



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:49 PM GMT

PDB ID : 4AKI  
Title : Dynein Motor Domain - LuAc derivative  
Authors : Schmidt, H.; Gleave, E.S.; Carter, A.P.  
Deposited on : 2012-02-22  
Resolution : 3.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

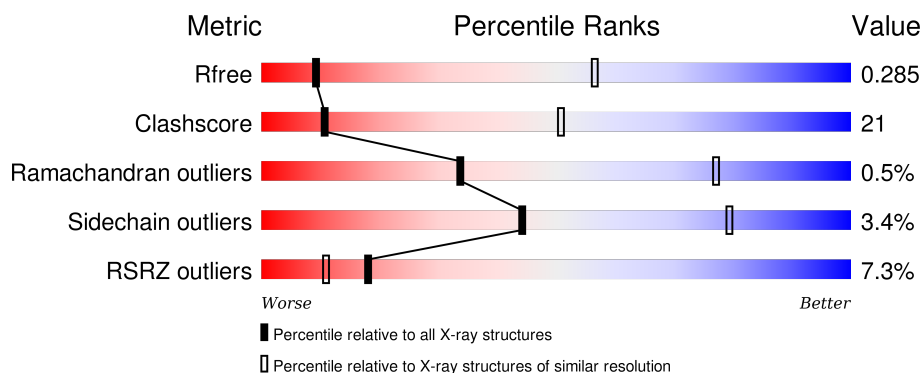
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2695	<div> <div>6%</div> <div>66%</div> <div>30%</div> <div>..</div> </div>
1	B	2695	<div> <div>8%</div> <div>68%</div> <div>29%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	5094	-	-	X	-
3	SO4	A	5095	-	-	X	X
3	SO4	A	5096	-	-	X	-
3	SO4	B	5095	-	-	X	-
4	MG	A	5097	-	-	-	X



In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

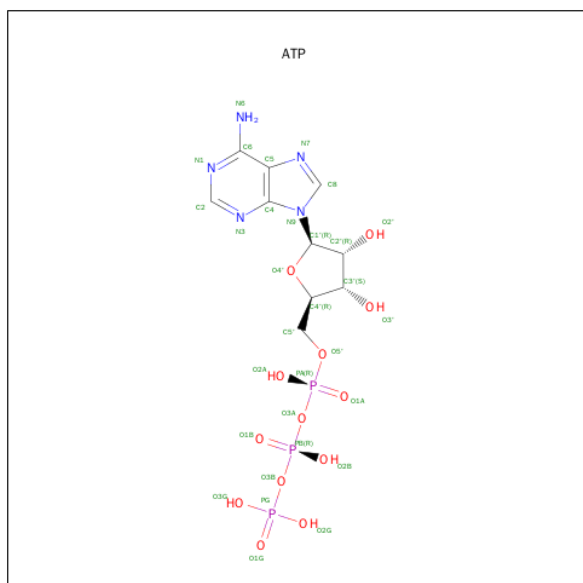
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2650	Total 20748	C 13268	N 3472	O 3915	S 93	0	0	0
1	B	2650	Total 20748	C 13268	N 3472	O 3915	S 93	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1630	ILE	LEU	CONFLICT	UNP P36022
A	3782	ASP	GLU	CONFLICT	UNP P36022
B	1630	ILE	LEU	CONFLICT	UNP P36022
B	3782	ASP	GLU	CONFLICT	UNP P36022

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$ ).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

