Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 01:06 AM EDT

PDB ID	:	6PD2
Title	:	PntC-AEPT: fusion protein of phosphonate-specific cytidylyltransferase and 2-aminoethylphosphonate (AEP) transaminase from Treponema denticola in complex with cytidine monophosphate-AEP
Authors	:	Suits, M.D.L.; Whiteside, J.
Deposited on	:	2019-06-18
Resolution	:	1.95 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 1.95 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 9 unique types of molecules in this entry. The entry contains 21090 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 Nucleotidyl transferase/aminotransferase, class V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	615	Total	C	N	O	S	0	0	0
			4831	3084	798	914	35			
1	B	615	Total	C	N	O	S	0	0	0
			4831	3084	798	914	35			
1	C	616	Total	C	N	O	S	0	0	0
			4838	3089	799	915	35			
1	D	608	Total	C	N	O	S	0	0	0
			4776	3051	786	904	35			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	617	LEU	-	expression tag	UNP Q73MU2
A	618	GLU	-	expression tag	UNP Q73MU2
A	619	HIS	-	expression tag	UNP Q73MU2
A	620	HIS	-	expression tag	UNP Q73MU2
A	621	HIS	-	expression tag	UNP Q73MU2
A	622	HIS	-	expression tag	UNP Q73MU2
A	623	HIS	-	expression tag	UNP Q73MU2
A	624	HIS	-	expression tag	UNP Q73MU2
B	617	LEU	-	expression tag	UNP Q73MU2
B	618	GLU	-	expression tag	UNP Q73MU2
B	619	HIS	-	expression tag	UNP Q73MU2
B	620	HIS	-	expression tag	UNP Q73MU2
B	621	HIS	-	expression tag	UNP Q73MU2
B	622	HIS	-	expression tag	UNP Q73MU2
B	623	HIS	-	expression tag	UNP Q73MU2
B	624	HIS	-	expression tag	UNP Q73MU2
C	617	LEU	-	expression tag	UNP Q73MU2
C	618	GLU	-	expression tag	UNP Q73MU2
C	619	HIS	-	expression tag	UNP Q73MU2
C	620	HIS	-	expression tag	UNP Q73MU2
C	621	HIS	-	expression tag	UNP Q73MU2

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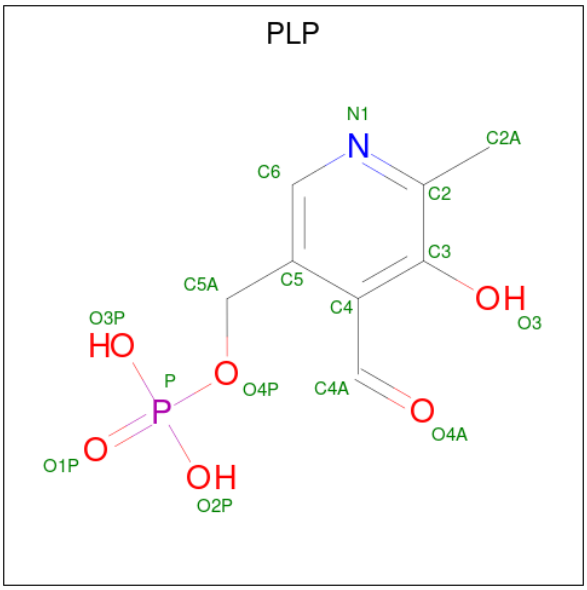
Chain	Residue	Modelled	Actual	Comment	Reference
C	622	HIS	-	expression tag	UNP Q73MU2
C	623	HIS	-	expression tag	UNP Q73MU2
C	624	HIS	-	expression tag	UNP Q73MU2
D	617	LEU	-	expression tag	UNP Q73MU2
D	618	GLU	-	expression tag	UNP Q73MU2
D	619	HIS	-	expression tag	UNP Q73MU2
D	620	HIS	-	expression tag	UNP Q73MU2
D	621	HIS	-	expression tag	UNP Q73MU2
D	622	HIS	-	expression tag	UNP Q73MU2
D	623	HIS	-	expression tag	UNP Q73MU2
D	624	HIS	-	expression tag	UNP Q73MU2

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).

