



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 03:52 pm BST

PDB ID : 5VRV  
Title : 2.05 Angstrom Resolution Crystal Structure of C-terminal Domain (DUF2156) of Putative Lysylphosphatidylglycerol Synthetase from *Agrobacterium fabrum*.  
Authors : Minasov, G.; Wawrzak, Z.; Skarina, T.; Grimshaw, S.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2017-05-11  
Resolution : 2.05 Å(reported)

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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.

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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 : 1.8.5 (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

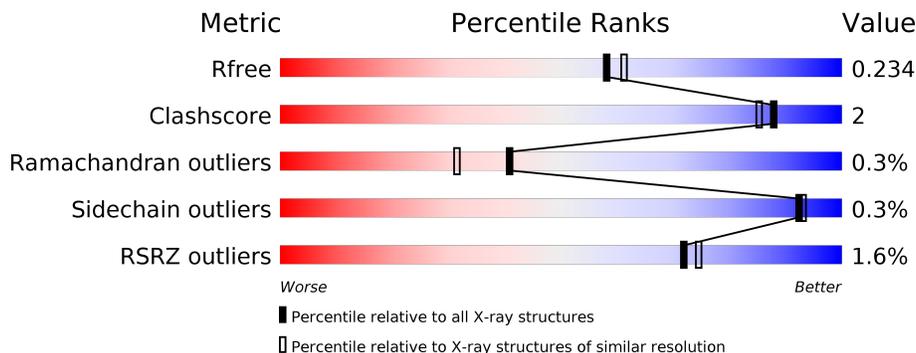
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	330	<p>2% 91% 6% .</p>
1	B	330	<p>0% 91% 5% .</p>
1	C	330	<p>0% 91% 5% .</p>
1	D	330	<p>2% 89% 6% 5%</p>
1	E	330	<p>2% 88% 7% .</p>
1	F	330	<p>2% 92% . .</p>

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 15622 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 regulated by acid pH.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	319	2531	1608	442	468	1	12	0	4	0
1	B	316	2508	1589	442	464	1	12	0	4	0
1	C	316	2469	1566	431	459	1	12	0	1	0
1	D	315	2455	1557	429	456	1	12	0	0	0
1	E	316	2472	1568	434	457	1	12	0	1	0
1	F	317	2471	1567	431	460	1	12	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

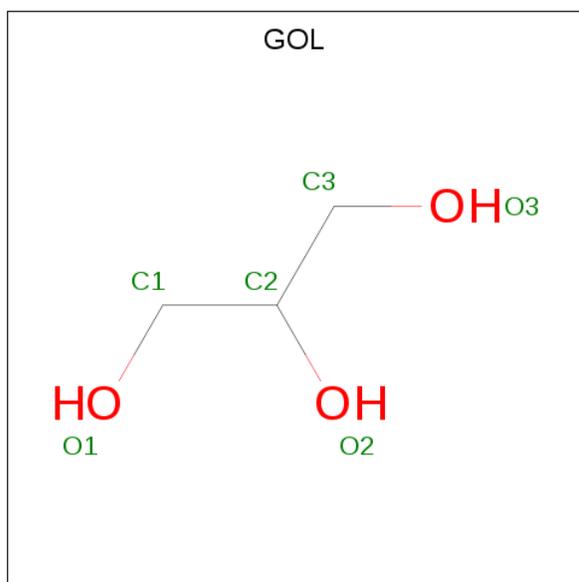
Chain	Residue	Modelled	Actual	Comment	Reference
A	537	SER	-	expression tag	UNP A9CHP8
A	538	ASN	-	expression tag	UNP A9CHP8
A	539	ALA	-	expression tag	UNP A9CHP8
B	537	SER	-	expression tag	UNP A9CHP8
B	538	ASN	-	expression tag	UNP A9CHP8
B	539	ALA	-	expression tag	UNP A9CHP8
C	537	SER	-	expression tag	UNP A9CHP8
C	538	ASN	-	expression tag	UNP A9CHP8
C	539	ALA	-	expression tag	UNP A9CHP8
D	537	SER	-	expression tag	UNP A9CHP8
D	538	ASN	-	expression tag	UNP A9CHP8
D	539	ALA	-	expression tag	UNP A9CHP8
E	537	SER	-	expression tag	UNP A9CHP8
E	538	ASN	-	expression tag	UNP A9CHP8
E	539	ALA	-	expression tag	UNP A9CHP8
F	537	SER	-	expression tag	UNP A9CHP8
F	538	ASN	-	expression tag	UNP A9CHP8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	539	ALA	-	expression tag	UNP A9CHP8