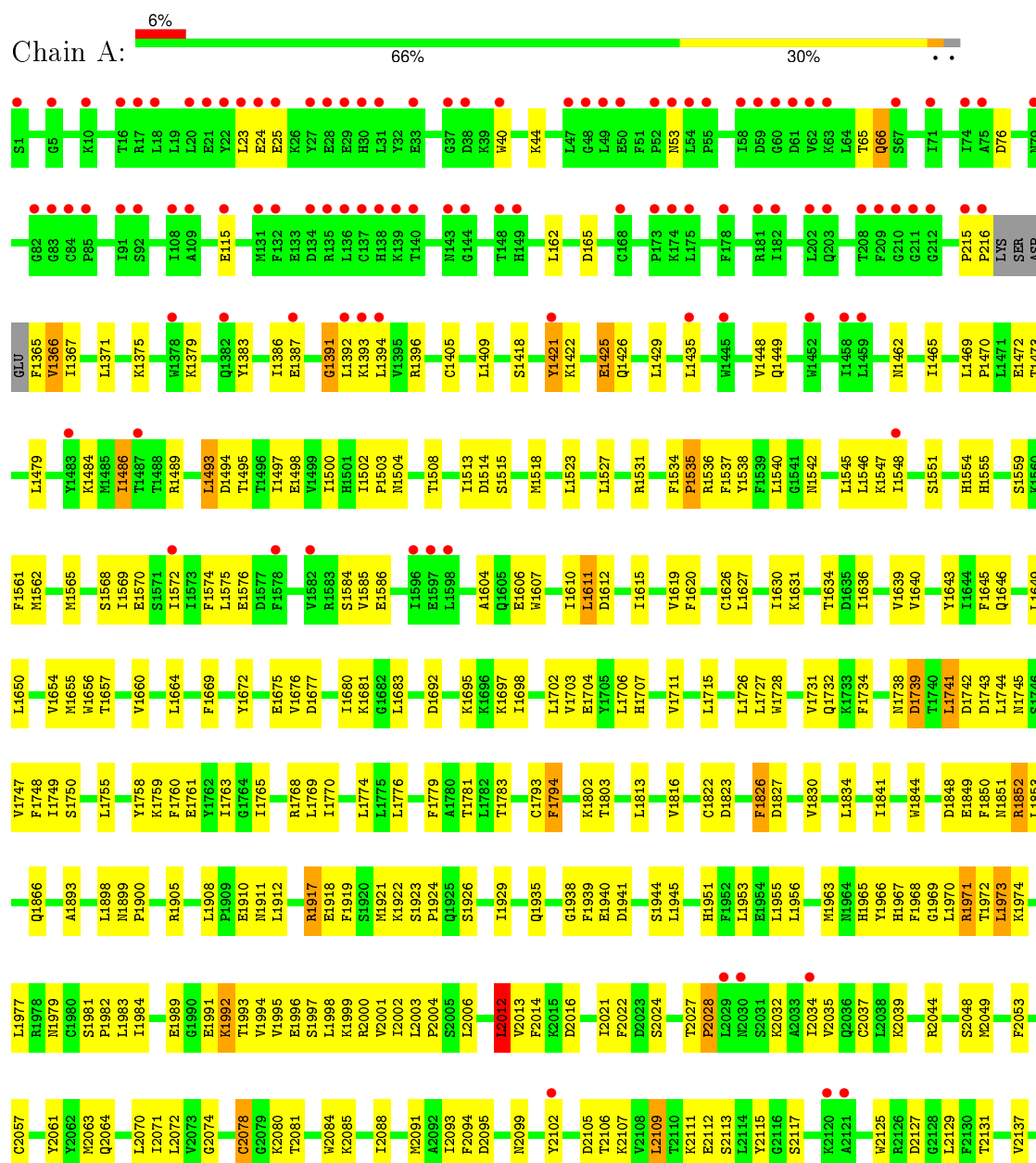
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC

