



## Full wwPDB EM Validation Report ⓘ

Apr 24, 2025 – 11:34 AM EDT

PDB ID : 9BN3 / pdb\_00009bn3  
EMDB ID : EMD-44720  
Title : The alpha registry-locked dynein motor domain mutant in 5mM ATP condition, class1  
Authors : Chai, P.; Zhang, K.  
Deposited on : 2024-05-02  
Resolution : 2.80 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

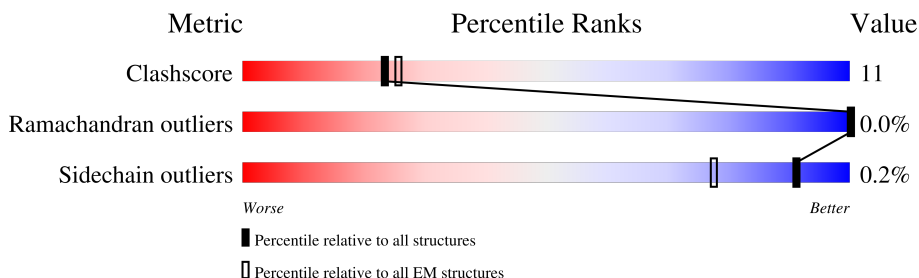
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	4646	<div> <div>10%</div> <div>46%</div> <div>16%</div> <div>38%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 23152 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.

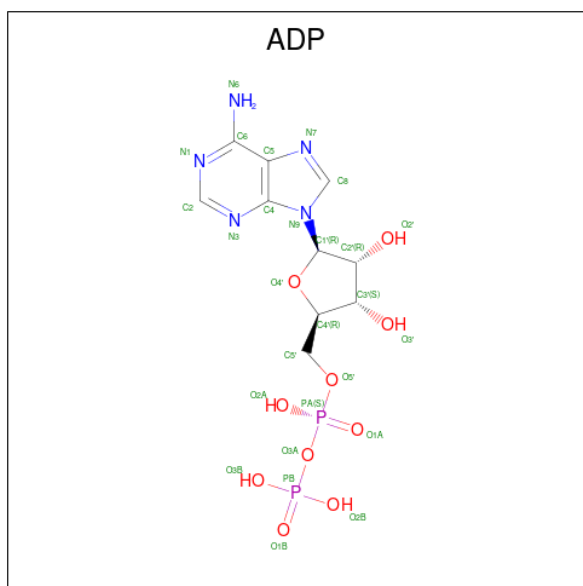
- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2866	23040	14688	3978	4259	115	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2389	ASP	GLU	conflict	UNP Q14204

- 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

- 
- The diagram illustrates the chemical structure of Adenosine Triphosphate (ATP). It consists of an adenine base (a purine ring system with an amino group at position 6) attached to a ribose sugar (a five-membered ring with hydroxyl groups at positions 2' and 3'). The ribose is linked to a chain of three phosphate groups (labeled alpha, beta, and gamma) via phosphodiester bonds. The alpha phosphate is directly attached to the 5' carbon of the ribose. The beta and gamma phosphates are linked in series. The structure is shown with stereochemistry, indicating the orientation of the hydroxyl groups and the phosphate chain. The atoms are labeled with their respective element symbols and positions (e.g., N1, N3, N7, N9, C2, C4, C5, C6, C1', C2', C3', C4', C5', O1, O2, O3, O4, O5, O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23, O24, O25, O26, O27, O28, O29, O30, O31, O32, O33, O34, O35, O36, O37, O38, O39, O40, O41, O42, O43, O44, O45, O46, O47, O48, O49, O50, O51, O52, O53, O54, O55, O56, O57, O58, O59, O60, O61, O62, O63, O64, O65, O66, O67, O68, O69, O70, O71, O72, O73, O74, O75, O76, O77, O78, O79, O80, O81, O82, O83, O84, O85, O86, O87, O88, O89, O90, O91, O92, O93, O94, O95, O96, O97, O98, O99, O100).



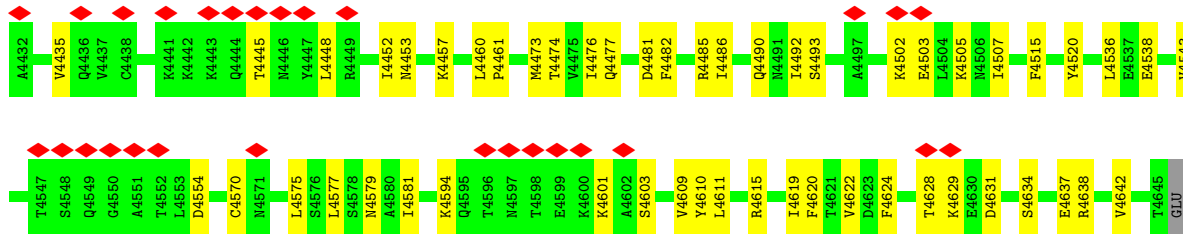




LEU	Q3156	E3073	D2995	D2885	D2787	K2673	L2591	L2449	R2358	Y2265	GLY	ARG
LYS	A3157	G3074	E2996	Q2886	W2802	F2682	V2592	L2450	F2364	D2269	GLU	SER
MET	N3158	L3075	S2997	E2887	W2806	M2686	L2593	R2451	S2365	P2270		ASN
VAL	K3163	K3076	N2998	R2890	L2806	M2697	P2596	C2454	V2368	R2273		K2034
ASP	R3164	D3077	L3000	K2894	A2809	D2697	L2605	S2457	L2369	D2277		L2035
GLN	M3169	R3078	L3000	K2894	L2810	V2701	L2609	L2458	S2370	F2280		F2036
GLN	T3172	A3079	D3001	K2898	T2815	R2702	R2610	L2462	T2371	F2280		S2038
ALA	Y3176	A3080	L3004	E2898	L2816	E2703	R2611	R2467	I2374	K2286		L2039
LYS	E3193	L3084	L3005	E2903	L2817	E2704	P2613	R2467	N2377	I2138		P2044
LYS	L3194	E3007	E3006	E2904	V2818	R2705	D2614	V2469	E2152	D2152		R2045
VAL	E3195	F3086	M3008	D2906	G2820	Q2707	E2616	Q2471	R2383	R2292		R2046
MET	E3196	N3087	G3015	V2910	L2821	F2706	V2617	Y2472	D2389	E2294		F2059
SER	Q3197	N3092	F3021	W2910	L2822	V2709	F2622	Y2472	GLY	E2294		L2065
GLN	Q3198	W3093	E3022	N2913	R2823	G2710	S2623	D2478	GLU	L2295		A2066
GLU	F3094	F3094	G3023	W2825	L2824	R2720	S2624	M2481	ASP	V2164		A2066
ILE	G3095	D3024	E3025	A2826	K2721	T2626	A2625	W2481	GLU	Q2296		R2067
GLU	H3200	D3096	Y3026	R2924	R2726	T2627	T2626	Q2485	GLN	W2300		W2069
GLN	L3201	A3101	L3029	I2925	L2830	V2731	P2628	Q2485	GLN	R2179		W2070
GLN	N3202	V3105	M3030	Q2928	R2831	P2732	E2629	R2488	ARG	D2306		P2071
LEU	V3203	V3105	Q3030	Q2930	F2833	V2734	L2630	R2488	ARG	V2307		P2071
HIS	G3204	K3113	T3031	V2838	V2735	Y2738	K2633	I2498	ARG	E2188		L2075
LYS	L3205	N3119	K3032	E2839	V2738	P2739	T2634	W2500	GLY	D2308		L2075
GLN	R3206	G3129	Q3032	D2840	E2738	G2740	D2635	S2501	GLY	E2205		Q2079
GLU	K3207	N3119	L2933	L2934	W2739	G2740	P2636	L2502	GLU	L2208		Y2086
VAL	L3208	P3123	K3034	L2936	R2844	G2740	D2636	L2502	ASP	Q2209		L2090
ILE	K3209	D3124	L3042	L2937	W2845	G2740	H2637	D2505	GLY	L2210		L2090
ALA	E3210	T3211	G3036	W2938	T2846	S2743	E2640	P2527	GLU	I2213		L2093
ASP	L3211	M3126	A3037	S2939	D2847	Y2747	E2640	P2527	GLU	D2320		L2097
LYS	V3212	P3127	Q3038	E2848	E2848	G2749	R2643	P2530	ALA	M2221		L2097
GLN	D3213	V3128	K3039	L2849	L2850	R2748	W2646	N2531	ALA	D2321		G2101
VAL	Q3214	V3129	E3040	D2851	L2852	G2749	Q2647	I2532	P2410	L2327		G2101
LYS	V3215	Y3130	G3041	T2852	T2853	R2763	H2646	P2533	P2411	L2327		K2104
GLU	E3216	D3131	L3042	V2853	A2854	L2756	Q2647	P2533	P2412	G2227		R2105
ASP	L3217	K3132	M3043	A2854	L2855	L2756	V2648	I2534	L2413	K2230		E2106
LEU	R3218	L3133	L3044	L2855	L2856	R2757	V2649	P2535	Q2416	S2231		E2106
LYS	R3219	P3134	D3045	R2863	L2864	L2758	A2651	W2545	R2417	R2332		Q2109
VAL	R3220	Q3135	S3046	R2864	E2864	L2759	P2652	Q2554	W2423	L2333		L2111
ASP	ASP	P3136	H3047	E2970	K2865	L2762	Q2654	D2566	Q2424	S2334		K2112
LEU	LEU	P3137	E3048	E2971	K2866	A2766	L2655	D2566	R2338	K2239		R2113
ALA	ALA	S3138	E3049	D2971	M2867	T2770	L2661	V2569	V2339	K2239		E2114
VAL	ALA	R3140	K3052	L2976	S2868	M2773	L2661	V2569	R2340	R2340		LYS
ILE	ILE	E3141	W3053	F3054	R2869	V2774	C2663	R2576	I2341	E2242		GLU
GLN	GLU	V3144	F3054	T3055	R2870	V2774	C2663	H2577	W2342	R2243		GLU
ASN	GLU	S3145	T3055	E2981	L2871	R2783	D2664	L2581	F2343	L2244		ARG
ALA	VAL	N3144	V3053	V2979	L2870	R2783	D2664	W2584	E2944	G2246		GLY
VAL	VAL	S3146	I3059	R2981	T2871	R2783	E2665	W2584	V2345	V2247		GLU
LYS	LYS	G3147	V3069	K2981	T2871	R2783	E2665	W2584	Q2346	E2248		ALA
SER	ASN	V3148	V3069	K2986	S2878	F2784	L2668	W2584	Y2350	K2261		VAL
ALA	ALA	H3151	F3066	E2988	K2879	T2785	P2669	P2590	A2351	K2261		ASP
ALA	ALA	Q3152	T3067	E2988	D2880	Q2786	D2670	—	T2352	—		GLU
ASN	ASN	T3153	N3069	—	—	—	—	—	L2353	—		—
ASP	ASP	L3154	P3070	—	—	—	—	—	A2354	—		—
LYS	LYS	H3155	S3071	—	—	—	—	—	—	—		—
LYS	LYS	S3072	S3072	—	—	—	—	—	—	—		—

T4333	G4300	V4099	M4004	N3912	V3797	G3736	A3564	K3480	GLU	LYS
G4336	W4201	H4100	M4007	L3916	Y3801	R3655	L3567	S3481	ASP	LYS
V4337	K4204	L4106	L4025	S3917	L3802	T3656	P3569	L3482	ILE	GLN
I4340	F4207	M4107	L4025	S3918	P3803	G3657	A3569	ARG	ILE	HIS
S4341	D4220	Q4108	H4029	G3919	T3806	G3658	D3570	GLU	VAL	VAL
L4342	D4220	L4109	I4030	G3920	T3806	R3659	D3571	LYS	VAL	GLU
M4343	A4227	E4111	T4033	T3921	T3811	R3660	K3581	MET	VAL	ARG
L4344	A4227	K4112	T4033	P3922	Y3812	L3661	L3581	GLN	GLN	VAL
K4345	E4230	L4113	E4034	R3923	L3818	L3662	R3585	LYS	LYS	ARG
M4346	E4230	L4113	P4037	R3924	L3818	T3663	P3587	ASN	ASN	ASN
Q4347	I4233	L4116	P4040	Q3925	T3821	G3665	L3590	TYR	ASN	ASN
MET	I4238	Q4117	M4043	Q3926	Q3826	D3666	D3591	ASN	ASN	ASN
GLU	M4247	P4118	C4044	E3930	L3829	Q3667	F3599	TYR	ASN	ASN
ASP	T4251	H4119	S4045	Q3931	L3829	D3668	K3497	ASP	ASP	ASP
ASP	Y4252	L4124	V4046	A3932	T3835	I3669	K3497	ASP	ASP	ASP
ASP	L4264	F4125	E4056	V3935	N3838	D3670	K3497	ASP	ASP	ASP
ALA	T4126	L4126	D4057	V3936	N3839	L3671	K3498	ASP	ASP	ASP
ALA	T4127	T4127	L4058	R3937	L3840	S3672	Q3499	ASP	ASP	ASP
ALA	M4128	M4128	L4058	R3937	L3841	S3672	Q3499	ASP	ASP	ASP
GLU	M4266	M4128	A4059	L3938	E3842	S3672	M3500	ASP	ASP	ASP
THR	E4270	K4133	A4060	L3938	N3843	D3606	S3501	ASP	ASP	ASP
GLU	F4278	V4134	E4061	P3942	N3844	R3607	T3502	ASP	ASP	ASP
LYS	L4284	P4135	Q4062	K3945	K3847	K3608	T3503	ASP	ASP	ASP
THR	L4284	L4139	T4064	D3946	V3849	T3610	C3507	ASP	ASP	ASP
ASP	K4287	R4140	Q4065	A3949	V3849	T3611	L3508	ASP	ASP	ASP
ASP	V4289	I4144	S4068	K3950	H3852	D3612	L3509	ASP	ASP	ASP
THR	D4289	F4145	T4069	V3951	T3853	R3613	S3510	ASP	ASP	ASP
THR	D4289	V4146	A4070	Q3952	R3854	F3614	T3507	ASP	ASP	ASP
ASP	Q4290	F4147	A4071	Q3953	R3855	D3617	Y3516	ASP	ASP	ASP
GLY	H4291	E4148	Q4072	A3953	L3856	F3619	F3620	ASP	ASP	ASP
ARG	M4296	K4154	Q4073	D3954	S3857	R3620	M3524	ASP	ASP	ASP
PRO	P4297	R4168	A4074	E3955	I3858	K3624	L3536	ASP	ASP	ASP
R4378	D4298	I4169	E4075	Q3956	F3864	R3624	Q3537	ASP	ASP	ASP
H4389	R4302	S4172	F4077	I3959	R3870	R3628	Q3538	ASP	ASP	ASP
Q4393	V4306	P4173	H4078	P3966	V3871	F3629	A3539	ASP	ASP	ASP
L4398	E4310	R4174	Q4079	Y3972	R3872	L3633	N3540	ASP	ASP	ASP
K4399	D4314	A4177	D4081	E3976	G3874	L3636	I3541	ASP	ASP	ASP
E4403	P4318	R4178	K4082	E3977	L3876	D3637	R3544	ASP	ASP	ASP
K4406	L4321	A4179	A4083	E3978	L3877	Y3638	T3545	ASP	ASP	ASP
F4412	P4324	W4185	T4084	E3979	H3880	E3639	D3546	ASP	ASP	ASP
E4416	N4325	A4188	N4085	E3980	L3892	S3640	Y3552	ASP	ASP	ASP
L4431	N4326	I4189	T4086	P3981	L3892	Y3641	L3553	ASP	ASP	ASP
	V4330	E4192	K4089	T3982	E3898	D3643	N3554	ASP	ASP	ASP
		Y4196	R4092	G3984	L3909	Y3644	S3556	ASP	ASP	ASP
			M4095	R3989		L3649	D3557	ASP	ASP	ASP
			L4096	R3997		E3652	E3558	ASP	ASP	ASP
			K4097	R4000		V3653	R3559	ASP	ASP	ASP
			N4098	A4003			L3560	ASP	ASP	ASP
							W3562	ASP	ASP	ASP
							Q3563	ASP	ASP	ASP





