



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 02:52 AM UTC

PDB ID : 9DH7 / pdb_00009dh7
EMDB ID : EMD-46858
Title : State-4 of the motor domain from full-length human dynein-1 in 5mM AMPPNP with 5mM Mg²⁺
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-09-03
Resolution : 3.40 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

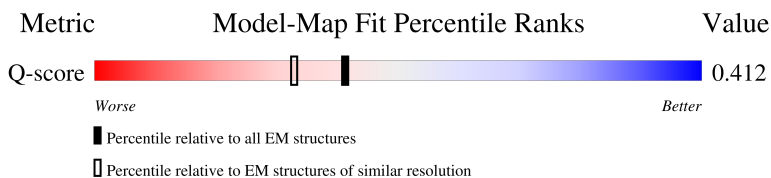
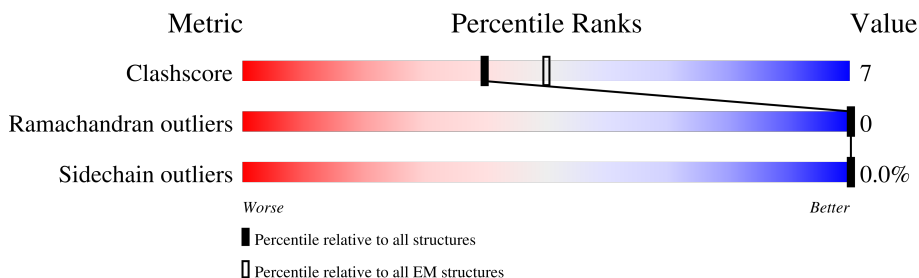
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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](#)

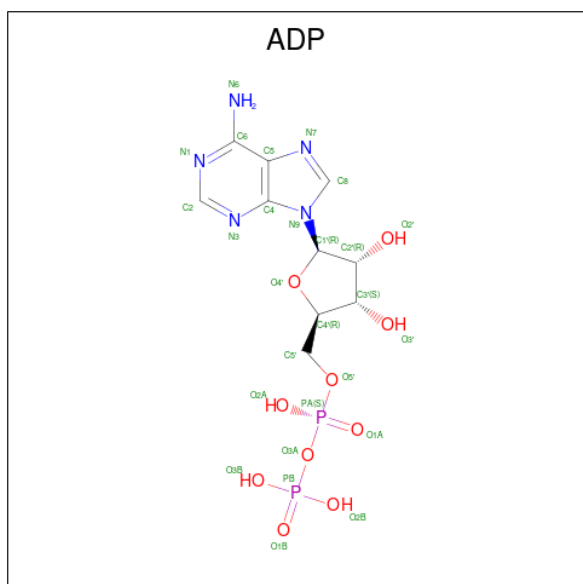
There are 4 unique types of molecules in this entry. The entry contains 23020 atoms, of which 0 are hydrogens and 0 are deuteriums.

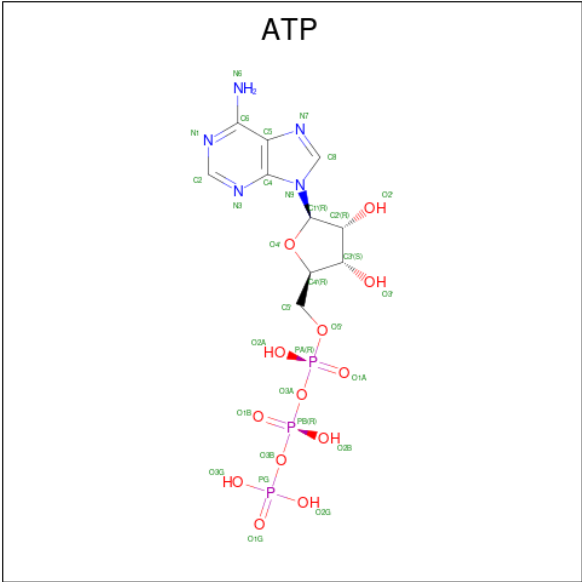
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- 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	2857	22907	14584	3957	4253	113	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).





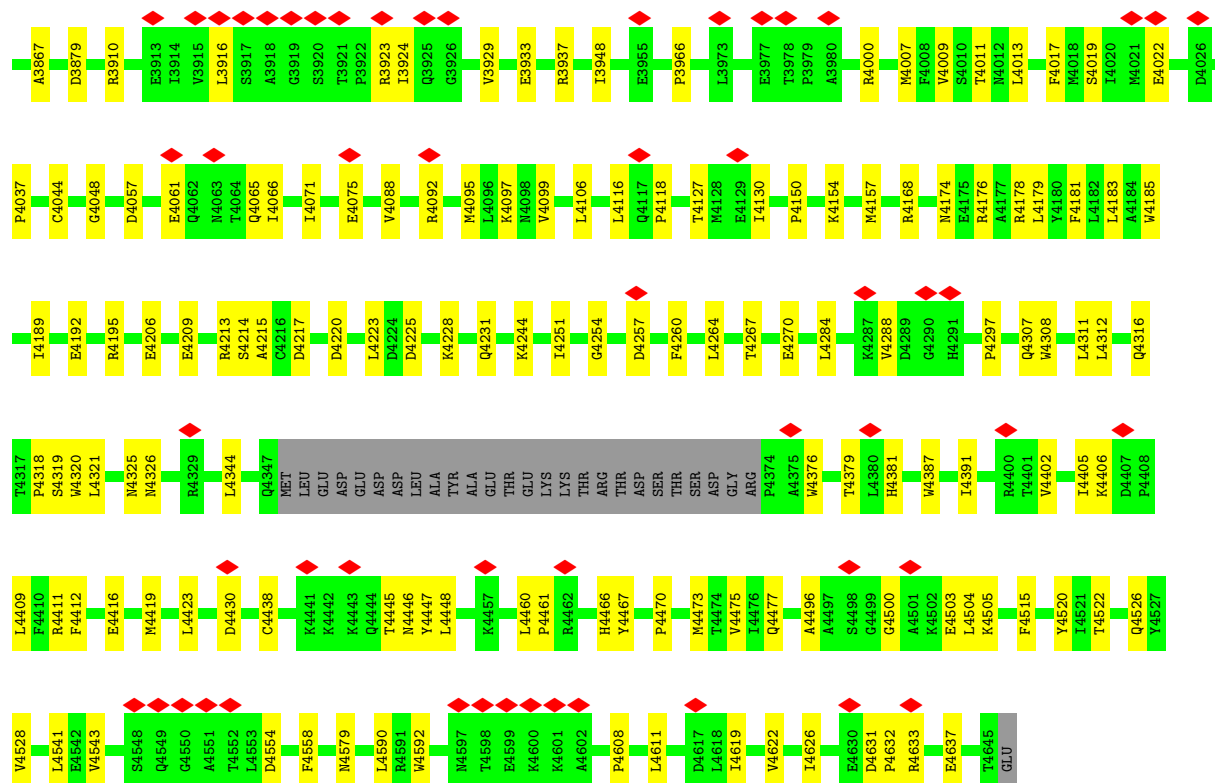
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

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

R2046	G1911	V1721	R1621	L1561	ILE	LYS	ALA	VAL	TRP	ARG	GLU	ALA	ASN	GLU	ASN	PHE
Q2047	E1914	V1724	E1622	P1562	ASN	ASN	SER	THR	GLU	PHE	PHE	LEU	LEU	ARG	LEU	PHE
L2048				V1563	VAL	ALA	GLU	ALA	LYS	THR	THR	GLU	ASP	ILE	THR	GLN
V2052	V1929	Y1738	S1625	E1564	ILE	VAL	PHE	VAL	PRO	PRO	ILE	LEU	GLY	ASN	GLY	LYS
F2059	D1933	L1749	P1627	T1565	ALA	LYS	GLN	GLN	SER	SER	SER	GLN	PRO	VAL	VAL	GLY
R2060	E1934	M1769	Y1630	Q1566	LYS	ASP	ARG	ASP	THR	TRP	TRP	ASP	ASP	GLU	ILE	VAL
L2065	T1935	F1631	V1632	R1567	VAL	VAL	LEU	LEU	GLY	TYR	TYR	GLY	GLY	ILE	LEU	LEU
A2066	Q1939	G1770	G1633	F1568	PRO	LEU	SER	ASN	ASN	ILE	ILE	GLY	VAL	VAL	GLY	LEU
I2069	Q1943	G1771	D1634	Q1569	TYR	ALA	GLY	VAL	ARG	ASN	ASN	LEU	LEU	ASN	ILE	ILE
V2070	R1943	G1772	D1635	S1570	LYS	GLN	MET	TRP	ILE	ILE	GLY	ASP	GLU	PRO	VAL	GLU
P2071	V1946	D1773	E1636	I1571	VAL	GLY	ILE	GLU	GLU	GLY	GLY	ASP	GLU	ASN	GLY	LYS
L2075	Q1950	A1775	L1637	T1573	GLU	ALA	MET	VAL	GLN	GLY	TRP	VAL	TYR	GLY	ALA	ASP
E2078	F1957	L1782	L1638	E1574	ASP	LEU	LEU	VAL	ALA	GLY	ALA	ASP	LEU	ARG	LEU	GLU
H2085	D1958	S1783	E1639	F1575	LEU	GLU	ILE	VAL	LEU	PHE	THR	THR	VAL	VAL	ARG	GLU
Y2086	E1959	E1786	I1641	L1576	GLU	PHE	GLU	ILE	THR	GLY	ALA	GLY	MET	ALA	VAL	VAL
D2087	R1962	V1787	G1642	A1577	TRP	LEU	SER	ILE	ILE	ILE	ASP	GLY	GLY	VAL	THR	THR
L2093	E1965	L1791	V1647	L1578	LYS	GLN	LYS	GLN	GLY	ARG	MET	GLN	ASP	VAL	GLU	GLU
K2104	H1985	L1797	K1645	M1579	ASN	ASN	ASP	ASP	LYS	LYS	GLY	GLY	GLY	VAL	GLU	THR
R2105	S1986	R1805	N1646	K1580	ARG	VAL	GLU	GLU	ASP	LYS	PHE	GLY	VAL	VAL	LEU	CYS
E2106	N1987	E1805	V1647	L1582	ILE	VAL	GLU	GLU	GLY	GLY	THR	THR	GLN	ALA	LEU	ILE
R2107	P1988	E1809	H1653	S1583	MET	TRP	TRP	GLN	ARG	ASP	ASP	ASP	GLY	THR	THR	THR
R2118	N1989	E1809	K1656	S1585	ALA	ASN	THR	ASP	LYS	SER	ALA	ALA	VAL	GLY	GLY	GLY
G2119	Y1990	E1814	L1650	P1586	LEU	GLU	TYR	TRP	ASP	ILE	ILE	GLN	VAL	VAL	VAL	VAL
E2120	D1991	L1815	I1664	V1588	PHE	ASP	GLU	GLN	GLN	GLN	GLN	GLN	TRP	ALA	ALA	ALA
A2121	K1992	V1816	I1665	M1589	V1536	VAL	LEU	LEU	VAL	VAL	VAL	VAL	GLN	VAL	VAL	VAL
V2122	T1993	D1831	L1666	D1590	Q1537	VAL	LEU	ASP	CYS	ALA	ALA	ASN	GLN	PRO	PRO	PRO
D2123	S1994	S1835	N1667	V1591	I1538	ASN	ASN	ASN	LYS	LYS	LYS	LYS	ASP	ARG	ARG	ARG
E2124	P1996	F1836	D1668	L1592	D1539	GLN	GLN	VAL	GLU	GLY	GLY	GLY	ASP	GLN	GLN	GLN
E2129	I1997	E1837	D1669	M1593	V1540	ASN	ASN	ASN	ALA	ILE	PHE	GLY	ASP	PRO	PRO	PRO
N2130	E2000	D1847	L1674	I1594	Q1541	CYS	LYS	TRP	ASP	VAL	GLU	GLN	ALA	GLN	ALA	ALA
L2131	V2006	P1848	G1675	Q1595	R1542	ARG	ARG	VAL	ALA	GLU	LYS	GLN	ALA	VAL	VAL	VAL
P2132	P2010	T1851	R1679	G1596	W1543	LEU	LEU	VAL	GLU	GLU	GLY	GLY	GLY	GLY	GLY	GLY
Q2134	P2010	D1852	M1685	V1597	W1544	ILE	ILE	SER	THR	ASP	VAL	VAL	ASN	VAL	VAL	VAL
E2135	P2011	V1853	F1686	Q1598	V1545	ARG	GLY	GLU	THR	ARG	GLU	GLY	ILE	ILE	ILE	ILE
I2138	I2016	Q1856	K1687	R1599	Y1546	TRP	TRP	LEU	GLY	VAL	VAL	TYR	ASN	ASN	ASN	ASN
Q2139	T2017	K1878	E1684	S1900	L1547	ASP	ASP	LEU	LEU	GLU	GLY	ARG	ARG	GLY	GLY	GLY
T2144	M2018	L1879	K1697	L1601	E1548	ASP	PHE	GLY	THR	ARG	VAL	GLY	GLY	GLY	GLY	GLY
M2145	S2026	L1879	L1698	E1602	G1549	LEU	ILE	GLN	SER	THR	VAL	GLN	GLY	GLY	GLY	GLY
K2148	T1882	T1882	K1697	R1603	T1550	ASN	ASN	TRP	ALA	THR	ASP	LEU	THR	ASP	GLY	GLY
L2149	D2030	C1888	N1699	A1805	F1551	VAL	LYS	ASP	VAL	ARG	LEU	LEU	LEU	ASP	LEU	LEU
L2157	S2038	P1904	E1700	D1606	T1552	LYS	VAL	VAL	ARG	LEU	LEU	LEU	LEU	ASN	LYS	LYS
D2163	L2039	F1905	E1708	L1607	G1553	GLY	GLY	ASP	ARG	THR	GLU	GLU	GLU	ASN	ASN	ASN
			V1711	L1608	S1554	ASN	GLN	GLN	THR	THR	GLY	GLY	GLY	GLY	GLY	GLY
			T1712	L1609	A1555	THR	THR	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
			L1717	K1610	D1556	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
				K1613	I1557	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
				L1614	K1558	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
				L1615	E1617	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
				G1616	L1618	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
				E1617	Y1619	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
				L1618	E1620	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20077	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.167	Depositor
Minimum map value	-0.523	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1573, 1.1573, 1.1573	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.21	0/23391	0.34	0/31705

