Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2023 – 08:08 PM EDT

PDB ID	:	6Q13
Title	:	CRYSTAL STRUCTURE OF LDHA IN COMPLEX WITH COMPOUND NCGC00420737-09 AT 2.00 A RESOLUTION
Authors	:	Davies, D.R.; Dranow, D.M.
Deposited on	:	2019-08-02
Resolution	:	2.00 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 2.00 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

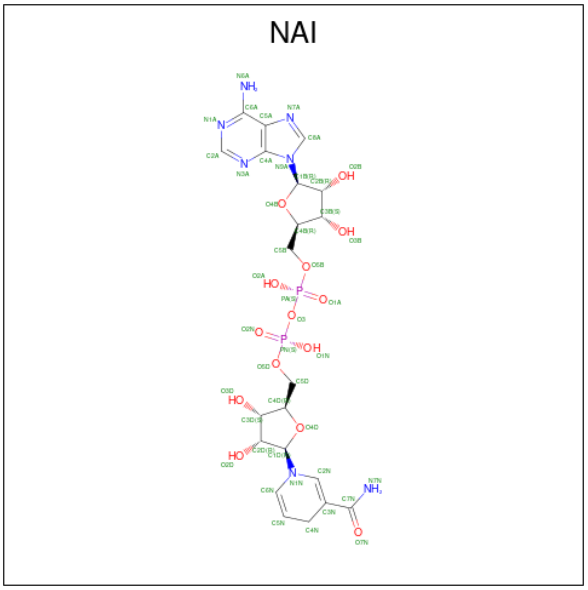
There are 5 unique types of molecules in this entry. The entry contains 11493 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-lactate dehydrogenase A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	2	0
			2533	1617	433	470	13			
1	B	331	Total	C	N	O	S	0	2	0
			2518	1610	427	468	13			
1	C	331	Total	C	N	O	S	0	2	0
			2537	1619	431	474	13			
1	D	331	Total	C	N	O	S	0	3	0
			2522	1604	427	478	13			

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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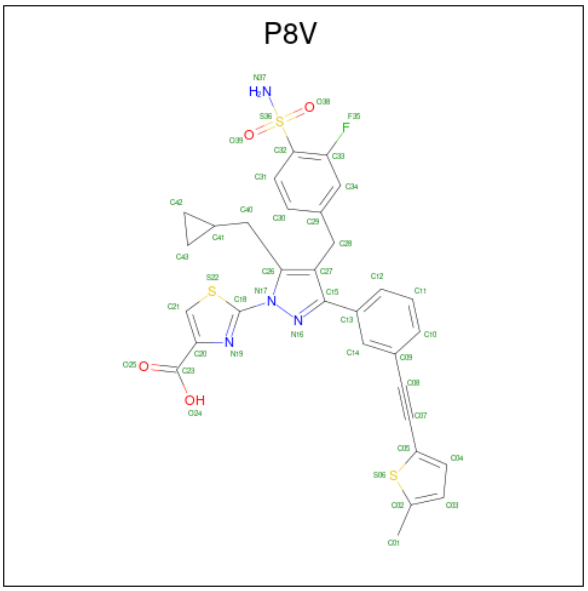
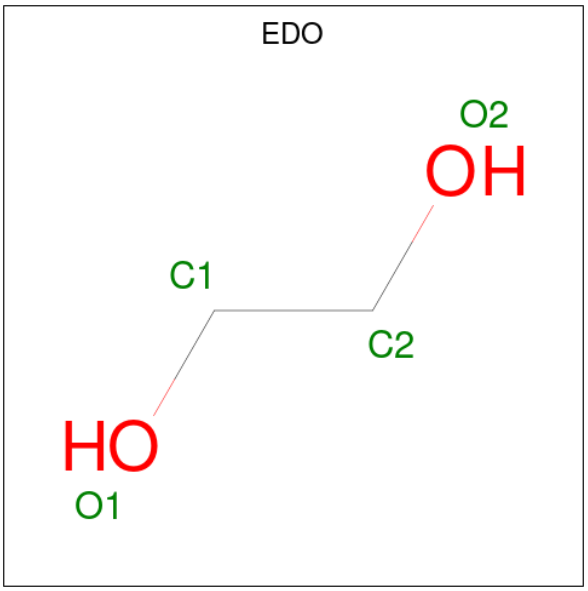
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 2-[5-(cyclopropylmethyl)-4-[(3-fluoro-4-sulfamoylphenyl)methyl]-3-{3-[(5-methylthiophen-2-yl)ethynyl]phenyl}-1H-pyrazol-1-yl]-1,3-thiazole-4-carboxylic acid (three-letter code: P8V) (formula: $C_{31}H_{25}FN_4O_4S_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			43	31	1	4	4	3		
3	B	1	Total	C	F	N	O	S	0	0
			43	31	1	4	4	3		
3	C	1	Total	C	F	N	O	S	0	0
			43	31	1	4	4	3		
3	D	1	Total	C	F	N	O	S	0	0
			43	31	1	4	4	3		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	280	Total O 288 288	0	8
5	B	255	Total O 255 255	0	0
5	C	226	Total O 231 231	0	5
5	D	200	Total O 205 205	0	5

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 2	Depositor
Cell constants a, b, c, α, β, γ	134.80Å 94.74Å 121.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.14 – 2.00	Depositor
% Data completeness (in resolution range)	99.0 (45.14-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.88 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.169 , 0.209	Depositor
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.334	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11493	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.07% 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

