Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 03:33 AM EDT

PDB ID	:	6MFW
Title	:	Crystal structure of a 4-domain construct of LgrA in the substrate donation state
Authors	:	Reimer, J.M.; Eivaskhani, M.; Schmeing, T.M.
Deposited on	:	2018-09-12
Resolution	:	2.50 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 ⓘ 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	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.50 Å.

There are no overall percentile quality scores available for this entry.

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

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 19072 atoms, of which 9373 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.

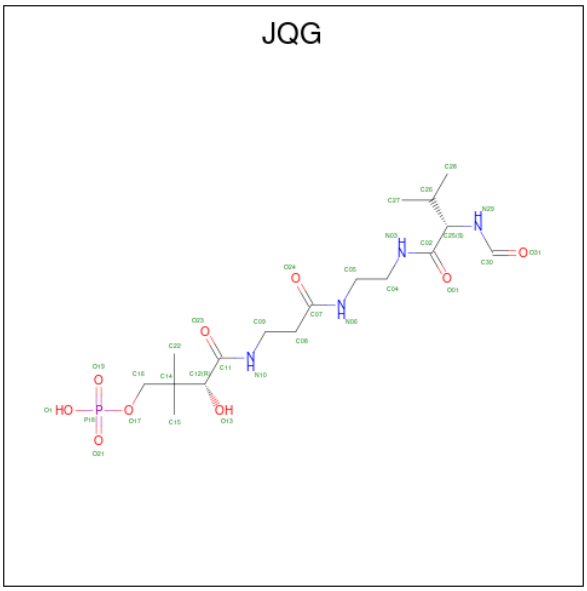
- Molecule 1 is a protein called Linear gramicidin synthase subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1181	Total	C	H	N	O	S	0	0	0
			18710	6017	9299	1602	1752	40			

There are 13 discrepancies between the modelled and reference sequences:

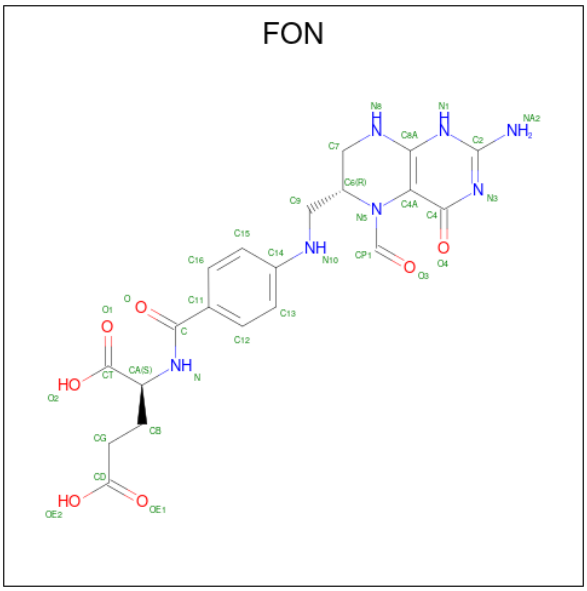
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q70LM7
A	0	ALA	-	expression tag	UNP Q70LM7
A	1	MET	-	expression tag	UNP Q70LM7
A	2	GLY	-	expression tag	UNP Q70LM7
A	1200	ALA	-	expression tag	UNP Q70LM7
A	1201	ALA	-	expression tag	UNP Q70LM7
A	1202	ALA	-	expression tag	UNP Q70LM7
A	1203	GLU	-	expression tag	UNP Q70LM7
A	1204	ASN	-	expression tag	UNP Q70LM7
A	1205	LEU	-	expression tag	UNP Q70LM7
A	1206	TYR	-	expression tag	UNP Q70LM7
A	1207	PHE	-	expression tag	UNP Q70LM7
A	1208	GLN	-	expression tag	UNP Q70LM7

- Molecule 2 is (2 {R})- {N}-[3-[2-[[(2 {S})-2-formamido-3-methyl-butanoyl]amino]ethylamino]-3-oxidanylidene-propyl]-3,3-dimethyl-2-oxidanyl-4-[oxidanyl-bis(oxidanylidene)-$l^{6}-phosphanyl]oxy-butanamide (three-letter code: JQG) (formula: $C_{17}H_{32}N_4O_9P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			61	17	31	4	8	1		

