Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2026 – 06:08 PM EST

PDB ID	:	36JR / pdb_000036jr
Title	:	Tri-complex of Compound 12, KRas Q61H, and CypA
Authors	:	Tomlinson, A.C.A.; Yano, J.K.
Deposited on	:	2026-06-14
Resolution	:	1.88 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

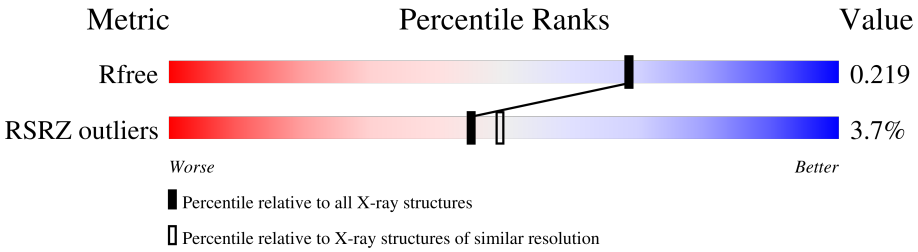
MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 1.88 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	1220 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5848 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 Isoform 2B of GTPase KRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	0	0
			1357	849	234	267	7			
1	B	170	Total	C	N	O	S	0	1	0
			1362	853	234	267	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P01116
A	61	HIS	GLN	engineered mutation	UNP P01116
B	0	SER	-	expression tag	UNP P01116
B	61	HIS	GLN	engineered mutation	UNP P01116

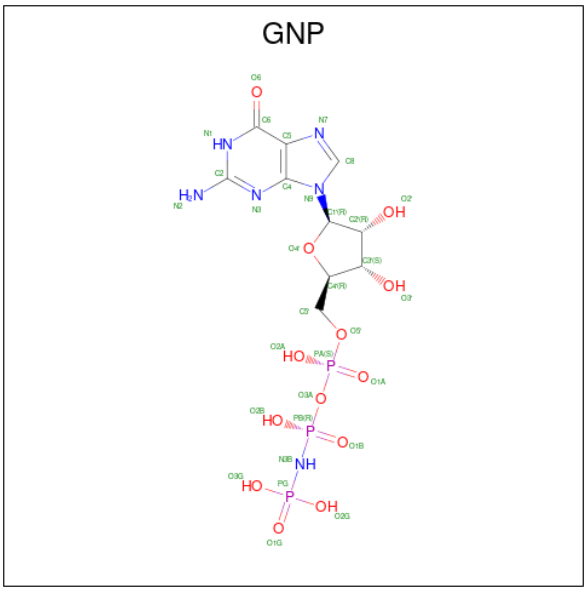
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	164	Total	C	N	O	S	0	0	0
			1257	797	217	235	8			
2	D	163	Total	C	N	O	S	0	0	0
			1248	792	216	232	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP P62937
D	0	SER	-	expression tag	UNP P62937

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).

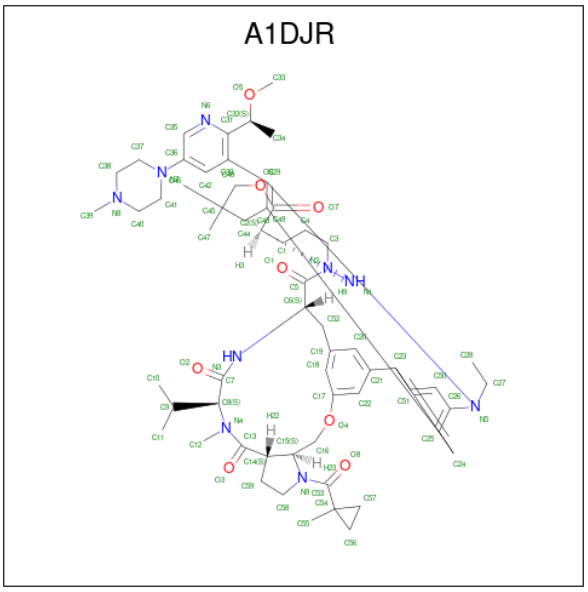


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is (1M,9S,13S,16S,19S,21S,25S,32M)-33-ethyl-32-{2-[(1S)-1-methoxyethyl]-5-(4-methylpiperazin-1-yl)pyridin-3-yl}-15,29,29-trimethyl-10-(1-methylcyclopropane-1-carbonyl)-16-(propan-2-yl)-7,27-dioxa-10,15,18,21,33,39-hexaazaheptacyclo[29.5.2.1 2,6 .1 4,19 .1 21,25 .0 9,13 .0 34,38]hentetraconta-1(36),2(41),3,5,31,34,37-heptaene-14,17,20,26-tetrone (non-preferred name) (CCD ID: A1DJR) (formula: $C_{59}H_{79}N_9O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O 76 59 9 8	0	0
5	D	1	Total C N O 76 59 9 8	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	111	Total O 111 111	0	0
6	B	138	Total O 138 138	0	0
6	C	64	Total O 64 64	0	0
6	D	93	Total O 93 93	0	0