22 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	$\#\|Z\| > 2$
4	EDO	A	403	-	3,3,3	0.40	0	2,2,2	0.44	0
4	EDO	D	405	-	3,3,3	0.45	0	2,2,2	0.28	0
2	NAI	B	401	-	42,48,48	4.93	22 (52%)	47,73,73	3.20	8 (17%)
4	EDO	D	407	-	3,3,3	0.53	0	2,2,2	0.33	0
4	EDO	D	403	-	3,3,3	0.50	0	2,2,2	0.25	0
2	NAI	C	401	-	42,48,48	4.98	23 (54%)	47,73,73	3.24	7 (14%)
3	P8V	A	402	-	39,48,48	2.44	8 (20%)	49,71,71	1.19	5 (10%)
3	P8V	B	402	-	39,48,48	2.47	7 (17%)	49,71,71	1.38	7 (14%)
4	EDO	C	404	-	3,3,3	0.71	0	2,2,2	0.32	0
4	EDO	C	406	-	3,3,3	0.46	0	2,2,2	0.40	0
2	NAI	A	401	-	42,48,48	4.80	24 (57%)	47,73,73	3.12	7 (14%)
4	EDO	C	405	-	3,3,3	0.50	0	2,2,2	0.11	0
3	P8V	D	402	-	39,48,48	2.44	7 (17%)	49,71,71	1.54	7 (14%)
4	EDO	D	406	-	3,3,3	0.50	0	2,2,2	0.45	0
4	EDO	A	404	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	A	406	-	3,3,3	0.45	0	2,2,2	0.49	0
4	EDO	A	405	-	3,3,3	0.49	0	2,2,2	0.27	0
4	EDO	C	403	-	3,3,3	0.42	0	2,2,2	0.41	0
4	EDO	D	404	-	3,3,3	0.37	0	2,2,2	0.55	0
2	NAI	D	401	-	42,48,48	5.02	24 (57%)	47,73,73	3.40	8 (17%)
4	EDO	B	403	-	3,3,3	0.47	0	2,2,2	0.39	0
3	P8V	C	402	-	39,48,48	2.45	7 (17%)	49,71,71	1.26	5 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	403	-	-	1/1/1/1	-
4	EDO	D	405	-	-	1/1/1/1	-
2	NAI	B	401	-	-	5/25/72/72	0/5/5/5
4	EDO	D	407	-	-	0/1/1/1	-
4	EDO	D	403	-	-	0/1/1/1	-
2	NAI	C	401	-	-	7/25/72/72	0/5/5/5
3	P8V	A	402	-	-	2/21/33/33	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	P8V	B	402	-	-	2/21/33/33	0/6/6/6
4	EDO	C	404	-	-	1/1/1/1	-
4	EDO	C	406	-	-	0/1/1/1	-
2	NAI	A	401	-	-	5/25/72/72	0/5/5/5
4	EDO	C	405	-	-	0/1/1/1	-
3	P8V	D	402	-	-	2/21/33/33	0/6/6/6
4	EDO	D	406	-	-	1/1/1/1	-
4	EDO	A	404	-	-	0/1/1/1	-
4	EDO	A	406	-	-	1/1/1/1	-
4	EDO	A	405	-	-	0/1/1/1	-
4	EDO	C	403	-	-	1/1/1/1	-
4	EDO	D	404	-	-	0/1/1/1	-
2	NAI	D	401	-	-	5/25/72/72	0/5/5/5
4	EDO	B	403	-	-	1/1/1/1	-
3	P8V	C	402	-	-	2/21/33/33	0/6/6/6

