



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2018 – 01:19 PM EDT

PDB ID : 5YC5  
Title : Crystal structure of human IgG-Fc in complex with aglycan and optimized Fc gamma receptor IIIa  
Authors : Caaveiro, J.M.M.; Tamura, H.; Tsumoto, K.; Kiyoshi, M.  
Deposited on : 2017-09-06  
Resolution : 2.71 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

<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 : rb-20030736  
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) : rb-20030736

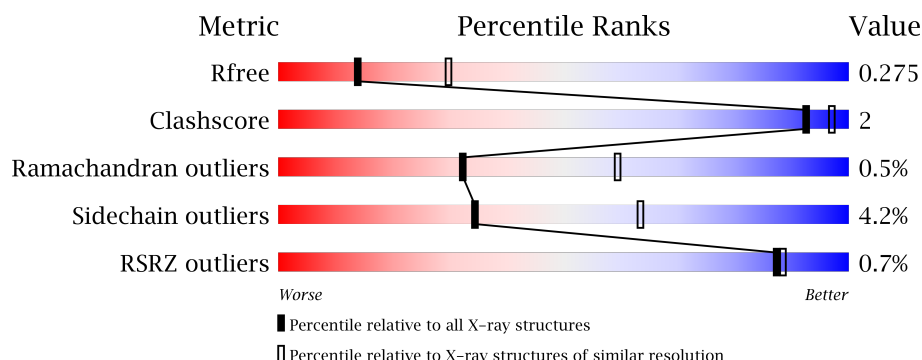
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




The reported resolution of this entry is 2.71 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	2649 (2.74-2.70)
Clashscore	112137	2993 (2.74-2.70)
Ramachandran outliers	110173	2946 (2.74-2.70)
Sidechain outliers	110143	2947 (2.74-2.70)
RSRZ outliers	101464	2665 (2.74-2.70)

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	223	
1	B	223	
2	C	182	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4995 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 Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1684	1073	283	322	6			
1	B	213	Total	C	N	O	S	0	0	0
			1700	1083	285	326	6			

- Molecule 2 is a protein called Low affinity immunoglobulin gamma Fc region receptor III-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	171	Total	C	N	O	S	0	0	0
			1366	859	238	265	4			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	9	GLU	VAL	engineered mutation	UNP P08637
C	11	ILE	PHE	engineered mutation	UNP P08637
C	17	ASN	TYR	engineered mutation	UNP P08637
C	30	ARG	GLN	engineered mutation	UNP P08637
C	57	LEU	PHE	engineered mutation	UNP P08637
C	74	SER	ASN	engineered mutation	UNP P08637
C	99	GLU	VAL	engineered mutation	UNP P08637
C	103	GLY	GLU	engineered mutation	UNP P08637
C	153	SER	PHE	engineered mutation	UNP P08637
C	158	VAL	PHE	variant	UNP P08637
C	176	GLY	-	expression tag	UNP P08637
C	177	HIS	-	expression tag	UNP P08637
C	178	HIS	-	expression tag	UNP P08637
C	179	HIS	-	expression tag	UNP P08637
C	180	HIS	-	expression tag	UNP P08637
C	181	HIS	-	expression tag	UNP P08637
C	182	HIS	-	expression tag	UNP P08637

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



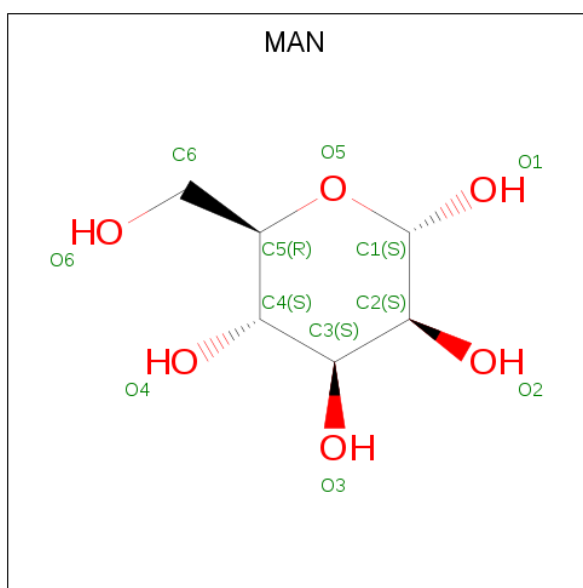
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



