



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3VKH / pdb_00003vkh
Title : X-ray structure of a functional full-length dynein motor domain
Authors : Kon, T.; Oyama, T.; Shimo-Kon, R.; Suto, K.; Kurisu, G.
Deposited on : 2011-11-16
Resolution : 3.80 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

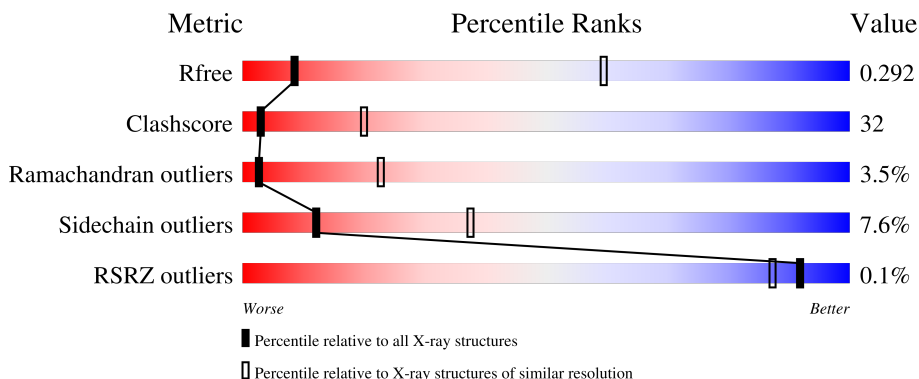
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	3367	
1	B	3367	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 45974 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	3042	Total	C	N	O	S	0	0	0
			23374	14951	3955	4368	100			
1	B	2908	Total	C	N	O	S	0	0	0
			22384	14307	3792	4190	95			

There are 48 discrepancies between the modelled and reference sequences:

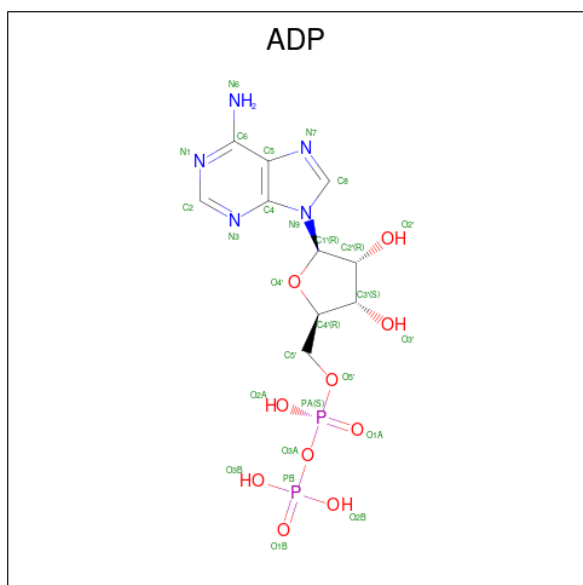
Chain	Residue	Modelled	Actual	Comment	Reference
A	1364	MET	-	expression tag	UNP P34036
A	1365	THR	-	expression tag	UNP P34036
A	1366	ARG	-	expression tag	UNP P34036
A	1367	HIS	-	expression tag	UNP P34036
A	1368	HIS	-	expression tag	UNP P34036
A	1369	HIS	-	expression tag	UNP P34036
A	1370	HIS	-	expression 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
B	1364	MET	-	expression tag	UNP P34036

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Chain	Residue	Modelled	Actual	Comment	Reference
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

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

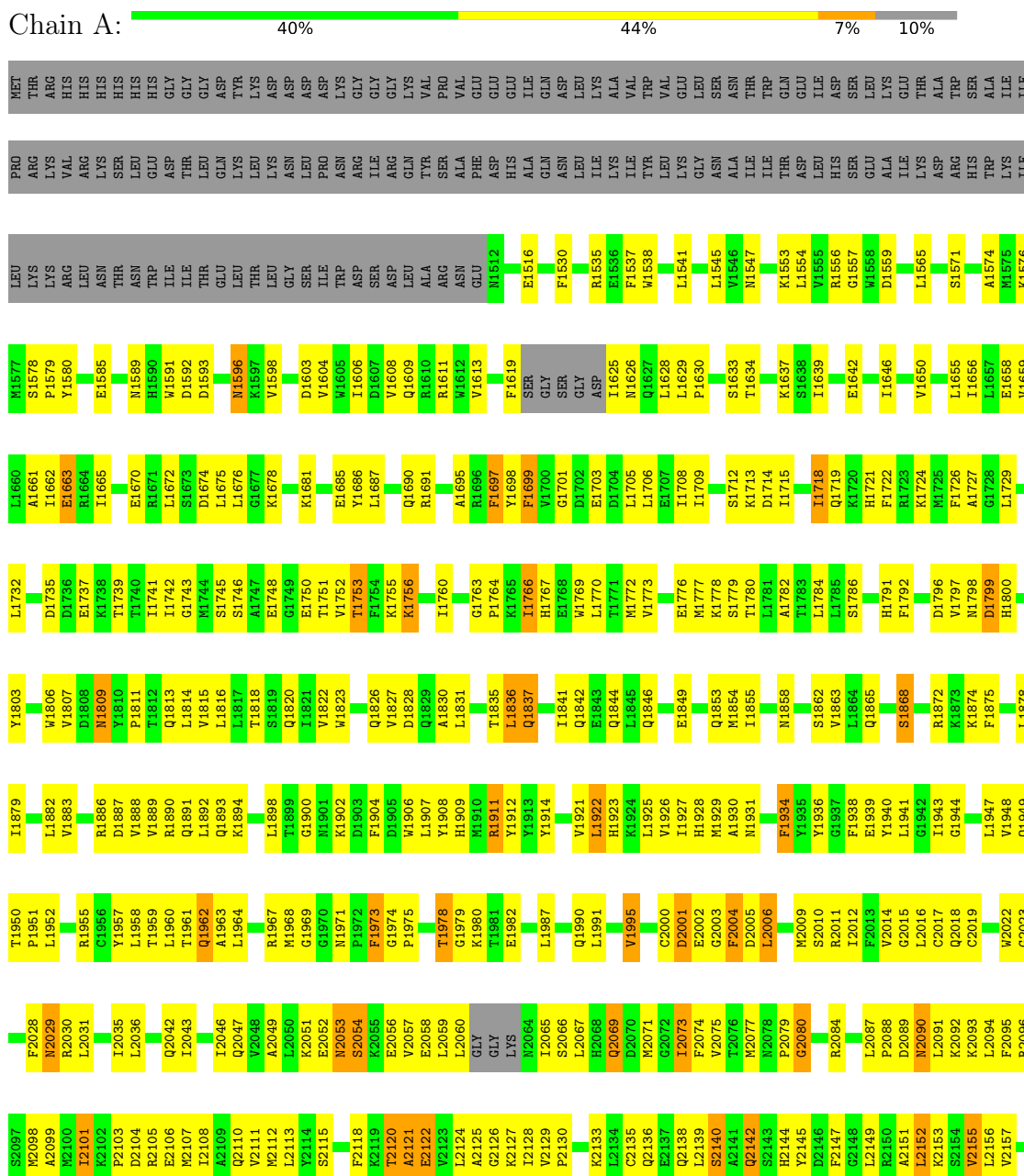


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B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

