



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 04:40 am BST

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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

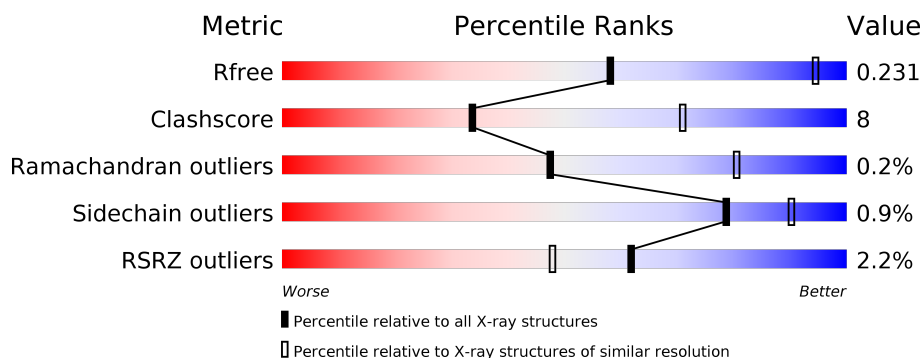
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.54 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 on 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	2661	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>••</div> </div> </div>
1	B	2661	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>•</div> </div> </div>

2 Entry composition

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

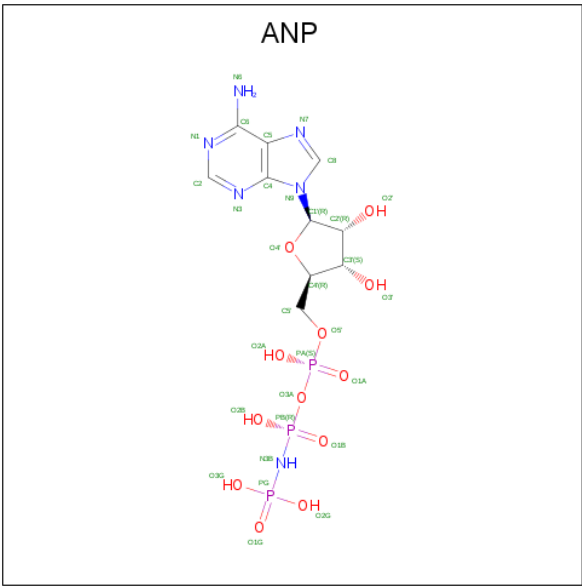
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Chain	Residue	Modelled	Actual	Comment	Reference
A	4097	GLY	-	linker	UNP P36022
A	4098	SER	-	linker	UNP P36022
A	4099	HIS	-	expression tag	UNP P36022
A	4100	HIS	-	expression tag	UNP P36022
A	4101	HIS	-	expression tag	UNP P36022
A	4102	HIS	-	expression 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: C₁₀H₁₇N₆O₁₂P₃).



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		

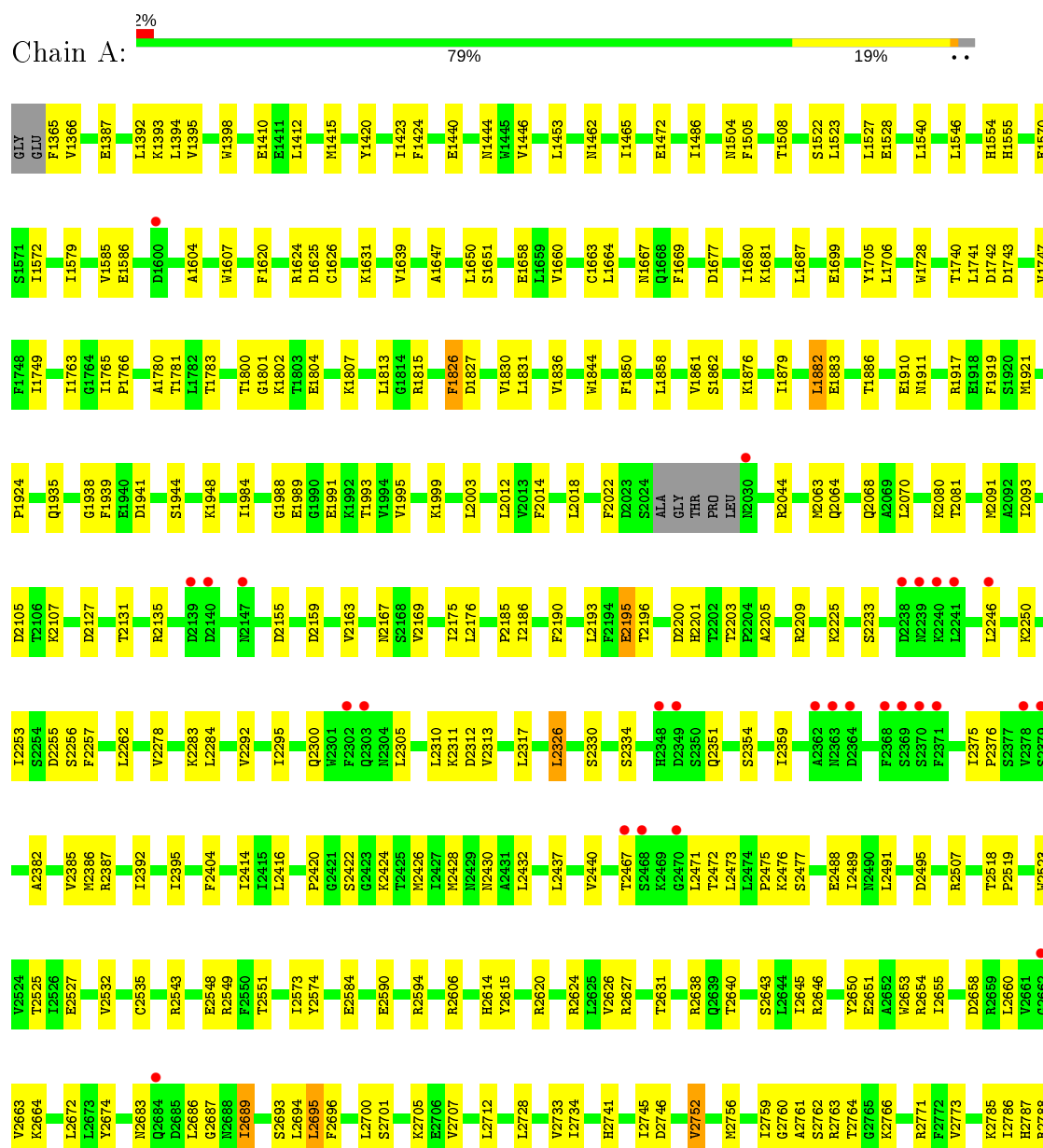
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