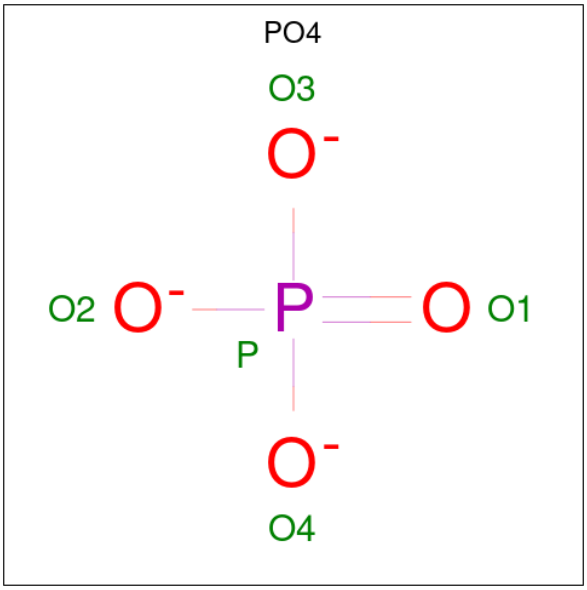


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	D	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	B	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0
3	D	2	Total Mg 2 2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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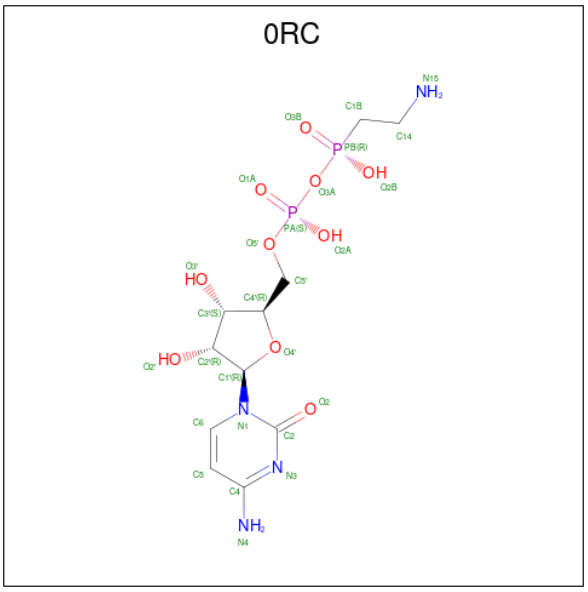
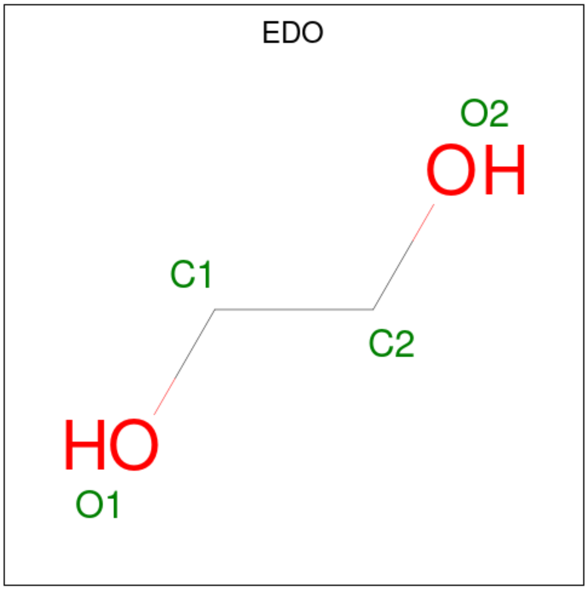
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0

- Molecule 5 is 5'-O-[(S)-{[(R)-(2-aminoethyl)(hydroxy)phosphoryl]oxy}(hydroxy)phosphoryl]cytidine (three-letter code: 0RC) (formula: $C_{11}H_{20}N_4O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 27 11 4 10 2	0	0
5	B	1	Total C N O P 27 11 4 10 2	0	0
5	C	1	Total C N O P 27 11 4 10 2	0	0
5	D	1	Total C N O P 27 11 4 10 2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0

