Full wwPDB X-ray Structure Validation Report (i)

Jan 24, 2017 – 11:33 AM EST

PDB ID	:	5HYE
Title	:	Glycosylated Knob-Knob Fc fragment (P212121)
Authors	:	Kuglstatter, A.; Stihle, M.; Benz, J.
Deposited on	:	2016-02-01
Resolution	:	1.89 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

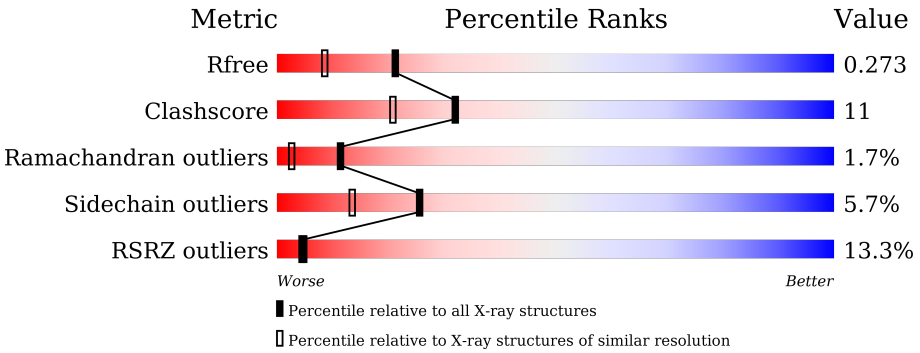
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.89 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	4% 74% 16% · 8%
1	C	227	20% 68% 18% 5% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BMA	A	504	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3705 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.

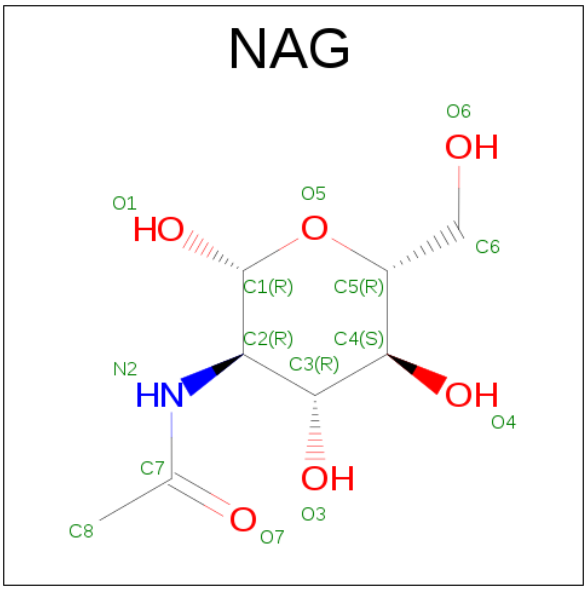
- Molecule 1 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	1	0
			1673	1068	281	317	7			
1	C	207	Total	C	N	O	S	0	0	0
			1665	1063	280	315	7			

There are 4 discrepancies between the modelled and reference sequences:

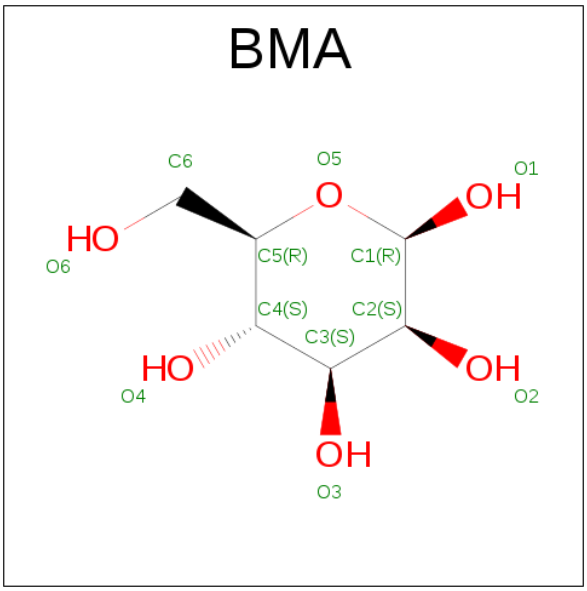
Chain	Residue	Modelled	Actual	Comment	Reference
A	354	CYS	SER	engineered mutation	UNP P01857
A	366	TRP	THR	engineered mutation	UNP P01857
C	354	CYS	SER	engineered mutation	UNP P01857
C	366	TRP	THR	engineered mutation	UNP P01857

