



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 21, 2025 – 04:26 PM JST

PDB ID : 9WLV / pdb\_00009wlv  
Title : The Crystal Structure of Alpha-Beta-fold\_hydrolase from *Microbunus sagamiensis*.  
Authors : Huang, J.; Smith, S.; Wang, Q.; Bao, X.  
Deposited on : 2025-09-02  
Resolution : 1.90 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 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 : 4-5-2 with Phenix2.0  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

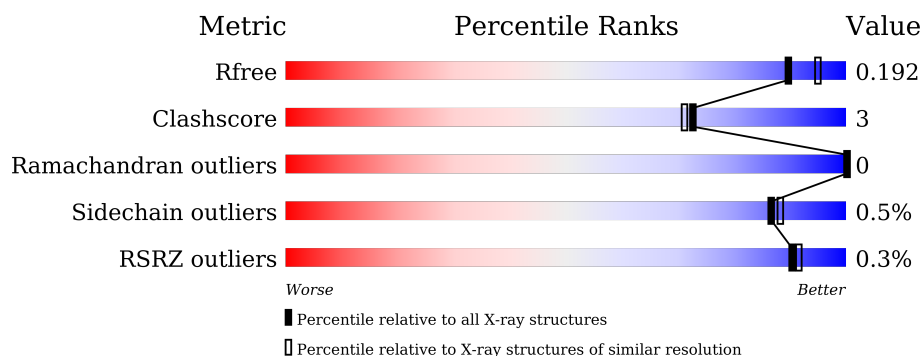
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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	AAA	290	<div> <div></div> <div>96%</div> <div>.</div> </div>
1	BBB	290	<div> <div></div> <div>93%</div> <div>7%</div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5003 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.

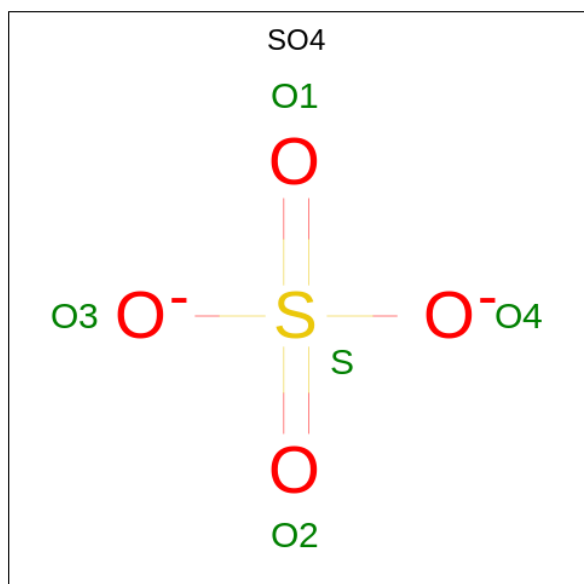
- Molecule 1 is a protein called Pimeloyl-ACP methyl ester carboxylesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	290	Total	C	N	O	S	0	4	0
			2148	1343	389	407	9			
1	BBB	290	Total	C	N	O	S	0	2	0
			2133	1335	383	406	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	0	GLY	-	expression tag	UNP A0A1H2MDS2
AAA	1	MET	-	expression tag	UNP A0A1H2MDS2
BBB	0	GLY	-	expression tag	UNP A0A1H2MDS2
BBB	1	MET	-	expression tag	UNP A0A1H2MDS2

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).