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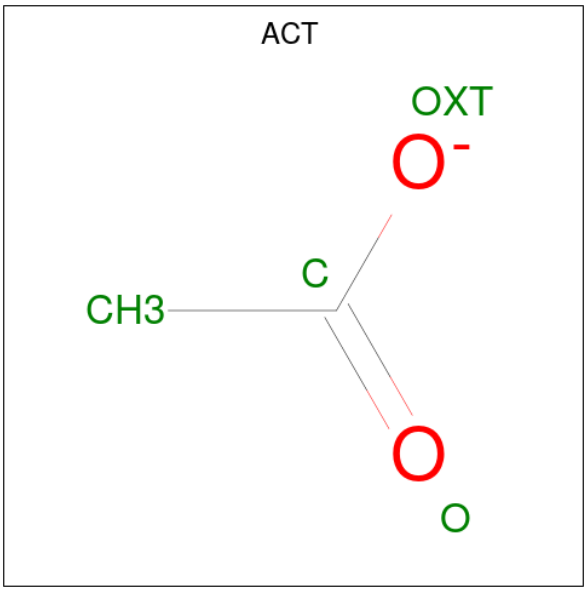
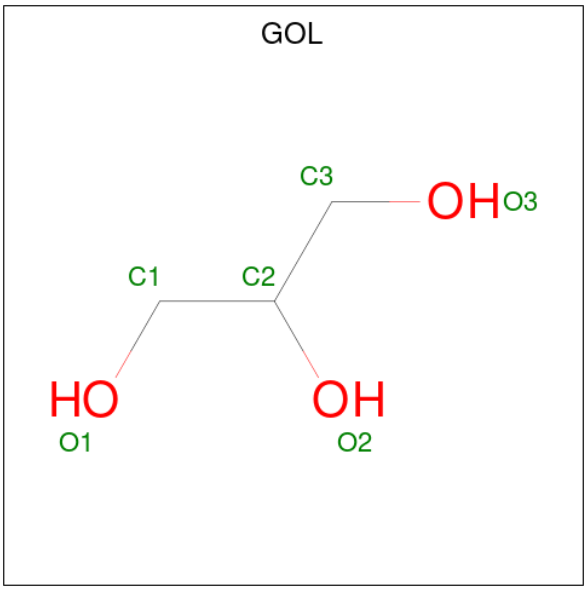
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 6 3 3	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	354	Total O 354 354	0	0
9	B	352	Total O 352 352	0	0
9	C	411	Total O 411 411	0	0
9	D	330	Total O 330 330	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 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.45Å 154.05Å 134.58Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	47.98 – 1.95	Depositor
% Data completeness (in resolution range)	98.0 (47.98-1.95)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.220 , 0.254	Depositor
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.768	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
Total number of atoms	21090	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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 59 ligands modelled in this entry, 8 are monoatomic - leaving 51 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	$\#\|Z\| > 2$
6	EDO	C	2214	-	3,3,3	0.53	0	2,2,2	0.59	0
4	PO4	D	709	-	4,4,4	1.05	0	6,6,6	0.79	0
6	EDO	D	711	-	3,3,3	0.31	0	2,2,2	0.82	0
4	PO4	C	2215	-	4,4,4	0.94	0	6,6,6	0.83	0
6	EDO	D	712	-	3,3,3	0.59	0	2,2,2	0.56	0
6	EDO	C	2210	-	3,3,3	0.58	0	2,2,2	0.51	0
6	EDO	A	713	-	3,3,3	0.43	0	2,2,2	0.31	0
6	EDO	A	706	-	3,3,3	0.74	0	2,2,2	0.24	0
7	ACT	A	715	-	3,3,3	1.22	0	3,3,3	1.37	0
8	GOL	B	711	-	5,5,5	1.81	3 (60%)	5,5,5	1.10	0
4	PO4	D	704	-	4,4,4	0.63	0	6,6,6	0.70	0
6	EDO	B	710	-	3,3,3	0.64	0	2,2,2	0.53	0
6	EDO	A	709	-	3,3,3	0.52	0	2,2,2	0.76	0
6	EDO	A	710	-	3,3,3	0.34	0	2,2,2	0.94	0
6	EDO	A	714	-	3,3,3	0.43	0	2,2,2	0.42	0
8	GOL	B	709	-	5,5,5	0.53	0	5,5,5	1.05	0
4	PO4	C	2207	-	4,4,4	0.72	0	6,6,6	0.68	0
6	EDO	B	706	-	3,3,3	0.25	0	2,2,2	0.37	0
6	EDO	A	708	-	3,3,3	0.56	0	2,2,2	0.25	0
6	EDO	C	2208	-	3,3,3	0.37	0	2,2,2	0.96	0
6	EDO	C	2206	-	3,3,3	0.42	0	2,2,2	0.67	0
7	ACT	C	2201	-	3,3,3	1.43	0	3,3,3	1.25	0
5	0RC	C	2205	3	27,28,28	4.12	13 (48%)	36,42,42	1.49	7 (19%)
5	0RC	A	705	3	27,28,28	4.21	12 (44%)	36,42,42	1.94	6 (16%)
2	PLP	B	701	-	16,16,16	1.24	1 (6%)	20,23,23	1.23	3 (15%)
6	EDO	C	2213	-	3,3,3	0.63	0	2,2,2	0.25	0
5	0RC	D	705	3	27,28,28	4.12	14 (51%)	36,42,42	1.40	5 (13%)
6	EDO	A	716	-	3,3,3	0.43	0	2,2,2	0.95	0
2	PLP	D	702	-	16,16,16	1.20	2 (12%)	20,23,23	1.21	2 (10%)
6	EDO	A	712	-	3,3,3	0.31	0	2,2,2	0.92	0
6	EDO	C	2209	-	3,3,3	0.79	0	2,2,2	0.16	0
6	EDO	D	706	-	3,3,3	0.46	0	2,2,2	0.76	0
6	EDO	A	717	-	3,3,3	0.26	0	2,2,2	0.31	0
4	PO4	B	712	-	4,4,4	0.32	0	6,6,6	0.79	0
7	ACT	A	707	-	3,3,3	1.98	1 (33%)	3,3,3	1.38	0
6	EDO	D	708	-	3,3,3	0.58	0	2,2,2	0.43	0
4	PO4	B	708	-	4,4,4	0.84	0	6,6,6	0.64	0
6	EDO	A	711	-	3,3,3	0.64	0	2,2,2	1.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	PO4	A	704	-	4,4,4	0.88	0	6,6,6	1.04	0
2	PLP	A	701	-	16,16,16	1.16	2 (12%)	20,23,23	1.46	4 (20%)
6	EDO	C	2212	-	3,3,3	0.57	0	2,2,2	0.09	0
4	PO4	C	2204	-	4,4,4	0.64	0	6,6,6	1.24	0
6	EDO	D	710	-	3,3,3	0.62	0	2,2,2	0.06	0
4	PO4	B	704	-	4,4,4	0.86	0	6,6,6	0.84	0
6	EDO	B	707	-	3,3,3	0.40	0	2,2,2	0.43	0
4	PO4	A	718	-	4,4,4	1.04	0	6,6,6	0.62	0
4	PO4	D	714	-	4,4,4	0.41	0	6,6,6	0.70	0
6	EDO	D	713	-	3,3,3	0.61	0	2,2,2	0.39	0
2	PLP	C	2202	-	16,16,16	1.08	1 (6%)	20,23,23	1.09	1 (5%)
6	EDO	D	707	-	3,3,3	0.52	0	2,2,2	0.54	0
5	0RC	B	705	3	27,28,28	4.21	14 (51%)	36,42,42	1.75	8 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	C	2214	-	-	0/1/1/1	-
6	EDO	D	711	-	-	0/1/1/1	-
6	EDO	D	712	-	-	0/1/1/1	-
6	EDO	C	2210	-	-	0/1/1/1	-
6	EDO	A	713	-	-	1/1/1/1	-
8	GOL	B	711	-	-	2/4/4/4	-
2	PLP	C	2202	-	-	2/8/8/8	0/1/1/1
6	EDO	B	710	-	-	1/1/1/1	-
6	EDO	A	709	-	-	1/1/1/1	-
6	EDO	A	710	-	-	0/1/1/1	-
6	EDO	A	714	-	-	1/1/1/1	-
8	GOL	B	709	-	-	2/4/4/4	-
6	EDO	B	706	-	-	1/1/1/1	-
6	EDO	A	708	-	-	0/1/1/1	-
6	EDO	C	2208	-	-	0/1/1/1	-
6	EDO	C	2206	-	-	1/1/1/1	-
5	0RC	C	2205	3	-	2/17/36/36	0/2/2/2
5	0RC	A	705	3	-	4/17/36/36	0/2/2/2
2	PLP	B	701	-	-	1/8/8/8	0/1/1/1
6	EDO	C	2213	-	-	0/1/1/1	-
5	0RC	D	705	3	-	4/17/36/36	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	716	-	-	0/1/1/1	-
2	PLP	D	702	-	-	1/8/8/8	0/1/1/1
6	EDO	A	712	-	-	1/1/1/1	-
6	EDO	C	2209	-	-	0/1/1/1	-
6	EDO	D	706	-	-	1/1/1/1	-
6	EDO	A	717	-	-	0/1/1/1	-
6	EDO	D	708	-	-	0/1/1/1	-
6	EDO	A	711	-	-	0/1/1/1	-
2	PLP	A	701	-	-	1/8/8/8	0/1/1/1
6	EDO	C	2212	-	-	1/1/1/1	-
6	EDO	D	710	-	-	0/1/1/1	-
6	EDO	B	707	-	-	1/1/1/1	-
6	EDO	D	713	-	-	0/1/1/1	-
6	EDO	A	706	-	-	0/1/1/1	-
6	EDO	D	707	-	-	0/1/1/1	-
5	0RC	B	705	3	-	3/17/36/36	0/2/2/2