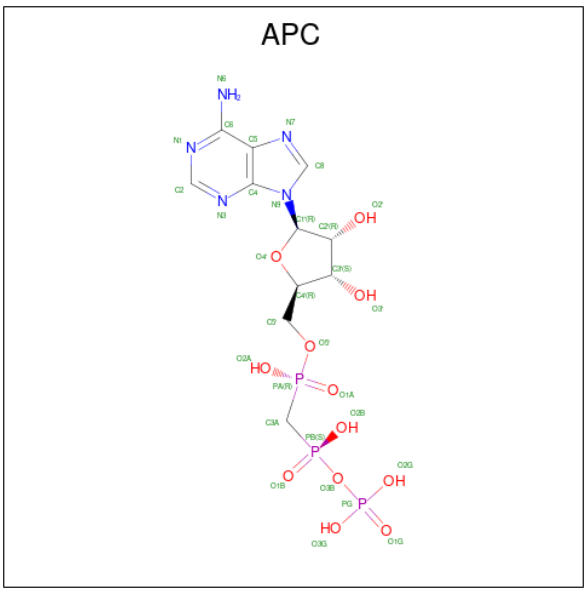
- Molecule 3 is N-{[4-({[(6R)-2-amino-5-formyl-4-oxo-1,4,5,6,7,8-hexahydropteridin-6-yl]methyl}amino)phenyl]carbonyl}-L-glutamic acid (three-letter code: FON) (formula: $C_{20}H_{23}N_7O_7$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			55	20	21	7	7		

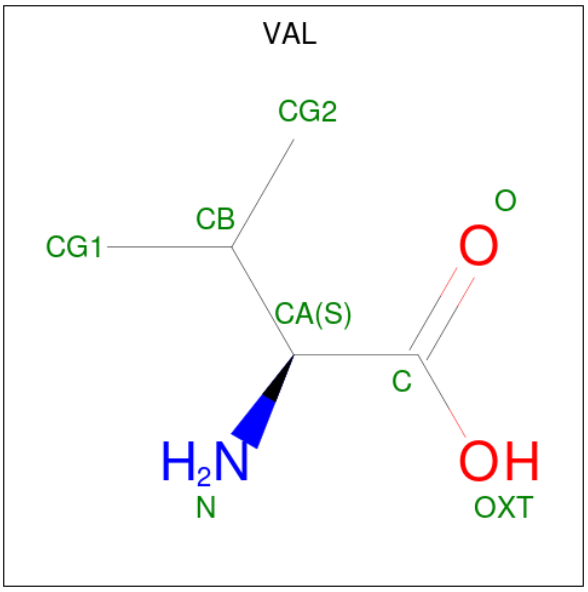
- Molecule 4 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-

letter code: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



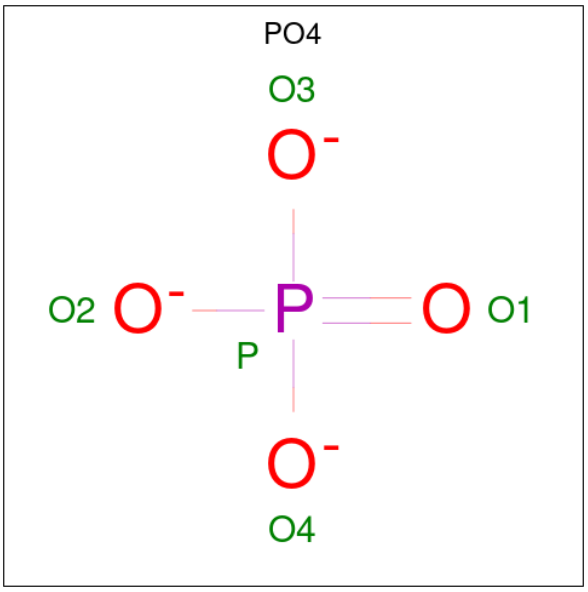
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	0	0
			45	11	14	5	12	3		

- Molecule 5 is VALINE (three-letter code: VAL) (formula: $C_5H_{11}NO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			16	5	8	1	2		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	179	Total O 179 179	0	0

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

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.37Å 133.87Å 162.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.33 – 2.50	Depositor
% Data completeness (in resolution range)	99.9 (69.33-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 2.37Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.200 , 0.243	Depositor
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.387	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	19072	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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 monosaccharides in this entry.

