wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 03:22 PM EST

PDB ID	:	4W8F
Title	:	Crystal structure of the dynein motor domain in the AMPPNP-bound state
Authors	:	Cheng, H.-C.; Bhabha, G.; Zhang, N.; Vale, R.D.
Deposited on	:	2014-08-24
Resolution	:	3.54 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:

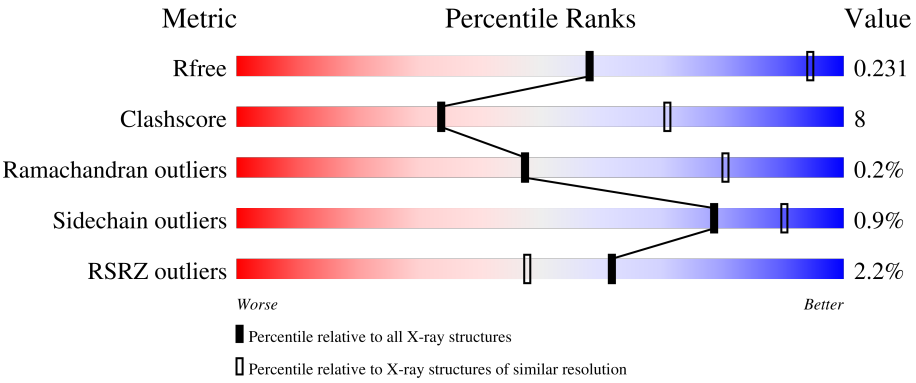
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.54 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	1028 (3.60-3.48)
Clashscore	141614	1109 (3.60-3.48)
Ramachandran outliers	138981	1073 (3.60-3.48)
Sidechain outliers	138945	1074 (3.60-3.48)
RSRZ outliers	127900	1079 (3.62-3.46)

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	2661	2% 79% 19%
1	B	2661	2% 79% 19%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 84822 atoms, of which 42429 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 lysozyme chimera.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	2608	Total	C	H	N	O	S	0	0	0
			42239	13515	21166	3504	3957	97			
1	B	2609	Total	C	H	N	O	S	0	0	0
			42236	13509	21166	3505	3959	97			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1363	GLY	-	expression tag	UNP P36022
A	1849	GLN	GLU	engineered mutation	UNP P36022
A	3120	GLY	-	linker	UNP P36022
A	3121	SER	-	linker	UNP P36022
A	3122	GLY	-	linker	UNP P36022
A	3123	SER	-	linker	UNP P36022
A	3124	GLY	-	linker	UNP P36022
A	3125	SER	-	linker	UNP P36022
A	3136	GLY	ARG	conflict	UNP P00720
A	3178	THR	CYS	conflict	UNP P00720
A	3221	ALA	CYS	conflict	UNP P00720
A	3261	ARG	ILE	conflict	UNP P00720
A	3286	GLY	-	linker	UNP P00720
A	3287	SER	-	linker	UNP P00720
A	3288	GLY	-	linker	UNP P00720
A	3289	SER	-	linker	UNP P00720
A	3290	GLY	-	linker	UNP P00720
A	3291	SER	-	linker	UNP P00720
A	3742	ASP	ASN	conflict	UNP P36022
A	3895	VAL	PHE	conflict	UNP P36022
A	4072	ASP	ASN	conflict	UNP P36022
A	4093	GLY	-	linker	UNP P36022
A	4094	SER	-	linker	UNP P36022
A	4095	GLY	-	linker	UNP P36022
A	4096	SER	-	linker	UNP P36022

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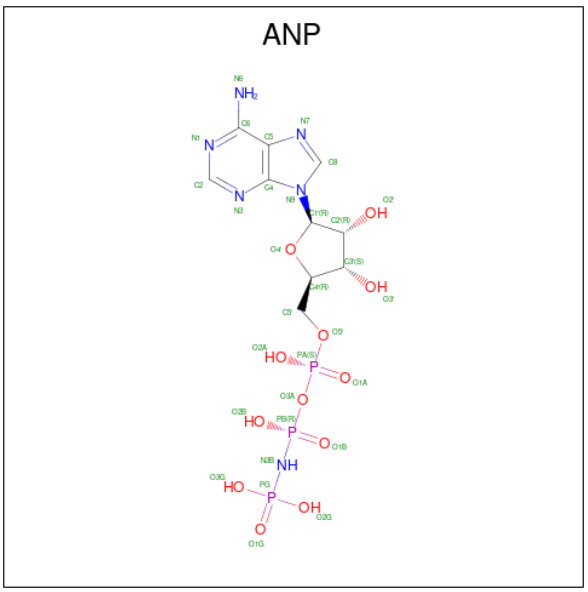
Chain	Residue	Modelled	Actual	Comment	Reference
A	4097	GLY	-	linker	UNP P36022
A	4098	SER	-	linker	UNP P36022
A	4099	HIS	-	expression tag	UNP P36022
A	4100	HIS	-	expression tag	UNP P36022
A	4101	HIS	-	expression tag	UNP P36022
A	4102	HIS	-	expression tag	UNP P36022
A	4103	HIS	-	expression tag	UNP P36022
A	4104	HIS	-	expression tag	UNP P36022
B	1363	GLY	-	expression tag	UNP P36022
B	1849	GLN	GLU	engineered mutation	UNP P36022
B	3120	GLY	-	linker	UNP P36022
B	3121	SER	-	linker	UNP P36022
B	3122	GLY	-	linker	UNP P36022
B	3123	SER	-	linker	UNP P36022
B	3124	GLY	-	linker	UNP P36022
B	3125	SER	-	linker	UNP P36022
B	3136	GLY	ARG	conflict	UNP P00720
B	3178	THR	CYS	conflict	UNP P00720
B	3221	ALA	CYS	conflict	UNP P00720
B	3261	ARG	ILE	conflict	UNP P00720
B	3286	GLY	-	linker	UNP P00720
B	3287	SER	-	linker	UNP P00720
B	3288	GLY	-	linker	UNP P00720
B	3289	SER	-	linker	UNP P00720
B	3290	GLY	-	linker	UNP P00720
B	3291	SER	-	linker	UNP P00720
B	3742	ASP	ASN	conflict	UNP P36022
B	3895	VAL	PHE	conflict	UNP P36022
B	4072	ASP	ASN	conflict	UNP P36022
B	4093	GLY	-	linker	UNP P36022
B	4094	SER	-	linker	UNP P36022
B	4095	GLY	-	linker	UNP P36022
B	4096	SER	-	linker	UNP P36022
B	4097	GLY	-	linker	UNP P36022
B	4098	SER	-	linker	UNP P36022
B	4099	HIS	-	expression tag	UNP P36022
B	4100	HIS	-	expression tag	UNP P36022
B	4101	HIS	-	expression tag	UNP P36022
B	4102	HIS	-	expression tag	UNP P36022
B	4103	HIS	-	expression tag	UNP P36022
B	4104	HIS	-	expression tag	UNP P36022

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter

code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			43	10	12	6	12	3		
2	A	1	Total	C	H	N	O	P	0	0
			43	10	12	6	12	3		
2	A	1	Total	C	H	N	O	P	0	0
			43	10	12	6	12	3		
2	A	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		
2	B	1	Total	C	H	N	O	P	0	0
			43	10	12	6	12	3		
2	B	1	Total	C	H	N	O	P	0	0
			43	10	12	6	12	3		
2	B	1	Total	C	H	N	O	P	0	0
			43	10	12	6	12	3		
2	B	1	Total	C	H	N	O	P	0	0
			43	10	12	6	12	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

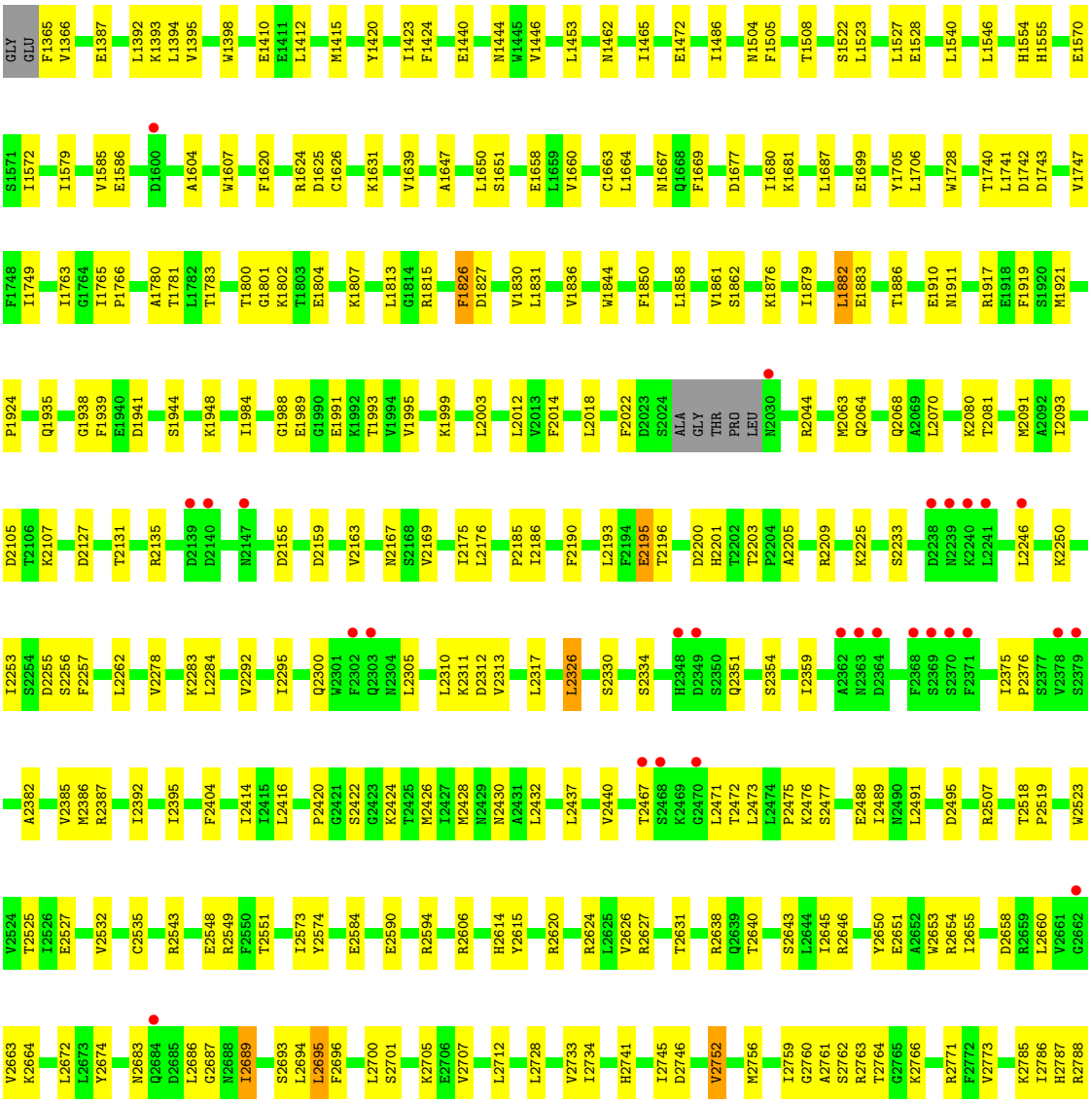
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

