



Full wwPDB EM Validation Report ⓘ

Apr 24, 2025 – 10:47 AM EDT

PDB ID : 9BMC / pdb_00009bmc
EMDB ID : EMD-44695
Title : Post-2 motor domain from full-length human dynein-1 bound to microtubules
in 5mM ADP condition
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.50 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

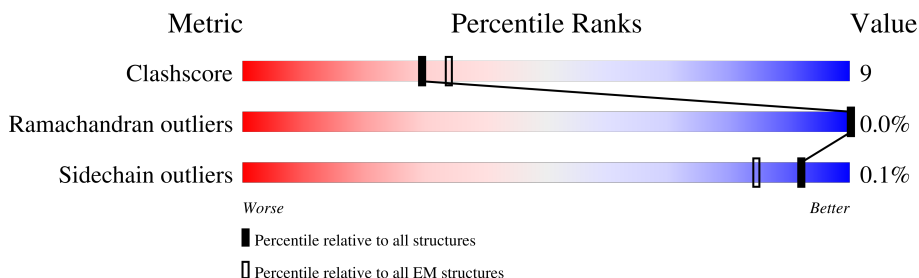
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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>8%</div> <div>51%</div> <div>15%</div> <div>35%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 24617 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	3043	24503	15606	4234	4541	122	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 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	2	Total 2	Mg 2	0



T3530	H3534	H3535	N3540	I3541	R3544	I3547	E3551	S3554	R3559	K3562	L3567	P3568	L3568	C3573	N3576	A3577	I3578	K3581	R3582	R3585	I3590	D3591	P3592	T3600	M3601	R3611	T3612	S3613	F3614	D3615	D3617	F3618	F3619	R3620	E3624	R3628	L3634	V3635	Q3636	D3637								
ALA	ARG	TYR	GLY	GLU	TYR	VAL	SER	GLN	ILE	ALA	ASP	ALA	VAL	GLU	ARG	GLY	ASN	GLU	LEU	GLN	LEU	GLU	ASP	GLY	ASP	GLN	GLN	GLY	GLN	GLY	GLY	VAL	GLU	GLN	PHO	MET	ILE	ASP	LEU	GLU	ALA	VAL	SER	ILE				
ALA	ARG	TYR	GLY	GLU	TYR	VAL	SER	GLN	ILE	ALA	ASP	ALA	VAL	GLU	ARG	GLY	ASN	GLU	LEU	GLN	LEU	GLU	ASP	GLY	ASP	GLN	GLN	GLY	GLN	GLY	GLY	VAL	GLU	GLN	PHO	MET	ILE	ASP	LEU	GLU	ALA	VAL	SER	ILE				
HIS	LYS	GLN	GLY	VAL	ILE	ASP	LYS	GLN	MET	LYS	GLN	GLY	VAL	GLY	ASN	GLY	ASN	GLY	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY				
H3200	R3206	K3207	I3208	T3211	V3212	D3213	Q3214	V3215	E3216	E3217	L3218	R3219	R3220	R3221	LEU	ARG	ILE	LYS	SER	GLN	GLY	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY				
F3086	N3087	V3090	L3091	N3092	K3093	F3094	W3097	E3100	A3101	L3102	L3103	Q3104	K3107	E3108	F3109	M3113	D3114	L3115	E3116	F3123	P3127	Y3130	D3131	K3132	R3140	E3141	A3142	I3143	V3144	L3154	A3162	T3168	M3169	F3066	T3067	M3068	S3071	E3073	G3074	L3075	K3076	D3077	R3078	A3079	A3080	T3081	A3084	L3085
E3006	T3010	L3011	L3012	G3015	P3018	F3021	E3022	G3023	D3024	E3025	L3029	C3033	G3036	A3037	Q3038	K3039	E3040	G3041	L3042	M3043	L3044	D3045	H3046	F3054	T3055	Q3057	V3058	I3059	R3060	V3064	V3065	F3066	T3067	M3068	S3071	E3073	G3074	L3075	K3076	D3077	R3078	A3079	A3080	T3081	A3084	L3085		
Y2901	E2902	E2903	L2909	V2910	V2915	V2919	L2925	Q2930	L2933	L2934	L2935	L2936	S2939	G2940	K2943	L2946	V2950	L2956	K2962	V2963	H2964	Y2967	E2970	D2975	L2976	T2977	V2979	R2982	N2987	E2988	K2989	L2990	K2991	F2992	N2998	V2999	L3000	D3001	L3005									
M2773	F2784	D2787	P2790	H2791	T2792	I2793	Y2794	M2799	F2807	L2816	P2817	G2820	R2823	L2824	W2825	Q2834	L2835	R2836	L2837	V2838	E2842	R2843	D2847	K2856	H2857	F2858	P2859	N2860	L2861	D2862	R2863	E2864	K2865	S2868	R2869	W2876	D2880	D2885	Q2886	K2898								
N2667	L2668	P2669	K2673	R2678	V2679	L2680	S2681	F2682	L2683	R2684	V2687	E2688	D2689	Q2690	T2699	R2705	V2709	C2712	R2720	L2723	R2726	F2727	L2728	V2731	V2736	D2737	Y2738	S2743	I2747	Y2748	G2749	T2750	M2755	L2756	R2757	L2758	L2759	L2762	R2763	E2767	P2768	L2769						
W2545	E2556	V2557	E2558	T2559	H2560	D2566	V2569	F2570	T2571	V2575	R2576	H2577	L2580	L2581	L2582	R2583	E2587	H2588	K2589	P2590	L2591	V2592	L2593	C2594	L2605	R2610	G2619	L2620	P2628	E2629	L2630	K2633	T2634	F2635	N2646	L2650	A2651	P2652	W2658	F2662	L2663	E2665	I2666					
L2413	Q2416	R2417	L2418	A2419	A2420	T2421	L2422	N2430	E2444	H2445	I2446	L2449	T2450	R2451	L2452	R2453	C2454	S2460	M2461	Q2464	A2465	C2466	R2467	N2468	V2469	N2481	E2487	R2492	Y2493	L2499	W2500	D2505	S2506	R2507	L2508	K2509	G2515	E2516	R2519	L2526	P2527	T2528	D2536					
D2308	W2311	L2315	D2320	D2321	L2324	R2332	N2338	F2343	Q2346	W2347	L2348	L2349	L2350	A2354	R2358	W2363	F2364	L2369	W2373	L2382	P2386	L2387	G2390	E2391	D2392	E2393	A2394	Q2395	R2396	R2397	R2398	K2399	G2400	W2401	E2402	D2403	E2404	G2405	E2406	E2407	A2408	A2409						



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	127909	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	1.446	Depositor
Minimum map value	-0.917	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.2	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

5.1 Standard geometry

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	0.28	0/25022	0.49	0/33900

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

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	24503	0	24573	441	0
2	A	81	0	36	5	0
3	A	31	0	12	1	0
4	A	2	0	0	0	0
All	All	24617	0	24621	441	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 9.