All (122) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	NAI	C2B-C1B	-17.40	1.27	1.53
2	C	401	NAI	C2B-C1B	-16.97	1.28	1.53
2	B	401	NAI	C2B-C1B	-16.77	1.28	1.53
2	A	401	NAI	C2B-C1B	-16.24	1.29	1.53
2	C	401	NAI	C6N-C5N	12.19	1.55	1.33
2	B	401	NAI	C6N-C5N	12.03	1.54	1.33
2	D	401	NAI	C6N-C5N	11.88	1.54	1.33
2	A	401	NAI	C6N-C5N	11.66	1.54	1.33
2	D	401	NAI	O4B-C1B	10.29	1.55	1.41
2	B	401	NAI	C3B-C4B	-9.98	1.27	1.53
2	C	401	NAI	C3B-C4B	-9.98	1.27	1.53
2	C	401	NAI	O4B-C1B	9.89	1.54	1.41
2	D	401	NAI	C3B-C4B	-9.83	1.27	1.53
2	A	401	NAI	C3B-C4B	-9.73	1.28	1.53
2	B	401	NAI	O4B-C1B	9.37	1.54	1.41
2	A	401	NAI	O4B-C1B	8.83	1.53	1.41
3	D	402	P8V	O39-S36	7.94	1.58	1.43
3	B	402	P8V	O38-S36	7.69	1.58	1.43
2	B	401	NAI	O4D-C1D	7.64	1.60	1.42
3	C	402	P8V	C21-S22	7.38	1.82	1.70
3	A	402	P8V	O39-S36	7.37	1.57	1.43
2	B	401	NAI	C2N-C3N	7.30	1.55	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	NAI	C2N-C3N	7.28	1.55	1.34
3	C	402	P8V	O39-S36	7.25	1.57	1.43
2	C	401	NAI	C2D-C1D	-7.20	1.30	1.53
2	D	401	NAI	O4D-C1D	7.19	1.59	1.42
2	A	401	NAI	O4D-C1D	7.19	1.59	1.42
3	C	402	P8V	O38-S36	7.18	1.57	1.43
2	D	401	NAI	C2D-C1D	-7.17	1.30	1.53
2	C	401	NAI	O4D-C1D	7.16	1.59	1.42
2	A	401	NAI	C2D-C1D	-7.15	1.30	1.53
3	A	402	P8V	C21-S22	7.12	1.81	1.70
2	A	401	NAI	C2N-C3N	7.07	1.54	1.34
2	B	401	NAI	C2D-C1D	-7.06	1.30	1.53
3	B	402	P8V	O39-S36	7.04	1.56	1.43
3	D	402	P8V	O38-S36	7.04	1.56	1.43
2	C	401	NAI	C2N-C3N	7.00	1.54	1.34
3	B	402	P8V	C21-S22	6.91	1.81	1.70
3	A	402	P8V	O38-S36	6.79	1.56	1.43
3	D	402	P8V	C21-S22	6.58	1.81	1.70
2	A	401	NAI	C7N-N7N	5.98	1.49	1.33
2	C	401	NAI	C7N-N7N	5.82	1.48	1.33
2	B	401	NAI	C7N-N7N	5.79	1.48	1.33
2	D	401	NAI	O4D-C4D	-5.76	1.32	1.45
2	C	401	NAI	O4D-C4D	-5.74	1.32	1.45
2	D	401	NAI	C7N-N7N	5.70	1.48	1.33
2	B	401	NAI	O4D-C4D	-5.61	1.32	1.45
2	C	401	NAI	O4B-C4B	5.52	1.57	1.45
2	C	401	NAI	C2B-C3B	5.51	1.68	1.53
2	D	401	NAI	O4B-C4B	5.49	1.57	1.45
2	A	401	NAI	O4D-C4D	-5.44	1.32	1.45
2	A	401	NAI	O4B-C4B	5.39	1.57	1.45
2	D	401	NAI	C2B-C3B	5.33	1.67	1.53
2	B	401	NAI	C2B-C3B	5.30	1.67	1.53
3	D	402	P8V	C15-N16	-5.28	1.31	1.35
3	B	402	P8V	C15-N16	-5.20	1.31	1.35
2	B	401	NAI	O4B-C4B	5.17	1.56	1.45
2	A	401	NAI	C2B-C3B	5.07	1.67	1.53
2	C	401	NAI	C6A-N6A	4.74	1.51	1.34
2	D	401	NAI	C6A-N6A	4.73	1.51	1.34
3	C	402	P8V	C15-N16	-4.65	1.31	1.35
3	A	402	P8V	C15-N16	-4.59	1.31	1.35
3	A	402	P8V	S36-N37	4.47	1.69	1.60
2	A	401	NAI	C6A-N6A	4.42	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAI	C6A-N6A	4.36	1.50	1.34
3	C	402	P8V	S36-N37	4.32	1.68	1.60
3	B	402	P8V	S36-N37	4.15	1.68	1.60
2	D	401	NAI	C6N-N1N	3.90	1.47	1.37
2	B	401	NAI	C2A-N3A	3.85	1.38	1.32
2	C	401	NAI	C2A-N3A	3.80	1.38	1.32
3	D	402	P8V	S36-N37	3.79	1.67	1.60
2	A	401	NAI	C6N-N1N	3.75	1.46	1.37
2	C	401	NAI	C6N-N1N	3.73	1.46	1.37
2	A	401	NAI	C2A-N3A	3.73	1.38	1.32
2	B	401	NAI	C6N-N1N	3.73	1.46	1.37
2	D	401	NAI	C2A-N3A	3.54	1.37	1.32
3	A	402	P8V	C02-S06	3.52	1.80	1.74
3	C	402	P8V	C02-S06	3.49	1.80	1.74
2	D	401	NAI	C7N-C3N	3.16	1.55	1.48
2	C	401	NAI	C4N-C5N	3.13	1.57	1.48
3	B	402	P8V	C02-S06	3.12	1.80	1.74
2	B	401	NAI	C7N-C3N	3.10	1.55	1.48
2	C	401	NAI	O2D-C2D	3.09	1.50	1.43
2	D	401	NAI	C4N-C5N	3.08	1.56	1.48
2	B	401	NAI	C4N-C5N	3.07	1.56	1.48
3	D	402	P8V	C02-S06	3.06	1.79	1.74
3	B	402	P8V	C33-C32	-2.97	1.37	1.39
2	A	401	NAI	O2D-C2D	2.92	1.49	1.43
2	A	401	NAI	C4N-C5N	2.91	1.56	1.48
3	A	402	P8V	C20-C23	2.91	1.54	1.50
2	D	401	NAI	O2D-C2D	2.80	1.49	1.43
2	B	401	NAI	O2D-C2D	2.79	1.49	1.43
2	C	401	NAI	C7N-C3N	2.73	1.54	1.48
2	A	401	NAI	C7N-C3N	2.71	1.54	1.48
2	B	401	NAI	O7N-C7N	-2.54	1.18	1.24
2	B	401	NAI	C5A-C4A	-2.48	1.34	1.40
2	D	401	NAI	C5B-C4B	2.48	1.59	1.51
2	A	401	NAI	C5A-C4A	-2.43	1.34	1.40
2	C	401	NAI	C5A-C4A	-2.39	1.34	1.40
2	B	401	NAI	PN-O5D	2.38	1.68	1.59
2	C	401	NAI	C5B-C4B	2.38	1.59	1.51
2	D	401	NAI	C5A-C4A	-2.34	1.34	1.40
2	D	401	NAI	PN-O5D	2.29	1.68	1.59
2	C	401	NAI	O7N-C7N	-2.27	1.19	1.24
3	C	402	P8V	C20-C23	2.27	1.54	1.50
2	B	401	NAI	C4N-C3N	2.27	1.54	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	P8V	C33-C32	-2.24	1.37	1.39
2	D	401	NAI	C4N-C3N	2.23	1.54	1.49
2	A	401	NAI	O3B-C3B	2.17	1.48	1.43
2	D	401	NAI	O7N-C7N	-2.15	1.19	1.24
2	B	401	NAI	C5B-C4B	2.12	1.58	1.51
2	A	401	NAI	O3D-C3D	-2.12	1.38	1.43
2	A	401	NAI	C4N-C3N	2.11	1.54	1.49
2	D	401	NAI	O3D-C3D	-2.10	1.38	1.43
2	D	401	NAI	O3B-C3B	2.10	1.47	1.43
2	C	401	NAI	PN-O5D	2.08	1.67	1.59
2	A	401	NAI	C2A-N1A	2.07	1.37	1.33
2	C	401	NAI	O3D-C3D	-2.07	1.38	1.43
2	C	401	NAI	C4N-C3N	2.06	1.54	1.49
2	A	401	NAI	C5B-C4B	2.05	1.58	1.51
2	A	401	NAI	PN-O5D	2.04	1.67	1.59
3	A	402	P8V	O24-C23	-2.03	1.24	1.30

