



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 01:15 AM UTC

PDB ID : 9BMD / pdb_00009bmd
EMDB ID : EMD-44696
Title : Motor domain from full-length human dynein-1 bound to microtubules in 5mM
AMPPNP condition
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 2.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

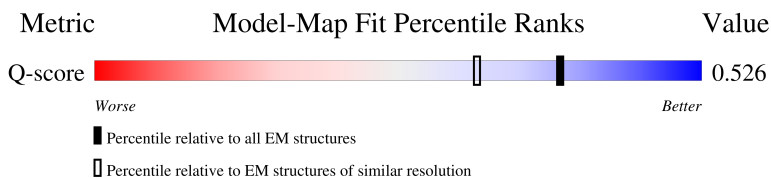
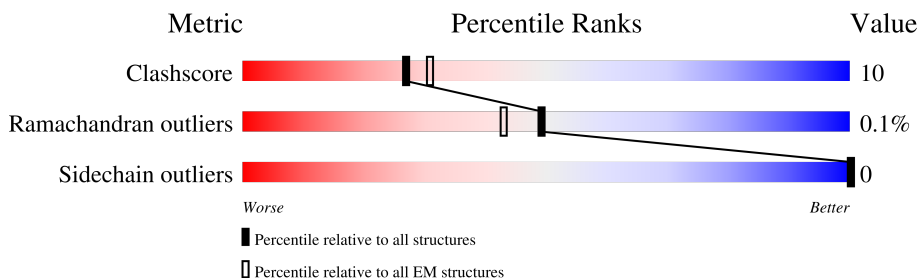
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	<p>21% (red), 49% (green), 17% (yellow), 35% (grey)</p>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 24603 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	3038	24479	15591	4228	4538	122	1	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

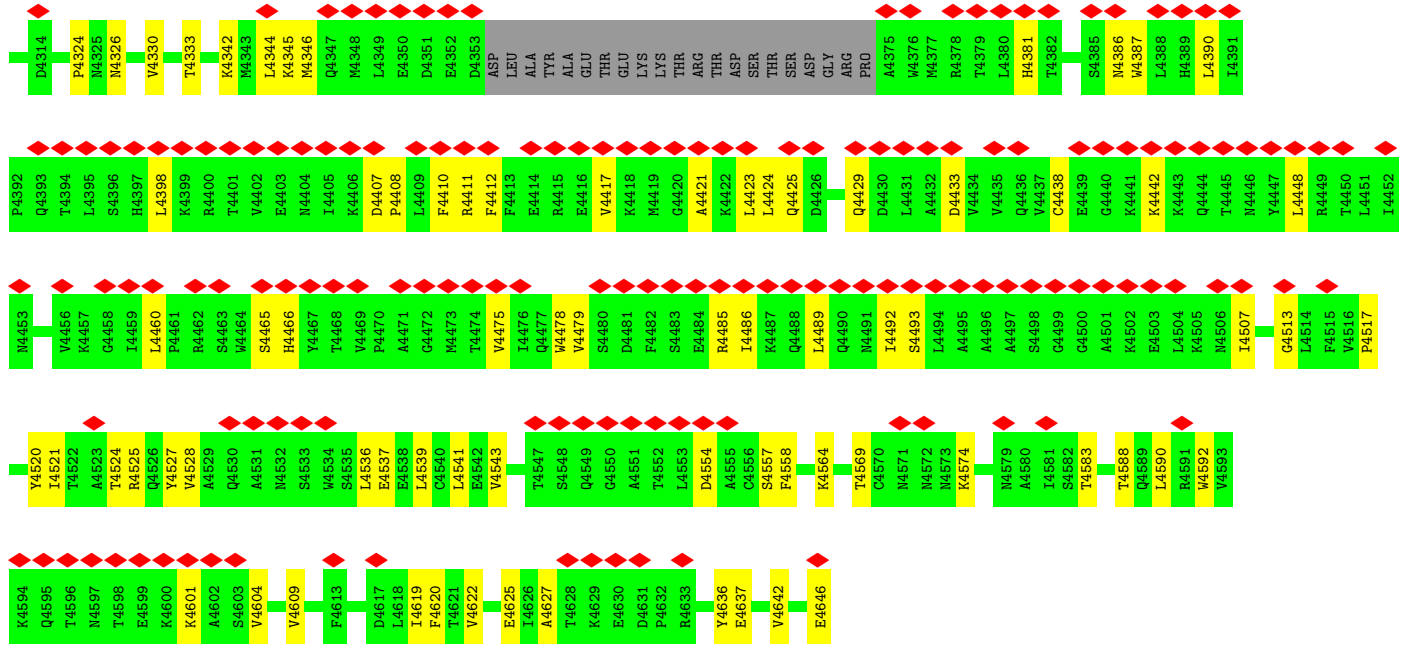
- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

L2090	S2162	L2244	S2334	A2409	R2485	H2560	N2667	D2787	V2884	T2961	Q3032	K3113
L2093	D2163	E2245	L2335	S2410	L2486	K2561	L2668	D2788	D2885	K2962	C3033	D3114
K2094	V2168	E2248	R2340	P2411	R2487	A2564	M2671	T2788	Q2886	V2963	K3034	L3115
L2097	Q2169	E2248	T2341	M2412	R2488	E2564	K2672	R2787	E2887	H2964	E3035	E3116
V2103	Y2170	S2260	F2342	Q2413	V2493	P2565	K2673	E2796	E2888	R2965	G3036	K3117
K2104	H2171	K2261	M2343	Q2414	L2494	D2566	Y2574	M2799	L2889	K2966	A3037	F3118
R2105	R2172	D2262	E2344	I2415	V2495	T2571	G2675	T2800	L2889	Y2967	G3038	N3119
E2106	G2173	T2267	Q2345	R2416	L2498	T2574	R2684	W2802	A2895	T2968	K3039	I3121
R2107	E2174	L2268	Q2346	R2417	L2499	T2577	T2695	E2808	R2896	T2968	E3040	I3122
T2108	M2175	L2268	D2347	A2419	L2502	H2577	D2697	E2809	L2897	E2970	G3041	F3123
Q2109	R2179	D2269	A2351	A2420	S2503	L2581	D2697	R2811	K2898	V2971	L3042	D3124
K2110	E2180	P2270	T2352	T2428	Q2504	Q2505	V2701	E2814	F2900	D2971	M3043	Y3125
T2111	E2181	N2271	L2353	S2429	D2505	R2507	F2708	T2815	Y2901	F2972	L3044	K3126
K2112	E2188	T2272	L2383	N2430	R2507	K2589	E2587	L2816	E2902	D2973	S3045	F3127
R2113	E2188	R2273	S2357	V2433	L2508	P2590	K2589	R2816	E2902	E2974	K3046	U3128
E2114	L2191	E2274	R2358	T2434	K2509	L2591	C2712	R2823	E2903	E2974	H3047	D3131
K2115	T2192	W2275	C2359	Q2434	L2510	V2592	P2714	R2828	E2904	D2975	E3048	K3132
E2116	D2195	T2276	G2360	T2437	R2511	V2592	P2714	E2829	L2905	R2982	E3048	K3133
E2117	E2196	D2277	M2361	E2438	A2512	E2513	P2718	A2829	D2906	K2986	K3052	F3134
R2118	E2197	G2278	V2362	H2439	E2513	L2514	R2719	R2836	V2907	K2989	Q3057	I3135
G2119	E2197	G2278	W2363	A2440	E2515	L2514	R2720	R2836	V2910	K2989	Q3057	F3136
E2120	M2202	H2282	D2367	F2441	G2515	L2605	L2723	D2840	V2910	D2985	R3060	R3140
A2121	W2204	R2285	V2368	Q2442	E2516	E2516	L2612	E2841	E2914	E2985	R3060	E3141
V2122	V2204	R2285	L2369	L2443	L2517	P2613	R2726	E2841	E2915	E2987	N3061	A3142
D2123	E2205	I2288	S2370	E2444	R2518	D2614	F2727	R2844	H2918	N2988	V3064	I3143
E2124	K2206	D2289	T2371	H2445	R2519	M2615	L2728	W2845	V2919	V2989	V3066	V3144
G2125	V2207	S2290	D2372	L2446	R2520	M2615	L2728	T2846	L2920	V2989	F3066	V3148
E2126	L2208	S2290	L2374	M2447	I2521	E2616	V2731	D2847	E2922	D3001	T3067	M3068
E2127	Q2210	W2291	L2374	D2448	T2522	L2620	P2732	E2848	R2922	S3002	N3069	N3070
T2127	L2210	R2292	L2382	L2449	T2523	L2620	P2733	E2848	I2924	G3003	P3070	SER
A2128	Q2212	G2293	T2386	T2450	V2524	E2629	V2734	D2851	R2924	F3004	SER	SER
E2129	T2214	E2294	P2386	R2452	V2524	E2629	V2734	D2851	Q2928	L3005	GLY	GLY
N2130	Q2215	L2295	L2387	R2453	P2527	K2633	L2747	L2854	P2929	E3006	LEU	LEU
L2131	N2217	Q2297	D2388	C2454	T2528	P2634	Y2748	K2855	D2949	R3007	LYS	LYS
F2132	N2217	K2297	E2389	S2460	A2529	P2636	G2749	H2855	M2950	M3008	ASP	ASP
E2133	H2218	D2306	E2389	A2465	W2531	H2637	T2750	P2858	P2859	N3009	ARG	ARG
Q2134	G2219	D2306	E2391	C2466	T2532	R2642	R2757	P2859	W2860	T3010	ALA	ALA
E2135	L2220	P2309	D2392	R2467	I2533	R2643	L2758	W2861	L2860	L3011	A3080	A3080
L2136	M2221	E2313	E2393	N2468	T2534	T2644	L2759	D2862	D2862	L3012	T3081	T3081
L2137	V2223	W2314	A2394	Q2471	I2535	T2644	T2759	D2862	R2863	A3013	S3082	S3082
Q2139	G2223	N2314	A2394	Y2472	L2541	P2645	P2760	R2863	R2863	N3014	S3082	S3082
S2140	G2227	W2314	Q2395	N2473	S2542	N2648	P2760	R2863	R2863	G3015	R3088	R3088
V2141	K2230	L2319	R2396	A2474	G2543	V2648	R2763	E2864	E2864	E3016	C3088	C3088
K2148	S2231	D2320	R2397	A2474	G2543	V2648	R2763	E2864	E2864	E3016	C3088	C3088
L2149	M2232	D2321	R2398	N2475	E2544	V2648	R2763	A2866	A2866	V3017	R3088	R3088
W2150	M2232	D2321	R2398	H2476	W2545	V2648	R2763	A2866	A2866	V3017	R3088	R3088
A2151	A2233	K2322	K2399	P2477	E2545	V2648	R2763	A2866	A2866	P3018	V3090	V3090
E2152	R2286	L2324	G2400	D2478	W2545	V2648	R2763	A2866	A2866	G3019	N3092	N3092
D2153	V2236	L2325	G2400	D2478	W2545	V2648	R2763	A2866	A2866	W3019	W3093	W3093
T2154	V2236	L2325	G2400	D2478	W2545	V2648	R2763	A2866	A2866	L3020	F3021	F3021
P2155	E2242	T2327	E2402	F2479	Q2554	K2657	L2655	L2877	L2877	G3022	F3021	F3021
L2156	R2243	L2327	E2402	P2480	E2556	K2657	G2656	L2877	L2877	G3023	Y3103	Y3103
L2157	R2243	P2328	E2404	M2481	E2557	K2657	G2656	L2877	L2877	D3024	E3108	E3108
L2160	G2330	N2329	G2406	Q2482	E2558	K2657	G2656	L2877	L2877	E3025	E3108	E3108
L2161	E2331	G2330	E2407	I2483	E2558	K2657	G2656	L2877	L2877	Y3026	K3112	K3112
	R2332	E2331	E2407	I2483	E2558	K2657	G2656	L2877	L2877	A3027		
	L2333	E2331	E2407	I2483	E2558	K2657	G2656	L2877	L2877	T3028		
										L3029		
										W3030		
										T3031		

D4224	Q4108	K3946	M3875	L3770	R3682	D3591	Q3499	ASP	TYR	LEU	GLU	ILE	ASP
D4225	L4109	D3946	L3876	E3771	T3685	F3692	M3500	LEU	GLU	ALA	ILE	LEU	LEU
T4226	E4110	L3947	H3877	M3772	V3686	S3593	I3503	ALA	VAL	GLU	GLN	GLN	GLU
A4227	K4111	L3948	Q3878	L3773	T3696	G3594	L3508	SER	ASN	SER	GLN	GLN	SER
K4228	K4112	A3949	D3879	K3774	E3687	Q3595	L3509	ILE	ARG	ILE	CYS	HIS	LEU
G4229	L4113	K3950	L3886	R3775	D3691	I3600	S3510	ALA	ALA	LEU	LEU	LEU	LEU
R4230	H4114	V3951	L3887	R3776	C3692	L3692	F3520	TYR	SER	LEU	LEU	LEU	LEU
Q4231	S4115	Q3952	A3888	A3777	C3693	M3601	D3521	LYS	ALA	LEU	LEU	LEU	LEU
M4232	L4116	A3953	R3889	A3778	S3694	R3602	Q3522	GLU	CYS	GLY	GLU	VAL	VAL
D4236	Q4117	D3954	K3891	E3779	R3695	E3603	Q3523	GLU	PRO	GLU	SER	ILE	ALA
H4119	P4118	E3955	L3886	R3782	V3604	K3605	M3524	VAL	MET	THR	THR	ALA	ASP
A1120	H4119	Q3956	L3887	E3785	M3700	K3605	D3524	LEU	LYS	ASP	ASP	LYS	LYS
A4242	A4061	F3957	L3888	E3786	S3706	H3534	T3211	ILE	TRP	TRP	GLN	GLN	LYS
A4248	Q4062	G3958	A3888	E3787	S3707	H3535	V3212	SER	ALA	LYS	LYS	MET	LYS
I4251	M4063	R3959	R3889	T3787	L3708	L3536	D3213	SER	GLN	GLN	SER	SER	SER
F4252	T4064	I3962	D3901	D3788	V3716	Q3538	Q3214	VAL	ALA	ILE	VAL	VAL	VAL
G4253	Q4065	D3962	D3902	M3791	D3723	A3539	V3215	ARG	GLN	ARG	GLN	GLN	GLN
E4259	T4066	P3866	A3903	Q3792	V3724	R3540	E3216	ILE	LEU	ILE	ASP	ASP	ASP
T4267	S4068	T3969	Q3906	E3794	E3726	I3541	E3217	ALA	TYR	ILE	LEU	ASP	ASP
K4133	A4070	Y3972	L3909	T3796	D3730	T3545	L3218	ARG	ASP	ARG	LYS	LYS	LYS
M4137	L4071	L3973	R3910	T3796	D3730	D3546	R3219	LEU	MET	GLU	VAL	VAL	VAL
L4138	G4072	W3974	G3911	V3797	F3738	A3548	R3220	ALA	LEU	ASN	PRO	PRO	PRO
F4145	S4073	S3975	N3912	Y3801	Q3739	R3549	R3221	VAL	LEU	ALA	VAL	VAL	VAL
F4146	A4074	E3976	E3913	Y3809	L3740	T3550	LEU	VAL	PRO	THR	THR	THR	THR
F4147	E4075	E3977	I3914	S3809	R3643	E3551	ARG	ILE	PRO	ILE	ILE	ILE	ILE
F4127	G4076	R3978	V3915	S3817	V3644	Y3552	LYS	GLN	ARG	VAL	VAL	VAL	VAL
E4129	F4077	P3979	L3916	S3817	L3645	L3553	GLU	ASN	ARG	ASN	GLN	GLN	GLN
I4130	N4078	A3980	L3917	Q3820	N3646	S3554	LEU	ASN	ASN	ASN	ASN	ASN	ASN
K4133	Q4079	I3981	A3918	I3821	F3647	R3474	LEU	ALA	GLY	GLY	GLY	GLY	GLY
M4137	L4079	A3995	A3919	I3829	V3648	S3475	LEU	ALA	LEU	LEU	LEU	LEU	LEU
L4138	D4081	F3996	G3919	L3835	L3649	T3476	VAL	ALA	GLU	GLU	GLU	GLU	GLU
F4145	D4082	R4000	S3920	Y3836	R3654	A3477	VAL	ALA	GLU	GLU	GLU	GLU	GLU
F4146	K4083	V4009	S3922	I3836	R3655	L3478	VAL	ALA	GLU	GLU	GLU	GLU	GLU
F4147	L4084	V4009	R3923	Y3836	R3656	L3479	VAL	ALA	GLU	GLU	GLU	GLU	GLU
C4170	M4085	V4009	I3924	V3839	R3657	K3480	VAL	ALA	GLU	GLU	GLU	GLU	GLU
K4171	T4086	N4012	I3925	P3844	G3658	K3481	VAL	ALA	GLU	GLU	GLU	GLU	GLU
S4172	V4088	L4013	Q3926	N3845	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
P4173	V4088	L4013	L3927	L3846	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
N4174	V4088	L4013	T3928	K3847	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
E4175	V4088	L4013	E3928	G3848	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
R4176	V4088	L4013	V3929	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
A4177	V4088	L4013	E3930	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
R4178	V4088	L4013	Q3931	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
S4090	V4088	L4013	A3932	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
Q4091	V4088	L4013	E3933	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
R4092	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
W4093	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
V4094	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
L4095	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
L4096	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
R4097	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
W4098	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
V4099	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
H4100	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
T4028	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
H4029	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
I4030	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
M4043	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
C4044	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
S4045	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
G4048	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
Y4049	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
D4050	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
A4051	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
H4054	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
V4055	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
A4056	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
E4057	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
L4058	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
A4059	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
A4060	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
A4061	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
Q4062	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
M4063	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
T4064	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
Q4065	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
T4066	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
S4067	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
A4068	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
A4069	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
A4070	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
L4071	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
G4072	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
S4073	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
A4074	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
E4075	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
G4076	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
F4077	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
N4078	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
Q4079	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
A4080	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
A4081	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
A4082	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
A4083	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
L4084	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
M4085	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
T4086	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
V4088	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
A4087	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
K4089	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
S4090	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
Q4091	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
R4092	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
W4093	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
L4094	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU
L4095	V4088	L4013	A3934	V3849	G3658	L3482	VAL	ALA	GLU	GLU	GLU	GLU	GLU



