



Full wwPDB EM Validation Report ⓘ

Apr 24, 2025 – 11:11 AM EDT

PDB ID : 9DH6 / pdb_00009dh6
EMDB ID : EMD-46857
Title : State-2 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.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

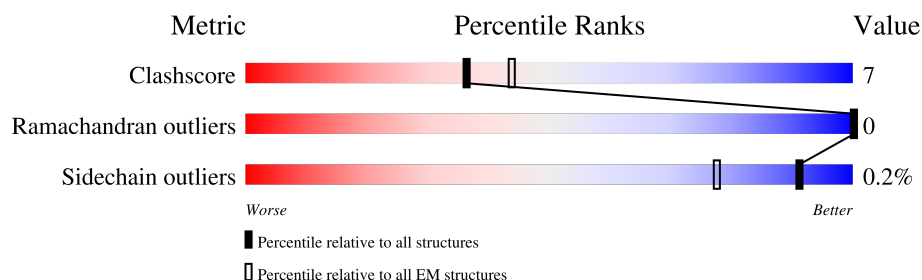
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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)
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	<div> <div>26%</div> <div>51%</div> <div>12%</div> <div>37%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 23689 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	2935	23575	15017	4067	4374	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	

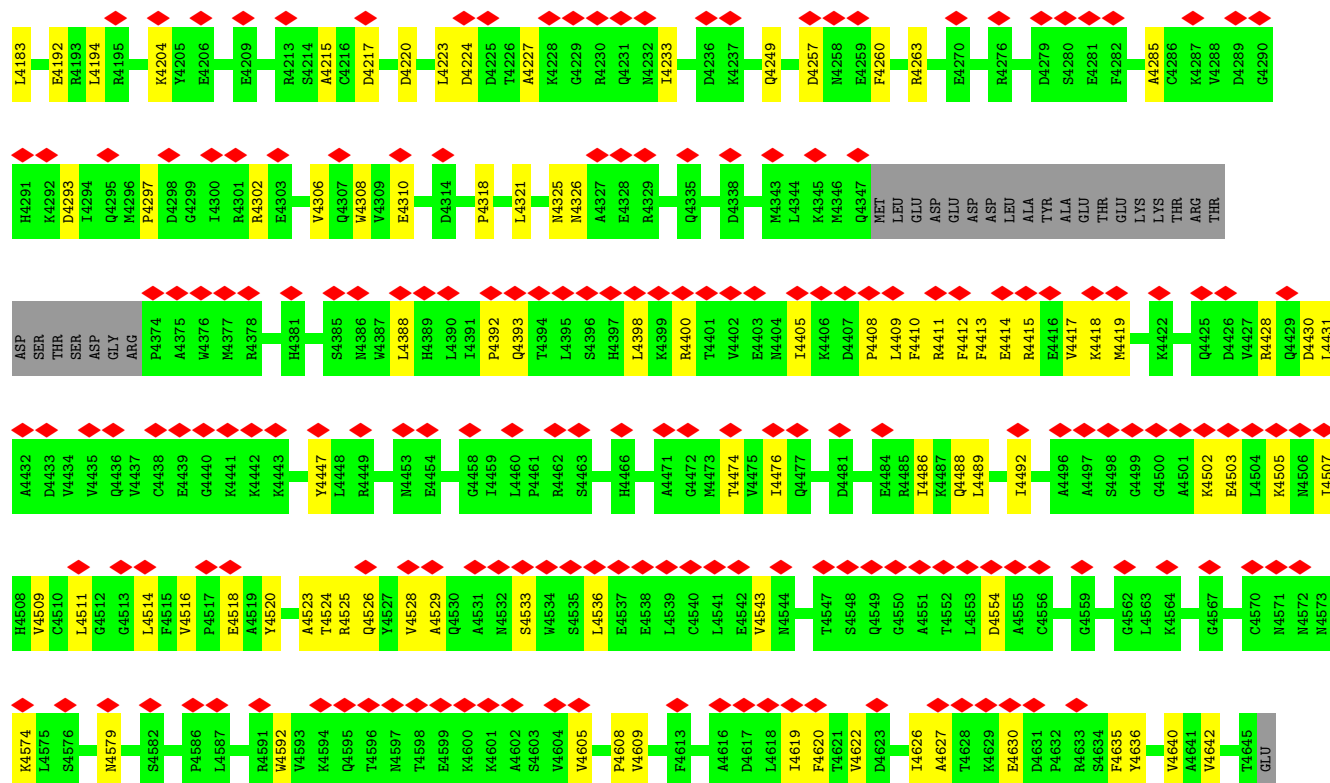
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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



G3041	H2857	L2502	I2422	N2338	D2255	L2149	A2066	L1982	Q1855
L3042	N2860	R2507	M2423	F2343	K2257	V2150	N2067	R1983	Q1856
K3043	L2605	L2508	Q2424	E2344	A2258	A2151	K2068	E1984	K1865
L3044	F2606	K2509	N2430	V2345	A2258	E2152	V2070	H1985	E1871
D3045	R2863	R2511	Q2431	Q2346	H2263	L2156	P2071	S1986	Q1876
S3046	E2864	A2512	L2432	D2347	L2268	F2158	L2075	P1988	D1877
H3047	K2865	E2516	V2433	V2349	D2269	S2159	D2077	N1989	K1878
E3048	S2868	R2519	E2438	T2352	P2270	L2160	D2078	Y1990	L1879
E3049	R2869	R2520	A2440	L2353	N2271	L2161	Q2079	D1991	V1880
K3052	S2877	F2524	Q2441	F2441	T2272	D2163	L2080	K1992	Q1881
R3060	K2878	V2524	L2443	F2363	R2273	V2165	S2081	T1993	D1886
N3069	S2879	P2525	E2444	E2366	E2274	P2166	S2082	A1994	R1887
S3072	D2880	L2526	H2445	E2366	T2276	G2167	Q2083	A1996	P1996
E3073	D2885	P2527	H2447	V2367	D2277	V2168	D2087	I1997	M1892
G3074	Q2886	T2528	D2448	L2369	R2285	Q2170	R2091	T1998	N1899
L3075	E2887	A2529	L2449	L2372	K2286	H2171	K2094	C1999	S1903
R3076	E2888	N2531	R2451	N2376	S2289	R2172	N2102	E2000	P1904
D3077	Q2889	L2532	L2452	L2382	V2291	G2173	V2103	L2001	A1908
R3078	R2896	T2535	S2457	P2386	R2292	E2174	K2104	N2002	K1912
A3079	Y2901	T2541	M2461	L2387	G2293	M2175	E2105	N2003	E1913
A3080	E2902	S2542	L2462	D2388	E2294	A2177	R2106	K2004	E1914
T3081	E2903	W2545	H2463	GLU	L2295	L2178	R2107	Q2005	H1921
L3085	E2904	Q2554	Q2464	GLY	L2296	E2180	I2108	V2006	
F3086	L2905	L2555	A2465	GLY	K2297	E2181	Q2109	D2011	
N3087	L2906	E2556	Q2466	ASP	R2298	Q2187	K2110	T2016	
R3088	D2907	E2557	R2467	ALA	D2304	D2195	K2112	T2017	
C3089	P2908	V2557	Q2467	ALA	G2305	G2196	E2113	G2021	
F3094	L2909	E2558	Q2471	GLN	G2305	E2197	E2114	Y2022	
G3095	E2914	E2559	H2475	ARG	V2307	E2198	K2115	A2023	
D3096	D2923	H2560	H2476	ARG	D2308	E2205	E2116	G2024	
K3097	R2924	A2563	D2477	LYS	P2309	E2205	E2117	R2025	
S3098	L2925	A2564	D2478	LYS	E2310	Q2212	R2118	S2026	
N3099	F2926	P2565	F2479	GLU	V2311	Q2221	G2119	N2027	
G3100	R2927	D2566	P2480	ASP	E2312	M2221	E2120	L2028	
Q3104	Q2930	T2571	M2481	GLY	E2313	G2224	A2121	P2029	
E3108	Q2931	L2572	Q2482	GLU	N2316	S2228	V2122	D2030	
F3109	G2932	D2573	I2483	ALA	D2320	E2231	D2123	N2031	
S3110	L2933	T2574	E2484	ALA	D2321	E2234	E2124	L2032	
K3112	L2936	V2575	Q2485	P2411	N2322	E2242	E2126	K2034	
N3113	L2936	R2576	E2486	W2412	L2324	R2243	T2127	T2042	
L3114	K2943	L2581	R2488	L2413	T2326	E2243	A2128	K2043	
L3115	A2951	Y2582	Y2493	Q2416	L2327	R2243	E2129	P2044	
E3116	L2956	T2583	V2495	D2418	N2328	L2244	D2045	D2045	
K3117	L2956	E2587	L2496		P2329	E2245	Q2047	Q2047	
P3118	L2961	H2588	K2589		E2330	E2248	E2135	V2052	
N3119	K2962	V2731	P2590		R2332		T2138	M2053	
Y3120	V2963	P2732			S2334		K2148	R2060	
T3121								E2063	
P3122									
P3123									
P3124									





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47152	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	1.222	Depositor
Minimum map value	-0.580	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: ATP, MG, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/24075	0.47	0/32628