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	22907	0	22979	329	0
2	A	81	0	36	3	0
3	A	31	0	12	2	0
4	A	1	0	0	0	0
All	All	23020	0	23027	329	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 (329) 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:3068:MET:HE1	1:A:3078:ARG:HG3	1.69	0.74
1:A:3557:ASP:OD1	1:A:3743:ARG:NH1	2.22	0.73
1:A:3655:ARG:HG2	1:A:3660:VAL:HG22	1.71	0.73
1:A:4225:ASP:O	1:A:4228:LYS:NZ	2.22	0.73
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.22	0.72
1:A:4267:THR:HG23	1:A:4633:ARG:HD2	1.71	0.71
1:A:2840:ASP:OD1	1:A:2843:ARG:NH2	2.24	0.71
1:A:4541:LEU:HD11	1:A:4590:LEU:HB3	1.72	0.69
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	1.74	0.69
1:A:3811:ILE:HG22	1:A:3815:MET:HE3	1.75	0.68
1:A:3851:ASP:HB3	1:A:3854:GLN:HG2	1.73	0.68
1:A:2621:ASN:ND2	1:A:3014:ASN:OD1	2.26	0.67
1:A:3178:ASP:OD2	1:A:3585:ARG:NE	2.28	0.67
1:A:3129:VAL:HG21	1:A:3149:PHE:HB2	1.75	0.67
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.76	0.66
1:A:1939:GLN:HB3	1:A:1943:ARG:HH12	1.61	0.65
1:A:2596:PRO:HB2	1:A:2738:TYR:CZ	2.32	0.65
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.78	0.65
1:A:2965:ARG:HH22	1:A:3614:PHE:HB3	1.63	0.64
1:A:1647:VAL:HG21	1:A:1666:LEU:HD22	1.78	0.64
1:A:1914:GLU:HG3	2:A:4701:ADP:H2'	1.80	0.64
1:A:1904:PRO:HG2	1:A:2017:THR:HG22	1.80	0.63
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.80	0.63
1:A:3910:ARG:HE	1:A:4344:LEU:HD11	1.63	0.63
1:A:1879:LEU:HD11	1:A:1914:GLU:HB3	1.78	0.63
1:A:2176:THR:O	1:A:2179:ARG:N	2.33	0.61
1:A:3005:LEU:HD12	1:A:3082:SER:HB2	1.83	0.61
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.82	0.61
1:A:1959:GLU:HB3	1:A:1962:ARG:HG3	1.83	0.61
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.34	0.61
1:A:1985:HIS:HD2	1:A:1997:ILE:HD13	1.66	0.60
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.82	0.59
1:A:2046:ARG:HG3	1:A:2093:LEU:HD22	1.83	0.59
1:A:2075:LEU:HD22	1:A:4522:THR:HG23	1.84	0.59
1:A:4088:VAL:HG11	1:A:4116:LEU:HD21	1.84	0.59
1:A:1708:GLU:HA	1:A:1711:VAL:HG12	1.83	0.59
1:A:2257:LYS:NZ	1:A:2308:ASP:OD2	2.28	0.58
1:A:2220:LEU:HD22	1:A:2342:MET:HE2	1.84	0.58
1:A:2457:SER:O	1:A:2461:MET:HG3	2.02	0.58
1:A:2967:TYR:OH	1:A:2975:ASP:OD2	2.18	0.58
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.83	0.58
1:A:1687:LYS:HG2	1:A:1712:THR:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3488:ARG:NH1	1:A:3746:GLU:OE1	2.36	0.58
1:A:2671:MET:HG2	1:A:2677:GLN:HG3	1.86	0.58
1:A:3045:ASP:OD1	1:A:3046:SER:N	2.36	0.58
1:A:2042:THR:HG21	1:A:4257:ASP:HB2	1.86	0.57
1:A:1939:GLN:NE2	1:A:4075:GLU:OE2	2.38	0.57
1:A:1965:GLU:HG2	1:A:2026:SER:HB3	1.85	0.57
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.87	0.57
1:A:1717:LEU:HB2	1:A:1749:LEU:HD22	1.86	0.57
1:A:2627:THR:OG1	1:A:2629:GLU:OE1	2.22	0.57
1:A:2648:VAL:HG12	1:A:2701:VAL:HG13	1.87	0.57
1:A:4473:MET:HG3	1:A:4477:GLN:HB2	1.85	0.57
1:A:3194:LEU:HD22	1:A:3500:MET:HE3	1.85	0.56
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.38	0.56
1:A:1636:ASP:O	1:A:1640:ILE:HD12	2.05	0.56
1:A:1946:VAL:HG22	1:A:2006:VAL:HG21	1.87	0.56
1:A:4496:ALA:HB2	1:A:4504:LEU:HD21	1.85	0.56
1:A:3017:VAL:HB	1:A:3020:LEU:HB2	1.87	0.56
1:A:2149:LEU:HD11	1:A:2157:LEU:HD13	1.86	0.56
1:A:4192:GLU:HB3	1:A:4321:LEU:HD21	1.88	0.55
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.89	0.55
1:A:2213:ILE:HG22	1:A:2220:LEU:HG	1.88	0.55
1:A:1699:ASN:OD1	1:A:1700:GLU:N	2.39	0.55
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.88	0.55
1:A:4409:LEU:HD11	1:A:4558:PHE:HE2	1.72	0.55
1:A:3815:MET:HA	1:A:3818:LEU:HD12	1.89	0.55
1:A:3499:GLN:O	1:A:3503:ILE:HG13	2.07	0.55
1:A:1805:ARG:HD3	1:A:2105:ARG:HH21	1.71	0.54
1:A:3001:ASP:OD1	1:A:3002:SER:N	2.39	0.54
1:A:1985:HIS:CD2	1:A:1997:ILE:HD13	2.42	0.54
1:A:2087:ASP:O	1:A:2148:LYS:NZ	2.40	0.54
1:A:2975:ASP:O	1:A:2979:VAL:HG23	2.07	0.54
1:A:2855:LEU:HD21	1:A:2863:ARG:HG3	1.90	0.54
1:A:1943:ARG:NH1	1:A:2273:ARG:HD2	2.23	0.53
1:A:2046:ARG:CG	1:A:2093:LEU:HD22	2.38	0.53
1:A:2221:MET:HG3	1:A:2343:PHE:HB2	1.89	0.53
1:A:2422:ILE:HD13	1:A:2487:GLU:HA	1.90	0.53
1:A:2242:GLU:HG3	1:A:2248:GLU:HA	1.90	0.53
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.08	0.53
1:A:3544:ARG:NH1	1:A:3547:ILE:HG13	2.24	0.53
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	1.90	0.52
1:A:3157:ALA:HB1	1:A:3524:MET:HE2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1582:VAL:HG23	1:A:1591:VAL:HG11	1.90	0.52
1:A:2751:PHE:HB3	1:A:2803:VAL:HG11	1.91	0.52
1:A:1939:GLN:HB3	1:A:1943:ARG:NH1	2.23	0.52
1:A:2232:MET:HG3	3:A:4702:ATP:C8	2.45	0.52
1:A:4179:LEU:HD12	1:A:4223:LEU:HD22	1.91	0.52
1:A:4264:LEU:O	1:A:4267:THR:HB	2.09	0.52
1:A:2564:ALA:HB3	1:A:2567:VAL:HG23	1.89	0.52
1:A:3021:PHE:CG	1:A:3029:LEU:HD22	2.45	0.52
1:A:3130:TYR:CZ	1:A:3132:LYS:HB2	2.44	0.52
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.90	0.52
1:A:2387:LEU:HB2	1:A:2412:MET:HE2	1.90	0.52
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.92	0.52
1:A:2784:PHE:HB2	1:A:2794:TYR:HE2	1.75	0.52
1:A:4430:ASP:OD2	1:A:4447:TYR:OH	2.28	0.52
1:A:4631:ASP:OD2	1:A:4633:ARG:HB3	2.10	0.52
1:A:2557:VAL:O	1:A:2757:ARG:NH2	2.42	0.51
1:A:2925:ILE:HG13	1:A:2933:LEU:HD21	1.90	0.51
1:A:3233:ASN:OD1	1:A:3234:ALA:N	2.43	0.51
1:A:3521:ASP:OD2	1:A:3523:GLN:NE2	2.43	0.51
1:A:4267:THR:HG23	1:A:4633:ARG:CD	2.39	0.51
1:A:1882:THR:HA	1:A:2048:LEU:HD23	1.92	0.51
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.92	0.51
1:A:2195:ASP:O	1:A:2198:GLU:HG3	2.11	0.51
1:A:2905:LEU:HD11	1:A:3652:GLU:HB3	1.91	0.51
1:A:3016:GLU:OE1	1:A:3051:TYR:OH	2.27	0.51
1:A:1674:LEU:HB3	1:A:1685:MET:HE1	1.91	0.50
1:A:3024:ASP:N	1:A:3024:ASP:OD1	2.43	0.50
1:A:3808:CYS:HB3	1:A:3832:PHE:HZ	1.76	0.50
1:A:2965:ARG:NH2	1:A:3614:PHE:HB3	2.25	0.50
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.44	0.50
1:A:3478:LEU:HD11	1:A:3767:ILE:HG23	1.94	0.50
1:A:1711:VAL:HG23	1:A:1853:VAL:HG21	1.93	0.50
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.44	0.50
1:A:3825:TYR:OH	1:A:3879:ASP:OD2	2.24	0.50
1:A:3176:TYR:O	1:A:3180:ILE:HG12	2.12	0.49
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	1.94	0.49
1:A:4500:GLY:H	1:A:4503:GLU:HB3	1.77	0.49
1:A:1664:ILE:HD12	1:A:1666:LEU:HD11	1.95	0.49
1:A:2213:ILE:HA	1:A:2216:ILE:HG22	1.93	0.49
1:A:2046:ARG:HD2	1:A:2070:VAL:HG13	1.94	0.49
1:A:2457:SER:OG	1:A:2732:PRO:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3124:ASP:OD1	1:A:3125:TYR:N	2.44	0.49
1:A:3916:LEU:HD11	1:A:3937:ARG:HG3	1.95	0.49
1:A:4065:GLN:HB3	1:A:4092:ARG:HH21	1.78	0.49
1:A:1814:GLU:HB2	1:A:1878:LYS:HE2	1.94	0.49
1:A:2131:LEU:HD12	1:A:2132:PRO:HD2	1.95	0.49
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.47	0.49
1:A:3653:VAL:HG11	1:A:3671:LEU:HD22	1.95	0.48
1:A:4402:VAL:O	1:A:4406:LYS:NZ	2.46	0.48
1:A:1543:ARG:HA	1:A:1546:TYR:CE2	2.48	0.48
1:A:1578:LEU:O	1:A:1582:VAL:HG12	2.13	0.48
1:A:2134:GLN:O	1:A:2138:ILE:HG12	2.13	0.48
1:A:3628:ARG:NH2	1:A:3667:GLN:OE1	2.46	0.48
1:A:1957:PHE:HB2	1:A:2016:ILE:HG22	1.95	0.48
1:A:3795:GLU:O	1:A:3799:GLN:HG2	2.14	0.48
1:A:3835:ILE:HD13	1:A:3867:ALA:HA	1.95	0.48
1:A:4185:TRP:O	1:A:4189:ILE:HG12	2.13	0.48
1:A:1769:MET:HE2	1:A:1831:ASP:HA	1.96	0.48
1:A:1783:SER:O	1:A:1787:VAL:HG13	2.14	0.48
1:A:2270:PRO:HA	1:A:2273:ARG:HH21	1.77	0.48
1:A:1630:TYR:CE1	1:A:1950:GLN:HG3	2.48	0.48
1:A:2581:LEU:HD11	1:A:2593:LEU:HD21	1.95	0.48
1:A:1835:SER:OG	1:A:1837:GLU:OE1	2.32	0.48
1:A:3575:GLU:O	1:A:3579:MET:HG3	2.13	0.48
1:A:3211:THR:O	1:A:3215:VAL:HG13	2.14	0.48
1:A:4470:PRO:HD2	1:A:4473:MET:HE3	1.95	0.48
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.14	0.48
1:A:2039:LEU:HD12	1:A:4254:GLY:HA2	1.96	0.48
1:A:3568:PRO:HG2	1:A:3573:CYS:SG	2.54	0.48
1:A:3725:ASP:HA	1:A:3728:ARG:HG2	1.96	0.47
1:A:4405:ILE:O	1:A:4411:ARG:NE	2.43	0.47
1:A:2221:MET:SD	1:A:2348:LEU:HD11	2.54	0.47
1:A:3738:PHE:CZ	1:A:3783:LYS:HE3	2.48	0.47
1:A:2257:LYS:HE3	1:A:2676:THR:HG21	1.97	0.47
1:A:2578:GLU:OE1	1:A:2607:SER:OG	2.26	0.47
1:A:4416:GLU:HA	1:A:4419:MET:HE2	1.97	0.47
1:A:4633:ARG:O	1:A:4637:GLU:HG3	2.15	0.47
1:A:2308:ASP:O	1:A:2312:VAL:HG12	2.15	0.47
1:A:2382:LEU:HD23	1:A:2420:ALA:HB2	1.95	0.47
1:A:4154:LYS:HD2	1:A:4312:LEU:HB2	1.97	0.47
1:A:2085:HIS:HB3	1:A:2348:LEU:HD12	1.96	0.47
1:A:2163:ASP:OD1	1:A:4526:GLN:NE2	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2571:THR:H	1:A:2574:THR:HB	1.80	0.47
1:A:3839:VAL:HG12	1:A:3859:ILE:HG23	1.97	0.47
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.97	0.47
1:A:3060:ARG:HG2	1:A:3060:ARG:HH11	1.80	0.47
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.48	0.47
1:A:2230:LYS:HE2	3:A:4702:ATP:O1B	2.15	0.46
1:A:4176:ARG:NH1	1:A:4220:ASP:OD1	2.48	0.46
1:A:1929:VAL:H	1:A:2332:ARG:HH22	1.63	0.46
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.98	0.46
1:A:3478:LEU:HD11	1:A:3767:ILE:HG12	1.97	0.46
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.50	0.46
1:A:2642:ARG:NH2	1:A:2704:GLU:OE2	2.48	0.46
1:A:4297:PRO:HG3	1:A:4308:TRP:CD2	2.50	0.46
1:A:2388:ASP:OD1	1:A:2388:ASP:N	2.48	0.46
1:A:4066:ILE:HD11	1:A:4095:MET:HB2	1.97	0.46
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.97	0.46
1:A:1797:LEU:HD11	1:A:2060:ARG:HH21	1.80	0.46
1:A:2232:MET:HE2	1:A:2232:MET:HA	1.97	0.46
1:A:2306:ASP:OD2	1:A:2676:THR:OG1	2.29	0.46
1:A:4019:SER:O	1:A:4022:GLU:HG2	2.16	0.46
1:A:1632:VAL:HG12	1:A:1656:LYS:HD2	1.97	0.46
1:A:1738:TYR:HE2	1:A:1792:LEU:HD21	1.80	0.46
1:A:2620:LEU:HD11	1:A:2634:THR:HG21	1.98	0.46
1:A:3846:LEU:HD22	1:A:3855:ARG:HG2	1.98	0.46
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.98	0.46
1:A:1543:ARG:HA	1:A:1546:TYR:CZ	2.51	0.45
1:A:3728:ARG:HB3	1:A:3794:VAL:HG11	1.97	0.45
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.96	0.45
1:A:3716:VAL:HB	1:A:3836:TYR:OH	2.16	0.45
1:A:2188:GLU:OE1	1:A:2243:ARG:NH2	2.47	0.45
1:A:3644:VAL:HG22	1:A:3664:LEU:HD22	1.99	0.45
1:A:3650:ASN:HD21	1:A:3695:ARG:NH1	2.14	0.45
1:A:2144:THR:HG22	1:A:2145:MET:HE2	1.98	0.45
1:A:3474:ARG:HE	1:A:3767:ILE:HG21	1.82	0.45
1:A:3612:THR:O	1:A:3635:VAL:HA	2.17	0.45
1:A:2517:TYR:CE2	1:A:2521:ILE:HD13	2.52	0.45
1:A:1797:LEU:HD11	1:A:2060:ARG:NH2	2.32	0.45
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.51	0.45
1:A:3855:ARG:O	1:A:3859:ILE:HG13	2.16	0.45
1:A:3929:VAL:O	1:A:3933:GLU:HG3	2.17	0.45
1:A:4288:VAL:O	1:A:4319:SER:OG	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	1.99	0.45
1:A:1905:PHE:CE1	1:A:2038:SER:HB2	2.52	0.44
1:A:2297:LYS:O	1:A:2338:ASN:ND2	2.35	0.44
1:A:3608:LYS:HB3	1:A:3608:LYS:HE3	1.71	0.44
1:A:2224:GLY:O	1:A:2346:GLN:HA	2.17	0.44
1:A:4095:MET:HE3	1:A:4097:LYS:HE3	1.99	0.44
1:A:3761:LEU:HA	1:A:3767:ILE:HD11	1.99	0.44
1:A:2461:MET:HE2	1:A:2461:MET:HB3	1.88	0.44
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.52	0.44
1:A:3601:MET:HE2	1:A:3634:LEU:HD23	2.00	0.44
1:A:1587:LEU:HB3	1:A:1590:ASP:HB2	2.00	0.44
1:A:1985:HIS:CE1	1:A:2010:PRO:HB3	2.52	0.44
1:A:2581:LEU:HD12	1:A:2604:THR:HG22	1.99	0.44
1:A:3113:MET:SD	1:A:3184:ALA:HA	2.58	0.44
1:A:4185:TRP:CD1	1:A:4284:LEU:HD22	2.53	0.44
1:A:4307:GLN:HE22	1:A:4311:LEU:HD11	1.82	0.44
1:A:3154:LEU:HG	1:A:3516:TYR:CD1	2.52	0.44
1:A:3923:ARG:HG3	1:A:3923:ARG:O	2.17	0.44
1:A:1541:GLN:O	1:A:1545:VAL:HG23	2.18	0.43
1:A:1848:PRO:HA	1:A:1856:GLN:HE21	1.82	0.43
1:A:3214:GLN:O	1:A:3218:LEU:HD23	2.17	0.43
1:A:4174:ASN:OD1	1:A:4231:GLN:NE2	2.49	0.43
1:A:2220:LEU:HB2	1:A:2342:MET:HG2	2.01	0.43
1:A:3160:ARG:NH2	1:A:3524:MET:HE1	2.34	0.43
1:A:3481:SER:HB3	1:A:3774:LYS:HE2	2.00	0.43
1:A:1550:ILE:O	1:A:1554:SER:OG	2.35	0.43
1:A:1911:GLY:HA2	2:A:4701:ADP:H5'1	2.00	0.43
1:A:4376:TRP:HA	1:A:4379:THR:HG22	2.00	0.43
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	2.01	0.43
1:A:2304:ASP:OD1	1:A:2726:ARG:NH2	2.51	0.43
1:A:4183:LEU:HD11	1:A:4215:ALA:HB1	2.00	0.43
1:A:4445:THR:H	1:A:4448:LEU:HB2	1.83	0.43
1:A:2139:GLN:HG3	1:A:2170:TYR:CZ	2.53	0.43
1:A:2414:GLN:NE2	1:A:2418:ASP:OD1	2.51	0.43
1:A:2804:ARG:HG3	1:A:2808:GLU:OE1	2.18	0.43
1:A:2872:LEU:HD22	1:A:2920:LEU:HD12	2.00	0.43
1:A:2018:MET:HE2	1:A:2018:MET:HB3	1.79	0.43
1:A:2951:ALA:HB1	1:A:2956:LEU:HB2	2.01	0.43
1:A:3146:SER:HA	1:A:3535:HIS:CE1	2.54	0.43
1:A:3948:ILE:H	1:A:3948:ILE:HD12	1.84	0.43
1:A:1782:LEU:O	1:A:1786:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2016:ILE:O	1:A:2016:ILE:HG13	2.19	0.43
1:A:2132:PRO:HB2	1:A:2135:GLU:HB3	2.01	0.43
1:A:4157:MET:HE2	1:A:4157:MET:HB3	1.91	0.43
1:A:3212:VAL:O	1:A:3215:VAL:HG22	2.19	0.42
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	2.00	0.42
1:A:4460:LEU:HA	1:A:4475:VAL:HG22	2.00	0.42
1:A:1543:ARG:HB3	1:A:1608:LEU:HD12	2.01	0.42
1:A:1959:GLU:HB3	1:A:1962:ARG:CG	2.49	0.42
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	2.01	0.42
1:A:2826:ALA:HB2	1:A:2867:MET:HE1	2.01	0.42
1:A:4007:MET:O	1:A:4011:THR:HG23	2.20	0.42
1:A:4214:SER:HB2	1:A:4251:ILE:HG23	2.02	0.42
1:A:4467:TYR:HB3	1:A:4515:PHE:HD2	1.84	0.42
1:A:2145:MET:O	1:A:2148:LYS:HG2	2.19	0.42
1:A:3782:ARG:O	1:A:3785:GLU:HG2	2.19	0.42
1:A:4048:GLY:HA3	1:A:4206:GLU:OE1	2.20	0.42
1:A:4097:LYS:HA	1:A:4127:THR:OG1	2.19	0.42
1:A:3491:LYS:HA	1:A:3491:LYS:HD3	1.80	0.42
1:A:4071:ILE:HG13	1:A:4099:VAL:HG12	2.01	0.42
1:A:4543:VAL:HG21	1:A:4622:VAL:HG12	2.02	0.42
1:A:3194:LEU:HD22	1:A:3500:MET:CE	2.47	0.42
1:A:4307:GLN:NE2	1:A:4311:LEU:HD11	2.34	0.42
1:A:4316:GLN:HG3	1:A:4320:TRP:CE3	2.55	0.42
1:A:4626:ILE:HD11	1:A:4632:PRO:HD3	2.02	0.42
1:A:1933:ASP:OD2	1:A:1935:THR:OG1	2.35	0.42
1:A:2290:SER:HB2	1:A:2295:LEU:HG	2.02	0.42
1:A:3597:THR:HG23	1:A:3634:LEU:HD21	2.02	0.42
1:A:4297:PRO:HG3	1:A:4308:TRP:CG	2.55	0.42
1:A:1805:ARG:O	1:A:1809:GLU:HG3	2.20	0.42
1:A:2925:ILE:HG21	1:A:2933:LEU:HG	2.01	0.42
1:A:3221:ASP:O	1:A:3225:LYS:HG2	2.20	0.42
1:A:3617:ASP:N	1:A:3617:ASP:OD1	2.52	0.42
1:A:1613:LYS:O	1:A:1617:GLU:HG2	2.20	0.41
1:A:1816:VAL:HG11	1:A:2052:VAL:HG22	2.02	0.41
1:A:2059:PHE:CZ	1:A:2104:LYS:HD3	2.55	0.41
1:A:3160:ARG:HH21	1:A:3524:MET:HE1	1.84	0.41
1:A:3732:LEU:HD22	1:A:3791:MET:HE1	2.01	0.41
1:A:1847:ASP:O	1:A:1856:GLN:HG3	2.21	0.41
1:A:1888:CYS:HA	1:A:2039:LEU:CD2	2.50	0.41
1:A:2065:LEU:HD11	1:A:2133:GLU:HB3	2.02	0.41
1:A:2536:ASP:OD1	1:A:2572:LEU:HD21	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2962:LYS:HG3	1:A:3665:GLY:HA2	2.02	0.41
1:A:2974:GLU:OE1	1:A:2977:ARG:NH1	2.53	0.41
1:A:3544:ARG:HH12	1:A:3547:ILE:HG13	1.85	0.41
1:A:4057:ASP:O	1:A:4061:GLU:HG2	2.21	0.41
1:A:3148:VAL:O	1:A:3152:GLN:HG3	2.20	0.41
1:A:3454:LEU:O	1:A:3457:GLU:HG2	2.21	0.41
1:A:3691:ASP:O	1:A:3695:ARG:HG3	2.21	0.41
1:A:3135:GLN:HB2	1:A:3136:PRO:HD3	2.02	0.41
1:A:4209:GLU:OE2	1:A:4213:ARG:NE	2.54	0.41
1:A:1560:LEU:O	1:A:1561:LEU:HD23	2.21	0.41
1:A:4044:CYS:HB3	1:A:4130:ILE:HG12	2.03	0.41
1:A:4423:LEU:HD13	1:A:4466:HIS:HD2	1.84	0.41
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	2.01	0.41
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.56	0.41
1:A:2548:TRP:CD1	1:A:2576:ARG:HG2	2.56	0.41
1:A:2569:VAL:HG11	1:A:2747:ILE:HA	2.02	0.41
1:A:3740:LEU:O	1:A:3744:GLN:HG3	2.21	0.41
1:A:3759:ARG:HH21	1:A:3761:LEU:HB2	1.85	0.41
1:A:4260:PHE:CZ	1:A:4608:PRO:HB3	2.56	0.41
1:A:2507:ARG:HE	1:A:2507:ARG:HB2	1.70	0.41
1:A:3650:ASN:HD21	1:A:3695:ARG:HH11	1.69	0.41
1:A:4157:MET:HE1	1:A:4181:PHE:CE1	2.56	0.41
1:A:2107:ARG:NH1	1:A:2135:GLU:OE2	2.54	0.40
1:A:3159:ALA:O	1:A:3163:LYS:HG2	2.21	0.40
1:A:4168:ARG:NH2	1:A:4217:ASP:OD2	2.48	0.40
1:A:1679:ARG:H	1:A:1679:ARG:HD2	1.86	0.40
1:A:3122:VAL:HG13	1:A:3126:MET:HE2	2.03	0.40
1:A:3716:VAL:HG21	1:A:3804:LEU:HD23	2.04	0.40
1:A:3924:ILE:HD12	1:A:3924:ILE:H	1.86	0.40
1:A:1914:GLU:HG2	2:A:4701:ADP:O1A	2.21	0.40
1:A:2912:PHE:CE2	1:A:2914:GLU:HB2	2.56	0.40
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	2.04	0.40
1:A:1848:PRO:HA	1:A:1856:GLN:NE2	2.36	0.40
1:A:3075:LEU:HD12	1:A:3075:LEU:HA	1.95	0.40
1:A:4013:LEU:HD13	1:A:4017:PHE:CE2	2.57	0.40
1:A:1787:VAL:O	1:A:1791:VAL:HG23	2.22	0.40
1:A:2046:ARG:HG2	1:A:2070:VAL:HG22	2.03	0.40
1:A:2717:ASP:O	1:A:4446:ASN:ND2	2.53	0.40
1:A:4150:PRO:O	1:A:4195:ARG:NH2	2.51	0.40
1:A:4244:LYS:NZ	1:A:4270:GLU:OE1	2.53	0.40
1:A:4387:TRP:O	1:A:4391:ILE:HG13	2.22	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	2849/4646 (61%)	2808 (99%)	41 (1%)	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	2530/4125 (61%)	2529 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2321	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1598	GLN
1	A	1856	GLN
1	A	1974	GLN
1	A	1985	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2047	GLN
1	A	2263	HIS
1	A	2414	GLN
1	A	2463	HIS
1	A	2464	GLN
1	A	2485	GLN
1	A	2549	GLN
1	A	2621	ASN
1	A	2781	GLN
1	A	2827	HIS
1	A	2960	GLN
1	A	3069	ASN
1	A	3152	GLN
1	A	3526	GLN
1	A	3714	ASN
1	A	3744	GLN
1	A	3754	ASN
1	A	3877	HIS
1	A	4098	ASN
1	A	4114	HIS
1	A	4295	GLN
1	A	4326	ASN
1	A	4386	ASN
1	A	4490	GLN
1	A	4491	ASN
1	A	4566	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	A	4704	-	28,29,29	0.47	0	43,45,45	0.47	0
2	ADP	A	4701	-	28,29,29	0.45	0	43,45,45	0.49	0
2	ADP	A	4703	-	28,29,29	0.45	0	43,45,45	0.49	0
3	ATP	A	4702	4	32,33,33	0.53	0	48,52,52	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	4704	-	-	3/16/32/32	0/3/3/3
2	ADP	A	4701	-	-	1/16/32/32	0/3/3/3
2	ADP	A	4703	-	-	0/16/32/32	0/3/3/3
3	ATP	A	4702	4	-	1/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