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	NAI	C5A-C6A-N6A	15.96	144.60	120.35
2	C	401	NAI	C5A-C6A-N6A	15.18	143.42	120.35
2	B	401	NAI	C5A-C6A-N6A	14.82	142.88	120.35
2	A	401	NAI	C5A-C6A-N6A	14.08	141.75	120.35
2	D	401	NAI	N6A-C6A-N1A	-11.14	95.46	118.57
2	B	401	NAI	N6A-C6A-N1A	-10.62	96.53	118.57
2	C	401	NAI	N6A-C6A-N1A	-10.46	96.86	118.57
2	A	401	NAI	N6A-C6A-N1A	-9.84	98.15	118.57
2	D	401	NAI	C1B-N9A-C4A	-9.09	110.68	126.64
2	C	401	NAI	C1B-N9A-C4A	-9.01	110.82	126.64
2	A	401	NAI	C1B-N9A-C4A	-8.53	111.65	126.64
2	B	401	NAI	C1B-N9A-C4A	-7.63	113.24	126.64
2	D	401	NAI	N3A-C2A-N1A	-5.48	120.12	128.68
2	A	401	NAI	N3A-C2A-N1A	-5.20	120.55	128.68
2	B	401	NAI	N3A-C2A-N1A	-5.20	120.55	128.68
3	D	402	P8V	C28-C27-C26	-4.94	122.05	126.41
2	C	401	NAI	N3A-C2A-N1A	-4.88	121.05	128.68
2	B	401	NAI	O4B-C1B-C2B	-4.81	99.90	106.93
3	B	402	P8V	O24-C23-O25	3.89	131.98	123.35
3	C	402	P8V	O24-C23-O25	3.84	131.86	123.35
2	A	401	NAI	O4B-C1B-C2B	-3.82	101.34	106.93
3	D	402	P8V	O24-C23-O25	3.79	131.75	123.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	402	P8V	O25-C23-C20	-3.69	113.76	121.24
3	B	402	P8V	O25-C23-C20	-3.64	113.85	121.24
3	D	402	P8V	O38-S36-N37	3.59	112.69	107.36
3	C	402	P8V	C28-C27-C26	-3.54	123.29	126.41
3	A	402	P8V	O24-C23-O25	3.46	131.03	123.35
3	D	402	P8V	O25-C23-C20	-3.33	114.48	121.24
3	B	402	P8V	C31-C32-C33	3.29	120.62	118.43
3	A	402	P8V	O25-C23-C20	-3.19	114.77	121.24
3	D	402	P8V	C40-C26-C27	-3.10	125.06	130.34
3	A	402	P8V	C40-C26-C27	-3.01	125.19	130.34
3	D	402	P8V	C28-C27-C15	3.01	131.93	127.36
3	B	402	P8V	C34-C33-C32	-2.97	121.38	123.10
2	D	401	NAI	O4B-C1B-C2B	-2.95	102.61	106.93
3	B	402	P8V	C28-C27-C26	-2.73	124.00	126.41
3	C	402	P8V	C40-C26-C27	-2.66	125.80	130.34
2	D	401	NAI	C3B-C2B-C1B	2.61	104.91	100.98
3	D	402	P8V	C31-C32-C33	2.52	120.11	118.43
3	A	402	P8V	C28-C27-C15	2.47	131.12	127.36
3	A	402	P8V	C13-C15-N16	-2.39	116.69	120.78
3	B	402	P8V	C28-C27-C15	2.33	130.89	127.36
2	A	401	NAI	C4D-O4D-C1D	-2.31	104.38	109.47
2	A	401	NAI	O4B-C4B-C5B	-2.28	101.88	109.37
3	C	402	P8V	C28-C27-C15	2.25	130.78	127.36
3	B	402	P8V	C40-C26-C27	-2.22	126.55	130.34
2	C	401	NAI	O4B-C1B-C2B	-2.20	103.72	106.93
2	B	401	NAI	O4D-C1D-C2D	-2.17	101.91	106.64
2	D	401	NAI	C4D-O4D-C1D	-2.16	104.71	109.47
2	C	401	NAI	C4D-O4D-C1D	-2.14	104.74	109.47
2	B	401	NAI	C4D-O4D-C1D	-2.14	104.76	109.47
2	B	401	NAI	C3B-C2B-C1B	2.09	104.12	100.98
2	C	401	NAI	PN-O3-PA	-2.05	125.79	132.83
2	D	401	NAI	O4D-C1D-C2D	-2.00	102.28	106.64

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	P8V	C12-C13-C15-C27
3	A	402	P8V	C14-C13-C15-C27
3	B	402	P8V	C12-C13-C15-C27
3	B	402	P8V	C14-C13-C15-C27
3	C	402	P8V	C12-C13-C15-C27

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Mol	Chain	Res	Type	Atoms
3	C	402	P8V	C14-C13-C15-C27
3	D	402	P8V	C12-C13-C15-C27
3	D	402	P8V	C14-C13-C15-C27
4	C	404	EDO	O1-C1-C2-O2
2	D	401	NAI	C2D-C1D-N1N-C2N
2	C	401	NAI	C2D-C1D-N1N-C2N
2	B	401	NAI	C2D-C1D-N1N-C2N
2	D	401	NAI	C2D-C1D-N1N-C6N
2	A	401	NAI	C2D-C1D-N1N-C2N
4	B	403	EDO	O1-C1-C2-O2
4	C	403	EDO	O1-C1-C2-O2
2	C	401	NAI	C2D-C1D-N1N-C6N
2	C	401	NAI	C5B-O5B-PA-O2A
2	B	401	NAI	O4D-C1D-N1N-C2N
2	A	401	NAI	C2D-C1D-N1N-C6N
2	A	401	NAI	O4D-C1D-N1N-C2N
2	D	401	NAI	O4D-C1D-N1N-C2N
2	B	401	NAI	C2D-C1D-N1N-C6N
2	C	401	NAI	O4D-C1D-N1N-C2N
4	A	406	EDO	O1-C1-C2-O2
4	D	406	EDO	O1-C1-C2-O2
2	A	401	NAI	O4B-C4B-C5B-O5B
2	C	401	NAI	O4B-C4B-C5B-O5B
2	B	401	NAI	O4B-C4B-C5B-O5B
2	A	401	NAI	O4D-C1D-N1N-C6N
2	D	401	NAI	O4D-C1D-N1N-C6N
4	D	405	EDO	O1-C1-C2-O2
2	B	401	NAI	O4D-C1D-N1N-C6N
2	C	401	NAI	O4D-C1D-N1N-C6N
2	C	401	NAI	C5B-O5B-PA-O3
2	D	401	NAI	O4B-C4B-C5B-O5B
4	A	403	EDO	O1-C1-C2-O2

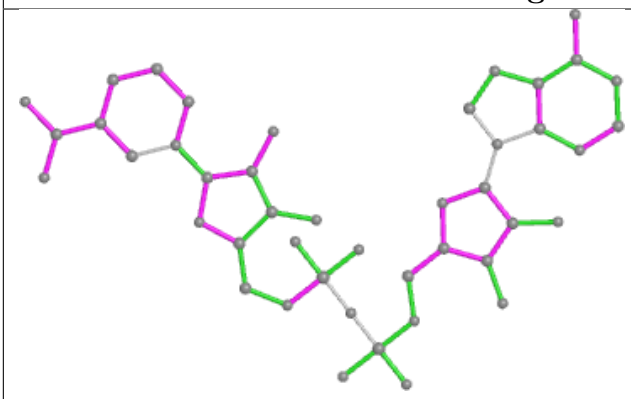
There are no ring outliers.

No monomer is involved in short contacts.

