



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 2, 2024 – 06:48 PM EST

PDB ID : 4GFH
Title : Topoisomerase II-DNA-AMPPNP complex
Authors : Schmidt, B.H.; Osheroff, N.; Berger, J.M.
Deposited on : 2012-08-03
Resolution : 4.41 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

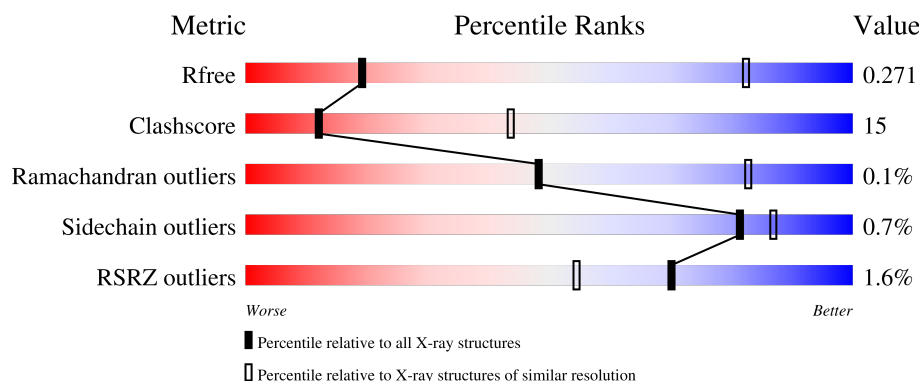
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.41 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}	164625	1013 (4.90-3.90)
Clashscore	180529	1066 (4.90-3.90)
Ramachandran outliers	177936	1019 (4.92-3.86)
Sidechain outliers	177891	1003 (4.92-3.86)
RSRZ outliers	164620	1010 (4.90-3.90)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1178	 2% 65% 27% • 6%
1	F	1178	 % 65% 27% • 7%
2	B	11	 45% 45% 9%
2	G	11	 55% 36% 9%
3	C	15	 53% 47%
3	H	15	 7% 53% 47%

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Mol	Chain	Length	Quality of chain
4	D	11	 82% 9% 9%
4	I	11	 64% 27% 9%
5	E	15	 73% 27%
5	J	15	 60% 40%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PTR	F	782[A]	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20236 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 topoisomerase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1102	Total	C	N	O	P	S	0	1	0
			9042	5804	1515	1687	1	35			
1	F	1098	Total	C	N	O	P	S	0	1	0
			9012	5788	1510	1678	1	35			

- Molecule 2 is a DNA chain called DNA (5'-D(P*CP*CP*TP*AP*CP*TP*GP*CP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	P	0	11	0
			219	105	36	67	11			
2	G	11	Total	C	N	O	P	0	11	0
			219	105	36	67	11			

- Molecule 3 is a DNA chain called DNA (5'-D(*CP*GP*CP*GP*GP*TP*AP*GP*CP*AP*GP*TP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	15	Total	C	N	O	P	0	15	0
			310	147	63	86	14			
3	H	15	Total	C	N	O	P	0	15	0
			310	147	63	86	14			

- Molecule 4 is a DNA chain called DNA (5'-D(P*GP*GP*AP*TP*GP*AP*CP*GP*AP*TP*(TSP))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	11	Total	C	N	O	P	S	0	11	0
			230	109	44	65	11	1			
4	I	11	Total	C	N	O	P	S	0	11	0
			230	109	44	65	11	1			

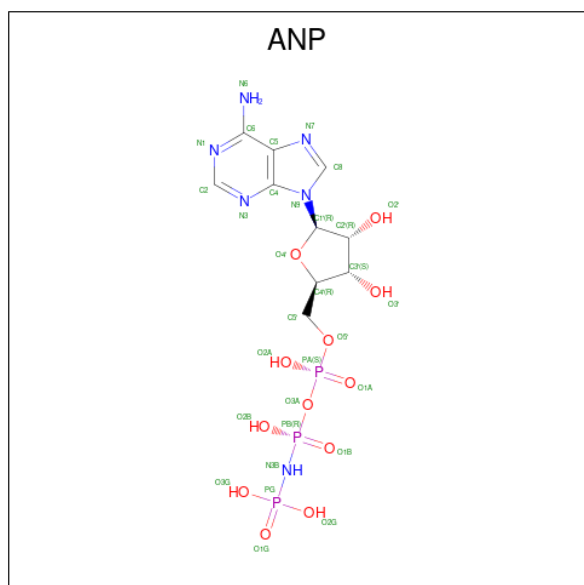
- Molecule 5 is a DNA chain called DNA (5'-D(*CP*GP*CP*GP*AP*AP*TP*CP*GP*TP*CP*AP*TP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	15	Total	C	N	O	P	0	15	0
			300	144	54	88	14			
5	J	15	Total	C	N	O	P	0	15	0
			300	144	54	88	14			

