



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:51 AM UTC

PDB ID : 3VKG / pdb_00003vkg
Title : X-ray structure of an MTBD truncation mutant of dynein motor domain
Authors : Kon, T.; Oyama, T.; Shimo-Kon, R.; Suto, K.; Kurisu, G.
Deposited on : 2011-11-16
Resolution : 2.81 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

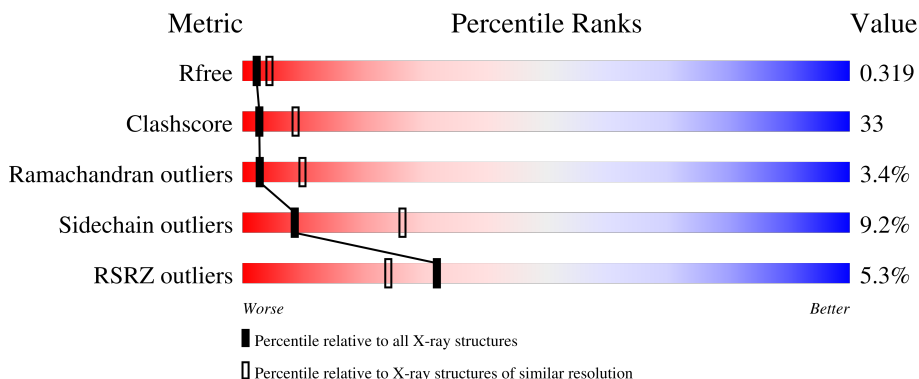
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	3245	
1	B	3245	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 45284 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2954	Total	C	N	O	S	0	0	0
			22821	14585	3870	4270	96			
1	B	2853	Total	C	N	O	S	0	0	0
			22146	14131	3745	4174	96			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1364	MET	-	expression tag	UNP P34036
A	1365	THR	-	expression tag	UNP P34036
A	1366	ARG	-	expression tag	UNP P34036
A	1367	HIS	-	expression tag	UNP P34036
A	1368	HIS	-	expression tag	UNP P34036
A	1369	HIS	-	expression tag	UNP P34036
A	1370	HIS	-	expression tag	UNP P34036
A	1371	HIS	-	expression tag	UNP P34036
A	1372	HIS	-	expression tag	UNP P34036
A	1373	GLY	-	expression tag	UNP P34036
A	1374	GLY	-	expression tag	UNP P34036
A	1375	GLY	-	expression tag	UNP P34036
A	1376	ASP	-	expression tag	UNP P34036
A	1377	TYR	-	expression tag	UNP P34036
A	1378	LYS	-	expression tag	UNP P34036
A	1379	ASP	-	expression tag	UNP P34036
A	1380	ASP	-	expression tag	UNP P34036
A	1381	ASP	-	expression tag	UNP P34036
A	1382	ASP	-	expression tag	UNP P34036
A	1383	LYS	-	expression tag	UNP P34036
A	1384	GLY	-	expression tag	UNP P34036
A	1385	GLY	-	expression tag	UNP P34036
A	1386	GLY	-	expression tag	UNP P34036
A	1387	LYS	-	expression tag	UNP P34036
A	3494	THR	-	linker	UNP P34036

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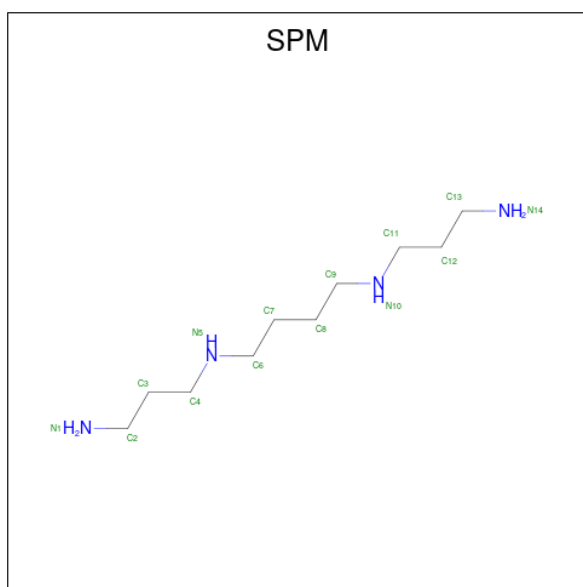
Chain	Residue	Modelled	Actual	Comment	Reference
A	3495	GLY	-	linker	UNP P34036
B	1364	MET	-	expression tag	UNP P34036
B	1365	THR	-	expression tag	UNP P34036
B	1366	ARG	-	expression tag	UNP P34036
B	1367	HIS	-	expression tag	UNP P34036
B	1368	HIS	-	expression tag	UNP P34036
B	1369	HIS	-	expression tag	UNP P34036
B	1370	HIS	-	expression tag	UNP P34036
B	1371	HIS	-	expression tag	UNP P34036
B	1372	HIS	-	expression tag	UNP P34036
B	1373	GLY	-	expression tag	UNP P34036
B	1374	GLY	-	expression tag	UNP P34036
B	1375	GLY	-	expression tag	UNP P34036
B	1376	ASP	-	expression tag	UNP P34036
B	1377	TYR	-	expression tag	UNP P34036
B	1378	LYS	-	expression tag	UNP P34036
B	1379	ASP	-	expression tag	UNP P34036
B	1380	ASP	-	expression tag	UNP P34036
B	1381	ASP	-	expression tag	UNP P34036
B	1382	ASP	-	expression tag	UNP P34036
B	1383	LYS	-	expression tag	UNP P34036
B	1384	GLY	-	expression tag	UNP P34036
B	1385	GLY	-	expression tag	UNP P34036
B	1386	GLY	-	expression tag	UNP P34036
B	1387	LYS	-	expression tag	UNP P34036
B	3494	THR	-	linker	UNP P34036
B	3495	GLY	-	linker	UNP P34036

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			14	10	4		
3	A	1	Total	C	N	0	0
			14	10	4		
3	B	1	Total	C	N	0	0
			14	10	4		
3	B	1	Total	C	N	0	0
			14	10	4		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	2	Total	Mg	0	0
			2	2		

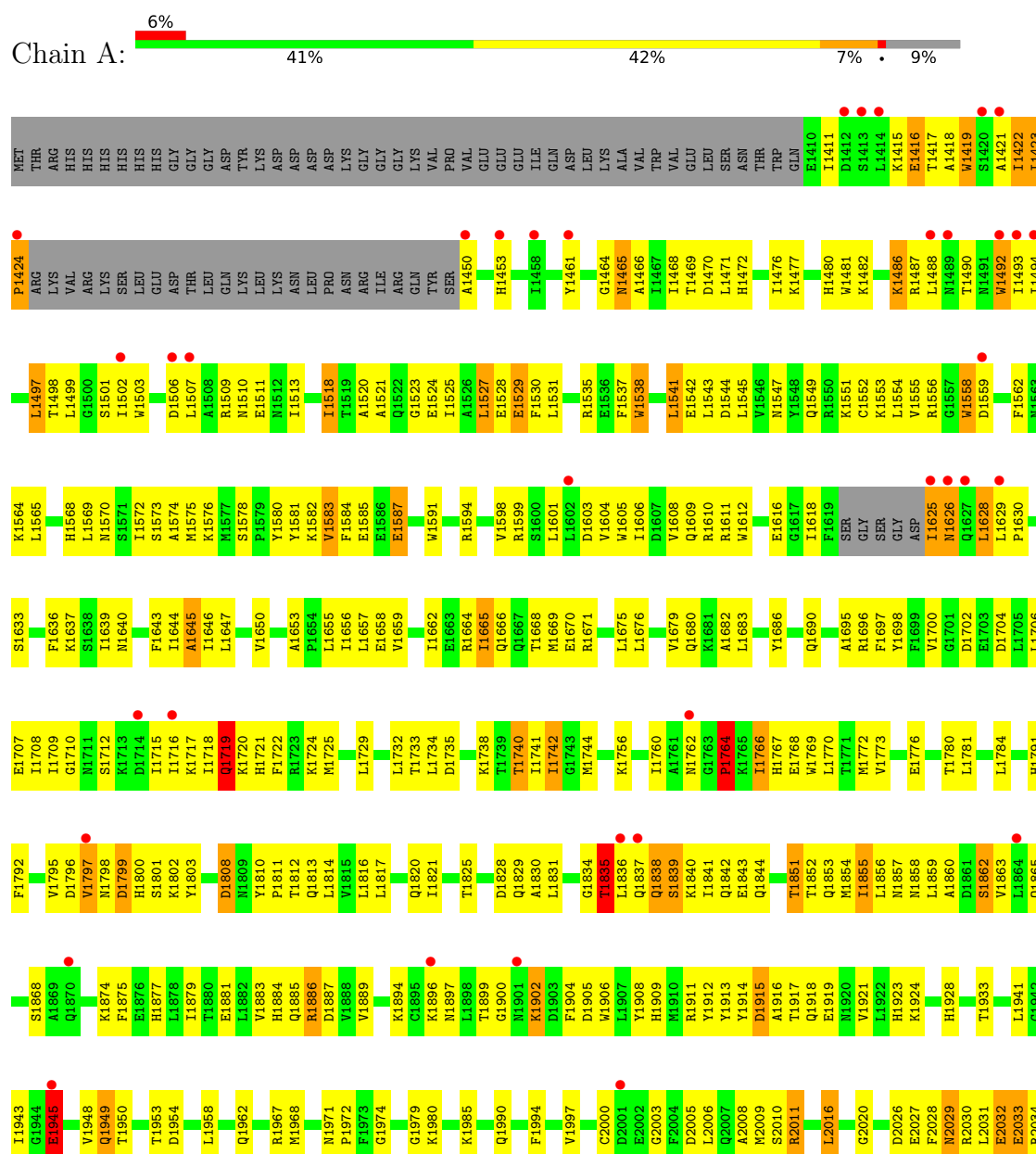
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	23	Total	O	0	0
			23	23		
5	B	19	Total	O	0	0
			19	19		

