



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 10:34 AM UTC

PDB ID : 9BMY / pdb_00009bmy
EMDB ID : EMD-44715
Title : State-1 of motor domain from full-length human dynein-1 in apo condition
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 2.86 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

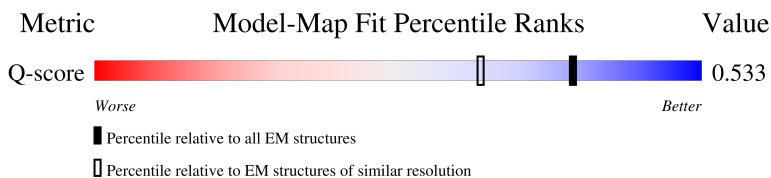
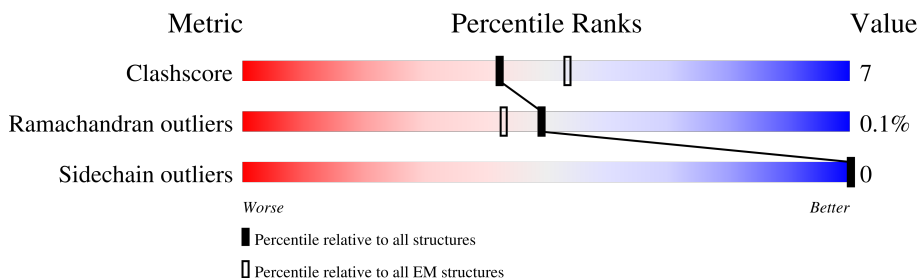
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.86 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	12017 (2.36 - 3.36)

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](#)

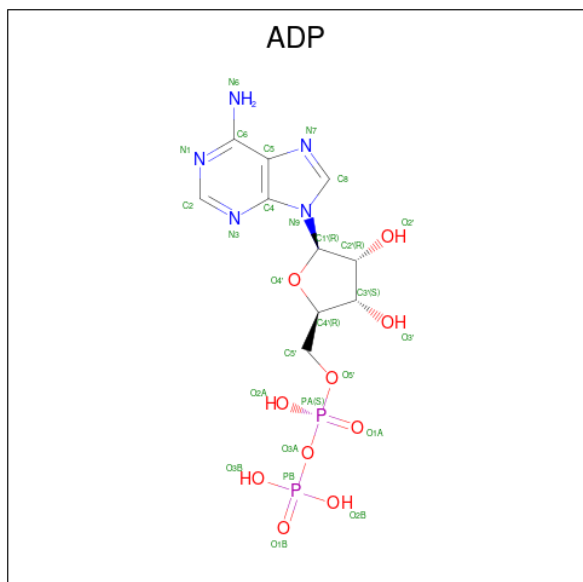
There are 4 unique types of molecules in this entry. The entry contains 23707 atoms, of which 0 are hydrogens and 0 are deuteriums.

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).





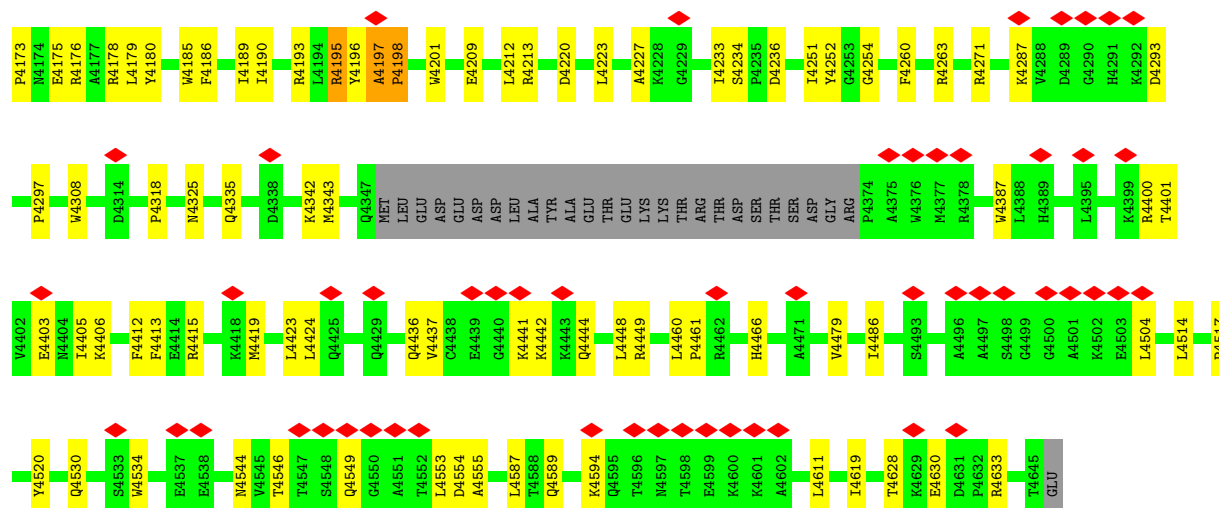
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

- 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

G2196	E2197	K2206	V2207	L2208	Y2211	T2214	M2221	G2224	P2225	S2226	K2230	D2269	P2270	N2271	L2279	S2290	E2294	L2295	N2316	S2317	V2318	L2319	D2320	D2321	R2332	F2343	Q2346	L2353	A2354	T2355	V2356	C2359	G2360	M2361	F2364	I2374	P2386	E2389	GLY									
Q2079	L2080	R2091	K2104	R2107	E2113	E2116	E2117	R2118	G2119	E2120	A2121	V2122	D2123	E2124	H1985	G2125	E2126	E2129	N2130	L2131	P2132	E2133	Q2134	E2135	I2136	L2137	I2138	Q2139	T2144	M2145	L2149	L2157	L2160	S2162	D2163	V2164	F2165	H2171	R2172	G2173	E2174	M2175	T2176	R2179	D2195			
T1693	A1908	E1914	V1929	F1930	N1931	D1937	D1958	E1959	R1962	E1965	A1966	M1967	E1980	R1983	E1984	H1985	S1986	N1987	P1988	N1989	Y1990	D1991	K1992	T1993	S1994	A1995	P1996	I1997	T1998	Q2005	S2026	W2027	L2028	L2032	R2037	S2038	L2039	Q2047	F2059	R2060	T2061	I2069	V2070	P2071				
S1554	A1555	D1556	H1559	R1567	I1571	F1575	M1579	V1591	Q1595	R1599	S1600	L1601	D1606	L1607	I1611	Q1612	R1621	E1622	R1623	S1624	S1625	F1629	Y1630	F1631	V1632	Q1634	E1635	L1638	M1646	V1647	A1648	K1649	L1666	N1667	E1668	D1669	M1670	S1671	V1672	V1673	K1687							
LYS	ASN	GLU	ALA	ILE	VAL	GLN	LYS	LEU	VAL	GLY	ASN	M1457	E1461	K1464	Q1465	I1466	R1467	L1475	V1478	L1486	I1487	R1488	G1489	W1490	D1491	H1500	K1508	L1509	S1510	Y1513	F1516	E1517	E1518	W1523	K1526	I1530	F1534	W1537	R1543									
ALA	SER	TYR	GLU	PHE	VAL	GLM	GLY	LEU	VAL	GLY	MET	MET	LEU	VAL	ILE	GLU	LEU	ILE	GLU	ASP	HIS	TRP	LYS	GLM	LEU	LYS	ARG	GLN	HIS	GLN	VAL	GLU	ASN	LEU	THR	LEU	GLN	ASP	TRP	ALA	ARG	GLY	GLN					
VAL	ALA	GLU	GLU	THR	LYS	PRO	PRO	GLY	TRP	VAL	VAL	TRP	VAL	GLU	ILE	ASP	GLY	GLY	PRO	TRP	LYS	VAL	GLN	GLN	PRO	LYS	ALA	VAL	GLN	ALA	GLU	THR	ASP	GLY	ASN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY				
TRP	GLU	LYS	PRO	VAL	PRO	VAL	ARG	GLY	GLY	ASN	LEU	GLN	ALA	THR	ILE	TYR	GLY	PHE	LYS	ASP	ASP	ASP	GLY	GLY	GLY	ALA	ALA	GLY	GLU	THR	LEU	LYS	GLY	LEU	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY			
ARG	PHE	GLN	PHE	PRO	PRO	SER	TRP	TRP	LEU	TYR	ILE	ASP	ASN	GLY	GLY	ARG	LYS	LYS	THR	PHE	ILE	GLY	ASP	THR	GLN	GLN	VAL	ALA	GLY	GLN	VAL	GLY	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY		
GLU	PHE	HIS	SER	GLN	ILE	SER	LYS	SER	ARG	GLY	VAL	VAL	THR	ASP	THR	GLY	ASP	GLY	THR	GLY	THR	LYS	VAL	GLN	SER	SER	GLY	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
ASN	LYS	LEU	ARG	THR	ASN	GLY	ASN	LEU	VAL	VAL	GLY	LEU	GLY	THR	TRP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY

