



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:14 AM GMT

PDB ID : 3OA5  
Title : The structure of chi1, a chitinase from Yersinia entomophaga  
Authors : Busby, J.N.; Lott, J.S.; Hurst, M.R.H.  
Deposited on : 2010-08-04  
Resolution : 1.74 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

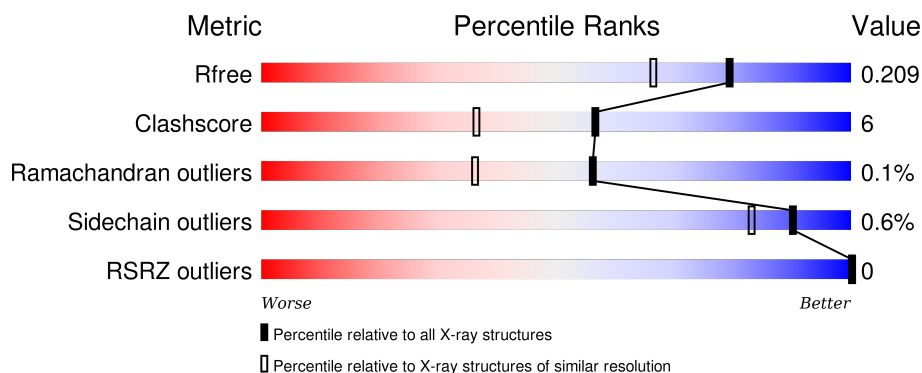
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 1.74 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))
$R_{free}$	91344	2417 (1.76-1.72)
Clashscore	102246	2570 (1.76-1.72)
Ramachandran outliers	100387	2544 (1.76-1.72)
Sidechain outliers	100360	2544 (1.76-1.72)
RSRZ outliers	91569	2420 (1.76-1.72)

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	574	 82% 8% 10%
1	B	574	 80% 9% 10%

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	2PE	A	543	-	-	-	X
2	2PE	B	543	-	-	-	X
3	GOL	A	544	-	-	-	X
3	GOL	A	545	-	-	X	-
3	GOL	A	546	-	-	X	X
3	GOL	B	544	-	-	-	X
3	GOL	B	545	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9006 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 Chi1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	14	0
			4076	2598	667	800	11			
1	B	514	Total	C	N	O	S	0	9	0
			4035	2563	663	799	10			

There are 64 discrepancies between the modelled and reference sequences:

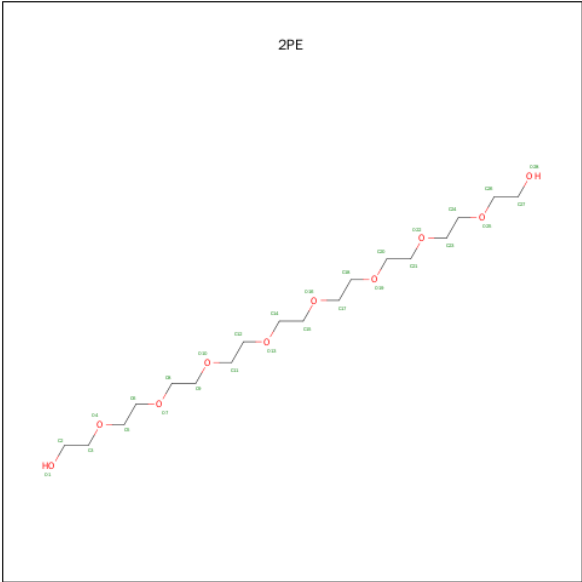
Chain	Residue	Modelled	Actual	Comment	Reference
A	-31	MET	-	EXPRESSION TAG	UNP B6A876
A	-30	SER	-	EXPRESSION TAG	UNP B6A876
A	-29	TYR	-	EXPRESSION TAG	UNP B6A876
A	-28	TYR	-	EXPRESSION TAG	UNP B6A876
A	-27	HIS	-	EXPRESSION TAG	UNP B6A876
A	-26	HIS	-	EXPRESSION TAG	UNP B6A876
A	-25	HIS	-	EXPRESSION TAG	UNP B6A876
A	-24	HIS	-	EXPRESSION TAG	UNP B6A876
A	-23	HIS	-	EXPRESSION TAG	UNP B6A876
A	-22	HIS	-	EXPRESSION TAG	UNP B6A876
A	-21	LEU	-	EXPRESSION TAG	UNP B6A876
A	-20	GLU	-	EXPRESSION TAG	UNP B6A876
A	-19	SER	-	EXPRESSION TAG	UNP B6A876
A	-18	THR	-	EXPRESSION TAG	UNP B6A876
A	-17	SER	-	EXPRESSION TAG	UNP B6A876
A	-16	LEU	-	EXPRESSION TAG	UNP B6A876
A	-15	TYR	-	EXPRESSION TAG	UNP B6A876
A	-14	LYS	-	EXPRESSION TAG	UNP B6A876
A	-13	LYS	-	EXPRESSION TAG	UNP B6A876
A	-12	ALA	-	EXPRESSION TAG	UNP B6A876
A	-11	GLY	-	EXPRESSION TAG	UNP B6A876
A	-10	PHE	-	EXPRESSION TAG	UNP B6A876
A	-9	GLU	-	EXPRESSION TAG	UNP B6A876
A	-8	ASN	-	EXPRESSION TAG	UNP B6A876
A	-7	LEU	-	EXPRESSION TAG	UNP B6A876