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	23575	0	23639	354	0
2	A	81	0	36	5	0
3	A	31	0	12	0	0
4	A	2	0	0	0	0
All	All	23689	0	23687	354	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 (354) 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:1497:VAL:HG13	1:A:1527:LEU:HD22	1.59	0.85
1:A:2156:LEU:HG	1:A:4411:ARG:HD2	1.59	0.83
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.62	0.81
1:A:2257:LYS:HE3	1:A:2676:THR:HG21	1.65	0.79
1:A:1810:HIS:HD2	1:A:1878:LYS:HG3	1.48	0.78
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.67	0.77
1:A:4260:PHE:HD1	1:A:4263:ARG:HH21	1.36	0.74
1:A:1526:LYS:HA	1:A:1529:ARG:HD3	1.68	0.74
1:A:3488:ARG:NH2	1:A:3746:GLU:OE1	2.21	0.74
1:A:1806:ARG:O	1:A:1810:HIS:ND1	2.21	0.73
1:A:3502:THR:HG21	1:A:3544:ARG:HG3	1.70	0.73
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.21	0.73
1:A:1652:LYS:HG3	1:A:1653:HIS:HD2	1.52	0.73
1:A:4413:PHE:CZ	1:A:4492:ILE:HG23	2.24	0.72
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.71	0.72
1:A:4574:LYS:HB3	1:A:4627:ALA:HB2	1.71	0.71
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.72	0.71
1:A:1523:TRP:HA	1:A:1526:LYS:HE3	1.73	0.69
1:A:1477:LEU:HB3	1:A:1485:ARG:HB3	1.74	0.69
1:A:4393:GLN:HG3	1:A:4428:ARG:HH12	1.58	0.68
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.74	0.68
1:A:3557:ASP:OD1	1:A:3743:ARG:NH1	2.27	0.68
1:A:3487:GLU:OE1	1:A:3491:LYS:NZ	2.27	0.67
1:A:3753:LEU:HD21	1:A:3770:LEU:HD21	1.78	0.65
1:A:3078:ARG:HA	1:A:3081:THR:HG22	1.78	0.65
1:A:2257:LYS:NZ	1:A:2308:ASP:OD2	2.30	0.65
1:A:1904:PRO:HG2	1:A:2017:THR:HG22	1.77	0.64
1:A:3481:SER:O	1:A:3774:LYS:NZ	2.30	0.64
1:A:3731:LEU:HD21	1:A:3790:VAL:HB	1.80	0.64
1:A:2925:ILE:HG21	1:A:2933:LEU:HG	1.78	0.63
1:A:3499:GLN:O	1:A:3503:ILE:HG13	1.99	0.62
1:A:2581:LEU:HD11	1:A:2593:LEU:HD21	1.79	0.62
1:A:2449:LEU:HA	1:A:2453:ARG:HH21	1.63	0.62
1:A:4619:ILE:HG22	1:A:4620:PHE:HD1	1.65	0.62
1:A:2382:LEU:HD12	1:A:2416:GLN:HE21	1.65	0.62
1:A:2485:GLN:OE1	1:A:2488:ARG:NH2	2.32	0.62
1:A:3825:TYR:CZ	1:A:3875:MET:HG3	2.35	0.62
1:A:2172:ARG:NH1	1:A:2205:GLU:OE2	2.33	0.62
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.83	0.61
1:A:3935:VAL:HG22	1:A:3996:PHE:HE1	1.65	0.61
1:A:3129:VAL:HG21	1:A:3149:PHE:HB2	1.81	0.61
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2172:ARG:NH2	1:A:2212:GLN:OE1	2.35	0.60
1:A:1543:ARG:HA	1:A:1546:TYR:CE1	2.37	0.60
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.83	0.60
1:A:1504:VAL:HG11	1:A:1524:GLU:HG3	1.84	0.60
1:A:2080:LEU:HD23	1:A:2156:LEU:HD22	1.83	0.59
1:A:2149:LEU:HD11	1:A:2157:LEU:HD13	1.82	0.59
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.82	0.59
1:A:3830:GLN:NE2	1:A:3834:ASP:OD1	2.35	0.59
1:A:1652:LYS:HG3	1:A:1653:HIS:CD2	2.36	0.59
1:A:2087:ASP:O	1:A:2148:LYS:NZ	2.36	0.59
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.84	0.59
1:A:1943:ARG:NH1	1:A:2329:ASN:O	2.36	0.59
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.85	0.59
1:A:3178:ASP:OD2	1:A:3585:ARG:NE	2.34	0.59
1:A:2307:VAL:HA	1:A:2311:TRP:HE1	1.68	0.59
1:A:3935:VAL:HG13	1:A:3947:LEU:HD23	1.85	0.58
1:A:1639:GLU:OE2	1:A:1643:ASN:ND2	2.36	0.58
1:A:3916:LEU:HD11	1:A:3937:ARG:HG3	1.85	0.58
1:A:2974:GLU:OE1	1:A:2977:ARG:NH1	2.37	0.58
1:A:1810:HIS:NE2	1:A:1876:GLN:O	2.31	0.58
1:A:3478:LEU:HD22	1:A:3767:ILE:HG23	1.86	0.58
1:A:2410:SER:HB3	1:A:2413:LEU:HD23	1.87	0.57
1:A:4088:VAL:HG11	1:A:4116:LEU:HD21	1.83	0.57
1:A:2327:LEU:HD12	1:A:2331:GLU:HB3	1.85	0.57
1:A:2995:ASP:OD1	1:A:2996:GLU:N	2.36	0.57
1:A:3114:ASP:O	1:A:3140:ARG:NH2	2.38	0.57
1:A:3581:LYS:HE3	1:A:3582:ARG:HG3	1.86	0.57
1:A:1930:PHE:HA	1:A:2326:THR:HG21	1.87	0.57
1:A:2313:GLU:OE1	1:A:2316:ASN:ND2	2.36	0.57
1:A:2864:GLU:OE1	1:A:2864:GLU:N	2.36	0.57
1:A:2094:LYS:NZ	2:A:4701:ADP:O2'	2.34	0.57
1:A:2519:ARG:HG3	1:A:2526:LEU:HD22	1.86	0.57
1:A:3597:THR:HG23	1:A:3634:LEU:HD21	1.86	0.57
1:A:3779:GLU:O	1:A:3783:LYS:HG2	2.04	0.57
1:A:3482:LEU:HD11	1:A:3770:LEU:HD23	1.86	0.56
1:A:1887:ARG:HD2	1:A:4249:GLN:HG2	1.87	0.56
1:A:1987:ASN:OD1	1:A:1989:ASN:ND2	2.38	0.56
1:A:4525:ARG:HD3	1:A:4536:LEU:HD23	1.88	0.56
1:A:1914:GLU:HG3	2:A:4701:ADP:H3'	1.88	0.56
1:A:2179:ARG:NH1	1:A:2195:ASP:OD1	2.39	0.55
1:A:1589:MET:SD	1:A:1589:MET:N	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.40	0.55
1:A:3611:ARG:NH1	1:A:3636:GLN:OE1	2.35	0.55
1:A:1763:GLU:OE1	1:A:1838:TRP:NE1	2.34	0.54
1:A:2773:MET:HG2	1:A:2825:TRP:HE1	1.71	0.54
1:A:3588:LEU:HD11	1:A:3638:VAL:HG11	1.88	0.54
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.88	0.54
1:A:3960:TRP:HD1	1:A:3969:THR:HG23	1.72	0.54
1:A:4489:LEU:HD23	1:A:4492:ILE:HD12	1.88	0.54
1:A:2080:LEU:HD11	1:A:2157:LEU:HD12	1.89	0.54
1:A:3459:GLN:HA	1:A:3462:LYS:HD2	1.89	0.54
1:A:4227:ALA:HB2	1:A:4233:ILE:HD12	1.90	0.54
1:A:4518:GLU:OE1	1:A:4518:GLU:N	2.33	0.54
1:A:4398:LEU:HD12	1:A:4414:GLU:HA	1.89	0.53
1:A:2694:ARG:NH2	1:A:2697:ASP:OD2	2.39	0.53
1:A:4409:LEU:O	1:A:4413:PHE:HB2	2.08	0.53
1:A:2063:GLU:O	1:A:2067:ASN:ND2	2.41	0.53
1:A:2138:ILE:HD11	1:A:2165:PHE:CG	2.43	0.53
1:A:3653:VAL:HG12	1:A:3662:ILE:HB	1.88	0.53
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.90	0.53
1:A:4543:VAL:HG21	1:A:4622:VAL:HG12	1.90	0.53
1:A:2623:SER:OG	1:A:3006:GLU:OE1	2.26	0.53
1:A:3655:ARG:HG2	1:A:3660:VAL:HG22	1.91	0.52
1:A:3970:VAL:HB	1:A:3989:ARG:HD3	1.91	0.52
1:A:4194:LEU:HD11	1:A:4204:LYS:HA	1.91	0.52
1:A:4605:VAL:HG23	1:A:4636:TYR:HE1	1.75	0.52
1:A:2495:VAL:HG21	1:A:2524:VAL:HG21	1.90	0.52
1:A:3216:GLU:HG2	1:A:3219:ARG:HH21	1.74	0.52
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.91	0.52
1:A:2654:GLN:NE2	1:A:3048:GLU:OE2	2.43	0.52
1:A:4474:THR:HG22	1:A:4476:ILE:H	1.75	0.52
1:A:3650:ASN:HD21	1:A:3695:ARG:HH11	1.58	0.51
1:A:4388:LEU:HD21	1:A:4431:LEU:HB3	1.93	0.51
1:A:2363:TRP:HE1	1:A:2365:SER:HG	1.54	0.51
1:A:2457:SER:OG	1:A:2732:PRO:HB3	2.09	0.51
1:A:2440:ALA:HB2	1:A:2502:LEU:HD23	1.92	0.51
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.93	0.51
1:A:4520:TYR:O	1:A:4524:THR:HG23	2.11	0.51
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.92	0.51
1:A:3990:LEU:HA	1:A:4004:MET:HG2	1.93	0.51
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.93	0.51
1:A:1847:ASP:N	1:A:1856:GLN:O	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3130:TYR:CZ	1:A:3132:LYS:HB3	2.45	0.51
1:A:3720:GLU:OE1	1:A:3855:ARG:NE	2.43	0.51
1:A:4081:ASP:OD1	1:A:4112:LYS:NZ	2.44	0.51
1:A:1527:LEU:HD23	1:A:1530:ILE:HD12	1.92	0.50
1:A:3160:ARG:HE	1:A:3164:ARG:HH21	1.60	0.50
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.93	0.50
1:A:3914:ILE:O	1:A:3937:ARG:NH1	2.44	0.50
1:A:4021:MET:HA	1:A:4021:MET:HE2	1.93	0.50
1:A:3835:ILE:HG12	1:A:3870:ARG:HD2	1.92	0.50
1:A:3892:LEU:HD13	1:A:3983:ILE:HG21	1.94	0.50
1:A:4408:PRO:HG3	1:A:4526:GLN:HB3	1.92	0.50
1:A:4412:PHE:HZ	1:A:4514:LEU:HD13	1.75	0.50
1:A:3931:GLN:O	1:A:3935:VAL:HG23	2.11	0.50
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.93	0.50
1:A:1535:ASP:O	1:A:2292:ARG:NH2	2.45	0.49
1:A:2485:GLN:NE2	1:A:2542:SER:O	2.45	0.49
1:A:4392:PRO:O	1:A:4428:ARG:NH1	2.45	0.49
1:A:4192:GLU:HB2	1:A:4321:LEU:HD21	1.95	0.49
1:A:4183:LEU:HD11	1:A:4215:ALA:HB1	1.95	0.49
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.13	0.49
1:A:4297:PRO:HG3	1:A:4308:TRP:CD2	2.47	0.49
1:A:4503:GLU:O	1:A:4507:ILE:HG23	2.13	0.49
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.93	0.49
1:A:3144:VAL:O	1:A:3148:VAL:HG23	2.13	0.48
1:A:4153:VAL:O	1:A:4157:MET:HG3	2.13	0.48
1:A:3639:GLU:OE2	1:A:3681:THR:OG1	2.30	0.48
1:A:4302:ARG:O	1:A:4306:VAL:HG23	2.14	0.48
1:A:2291:VAL:HG13	1:A:2292:ARG:HG3	1.95	0.48
1:A:3775:ARG:O	1:A:3779:GLU:HG2	2.12	0.48
1:A:3786:GLU:O	1:A:3790:VAL:HG23	2.14	0.48
1:A:4176:ARG:NH2	1:A:4224:ASP:OD1	2.35	0.48
1:A:3160:ARG:HE	1:A:3164:ARG:NH2	2.11	0.48
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.46	0.48
1:A:3585:ARG:NH1	1:A:3694:SER:O	2.41	0.48
1:A:4525:ARG:HG3	1:A:4592:TRP:CH2	2.48	0.48
1:A:2297:LYS:O	1:A:2338:ASN:ND2	2.46	0.48
1:A:2901:TYR:OH	1:A:2909:LEU:N	2.47	0.48
1:A:3135:GLN:HB2	1:A:3136:PRO:HD3	1.94	0.48
1:A:1853:VAL:HA	1:A:1856:GLN:HG3	1.95	0.47
1:A:1980:GLU:O	1:A:1984:GLU:HG2	2.14	0.47
1:A:3639:GLU:HG3	1:A:3686:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1912:LYS:NZ	2:A:4701:ADP:O3B	2.33	0.47
1:A:1985:HIS:CE1	1:A:2010:PRO:HG3	2.49	0.47
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.48	0.47
1:A:2644:THR:OG1	1:A:2647:GLY:O	2.20	0.47
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.94	0.47
1:A:2605:LEU:HD13	1:A:2709:VAL:HG11	1.96	0.47
1:A:3716:VAL:HB	1:A:3836:TYR:OH	2.14	0.47
1:A:3891:LYS:HD2	1:A:4013:LEU:HD23	1.96	0.47
1:A:2042:THR:HG21	1:A:4257:ASP:HB2	1.97	0.47
1:A:2224:GLY:O	1:A:2346:GLN:HA	2.14	0.47
1:A:2951:ALA:HB1	1:A:2956:LEU:HB2	1.96	0.47
1:A:4430:ASP:OD2	1:A:4447:TYR:OH	2.31	0.47
1:A:2290:SER:HB2	1:A:2295:LEU:HG	1.97	0.47
1:A:2463:HIS:O	1:A:2467:ARG:HG3	2.14	0.47
1:A:2816:LEU:HD23	1:A:2817:PRO:O	2.14	0.47
1:A:2967:TYR:OH	1:A:2975:ASP:OD2	2.25	0.47
1:A:3174:ARG:NH1	1:A:3650:ASN:OD1	2.48	0.47
1:A:1698:ILE:HD12	1:A:1701:TRP:NE1	2.30	0.47
1:A:4509:VAL:HG11	1:A:4514:LEU:HD11	1.96	0.47
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.50	0.47