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

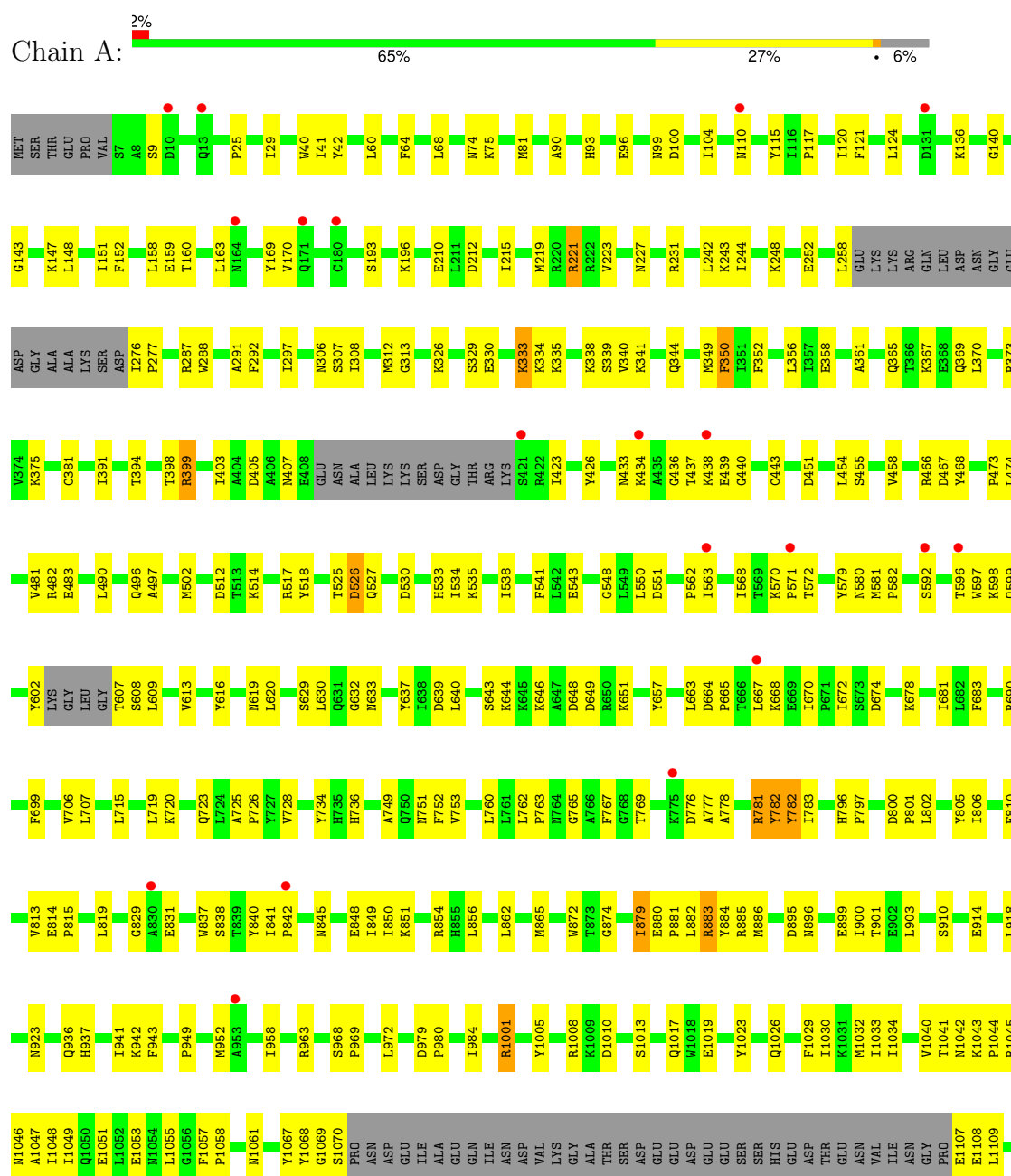


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
7	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

