



## Full wwPDB EM Validation Report ⓘ

Aug 14, 2025 – 01:43 PM EDT

PDB ID : 9BMV / pdb\_00009bmv  
EMDB ID : EMD-44712  
Title : State-7a-post1 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](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.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.45.1

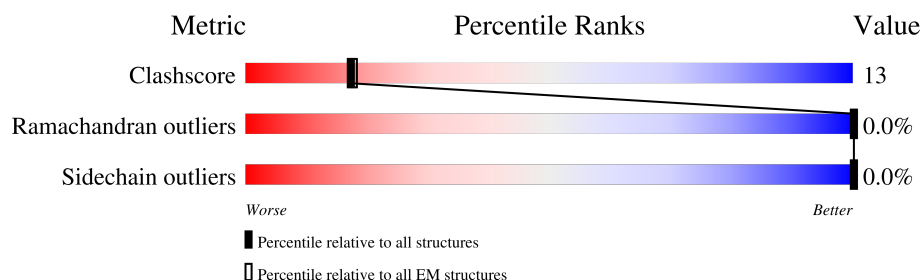
# 1 Overall quality at a glance

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)
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	

## 2 Entry composition [i](#)

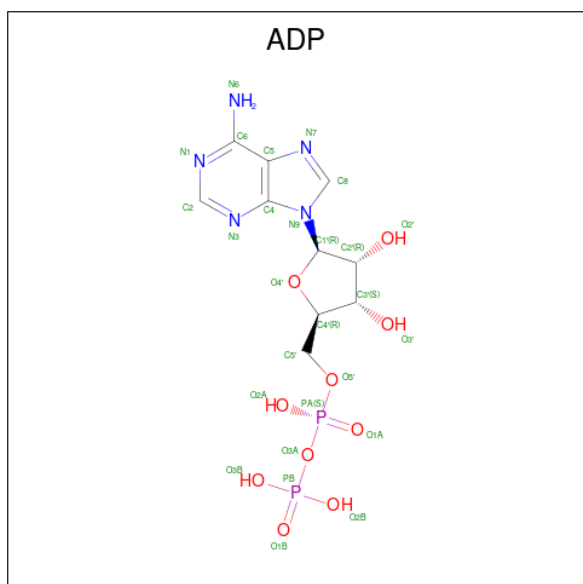
There are 4 unique types of molecules in this entry. The entry contains 24616 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

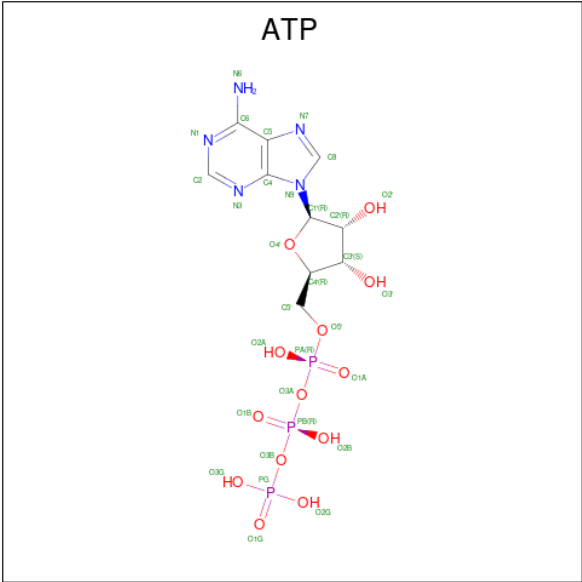
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3043	24503	15606	4234	4541	122	0	0

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



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

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



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

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





SER	L3115	L3020	F2926	V2838	L2723	R2643	R2519	A2420	L2335	H2252	E2133	G2021
GLN	E3116	F3021	R2927	E2859	R2726	T2644	T2519	A2421	P2336	I2253	I2136	TYR
GLU	Y3125	E3022	Q2930	D2840	F2727	P2645	T2522	I2422	P2337	A2258	L2137	ALA
VAL	G3023	E2841	G2931	E2842	L2728	G2647	V2524	S2429	M2338	I2259	I2138	GLY
LYS	D3024	E2843	H2932	R2844	R2729	V2648	P2527	R2430	I2341	K2260	V2141	ARG
ASN	E3025	R2844	L2935	E2844	H2730	V2649	D2536	K2435	M2342	K2261	V2146	P2029
ASN	L3029	I2850	G2940	D2851	V2731	A2651	P2544	L2437	E2344	D2262	V2146	D2030
ALA	M3030	D2851	K2943	H2857	V2732	P2652	V2545	E2438	V2345	L2264	L2149	L2035
ALA	T3031	H2857	K2943	H2857	L2744	K2657	V2545	H2439	D2347	Y2265	L2156	M2041
ASP	Q3032								L2348	D2269	L2156	P2044
LYS	Q3038	H2860	L2946	H2860	I2747	V2660	V2557	Q2442	T2352	P2270	L2161	P2044
LEU	K3039	I2861	L2956	I2861	A2754	F2662	E2558	T2452	L2353	M2271	L2176	M2053
LYS	E3040	D2862	S2957	D2862	R2757	G2663	T2559	R2451	A2354	T2272	E2181	L2054
MET	G3041	R2863	V2958	R2863	E2761	D2664	T2571	L2455	R2358	E2274	C2186	Y2055
VAL	L3042	E2864		E2864	S2761	E2665	L2571	S2457	M2361	T2276	L2191	S2056
LYS	L3043	M2867	K2962	M2867	M2773	E2666	T2576	S2460	F2364	G2278	T2192	R2060
ASP	L3044	R2868	V2963	R2868	V2774	L2668	R2576	M2461	V2368	L2281	W2203	L2065
GLN	D3045	S2869	H2964	S2869	E2782	P2669	H2577	L2462	L2369	L2284	V2204	A2066
GLN	S3046	R2869	R2965	R2869	E2782	T2676	E2578	A2465	D2372	L2287	K2206	L2069
ALA	A3162	K2966	K2966	Y2873	D2787	D2670	E2578	M2473	L2382	R2292	Q2209	L2080
ALA	E3049	S2874	G2969	S2874	T2788	M2671	L2585	M2481	P2386	G2293	L2210	Q2083
GLU	L3050	M2875	E2970	D2880	Q2789	D2672	L2581	L2486	L2387	E2294	L2211	Y2086
LYS	N3061	R2876	E2970	D2880	H2791	K2673	L2581	E2487	L2295	Q2296	T2214	R2091
VAL	T3067	S2878	D2973	K2879	Y2792	G2675	T2583	L2489	D2388	K2297	L2220	A2092
MET		K2879	L2976	D2880	Y2792	T2676	L2585	Q2491	E2391	R2298	M2221	L2093
SER	F3179	S3072	L2976	D2880	Q2789	F2682	K2589	R2492	E2392	T2301	M2222	K2094
GLN	I3180	E3073	V2979	D2880	H2791	G2684	P2590	Y2493	E2393	D2304	G2224	L2097
ILE	G3074	R2881	L2980	D2881	Y2792	Q2685	L2591	L2494	Q2395	G2305	K2230	N2102
GLU	L3075	D2885	R2981	D2885	Y2792	M2686	V2592	V2495	R2396	D2306	S2231	V2103
GLN	K3076	R2885	R2982	D2885	E2798	V2687	P2596	L2496	R2397	D2307	R2104	R2105
LEU	S3077	E2888	C2985	E2888	M2799	H2688	K2601	L2499	R2398	W2234	W2234	K2110
HIS	R3078	L2889	N2986	L2889	R2804	E2694	T2602	Y2493	K2399	E2310	R2235	I2111
LYS	A3079	V2893	E2988	V2893	R2811	D2697	W2603	L2495	K2399	W2311	K2239	R2112
GLN	A3080	L2897	A2991	L2897	P2812	K2702	S2607	L2499	G2400	E2312	A2240	R2113
GLU	P3083	Y2901	F2992	E2901	L2816	L2703	P2613	S2503	G2400	E2313	A2240	E2114
VAL	I3208	I2993	I2993	E2902	P2817	E2704	D2614	D2505	K2401	N2314	E2242	K2115
ILE	K3209	M2994	M2994	E2903	V2818	R2705	W2615	D2506	E2402	L2315	E2242	E2116
ASP	E3210	E2995	E2995	E2904	L2706	Q2707	G2619	L2508	D2403	V2312	E2242	
LYS	T3211	E2996	E2996	L2905	F2708	V2709	L2650	K2509	E2404	E2315	E2242	
GLN	V3212	S2997	S2997	D2906	G2820	V2709	S2623	M2510	G2405	V2318	E2244	
MET	D3213	N2998	N2998	L2909	R2823	C2712	E2629	L2514	E2406	E2245	E2245	
SER	Q3214	V2999	V2999	V2910	L2830	D2717	L2630	G2515	E2407	G2246	G2246	
LYS	V3215	L3000	L3000	V2910	R2831	P2718	L2630	E2516	A2408	L2325	E2248	
GLU	E3216	G3095	G3095	V2910	F2833	G2719	T2634	Y2517	A2409	L2333	P2132	
ASP	E3217	W3097	W3097	V2910	Q2834	R2720	F2635	L2518		S2334		
LEU	L3218	E3100	F3004	L2916	Q2834	R2720	F2635					
LYS	R3219	E3006	E3006	L2920	D2835	R2720	F2635					
VAL	R3220	R3007	R3007	R2921	R2836	R2720	F2635					
	D3221	V3017	V3017	I2925	L2837							
	LEU	K3112	K3112									
	ARG	D3114	D3114									
	ILE											
	LYS											

M4597 T4598 E4599	S4465 H4466	P4470 A4471 G4472 M4473 T4474 V4475 I4476 Q4477 W4478	THR ARG ASP THR SER ASP GLY ARG PRO	R4230 L4243 M4247 A4248 I4251 Y4252 F4260 L4269 S4277 F4281 F4282 K4287 G4290 H4291 I4294 I4300 E4304 W4320 L4321 P4324 W4325 W4326 L4332 K4342 M4343 L4344 K4345 M4346	E3930 Q3931 E3932 E3933 R3937 Q3952 P3966 V3970 L3973 E3977 P3982 I3983 Q3984 Q3985 R3989 L3992 F3996 D3999 R4000 L4001 L4002 H4006 M4012 L4025 D4026 L4027 I4030 V4031 P4037 M4038 T4039 P4040 V4041 M4042 C4044 S4045 V4046 D4050 A4051 L4071	I3835 V3839 L3840 N3845 D3851 H3852 T3853 Q3854 R3855 I3858 L3863 F3864 Q3865 V3866 N3869 R3870 V3871 A3872 R3873 G3874 M3875 H3880 F3883 L3886 L3887 A3888 R3889 I3890 K3891 L3892 D3902 A3903 Q3906 L3909 R3910 E3913 I3914 V3915 L3916 S3917 A3918 G3919 I3811 T3814 L3818 I3821 L3824 S3828 F3831	E3746 K3747 S3748 L3749 L3750 Q3751 A3752 L3753 I3754 E3755 V3756 K3757 G3758 R3759 I3760 L3761 D3762 D3763 D3764 T3765 I3766 I3767 T3768 T3769 L3770 E3771 N3772 L3773 K3774 R3775 F3776 A3777 A3778 E3779 V3780 T3781 R3782 V3784 E3785 E3786 T3787 D3788 S3809 S3810 I3811 T3814 L3818 I3821 L3824 S3828 F3831	L3649 N3650 E3651 V3652 R3653 R3654 R3655 T3656 G3657 G3658 R3659 I3662 T3663 L3664 G3665 D3666 Q3667 P3673 L3679 S3680 T3681 T3685 P3689 P3690 D3691 L3692 C3693 S3694 R3695 F3698 V3699 N3700 F3701 R3704 R3705 L3708 E3720 D3723 E3726 Q3735 G3736 L3740 R3741 L3742 Q3744 L3745	R3561 W3562 L3567 T3574 E3575 N3576 A3577 I3578 G3579 R3582 R3585 L3588 G3599 I3600 M3601 N3602 E3603 K3608 L3609 T3610 L3611 T3612 L3615 D3616 A3618 F3619 R3620 N3622 L3623 A3626 L3627 R3629 G3630 N3631 P3632 V3635 V3638 E3639 V3648 D3657 E3558	ALA ALA VAL GLU A3470 K3471 V3472 N3473 R3474 V3475 T3476 A3477 L3478 L3479 K3480 S3481 L3482 S3483 A3484 E3485 R3486 E3487 R3488 W3489 T3492 T3502 L3508 L3509 S3510 A3511 I3514 A3515 Y3516 A3517 G3518 Y3519 F3520 M3524 R3525 W3532 L3536 F3543 R3544 T3545 D3546 R3549 L3553 D3557 E3558	LEU LYS ARG VAL GLU PRO ILE GLU ALA GLN ASN PHE SER ALA VAL GLN LYS SER ILE LEU GLU SER ASP ALA GLN HIS VAL GLU ASN LYS VAL MET ALA MET SER PRO ASN PRO ALA ALA VAL TYR ASN MET GLY GLU GLY GLU THR THR LYS TRP ALA GLN ILE ALA GLN ARG SER LEU ILE TYR ALA ASP MET LEU	ASN PHE ILE PRO VAL THR ILE PRO GLU VAL ALA GLN ASN PHE SER ALA VAL GLN LYS SER ILE LEU GLU SER ASP ALA GLN HIS VAL GLU ASN LYS VAL MET ARG LYS SER MET ALA TYR MET SER PRO ASN PRO ALA ALA VAL TYR ASN MET GLY GLU GLY GLU THR THR LYS TRP ALA GLN ILE ALA GLN ARG SER LEU ILE TYR ALA ASP MET LEU
M4600 V4604 L4607 P4608 V4609 M4612 I4619 F4620 D4623 F4624 A4627 E4630 F4635 E4637 R4638 V4639 V4640 V4641 V4642 E4646	S4465 H4466 P4470 A4471 G4472 M4473 T4474 V4475 I4476 Q4477 W4478 V4479 S4480 D4481 F4482 S4483 E4484 R4485 I4486 S4493 A4496 A4501 L4504 L4511 E4518 V4528 L4541 Q4549 D4554 A4555 C4556 S4557 V4560 K4564 K4574 L4577 S4578 N4579 L4590 R4591 W4592 Q4595 T4596	G4472 T4474 I4476 Q4477 W4478 V4479 S4480 D4481 F4482 S4483 E4484 R4485 I4486 S4493 A4496 A4501 L4504 L4511 E4518 V4528 L4541 Q4549 D4554 A4555 C4556 S4557 V4560 K4564 K4574 L4577 S4578 N4579 L4590 R4591 W4592 Q4595 T4596	THR ARG ASP THR SER ASP GLY ARG PRO	R4230 L4243 M4247 A4248 I4251 Y4252 F4260 L4269 S4277 F4281 F4282 K4287 G4290 H4291 I4294 I4300 E4304 W4320 L4321 P4324 W4325 W4326 L4332 K4342 M4343 L4344 K4345 M4346	E3930 Q3931 E3932 E3933 R3937 Q3952 P3966 V3970 L3973 E3977 P3982 I3983 Q3984 Q3985 R3989 L3992 F3996 D3999 R4000 L4001 L4002 H4006 M4012 L4025 D4026 L4027 I4030 V4031 P4037 M4038 T4039 P4040 V4041 M4042 C4044 S4045 V4046 D4050 A4051 L4071	I3835 V3839 L3840 N3845 D3851 H3852 T3853 Q3854 R3855 I3858 L3863 F3864 Q3865 V3866 N3869 R3870 V3871 A3872 R3873 G3874 M3875 H3880 F3883 L3886 L3887 A3888 R3889 I3890 K3891 L3892 D3902 A3903 Q3906 L3909 R3910 E3913 I3914 V3915 L3916 S3917 A3918 G3919 I3811 T3814 L3818 I3821 L3824 S3828 F3831	E3746 K3747 S3748 L3749 L3750 Q3751 A3752 L3753 I3754 E3755 V3756 K3757 G3758 R3759 I3760 L3761 D3762 D3763 D3764 T3765 I3766 I3767 T3768 T3769 L3770 E3771 N3772 L3773 K3774 R3775 F3776 A3777 A3778 E3779 V3780 T3781 R3782 V3784 E3785 E3786 T3787 D3788 S3809 S3810 I3811 T3814 L3818 I3821 L3824 S3828 F3831	L3649 N3650 E3651 V3652 R3653 R3654 R3655 T3656 G3657 G3658 R3659 I3662 T3663 L3664 G3665 D3666 Q3667 P3673 L3679 S3680 T3681 T3685 P3689 P3690 D3691 L3692 C3693 S3694 R3695 F3698 V3699 N3700 F3701 R3704 R3705 L3708 E3720 D3723 E3726 Q3735 G3736 L3740 R3741 L3742 Q3744 L3745	R3561 W3562 L3567 T3574 E3575 N3576 A3577 I3578 G3579 R3582 R3585 L3588 G3599 I3600 M3601 N3602 E3603 K3608 L3609 T3610 L3611 T3612 L3615 D3616 A3618 F3619 R3620 N3622 L3623 A3626 L3627 R3629 G3630 N3631 P3632 V3635 V3638 E3639 V3648 D3657 E3558	ALA ALA VAL GLU A3470 K3471 V3472 N3473 R3474 V3475 T3476 A3477 L3478 L3479 K3480 S3481 L3482 S3483 A3484 E3485 R3486 E3487 R3488 W3489 T3492 T3502 L3508 L3509 S3510 A3511 I3514 A3515 Y3516 A3517 G3518 Y3519 F3520 M3524 R3525 W3532 L3536 F3543 R3544 T3545 D3546 R3549 L3553 D3557 E3558	LEU LYS ARG VAL GLU PRO ILE GLU ALA GLN ASN PHE SER ALA VAL GLN LYS SER ILE LEU GLU SER ASP ALA GLN HIS VAL GLU ASN LYS VAL MET ARG LYS SER MET ALA TYR MET SER PRO ASN PRO ALA ALA VAL TYR ASN MET GLY GLU GLY GLU THR THR LYS TRP ALA GLN ILE ALA GLN ARG SER LEU ILE TYR ALA ASP MET LEU	ASN PHE ILE PRO VAL THR ILE PRO GLU VAL ALA GLN ASN PHE SER ALA VAL GLN LYS SER ILE LEU GLU SER ASP ALA GLN HIS VAL GLU ASN LYS VAL MET ARG LYS SER MET ALA TYR MET SER PRO ASN PRO ALA ALA VAL TYR ASN MET GLY GLU GLY GLU THR THR LYS TRP ALA GLN ILE ALA GLN ARG SER LEU ILE TYR ALA ASP MET LEU