1:A:2231:SER:OG	1:A:2344:GLU:OE2	2.33	0.47
1:A:3570:ASP:OD1	1:A:3571:ASP:N	2.48	0.47
1:A:3960:TRP:CD1	1:A:3969:THR:HG23	2.49	0.47
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	1.97	0.47
1:A:2075:LEU:HD13	1:A:2160:LEU:HD11	1.96	0.46
1:A:2275:TRP:NE1	1:A:2277:ASP:OD1	2.48	0.46
1:A:2308:ASP:O	1:A:2312:VAL:HG12	2.16	0.46
1:A:4413:PHE:O	1:A:4417:VAL:HG23	2.14	0.46
1:A:1738:TYR:CE2	1:A:1792:LEU:HD11	2.50	0.46
1:A:3109:PHE:HD2	1:A:3180:ILE:HG22	1.80	0.46
1:A:3780:VAL:O	1:A:3784:VAL:HG23	2.15	0.46
1:A:4408:PRO:HB3	1:A:4411:ARG:HH21	1.79	0.46
1:A:3791:MET:O	1:A:3795:GLU:HG3	2.14	0.46
1:A:3912:ASN:O	1:A:3937:ARG:NH1	2.49	0.46
1:A:1490:TRP:HZ3	1:A:1534:PHE:HD1	1.64	0.46
1:A:1903:SER:HA	1:A:2016:ILE:O	2.15	0.46
1:A:3876:LEU:HD23	1:A:4146:VAL:HG11	1.98	0.46
1:A:1467:ARG:HB2	1:A:1523:TRP:HH2	1.80	0.46
1:A:1550:ILE:O	1:A:1554:SER:OG	2.29	0.46
1:A:3161:LEU:HB3	1:A:3168:THR:HG22	1.98	0.46
1:A:3624:GLU:HG3	1:A:3669:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4171:LYS:HG3	1:A:4172:SER:H	1.81	0.46
1:A:2446:ILE:HG13	1:A:2735:TYR:CD1	2.51	0.46
1:A:1508:LYS:HA	1:A:1513:TYR:CG	2.51	0.45
1:A:3100:GLU:HG2	1:A:3130:TYR:HE1	1.80	0.45
1:A:2983:SER:HB2	1:A:2990:ILE:HD12	1.99	0.45
1:A:4412:PHE:HE1	1:A:4516:VAL:HG23	1.81	0.45
1:A:2606:PHE:HE1	1:A:2617:VAL:HG21	1.81	0.45
1:A:2885:ASP:HB3	1:A:2888:GLU:OE1	2.16	0.45
1:A:4412:PHE:CZ	1:A:4514:LEU:HD13	2.51	0.45
1:A:2104:LYS:HG3	1:A:2131:LEU:HD21	1.99	0.45
1:A:3843:ASN:ND2	1:A:3862:ASP:OD2	2.48	0.45
1:A:4410:PHE:HA	1:A:4413:PHE:HB3	1.99	0.45
1:A:2624:SER:HB3	1:A:3081:THR:HA	1.98	0.45
1:A:2818:VAL:O	1:A:2822:ILE:HG12	2.17	0.45
1:A:2901:TYR:CZ	1:A:2908:PRO:HA	2.50	0.45
1:A:4409:LEU:HA	1:A:4523:ALA:HB1	1.99	0.45
1:A:3044:LEU:HB3	1:A:3049:GLU:HG3	1.98	0.45
1:A:1526:LYS:O	1:A:1530:ILE:HG13	2.17	0.45
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.17	0.45
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.48	0.45
1:A:2103:VAL:HA	1:A:2106:GLU:HG2	1.99	0.45
1:A:3551:GLU:HA	1:A:3559:ARG:NH1	2.32	0.45
1:A:4489:LEU:HA	1:A:4492:ILE:HD12	1.98	0.45
1:A:1640:ILE:HD11	1:A:1653:HIS:HB3	1.99	0.45
1:A:1640:ILE:HA	1:A:1650:LEU:HD22	2.00	0.44
1:A:3114:ASP:O	1:A:3116:GLU:HG2	2.17	0.44
1:A:3837:HIS:CE1	1:A:3841:TYR:HD2	2.35	0.44
1:A:1626:PHE:HB3	1:A:1629:PHE:CD2	2.53	0.44
1:A:2965:ARG:HH12	1:A:3640:SER:HB3	1.81	0.44
1:A:3151:HIS:ND1	1:A:3516:TYR:OH	2.33	0.44
1:A:1572:SER:O	1:A:1576:LEU:HG	2.18	0.44
1:A:2324:LEU:HD23	1:A:2334:SER:HA	1.99	0.44
1:A:2527:PRO:HD3	1:A:2545:TRP:CE2	2.53	0.44
1:A:2571:THR:O	1:A:2575:VAL:HG22	2.16	0.44
1:A:2697:ASP:N	1:A:2697:ASP:OD1	2.50	0.44
1:A:4488:GLN:O	1:A:4492:ILE:HG13	2.18	0.44
1:A:2511:ARG:HD3	1:A:2535:ILE:HD13	1.99	0.44
1:A:4400:ARG:HD2	1:A:4405:ILE:HD11	1.98	0.44
1:A:3013:ALA:HA	1:A:3088:ARG:HG3	2.00	0.44
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.51	0.44
1:A:1568:PHE:HB2	1:A:1611:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1623:ARG:HA	1:A:1629:PHE:HB2	2.01	0.43
1:A:2159:SER:OG	1:A:4411:ARG:NH1	2.52	0.43
1:A:2527:PRO:HD3	1:A:2545:TRP:CD2	2.54	0.43
1:A:2816:LEU:HD21	1:A:2821:LEU:N	2.33	0.43
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	2.00	0.43
1:A:1724:VAL:HG11	1:A:1753:SER:HB3	2.00	0.43
1:A:1960:PHE:HE2	1:A:2032:LEU:HD21	1.82	0.43
1:A:3026:TYR:O	1:A:3030:MET:HG2	2.19	0.43
1:A:3575:GLU:O	1:A:3579:MET:HG3	2.18	0.43
1:A:4626:ILE:HD12	1:A:4630:GLU:O	2.18	0.43
1:A:1800:GLN:OE1	1:A:1804:ARG:NH1	2.45	0.43
1:A:1816:VAL:HG11	1:A:2052:VAL:HG22	2.00	0.43
1:A:4223:LEU:HD12	1:A:4223:LEU:HA	1.86	0.43
1:A:1558:LYS:HD3	1:A:1565:THR:HG21	2.00	0.43
1:A:4013:LEU:HD13	1:A:4017:PHE:CE2	2.54	0.43
1:A:4525:ARG:HG3	1:A:4592:TRP:CZ3	2.54	0.43
1:A:1507:MET:O	1:A:1513:TYR:HB2	2.18	0.43
1:A:2418:ASP:O	1:A:2422:ILE:HG12	2.18	0.43
1:A:3597:THR:HG21	1:A:3611:ARG:HH12	1.84	0.43
1:A:3873:ARG:HD3	1:A:3873:ARG:HA	1.81	0.43
1:A:1738:TYR:HE2	1:A:1792:LEU:HD11	1.83	0.43
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.51	0.43
1:A:1542:ARG:O	1:A:1546:TYR:HD1	2.02	0.43
1:A:2976:LEU:HA	1:A:2979:VAL:HG12	2.01	0.43
1:A:1717:LEU:HB2	1:A:1749:LEU:HD22	2.01	0.42
1:A:2507:ARG:HH21	1:A:2509:LYS:HE2	1.83	0.42
1:A:2936:ILE:O	1:A:3094:PHE:N	2.52	0.42
1:A:4630:GLU:HB3	1:A:4635:PHE:HE1	1.84	0.42
1:A:1933:ASP:OD1	1:A:1935:THR:HG22	2.19	0.42
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.44	0.42
1:A:2138:ILE:HD12	1:A:2161:LEU:HD22	2.00	0.42
1:A:3207:LYS:HD3	1:A:3207:LYS:HA	1.85	0.42
1:A:3214:GLN:HB3	1:A:3761:LEU:HD12	2.00	0.42
1:A:3951:VAL:HG12	1:A:3973:LEU:HD21	2.00	0.42
1:A:1543:ARG:HA	1:A:1546:TYR:CD1	2.55	0.42
1:A:1957:PHE:HB2	1:A:2016:ILE:HG22	2.00	0.42
1:A:2308:ASP:OD1	1:A:2311:TRP:HD1	2.03	0.42
1:A:2386:PRO:HG3	1:A:2413:LEU:HD21	2.00	0.42
1:A:3900:THR:HG23	1:A:3902:ASP:H	1.84	0.42
1:A:1814:GLU:OE1	1:A:1878:LYS:NZ	2.52	0.42
1:A:3457:GLU:O	1:A:3461:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4529:ALA:O	1:A:4533:SER:N	2.53	0.42
1:A:1879:LEU:HD22	2:A:4701:ADP:C4	2.55	0.42
1:A:3039:LYS:HB3	1:A:3039:LYS:HE3	1.78	0.42
1:A:3906:GLN:NE2	1:A:3910:ARG:HD2	2.34	0.42
1:A:4415:ARG:HE	1:A:4419:MET:HE1	1.85	0.42
1:A:2083:GLN:HE21	1:A:2150:VAL:HG11	1.85	0.42
1:A:3454:LEU:O	1:A:3457:GLU:HG2	2.20	0.42
1:A:4525:ARG:NH2	1:A:4536:LEU:O	2.47	0.42
1:A:1561:LEU:HB3	1:A:1564:GLU:OE2	2.19	0.42
1:A:1587:LEU:HD12	1:A:1587:LEU:HA	1.94	0.41
1:A:1680:GLU:HG2	1:A:1803:LEU:HD13	2.02	0.41
1:A:2163:ASP:HB3	1:A:4526:GLN:HE21	1.84	0.41
1:A:2465:ALA:HB2	1:A:2493:TYR:CE1	2.54	0.41
1:A:4486:ILE:HD13	1:A:4486:ILE:HA	1.90	0.41
1:A:1501:ILE:HG13	1:A:1527:LEU:HD13	2.01	0.41
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.53	0.41
1:A:3924:ILE:HD12	1:A:3924:ILE:H	1.85	0.41
1:A:4400:ARG:NE	1:A:4414:GLU:OE1	2.53	0.41
1:A:1661:VAL:HG22	1:A:1676:ILE:HD12	2.02	0.41
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	2.03	0.41
1:A:2313:GLU:OE2	1:A:2352:THR:OG1	2.37	0.41
1:A:3085:LEU:O	1:A:3089:CYS:HB2	2.21	0.41
1:A:1658:PHE:HB2	1:A:1661:VAL:HB	2.03	0.41
1:A:1814:GLU:O	1:A:1818:GLN:HG3	2.21	0.41
1:A:2091:ARG:HH21	2:A:4701:ADP:PA	2.44	0.41
1:A:2766:ALA:O	1:A:2770:THR:HG22	2.21	0.41
1:A:3692:LEU:O	1:A:3696:VAL:HG22	2.21	0.41
1:A:3825:TYR:OH	1:A:3879:ASP:OD2	2.28	0.41
1:A:1645:LYS:HA	1:A:1645:LYS:HD2	1.77	0.41
1:A:3608:LYS:HD2	1:A:3608:LYS:HA	1.67	0.41
1:A:2671:MET:HA	1:A:2676:THR:O	2.19	0.41
1:A:3955:GLU:OE1	1:A:3955:GLU:N	2.52	0.41
1:A:1672:VAL:HG22	1:A:1691:SER:HB3	2.03	0.41
1:A:1810:HIS:CD2	1:A:1878:LYS:HG3	2.39	0.41
1:A:3521:ASP:OD1	1:A:3521:ASP:N	2.45	0.41
1:A:2079:GLN:O	1:A:4415:ARG:NH1	2.47	0.41
1:A:2228:SER:HB2	1:A:2364:PHE:HB3	2.01	0.41
1:A:2541:ILE:HD12	1:A:2541:ILE:HA	1.95	0.41
1:A:3550:THR:HG22	1:A:3575:GLU:HG3	2.03	0.41
1:A:3723:ASP:O	1:A:3726:GLU:HG2	2.21	0.41
1:A:4260:PHE:CZ	1:A:4608:PRO:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.36	0.41
1:A:1749:LEU:HD23	1:A:1749:LEU:HA	1.86	0.41
1:A:3570:ASP:OD2	1:A:3707:SER:HB3	2.21	0.41
1:A:3612:THR:O	1:A:3635:VAL:HA	2.20	0.41
1:A:3718:LYS:HB2	1:A:3725:ASP:OD2	2.20	0.41
1:A:4180:TYR:OH	1:A:4220:ASP:OD1	2.33	0.41
1:A:4285:ALA:O	1:A:4293:ASP:HB2	2.20	0.41
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.55	0.41
1:A:4418:LYS:HE3	1:A:4418:LYS:HB2	1.88	0.41
1:A:4511:LEU:HD23	1:A:4511:LEU:HA	1.89	0.41
1:A:3182:HIS:NE2	1:A:3582:ARG:O	2.53	0.40
1:A:3886:LEU:O	1:A:3890:ILE:HG12	2.21	0.40
1:A:4002:LEU:HD23	1:A:4002:LEU:HA	1.92	0.40
1:A:3109:PHE:CD2	1:A:3180:ILE:HG22	2.56	0.40
1:A:3717:LEU:HD23	1:A:3717:LEU:HA	1.94	0.40
1:A:1467:ARG:HB2	1:A:1523:TRP:CH2	2.57	0.40
1:A:1564:GLU:HA	1:A:1567:ARG:HB2	2.04	0.40
1:A:2029:PRO:HB2	1:A:2031:ASN:OD1	2.22	0.40
1:A:2075:LEU:HB3	1:A:2160:LEU:HD21	2.02	0.40
1:A:4158:LEU:HD21	1:A:4310:GLU:HG3	2.03	0.40
1:A:4605:VAL:HG23	1:A:4636:TYR:CE1	2.55	0.40
1:A:4635:PHE:HD2	1:A:4640:VAL:HG11	1.85	0.40
1:A:2943:LYS:HG2	1:A:3094:PHE:HD2	1.86	0.40
1:A:3485:GLU:HG3	1:A:3488:ARG:HH21	1.86	0.40
1:A:4172:SER:HB2	1:A:4173:PRO:HD3	2.03	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	2927/4646 (63%)	2883 (98%)	44 (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	2603/4125 (63%)	2599 (100%)	4 (0%)	92 96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2332	ARG
1	A	2863	ARG
1	A	3233	ASN
1	A	4502	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1643	ASN
1	A	1653	HIS
1	A	1989	ASN
1	A	2416	GLN
1	A	2752	ASN
1	A	2827	HIS
1	A	3237	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	4701	4	24,29,29	0.86	0	29,45,45	1.23	2 (6%)
2	ADP	A	4704	-	24,29,29	0.88	0	29,45,45	1.18	2 (6%)
2	ADP	A	4703	-	24,29,29	0.86	0	29,45,45	1.20	2 (6%)
3	ATP	A	4702	4	28,33,33	0.67	0	34,52,52	0.59	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	4701	4	-	0/12/32/32	0/3/3/3
2	ADP	A	4704	-	-	1/12/32/32	0/3/3/3
2	ADP	A	4703	-	-	0/12/32/32	0/3/3/3
3	ATP	A	4702	4	-	7/18/38/38	0/3/3/3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	N3-C2-N1	-3.68	123.68	128.67
2	A	4701	ADP	N3-C2-N1	-3.61	123.77	128.67
2	A	4704	ADP	N3-C2-N1	-3.61	123.78	128.67
2	A	4704	ADP	C4-C5-N7	-2.57	106.62	109.34
2	A	4703	ADP	C4-C5-N7	-2.45	106.74	109.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	ADP	C4-C5-N7	-2.43	106.77	109.34
3	A	4702	ATP	C5-C6-N6	2.32	123.84	120.31