3 Residue-property plots

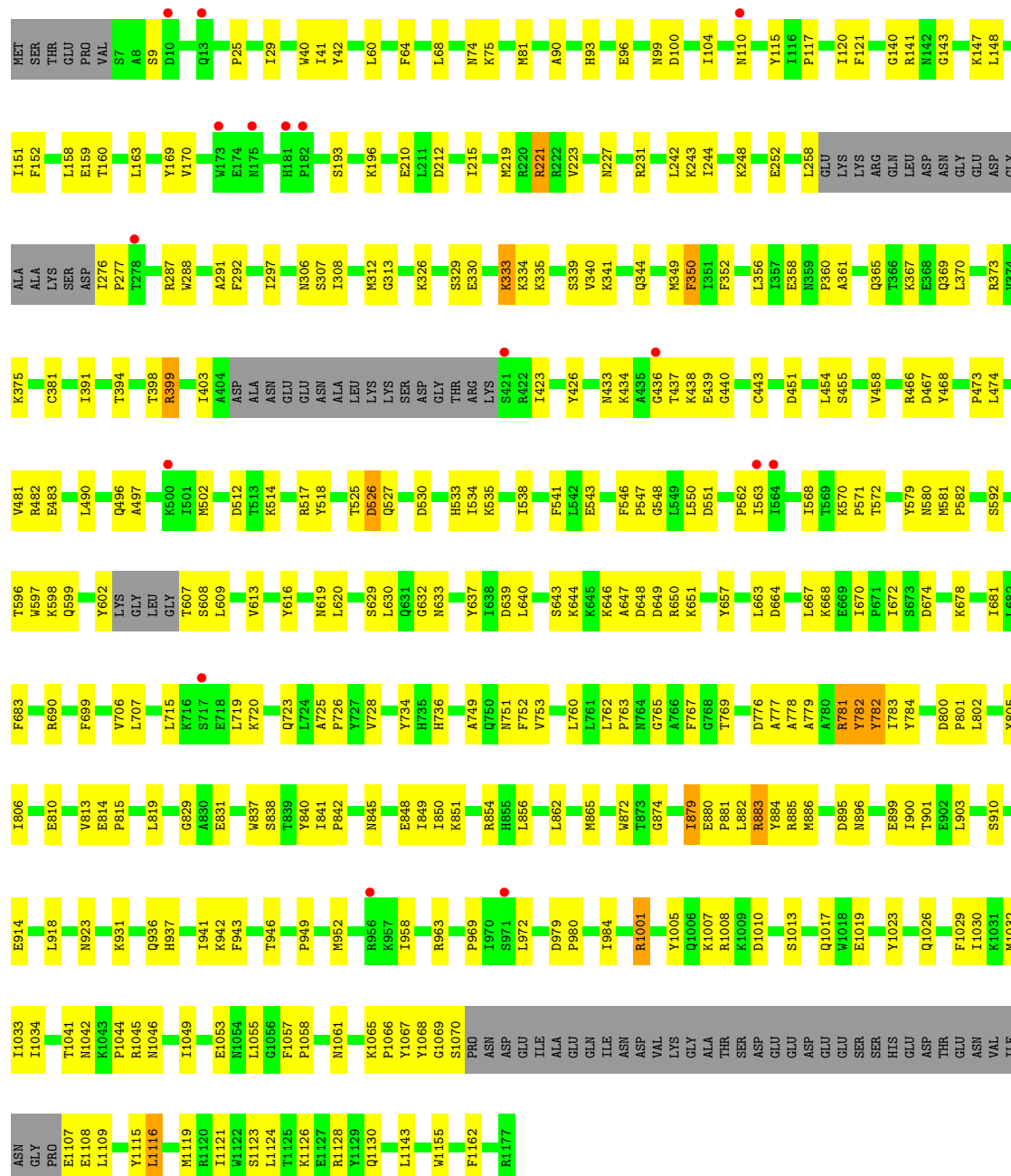
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: DNA topoisomerase 2



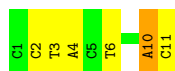


• Molecule 1: DNA topoisomerase 2

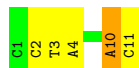


• Molecule 2: DNA (5'-D(P*CP*CP*TP*AP*CP*TP*GP*CP*TP*AP*C)-3')





- Molecule 2: DNA (5'-D(P*CP*CP*TP*AP*CP*TP*GP*CP*TP*AP*C)-3')



