



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 05:58 AM UTC

PDB ID : 9BMT / pdb_00009bmt
EMDB ID : EMD-44710
Title : State-5 of motor domain from full-length human dynein-1 in 5 mM ADP
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.70 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

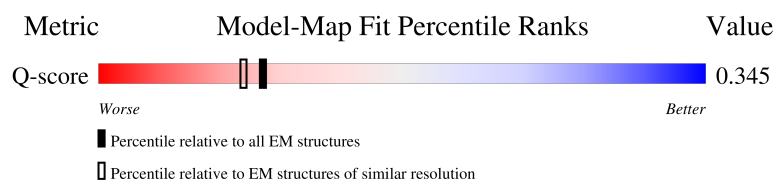
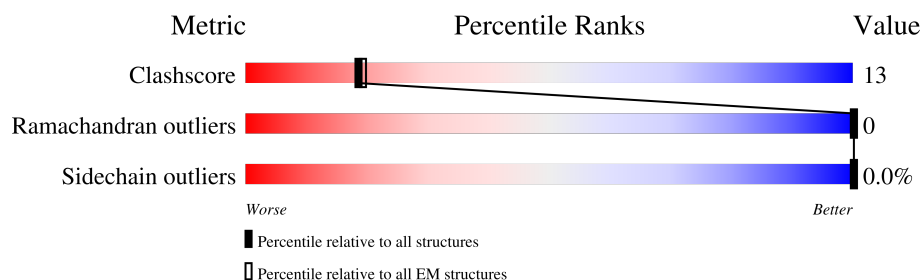
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

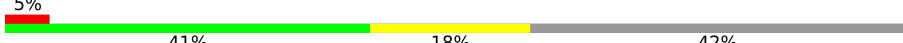
The reported resolution of this entry is 3.70 Å.

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	11569 (3.20 - 4.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4646	

2 Entry composition [i](#)

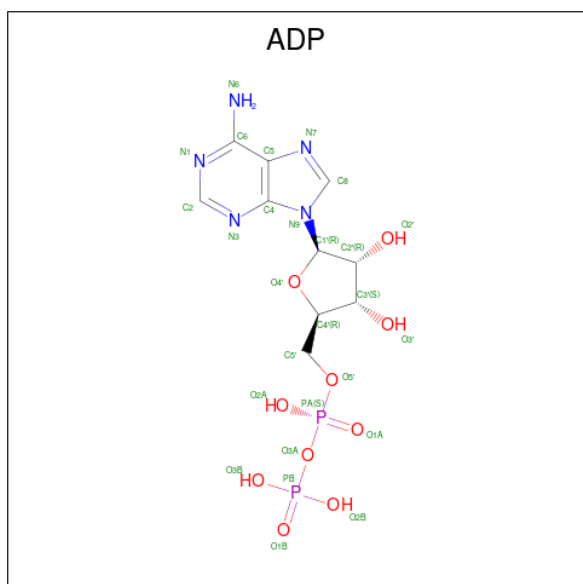
There are 3 unique types of molecules in this entry. The entry contains 21867 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	2711	21755	13852	3757	4035	111	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0
2	A	1	27	10	5	10	2	0
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).



PRO	LYS	E3193	Y3103	L3020	N2913	L2813	Q2707	L2630	S2503	ALA	L2335	L2336	L2127
PRO	LYS	L3194	Q3104	F3021	L2916	L2816	F2708	L2637	S2504	S2410	F2336	F2337	L2131
ALA	MET	E3195	V3105	E3022	D2917	P2817	C2712	H2637	D2505	P2411	P2338	P2339	P2132
VAL	SER	Q3196	G3106	Y3026	H2918	E2818	N2713	Y2638	M2510	M2412	V2339	R2340	E2135
LEU	GLN	Q3197	K3107	A3027	V2919	E2819	P2714	C2639	R2511	A2419	R2341	R2342	Q2139
ALA	ILE	Q3198	T3110	T3028	L2920	G2820	P2718	E2640	A2512	A2420	M2342	M2343	M2145
LEU	ILE	M3199	S3111	M3030	R2922	L2821	P2718	Y2641	E2513	Q2424	T2271	T2272	V2146
GLU	GLN	H3200	L3115	L3031	F2926	W2825	K2721	T2644	L2514	M2423	T2273	T2274	P2147
SER	GLN	L3201	Q3032	Q3033	L2933	A2826	P2722	Q2647	G2515	N2430	R2273	R2274	K2148
LEU	GLN	V3203	C3033	K3034	L2935	L2830	L2723	V2648	E2516	T2434	E2275	E2276	T2154
LEU	GLN	G3204	E3035	E3036	L2936	L2831	F2727	V2649	L2517	T2435	W2276	W2277	E2174
GLY	GLU	L3205	A3037	A3038	G2937	Q2834	P2731	L2650	R2519	A2436	D2278	D2279	M2175
GLU	GLU	R3206	L3206	L3039	C2937	E2841	V2732	K2651	L2520	T2437	F2280	F2281	T2176
THR	ILE	L3208	V3125	E3040	K2943	E2842	W2733	P2652	P2527	E2438	T2282	T2283	L2177
SER	ALA	K3209	P3128	E3041	L2948	R2843	V2734	W2657	W2545	E2444	H2282	H2283	L2178
THR	ASP	E3210	Y3129	E3042	R2948	E2844	W2735	W2658	W2546	H2445	V2284	V2285	E2180
ASP	LYS	T3211	L3131	E3043	V2958	R2845	V2736	V2659	P2547	M2446	C2359	C2360	E2181
GLN	LYS	V3212	K3132	E3044	Q2960	R2847	Q2746	L2661	K2551	D2448	W2361	W2362	L2182
ILE	VAL	Q3213	L3133	E3045	H2964	L2850	L2747	D2664	Q2554	L2449	W2363	W2364	K2183
GLY	VAL	Q3214	Q3135	K3052	R2964	H2857	L2756	E2665	Q2554	R2453	F2364	F2365	L2191
ILE	ASP	V3215	P3136	W3053	Y2967	R2857	R2757	L2666	V2562	C2454	S2365	S2366	T2192
LEU	LEU	E3216	P3137	Q3057	L2967	L2861	L2762	L2668	W2568	L2455	S2370	S2371	W2202
ASP	ASP	E3217	R3140	Q3057	D2973	E2864	R2763	P2669	V2569	F2459	E2294	E2295	K2206
LYS	LYS	L3218	T3143	R3060	L2976	R2869	A2766	D2670	T2583	S2460	Q2292	Q2293	K2209
VAL	VAL	R3219	V3144	R2977	R2977	P2870	L2769	M2671	L2590	L2462	R2297	R2298	Q2209
PRO	ALA	R3220	H3063	V2979	V2979	L2871	L2773	C2673	L2591	H2463	K2381	K2382	L2220
THR	ILE	ASP	V3064	F3066	K2989	L2877	V2774	Y2674	V2592	Q2466	S2384	S2385	W2221
ILE	ILE	LEU	V3150	F3066	L2989	L2877	E2775	G2675	L2593	R2467	I2385	I2386	R2222
VAL	ALA	ILE	Q3152	F3070	F2992	L2882	T2778	Q2677	P2596	N2468	D2304	D2305	V2223
ASN	ASN	LYS	T3153	I2993	I2993	L2882	T2779	T2680	G2600	V2469	D2306	D2307	S2226
SER	ASN	GLN	L3154	M2994	M2994	Q2886	M2779	S2681	K2601	K2470	W2311	W2312	Q2227
ALA	ALA	GLU	K3076	E2996	E2996	L2889	Q2780	F2682	T2602	Q2471	GLU	GLU	S2228
VAL	VAL	LEU	R3077	R3077	R3077	R2890	Q2781	F2683	M2603	M2481	ASP	ASP	M2232
GLU	LYS	GLU	R3078	R3078	R3078	R2891	E2782	L2684	L2605	Q2482	GLU	GLU	R2232
ILE	ILE	LYS	A3079	N2998	N2998	E2892	R2783	R2685	L2605	T2483	ALA	ALA	R2235
SER	LYS	ASN	A3080	V2999	V2999	V2893	F2784	W2686	L2609	E2487	GLN	GLN	R2236
LYS	LYS	ALA	L3085	L3000	L3000	R2896	H2791	V2687	L2609	E2487	ARG	ARG	L2238
ALA	ALA	ALA	F3086	G3003	G3003	Q2896	Y2794	Q2691	M2615	R2487	D2321	D2322	R2243
ASN	ASN	ASN	N3087	F3004	F3004	V2899	Y2794	F2692	E2616	R2487	N2322	N2323	L2244
VAL	VAL	ASP	R3088	L3005	L3005	F2900	R2797	Y2693	Y2493	R2487	L2324	L2325	E2245
LYS	LYS	LYS	C3089	E3006	E3006	V2901	E2798	R2694	V2617	Y2493	LYS	LYS	L2253
VAL	VAL	ARG	V3090	M3007	M3007	E2902	M2799	T2695	N2621	V2496	T2326	T2327	R2257
LYS	LYS	LYS	L3091	M3008	M3008	L2909	W2802	W2700	F2622	A2497	GLU	GLU	A2258
LYS	SER	ASN	N3092	L3012	L3012	V2910	R2803	L2703	S2623	T2499	ASP	ASP	K2257
ASN	ASN	TYR	T3099	L3017	L3017	L2911	R2804	E2704	T2626	L2499	GLU	GLU	A2258
VAL	VAL	LYS	E3100	A3101	A3101	F2912	W2804	R2705	L2706	W2500	GLU	GLU	R2259
ASP	ASP	ASN	A3101	L3102	L3102	F2912	W2804	R2705	L2706	W2500	E2331	E2332	L2333
GLN	GLN	GLU	R3191	S3192	S3192	F2912	W2804	R2705	L2706	W2500	R2332	R2333	S2334
ALA	ALA	LYS	S3192	S3192	S3192	F2912	W2804	R2705	L2706	W2500	R2332	R2333	S2334

M4597	E4439	M4339	M4185	R4000	L3773	T3697	L3688	S3493	VAL
T4598	G4440	I4340	F4186	M4009	K3774	F3698	D3591	E3494	GLU
E4599	K4441			M3875	R3775	F3699		T3495	GLN
								M396	PRO
L4618	T4444	M4343	T4190	S4019	R3776	T3704	A3596	F3496	ILE
F4620	T4445	L4344	Q4191	I4020	A3777	R3705	T3597	T3497	ASN
		K4345	E4192	M4021	R3778	S3706		A397	ARG
		M4346	E4022	A4022	A3779	S3707		A398	ASP
R4638	R4449	M4347	Q4023	Q4023	R3779			A399	LEU
		MET	R4195	Q4024	E3779			M3601	GLU
		LEU	R4196	L3886	E3780	K3718		M3500	ILE
K4457				L3887	T3781			S3501	ALA
		GLU	M4201		R3782	V3724		T3502	ASN
F4482		ASP	L4027	I3890		D3725			ARG
		GLU	T4028		K3783	E3726		S3510	ALA
R4485		ASP	F4207	E3898	V3784	K3727			LEU
T4486		ASP	H4029		E3785	K3728		I3514	ALA
L4487		LEU	F3908		E3786	R3729		A3515	GLY
Q4488		ALA	S4210	L3909	E3787	S3729		Y3516	GLU
L4489		TYR	L4211		D3788	D3730		A3517	TYR
Q4490		ALA	R4212		T3787	E3624		G3518	ALA
M4491		GLU	L4213		L3731			Y3519	VAL
T4492		THR	S4234		L3732			F3520	LEU
		GLU	L4068		K3733				ILE
E4503		LYS	K4237		R3734			Q3523	ALA
		LYS			K3735			K3524	SER
L4511		THR	Y4252		L3734			R3525	GLU
G4512		ARG			Q3732			R3526	ALA
G4513		THR	D4257		Q3735				GLN
L4514		ASP	M4258		Q3736			N3527	ALA
		SER	E4259		E3737			L3528	ILE
		THR	F4260		F3738				ASN
P4517		THR	Q4097		Q3739				LYS
E4518		SER	M4098		L3740			N3532	ALA
		ASP	Q4099		R3741				ASP
T4521		GLY	V3935		L3742			Q3542	LEU
		ARG	L4284		R3743			R3549	ALA
V4528		ARG	A4285		Q3744			T3550	ARG
			C4286		Q3745			E3551	VAL
S4535			K4287		L3745			L3552	GLU
L4536					E3746			S3554	LEU
E4537			E4110		R3747			N3555	ASN
			P4118		K3748			A3556	GLU
V4543			L4126		K3819			D3557	LEU
			E4304					E3558	GLN
T4547			P4135		Q3826			L3560	LYS
			L4138		F3831			R3561	LEU
					F3832			L3478	GLU
A4551			R4143		L3818			L3477	ASP
V4560			T4144		K3819			L3479	ASP
C4570			T4315		Q3826			K3480	ALA
			F4145		I3835			S3481	LYS
			V4146		N3838			L3482	ASP
F4147			F4147		V3756			S3483	ASN
			E3976		K3757			K3579	GLN
			E3977		E3757			L3580	LYS
L4575					I3835			E3485	GLN
			L4323		N3838			R3486	LYS
M4579			P4324		L3840			E3487	ASN
			M4325		Y3841			R3488	
			M4326		E3842			Y3586	
P4586			L4331		N3843			E3489	
T4587			V4417		R3759			E3490	
			S4172		I3760			K3491	
			R4178		L3761			T3492	
			L4179		L3762				
					L3763				
					D3764				
					T3765				
					I3766				
					T3767				
					T3768				
					T3769				
					L3770				
					E3771				
					N3772				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40399	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.679	Depositor
Minimum map value	-0.444	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.11	Depositor
Map size ($\text{\AA}$)	329.984, 329.984, 329.984	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0312, 1.0312, 1.0312	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: ADP, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.14	0/22220	0.33	0/30121

