Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 07:46 am BST

PDB ID	:	2W3B
Title	:	HUMAN DIHYDROFOLATE REDUCTASE COMPLEXED WITH NADPH AND A LIPOPHILIC ANTIFOLATE SELECTIVE FOR MYCOBACTERIUM AVIUM DHFR, 6-((2,5- DIETHOXYPHENYL)AMINOMETHYL)-2,4-DIAMINO-5-METHYLPYRIDO(2,3-D) PYRIMIDINE (SRI-8686)
Authors	:	Leung, A.K.W.; Reynolds, R.C.; Borhani, D.W.
Deposited on	:	2008-11-11
Resolution	:	1.27 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 following versions of software and data (see references (i)) were used in the production of this report:

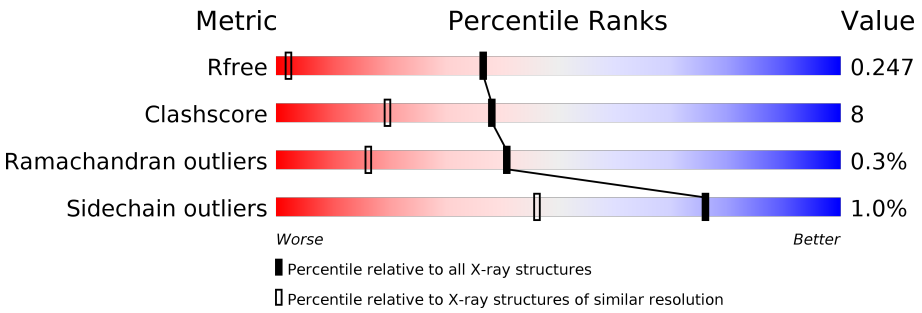
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.27 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1850 (1.30-1.26)
Clashscore	141614	1926 (1.30-1.26)
Ramachandran outliers	138981	1860 (1.30-1.26)
Sidechain outliers	138945	1859 (1.30-1.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	187	87% 11% ••
1	B	187	94% 6% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	VG9	A	301[A]	-	-	X	-

2 Entry composition (i)

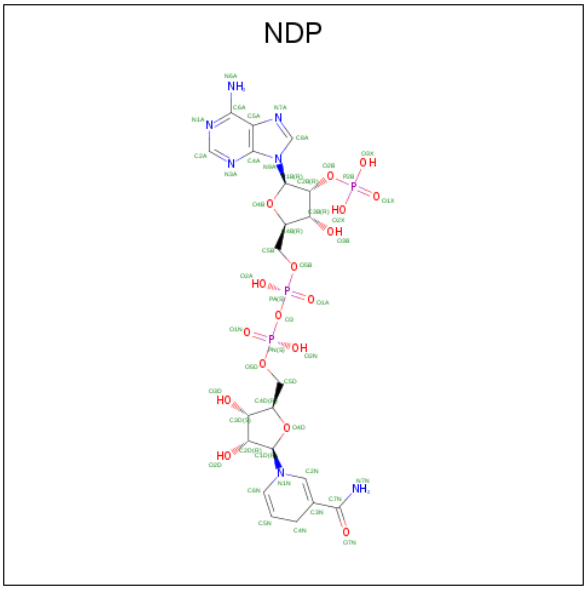
There are 6 unique types of molecules in this entry. The entry contains 3848 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DIHYDROFOLATE REDUCTASE.

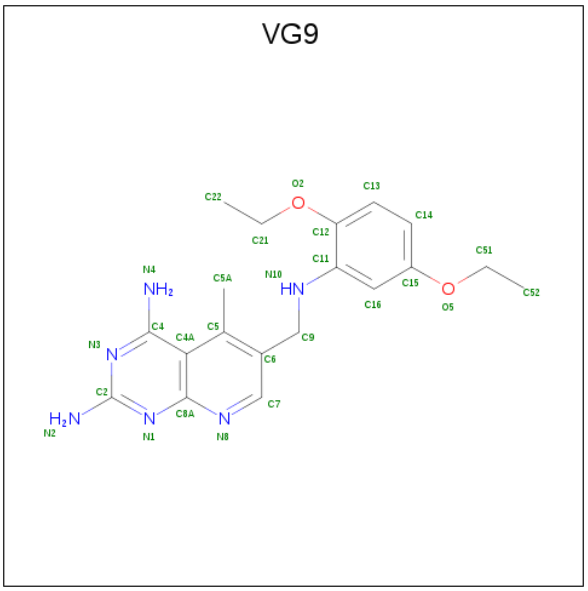
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	185	1549	996	258	288	7	0	11	0
1	B	186	1506	975	248	275	8	0	8	1

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



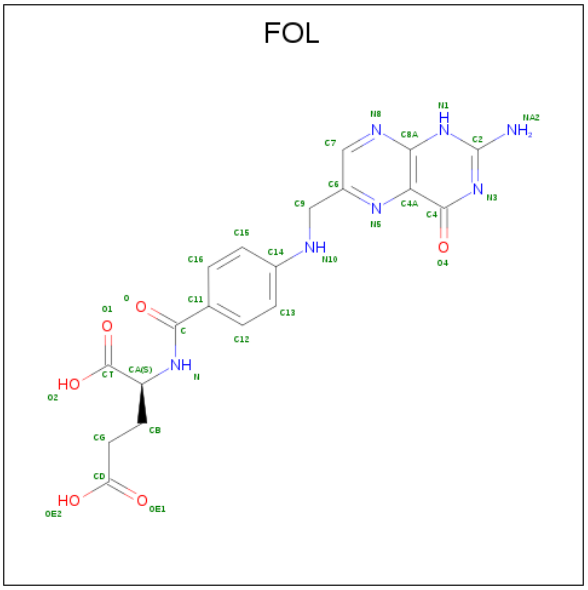
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0
2	B	1	48	21	7	17	3	0	0

- Molecule 3 is 6-{[(2,5-DIETHOXYPHENYL)AMINO]METHYL}-5-METHYLPYRIDO[2,3-D]PYRIMIDINE-2,4-DIAMINE (three-letter code: VG9) (formula: $C_{19}H_{24}N_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	27	19	6	2	0	1
			Total	C	N	O		
3	B	1	27	19	6	2	0	1

- Molecule 4 is FOLIC ACID (three-letter code: FOL) (formula: $C_{19}H_{19}N_7O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	32	19	7	6	0	1
			Total	C	N	O		
4	B	1	32	19	7	6	0	1

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
5	B	1	1	1	0	0
			Total	K		
5	A	1	1	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	306	310	310	0	4
			Total	O		
6	B	267	267	267	0	0

3 Residue-property plots (i)

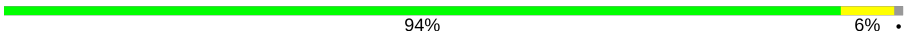
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DIHYDROFOLATE REDUCTASE

