



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:41 am GMT

PDB ID : 5F93  
Title : Blood group antigen binding adhesin BabA of Helicobacter pylori strain A730  
in complex with blood group H Lewis b hexasaccharide  
Authors : Moonens, K.; Gideonsson, P.; Subedi, S.; Romao, E.; Oscarson, S.; Muylder-  
mans, S.; Boren, T.; Remaut, H.  
Deposited on : 2015-12-09  
Resolution : 2.99 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

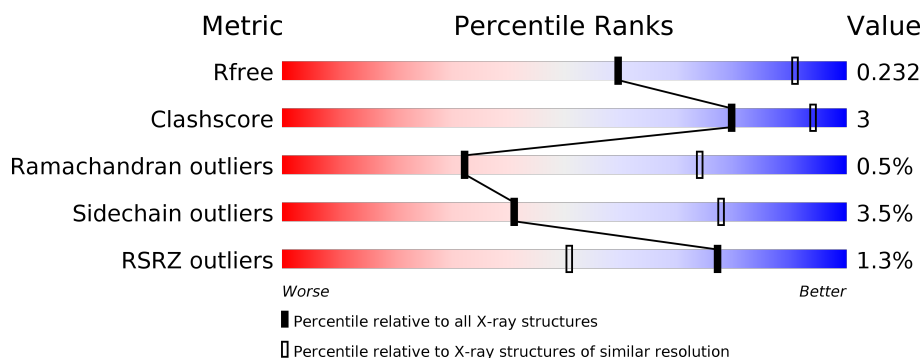
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 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))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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. 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	469	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>80%</span> <span>10%</span> <span>10%</span> </div> </div>
1	B	469	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>82%</span> <span>9%</span> <span>9%</span> </div> </div>
1	E	469	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>81%</span> <span>8%</span> <span>10%</span> </div> </div>
1	G	469	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 96%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>2%</span> <span>79%</span> <span>10%</span> <span>10%</span> </div> </div>
2	C	120	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 95%, yellow 5%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span></span> <span>80%</span> <span>15%</span> <span>5%</span> </div> </div>
2	D	120	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 97%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>85%</span> <span>10%</span> <span>5%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	120	<div><div></div><div>88%</div><div>8%5%</div></div>
2	H	120	<div>%<div><div></div><div>84%</div><div>10%• 5%</div></div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16509 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 Adhesin binding fucosylated histo-blood group antigen,Adhesin,Adhesin binding fucosylated histo-blood group antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3184	1970	544	657	13			
1	B	426	Total	C	N	O	S	0	2	0
			3205	1981	547	664	13			
1	E	420	Total	C	N	O	S	0	0	0
			3149	1947	538	651	13			
1	G	422	Total	C	N	O	S	0	1	0
			3165	1956	541	655	13			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ALA	-	expression tag	UNP O52269
A	4	SER	-	expression tag	UNP O52269
A	5	TRP	-	expression tag	UNP O52269
A	6	SER	-	expression tag	UNP O52269
A	7	HIS	-	expression tag	UNP O52269
A	8	PRO	-	expression tag	UNP O52269
A	9	GLN	-	expression tag	UNP O52269
A	10	PHE	-	expression tag	UNP O52269
A	11	GLU	-	expression tag	UNP O52269
A	12	LYS	-	expression tag	UNP O52269
A	13	SER	-	expression tag	UNP O52269
A	14	GLY	-	expression tag	UNP O52269
A	15	GLY	-	expression tag	UNP O52269
A	16	GLY	-	expression tag	UNP O52269
A	17	GLY	-	expression tag	UNP O52269
A	18	GLY	-	expression tag	UNP O52269
A	19	LEU	-	expression tag	UNP O52269
A	20	VAL	-	expression tag	UNP O52269
A	21	PRO	-	expression tag	UNP O52269
A	22	ARG	-	expression tag	UNP O52269