All (441) 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:4326:ASN:HD22	1:A:4581:ILE:HD13	1.41	0.83
1:A:2665:GLU:HB3	1:A:2668:LEU:HD23	1.63	0.80
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.17	0.77
1:A:4206:GLU:O	1:A:4255:ARG:NH1	2.17	0.76
1:A:1511:PRO:HG2	1:A:3659:ARG:HE	1.52	0.75
1:A:4574:LYS:HB3	1:A:4627:ALA:HB2	1.69	0.75
1:A:4069:ILE:HD13	1:A:4079:GLN:HG3	1.72	0.72
1:A:2131:LEU:HD12	1:A:2132:PRO:HD2	1.71	0.72
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.72	0.72
1:A:2172:ARG:NH1	1:A:2173:GLY:O	2.23	0.72
1:A:2943:LYS:NZ	2:A:4704:ADP:O1B	2.23	0.71
1:A:2999:VAL:HG13	1:A:3005:LEU:HD21	1.72	0.71
1:A:4025:LEU:HD22	1:A:4027:LEU:HD22	1.72	0.70
1:A:1467:ARG:NH2	1:A:1519:ASP:OD2	2.24	0.70
1:A:3742:LEU:HD11	1:A:3780:VAL:HG21	1.74	0.69
1:A:1454:GLN:HA	1:A:1457:MET:SD	2.31	0.69
1:A:1880:VAL:HG11	1:A:2049:ILE:HA	1.75	0.69
1:A:1332:VAL:HB	1:A:1377:LEU:HD22	1.74	0.69
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.75	0.67
1:A:2588:HIS:CE1	1:A:2658:TRP:HZ3	2.12	0.67
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.76	0.67
1:A:3725:ASP:OD1	1:A:3728:ARG:NH2	2.28	0.67
1:A:2925:ILE:HD12	1:A:3090:VAL:HG11	1.77	0.67
1:A:1626:PHE:HE2	1:A:1628:ARG:HB2	1.61	0.66
1:A:3756:VAL:HG23	1:A:3760:ILE:HG21	1.78	0.66
1:A:3113:MET:O	1:A:3140:ARG:NH2	2.29	0.66
1:A:2581:LEU:HD22	1:A:2591:LEU:HD21	1.78	0.66
1:A:3910:ARG:NH2	1:A:4348:MET:SD	2.68	0.65
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.79	0.65
1:A:3544:ARG:NH1	1:A:3735:GLN:OE1	2.30	0.65
1:A:1698:ILE:HD13	1:A:1701:TRP:HE1	1.62	0.65
1:A:2556:GLU:OE2	1:A:2757:ARG:NH2	2.30	0.64
1:A:2943:LYS:HG2	1:A:3094:PHE:HE2	1.61	0.64
1:A:2320:ASP:OD1	1:A:2321:ASP:N	2.30	0.64
1:A:2182:LEU:HD11	1:A:2207:VAL:HG11	1.79	0.63
1:A:2992:PHE:HD2	1:A:3064:VAL:HG13	1.64	0.63
1:A:4564:LYS:HG3	1:A:4646:GLU:HB2	1.81	0.63
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.81	0.63
1:A:2936:ILE:HD13	1:A:3068:MET:HB2	1.80	0.63
1:A:3914:ILE:H	1:A:3937:ARG:HH12	1.47	0.63
1:A:3772:ASN:HA	1:A:3775:ARG:HH11	1.64	0.62
1:A:2668:LEU:HD21	1:A:2720:ARG:HH11	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2536:ASP:OD1	1:A:2576:ARG:NH1	2.33	0.62
1:A:4547:THR:HG22	1:A:4586:PRO:HG2	1.82	0.62
1:A:1571:ILE:HD11	1:A:1607:LEU:HB3	1.82	0.62
1:A:2930:GLN:HB2	1:A:3059:ILE:HG23	1.81	0.62
1:A:1816:VAL:HG11	1:A:2052:VAL:HG22	1.82	0.61
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.81	0.61
1:A:3079:ALA:HB2	1:A:3086:PHE:HE2	1.66	0.61
1:A:1626:PHE:HB2	1:A:1699:ASN:ND2	2.16	0.61
1:A:3103:TYR:OH	1:A:3141:GLU:OE1	2.15	0.61
1:A:1529:ARG:HH21	1:A:1592:LEU:HG	1.66	0.60
1:A:1661:VAL:HG22	1:A:1676:ILE:HG21	1.82	0.60
1:A:4031:VAL:HG11	1:A:4058:LEU:HD21	1.83	0.60
1:A:2620:LEU:HD12	1:A:2630:LEU:HD21	1.83	0.60
1:A:3763:ASP:OD2	1:A:3765:THR:OG1	2.19	0.60
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.83	0.60
1:A:2191:LEU:HD12	3:A:4702:ATP:C6	2.36	0.60
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.82	0.60
1:A:1626:PHE:CE2	1:A:1628:ARG:HB2	2.37	0.59
1:A:3739:GLN:HA	1:A:3742:LEU:HD12	1.83	0.59
1:A:3889:ARG:HH22	1:A:4347:GLN:HG3	1.65	0.59
1:A:2258:ALA:HB1	1:A:2682:PHE:HD1	1.66	0.59
1:A:2291:VAL:HG23	1:A:2292:ARG:HG2	1.83	0.59
1:A:3592:PRO:HD3	1:A:3702:THR:HG22	1.85	0.59
1:A:4460:LEU:HA	1:A:4475:VAL:HG22	1.84	0.59
1:A:2189:MET:HG3	1:A:2191:LEU:HD23	1.83	0.59
1:A:3530:THR:O	1:A:3534:HIS:ND1	2.36	0.59
1:A:2593:LEU:HD13	1:A:2605:LEU:HD12	1.85	0.59
1:A:3755:GLU:OE2	1:A:3759:ARG:NH1	2.36	0.59
1:A:4511:LEU:HD23	1:A:4560:VAL:HG13	1.84	0.59
1:A:4113:LEU:HD13	1:A:4116:LEU:HD12	1.85	0.58
1:A:2382:LEU:HD23	1:A:2420:ALA:HB2	1.83	0.58
1:A:3611:ARG:NH1	1:A:3636:GLN:OE1	2.37	0.58
1:A:2324:LEU:HD11	1:A:2332:ARG:HB3	1.86	0.58
1:A:3684:PRO:HB3	1:A:3702:THR:HG21	1.86	0.58
1:A:3600:ILE:HD11	1:A:3634:LEU:HD13	1.85	0.58
1:A:1478:VAL:HB	1:A:1488:ARG:HE	1.68	0.57
1:A:2666:ILE:HG22	1:A:2723:LEU:HD21	1.87	0.57
1:A:2369:LEU:HD12	1:A:2373:MET:HE3	1.87	0.57
1:A:2823:ARG:HH12	1:A:2868:SER:H	1.51	0.57
1:A:2970:GLU:N	1:A:2970:GLU:OE1	2.37	0.57
1:A:2221:MET:HE1	1:A:2348:LEU:HD21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3612:THR:HG21	1:A:3619:PHE:HA	1.86	0.57
1:A:3873:ARG:HD2	1:A:4025:LEU:HD12	1.87	0.57
1:A:2265:TYR:OH	1:A:2311:TRP:O	2.11	0.57
1:A:2668:LEU:HD21	1:A:2720:ARG:NH1	2.19	0.57
1:A:3486:ARG:O	1:A:3490:GLU:HG2	2.05	0.56
1:A:2112:LYS:HG3	1:A:2122:VAL:HG11	1.87	0.56
1:A:4071:ILE:HG23	1:A:4077:PHE:HE1	1.71	0.56
1:A:2910:VAL:HG22	1:A:3108:GLU:HG2	1.87	0.56
1:A:4183:LEU:HD11	1:A:4215:ALA:HB1	1.87	0.56
1:A:1755:GLN:HG3	1:A:1814:GLU:OE2	2.06	0.55
1:A:1961:ASN:HD21	1:A:2019:ASN:HB3	1.71	0.55
1:A:2577:HIS:O	1:A:2581:LEU:HG	2.07	0.55
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.88	0.55
1:A:3103:TYR:CE2	1:A:3107:LYS:HD2	2.41	0.55
1:A:3208:ILE:HG23	1:A:3482:LEU:HD12	1.88	0.55
1:A:1411:ARG:NH2	1:A:1456:GLU:OE1	2.35	0.55
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.87	0.55
1:A:1349:GLN:NE2	1:A:1353:SER:O	2.40	0.55
1:A:1622:GLU:OE2	1:A:1697:LYS:NZ	2.36	0.55
1:A:1959:GLU:OE2	1:A:2019:ASN:ND2	2.39	0.55
1:A:4303:GLU:OE1	1:A:4303:GLU:N	2.32	0.54
1:A:1451:LEU:HD12	1:A:3656:THR:HG21	1.90	0.54
1:A:2192:THR:HB	1:A:2373:MET:HG2	1.88	0.54
1:A:4176:ARG:NH2	1:A:4224:ASP:OD1	2.39	0.54
1:A:1479:ASN:HD21	1:A:1482:ASN:H	1.55	0.54
1:A:2619:GLY:HA2	1:A:2662:PHE:HB3	1.89	0.54
1:A:2987:ASN:OD1	1:A:3057:GLN:NE2	2.38	0.54
1:A:2346:GLN:HB2	1:A:2726:ARG:HD2	1.89	0.54
1:A:2629:GLU:O	1:A:2633:LYS:HG2	2.07	0.54
1:A:1420:LEU:HD13	1:A:1437:VAL:HG11	1.90	0.54
1:A:2464:GLN:HG2	1:A:2583:THR:HG23	1.90	0.54
1:A:3130:TYR:CZ	1:A:3132:LYS:HB2	2.43	0.54
1:A:4324:PRO:HB3	1:A:4638:ARG:HH11	1.72	0.54
1:A:1374:PRO:HD2	1:A:1377:LEU:HD12	1.90	0.53
1:A:2834:GLN:HG2	1:A:2843:ARG:HG2	1.90	0.53
1:A:4398:LEU:HG	1:A:4417:VAL:HG21	1.90	0.53
1:A:3715:GLU:OE2	1:A:3837:HIS:NE2	2.37	0.53
1:A:1907:PRO:O	1:A:1912:LYS:NZ	2.41	0.53
1:A:2222:MET:HG2	1:A:2364:PHE:CE1	2.44	0.53
1:A:3851:ASP:OD2	1:A:3853:THR:OG1	2.23	0.53
1:A:2747:ILE:O	1:A:2750:THR:OG1	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3055:THR:O	1:A:3059:ILE:HD12	2.08	0.53
1:A:2453:ARG:NH1	1:A:2505:ASP:OD2	2.25	0.53
1:A:2149:LEU:HD11	1:A:2157:LEU:HD22	1.91	0.53
1:A:2304:ASP:OD1	1:A:2726:ARG:NH2	2.43	0.53
1:A:3554:SER:HB3	1:A:3578:ILE:HD11	1.90	0.53
1:A:3654:ARG:HH21	1:A:3661:LEU:HG	1.74	0.52
1:A:3828:SER:HB3	1:A:4140:ARG:HG2	1.90	0.52
1:A:3909:LEU:HB3	1:A:4344:LEU:HD13	1.91	0.52
1:A:4560:VAL:HB	1:A:4588:THR:HB	1.91	0.52
1:A:3879:ASP:OD1	1:A:4342:LYS:NZ	2.31	0.52
1:A:1579:MET:HA	1:A:1582:VAL:HG12	1.92	0.52
1:A:3590:ILE:HD11	1:A:3700:ASN:ND2	2.24	0.52
1:A:3143:ILE:HD13	1:A:3541:ILE:HD13	1.90	0.52
1:A:3482:LEU:O	1:A:3485:GLU:HG3	2.10	0.52
1:A:2569:VAL:HB	1:A:2747:ILE:HG13	1.92	0.52
1:A:4096:LEU:HD13	1:A:4105:TRP:HH2	1.75	0.52
1:A:1405:SER:OG	1:A:1406:GLU:N	2.43	0.52
1:A:2449:LEU:HD11	1:A:2454:CYS:SG	2.50	0.52
1:A:2464:GLN:NE2	1:A:2468:ASN:OD1	2.43	0.52
1:A:1750:VAL:HG12	1:A:1811:LEU:HD21	1.91	0.52
1:A:1927:VAL:HG22	1:A:1954:TRP:HB2	1.90	0.51
1:A:1486:LEU:HB3	1:A:1541:GLN:NE2	2.25	0.51
1:A:3174:ARG:HH12	1:A:3695:ARG:CZ	2.23	0.51
1:A:1979:GLN:HB3	1:A:2035:LEU:HD13	1.93	0.51
1:A:2628:PRO:HG3	1:A:2679:VAL:HA	1.90	0.51
1:A:4180:TYR:OH	1:A:4220:ASP:OD2	2.28	0.51
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	1.91	0.51
1:A:4069:ILE:HD12	1:A:4080:ALA:HA	1.93	0.51
1:A:1652:LYS:HB2	1:A:2332:ARG:HH22	1.76	0.51
1:A:2919:VAL:HG13	1:A:2950:VAL:HG22	1.92	0.51
1:A:3591:ASP:HB3	1:A:3701:PHE:HB2	1.92	0.50
1:A:2065:LEU:HD11	1:A:2133:GLU:HB3	1.92	0.50
1:A:1336:LEU:HD11	1:A:1386:VAL:HG21	1.93	0.50
1:A:1547:LEU:HD11	1:A:1612:GLN:HB2	1.93	0.50
1:A:3097:TRP:HB3	1:A:3101:ALA:HB3	1.94	0.50
1:A:2507:ARG:HD2	1:A:2509:LYS:NZ	2.27	0.50
1:A:4202:SER:OG	1:A:4261:ASP:OD2	2.25	0.50
1:A:4535:SER:OG	1:A:4537:GLU:OE1	2.28	0.50
1:A:2748:TYR:CE2	1:A:2799:MET:HG2	2.47	0.50
1:A:2382:LEU:O	1:A:2416:GLN:NE2	2.38	0.50
1:A:1356:PRO:HB3	1:A:1401:ILE:HG12	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.94	0.49
1:A:1717:LEU:HB2	1:A:1749:LEU:HD22	1.94	0.49
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.93	0.49
1:A:1438:ASP:HB3	1:A:1441:LYS:HB3	1.94	0.49
1:A:2915:VAL:HG13	1:A:2946:LEU:HD21	1.93	0.49
1:A:4038:ASN:HB3	1:A:4118:PRO:HG3	1.95	0.49
1:A:3084:ALA:HA	1:A:3087:ASN:HB2	1.94	0.49
1:A:3113:MET:HB3	1:A:3115:LEU:HD13	1.95	0.49
1:A:2146:VAL:HA	1:A:2149:LEU:HD12	1.94	0.49
1:A:4040:PRO:HB3	1:A:4124:LEU:HD23	1.94	0.49
1:A:1961:ASN:ND2	1:A:2019:ASN:O	2.46	0.49
1:A:3193:GLU:O	1:A:3196:GLU:HG3	2.13	0.49
1:A:3973:LEU:HB3	1:A:3992:LEU:HD11	1.93	0.49
1:A:2581:LEU:CD2	1:A:2591:LEU:HD21	2.41	0.49
1:A:3178:ASP:OD2	1:A:3585:ARG:NE	2.45	0.49
1:A:3716:VAL:HG23	1:A:3836:TYR:OH	2.13	0.49
1:A:2964:HIS:HB2	1:A:3644:VAL:HB	1.95	0.49
1:A:3162:ALA:HB2	1:A:3168:THR:HG21	1.94	0.49
1:A:3910:ARG:CZ	1:A:4344:LEU:HD11	2.43	0.49
1:A:2666:ILE:HB	1:A:2712:CYS:SG	2.53	0.48
1:A:2728:LEU:HA	1:A:2731:VAL:HG22	1.95	0.48
1:A:3591:ASP:N	1:A:3591:ASP:OD1	2.46	0.48
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.95	0.48
1:A:2222:MET:HG2	1:A:2364:PHE:HE1	1.79	0.48
1:A:2395:GLN:HB3	1:A:2398:ARG:HH22	1.78	0.48
1:A:2784:PHE:CE1	1:A:2842:GLU:HB3	2.48	0.48
1:A:3108:GLU:HG3	1:A:3109:PHE:HD1	1.78	0.48
1:A:2963:VAL:HB	1:A:2998:ASN:HB3	1.95	0.48
1:A:2290:SER:HB3	1:A:2295:LEU:HG	1.96	0.48
1:A:1582:VAL:HG23	1:A:1591:VAL:HG22	1.94	0.48
1:A:1785:VAL:HG13	1:A:1815:LEU:HD12	1.95	0.48
1:A:1800:GLN:OE1	1:A:1804:ARG:NH1	2.47	0.48
1:A:2847:ASP:OD2	1:A:2869:ARG:NH1	2.41	0.48
1:A:2214:THR:HG22	1:A:2220:LEU:HD21	1.96	0.48
1:A:2628:PRO:HG2	1:A:2678:ARG:HG2	1.96	0.48
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.49	0.48
1:A:2324:LEU:HD21	1:A:2332:ARG:HE	1.78	0.48
1:A:3154:LEU:HD13	1:A:3516:TYR:CD1	2.49	0.48
1:A:1652:LYS:HD2	1:A:2332:ARG:HH12	1.79	0.48
1:A:2224:GLY:H	1:A:2230:LYS:HD3	1.78	0.48
1:A:2784:PHE:HB2	1:A:2794:TYR:HE2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3567:LEU:HD12	1:A:3568:PRO:HD2	1.95	0.48
1:A:2999:VAL:HG21	1:A:3068:MET:HE1	1.96	0.47
1:A:3765:THR:HB	1:A:3767:ILE:HG12	1.96	0.47
1:A:1632:VAL:HG22	1:A:1636:ASP:HB2	1.95	0.47
1:A:2823:ARG:HH22	1:A:2868:SER:HB3	1.78	0.47
1:A:1857:LEU:HD22	1:A:1868:TYR:HB2	1.95	0.47
1:A:2446:ILE:HD13	1:A:2594:CYS:SG	2.54	0.47
1:A:2001:LEU:HD12	1:A:2006:VAL:HG21	1.97	0.47
1:A:4065:GLN:HG2	1:A:4092:ARG:NH2	2.28	0.47
1:A:1892:MET:SD	1:A:1902:GLY:HA3	2.55	0.47
1:A:4404:ASN:ND2	1:A:4501:ALA:HB2	2.30	0.47
1:A:1355:GLN:HG3	1:A:1358:LYS:H	1.79	0.47
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.47	0.47
1:A:2519:ARG:HG3	1:A:2526:LEU:HD12	1.97	0.47
1:A:3174:ARG:NH2	2:A:4704:ADP:O3A	2.48	0.47
1:A:3562:TRP:HB3	1:A:3567:LEU:HD23	1.95	0.47
1:A:2581:LEU:HD13	1:A:2605:LEU:HA	1.97	0.47
1:A:2635:PHE:HB3	1:A:2650:LEU:HD11	1.96	0.47
1:A:3056:SER:O	1:A:3060:ARG:HG3	2.15	0.47
1:A:3590:ILE:HD11	1:A:3700:ASN:HD22	1.80	0.47
1:A:4247:MET:HA	1:A:4251:ILE:HB	1.97	0.47
1:A:2467:ARG:NH2	1:A:2587:GLU:OE1	2.48	0.47
1:A:2967:TYR:OH	1:A:2975:ASP:OD2	2.33	0.47
1:A:1388:ARG:HA	1:A:1391:LYS:HE2	1.95	0.46
1:A:2784:PHE:HB3	1:A:2792:TYR:CD2	2.49	0.46
1:A:3100:GLU:OE2	1:A:3104:GLN:NE2	2.39	0.46
1:A:3781:THR:HG22	1:A:3785:GLU:OE1	2.15	0.46
1:A:3888:ALA:HA	1:A:4013:LEU:HD21	1.97	0.46
1:A:1466:ILE:HG12	1:A:1500:HIS:ND1	2.30	0.46
1:A:2759:ILE:HG21	1:A:2762:LEU:HD23	1.97	0.46
1:A:4395:LEU:HD11	1:A:4486:ILE:HD12	1.98	0.46
1:A:2079:GLN:HB2	1:A:2160:LEU:HD11	1.98	0.46
1:A:4112:LYS:O	1:A:4116:LEU:HG	2.16	0.46
1:A:2354:ALA:HB1	1:A:2358:ARG:HH21	1.80	0.46
1:A:3010:THR:HG21	1:A:3018:PRO:HD2	1.97	0.46
1:A:1469:VAL:O	1:A:1473:TYR:HB2	2.16	0.46
1:A:2651:ALA:HB1	1:A:2705:ARG:HH21	1.81	0.46
1:A:4054:HIS:CD2	1:A:4147:PHE:HE2	2.33	0.46
1:A:3620:ARG:O	1:A:3624:GLU:HG2	2.16	0.46
1:A:2838:VAL:HG13	1:A:3093:TRP:CZ2	2.51	0.46
1:A:3601:MET:CE	1:A:3611:ARG:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3767:ILE:HA	1:A:3770:LEU:HG	1.98	0.46
1:A:1408:LEU:HB3	1:A:1413:TRP:CD1	2.52	0.45
1:A:2943:LYS:HE2	1:A:3067:THR:HB	1.98	0.45
1:A:1657:MET:HE1	1:A:1702:LEU:HD21	1.98	0.45
1:A:3568:PRO:HG2	1:A:3573:CYS:SG	2.56	0.45
1:A:1483:LYS:HE3	1:A:1548:GLU:OE1	2.17	0.45
1:A:1789:LEU:HD23	1:A:1789:LEU:HA	1.80	0.45
1:A:2181:GLU:HG3	1:A:2244:LEU:HD13	1.99	0.45
1:A:1526:LYS:O	1:A:1530:ILE:HG22	2.16	0.45
1:A:2605:LEU:HD13	1:A:2662:PHE:CE2	2.52	0.45
1:A:2683:ILE:O	1:A:2687:VAL:HG22	2.16	0.45
1:A:3562:TRP:HZ2	1:A:3581:LYS:HD3	1.81	0.45
1:A:1546:TYR:CE2	1:A:1550:ILE:HD11	2.51	0.45
1:A:2075:LEU:HB3	1:A:2160:LEU:HD13	1.98	0.45
1:A:2876:TRP:HH2	1:A:2919:VAL:HG12	1.81	0.45
1:A:3073:GLU:HG2	1:A:3074:GLY:N	2.32	0.45
1:A:2956:LEU:HD23	1:A:2989:LYS:HB3	1.97	0.45
1:A:3780:VAL:O	1:A:3784:VAL:HG23	2.16	0.45
1:A:4087:ALA:HA	1:A:4092:ARG:HB2	1.98	0.45
1:A:4088:VAL:HG13	1:A:4118:PRO:HA	1.97	0.45
1:A:4281:GLU:N	1:A:4281:GLU:OE1	2.50	0.45
1:A:1928:LEU:HD13	1:A:1948:LEU:HD21	1.98	0.45
1:A:2369:LEU:HD23	1:A:2451:ARG:HH21	1.81	0.45
1:A:3123:PRO:HB3	1:A:3540:ASN:OD1	2.16	0.45
1:A:4097:LYS:HA	1:A:4127:THR:OG1	2.17	0.45
1:A:4324:PRO:HB2	1:A:4326:ASN:OD1	2.17	0.45
1:A:4457:LYS:HB2	1:A:4457:LYS:HE2	1.70	0.45
1:A:1652:LYS:HD2	1:A:2332:ARG:NH1	2.32	0.45
1:A:1937:ASP:OD2	1:A:1940:ALA:HB3	2.16	0.45
1:A:2666:ILE:O	1:A:2669:PRO:HD2	2.17	0.45
1:A:3114:ASP:O	1:A:3140:ARG:NH2	2.49	0.45
1:A:4037:PRO:HB2	1:A:4118:PRO:HB2	1.99	0.45
1:A:4191:GLN:O	1:A:4194:LEU:HB2	2.17	0.44
1:A:4192:GLU:OE2	1:A:4195:ARG:HD3	2.17	0.44
1:A:1947:GLY:O	1:A:1951:VAL:HG12	2.17	0.44
1:A:2054:LEU:HG	1:A:2097:LEU:HD13	1.98	0.44
1:A:2898:LYS:O	1:A:2902:GLU:HG2	2.16	0.44
1:A:4031:VAL:O	1:A:4123:ARG:NH1	2.49	0.44
1:A:4324:PRO:HD3	1:A:4638:ARG:HG2	2.00	0.44
1:A:1925:ARG:NH1	1:A:2011:ASP:HB3	2.32	0.44
1:A:2943:LYS:HG2	1:A:3094:PHE:CE2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1479:ASN:ND2	1:A:1482:ASN:H	2.14	0.44
1:A:3779:GLU:O	1:A:3783:LYS:HG3	2.17	0.44
1:A:2191:LEU:HD11	1:A:2232:MET:HG2	1.99	0.44
1:A:2500:TRP:CD2	1:A:2580:LEU:HD11	2.53	0.44
1:A:2757:ARG:HG3	1:A:2763:ARG:HH22	1.81	0.44
1:A:2773:MET:HG2	1:A:2825:TRP:HE1	1.83	0.44
1:A:2915:VAL:HG21	2:A:4704:ADP:HN61	1.82	0.44
1:A:2940:GLY:HA3	1:A:3174:ARG:HG3	1.99	0.44
1:A:4577:LEU:HD22	1:A:4638:ARG:HD2	1.98	0.44
1:A:2324:LEU:HD21	1:A:2332:ARG:NE	2.33	0.44
1:A:2935:LEU:HD23	1:A:3092:ASN:HB3	2.00	0.44
1:A:1626:PHE:HB3	1:A:1629:PHE:CD2	2.53	0.44
1:A:1914:GLU:HG3	2:A:4701:ADP:H3'	2.00	0.44
1:A:4179:LEU:HD12	1:A:4223:LEU:HD22	1.99	0.44
1:A:2053:MET:HE3	1:A:2094:LYS:HA	2.00	0.44
1:A:2499:LEU:HD11	1:A:2515:GLY:HA2	2.00	0.44
1:A:2933:LEU:O	1:A:3065:VAL:HA	2.18	0.44
1:A:2506:SER:OG	1:A:2507:ARG:N	2.51	0.43
1:A:1397:ASN:O	1:A:1401:ILE:HG13	2.17	0.43
1:A:1844:PHE:CD2	1:A:1859:ILE:HG12	2.54	0.43
1:A:3169:MET:HB3	1:A:3693:CYS:SG	2.58	0.43
1:A:3824:LEU:HD22	1:A:4130:ILE:HD12	2.00	0.43
1:A:1658:PHE:HB2	1:A:1661:VAL:HB	2.00	0.43
1:A:2386:PRO:HG3	1:A:2413:LEU:HD21	2.01	0.43
1:A:2755:MET:HG3	1:A:2807:PHE:HB2	2.00	0.43
1:A:3767:ILE:HG13	1:A:3771:GLU:OE2	2.18	0.43
1:A:1419:ARG:HD2	1:A:1445:ILE:HG23	1.99	0.43
1:A:1513:TYR:O	1:A:1517:GLU:HG2	2.19	0.43
1:A:2605:LEU:HD13	1:A:2662:PHE:HE2	1.83	0.43
1:A:3130:TYR:CE2	1:A:3132:LYS:HB2	2.53	0.43
1:A:4243:LEU:HB3	1:A:4247:MET:HE3	1.98	0.43
1:A:2265:TYR:OH	1:A:2315:LEU:HG	2.18	0.43
1:A:2396:ARG:NH1	1:A:2406:GLU:OE2	2.51	0.43
1:A:2422:ILE:HG21	1:A:2487:GLU:HA	2.00	0.43
1:A:2460:SER:OG	1:A:2589:LYS:HD2	2.19	0.43
1:A:2901:TYR:OH	1:A:2909:LEU:N	2.26	0.43
1:A:3079:ALA:HB2	1:A:3086:PHE:CE2	2.50	0.43
1:A:2658:TRP:CD1	1:A:2705:ARG:HD2	2.53	0.43
1:A:2976:LEU:HA	1:A:2979:VAL:HG12	1.99	0.43
1:A:1756:ILE:HD11	1:A:1857:LEU:HD11	2.00	0.43
1:A:2571:THR:O	1:A:2575:VAL:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3913:GLU:N	1:A:3913:GLU:OE1	2.52	0.43
1:A:1409:LYS:HB3	1:A:1410:ASP:H	1.61	0.43
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	2.01	0.43
1:A:2836:ARG:HB2	1:A:3091:LEU:HD11	2.01	0.43
1:A:3140:ARG:O	1:A:3144:VAL:HG23	2.18	0.43
1:A:2393:GLU:O	1:A:2397:ARG:NH1	2.51	0.43
1:A:2962:LYS:HG3	1:A:3665:GLY:O	2.19	0.43
1:A:3792:GLN:O	1:A:3796:THR:HG23	2.19	0.43
1:A:1350:PRO:HA	1:A:1430:THR:HA	2.00	0.43
1:A:1425:VAL:HB	1:A:1428:GLU:HB2	2.01	0.43
1:A:1698:ILE:HD13	1:A:1701:TRP:NE1	2.30	0.43
1:A:3614:PHE:HE2	1:A:3642:ASP:H	1.66	0.43
1:A:2012:MET:HE3	1:A:2012:MET:HB3	1.90	0.42
1:A:2213:ILE:HG22	1:A:2220:LEU:HD22	2.00	0.42
1:A:3641:TYR:CD2	1:A:3692:LEU:HD12	2.54	0.42
1:A:4511:LEU:HD23	1:A:4560:VAL:CG1	2.49	0.42
1:A:2769:LEU:HA	1:A:2858:PHE:HZ	1.84	0.42
1:A:3127:PRO:HB2	1:A:3535:HIS:CE1	2.54	0.42
1:A:2680:ILE:HD13	1:A:2680:ILE:HA	1.86	0.42
1:A:3033:CYS:SG	1:A:3054:PHE:HB2	2.60	0.42
1:A:3544:ARG:HH21	1:A:3547:ILE:HG13	1.85	0.42
1:A:4065:GLN:HG2	1:A:4092:ARG:HH21	1.84	0.42
1:A:1598:GLN:HG2	1:A:1599:ARG:HH21	1.85	0.42
1:A:1724:VAL:HA	1:A:1727:PHE:HB2	2.01	0.42
1:A:2469:VAL:HG13	1:A:2481:MET:SD	2.59	0.42
1:A:2737:ASP:OD1	1:A:2738:TYR:N	2.47	0.42
1:A:3211:THR:O	1:A:3215:VAL:HG23	2.19	0.42
1:A:1403:LEU:HD23	1:A:1408:LEU:HD21	2.02	0.42
1:A:1486:LEU:HB3	1:A:1541:GLN:HE22	1.84	0.42
1:A:1509:LEU:HD11	1:A:3628:ARG:HB2	2.00	0.42
1:A:2387:LEU:HD23	1:A:2467:ARG:NH2	2.35	0.42
1:A:2898:LYS:O	1:A:2901:TYR:HB2	2.20	0.42
1:A:4235:PRO:HB2	1:A:4275:THR:HG23	2.01	0.42
1:A:1905:PHE:HB2	1:A:2020:PRO:HD3	2.02	0.42
1:A:2982:ARG:HE	1:A:2990:ILE:HD11	1.84	0.42
1:A:3215:VAL:HG11	1:A:3478:LEU:HD23	2.02	0.42
1:A:3474:ARG:HE	1:A:3764:ASP:HB3	1.84	0.42
1:A:1463:LEU:O	1:A:1467:ARG:HD3	2.20	0.42
1:A:1663:SER:OG	1:A:1664:ILE:N	2.53	0.42
1:A:2206:LYS:HA	1:A:2206:LYS:HD3	1.86	0.42
1:A:2223:VAL:HG23	1:A:2363:TRP:CE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2500:TRP:CE3	1:A:2580:LEU:HD11	2.55	0.42
1:A:2527:PRO:HD3	1:A:2545:TRP:CE2	2.54	0.42
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	2.01	0.42
1:A:1351:TRP:CH2	1:A:1400:VAL:HG13	2.55	0.42
1:A:2231:SER:HA	1:A:2234:TRP:NE1	2.35	0.42
1:A:2605:LEU:HD11	1:A:2709:VAL:HG12	2.01	0.42
1:A:2743:SER:O	1:A:2747:ILE:HG22	2.19	0.42
1:A:2939:SER:O	1:A:3172:THR:HB	2.20	0.42
1:A:3821:ILE:HD11	1:A:4346:MET:HG2	2.01	0.42
1:A:1912:LYS:HG2	1:A:2041:MET:HG3	2.00	0.42
1:A:2418:ASP:O	1:A:2422:ILE:HG12	2.20	0.42
1:A:3015:GLY:HA3	1:A:3059:ILE:HD11	2.00	0.42
1:A:1391:LYS:HE2	1:A:1391:LYS:HB3	1.81	0.41
1:A:3021:PHE:CD2	1:A:3029:LEU:HD22	2.55	0.41
1:A:3551:GLU:OE2	1:A:3559:ARG:NH1	2.53	0.41
1:A:3840:LEU:HD23	1:A:3840:LEU:HA	1.87	0.41
1:A:3923:ARG:HE	1:A:3923:ARG:HB3	1.70	0.41
1:A:4524:THR:HB	1:A:4558:PHE:CE2	2.55	0.41
1:A:1879:LEU:HD12	2:A:4701:ADP:C6	2.54	0.41
1:A:3012:LEU:HD11	1:A:3066:PHE:CE2	2.54	0.41
1:A:3190:LYS:CB	1:A:3503:ILE:HD11	2.50	0.41
1:A:2297:LYS:O	1:A:2338:ASN:ND2	2.54	0.41
1:A:4594:LYS:HE3	1:A:4594:LYS:HB2	1.94	0.41
1:A:1746:GLN:O	1:A:1750:VAL:HG23	2.21	0.41
1:A:2306:ASP:OD1	1:A:2307:VAL:N	2.53	0.41
1:A:2697:ASP:HB3	1:A:2699:THR:HG22	2.01	0.41
1:A:1546:TYR:CZ	1:A:1550:ILE:HD11	2.54	0.41
1:A:2684:ARG:NH1	1:A:2688:GLU:OE1	2.37	0.41
1:A:3108:GLU:HG3	1:A:3109:PHE:CD1	2.55	0.41
1:A:3512:ALA:O	1:A:3516:TYR:HB2	2.21	0.41
1:A:3190:LYS:HB3	1:A:3503:ILE:HD11	2.02	0.41
1:A:1571:ILE:HD11	1:A:1607:LEU:CB	2.50	0.41
1:A:2577:HIS:ND1	1:A:2736:VAL:HG22	2.35	0.41
1:A:3078:ARG:HA	1:A:3081:THR:HG22	2.01	0.41
1:A:3576:ASN:ND2	1:A:3700:ASN:O	2.40	0.41
1:A:3659:ARG:CZ	1:A:3661:LEU:HD21	2.51	0.41
1:A:4178:ARG:NH2	1:A:4299:GLY:O	2.39	0.41
1:A:1416:LEU:HG	1:A:1449:VAL:HG21	2.01	0.41
1:A:1678:SER:OG	1:A:1679:ARG:N	2.52	0.41
1:A:2885:ASP:OD1	1:A:2886:GLN:N	2.53	0.41
1:A:3644:VAL:O	1:A:3647:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3945:LYS:HE2	1:A:3945:LYS:HB2	1.93	0.41
1:A:4246:LEU:HD23	1:A:4246:LEU:HA	1.89	0.41
1:A:4284:LEU:HD23	1:A:4284:LEU:HA	1.90	0.41
1:A:4423:LEU:HD13	1:A:4466:HIS:CD2	2.56	0.41
1:A:2206:LYS:HB3	1:A:2364:PHE:CE2	2.56	0.41
1:A:2406:GLU:HG2	1:A:2409:ALA:HB2	2.02	0.41
1:A:2492:ARG:HG3	1:A:2545:TRP:CE2	2.56	0.41
1:A:3947:LEU:O	1:A:3951:VAL:HG23	2.20	0.41
1:A:1459:LEU:O	1:A:1463:LEU:HD23	2.20	0.40
1:A:2096:VAL:HG11	1:A:2141:VAL:HG22	2.03	0.40
1:A:2558:GLU:HG3	1:A:2560:HIS:CE1	2.56	0.40
1:A:2652:PRO:HD2	1:A:2705:ARG:NH2	2.36	0.40
1:A:2977:ARG:HD3	1:A:3025:GLU:HG2	2.03	0.40
1:A:1478:VAL:HB	1:A:1488:ARG:NE	2.34	0.40
1:A:2308:ASP:HA	1:A:2350:TYR:O	2.21	0.40
1:A:2395:GLN:HB3	1:A:2398:ARG:NH2	2.36	0.40
1:A:2758:LEU:HD11	1:A:2807:PHE:HE1	1.86	0.40
1:A:4430:ASP:OD2	1:A:4447:TYR:OH	2.30	0.40
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.56	0.40
1:A:3114:ASP:O	1:A:3116:GLU:HG3	2.21	0.40
1:A:3601:MET:HE1	1:A:3611:ARG:HB2	2.04	0.40
1:A:3802:LEU:N	1:A:3803:PRO:HD2	2.37	0.40
1:A:4288:VAL:O	1:A:4319:SER:OG	2.30	0.40
1:A:4391:ILE:O	1:A:4428:ARG:NH2	2.54	0.40
1:A:2663:CYS:HB2	1:A:2666:ILE:HD11	2.03	0.40
1:A:2790:PRO:HG2	1:A:3075:LEU:HD23	2.02	0.40
1:A:3189:GLU:OE2	1:A:3582:ARG:NH2	2.55	0.40
1:A:3211:THR:HG21	1:A:3753:LEU:HD11	2.03	0.40
1:A:2915:VAL:O	1:A:2919:VAL:HG23	2.22	0.40
1:A:3635:VAL:O	1:A:3680:SER:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3035/4646 (65%)	2959 (98%)	75 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1510	SER