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	21755	0	21789	570	0
2	A	81	0	36	7	0
3	A	31	0	12	2	0
All	All	21867	0	21837	570	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (570) 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:3195:GLU:HA	1:A:3198:GLN:HG2	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1950:GLN:HG2	1:A:2006:VAL:HG13	1.63	0.80
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.63	0.80
1:A:3073:GLU:HA	1:A:3076:LYS:HE2	1.65	0.79
1:A:3499:GLN:HA	1:A:3502:THR:HG22	1.64	0.79
1:A:3790:VAL:HG13	1:A:3794:VAL:HB	1.64	0.78
1:A:4055:VAL:HG11	1:A:4095:MET:HE1	1.64	0.77
1:A:2762:LEU:HD21	1:A:2821:LEU:HD22	1.66	0.76
1:A:2280:PHE:HE1	1:A:2315:LEU:HD21	1.52	0.74
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	1.68	0.74
1:A:2839:GLU:HB3	1:A:2842:GLU:HG2	1.70	0.74
1:A:2053:MET:HE1	1:A:2094:LYS:HA	1.70	0.72
1:A:3871:VAL:HG12	1:A:3875:MET:HE3	1.72	0.71
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.72	0.71
1:A:4400:ARG:HE	1:A:4405:ILE:HD11	1.55	0.71
1:A:1888:CYS:HB2	1:A:2041:MET:HE1	1.71	0.70
1:A:2913:ASN:HA	1:A:2916:LEU:HD12	1.73	0.70
1:A:2449:LEU:HA	1:A:2453:ARG:HH21	1.57	0.69
1:A:4027:LEU:HB3	1:A:4058:LEU:HD22	1.71	0.69
1:A:2253:ILE:O	1:A:2693:TYR:OH	2.09	0.69
1:A:2444:GLU:HB3	1:A:2510:MET:HE1	1.73	0.69
1:A:1880:VAL:HG21	1:A:2052:VAL:HG11	1.73	0.69
1:A:3197:GLN:HG2	1:A:3496:PHE:HZ	1.56	0.69
1:A:2245:GLU:OE1	1:A:2298:ARG:NH2	2.26	0.69
1:A:1927:VAL:HG12	1:A:1954:TRP:HB2	1.76	0.68
1:A:2148:LYS:HB2	1:A:2361:MET:HE2	1.76	0.68
1:A:3154:LEU:HB3	1:A:3171:ILE:HD13	1.76	0.68
1:A:1698:ILE:HD12	1:A:1701:TRP:HE1	1.58	0.68
1:A:4019:SER:O	1:A:4023:GLN:NE2	2.22	0.67
1:A:3191:ARG:NH1	1:A:3500:MET:SD	2.67	0.67
1:A:2979:VAL:HG21	1:A:2992:PHE:HE2	1.60	0.67
1:A:1647:VAL:HA	1:A:1650:LEU:HD13	1.77	0.66
1:A:2258:ALA:HB1	1:A:2682:PHE:HD1	1.60	0.66
1:A:2232:MET:HA	1:A:2235:ARG:HB3	1.78	0.66
1:A:1928:LEU:HD23	1:A:1948:LEU:HD21	1.77	0.65
1:A:1961:ASN:ND2	1:A:2019:ASN:O	2.29	0.65
1:A:1630:TYR:HE2	1:A:1946:VAL:HG23	1.61	0.65
1:A:3558:GLU:HG3	1:A:3561:ARG:HH21	1.62	0.65
1:A:4403:GLU:HA	1:A:4406:LYS:HD2	1.77	0.65
1:A:3175:HIS:HB3	1:A:3516:TYR:HE1	1.62	0.65
1:A:2779:MET:HA	1:A:2782:GLU:HG2	1.77	0.65
1:A:4234:SER:HB3	1:A:4237:LYS:HG2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1713:LEU:HD11	1:A:1872:TYR:HB2	1.79	0.64
1:A:3485:GLU:OE2	1:A:3489:TRP:NE1	2.29	0.64
1:A:2615:MET:HG3	1:A:2658:TRP:HB2	1.79	0.64
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.81	0.63
1:A:4191:GLN:NE2	1:A:4207:PHE:O	2.31	0.63
1:A:2226:SER:HB2	1:A:2726:ARG:HG2	1.80	0.63
1:A:4313:PRO:HB2	1:A:4315:THR:HG22	1.80	0.63
1:A:2677:GLN:HB2	1:A:2680:ILE:HG12	1.81	0.62
1:A:3004:PHE:O	1:A:3008:MET:HG2	1.99	0.62
1:A:2964:HIS:H	1:A:2967:TYR:HB2	1.64	0.62
1:A:2295:LEU:O	1:A:2338:ASN:ND2	2.33	0.62
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.33	0.62
1:A:4027:LEU:HD23	1:A:4030:ILE:HD11	1.81	0.62
1:A:2784:PHE:HB2	1:A:2794:TYR:HE2	1.65	0.62
1:A:3653:VAL:HG12	1:A:3662:ILE:HD11	1.82	0.61
1:A:3115:LEU:HD22	1:A:3143:ILE:HD13	1.82	0.61
1:A:2499:LEU:HD21	1:A:2518:ILE:HG21	1.82	0.61
1:A:4196:TYR:HE1	1:A:4331:LEU:HD22	1.66	0.61
1:A:3197:GLN:HG2	1:A:3496:PHE:CZ	2.36	0.61
1:A:2590:PRO:HG3	1:A:2687:VAL:HG21	1.82	0.61
1:A:4106:LEU:HD23	1:A:4135:PRO:HD2	1.83	0.61
1:A:3485:GLU:HG2	1:A:3770:LEU:HD21	1.82	0.60
1:A:2027:ASN:OD1	1:A:2028:LEU:N	2.33	0.60
1:A:3909:LEU:HD23	1:A:4344:LEU:HA	1.83	0.60
1:A:3518:GLY:HA2	1:A:3579:MET:HE1	1.82	0.60
1:A:2430:ASN:O	1:A:2435:LYS:NZ	2.33	0.60
1:A:2437:LEU:HD21	1:A:2455:LEU:HD21	1.83	0.60
1:A:2797:ARG:NH1	1:A:3087:ASN:OD1	2.35	0.60
1:A:3818:LEU:HD21	1:A:3875:MET:HE2	1.83	0.60
1:A:2445:HIS:ND1	1:A:2505:ASP:OD1	2.34	0.60
1:A:4297:PRO:HG3	1:A:4308:TRP:CG	2.36	0.60
1:A:2113:ARG:O	1:A:2116:GLU:HG3	2.02	0.60
1:A:2131:LEU:HD12	1:A:2132:PRO:HD2	1.83	0.59
1:A:3691:ASP:O	1:A:3695:ARG:HG3	2.03	0.59
1:A:1643:ASN:HD21	1:A:1649:LYS:HD2	1.67	0.59
1:A:3126:MET:HG2	1:A:3128:VAL:HG13	1.84	0.59
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.84	0.59
1:A:3731:LEU:HD12	1:A:3790:VAL:HG21	1.83	0.59
1:A:2933:LEU:HB2	1:A:3065:VAL:HG23	1.84	0.59
1:A:3207:LYS:NZ	1:A:3750:LEU:O	2.34	0.59
1:A:3704:THR:H	1:A:3707:SER:HB3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1631:PHE:HD1	1:A:1657:MET:HG2	1.67	0.59
1:A:1633:GLY:HA2	1:A:1943:ARG:HD2	1.85	0.59
1:A:3580:LEU:HD21	1:A:3699:VAL:HG21	1.84	0.59
1:A:4192:GLU:OE1	1:A:4195:ARG:NH1	2.34	0.59
1:A:3185:ASN:O	1:A:3189:GLU:HG3	2.03	0.58
1:A:4535:SER:OG	1:A:4537:GLU:OE1	2.20	0.58
1:A:1655:LYS:HD2	1:A:2332:ARG:NE	2.18	0.58
1:A:2623:SER:N	1:A:2626:THR:OG1	2.35	0.58
1:A:3689:PRO:HG2	1:A:3692:LEU:HD23	1.85	0.58
1:A:3654:ARG:NH1	1:A:3668:ASP:OD1	2.35	0.58
1:A:3734:LEU:HA	1:A:3738:PHE:HB2	1.85	0.58
1:A:3007:ARG:HD3	1:A:3020:LEU:HD21	1.85	0.58
1:A:3154:LEU:HD21	1:A:3532:TRP:HZ2	1.68	0.58
1:A:2569:VAL:HB	1:A:2747:ILE:HG13	1.85	0.58
1:A:2446:ILE:HG23	1:A:2447:MET:HG2	1.85	0.58
1:A:1746:GLN:HB2	1:A:1749:LEU:HD23	1.85	0.57
1:A:2935:LEU:HB3	1:A:2943:LYS:HD2	1.86	0.57
1:A:3882:THR:HG22	1:A:4339:MET:HG2	1.86	0.57
1:A:4414:GLU:HA	1:A:4417:VAL:HG22	1.87	0.57
1:A:3100:GLU:HA	1:A:3130:TYR:HE1	1.68	0.57
1:A:3935:VAL:HG22	1:A:3996:PHE:HE1	1.69	0.57
1:A:2382:LEU:HD23	1:A:2420:ALA:HB2	1.86	0.57
1:A:1916:VAL:HG13	1:A:2015:PHE:HD2	1.70	0.57
1:A:2684:ARG:HA	1:A:2687:VAL:HG12	1.85	0.57
1:A:2323:LYS:HB3	1:A:2335:LEU:HB3	1.86	0.57
1:A:2797:ARG:NH2	2:A:4703:ADP:O3A	2.37	0.57
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.87	0.57
1:A:3523:GLN:OE1	1:A:3523:GLN:N	2.35	0.56
1:A:4171:LYS:HG3	1:A:4172:SER:H	1.69	0.56
1:A:1899:ARG:HG2	1:A:1986:SER:HB3	1.88	0.56
1:A:2220:LEU:HB2	1:A:2342:MET:HG2	1.87	0.56
1:A:2232:MET:HE2	3:A:4702:ATP:H2'	1.87	0.56
1:A:1711:VAL:HG23	1:A:1853:VAL:HG11	1.87	0.56
1:A:2769:LEU:O	1:A:2773:MET:HG3	2.06	0.56
1:A:3021:PHE:CD1	1:A:3029:LEU:HD22	2.40	0.56
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.37	0.56
1:A:2271:ASN:OD1	1:A:2272:THR:N	2.39	0.56
1:A:2278:GLY:O	1:A:2282:HIS:N	2.29	0.56
1:A:2943:LYS:N	2:A:4704:ADP:O1B	2.35	0.56
1:A:3488:ARG:NH1	1:A:3746:GLU:OE2	2.39	0.56
1:A:4186:PHE:O	1:A:4190:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2669:PRO:O	1:A:2677:GLN:NE2	2.36	0.56
1:A:3048:GLU:O	1:A:3052:LYS:HG2	2.06	0.56
1:A:3746:GLU:O	1:A:3750:LEU:HG	2.06	0.55
1:A:2300:TRP:CD1	1:A:2340:ARG:HB2	2.41	0.55
1:A:3178:ASP:OD2	1:A:3585:ARG:NE	2.39	0.55
1:A:2626:THR:HG23	1:A:2630:LEU:HD12	1.87	0.55
1:A:2979:VAL:HG21	1:A:2992:PHE:CE2	2.42	0.55
1:A:2667:ASN:HB3	1:A:2723:LEU:HD11	1.89	0.55
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	1.87	0.55
1:A:3126:MET:SD	1:A:3126:MET:N	2.80	0.55
1:A:2299:GLN:N	1:A:2299:GLN:OE1	2.40	0.55
1:A:4503:GLU:OE2	1:A:4503:GLU:N	2.38	0.55
1:A:3135:GLN:HB3	1:A:3136:PRO:HD3	1.89	0.55
1:A:1866:PHE:HE2	1:A:1893:THR:HG23	1.72	0.54
1:A:2819:GLU:HA	1:A:2861:ILE:HD11	1.88	0.54
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.40	0.54
1:A:2492:ARG:HG2	1:A:2545:TRP:CE2	2.43	0.54
1:A:4398:LEU:HG	1:A:4417:VAL:HG21	1.89	0.54
1:A:1843:ARG:HH12	1:A:1861:MET:HA	1.73	0.54
1:A:2287:ILE:HD12	1:A:2294:GLU:HG3	1.89	0.54
1:A:3971:PRO:HG2	1:A:3973:LEU:HD11	1.90	0.54
1:A:3003:GLY:HA2	1:A:3006:GLU:HG2	1.88	0.54
1:A:2287:ILE:HG12	1:A:2299:GLN:HE21	1.73	0.54
1:A:2644:THR:OG1	1:A:2647:GLY:O	2.21	0.54
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.90	0.54
1:A:1934:GLU:OE2	1:A:1934:GLU:N	2.27	0.54
1:A:2461:MET:HG2	1:A:2493:TYR:HE1	1.73	0.54
1:A:2791:HIS:CD2	1:A:3091:LEU:HD11	2.43	0.54
1:A:4186:PHE:HE1	1:A:4268:PHE:HB3	1.71	0.54
1:A:1630:TYR:HD2	1:A:1947:GLY:HA2	1.72	0.54
1:A:4445:THR:O	1:A:4449:ARG:N	2.36	0.54
1:A:2660:VAL:HG22	1:A:2707:GLN:HE21	1.72	0.53
1:A:3614:PHE:HE2	1:A:3641:TYR:HD2	1.56	0.53
1:A:4068:SER:HB2	1:A:4097:LYS:HE2	1.90	0.53
1:A:4209:GLU:OE1	1:A:4213:ARG:NH2	2.40	0.53
1:A:1860:GLN:HE22	1:A:1865:LYS:HB3	1.74	0.53
1:A:2901:TYR:OH	1:A:2909:LEU:N	2.35	0.53
1:A:2976:LEU:HA	1:A:2979:VAL:HG22	1.89	0.53
1:A:3831:PHE:O	1:A:3835:ILE:HD12	2.08	0.53
1:A:1945:PHE:HA	1:A:1948:LEU:HD12	1.89	0.53
1:A:2918:HIS:O	1:A:2922:ILE:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2976:LEU:HD22	1:A:3020:LEU:HG	1.90	0.53
1:A:3106:GLY:O	1:A:3110:THR:OG1	2.22	0.53
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.91	0.53
1:A:1755:GLN:OE1	1:A:1922:GLN:NE2	2.37	0.53
1:A:1879:LEU:HD11	2:A:4701:ADP:C6	2.43	0.53
1:A:2596:PRO:O	1:A:2601:LYS:NZ	2.40	0.53
1:A:2877:LEU:HD21	1:A:2892:TYR:HB2	1.90	0.53
1:A:3481:SER:OG	1:A:3767:ILE:HD12	2.09	0.53
1:A:4099:VAL:HG21	1:A:4126:LEU:HD12	1.91	0.53
1:A:2192:THR:HG21	1:A:2373:MET:HG3	1.91	0.53
1:A:2592:VAL:HB	1:A:2733:VAL:HG22	1.91	0.53
1:A:1931:ASN:OD1	1:A:1962:ARG:NH2	2.42	0.53
1:A:3555:ASN:OD1	1:A:3556:ALA:N	2.42	0.53
1:A:3635:VAL:HB	1:A:3679:LEU:HD13	1.90	0.53
1:A:1698:ILE:HD12	1:A:1701:TRP:NE1	2.23	0.52
1:A:1864:ALA:HB2	1:A:1897:GLU:HB2	1.91	0.52
1:A:4026:ASP:OD1	1:A:4028:THR:OG1	2.23	0.52
1:A:3044:LEU:HB3	1:A:3049:GLU:HG3	1.91	0.52
1:A:3974:TRP:NE1	1:A:3976:GLU:OE2	2.42	0.52
1:A:3737:GLU:O	1:A:3741:ARG:N	2.33	0.52
1:A:3933:GLU:HA	1:A:3936:VAL:HG22	1.92	0.52
1:A:1949:CYS:SG	1:A:1978:ILE:HD13	2.49	0.52
1:A:2483:ILE:O	1:A:2487:GLU:HG3	2.10	0.52
1:A:3144:VAL:O	1:A:3148:VAL:HG23	2.10	0.52
1:A:1979:GLN:O	1:A:1983:ARG:HG3	2.10	0.52
1:A:2075:LEU:HD11	1:A:4536:LEU:HD13	1.92	0.52
1:A:2280:PHE:CE1	1:A:2315:LEU:HD21	2.38	0.52
1:A:2889:LEU:HG	1:A:2916:LEU:HD22	1.92	0.52
1:A:3843:ASN:HB3	1:A:3846:LEU:HD12	1.92	0.52
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.90	0.52
1:A:2174:GLU:N	1:A:2174:GLU:OE1	2.41	0.52
1:A:3913:GLU:N	1:A:3913:GLU:OE1	2.43	0.52
1:A:3898:GLU:OE2	1:A:3981:THR:OG1	2.28	0.52
1:A:4512:GLY:HA3	1:A:4645:THR:HG23	1.92	0.52
1:A:2191:LEU:HD21	1:A:2232:MET:HG3	1.92	0.51
1:A:2316:ASN:O	1:A:2358:ARG:NH2	2.43	0.51
1:A:2834:GLN:NE2	1:A:2843:ARG:HD2	2.24	0.51
1:A:2132:PRO:HB2	1:A:2135:GLU:OE2	2.10	0.51
1:A:2683:ILE:HG23	1:A:2708:PHE:HD2	1.75	0.51
1:A:3886:LEU:HD11	1:A:4346:MET:HG3	1.91	0.51
1:A:1939:GLN:H	1:A:1939:GLN:CD	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1687:LYS:HG2	1:A:1712:THR:HG22	1.91	0.51
1:A:2232:MET:SD	1:A:2232:MET:N	2.76	0.51
1:A:2547:PRO:O	1:A:2551:LYS:NZ	2.40	0.51
1:A:2813:LEU:HD13	1:A:2816:LEU:HD13	1.92	0.51
1:A:3743:ARG:NH1	1:A:3743:ARG:O	2.39	0.51
1:A:4402:VAL:HG22	1:A:4406:LYS:HE3	1.92	0.51
1:A:2114:GLU:O	1:A:2117:GLU:HG3	2.11	0.51
1:A:2311:TRP:H	1:A:2311:TRP:CD1	2.29	0.51
1:A:3204:GLY:O	1:A:3208:ILE:HG12	2.11	0.51
1:A:3808:CYS:HB2	1:A:3832:PHE:HZ	1.76	0.51
1:A:3856:LEU:O	1:A:3859:ILE:HG22	2.11	0.51
1:A:4487:LYS:NZ	1:A:4491:ASN:HB2	2.25	0.51
1:A:2839:GLU:HG3	1:A:2841:GLU:H	1.75	0.51
1:A:3729:SER:O	1:A:3733:LYS:HG2	2.11	0.51
1:A:3785:GLU:O	1:A:3789:ILE:HG13	2.11	0.51
1:A:3950:LYS:NZ	1:A:3973:LEU:O	2.38	0.51
1:A:2464:GLN:HG2	1:A:2583:THR:HG22	1.93	0.51
1:A:1686:PHE:HA	1:A:1712:THR:HG21	1.94	0.50
1:A:2263:HIS:CG	1:A:2695:THR:HB	2.46	0.50
1:A:2503:SER:HB3	1:A:2514:LEU:HD22	1.92	0.50
1:A:3731:LEU:O	1:A:3734:LEU:HG	2.11	0.50
1:A:3846:LEU:HD11	1:A:3859:ILE:HD13	1.93	0.50
1:A:2593:LEU:HD11	1:A:2605:LEU:HB2	1.93	0.50
1:A:3017:VAL:HB	1:A:3020:LEU:HD23	1.93	0.50
1:A:2826:ALA:HA	1:A:2850:ILE:HD11	1.93	0.50
1:A:4417:VAL:HG12	1:A:4489:LEU:HD12	1.93	0.50
1:A:3667:GLN:NE2	1:A:3668:ASP:O	2.45	0.50
1:A:2494:LEU:O	1:A:2498:ILE:HD12	2.12	0.50
1:A:1903:SER:N	1:A:2037:ARG:O	2.38	0.50
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.46	0.50
1:A:2948:ARG:HG2	1:A:2958:VAL:HG21	1.93	0.50
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.93	0.50
1:A:2299:GLN:NE2	1:A:2338:ASN:OD1	2.44	0.50
1:A:2773:MET:HG2	1:A:2825:TRP:HE1	1.77	0.50
1:A:3100:GLU:HA	1:A:3130:TYR:CE1	2.47	0.50
1:A:3488:ARG:HG2	1:A:3491:LYS:HE3	1.94	0.50
1:A:2054:LEU:HD21	1:A:2097:LEU:HD22	1.93	0.49
1:A:2363:TRP:HE1	1:A:2365:SER:HB2	1.77	0.49
1:A:2995:ASP:OD2	1:A:2996:GLU:N	2.45	0.49
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.12	0.49
1:A:3032:GLN:O	1:A:3035:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3875:MET:HE1	1:A:3883:PHE:CG	2.47	0.49
1:A:1630:TYR:CE2	1:A:1946:VAL:HG23	2.44	0.49
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.95	0.49
1:A:1647:VAL:HG11	1:A:1692:ILE:HD13	1.94	0.49
1:A:1779:HIS:CE1	1:A:1826:ILE:HD12	2.48	0.49
1:A:3884:ALA:HB1	1:A:4009:VAL:HG11	1.94	0.49
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.95	0.49
1:A:2455:LEU:HD12	1:A:2459:PHE:CZ	2.47	0.49
1:A:2890:ARG:NH1	1:A:2911:LEU:O	2.46	0.49
1:A:4511:LEU:HD23	1:A:4560:VAL:HG13	1.94	0.49
1:A:1913:THR:O	1:A:1917:LYS:HG3	2.12	0.49
1:A:2773:MET:HB2	1:A:2799:MET:HE3	1.93	0.49
1:A:2306:ASP:OD1	1:A:2307:VAL:N	2.46	0.49
1:A:3492:THR:O	1:A:3496:PHE:HB2	2.13	0.49
1:A:1751:VAL:HG21	1:A:1878:LYS:HZ1	1.78	0.49
1:A:2286:LYS:HZ2	1:A:2291:VAL:HB	1.78	0.49
1:A:3201:LEU:HD22	1:A:3496:PHE:CD2	2.48	0.48
1:A:2387:LEU:H	1:A:2412:MET:HE1	1.76	0.48
1:A:2658:TRP:CE3	1:A:2705:ARG:HA	2.48	0.48
1:A:2718:PRO:HB2	1:A:3080:ALA:HB2	1.95	0.48
1:A:2886:GLN:OE1	1:A:2886:GLN:N	2.35	0.48
1:A:4190:ILE:HG23	1:A:4201:TRP:CZ2	2.48	0.48
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.94	0.48
1:A:1724:VAL:O	1:A:1728:GLY:N	2.45	0.48
1:A:2517:TYR:HA	1:A:2520:ARG:HD3	1.95	0.48
1:A:3838:ASN:ND2	1:A:3842:GLU:OE2	2.47	0.48
1:A:2387:LEU:HD11	1:A:2463:HIS:HB3	1.95	0.48
1:A:2453:ARG:NH1	1:A:2505:ASP:OD2	2.47	0.48
1:A:3524:MET:O	1:A:3528:LEU:HG	2.13	0.48
1:A:3624:GLU:OE1	1:A:3669:ILE:HD13	2.14	0.48
1:A:4257:ASP:OD1	1:A:4258:ASN:N	2.47	0.48
1:A:2641:TYR:CD1	1:A:2650:LEU:HD13	2.48	0.48
1:A:3037:ALA:HA	1:A:3040:GLU:HG2	1.96	0.48
1:A:3007:ARG:HH11	1:A:3020:LEU:HD22	1.79	0.48
1:A:3028:THR:HG22	1:A:3032:GLN:HE21	1.78	0.48
1:A:3196:GLU:O	1:A:3200:HIS:ND1	2.37	0.48
1:A:3553:LEU:HD12	1:A:3582:ARG:NH1	2.29	0.48
1:A:1632:VAL:HB	1:A:1636:ASP:HB2	1.96	0.48
1:A:1769:MET:HG3	1:A:1831:ASP:HA	1.95	0.48
1:A:3510:SER:O	1:A:3514:ILE:HG12	2.13	0.48
1:A:4393:GLN:HG2	1:A:4428:ARG:HH21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4570:CYS:HB3	1:A:4575:LEU:HD23	1.95	0.48
1:A:2322:ASN:OD1	1:A:2323:LYS:N	2.47	0.48
1:A:2091:ARG:HD2	1:A:2357:SER:HB2	1.96	0.47
1:A:2600:GLY:H	2:A:4703:ADP:H5'2	1.79	0.47
1:A:3935:VAL:HG13	1:A:3947:LEU:HD23	1.96	0.47
1:A:4190:ILE:HG23	1:A:4201:TRP:HZ2	1.79	0.47
1:A:2387:LEU:N	1:A:2412:MET:HE1	2.29	0.47
1:A:3743:ARG:HH12	1:A:3747:LYS:HB3	1.79	0.47
1:A:1708:GLU:HA	1:A:1711:VAL:HG12	1.96	0.47
1:A:2297:LYS:O	1:A:2338:ASN:ND2	2.48	0.47
1:A:4518:GLU:OE2	1:A:4518:GLU:N	2.35	0.47
1:A:2869:ARG:O	1:A:2871:ILE:HD12	2.15	0.47
1:A:2937:GLY:C	1:A:3070:PRO:HD3	2.39	0.47
1:A:3840:LEU:HA	1:A:3859:ILE:HD11	1.95	0.47
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.96	0.47
1:A:2465:ALA:HB2	1:A:2493:TYR:CE1	2.49	0.47
1:A:3944:PHE:CZ	1:A:3974:TRP:HB3	2.50	0.47
1:A:4071:ILE:HG13	1:A:4099:VAL:HG12	1.97	0.47
1:A:1756:ILE:HG13	1:A:1844:PHE:HB3	1.96	0.47
1:A:2063:GLU:OE1	1:A:2063:GLU:N	2.39	0.47
1:A:3026:TYR:CE1	1:A:3030:MET:HE3	2.48	0.47
1:A:3133:LEU:HD12	1:A:3134:PRO:HD2	1.96	0.47
1:A:3591:ASP:OD1	1:A:3591:ASP:N	2.47	0.47
1:A:2029:PRO:HG2	1:A:2032:LEU:HD12	1.97	0.47
1:A:2238:LEU:HD12	1:A:2300:TRP:CE3	2.50	0.47
1:A:2899:VAL:HA	1:A:2902:GLU:HG2	1.97	0.47
1:A:3057:GLN:HE22	1:A:3060:ARG:HH21	1.63	0.47
1:A:3751:GLN:HA	1:A:3754:ASN:HD22	1.80	0.47
1:A:1914:GLU:OE1	2:A:4701:ADP:H3'	2.15	0.47
1:A:2960:GLN:HG3	1:A:2993:ILE:HB	1.96	0.47
1:A:3195:GLU:O	1:A:3198:GLN:HB2	2.15	0.47
1:A:3787:THR:O	1:A:3790:VAL:HB	2.15	0.47
1:A:3140:ARG:HA	1:A:3143:ILE:HG12	1.96	0.47
1:A:3526:GLN:OE1	1:A:3549:ARG:NH2	2.39	0.47
1:A:4374:PRO:HB2	1:A:4376:TRP:CD1	2.50	0.47
1:A:4543:VAL:HG13	1:A:4588:THR:HG23	1.97	0.47
1:A:2893:VAL:HG13	1:A:2911:LEU:HD13	1.97	0.46
1:A:3553:LEU:O	1:A:3582:ARG:NH2	2.47	0.46
1:A:1752:LEU:O	1:A:1756:ILE:HD12	2.15	0.46
1:A:1763:GLU:OE2	1:A:1845:TYR:OH	2.29	0.46
1:A:2461:MET:SD	1:A:2497:ALA:HA	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.49	0.46
1:A:1643:ASN:OD1	1:A:1646:ASN:HB2	2.15	0.46
1:A:2180:GLU:O	1:A:2183:LYS:HG2	2.15	0.46
1:A:3695:ARG:HH11	1:A:3695:ARG:HG2	1.80	0.46
1:A:3870:ARG:HD3	1:A:4143:ARG:HH12	1.80	0.46
1:A:3883:PHE:O	1:A:3887:LEU:HD23	2.16	0.46
1:A:1722:THR:O	1:A:1726:ILE:HG12	2.15	0.46
1:A:1788:THR:HA	1:A:1791:VAL:HG22	1.98	0.46
1:A:3692:LEU:O	1:A:3696:VAL:HG22	2.15	0.46
1:A:3766:ILE:O	1:A:3769:THR:OG1	2.29	0.46
1:A:4143:ARG:HG2	1:A:4145:PHE:CE2	2.50	0.46
1:A:1631:PHE:CD1	1:A:1657:MET:HG2	2.50	0.46
1:A:1917:LYS:HA	1:A:1927:VAL:HG21	1.96	0.46
1:A:2115:LYS:HE3	1:A:2121:ALA:O	2.15	0.46
1:A:2596:PRO:HD3	1:A:2735:TYR:HE1	1.81	0.46
1:A:3488:ARG:O	1:A:3491:LYS:HG3	2.15	0.46
1:A:1900:LEU:HD21	1:A:2037:ARG:HH21	1.81	0.46
1:A:1784:ASN:O	1:A:1788:THR:HG22	2.16	0.46
1:A:1866:PHE:CE2	1:A:1893:THR:HG23	2.50	0.46
1:A:2472:TYR:HD2	1:A:2481:MET:HE2	1.79	0.46
1:A:2609:LEU:HD13	1:A:2617:VAL:HG22	1.96	0.46
1:A:2284:LEU:O	1:A:2287:ILE:HG22	2.16	0.46
1:A:4178:ARG:NH1	1:A:4296:MET:HE1	2.30	0.46
1:A:2926:PHE:HD1	1:A:3063:HIS:CD2	2.34	0.46
1:A:3759:ARG:HG3	1:A:3760:ILE:HG12	1.97	0.46
1:A:2228:SER:N	3:A:4702:ATP:O1B	2.48	0.46
1:A:2346:GLN:HB3	1:A:2726:ARG:HD2	1.98	0.46
1:A:2670:ASP:HA	1:A:2721:LYS:HE3	1.97	0.46
1:A:2300:TRP:HE1	1:A:2340:ARG:HG3	1.82	0.45
1:A:2554:GLN:OE1	1:A:2746:GLN:NE2	2.49	0.45
1:A:1788:THR:O	1:A:1792:LEU:HD23	2.17	0.45
1:A:2664:ASP:OD1	1:A:2665:GLU:N	2.48	0.45
1:A:4211:ASP:OD1	1:A:4212:LEU:N	2.49	0.45
1:A:1810:HIS:NE2	1:A:1876:GLN:O	2.47	0.45
1:A:2286:LYS:NZ	1:A:2291:VAL:HB	2.32	0.45
1:A:2661:LEU:HB3	1:A:2708:PHE:CD1	2.51	0.45
1:A:1945:PHE:HE2	1:A:1978:ILE:HD12	1.82	0.45
1:A:2028:LEU:HD21	1:A:2036:PHE:HB2	1.99	0.45
1:A:3886:LEU:O	1:A:3890:ILE:HG12	2.17	0.45
1:A:1940:ALA:HA	1:A:1943:ARG:NE	2.32	0.45
1:A:2050:ALA:O	1:A:2054:LEU:HD23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1627:PRO:HB2	1:A:1950:GLN:HB3	1.99	0.45
1:A:2145:MET:O	1:A:2148:LYS:HG2	2.17	0.45
1:A:2562:VAL:O	1:A:2804:ARG:NH1	2.49	0.45
1:A:2592:VAL:HG23	1:A:2731:VAL:HG11	1.99	0.45
1:A:3206:ARG:O	1:A:3210:GLU:HG2	2.17	0.45
1:A:4186:PHE:HE2	1:A:4252:TYR:CD2	2.34	0.45
1:A:4324:PRO:HB3	1:A:4638:ARG:NH2	2.32	0.45
1:A:4412:PHE:HZ	1:A:4514:LEU:HD13	1.82	0.45
1:A:1959:GLU:HB3	1:A:1962:ARG:HG3	1.99	0.45
1:A:2652:PRO:HD2	1:A:2705:ARG:CZ	2.47	0.45
1:A:2756:LEU:HD12	1:A:2766:ALA:HB2	1.98	0.45
1:A:2115:LYS:HD2	1:A:2118:ARG:NH1	2.32	0.45
1:A:3744:GLN:O	1:A:3747:LYS:HG3	2.17	0.45
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.98	0.45
1:A:4411:ARG:O	1:A:4414:GLU:HG3	2.17	0.45
1:A:4444:GLN:O	1:A:4449:ARG:NH1	2.49	0.45
1:A:2896:ARG:HA	1:A:2896:ARG:HD2	1.76	0.45
1:A:2973:ASP:O	1:A:2977:ARG:HD3	2.17	0.45
1:A:3796:THR:HA	1:A:3799:GLN:HG3	1.99	0.45
1:A:3908:PHE:HD2	1:A:3909:LEU:HD12	1.82	0.45
1:A:3922:PRO:HG2	1:A:3924:ILE:HD11	1.99	0.45
1:A:4336:GLY:O	1:A:4340:ILE:HG12	2.16	0.45
1:A:4489:LEU:HA	1:A:4492:ILE:HG22	1.98	0.45
1:A:1882:THR:HG23	1:A:1885:THR:H	1.81	0.44
1:A:2223:VAL:HG13	1:A:2363:TRP:HE3	1.82	0.44
1:A:3553:LEU:HD12	1:A:3582:ARG:CZ	2.47	0.44
1:A:3870:ARG:HD3	1:A:4143:ARG:NH1	2.32	0.44
1:A:1683:GLU:OE2	1:A:1683:GLU:N	2.50	0.44
1:A:2778:THR:O	1:A:2781:GLN:HG3	2.17	0.44
1:A:1946:VAL:HG12	1:A:2001:LEU:HD13	2.00	0.44
1:A:2472:TYR:CD2	1:A:2481:MET:HE2	2.52	0.44
1:A:3747:LYS:HA	1:A:3750:LEU:HD12	1.99	0.44
1:A:4021:MET:HA	1:A:4021:MET:HE2	1.99	0.44
1:A:4619:ILE:HG22	1:A:4620:PHE:HD1	1.82	0.44
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.50	0.44
1:A:2148:LYS:HB2	1:A:2361:MET:CE	2.45	0.44
1:A:2469:VAL:HG13	1:A:2481:MET:CE	2.47	0.44
1:A:3012:LEU:HD13	1:A:3089:CYS:SG	2.57	0.44
1:A:3117:LYS:NZ	1:A:3542:GLN:OE1	2.32	0.44
1:A:1751:VAL:HG13	1:A:1814:GLU:HG3	1.99	0.44
1:A:2370:SER:H	1:A:2373:MET:CE	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2756:LEU:HD13	1:A:2762:LEU:HD23	2.00	0.44
1:A:3078:ARG:CZ	1:A:3078:ARG:HA	2.48	0.44
1:A:3596:ALA:O	1:A:3600:ILE:HG12	2.17	0.44
1:A:1850:GLN:HB3	1:A:1856:GLN:HG2	1.99	0.44
1:A:3938:LEU:HD13	1:A:3995:ALA:HB2	2.00	0.44
1:A:2012:MET:HE2	1:A:2012:MET:HB2	1.91	0.44
1:A:2381:ARG:HH21	1:A:2385:ILE:HG21	1.82	0.44
1:A:2681:SER:HA	1:A:2684:ARG:HG2	2.00	0.44
1:A:2992:PHE:HE1	1:A:2994:MET:SD	2.41	0.44
1:A:3172:THR:HG21	1:A:3694:SER:HB2	2.00	0.44
1:A:4485:ARG:HG2	1:A:4513:GLY:HA2	1.99	0.44
1:A:2123:ASP:O	1:A:2127:ILE:HG13	2.17	0.44
1:A:2307:VAL:HG23	1:A:2311:TRP:CZ2	2.53	0.44
1:A:2467:ARG:O	1:A:2471:GLN:HG2	2.18	0.44
1:A:2639:CYS:HA	1:A:2652:PRO:HA	1.99	0.44
1:A:3161:LEU:HD11	1:A:3524:MET:HE3	1.99	0.44
1:A:3705:ARG:HG2	1:A:3813:PHE:CE2	2.53	0.44
1:A:1846:PHE:CE1	1:A:1856:GLN:HB3	2.53	0.43
1:A:2568:VAL:HG23	1:A:2603:MET:HE1	2.00	0.43
1:A:1843:ARG:NH1	1:A:1861:MET:HA	2.33	0.43
1:A:2757:ARG:HA	1:A:2763:ARG:HE	1.83	0.43
1:A:3718:LYS:HA	1:A:3725:ASP:OD1	2.18	0.43
1:A:2175:MET:HB3	1:A:2178:LEU:HB3	2.00	0.43
1:A:2601:LYS:HG2	1:A:2736:VAL:HB	1.98	0.43
1:A:3551:GLU:OE1	1:A:3559:ARG:NH1	2.51	0.43
1:A:4343:MET:HE2	1:A:4343:MET:HB3	1.80	0.43
1:A:4517:PRO:O	1:A:4521:ILE:HD12	2.18	0.43
1:A:1751:VAL:HG11	1:A:1878:LYS:HZ1	1.82	0.43
1:A:2315:LEU:HD23	1:A:2315:LEU:HA	1.73	0.43
1:A:3793:GLU:OE2	1:A:3794:VAL:HG23	2.17	0.43
1:A:3819:LYS:HE3	1:A:3826:GLN:OE1	2.17	0.43
1:A:4067:THR:O	1:A:4095:MET:N	2.49	0.43
1:A:4196:TYR:HD2	1:A:4323:LEU:HD22	1.83	0.43
1:A:4286:CYS:C	1:A:4287:LYS:HG2	2.43	0.43
1:A:1628:ARG:CZ	1:A:1951:VAL:HG13	2.48	0.43
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	2.01	0.43
1:A:3644:VAL:HG23	1:A:3645:LEU:HD22	2.00	0.43
1:A:4106:LEU:HD11	1:A:4138:LEU:HD22	2.00	0.43
1:A:1842:MET:HA	1:A:1861:MET:HB2	2.01	0.43
1:A:2693:TYR:CE1	1:A:2700:TRP:HE3	2.36	0.43
1:A:2813:LEU:HD21	1:A:2882:ILE:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3103:TYR:CE2	1:A:3107:LYS:HD2	2.53	0.43
1:A:2691:GLY:HA2	1:A:2703:LEU:HG	2.00	0.43
1:A:2830:LEU:O	1:A:2834:GLN:HB3	2.18	0.43
1:A:3568:PRO:HG2	1:A:3573:CYS:SG	2.59	0.43
1:A:1836:PHE:HA	1:A:1839:LEU:HB2	2.00	0.43
1:A:2147:PRO:HG3	1:A:2209:GLN:HB3	2.01	0.43
1:A:2419:ALA:O	1:A:2423:MET:HG2	2.19	0.43
1:A:3149:PHE:O	1:A:3153:THR:HG23	2.18	0.43
1:A:3204:GLY:HA3	1:A:3489:TRP:CH2	2.54	0.43
1:A:4179:LEU:HD23	1:A:4179:LEU:HA	1.85	0.43
1:A:4185:TRP:CD2	1:A:4284:LEU:HD21	2.54	0.43
1:A:1629:PHE:O	1:A:1632:VAL:HG22	2.18	0.43
1:A:1713:LEU:HD22	1:A:1749:LEU:HD21	1.99	0.43
1:A:1942:GLY:O	1:A:1946:VAL:HG22	2.19	0.43
1:A:2076:CYS:HB3	1:A:2088:PHE:CE2	2.54	0.43
1:A:2383:ARG:NH2	1:A:2424:GLN:OE1	2.24	0.43
1:A:4260:PHE:HE2	1:A:4618:LEU:HD11	1.84	0.43
1:A:2648:VAL:HG21	1:A:2694:ARG:HH22	1.82	0.42
1:A:2666:ILE:HG22	1:A:2712:CYS:HB3	2.00	0.42
1:A:3555:ASN:HB3	1:A:3558:GLU:OE2	2.19	0.42
1:A:4547:THR:HA	1:A:4586:PRO:HB2	2.01	0.42
1:A:2181:GLU:OE1	1:A:2243:ARG:NH1	2.53	0.42
1:A:3561:ARG:NH1	1:A:3603:GLU:OE2	2.52	0.42
1:A:3606:ASP:N	1:A:3606:ASP:OD1	2.49	0.42
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	2.01	0.42
1:A:2135:GLU:H	1:A:2135:GLU:CD	2.24	0.42
1:A:2381:ARG:O	1:A:2385:ILE:HG22	2.19	0.42
1:A:2446:ILE:HD11	1:A:2714:PRO:HB3	1.99	0.42
1:A:2683:ILE:HG23	1:A:2708:PHE:CD2	2.53	0.42
1:A:2686:MET:HA	1:A:2691:GLY:O	2.19	0.42
1:A:3101:ALA:O	1:A:3105:VAL:HG23	2.20	0.42
1:A:1845:TYR:HE1	1:A:1860:GLN:HB2	1.84	0.42
1:A:2723:LEU:HD23	1:A:2727:PHE:CE1	2.54	0.42
1:A:3597:THR:HG21	1:A:3611:ARG:HH12	1.85	0.42
1:A:3950:LYS:NZ	1:A:3975:SER:HB3	2.34	0.42
1:A:4482:PHE:O	1:A:4486:ILE:HG12	2.18	0.42
1:A:2146:VAL:HG13	1:A:2154:ILE:HD12	1.99	0.42
1:A:2238:LEU:HB2	1:A:2300:TRP:CZ3	2.54	0.42
1:A:2492:ARG:HG2	1:A:2545:TRP:NE1	2.34	0.42
1:A:2864:GLU:OE1	1:A:2864:GLU:N	2.46	0.42
1:A:3160:ARG:HH12	1:A:3524:MET:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2496:TYR:CE1	1:A:2500:TRP:HD1	2.38	0.42
1:A:2512:ALA:O	1:A:2516:GLU:HG2	2.19	0.42
1:A:3207:LYS:HD2	1:A:3754:ASN:OD1	2.20	0.42
1:A:2102:ASN:HA	1:A:2105:ARG:NH1	2.34	0.42
1:A:2117:GLU:OE2	1:A:2118:ARG:HD2	2.19	0.42
1:A:2989:LYS:HE2	1:A:3060:ARG:HH12	1.83	0.42
1:A:3586:TYR:HD2	1:A:3649:LEU:HD23	1.84	0.42
1:A:1853:VAL:HA	1:A:1856:GLN:HG3	2.02	0.42
1:A:1899:ARG:HD3	1:A:1899:ARG:HA	1.83	0.42
1:A:2114:GLU:HA	1:A:2117:GLU:HG3	2.02	0.42
1:A:2935:LEU:N	1:A:3066:PHE:O	2.52	0.42
1:A:3150:VAL:O	1:A:3154:LEU:HD23	2.20	0.42
1:A:3655:ARG:NE	1:A:3660:VAL:HG22	2.35	0.42
1:A:4107:MET:HE3	1:A:4110:GLU:HB3	2.01	0.42
1:A:2287:ILE:CG1	1:A:2299:GLN:HE21	2.33	0.42
1:A:2747:ILE:HD11	2:A:4703:ADP:C2	2.55	0.42
1:A:1850:GLN:OE1	1:A:1851:THR:N	2.53	0.42
1:A:3518:GLY:CA	1:A:3579:MET:HE1	2.49	0.42
1:A:3789:ILE:HG22	1:A:3793:GLU:HG2	2.00	0.42
1:A:4055:VAL:CG1	1:A:4095:MET:HE1	2.43	0.42
1:A:2221:MET:HE1	1:A:2343:PHE:HB2	2.02	0.41
1:A:3885:MET:HE3	1:A:3885:MET:HB3	1.85	0.41
1:A:2073:PHE:HE2	1:A:2093:LEU:HA	1.84	0.41
1:A:2202:MET:SD	1:A:2202:MET:N	2.94	0.41
1:A:3040:GLU:OE2	1:A:3053:TRP:NE1	2.53	0.41
1:A:4025:LEU:HD21	1:A:4147:PHE:CE2	2.55	0.41
1:A:2176:THR:O	1:A:2180:GLU:HG2	2.21	0.41
1:A:3003:GLY:O	1:A:3006:GLU:HG2	2.20	0.41
1:A:3151:HIS:CE1	1:A:3176:TYR:HB2	2.55	0.41
1:A:3196:GLU:HG2	1:A:3200:HIS:CE1	2.56	0.41
1:A:3614:PHE:CE2	1:A:3638:VAL:HG23	2.55	0.41
1:A:3783:LYS:O	1:A:3787:THR:HG23	2.20	0.41
1:A:1847:ASP:N	1:A:1856:GLN:O	2.45	0.41
1:A:2847:ASP:O	1:A:2850:ILE:HG22	2.20	0.41
1:A:3570:ASP:HB3	1:A:3573:CYS:SG	2.60	0.41
1:A:1652:LYS:HA	1:A:1655:LYS:HE3	2.02	0.41
1:A:1846:PHE:HE1	1:A:1856:GLN:HB3	1.86	0.41
1:A:1999:CYS:SG	1:A:2000:GLU:N	2.94	0.41
1:A:2206:LYS:HD3	1:A:2206:LYS:HA	1.85	0.41
1:A:2671:MET:HG2	1:A:2672:ASP:O	2.20	0.41
1:A:2920:LEU:HD23	1:A:2920:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3005:LEU:HD12	1:A:3085:LEU:HD11	2.02	0.41
1:A:3030:MET:HA	1:A:3033:CYS:SG	2.61	0.41
1:A:3807:ALA:O	1:A:3811:ILE:HG12	2.20	0.41
1:A:3856:LEU:HA	1:A:3859:ILE:HG22	2.03	0.41
1:A:4528:VAL:HG11	1:A:4592:TRP:CB	2.51	0.41
1:A:2348:LEU:HD23	1:A:2348:LEU:HA	1.87	0.41
1:A:2590:PRO:HG2	1:A:2731:VAL:HG22	2.01	0.41
1:A:3780:VAL:O	1:A:3784:VAL:HG23	2.21	0.41
1:A:3950:LYS:HZ2	1:A:3975:SER:HB3	1.86	0.41
1:A:3993:ILE:HD13	1:A:3993:ILE:HA	1.92	0.41
1:A:2018:MET:HB3	1:A:2018:MET:HE2	1.80	0.41
1:A:2434:THR:HG22	1:A:2438:GLU:OE2	2.21	0.41
1:A:3128:VAL:HG12	1:A:3133:LEU:HD23	2.02	0.41
1:A:3177:LEU:HD11	2:A:4704:ADP:HI'	2.02	0.41
1:A:3588:LEU:HD23	1:A:3698:PHE:CE1	2.55	0.41
1:A:3624:GLU:OE1	1:A:3624:GLU:HA	2.20	0.41
1:A:2519:ARG:HG2	1:A:2526:LEU:HD13	2.03	0.41
1:A:3724:VAL:HG11	1:A:3797:VAL:HG21	2.02	0.41
1:A:1738:TYR:HE1	1:A:1792:LEU:HD21	1.86	0.40
1:A:1739:ILE:HG23	1:A:1804:ARG:HD3	2.03	0.40
1:A:2527:PRO:HG3	1:A:2545:TRP:CG	2.56	0.40
1:A:3112:LYS:HA	1:A:3112:LYS:HD3	1.94	0.40
1:A:3841:TYR:O	1:A:3842:GLU:HG2	2.20	0.40
1:A:4304:GLU:OE2	1:A:4304:GLU:N	2.37	0.40
1:A:1792:LEU:HB3	1:A:1812:ILE:HG12	2.04	0.40
1:A:1888:CYS:HA	1:A:2039:LEU:HD21	2.03	0.40
1:A:2114:GLU:O	1:A:2118:ARG:HD3	2.21	0.40
1:A:3601:MET:HE1	1:A:3611:ARG:HB2	2.04	0.40
1:A:1697:LYS:O	1:A:1701:TRP:HD1	2.05	0.40
1:A:1904:PRO:O	1:A:1912:LYS:HD2	2.21	0.40
1:A:2115:LYS:HD2	1:A:2118:ARG:HH12	1.86	0.40
1:A:3765:THR:C	1:A:3767:ILE:H	2.28	0.40
1:A:1936:PHE:CZ	1:A:1941:MET:HG3	2.56	0.40
1:A:2257:LYS:HD2	1:A:2257:LYS:HA	1.77	0.40
1:A:3653:VAL:HA	1:A:3662:ILE:HG13	2.02	0.40
1:A:3755:GLU:HB3	1:A:3757:LYS:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2699/4646 (58%)	2645 (98%)	54 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2407/4125 (58%)	2406 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3092	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1779	HIS
1	A	1856	GLN
1	A	1863	ASN
1	A	1894	GLN
1	A	1939	GLN
1	A	1974	GLN
1	A	2051	GLN

