Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2017 – 12:48 PM EST

PDB ID	:	5HY9
Title	:	Glycosylated, disulfide-linked Knob-into-Hole Fc fragment
Authors	:	Kuglstatter, A.; Stihle, M.; Benz, J.
Deposited on	:	2016-02-01
Resolution	:	2.70 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*
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:

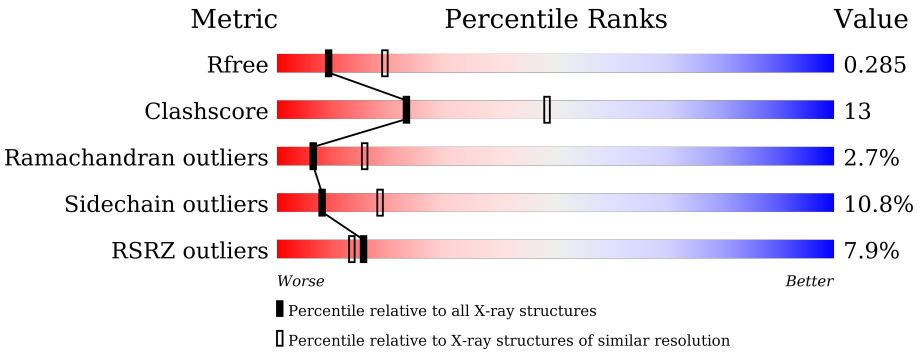
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 >=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 <=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	227	% 69% 17% 5% 9%
2	B	227	13% 52% 28% 7% • 12%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3470 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	207	Total	C	N	O	S	0	0	0
			1665	1063	280	315	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	354	CYS	SER	engineered mutation	UNP P01857
A	366	TRP	THR	engineered mutation	UNP P01857

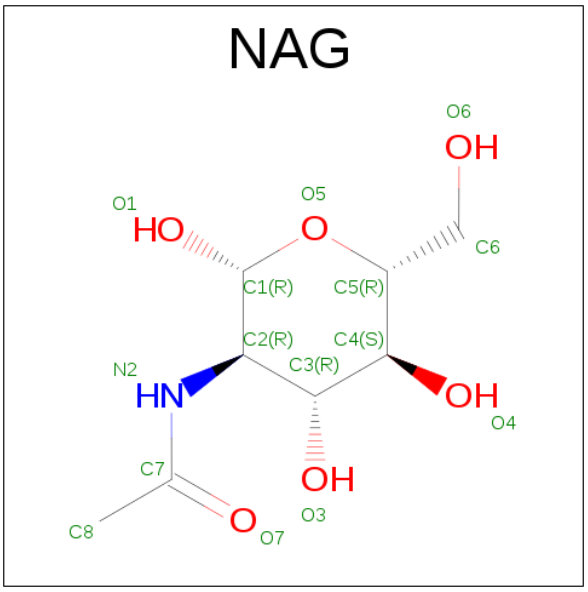
- Molecule 2 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	200	Total	C	N	O	S	0	0	0
			1582	1005	268	302	7			

There are 4 discrepancies between the modelled and reference sequences:

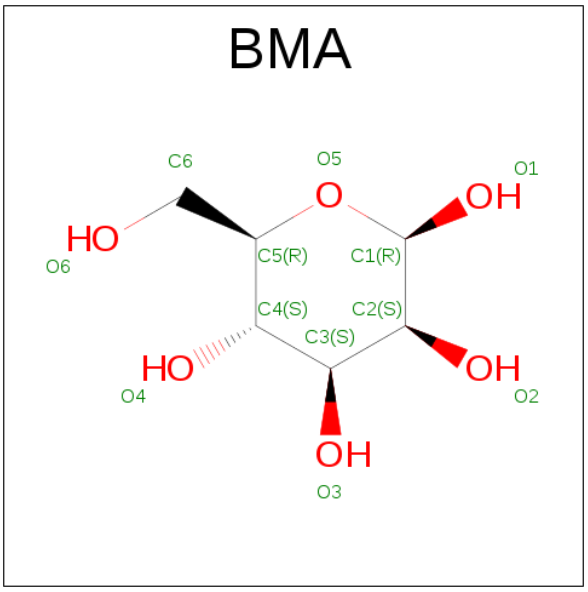
Chain	Residue	Modelled	Actual	Comment	Reference
B	349	CYS	TYR	engineered mutation	UNP P01857
B	366	SER	THR	engineered mutation	UNP P01857
B	368	ALA	LEU	engineered mutation	UNP P01857
B	407	VAL	TYR	engineered mutation	UNP P01857