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Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLY	-	expression tag	UNP O52269
A	24	SER	-	expression tag	UNP O52269
A	464	GLY	-	expression tag	UNP O52269
A	465	SER	-	expression tag	UNP O52269
A	466	HIS	-	expression tag	UNP O52269
A	467	HIS	-	expression tag	UNP O52269
A	468	HIS	-	expression tag	UNP O52269
A	469	HIS	-	expression tag	UNP O52269
A	470	HIS	-	expression tag	UNP O52269
A	471	HIS	-	expression tag	UNP O52269
B	3	ALA	-	expression tag	UNP O52269
B	4	SER	-	expression tag	UNP O52269
B	5	TRP	-	expression tag	UNP O52269
B	6	SER	-	expression tag	UNP O52269
B	7	HIS	-	expression tag	UNP O52269
B	8	PRO	-	expression tag	UNP O52269
B	9	GLN	-	expression tag	UNP O52269
B	10	PHE	-	expression tag	UNP O52269
B	11	GLU	-	expression tag	UNP O52269
B	12	LYS	-	expression tag	UNP O52269
B	13	SER	-	expression tag	UNP O52269
B	14	GLY	-	expression tag	UNP O52269
B	15	GLY	-	expression tag	UNP O52269
B	16	GLY	-	expression tag	UNP O52269
B	17	GLY	-	expression tag	UNP O52269
B	18	GLY	-	expression tag	UNP O52269
B	19	LEU	-	expression tag	UNP O52269
B	20	VAL	-	expression tag	UNP O52269
B	21	PRO	-	expression tag	UNP O52269
B	22	ARG	-	expression tag	UNP O52269
B	23	GLY	-	expression tag	UNP O52269
B	24	SER	-	expression tag	UNP O52269
B	464	GLY	-	expression tag	UNP O52269
B	465	SER	-	expression tag	UNP O52269
B	466	HIS	-	expression tag	UNP O52269
B	467	HIS	-	expression tag	UNP O52269
B	468	HIS	-	expression tag	UNP O52269
B	469	HIS	-	expression tag	UNP O52269
B	470	HIS	-	expression tag	UNP O52269
B	471	HIS	-	expression tag	UNP O52269
E	3	ALA	-	expression tag	UNP O52269
E	4	SER	-	expression tag	UNP O52269

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Chain	Residue	Modelled	Actual	Comment	Reference
E	5	TRP	-	expression tag	UNP O52269
E	6	SER	-	expression tag	UNP O52269
E	7	HIS	-	expression tag	UNP O52269
E	8	PRO	-	expression tag	UNP O52269
E	9	GLN	-	expression tag	UNP O52269
E	10	PHE	-	expression tag	UNP O52269
E	11	GLU	-	expression tag	UNP O52269
E	12	LYS	-	expression tag	UNP O52269
E	13	SER	-	expression tag	UNP O52269
E	14	GLY	-	expression tag	UNP O52269
E	15	GLY	-	expression tag	UNP O52269
E	16	GLY	-	expression tag	UNP O52269
E	17	GLY	-	expression tag	UNP O52269
E	18	GLY	-	expression tag	UNP O52269
E	19	LEU	-	expression tag	UNP O52269
E	20	VAL	-	expression tag	UNP O52269
E	21	PRO	-	expression tag	UNP O52269
E	22	ARG	-	expression tag	UNP O52269
E	23	GLY	-	expression tag	UNP O52269
E	24	SER	-	expression tag	UNP O52269
E	464	GLY	-	expression tag	UNP O52269
E	465	SER	-	expression tag	UNP O52269
E	466	HIS	-	expression tag	UNP O52269
E	467	HIS	-	expression tag	UNP O52269
E	468	HIS	-	expression tag	UNP O52269
E	469	HIS	-	expression tag	UNP O52269
E	470	HIS	-	expression tag	UNP O52269
E	471	HIS	-	expression tag	UNP O52269
G	3	ALA	-	expression tag	UNP O52269
G	4	SER	-	expression tag	UNP O52269
G	5	TRP	-	expression tag	UNP O52269
G	6	SER	-	expression tag	UNP O52269
G	7	HIS	-	expression tag	UNP O52269
G	8	PRO	-	expression tag	UNP O52269
G	9	GLN	-	expression tag	UNP O52269
G	10	PHE	-	expression tag	UNP O52269
G	11	GLU	-	expression tag	UNP O52269
G	12	LYS	-	expression tag	UNP O52269
G	13	SER	-	expression tag	UNP O52269
G	14	GLY	-	expression tag	UNP O52269
G	15	GLY	-	expression tag	UNP O52269
G	16	GLY	-	expression tag	UNP O52269