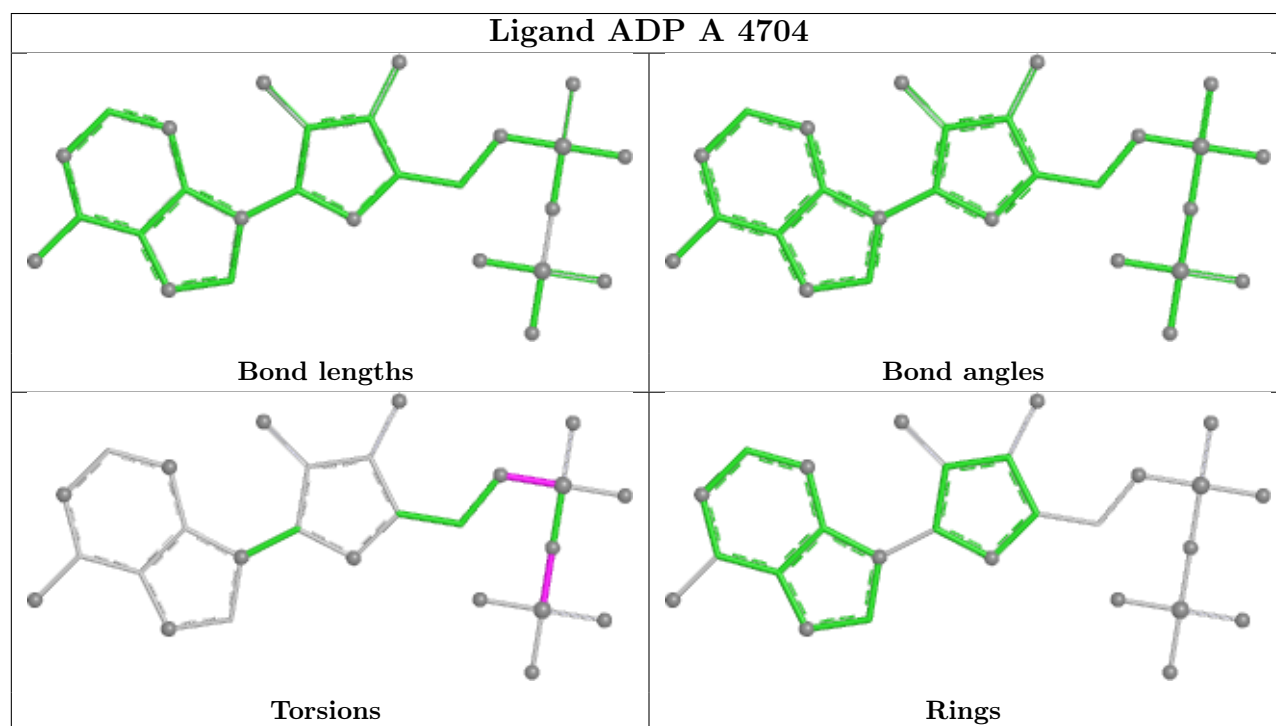
Mol	Chain	Res	Type	Atoms
2	A	4704	ADP	PA-O3A-PB-O2B
2	A	4704	ADP	PA-O3A-PB-O3B
3	A	4702	ATP	O4'-C4'-C5'-O5'
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4701	ADP	O4'-C4'-C5'-O5'