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Mol	Chain	Res	Type
1	A	2109	GLN
1	A	2171	HIS
1	A	2464	GLN
1	A	2471	GLN
1	A	2482	GLN
1	A	2531	ASN
1	A	2560	HIS
1	A	2707	GLN
1	A	2789	GLN
1	A	2834	GLN
1	A	3032	GLN
1	A	3135	GLN
1	A	3181	ASN
1	A	3182	HIS
1	A	3188	HIS
1	A	3535	HIS
1	A	3563	GLN
1	A	3584	ASN
1	A	3754	ASN
1	A	3772	ASN
1	A	3800	GLN
1	A	4231	GLN
1	A	4397	HIS
1	A	4589	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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	4703	-	28,29,29	1.40	4 (14%)	43,45,45	1.89	8 (18%)
2	ADP	A	4704	-	28,29,29	1.39	4 (14%)	43,45,45	1.81	9 (20%)
2	ADP	A	4701	-	28,29,29	1.40	5 (17%)	43,45,45	1.71	7 (16%)
3	ATP	A	4702	-	32,33,33	0.50	1 (3%)	48,52,52	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	4703	-	-	4/16/32/32	0/3/3/3
2	ADP	A	4704	-	-	1/16/32/32	0/3/3/3
2	ADP	A	4701	-	-	1/16/32/32	0/3/3/3
3	ATP	A	4702	-	-	4/22/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4701	ADP	C5-C4	4.74	1.47	1.39
2	A	4703	ADP	C5-C4	4.70	1.47	1.39
2	A	4704	ADP	C5-C4	4.61	1.47	1.39
2	A	4704	ADP	C5-C6	2.69	1.48	1.41
2	A	4703	ADP	C5-C6	2.67	1.48	1.41
2	A	4701	ADP	C5-C6	2.51	1.48	1.41
2	A	4703	ADP	C5-N7	-2.38	1.34	1.39
2	A	4704	ADP	C8-N7	2.37	1.36	1.31
2	A	4701	ADP	C5-N7	-2.36	1.34	1.39
2	A	4701	ADP	C8-N7	2.29	1.36	1.31
2	A	4704	ADP	C5-N7	-2.27	1.34	1.39
2	A	4703	ADP	C8-N7	2.20	1.35	1.31
2	A	4701	ADP	C4-N9	-2.05	1.33	1.37
3	A	4702	ATP	PA-O3A	-2.03	1.57	1.59