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





D4311	D4241	L4170	L4083	L4091	L4021	L3951	E3878	R3806	ARG	P3672	A3595	D3516	A3451	K3385	L3289
Y4312	P4242	A4171	L4084	S4091	C4022	F3952	E3878	P3607	LYS	L3673	S3596	D3516	L3452	K3386	K3290
W4313	G4243	E4172	L4085	P4029	R4022	F3952	L3879	D3808	LYS	V3674	A3597	T3521	T3453	H3387	K3291
W4314	W4244	L4086	R4023	D4092	R4024	K3954	L3879	T3809	GLY	I3675	F3598	T3522	K3454	L3388	L3292
D4315	K4245	A4178	K4087	W4094	Q4026	V3955	V3882	H3810	GLY	P3676	L3599	L3525	G3455	D3389	R3293
S4318	K4246	A4179	Q4026	L4096	Q4026	K3811	Y3886	K3811	ARG	P3677	A3600	L3525	Y3456	E3390	
K4319	W4247	Q4027	W4027	W4027	W4027	K3812	N3867	K3812	ILE	S3678	Y3601	L3525	L3457	I3391	E3296
G4320	L4248	G4182	S4091	P4029	P4029	R3813	N3867	R3813	LEU		I3602	S3528	E3458	L3394	
R4321	D4092	T4183	L3959	S4029	S4029	R3814	N3868	R3814	ILE	A3681	G3603	S3529	D3459	K3399	Y3299
S4322	W4094	W4184	N3961	F4030	R4023	D3815	A3889	D3815	ARG	M3682	A3530	T3529	P3460	K3300	K3300
	T4251	V4094	K3964	S4031	S4031	L3816	A3890	L3816	LEU	E3683	F3605	T3531	G3461	K3396	
	P4252	L4095	L3965	K4032	K4032	L3817	L3891	L3817	GLY	F3684	D3606	Y3532	F3462	P3397	K3309
	L4253	L4187	L3965	L4033	L4033	ASP	S3882	L3817	ASP	I3685		K3533	D3463	P3398	
P4326	G4254	K4188	L3969	W4034	W4034	GLN	C3883	I3819	GLN	M3686	R3610	Y3536	Y3467	T3399	L3313
I4329	L4255	N4189	L3969	D4035	D4035	ASP	S3894	Q3820	ASP	Y3689	T3611	Y3536	D3314	P3400	L3313
P4330	P4256	H4190	H4099	D4035	H4036	VAL	R3895	G3821	VAL	D3612	D3612				V3315
W4331	A4257	H4191	S4100	G3821	H4036	ASP	R3895	G3821	ASP	D3612	D3612			A3404	
V4334	T4258	A4192	C4103	I3974	Q4039	ASP	V3896	V3825	PHE	K3691	L3614	L3539	S3470	M3405	Q3319
R4335	R4258	A4193	S4104	V3976	M4040	SER	F3898	K3826	SER	D3692	K3614	R3541	S3472		
L4336	W4260	L4197	V4105	K3977	D4043	P3768	A3899	L3827		K3693	S3623	E3542	A3473	K3323	K3323
L4338	P4263	L4200	E4108	G3978	W4044	R3828	M3900	R3828	K3694	I3694	S3623	I3546	C3474	C3409	L3324
	Q4263	E4201	D4109	K3980	K4045	R3829	E3902	L3830	M3761	T3695	S3623	I3546	P3476	M3411	L3410
	R4267	E4202	F4110	N3981	Q4046	E3831	L3903	E3831	F3704	T3697	S3623	E3549	L3477	M3412	L3412
S4268	S4268	K4203	L4111	E3985	F4047	L3834	Q3905	L3834	I3764	S3698	V3624	K3550	V3478	G3413	G3413
Y4343	R4269	L4204	N4112	S3986	G4049	L3835	F3906	L3835	F3765	F3699	V3624	S3551	K3479	K3414	K3337
Y4271	W4270	H4205		E3987	K4050	R3836	H3907	L3836	A3481	D3701	L3700	K3552	W3480	K3415	Q3338
L4273	Y4271	S4206	L4116	W3988	D4051	A3837	Y3909	A3837	R3767	D3701	F3628	K3554	G3489	L3416	L3416
	L4273	S4208	D4117	D3989	Q4052	L3838	F3909	L3838	R3767	F3704	S3639	K3554	T3482	L3417	L3417
		P4209	W4118	F3990	W4053	S3839	Q3910	S3839	D3768		S3639	K3554	A3483	E3418	A3418
		P4211	A4119	L3991	G4054	Q3840	F3911	Q3840	A3771	N3707	V3634	K3554	Q3484	W3419	R3342
		P4211	E4120	L3992	E4055	R3841	S3912	R3841			P3635	D3557	T3485		Q3345
		S4212	L4121	L3992	P4056	S3942	R3913	S3942	T3774	A3711	L3638	D3558	Y3487	I3422	I3422
		F4213	V4122	G3994	I4057	R3943	L3914	R3943	P3775	E3488	S3560	R3559	S3488	R3423	R3423
		E4123	E4123	G3995	A4058	S3944	A3915	S3944	D3776	L3712	I3561	K3562	E3489	K3425	K3425
		L4124	E4125	R3996	P4059	L3845	F3916	L3845		G3715	A3562	I3490	T3490	I3426	I3426
		L4215	E4126	N3997	E4060	L3845	L3917	L3845	S3779	C3716	L3563	L3563	L3491	M3497	M3497
		F4216	V4126	L3998	S4061	D3848	D3918	D3848	R3780	P3717	L3564	L3564	ASP	E3428	E3428
		M4217	K4127	L3999	W4062	D3849	I3919	D3849	V3781	L3718	W3647	D3565	ARG	P3429	P3429
		T4218	S4128	T3999	I4063	S3850	F3920	S3850	F3782	L3719	R3648	L3567	ILE	N3430	N3430
		S4219	S4129	S4000	V4064	V3851	Y3921	V3851	F3783	V3720	L3567	L3567	LYS	F3431	F3431
		E4220	A4065	L4001	A4065	N3922	N3922	N3922	V3784	Q3721	L3652	K3568	PRO	I3432	I3432
		L4221	Q4066	K4002	A4066	L3923	L3923	L3923	N3785	D3722	P3653	E3570	LEU	T3433	T3433
		H4222	A4067	E4003	A4067	T4004	L3924	L3924	F3786	V3723	S3654	R3571	ARG	S3434	S3434
		P4223	Q4068	L4005	Q4068	N3926	N3926	N3926	V3788	E3724	D3655		GLU	I3436	I3436
		L4224	L4134	P4006	L4069	L3858	N3927	L3858	T3789	N3725	C3568		GLU	I3436	I3436
		L4225	E4135	Q4007	S4070	K3859	N3927	K3859	P3790	I3726	S3578		VAL	N3437	N3437
			S4136	L4008	N4071				P3728	D3727	I3659		GLU	Y3438	Y3438
			L4149	L4011	Q4072	T3862	L3930	T3862	S3791	F3728	K3660		GLN	D3439	D3439
			L4149	L4012	Q4073	T3863	L3930	T3863	S3792	V3729	N3661		LEU	T3440	T3440
			W4157	L4013	S4074	E3864	K3933	E3864	L3793	L3730	A3662		GLU	K3441	K3441
			K4158	T4013	T4075	T3865	L3939	T3865	Q3794	N3731	I3663		ASN	I3373	I3373
			L4158	T4014	T4076	A3866	R3939	A3866	L3798	P3732	K3664		ALA	M3443	M3443
			L4158	T4015	T4077	L3867	L3943	L3867	L3733	V3734	S3586		ALA	M3444	M3444
			L4162	Q4016	S4078	K3868	L3943	K3868	L3734	T3587	ASN		ASN	T3445	T3445
			G4163	Q4017	M4079	V3869	L3943	V3869	L3734	N3735	F3668		GLU	P3446	P3446
			F4168	R4018	F4080	E3870	T3947	E3870	L3802	K3736	N3669		LEU	V3380	V3380
			E4169	W4019	F4080	E3870	F3948	E3870	K3803	GLU	R3670		K3512	S3351	S3351
				L4020	K4082	V3875		V3875	E3805	ILE	Y3671			R3449	R3449
														E3450	E3450