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	241362	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	1.441	Depositor
Minimum map value	-0.841	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	316.8, 316.8, 316.8	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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, ANP, 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	0.18	0/25000	0.33	0/33870

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	24479	0	24538	487	0
2	A	27	0	12	2	0
3	A	31	0	12	2	0
4	A	62	0	26	3	0
5	A	4	0	0	0	0
All	All	24603	0	24588	487	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 10.

All (487) 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:2598:GLY:H	4:A:4703:ANP:HNB1	1.23	0.82
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.64	0.80
1:A:2581:LEU:HD21	1:A:2605:LEU:HD23	1.68	0.75
1:A:1397:ASN:O	1:A:1401:ILE:HD12	1.91	0.70
1:A:2506:SER:HB3	1:A:2510:MET:HB2	1.71	0.70
1:A:4079:GLN:HA	1:A:4082:LYS:HE3	1.73	0.69
1:A:1898:ALA:O	1:A:1983:ARG:NH1	2.26	0.68
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.75	0.68
1:A:3691:ASP:OD1	1:A:3695:ARG:NH1	2.28	0.68
1:A:2481:MET:HE2	1:A:2486:LEU:HA	1.76	0.67
1:A:2179:ARG:NH2	1:A:2195:ASP:OD1	2.28	0.67
1:A:3474:ARG:HE	1:A:3764:ASP:HB3	1.59	0.66
1:A:3194:LEU:HD22	1:A:3500:MET:HE3	1.75	0.66
1:A:4408:PRO:HA	1:A:4411:ARG:HE	1.59	0.66
1:A:4541:LEU:HD11	1:A:4590:LEU:HB3	1.77	0.66
1:A:2148:LYS:HG2	1:A:2361:MET:HB3	1.78	0.65
1:A:1462:PHE:HB2	1:A:3628:ARG:HD2	1.79	0.65
1:A:2925:ILE:HG21	1:A:2933:LEU:HB2	1.78	0.65
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.78	0.65
1:A:4276:ARG:NH2	1:A:4279:ASP:OD2	2.30	0.65
1:A:3113:MET:HE2	1:A:3184:ALA:HA	1.78	0.65
1:A:2221:MET:HE3	1:A:2343:PHE:HD2	1.61	0.64
1:A:2925:ILE:HG13	1:A:2933:LEU:HD13	1.79	0.64
1:A:2324:LEU:HD11	1:A:2332:ARG:HB3	1.80	0.64
1:A:3820:GLN:HE21	1:A:4345:LYS:HG2	1.62	0.64
1:A:1571:ILE:HG23	1:A:1604:LEU:HD22	1.80	0.63
1:A:2382:LEU:HD23	1:A:2420:ALA:HB2	1.80	0.63
1:A:4574:LYS:HB3	1:A:4627:ALA:HB2	1.80	0.63
1:A:2320:ASP:OD1	1:A:2321:ASP:N	2.31	0.62
1:A:1688:THR:OG1	1:A:1708:GLU:OE2	2.16	0.62
1:A:3113:MET:O	1:A:3140:ARG:NH2	2.32	0.62
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.82	0.62
1:A:3871:VAL:HG12	1:A:3875:MET:HE2	1.80	0.62
1:A:3113:MET:HB3	1:A:3115:LEU:HG	1.82	0.62
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.33	0.61
1:A:4172:SER:O	1:A:4176:ARG:NH1	2.33	0.61
1:A:1417:MET:HE1	1:A:1423:ASN:HA	1.83	0.61
1:A:2149:LEU:HD11	1:A:2157:LEU:HD22	1.82	0.61
1:A:2453:ARG:NH1	1:A:2505:ASP:OD2	2.33	0.61
1:A:2889:LEU:HD13	1:A:2920:LEU:HD11	1.82	0.60
1:A:2138:ILE:HG13	1:A:2161:LEU:HD21	1.82	0.60
1:A:2385:ILE:O	1:A:2416:GLN:NE2	2.32	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3749:LEU:HD11	1:A:3770:LEU:HG	1.83	0.60
1:A:4564:LYS:HG3	1:A:4646:GLU:HB2	1.84	0.60
1:A:2290:SER:HB2	1:A:2295:LEU:HD23	1.85	0.59
1:A:4176:ARG:NH2	1:A:4224:ASP:OD1	2.30	0.59
1:A:2728:LEU:HA	1:A:2731:VAL:HG22	1.84	0.59
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	1.85	0.59
1:A:2230:LYS:NZ	1:A:2345:VAL:O	2.35	0.59
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.85	0.58
1:A:1964:GLU:HG2	1:A:1967:MET:HE2	1.85	0.58
1:A:2605:LEU:HD13	1:A:2662:PHE:HE1	1.67	0.58
1:A:3553:LEU:HB2	1:A:3578:ILE:HD13	1.85	0.58
1:A:4071:ILE:HG13	1:A:4099:VAL:HG12	1.84	0.58
1:A:1419:ARG:HD2	1:A:1445:ILE:HG23	1.86	0.58
1:A:3211:THR:HG21	1:A:3753:LEU:HD11	1.86	0.58
1:A:3488:ARG:HA	1:A:3491:LYS:HE2	1.85	0.57
1:A:2386:PRO:HG3	1:A:2413:LEU:HD22	1.85	0.57
1:A:3624:GLU:HG2	1:A:3664:LEU:HD23	1.87	0.57
1:A:2593:LEU:HD23	1:A:2734:VAL:HB	1.86	0.57
1:A:2776:PHE:HZ	1:A:2846:THR:HG23	1.69	0.57
1:A:3008:MET:HG2	1:A:3066:PHE:HZ	1.69	0.57
1:A:3886:LEU:HD11	1:A:4346:MET:HG3	1.86	0.57
1:A:2914:GLU:O	1:A:2918:HIS:ND1	2.28	0.57
1:A:4300:ILE:HG13	1:A:4301:ARG:HD3	1.85	0.57
1:A:2447:MET:HG3	1:A:2733:VAL:HG11	1.86	0.57
1:A:4193:ARG:NH2	1:A:4637:GLU:O	2.25	0.57
1:A:1961:ASN:ND2	1:A:2019:ASN:O	2.37	0.57
1:A:2968:THR:HG22	1:A:2970:GLU:H	1.70	0.57
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.86	0.56
1:A:2324:LEU:HD21	1:A:2332:ARG:HG2	1.87	0.56
1:A:3620:ARG:NH2	1:A:3642:ASP:OD2	2.39	0.56
1:A:3661:LEU:HD12	1:A:3668:ASP:HB3	1.86	0.56
1:A:3771:GLU:OE1	1:A:3774:LYS:NZ	2.34	0.56
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.87	0.56
1:A:2396:ARG:NH1	1:A:2406:GLU:OE2	2.39	0.56
1:A:4386:ASN:O	1:A:4390:LEU:HG	2.05	0.56
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.33	0.56
1:A:4175:GLU:OE1	1:A:4175:GLU:N	2.38	0.56
1:A:2472:TYR:CD1	1:A:2541:ILE:HG21	2.40	0.56
1:A:4088:VAL:HG23	1:A:4118:PRO:HA	1.88	0.56
1:A:1374:PRO:HD2	1:A:1377:LEU:HD12	1.88	0.55
1:A:2188:GLU:OE1	1:A:2243:ARG:NH1	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2694:ARG:HG3	1:A:2701:VAL:HG21	1.87	0.55
1:A:3931:GLN:O	1:A:3935:VAL:HG23	2.06	0.55
1:A:3889:ARG:HH12	1:A:3909:LEU:HD11	1.71	0.55
1:A:3879:ASP:OD1	1:A:4342:LYS:NZ	2.35	0.55
1:A:2511:ARG:HD3	1:A:2535:ILE:HD13	1.87	0.55
1:A:4424:LEU:HD13	1:A:4486:ILE:HG13	1.89	0.55
1:A:1510:SER:HB2	1:A:3629:PHE:HB3	1.87	0.55
1:A:1925:ARG:HG2	1:A:1954:TRP:CD1	2.42	0.55
1:A:1545:VAL:O	1:A:1548:GLU:HG3	2.06	0.55
1:A:1947:GLY:O	1:A:1951:VAL:HG12	2.07	0.55
1:A:4527:TYR:CD2	1:A:4558:PHE:HZ	2.25	0.55
1:A:2075:LEU:HD11	1:A:4536:LEU:HD22	1.88	0.54
1:A:2965:ARG:HG3	1:A:2966:LYS:HD2	1.89	0.54
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.89	0.54
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.87	0.54
1:A:2192:THR:HB	1:A:2373:MET:HG2	1.89	0.54
1:A:2075:LEU:HD11	1:A:4536:LEU:CD2	2.38	0.54
1:A:2081:SER:O	1:A:2083:GLN:HG2	2.08	0.54
1:A:3716:VAL:HG23	1:A:3836:TYR:OH	2.06	0.54
1:A:4271:ARG:NH1	1:A:4284:LEU:O	2.38	0.54
1:A:2374:ILE:HD13	1:A:2452:LEU:HD21	1.89	0.54
1:A:2851:ASP:OD1	1:A:2867:MET:HG2	2.08	0.54
1:A:2557:VAL:O	1:A:2757:ARG:NH2	2.39	0.54
1:A:4398:LEU:HG	1:A:4417:VAL:HG21	1.90	0.54
1:A:2718:PRO:HG2	1:A:3082:SER:HA	1.90	0.54
1:A:3551:GLU:HG3	1:A:3559:ARG:NH1	2.23	0.54
1:A:4465:SER:OG	1:A:4478:TRP:NE1	2.41	0.54
1:A:1765:ALA:O	1:A:1769:MET:HG3	2.08	0.53
1:A:4525:ARG:HE	1:A:4539:LEU:HB2	1.73	0.53
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.89	0.53
1:A:2309:PRO:HB3	1:A:2352:THR:HG23	1.90	0.53
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.89	0.53
1:A:2823:ARG:HH12	1:A:2868:SER:H	1.56	0.53
1:A:3499:GLN:O	1:A:3503:ILE:HG13	2.08	0.53
1:A:3835:ILE:HG23	1:A:3866:VAL:HG12	1.90	0.53
1:A:2591:LEU:HA	1:A:2732:PRO:HD2	1.91	0.53
1:A:2910:VAL:HG22	1:A:3108:GLU:HG2	1.90	0.53
1:A:3088:ARG:NH1	4:A:4703:ANP:O1G	2.42	0.53
1:A:3644:VAL:HG22	1:A:3664:LEU:HD12	1.91	0.53
1:A:3659:ARG:HG3	1:A:3661:LEU:HD21	1.90	0.53
1:A:2218:HIS:HA	1:A:2340:ARG:HD3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1632:VAL:HG12	1:A:1656:LYS:HD2	1.90	0.53
1:A:2104:LYS:HA	1:A:2136:ILE:HD13	1.89	0.53
1:A:2154:ILE:N	1:A:2155:PRO:HD2	2.24	0.53
1:A:2248:GLU:HG2	1:A:2297:LYS:NZ	2.23	0.53
1:A:2936:ILE:HG23	1:A:3093:TRP:HE3	1.73	0.53
1:A:3891:LYS:HD2	1:A:4013:LEU:HD23	1.91	0.53
1:A:1755:GLN:HG3	1:A:1814:GLU:OE2	2.09	0.52
1:A:2747:ILE:O	1:A:2750:THR:OG1	2.27	0.52
1:A:1457:MET:HE2	1:A:3659:ARG:HB3	1.90	0.52
1:A:3194:LEU:HD11	1:A:3499:GLN:HB2	1.89	0.52
1:A:2060:ARG:HG3	1:A:2061:THR:HG23	1.92	0.52
1:A:2446:ILE:HD11	1:A:2714:PRO:HB3	1.91	0.52
1:A:2156:LEU:O	1:A:2160:LEU:HG	2.09	0.52
1:A:2896:ARG:HG3	1:A:2953:MET:HE3	1.92	0.52
1:A:2488:ARG:HH21	1:A:2543:GLY:H	1.57	0.52
1:A:3835:ILE:HG12	1:A:3870:ARG:HG3	1.91	0.52
1:A:2080:LEU:HD12	1:A:2088:PHE:CZ	2.44	0.52
1:A:3593:SER:O	1:A:3682:ARG:NH2	2.43	0.52
1:A:2449:LEU:HD11	1:A:2454:CYS:SG	2.49	0.52
1:A:2797:ARG:NH1	4:A:4703:ANP:O1G	2.36	0.52
1:A:2053:MET:HE1	1:A:2094:LYS:HB3	1.91	0.51
1:A:3581:LYS:NZ	1:A:3582:ARG:HH11	2.06	0.51
1:A:3762:ASP:OD1	1:A:3763:ASP:N	2.43	0.51
1:A:4574:LYS:HE2	1:A:4625:GLU:HG2	1.91	0.51
1:A:1360:ARG:NH2	1:A:2899:VAL:HG22	2.26	0.51
1:A:1825:LEU:HA	1:A:1830:ILE:HD13	1.92	0.51
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.75	0.51
1:A:1882:THR:HG22	1:A:2048:LEU:HD23	1.92	0.51
1:A:1420:LEU:HD13	1:A:1437:VAL:HG11	1.93	0.51
1:A:4520:TYR:O	1:A:4524:THR:HG23	2.10	0.51
1:A:2065:LEU:HD11	1:A:2133:GLU:HB3	1.91	0.51
1:A:3131:ASP:OD1	1:A:3132:LYS:N	2.44	0.51
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.40	0.51
1:A:1513:TYR:CZ	1:A:1517:GLU:HG2	2.45	0.51
1:A:2072:PHE:HE2	1:A:2141:VAL:HG11	1.75	0.51
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.92	0.51
1:A:3561:ARG:NH1	1:A:3603:GLU:OE1	2.44	0.51
1:A:2644:THR:OG1	1:A:2647:GLY:O	2.26	0.50
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.93	0.50
