



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 08:19 am GMT

PDB ID : 2DTS
Title : Crystal Structure of the Defucosylated Fc Fragment from Human Immunoglobulin G1
Authors : Matsumiya, S.; Yamaguchi, Y.; Saito, J.; Nagano, M.; Sasakawa, H.; Otaki, S.; Satoh, M.; Shitara, K.; Kato, K.
Deposited on : 2006-07-14
Resolution : 2.20 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

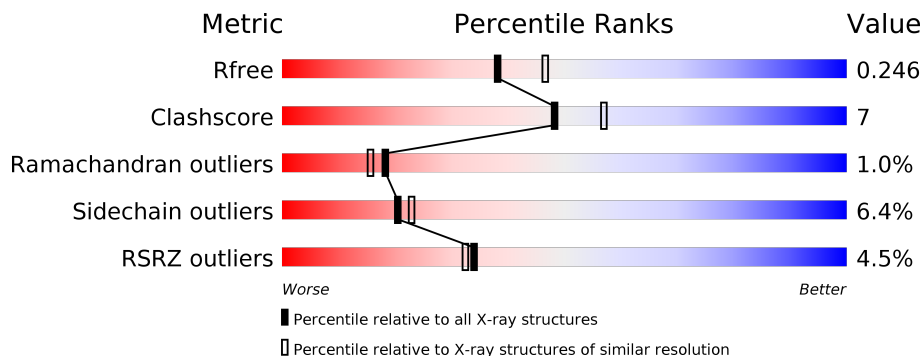
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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 ≥ 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	 8% 71% 20% • 5%
1	B	223	 8% 68% 23% • 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3620 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 Ig gamma-1 chain C region.

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	208	Total	C	N	O	S	0	0	0
			1664	1059	280	319	6			

- Molecule 2 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	6	Total	C	N	O	0	0
			75	42	3	30		

- Molecule 3 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	6	Total	C	N	O	0	0
			75	42	3	30		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is water.

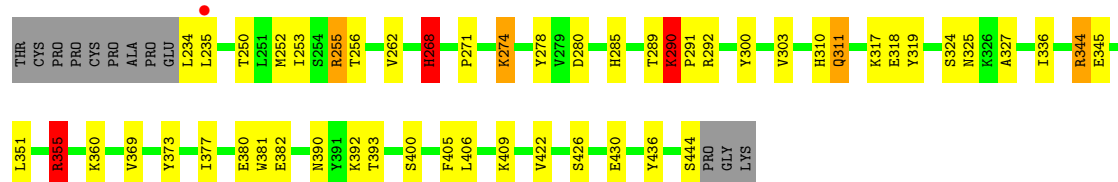
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	57	Total	O	0	0
			57	57		
5	B	51	Total	O	0	0
			51	51		

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.

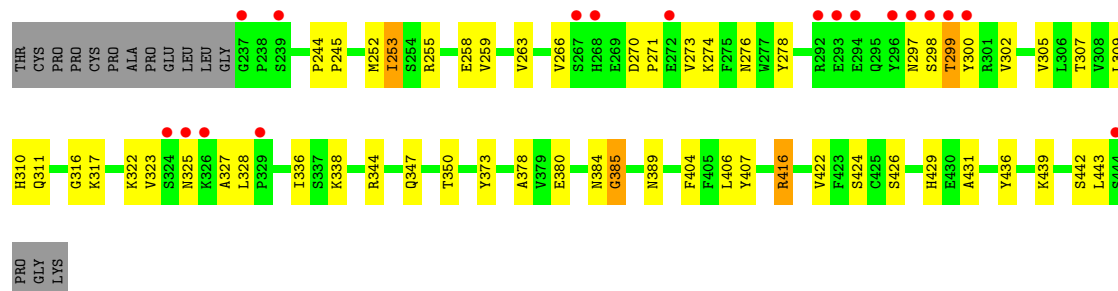
- Molecule 1: Ig gamma-1 chain C region

Chain A: 