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	127.06Å 127.06Å 106.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	55.02 – 1.88 55.02 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.9 (55.02-1.88) 100.0 (55.02-1.88)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.182 , 0.218 0.182 , 0.219	Depositor DCC
R_{free} test set	3980 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	37.1	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.036 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5848	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no oligosaccharides in this entry.

4.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
5	A1DJR	D	201	-	83,85,85	0.62	1 (1%)	105,129,129	0.80	2 (1%)
3	GNP	A	201	4	34,34,34	1.90	6 (17%)	47,54,54	1.57	6 (12%)
3	GNP	B	201	4	34,34,34	1.78	4 (11%)	47,54,54	1.60	6 (12%)
5	A1DJR	C	201	-	83,85,85	0.64	1 (1%)	105,129,129	0.78	3 (2%)

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
5	A1DJR	D	201	-	-	13/85/123/123	0/3/10/10
3	GNP	A	201	4	-	5/18/38/38	0/3/3/3
3	GNP	B	201	4	-	3/18/38/38	0/3/3/3
5	A1DJR	C	201	-	-	12/85/123/123	0/3/10/10

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201	GNP	PB-O3A	6.21	1.66	1.59
3	A	201	GNP	PG-N3B	6.12	1.79	1.63
3	B	201	GNP	PG-N3B	5.86	1.78	1.63
3	B	201	GNP	PG-O1G	4.50	1.53	1.46
3	B	201	GNP	PB-O3A	4.26	1.64	1.59
3	A	201	GNP	PG-O1G	3.38	1.51	1.46
5	C	201	A1DJR	C5-N2	3.14	1.39	1.35
5	D	201	A1DJR	C5-N2	2.65	1.39	1.35
3	A	201	GNP	PG-O3G	-2.33	1.50	1.56
3	A	201	GNP	PB-O1B	2.31	1.49	1.46
3	B	201	GNP	PG-O3G	-2.30	1.50	1.56
3	A	201	GNP	PG-O2G	-2.01	1.51	1.56

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	201	GNP	O1G-PG-N3B	-7.89	100.15	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	201	GNP	O1G-PG-N3B	-6.11	102.78	111.77
3	A	201	GNP	O1B-PB-N3B	4.94	119.04	111.77
3	A	201	GNP	O2G-PG-O3G	3.99	118.31	107.59
3	B	201	GNP	O2B-PB-O1B	3.71	117.83	109.87
3	B	201	GNP	O2G-PG-O3G	3.39	116.71	107.59
3	A	201	GNP	O2B-PB-O1B	3.35	117.06	109.87
3	A	201	GNP	O3A-PB-N3B	-3.25	97.58	106.59
5	D	201	A1DJR	C41-N7-C37	3.11	118.56	111.57
3	B	201	GNP	O1B-PB-N3B	2.90	116.04	111.77
5	C	201	A1DJR	C41-N7-C37	2.67	117.58	111.57
3	B	201	GNP	O2A-PA-O1A	2.65	124.78	112.44
3	B	201	GNP	O3A-PB-N3B	-2.45	99.80	106.59
5	C	201	A1DJR	O6-C48-C45	-2.34	105.22	109.25
5	D	201	A1DJR	C59-C58-N9	-2.24	100.76	103.22
3	A	201	GNP	O2A-PA-O1A	2.17	122.54	112.44
5	C	201	A1DJR	C30-C29-C43	-2.12	126.14	128.34

