



Full wwPDB EM Validation Report ⓘ

Apr 24, 2025 – 12:28 PM EDT

PDB ID : 9BM4 / pdb_00009bm4
EMDB ID : EMD-44687
Title : State-5b of motor domain from full-length human dynein-1 in 5 mM ATP
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.48 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

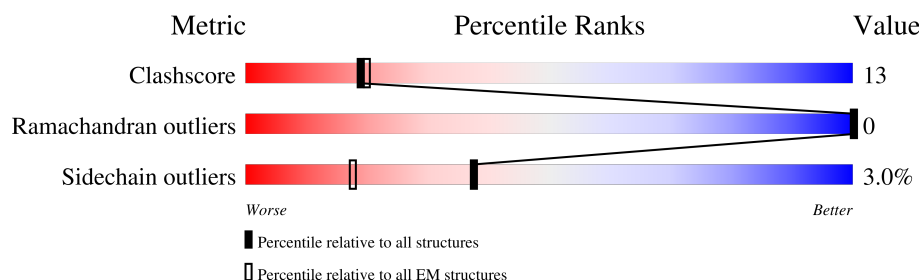
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.48 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	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 21801 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	2701	21684	13811	3743	4019	111	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

- 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 31	C 10	N 5	O 13	P 3	0
3	A	1	Total 31	C 10	N 5	O 13	P 3	0

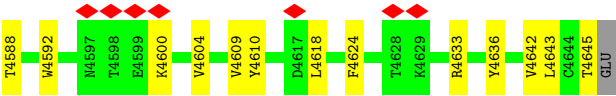
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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



T3211	D3114	Q3032	L2920	E2839	12747	R2610	L2499	D2388	Q2299	L2191	E2078	K2007
V3212	L3115	E3035	D2923	D2840	Y2748	P2613	W2500	E2389	F2303	T2192	Q2079	P2010
D3213	E3116	D2841	F2926	E2842	G2749	D2614	S2501	GLU	D2308	K2206	H2085	D2011
Q3214	P3123	R2843	R2927	R2844	T2750	M2615	D2502	ASP	P2309	Q2212	Y2086	D2012
V3215	D3124	R2845	Q2928	W2846	A2754	S2623	D2505	GLU	E2310	T2216	D2087	A2013
E3216	G3041	G3041	Q2929	T2846	R2757	T2626	S2506	ALA	W2311	L2220	F2088	A2014
E3217	Y3125	L3042	Q2930	T2846	R2757	T2626	R2507	GLN	W2312	L2220	G2089	F2015
L3218	M3043	L3044	G2931	T2850	R2759	L2630	R2511	ARG	E2313	L2221	L2090	T2016
R3219	H3047	L2933	H2932	H2857	R2763	Y2641	L2514	LYS	M2314	W2222	V2096	T2017
R3220	E3048	L2934	L2933	F2858	T2770	G2647	E2515	GLY	D2320	G2223	L2097	N2018
ASP	K3132	E3048	L2935	D2861	T2770	G2647	E2516	LYS	D2321	V2227	S2089	P2020
LEU	L3133	E3049	L2936	D2862	T2774	V2648	Y2517	ASP	N2322	S2228	A2100	TVR
ARG	P3134	I3059	G2937	R2863	E2775	V2649	L2518	GLU	K2323	S2231	V2103	ALA
ILE	Q3135	H3063	V2938	E2864	E2779	L2650	T2521	GLY	L2324	M2232	R2107	GLY
SER	P3136	F3066	V2963	S2868	W2779	K2657	T2526	GLU	L2325	A2233	E2114	ARG
GLN	R3140	T3067	R2964	T2871	E2782	W2658	P2527	ALA	P2328	W2234	K2115	SER
GLU	S3146	K2965	K2966	T2872	R2783	V2658	T2528	ALA	N2329	L2244	E2116	L2028
LEU	G3147	Y2967	Y2967	Y2872	F2784	D2664	T2528	S2410	G2330	E2245	P2029	P2029
VAL	V3148	S3070	T2968	Y2873	T2785	E2665	W2531	P2411	E2331	E2265	E2117	D2030
LYS	F3149	SER	G2969	Y2876	Q2786	E2665	W2531	M2412	R2332	P2256	R2118	N2031
ASN	V3150	SER	E2974	W2876	D2787	E2665	W2531	L2413	L2333	S2260	E2119	L2032
ALA	G3151	GLU	D2975	K2879	T2788	P2689	T2534	Q2416	P2337	K2261	E2120	F2036
ALA	Q3152	LEU	L2976	D2880	Q2789	D2670	T2535	R2417	N2338	R2261	E2120	R2037
ASN	T3153	LYS	R2977	T2881	R2790	Y2674	E2538	D2418	V2339	D2262	A2121	S2038
ASP	L3154	ASP	T2978	Y2882	H2791	Y2674	E2538	A2419	R2340	R2263	L2039	L2039
LYS	N3158	ARG	R2981	P2883	T2792	Y2679	W2548	I2422	I2341	L2264	D2123	A2040
LEU	T3168	ALA	D2995	Q2886	Y2794	V2679	V2557	M2423	M2342	Y2265	E2126	N2041
LYS	M3169	LYS	E2996	E2887	R2797	R2684	V2557	S2429	F2343	L2268	I2127	T2042
MET	A3170	E2888	E2996	E2888	Q2686	Q2686	T2559	V2345	E2345	L2137	L2137	R2046
VAL	I3171	L2889	S2997	E2889	V2687	V2687	A2563	V2350	Y2350	I2138	Q2139	I2049
ASP	H3175	R2890	N2998	R2890	E2688	E2688	D2566	A2351	A2351	S2140	V2141	V2052
GLN	A3184	D2891	G3002	D2891	H2689	H2689	D2566	L2352	T2352	C2142	C2142	M2053
ALA	K3190	Y2892	F3004	V2893	Q2692	Q2692	V2569	A2354	A2354	E2274	E2143	L2054
LYS	R3191	K2894	L3005	K2894	Q2698	Q2698	V2569	R2451	V2355	W2275	K2148	Y2055
LYS	E3195	R2896	E3006	A2895	V2701	V2701	L2581	L2452	S2357	G2278	L2161	S2056
VAL	E3196	L2897	R3007	L2895	G2710	G2710	L2581	S2457	M2361	L2279	L2161	R2060
MET	Q3197	E2902	M3008	E2902	K2721	K2721	L2584	M2461	M2361	H2282	Q2169	L2065
SER	Q3198	E2903	N3009	E2903	R2729	R2729	L2585	Q2471	V2362	V2283	Y2170	A2066
GLN	M3199	D2906	L3012	D2906	H2730	H2730	H2588	D2478	W2363	L2284	T2176	V2067
ILE	H3200	V2907	A3013	V2907	R2732	R2732	K2589	F2479	F2364	I2287	A2177	K2068
GLN	L3201	W2908	N3014	W2908	Y2731	Y2731	P2590	D2478	S2365	L2288	R2179	I2069
GLU	V3105	L2909	F3021	L2909	V2733	V2733	L2593	F2479	E2366	D2289	E2180	V2070
GLN	K3106	V2910	D3024	V2910	Q2834	Q2834	L2593	I2490	L2369	R2292	E2181	F2071
LEU	E3107	L2911	E3025	L2911	R2835	R2835	M2603	I2490	M2373	E2293	E2181	F2072
LYS	F3109	L2916	E3025	L2916	R2836	R2836	L2604	V2495	W2373	G2294	Q2187	K2074
LYS	G3204	D2917	M3030	D2917	L2837	L2837	T2606	V2495	I2385	E2294	E2188	L2075
GLN	R3206	H2918	M3030	H2918	Y2838	Y2838	F2606	I2498	P2386	L2295	M2189	C2076
GLU	I3208	V2919	T3031	V2919					L2387	R2298	Y2190	D2077
K3209	E3210											
E3210												





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114327	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.703	Depositor
Minimum map value	-0.410	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	332.80002, 332.80002, 332.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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	0.27	0/22148	0.51	3/30024 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1766	LEU	CA-CB-CG	6.52	130.29	115.30
1	A	4451	LEU	CA-CB-CG	5.96	129.01	115.30
1	A	4224	ASP	CB-CG-OD1	5.18	122.97	118.30

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	21684	0	21717	549	0
2	A	54	0	24	4	0
3	A	62	0	24	5	0
4	A	1	0	0	0	0
All	All	21801	0	21765	549	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 13.