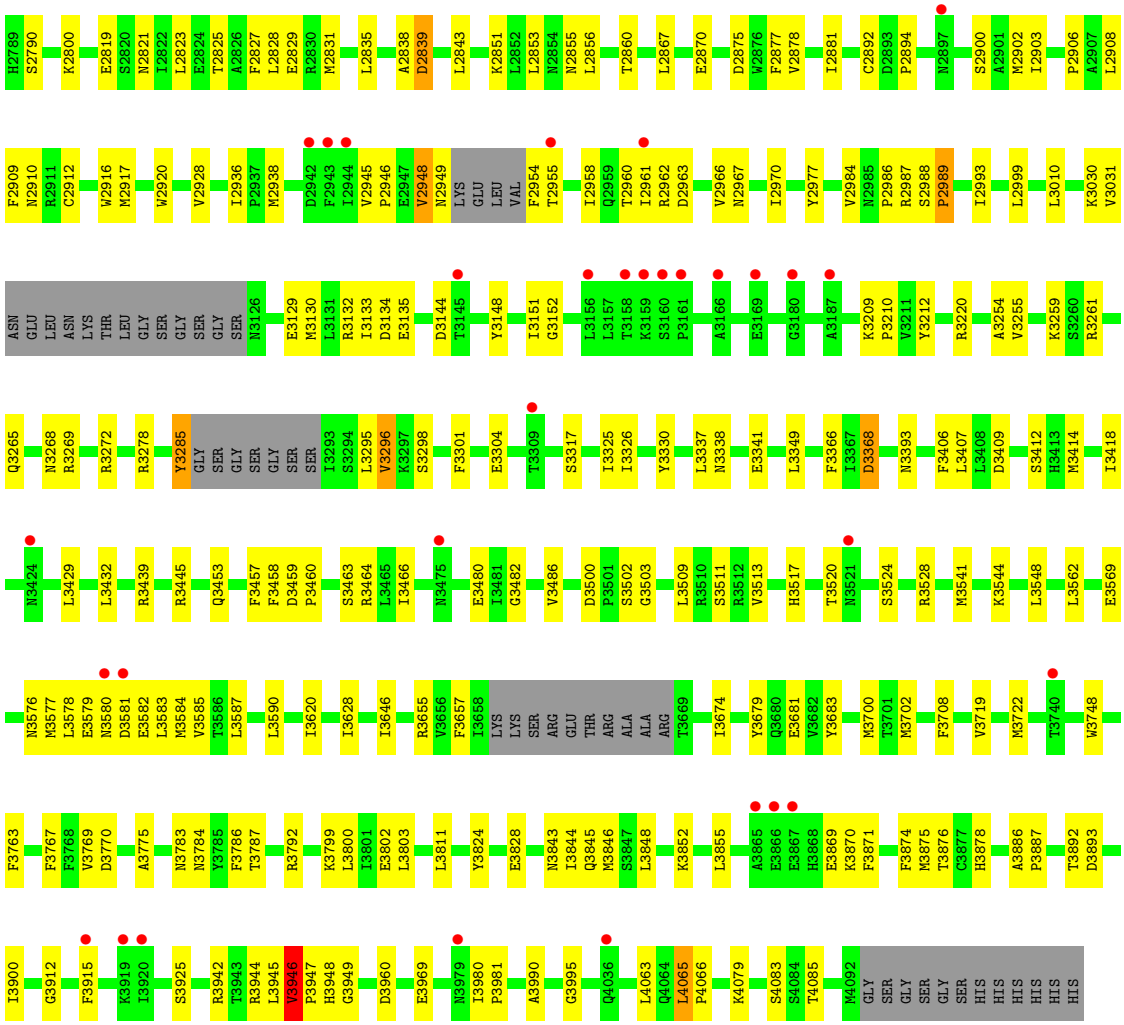
3 Residue-property plots (i)

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 lysozyme chimera

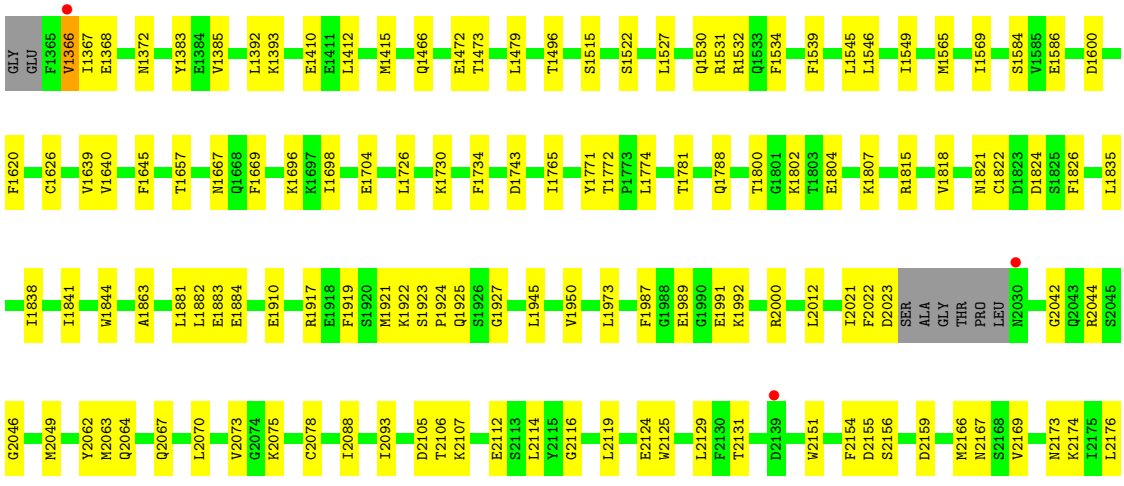
Chain A:

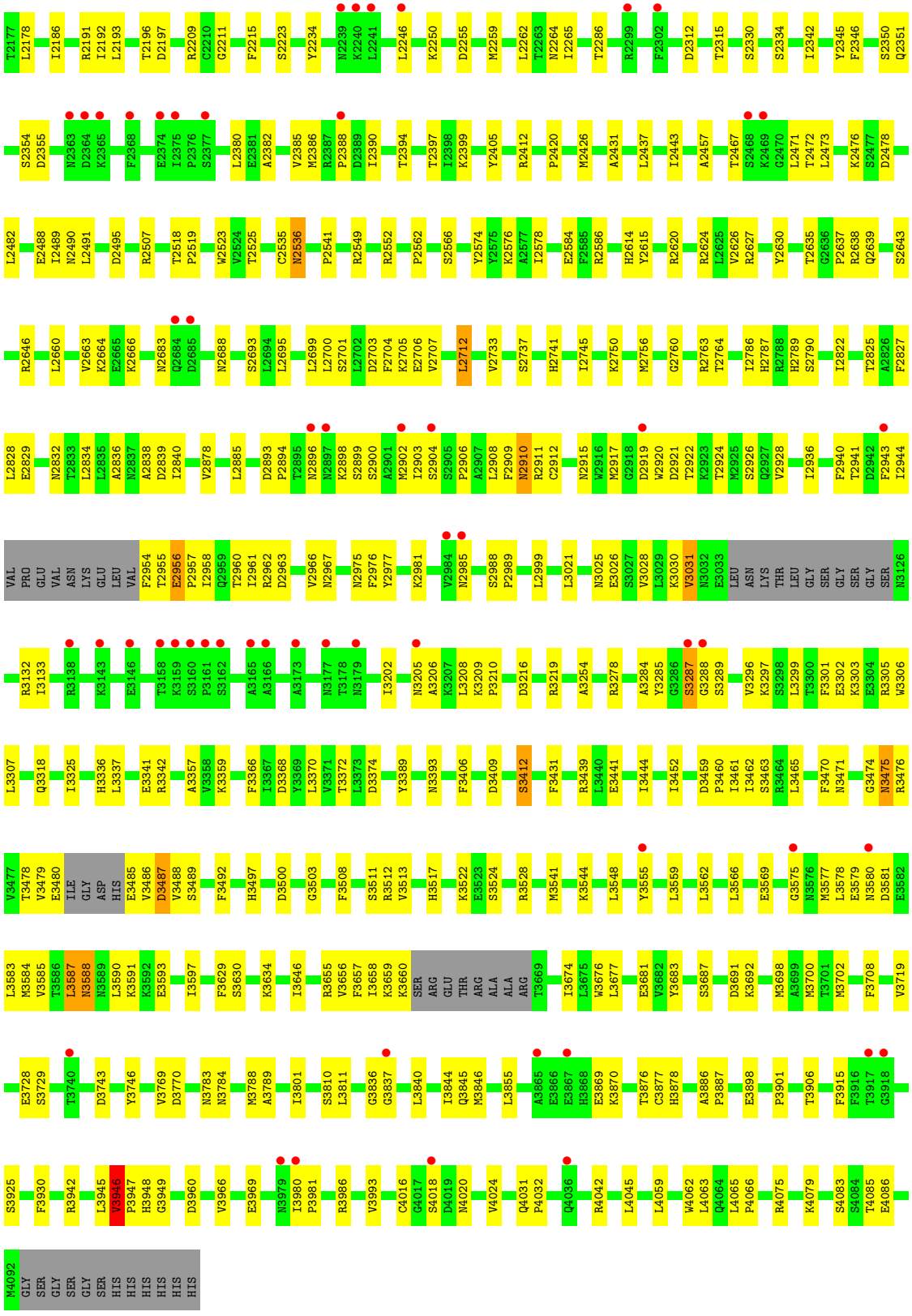




• Molecule 1: Dynein heavy chain lysozyme chimera

Chain B:




T2177 L2178 I2186 R2191 I2192 L2193 T2196 D2197 R2209 G2210 G2211 F2215 S2223 Y2234 N2239 K2240 L2241 L2246 K2250 D2255 M2259 L2262 T2263 N2264 I2265 T2286 R2299 F2302 D2312 T2315 S2330 S2334 I2342 Y2345 F2346 S2350 Q2351
S2354 D2355 N2363 D2364 K2365 F2368 E2374 I2375 P2376 S2377 L2380 E2381 A2382 V2385 M2386 R2387 P2388 D2389 I2390 T2394 T2397 I2398 K2399 Y2405 R2412 P2420 M2426 A2431 L2437 I2443 A2457 T2467 S2468 K2469 G2470 L2471 T2472 L2473 K2476 S2477 D2478
L2482 E2488 I2489 N2490 L2491 D2495 R2507 T2518 P2519 W2523 V2524 T2525 C2535 N2536 P2541 R2549 R2552 P2562 S2566 Y2574 Y2575 K2576 A2577 I2578 E2584 F2585 R2586 H2614 Y2615 R2620 R2624 L2625 V2626 R2627 Y2630 T2635 G2636 P2637 R2638 Q2639 S2643
R2646 L2660 V2663 K2664 E2665 K2666 N2683 Q2684 D2685 N2688 S2693 L2694 L2695 L2699 L2700 S2701 L2702 D2703 F2704 K2705 E2706 V2707 L2712 V2733 S2737 H2741 I2745 K2750 M2756 G2760 R2763 T2764 I2786 H2787 R2788 H2789 S2790 I2822 T2825 A2826 F2827
L2828 E2829 N2832 T2833 L2834 L2835 A2836 N2837 A2838 D2839 I2840 W2878 L2885 D2893 P2894 T2895 N2896 N2897 K2898 S2899 S2900 A2901 M2902 I2903 S2904 S2905 P2906 A2907 L2908 F2909 N2910 R2911 C2912 N2915 W2916 M2917 G2918 D2919 W2920 D2921 T2922 K2923 T2924 M2925 S2926 Q2927 V2928 I2936 F2940 T2941 D2942 F2943 I2944
VAL PRO GLU VAL ASN LYS GLU LEU VAL F2954 T2955 E2956 P2957 I2958 Q2959 T2960 I2961 R2962 D2963 V2966 N2967 N2975 F2976 Y2977 K2981 V2984 N2985 S2988 P2989 L2999 L3021 N3025 E3026 S3027 V3028 L3029 K3030 V3031 N3032 E3033 LEU ASN LYS THR LEU GLY SER GLY SER GLY SER N3126
R3132 I3133 R3138 K3143 E3146 T3158 K3159 S3160 P3161 S3162 A3165 A3166 A3173 N3177 T3178 N3179 I3202 N3205 A3206 K3207 L3208 K3209 P3210 D3216 R3219 A3254 R3278 A3284 Y3285 G3286 S3287 G3288 S3289 V3296 K3297 S3298 L3299 T3300 F3301 E3302 K3303 E3304 R3305 W3306
L3307 Q3318 I3325 H3336 L3337 E3341 R3342 A3357 V3358 K3359 F3366 I3367 D3368 Y3369 L3370 V3371 T3372 L3373 D3374 Y3389 N3393 F3406 D3409 S3412 F3431 R3439 L3440 E3441 I3444 I3452 D3459 P3460 I3461 I3462 S3463 R3464 L3465 F3470 N3471 G3474 N3475 R3476
V3477 T3478 V3479 E3480 ILE GLY ASP HIS E3485 V3486 D3487 V3488 S3489 F3492 H3497 D3500 G3503 F3508 S3511 R3512 V3513 H3517 K3522 E3523 S3524 R3528 M3541 K3544 L3548 Y3555 L3559 L3562 L3566 E3569 G3575 N3576 M3577 L3578 E3579 N3580 D3581 E3582
L3583 M3584 V3585 T3586 L3587 N3588 N3589 L3590 K3591 K3592 E3593 I3597 F3629 S3630 K3634 I3646 R3655 V3656 F3657 I3658 K3659 K3660 SER ARG GLU THR ARG ALA ALA ARG T3669 I3674 L3675 W3676 L3677 E3681 V3682 Y3683 S3687 D3691 K3692 M3698 A3699 M3700 T3701 M3702 F3708 V3719
E3728 S3729 T3740 D3743 Y3746 V3769 D3770 N3783 N3784 M3788 A3789 I3801 S3810 L3811 G3836 G3837 L3840 I3844 Q3845 M3846 L3855 A3865 E3866 E3867 H3868 E3869 K3870 T3876 C3877 H3878 A3886 P3887 E3898 P3901 T3906 F3915 F3916 T3917 G3918
S3925 F3930 R3942 L3945 V3946 P3947 H3948 G3949 D3960 V3966 E3969 N3979 I3980 P3981 R3986 V3993 C4016 G4017 S4018 D4019 N4020 V4024 Q4031 P4032 Q4036 R4042 L4045 L4059 W4062 L4063 Q4064 L4065 P4066 R4075 K4079 S4083 S4084 T4085 E4086
M4092 GLY SER GLY SER GLY SER HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	137.73Å 154.38Å 177.55Å 90.00° 96.59° 90.00°	Depositor
Resolution (Å)	49.40 – 3.54 49.40 – 3.54	Depositor EDS
% Data completeness (in resolution range)	92.2 (49.40-3.54) 92.3 (49.40-3.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1769)	Depositor
R, R_{free}	0.228 , 0.262 0.234 , 0.231	Depositor DCC
R_{free} test set	4148 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	54.3	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 25.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	84822	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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: ANP, 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	0.32	0/21492	0.58	5/29041 (0.0%)
1	B	0.32	0/21487	0.57	2/29028 (0.0%)
All	All	0.32	0/42979	0.57	7/58069 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	3575	GLY	N-CA-C	-6.92	95.81	113.10
1	A	3296	VAL	N-CA-C	-6.30	93.98	111.00
1	B	3587	LEU	CA-CB-CG	6.22	129.60	115.30
1	A	1882	LEU	CB-CG-CD2	5.96	121.13	111.00
1	A	1882	LEU	CA-CB-CG	5.91	128.90	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3946	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	B	3946	VAL	Peptide

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	21073	21166	21167	354	0
1	B	21070	21166	21167	361	0
2	A	124	49	52	8	0
2	B	124	48	52	8	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	42393	42429	42438	721	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 8.

The worst 5 of 721 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:B:3692:LYS:N	1:B:3898:GLU:OE2	1.95	0.99
1:A:2946:PRO:HG3	1:A:2958:ILE:HG23	1.51	0.89
1:A:3134:ASP:OD2	1:A:3269:ARG:NE	2.08	0.86
1:A:2387:ARG:NH2	1:A:2875:ASP:OD2	2.10	0.84
1:A:3945:LEU:HD13	1:A:4065:LEU:HD21	1.62	0.82

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	2596/2661 (98%)	2473 (95%)	118 (4%)	5 (0%)	47 80
1	B	2597/2661 (98%)	2476 (95%)	116 (4%)	5 (0%)	47 80
All	All	5193/5322 (98%)	4949 (95%)	234 (4%)	10 (0%)	47 80

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1366	VAL
1	A	3946	VAL
1	B	1366	VAL
1	B	3031	VAL
1	B	3946	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	2367/2406 (98%)	2347 (99%)	20 (1%)	81 92
1	B	2366/2406 (98%)	2345 (99%)	21 (1%)	78 90
All	All	4733/4812 (98%)	4692 (99%)	41 (1%)	78 90

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2712	LEU
1	B	3287	SER
1	B	2786	ILE
1	B	2975	ASN
1	B	3471	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3962	GLN
1	B	2201	HIS
1	B	2444	ASN
1	B	3318	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ANP	A	5001	-	29,33,33	1.11	3 (10%)	31,52,52	1.07	2 (6%)
2	ANP	B	5004	-	29,33,33	1.63	5 (17%)	31,52,52	1.19	2 (6%)
2	ANP	A	5002	3	29,33,33	1.01	3 (10%)	31,52,52	1.10	2 (6%)
2	ANP	B	5002	3	29,33,33	1.82	5 (17%)	31,52,52	1.26	3 (9%)
2	ANP	A	5004	-	29,33,33	1.81	5 (17%)	31,52,52	1.30	3 (9%)
2	ANP	B	5001	-	29,33,33	2.14	6 (20%)	31,52,52	1.32	2 (6%)
2	ANP	B	5003	-	29,33,33	1.80	5 (17%)	31,52,52	1.05	2 (6%)
2	ANP	A	5003	-	29,33,33	2.07	5 (17%)	31,52,52	1.21	3 (9%)

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	ANP	A	5001	-	-	4/14/38/38	0/3/3/3
2	ANP	B	5004	-	-	5/14/38/38	0/3/3/3
2	ANP	A	5002	3	-	5/14/38/38	0/3/3/3
2	ANP	B	5002	3	-	3/14/38/38	0/3/3/3
2	ANP	A	5004	-	-	8/14/38/38	0/3/3/3
2	ANP	B	5001	-	-	7/14/38/38	0/3/3/3
2	ANP	B	5003	-	-	5/14/38/38	0/3/3/3
2	ANP	A	5003	-	-	7/14/38/38	0/3/3/3

