wwPDB X-ray Structure Validation Summary Report (i)

Nov 3, 2023 – 05:59 AM EDT

PDB ID	:	3VKH
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 (i) 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 (i)) were used in the production of this report:

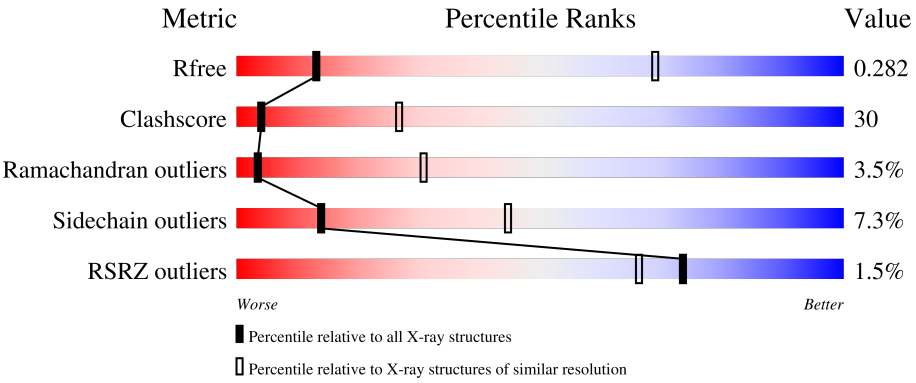
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 <=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	2% 42% 42% 6% 10%
1	B	3367	% 46% 37% • 14%

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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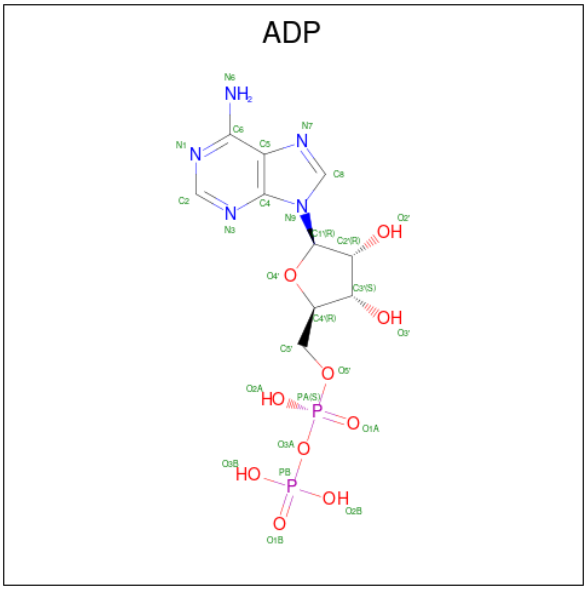
Chain	Residue	Modelled	Actual	Comment	Reference
B	1365	THR	-	expression tag	UNP P34036
B	1366	ARG	-	expression tag	UNP P34036
B	1367	HIS	-	expression tag	UNP P34036
B	1368	HIS	-	expression tag	UNP P34036
B	1369	HIS	-	expression tag	UNP P34036
B	1370	HIS	-	expression tag	UNP P34036
B	1371	HIS	-	expression 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 (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



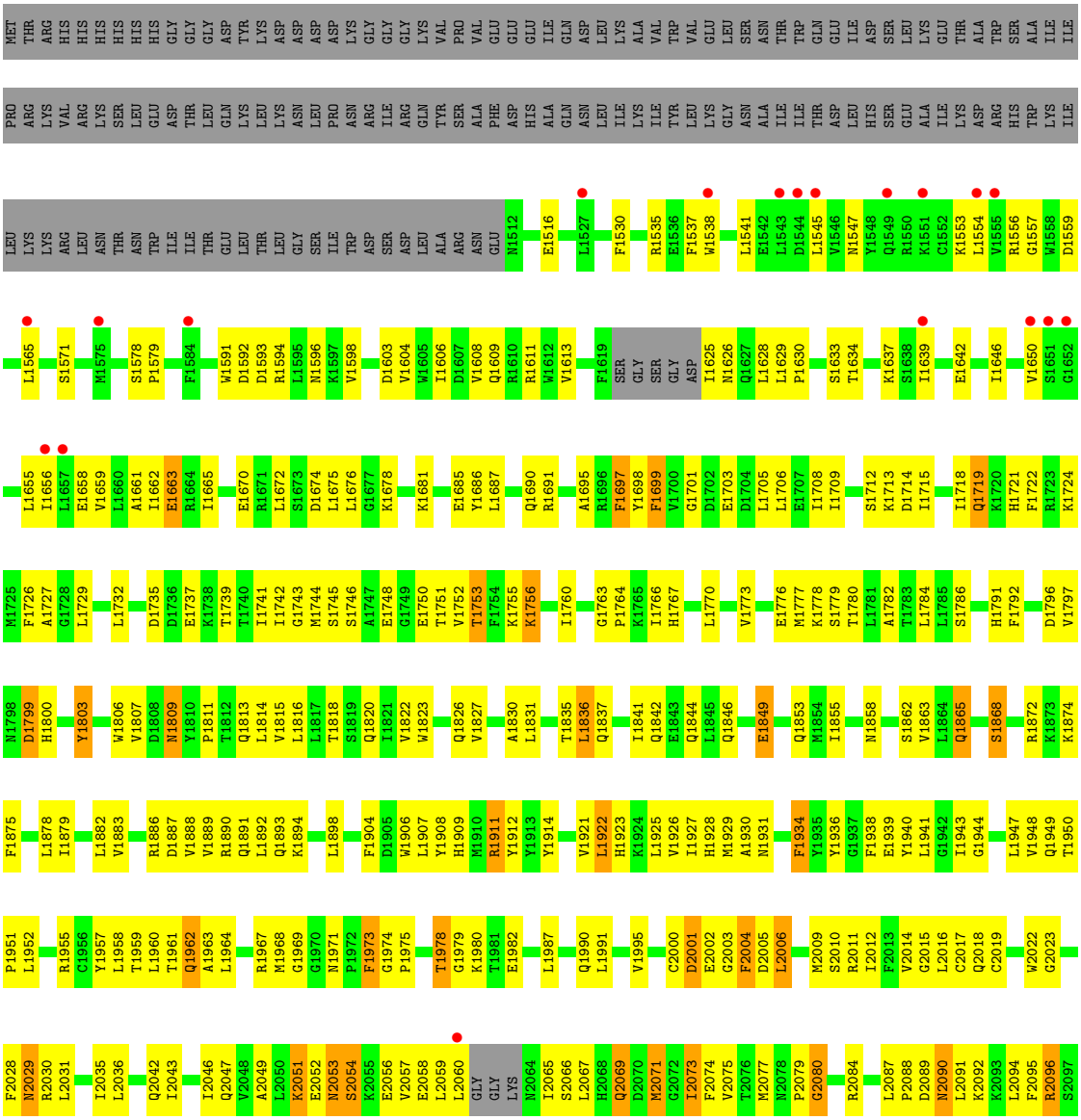
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B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

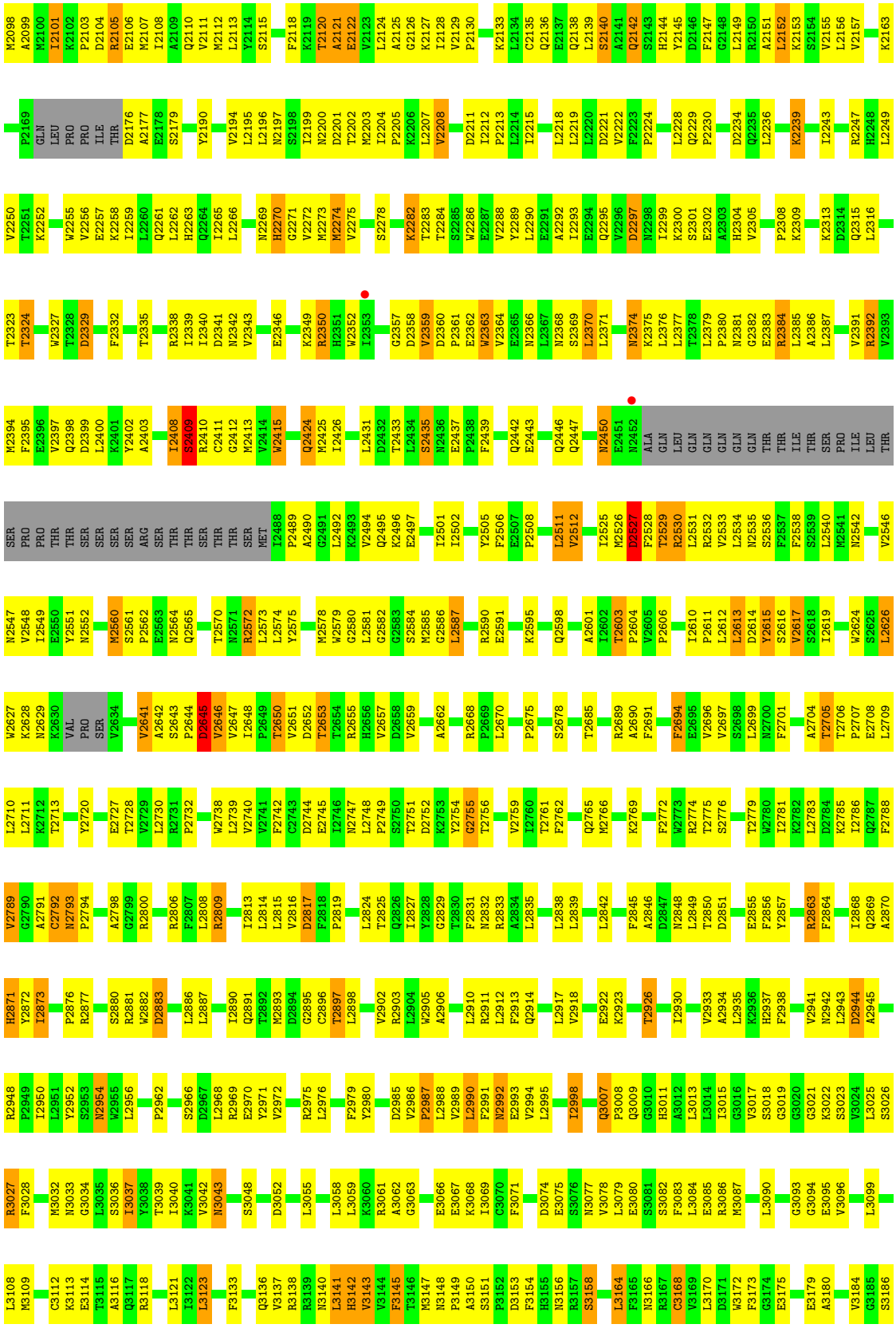
3 Residue-property plots (i)

