Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 06:04 pm GMT

PDB ID	:	2WWG
Title	:	Plasmodium falciparum thymidylate kinase in complex with dGMP and ADP
Authors	:	Whittingham, J.L.; Carrero-Lerida, J.; Brannigan, J.A.; Ruiz-Perez, L.M.; Silva, A.P.; Fogg, M.J.; Wilkinson, A.J.; Gilbert, I.H.; Wilson, K.S.; Gonzalez-Pacanowska, D.
Deposited on	:	2009-10-23
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

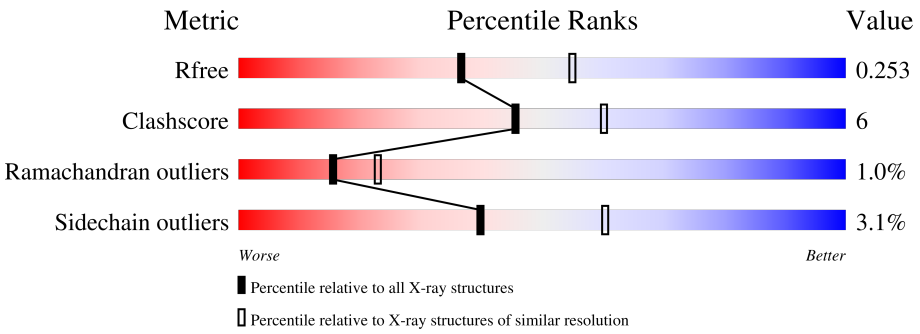
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 of 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	212	79% 18% ••
1	B	212	81% 17% ••
1	C	212	80% 16% ••

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5654 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.

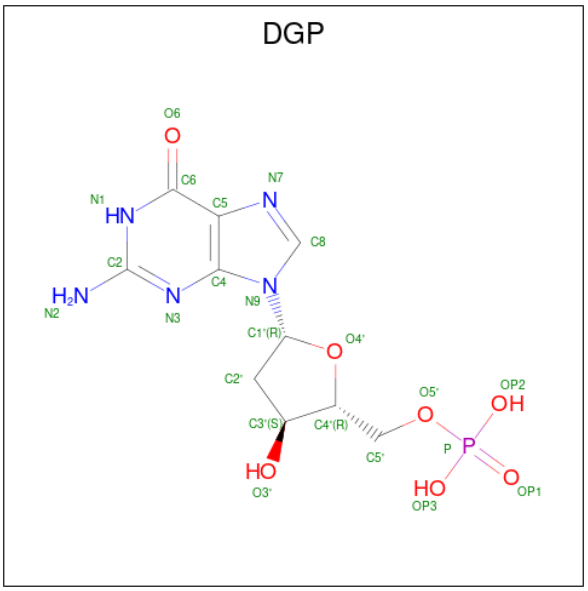
- Molecule 1 is a protein called THYMIDILATE KINASE, PUTATIVE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	209	1735	1114	288	327	6	14	0	0
1	B	210	1750	1124	291	328	7	12	1	0
1	C	210	1743	1119	289	328	7	23	0	0

There are 6 discrepancies between the modelled and reference sequences:

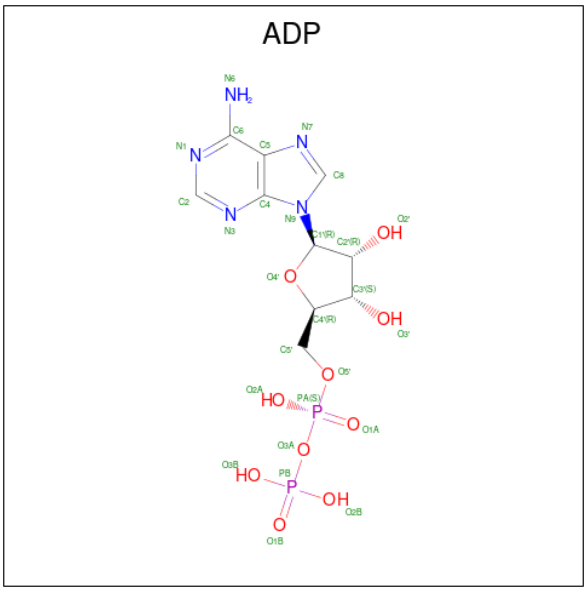
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP Q8I4S1
A	0	HIS	-	expression tag	UNP Q8I4S1
B	-1	SER	-	expression tag	UNP Q8I4S1
B	0	HIS	-	expression tag	UNP Q8I4S1
C	-1	SER	-	expression tag	UNP Q8I4S1
C	0	HIS	-	expression tag	UNP Q8I4S1

- Molecule 2 is 2'-DEOXYGUANOSINE-5'-MONOPHOSPHATE (three-letter code: DGP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	23	10	5	7	1	0	0
			Total	C	N	O	P		
2	B	1	23	10	5	7	1	0	0
			Total	C	N	O	P		
2	C	1	23	10	5	7	1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

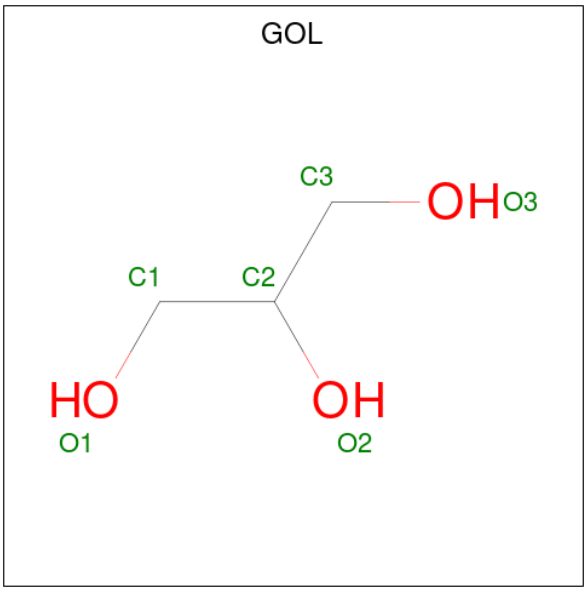


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
3	B	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
3	C	1	27	10	5	10	2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	A	2	2	2	0	0
			Total	Na		
4	B	2	2	2	0	0
			Total	Na		
4	C	2	2	2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	6	3	3	0	0
			Total	C	O		
5	A	1	6	3	3	0	0
			Total	C	O		
5	A	1	6	3	3	0	0
			Total	C	O		
5	A	1	6	3	3	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 6 is water.