There are no chirality outliers.

All (8) torsion outliers are listed below:

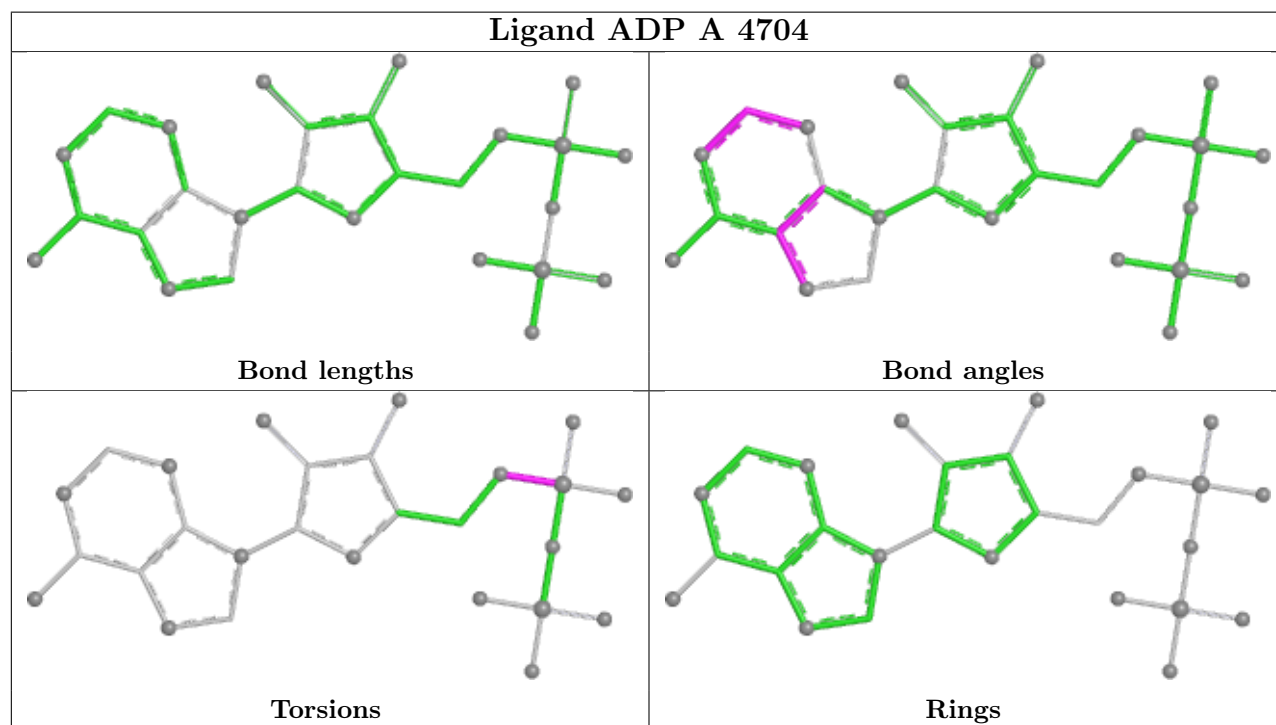
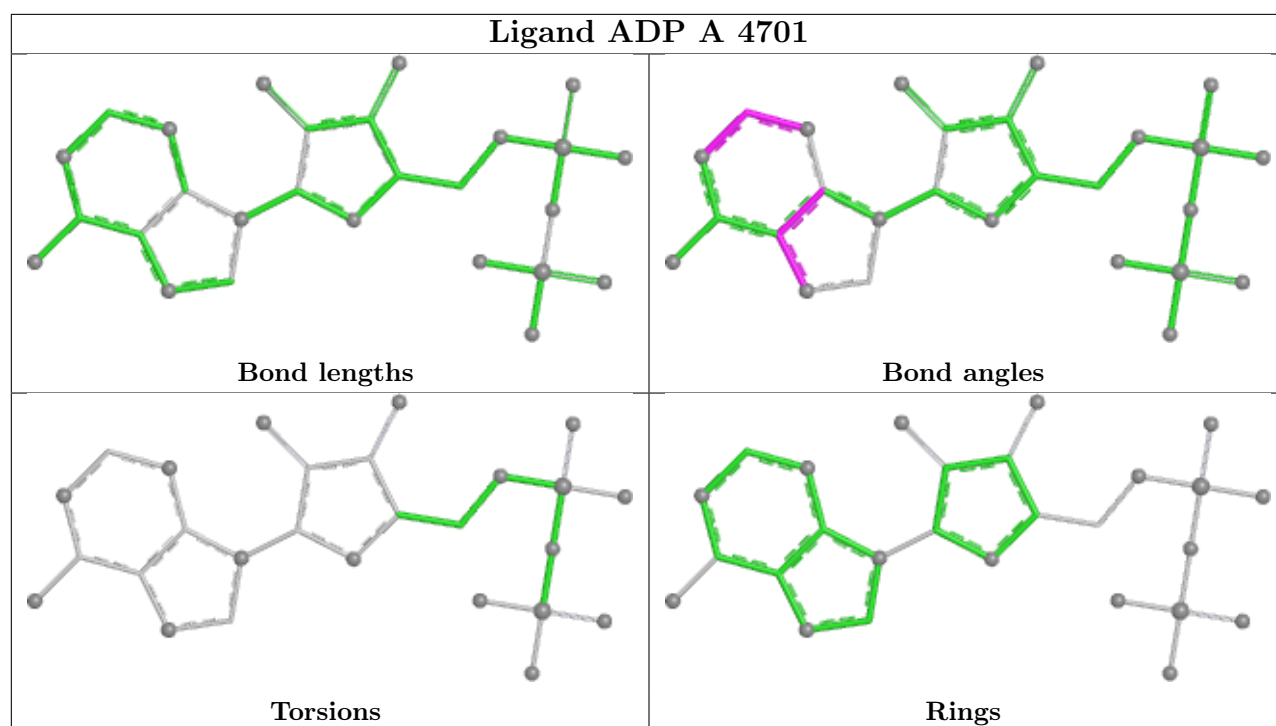
Mol	Chain	Res	Type	Atoms
3	A	4702	ATP	C5'-O5'-PA-O2A
3	A	4702	ATP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'
2	A	4704	ADP	C5'-O5'-PA-O1A
3	A	4702	ATP	C5'-O5'-PA-O1A
3	A	4702	ATP	C5'-O5'-PA-O3A
3	A	4702	ATP	PA-O3A-PB-O1B
3	A	4702	ATP	PA-O3A-PB-O2B