All (549) 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:1659:ALA:HA	1:A:1926:PHE:HE1	1.24	1.00
1:A:1659:ALA:HA	1:A:1926:PHE:CE1	2.07	0.88
1:A:3759:ARG:HG3	1:A:3760:ILE:HG13	1.56	0.88
1:A:3030:MET:SD	1:A:3047:HIS:ND1	2.49	0.84
1:A:3845:ASN:HB3	1:A:3858:ILE:HD11	1.61	0.83
1:A:2461:MET:HG3	1:A:2583:THR:HG21	1.62	0.80
1:A:3721:ARG:HH12	1:A:3852:HIS:CE1	1.99	0.80
1:A:2325:LEU:HB3	1:A:2333:LEU:HB2	1.63	0.79
1:A:2386:PRO:HA	1:A:2416:GLN:HE22	1.48	0.78
1:A:3474:ARG:HD2	1:A:3762:ASP:HB3	1.67	0.76
1:A:1842:MET:HA	1:A:1861:MET:HB2	1.68	0.76
1:A:3721:ARG:HG3	1:A:3724:VAL:HB	1.67	0.76
1:A:2452:LEU:HD11	3:A:4702:ATP:H4'	1.70	0.74
1:A:3796:THR:HA	1:A:3799:GLN:HG3	1.72	0.72
1:A:4377:MET:HE2	1:A:4438:CYS:HA	1.72	0.72
1:A:4027:LEU:HB3	1:A:4058:LEU:HD22	1.72	0.72
1:A:1950:GLN:HG2	1:A:2006:VAL:HG13	1.72	0.72
1:A:1655:LYS:HB3	1:A:2332:ARG:HD2	1.74	0.70
1:A:3721:ARG:O	1:A:3725:ASP:N	2.24	0.69
1:A:1859:ILE:HD12	1:A:1923:LEU:HD23	1.73	0.69
1:A:1792:LEU:HD12	1:A:1812:ILE:HG13	1.75	0.68
1:A:2910:VAL:HG11	1:A:3105:VAL:HG13	1.76	0.68
1:A:2670:ASP:HA	1:A:2721:LYS:HE3	1.75	0.68
1:A:2918:HIS:HE1	1:A:3094:PHE:HA	1.57	0.68
1:A:4374:PRO:HG2	1:A:4377:MET:HB2	1.75	0.67
1:A:1843:ARG:HH12	1:A:1861:MET:HA	1.59	0.67
1:A:4113:LEU:HD11	1:A:4124:LEU:HD23	1.76	0.67
1:A:3013:ALA:HB2	1:A:3088:ARG:HE	1.59	0.67
1:A:3005:LEU:HD11	1:A:3085:LEU:HD22	1.78	0.66
1:A:3101:ALA:O	1:A:3105:VAL:HG23	1.96	0.65
1:A:3631:ASN:ND2	1:A:3632:PRO:O	2.28	0.65
1:A:4299:GLY:HA3	1:A:4304:GLU:HG2	1.78	0.65
1:A:2275:TRP:CH2	1:A:2328:PRO:HD2	2.32	0.65
1:A:4281:GLU:OE2	1:A:4281:GLU:N	2.30	0.65
1:A:4211:ASP:OD1	1:A:4255:ARG:NH1	2.30	0.65
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.29	0.65
1:A:2227:GLY:HA2	1:A:2452:LEU:HD12	1.80	0.64
1:A:2444:GLU:OE1	1:A:2507:ARG:NH1	2.28	0.64
1:A:2893:VAL:HG13	1:A:2911:LEU:HD21	1.80	0.64
1:A:1982:LEU:HD21	1:A:2012:MET:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1746:GLN:N	1:A:1746:GLN:OE1	2.31	0.64
1:A:2499:LEU:HD13	1:A:2514:LEU:HD23	1.79	0.64
1:A:2757:ARG:HA	1:A:2763:ARG:HD3	1.78	0.64
1:A:2295:LEU:O	1:A:2338:ASN:ND2	2.31	0.64
1:A:2452:LEU:HD13	1:A:2729:ARG:HE	1.63	0.63
1:A:2099:SER:OG	1:A:2140:SER:OG	2.17	0.63
1:A:2890:ARG:O	1:A:2894:LYS:HG3	1.99	0.63
1:A:1801:PRO:HD2	1:A:1804:ARG:HE	1.64	0.63
1:A:1632:VAL:HB	1:A:1636:ASP:HB2	1.81	0.62
1:A:1847:ASP:N	1:A:1856:GLN:O	2.31	0.62
1:A:1820:ASP:OD1	1:A:1823:ARG:NH2	2.33	0.62
1:A:3931:GLN:O	1:A:3935:VAL:HG23	1.99	0.62
1:A:2977:ARG:HG3	1:A:3020:LEU:HB3	1.80	0.61
1:A:3116:GLU:HG2	1:A:3140:ARG:HH12	1.65	0.61
1:A:3790:VAL:HG13	1:A:3794:VAL:HB	1.82	0.61
1:A:4176:ARG:NH1	1:A:4220:ASP:OD1	2.32	0.61
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.81	0.61
1:A:1686:PHE:HA	1:A:1712:THR:HG21	1.81	0.61
1:A:3576:ASN:ND2	1:A:3700:ASN:O	2.33	0.61
1:A:3909:LEU:HD21	1:A:4343:MET:HE2	1.82	0.61
1:A:1762:VAL:O	1:A:1766:LEU:HD22	2.01	0.60
1:A:1912:LYS:HD3	1:A:2017:THR:HB	1.82	0.60
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.82	0.60
1:A:2498:ILE:HG23	1:A:2502:LEU:HD22	1.83	0.60
1:A:3175:HIS:HB3	1:A:3516:TYR:HE1	1.65	0.60
1:A:1684:VAL:HG12	1:A:1746:GLN:HE21	1.66	0.60
1:A:3731:LEU:HA	1:A:3734:LEU:HD23	1.84	0.60
1:A:4257:ASP:OD2	1:A:4258:ASN:N	2.34	0.60
1:A:1880:VAL:HG21	1:A:2049:ILE:HG13	1.83	0.60
1:A:3214:GLN:HB2	1:A:3759:ARG:HH12	1.65	0.60
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	1.84	0.60
1:A:2142:CYS:SG	1:A:2143:GLU:N	2.75	0.60
1:A:2419:ALA:O	1:A:2423:MET:HG2	2.00	0.60
1:A:1812:ILE:HG21	1:A:2056:SER:HA	1.84	0.60
1:A:2245:GLU:OE2	1:A:2298:ARG:NH2	2.35	0.60
1:A:3724:VAL:HA	1:A:3727:LYS:HB3	1.82	0.60
1:A:1846:PHE:HD2	1:A:1857:LEU:HB2	1.67	0.60
1:A:2499:LEU:HD21	1:A:2518:ILE:HG21	1.81	0.60
1:A:3808:CYS:HG	1:A:3836:TYR:HE2	1.50	0.59
1:A:2014:ILE:HG23	1:A:2036:PHE:HZ	1.66	0.59
1:A:2231:SER:OG	1:A:2344:GLU:OE2	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2413:LEU:HG	1:A:2417:ARG:HE	1.68	0.59
1:A:3551:GLU:OE1	1:A:3559:ARG:NH1	2.36	0.59
1:A:4190:ILE:HD12	1:A:4201:TRP:HZ2	1.68	0.59
1:A:2191:LEU:HD21	1:A:2232:MET:HG2	1.83	0.59
1:A:3517:ALA:HA	1:A:3520:PHE:HD1	1.67	0.58
1:A:3638:VAL:HG22	1:A:3681:THR:HG22	1.85	0.58
1:A:3825:TYR:CZ	1:A:3875:MET:HG3	2.39	0.58
1:A:2968:THR:OG1	1:A:2969:GLY:N	2.37	0.58
1:A:2325:LEU:HD23	1:A:2333:LEU:HD23	1.84	0.58
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.84	0.58
1:A:3793:GLU:O	1:A:3797:VAL:HG23	2.03	0.58
1:A:2320:ASP:HB3	1:A:2358:ARG:HD3	1.84	0.58
1:A:3951:VAL:HG13	1:A:3957:PHE:CE2	2.40	0.57
1:A:2534:ILE:HD12	1:A:2534:ILE:H	1.68	0.57
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.69	0.57
1:A:3971:PRO:HG2	1:A:3973:LEU:HD11	1.84	0.57
1:A:2337:PRO:O	1:A:2340:ARG:NH1	2.37	0.57
1:A:2789:GLN:HB2	1:A:2792:TYR:CD1	2.40	0.57
1:A:2075:LEU:HD22	1:A:4526:GLN:HE21	1.68	0.57
1:A:2770:THR:O	1:A:2774:VAL:HG22	2.05	0.57
1:A:2873:TYR:CE2	1:A:2883:PRO:HD3	2.38	0.57
1:A:1710:ARG:HH11	1:A:1854:LEU:HD11	1.69	0.57
1:A:2065:LEU:HD13	1:A:2137:LEU:HD22	1.87	0.57
1:A:3521:ASP:OD1	1:A:3521:ASP:N	2.33	0.57
1:A:3096:ASP:OD2	1:A:3097:TRP:N	2.39	0.56
1:A:3623:LEU:O	1:A:3627:LEU:HG	2.05	0.56
1:A:2068:LYS:NZ	1:A:4535:SER:OG	2.39	0.56
1:A:3035:GLU:O	1:A:3039:LYS:HG3	2.05	0.56
1:A:4260:PHE:HE2	1:A:4618:LEU:HD11	1.69	0.56
1:A:4600:LYS:HB2	1:A:4604:VAL:HG11	1.87	0.56
1:A:1810:HIS:NE2	1:A:1876:GLN:O	2.39	0.56
1:A:1896:LEU:HD11	1:A:2013:ALA:HB2	1.88	0.56
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.38	0.56
1:A:2354:ALA:O	1:A:2358:ARG:NH1	2.38	0.56
1:A:2686:MET:HE2	1:A:2692:PHE:HB3	1.87	0.56
1:A:3787:THR:O	1:A:3790:VAL:HB	2.05	0.56
1:A:2842:GLU:O	1:A:2846:THR:HG23	2.06	0.56
1:A:4554:ASP:OD1	1:A:4555:ALA:N	2.38	0.56
1:A:3485:GLU:OE2	1:A:3489:TRP:NE1	2.30	0.55
1:A:1951:VAL:HG13	1:A:1953:ALA:H	1.71	0.55
1:A:2981:ARG:NH1	1:A:3025:GLU:OE2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3002:SER:O	1:A:3006:GLU:HG2	2.07	0.55
1:A:1687:LYS:HG2	1:A:1712:THR:HG22	1.88	0.55
1:A:3886:LEU:HD11	1:A:4346:MET:HG3	1.88	0.55
1:A:3758:GLY:O	1:A:3761:LEU:HB2	2.07	0.55
1:A:2075:LEU:HD22	1:A:4526:GLN:NE2	2.23	0.54
1:A:1888:CYS:HA	1:A:2039:LEU:HD21	1.89	0.54
1:A:4293:ASP:N	1:A:4293:ASP:OD1	2.38	0.54
1:A:1860:GLN:HG2	1:A:1865:LYS:HG2	1.88	0.54
1:A:1912:LYS:O	1:A:1916:VAL:HG23	2.07	0.54
1:A:3959:ILE:O	1:A:3963:SER:OG	2.22	0.54
1:A:3552:TYR:HB3	1:A:3553:LEU:HD12	1.90	0.54
1:A:4031:VAL:HG21	1:A:4058:LEU:HD21	1.89	0.54
1:A:1623:ARG:HH21	1:A:1637:LEU:HD22	1.72	0.54
1:A:3951:VAL:HG13	1:A:3957:PHE:HE2	1.71	0.54
1:A:3851:ASP:HB3	1:A:3854:GLN:HG2	1.89	0.54
1:A:4094:VAL:HG13	1:A:4124:LEU:HD13	1.87	0.54
1:A:4452:ILE:O	1:A:4456:VAL:HG12	2.07	0.54
1:A:2511:ARG:HB3	1:A:2535:ILE:HD12	1.90	0.54
1:A:3854:GLN:O	1:A:3858:ILE:HG22	2.08	0.54
1:A:1665:ILE:N	1:A:1675:GLY:O	2.41	0.53
1:A:2388:ASP:HB3	1:A:2412:MET:HE1	1.90	0.53
1:A:1957:PHE:HB2	1:A:2016:ILE:HA	1.89	0.53
1:A:2123:ASP:HB3	1:A:2126:GLU:HG2	1.90	0.53
1:A:3113:MET:SD	1:A:3184:ALA:HA	2.48	0.53
1:A:2495:VAL:HG11	1:A:2526:LEU:HD21	1.89	0.53
1:A:2759:ILE:HG13	1:A:2759:ILE:O	2.09	0.53
1:A:4025:LEU:HD22	1:A:4027:LEU:HG	1.88	0.53
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.91	0.53
1:A:3892:LEU:HD13	1:A:3983:ILE:HG21	1.90	0.53
1:A:1912:LYS:HB3	1:A:2041:MET:HG3	1.91	0.53
1:A:2826:ALA:HA	1:A:2850:ILE:HD11	1.89	0.53
1:A:2178:LEU:HD13	1:A:2244:LEU:HD22	1.90	0.53
1:A:3123:PRO:HG3	1:A:3539:ALA:HA	1.90	0.53
1:A:4106:LEU:HD23	1:A:4135:PRO:HD2	1.89	0.53
1:A:2261:LYS:NZ	1:A:2313:GLU:OE1	2.35	0.53
1:A:2935:LEU:HD22	1:A:3094:PHE:HE1	1.73	0.53
1:A:3638:VAL:HG11	1:A:3679:LEU:HB3	1.91	0.53
1:A:3870:ARG:CZ	1:A:4034:GLU:HG3	2.39	0.53
1:A:1961:ASN:HD21	1:A:2019:ASN:HB3	1.73	0.52
1:A:1746:GLN:HG2	1:A:1872:TYR:HE1	1.74	0.52
1:A:1961:ASN:OD1	1:A:1962:ARG:NH1	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4260:PHE:CE2	1:A:4618:LEU:HD11	2.44	0.52
1:A:1789:LEU:HD21	1:A:1815:LEU:HB3	1.91	0.52
1:A:2684:ARG:NH1	1:A:2688:GLU:OE2	2.40	0.52
1:A:2581:LEU:HD21	1:A:2605:LEU:HD23	1.91	0.52
1:A:2974:GLU:O	1:A:2978:THR:HG23	2.09	0.52
1:A:4042:LEU:HD13	1:A:4126:LEU:HB2	1.92	0.52
1:A:2557:VAL:HG12	1:A:2750:THR:HG22	1.92	0.52
1:A:2918:HIS:CE1	1:A:3094:PHE:HA	2.42	0.52
1:A:3133:LEU:HD12	1:A:3134:PRO:HD2	1.91	0.52
1:A:4565:LEU:HD13	1:A:4642:VAL:HG22	1.92	0.52
1:A:2260:SER:OG	1:A:2263:HIS:ND1	2.39	0.52
1:A:2666:ILE:HD12	1:A:2710:GLY:HA3	1.91	0.52
1:A:2964:HIS:CD2	1:A:2966:LYS:HB3	2.45	0.52
1:A:2279:LEU:HA	1:A:2698:GLN:HG2	1.91	0.52
1:A:2457:SER:HB2	1:A:2732:PRO:HB3	1.92	0.52
1:A:4106:LEU:HG	1:A:4138:LEU:HD22	1.92	0.52
1:A:4400:ARG:NE	1:A:4405:ILE:HD11	2.25	0.52
1:A:2079:GLN:O	1:A:4415:ARG:NH2	2.43	0.51
1:A:2278:GLY:O	1:A:2282:HIS:N	2.40	0.51
1:A:2603:MET:CE	3:A:4703:ATP:H2'	2.39	0.51
1:A:2963:VAL:HG11	1:A:2998:ASN:HA	1.91	0.51
1:A:1647:VAL:HG11	1:A:1692:ILE:HD13	1.91	0.51
1:A:2054:LEU:HG	1:A:2097:LEU:HD22	1.92	0.51
1:A:1659:ALA:HB3	1:A:1872:TYR:O	2.09	0.51
1:A:3488:ARG:O	1:A:3491:LYS:HG3	2.10	0.51
1:A:3724:VAL:HG13	1:A:3727:LYS:HD3	1.93	0.51
1:A:4030:ILE:HG21	1:A:4145:PHE:CZ	2.45	0.51
1:A:4446:ASN:O	1:A:4450:THR:HG22	2.11	0.51
1:A:3947:LEU:O	1:A:3951:VAL:HG23	2.11	0.51
1:A:2862:ASP:OD1	1:A:2862:ASP:N	2.41	0.51
1:A:3721:ARG:CG	1:A:3724:VAL:HB	2.39	0.51
1:A:2593:LEU:HD23	1:A:2736:VAL:HG21	1.91	0.51
1:A:2886:GLN:H	1:A:2886:GLN:CD	2.14	0.50
1:A:3612:THR:O	1:A:3635:VAL:HA	2.11	0.50
1:A:1843:ARG:NH1	1:A:1861:MET:HA	2.23	0.50
1:A:1959:GLU:O	1:A:1959:GLU:HG3	2.12	0.50
1:A:3513:PHE:HZ	1:A:3575:GLU:HB3	1.77	0.50
1:A:3705:ARG:HG2	1:A:3813:PHE:HE1	1.76	0.50
1:A:2688:GLU:OE1	1:A:2689:HIS:NE2	2.45	0.50
1:A:4381:HIS:NE2	1:A:4439:GLU:OE2	2.41	0.50
1:A:1846:PHE:HA	1:A:1857:LEU:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1880:VAL:HG22	2:A:4701:ADP:N1	2.27	0.50
1:A:1903:SER:N	1:A:2037:ARG:O	2.44	0.50
1:A:3764:ASP:O	1:A:3767:ILE:HG12	2.11	0.50
1:A:3870:ARG:NH2	1:A:4034:GLU:HG3	2.26	0.50
1:A:2935:LEU:HB2	1:A:3067:THR:HG22	1.93	0.50
1:A:2563:ALA:HB3	1:A:2804:ARG:HG2	1.93	0.50
1:A:4187:HIS:CD2	1:A:4212:LEU:HD22	2.47	0.50
1:A:2977:ARG:HG2	1:A:3021:PHE:CE1	2.47	0.49
1:A:3114:ASP:OD1	1:A:3114:ASP:N	2.45	0.49
1:A:2039:LEU:HD12	1:A:2040:ALA:H	1.77	0.49
1:A:2775:GLU:O	1:A:2779:MET:HE3	2.12	0.49
1:A:3044:LEU:HD22	1:A:3049:GLU:HB3	1.92	0.49
1:A:3737:GLU:HG3	1:A:3741:ARG:NH2	2.27	0.49
1:A:3835:ILE:HD13	1:A:3867:ALA:HA	1.93	0.49
1:A:4430:ASP:OD1	1:A:4451:LEU:HD11	2.12	0.49
1:A:4128:MET:SD	1:A:4134:VAL:HG21	2.52	0.49
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.45	0.49
1:A:2049:ILE:HG21	1:A:2090:LEU:HD11	1.93	0.49
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.94	0.49
1:A:3514:ILE:HD13	1:A:3579:MET:HG2	1.95	0.49
1:A:1628:ARG:HD2	1:A:1951:VAL:HG23	1.95	0.49
1:A:1710:ARG:HG3	1:A:1870:PHE:HB3	1.94	0.49
1:A:2071:PRO:O	1:A:2075:LEU:HG	2.13	0.49
1:A:2822:ILE:HG13	1:A:2861:ILE:HD13	1.95	0.49
1:A:3103:TYR:CE2	1:A:3107:LYS:HD2	2.47	0.49
1:A:3654:ARG:NH1	1:A:3668:ASP:OD1	2.46	0.49
1:A:1747:ALA:HB2	1:A:1807:LYS:HG2	1.94	0.49
1:A:2181:GLU:OE2	1:A:2244:LEU:HB2	2.13	0.49
1:A:3506:ASP:HB3	1:A:3552:TYR:CE2	2.48	0.49
1:A:3721:ARG:NH1	1:A:3852:HIS:CE1	2.76	0.49
1:A:2287:ILE:HG12	1:A:2299:GLN:OE1	2.13	0.49
1:A:3086:PHE:CD1	1:A:3091:LEU:HD21	2.48	0.49
1:A:3808:CYS:SG	1:A:3836:TYR:HE2	2.35	0.49
1:A:1684:VAL:HG12	1:A:1746:GLN:NE2	2.27	0.49
1:A:1843:ARG:HG3	1:A:1843:ARG:HH11	1.78	0.48
1:A:2606:PHE:O	1:A:2610:ARG:HG2	2.13	0.48
1:A:3776:GLU:O	1:A:3780:VAL:HG23	2.13	0.48
1:A:4554:ASP:N	1:A:4557:SER:OG	2.46	0.48
1:A:1743:ASP:OD1	1:A:1804:ARG:HD3	2.13	0.48
1:A:2046:ARG:O	1:A:2049:ILE:HG22	2.13	0.48
1:A:2087:ASP:OD1	1:A:2357:SER:OG	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2623:SER:N	1:A:2626:THR:OG1	2.46	0.48
1:A:3218:LEU:HD21	1:A:3760:ILE:HG23	1.95	0.48
1:A:2115:LYS:NZ	1:A:2126:GLU:OE2	2.47	0.48
1:A:2029:PRO:HG2	1:A:2032:LEU:HD12	1.95	0.48
1:A:2969:GLY:HA2	1:A:3004:PHE:HE1	1.78	0.48
1:A:3689:PRO:HG2	1:A:3692:LEU:HD23	1.94	0.48
1:A:2223:VAL:HG22	1:A:2345:VAL:HG23	1.95	0.48
1:A:2350:TYR:CD2	1:A:2674:TYR:HA	2.49	0.48
1:A:2822:ILE:HD11	1:A:2858:PHE:CG	2.48	0.48
1:A:3614:PHE:HZ	1:A:3645:LEU:HD11	1.78	0.48
1:A:1789:LEU:CD2	1:A:1815:LEU:HB3	2.44	0.48
1:A:3214:GLN:HB2	1:A:3759:ARG:NH1	2.27	0.48
1:A:4309:VAL:HA	1:A:4312:LEU:HG	1.95	0.48
1:A:2042:THR:HG22	1:A:2043:LYS:HE3	1.96	0.48
1:A:2284:LEU:O	1:A:2288:ILE:HG12	2.14	0.48
1:A:4038:ASN:HA	1:A:4118:PRO:HG2	1.96	0.48
1:A:3008:MET:O	1:A:3012:LEU:HG	2.14	0.47
1:A:3154:LEU:HD21	1:A:3532:TRP:HZ2	1.78	0.47
1:A:2886:GLN:OE1	1:A:2886:GLN:N	2.42	0.47
1:A:4013:LEU:HD23	1:A:4017:PHE:CZ	2.48	0.47
1:A:3888:ALA:HB1	1:A:4012:ASN:HD22	1.80	0.47
1:A:4283:LYS:NZ	1:A:4293:ASP:OD2	2.41	0.47
1:A:4387:TRP:HZ2	1:A:4476:ILE:HG13	1.79	0.47
1:A:2049:ILE:HD11	2:A:4701:ADP:C4	2.49	0.47
1:A:4446:ASN:OD1	1:A:4446:ASN:N	2.47	0.47
1:A:2077:ASP:HA	1:A:2088:PHE:HD2	1.80	0.47
1:A:2559:THR:CG2	1:A:2757:ARG:HD2	2.44	0.47
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.14	0.47
1:A:3811:ILE:HD11	1:A:3864:PHE:CE1	2.49	0.47