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47280	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	0.717	Depositor
Minimum map value	-0.337	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.12	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, MG

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	0.16	0/25022	0.34	0/33900

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1567	ARG	Sidechain

### 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	24503	0	24574	659	0
2	A	81	0	36	9	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	12	3	0
4	A	1	0	0	0	0
All	All	24616	0	24622	659	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 (659) 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:4189:ILE:HD11	1:A:4321:LEU:HA	1.55	0.88
1:A:3818:LEU:HA	1:A:4346:MET:HE1	1.61	0.81
1:A:1551:PHE:HA	1:A:1557:ILE:HD11	1.63	0.80
1:A:3178:ASP:HB2	1:A:3585:ARG:HH21	1.48	0.78
1:A:1632:VAL:HB	1:A:1657:MET:HE1	1.66	0.78
1:A:4609:VAL:HG12	1:A:4642:VAL:HB	1.66	0.75
1:A:3502:THR:HG21	1:A:3544:ARG:HG3	1.67	0.74
1:A:2252:HIS:HB2	1:A:2301:ILE:HG22	1.70	0.73
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.72	0.72
1:A:4398:LEU:HB2	1:A:4414:GLU:HG3	1.70	0.72
1:A:2503:SER:HB3	1:A:2514:LEU:HD13	1.71	0.72
1:A:4193:ARG:NH2	1:A:4637:GLU:O	2.21	0.72
1:A:2851:ASP:HB3	1:A:2867:MET:HE1	1.72	0.70
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.72	0.70
1:A:2413:LEU:HA	1:A:2416:GLN:HE21	1.55	0.70
1:A:1912:LYS:HG2	1:A:2041:MET:HG3	1.75	0.69
1:A:2720:ARG:HH22	1:A:3083:PRO:HG3	1.57	0.69
1:A:2053:MET:HE3	1:A:2094:LYS:HE3	1.75	0.69
1:A:1857:LEU:HD22	1:A:1868:TYR:HB2	1.74	0.69
1:A:2879:LYS:HG3	1:A:2880:ASP:H	1.58	0.68
1:A:1346:MET:HE1	1:A:1366:LEU:HD11	1.75	0.68
1:A:2186:CYS:HA	1:A:2191:LEU:HD12	1.75	0.68
1:A:3588:LEU:HD11	1:A:3638:VAL:HG11	1.75	0.68
1:A:2747:ILE:HD11	2:A:4703:ADP:C6	2.30	0.67
1:A:3100:GLU:HG3	1:A:3130:TYR:HE1	1.58	0.67
1:A:3924:ILE:HB	1:A:3927:LEU:HD23	1.75	0.67
1:A:1925:ARG:HH12	1:A:2011:ASP:HB3	1.60	0.67
1:A:3167:ARG:NH1	1:A:3519:TYR:OH	2.26	0.67
1:A:4187:HIS:ND1	1:A:4252:TYR:OH	2.27	0.66
1:A:2943:LYS:HE2	1:A:3067:THR:HB	1.78	0.66
1:A:2030:ASP:OD2	1:A:4131:ASN:ND2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2935:LEU:HD22	1:A:3094:PHE:HE1	1.61	0.66
1:A:3546:ASP:O	1:A:3735:GLN:NE2	2.24	0.66
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.23	0.65
1:A:2113:ARG:HA	1:A:2116:GLU:HG2	1.78	0.65
1:A:3486:ARG:HA	1:A:3489:TRP:HD1	1.62	0.65
1:A:2261:LYS:NZ	1:A:2310:GLU:O	2.28	0.65
1:A:2581:LEU:HD13	1:A:2591:LEU:HD13	1.79	0.65
1:A:2958:VAL:HA	1:A:2991:ALA:HB3	1.78	0.65
1:A:1728:GLY:O	1:A:1784:ASN:ND2	2.31	0.64
1:A:2304:ASP:OD1	1:A:2726:ARG:NH2	2.31	0.64
1:A:3821:ILE:HG12	1:A:4346:MET:HE2	1.80	0.64
1:A:1406:GLU:HG3	1:A:3658:GLY:HA3	1.77	0.64
1:A:1714:ALA:HA	1:A:1870:PHE:HE2	1.63	0.64
1:A:2348:LEU:HD11	1:A:2361:MET:HE1	1.79	0.64
1:A:2620:LEU:HD11	1:A:2634:THR:HG21	1.79	0.64
1:A:4408:PRO:HA	1:A:4411:ARG:HE	1.63	0.63
1:A:1695:HIS:HB3	1:A:1700:GLU:HG3	1.81	0.63
1:A:3845:ASN:HB3	1:A:3858:ILE:HD11	1.81	0.63
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.31	0.63
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.80	0.63
1:A:3886:LEU:HD11	1:A:4346:MET:HG3	1.81	0.63
1:A:4031:VAL:O	1:A:4123:ARG:NH1	2.32	0.63
1:A:3576:ASN:ND2	1:A:3700:ASN:O	2.32	0.63
1:A:4105:TRP:CD1	1:A:4108:GLN:HE21	2.16	0.63
1:A:2387:LEU:HD13	1:A:2412:MET:HE3	1.81	0.63
1:A:3910:ARG:HE	1:A:4344:LEU:HD11	1.64	0.63
1:A:4600:LYS:NZ	1:A:4604:VAL:O	2.32	0.63
1:A:3209:LYS:HA	1:A:3486:ARG:HH12	1.65	0.62
1:A:4105:TRP:HD1	1:A:4108:GLN:HE21	1.46	0.62
1:A:3005:LEU:HD11	1:A:3078:ARG:HH11	1.65	0.62
1:A:4564:LYS:HG3	1:A:4646:GLU:HG3	1.80	0.62
1:A:2897:LEU:HD21	1:A:2909:LEU:HB2	1.81	0.62
1:A:2258:ALA:HB1	1:A:2682:PHE:HD1	1.65	0.62
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.82	0.62
1:A:4046:VAL:HG21	1:A:4148:GLU:HG3	1.81	0.62
1:A:1797:LEU:HD22	1:A:2060:ARG:HH22	1.64	0.61
1:A:1888:CYS:HB2	1:A:2041:MET:HE1	1.82	0.61
1:A:2629:GLU:N	1:A:2629:GLU:OE1	2.31	0.61
1:A:2603:MET:HE1	2:A:4703:ADP:C4	2.36	0.61
1:A:2823:ARG:HH22	1:A:2868:SER:HB3	1.65	0.61
1:A:2009:SER:HB2	1:A:2012:MET:HE3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2660:VAL:HG22	1:A:2707:GLN:HB2	1.82	0.61
1:A:4040:PRO:HB3	1:A:4124:LEU:HD23	1.83	0.61
1:A:1452:VAL:HG22	1:A:1512:TYR:HE1	1.66	0.61
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.34	0.61
1:A:3914:ILE:H	1:A:3937:ARG:HH12	1.47	0.61
1:A:1941:MET:HG2	1:A:1944:ILE:HD12	1.83	0.61
1:A:3209:LYS:HB2	1:A:3486:ARG:HH22	1.66	0.61
1:A:3743:ARG:NE	1:A:3746:GLU:OE2	2.23	0.60
1:A:4186:PHE:O	1:A:4189:ILE:HG22	2.00	0.60
1:A:3508:LEU:HD23	1:A:3536:LEU:HD21	1.83	0.60
1:A:3567:LEU:HD12	1:A:3595:GLN:HE22	1.66	0.60
1:A:2065:LEU:HD11	1:A:2133:GLU:HB3	1.83	0.60
1:A:2112:LYS:HG3	1:A:2122:VAL:HG11	1.83	0.60
1:A:4619:ILE:HG22	1:A:4620:PHE:HD1	1.67	0.60
1:A:2603:MET:HE1	2:A:4703:ADP:H2'	1.84	0.60
1:A:2915:VAL:HG23	1:A:2946:LEU:HD11	1.83	0.60
1:A:3518:GLY:HA3	1:A:3579:MET:HE1	1.83	0.60
1:A:2717:ASP:HB3	1:A:2720:ARG:HG3	1.84	0.59
1:A:3207:LYS:NZ	1:A:3210:GLU:OE1	2.35	0.59
1:A:3871:VAL:HG12	1:A:3875:MET:HE2	1.85	0.59
1:A:2451:ARG:O	1:A:2455:LEU:HD12	2.02	0.59
1:A:3608:LYS:HE3	1:A:3631:ASN:HB3	1.84	0.59
1:A:1800:GLN:OE1	1:A:1804:ARG:NH1	2.36	0.59
1:A:2495:VAL:HG21	1:A:2524:VAL:HG11	1.84	0.59
1:A:2613:PRO:O	1:A:2657:LYS:NZ	2.35	0.59
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.68	0.59
1:A:1965:GLU:N	1:A:1965:GLU:OE1	2.34	0.59
1:A:2464:GLN:HG2	1:A:2583:THR:HG23	1.85	0.59
1:A:1403:LEU:HD23	1:A:1450:LEU:HD21	1.85	0.58
1:A:2297:LYS:O	1:A:2338:ASN:ND2	2.36	0.58
1:A:4454:GLU:OE1	1:A:4461:PRO:HA	2.04	0.58
1:A:2373:MET:HE1	3:A:4702:ATP:C4	2.38	0.58
1:A:2451:ARG:HG2	1:A:2455:LEU:HD11	1.86	0.58
1:A:2790:PRO:HB3	1:A:3076:LYS:HE2	1.86	0.58
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.85	0.58
1:A:2325:LEU:HB3	1:A:2333:LEU:HB2	1.85	0.58
1:A:3208:ILE:O	1:A:3212:VAL:HG23	2.04	0.58
1:A:2386:PRO:HA	1:A:2416:GLN:HE22	1.68	0.57
1:A:2592:VAL:HB	1:A:2733:VAL:HG12	1.85	0.57
1:A:3525:ARG:NH1	1:A:3576:ASN:OD1	2.37	0.57
1:A:4398:LEU:HD21	1:A:4493:SER:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2083:GLN:HB2	1:A:2086:TYR:CD1	2.39	0.57
1:A:2830:LEU:HD22	1:A:2850:ILE:HD13	1.85	0.57
1:A:3154:LEU:HD13	1:A:3516:TYR:CD1	2.40	0.57
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.86	0.57
1:A:2578:GLU:OE2	1:A:2607:SER:OG	2.21	0.57
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.85	0.57
1:A:2287:ILE:HA	1:A:2294:GLU:HG3	1.85	0.57
1:A:2615:MET:SD	1:A:2615:MET:N	2.78	0.57
1:A:2818:VAL:HG11	1:A:2861:ILE:HD12	1.87	0.57
1:A:3553:LEU:O	1:A:3582:ARG:NH1	2.32	0.56
1:A:2744:LEU:HA	1:A:2747:ILE:HG22	1.86	0.56
1:A:1416:LEU:HD23	1:A:1449:VAL:HG11	1.87	0.56
1:A:2175:MET:SD	1:A:2175:MET:N	2.78	0.56
1:A:2694:ARG:HD3	1:A:2697:ASP:HB3	1.87	0.56
1:A:1911:GLY:O	1:A:1915:SER:OG	2.15	0.56
1:A:3763:ASP:OD2	1:A:3765:THR:OG1	2.22	0.56
1:A:1543:ARG:NH1	1:A:1609:GLY:HA2	2.21	0.56
1:A:2623:SER:HA	1:A:2668:LEU:HB3	1.88	0.56
1:A:1960:PHE:HE1	1:A:1968:LEU:HG	1.71	0.56
1:A:3756:VAL:HG13	1:A:3757:LYS:H	1.70	0.56
1:A:2964:HIS:ND1	1:A:2965:ARG:O	2.38	0.56
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.39	0.56
1:A:4496:ALA:HB2	1:A:4504:LEU:HD21	1.88	0.56
1:A:1415:GLN:O	1:A:1419:ARG:HG2	2.06	0.55
1:A:2993:ILE:C	1:A:2994:MET:HE2	2.30	0.55
1:A:2102:ASN:OD1	1:A:2105:ARG:NH2	2.33	0.55
1:A:1396:ILE:HD12	1:A:1439:LEU:HD12	1.86	0.55
1:A:3562:TRP:HB3	1:A:3567:LEU:HD22	1.88	0.55
1:A:3756:VAL:HG23	1:A:3760:ILE:HB	1.89	0.55
1:A:2091:ARG:NH1	2:A:4701:ADP:O3'	2.40	0.55
1:A:2910:VAL:N	2:A:4704:ADP:N1	2.50	0.55
1:A:1982:LEU:HD21	1:A:2012:MET:HB2	1.88	0.55
1:A:2505:ASP:OD1	1:A:2733:VAL:HG23	2.07	0.55
1:A:2965:ARG:O	1:A:2966:LYS:HG2	2.06	0.55
1:A:1979:GLN:HB3	1:A:2035:LEU:HD13	1.89	0.55
1:A:4574:LYS:HB3	1:A:4627:ALA:HB2	1.89	0.55
1:A:1571:ILE:HD11	1:A:1607:LEU:HD12	1.89	0.55
1:A:1501:ILE:HA	1:A:1504:VAL:HG22	1.89	0.55
1:A:1684:VAL:C	1:A:1685:MET:HE2	2.32	0.55
1:A:3902:ASP:OD1	1:A:3903:ALA:N	2.40	0.55
1:A:2270:PRO:HA	1:A:2273:ARG:HH22	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2323:LYS:HB3	1:A:2335:LEU:HB3	1.89	0.54
1:A:4480:SER:O	1:A:4483:SER:OG	2.16	0.54
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.89	0.54
1:A:1332:VAL:HB	1:A:1377:LEU:HD22	1.89	0.54
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.88	0.54
1:A:2999:VAL:HG13	1:A:3005:LEU:HD21	1.89	0.54
1:A:3851:ASP:OD2	1:A:3853:THR:OG1	2.25	0.54
1:A:3755:GLU:OE2	1:A:3759:ARG:NH1	2.41	0.54
1:A:4096:LEU:HD13	1:A:4105:TRP:HH2	1.73	0.54
1:A:1925:ARG:NH2	1:A:1952:GLY:O	2.40	0.54
1:A:2925:ILE:HD12	1:A:3090:VAL:HG11	1.88	0.54
1:A:2976:LEU:HA	1:A:2979:VAL:HG12	1.88	0.54
1:A:2325:LEU:HD23	1:A:2333:LEU:HD12	1.90	0.54
1:A:3828:SER:HB3	1:A:4140:ARG:HG2	1.90	0.54
1:A:4414:GLU:HA	1:A:4417:VAL:HG22	1.90	0.54
1:A:1510:SER:O	1:A:1512:TYR:N	2.41	0.53
1:A:4281:GLU:N	1:A:4281:GLU:OE1	2.41	0.53
1:A:1810:HIS:NE2	1:A:1876:GLN:O	2.40	0.53
1:A:2422:ILE:HG23	1:A:2487:GLU:HG2	1.90	0.53
1:A:3502:THR:HG23	1:A:3543:PHE:HA	1.90	0.53
1:A:2481:MET:SD	1:A:2481:MET:N	2.81	0.53
1:A:3909:LEU:HD11	1:A:4343:MET:HE3	1.89	0.53
1:A:1658:PHE:HB2	1:A:1661:VAL:HB	1.90	0.53
1:A:2619:GLY:HA2	1:A:2662:PHE:HB3	1.90	0.53
1:A:4511:LEU:HD23	1:A:4560:VAL:HG13	1.89	0.53
1:A:2230:LYS:NZ	3:A:4702:ATP:O2B	2.33	0.53
1:A:2499:LEU:O	1:A:2503:SER:OG	2.22	0.53
1:A:3690:PRO:HA	1:A:3693:CYS:HB3	1.91	0.53
1:A:2684:ARG:HH12	1:A:2726:ARG:HE	1.55	0.53
1:A:2842:GLU:OE1	1:A:2842:GLU:N	2.33	0.53
1:A:3200:HIS:NE2	1:A:3747:LYS:HG3	2.24	0.53
1:A:2838:VAL:HG13	1:A:3093:TRP:CZ2	2.43	0.53
1:A:3474:ARG:HB2	1:A:3764:ASP:HB3	1.89	0.53
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	1.89	0.53
1:A:1946:VAL:HG13	1:A:2006:VAL:HG21	1.91	0.53
1:A:1968:LEU:HD21	1:A:2029:PRO:HG3	1.91	0.53
1:A:3162:ALA:HB2	1:A:3168:THR:HG21	1.91	0.53
1:A:3208:ILE:HG22	1:A:3486:ARG:NH1	2.23	0.53
1:A:3824:LEU:HD11	1:A:4044:CYS:SG	2.48	0.53
1:A:4470:PRO:HG3	1:A:4612:ASN:HD22	1.74	0.53
1:A:1478:VAL:HG11	1:A:1488:ARG:HE	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.91	0.53
1:A:1398:MET:SD	1:A:1399:LEU:HD22	2.49	0.52
1:A:3635:VAL:HB	1:A:3679:LEU:HD23	1.89	0.52
1:A:3474:ARG:HB3	1:A:3765:THR:HG23	1.91	0.52
1:A:2644:THR:OG1	1:A:2647:GLY:O	2.27	0.52
1:A:3021:PHE:CD2	1:A:3029:LEU:HD22	2.45	0.52
1:A:4183:LEU:HD11	1:A:4215:ALA:HB1	1.91	0.52
1:A:4595:GLN:NE2	1:A:4596:THR:O	2.42	0.52
1:A:1752:LEU:HD11	1:A:1868:TYR:CZ	2.45	0.52
1:A:1959:GLU:OE2	1:A:2019:ASN:ND2	2.35	0.52
1:A:1959:GLU:OE1	1:A:1962:ARG:NH1	2.43	0.52
1:A:1477:LEU:HD23	1:A:1487:ILE:HD13	1.91	0.52