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



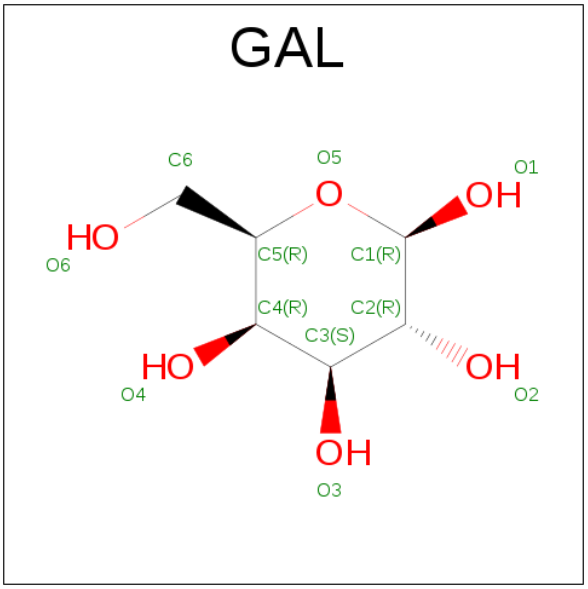
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

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



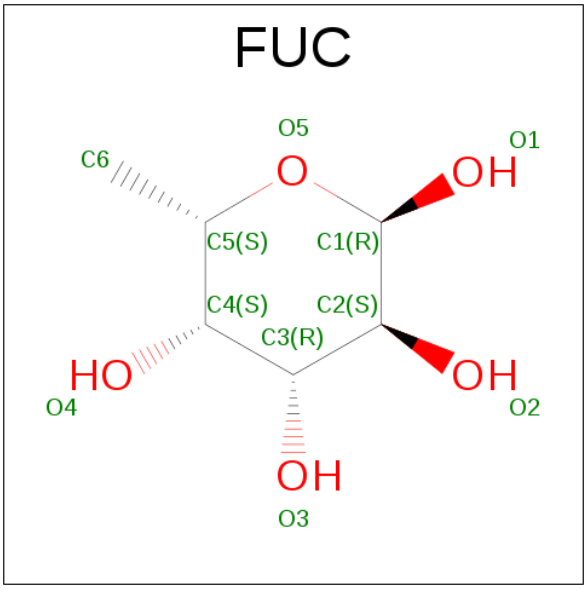
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	B	1	Total C O 11 6 5	0	0
4	B	1	Total C O 11 6 5	0	0

- Molecule 5 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



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

- 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 10 6 4	0	0
6	B	1	Total C O 10 6 4	0	0

- Molecule 7 is water.

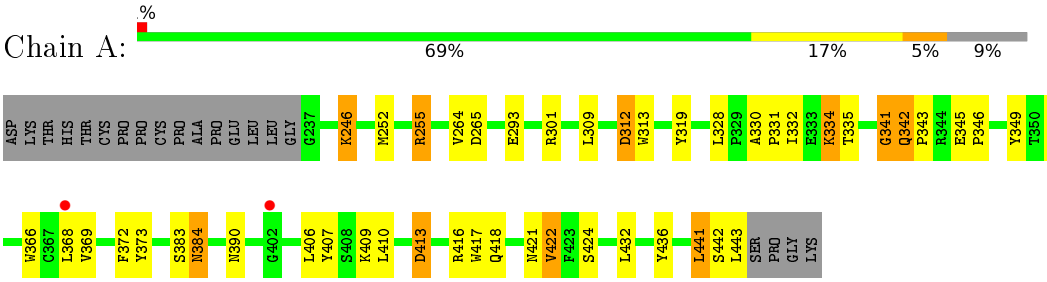
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	34	Total O 34 34	0	0
7	B	5	Total O 5 5	0	0

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 errors 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.