Chain A:

- Molecule 1: DIHYDROFOLATE REDUCTASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	87.72Å 94.39Å 95.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.95 – 1.27 14.94 – 1.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (14.95-1.27) 99.7 (14.94-1.25)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 1.25Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.171 , 0.203 0.217 , 0.247	Depositor DCC
R_{free} test set	5467 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	16.2	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3848	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FOL, NDP, K, VG9

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.57	0/1595	0.78	2/2156 (0.1%)
1	B	0.54	0/1542	0.67	0/2087
All	All	0.56	0/3137	0.73	2/4243 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	65	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	21	ASP	CB-CG-OD1	5.35	123.12	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1549	0	1530	27	0
1	B	1506	0	1484	11	0
2	A	48	0	26	3	0
2	B	48	0	26	4	0
3	A	27	0	24	10	0
3	B	27	0	24	6	0
4	A	32	0	17	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	32	0	17	5	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	310	0	0	7	0
6	B	267	0	0	4	0
All	All	3848	0	3148	49	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (49) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ASP:OD1	3:A:301[A]:VG9:H222	1.65	0.94
1:B:132:LYS:NZ	1:B:162:TYR:OH	2.00	0.93
2:A:201:NDP:H42N	4:A:401[B]:FOL:C7	2.02	0.90
2:B:201:NDP:H42N	4:B:401[B]:FOL:C7	2.08	0.83
3:A:301[A]:VG9:H223	6:A:2305:HOH:O	1.79	0.82
3:B:301[A]:VG9:H42N	3:B:301[A]:VG9:H5A1	1.46	0.81
3:A:301[A]:VG9:H5A1	3:A:301[A]:VG9:H42N	1.44	0.81
1:A:79:LEU:HA	1:A:80:LYS:CB	2.19	0.73
1:B:162:TYR:HE2	6:B:2163:HOH:O	1.70	0.73
1:A:79:LEU:HA	1:A:80:LYS:HB2	1.72	0.70
1:A:115:VAL:O	4:A:401[B]:FOL:H7	1.93	0.69
1:A:79:LEU:O	6:A:2160:HOH:O	2.09	0.69
1:B:119[B]:SER:OG	2:B:201:NDP:N7A	2.31	0.64
2:A:201:NDP:H42N	4:A:401[B]:FOL:C6	2.28	0.63
3:A:301[A]:VG9:C22	6:A:2305:HOH:O	2.42	0.60
3:B:301[A]:VG9:H222	6:B:2038:HOH:O	2.04	0.58
1:A:19:ASN:OD1	1:B:178:LYS:NZ	2.36	0.57
1:A:79:LEU:CA	1:A:80:LYS:CB	2.82	0.56
3:B:301[A]:VG9:N4	3:B:301[A]:VG9:H5A1	2.14	0.55
3:B:301[A]:VG9:H221	6:B:2012:HOH:O	2.05	0.55
1:A:80:LYS:NZ	6:A:2161:HOH:O	2.41	0.54
1:B:16:ILE:O	2:B:201:NDP:H2N	2.07	0.54
1:B:115:VAL:O	4:B:401[B]:FOL:H7	2.07	0.54
1:A:79:LEU:CA	1:A:80:LYS:HB3	2.37	0.54
1:B:70:ARG:HH12	3:B:301[A]:VG9:H522	1.72	0.54
1:A:22:LEU:HG	3:A:301[A]:VG9:C22	2.37	0.54
1:A:21:ASP:OD1	3:A:301[A]:VG9:C22	2.49	0.52
3:A:301[A]:VG9:H5A1	3:A:301[A]:VG9:N4	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LYS:HD3	6:A:2163:HOH:O	2.10	0.51
1:A:16:ILE:O	2:A:201:NDP:H2N	2.12	0.50
1:B:30:GLU:OE1	4:B:401[B]:FOL:N3	2.45	0.49
1:A:79:LEU:HA	1:A:80:LYS:HB3	1.90	0.49
1:A:21:ASP:HA	3:A:301[A]:VG9:H221	1.95	0.48
1:B:31:PHE:HE1	3:B:301[A]:VG9:H7	1.78	0.48
1:A:80:LYS:HG2	1:A:81:GLU:HG2	1.96	0.48
1:A:10[B]:VAL:CG2	1:A:14:MET:HA	2.44	0.47
1:B:34:PHE:CE2	4:B:401[B]:FOL:H16	2.51	0.46
1:A:22:LEU:HG	3:A:301[A]:VG9:H223	1.97	0.46
1:A:79:LEU:HB3	1:A:80:LYS:HB3	1.97	0.46
1:A:114:ILE:HG23	1:A:120:VAL:HG12	1.98	0.46
1:A:32[B]:ARG:HG3	6:A:2078:HOH:O	2.16	0.46
2:B:201:NDP:H42N	4:B:401[B]:FOL:C6	2.45	0.45
1:A:34:PHE:CE2	4:A:401[B]:FOL:H16	2.52	0.45
1:A:22:LEU:HG	3:A:301[A]:VG9:H222	1.99	0.43
1:A:102:GLN:HB3	1:A:103:PRO:CD	2.49	0.43
1:A:148:PHE:HA	6:A:2235:HOH:O	2.19	0.42
1:A:30:GLU:OE1	4:A:401[B]:FOL:N3	2.53	0.42
1:A:130:HIS:HE1	1:A:132:LYS:NZ	2.19	0.41
1:B:162:TYR:HE1	6:B:2256:HOH:O	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	194/187 (104%)	191 (98%)	2 (1%)	1 (0%)	29 6
1	B	192/187 (103%)	190 (99%)	2 (1%)	0	100 100
All	All	386/374 (103%)	381 (99%)	4 (1%)	1 (0%)	41 16

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	171/169 (101%)	168 (98%)	3 (2%)	59	22
1	B	161/169 (95%)	160 (99%)	1 (1%)	86	64
All	All	332/338 (98%)	328 (99%)	4 (1%)	76	38

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94[A]	ASP
1	A	94[B]	ASP
1	A	131	LEU
1	B	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	B	35	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
4	FOL	B	401[B]	-	28,34,34	2.19	5 (17%)	36,47,47	1.84	10 (27%)
3	VG9	B	301[A]	-	29,29,29	0.67	0	37,40,40	1.82	9 (24%)
3	VG9	A	301[A]	-	29,29,29	0.58	0	37,40,40	1.75	7 (18%)
2	NDP	B	201	-	45,52,52	1.33	5 (11%)	53,80,80	1.41	7 (13%)
4	FOL	A	401[B]	-	28,34,34	2.09	5 (17%)	36,47,47	1.58	6 (16%)
2	NDP	A	201	-	45,52,52	1.24	4 (8%)	53,80,80	1.32	6 (11%)