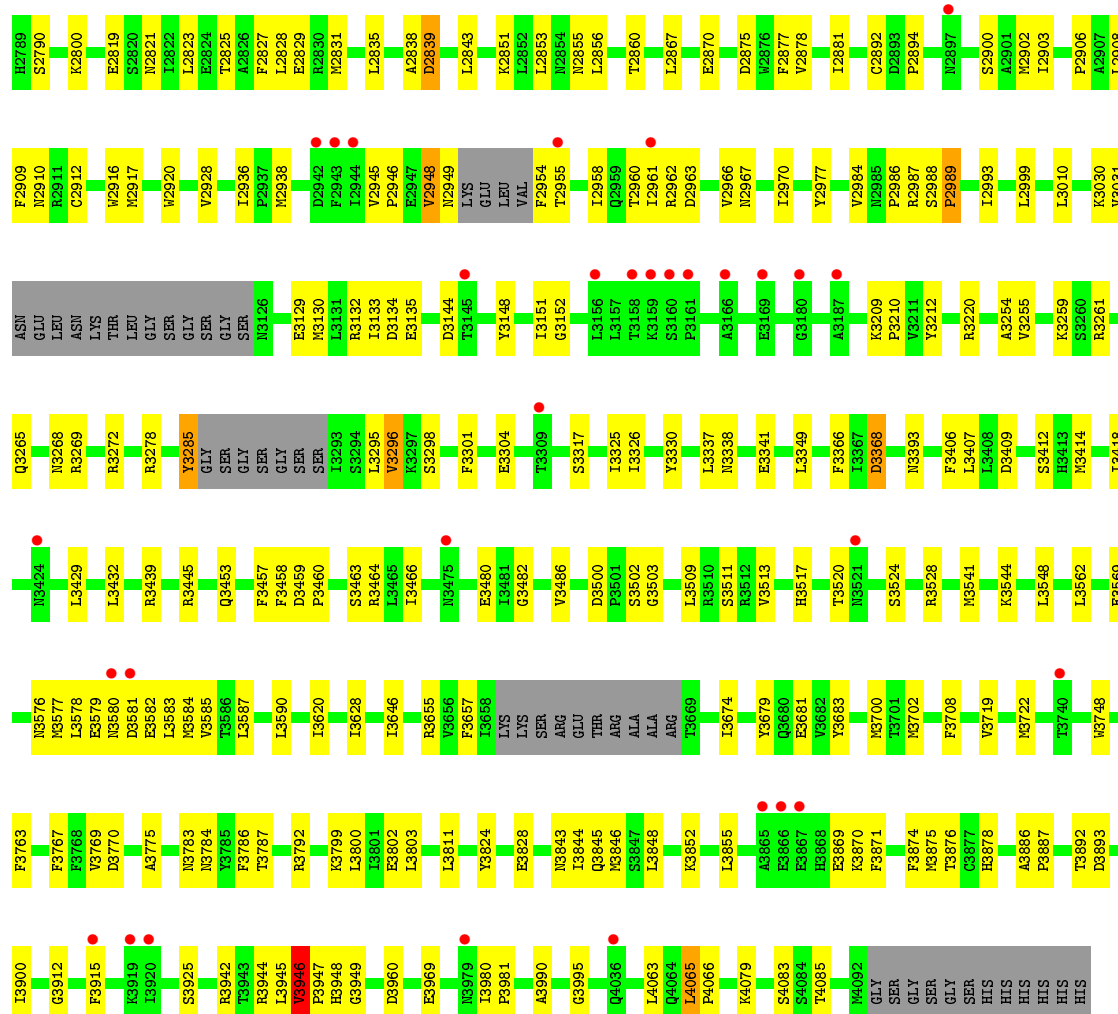
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

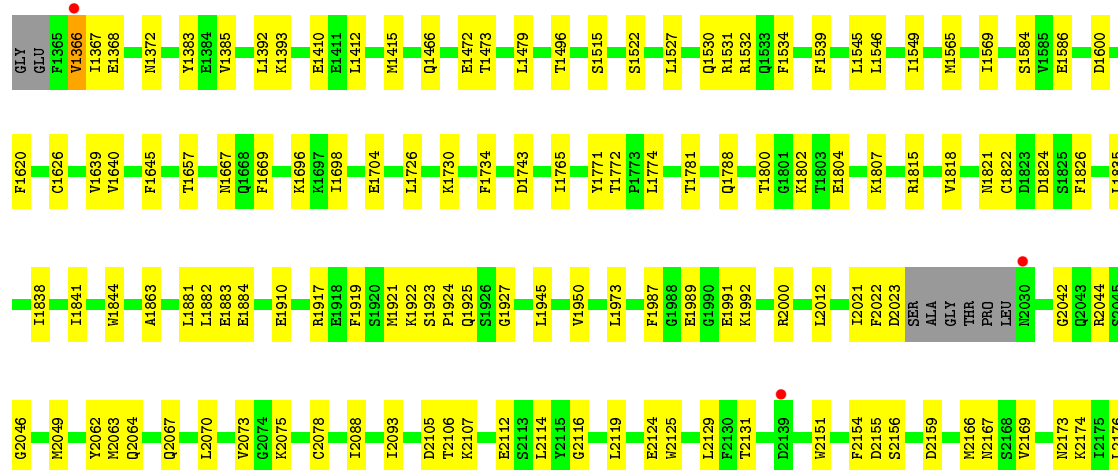
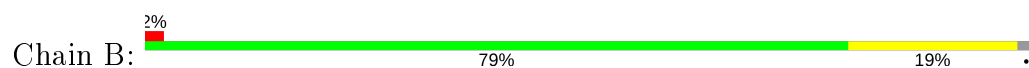
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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





• Molecule 1: Dynein heavy chain lysozyme chimera



H4092	S9925	E3728	L3583	V8477	L3307	R3132	VAL	L2828	R2646	L482	S2354	T2177
GLY	F9930	S3729	K3584	T3478	Q3318	I3133	PRO	E829	R2660	E488	D2355	L2178
GLY			V3585	V3479			GLU	N2832		I2489		I2186
GLY	R3942	T3740	T3586	E3480	I3325	R3138	ASN	T2833	V2663	N2490	N2363	R2191
GLY	L3945	D3743	L3587	ILE	H3336	R3143	LYS	L2834	K2664	L2491	K2364	I2192
SER	L3946		N3588	ASP	L3337	R3146	GLU	L2835	K2665		K2365	L2193
HIS	L3947		N3589	HIS		E3146	LEU	A2836	K2666	D2495	F2368	
HIS	P3947		L3590	E3485	E3341		VAL	D2837		R2507		T2196
HIS	H9948	Y3746	K3591	E3486	R3342	T3158	T2955	A2838	N2683	T2518	E2374	D2197
HIS	G3949	V3769	E3592	D3487	R3442	K3159	E2956	D2839	Q2684	P2519	I2375	
HIS		D3770	E3593	V3488	A3357	S3160	P2957	L2840	D2685		P2376	R2209
HIS	D3960		I3597	S3489	F3358	P3161	L2958	V2878			S2377	G2210
		N3783		F3492	K3359	S3162	Q2959		N2688	V2523		G2211
	V3966	N3784	F3629	H3497	F3366	A3165	T2960	L2885	S2693	V2524	L2380	
	E3969	K3788	S3630	H3497	I3367	A3166	T2961	T2525	L2694	E2381	F2215	
	K3789	A3789	K3634	D3500	D3368	A3173	R2962	D2893	L2695	A2382		S2223
	I3801		I3646		F3369		D2963	P2894		V2385		Y2234
		I3810		G3503	L3370	N3177	V2966	T2896	L2699	M2386		
	S3810	L3811	R3655	F3508	L3371	K3177	N2967	N2897	L2700	R2387	N2239	
			F3656		T3372	T3178	K2975	K2898	S2701	P2541	K2240	
	G3836		I3657	S3511	L3373	N3179	N2976	S2899	D2702	R2549	L2241	
	G3837		K3658	R3512	D3374		Y2977	S2900	D2703		L2390	
			K3659	V3513		I3202		K2901	F2704	R2582		
	L3840		SER		Y3389	N3205		N2902	K2705		T2394	L2246
		L3844	ARG	H3517	N3393	A3206	K2981	I2903	E2706	P2562	T2397	K2250
		Q3845	GLU		F3406	K3207	V2984	S2905	V2707	S2566	T2398	D2255
	K3846		THR	K3522		L3208	N2985	P2906		Y2574	Y2405	N2259
			ARG	E3523	D3409	K3209	S2988	L2908	V2733	T2575		
	L3855		ALA	S3524		P3210	P2989	N2910	A2577	K2576	R2412	L2262
			ALA	R3528	S3412	D3216	L2999	R2911	S2737	I2578	P2420	N2263
			ARG					C2912	E2741			L2285
				M3541	F3431	R3219	L3021			E2584	M2426	T2286
			I3674	K3544	R3439	A3254	N3025	N2915	I2745	F2585		
			L3675	L3548	L3440	R3278	E3026	N2917	K2750	R2586	A2431	
			L3677		E3441		S3027	G2918		E2614	L2437	R2299
				Y3555	I3444	A3284	V3028	D2919	K2756	Y2615		F2302
				L3559	I3452	Y3285	L3028	V2920	G2760		I2443	
						G3286	K3030	D2921	R2763	R2624	A2457	D2312
				L3562	D3459	S3287	N3032	T2924	T2764	L2625		T2315
				L3566	P3460	S3289	E3033	T2922		V2626	T2467	
					I3461		LEU	K2925	I2786	R2627	S2468	S2330
				E3569	I3462	K3297	ASN	S2926	E2787		K2469	
					S3463	K3297	LYS	Q2827	R2788	Y2630	K2470	S2334
				G3575	R3465	S3298	THR	V2928	E2789	T2635	L2471	
				N3576	L3465	T3300	LEU	I2936	K2790	T2636	L2473	I2342
				M3577	F3470	F3301	GLY		S2790	G2636		Y2345
				L3578	N3471	E3302	SER	F2940	P2637	R2638	K2476	F2346
				E3579	K3471	K3303	GLY	T2941		Q2639	S2477	
				N3580	G3474	E3304	GLY	T2942	T2825		D2478	S2350
				N3581	N3475	R3305	SER	F2943	A2826			
				E3582	R3476	N3306	N3126	I2944	F2827	S2643		

