



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 12:44 PM BST

PDB ID : 1MFE  
Title : RECOGNITION OF A CELL-SURFACE OLIGO-SACCHARIDE OF PATHOGENIC SALMONELLA BY AN ANTIBODY FAB FRAGMENT  
Authors : Cygler, M.  
Deposited on : 1993-10-25  
Resolution : 2.00 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.

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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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

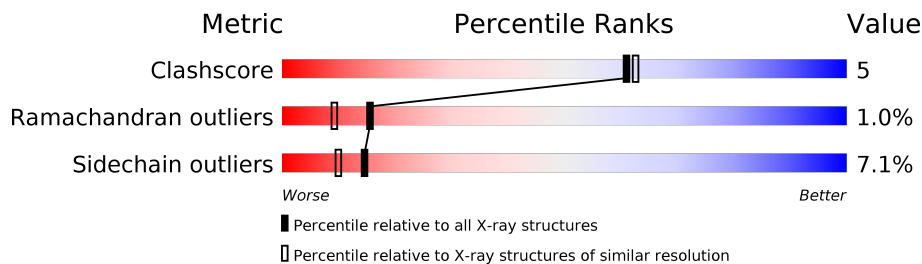
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	215	
2	H	219	
3	A	3	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3434 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 IGG1-LAMBDA SE155-4 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	211	1604	999	273	323	9	0	2	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	28	THR	ALA	conflict	GB 387376
L	31	SER	THR	conflict	GB 387376
L	32	GLY	SER	conflict	GB 387376
L	34	HIS	TYR	conflict	GB 387376
L	52	ASP	GLY	conflict	GB 387376
L	82	PRO	THR	conflict	GB 387376
L	94	CYS	TYR	conflict	GB 387376
L	95	ASN	SER	conflict	GB 387376
L	99	ILE	VAL	conflict	GB 387376

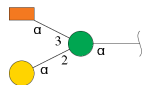
- Molecule 2 is a protein called IGG1-LAMBDA SE155-4 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	212	1614	1028	270	304	12	0	4	2

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	ALA	deletion	GB 208365
H	468	ARG	ASP	conflict	GB 208365

- Molecule 3 is an oligosaccharide called alpha-D-galactopyranose-(1-2)-[alpha-D-Abequopyranose-(1-3)]alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
3	A	3	32	18	14	0	0	0

- Molecule 4 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	L	102	102	102	0	0
4	H	82	82	82	0	0

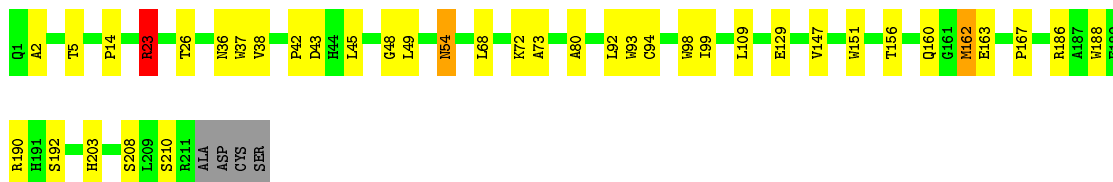
### 3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

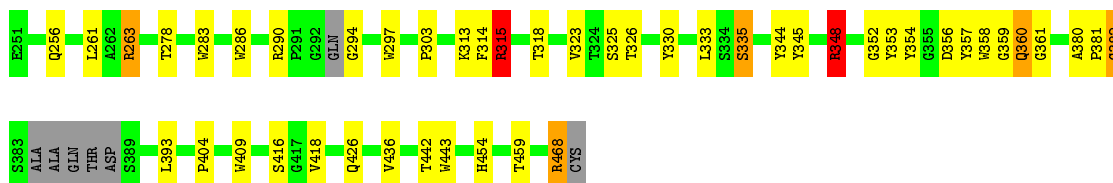
- Molecule 1: IGG1-LAMBDA SE155-4 FAB (LIGHT CHAIN)

Chain L: 

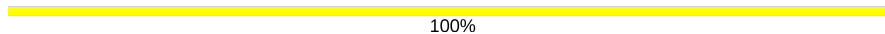


- Molecule 2: IGG1-LAMBDA SE155-4 FAB (HEAVY CHAIN)

Chain H: 



- Molecule 3: alpha-D-galactopyranose-(1-2)-[alpha-D-Abeguopyranose-(1-3)]alpha-D-mannopyranose

Chain A: 



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.30Å 128.60Å 79.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3434	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

