



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:07 PM UTC

PDB ID : 3ZKD / pdb_00003zkd
Title : CRYSTAL STRUCTURE OF THE ATPASE REGION OF Mycobacterium tuberculosis GyrB WITH AMPPNP
Authors : Agrawal, A.; Roue, M.; Spitzfaden, C.; Petrella, S.; Aubry, A.; Volker, C.; Mossakowska, D.; Hann, M.; Bax, B.; Mayer, C.
Deposited on : 2013-01-22
Resolution : 2.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

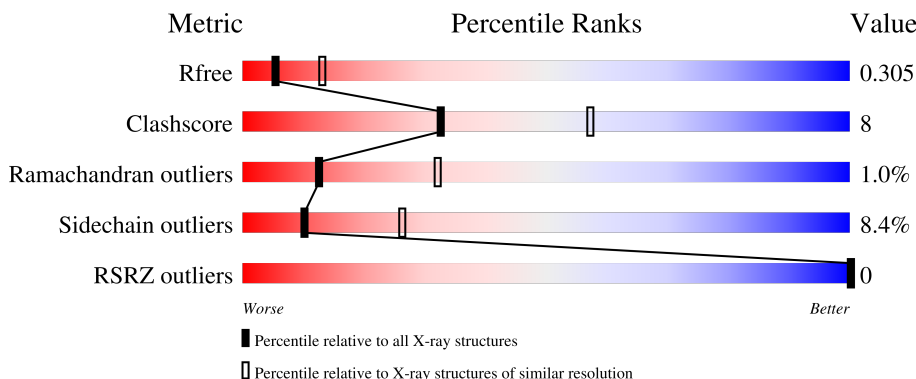
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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

Mol	Chain	Length	Quality of chain
1	A	432	
1	B	432	
1	C	432	
1	D	432	

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Mol	Chain	Length	Quality of chain
1	E	432	 69%18%•12%
1	F	432	 62%21%•13%
1	G	432	 65%21%•12%
1	H	432	 66%20%•12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23192 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 DNA GYRASE SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			2855	1789	503	557	6			
1	B	375	Total	C	N	O	S	0	0	0
			2843	1783	498	556	6			
1	C	390	Total	C	N	O	S	0	0	0
			2927	1835	519	567	6			
1	D	379	Total	C	N	O	S	0	0	0
			2817	1766	489	556	6			
1	E	382	Total	C	N	O	S	0	0	0
			2878	1803	506	563	6			
1	F	376	Total	C	N	O	S	0	0	0
			2821	1768	497	550	6			
1	G	378	Total	C	N	O	S	0	0	0
			2845	1786	497	556	6			
1	H	378	Total	C	N	O	S	0	0	0
			2835	1776	494	559	6			

There are 40 discrepancies between the modelled and reference sequences:

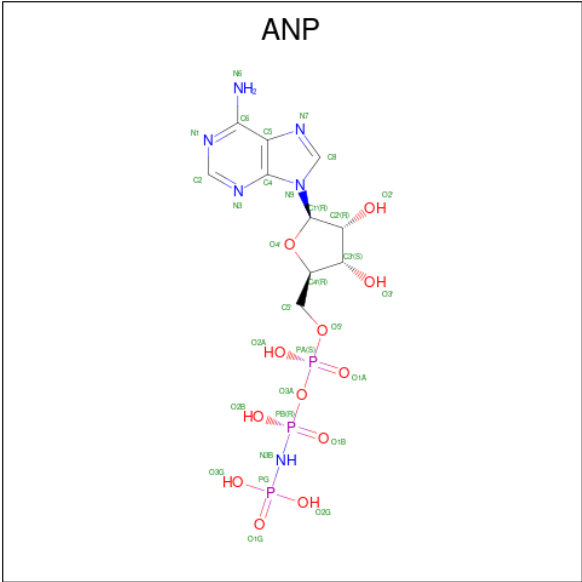
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP I6WX66
A	-3	PRO	-	expression tag	UNP I6WX66
A	-2	LEU	-	expression tag	UNP I6WX66
A	-1	GLY	-	expression tag	UNP I6WX66
A	0	SER	-	expression tag	UNP I6WX66
B	-4	GLY	-	expression tag	UNP I6WX66
B	-3	PRO	-	expression tag	UNP I6WX66
B	-2	LEU	-	expression tag	UNP I6WX66
B	-1	GLY	-	expression tag	UNP I6WX66
B	0	SER	-	expression tag	UNP I6WX66
C	-4	GLY	-	expression tag	UNP I6WX66
C	-3	PRO	-	expression tag	UNP I6WX66
C	-2	LEU	-	expression tag	UNP I6WX66

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP I6WX66
C	0	SER	-	expression tag	UNP I6WX66
D	-4	GLY	-	expression tag	UNP I6WX66
D	-3	PRO	-	expression tag	UNP I6WX66
D	-2	LEU	-	expression tag	UNP I6WX66
D	-1	GLY	-	expression tag	UNP I6WX66
D	0	SER	-	expression tag	UNP I6WX66
E	-4	GLY	-	expression tag	UNP I6WX66
E	-3	PRO	-	expression tag	UNP I6WX66
E	-2	LEU	-	expression tag	UNP I6WX66
E	-1	GLY	-	expression tag	UNP I6WX66
E	0	SER	-	expression tag	UNP I6WX66
F	-4	GLY	-	expression tag	UNP I6WX66
F	-3	PRO	-	expression tag	UNP I6WX66
F	-2	LEU	-	expression tag	UNP I6WX66
F	-1	GLY	-	expression tag	UNP I6WX66
F	0	SER	-	expression tag	UNP I6WX66
G	-4	GLY	-	expression tag	UNP I6WX66
G	-3	PRO	-	expression tag	UNP I6WX66
G	-2	LEU	-	expression tag	UNP I6WX66
G	-1	GLY	-	expression tag	UNP I6WX66
G	0	SER	-	expression tag	UNP I6WX66
H	-4	GLY	-	expression tag	UNP I6WX66
H	-3	PRO	-	expression tag	UNP I6WX66
H	-2	LEU	-	expression tag	UNP I6WX66
H	-1	GLY	-	expression tag	UNP I6WX66
H	0	SER	-	expression tag	UNP I6WX66

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: 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	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

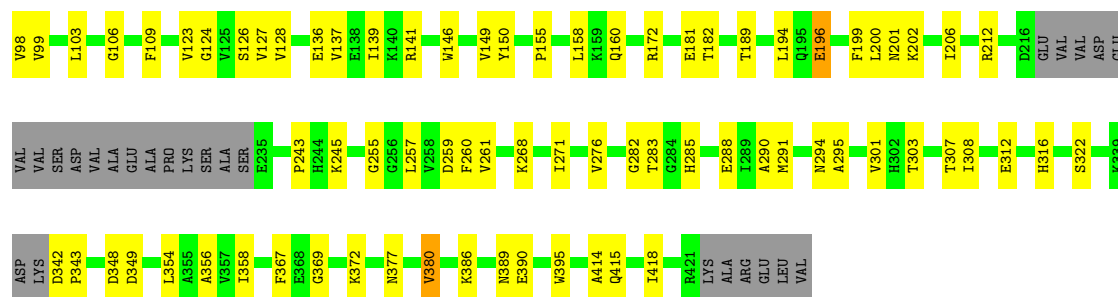
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0
3	G	1	Total 1	Mg 1	0	0
3	H	1	Total 1	Mg 1	0	0

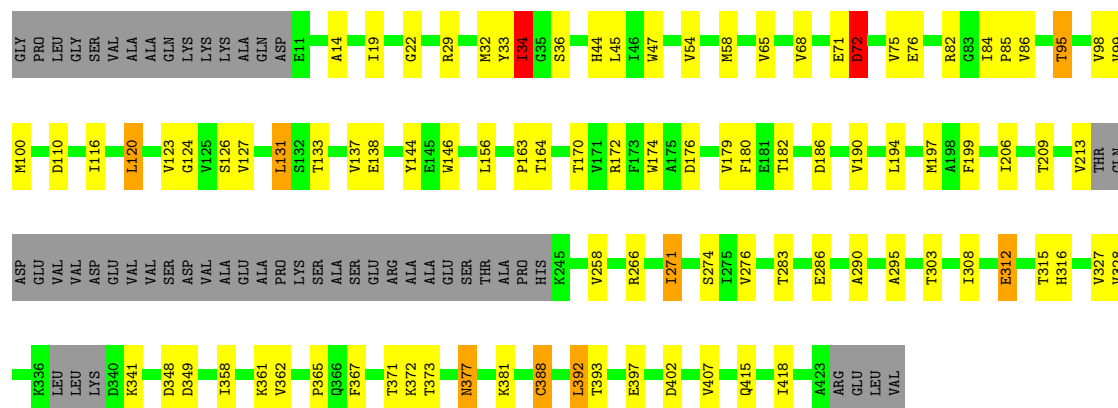
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total 20	O 20	0	0
4	B	11	Total 11	O 11	0	0
4	C	20	Total 20	O 20	0	0
4	D	8	Total 8	O 8	0	0
4	E	15	Total 15	O 15	0	0
4	F	12	Total 12	O 12	0	0
4	G	22	Total 22	O 22	0	0
4	H	7	Total 7	O 7	0	0