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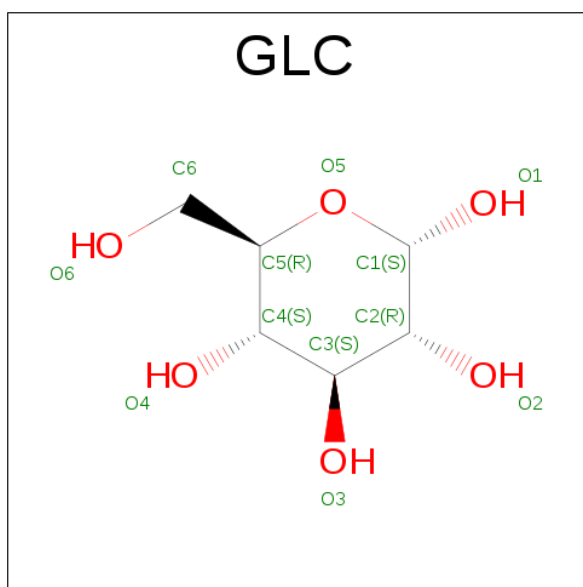
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Chain	Residue	Modelled	Actual	Comment	Reference
G	17	GLY	-	expression tag	UNP O52269
G	18	GLY	-	expression tag	UNP O52269
G	19	LEU	-	expression tag	UNP O52269
G	20	VAL	-	expression tag	UNP O52269
G	21	PRO	-	expression tag	UNP O52269
G	22	ARG	-	expression tag	UNP O52269
G	23	GLY	-	expression tag	UNP O52269
G	24	SER	-	expression tag	UNP O52269
G	464	GLY	-	expression tag	UNP O52269
G	465	SER	-	expression tag	UNP O52269
G	466	HIS	-	expression tag	UNP O52269
G	467	HIS	-	expression tag	UNP O52269
G	468	HIS	-	expression tag	UNP O52269
G	469	HIS	-	expression tag	UNP O52269
G	470	HIS	-	expression tag	UNP O52269
G	471	HIS	-	expression tag	UNP O52269

- Molecule 2 is a protein called Nanobody Nb-ER19.

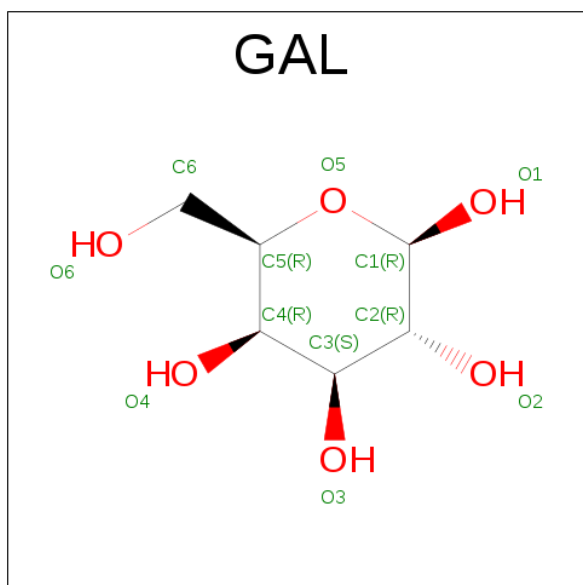
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	114	Total 873	C 546	N 158	O 164	S 5	0	0	0
2	D	114	Total 873	C 546	N 158	O 164	S 5	0	0	0
2	F	114	Total 873	C 546	N 158	O 164	S 5	0	0	0
2	H	114	Total 873	C 546	N 158	O 164	S 5	0	0	0

