Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 04:10 PM BST

PDB ID	:	3WB2
Title	:	HcgB from Methanocaldococcus jannaschii in complex with the guanylyl-pyridinol product in a model reaction of [Fe]-hydrogenase cofactor biosynthesis
Authors	:	Fujishiro, T.; Ermler, U.; Shima, S.
Deposited on	:	2013-05-11
Resolution	:	2.44 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 following versions of software and data (see references ⓘ) were used in the production of this report:

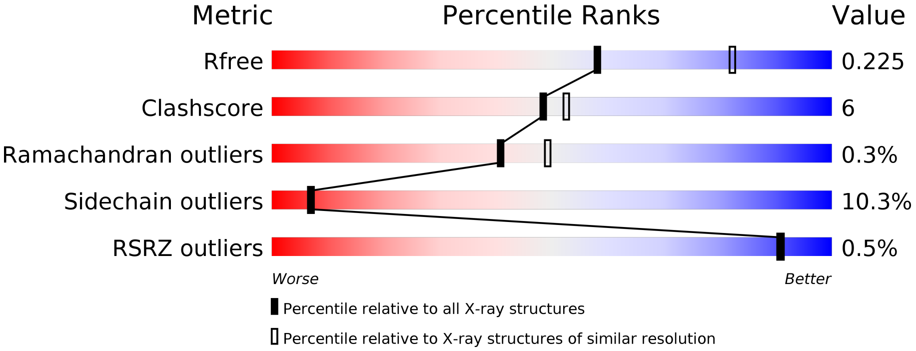
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

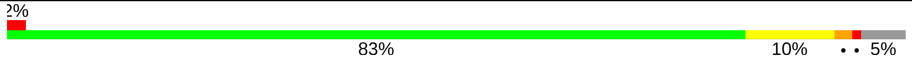
The reported resolution of this entry is 2.44 Å.

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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	166	
1	B	166	
1	C	166	
1	D	166	

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 5284 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 Uncharacterized protein MJ0488.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	160	1260	798	223	233	6	0	0	0
1	B	157	1233	781	218	228	6	0	0	0
1	C	157	1233	781	218	228	6	0	0	0
1	D	160	1260	798	223	233	6	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q57912
A	2	VAL	-	EXPRESSION TAG	UNP Q57912
A	159	LEU	-	EXPRESSION TAG	UNP Q57912
A	160	GLU	-	EXPRESSION TAG	UNP Q57912
A	161	HIS	-	EXPRESSION TAG	UNP Q57912
A	162	HIS	-	EXPRESSION TAG	UNP Q57912
A	163	HIS	-	EXPRESSION TAG	UNP Q57912
A	164	HIS	-	EXPRESSION TAG	UNP Q57912
A	165	HIS	-	EXPRESSION TAG	UNP Q57912
A	166	HIS	-	EXPRESSION TAG	UNP Q57912
B	1	MET	-	EXPRESSION TAG	UNP Q57912
B	2	VAL	-	EXPRESSION TAG	UNP Q57912
B	159	LEU	-	EXPRESSION TAG	UNP Q57912
B	160	GLU	-	EXPRESSION TAG	UNP Q57912
B	161	HIS	-	EXPRESSION TAG	UNP Q57912
B	162	HIS	-	EXPRESSION TAG	UNP Q57912
B	163	HIS	-	EXPRESSION TAG	UNP Q57912
B	164	HIS	-	EXPRESSION TAG	UNP Q57912
B	165	HIS	-	EXPRESSION TAG	UNP Q57912
B	166	HIS	-	EXPRESSION TAG	UNP Q57912
C	1	MET	-	EXPRESSION TAG	UNP Q57912

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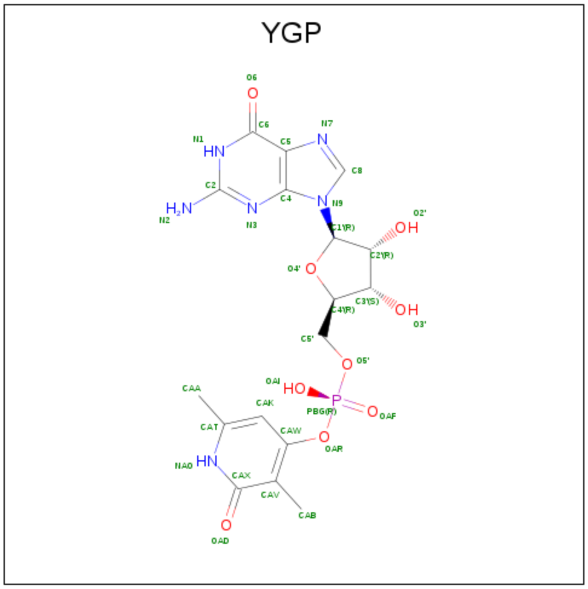
Chain	Residue	Modelled	Actual	Comment	Reference
C	2	VAL	-	EXPRESSION TAG	UNP Q57912
C	159	LEU	-	EXPRESSION TAG	UNP Q57912
C	160	GLU	-	EXPRESSION TAG	UNP Q57912
C	161	HIS	-	EXPRESSION TAG	UNP Q57912
C	162	HIS	-	EXPRESSION TAG	UNP Q57912
C	163	HIS	-	EXPRESSION TAG	UNP Q57912
C	164	HIS	-	EXPRESSION TAG	UNP Q57912
C	165	HIS	-	EXPRESSION TAG	UNP Q57912
C	166	HIS	-	EXPRESSION TAG	UNP Q57912
D	1	MET	-	EXPRESSION TAG	UNP Q57912
D	2	VAL	-	EXPRESSION TAG	UNP Q57912
D	159	LEU	-	EXPRESSION TAG	UNP Q57912
D	160	GLU	-	EXPRESSION TAG	UNP Q57912
D	161	HIS	-	EXPRESSION TAG	UNP Q57912
D	162	HIS	-	EXPRESSION TAG	UNP Q57912
D	163	HIS	-	EXPRESSION TAG	UNP Q57912
D	164	HIS	-	EXPRESSION TAG	UNP Q57912
D	165	HIS	-	EXPRESSION TAG	UNP Q57912
D	166	HIS	-	EXPRESSION TAG	UNP Q57912

- Molecule 2 is 5'-O-[(R)-[(3,6-dimethyl-2-oxo-1,2-dihydropyridin-4-yl)oxy](hydroxy)phosphoryl]guanosine (three-letter code: YGP) (formula: $C_{17}H_{21}N_6O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	33	17	6	9	1	0	0

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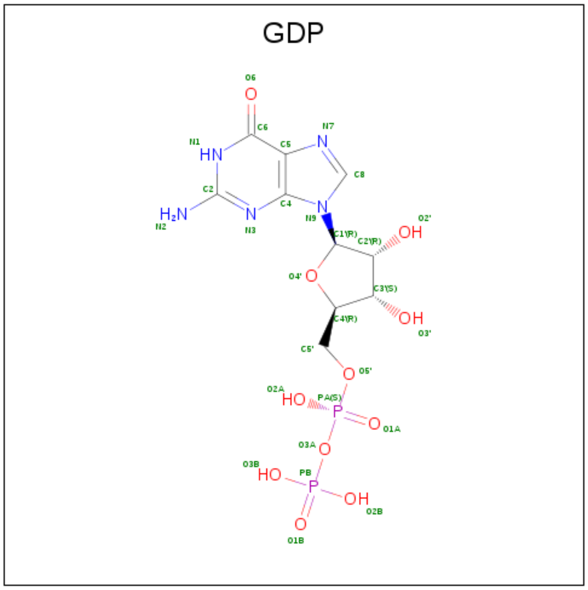
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	33	17	6	9	1	0	0
2	C	1	33	17	6	9	1	0	0
2	C	1	33	17	6	9	1	0	0