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



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

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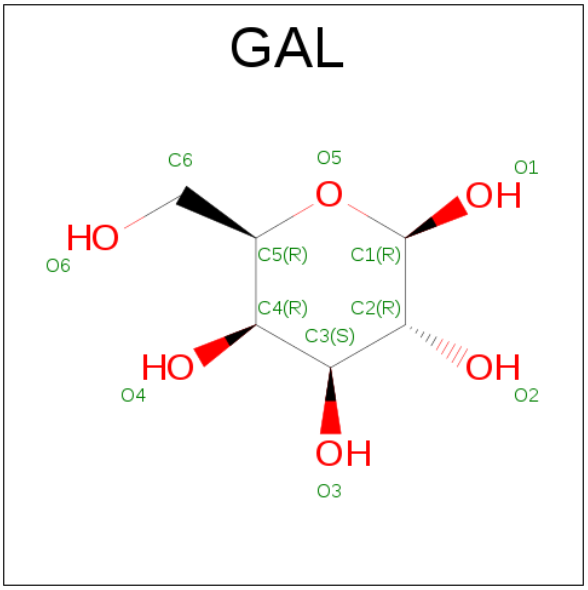
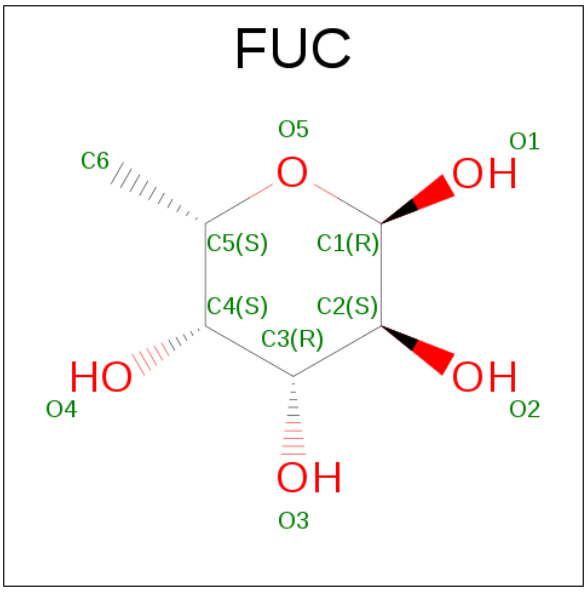
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 11 6 5	0	0
3	C	1	Total C O 11 6 5	0	0

- 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 11 6 5	0	0
4	C	1	Total C O 11 6 5	0	0

- Molecule 5 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



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

- Molecule 6 is water.

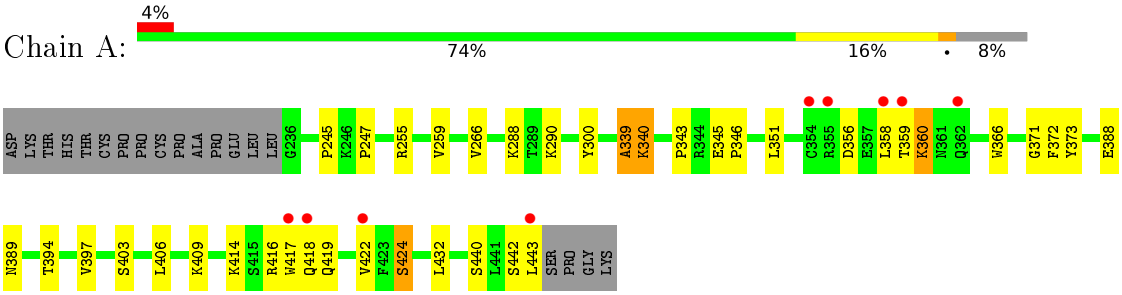
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	109	Total O 109 109	0	0
6	C	38	Total O 38 38	0	0

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.