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	FOL	B	401[B]	-	-	0/16/22/22	0/3/3/3
3	VG9	B	301[A]	-	-	2/11/11/11	0/3/3/3
3	VG9	A	301[A]	-	-	6/11/11/11	0/3/3/3
2	NDP	B	201	-	-	4/30/77/77	0/5/5/5
4	FOL	A	401[B]	-	-	0/16/22/22	0/3/3/3
2	NDP	A	201	-	-	4/30/77/77	0/5/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401[B]	FOL	O-C	8.88	1.41	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401[B]	FOL	O-C	8.76	1.41	1.23
2	B	201	NDP	C2A-N3A	4.63	1.39	1.32
2	A	201	NDP	O7N-C7N	4.07	1.34	1.24
4	B	401[B]	FOL	C6-N5	3.85	1.39	1.32
2	A	201	NDP	C2A-N3A	3.73	1.38	1.32
4	B	401[B]	FOL	C4A-N5	3.72	1.38	1.33
2	B	201	NDP	O7N-C7N	3.65	1.33	1.24
4	B	401[B]	FOL	C7-N8	3.53	1.37	1.31
4	A	401[B]	FOL	C6-N5	3.08	1.38	1.32
4	A	401[B]	FOL	C7-N8	2.93	1.36	1.31
2	B	201	NDP	C2A-N1A	2.91	1.39	1.33
4	A	401[B]	FOL	C4A-N5	2.87	1.37	1.33
2	B	201	NDP	C6N-C5N	2.69	1.38	1.33
4	B	401[B]	FOL	C4-N3	2.68	1.37	1.33
2	A	201	NDP	C6N-C5N	2.58	1.37	1.33
4	A	401[B]	FOL	C4-N3	2.57	1.37	1.33
2	A	201	NDP	C2A-N1A	2.56	1.38	1.33
2	B	201	NDP	P2B-O2B	2.31	1.63	1.59

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	NDP	N3A-C2A-N1A	-5.02	120.83	128.68
4	B	401[B]	FOL	N1-C2-N3	-4.88	120.71	127.22
2	B	201	NDP	N3A-C2A-N1A	-4.87	121.07	128.68
4	A	401[B]	FOL	N1-C2-N3	-4.68	120.98	127.22
3	B	301[A]	VG9	N1-C2-N3	-4.63	121.04	127.22
3	A	301[A]	VG9	N1-C2-N3	-4.45	121.29	127.22
4	A	401[B]	FOL	C4A-C4-N3	-4.44	117.36	123.43
3	A	301[A]	VG9	C2-N1-C8A	4.28	120.25	115.36
3	B	301[A]	VG9	O2-C12-C11	3.97	121.45	114.92
2	B	201	NDP	C3N-C7N-N7N	3.96	124.71	117.67
3	A	301[A]	VG9	C7-N8-C8A	3.96	120.67	116.69
3	B	301[A]	VG9	C7-N8-C8A	3.86	120.58	116.69
4	B	401[B]	FOL	C2-N1-C8A	3.79	119.69	115.36
4	A	401[B]	FOL	C4-N3-C2	3.60	121.64	115.93
3	B	301[A]	VG9	C2-N1-C8A	3.37	119.21	115.36
2	B	201	NDP	C1D-N1N-C2N	-3.32	115.58	121.11
2	A	201	NDP	C3N-C7N-N7N	3.10	123.18	117.67
3	A	301[A]	VG9	C5A-C5-C6	-3.10	117.25	120.80
4	B	401[B]	FOL	C4-N3-C2	2.97	120.65	115.93
4	B	401[B]	FOL	C4A-C4-N3	-2.91	119.45	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	201	NDP	C3N-C2N-N1N	-2.87	119.01	123.10
4	B	401[B]	FOL	C9-C6-N5	2.83	121.69	116.66
3	B	301[A]	VG9	C9-C6-C7	-2.83	117.43	121.30
2	A	201	NDP	O7N-C7N-C3N	-2.77	115.69	120.90
3	B	301[A]	VG9	C5A-C5-C6	-2.76	117.64	120.80
3	A	301[A]	VG9	O2-C12-C11	2.76	119.45	114.92
3	B	301[A]	VG9	O2-C12-C13	-2.75	118.03	123.97
4	A	401[B]	FOL	C2-N1-C8A	2.66	118.40	115.36
3	A	301[A]	VG9	C7-C6-C5	2.63	120.23	118.16
4	B	401[B]	FOL	C4-C4A-N5	2.63	121.61	118.60
4	B	401[B]	FOL	C7-N8-C8A	2.57	119.28	116.69
2	B	201	NDP	O4D-C1D-N1N	2.47	112.88	108.06
4	A	401[B]	FOL	C9-C6-C7	-2.44	117.29	121.55
4	A	401[B]	FOL	C9-C6-N5	2.40	120.93	116.66
4	B	401[B]	FOL	C8A-C4A-N5	-2.34	119.68	122.33
2	B	201	NDP	O7N-C7N-C3N	-2.34	116.49	120.90
4	B	401[B]	FOL	C7-C6-N5	-2.31	119.34	120.85
2	A	201	NDP	O2N-PN-O1N	2.19	123.08	112.24
2	A	201	NDP	O3X-P2B-O2X	2.12	115.75	107.64
4	B	401[B]	FOL	C6-C7-N8	-2.12	121.05	123.13
3	A	301[A]	VG9	O2-C12-C13	-2.09	119.45	123.97
2	A	201	NDP	O4D-C1D-N1N	2.06	112.08	108.06
3	B	301[A]	VG9	C7-C6-C5	2.04	119.77	118.16
3	B	301[A]	VG9	C5-C4A-C8A	2.03	120.04	118.22
2	B	201	NDP	O2N-PN-O1N	2.01	122.16	112.24

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301[A]	VG9	C11-C12-O2-C21
3	A	301[A]	VG9	C52-C51-O5-C15
3	A	301[A]	VG9	C14-C15-O5-C51
3	A	301[A]	VG9	C16-C15-O5-C51
3	A	301[A]	VG9	C22-C21-O2-C12
2	A	201	NDP	PA-O3-PN-O5D
3	A	301[A]	VG9	C13-C12-O2-C21
2	B	201	NDP	C4D-C5D-O5D-PN
2	A	201	NDP	C4D-C5D-O5D-PN
2	B	201	NDP	O4D-C1D-N1N-C2N
2	A	201	NDP	O4D-C1D-N1N-C2N
2	B	201	NDP	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	B	201	NDP	C2N-C3N-C7N-N7N
2	A	201	NDP	C2N-C3N-C7N-N7N
3	B	301[A]	VG9	C11-C12-O2-C21
3	B	301[A]	VG9	C13-C12-O2-C21

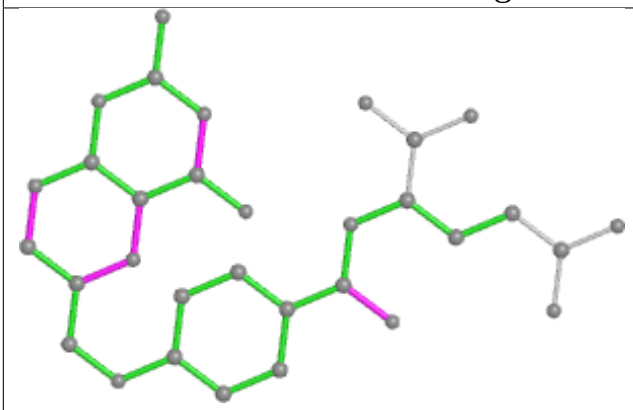
There are no ring outliers.