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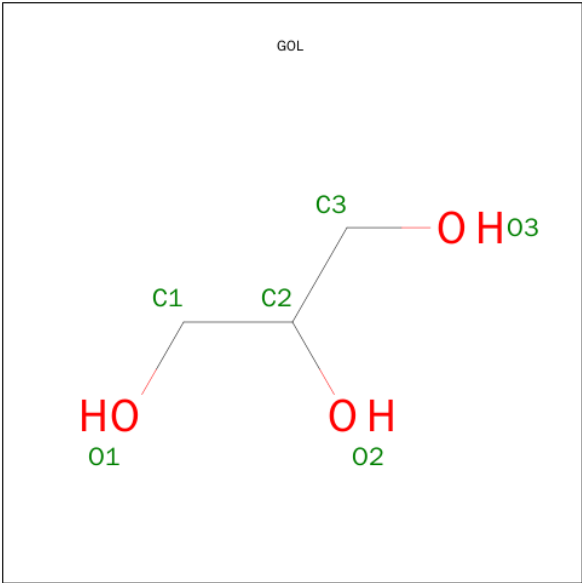
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	TYR	-	EXPRESSION TAG	UNP B6A876
A	-5	PHE	-	EXPRESSION TAG	UNP B6A876
A	-4	GLN	-	EXPRESSION TAG	UNP B6A876
A	-3	GLY	-	EXPRESSION TAG	UNP B6A876
A	-2	SER	-	EXPRESSION TAG	UNP B6A876
A	-1	GLY	-	EXPRESSION TAG	UNP B6A876
A	0	ALA	-	EXPRESSION TAG	UNP B6A876
B	-31	MET	-	EXPRESSION TAG	UNP B6A876
B	-30	SER	-	EXPRESSION TAG	UNP B6A876
B	-29	TYR	-	EXPRESSION TAG	UNP B6A876
B	-28	TYR	-	EXPRESSION TAG	UNP B6A876
B	-27	HIS	-	EXPRESSION TAG	UNP B6A876
B	-26	HIS	-	EXPRESSION TAG	UNP B6A876
B	-25	HIS	-	EXPRESSION TAG	UNP B6A876
B	-24	HIS	-	EXPRESSION TAG	UNP B6A876
B	-23	HIS	-	EXPRESSION TAG	UNP B6A876
B	-22	HIS	-	EXPRESSION TAG	UNP B6A876
B	-21	LEU	-	EXPRESSION TAG	UNP B6A876
B	-20	GLU	-	EXPRESSION TAG	UNP B6A876
B	-19	SER	-	EXPRESSION TAG	UNP B6A876
B	-18	THR	-	EXPRESSION TAG	UNP B6A876
B	-17	SER	-	EXPRESSION TAG	UNP B6A876
B	-16	LEU	-	EXPRESSION TAG	UNP B6A876
B	-15	TYR	-	EXPRESSION TAG	UNP B6A876
B	-14	LYS	-	EXPRESSION TAG	UNP B6A876
B	-13	LYS	-	EXPRESSION TAG	UNP B6A876
B	-12	ALA	-	EXPRESSION TAG	UNP B6A876
B	-11	GLY	-	EXPRESSION TAG	UNP B6A876
B	-10	PHE	-	EXPRESSION TAG	UNP B6A876
B	-9	GLU	-	EXPRESSION TAG	UNP B6A876
B	-8	ASN	-	EXPRESSION TAG	UNP B6A876
B	-7	LEU	-	EXPRESSION TAG	UNP B6A876
B	-6	TYR	-	EXPRESSION TAG	UNP B6A876
B	-5	PHE	-	EXPRESSION TAG	UNP B6A876
B	-4	GLN	-	EXPRESSION TAG	UNP B6A876
B	-3	GLY	-	EXPRESSION TAG	UNP B6A876
B	-2	SER	-	EXPRESSION TAG	UNP B6A876
B	-1	GLY	-	EXPRESSION TAG	UNP B6A876
B	0	ALA	-	EXPRESSION TAG	UNP B6A876

- Molecule 2 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: C<sub>18</sub>H<sub>38</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			14	9	5		
2	B	1	Total	C	O	0	0
			16	10	6		