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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(°)	Ideal(°)
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 ⓘ

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	A	3811	LEU
1	B	2012	LEU
1	B	3471	ASN
1	A	3871	PHE
1	B	1818	VAL

Some 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ANP	B	5001	-	29,33,33	2.14	6 (20%)	31,52,52	1.32	2 (6%)
2	ANP	A	5004	-	29,33,33	1.81	5 (17%)	31,52,52	1.30	3 (9%)
2	ANP	B	5004	-	29,33,33	1.63	5 (17%)	31,52,52	1.19	2 (6%)
2	ANP	A	5001	-	29,33,33	1.11	3 (10%)	31,52,52	1.07	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	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	B	5001	-	-	7/14/38/38	0/3/3/3
2	ANP	A	5004	-	-	8/14/38/38	0/3/3/3
2	ANP	B	5004	-	-	5/14/38/38	0/3/3/3
2	ANP	A	5001	-	-	4/14/38/38	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	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(°)	Ideal(°)
2	B	5001	ANP	PA-O3A-PB	-5.09	114.69	132.62
2	B	5002	ANP	PA-O3A-PB	-4.73	115.97	132.62
2	A	5004	ANP	PA-O3A-PB	-4.64	116.27	132.62
2	B	5004	ANP	PA-O3A-PB	-4.24	117.70	132.62
2	A	5003	ANP	PA-O3A-PB	-4.01	118.51	132.62

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

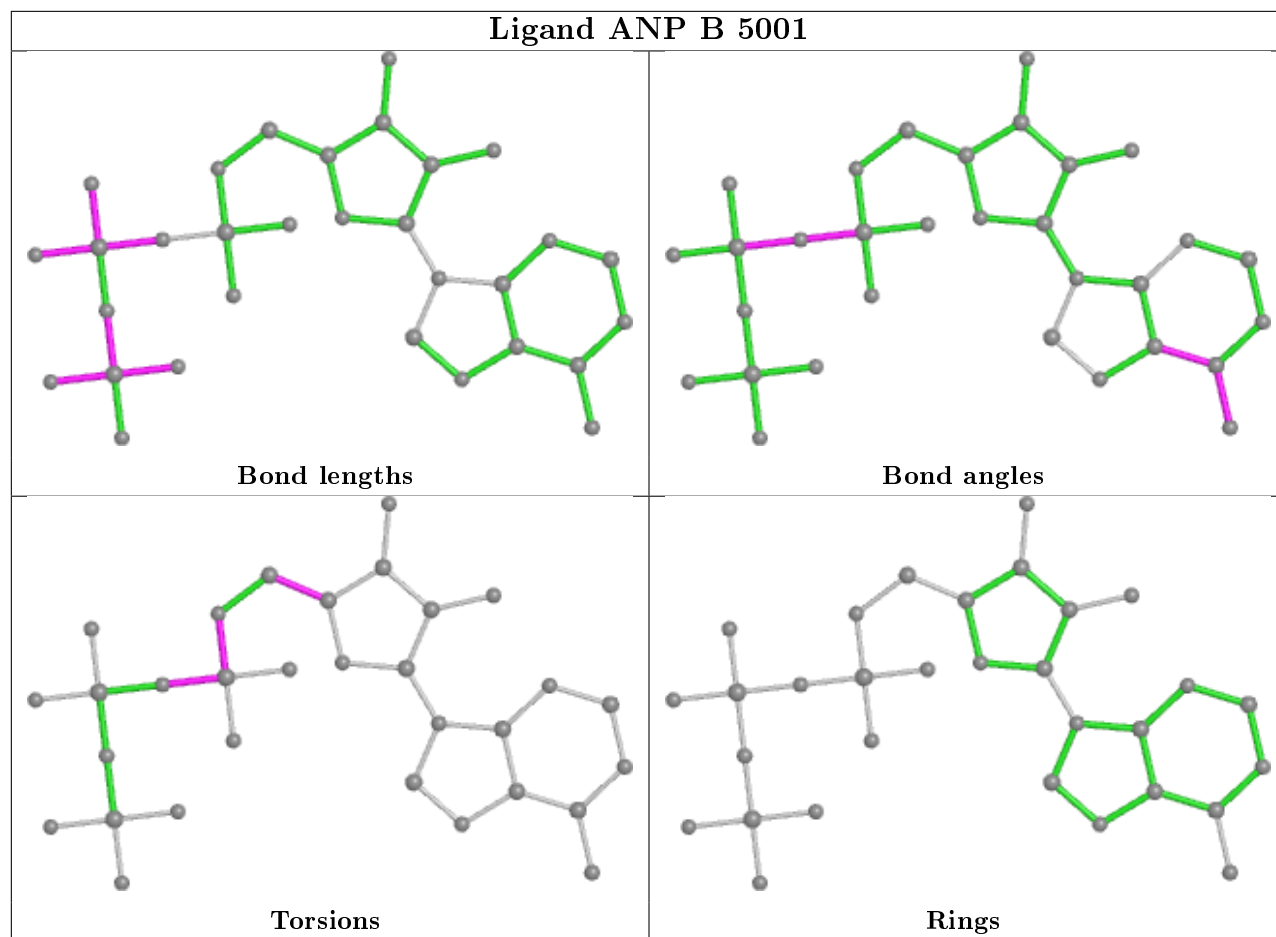
Mol	Chain	Res	Type	Atoms
2	B	5001	ANP	C5'-O5'-PA-O1A
2	B	5001	ANP	C5'-O5'-PA-O2A
2	A	5004	ANP	PB-N3B-PG-O1G
2	A	5004	ANP	PG-N3B-PB-O1B
2	A	5004	ANP	PA-O3A-PB-O1B