6 monomers are involved in 29 short contacts:

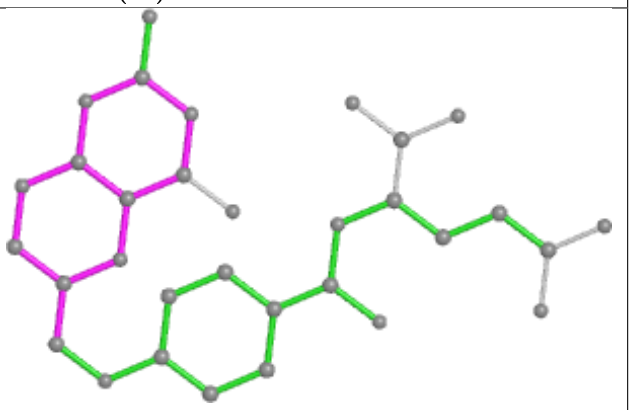
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401[B]	FOL	5	0
3	B	301[A]	VG9	6	0
3	A	301[A]	VG9	10	0
2	B	201	NDP	4	0
4	A	401[B]	FOL	5	0
2	A	201	NDP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

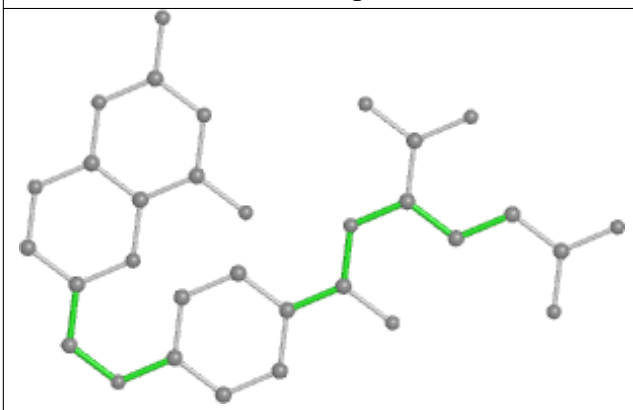
Ligand FOL B 401 (B)



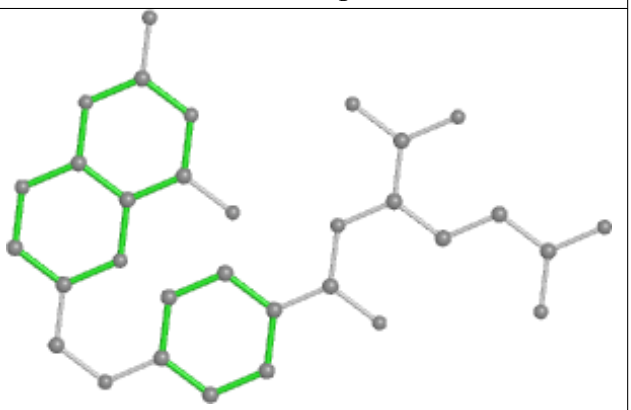
Bond lengths



Bond angles

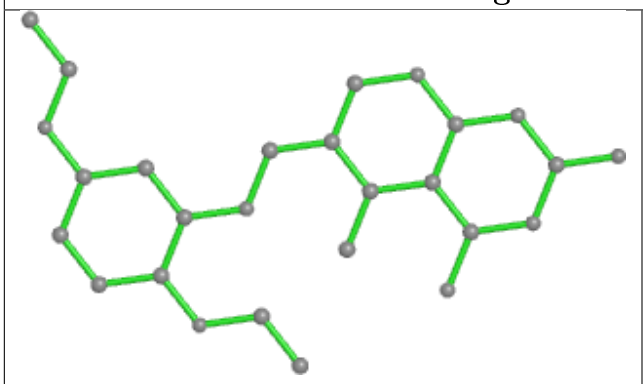


Torsions

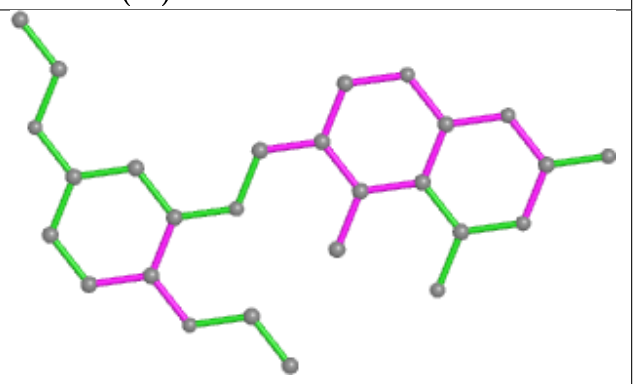


Rings

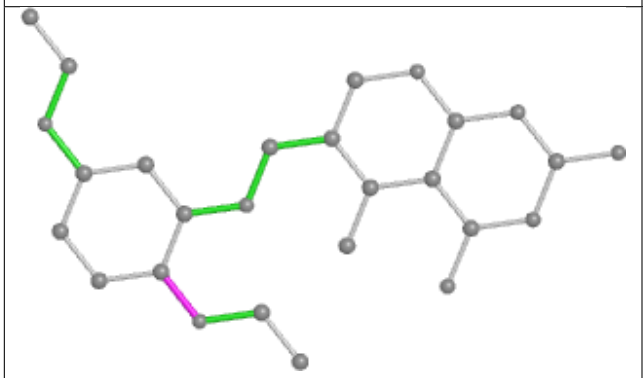
Ligand VG9 B 301 (A)