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	GNP	PB-N3B-PG-O1G
3	A	201	GNP	PG-N3B-PB-O1B
3	A	201	GNP	PG-N3B-PB-O3A
3	B	201	GNP	PB-N3B-PG-O1G
3	B	201	GNP	PG-N3B-PB-O1B
3	B	201	GNP	PG-N3B-PB-O3A
5	C	201	A1DJR	C18-C17-O4-C16
5	C	201	A1DJR	C22-C17-O4-C16
5	D	201	A1DJR	C18-C17-O4-C16
5	D	201	A1DJR	C22-C17-O4-C16
5	C	201	A1DJR	C30-C31-C32-C34
5	D	201	A1DJR	C30-C31-C32-C34
5	C	201	A1DJR	C30-C31-C32-O5
5	D	201	A1DJR	C30-C31-C32-O5
5	C	201	A1DJR	C19-C52-C6-N3
5	C	201	A1DJR	C31-C32-O5-C33
5	D	201	A1DJR	C31-C32-O5-C33
5	D	201	A1DJR	C19-C52-C6-N3
5	C	201	A1DJR	O3-C13-C14-C15
5	C	201	A1DJR	N4-C13-C14-C15
5	D	201	A1DJR	C19-C52-C6-C5

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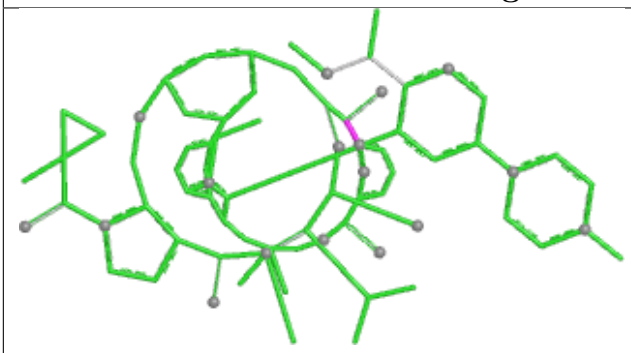
Mol	Chain	Res	Type	Atoms
5	C	201	A1DJR	N4-C13-C14-C59
5	D	201	A1DJR	N4-C13-C14-C59
5	C	201	A1DJR	C19-C52-C6-C5
5	C	201	A1DJR	C15-C16-O4-C17
5	D	201	A1DJR	C15-C16-O4-C17
3	A	201	GNP	PA-O3A-PB-O2B
5	C	201	A1DJR	O3-C13-C14-C59
5	D	201	A1DJR	O3-C13-C14-C59
5	D	201	A1DJR	O8-C53-C54-C55
5	D	201	A1DJR	O3-C13-C14-C15
3	A	201	GNP	PA-O3A-PB-O1B
5	D	201	A1DJR	N4-C13-C14-C15

There are no ring outliers.

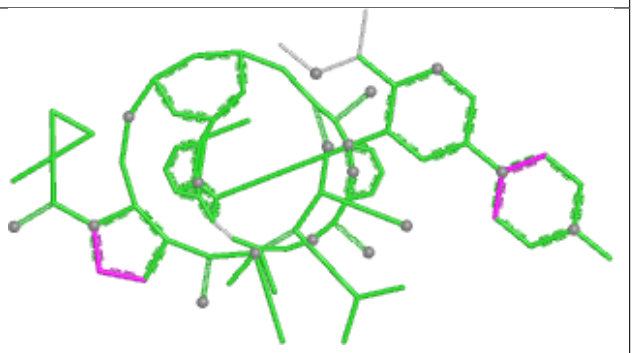
No monomer is involved in short contacts.

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.

