



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 06:06 pm GMT

PDB ID : 4JTW  
Title : Crystal structure of HCV NS5B polymerase in complex with compound 1  
Authors : Coulombe, R.  
Deposited on : 2013-03-24  
Resolution : 3.00 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

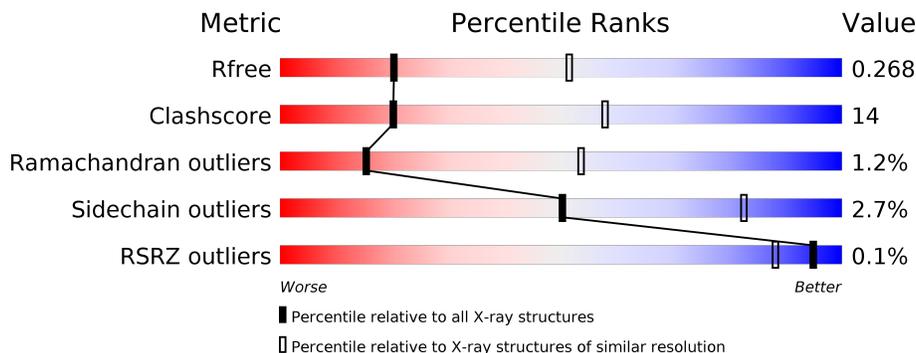
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	576	
1	B	576	

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
2	GOL	A	3001	-	-	-	X
2	GOL	B	601	-	-	-	X
3	1NU	B	602	-	-	-	X
4	MG	A	3004	-	-	-	X
4	MG	B	603	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9122 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.

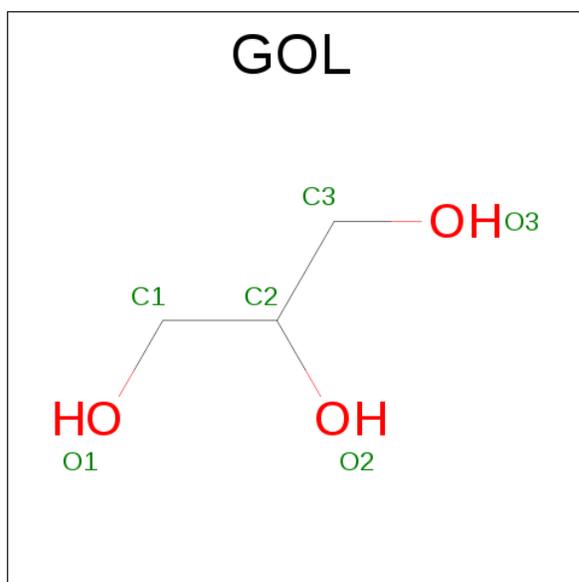
- Molecule 1 is a protein called Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	560	4362	2747	771	812	32	0	0	0
1	B	560	4362	2747	771	812	32	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

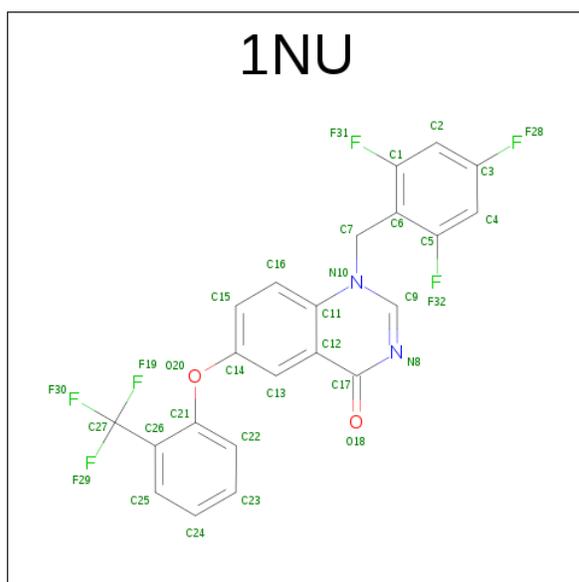
Chain	Residue	Modelled	Actual	Comment	Reference
A	571	HIS	-	EXPRESSION TAG	UNP O92972
A	572	HIS	-	EXPRESSION TAG	UNP O92972
A	573	HIS	-	EXPRESSION TAG	UNP O92972
A	574	HIS	-	EXPRESSION TAG	UNP O92972
A	575	HIS	-	EXPRESSION TAG	UNP O92972
A	576	HIS	-	EXPRESSION TAG	UNP O92972
B	571	HIS	-	EXPRESSION TAG	UNP O92972
B	572	HIS	-	EXPRESSION TAG	UNP O92972
B	573	HIS	-	EXPRESSION TAG	UNP O92972
B	574	HIS	-	EXPRESSION TAG	UNP O92972
B	575	HIS	-	EXPRESSION TAG	UNP O92972
B	576	HIS	-	EXPRESSION TAG	UNP O92972

