wwPDB X-ray Structure Validation Summary Report (i)

Aug 19, 2023 – 06:26 PM EDT

PDB ID	:	2GL0
Title	:	Structure of PAE2307 in complex with adenosine
Authors	:	Lott, J.S.; Paget, B.; Johnston, J.M.; Baker, E.N.
Deposited on	:	2006-04-04
Resolution	:	2.25 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:

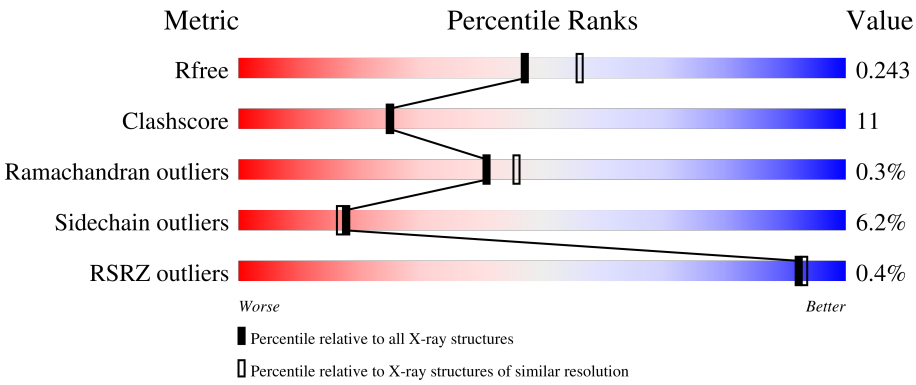
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	167	% 77% 19% • • •
1	B	167	72% 22% • • •
1	C	167	71% 22% • • •
1	D	167	77% 17% • • •
1	E	167	75% 19% • • •

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Mol	Chain	Length	Quality of chain
1	F	167	% 71% 21% 5%

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
3	PO4	C	502	-	-	X	-
3	PO4	D	501	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8217 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 conserved hypothetical protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	163	1283	826	225	230	2	0	0	0
1	B	163	1283	826	225	230	2	0	0	0
1	C	162	1277	823	224	228	2	0	0	0
1	D	163	1283	826	225	230	2	0	0	0
1	E	163	1283	826	225	230	2	0	0	0
1	F	162	1277	823	224	228	2	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP Q8ZVF7
A	2	THR	-	cloning artifact	UNP Q8ZVF7
A	3	ASP	-	cloning artifact	UNP Q8ZVF7
B	1	MET	-	cloning artifact	UNP Q8ZVF7
B	2	THR	-	cloning artifact	UNP Q8ZVF7
B	3	ASP	-	cloning artifact	UNP Q8ZVF7
C	1	MET	-	cloning artifact	UNP Q8ZVF7
C	2	THR	-	cloning artifact	UNP Q8ZVF7
C	3	ASP	-	cloning artifact	UNP Q8ZVF7
D	1	MET	-	cloning artifact	UNP Q8ZVF7
D	2	THR	-	cloning artifact	UNP Q8ZVF7
D	3	ASP	-	cloning artifact	UNP Q8ZVF7
E	1	MET	-	cloning artifact	UNP Q8ZVF7
E	2	THR	-	cloning artifact	UNP Q8ZVF7
E	3	ASP	-	cloning artifact	UNP Q8ZVF7
F	1	MET	-	cloning artifact	UNP Q8ZVF7
F	2	THR	-	cloning artifact	UNP Q8ZVF7

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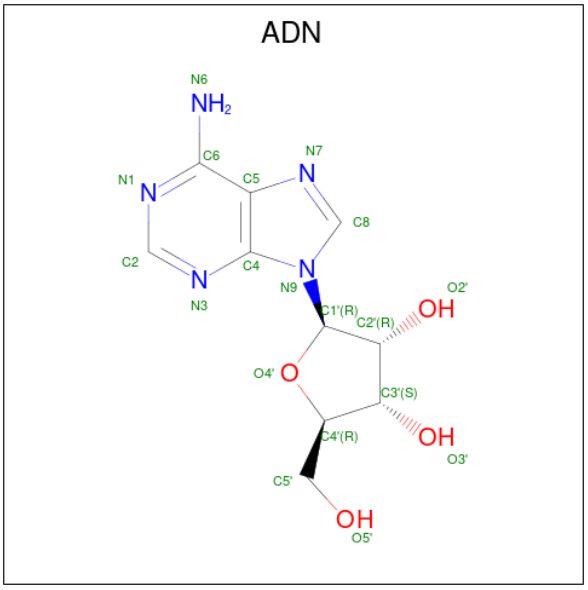
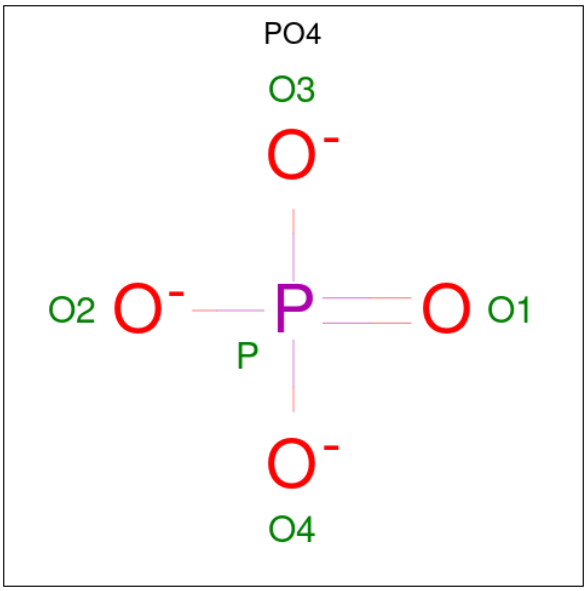
Chain	Residue	Modelled	Actual	Comment	Reference
F	3	ASP	-	cloning artifact	UNP Q8ZVF7