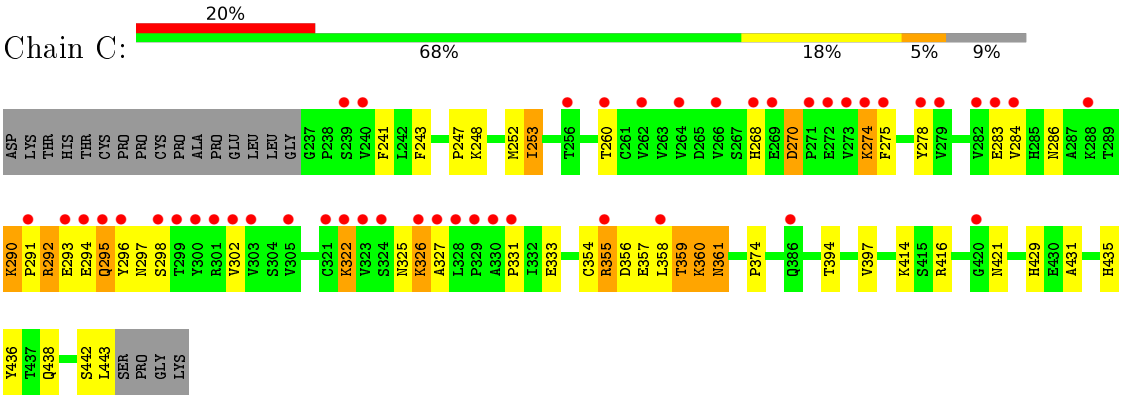
- Molecule 1: Ig gamma-1 chain C region

Chain A:



- Molecule 1: Ig gamma-1 chain C region

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	49.03Å 81.62Å 136.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.17 – 1.89 46.13 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.17-1.89) 99.6 (46.13-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.224 , 0.275 0.220 , 0.273	Depositor DCC
R_{free} test set	2236 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	43.3	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3705	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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	0.95	0/1724	0.96	0/2350
1	C	0.82	1/1713 (0.1%)	0.86	0/2335
All	All	0.89	1/3437 (0.0%)	0.91	0/4685

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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	274	LYS	CE-NZ	8.53	1.70	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	354	CYS	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	1673	0	1638	26	0
1	C	1665	0	1628	47	0
2	A	56	0	48	1	0
2	C	56	0	48	4	0
3	A	33	0	26	1	0
3	C	33	0	26	2	0
4	A	11	0	10	0	0
4	C	11	0	10	0	0
5	A	10	0	10	0	0
5	C	10	0	10	1	0
6	A	109	0	0	3	0
6	C	38	0	0	3	0
All	All	3705	0	3454	74	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 11.