P3979	H3880	L3692	F3520	ILE	TYR	VAL	SER	R3167	M3030	D2851	R2694	E2513	GLU
A3980	K3891	C3693	M3524	ARG	ASN	LYS	GLN	+	Q3038	A2854	D2697	N2531	ASP
Q3985	T3895	S3694	D3546	LEU	TYR	ALA	ILE	T3172	M3043	H2857	Q2698	D2536	ALA
R3989	E3898	V3703	I3547	GLU	ILE	LEU	GLN	H3175	L3044	E2864	C2712	Y2537	GLN
R3997	E3898	V3716	I3547	SER	ASN	SER	GLN	H3182	D3045	E2864	R2720	E2538	ARG
L4001	D3902	L3731	L3553	ILE	ARG	ILE	LEU	H3183	E3049	M2867	R2729	W2548	ARG
L4002	F3908	L3740	D3557	ALA	ALA	LEU	GLN	Y3183	I3059	S2868	W2730	W2557	LYS
V4009	L3909	R3741	E3558	TYR	LEU	LEU	GLN	A3184	E3049	R2869	V2731	V2562	GLU
L4013	R3910	L3742	W3562	GLY	CYS	GLY	VAL	L3194	I3059	T2882	P2732	V2567	ASP
M4021	N3912	R3743	L3578	R3206	ASP	GLU	ILE	R3206	F3066	P2883	Y2738	A2563	GLY
E4034	E3913	Q3744	M3579	T3211	THR	SER	ALA	+	E3073	L2905	R2756	A2564	GLU
P4037	I3914	L3745	R3581	D3213	VAL	THR	ASP	Y3212	K3076	D2906	L2756	P2565	ALA
M4043	V3915	L3750	K3583	E3216	TRP	TRP	GLN	D3213	D3077	F2912	R2757	V2567	ALA
A4051	L3916	N3754	F3584	E3217	ALA	GLN	MET	+	N3092	M2913	M2755	D2567	ALA
I4071	S3917	K3757	R3585	E3218	ILE	ALA	SER	E3216	D3096	E2914	L2756	D2567	ALA
M4087	A3918	G3758	R3585	E3219	ALA	ARG	LYS	E3217	W3097	E2914	R2757	D2567	ALA
V4088	G3919	L3760	L3588	E3220	ASN	ILE	GLU	E3218	D3096	E2914	R2757	D2567	ALA
R4092	S3920	L3761	T3597	E3221	TYR	ILE	LEU	E3219	W3097	E2914	R2757	D2567	ALA
L4096	T3921	D3762	L3600	E3222	ALA	MET	ASP	E3220	T3110	E2914	R2757	D2567	ALA
M4097	P3922	G3763	M3601	E3223	ASP	ARG	LYS	E3221	S3111	E2914	R2757	D2567	ALA
V4099	R3923	D3764	K3608	E3224	MET	GLU	VAL	E3222	K3112	E2914	R2757	D2567	ALA
H4100	I3924	T3765	K3608	E3225	LEU	ASN	GLU	E3223	M3113	E2914	R2757	D2567	ALA
G4104	Q3925	L3766	R3611	E3226	LYS	PHE	PRO	E3224	L3114	E2914	R2757	D2567	ALA
W4105	G3926	L3767	R3611	E3227	VAL	ILE	ALA	E3225	L3115	E2914	R2757	D2567	ALA
L4106	R3926	L3774	D3617	E3228	GLU	PRO	VAL	E3226	F3116	E2914	R2757	D2567	ALA
M4107	E3930	R3775	E3617	E3229	LEU	THR	ILE	E3227	K3117	E2914	R2757	D2567	ALA
L4116	E3933	E3776	E3624	E3230	ASN	ILE	ALA	E3228	P3118	E2914	R2757	D2567	ALA
Q4117	A3934	A3777	L3634	E3231	GLU	ALA	VAL	E3229	K3124	E2914	R2757	D2567	ALA
P4118	V3935	R3782	V3638	E3232	LYS	GLU	LYS	E3230	Y3125	E2914	R2757	D2567	ALA
T4127	R3937	L3788	P3643	E3233	LEU	ILE	ILE	E3231	L3133	E2914	R2757	D2567	ALA
M4128	L3938	I3789	R3643	E3234	GLU	SER	SER	E3232	P3134	E2914	R2757	D2567	ALA
R4143	S3939	V3790	R3651	E3235	ASP	SER	LYS	E3233	Q3135	E2914	R2757	D2567	ALA
P4150	F3944	I3821	R3652	E3236	ASP	ALA	HIS	E3234	H3139	E2914	R2757	D2567	ALA
T4160	K3945	L3829	R3655	E3237	LYS	ASP	LEU	E3235	R3140	E2914	R2757	D2567	ALA
R4168	D3946	L3835	R3660	E3238	ASN	GLY	VAL	E3236	E3141	E2914	R2757	D2567	ALA
S4172	V3950	Y3836	L3661	E3239	GLN	LYS	GLU	E3237	A3142	E2914	R2757	D2567	ALA
	Y3951	Y3836	V3666	E3240	GLN	MET	VAL	E3238	I3143	E2914	R2757	D2567	ALA
	Q3952	V3839	D3666	E3241	LYS	LYS	VAL	E3239	V3148	E2914	R2757	D2567	ALA
	A3953	D3862	Q3667	E3242	ALA	SER	ARG	E3240	Q3152	E2914	R2757	D2567	ALA
	D3954	L3863	I3669	E3243	ASN	TYR	ALA	E3241	L3153	E2914	R2757	D2567	ALA
	E3955	L3863	I3669	E3244	GLY	MET	ALA	E3242	L3154	E2914	R2757	D2567	ALA
	Q3956	V3866	T3681	E3245	VAL	SER	PRO	E3243	A3157	E2914	R2757	D2567	ALA
	P3966	R3870	D3691	E3246	GLN	ASN	ALA	E3244	R3160	E2914	R2757	D2567	ALA
	L3973			E3247	ASN	VAL	ALA	E3245	K3163	E2914	R2757	D2567	ALA
	H3974			E3248	GLY	VAL	ALA	E3246	R3164	E2914	R2757	D2567	ALA
	S3975			E3249	GLY	VAL	ALA	E3247		E2914	R2757	D2567	ALA
	E3976			E3250	LYS	VAL	LYS	E3248		E2914	R2757	D2567	ALA
	E3977			E3251	LYS	VAL	LYS	E3249		E2914	R2757	D2567	ALA
	T3978			E3252	VAL	VAL	ALA	E3250		E2914	R2757	D2567	ALA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136324	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)	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	2.445	Depositor
Minimum map value	-1.410	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.35	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	0.18	0/24093	0.32	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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4195	ARG	Sidechain