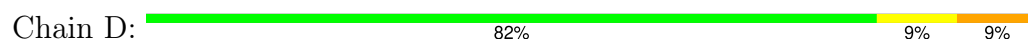
- Molecule 3: DNA (5'-D(*CP*GP*CP*GP*GP*TP*AP*GP*CP*AP*GP*TP*AP*GP*G)-3')



- Molecule 3: DNA (5'-D(*CP*GP*CP*GP*GP*TP*AP*GP*CP*AP*GP*TP*AP*GP*G)-3')



- Molecule 4: DNA (5'-D(P*GP*GP*AP*TP*GP*AP*CP*GP*AP*TP*(TSP))-3')



- Molecule 4: DNA (5'-D(P*GP*GP*AP*TP*GP*AP*CP*GP*AP*TP*(TSP))-3')



- Molecule 5: DNA (5'-D(*CP*GP*CP*GP*AP*AP*TP*CP*GP*TP*CP*AP*TP*CP*C)-3')



- Molecule 5: DNA (5'-D(*CP*GP*CP*GP*AP*AP*TP*CP*GP*TP*CP*AP*TP*CP*C)-3')

Chain J:  60% 40%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	169.13Å 169.88Å 169.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.99 – 4.41 46.99 – 4.41	Depositor EDS
% Data completeness (in resolution range)	91.2 (46.99-4.41) 90.9 (46.99-4.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 4.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.239 , 0.275 0.236 , 0.271	Depositor DCC
R_{free} test set	1448 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	185.0	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 875.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -k,-h,l 0.389 for l,-k,h 0.000 for l,h,k 0.000 for k,l,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	20236	wwPDB-VP
Average B, all atoms (Å ²)	248.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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: TSP, ANP, MG, PTR

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	0.23	0/9218	0.45	2/12428 (0.0%)
1	F	0.23	0/9188	0.45	2/12387 (0.0%)
2	B	0.39	0/243	1.00	1/371 (0.3%)
2	G	0.39	0/243	0.99	1/371 (0.3%)
3	C	0.58	2/349 (0.6%)	0.96	0/539
3	H	0.46	0/349	0.98	0/539
4	D	0.47	0/236	0.94	1/363 (0.3%)
4	I	0.41	0/236	0.97	2/363 (0.6%)
5	E	0.43	0/335	0.98	0/514
5	J	0.43	0/335	0.95	0/514
All	All	0.26	2/20732 (0.0%)	0.54	9/28389 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1[A]	DC	C4'-O4'	5.23	1.50	1.45
3	C	1[A]	DC	O3'-P	-5.03	1.55	1.61

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	10[B]	DT	C4'-C3'-O3'	6.17	125.13	109.70
2	G	10[A]	DA	O4'-C4'-C3'	-5.83	102.17	104.50
2	B	10[A]	DA	O4'-C4'-C3'	-5.75	102.20	104.50
1	A	879	ILE	CB-CA-C	-5.57	100.45	111.60
1	F	879	ILE	CB-CA-C	-5.56	100.48	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9042	0	9077	308	0
1	F	9012	0	9056	306	0
2	B	219	0	114	6	0
2	G	219	0	118	6	0
3	C	310	0	146	5	0
3	H	310	0	147	7	0
4	D	230	0	108	1	0
4	I	230	0	108	6	0
5	E	300	0	154	3	0
5	J	300	0	153	7	0
6	A	1	0	0	0	0
6	F	1	0	0	0	0
7	A	31	0	13	2	0
7	F	31	0	13	3	0
All	All	20236	0	19207	606	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 15.

The worst 5 of 606 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:F:29:ILE:HD13	1:F:152:PHE:CE2	1.73	1.24
1:A:29:ILE:HD13	1:A:152:PHE:CE2	1.73	1.23
1:F:29:ILE:CD1	1:F:152:PHE:CZ	2.38	1.06
1:A:29:ILE:CD1	1:A:152:PHE:CZ	2.38	1.05
1:A:29:ILE:HD13	1:A:152:PHE:CZ	1.93	1.02

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	1091/1178 (93%)	1038 (95%)	52 (5%)	1 (0%)	48	83
1	F	1087/1178 (92%)	1034 (95%)	52 (5%)	1 (0%)	48	83
All	All	2178/2356 (92%)	2072 (95%)	104 (5%)	2 (0%)	48	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	526	ASP
1	F	526	ASP