1:A:1579:MET:HA	1:A:1582:VAL:HG12	1.91	0.52
1:A:3131:ASP:OD1	1:A:3132:LYS:HG3	2.10	0.52
1:A:4541:LEU:HD11	1:A:4590:LEU:HB3	1.92	0.52
1:A:1925:ARG:NH1	1:A:2011:ASP:HB3	2.25	0.52
1:A:2843:ARG:HH21	1:A:3093:TRP:HD1	1.58	0.52
1:A:4002:LEU:O	1:A:4006:HIS:ND1	2.41	0.52
1:A:3910:ARG:NE	1:A:4344:LEU:HD11	2.24	0.52
1:A:4577:LEU:HD22	1:A:4638:ARG:HD2	1.92	0.52
1:A:4287:LYS:HD3	1:A:4290:GLY:HA2	1.91	0.51
1:A:1504:VAL:HA	1:A:1507:MET:HG3	1.92	0.51
1:A:2111:ILE:O	1:A:2115:LYS:HG3	2.10	0.51
1:A:2307:VAL:HG23	1:A:2345:VAL:HG11	1.91	0.51
1:A:2536:ASP:OD1	1:A:2576:ARG:NH1	2.43	0.51
1:A:4042:LEU:HD11	1:A:4138:LEU:HG	1.91	0.51
1:A:1418:LYS:HD2	1:A:1419:ARG:HD2	1.92	0.51
1:A:2666:ILE:O	1:A:2669:PRO:HD2	2.10	0.51
1:A:3481:SER:HB2	1:A:3770:LEU:HD11	1.92	0.51
1:A:1881:GLN:HE22	1:A:1889:TYR:HE2	1.59	0.51
1:A:1690:VAL:HG11	1:A:1705:VAL:HG22	1.93	0.51
1:A:2265:TYR:CZ	1:A:2314:ASN:HB2	2.46	0.51
1:A:2666:ILE:HG22	1:A:2723:LEU:HD21	1.91	0.51
1:A:4247:MET:HA	1:A:4251:ILE:HB	1.93	0.51
1:A:1748:GLN:O	1:A:1752:LEU:HG	2.11	0.51
1:A:1938:PHE:CE1	1:A:1967:MET:HG2	2.46	0.51
1:A:3873:ARG:NH1	1:A:4025:LEU:HB3	2.25	0.51
1:A:2623:SER:OG	1:A:3006:GLU:OE1	2.28	0.51
1:A:1390:LEU:HD23	1:A:1393:TYR:HD2	1.75	0.51
1:A:1634:ASP:OD1	1:A:1635:GLU:N	2.43	0.51
1:A:2406:GLU:HG2	1:A:2409:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3821:ILE:HD12	1:A:4342:LYS:HG2	1.92	0.51
1:A:2223:VAL:HG21	1:A:2348:LEU:HG	1.93	0.51
1:A:2248:GLU:OE2	1:A:2292:ARG:NH1	2.39	0.51
1:A:2203:TRP:CH2	1:A:2236:VAL:HG11	2.46	0.51
1:A:2473:ASN:HB2	1:A:2481:MET:HE1	1.91	0.51
1:A:3044:LEU:HD13	1:A:3049:GLU:HG3	1.92	0.51
1:A:3549:ARG:NH2	1:A:3575:GLU:OE2	2.33	0.51
1:A:2393:GLU:O	1:A:2397:ARG:NH1	2.44	0.50
1:A:2992:PHE:CE2	1:A:2994:MET:HE3	2.46	0.50
1:A:2192:THR:HB	1:A:2373:MET:HG2	1.93	0.50
1:A:3024:ASP:OD1	1:A:3025:GLU:N	2.43	0.50
1:A:1797:LEU:HD13	1:A:2060:ARG:HH12	1.76	0.50
1:A:2976:LEU:O	1:A:2980:LEU:HD23	2.10	0.50
1:A:2292:ARG:O	1:A:2292:ARG:HD3	2.12	0.50
1:A:2571:THR:H	1:A:2574:THR:HB	1.75	0.50
1:A:4404:ASN:HB3	1:A:4410:PHE:CE2	2.46	0.50
1:A:2596:PRO:O	1:A:2601:LYS:NZ	2.45	0.50
1:A:2973:ASP:OD1	1:A:3007:ARG:NE	2.44	0.50
1:A:4404:ASN:HB3	1:A:4410:PHE:CZ	2.46	0.50
1:A:1557:ILE:HA	1:A:1560:LEU:HB2	1.93	0.50
1:A:1882:THR:O	1:A:1885:THR:OG1	2.27	0.50
1:A:2396:ARG:HG3	1:A:2399:LYS:HE2	1.94	0.50
1:A:1651:GLN:OE1	1:A:1663:SER:HA	2.12	0.50
1:A:1701:TRP:O	1:A:1705:VAL:HG23	2.11	0.50
1:A:1936:PHE:CD2	1:A:1938:PHE:CE1	3.00	0.50
1:A:2559:THR:HG22	1:A:2757:ARG:HB3	1.92	0.50
1:A:2969:GLY:HA2	1:A:3004:PHE:HE1	1.77	0.50
1:A:2275:TRP:NE1	1:A:2277:ASP:OD1	2.45	0.49
1:A:3909:LEU:HB3	1:A:4344:LEU:HD13	1.94	0.49
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	1.93	0.49
1:A:2492:ARG:HD2	1:A:2545:TRP:CE2	2.47	0.49
1:A:2643:ARG:NH1	1:A:2644:THR:O	2.45	0.49
1:A:3561:ARG:NH2	1:A:3603:GLU:OE2	2.44	0.49
1:A:4176:ARG:NH2	1:A:4220:ASP:OD1	2.40	0.49
1:A:1391:LYS:O	1:A:1395:LYS:HG2	2.12	0.49
1:A:1814:GLU:O	1:A:1818:GLN:HG2	2.12	0.49
1:A:2585:LEU:HD21	1:A:2709:VAL:HG11	1.94	0.49
1:A:1698:ILE:HD13	1:A:1701:TRP:HE1	1.77	0.49
1:A:1769:MET:HE3	1:A:1769:MET:HA	1.94	0.49
1:A:2294:GLU:HA	1:A:2297:LYS:HD3	1.95	0.49
1:A:2461:MET:HG3	1:A:2584:TRP:HE1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3756:VAL:HG13	1:A:3757:LYS:N	2.28	0.49
1:A:1424:TRP:CZ3	1:A:1434:ILE:HG12	2.48	0.49
1:A:2789:GLN:HB2	1:A:2792:TYR:CE1	2.48	0.49
1:A:3916:LEU:HD12	1:A:3933:GLU:HG3	1.94	0.49
1:A:3970:VAL:HB	1:A:3989:ARG:HG2	1.93	0.49
1:A:1657:MET:HE2	1:A:1657:MET:N	2.27	0.49
1:A:2346:GLN:HB2	1:A:2726:ARG:HD2	1.94	0.49
1:A:2372:ASP:OD1	1:A:2429:SER:HA	2.12	0.49
1:A:2439:HIS:O	1:A:2442:GLN:HG2	2.12	0.49
1:A:2672:ASP:OD1	1:A:2673:LYS:N	2.41	0.49
1:A:1511:PRO:O	1:A:1514:LYS:HG2	2.12	0.49
1:A:2395:GLN:HB3	1:A:2398:ARG:HH22	1.77	0.49
1:A:3627:LEU:HD23	1:A:3662:ILE:HG21	1.94	0.49
1:A:2296:GLN:N	1:A:2296:GLN:OE1	2.46	0.49
1:A:2811:ARG:HB3	1:A:2812:PRO:HD3	1.93	0.49
1:A:1349:GLN:O	1:A:1430:THR:OG1	2.28	0.48
1:A:2514:LEU:O	1:A:2518:ILE:HG12	2.12	0.48
1:A:3788:ASP:N	1:A:3788:ASP:OD1	2.46	0.48
1:A:1747:ALA:O	1:A:1750:VAL:HG12	2.14	0.48
1:A:2718:PRO:HB2	1:A:3080:ALA:HB2	1.95	0.48
1:A:1466:ILE:HA	1:A:1469:VAL:HG22	1.95	0.48
1:A:1503:SER:O	1:A:1507:MET:HG2	2.14	0.48
1:A:2131:LEU:HD12	1:A:2132:PRO:HD2	1.95	0.48
1:A:3133:LEU:HD12	1:A:3134:PRO:HD2	1.95	0.48
1:A:2488:ARG:O	1:A:2492:ARG:HG2	2.14	0.48
1:A:2965:ARG:HD3	1:A:2966:LYS:H	1.78	0.48
1:A:3609:ILE:HB	1:A:3632:PRO:HG2	1.95	0.48
1:A:3831:PHE:O	1:A:3835:ILE:HD12	2.13	0.48
1:A:1336:LEU:HD11	1:A:1386:VAL:HG21	1.95	0.48
1:A:1868:TYR:HD2	1:A:1870:PHE:CD1	2.32	0.48
1:A:2993:ILE:O	1:A:2994:MET:HE2	2.13	0.48
1:A:3635:VAL:O	1:A:3680:SER:N	2.47	0.48
1:A:2671:MET:HG2	1:A:2675:GLY:HA2	1.95	0.48
1:A:2901:TYR:OH	1:A:2909:LEU:N	2.40	0.48
1:A:3818:LEU:HD23	1:A:4346:MET:HE3	1.96	0.48
1:A:4324:PRO:HB3	1:A:4638:ARG:HH11	1.79	0.48
1:A:1571:ILE:HG23	1:A:1604:LEU:HD22	1.96	0.48
1:A:1933:ASP:OD2	1:A:1962:ARG:NH1	2.47	0.48
1:A:2080:LEU:HD23	1:A:2156:LEU:HD22	1.95	0.48
1:A:2963:VAL:HB	1:A:2998:ASN:HB3	1.96	0.48
1:A:3767:ILE:O	1:A:3771:GLU:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1698:ILE:HA	1:A:1701:TRP:NE1	2.28	0.47
1:A:4395:LEU:HD11	1:A:4486:ILE:HD12	1.96	0.47
1:A:2265:TYR:OH	1:A:2311:TRP:O	2.19	0.47
1:A:3588:LEU:HD23	1:A:3698:PHE:CE1	2.50	0.47
1:A:3982:PRO:HA	1:A:3985:GLN:HG2	1.96	0.47
1:A:3992:LEU:HD22	1:A:3996:PHE:HE2	1.79	0.47
1:A:1498:LYS:HA	1:A:1501:ILE:HG12	1.96	0.47
1:A:2527:PRO:HD3	1:A:2545:TRP:CE2	2.49	0.47
1:A:2879:LYS:HG3	1:A:2880:ASP:N	2.28	0.47
1:A:2373:MET:HE1	3:A:4702:ATP:C5	2.50	0.47
1:A:2382:LEU:HD23	1:A:2420:ALA:HB2	1.96	0.47
1:A:2834:GLN:HA	1:A:2837:LEU:HD13	1.95	0.47
1:A:1356:PRO:HB3	1:A:1401:ILE:HG12	1.95	0.47
1:A:1748:GLN:HE22	1:A:1872:TYR:HA	1.79	0.47
1:A:2284:LEU:HA	1:A:2287:ILE:HG12	1.97	0.47
1:A:2301:ILE:HD11	1:A:2341:ILE:HG12	1.95	0.47
1:A:2649:VAL:HG22	1:A:2702:LYS:HB3	1.95	0.47
1:A:2841:GLU:CD	1:A:2844:ARG:HH21	2.22	0.47
1:A:1507:MET:HE3	1:A:1507:MET:HB3	1.81	0.47
1:A:1964:GLU:OE1	1:A:1967:MET:N	2.38	0.47
1:A:2104:LYS:HB2	1:A:2136:ILE:HG21	1.96	0.47
1:A:2110:LYS:O	1:A:2114:GLU:HG2	2.14	0.47
1:A:2635:PHE:CZ	1:A:2650:LEU:HD22	2.49	0.47
1:A:2956:LEU:HG	1:A:2991:ALA:HB2	1.96	0.47
1:A:3865:GLN:NE2	1:A:3869:ASN:OD1	2.47	0.47
1:A:3892:LEU:HD13	1:A:3983:ILE:HG12	1.96	0.47
1:A:4401:THR:O	1:A:4405:ILE:HG12	2.15	0.47
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	1.97	0.47
1:A:4473:MET:SD	1:A:4477:GLN:HB2	2.55	0.47
1:A:2987:ASN:OD1	1:A:3061:ASN:ND2	2.47	0.47
1:A:4391:ILE:HD11	1:A:4479:VAL:HG23	1.95	0.47
1:A:1789:LEU:HD11	1:A:2055:TYR:HE2	1.80	0.47
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.50	0.47
1:A:2239:LYS:O	1:A:2242:GLU:HG3	2.14	0.47
1:A:2652:PRO:HD2	1:A:2705:ARG:HH11	1.79	0.47
1:A:2903:GLU:HG3	1:A:2904:GLU:OE1	2.15	0.47
1:A:2506:SER:OG	1:A:2507:ARG:N	2.47	0.47
1:A:2557:VAL:HG13	1:A:2754:ALA:HB2	1.97	0.47
1:A:4219:VAL:HG22	1:A:4243:LEU:HD22	1.96	0.47
1:A:4393:GLN:OE1	1:A:4393:GLN:N	2.39	0.47
1:A:1683:GLU:O	1:A:1746:GLN:NE2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3140:ARG:HA	1:A:3143:ILE:HG22	1.97	0.46
1:A:3872:ALA:O	1:A:3880:HIS:NE2	2.47	0.46
1:A:1998:THR:HG21	1:A:2005:GLN:HB3	1.97	0.46
1:A:2940:GLY:HA3	1:A:3174:ARG:HG3	1.97	0.46
1:A:3039:LYS:HA	1:A:3039:LYS:HD3	1.71	0.46
1:A:1812:ILE:HD13	1:A:2056:SER:HA	1.96	0.46
1:A:2220:LEU:O	1:A:2342:MET:HA	2.15	0.46
1:A:4324:PRO:HD3	1:A:4638:ARG:HG3	1.96	0.46
1:A:1343:ILE:HA	1:A:1346:MET:HE2	1.98	0.46
1:A:2083:GLN:HB2	1:A:2086:TYR:HD1	1.81	0.46
1:A:3618:ALA:HA	1:A:3621:LYS:NZ	2.31	0.46
1:A:3772:ASN:HA	1:A:3775:ARG:HE	1.79	0.46
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.49	0.46
1:A:1941:MET:HA	1:A:1944:ILE:HB	1.96	0.46
1:A:3601:MET:HG3	1:A:3611:ARG:HH21	1.80	0.46
1:A:4095:MET:HE1	1:A:4097:LYS:NZ	2.30	0.46
1:A:1451:LEU:HG	1:A:3673:PRO:HG2	1.97	0.46
1:A:2465:ALA:HB2	1:A:2493:TYR:CD2	2.51	0.46
1:A:2507:ARG:HE	1:A:2509:LYS:NZ	2.13	0.46
1:A:3650:ASN:OD1	1:A:3695:ARG:NH1	2.49	0.46
1:A:4609:VAL:HG23	1:A:4619:ILE:HB	1.98	0.46
1:A:3115:LEU:HD13	1:A:3143:ILE:HG21	1.97	0.46
1:A:3511:ALA:HA	1:A:3514:ILE:HG22	1.97	0.46
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.98	0.46
1:A:4577:LEU:HG	1:A:4630:GLU:OE1	2.15	0.46
1:A:1633:GLY:HA2	1:A:1943:ARG:NH1	2.30	0.46
1:A:1661:VAL:HG22	1:A:1676:ILE:HG21	1.98	0.46
1:A:1910:THR:HG22	1:A:2044:PRO:HD3	1.98	0.46
1:A:1942:GLY:HA3	1:A:2002:LEU:HD21	1.98	0.46
1:A:1351:TRP:H	1:A:1430:THR:HA	1.81	0.46
1:A:1630:TYR:O	1:A:1943:ARG:NE	2.34	0.46
1:A:1964:GLU:O	1:A:1968:LEU:N	2.28	0.46
1:A:2262:ASP:OD2	1:A:2263:HIS:N	2.49	0.46
1:A:2307:VAL:HA	1:A:2311:TRP:CZ2	2.51	0.46
1:A:2686:MET:SD	1:A:2703:LEU:HD11	2.56	0.46
1:A:3591:ASP:N	1:A:3591:ASP:OD1	2.48	0.46
1:A:3557:ASP:OD1	1:A:3558:GLU:N	2.49	0.46
1:A:3704:THR:HG22	1:A:3705:ARG:H	1.81	0.46
1:A:4405:ILE:O	1:A:4411:ARG:NH2	2.49	0.46
1:A:1388:ARG:HA	1:A:1391:LYS:HE2	1.98	0.45
1:A:2422:ILE:HD13	1:A:2487:GLU:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2584:TRP:CH2	1:A:2732:PRO:HB2	2.51	0.45
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.49	0.45
1:A:4186:PHE:O	1:A:4190:ILE:HD12	2.16	0.45
1:A:4413:PHE:CD2	1:A:4504:LEU:HD22	2.50	0.45
1:A:3567:LEU:HB2	1:A:3599:PHE:CD1	2.51	0.45
1:A:1582:VAL:HG23	1:A:1591:VAL:HG22	1.98	0.45
1:A:2577:HIS:O	1:A:2581:LEU:HD23	2.17	0.45
1:A:2804:ARG:HH12	1:A:2811:ARG:HH22	1.64	0.45
1:A:2982:ARG:NH2	1:A:2988:GLU:OE2	2.40	0.45
1:A:3174:ARG:HH12	1:A:3695:ARG:CZ	2.28	0.45
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.98	0.45
1:A:4037:PRO:HB2	1:A:4118:PRO:HB2	1.97	0.45
1:A:4401:THR:OG1	1:A:4404:ASN:OD1	2.34	0.45
1:A:4410:PHE:O	1:A:4414:GLU:OE1	2.35	0.45
1:A:4518:GLU:HG3	1:A:4619:ILE:HG23	1.99	0.45
1:A:1507:MET:SD	1:A:3629:PHE:HE1	2.39	0.45
1:A:1510:SER:N	1:A:3608:LYS:HZ3	2.14	0.45
1:A:1881:GLN:NE2	1:A:1889:TYR:HE2	2.14	0.45
1:A:2839:GLU:N	1:A:2839:GLU:OE1	2.49	0.45
1:A:3619:PHE:CE2	1:A:3623:LEU:HD11	2.52	0.45
1:A:1498:LYS:HE2	1:A:1531:MET:HE1	1.97	0.45
1:A:2224:GLY:H	1:A:2230:LYS:HD3	1.80	0.45
1:A:1755:GLN:OE1	1:A:1922:GLN:NE2	2.50	0.45
1:A:2260:SER:OG	1:A:2262:ASP:OD2	2.28	0.45
1:A:2837:LEU:HD23	1:A:2842:GLU:HG2	1.98	0.45
1:A:3167:ARG:HH11	1:A:3519:TYR:HH	1.60	0.45
1:A:3174:ARG:NH2	2:A:4704:ADP:O3A	2.49	0.45
1:A:3574:THR:O	1:A:3578:ILE:HG12	2.15	0.45
1:A:3875:MET:HE1	1:A:3883:PHE:HB2	1.98	0.45
1:A:3909:LEU:HD23	1:A:4344:LEU:HA	1.98	0.45
1:A:4227:ALA:O	1:A:4230:ARG:HG3	2.17	0.45
1:A:4445:THR:O	1:A:4449:ARG:HG3	2.16	0.45
1:A:4609:VAL:HG22	1:A:4620:PHE:O	2.17	0.45
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.98	0.45