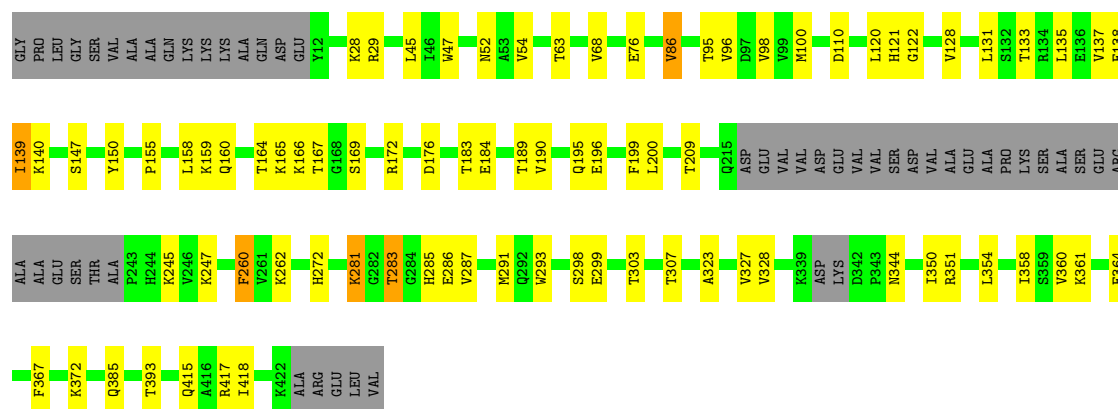
• Molecule 1: DNA GYRASE SUBUNIT B

Chain D: 66% 20% 12%



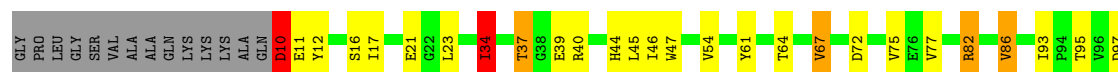
• Molecule 1: DNA GYRASE SUBUNIT B

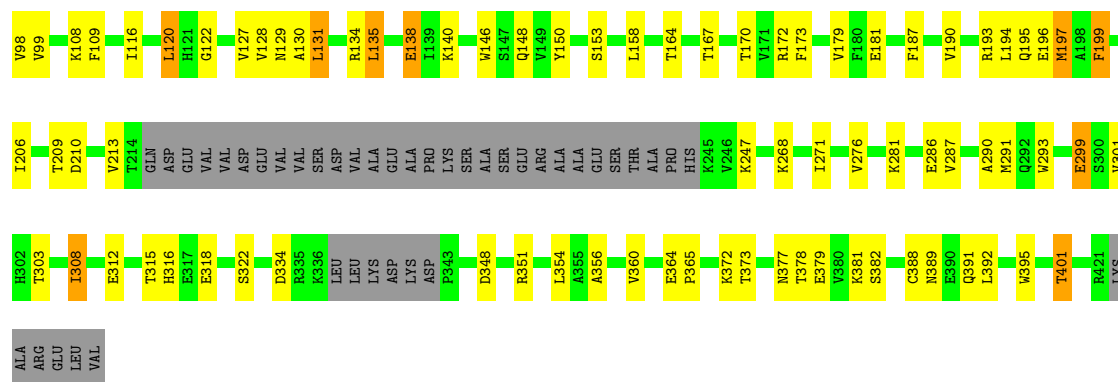
Chain E: 69% 18% 12%



• Molecule 1: DNA GYRASE SUBUNIT B

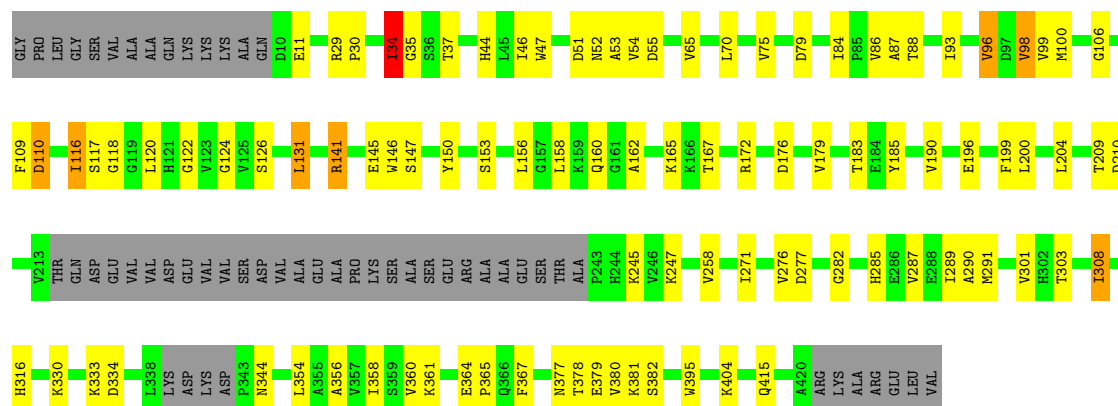
Chain F: 62% 21% 13%





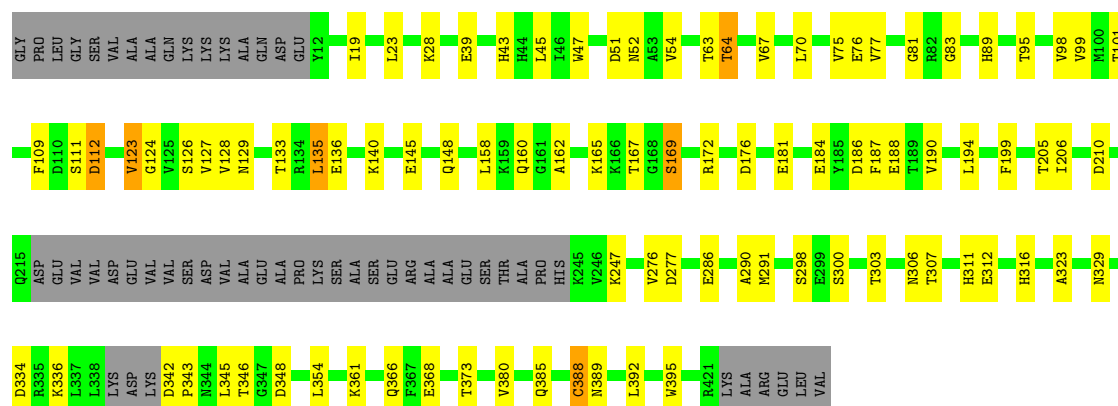
• Molecule 1: DNA GYRASE SUBUNIT B

Chain G: 65% 21% 12%



• Molecule 1: DNA GYRASE SUBUNIT B

Chain H: 66% 20% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.95Å 97.85Å 138.07Å 108.21° 105.18° 91.04°	Depositor
Resolution (Å)	24.81 – 2.95 24.81 – 2.95	Depositor EDS
% Data completeness (in resolution range)	84.6 (24.81-2.95) 84.6 (24.81-2.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.94Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.182 , 0.257 (Not available) , 0.305	Depositor DCC
R_{free} test set	2459 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.705	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 26.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.168 for h,-k,-h-l 0.015 for -h,k,-k-l 0.009 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	23192	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.78	0/2907	1.40	16/3940 (0.4%)
1	B	0.78	0/2896	1.38	15/3928 (0.4%)
1	C	0.81	0/2981	1.41	13/4044 (0.3%)
1	D	0.77	0/2869	1.40	15/3901 (0.4%)
1	E	0.77	1/2932 (0.0%)	1.38	8/3979 (0.2%)
1	F	0.81	1/2873 (0.0%)	1.41	11/3900 (0.3%)
1	G	0.78	0/2898	1.43	19/3932 (0.5%)
1	H	0.78	0/2886	1.38	12/3919 (0.3%)
All	All	0.79	2/23242 (0.0%)	1.40	109/31543 (0.3%)

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	2
1	C	0	1
1	H	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	364	GLU	CA-C	5.21	1.58	1.52
1	F	364	GLU	CA-C	5.08	1.58	1.52

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	51	ASP	CA-CB-CG	7.90	120.50	112.60
1	D	72	ASP	CA-CB-CG	7.39	119.99	112.60
1	G	34	ILE	N-CA-CB	-7.37	102.58	112.16
1	G	30	PRO	CA-C-N	7.34	128.25	120.03
1	G	30	PRO	C-N-CA	7.34	128.25	120.03

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	342	ASP	Mainchain,Peptide
1	C	342	ASP	Mainchain
1	H	342	ASP	Mainchain

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	2855	0	2774	51	0
1	B	2843	0	2764	57	0
1	C	2927	0	2837	47	0
1	D	2817	0	2690	45	0
1	E	2878	0	2780	40	0
1	F	2821	0	2726	54	0
1	G	2845	0	2756	45	0
1	H	2835	0	2723	43	0
2	A	31	0	13	3	0
2	B	31	0	13	1	0
2	C	31	0	13	1	0
2	D	31	0	13	1	0
2	E	31	0	13	2	0
2	F	31	0	13	1	0
2	G	31	0	13	2	0
2	H	31	0	13	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	20	0	0	0	0
4	B	11	0	0	0	0
4	C	20	0	0	0	0
4	D	8	0	0	0	0
4	E	15	0	0	0	0
4	F	12	0	0	0	0
4	G	22	0	0	0	0
4	H	7	0	0	0	0
All	All	23192	0	22154	358	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 358 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:93:ILE:HG13	1:B:94:PRO:HD2	1.53	0.90
1:C:308:ILE:HD13	1:C:372:LYS:HD3	1.61	0.82
1:D:312:GLU:CG	1:D:373:THR:HB	2.13	0.78
1:D:312:GLU:HG3	1:D:373:THR:HB	1.67	0.76
2:A:601:ANP:H8	2:A:601:ANP:H5'2	1.68	0.75

