



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:40 am BST

PDB ID : 4ELZ  
Title : CCDBVFI:GYRA14VFI  
Authors : De Jonge, N.; Simic, M.; Buts, L.; Haesaerts, S.; Roelants, K.; Garcia-Pino, A.; Sterckx, Y.; De Greve, H.; Lah, J.; Loris, R.  
Deposited on : 2012-04-11  
Resolution : 2.20 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](mailto: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 : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

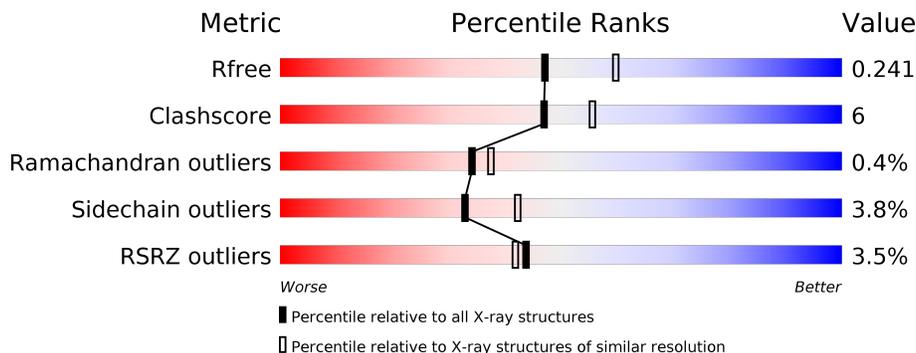
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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  $\leq 5\%$ . 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	153	 3% 76% 14% 7%
1	B	153	 2% 75% 10% 14%
2	C	105	 5% 81% 18%
2	D	105	 4% 81% 15%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	501	-	-	X	-

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 3866 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 DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	143	1085	693	191	198	3	0	1	0
1	B	131	1002	646	174	180	2	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	342	MET	-	INITIATING METHIONINE	UNP Q5E5J7
A	343	GLY	-	EXPRESSION TAG	UNP Q5E5J7
A	344	SER	-	EXPRESSION TAG	UNP Q5E5J7
A	345	SER	-	EXPRESSION TAG	UNP Q5E5J7
A	346	HIS	-	EXPRESSION TAG	UNP Q5E5J7
A	347	HIS	-	EXPRESSION TAG	UNP Q5E5J7
A	348	HIS	-	EXPRESSION TAG	UNP Q5E5J7
A	349	HIS	-	EXPRESSION TAG	UNP Q5E5J7
A	350	HIS	-	EXPRESSION TAG	UNP Q5E5J7
A	351	HIS	-	EXPRESSION TAG	UNP Q5E5J7
A	352	SER	-	EXPRESSION TAG	UNP Q5E5J7
A	353	SER	-	EXPRESSION TAG	UNP Q5E5J7
A	354	GLY	-	EXPRESSION TAG	UNP Q5E5J7
A	355	LEU	-	EXPRESSION TAG	UNP Q5E5J7
A	356	VAL	-	EXPRESSION TAG	UNP Q5E5J7
A	357	PRO	-	EXPRESSION TAG	UNP Q5E5J7
A	358	ARG	-	EXPRESSION TAG	UNP Q5E5J7
A	359	GLY	-	EXPRESSION TAG	UNP Q5E5J7
A	360	SER	-	EXPRESSION TAG	UNP Q5E5J7
A	361	HIS	-	EXPRESSION TAG	UNP Q5E5J7
A	362	MET	-	EXPRESSION TAG	UNP Q5E5J7
B	342	MET	-	INITIATING METHIONINE	UNP Q5E5J7
B	343	GLY	-	EXPRESSION TAG	UNP Q5E5J7
B	344	SER	-	EXPRESSION TAG	UNP Q5E5J7
B	345	SER	-	EXPRESSION TAG	UNP Q5E5J7