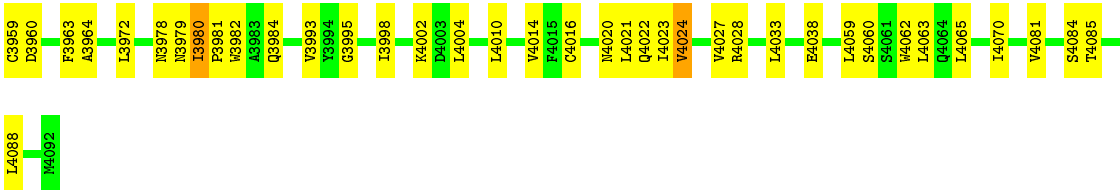


G3877	G3878	L3884	P3885	A3886	P3887	L3888	L3889	Q3890	R3894	F3895	E3898	D3899	T3906	V3911	G3912	F3915	F3916	T3917	K3919	V3923	K3924	S3925	V3927	W3934	F3935	T3939	T3943	L3945	V3946	P3947	H3948	G3949	S3951	Y3955	D3960	F3963	A3964	Y3967	N3978																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
F3786	I3787	R3792	K3799	L3803	S3807	K3808	K3809	S3810	L3811	L3816	G3817	S3818	L3819	N3821	L3822	N3823	V3824	A3825	S3832	G3833	G3836	G3837	S3838	I3839	Q3845	K3846	S3847	L3848	S3849	W3850	K3851	T3852	L3853	V3854	H3858	F3859	T3862	A3865	E3869	K3870	A3964	K3872	K3873	N3875																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
S3687	L3690	D3691	K3692	K3693	F3694	K3695	L3696	K3697	K3698	L3601	F3607	D3612	N3613	L3614	V3615	Y3618	G3622	S3628	M3631	F3641	S3645	L3646	V3656	F3657	L3658	L3659	S3662	S3663	K3664	L3665	L3666	L3667	E3668	L3669	N3671	V3674	V3777	K3778	A3779	N3780	N3784	Y3785																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
E3582	L3583	M3584	L3587	K3588	L3589	K3591	K3592	E3593	A3594	M3595	F3518	V3519	T3520	N3521	L3524	E3525	F3530	D3531	L3534	E3537	N3538	M3541	L3542	K3543	K3544	D3547	L3548	L3549	K3550	Y3555	K3556	N3561	L3562	E3563	K3564	L3565	L3566	L3567	E3568	F3569	N3571	N3572	S3573	M3577	L3578	E3579	N3580	D3581																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
E3022	F3023	L3024	N3025	V3028	L3029	L3030	V3031	L3032	L3033	L3034	L3035	L3036	L3037	L3038	L3039	L3040	F3406	L3407	L3408	D3409	R3413	M3414	L3415	T3416	V3417	L3418	L3419	R3439	L3440	F3446	Q3453	D3459	P3460	L3461	L3462	S3463	L3464	L3465	L3466	S3467	F3470	A3473	G3474	N3475	R3476	L3481	G3482																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
T2881	T2890	L2891	C2892	W2902	L2903	L2908	C2911	C2912	W2916	N2917	W2920	M2938	T2941	D2942	I2943	S2948	L2949	V2950	L2951	L2952	L2953	L2954	L2955	L2956	L2957	L2958	L2959	L2960	L2961	D2962	L2963	V2982	G2983	W2984	N2985	R2986	L2987	S2988	P2989	G2990	L3010	F3016	V3017	N3018	L3021																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
L2786	R2787	R2788	F2795	L2799	L2808	R2812	T2813	L2816	L2817	L2818	E2819	S2820	N2821	L2822	L2828	E2829	N2832	T2833	L2834	L2835	L2836	L2837	L2838	L2839	L2840	L2841	L2842	L2843	L2844	Q2845	G2846	Y2849	L2852	L2853	L2856	T2860	R2861	L2865	L2866	L2867	D2868	E2872	L2873	V2874	D2875	V2878																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
S2643	L2644	L2645	R2646	L2647	R2654	D2658	V2661	V2677	L2686	G2687	S2691	L2694	L2694	L2694	L2697	L2698	L2699	L2700	L2701	L2702	L2703	L2704	L2705	L2706	L2707	L2708	L2709	L2710	L2711	L2712	L2713	L2714	L2715	L2716	L2717	L2718	L2719	L2720	L2721	L2722	L2723	L2724	L2725	L2726	L2727	L2728	L2729	L2730	L2731	L2732	L2733	L2734	L2735	L2736	L2737	L2738	L2739	L2740	L2741	L2742	L2743	L2744	L2745	L2746	L2747	L2748	L2749	L2750	L2751	L2752	L2753	L2754	