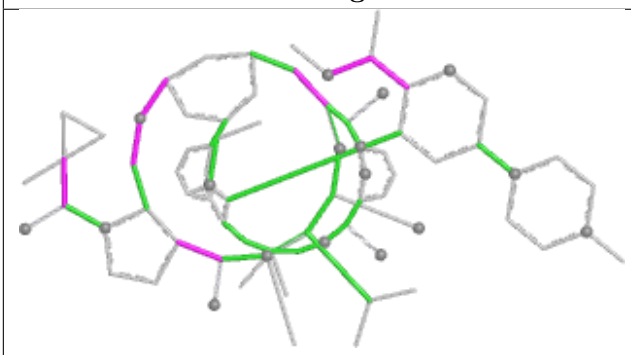
Ligand A1DJR D 201



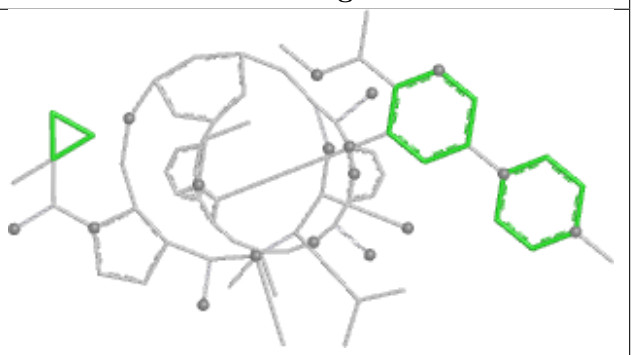
Bond lengths



Bond angles

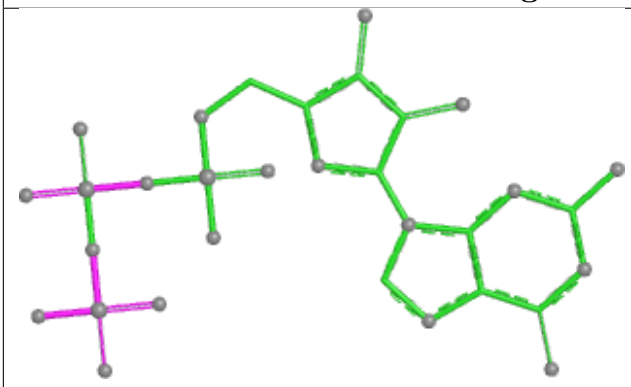


Torsions

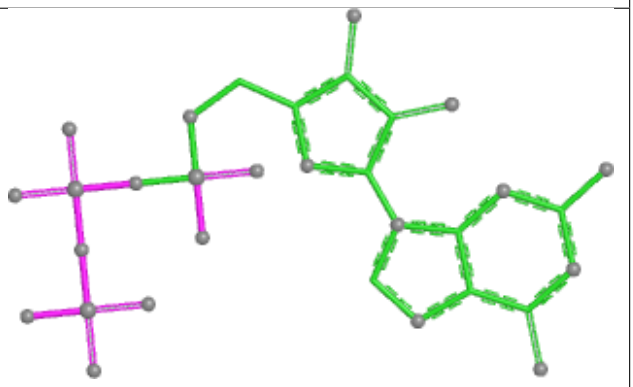


Rings

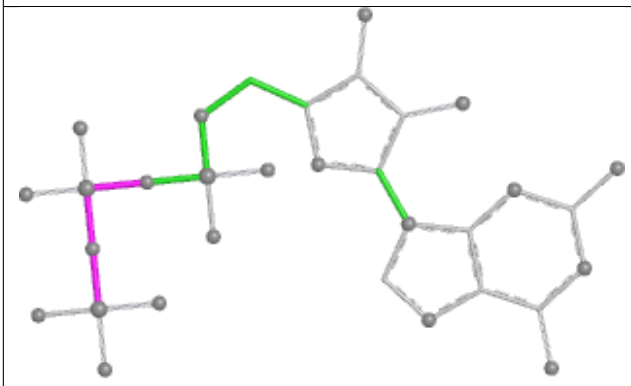
Ligand GNP A 201



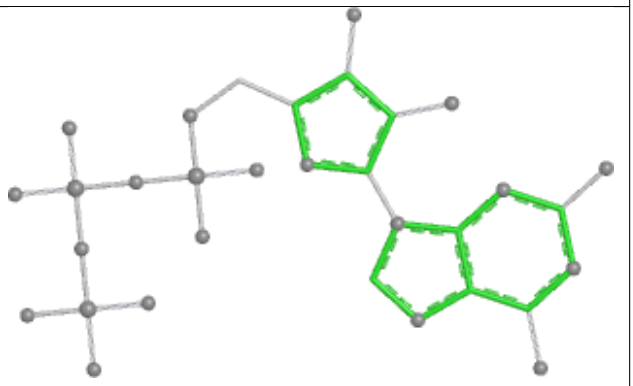
Bond lengths



Bond angles

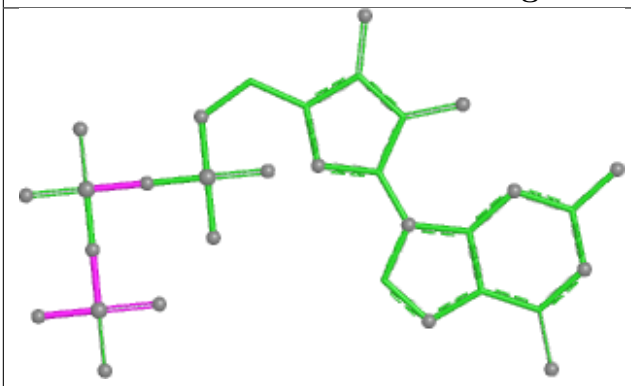


Torsions

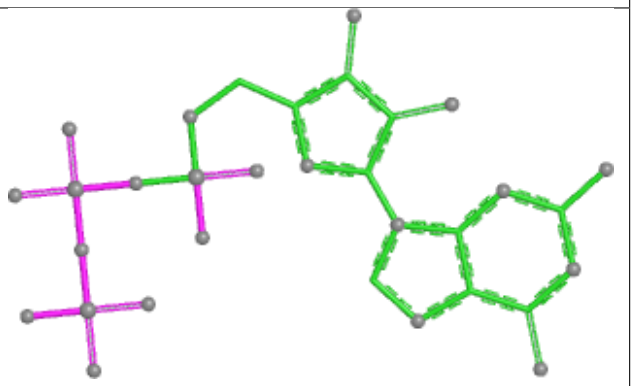


Rings

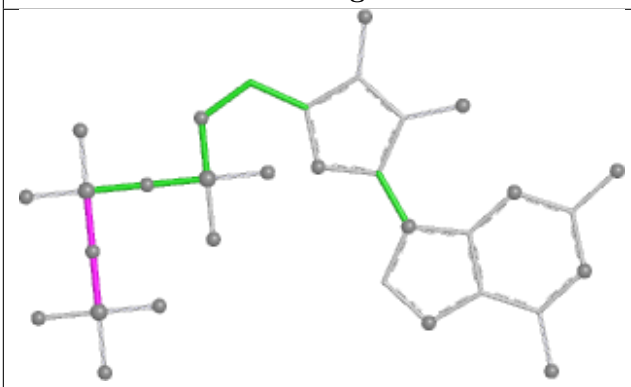
Ligand GNP B 201



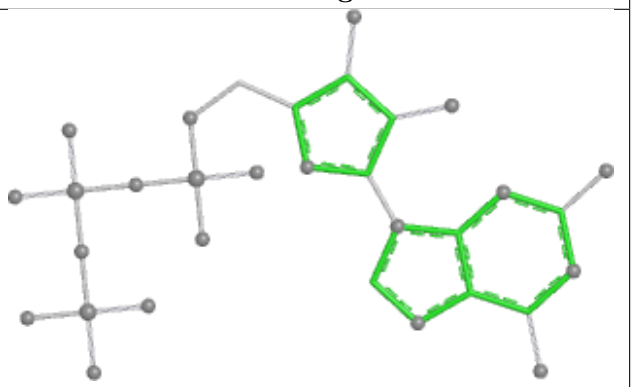
Bond lengths



Bond angles

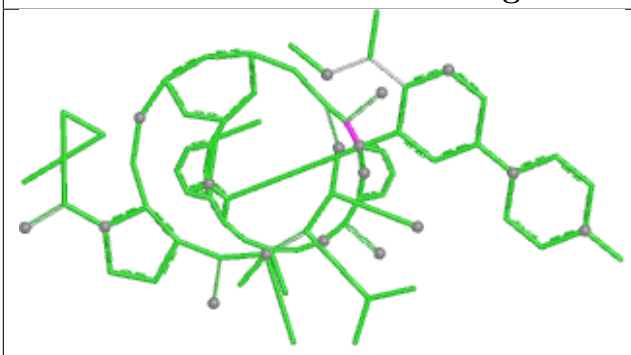


Torsions

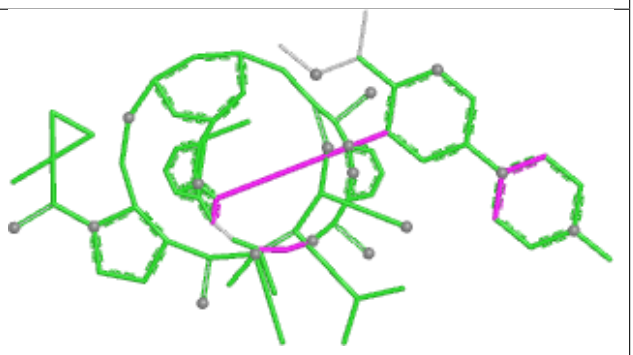


Rings

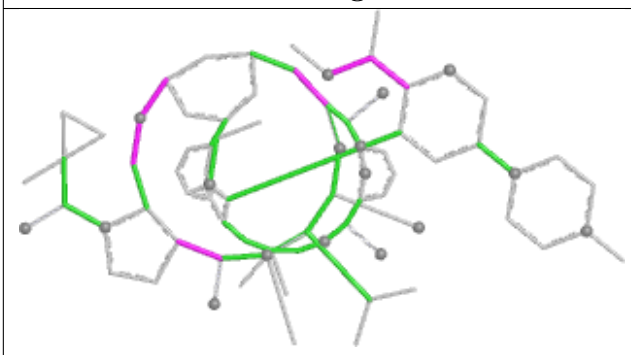