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5001	ANP	PG-O1G	7.80	1.58	1.46
2	B	5002	ANP	PG-O1G	7.77	1.58	1.46
2	B	5003	ANP	PG-O1G	7.72	1.58	1.46
2	A	5004	ANP	PG-O1G	7.71	1.58	1.46
2	A	5003	ANP	PG-O1G	7.35	1.57	1.46

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	5001	ANP	PB-O3A-PA	-5.09	114.69	132.62
2	B	5002	ANP	PB-O3A-PA	-4.73	115.97	132.62
2	A	5004	ANP	PB-O3A-PA	-4.64	116.27	132.62
2	B	5004	ANP	PB-O3A-PA	-4.24	117.70	132.62
2	A	5003	ANP	PB-O3A-PA	-4.01	118.51	132.62

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5001	ANP	PG-N3B-PB-O1B
2	A	5001	ANP	PA-O3A-PB-O1B
2	A	5002	ANP	PB-N3B-PG-O1G
2	A	5002	ANP	PG-N3B-PB-O1B
2	A	5002	ANP	PG-N3B-PB-O3A

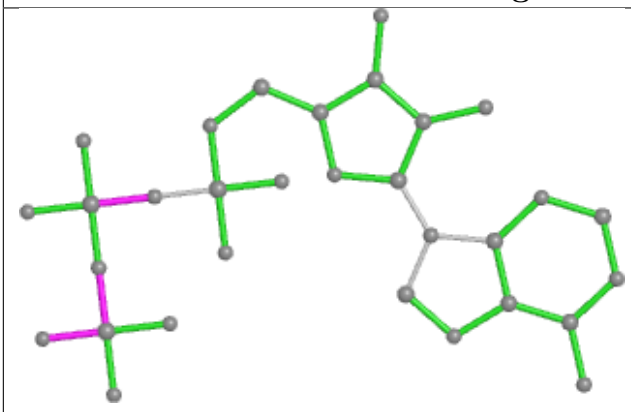
There are no ring outliers.

8 monomers are involved in 16 short contacts:

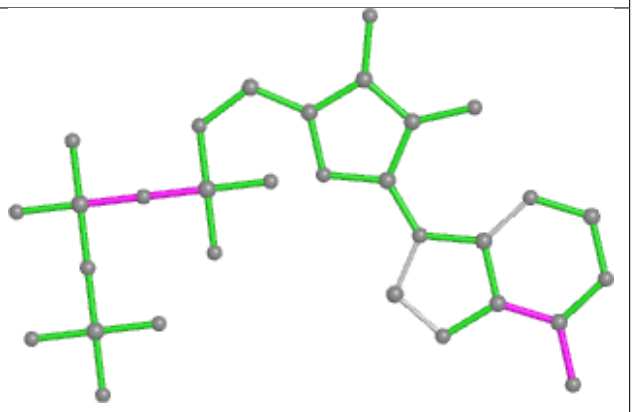
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5001	ANP	1	0
2	B	5004	ANP	1	0
2	A	5002	ANP	2	0
2	B	5002	ANP	2	0
2	A	5004	ANP	2	0
2	B	5001	ANP	2	0
2	B	5003	ANP	3	0
2	A	5003	ANP	3	0

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 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.