- 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		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	S	0	0
			5	4	1		

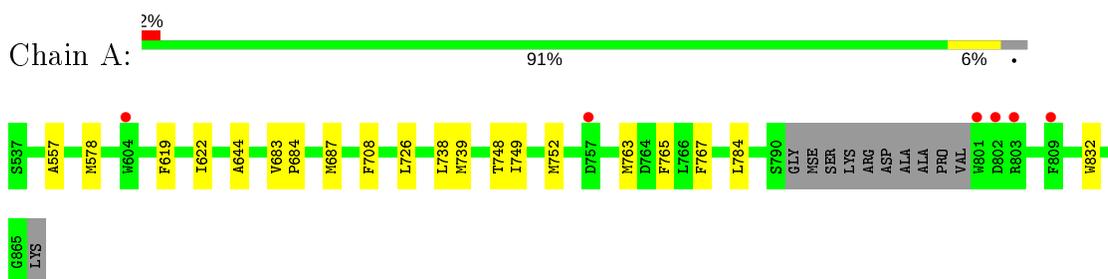
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	159	Total	O	0	5
			163	163		
4	B	118	Total	O	0	6
			121	121		
4	C	126	Total	O	0	5
			131	131		
4	D	82	Total	O	0	2
			84	84		
4	E	78	Total	O	0	3
			81	81		
4	F	106	Total	O	0	1
			107	107		

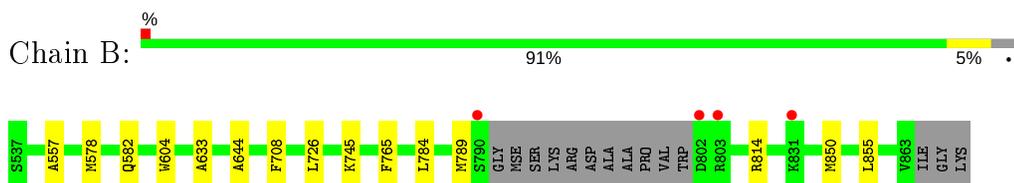
### 3 Residue-property plots [i](#)

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.

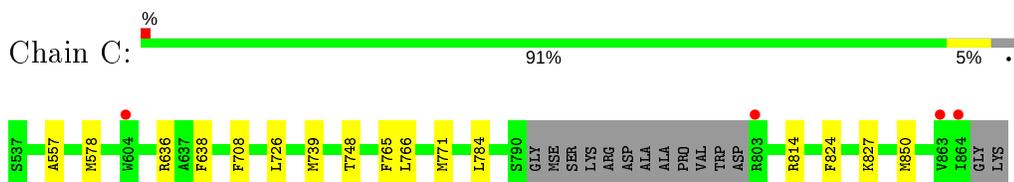
- Molecule 1: Protein regulated by acid pH



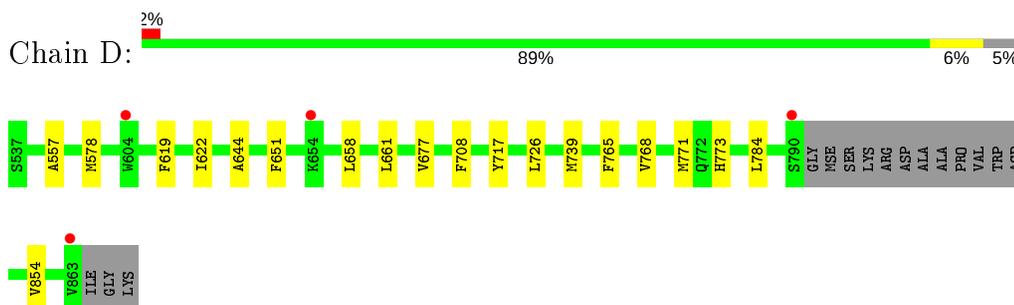
- Molecule 1: Protein regulated by acid pH