All (74) 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:C:274:LYS:CE	1:C:274:LYS:NZ	1.70	1.51
1:C:248:LYS:HG3	1:C:252:MET:HE1	1.38	0.99
1:A:255:ARG:HD2	6:A:601:HOH:O	1.81	0.79
1:C:292:ARG:HG2	1:C:292:ARG:HH11	1.47	0.78
1:C:248:LYS:HG3	1:C:252:MET:CE	2.14	0.74
1:C:243:PHE:CD2	2:C:505:NAG:H61	2.25	0.70
1:C:436:TYR:OH	1:C:438:GLN:NE2	2.21	0.70
1:C:435:HIS:HE1	6:C:629:HOH:O	1.77	0.68
3:A:506:BMA:O3	2:A:509:NAG:C1	2.43	0.67
2:C:502:NAG:H82	5:C:508:FUC:C1	2.31	0.60
1:C:325:ASN:OD1	1:C:327:ALA:HB3	2.01	0.60
1:C:359:THR:OG1	1:C:360:LYS:HE3	2.01	0.60
1:C:290:LYS:HE3	1:C:291:PRO:HD2	1.84	0.59
1:A:417:TRP:O	1:A:443:LEU:HB2	2.02	0.58
1:A:424:SER:OG	1:A:440:SER:OG	2.19	0.58
1:A:422:VAL:HA	1:A:442:SER:HB3	1.87	0.57
1:C:248:LYS:CG	1:C:252:MET:HE1	2.24	0.56
1:A:416:ARG:HA	1:A:419:GLN:HB2	1.86	0.55
1:A:366:TRP:CH2	1:A:409:LYS:HD2	2.40	0.55
1:C:429:HIS:CD2	1:C:431:ALA:H	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ASP:OD2	1:C:327:ALA:HB2	2.07	0.55
1:C:248:LYS:CG	1:C:252:MET:CE	2.83	0.54
1:A:351:LEU:HB2	1:A:366:TRP:HB2	1.88	0.54
1:C:322:LYS:HE3	1:C:333:GLU:HG3	1.90	0.54
1:C:292:ARG:HG2	1:C:292:ARG:NH1	2.16	0.54
1:C:360:LYS:HA	1:C:360:LYS:HE2	1.90	0.54
1:A:406:LEU:HD12	1:A:406:LEU:C	2.29	0.53
1:C:274:LYS:CD	1:C:274:LYS:NZ	2.62	0.53
1:A:339:ALA:N	6:A:602:HOH:O	2.26	0.53
1:A:371:GLY:HA2	1:A:403:SER:OG	2.09	0.52
1:C:243:PHE:HD2	2:C:505:NAG:H61	1.74	0.52
1:A:290:LYS:HE3	6:A:675:HOH:O	2.09	0.51
1:C:361:ASN:H	1:C:361:ASN:ND2	2.09	0.51
1:C:360:LYS:CA	1:C:360:LYS:HE2	2.40	0.51
1:C:442:SER:O	1:C:443:LEU:C	2.49	0.50
1:A:417:TRP:CZ3	1:A:442:SER:HA	2.46	0.50
1:A:394:THR:HG22	1:C:397:VAL:HG21	1.93	0.49
1:A:359:THR:HA	1:A:414:LYS:HZ3	1.76	0.49
1:A:359:THR:HA	1:A:414:LYS:NZ	2.28	0.48
1:C:286:ASN:N	6:C:602:HOH:O	2.38	0.48
1:C:290:LYS:HE3	1:C:290:LYS:HB3	1.52	0.48
1:C:292:ARG:C	1:C:293:GLU:HG3	2.33	0.48
1:C:374:PRO:O	1:C:429:HIS:HE1	1.95	0.48
1:C:292:ARG:CB	1:C:302:VAL:HG22	2.44	0.47
1:A:360:LYS:NZ	1:A:360:LYS:HB2	2.29	0.47
1:C:357:GLU:O	1:C:360:LYS:HB2	2.15	0.47
1:C:241:PHE:CE1	3:C:503:BMA:H2	2.50	0.47
1:C:322:LYS:HE2	1:C:331:PRO:HB2	1.96	0.47
1:A:343:PRO:HA	1:A:373:TYR:O	2.15	0.46
1:A:418:GLN:HA	1:A:443:LEU:HD13	1.98	0.46
1:C:295:GLN:HB2	1:C:297:ASN:OD1	2.15	0.46
1:C:435:HIS:CE1	6:C:629:HOH:O	2.61	0.46
1:A:360:LYS:O	1:A:414:LYS:HD2	2.16	0.45
1:C:325:ASN:C	1:C:327:ALA:H	2.18	0.45
1:C:248:LYS:O	1:C:252:MET:HE2	2.16	0.45
1:C:360:LYS:O	1:C:414:LYS:HD3	2.17	0.45
1:A:442:SER:O	1:A:443:LEU:C	2.56	0.45
1:C:292:ARG:HB3	1:C:302:VAL:HG22	1.99	0.44
1:C:283:GLU:HG3	1:C:284:VAL:N	2.32	0.44
1:C:274:LYS:HG2	1:C:275:PHE:N	2.31	0.44
3:C:503:BMA:O2	3:C:506:BMA:C1	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:THR:HG21	2:C:505:NAG:O6	2.18	0.43
1:A:346:PRO:HB3	1:A:372:PHE:HB3	2.00	0.43
1:C:253:ILE:H	1:C:253:ILE:HG12	1.59	0.42
1:A:397:VAL:HG21	1:C:394:THR:HA	2.00	0.42
1:C:295:GLN:H	1:C:295:GLN:HG2	1.69	0.42
1:C:416:ARG:O	1:C:421:ASN:ND2	2.53	0.42
1:C:290:LYS:CE	1:C:291:PRO:HD2	2.49	0.41
1:C:356:ASP:OD2	1:C:356:ASP:N	2.49	0.41
1:A:358:LEU:O	1:A:359:THR:CG2	2.68	0.41
1:A:266:VAL:HB	1:A:300:TYR:HB2	2.03	0.41
1:C:268:HIS:N	1:C:268:HIS:CD2	2.87	0.41
1:A:245:PRO:HD3	1:A:259:VAL:HG22	2.03	0.40
1:A:345:GLU:HG3	1:A:432:LEU:HD23	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	207/227 (91%)	196 (95%)	7 (3%)	4 (2%)	10 2
1	C	205/227 (90%)	193 (94%)	9 (4%)	3 (2%)	13 3
All	All	412/454 (91%)	389 (94%)	16 (4%)	7 (2%)	11 2