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	C5-C4-N3	-6.19	118.19	126.72
2	A	4704	ADP	C5-C4-N3	-5.74	118.82	126.72
2	A	4701	ADP	C5-C4-N3	-5.32	119.39	126.72
2	A	4703	ADP	N3-C4-N9	4.96	135.61	127.17
2	A	4704	ADP	N3-C4-N9	4.53	134.88	127.17
2	A	4701	ADP	N3-C4-N9	4.37	134.60	127.17
2	A	4703	ADP	C2-N3-C4	3.89	121.34	111.83
2	A	4704	ADP	C2-N3-C4	3.65	120.74	111.83
2	A	4704	ADP	C4-C5-N7	-3.42	106.67	110.58
2	A	4701	ADP	C2-N3-C4	3.38	120.08	111.83
2	A	4703	ADP	N3-C2-N1	-3.34	123.53	128.58
2	A	4703	ADP	C4-C5-N7	-3.32	106.78	110.58
2	A	4704	ADP	N3-C2-N1	-3.16	123.79	128.58
2	A	4701	ADP	C4-C5-N7	-3.06	107.08	110.58
2	A	4701	ADP	N3-C2-N1	-3.04	123.99	128.58
2	A	4703	ADP	C3'-C2'-C1'	2.80	106.75	101.46
2	A	4701	ADP	C4-N9-C8	2.70	108.58	105.74
2	A	4704	ADP	C4-N9-C8	2.66	108.53	105.74
2	A	4704	ADP	C5-N7-C8	2.49	107.36	103.45
2	A	4703	ADP	C5-N7-C8	2.47	107.33	103.45
2	A	4703	ADP	C4-N9-C8	2.36	108.22	105.74
2	A	4704	ADP	C3'-C2'-C1'	2.23	105.69	101.46
2	A	4701	ADP	C5-N7-C8	2.19	106.89	103.45
2	A	4704	ADP	C6-C5-N7	2.09	136.11	132.09