1:A:3679:LEU:HD12	1:A:3696:VAL:HG11	1.93	0.50
1:A:3143:ILE:HD13	1:A:3541:ILE:HD13	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4071:ILE:HD11	1:A:4096:LEU:HD22	1.93	0.50
1:A:2666:ILE:HB	1:A:2712:CYS:SG	2.52	0.50
1:A:3044:LEU:HD22	1:A:3049:GLU:HG2	1.93	0.50
1:A:2808:GLU:OE1	1:A:2811:ARG:NH2	2.43	0.50
1:A:4342:LYS:O	1:A:4346:MET:HG2	2.12	0.50
1:A:3133:LEU:HD21	1:A:3137:PRO:HB3	1.93	0.50
1:A:3024:ASP:O	1:A:3028:THR:HG23	2.12	0.50
1:A:4460:LEU:HA	1:A:4475:VAL:HG22	1.93	0.50
1:A:1425:VAL:HB	1:A:1428:GLU:HB2	1.94	0.50
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.46	0.50
1:A:3191:ARG:O	1:A:3195:GLU:HG3	2.12	0.50
1:A:4045:SER:HB3	1:A:4049:TYR:HB3	1.93	0.50
1:A:4398:LEU:HD21	1:A:4493:SER:HA	1.93	0.50
1:A:4099:VAL:HG21	1:A:4126:LEU:HB3	1.94	0.50
1:A:4442:LYS:HE2	1:A:4448:LEU:HD11	1.94	0.50
1:A:4601:LYS:HB2	1:A:4604:VAL:HG23	1.93	0.50
1:A:1339:VAL:HG11	1:A:1370:LEU:HD21	1.94	0.49
1:A:2179:ARG:HD3	1:A:2208:LEU:HD11	1.94	0.49
1:A:2434:THR:O	1:A:2438:GLU:HG2	2.12	0.49
1:A:1964:GLU:OE2	1:A:1966:ARG:NH1	2.45	0.49
1:A:2787:ASP:OD1	1:A:2788:THR:N	2.45	0.49
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.93	0.49
1:A:3127:PRO:HG3	1:A:3538:GLN:HB3	1.94	0.49
1:A:3551:GLU:HG3	1:A:3559:ARG:HH12	1.77	0.49
1:A:2495:VAL:HG21	1:A:2524:VAL:HG11	1.95	0.49
1:A:1751:VAL:HG11	1:A:1878:LYS:HD2	1.94	0.49
1:A:2527:PRO:HD3	1:A:2545:TRP:CE2	2.48	0.49
1:A:3591:ASP:OD2	1:A:3596:ALA:HB3	2.12	0.49
1:A:2209:GLN:O	1:A:2212:GLN:HG2	2.13	0.49
1:A:3194:LEU:HD13	1:A:3500:MET:HE2	1.94	0.49
1:A:4288:VAL:HG21	1:A:4294:ILE:HG13	1.94	0.49
1:A:3597:THR:O	1:A:3601:MET:HG2	2.13	0.49
1:A:2919:VAL:HG13	1:A:2950:VAL:HG22	1.94	0.49
1:A:3767:ILE:HA	1:A:3770:LEU:HD13	1.94	0.49
1:A:2446:ILE:HG23	1:A:2447:MET:HG2	1.95	0.48
1:A:2844:ARG:O	1:A:2848:GLU:HG3	2.13	0.48
1:A:2918:HIS:O	1:A:2922:ILE:HG13	2.13	0.48
1:A:4069:ILE:HD13	1:A:4079:GLN:HG2	1.95	0.48
1:A:1540:VAL:HG13	1:A:1608:LEU:HD12	1.94	0.48
1:A:3888:ALA:O	1:A:4012:ASN:ND2	2.46	0.48
1:A:1332:VAL:HB	1:A:1377:LEU:HD22	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1661:VAL:HG22	1:A:1676:ILE:HD12	1.94	0.48
1:A:2872:LEU:HD13	1:A:2889:LEU:HD12	1.95	0.48
1:A:2223:VAL:HG11	1:A:2348:LEU:HG	1.94	0.48
1:A:2248:GLU:HG2	1:A:2297:LYS:HZ2	1.76	0.48
1:A:2472:TYR:HB2	1:A:2541:ILE:HD12	1.95	0.48
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.94	0.48
1:A:1816:VAL:HG11	1:A:2052:VAL:HG22	1.93	0.48
1:A:2053:MET:SD	1:A:2094:LYS:HG2	2.54	0.48
1:A:2094:LYS:NZ	2:A:4701:ADP:O2'	2.32	0.48
1:A:1556:ASP:O	1:A:1560:LEU:HG	2.13	0.48
1:A:2232:MET:HG3	3:A:4702:ATP:C8	2.48	0.48
1:A:2499:LEU:O	1:A:2503:SER:OG	2.25	0.48
1:A:2666:ILE:HG22	1:A:2723:LEU:HD21	1.94	0.48
1:A:3193:GLU:O	1:A:3196:GLU:HG3	2.13	0.48
1:A:2206:LYS:NZ	1:A:2363:TRP:O	2.32	0.48
1:A:2415:ILE:HD11	1:A:2473:ASN:HD22	1.79	0.48
1:A:3659:ARG:HG3	1:A:3661:LEU:CD2	2.44	0.48
1:A:3817:SER:C	1:A:4346:MET:HE1	2.39	0.48
1:A:2760:PRO:HB3	1:A:2763:ARG:HH21	1.79	0.48
1:A:3575:GLU:O	1:A:3579:MET:HG3	2.14	0.48
1:A:4081:ASP:OD1	1:A:4082:LYS:N	2.47	0.48
1:A:2534:ILE:HD12	1:A:2534:ILE:H	1.79	0.47
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.49	0.47
1:A:2484:GLU:O	1:A:2488:ARG:HG3	2.14	0.47
1:A:2965:ARG:HE	1:A:2966:LYS:HD2	1.78	0.47
1:A:3591:ASP:O	1:A:3682:ARG:HA	2.15	0.47
1:A:3972:TYR:OH	1:A:3976:GLU:OE1	2.30	0.47
1:A:4055:VAL:HB	1:A:4095:MET:HE1	1.96	0.47
1:A:1628:ARG:NH2	1:A:1871:GLU:OE1	2.47	0.47
1:A:2956:LEU:HG	1:A:2989:LYS:HB3	1.97	0.47
1:A:3488:ARG:HH12	1:A:3773:LEU:HB3	1.79	0.47
1:A:3935:VAL:HG22	1:A:3996:PHE:HE1	1.79	0.47
1:A:4302:ARG:O	1:A:4306:VAL:HG23	2.14	0.47
1:A:3194:LEU:HD13	1:A:3500:MET:CE	2.44	0.47
1:A:4178:ARG:NH2	1:A:4299:GLY:O	2.46	0.47
1:A:3766:ILE:O	1:A:3769:THR:HG22	2.14	0.47
1:A:4044:CYS:HB3	1:A:4130:ILE:HG12	1.96	0.47
1:A:2268:LEU:HB3	1:A:2275:TRP:HE3	1.79	0.47
1:A:2371:THR:HG22	1:A:2451:ARG:HD2	1.97	0.47
1:A:2454:CYS:HB3	1:A:2502:LEU:HD23	1.97	0.47
1:A:3724:VAL:HG13	1:A:3794:VAL:HG12	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3909:LEU:HB3	1:A:4344:LEU:HD21	1.97	0.47
1:A:1403:LEU:HD23	1:A:1450:LEU:HD11	1.96	0.47
1:A:3157:ALA:HB1	1:A:3524:MET:HE2	1.96	0.47
1:A:4027:LEU:HD11	1:A:4043:MET:HE1	1.96	0.47
1:A:1667:ASN:HB2	1:A:1672:VAL:HB	1.97	0.47
1:A:1571:ILE:HD11	1:A:1607:LEU:HB3	1.97	0.47
1:A:3915:VAL:HG21	1:A:4390:LEU:HD22	1.97	0.47
1:A:4137:ASN:OD1	1:A:4138:LEU:N	2.48	0.46
1:A:4543:VAL:HG21	1:A:4622:VAL:HG12	1.96	0.46
1:A:1336:LEU:HD11	1:A:1386:VAL:HG21	1.97	0.46
1:A:1701:TRP:O	1:A:1705:VAL:HG23	2.15	0.46
1:A:1847:ASP:OD1	1:A:1849:LYS:HG2	2.15	0.46
1:A:1859:ILE:HD11	1:A:1868:TYR:HD1	1.80	0.46
1:A:2884:VAL:HG13	1:A:2889:LEU:HD11	1.98	0.46
1:A:3044:LEU:HD13	1:A:3049:GLU:HG3	1.97	0.46
1:A:2135:GLU:HA	1:A:2138:ILE:HG22	1.97	0.46
1:A:2445:HIS:NE2	1:A:2449:LEU:HD22	2.31	0.46
1:A:2726:ARG:NH1	3:A:4702:ATP:O3G	2.48	0.46
1:A:3178:ASP:OD1	1:A:3584:ASN:HB2	2.15	0.46
1:A:2227:GLY:HA3	1:A:2452:LEU:HD12	1.97	0.46
1:A:2924:ARG:O	1:A:2928:GLN:HG2	2.16	0.46
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	1.98	0.46
1:A:2453:ARG:HD3	1:A:2728:LEU:O	2.16	0.46
1:A:3196:GLU:HA	1:A:3199:MET:HG3	1.97	0.46
1:A:4267:THR:HG21	1:A:4636:TYR:HD2	1.79	0.46
1:A:1769:MET:SD	1:A:1775:ALA:HA	2.56	0.46
1:A:3123:PRO:HG2	1:A:3126:MET:HG3	1.96	0.46
1:A:1469:VAL:HG11	1:A:1500:HIS:CE1	2.50	0.46
1:A:2936:ILE:HA	1:A:3068:MET:O	2.16	0.46
1:A:2191:LEU:HD12	1:A:2236:VAL:HG21	1.98	0.46
1:A:2934:LEU:HD23	1:A:3091:LEU:CD2	2.46	0.46
1:A:4554:ASP:H	1:A:4557:SER:HB2	1.81	0.46
1:A:1456:GLU:HG2	1:A:1512:TYR:HB3	1.97	0.45
1:A:2080:LEU:HD22	1:A:2153:ASP:HB3	1.97	0.45
1:A:4214:SER:HB2	1:A:4251:ILE:HG23	1.98	0.45
1:A:2135:GLU:HG2	1:A:2168:VAL:HG13	1.97	0.45
1:A:2323:LYS:HB3	1:A:2335:LEU:HB3	1.98	0.45
1:A:2935:LEU:HD23	1:A:3092:ASN:HB3	1.99	0.45
1:A:4094:VAL:HB	1:A:4124:LEU:HD12	1.98	0.45
1:A:3876:LEU:HD23	1:A:4146:VAL:HG11	1.98	0.45
1:A:2748:TYR:CD2	1:A:2799:MET:HE3	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4429:GLN:NE2	1:A:4433:ASP:OD1	2.48	0.45
1:A:1599:ARG:HG3	1:A:1599:ARG:HH11	1.81	0.45
1:A:2093:LEU:O	1:A:2097:LEU:HG	2.17	0.45
1:A:2369:LEU:HD12	1:A:2373:MET:HE2	1.99	0.45
1:A:2643:ARG:HE	1:A:2648:VAL:HG22	1.80	0.45
1:A:2996:GLU:HA	1:A:2999:VAL:HB	1.99	0.45
1:A:4407:ASP:HB3	1:A:4410:PHE:HB3	1.99	0.45
1:A:1619:LEU:HD22	1:A:1637:LEU:HD23	1.97	0.45
1:A:2065:LEU:HD21	1:A:2134:GLN:HG2	1.99	0.45
1:A:3568:PRO:HG2	1:A:3573:CYS:SG	2.56	0.45
1:A:1721:VAL:O	1:A:1725:GLU:HG3	2.17	0.45
1:A:1850:GLN:HB2	1:A:1856:GLN:HG2	1.97	0.45
1:A:2560:HIS:O	1:A:2561:LYS:HG2	2.17	0.45
1:A:2775:GLU:O	1:A:2778:THR:OG1	2.35	0.45
1:A:1459:LEU:HD22	1:A:1507:MET:HG3	1.99	0.45
1:A:2072:PHE:CE2	1:A:2141:VAL:HG11	2.52	0.45
1:A:3801:TYR:HD1	1:A:3856:LEU:HD13	1.80	0.45
1:A:1635:GLU:HG2	1:A:1636:ASP:N	2.32	0.45
1:A:1687:LYS:HG3	1:A:1715:LYS:HD2	1.97	0.45
1:A:2798:GLU:HG3	1:A:2801:ARG:HH21	1.81	0.45
1:A:3692:LEU:O	1:A:3696:VAL:HG22	2.16	0.45
1:A:3821:ILE:HD12	1:A:4342:LYS:HG2	1.97	0.45
1:A:1408:LEU:HD12	1:A:1408:LEU:HA	1.87	0.45
1:A:1793:ALA:HA	1:A:1796:VAL:HG12	1.98	0.45
1:A:1468:GLU:O	1:A:1472:THR:HG22	2.17	0.44
1:A:2202:MET:O	1:A:2205:GLU:HG2	2.18	0.44
1:A:2905:LEU:HD23	1:A:2948:ARG:HH22	1.82	0.44
1:A:2346:GLN:HB2	1:A:2726:ARG:HD2	1.97	0.44
1:A:2778:THR:O	1:A:2782:GLU:HG3	2.17	0.44
1:A:3057:GLN:O	1:A:3061:ASN:HB2	2.16	0.44
1:A:4423:LEU:HD13	1:A:4466:HIS:ND1	2.32	0.44
1:A:2211:TYR:O	1:A:2214:THR:OG1	2.29	0.44
1:A:3008:MET:HE2	1:A:3064:VAL:HG21	1.99	0.44
1:A:3708:LEU:HD13	1:A:3829:LEU:HD11	1.99	0.44
1:A:3878:GLN:HG3	1:A:3879:ASP:OD1	2.17	0.44
1:A:2134:GLN:HE21	1:A:2168:VAL:HG21	1.82	0.44
1:A:2671:MET:HB3	1:A:2675:GLY:HA2	1.99	0.44
1:A:1561:LEU:HB3	1:A:1564:GLU:HB2	2.00	0.44
1:A:2049:ILE:HD13	1:A:2090:LEU:HD21	2.00	0.44
1:A:2204:VAL:O	1:A:2207:VAL:HG12	2.18	0.44
1:A:3724:VAL:HG21	1:A:3797:VAL:HG21	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4093:TRP:CD1	1:A:4123:ARG:HB2	2.53	0.44
1:A:4191:GLN:O	1:A:4194:LEU:HB2	2.18	0.44
1:A:4485:ARG:NH1	1:A:4513:GLY:O	2.51	0.44
1:A:4517:PRO:O	1:A:4521:ILE:HG12	2.17	0.44
1:A:1409:LYS:O	1:A:1413:TRP:HD1	2.01	0.44
1:A:2938:VAL:O	1:A:2943:LYS:NZ	2.51	0.44
1:A:4277:SER:HA	1:A:4282:PHE:CG	2.52	0.44
1:A:4324:PRO:HB2	1:A:4326:ASN:OD1	2.18	0.44
1:A:1646:ASN:ND2	1:A:1649:LYS:HE2	2.33	0.44
1:A:2915:VAL:HG13	1:A:2946:LEU:HD21	2.00	0.44
1:A:1911:GLY:N	2:A:4701:ADP:O1B	2.47	0.44
1:A:1974:GLN:O	1:A:1978:ILE:HG13	2.18	0.44
1:A:3643:PRO:O	1:A:3646:ASN:ND2	2.50	0.44
1:A:3581:LYS:HZ2	1:A:3582:ARG:HH11	1.65	0.43
1:A:3922:PRO:HD2	1:A:3936:VAL:HG21	1.99	0.43
1:A:2232:MET:HE2	1:A:2232:MET:HA	1.99	0.43