Ligand A1DJR C 201



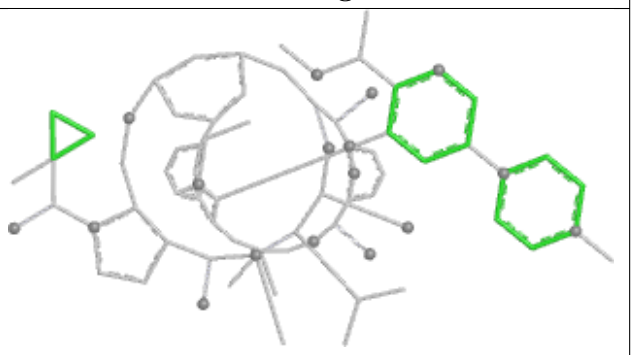
Bond lengths



Bond angles



Torsions



Rings

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	170/170 (100%)	0.14	8 (4%)	36	38	28, 43, 65, 112	0
1	B	170/170 (100%)	0.06	9 (5%)	32	34	28, 40, 62, 94	1 (0%)
2	C	164/166 (98%)	0.42	6 (3%)	45	49	30, 57, 84, 112	1 (0%)
2	D	163/166 (98%)	0.14	2 (1%)	76	81	28, 51, 73, 88	1 (0%)
All	All	667/672 (99%)	0.19	25 (3%)	45	49	28, 47, 77, 112	3 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	2	VAL	6.3
2	D	2	VAL	4.2
1	A	0	SER	3.3
1	B	65	SER	2.9
1	A	62	GLU	2.9
1	A	169	LYS	2.9
2	D	164	LEU	2.8
2	C	165	GLU	2.8
2	C	70	HIS	2.7
1	A	68	ARG	2.6
1	B	66	ALA	2.5
2	C	164	LEU	2.5
1	B	169	LYS	2.5
1	A	71	TYR	2.4
1	B	122	SER	2.4
1	B	62	GLU	2.4
1	B	94	HIS	2.3