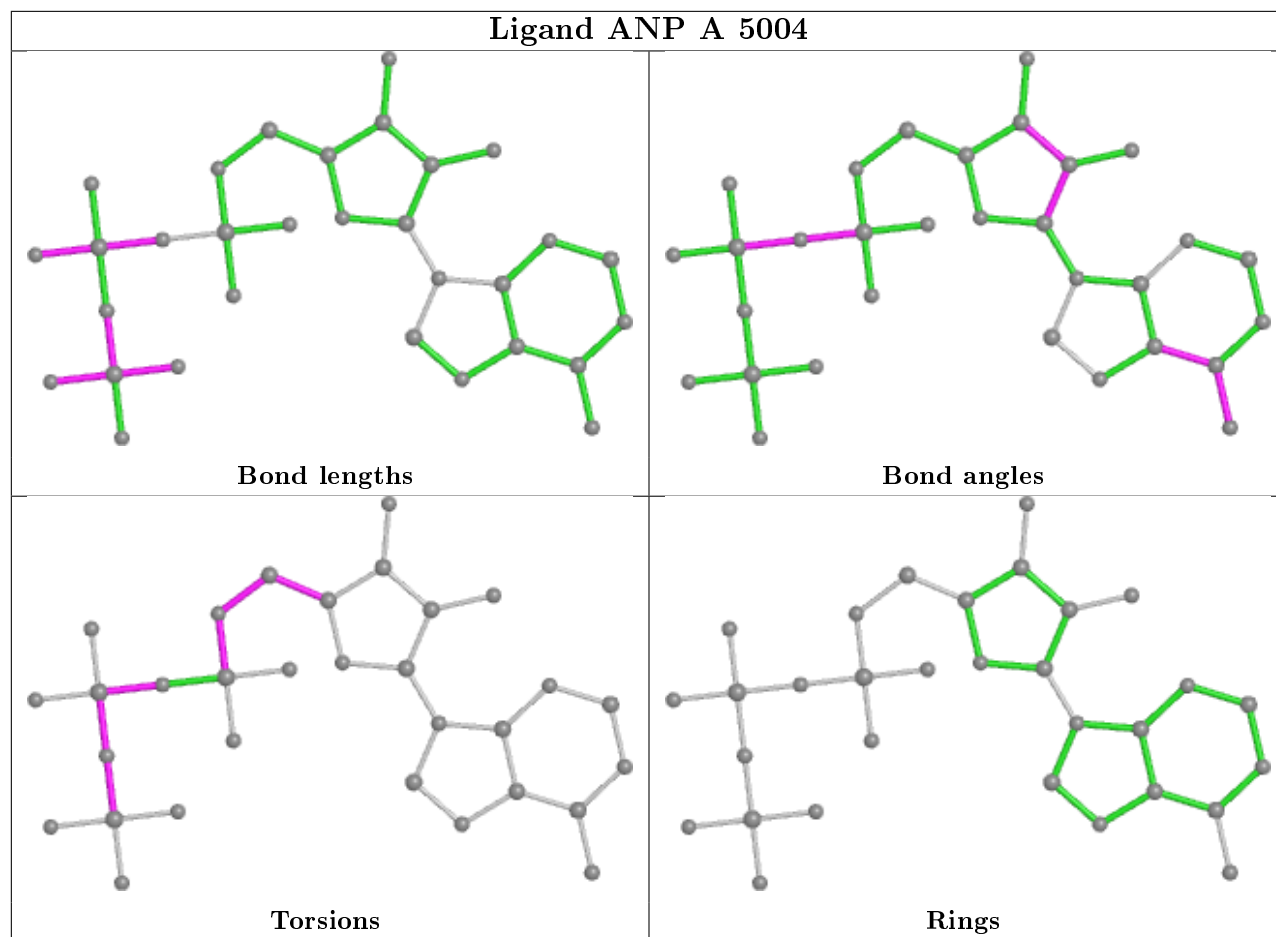
There are no ring outliers.

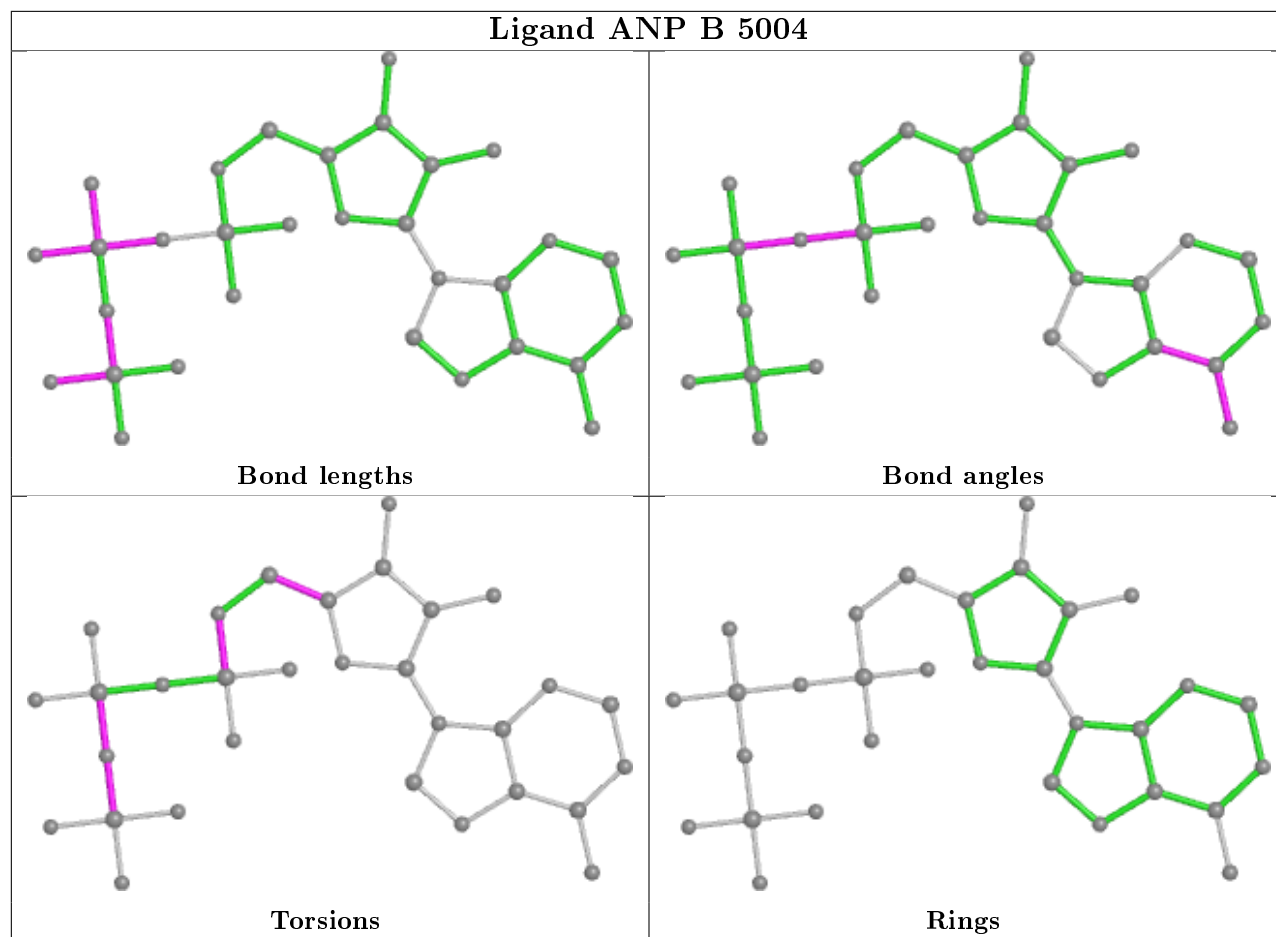
8 monomers are involved in 16 short contacts:

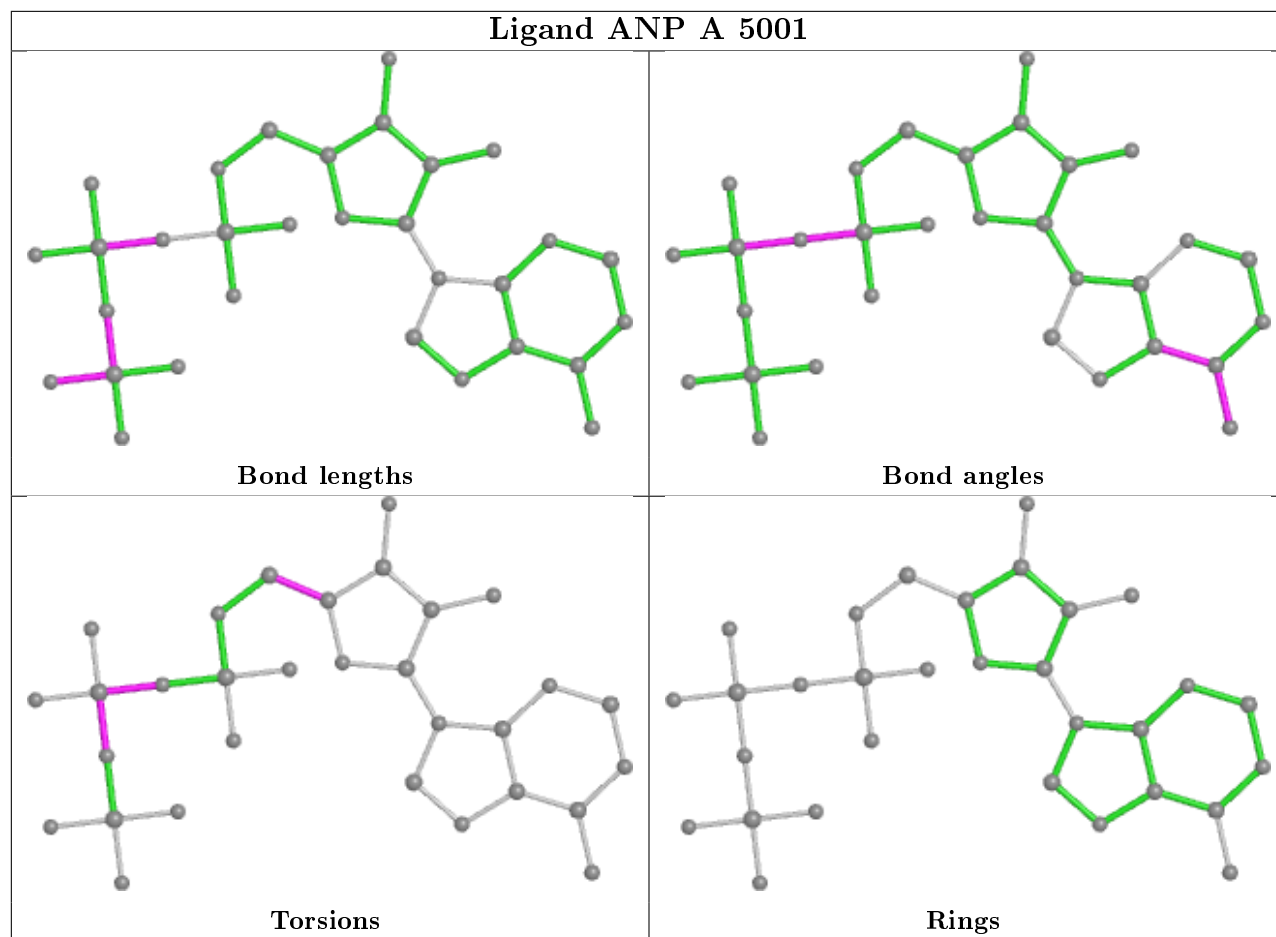
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5001	ANP	2	0
2	A	5004	ANP	2	0
2	B	5004	ANP	1	0
2	A	5001	ANP	1	0
2	A	5002	ANP	2	0
2	B	5002	ANP	2	0
2	B	5003	ANP	3	0
2	A	5003	ANP	3	0

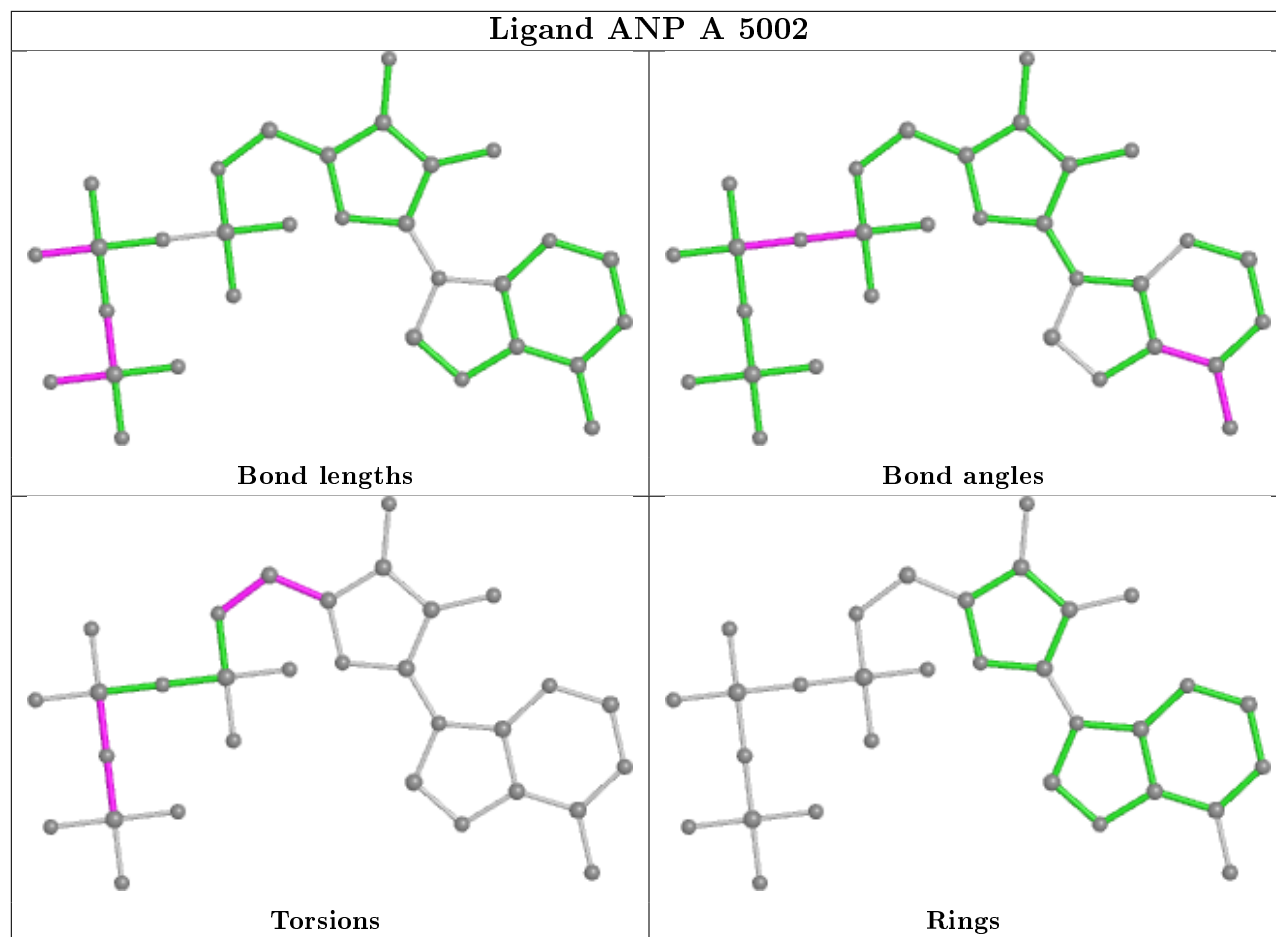
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