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	428	Total	O	0	0
			428	428		
4	B	407	Total	O	0	0
			407	407		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.01Å 67.17Å 81.68Å 102.85° 108.06° 92.10°	Depositor
Resolution (Å)	75.27 – 1.74 53.85 – 1.74	Depositor EDS
% Data completeness (in resolution range)	96.9 (75.27-1.74) 89.7 (53.85-1.74)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.165 , 0.210 0.165 , 0.209	Depositor DCC
$R_{free}$ test set	5541 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.3	EDS
Estimated twinning fraction	0.045 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 110382 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9006	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, 2PE

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	0.84	1/4210 (0.0%)	0.83	1/5710 (0.0%)
1	B	0.82	1/4151 (0.0%)	0.80	3/5635 (0.1%)
All	All	0.83	2/8361 (0.0%)	0.81	4/11345 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	CYS	CB-SG	-5.53	1.72	1.81
1	B	248	PHE	CE2-CZ	5.15	1.47	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	183	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	B	368	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	271	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	462	LEU	CA-CB-CG	5.03	126.87	115.30

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	A	4076	0	3918	57	0
1	B	4035	0	3841	36	0
2	A	14	0	16	6	0
2	B	16	0	20	8	0
3	A	18	0	24	9	0
3	B	12	0	16	0	0
4	A	428	0	0	2	0
4	B	407	0	0	6	1
All	All	9006	0	7835	98	1

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.

The worst 5 of 98 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:427[B]:MET:CE	1:A:434:GLY:HA2	1.41	1.48
1:A:427[B]:MET:CE	1:A:427[B]:MET:HA	1.31	1.48
1:A:427[B]:MET:HE1	1:A:434:GLY:CA	1.48	1.43
1:A:427[B]:MET:HA	1:A:427[B]:MET:HE2	1.16	1.14
1:A:427[B]:MET:CE	1:A:427[B]:MET:CA	2.19	1.14

All (1) 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)
4:B:606:HOH:O	4:B:785:HOH:O[1_455]	2.11	0.09

## 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	527/574 (92%)	510 (97%)	17 (3%)	0	100	100
1	B	521/574 (91%)	500 (96%)	19 (4%)	2 (0%)	39	20
All	All	1048/1148 (91%)	1010 (96%)	36 (3%)	2 (0%)	56	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	404[A]	ASP
1	B	404[B]	ASP

### 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	A	427/482 (89%)	425 (100%)	2 (0%)	92	87
1	B	421/482 (87%)	418 (99%)	3 (1%)	88	80
All	All	848/964 (88%)	843 (99%)	5 (1%)	90	83

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

Mol	Chain	Res	Type
1	A	338	HIS
1	A	440	LEU
1	B	12	ASP
1	B	338	HIS
1	B	462	LEU

Some 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

7 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	2PE	A	543	-	13,13,27	0.67	0	12,12,26	0.77	0
3	GOL	A	544	-	5,5,5	0.32	0	5,5,5	0.60	0
3	GOL	A	545	-	5,5,5	0.36	0	5,5,5	0.35	0
3	GOL	A	546	-	5,5,5	0.40	0	5,5,5	0.65	0
2	2PE	B	543	-	15,15,27	0.52	0	14,14,26	1.53	3 (21%)
3	GOL	B	544	-	5,5,5	0.25	0	5,5,5	0.72	0
3	GOL	B	545	-	5,5,5	0.27	0	5,5,5	0.53	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	2PE	A	543	-	-	0/11/11/25	0/0/0/0
3	GOL	A	544	-	-	0/4/4/4	0/0/0/0
3	GOL	A	545	-	-	0/4/4/4	0/0/0/0
3	GOL	A	546	-	-	0/4/4/4	0/0/0/0
2	2PE	B	543	-	-	0/13/13/25	0/0/0/0
3	GOL	B	544	-	-	0/4/4/4	0/0/0/0
3	GOL	B	545	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	543	2PE	C14-O13-C12	-2.37	103.11	113.31
2	B	543	2PE	O13-C12-C11	2.19	120.12	110.36
2	B	543	2PE	O13-C14-C15	3.69	126.78	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	543	2PE	6	0
3	A	545	GOL	4	0
3	A	546	GOL	5	0
2	B	543	2PE	8	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	515/574 (89%)	-0.43	0 100 100	11, 19, 32, 47	0
1	B	514/574 (89%)	-0.39	0 100 100	13, 21, 35, 43	0
All	All	1029/1148 (89%)	-0.41	0 100 100	11, 20, 33, 47	0

There are no RSRZ outliers to report.

### 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
3	GOL	A	546	6/6	0.90	0.16	8.96	25,40,42,49	0
3	GOL	B	545	6/6	0.96	0.20	7.79	29,36,38,47	0
2	2PE	B	543	16/28	0.94	0.14	6.90	15,28,41,42	0
3	GOL	B	544	6/6	0.94	0.12	6.55	30,33,36,36	0
2	2PE	A	543	14/28	0.90	0.15	6.27	16,26,31,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	544	6/6	0.92	0.12	3.92	25,29,31,32	0
3	GOL	A	545	6/6	0.90	0.18	-	45,48,50,52	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.