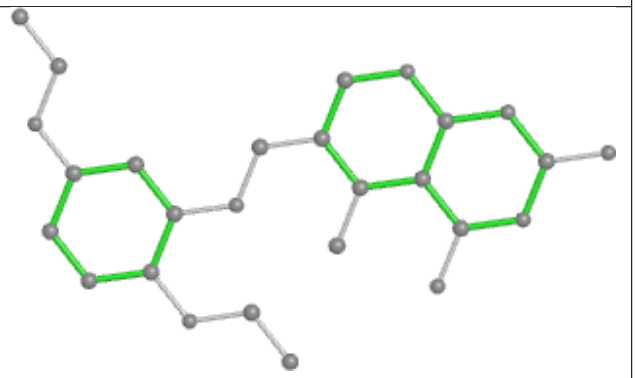
Bond lengths



Bond angles

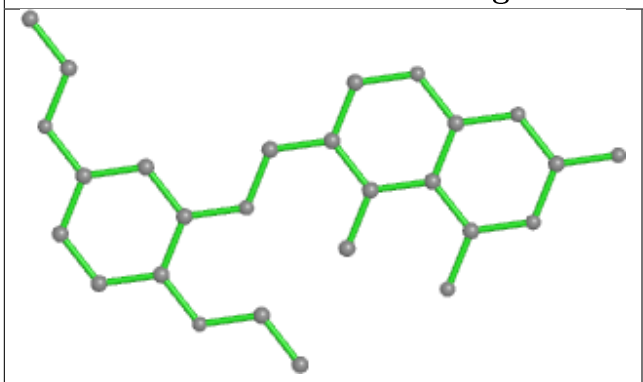


Torsions

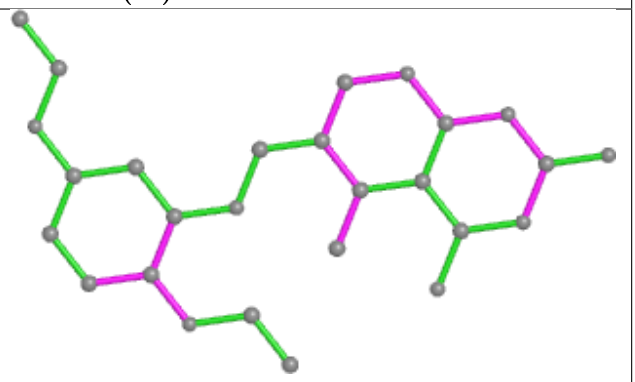


Rings

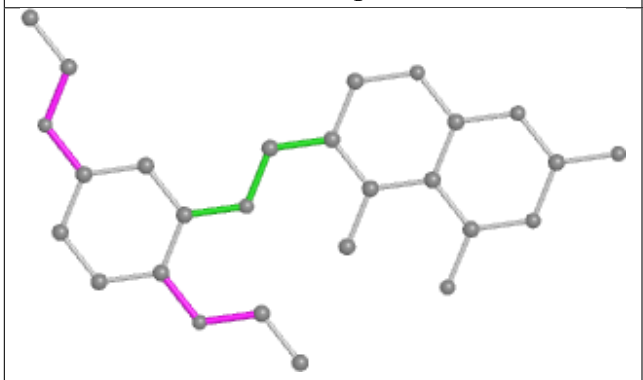
Ligand VG9 A 301 (A)