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	23593	0	23657	315	0
2	A	81	0	36	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	12	3	0
4	A	2	0	0	0	0
All	All	23707	0	23705	317	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 (317) 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:2221:MET:HG2	1:A:2343:PHE:HB2	1.55	0.89
1:A:2629:GLU:OE2	1:A:2633:LYS:NZ	2.12	0.83
1:A:4271:ARG:HD3	1:A:4633:ARG:HH12	1.43	0.82
1:A:1490:TRP:HH2	1:A:1537:TRP:HD1	1.29	0.79
1:A:4088:VAL:HG11	1:A:4116:LEU:HD21	1.67	0.76
1:A:1571:ILE:HD13	1:A:1607:LEU:HB3	1.69	0.74
1:A:2149:LEU:HD11	1:A:2157:LEU:HD13	1.68	0.74
1:A:1490:TRP:CH2	1:A:1537:TRP:HD1	2.08	0.72
1:A:2788:THR:HG22	1:A:2789:GLN:HG2	1.72	0.72
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.71	0.71
1:A:2562:VAL:O	1:A:2804:ARG:NH1	2.21	0.71
1:A:2581:LEU:HD11	1:A:2593:LEU:HD21	1.72	0.71
1:A:2930:GLN:HG3	1:A:3059:ILE:HG23	1.73	0.71
1:A:4190:ILE:HD12	1:A:4201:TRP:HZ2	1.56	0.71
1:A:4549:GLN:HG3	1:A:4587:LEU:HB2	1.73	0.70
1:A:1466:ILE:HG12	1:A:1500:HIS:HD1	1.57	0.69
1:A:4197:ALA:HB3	1:A:4198:PRO:HD3	1.75	0.67
1:A:2444:GLU:H	1:A:2510:MET:HE3	1.61	0.66
1:A:3661:LEU:HD12	1:A:3668:ASP:HB2	1.76	0.65
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.24	0.64
1:A:2906:ASP:OD2	1:A:3655:ARG:NH1	2.29	0.64
1:A:2452:LEU:HD13	1:A:2729:ARG:HH21	1.63	0.64
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.79	0.64
1:A:2138:ILE:HD12	1:A:2161:LEU:HD22	1.79	0.64
1:A:2536:ASP:OD1	1:A:2576:ARG:NH1	2.31	0.63
1:A:4097:LYS:HA	1:A:4127:THR:HB	1.79	0.63
1:A:4176:ARG:NH1	1:A:4220:ASP:OD2	2.27	0.62
1:A:1487:ILE:HD12	1:A:1537:TRP:NE1	2.14	0.62
1:A:1908:ALA:HB3	1:A:2353:LEU:HD22	1.81	0.62
1:A:2080:LEU:O	1:A:4415:ARG:NH1	2.33	0.62
3:A:4702:ATP:H8	3:A:4702:ATP:H5'1	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3557:ASP:OD1	1:A:3743:ARG:NH1	2.32	0.62
3:A:4702:ATP:H5'1	3:A:4702:ATP:C8	2.34	0.62
1:A:1490:TRP:HH2	1:A:1537:TRP:CD1	2.17	0.61
1:A:1751:VAL:HG21	1:A:1878:LYS:HE3	1.83	0.61
1:A:2226:SER:HA	3:A:4702:ATP:O1G	2.00	0.61
1:A:2905:LEU:HD11	1:A:3652:GLU:HB3	1.83	0.60
1:A:2457:SER:HB2	1:A:2732:PRO:HB3	1.82	0.60
1:A:3761:LEU:HA	1:A:3767:ILE:HD11	1.82	0.60
1:A:4436:GLN:HG3	1:A:4441:LYS:HB2	1.84	0.60
1:A:2488:ARG:HG3	1:A:2492:ARG:HH12	1.65	0.59
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.85	0.59
1:A:4287:LYS:H	1:A:4293:ASP:HB3	1.68	0.59
1:A:1466:ILE:HG12	1:A:1500:HIS:ND1	2.17	0.59
1:A:1623:ARG:HD3	1:A:1630:TYR:HA	1.84	0.59
1:A:3909:LEU:HD21	1:A:4343:MET:HE2	1.84	0.59
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.85	0.59
1:A:2562:VAL:HG11	1:A:2755:MET:HB2	1.85	0.58
1:A:2841:GLU:OE1	1:A:2844:ARG:NH1	2.36	0.58
1:A:2356:VAL:HG13	1:A:2361:MET:HE3	1.84	0.58
1:A:2279:LEU:HA	1:A:2698:GLN:HG3	1.86	0.58
1:A:2422:ILE:HD13	1:A:2487:GLU:HA	1.85	0.58
1:A:3951:VAL:CG2	1:A:3973:LEU:HD21	2.33	0.58
1:A:2039:LEU:HD12	1:A:4254:GLY:HA2	1.84	0.58
1:A:4071:ILE:HD11	1:A:4096:LEU:HB3	1.86	0.57
1:A:3597:THR:HG23	1:A:3634:LEU:HD21	1.86	0.57
1:A:3655:ARG:HG2	1:A:3660:VAL:HG22	1.86	0.57
1:A:4544:ASN:HD22	1:A:4589:GLN:HG3	1.70	0.57
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.38	0.57
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.85	0.57
1:A:1931:ASN:HD22	1:A:2317:SER:H	1.51	0.56
1:A:2449:LEU:HD11	1:A:2454:CYS:SG	2.46	0.56
1:A:1567:ARG:O	1:A:1571:ILE:HG13	2.05	0.56
1:A:3951:VAL:HG22	1:A:3973:LEU:HD21	1.87	0.56
1:A:4168:ARG:NE	1:A:4220:ASP:OD1	2.30	0.56
1:A:1985:HIS:CD2	1:A:1997:ILE:HD13	2.41	0.56
1:A:3601:MET:HG3	1:A:3611:ARG:NH2	2.21	0.56
1:A:3891:LYS:HD2	1:A:4013:LEU:HD23	1.87	0.56
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.87	0.56
1:A:4444:GLN:O	1:A:4449:ARG:NH1	2.38	0.56
1:A:1537:TRP:CE3	1:A:1601:LEU:HD11	2.41	0.56
1:A:4554:ASP:OD1	1:A:4555:ALA:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.88	0.55
1:A:4071:ILE:HG13	1:A:4099:VAL:HG12	1.87	0.55
1:A:2319:LEU:HD13	1:A:2359:CYS:SG	2.45	0.55
1:A:4104:GLY:HA2	1:A:4107:MET:HE3	1.88	0.55
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.40	0.55
1:A:1998:THR:HG21	1:A:2005:GLN:HB3	1.88	0.55
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.89	0.54
1:A:2144:THR:HG22	1:A:2145:MET:HE2	1.89	0.54
1:A:2694:ARG:NH1	1:A:2697:ASP:OD2	2.40	0.54
1:A:1543:ARG:NH1	1:A:1612:GLN:OE1	2.41	0.53
1:A:2665:GLU:HB3	1:A:2668:LEU:HD12	1.90	0.53
1:A:3914:ILE:O	1:A:3937:ARG:NH1	2.42	0.53
1:A:2596:PRO:HB2	1:A:2738:TYR:CZ	2.43	0.53
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.89	0.53
1:A:3916:LEU:HD11	1:A:3937:ARG:HG3	1.91	0.53
1:A:1571:ILE:HD12	1:A:1611:ILE:HD11	1.90	0.53
1:A:1887:ARG:HE	1:A:2039:LEU:HD11	1.74	0.53
1:A:1487:ILE:HD12	1:A:1537:TRP:HE1	1.73	0.53
1:A:3044:LEU:HD22	1:A:3049:GLU:HB3	1.90	0.53
1:A:3750:LEU:O	1:A:3754:ASN:ND2	2.42	0.53
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.42	0.52
1:A:2621:ASN:OD1	1:A:3014:ASN:ND2	2.43	0.52
1:A:4196:TYR:O	1:A:4197:ALA:C	2.52	0.52
1:A:1832:ASN:HD21	1:A:1834:LYS:HB2	1.72	0.52
1:A:2620:LEU:HD22	1:A:2631:LEU:HD23	1.91	0.52
1:A:1687:LYS:HD3	1:A:1712:THR:HG23	1.91	0.52
1:A:4209:GLU:OE2	1:A:4213:ARG:NE	2.36	0.52
1:A:1929:VAL:H	1:A:2332:ARG:NH2	2.09	0.51
1:A:1965:GLU:HG2	1:A:2026:SER:HB3	1.91	0.51
1:A:3182:HIS:NE2	1:A:3582:ARG:O	2.40	0.51
1:A:1467:ARG:HE	1:A:1523:TRP:HZ2	1.56	0.51
1:A:2835:ASP:HB3	1:A:3092:ASN:HD22	1.74	0.51
1:A:2973:ASP:OD2	1:A:3007:ARG:NH2	2.43	0.51
1:A:3194:LEU:HD23	1:A:3500:MET:SD	2.51	0.51
1:A:4179:LEU:HD12	1:A:4223:LEU:HD22	1.92	0.51
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.91	0.51
1:A:4413:PHE:HD2	1:A:4504:LEU:HD13	1.75	0.51
1:A:4517:PRO:HG3	1:A:4611:LEU:HD13	1.93	0.51
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.43	0.51
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	1.93	0.51
1:A:3750:LEU:HG	1:A:3754:ASN:HD21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1671:SER:HB2	1:A:1693:THR:HG23	1.92	0.50
1:A:2487:GLU:O	1:A:2491:GLN:HG3	2.11	0.50
1:A:3624:GLU:HG3	1:A:3669:ILE:HD13	1.93	0.50
1:A:2807:PHE:CE2	1:A:2811:ARG:HD3	2.46	0.50
1:A:2211:TYR:O	1:A:2214:THR:OG1	2.29	0.50
1:A:1929:VAL:H	1:A:2332:ARG:HH21	1.59	0.50
1:A:2224:GLY:O	1:A:2346:GLN:HA	2.12	0.50
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	1.92	0.50
1:A:1860:GLN:HG2	1:A:1865:LYS:HG2	1.93	0.50
1:A:2294:GLU:OE1	1:A:2294:GLU:N	2.39	0.50
1:A:3211:THR:HG23	1:A:3761:LEU:HD11	1.93	0.50
1:A:1575:PHE:O	1:A:1579:MET:HG2	2.12	0.49
1:A:2638:TYR:HB3	1:A:2659:LEU:HD11	1.93	0.49
1:A:2917:ASP:OD2	1:A:2921:ARG:NH2	2.45	0.49
1:A:1929:VAL:HG13	1:A:1958:ASP:OD2	2.12	0.49
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.48	0.49
1:A:2773:MET:HE2	1:A:2802:TRP:CG	2.48	0.49
1:A:2564:ALA:HB3	1:A:2567:VAL:HG23	1.94	0.49
1:A:2773:MET:HB3	1:A:2799:MET:HE1	1.94	0.49
1:A:4180:TYR:OH	1:A:4220:ASP:OD1	2.31	0.49
1:A:4387:TRP:CD1	1:A:4479:VAL:HG11	2.47	0.49
1:A:1914:GLU:HG2	2:A:4701:ADP:O1A	2.13	0.49
1:A:2174:GLU:OE1	1:A:2176:THR:OG1	2.30	0.49
1:A:2374:ILE:HD13	1:A:2452:LEU:HD21	1.95	0.49
1:A:4403:GLU:HA	1:A:4406:LYS:HE2	1.95	0.49
1:A:2061:THR:OG1	1:A:2133:GLU:OE1	2.28	0.49
1:A:2994:MET:HE1	1:A:3008:MET:HG3	1.95	0.49
1:A:1556:ASP:OD2	1:A:1621:ARG:NH2	2.43	0.48
1:A:4043:MET:HB3	1:A:4051:ALA:HB3	1.95	0.48
1:A:4436:GLN:HG2	1:A:4442:LYS:HG2	1.95	0.48
1:A:1647:VAL:HG21	1:A:1670:ASN:HB3	1.95	0.48
1:A:2069:ILE:HB	1:A:2137:LEU:HD21	1.96	0.48
1:A:1959:GLU:HB3	1:A:1962:ARG:HG3	1.96	0.48
1:A:3944:PHE:CE1	1:A:3974:TRP:HB3	2.48	0.48
1:A:2869:ARG:HA	1:A:2869:ARG:NE	2.28	0.48
1:A:2445:HIS:NE2	1:A:2449:LEU:HD22	2.28	0.48
1:A:4251:ILE:HG22	1:A:4252:TYR:CD2	2.49	0.48
1:A:2443:LEU:HD21	1:A:2513:GLU:OE1	2.14	0.47
1:A:3485:GLU:OE2	1:A:3774:LYS:NZ	2.43	0.47
1:A:2445:HIS:HB3	1:A:2505:ASP:OD2	2.15	0.47
1:A:4400:ARG:HE	1:A:4405:ILE:HD11	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1761:ASN:HB3	1:A:1781:VAL:HG22	1.96	0.47
1:A:1931:ASN:HD21	1:A:2316:ASN:HB2	1.79	0.47
1:A:3030:MET:HE2	1:A:3030:MET:HA	1.97	0.47
1:A:3175:HIS:CD2	1:A:3585:ARG:HH22	2.32	0.47
1:A:3835:ILE:HG12	1:A:3870:ARG:HD2	1.95	0.47
1:A:2138:ILE:HD11	1:A:2165:PHE:CG	2.50	0.47
1:A:2751:PHE:HB3	1:A:2803:VAL:HG11	1.96	0.47
1:A:3950:LYS:HB3	1:A:3973:LEU:CD1	2.43	0.47
1:A:2386:PRO:HG3	1:A:2413:LEU:HD13	1.97	0.47
1:A:2850:ILE:HG22	1:A:2867:MET:HE1	1.95	0.47
1:A:3731:LEU:HD11	1:A:3790:VAL:HG12	1.96	0.47
1:A:4628:THR:OG1	1:A:4630:GLU:HG2	2.15	0.47
1:A:2134:GLN:O	1:A:2138:ILE:HG12	2.15	0.47
1:A:4175:GLU:OE1	1:A:4175:GLU:N	2.48	0.47
1:A:2175:MET:HE3	1:A:2208:LEU:HD22	1.97	0.46
1:A:2592:VAL:HG23	1:A:2731:VAL:HG11	1.97	0.46
1:A:3703:VAL:HG21	1:A:3829:LEU:HD22	1.97	0.46
1:A:1623:ARG:NH1	1:A:1632:VAL:O	2.48	0.46
1:A:3966:PRO:HG3	1:A:3997:ARG:HG3	1.97	0.46
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.15	0.46
1:A:3110:THR:O	1:A:3140:ARG:NH1	2.49	0.46
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.98	0.46
1:A:2790:PRO:HB3	1:A:3076:LYS:HG2	1.98	0.46
1:A:1937:ASP:HA	1:A:1967:MET:HG3	1.98	0.46
1:A:2994:MET:HE3	1:A:3066:PHE:HE1	1.81	0.46
1:A:3117:LYS:HE2	1:A:3139:HIS:CD2	2.51	0.46
1:A:3553:LEU:HB2	1:A:3578:ILE:HD13	1.97	0.46
1:A:3921:THR:HG21	1:A:3933:GLU:HG2	1.98	0.46
1:A:4172:SER:HB2	1:A:4173:PRO:HD3	1.99	0.46
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.98	0.45
1:A:3175:HIS:HB3	1:A:3516:TYR:CE1	2.50	0.45
1:A:4087:ALA:HA	1:A:4092:ARG:HB3	1.99	0.45
1:A:1879:LEU:HD22	2:A:4701:ADP:C4	2.52	0.45
1:A:2688:GLU:OE1	1:A:2689:HIS:CE1	2.69	0.45
1:A:2179:ARG:NH2	1:A:2195:ASP:OD1	2.43	0.45
1:A:2912:PHE:CE2	1:A:2914:GLU:HB2	2.52	0.45
1:A:4423:LEU:HD13	1:A:4466:HIS:ND1	2.31	0.45
1:A:1931:ASN:ND2	1:A:2316:ASN:HB2	2.31	0.45
1:A:2851:ASP:HA	1:A:2867:MET:HE3	1.99	0.45
1:A:4517:PRO:HG2	1:A:4619:ILE:HD12	1.98	0.45
1:A:4415:ARG:HE	1:A:4415:ARG:HB3	1.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2668:LEU:HD21	1:A:2720:ARG:CZ	2.47	0.45
1:A:4100:HIS:HB3	1:A:4128:MET:HB2	1.99	0.45
1:A:1635:GLU:HA	1:A:1638:LEU:HD12	1.98	0.45
1:A:2963:VAL:HG23	1:A:3643:PRO:HB2	1.99	0.45
1:A:4185:TRP:O	1:A:4189:ILE:HG12	2.18	0.44
1:A:3601:MET:HG3	1:A:3611:ARG:HH21	1.80	0.44
1:A:4189:ILE:O	1:A:4193:ARG:HG3	2.17	0.44
1:A:1697:LYS:HB3	1:A:1700:GLU:OE1	2.18	0.44
1:A:3217:GLU:HB2	1:A:3220:ARG:HH21	1.82	0.44
1:A:2975:ASP:O	1:A:2979:VAL:HG23	2.18	0.44
1:A:3232:LYS:HA	1:A:3232:LYS:HD3	1.76	0.44
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.99	0.44
1:A:1980:GLU:OE2	1:A:1983:ARG:NH1	2.51	0.44
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	2.00	0.44
1:A:2548:TRP:CD1	1:A:2576:ARG:HG2	2.53	0.44
1:A:3485:GLU:HG3	1:A:3488:ARG:HH22	1.83	0.44
1:A:4412:PHE:HZ	1:A:4514:LEU:HD13	1.82	0.44
1:A:2079:GLN:HB2	1:A:2160:LEU:HD11	2.00	0.44
1:A:4186:PHE:O	1:A:4190:ILE:HG12	2.18	0.44
1:A:1625:SER:HB2	1:A:1699:ASN:ND2	2.33	0.43
1:A:2290:SER:HB2	1:A:2295:LEU:HG	1.99	0.43
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.50	0.43
1:A:4401:THR:O	1:A:4405:ILE:HG12	2.17	0.43
1:A:1623:ARG:NH1	1:A:1629:PHE:O	2.47	0.43
1:A:3910:ARG:HE	1:A:3913:GLU:CD	2.27	0.43
1:A:4227:ALA:HB2	1:A:4233:ILE:HD12	2.01	0.43
1:A:1724:VAL:HG11	1:A:1753:SER:HB3	2.00	0.43
1:A:1997:ILE:H	1:A:1997:ILE:HD12	1.83	0.43
1:A:3160:ARG:O	1:A:3163:LYS:HG2	2.17	0.43
1:A:4034:GLU:OE1	1:A:4143:ARG:NH1	2.41	0.43
1:A:4415:ARG:O	1:A:4419:MET:HG2	2.18	0.43
1:A:1666:LEU:HD23	1:A:1673:VAL:HA	2.00	0.43
1:A:2457:SER:O	1:A:2461:MET:HG3	2.18	0.43
1:A:2994:MET:HG3	1:A:2998:ASN:HD22	1.84	0.43
1:A:2776:PHE:HZ	1:A:2846:THR:HG23	1.83	0.43
1:A:3880:HIS:ND1	1:A:4021:MET:HG3	2.33	0.43
1:A:1834:LYS:HA	1:A:1834:LYS:HD3	1.88	0.43
1:A:2538:GLU:HB3	1:A:2548:TRP:CZ2	2.54	0.43
1:A:4173:PRO:HD2	1:A:4176:ARG:HH21	1.84	0.43
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	2.00	0.43
1:A:3936:VAL:O	1:A:3939:SER:OG	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3148:VAL:O	1:A:3152:GLN:HG3	2.19	0.43
1:A:3154:LEU:HG	1:A:3516:TYR:CD1	2.54	0.43
1:A:2028:LEU:HG	1:A:2032:LEU:HD23	1.99	0.42
1:A:2961:ILE:HG13	1:A:2963:VAL:HG13	2.00	0.42
1:A:4234:SER:OG	1:A:4236:ASP:OD1	2.31	0.42
1:A:4297:PRO:HB3	1:A:4308:TRP:CD1	2.54	0.42
1:A:4437:VAL:HG21	1:A:4448:LEU:HD13	2.00	0.42
1:A:3514:ILE:HD11	1:A:3553:LEU:HD13	2.00	0.42
1:A:3745:LEU:HD13	1:A:3777:ALA:HA	2.01	0.42
1:A:4196:TYR:CZ	1:A:4318:PRO:HB3	2.54	0.42
1:A:1853:VAL:HA	1:A:1856:GLN:HG3	2.01	0.42
1:A:2230:LYS:HG2	1:A:2364:PHE:CG	2.54	0.42
1:A:2825:TRP:CZ3	1:A:2854:ALA:HB2	2.55	0.42
1:A:2882:ILE:HB	1:A:2883:PRO:HD2	2.01	0.42
1:A:3194:LEU:HD21	1:A:3499:GLN:HB2	2.01	0.42
1:A:2488:ARG:CG	1:A:2492:ARG:HH12	2.32	0.42
1:A:2557:VAL:O	1:A:2757:ARG:NH2	2.52	0.42
1:A:2446:ILE:HD12	1:A:2446:ILE:HA	1.92	0.42
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.55	0.42
1:A:4546:THR:HG21	1:A:4589:GLN:HE21	1.84	0.42
1:A:1490:TRP:HZ3	1:A:1534:PHE:HB3	1.83	0.42
1:A:2784:PHE:HB3	1:A:2792:TYR:CD2	2.54	0.42
1:A:3558:GLU:HG2	1:A:3562:TRP:CE2	2.54	0.42
1:A:1738:TYR:HE2	1:A:1792:LEU:HD21	1.85	0.41
1:A:2059:PHE:CZ	1:A:2104:LYS:HD3	2.55	0.41
1:A:3110:THR:O	1:A:3113:MET:HB2	2.19	0.41
1:A:2163:ASP:OD1	1:A:4530:GLN:NE2	2.54	0.41
1:A:2221:MET:HE1	1:A:2355:THR:HG22	2.02	0.41
1:A:2864:GLU:O	1:A:2868:SER:OG	2.30	0.41
1:A:4106:LEU:HD23	1:A:4106:LEU:HA	1.93	0.41
1:A:4423:LEU:HD22	1:A:4466:HIS:HB2	2.01	0.41
1:A:4553:LEU:HD23	1:A:4553:LEU:HA	1.87	0.41
1:A:1526:LYS:O	1:A:1530:ILE:HG13	2.20	0.41
1:A:1623:ARG:NH2	1:A:1634:ASP:OD1	2.54	0.41
1:A:2107:ARG:HD2	1:A:2136:ILE:HG12	2.02	0.41
1:A:3862:ASP:OD1	1:A:3866:VAL:HG23	2.20	0.41
1:A:4190:ILE:HD12	1:A:4201:TRP:CZ2	2.45	0.41
1:A:1475:LEU:HD12	1:A:1591:VAL:HG21	2.02	0.41
1:A:1895:ALA:HB2	1:A:2037:ARG:HB2	2.02	0.41
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	2.02	0.41
1:A:3017:VAL:HB	1:A:3020:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2471:GLN:HE21	1:A:2471:GLN:HB3	1.73	0.41
1:A:3115:LEU:HD13	1:A:3143:ILE:HG21	2.01	0.41
1:A:3955:GLU:H	1:A:3955:GLU:CD	2.28	0.41
1:A:2581:LEU:HD12	1:A:2604:THR:HG22	2.02	0.41
1:A:2667:ASN:OD1	1:A:2712:CYS:HB2	2.20	0.41
1:A:3584:ASN:O	1:A:3651:ARG:NH2	2.53	0.41
1:A:3716:VAL:HB	1:A:3836:TYR:OH	2.20	0.41
1:A:3908:PHE:HE1	1:A:4001:LEU:HD11	1.86	0.41
1:A:3951:VAL:HG23	1:A:3973:LEU:HD21	2.01	0.41
1:A:2912:PHE:HE2	1:A:2914:GLU:HB2	1.86	0.41
1:A:2206:LYS:HA	1:A:2206:LYS:HD3	1.86	0.41
1:A:3912:ASN:O	1:A:3937:ARG:NH1	2.54	0.41
1:A:1508:LYS:HG2	1:A:1513:TYR:CZ	2.56	0.41
1:A:1899:ARG:N	1:A:1899:ARG:HD2	2.34	0.41
1:A:2582:TYR:CE2	1:A:2612:LEU:HD13	2.56	0.41
1:A:3985:GLN:HB3	1:A:3989:ARG:NH1	2.36	0.41
1:A:1478:VAL:CG2	1:A:1488:ARG:HH21	2.34	0.41
1:A:1486:LEU:HD23	1:A:1579:MET:HE2	2.03	0.41
1:A:2132:PRO:HB2	1:A:2135:GLU:HB3	2.02	0.41
1:A:3157:ALA:HB1	1:A:3524:MET:HE2	2.03	0.41
1:A:4424:LEU:HD13	1:A:4486:ILE:HG13	2.03	0.41
1:A:4534:TRP:CD2	1:A:4594:LYS:HD3	2.56	0.41
1:A:2290:SER:HA	1:A:2294:GLU:OE1	2.21	0.40
1:A:3588:LEU:HD21	1:A:3638:VAL:HG11	2.02	0.40
1:A:3821:ILE:HB	1:A:4342:LYS:HG2	2.04	0.40
1:A:4150:PRO:O	1:A:4195:ARG:NH2	2.53	0.40
1:A:2091:ARG:NH1	2:A:4701:ADP:H5'2	2.36	0.40
1:A:2353:LEU:C	1:A:2353:LEU:HD23	2.46	0.40
1:A:3133:LEU:HD11	1:A:3141:GLU:HB3	2.03	0.40
1:A:4099:VAL:HG23	1:A:4106:LEU:HD11	2.02	0.40
1:A:4260:PHE:HD1	1:A:4263:ARG:NH2	2.19	0.40
1:A:1744:LYS:HD3	1:A:1745:TYR:CE2	2.55	0.40
1:A:3113:MET:HE3	1:A:3184:ALA:HA	2.02	0.40
1:A:3229:LEU:HD12	1:A:3465:LEU:HD13	2.03	0.40
1:A:4002:LEU:HD11	1:A:4335:GLN:HB3	2.04	0.40
1:A:2925:ILE:HG13	1:A:2933:LEU:HD21	2.03	0.40
1:A:3001:ASP:OD1	1:A:3002:SER:N	2.54	0.40
1:A:3731:LEU:HD11	1:A:3790:VAL:CG1	2.52	0.40
1:A:3740:LEU:O	1:A:3744:GLN:HG3	2.20	0.40
1:A:3741:ARG:NH2	1:A:3776:GLU:OE1	2.53	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	2929/4646 (63%)	2882 (98%)	45 (2%)	2 (0%)	48	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4197	ALA
1	A	4198	PRO