*Continued on next page...*

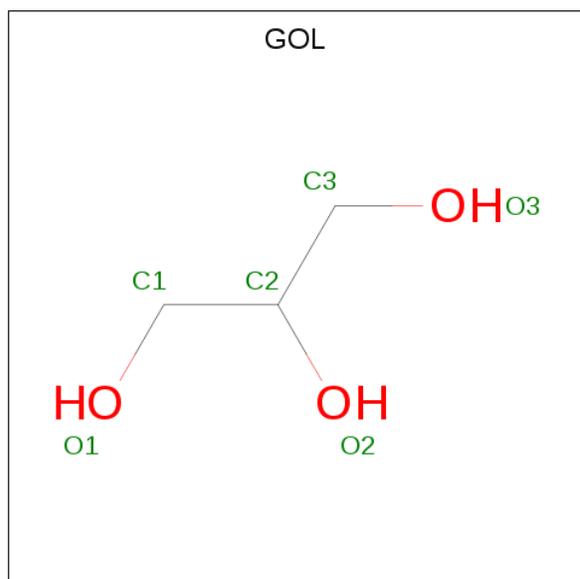
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	346	HIS	-	EXPRESSION TAG	UNP Q5E5J7
B	347	HIS	-	EXPRESSION TAG	UNP Q5E5J7
B	348	HIS	-	EXPRESSION TAG	UNP Q5E5J7
B	349	HIS	-	EXPRESSION TAG	UNP Q5E5J7
B	350	HIS	-	EXPRESSION TAG	UNP Q5E5J7
B	351	HIS	-	EXPRESSION TAG	UNP Q5E5J7
B	352	SER	-	EXPRESSION TAG	UNP Q5E5J7
B	353	SER	-	EXPRESSION TAG	UNP Q5E5J7
B	354	GLY	-	EXPRESSION TAG	UNP Q5E5J7
B	355	LEU	-	EXPRESSION TAG	UNP Q5E5J7
B	356	VAL	-	EXPRESSION TAG	UNP Q5E5J7
B	357	PRO	-	EXPRESSION TAG	UNP Q5E5J7
B	358	ARG	-	EXPRESSION TAG	UNP Q5E5J7
B	359	GLY	-	EXPRESSION TAG	UNP Q5E5J7
B	360	SER	-	EXPRESSION TAG	UNP Q5E5J7
B	361	HIS	-	EXPRESSION TAG	UNP Q5E5J7
B	362	MET	-	EXPRESSION TAG	UNP Q5E5J7

- Molecule 2 is a protein called CcdB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	104	Total	C	N	O	S	0	0	0
			796	515	124	154	3			
2	D	102	Total	C	N	O	S	0	1	0
			784	506	122	153	3			

- Molecule 3 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
3	A	1	Total	C	O	0	0
			6	3	3		

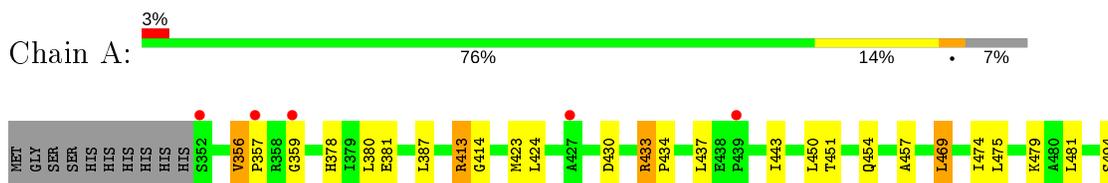
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total	O	0	0
			61	61		
4	B	48	Total	O	0	0
			48	48		
4	C	45	Total	O	0	0
			45	45		
4	D	39	Total	O	0	0
			39	39		

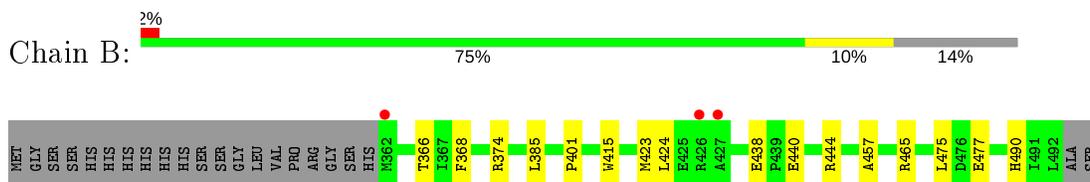
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