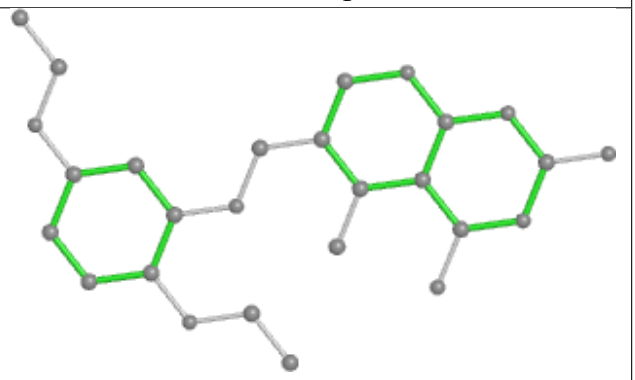
Bond lengths



Bond angles

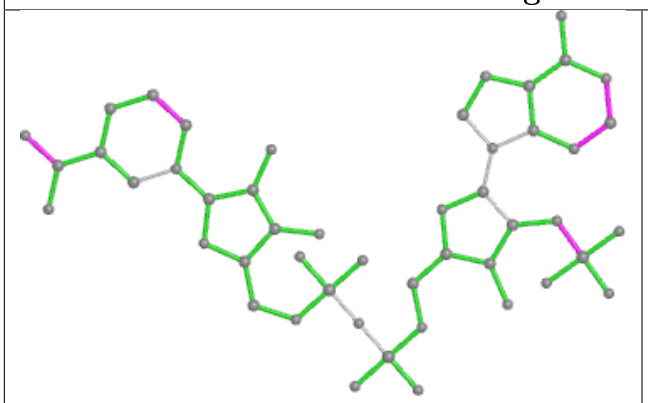


Torsions

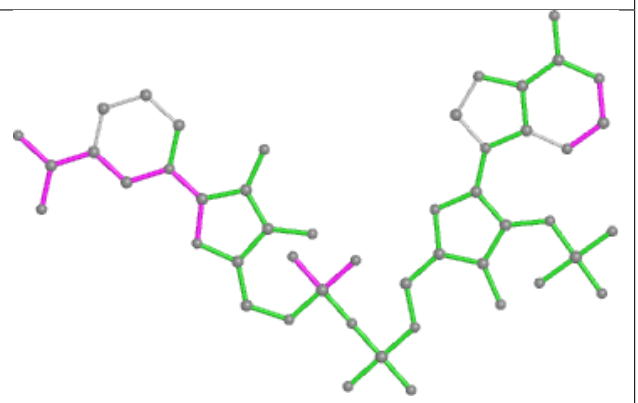


Rings

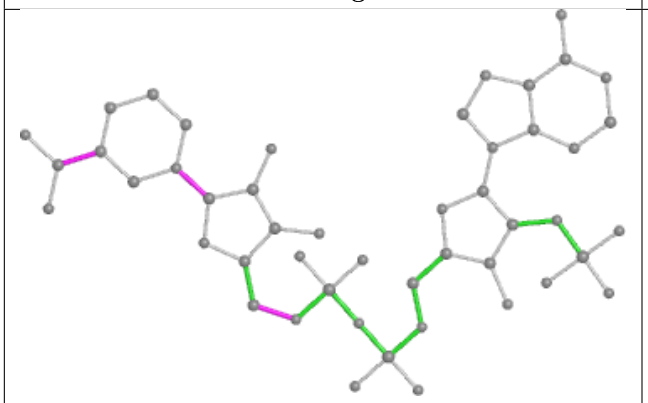
Ligand NDP B 201



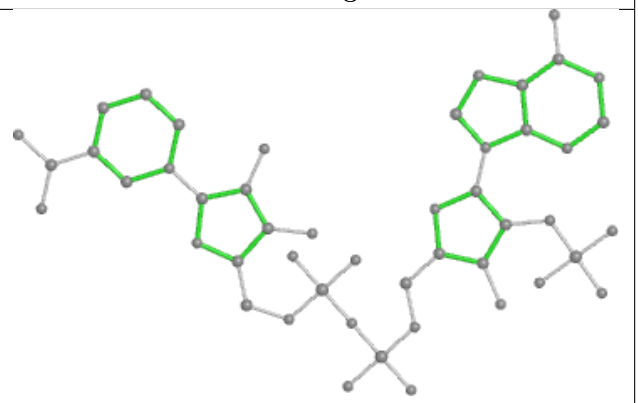
Bond lengths



Bond angles

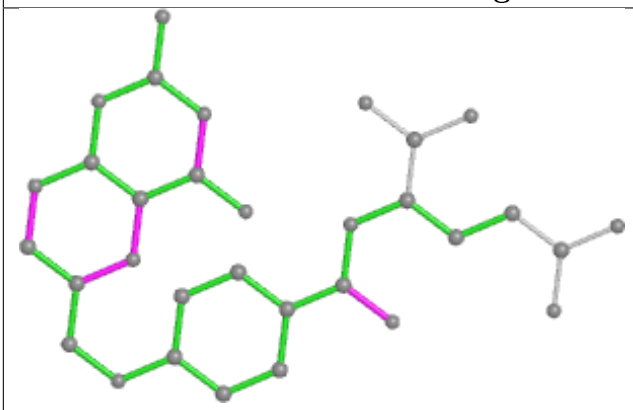


Torsions

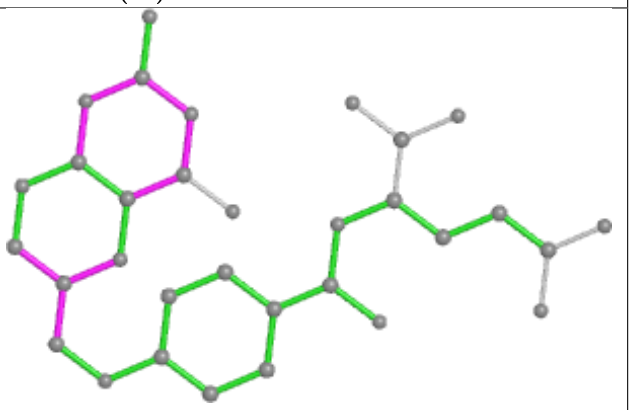


Rings

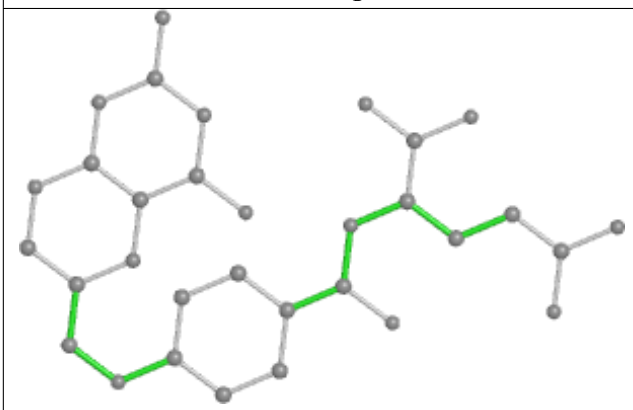
Ligand FOL A 401 (B)