1:A:2620:LEU:HD11	1:A:2634:THR:HG21	2.00	0.43
1:A:2828:GLU:OE1	1:A:2924:ARG:NH1	2.50	0.43
1:A:2923:ASP:OD1	1:A:2927:ARG:NH2	2.50	0.43
1:A:4086:THR:HG23	1:A:4089:LYS:HZ3	1.83	0.43
1:A:2288:ILE:HD12	1:A:2333:LEU:HD22	2.00	0.43
1:A:2309:PRO:HB3	1:A:2352:THR:CG2	2.49	0.43
1:A:2884:VAL:HG11	1:A:2889:LEU:HD21	1.99	0.43
1:A:2219:GLY:HA2	1:A:2341:ILE:O	2.19	0.43
1:A:2319:LEU:HD13	1:A:2359:CYS:SG	2.58	0.43
1:A:4330:VAL:O	1:A:4333:THR:HG22	2.18	0.43
1:A:4492:ILE:HD12	1:A:4507:ILE:HD13	2.01	0.43
1:A:1350:PRO:O	1:A:1354:VAL:HG23	2.18	0.43
1:A:2468:ASN:HA	1:A:2471:GLN:HG2	1.99	0.43
1:A:4209:GLU:O	1:A:4213:ARG:HG3	2.19	0.43
1:A:2467:ARG:NH1	1:A:2587:GLU:OE2	2.51	0.43
1:A:2895:ALA:O	1:A:2899:VAL:HG23	2.19	0.43
1:A:2388:ASP:OD1	1:A:2389:GLU:N	2.52	0.43
1:A:2905:LEU:HD23	1:A:2948:ARG:NH2	2.32	0.43
1:A:2936:ILE:HG23	1:A:3093:TRP:CE3	2.54	0.43
1:A:3648:VAL:HA	1:A:3662:ILE:HD11	2.01	0.43
1:A:1547:LEU:HD22	1:A:1608:LEU:HD22	2.00	0.43
1:A:2483:ILE:O	1:A:2487:GLU:HG3	2.19	0.43
1:A:3008:MET:HE3	1:A:3011:LEU:HD23	2.01	0.43
1:A:4100:HIS:CD2	1:A:4129:GLU:HG2	2.54	0.43
1:A:1741:TRP:CH2	1:A:1750:VAL:HG13	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2221:MET:HE3	1:A:2343:PHE:CD2	2.48	0.43
1:A:2460:SER:OG	1:A:2589:LYS:HD2	2.18	0.43
1:A:4096:LEU:HD13	1:A:4105:TRP:HH2	1.84	0.43
1:A:4489:LEU:O	1:A:4492:ILE:HG22	2.19	0.43
1:A:2413:LEU:HG	1:A:2417:ARG:HE	1.84	0.43
1:A:1370:LEU:HD11	1:A:1390:LEU:HD12	2.01	0.42
1:A:1927:VAL:HG22	1:A:1954:TRP:HB2	2.02	0.42
1:A:3576:ASN:ND2	1:A:3700:ASN:O	2.50	0.42
1:A:4097:LYS:HA	1:A:4127:THR:OG1	2.18	0.42
1:A:2982:ARG:HA	1:A:2986:LYS:HD2	2.00	0.42
1:A:4087:ALA:HB1	1:A:4092:ARG:O	2.18	0.42
1:A:2514:LEU:O	1:A:2518:ILE:HG12	2.19	0.42
1:A:3500:MET:HE2	1:A:3503:ILE:HD12	2.01	0.42
1:A:4087:ALA:O	1:A:4091:GLY:N	2.51	0.42
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	2.00	0.42
1:A:4421:ALA:O	1:A:4425:GLN:HG2	2.19	0.42
1:A:2071:PRO:O	1:A:2075:LEU:HG	2.19	0.42
1:A:2668:LEU:HD23	1:A:2668:LEU:HA	1.88	0.42
1:A:2175:MET:HE1	1:A:2211:TYR:HD2	1.84	0.42
1:A:2559:THR:HG22	1:A:2757:ARG:HB3	2.02	0.42
1:A:1408:LEU:O	1:A:1412:HIS:HB2	2.19	0.42
1:A:1952:GLY:HA2	1:A:2012:MET:HB3	2.01	0.42
1:A:2925:ILE:HD11	1:A:3090:VAL:HG11	2.01	0.42
1:A:3113:MET:HE2	1:A:3184:ALA:CA	2.48	0.42
1:A:1356:PRO:CB	1:A:1401:ILE:HG13	2.49	0.42
1:A:1411:ARG:O	1:A:1415:GLN:HG3	2.19	0.42
1:A:1838:TRP:CZ2	1:A:1843:ARG:HG2	2.55	0.42
1:A:1481:GLN:N	1:A:2271:ASN:O	2.51	0.42
1:A:2278:GLY:N	1:A:2281:THR:OG1	2.53	0.42
1:A:2999:VAL:HG13	1:A:3005:LEU:HD21	2.02	0.42
1:A:3620:ARG:O	1:A:3624:GLU:HG3	2.20	0.42
1:A:1454:GLN:NE2	1:A:3671:LEU:O	2.41	0.42
1:A:1910:THR:HG22	1:A:2044:PRO:HD3	2.02	0.42
1:A:3605:LYS:HE3	1:A:3605:LYS:HB2	1.86	0.42
1:A:3787:THR:O	1:A:3791:MET:HG3	2.19	0.42
1:A:3944:PHE:CE1	1:A:3974:TRP:HB3	2.55	0.42
1:A:4043:MET:HE2	1:A:4147:PHE:CE1	2.54	0.42
1:A:4460:LEU:HD21	1:A:4465:SER:OG	2.20	0.42
1:A:2449:LEU:HA	1:A:2449:LEU:HD12	1.79	0.42
1:A:2863:ARG:CZ	1:A:2867:MET:HB2	2.50	0.42
1:A:3140:ARG:O	1:A:3144:VAL:HG23	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1414:LYS:O	1:A:1417:MET:HB3	2.20	0.41
1:A:1511:PRO:O	1:A:1514:LYS:NZ	2.37	0.41
1:A:1873:LEU:HD13	1:A:1921:HIS:HB3	2.01	0.41
1:A:2068:LYS:HG2	1:A:4537:GLU:OE2	2.20	0.41
1:A:2440:ALA:HB2	1:A:2502:LEU:HB3	2.02	0.41
1:A:3767:ILE:O	1:A:3771:GLU:HG2	2.19	0.41
1:A:2571:THR:H	1:A:2574:THR:HB	1.85	0.41
1:A:2836:ARG:NH1	1:A:3091:LEU:HD12	2.35	0.41
1:A:3740:LEU:O	1:A:3743:ARG:HG2	2.20	0.41
1:A:3927:LEU:HD11	1:A:3957:PHE:HE2	1.85	0.41
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.55	0.41
1:A:2214:THR:HG22	1:A:2220:LEU:HD21	2.03	0.41
1:A:2593:LEU:HD12	1:A:2605:LEU:HG	2.03	0.41
1:A:3123:PRO:HB3	1:A:3540:ASN:OD1	2.20	0.41
1:A:3739:GLN:HB3	1:A:3743:ARG:HH21	1.85	0.41
1:A:3972:TYR:C	1:A:3973:LEU:HD12	2.45	0.41
1:A:2175:MET:O	1:A:2179:ARG:HG2	2.21	0.41
1:A:2529:ALA:HB1	1:A:2532:ILE:HB	2.02	0.41
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.56	0.41
1:A:4028:THR:HA	1:A:4058:LEU:HD11	2.01	0.41
1:A:1425:VAL:O	1:A:1429:LEU:N	2.53	0.41
1:A:1990:TYR:HE2	1:A:1995:ALA:HA	1.85	0.41
1:A:4239:PRO:HB2	1:A:4242:ALA:HB3	2.03	0.41
1:A:1484:CYS:HB3	1:A:1576:LEU:HD22	2.03	0.41
1:A:1738:TYR:HE2	1:A:1792:LEU:HD21	1.86	0.41
1:A:1878:LYS:HE3	1:A:1878:LYS:HB3	1.84	0.41
1:A:2115:LYS:HE2	1:A:2127:ILE:HD11	2.02	0.41
1:A:2668:LEU:HD21	1:A:2720:ARG:HH11	1.85	0.41
1:A:3158:ASN:OD1	1:A:3168:THR:HB	2.21	0.41
1:A:4086:THR:O	1:A:4090:SER:OG	2.26	0.41
1:A:1464:LYS:HB2	1:A:1464:LYS:HE3	1.78	0.41
1:A:2077:ASP:OD2	1:A:2088:PHE:HB2	2.21	0.41
1:A:2103:VAL:O	1:A:2106:GLU:HG2	2.21	0.41
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	2.03	0.41
1:A:4543:VAL:HG13	1:A:4588:THR:HG23	2.02	0.41
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	2.02	0.41
1:A:1397:ASN:O	1:A:1400:VAL:HB	2.20	0.41
1:A:1987:ASN:OD1	1:A:1987:ASN:N	2.54	0.41
1:A:2231:SER:HA	1:A:2234:TRP:NE1	2.36	0.41
1:A:2673:LYS:NZ	1:A:2674:TYR:OH	2.53	0.41
1:A:3013:ALA:HB2	1:A:3088:ARG:NE	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3103:TYR:OH	1:A:3141:GLU:HG2	2.20	0.41
1:A:3114:ASP:O	1:A:3140:ARG:NH2	2.54	0.41
1:A:3523:GLN:HG2	1:A:3706:SER:CB	2.50	0.41
1:A:4248:ALA:O	1:A:4253:GLY:HA3	2.21	0.41
1:A:4387:TRP:NE1	1:A:4479:VAL:HG21	2.35	0.41
1:A:4485:ARG:HG2	1:A:4513:GLY:HA2	2.03	0.41
1:A:1698:ILE:O	1:A:1702:LEU:HB2	2.20	0.41
1:A:2518:ILE:O	1:A:2522:THR:HG22	2.21	0.41
1:A:3007:ARG:HH21	1:A:3020:LEU:HD13	1.85	0.41
1:A:3550:THR:O	1:A:3554:SER:OG	2.35	0.41
1:A:3645:LEU:HG	1:A:3649:LEU:HG	2.02	0.41
1:A:4619:ILE:HG22	1:A:4620:PHE:HD1	1.84	0.41
1:A:2577:HIS:CD2	1:A:2736:VAL:HG22	2.56	0.40
1:A:2590:PRO:HA	1:A:2708:PHE:O	2.21	0.40
1:A:2667:ASN:HB3	1:A:2720:ARG:HB3	2.02	0.40
1:A:2854:ALA:O	1:A:2858:PHE:HB2	2.21	0.40
1:A:2920:LEU:HD23	1:A:2920:LEU:HA	1.86	0.40
1:A:3508:LEU:HD22	1:A:3536:LEU:HD11	2.02	0.40
1:A:1461:GLU:O	1:A:1465:GLN:HG3	2.21	0.40
1:A:2445:HIS:CD2	1:A:2449:LEU:HD22	2.56	0.40
1:A:4528:VAL:HG21	1:A:4592:TRP:HB2	2.03	0.40
1:A:1354:VAL:HG21	1:A:1431:LEU:HB2	2.03	0.40
1:A:1810:HIS:NE2	1:A:1876:GLN:O	2.52	0.40
1:A:1876:GLN:HG2	1:A:1921:HIS:CD2	2.57	0.40
1:A:1899:ARG:HD3	1:A:1899:ARG:HA	1.86	0.40
1:A:1912:LYS:HE3	1:A:1912:LYS:HB2	1.84	0.40
1:A:3548:ALA:HB1	1:A:3551:GLU:OE1	2.22	0.40
1:A:3756:VAL:HG12	1:A:3760:ILE:HD13	2.03	0.40
1:A:4307:GLN:O	1:A:4311:LEU:HG	2.21	0.40
1:A:1359:LEU:HD11	1:A:1435:TRP:CZ2	2.57	0.40
1:A:1698:ILE:HD13	1:A:1701:TRP:HE1	1.86	0.40
1:A:1713:LEU:HD23	1:A:1713:LEU:HA	1.92	0.40
1:A:3012:LEU:HD11	1:A:3066:PHE:HE2	1.87	0.40
1:A:3143:ILE:HG23	1:A:3508:LEU:HD12	2.04	0.40
1:A:4569:THR:HG22	1:A:4583:THR:HG21	2.04	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	3029/4646 (65%)	2974 (98%)	53 (2%)	2 (0%)	48 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4292	LYS
1	A	4130	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2704/4125 (66%)	2704 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1368	ASN
1	A	1421	HIS
1	A	1482	ASN
1	A	1528	ASN
1	A	1646	ASN
1	A	1670	ASN
1	A	1755	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1817	HIS
1	A	1863	ASN
1	A	1876	GLN
1	A	1894	GLN
1	A	1922	GLN
1	A	2215	GLN
1	A	2263	HIS
1	A	2377	ASN
1	A	2476	HIS
1	A	2482	GLN
1	A	2637	HIS
1	A	2685	GLN
1	A	2752	ASN
1	A	2786	GLN
1	A	2834	GLN
1	A	2849	ASN
1	A	2886	GLN
1	A	3057	GLN
1	A	3473	ASN
1	A	3535	HIS
1	A	3584	ASN
1	A	3772	ASN
1	A	3799	GLN
1	A	3820	GLN
1	A	4012	ASN
1	A	4054	HIS
1	A	4078	ASN
1	A	4131	ASN
1	A	4174	ASN
1	A	4579	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 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
4	ANP	A	4704	5	33,33,33	2.29	5 (15%)	45,52,52	1.20	3 (6%)
4	ANP	A	4703	5	33,33,33	2.28	5 (15%)	45,52,52	1.17	3 (6%)
2	ADP	A	4701	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	8 (18%)
3	ATP	A	4702	5	32,33,33	0.38	0	48,52,52	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	A	4704	5	-	8/18/38/38	0/3/3/3
4	ANP	A	4703	5	-	4/18/38/38	0/3/3/3
2	ADP	A	4701	-	-	3/16/32/32	0/3/3/3
3	ATP	A	4702	5	-	3/22/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4704	ANP	PB-O3A	8.86	1.70	1.59
4	A	4703	ANP	PB-O3A	8.78	1.70	1.59
4	A	4703	ANP	PG-N3B	6.25	1.79	1.63
4	A	4704	ANP	PG-N3B	6.20	1.79	1.63
4	A	4704	ANP	PG-O1G	4.70	1.53	1.46
4	A	4703	ANP	PG-O1G	4.64	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4701	ADP	C5-C4	4.54	1.47	1.39
4	A	4704	ANP	PB-O1B	2.65	1.50	1.46
2	A	4701	ADP	C5-C6	2.63	1.48	1.41
4	A	4703	ANP	PB-O1B	2.61	1.50	1.46
2	A	4701	ADP	C5-N7	-2.37	1.34	1.39
2	A	4701	ADP	C8-N7	2.24	1.36	1.31
4	A	4703	ANP	PB-O2B	-2.23	1.50	1.56
4	A	4704	ANP	PB-O2B	-2.22	1.50	1.56