There are no chirality outliers.

All (10) torsion outliers are listed below:

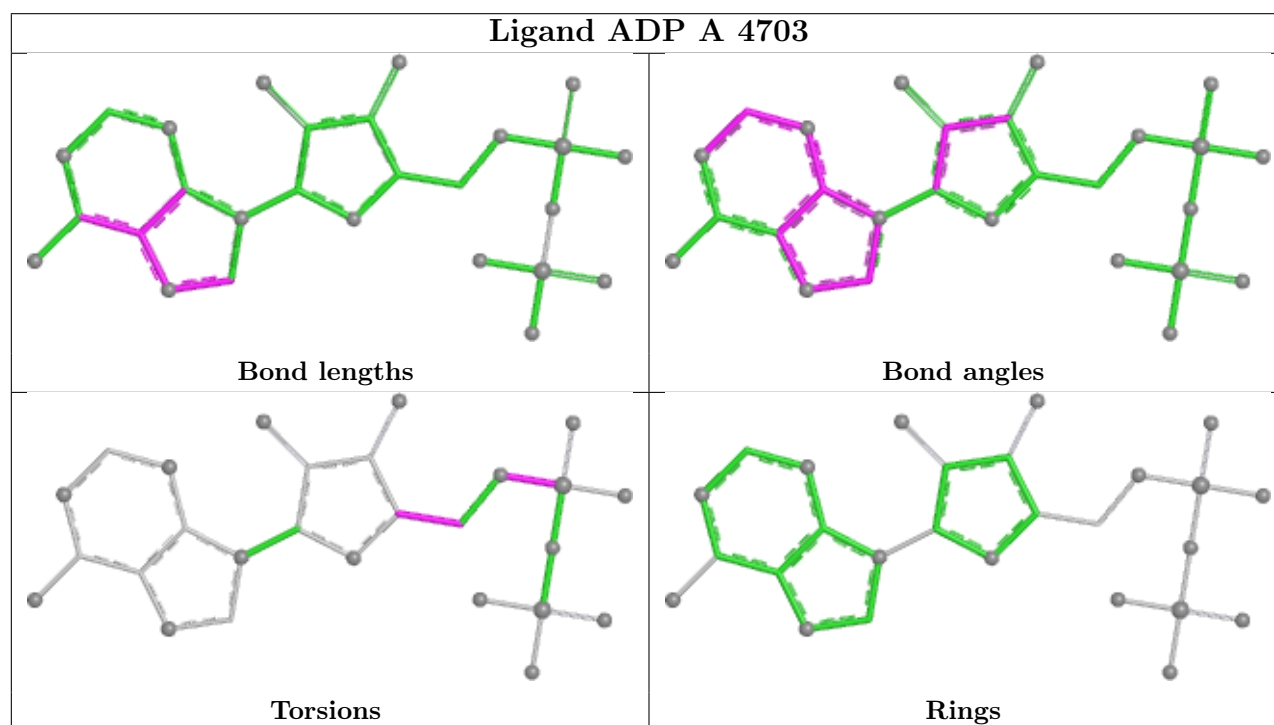
Mol	Chain	Res	Type	Atoms
2	A	4703	ADP	C5'-O5'-PA-O1A
2	A	4703	ADP	C5'-O5'-PA-O2A
2	A	4703	ADP	C5'-O5'-PA-O3A
3	A	4702	ATP	PG-O3B-PB-O2B
2	A	4704	ADP	C5'-O5'-PA-O1A
3	A	4702	ATP	PA-O3A-PB-O2B
3	A	4702	ATP	PG-O3B-PB-O1B
2	A	4703	ADP	O4'-C4'-C5'-O5'
3	A	4702	ATP	PA-O3A-PB-O1B
2	A	4701	ADP	O4'-C4'-C5'-O5'

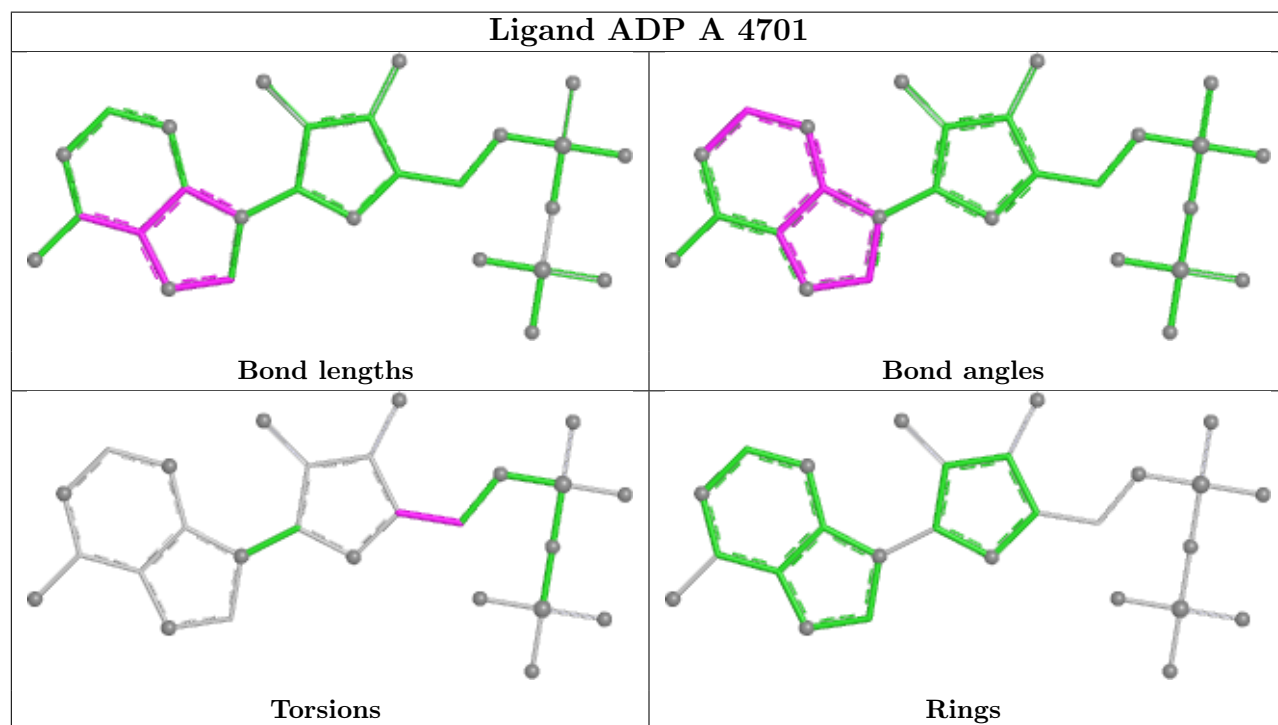
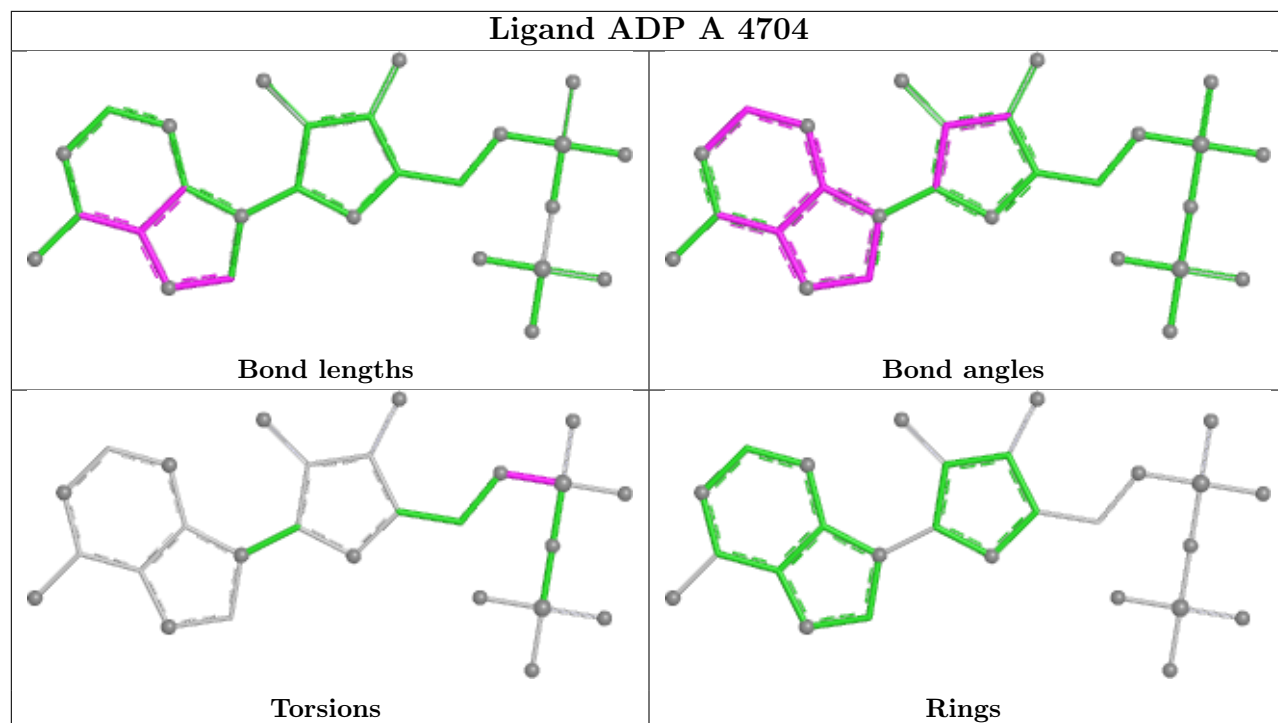
There are no ring outliers.