1:A:3043:MET:SD	1:A:3043:MET:N	2.87	0.45
1:A:2451:ARG:HG2	1:A:2455:LEU:CD1	2.46	0.45
1:A:2921:ARG:O	1:A:2925:ILE:HG12	2.16	0.45
1:A:3154:LEU:HD13	1:A:3516:TYR:HD1	1.79	0.44
1:A:4027:LEU:HD21	1:A:4043:MET:HE2	1.98	0.44
1:A:4395:LEU:HD21	1:A:4486:ILE:HG23	1.99	0.44
1:A:1397:ASN:O	1:A:1401:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1523:TRP:HA	1:A:1526:LYS:HG2	1.98	0.44
1:A:2210:LEU:O	1:A:2214:THR:HG23	2.17	0.44
1:A:2875:ASN:HD21	1:A:2927:ARG:NH1	2.15	0.44
1:A:4248:ALA:HB2	1:A:4269:LEU:HD12	1.99	0.44
1:A:4600:LYS:HE2	1:A:4604:VAL:HG12	2.00	0.44
1:A:2704:GLU:O	1:A:2706:ILE:HG12	2.16	0.44
1:A:2798:GLU:OE1	1:A:2836:ARG:NH2	2.50	0.44
1:A:3510:SER:HB2	1:A:3553:LEU:HD11	1.98	0.44
1:A:4391:ILE:O	1:A:4428:ARG:NH2	2.50	0.44
1:A:1868:TYR:HB3	1:A:1870:PHE:CD1	2.52	0.44
1:A:4460:LEU:HA	1:A:4475:VAL:HG22	2.00	0.44
1:A:2506:SER:OG	1:A:2510:MET:HB3	2.18	0.44
1:A:2516:GLU:O	1:A:2519:ARG:HG2	2.17	0.44
1:A:3596:ALA:HB2	1:A:3701:PHE:CE2	2.52	0.44
1:A:3906:GLN:OE1	1:A:3910:ARG:HG3	2.17	0.44
1:A:4071:ILE:HG13	1:A:4099:VAL:HG12	2.00	0.44
1:A:1367:LEU:HD21	1:A:1394:MET:HE1	2.00	0.44
1:A:1727:PHE:HE2	1:A:1741:TRP:CG	2.36	0.44
1:A:1863:ASN:OD1	1:A:1894:GLN:NE2	2.39	0.44
1:A:1888:CYS:O	1:A:1892:MET:HG2	2.17	0.44
1:A:2231:SER:HA	1:A:2234:TRP:NE1	2.32	0.44
1:A:2527:PRO:HD3	1:A:2545:TRP:CD1	2.53	0.44
1:A:2744:LEU:O	1:A:2747:ILE:HG22	2.18	0.44
1:A:2874:SER:HB2	1:A:2920:LEU:HD11	2.00	0.44
1:A:3114:ASP:O	1:A:3140:ARG:NH2	2.51	0.44
1:A:3612:THR:O	1:A:3635:VAL:HA	2.18	0.44
1:A:3720:GLU:OE2	1:A:3855:ARG:HD3	2.17	0.44
1:A:4635:PHE:CD2	1:A:4640:VAL:HG11	2.53	0.44
1:A:1374:PRO:HD2	1:A:1377:LEU:HD12	2.00	0.44
1:A:1417:MET:HE1	1:A:1424:TRP:CE3	2.53	0.44
1:A:1608:LEU:O	1:A:1611:ILE:HG22	2.18	0.44
1:A:2253:ILE:HG21	1:A:2689:HIS:CE1	2.53	0.44
1:A:3626:ALA:HA	1:A:3631:ASN:OD1	2.17	0.44
1:A:4481:ASP:OD2	1:A:4485:ARG:NE	2.36	0.44
1:A:3109:PHE:HD2	1:A:3180:ILE:HG21	1.83	0.43
1:A:3973:LEU:HB2	1:A:3992:LEU:HD11	1.99	0.43
1:A:2094:LYS:HD3	2:A:4701:ADP:O2'	2.18	0.43
1:A:2368:VAL:HG12	1:A:2369:LEU:HD22	2.00	0.43
1:A:4332:LEU:HD23	1:A:4332:LEU:HA	1.85	0.43
1:A:1536:VAL:HG12	1:A:1601:LEU:HG	2.00	0.43
1:A:1626:PHE:CE2	1:A:1628:ARG:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2146:VAL:HA	1:A:2149:LEU:HD23	1.99	0.43
1:A:3689:PRO:HB2	1:A:3691:ASP:OD1	2.18	0.43
1:A:1413:TRP:O	1:A:1417:MET:HG2	2.18	0.43
1:A:1417:MET:HE1	1:A:1424:TRP:CZ3	2.53	0.43
1:A:1491:ASP:OD1	1:A:1495:ASN:ND2	2.48	0.43
1:A:1504:VAL:HA	1:A:1507:MET:CG	2.48	0.43
1:A:1714:ALA:HA	1:A:1870:PHE:CE2	2.49	0.43
1:A:2306:ASP:HB2	1:A:2676:THR:HG21	1.99	0.43
1:A:4393:GLN:HG2	1:A:4394:THR:N	2.33	0.43
1:A:1349:GLN:NE2	1:A:1353:SER:O	2.52	0.43
1:A:1678:SER:HB2	1:A:1872:TYR:HE2	1.84	0.43
1:A:2893:VAL:HG11	1:A:2916:LEU:HD13	2.01	0.43
1:A:3886:LEU:O	1:A:3890:ILE:HG12	2.19	0.43
1:A:3916:LEU:HD23	1:A:3916:LEU:HA	1.88	0.43
1:A:4172:SER:O	1:A:4176:ARG:NH1	2.50	0.43
1:A:1699:ASN:C	1:A:1699:ASN:HD22	2.26	0.43
1:A:2110:LYS:HA	1:A:2113:ARG:CZ	2.48	0.43
1:A:2206:LYS:HB3	1:A:2364:PHE:CE2	2.53	0.43
1:A:2435:LYS:O	1:A:2438:GLU:HG3	2.18	0.43
1:A:2465:ALA:HB2	1:A:2493:TYR:CE2	2.54	0.43
1:A:2590:PRO:HG2	1:A:2687:VAL:HG21	2.00	0.43
1:A:2241:LEU:HB3	1:A:2298:ARG:NH2	2.34	0.43
1:A:3202:ASN:O	1:A:3206:ARG:HG3	2.18	0.43
1:A:3576:ASN:CB	1:A:3701:PHE:HE1	2.31	0.43
1:A:3888:ALA:HB1	1:A:4012:ASN:HD22	1.83	0.43
1:A:4050:ASP:OD1	1:A:4051:ALA:N	2.49	0.43
1:A:4423:LEU:HD21	1:A:4466:HIS:ND1	2.33	0.43
1:A:1914:GLU:OE1	2:A:4701:ADP:H3'	2.19	0.43
1:A:2354:ALA:HB1	1:A:2358:ARG:HH21	1.83	0.43
1:A:2995:ASP:OD1	1:A:3067:THR:OG1	2.35	0.43
1:A:3030:MET:SD	1:A:3050:LEU:HD11	2.59	0.43
1:A:3723:ASP:O	1:A:3726:GLU:HG3	2.17	0.43
1:A:1671:SER:O	1:A:1692:ILE:HG22	2.19	0.43
1:A:2309:PRO:HB3	1:A:2352:THR:HG23	2.01	0.43
1:A:2522:THR:OG1	1:A:2524:VAL:HG12	2.19	0.43
1:A:2727:PHE:O	1:A:2731:VAL:HG22	2.18	0.43
1:A:4109:LEU:HD23	1:A:4113:LEU:HD23	2.01	0.43
1:A:1367:LEU:HD11	1:A:1394:MET:SD	2.58	0.42
1:A:1412:HIS:CE1	1:A:1453:ALA:HA	2.54	0.42
1:A:1587:LEU:HD23	1:A:1589:MET:H	1.83	0.42
1:A:2222:MET:HE2	1:A:2222:MET:HB2	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2457:SER:OG	1:A:2584:TRP:HZ2	2.01	0.42
1:A:2985:CYS:SG	1:A:3032:GLN:HB3	2.58	0.42
1:A:3650:ASN:HB3	1:A:3652:GLU:HG2	1.99	0.42
1:A:1467:ARG:HA	1:A:1523:TRP:CH2	2.55	0.42
1:A:2309:PRO:HA	1:A:2312:VAL:HG12	2.01	0.42
1:A:3169:MET:HB3	1:A:3693:CYS:SG	2.60	0.42
1:A:1882:THR:HG23	1:A:1885:THR:H	1.84	0.42
1:A:1940:ALA:HB1	1:A:1943:ARG:CZ	2.49	0.42
1:A:1961:ASN:ND2	1:A:2019:ASN:O	2.51	0.42
1:A:2885:ASP:HB3	1:A:2888:GLU:OE1	2.19	0.42
1:A:3130:TYR:CZ	1:A:3132:LYS:HB2	2.54	0.42
1:A:3999:ASP:OD1	1:A:4000:ARG:HG2	2.19	0.42
1:A:1626:PHE:HB3	1:A:1629:PHE:CD2	2.54	0.42
1:A:1629:PHE:HE1	1:A:1640:ILE:HG21	1.84	0.42
1:A:2666:ILE:HB	1:A:2712:CYS:SG	2.59	0.42
1:A:1608:LEU:HA	1:A:1611:ILE:HG22	2.01	0.42
1:A:1931:ASN:O	1:A:1936:PHE:HD1	2.03	0.42
1:A:2138:ILE:HG13	1:A:2161:LEU:HD21	2.01	0.42
1:A:2863:ARG:NH2	1:A:2864:GLU:OE2	2.52	0.42
1:A:3930:GLU:HG2	1:A:3931:GLN:N	2.34	0.42
1:A:2823:ARG:HH12	1:A:2868:SER:N	2.18	0.42
1:A:2843:ARG:HH21	1:A:3093:TRP:CD1	2.37	0.42
1:A:3211:THR:HG21	1:A:3753:LEU:HD21	2.01	0.42
1:A:3840:LEU:HD23	1:A:3840:LEU:HA	1.85	0.42
1:A:1983:ARG:HB3	1:A:1983:ARG:NH1	2.35	0.42
1:A:2138:ILE:HA	1:A:2141:VAL:HG12	2.01	0.42
1:A:2412:MET:O	1:A:2416:GLN:HG2	2.19	0.42
1:A:2779:MET:HA	1:A:2782:GLU:HG3	2.02	0.42
1:A:3112:LYS:HE3	1:A:3113:MET:HE3	2.02	0.42
1:A:3150:VAL:HG13	1:A:3532:TRP:CE2	2.54	0.42
1:A:3780:VAL:O	1:A:3784:VAL:HG23	2.20	0.42
1:A:3782:ARG:O	1:A:3786:GLU:HG2	2.19	0.42
1:A:3814:THR:O	1:A:3818:LEU:HG	2.20	0.42
1:A:2486:LEU:O	1:A:2490:ILE:HG12	2.20	0.42
1:A:2686:MET:HE1	1:A:2708:PHE:CZ	2.55	0.42
1:A:2962:LYS:HE3	1:A:3663:THR:HG21	2.00	0.42
1:A:3146:SER:O	1:A:3150:VAL:HG23	2.20	0.42
1:A:3596:ALA:HB2	1:A:3701:PHE:CD2	2.55	0.42
1:A:3736:GLY:O	1:A:3740:LEU:N	2.40	0.42
1:A:4173:PRO:HB2	1:A:4175:GLU:OE1	2.20	0.42
1:A:4294:ILE:HD11	1:A:4320:TRP:NE1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4623:ASP:OD2	1:A:4624:PHE:N	2.53	0.42
1:A:1416:LEU:HD12	1:A:1417:MET:HE2	2.01	0.42
1:A:1539:ASP:HA	1:A:1542:ARG:HD3	2.00	0.42
1:A:3133:LEU:HD11	1:A:3141:GLU:HB3	2.01	0.42
1:A:3212:VAL:HA	1:A:3215:VAL:HG12	2.02	0.42
1:A:3704:THR:HG22	1:A:3705:ARG:N	2.35	0.42
1:A:1390:LEU:O	1:A:1394:MET:HE3	2.20	0.41
1:A:1623:ARG:HB3	1:A:1630:TYR:CZ	2.55	0.41
1:A:2460:SER:OG	1:A:2589:LYS:HD2	2.20	0.41
1:A:3209:LYS:HE2	1:A:3486:ARG:NH2	2.34	0.41
1:A:2278:GLY:N	1:A:2281:THR:OG1	2.52	0.41
1:A:2387:LEU:HD21	1:A:2463:HIS:ND1	2.35	0.41
1:A:4461:PRO:HG2	1:A:4464:TRP:CE3	2.55	0.41
1:A:4607:LEU:HD22	1:A:4640:VAL:HG13	2.02	0.41
1:A:2205:GLU:O	1:A:2209:GLN:HG3	2.19	0.41
1:A:2211:TYR:CE1	1:A:2241:LEU:HD21	2.54	0.41
1:A:3178:ASP:OD2	1:A:3585:ARG:NE	2.52	0.41
1:A:4107:MET:O	1:A:4110:GLU:HG2	2.21	0.41
1:A:1678:SER:OG	1:A:1679:ARG:N	2.53	0.41
1:A:2723:LEU:HD23	1:A:2723:LEU:HA	1.84	0.41
1:A:3470:ALA:O	1:A:3474:ARG:HG3	2.20	0.41
1:A:1464:LYS:HE2	1:A:1464:LYS:HB2	1.89	0.41
1:A:2269:ASP:O	1:A:2273:ARG:NH2	2.54	0.41
1:A:2684:ARG:O	1:A:2688:GLU:HG3	2.20	0.41
1:A:3209:LYS:HB2	1:A:3486:ARG:NH2	2.35	0.41
1:A:4260:PHE:CE2	1:A:4608:PRO:HB3	2.56	0.41
1:A:1650:LEU:HD23	1:A:1650:LEU:HA	1.90	0.41
1:A:2729:ARG:HE	1:A:2730:HIS:CD2	2.38	0.41
1:A:2773:MET:HB3	1:A:2799:MET:HE3	2.01	0.41
1:A:2832:LEU:HD23	1:A:2832:LEU:HA	1.92	0.41
1:A:2884:VAL:HG21	1:A:2889:LEU:HD12	2.01	0.41
1:A:4038:ASN:HB3	1:A:4118:PRO:HG2	2.02	0.41
1:A:4554:ASP:N	1:A:4557:SER:OG	2.53	0.41
1:A:1431:LEU:HD21	1:A:1435:TRP:CZ2	2.56	0.41
1:A:1940:ALA:HB1	1:A:1943:ARG:NH2	2.35	0.41
1:A:1980:GLU:O	1:A:1984:GLU:HG3	2.21	0.41
1:A:2094:LYS:HE2	1:A:2094:LYS:HB3	1.80	0.41
1:A:2413:LEU:HD13	1:A:2416:GLN:NE2	2.35	0.41
1:A:3017:VAL:O	1:A:3020:LEU:HD22	2.21	0.41
1:A:4277:SER:HA	1:A:4282:PHE:CD2	2.56	0.41
1:A:1661:VAL:HG13	1:A:1676:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1788:THR:O	1:A:1792:LEU:HD23	2.21	0.41
1:A:1973:GLN:HA	1:A:1976:GLN:HE21	1.86	0.41
1:A:3042:LEU:O	1:A:3044:LEU:HG	2.20	0.41
1:A:3167:ARG:NH2	1:A:3685:THR:HA	2.36	0.41
1:A:1390:LEU:C	1:A:1394:MET:HE3	2.45	0.41
1:A:1470:TRP:CE3	1:A:1470:TRP:HA	2.56	0.41
1:A:1786:GLU:OE2	1:A:1790:ASN:ND2	2.54	0.41
1:A:2054:LEU:HG	1:A:2097:LEU:HD12	2.03	0.41
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	2.02	0.41
1:A:2253:ILE:HG21	1:A:2689:HIS:NE2	2.36	0.41
1:A:2265:TYR:OH	1:A:2315:LEU:HG	2.21	0.41
1:A:2335:LEU:HD23	1:A:2336:PRO:O	2.21	0.41
1:A:2873:TYR:HB3	1:A:2881:TYR:CE2	2.56	0.41
1:A:2876:TRP:HA	1:A:2876:TRP:CE3	2.56	0.41
1:A:2909:LEU:HA	2:A:4704:ADP:C2	2.56	0.41
1:A:2927:ARG:O	1:A:2927:ARG:HG3	2.21	0.41
1:A:2930:GLN:HG3	1:A:2932:HIS:CD2	2.55	0.41
1:A:3481:SER:HB2	1:A:3770:LEU:CD1	2.51	0.41
1:A:4400:ARG:HB3	1:A:4405:ILE:HD11	2.03	0.41
1:A:4404:ASN:ND2	1:A:4501:ALA:HB2	2.36	0.41
1:A:1351:TRP:CE3	1:A:1434:ILE:HD12	2.56	0.41
1:A:1931:ASN:O	1:A:1936:PHE:CD1	2.74	0.41
1:A:2009:SER:O	1:A:2012:MET:HG2	2.21	0.41
1:A:2395:GLN:HB3	1:A:2398:ARG:NH2	2.36	0.41
1:A:2591:LEU:H	1:A:2709:VAL:HG12	1.86	0.41
1:A:2916:LEU:HD12	1:A:2916:LEU:HA	1.91	0.41
1:A:3045:ASP:OD1	1:A:3046:SER:N	2.53	0.41
1:A:3924:ILE:HG23	1:A:3952:GLN:OE1	2.21	0.41
1:A:2206:LYS:HD3	1:A:2206:LYS:HA	1.89	0.40
1:A:2646:ASN:OD1	1:A:2647:GLY:N	2.54	0.40
1:A:2935:LEU:HD23	1:A:3092:ASN:HB3	2.03	0.40
1:A:3174:ARG:HD2	1:A:3694:SER:OG	2.21	0.40
1:A:3811:ILE:HD11	1:A:3864:PHE:CE1	2.55	0.40
1:A:1344:ASP:O	1:A:1348:GLU:HG2	2.21	0.40
1:A:2093:LEU:O	1:A:2097:LEU:HD23	2.22	0.40
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	2.04	0.40
1:A:4300:ILE:N	1:A:4304:GLU:OE2	2.45	0.40
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	2.02	0.40
1:A:2224:GLY:N	1:A:2230:LYS:HD3	2.36	0.40
1:A:2789:GLN:HB2	1:A:2792:TYR:HE1	1.87	0.40
1:A:2888:GLU:OE1	1:A:2888:GLU:N	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3627:LEU:HD21	1:A:3648:VAL:HG22	2.03	0.40
1:A:3749:LEU:HD13	1:A:3773:LEU:HD22	2.02	0.40
1:A:3835:ILE:HG23	1:A:3866:VAL:HG12	2.04	0.40
1:A:1477:LEU:HB3	1:A:1485:ARG:HG2	2.04	0.40
1:A:1739:ILE:HD13	1:A:1739:ILE:HA	1.91	0.40
1:A:2315:LEU:HA	1:A:2318:VAL:HG22	2.02	0.40
1:A:3209:LYS:CA	1:A:3486:ARG:HH12	2.33	0.40
1:A:3772:ASN:O	1:A:3775:ARG:HG2	2.21	0.40
1:A:4277:SER:HA	1:A:4282:PHE:CG	2.56	0.40
1:A:1523:TRP:CE3	1:A:1526:LYS:HD2	2.56	0.40
1:A:2877:LEU:HD12	1:A:2884:VAL:HB	2.02	0.40
1:A:3746:GLU:HA	1:A:3773:LEU:HD21	2.04	0.40
1:A:4186:PHE:CE1	1:A:4190:ILE:HD11	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3035/4646 (65%)	2956 (97%)	78 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1511	PRO