- Molecule 3 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	E	1	Total	C	O	0	0
			12	6	6		
3	G	1	Total	C	O	0	0
			12	6	6		

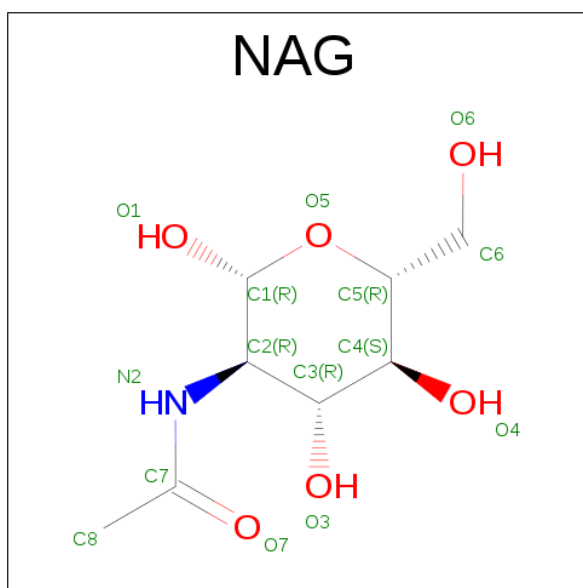
- Molecule 4 is BETA-D-GALACTOSE (three-letter code: GAL) (formula:  $C_6H_{12}O_6$ ).





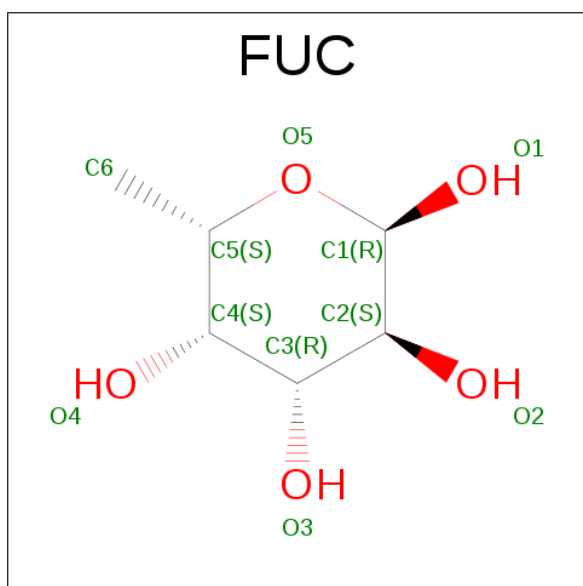
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	E	1	Total	C	O	0	0
			11	6	5		
4	E	1	Total	C	O	0	0
			11	6	5		
4	G	1	Total	C	O	0	0
			11	6	5		
4	G	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula:  $C_6H_{12}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	A	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		
6	E	1	Total	C	O	0	0
			10	6	4		
6	E	1	Total	C	O	0	0
			10	6	4		
6	G	1	Total	C	O	0	0
			10	6	4		
6	G	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	8	Total	O	0	0
			8	8		
7	B	13	Total	O	0	0
			13	13		
7	E	6	Total	O	0	0
			6	6		

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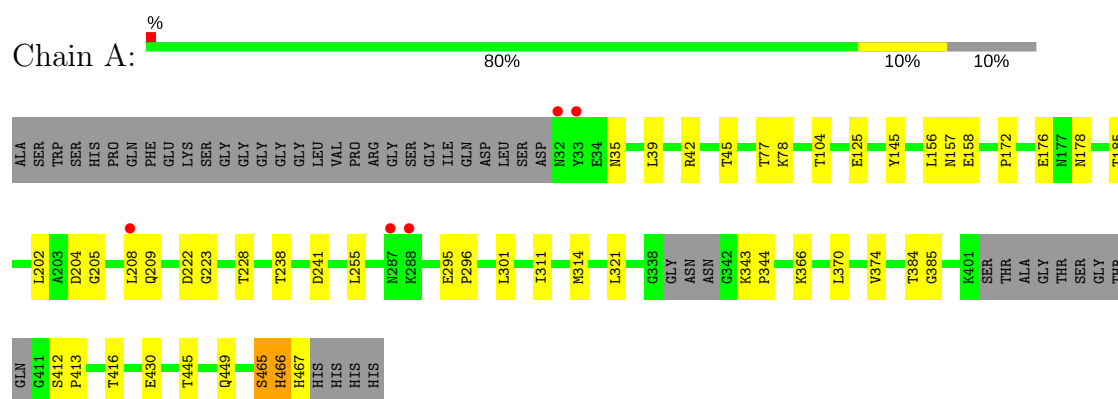
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	7	Total 7	O 7	0	0
7	C	2	Total 2	O 2	0	0
7	F	3	Total 3	O 3	0	0
7	H	3	Total 3	O 3	0	0