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	2605/4125 (63%)	2605 (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 (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1465	GLN
1	A	1559	HIS
1	A	1569	GLN
1	A	1643	ASN
1	A	1646	ASN
1	A	1670	ASN
1	A	1855	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1894	GLN
1	A	1931	ASN
1	A	1974	GLN
1	A	1976	GLN
1	A	2067	ASN
1	A	2171	HIS
1	A	2296	GLN
1	A	2463	HIS
1	A	2464	GLN
1	A	2471	GLN
1	A	2475	ASN
1	A	2554	GLN
1	A	2685	GLN
1	A	2713	ASN
1	A	2930	GLN
1	A	3069	ASN
1	A	3092	ASN
1	A	3200	HIS
1	A	3214	GLN
1	A	3523	GLN
1	A	3526	GLN
1	A	3602	ASN
1	A	3636	GLN
1	A	3735	GLN
1	A	3754	ASN
1	A	3877	HIS
1	A	3878	GLN
1	A	3956	GLN
1	A	4054	HIS
1	A	4335	GLN
1	A	4425	GLN
1	A	4429	GLN
1	A	4453	ASN
1	A	4532	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 [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	4704	-	28,29,29	0.47	0	43,45,45	0.47	0
3	ATP	A	4702	4	32,33,33	0.56	0	48,52,52	0.58	0
2	ADP	A	4703	-	28,29,29	0.47	0	43,45,45	0.46	0
2	ADP	A	4701	4	28,29,29	0.45	0	43,45,45	0.49	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	-	-	2/16/32/32	0/3/3/3
3	ATP	A	4702	4	-	2/22/38/38	0/3/3/3
2	ADP	A	4703	-	-	1/16/32/32	0/3/3/3
2	ADP	A	4701	4	-	0/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

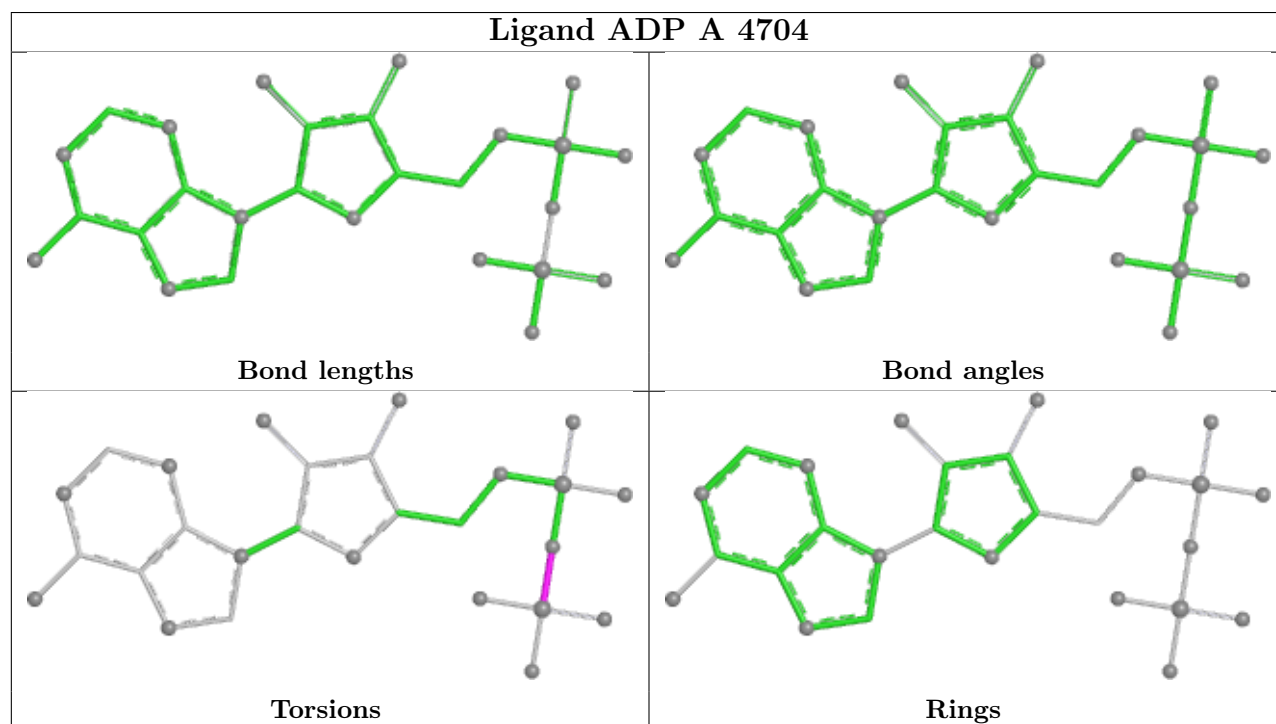
Mol	Chain	Res	Type	Atoms
2	A	4704	ADP	PA-O3A-PB-O2B
3	A	4702	ATP	O4'-C4'-C5'-O5'
2	A	4704	ADP	PA-O3A-PB-O1B
3	A	4702	ATP	C3'-C4'-C5'-O5'
2	A	4703	ADP	PA-O3A-PB-O3B