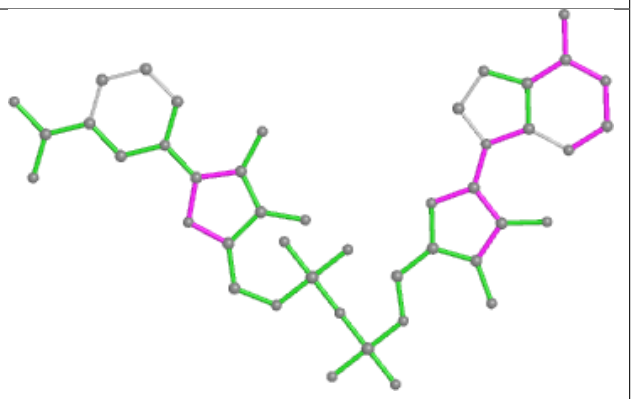
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

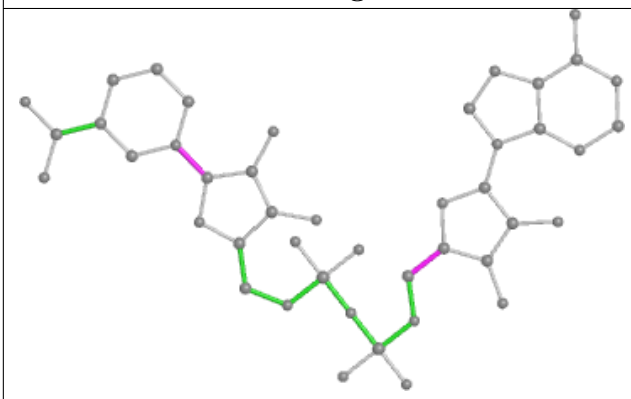
Ligand NAI B 401



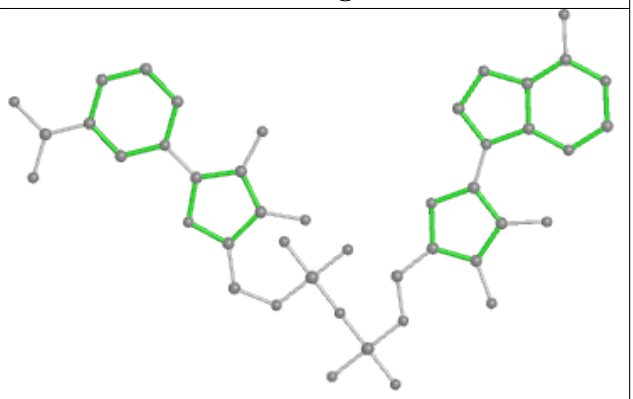
Bond lengths



Bond angles

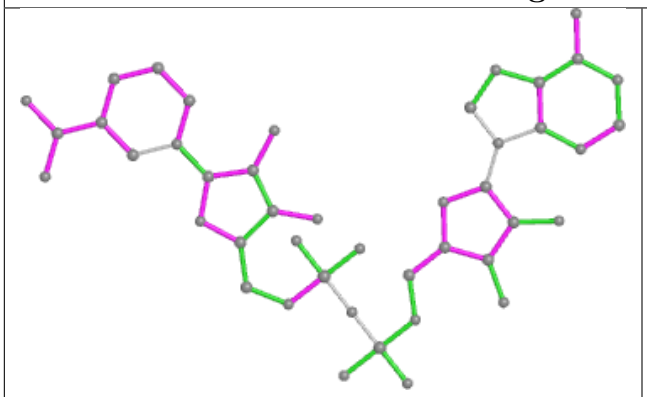


Torsions



Rings

Ligand NAI C 401



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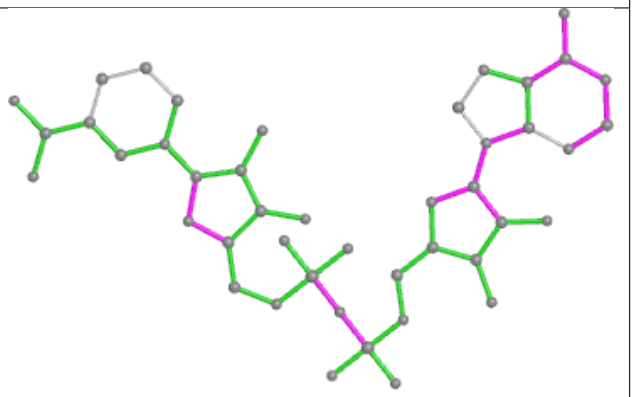
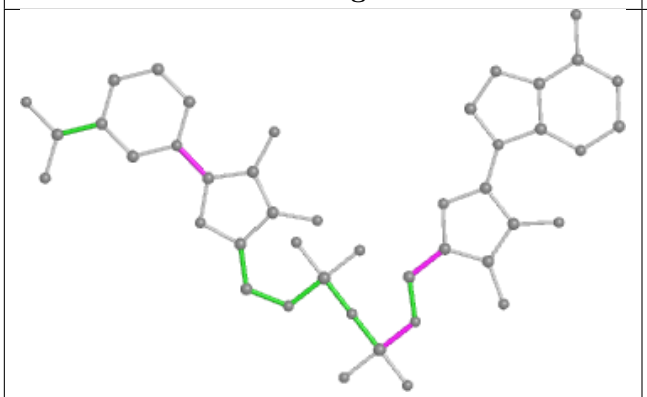


Bond angles



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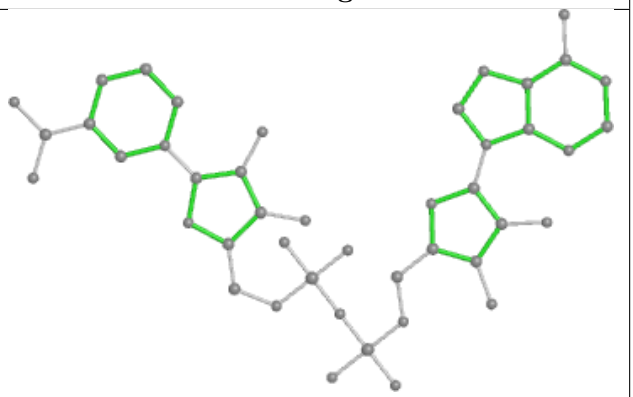
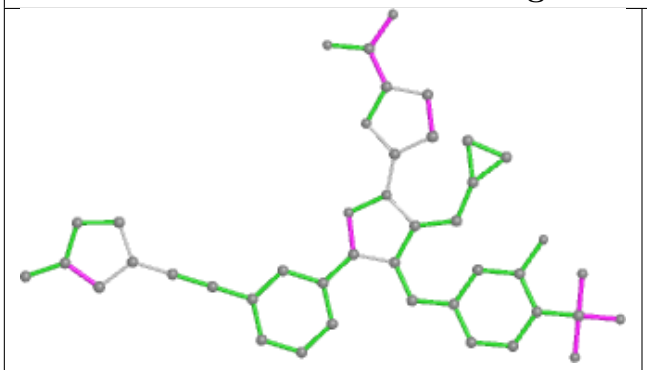
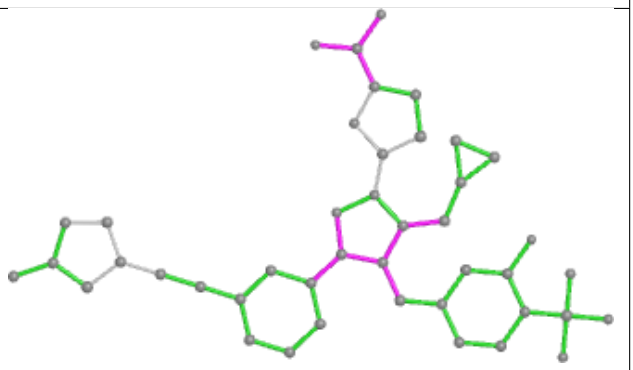