L2755	L2756	L2757	L2758	L2759	L2760	L2761	L2762	L2763	L2764	L2765	L2766	L2767	L2768	L2769	L2770	L2771	L2772	L2773	L2774	L2775	L2776	L2777	L2778	L2779	L2780	L2781	L2782	L2783	L2784	L2785	L2786	L2787	L2788	L2789	L2790	L2791	L2792	L2793	L2794	L2795	L2796	L2797	L2798	L2799	L2800	L2801	L2802	L2803	L2804	L2805	L2806	L2807	L2808	L2809	L2810	L2811	L2812	L2813	L2814	L2815	L2816	L2817	L2818	L2819	L2820	L2821	L2822	L2823	L2824	L2825	L2826	L2827	L2828	L2829	L2830	L2831	L2832	L2833	L2834	L2835	L2836	L2837	L2838	L2839	L2840	L2841	L2842	L2843	L2844	L2845	L2846	L2847	L2848	L2849	L2850	L2851	L2852	L2853	L2854	L2855	L2856	L2857	L2858	L2859	L2860	L2861	L2862	L2863	L2864	L2865	L2866	L2867	L2868	L2869	L2870	L2871	L2872	L2873	L2874	L2875	L2876	L2877	L2878	L2879	L2880	L2881	L2882	L2883	L2884	L2885	L2886	L2887	L2888	L2889	L2890	L2891	L2892	L2893	L2894	L2895	L2896	L2897	L2898	L2899	L2900	L2901	L2902	L2903	L2904	L2905	L2906	L2907	L2908	L2909	L2910	L2911	L2912	L2913	L2914	L2915	L2916	L2917	L2918	L2919	L2920	L2921	L2922	L2923	L2924	L2925	L2926	L2927	L2928	L2929	L2930	L2931	L2932	L2933	L2934	L2935	L2936	L2937	L2938	L2939	L2940	L2941	L2942	L2943	L2944	L2945	L2946	L2947	L2948	L2949	L2950	L2951	L2952	L2953	L2954	L2955	L2956	L2957	L2958	L2959	L2960	L2961	L2962	L2963	L2964	L2965	L2966	L2967	L2968	L2969	L2970	L2971	L2972	L2973	L2974	L2975	L2976	L2977	L2978	L2979	L2980	L2981	L2982	L2983	L2984	L2985	L2986	L2987	L2988	L2989	L2990	L2991	L2992	L2993	L2994	L2995	L2996	L2997	L2998	L2999	L3000	L3001	L3002	L3003	L3004	L3005	L3006	L3007	L3008	L3009	L3010	L3011	L3012	L3013	L3014	L3015	L3016	L3017	L3018	L3019	L3020	L3021	L3022	L3023	L3024	L3025	L3026	L3027	L3028	L3029	L3030	L3031	L3032	L3033	L3034	L3035	L3036	L3037	L3038	L3039	L3040	L3041	L3042	L3043	L3044	L3045	L3046	L3047	L3048	L3049	L3050	L3051	L3052	L3053	L3054	L3055	L3056	L3057	L3058	L3059	L3060	L3061	L3062	L3063	L3064	L3065	L3066	L3067	L3068	L3069	L3070	L3071	L3072	L3073	L3074	L3075	L3076	L3077	L3078	L3079	L3080	L3081	L3082	L3083	L3084	L3085	L3086	L3087	L3088	L3089	L3090	L3091	L3092	L3093	L3094	L3095	L3096	L3097	L3098	L3099	L3100	L3101	L3102	L3103	L3104	L3105	L3106	L3107	L3108	L3109	L3110	L3111	L3112	L3113	L3114	L3115	L3116	L3117	L3118	L3119	L3120	L3121	L3122	L3123	L3124	L3125	L3126	L3127	L3128	L3129	L3130	L3131	L3132	L3133	L3134	L3135	L3136	L3137	L3138	L3139	L3140	L3141	L3142	L3143	L3144	L3145	L3146	L3147	L3148	L3149	L3150	L3151	L3152	L3153	L3154	L3155	L3156	L3157	L3158	L3159	L3160	L3161	L3162	L3163	L3164	L3165	L3166	L3167	L3168	L3169	L3170	L3171	L3172	L3173	L3174	L3175	L3176	L3177	L3178	L3179	L3180	L3181	L3182	L3183	L3184	L3185	L3186	L3187	L3188	L3189	L3190	L3191	L3192	L3193	L3194	L3195	L3196	L3197	L3198	L3199	L3200	L3201	L3202	L3203	L3204	L3205	L3206	L3207	L3208	L3209	L3210	L3211	L3212	L3213	L3214	L3215	L3216	L3217	L3218	L3219	L3220	L3221	L3222	L3223	L3224	L3225	L3226	L3227	L3228	L3229	L3230	L3231	L3232	L3233	