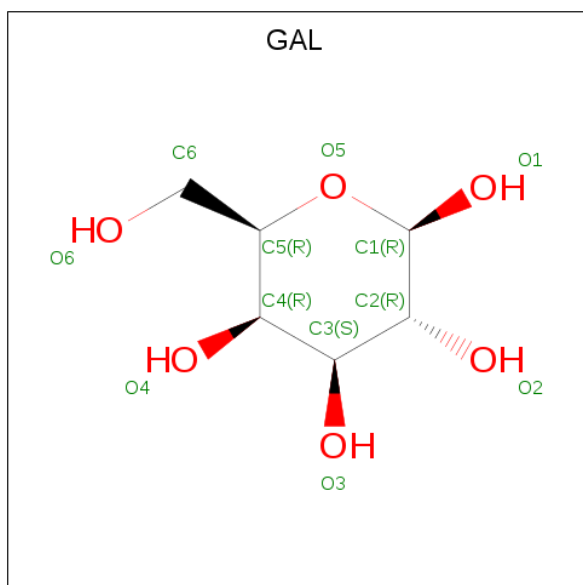
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is BETA-D-GALACTOSE (three-letter code: GAL) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula:  $C_6H_{12}O_5$ ).



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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		

- Molecule 9 is water.

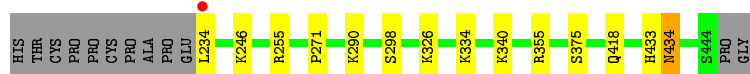
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	18	Total	O	0	0
			18	18		
9	B	10	Total	O	0	0
			10	10		
9	C	7	Total	O	0	0
			7	7		

### 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.

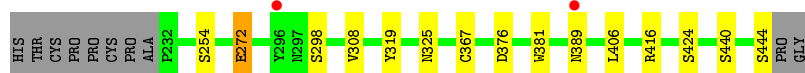
- Molecule 1: Immunoglobulin gamma-1 heavy chain

Chain A: 




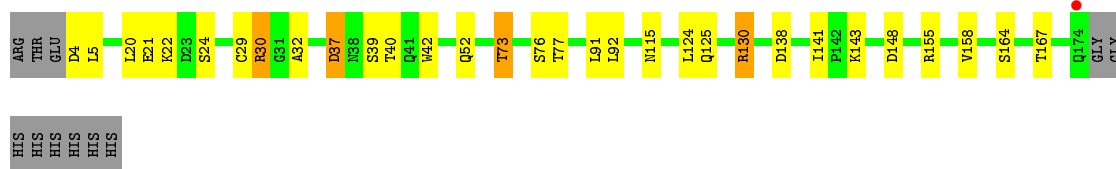
- Molecule 1: Immunoglobulin gamma-1 heavy chain

Chain B: 



- Molecule 2: Low affinity immunoglobulin gamma Fc region receptor III-A

Chain C: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.79Å 101.42Å 122.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.90 – 2.71 46.89 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.90-2.71) 100.0 (46.89-2.71)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.209 , 0.273 0.214 , 0.275	Depositor DCC
$R_{free}$ test set	1259 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.0	Xtriage
Anisotropy	0.866	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 18.6	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	0.93	EDS
Total number of atoms	4995	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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: BMA, NAG, CL, GAL, FUC, 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	A	0.83	0/1730	0.96	3/2357 (0.1%)
1	B	0.79	0/1747	0.92	1/2380 (0.0%)
2	C	0.84	0/1400	0.95	4/1902 (0.2%)
All	All	0.82	0/4877	0.94	8/6639 (0.1%)

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
2	C	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	130	ARG	NE-CZ-NH1	6.54	123.57	120.30
2	C	138	ASP	CB-CG-OD1	6.25	123.93	118.30
1	B	416	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	234	LEU	CA-CB-CG	5.39	127.69	115.30
1	A	255	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	A	355	ARG	NE-CZ-NH2	5.22	122.91	120.30
2	C	30	ARG	NE-CZ-NH1	5.09	122.84	120.30
2	C	37	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	76	SER	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	1684	0	1655	3	0
1	B	1700	0	1669	4	0
2	C	1366	0	1317	11	0
3	A	56	0	48	1	0
3	B	56	0	49	0	0
4	A	11	0	8	0	0
4	B	11	0	8	0	0
5	A	22	0	18	0	0
5	B	22	0	18	0	0
6	A	11	0	10	1	0
7	A	10	0	10	0	0
7	B	10	0	10	0	0
8	A	1	0	0	0	0
9	A	18	0	0	0	0
9	B	10	0	0	0	0
9	C	7	0	0	0	0
All	All	4995	0	4820	18	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 2.