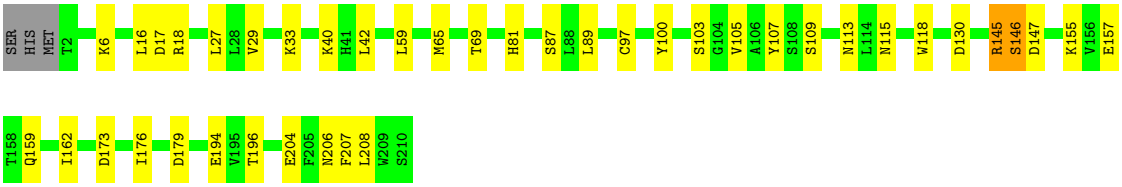
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	85	85	85	0	0
			Total	O		
6	B	64	64	64	0	0
			Total	O		
6	C	31	31	31	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

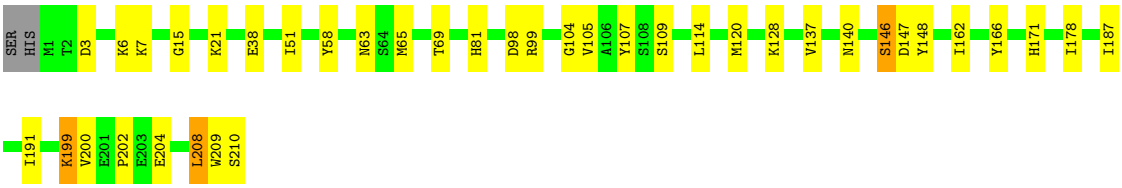
• Molecule 1: THYMIDILATE KINASE, PUTATIVE

Chain A:



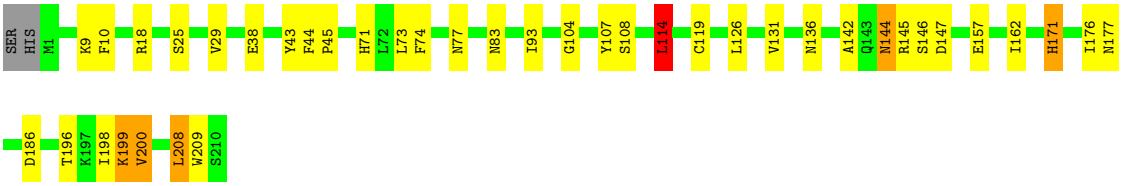
• Molecule 1: THYMIDILATE KINASE, PUTATIVE

Chain B:



• Molecule 1: THYMIDILATE KINASE, PUTATIVE

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	110.74Å 110.74Å 119.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	95.90 – 2.40 34.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (95.90-2.40) 99.2 (34.68-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.75 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.190 , 0.258 0.249 , 0.253	Depositor DCC
R_{free} test set	869 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	44.4	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	5654	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: ADP, NA, DGP, GOL

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	1.04	2/1777 (0.1%)	0.92	4/2399 (0.2%)
1	B	0.96	2/1796 (0.1%)	0.85	1/2424 (0.0%)
1	C	0.97	2/1785 (0.1%)	0.87	2/2409 (0.1%)
All	All	0.99	6/5358 (0.1%)	0.88	7/7232 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	1	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	199	LYS	CA-CB	-9.88	1.32	1.53
1	B	200	VAL	CA-CB	9.62	1.75	1.54
1	C	157	GLU	CB-CG	-6.23	1.40	1.52
1	C	209	TRP	CB-CG	-5.66	1.40	1.50
1	A	207	PHE	CE1-CZ	5.44	1.47	1.37
1	A	157	GLU	CB-CG	5.22	1.62	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	VAL	CB-CA-C	-7.42	97.31	111.40
1	A	204	GLU	CA-CB-CG	-6.97	98.06	113.40
1	C	171	HIS	CB-CA-C	6.87	124.14	110.40
1	A	155	LYS	CG-CD-CE	5.92	129.65	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	179	ASP	CB-CG-OD1	5.64	123.38	118.30
1	C	114	LEU	CA-CB-CG	5.36	127.62	115.30
1	A	173	ASP	CB-CG-OD2	-5.34	113.49	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	171	HIS	CA

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	1735	0	1702	21	0
1	B	1750	0	1721	25	0
1	C	1743	0	1715	23	0
2	A	23	0	12	2	0
2	B	23	0	12	1	0
2	C	23	0	12	2	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	A	48	0	64	2	0
5	B	36	0	48	2	0
5	C	6	0	8	1	0
6	A	85	0	0	1	0
6	B	64	0	0	1	0
6	C	31	0	0	0	0
All	All	5654	0	5330	68	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 6.

All (68) 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:B:65:MET:CE	1:B:69:THR:HG22	2.18	0.73
1:C:199:LYS:O	1:C:200:VAL:HB	1.98	0.64
1:B:65:MET:HE2	1:B:69:THR:HG22	1.79	0.64
1:A:115:ASN:HD22	1:A:118:TRP:H	1.46	0.64
1:A:18:ARG:HH21	1:A:147:ASP:HB2	1.67	0.60
1:C:114:LEU:HD12	5:C:1001:GOL:H12	1.84	0.59
1:A:65:MET:CE	1:A:69:THR:HG22	2.34	0.57
1:B:65:MET:CE	1:B:69:THR:CG2	2.83	0.56
1:C:146:SER:O	1:C:147:ASP:HB2	2.06	0.55
1:C:131:VAL:HG21	1:C:176:ILE:HD12	1.89	0.55
1:B:81:HIS:CD2	5:B:1006:GOL:H32	2.43	0.54
1:C:107:TYR:CE1	2:C:211:DGP:H2'	2.43	0.54
1:A:176:ILE:HD13	1:A:194:GLU:HG2	1.90	0.53
1:B:137:VAL:HG23	1:B:137:VAL:O	2.09	0.52
1:B:105:VAL:O	1:B:109:SER:HB3	2.11	0.50
1:B:128:LYS:NZ	1:B:210:SER:O	2.35	0.49
1:A:16:LEU:HB3	1:A:159:GLN:NE2	2.28	0.49
1:C:136:ASN:HD22	1:C:177:ASN:HD21	1.59	0.49
1:A:107:TYR:CE1	2:A:211:DGP:H2'	2.48	0.49
1:A:145:ARG:O	1:A:146:SER:C	2.50	0.49
1:C:126:LEU:HB2	1:C:208:LEU:HD22	1.94	0.49
1:B:15:GLY:O	1:B:21:LYS:HE3	2.12	0.49
1:C:144:ASN:HD22	1:C:144:ASN:H	1.59	0.49
1:B:146:SER:C	1:B:148:TYR:H	2.16	0.48
1:A:6:LYS:HZ1	1:A:130:ASP:CG	2.16	0.48
1:C:43:TYR:CD1	1:C:43:TYR:N	2.81	0.48
1:A:59:LEU:HD13	2:A:211:DGP:H5'	1.95	0.47
1:A:17:ASP:H	1:A:159:GLN:HE22	1.61	0.47
1:A:196:THR:HA	5:A:1006:GOL:H12	1.96	0.47
1:C:38:GLU:HB2	1:C:93:ILE:HA	1.96	0.46
1:B:65:MET:HE2	1:B:69:THR:CG2	2.43	0.46
1:B:6:LYS:O	1:B:202:PRO:HA	2.16	0.46
1:B:98:ASP:O	1:B:99:ARG:HB2	2.17	0.45
1:B:208:LEU:HA	1:B:209:TRP:HA	1.73	0.45
1:B:187:ILE:HG22	1:B:191:ILE:HD12	1.99	0.44
1:A:42:LEU:O	1:A:97:CYS:HA	2.18	0.44
1:A:89:LEU:HA	1:A:89:LEU:HD23	1.79	0.44
1:C:142:ALA:HB1	1:C:145:ARG:HD2	1.99	0.44
1:A:107:TYR:CE1	1:A:162:ILE:HD13	2.51	0.44
1:C:107:TYR:CE1	1:C:162:ILE:HD13	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:TYR:O	1:A:103:SER:HB2	2.17	0.44
1:C:108:SER:O	1:C:114:LEU:HB2	2.18	0.43
1:A:40:LYS:NZ	6:A:2018:HOH:O	2.40	0.43
1:C:18:ARG:HA	3:C:212:ADP:O3B	2.17	0.43
1:C:74:PHE:O	1:C:77:ASN:HB3	2.19	0.43
1:A:105:VAL:O	1:A:109:SER:HB3	2.19	0.43
1:B:107:TYR:CE1	1:B:162:ILE:HD13	2.54	0.43
1:B:21:LYS:HE2	1:B:99:ARG:CZ	2.48	0.42
1:A:27:LEU:HD23	1:A:27:LEU:HA	1.94	0.42
1:B:140:ASN:ND2	6:B:2045:HOH:O	2.52	0.42
1:C:104:GLY:O	1:C:108:SER:HB2	2.19	0.42
1:B:51:ILE:HG12	1:C:73:LEU:HD21	2.02	0.42
1:B:58:TYR:HA	1:B:63:ASN:OD1	2.20	0.42
1:C:25:SER:O	1:C:29:VAL:HG23	2.19	0.42
1:A:65:MET:HE3	1:A:69:THR:CG2	2.50	0.41
1:B:104:GLY:HA2	2:B:211:DGP:O6	2.19	0.41
1:B:178:ILE:HG21	1:B:187:ILE:HG23	2.01	0.41
1:C:44:PHE:HA	1:C:45:PRO:C	2.40	0.41
1:A:81:HIS:CD2	5:A:1005:GOL:H32	2.56	0.41
1:C:9:LYS:HA	1:C:9:LYS:HD2	1.83	0.41
1:C:107:TYR:CD1	2:C:211:DGP:H2'	2.56	0.41
1:B:105:VAL:CG2	1:B:120:MET:HG3	2.51	0.41
1:B:3:ASP:OD2	1:B:7:LYS:NZ	2.52	0.41
1:A:29:VAL:HG12	1:A:33:LYS:HE2	2.02	0.40
1:C:108:SER:HB3	1:C:114:LEU:HD23	2.03	0.40
1:B:171:HIS:CD2	1:B:171:HIS:H	2.38	0.40
1:C:71:HIS:CE1	1:C:119:CYS:HB3	2.56	0.40
1:B:38:GLU:OE1	5:B:1002:GOL:O2	2.39	0.40