1:A:4435:VAL:O	1:A:4439:GLU:HG2	2.14	0.47
1:A:3641:TYR:CD2	1:A:3692:LEU:HD21	2.49	0.47
1:A:1746:GLN:O	1:A:1750:VAL:HG12	2.14	0.47
1:A:2114:GLU:OE2	1:A:2118:ARG:NH2	2.47	0.47
1:A:2669:PRO:HG2	1:A:2679:VAL:HG21	1.97	0.47
1:A:2930:GLN:HB2	1:A:3059:ILE:HG13	1.96	0.47
1:A:3630:GLY:O	1:A:3674:SER:OG	2.26	0.47
1:A:4276:ARG:NH2	1:A:4279:ASP:HB2	2.30	0.47
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.97	0.47
1:A:1652:LYS:HA	1:A:1655:LYS:HE3	1.96	0.47
1:A:2603:MET:HE3	3:A:4703:ATP:H2'	1.96	0.47
1:A:3592:PRO:HG3	1:A:3702:THR:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3619:PHE:HZ	1:A:3645:LEU:HD21	1.80	0.47
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.97	0.47
1:A:1676:ILE:HD11	1:A:1709:MET:HB2	1.96	0.47
1:A:1964:GLU:O	1:A:1968:LEU:N	2.35	0.47
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.97	0.47
1:A:4289:ASP:N	1:A:4289:ASP:OD1	2.47	0.47
1:A:2896:ARG:HA	1:A:2896:ARG:HD2	1.75	0.46
1:A:3983:ILE:HD13	1:A:4011:THR:HG22	1.97	0.46
1:A:2836:ARG:HG2	1:A:2837:LEU:HD22	1.97	0.46
1:A:3690:PRO:HA	1:A:3693:CYS:SG	2.54	0.46
1:A:3767:ILE:HA	1:A:3770:LEU:HD12	1.96	0.46
1:A:4305:PHE:O	1:A:4309:VAL:HG12	2.15	0.46
1:A:1698:ILE:HA	1:A:1701:TRP:CD1	2.50	0.46
1:A:3716:VAL:HB	1:A:3836:TYR:OH	2.15	0.46
1:A:4276:ARG:HH21	1:A:4279:ASP:HB2	1.80	0.46
1:A:1741:TRP:CH2	1:A:1750:VAL:HG23	2.50	0.46
1:A:1985:HIS:NE2	1:A:2010:PRO:HB3	2.31	0.46
1:A:2320:ASP:OD2	1:A:2322:ASN:N	2.42	0.46
1:A:2743:SER:O	1:A:2747:ILE:HG22	2.15	0.46
1:A:2928:GLN:O	1:A:3063:HIS:NE2	2.44	0.46
1:A:1626:PHE:CE2	1:A:1629:PHE:HB3	2.51	0.46
1:A:1680:GLU:OE1	1:A:1682:GLU:N	2.46	0.46
1:A:2841:GLU:OE1	1:A:2844:ARG:NH1	2.49	0.46
1:A:3791:MET:HG2	1:A:3792:GLN:HG2	1.97	0.46
1:A:4026:ASP:O	1:A:4030:ILE:HG12	2.15	0.46
1:A:2934:LEU:HD12	1:A:3066:PHE:CB	2.46	0.46
1:A:3024:ASP:N	1:A:3024:ASP:OD1	2.49	0.46
1:A:1717:LEU:HB2	1:A:1749:LEU:HD21	1.97	0.46
1:A:2072:PHE:HA	1:A:2075:LEU:HD12	1.97	0.46
1:A:3013:ALA:HB2	1:A:3088:ARG:NE	2.27	0.46
1:A:1941:MET:SD	1:A:1945:PHE:HD2	2.39	0.46
1:A:3158:ASN:OD1	1:A:3168:THR:HB	2.15	0.46
1:A:2228:SER:OG	1:A:2364:PHE:HB3	2.16	0.46
1:A:3499:GLN:HA	1:A:3502:THR:HG22	1.97	0.46
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.98	0.46
1:A:1769:MET:SD	1:A:1777:PRO:HD2	2.55	0.45
1:A:2268:LEU:HD13	1:A:2275:TRP:HE3	1.81	0.45
1:A:1635:GLU:HG3	1:A:2273:ARG:HB3	1.97	0.45
1:A:1836:PHE:HA	1:A:1839:LEU:HB2	1.97	0.45
1:A:2412:MET:O	1:A:2416:GLN:HG3	2.16	0.45
1:A:3629:PHE:CE1	1:A:3631:ASN:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3884:ALA:HB1	1:A:4009:VAL:HG11	1.98	0.45
1:A:4388:LEU:HD23	1:A:4388:LEU:HA	1.81	0.45
1:A:4575:LEU:HG	1:A:4624:PHE:HB3	1.98	0.45
1:A:2148:LYS:HB2	1:A:2361:MET:HB3	1.98	0.45
1:A:2834:GLN:HA	1:A:2837:LEU:HD23	1.97	0.45
1:A:1738:TYR:HE1	1:A:1792:LEU:HD21	1.82	0.45
1:A:1832:ASN:HD21	1:A:1834:LYS:HB2	1.81	0.45
1:A:3632:PRO:HA	1:A:3676:VAL:O	2.16	0.45
1:A:4645:THR:O	1:A:4645:THR:OG1	2.29	0.45
1:A:2785:THR:HG23	1:A:2787:ASP:H	1.82	0.45
1:A:2797:ARG:HA	3:A:4703:ATP:O3'	2.16	0.45
1:A:2935:LEU:N	1:A:3066:PHE:O	2.41	0.45
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.99	0.45
1:A:3190:LYS:HD2	1:A:3552:TYR:HE1	1.82	0.45
1:A:3790:VAL:CG1	1:A:3794:VAL:HB	2.46	0.45
1:A:2916:LEU:O	1:A:2919:VAL:HG12	2.16	0.45
1:A:3705:ARG:HG2	1:A:3813:PHE:CE1	2.52	0.45
1:A:4610:TYR:HB2	1:A:4643:LEU:HD22	1.99	0.45
1:A:2585:LEU:HD13	1:A:2615:MET:HE1	1.98	0.45
1:A:2593:LEU:HD13	1:A:2605:LEU:HD11	1.98	0.45
1:A:2809:ALA:HB1	1:A:2824:ILE:HD11	1.98	0.45
1:A:2932:HIS:ND1	1:A:3012:LEU:HD22	2.31	0.45
1:A:1716:LEU:HB3	1:A:1745:TYR:HE1	1.82	0.45
1:A:1816:VAL:HG11	1:A:2052:VAL:HG22	1.97	0.45
1:A:2220:LEU:O	1:A:2342:MET:HA	2.16	0.45
1:A:3198:GLN:HE22	1:A:3496:PHE:HB3	1.81	0.45
1:A:3474:ARG:CD	1:A:3762:ASP:HB3	2.43	0.45
1:A:3914:ILE:HB	1:A:3937:ARG:HD3	1.99	0.45
1:A:4380:LEU:HD11	1:A:4455:LEU:HB3	1.99	0.45
1:A:3204:GLY:O	1:A:3208:ILE:HG12	2.17	0.45
1:A:1667:ASN:HB3	1:A:1674:LEU:HD11	1.99	0.44
1:A:2049:ILE:HD11	2:A:4701:ADP:C5	2.53	0.44
1:A:2557:VAL:HG13	1:A:2754:ALA:HB2	1.99	0.44
1:A:3020:LEU:H	1:A:3020:LEU:HD22	1.82	0.44
1:A:1947:GLY:O	1:A:1951:VAL:HG12	2.17	0.44
1:A:2324:LEU:HD23	1:A:2324:LEU:H	1.82	0.44
1:A:2369:LEU:HD12	1:A:2373:MET:HE2	1.99	0.44
1:A:2176:THR:O	1:A:2180:GLU:HG2	2.17	0.44
1:A:2256:PRO:HG3	1:A:2303:PHE:CD1	2.53	0.44
1:A:2518:ILE:HA	1:A:2521:ILE:HG12	1.98	0.44
1:A:2688:GLU:HB2	1:A:2730:HIS:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2934:LEU:HD12	1:A:3066:PHE:HB3	2.00	0.44
1:A:1896:LEU:HD13	1:A:1896:LEU:HA	1.84	0.44
1:A:2452:LEU:HD23	1:A:2452:LEU:HA	1.80	0.44
1:A:2935:LEU:HD22	1:A:3094:PHE:CE1	2.52	0.44
1:A:1743:ASP:OD2	1:A:1804:ARG:NH1	2.50	0.44
1:A:2221:MET:HE2	1:A:2361:MET:SD	2.58	0.44
1:A:2231:SER:HA	1:A:2234:TRP:NE1	2.32	0.44
1:A:2500:TRP:NE1	1:A:2535:ILE:HG23	2.32	0.44
1:A:4081:ASP:O	1:A:4085:ASN:ND2	2.51	0.44
1:A:3641:TYR:HE1	1:A:3645:LEU:HD12	1.82	0.44
1:A:4297:PRO:HG3	1:A:4308:TRP:CG	2.52	0.44
1:A:2085:HIS:HB2	1:A:2361:MET:HG2	2.00	0.44
1:A:1746:GLN:HG2	1:A:1872:TYR:CE1	2.53	0.44
1:A:1749:LEU:HD23	1:A:1749:LEU:HA	1.70	0.44
1:A:1933:ASP:N	1:A:1933:ASP:OD1	2.50	0.44
1:A:1972:SER:HB2	1:A:2031:ASN:HD21	1.83	0.44
1:A:2816:LEU:HD23	1:A:2817:PRO:O	2.18	0.44
1:A:4233:ILE:HD11	1:A:4237:LYS:HB2	1.99	0.44
1:A:1623:ARG:HB3	1:A:1630:TYR:HD2	1.83	0.43
1:A:3957:PHE:HZ	1:A:3996:PHE:CE2	2.36	0.43
1:A:1948:LEU:HA	1:A:1951:VAL:HG12	2.00	0.43
1:A:2363:TRP:HE1	1:A:2365:SER:HB2	1.83	0.43
1:A:3154:LEU:HB3	1:A:3171:ILE:HD13	2.00	0.43
1:A:3198:GLN:NE2	1:A:3496:PHE:HB3	2.32	0.43
1:A:3575:GLU:O	1:A:3579:MET:HG3	2.19	0.43
1:A:3588:LEU:HD11	1:A:3638:VAL:HG21	2.00	0.43
1:A:4288:VAL:HG22	1:A:4293:ASP:HA	2.00	0.43
1:A:3148:VAL:O	1:A:3152:GLN:HG2	2.17	0.43
1:A:4412:PHE:HZ	1:A:4514:LEU:HD13	1.83	0.43
1:A:1653:HIS:O	1:A:1656:LYS:N	2.52	0.43
1:A:2518:ILE:O	1:A:2522:THR:HG22	2.18	0.43
1:A:1660:GLY:O	1:A:1678:SER:HA	2.18	0.43
1:A:1702:LEU:HD23	1:A:1702:LEU:HA	1.91	0.43
1:A:3151:HIS:ND1	1:A:3516:TYR:OH	2.36	0.43
1:A:3954:ASP:OD1	1:A:3956:GLN:N	2.51	0.43
1:A:4375:ALA:O	1:A:4379:THR:HG23	2.19	0.43
1:A:1880:VAL:CG2	1:A:2049:ILE:HG13	2.47	0.43
1:A:1971:VAL:O	1:A:1975:VAL:HG13	2.18	0.43
1:A:2049:ILE:HD11	2:A:4701:ADP:C2	2.53	0.43
1:A:2721:LYS:HE2	1:A:2721:LYS:HB2	1.80	0.43
1:A:3474:ARG:O	1:A:3478:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3793:GLU:O	1:A:3796:THR:OG1	2.32	0.43
1:A:1710:ARG:HE	1:A:1710:ARG:HB2	1.64	0.43
1:A:2784:PHE:HB2	1:A:2794:TYR:HE2	1.84	0.43
1:A:3154:LEU:HD12	1:A:3171:ILE:HD11	1.99	0.43
1:A:4171:LYS:HA	1:A:4171:LYS:HD3	1.83	0.43
1:A:1910:THR:OG1	1:A:1912:LYS:NZ	2.37	0.43
1:A:2123:ASP:O	1:A:2127:ILE:HG12	2.19	0.43
1:A:3154:LEU:HG	1:A:3516:TYR:CD2	2.53	0.43
1:A:3635:VAL:O	1:A:3680:SER:OG	2.27	0.43
1:A:3744:GLN:O	1:A:3747:LYS:HG3	2.18	0.43
1:A:2212:GLN:O	1:A:2216:ILE:HG23	2.19	0.43
1:A:2588:HIS:HE1	1:A:2658:TRP:CE2	2.36	0.43
1:A:4188:ALA:O	1:A:4192:GLU:HG2	2.18	0.43
1:A:4192:GLU:OE1	1:A:4192:GLU:HA	2.19	0.43
1:A:4436:GLN:NE2	1:A:4442:LYS:HB2	2.34	0.43
1:A:2791:HIS:HB2	1:A:3091:LEU:CD2	2.49	0.43
1:A:4525:ARG:HD3	1:A:4592:TRP:CZ3	2.54	0.43
1:A:3801:TYR:HD1	1:A:3856:LEU:HD13	1.84	0.42
1:A:2189:MET:HB3	1:A:2191:LEU:HD13	2.01	0.42
1:A:2615:MET:HG3	1:A:2658:TRP:O	2.19	0.42
1:A:2871:ILE:O	1:A:2872:LEU:HD23	2.19	0.42
1:A:3032:GLN:O	1:A:3035:GLU:HG2	2.19	0.42
1:A:3726:GLU:HA	1:A:3729:SER:HB3	2.01	0.42
1:A:3910:ARG:O	1:A:3913:GLU:HG2	2.18	0.42
1:A:4223:LEU:HD12	1:A:4223:LEU:HA	1.76	0.42
1:A:1631:PHE:HE2	1:A:1656:LYS:HB3	1.83	0.42
1:A:2265:TYR:OH	1:A:2311:TRP:O	2.27	0.42
1:A:2868:SER:O	1:A:2871:ILE:HG13	2.20	0.42
1:A:2897:LEU:HD23	1:A:2897:LEU:HA	1.92	0.42
1:A:4044:CYS:O	1:A:4146:VAL:HA	2.19	0.42
1:A:3614:PHE:HE2	1:A:3641:TYR:HD1	1.65	0.42
1:A:1736:ASN:O	1:A:1740:THR:OG1	2.31	0.42
1:A:3485:GLU:O	1:A:3489:TRP:HD1	2.02	0.42
1:A:3500:MET:O	1:A:3503:ILE:HG22	2.18	0.42
1:A:3787:THR:HA	1:A:3790:VAL:CG2	2.49	0.42
1:A:2747:ILE:HG23	1:A:2748:TYR:CD2	2.55	0.42
1:A:2936:ILE:O	1:A:3094:PHE:N	2.49	0.42
1:A:3588:LEU:HD23	1:A:3698:PHE:CE1	2.55	0.42
1:A:4037:PRO:HB2	1:A:4118:PRO:HB2	2.02	0.42
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.55	0.42
1:A:2308:ASP:OD2	1:A:2311:TRP:NE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2926:PHE:HA	1:A:3063:HIS:CD2	2.54	0.42
1:A:1630:TYR:HD1	1:A:1947:GLY:HA2	1.84	0.42
1:A:1714:ALA:HB1	1:A:1856:GLN:OE1	2.20	0.42
1:A:1792:LEU:HD13	1:A:1808:LEU:HD13	2.02	0.42
1:A:2908:PRO:HB2	1:A:3109:PHE:CZ	2.54	0.42
1:A:3211:THR:O	1:A:3215:VAL:HG23	2.19	0.42
1:A:4295:GLN:HA	1:A:4295:GLN:NE2	2.35	0.42
1:A:4429:GLN:NE2	1:A:4433:ASP:OD2	2.52	0.42
1:A:1698:ILE:HD12	1:A:1701:TRP:NE1	2.35	0.42
1:A:2613:PRO:O	1:A:2657:LYS:NZ	2.52	0.42
1:A:2648:VAL:HG12	1:A:2701:VAL:HG22	2.01	0.42
1:A:2893:VAL:CG1	1:A:2911:LEU:HD21	2.48	0.42
1:A:4100:HIS:HB2	1:A:4131:ASN:HD21	1.84	0.42
1:A:3935:VAL:HG22	1:A:3996:PHE:HE1	1.85	0.42
1:A:4119:HIS:HE2	1:A:4121:CYS:HG	1.64	0.42
1:A:1964:GLU:HB2	1:A:1967:MET:HB2	2.01	0.41
1:A:2569:VAL:HG11	1:A:2747:ILE:HA	2.01	0.41
1:A:2995:ASP:OD2	1:A:2996:GLU:N	2.53	0.41
1:A:3787:THR:HA	1:A:3790:VAL:HG23	2.02	0.41
1:A:4543:VAL:HG13	1:A:4588:THR:HG23	2.01	0.41
1:A:2559:THR:HG22	1:A:2754:ALA:O	2.19	0.41
1:A:2876:TRP:HB3	1:A:2892:TYR:CE2	2.55	0.41
1:A:2888:GLU:OE1	1:A:2888:GLU:N	2.44	0.41
1:A:2911:LEU:HD12	1:A:2911:LEU:HA	1.91	0.41
1:A:3113:MET:HE2	1:A:3113:MET:HB2	1.87	0.41
1:A:3740:LEU:O	1:A:3744:GLN:HG2	2.20	0.41
1:A:4169:ILE:HD12	1:A:4302:ARG:HH11	1.84	0.41
1:A:4189:ILE:HD12	1:A:4321:LEU:HA	2.02	0.41
1:A:4313:PRO:HD2	1:A:4320:TRP:HH2	1.85	0.41
1:A:2505:ASP:HB3	1:A:2733:VAL:O	2.20	0.41
1:A:2920:LEU:HD23	1:A:2920:LEU:HA	1.80	0.41
1:A:4166:VAL:HG13	1:A:4302:ARG:NH2	2.35	0.41
1:A:4228:LYS:HE2	1:A:4228:LYS:HB2	1.89	0.41
1:A:4510:CYS:HG	1:A:4561:THR:HG1	1.65	0.41
1:A:1631:PHE:HA	1:A:1947:GLY:HA3	2.02	0.41
1:A:1739:ILE:HD11	1:A:1804:ARG:HD2	2.02	0.41
1:A:1938:PHE:O	1:A:1942:GLY:N	2.36	0.41
1:A:1954:TRP:CE3	1:A:2015:PHE:HE1	2.38	0.41
1:A:2614:ASP:OD1	1:A:2614:ASP:N	2.45	0.41
1:A:2809:ALA:CB	1:A:2824:ILE:HD11	2.50	0.41
1:A:2784:PHE:CE1	1:A:2837:LEU:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2976:LEU:HD12	1:A:2976:LEU:HA	1.87	0.41
1:A:3149:PHE:O	1:A:3153:THR:HG23	2.20	0.41
1:A:3721:ARG:HD3	1:A:3797:VAL:HG13	2.02	0.41
1:A:4118:PRO:HB3	1:A:4122:PHE:CD2	2.55	0.41
1:A:4486:ILE:HD13	1:A:4486:ILE:HA	1.86	0.41
1:A:2100:ALA:O	1:A:2103:VAL:HG12	2.21	0.41
1:A:3100:GLU:OE1	1:A:3130:TYR:OH	2.20	0.41
1:A:3747:LYS:O	1:A:3751:GLN:HG2	2.19	0.41
1:A:1650:LEU:HA	1:A:1653:HIS:HD2	1.86	0.41
1:A:1665:ILE:HD11	1:A:1677:SER:HB2	2.02	0.41
1:A:2938:VAL:HG12	1:A:3095:GLY:O	2.21	0.41
1:A:3624:GLU:HA	1:A:3627:LEU:HD12	2.01	0.41
1:A:4633:ARG:HA	1:A:4636:TYR:HD2	1.86	0.41
1:A:1784:ASN:O	1:A:1787:VAL:HG12	2.20	0.41
1:A:2534:ILE:HD12	1:A:2534:ILE:N	2.33	0.41
1:A:2964:HIS:NE2	1:A:2966:LYS:HD2	2.35	0.41
1:A:3191:ARG:O	1:A:3195:GLU:HB2	2.21	0.41
1:A:3567:LEU:HB2	1:A:3599:PHE:CE2	2.55	0.41
1:A:4119:HIS:CD2	1:A:4121:CYS:H	2.38	0.41
1:A:4171:LYS:HG3	1:A:4172:SER:H	1.86	0.41
1:A:1684:VAL:O	1:A:1685:MET:HE2	2.21	0.41
1:A:1717:LEU:HD11	1:A:1756:ILE:HD12	2.02	0.41
1:A:2324:LEU:HD23	1:A:2324:LEU:N	2.35	0.41
1:A:2385:ILE:HA	1:A:2386:PRO:HD3	1.96	0.41
1:A:2490:ILE:HD13	1:A:2490:ILE:HA	1.96	0.41
1:A:3099:THR:OG1	1:A:3152:GLN:NE2	2.53	0.41
1:A:3609:ILE:HD11	1:A:3634:LEU:HB2	2.03	0.41
1:A:4149:PRO:HA	1:A:4150:PRO:HD3	1.96	0.41
1:A:4154:LYS:HD2	1:A:4312:LEU:HB2	2.03	0.41
1:A:2641:TYR:CE1	1:A:2650:LEU:HD13	2.56	0.41
1:A:3549:ARG:NE	1:A:3575:GLU:OE2	2.54	0.41
1:A:1653:HIS:HA	1:A:1656:LYS:HD2	2.03	0.40
1:A:1907:PRO:O	1:A:1912:LYS:NZ	2.54	0.40
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.56	0.40
1:A:2626:THR:HG23	1:A:2630:LEU:HD13	2.02	0.40
1:A:4380:LEU:HA	1:A:4383:THR:HG22	2.03	0.40
1:A:4388:LEU:HG	1:A:4431:LEU:HB3	2.03	0.40
1:A:4577:LEU:HD23	1:A:4577:LEU:HA	1.84	0.40
1:A:1702:LEU:O	1:A:1706:GLU:HG3	2.21	0.40
1:A:2192:THR:HG22	3:A:4702:ATP:N1	2.36	0.40
1:A:4404:ASN:HB3	1:A:4410:PHE:CG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	2.02	0.40
1:A:2161:LEU:HD23	1:A:2161:LEU:HA	1.91	0.40
1:A:2969:GLY:HA2	1:A:3004:PHE:CE1	2.55	0.40
1:A:3742:LEU:HD22	1:A:3777:ALA:HA	2.04	0.40
1:A:3888:ALA:HB1	1:A:4012:ASN:ND2	2.36	0.40
1:A:2073:PHE:HZ	1:A:2096:VAL:HG21	1.87	0.40
1:A:2352:THR:O	1:A:2356:VAL:HG23	2.22	0.40
1:A:2419:ALA:HA	1:A:2422:ILE:HD12	2.02	0.40
1:A:2802:TRP:HE1	1:A:2806:ILE:HD11	1.86	0.40
1:A:2816:LEU:HD21	1:A:2821:LEU:N	2.36	0.40
1:A:3009:ASN:OD1	1:A:3088:ARG:HD2	2.22	0.40
1:A:3042:LEU:HD23	1:A:3042:LEU:HA	1.91	0.40
1:A:3630:GLY:HA2	1:A:3675:PHE:HB2	2.03	0.40
1:A:3801:TYR:CD1	1:A:3856:LEU:HD13	2.57	0.40
1:A:2206:LYS:HD3	1:A:2206:LYS:HA	1.86	0.40
1:A:3135:GLN:HB3	1:A:3136:PRO:HD3	2.03	0.40
1:A:3721:ARG:CZ	1:A:3724:VAL:HG11	2.51	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	2687/4646 (58%)	2624 (98%)	63 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2400/4125 (58%)	2329 (97%)	71 (3%)	36	63