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 3 is 1-(2,4,6-TRIFLUOROBENZYL)-6-[2-(TRIFLUOROMETHYL)PHENOXY]QUINAZOLIN-4(1H)-ONE (three-letter code: 1NU) (formula: C<sub>22</sub>H<sub>12</sub>F<sub>6</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			32	22	6	2	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	B	1	32	22	6	2	2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

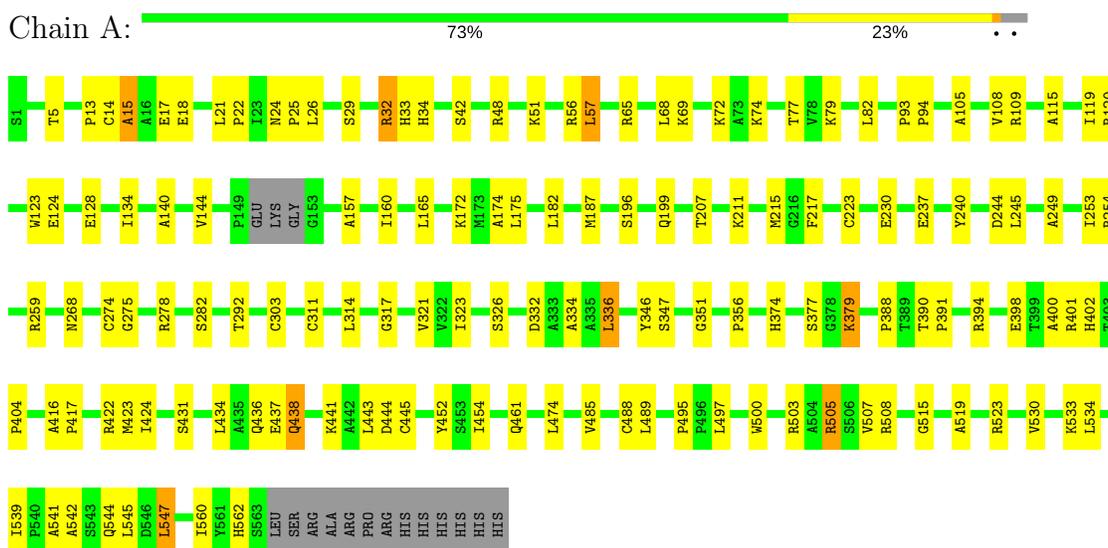
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	169	169	169	0	0
5	B	149	149	149	0	0

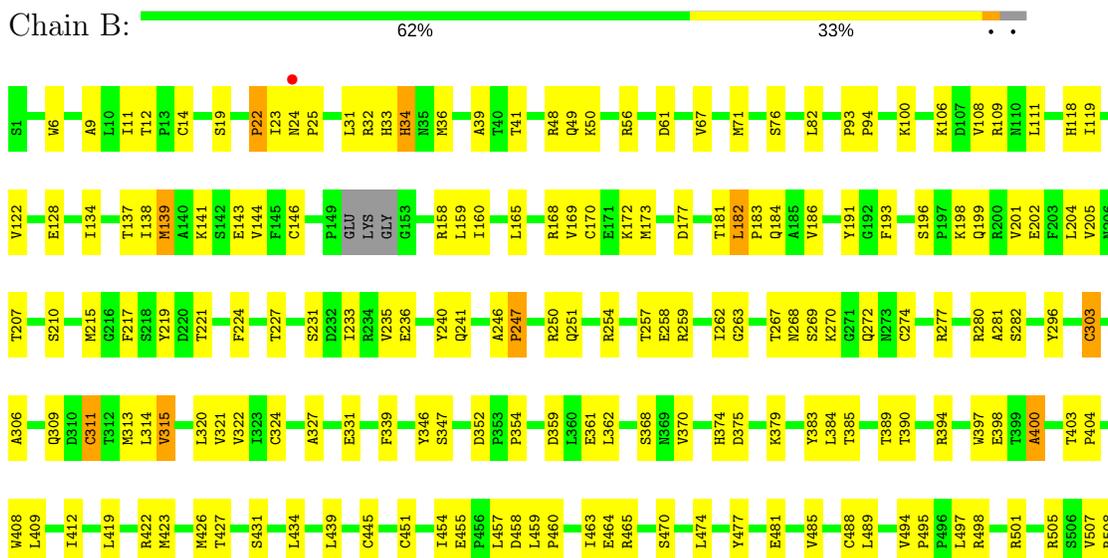
### 3 Residue-property plots

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



- Molecule 1: Genome polyprotein



L511	G515	A519	T620	G521	G522	R523	Y524	L525	A529	V530	K533	L534	K535	P538	I539	P540	A541	A542	L545	D546	L547	V550	I560	Y561	H562	S563	LEU	SER	ARG	ALA	ARG	ARG	PRO	ARG	HIS	HIS	HIS	HIS	HIS
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## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.43Å 108.00Å 134.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 39.19 – 2.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.00) 97.1 (39.19-2.99)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 3.01Å)	Xtrriage
Refinement program	CNX 2002	Depositor
R, $R_{free}$	0.200 , 0.274 0.197 , 0.268	Depositor DCC
$R_{free}$ test set	3118 reflections (11.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.0	Xtrriage
Anisotropy	0.343	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 45.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.008 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9122	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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, 0.333 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: 1NU, MG, 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	0.37	0/4457	0.63	1/6049 (0.0%)
1	B	0.34	0/4457	0.60	0/6049
All	All	0.35	0/8914	0.61	1/12098 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	GLY	N-CA-C	-5.18	100.15	113.10