- Molecule 2 is ADENOSINE (three-letter code: ADN) (formula: $C_{10}H_{13}N_5O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	19	10	5	4	0	0
2	B	1	19	10	5	4	0	0
2	C	1	19	10	5	4	0	0
2	D	1	19	10	5	4	0	0
2	E	1	19	10	5	4	0	0
2	F	1	19	10	5	4	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

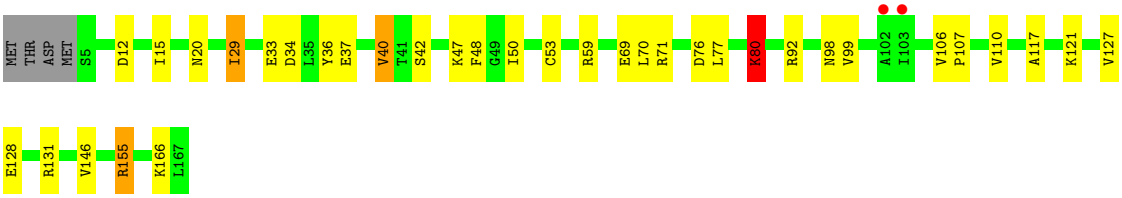
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	70	Total O 70 70	0	0
4	B	72	Total O 72 72	0	0
4	C	81	Total O 81 81	0	0
4	D	60	Total O 60 60	0	0
4	E	53	Total O 53 53	0	0
4	F	71	Total O 71 71	0	0

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.

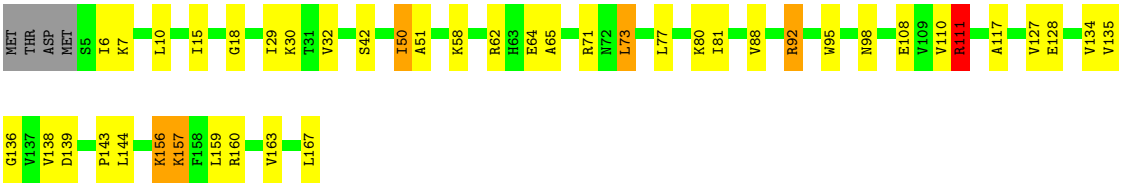
- Molecule 1: conserved hypothetical protein

Chain A:



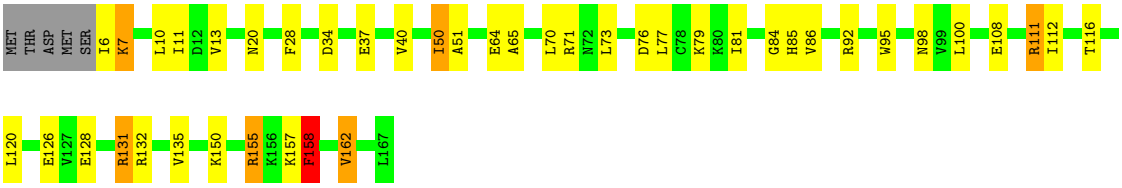
- Molecule 1: conserved hypothetical protein

Chain B:



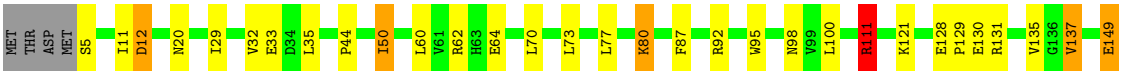
- Molecule 1: conserved hypothetical protein

Chain C:



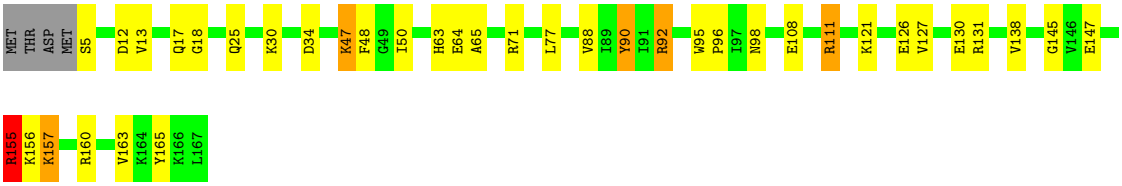
- Molecule 1: conserved hypothetical protein

Chain D:



• Molecule 1: conserved hypothetical protein

Chain E:



• Molecule 1: conserved hypothetical protein

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.86Å 109.83Å 112.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.33 – 2.25 45.39 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.33-2.25) 98.1 (45.39-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.19 (at 2.24Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.170 , 0.245 0.170 , 0.243	Depositor DCC
R_{free} test set	2271 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.026 for -h,l,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8217	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.51 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0942e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ADN

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	1.32	3/1306 (0.2%)	1.09	4/1768 (0.2%)
1	B	1.18	1/1306 (0.1%)	1.11	4/1768 (0.2%)
1	C	1.35	6/1300 (0.5%)	1.15	7/1760 (0.4%)
1	D	1.25	3/1306 (0.2%)	1.16	6/1768 (0.3%)
1	E	1.15	1/1306 (0.1%)	1.05	1/1768 (0.1%)
1	F	1.28	2/1300 (0.2%)	1.11	2/1760 (0.1%)
All	All	1.25	16/7824 (0.2%)	1.11	24/10592 (0.2%)

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	C	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	158	PHE	C-N	-17.48	0.93	1.34
1	C	157	LYS	C-N	-12.78	1.04	1.34
1	A	110	VAL	CB-CG2	-6.34	1.39	1.52
1	F	109	VAL	CB-CG2	6.32	1.66	1.52
1	E	90	TYR	CD1-CE1	6.10	1.48	1.39