L3234	L3235	L3236	L3237	L3238	L3239	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259	L3260	L3261	L3262	L3263	L3264	L3265	L3266	L3267	L3268	L3269	L3270	L3271	L3272	L3273	L3274	L3275	L3276	L3277	L3278	L3279	L3280	L3281	L3282	L3283	L3284	L3285	L3286	L3287	L3288	L3289	L3290	L3291	L3292	L3293	L3294	L3295	L3296	L3297	L3298	L3299	L3300	L3301	L3302	L3303	L3304	L3305	L3306	L3307	L3308	L3309	L3310	L3311	L3312	L3313	L3314	L3315	L3316	L3317	L3318	L3319	L3320	L3321	L3322	L3323	L3324	L3325	L3326	L3327	L3328	L3329	L3330	L3331	L3332	L3333	L3334	L3335	L3336	L3337	L3338	L3339	L3340	L3341	L3342	L3343	L3344	L3345	L3346	L3347	L3348	L3349	L3350	L3351	L3352	L3353	L3354	L3355	L3356	L3357	L3358	L3359	L3360	L3361	L3362	L3363	L3364	L3365	L3366	L3367	L3368	L3369	L3370	L3371	L3372	L3373	L3374	L3375	L3376	L3377	L3378	L3379	L3380	L3381	L3382	L3383	L3384	L3385	L3386	L3387	L3388	L3389	L3390	L3391	L3392	L3393	L3394	L3395	L3396	L3397	L3398	L3399	L3400	L3401	L3402	L3403	L3404	L3405	L3406	L3407	L3408	L3409	L3410	L3411	L3412	L3413	L3414	L3415	L3416	L3417	L3418	L3419	L3420	L3421	L3422	L3423	L3424	L3425	L3426	L3427	L3428	L3429	L3430	L3431	L3432	L3433	L3434	L3435	L3436	L3437	L3438	L3439	L3440	L3441	L3442	L3443	L3444	L3445	L3446	L3447	L3448	L3449	L3450	L3451	L3452	L3453	L3454	L3455	L3456	L3457	L3458	L3459	L3460	L3461	L3462	L3463	L3464	L3465	L3466	L3467	L3468	L3469	L3470	L3471	L3472	L3473	L3474	L3475	L3476	L3477	L3478	L3479	L3480	L3481	L3482	L3483	L3484	L3485	L3486	L3487	L3488	L3489	L3490	L3491	L3492	L3493	L3494	L3495	L3496	L3497	L3498	L3499	L3500	L3501	L3502	L3503	L3504	L3505	L3506	L3507	L3508	L3509	L3510	L3511	L3512	L3513	L3514	L3515	L3516	L3517	L3518	L3519	L3520	L3521	L3522	L3523	L3524	L3525	L3526	L3527	L3528	L3529	L3530	L3531	L3532	L3533	L3534	L3535	L3536	L3537	L3538	L3539	L3540	L3541	L3542	L3543	L3544	L3545	L3546	L3547	L3548	L3549	L3550	L3551	L3552	L3553	L3554	L3555	L3556	L3557	L3558	L3559	L3560	L3561	L3562	L3563	L3564	L3565	L3566	L3567	L3568	L3569	L3570	L3571	L3572	L3573	L3574	L3575	L3576	L3577	L3578	L3579	L3580	L3581	L3582	L3583	L3584	L3585	L3586	L3587	L3588	L3589	L3590	L3591	L3592	L3593	L3594	L3595	L3596	L3597	L3598	L3599	L3600	L3601	L3602	L3603	L3604	L3605	L3606	L3607	L3608	L3609	L3610	L3611	L3612	L3613	L3614	L3615	L3616	L3617	L3618	L3619	L3620	L3621	L3622	L3623	L3624	L3625	L3626	L3627	L3628	L3629	L3630	L3631	L3632	L3633	L3634	L3635	L3636	L3637	L3638	L3639	L3640	L3641	L3642	L3643	L3644	L3645	L3646	L3647	L3648	L3649	L3650	L3651	L3652	L3653	L3654	L3655	L3656	L3657	L3658	L3659	L3660	L3661	L3662	L3663	L3664	L3665	L3666	L3667	L3668	L3669	L3670	L3671	L3672	L3673	L3674	L3675	L3676	L3677	L3678	L3679	L3680	L3681	L3682	L3683	L3684	L3685	L3686	L3687	L3688	L3689	L3690	L3691	L3692	L3693	L3694	L3695	L3696	L3697	L3698	L3699	L3700	L3701	L3702	L3703	L3704	L3705	L3706	L3707	L3708	L3709	L3710	L3711	L3712	L3713	L3714	L3715	L3716	L3717	L3718	L3719	L3720</