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

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

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	28	10	5	11	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	42	42	42	0	0

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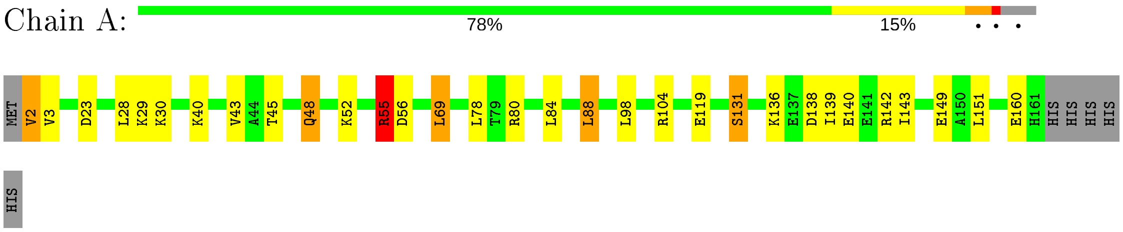
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	43	Total O 43 43	0	0
5	C	28	Total O 28 28	0	0
5	D	23	Total O 23 23	0	0

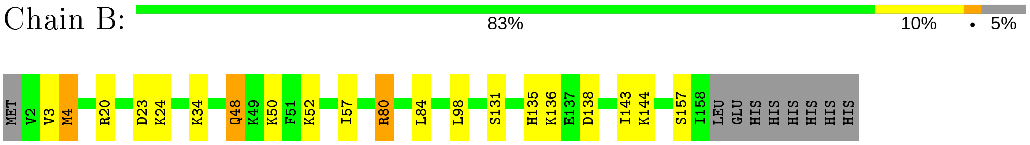
3 Residue-property plots ⓘ

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

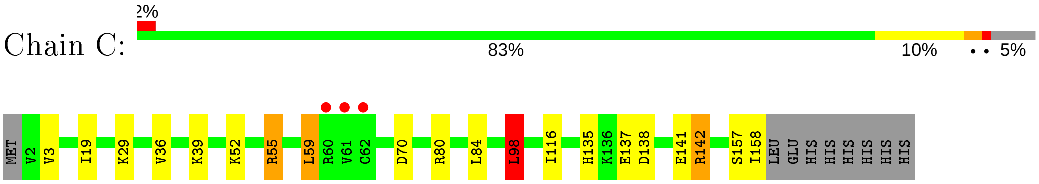
- Molecule 1: Uncharacterized protein MJ0488



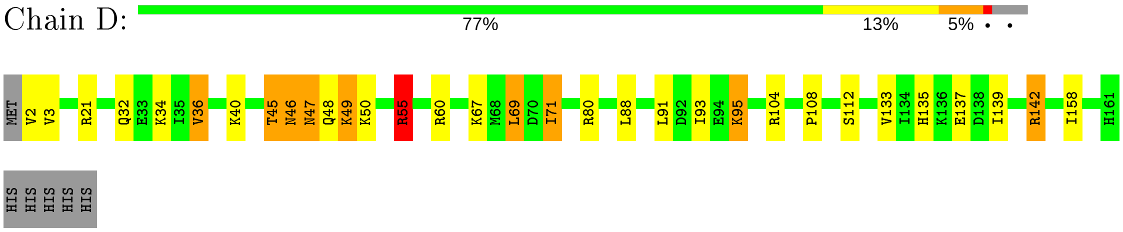
- Molecule 1: Uncharacterized protein MJ0488



- Molecule 1: Uncharacterized protein MJ0488



- Molecule 1: Uncharacterized protein MJ0488



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	115.01Å 97.37Å 63.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.51 – 2.44 49.51 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.51-2.44) 99.3 (49.51-2.44)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.45Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.172 , 0.226 0.172 , 0.225	Depositor DCC
R_{free} test set	1362 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 57.4	EDS
L-test for twinning[2]	$< \|L\| >$ = 0.48, $< L^2 >$ = 0.31	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5284	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 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, YGP