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	371/432 (86%)	342 (92%)	22 (6%)	7 (2%)	6	17
1	B	369/432 (85%)	346 (94%)	22 (6%)	1 (0%)	36	59
1	C	384/432 (89%)	359 (94%)	21 (6%)	4 (1%)	12	32
1	D	373/432 (86%)	351 (94%)	15 (4%)	7 (2%)	6	17
1	E	376/432 (87%)	355 (94%)	20 (5%)	1 (0%)	36	59
1	F	370/432 (86%)	349 (94%)	19 (5%)	2 (0%)	24	49
1	G	372/432 (86%)	349 (94%)	18 (5%)	5 (1%)	9	26
1	H	372/432 (86%)	349 (94%)	19 (5%)	4 (1%)	11	29
All	All	2987/3456 (86%)	2800 (94%)	156 (5%)	31 (1%)	12	32

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	343	PRO
1	C	343	PRO
1	H	343	PRO
1	A	87	ALA
1	A	124	GLY

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	297/350 (85%)	278 (94%)	19 (6%)	16	38
1	B	298/350 (85%)	271 (91%)	27 (9%)	9	23
1	C	301/350 (86%)	277 (92%)	24 (8%)	11	28
1	D	289/350 (83%)	268 (93%)	21 (7%)	13	33
1	E	299/350 (85%)	277 (93%)	22 (7%)	13	32
1	F	292/350 (83%)	255 (87%)	37 (13%)	4	13
1	G	296/350 (85%)	269 (91%)	27 (9%)	9	23
1	H	293/350 (84%)	272 (93%)	21 (7%)	13	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2365/2800 (84%)	2167 (92%)	198 (8%)	10	26

5 of 198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	34	ILE
1	F	348	ASP
1	F	64	THR
1	F	135	LEU
1	G	34	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	309	ASN
1	F	44	HIS
1	H	285	HIS
1	D	399	ASN
1	E	272	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 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	601	3	33,33,33	3.53	15 (45%)	45,52,52	2.19	14 (31%)
2	ANP	E	601	3	33,33,33	3.53	14 (42%)	45,52,52	1.94	8 (17%)
2	ANP	F	601	3	33,33,33	3.52	14 (42%)	45,52,52	2.22	13 (28%)
2	ANP	D	601	3	33,33,33	3.53	14 (42%)	45,52,52	2.04	12 (26%)
2	ANP	B	601	3	33,33,33	3.48	15 (45%)	45,52,52	2.03	13 (28%)
2	ANP	H	601	3	33,33,33	3.49	14 (42%)	45,52,52	2.08	12 (26%)
2	ANP	C	601	3	33,33,33	3.56	14 (42%)	45,52,52	2.06	11 (24%)
2	ANP	G	601	3	33,33,33	3.54	14 (42%)	45,52,52	2.09	10 (22%)

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	601	3	-	1/18/38/38	0/3/3/3
2	ANP	E	601	3	-	3/18/38/38	0/3/3/3
2	ANP	F	601	3	-	4/18/38/38	0/3/3/3
2	ANP	D	601	3	-	3/18/38/38	0/3/3/3
2	ANP	B	601	3	-	2/18/38/38	0/3/3/3
2	ANP	H	601	3	-	2/18/38/38	0/3/3/3
2	ANP	C	601	3	-	4/18/38/38	0/3/3/3
2	ANP	G	601	3	-	2/18/38/38	0/3/3/3

The worst 5 of 114 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	ANP	PB-O1B	11.26	1.63	1.46
2	A	601	ANP	PB-O1B	11.11	1.63	1.46
2	G	601	ANP	PB-O1B	10.88	1.62	1.46
2	D	601	ANP	PB-O1B	10.87	1.62	1.46
2	E	601	ANP	PB-O1B	10.64	1.62	1.46

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	ANP	C5-C4-N3	-6.33	118.00	126.72
2	G	601	ANP	C5-C4-N3	-6.24	118.13	126.72
2	A	601	ANP	C5-C4-N3	-6.15	118.25	126.72
2	D	601	ANP	C5-C4-N3	-6.05	118.39	126.72
2	F	601	ANP	C5-C4-N3	-6.02	118.42	126.72

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

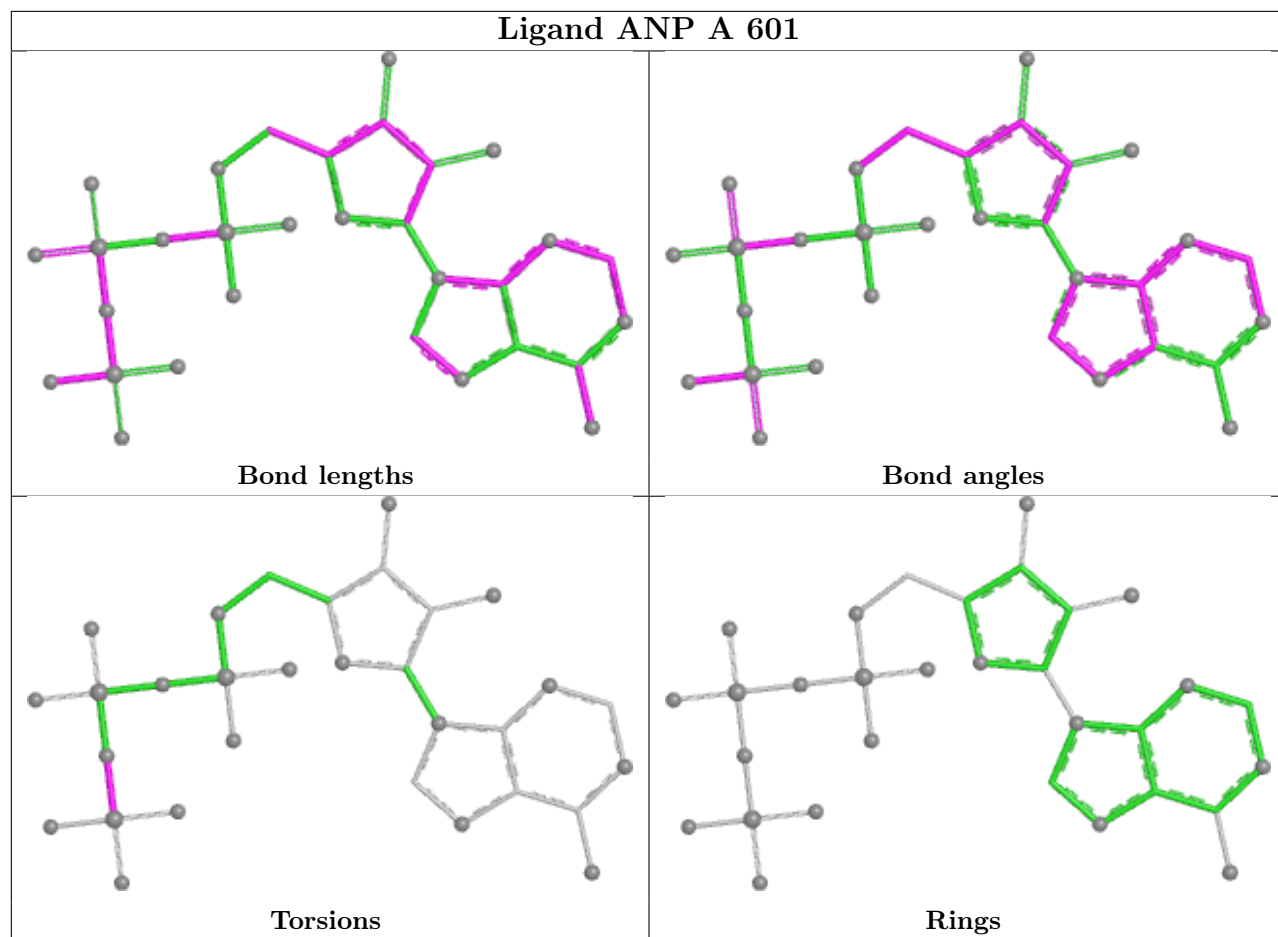
Mol	Chain	Res	Type	Atoms
2	A	601	ANP	PB-N3B-PG-O1G
2	B	601	ANP	PA-O3A-PB-O2B
2	C	601	ANP	PG-N3B-PB-O1B
2	C	601	ANP	PG-N3B-PB-O3A
2	C	601	ANP	PA-O3A-PB-O2B