Rings

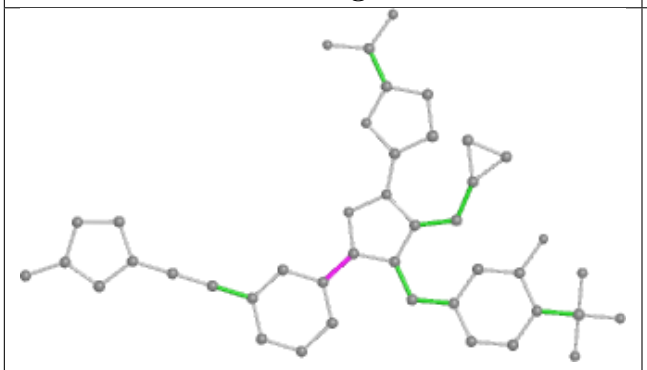
Ligand P8V A 402



Bond lengths



Bond angles



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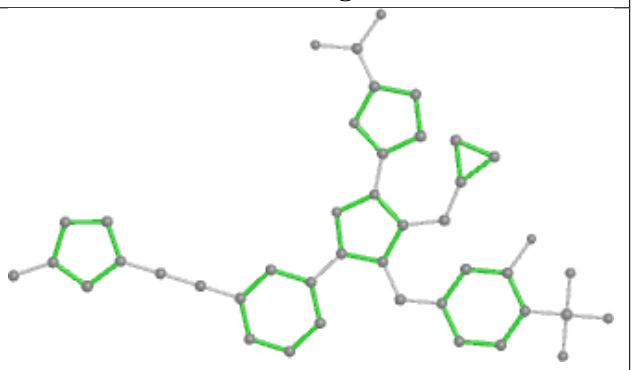
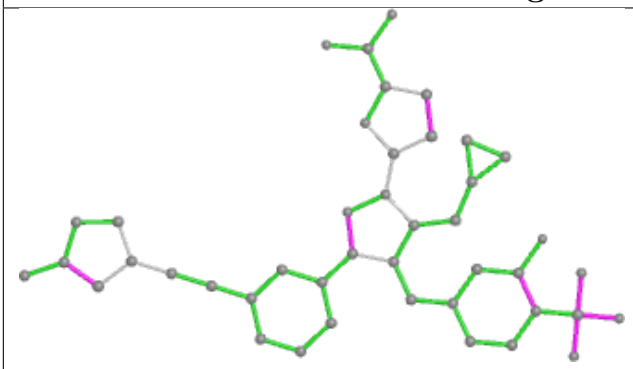
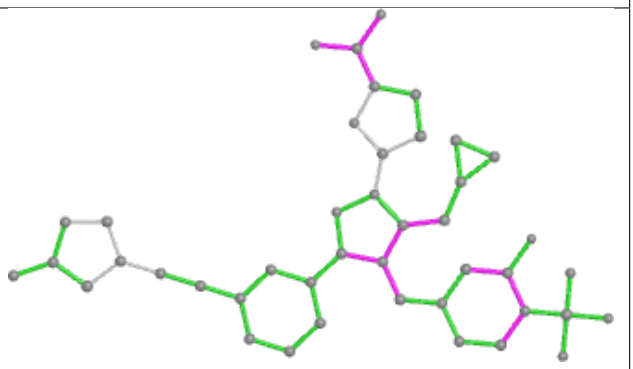