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	ADP	C5-C4-N3	-5.80	118.74	126.72
4	A	4703	ANP	O2B-PB-O1B	4.89	120.35	109.87
4	A	4704	ANP	O2B-PB-O1B	4.81	120.17	109.87
2	A	4701	ADP	N3-C4-N9	4.60	135.00	127.17
4	A	4704	ANP	O1G-PG-N3B	-4.10	105.73	111.77
4	A	4703	ANP	O1G-PG-N3B	-3.87	106.07	111.77
2	A	4701	ADP	C2-N3-C4	3.71	120.90	111.83
2	A	4701	ADP	C4-C5-N7	-3.44	106.65	110.58
2	A	4701	ADP	N3-C2-N1	-3.28	123.62	128.58
2	A	4701	ADP	C4-N9-C8	2.70	108.58	105.74
4	A	4704	ANP	O2G-PG-O3G	2.56	114.47	107.59
2	A	4701	ADP	C5-N7-C8	2.51	107.39	103.45
4	A	4703	ANP	O2G-PG-O3G	2.47	114.23	107.59
2	A	4701	ADP	C6-C5-N7	2.07	136.08	132.09

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	4703	ANP	PB-N3B-PG-O1G
4	A	4703	ANP	PA-O3A-PB-O2B
4	A	4704	ANP	PB-N3B-PG-O1G
4	A	4704	ANP	PG-N3B-PB-O1B
4	A	4704	ANP	C5'-O5'-PA-O2A
4	A	4704	ANP	C5'-O5'-PA-O3A
4	A	4704	ANP	O4'-C4'-C5'-O5'
4	A	4704	ANP	C3'-C4'-C5'-O5'
2	A	4701	ADP	O4'-C4'-C5'-O5'
3	A	4702	ATP	PB-O3B-PG-O1G
3	A	4702	ATP	PB-O3B-PG-O2G

Continued on next page...

Continued from previous page...

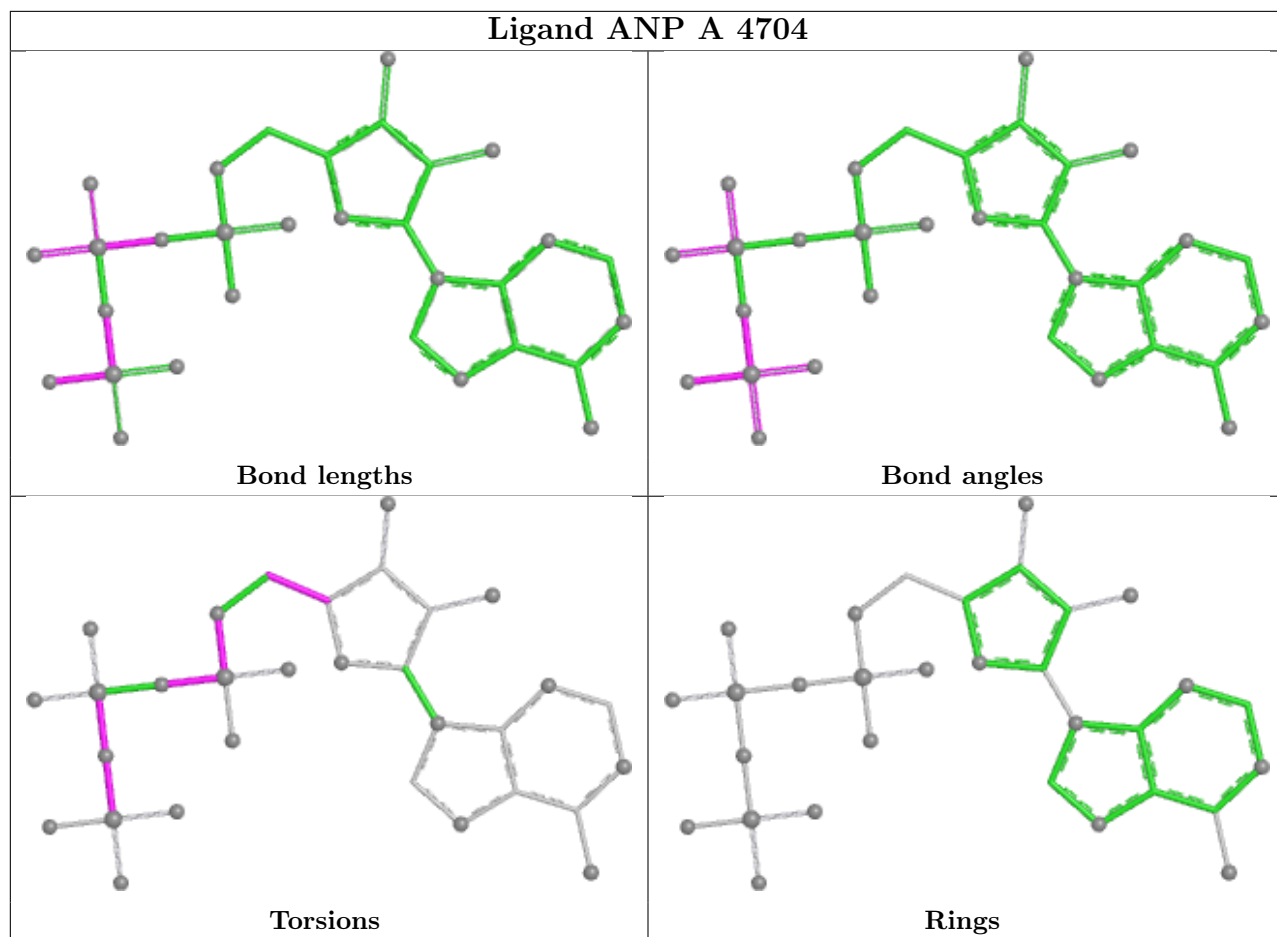
Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	PB-O3A-PA-O2A
2	A	4701	ADP	PB-O3A-PA-O1A
4	A	4703	ANP	O4'-C4'-C5'-O5'
4	A	4704	ANP	PB-O3A-PA-O2A
4	A	4703	ANP	PA-O3A-PB-O1B
4	A	4704	ANP	PG-N3B-PB-O3A
3	A	4702	ATP	PG-O3B-PB-O2B

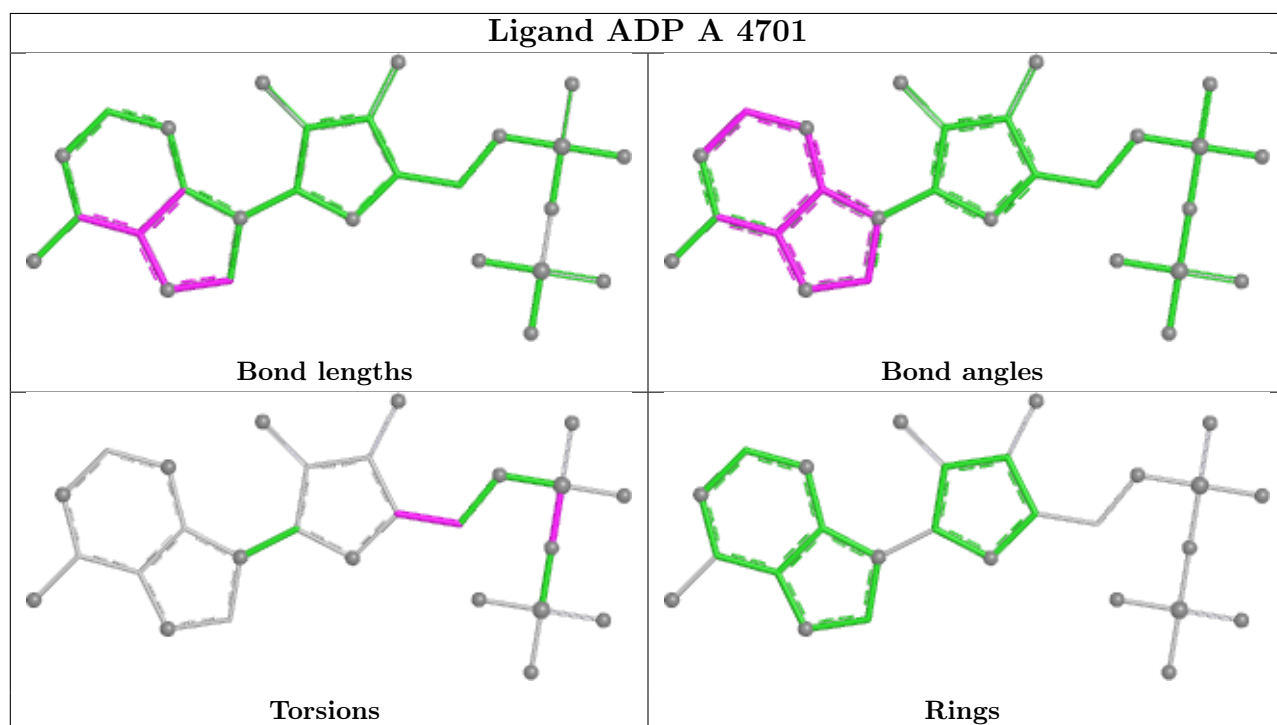
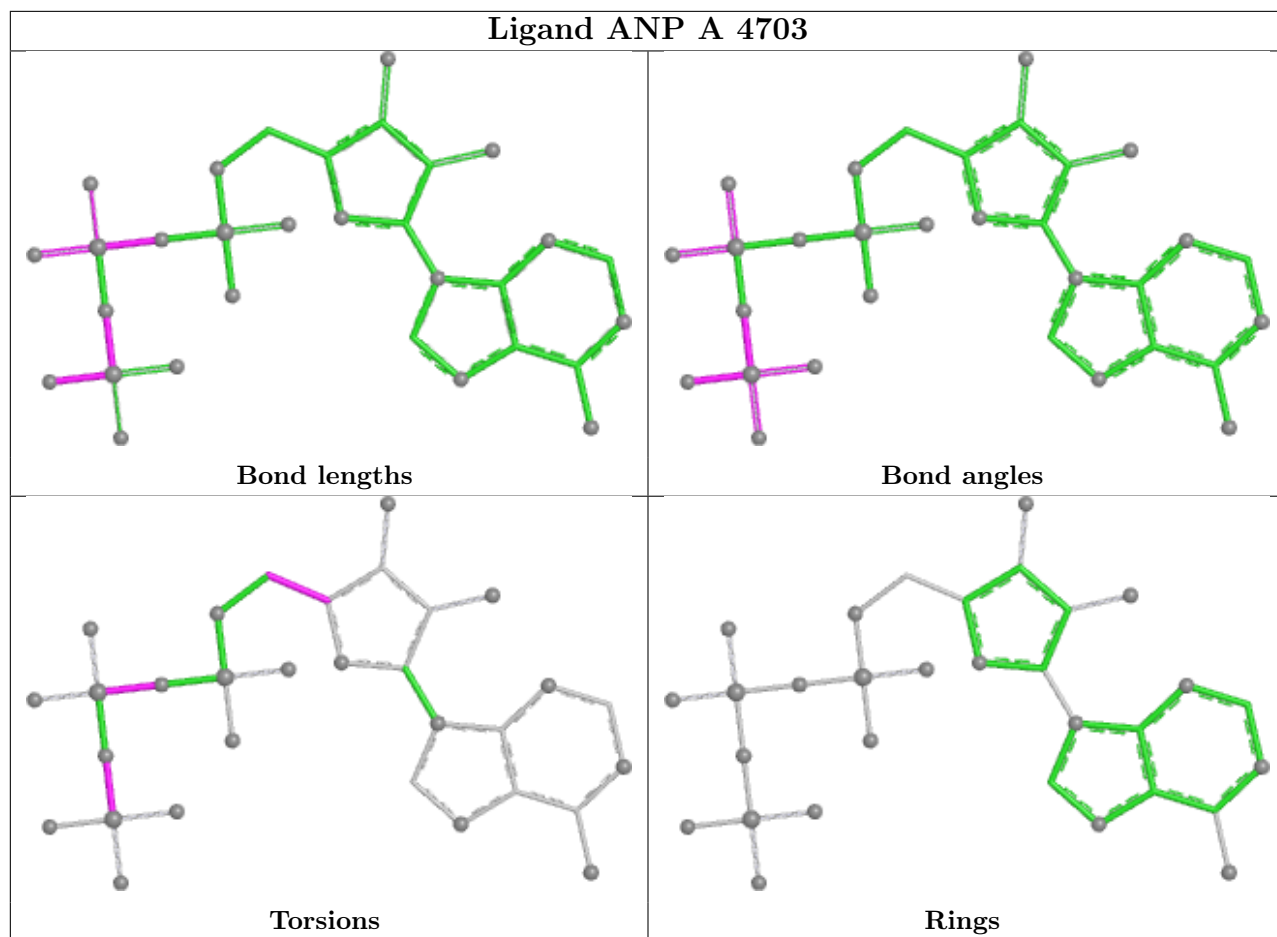
There are no ring outliers.