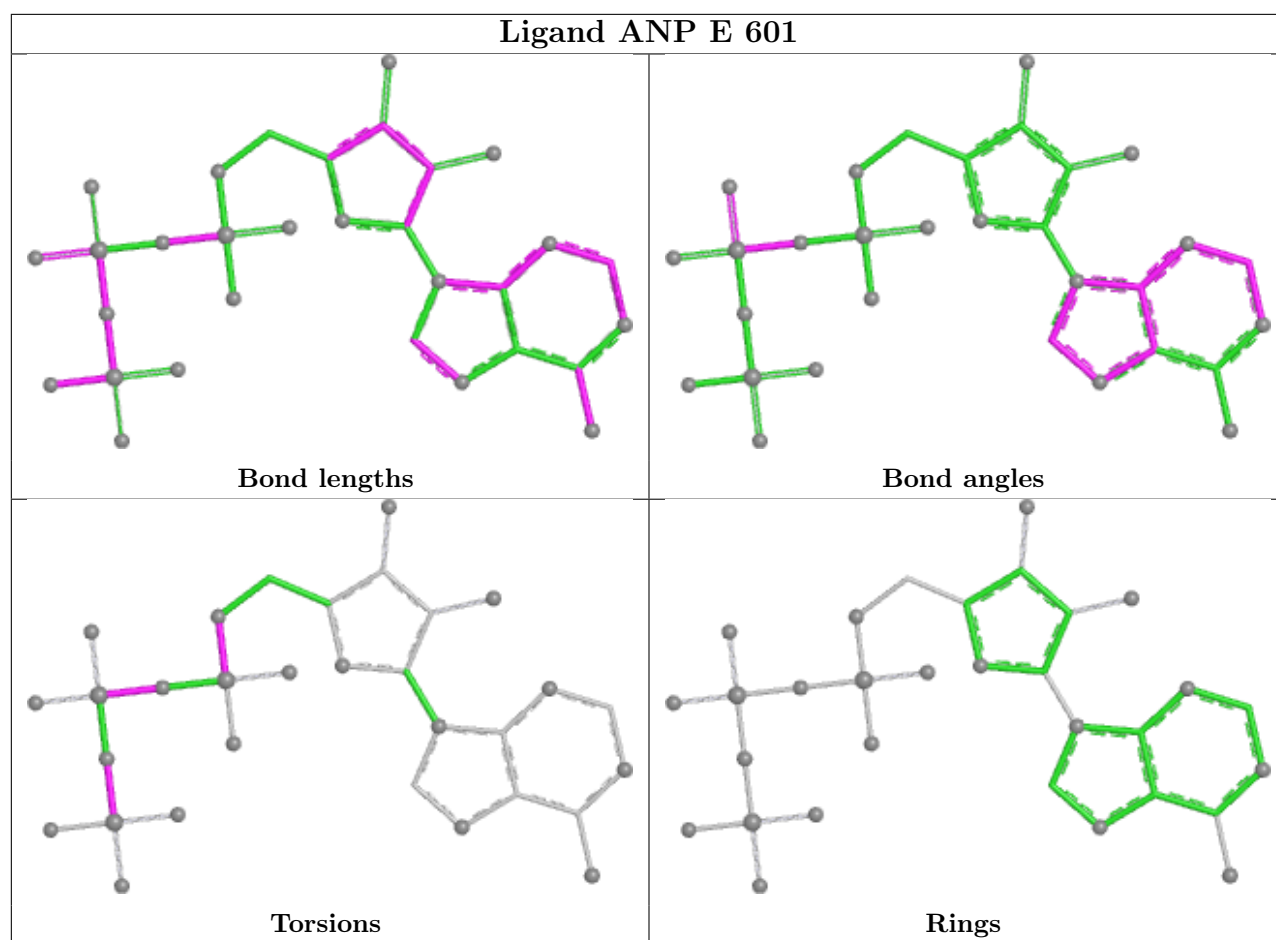
There are no ring outliers.

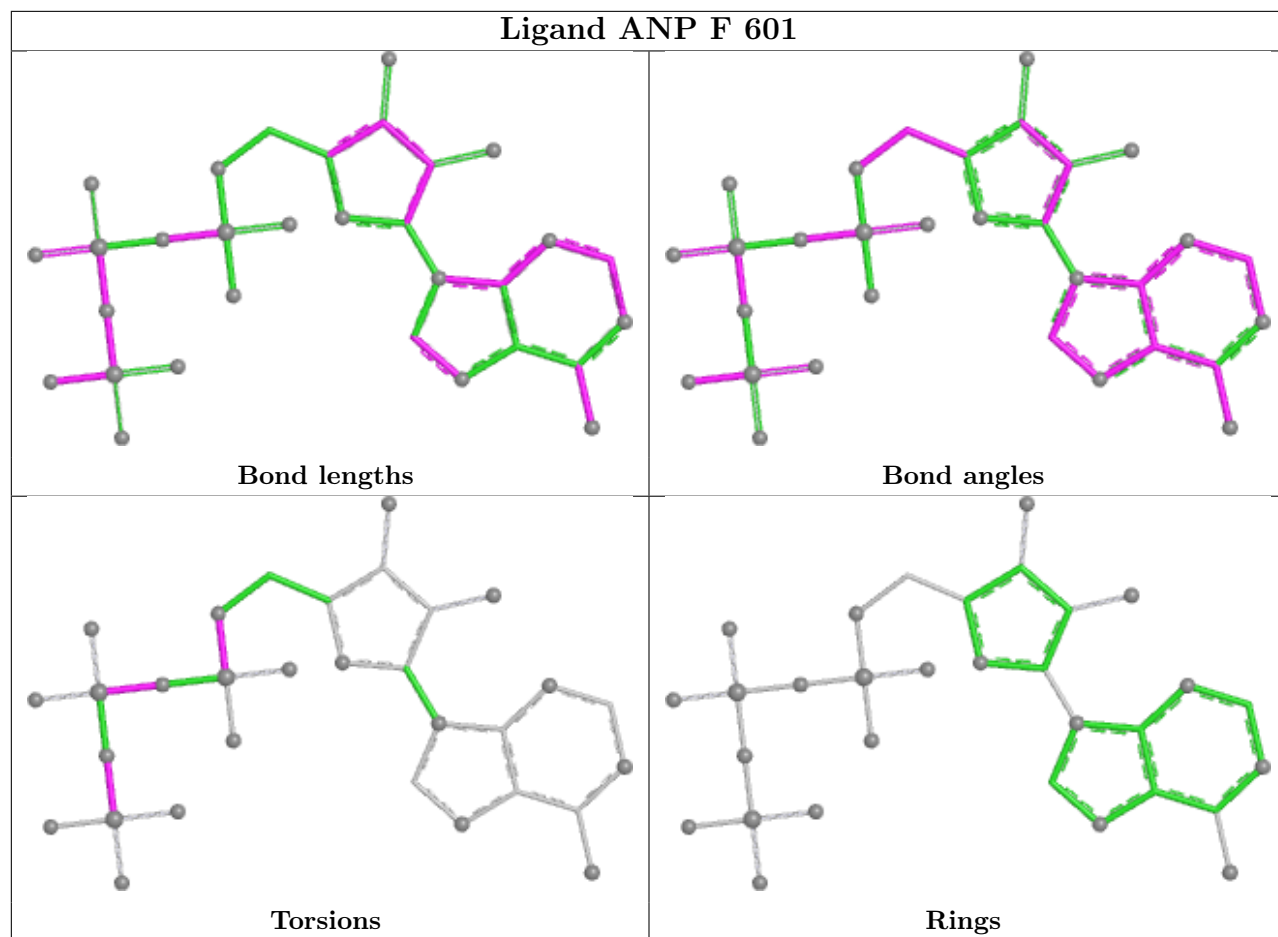
8 monomers are involved in 12 short contacts:

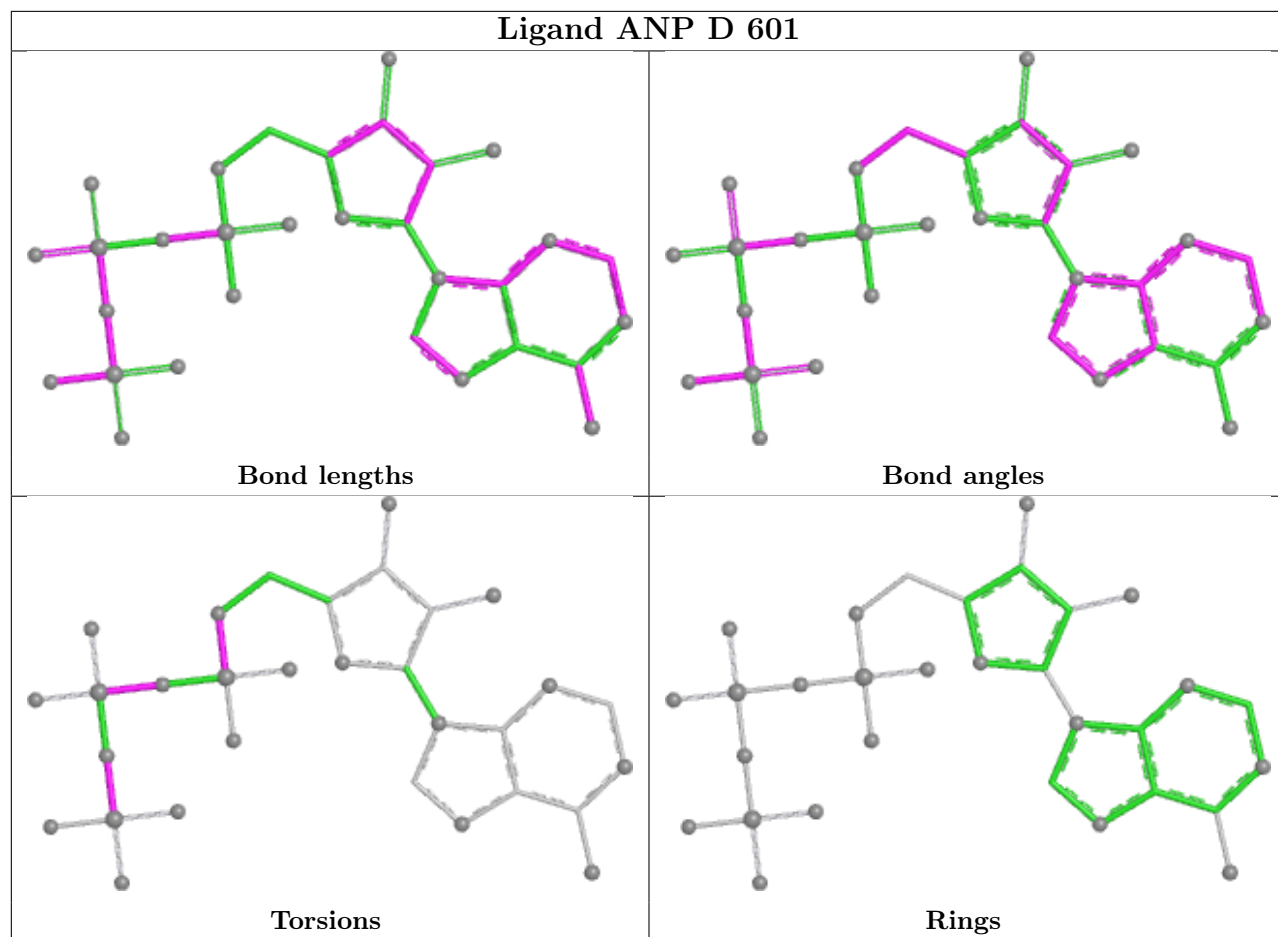
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	ANP	3	0
2	E	601	ANP	2	0
2	F	601	ANP	1	0
2	D	601	ANP	1	0
2	B	601	ANP	1	0
2	H	601	ANP	1	0
2	C	601	ANP	1	0
2	G	601	ANP	2	0

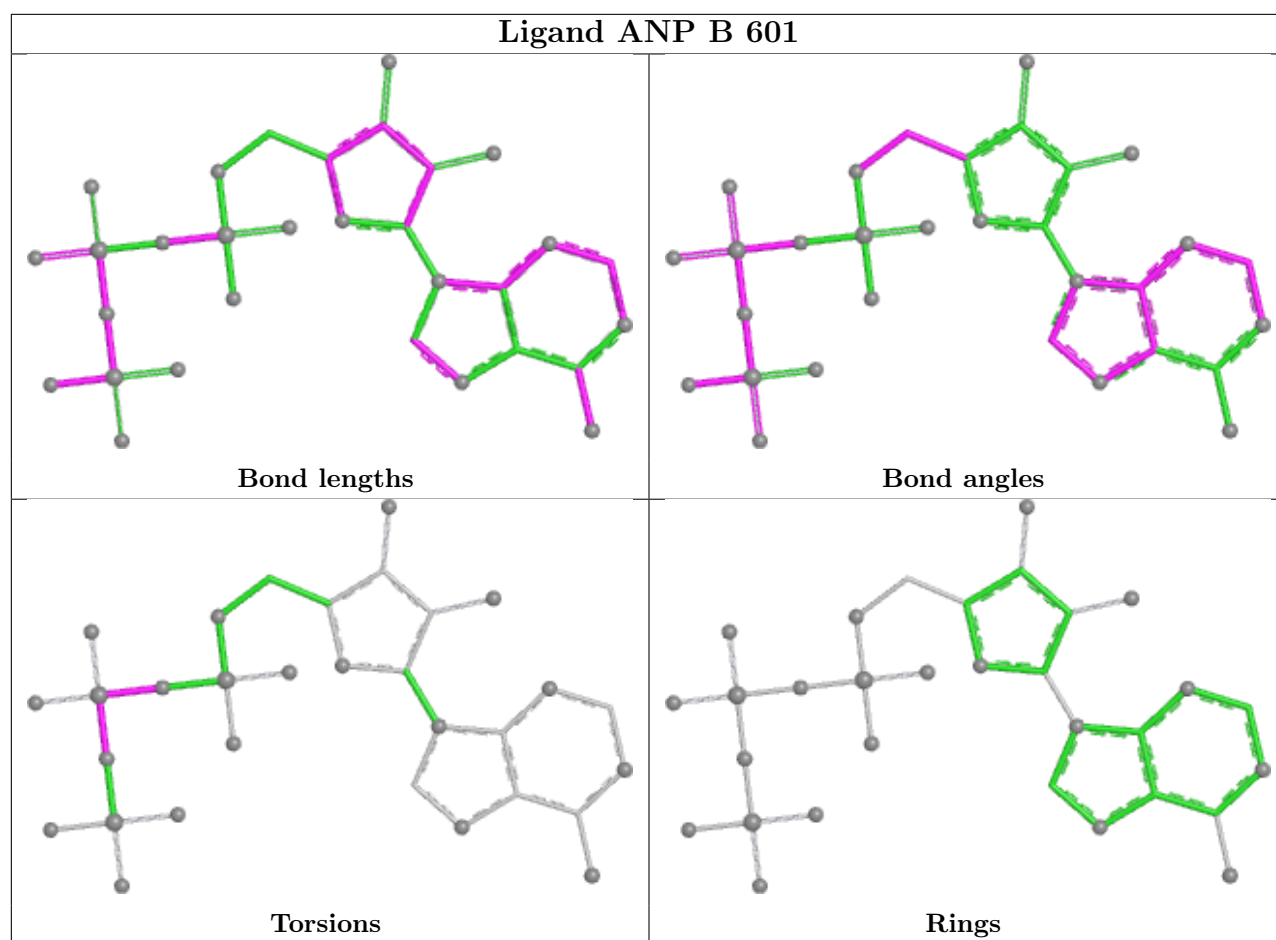
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