All (18) 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:C:20:LEU:HD21	2:C:92:LEU:HB2	1.78	0.64
1:B:272:GLU:O	1:B:325:ASN:ND2	2.33	0.59
2:C:155:ARG:HB3	2:C:164:SER:HB3	1.89	0.54
2:C:4:ASP:OD1	2:C:5:LEU:N	2.43	0.52
2:C:37:ASP:OD1	2:C:39:SER:OG	2.27	0.50
2:C:91:LEU:HD12	2:C:164:SER:HA	1.95	0.48
1:B:406:LEU:HD12	1:B:406:LEU:C	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:32:ALA:O	2:C:73:THR:CG2	2.62	0.47
2:C:141:ILE:HG21	2:C:148:ASP:OD1	2.15	0.47
1:A:246:LYS:HG2	6:A:1009:GAL:O4	2.16	0.46
2:C:29:CYS:HB2	2:C:42:TRP:CZ2	2.52	0.45
1:A:433:HIS:CD2	1:A:434:ASN:ND2	2.86	0.44
2:C:158:VAL:O	2:C:158:VAL:HG12	2.17	0.44
1:B:308:VAL:HG12	1:B:319:TYR:CE1	2.53	0.43
2:C:21:GLU:O	2:C:22:LYS:HB2	2.18	0.42
1:B:367:CYS:HB2	1:B:381:TRP:CZ2	2.54	0.42
2:C:125:GLN:OE1	2:C:130:ARG:NH1	2.44	0.41
1:A:334:LYS:HE3	3:A:1005:NAG:H82	2.02	0.41

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	209/223 (94%)	203 (97%)	4 (2%)	2 (1%)	18	41
1	B	211/223 (95%)	200 (95%)	11 (5%)	0	100	100
2	C	169/182 (93%)	166 (98%)	2 (1%)	1 (1%)	28	55
All	All	589/628 (94%)	569 (97%)	17 (3%)	3 (0%)	32	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	ASN
2	C	77	THR
1	A	271	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	A	196/206 (95%)	190 (97%)	6 (3%)	45	74
1	B	198/206 (96%)	190 (96%)	8 (4%)	36	65
2	C	154/163 (94%)	145 (94%)	9 (6%)	23	48
All	All	548/575 (95%)	525 (96%)	23 (4%)	34	63

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	LYS
1	A	298	SER
1	A	326	LYS
1	A	340	LYS
1	A	375	SER
1	A	418	GLN
1	B	254	SER
1	B	272	GLU
1	B	298	SER
1	B	376	ASP
1	B	389	ASN
1	B	424	SER
1	B	440	SER
1	B	444	SER
2	C	24	SER
2	C	30	ARG
2	C	40	THR
2	C	52	GLN
2	C	73	THR
2	C	115	ASN
2	C	124	LEU
2	C	143	LYS
2	C	167	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	342	GLN
1	A	386	GLN
1	A	390	ASN
1	A	434	ASN
1	B	386	GLN
1	B	434	ASN
2	C	15	GLN
2	C	52	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

15 non-standard protein/DNA/RNA residues 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	NAG	A	1001	1,3,7	14,14,15	0.82	1 (7%)	15,19,21	1.89	3 (20%)
3	NAG	A	1002	3,4	14,14,15	0.62	0	15,19,21	0.82	0
5	MAN	A	1004	3,4	11,11,12	0.61	0	13,15,17	2.43	3 (23%)
3	NAG	A	1005	5	14,14,15	1.29	1 (7%)	15,19,21	1.59	4 (26%)
5	MAN	A	1007	3,4	11,11,12	0.58	0	13,15,17	2.10	4 (30%)
3	NAG	A	1008	5,6	14,14,15	0.93	0	15,19,21	2.69	7 (46%)
6	GAL	A	1009	3	11,11,12	1.53	4 (36%)	13,15,17	1.67	3 (23%)
7	FUC	A	1011	3	9,10,11	1.19	0	13,14,16	2.72	5 (38%)
3	NAG	B	1001	1,3,7	14,14,15	0.68	0	15,19,21	1.13	0
3	NAG	B	1002	3,4	14,14,15	0.98	1 (7%)	15,19,21	1.45	3 (20%)
5	MAN	B	1004	3,4	11,11,12	0.69	0	13,15,17	2.14	3 (23%)
3	NAG	B	1005	5	14,14,15	0.66	0	15,19,21	1.59	4 (26%)
5	MAN	B	1007	3,4	11,11,12	0.67	0	13,15,17	1.75	4 (30%)
3	NAG	B	1008	5	14,14,15	0.40	0	15,19,21	1.60	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	FUC	B	1011	3	9,10,11	0.87	0	13,14,16	1.53	2 (15%)