3 Residue-property plots

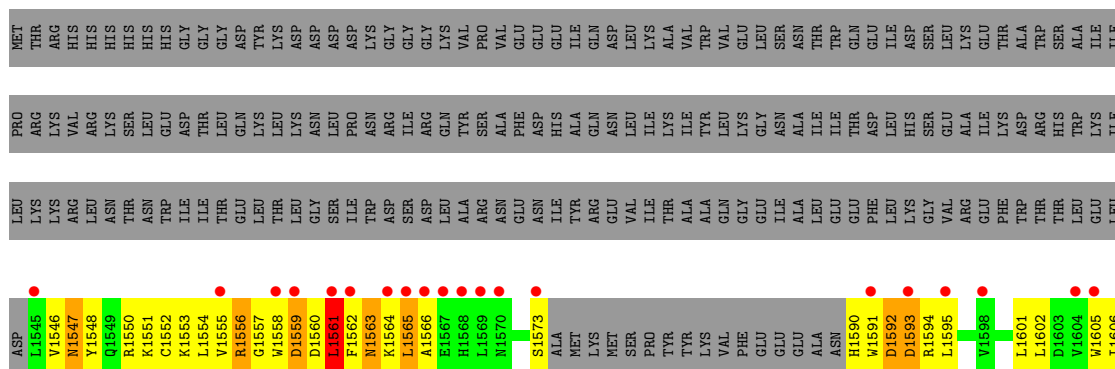
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Dynein heavy chain, cytoplasmic



H2937	F2938	P2939	S2940	N2941	P2942	L2943	D2944	A2945	L2946	R2947	K2948	P2949	L2950	L2951	Y2952	S2953	L2956	L2957	LYS	ASP	TYR	GLN	P2962	R2965	S2966	D2967	L2968	R2969	Y2972	R2975	L2976	K2977	V2978	F2979	Y2980	GLU	GLU	LEU	ASP	VAL	L2988	V2989	L2990	F2991	E2993	V2994	L2995	D2996	H2997	L2998	L2999	R3000																																																																																																																																																																																																																																																																																																																																																																																																																																						
E2637	T2638	H2639	K2640	V2641	S2642	S2643	F2644	L2645	V2646	L2647	L2648	V2651	D2652	T2653	T2654	R2655	H2656	V2657	D2658	L2659	L2660	H2661	H2667	R2668	L2669	L2670	L2671	L2672	C2673	T2756	Q2757	R2758	V2759	I2760	T2761	T2683	L2684	T2687	L2688	R2689	A2690	F2691	P2692	V2696	V2697	S2698	L2699	F2788	V2789	G2790	A2791	C2792	N2793	T2796	F2797	S2798																																																																																																																																																																																																																																																																																																																																																																																																																																		
L2709	L2710	L2711	F2714	H2717	C2718	T2723	P2724	S2725	G2726	E2727	V2728	V2729	L2730	R2731	L2738	V2740	V2741	D2744	E2745	L2746	N2747	P2749	S2750	T2751	T2756	Q2757	R2758	V2759	I2760	T2761	F2762	I2763	V2767	G2771	F2772	W2773	T2779	W2780	L2781	K2782	F2788	V2789	G2790	A2791	C2792	N2793	T2796	H2871	T2872																																																																																																																																																																																																																																																																																																																																																																																																																																									
D2797	A2798	G2799	R2800	L2803	T2804	H2805	R2806	F2807	L2808	R2809	H2810	A2811	P2812	L2813	L2814	L2815	P2819	S2823	S2823	L2827	V2828	G2829	T2830	F2831	R2832	L2833	A2834	L2835	L2836	K2837	H2838	L2839	P2840	R2843	S2844	F2845	D2847	N2848	M2853	E2854	E2855	F2856	E2859	R2863	F2864	L2865	P2866	D2867	A2870	H2871																																																																																																																																																																																																																																																																																																																																																																																																																																								
Y2872	L2873	Y2874	S2875	P2876	E2877	L2878	S2880	R2881	V2882	R2883	A2884	A2885	L2886	L2887	L2888	A2889	L2890	Q2891	M2893	D2894	G2895	L2896	T2897	E2898	V2902	R2903	L2904	W2905	H2907	E2908	L2910	L2911	L2912	F2913	D2914	R2915	L2916	L2917	L2918	E2919	K2923	W2924	W2925	T2926	K2929	V2934	L2935	V2936	L2937	L2938	L2939	K2936																																																																																																																																																																																																																																																																																																																																																																																																																																						
L2936	L2936	S2940	Q2944	T2945	L2946	T2948	A2948	K2951	E2952	N2953	E2956	V2957	L2958	GLY	GLY	LYS	N2964	L2965	S2966	L2967	L2968	L2969	Y2972	R2975	L2976	K2977	V2978	F2979	Y2980	GLU	GLY	LEU	ASP	VAL	L2988	V2989	L2990	F2991	E2993	V2994	L2995	D2996	H2997	L2998	L2999	R3000																																																																																																																																																																																																																																																																																																																																																																																																																																												
L2204	P2205	K2206	L2207	V2208	A2209	D2210	D2211	D2212	P2213	L2214	Q2215	Q2216	L2219	V2222	F2223	G2224	S2226	Q2227	L2228	Q2229	Q2235	L2236	K2239	L2243	R2247	T2251	K2252	E2257	K2258	S2179	K2180	L2186	Y2187	C2188	Q2189	V2190	E2191	I2192	G2271	V2272	M2273	M2274	V2275	G2276	K2282	T2283	T2284	S2285																																																																																																																																																																																																																																																																																																																																																																																																																																										
W2286	E2287	V2288	Y2289	L2290	E2291	A2292	Q2295	Q2296	D2297	V2305	M2306	D2307	P2308	K2309	A2310	T2311	T2312	K2313	D2314	Q2315	L2316	S2319	W2327	T2328	L2331	R2337	R2338	I2339	D2341	N2342	V2343	E2346	R2350	H2351	W2352	I2353	I2354	G2357	D2358	V2359	D2360	P2361	E2362	W2363	V2364	E2365	L2366	N2368																																																																																																																																																																																																																																																																																																																																																																																																																																										
S2369	L2370	L2371	D2372	D2373	V2374	K2375	L2376	L2377	T2378	L2379	P2380	V2381	G2382	E2383	R2384	L2385	A2386	L2387	P2388	R2389	M2526	V2391	R2392	V2393	H2394	F2395	E2396	V2397	Q2398	N2399	L2400	K2401	Y2402	L2403	T2404	L2405	L2406	T2407	L2408	S2409	G2412	W2413	V2414	W2415	F2416	S2417	L2421	T2422	T2423	S2566	N2567	L2426	F2427	Y2430	L2431	D2432																																																																																																																																																																																																																																																																																																																																																																																																																																		
T2433	L2434	S2435	N2436	D2437	E2438	F2439	D2440	P2441	Q2442	E2443	Q2446	Q2447	K2448	R2449	A2453	GLN	LEU	GLN	GLN	GLN	THR	THR	ILE	THR	SER	PRO	ILE	LEU	THR	SER	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR