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	2706/4125 (66%)	2704 (100%)	2 (0%)	92	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2172	ARG
1	A	3092	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1482	ASN
1	A	1541	GLN
1	A	1699	ASN
1	A	3865	GLN
1	A	3869	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	A	4701	-	24,29,29	0.84	0	29,45,45	1.23	3 (10%)
2	ADP	A	4703	-	24,29,29	0.87	0	29,45,45	1.23	2 (6%)
2	ADP	A	4704	-	24,29,29	0.85	0	29,45,45	1.24	2 (6%)
3	ATP	A	4702	4	28,33,33	0.78	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	-	-	3/12/32/32	0/3/3/3
2	ADP	A	4703	-	-	4/12/32/32	0/3/3/3
2	ADP	A	4704	-	-	4/12/32/32	0/3/3/3
3	ATP	A	4702	4	-	1/18/38/38	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	N3-C2-N1	-3.81	123.50	128.67
2	A	4701	ADP	N3-C2-N1	-3.71	123.64	128.67
2	A	4704	ADP	N3-C2-N1	-3.67	123.69	128.67
2	A	4701	ADP	C4-C5-N7	-2.37	106.83	109.34
3	A	4702	ATP	C5-C6-N6	2.30	123.81	120.31
2	A	4704	ADP	C4-C5-N7	-2.28	106.93	109.34
2	A	4703	ADP	C4-C5-N7	-2.23	106.98	109.34
2	A	4701	ADP	C2'-C3'-C4'	2.04	106.56	102.61