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2205	0RC	PB-O3A	10.60	1.70	1.58
5	A	705	0RC	PB-O3A	10.40	1.70	1.58
5	B	705	0RC	PB-O3A	9.65	1.69	1.58
5	D	705	0RC	PB-O3A	9.41	1.68	1.58
5	B	705	0RC	C2'-C3'	-7.98	1.31	1.53
5	D	705	0RC	C2'-C3'	-7.98	1.31	1.53
5	A	705	0RC	O4'-C1'	7.83	1.60	1.42
5	C	2205	0RC	C2'-C3'	-7.70	1.32	1.53
5	B	705	0RC	O4'-C4'	-7.69	1.27	1.45
5	D	705	0RC	O4'-C1'	7.58	1.60	1.42
5	B	705	0RC	O4'-C1'	7.54	1.59	1.42
5	A	705	0RC	C2'-C3'	-7.46	1.32	1.53
5	A	705	0RC	O4'-C4'	-7.40	1.28	1.45
5	C	2205	0RC	O4'-C1'	7.17	1.59	1.42
5	D	705	0RC	C3'-C4'	6.98	1.70	1.53
5	D	705	0RC	O4'-C4'	-6.95	1.29	1.45
5	C	2205	0RC	O4'-C4'	-6.83	1.29	1.45
5	C	2205	0RC	C3'-C4'	6.80	1.70	1.53
5	A	705	0RC	C3'-C4'	6.53	1.69	1.53
5	B	705	0RC	C3'-C4'	6.29	1.69	1.53
5	D	705	0RC	C1'-N1	-5.89	1.30	1.47
5	C	2205	0RC	C1'-N1	-5.68	1.31	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	705	0RC	C1'-N1	-5.64	1.31	1.47
5	A	705	0RC	C4-N4	5.51	1.46	1.33
5	B	705	0RC	C1'-N1	-5.46	1.31	1.47
5	B	705	0RC	C4-N4	5.40	1.46	1.33
5	D	705	0RC	C4-N4	5.38	1.46	1.33
5	A	705	0RC	C1B-C14	5.19	1.60	1.53
5	C	2205	0RC	C4-N4	5.06	1.45	1.33
5	B	705	0RC	C2-N1	-5.05	1.29	1.40
5	A	705	0RC	C2-N1	-4.71	1.29	1.40
5	B	705	0RC	C1B-C14	4.70	1.60	1.53
5	B	705	0RC	O2-C2	-4.24	1.15	1.23
5	C	2205	0RC	C2-N1	-4.07	1.31	1.40
5	D	705	0RC	C2-N1	-4.01	1.31	1.40
5	D	705	0RC	O2-C2	-3.95	1.16	1.23
5	C	2205	0RC	C1B-C14	3.78	1.58	1.53
5	D	705	0RC	O5'-C5'	-3.66	1.30	1.44
5	C	2205	0RC	O2-C2	-3.64	1.17	1.23
5	B	705	0RC	O5'-C5'	-3.61	1.30	1.44
5	C	2205	0RC	O5'-C5'	-3.61	1.30	1.44
5	A	705	0RC	O2-C2	-3.42	1.17	1.23
7	A	707	ACT	CH3-C	3.30	1.62	1.49
5	A	705	0RC	O5'-C5'	-3.10	1.32	1.44
2	B	701	PLP	C2-N1	2.86	1.39	1.33
2	A	701	PLP	C4-C5	-2.76	1.38	1.42
5	D	705	0RC	PB-O3B	2.67	1.58	1.51
5	D	705	0RC	C1B-C14	2.61	1.56	1.53
5	D	705	0RC	PA-O1A	2.57	1.60	1.50
8	B	711	GOL	O2-C2	-2.50	1.35	1.43
5	C	2205	0RC	PA-O1A	2.42	1.59	1.50
5	A	705	0RC	PA-O1A	2.38	1.59	1.50
8	B	711	GOL	O3-C3	-2.32	1.32	1.42
2	D	702	PLP	C3-C2	-2.29	1.38	1.40
5	B	705	0RC	C4-N3	-2.19	1.30	1.34
2	C	2202	PLP	C4-C4A	2.19	1.51	1.46
5	D	705	0RC	C4-N3	-2.18	1.30	1.34
2	D	702	PLP	C2-N1	2.16	1.37	1.33
5	B	705	0RC	PA-O1A	2.14	1.58	1.50
5	B	705	0RC	PB-O3B	2.11	1.56	1.51
2	A	701	PLP	C4-C4A	2.09	1.51	1.46
5	C	2205	0RC	PA-O5'	2.08	1.67	1.59
8	B	711	GOL	C1-C2	2.01	1.60	1.51