- Molecule 1: Ig gamma-1 chain C region

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.47Å 77.69Å 143.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 40.72 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-2.20) 98.3 (40.72-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.192 , 0.251 0.198 , 0.246	Depositor DCC
R_{free} test set	1434 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3620	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, 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	1.75	22/1730 (1.3%)	1.31	13/2357 (0.6%)
1	B	1.39	12/1710 (0.7%)	1.20	5/2330 (0.2%)
All	All	1.58	34/3440 (1.0%)	1.26	18/4687 (0.4%)

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

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	430	GLU	CD-OE1	15.91	1.43	1.25
1	A	290	LYS	CB-CG	9.78	1.78	1.52
1	A	278	TYR	CD1-CE1	-8.40	1.26	1.39
1	B	426	SER	CB-OG	-8.29	1.31	1.42
1	A	380	GLU	CD-OE2	8.21	1.34	1.25

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	ARG	NE-CZ-NH1	11.79	126.20	120.30
1	B	416	ARG	NE-CZ-NH1	11.17	125.88	120.30
1	A	430	GLU	OE1-CD-OE2	8.31	133.28	123.30
1	A	280	ASP	CB-CG-OD2	-8.23	110.89	118.30
1	A	280	ASP	CB-CG-OD1	7.84	125.35	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	268	HIS	Sidechain

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	24	1
1	B	1664	0	1630	22	0
2	A	75	0	64	0	0
3	B	75	0	63	1	0
4	B	14	0	13	1	0
5	A	57	0	0	4	0
5	B	51	0	0	0	0
All	All	3620	0	3425	48	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 48 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:LYS:CG	1:A:290:LYS:CB	1.78	1.55
1:A:290:LYS:HE2	1:A:291:PRO:O	1.70	0.90
1:A:268:HIS:ND1	5:A:456:HOH:O	2.13	0.81
1:A:290:LYS:CE	1:A:291:PRO:O	2.32	0.77
1:B:429:HIS:CD2	1:B:431:ALA:H	2.06	0.73

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:HIS:NE2	1:A:285:HIS:ND1[4_456]	1.67	0.53

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	A	209/223 (94%)	205 (98%)	4 (2%)	0	100	100
1	B	206/223 (92%)	193 (94%)	9 (4%)	4 (2%)	9	6
All	All	415/446 (93%)	398 (96%)	13 (3%)	4 (1%)	18	16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	298	SER
1	B	327	ALA
1	B	385	GLY
1	B	443	LEU

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%)	181 (92%)	15 (8%)	15	15
1	B	194/206 (94%)	184 (95%)	10 (5%)	27	32
All	All	390/412 (95%)	365 (94%)	25 (6%)	20	23

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	360	LYS
1	A	400	SER

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Mol	Chain	Res	Type
1	B	416	ARG
1	A	390	ASN
1	A	422	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	390	ASN
1	A	418	GLN
1	B	421	ASN
1	A	361	ASN
1	B	347	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 ⓘ