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	175.77Å 118.19Å 202.68Å 90.00° 90.91° 90.00°	Depositor
Resolution (Å)	49.14 – 3.70 49.09 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.14-3.70) 99.9 (49.09-3.70)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.7.0019	Depositor
R, $R_{free}$	0.231 , 0.289 0.226 , 0.285	Depositor DCC
$R_{free}$ test set	4446 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	142.7	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 138.7	EDS
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 88912 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	41590	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, 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	0.58	1/21146 (0.0%)	0.80	12/28618 (0.0%)
1	B	0.47	0/21146	0.68	4/28618 (0.0%)
All	All	0.53	1/42292 (0.0%)	0.74	16/57236 (0.0%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2872	GLU	CG-CD	7.57	1.63	1.51

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1741	LEU	CB-CG-CD1	8.44	125.34	111.00
1	A	1973	LEU	CB-CG-CD1	-7.38	98.45	111.00
1	A	2872	GLU	OE1-CD-OE2	-7.25	114.59	123.30
1	A	2866	LEU	CA-CB-CG	6.12	129.38	115.30
1	A	1769	LEU	CA-CB-CG	6.06	129.24	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1739	ASP	Peptide

## 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	20748	0	20207	891	0
1	B	20748	0	20206	851	0
2	A	31	0	12	4	0
2	B	31	0	12	7	0
3	A	15	0	0	9	0
3	B	15	0	0	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	41590	0	40437	1741	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 21.

The worst 5 of 1741 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:216:PRO:C	1:A:3475:ASN:HB3	1.39	1.40
1:B:1620:PHE:HD1	1:B:1760:PHE:CZ	1.53	1.24
1:A:1620:PHE:HD1	1:A:1760:PHE:CZ	1.58	1.21
1:B:3534:LEU:CD1	1:B:3618:TYR:HE2	1.53	1.21
1:B:1409:LEU:HD21	1:B:1435:LEU:HB3	1.24	1.18

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 X-ray entries followed by that with respect to entries of similar resolution.

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	2640/2695 (98%)	2519 (95%)	107 (4%)	14 (0%)	34	77
1	B	2640/2695 (98%)	2522 (96%)	104 (4%)	14 (0%)	34	77
All	All	5280/5390 (98%)	5041 (96%)	211 (4%)	28 (0%)	34	77

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1391	GLY
1	B	214	HIS
1	B	1366	VAL
1	B	1391	GLY
1	A	1366	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	2218/2453 (90%)	2140 (96%)	78 (4%)	43	78
1	B	2218/2453 (90%)	2144 (97%)	74 (3%)	45	79
All	All	4436/4906 (90%)	4284 (97%)	152 (3%)	44	79