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	298	SER
1	C	355	ARG
1	A	388	GLU
1	A	389	ASN
1	A	339	ALA

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Mol	Chain	Res	Type
1	C	326	LYS
1	A	340	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	194/210 (92%)	188 (97%)	6 (3%)	47 37
1	C	193/210 (92%)	177 (92%)	16 (8%)	14 5
All	All	387/420 (92%)	365 (94%)	22 (6%)	25 13

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	247	PRO
1	A	288	LYS
1	A	340	LYS
1	A	356	ASP
1	A	360	LYS
1	A	424	SER
1	C	247	PRO
1	C	253	ILE
1	C	270	ASP
1	C	278	TYR
1	C	290	LYS
1	C	292	ARG
1	C	294	GLU
1	C	295	GLN
1	C	296	TYR
1	C	322	LYS
1	C	326	LYS
1	C	355	ARG
1	C	358	LEU
1	C	359	THR
1	C	360	LYS

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Mol	Chain	Res	Type
1	C	361	ASN

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

Mol	Chain	Res	Type
1	C	268	HIS
1	C	361	ASN
1	C	429	HIS
1	C	438	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

10 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	$\#\|Z\| > 2$
2	NAG	A	501	1,2,5	14,14,15	0.84	0	15,19,21	1.36	3 (20%)
2	NAG	A	502	3,2	14,14,15	1.31	3 (21%)	15,19,21	1.29	1 (6%)
2	NAG	A	505	3,4	14,14,15	1.06	1 (7%)	15,19,21	1.35	3 (20%)
4	GAL	A	507	2	11,11,12	1.36	3 (27%)	15,15,17	1.84	4 (26%)
2	NAG	A	509	3	14,14,15	0.67	0	15,19,21	1.51	2 (13%)
2	NAG	C	501	1,2,5	14,14,15	0.80	0	15,19,21	1.79	5 (33%)
2	NAG	C	502	3,2	14,14,15	0.69	0	15,19,21	1.40	2 (13%)
2	NAG	C	505	3,4	14,14,15	0.97	1 (7%)	15,19,21	1.49	3 (20%)
4	GAL	C	507	2	11,11,12	0.88	1 (9%)	15,15,17	1.67	6 (40%)
2	NAG	C	509	3	14,14,15	0.60	0	15,19,21	1.72	2 (13%)