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	0.78	0/1268	1.02	5/1695 (0.3%)
1	B	0.77	0/1240	0.96	1/1657 (0.1%)
1	C	0.68	0/1240	0.87	1/1657 (0.1%)
1	D	0.73	0/1268	0.93	1/1695 (0.1%)
All	All	0.74	0/5016	0.95	8/6704 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	104	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	A	98	LEU	CA-CB-CG	6.29	129.77	115.30
1	A	55	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	69	LEU	CB-CG-CD1	-5.93	100.92	111.00
1	C	98	LEU	CB-CG-CD1	-5.29	102.00	111.00
1	A	88	LEU	CA-CB-CG	5.24	127.36	115.30
1	B	20	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	D	55	ARG	NE-CZ-NH2	5.13	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1260	0	1364	17	0
1	B	1233	0	1340	11	0
1	C	1233	0	1340	12	0
1	D	1260	0	1364	30	0
2	A	66	0	40	0	0
2	C	66	0	40	1	0
3	A	2	0	0	0	0
4	A	28	0	12	0	0
5	A	42	0	0	1	0
5	B	43	0	0	1	0
5	C	28	0	0	2	0
5	D	23	0	0	1	0
All	All	5284	0	5500	64	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 (64) 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:D:55:ARG:HG2	1:D:55:ARG:HH21	1.37	0.88
1:A:3:VAL:HG21	1:D:95:LYS:NZ	1.91	0.85
1:D:135:HIS:HD2	1:D:137:GLU:H	1.28	0.81
1:C:98:LEU:HD11	1:C:116:ILE:CG2	2.12	0.79
1:C:98:LEU:HD11	1:C:116:ILE:HG23	1.66	0.77
1:A:55:ARG:HH11	1:A:55:ARG:HG2	1.52	0.73
1:B:4:MET:HG3	1:B:34:LYS:HE3	1.73	0.71
1:D:50:LYS:HE2	1:D:139:ILE:HD13	1.74	0.70
1:C:19:ILE:HG22	1:C:19:ILE:O	1.93	0.68
1:A:3:VAL:HG21	1:D:95:LYS:HZ1	1.59	0.67
1:D:67:LYS:NZ	5:D:223:HOH:O	2.28	0.67
1:C:98:LEU:CD1	1:C:116:ILE:HG23	2.25	0.66
1:B:57:ILE:HD11	1:B:144:LYS:HG3	1.78	0.66
1:A:55:ARG:HH11	1:A:55:ARG:CG	2.08	0.65
1:D:45:THR:HB	1:D:46:ASN:O	1.95	0.65
1:A:43:VAL:HG12	1:A:45:THR:HG22	1.79	0.64
1:A:48:GLN:HB2	5:A:316:HOH:O	1.96	0.64
1:D:55:ARG:CG	1:D:55:ARG:HH21	2.10	0.62
1:A:2:VAL:O	1:A:30:LYS:HE2	2.00	0.62
1:D:71:ILE:HG22	1:D:71:ILE:O	2.00	0.60
1:D:46:ASN:C	1:D:46:ASN:HD22	2.05	0.60
1:B:48:GLN:HG3	1:B:52:LYS:HE3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:VAL:HG21	1:D:95:LYS:HZ2	1.66	0.58
1:C:19:ILE:CG2	1:C:19:ILE:O	2.51	0.58
5:C:317:HOH:O	1:D:50:LYS:CE	2.52	0.58
1:D:69:LEU:HD11	1:D:93:ILE:HD11	1.85	0.58
1:C:135:HIS:HD2	1:C:137:GLU:H	1.51	0.58
5:C:317:HOH:O	1:D:50:LYS:HE2	2.06	0.56
1:B:80:ARG:NH2	1:D:91:LEU:HD23	2.21	0.55
1:B:138:ASP:HB3	5:B:227:HOH:O	2.06	0.55
1:D:69:LEU:HD13	1:D:71:ILE:HD12	1.87	0.55
1:B:48:GLN:CG	1:B:52:LYS:HE3	2.41	0.51
1:D:48:GLN:HG3	1:D:48:GLN:O	2.11	0.50
1:A:138:ASP:HB3	1:A:140:GLU:OE2	2.12	0.49
1:C:138:ASP:HB3	1:C:141:GLU:HB2	1.93	0.49
1:A:3:VAL:CG2	1:D:95:LYS:NZ	2.71	0.49
1:D:71:ILE:O	1:D:71:ILE:CG2	2.60	0.48
1:D:46:ASN:HD22	1:D:47:ASN:HB3	1.77	0.48
1:D:46:ASN:HD22	1:D:47:ASN:CB	2.26	0.48
1:D:60:ARG:HB2	1:D:158:ILE:HD11	1.96	0.48
1:B:50:LYS:HG2	1:B:143:ILE:HD13	1.96	0.47
1:B:144:LYS:HE3	1:B:144:LYS:HB2	1.51	0.47
1:C:135:HIS:CD2	1:C:137:GLU:H	2.31	0.47
1:D:46:ASN:ND2	1:D:47:ASN:CB	2.78	0.46
1:D:46:ASN:ND2	1:D:47:ASN:HB2	2.31	0.46
1:B:135:HIS:O	1:B:136:LYS:HB2	2.17	0.45
1:D:47:ASN:OD1	1:D:49:LYS:HG2	2.16	0.45
1:A:55:ARG:NH1	1:A:55:ARG:HG2	2.24	0.44
1:A:55:ARG:NH1	1:A:56:ASP:OD1	2.50	0.44
1:A:139:ILE:O	1:A:143:ILE:HG12	2.18	0.44
1:D:142:ARG:HA	1:D:142:ARG:HD2	1.77	0.44
1:D:55:ARG:CG	1:D:55:ARG:NH2	2.77	0.44
1:D:32:GLN:O	1:D:36:VAL:HG13	2.17	0.43
1:A:2:VAL:O	1:A:30:LYS:CE	2.66	0.43
1:C:142:ARG:HA	1:C:142:ARG:HD2	1.65	0.43
1:C:55:ARG:HD2	1:C:59:LEU:HD22	2.00	0.42
1:C:158:ILE:O	1:C:158:ILE:HG22	2.19	0.42
1:D:135:HIS:CD2	1:D:137:GLU:H	2.19	0.42
1:A:55:ARG:HH11	1:A:55:ARG:CB	2.34	0.41
1:A:23:ASP:HB2	1:B:131:SER:HB3	2.03	0.41
1:A:131:SER:HB3	1:B:23:ASP:HB2	2.03	0.41
1:C:59:LEU:HD12	1:C:59:LEU:HA	1.92	0.40
2:C:201:YGP:H21	2:C:201:YGP:H12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ARG:HD2	1:D:108:PRO:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	158/166 (95%)	154 (98%)	3 (2%)	1 (1%)	25	29
1	B	155/166 (93%)	150 (97%)	5 (3%)	0	100	100
1	C	155/166 (93%)	151 (97%)	4 (3%)	0	100	100
1	D	158/166 (95%)	151 (96%)	6 (4%)	1 (1%)	25	29
All	All	626/664 (94%)	606 (97%)	18 (3%)	2 (0%)	41	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	GLU
1	D	47	ASN

5.3.2 Protein sidechains ⓘ

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	140/146 (96%)	122 (87%)	18 (13%)	4	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	137/146 (94%)	129 (94%)	8 (6%)	20	26
1	C	137/146 (94%)	124 (90%)	13 (10%)	8	9
1	D	140/146 (96%)	122 (87%)	18 (13%)	4	3
All	All	554/584 (95%)	497 (90%)	57 (10%)	7	7

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	28	LEU
1	A	29	LYS
1	A	40	LYS
1	A	48	GLN
1	A	52	LYS
1	A	55	ARG
1	A	69	LEU
1	A	78	LEU
1	A	80	ARG
1	A	84	LEU
1	A	88	LEU
1	A	119	GLU
1	A	131	SER
1	A	136	LYS
1	A	142	ARG
1	A	149	GLU
1	A	151	LEU
1	B	3	VAL
1	B	4	MET
1	B	24	LYS
1	B	48	GLN
1	B	80	ARG
1	B	84	LEU
1	B	98	LEU
1	B	157	SER
1	C	3	VAL
1	C	29	LYS
1	C	36	VAL
1	C	39	LYS
1	C	52	LYS
1	C	55	ARG
1	C	59	LEU

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Mol	Chain	Res	Type
1	C	70	ASP
1	C	80	ARG
1	C	84	LEU
1	C	98	LEU
1	C	142	ARG
1	C	157	SER
1	D	2	VAL
1	D	3	VAL
1	D	21	ARG
1	D	34	LYS
1	D	36	VAL
1	D	40	LYS
1	D	45	THR
1	D	46	ASN
1	D	49	LYS
1	D	55	ARG
1	D	69	LEU
1	D	71	ILE
1	D	80	ARG
1	D	88	LEU
1	D	95	LYS
1	D	112	SER
1	D	133	VAL
1	D	142	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	B	48	GLN
1	C	135	HIS
1	D	46	ASN
1	D	48	GLN
1	D	135	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	YGP	A	202	-	32,36,36	2.52	12 (37%)	38,55,55	2.20	14 (36%)
4	GDP	A	204	3	24,30,30	1.43	3 (12%)	31,47,47	2.05	6 (19%)
2	YGP	A	201	-	32,36,36	2.35	9 (28%)	38,55,55	1.96	9 (23%)
2	YGP	C	202	-	32,36,36	2.25	12 (37%)	38,55,55	2.04	8 (21%)
2	YGP	C	201	-	32,36,36	2.44	10 (31%)	38,55,55	2.24	9 (23%)

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	YGP	A	202	-	-	2/11/31/31	0/4/4/4
4	GDP	A	204	3	-	2/12/32/32	0/3/3/3
2	YGP	A	201	-	-	1/11/31/31	0/4/4/4
2	YGP	C	202	-	-	0/11/31/31	0/4/4/4
2	YGP	C	201	-	-	0/11/31/31	0/4/4/4