Q4017	D3935	K3860	S3779	L3719	K3647	K3554	V3360	K3290	ASN	M3147	I3069	I3001
K4018	P3936	E3861	R3750	V3720	H3648	N3555	K3561	K3291	L3216	M3148	C3070	V3004
V4019	N3937	T3862	T3781	Q3721			K3562		M3217	P3149		
L4020	E3938	T3863	T3782	D3722			V3363	T3295	A3218	A3150	D3074	F3005
I4021	R3939	E3864	F3783	V3723	S3651		V3364		I3219	P3151	E3075	Q3007
	L3940	I3865		E3724	E3656		D3365	Q3298	P3220	S3152	S3076	Q3006
V4027	V3943	A3866	V3788	ASN			L3366	V3299	P3221	P3153	N3077	P3008
L4033	Y3942	L3867	T3789	ILE	E3660		GLU	K3300	S3222	F3154	V3078	Q3009
V4034	N3943	K3868	P3790	ASP	N3661		LYS	D3301	H3223	H3155	L3079	
D4035	S3791	V3869	S3791	PRO	ALA		GLU	Q3302	A3226	N3156	E3080	L3013
H4036	I3947	E3870	S3792	VAL	M3664		THR	A3307	V3227	ARG	F3083	L3014
I4037	F3948	T3871		ASN	L3665		PRO	Q3308	V3227	ALA	L3084	I3015
Q4038	T3951	E3873	P3807	PRO	K3666		THR	R3309	Y3228	THR	G3016	G3016
Q4039		T3874	D3808	VAL	K3667		GLY	R3310	Y3233	P3161	E3085	V3017
N4040	V3955	V3875	T3809	LEU	F3668		L3497	R3311	I3234	S3162	R3086	S3018
		K3876	H3810	ASN	S3670		R3498	E3312	T3237	A3163	N3088	G3019
D4043	L3959	K3877		LYS	V3671		E3500		I3238	L3164	T3089	K3022
K4044	L3960	E3878	R3813	GLU	P3672		V3501	V3315	Q3249	R3167	L3090	S3023
K4045	N3961	I3879	S3814	ILE	L3673		E3502	K3316	G3250		L3091	V3024
Q4046		D3815	D3815	ARG	V3674		S3501	R3317	G3251	L3170	E3095	L3025
F4047	L3965	E3880	L3816	LYS	L3675		Q3503	E3318	Q3252	D3171	S3026	R3027
F4048	V3882	L3817	S3586	LYS	D3676		L3504	R3319	N3246	W3172	V3096	R3027
G4049	V3883	K3818	T3587	GLY	F3677		E3505		L3246		P3097	F3028
K4050	A3884	L3819	V3588	GLY	S3678		N3506	A3320	Q3249	E3175	G3098	V3029
D4051	L3885	Q3820		ARG			E3507	N3321	G3250		L3099	A3030
Q4052	Y3886	G3821	V3592	LEU	M3682		A3508	Q3322	G3250			W3031
Q4053	N3887	E3822	V3593	LEU	E3683		N3509		G3251	P3178	F3105	M3032
G4054	F3888	F3823		ILE	F3684		E3510	K3326	Q3252	E3179	T3106	
V3976	V3888	Q3824	S3596	ARG	L3511		L3511	R3327	N3253	A3180	A3107	I3037
K3977	N3889	L3824	A3597	LEU	K3686		K3512	V3328	Y3254	L3181	L3108	Y3038
		K3826	F3598	GLY	N3687		L3513	R3329	V3255	F3182	N3109	T3039
N3881	S3894	L3827		ASP	Q3688		K3514	D3330	T3256	Q3183		L3040
E3982	K3895			GLN	K3689		D3516	Q3332	R3258	V3184	K3113	K3041
I3983	V3896	L3830	Y3601	ASP	A3690		E3517	A3333	H3259	G3185	E3114	ASN
E3987	F3897	E3831	G3603	VAL	F3691		F3518	A3334	Y3260	S3186	T3115	ASN
W3988	A3899	L3834	F3604	PHE	I3694		V3519	E3335	F3263	A3116	Q3117	ASN
D3989	E3901	L3835	F3609	SER	T3695		A3520	I3336	I3264	R3118	R3118	Y3046
F3990	E3902	N3836	R3610	PRO	K3696		T3521	K3337	N3265	N3119	G3120	K3047
L3992		A3837	S3698	F3759	T3697		T3522	Q3338		L3192	L3121	S3048
K3993		L3838		F3760	S3698		T3523		V3268	L3193	L3122	S3049
G3994	I3907	M3761	V3624	M3761	PHE		A3524	A3341	L3269	L3194	I3122	D3050
G3995	L3908	L3762		L3762	LEU		L3525	R3342	L3270	F3051	I3123	F3051
D3996	Q3910	F3763	F3628	F3763	ASP		E3526	Q3345	L3275	N3196	D3124	D3052
F3911	F3911	L3764	K3629	L3764	SER		K3527	V3346	R3276	Q3197	S3125	D3053
S3912	S3912	F3765	S3630	F3765	SER		S3528	Q3347	R3275	Y3199	E3126	D3054
L3913	L3913	T3766	D3631	T3766	F3704		L3632	D3349	D3276	I3200	F3133	L3055
S4000	S4000	R3767	S3633	R3767	K3705		A3530	V3350		A3201		R3056
		D3847	V3634	D3768	K3706		T3531	V3532	E3279	P3202		
I3919	I3919	P3769	V3635	P3769	N3707		V3536	V3536	E3280	P3202	V3137	L3059
		D3848	P3636	T3770	L3708		A3537	R3351	E3281	P3203	R3138	K3060
K4002	K4002	S3851	S3636	S3771	A3711		L3538	K3352	Q3282	V3204	R3139	K3061
E4003	E4003	I3852	F3641	I3852			A3539	K3353	L3283		N3140	A3062
L4005	L4005	T3773	P3642	T3773	F3714		L3539	E3354	H3284	Q3207	L3141	G3063
F4006	F4006	T3774	E2643	T3774	E3642		L3540	L3355	H3285		H3142	G3064
Q4007	Q4007	P3775	E2643	P3775	G3715		I3546	A3356	N3286	I3211	V3143	K3065
		D3776	R3644	D3776	C3716			V3357	I3287	MEI	F3144	E3066
L4011	L4011	L3777	L3645	L3777	P3717			K3358	G3288	GLY	F3145	E3067
F4106	F4106	L3778	N3646	L3778	L3718			K3359	L3289	ASN	T3146	K3068
G4107	G4107											
E4108	E4108											





Q3824	P3677	A3597	Q3332	R3251	F3185	G3102	T3039	R2965	Y2874	R2774	N2700
V3825	E3517	A3598	A3333	Q3252	N3166	E3103	G3042	L2968	S2875	T2775	A2704
L3827	E3518	F3598	A3334	N3253	L3170	F3104	N3043	L2969	R2876	T2781	T2705
R3828	T3523		E3335	Y3254	D3171	F3105	N3044	E2970	P2877	K2782	P2706
L3829	F3528	Y3601	Q3338	V3255	N3172	T3106	N3045	E2971	D2883	L2783	T2707
M3686	I3529	F3602	R3339	T3256	F3173	A3107	Y3046	Y2972	R2884	D2784	
Q3604	F3529	G3603	D3340	R3256	F3174	L3108	K3047	K2973	K2785	K2785	L2711
F3605	K3533	F3604	A3341	H3259	E3175	H3110	K3047	K2974	L2887	L2786	K2712
ASP	E3534	ASP	R3342		Q3183	A3111	S3049	K2975	L2888	F2782	F2713
F3609	E3535	R3610	A3343	I3264	V3184	C3112	S3050	L2976	A2889	F2788	F2714
R3611	E3536	R3611	L3344	V3268	G3185	K3113	F3051	L2890	L2890		D2715
D3612	A3537	D3612	V3346	L3269	S3186	F3114	D3052	K2977	Q2891	A2791	H2716
	T3538		Q3347	L3270	E3187	T3115	D3053	E2982	T2897	E2792	H2717
	L3539		L3348		F3188	A3116	D3054	E2983	L2898	N2793	C2718
	I3540		D3349	R3275	R3189	C3117	L3055	P2794	E2719	E2795	E2719
	K3541		D3350		T3190	ASN	K3056	V2986	L2904	T2796	K2721
	E3542		R3351	L3278	N3191	GLY	L3058	D2997	H2907	D2797	R2722
	T3543		K3352	E3279	L3192	LEU	L3059	L2990	L2907	A2798	T2723
	E3544		N3353	E3280	D3193	ILE	K3060	F2991	E2908	R2799	P2724
	Q3545		E3354	E3281	L3194	LEU	R3061	L2999	A2909	R2800	S2725
	I3546		I3355	Q3282	E3195	ASP	A3062	L2995	L2910	V2801	G2726
	K3547		A3356	L3283		S3125	G3063	D2996	R2911	K2727	E2727
	T3548		V3357		F3205	E3126	C3064	H2997	L2912	H2810	T2728
	E3549		Q3358	Q3288	I3286	E3127	K3065	L2998	F2913	L2811	V2729
	S3550		L3359	L3289	Q2207	E3128	E3066	L2999	R2916	P2812	L2730
			VAL		E3210	E3129	E3067	K3000	R2917	E2731	R2732
	V3553		LVS	R3292		Y3130	K3068	L2995	L2917	S2823	P2732
	K3554		ALA	R3293	N3211	K3131	L3069	K3003	V2918	L2827	Q2734
	N3555		TYR	R3296	GLY	F3132	C3070	V3004	E2921	L2827	Q2734
			ALA	E3296	ASN	F3073		P3008		F2831	L2735
	R3559		ASP	A3297	ASN	T3134	F3073	P3008		F2831	L2735
			LEU	Q3298	ASN	D3074	D3074	Q3009	W2925	L2835	K2737
	L3563		GLU	V3299	LEU	Q3136	E3075	G3010		L2835	W2738
	L3564		LVS			V3137	S3076	H3011	H2937	N2836	L2739
			LVS			R3137	N3077	A3012	P2938	K2837	L2740
	L3567		ALA	L3302		R3138	V3078	L3013	P2939	L2838	
	N3568		GLU			R3139		L3014	S2940	L2839	
	S3569		PRO	Q3308		N3140	L3079	L3014	V2941	P2840	
			THR	K3309		V3143	E3080	V3017	N2942	N2841	E2745
	R3570		GLY	N3310	H3223	F3144		G3018	N2943	L2842	L2746
	R3571		PRO	R3311	R3224	S3018		G3018	L2943	L2842	L2747
			VAL	E3312	D3225	F3145		G3019	L2944	L2843	L2748
	R3572		ARG	E3313	A3226	T3146		E3085	A2945	S2844	P2749
	K3573		GLU	D3314		K3147		K3022	L2946	S2844	S2750
	W3574		GLU	V3315	V3232	N3148		S3023	L2946	F2845	T2751
	E3575		VAL	K3316	Y3233	N3148		S3023	R2947	N2848	T2756
	Q3576		VAL	R3317	R3234	P3149		V3024	R2948	Q2861	Q2757
	Q3577		Q3502	N3318	H3235	T3089		L3025	P2949	R2863	R2758
	S3578		R3503	E3318	H3235	S3151		L2950	L2950	V2863	V2759
	E3579		L3504	Q3319	Q3236	P3152		L2952	L2952	F2864	
	N3580		E3505	A3320	T3237	D3153		F3028	L2952	R2865	L2760
			N3506		T3238			F3029	W2952	F2866	
	Q3584		N3509	L3324	R3157	R3157		G3030	W2955	P2866	T2761
	M3585		E3510	K3325	S3158	S3158		K3031		P2866	
			R3510	Q3326	E3240	C3094		N3032		P2866	
	V3588		L3511	M3327	A3241	PRO		N3033		Q2869	M2766
			K3512	N3242	N3242	GLY		L3035		A2870	V2767
	V3592		L3513	V3328	S3161	LEU		L3035		H2871	E2768
	V3593		L3514	Q3329	P3162	PHE		S3036		V2862	
	I3594		K3514	D3330	L3164			L3037		Y2863	
			Q3515	Q3331	L3164			Y3038		L2873	