F4252	I4162	K4087	Q4016	N3927	L3835	P3672	T3583	SER	GLU	LYS	P3672	T3583	GLU	LYS	Y3254	A3159	E3066
I4253	G4163	S4091	L4020	F3928	A3841	L3673	N3584	ILE	PRO	LYS	L3674	N3584	PRO	ALA	V3255	T3160	E3067
I4255	G4167	D4092	I4021	N3929	S3842	V3674	M3585	ILE	ASN	GLY	V3675	M3585	PHE	GLU	P3256	S3161	K3068
A4257	L4170	R4093	C4022	L3930	G3843	L3675	S3586	ARG	PHE	ARG	L3676	S3586	ILE	ALA	P3257	P3162	I3069
A4258	A4171	V4094	L4023	D3931	N3844	D3677	T3587	ASP	THR	ILE	P3677	T3587	THR	ILE	H3258	L3164	I3072
R4259	L4095	L4095	R4024	D3932	T3845	L3677	V3588	ILE	THR	ILE	P3677	V3588	THR	ILE	H3259	F3165	I3072
M4260	Q4025	Q4025	Q4025	D3935	L3846	A3681	V3589	PRO	ILE	GLY	A3681	V3589	ILE	GLY	Y3260	N3166	V3078
Q4263	V4027	D3947	Q4026	D3939	D3847	M3682	V3592	ASP	ILE	ALA	M3682	V3592	ILE	ALA	F3263	L3170	L3079
P4264	V4027	F3948	V4027	R3939	D3848	E3683	V3592	LEU	ALA	ASN	E3683	V3592	LEU	ASN	L3170	D3171	E3080
A4265	L3940	D3849	L3940	D3849	D3849	F3684	A3595	GLY	TYR	GLN	F3684	A3595	GLY	TYR	V3267	W3172	S3082
E4266	S3850	S3850	S3850	S3850	S3850	L3685	F3598	ASP	ASP	VAL	L3685	F3598	GLU	VAL	V3268	F3173	S3083
R4267	S4031	V3852	S4031	L3943	L3852	M3686	F3598	GLN	THR	LYS	M3686	F3598	GLU	THR	G3174	L3084	L3084
F4270	F4105	F4105	F4105	F4105	F4105	N3687	F3598	ASP	LYS	THR	N3687	F3598	VAL	LYS	E3175	E3085	R3086
H4191	F4106	F4106	F4106	F4106	F4106	Q3688	Y3601	VAL	GLY	THR	Q3688	Y3601	GLY	THR	N3272	L3181	M3087
L4192	G4107	G4107	G4107	G4107	G4107	Y3689	I3602	ASP	MET	ILE	Y3689	I3602	MET	ILE	E3273	F3182	N3088
A4193	E4108	E4108	E4108	E4108	E4108	D3691	G3603	LEU	THR	LYS	D3691	G3603	LEU	THR	K3274	L3182	T3089
P4194	D4109	D4109	D4109	D4109	D4109	K3692	F3604	ASN	PRO	LYS	K3692	F3604	ASN	PRO	G3268	Q3183	T3089
L4197	F4110	F4110	F4110	F4110	F4110	K3693	F3605	ALA	LYS	HIS	K3693	F3605	ALA	LYS	L3289	V3184	L3090
L4200	L4111	L4111	L4111	L4111	L4111	L3694	D3606	ALA	ILE	LEU	L3694	D3606	ALA	ILE	K3291	G3185	L3091
E4201	M4112	M4112	M4112	M4112	M4112	T3695	Q3607	GLU	ARG	ASP	T3695	Q3607	GLU	ARG	L3292	S3186	A3092
S4206	T4113	T4113	T4113	T4113	T4113	K3696	N3608	LEU	GLU	THR	K3696	N3608	LEU	GLU	E3187	G3093	G3093
L4280	M4118	M4118	M4118	M4118	M4118	T3697	F3609	LEU	ALA	ILE	T3697	F3609	LEU	ALA	D3284	G3094	G3094
L4281	A4119	A4119	A4119	A4119	A4119	S3698	R3610	ILE	THR	SER	S3698	R3610	ILE	THR	T3295	E3095	E3095
L4282	H4120	H4120	H4120	H4120	H4120	F3699	M3614	THR	LYS	LEU	F3699	M3614	THR	LYS	T3295	VAL	VAL
P4209	K3877	K3877	K3877	K3877	K3877	D3701	Y3536	GLY	PRO	GLY	D3701	Y3536	GLY	PRO	V3299	E3195	PRO
E4283	L4121	L4121	L4121	L4121	L4121	S3702	M3617	TYR	TYR	LYS	S3702	M3617	TYR	TYR	N3196	N3196	LEU
R4284	V4122	V4122	V4122	V4122	V4122	F3703	I3619	LEU	PRO	PRO	F3703	I3619	LEU	PRO	P3302	Y3199	PHE
L4285	F3967	F3967	F3967	F3967	F3967	M3705	R3620	ASP	GLU	THR	M3705	R3620	ASP	GLU	P3306	P3202	GLY
L4288	I3973	I3973	I3973	I3973	I3973	L3708	S3623	PRO	PRO	PRO	L3708	S3623	PRO	PRO	L3313	E3103	E3103
P4289	V3976	V3976	V3976	V3976	V3976	G3715	F3628	GLY	PHE	VAL	G3715	F3628	GLY	PHE	D3314	M3212	F3105
W4292	K3887	K3887	K3887	K3887	K3887	C3716	Y3542	ASP	ASN	ASN	C3716	Y3542	ASP	ASN	V3315	E3410	F3105
T4293	P3888	P3888	P3888	P3888	P3888	L3717	I3545	TYR	TYR	ALA	L3717	I3545	TYR	ALA	K3316	M3109	M3109
E4294	N3890	N3890	N3890	N3890	N3890	P3717	V3634	GLU	GLU	MET	P3717	V3634	GLU	GLU	Q3322	R3217	R3118
F4295	L3891	L3891	L3891	L3891	L3891	L3718	P3635	THR	THR	GLY	L3718	P3635	THR	THR	Q3322	A3218	ASN
F4296	S3892	S3892	S3892	S3892	S3892	L3719	S3636	VAL	VAL	ALA	L3719	S3636	VAL	VAL	A3218	G3219	GLY
E4297	C3893	C3893	C3893	C3893	C3893	F3720	F3637	ARG	ARG	VAL	F3720	F3637	ARG	ARG	P3220	P3220	LEU
L4298	S3894	S3894	S3894	S3894	S3894	Q3721	L3638	ALA	ALA	CYS	Q3721	L3638	ALA	ALA	P3221	I3221	ILE
A4299	R3895	R3895	R3895	R3895	R3895	D3722	S3639	SER	SER	LYS	D3722	S3639	SER	LYS	S3222	S3222	LEU
R4303	V3896	V3896	V3896	V3896	V3896	V3723	W3647	LEU	LEU	LYS	V3723	W3647	LEU	LEU	Q3345	S3125	ASP
P4304	Y3897	Y3897	Y3897	Y3897	Y3897	E3724	N3650	GLY	GLY	ALA	E3724	N3650	GLY	GLY	V3228	V3228	ASP
E4305	F3898	F3898	F3898	F3898	F3898	N3725	S3558	GLY	CYS	CYS	N3725	S3558	GLY	CYS	S3229	S3229	LEU
A4306	L3998	L3998	L3998	L3998	L3998	I3726	R3559	PRO	PRO	LYS	I3726	R3559	PRO	PRO	L3129	L3129	LEU
L4307	E3902	E3902	E3902	E3902	E3902	D3727	S3560	LEU	LEU	LYS	D3727	S3560	LEU	LEU	S3230	S3230	LEU
I4310	S3904	S3904	S3904	S3904	S3904	V3729	L3563	VAL	VAL	GLY	V3729	L3563	VAL	VAL	E3354	L3231	S3135
R4311	L3908	L3908	L3908	L3908	L3908	L3730	L3564	GLY	GLY	GLY	L3730	L3564	GLY	GLY	Q3358	V3232	Q3136
P4312	Y3909	Y3909	Y3909	Y3909	Y3909	N3731	D3565	TRP	TRP	LYS	N3731	D3565	TRP	TRP	V3233	F3233	Y3137
F4313	Q3910	Q3910	Q3910	Q3910	Q3910	P3732	L3567	ALA	ALA	ALA	P3732	L3567	ALA	ALA	I3234	R3138	R3138
D4315	F3911	F3911	F3911	F3911	F3911	V3733	M3664	THR	THR	ILE	V3733	M3664	THR	THR	H3235	R3139	LYS
Y4238	S3912	S3912	S3912	S3912	S3912	L3734	R3571	ALA	ALA	ARG	L3734	R3571	ALA	ALA	T3237	N3140	N3140
E4239	L3913	L3913	L3913	L3913	L3913	K3736	R3572	LYS	LYS	LYS	K3736	R3572	LYS	LYS	I3238	F3145	F3145
W4244	L4011	L4011	L4011	L4011	L4011	I3736	F3668	THR	THR	GLN	I3736	F3668	THR	THR	L3248	R3248	S3151
N4323	L4012	L4012	L4012	L4012	L4012	ILE	Y3574	ILE	ILE	LYS	ILE	Y3574	ILE	ILE	LEU	ASP	ASP
I4324	S4013	S4013	S4013	S4013	S4013	ARG	Y3671	ARG	ARG	TYR	Y3671	Y3671	TYR	TYR	GLU	S3151	S3151

M4693	I4E	E4549	THR	L4399	D4327
	SER	W4550	ILE	P4400	K4328
	SER	K4551	THR	E4401	F4329
	GLU	W4552	GLU	I4402	P4330
	GLY	W4553	TRP	S4403	W4331
	GLY	S4554	THR	T4404	I4332
	ALA	W4555	LYS	P4405	K4333
	S4636	W4556	LEU	I4406	A4334
	P4637	E4557	LEU	W4407	R4335
	L4703	T4558	PRO	L4408	T4336
F4701	W4702	W4639	LYS	G4409	L4337
	I4703	L4642	PRO	L4410	L4338
	L4643	F4568	LEU	P4411	G4339
	E4645	L4644	LYS	E4412	S4340
	T4711	R4571	GLN	M4413	T4341
	L4647	M4572	LEU	A4414	T4342
	W4648	Q4573	LYS	E4415	Y4343
	W4649	Q4574	ARG	K4422	G4344
	W4650	L4575	THR	A4423	G4345
	Q4653	S4581	GLN	R4424	R4346
F4717	Q4653	ASN	K4425	M4249	F4350
	ASP	SER	ILE	M4236	F4351
	TYR	ASP	K4492	I4427	D4352
	SER	SER	P4494	A4429	L4355
	ILE	ILE	F4499	L4430	L4356
	S4661	Q4588	F4500	Q4431	Y4357
	T4662	W4589	R4501	K4432	S4358
	P4663	W4590	E4502	M4433	F4359
	L4664	L4591	I4503	Q4434	L4360
	S4665	G4592	L4506	E4437	F4361
S4725	T4666	G4593	G4506	GLU	Q4362
	A4667	W4596	L4509	ASP	L4363
	T4668	P4597	W4510	GLY	F4364
	L4669	I4601	I4513	ASP	T4365
	W4670	T4604	L4523	ASP	W4369
	K4671	T4604	ILE	GLN	M4370
	D4672	S4607	ILE	VAL	P4371
	K4674	L4611	SER	SER	D4372
	D4675	L4611	GLY	GLY	F4373
	ASP	L4611	ASN	ASN	P4374
F4702	PRO	L4611	ILE	LYS	P4377
	ILE	W4614	K4529	LYS	S4378
	PHE	S4614	S4530	GLU	I4379
	ASN	SER	S4530	GLU	G4380
	ASN	LEU	T4531	SER	L4381
	E4617	M4618	R4535	SER	T4388
	SER	SER	R4535	SER	R4389
	SER	L4621	S4540	E4459	A4390
	K4695	K4622	I4541	K4464	H4391
	L4686	A4623	S4542	A4464	I4396
S4728	S4687	S4624	K4543	K4485	F4397
	W4688	SER	G4544	LEU	I4397
	P4689	SER	I4545	ARG	A4203
	W4690	LEU	GLY	ALA	
	Y4691	L4692	THR	ALA	
	I4E				

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	195.73Å 228.96Å 201.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.79 – 3.80 48.79 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.79-3.80) 99.3 (48.79-3.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.52 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.292 0.220 , 0.292	Depositor DCC
R_{free} test set	4469 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	125.1	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 128.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	45974	wwPDB-VP
Average B, all atoms (Å ²)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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	0.28	0/23866	0.75	10/32482 (0.0%)
1	B	0.27	0/22846	0.73	4/31076 (0.0%)
All	All	0.27	0/46712	0.74	14/63558 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1737	GLU	N-CA-C	-6.59	105.21	113.18
1	A	3671	TYR	CA-C-N	6.24	126.27	119.90
1	A	3671	TYR	C-N-CA	6.24	126.27	119.90
1	A	3371	PRO	N-CA-CB	6.12	109.68	103.25
1	A	4005	ILE	CA-C-N	5.85	125.05	118.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	23374	0	22545	1654	0
1	B	22384	0	21550	1231	0
2	A	108	0	48	7	0
2	B	108	0	48	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	45974	0	44191	2881	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 32.