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	433112	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	2.677	Depositor
Minimum map value	-1.892	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	412.488, 412.488, 412.488	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1458, 1.1458, 1.1458	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	0.26	1/23533 (0.0%)	0.51	3/31898 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3587	PRO	CG-CD	-6.12	1.30	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3587	PRO	N-CD-CG	-10.98	86.73	103.20
1	A	3587	PRO	CA-CB-CG	-8.39	88.05	104.00
1	A	3587	PRO	CA-N-CD	-5.11	104.34	111.50

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	23040	0	23108	497	0
2	A	81	0	36	0	0
3	A	31	0	12	1	0
All	All	23152	0	23156	497	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 11.

All (497) 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:2423:MET:HE1	1:A:2462:LEU:HD13	1.62	0.81
1:A:3151:HIS:HD1	1:A:3516:TYR:HH	1.26	0.79
1:A:4043:MET:HB2	1:A:4127:THR:HA	1.63	0.79
1:A:1511:PRO:HG3	1:A:3628:ARG:HE	1.47	0.78
1:A:3209:LYS:HG3	1:A:3486:ARG:HH21	1.48	0.78
1:A:3137:PRO:HB3	1:A:3141:GLU:HB2	1.66	0.77
1:A:3113:MET:O	1:A:3140:ARG:NH2	2.18	0.76
1:A:1814:GLU:HG2	1:A:1878:LYS:HE2	1.67	0.76
1:A:2261:LYS:HE3	1:A:2311:TRP:HB3	1.68	0.75
1:A:3942:PRO:HA	1:A:3945:LYS:HE3	1.69	0.75
1:A:1582:VAL:HG23	1:A:1591:VAL:HG11	1.69	0.74
1:A:2822:ILE:HD11	1:A:2854:ALA:HB1	1.70	0.73
1:A:3730:ASP:OD1	1:A:3733:LYS:NZ	2.21	0.73
1:A:3158:ASN:ND2	1:A:3169:MET:O	2.20	0.73
1:A:4326:ASN:HD21	1:A:4581:ILE:HG23	1.53	0.73
1:A:3839:VAL:O	1:A:3843:ASN:ND2	2.23	0.71
1:A:2500:TRP:HZ2	1:A:2576:ARG:HD3	1.55	0.71
1:A:3826:GLN:HB3	1:A:4140:ARG:HD2	1.73	0.71
1:A:3585:ARG:HB2	1:A:3697:THR:HG23	1.72	0.70
1:A:2294:GLU:O	1:A:2338:ASN:ND2	2.25	0.70
1:A:2467:ARG:O	1:A:2471:GLN:NE2	2.25	0.70
1:A:3602:ASN:HA	1:A:3605:LYS:HE3	1.74	0.70
1:A:1751:VAL:HG13	1:A:1814:GLU:HG3	1.71	0.70
1:A:2829:ALA:O	1:A:2833:PHE:HB2	1.91	0.69
1:A:2640:GLU:HG2	1:A:2653:VAL:HG22	1.74	0.69
1:A:2138:ILE:HD12	1:A:2161:LEU:HD22	1.74	0.69
1:A:2354:ALA:HB1	1:A:2358:ARG:HH21	1.57	0.69
1:A:1978:ILE:HD11	1:A:2001:LEU:HD11	1.76	0.68
1:A:2625:ALA:HB3	1:A:3006:GLU:HG3	1.76	0.67
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.75	0.67
1:A:4176:ARG:NH1	1:A:4220:ASP:OD1	2.28	0.67
1:A:2885:ASP:OD2	1:A:2886:GLN:N	2.28	0.66
1:A:2485:GLN:OE1	1:A:2488:ARG:NH2	2.27	0.66
1:A:4037:PRO:HG2	1:A:4117:GLN:HE21	1.61	0.66
1:A:1795:SER:O	1:A:1800:GLN:NE2	2.28	0.66
1:A:4324:PRO:HD3	1:A:4638:ARG:HG3	1.78	0.65
1:A:3912:ASN:O	1:A:3937:ARG:NH1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4033:THR:OG1	1:A:4034:GLU:OE1	2.15	0.65
1:A:2867:MET:SD	1:A:2868:SER:N	2.69	0.64
1:A:3194:LEU:HD13	1:A:3503:ILE:HD11	1.79	0.64
1:A:1808:LEU:O	1:A:1812:ILE:HD12	1.98	0.64
1:A:4065:GLN:HE21	1:A:4092:ARG:HD3	1.62	0.64
1:A:4448:LEU:O	1:A:4452:ILE:HG12	1.98	0.64
1:A:3736:GLY:O	1:A:3740:LEU:N	2.31	0.64
1:A:1711:VAL:O	1:A:1715:LYS:HG2	1.98	0.64
1:A:2937:GLY:HA3	1:A:3094:PHE:HB2	1.80	0.63
1:A:3004:PHE:O	1:A:3008:MET:HG2	1.98	0.63
1:A:3691:ASP:HB2	1:A:3695:ARG:HH12	1.65	0.62
1:A:2068:LYS:NZ	1:A:2164:VAL:O	2.32	0.62
1:A:2759:ILE:HD12	1:A:2762:LEU:HD12	1.82	0.62
1:A:3854:GLN:O	1:A:3858:ILE:HG13	2.00	0.61
1:A:3877:HIS:HA	1:A:3880:HIS:CD2	2.35	0.61
1:A:4577:LEU:HD22	1:A:4638:ARG:HD2	1.81	0.61
1:A:3561:ARG:NH1	1:A:3603:GLU:OE2	2.33	0.61
1:A:2505:ASP:HB3	1:A:2733:VAL:HG23	1.81	0.61
1:A:1752:LEU:HD11	1:A:1868:TYR:CZ	2.36	0.61
1:A:2413:LEU:O	1:A:2417:ARG:HG3	2.01	0.61
1:A:1659:ALA:HB2	1:A:1926:PHE:HD1	1.64	0.60
1:A:2704:GLU:HG3	1:A:2705:ARG:HG3	1.84	0.60
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.84	0.60
1:A:2265:TYR:OH	1:A:2311:TRP:O	2.19	0.60
1:A:2930:GLN:OE1	1:A:2930:GLN:N	2.27	0.60
1:A:3508:LEU:HD23	1:A:3536:LEU:HD21	1.81	0.60
1:A:3923:ARG:HH12	1:A:3952:GLN:HB2	1.67	0.60
1:A:2663:CYS:HB2	1:A:2710:GLY:HA2	1.84	0.60
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.84	0.60
1:A:3826:GLN:HB2	1:A:4139:LEU:HB3	1.85	0.59
1:A:2270:PRO:HA	1:A:2273:ARG:HH21	1.67	0.59
1:A:1760:GLU:O	1:A:1764:THR:HG23	2.02	0.59
1:A:3215:VAL:HG11	1:A:3478:LEU:HD11	1.83	0.59
1:A:4040:PRO:HB3	1:A:4124:LEU:HD22	1.85	0.59
1:A:4172:SER:HB2	1:A:4173:PRO:HD2	1.84	0.59
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.84	0.58
1:A:1587:LEU:HB3	1:A:1590:ASP:HB2	1.85	0.58
1:A:3849:VAL:HG12	1:A:3855:ARG:HG3	1.85	0.58
1:A:2622:PHE:CD1	1:A:2626:THR:HG21	2.38	0.58
1:A:3818:LEU:HD23	1:A:4346:MET:HE2	1.85	0.58
1:A:1734:ASP:HB3	1:A:1737:THR:HG22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3981:THR:HG23	1:A:3984:GLY:H	1.67	0.58
1:A:2280:PHE:HE1	1:A:2315:LEU:HD21	1.68	0.58
1:A:2179:ARG:HE	1:A:2208:LEU:HD11	1.69	0.58
1:A:1588:VAL:HG13	1:A:1589:MET:HE3	1.86	0.58
1:A:3972:TYR:HE1	1:A:3989:ARG:HH21	1.51	0.58
1:A:1910:THR:HG23	1:A:2044:PRO:HD3	1.85	0.57
1:A:1852:ASP:OD2	1:A:1855:GLN:NE2	2.31	0.57
1:A:1887:ARG:HD3	1:A:2039:LEU:HD11	1.85	0.57
1:A:3909:LEU:HB3	1:A:4344:LEU:HD13	1.86	0.57
1:A:1561:LEU:HD23	1:A:1564:GLU:HG3	1.87	0.57
1:A:3873:ARG:HD2	1:A:4025:LEU:HD13	1.87	0.57
1:A:4201:TRP:HZ3	1:A:4207:PHE:HE1	1.52	0.57
1:A:2773:MET:HG3	1:A:2825:TRP:HE1	1.68	0.57
1:A:2890:ARG:HG2	1:A:2894:LYS:HE2	1.87	0.57
1:A:2933:LEU:HD12	1:A:3065:VAL:HG22	1.87	0.57
1:A:4445:THR:HG22	1:A:4448:LEU:HD23	1.86	0.57
1:A:2210:LEU:HG	1:A:2220:LEU:HD21	1.87	0.57
1:A:2533:PRO:HB2	1:A:2535:ILE:HG22	1.87	0.57
1:A:2623:SER:HA	1:A:2668:LEU:HD23	1.87	0.57
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	1.86	0.57
1:A:2961:ILE:HB	1:A:2998:ASN:HD21	1.68	0.57
1:A:4176:ARG:HH12	1:A:4220:ASP:HA	1.68	0.57
1:A:2851:ASP:OD1	1:A:2865:LYS:NZ	2.38	0.56
1:A:4106:LEU:HD23	1:A:4135:PRO:HD2	1.87	0.56
1:A:1511:PRO:HG2	1:A:3670:ASP:HB3	1.86	0.56
1:A:1814:GLU:OE2	1:A:1878:LYS:NZ	2.29	0.56
1:A:4399:LYS:NZ	1:A:4493:SER:OG	2.38	0.56
1:A:4453:ASN:O	1:A:4457:LYS:NZ	2.38	0.56
1:A:2292:ARG:H	1:A:2292:ARG:HH11	1.53	0.56
1:A:3208:ILE:HB	1:A:3486:ARG:HH22	1.71	0.56
1:A:4172:SER:OG	1:A:4176:ARG:NE	2.28	0.56
1:A:2280:PHE:CE1	1:A:2315:LEU:HD21	2.41	0.55
1:A:2826:ALA:HA	1:A:2850:ILE:HD11	1.88	0.55
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.87	0.55
1:A:2665:GLU:HB3	1:A:2668:LEU:HB2	1.88	0.55
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.89	0.55
1:A:1846:PHE:CE2	1:A:1848:PRO:HG3	2.41	0.55
1:A:2308:ASP:HB3	1:A:2311:TRP:NE1	2.21	0.55
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.41	0.55
1:A:2320:ASP:HB3	1:A:2358:ARG:HD3	1.87	0.55
1:A:2622:PHE:HD1	1:A:2626:THR:HG21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2849:ASN:HA	1:A:2852:THR:HG22	1.87	0.55
1:A:2065:LEU:HD11	1:A:2133:GLU:HB3	1.88	0.55
1:A:3734:LEU:HD21	1:A:3783:LYS:HB3	1.89	0.54
1:A:4069:ILE:HD13	1:A:4080:ALA:HA	1.89	0.54
1:A:2925:ILE:HG21	1:A:2933:LEU:HG	1.87	0.54
1:A:3033:CYS:HB2	1:A:3053:TRP:HZ3	1.72	0.54
1:A:2922:ILE:HG23	1:A:2933:LEU:HD11	1.89	0.54
1:A:1626:PHE:CE1	1:A:1628:ARG:HB2	2.42	0.54
1:A:3126:MET:SD	1:A:3539:ALA:HB2	2.48	0.54
1:A:2457:SER:HB3	1:A:2732:PRO:HB3	1.88	0.54
1:A:3691:ASP:O	1:A:3695:ARG:NH1	2.40	0.54
1:A:3567:LEU:HB2	1:A:3599:PHE:CE1	2.42	0.54
1:A:4227:ALA:HB2	1:A:4233:ILE:HD13	1.89	0.54
1:A:3207:LYS:HE3	1:A:3753:LEU:HB3	1.90	0.54
1:A:4004:MET:HE3	1:A:4007:MET:HB2	1.90	0.54
1:A:4247:MET:HG2	1:A:4251:ILE:HD11	1.90	0.54
1:A:3614:PHE:HE2	1:A:3638:VAL:HG12	1.73	0.53
1:A:3724:VAL:HA	1:A:3727:LYS:HG2	1.89	0.53
1:A:4169:ILE:HG21	1:A:4302:ARG:HE	1.73	0.53
1:A:2441:PHE:HA	1:A:2449:LEU:HD23	1.90	0.53
1:A:3502:THR:OG1	1:A:3544:ARG:N	2.42	0.53
1:A:3034:LYS:O	1:A:3038:GLN:HG2	2.09	0.53
1:A:3148:VAL:O	1:A:3152:GLN:HG2	2.08	0.53
1:A:3055:THR:O	1:A:3059:ILE:HG12	2.08	0.53
1:A:3638:VAL:HG11	1:A:3679:LEU:HB3	1.91	0.53
1:A:3730:ASP:HA	1:A:3733:LYS:HZ2	1.73	0.53
1:A:4201:TRP:CZ3	1:A:4207:PHE:HE1	2.26	0.53
1:A:2630:LEU:HA	1:A:2633:LYS:NZ	2.23	0.53
1:A:1806:ARG:NH2	1:A:1876:GLN:O	2.42	0.53
1:A:2113:ARG:O	1:A:2113:ARG:HG3	2.08	0.53
1:A:2221:MET:HG3	1:A:2343:PHE:HB2	1.91	0.53
1:A:3731:LEU:HD11	1:A:3790:VAL:HG12	1.90	0.53
1:A:2648:VAL:HG12	1:A:2701:VAL:HG23	1.90	0.53