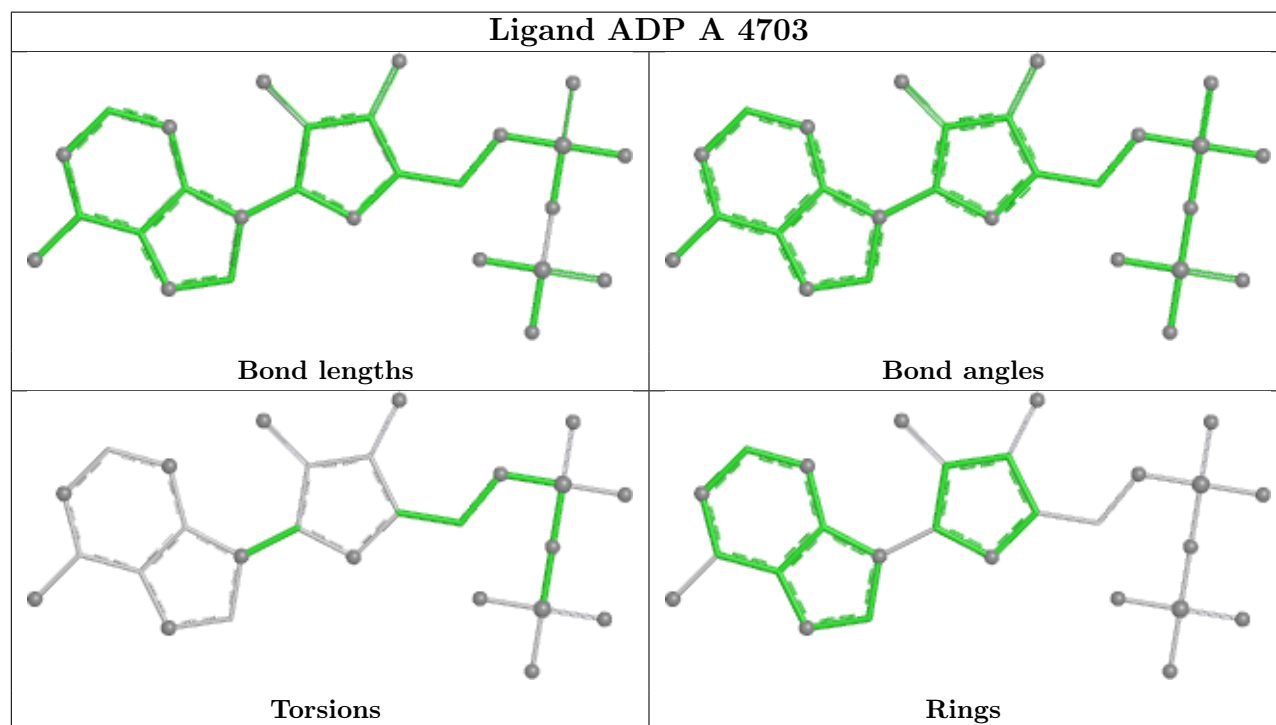
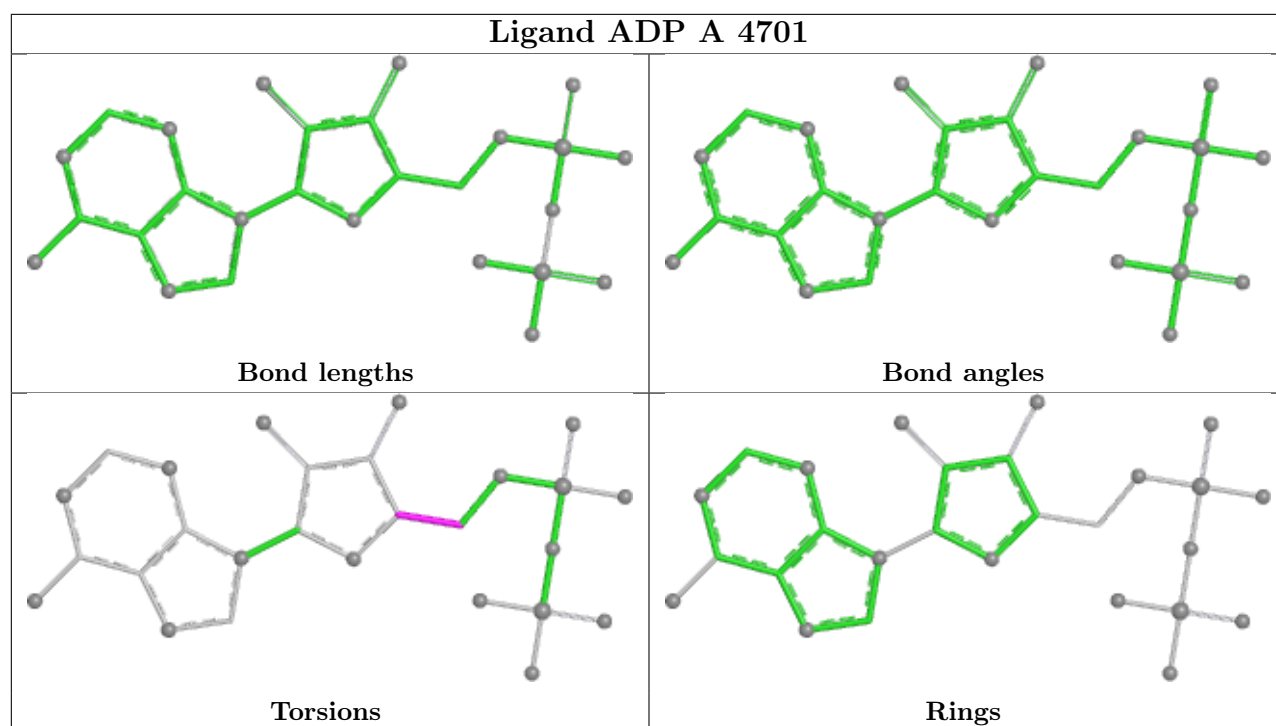
There are no ring outliers.