The worst 5 of 2881 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:3689:TYR:HB2	1:A:3694:ILE:HD11	1.29	1.14
1:A:3337:LYS:HB3	1:A:3525:LEU:HD13	1.35	1.07
1:B:3841:ALA:O	1:B:3842:SER:HB2	1.54	1.04
1:A:4242:PRO:HA	1:A:4286:ARG:HH12	1.22	1.03
1:A:4109:ASP:HA	1:A:4112:ASN:HD22	1.22	1.00

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	3010/3367 (89%)	2424 (80%)	448 (15%)	138 (5%)	2	18
1	B	2870/3367 (85%)	2476 (86%)	327 (11%)	67 (2%)	5	30
All	All	5880/6734 (87%)	4900 (83%)	775 (13%)	205 (4%)	3	23

5 of 205 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1836	LEU
1	A	2121	ALA
1	A	2409	SER
1	A	2560	MET

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Mol	Chain	Res	Type
1	A	2617	VAL

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 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	2457/3028 (81%)	2242 (91%)	215 (9%)	9	33
1	B	2353/3028 (78%)	2202 (94%)	151 (6%)	16	42
All	All	4810/6056 (79%)	4444 (92%)	366 (8%)	12	37

5 of 366 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1867	LEU
1	B	2883	ASP
1	B	2031	LEU
1	B	2320	LEU
1	B	3050	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 226 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4323	ASN
1	B	4596	ASN
1	B	1877	HIS
1	B	4573	GLN
1	B	3794	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	B	9007	-	28,29,29	1.68	5 (17%)	43,45,45	1.93	11 (25%)
2	ADP	B	9008	-	28,29,29	1.67	5 (17%)	43,45,45	1.92	11 (25%)
2	ADP	A	9001	-	28,29,29	1.67	5 (17%)	43,45,45	1.92	10 (23%)
2	ADP	A	9003	-	28,29,29	1.69	5 (17%)	43,45,45	1.94	10 (23%)
2	ADP	B	9010	-	28,29,29	1.68	5 (17%)	43,45,45	1.94	12 (27%)
2	ADP	B	9009	-	28,29,29	1.68	5 (17%)	43,45,45	1.93	10 (23%)
2	ADP	A	9002	-	28,29,29	1.66	5 (17%)	43,45,45	1.91	11 (25%)
2	ADP	A	9004	-	28,29,29	1.68	5 (17%)	43,45,45	1.94	11 (25%)

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	-	-	5/16/32/32	0/3/3/3
2	ADP	B	9008	-	-	3/16/32/32	0/3/3/3
2	ADP	A	9001	-	-	6/16/32/32	0/3/3/3
2	ADP	A	9003	-	-	6/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	9010	-	-	6/16/32/32	0/3/3/3
2	ADP	B	9009	-	-	6/16/32/32	0/3/3/3
2	ADP	A	9002	-	-	4/16/32/32	0/3/3/3
2	ADP	A	9004	-	-	3/16/32/32	0/3/3/3

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	9002	ADP	C5-C4	5.47	1.48	1.39
2	B	9008	ADP	C5-C4	5.41	1.48	1.39
2	B	9009	ADP	C5-C4	5.38	1.48	1.39
2	A	9003	ADP	C5-C4	5.37	1.48	1.39
2	A	9004	ADP	C5-C4	5.35	1.48	1.39

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9003	ADP	C5-C4-N3	-5.67	118.91	126.72
2	A	9002	ADP	C5-C4-N3	-5.67	118.91	126.72
2	B	9008	ADP	C5-C4-N3	-5.67	118.91	126.72
2	B	9009	ADP	C5-C4-N3	-5.62	118.98	126.72
2	B	9010	ADP	C5-C4-N3	-5.60	119.00	126.72

There are no chirality outliers.

5 of 39 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
2	A	9003	ADP	C5'-O5'-PA-O1A
2	A	9003	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

5 monomers are involved in 10 short contacts:

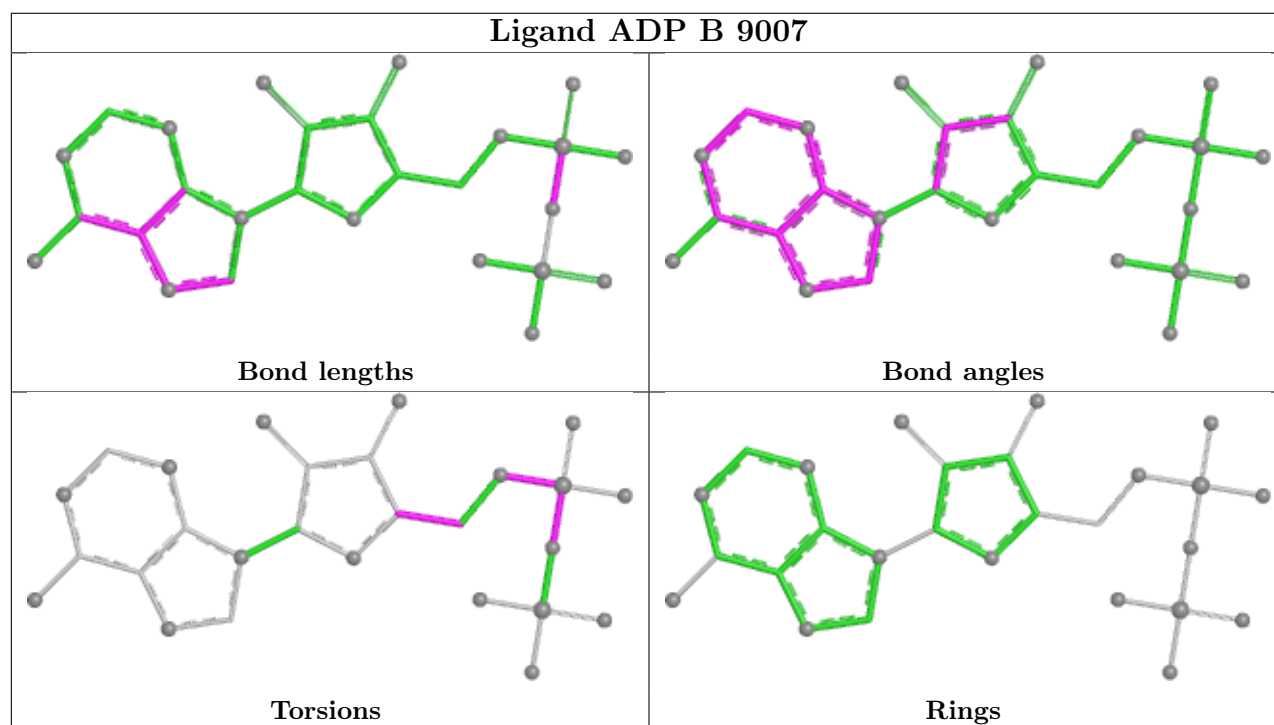
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9001	ADP	1	0
2	B	9010	ADP	2	0
2	B	9009	ADP	1	0

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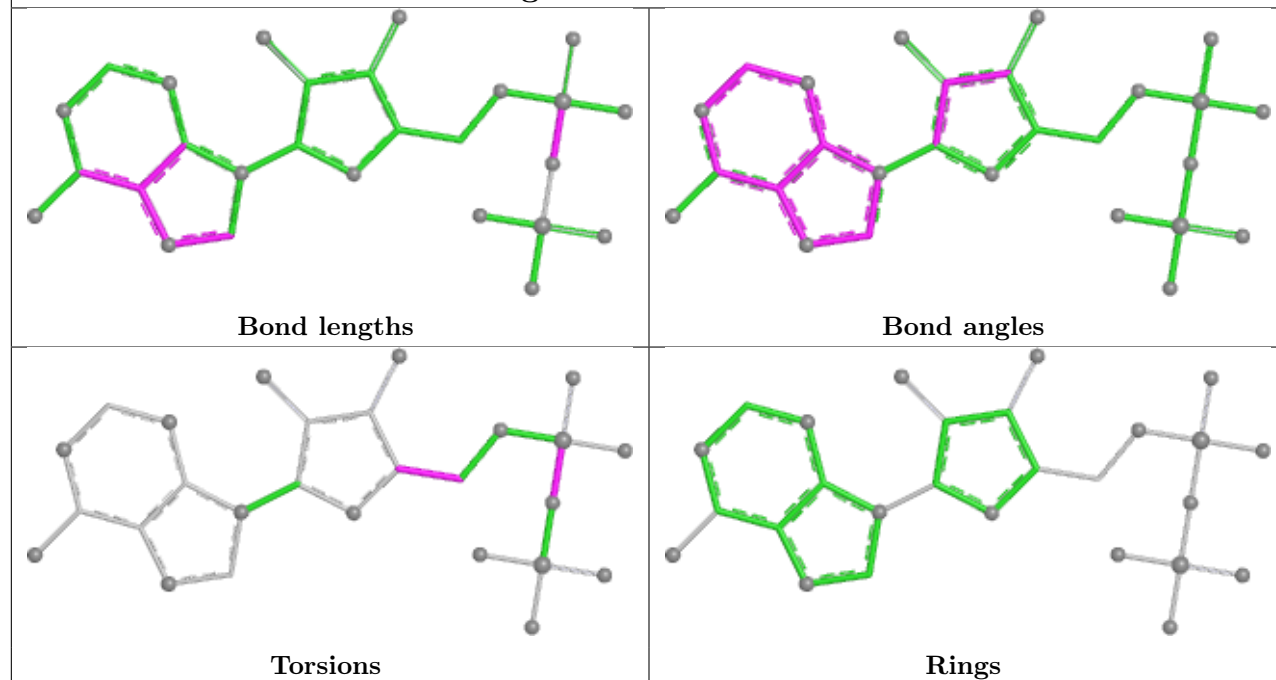
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9002	ADP	4	0
2	A	9004	ADP	2	0