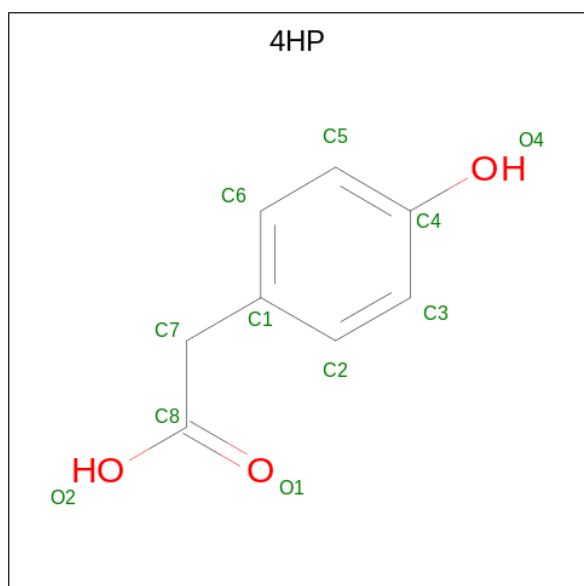


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	O	S	0	0
			5	4	1		
2	AAA	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 4-HYDROXYPHENYLACETATE (CCD ID: 4HP) (formula: C<sub>8</sub>H<sub>8</sub>O<sub>3</sub>).



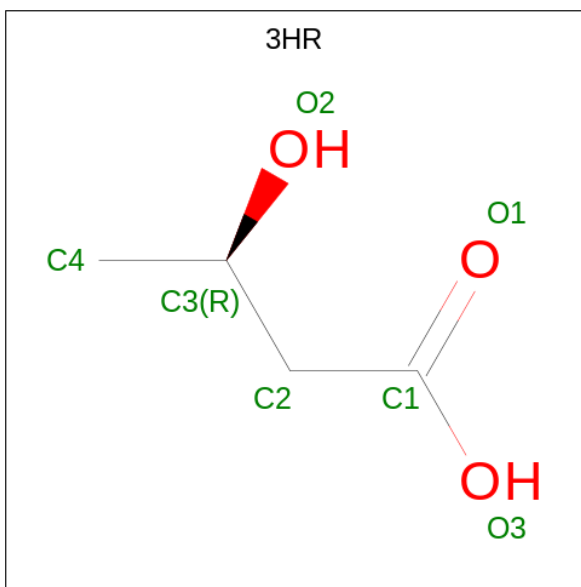
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			11	8	3		
4	BBB	1	Total	C	O	0	0
			11	8	3		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 6 is (3R)-3-hydroxybutanoic acid (CCD ID: 3HR) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	BBB	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	356	Total	O	0	0
			356	356		
7	BBB	278	Total	O	0	0
			278	278		

### 3 Residue-property plots

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: Pimeloyl-ACP methyl ester carboxylesterase

Chain AAA:  96%



- Molecule 1: Pimeloyl-ACP methyl ester carboxylesterase

Chain BBB:  93%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.21Å 125.21Å 79.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 1.90 49.29 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.29-1.90) 100.0 (49.29-1.90)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.21 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.144 , 0.179 0.157 , 0.192	Depositor DCC
$R_{free}$ test set	2527 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.3	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 37.4	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	5003	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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: 4HP, CL, SO4, GOL, 3HR

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	AAA	1.09	0/2206	1.18	0/3009
1	BBB	1.11	0/2185	1.18	0/2982
All	All	1.10	0/4391	1.18	0/5991

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

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	AAA	2148	0	2113	9	0
1	BBB	2133	0	2091	16	0
2	AAA	10	0	0	0	0
3	AAA	1	0	0	0	0
4	AAA	11	0	6	1	0
4	BBB	11	0	6	2	0
5	AAA	36	0	48	2	0
5	BBB	12	0	16	1	0
6	BBB	7	0	7	1	0
7	AAA	356	0	0	3	0
7	BBB	278	0	0	5	0
All	All	5003	0	4287	27	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 3.