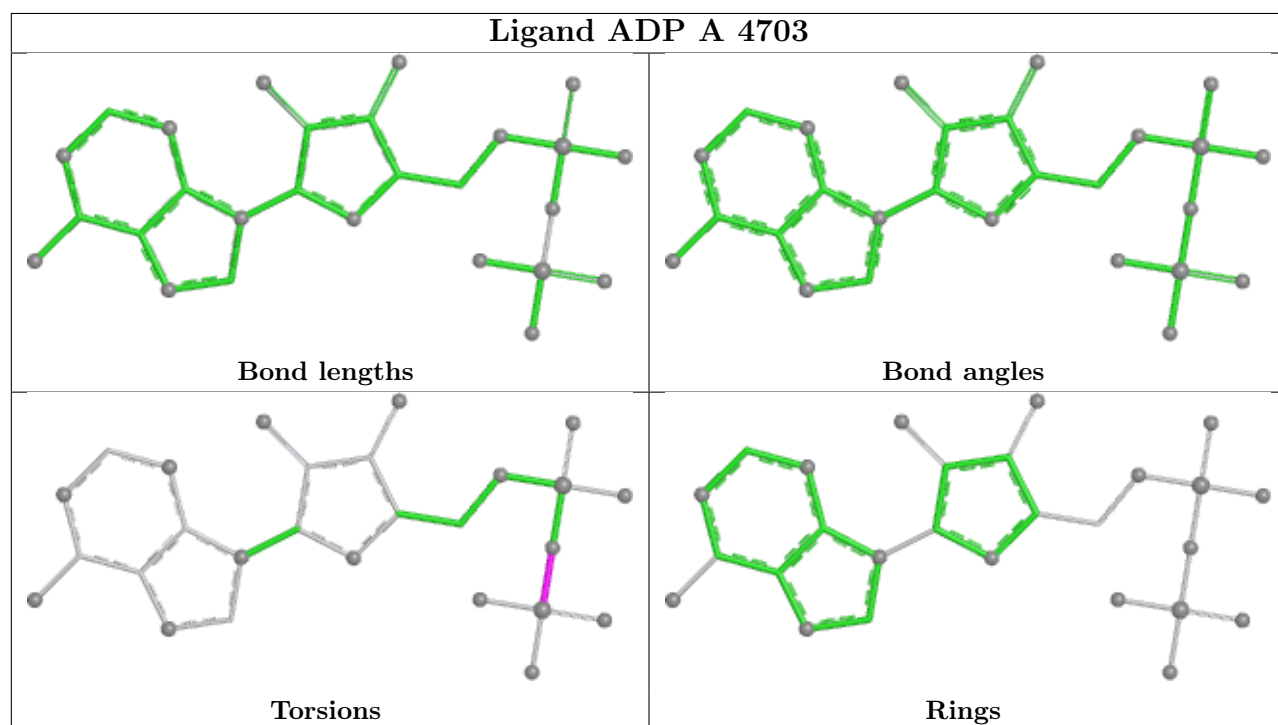
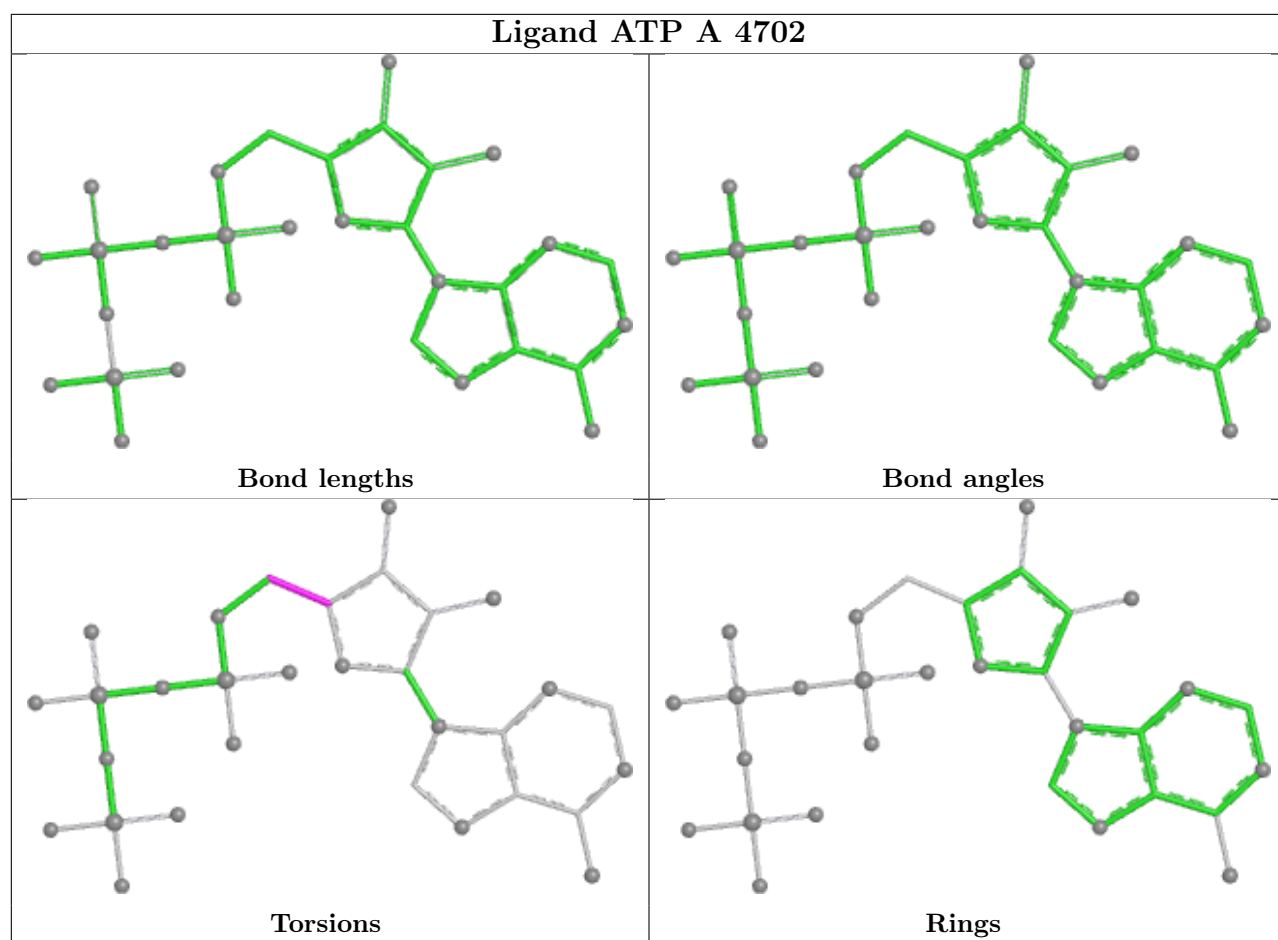
There are no ring outliers.

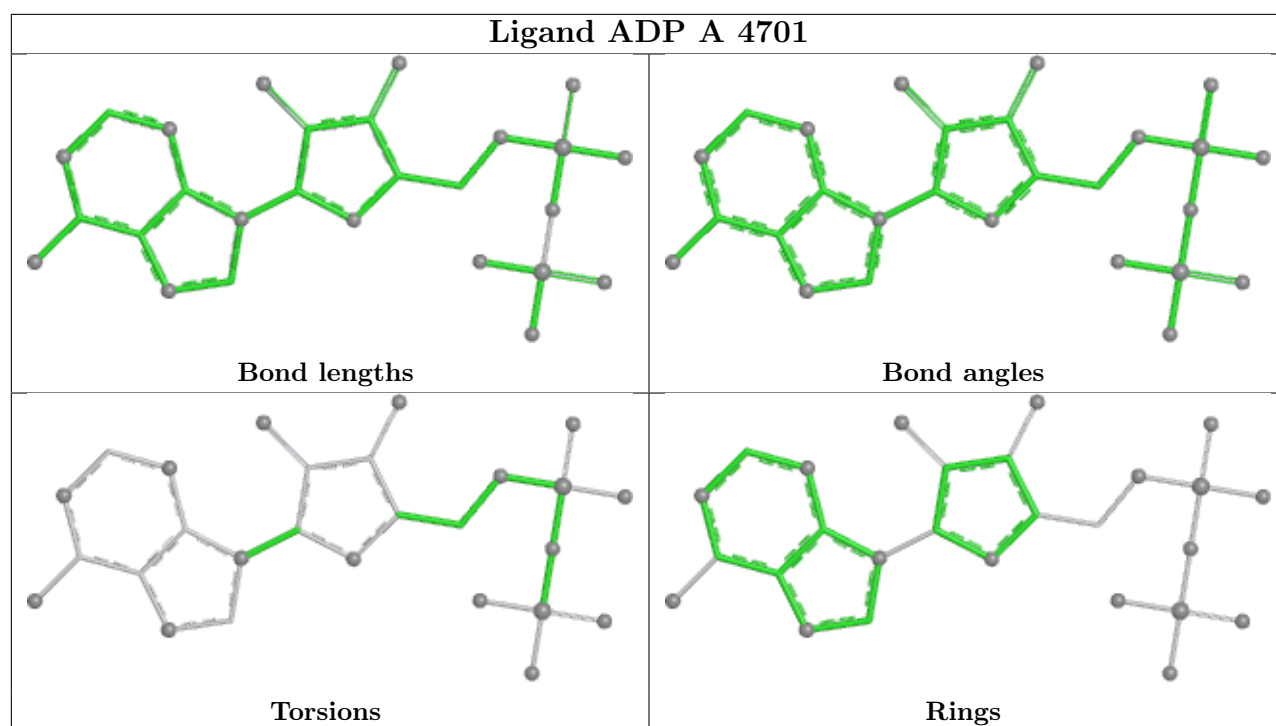
2 monomers are involved in 6 short contacts:

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

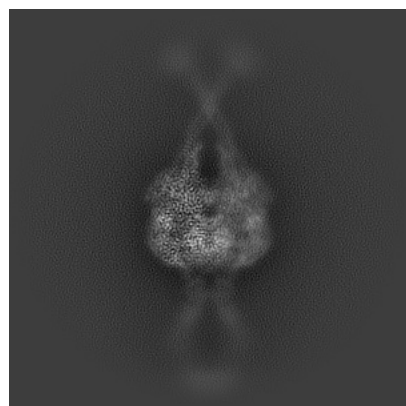
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44715. These allow visual inspection of the internal detail of the map and identification of artifacts.

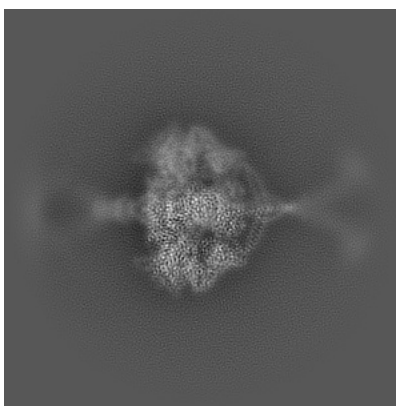
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