### 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	2706/4125 (66%)	2705 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
1	A	1567	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1566	GLN
1	A	1755	GLN
1	A	1876	GLN
1	A	1922	GLN
1	A	1950	GLN
1	A	2051	GLN
1	A	2263	HIS
1	A	2282	HIS
1	A	2299	GLN
1	A	2377	ASN
1	A	2414	GLN
1	A	2416	GLN
1	A	2439	HIS
1	A	2442	GLN
1	A	2475	ASN
1	A	2677	GLN
1	A	2698	GLN
1	A	2786	GLN
1	A	3032	GLN
1	A	3038	GLN
1	A	3202	ASN
1	A	3535	HIS
1	A	3646	ASN
1	A	4156	ASN
1	A	4191	GLN
1	A	4262	GLN
1	A	4446	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 ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	ADP	A	4701	-	24,29,29	0.87	0	29,45,45	1.26	3 (10%)
3	ATP	A	4702	4	28,33,33	0.75	0	34,52,52	0.61	1 (2%)
2	ADP	A	4704	-	24,29,29	0.85	0	29,45,45	1.24	2 (6%)
2	ADP	A	4703	-	24,29,29	0.87	0	29,45,45	1.29	3 (10%)

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
3	ATP	A	4702	4	-	5/18/38/38	0/3/3/3
2	ADP	A	4704	-	-	2/12/32/32	0/3/3/3
2	ADP	A	4703	-	-	5/12/32/32	0/3/3/3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	N3-C2-N1	-3.62	123.76	128.67
2	A	4704	ADP	N3-C2-N1	-3.57	123.83	128.67
2	A	4701	ADP	N3-C2-N1	-3.54	123.86	128.67
2	A	4704	ADP	C4-C5-N7	-2.53	106.67	109.34
2	A	4701	ADP	C4-C5-N7	-2.48	106.72	109.34
2	A	4703	ADP	C4-C5-N7	-2.45	106.75	109.34
3	A	4702	ATP	C5-C6-N6	2.41	123.98	120.31
2	A	4701	ADP	C4'-O4'-C1'	2.34	112.07	109.92
2	A	4703	ADP	C4'-O4'-C1'	2.26	112.00	109.92

There are no chirality outliers.

All (15) torsion outliers are listed below:

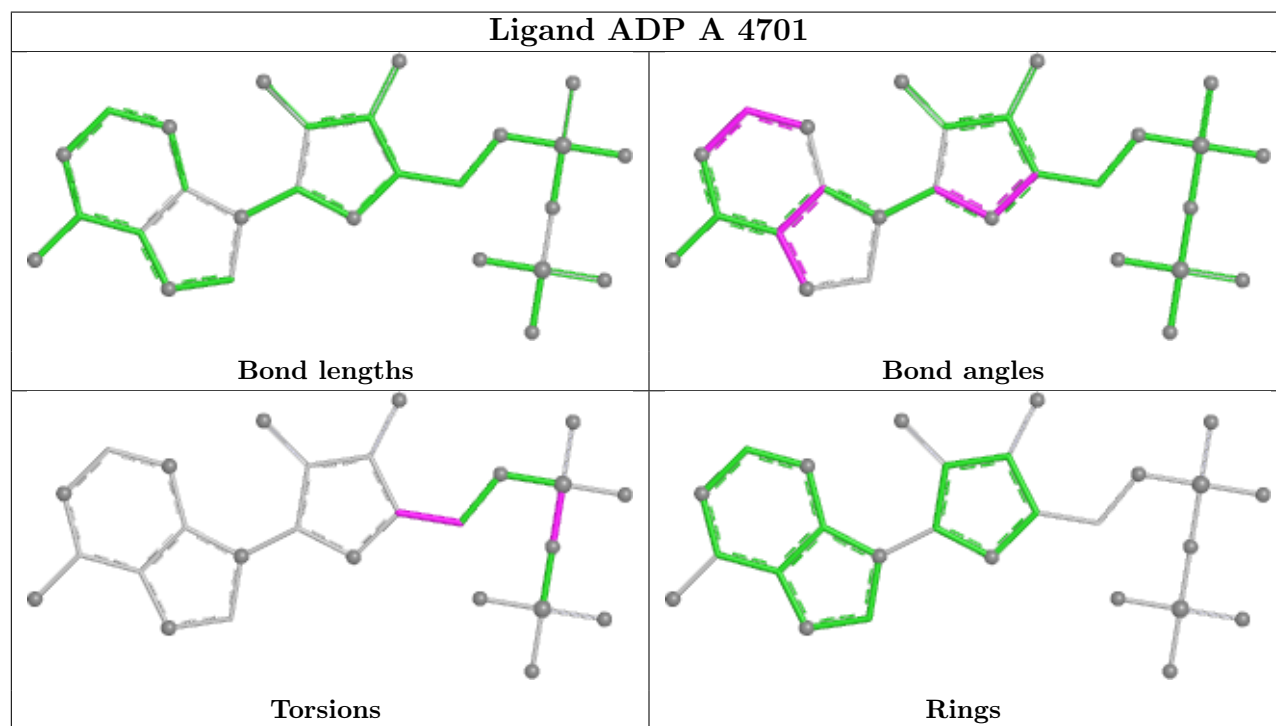
Mol	Chain	Res	Type	Atoms
2	A	4703	ADP	C5'-O5'-PA-O1A
2	A	4703	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A
3	A	4702	ATP	PB-O3B-PG-O3G
2	A	4703	ADP	O4'-C4'-C5'-O5'
2	A	4703	ADP	C3'-C4'-C5'-O5'
3	A	4702	ATP	PB-O3B-PG-O1G
3	A	4702	ATP	O4'-C4'-C5'-O5'
2	A	4701	ADP	PB-O3A-PA-O2A
3	A	4702	ATP	PA-O3A-PB-O1B
3	A	4702	ATP	C3'-C4'-C5'-O5'
2	A	4703	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	O4'-C4'-C5'-O5'
2	A	4701	ADP	PB-O3A-PA-O1A