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	YGP	O4'-C1'	6.89	1.50	1.41
2	A	202	YGP	O4'-C1'	6.07	1.49	1.41
2	A	201	YGP	C6-N1	5.56	1.42	1.33
2	A	202	YGP	C6-N1	5.55	1.42	1.33
2	A	201	YGP	O4'-C1'	5.39	1.48	1.41
2	A	202	YGP	CAX-NAO	5.30	1.42	1.33
4	A	204	GDP	C6-C5	5.16	1.50	1.41
2	C	202	YGP	O4'-C1'	5.14	1.48	1.41
2	C	201	YGP	C6-N1	4.89	1.41	1.33
2	A	201	YGP	CAT-NAO	4.77	1.43	1.34
2	C	201	YGP	CAX-NAO	4.67	1.41	1.33
2	C	202	YGP	CAX-NAO	4.66	1.41	1.33
2	A	202	YGP	C2-N1	4.49	1.43	1.35
2	A	201	YGP	CAX-NAO	4.42	1.40	1.33
2	C	202	YGP	C6-N1	4.36	1.40	1.33
2	C	201	YGP	CAA-CAT	-4.34	1.40	1.50
2	A	201	YGP	CAA-CAT	-4.07	1.40	1.50
2	A	202	YGP	CAB-CAV	-4.05	1.41	1.51
2	A	201	YGP	C6-C5	-4.00	1.34	1.41
2	C	202	YGP	C6-C5	-3.77	1.34	1.41
2	A	202	YGP	CAT-NAO	3.60	1.41	1.34
2	C	202	YGP	C2-N1	3.60	1.41	1.35
2	C	201	YGP	C2-N1	3.55	1.41	1.35
2	C	201	YGP	CAT-NAO	3.51	1.41	1.34
2	C	201	YGP	CAB-CAV	-3.47	1.43	1.51
2	C	201	YGP	C6-C5	-3.35	1.35	1.41
2	C	202	YGP	CAT-NAO	3.35	1.41	1.34
2	C	202	YGP	CAB-CAV	-3.20	1.43	1.51
2	A	201	YGP	C2-N1	3.19	1.41	1.35
2	A	201	YGP	CAB-CAV	-3.10	1.44	1.51
2	C	202	YGP	CAW-CAV	3.07	1.44	1.40
4	A	204	GDP	C5-C4	3.07	1.49	1.40
2	A	202	YGP	CAA-CAT	-3.04	1.43	1.50
2	C	202	YGP	CAA-CAT	-2.92	1.43	1.50
2	A	202	YGP	O4'-C4'	2.83	1.51	1.45
2	A	202	YGP	PBG-O5'	2.74	1.70	1.59
2	A	201	YGP	PBG-OAR	2.55	1.65	1.60
2	A	202	YGP	PBG-OAI	2.48	1.66	1.55
2	C	202	YGP	C5-C4	-2.44	1.34	1.40
2	A	202	YGP	PBG-OAR	2.28	1.65	1.60
2	C	202	YGP	O4'-C4'	2.23	1.50	1.45
2	C	202	YGP	PBG-OAR	2.22	1.65	1.60
2	C	201	YGP	O4'-C4'	2.18	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	YGP	C5-C4	-2.12	1.35	1.40
2	A	202	YGP	CAK-CAW	2.05	1.42	1.38
4	A	204	GDP	O4'-C1'	2.01	1.43	1.41

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	201	YGP	N3-C2-N1	-6.67	118.32	127.22
2	A	201	YGP	N3-C2-N1	-6.28	118.84	127.22
2	C	202	YGP	N3-C2-N1	-6.21	118.94	127.22
2	C	201	YGP	C2-N3-C4	5.95	122.15	115.36
2	C	201	YGP	CAV-CAX-NAO	-5.64	117.58	125.25
2	C	202	YGP	C2-N3-C4	5.37	121.49	115.36
2	A	202	YGP	N3-C2-N1	-5.20	120.29	127.22
2	A	202	YGP	CAV-CAX-NAO	-5.08	118.35	125.25
2	A	201	YGP	C2-N3-C4	5.05	121.13	115.36
2	A	202	YGP	C2-N3-C4	5.01	121.08	115.36
4	A	204	GDP	C6-C5-C4	-4.96	116.07	120.80
4	A	204	GDP	C6-N1-C2	4.55	123.16	115.93
2	C	202	YGP	CAV-CAX-NAO	-4.49	119.14	125.25
4	A	204	GDP	C2-N3-C4	4.45	120.44	115.36
2	A	201	YGP	CAV-CAX-NAO	-4.14	119.63	125.25
2	A	202	YGP	CAX-NAO-CAT	4.06	122.60	116.89
4	A	204	GDP	C5-C6-N1	-4.01	117.94	123.43
2	C	202	YGP	CAX-NAO-CAT	3.90	122.36	116.89
2	A	202	YGP	C5-C6-N1	-3.77	118.27	123.43
2	C	201	YGP	CAX-NAO-CAT	3.58	121.92	116.89
4	A	204	GDP	N3-C2-N1	-3.51	122.55	127.22
2	A	202	YGP	O4'-C1'-C2'	-3.15	102.32	106.93
2	A	201	YGP	CAX-NAO-CAT	3.11	121.25	116.89
2	C	201	YGP	N2-C2-N1	3.06	122.00	117.25
2	C	201	YGP	PBG-OAR-CAW	2.95	131.58	124.07
2	C	202	YGP	OAI-PBG-OAR	2.84	113.42	104.14
2	A	202	YGP	C1'-N9-C4	2.83	131.61	126.64
2	C	201	YGP	CAB-CAV-CAW	-2.81	116.47	120.68
2	C	201	YGP	C5-C6-N1	-2.80	119.61	123.43
2	A	202	YGP	OAR-CAW-CAK	2.73	125.06	119.46
2	A	201	YGP	N2-C2-N3	2.68	122.16	117.79
2	C	202	YGP	PBG-OAR-CAW	2.66	130.85	124.07
2	A	202	YGP	PBG-OAR-CAW	2.61	130.72	124.07
2	C	201	YGP	C4-C5-N7	-2.51	106.78	109.40
2	C	202	YGP	C5-C6-N1	-2.37	120.20	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	202	YGP	N2-C2-N1	2.35	120.90	117.25
2	A	201	YGP	OAR-CAW-CAK	2.29	124.16	119.46
2	A	202	YGP	CAX-CAV-CAW	2.25	119.41	116.51
2	A	201	YGP	CAK-CAT-NAO	-2.21	118.27	121.49
4	A	204	GDP	O3'-C3'-C4'	2.18	117.36	111.05
2	A	201	YGP	CAA-CAT-NAO	2.17	120.03	116.56
2	A	202	YGP	CAK-CAT-NAO	-2.14	118.37	121.49
2	A	202	YGP	CAA-CAT-NAO	2.09	119.89	116.56
2	A	201	YGP	C5'-C4'-C3'	-2.05	107.51	115.18
2	A	202	YGP	C4-C5-N7	-2.04	107.27	109.40
2	C	202	YGP	N2-C2-N1	2.01	120.38	117.25

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	204	GDP	PA-O3A-PB-O1B
4	A	204	GDP	O4'-C4'-C5'-O5'
2	A	202	YGP	CAW-OAR-PBG-O5'
2	A	202	YGP	CAW-OAR-PBG-OAF
2	A	201	YGP	C5'-O5'-PBG-OAF