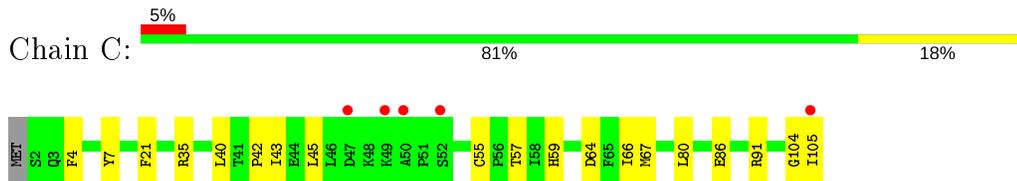
- Molecule 1: DNA gyrase subunit A



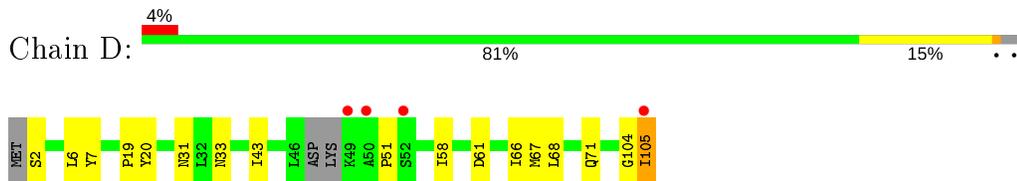
- Molecule 1: DNA gyrase subunit A



- Molecule 2: CcdB



- Molecule 2: CcdB



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.51Å 94.59Å 120.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.94 – 2.20 16.94 – 2.13	Depositor EDS
% Data completeness (in resolution range)	95.8 (16.94-2.20) 94.2 (16.94-2.13)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.17 (at 2.12Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.195 , 0.247 0.190 , 0.241	Depositor DCC
$R_{free}$ test set	1652 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtrriage
Anisotropy	0.200	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 65.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3866	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.00% 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: 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	0.40	0/1106	0.56	0/1498
1	B	0.37	0/1018	0.52	0/1376
2	C	0.36	0/812	0.54	0/1111
2	D	0.37	0/802	0.55	0/1096
All	All	0.38	0/3738	0.54	0/5081

There are no bond length outliers.

There are no bond angle outliers.

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	1085	0	1083	18	0
1	B	1002	0	1004	9	0
2	C	796	0	776	14	0
2	D	784	0	767	10	0
3	A	6	0	8	5	0
4	A	61	0	0	0	0
4	B	48	0	0	1	0
4	C	45	0	0	1	0
4	D	39	0	0	2	0
All	All	3866	0	3638	45	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 (45) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:PRO:HD3	3:A:501:GOL:H31	1.59	0.83
1:A:378:HIS:HA	3:A:501:GOL:H11	1.64	0.80
2:C:40:LEU:HD22	2:C:67:MET:HG2	1.68	0.72
1:A:430:ASP:O	1:A:433:ARG:HD2	1.91	0.69
2:D:43:ILE:HG12	2:D:66:ILE:HG12	1.74	0.67
1:A:381:GLU:OE1	3:A:501:GOL:H12	1.97	0.64
1:A:433:ARG:HA	3:A:501:GOL:H31	1.81	0.63
1:B:385:LEU:HD21	1:B:415:TRP:HB2	1.81	0.63
1:A:380:LEU:HD12	1:A:481:LEU:HD12	1.80	0.62
2:C:59:HIS:ND1	2:C:64:ASP:OD1	2.28	0.58
1:A:457:ALA:O	2:D:105:ILE:HD11	2.03	0.58
1:B:368:PHE:CZ	2:D:31:ASN:HB3	2.39	0.57
1:A:423:MET:SD	1:A:479:LYS:HG2	2.47	0.55
2:C:4:PHE:CZ	2:C:91:ARG:HG3	2.42	0.55
1:B:423:MET:HE1	1:B:475:LEU:HD22	1.87	0.54
1:A:413:ARG:HG2	1:A:414:GLY:N	2.23	0.54
1:B:457:ALA:HB1	2:C:105:ILE:HD11	1.90	0.53
2:D:19:PRO:HB2	2:D:20:TYR:CD2	2.45	0.52
2:C:21:PHE:HE1	2:C:80:LEU:HD22	1.76	0.50
1:B:440:GLU:O	1:B:444:ARG:NH1	2.44	0.49
2:C:104:GLY:HA2	4:C:241:HOH:O	2.12	0.48
1:A:434:PRO:HD3	3:A:501:GOL:C3	2.39	0.48
1:A:437:LEU:HD11	1:A:451:THR:HG21	1.94	0.48
2:C:7:TYR:CE1	2:C:80:LEU:HB3	2.48	0.48
1:A:469:LEU:HB2	1:B:401:PRO:O	2.13	0.48
2:D:61:ASP:HA	4:D:239:HOH:O	2.15	0.47
2:D:58:ILE:HD11	2:D:67:MET:HE3	1.95	0.47
2:D:104:GLY:HA2	4:D:209:HOH:O	2.14	0.47
2:C:35:ARG:HG3	2:C:80:LEU:HD11	1.97	0.46
1:B:374:ARG:NH1	4:B:542:HOH:O	2.46	0.46
2:C:43:ILE:HD11	2:C:57:THR:HG23	1.97	0.45
1:A:356:VAL:HA	1:A:357:PRO:HD3	1.91	0.44
1:A:475:LEU:O	1:A:479:LYS:HG3	2.18	0.43
1:B:465:ARG:HH22	2:C:105:ILE:HG22	1.83	0.43
2:C:40:LEU:CD2	2:C:67:MET:HG2	2.43	0.43
2:C:55:CYS:HB3	2:C:66:ILE:HG23	2.00	0.43
2:C:43:ILE:HG12	2:C:66:ILE:HD12	2.01	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:LEU:HD11	1:A:474:ILE:HD12	2.01	0.43
1:A:424:LEU:HB3	1:A:443:ILE:HD11	2.01	0.43
2:D:2:SER:N	2:D:7:TYR:HH	2.17	0.42
1:A:450:LEU:HD22	1:A:454:GLN:HG3	2.01	0.42
2:C:42:PRO:HB2	2:C:45:LEU:HG	2.01	0.41
2:D:68:LEU:HB3	2:D:71:GLN:HG3	2.02	0.41
1:A:433:ARG:HD3	1:A:433:ARG:O	2.21	0.41
1:B:368:PHE:CE2	2:D:31:ASN:HB3	2.57	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	142/153 (93%)	140 (99%)	1 (1%)	1 (1%)	22	22
1	B	129/153 (84%)	127 (98%)	2 (2%)	0	100	100
2	C	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
2	D	99/105 (94%)	94 (95%)	4 (4%)	1 (1%)	15	14
All	All	472/516 (92%)	461 (98%)	9 (2%)	2 (0%)	34	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	51	PRO
1	A	359	GLY