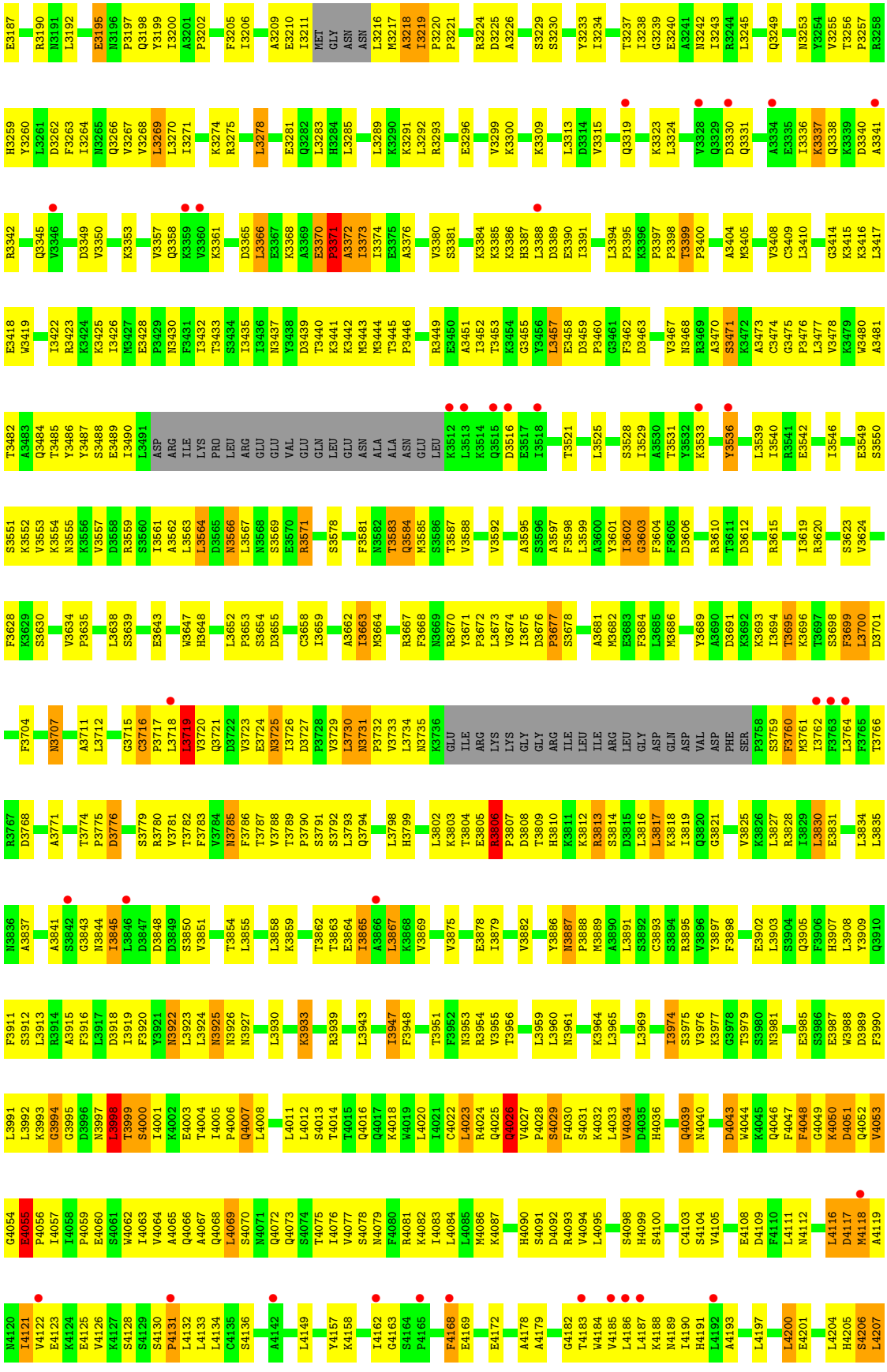
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

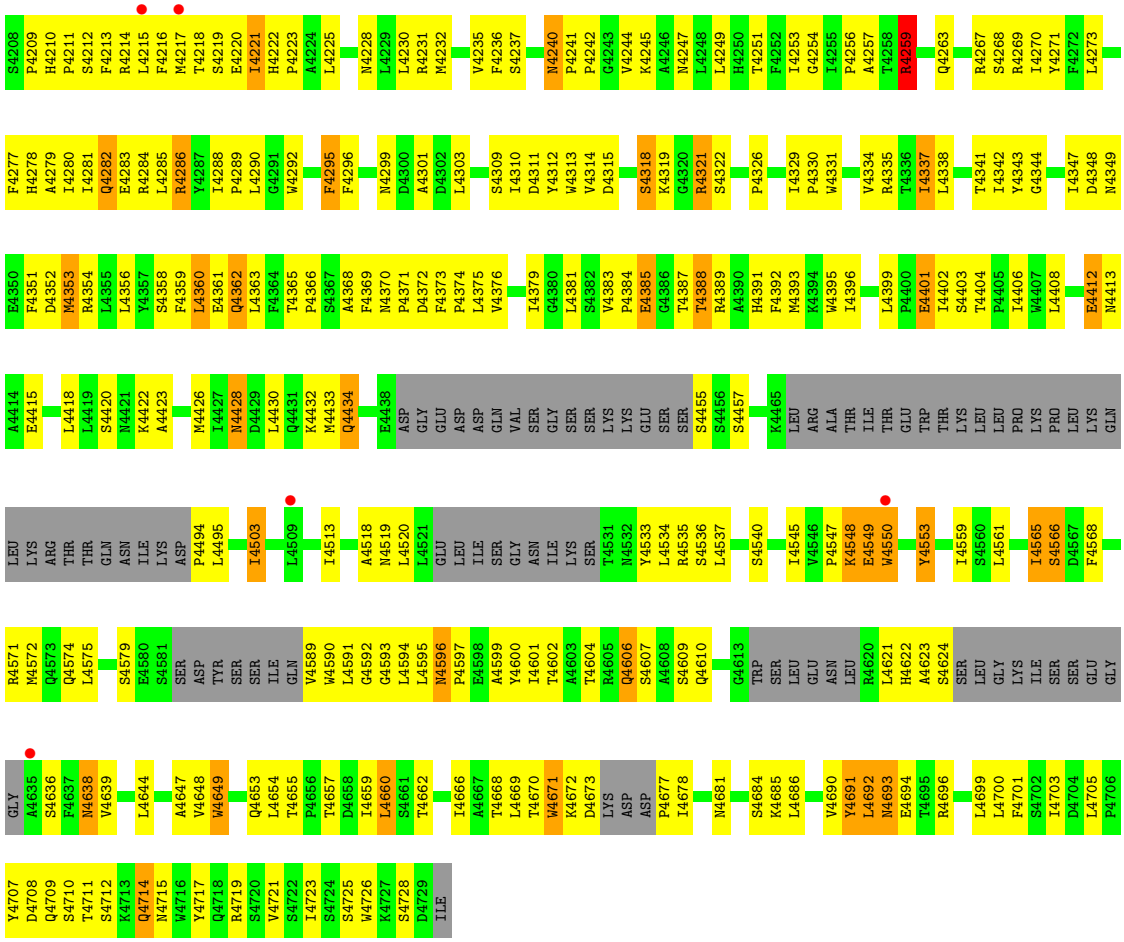
• Molecule 1: Dynein heavy chain, cytoplasmic

Chain A:



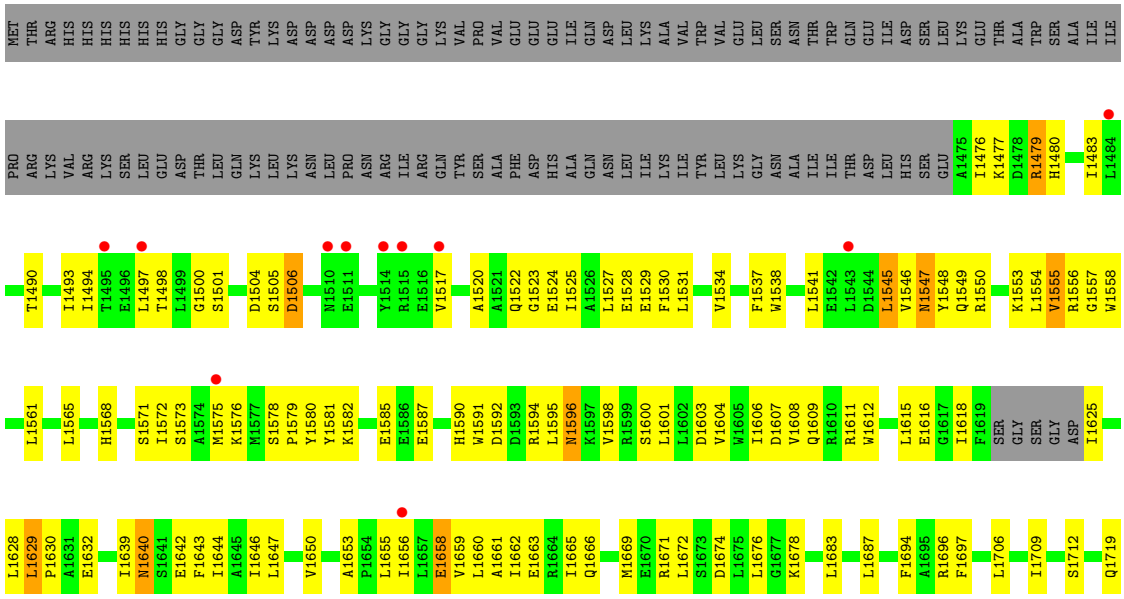


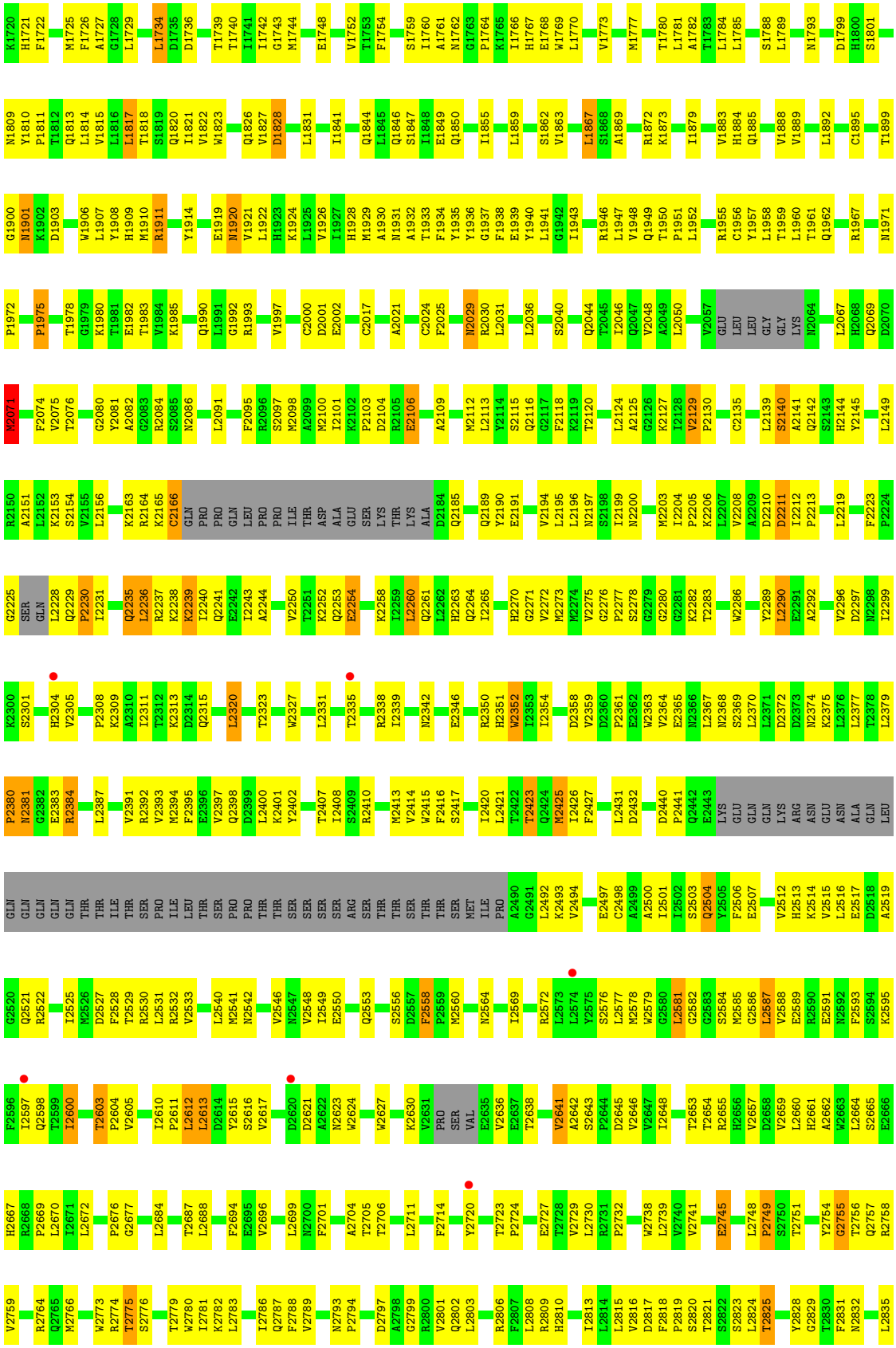


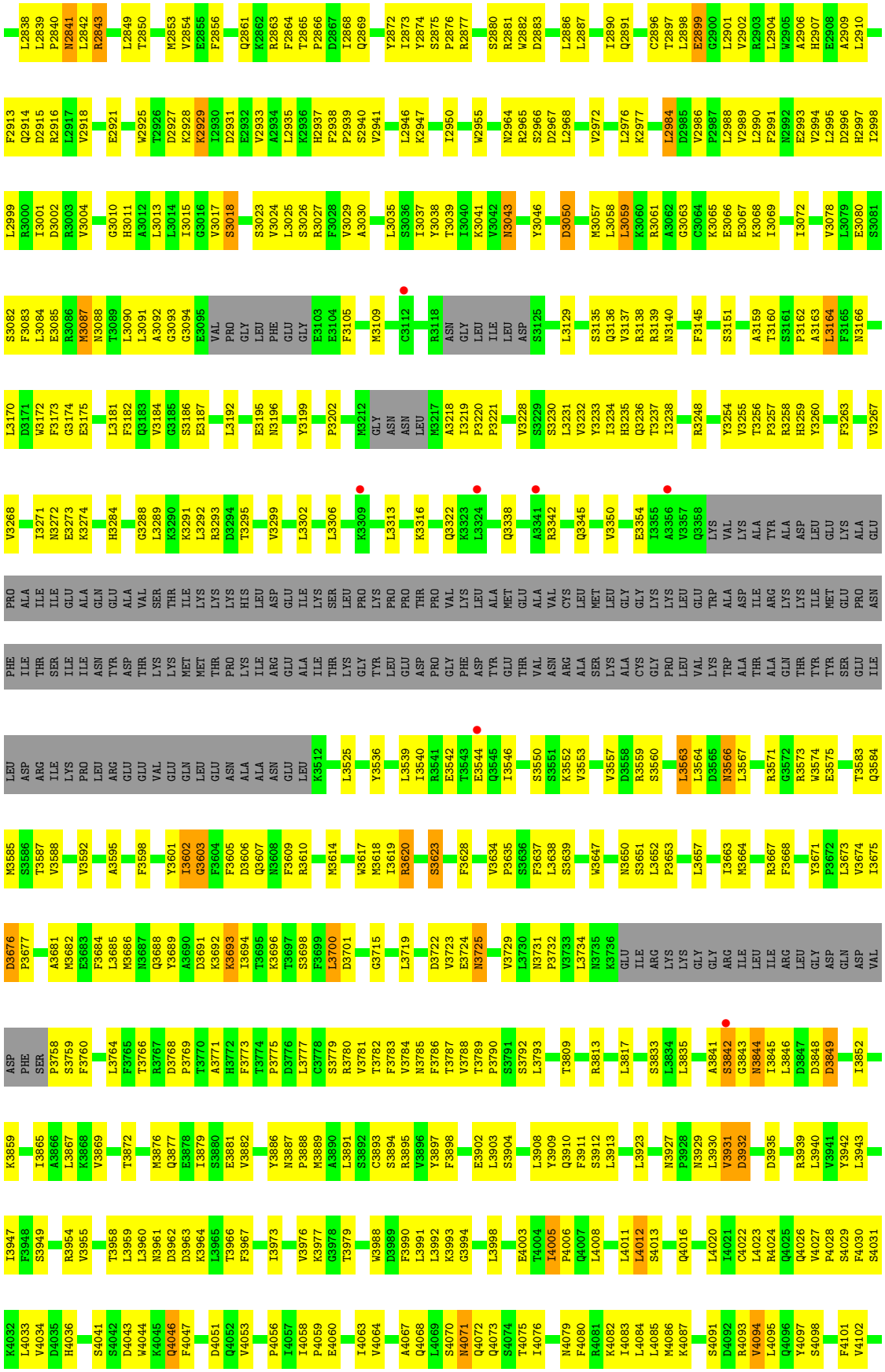


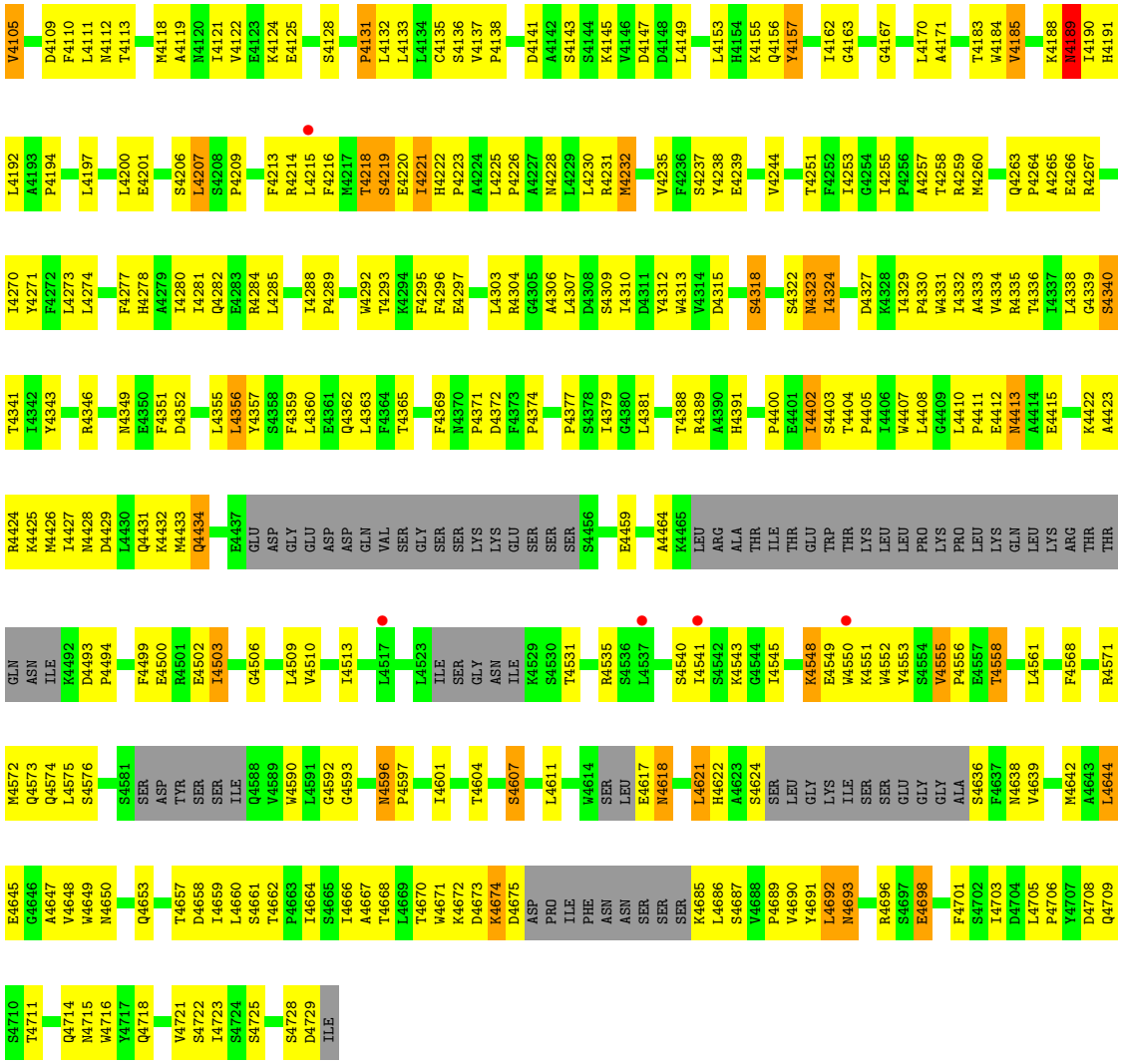
• Molecule 1: Dynein heavy chain, cytoplasmic

Chain B:






L2838 L2839 P2840 N2841 L2842 R2843 L2849 T2850 M2853 V2854 E2855 F2856 Q2861 K2862 R2863 F2864 T2865 P2866 D2867 I2868 Q2869 Y2872 I2873 Y2874 S2875 P2876 R2877 S2880 R2881 W2882 D2883 L2886 L2887 I2890 Q2891 C2896 T2897 L2898 E2899 G2900 L2901 V2902 R2903 L2904 W2905 A2906 H2907 E2908 A2909 L2910
F2913 Q2914 D2915 R2916 L2917 V2918 E2921 W2925 T2926 D2927 K2928 K2929 I2930 D2931 E2932 V2933 A2934 L2935 K2936 H2937 F2938 P2939 S2940 V2941 L2946 K2947 I2950 W2955 N2964 R2965 S2966 D2967 L2968 V2972 L2976 K2977 L2984 D2985 V2986 P2987 L2988 V2989 L2990 F2991 N2992 E2993 V2994 L2995 D2996 H2997 I2998
L2999 R3000 I3001 D3002 R3003 V3004 G3010 H3011 A3012 L3013 L3014 I3015 G3016 V3017 S3018 S3023 V3024 L3025 S3026 R3027 F3028 V3029 A3030 L3035 S3036 I3037 Y3038 T3039 I3040 K3041 V3042 N3043 Y3046 D3050 M3057 L3058 L3059 K3060 R3061 A3062 G3063 G3064 K3065 E3066 E3067 K3068 I3069 I3072 V3078 L3079 E3080 S3081
S3082 F3083 L3084 E3085 R3086 M3087 N3088 T3089 L3090 L3091 A3092 G3093 G3094 E3095 VAL PRO GLY LEU PHE GLU GLY E3103 E3104 F3105 M3109 C3112 R3118 ASN GLY LEU ILE LEU ASP S3125 L3129 S3135 Q3136 V3137 R3138 R3139 N3140 F3145 S3151 A3159 T3160 S3161 P3162 A3163 L3164 F3165 N3166
L3170 D3171 W3172 F3173 G3174 E3175 L3181 F3182 Q3183 V3184 G3185 S3186 E3187 L3192 E3195 N3196 Y3199 P3202 M3212 GLY ASN ASN LEU M3217 A3218 I3219 P3220 P3221 V3228 S3229 S3230 L3231 V3232 Y3233 I3234 H3235 Q3236 T3237 I3238 R3248 Y3254 V3255 T3256 P3257 R3258 H3259 Y3260 F3263 V3267
V3268 I3271 N3272 E3273 K3274 H3284 G3288 L3289 K3290 K3291 L3292 R3293 D3294 T3295 V3299 L3302 L3306 K3309 L3313 K3316 Q3322 K3323 L3324 Q3338 A3341 R3342 Q3345 V3350 E3354 I3355 A3356 V3357 Q3358 LYS VAL LYS ALA TYR ALA ASP LEU GLU LYS ALA GLU
PRO ALA ILE ILE GLU ALA GLN GLU GLU ALA VAL SER THR ILE LYS LYS LYS HIS LEU ASP GLU ILE LYS SER LEU PRO LYS PRO PRO THR PRO VAL LYS LEU ALA MET GLU ALA VAL CYS LEU MET LEU GLY GLY LYS LYS LEU LEU GLU TRP ALA ASP ILE ARG LYS LYS ILE MET GLU PRO ASN
PHE ILE THR SER ILE ILE ASN TYR ASP THR LYS LYS MET MET THR PRO LYS ILE ARG GLU ALA ILE THR LYS GLY TYR LEU GLU ASP PRO GLY TYR ASP ASP TYR GLU THR VAL ASN ARG ALA SER LYS ALA CYS GLY PRO LEU VAL LYS TRP ALA ALA THR ALA GLN THR TYR TYR SER GLU ILE
LEU ASP ARG ILE LYS PRO LEU ARG GLU VAL GLU GLN LEU GLU GLU ASN ALA ALA ASN GLU LEU K3512 L3525 Y3536 L3539 I3540 R3541 E3542 T3543 E3544 Q3545 I3546 S3550 S3551 K3552 V3553 V3557 D3558 R3559 S3560 L3563 L3564 D3565 N3566 L3567 R3571 G3572 R3573 W3574 E3575 T3583 Q3584
M3585 S3586 T3587 V3588 V3592 A3595 F3598 Y3601 I3602 G3603 F3604 F3605 D3606 Q3607 M3608 F3609 R3610 M3614 W3617 M3618 I3619 R3620 S3623 F3628 V3634 P3635 S3636 F3637 L3638 S3639 W3647 N3650 S3651 L3652 P3653 L3657 I3663 M3664 R3667 F3668 Y3671 P3672 L3673 V3674 I3675
D3676 P3677 A3681 M3682 E3683 F3684 L3685 M3686 N3687 Q3688 Y3689 A3690 D3691 K3692 K3693 I3694 T3695 K3696 T3697 S3698 F3699 L3700 D3701 G3715 L3719 D3722 V3723 E3724 N3725 V3729 L3730 N3731 P3732 V3733 L3734 N3735 K3736 GLU ILE ARG LYS GLY GLY ARG ILE LEU ILE ARG LEU GLY ASP GLN ASP VAL
ASP PHE SER P3758 S3759 F3760 L3764 F3765 T3766 R3767 D3768 P3769 T3770 A3771 H3772 F3773 T3774 P3775 D3776 L3777 C3778 S3779 R3780 V3781 T3782 F3783 V3784 N3785 F3786 T3787 V3788 T3789 P3790 S3791 S3792 L3793 T3809 R3813 L3817 S3833 L3834 L3835 A3841 S3842 G3843 N3844 I3845 L3846 D3847 D3848 D3849 I3852
K3859 I3865 A3866 L3867 K3868 V3869 T3872 M3876 Q3877 E3878 I3879 S3880 E3881 V3882 Y3886 N3887 P3888 M3889 A3890 L3891 S3892 C3893 S3894 R3895 V3896 Y3897 F3898 E3902 L3903 S3904 L3908 Y3909 Q3910 F3911 S3912 L3913 L3923 N3927 P3928 N3929 L3930 V3931 D3932 D3935 R3939 L3940 V3941 Y3942 L3943
I3947 F3948 S3949 R3954 V3955 T3958 L3959 L3960 N3961 D3962 D3963 K3964 L3965 T3966 F3967 I3973 V3976 K3977 G3978 T3979 W3988 D3989 F3990 L3991 L3992 K3993 G3994 L3998 E4003 T4004 I4005 P4006 Q4007 L4008 L4011 L4012 S4013 Q4016 L4020 I4021 C4022 L4023 R4024 Q4025 Q4026 V4027 P4028 S4029 S4031
K4032 L4033 V4034 D4035 H4036 S4041 S4042 D4043 W4044 K4045 Q4046 F4047 D4051 Q4052 V4053 P4056 I4057 I4058 P4059 E4060 I4063 V4064 A4067 Q4068 L4069 S4070 N4071 Q4072 Q4073 S4074 T4075 I4076 N4079 F4080 R4081 K4082 I4083 L4084 L4085 M4086 K4087 S4091 D4092 R4093 V4094 L4095 Q4096 Y4097 S4098 F4101 V4102


V4106 D4109 F4110 L4111 N4112 T4113 M4118 A4119 N4120 I4121 V4122 E4123 K4124 E4125 S4128 P4131 L4132 L4133 L4134 C4135 S4136 V4137 P4138 D4141 A4142 S4143 S4144 K4145 V4146 D4147 D4148 L4149 L4153 H4154 K4155 Q4156 Y4157 I4162 G4163 G4167 L4170 A4171 T4183 W4184 V4185 K4188 N4189 I4190 H4191
L4192 A4193 P4194 L4197 L4200 E4201 S4206 L4207 S4208 P4209 F4213 R4214 L4215 F4216 M4217 T4218 S4219 E4220 I4221 H4222 P4223 A4224 L4225 P4226 A4227 N4228 L4229 L4230 R4231 M4232 V4235 F4236 S4237 Y4238 E4239 V4244 T4251 F4252 I4253 G4254 I4255 P4256 A4257 T4258 R4259 M4260 Q4263 P4264 A4265 E4266 R4267
I4270 Y4271 F4272 L4273 L4274 F4277 H4278 A4279 I4280 I4281 Q4282 E4283 R4284 L4285 I4288 P4289 W4292 T4293 K4294 F4295 F4296 E4297 L4303 R4304 G4305 A4306 L4307 D4308 S4309 I4310 D4311 Y4312 W4313 V4314 D4315 S4318 S4322 N4323 I4324 D4327 K4328 I4329 P4330 W4331 I4332 A4333 V4334 R4335 T4336 I4337 L4338 G4339 S4340
T4341 I4342 Y4343 R4346 N4349 E4350 F4351 D4352 L4355 L4356 Y4357 S4358 F4359 L4360 E4361 Q4362 L4363 F4364 T4365 F4369 N4370 P4371 D4372 F4373 P4374 P4377 S4378 I4379 G4380 L4381 T4388 R4389 A4390 H4391 P4400 E4401 I4402 S4403 T4404 P4405 I4406 W4407 L4408 G4409 L4410 P4411 E4412 N4413 A4414 E4415 K4422 A4423
R4424 K4425 M4426 I4427 N4428 D4429 L4430 Q4431 K4432 M4433 Q4434 E4437 GLU ASP GLY GLU ASP ASP GLN VAL SER GLY SER SER LYS LYS GLU SER SER SER S4456 E4459 A4464 K4465 LEU ARG ALA THR ILE THR GLU TRP THR LYS LEU LEU PRO LYS PRO LEU LYS GLN LEU LYS ARG THR THR
GLN ASN ILE K4492 D4493 P4494 F4499 E4500 R4501 E4502 I4503 G4506 L4509 V4510 I4513 L4517 L4523 ILE SER GLY ASN ILE K4529 S4530 T4531 R4535 S4536 L4537 S4540 I4541 S4542 K4543 G4544 I4545 K4548 E4549 W4550 K4551 W4552 Y4553 S4554 V4555 P4556 E4557 T4558 L4561 F4568 R4571
M4572 Q4573 Q4574 L4575 S4576 S4581 SER ASP TYR SER SER ILE Q4588 V4589 W4590 L4591 G4592 G4593 N4596 P4597 I4601 T4604 S4607 L4611 W4614 SER LEU E4617 N4618 L4621 H4622 A4623 S4624 SER LEU GLY LYS ILE SER SER GLU GLY GLY ALA S4636 F4637 N4638 V4639 M4642 A4643 L4644
E4645 G4646 A4647 V4648 W4649 N4650 Q4653 T4657 D4658 I4659 L4660 S4661 T4662 P4663 I4664 S4665 I4666 A4667 T4668 L4669 T4670 W4671 K4672 D4673 K4674 D4675 ASP PRO ILE PHE ASN ASN SER SER SER K4685 L4686 S4687 V4688 P4689 V4690 Y4691 L4692 N4693 R4696 S4697 E4698 F4701 S4702 I4703 D4704 L4705 P4706 Y4707 D4708 Q4709
S4710 T4711 Q4714 N4715 W4716 Y4717 Q4718 V4721 S4722 I4723 S4724 S4725 S4728 D4729 ILE

4 Data and refinement statistics (i)

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 48.78 – 3.79	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.79-3.80) 99.0 (48.78-3.79)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.52 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.292 0.211 , 0.282	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)	0.28 , 112.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.24	0/23866	0.44	1/32482 (0.0%)
1	B	0.24	0/22846	0.43	0/31076
All	All	0.24	0/46712	0.44	1/63558 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3371	PRO	N-CA-CB	5.32	109.68	103.30

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	1559	0
1	B	22384	0	21550	1149	0
2	A	108	0	48	7	0
2	B	108	0	48	3	0
All	All	45974	0	44191	2704	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 30.