Rings

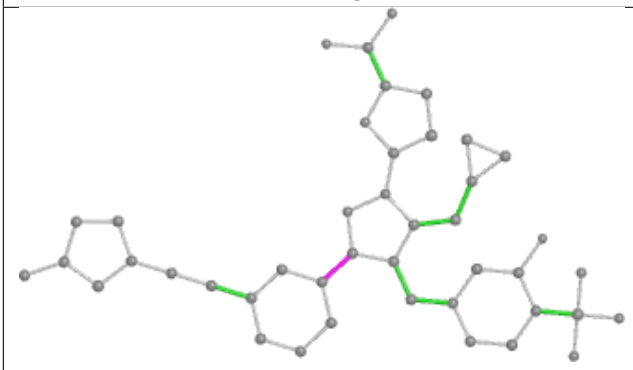
Ligand P8V B 402



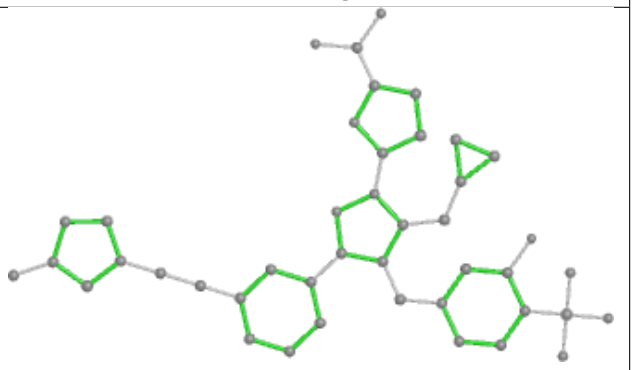
Bond lengths



Bond angles

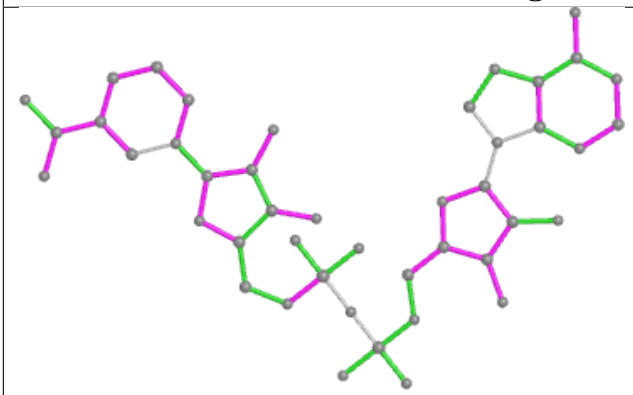


Torsions

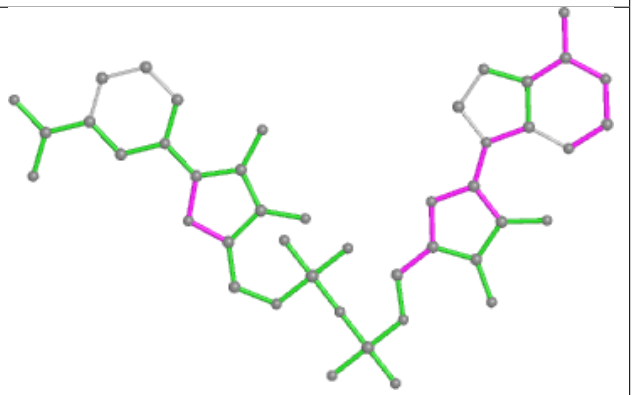


Rings

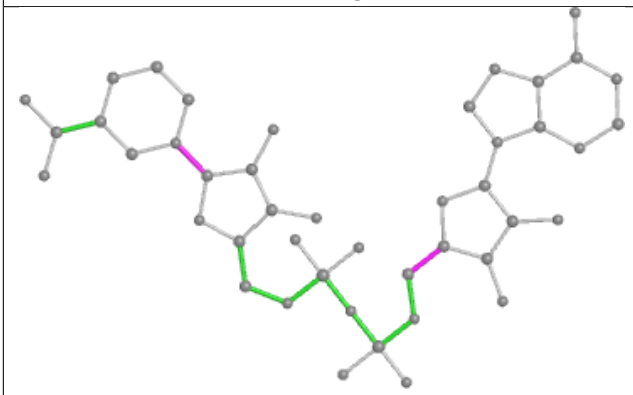
Ligand NAI A 401



Bond lengths



Bond angles



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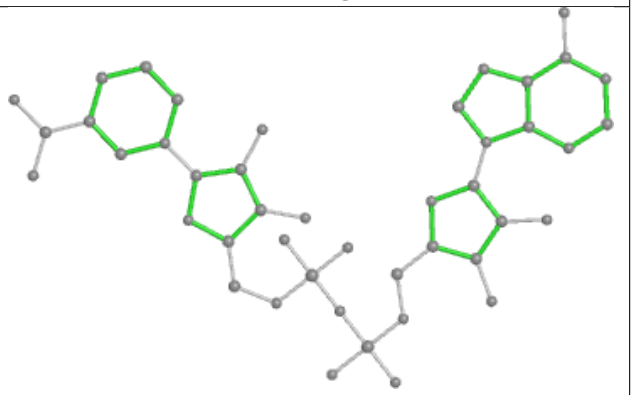
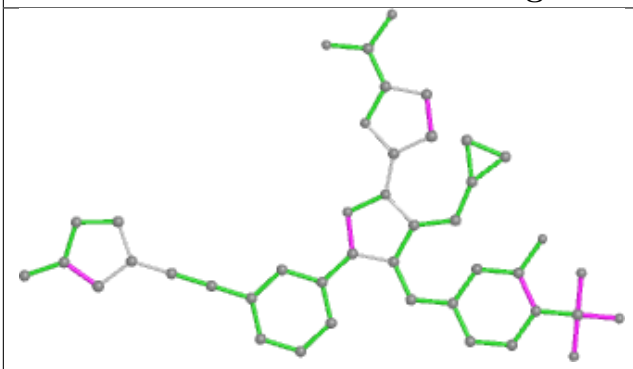


Rings

Ligand P8V D 402



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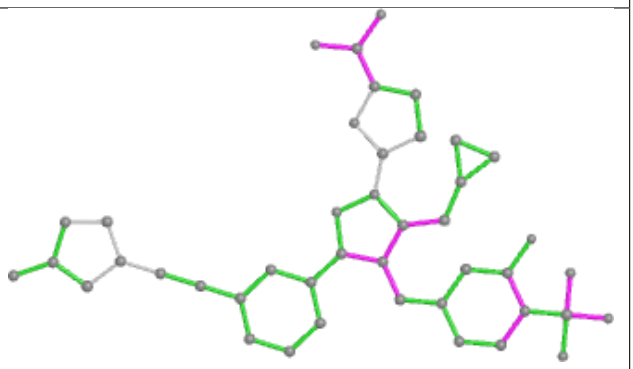
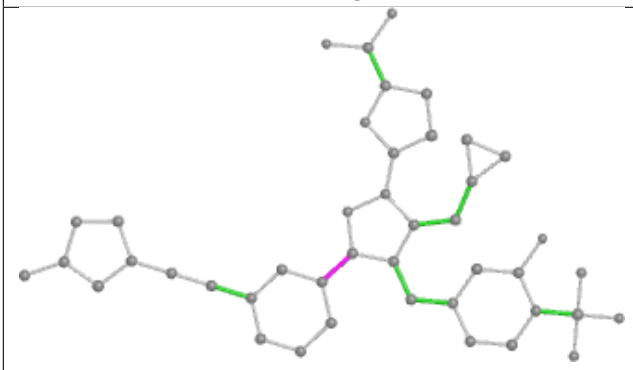


Bond angles



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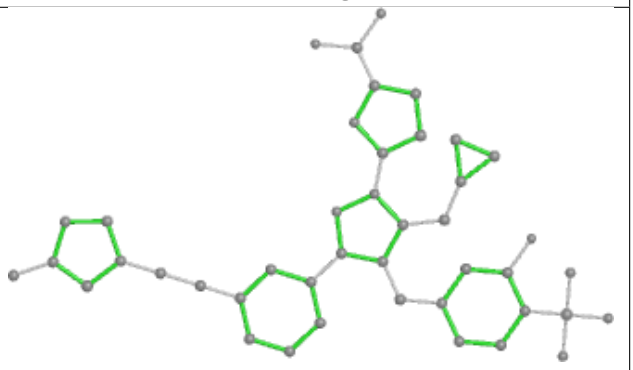
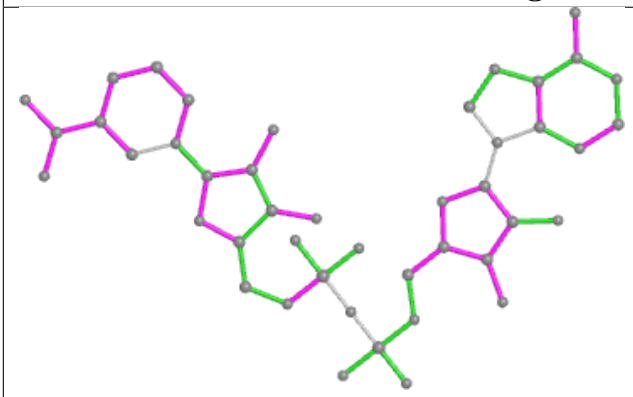