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1629	PHE
1	A	1657	MET
1	A	1738	TYR
1	A	1886	ASP
1	A	1900	LEU
1	A	1925	ARG
1	A	1926	PHE
1	A	1931	ASN
1	A	1937	ASP
1	A	1938	PHE
1	A	1945	PHE
1	A	2012	MET
1	A	2036	PHE
1	A	2043	LYS
1	A	2055	TYR
1	A	2060	ARG
1	A	2142	CYS
1	A	2169	GLN
1	A	2170	TYR
1	A	2187	GLN
1	A	2228	SER
1	A	2289	ASP
1	A	2322	ASN
1	A	2332	ARG
1	A	2366	GLU
1	A	2429	SER
1	A	2444	GLU
1	A	2471	GLN
1	A	2615	MET
1	A	2779	MET
1	A	2843	ARG
1	A	2881	TYR
1	A	2923	ASP
1	A	2975	ASP
1	A	3014	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3087	ASN
1	A	3103	TYR
1	A	3146	SER
1	A	3158	ASN
1	A	3169	MET
1	A	3474	ARG
1	A	3491	LYS
1	A	3496	PHE
1	A	3521	ASP
1	A	3529	PHE
1	A	3552	TYR
1	A	3629	PHE
1	A	3721	ARG
1	A	3741	ARG
1	A	3747	LYS
1	A	3770	LEU
1	A	3776	GLU
1	A	3791	MET
1	A	3847	LYS
1	A	3923	ARG
1	A	3945	LYS
1	A	3946	ASP
1	A	3957	PHE
1	A	3972	TYR
1	A	4095	MET
1	A	4128	MET
1	A	4140	ARG
1	A	4171	LYS
1	A	4268	PHE
1	A	4276	ARG
1	A	4314	ASP
1	A	4399	LYS
1	A	4419	MET
1	A	4498	SER
1	A	4540	CYS
1	A	4573	ASN