The worst 5 of 2704 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 24
1	B	2870/3367 (85%)	2476 (86%)	327 (11%)	67 (2%)	6 38
All	All	5880/6734 (87%)	4900 (83%)	775 (13%)	205 (4%)	3 31

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
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%)	2249 (92%)	208 (8%)	10 40
1	B	2353/3028 (78%)	2210 (94%)	143 (6%)	18 50
All	All	4810/6056 (79%)	4459 (93%)	351 (7%)	14 45

5 of 351 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2029	ASN
1	B	3050	ASP
1	B	2189	GLN
1	B	2581	LEU
1	B	3620	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 198 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1568	HIS
1	B	2504	GLN
1	B	1690	GLN
1	B	2029	ASN
1	B	2832	ASN

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 monosaccharides 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	A	9001	-	24,29,29	1.26	3 (12%)	29,45,45	1.57	5 (17%)
2	ADP	B	9010	-	24,29,29	1.24	3 (12%)	29,45,45	1.56	5 (17%)
2	ADP	B	9007	-	24,29,29	1.23	3 (12%)	29,45,45	1.54	5 (17%)
2	ADP	B	9008	-	24,29,29	1.23	3 (12%)	29,45,45	1.55	5 (17%)
2	ADP	A	9003	-	24,29,29	1.26	3 (12%)	29,45,45	1.56	5 (17%)
2	ADP	A	9002	-	24,29,29	1.23	2 (8%)	29,45,45	1.56	5 (17%)
2	ADP	B	9009	-	24,29,29	1.25	3 (12%)	29,45,45	1.56	5 (17%)
2	ADP	A	9004	-	24,29,29	1.23	3 (12%)	29,45,45	1.56	5 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	9001	-	-	5/12/32/32	0/3/3/3
2	ADP	B	9010	-	-	6/12/32/32	0/3/3/3
2	ADP	B	9007	-	-	4/12/32/32	0/3/3/3
2	ADP	B	9008	-	-	2/12/32/32	0/3/3/3
2	ADP	A	9003	-	-	5/12/32/32	0/3/3/3
2	ADP	A	9002	-	-	3/12/32/32	0/3/3/3
2	ADP	B	9009	-	-	5/12/32/32	0/3/3/3
2	ADP	A	9004	-	-	3/12/32/32	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	9002	ADP	C5-C4	2.99	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9008	ADP	C5-C4	2.95	1.48	1.40
2	B	9009	ADP	C5-C4	2.93	1.48	1.40
2	A	9003	ADP	C5-C4	2.93	1.48	1.40
2	A	9004	ADP	C5-C4	2.91	1.48	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	9004	ADP	N3-C2-N1	-4.33	121.91	128.68
2	A	9003	ADP	N3-C2-N1	-4.30	121.96	128.68
2	B	9007	ADP	N3-C2-N1	-4.29	121.97	128.68
2	B	9010	ADP	N3-C2-N1	-4.27	122.00	128.68
2	A	9001	ADP	N3-C2-N1	-4.27	122.00	128.68

There are no chirality outliers.

5 of 33 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	9003	ADP	C5'-O5'-PA-O1A
2	A	9003	ADP	C5'-O5'-PA-O2A
2	B	9007	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

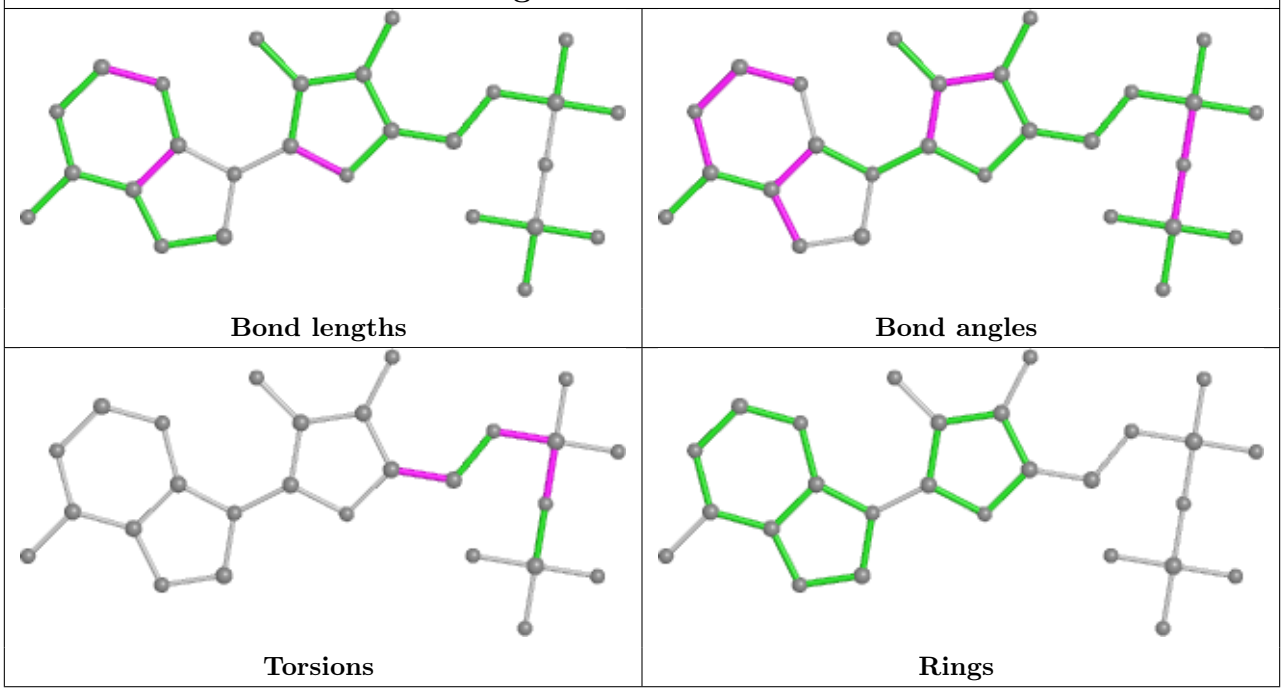
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9001	ADP	1	0
2	B	9010	ADP	2	0
2	A	9002	ADP	4	0
2	B	9009	ADP	1	0
2	A	9004	ADP	2	0

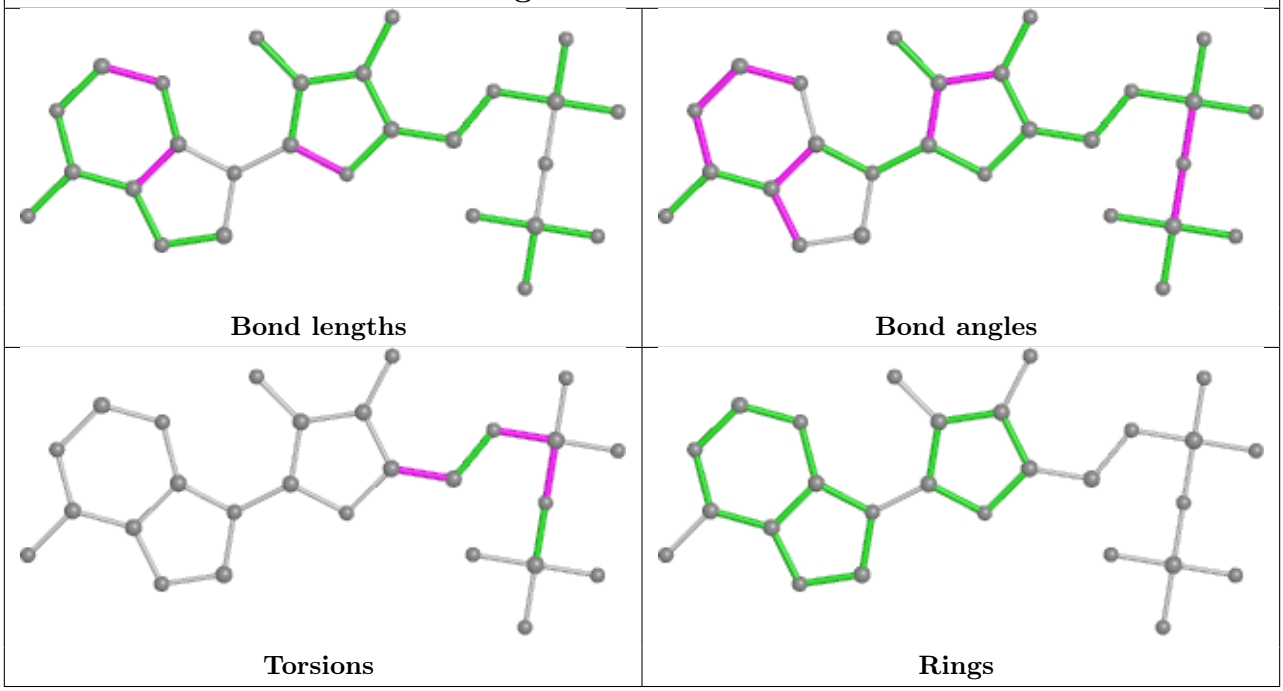
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

