



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 29, 2024 – 01:23 PM EDT

PDB ID : 4M1J  
Title : Crystal structure of Pseudomonas aeruginosa PvdQ in complex with a transition state analogue  
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Deposited on : 2013-08-02  
Resolution : 1.80 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

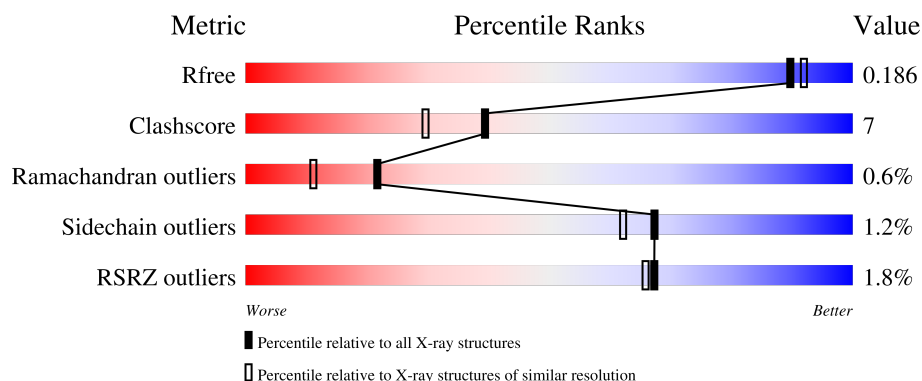
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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 of 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	C	548	
2	A	165	

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
4	GOL	A	204	-	-	X	-
4	GOL	C	804	-	-	X	-
4	GOL	C	806	-	-	X	-
4	GOL	C	807	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6303 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 Acyl-homoserine lactone acylase PvdQ subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	548	4276	2689	782	794	11	0	3	0

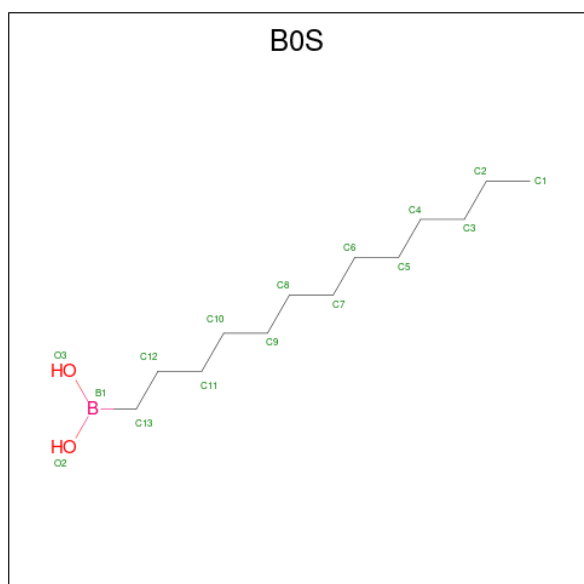
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	763	ALA	-	expression tag	UNP Q9I194
C	764	ALA	-	expression tag	UNP Q9I194

- Molecule 2 is a protein called Acyl-homoserine lactone acylase PvdQ subunit alpha.

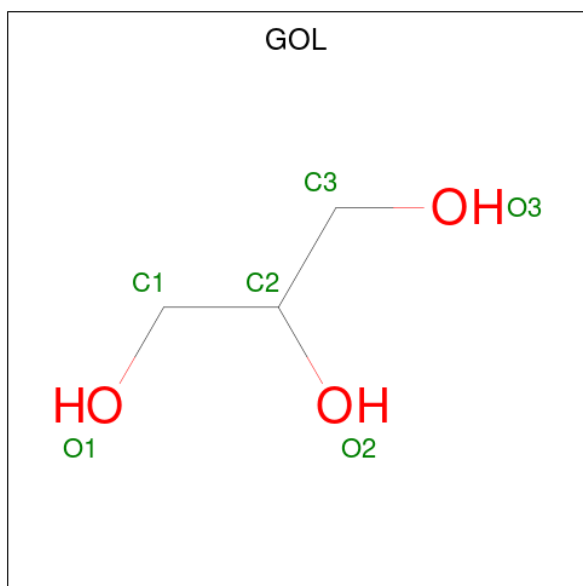
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	165	1293	819	231	241	2	0	4	0