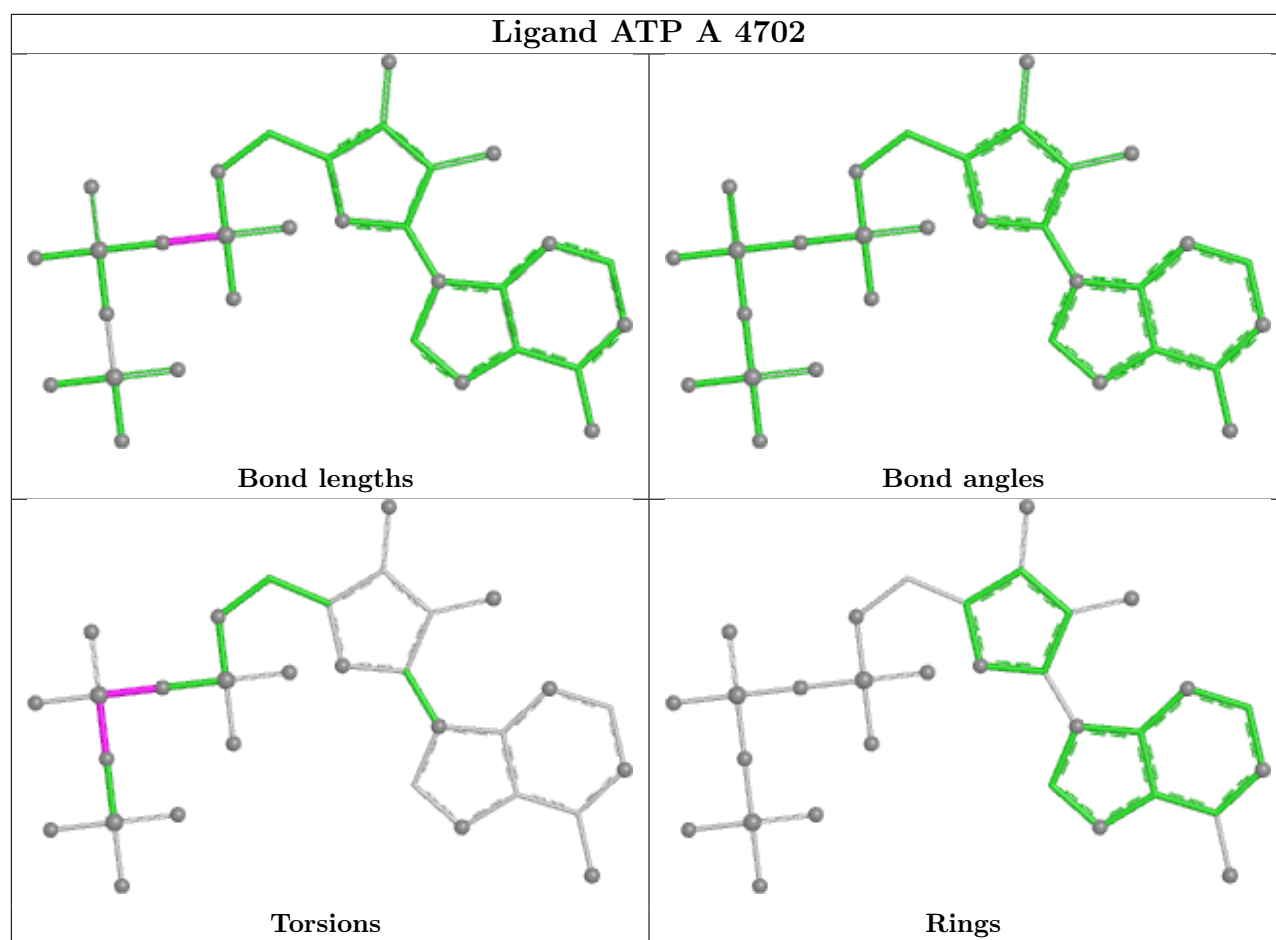
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4703	ADP	3	0
2	A	4704	ADP	2	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.

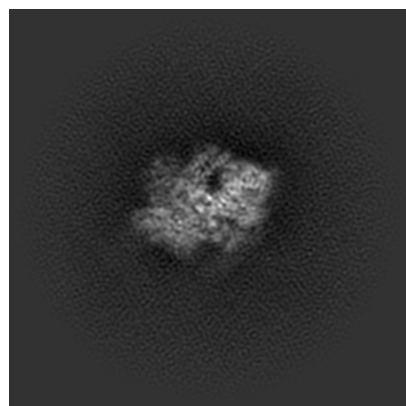
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44710. These allow visual inspection of the internal detail of the map and identification of artifacts.

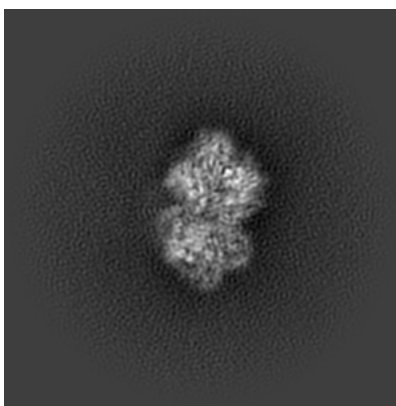
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

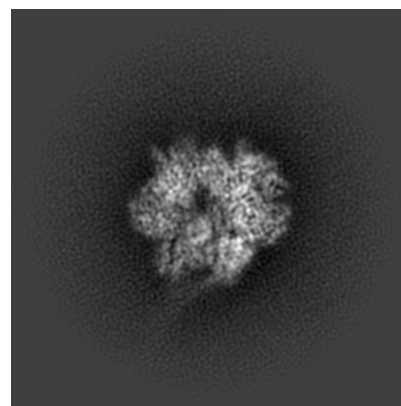
6.1.1 Primary map



X

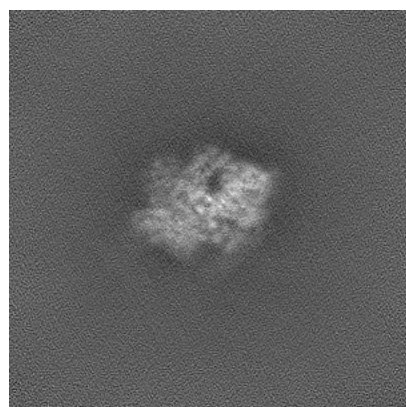


Y

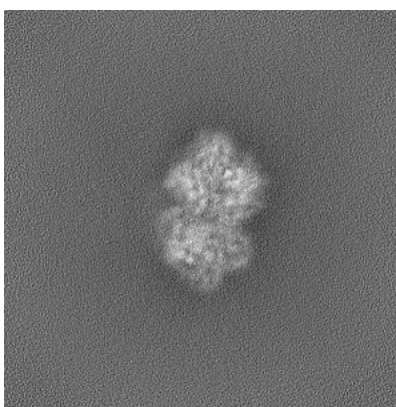


Z

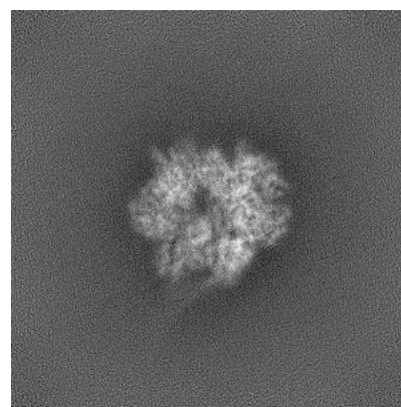
6.1.2 Raw map



X



Y

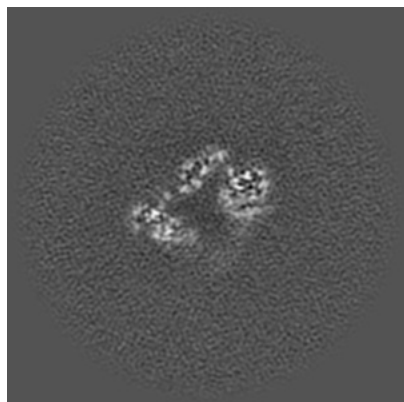


Z

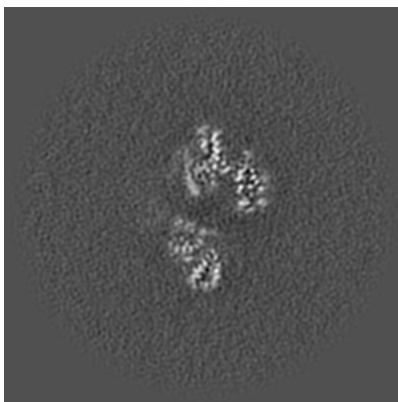
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

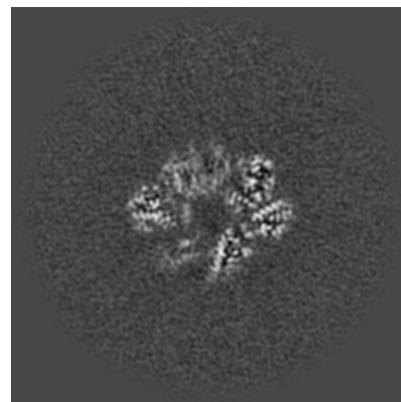
6.2.1 Primary map



X Index: 160

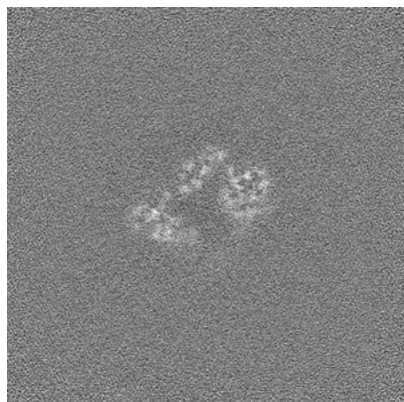


Y Index: 160

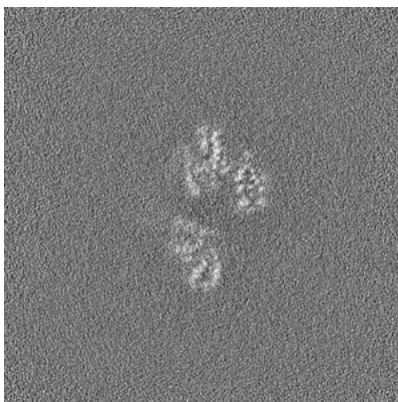


Z Index: 160

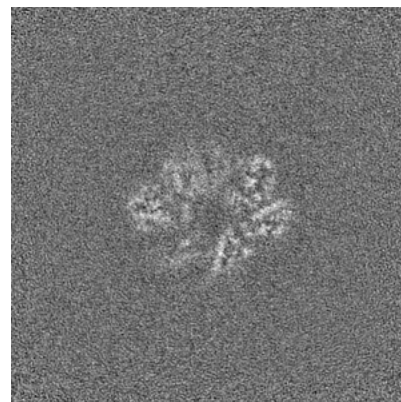
6.2.2 Raw map



X Index: 160



Y Index: 160

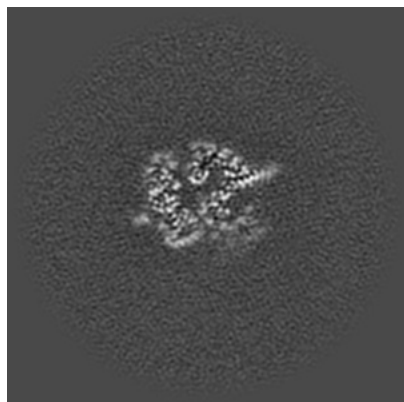


Z Index: 160

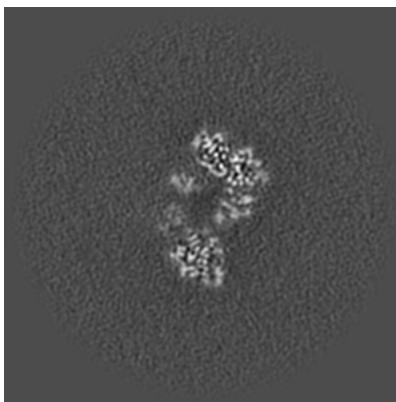
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

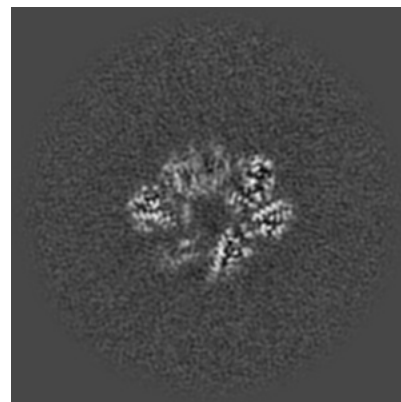
6.3.1 Primary map



X Index: 181

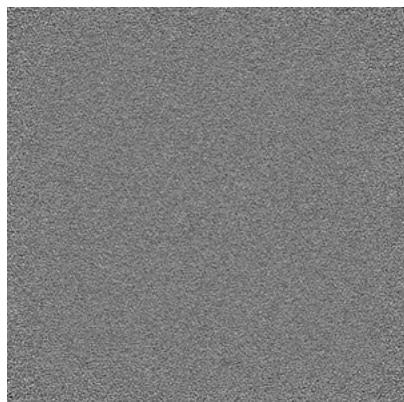


Y Index: 150

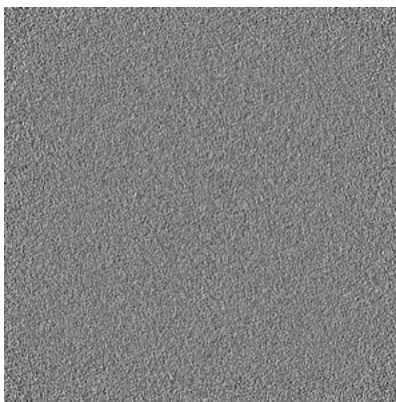


Z Index: 160

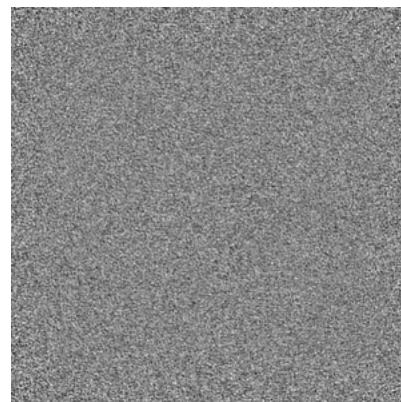
6.3.2 Raw map



X Index: 0



Y Index: 0

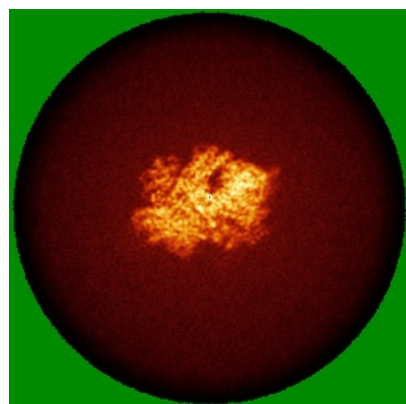


Z Index: 0

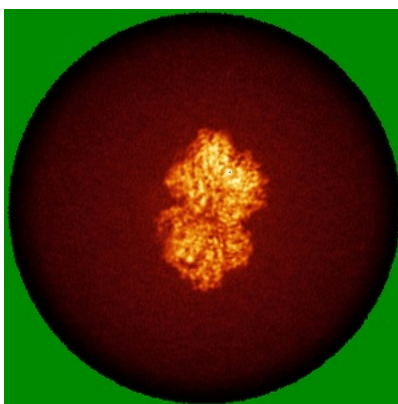
The images above show the largest variance slices of the map in three orthogonal directions.