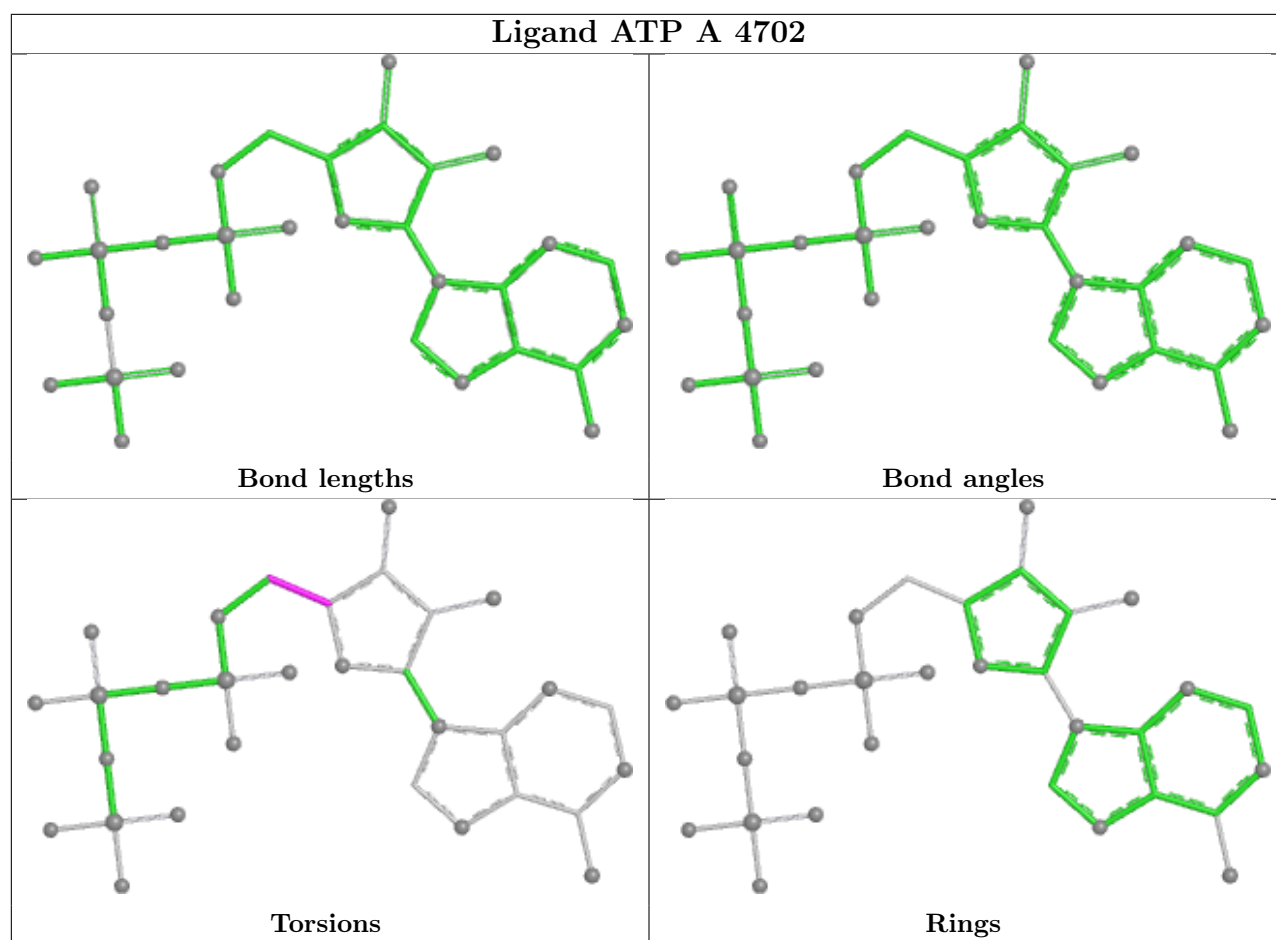
2 monomers are involved in 5 short contacts:

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

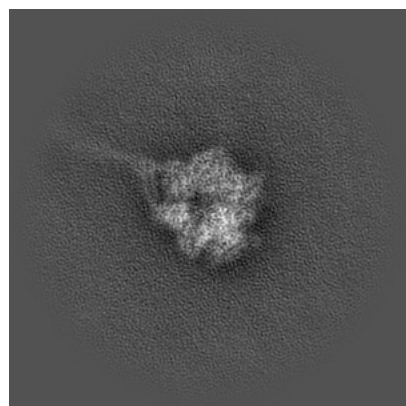
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46858. These allow visual inspection of the internal detail of the map and identification of artifacts.

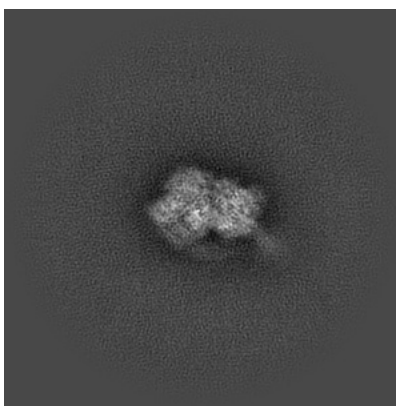
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

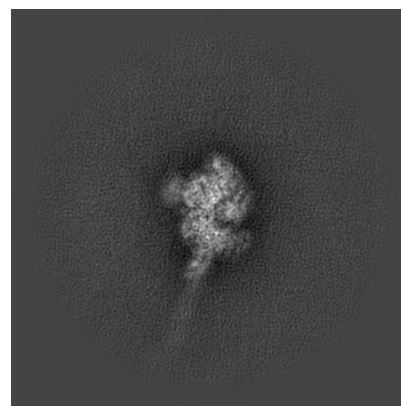
6.1.1 Primary map



X

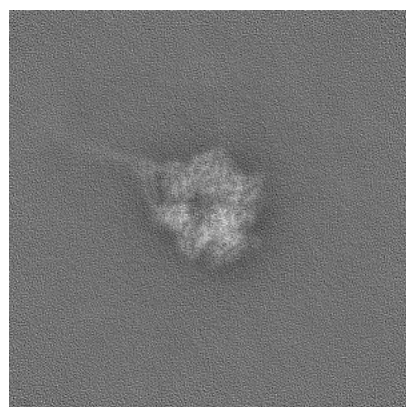


Y

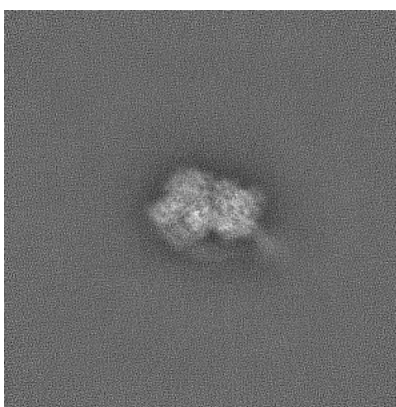


Z

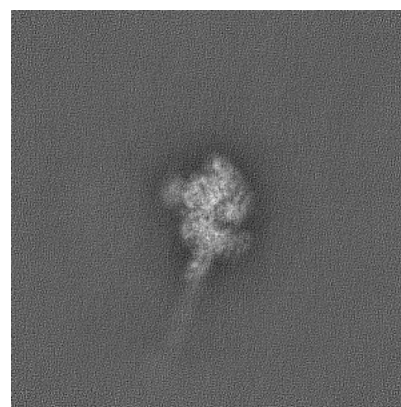
6.1.2 Raw map



X



Y

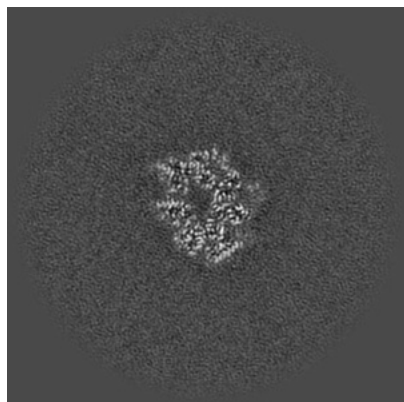


Z

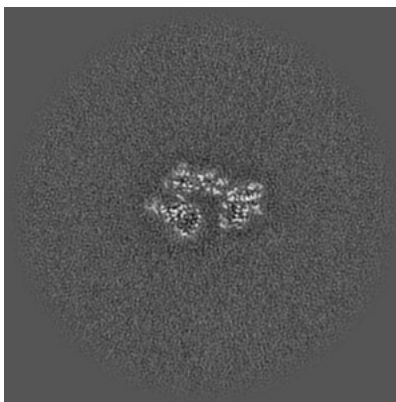
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