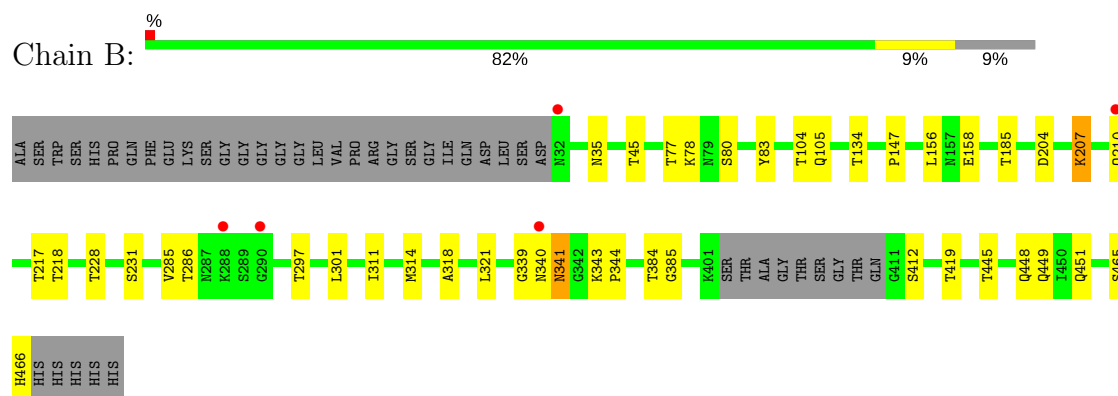
### 3 Residue-property plots [i](#)

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.

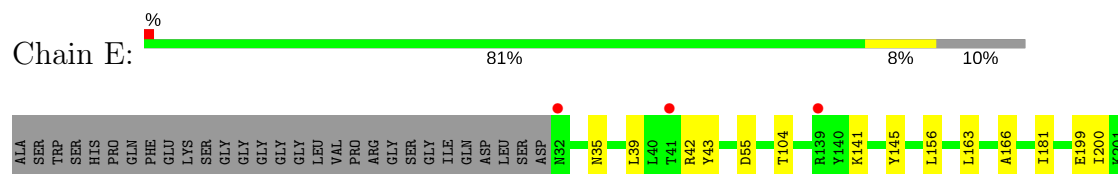
- Molecule 1: Adhesin binding fucosylated histo-blood group antigen,Adhesin,Adhesin binding fucosylated histo-blood group antigen



- Molecule 1: Adhesin binding fucosylated histo-blood group antigen,Adhesin,Adhesin binding fucosylated histo-blood group antigen



- Molecule 1: Adhesin binding fucosylated histo-blood group antigen,Adhesin,Adhesin binding fucosylated histo-blood group antigen





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.17Å 134.47Å 123.98Å 90.00° 102.30° 90.00°	Depositor
Resolution (Å)	48.64 – 2.99 48.64 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.9 (48.64-2.99) 97.9 (48.64-2.99)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.181 , 0.234 0.185 , 0.232	Depositor DCC
$R_{free}$ test set	3241 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.2	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 49.0	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	0.95	EDS
Total number of atoms	16509	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.54 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.7101e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: GLC, GAL, NAG, FUC