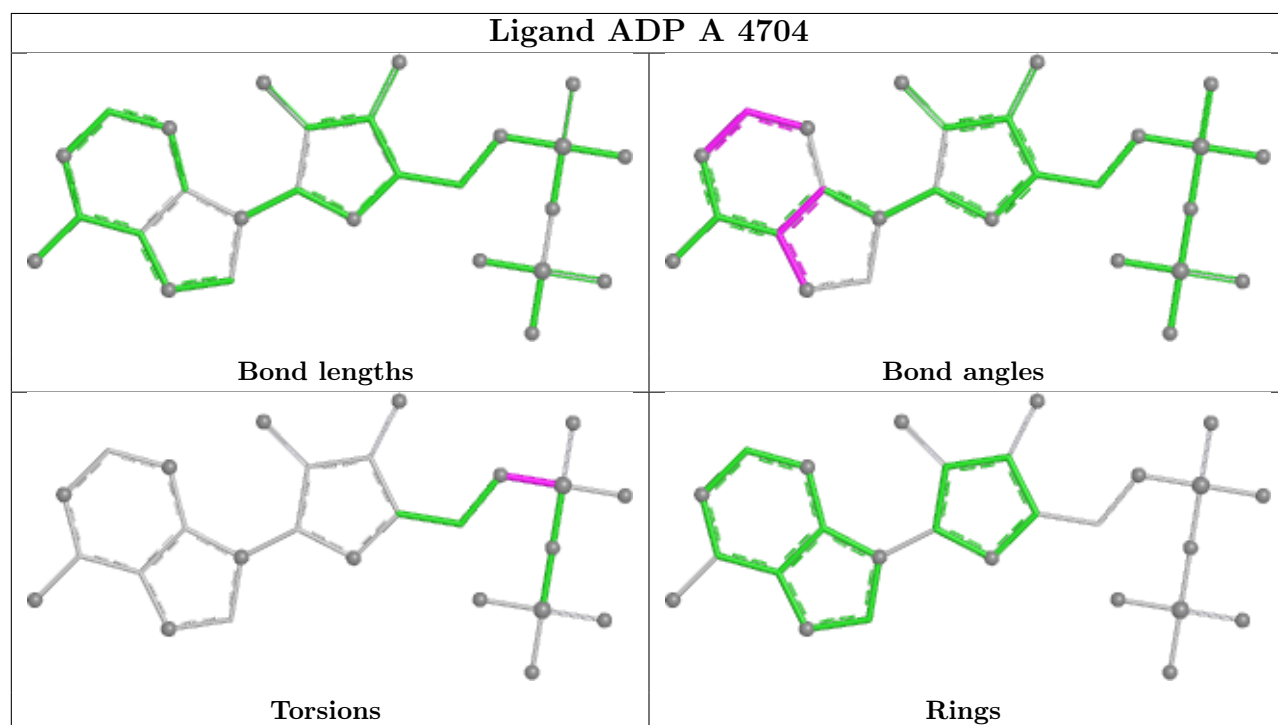
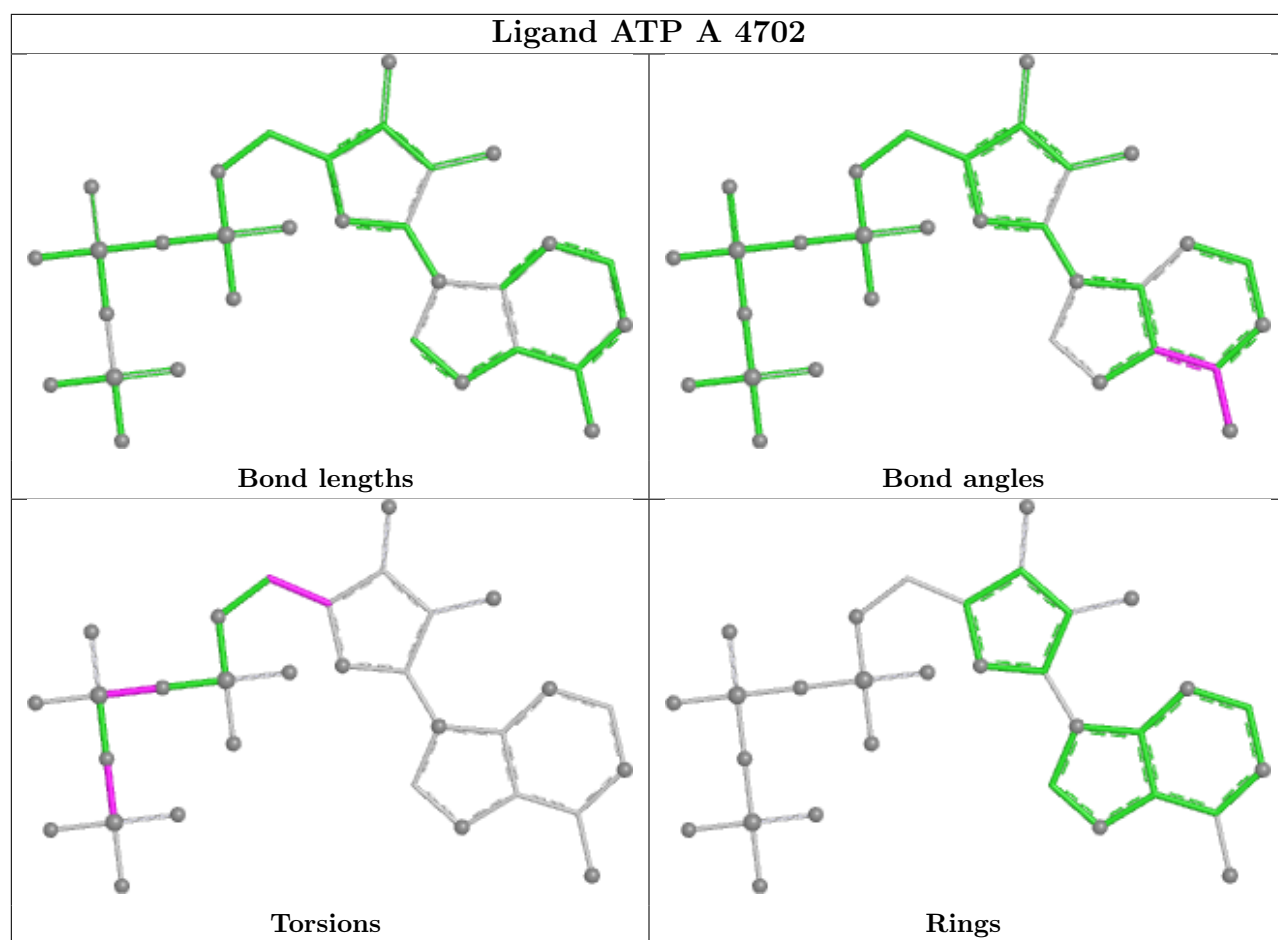
There are no ring outliers.

4 monomers are involved in 12 short contacts:

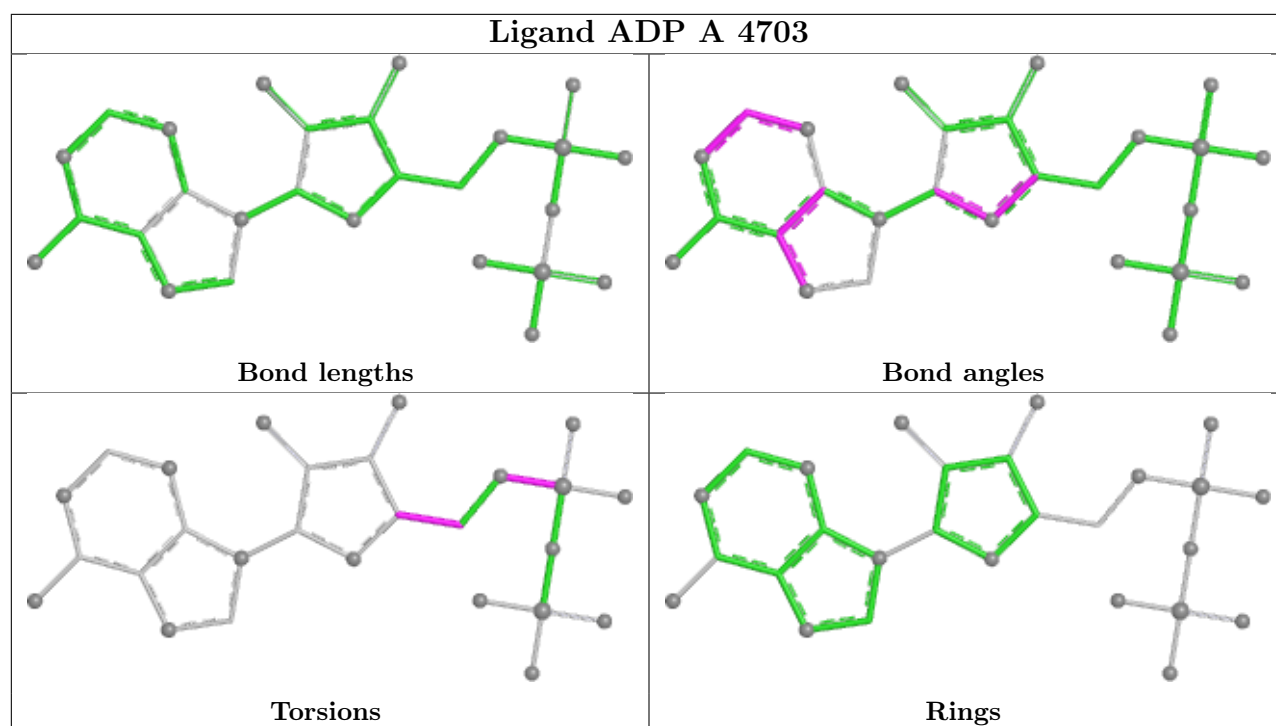
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	3	0
3	A	4702	ATP	3	0
2	A	4704	ADP	3	0
2	A	4703	ADP	3	0

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.

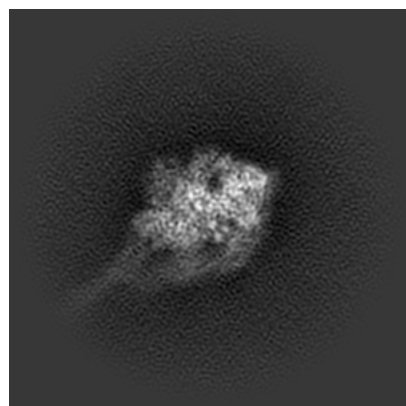
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44712. These allow visual inspection of the internal detail of the map and identification of artifacts.

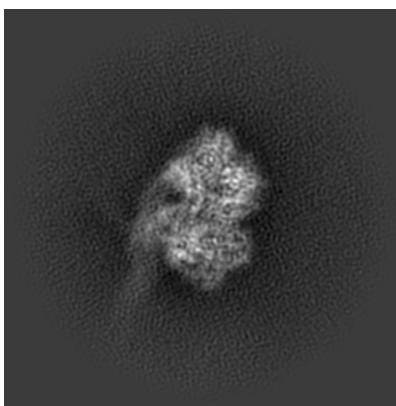
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

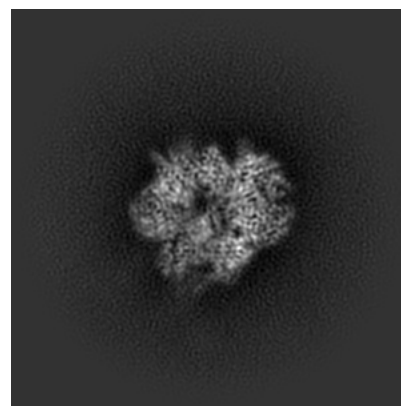
#### 6.1.1 Primary map



X

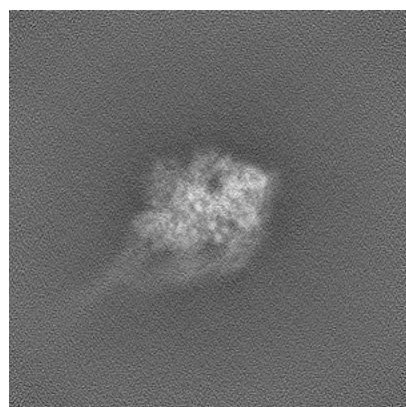


Y

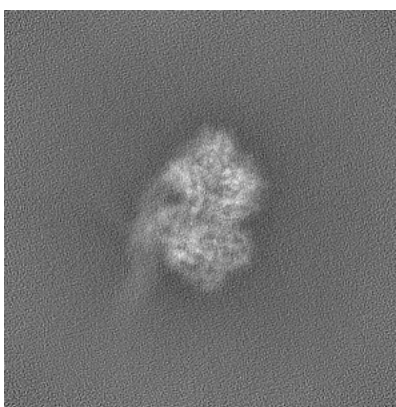


Z

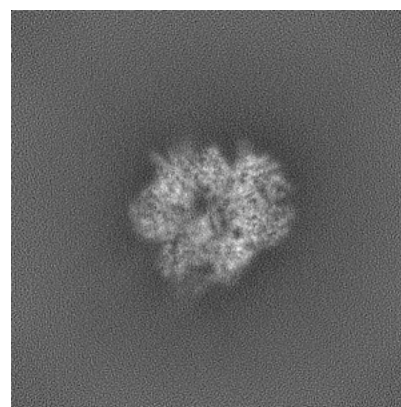
#### 6.1.2 Raw map



X



Y

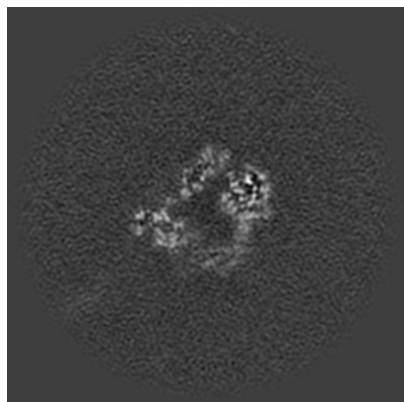


Z

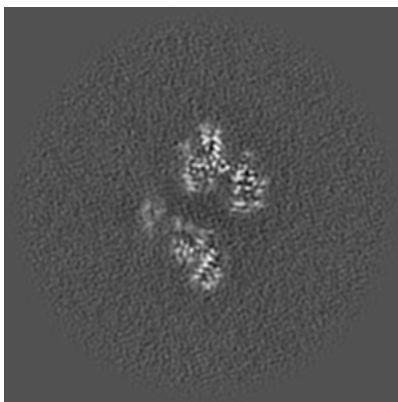
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

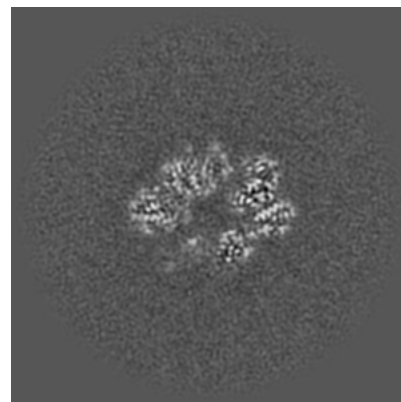
### 6.2.1 Primary map



X Index: 160

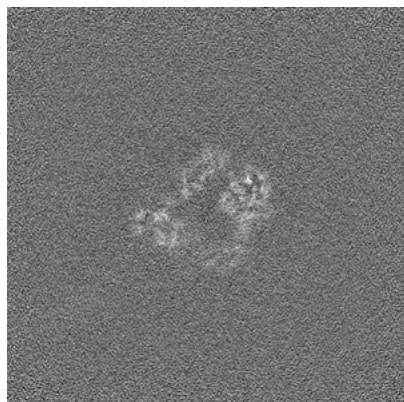


Y Index: 160

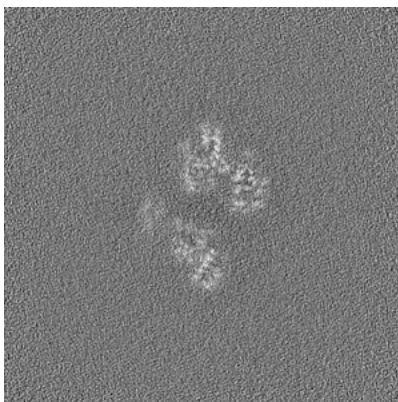


Z Index: 160

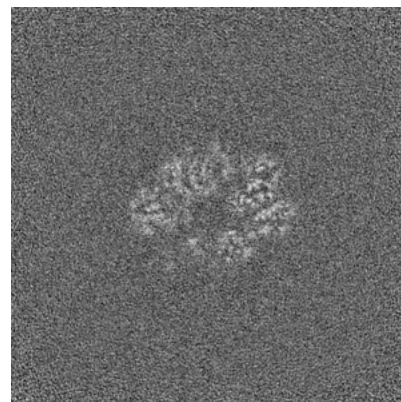
### 6.2.2 Raw map



X Index: 160



Y Index: 160

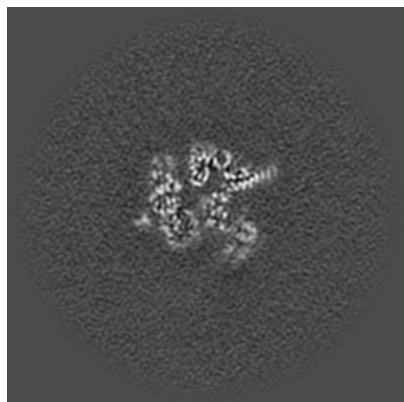


Z Index: 160

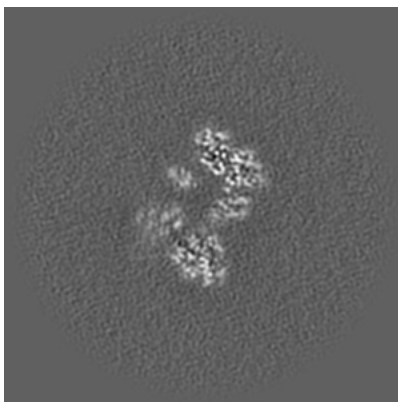
The images above show central slices of the map in three orthogonal directions.