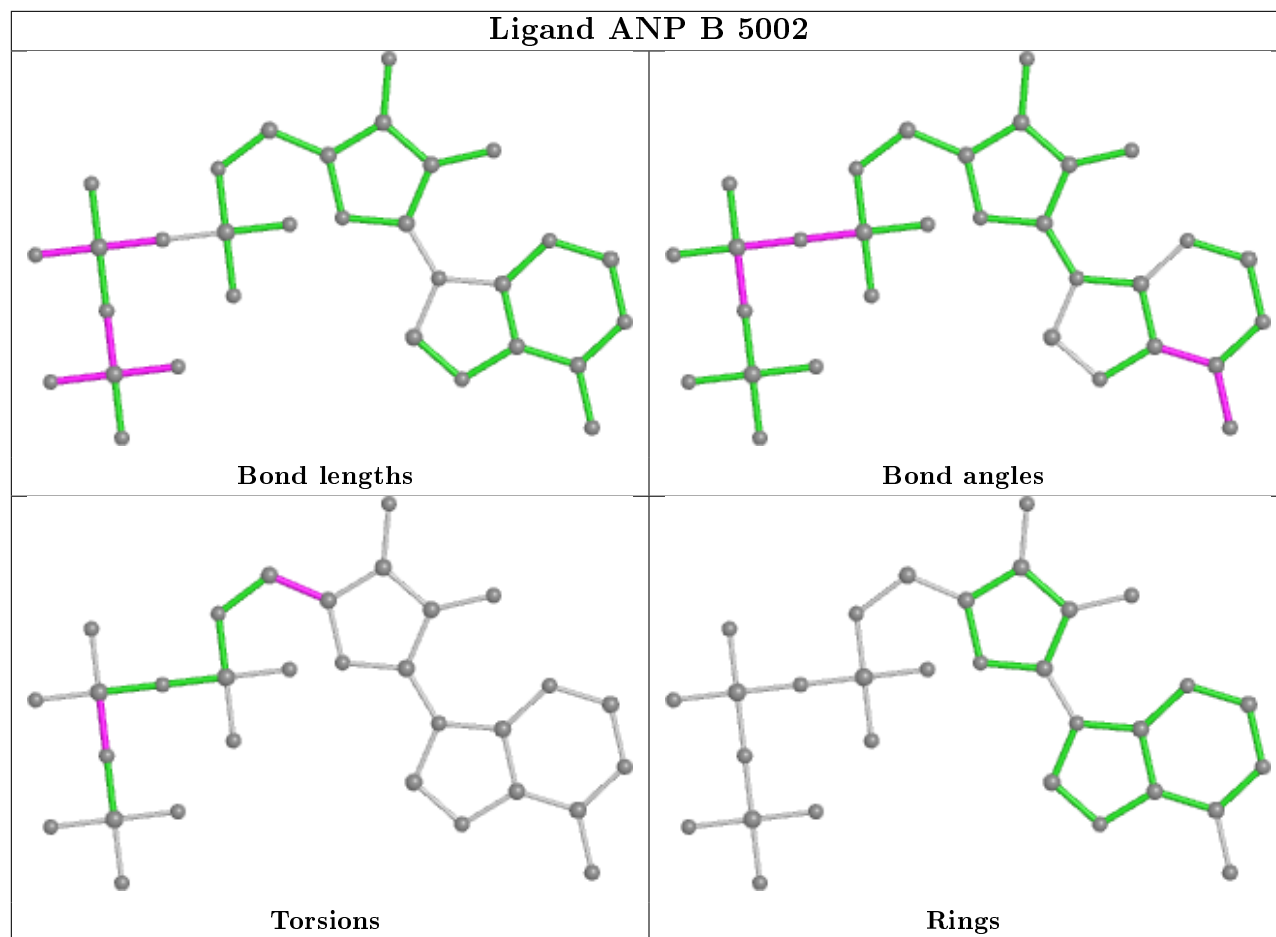


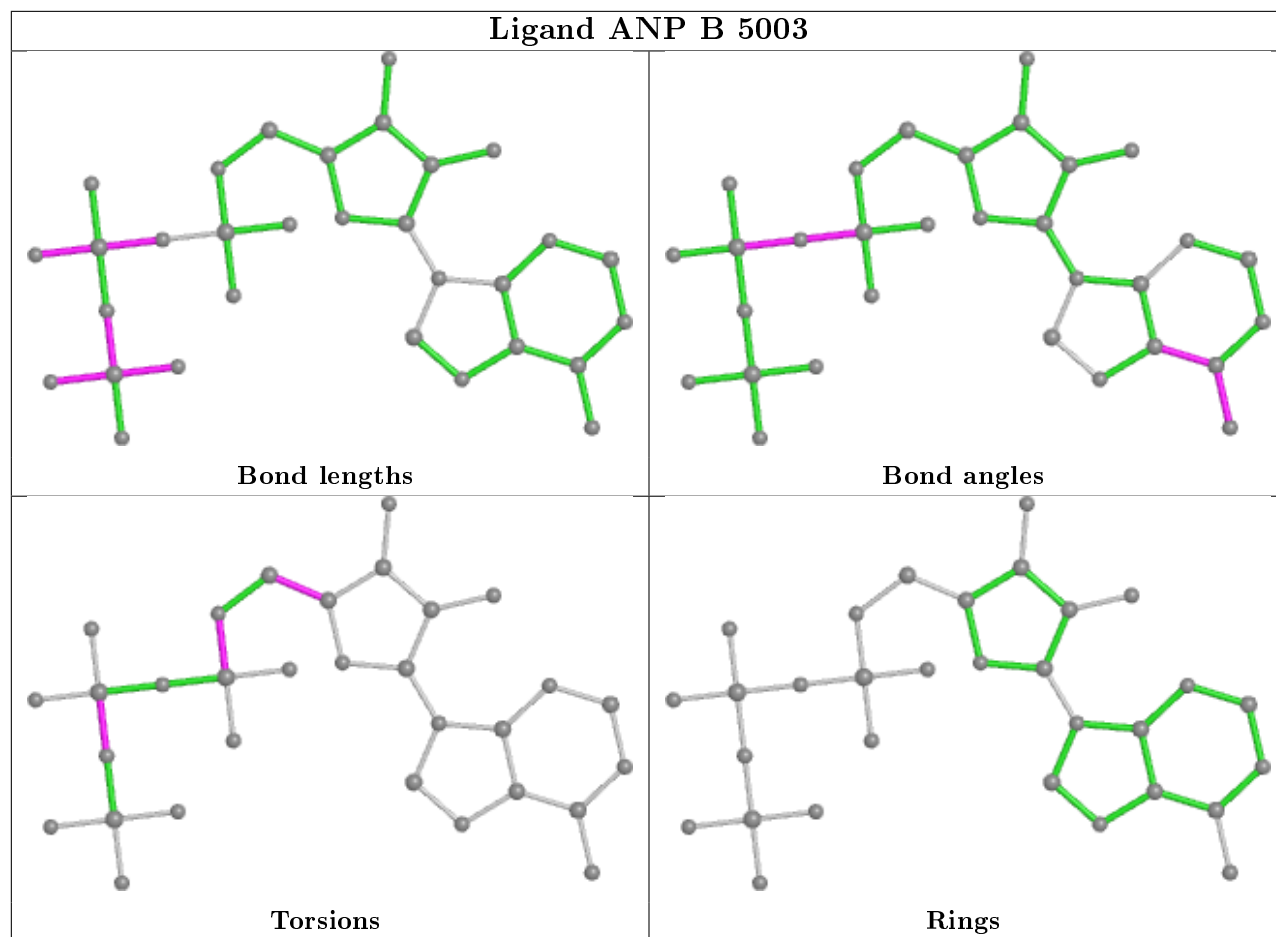


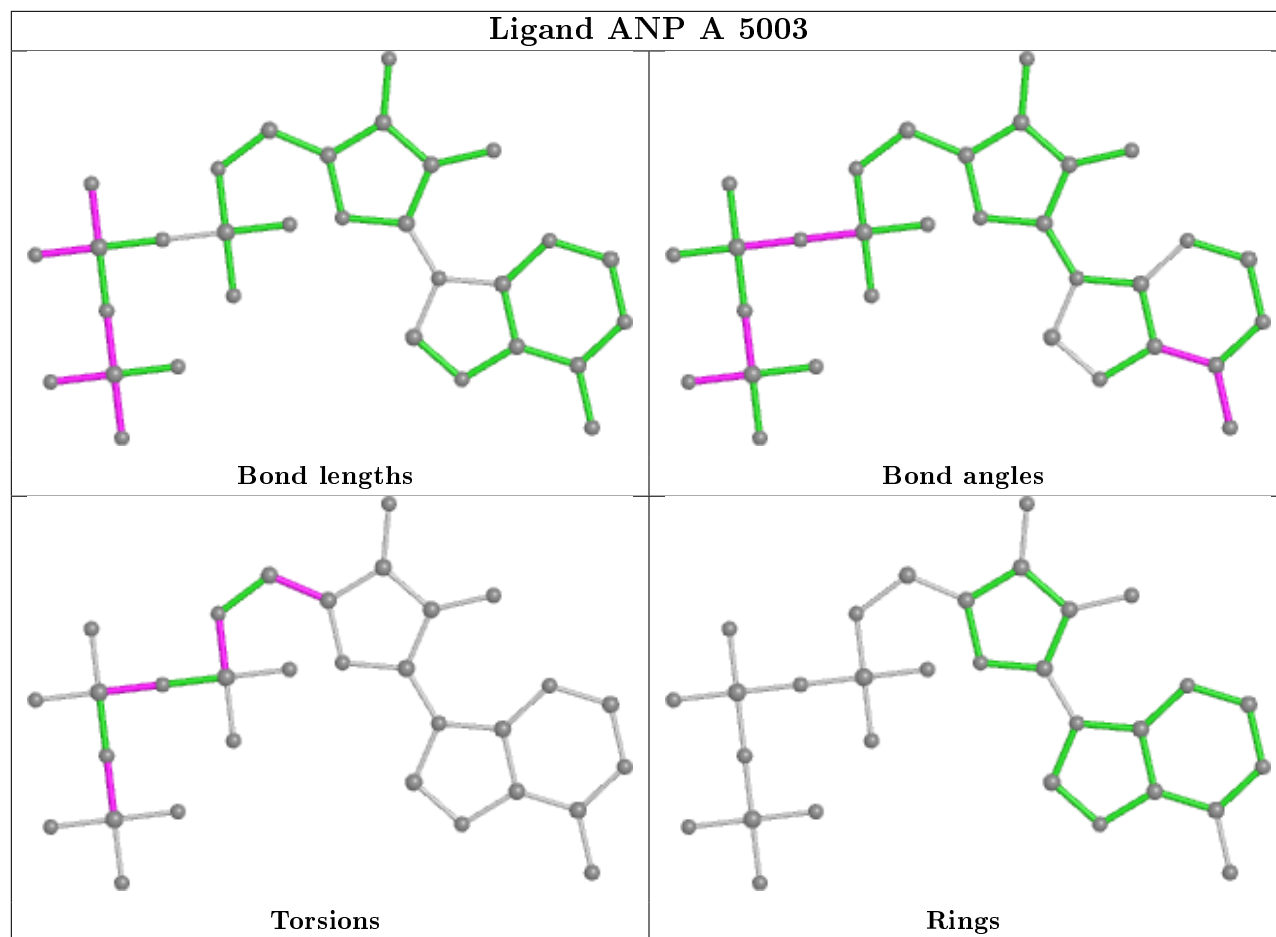












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	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 [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

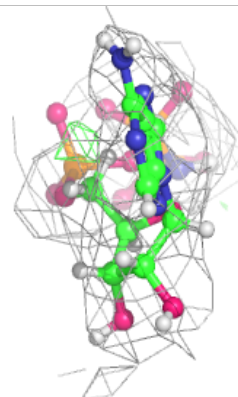
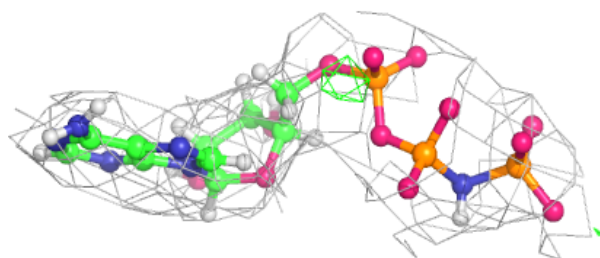
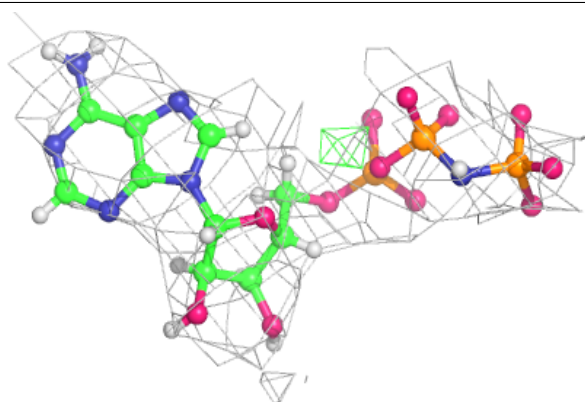
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ANP	A	5004	31/31	0.91	0.27	49,72,160,227	0