1:A:3499:GLN:O	1:A:3503:ILE:HG13	2.09	0.53
1:A:4201:TRP:HE1	1:A:4264:LEU:HD23	1.74	0.53
1:A:1618:TYR:HA	1:A:1621:ARG:HG2	1.91	0.52
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.44	0.52
1:A:1959:GLU:HB3	1:A:1962:ARG:HG3	1.90	0.52
1:A:3723:ASP:O	1:A:3726:GLU:HG3	2.10	0.52
1:A:3729:SER:O	1:A:3733:LYS:HG3	2.09	0.52
1:A:3741:ARG:HH12	1:A:3776:GLU:HG2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3559:ARG:O	1:A:3563:GLN:HG2	2.08	0.52
1:A:2963:VAL:HG11	1:A:2998:ASN:HA	1.92	0.52
1:A:2944:THR:O	1:A:2948:ARG:HG3	2.10	0.52
1:A:2382:LEU:O	1:A:2416:GLN:NE2	2.39	0.52
1:A:4247:MET:O	1:A:4252:TYR:HB2	2.10	0.52
1:A:2910:VAL:HG21	1:A:3105:VAL:HG22	1.92	0.51
1:A:4492:ILE:HG12	1:A:4507:ILE:HD13	1.91	0.51
1:A:4070:ALA:HA	1:A:4097:LYS:HB2	1.92	0.51
1:A:2079:GLN:HG2	1:A:2160:LEU:HD21	1.91	0.51
1:A:2220:LEU:HD23	1:A:2342:MET:HE3	1.92	0.51
1:A:2581:LEU:HD13	1:A:2605:LEU:HD12	1.92	0.51
1:A:4188:ALA:O	1:A:4192:GLU:HG2	2.10	0.51
1:A:1659:ALA:HB2	1:A:1926:PHE:CD1	2.43	0.51
1:A:1666:LEU:HB3	1:A:1670:ASN:HA	1.92	0.51
1:A:3556:ALA:HB2	1:A:3737:GLU:OE1	2.11	0.51
1:A:4306:VAL:O	1:A:4310:GLU:HG3	2.11	0.51
1:A:2635:PHE:HB3	1:A:2650:LEU:HD11	1.91	0.51
1:A:3876:LEU:HD23	1:A:4146:VAL:HG11	1.90	0.51
1:A:2346:GLN:HB2	1:A:2726:ARG:HD2	1.92	0.51
1:A:2383:ARG:NH2	1:A:2424:GLN:OE1	2.43	0.51
1:A:1599:ARG:O	1:A:1602:GLU:HG3	2.10	0.51
1:A:2823:ARG:HE	1:A:2871:ILE:HG23	1.75	0.51
1:A:4201:TRP:HZ3	1:A:4207:PHE:CE1	2.29	0.51
1:A:2818:VAL:O	1:A:2822:ILE:HG22	2.11	0.51
1:A:3649:LEU:HB3	1:A:3695:ARG:HB3	1.93	0.51
1:A:1533:LEU:HD11	1:A:1597:VAL:HG12	1.93	0.51
1:A:2354:ALA:HB1	1:A:2358:ARG:NH2	2.25	0.51
1:A:3704:THR:H	1:A:3707:SER:HB3	1.76	0.50
1:A:4168:ARG:NH1	1:A:4220:ASP:OD2	2.41	0.50
1:A:3487:GLU:O	1:A:3490:GLU:HG3	2.11	0.50
1:A:3488:ARG:HH12	1:A:3773:LEU:HD22	1.77	0.50
1:A:1619:LEU:HG	1:A:1637:LEU:HD23	1.94	0.50
1:A:2071:PRO:O	1:A:2075:LEU:HG	2.12	0.50
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	1.93	0.50
1:A:3690:PRO:HA	1:A:3693:CYS:HB2	1.94	0.50
1:A:1698:ILE:HA	1:A:1701:TRP:CD1	2.47	0.49
1:A:1933:ASP:OD1	1:A:1934:GLU:N	2.43	0.49
1:A:3128:VAL:HG22	1:A:3145:ASN:OD1	2.12	0.49
1:A:1904:PRO:HB2	1:A:1912:LYS:HB3	1.94	0.49
1:A:2308:ASP:HB3	1:A:2311:TRP:CD1	2.47	0.49
1:A:1899:ARG:HB3	1:A:1983:ARG:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2862:ASP:OD1	1:A:2863:ARG:N	2.45	0.49
1:A:2935:LEU:HD23	1:A:3092:ASN:HB2	1.94	0.49
1:A:3193:GLU:O	1:A:3196:GLU:HG3	2.12	0.49
1:A:2868:SER:OG	1:A:2870:PRO:HD2	2.12	0.49
1:A:3923:ARG:NH1	1:A:3952:GLN:HB2	2.28	0.49
1:A:2527:PRO:HD3	1:A:2545:TRP:CD2	2.48	0.49
1:A:2756:LEU:HD12	1:A:2766:ALA:HB2	1.94	0.49
1:A:4486:ILE:O	1:A:4490:GLN:HG3	2.12	0.49
1:A:1926:PHE:CE2	1:A:1928:LEU:HD11	2.47	0.49
1:A:2759:ILE:HG13	1:A:2759:ILE:O	2.13	0.49
1:A:4474:THR:HG22	1:A:4476:ILE:H	1.78	0.49
1:A:1888:CYS:HA	1:A:2039:LEU:HD22	1.95	0.49
1:A:2188:GLU:OE2	1:A:2243:ARG:NH2	2.46	0.49
1:A:2327:LEU:HD12	1:A:2331:GLU:HB3	1.95	0.49
1:A:2838:VAL:HG13	1:A:3093:TRP:CZ2	2.47	0.49
1:A:3628:ARG:HD3	1:A:3628:ARG:O	2.12	0.49
1:A:2457:SER:OG	1:A:2501:SER:HB2	2.13	0.49
1:A:2671:MET:HB2	1:A:2721:LYS:HG2	1.95	0.49
1:A:3133:LEU:N	1:A:3134:PRO:HD3	2.27	0.49
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.95	0.49
1:A:4140:ARG:HG3	1:A:4140:ARG:HH11	1.78	0.49
1:A:1927:VAL:HG22	1:A:1954:TRP:HB2	1.95	0.49
1:A:2134:GLN:O	1:A:2138:ILE:HG12	2.13	0.49
1:A:3724:VAL:HG21	1:A:3797:VAL:HG11	1.93	0.49
1:A:4046:VAL:HG21	1:A:4148:GLU:HG2	1.93	0.49
1:A:1698:ILE:HA	1:A:1701:TRP:NE1	2.28	0.48
1:A:4481:ASP:OD1	1:A:4482:PHE:N	2.46	0.48
1:A:2269:ASP:OD1	1:A:2269:ASP:N	2.46	0.48
1:A:2617:VAL:HG13	1:A:2660:VAL:HG23	1.95	0.48
1:A:3587:PRO:O	1:A:3587:PRO:HG2	2.12	0.48
1:A:3931:GLN:O	1:A:3935:VAL:HG23	2.13	0.48
1:A:4175:GLU:HG3	1:A:4278:PHE:CE2	2.48	0.48
1:A:1711:VAL:HG13	1:A:1715:LYS:HE3	1.95	0.48
1:A:2449:LEU:HD11	1:A:2454:CYS:SG	2.53	0.48
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.95	0.48
1:A:2831:ARG:HA	1:A:2831:ARG:NE	2.28	0.48
1:A:2849:ASN:O	1:A:2853:VAL:HG22	2.13	0.48
1:A:4445:THR:H	1:A:4448:LEU:HB2	1.79	0.48
1:A:2660:VAL:HG12	1:A:2707:GLN:HB3	1.94	0.48
1:A:2740:GLY:N	1:A:2743:SER:OG	2.47	0.48
1:A:3591:ASP:HB3	1:A:3701:PHE:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2785:THR:OG1	1:A:2787:ASP:OD1	2.27	0.48
1:A:2809:ALA:HB1	1:A:2824:ILE:HD13	1.96	0.48
1:A:3151:HIS:CE1	1:A:3176:TYR:HB2	2.48	0.48
1:A:3642:ASP:OD2	1:A:3644:VAL:HG12	2.14	0.48
1:A:2309:PRO:HD3	1:A:2350:TYR:O	2.13	0.47
1:A:4100:HIS:HB3	1:A:4128:MET:HB2	1.96	0.47
1:A:1721:VAL:O	1:A:1725:GLU:HG2	2.15	0.47
1:A:2340:ARG:HG2	1:A:2340:ARG:HH11	1.78	0.47
1:A:2472:TYR:CE2	1:A:2481:MET:HB3	2.50	0.47
1:A:3801:TYR:CD1	1:A:3856:LEU:HD13	2.49	0.47
1:A:4178:ARG:HD2	1:A:4278:PHE:CE2	2.49	0.47
1:A:2365:SER:O	1:A:2368:VAL:HG22	2.14	0.47
1:A:3034:LYS:NZ	1:A:3035:GLU:OE2	2.46	0.47
1:A:2309:PRO:HG3	1:A:2352:THR:HG23	1.96	0.47
1:A:3555:ASN:HB2	1:A:3558:GLU:OE1	2.15	0.47
1:A:2999:VAL:HG11	1:A:3078:ARG:HH12	1.78	0.47
1:A:3144:VAL:O	1:A:3148:VAL:HG23	2.14	0.47
1:A:1938:PHE:HZ	1:A:1970:ALA:HB3	1.79	0.47
1:A:2609:LEU:HD22	1:A:2660:VAL:HG21	1.97	0.47
1:A:3872:ALA:HB1	1:A:3880:HIS:ND1	2.30	0.47
1:A:4575:LEU:HG	1:A:4624:PHE:HB3	1.97	0.47
1:A:1575:PHE:HD1	1:A:1604:LEU:HD21	1.80	0.47
1:A:2654:GLN:O	1:A:2705:ARG:NH2	2.48	0.47
1:A:2939:SER:O	1:A:3172:THR:HB	2.15	0.47
1:A:4416:GLU:OE2	1:A:4515:PHE:N	2.31	0.47
1:A:1682:GLU:OE1	1:A:1872:TYR:OH	2.27	0.47
1:A:2059:PHE:HE1	1:A:2101:GLY:HA2	1.80	0.47
1:A:2308:ASP:HB3	1:A:2311:TRP:HE1	1.80	0.47
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.15	0.47
1:A:2686:MET:SD	1:A:2703:LEU:HD11	2.55	0.47
1:A:2935:LEU:HD22	1:A:3094:PHE:CE1	2.50	0.47
1:A:3872:ALA:O	1:A:3880:HIS:HE1	1.98	0.47
1:A:1463:LEU:HD21	1:A:1519:ASP:HB3	1.97	0.47
1:A:4296:MET:SD	1:A:4297:PRO:HD2	2.55	0.47
1:A:4538:GLU:HB3	1:A:4594:LYS:HE2	1.96	0.47
1:A:1520:ALA:O	1:A:1524:GLU:N	2.47	0.46
1:A:3152:GLN:O	1:A:3156:GLN:HG2	2.14	0.46
1:A:2132:PRO:HB2	1:A:2135:GLU:OE1	2.15	0.46
1:A:3838:ASN:HA	1:A:3842:GLU:CD	2.36	0.46
1:A:2306:ASP:HA	1:A:2345:VAL:HG23	1.97	0.46
1:A:4175:GLU:HG3	1:A:4278:PHE:HE2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2890:ARG:NH2	1:A:2913:ASN:OD1	2.44	0.46
1:A:3197:GLN:HG3	1:A:3496:PHE:CE2	2.50	0.46
1:A:4266:ASN:O	1:A:4270:GLU:HG3	2.15	0.46
1:A:1804:ARG:O	1:A:1808:LEU:HD23	2.16	0.46
1:A:1998:THR:HG22	1:A:2007:LYS:HA	1.98	0.46
1:A:2034:LYS:HG3	1:A:2035:LEU:HG	1.97	0.46
1:A:2179:ARG:NH1	1:A:2195:ASP:OD1	2.49	0.46
1:A:2624:SER:HA	1:A:2669:PRO:HA	1.98	0.46
1:A:3739:GLN:O	1:A:3743:ARG:HG2	2.16	0.46
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.81	0.46
1:A:4201:TRP:NE1	1:A:4264:LEU:HD23	2.30	0.46
1:A:1503:SER:O	1:A:1507:MET:HG3	2.16	0.46
1:A:2138:ILE:HD11	1:A:2165:PHE:CG	2.51	0.46
1:A:2577:HIS:O	1:A:2581:LEU:HG	2.15	0.46
1:A:3659:ARG:HG3	1:A:3661:LEU:HG	1.96	0.46
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.98	0.46
1:A:2152:GLU:OE2	1:A:2152:GLU:N	2.42	0.45
1:A:4570:CYS:HB3	1:A:4575:LEU:HD23	1.98	0.45
1:A:2650:LEU:HD22	1:A:2703:LEU:HD22	1.98	0.45
1:A:4136:VAL:O	1:A:4140:ARG:HG2	2.17	0.45
1:A:1699:ASN:OD1	1:A:1700:GLU:N	2.49	0.45
1:A:3084:ALA:HA	1:A:3087:ASN:HB3	1.99	0.45
1:A:2209:GLN:O	1:A:2213:ILE:HG12	2.16	0.45
1:A:1789:LEU:HD13	1:A:1815:LEU:HB3	1.99	0.45
1:A:2037:ARG:HH21	1:A:4251:ILE:HA	1.81	0.45
1:A:2890:ARG:O	1:A:2894:LYS:HG3	2.15	0.45
1:A:1492:ASP:OD1	1:A:1492:ASP:N	2.50	0.45
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.50	0.45
1:A:2309:PRO:HA	1:A:2312:VAL:HG22	1.99	0.45
1:A:3204:GLY:HA2	1:A:3750:LEU:HD21	1.99	0.45
1:A:1501:ILE:HA	1:A:1504:VAL:HG22	1.98	0.45
1:A:1579:MET:HA	1:A:1582:VAL:HG12	1.99	0.45
1:A:2469:VAL:HG13	1:A:2481:MET:SD	2.57	0.45
1:A:1680:GLU:CD	1:A:1680:GLU:H	2.20	0.45
1:A:2242:GLU:HG3	1:A:2248:GLU:HA	1.99	0.45
1:A:4611:LEU:HD23	1:A:4611:LEU:H	1.82	0.45
1:A:1561:LEU:HD11	1:A:1618:TYR:CG	2.52	0.44
1:A:1713:LEU:HD13	1:A:1749:LEU:HD11	1.99	0.44
1:A:3715:GLU:OE2	1:A:3841:TYR:OH	2.29	0.44
1:A:4502:LYS:HE2	1:A:4502:LYS:HB2	1.69	0.44
1:A:2445:HIS:NE2	1:A:2449:LEU:HD22	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3590:ILE:HB	1:A:3700:ASN:HA	2.00	0.44