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	204.26Å 221.81Å 192.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.45 – 2.81 96.45 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.0 (96.45-2.81) 98.3 (96.45-2.81)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.82Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.262 , 0.319 0.263 , 0.319	Depositor DCC
R_{free} test set	10425 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	45284	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

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, SPM, 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	0.62	1/23297 (0.0%)	1.06	132/31692 (0.4%)
1	B	0.60	2/22599 (0.0%)	1.05	135/30724 (0.4%)
All	All	0.61	3/45896 (0.0%)	1.06	267/62416 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2129	VAL	CA-CB	7.69	1.58	1.54
1	A	3862	THR	CA-CB	5.60	1.60	1.53
1	B	3109	MET	SD-CE	5.24	1.92	1.79

The worst 5 of 267 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2744	ASP	N-CA-C	11.20	123.49	111.28
1	A	4027	VAL	N-CA-C	8.68	116.15	107.55
1	A	2310	ALA	N-CA-C	-8.66	102.15	112.89
1	B	3030	ALA	N-CA-C	-8.44	102.16	111.36
1	B	4436	SER	N-CA-C	-8.43	102.93	113.55

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	22821	0	21998	1468	0
1	B	22146	0	21438	1492	0
2	A	108	0	48	14	0
2	B	108	0	48	9	0
3	A	28	0	52	2	0
3	B	28	0	52	5	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
5	A	23	0	0	1	0
5	B	19	0	0	1	0
All	All	45284	0	43636	2954	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 33.

The worst 5 of 2954 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:3330:ASP:HB3	1:A:3532:TYR:HE2	1.12	1.12
1:A:2902:VAL:HG21	1:A:2941:VAL:HG21	1.31	1.12
1:A:3766:THR:HG22	1:A:3768:ASP:H	1.14	1.09
1:A:2548:VAL:HG11	1:A:2565:GLN:HE21	1.20	1.06
1:B:1655:LEU:H	1:B:1655:LEU:HD22	1.20	1.05

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	2908/3245 (90%)	2474 (85%)	332 (11%)	102 (4%)	3	9
1	B	2813/3245 (87%)	2376 (84%)	347 (12%)	90 (3%)	3	10
All	All	5721/6490 (88%)	4850 (85%)	679 (12%)	192 (3%)	3	10

5 of 192 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1465	ASN
1	A	1583	VAL
1	A	1797	VAL
1	A	1835	THR
1	A	1839	SER

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	2408/2921 (82%)	2199 (91%)	209 (9%)	9	29
1	B	2369/2921 (81%)	2140 (90%)	229 (10%)	8	24
All	All	4777/5842 (82%)	4339 (91%)	438 (9%)	8	26

5 of 438 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1887	ASP
1	B	2670	LEU
1	B	4162	ILE
1	B	1959	THR
1	B	2260	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 224 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4650	ASN
1	B	4651	ASN
1	B	2110	GLN
1	B	4618	ASN
1	B	4025	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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	B	9007	4	28,29,29	1.58	3 (10%)	43,45,45	1.87	11 (25%)
2	ADP	A	9004	-	28,29,29	1.72	6 (21%)	43,45,45	1.85	10 (23%)
2	ADP	B	9008	4	28,29,29	1.85	6 (21%)	43,45,45	1.87	11 (25%)
3	SPM	B	9018	-	13,13,13	0.56	0	12,12,12	0.86	0
2	ADP	B	9010	-	28,29,29	1.71	5 (17%)	43,45,45	1.87	11 (25%)
2	ADP	B	9009	-	28,29,29	1.80	5 (17%)	43,45,45	1.86	11 (25%)
3	SPM	A	9016	-	13,13,13	0.52	0	12,12,12	0.88	0
2	ADP	A	9003	-	28,29,29	1.78	6 (21%)	43,45,45	2.03	13 (30%)
2	ADP	A	9001	-	28,29,29	1.64	5 (17%)	43,45,45	1.88	12 (27%)
2	ADP	A	9002	4	28,29,29	1.73	5 (17%)	43,45,45	1.95	10 (23%)
3	SPM	A	9012	-	13,13,13	0.59	0	12,12,12	0.81	0
3	SPM	B	9022	-	13,13,13	0.40	0	12,12,12	0.95	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	9007	4	-	6/16/32/32	0/3/3/3
2	ADP	A	9004	-	-	3/16/32/32	0/3/3/3
2	ADP	B	9008	4	-	5/16/32/32	0/3/3/3
3	SPM	B	9018	-	-	7/11/11/11	-
2	ADP	B	9010	-	-	6/16/32/32	0/3/3/3
2	ADP	B	9009	-	-	6/16/32/32	0/3/3/3
3	SPM	A	9016	-	-	11/11/11/11	-
2	ADP	A	9003	-	-	5/16/32/32	0/3/3/3
2	ADP	A	9001	-	-	6/16/32/32	0/3/3/3
2	ADP	A	9002	4	-	5/16/32/32	0/3/3/3
3	SPM	A	9012	-	-	5/11/11/11	-
3	SPM	B	9022	-	-	7/11/11/11	-

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9009	ADP	C5-C4	5.65	1.49	1.39
2	B	9008	ADP	C5-C4	5.40	1.48	1.39
2	A	9004	ADP	C5-C4	5.30	1.48	1.39
2	A	9001	ADP	C5-C4	5.20	1.48	1.39
2	A	9003	ADP	C5-C4	5.18	1.48	1.39

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9002	ADP	C5-C4-N3	-5.96	118.52	126.72
2	A	9003	ADP	C5-C4-N3	-5.79	118.74	126.72
2	B	9009	ADP	C5-C4-N3	-5.55	119.07	126.72
2	B	9008	ADP	C5-C4-N3	-5.38	119.30	126.72
2	A	9004	ADP	C5-C4-N3	-5.26	119.47	126.72

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	9001	ADP	C5'-O5'-PA-O1A
2	A	9001	ADP	C5'-O5'-PA-O2A
2	A	9001	ADP	C5'-O5'-PA-O3A