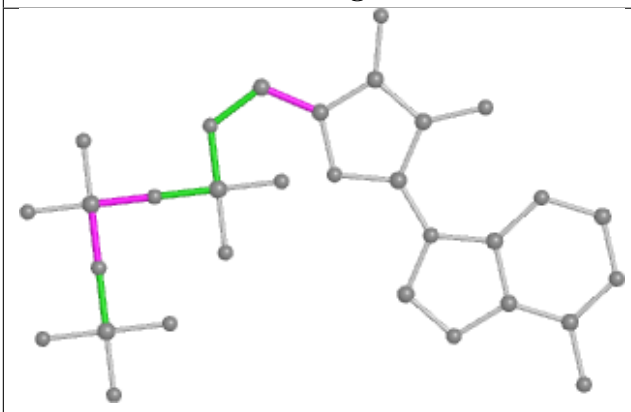
Ligand ANP A 5001



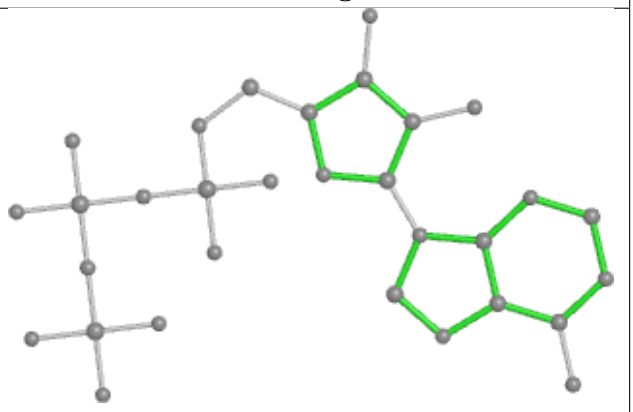
Bond lengths



Bond angles

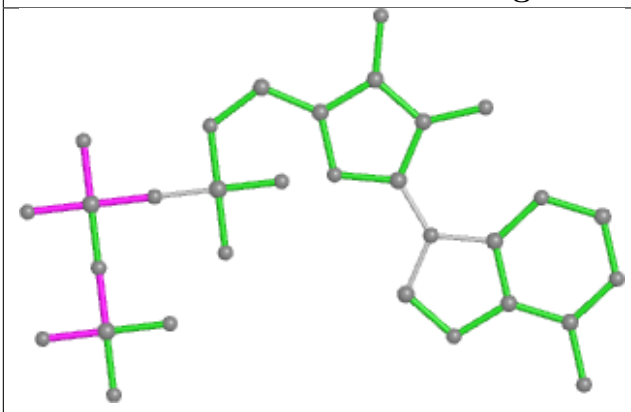


Torsions

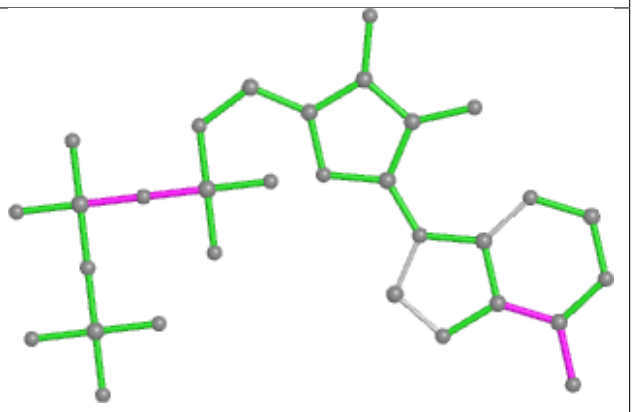


Rings

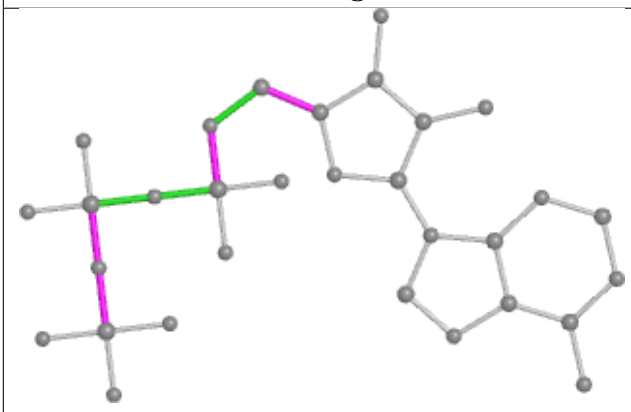
Ligand ANP B 5004



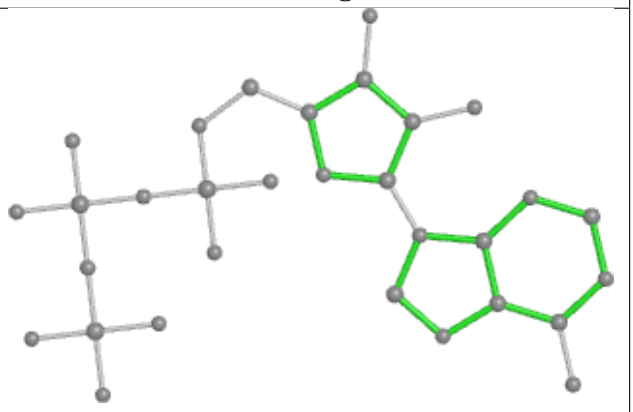
Bond lengths



Bond angles

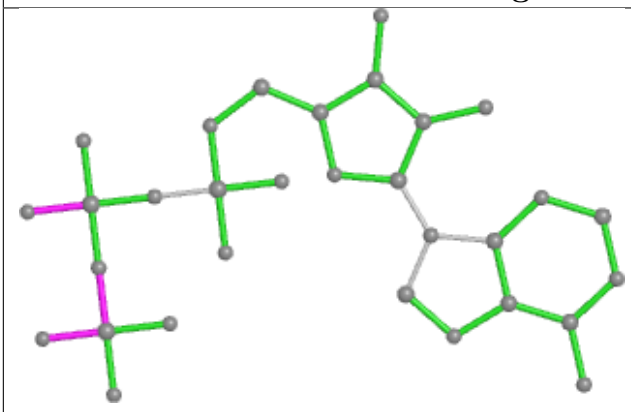


Torsions

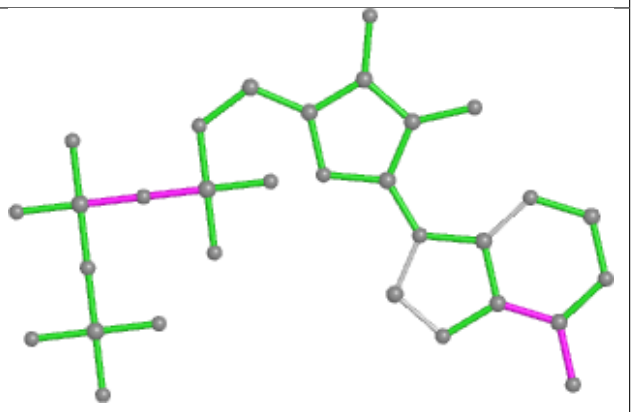


Rings

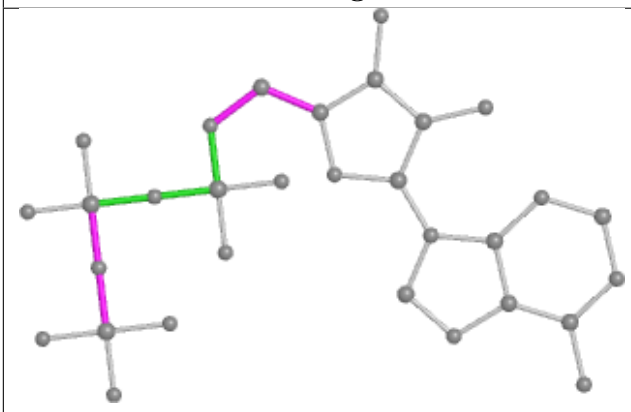
Ligand ANP A 5002



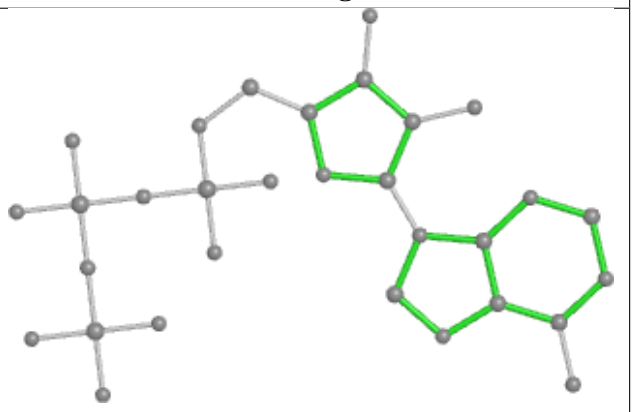
Bond lengths



Bond angles

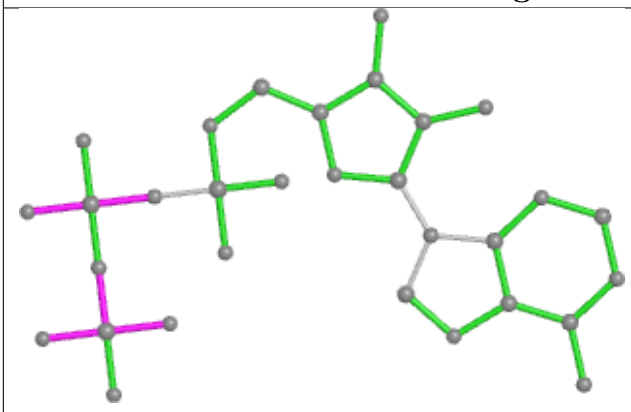


Torsions

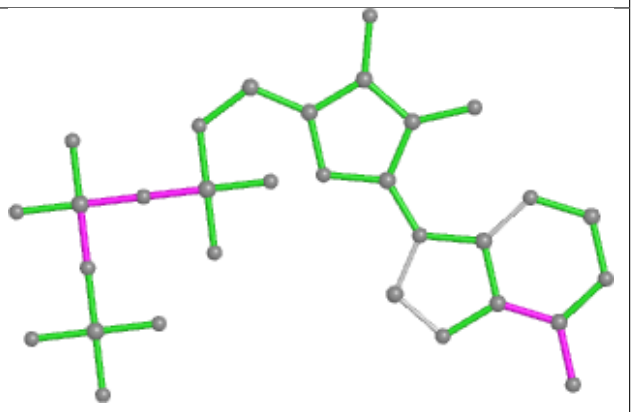


Rings

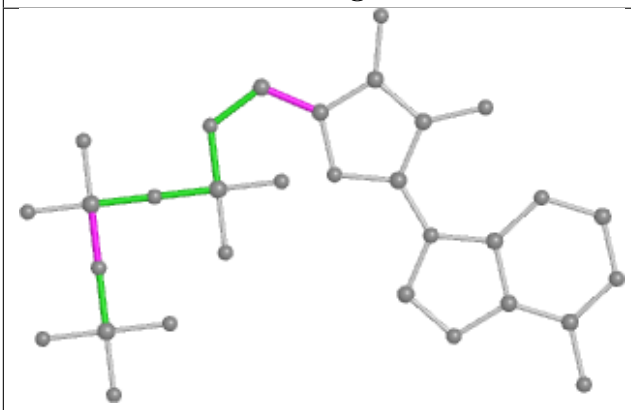
Ligand ANP B 5002



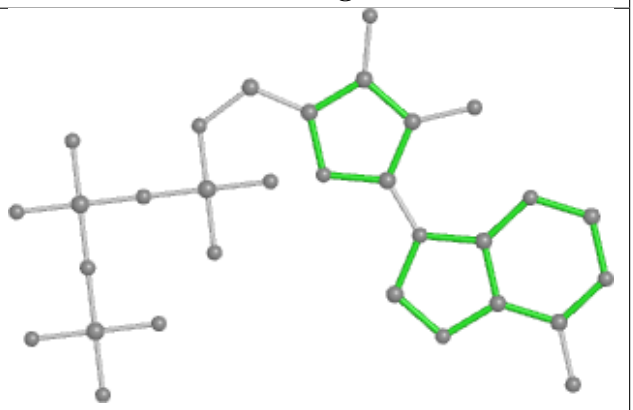
Bond lengths



Bond angles

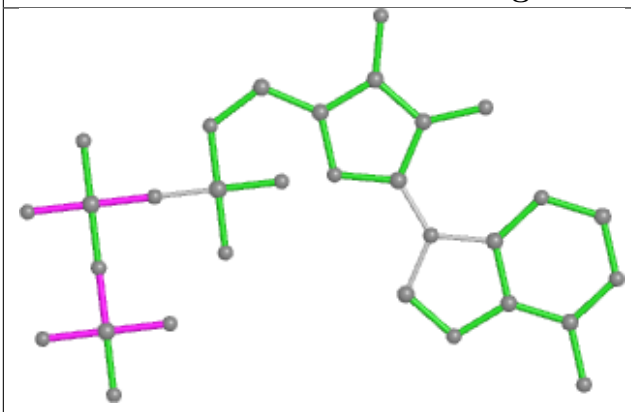


Torsions

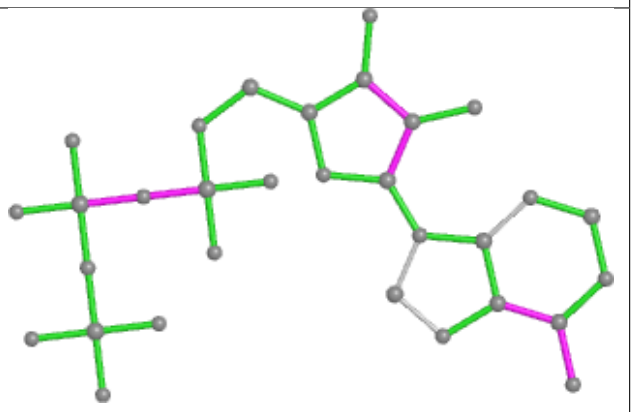


Rings

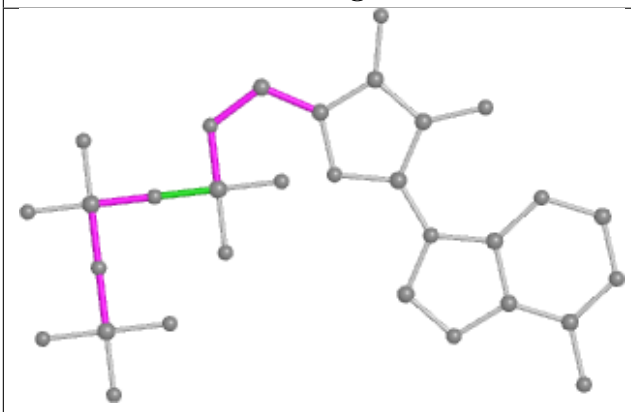
Ligand ANP A 5004