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4703	ADP	C5'-O5'-PA-O1A
2	A	4703	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C3'-C4'-C5'-O5'
2	A	4704	ADP	O4'-C4'-C5'-O5'
2	A	4701	ADP	PB-O3A-PA-O1A
2	A	4703	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	O4'-C4'-C5'-O5'
2	A	4701	ADP	PB-O3A-PA-O2A
2	A	4703	ADP	O4'-C4'-C5'-O5'
3	A	4702	ATP	PA-O3A-PB-O2B

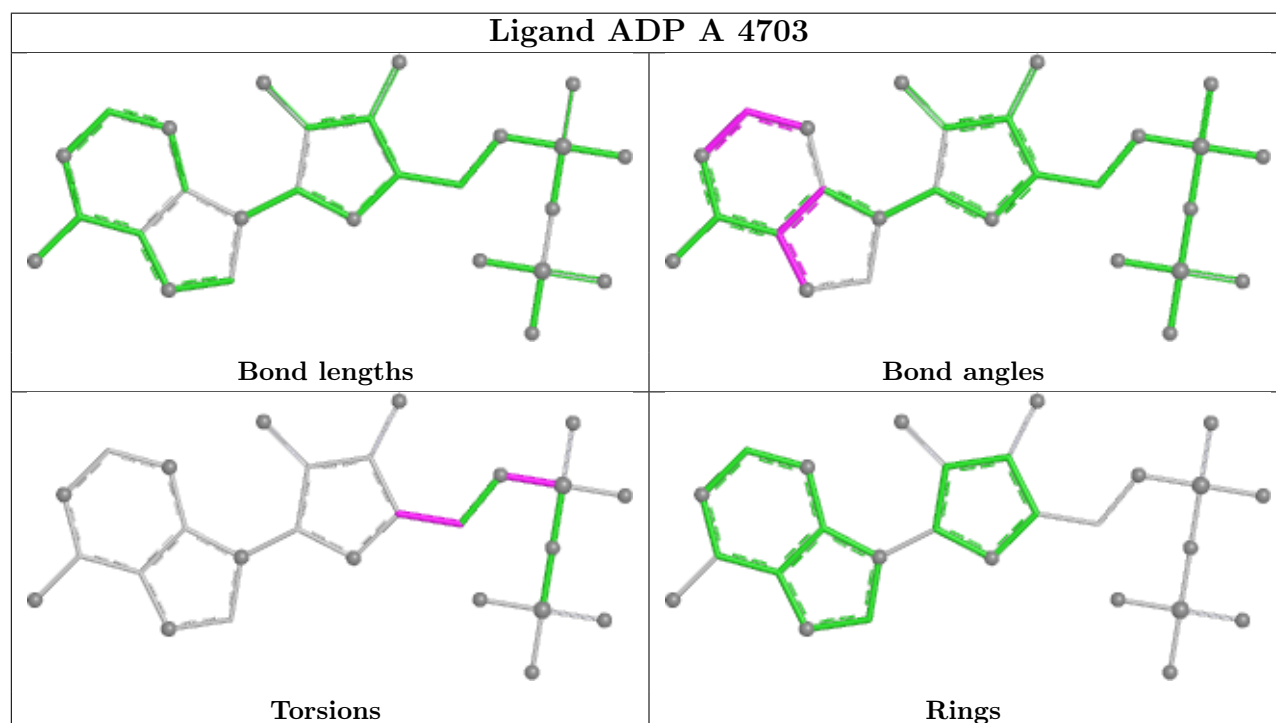
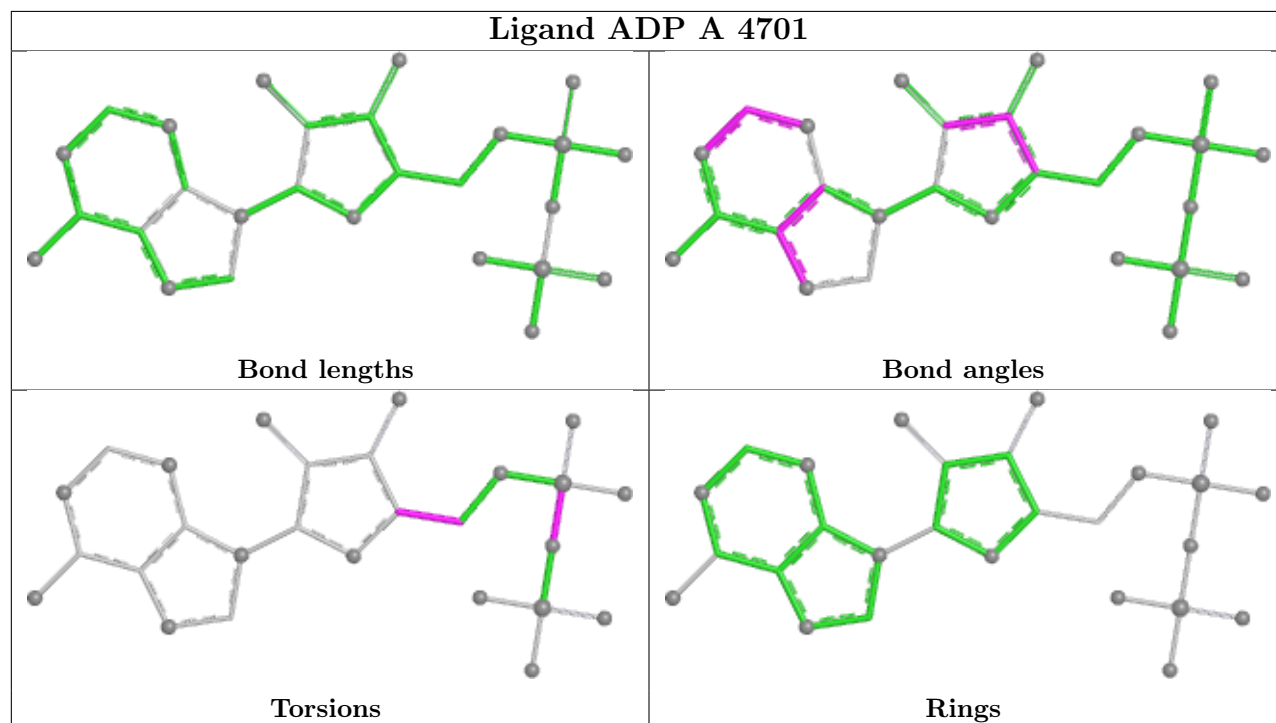
There are no ring outliers.