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	1653	HIS
1	A	2416	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2588	HIS
1	A	3198	GLN
1	A	3631	ASN
1	A	3852	HIS
1	A	4526	GLN

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	A	4701	-	24,29,29	0.73	0	29,45,45	0.74	1 (3%)
3	ATP	A	4703	4	28,33,33	0.71	0	34,52,52	0.83	1 (2%)
2	ADP	A	4704	-	24,29,29	0.85	0	29,45,45	1.18	2 (6%)
3	ATP	A	4702	-	28,33,33	0.73	0	34,52,52	0.61	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	-	-	2/12/32/32	0/3/3/3
3	ATP	A	4703	4	-	3/18/38/38	0/3/3/3
2	ADP	A	4704	-	-	1/12/32/32	0/3/3/3
3	ATP	A	4702	-	-	1/18/38/38	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4704	ADP	N3-C2-N1	-3.56	123.84	128.67
2	A	4704	ADP	C4-C5-N7	-2.48	106.72	109.34
3	A	4702	ATP	C5-C6-N6	2.32	123.84	120.31
2	A	4701	ADP	C5-C6-N6	2.26	123.76	120.31
3	A	4703	ATP	C5-C6-N6	2.25	123.75	120.31

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4704	ADP	C5'-O5'-PA-O1A
3	A	4703	ATP	PB-O3B-PG-O3G
2	A	4701	ADP	O4'-C4'-C5'-O5'
2	A	4701	ADP	C3'-C4'-C5'-O5'
3	A	4702	ATP	O4'-C4'-C5'-O5'
3	A	4703	ATP	C5'-O5'-PA-O1A
3	A	4703	ATP	PB-O3B-PG-O1G

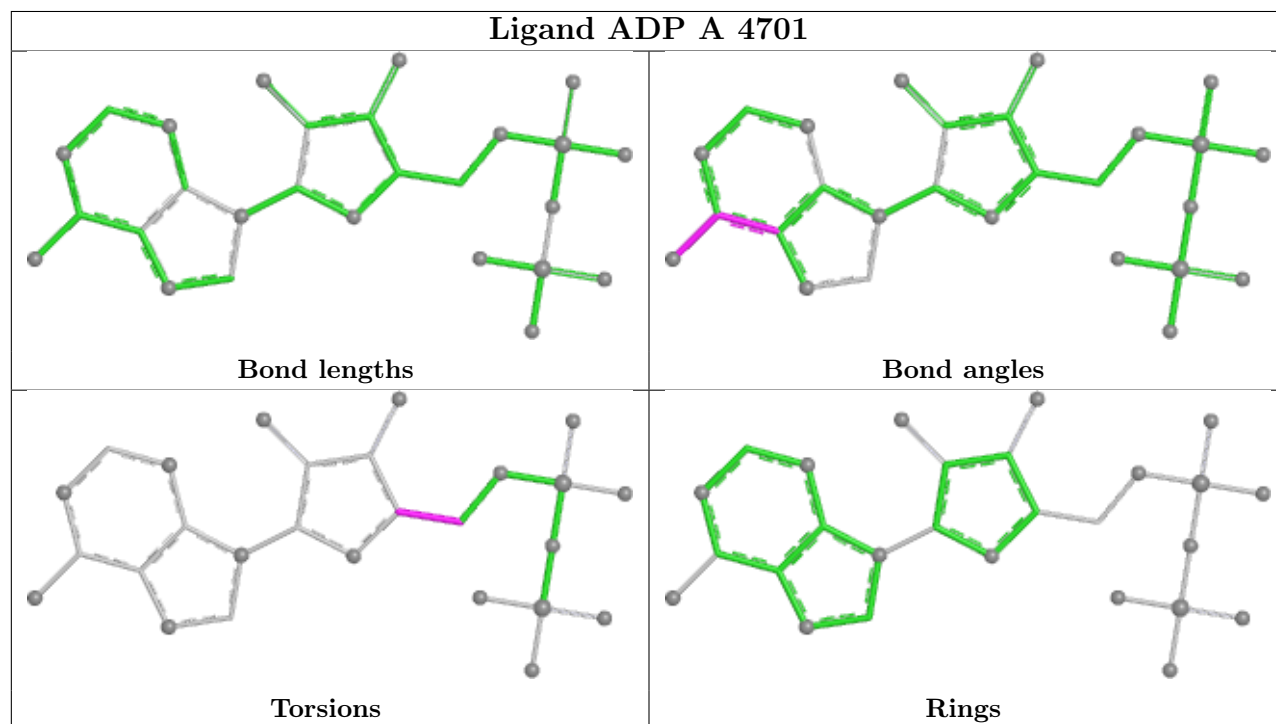
There are no ring outliers.

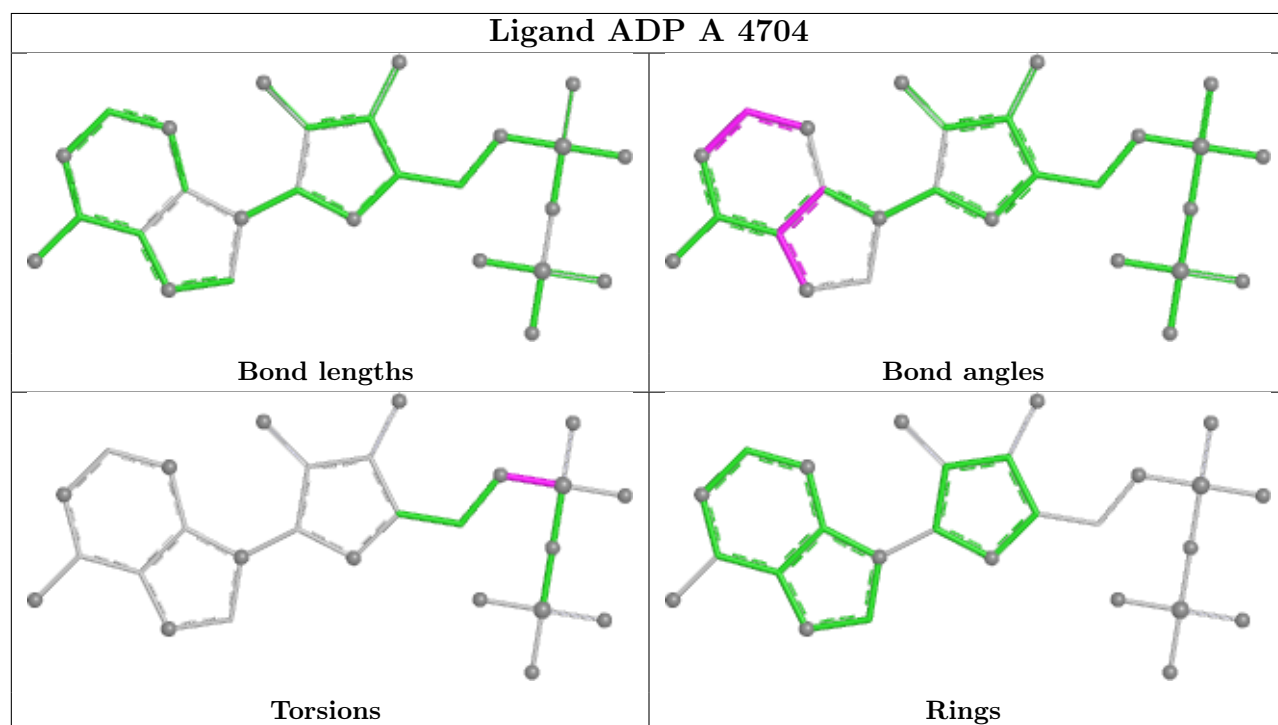
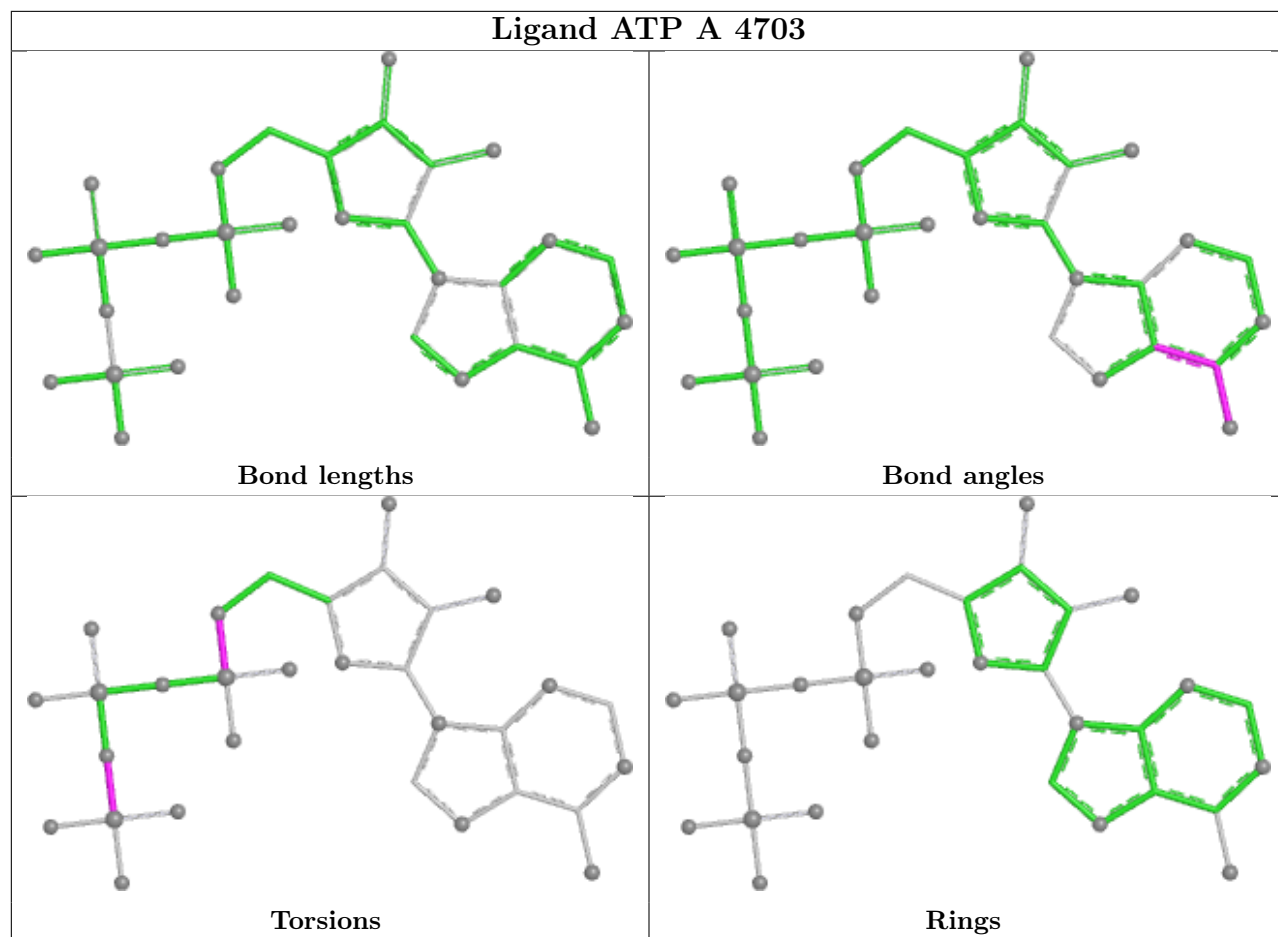
3 monomers are involved in 9 short contacts:

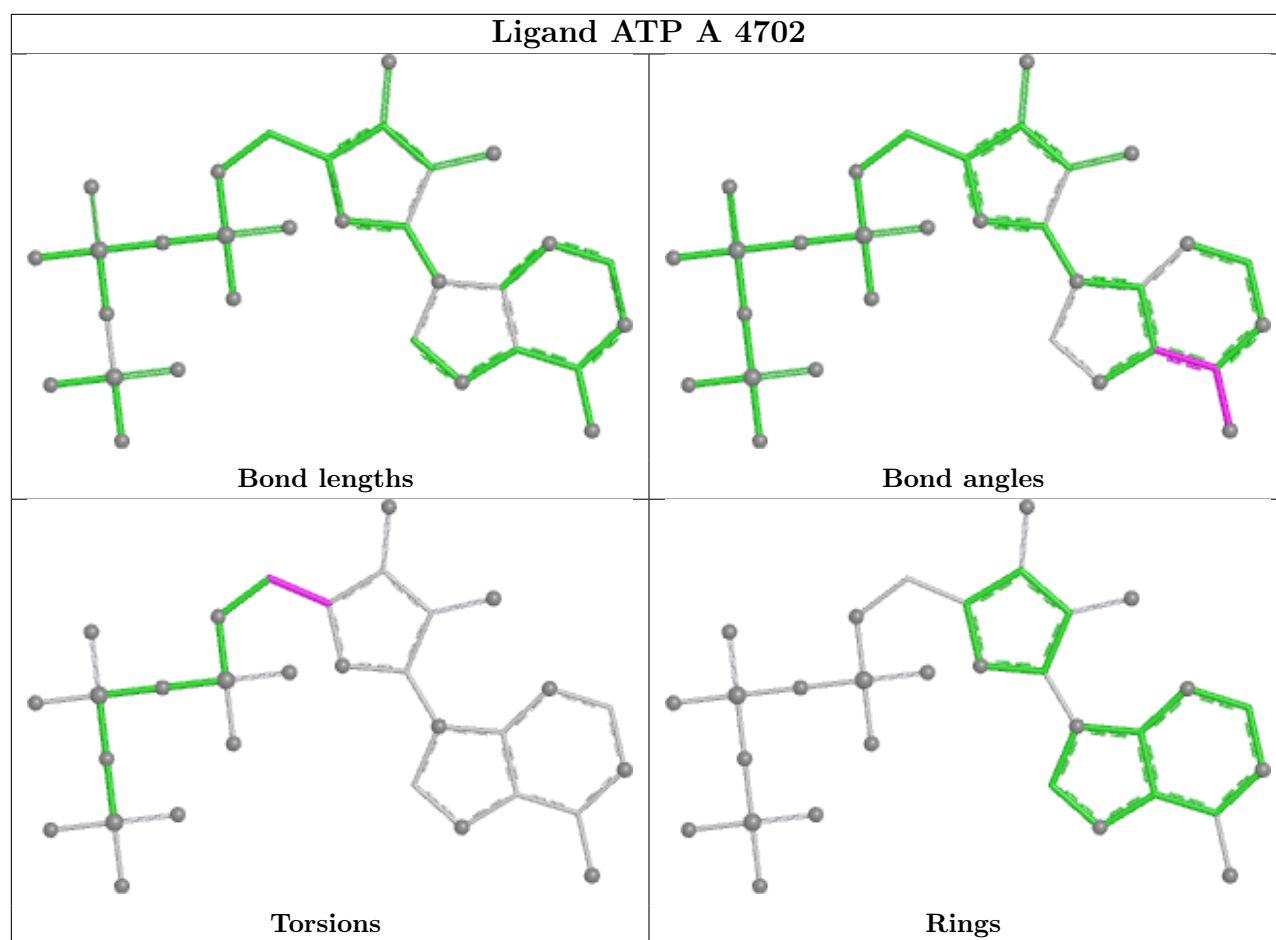
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	4	0
3	A	4703	ATP	3	0
3	A	4702	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

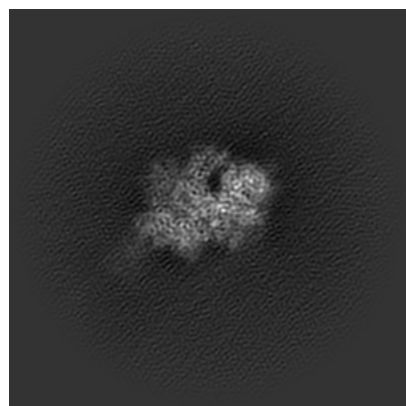
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44687. These allow visual inspection of the internal detail of the map and identification of artifacts.