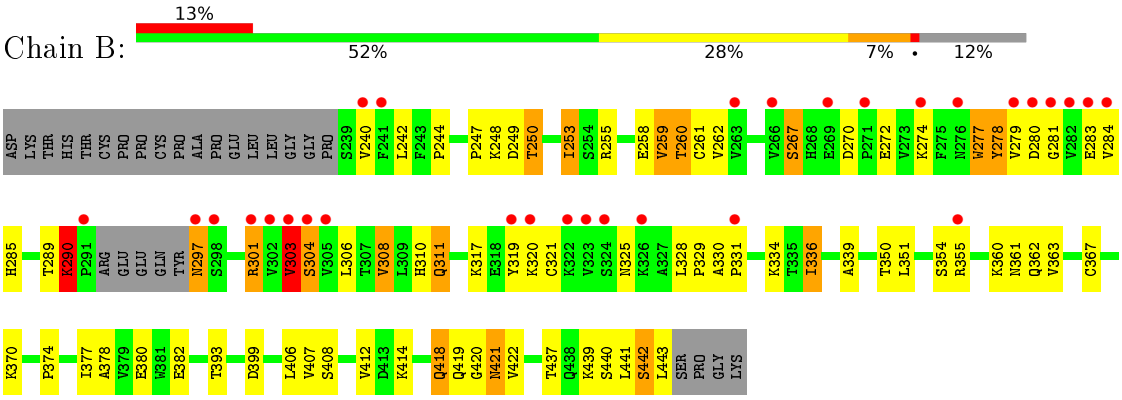
- Molecule 1: Ig gamma-1 chain C region

Chain A:



- Molecule 2: Ig gamma-1 chain C region

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	151.81Å 151.81Å 113.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.59 – 2.70 45.55 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.59-2.70) 99.8 (45.55-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.212 , 0.272 0.225 , 0.285	Depositor DCC
R_{free} test set	1109 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	85.5	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3470	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FUC, GAL, BMA, NAG

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	0.86	0/1713	0.98	4/2335 (0.2%)
2	B	0.66	0/1623	0.81	0/2210
All	All	0.77	0/3336	0.90	4/4545 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	301	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	A	312	ASP	CB-CG-OD2	7.23	124.81	118.30
1	A	312	ASP	CB-CG-OD1	-5.74	113.13	118.30
1	A	334	LYS	CD-CE-NZ	-5.50	99.06	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1665	0	1627	33	0
2	B	1582	0	1559	59	0
3	A	56	0	48	1	0
3	B	42	0	36	2	0
4	A	33	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	22	0	18	2	0
5	A	11	0	10	3	0
6	A	10	0	10	0	0
6	B	10	0	10	0	0
7	A	34	0	0	1	0
7	B	5	0	0	0	0
All	All	3470	0	3344	91	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 13.