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	NAG	A	1001	1,3,7	-	0/6/23/26	0/1/1/1
3	NAG	A	1002	3,4	-	0/6/23/26	0/1/1/1
5	MAN	A	1004	3,4	-	0/2/19/22	0/1/1/1
3	NAG	A	1005	5	-	0/6/23/26	0/1/1/1
5	MAN	A	1007	3,4	-	0/2/19/22	0/1/1/1
3	NAG	A	1008	5,6	-	0/6/23/26	0/1/1/1
6	GAL	A	1009	3	-	0/2/19/22	0/1/1/1
7	FUC	A	1011	3	-	0/0/17/20	0/1/1/1
3	NAG	B	1001	1,3,7	-	0/6/23/26	0/1/1/1
3	NAG	B	1002	3,4	-	0/6/23/26	0/1/1/1
5	MAN	B	1004	3,4	-	0/2/19/22	0/1/1/1
3	NAG	B	1005	5	-	0/6/23/26	0/1/1/1
5	MAN	B	1007	3,4	-	0/2/19/22	0/1/1/1
3	NAG	B	1008	5	-	0/6/23/26	0/1/1/1
7	FUC	B	1011	3	-	0/0/17/20	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	NAG	O5-C1	-2.04	1.40	1.43
3	A	1005	NAG	C3-C2	2.02	1.56	1.52
6	A	1009	GAL	O2-C2	2.04	1.47	1.43
6	A	1009	GAL	O5-C1	2.06	1.47	1.43
3	A	1001	NAG	O4-C4	2.18	1.48	1.43
6	A	1009	GAL	C2-C3	2.32	1.55	1.52
6	A	1009	GAL	C1-C2	2.70	1.58	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1004	MAN	O5-C1-C2	-6.92	99.95	110.79
7	A	1011	FUC	O4-C4-C3	-4.32	100.95	110.36
3	A	1008	NAG	O7-C7-N2	-4.16	113.91	121.92
5	B	1004	MAN	O4-C4-C3	-3.76	102.18	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1008	NAG	O4-C4-C3	-3.72	102.27	110.36
5	A	1004	MAN	O4-C4-C3	-3.29	103.20	110.36
5	A	1007	MAN	O2-C2-C3	-3.22	103.85	110.17
5	A	1007	MAN	C6-C5-C4	-3.12	105.71	113.00
3	B	1008	NAG	C3-C4-C5	-3.09	104.76	110.22
5	A	1004	MAN	O3-C3-C4	-3.02	103.79	110.36
5	B	1004	MAN	O2-C2-C3	-2.91	104.46	110.17
3	B	1008	NAG	O5-C1-C2	-2.80	107.57	111.47
5	B	1007	MAN	O2-C2-C3	-2.79	104.70	110.17
3	B	1002	NAG	O5-C1-C2	-2.69	107.73	111.47
3	A	1008	NAG	C4-C3-C2	-2.64	107.14	111.02
3	A	1008	NAG	C1-O5-C5	-2.56	108.64	112.17
3	A	1005	NAG	O7-C7-C8	-2.38	117.72	122.06
5	A	1007	MAN	O3-C3-C4	-2.17	105.63	110.36
3	B	1005	NAG	C4-C3-C2	-2.10	107.93	111.02
5	B	1007	MAN	O6-C6-C5	-2.08	104.33	111.34
3	B	1005	NAG	O3-C3-C2	-2.02	105.06	109.39
5	B	1007	MAN	O3-C3-C2	-2.02	106.36	110.02
3	A	1005	NAG	C6-C5-C4	2.10	117.92	113.00
3	A	1001	NAG	O4-C4-C5	2.20	114.82	109.28
3	B	1002	NAG	O7-C7-N2	2.25	126.26	121.92
3	A	1005	NAG	O3-C3-C2	2.30	114.31	109.39
7	B	1011	FUC	O5-C1-C2	2.30	114.39	110.79
7	A	1011	FUC	O5-C5-C4	2.43	113.63	109.62
3	B	1002	NAG	C2-N2-C7	2.51	126.61	122.94
3	A	1008	NAG	C3-C4-C5	2.55	114.72	110.22
3	B	1008	NAG	O4-C4-C3	2.59	115.99	110.36
3	A	1008	NAG	C1-C2-N2	2.64	115.00	110.49
3	B	1005	NAG	O3-C3-C4	2.70	116.23	110.36
3	A	1001	NAG	C1-O5-C5	2.76	115.97	112.17
3	B	1005	NAG	O5-C1-C2	2.77	115.33	111.47
6	A	1009	GAL	O2-C2-C1	2.92	115.12	109.18
6	A	1009	GAL	C1-O5-C5	2.92	116.20	112.17
5	B	1007	MAN	O2-C2-C1	3.00	115.27	109.18
3	A	1005	NAG	C2-N2-C7	3.06	127.41	122.94
7	A	1011	FUC	O2-C2-C1	3.22	115.73	109.18
7	B	1011	FUC	C3-C4-C5	3.34	114.93	109.68
7	A	1011	FUC	O5-C1-C2	3.40	116.12	110.79
6	A	1009	GAL	O5-C1-C2	3.62	116.46	110.79
5	A	1007	MAN	C1-C2-C3	4.56	115.44	109.65
5	B	1004	MAN	C1-C2-C3	5.02	116.02	109.65
3	A	1001	NAG	C1-C2-N2	5.07	119.15	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1008	NAG	C8-C7-N2	5.89	126.75	116.11
7	A	1011	FUC	C3-C4-C5	6.51	119.91	109.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1005	NAG	1	0
6	A	1009	GAL	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 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	$\# Z  > 2$
3	NAG	A	1001	1,3,7	14,14,15	0.82	1 (7%)	15,19,21	1.89	3 (20%)
3	NAG	A	1002	3,4	14,14,15	0.62	0	15,19,21	0.82	0
4	BMA	A	1003	3,5	11,11,12	0.84	0	13,15,17	1.78	3 (23%)
5	MAN	A	1004	3,4	11,11,12	0.61	0	13,15,17	2.43	3 (23%)
3	NAG	A	1005	5	14,14,15	1.29	1 (7%)	15,19,21	1.59	4 (26%)
5	MAN	A	1007	3,4	11,11,12	0.58	0	13,15,17	2.10	4 (30%)
3	NAG	A	1008	5,6	14,14,15	0.93	0	15,19,21	2.69	7 (46%)
6	GAL	A	1009	3	11,11,12	1.53	4 (36%)	13,15,17	1.67	3 (23%)
7	FUC	A	1011	3	9,10,11	1.19	0	13,14,16	2.72	5 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	B	1001	1,3,7	14,14,15	0.68	0	15,19,21	1.13	0
3	NAG	B	1002	3,4	14,14,15	0.98	1 (7%)	15,19,21	1.45	3 (20%)
4	BMA	B	1003	3,5	11,11,12	0.89	1 (9%)	13,15,17	1.13	1 (7%)
5	MAN	B	1004	3,4	11,11,12	0.69	0	13,15,17	2.14	3 (23%)
3	NAG	B	1005	5	14,14,15	0.66	0	15,19,21	1.59	4 (26%)
5	MAN	B	1007	3,4	11,11,12	0.67	0	13,15,17	1.75	4 (30%)
3	NAG	B	1008	5	14,14,15	0.40	0	15,19,21	1.60	3 (20%)
7	FUC	B	1011	3	9,10,11	0.87	0	13,14,16	1.53	2 (15%)