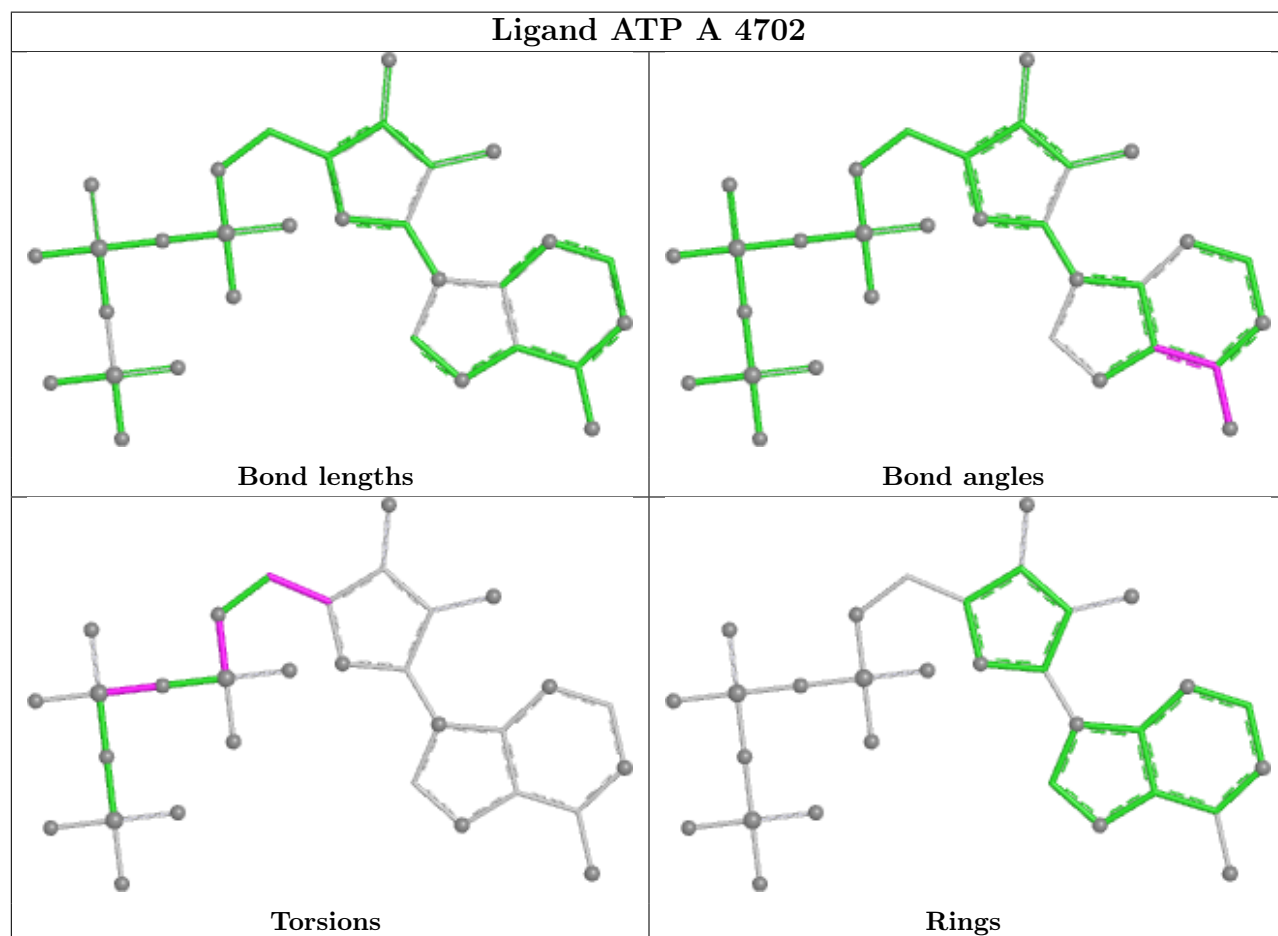
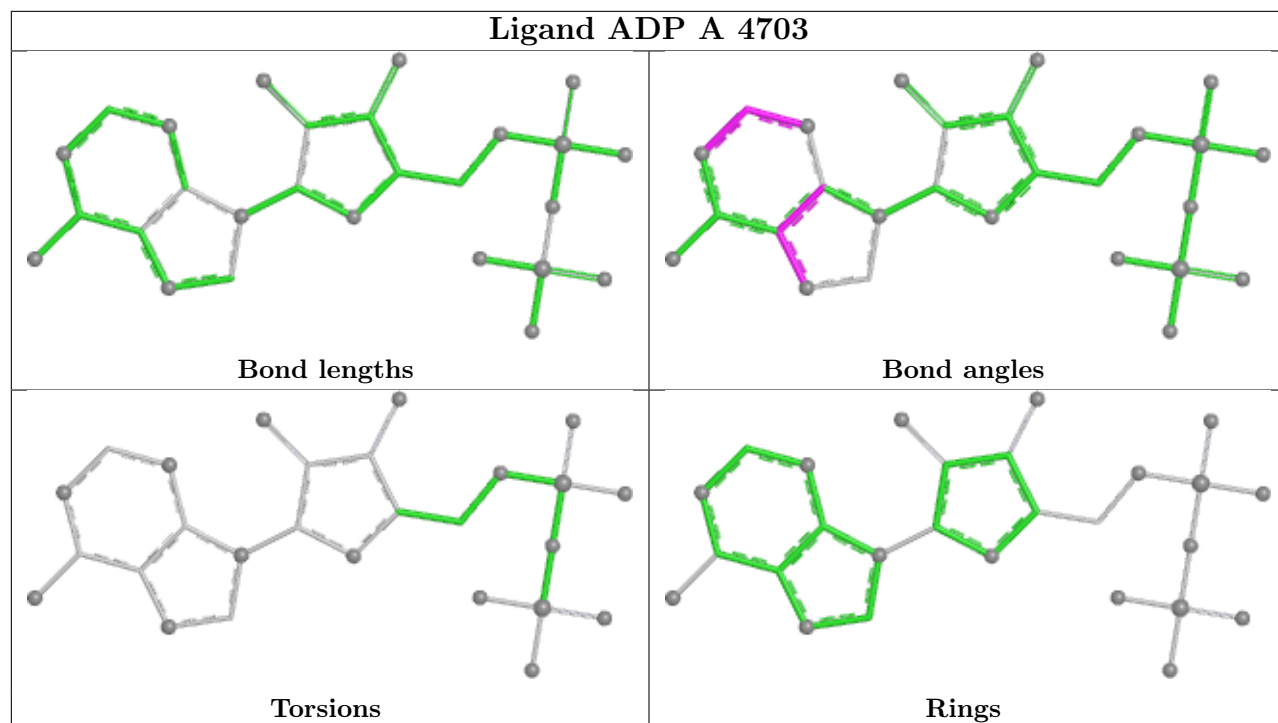
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

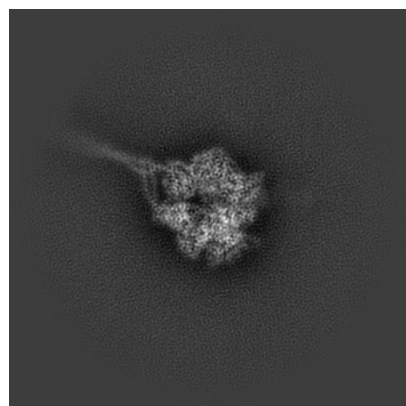
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46857. These allow visual inspection of the internal detail of the map and identification of artifacts.

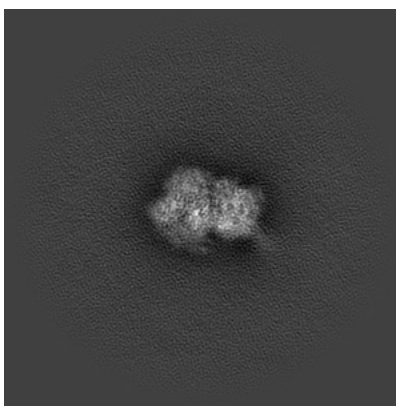
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

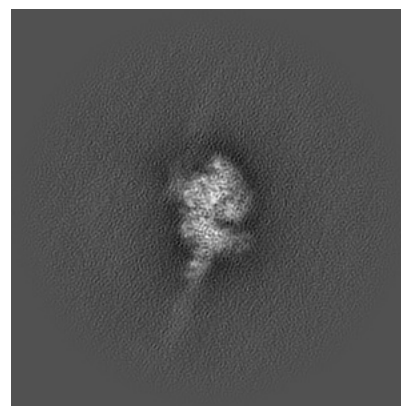
6.1.1 Primary map



X

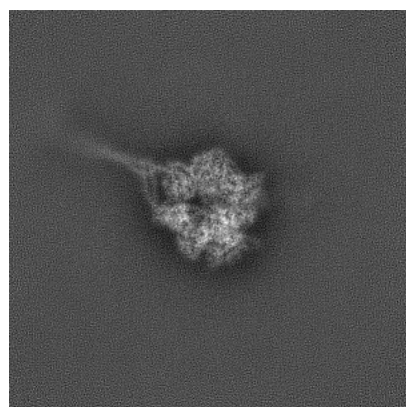


Y

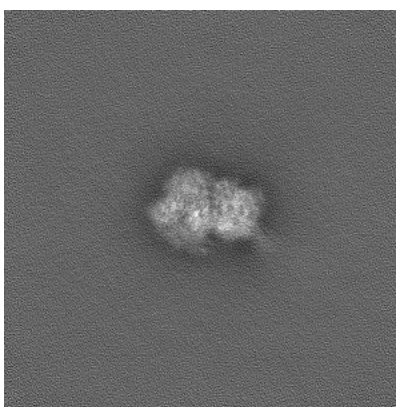


Z

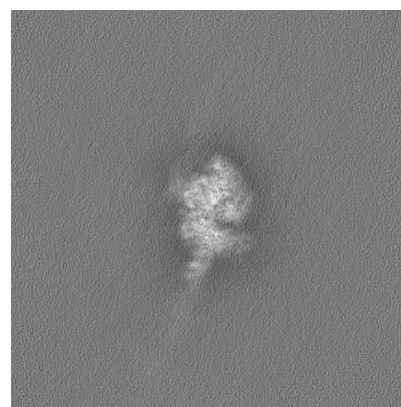
6.1.2 Raw map



X



Y

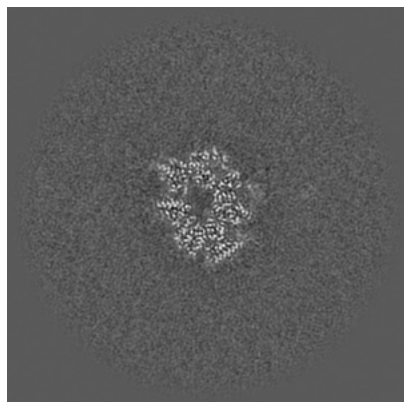


Z

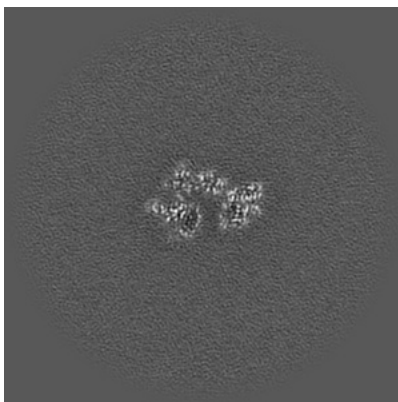
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

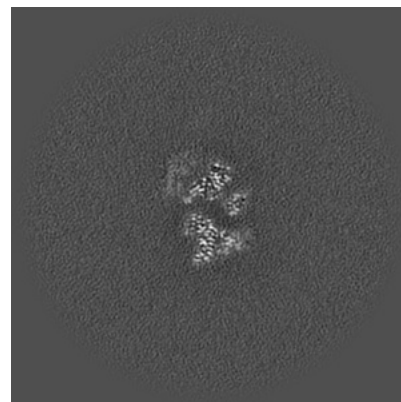
6.2.1 Primary map



X Index: 192

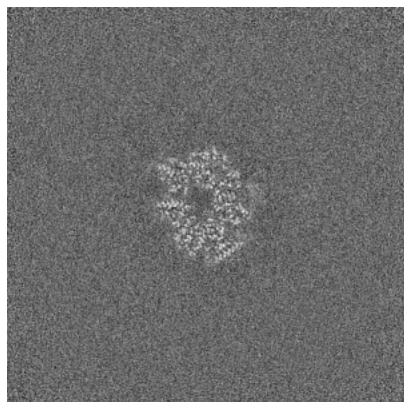


Y Index: 192

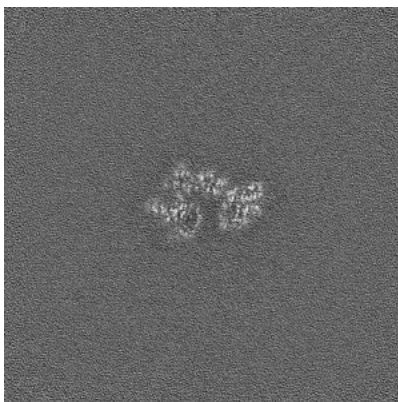


Z Index: 192

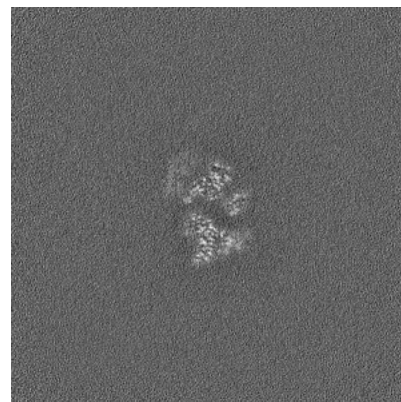
6.2.2 Raw map



X Index: 192



Y Index: 192

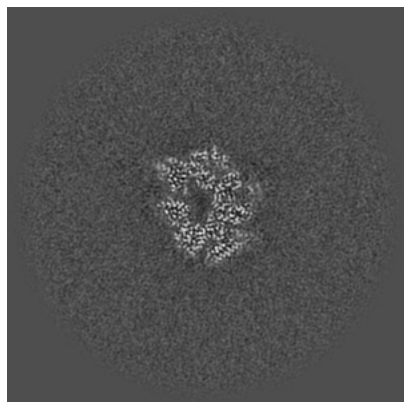


Z Index: 192

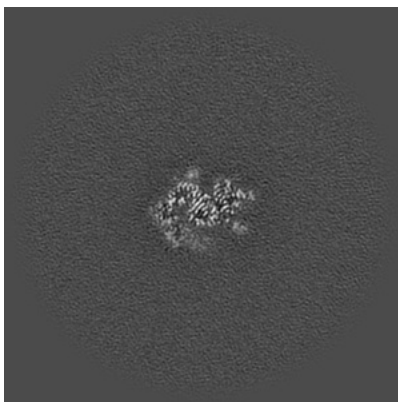
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