4.6 Ligand geometry

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	JQG	A	1301	1	23,29,30	2.48	7 (30%)	30,38,41	1.07	1 (3%)
3	FON	A	1302	-	34,36,36	3.90	15 (44%)	36,50,50	2.00	6 (16%)
5	VAL	A	1304	-	5,7,7	1.07	1 (20%)	7,9,9	0.70	0
4	APC	A	1303	7	27,33,33	3.60	10 (37%)	31,52,52	1.43	5 (16%)
6	PO4	A	1305	-	4,4,4	0.86	0	6,6,6	0.42	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
3	FON	A	1302	-	-	8/24/37/37	0/2/3/3
5	VAL	A	1304	-	-	2/8/8/8	-
4	APC	A	1303	7	-	4/15/38/38	0/3/3/3
2	JQG	A	1301	1	-	6/38/40/41	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1302	FON	C4A-N5	10.77	1.56	1.41
4	A	1303	APC	PB-O3B	10.02	1.69	1.58
3	A	1302	FON	C2-N1	8.35	1.50	1.35
4	A	1303	APC	C3'-C4'	-8.17	1.32	1.53
4	A	1303	APC	O4'-C4'	7.77	1.62	1.45
3	A	1302	FON	C4-N3	7.65	1.46	1.33
3	A	1302	FON	CP1-N5	7.39	1.45	1.35
4	A	1303	APC	O4'-C1'	-6.95	1.31	1.41
3	A	1302	FON	C7-C6	-6.00	1.45	1.52
2	A	1301	JQG	C07-N06	5.90	1.46	1.33
3	A	1302	FON	C2-NA2	5.88	1.45	1.33
2	A	1301	JQG	C02-N03	5.85	1.46	1.33
2	A	1301	JQG	C11-N10	5.75	1.46	1.33
3	A	1302	FON	C7-N8	-5.58	1.35	1.44
3	A	1302	FON	C8A-N1	5.35	1.44	1.34
3	A	1302	FON	C4A-C4	4.96	1.48	1.41
3	A	1302	FON	C-N	4.89	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1303	APC	PA-O5'	4.19	1.63	1.57
2	A	1301	JQG	C30-N29	3.86	1.46	1.33
4	A	1303	APC	C6-N6	3.86	1.48	1.34
3	A	1302	FON	C4A-C8A	-3.36	1.34	1.41
4	A	1303	APC	PB-O2B	-3.14	1.49	1.56
4	A	1303	APC	O2'-C2'	-2.80	1.36	1.43
4	A	1303	APC	PA-O1A	-2.69	1.45	1.51
4	A	1303	APC	O3'-C3'	2.63	1.49	1.43
2	A	1301	JQG	O23-C11	-2.44	1.18	1.23
3	A	1302	FON	C2-N3	-2.40	1.31	1.35
3	A	1302	FON	O4-C4	-2.23	1.18	1.24
2	A	1301	JQG	O01-C02	-2.20	1.19	1.23
5	A	1304	VAL	OXT-C	-2.13	1.23	1.30
3	A	1302	FON	O-C	-2.11	1.19	1.23
2	A	1301	JQG	O24-C07	-2.02	1.19	1.23
3	A	1302	FON	C14-N10	2.01	1.44	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1302	FON	C8A-C4A-C4	7.03	119.94	114.44
4	A	1303	APC	N3-C2-N1	-4.88	121.06	128.68
3	A	1302	FON	O3-CP1-N5	-3.87	119.75	125.36
3	A	1302	FON	N1-C2-N3	-3.48	119.96	125.42
3	A	1302	FON	C2-N3-C4	3.07	120.80	115.93
4	A	1303	APC	PB-O3B-PG	-2.95	122.21	132.62
3	A	1302	FON	C4A-N5-C6	-2.84	114.28	119.31
3	A	1302	FON	C2-N1-C8A	2.31	119.71	114.54
4	A	1303	APC	C1'-N9-C4	-2.27	122.66	126.64
4	A	1303	APC	C4-C5-N7	-2.25	107.05	109.40
2	A	1301	JQG	O31-C30-N29	-2.12	119.69	125.27
4	A	1303	APC	C2-N1-C6	2.04	122.25	118.75

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1303	APC	PB-C3A-PA-O1A
4	A	1303	APC	C5'-O5'-PA-O1A
2	A	1301	JQG	N29-C25-C26-C27
2	A	1301	JQG	C02-C25-C26-C27
2	A	1301	JQG	N29-C25-C26-C28