1:A:3612:THR:O	1:A:3635:VAL:HA	2.16	0.44
1:A:4154:LYS:HE3	1:A:4310:GLU:HA	1.98	0.44
1:A:1860:GLN:HG2	1:A:1865:LYS:HG2	2.00	0.44
1:A:2371:THR:HG22	1:A:2451:ARG:HD2	1.99	0.44
1:A:3976:GLU:HB3	1:A:3979:PRO:HD2	1.99	0.44
1:A:4185:TRP:CD1	1:A:4284:LEU:HD12	2.53	0.44
1:A:1697:LYS:HD2	1:A:1698:ILE:H	1.82	0.44
1:A:1888:CYS:O	1:A:1892:MET:HG2	2.18	0.44
1:A:2046:ARG:HG2	1:A:2090:LEU:HD13	2.00	0.44
1:A:2086:TYR:OH	1:A:2153:ASP:OD2	2.24	0.44
1:A:2663:CYS:N	1:A:2709:VAL:O	2.47	0.44
1:A:2770:THR:O	1:A:2774:VAL:HG23	2.18	0.44
1:A:4326:ASN:O	1:A:4330:VAL:HG23	2.18	0.44
1:A:1588:VAL:HG13	1:A:1589:MET:CE	2.48	0.44
1:A:1613:LYS:O	1:A:1617:GLU:HG2	2.18	0.44
1:A:2245:GLU:HB2	1:A:2247:VAL:HG12	2.00	0.44
1:A:2454:CYS:HB3	1:A:2502:LEU:HD12	1.98	0.44
1:A:3015:GLY:HA3	1:A:3059:ILE:HD11	2.00	0.44
1:A:3628:ARG:HD3	1:A:3628:ARG:C	2.38	0.44
1:A:4117:GLN:OE1	1:A:4117:GLN:N	2.50	0.44
1:A:1651:GLN:N	1:A:1651:GLN:OE1	2.49	0.44
1:A:2593:LEU:HD23	1:A:2734:VAL:HB	1.99	0.44
1:A:1920:GLY:HA3	1:A:1927:VAL:HG21	1.99	0.43
1:A:2106:GLU:OE1	1:A:2109:GLN:NE2	2.50	0.43
1:A:4503:GLU:O	1:A:4507:ILE:HG13	2.17	0.43
1:A:2569:VAL:HG21	1:A:2747:ILE:HA	2.01	0.43
1:A:2845:TRP:CE2	1:A:2849:ASN:ND2	2.87	0.43
1:A:2374:ILE:HA	3:A:4702:ATP:H8	1.83	0.43
1:A:2806:ILE:O	1:A:2810:LEU:HG	2.18	0.43
1:A:3507:CYS:HG	1:A:3552:TYR:HH	1.61	0.43
1:A:3724:VAL:HG11	1:A:3797:VAL:HG21	2.01	0.43
1:A:3811:ILE:HD11	1:A:3864:PHE:CE1	2.53	0.43
1:A:4099:VAL:HG11	1:A:4126:LEU:HB3	2.01	0.43
1:A:4113:LEU:HD23	1:A:4113:LEU:HA	1.86	0.43
1:A:2831:ARG:HG3	1:A:2924:ARG:NH1	2.33	0.43
1:A:3609:ILE:HD11	1:A:3634:LEU:HB2	2.01	0.43
1:A:2458:LEU:O	1:A:2462:LEU:HG	2.19	0.43
1:A:2749:GLY:O	1:A:2753:ARG:HG3	2.18	0.43
1:A:3555:ASN:O	1:A:3559:ARG:HG3	2.19	0.43
1:A:3633:LEU:HB3	1:A:3677:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3638:VAL:HG22	1:A:3681:THR:HB	2.01	0.43
1:A:1903:SER:N	1:A:2037:ARG:O	2.48	0.43
1:A:2354:ALA:O	1:A:2358:ARG:HB2	2.18	0.43
1:A:2596:PRO:HB2	1:A:2738:TYR:CE1	2.53	0.43
1:A:3620:ARG:HE	1:A:3620:ARG:HB3	1.56	0.43
1:A:3721:ARG:HG2	1:A:3852:HIS:CE1	2.53	0.43
1:A:4196:TYR:O	1:A:4200:GLY:N	2.51	0.43
1:A:4473:MET:HB2	1:A:4477:GLN:OE1	2.19	0.43
1:A:3812:TYR:CZ	1:A:3829:LEU:HD13	2.54	0.43
1:A:3877:HIS:O	1:A:3877:HIS:ND1	2.49	0.43
1:A:4601:LYS:HE2	1:A:4603:SER:HB3	2.01	0.43
1:A:2075:LEU:HD11	1:A:4536:LEU:HD13	2.01	0.43
1:A:2981:ARG:NH1	1:A:3032:GLN:OE1	2.50	0.43
1:A:2995:ASP:OD2	1:A:2998:ASN:HB2	2.19	0.43
1:A:3562:TRP:CZ2	1:A:3581:LYS:HD2	2.54	0.43
1:A:4172:SER:CB	1:A:4176:ARG:HH21	2.32	0.43
1:A:4333:THR:O	1:A:4337:VAL:HG23	2.19	0.42
1:A:1588:VAL:HA	1:A:1591:VAL:HG22	2.01	0.42
1:A:3745:LEU:HD12	1:A:3745:LEU:HA	1.88	0.42
1:A:4003:ALA:O	1:A:4007:MET:HG3	2.19	0.42
1:A:1544:TRP:HE1	1:A:1572:SER:HA	1.84	0.42
1:A:1635:GLU:OE1	1:A:1635:GLU:N	2.33	0.42
1:A:3029:LEU:HD11	1:A:3054:PHE:CZ	2.55	0.42
1:A:3803:PRO:HA	1:A:3806:THR:HG22	2.01	0.42
1:A:3844:PRO:HA	1:A:3847:LYS:HE3	2.00	0.42
1:A:4543:VAL:HG21	1:A:4622:VAL:HG23	2.01	0.42
1:A:1554:SER:OG	1:A:1642:GLY:HA3	2.18	0.42
1:A:2232:MET:HE1	1:A:2235:ARG:HD2	2.01	0.42
1:A:3892:LEU:HD13	1:A:3983:ILE:HG21	2.00	0.42
1:A:2410:SER:HB3	1:A:2411:PRO:HD3	2.01	0.42
1:A:4044:CYS:SG	1:A:4144:ILE:HG23	2.59	0.42
1:A:2668:LEU:HD13	1:A:2720:ARG:HH12	1.85	0.42
1:A:3005:LEU:HD21	1:A:3078:ARG:NH1	2.35	0.42
1:A:3146:SER:OG	1:A:3508:LEU:HD21	2.19	0.42
1:A:4179:LEU:HD11	1:A:4238:ILE:HD12	2.01	0.42
1:A:4189:ILE:HD13	1:A:4321:LEU:HD23	2.01	0.42
1:A:2227:GLY:O	1:A:2369:LEU:HD23	2.20	0.42
1:A:2852:THR:HA	1:A:2855:LEU:HG	2.01	0.42
1:A:2965:ARG:NH2	1:A:3640:SER:O	2.53	0.42
1:A:3562:TRP:HB3	1:A:3567:LEU:HD22	2.02	0.42
1:A:1692:ILE:HG23	1:A:1701:TRP:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2592:VAL:HB	1:A:2733:VAL:HG12	2.02	0.42
1:A:2783:ARG:HD3	1:A:2845:TRP:CE2	2.54	0.42
1:A:2820:GLY:O	1:A:2824:ILE:HG13	2.20	0.42
1:A:2935:LEU:N	1:A:3066:PHE:O	2.45	0.42
1:A:3139:HIS:NE2	1:A:3541:ILE:HG23	2.34	0.42
1:A:3512:ALA:O	1:A:3516:TYR:HB2	2.19	0.42
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	2.02	0.42
1:A:2277:ASP:OD1	1:A:2277:ASP:N	2.52	0.42
1:A:2300:TRP:CD1	1:A:2340:ARG:HB2	2.55	0.42
1:A:2961:ILE:HB	1:A:2998:ASN:ND2	2.34	0.42
1:A:3126:MET:HE1	1:A:3538:GLN:HG2	2.02	0.42
1:A:3740:LEU:O	1:A:3744:GLN:HG2	2.20	0.42
1:A:3997:ARG:HH21	1:A:4000:ARG:HD3	1.85	0.42
1:A:2627:THR:OG1	1:A:2629:GLU:HG2	2.20	0.42
1:A:3604:TYR:HD1	1:A:3607:ARG:HD3	1.85	0.42
1:A:4634:SER:HA	1:A:4637:GLU:HG2	2.01	0.42
1:A:1814:GLU:O	1:A:1818:GLN:HG3	2.20	0.41
1:A:2457:SER:HB2	1:A:2584:TRP:CZ2	2.55	0.41
1:A:2628:PRO:HB3	1:A:2682:PHE:CD2	2.55	0.41
1:A:2635:PHE:HE1	1:A:2661:LEU:HD11	1.85	0.41
1:A:3154:LEU:HA	1:A:3154:LEU:HD12	1.73	0.41
1:A:3030:MET:HA	1:A:3033:CYS:SG	2.60	0.41
1:A:3966:PRO:CD	1:A:4000:ARG:HG3	2.50	0.41
1:A:2179:ARG:NH2	1:A:2205:GLU:OE2	2.53	0.41
1:A:2633:LYS:NZ	1:A:2633:LYS:HB2	2.36	0.41
1:A:2851:ASP:OD2	1:A:2869:ARG:NH1	2.52	0.41
1:A:3196:GLU:HA	1:A:3199:MET:HG3	2.02	0.41
1:A:3611:ARG:NH2	1:A:3636:GLN:OE1	2.53	0.41
1:A:2847:ASP:O	1:A:2850:ILE:HG22	2.21	0.41
1:A:3835:ILE:HG12	1:A:3870:ARG:HD2	2.02	0.41
1:A:4178:ARG:HD2	1:A:4278:PHE:CD2	2.55	0.41
1:A:4631:ASP:OD1	1:A:4631:ASP:N	2.53	0.41
1:A:2230:LYS:HG2	1:A:2364:PHE:CD1	2.56	0.41
1:A:2925:ILE:O	1:A:2928:GLN:HG2	2.20	0.41
1:A:2935:LEU:O	1:A:3067:THR:HA	2.20	0.41
1:A:2936:ILE:HG12	1:A:3068:MET:HB3	2.03	0.41
1:A:2937:GLY:C	1:A:3070:PRO:HD3	2.41	0.41
1:A:3101:ALA:O	1:A:3105:VAL:HG23	2.20	0.41
1:A:3818:LEU:HD23	1:A:3818:LEU:HA	1.93	0.41
1:A:3821:ILE:HD13	1:A:4345:LYS:HD3	2.03	0.41
1:A:3932:ALA:O	1:A:3936:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4342:LYS:O	1:A:4345:LYS:HG2	2.20	0.41
1:A:1834:LYS:HA	1:A:1834:LYS:HD2	1.90	0.41
1:A:2235:ARG:O	1:A:2239:LYS:HG2	2.20	0.41
1:A:2505:ASP:HA	1:A:2735:TYR:HB2	2.02	0.41
1:A:2976:LEU:HA	1:A:2979:VAL:HG12	2.02	0.41
1:A:3085:LEU:HD23	1:A:3085:LEU:HA	1.92	0.41
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.40	0.41
1:A:4628:THR:HG23	1:A:4629:LYS:HG3	2.02	0.41
1:A:1806:ARG:HE	1:A:1875:VAL:HG11	1.86	0.41
1:A:1985:HIS:ND1	1:A:1997:ILE:HD12	2.35	0.41
1:A:2498:ILE:HG23	1:A:2502:LEU:HD22	2.03	0.41
1:A:2668:LEU:HD13	1:A:2720:ARG:NH1	2.36	0.41
1:A:3743:ARG:HA	1:A:3743:ARG:HD3	1.93	0.41
1:A:3764:ASP:HA	1:A:3767:ILE:HB	2.02	0.41
1:A:3959:ILE:HD12	1:A:3959:ILE:H	1.85	0.41
1:A:4431:LEU:O	1:A:4435:VAL:HG23	2.20	0.41
1:A:2104:LYS:NZ	1:A:2133:GLU:OE2	2.47	0.41
1:A:2111:ILE:CD1	1:A:2131:LEU:HD21	2.51	0.41
1:A:3015:GLY:HA3	1:A:3059:ILE:CD1	2.51	0.41
1:A:3127:PRO:HG2	1:A:3130:TYR:CD1	2.55	0.41
1:A:3133:LEU:HD23	1:A:3141:GLU:OE2	2.21	0.41
1:A:3606:ASP:OD1	1:A:3607:ARG:HG3	2.20	0.41
1:A:3873:ARG:HA	1:A:3873:ARG:HD3	1.76	0.41
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	2.03	0.41
1:A:4629:LYS:HE2	1:A:4629:LYS:HB2	1.90	0.41
1:A:3791:MET:HA	1:A:3794:VAL:HB	2.03	0.41
1:A:3871:VAL:HG12	1:A:3875:MET:SD	2.61	0.41
1:A:4204:LYS:HE2	1:A:4204:LYS:HB2	1.97	0.41
1:A:2605:LEU:HD11	1:A:2709:VAL:HG11	2.02	0.40
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.57	0.40
1:A:4610:TYR:CZ	1:A:4615:ARG:HB3	2.56	0.40
1:A:2093:LEU:O	1:A:2097:LEU:HG	2.21	0.40
1:A:2500:TRP:CZ2	1:A:2576:ARG:HD3	2.45	0.40
1:A:3664:LEU:HB3	1:A:3669:ILE:HD13	2.02	0.40
1:A:1783:SER:O	1:A:1787:VAL:HG23	2.22	0.40
1:A:2439:HIS:O	1:A:2442:GLN:HG2	2.22	0.40
1:A:3154:LEU:HD22	1:A:3516:TYR:CD1	2.56	0.40
1:A:3205:LEU:HG	1:A:3489:TRP:HE3	1.86	0.40
1:A:4111:LYS:HD3	1:A:4111:LYS:HA	1.81	0.40
1:A:4481:ASP:O	1:A:4485:ARG:HG3	2.22	0.40
1:A:4619:ILE:HG22	1:A:4620:PHE:HD1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1702:LEU:HA	1:A:1702:LEU:HD23	1.89	0.40
1:A:2018:MET:SD	1:A:2028:LEU:HB3	2.62	0.40
1:A:2527:PRO:HD3	1:A:2545:TRP:CE2	2.56	0.40
1:A:4336:GLY:O	1:A:4340:ILE:HG12	2.21	0.40
1:A:1842:MET:SD	1:A:1922:GLN:HG2	2.61	0.40
1:A:1912:LYS:HB2	1:A:1912:LYS:HE2	1.92	0.40
1:A:2231:SER:HA	1:A:2234:TRP:NE1	2.36	0.40
1:A:2880:ASP:OD2	1:A:2880:ASP:N	2.44	0.40
1:A:4058:LEU:O	1:A:4061:GLU:HG3	2.21	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	2854/4646 (61%)	2750 (96%)	103 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4172	SER