1	B	71	TYR	2.2
1	B	95	HIS	2.2
1	A	65	SER	2.2
2	C	69	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	137	ASN	2.1
1	A	29	VAL	2.1
1	A	122	SER	2.0
1	B	68	ARG	2.0

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

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

5.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.4 Ligands (i)

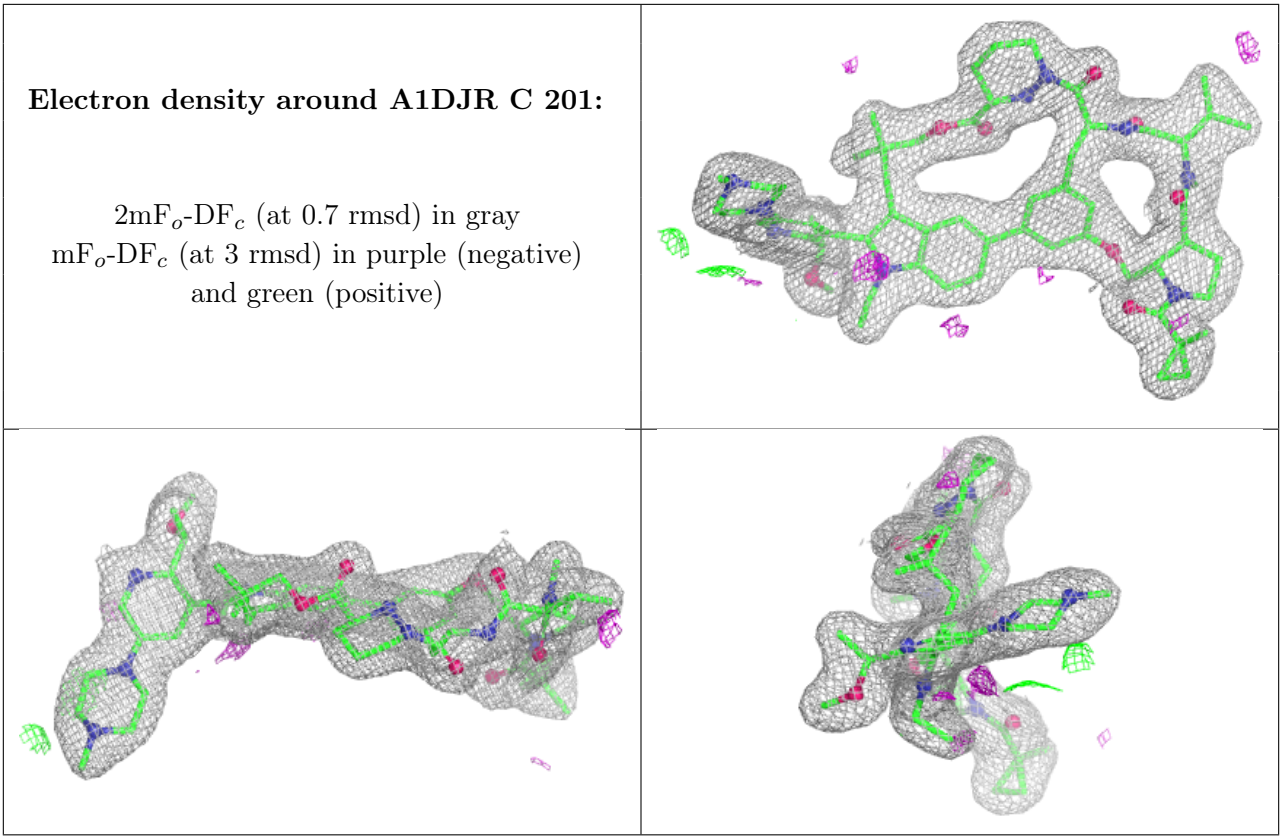
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	A1DJR	C	201	76/76	0.97	0.07	31,37,47,51	0
5	A1DJR	D	201	76/76	0.97	0.06	26,31,36,38	0
3	GNP	A	201	32/32	0.98	0.05	30,36,43,45	0
4	MG	B	202	1/1	0.99	0.03	30,30,30,30	0
3	GNP	B	201	32/32	0.99	0.05	30,36,40,43	0
4	MG	A	202	1/1	0.99	0.02	31,31,31,31	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.