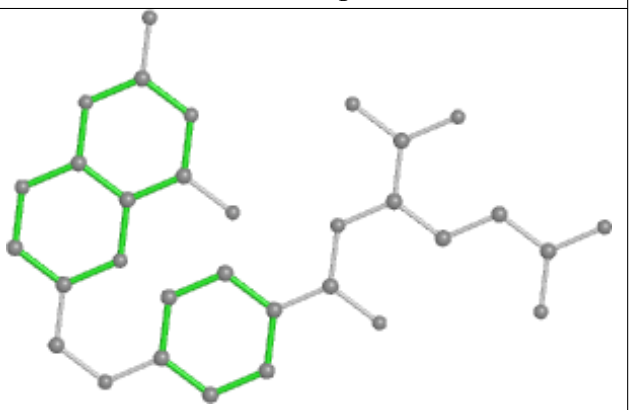
Bond lengths



Bond angles

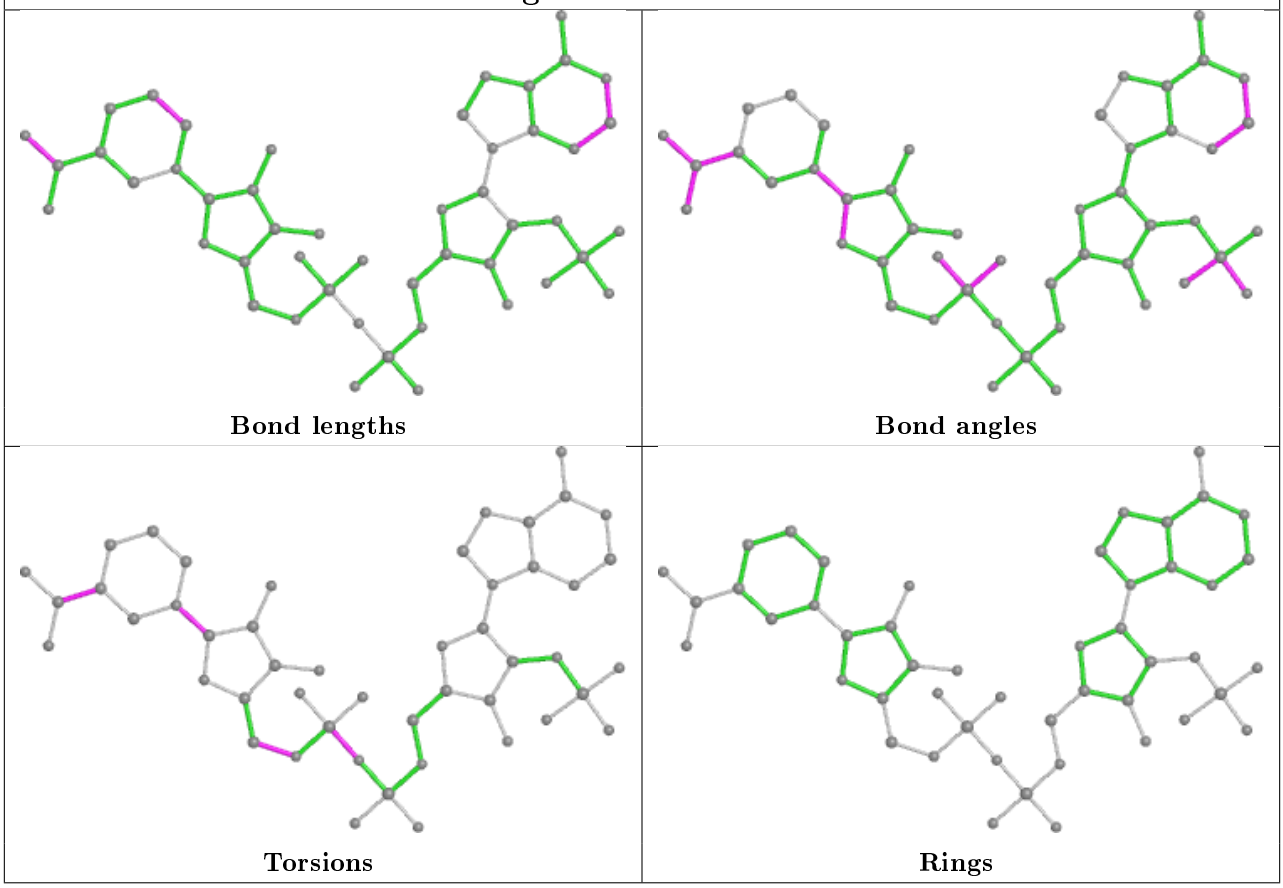


Torsions



Rings

Ligand NDP A 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

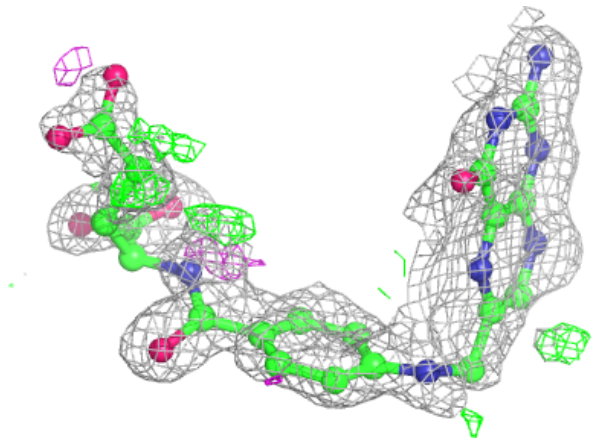
6.4 Ligands (i)

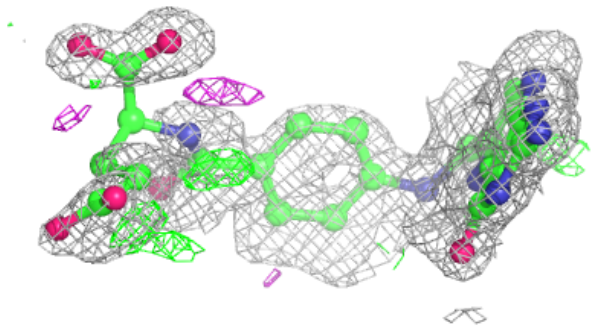
Unable to reproduce the depositors R factor - this section is therefore empty.

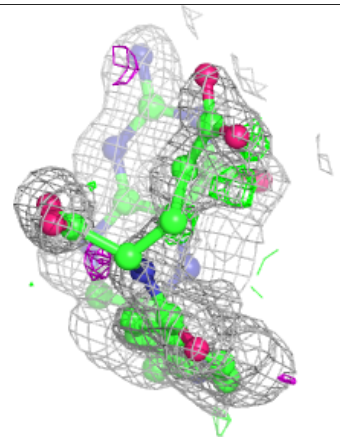
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FOL B 401 (B):

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

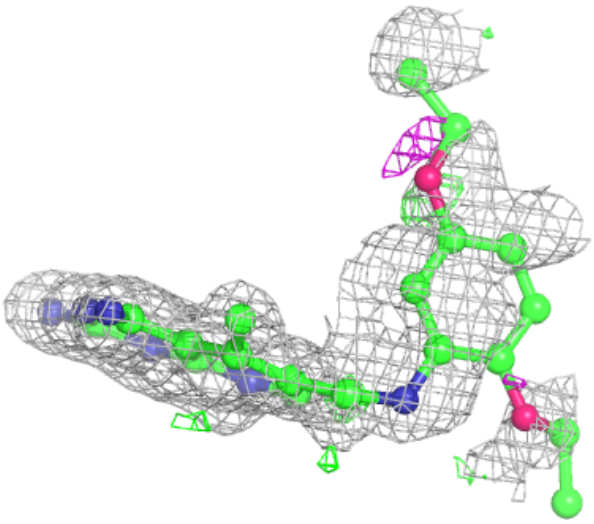


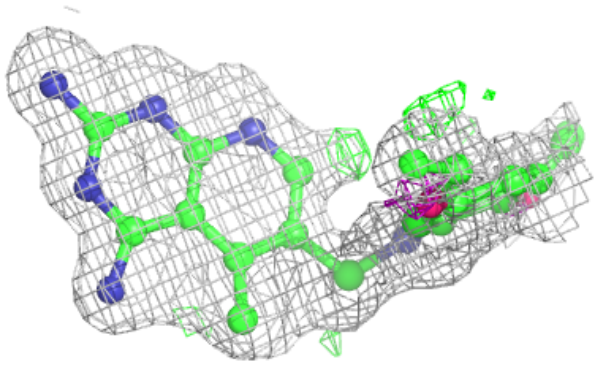


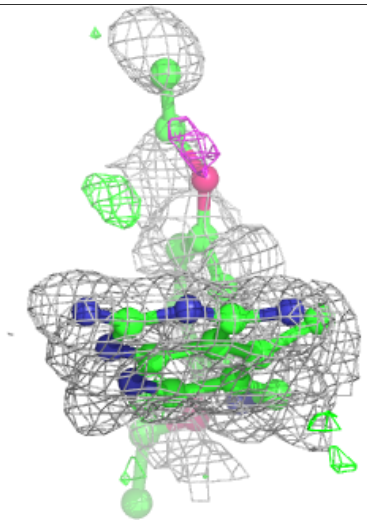


Electron density around VG9 B 301 (A):

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

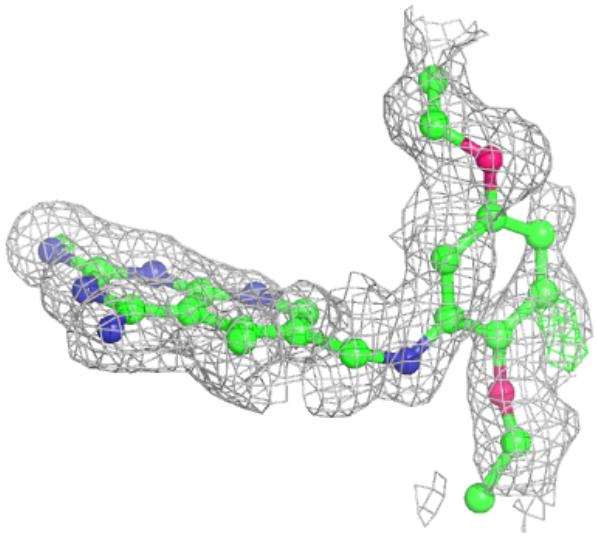


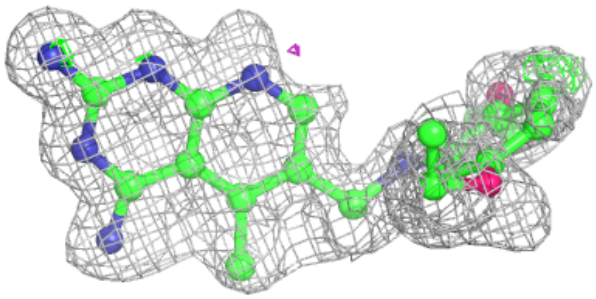


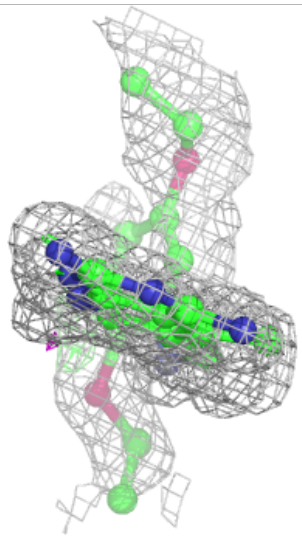


Electron density around VG9 A 301 (A):