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

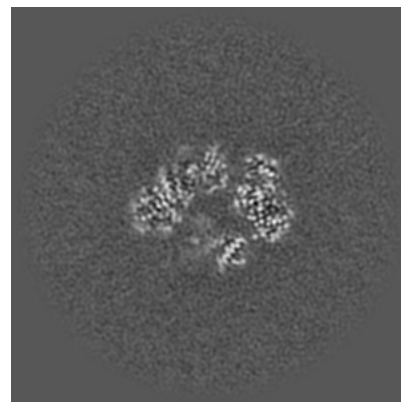
### 6.3.1 Primary map



X Index: 182

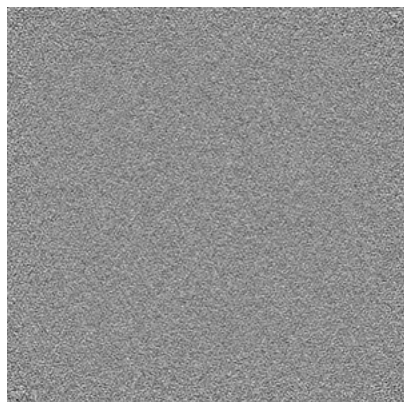


Y Index: 150

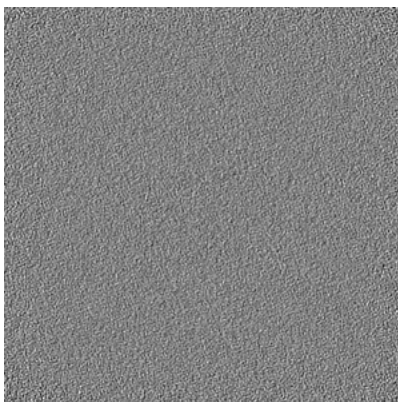


Z Index: 165

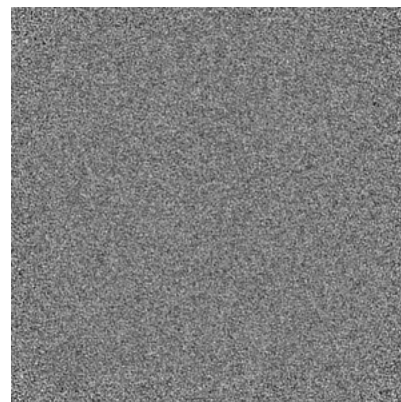
### 6.3.2 Raw map



X Index: 0



Y Index: 0



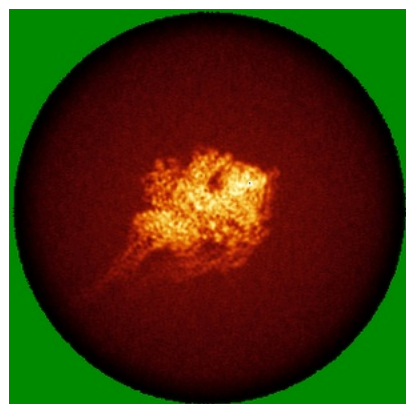
Z Index: 0

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

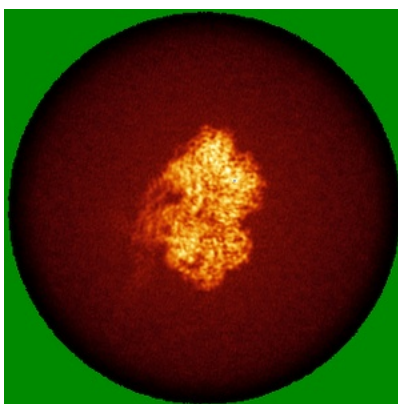


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

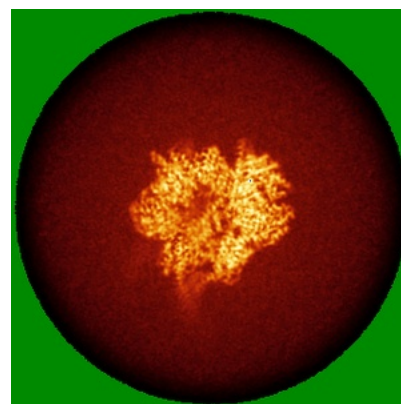
### 6.4.1 Primary map



X

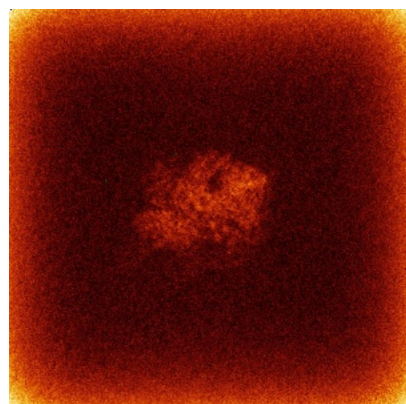


Y

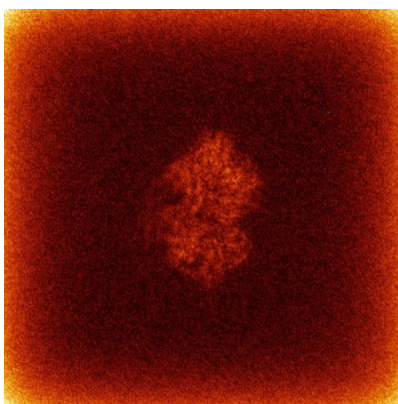


Z

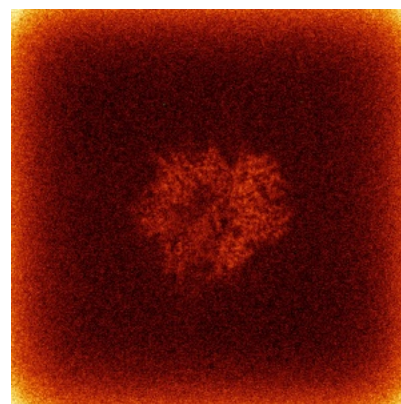
### 6.4.2 Raw map



X



Y

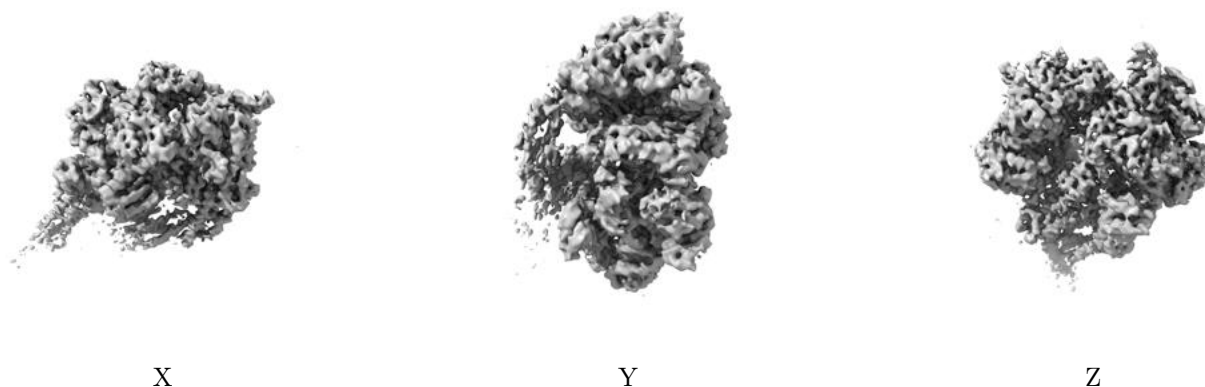


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

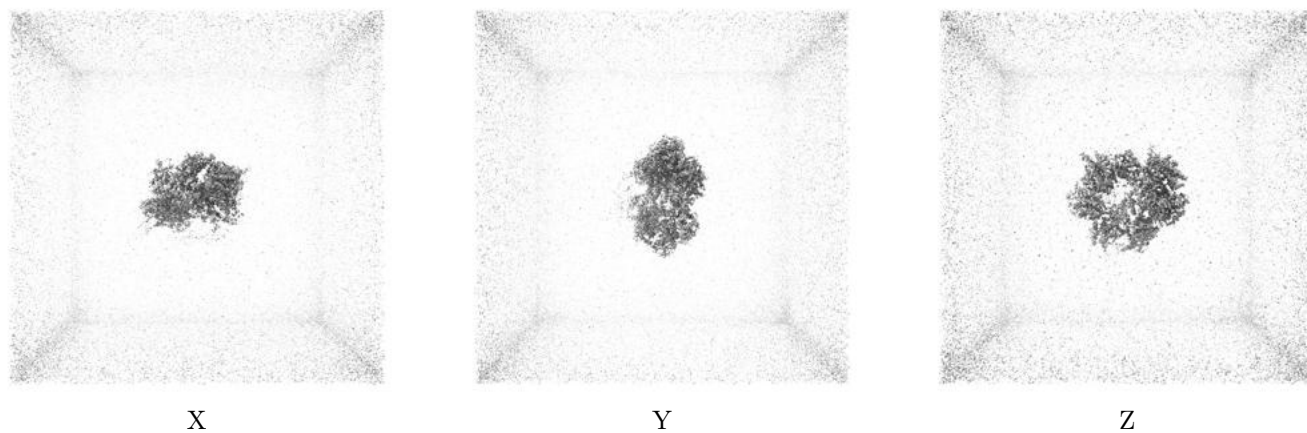
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

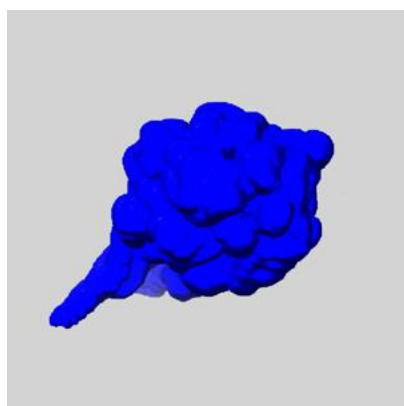
## 6.6 Mask visualisation [i](#)

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

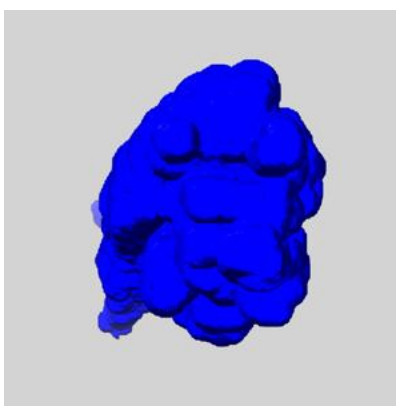
A mask typically either:

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

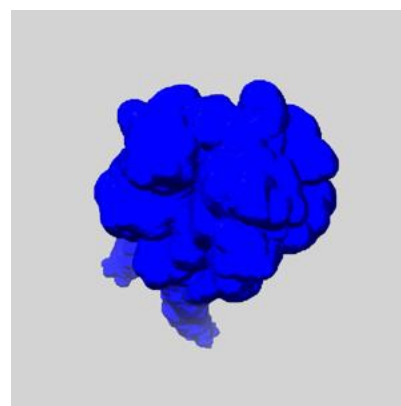
### 6.6.1 emd\_44712\_msk\_1.map [i](#)



X



Y

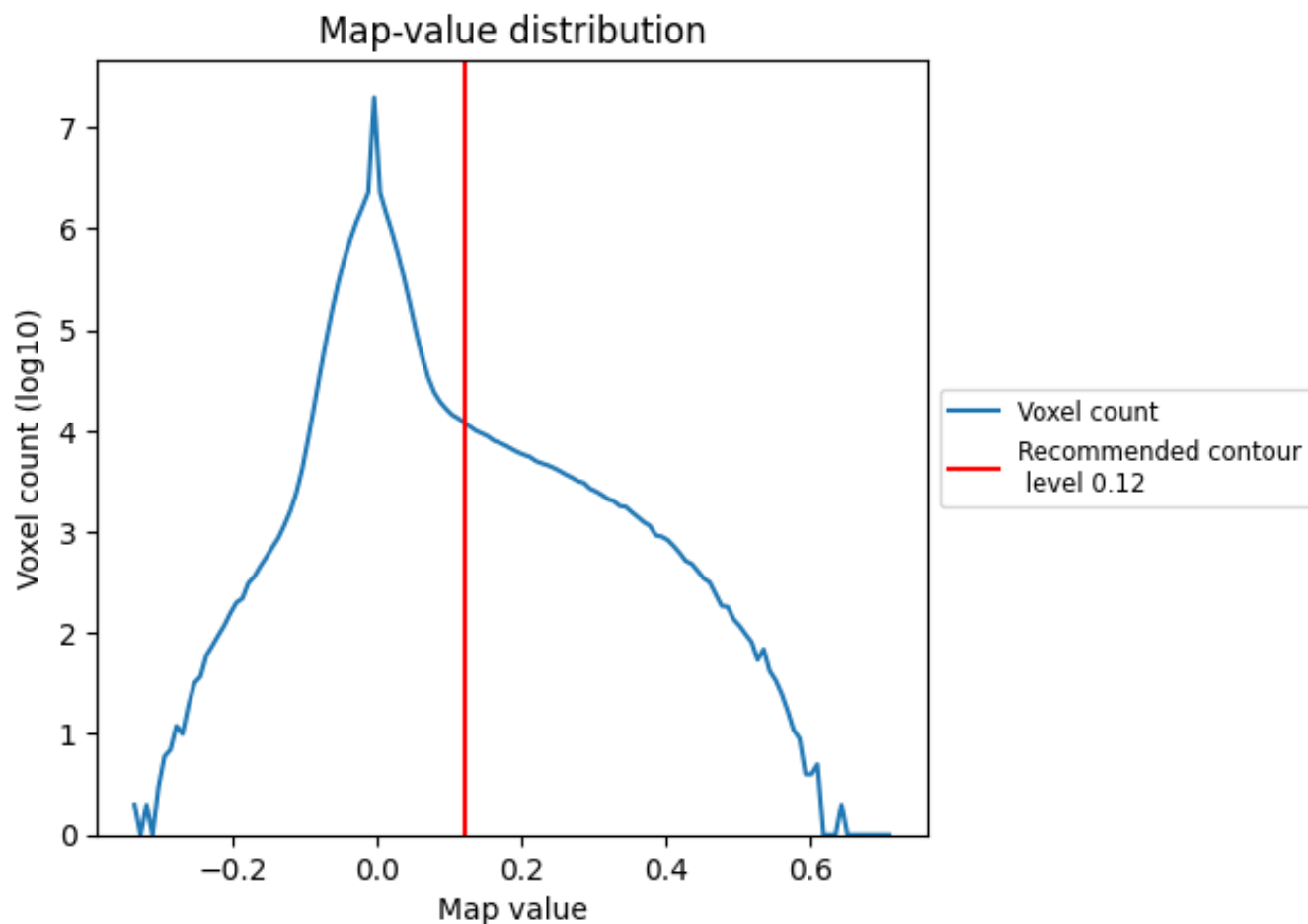


Z

## 7 Map analysis [i](#)

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

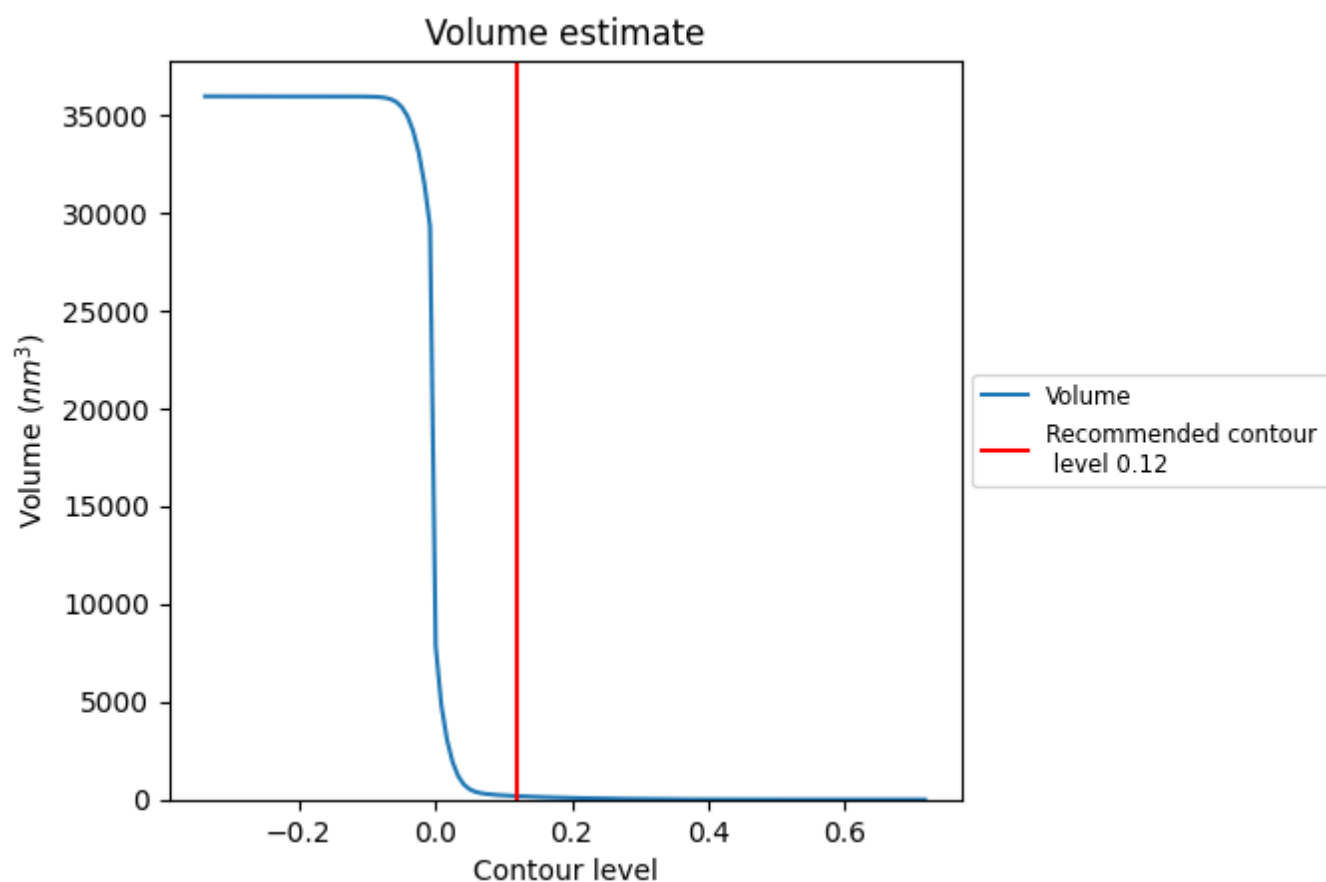
### 7.1 Map-value distribution [i](#)



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.