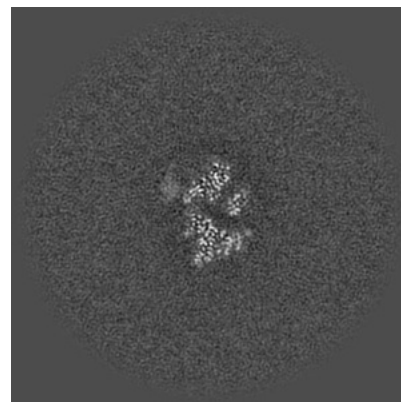
6.2.1 Primary map



X Index: 192

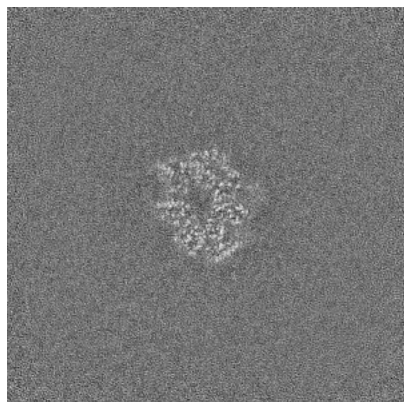


Y Index: 192

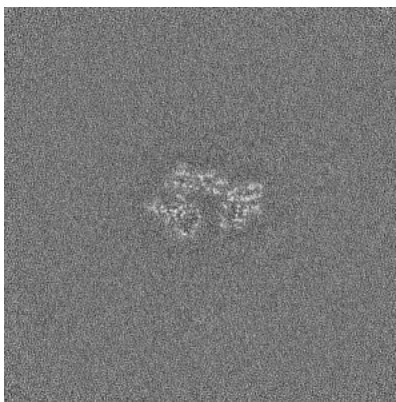


Z Index: 192

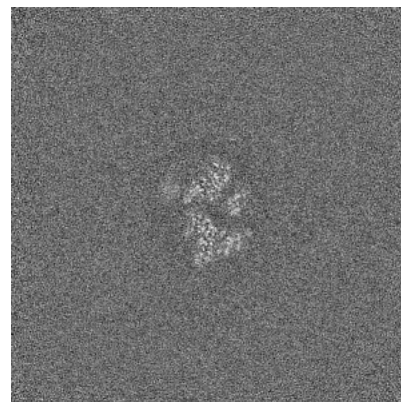
6.2.2 Raw map



X Index: 192



Y Index: 192

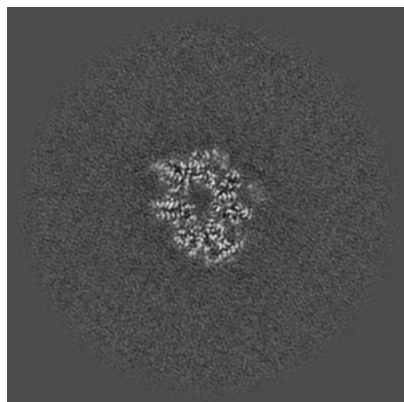


Z Index: 192

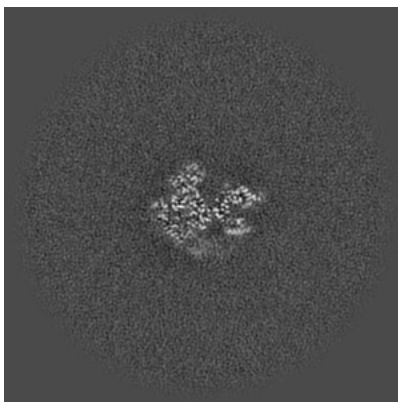
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

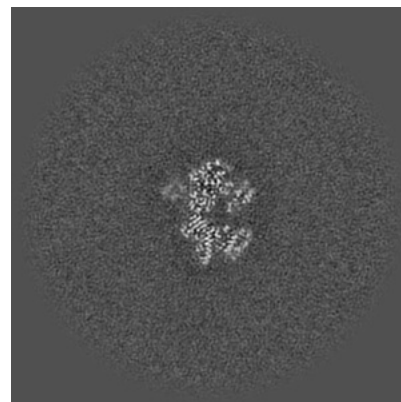
6.3.1 Primary map



X Index: 191

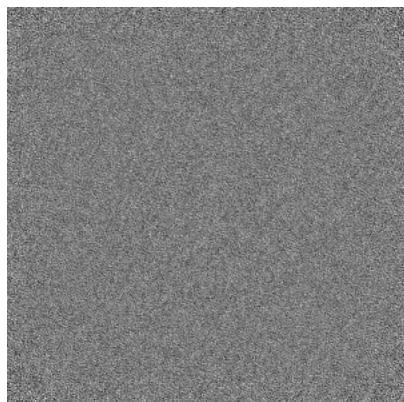


Y Index: 206

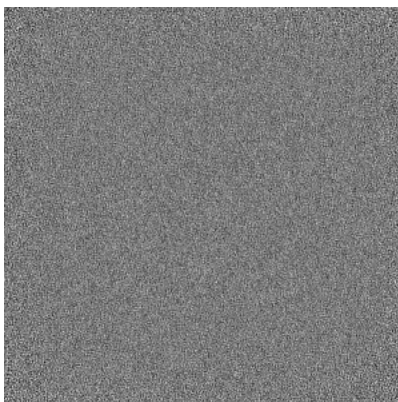


Z Index: 184

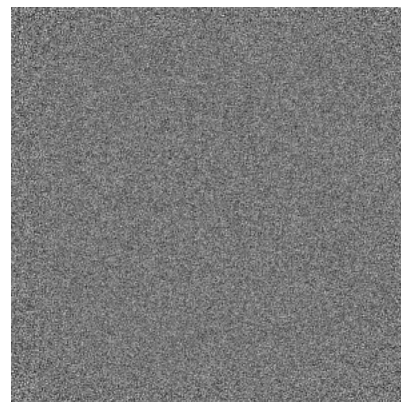
6.3.2 Raw map



X Index: 0



Y Index: 0

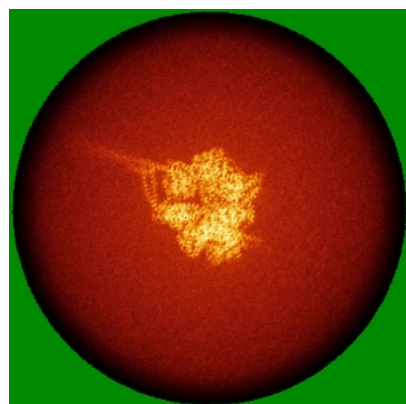


Z Index: 0

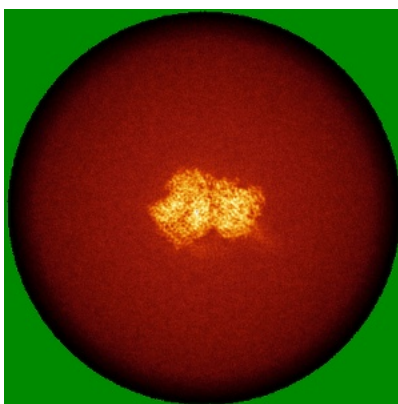
The images above show the largest variance slices of the map in three orthogonal directions.

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

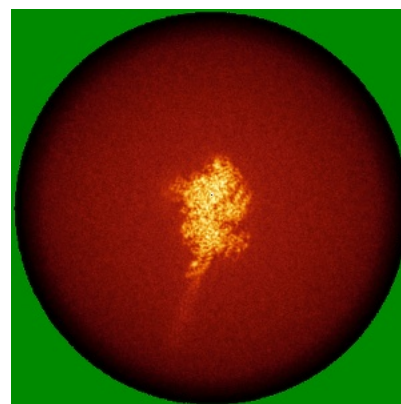
6.4.1 Primary map



X

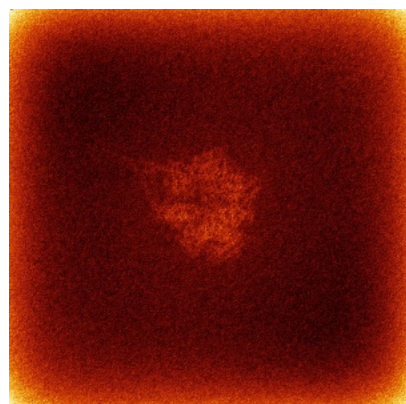


Y

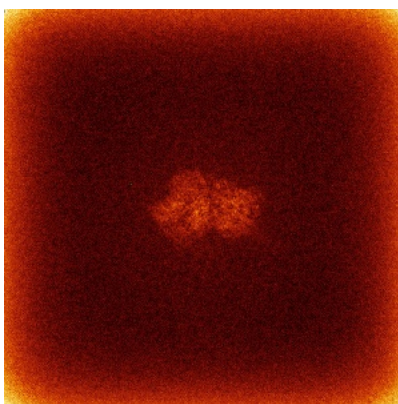


Z

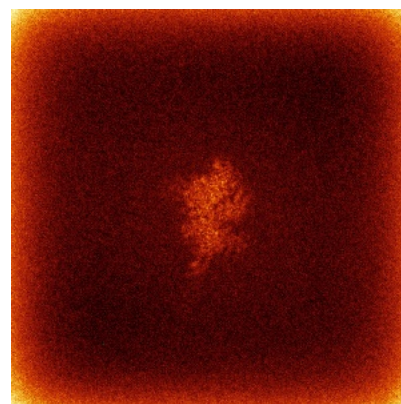
6.4.2 Raw map



X



Y

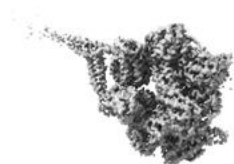


Z

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



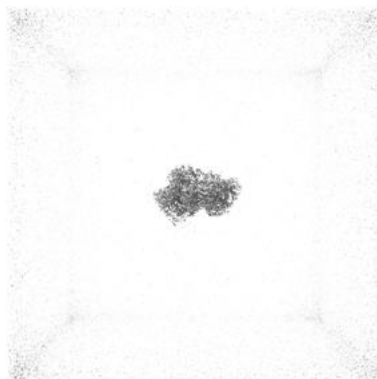
Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

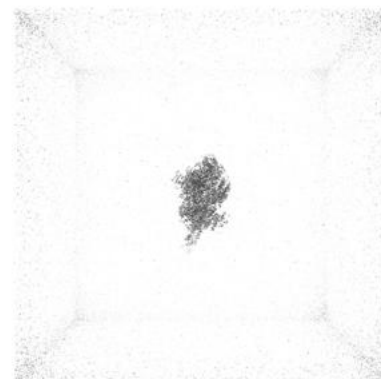
6.5.2 Raw map



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.

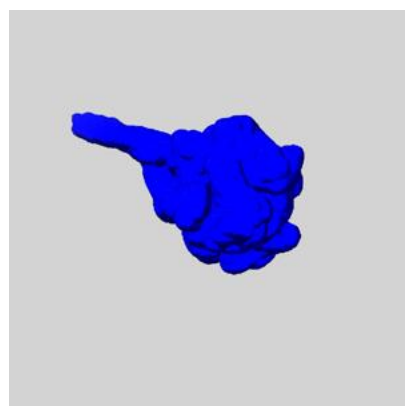
6.6 Mask visualisation [i](#)

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

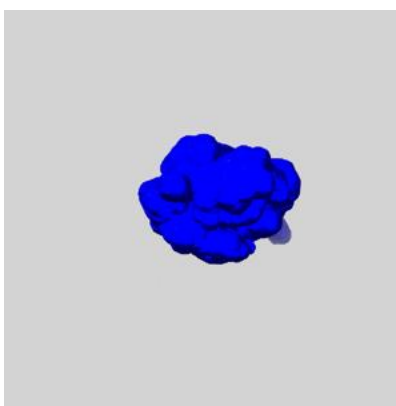
A mask typically either:

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

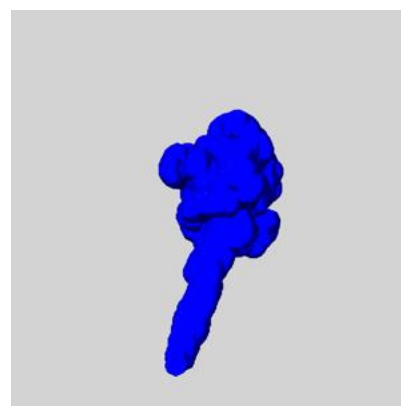
6.6.1 emd_46858_msk_1.map [i](#)