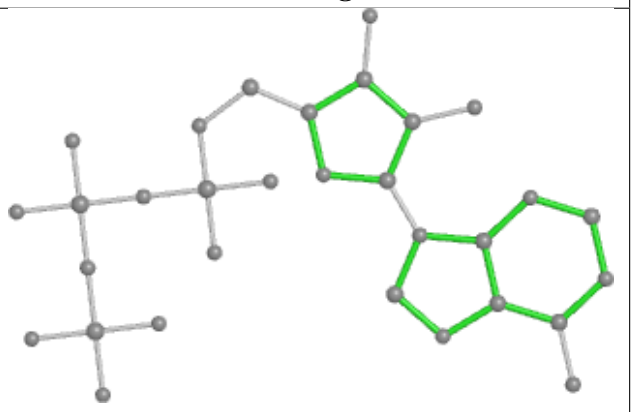
Bond lengths



Bond angles

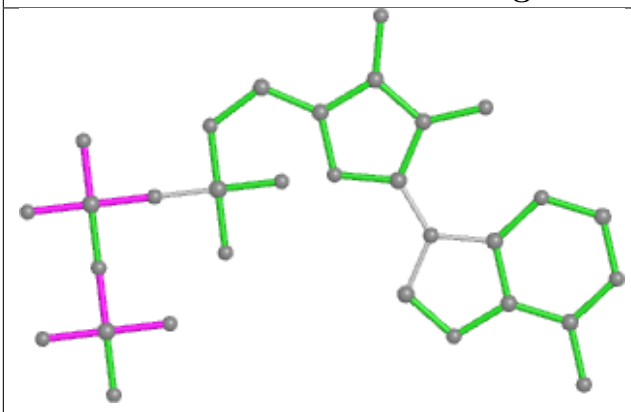


Torsions

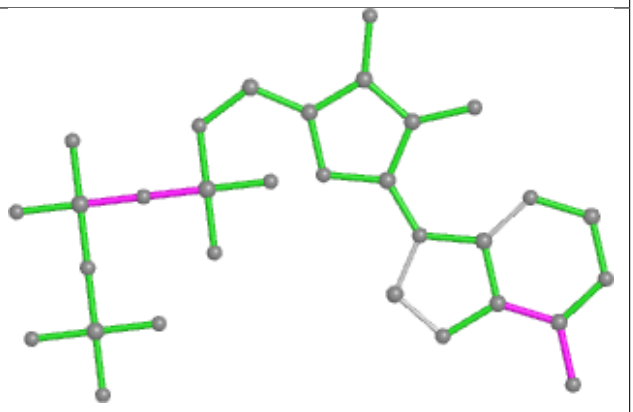


Rings

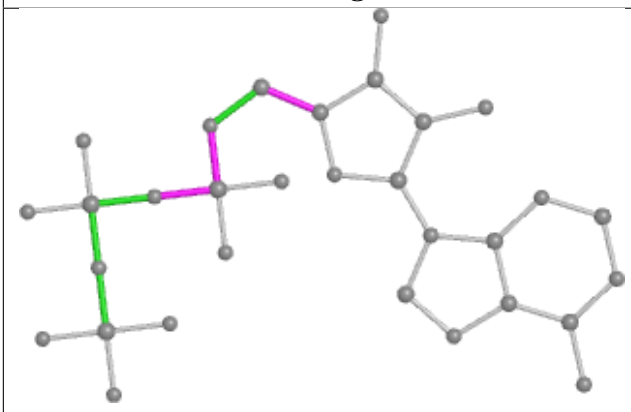
Ligand ANP B 5001



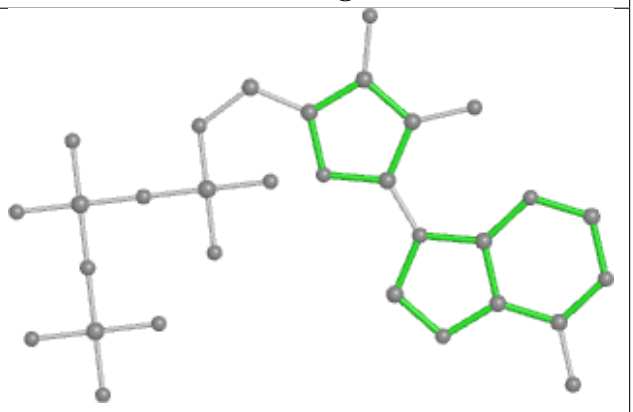
Bond lengths



Bond angles

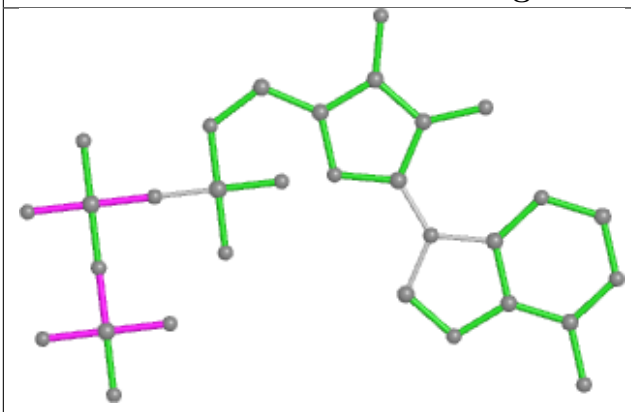


Torsions

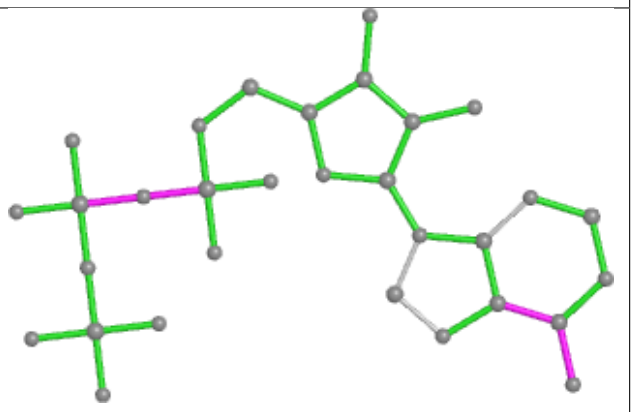


Rings

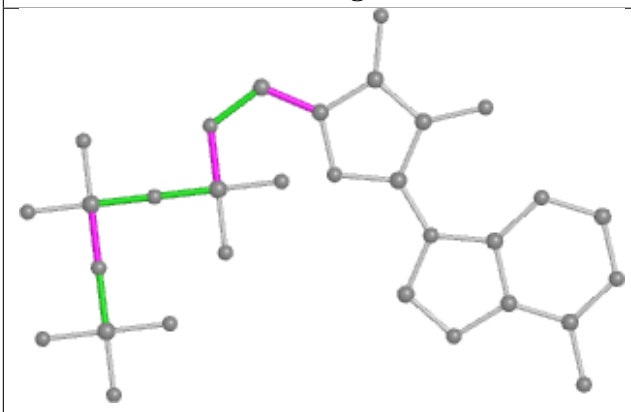
Ligand ANP B 5003



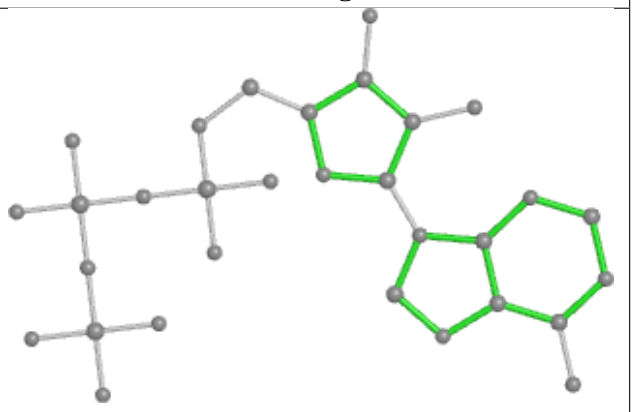
Bond lengths



Bond angles

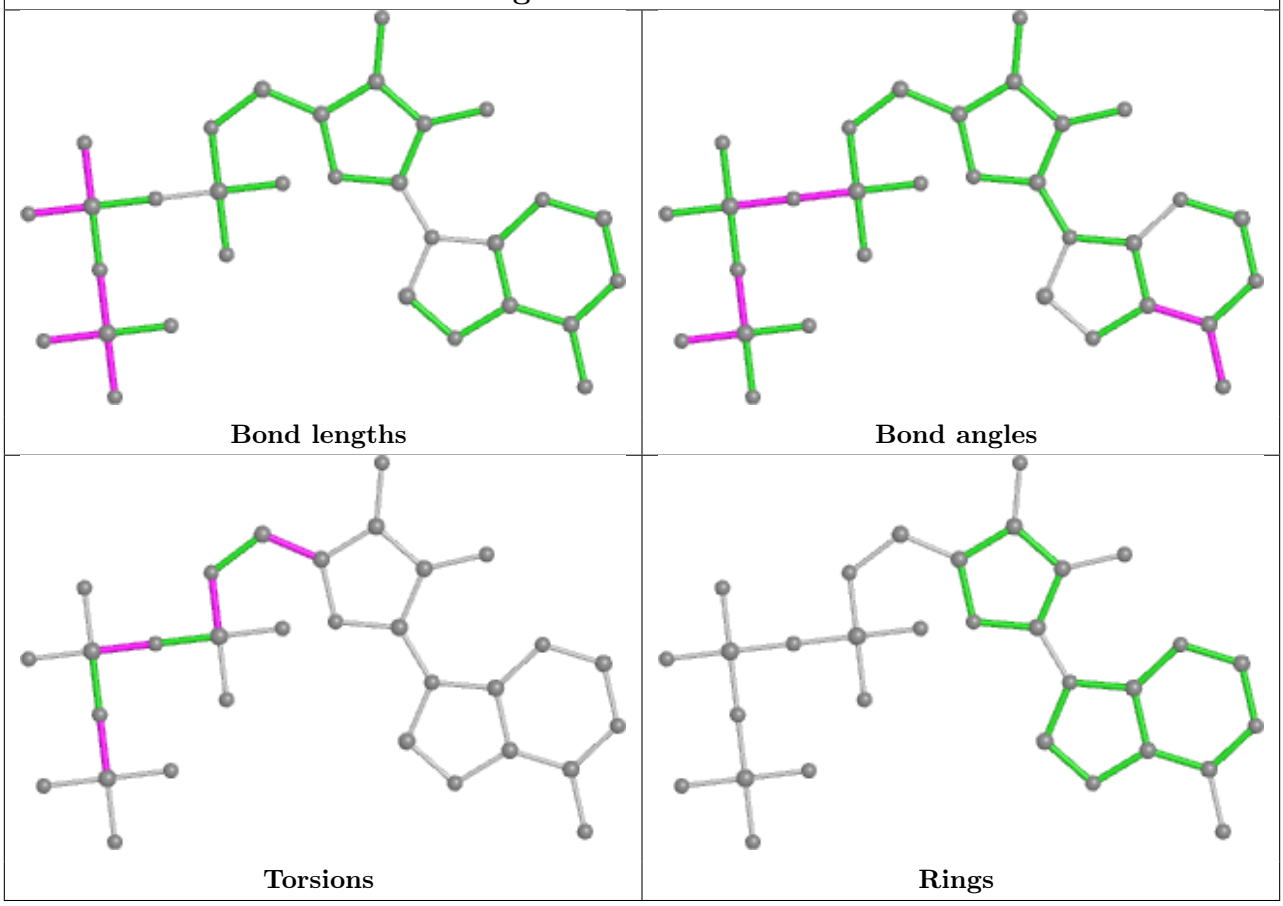


Torsions



Rings

Ligand ANP A 5003



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	2608/2661 (98%)	-0.10	59 (2%)	60	46	20, 50, 119, 275	0
1	B	2609/2661 (98%)	-0.09	58 (2%)	62	48	23, 54, 121, 247	0
All	All	5217/5322 (98%)	-0.10	117 (2%)	62	48	20, 52, 120, 275	0

The worst 5 of 117 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3166	ALA	6.8
1	B	2364	ASP	6.5
1	A	2363	ASN	6.5
1	B	3159	LYS	5.5
1	B	2363	ASN	5.5