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	0.62	0/3234	0.74	0/4395
1	B	0.63	0/3261	0.75	0/4433
1	E	0.55	0/3198	0.70	0/4347
1	G	0.54	0/3217	0.70	0/4373
2	C	0.62	0/893	0.82	0/1210
2	D	0.60	0/893	0.78	0/1210
2	F	0.69	0/893	0.86	0/1210
2	H	0.71	0/893	0.82	0/1210
All	All	0.60	0/16482	0.74	0/22388

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	G	0	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	466	HIS	Peptide
1	G	226	VAL	Peptide
1	G	340	ASN	Peptide

## 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	3184	0	3085	20	0
1	B	3205	0	3106	23	0
1	E	3149	0	3047	20	0
1	G	3165	0	3063	20	0
2	C	873	0	852	7	0
2	D	873	0	852	5	0
2	F	873	0	852	3	0
2	H	873	0	852	6	0
3	A	12	0	11	0	0
3	B	12	0	11	0	0
3	E	12	0	11	2	0
3	G	12	0	11	0	0
4	A	22	0	18	0	0
4	B	22	0	18	0	0
4	E	22	0	18	2	0
4	G	22	0	18	0	0
5	A	14	0	11	0	0
5	B	14	0	11	0	0
5	E	14	0	11	0	0
5	G	14	0	11	0	0
6	A	20	0	20	0	0
6	B	20	0	20	1	0
6	E	20	0	20	1	0
6	G	20	0	20	0	0
7	A	8	0	0	0	0
7	B	13	0	0	0	0
7	C	2	0	0	0	0
7	E	6	0	0	0	0
7	F	3	0	0	0	0
7	G	7	0	0	0	0
7	H	3	0	0	0	0
All	All	16509	0	15949	102	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.

The worst 5 of 102 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:F:3:VAL:N	2:F:26:SER:HG	1.86	0.74
1:G:202:LEU:HD23	1:G:206:GLN:O	1.90	0.71
1:B:339:GLY:O	1:B:341:ASN:N	2.30	0.64
1:A:35:ASN:OD1	1:A:35:ASN:C	2.38	0.62
1:B:465:SER:O	1:B:466:HIS:HB2	2.01	0.61

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	418/469 (89%)	394 (94%)	23 (6%)	1 (0%)	51	86
1	B	424/469 (90%)	401 (95%)	22 (5%)	1 (0%)	51	86
1	E	414/469 (88%)	383 (92%)	30 (7%)	1 (0%)	51	86
1	G	417/469 (89%)	385 (92%)	28 (7%)	4 (1%)	18	59
2	C	112/120 (93%)	107 (96%)	4 (4%)	1 (1%)	20	62
2	D	112/120 (93%)	109 (97%)	2 (2%)	1 (1%)	20	62
2	F	112/120 (93%)	108 (96%)	3 (3%)	1 (1%)	20	62
2	H	112/120 (93%)	104 (93%)	7 (6%)	1 (1%)	20	62
All	All	2121/2356 (90%)	1991 (94%)	119 (6%)	11 (0%)	32	74

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	340	ASN
1	E	341	ASN
2	C	115	SER
2	D	115	SER
1	A	465	SER

### 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	350/384 (91%)	337 (96%)	13 (4%)	39	76
1	B	353/384 (92%)	342 (97%)	11 (3%)	45	80
1	E	346/384 (90%)	334 (96%)	12 (4%)	41	78
1	G	348/384 (91%)	336 (97%)	12 (3%)	42	78
2	C	93/99 (94%)	89 (96%)	4 (4%)	33	72
2	D	93/99 (94%)	90 (97%)	3 (3%)	44	79
2	F	93/99 (94%)	90 (97%)	3 (3%)	44	79
2	H	93/99 (94%)	90 (97%)	3 (3%)	44	79
All	All	1769/1932 (92%)	1708 (97%)	61 (3%)	41	78

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	202	LEU
1	E	419	THR
2	F	85	SER
1	E	227	SER
1	E	334	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	124	ASN
1	G	161	GLN
2	D	77	ASN
1	G	109	ASN
2	F	55	GLN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