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	NAG	A	1001	1,3,7	-	0/6/23/26	0/1/1/1
3	NAG	A	1002	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	1003	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	1004	3,4	-	0/2/19/22	0/1/1/1
3	NAG	A	1005	5	-	0/6/23/26	0/1/1/1
5	MAN	A	1007	3,4	-	0/2/19/22	0/1/1/1
3	NAG	A	1008	5,6	-	0/6/23/26	0/1/1/1
6	GAL	A	1009	3	-	0/2/19/22	0/1/1/1
7	FUC	A	1011	3	-	0/0/17/20	0/1/1/1
3	NAG	B	1001	1,3,7	-	0/6/23/26	0/1/1/1
3	NAG	B	1002	3,4	-	0/6/23/26	0/1/1/1
4	BMA	B	1003	3,5	-	0/2/19/22	0/1/1/1
5	MAN	B	1004	3,4	-	0/2/19/22	0/1/1/1
3	NAG	B	1005	5	-	0/6/23/26	0/1/1/1
5	MAN	B	1007	3,4	-	0/2/19/22	0/1/1/1
3	NAG	B	1008	5	-	0/6/23/26	0/1/1/1
7	FUC	B	1011	3	-	0/0/17/20	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1003	BMA	O5-C1	-2.17	1.40	1.43
3	B	1002	NAG	O5-C1	-2.04	1.40	1.43
3	A	1005	NAG	C3-C2	2.02	1.56	1.52
6	A	1009	GAL	O2-C2	2.04	1.47	1.43
6	A	1009	GAL	O5-C1	2.06	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	NAG	O4-C4	2.18	1.48	1.43
6	A	1009	GAL	C2-C3	2.32	1.55	1.52
6	A	1009	GAL	C1-C2	2.70	1.58	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1004	MAN	O5-C1-C2	-6.92	99.95	110.79
7	A	1011	FUC	O4-C4-C3	-4.32	100.95	110.36
3	A	1008	NAG	O7-C7-N2	-4.16	113.91	121.92
5	B	1004	MAN	O4-C4-C3	-3.76	102.18	110.36
3	A	1008	NAG	O4-C4-C3	-3.72	102.27	110.36
5	A	1004	MAN	O4-C4-C3	-3.29	103.20	110.36
5	A	1007	MAN	O2-C2-C3	-3.22	103.85	110.17
5	A	1007	MAN	C6-C5-C4	-3.12	105.71	113.00
3	B	1008	NAG	C3-C4-C5	-3.09	104.76	110.22
5	A	1004	MAN	O3-C3-C4	-3.02	103.79	110.36
5	B	1004	MAN	O2-C2-C3	-2.91	104.46	110.17
3	B	1008	NAG	O5-C1-C2	-2.80	107.57	111.47
5	B	1007	MAN	O2-C2-C3	-2.79	104.70	110.17
4	B	1003	BMA	O3-C3-C2	-2.71	105.09	110.02
3	B	1002	NAG	O5-C1-C2	-2.69	107.73	111.47
3	A	1008	NAG	C4-C3-C2	-2.64	107.14	111.02
3	A	1008	NAG	C1-O5-C5	-2.56	108.64	112.17
3	A	1005	NAG	O7-C7-C8	-2.38	117.72	122.06
5	A	1007	MAN	O3-C3-C4	-2.17	105.63	110.36
4	A	1003	BMA	O6-C6-C5	-2.15	104.09	111.34
3	B	1005	NAG	C4-C3-C2	-2.10	107.93	111.02
5	B	1007	MAN	O6-C6-C5	-2.08	104.33	111.34
3	B	1005	NAG	O3-C3-C2	-2.02	105.06	109.39
5	B	1007	MAN	O3-C3-C2	-2.02	106.36	110.02
4	A	1003	BMA	C3-C4-C5	2.04	113.81	110.22
3	A	1005	NAG	C6-C5-C4	2.10	117.92	113.00
3	A	1001	NAG	O4-C4-C5	2.20	114.82	109.28
3	B	1002	NAG	O7-C7-N2	2.25	126.26	121.92
