



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2020 – 06:28 am BST

PDB ID : 4R40  
Title : Crystal Structure of TolB/Pal complex from Yersinia pestis.  
Authors : Maltseva, N.; Kim, Y.; Osipiuk, J.; Anderson, W.F.; Joachimiak, A.; Center  
for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2014-08-18  
Resolution : 2.50 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

<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

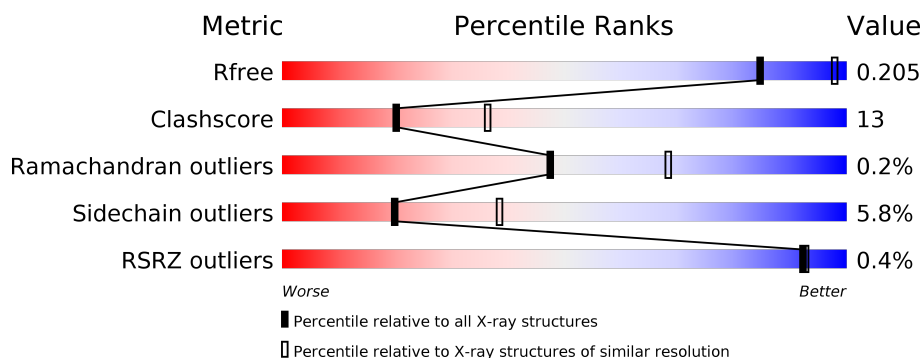
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	411	 66% 30% ..
1	C	411	 71% 24% ..
2	B	141	 68% 17% • 12%
2	D	141	 % 65% 20% .. 12%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8156 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 Protein TolB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	Se	0	2	0
			3079	1941	533	599	6			
1	C	405	Total	C	N	O	Se	0	1	0
			3063	1931	531	596	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	SER	-	EXPRESSION TAG	UNP Q8ZGZ1
A	21	ASN	-	EXPRESSION TAG	UNP Q8ZGZ1
A	22	ALA	-	EXPRESSION TAG	UNP Q8ZGZ1
C	20	SER	-	EXPRESSION TAG	UNP Q8ZGZ1
C	21	ASN	-	EXPRESSION TAG	UNP Q8ZGZ1
C	22	ALA	-	EXPRESSION TAG	UNP Q8ZGZ1

- Molecule 2 is a protein called Peptidoglycan-associated lipoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	124	Total	C	N	O	Se	0	0	0
			967	604	172	188	3			
2	D	124	Total	C	N	O	Se	0	0	0
			967	604	172	188	3			

There are 6 discrepancies between the modelled and reference sequences:

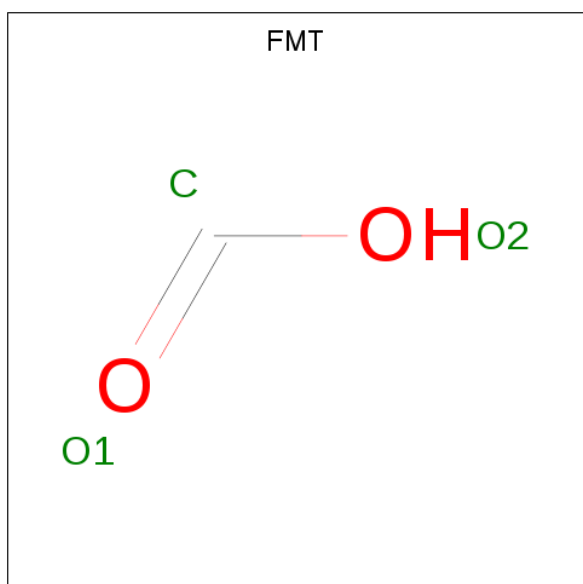
Chain	Residue	Modelled	Actual	Comment	Reference
B	28	SER	-	EXPRESSION TAG	UNP Q7CH55
B	29	ASN	-	EXPRESSION TAG	UNP Q7CH55
B	30	ALA	-	EXPRESSION TAG	UNP Q7CH55
D	28	SER	-	EXPRESSION TAG	UNP Q7CH55
D	29	ASN	-	EXPRESSION TAG	UNP Q7CH55
D	30	ALA	-	EXPRESSION TAG	UNP Q7CH55