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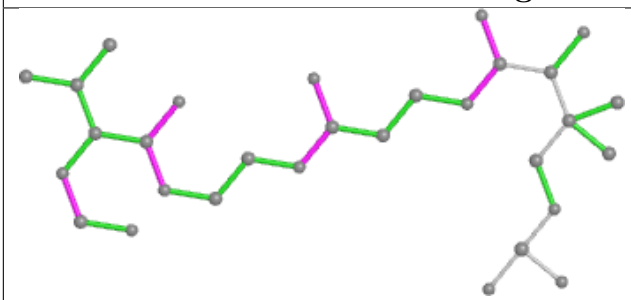
Mol	Chain	Res	Type	Atoms
2	A	1301	JQG	C02-C25-C26-C28
3	A	1302	FON	N-C-C11-C12
3	A	1302	FON	O-C-C11-C12
5	A	1304	VAL	O-C-CA-CB
5	A	1304	VAL	OXT-C-CA-CB
3	A	1302	FON	O-C-C11-C16
3	A	1302	FON	N-C-C11-C16
3	A	1302	FON	N-CA-CB-CG
4	A	1303	APC	PB-C3A-PA-O5'
3	A	1302	FON	CA-CB-CG-CD
2	A	1301	JQG	C07-C08-C09-N10
3	A	1302	FON	OE1-CD-CG-CB
3	A	1302	FON	OE2-CD-CG-CB
4	A	1303	APC	C5'-O5'-PA-O2A
2	A	1301	JQG	C04-C05-N06-C07

There are no ring outliers.

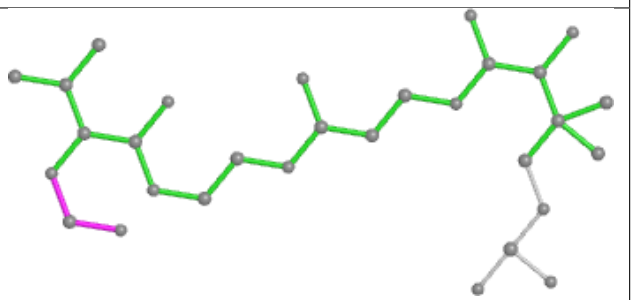
No monomer is involved in short contacts.

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.