All (91) 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:B:290:LYS:HE3	2:B:303:VAL:HG11	1.33	1.10
2:B:240:VAL:HG12	2:B:334:LYS:HG2	1.38	1.03
2:B:253:ILE:H	2:B:253:ILE:HD12	1.31	0.95
2:B:277:TRP:HZ2	2:B:304:SER:HG	1.18	0.87
2:B:267:SER:HB2	2:B:270:ASP:H	1.43	0.81
2:B:361:ASN:O	2:B:414:LYS:HB2	1.83	0.79
2:B:277:TRP:HZ2	2:B:304:SER:OG	1.67	0.78
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.66	0.76
2:B:290:LYS:CE	2:B:303:VAL:HG11	2.17	0.72
2:B:301:ARG:HH21	2:B:303:VAL:HG22	1.55	0.71
2:B:406:LEU:HD12	2:B:406:LEU:C	2.13	0.69
2:B:260:THR:HG22	2:B:262:VAL:HG23	1.76	0.68
2:B:308:VAL:HB	2:B:319:TYR:OH	1.96	0.66
2:B:319:TYR:HB2	2:B:336:ILE:HG22	1.86	0.58
1:A:407:TYR:CZ	2:B:407:VAL:HG11	2.39	0.57
2:B:289:THR:HG22	2:B:289:THR:O	2.05	0.57
1:A:383:SER:O	1:A:384:ASN:C	2.43	0.56
2:B:377:ILE:CG1	2:B:378:ALA:H	2.18	0.56
2:B:244:PRO:HD3	2:B:336:ILE:HD11	1.87	0.56
4:B:504:BMA:H4	3:B:506:NAG:C1	2.36	0.55
2:B:308:VAL:HB	2:B:319:TYR:CZ	2.41	0.55
2:B:260:THR:CG2	2:B:262:VAL:HG23	2.36	0.55
1:A:368:LEU:HD23	1:A:369:VAL:N	2.21	0.55
2:B:278:TYR:CD1	2:B:278:TYR:N	2.76	0.54
1:A:341:GLY:HA3	1:A:373:TYR:CE2	2.44	0.53
1:A:409:LYS:NZ	2:B:399:ASP:OD2	2.40	0.53
2:B:290:LYS:HB2	2:B:303:VAL:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:GLY:HA2	2:B:320:LYS:HE3	1.91	0.52
2:B:297:ASN:N	2:B:297:ASN:OD1	2.41	0.52
2:B:253:ILE:CD1	2:B:253:ILE:H	2.02	0.52
2:B:367:CYS:O	2:B:407:VAL:HA	2.11	0.51
1:A:421:ASN:O	1:A:442:SER:HB3	2.11	0.51
2:B:419:GLN:O	2:B:421:ASN:N	2.45	0.50
2:B:301:ARG:NE	2:B:301:ARG:O	2.44	0.49
2:B:377:ILE:CG1	2:B:378:ALA:N	2.76	0.49
1:A:345:GLU:HG2	1:A:432:LEU:HD23	1.95	0.49
2:B:242:LEU:HD21	2:B:319:TYR:O	2.12	0.49
2:B:262:VAL:HG11	2:B:301:ARG:NH1	2.29	0.48
2:B:283:GLU:OE1	2:B:283:GLU:HA	2.13	0.48
2:B:350:THR:HB	2:B:441:LEU:HD22	1.95	0.48
2:B:249:ASP:HA	2:B:255:ARG:HD3	1.95	0.48
1:A:351:LEU:HB2	1:A:366:TRP:HB2	1.95	0.47
1:A:407:TYR:CE1	2:B:407:VAL:HG11	2.48	0.47
2:B:325:ASN:H	2:B:328:LEU:HD12	1.79	0.47
2:B:422:VAL:HA	2:B:442:SER:HB3	1.96	0.47
2:B:350:THR:O	2:B:351:LEU:HD23	2.15	0.47
2:B:377:ILE:HG12	2:B:378:ALA:H	1.79	0.47
1:A:246:LYS:CD	5:A:507:GAL:O4	2.63	0.47
2:B:259:VAL:O	2:B:260:THR:OG1	2.31	0.47
2:B:259:VAL:CG2	2:B:306:LEU:HB3	2.46	0.46
2:B:277:TRP:HA	2:B:320:LYS:O	2.16	0.46
1:A:417:TRP:CH2	1:A:442:SER:O	2.68	0.46
1:A:390:ASN:O	1:A:410:LEU:HD12	2.15	0.46
2:B:277:TRP:O	2:B:283:GLU:OE1	2.34	0.46
1:A:264:VAL:O	1:A:265:ASP:HB2	2.15	0.46
1:A:328:LEU:HD13	1:A:332:ILE:HG13	1.97	0.45
2:B:418:GLN:HA	2:B:443:LEU:HD13	1.96	0.45
1:A:422:VAL:HG12	1:A:422:VAL:O	2.16	0.45
1:A:436:TYR:C	1:A:436:TYR:CD1	2.89	0.45
1:A:362:GLN:HG3	1:A:413:ASP:HA	1.97	0.45
2:B:339:ALA:HB3	2:B:374:PRO:HB3	1.97	0.45
1:A:330:ALA:O	1:A:331:PRO:C	2.54	0.45
1:A:349:TYR:HB3	2:B:354:SER:CB	2.47	0.45
2:B:303:VAL:O	2:B:304:SER:CB	2.65	0.45
1:A:406:LEU:HD12	1:A:406:LEU:C	2.37	0.45
1:A:351:LEU:HA	1:A:352:PRO:HD3	1.79	0.44
1:A:312:ASP:O	1:A:313:TRP:C	2.54	0.44
2:B:334:LYS:HA	2:B:334:LYS:HD3	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:MET:HB2	1:A:255:ARG:HG3	1.99	0.44
1:A:416:ARG:O	1:A:421:ASN:ND2	2.41	0.43
1:A:246:LYS:HD2	5:A:507:GAL:O4	2.19	0.43
2:B:393:THR:OG1	2:B:408:SER:OG	2.36	0.43
4:B:504:BMA:C4	3:B:506:NAG:C1	2.97	0.42
1:A:309:LEU:HD23	1:A:309:LEU:N	2.35	0.42
1:A:441:LEU:HB2	7:A:630:HOH:O	2.19	0.42
2:B:311:GLN:HB3	2:B:311:GLN:HE21	1.59	0.42
2:B:301:ARG:NH2	2:B:303:VAL:HG22	2.27	0.42
2:B:279:VAL:O	2:B:280:ASP:HB2	2.19	0.42
2:B:303:VAL:O	2:B:304:SER:HB2	2.20	0.41
3:A:505:NAG:H61	5:A:507:GAL:C1	2.50	0.41
2:B:377:ILE:HG12	2:B:378:ALA:N	2.35	0.41
2:B:242:LEU:HD13	2:B:321:CYS:HB2	2.03	0.41
1:A:443:LEU:N	1:A:443:LEU:HD12	2.36	0.41
2:B:250:THR:O	2:B:310:HIS:HD2	2.04	0.41
2:B:360:LYS:HA	2:B:360:LYS:HD3	1.59	0.41
1:A:252:MET:CE	1:A:255:ARG:HD3	2.50	0.41
2:B:330:ALA:HB1	2:B:331:PRO:HD2	2.02	0.41
2:B:362:GLN:HB3	2:B:412:VAL:O	2.20	0.41
1:A:319:TYR:O	1:A:335:THR:HA	2.21	0.40
1:A:346:PRO:CB	1:A:372:PHE:HB3	2.46	0.40
1:A:342:GLN:HA	1:A:343:PRO:HD3	1.95	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	A	205/227 (90%)	191 (93%)	12 (6%)	2 (1%)	19 45
2	B	196/227 (86%)	178 (91%)	9 (5%)	9 (5%)	3 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	401/454 (88%)	369 (92%)	21 (5%)	11 (3%)	6 16