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	207/212 (98%)	197 (95%)	9 (4%)	1 (0%)	29	41
1	B	209/212 (99%)	196 (94%)	11 (5%)	2 (1%)	15	23
1	C	208/212 (98%)	193 (93%)	12 (6%)	3 (1%)	11	15
All	All	624/636 (98%)	586 (94%)	32 (5%)	6 (1%)	15	23

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	146	SER
1	C	199	LYS
1	C	200	VAL
1	A	146	SER
1	B	147	ASP
1	C	198	ILE

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	192/195 (98%)	187 (97%)	5 (3%)	46	66
1	B	194/195 (100%)	189 (97%)	5 (3%)	46	66
1	C	193/195 (99%)	185 (96%)	8 (4%)	30	48
All	All	579/585 (99%)	561 (97%)	18 (3%)	40	60

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	SER
1	A	113	ASN
1	A	145	ARG
1	A	206	ASN
1	A	208	LEU
1	B	114	LEU
1	B	166	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	199	LYS
1	B	204	GLU
1	B	208	LEU
1	C	10	PHE
1	C	83	ASN
1	C	114	LEU
1	C	144	ASN
1	C	171	HIS
1	C	186	ASP
1	C	196	THR
1	C	208	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	41	HIS
1	A	115	ASN
1	A	159	GLN
1	A	206	ASN
1	B	41	HIS
1	B	77	ASN
1	B	159	GLN
1	C	77	ASN
1	C	113	ASN
1	C	144	ASN
1	C	177	ASN
1	C	206	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 6 are monoatomic - leaving 21 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	DGP	B	211	4	22,25,25	1.51	3 (13%)	26,38,38	1.90	7 (26%)
5	GOL	B	1002	-	5,5,5	0.72	0	5,5,5	0.67	0
3	ADP	A	212	4	24,29,29	1.59	5 (20%)	29,45,45	1.57	4 (13%)
5	GOL	B	1001	-	5,5,5	0.44	0	5,5,5	0.48	0
5	GOL	A	1003	-	5,5,5	0.35	0	5,5,5	0.53	0
5	GOL	B	1006	-	5,5,5	0.32	0	5,5,5	0.94	0
5	GOL	A	1007	-	5,5,5	0.49	0	5,5,5	0.05	0
5	GOL	A	1006	-	5,5,5	0.36	0	5,5,5	0.34	0
2	DGP	A	211	4	22,25,25	1.84	5 (22%)	26,38,38	2.33	11 (42%)
5	GOL	C	1001	-	5,5,5	0.25	0	5,5,5	0.37	0
5	GOL	A	1004	-	5,5,5	0.46	0	5,5,5	0.42	0
5	GOL	A	1002	-	5,5,5	0.60	0	5,5,5	0.82	0
3	ADP	B	212	4	24,29,29	1.49	3 (12%)	29,45,45	1.69	6 (20%)
5	GOL	B	1005	-	5,5,5	0.40	0	5,5,5	0.50	0
5	GOL	A	1008	-	5,5,5	0.40	0	5,5,5	0.47	0
5	GOL	B	1004	-	5,5,5	0.59	0	5,5,5	0.49	0
5	GOL	A	1001	-	5,5,5	0.65	0	5,5,5	0.76	0
2	DGP	C	211	4	22,25,25	2.16	5 (22%)	26,38,38	1.93	9 (34%)
3	ADP	C	212	4	24,29,29	2.05	4 (16%)	29,45,45	1.63	5 (17%)
5	GOL	A	1005	-	5,5,5	0.30	0	5,5,5	0.82	0
5	GOL	B	1003	-	5,5,5	0.53	0	5,5,5	1.24	1 (20%)