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

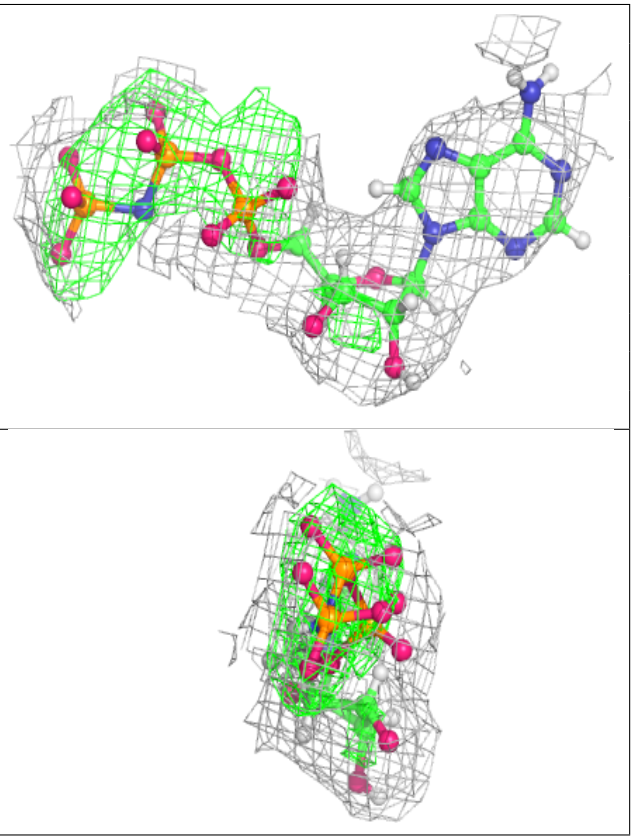
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	ANP	A	5002	31/31	0.91	0.28	36,66,98,149	0
2	ANP	A	5003	31/31	0.91	0.28	21,52,121,134	0
2	ANP	A	5004	31/31	0.91	0.27	49,72,160,227	0
2	ANP	B	5003	31/31	0.92	0.34	43,75,101,161	0
2	ANP	B	5002	31/31	0.93	0.25	28,67,122,162	0
2	ANP	A	5001	31/31	0.94	0.24	23,51,183,503	0
2	ANP	B	5001	31/31	0.94	0.24	31,57,180,372	0
2	ANP	B	5004	31/31	0.94	0.24	47,78,162,183	0
3	MG	B	5005	1/1	0.97	0.26	54,54,54,54	0
3	MG	A	5005	1/1	0.98	0.36	50,50,50,50	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.

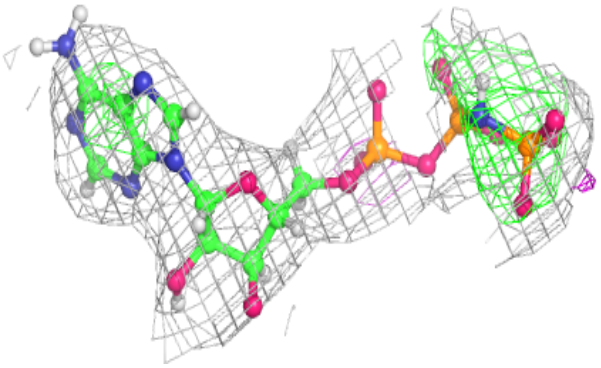
Electron density around ANP A 5002:

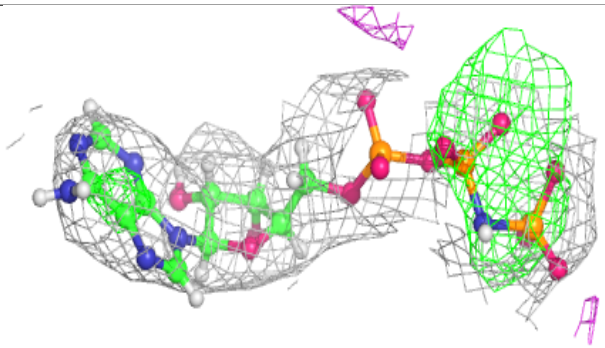
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

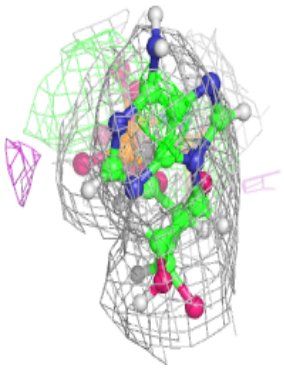


Electron density around ANP A 5003:

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

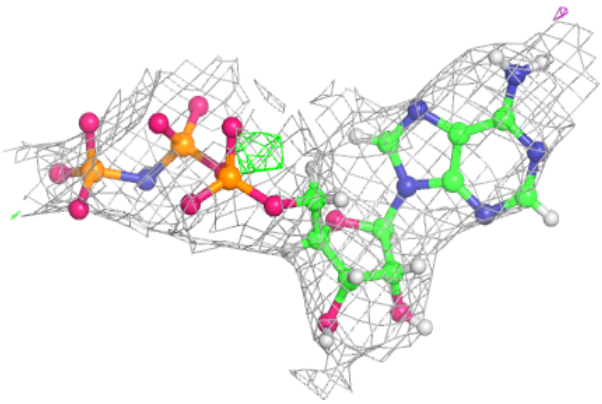


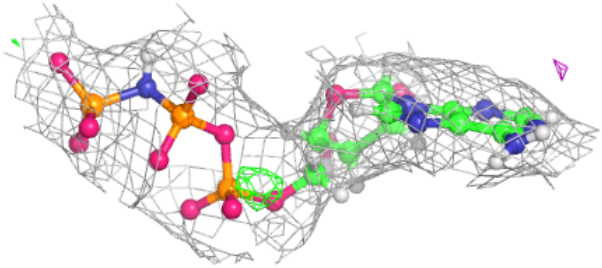


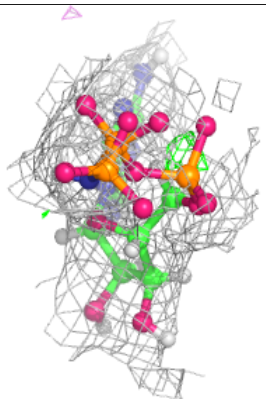


Electron density around ANP A 5004:

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

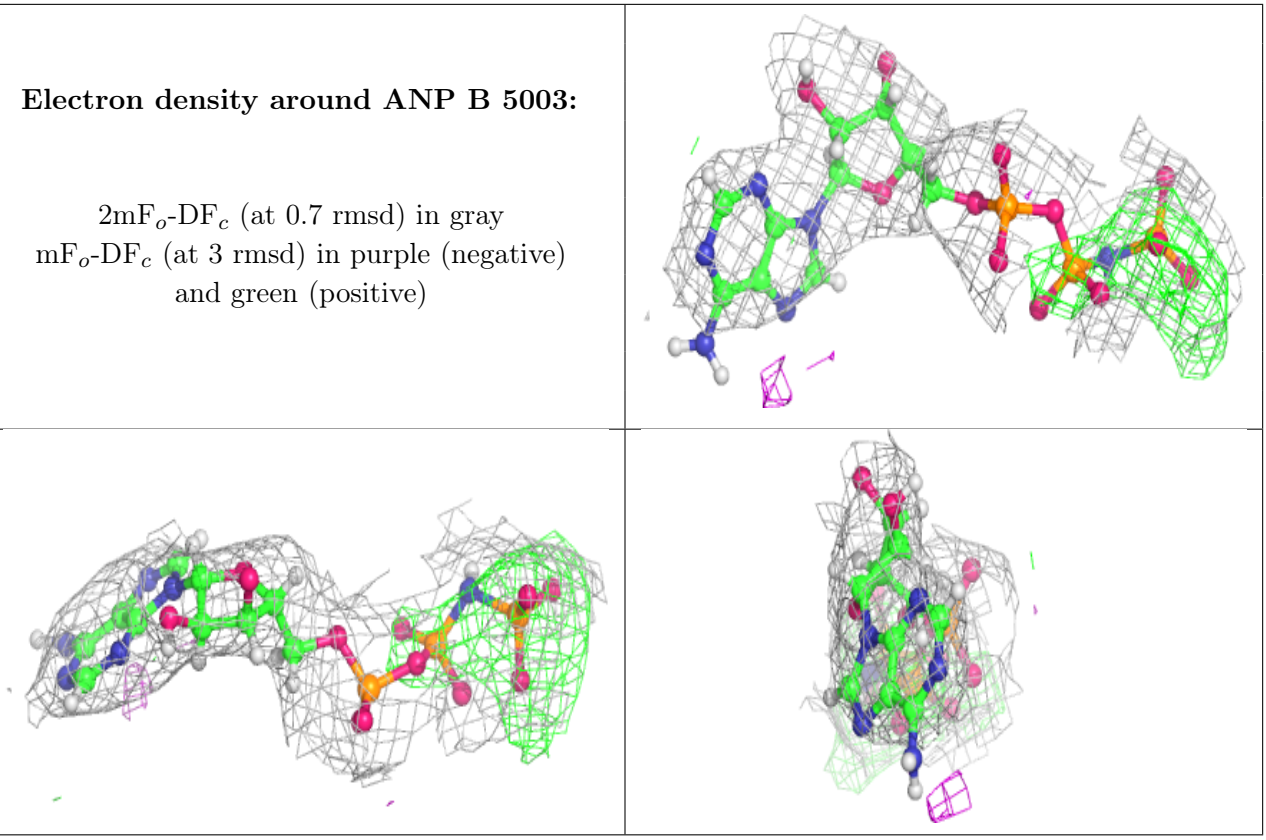






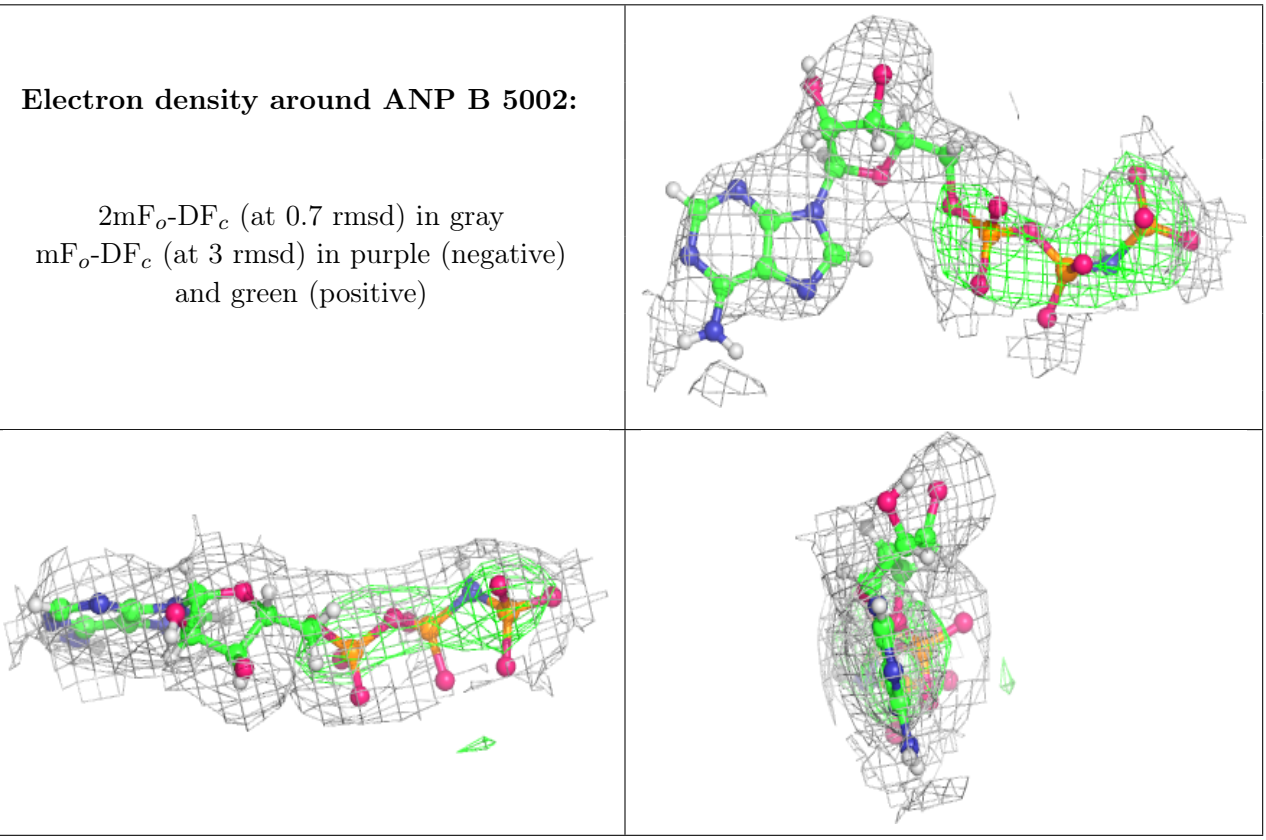
Electron density around ANP B 5003:

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



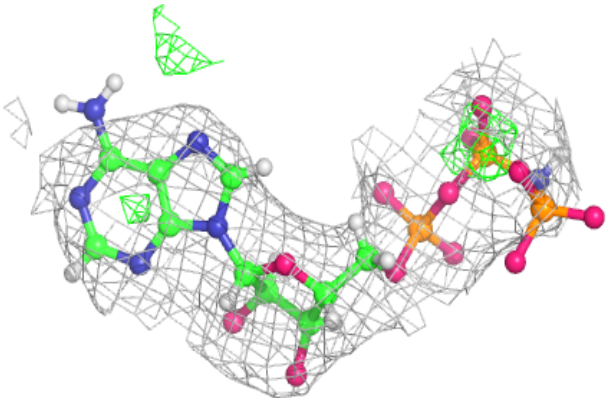
Electron density around ANP B 5002:

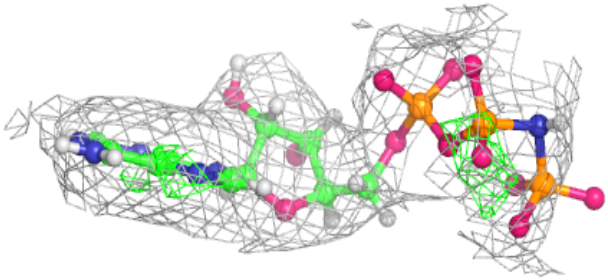
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

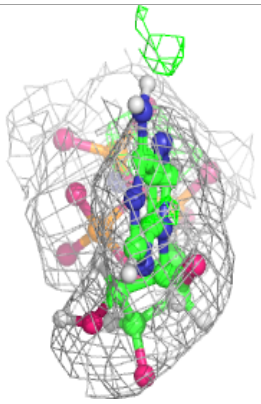


Electron density around ANP A 5001:

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

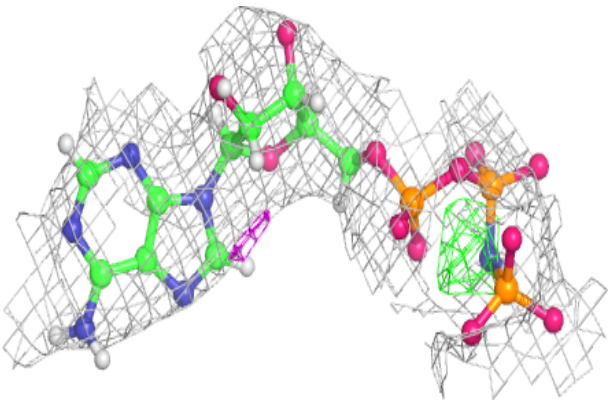


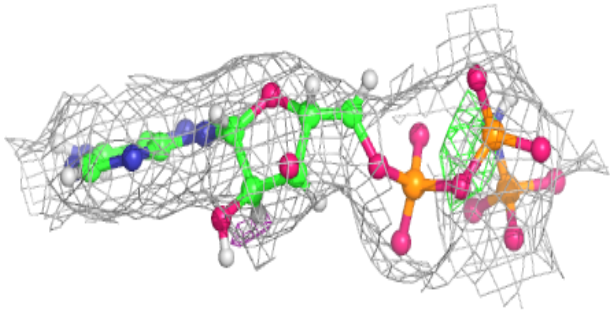


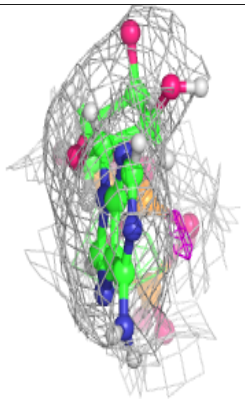


Electron density around ANP B 5001:

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

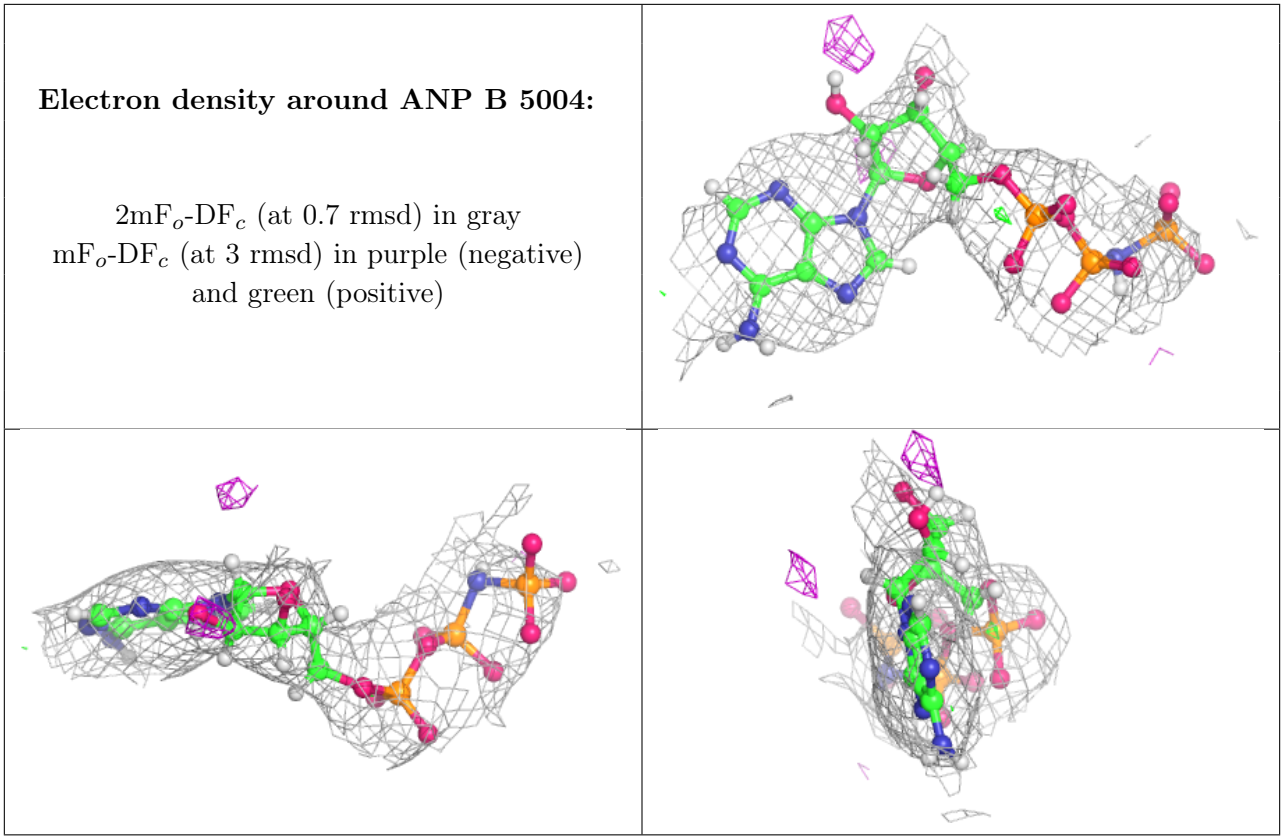






Electron density around ANP B 5004:

$2mF_o$-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.