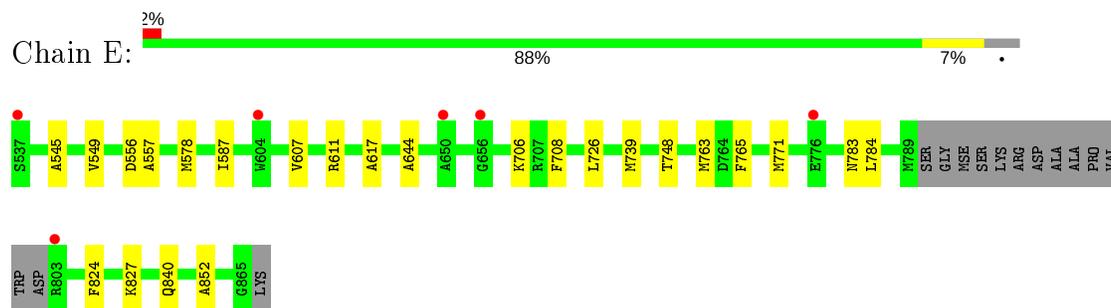
- Molecule 1: Protein regulated by acid pH



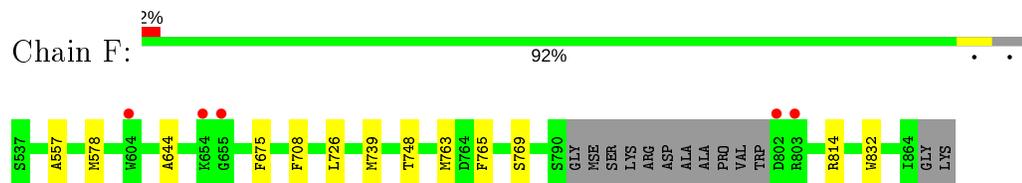
- Molecule 1: Protein regulated by acid pH



- Molecule 1: Protein regulated by acid pH



- Molecule 1: Protein regulated by acid pH



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	194.40 Å 194.40 Å 50.23 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.65 – 2.05 29.65 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.65-2.05) 100.0 (29.65-2.05)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.04 Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.190 , 0.228 0.201 , 0.234	Depositor DCC
$R_{free}$ test set	6697 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.3	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 27.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.064 for -h,-k,l 0.064 for h,-h-k,-l 0.199 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15622	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 3.66% 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, 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	0.47	0/2573	0.75	0/3450
1	B	0.47	0/2549	0.73	0/3416
1	C	0.47	0/2508	0.74	0/3361
1	D	0.45	0/2494	0.69	0/3342
1	E	0.46	0/2511	0.70	0/3364
1	F	0.46	0/2510	0.71	0/3364
All	All	0.46	0/15145	0.72	0/20297

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	2531	0	2468	11	0
1	B	2508	0	2447	8	0
1	C	2469	0	2418	10	0
1	D	2455	0	2403	14	0
1	E	2472	0	2424	12	0
1	F	2471	0	2418	7	0
2	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
3	E	5	0	0	0	0
4	A	163	0	0	1	0
4	B	121	0	0	1	0
4	C	131	0	0	0	0
4	D	84	0	0	0	0
4	E	81	0	0	1	0
4	F	107	0	0	1	0
All	All	15622	0	14610	60	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 2.