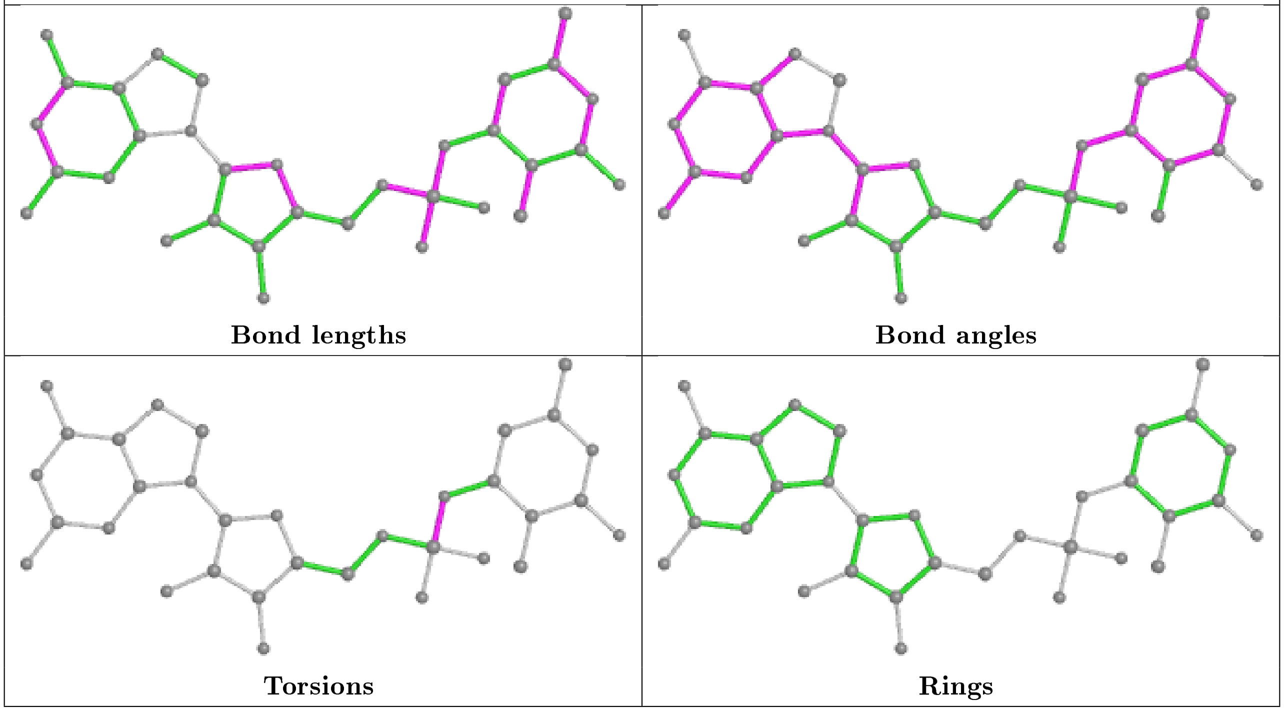
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	201	YGP	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 YGP A 202



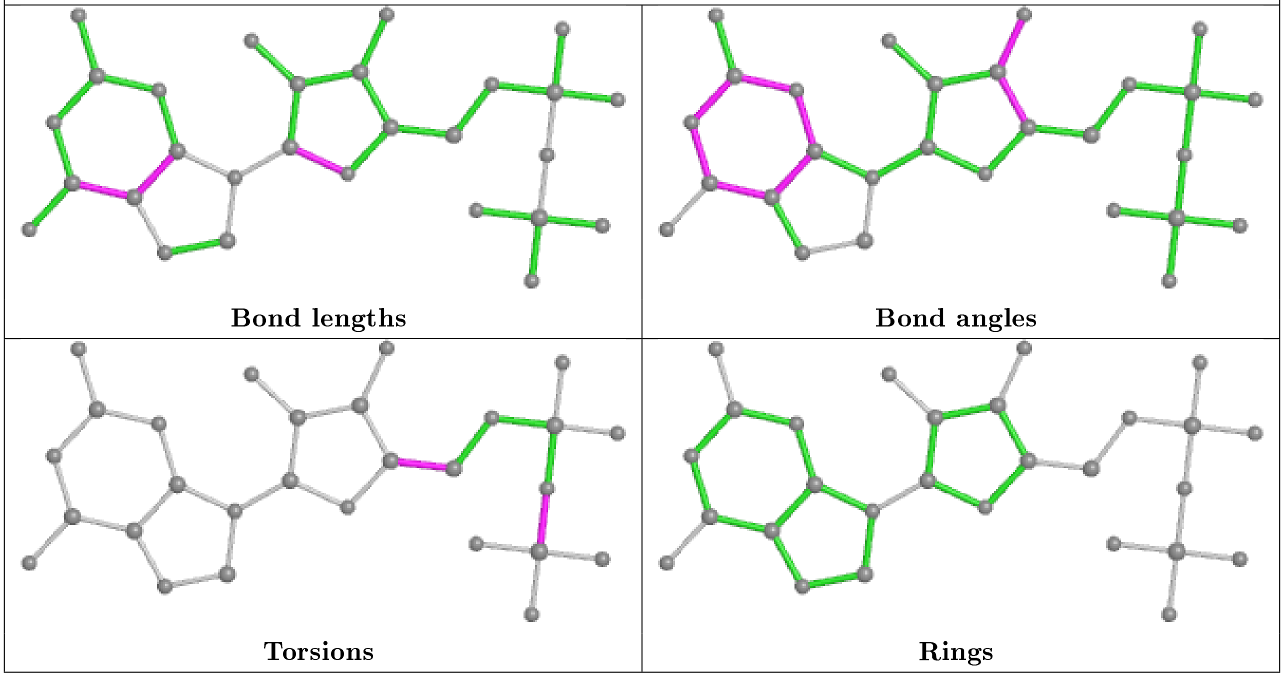
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP A 204