- Molecule 3 is tridecylboronic acid (three-letter code: B0S) (formula:  $C_{13}H_{29}BO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	B	C	O	0	0
			16	1	13	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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

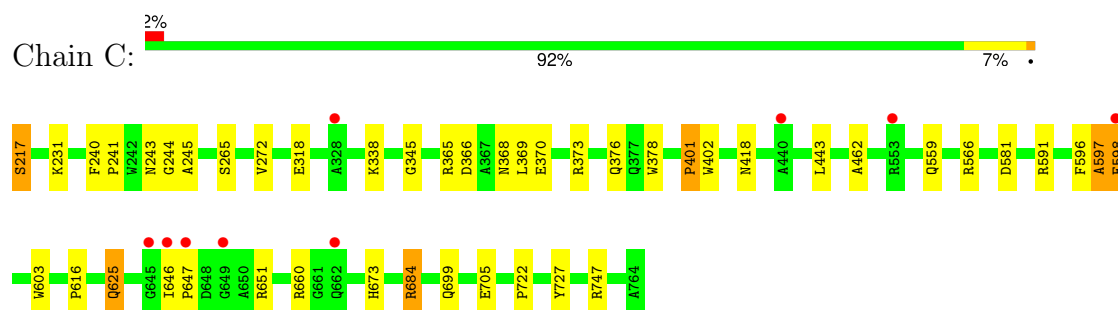
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	428	Total 428	O 428	0	0
5	A	170	Total 170	O 170	0	0

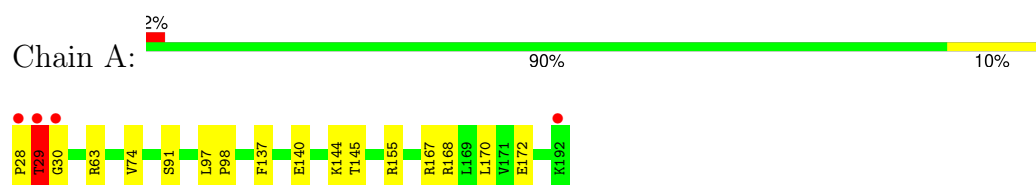
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Acyl-homoserine lactone acylase PvdQ subunit beta



- Molecule 2: Acyl-homoserine lactone acylase PvdQ subunit alpha



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.95Å 166.43Å 94.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.00 – 1.80 41.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (41.00-1.80) 93.4 (41.00-1.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, $R_{free}$	0.162 , 0.188 0.161 , 0.186	Depositor DCC
$R_{free}$ test set	4356 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.4	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6303	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: B0S, 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	C	0.60	3/4386 (0.1%)	0.56	4/5967 (0.1%)
2	A	0.56	0/1334	0.66	1/1811 (0.1%)
All	All	0.59	3/5720 (0.1%)	0.58	5/7778 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	597	ALA	C-N	-28.13	0.69	1.34
1	C	598	GLU	C-N	-13.34	1.03	1.34
1	C	217	SER	C-N	10.05	1.57	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	598	GLU	O-C-N	-7.23	111.14	122.70
1	C	597	ALA	O-C-N	-7.00	111.51	122.70
2	A	29	THR	N-CA-CB	5.29	120.34	110.30
1	C	597	ALA	C-N-CA	5.25	134.82	121.70
1	C	598	GLU	CA-C-N	5.22	128.69	117.20

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

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	C	4276	0	4188	56	0
2	A	1293	0	1262	18	0
3	C	16	0	29	1	0
4	A	36	0	48	7	0
4	C	84	0	112	35	0
5	A	170	0	0	4	3
5	C	428	0	0	12	2
All	All	6303	0	5639	75	3

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 7.