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	705	0RC	PB-C1B-C14	-7.59	97.86	114.06
5	B	705	0RC	PB-O3A-PA	-4.41	118.57	132.56
5	A	705	0RC	PB-O3A-PA	-4.17	119.35	132.56
5	B	705	0RC	C3'-C2'-C1'	4.03	109.08	101.43
5	B	705	0RC	O4'-C1'-C2'	-3.85	98.26	106.64
5	D	705	0RC	PB-O3A-PA	-3.15	122.58	132.56
2	A	701	PLP	O4A-C4A-C4	-3.12	118.10	124.91
5	B	705	0RC	PB-C1B-C14	-3.10	107.44	114.06
5	A	705	0RC	C3'-C2'-C1'	3.07	107.25	101.43
5	C	2205	0RC	C3'-C2'-C1'	3.02	107.17	101.43
2	D	702	PLP	C5-C6-N1	-2.98	118.85	123.82
5	D	705	0RC	O2-C2-N3	-2.97	117.50	122.33
5	C	2205	0RC	O3B-PB-C1B	2.91	117.38	109.05
5	C	2205	0RC	O2B-PB-O3B	2.88	119.68	110.07
5	C	2205	0RC	PB-O3A-PA	-2.73	123.92	132.56
5	B	705	0RC	O4'-C1'-N1	2.67	114.45	108.36
5	D	705	0RC	O4'-C1'-C2'	-2.64	100.88	106.64
2	C	2202	PLP	O4A-C4A-C4	-2.64	119.16	124.91
2	B	701	PLP	O4A-C4A-C4	-2.59	119.26	124.91
5	A	705	0RC	O4'-C1'-N1	2.55	114.20	108.36
2	B	701	PLP	C5-C6-N1	-2.49	119.67	123.82
5	C	2205	0RC	O4'-C1'-N1	2.42	113.89	108.36
5	B	705	0RC	O2'-C2'-C1'	2.39	118.01	110.02
2	A	701	PLP	O2P-P-O1P	2.38	119.99	110.68
5	A	705	0RC	C5-C4-N3	-2.38	117.28	121.33
2	A	701	PLP	C4-C3-C2	2.35	121.64	120.19
2	A	701	PLP	C2A-C2-C3	2.35	123.79	120.89
5	C	2205	0RC	O2-C2-N3	-2.35	118.51	122.33
5	A	705	0RC	O4'-C4'-C3'	2.33	109.72	105.11
2	D	702	PLP	O4A-C4A-C4	-2.27	119.95	124.91
5	B	705	0RC	O2B-PB-C1B	-2.26	100.40	105.63
2	B	701	PLP	O3P-P-O4P	2.22	112.63	106.73
5	D	705	0RC	C3'-C2'-C1'	2.17	105.55	101.43
5	D	705	0RC	C5'-C4'-C3'	-2.15	107.14	115.18
5	B	705	0RC	C5-C4-N3	-2.14	117.68	121.33
5	C	2205	0RC	O4'-C4'-C3'	2.02	109.11	105.11

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	705	0RC	C14-C1B-PB-O3B
5	A	705	0RC	C14-C1B-PB-O3A

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Mol	Chain	Res	Type	Atoms
5	B	705	0RC	C14-C1B-PB-O3B
5	B	705	0RC	C14-C1B-PB-O2B
5	B	705	0RC	C14-C1B-PB-O3A
5	C	2205	0RC	C14-C1B-PB-O2B
5	D	705	0RC	C5'-O5'-PA-O1A
8	B	709	GOL	O1-C1-C2-C3
8	B	711	GOL	O1-C1-C2-O2
8	B	711	GOL	O1-C1-C2-C3
2	C	2202	PLP	C3-C4-C4A-O4A
2	B	701	PLP	C3-C4-C4A-O4A
6	A	709	EDO	O1-C1-C2-O2
6	A	712	EDO	O1-C1-C2-O2
6	C	2206	EDO	O1-C1-C2-O2
8	B	709	GOL	O1-C1-C2-O2
6	A	714	EDO	O1-C1-C2-O2
6	D	706	EDO	O1-C1-C2-O2
5	A	705	0RC	C14-C1B-PB-O2B
5	D	705	0RC	C5'-O5'-PA-O3A
2	C	2202	PLP	C5-C4-C4A-O4A
5	D	705	0RC	C3'-C4'-C5'-O5'
2	A	701	PLP	C5A-O4P-P-O2P
5	D	705	0RC	O4'-C4'-C5'-O5'
6	A	713	EDO	O1-C1-C2-O2
6	B	706	EDO	O1-C1-C2-O2
6	B	707	EDO	O1-C1-C2-O2
6	B	710	EDO	O1-C1-C2-O2
2	D	702	PLP	C5-C4-C4A-O4A
5	A	705	0RC	C5'-O5'-PA-O1A
5	C	2205	0RC	C5'-O5'-PA-O1A
6	C	2212	EDO	O1-C1-C2-O2