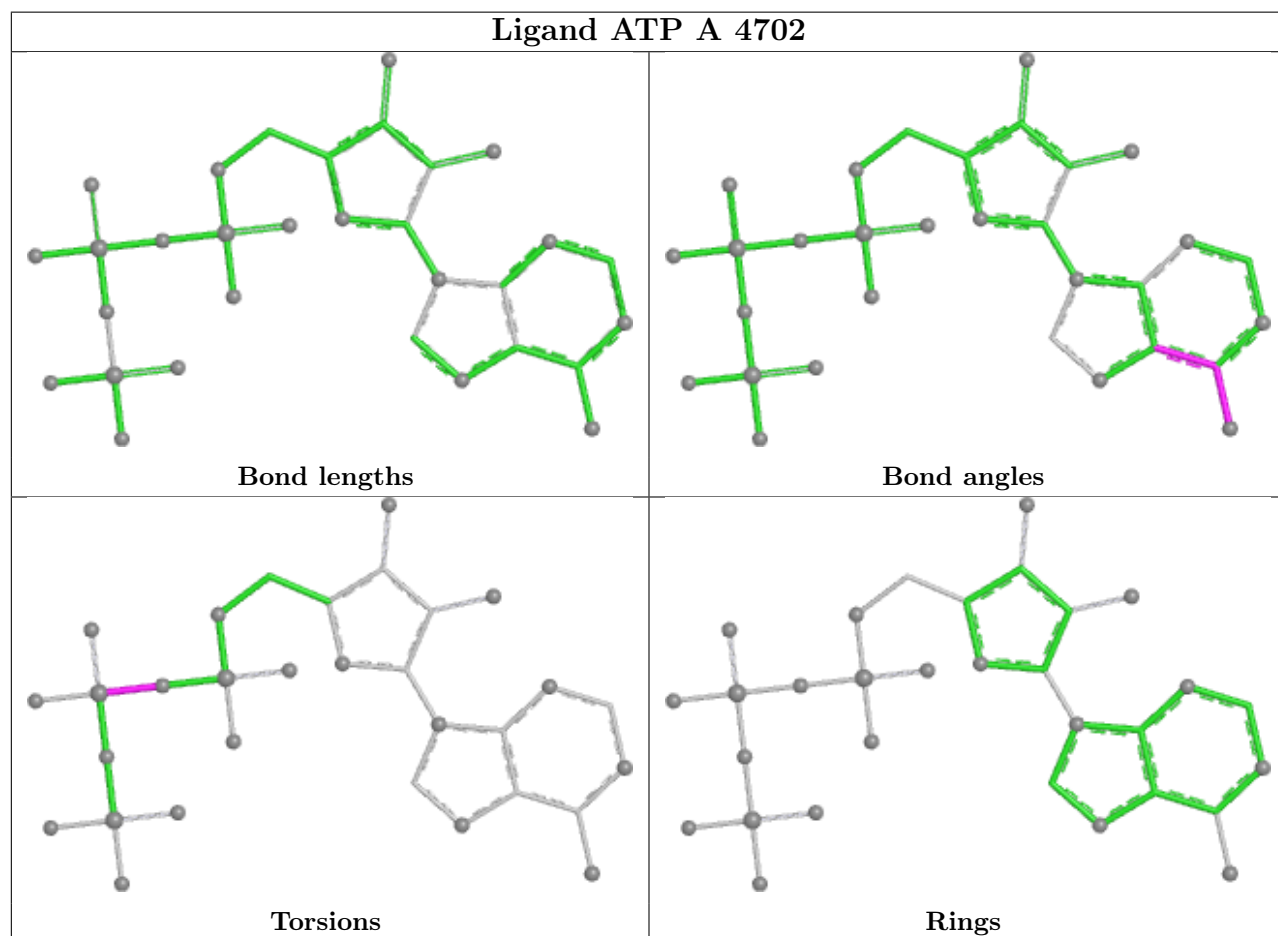
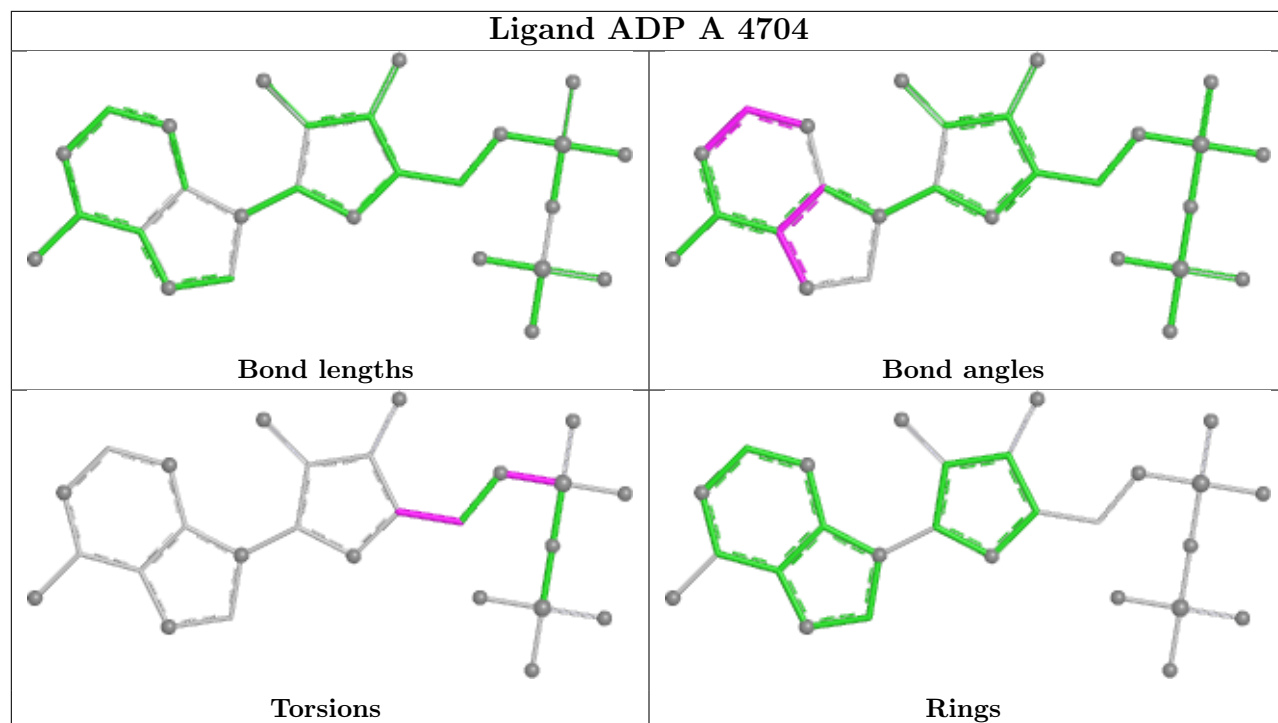
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	2	0
2	A	4704	ADP	3	0
3	A	4702	ATP	1	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.

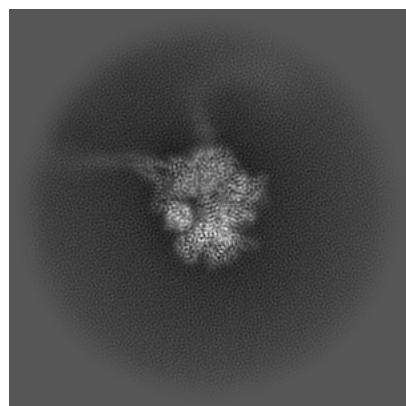
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44695. These allow visual inspection of the internal detail of the map and identification of artifacts.

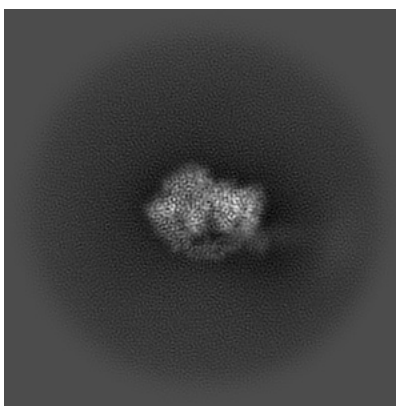
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

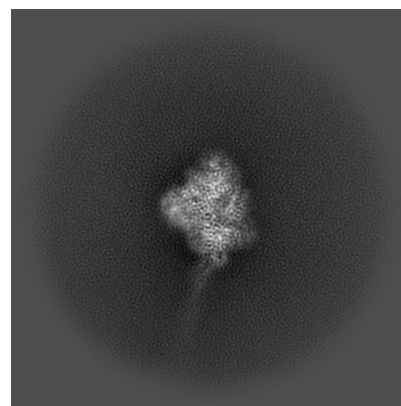
6.1.1 Primary map



X

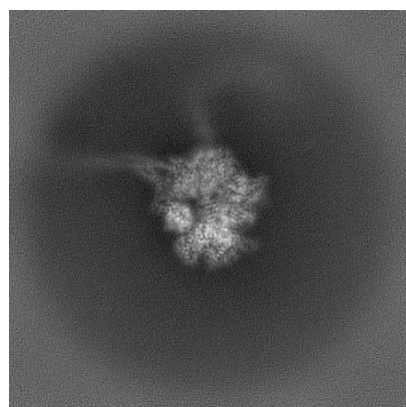


Y

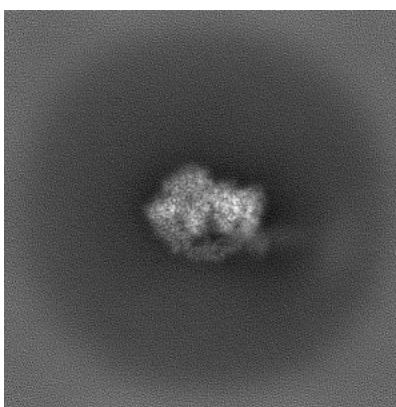


Z

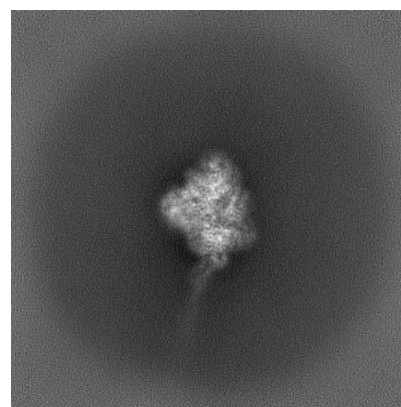
6.1.2 Raw map



X



Y

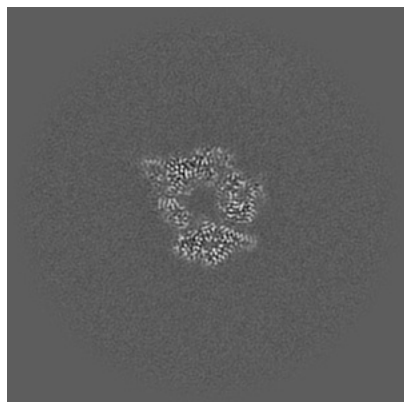


Z

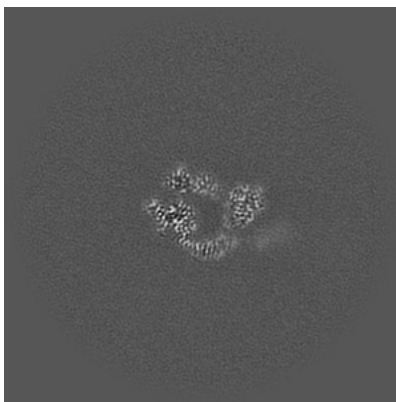
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