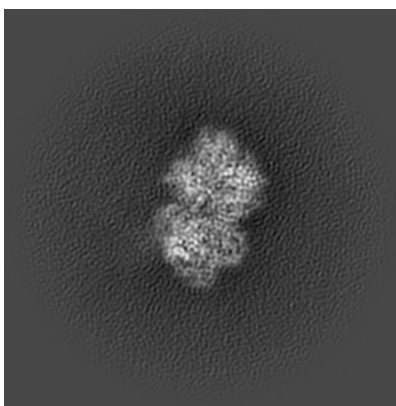
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

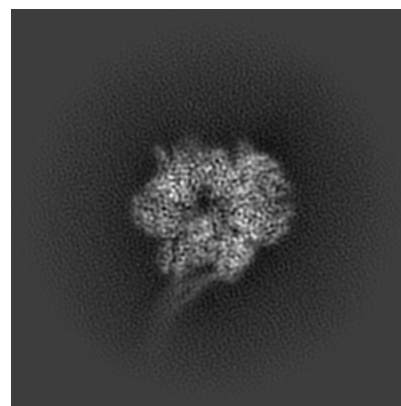
6.1.1 Primary map



X

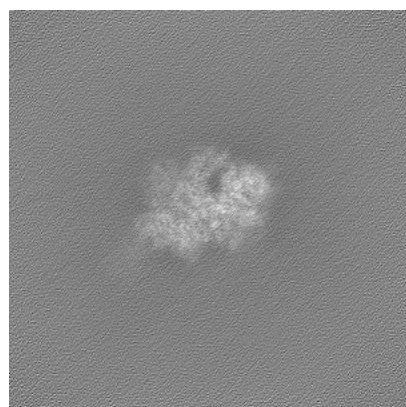


Y

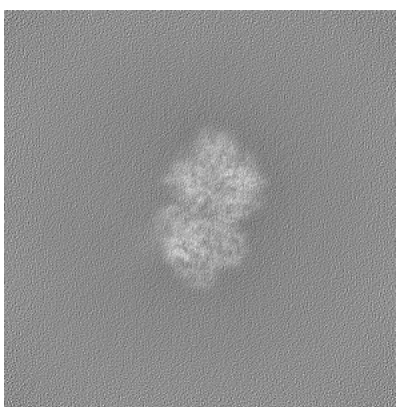


Z

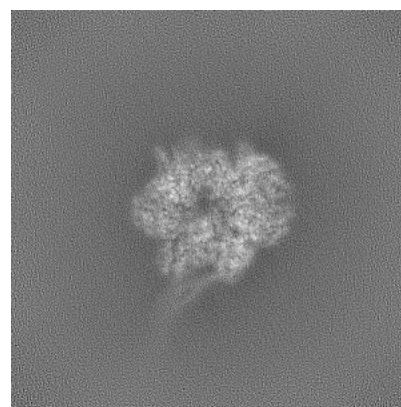
6.1.2 Raw map



X



Y

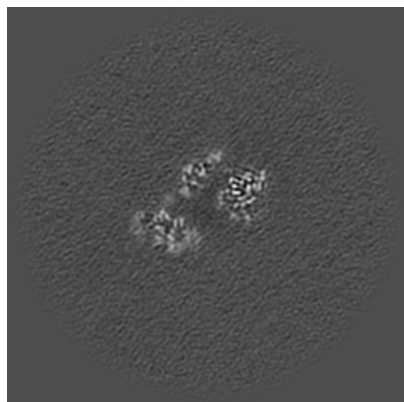


Z

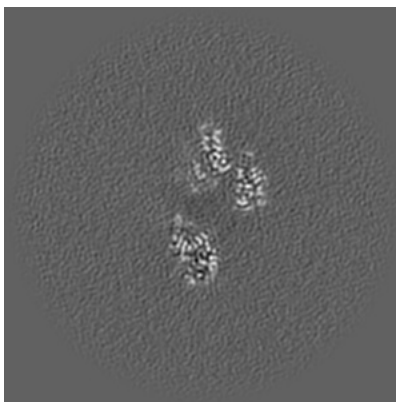
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

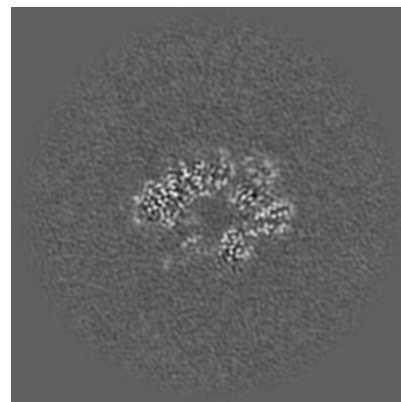
6.2.1 Primary map



X Index: 200

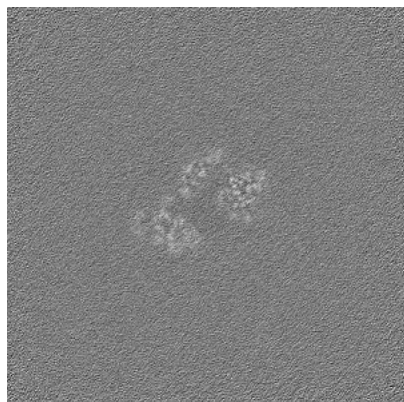


Y Index: 200

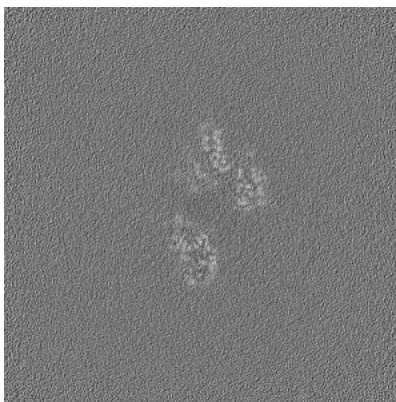


Z Index: 200

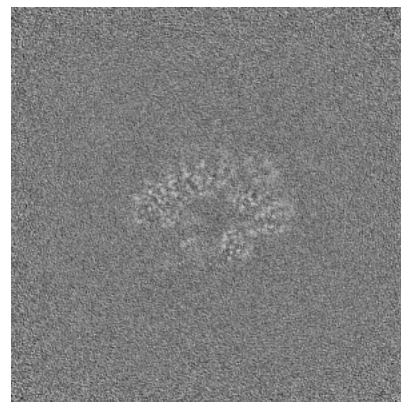
6.2.2 Raw map



X Index: 200



Y Index: 200

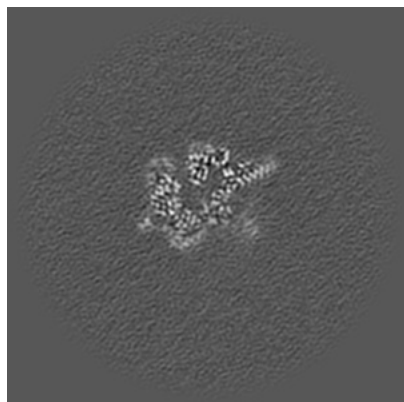


Z Index: 200

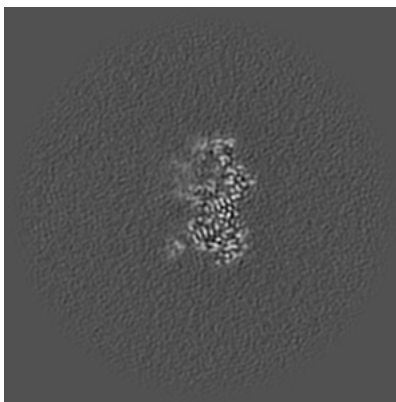
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

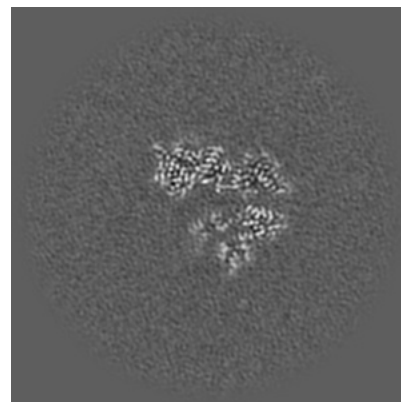
6.3.1 Primary map



X Index: 229

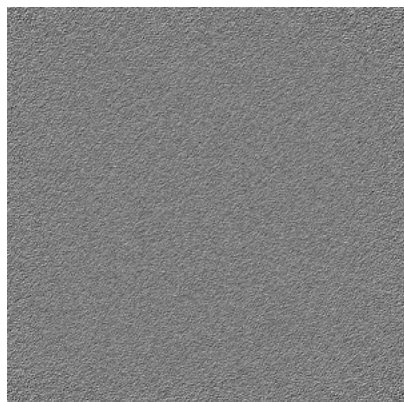


Y Index: 231

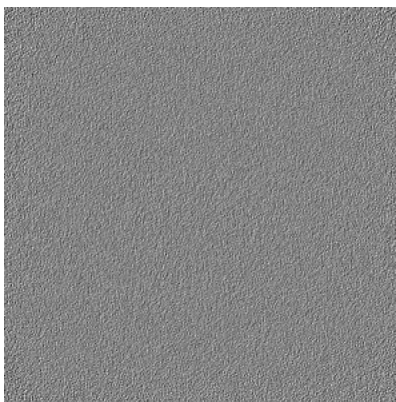


Z Index: 222

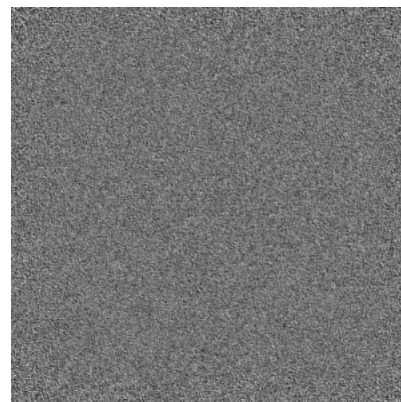
6.3.2 Raw map



X Index: 0



Y Index: 0

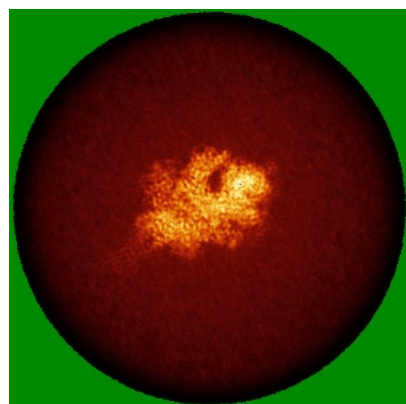


Z Index: 0

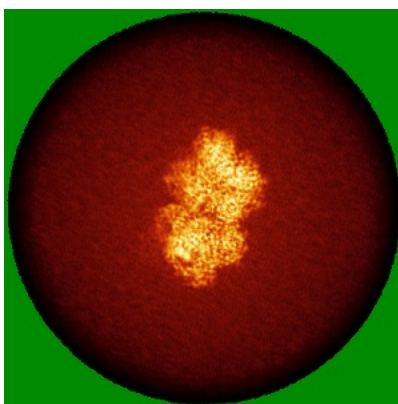
The images above show the largest variance slices of the map in three orthogonal directions.

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

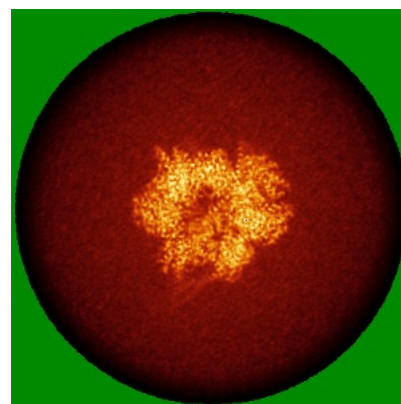
6.4.1 Primary map



X

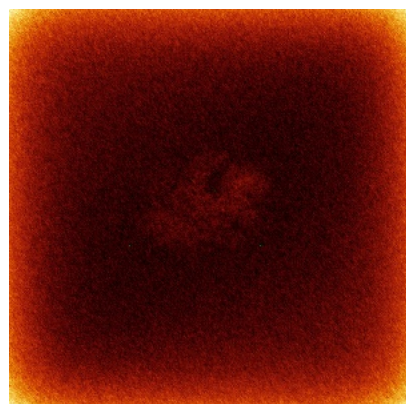


Y

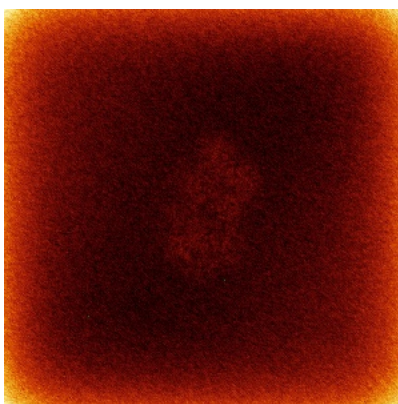


Z

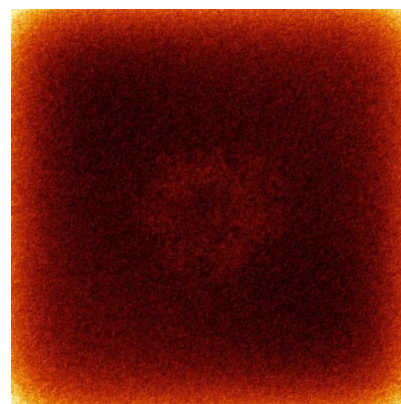
6.4.2 Raw map



X



Y

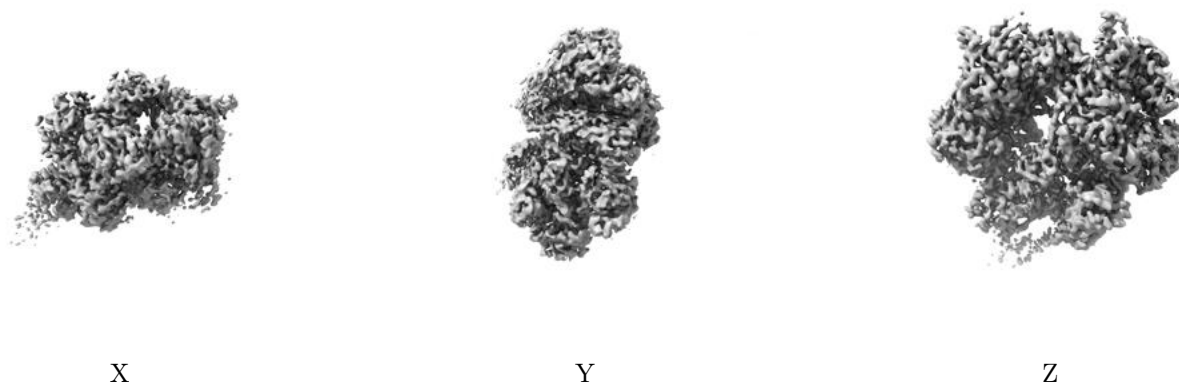


Z

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.