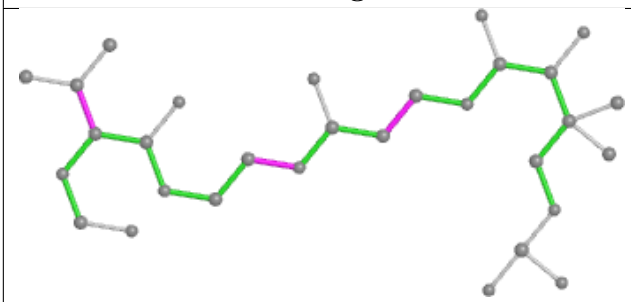
Ligand JQG A 1301



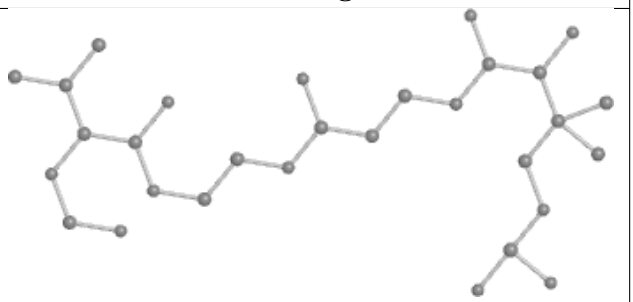
Bond lengths



Bond angles

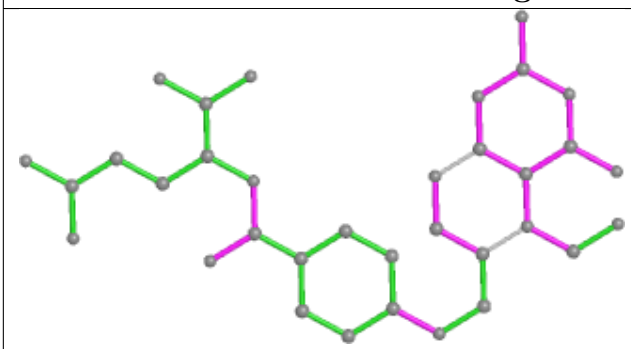


Torsions

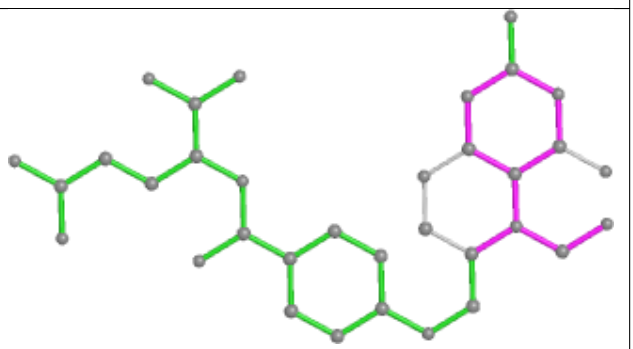


Rings

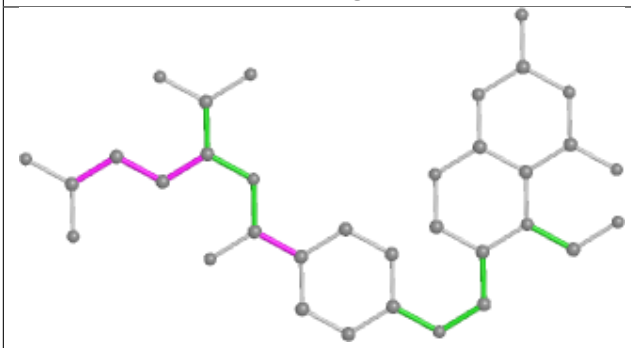
Ligand FON A 1302



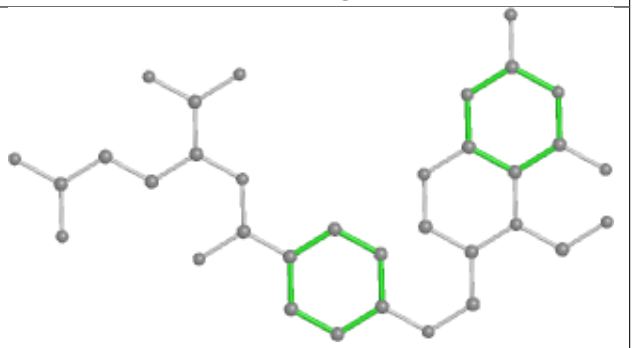
Bond lengths



Bond angles

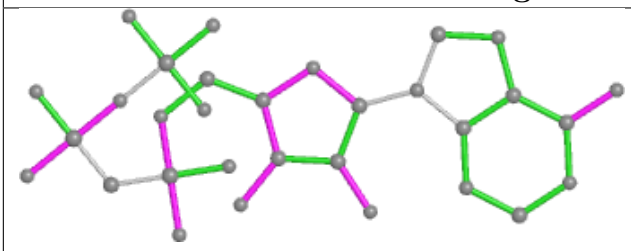


Torsions

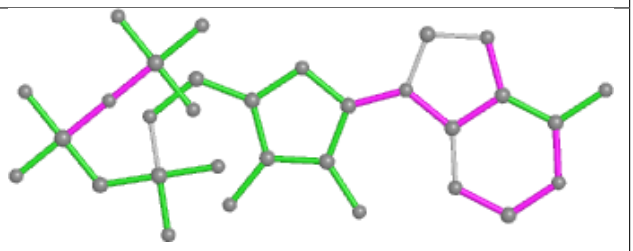


Rings

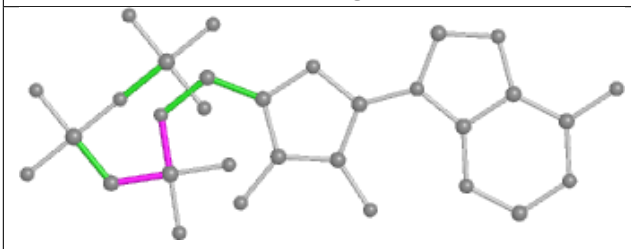
Ligand APC A 1303



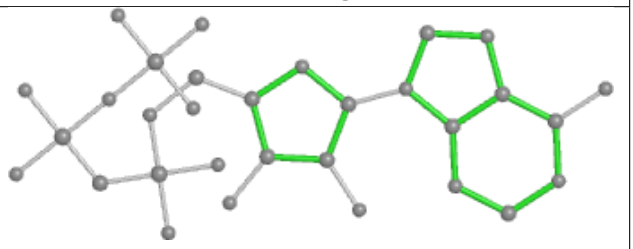
Bond lengths



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

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

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

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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