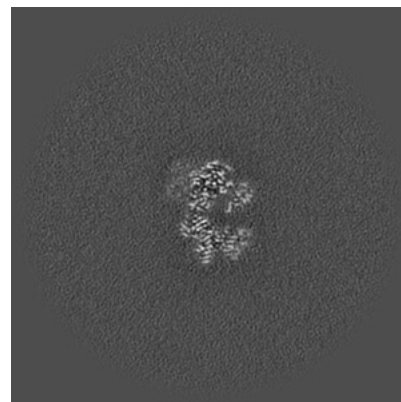
6.3.1 Primary map



X Index: 193

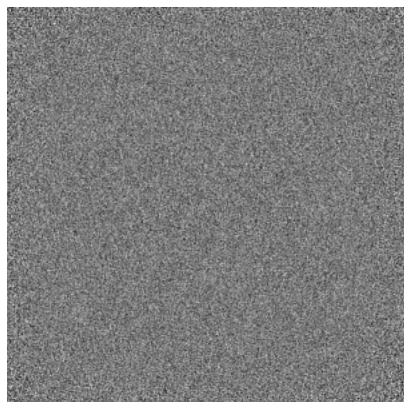


Y Index: 214

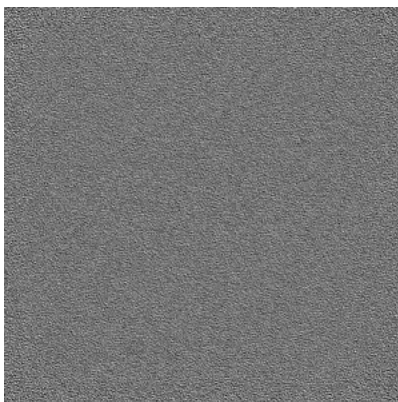


Z Index: 185

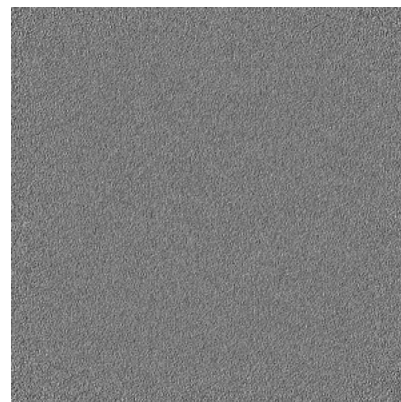
6.3.2 Raw map



X Index: 0



Y Index: 0

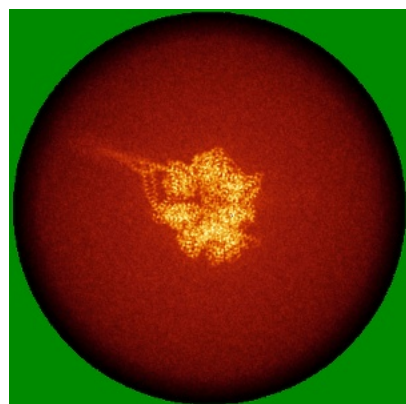


Z Index: 0

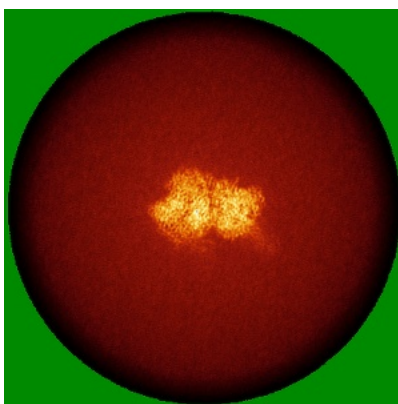
The images above show the largest variance slices of the map in three orthogonal directions.

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

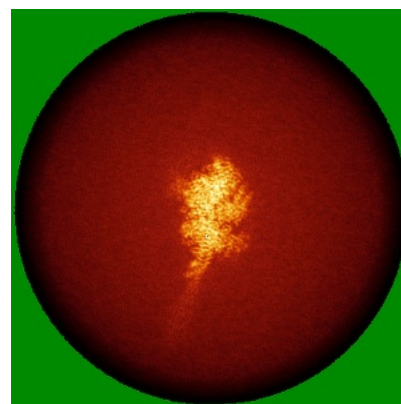
6.4.1 Primary map



X

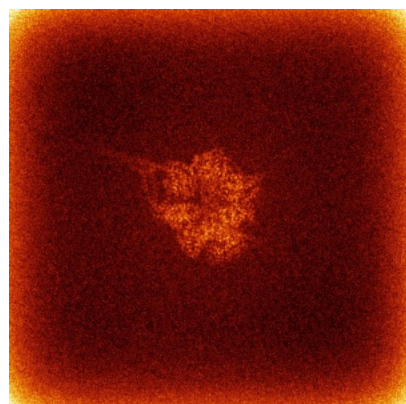


Y

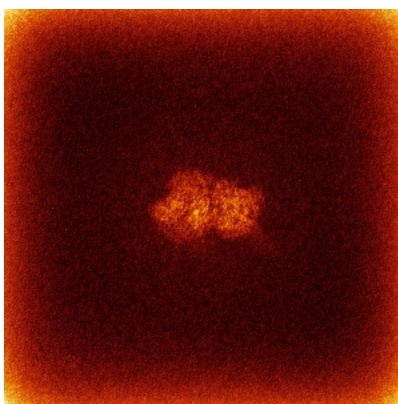


Z

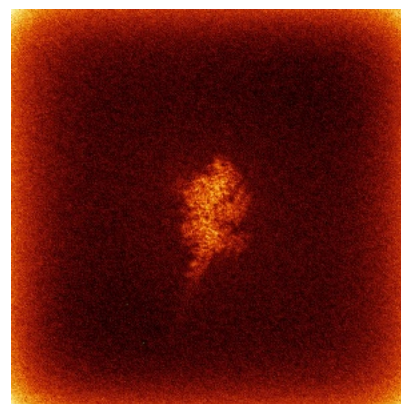
6.4.2 Raw map



X



Y

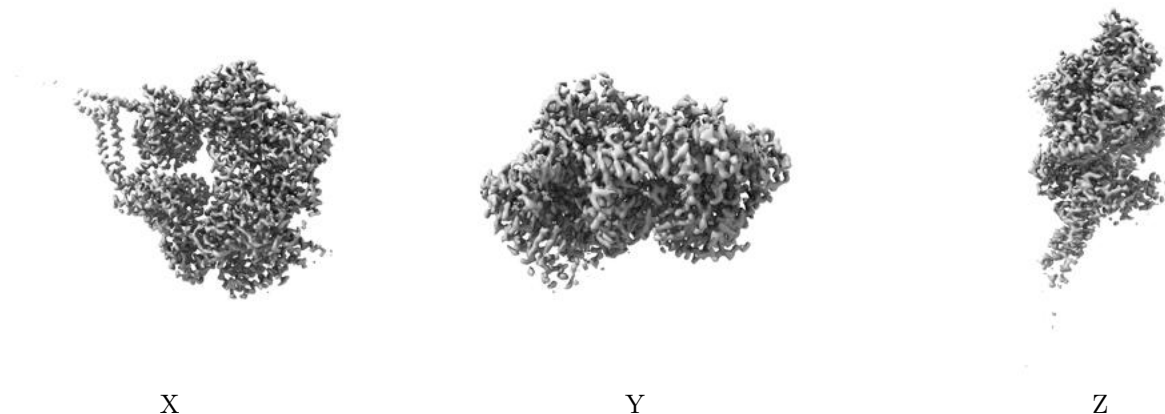


Z

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.

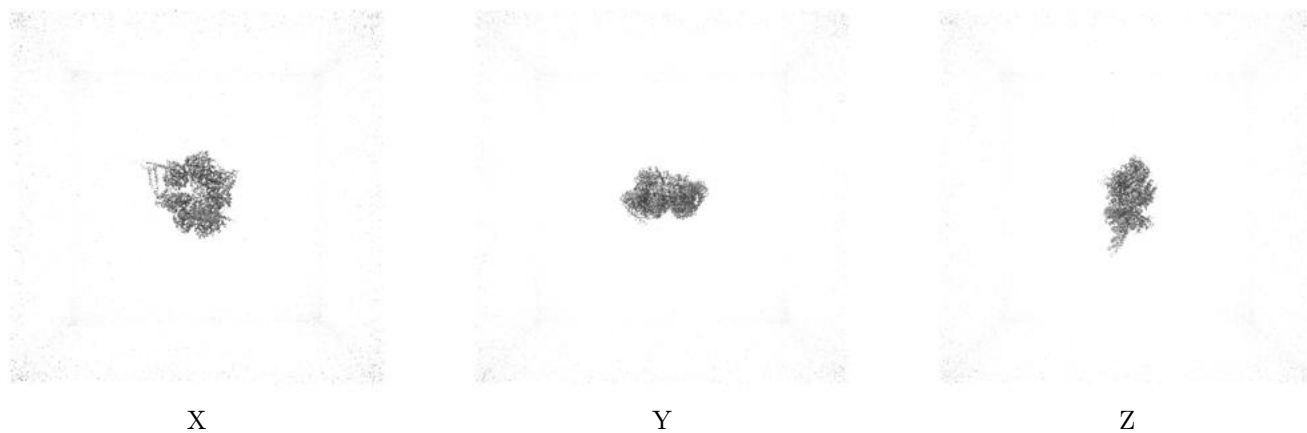
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

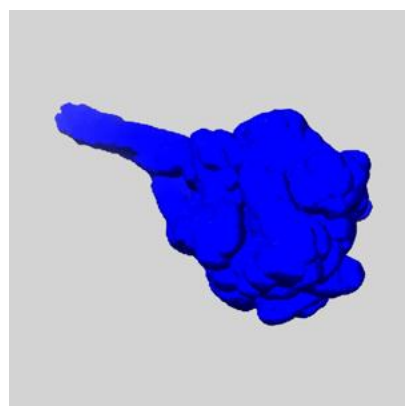
6.6 Mask visualisation [i](#)

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

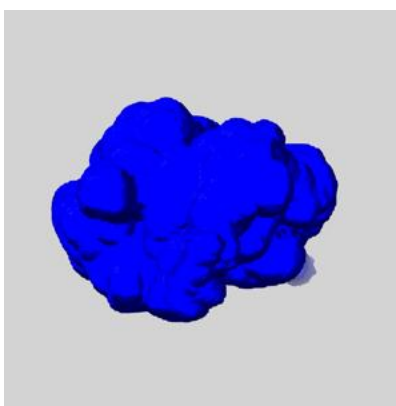
A mask typically either:

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

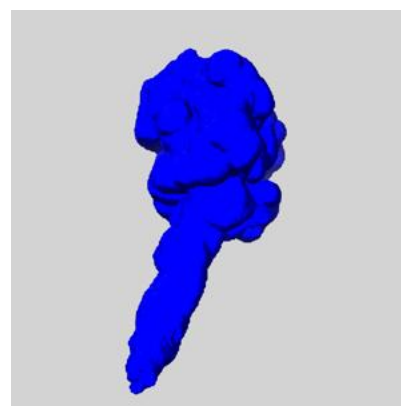
6.6.1 emd_46857_msk_1.map [i](#)