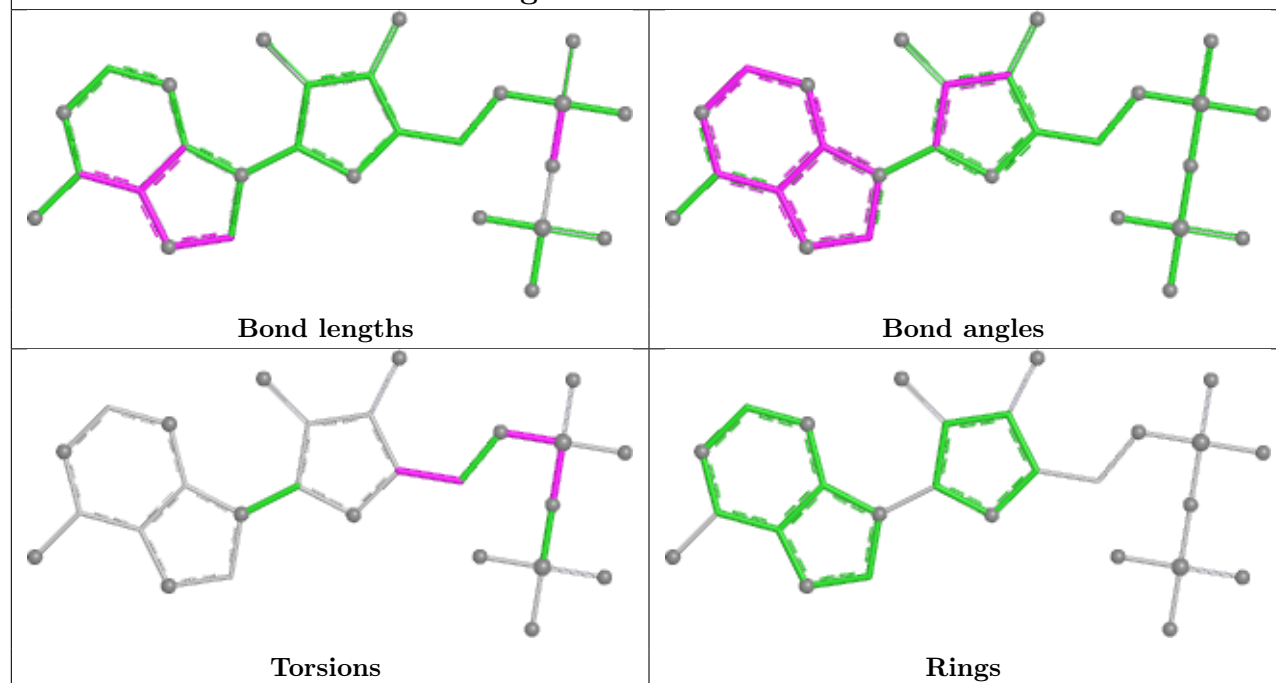
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

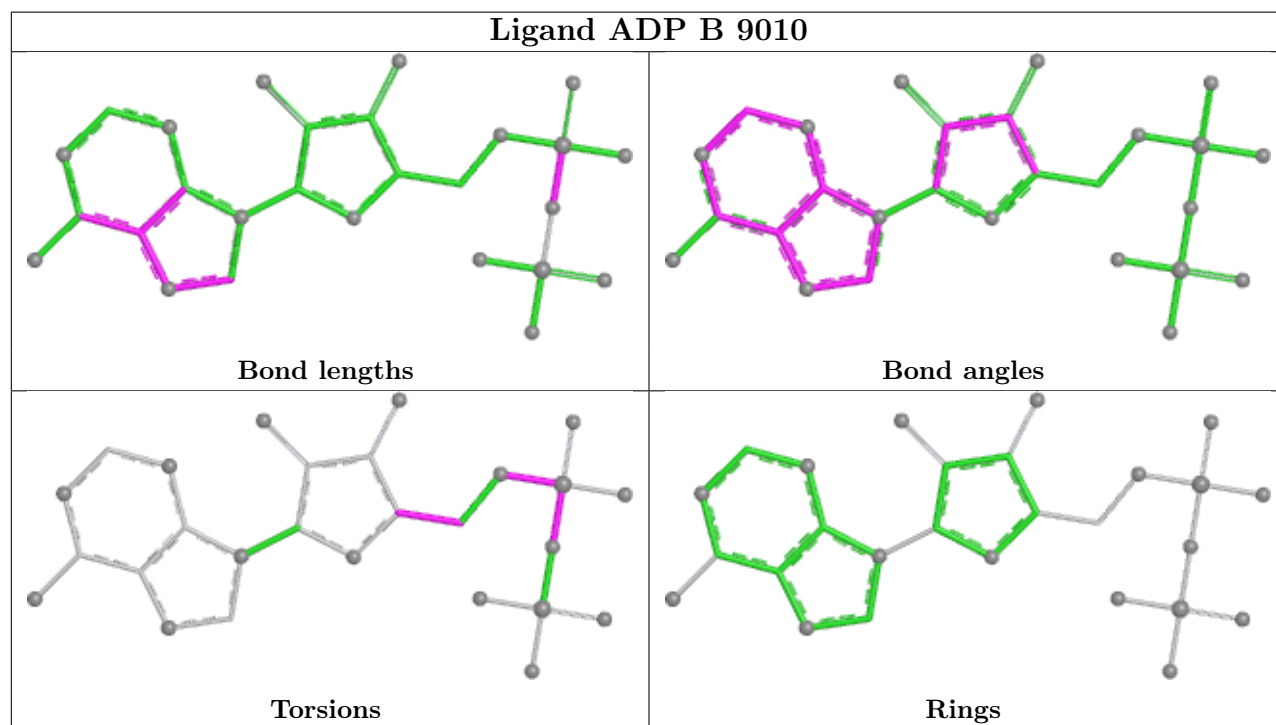
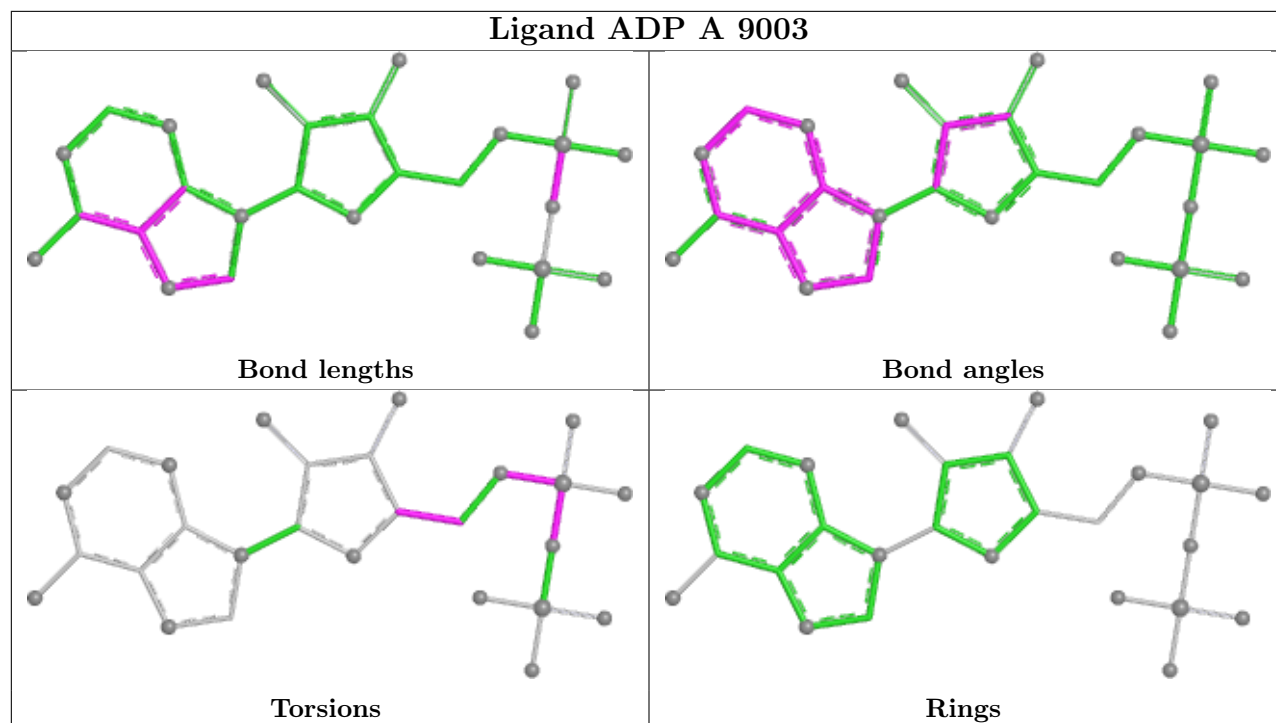


