



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:10 PM GMT

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

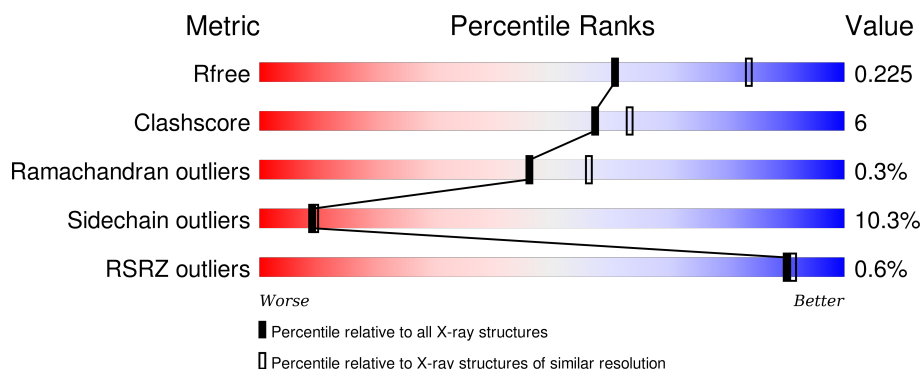
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1003 (2.46-2.42)
Clashscore	102246	1071 (2.46-2.42)
Ramachandran outliers	100387	1065 (2.46-2.42)
Sidechain outliers	100360	1065 (2.46-2.42)
RSRZ outliers	91569	1005 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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
1	A	160	Total	C	N	O	S	0	0	0
			1260	798	223	233	6			
1	B	157	Total	C	N	O	S	0	0	0
			1233	781	218	228	6			
1	C	157	Total	C	N	O	S	0	0	0
			1233	781	218	228	6			
1	D	160	Total	C	N	O	S	0	0	0
			1260	798	223	233	6			

There are 40 discrepancies between the modelled and reference sequences:

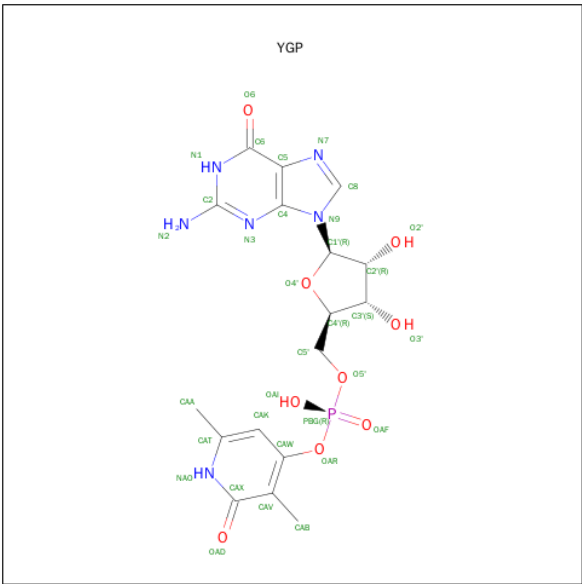
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q57912
A	2	VAL	-	EXPRESSION TAG	UNP Q57912
A	159	LEU	-	EXPRESSION TAG	UNP Q57912
A	160	GLU	-	EXPRESSION TAG	UNP Q57912
A	161	HIS	-	EXPRESSION TAG	UNP Q57912
A	162	HIS	-	EXPRESSION TAG	UNP Q57912
A	163	HIS	-	EXPRESSION TAG	UNP 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<sub>17</sub>H<sub>21</sub>N<sub>6</sub>O<sub>9</sub>P).