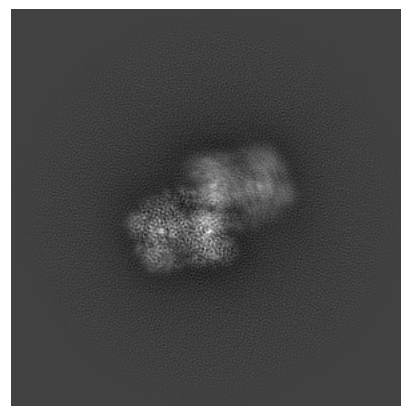
6.1.1 Primary map



X

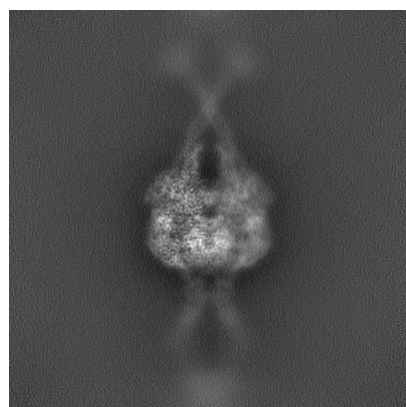


Y

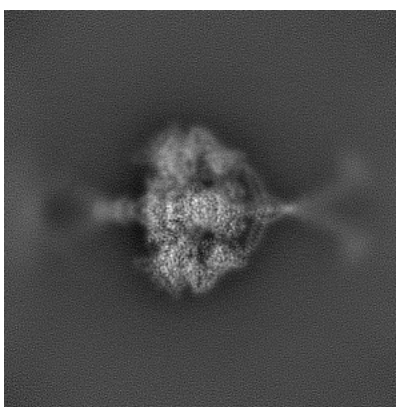


Z

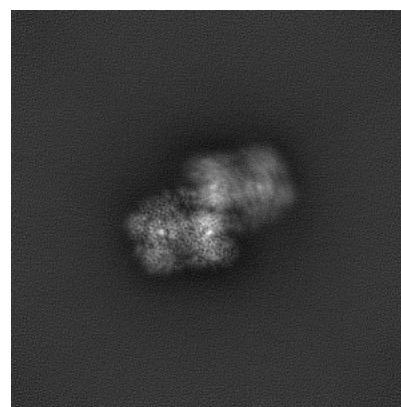
6.1.2 Raw map



X



Y

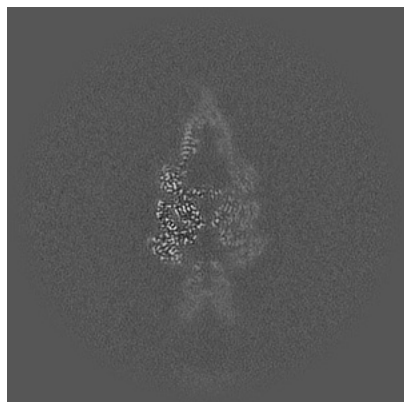


Z

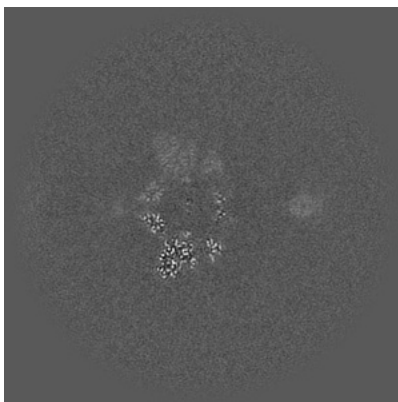
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 192

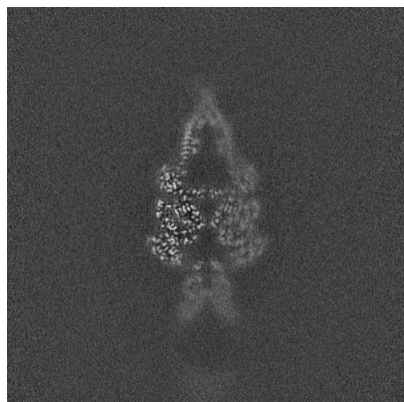


Y Index: 192

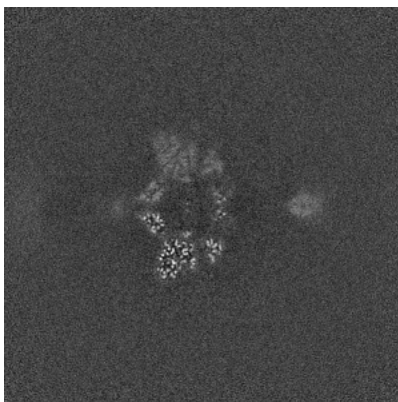


Z Index: 192

6.2.2 Raw map



X Index: 192



Y Index: 192

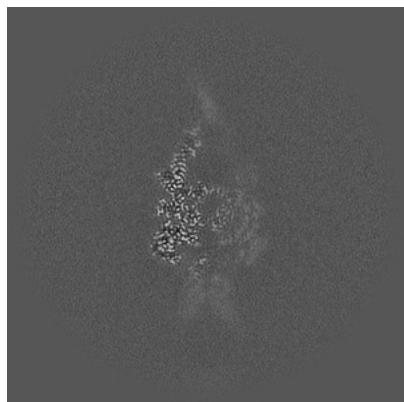


Z Index: 192

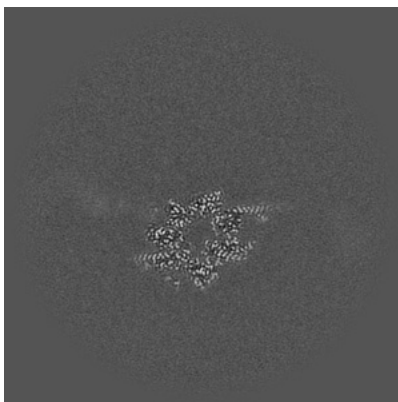
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

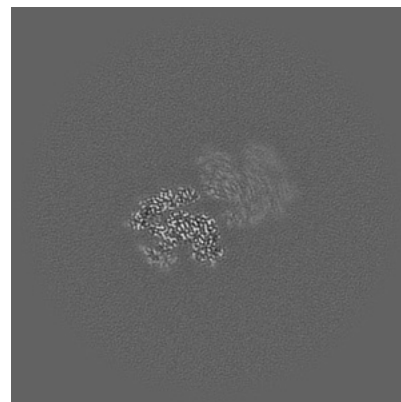
6.3.1 Primary map



X Index: 187

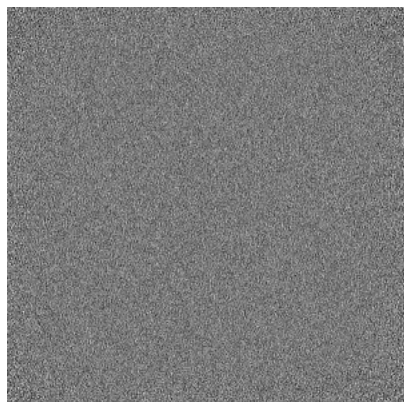


Y Index: 169

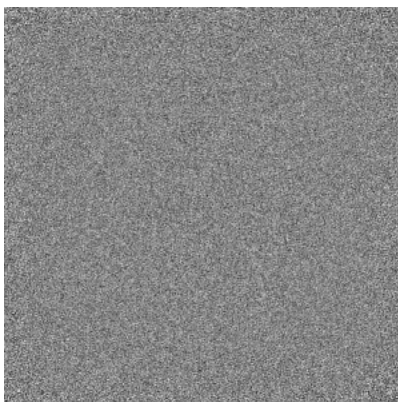


Z Index: 161

6.3.2 Raw map



X Index: 0



Y Index: 0

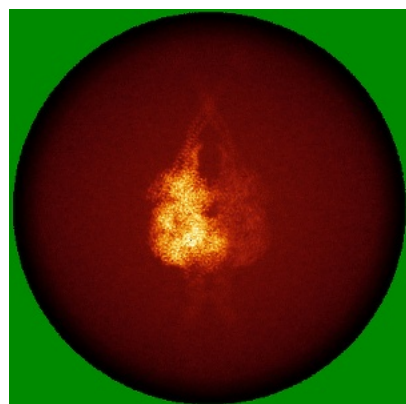


Z Index: 161

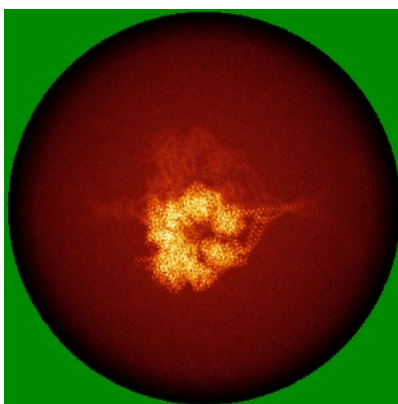
The images above show the largest variance slices of the map in three orthogonal directions.

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

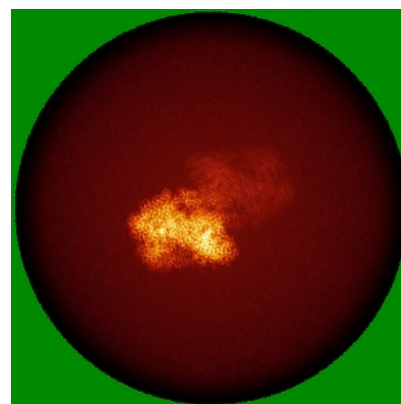
6.4.1 Primary map



X

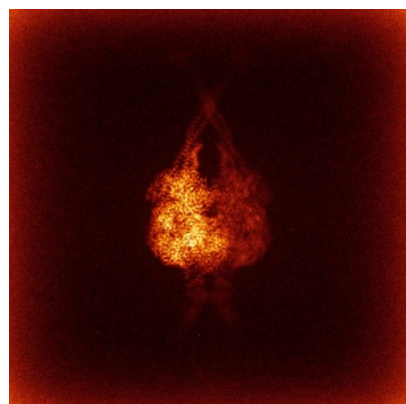


Y

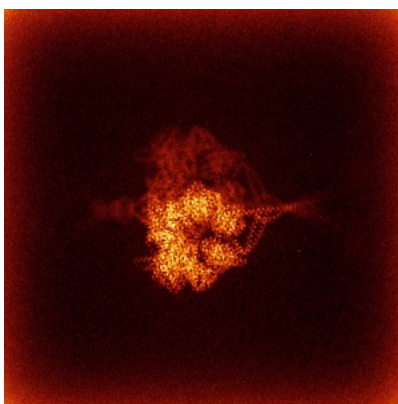


Z

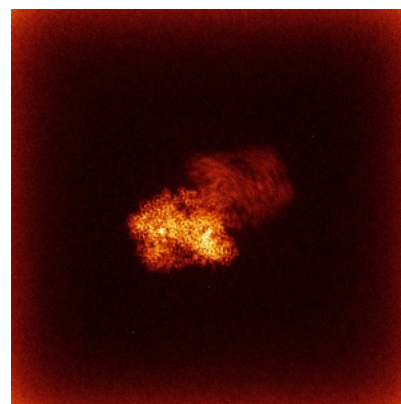
6.4.2 Raw map



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 0.35. 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.

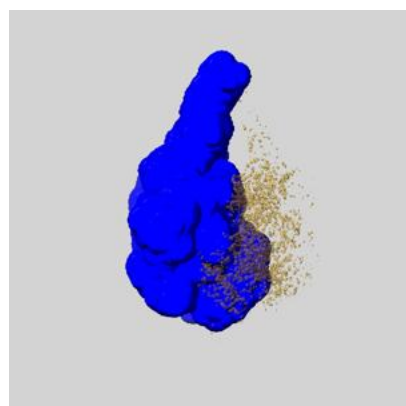
6.6 Mask visualisation [i](#)

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

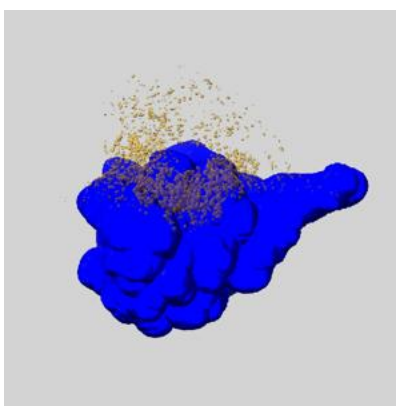
A mask typically either:

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

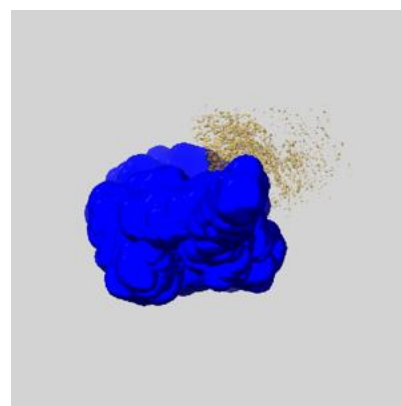
6.6.1 emd_44715_msk_1.map [i](#)