X



Y

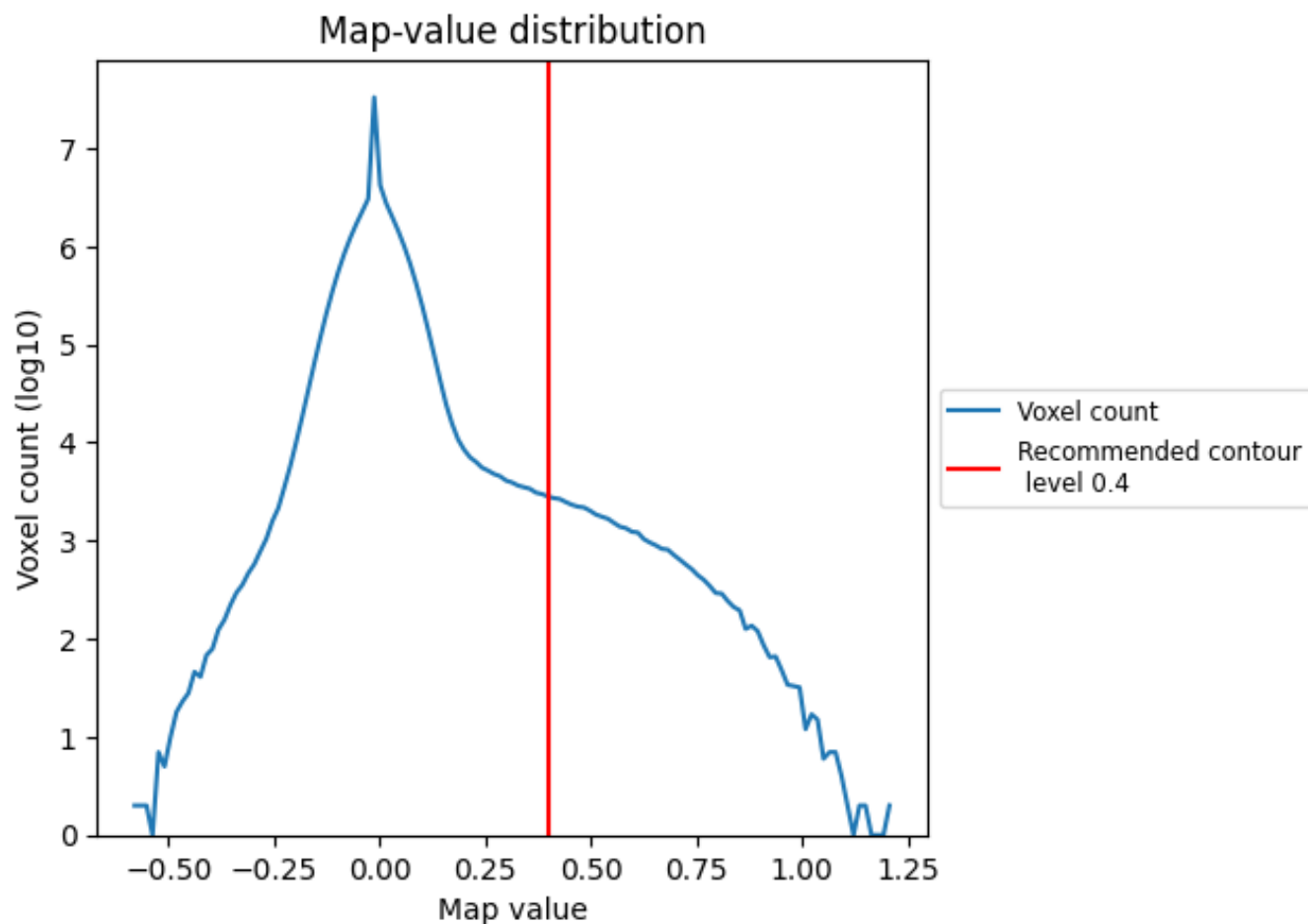


Z

7 Map analysis [i](#)

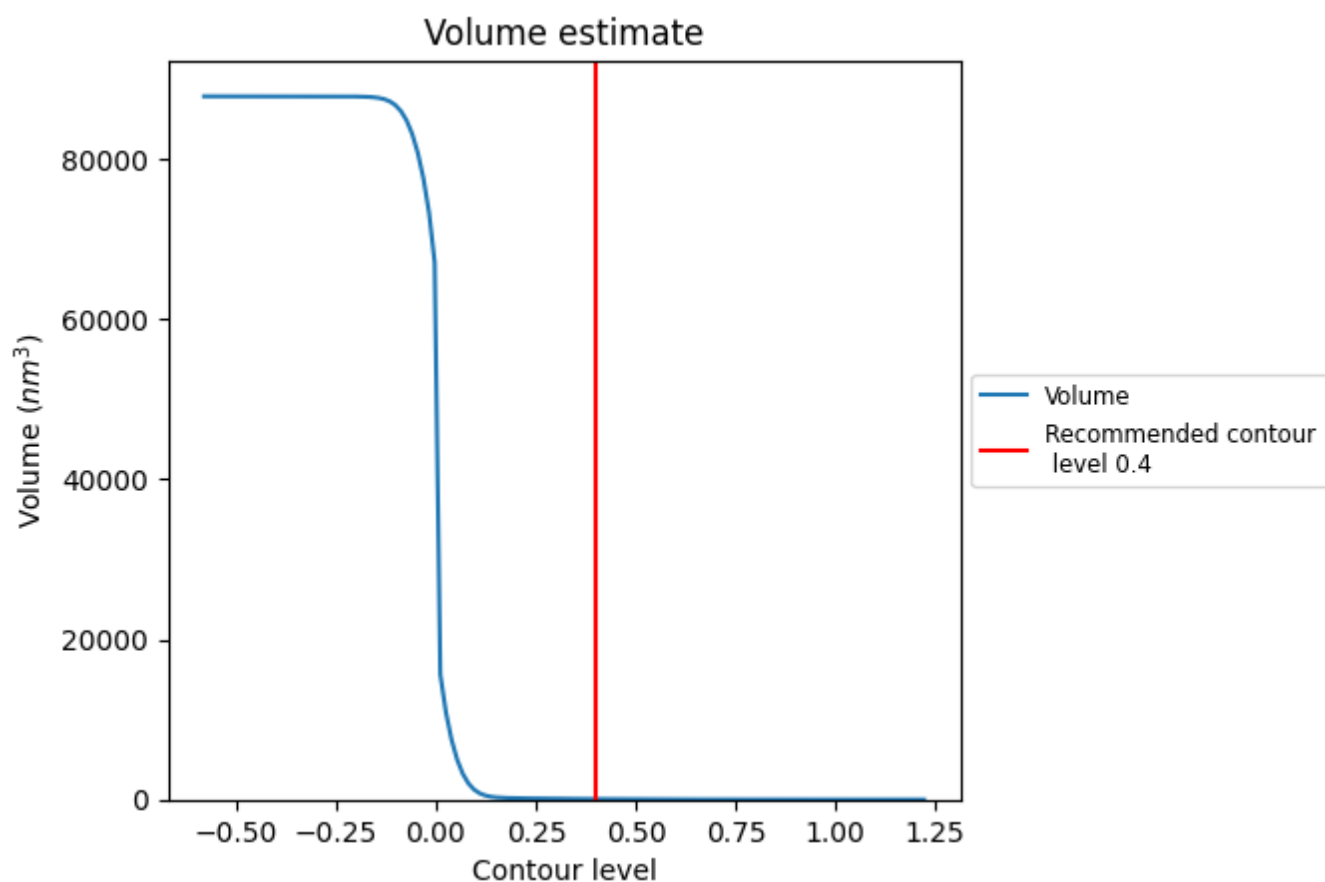
This section contains the results of statistical analysis of the map.

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.

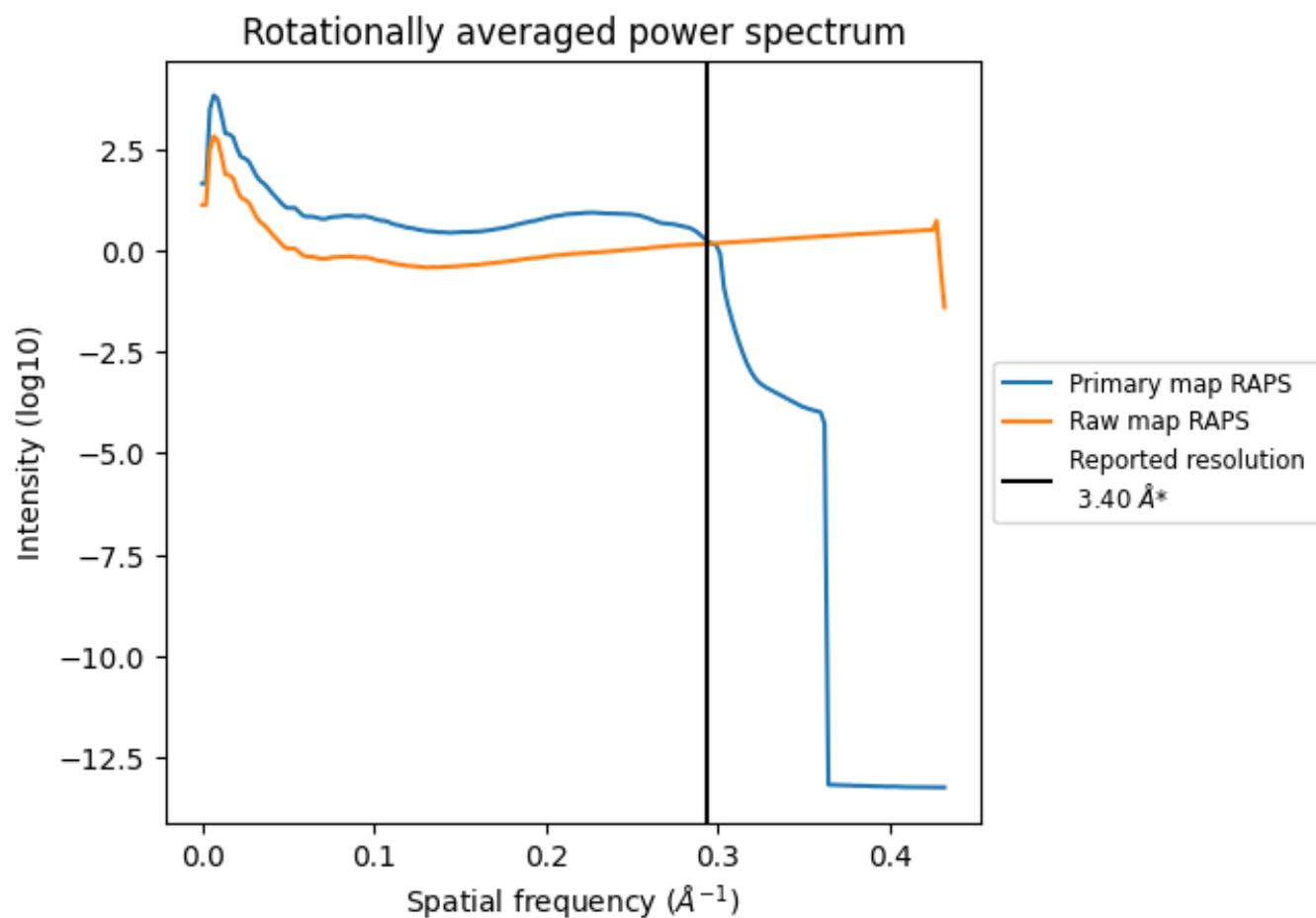
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 64 nm^3 ; this corresponds to an approximate mass of 58 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 ⓘ