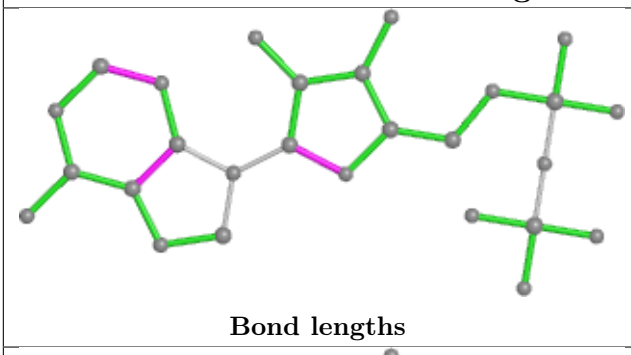
Ligand ADP A 9001



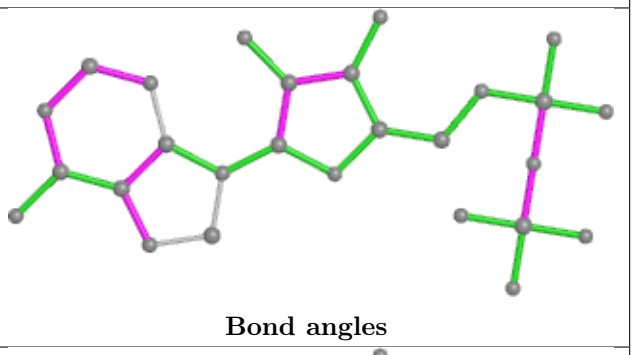
Ligand ADP B 9010



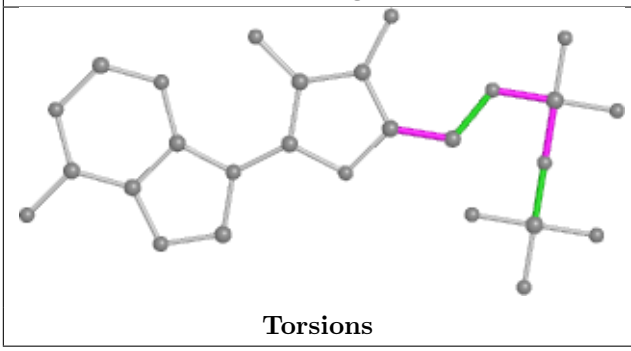
Ligand ADP B 9007



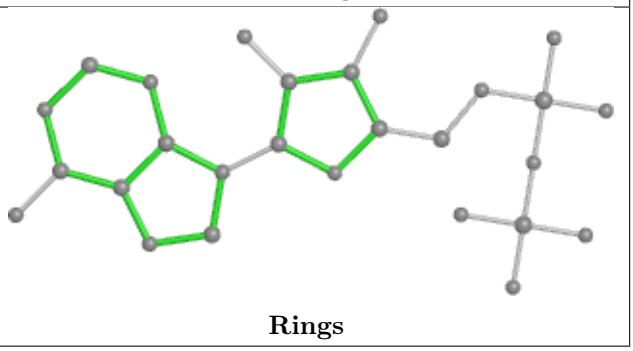
Bond lengths



Bond angles

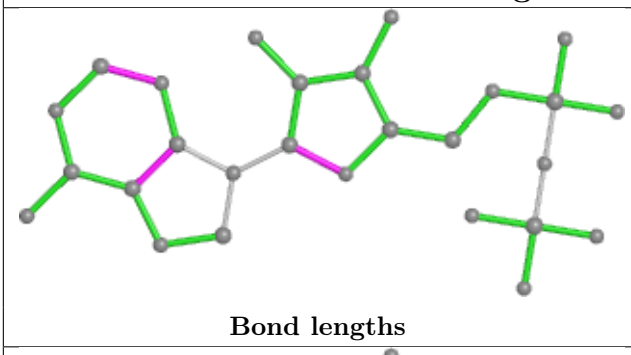


Torsions

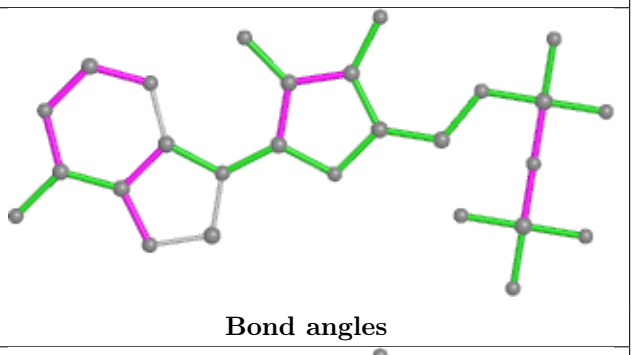


Rings

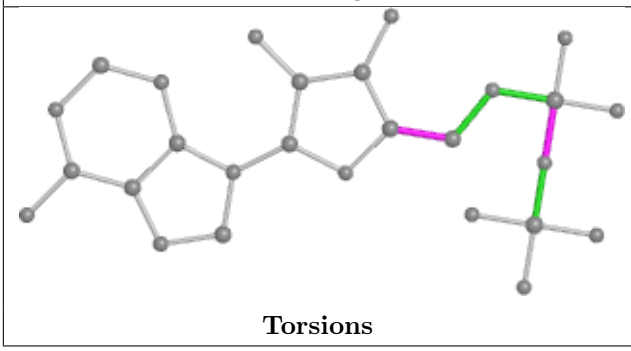
Ligand ADP B 9008



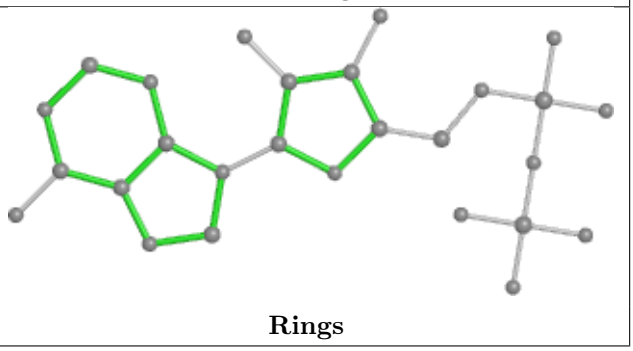
Bond lengths



Bond angles

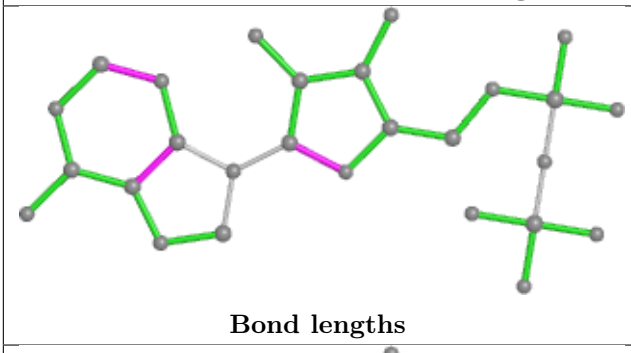


Torsions

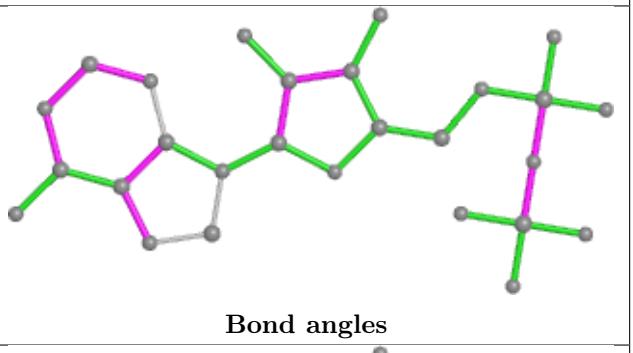


Rings

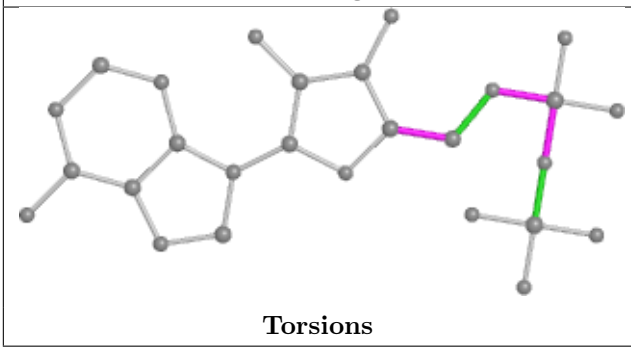
Ligand ADP A 9003



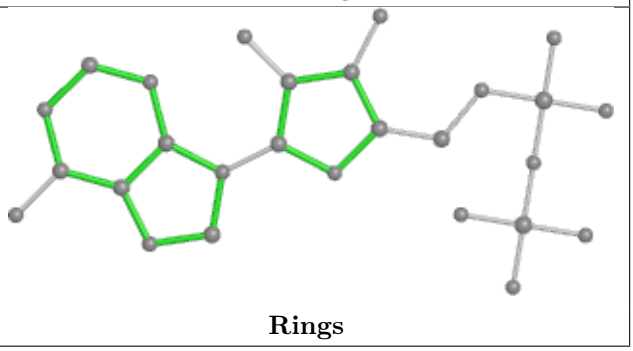
Bond lengths



Bond angles

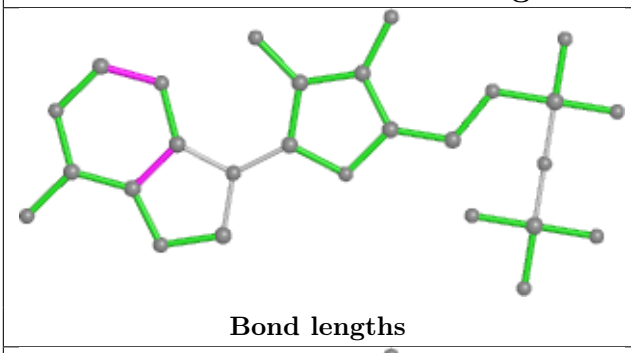


Torsions

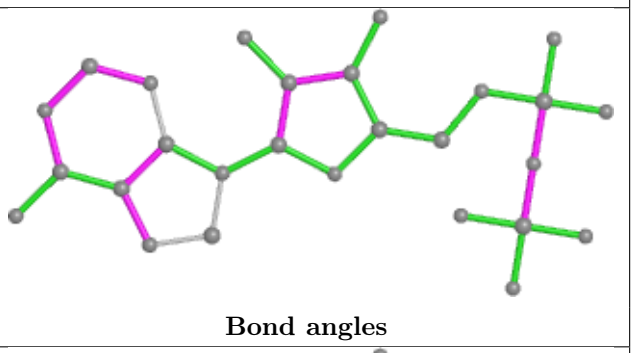


Rings

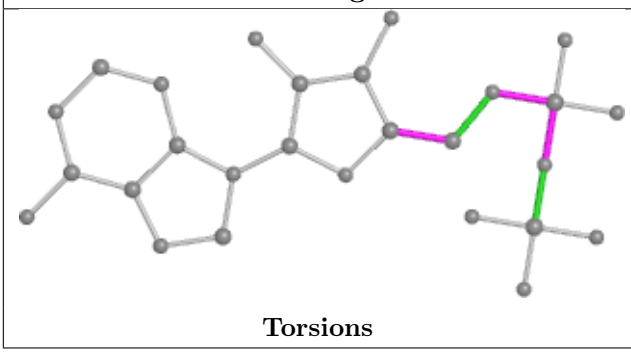
Ligand ADP A 9002



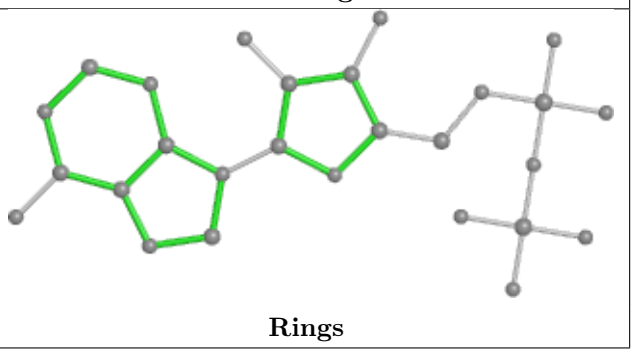
Bond lengths



Bond angles

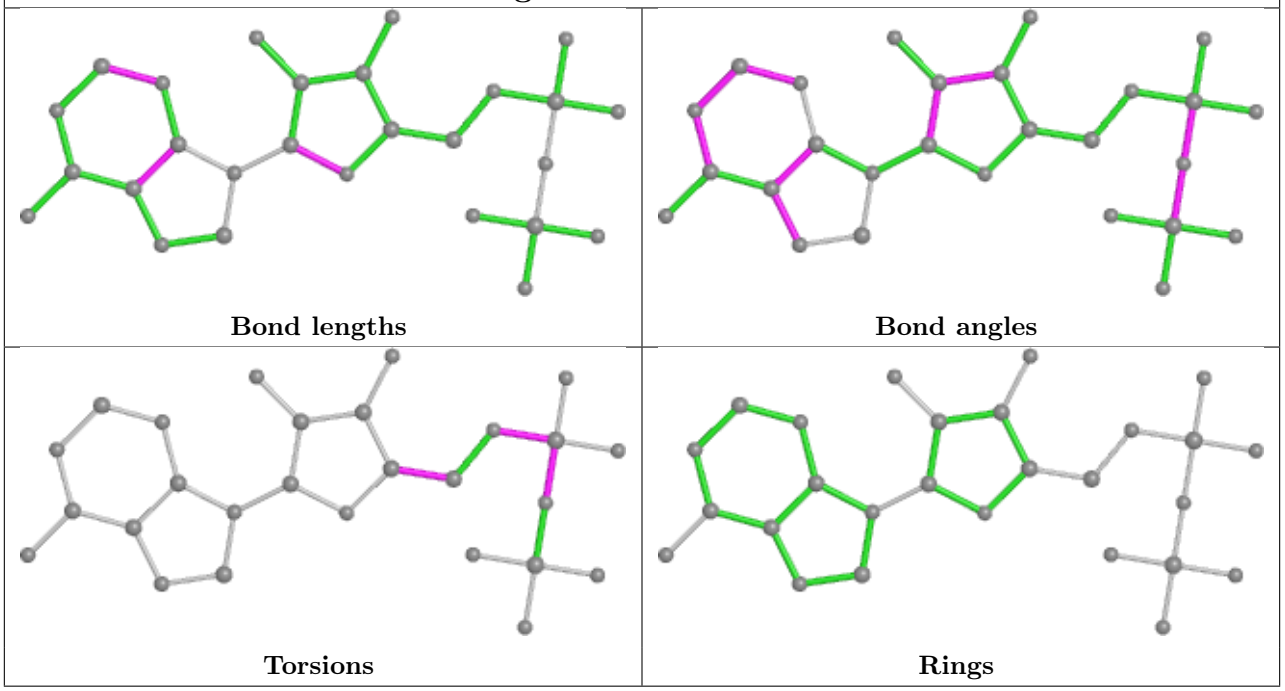


Torsions

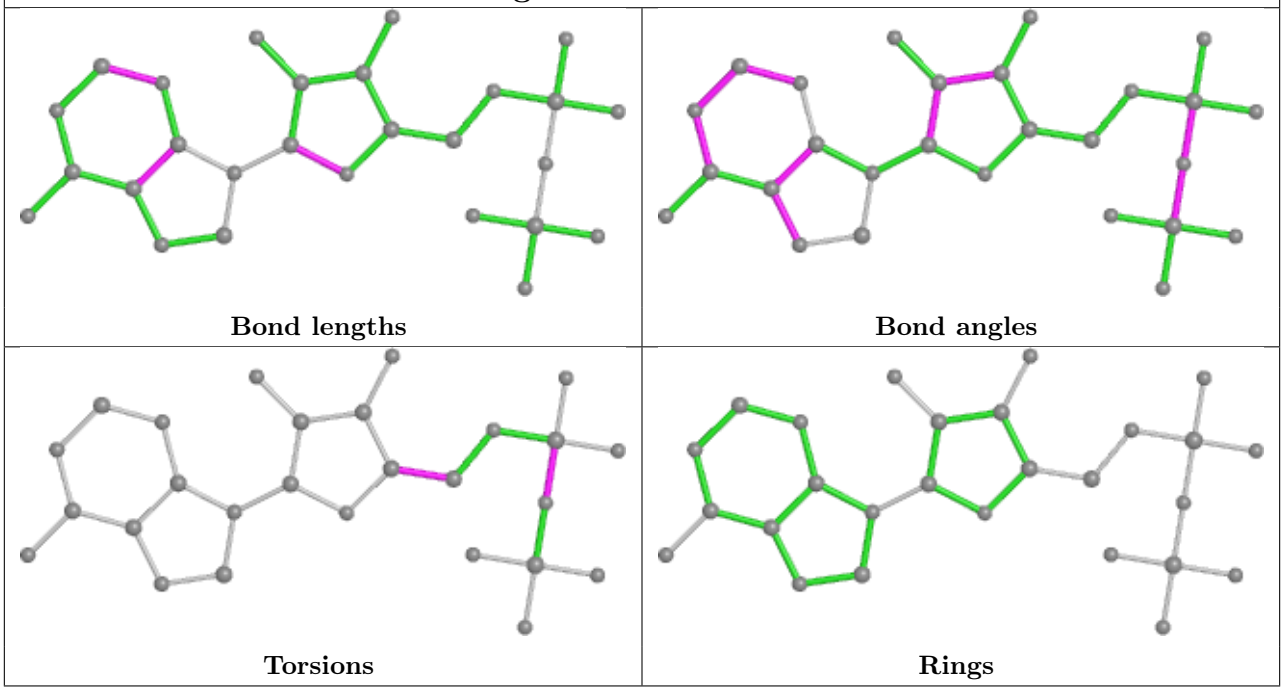


Rings

Ligand ADP B 9009



Ligand ADP A 9004



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

6.1 Protein, DNA and RNA chains

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^{th} 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%)	-0.14	61 (2%)	65	58	64, 130, 209, 322	0