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	111	ARG	NE-CZ-NH2	-13.18	113.71	120.30
1	F	111	ARG	NE-CZ-NH2	-12.64	113.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	158	PHE	O-C-N	-10.34	106.16	122.70
1	F	111	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	A	155	ARG	NE-CZ-NH1	7.57	124.08	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	158	PHE	Mainchain

5.2 Too-close contacts (i)

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	1283	0	1335	32	0
1	B	1283	0	1335	34	0
1	C	1277	0	1328	35	0
1	D	1283	0	1335	28	0
1	E	1283	0	1335	39	0
1	F	1277	0	1330	29	0
2	A	19	0	13	0	0
2	B	19	0	13	1	0
2	C	19	0	13	0	0
2	D	19	0	13	1	0
2	E	19	0	13	0	0
2	F	19	0	13	1	0
3	C	5	0	0	2	0
3	D	5	0	0	7	0
4	A	70	0	0	3	1
4	B	72	0	0	4	1
4	C	81	0	0	3	0
4	D	60	0	0	4	0
4	E	53	0	0	7	0
4	F	71	0	0	5	0
All	All	8217	0	8076	171	1

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 11.

The worst 5 of 171 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:E:157:LYS:HB2	1:E:157:LYS:NZ	1.46	1.17
1:A:121:LYS:HE3	4:C:967:HOH:O	1.47	1.15
4:A:971:HOH:O	1:B:163:VAL:HG12	1.59	1.01
1:C:131:ARG:HG2	1:C:131:ARG:HH11	1.22	1.00
1:E:126:GLU:CB	4:E:957:HOH:O	2.10	0.98

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:942:HOH:O	4:B:971:HOH:O[2_555]	1.94	0.26

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	161/167 (96%)	154 (96%)	7 (4%)	0	100	100
1	B	161/167 (96%)	151 (94%)	10 (6%)	0	100	100
1	C	160/167 (96%)	151 (94%)	8 (5%)	1 (1%)	25	25
1	D	161/167 (96%)	155 (96%)	6 (4%)	0	100	100
1	E	161/167 (96%)	150 (93%)	11 (7%)	0	100	100
1	F	160/167 (96%)	154 (96%)	4 (2%)	2 (1%)	12	8
All	All	964/1002 (96%)	915 (95%)	46 (5%)	3 (0%)	41	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	28	PHE
1	C	28	PHE
1	F	46	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	139/143 (97%)	134 (96%)	5 (4%)	35	42
1	B	139/143 (97%)	130 (94%)	9 (6%)	17	16
1	C	138/143 (96%)	130 (94%)	8 (6%)	20	20
1	D	139/143 (97%)	133 (96%)	6 (4%)	29	33
1	E	139/143 (97%)	131 (94%)	8 (6%)	20	20
1	F	138/143 (96%)	122 (88%)	16 (12%)	5	3
All	All	832/858 (97%)	780 (94%)	52 (6%)	18	17

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	5	SER
1	E	157	LYS
1	F	152	ARG
1	E	47	LYS
1	E	111	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	98	ASN
1	E	20	ASN
1	F	98	ASN
1	F	17	GLN
1	F	20	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADN	E	905	-	18,21,21	1.47	3 (16%)	18,31,31	1.80	4 (22%)
2	ADN	F	906	-	18,21,21	1.07	2 (11%)	18,31,31	1.48	4 (22%)
2	ADN	D	904	-	18,21,21	1.51	4 (22%)	18,31,31	1.68	4 (22%)
2	ADN	A	901	-	18,21,21	1.77	3 (16%)	18,31,31	2.19	7 (38%)
3	PO4	D	501	-	4,4,4	1.74	2 (50%)	6,6,6	1.00	0
3	PO4	C	502	-	4,4,4	1.24	0	6,6,6	0.70	0
2	ADN	B	902	-	18,21,21	1.28	3 (16%)	18,31,31	1.84	5 (27%)
2	ADN	C	903	-	18,21,21	1.57	3 (16%)	18,31,31	2.51	6 (33%)

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	ADN	E	905	-	-	0/2/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADN	F	906	-	-	0/2/22/22	0/3/3/3
2	ADN	D	904	-	-	0/2/22/22	0/3/3/3
2	ADN	A	901	-	-	2/2/22/22	0/3/3/3
2	ADN	B	902	-	-	0/2/22/22	0/3/3/3
2	ADN	C	903	-	-	0/2/22/22	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	ADN	C2'-C1'	-5.29	1.45	1.53
2	C	903	ADN	C5-C4	3.77	1.50	1.40
2	E	905	ADN	C2'-C1'	-3.74	1.48	1.53
2	D	904	ADN	C5-C4	3.34	1.49	1.40
2	B	902	ADN	C5-C4	3.22	1.49	1.40

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	903	ADN	C5'-C4'-C3'	-7.60	96.77	115.09
2	A	901	ADN	O2'-C2'-C1'	-4.99	92.41	110.85
2	E	905	ADN	C3'-C2'-C1'	4.00	107.00	100.98
2	C	903	ADN	C4-C5-N7	-3.95	105.28	109.40
2	B	902	ADN	C5'-C4'-C3'	-3.86	105.77	115.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	ADN	O4'-C4'-C5'-O5'
2	A	901	ADN	C3'-C4'-C5'-O5'