### 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	2548/4125 (62%)	2543 (100%)	5 (0%)	92 97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1729	LYS
1	A	2377	ASN
1	A	3741	ARG
1	A	3937	ARG
1	A	4029	HIS

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

Mol	Chain	Res	Type
1	A	2471	GLN
1	A	3602	ASN
1	A	3843	ASN
1	A	3880	HIS
1	A	4065	GLN
1	A	4117	GLN
1	A	4326	ASN

### 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	4701	-	24,29,29	0.87	0	29,45,45	1.28	2 (6%)
2	ADP	A	4704	-	24,29,29	0.86	0	29,45,45	1.24	2 (6%)
2	ADP	A	4703	-	24,29,29	0.91	0	29,45,45	1.23	3 (10%)
3	ATP	A	4702	-	28,33,33	0.67	0	34,52,52	0.61	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	4701	-	-	3/12/32/32	0/3/3/3
2	ADP	A	4704	-	-	3/12/32/32	0/3/3/3
2	ADP	A	4703	-	-	1/12/32/32	0/3/3/3
3	ATP	A	4702	-	-	5/18/38/38	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4704	ADP	N3-C2-N1	-3.84	123.47	128.67
2	A	4701	ADP	N3-C2-N1	-3.76	123.56	128.67
2	A	4703	ADP	N3-C2-N1	-3.68	123.68	128.67
2	A	4701	ADP	C4-C5-N7	-2.75	106.43	109.34
2	A	4704	ADP	C4-C5-N7	-2.56	106.63	109.34
2	A	4703	ADP	C4-C5-N7	-2.38	106.83	109.34
2	A	4703	ADP	O4'-C1'-N9	2.34	111.85	108.75
3	A	4702	ATP	C5-C6-N6	2.30	123.82	120.31

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O1A

*Continued on next page...*

*Continued from previous page...*

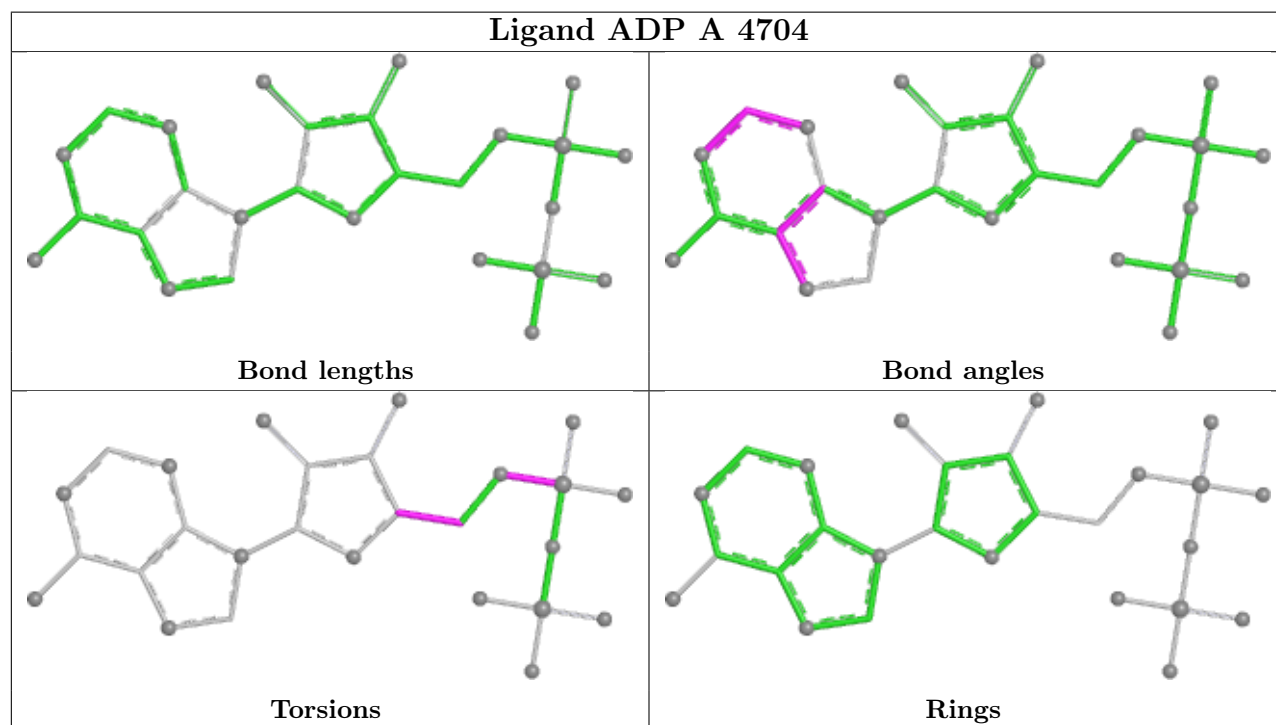
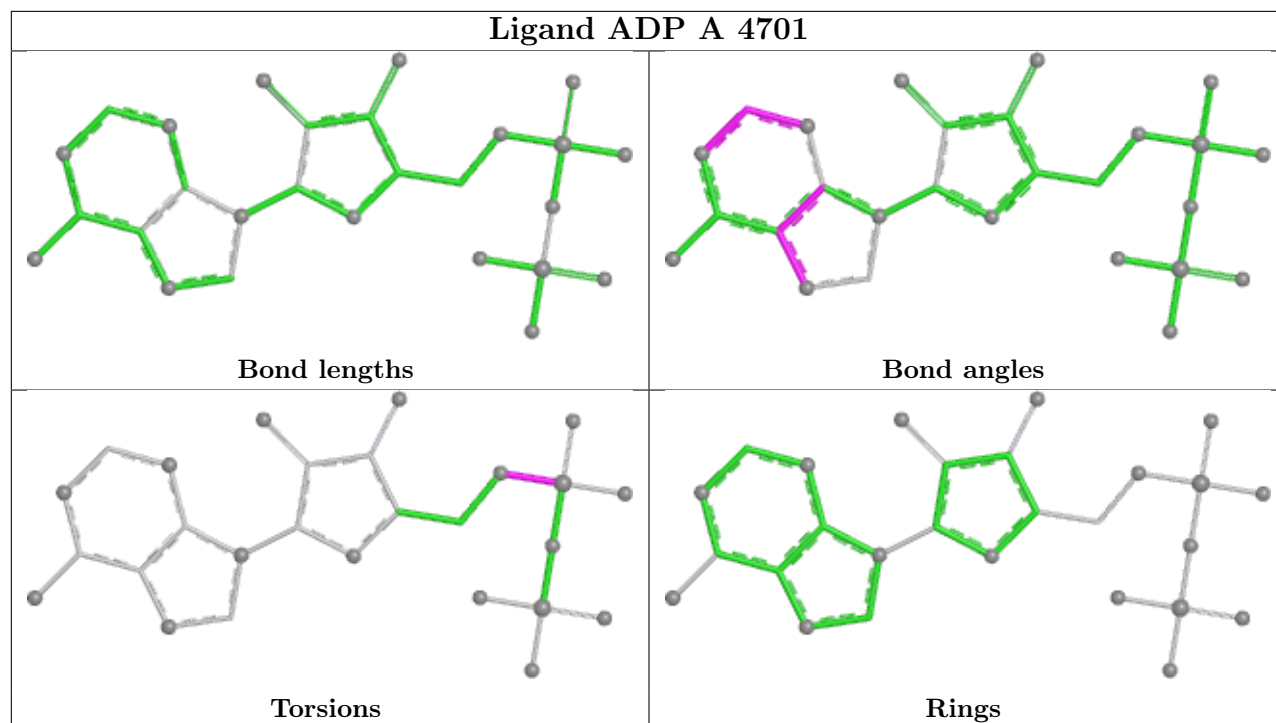
Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4704	ADP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C5'-O5'-PA-O2A
3	A	4702	ATP	C5'-O5'-PA-O3A
2	A	4704	ADP	C3'-C4'-C5'-O5'
3	A	4702	ATP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'
2	A	4703	ADP	O4'-C4'-C5'-O5'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

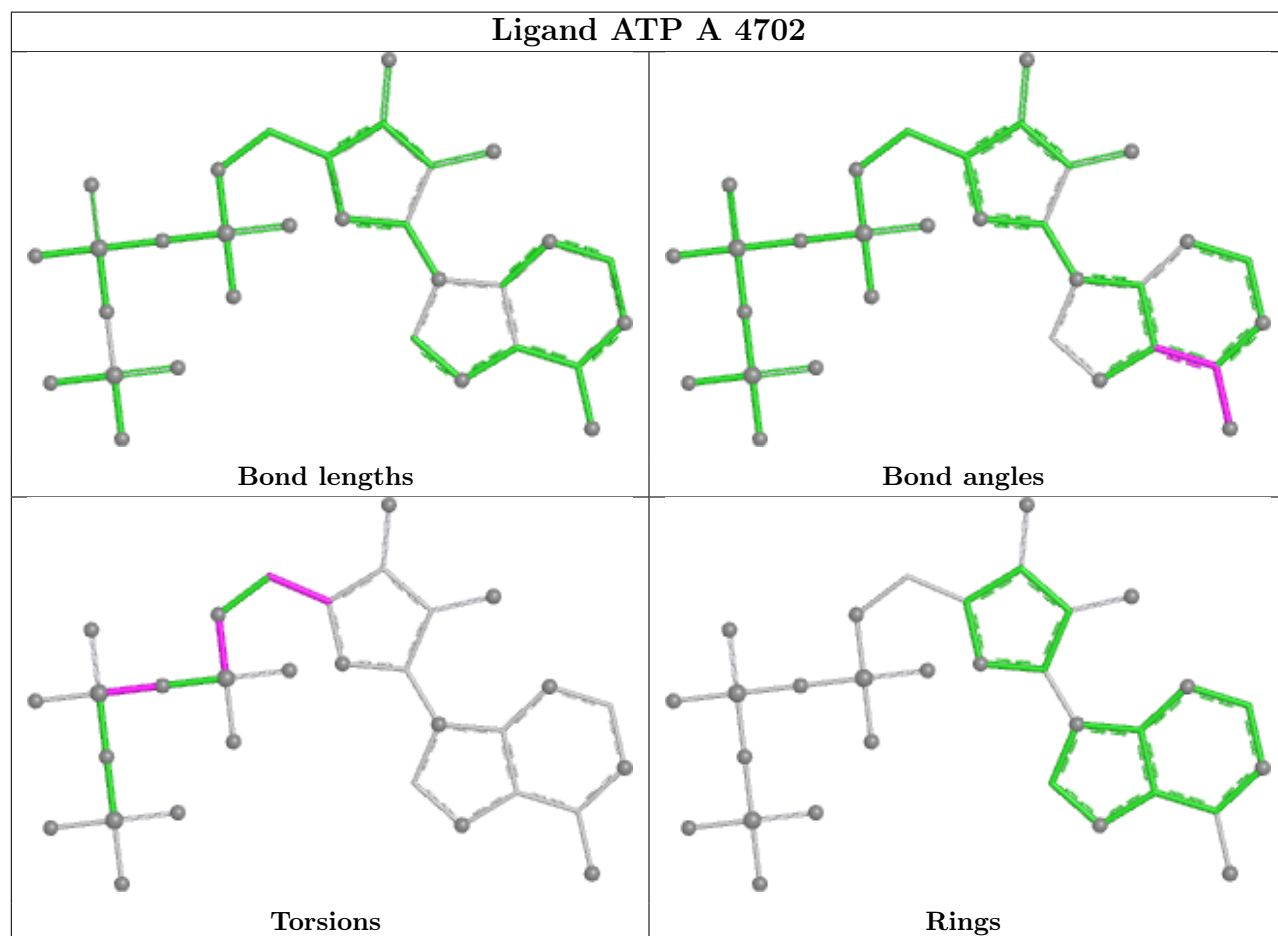
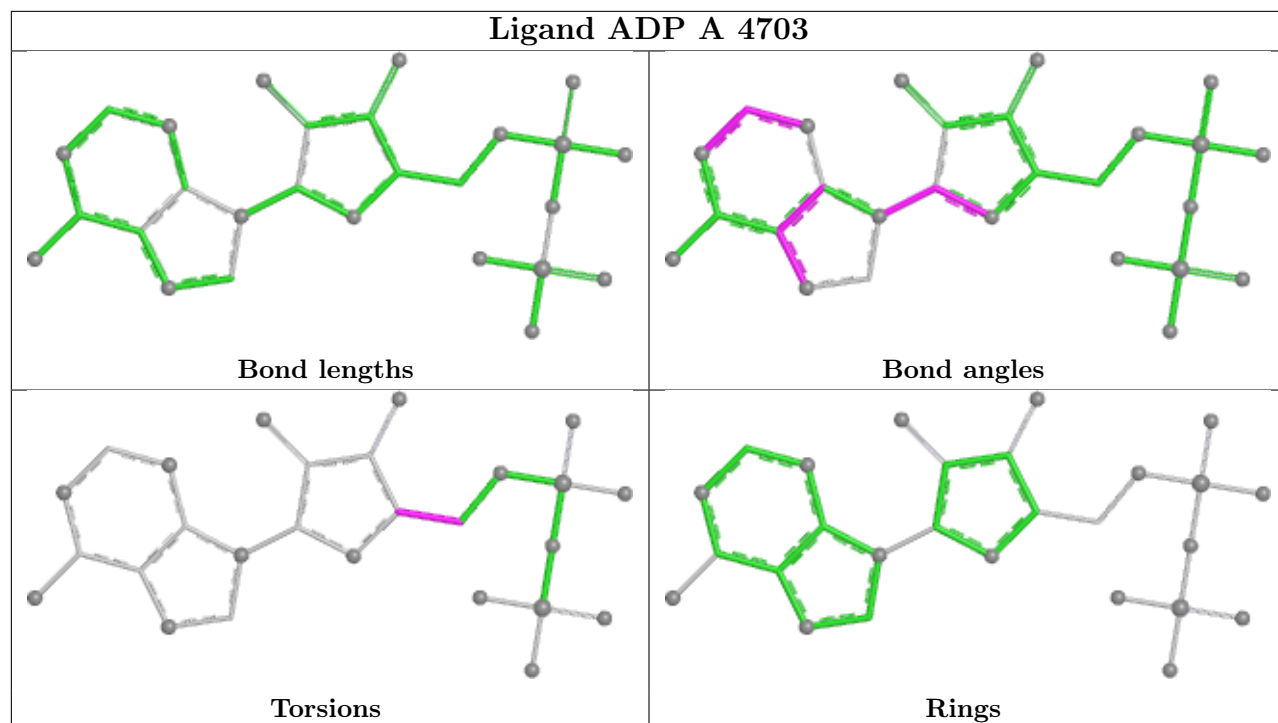
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4702	ATP	1	0