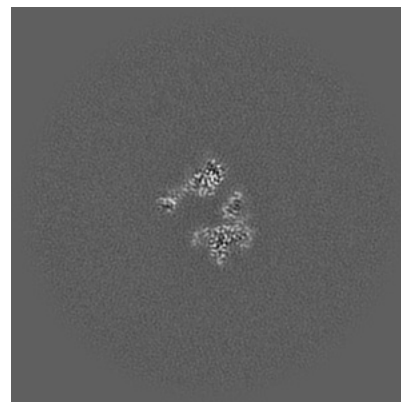
6.2.1 Primary map



X Index: 192

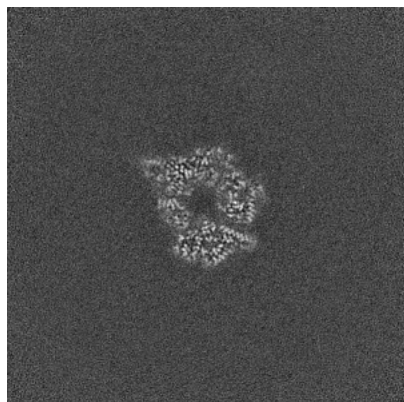


Y Index: 192

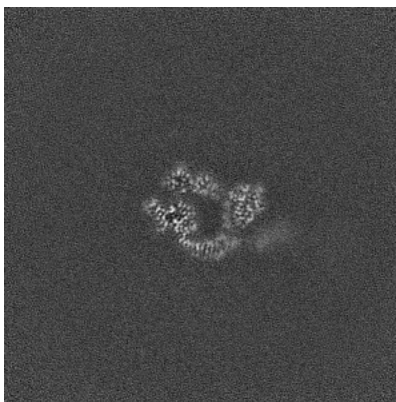


Z Index: 192

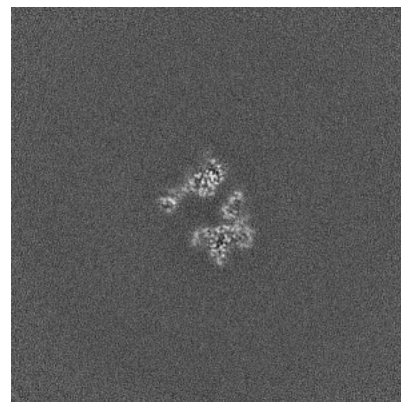
6.2.2 Raw map



X Index: 192



Y Index: 192

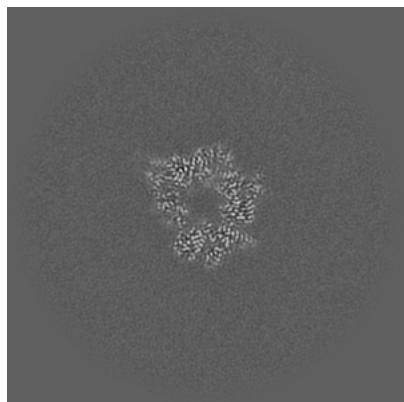


Z Index: 192

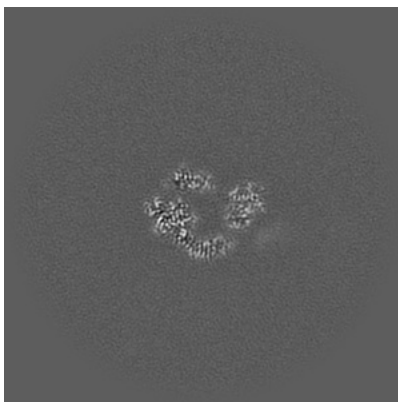
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

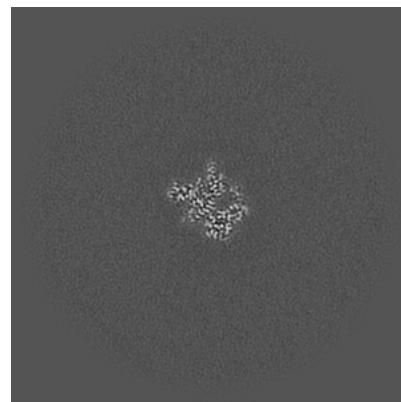
6.3.1 Primary map



X Index: 194

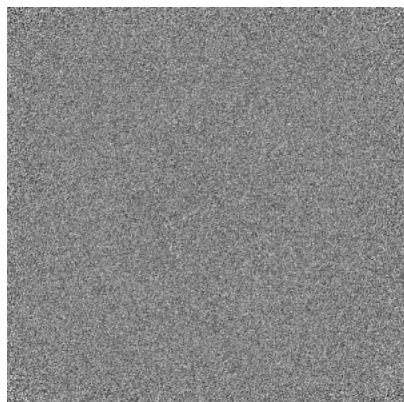


Y Index: 196

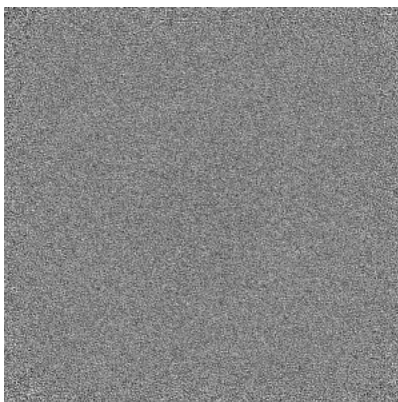


Z Index: 162

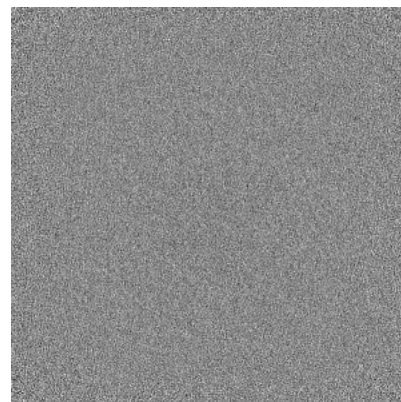
6.3.2 Raw map



X Index: 0



Y Index: 0

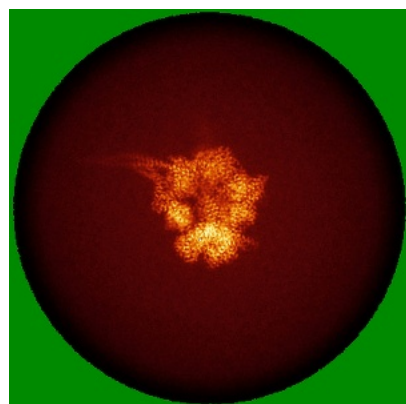


Z Index: 0

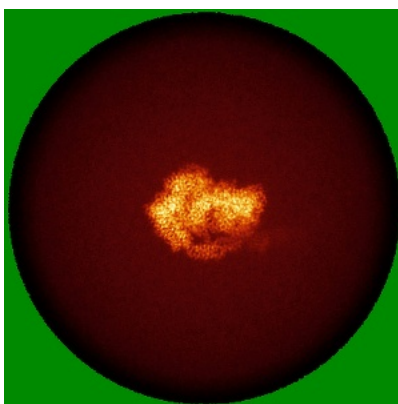
The images above show the largest variance slices of the map in three orthogonal directions.

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

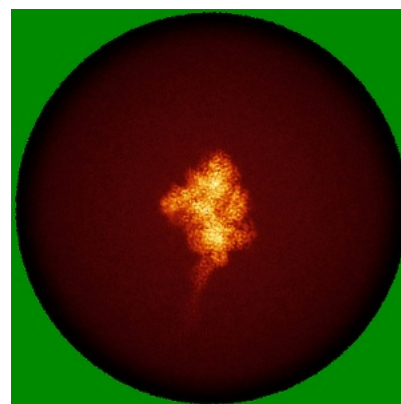
6.4.1 Primary map



X

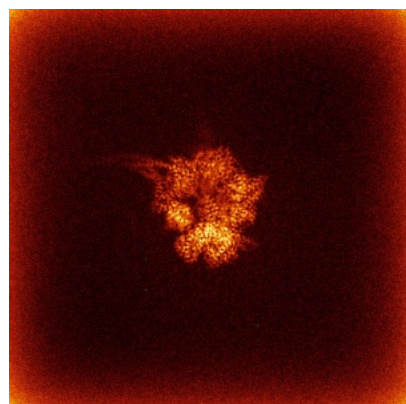


Y

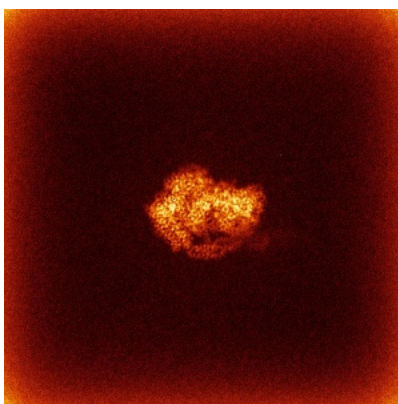


Z

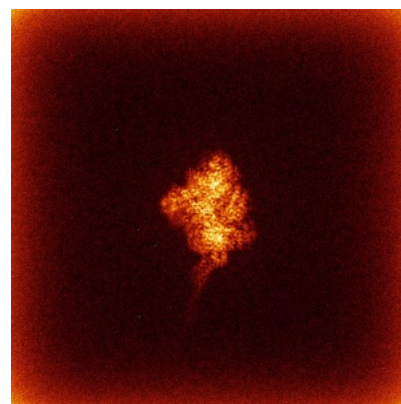
6.4.2 Raw map



X



Y

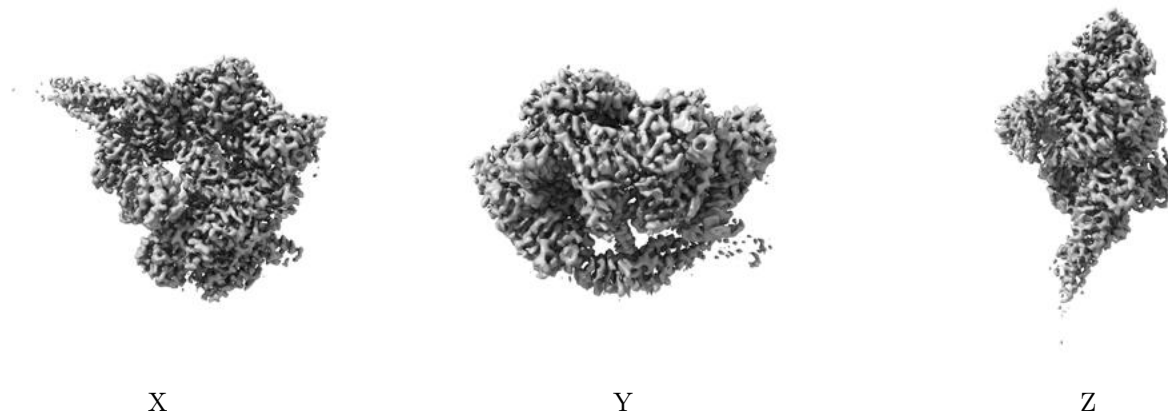


Z

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.

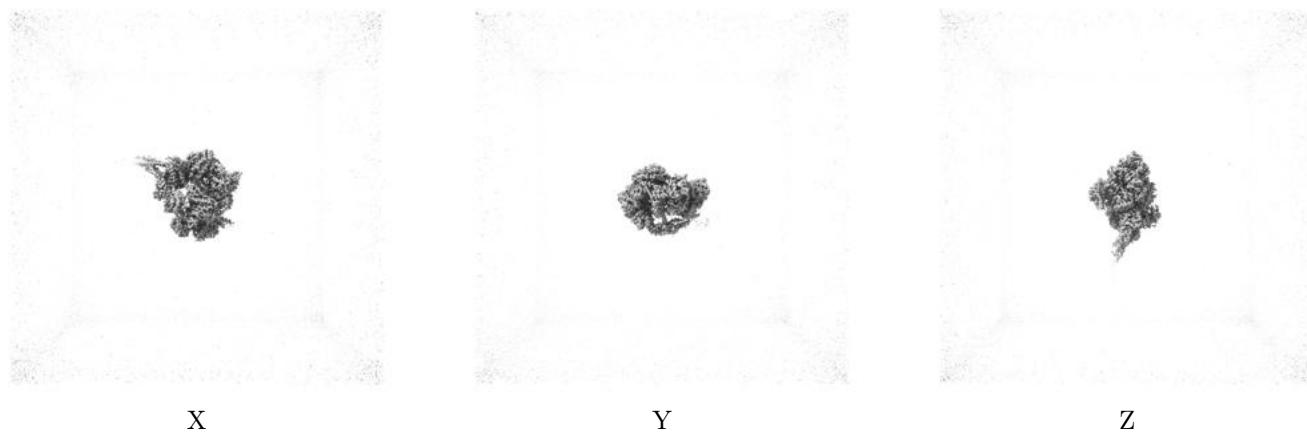
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

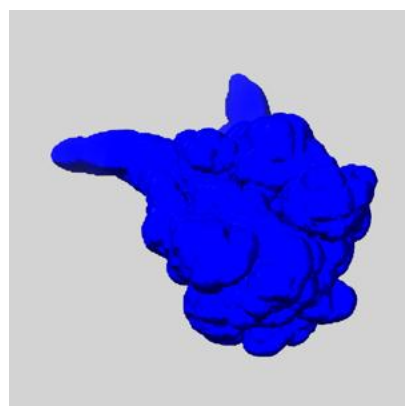
6.6 Mask visualisation [i](#)