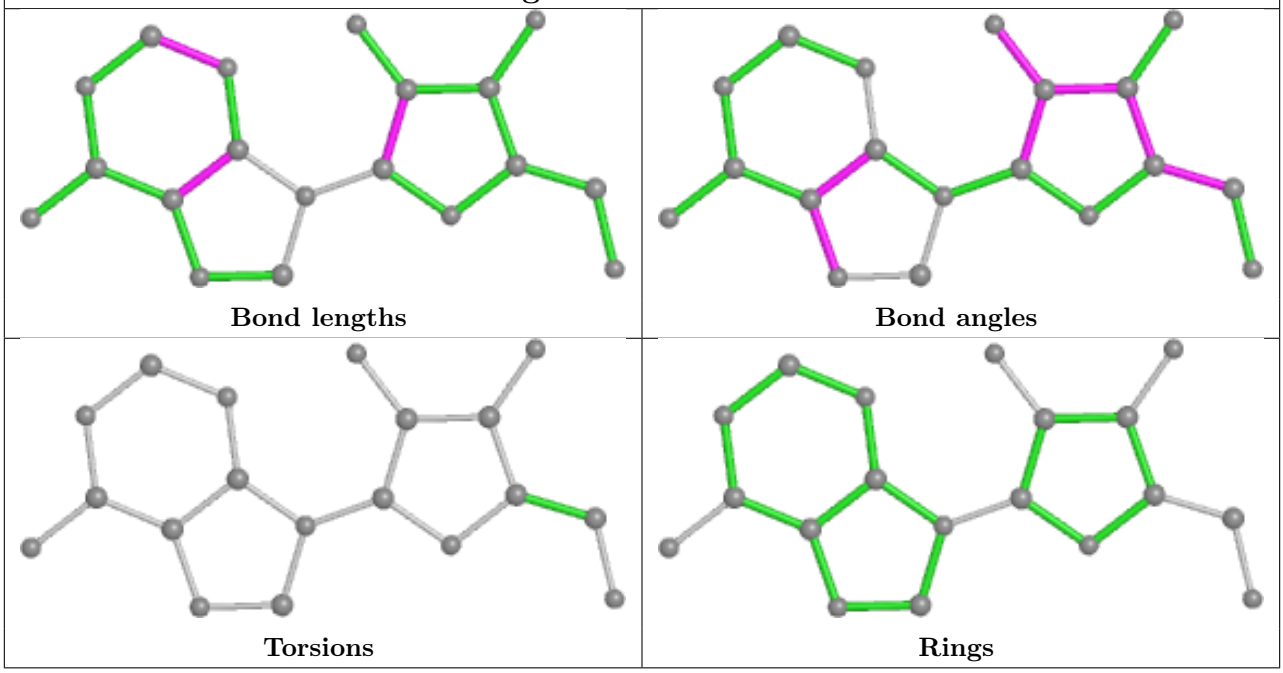
There are no ring outliers.

5 monomers are involved in 12 short contacts:

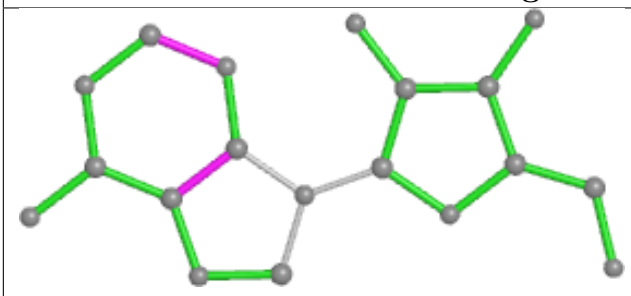
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	906	ADN	1	0
2	D	904	ADN	1	0
3	D	501	PO4	7	0
3	C	502	PO4	2	0
2	B	902	ADN	1	0

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.