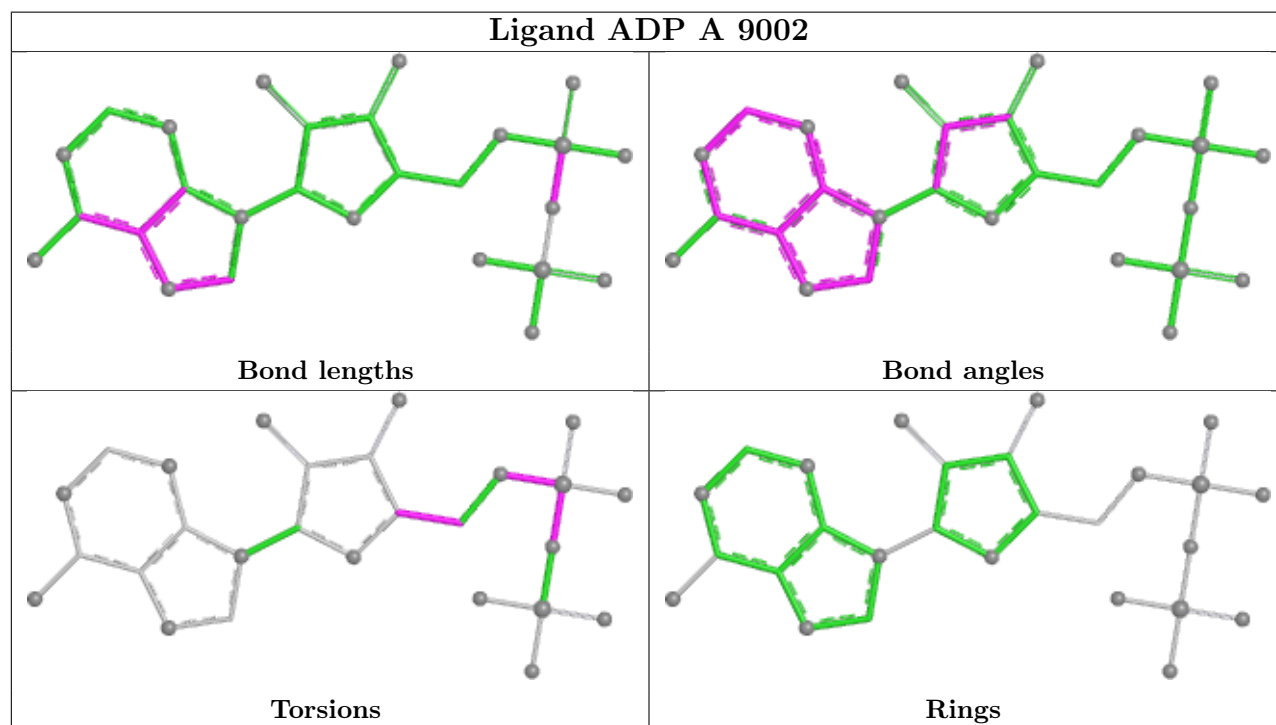
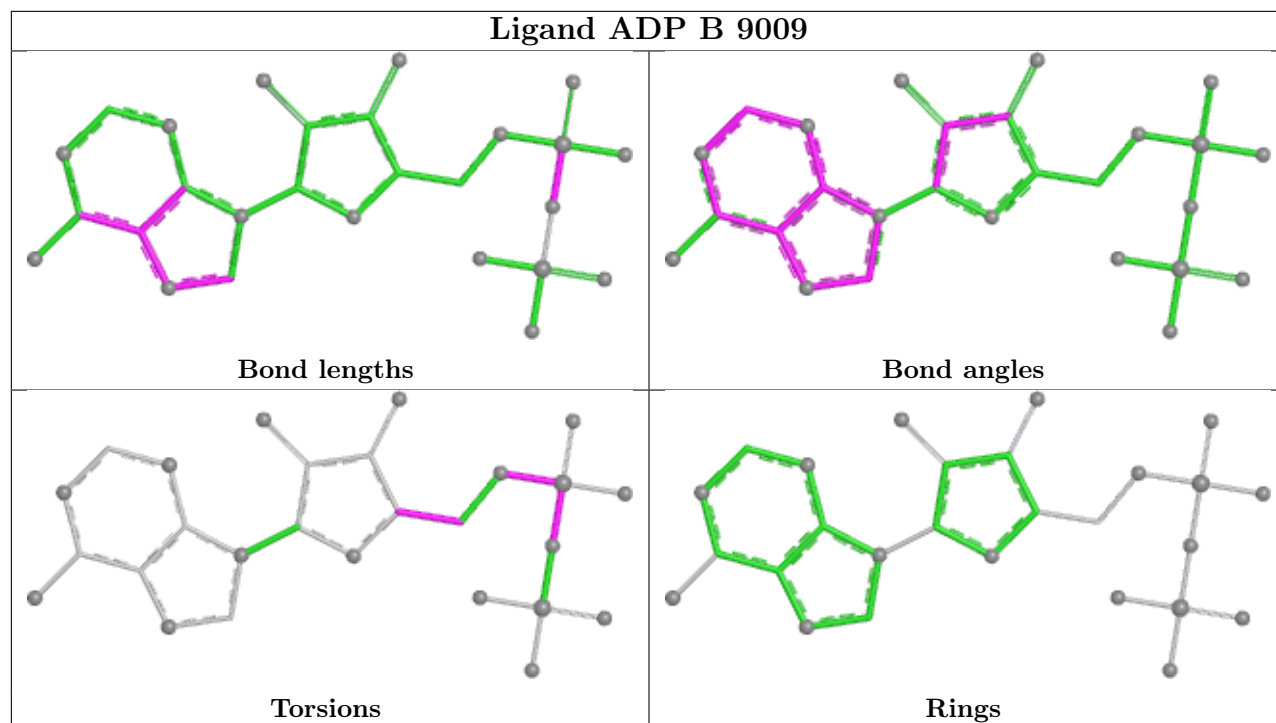
Ligand ADP B 9008

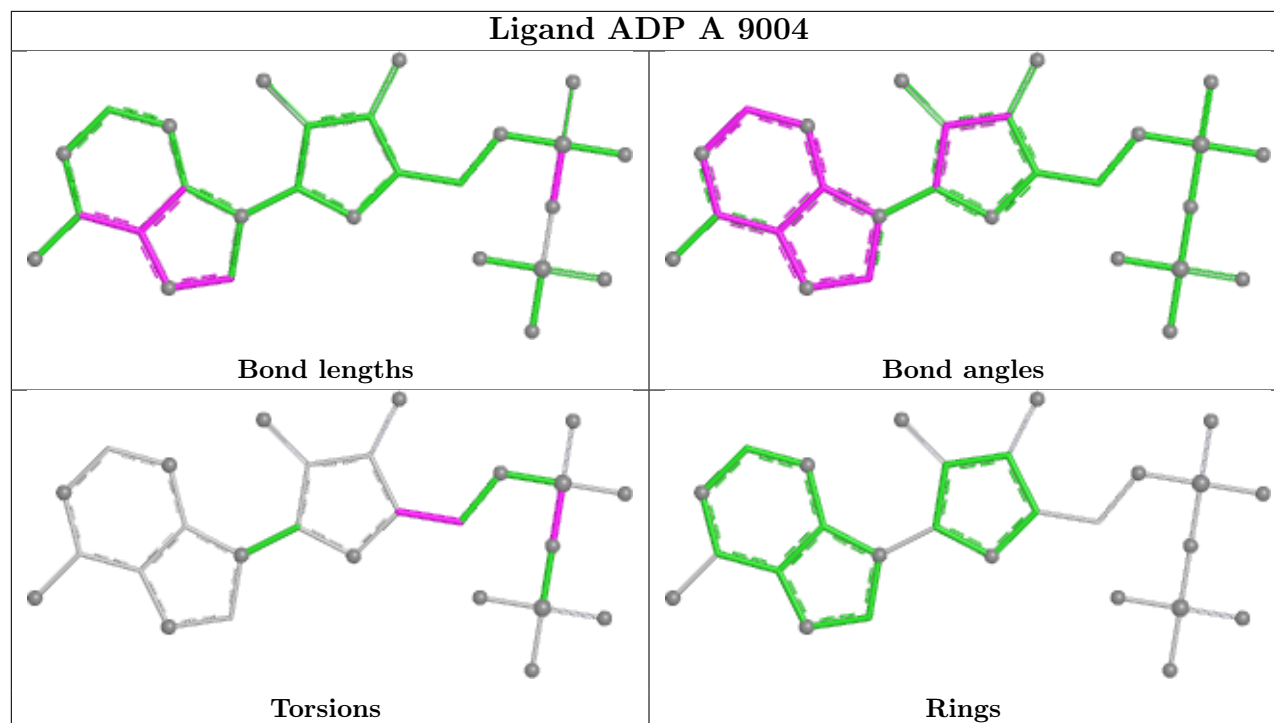


Ligand ADP A 9001









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, 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	3042/3367 (90%)	-0.48	2 (0%) 92 87	64, 130, 209, 322	0
1	B	2908/3367 (86%)	-0.46	6 (0%) 91 81	72, 136, 208, 335	0
All	All	5950/6734 (88%)	-0.47	8 (0%) 92 87	64, 133, 209, 335	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4550	TRP	2.8
1	B	3094	GLY	2.7
1	B	3727	ASP	2.6
1	B	3095	GLU	2.5
1	B	3708	LEU	2.5