The worst 5 of 60 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:F:726:LEU:HD11	1:F:765:PHE:HD2	1.50	0.75
1:B:814[B]:ARG:NH1	4:B:1001[B]:HOH:O	2.27	0.63
1:D:771:MSE:HE1	1:D:828:PHE:CD1	2.34	0.62
1:B:557:ALA:HA	1:B:578:MSE:HE1	1.81	0.61
1:D:717:TYR:OH	1:D:739:MSE:HE3	2.01	0.60

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	319/330 (97%)	311 (98%)	7 (2%)	1 (0%)	41 31
1	B	316/330 (96%)	306 (97%)	9 (3%)	1 (0%)	41 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	313/330 (95%)	306 (98%)	6 (2%)	1 (0%)	41	31
1	D	311/330 (94%)	304 (98%)	6 (2%)	1 (0%)	41	31
1	E	313/330 (95%)	304 (97%)	8 (3%)	1 (0%)	41	31
1	F	313/330 (95%)	306 (98%)	6 (2%)	1 (0%)	41	31
All	All	1885/1980 (95%)	1837 (98%)	42 (2%)	6 (0%)	41	31

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	708	PHE
1	A	708	PHE
1	B	708	PHE
1	C	708	PHE
1	E	708	PHE

### 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	258/249 (104%)	257 (100%)	1 (0%)	91	91
1	B	256/249 (103%)	254 (99%)	2 (1%)	81	82
1	C	253/249 (102%)	253 (100%)	0	100	100
1	D	251/249 (101%)	251 (100%)	0	100	100
1	E	252/249 (101%)	251 (100%)	1 (0%)	91	91
1	F	253/249 (102%)	252 (100%)	1 (0%)	91	91
All	All	1523/1494 (102%)	1518 (100%)	5 (0%)	92	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	763	MSE
1	B	745	LYS

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Mol	Chain	Res	Type
1	B	789	MSE
1	E	763	MSE
1	F	763	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	621	GLN
1	A	773	HIS
1	C	621	GLN
1	F	621	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](#)

5 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	$\# Z  > 2$
2	GOL	D	901	-	5,5,5	0.34	0	5,5,5	0.21	0
2	GOL	B	901	-	5,5,5	0.25	0	5,5,5	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	E	901	-	4,4,4	0.36	0	6,6,6	0.06	0
2	GOL	C	901	-	5,5,5	0.32	0	5,5,5	0.19	0
2	GOL	A	901	-	5,5,5	0.22	0	5,5,5	0.36	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
2	GOL	D	901	-	-	2/4/4/4	-
2	GOL	B	901	-	-	2/4/4/4	-
2	GOL	C	901	-	-	2/4/4/4	-
2	GOL	A	901	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	901	GOL	C1-C2-C3-O3
2	D	901	GOL	O2-C2-C3-O3
2	B	901	GOL	C1-C2-C3-O3
2	B	901	GOL	O2-C2-C3-O3
2	C	901	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

## 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	307/330 (93%)	-0.07	6 (1%) 65 69	24, 36, 57, 96	0
1	B	304/330 (92%)	-0.06	4 (1%) 77 79	25, 37, 58, 93	0
1	C	304/330 (92%)	-0.23	4 (1%) 77 79	29, 39, 57, 76	0
1	D	303/330 (91%)	-0.08	5 (1%) 70 73	30, 47, 69, 85	0
1	E	304/330 (92%)	0.05	6 (1%) 65 69	29, 47, 70, 89	0
1	F	305/330 (92%)	-0.02	5 (1%) 72 74	30, 41, 62, 91	0
All	All	1827/1980 (92%)	-0.07	30 (1%) 72 74	24, 41, 64, 96	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	790	SER	8.5
1	A	801	TRP	5.9
1	C	864	ILE	5.4
1	C	863	VAL	4.8
1	B	802	ASP	4.6

### 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
2	GOL	C	901	6/6	0.67	0.25	59,64,66,71	0
2	GOL	D	901	6/6	0.74	0.12	74,75,76,77	0
3	SO4	E	901	5/5	0.81	0.13	86,88,91,100	0
2	GOL	A	901	6/6	0.82	0.14	53,60,63,68	0
2	GOL	B	901	6/6	0.85	0.15	56,61,64,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.