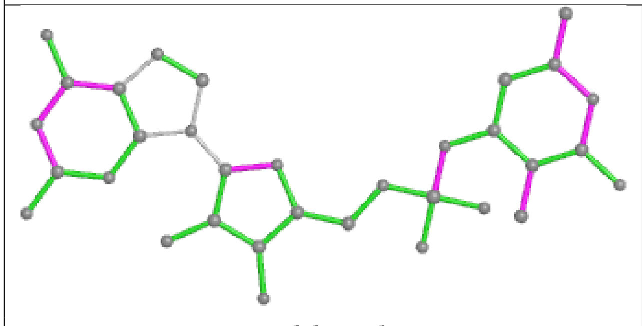
Bond lengths

Bond angles

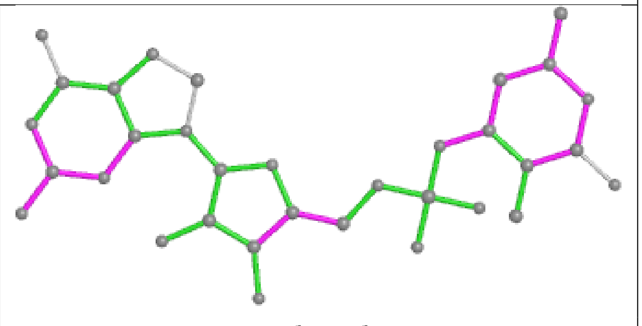
Torsions

Rings

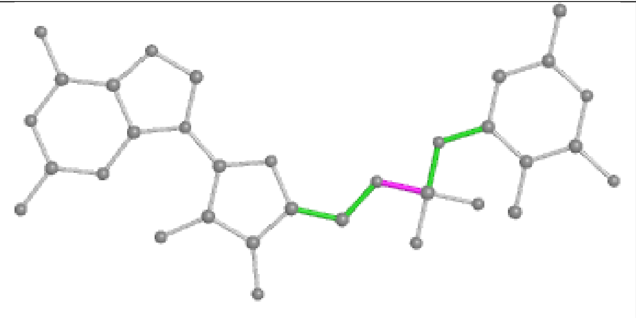
Ligand YGP A 201



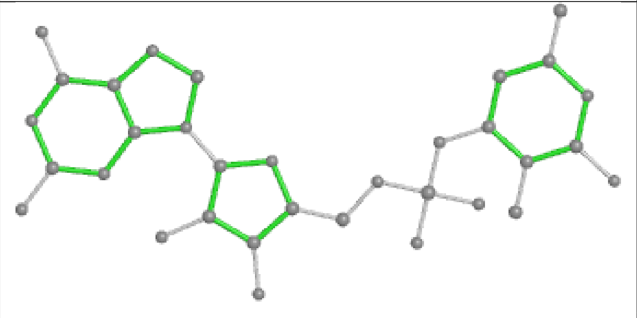
Bond lengths



Bond angles

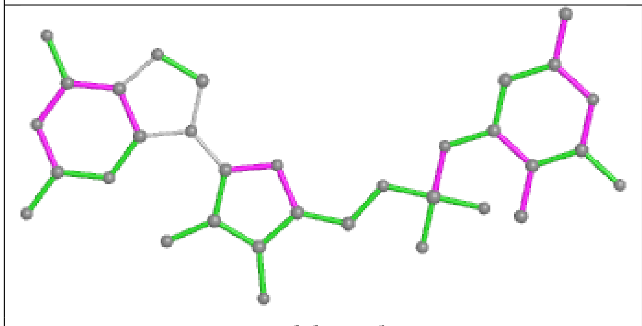


Torsions

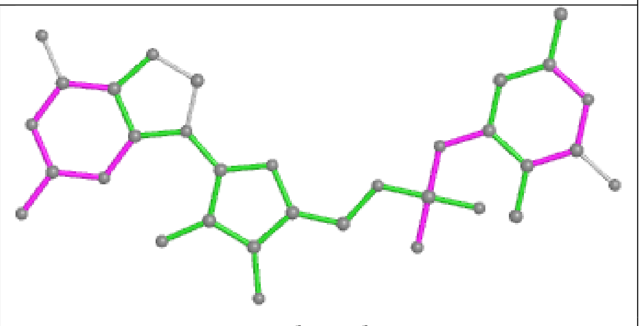


Rings

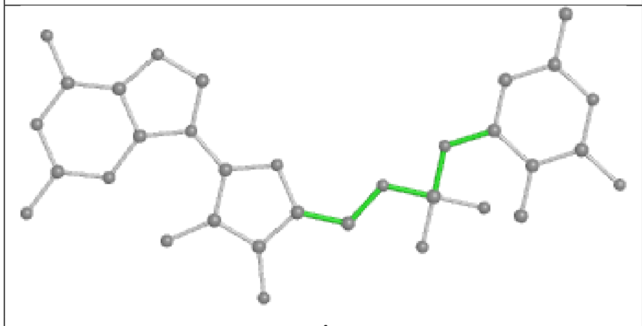
Ligand YGP C 202



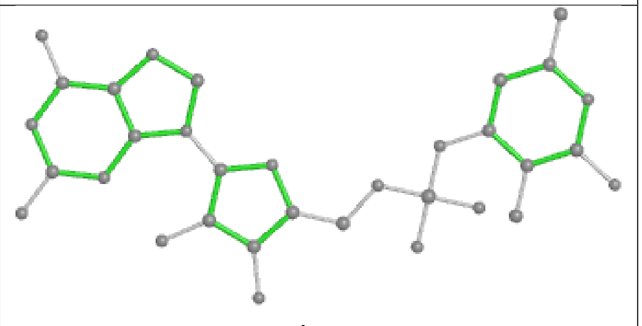
Bond lengths



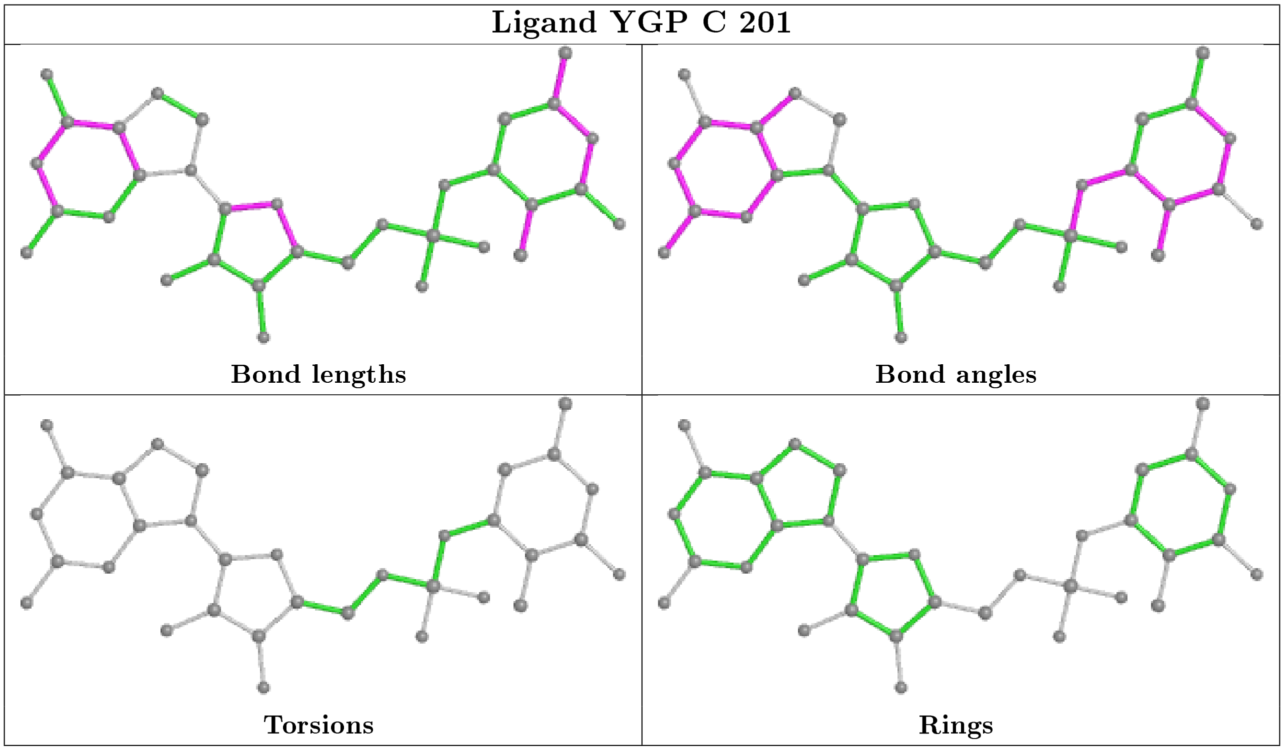
Bond angles



Torsions



Rings



Ligand YGP C 201

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	160/166 (96%)	-0.61	0	100	100	22, 37, 62, 81	0
1	B	157/166 (94%)	-0.64	0	100	100	24, 36, 58, 65	0
1	C	157/166 (94%)	-0.32	3 (1%)	66	63	30, 47, 70, 83	1 (0%)
1	D	160/166 (96%)	-0.62	0	100	100	27, 41, 74, 82	0
All	All	634/664 (95%)	-0.55	3 (0%)	91	91	22, 40, 65, 83	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	61	VAL	2.7
1	C	60	ARG	2.4
1	C	62	CYS	2.4