12 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	1	1,2	14,14,15	1.09	1 (7%)	15,19,21	1.82	4 (26%)
2	NAG	A	2	2	14,14,15	1.25	2 (14%)	15,19,21	2.31	6 (40%)
2	BMA	A	3	2	11,11,12	1.30	2 (18%)	13,15,17	2.42	9 (69%)
2	MAN	A	4	2	11,11,12	1.08	1 (9%)	13,15,17	1.76	3 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	A	7	2	11,11,12	0.79	0	13,15,17	2.33	4 (30%)
2	NAG	A	8	2	14,14,15	1.28	1 (7%)	15,19,21	2.89	8 (53%)
3	NAG	B	1	1,3	14,14,15	0.64	0	15,19,21	1.06	0
3	NAG	B	2	3	14,14,15	0.60	0	15,19,21	1.64	4 (26%)
3	BMA	B	3	3	11,11,12	0.66	0	13,15,17	2.02	4 (30%)
3	MAN	B	4	3	11,11,12	0.84	0	13,15,17	1.62	3 (23%)
3	NAG	B	5	3	14,14,15	0.95	0	15,19,21	1.85	5 (33%)
3	MAN	B	7	3,4	11,11,12	0.62	0	13,15,17	2.43	4 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	0/6/23/26	0/1/1/1
2	BMA	A	3	2	-	0/2/19/22	0/1/1/1
2	MAN	A	4	2	-	0/2/19/22	0/1/1/1
2	MAN	A	7	2	-	0/2/19/22	0/1/1/1
2	NAG	A	8	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
3	BMA	B	3	3	-	0/2/19/22	0/1/1/1
3	MAN	B	4	3	-	0/2/19/22	0/1/1/1
3	NAG	B	5	3	-	0/6/23/26	0/1/1/1
3	MAN	B	7	3,4	-	0/2/19/22	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3	BMA	C4-C5	-2.94	1.46	1.53
2	A	1	NAG	O5-C1	-2.69	1.39	1.43
2	A	2	NAG	O5-C1	-2.17	1.40	1.43
2	A	3	BMA	C2-C3	2.08	1.55	1.52
2	A	4	MAN	C1-C2	2.65	1.58	1.52

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	8	NAG	O3-C3-C2	-5.97	96.59	109.39
2	A	3	BMA	O3-C3-C4	-5.36	98.69	110.36
3	B	5	NAG	O5-C1-C2	-3.38	106.77	111.47
2	A	1	NAG	O7-C7-C8	-3.28	116.08	122.06
3	B	5	NAG	O3-C3-C2	-3.22	102.49	109.39

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1	NAG	C8-C7-N2-C2
3	B	1	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	NAG	1	0
3	B	2	NAG	1	0

5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z > 2$
4	NAG	B	8	3	14,14,15	0.85	0	15,19,21	1.54	3 (20%)

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	NAG	B	8	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	8	NAG	C2-N2-C7	-2.75	118.93	122.94
4	B	8	NAG	C1-C2-N2	-2.69	105.89	110.49
4	B	8	NAG	O4-C4-C3	3.00	116.89	110.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	8	NAG	C8-C7-N2-C2
4	B	8	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	8	NAG	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, 95th 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 ²)	Q<0.9
1	A	211/223 (94%)	-0.25	1 (0%) 90 90	25, 40, 50, 63	0
1	B	208/223 (93%)	0.31	18 (8%) 11 10	29, 39, 48, 56	0
All	All	419/446 (93%)	0.03	19 (4%) 34 32	25, 40, 49, 63	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	TYR	4.4
1	B	298	SER	4.0
1	B	296	TYR	3.9
1	B	268	HIS	3.7
1	B	267	SER	3.3

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](#)

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, 95th 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 ²)	Q<0.9
2	NAG	A	8	14/15	0.89	0.15	1.71	34,43,50,51	0
3	NAG	B	2	14/15	0.90	0.12	-1.03	29,33,36,37	0
2	MAN	A	4	11/12	0.91	0.13	-	30,33,35,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MAN	B	7	11/12	0.89	0.12	-	26,30,35,37	0
2	MAN	A	7	11/12	0.93	0.09	-	36,40,43,45	0
2	NAG	A	1	14/15	0.94	0.09	-	28,34,43,44	0
3	NAG	B	5	14/15	0.90	0.16	-	37,38,40,40	0
2	BMA	A	3	11/12	0.95	0.11	-	30,32,36,41	0
2	NAG	A	2	14/15	0.96	0.09	-	33,40,44,49	0
3	BMA	B	3	11/12	0.86	0.11	-	27,30,33,35	0
3	MAN	B	4	11/12	0.87	0.12	-	28,30,31,35	0
3	NAG	B	1	14/15	0.93	0.21	-	26,32,35,35	0

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, 95th 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(\AA^2)	Q<0.9
4	NAG	B	8	14/15	0.94	0.16	1.12	15,24,31,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.