## 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: GLA, PCA, ABE, MAN

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	L	0.86	0/1635	1.60	21/2236 (0.9%)
2	H	0.86	0/1660	1.69	33/2270 (1.5%)
All	All	0.86	0/3295	1.65	54/4506 (1.2%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	315	ARG	NE-CZ-NH1	12.59	126.59	120.30
2	H	348	ARG	NE-CZ-NH1	10.22	125.41	120.30
2	H	348	ARG	NE-CZ-NH2	-9.86	115.37	120.30
2	H	468	ARG	NE-CZ-NH1	9.69	125.14	120.30
2	H	286	TRP	CD1-CG-CD2	9.10	113.58	106.30
2	H	443	TRP	CD1-CG-CD2	8.56	113.15	106.30
2	H	286	TRP	CE2-CD2-CG	-8.50	100.50	107.30
1	L	23	ARG	NE-CZ-NH1	8.32	124.46	120.30
2	H	409	TRP	CD1-CG-CD2	8.27	112.91	106.30
1	L	93	TRP	CD1-CG-CD2	8.15	112.82	106.30
2	H	315	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	L	98	TRP	CD1-CG-CD2	7.72	112.47	106.30
1	L	93	TRP	CE2-CD2-CG	-7.67	101.17	107.30
2	H	297	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	L	23	ARG	NE-CZ-NH2	-7.56	116.52	120.30
2	H	358	TRP	CD1-CG-CD2	7.45	112.26	106.30
1	L	93	TRP	CG-CD2-CE3	7.45	140.60	133.90
1	L	93	TRP	CB-CG-CD1	-7.39	117.40	127.00
1	L	37	TRP	CD1-CG-CD2	7.35	112.18	106.30
2	H	283	TRP	CD1-CG-CD2	7.30	112.14	106.30
1	L	188	TRP	CE2-CD2-CG	-7.18	101.55	107.30
1	L	151	TRP	CD1-CG-CD2	7.03	111.92	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	443	TRP	CE2-CD2-CG	-7.01	101.69	107.30
2	H	358	TRP	CE2-CD2-CG	-6.93	101.76	107.30
2	H	283	TRP	CE2-CD2-CG	-6.86	101.81	107.30
2	H	263	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	L	188	TRP	CD1-CG-CD2	6.74	111.69	106.30
1	L	98	TRP	CE2-CD2-CG	-6.71	101.93	107.30
2	H	409	TRP	CE2-CD2-CG	-6.71	101.93	107.30
2	H	286	TRP	CG-CD2-CE3	6.58	139.82	133.90
2	H	286	TRP	CG-CD1-NE1	-6.53	103.57	110.10
1	L	151	TRP	CE2-CD2-CG	-6.52	102.08	107.30
2	H	353	TYR	CB-CG-CD2	-6.47	117.12	121.00
2	H	468	ARG	NE-CZ-NH2	-6.40	117.10	120.30
2	H	354	TYR	CB-CG-CD1	-6.36	117.18	121.00
2	H	344	TYR	CB-CG-CD2	-6.21	117.27	121.00
2	H	335	SER	CA-CB-OG	-6.14	94.63	111.20
1	L	129	GLU	CA-CB-CG	6.06	126.74	113.40
2	H	286	TRP	CB-CG-CD1	-6.06	119.12	127.00
2	H	297	TRP	CG-CD1-NE1	-6.03	104.07	110.10
1	L	37	TRP	CE2-CD2-CG	-6.03	102.48	107.30
1	L	188	TRP	CG-CD2-CE3	5.99	139.29	133.90
2	H	357	TYR	CB-CG-CD2	-5.96	117.42	121.00
1	L	188	TRP	CB-CG-CD1	-5.88	119.35	127.00
2	H	443	TRP	CG-CD1-NE1	-5.78	104.32	110.10
1	L	162	MET	CG-SD-CE	-5.72	91.04	100.20
1	L	190	ARG	NE-CZ-NH2	-5.51	117.55	120.30
2	H	409	TRP	CG-CD1-NE1	-5.30	104.80	110.10
2	H	330	TYR	CB-CA-C	-5.29	99.81	110.40
2	H	297	TRP	CE2-CD2-CG	-5.28	103.08	107.30
2	H	381	PRO	CA-C-N	-5.20	105.80	116.20
1	L	54	ASN	OD1-CG-ND2	-5.20	109.95	121.90
1	L	54	ASN	CB-CG-ND2	5.11	128.96	116.70
2	H	352	GLY	O-C-N	-5.04	114.63	122.70

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	L	1604	0	1538	13	0
2	H	1614	0	1554	17	0
3	A	32	0	30	0	0
4	H	82	0	0	1	0
4	L	102	0	0	3	0
All	All	3434	0	3122	29	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 5.