5 of 152 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3884	LEU
1	B	1554	HIS
1	B	3744	LEU
1	A	3917	THR
1	A	4040	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3624	HIS
1	B	1646	GLN
1	B	3780	ASN
1	A	3780	ASN
1	A	4077	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	ATP	A	5093	4	24,33,33	1.10	2 (8%)	31,52,52	2.57	7 (22%)
3	SO4	A	5094	-	4,4,4	0.60	0	6,6,6	0.54	0
3	SO4	A	5095	-	4,4,4	0.78	0	6,6,6	0.80	0
3	SO4	A	5096	-	4,4,4	0.41	0	6,6,6	0.45	0
2	ATP	B	5093	4	24,33,33	1.01	2 (8%)	31,52,52	2.01	5 (16%)
3	SO4	B	5094	-	4,4,4	0.56	0	6,6,6	0.56	0
3	SO4	B	5095	-	4,4,4	0.42	0	6,6,6	0.29	0
3	SO4	B	5096	-	4,4,4	0.23	0	6,6,6	0.20	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	5093	4	-	0/18/38/38	0/3/3/3
3	SO4	A	5094	-	-	0/0/0/0	0/0/0/0
3	SO4	A	5095	-	-	0/0/0/0	0/0/0/0
3	SO4	A	5096	-	-	0/0/0/0	0/0/0/0
2	ATP	B	5093	4	-	0/18/38/38	0/3/3/3
3	SO4	B	5094	-	-	0/0/0/0	0/0/0/0
3	SO4	B	5095	-	-	0/0/0/0	0/0/0/0
3	SO4	B	5096	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5093	ATP	PG-O2G	-2.08	1.47	1.54
2	B	5093	ATP	O4'-C1'	2.31	1.44	1.41
2	A	5093	ATP	C5-C4	2.31	1.45	1.40
2	B	5093	ATP	C5-C4	2.94	1.47	1.40

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5093	ATP	N3-C2-N1	-8.68	122.25	128.89
2	B	5093	ATP	N3-C2-N1	-7.44	123.20	128.89
2	A	5093	ATP	PA-O3A-PB	-5.37	117.66	132.73
2	A	5093	ATP	PB-O3B-PG	-4.21	118.56	132.67
2	B	5093	ATP	PB-O3B-PG	-3.78	119.98	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5093	ATP	4	0
3	A	5094	SO4	4	0
3	A	5095	SO4	3	0
3	A	5096	SO4	2	0
2	B	5093	ATP	7	0

*Continued on next page...*



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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5095	SO4	2	0
3	B	5096	SO4	1	0

## 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 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	2650/2695 (98%)	0.16	160 (6%)	25 15	80, 163, 325, 500	0
1	B	2650/2695 (98%)	0.40	229 (8%)	13 9	117, 210, 355, 500	0
All	All	5300/5390 (98%)	0.28	389 (7%)	18 11	80, 189, 342, 500	0

The worst 5 of 389 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	148	THR	18.5
1	B	35	ASP	17.4
1	B	155	TYR	17.3
1	B	143	ASN	16.6
1	B	67	SER	16.2

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	A	5097	1/1	0.99	0.40	3.20	59,59,59,59	0
3	SO4	A	5095	5/5	0.95	0.40	2.26	108,128,132,133	0
2	ATP	A	5093	31/31	0.95	0.32	1.55	72,125,180,196	0
3	SO4	B	5095	5/5	0.90	0.24	1.14	155,178,186,207	0
3	SO4	A	5094	5/5	0.95	0.29	0.93	109,114,153,161	0
2	ATP	B	5093	31/31	0.93	0.28	0.68	115,184,238,261	0
4	MG	B	5097	1/1	0.98	0.24	0.43	127,127,127,127	0
3	SO4	B	5094	5/5	0.86	0.30	0.27	151,165,190,192	0
3	SO4	A	5096	5/5	0.83	0.22	0.14	128,136,144,154	0
3	SO4	B	5096	5/5	0.96	0.14	-0.53	158,193,224,235	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.