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	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	B	5004	31/31	0.94	0.24	47,78,162,183	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
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.

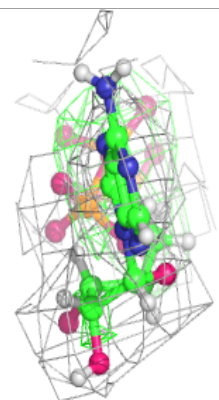
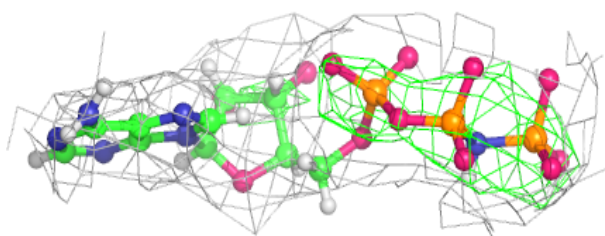
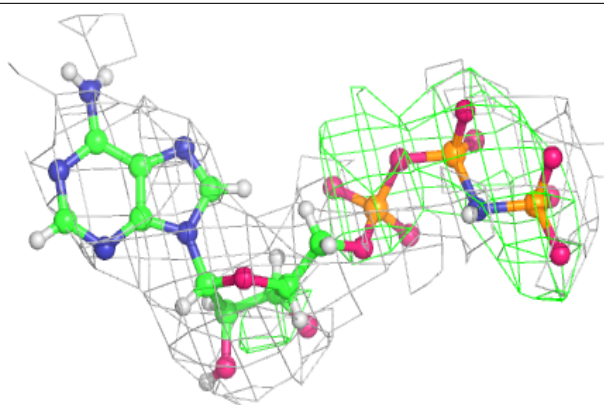
Electron density around ANP A 5004:

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

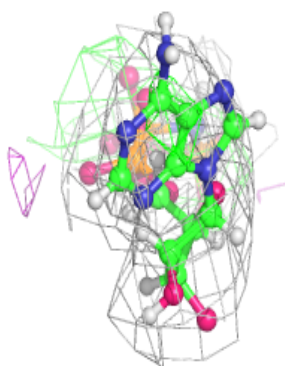
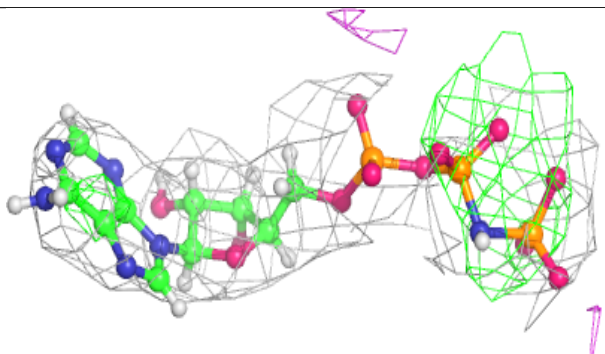
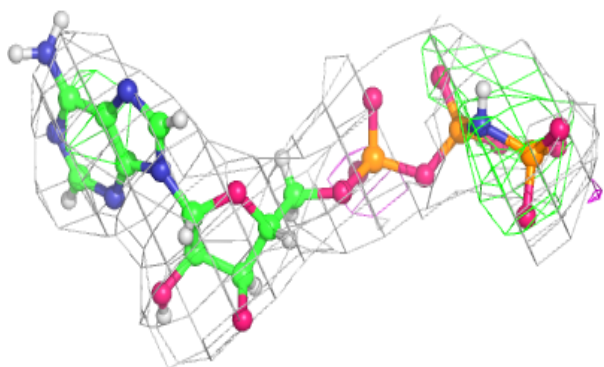


Electron density around ANP A 5002:

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

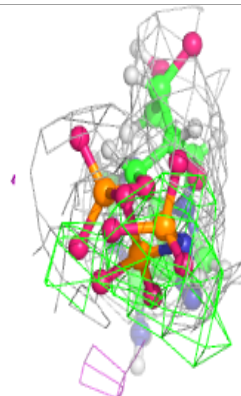
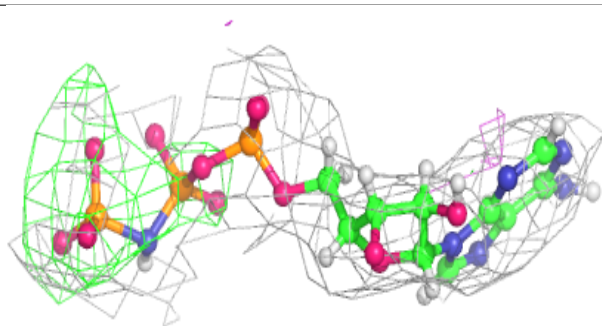
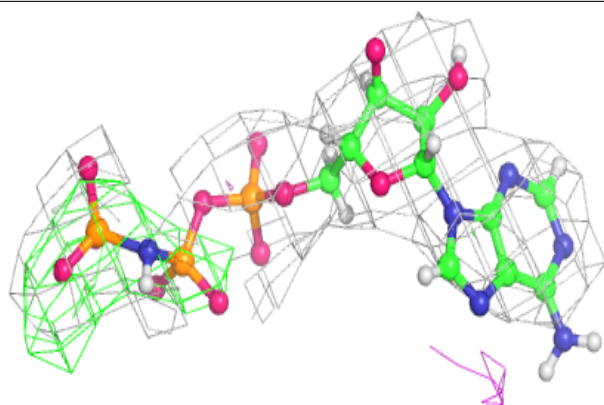
**Electron density around ANP A 5003:**

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

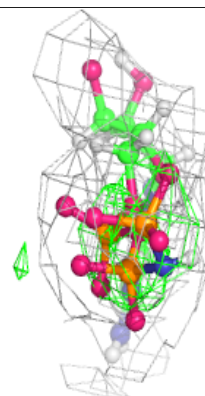
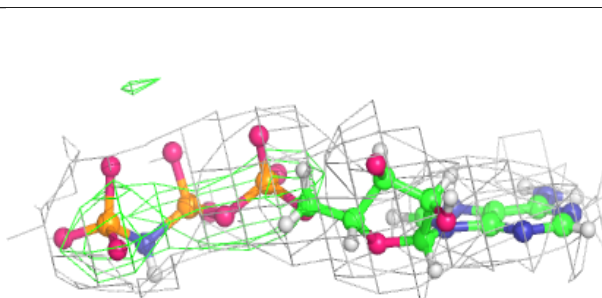
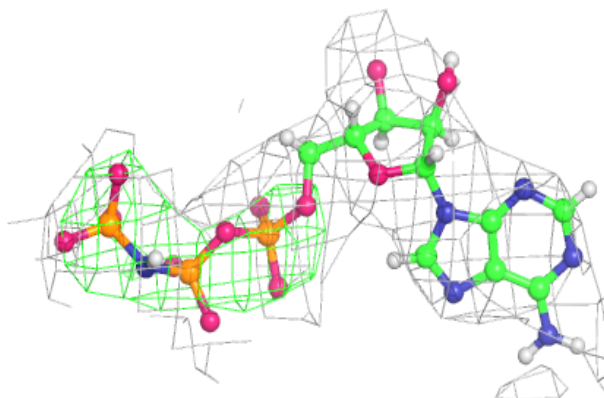


Electron density around ANP B 5003:

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

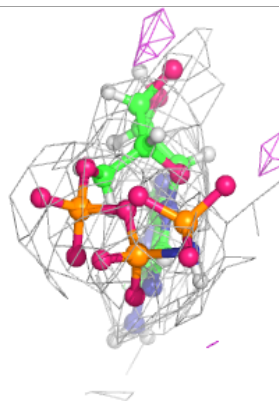
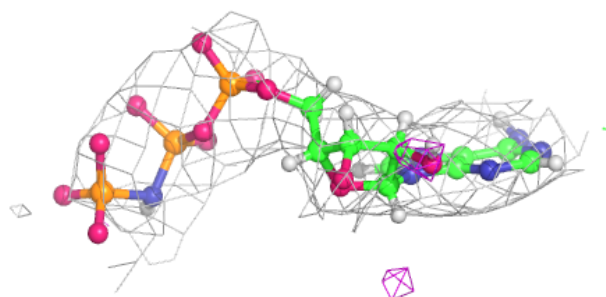
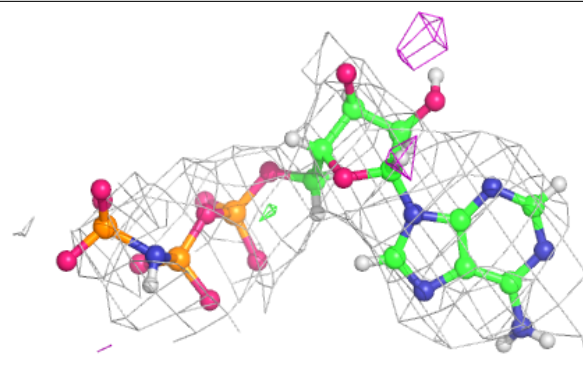
**Electron density around ANP B 5002:**

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

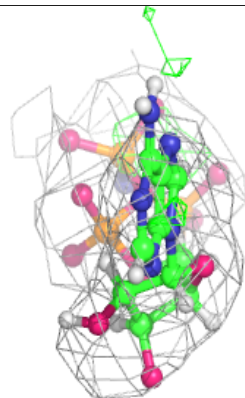
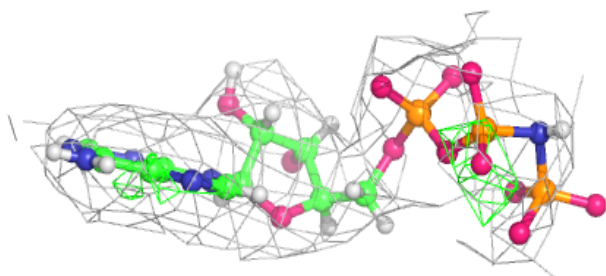
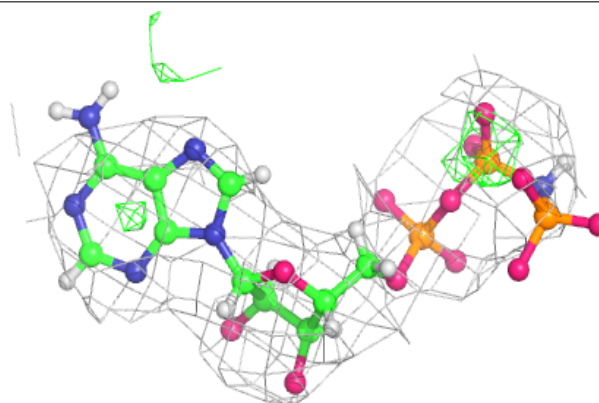


Electron density around ANP B 5004:

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

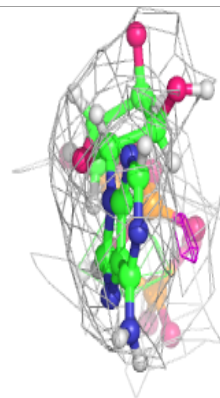
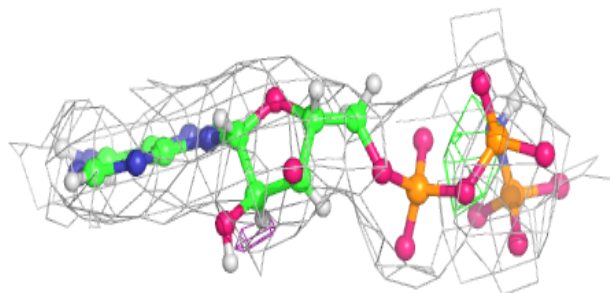
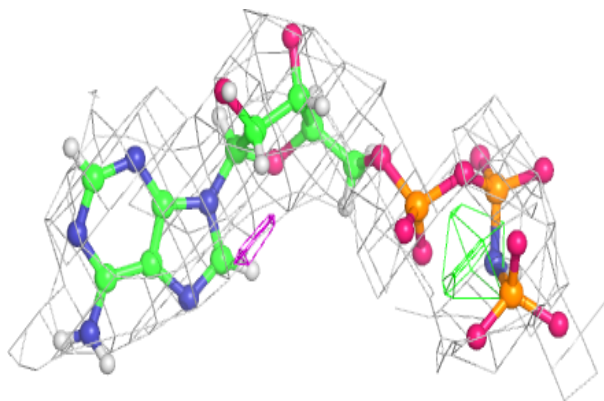
**Electron density around ANP A 5001:**

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.