X



Y

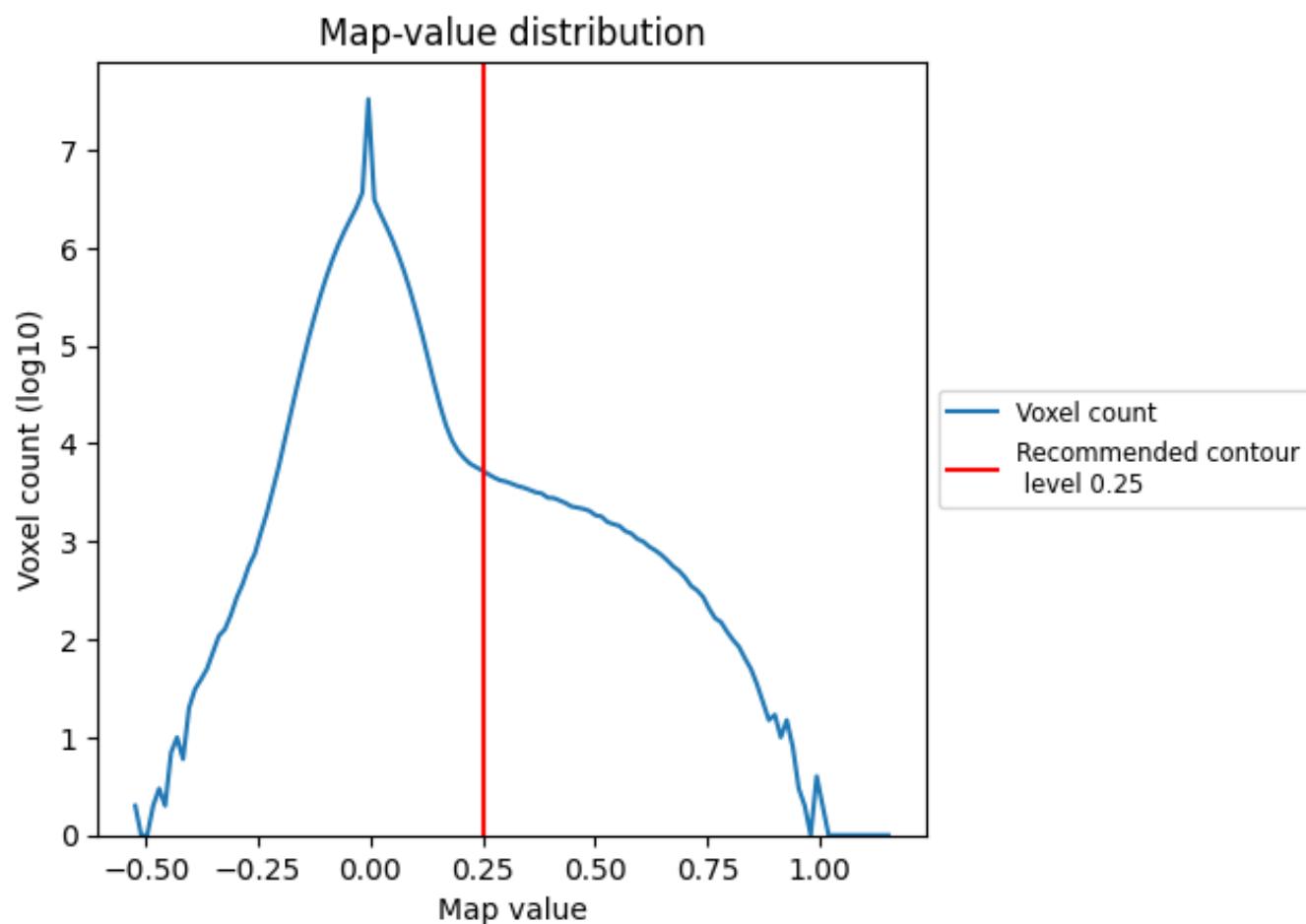


Z

7 Map analysis [i](#)

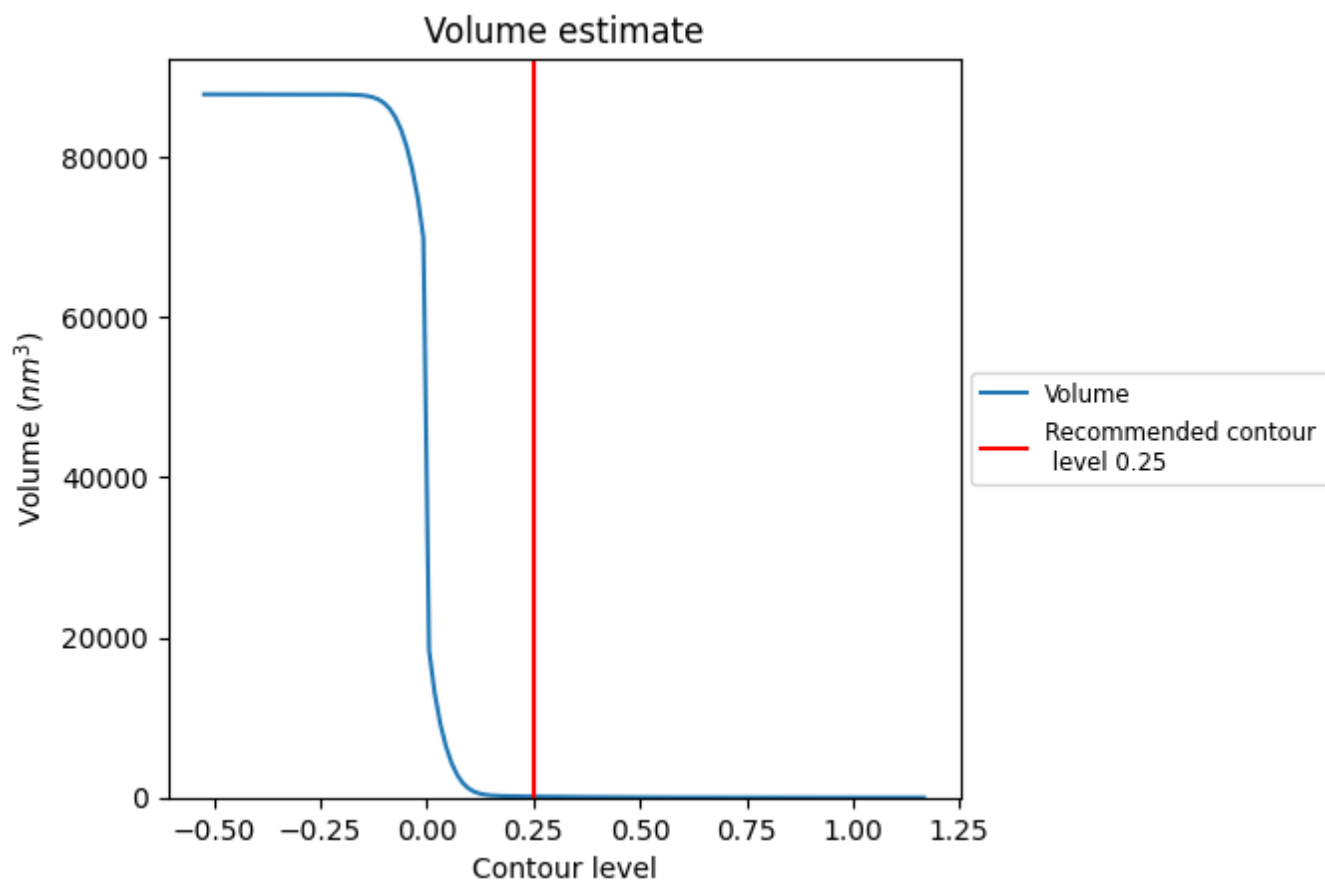
This section contains the results of statistical analysis of the map.

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.

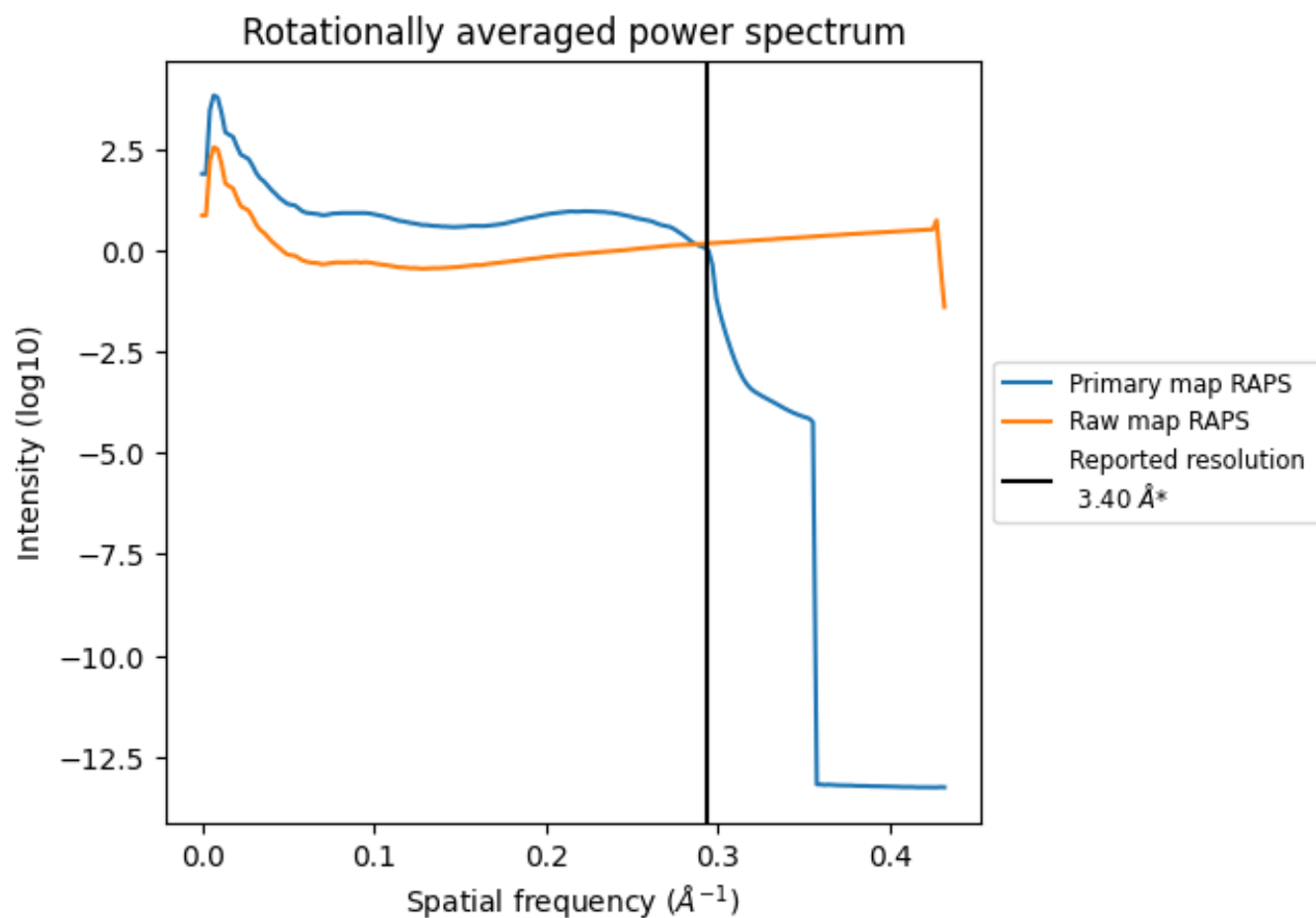
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 127 nm³; this corresponds to an approximate mass of 115 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 ⓘ