The worst 5 of 75 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:C:597:ALA:C	1:C:598:GLU:CA	2.01	1.28
1:C:597:ALA:O	1:C:598:GLU:N	1.62	1.26
1:C:597:ALA:CA	1:C:598:GLU:N	2.02	1.20
1:C:462:ALA:O	4:C:807:GOL:O2	1.67	1.12
1:C:245:ALA:H	4:C:806:GOL:H32	1.10	1.08

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:1298:HOH:O	5:A:464:HOH:O[6_554]	1.78	0.42
5:C:1298:HOH:O	5:A:455:HOH:O[6_554]	1.88	0.32
5:A:458:HOH:O	5:A:460:HOH:O[6_555]	2.00	0.20

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	C	549/548 (100%)	527 (96%)	20 (4%)	2 (0%)	30	19
2	A	167/165 (101%)	161 (96%)	4 (2%)	2 (1%)	11	3
All	All	716/713 (100%)	688 (96%)	24 (3%)	4 (1%)	22	11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	29	THR
1	C	647	PRO
2	A	30	GLY
1	C	401	PRO

### 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	C	444/447 (99%)	437 (98%)	7 (2%)	58	50
2	A	124/121 (102%)	124 (100%)	0	100	100
All	All	568/568 (100%)	561 (99%)	7 (1%)	67	62

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	559	GLN
1	C	625	GLN
1	C	705	GLU
1	C	684	ARG
1	C	418	ASN

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

### 5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

21 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	$\# Z  > 2$
3	B0S	C	801	1	15,15,15	0.53	0	13,15,15	1.20	1 (7%)
4	GOL	C	806	-	5,5,5	0.27	0	5,5,5	0.32	0
4	GOL	C	811	-	5,5,5	0.25	0	5,5,5	0.32	0
4	GOL	C	814	-	5,5,5	0.26	0	5,5,5	0.31	0
4	GOL	A	202	-	5,5,5	0.26	0	5,5,5	0.34	0
4	GOL	C	807	-	5,5,5	0.25	0	5,5,5	0.31	0
4	GOL	C	810	-	5,5,5	0.26	0	5,5,5	0.32	0
4	GOL	C	805	-	5,5,5	0.36	0	5,5,5	0.48	0
4	GOL	C	809	-	5,5,5	0.26	0	5,5,5	0.31	0
4	GOL	A	206	-	5,5,5	0.65	0	5,5,5	0.54	0
4	GOL	C	808	-	5,5,5	0.26	0	5,5,5	0.31	0
4	GOL	A	203	-	5,5,5	0.40	0	5,5,5	0.45	0
4	GOL	C	803	-	5,5,5	0.35	0	5,5,5	0.32	0
4	GOL	C	804	-	5,5,5	0.36	0	5,5,5	0.46	0
4	GOL	C	802	-	5,5,5	0.36	0	5,5,5	0.38	0
4	GOL	A	204	-	5,5,5	0.52	0	5,5,5	1.43	1 (20%)
4	GOL	A	205	-	5,5,5	0.32	0	5,5,5	0.38	0
4	GOL	C	812	-	5,5,5	0.26	0	5,5,5	0.31	0
4	GOL	C	815	-	5,5,5	0.26	0	5,5,5	0.31	0
4	GOL	A	201	-	5,5,5	0.38	0	5,5,5	0.38	0
4	GOL	C	813	-	5,5,5	0.26	0	5,5,5	0.32	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	B0S	C	801	1	-	6/11/13/13	-
4	GOL	C	806	-	-	0/4/4/4	-
4	GOL	C	811	-	-	0/4/4/4	-
4	GOL	C	814	-	-	0/4/4/4	-
4	GOL	A	202	-	-	2/4/4/4	-
4	GOL	C	807	-	-	0/4/4/4	-
4	GOL	C	810	-	-	1/4/4/4	-
4	GOL	C	805	-	-	2/4/4/4	-
4	GOL	C	809	-	-	0/4/4/4	-
4	GOL	A	206	-	-	4/4/4/4	-
4	GOL	C	808	-	-	2/4/4/4	-
4	GOL	A	203	-	-	2/4/4/4	-
4	GOL	C	803	-	-	4/4/4/4	-
4	GOL	C	804	-	-	0/4/4/4	-
4	GOL	C	802	-	-	2/4/4/4	-
4	GOL	A	204	-	-	2/4/4/4	-
4	GOL	A	205	-	-	1/4/4/4	-
4	GOL	C	812	-	-	0/4/4/4	-
4	GOL	C	815	-	-	1/4/4/4	-
4	GOL	A	201	-	-	0/4/4/4	-
4	GOL	C	813	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	801	B0S	O3-B1-C13	-3.27	113.80	121.06
4	A	204	GOL	O1-C1-C2	2.37	121.06	110.38