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

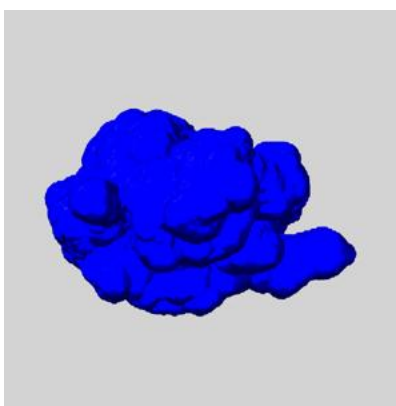
A mask typically either:

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

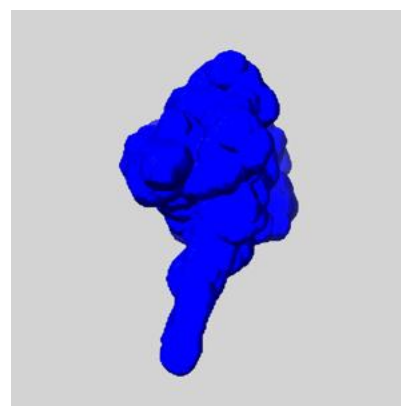
6.6.1 emd_44695_msk_1.map [i](#)



X



Y

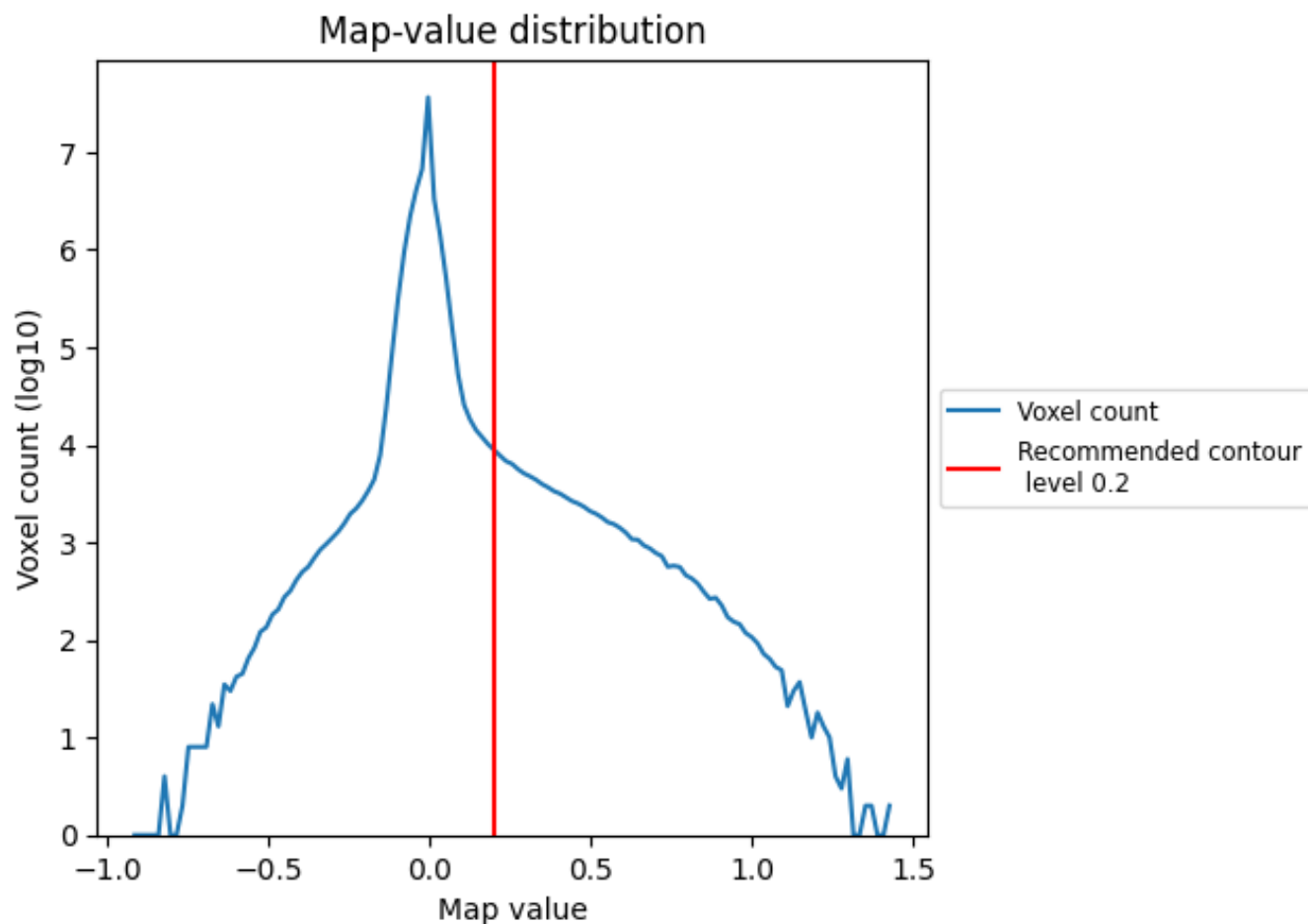


Z

7 Map analysis [i](#)

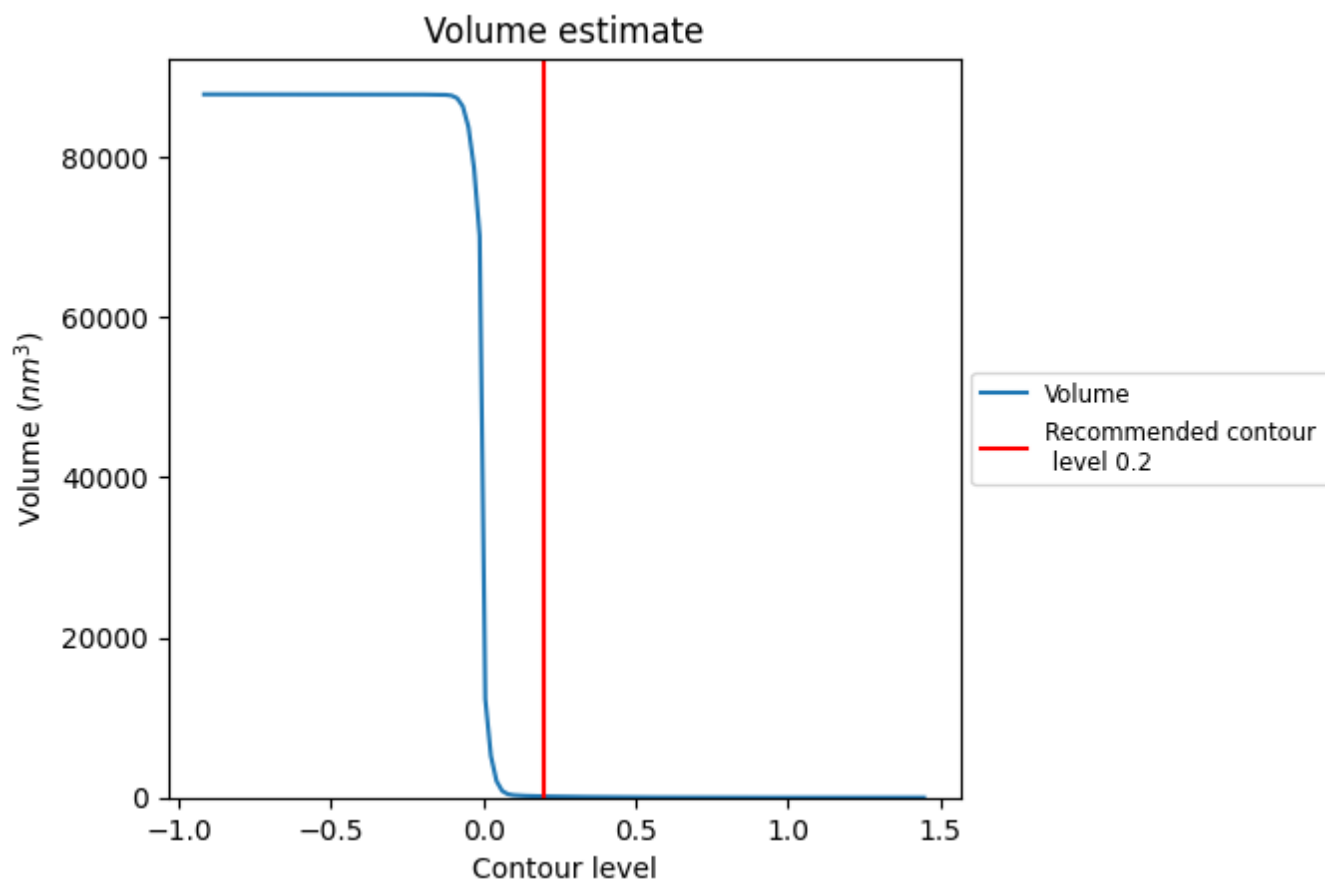
This section contains the results of statistical analysis of the map.

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.

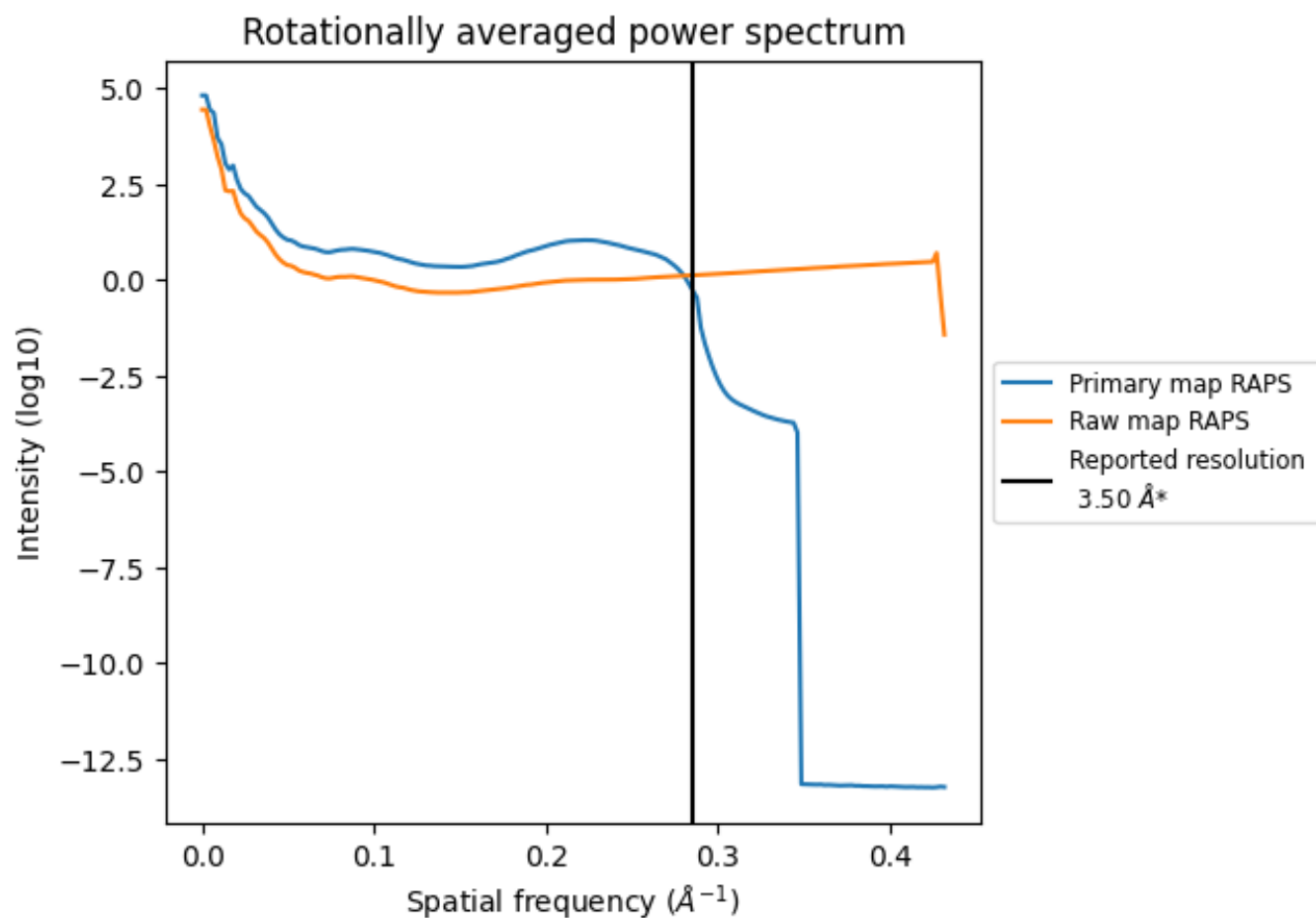
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 150 nm³; this corresponds to an approximate mass of 135 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 ⓘ