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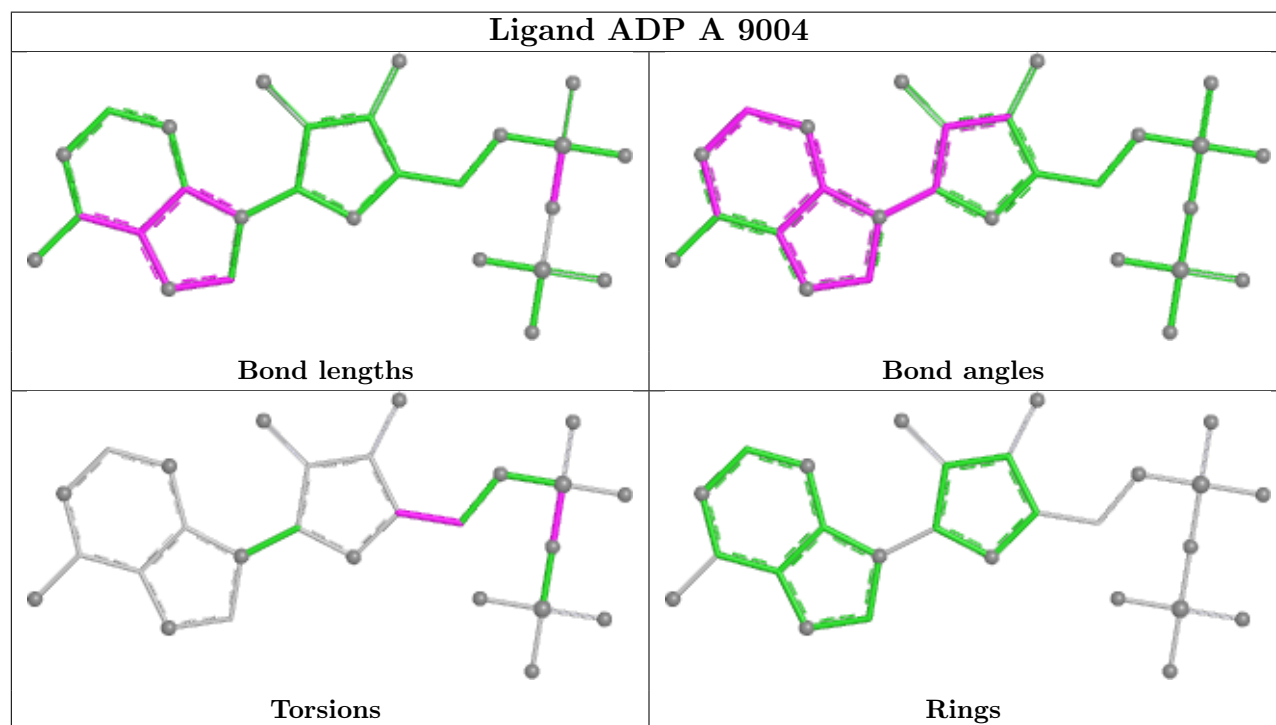
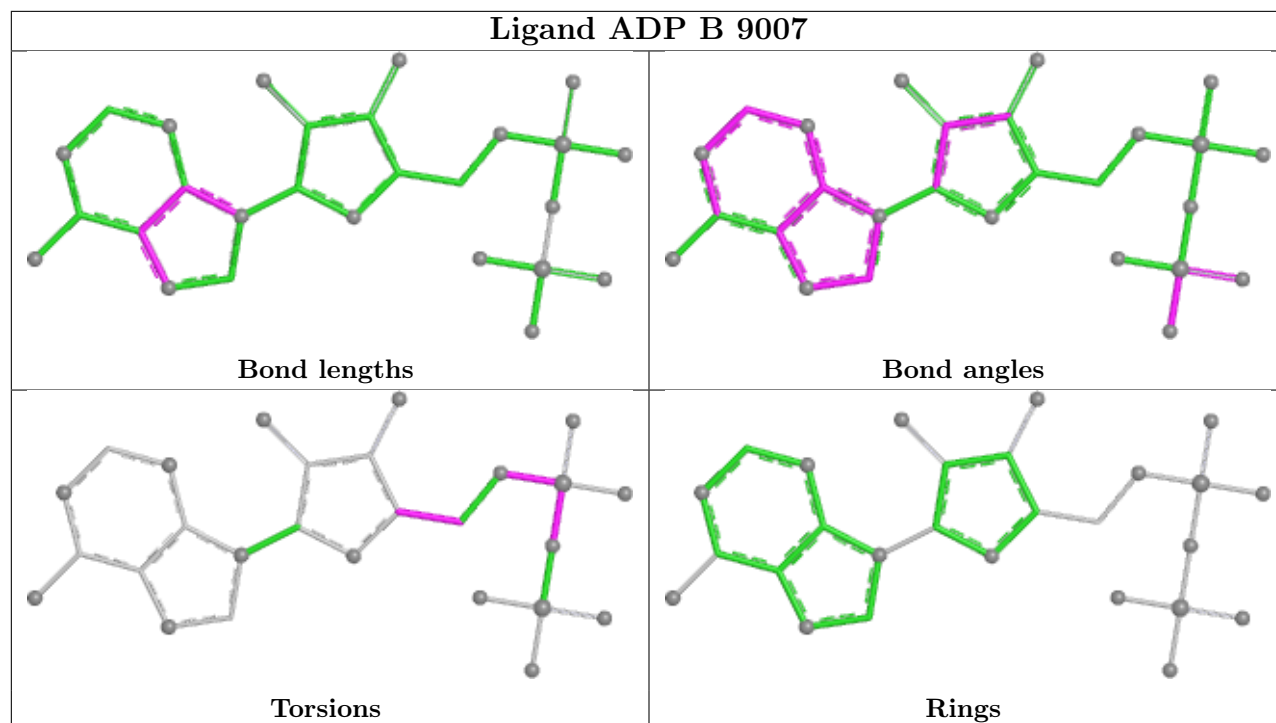
Mol	Chain	Res	Type	Atoms
2	A	9002	ADP	C5'-O5'-PA-O3A
2	A	9003	ADP	C5'-O5'-PA-O1A

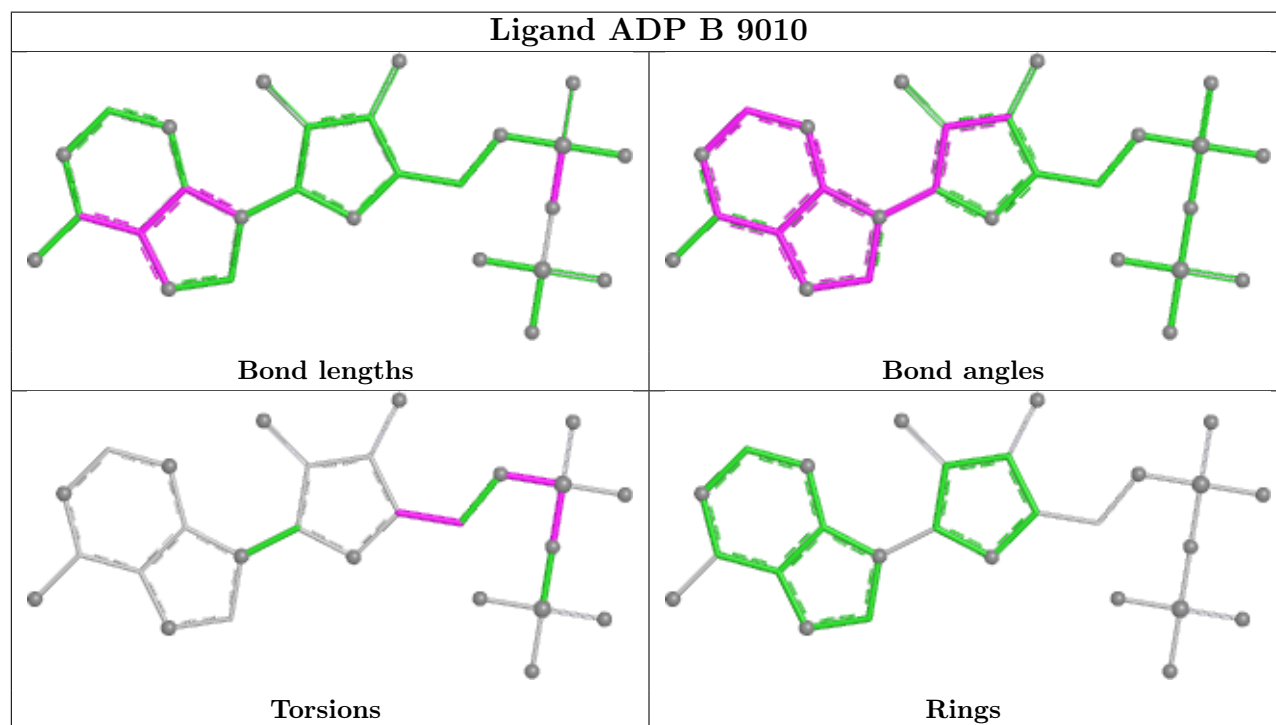
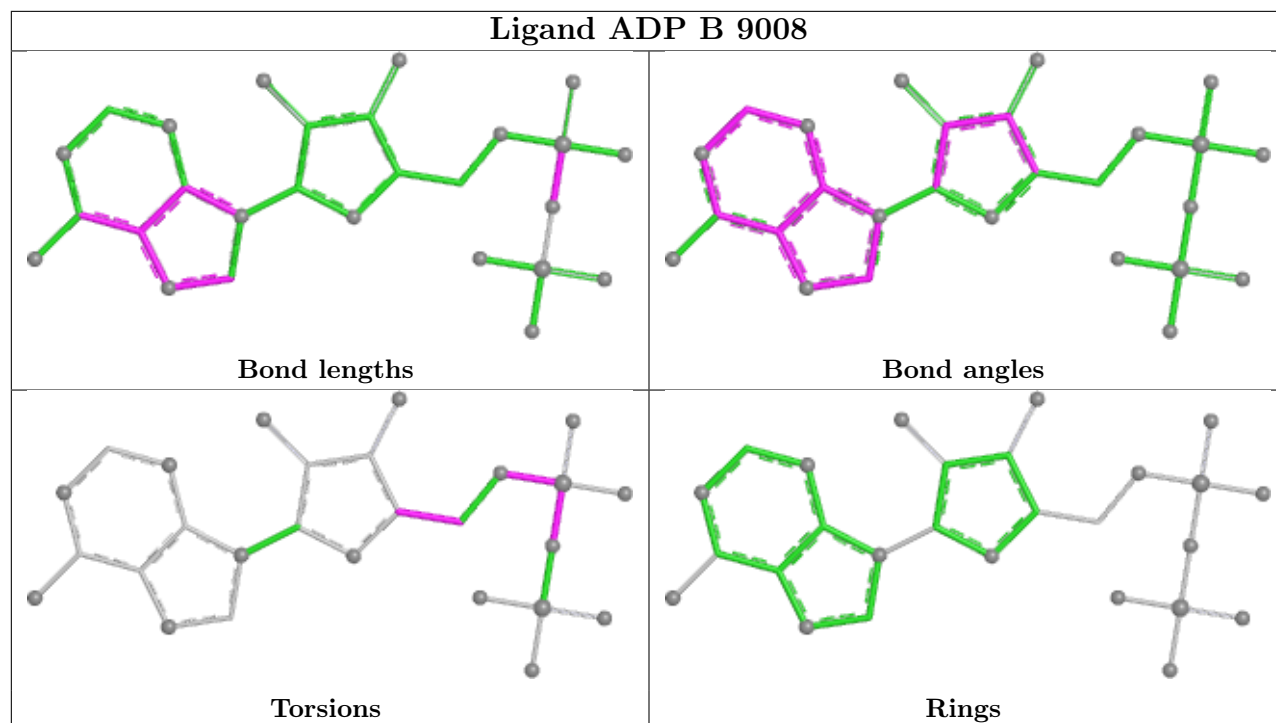
There are no ring outliers.