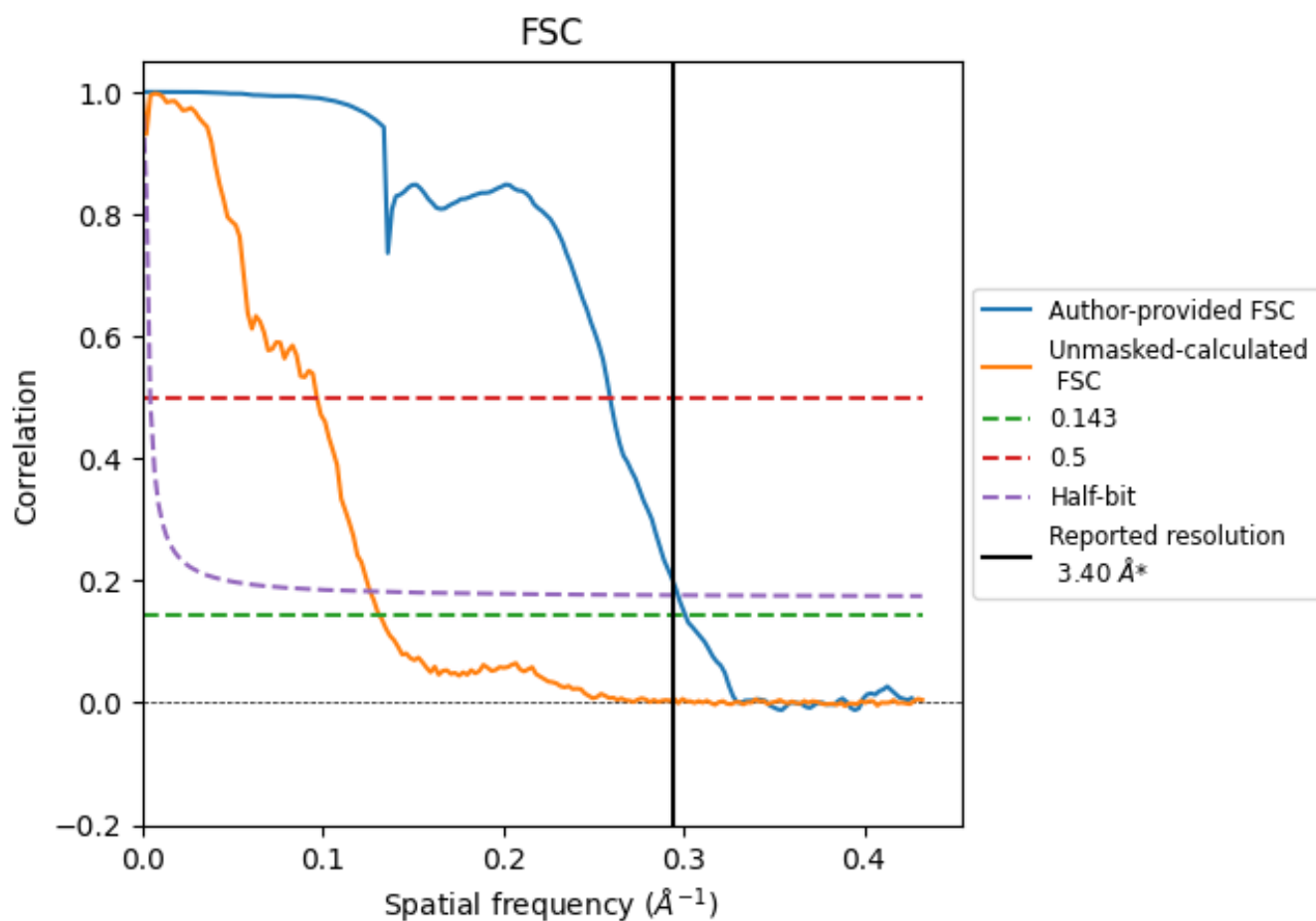


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

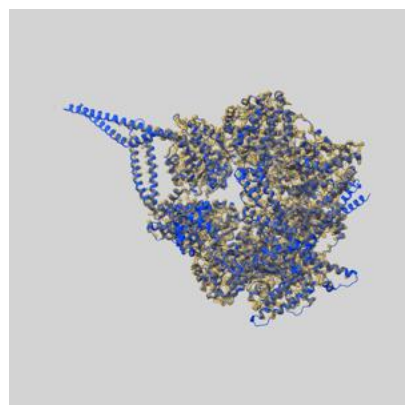
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.32	3.86	3.37
Unmasked-calculated*	7.60	10.33	7.92

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

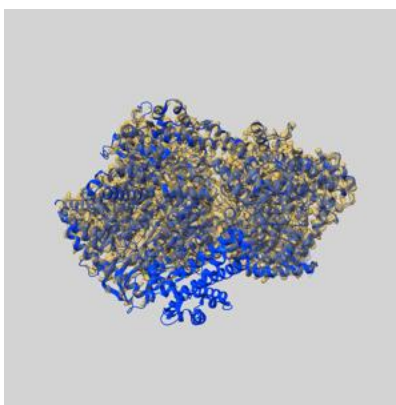
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46857 and PDB model 9DH6. Per-residue inclusion information can be found in section [3](#) on page [5](#).

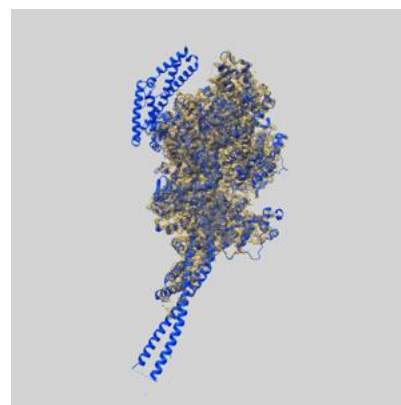
9.1 Map-model overlay [i](#)



X



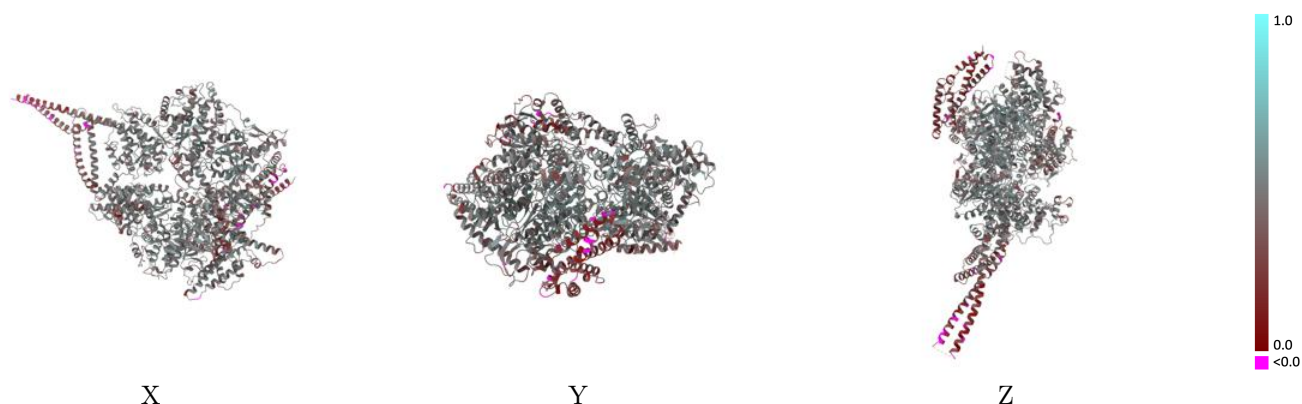
Y



Z

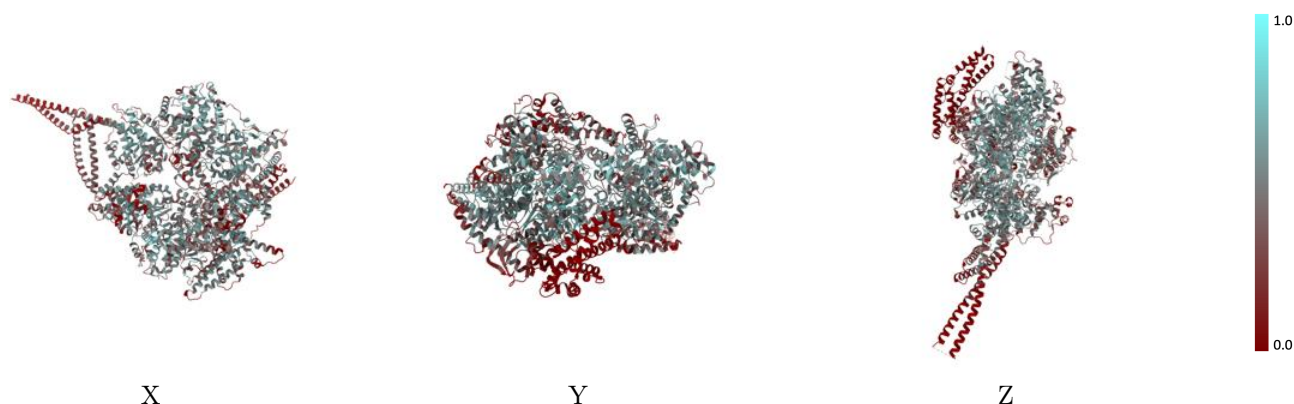
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



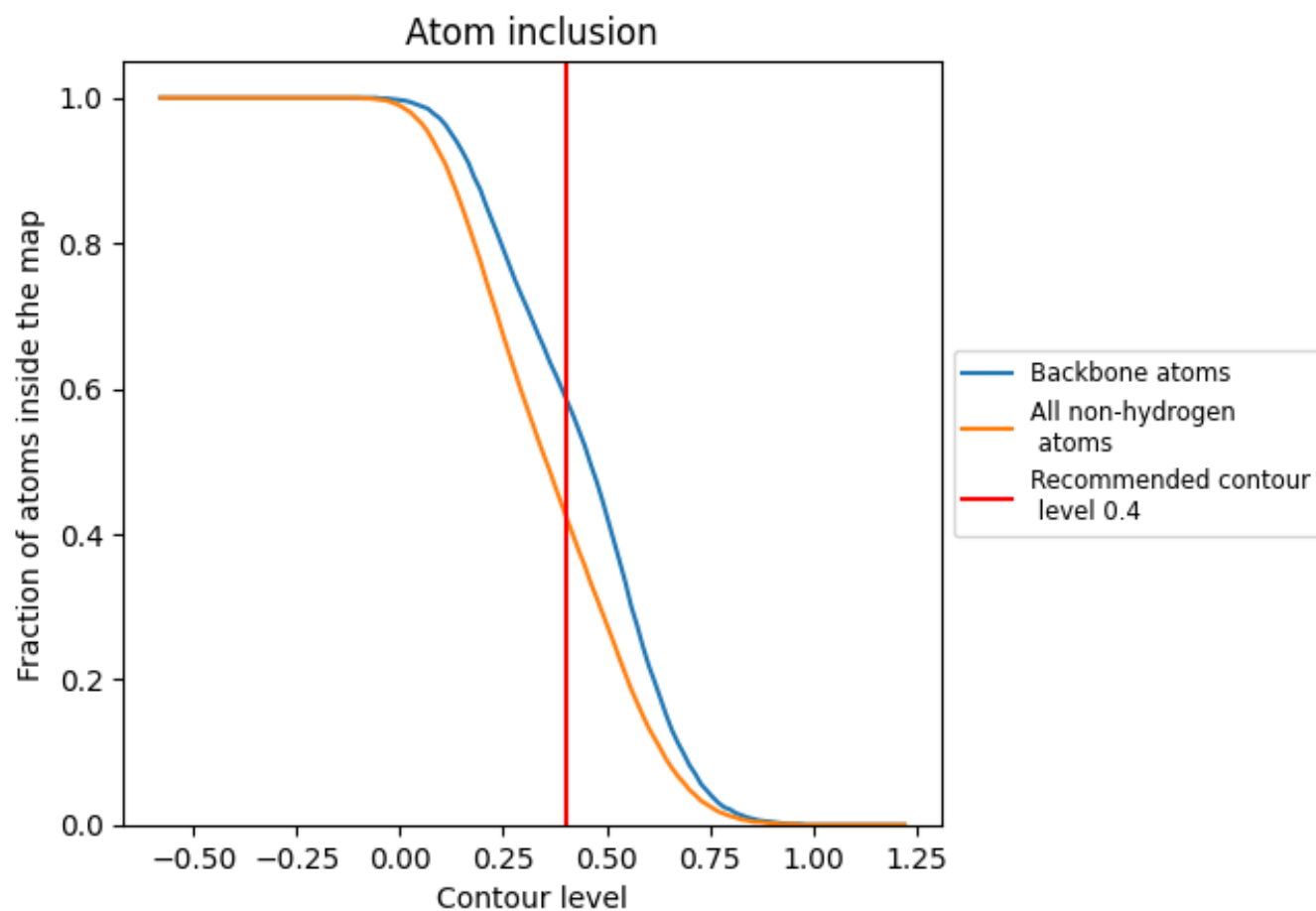
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 43% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4270	<div></div> 0.4420
A	<div></div> 0.4270	<div></div> 0.4420