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](#)

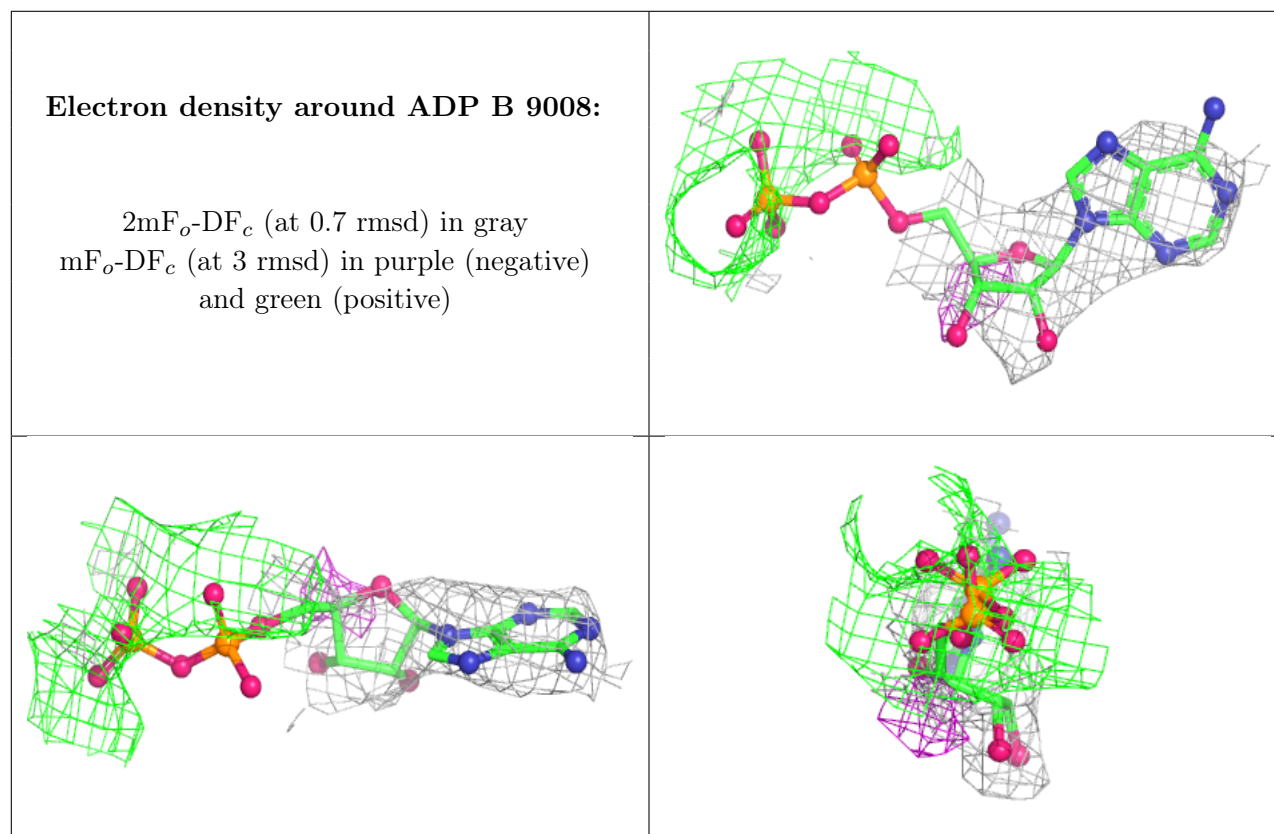
There are no oligosaccharides in this entry.

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.

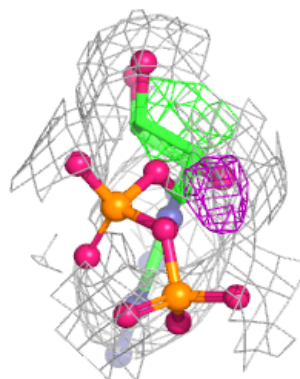
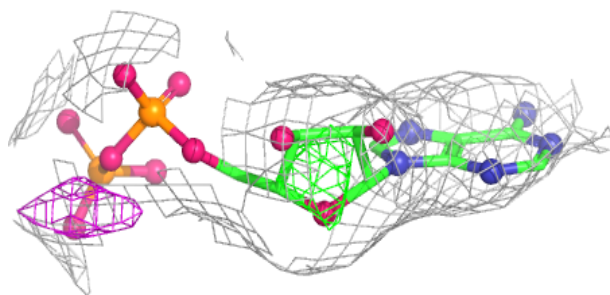
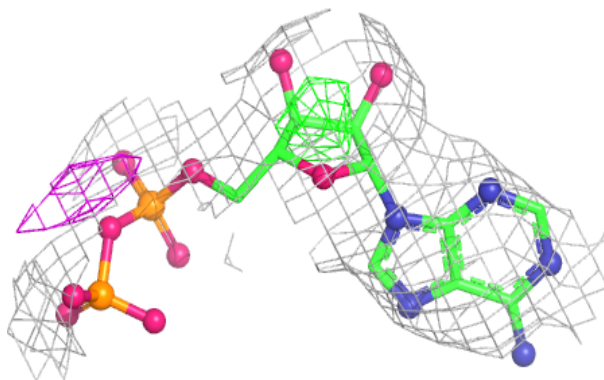
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	B	9008	27/27	0.88	0.12	129,129,129,129	0
2	ADP	A	9004	27/27	0.93	0.09	129,129,129,129	0
2	ADP	B	9010	27/27	0.93	0.09	129,129,129,129	0
2	ADP	A	9001	27/27	0.94	0.12	129,129,129,129	0
2	ADP	A	9002	27/27	0.95	0.10	129,129,129,129	0
2	ADP	A	9003	27/27	0.96	0.09	129,129,129,129	0
2	ADP	B	9007	27/27	0.96	0.10	129,129,129,129	0
2	ADP	B	9009	27/27	0.97	0.08	129,129,129,129	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.

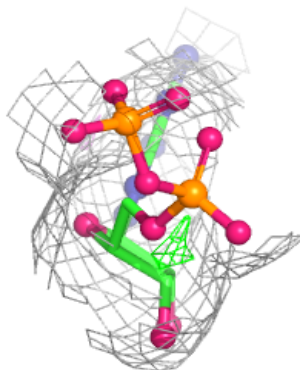
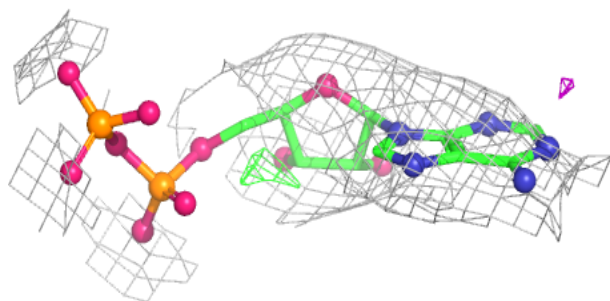
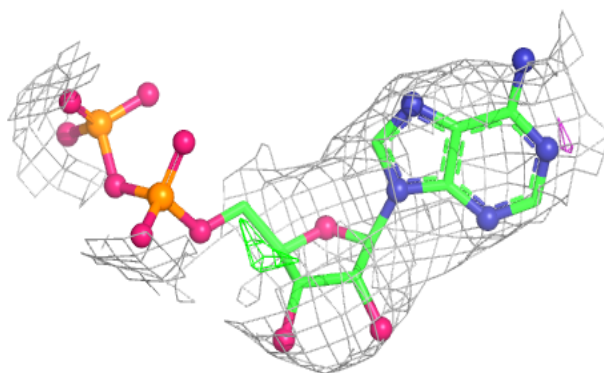


Electron density around ADP A 9004:

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

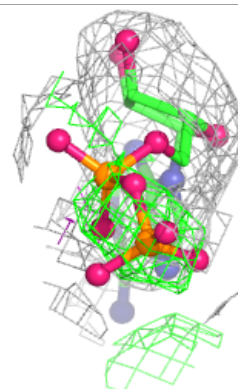
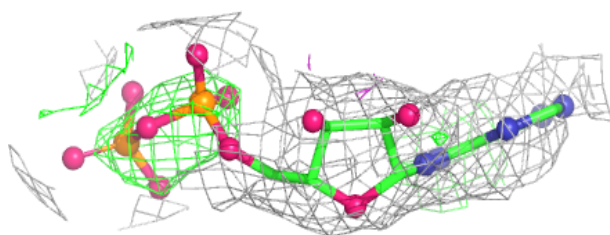
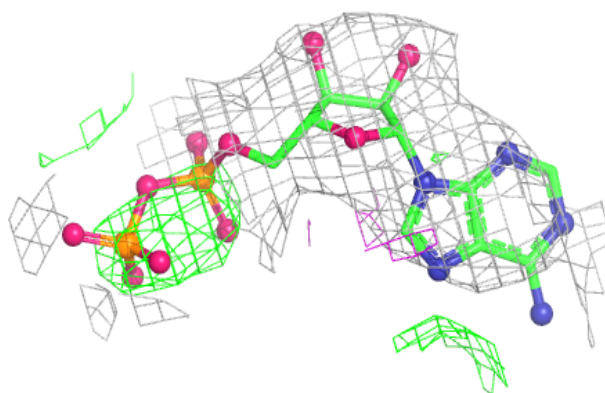
**Electron density around ADP B 9010:**