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



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

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



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

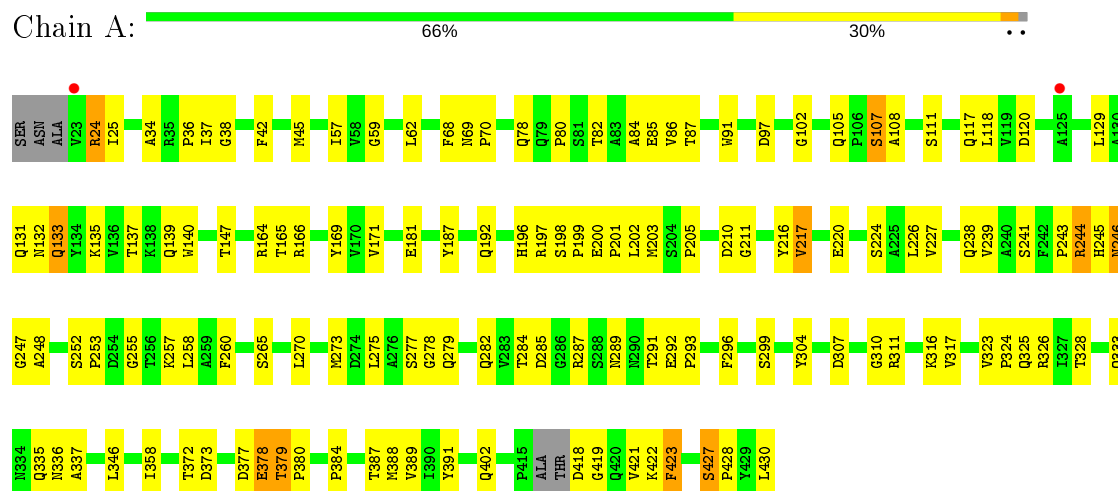
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	14	Total	O	0	0
			14	14		
6	B	7	Total	O	0	0
			7	7		
6	C	12	Total	O	0	0
			12	12		
6	D	3	Total	O	0	0
			3	3		