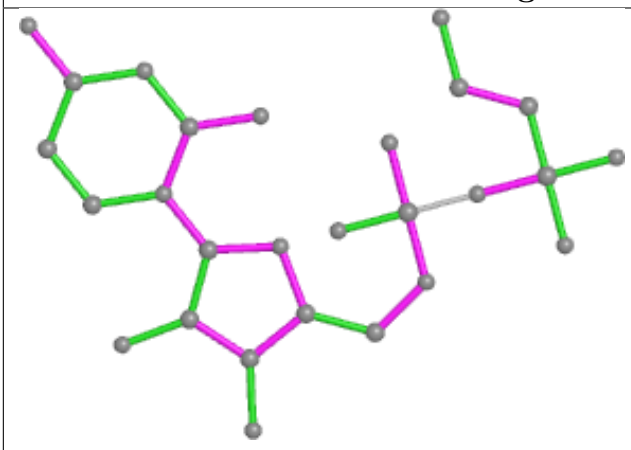
There are no ring outliers.

No monomer is involved in short contacts.

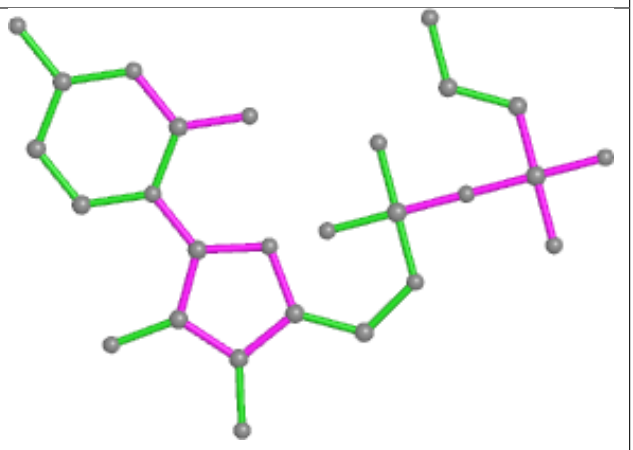
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