24 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	GLC	A	501	4	12,12,12	0.59	0	17,17,17	1.42	3 (17%)
4	GAL	A	502	3,5	11,11,12	0.57	0	13,15,17	1.09	1 (7%)
5	NAG	A	503	4,6	14,14,15	0.55	0	15,19,21	1.74	5 (33%)
4	GAL	A	504	5,6	11,11,12	0.84	0	13,15,17	1.31	2 (15%)
6	FUC	A	505	4	9,10,11	0.75	0	13,14,16	1.41	2 (15%)
6	FUC	A	506	5	9,10,11	0.65	0	13,14,16	1.18	2 (15%)
3	GLC	B	501	4	12,12,12	0.53	0	17,17,17	2.03	7 (41%)
4	GAL	B	502	3,5	11,11,12	0.60	0	13,15,17	1.50	3 (23%)
5	NAG	B	503	4,6	14,14,15	0.83	1 (7%)	15,19,21	2.49	7 (46%)
4	GAL	B	504	5,6	11,11,12	0.65	0	13,15,17	1.29	2 (15%)
6	FUC	B	505	4	9,10,11	0.80	0	13,14,16	1.45	2 (15%)
6	FUC	B	506	5	9,10,11	0.88	0	13,14,16	2.13	6 (46%)
3	GLC	E	501	4	12,12,12	0.44	0	17,17,17	0.51	0
4	GAL	E	502	3,5	11,11,12	0.46	0	13,15,17	0.78	0
5	NAG	E	503	4,6	14,14,15	0.52	0	15,19,21	1.28	1 (6%)
4	GAL	E	504	5,6	11,11,12	0.82	0	13,15,17	1.73	4 (30%)
6	FUC	E	505	4	9,10,11	0.80	0	13,14,16	1.33	2 (15%)
6	FUC	E	506	5	9,10,11	0.79	0	13,14,16	1.59	3 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GLC	G	501	4	12,12,12	0.59	0	17,17,17	1.07	2 (11%)
4	GAL	G	502	3,5	11,11,12	0.64	0	13,15,17	1.17	1 (7%)
5	NAG	G	503	4,6	14,14,15	0.45	0	15,19,21	1.50	4 (26%)
4	GAL	G	504	5,6	11,11,12	0.96	1 (9%)	13,15,17	1.54	3 (23%)
6	FUC	G	505	4	9,10,11	0.81	0	13,14,16	1.71	3 (23%)
6	FUC	G	506	5	9,10,11	0.60	0	13,14,16	1.44	3 (23%)

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	GLC	A	501	4	-	0/2/22/22	0/1/1/1
4	GAL	A	502	3,5	-	0/2/19/22	0/1/1/1
5	NAG	A	503	4,6	-	0/6/23/26	0/1/1/1
4	GAL	A	504	5,6	-	0/2/19/22	0/1/1/1
6	FUC	A	505	4	-	0/0/17/20	0/1/1/1
6	FUC	A	506	5	-	0/0/17/20	0/1/1/1
3	GLC	B	501	4	-	0/2/22/22	0/1/1/1
4	GAL	B	502	3,5	-	0/2/19/22	0/1/1/1
5	NAG	B	503	4,6	-	0/6/23/26	0/1/1/1
4	GAL	B	504	5,6	-	0/2/19/22	0/1/1/1
6	FUC	B	505	4	-	0/0/17/20	0/1/1/1
6	FUC	B	506	5	-	0/0/17/20	0/1/1/1
3	GLC	E	501	4	-	0/2/22/22	0/1/1/1
4	GAL	E	502	3,5	-	0/2/19/22	0/1/1/1
5	NAG	E	503	4,6	-	0/6/23/26	0/1/1/1
4	GAL	E	504	5,6	-	0/2/19/22	0/1/1/1
6	FUC	E	505	4	-	0/0/17/20	0/1/1/1
6	FUC	E	506	5	-	0/0/17/20	0/1/1/1
3	GLC	G	501	4	-	0/2/22/22	0/1/1/1
4	GAL	G	502	3,5	-	0/2/19/22	0/1/1/1
5	NAG	G	503	4,6	-	0/6/23/26	0/1/1/1
4	GAL	G	504	5,6	-	0/2/19/22	0/1/1/1
6	FUC	G	505	4	-	0/0/17/20	0/1/1/1
6	FUC	G	506	5	-	0/0/17/20	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	504	GAL	C1-C2	2.01	1.57	1.52
5	B	503	NAG	C1-C2	2.06	1.55	1.52