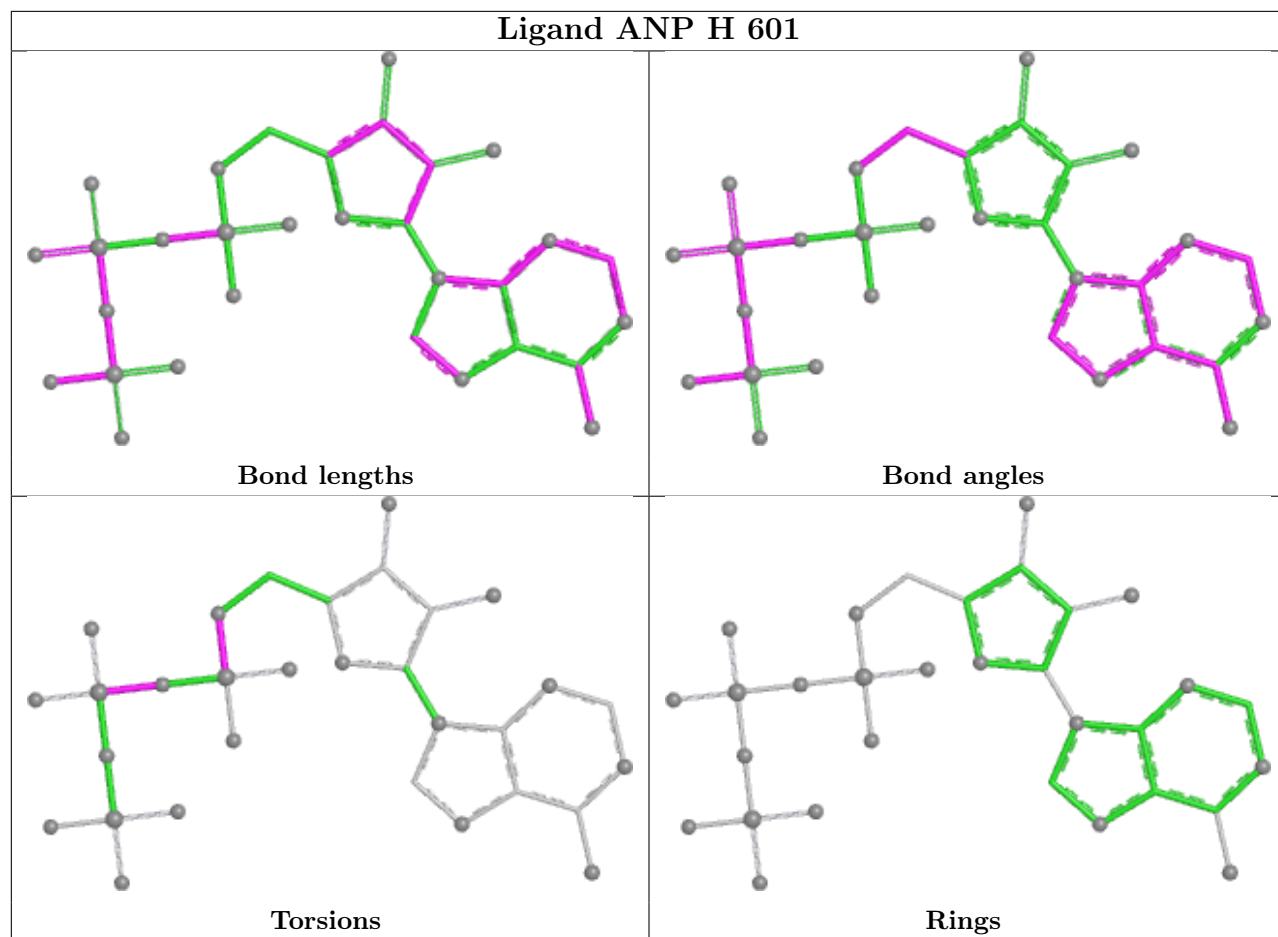


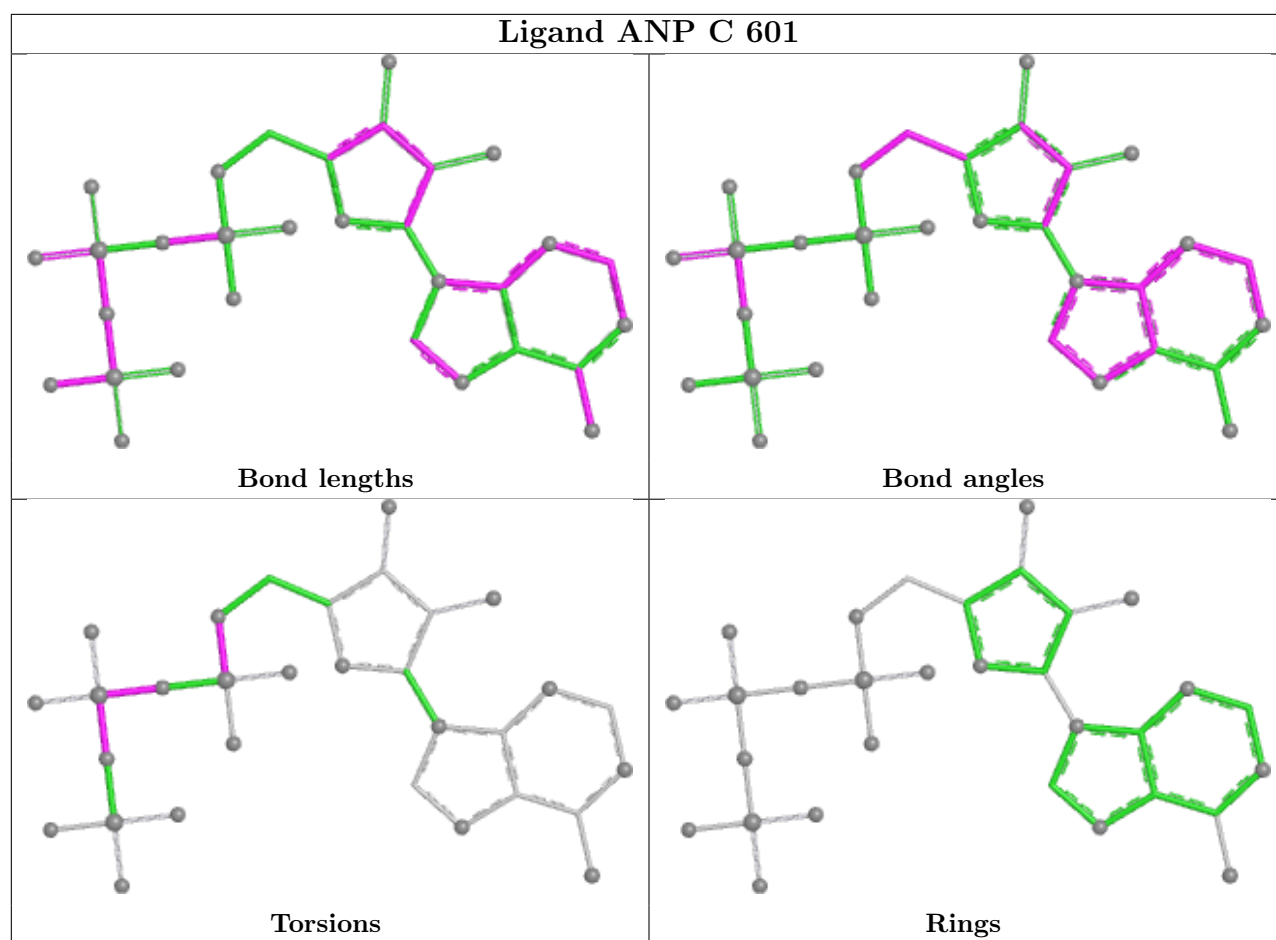


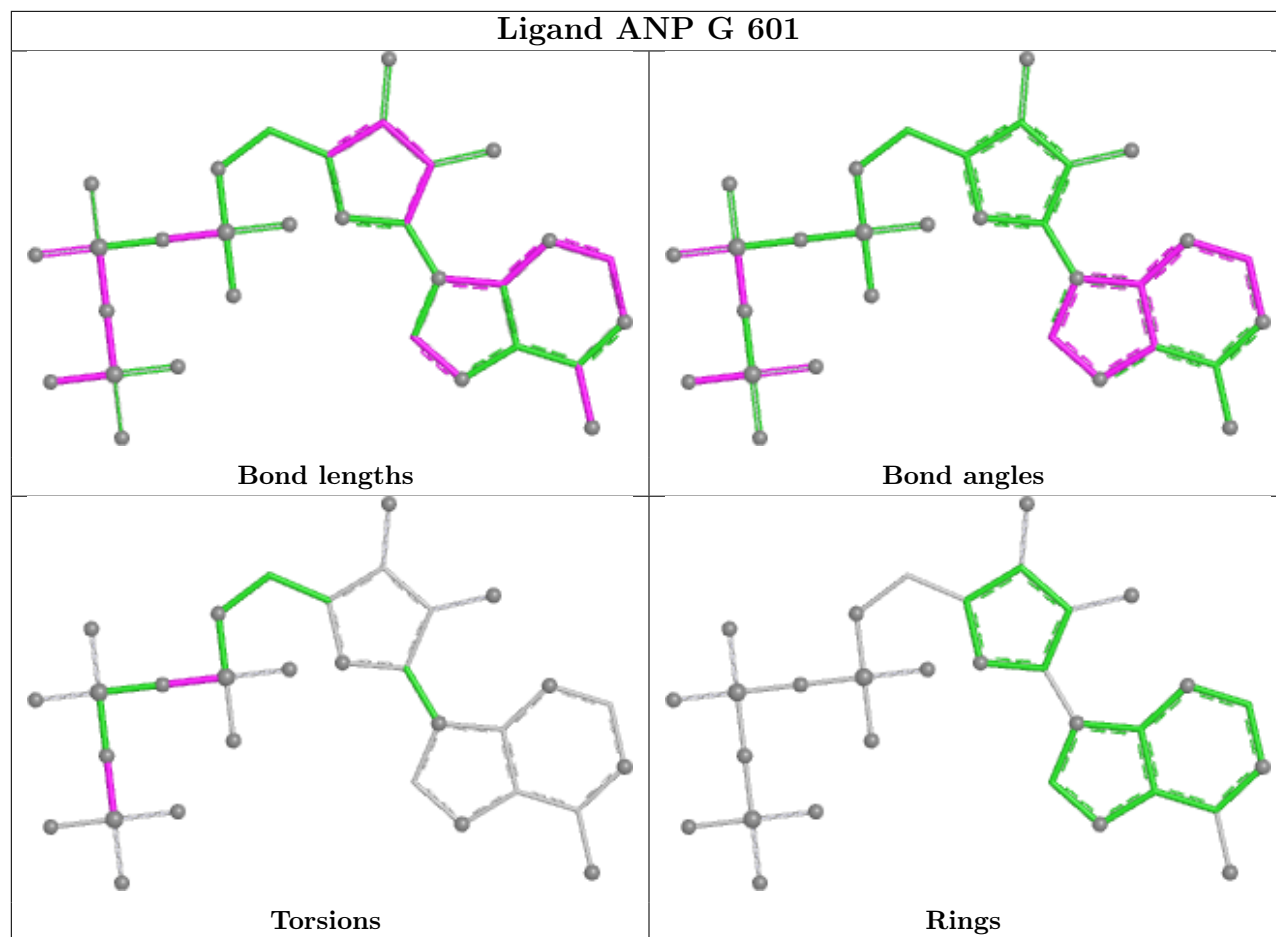












5.7 Other polymers [i](#)

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	377/432 (87%)	-1.55	0 100 100	47, 74, 130, 156	0
1	B	375/432 (86%)	-1.59	0 100 100	46, 75, 110, 129	0
1	C	390/432 (90%)	-1.58	0 100 100	39, 71, 129, 179	0
1	D	379/432 (87%)	-1.47	0 100 100	51, 83, 124, 160	0
1	E	382/432 (88%)	-1.60	0 100 100	41, 70, 135, 171	0
1	F	376/432 (87%)	-1.61	0 100 100	44, 72, 123, 160	0
1	G	378/432 (87%)	-1.57	0 100 100	41, 70, 132, 155	0
1	H	378/432 (87%)	-1.44	0 100 100	49, 82, 130, 149	0
All	All	3035/3456 (87%)	-1.55	0 100 100	39, 75, 128, 179	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