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	801	B0S	C10-C11-C12-C13
3	C	801	B0S	C11-C12-C13-B1
4	C	803	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	C	803	GOL	O1-C1-C2-C3
4	A	203	GOL	O1-C1-C2-C3

There are no ring outliers.

11 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	801	B0S	1	0
4	C	806	GOL	10	0
4	C	814	GOL	3	0
4	C	807	GOL	6	0
4	C	809	GOL	1	0
4	A	206	GOL	1	0
4	C	808	GOL	3	0
4	C	804	GOL	8	0
4	A	204	GOL	6	0
4	C	812	GOL	2	0
4	C	815	GOL	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	598:GLU	C	599:LEU	N	1.03
1	C	597:ALA	C	598:GLU	N	0.69

## 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	C	548/548 (100%)	-0.33	9 (1%) 70 69	8, 26, 53, 87	3 (0%)
2	A	165/165 (100%)	-0.59	4 (2%) 59 58	13, 19, 38, 94	4 (2%)
All	All	713/713 (100%)	-0.39	13 (1%) 67 66	8, 24, 52, 94	7 (0%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	28	PRO	6.0
2	A	29	THR	5.2
1	C	645	GLY	3.1
2	A	30	GLY	2.8
1	C	553	ARG	2.6

### 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 monosaccharides 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
4	GOL	C	815	6/6	0.71	0.21	56,68,70,72	0
4	GOL	C	813	6/6	0.73	0.20	65,75,77,79	0
4	GOL	C	810	6/6	0.75	0.21	56,64,67,78	0
4	GOL	C	811	6/6	0.76	0.20	54,62,67,67	0
4	GOL	C	808	6/6	0.76	0.19	53,60,66,69	0
4	GOL	C	814	6/6	0.76	0.20	65,70,76,87	0
4	GOL	C	807	6/6	0.76	0.22	27,44,64,74	0
4	GOL	C	809	6/6	0.78	0.21	54,58,67,68	0
4	GOL	C	803	6/6	0.80	0.18	38,48,51,61	0
4	GOL	C	806	6/6	0.84	0.15	22,28,37,57	0
4	GOL	A	203	6/6	0.84	0.15	28,46,49,54	0
4	GOL	A	205	6/6	0.85	0.12	36,43,45,54	0
4	GOL	C	812	6/6	0.86	0.14	55,64,70,75	0
4	GOL	C	805	6/6	0.89	0.11	25,38,41,43	0
4	GOL	A	204	6/6	0.89	0.22	19,25,42,45	0
4	GOL	A	201	6/6	0.89	0.12	36,44,48,54	0
4	GOL	C	804	6/6	0.90	0.11	23,36,44,47	0
4	GOL	A	206	6/6	0.91	0.14	22,31,44,45	0
3	B0S	C	801	16/16	0.93	0.11	21,29,41,44	0
4	GOL	C	802	6/6	0.93	0.10	20,40,47,47	0
4	GOL	A	202	6/6	0.94	0.08	21,29,35,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.