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	505	FUC	O5-C1-C2	-3.91	104.66	110.79
4	B	502	GAL	C2-C3-C4	-3.43	104.89	110.88
5	B	503	NAG	O5-C1-C2	-3.16	107.07	111.47
5	B	503	NAG	O7-C7-C8	-3.12	116.38	122.06
6	B	506	FUC	O5-C1-C2	-3.02	106.06	110.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	506	FUC	1	0
3	E	501	GLC	2	0
4	E	502	GAL	2	0
6	E	505	FUC	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	A	424/469 (90%)	-0.15	5 (1%) 79 53	39, 62, 113, 136	0
1	B	426/469 (90%)	-0.21	5 (1%) 79 53	38, 61, 106, 142	0
1	E	420/469 (89%)	-0.11	6 (1%) 75 49	41, 69, 123, 146	0
1	G	422/469 (89%)	-0.03	9 (2%) 64 34	41, 71, 127, 146	0
2	C	114/120 (95%)	-0.18	0 100 100	45, 69, 96, 135	0
2	D	114/120 (95%)	-0.26	1 (0%) 84 61	44, 66, 90, 127	0
2	F	114/120 (95%)	-0.26	0 100 100	38, 56, 78, 116	0
2	H	114/120 (95%)	-0.29	1 (0%) 84 61	41, 59, 80, 119	0
All	All	2148/2356 (91%)	-0.15	27 (1%) 77 51	38, 65, 119, 146	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	32	ASN	4.9
1	B	32	ASN	4.4
1	G	290	GLY	4.2
1	E	32	ASN	3.6
2	H	3	VAL	3.6

### 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. 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
6	FUC	B	505	10/11	0.95	0.30	0.74	58,63,68,73	0
6	FUC	E	505	10/11	0.95	0.25	0.41	69,79,83,85	0
6	FUC	G	505	10/11	0.94	0.26	0.36	78,85,90,91	0
4	GAL	A	502	11/12	0.94	0.23	-0.29	74,87,91,94	0
4	GAL	B	502	11/12	0.87	0.21	-0.31	68,93,107,110	0
6	FUC	A	505	10/11	0.98	0.18	-0.81	46,48,50,50	0
5	NAG	B	503	14/15	0.93	0.16	-1.39	48,65,68,68	0
3	GLC	G	501	12/12	0.85	0.39	-	93,104,117,122	0
3	GLC	A	501	12/12	0.84	0.35	-	92,98,104,107	0
6	FUC	B	506	10/11	0.96	0.21	-	67,72,81,82	0
6	FUC	A	506	10/11	0.94	0.26	-	72,77,79,81	0
4	GAL	G	504	11/12	0.89	0.34	-	73,90,95,95	0
5	NAG	E	503	14/15	0.95	0.19	-	80,88,93,95	0
3	GLC	E	501	12/12	0.77	0.31	-	89,110,130,135	0
4	GAL	E	504	11/12	0.88	0.19	-	71,83,89,91	0
4	GAL	B	504	11/12	0.95	0.17	-	57,62,67,69	0
4	GAL	E	502	11/12	0.85	0.26	-	85,112,123,125	0
5	NAG	A	503	14/15	0.96	0.14	-	55,63,64,67	0
6	FUC	E	506	10/11	0.91	0.33	-	83,91,102,108	0
5	NAG	G	503	14/15	0.94	0.25	-	78,90,101,101	0
6	FUC	G	506	10/11	0.89	0.34	-	100,102,105,109	0
4	GAL	G	502	11/12	0.84	0.32	-	96,113,123,125	0
3	GLC	B	501	12/12	0.79	0.54	-	103,118,124,124	0
4	GAL	A	504	11/12	0.95	0.17	-	54,59,65,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.