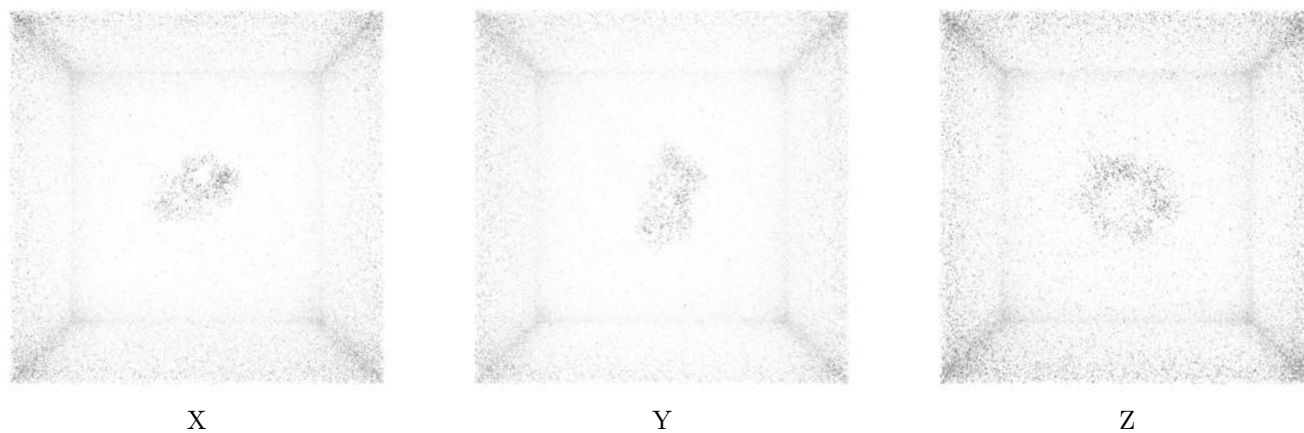
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

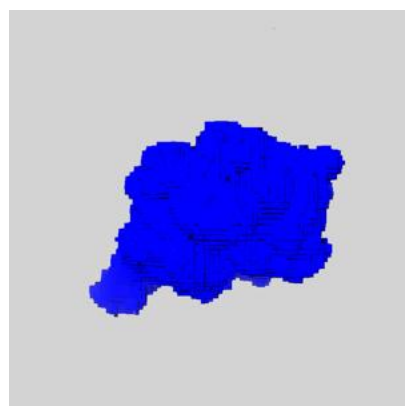
6.6 Mask visualisation [i](#)

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

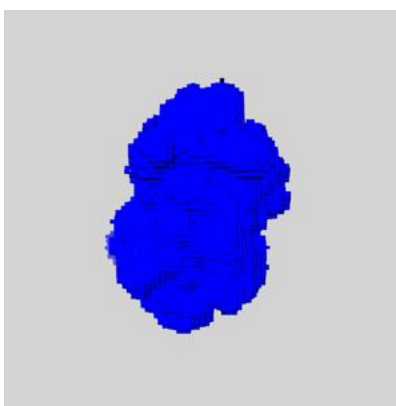
A mask typically either:

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

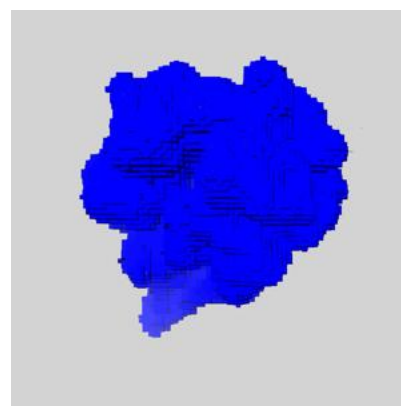
6.6.1 emd_44687_msk_1.map [i](#)



X



Y

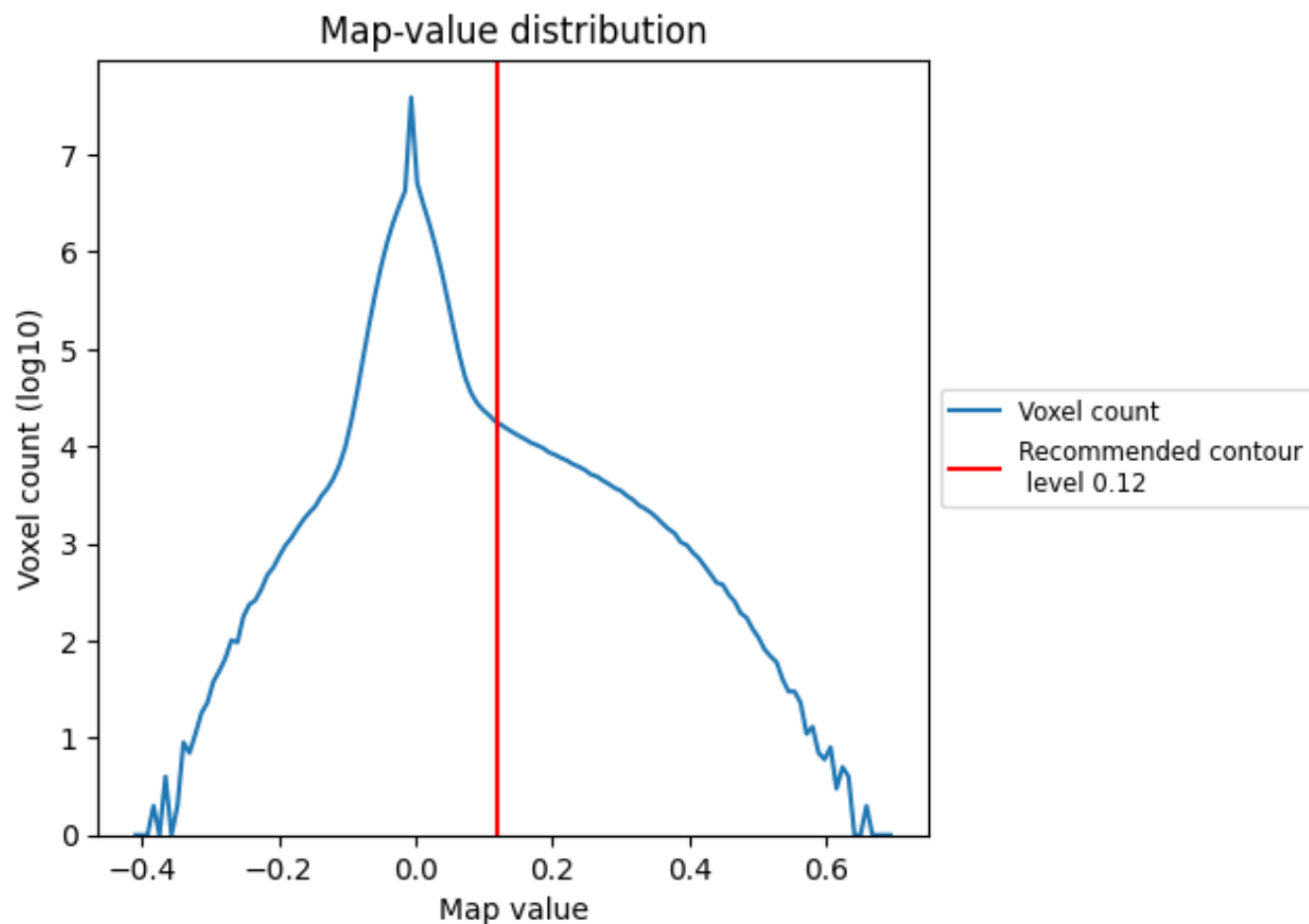


Z

7 Map analysis [i](#)

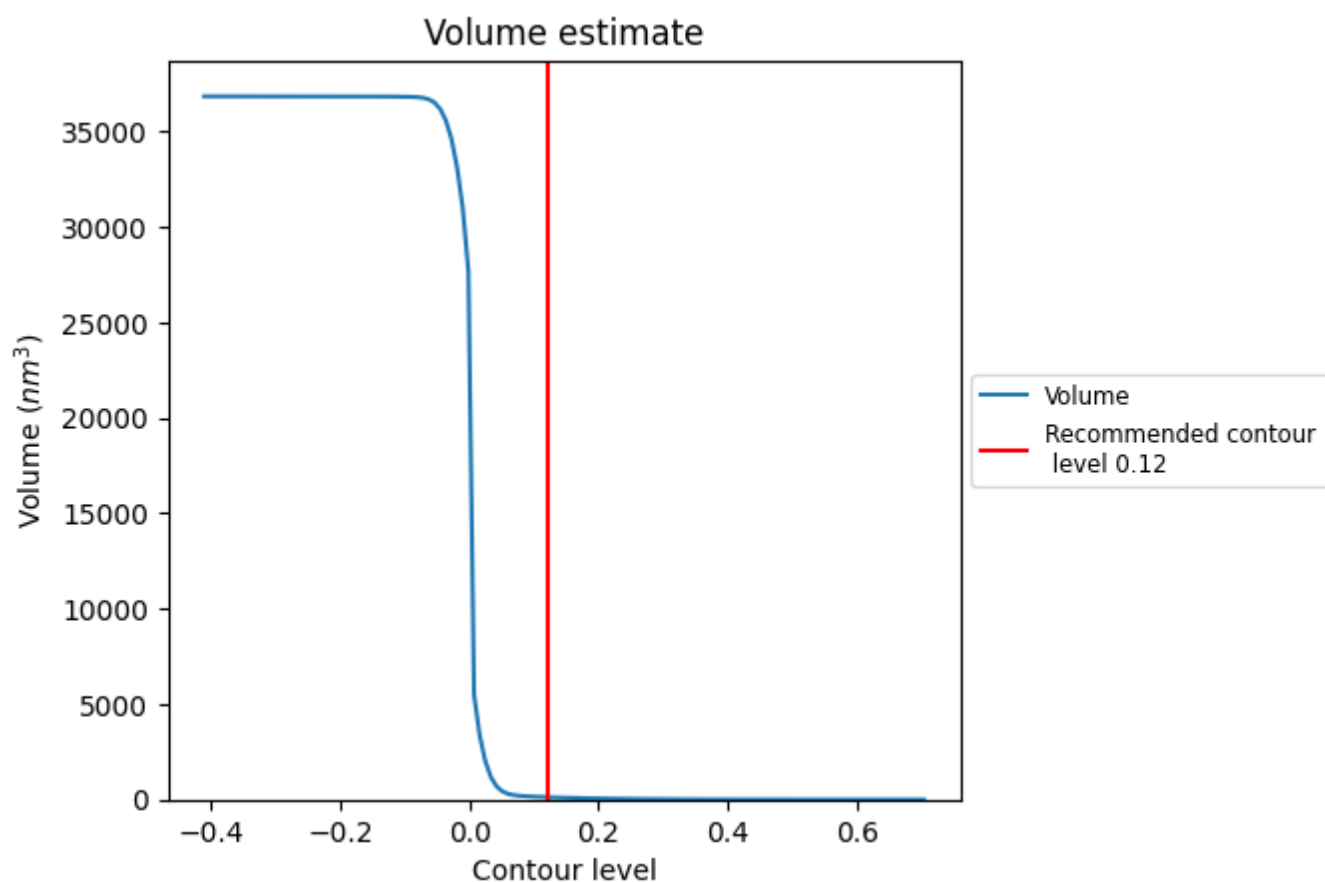
This section contains the results of statistical analysis of the map.

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.

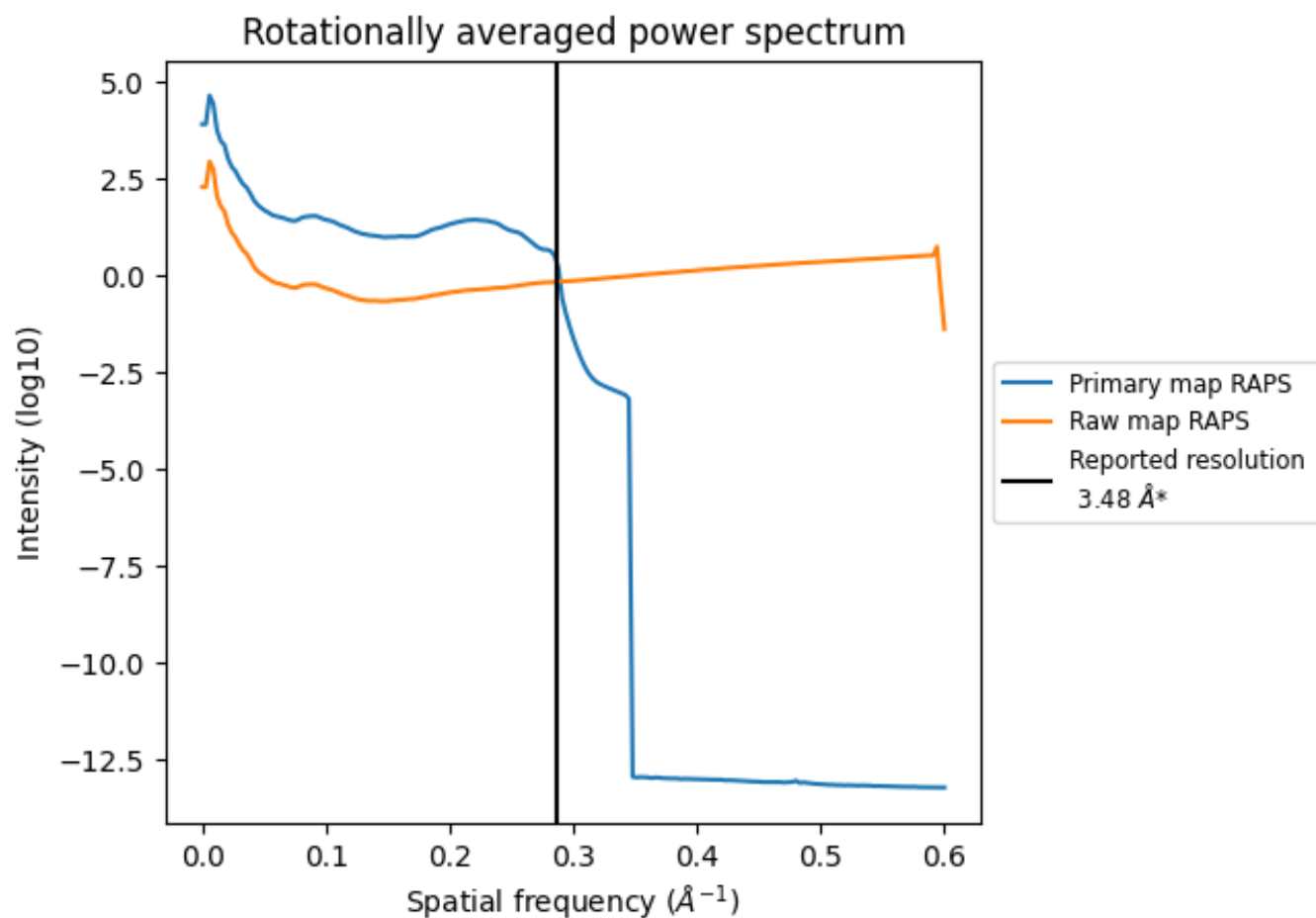
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 122 nm³; this corresponds to an approximate mass of 110 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 ⓘ