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
2	DGP	B	211	4	-	1/6/22/22	0/3/3/3
5	GOL	B	1002	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	212	4	-	1/12/32/32	0/3/3/3
5	GOL	B	1001	-	-	0/4/4/4	-
5	GOL	A	1003	-	-	0/4/4/4	-
5	GOL	B	1006	-	-	2/4/4/4	-
5	GOL	A	1007	-	-	4/4/4/4	-
5	GOL	A	1006	-	-	2/4/4/4	-
2	DGP	A	211	4	-	3/6/22/22	0/3/3/3
5	GOL	C	1001	-	-	2/4/4/4	-
5	GOL	A	1004	-	-	0/4/4/4	-
5	GOL	A	1002	-	-	4/4/4/4	-
3	ADP	B	212	4	-	7/12/32/32	0/3/3/3
5	GOL	B	1005	-	-	0/4/4/4	-
5	GOL	A	1008	-	-	2/4/4/4	-
5	GOL	B	1004	-	-	0/4/4/4	-
5	GOL	A	1001	-	-	2/4/4/4	-
2	DGP	C	211	4	-	1/6/22/22	0/3/3/3
3	ADP	C	212	4	-	5/12/32/32	0/3/3/3
5	GOL	A	1005	-	-	2/4/4/4	-
5	GOL	B	1003	-	-	1/4/4/4	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	212	ADP	PB-O1B	6.93	1.72	1.50
2	C	211	DGP	P-OP1	6.58	1.71	1.50
3	C	212	ADP	O4'-C1'	5.65	1.49	1.41
2	C	211	DGP	C5-C6	-4.38	1.38	1.47
2	A	211	DGP	C5-C6	-4.14	1.39	1.47
2	B	211	DGP	C5-C6	-4.10	1.39	1.47
2	A	211	DGP	O5'-C5'	-4.09	1.29	1.44
3	B	212	ADP	PA-O1A	3.83	1.64	1.50
3	B	212	ADP	O4'-C1'	3.62	1.46	1.41
3	A	212	ADP	O4'-C1'	3.58	1.46	1.41
3	B	212	ADP	PB-O1B	3.18	1.60	1.50
2	A	211	DGP	P-O5'	3.06	1.70	1.60
2	C	211	DGP	P-OP2	2.84	1.65	1.54
3	A	212	ADP	PA-O1A	2.79	1.60	1.50
2	B	211	DGP	O4'-C1'	2.72	1.48	1.42
2	C	211	DGP	C2-N1	2.70	1.44	1.37
3	A	212	ADP	PB-O3B	-2.70	1.44	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	211	DGP	P-OP3	-2.65	1.44	1.54
2	B	211	DGP	C2-N1	2.62	1.44	1.37
3	A	212	ADP	O4'-C4'	2.61	1.50	1.45
2	A	211	DGP	P-OP1	2.61	1.59	1.50
3	A	212	ADP	C2'-C1'	-2.38	1.50	1.53
3	C	212	ADP	C5'-C4'	2.37	1.59	1.51
3	C	212	ADP	PA-O1A	2.10	1.58	1.50
2	C	211	DGP	C5-C4	-2.00	1.38	1.43

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	211	DGP	OP3-P-O5'	6.97	125.28	106.73
3	B	212	ADP	N3-C2-N1	-5.34	120.33	128.68
3	A	212	ADP	N3-C2-N1	-4.79	121.19	128.68
3	C	212	ADP	PA-O3A-PB	-4.77	116.44	132.83
2	B	211	DGP	C2-N1-C6	-4.68	116.48	125.10
3	C	212	ADP	N3-C2-N1	-4.53	121.59	128.68
2	B	211	DGP	C5-C6-N1	3.87	120.79	113.95
2	C	211	DGP	C2-N1-C6	-3.70	118.29	125.10
2	C	211	DGP	C5-C6-N1	3.61	120.33	113.95
3	B	212	ADP	O3B-PB-O3A	3.53	116.47	104.64
3	B	212	ADP	PA-O3A-PB	-3.48	120.88	132.83
2	A	211	DGP	C2'-C1'-N9	-3.42	106.38	114.27
2	A	211	DGP	C8-N7-C5	3.34	109.35	102.99
2	B	211	DGP	C8-N7-C5	3.34	109.35	102.99
2	C	211	DGP	OP3-P-O5'	3.32	115.57	106.73
2	C	211	DGP	O6-C6-C5	-3.31	117.90	124.37
2	B	211	DGP	OP3-P-O5'	3.16	115.13	106.73
2	A	211	DGP	O3'-C3'-C4'	-3.03	98.50	110.10
3	A	212	ADP	O2B-PB-O3A	2.95	114.53	104.64
2	C	211	DGP	N2-C2-N1	2.84	122.77	116.71
2	C	211	DGP	C8-N7-C5	2.80	108.33	102.99
3	C	212	ADP	O2A-PA-O5'	2.75	120.51	107.75
2	C	211	DGP	C2'-C1'-N9	-2.70	108.03	114.27
3	C	212	ADP	O5'-PA-O1A	-2.62	98.84	109.07
2	A	211	DGP	OP2-P-O5'	-2.61	99.80	106.73
2	A	211	DGP	C2-N1-C6	-2.53	120.44	125.10
2	A	211	DGP	C5-C6-N1	2.52	118.40	113.95
2	A	211	DGP	OP2-P-OP1	-2.50	100.91	110.68
2	C	211	DGP	P-O5'-C5'	2.39	124.87	118.30
3	A	212	ADP	N6-C6-N1	2.37	123.49	118.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	212	ADP	O2B-PB-O1B	-2.34	101.53	110.68
2	C	211	DGP	N1-C2-N3	-2.30	119.02	123.32
2	A	211	DGP	C4'-O4'-C1'	-2.27	103.96	109.45
3	C	212	ADP	C4-C5-N7	-2.25	107.05	109.40
2	B	211	DGP	O6-C6-C5	-2.14	120.18	124.37
2	B	211	DGP	O3'-C3'-C4'	-2.14	101.93	110.10
3	A	212	ADP	C2-N1-C6	2.13	122.40	118.75
3	B	212	ADP	C2-N1-C6	2.11	122.36	118.75
2	B	211	DGP	OP2-P-OP1	-2.10	102.45	110.68
5	B	1003	GOL	C3-C2-C1	2.09	119.83	111.70
2	A	211	DGP	O4'-C4'-C5'	2.06	116.14	109.37
3	B	212	ADP	C4-C5-N7	-2.05	107.26	109.40
2	A	211	DGP	O4'-C1'-C2'	-2.04	102.40	106.25

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	211	DGP	C5'-O5'-P-OP1
2	A	211	DGP	C5'-O5'-P-OP2
2	A	211	DGP	C5'-O5'-P-OP3
3	B	212	ADP	PA-O3A-PB-O2B
3	B	212	ADP	PA-O3A-PB-O3B
3	B	212	ADP	C5'-O5'-PA-O3A
3	C	212	ADP	C5'-O5'-PA-O1A
3	C	212	ADP	C5'-O5'-PA-O2A
3	C	212	ADP	C5'-O5'-PA-O3A
5	A	1001	GOL	O1-C1-C2-C3
5	A	1002	GOL	O1-C1-C2-C3
5	A	1006	GOL	O1-C1-C2-C3
5	A	1007	GOL	C1-C2-C3-O3
5	A	1008	GOL	C1-C2-C3-O3
5	B	1002	GOL	C1-C2-C3-O3
5	B	1006	GOL	O1-C1-C2-C3
5	A	1005	GOL	O1-C1-C2-O2
3	C	212	ADP	O4'-C4'-C5'-O5'
3	C	212	ADP	C3'-C4'-C5'-O5'
5	A	1002	GOL	C1-C2-C3-O3
5	A	1005	GOL	O1-C1-C2-C3
5	C	1001	GOL	O1-C1-C2-C3
5	A	1001	GOL	O1-C1-C2-O2
5	A	1002	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	1002	GOL	O2-C2-C3-O3
5	B	1002	GOL	O2-C2-C3-O3
5	B	1006	GOL	O1-C1-C2-O2
5	C	1001	GOL	O1-C1-C2-O2
3	B	212	ADP	O4'-C4'-C5'-O5'
5	A	1008	GOL	O2-C2-C3-O3
3	B	212	ADP	C3'-C4'-C5'-O5'
5	A	1006	GOL	O1-C1-C2-O2
5	A	1007	GOL	O1-C1-C2-O2
3	B	212	ADP	C5'-O5'-PA-O1A
3	B	212	ADP	C5'-O5'-PA-O2A
5	A	1007	GOL	O2-C2-C3-O3
5	A	1007	GOL	O1-C1-C2-C3
5	B	1003	GOL	C1-C2-C3-O3
2	B	211	DGP	O4'-C4'-C5'-O5'
2	C	211	DGP	O4'-C4'-C5'-O5'
3	A	212	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