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

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

6.3 Carbohydrates ⓘ

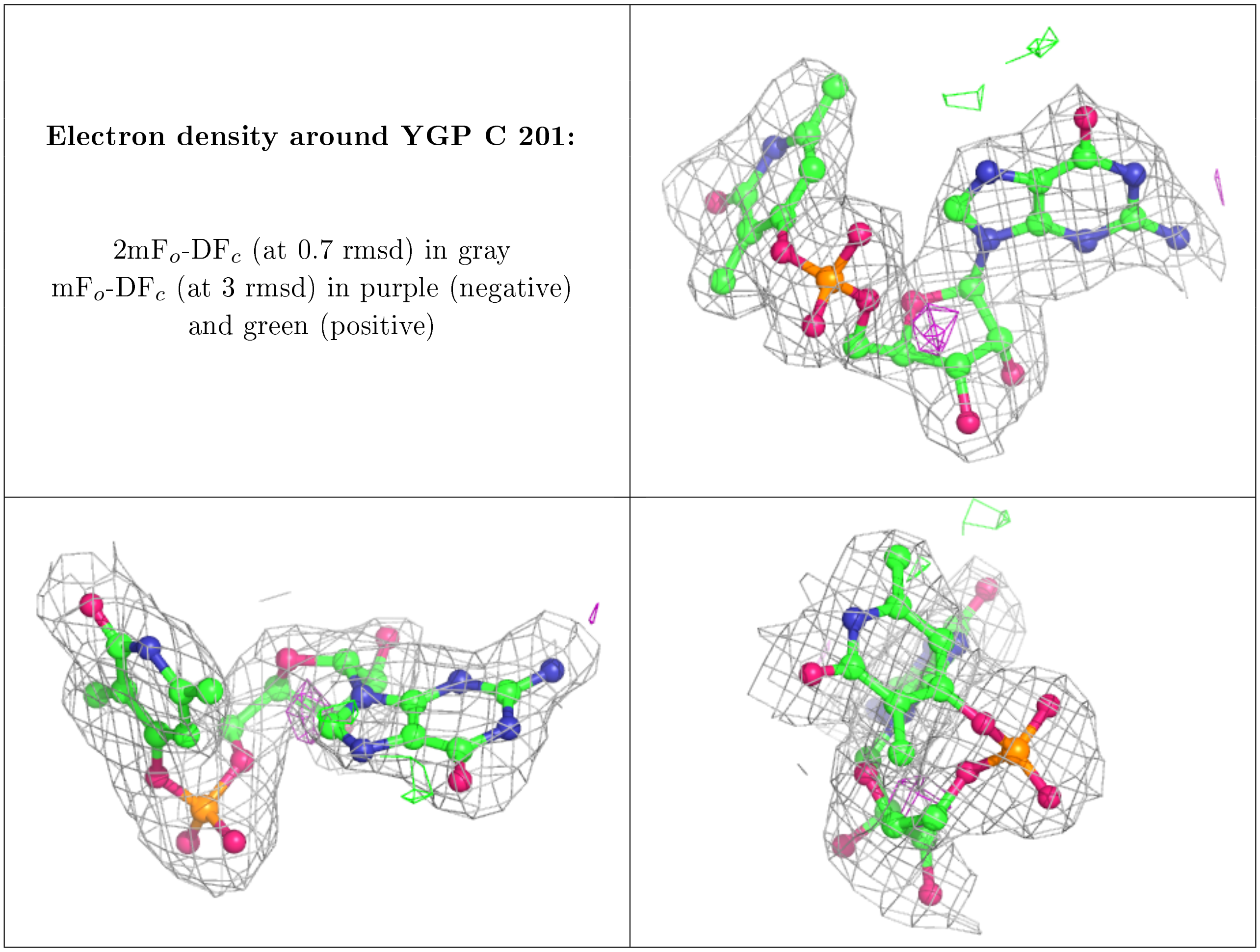
There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

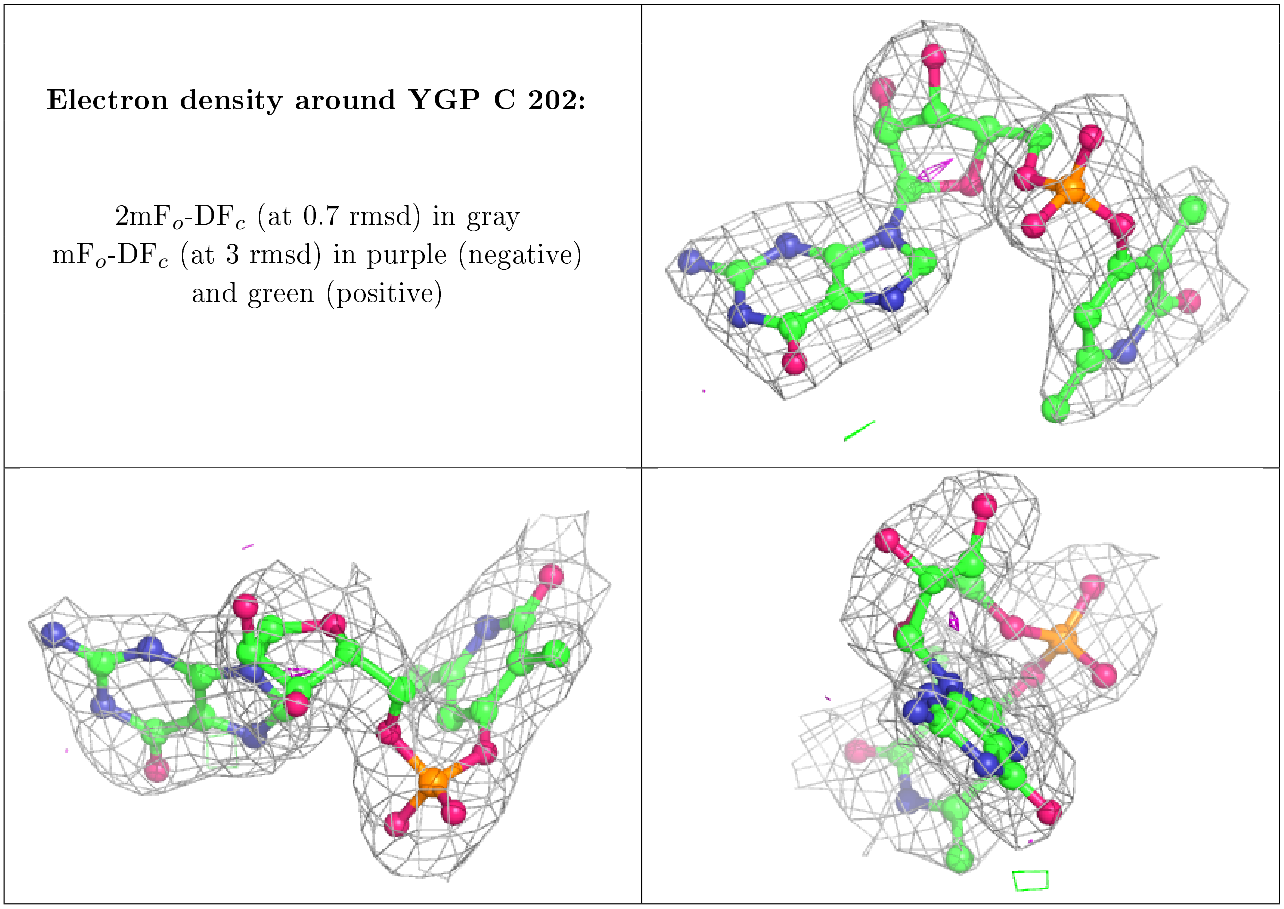
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	YGP	C	201	33/33	0.94	0.13	34,67,89,90	0
2	YGP	C	202	33/33	0.96	0.12	38,54,66,72	0
2	YGP	A	202	33/33	0.96	0.14	36,42,55,56	0
3	MG	A	203	1/1	0.97	0.07	49,49,49,49	0
4	GDP	A	204	28/28	0.97	0.10	36,48,70,76	0
3	MG	A	205	1/1	0.99	0.13	19,19,19,19	0
2	YGP	A	201	33/33	0.99	0.12	24,31,37,45	0

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.