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	NAG	O5-C1	-2.73	1.39	1.43
4	A	507	GAL	O3-C3	-2.41	1.37	1.43
4	C	507	GAL	O5-C1	-2.30	1.40	1.43
2	A	505	NAG	O5-C5	-2.26	1.38	1.43
4	A	507	GAL	C4-C5	2.06	1.57	1.53
2	A	502	NAG	C8-C7	2.17	1.55	1.50
4	A	507	GAL	C2-C3	2.17	1.55	1.52
2	C	505	NAG	C1-C2	2.27	1.55	1.52
2	A	502	NAG	C1-C2	2.59	1.56	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	507	GAL	C3-C4-C5	-3.46	104.06	110.23
2	C	502	NAG	C3-C4-C5	-2.96	104.96	110.23
2	A	501	NAG	C3-C4-C5	-2.42	105.91	110.23
2	A	509	NAG	O5-C5-C4	-2.41	106.14	110.13
2	A	505	NAG	O5-C5-C6	-2.34	102.32	107.34
2	C	501	NAG	O7-C7-C8	-2.30	117.83	122.07
2	C	501	NAG	C3-C4-C5	-2.25	106.21	110.23
4	C	507	GAL	C3-C4-C5	-2.11	106.46	110.23
4	C	507	GAL	O5-C5-C6	-2.11	102.83	107.34
4	C	507	GAL	O5-C1-C2	-2.10	107.53	110.89
2	A	505	NAG	O4-C4-C3	-2.08	105.66	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	505	NAG	O7-C7-C8	-2.07	118.25	122.07
2	A	505	NAG	C2-N2-C7	-2.04	120.45	123.11
2	A	501	NAG	O7-C7-C8	-2.03	118.33	122.07
2	C	505	NAG	O5-C5-C4	2.00	113.45	110.13
4	C	507	GAL	C1-C2-C3	2.02	112.00	109.55
4	C	507	GAL	O2-C2-C1	2.09	113.42	109.23
2	A	501	NAG	C8-C7-N2	2.12	120.16	116.10
2	C	501	NAG	C1-O5-C5	2.36	115.61	112.14
4	A	507	GAL	C2-C3-C4	2.61	115.60	111.05
2	C	501	NAG	C4-C3-C2	2.63	115.41	111.34
2	C	509	NAG	C2-N2-C7	2.74	126.66	123.11
2	C	502	NAG	C1-O5-C5	2.83	116.30	112.14
4	A	507	GAL	O3-C3-C2	2.93	115.38	110.01
2	C	505	NAG	C4-C3-C2	3.37	116.57	111.34
4	C	507	GAL	C1-O5-C5	3.49	117.27	112.14
2	A	502	NAG	C2-N2-C7	3.54	127.71	123.11
2	A	509	NAG	C1-O5-C5	3.57	117.39	112.14
2	C	501	NAG	C2-N2-C7	3.93	128.22	123.11
4	A	507	GAL	O2-C2-C1	4.22	117.69	109.23
2	C	509	NAG	C1-O5-C5	5.67	120.48	112.14

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
2	A	509	NAG	1	0
2	C	502	NAG	1	0
2	C	505	NAG	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