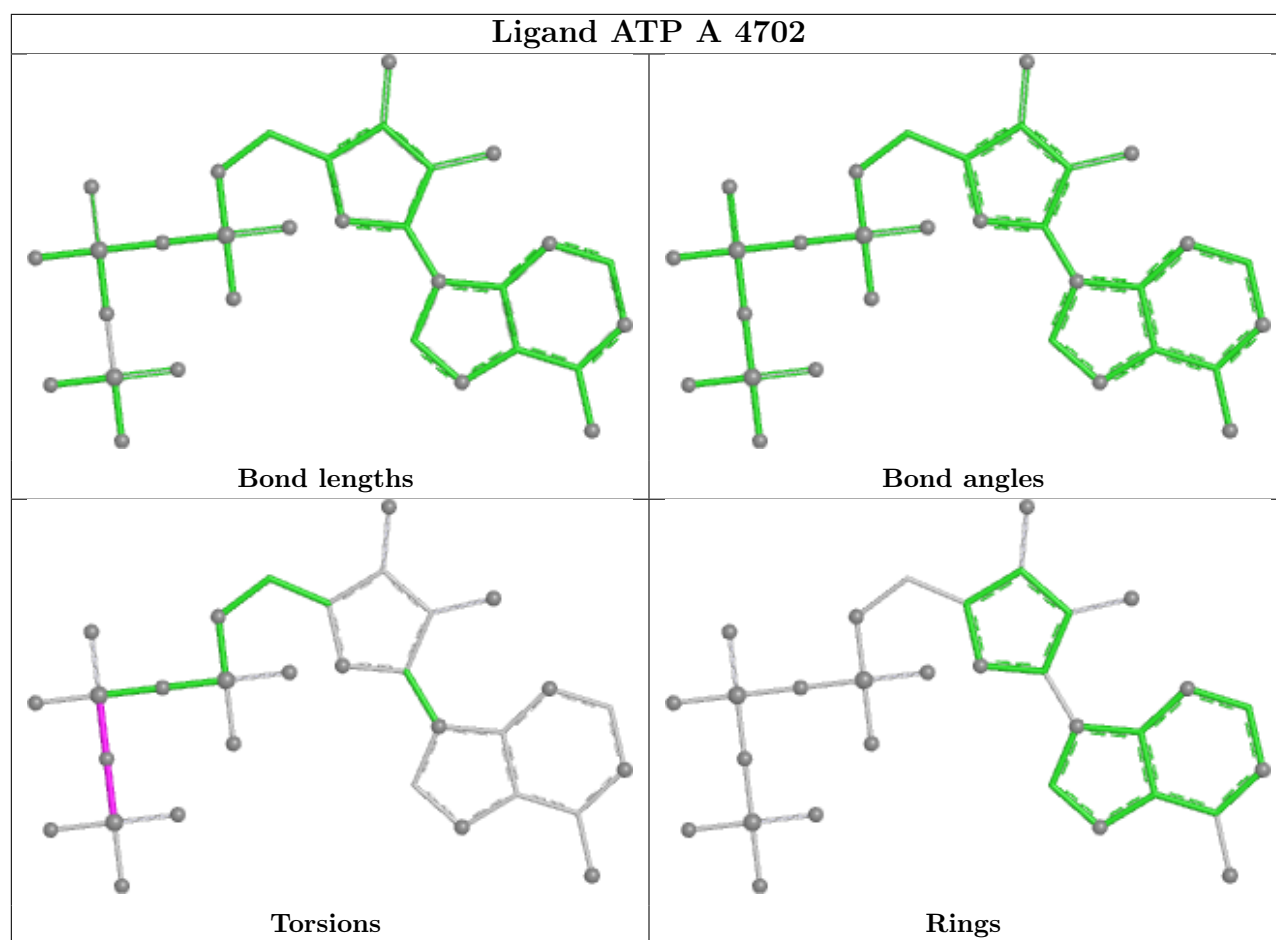
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4703	ANP	3	0
2	A	4701	ADP	2	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.

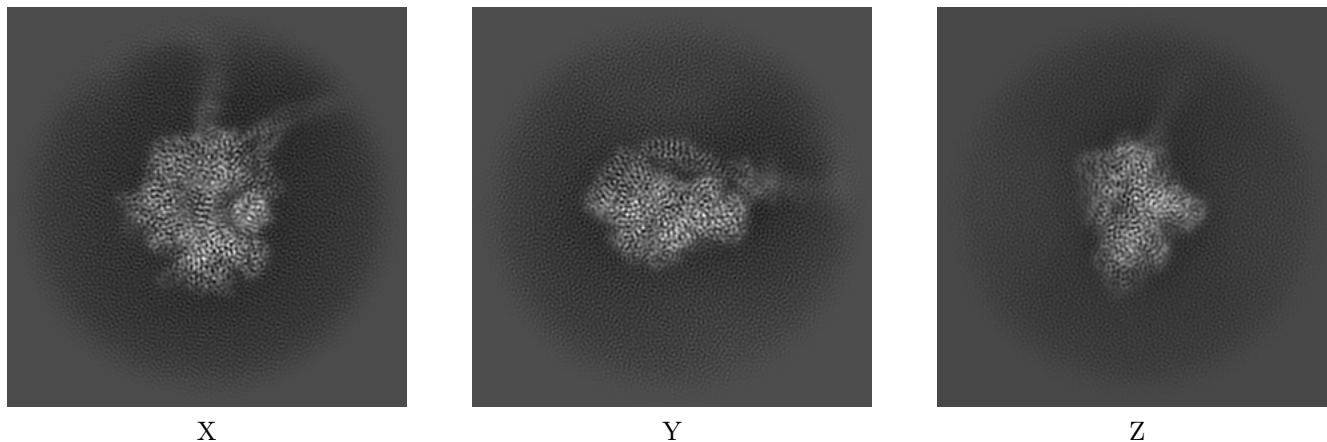
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44696. These allow visual inspection of the internal detail of the map and identification of artifacts.

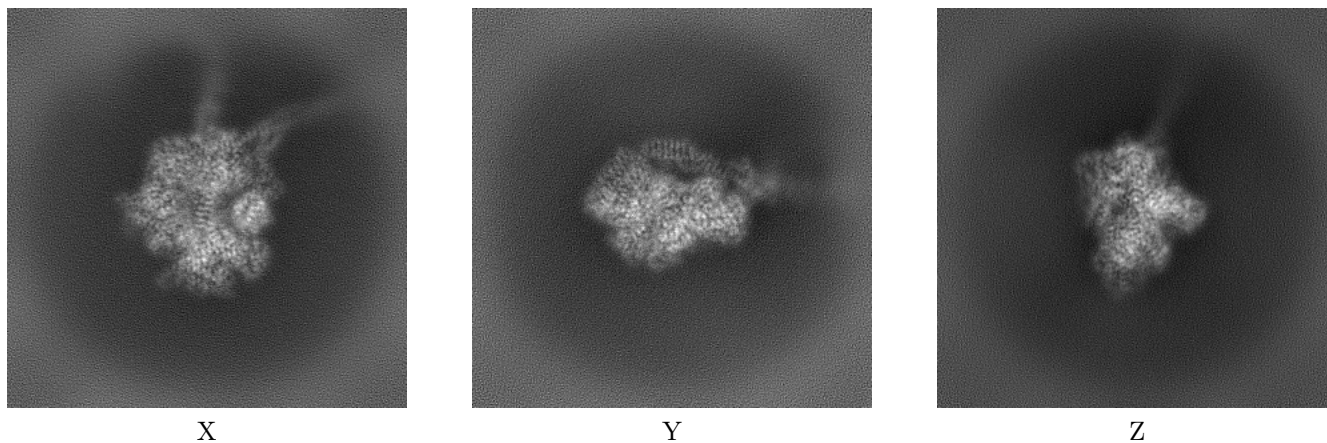
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



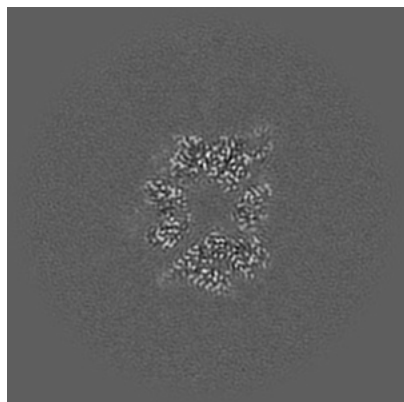
6.1.2 Raw map



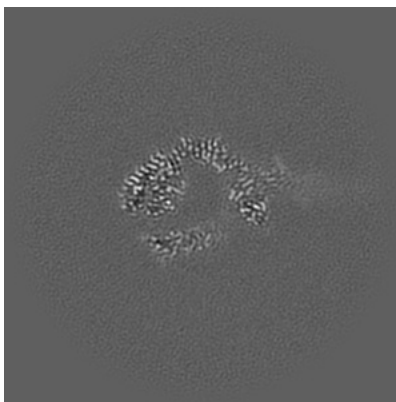
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

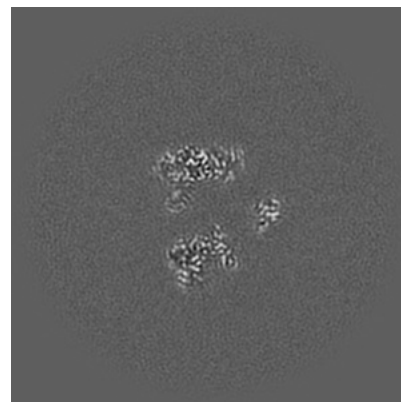
6.2.1 Primary map



X Index: 192

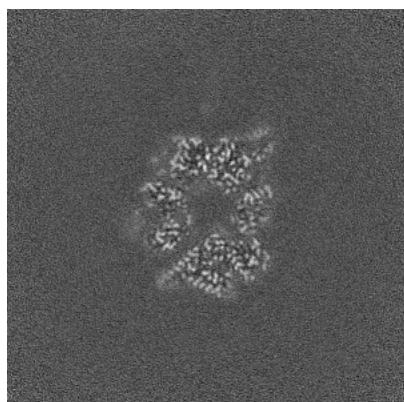


Y Index: 192

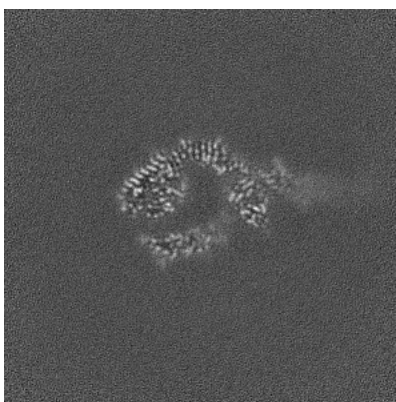


Z Index: 192

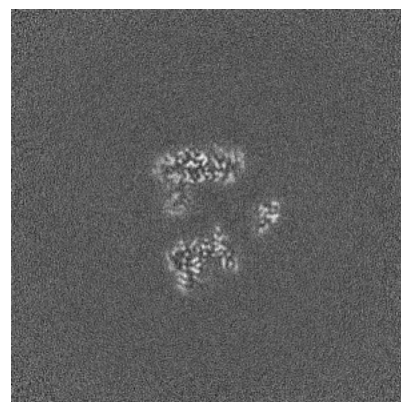
6.2.2 Raw map



X Index: 192



Y Index: 192

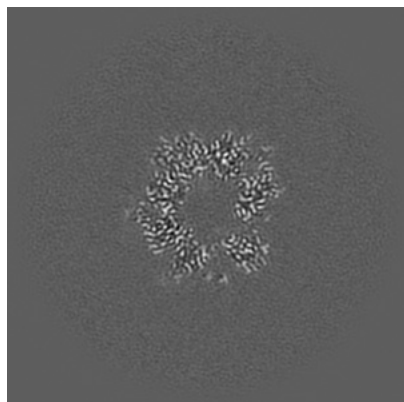


Z Index: 192

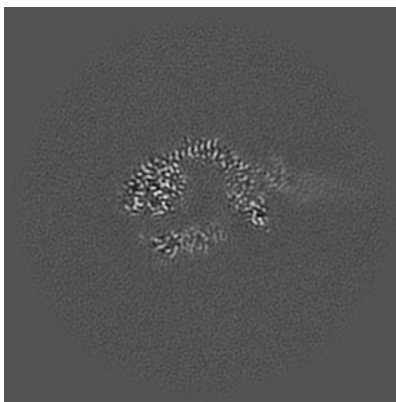
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