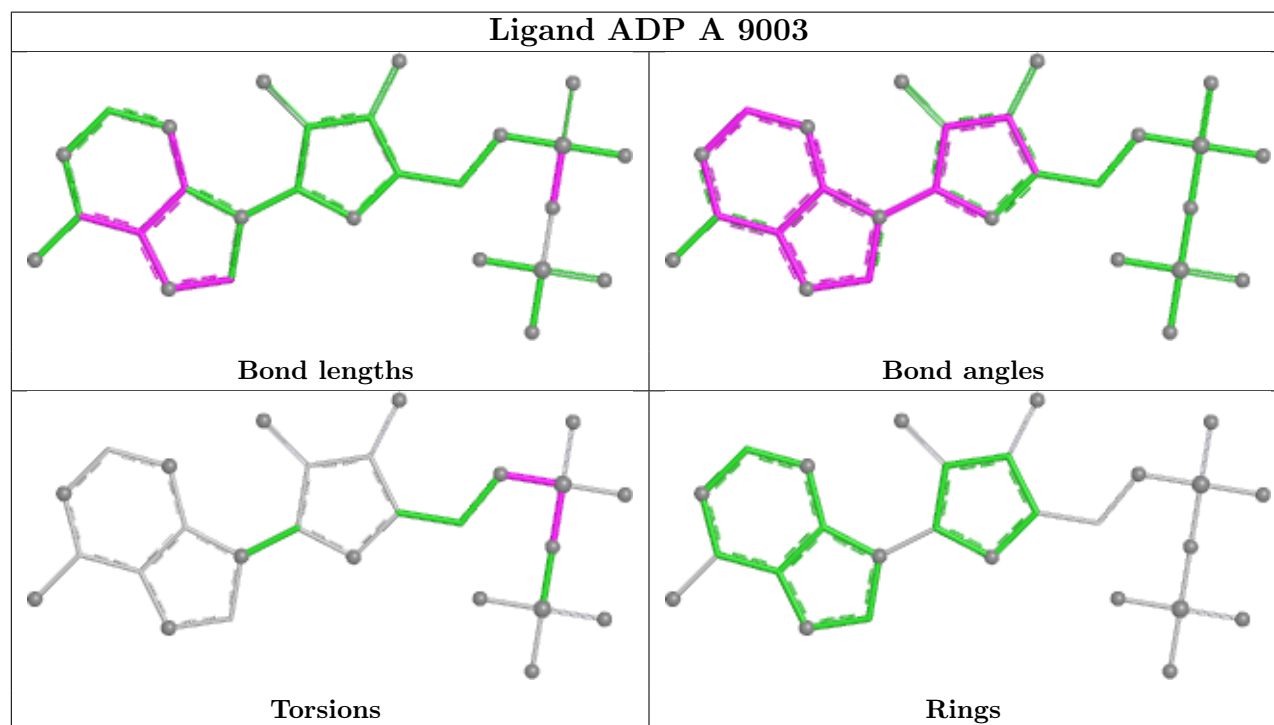
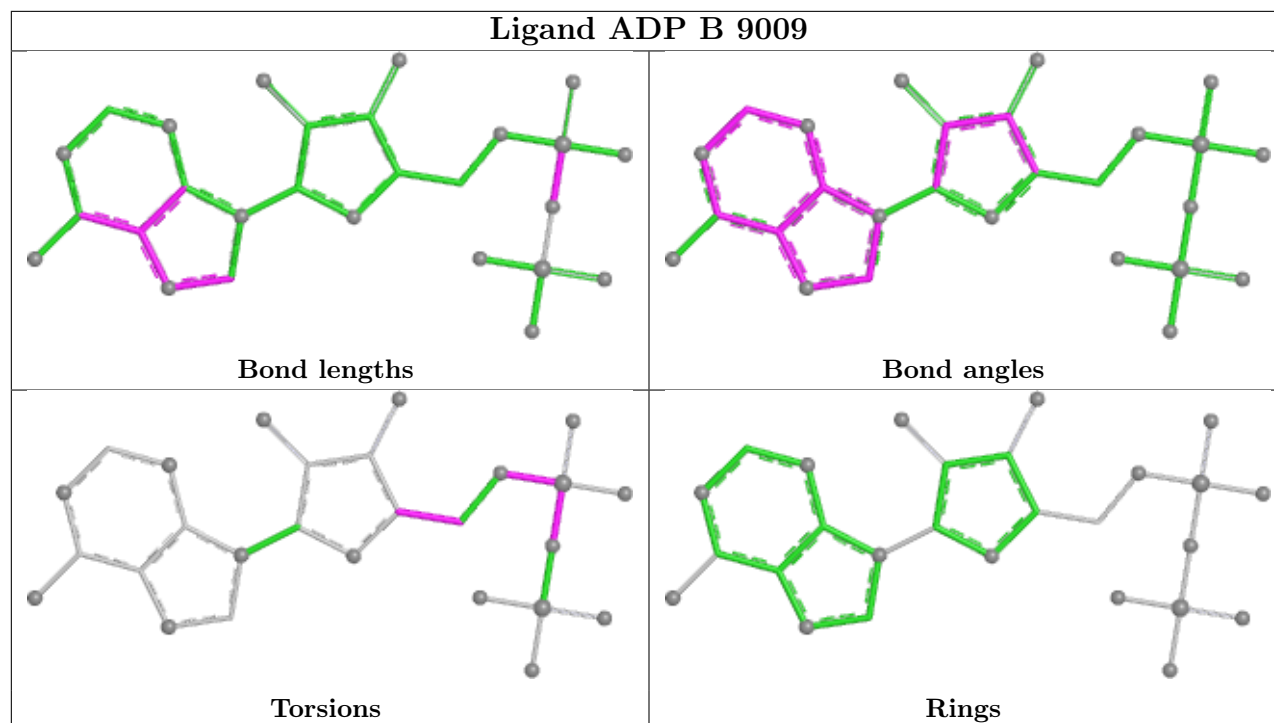
12 monomers are involved in 30 short contacts:

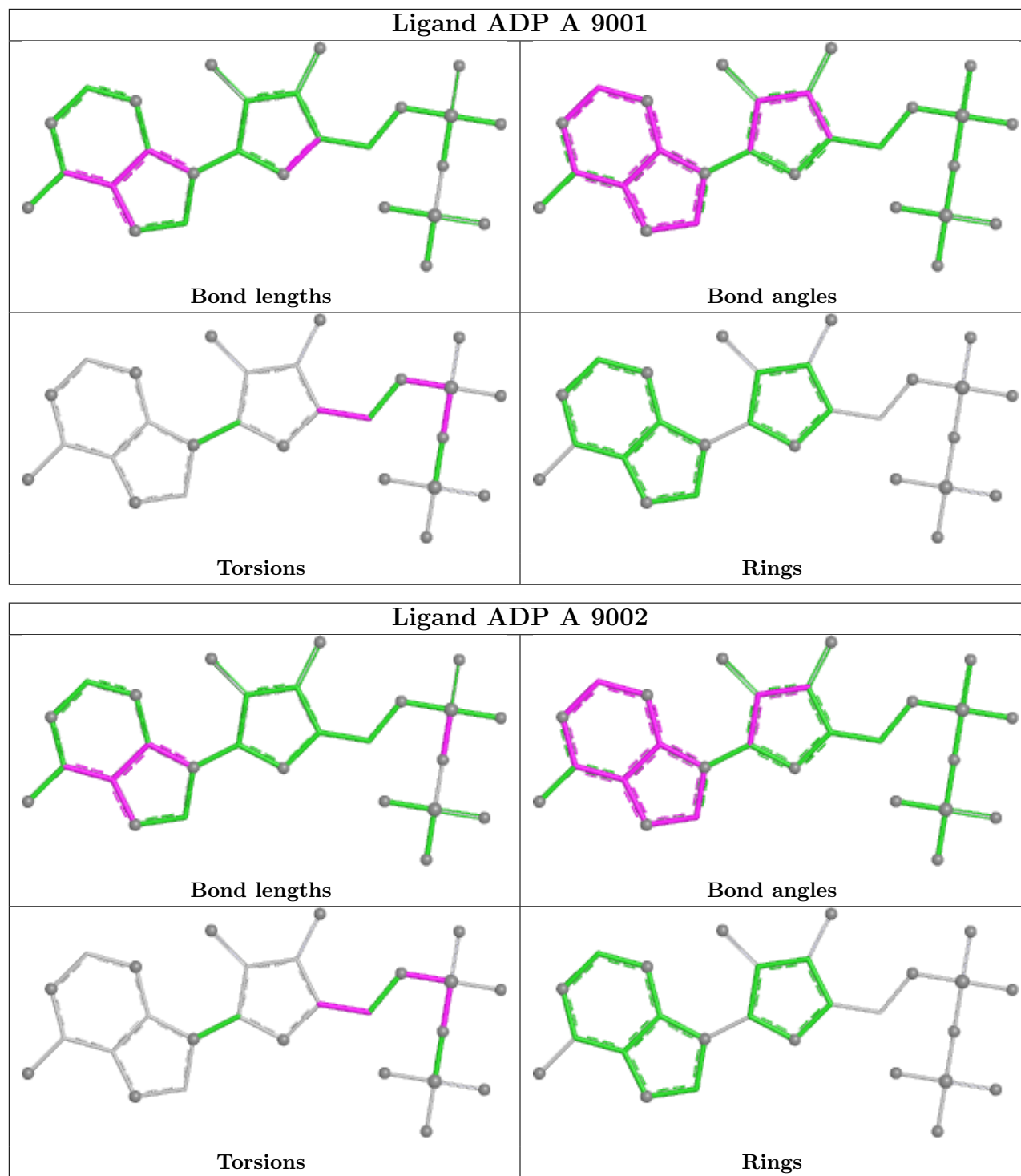
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	9007	ADP	2	0
2	A	9004	ADP	6	0
2	B	9008	ADP	2	0
3	B	9018	SPM	2	0
2	B	9010	ADP	3	0
2	B	9009	ADP	2	0
3	A	9016	SPM	1	0
2	A	9003	ADP	4	0
2	A	9001	ADP	1	0
2	A	9002	ADP	3	0
3	A	9012	SPM	1	0
3	B	9022	SPM	3	0