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	4362	0	4374	104	0
1	B	4362	0	4374	145	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
3	A	32	0	12	1	0
3	B	32	0	12	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	169	0	0	7	0
5	B	149	0	0	12	0
All	All	9122	0	8788	247	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 14.

The worst 5 of 247 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:515:GLY:HA2	1:B:519:ALA:HB2	1.48	0.92
1:B:314:LEU:HB3	1:B:321:VAL:HG13	1.52	0.90
1:A:18:GLU:HG2	1:A:401:ARG:NH2	1.84	0.90
1:B:233:ILE:HD12	1:B:262:ILE:HA	1.59	0.84
1:A:394:ARG:O	1:A:398:GLU:HG3	1.77	0.84

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	556/576 (96%)	515 (93%)	38 (7%)	3 (0%)	32 74
1	B	556/576 (96%)	499 (90%)	47 (8%)	10 (2%)	10 43
All	All	1112/1152 (96%)	1014 (91%)	85 (8%)	13 (1%)	15 53

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	ALA
1	B	33	HIS

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Mol	Chain	Res	Type
1	B	525	LEU
1	B	530	VAL
1	B	541	ALA

### 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	477/491 (97%)	463 (97%)	14 (3%)	48	82
1	B	477/491 (97%)	465 (98%)	12 (2%)	53	84
All	All	954/982 (97%)	928 (97%)	26 (3%)	50	82

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	505	ARG
1	B	34	HIS
1	B	521	CYS
1	A	544	GLN
1	A	547	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	562	HIS
1	B	34	HIS
1	B	446	GLN
1	A	544	GLN
1	B	251	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, 4 are monoatomic - leaving 4 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	GOL	A	3001	-	5,5,5	0.41	0	5,5,5	0.18	0
3	1NU	A	3002	-	34,35,35	2.12	12 (35%)	48,52,52	1.86	9 (18%)
2	GOL	B	601	-	5,5,5	0.38	0	5,5,5	0.18	0
3	1NU	B	602	-	34,35,35	2.46	14 (41%)	48,52,52	2.03	10 (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	GOL	A	3001	-	-	0/4/4/4	0/0/0/0
3	1NU	A	3002	-	-	0/14/14/14	0/4/4/4
2	GOL	B	601	-	-	0/4/4/4	0/0/0/0
3	1NU	B	602	-	-	0/14/14/14	0/4/4/4

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3002	1NU	C2-C1	2.02	1.41	1.37
3	B	602	1NU	C4-C3	2.08	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3002	1NU	C6-C5	2.09	1.41	1.38
3	A	3002	1NU	C24-C25	2.09	1.42	1.38
3	B	602	1NU	C13-C14	2.29	1.41	1.37

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3002	1NU	C4-C5-C6	-7.04	121.55	124.78
3	B	602	1NU	C4-C5-C6	-6.51	121.79	124.78
3	B	602	1NU	C2-C1-C6	-6.31	121.88	124.78
3	A	3002	1NU	C2-C1-C6	-5.13	122.42	124.78
3	B	602	1NU	C16-C11-C12	-3.50	115.27	120.01

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
3	A	3002	1NU	1	0

## 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](#)

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	560/576 (97%)	-0.67	0 <b>100</b>   <b>100</b>	16, 36, 59, 79	0
1	B	560/576 (97%)	-0.41	1 (0%) <b>94</b>   <b>85</b>	19, 50, 91, 103	0
All	All	1120/1152 (97%)	-0.54	1 (0%) <b>95</b>   <b>88</b>	16, 42, 80, 103	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	24	ASN	2.4

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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(Å <sup>2</sup> )	Q<0.9
2	GOL	A	3001	6/6	0.92	0.24	<b>4.39</b>	50,52,53,53	0
4	MG	B	603	1/1	0.94	0.28	<b>3.25</b>	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	B	601	6/6	0.92	0.26	2.17	44,46,47,48	0
4	MG	A	3004	1/1	0.90	0.26	2.15	44,44,44,44	0
3	1NU	B	602	32/32	0.91	0.25	2.15	57,64,70,72	0
4	MG	A	3003	1/1	0.78	0.24	1.82	46,46,46,46	0
3	1NU	A	3002	32/32	0.96	0.18	1.74	37,43,52,54	0
4	MG	B	604	1/1	0.74	0.38	-	56,56,56,56	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.