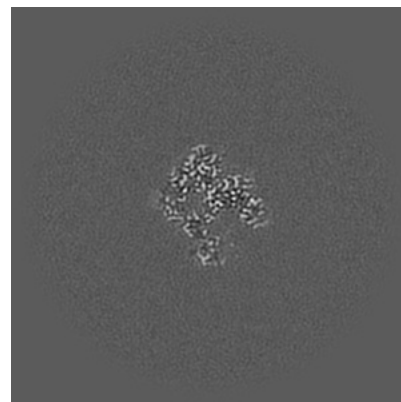
6.3.1 Primary map



X Index: 184

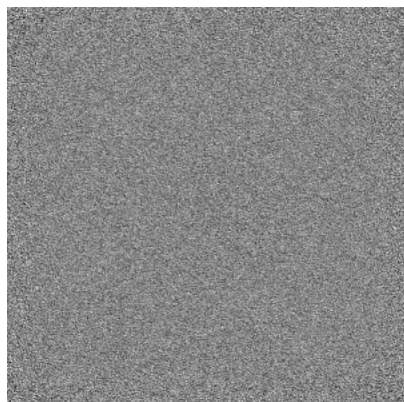


Y Index: 194

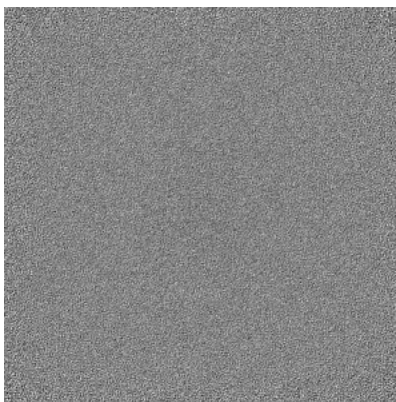


Z Index: 154

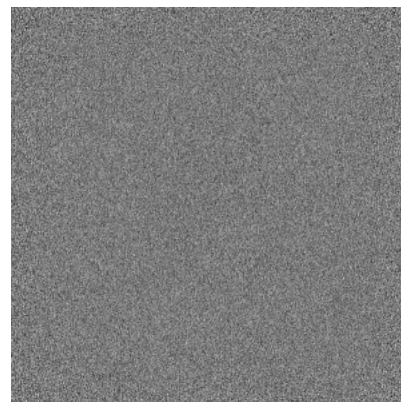
6.3.2 Raw map



X Index: 0



Y Index: 0

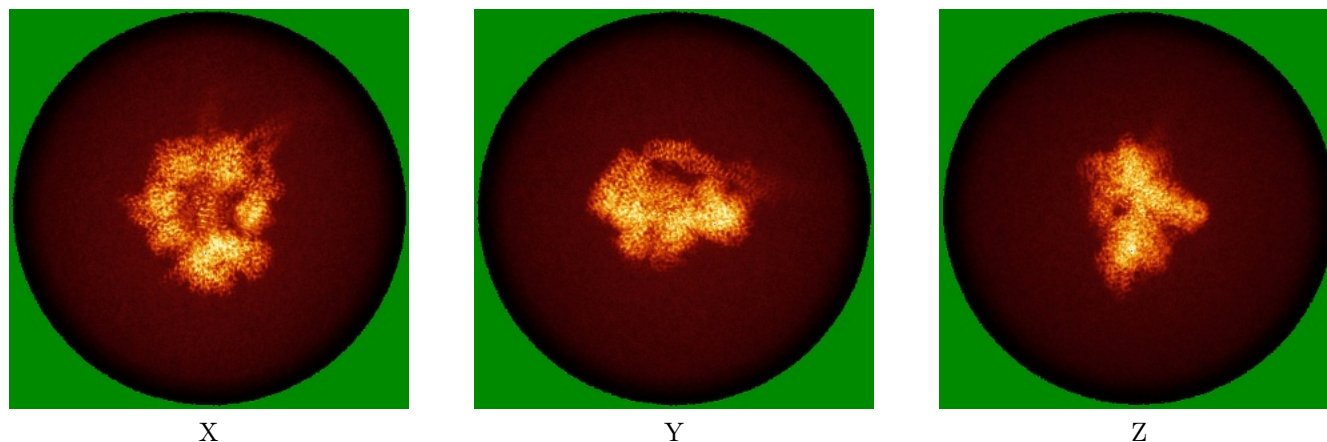


Z Index: 0

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

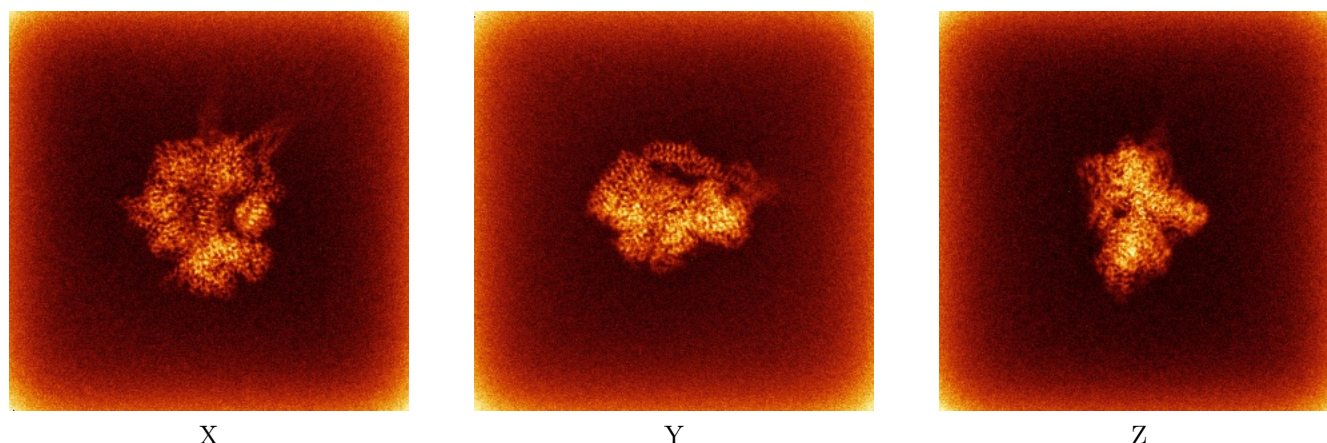


X

Y

Z

6.4.2 Raw map



X

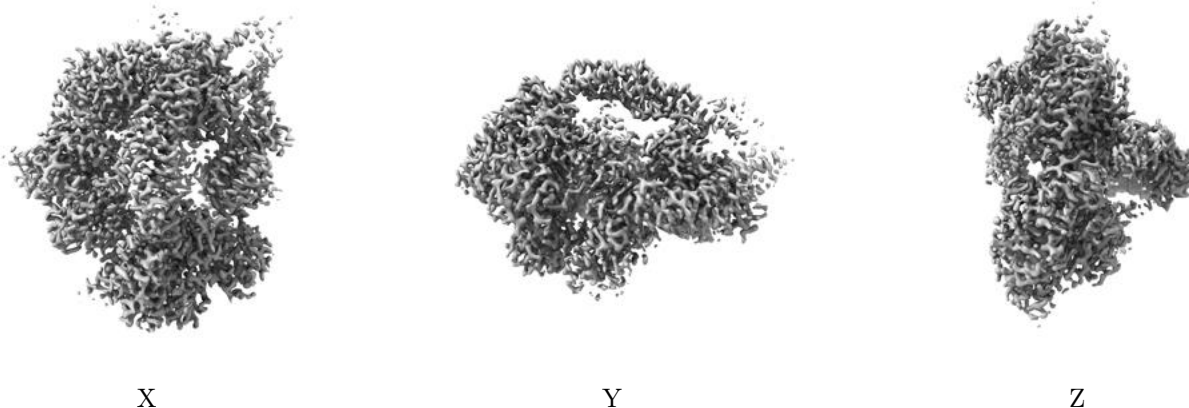
Y

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.

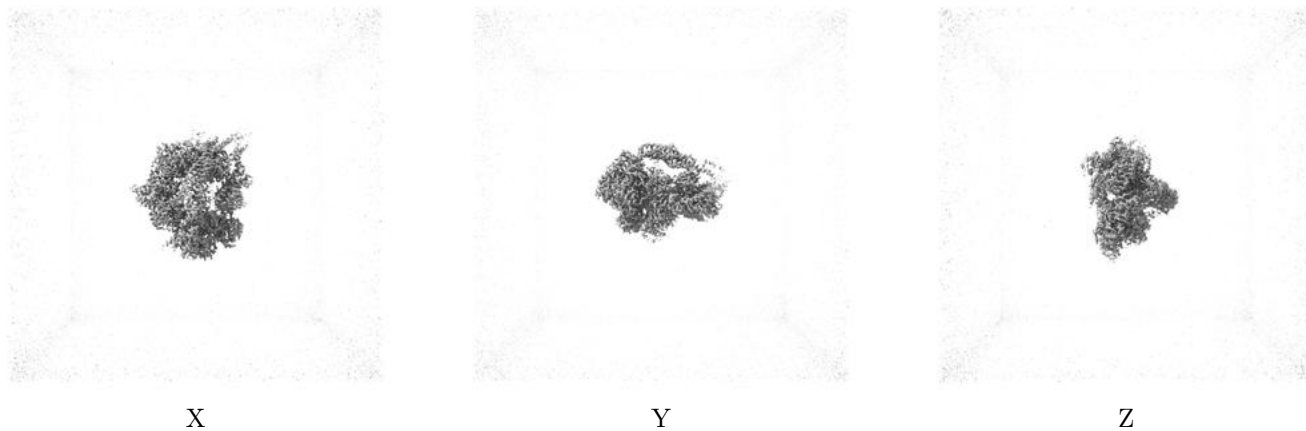
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

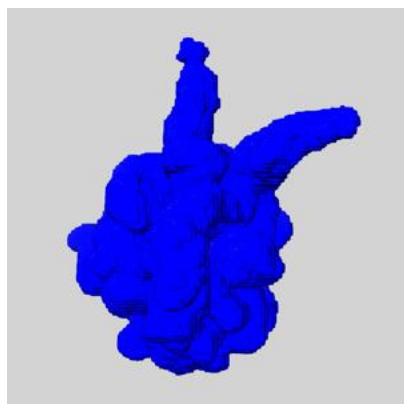
6.6 Mask visualisation [i](#)

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

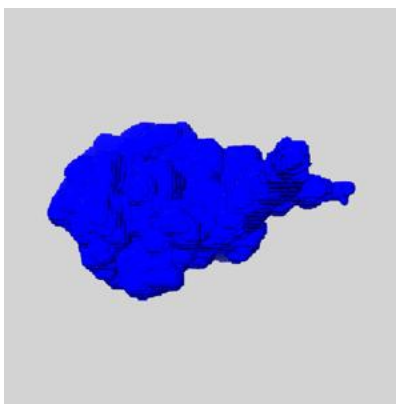
A mask typically either:

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

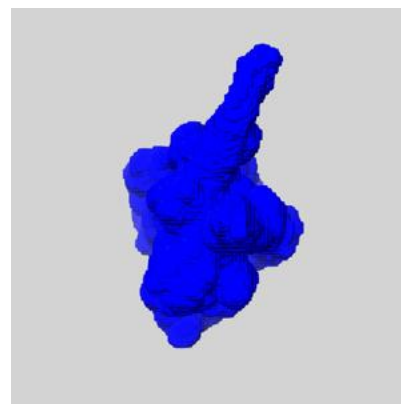
6.6.1 emd_44696_msk_1.map [i](#)



X



Y

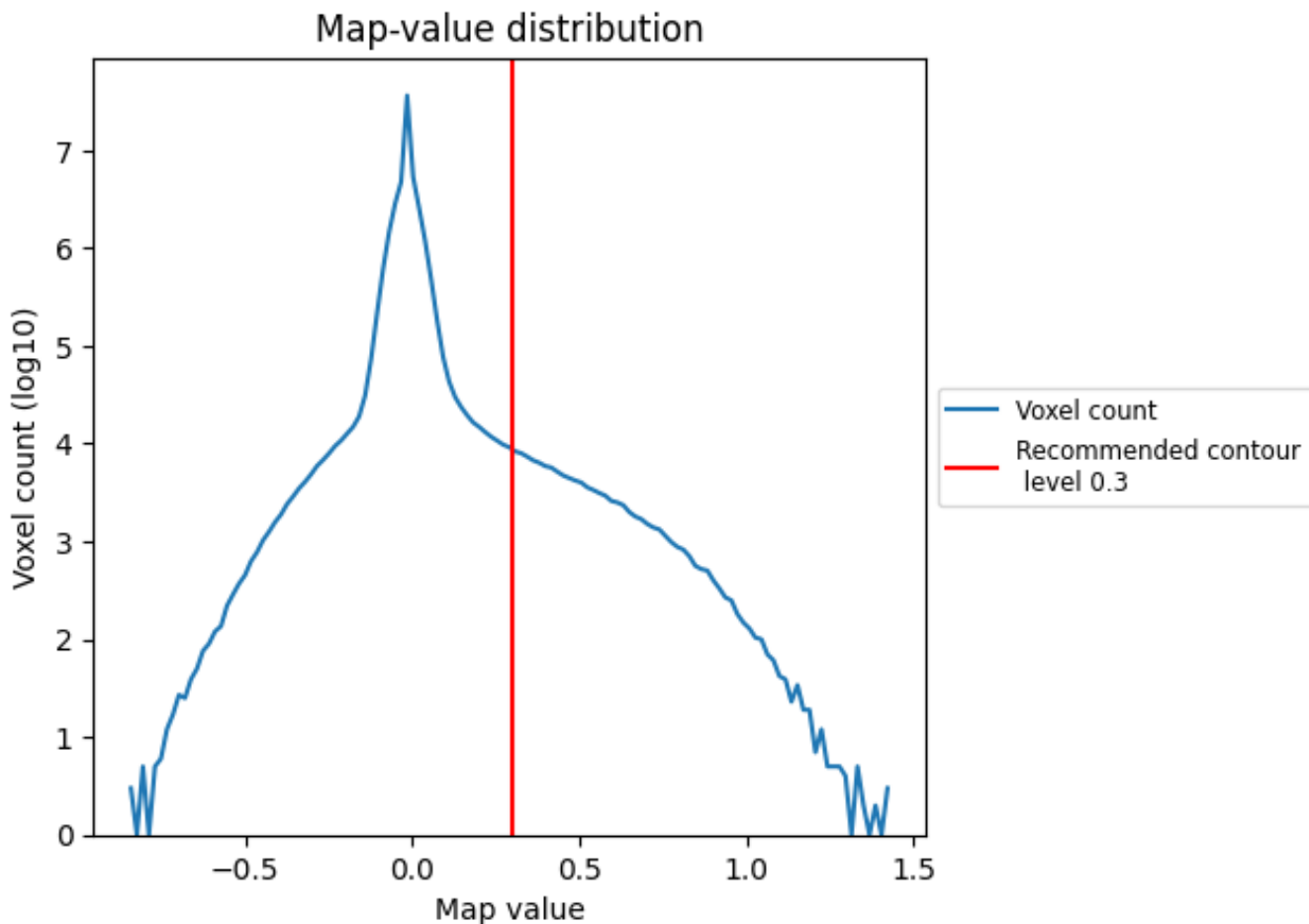


Z

7 Map analysis [i](#)

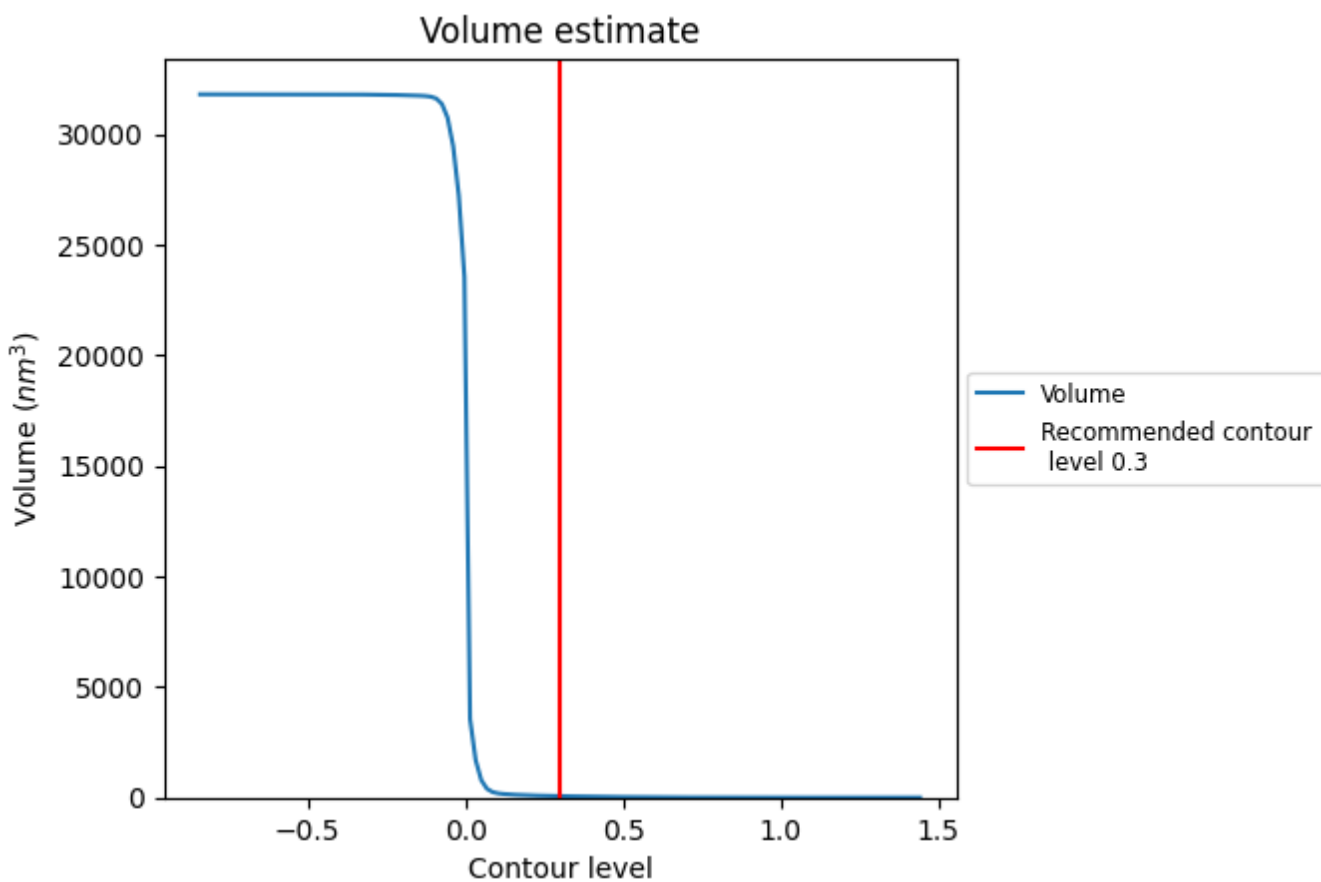
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