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	992/1055 (94%)	985 (99%)	7 (1%)	81	87
1	F	989/1055 (94%)	982 (99%)	7 (1%)	81	87
All	All	1981/2110 (94%)	1967 (99%)	14 (1%)	81	87

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	221	ARG
1	F	333	LYS
1	F	1001	ARG
1	F	781	ARG

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Mol	Chain	Res	Type
1	F	883	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	619	ASN
1	F	1167	GLN
1	A	619	ASN
1	A	1167	GLN
1	F	99	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	TSP	I	11[B]	4	17,21,22	3.30	6 (35%)	21,30,33	2.57	7 (33%)
4	TSP	D	11[B]	4	17,21,22	3.30	6 (35%)	21,30,33	2.50	7 (33%)
1	PTR	A	782[A]	1	15,16,17	2.03	1 (6%)	17,22,24	0.60	0
1	PTR	F	782[A]	1	15,16,17	2.03	1 (6%)	17,22,24	0.61	0

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
4	TSP	I	11[B]	4	-	2/7/21/22	0/2/2/2
4	TSP	D	11[B]	4	-	2/7/21/22	0/2/2/2
1	PTR	A	782[A]	1	-	2/10/11/13	0/1/1/1
1	PTR	F	782[A]	1	-	2/10/11/13	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	782[A]	PTR	OH-CZ	-7.69	1.23	1.40
1	A	782[A]	PTR	OH-CZ	-7.65	1.23	1.40
4	I	11[B]	TSP	O4-C4	7.10	1.37	1.23
4	D	11[B]	TSP	O4-C4	7.06	1.37	1.23
4	I	11[B]	TSP	C2'-C3'	-6.15	1.36	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	11[B]	TSP	C5-C4-N3	5.68	120.26	115.32
4	D	11[B]	TSP	C5-C4-N3	5.52	120.12	115.32
4	I	11[B]	TSP	C4-N3-C2	-5.41	120.25	127.34
4	D	11[B]	TSP	C4-N3-C2	-5.33	120.36	127.34
4	I	11[B]	TSP	O4-C4-C5	-4.85	119.37	124.92

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	11[B]	TSP	O4'-C4'-C5'-O5'
4	I	11[B]	TSP	O4'-C4'-C5'-O5'
4	I	11[B]	TSP	C3'-C4'-C5'-O5'
4	D	11[B]	TSP	C3'-C4'-C5'-O5'
1	F	782[A]	PTR	CA-CB-CG-CD2

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	782[A]	PTR	1	0
1	F	782[A]	PTR	6	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
7	ANP	F	1202	6	29,33,33	1.61	8 (27%)	31,52,52	1.44	3 (9%)
7	ANP	A	1202	6	29,33,33	1.60	8 (27%)	31,52,52	1.44	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
7	ANP	F	1202	6	-	4/14/38/38	0/3/3/3
7	ANP	A	1202	6	-	4/14/38/38	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1202	ANP	C6-N6	2.70	1.43	1.34
7	F	1202	ANP	C6-N6	2.68	1.43	1.34
7	F	1202	ANP	PG-O3G	-2.55	1.50	1.56
7	A	1202	ANP	PG-O3G	-2.54	1.50	1.56
7	F	1202	ANP	PB-O1B	2.52	1.50	1.46

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	1202	ANP	C4'-O4'-C1'	4.15	113.72	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1202	ANP	C4'-O4'-C1'	4.14	113.72	109.92
7	A	1202	ANP	N3-C2-N1	-4.06	123.16	128.67
7	F	1202	ANP	N3-C2-N1	-4.02	123.21	128.67
7	F	1202	ANP	O4'-C1'-N9	2.25	111.72	108.75