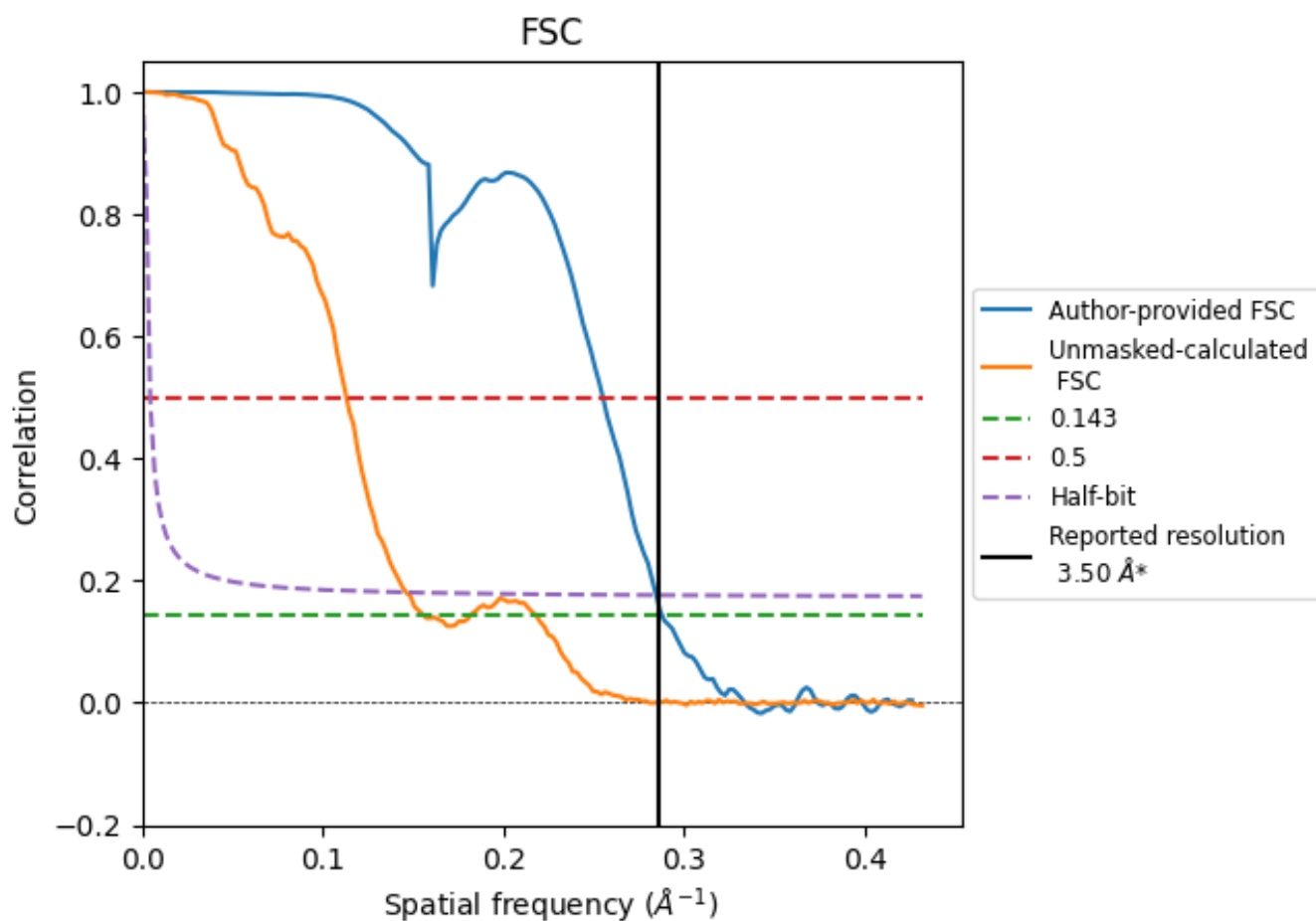


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 \AA^{-1}

8.2 Resolution estimates [i](#)

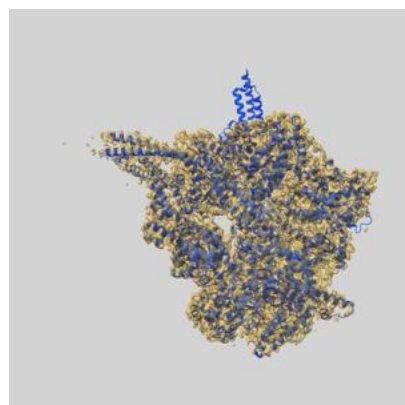
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.47	3.92	3.51
Unmasked-calculated*	6.41	8.83	6.84

*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 6.41 differs from the reported value 3.5 by more than 10 %

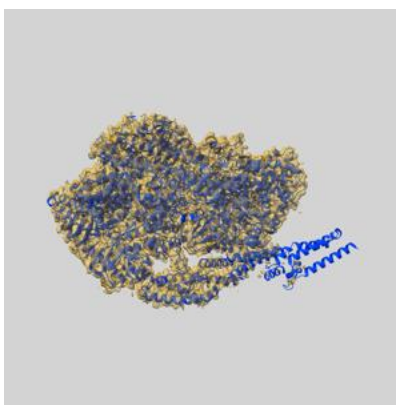
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44695 and PDB model 9BMC. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

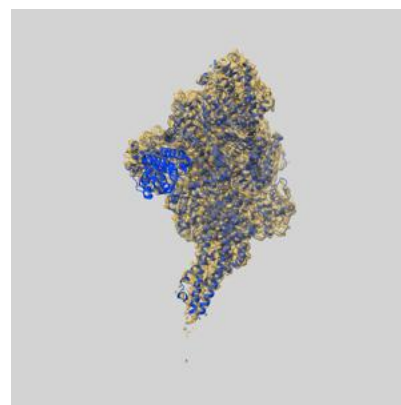
9.1 Map-model overlay [i](#)



X



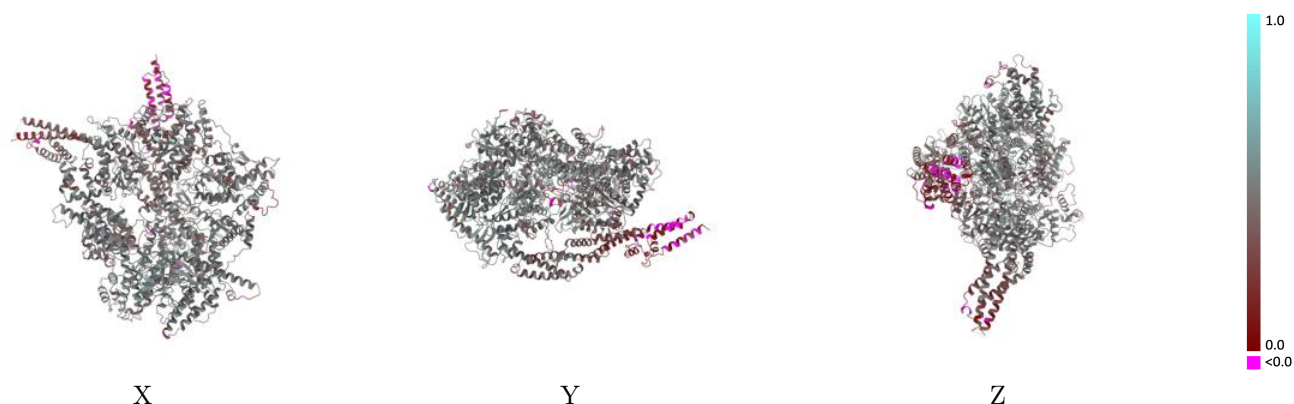
Y



Z

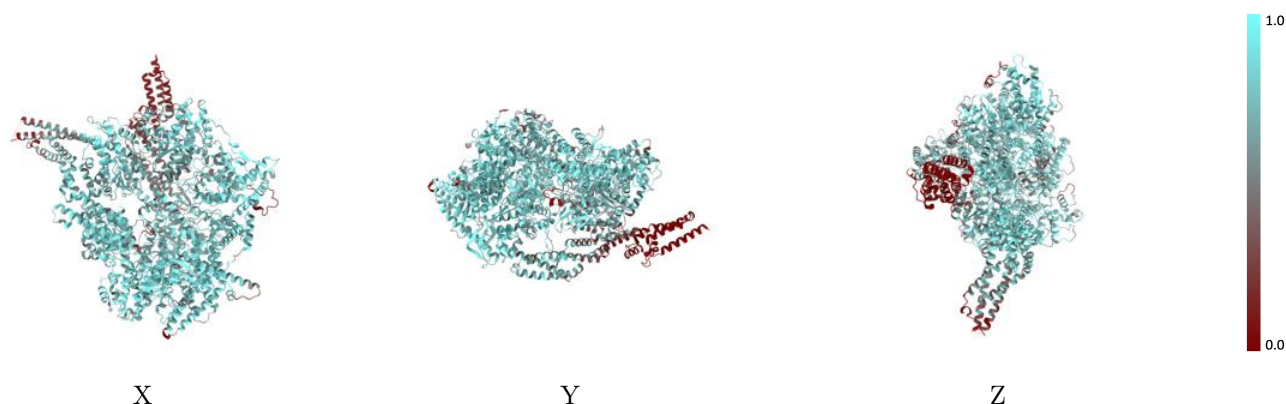
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



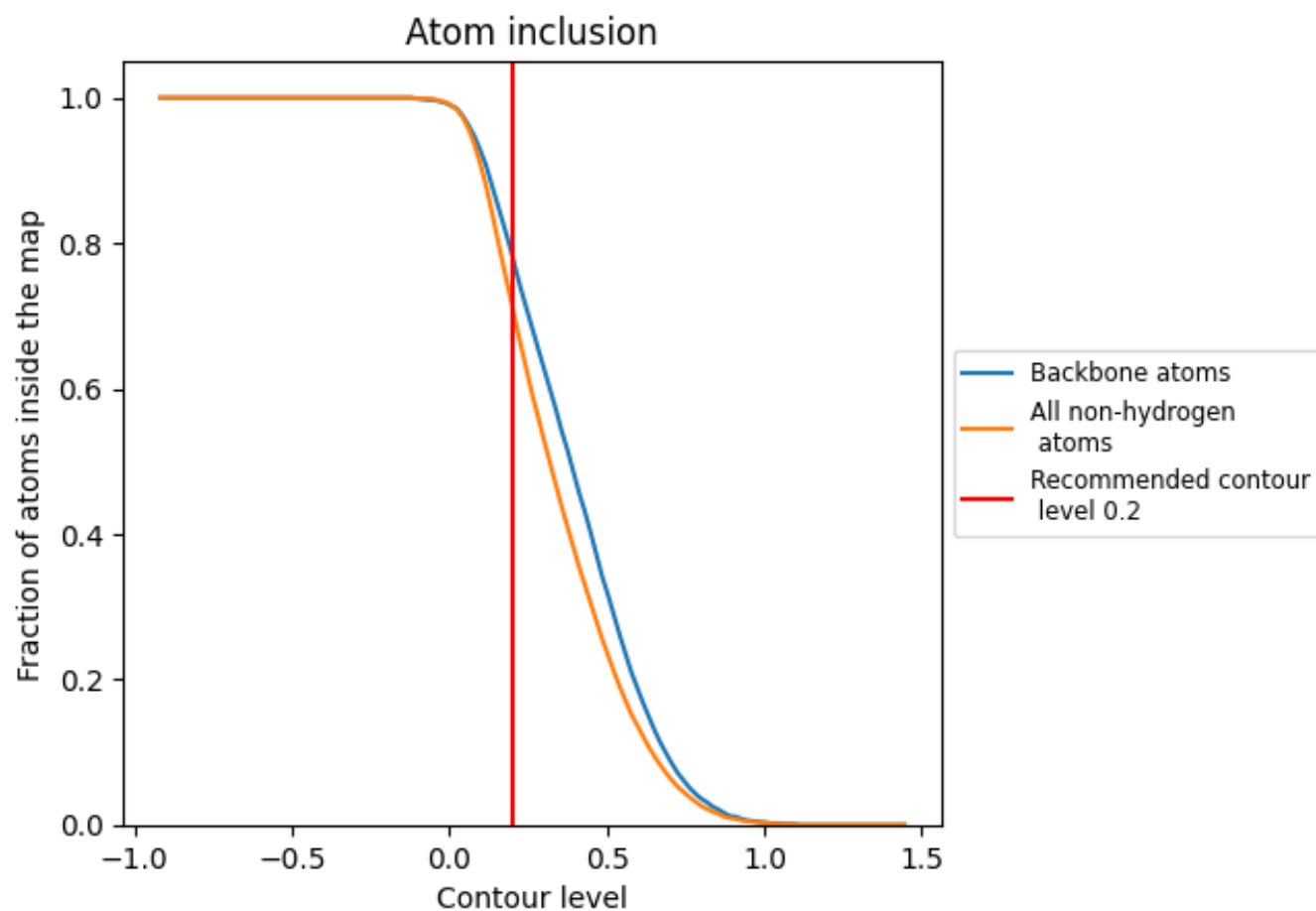
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 71% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7140	<div></div> 0.4420
A	<div></div> 0.7140	<div></div> 0.4420