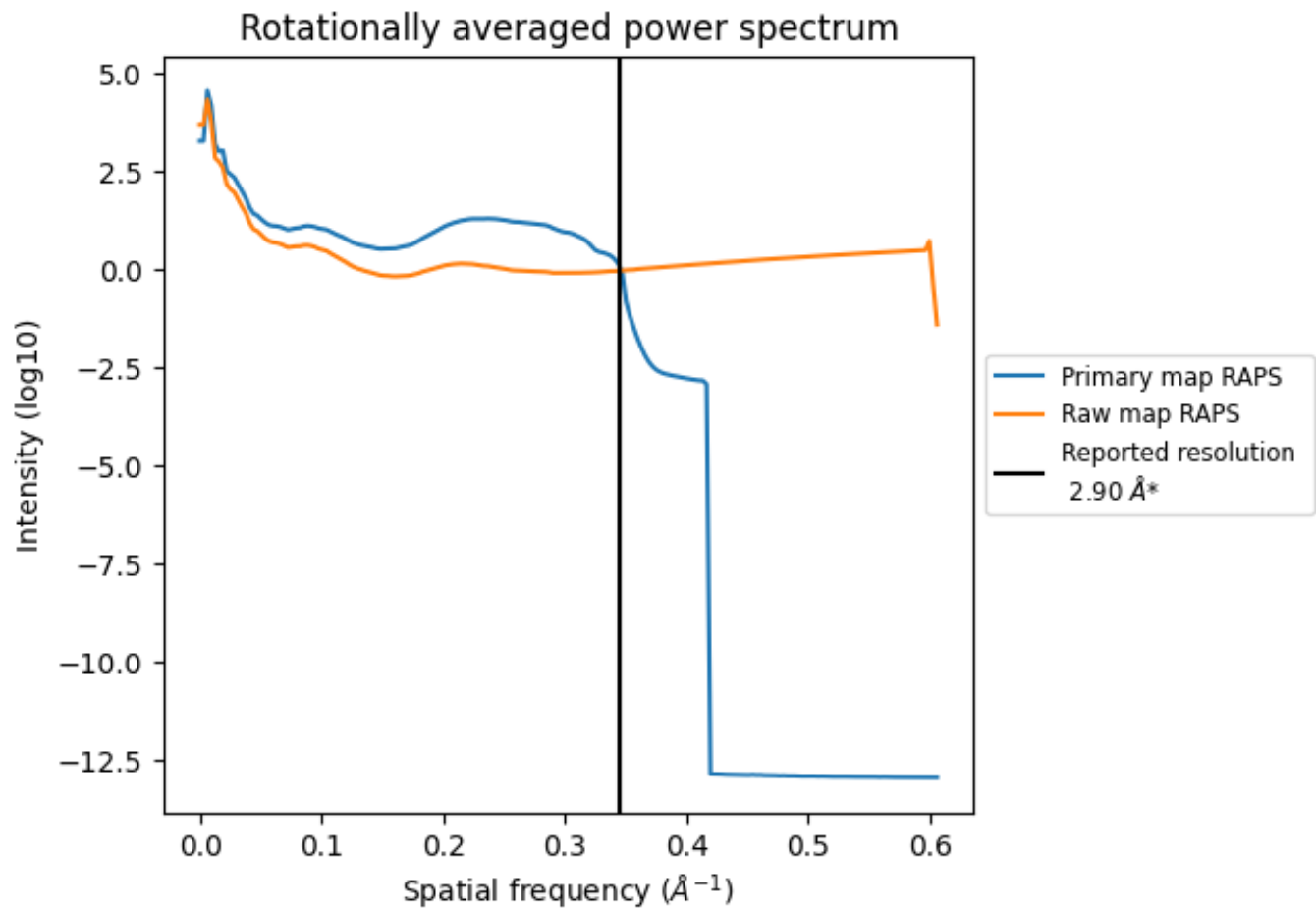
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 64 nm³; this corresponds to an approximate mass of 58 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

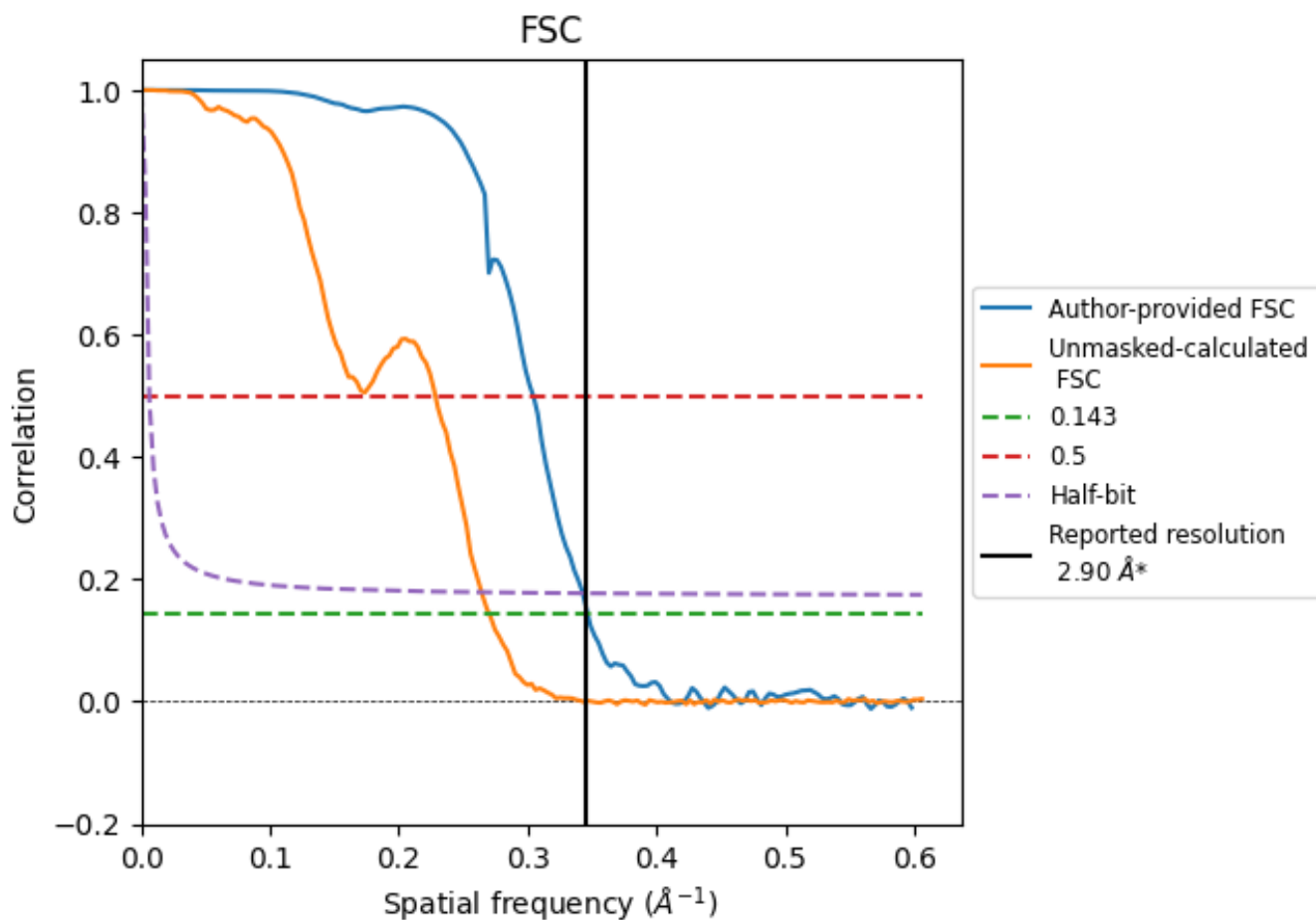


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

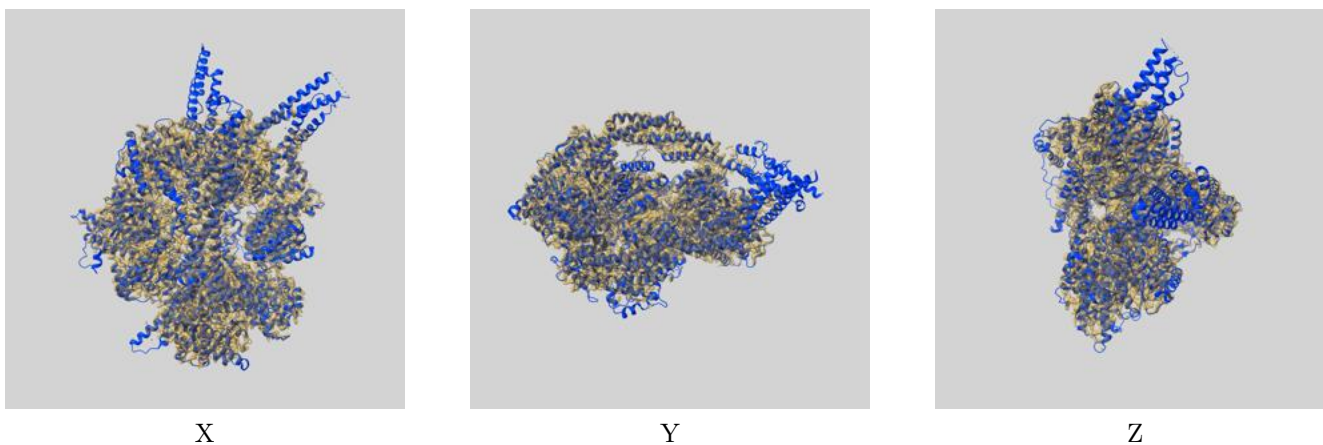
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.88	3.29	2.92
Unmasked-calculated*	3.70	4.38	3.79

*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 3.70 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

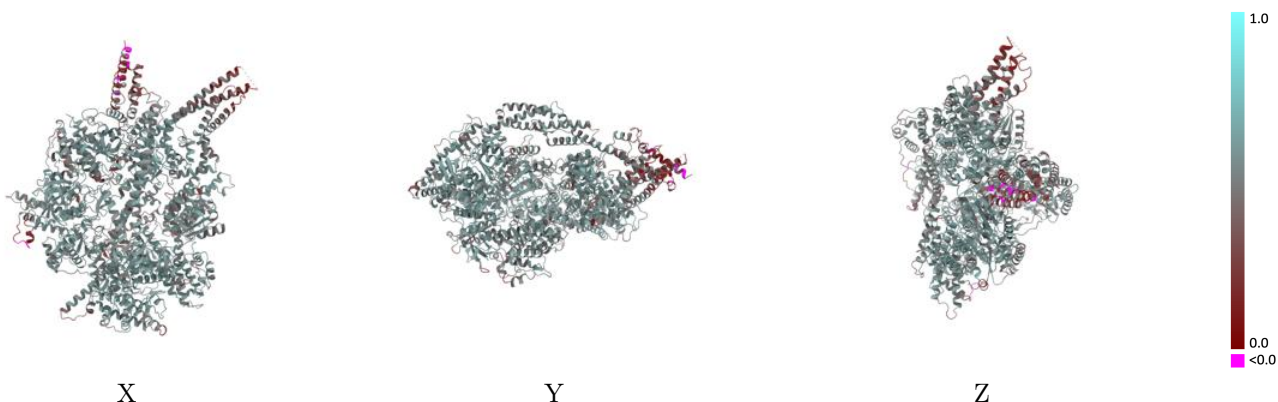
This section contains information regarding the fit between EMDB map EMD-44696 and PDB model 9BMD. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



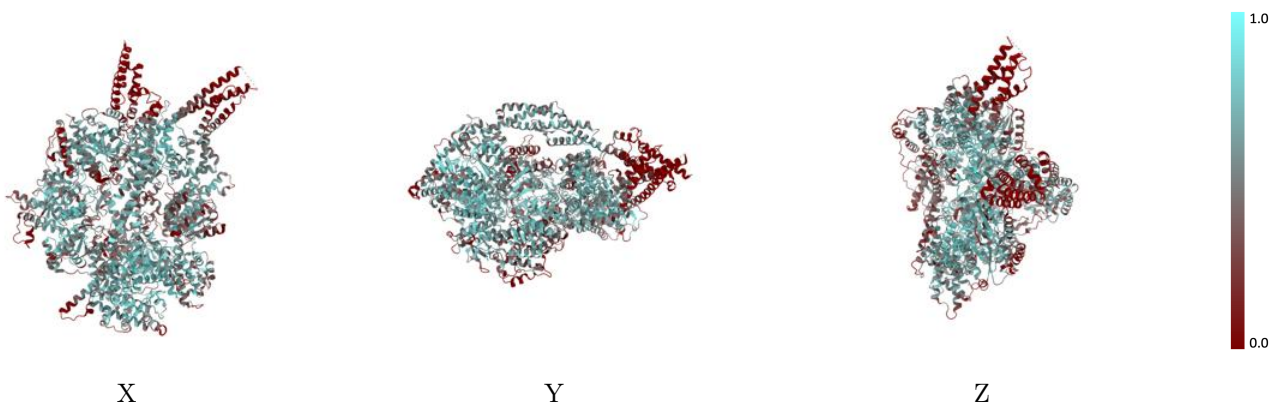
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



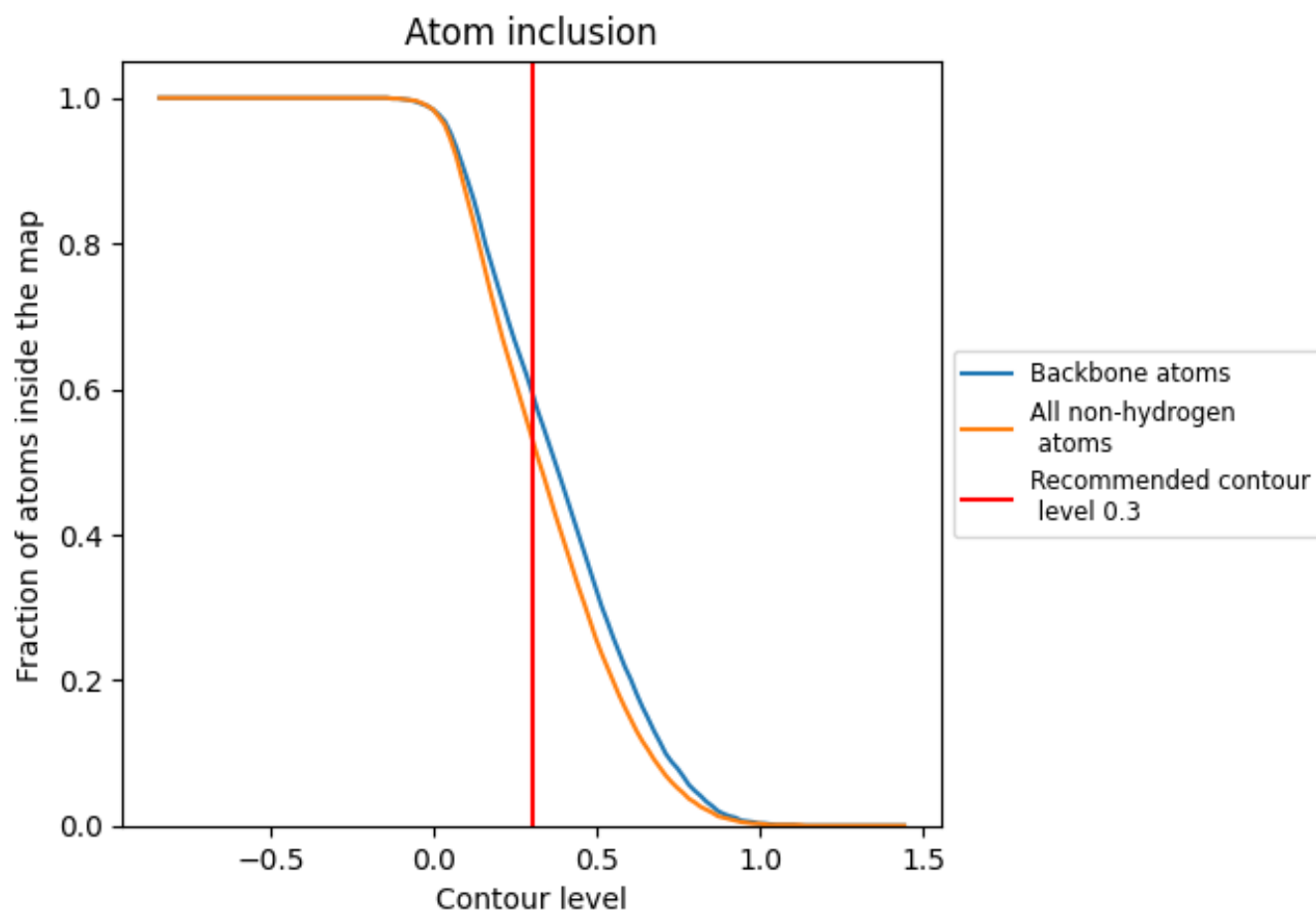
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).





9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5330	 0.5260
A	 0.5330	 0.5260