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

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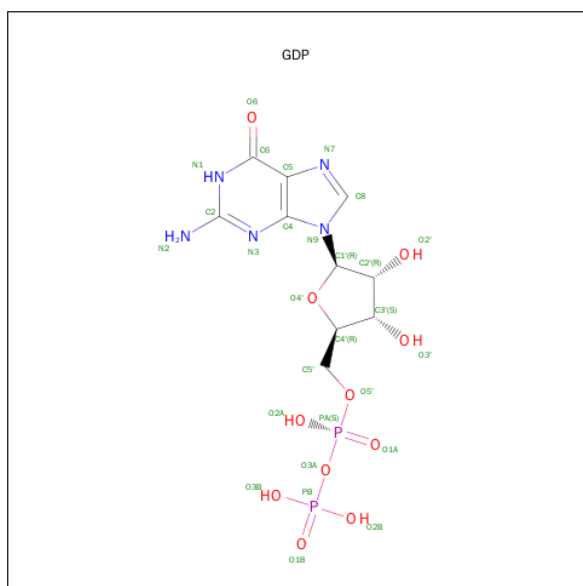
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			33	17	6	9	1		
2	C	1	Total	C	N	O	P	0	0
			33	17	6	9	1		
2	C	1	Total	C	N	O	P	0	0
			33	17	6	9	1		

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

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

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



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

- Molecule 5 is water.

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

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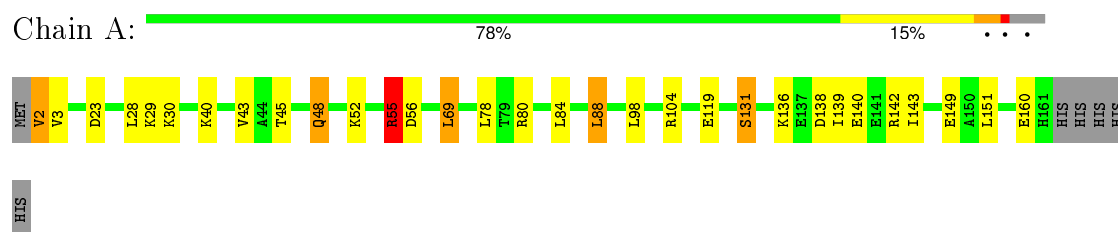
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	43	Total 43	O 43	0	0
5	C	28	Total 28	O 28	0	0
5	D	23	Total 23	O 23	0	0

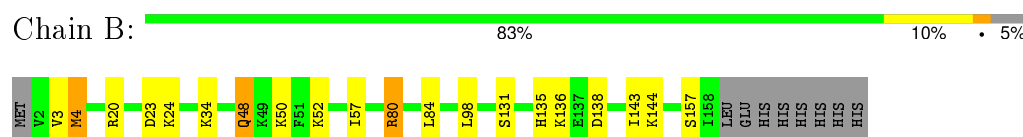
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

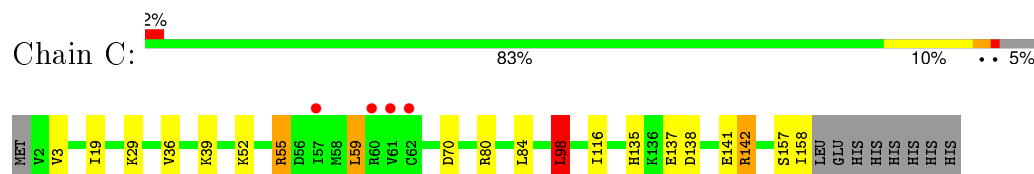
- Molecule 1: Uncharacterized protein MJ0488



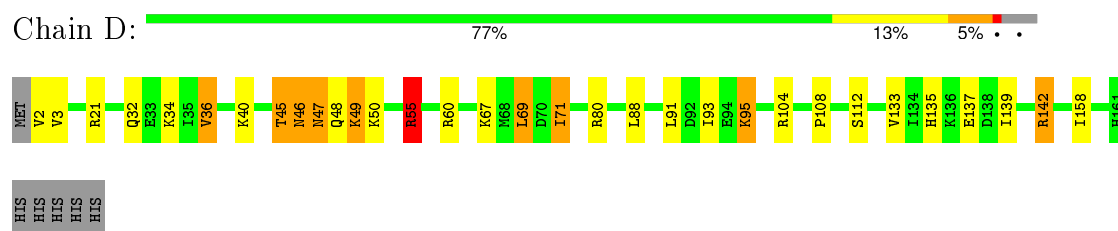
- Molecule 1: Uncharacterized protein MJ0488



- Molecule 1: Uncharacterized protein MJ0488



- Molecule 1: Uncharacterized protein MJ0488



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.01 Å 97.37 Å 63.54 Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.45 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.172 , 0.226 0.172 , 0.225	Depositor DCC
$R_{free}$ test set	1358 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.8	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 27164 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5284	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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	1260	0	1364	17	0
1	B	1233	0	1340	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