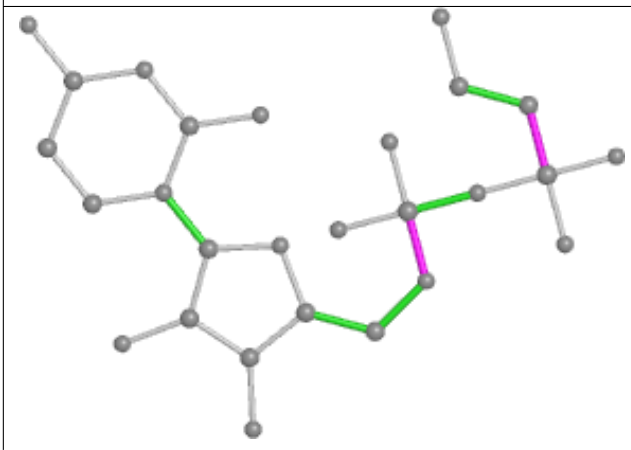
Ligand 0RC C 2205



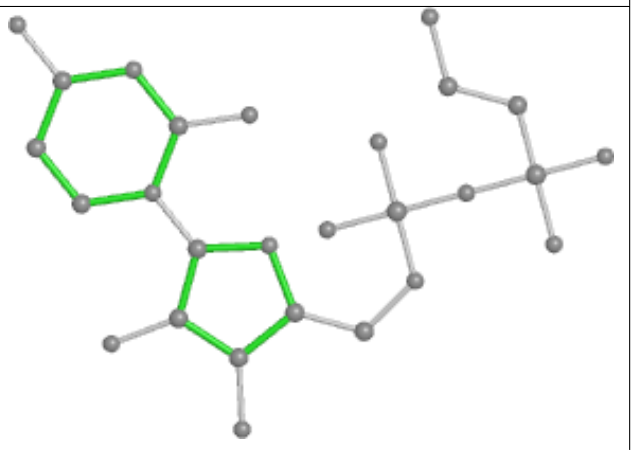
Bond lengths



Bond angles

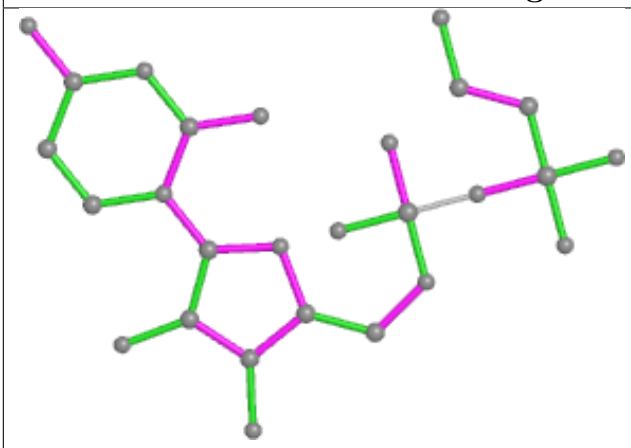


Torsions

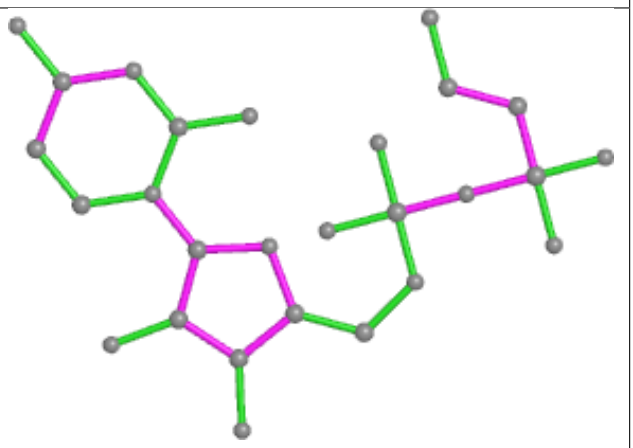


Rings

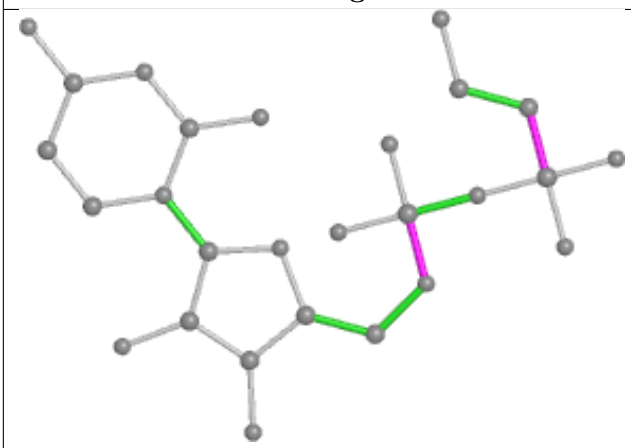
Ligand 0RC A 705



Bond lengths



Bond angles



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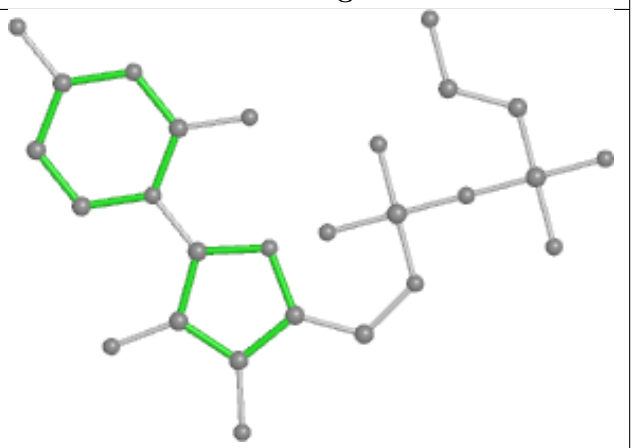
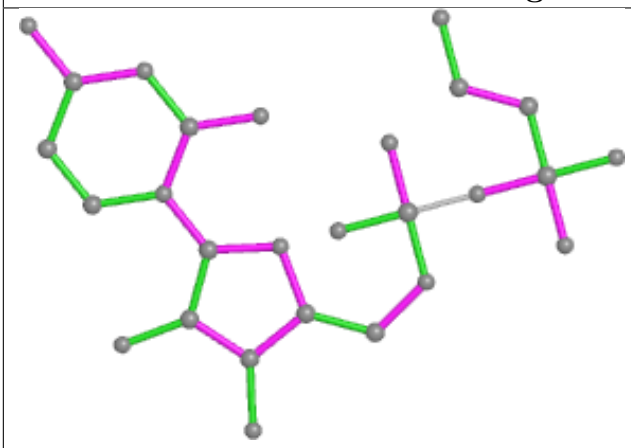
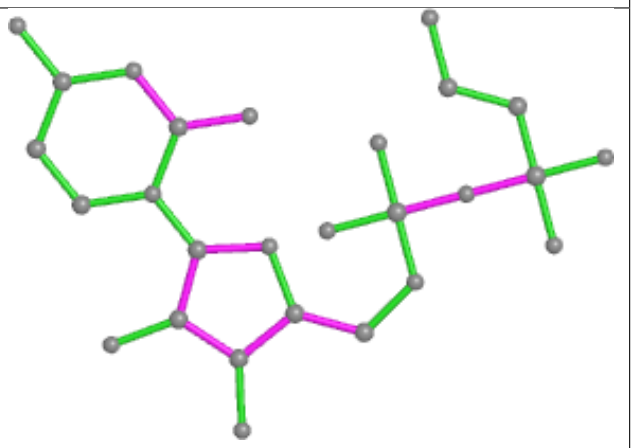