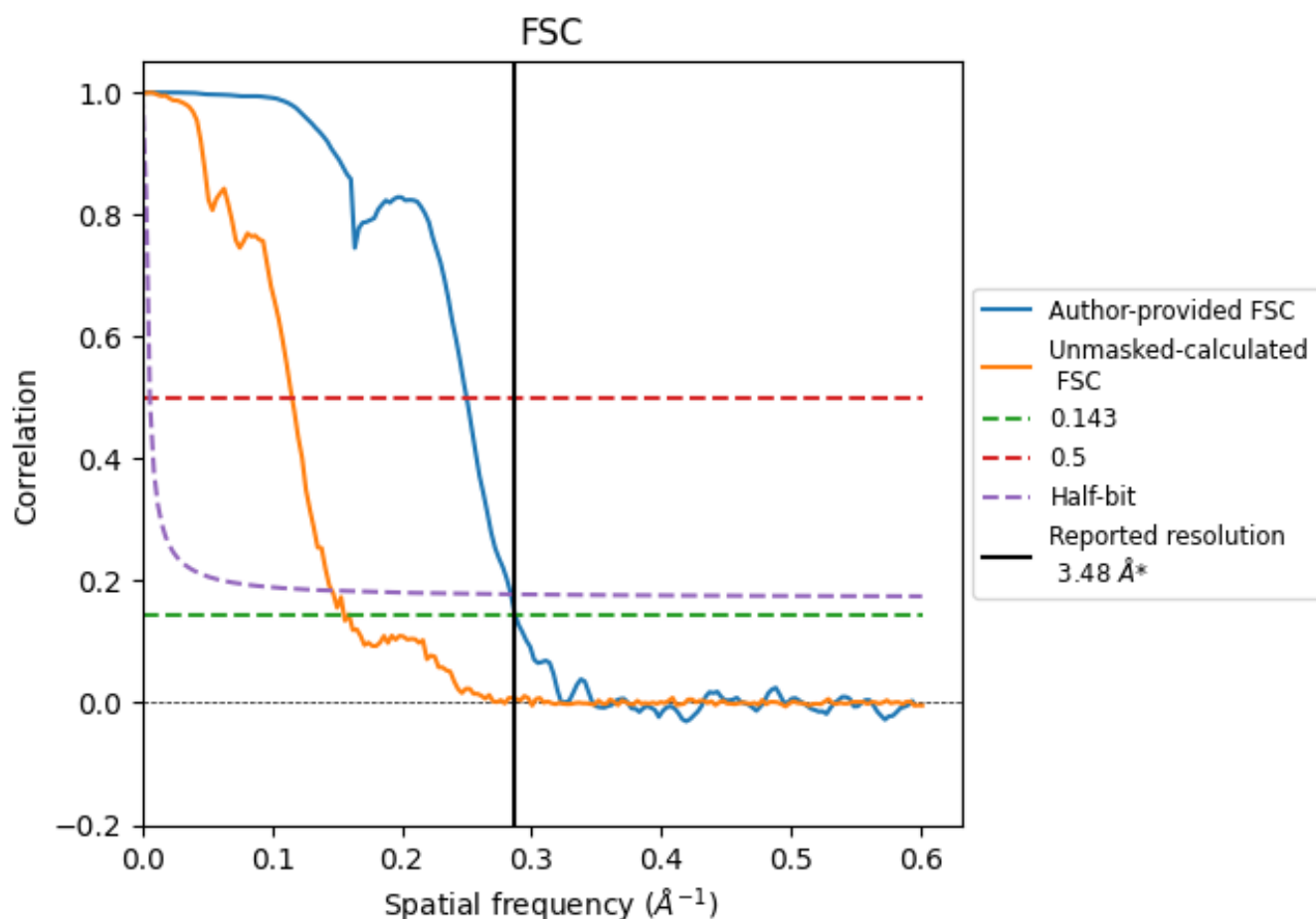


*Reported resolution corresponds to spatial frequency of 0.287 \AA^{-1}

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 0.287 \AA^{-1}

8.2 Resolution estimates [i](#)

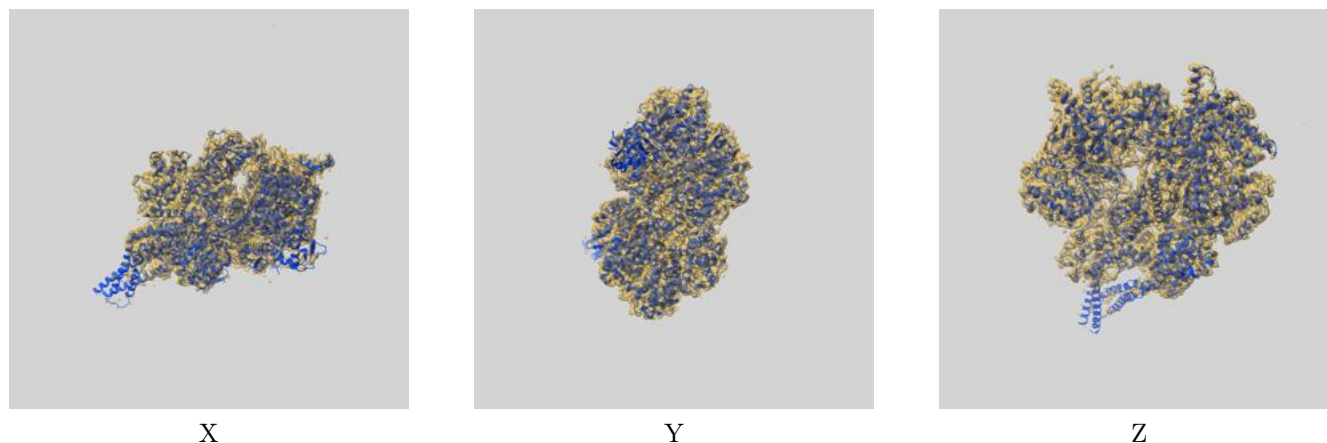
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.48	-	-
Author-provided FSC curve	3.48	4.00	3.52
Unmasked-calculated*	6.43	8.67	6.84

*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 6.43 differs from the reported value 3.48 by more than 10 %

9 Map-model fit [i](#)

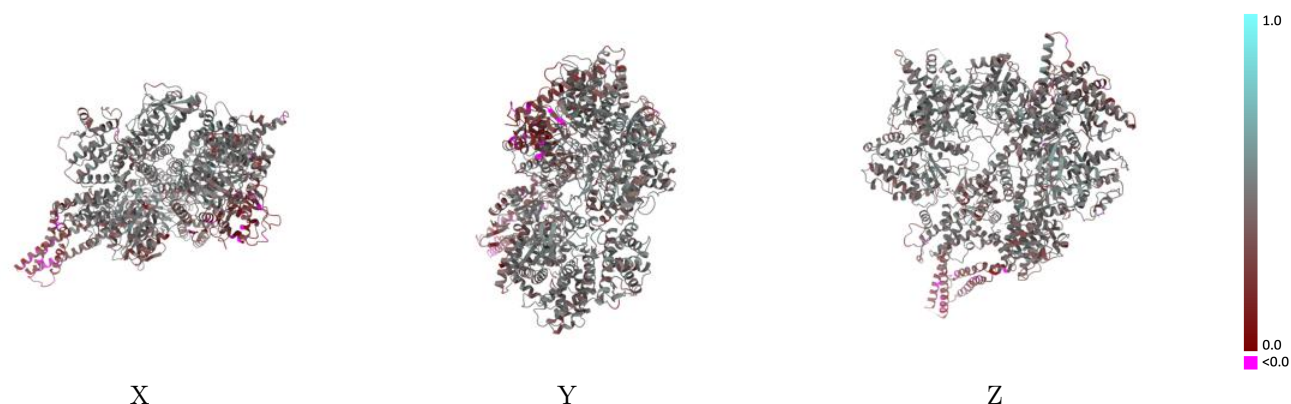
This section contains information regarding the fit between EMDB map EMD-44687 and PDB model 9BM4. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



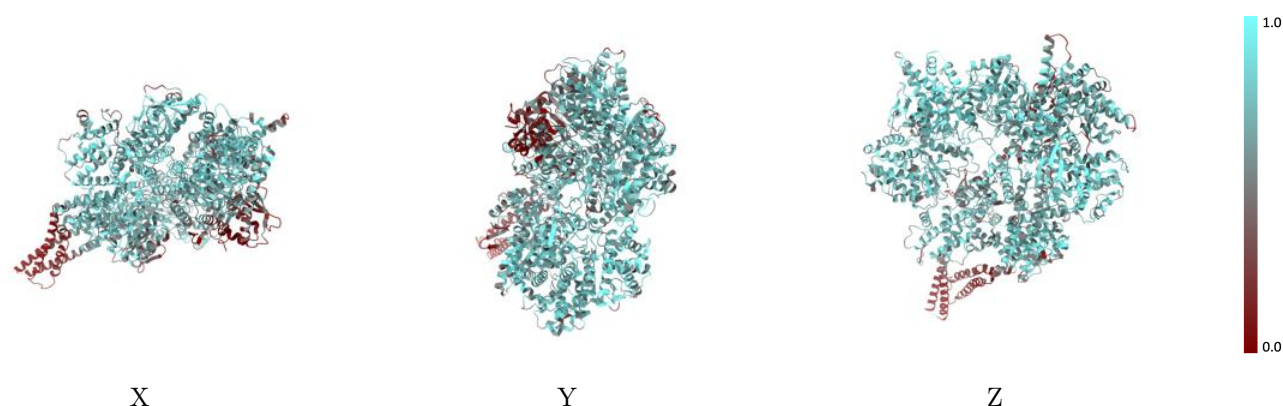
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



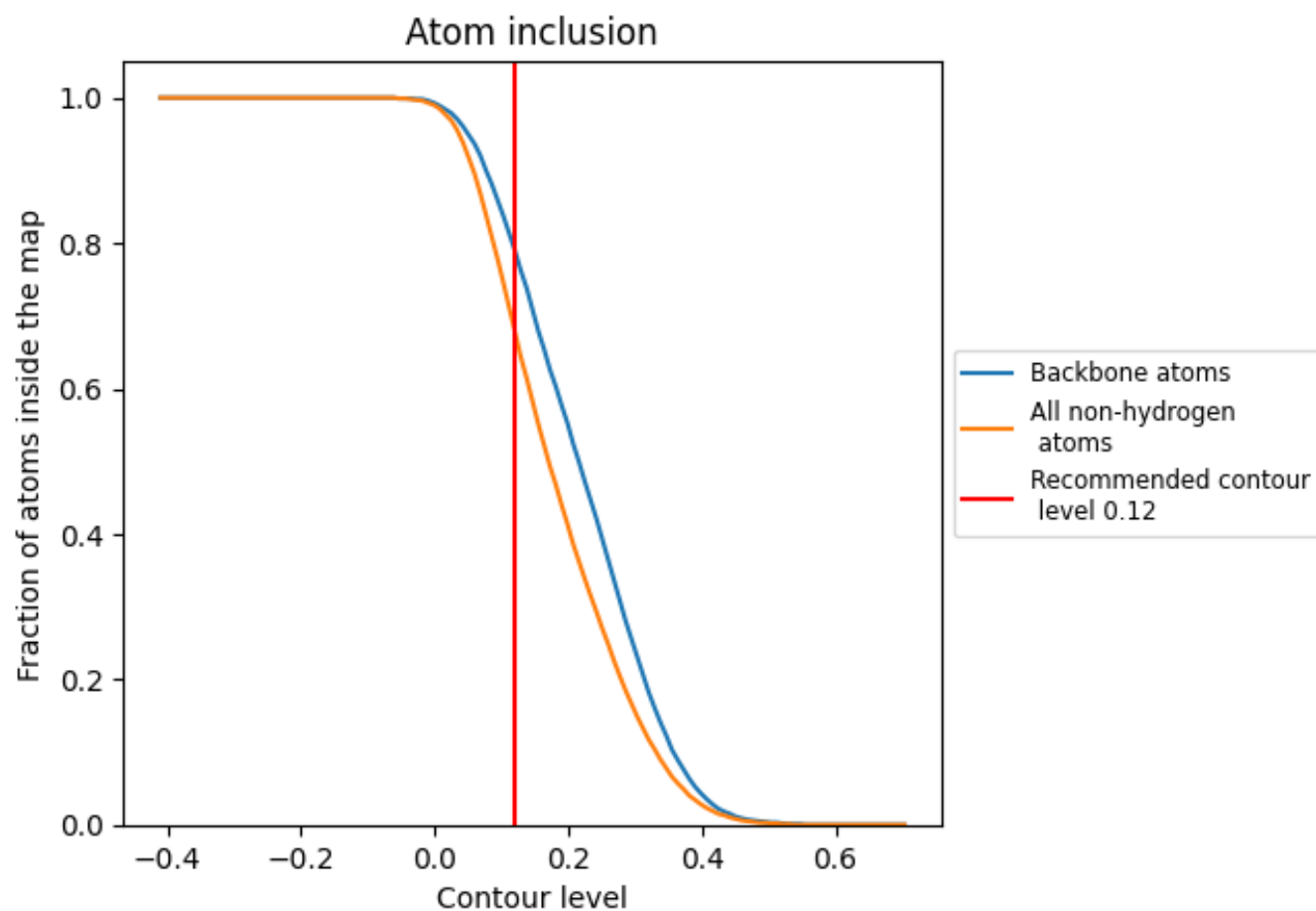
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 68% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.6780	<div><div></div></div> 0.4220
A	<div><div></div></div> 0.6780	<div><div></div></div> 0.4220