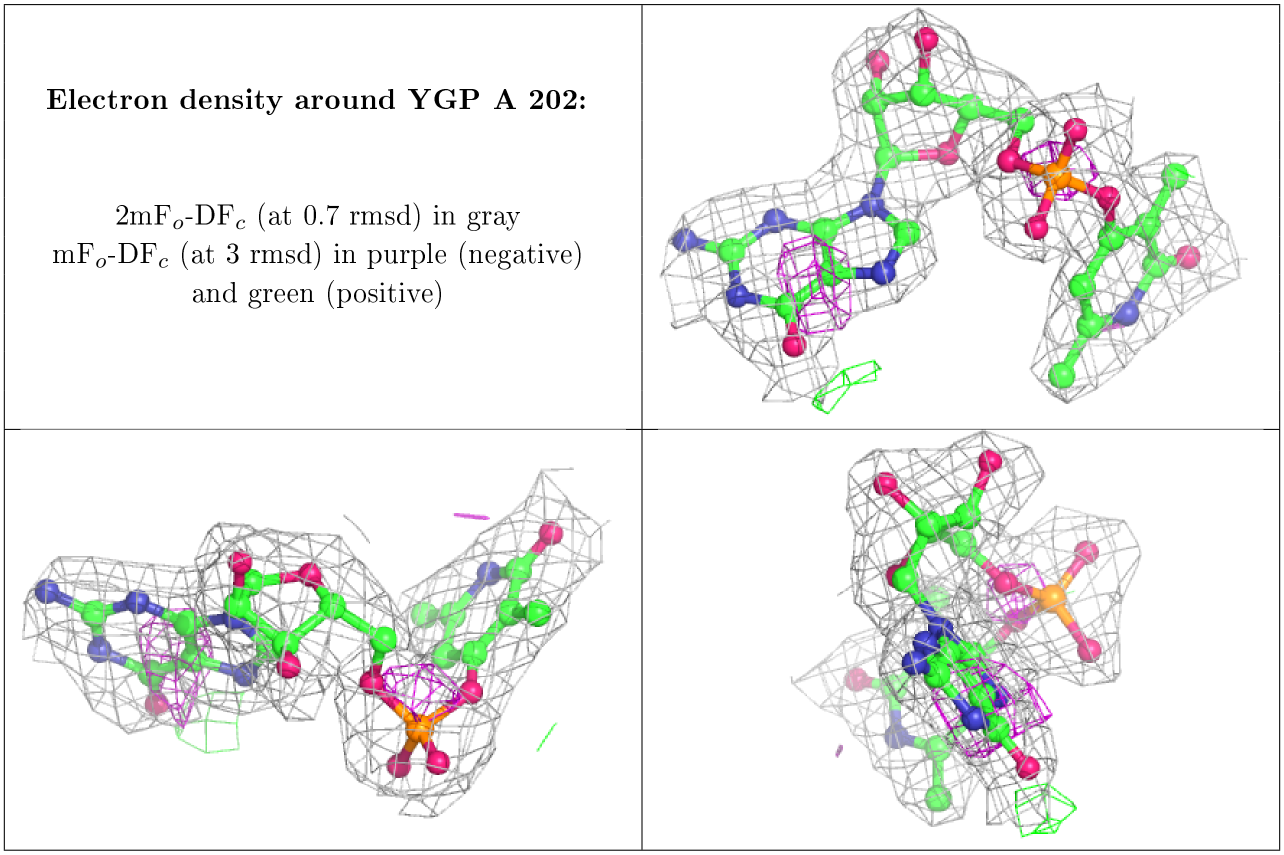
Electron density around YGP C 201:

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



Electron density around YGP C 202:

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

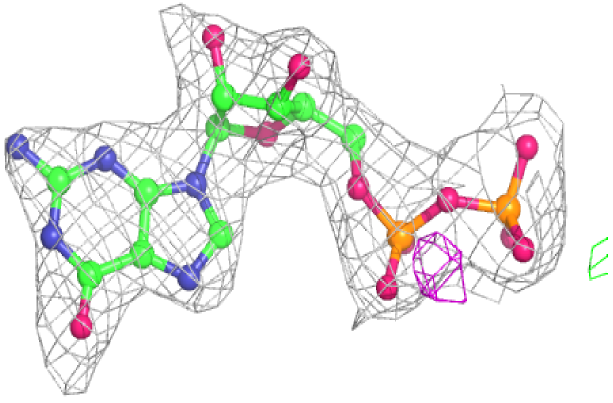


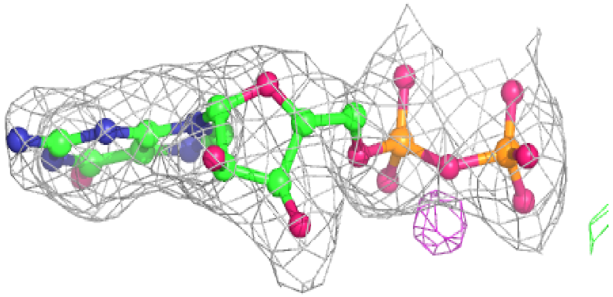
Electron density around YGP A 202:

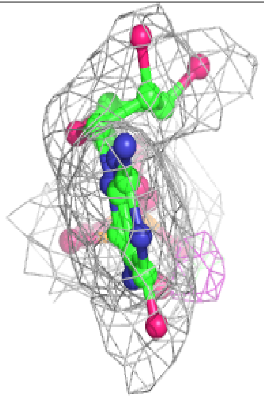
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around GDP A 204:

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

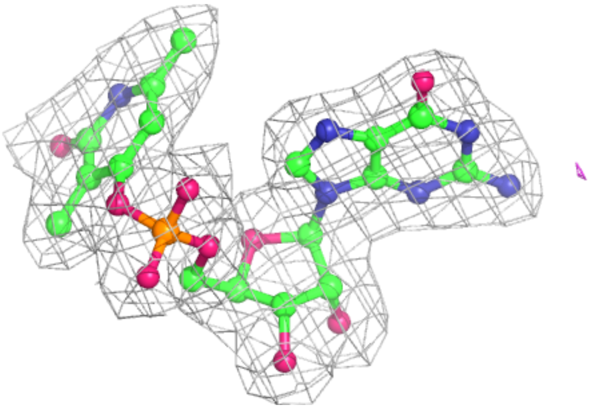


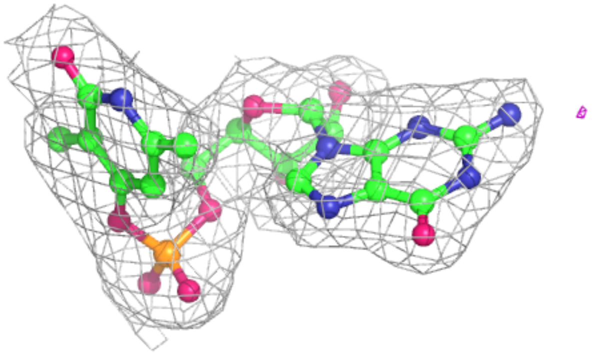




Electron density around YGP A 201:

$2mF_o$-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 ⓘ

There are no such residues in this entry.