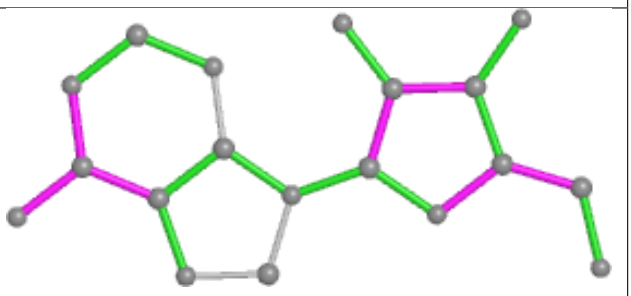
Ligand ADN E 905



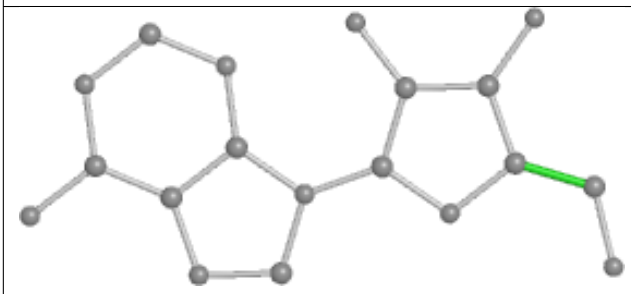
Ligand ADN F 906



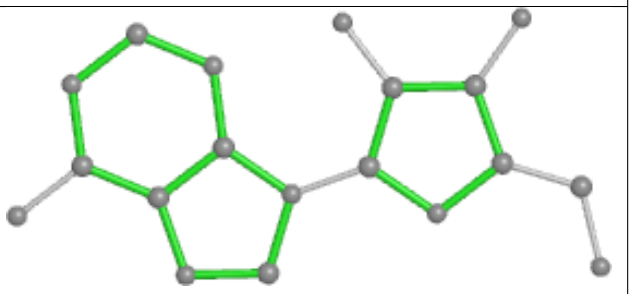
Bond lengths



Bond angles

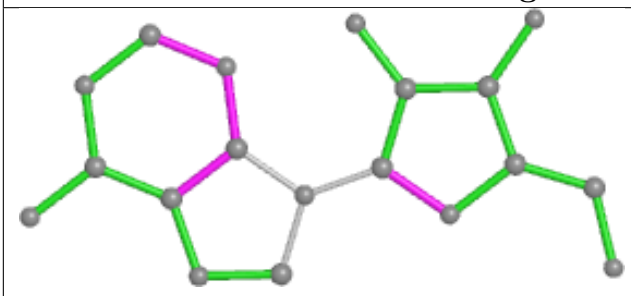


Torsions

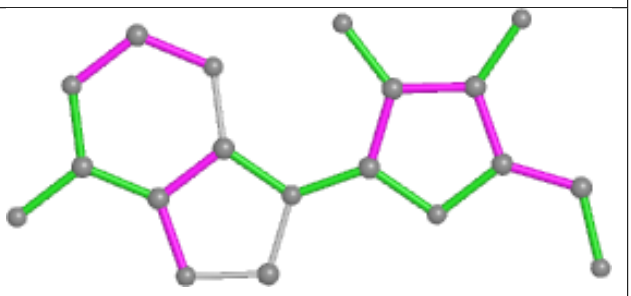


Rings

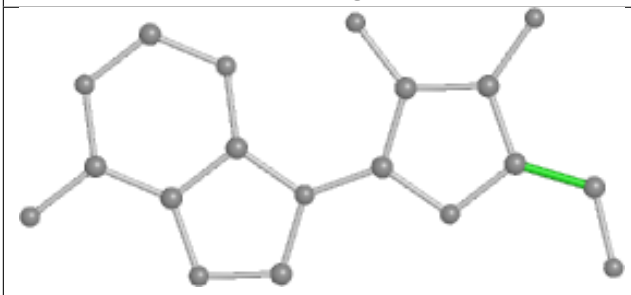
Ligand ADN D 904



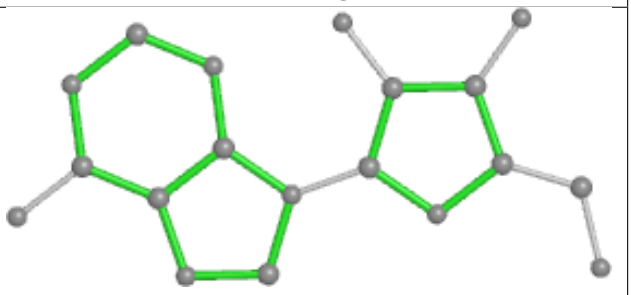
Bond lengths



Bond angles

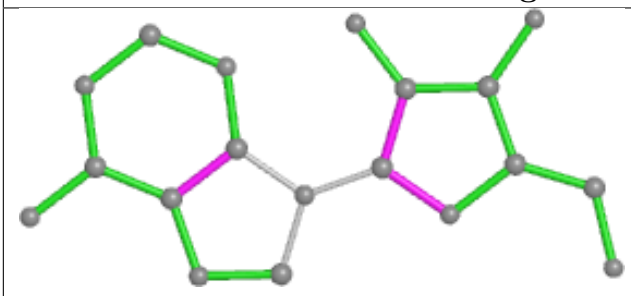


Torsions

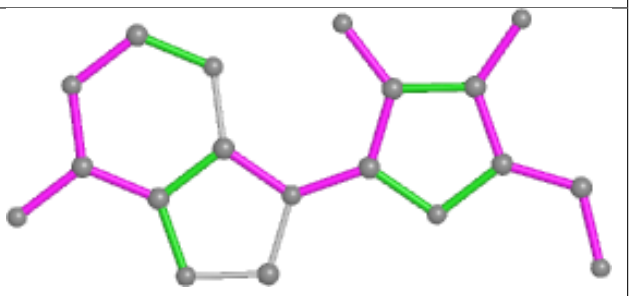


Rings

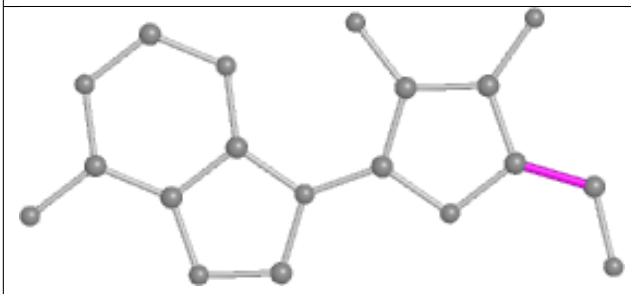
Ligand ADN A 901



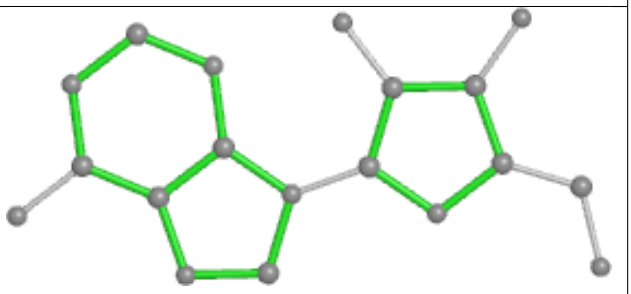
Bond lengths



Bond angles

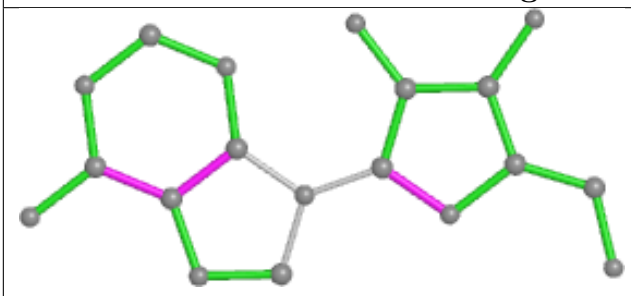


Torsions

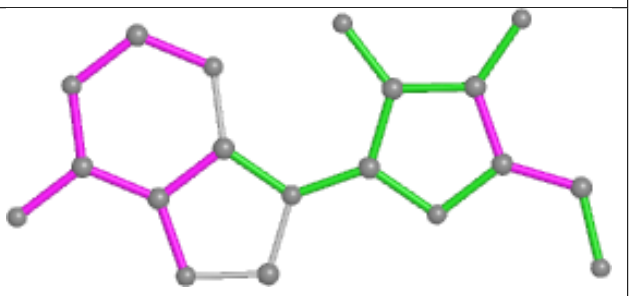


Rings

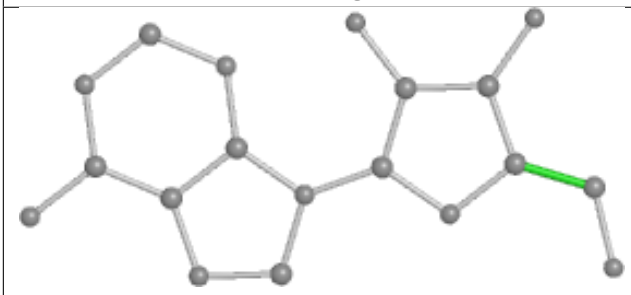
Ligand ADN B 902