18 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	$\#\|Z\| > 2$
2	NAG	A	501	1,2,5	14,14,15	0.84	0	15,19,21	1.36	3 (20%)
2	NAG	A	502	3,2	14,14,15	1.31	3 (21%)	15,19,21	1.29	1 (6%)
3	BMA	A	503	3,2	11,11,12	1.12	1 (9%)	15,15,17	2.84	5 (33%)
3	BMA	A	504	3,2	11,11,12	1.00	0	15,15,17	1.92	5 (33%)
2	NAG	A	505	3,4	14,14,15	1.06	1 (7%)	15,19,21	1.35	3 (20%)
3	BMA	A	506	3,2	11,11,12	1.20	1 (9%)	15,15,17	3.57	5 (33%)
4	GAL	A	507	2	11,11,12	1.36	3 (27%)	15,15,17	1.84	4 (26%)
5	FUC	A	508	2	10,10,11	1.08	1 (10%)	13,14,16	1.35	1 (7%)
2	NAG	A	509	3	14,14,15	0.67	0	15,19,21	1.51	2 (13%)
2	NAG	C	501	1,2,5	14,14,15	0.80	0	15,19,21	1.79	5 (33%)
2	NAG	C	502	3,2	14,14,15	0.69	0	15,19,21	1.40	2 (13%)
3	BMA	C	503	3,2	11,11,12	0.69	0	15,15,17	2.22	5 (33%)
3	BMA	C	504	3,2	11,11,12	0.67	0	15,15,17	2.42	6 (40%)
2	NAG	C	505	3,4	14,14,15	0.97	1 (7%)	15,19,21	1.49	3 (20%)
3	BMA	C	506	3,2	11,11,12	0.82	0	15,15,17	1.43	2 (13%)
4	GAL	C	507	2	11,11,12	0.88	1 (9%)	15,15,17	1.67	6 (40%)
5	FUC	C	508	2	10,10,11	0.77	0	13,14,16	1.61	4 (30%)
2	NAG	C	509	3	14,14,15	0.60	0	15,19,21	1.72	2 (13%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FUC	A	508	2	-	0/0/17/20	0/1/1/1
2	NAG	A	509	3	-	0/6/23/26	0/1/1/1
2	NAG	C	501	1,2,5	-	0/6/23/26	0/1/1/1
2	NAG	C	502	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	503	3,2	-	0/2/19/22	0/1/1/1
3	BMA	C	504	3,2	-	0/2/19/22	0/1/1/1
2	NAG	C	505	3,4	-	0/6/23/26	0/1/1/1
3	BMA	C	506	3,2	-	0/2/19/22	0/1/1/1
4	GAL	C	507	2	-	0/2/19/22	0/1/1/1
5	FUC	C	508	2	-	0/0/17/20	0/1/1/1
2	NAG	C	509	3	-	0/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	506	BMA	O5-C1	-3.04	1.38	1.43
2	A	502	NAG	O5-C1	-2.73	1.39	1.43
4	A	507	GAL	O3-C3	-2.41	1.37	1.43
4	C	507	GAL	O5-C1	-2.30	1.40	1.43
2	A	505	NAG	O5-C5	-2.26	1.38	1.43
4	A	507	GAL	C4-C5	2.06	1.57	1.53
5	A	508	FUC	C6-C5	2.07	1.56	1.51
2	A	502	NAG	C8-C7	2.17	1.55	1.50
4	A	507	GAL	C2-C3	2.17	1.55	1.52
2	C	505	NAG	C1-C2	2.27	1.55	1.52
3	A	503	BMA	O5-C1	2.46	1.47	1.43
2	A	502	NAG	C1-C2	2.59	1.56	1.52