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	259	VAL
2	B	290	LYS
2	B	304	SER
2	B	420	GLY
1	A	341	GLY
1	A	384	ASN
2	B	247	PRO
2	B	329	PRO
2	B	303	VAL
2	B	260	THR
2	B	253	ILE

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	193/210 (92%)	182 (94%)	11 (6%)	25 53
2	B	186/209 (89%)	156 (84%)	30 (16%)	3 7
All	All	379/419 (90%)	338 (89%)	41 (11%)	8 18

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	LYS
1	A	255	ARG
1	A	293	GLU
1	A	334	LYS
1	A	342	GLN
1	A	362	GLN
1	A	413	ASP

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Mol	Chain	Res	Type
1	A	418	GLN
1	A	422	VAL
1	A	424	SER
1	A	441	LEU
2	B	248	LYS
2	B	250	THR
2	B	258	GLU
2	B	261	CYS
2	B	267	SER
2	B	272	GLU
2	B	274	LYS
2	B	277	TRP
2	B	278	TYR
2	B	284	VAL
2	B	285	HIS
2	B	290	LYS
2	B	297	ASN
2	B	301	ARG
2	B	303	VAL
2	B	308	VAL
2	B	311	GLN
2	B	317	LYS
2	B	336	ILE
2	B	355	ARG
2	B	363	VAL
2	B	370	LYS
2	B	380	GLU
2	B	382	GLU
2	B	418	GLN
2	B	421	ASN
2	B	437	THR
2	B	439	LYS
2	B	440	SER
2	B	442	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	362	GLN
2	B	285	HIS
2	B	310	HIS
2	B	311	GLN

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Mol	Chain	Res	Type
2	B	421	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 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	501	1,3,6	14,14,15	0.62	0	15,19,21	1.44	1 (6%)
3	NAG	A	502	3,4	14,14,15	0.68	0	15,19,21	1.94	5 (33%)
3	NAG	A	505	5,4	14,14,15	1.13	1 (7%)	15,19,21	2.10	4 (26%)
5	GAL	A	507	3	11,11,12	1.11	1 (9%)	15,15,17	1.81	5 (33%)
3	NAG	A	509	4	14,14,15	0.72	0	15,19,21	1.33	1 (6%)
3	NAG	B	501	3,2,6	14,14,15	0.62	0	15,19,21	1.87	4 (26%)
3	NAG	B	502	3,4	14,14,15	1.10	2 (14%)	15,19,21	2.66	3 (20%)
3	NAG	B	506	4	14,14,15	0.68	1 (7%)	15,19,21	1.79	4 (26%)