All (27) 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:BBB:31:THR:O	4:BBB:301:4HP:H71	1.98	0.62
1:BBB:166:ARG:NH1	7:BBB:402:HOH:O	2.32	0.61
1:BBB:188:ALA:HB1	1:BBB:275[B]:LEU:HD12	1.84	0.60
1:BBB:50:LEU:HD11	1:BBB:286:VAL:HG12	1.86	0.57
1:BBB:50:LEU:HD11	1:BBB:286:VAL:CG1	2.37	0.54
1:BBB:244:MET:HE1	4:BBB:301:4HP:H6	1.91	0.52
1:BBB:247:PHE:CE1	1:BBB:264:LEU:HB3	2.47	0.50
6:BBB:303:3HR:H3	7:BBB:457:HOH:O	2.12	0.50
1:AAA:247:PHE:CE1	1:AAA:264:LEU:HB3	2.48	0.49
1:BBB:189:LEU:HG	1:BBB:271:LEU:HD13	1.95	0.48
1:AAA:166:ARG:NH2	7:AAA:609:HOH:O	2.46	0.47
1:BBB:244:MET:HE2	7:BBB:567:HOH:O	2.15	0.46
1:AAA:3[B]:THR:HG21	7:AAA:771:HOH:O	2.16	0.46
5:AAA:306:GOL:H12	7:AAA:783:HOH:O	2.15	0.46
1:AAA:32:PRO:O	4:AAA:304:4HP:H6	2.16	0.45
1:BBB:93:ALA:HA	1:BBB:117:LEU:O	2.16	0.45
1:AAA:39:ARG:CZ	1:AAA:192:GLU:HG3	2.47	0.45
1:AAA:206:ARG:HH12	5:AAA:306:GOL:C3	2.31	0.43
1:BBB:275[B]:LEU:HD23	1:BBB:275[B]:LEU:HA	1.70	0.42
1:AAA:5[B]:ARG:HH21	1:AAA:5[B]:ARG:HG3	1.84	0.42
1:BBB:284:GLU:OE1	5:BBB:302:GOL:O3	2.35	0.42
1:AAA:93:ALA:HA	1:AAA:117:LEU:O	2.20	0.42
1:BBB:139:GLN:OE1	1:BBB:179:SER:HB3	2.20	0.41
1:AAA:41:MET:HA	1:AAA:278:LEU:HD21	2.02	0.41
1:BBB:49:GLY:O	7:BBB:401:HOH:O	2.22	0.40
1:BBB:6:THR:HB	1:BBB:7:PRO:HD2	2.03	0.40
1:BBB:105:GLY:HA3	7:BBB:555:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 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	AAA	292/290 (101%)	284 (97%)	8 (3%)	0	100	100
1	BBB	290/290 (100%)	286 (99%)	4 (1%)	0	100	100
All	All	582/580 (100%)	570 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	AAA	213/209 (102%)	213 (100%)	0	100	100
1	BBB	211/209 (101%)	209 (99%)	2 (1%)	75	77
All	All	424/418 (101%)	422 (100%)	2 (0%)	86	88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	179	SER
1	BBB	213	LEU

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 ⓘ

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](#)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 for Mogul analysis.

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	$\# Z  > 2$
4	4HP	BBB	301	-	11,11,11	1.28	1 (9%)	14,14,14	1.66	1 (7%)
5	GOL	AAA	310	-	5,5,5	0.18	0	5,5,5	0.56	0
5	GOL	AAA	307	-	5,5,5	0.16	0	5,5,5	0.48	0
5	GOL	BBB	304	-	5,5,5	0.15	0	5,5,5	0.39	0
6	3HR	BBB	303	-	6,6,6	0.63	0	6,7,7	1.17	0
2	SO4	AAA	301	-	4,4,4	0.36	0	6,6,6	0.09	0
5	GOL	AAA	305	-	5,5,5	0.16	0	5,5,5	0.28	0
2	SO4	AAA	302	-	4,4,4	0.35	0	6,6,6	0.45	0
5	GOL	BBB	302	-	5,5,5	0.24	0	5,5,5	0.51	0
5	GOL	AAA	306	-	5,5,5	0.10	0	5,5,5	0.21	0
5	GOL	AAA	309	-	5,5,5	0.13	0	5,5,5	0.40	0
5	GOL	AAA	308	-	5,5,5	0.11	0	5,5,5	0.29	0
4	4HP	AAA	304	-	11,11,11	0.94	0	14,14,14	2.05	2 (14%)