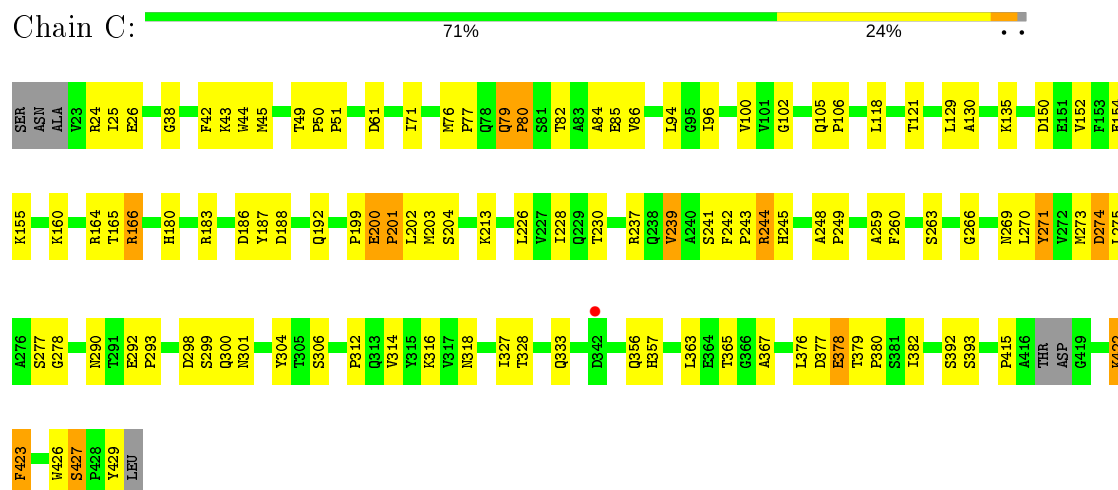
### 3 Residue-property plots

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: Protein TolB

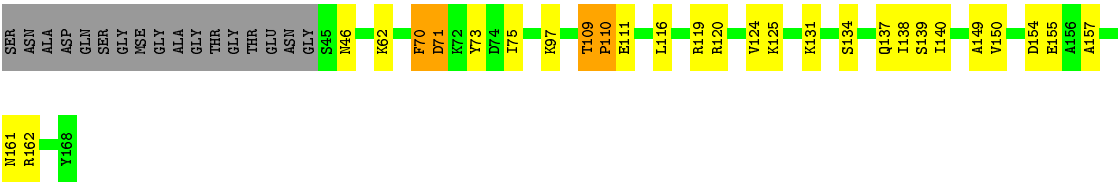


#### • Molecule 1: Protein TolB

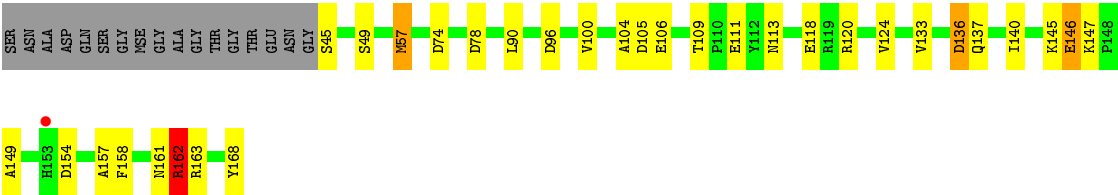


#### • Molecule 2: Peptidoglycan-associated lipoprotein





• Molecule 2: Peptidoglycan-associated lipoprotein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.39Å 175.25Å 66.27Å 90.00° 89.83° 90.00°	Depositor
Resolution (Å)	43.82 – 2.50 43.82 – 2.50	Depositor EDS
% Data completeness (in resolution range)	81.2 (43.82-2.50) 80.8 (43.82-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1593)	Depositor
R, $R_{free}$	0.170 , 0.214 0.170 , 0.205	Depositor DCC
$R_{free}$ test set	1550 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.6	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 25.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.440 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8156	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FMT, SO4

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	0.44	3/3146 (0.1%)	0.54	4/4281 (0.1%)
1	C	0.42	4/3130 (0.1%)	0.53	5/4259 (0.1%)
2	B	0.40	1/980 (0.1%)	0.47	1/1313 (0.1%)
2	D	0.33	0/980	0.42	0/1313
All	All	0.42	8/8236 (0.1%)	0.51	10/11166 (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
2	D	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	243	PRO	N-CD	5.36	1.55	1.47
1	A	428	PRO	N-CD	5.31	1.55	1.47
1	C	80	PRO	N-CD	5.30	1.55	1.47
2	B	110	PRO	N-CD	5.29	1.55	1.47
1	A	201	PRO	N-CD	5.21	1.55	1.47

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	PHE	C-N-CD	5.75	140.48	128.40
1	C	379	THR	C-N-CD	5.65	140.27	128.40
1	C	423	PHE	C-N-CD	5.63	140.22	128.40
1	A	427	SER	C-N-CD	5.55	140.06	128.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	109	THR	C-N-CD	5.49	139.92	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	162	ARG	Sidechain

## 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	3079	0	3020	85	0
1	C	3063	0	3002	80	0
2	B	967	0	943	21	0
2	D	967	0	943	23	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	3	0	1	0	0
4	B	3	0	1	0	0
5	B	12	0	16	1	0
5	C	6	0	8	0	0
6	A	14	0	0	0	0
6	B	7	0	0	0	0
6	C	12	0	0	0	0
6	D	3	0	0	0	0
All	All	8156	0	7934	201	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 13.