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

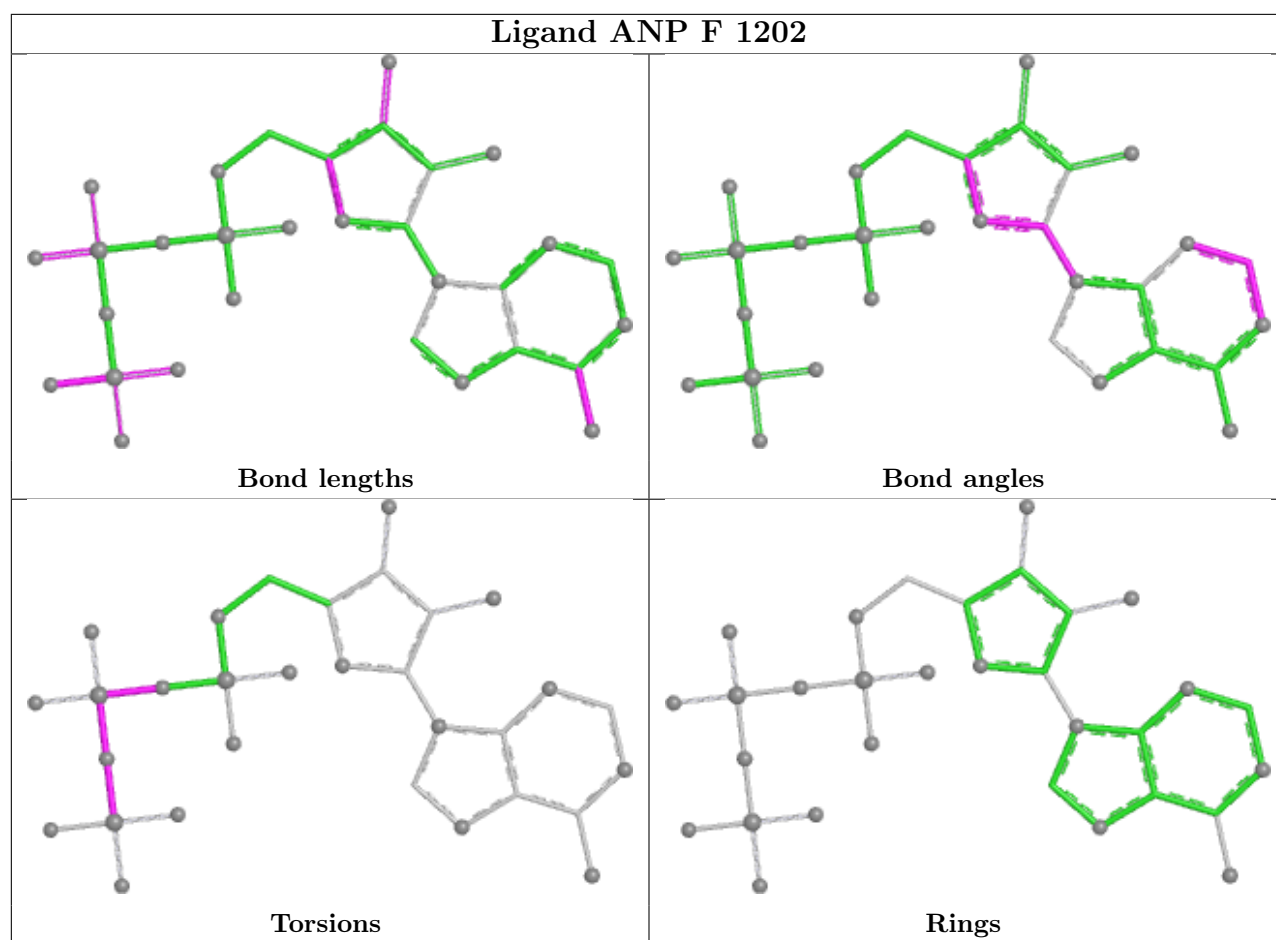
Mol	Chain	Res	Type	Atoms
7	A	1202	ANP	PB-N3B-PG-O1G
7	A	1202	ANP	PA-O3A-PB-O2B
7	F	1202	ANP	PB-N3B-PG-O1G
7	F	1202	ANP	PA-O3A-PB-O2B
7	A	1202	ANP	PA-O3A-PB-O1B