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

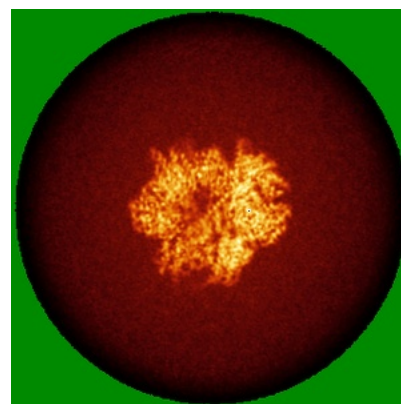
6.4.1 Primary map



X

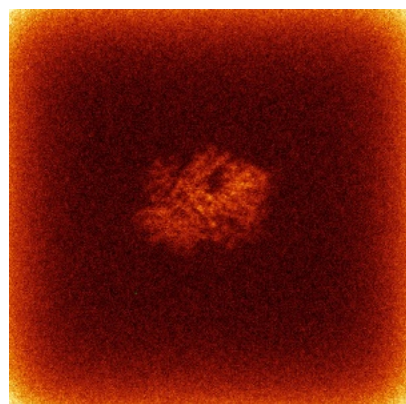


Y

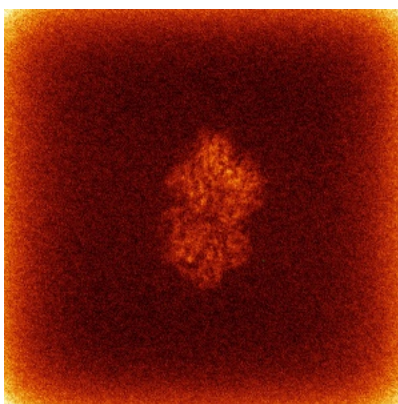


Z

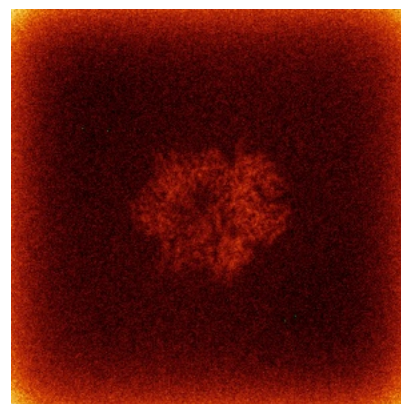
6.4.2 Raw map



X



Y

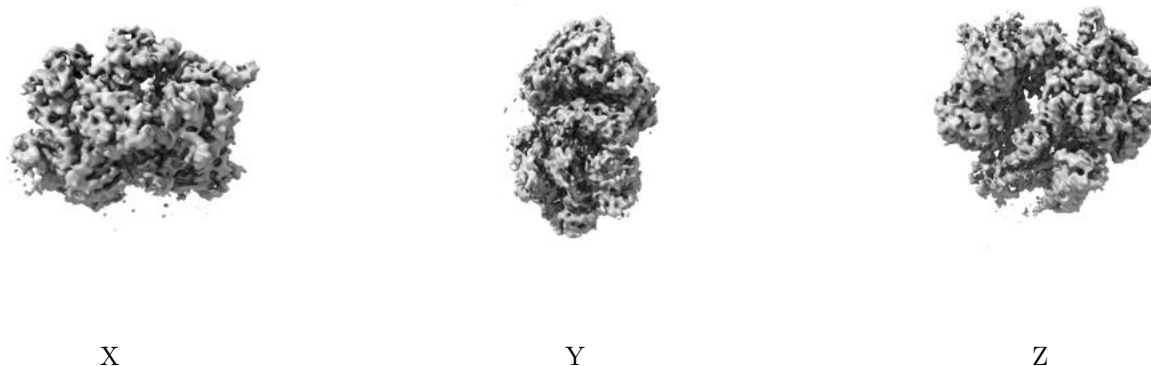


Z

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.

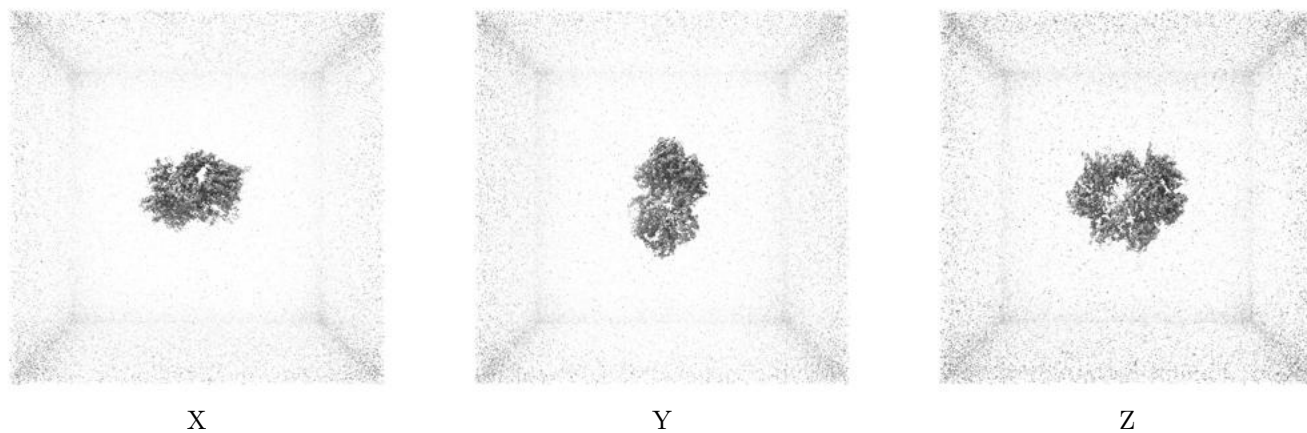
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. 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.

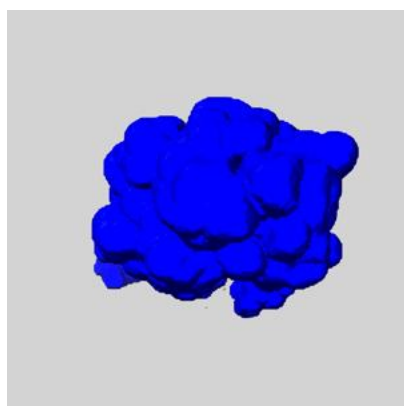
6.6 Mask visualisation [i](#)

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

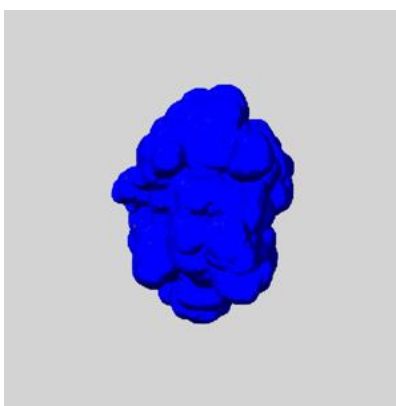
A mask typically either:

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

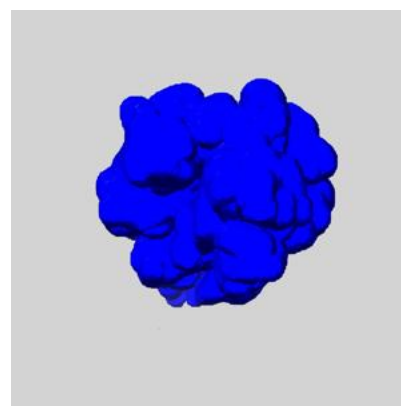
6.6.1 emd_44710_msk_1.map [i](#)



X



Y

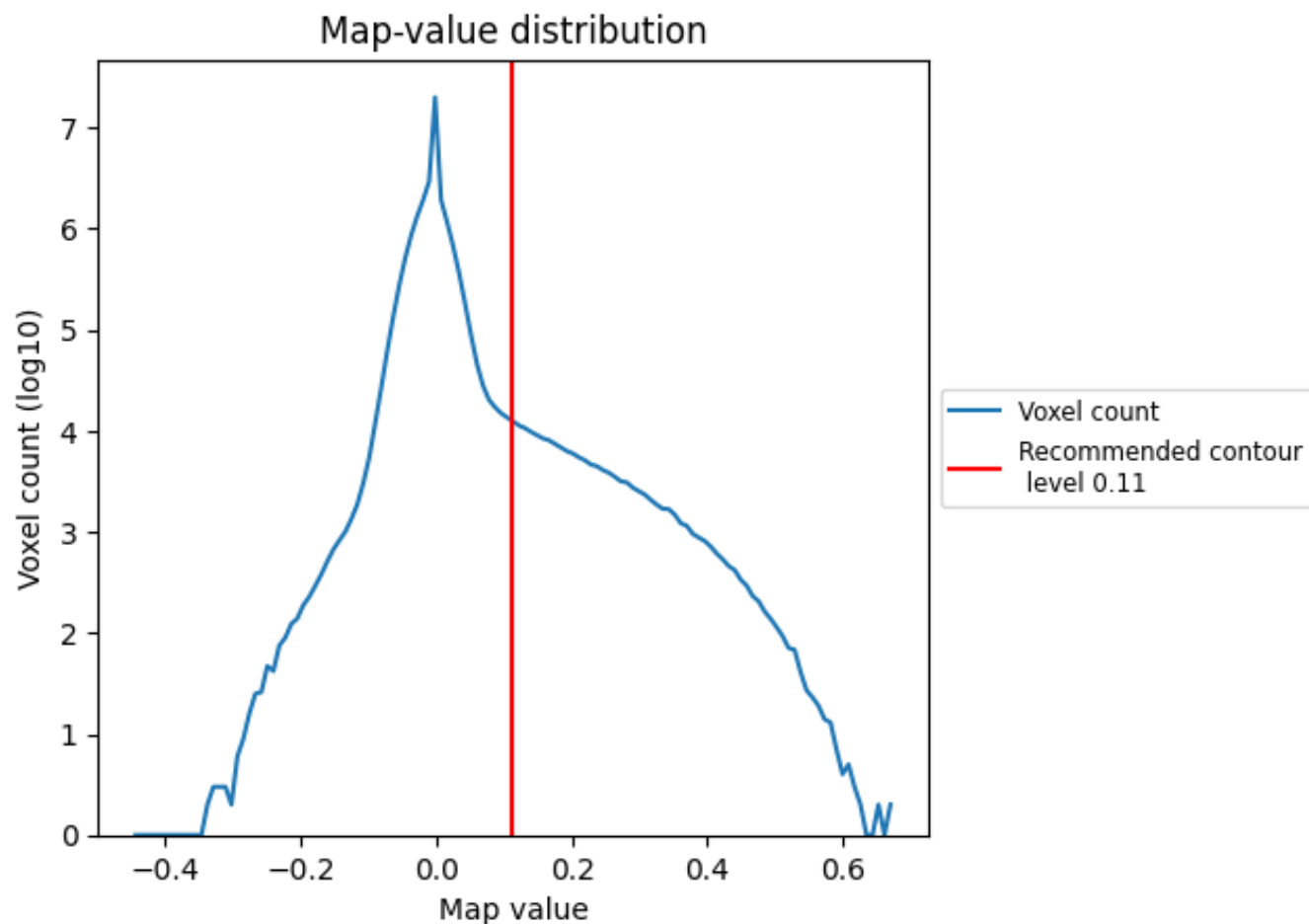


Z

7 Map analysis [i](#)

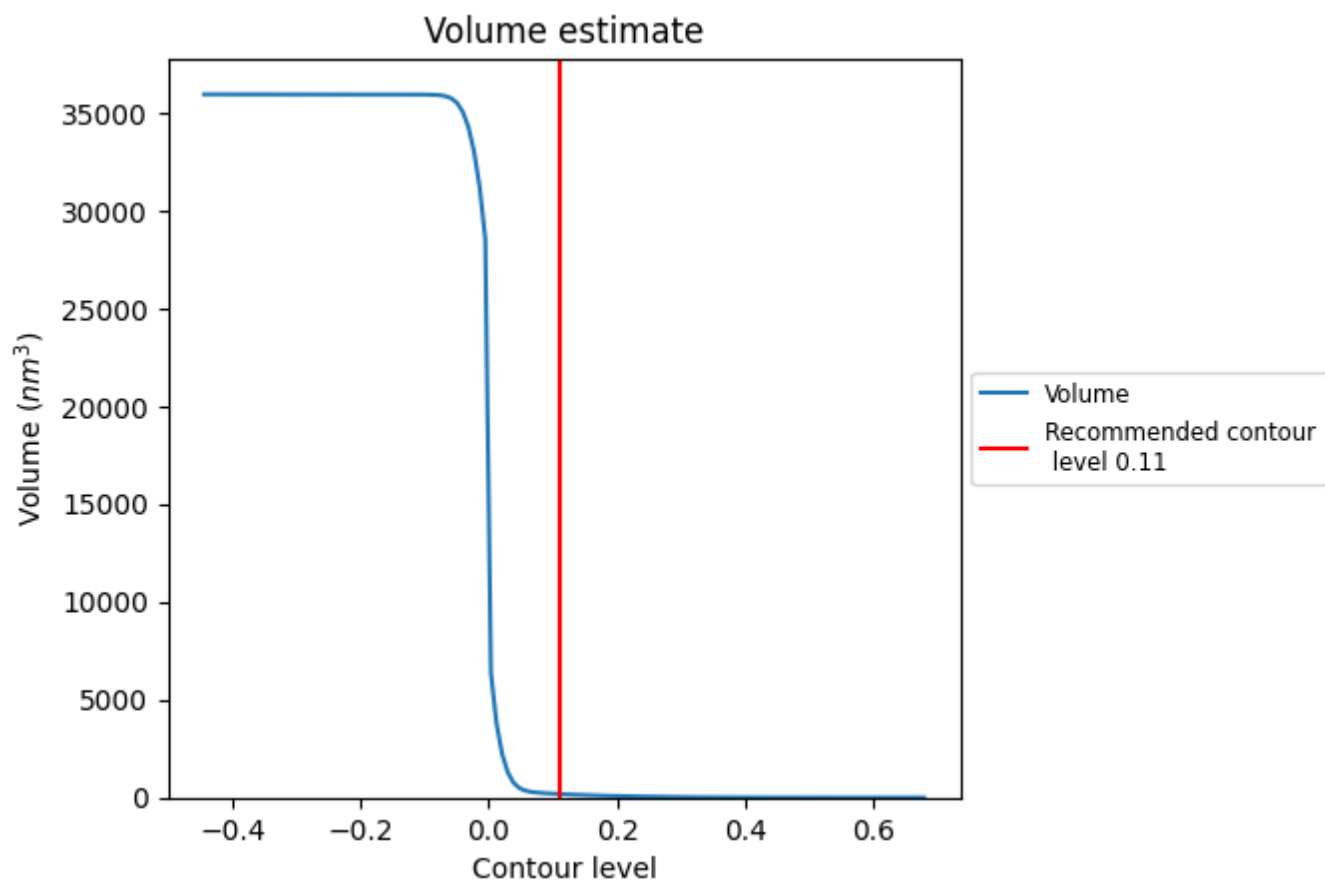
This section contains the results of statistical analysis of the map.

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.