3	A	1005	NAG	O3-C3-C2	2.30	114.31	109.39
7	B	1011	FUC	O5-C1-C2	2.30	114.39	110.79
7	A	1011	FUC	O5-C5-C4	2.43	113.63	109.62
3	B	1002	NAG	C2-N2-C7	2.51	126.61	122.94
3	A	1008	NAG	C3-C4-C5	2.55	114.72	110.22
3	B	1008	NAG	O4-C4-C3	2.59	115.99	110.36
3	A	1008	NAG	C1-C2-N2	2.64	115.00	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1005	NAG	O3-C3-C4	2.70	116.23	110.36
3	A	1001	NAG	C1-O5-C5	2.76	115.97	112.17
3	B	1005	NAG	O5-C1-C2	2.77	115.33	111.47
6	A	1009	GAL	O2-C2-C1	2.92	115.12	109.18
6	A	1009	GAL	C1-O5-C5	2.92	116.20	112.17
5	B	1007	MAN	O2-C2-C1	3.00	115.27	109.18
3	A	1005	NAG	C2-N2-C7	3.06	127.41	122.94
7	A	1011	FUC	O2-C2-C1	3.22	115.73	109.18
7	B	1011	FUC	C3-C4-C5	3.34	114.93	109.68
7	A	1011	FUC	O5-C1-C2	3.40	116.12	110.79
6	A	1009	GAL	O5-C1-C2	3.62	116.46	110.79
4	A	1003	BMA	C1-C2-C3	3.81	114.47	109.65
5	A	1007	MAN	C1-C2-C3	4.56	115.44	109.65
5	B	1004	MAN	C1-C2-C3	5.02	116.02	109.65
3	A	1001	NAG	C1-C2-N2	5.07	119.15	110.49
3	A	1008	NAG	C8-C7-N2	5.89	126.75	116.11
7	A	1011	FUC	C3-C4-C5	6.51	119.91	109.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1005	NAG	1	0
6	A	1009	GAL	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	211/223 (94%)	-0.06	1 (0%) 90 92	36, 53, 76, 90	0
1	B	213/223 (95%)	-0.10	2 (0%) 84 85	38, 51, 78, 92	0
2	C	171/182 (93%)	-0.05	1 (0%) 89 90	38, 54, 78, 107	0
All	All	595/628 (94%)	-0.07	4 (0%) 87 88	36, 53, 78, 107	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	296	TYR	3.1
1	B	389	ASN	2.5
1	A	234	LEU	2.1
2	C	174	GLN	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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	GAL	A	1009	11/12	0.91	0.21	1.06	68,71,72,72	0
3	NAG	B	1008	14/15	0.95	0.14	-0.60	48,52,54,55	0
3	NAG	A	1008	14/15	0.95	0.15	-0.76	51,53,54,58	0
3	NAG	A	1001	14/15	0.97	0.14	-0.83	46,54,63,66	0
3	NAG	B	1001	14/15	0.96	0.13	-1.44	55,65,68,69	0
5	MAN	A	1004	11/12	0.94	0.12	-	65,70,73,74	0
5	MAN	B	1004	11/12	0.94	0.14	-	65,69,70,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	1005	14/15	0.78	0.27	-	79,86,88,88	0
5	MAN	A	1007	11/12	0.97	0.17	-	45,47,52,57	0
3	NAG	A	1002	14/15	0.97	0.16	-	40,42,44,44	0
3	NAG	B	1002	14/15	0.95	0.15	-	47,50,58,59	0
7	FUC	A	1011	10/11	0.95	0.11	-	55,59,62,65	0
5	MAN	B	1007	11/12	0.95	0.12	-	50,53,55,59	0
3	NAG	B	1005	14/15	0.91	0.14	-	79,82,88,89	0
7	FUC	B	1011	10/11	0.95	0.16	-	59,67,72,72	0