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





## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

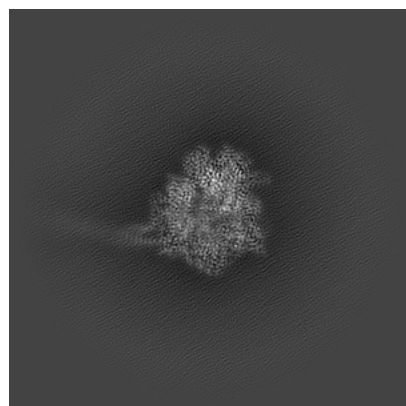
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44720. These allow visual inspection of the internal detail of the map and identification of artifacts.

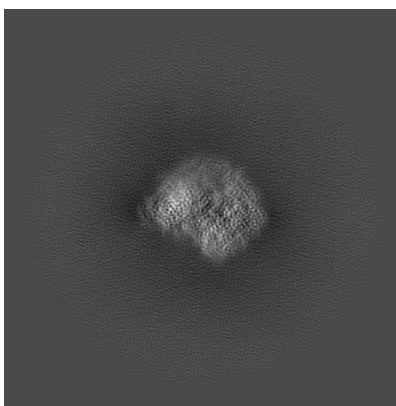
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

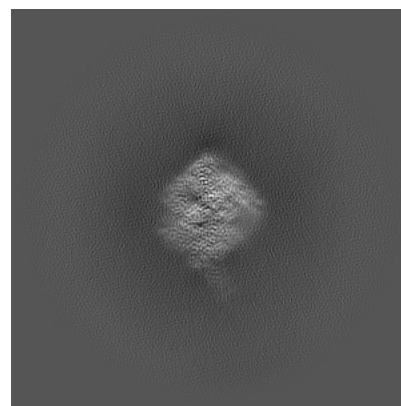
#### 6.1.1 Primary map



X

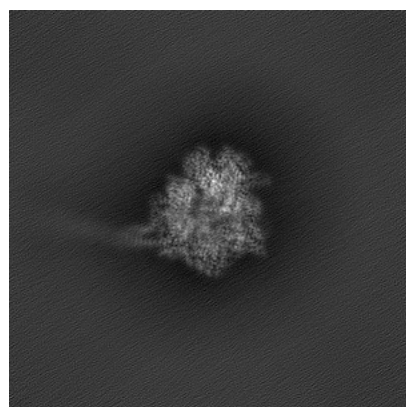


Y

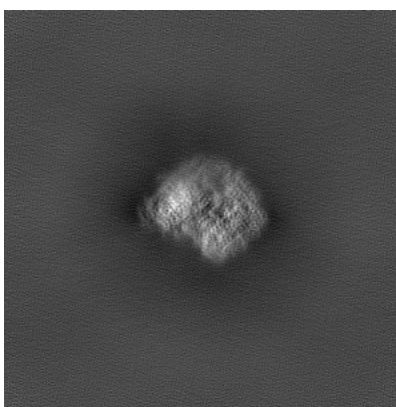


Z

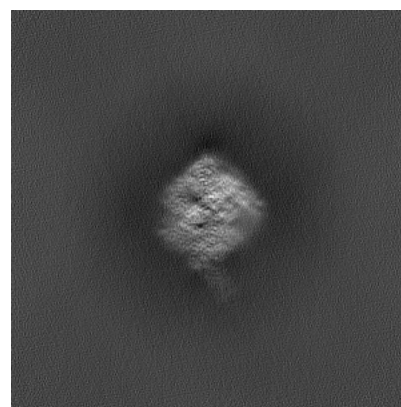
#### 6.1.2 Raw map



X



Y



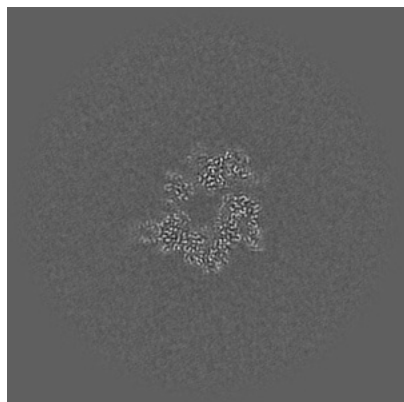
Z

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

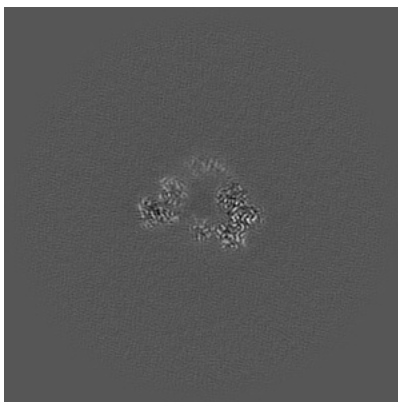


## 6.2 Central slices [i](#)

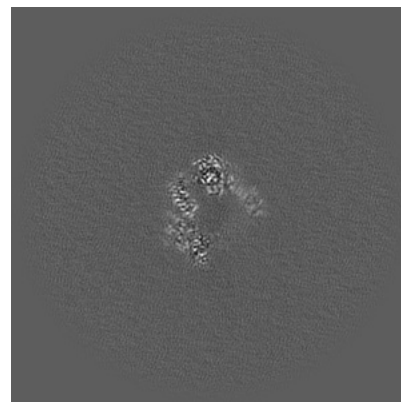
### 6.2.1 Primary map



X Index: 180

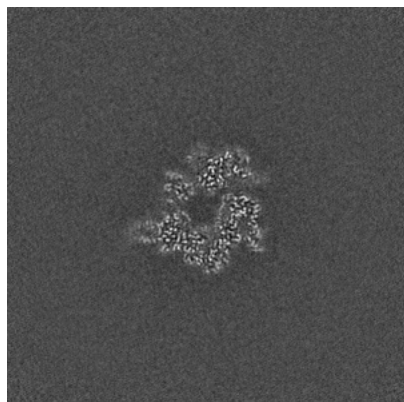


Y Index: 180

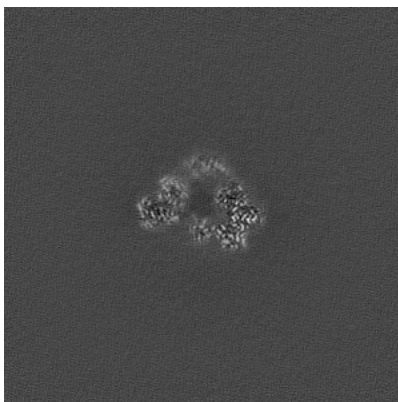


Z Index: 180

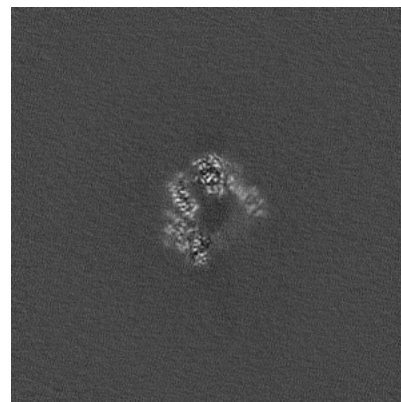
### 6.2.2 Raw map



X Index: 180



Y Index: 180



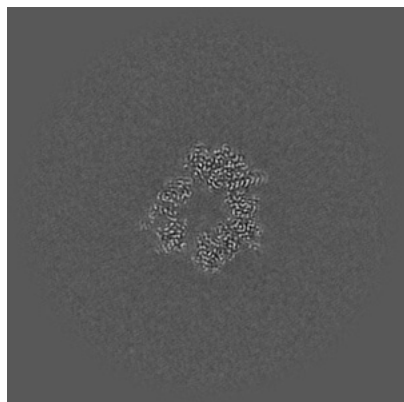
Z Index: 180

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

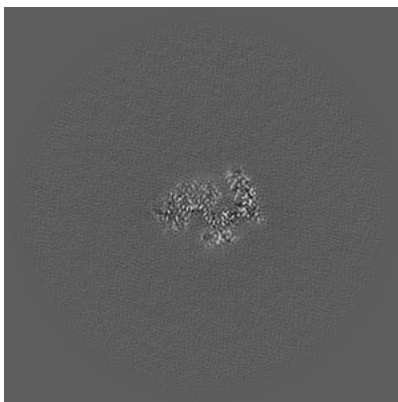


## 6.3 Largest variance slices [i](#)

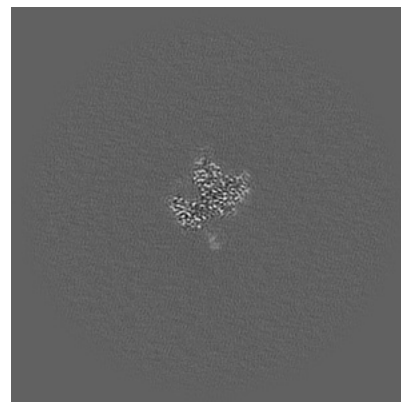
### 6.3.1 Primary map



X Index: 174

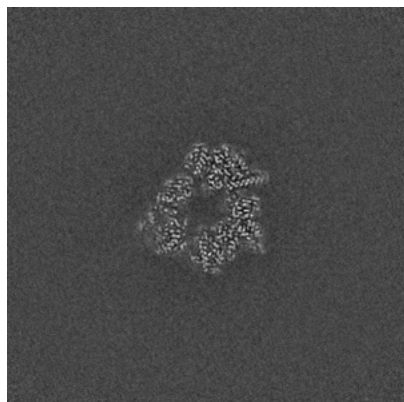


Y Index: 202

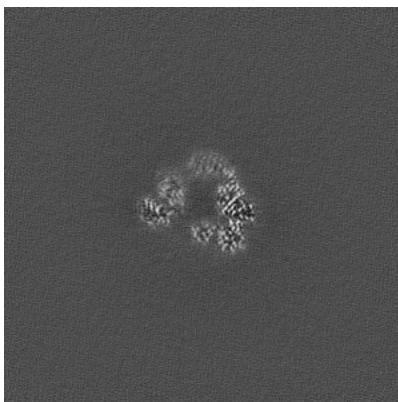


Z Index: 209

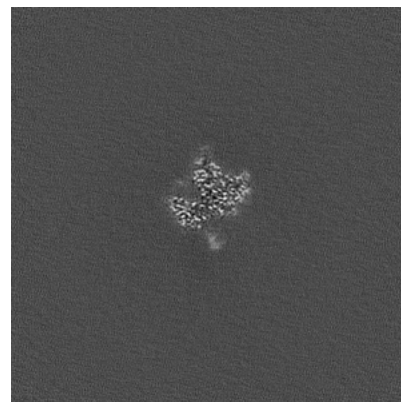
### 6.3.2 Raw map



X Index: 175



Y Index: 183

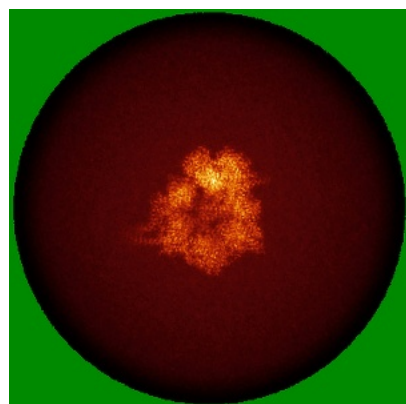


Z Index: 209

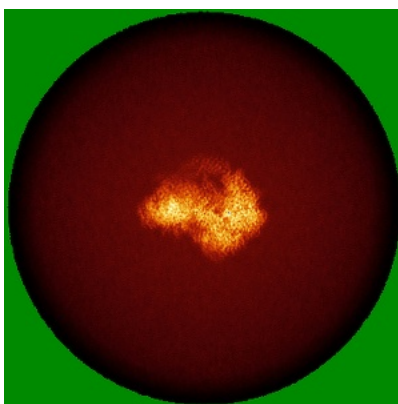
The images above show the largest variance slices of the map in three orthogonal directions.