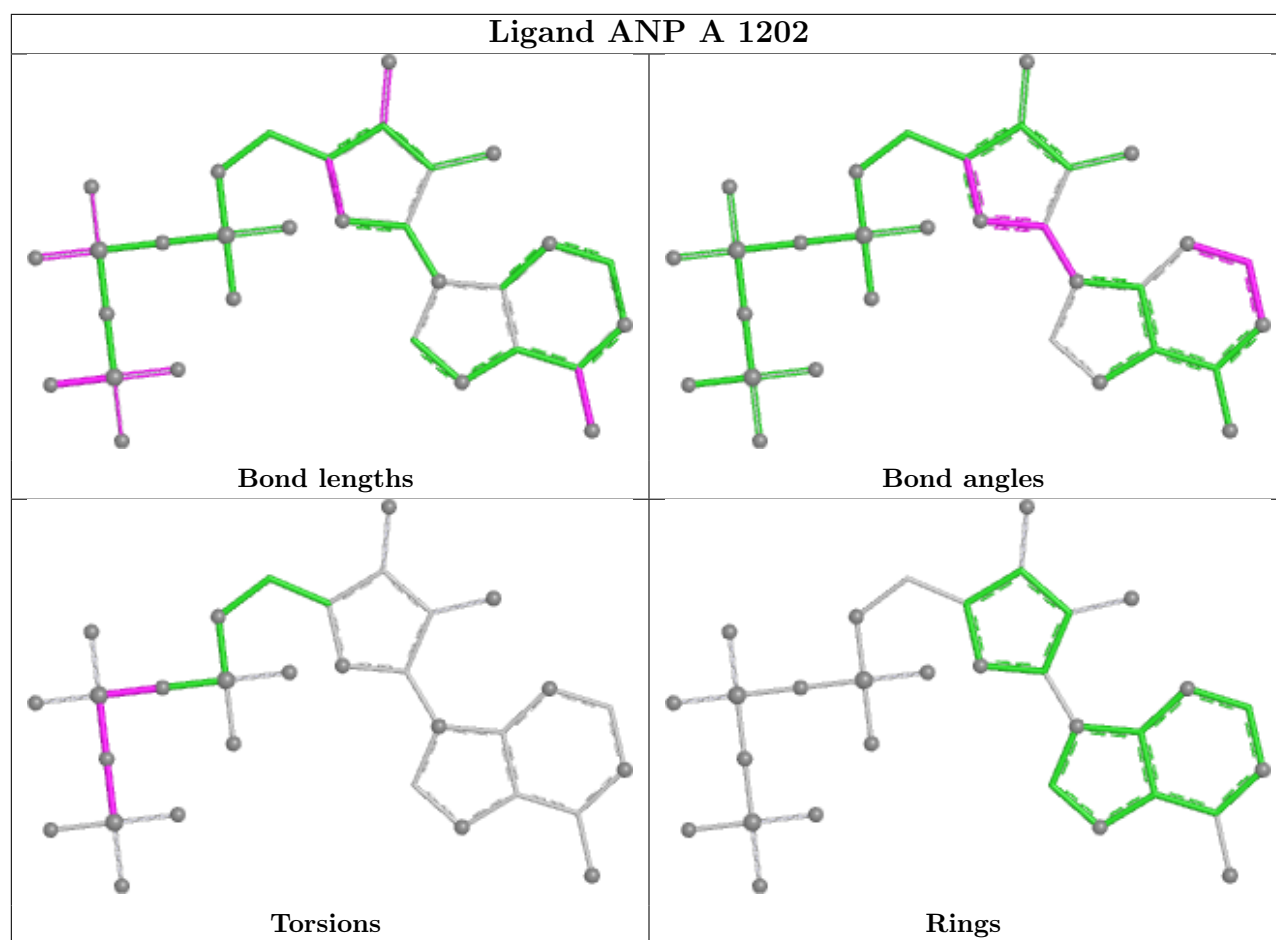
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	1202	ANP	3	0
7	A	1202	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](#)

Warning: The R factor obtained from EDS is 0.3011, which does not match the depositor's R factor of 0.2391. Please interpret the results in this section carefully.

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	1101/1178 (93%)	-0.19	19 (1%) 69 53	150, 238, 317, 403	0
1	F	1097/1178 (93%)	-0.20	16 (1%) 71 56	146, 240, 314, 414	0
2	B	11/11 (100%)	0.48	0 100 100	87, 134, 174, 182	11 (100%)
2	G	11/11 (100%)	0.58	0 100 100	79, 113, 165, 166	11 (100%)
3	C	15/15 (100%)	0.69	0 100 100	108, 136, 213, 215	15 (100%)
3	H	15/15 (100%)	0.45	1 (6%) 25 22	101, 132, 188, 216	15 (100%)
4	D	10/11 (90%)	0.50	0 100 100	82, 122, 182, 214	10 (100%)
4	I	10/11 (90%)	0.68	0 100 100	84, 137, 201, 209	10 (100%)
5	E	15/15 (100%)	0.63	0 100 100	81, 127, 180, 191	15 (100%)
5	J	15/15 (100%)	0.42	0 100 100	90, 146, 166, 188	15 (100%)
All	All	2300/2460 (93%)	-0.16	36 (1%) 70 54	79, 236, 315, 414	102 (4%)