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

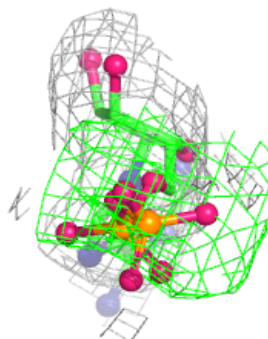
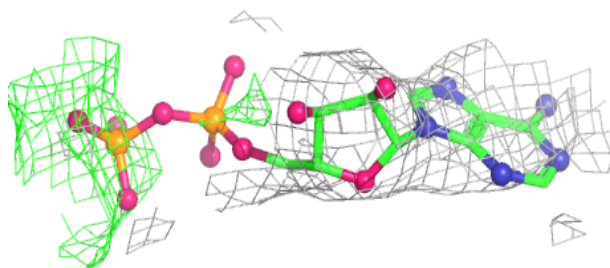
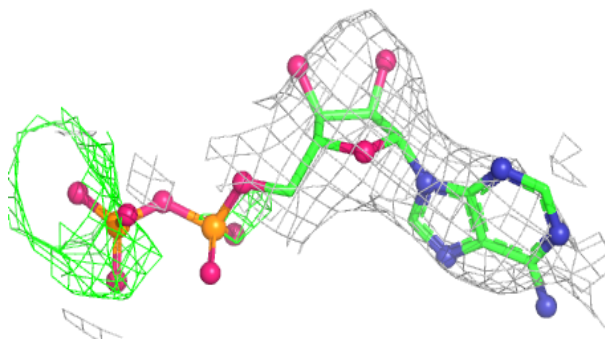


Electron density around ADP A 9001:

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

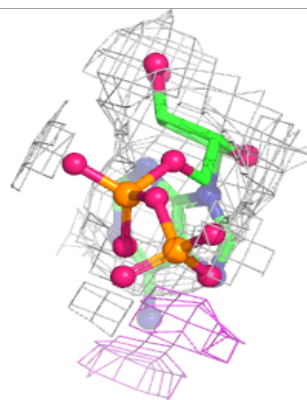
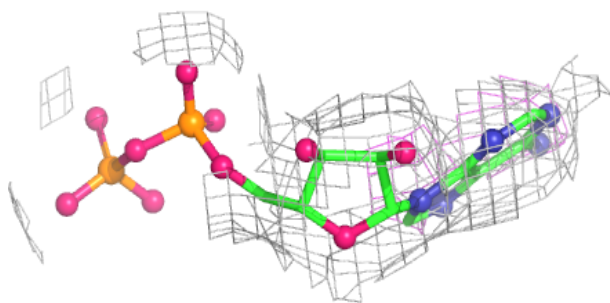
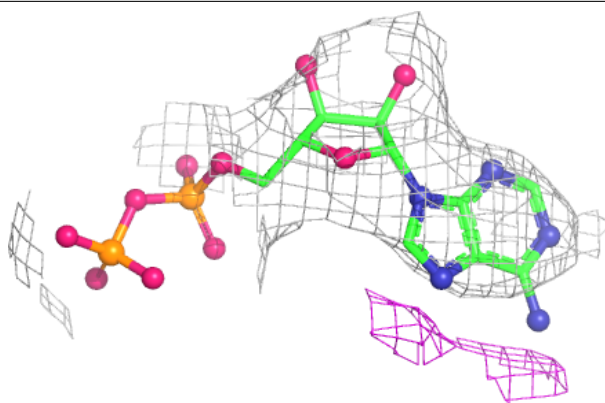
**Electron density around ADP A 9002:**

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

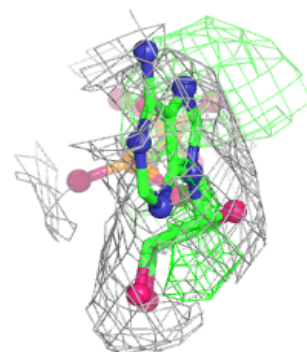
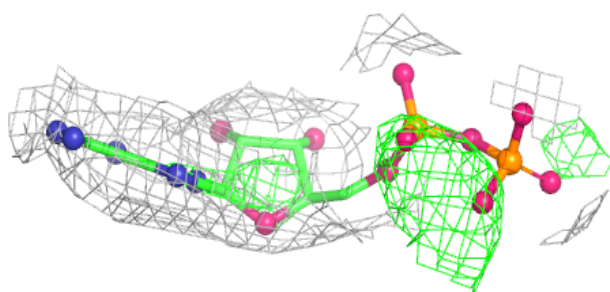
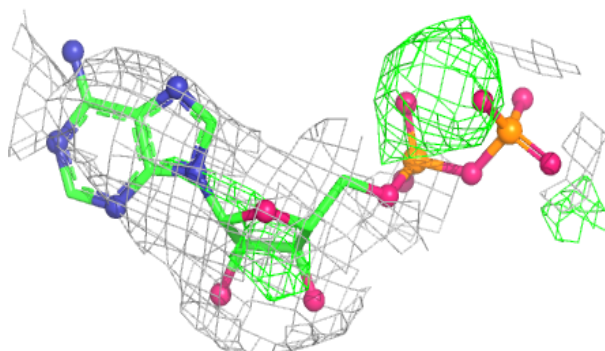


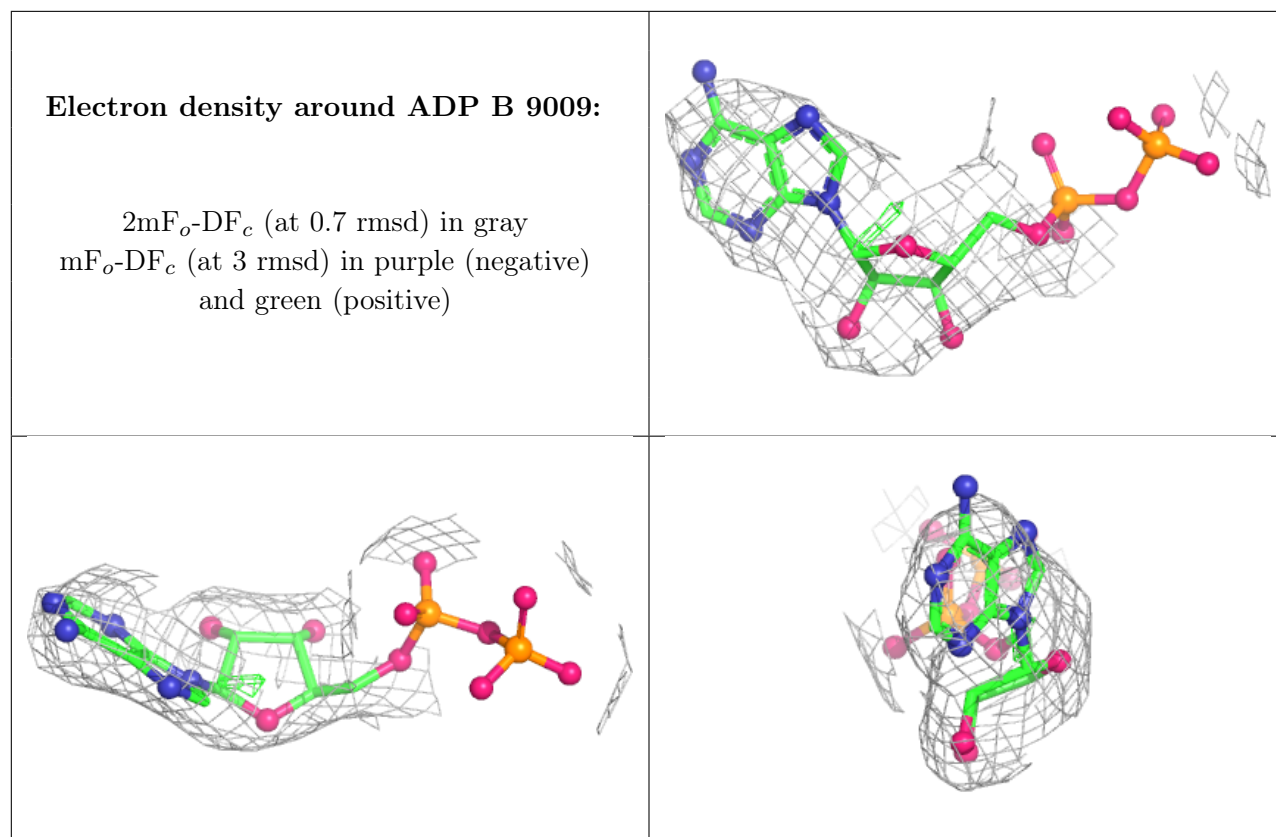
Electron density around ADP A 9003:

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

**Electron density around ADP B 9007:**

$2mF_o-DF_c$ (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.