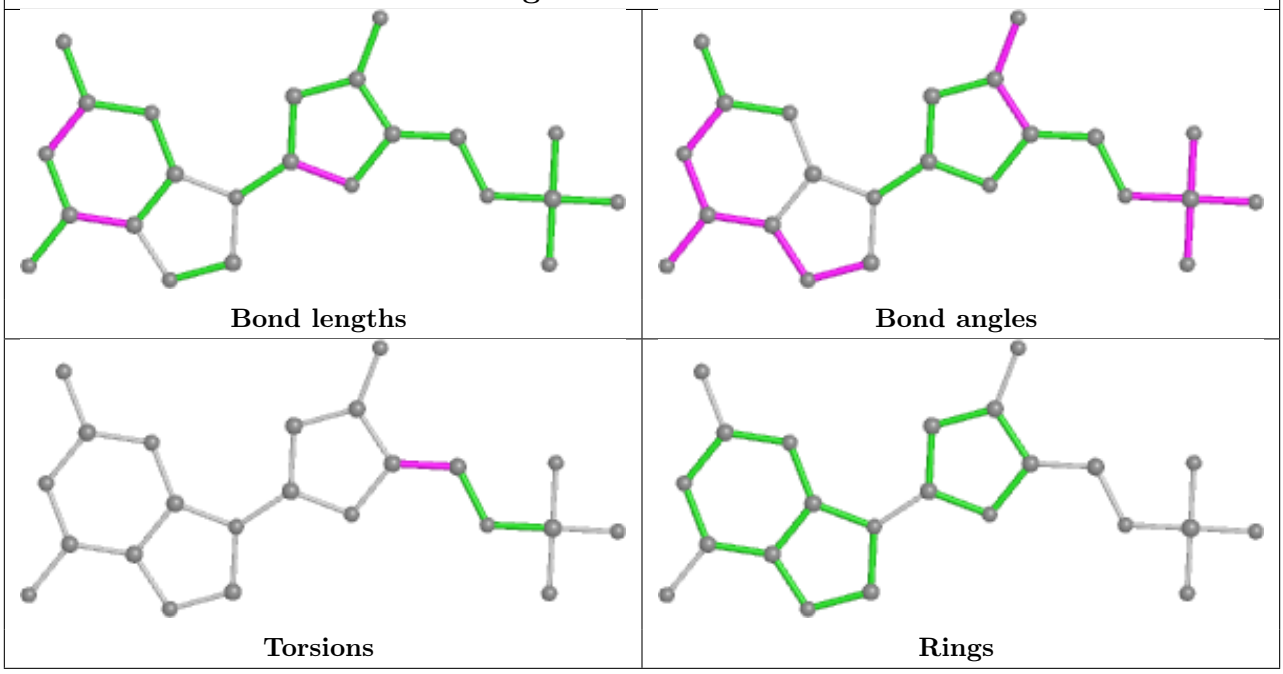
9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	211	DGP	1	0
5	B	1002	GOL	1	0
5	B	1006	GOL	1	0
5	A	1006	GOL	1	0
2	A	211	DGP	2	0
5	C	1001	GOL	1	0
2	C	211	DGP	2	0
3	C	212	ADP	1	0
5	A	1005	GOL	1	0

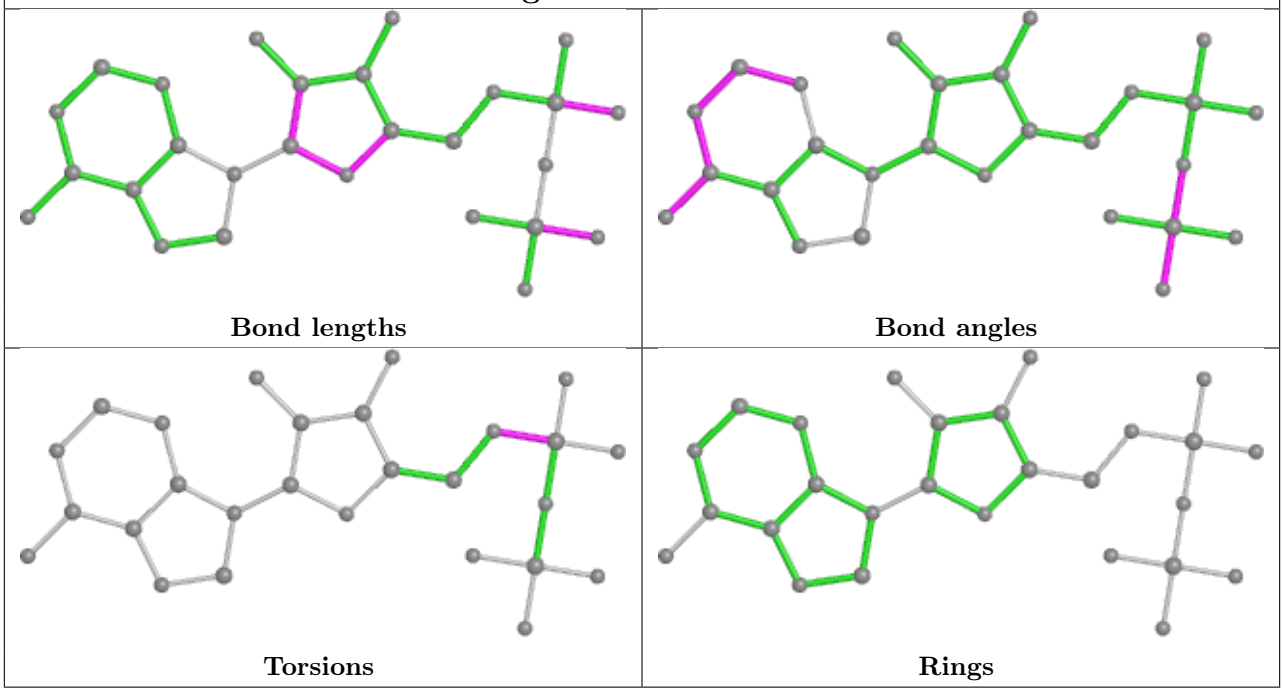
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