X



Y

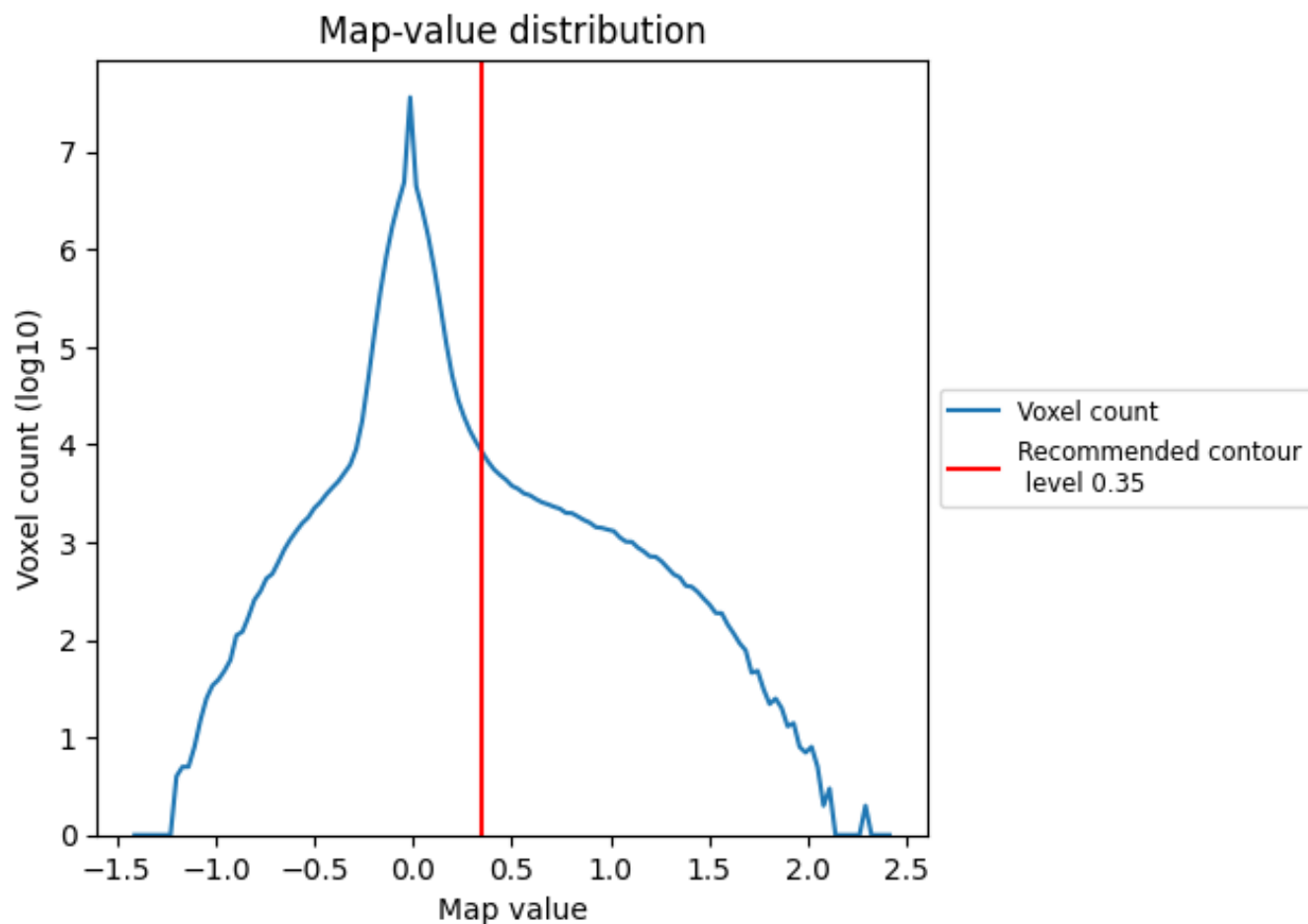


Z

7 Map analysis [i](#)

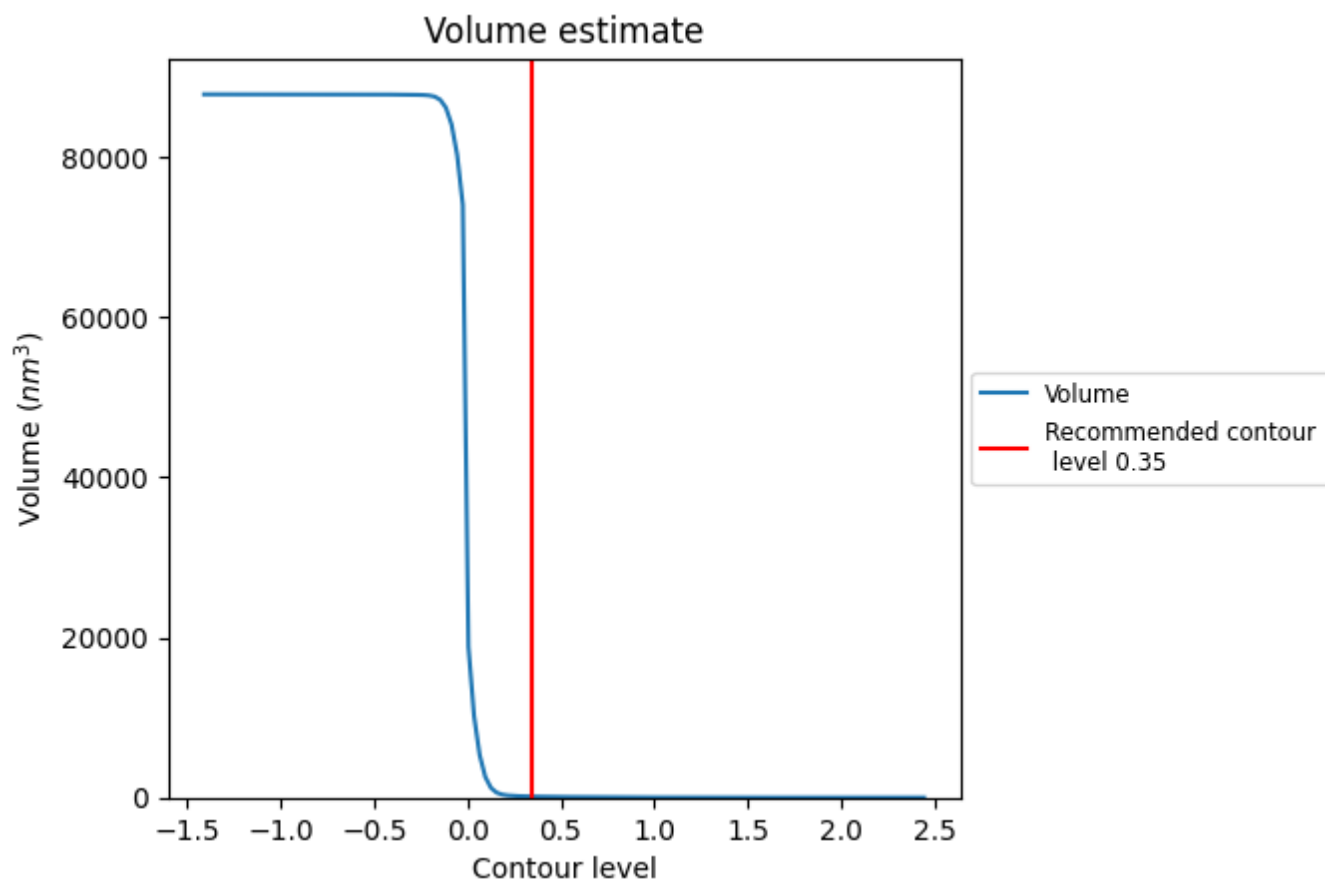
This section contains the results of statistical analysis of the map.

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.

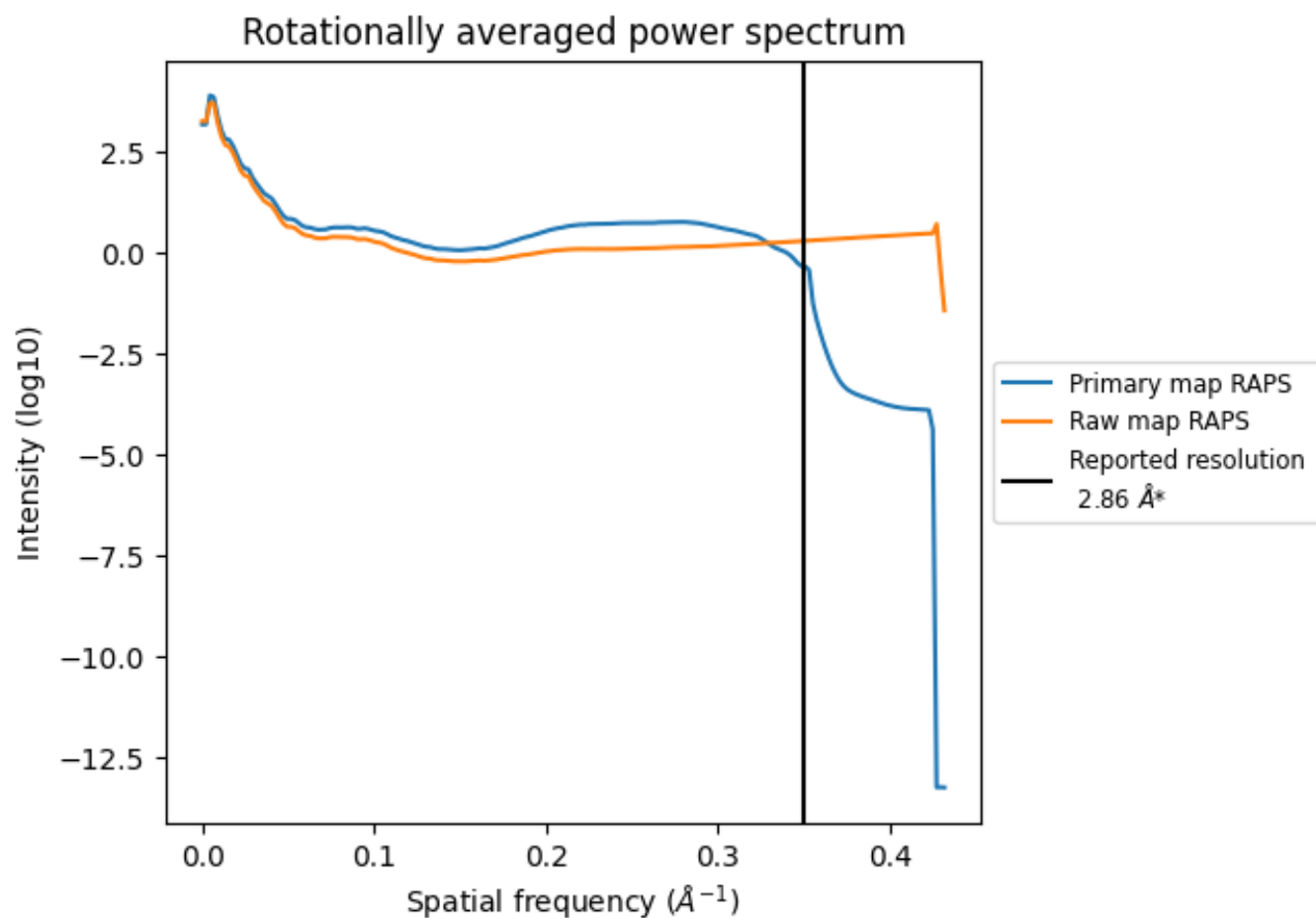
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 126 nm³; this corresponds to an approximate mass of 114 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 ⓘ