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
4	4HP	BBB	301	-	-	3/4/4/4	0/1/1/1
5	GOL	AAA	310	-	-	2/4/4/4	-
5	GOL	AAA	307	-	-	0/4/4/4	-
5	GOL	BBB	304	-	-	4/4/4/4	-
6	3HR	BBB	303	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	AAA	305	-	-	0/4/4/4	-
5	GOL	BBB	302	-	-	2/4/4/4	-
5	GOL	AAA	306	-	-	4/4/4/4	-
5	GOL	AAA	309	-	-	4/4/4/4	-
5	GOL	AAA	308	-	-	0/4/4/4	-
4	4HP	AAA	304	-	-	2/4/4/4	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BBB	301	4HP	O1-C8	3.16	1.32	1.22

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AAA	304	4HP	C1-C7-C8	6.09	131.32	113.67
4	BBB	301	4HP	C1-C7-C8	5.05	128.32	113.67
4	AAA	304	4HP	C7-C1-C2	2.66	124.71	120.89

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	AAA	310	GOL	C1-C2-C3-O3
5	BBB	302	GOL	C1-C2-C3-O3
5	BBB	304	GOL	O1-C1-C2-C3
5	BBB	304	GOL	O2-C2-C3-O3
6	BBB	303	3HR	C1-C2-C3-O2
6	BBB	303	3HR	C1-C2-C3-C4
5	AAA	306	GOL	O1-C1-C2-C3
5	AAA	306	GOL	C1-C2-C3-O3
5	AAA	309	GOL	O1-C1-C2-C3
5	AAA	309	GOL	C1-C2-C3-O3
5	BBB	304	GOL	C1-C2-C3-O3
5	AAA	306	GOL	O2-C2-C3-O3
5	BBB	302	GOL	O2-C2-C3-O3
5	AAA	309	GOL	O1-C1-C2-O2
5	BBB	304	GOL	O1-C1-C2-O2
5	AAA	309	GOL	O2-C2-C3-O3
5	AAA	310	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	AAA	304	4HP	C6-C1-C7-C8
4	BBB	301	4HP	C2-C1-C7-C8
4	AAA	304	4HP	C2-C1-C7-C8
6	BBB	303	3HR	O3-C1-C2-C3
4	BBB	301	4HP	C6-C1-C7-C8
5	AAA	306	GOL	O1-C1-C2-O2
4	BBB	301	4HP	C1-C7-C8-O1

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	BBB	301	4HP	2	0
6	BBB	303	3HR	1	0
5	BBB	302	GOL	1	0
5	AAA	306	GOL	2	0
4	AAA	304	4HP	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	AAA	290/290 (100%)	-0.53	1 (0%) 90 91	10, 19, 31, 45	4 (1%)
1	BBB	290/290 (100%)	-0.15	1 (0%) 90 91	12, 24, 45, 62	2 (0%)
All	All	580/580 (100%)	-0.34	2 (0%) 90 91	10, 21, 41, 62	6 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	247	PHE	3.1
1	AAA	179	SER	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 oligosaccharides 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	SO4	AAA	302	5/5	0.83	0.12	46,49,70,70	0
2	SO4	AAA	301	5/5	0.85	0.13	75,76,80,81	5
5	GOL	AAA	308	6/6	0.85	0.13	42,48,53,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	AAA	309	6/6	0.85	0.17	38,55,62,63	0
5	GOL	BBB	304	6/6	0.85	0.16	50,56,58,58	0
6	3HR	BBB	303	7/7	0.85	0.14	43,49,56,58	0
5	GOL	AAA	306	6/6	0.86	0.13	37,53,55,57	0
5	GOL	AAA	307	6/6	0.86	0.16	54,57,59,61	0
4	4HP	BBB	301	11/11	0.86	0.14	27,49,55,64	0
3	CL	AAA	303	1/1	0.87	0.14	68,68,68,68	0
4	4HP	AAA	304	11/11	0.88	0.14	32,42,48,50	0
5	GOL	AAA	305	6/6	0.89	0.14	39,53,55,57	0
5	GOL	BBB	302	6/6	0.89	0.11	28,39,41,43	0
5	GOL	AAA	310	6/6	0.96	0.07	24,31,33,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.