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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	2954/3245 (91%)	0.50	187 (6%) 26 19	17, 53, 78, 102	0
1	B	2853/3245 (87%)	0.39	121 (4%) 40 32	24, 52, 75, 100	0
All	All	5807/6490 (89%)	0.44	308 (5%) 32 24	17, 52, 77, 102	0

The worst 5 of 308 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4677	PRO	5.9
1	B	3108	LEU	4.8
1	B	4456	SER	4.8
1	A	4613	GLY	4.7
1	B	2323	THR	4.6

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

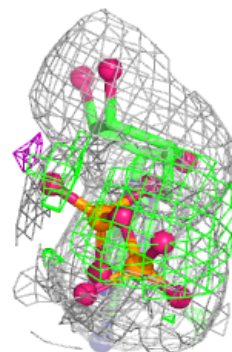
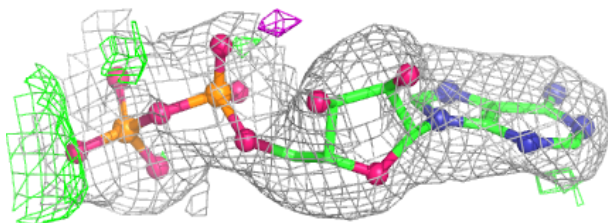
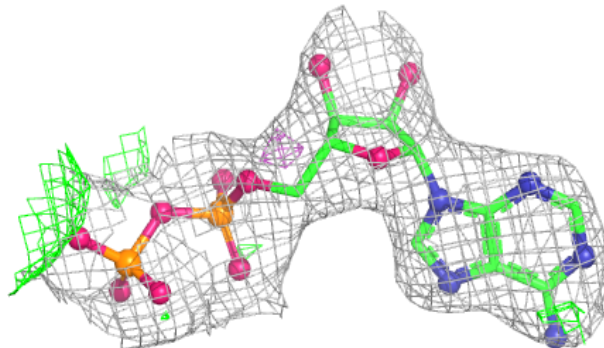
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	B	2	1/1	0.85	0.13	50,50,50,50	0
3	SPM	A	9016	14/14	0.86	0.17	43,50,54,55	0
3	SPM	B	9018	14/14	0.88	0.15	57,57,59,59	0
2	ADP	B	9008	27/27	0.89	0.13	41,51,53,54	0
3	SPM	A	9012	14/14	0.90	0.14	37,41,45,47	0
2	ADP	A	9002	27/27	0.90	0.12	47,49,52,54	0
3	SPM	B	9022	14/14	0.91	0.13	37,43,49,49	0
2	ADP	A	9003	27/27	0.91	0.11	41,45,50,52	0
2	ADP	A	9004	27/27	0.92	0.09	44,49,54,56	0
4	MG	B	3	1/1	0.92	0.15	28,28,28,28	0
2	ADP	B	9007	27/27	0.94	0.11	38,47,50,52	0
2	ADP	A	9001	27/27	0.94	0.11	32,38,42,44	0
2	ADP	B	9009	27/27	0.95	0.09	39,45,48,51	0
2	ADP	B	9010	27/27	0.95	0.09	31,37,46,48	0
4	MG	A	1	1/1	0.98	0.11	44,44,44,44	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

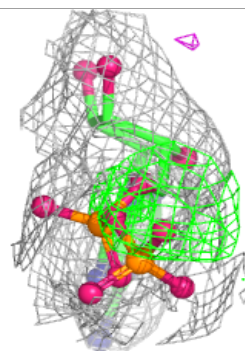
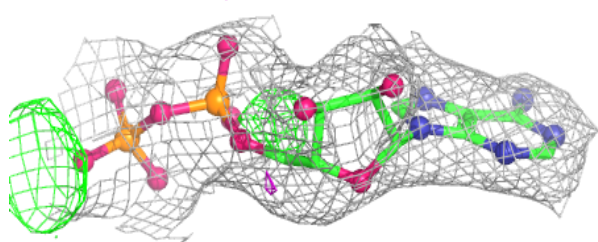
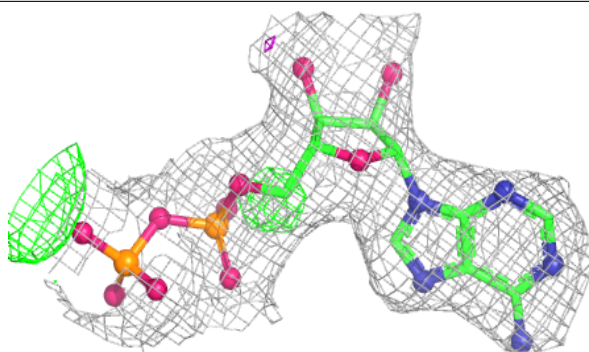
Electron density around ADP B 9008:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

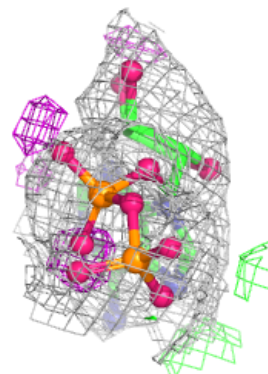
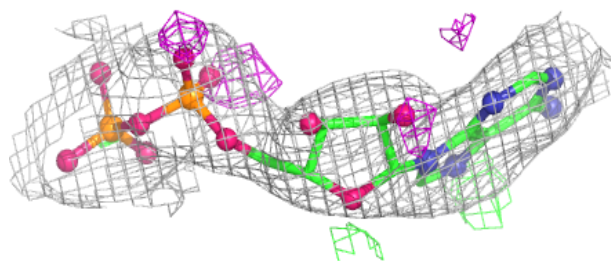
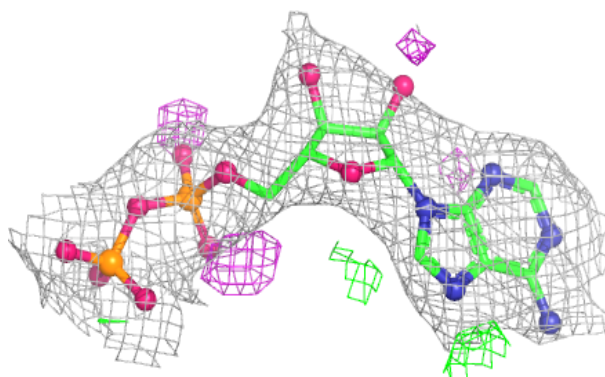


Electron density around ADP A 9002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

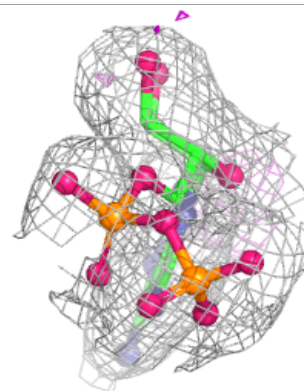
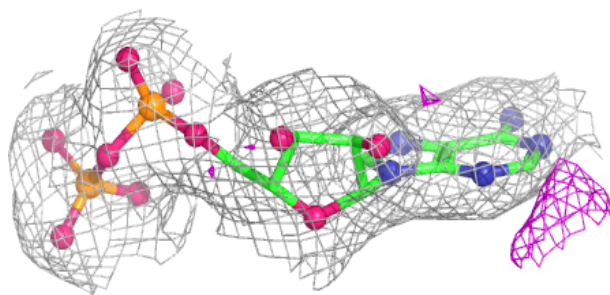
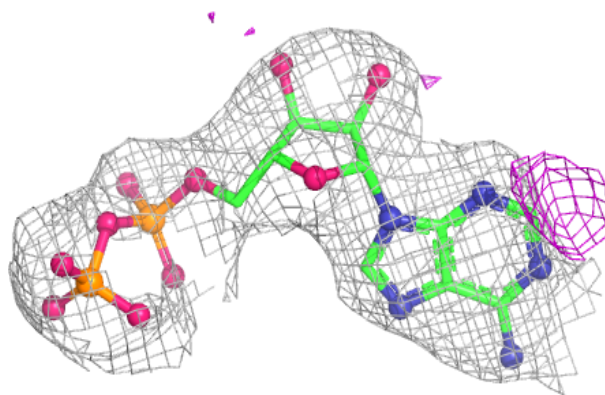
**Electron density around ADP A 9003:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