Rings

Ligand NAI D 401



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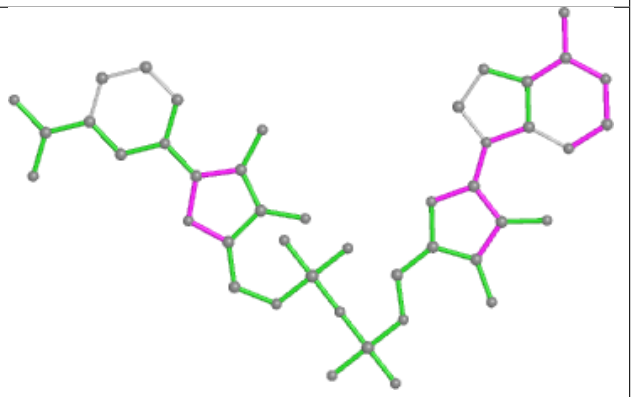
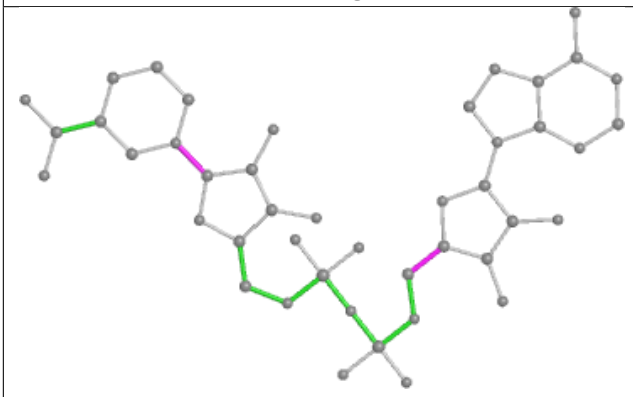


Bond angles



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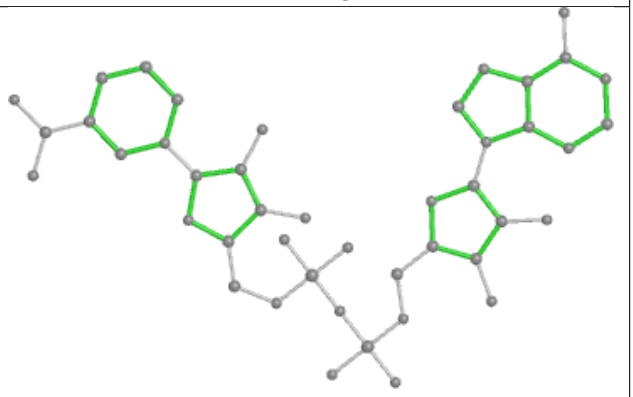
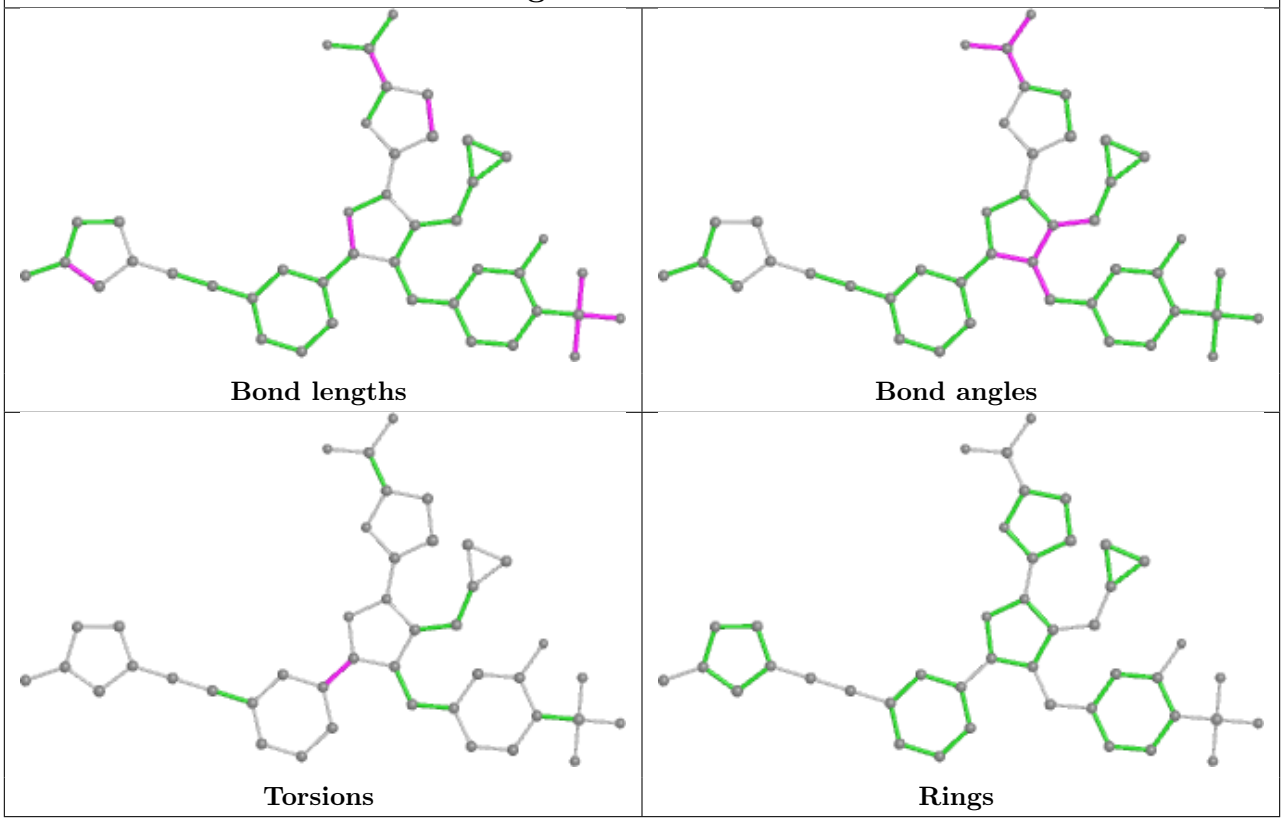


Rings

Ligand P8V C 402



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.