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	ASN	5.5
1	A	13	GLN	5.2
1	F	182	PRO	4.4
1	F	563	ILE	4.4
1	A	180	CYS	4.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	PTR	A	782[A]	16/17	0.92	0.14	281,285,288,289	16
1	PTR	F	782[A]	16/17	0.96	0.16	299,305,310,312	16
4	TSP	D	11[B]	20/21	0.97	0.13	501,508,514,517	20
4	TSP	I	11[B]	20/21	0.99	0.13	429,437,440,441	20

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

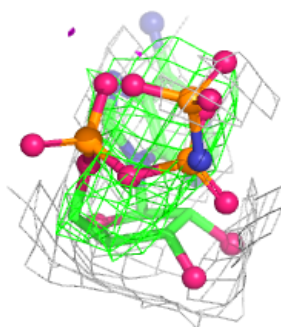
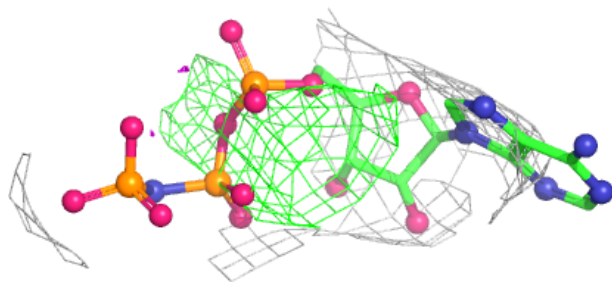
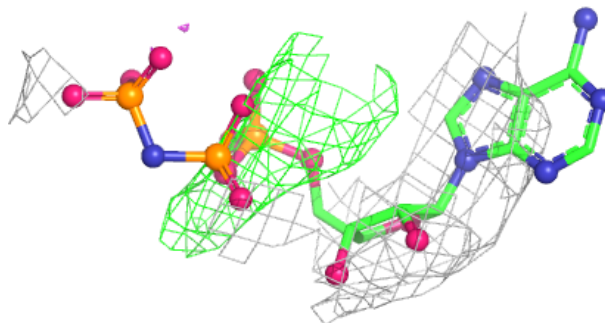
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	A	1201	1/1	0.98	0.05	115,115,115,115	0
6	MG	F	1201	1/1	0.98	0.05	114,114,114,114	0
7	ANP	A	1202	31/31	0.98	0.08	230,235,236,237	0
7	ANP	F	1202	31/31	0.99	0.07	229,235,247,251	0

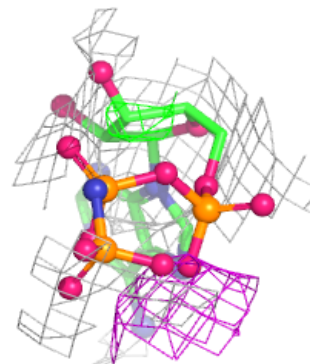
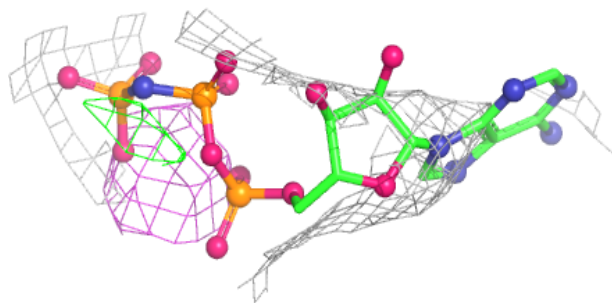
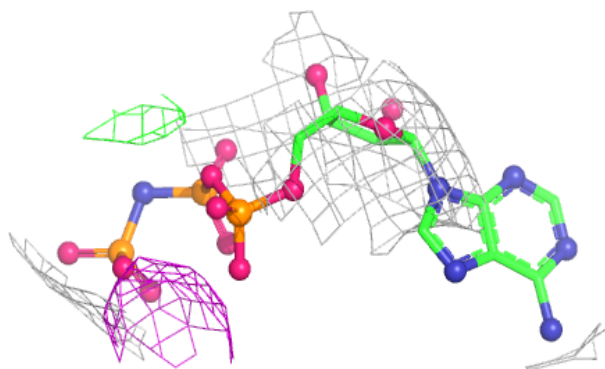
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ANP A 1202:

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

**Electron density around ANP F 1202:**

$2mF_o-DF_c$ (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.