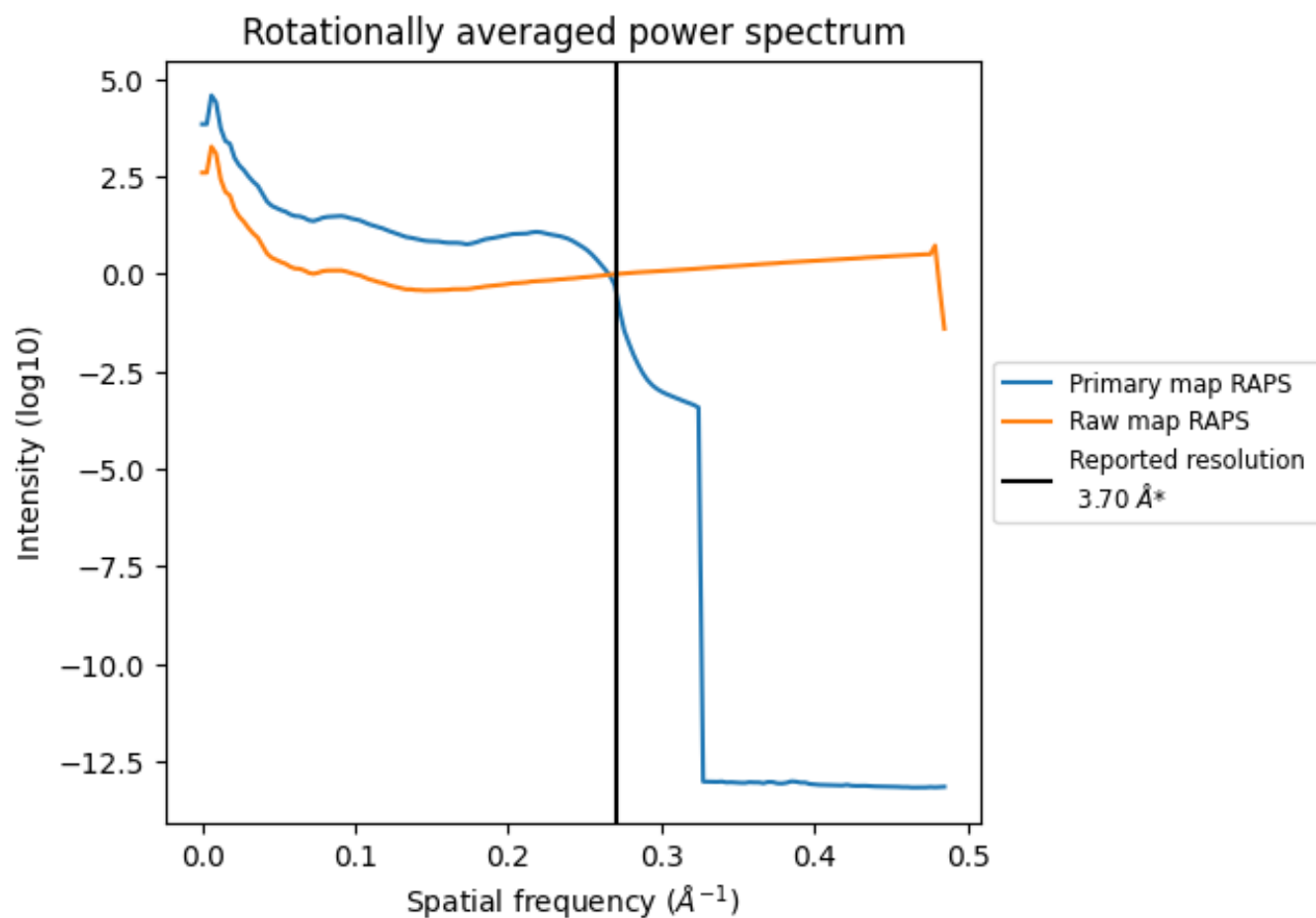
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 180 nm³; this corresponds to an approximate mass of 163 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 ⓘ

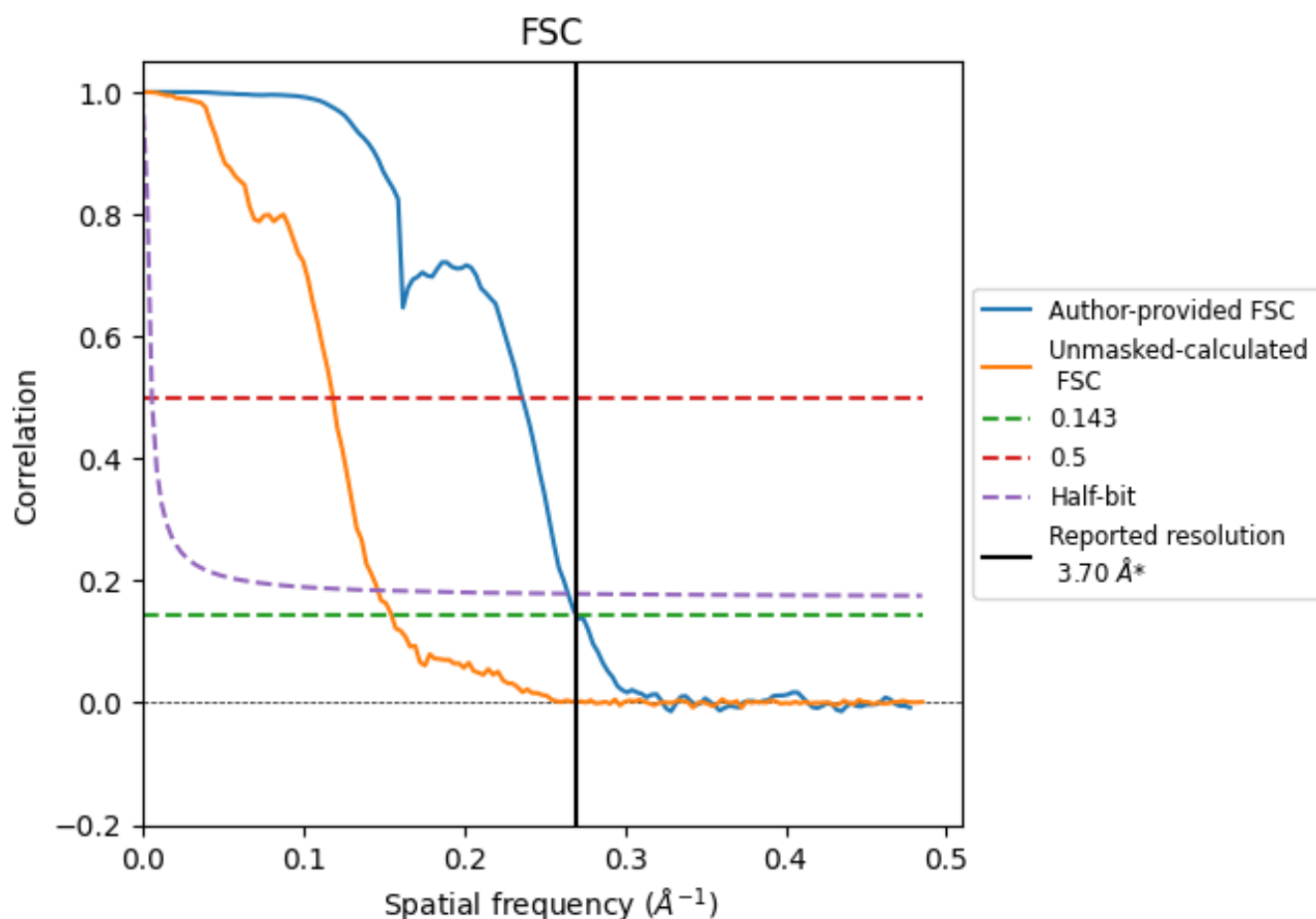


*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

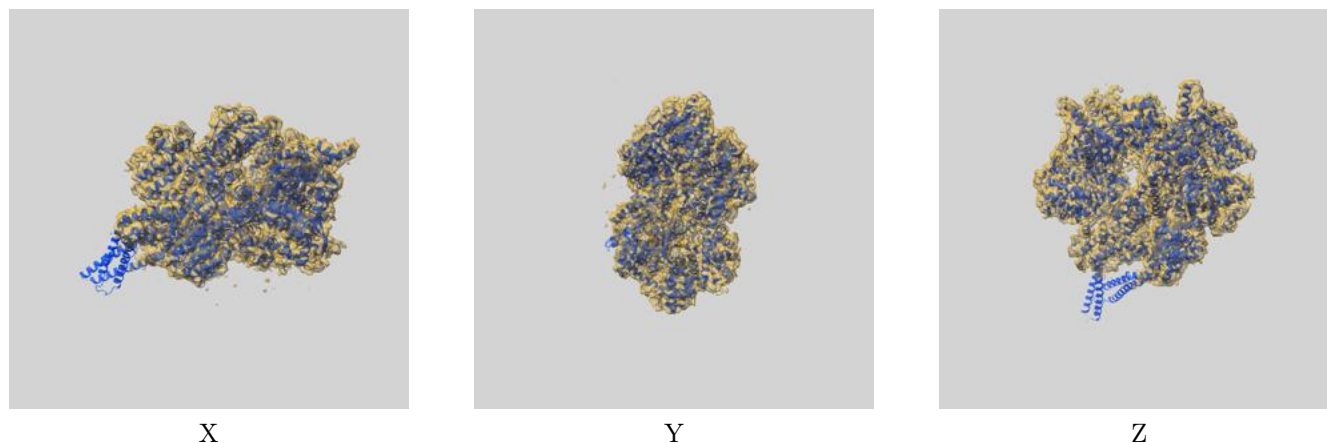
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.70	4.23	3.78
Unmasked-calculated*	6.45	8.44	6.83

*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 6.45 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

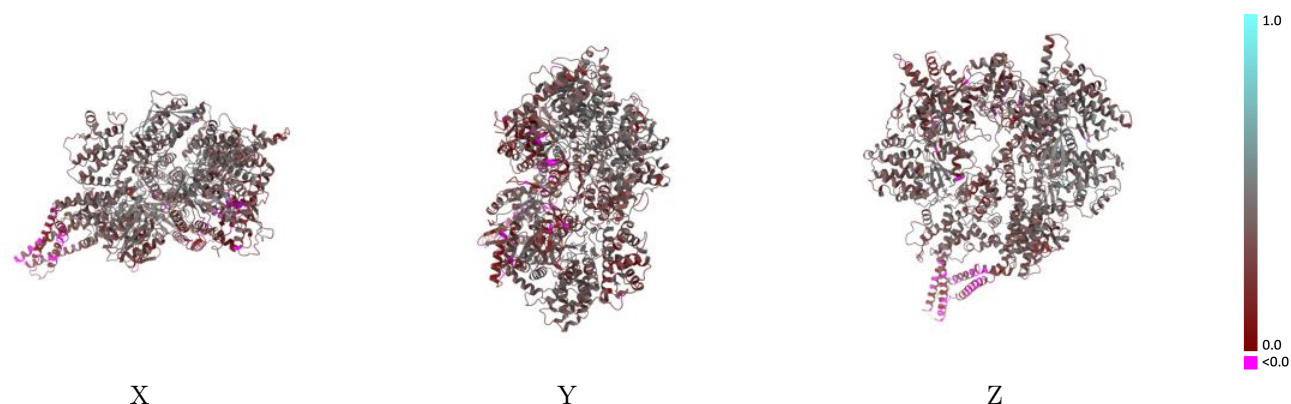
This section contains information regarding the fit between EMDB map EMD-44710 and PDB model 9BMT. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



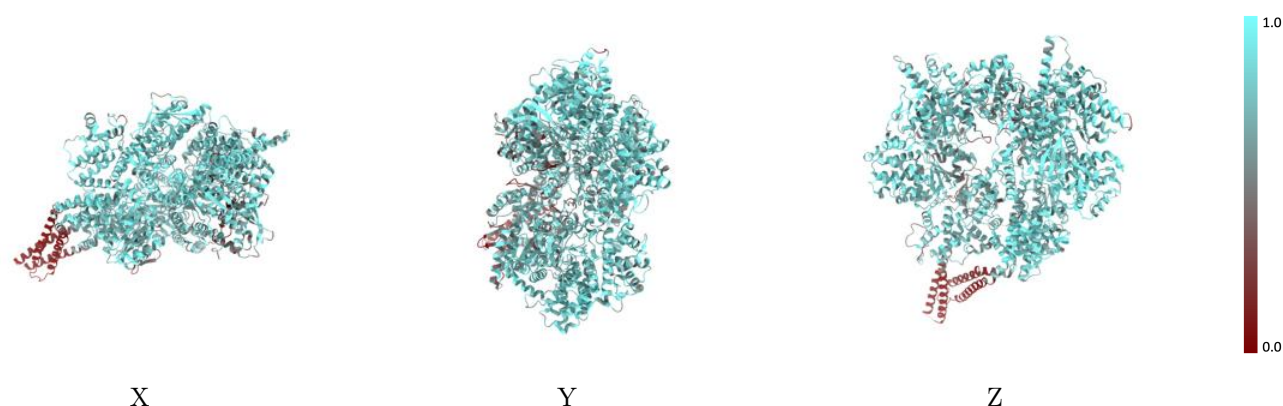
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



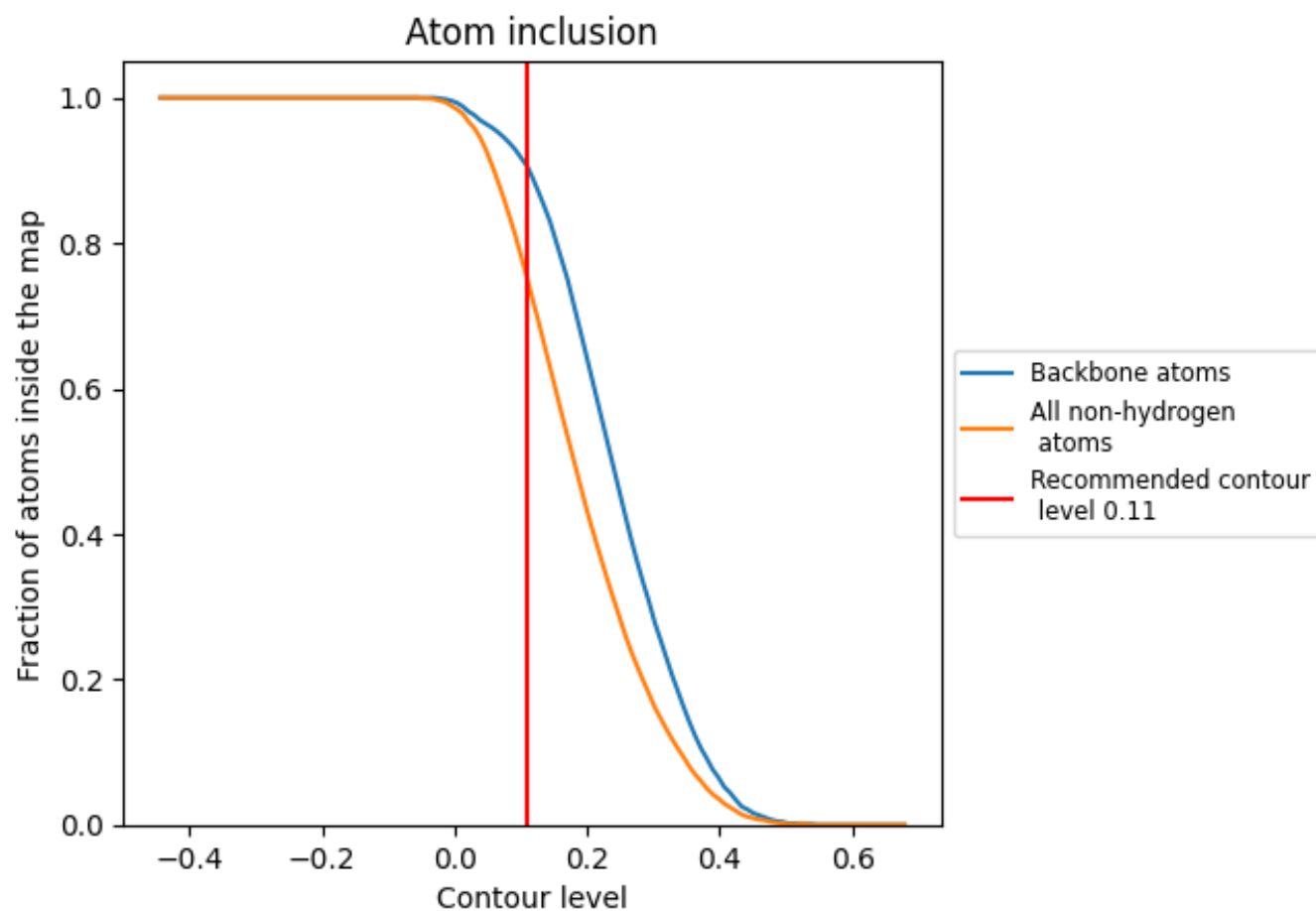
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 75% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7500	0.3450
A	0.7500	0.3450