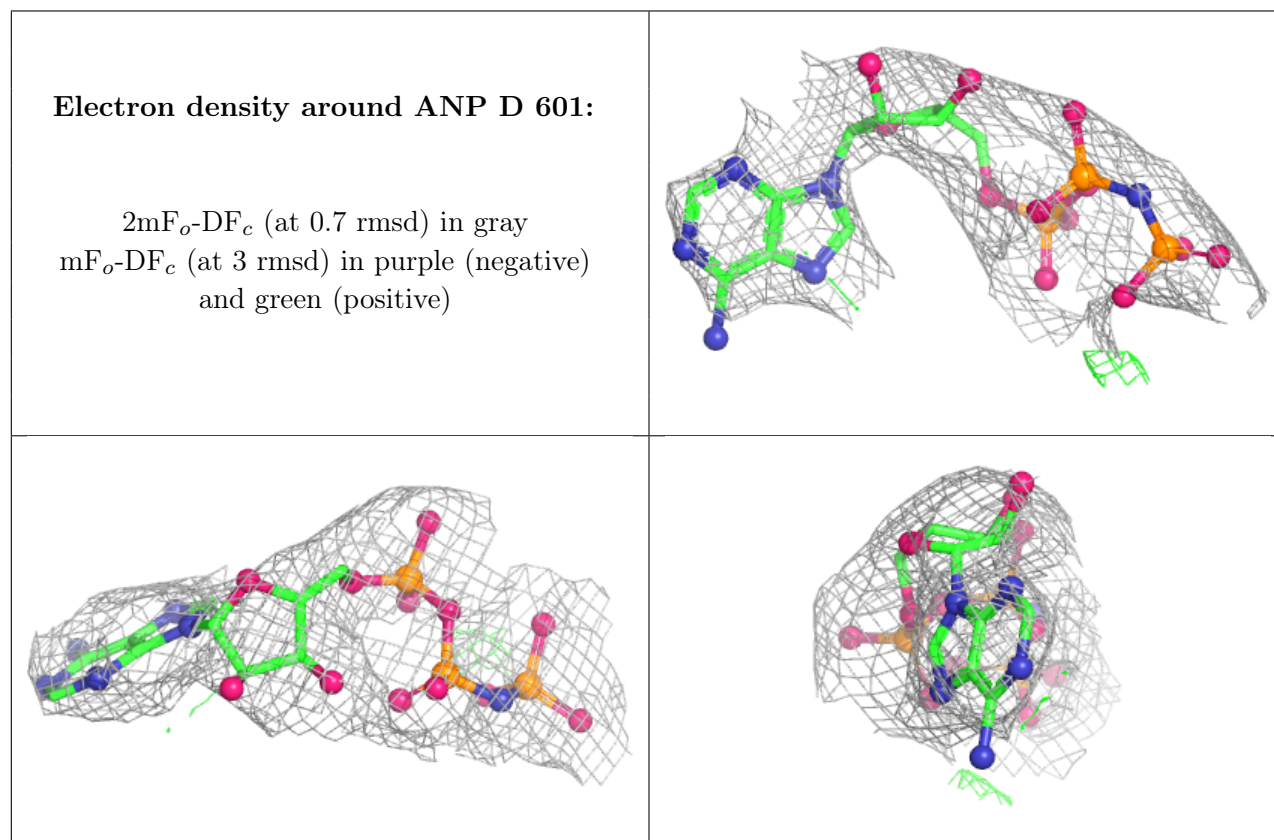
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

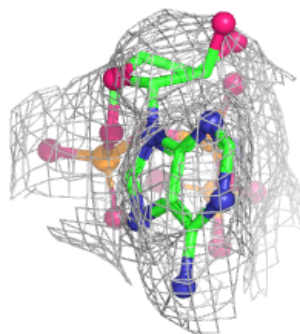
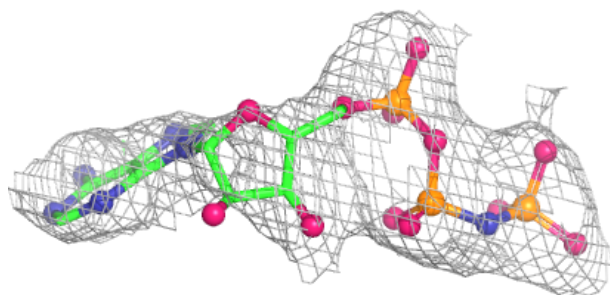
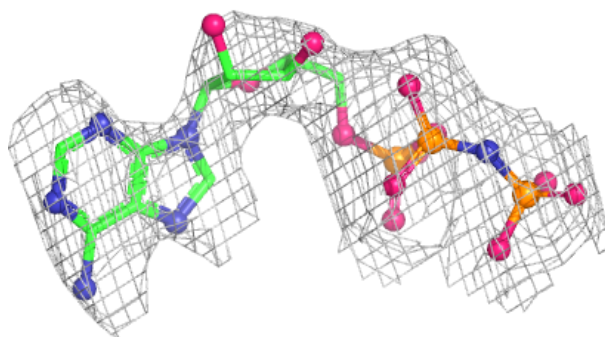
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	D	602	1/1	0.99	0.05	60,60,60,60	0
3	MG	F	602	1/1	0.99	0.05	48,48,48,48	0
3	MG	H	602	1/1	0.99	0.03	37,37,37,37	0
2	ANP	D	601	31/31	1.00	0.02	49,76,86,87	0
2	ANP	E	601	31/31	1.00	0.03	42,51,57,58	0
2	ANP	F	601	31/31	1.00	0.03	38,54,60,61	0
2	ANP	G	601	31/31	1.00	0.02	44,49,55,58	0
2	ANP	H	601	31/31	1.00	0.03	51,80,88,92	0
3	MG	A	602	1/1	1.00	0.03	38,38,38,38	0
3	MG	B	602	1/1	1.00	0.02	37,37,37,37	0
3	MG	C	602	1/1	1.00	0.01	35,35,35,35	0
2	ANP	A	601	31/31	1.00	0.03	49,58,62,63	0
3	MG	E	602	1/1	1.00	0.04	51,51,51,51	0
2	ANP	B	601	31/31	1.00	0.02	52,64,69,71	0
3	MG	G	602	1/1	1.00	0.02	35,35,35,35	0
2	ANP	C	601	31/31	1.00	0.02	48,59,66,69	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.

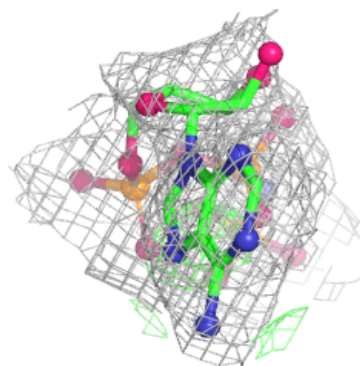
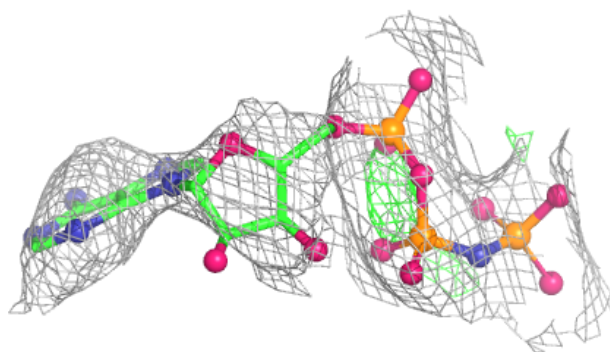
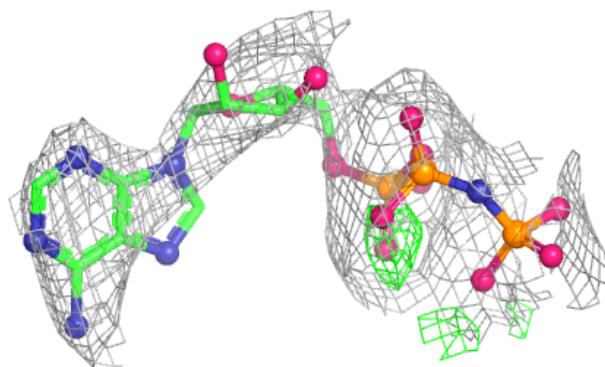


Electron density around ANP E 601:

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

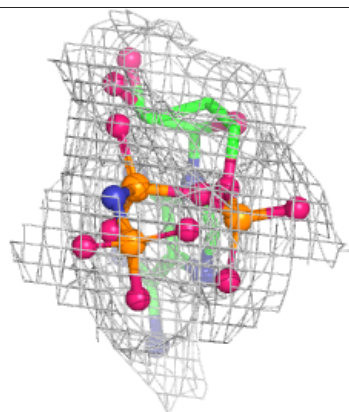
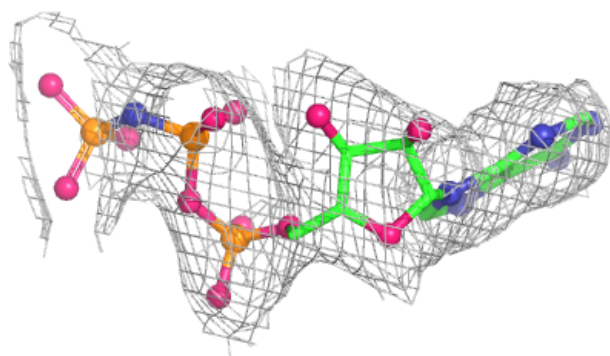
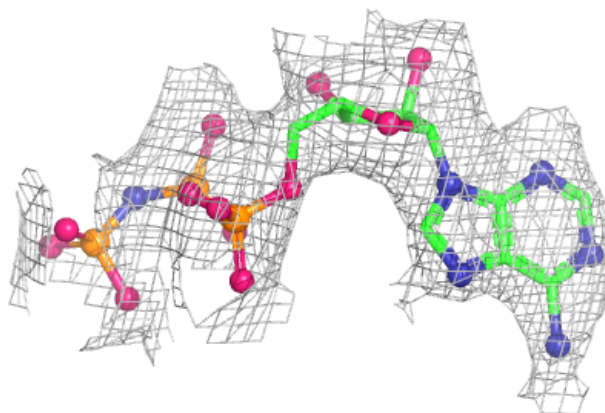
**Electron density around ANP F 601:**

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

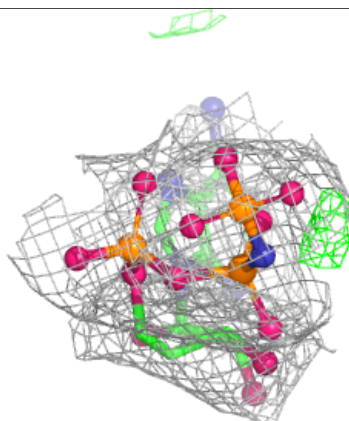
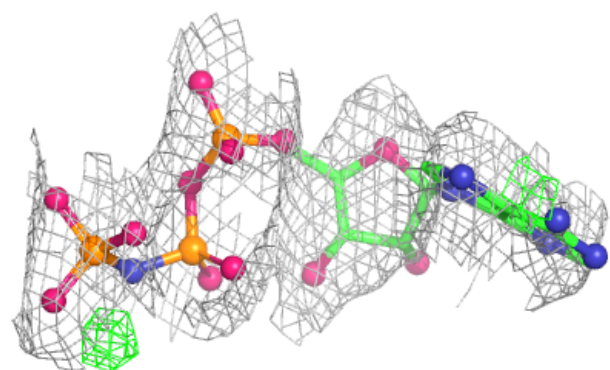
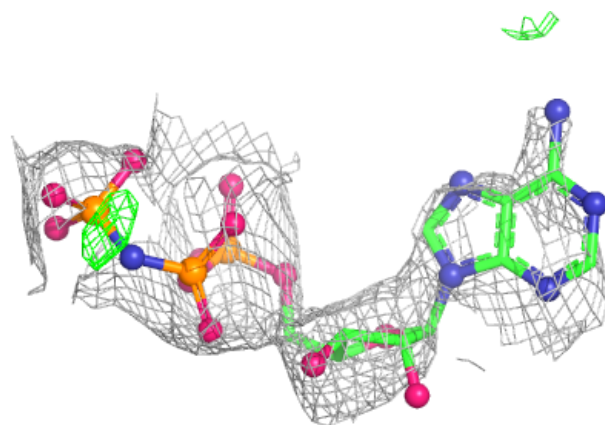


Electron density around ANP G 601:

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

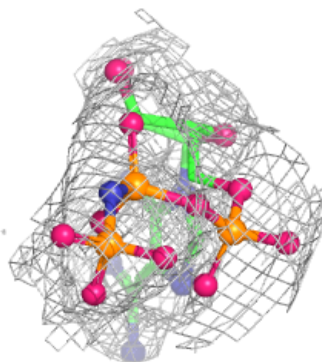
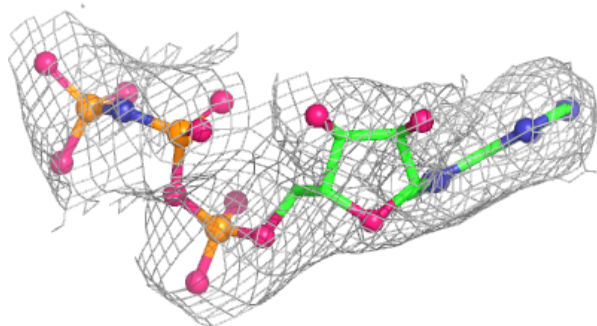
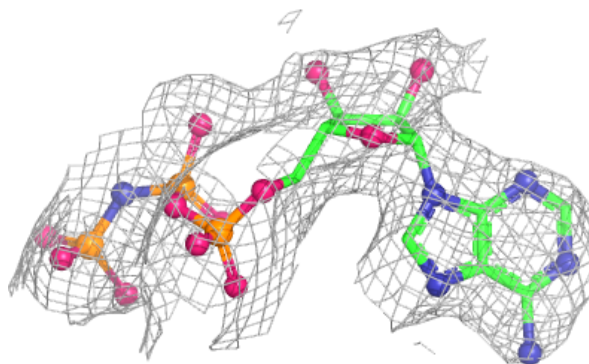
**Electron density around ANP H 601:**

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

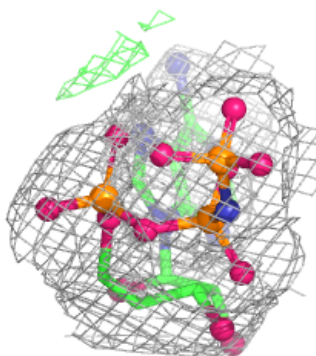
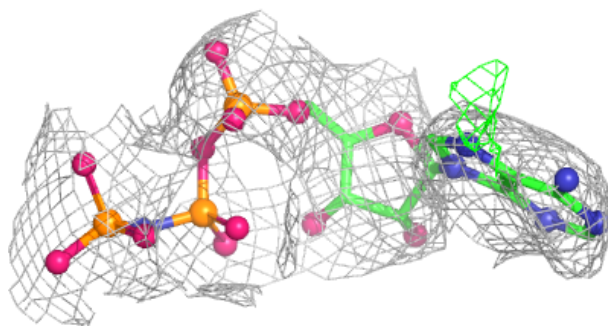
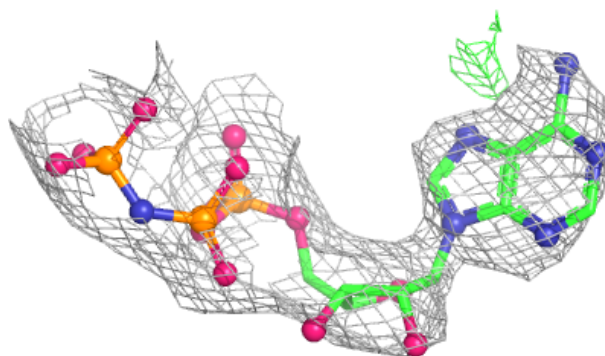


Electron density around ANP A 601:

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

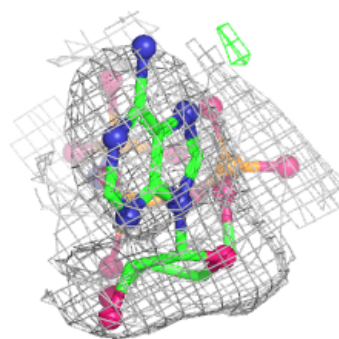
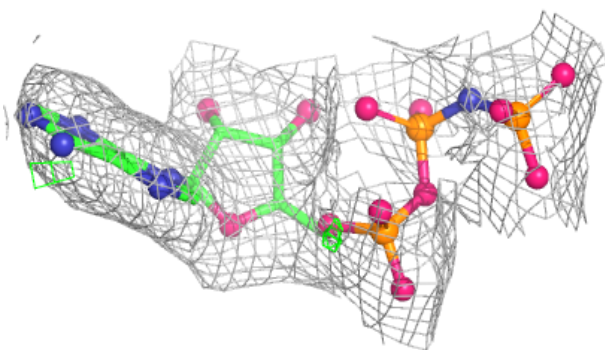
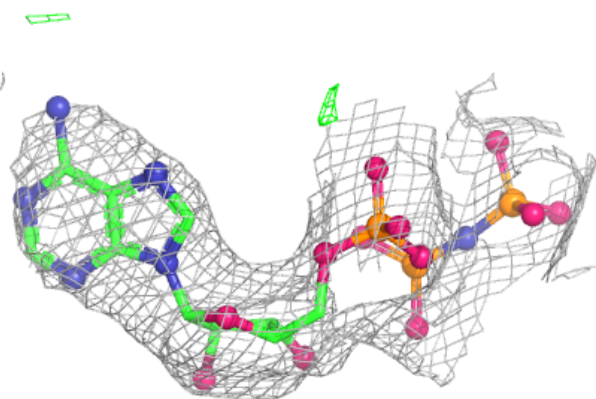
**Electron density around ANP B 601:**

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



Electron density around ANP C 601:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.