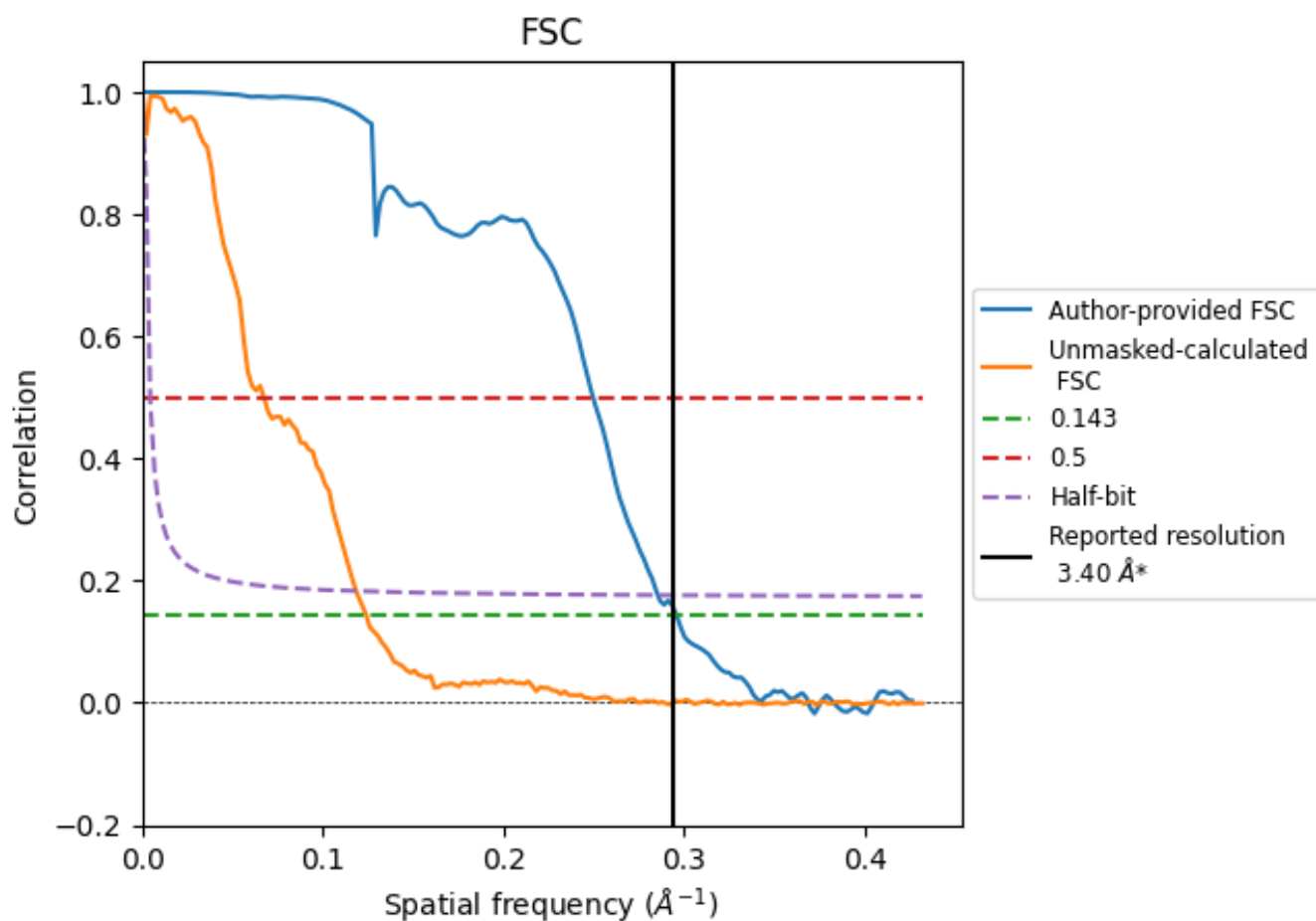


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 $0.294 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

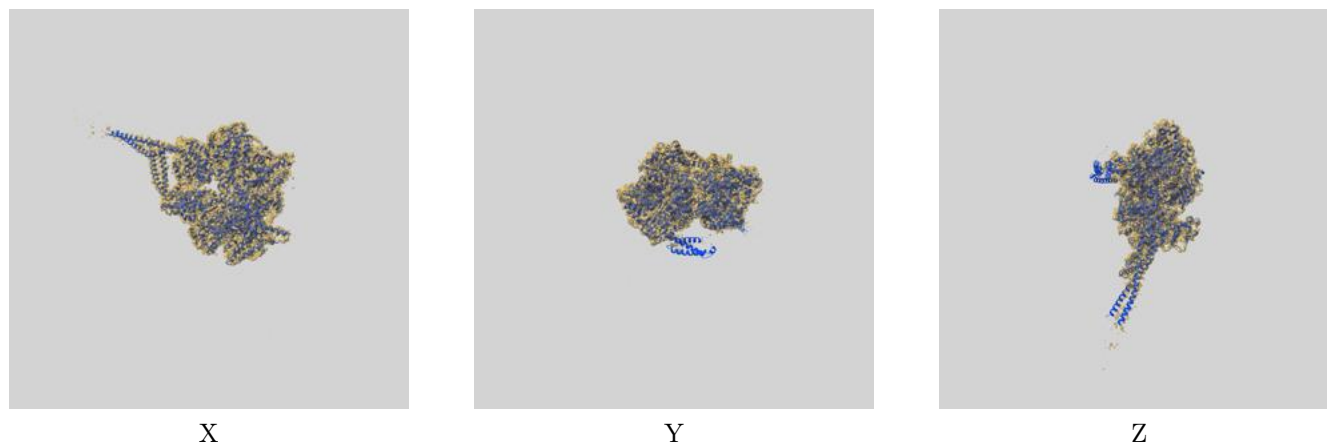
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.38	4.00	3.50
Unmasked-calculated*	8.06	14.84	8.43

*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 8.06 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

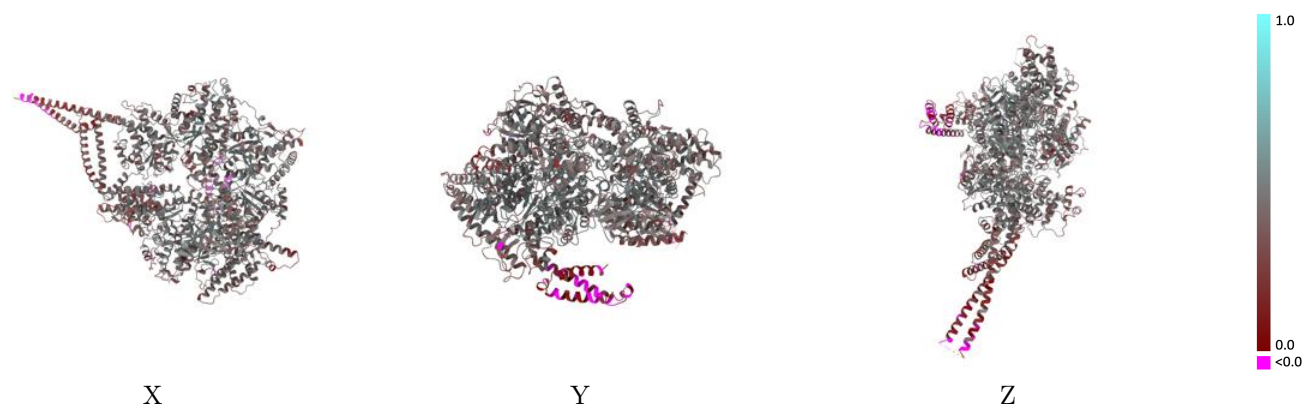
This section contains information regarding the fit between EMDB map EMD-46858 and PDB model 9DH7. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



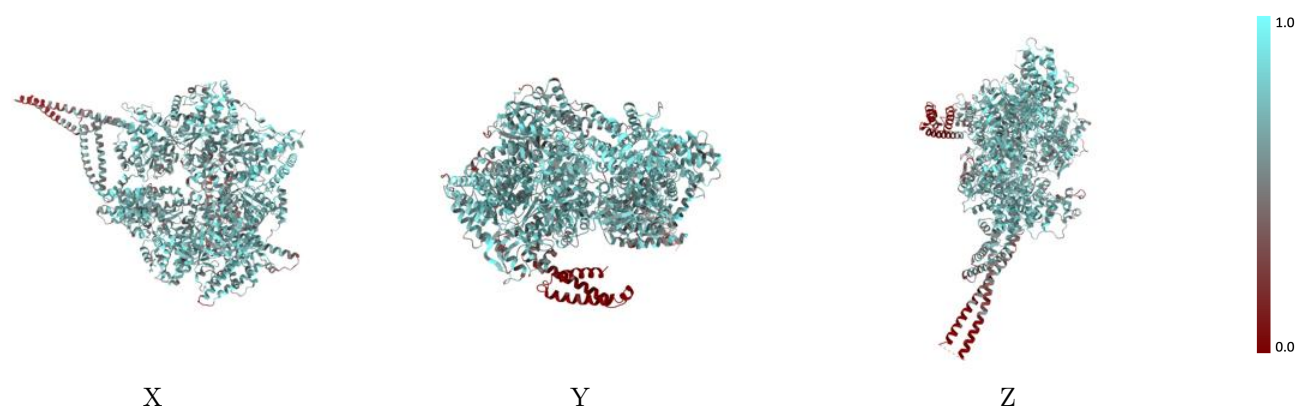
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



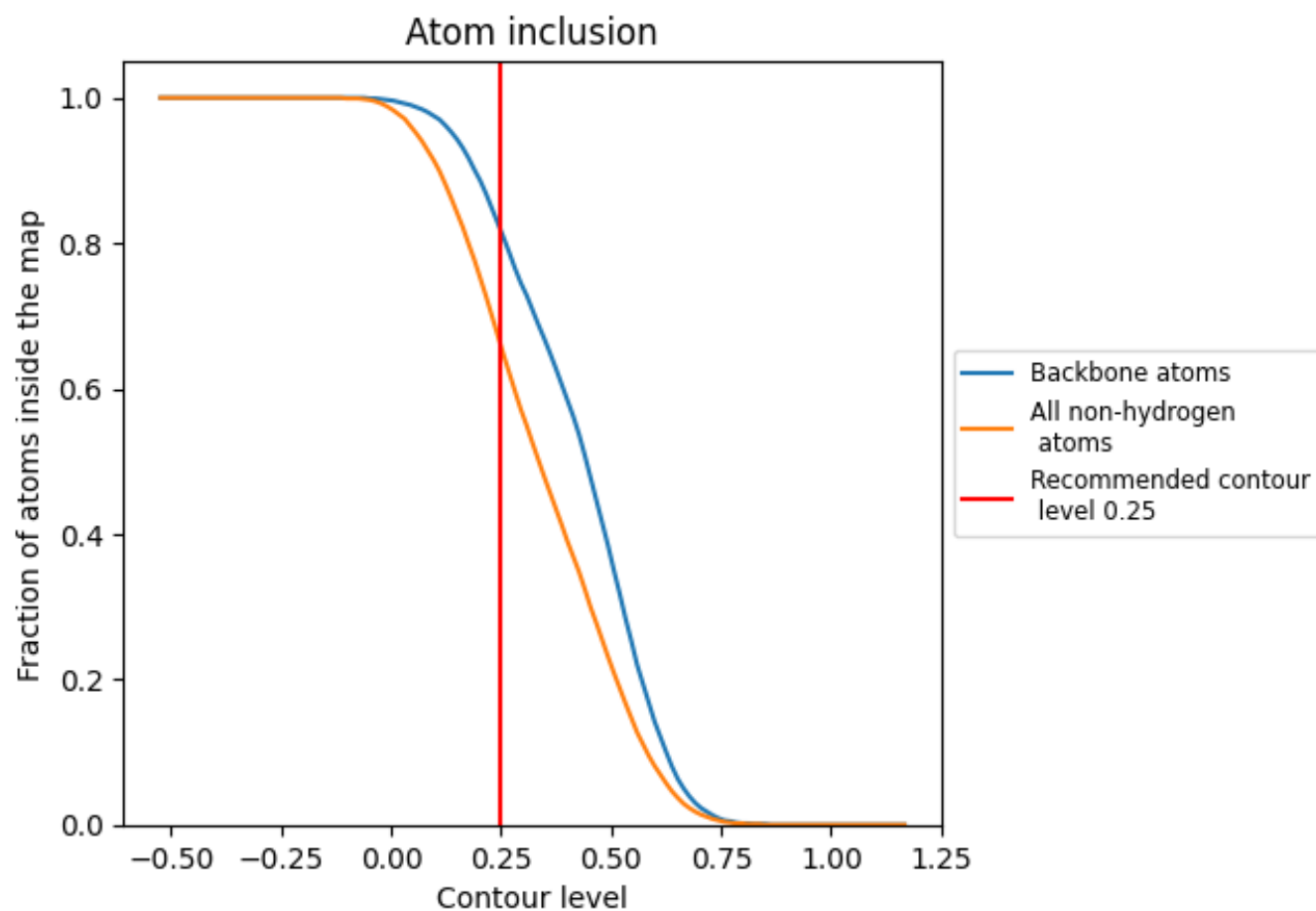
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 66% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6580	0.4120
A	0.6580	0.4120