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

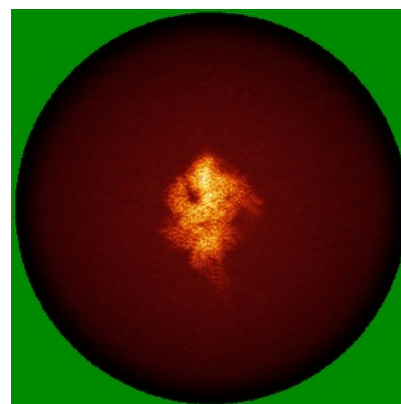
### 6.4.1 Primary map



X

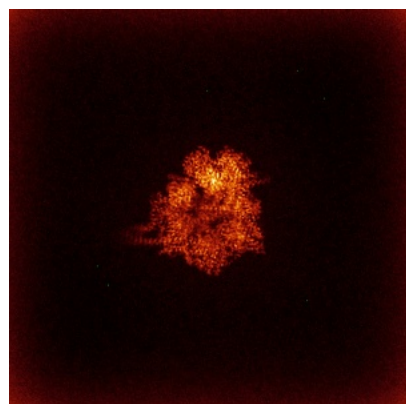


Y

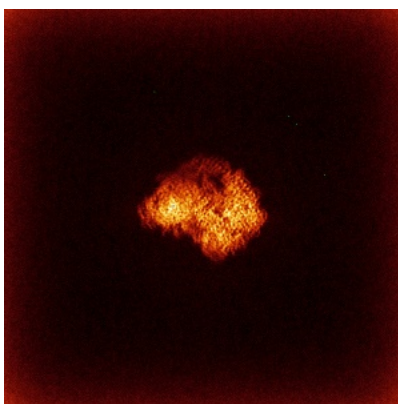


Z

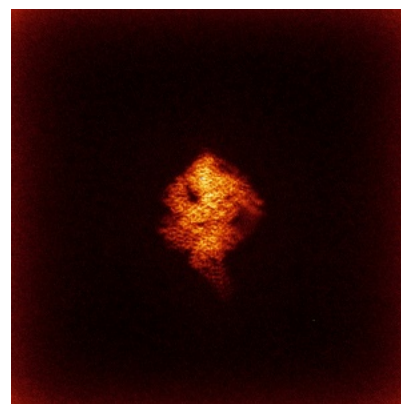
### 6.4.2 Raw map



X



Y

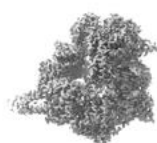


Z

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



X



Y



Z

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



X



Y



Z

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.

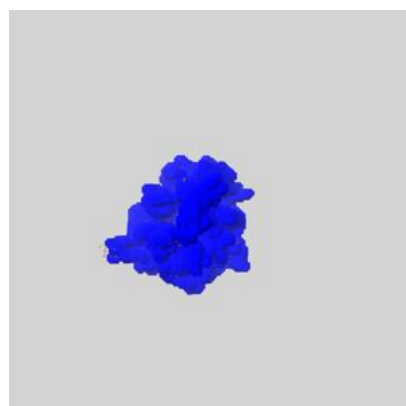
## 6.6 Mask visualisation [i](#)

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

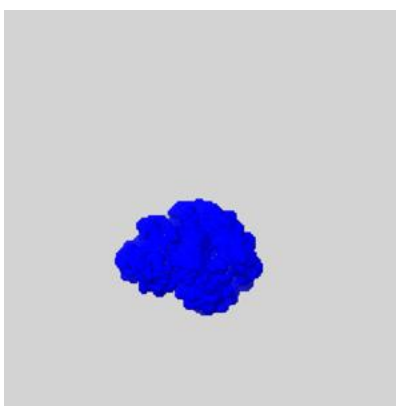
A mask typically either:

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

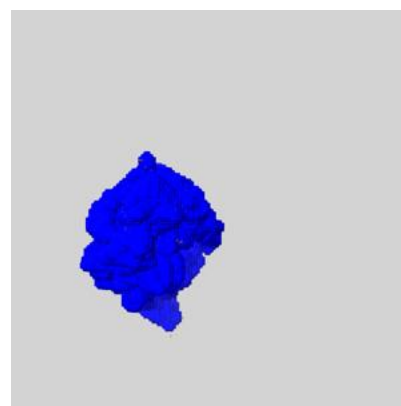
### 6.6.1 emd\_44720\_msk\_1.map [i](#)



X



Y

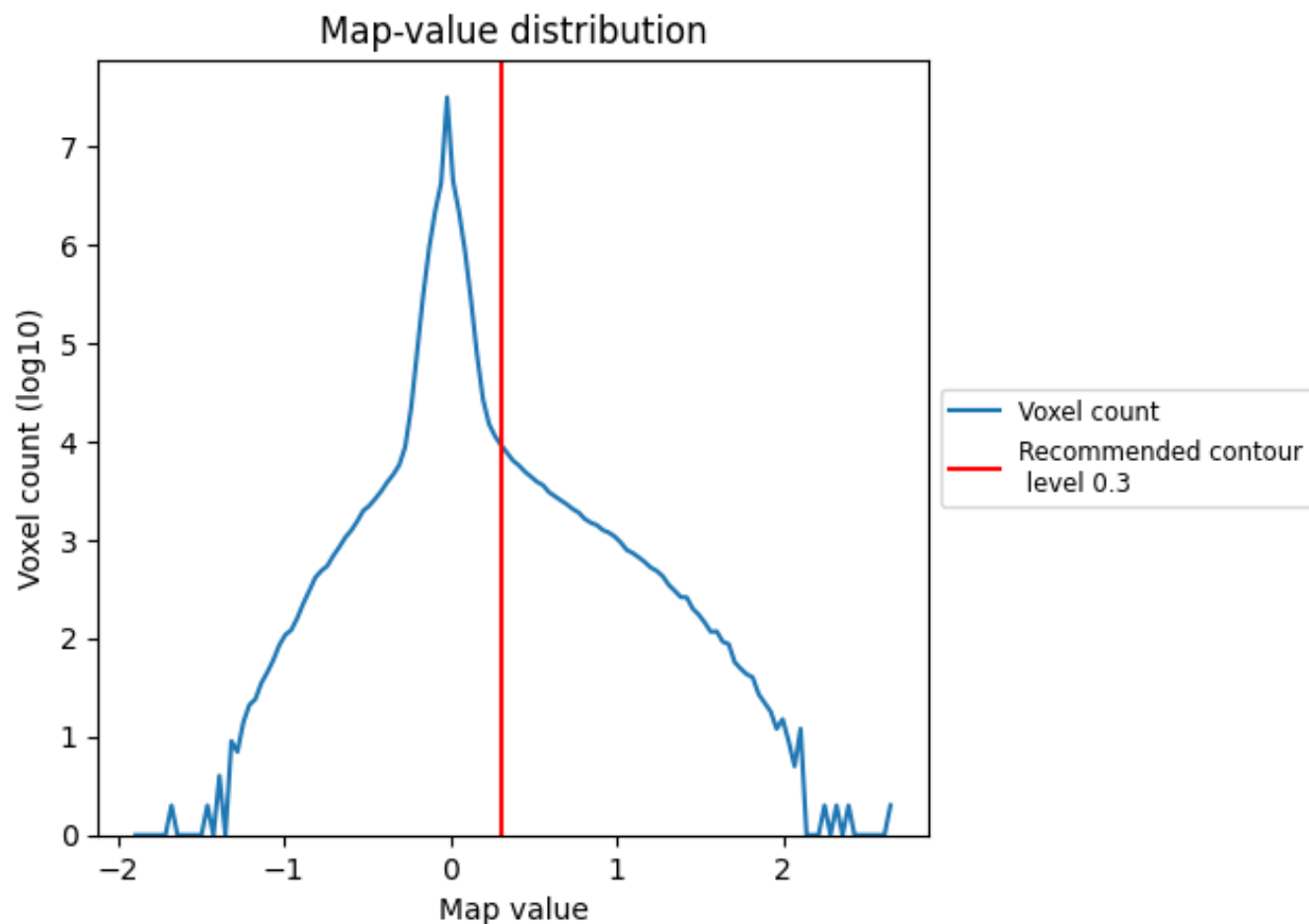


Z

## 7 Map analysis [i](#)

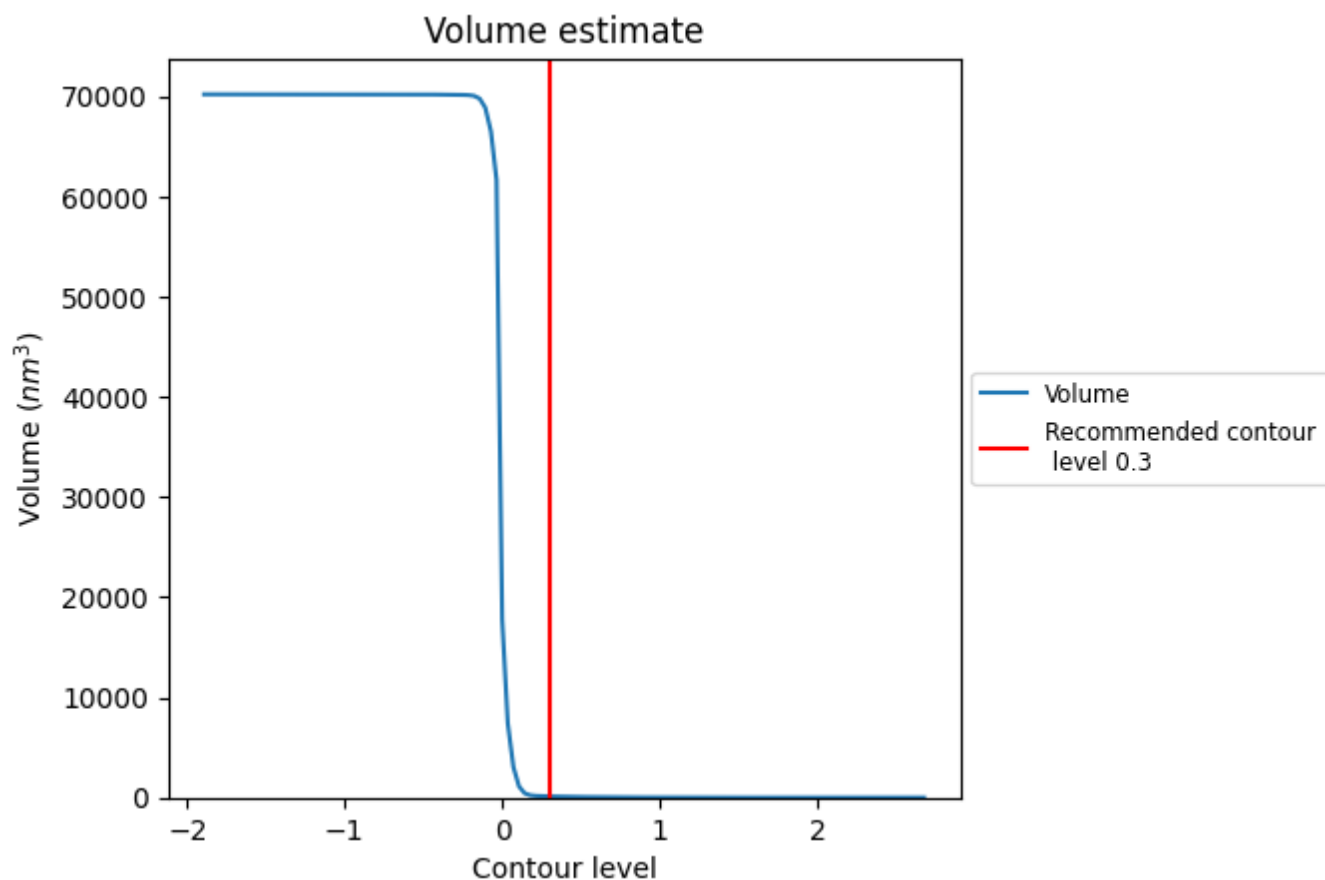
This section contains the results of statistical analysis of the map.

### 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.

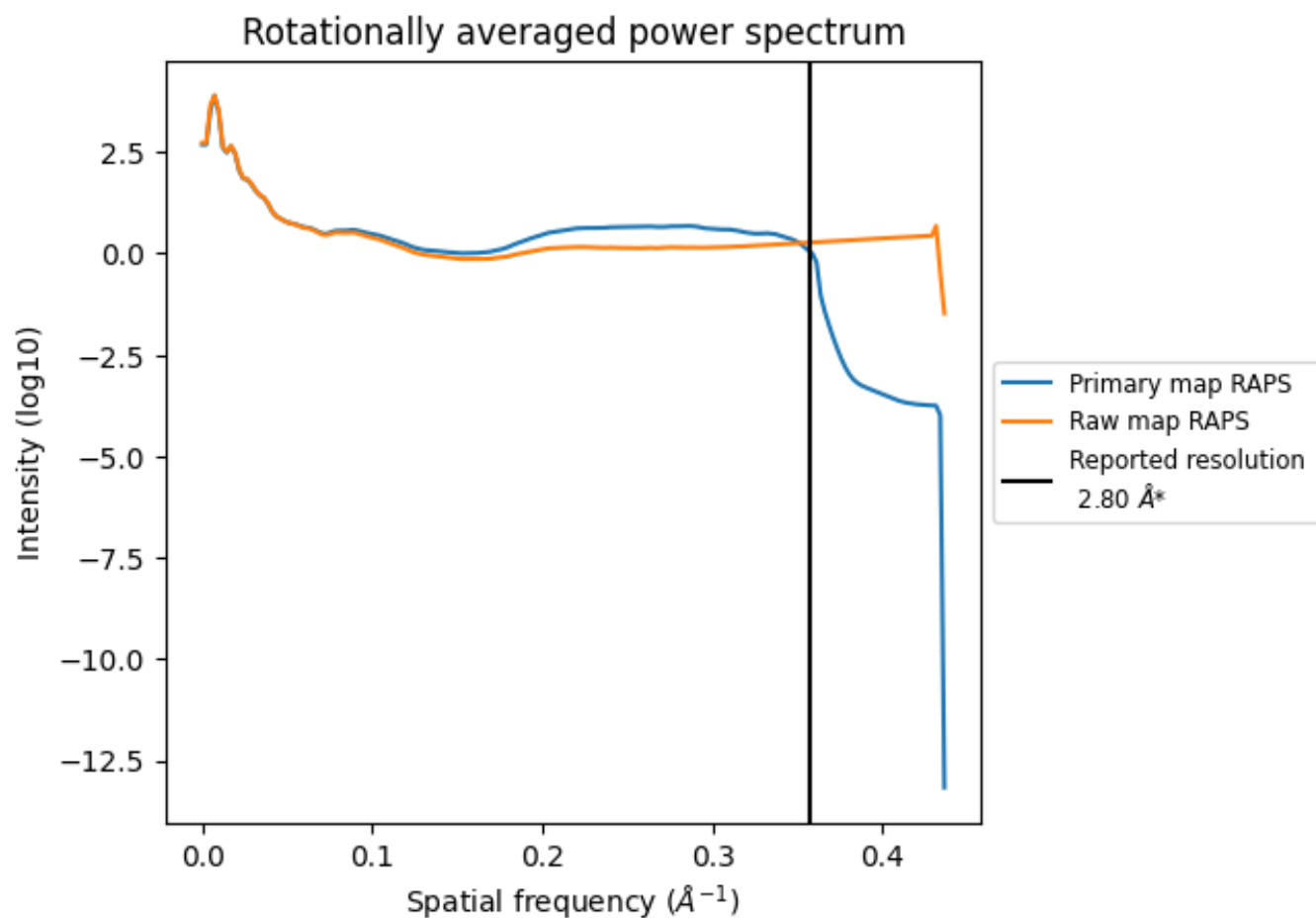
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115 nm<sup>3</sup>; this corresponds to an approximate mass of 104 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 ⓘ