The worst 5 of 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

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	158/166 (95%)	154 (98%)	3 (2%)	1 (1%)	30	36
1	B	155/166 (93%)	150 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	155/166 (93%)	151 (97%)	4 (3%)	0	100	100
1	D	158/166 (95%)	151 (96%)	6 (4%)	1 (1%)	30	36
All	All	626/664 (94%)	606 (97%)	18 (3%)	2 (0%)	46	56

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%)	5	4
1	B	137/146 (94%)	129 (94%)	8 (6%)	25	34
1	C	137/146 (94%)	124 (90%)	13 (10%)	11	12
1	D	140/146 (96%)	122 (87%)	18 (13%)	5	4
All	All	554/584 (95%)	497 (90%)	57 (10%)	9	9

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	157	SER
1	C	55	ARG
1	D	88	LEU
1	C	3	VAL
1	C	36	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	135	HIS
1	D	135	HIS
1	D	46	ASN
1	B	48	GLN
1	D	48	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 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	201	-	30,36,36	2.35	9 (30%)	35,55,55	1.85	11 (31%)
2	YGP	A	202	-	30,36,36	2.58	12 (40%)	35,55,55	1.81	10 (28%)
4	GDP	A	204	3	23,30,30	1.43	3 (13%)	30,47,47	2.28	8 (26%)
2	YGP	C	201	-	30,36,36	2.46	10 (33%)	35,55,55	1.99	9 (25%)
2	YGP	C	202	-	30,36,36	2.29	12 (40%)	35,55,55	1.82	8 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	YGP	A	201	-	-	0/11/31/31	0/4/4/4
2	YGP	A	202	-	-	0/11/31/31	0/4/4/4
4	GDP	A	204	3	-	0/12/32/32	0/3/3/3
2	YGP	C	201	-	-	0/11/31/31	0/4/4/4
2	YGP	C	202	-	-	0/11/31/31	0/4/4/4

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	202	YGP	CAB-CAV	-4.45	1.41	1.51
2	C	201	YGP	CAA-CAT	-4.04	1.40	1.50
2	C	201	YGP	CAB-CAV	-3.81	1.43	1.51
2	A	201	YGP	CAA-CAT	-3.79	1.40	1.50
2	C	202	YGP	CAB-CAV	-3.52	1.43	1.51

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	204	GDP	C2'-C1'-N9	-6.54	104.31	114.29
2	C	201	YGP	N3-C2-N1	-5.99	118.32	127.44
2	A	201	YGP	N3-C2-N1	-5.65	118.84	127.44
2	C	202	YGP	N3-C2-N1	-5.58	118.94	127.44
2	A	202	YGP	N3-C2-N1	-4.70	120.29	127.44

There are no chirality outliers.

There are no torsion outliers.

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

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	160/166 (96%)	-0.57	0	100 100	22, 37, 62, 81	0
1	B	157/166 (94%)	-0.60	0	100 100	24, 36, 58, 65	0
1	C	157/166 (94%)	-0.27	4 (2%)	61 59	30, 47, 70, 83	1 (0%)
1	D	160/166 (96%)	-0.58	0	100 100	27, 41, 74, 82	0
All	All	634/664 (95%)	-0.51	4 (0%)	90 91	22, 40, 65, 83	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	61	VAL	2.9
1	C	60	ARG	2.6
1	C	62	CYS	2.5
1	C	57	ILE	2.1

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	YGP	A	202	33/33	0.96	0.14	0.63	36,42,55,56	0
2	YGP	C	201	33/33	0.94	0.13	0.38	34,67,89,90	0
2	YGP	C	202	33/33	0.96	0.12	0.02	38,54,66,72	0
2	YGP	A	201	33/33	0.99	0.12	-0.31	24,31,37,45	0
4	GDP	A	204	28/28	0.97	0.10	-1.61	36,48,70,76	0
3	MG	A	205	1/1	0.99	0.13	-	19,19,19,19	0
3	MG	A	203	1/1	0.97	0.07	-	49,49,49,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.