### 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( $\text{\AA}^2$ )	Q<0.9
6	GAL	A	1009	11/12	0.91	0.21	1.06	68,71,72,72	0
3	NAG	B	1008	14/15	0.95	0.14	-0.60	48,52,54,55	0
3	NAG	A	1008	14/15	0.95	0.15	-0.76	51,53,54,58	0
3	NAG	A	1001	14/15	0.97	0.14	-0.83	46,54,63,66	0
3	NAG	B	1001	14/15	0.96	0.13	-1.44	55,65,68,69	0
3	NAG	B	1005	14/15	0.91	0.14	-	79,82,88,89	0
4	BMA	B	1003	11/12	0.98	0.14	-	47,49,52,58	0
5	MAN	A	1007	11/12	0.97	0.17	-	45,47,52,57	0
7	FUC	A	1011	10/11	0.95	0.11	-	55,59,62,65	0
3	NAG	A	1005	14/15	0.78	0.27	-	79,86,88,88	0
5	MAN	A	1004	11/12	0.94	0.12	-	65,70,73,74	0
4	BMA	A	1003	11/12	0.97	0.14	-	46,47,51,57	0
3	NAG	A	1002	14/15	0.97	0.16	-	40,42,44,44	0
3	NAG	B	1002	14/15	0.95	0.15	-	47,50,58,59	0
5	MAN	B	1004	11/12	0.94	0.14	-	65,69,70,74	0
5	MAN	B	1007	11/12	0.95	0.12	-	50,53,55,59	0
7	FUC	B	1011	10/11	0.95	0.16	-	59,67,72,72	0
8	CL	A	1012	1/1	0.94	0.09	-	78,78,78,78	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.