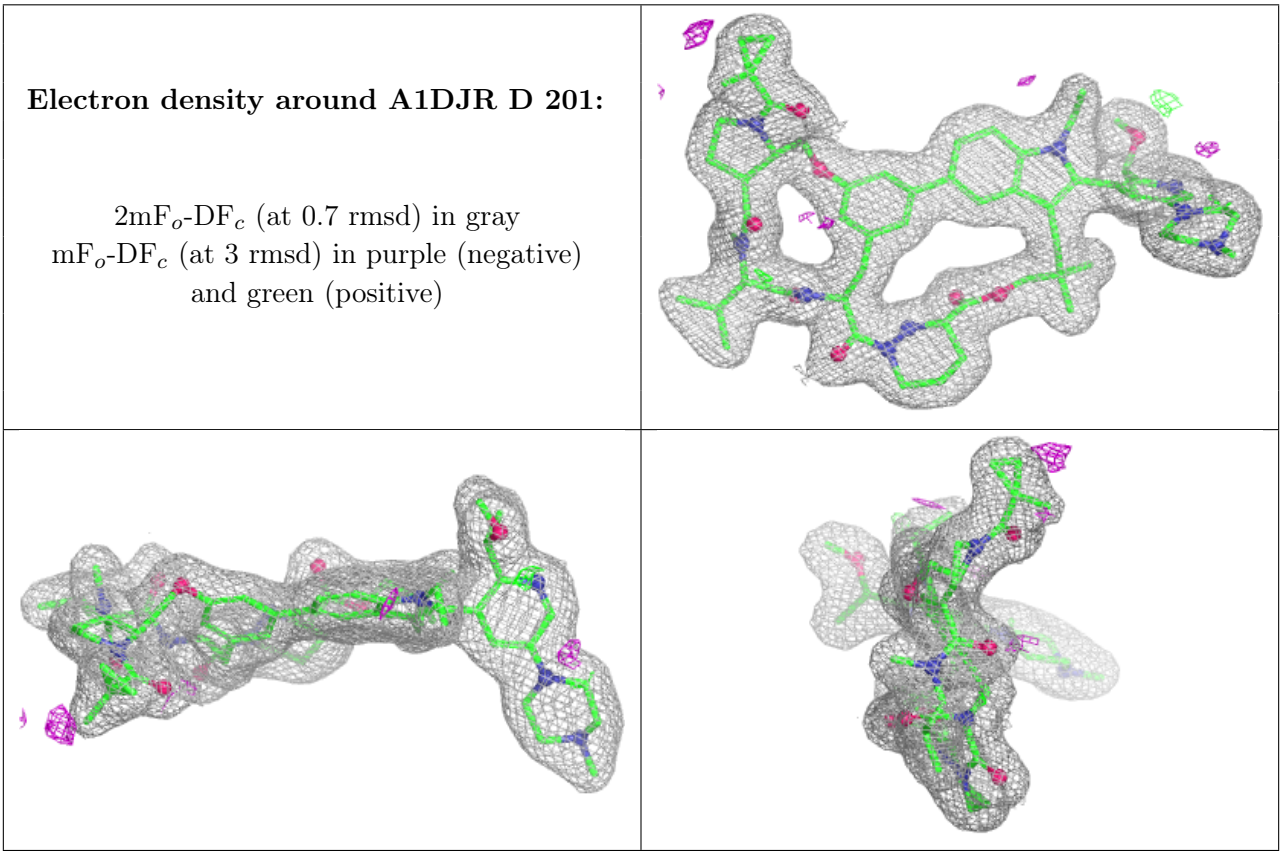
Electron density around A1DJR C 201:

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



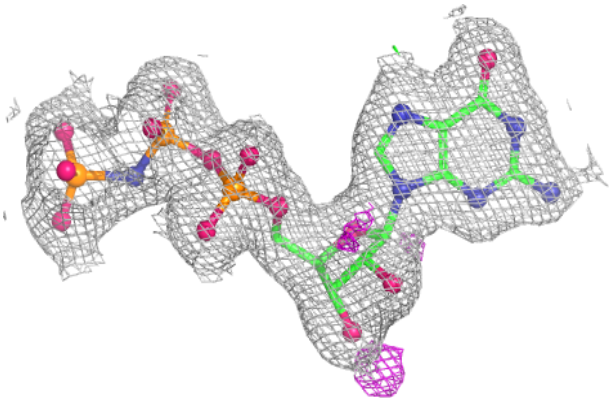
Electron density around A1DJR D 201:

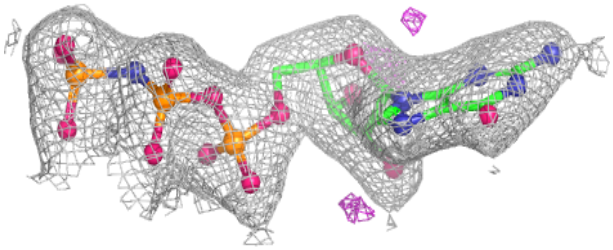
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

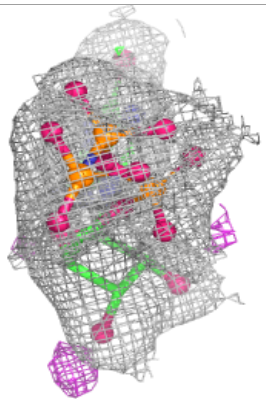


Electron density around GNP A 201:

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

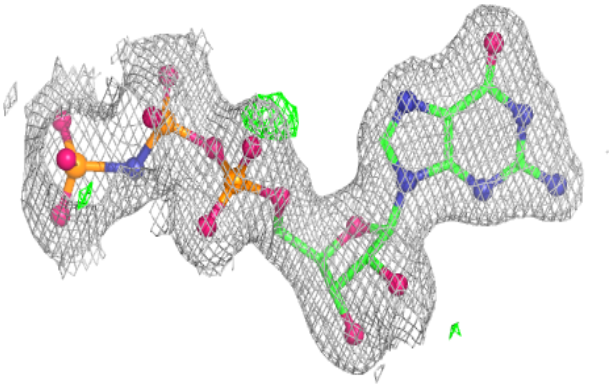


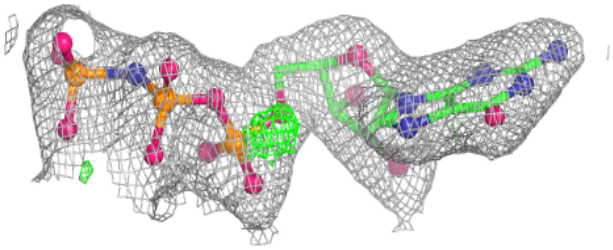


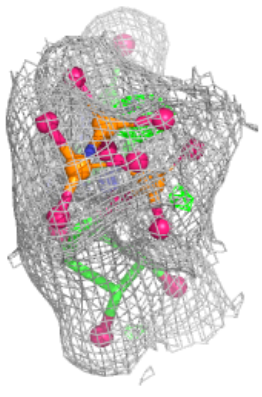


Electron density around GNP B 201:

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







5.5 Other polymers (i)

There are no such residues in this entry.