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	501	1,3,6	-	0/6/23/26	0/1/1/1
3	NAG	A	502	3,4	-	0/6/23/26	0/1/1/1
3	NAG	A	505	5,4	-	0/6/23/26	0/1/1/1
5	GAL	A	507	3	-	0/2/19/22	0/1/1/1
3	NAG	A	509	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	501	3,2,6	-	0/6/23/26	0/1/1/1
3	NAG	B	502	3,4	-	0/6/23/26	0/1/1/1
3	NAG	B	506	4	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	505	NAG	O5-C1	-3.13	1.38	1.43
5	A	507	GAL	O4-C4	-2.01	1.38	1.43
3	B	502	NAG	C3-C2	2.04	1.57	1.52
3	B	506	NAG	C1-C2	2.05	1.55	1.52
3	B	502	NAG	C1-C2	2.30	1.55	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	NAG	C1-O5-C5	-6.58	102.47	112.14
3	A	505	NAG	C3-C4-C5	-3.38	104.21	110.23
3	B	501	NAG	O4-C4-C3	-3.28	102.96	110.36
3	A	505	NAG	C6-C5-C4	-2.86	105.83	112.99
3	A	502	NAG	O7-C7-C8	-2.57	117.33	122.07
5	A	507	GAL	O5-C5-C4	-2.39	106.17	110.13
3	A	502	NAG	C3-C4-C5	-2.21	106.29	110.23
3	A	502	NAG	O4-C4-C5	-2.14	103.58	109.23
3	A	509	NAG	O3-C3-C2	2.09	113.85	109.37
3	B	506	NAG	C4-C3-C2	2.20	114.76	111.34
5	A	507	GAL	C1-O5-C5	2.56	115.90	112.14
5	A	507	GAL	C1-C2-C3	2.57	112.67	109.55
3	A	502	NAG	C2-N2-C7	2.58	126.46	123.11
5	A	507	GAL	C3-C4-C5	2.59	114.84	110.23
3	B	501	NAG	C2-N2-C7	2.92	126.90	123.11
3	B	506	NAG	C3-C4-C5	3.15	115.84	110.23
3	B	501	NAG	C3-C4-C5	3.18	115.90	110.23
3	B	501	NAG	C4-C3-C2	3.25	116.38	111.34
3	B	506	NAG	O5-C5-C4	3.26	115.53	110.13
5	A	507	GAL	O2-C2-C1	3.44	116.12	109.23
3	B	506	NAG	C1-O5-C5	3.54	117.34	112.14
3	A	501	NAG	C1-O5-C5	3.60	117.44	112.14
3	A	505	NAG	O5-C5-C6	3.71	115.29	107.34
3	B	502	NAG	C4-C3-C2	3.79	117.23	111.34
3	A	502	NAG	C1-O5-C5	4.75	119.13	112.14
3	A	505	NAG	C1-O5-C5	4.94	119.41	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	NAG	C2-N2-C7	5.44	130.18	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	505	NAG	1	0
5	A	507	GAL	3	0
3	B	506	NAG	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

15 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	NAG	A	501	1,3,6	14,14,15	0.62	0	15,19,21	1.44	1 (6%)
3	NAG	A	502	3,4	14,14,15	0.68	0	15,19,21	1.94	5 (33%)
4	BMA	A	503	3,4	11,11,12	0.46	0	15,15,17	2.84	7 (46%)
4	BMA	A	504	3,4	11,11,12	1.12	1 (9%)	15,15,17	4.51	5 (33%)
3	NAG	A	505	5,4	14,14,15	1.13	1 (7%)	15,19,21	2.10	4 (26%)
4	BMA	A	506	3,4	11,11,12	0.87	1 (9%)	15,15,17	2.05	3 (20%)
5	GAL	A	507	3	11,11,12	1.11	1 (9%)	15,15,17	1.81	5 (33%)
6	FUC	A	508	3	10,10,11	1.17	1 (10%)	13,14,16	2.20	3 (23%)
3	NAG	A	509	4	14,14,15	0.72	0	15,19,21	1.33	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	B	501	3,2,6	14,14,15	0.62	0	15,19,21	1.87	4 (26%)
3	NAG	B	502	3,4	14,14,15	1.10	2 (14%)	15,19,21	2.66	3 (20%)
4	BMA	B	503	3,4	11,11,12	1.63	2 (18%)	15,15,17	2.62	5 (33%)
4	BMA	B	504	3,4	11,11,12	1.18	1 (9%)	15,15,17	2.08	6 (40%)
6	FUC	B	505	3	10,10,11	0.88	0	13,14,16	1.87	4 (30%)
3	NAG	B	506	4	14,14,15	0.68	1 (7%)	15,19,21	1.79	4 (26%)