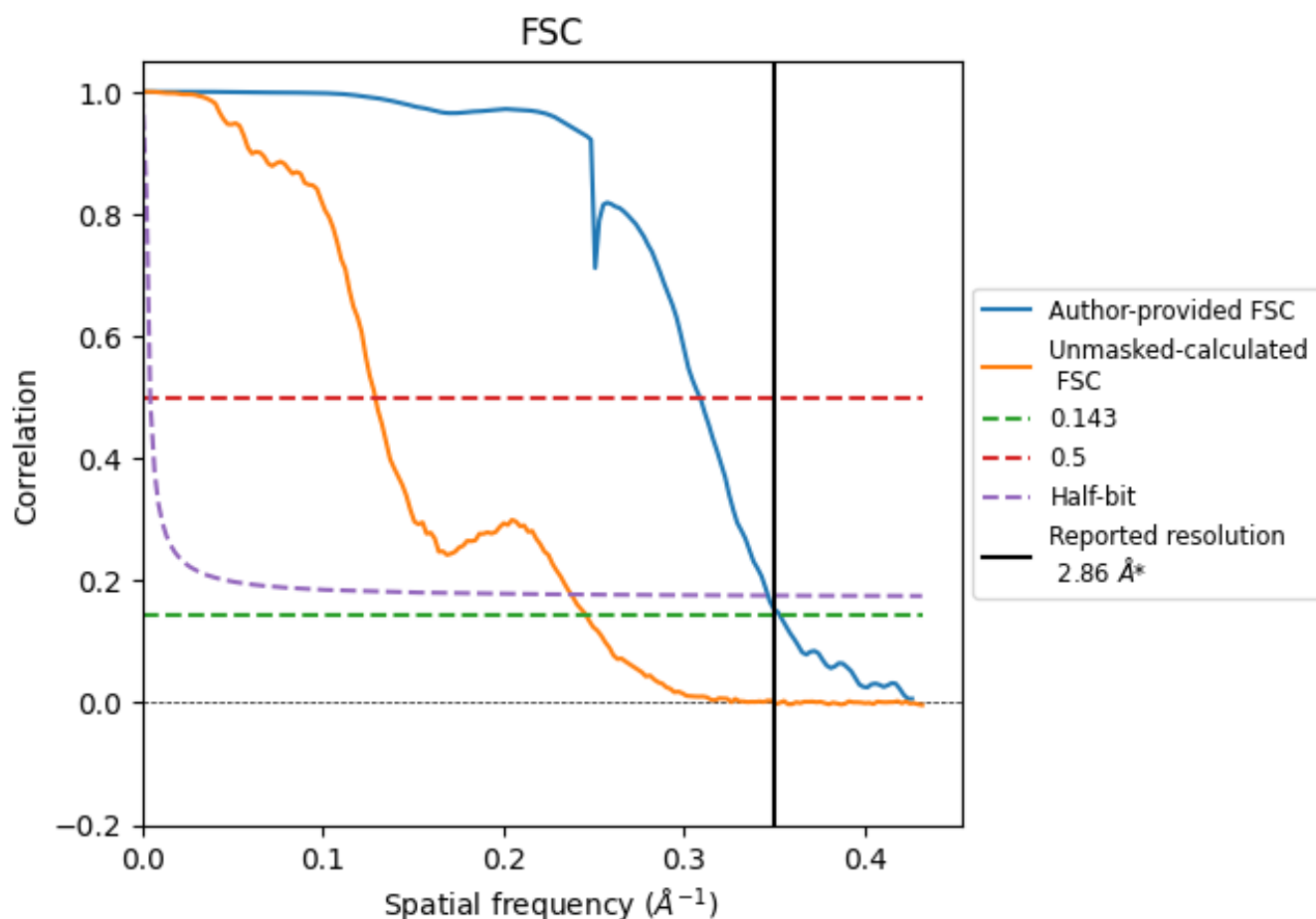


*Reported resolution corresponds to spatial frequency of 0.350 $\text{\AA}^{-1}$

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 0.350 $\text{\AA}^{-1}$

8.2 Resolution estimates

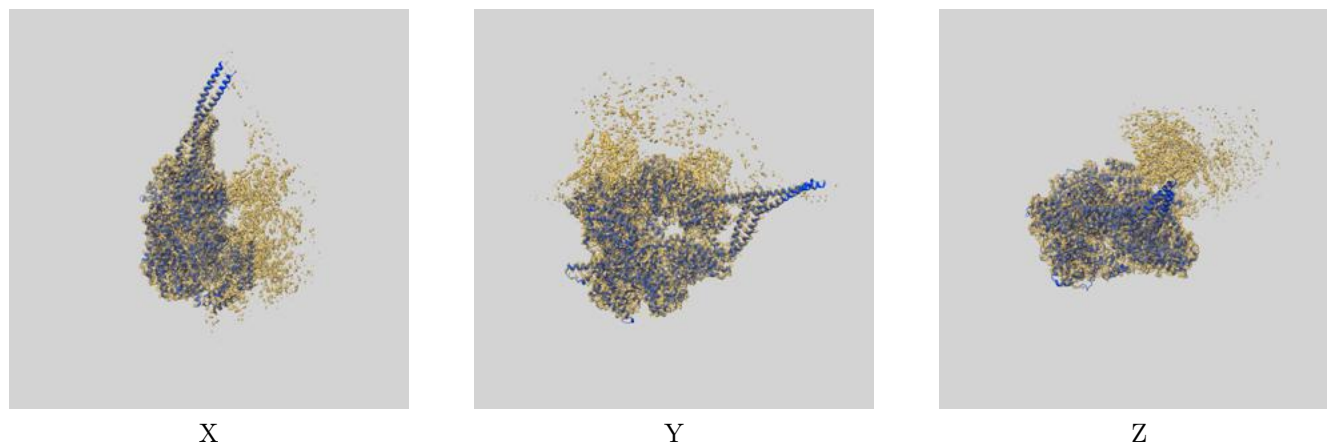
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	2.83	3.24	2.89
Unmasked-calculated*	4.07	7.75	4.21

*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 4.07 differs from the reported value 2.86 by more than 10 %

9 Map-model fit [i](#)

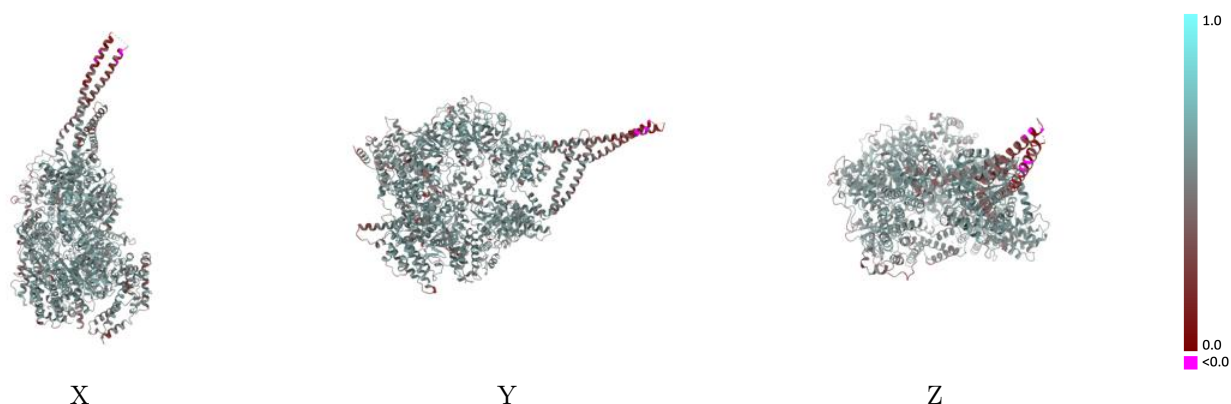
This section contains information regarding the fit between EMDB map EMD-44715 and PDB model 9BMY. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



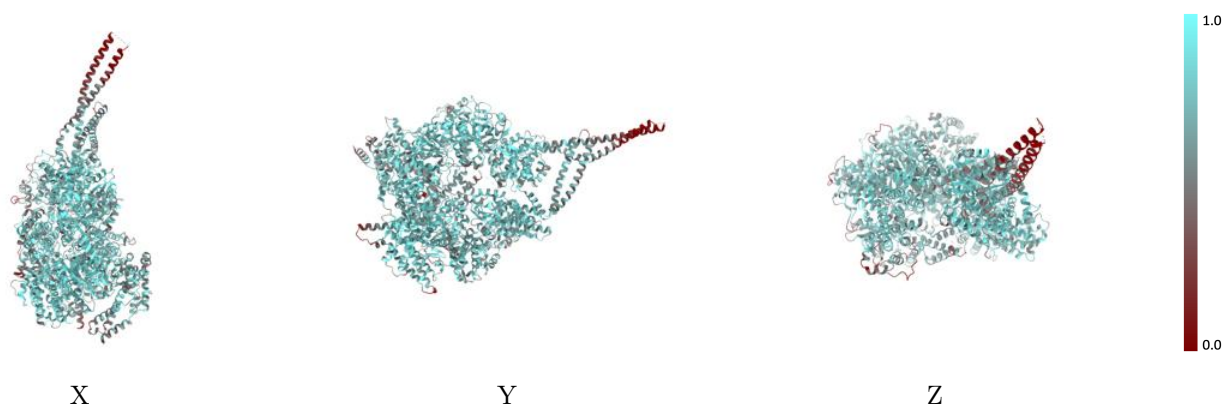
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



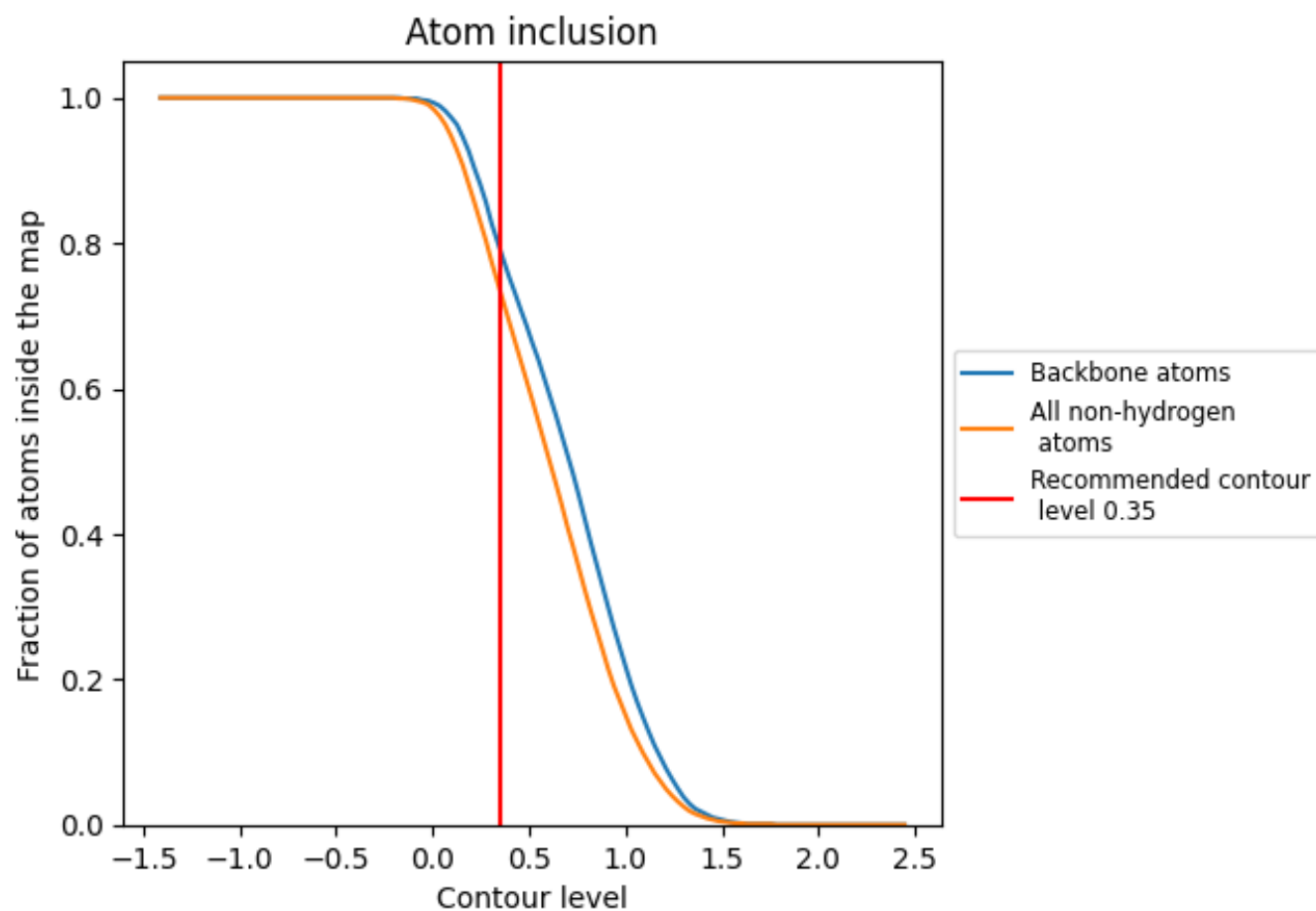
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 73% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7340	0.5330
A	0.7340	0.5330