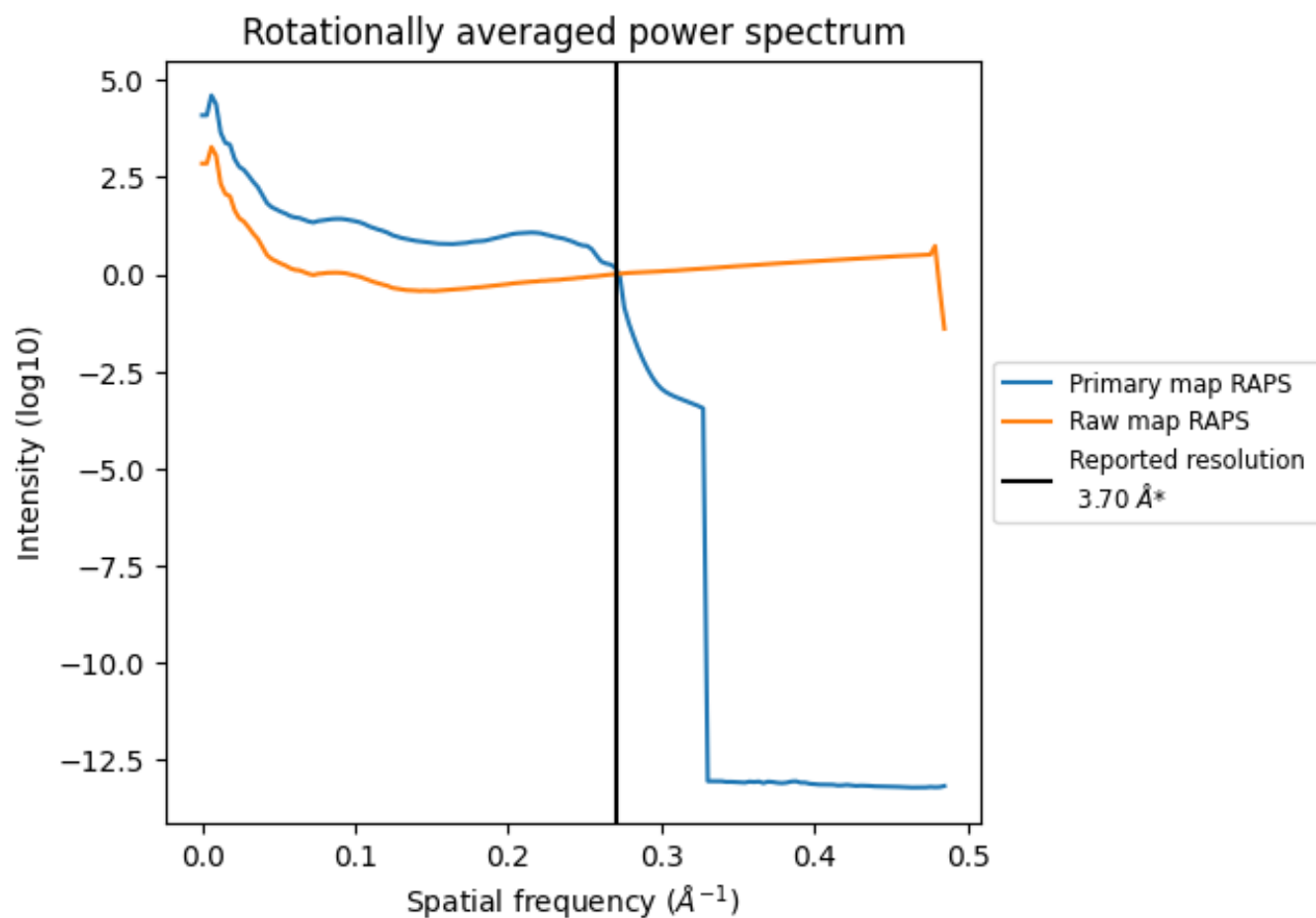
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177 nm<sup>3</sup>; this corresponds to an approximate mass of 159 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 ⓘ

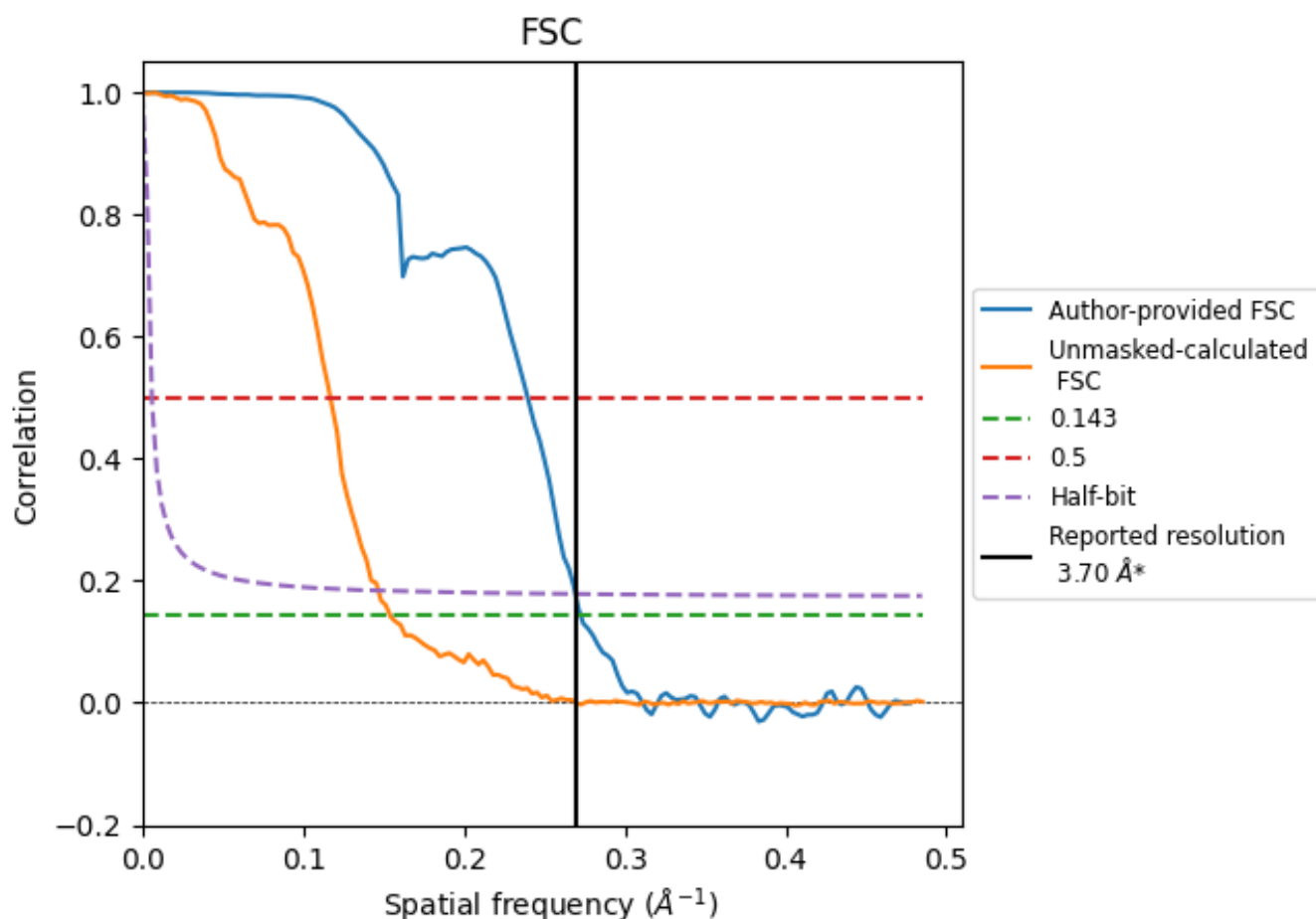


\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

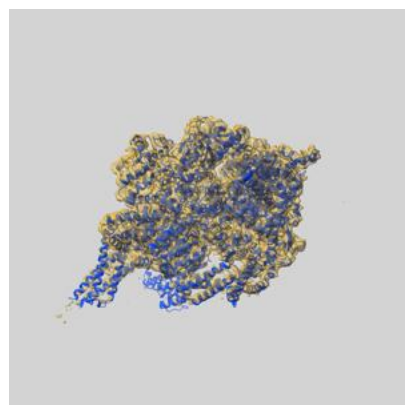
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.67	4.17	3.71
Unmasked-calculated*	6.49	8.55	6.81

\*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 6.49 differs from the reported value 3.7 by more than 10 %

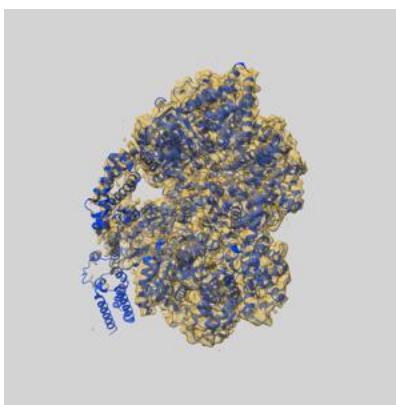
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44712 and PDB model 9BMV. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

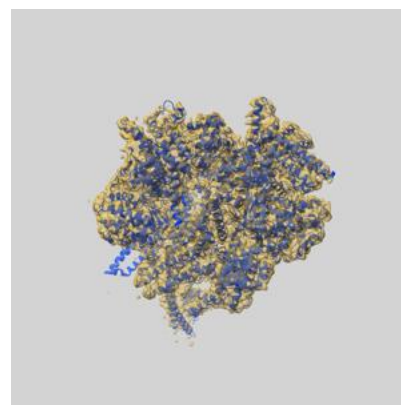
### 9.1 Map-model overlay [i](#)



X



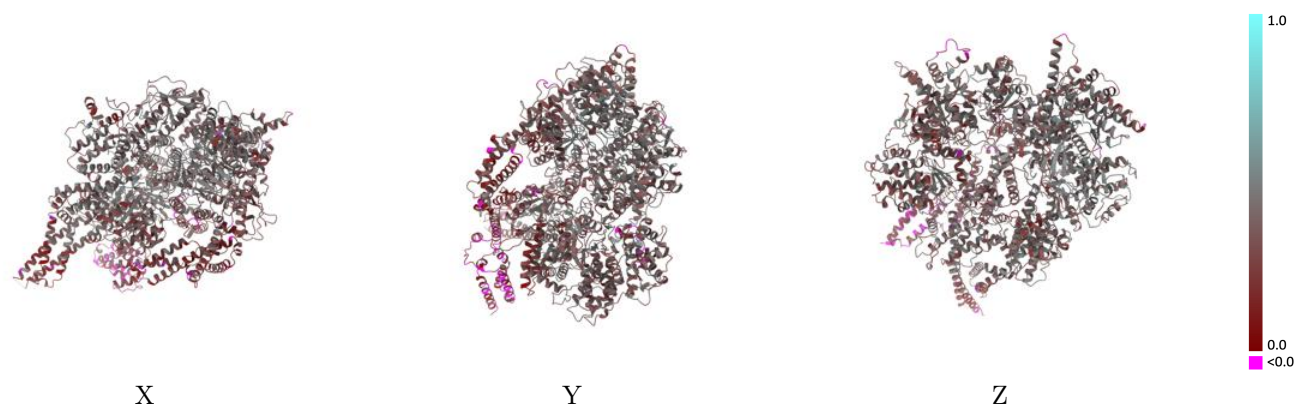
Y



Z

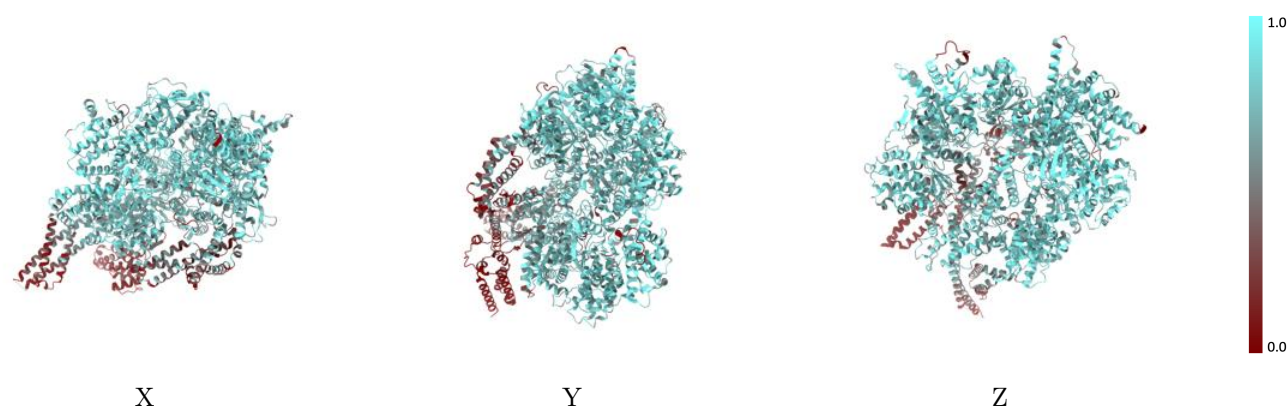
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



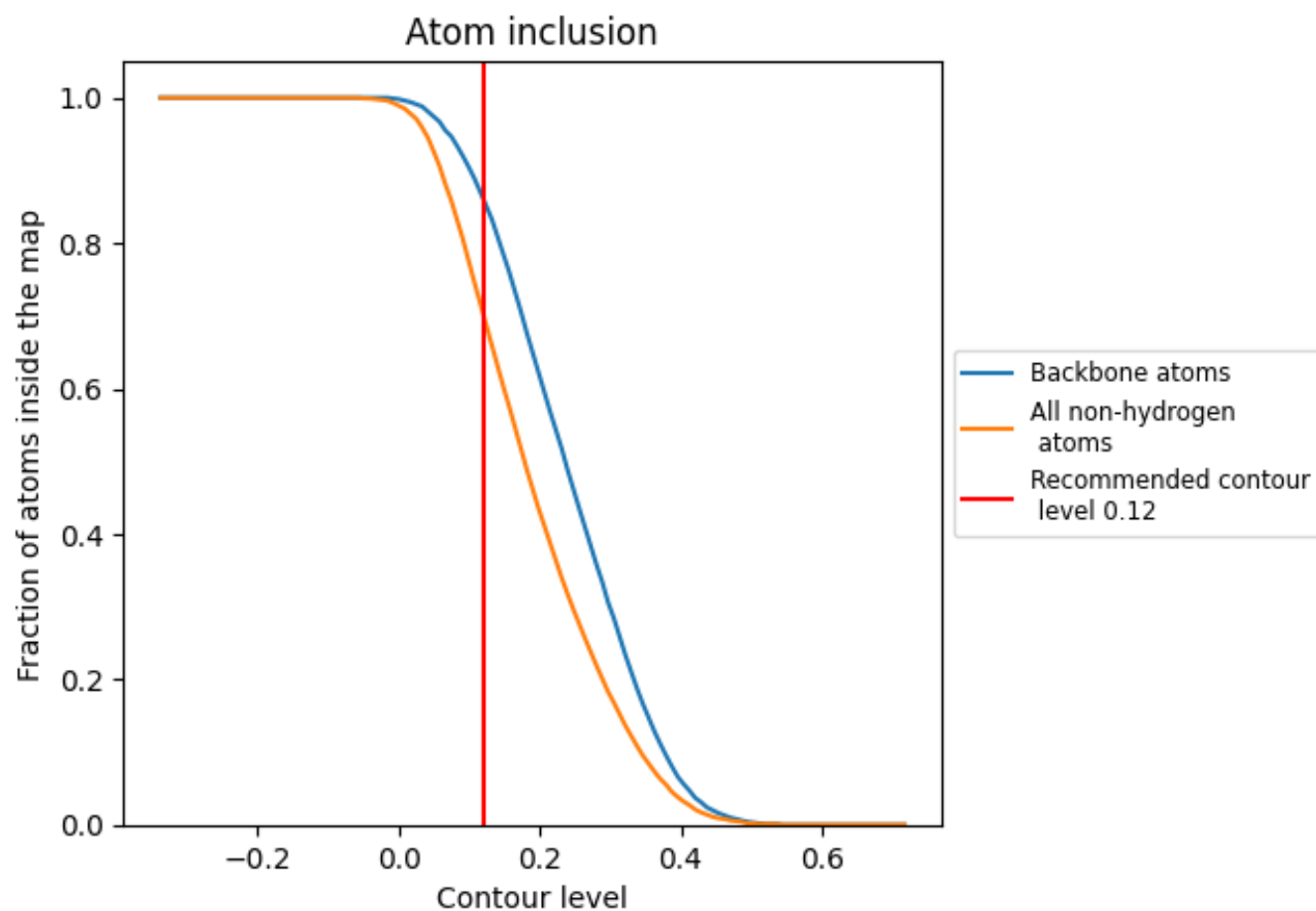
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7030	<div></div> 0.3600
A	<div></div> 0.7030	<div></div> 0.3600