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	501	1,3,6	-	0/6/23/26	0/1/1/1
3	NAG	A	502	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	503	3,4	-	0/2/19/22	0/1/1/1
4	BMA	A	504	3,4	-	0/2/19/22	0/1/1/1
3	NAG	A	505	5,4	-	0/6/23/26	0/1/1/1
4	BMA	A	506	3,4	-	0/2/19/22	0/1/1/1
5	GAL	A	507	3	-	0/2/19/22	0/1/1/1
6	FUC	A	508	3	-	0/0/17/20	0/1/1/1
3	NAG	A	509	4	-	0/6/23/26	0/1/1/1
3	NAG	B	501	3,2,6	-	0/6/23/26	0/1/1/1
3	NAG	B	502	3,4	-	0/6/23/26	0/1/1/1
4	BMA	B	503	3,4	-	0/2/19/22	0/1/1/1
4	BMA	B	504	3,4	-	0/2/19/22	0/1/1/1
6	FUC	B	505	3	-	0/0/17/20	0/1/1/1
3	NAG	B	506	4	-	0/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	508	FUC	C2-C3	-3.38	1.48	1.52
3	A	505	NAG	O5-C1	-3.13	1.38	1.43
4	A	504	BMA	O5-C1	-2.57	1.39	1.43
5	A	507	GAL	O4-C4	-2.01	1.38	1.43
4	A	506	BMA	O5-C1	-2.01	1.40	1.43
3	B	502	NAG	C3-C2	2.04	1.57	1.52
3	B	506	NAG	C1-C2	2.05	1.55	1.52
3	B	502	NAG	C1-C2	2.30	1.55	1.52
4	B	504	BMA	C2-C3	3.03	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	BMA	O3-C3	3.12	1.50	1.43
4	B	503	BMA	C2-C3	3.48	1.57	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	504	BMA	C1-O5-C5	-12.88	93.19	112.14
4	A	504	BMA	C1-C2-C3	-10.38	96.97	109.55
3	B	502	NAG	C1-O5-C5	-6.58	102.47	112.14
4	A	506	BMA	C1-O5-C5	-5.36	104.25	112.14
6	A	508	FUC	O2-C2-C3	-5.34	99.43	110.19
6	A	508	FUC	O3-C3-C2	-4.45	101.86	110.01
4	B	504	BMA	C1-C2-C3	-3.90	104.83	109.55
4	A	503	BMA	O6-C6-C5	-3.70	98.94	111.30
3	A	505	NAG	C3-C4-C5	-3.38	104.21	110.23
4	A	506	BMA	O4-C4-C3	-3.32	102.86	110.36
3	B	501	NAG	O4-C4-C3	-3.28	102.96	110.36
3	A	505	NAG	C6-C5-C4	-2.86	105.83	112.99
4	A	504	BMA	O6-C6-C5	-2.82	101.89	111.30
4	A	504	BMA	O5-C5-C4	-2.74	105.59	110.13
4	B	504	BMA	O5-C1-C2	-2.70	106.58	110.89
4	A	503	BMA	C1-C2-C3	-2.68	106.31	109.55
4	A	503	BMA	O4-C4-C3	-2.65	104.39	110.36
3	A	502	NAG	O7-C7-C8	-2.57	117.33	122.07
4	A	503	BMA	O2-C2-C3	-2.46	105.22	110.19
6	A	508	FUC	O5-C1-C2	-2.46	106.96	110.89
5	A	507	GAL	O5-C5-C4	-2.39	106.17	110.13
3	A	502	NAG	C3-C4-C5	-2.21	106.29	110.23
4	B	503	BMA	C1-O5-C5	-2.14	108.99	112.14
3	A	502	NAG	O4-C4-C5	-2.14	103.58	109.23
4	B	504	BMA	O6-C6-C5	-2.12	104.21	111.30
4	B	503	BMA	O2-C2-C3	2.03	114.27	110.19
4	A	504	BMA	C6-C5-C4	2.06	118.15	112.99
3	A	509	NAG	O3-C3-C2	2.09	113.85	109.37
3	B	506	NAG	C4-C3-C2	2.20	114.76	111.34
4	B	504	BMA	O2-C2-C1	2.42	114.07	109.23
6	B	505	FUC	C1-C2-C3	2.54	112.63	109.55
5	A	507	GAL	C1-O5-C5	2.56	115.90	112.14
5	A	507	GAL	C1-C2-C3	2.57	112.67	109.55
3	A	502	NAG	C2-N2-C7	2.58	126.46	123.11
5	A	507	GAL	C3-C4-C5	2.59	114.84	110.23
3	B	501	NAG	C2-N2-C7	2.92	126.90	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	505	FUC	C3-C4-C5	2.94	114.05	109.66
4	B	504	BMA	O2-C2-C3	3.11	116.46	110.19
3	B	506	NAG	C3-C4-C5	3.15	115.84	110.23
3	B	501	NAG	C3-C4-C5	3.18	115.90	110.23
6	B	505	FUC	C2-C3-C4	3.23	116.69	111.05
3	B	501	NAG	C4-C3-C2	3.25	116.38	111.34
4	A	506	BMA	O2-C2-C3	3.25	116.73	110.19
3	B	506	NAG	O5-C5-C4	3.26	115.53	110.13
4	B	504	BMA	O3-C3-C2	3.29	116.04	110.01
5	A	507	GAL	O2-C2-C1	3.44	116.12	109.23
6	B	505	FUC	O5-C5-C6	3.52	112.60	106.28
3	B	506	NAG	C1-O5-C5	3.54	117.34	112.14
3	A	501	NAG	C1-O5-C5	3.60	117.44	112.14
3	A	505	NAG	O5-C5-C6	3.71	115.29	107.34
3	B	502	NAG	C4-C3-C2	3.79	117.23	111.34
4	A	503	BMA	O5-C5-C4	3.95	116.68	110.13
4	B	503	BMA	C3-C4-C5	4.06	117.46	110.23
3	A	502	NAG	C1-O5-C5	4.75	119.13	112.14
3	A	505	NAG	C1-O5-C5	4.94	119.41	112.14
4	B	503	BMA	C1-C2-C3	5.00	115.61	109.55
4	A	503	BMA	O3-C3-C2	5.10	119.35	110.01
3	B	502	NAG	C2-N2-C7	5.44	130.18	123.11
4	A	503	BMA	C1-O5-C5	5.93	120.86	112.14
4	B	503	BMA	O3-C3-C2	6.40	121.73	110.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	505	NAG	1	0
5	A	507	GAL	3	0
4	B	504	BMA	2	0
3	B	506	NAG	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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	207/227 (91%)	0.10	2 (0%) 84 85	41, 63, 132, 176	0
2	B	200/227 (88%)	0.71	30 (15%) 3 2	59, 111, 161, 190	0
All	All	407/454 (89%)	0.40	32 (7%) 15 13	41, 90, 154, 190	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	302	VAL	7.0
2	B	324	SER	6.1
2	B	301	ARG	5.9
2	B	263	VAL	4.6
2	B	279	VAL	4.6
2	B	297	ASN	4.2
2	B	291	PRO	4.2
2	B	241	PHE	4.0
2	B	266	VAL	3.6
2	B	319	TYR	3.6
2	B	269	GLU	3.5
2	B	322	LYS	3.4
2	B	331	PRO	3.2
2	B	271	PRO	3.1
2	B	276	ASN	3.1
2	B	326	LYS	2.9
2	B	298	SER	2.8
2	B	274	LYS	2.8
2	B	303	VAL	2.5
2	B	281	GLY	2.5
2	B	323	VAL	2.5
2	B	304	SER	2.5
2	B	283	GLU	2.5
1	A	402	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	368	LEU	2.2
2	B	282	VAL	2.2
2	B	240	VAL	2.2
2	B	320	LYS	2.1
2	B	280	ASP	2.1
2	B	355	ARG	2.0
2	B	284	VAL	2.0
2	B	305	VAL	2.0