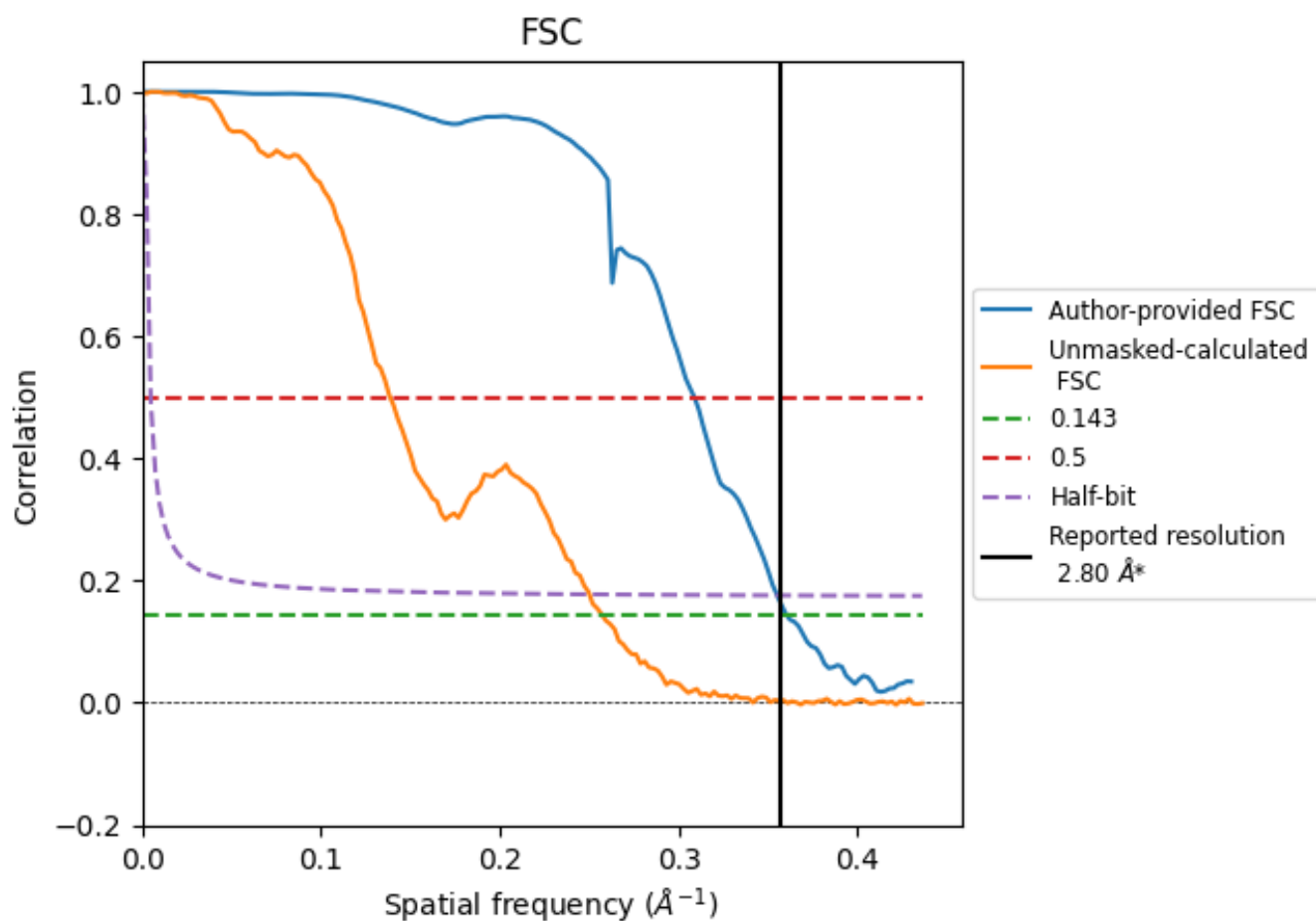


\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

## 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  $0.357 \text{ \AA}^{-1}$



## 8.2 Resolution estimates [i](#)

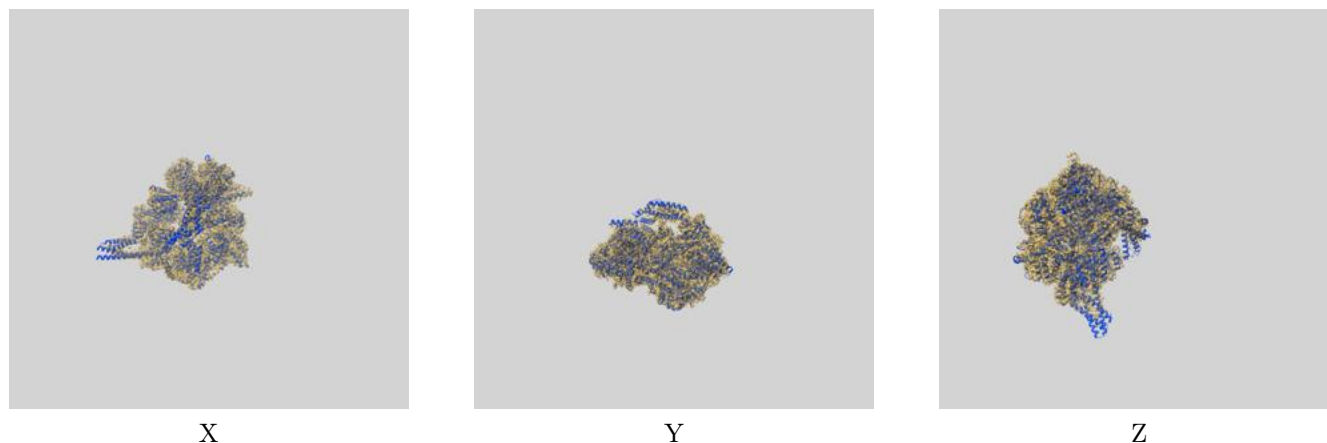
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.77	3.24	2.81
Unmasked-calculated*	3.89	7.21	4.00

\*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 3.89 differs from the reported value 2.8 by more than 10 %

## 9 Map-model fit [i](#)

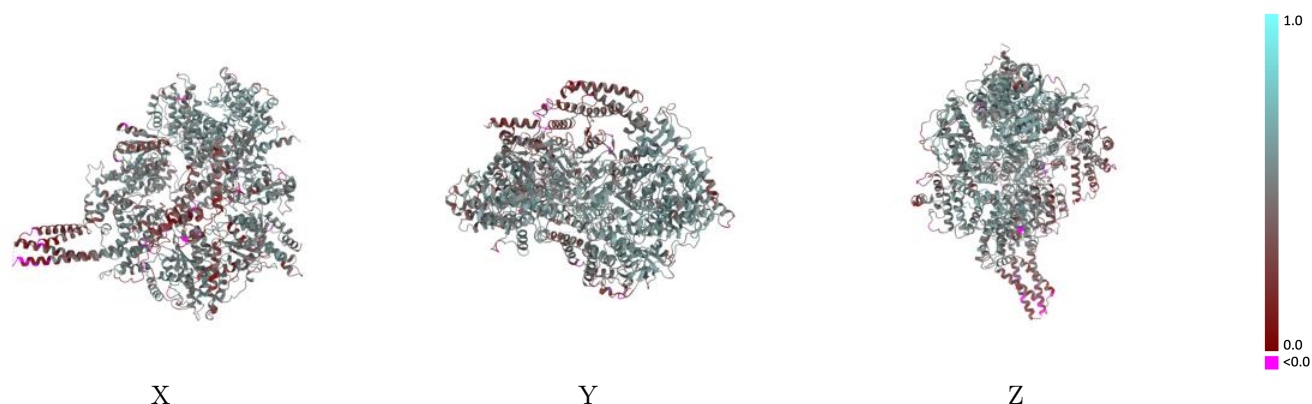
This section contains information regarding the fit between EMDB map EMD-44720 and PDB model 9BN3. Per-residue inclusion information can be found in section [3](#) on page [5](#).

### 9.1 Map-model overlay [i](#)



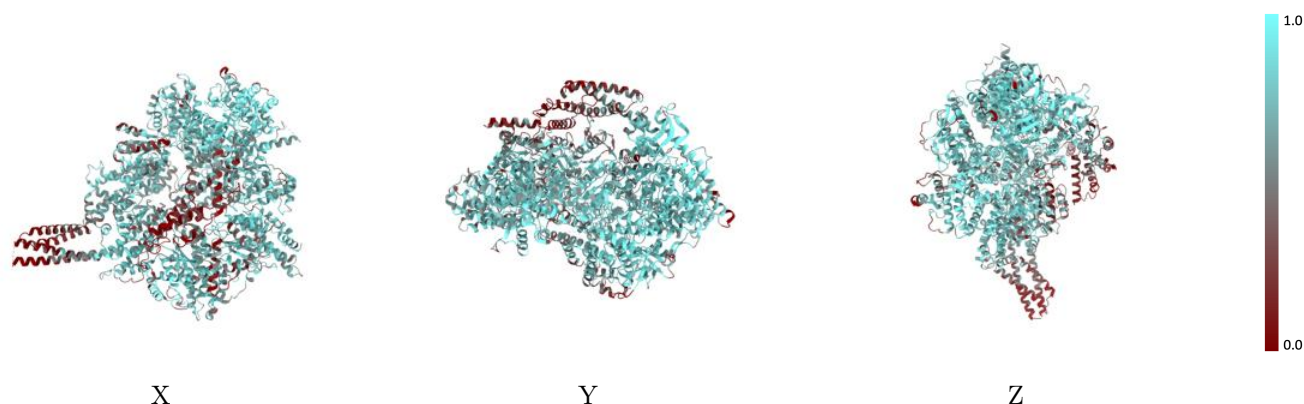
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



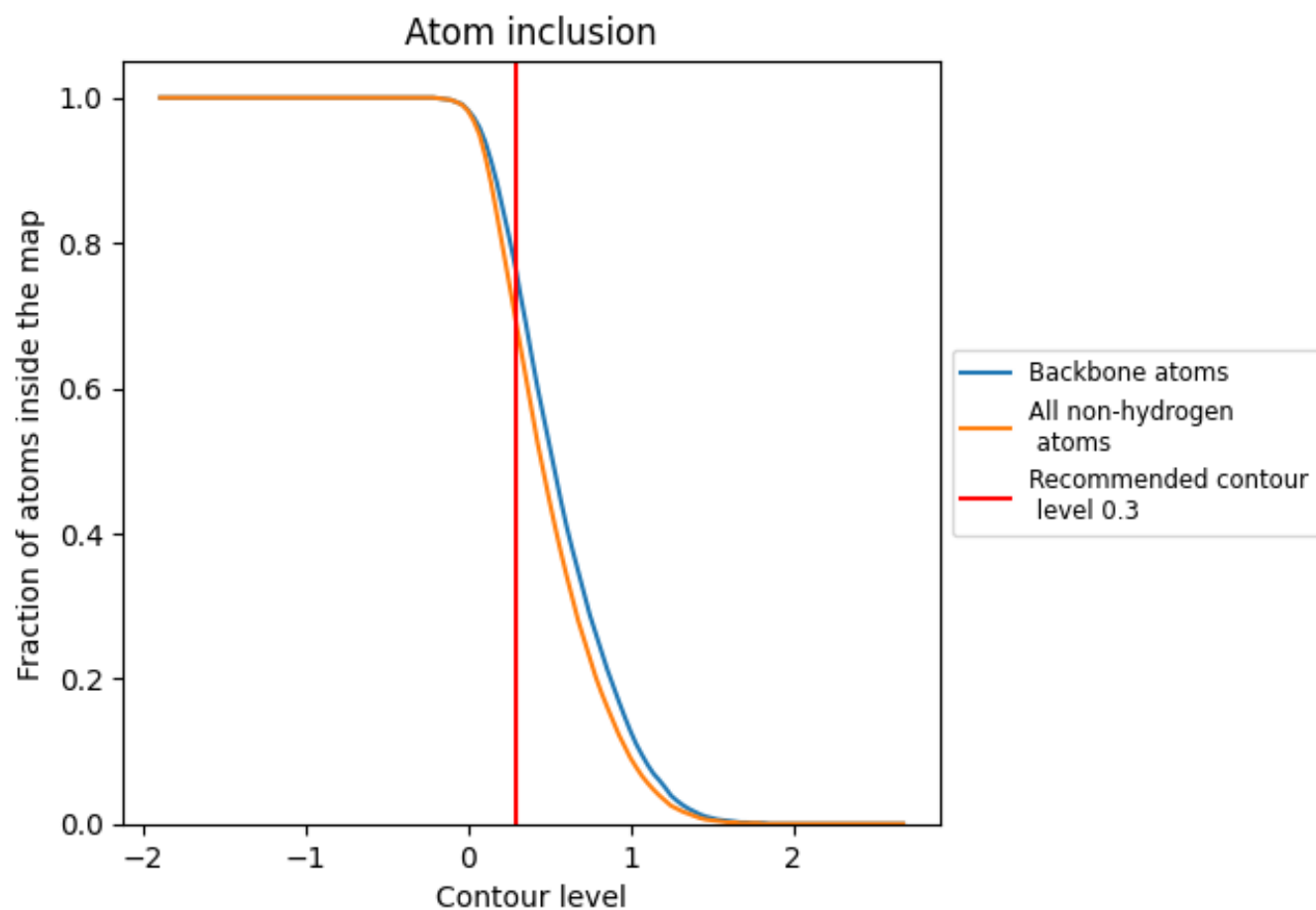
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 76% of all backbone atoms, 69% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.6880	<div><div></div></div> 0.4770
A	<div><div></div></div> 0.6880	<div><div></div></div> 0.4770