1	B	2908/3367 (86%)	-0.18	29 (0%)	82	76	72, 136, 208, 335	0
All	All	5950/6734 (88%)	-0.16	90 (1%)	73	66	64, 133, 209, 335	0

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1543	LEU	5.7
1	B	1517	VAL	4.8
1	A	1652	GLY	4.7
1	A	4187	LEU	4.5
1	A	1651	SER	4.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

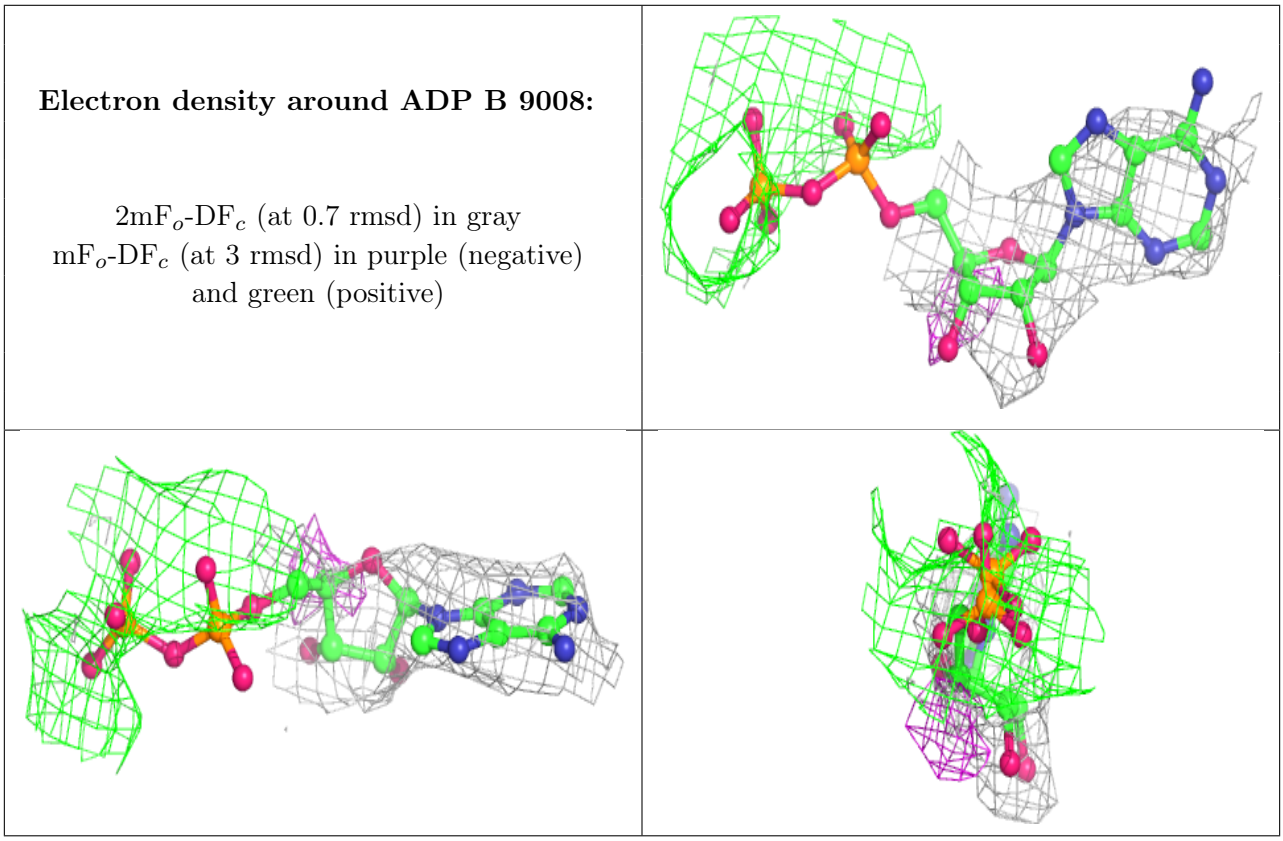
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	B	9008	27/27	0.85	0.40	129,129,129,129	0
2	ADP	B	9010	27/27	0.86	0.31	129,129,129,129	0
2	ADP	A	9002	27/27	0.90	0.30	129,129,129,129	0
2	ADP	B	9007	27/27	0.90	0.37	129,129,129,129	0
2	ADP	A	9004	27/27	0.91	0.30	129,129,129,129	0
2	ADP	A	9003	27/27	0.91	0.33	129,129,129,129	0
2	ADP	A	9001	27/27	0.94	0.38	129,129,129,129	0
2	ADP	B	9009	27/27	0.95	0.31	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.

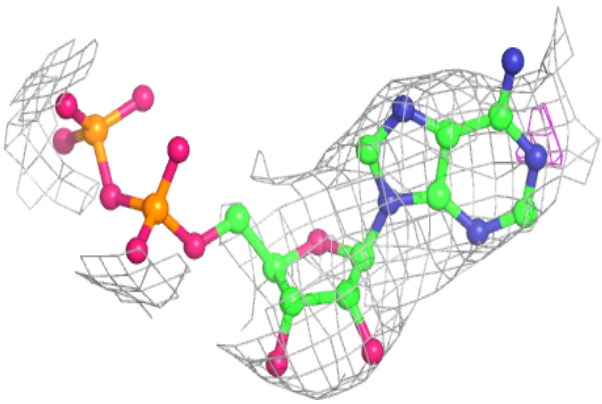
Electron density around ADP B 9008:

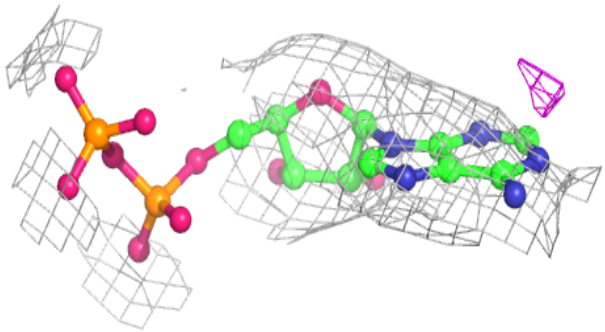
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

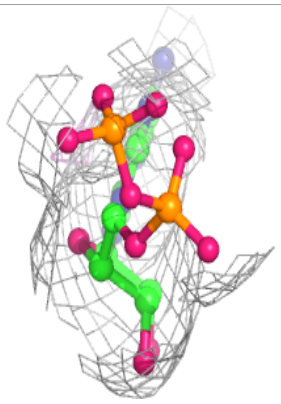


Electron density around ADP B 9010:

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

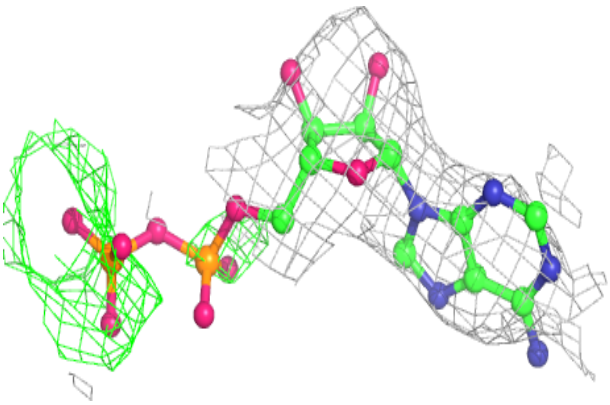


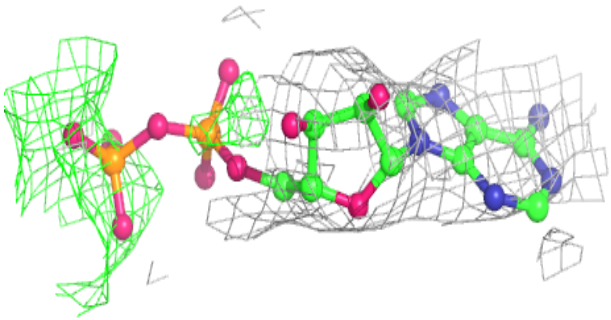


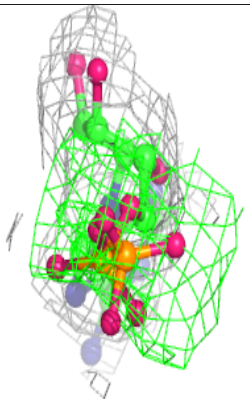


Electron density around ADP A 9002:

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

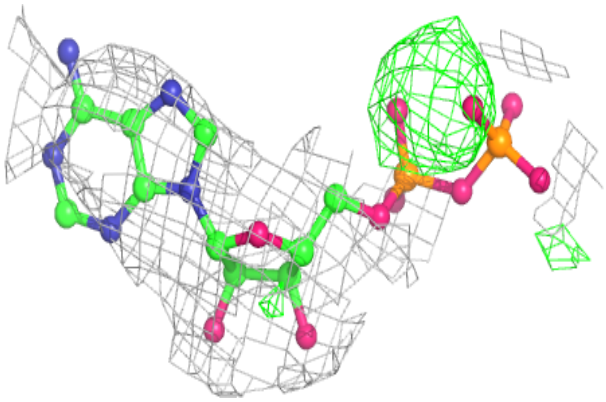


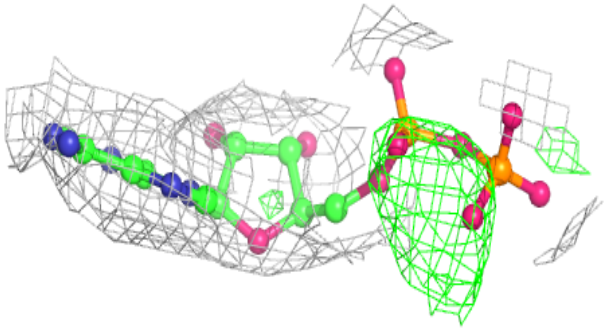


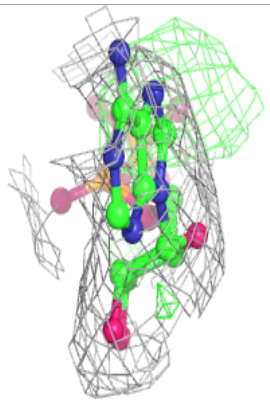


Electron density around ADP B 9007:

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

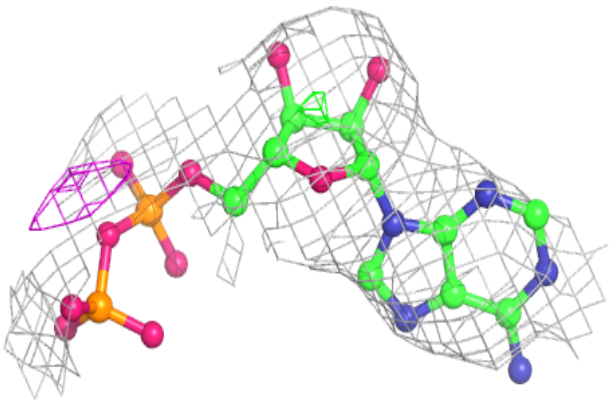


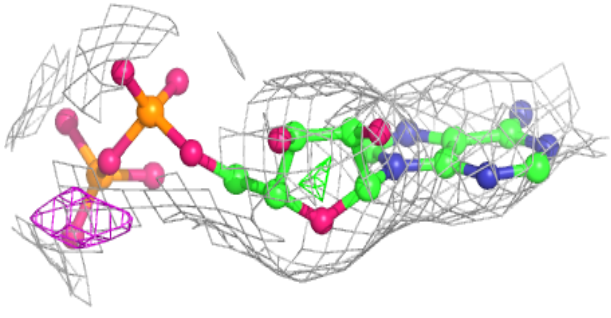


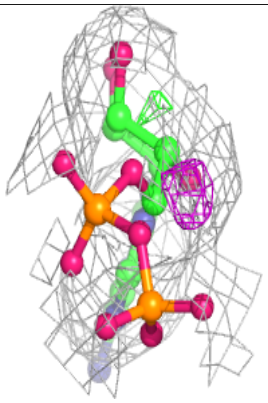


Electron density around ADP A 9004:

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

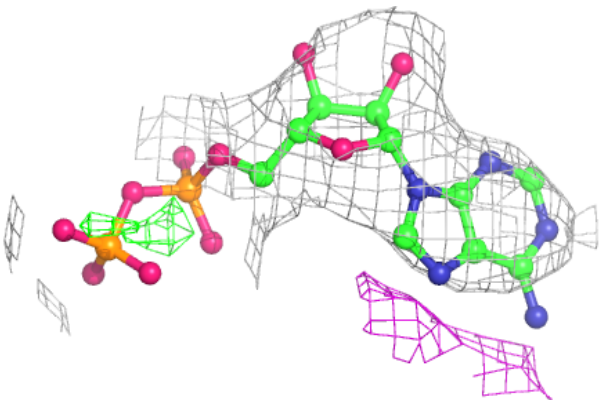


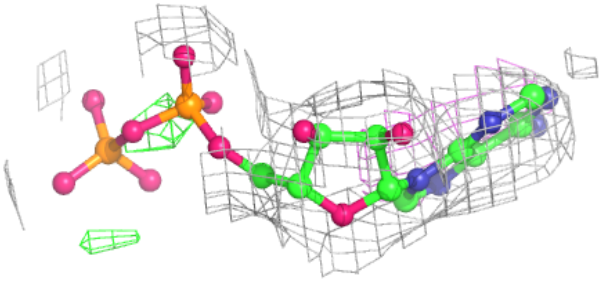


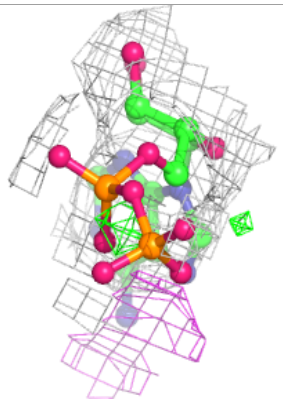


Electron density around ADP A 9003:

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

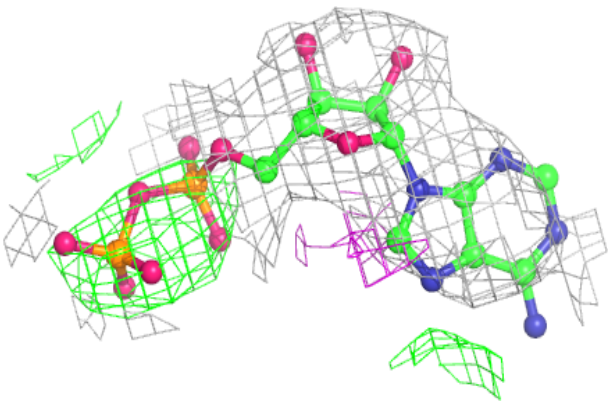


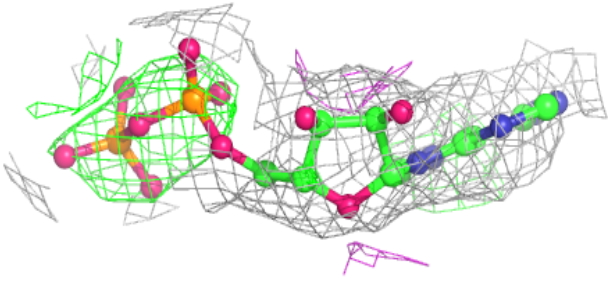


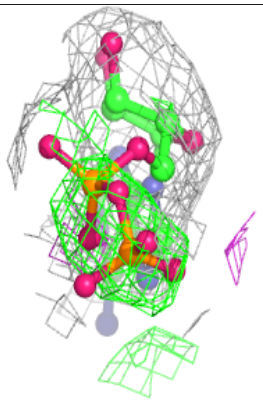


Electron density around ADP A 9001:

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

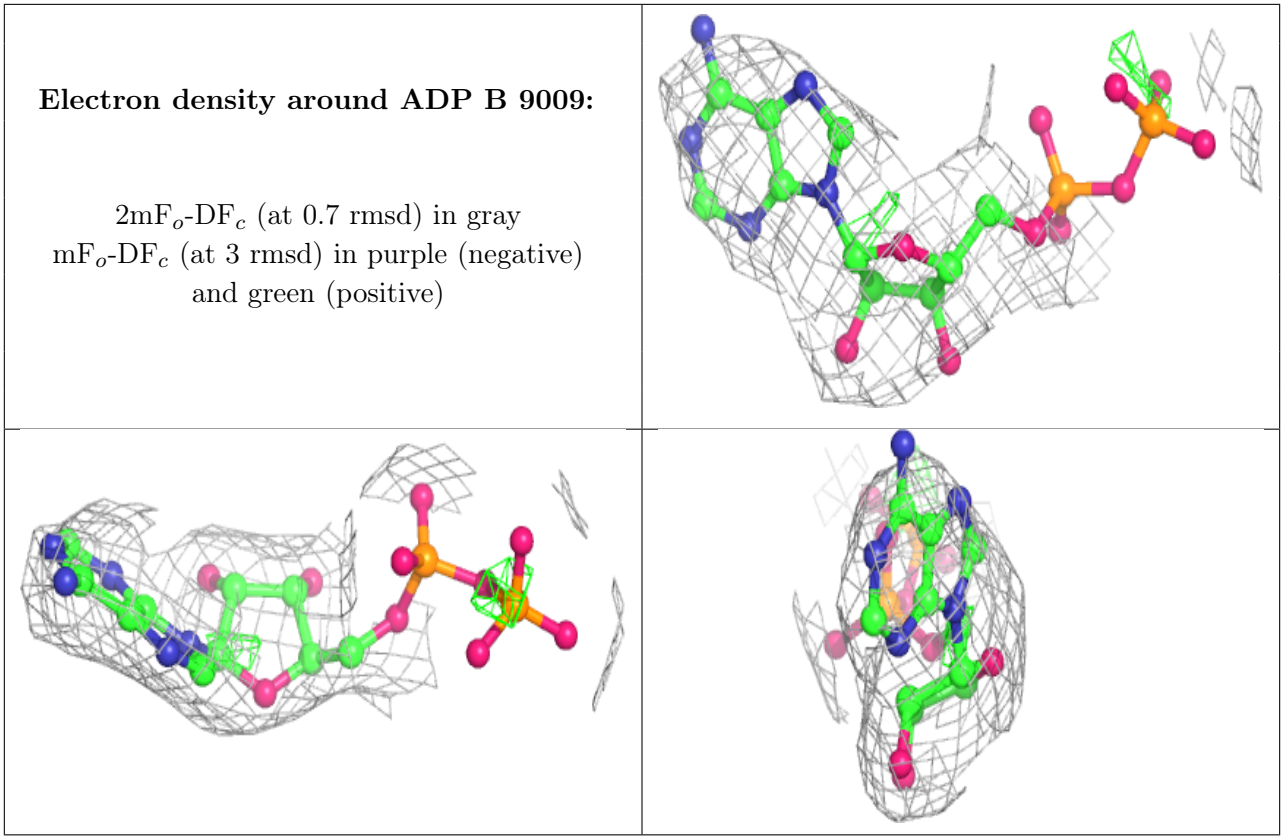






Electron density around ADP B 9009:

$2mF_o$-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.