Rings

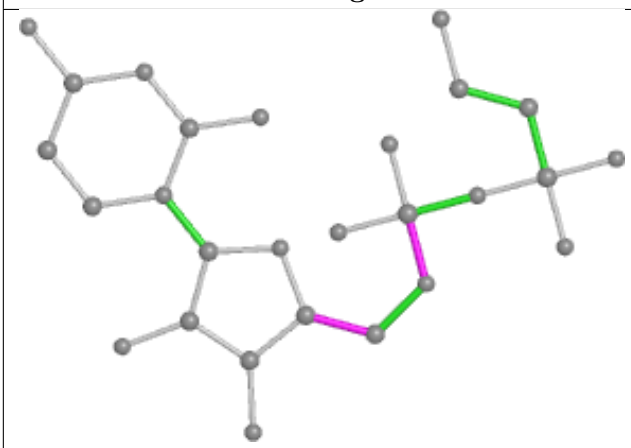
Ligand 0RC D 705



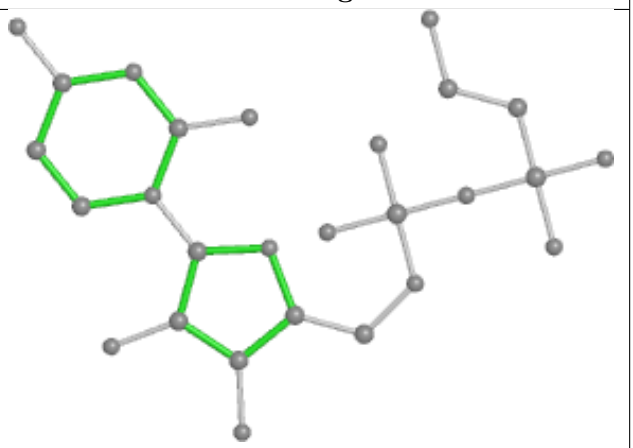
Bond lengths



Bond angles

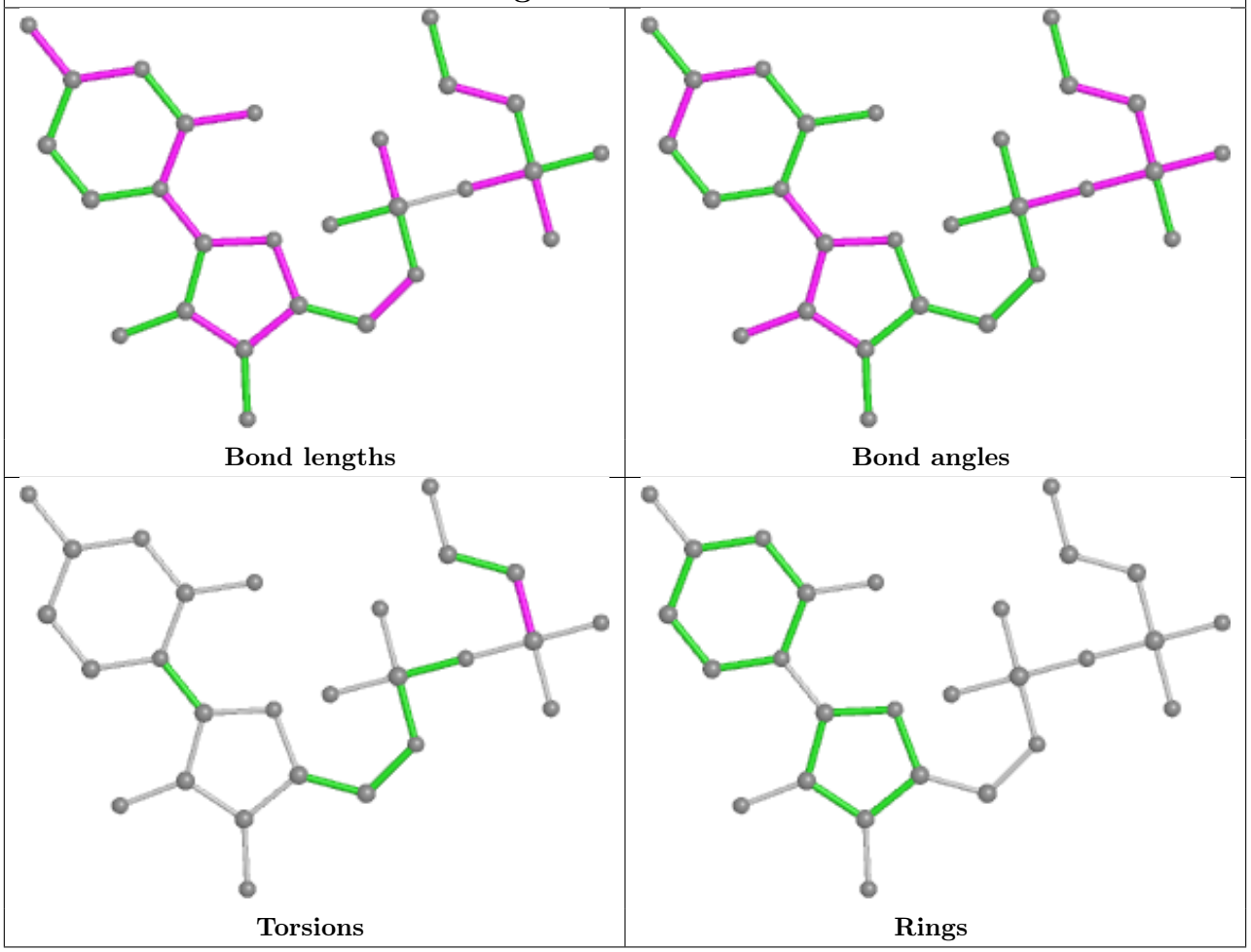


Torsions



Rings

Ligand 0RC B 705



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.