All (29) 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)
2:H:318:THR:HG22	2:H:333:LEU:HD23	1.76	0.67
1:L:156:THR:HG23	4:L:746:HOH:O	1.94	0.67
1:L:23:ARG:NH2	1:L:72:LYS:HE3	2.15	0.62
1:L:38:VAL:HG12	1:L:48:GLY:HA2	1.85	0.58
1:L:94:CYS:HB3	1:L:99:ILE:HD12	1.85	0.58
2:H:323:VAL:HB	2:H:326:THR:HG22	1.85	0.57
2:H:318:THR:HG22	2:H:333:LEU:CD2	2.35	0.55
2:H:382:GLY:HA2	2:H:468:ARG:HB2	1.89	0.54
2:H:256:GLN:HE22	2:H:345:TYR:HA	1.73	0.53
2:H:348:ARG:HD2	2:H:356:ASP:OD1	2.08	0.53
2:H:454:HIS:HB3	2:H:459:THR:HB	1.90	0.52
2:H:360:GLN:NE2	2:H:360:GLN:H	2.07	0.52
2:H:418:VAL:HG22	2:H:436:VAL:HG23	1.91	0.52
2:H:313:LYS:HD3	2:H:314:PHE:CE2	2.46	0.49
1:L:26:THR:HB	4:L:749:HOH:O	2.15	0.47
2:H:380:ALA:HB3	2:H:468:ARG:HG3	1.97	0.46
1:L:163:GLU:HG3	2:H:426:GLN:HG2	1.96	0.46
2:H:315:ARG:HH11	2:H:315:ARG:HG3	1.82	0.45
1:L:5:THR:HB	1:L:23:ARG:HG3	1.98	0.45
1:L:192:SER:O	1:L:210:SER:HA	2.18	0.44
2:H:256:GLN:NE2	2:H:361:GLY:H	2.16	0.43
1:L:23:ARG:CZ	1:L:72:LYS:HE3	2.48	0.43
1:L:42:PRO:HD3	4:L:715:HOH:O	2.18	0.43
1:L:23:ARG:HG2	1:L:23:ARG:HH11	1.84	0.43
2:H:303:PRO:HD2	4:H:751:HOH:O	2.21	0.41
1:L:14:PRO:HA	1:L:80:ALA:O	2.19	0.41
2:H:290:ARG:O	2:H:294:GLY:N	2.54	0.41
2:H:256:GLN:HE21	2:H:359:GLY:HA3	1.86	0.40
1:L:68:LEU:HD23	1:L:73:ALA:HA	2.02	0.40

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	L	211/215 (98%)	201 (95%)	8 (4%)	2 (1%)	17	11
2	H	210/219 (96%)	198 (94%)	10 (5%)	2 (1%)	15	9
All	All	421/434 (97%)	399 (95%)	18 (4%)	4 (1%)	15	9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	109	LEU
2	H	325	SER
1	L	2	ALA
2	H	382	GLY

### 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	L	180/182 (99%)	166 (92%)	14 (8%)	12	8
2	H	178/184 (97%)	167 (94%)	11 (6%)	18	13
All	All	358/366 (98%)	333 (93%)	25 (7%)	14	10

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	23	ARG
1	L	36	ASN
1	L	43	ASP
1	L	45	LEU
1	L	49	LEU
1	L	54	ASN
1	L	92	LEU
1	L	147	VAL
1	L	160	GLN
1	L	162	MET
1	L	167	PRO
1	L	186	ARG
1	L	203	HIS
1	L	208	SER
2	H	261	LEU
2	H	263	ARG
2	H	278	THR
2	H	315	ARG
2	H	335	SER
2	H	348	ARG
2	H	360	GLN
2	H	393	LEU
2	H	404	PRO
2	H	416	SER
2	H	442	THR

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

Mol	Chain	Res	Type
1	L	54	ASN
1	L	173	ASN
2	H	256	GLN
2	H	289	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](#)

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
1	PCA	L	1	1	7,8,9	0.70	0	9,10,12	0.87	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
1	PCA	L	1	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

3 monosaccharides 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	MAN	A	1	3	12,12,12	0.83	0	17,17,17	1.21	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GLA	A	2	3	11,11,12	1.40	2 (18%)	15,15,17	1.73	5 (33%)
3	ABE	A	3	3	9,9,10	1.54	1 (11%)	10,12,14	1.17	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	MAN	A	1	3	-	2/2/22/22	0/1/1/1
3	GLA	A	2	3	-	1/2/19/22	0/1/1/1
3	ABE	A	3	3	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3	ABE	C4-C5	3.54	1.58	1.52
3	A	2	GLA	C2-C3	2.48	1.56	1.52
3	A	2	GLA	C4-C3	2.27	1.58	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2	GLA	C6-C5-C4	3.54	121.30	113.00
3	A	2	GLA	O5-C5-C4	-2.98	103.57	110.83
3	A	2	GLA	O5-C5-C6	2.63	111.32	107.20
3	A	2	GLA	O2-C2-C1	2.38	114.03	109.15
3	A	1	MAN	C1-O5-C5	2.38	118.15	113.66
3	A	1	MAN	O2-C2-C3	-2.37	104.86	110.35
3	A	2	GLA	O5-C1-C2	2.26	114.27	110.77

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	MAN	C4-C5-C6-O6
3	A	1	MAN	O5-C5-C6-O6
3	A	2	GLA	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.