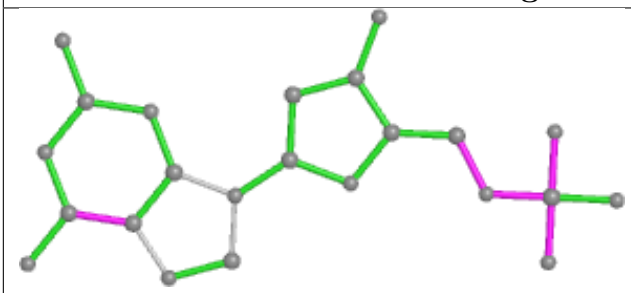
Ligand DGP B 211



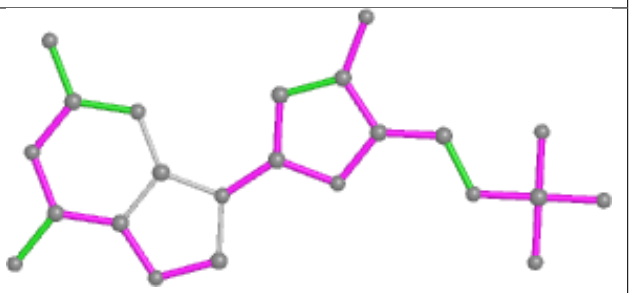
Ligand ADP A 212



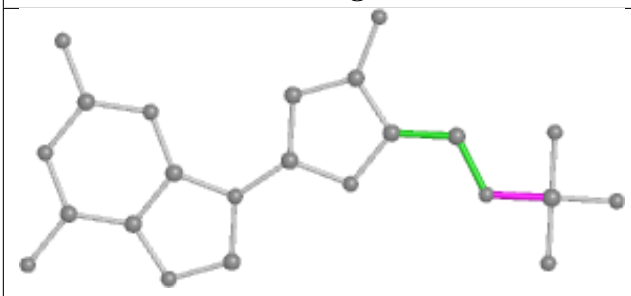
Ligand DGP A 211



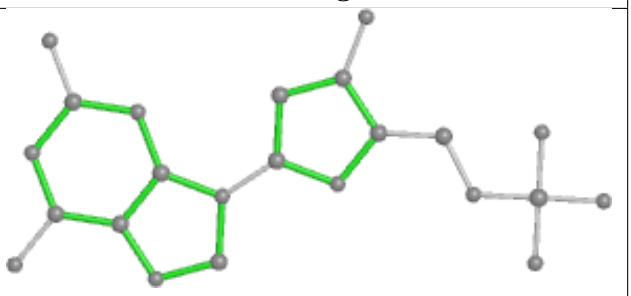
Bond lengths



Bond angles

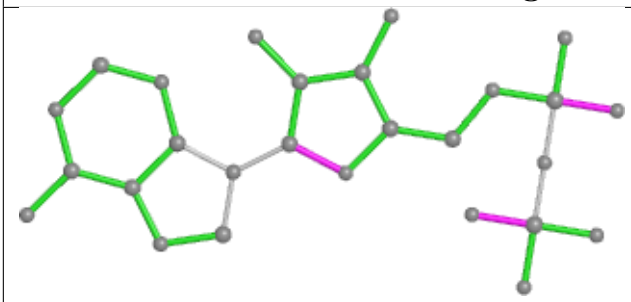


Torsions

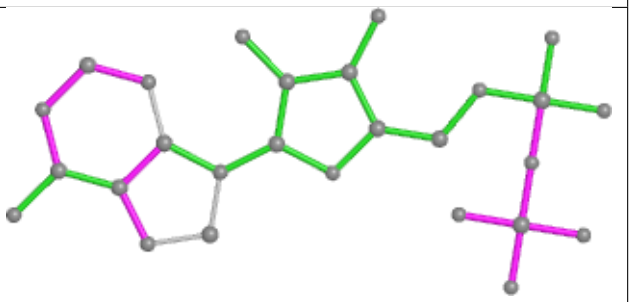


Rings

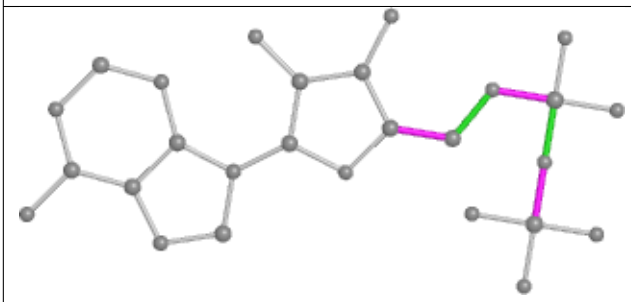
Ligand ADP B 212



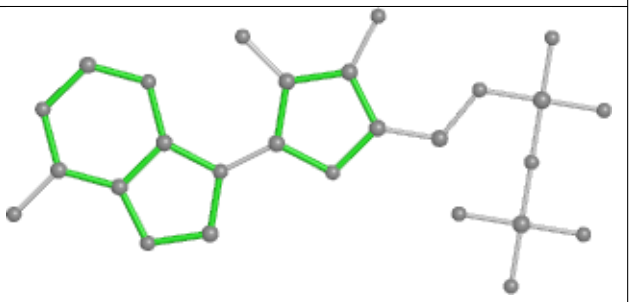
Bond lengths



Bond angles

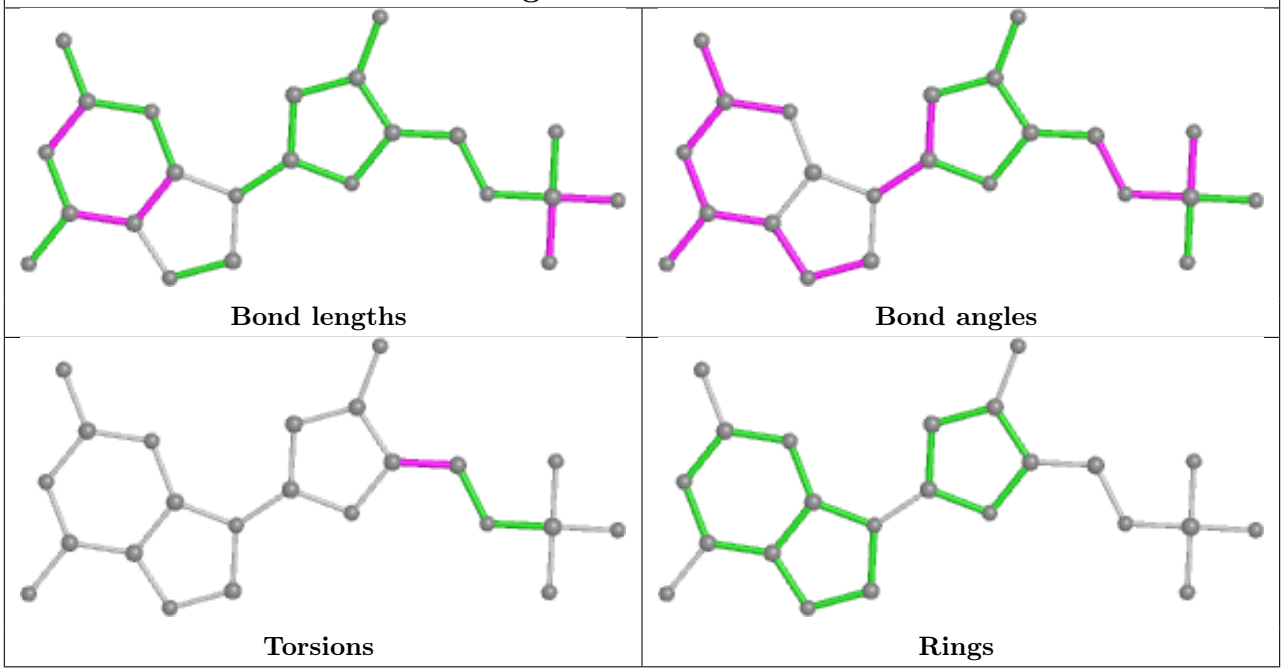


Torsions

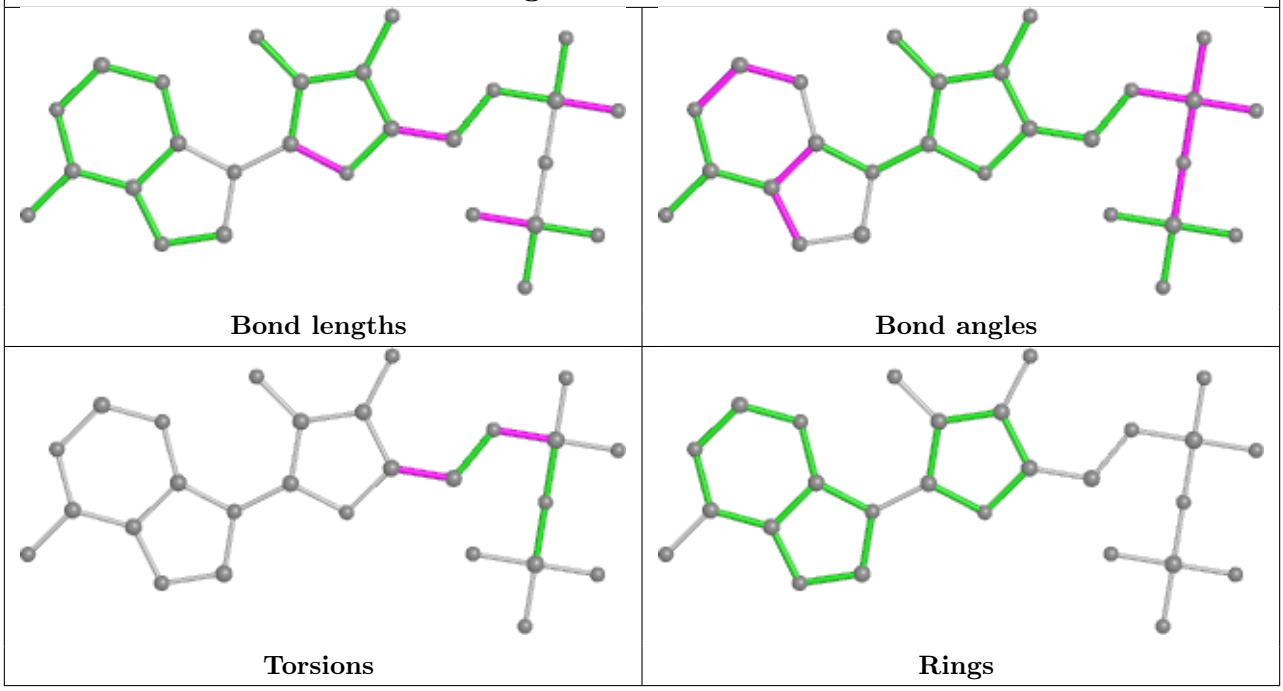