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

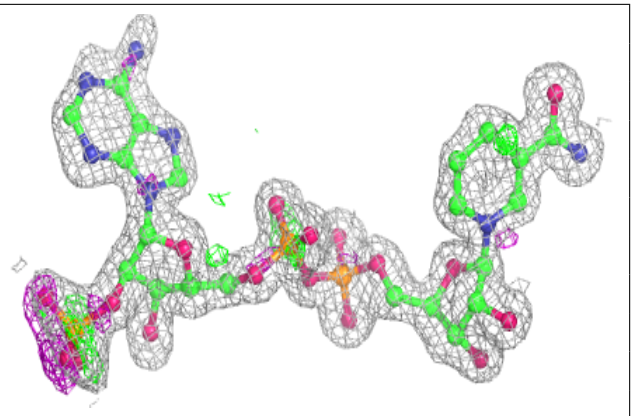


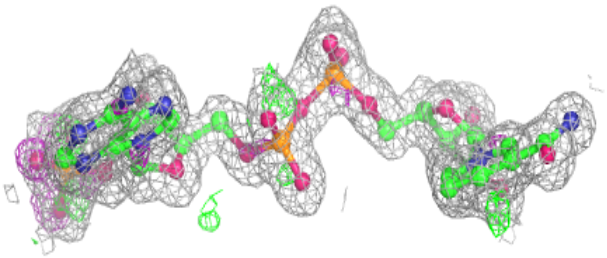


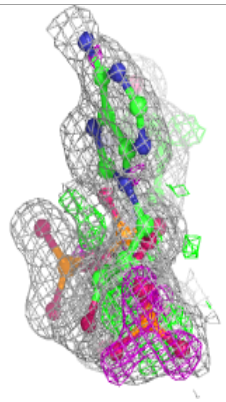


Electron density around NDP B 201:

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

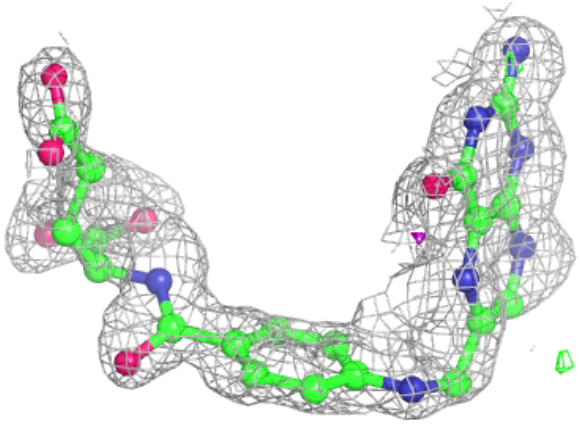


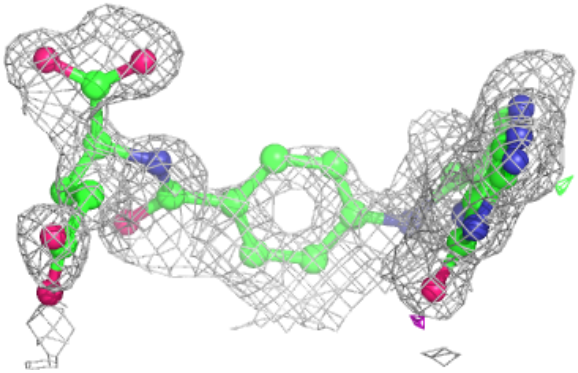


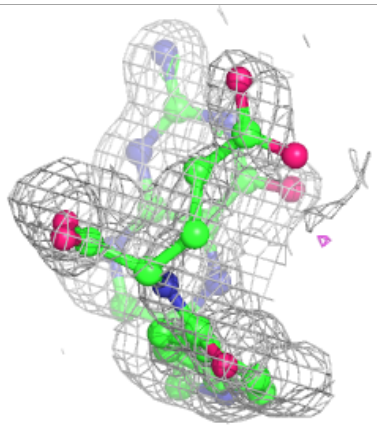


Electron density around FOL A 401 (B):

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

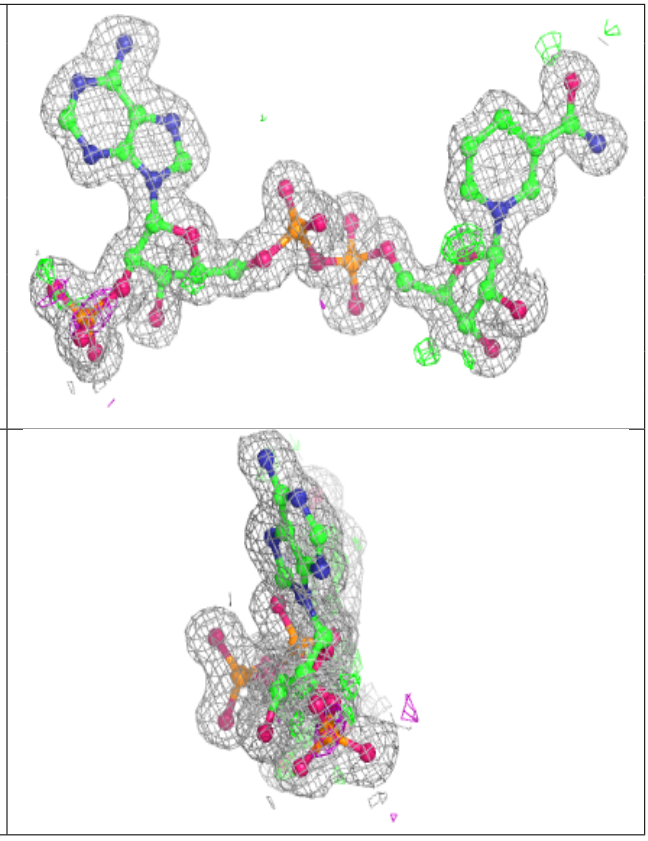






Electron density around NDP A 201:

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



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.