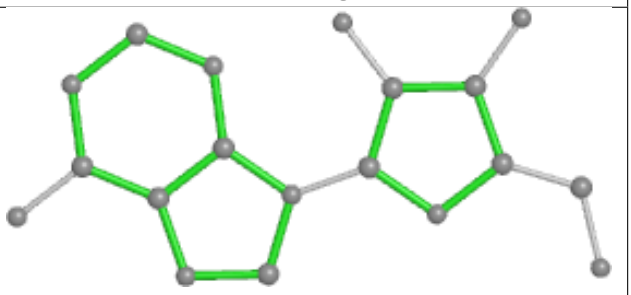
Bond lengths



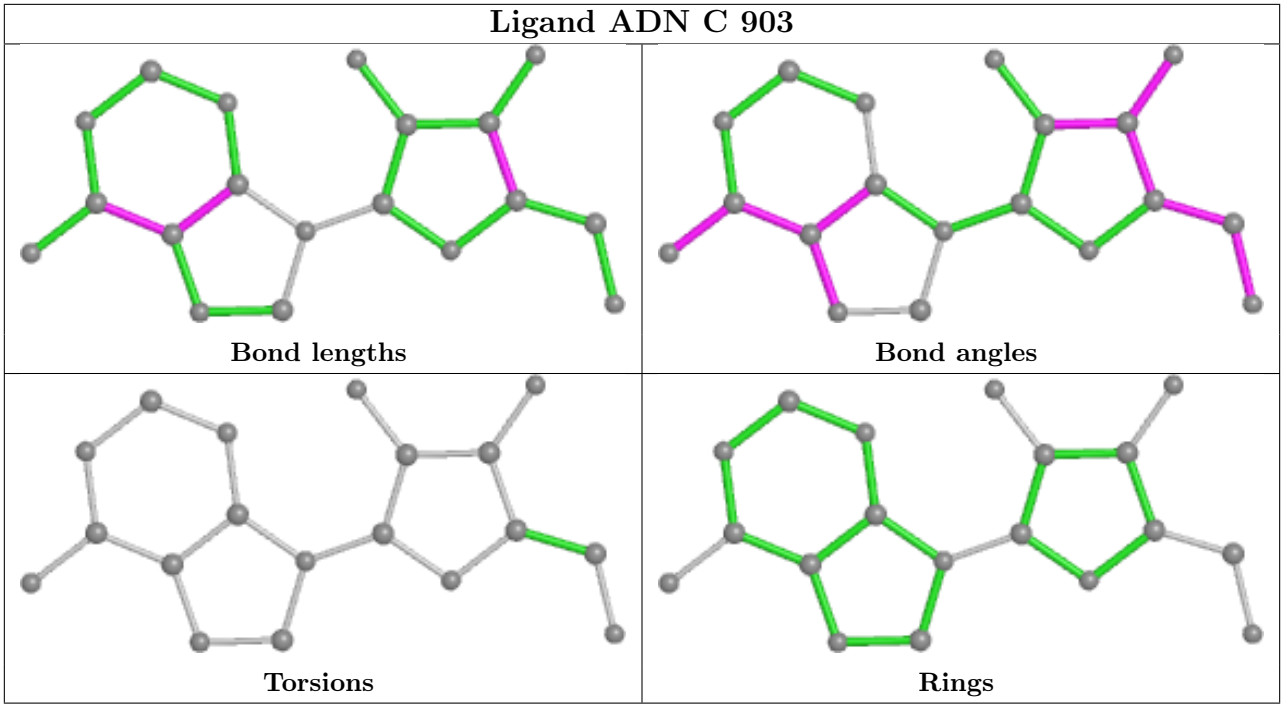
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	157:LYS	C	158:PHE	N	1.04
1	C	158:PHE	C	159:LEU	N	0.93

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	163/167 (97%)	-0.43	2 (1%)	79	81	8, 15, 22, 28	0
1	B	163/167 (97%)	-0.41	0	100	100	9, 15, 22, 29	0
1	C	162/167 (97%)	-0.31	0	100	100	13, 20, 27, 31	0
1	D	163/167 (97%)	-0.39	0	100	100	11, 17, 24, 29	0
1	E	163/167 (97%)	-0.23	0	100	100	11, 19, 27, 30	0
1	F	162/167 (97%)	-0.27	2 (1%)	79	81	9, 15, 22, 27	0
All	All	976/1002 (97%)	-0.34	4 (0%)	92	93	8, 17, 25, 31	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	145	GLY	3.4
1	F	144	LEU	2.1
1	A	103	ILE	2.1
1	A	102	ALA	2.1

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 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,