Rings

Ligand DGP C 211



Ligand ADP C 212



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.

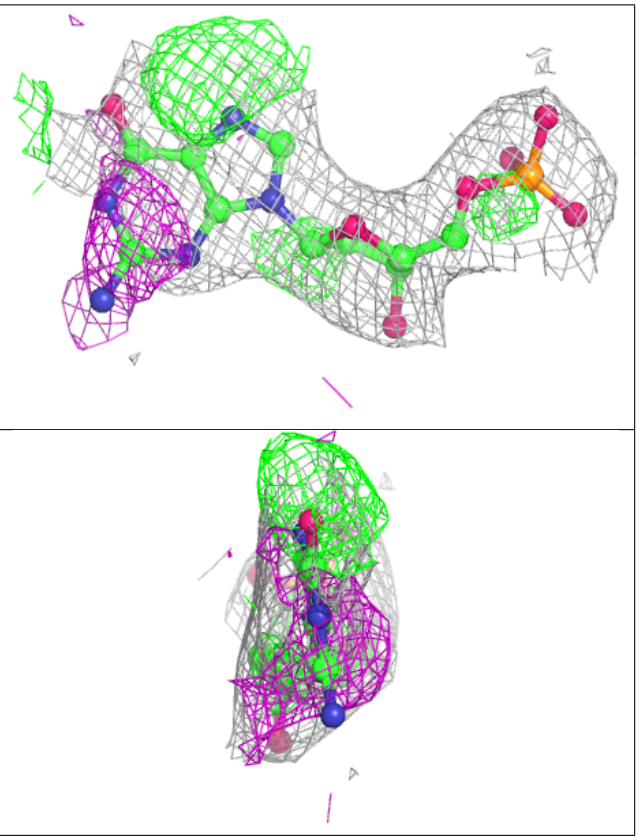
6.4 Ligands (i)

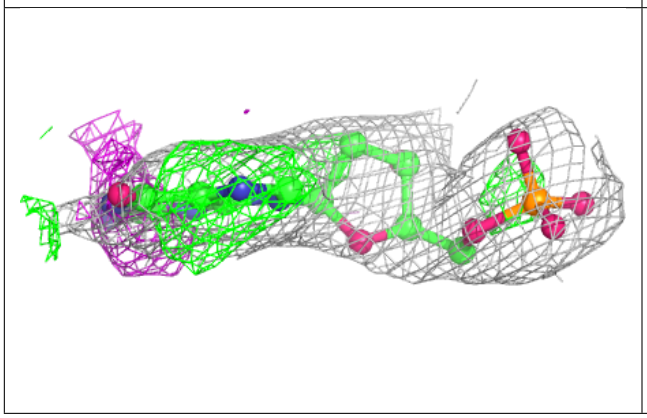
Unable to reproduce the depositors R factor - this section is therefore empty.

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 DGP A 211:

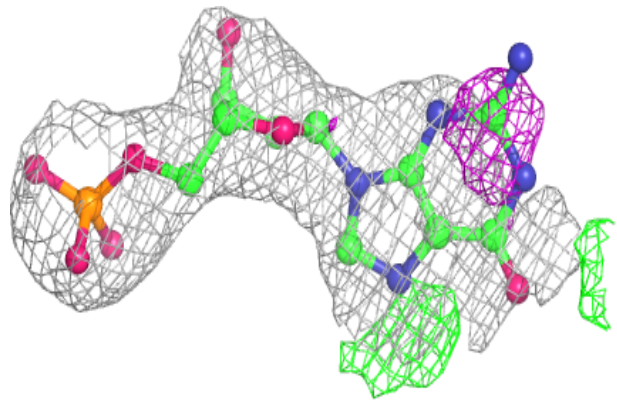
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

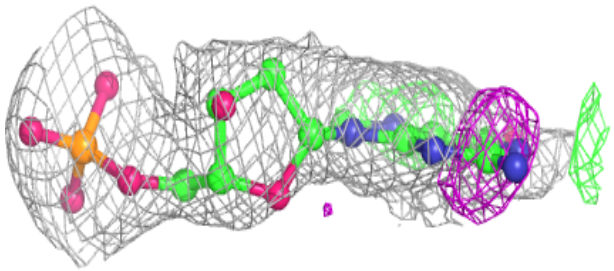


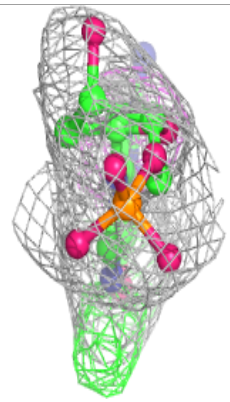


Electron density around DGP B 211:

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

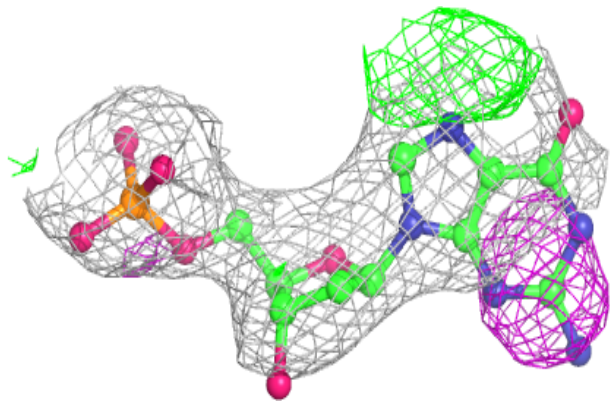


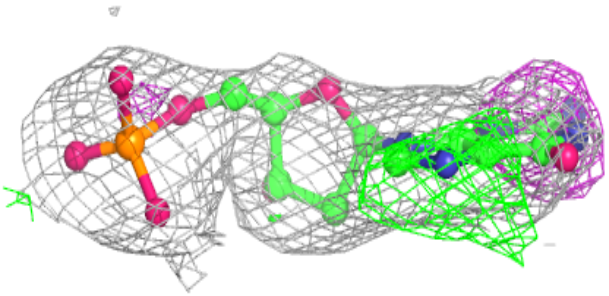


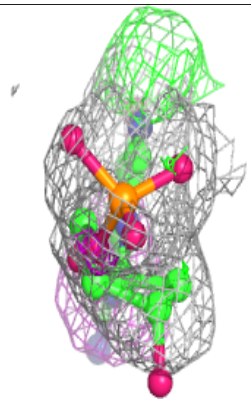


Electron density around DGP C 211:

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

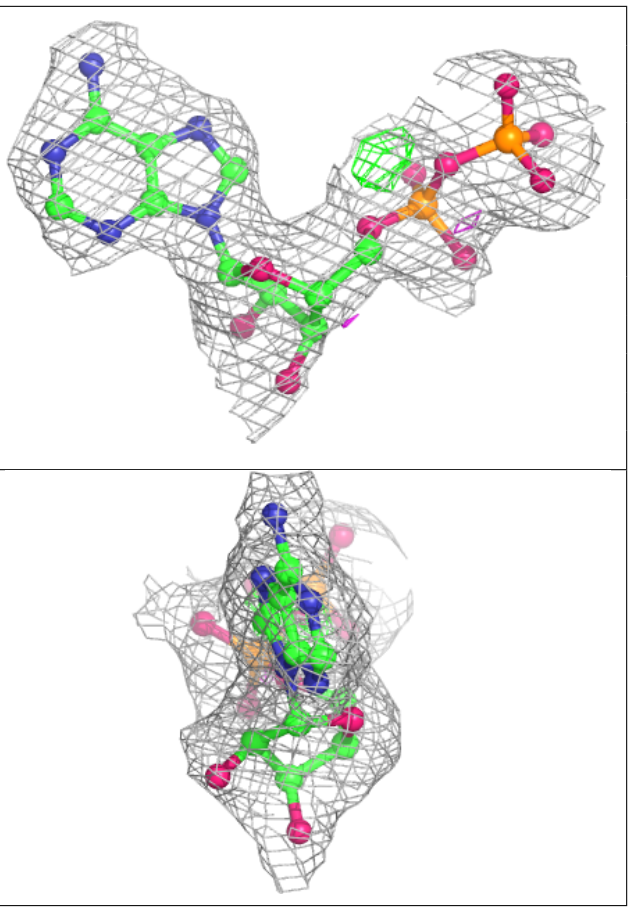






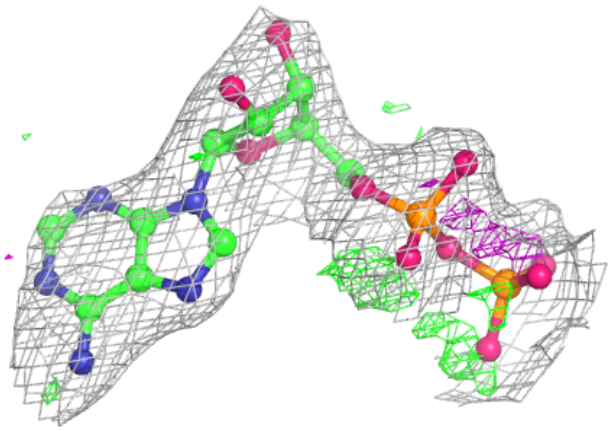
Electron density around ADP A 212:

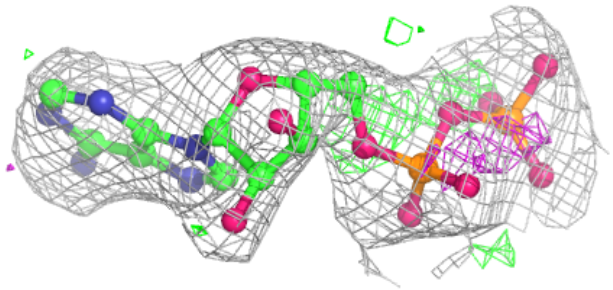
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

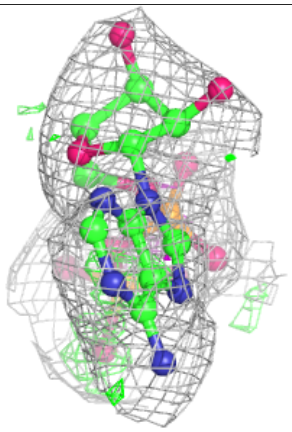


Electron density around ADP B 212:

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

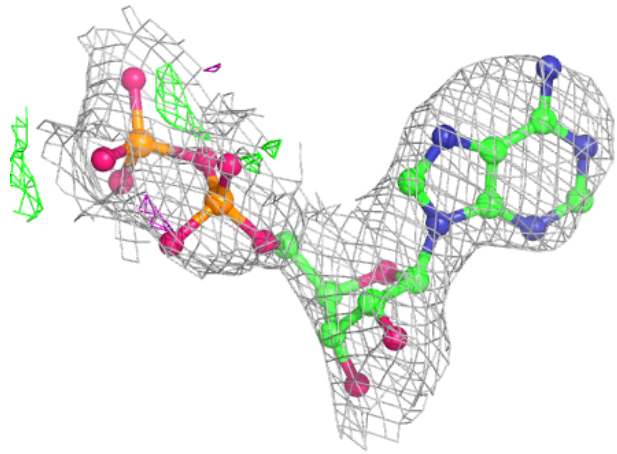


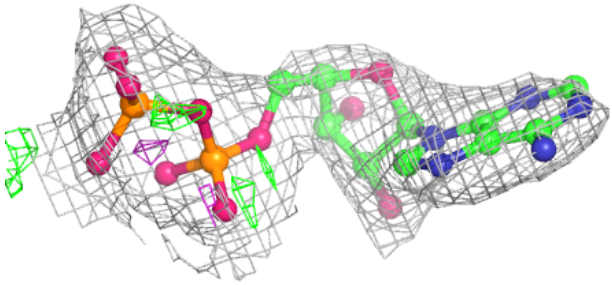


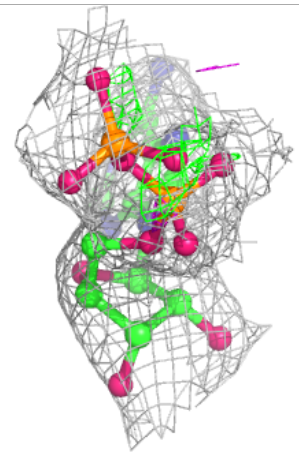


Electron density around ADP C 212:

$2mF_o$-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.