The worst 5 of 201 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:273[A]:MSE:HE3	1:A:278:GLY:HA2	1.56	0.88
2:D:105:ASP:HB2	2:D:158:PHE:CD1	2.15	0.80
1:C:422:LYS:HG3	1:C:423:PHE:HD2	1.48	0.79
1:A:277:SER:OG	1:A:279:GLN:HG3	1.84	0.78
1:C:365:THR:HG21	1:C:367:ALA:HB2	1.67	0.76

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	404/411 (98%)	394 (98%)	8 (2%)	2 (0%)	29	48
1	C	402/411 (98%)	395 (98%)	7 (2%)	0	100	100
2	B	122/141 (86%)	121 (99%)	1 (1%)	0	100	100
2	D	122/141 (86%)	117 (96%)	5 (4%)	0	100	100
All	All	1050/1104 (95%)	1027 (98%)	21 (2%)	2 (0%)	47	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	244	ARG

### 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	333/329 (101%)	316 (95%)	17 (5%)	24	45
1	C	330/329 (100%)	310 (94%)	20 (6%)	18	36
2	B	100/106 (94%)	95 (95%)	5 (5%)	24	46
2	D	100/106 (94%)	92 (92%)	8 (8%)	12	23
All	All	863/870 (99%)	813 (94%)	50 (6%)	20	38

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	24	ARG
1	C	202	LEU
2	D	136	ASP
1	C	135	LYS
1	C	155	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	402	GLN
2	B	113	ASN
1	C	308	GLN
1	A	335	GLN
1	A	336	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

9 ligands are 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	$\# Z  > 2$
5	GOL	C	501	-	5,5,5	0.36	0	5,5,5	0.28	0
3	SO4	D	201	-	4,4,4	0.14	0	6,6,6	0.17	0
4	FMT	A	502	-	0,2,2	0.00	-	0,1,1	0.00	-
3	SO4	B	204	-	4,4,4	0.36	0	6,6,6	0.15	0
3	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.05	0
4	FMT	B	201	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	B	203	-	5,5,5	0.38	0	5,5,5	0.22	0
5	GOL	B	202	-	5,5,5	0.35	0	5,5,5	0.26	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
5	GOL	C	501	-	-	2/4/4/4	-
5	GOL	B	203	-	-	2/4/4/4	-
5	GOL	B	202	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	501	GOL	O1-C1-C2-C3
5	B	202	GOL	O1-C1-C2-C3
5	B	202	GOL	C1-C2-C3-O3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	B	202	GOL	O1-C1-C2-O2
5	B	202	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	203	GOL	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	401/411 (97%)	-0.46	2 (0%) 91 91	27, 43, 64, 87	9 (2%)
1	C	400/411 (97%)	-0.45	1 (0%) 94 94	28, 45, 64, 81	10 (2%)
2	B	121/141 (85%)	-0.51	0 100 100	30, 43, 66, 82	9 (7%)
2	D	121/141 (85%)	-0.45	1 (0%) 86 87	30, 44, 64, 70	7 (5%)
All	All	1043/1104 (94%)	-0.46	4 (0%) 92 93	27, 44, 64, 87	35 (3%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	VAL	7.9
1	A	125	ALA	2.8
1	C	342	ASP	2.8
2	D	153	HIS	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. 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( $\text{\AA}^2$ )	Q<0.9
5	GOL	B	202	6/6	0.94	0.13	32,49,51,54	0
3	SO4	C	502	5/5	0.95	0.14	43,54,58,63	5
4	FMT	A	502	3/3	0.96	0.15	58,58,60,63	0
5	GOL	C	501	6/6	0.96	0.08	44,46,50,51	0
5	GOL	B	203	6/6	0.96	0.14	22,47,56,57	0
3	SO4	D	201	5/5	0.96	0.23	17,25,29,31	5
3	SO4	A	501	5/5	0.97	0.08	73,79,85,94	0
4	FMT	B	201	3/3	0.98	0.10	42,42,49,54	0
3	SO4	B	204	5/5	1.00	0.10	23,29,35,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.