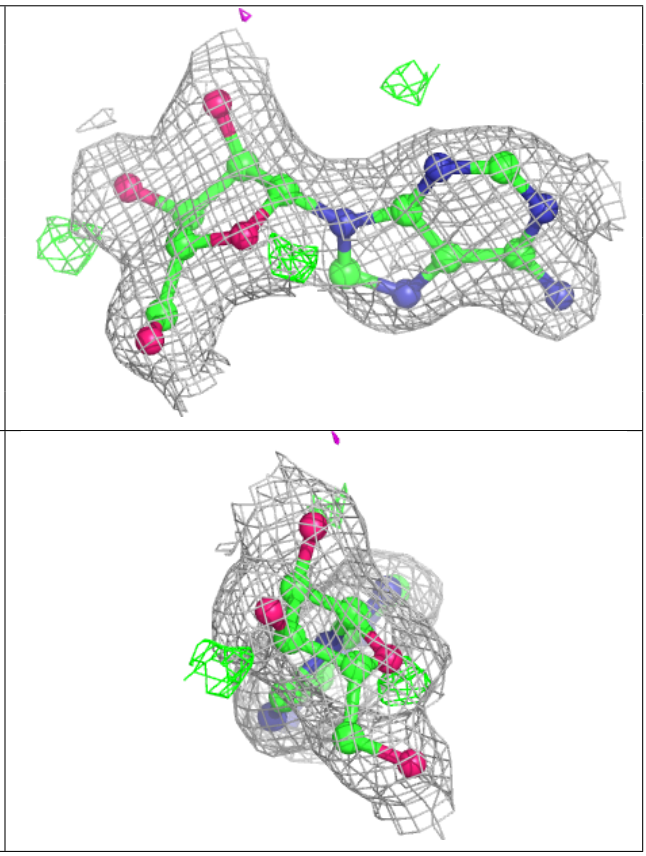
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADN	D	904	19/19	0.94	0.10	29,40,43,44	0
2	ADN	E	905	19/19	0.94	0.10	29,36,40,42	0
2	ADN	B	902	19/19	0.95	0.11	33,37,41,46	0
3	PO4	C	502	5/5	0.95	0.30	54,55,56,56	5
2	ADN	C	903	19/19	0.96	0.10	22,25,35,37	0
2	ADN	A	901	19/19	0.96	0.10	22,30,33,34	0
3	PO4	D	501	5/5	0.96	0.18	27,31,32,34	5
2	ADN	F	906	19/19	0.97	0.08	24,26,30,30	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.

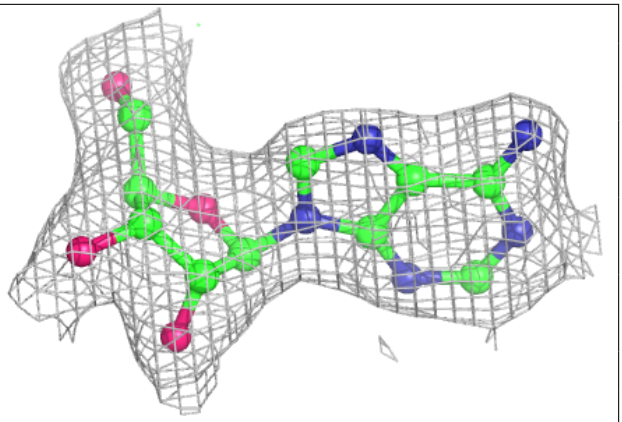
Electron density around ADN D 904:

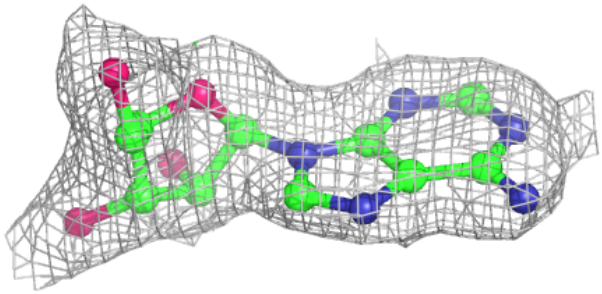
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

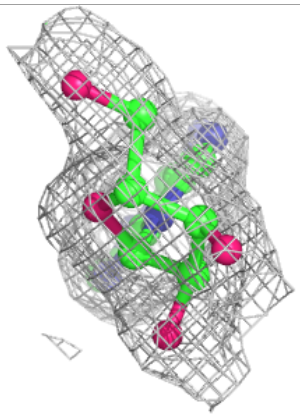


Electron density around ADN E 905:

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

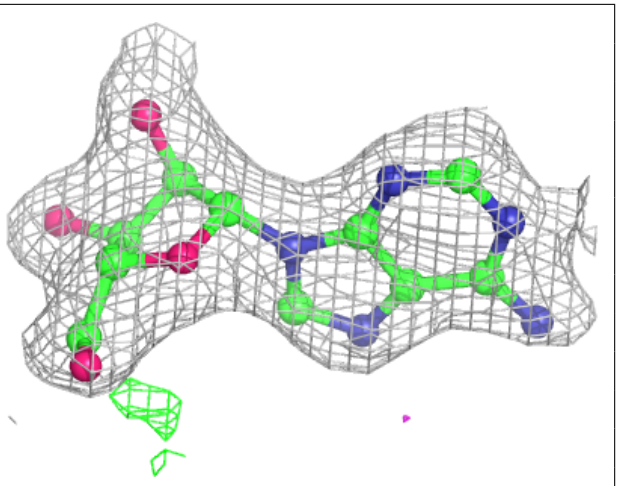


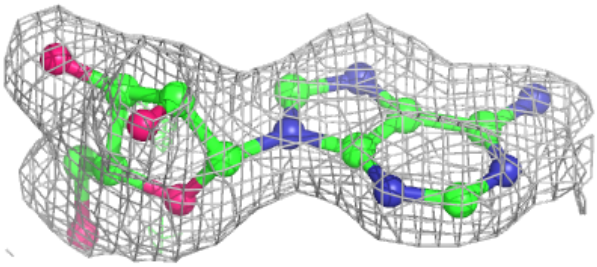


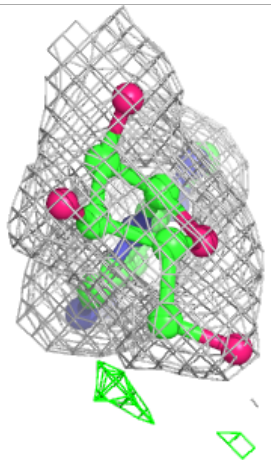


Electron density around ADN B 902:

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

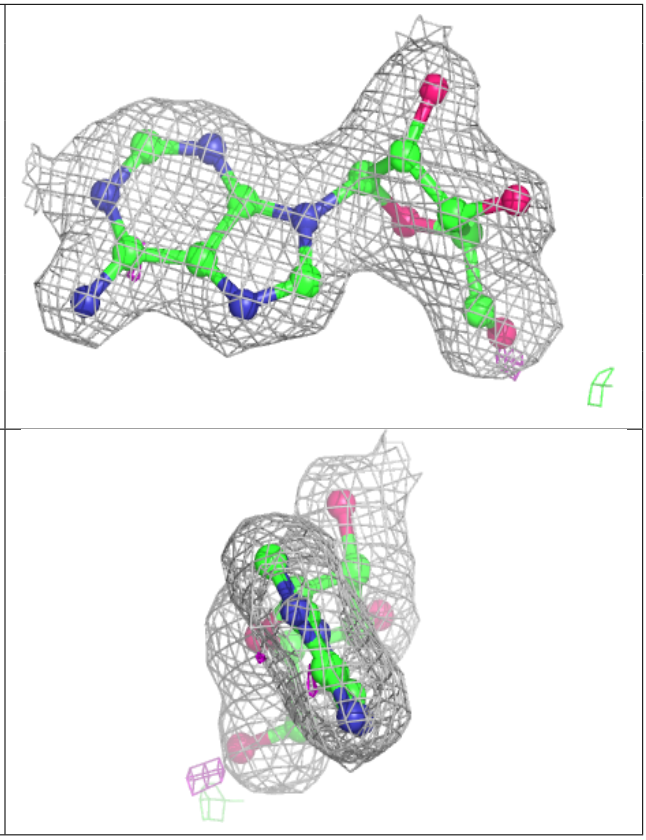






Electron density around ADN C 903:

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



Electron density around ADN A 901:

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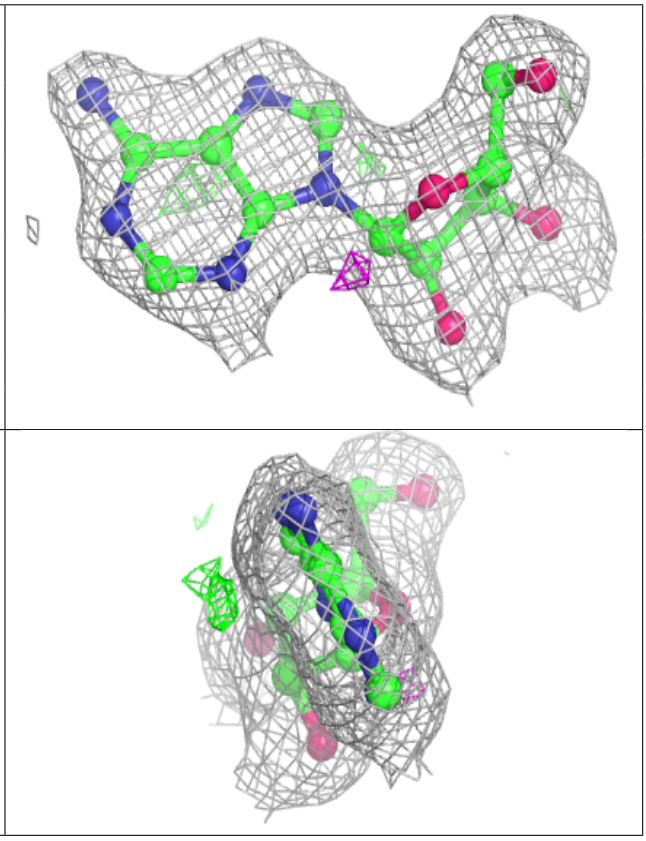
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADN F 906:

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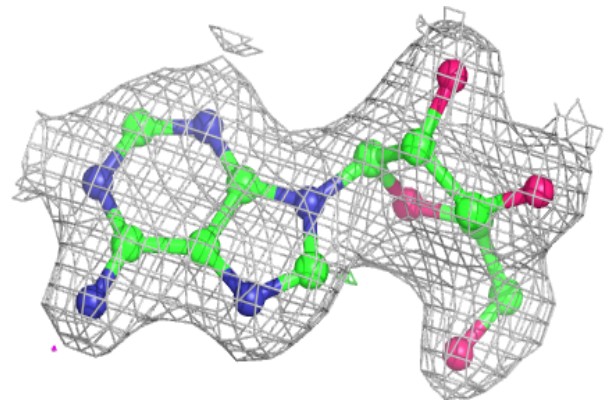
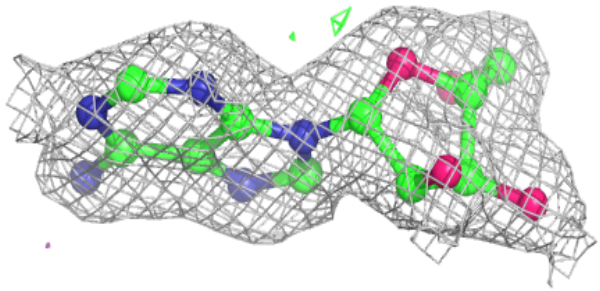
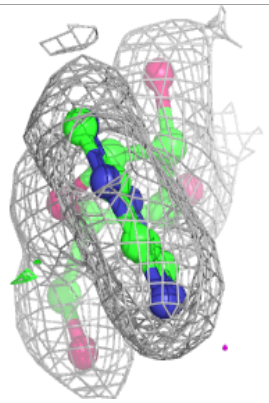
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.