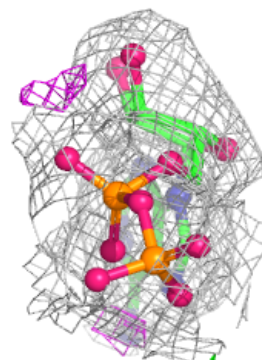
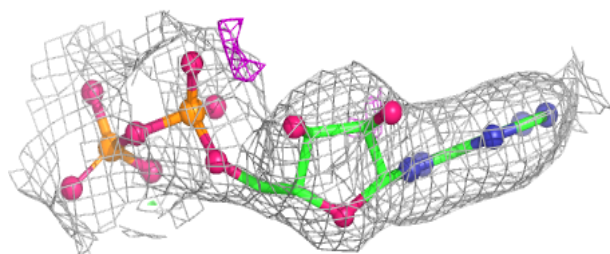
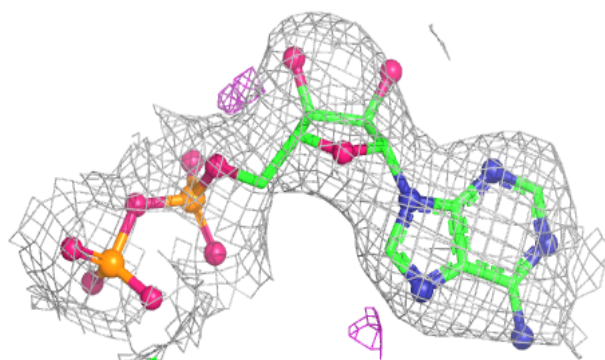


Electron density around ADP A 9004:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

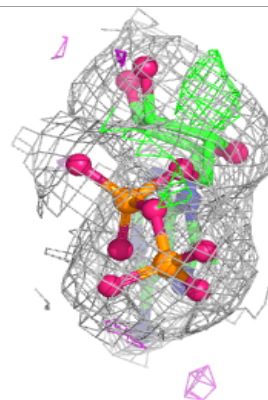
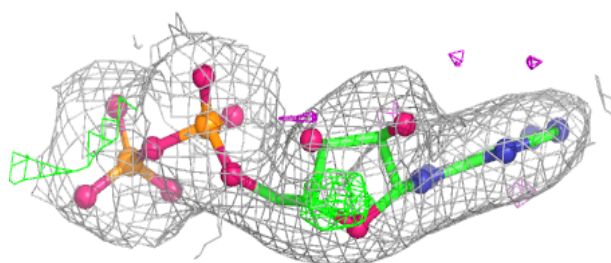
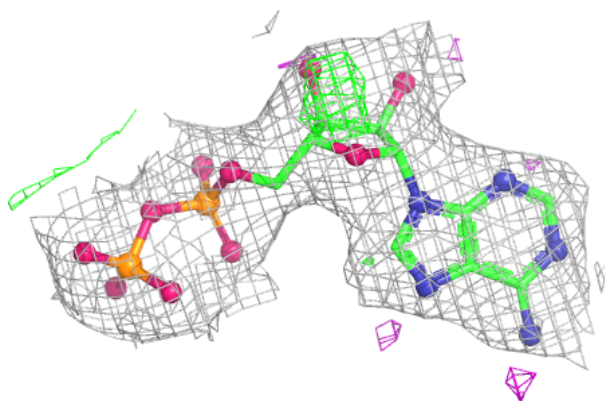
**Electron density around ADP B 9007:**

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and green (positive)

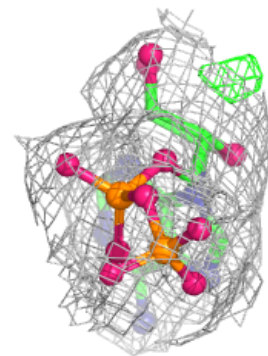
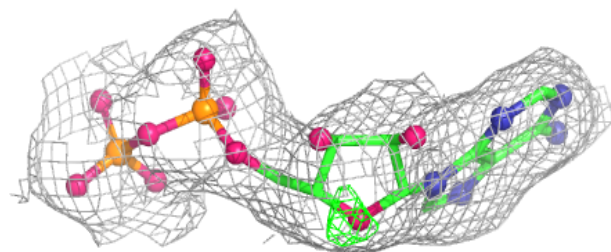
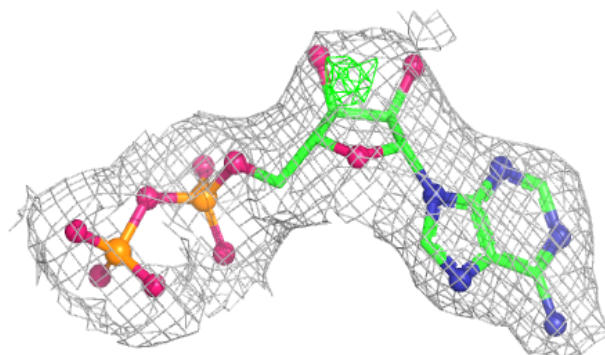


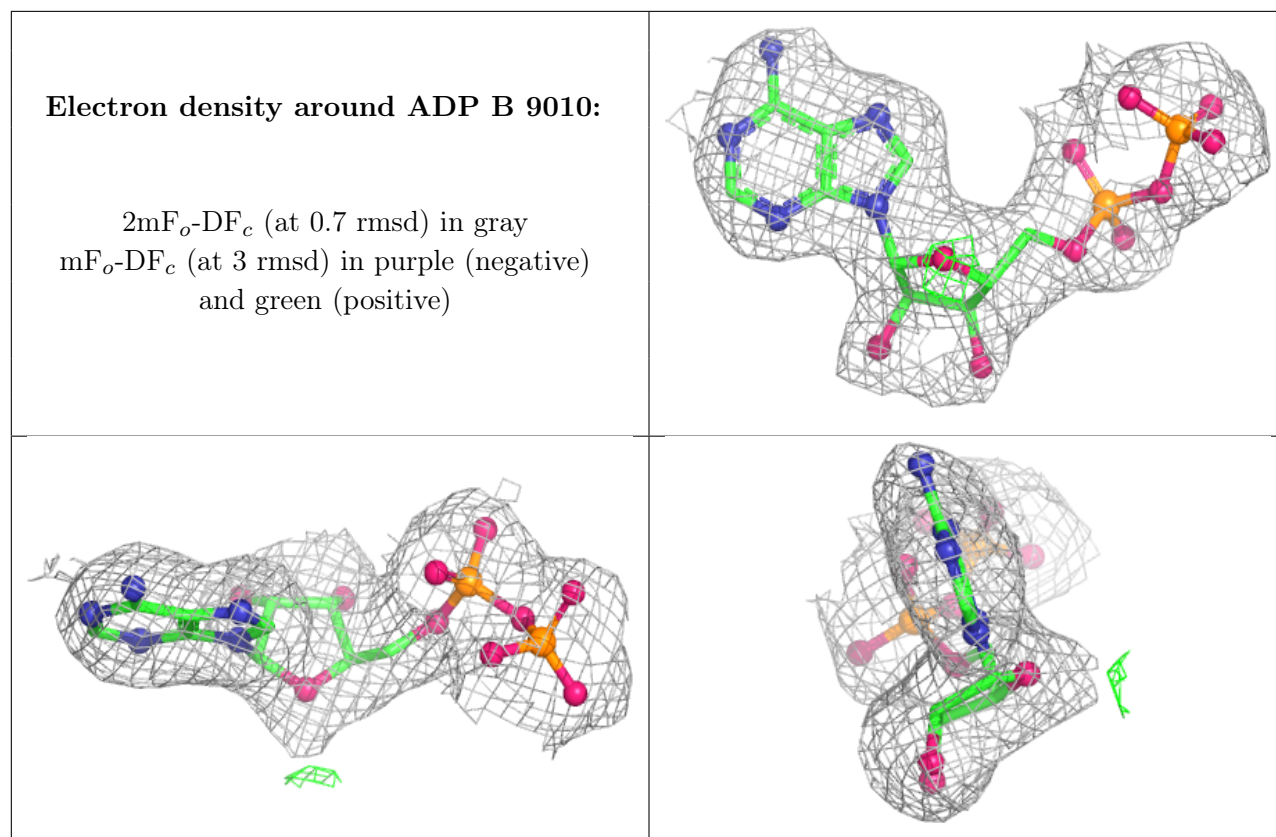
Electron density around ADP A 9001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP B 9009:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.