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^{th} 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
3	NAG	A	505	14/15	0.96	0.14	-1.95	38,44,50,52	0
5	GAL	A	507	11/12	0.94	0.14	-2.73	45,56,64,65	0
3	NAG	A	501	14/15	0.96	0.12	-3.66	28,31,36,43	0
3	NAG	A	509	14/15	0.85	0.16	-	62,73,90,91	0
3	NAG	A	502	14/15	0.96	0.11	-	30,33,39,40	0
3	NAG	B	501	14/15	0.76	0.37	-	73,79,83,84	0
3	NAG	B	506	14/15	0.63	0.30	-	77,92,107,112	0
3	NAG	B	502	14/15	0.78	0.38	-	87,102,107,107	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^{th} 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
6	FUC	B	505	10/11	0.85	0.33	-0.11	73,78,79,82	0
3	NAG	A	505	14/15	0.96	0.14	-1.95	38,44,50,52	0
5	GAL	A	507	11/12	0.94	0.14	-2.73	45,56,64,65	0
3	NAG	A	501	14/15	0.96	0.12	-3.66	28,31,36,43	0
3	NAG	B	501	14/15	0.76	0.37	-	73,79,83,84	0
3	NAG	B	506	14/15	0.63	0.30	-	77,92,107,112	0
4	BMA	A	504	11/12	0.96	0.10	-	36,39,47,49	0
3	NAG	A	509	14/15	0.85	0.16	-	62,73,90,91	0
4	BMA	A	503	11/12	0.97	0.07	-	35,39,44,47	0
3	NAG	A	502	14/15	0.96	0.11	-	30,33,39,40	0
4	BMA	A	506	11/12	0.93	0.10	-	62,70,78,80	0
4	BMA	B	503	11/12	0.57	0.31	-	73,93,105,115	0
4	BMA	B	504	11/12	0.54	0.41	-	88,101,115,115	0
6	FUC	A	508	10/11	0.97	0.11	-	31,35,40,46	0
3	NAG	B	502	14/15	0.78	0.38	-	87,102,107,107	0

6.5 Other polymers (i)

There are no such residues in this entry.