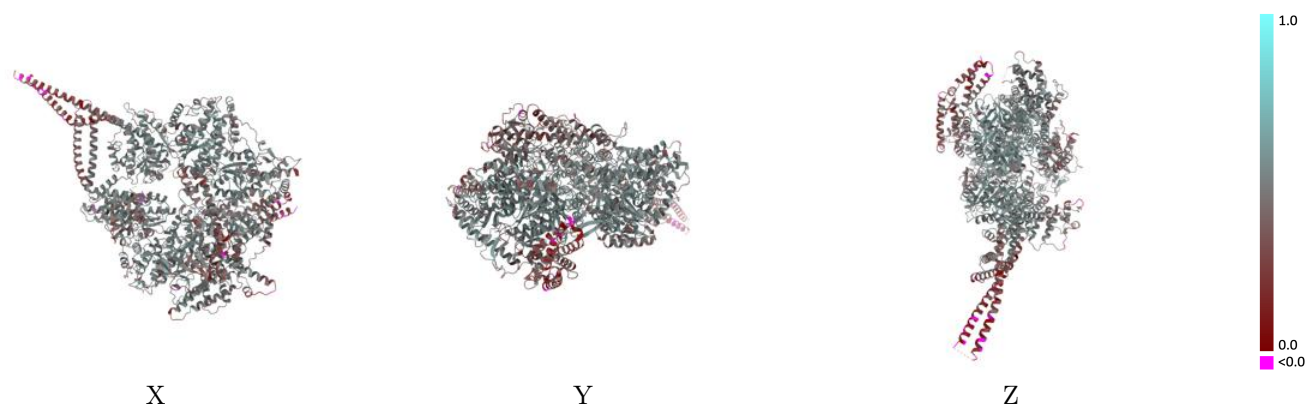
This section contains information regarding the fit between EMDB map EMD-44709 and PDB model 9BMS. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



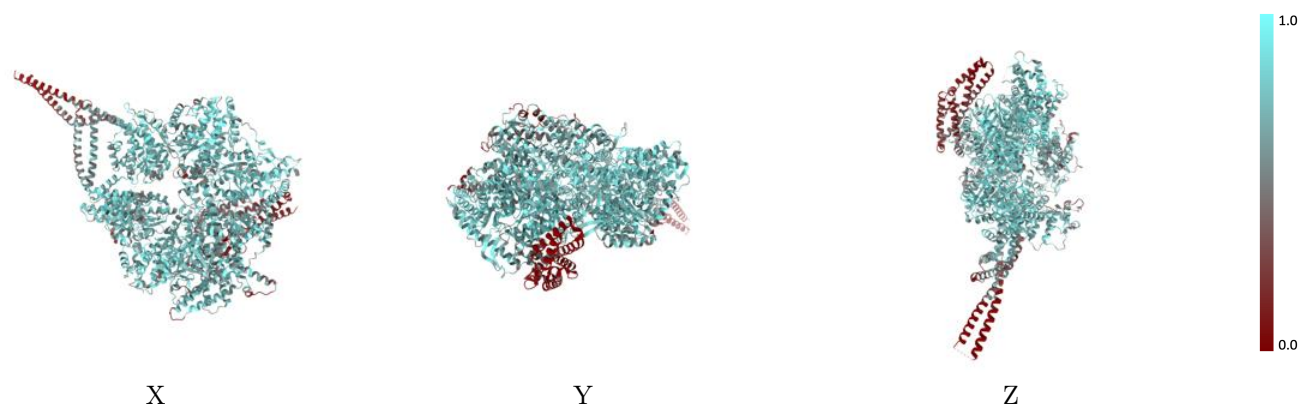
The images above show the 3D surface view of the map at the recommended contour level 0.21 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



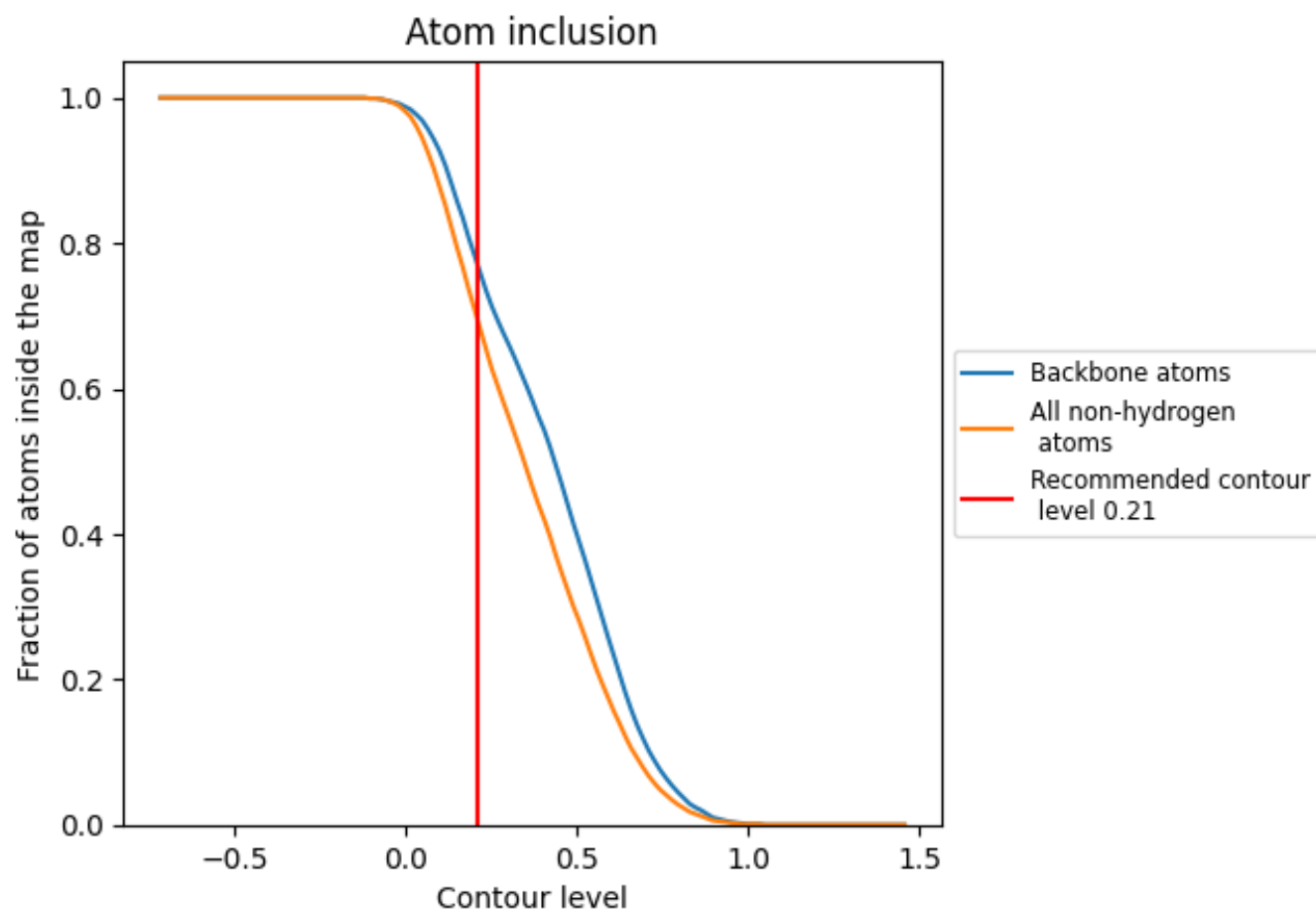
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.21).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% 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 (0.21) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6940	0.4670
A	0.6940	0.4670