### 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	105/125 (84%)	100 (95%)	5 (5%)	25	32
1	B	93/125 (74%)	88 (95%)	5 (5%)	22	26
2	C	88/99 (89%)	87 (99%)	1 (1%)	73	85
2	D	89/99 (90%)	86 (97%)	3 (3%)	37	47
All	All	375/448 (84%)	361 (96%)	14 (4%)	33	43

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	356	VAL
1	A	413	ARG
1	A	433	ARG
1	A	469	LEU
1	A	494	SER
1	B	366	THR
1	B	424	LEU
1	B	438	GLU
1	B	477	GLU
1	B	490	HIS
2	C	86	GLU
2	D	6	LEU
2	D	33	ASN
2	D	105	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

1 ligand is modelled in this entry.

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
3	GOL	A	501	-	5,5,5	0.35	0	5,5,5	0.80	0

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
3	GOL	A	501	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	GOL	5	0

## 5.7 Other polymers [i](#)

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 [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	143/153 (93%)	-0.28	5 (3%) 44 42	17, 35, 65, 99	0
1	B	131/153 (85%)	-0.32	3 (2%) 60 58	21, 38, 68, 101	0
2	C	104/105 (99%)	-0.22	5 (4%) 30 29	23, 38, 73, 88	0
2	D	102/105 (97%)	-0.11	4 (3%) 39 37	22, 41, 78, 97	0
All	All	480/516 (93%)	-0.24	17 (3%) 44 42	17, 38, 74, 101	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	50	ALA	5.4
1	A	359	GLY	5.0
1	B	427	ALA	4.8
2	D	105	ILE	4.7
1	A	357	PRO	3.8
2	D	50	ALA	3.8
1	A	439	PRO	3.2
2	C	49	LYS	2.9
2	C	47	ASP	2.8
2	D	49	LYS	2.8
1	A	427	ALA	2.8
2	D	52	SER	2.8
1	B	362	MET	2.5
2	C	52	SER	2.4
1	A	352	SER	2.4
2	C	105	ILE	2.3
1	B	426	ARG	2.1

### 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	A	501	6/6	0.88	0.23	50,52,59,63	0

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

There are no such residues in this entry.