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	506	BMA	C1-O5-C5	-11.96	94.55	112.14
3	A	503	BMA	O3-C3-C4	-7.43	93.61	110.36
3	A	503	BMA	C1-C2-C3	-5.45	102.95	109.55
3	C	503	BMA	C3-C4-C5	-5.25	100.86	110.23
3	C	504	BMA	O2-C2-C3	-4.25	101.63	110.19
3	C	504	BMA	C1-C2-C3	-4.19	104.47	109.55
3	C	504	BMA	C1-O5-C5	-3.53	106.95	112.14
4	A	507	GAL	C3-C4-C5	-3.46	104.06	110.23
3	A	504	BMA	O2-C2-C3	-3.32	103.50	110.19
3	A	504	BMA	O6-C6-C5	-3.22	100.54	111.30
3	A	506	BMA	O4-C4-C3	-3.11	103.35	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	502	NAG	C3-C4-C5	-2.96	104.96	110.23
5	A	508	FUC	C1-C2-C3	-2.75	106.22	109.55
3	A	506	BMA	O6-C6-C5	-2.57	102.73	111.30
3	C	503	BMA	C2-C3-C4	-2.56	106.58	111.05
3	C	503	BMA	O5-C5-C4	-2.46	106.06	110.13
2	A	501	NAG	C3-C4-C5	-2.42	105.91	110.23
2	A	509	NAG	O5-C5-C4	-2.41	106.14	110.13
2	A	505	NAG	O5-C5-C6	-2.34	102.32	107.34
2	C	501	NAG	O7-C7-C8	-2.30	117.83	122.07
3	A	503	BMA	C6-C5-C4	-2.28	107.27	112.99
2	C	501	NAG	C3-C4-C5	-2.25	106.21	110.23
4	C	507	GAL	C3-C4-C5	-2.11	106.46	110.23
4	C	507	GAL	O5-C5-C6	-2.11	102.83	107.34
4	C	507	GAL	O5-C1-C2	-2.10	107.53	110.89
2	A	505	NAG	O4-C4-C3	-2.08	105.66	110.36
2	C	505	NAG	O7-C7-C8	-2.07	118.25	122.07
2	A	505	NAG	C2-N2-C7	-2.04	120.45	123.11
2	A	501	NAG	O7-C7-C8	-2.03	118.33	122.07
3	A	503	BMA	O2-C2-C1	-2.01	105.20	109.23
2	C	505	NAG	O5-C5-C4	2.00	113.45	110.13
4	C	507	GAL	C1-C2-C3	2.02	112.00	109.55
5	C	508	FUC	O5-C1-C2	2.04	114.16	110.89
4	C	507	GAL	O2-C2-C1	2.09	113.42	109.23
2	A	501	NAG	C8-C7-N2	2.12	120.16	116.10
5	C	508	FUC	C1-C2-C3	2.13	112.13	109.55
3	C	506	BMA	O2-C2-C1	2.29	113.82	109.23
3	C	504	BMA	O2-C2-C1	2.33	113.89	109.23
3	A	504	BMA	C3-C4-C5	2.36	114.44	110.23
2	C	501	NAG	C1-O5-C5	2.36	115.61	112.14
3	A	504	BMA	O5-C5-C6	2.42	112.52	107.34
3	C	504	BMA	C2-C3-C4	2.50	115.41	111.05
3	A	506	BMA	O2-C2-C3	2.57	115.37	110.19
3	C	503	BMA	O4-C4-C5	2.59	116.06	109.23
4	A	507	GAL	C2-C3-C4	2.61	115.60	111.05
2	C	501	NAG	C4-C3-C2	2.63	115.41	111.34
2	C	509	NAG	C2-N2-C7	2.74	126.66	123.11
2	C	502	NAG	C1-O5-C5	2.83	116.30	112.14
3	A	506	BMA	C3-C4-C5	2.84	115.28	110.23
5	C	508	FUC	O5-C5-C6	2.90	111.49	106.28
4	A	507	GAL	O3-C3-C2	2.93	115.38	110.01
5	C	508	FUC	C3-C4-C5	2.99	114.13	109.66
3	A	504	BMA	O5-C1-C2	3.20	116.02	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	505	NAG	C4-C3-C2	3.37	116.57	111.34
4	C	507	GAL	C1-O5-C5	3.49	117.27	112.14
2	A	502	NAG	C2-N2-C7	3.54	127.71	123.11
2	A	509	NAG	C1-O5-C5	3.57	117.39	112.14
2	C	501	NAG	C2-N2-C7	3.93	128.22	123.11
3	C	503	BMA	O3-C3-C2	4.15	117.61	110.01
3	C	504	BMA	C3-C4-C5	4.16	117.64	110.23
3	C	506	BMA	O2-C2-C3	4.17	118.58	110.19
4	A	507	GAL	O2-C2-C1	4.22	117.69	109.23
3	A	503	BMA	O3-C3-C2	4.23	117.76	110.01
2	C	509	NAG	C1-O5-C5	5.67	120.48	112.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	504	BMA	C1

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	506	BMA	1	0
2	A	509	NAG	1	0
2	C	502	NAG	1	0
3	C	503	BMA	2	0
2	C	505	NAG	3	0
3	C	506	BMA	1	0
5	C	508	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

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	208/227 (91%)	0.46	9 (4%) 39 42	29, 44, 94, 109	0
1	C	207/227 (91%)	1.19	46 (22%) 1 1	35, 67, 124, 152	0
All	All	415/454 (91%)	0.83	55 (13%) 4 5	29, 54, 109, 152	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	296	TYR	10.0
1	C	298	SER	7.3
1	C	330	ALA	6.2
1	C	323	VAL	5.6
1	C	273	VAL	5.5
1	C	358	LEU	5.3
1	C	326	LYS	5.2
1	C	328	LEU	5.1
1	A	355	ARG	5.0
1	C	278	TYR	5.0
1	C	302	VAL	4.8
1	C	324	SER	4.8
1	C	272	GLU	4.6
1	C	239	SER	4.5
1	A	358	LEU	4.4
1	C	268	HIS	4.3
1	C	331	PRO	4.1
1	C	300	TYR	4.1
1	C	299	THR	4.1
1	C	274	LYS	3.8
1	C	262	VAL	3.8
1	C	294	GLU	3.4
1	C	266	VAL	3.4
1	C	279	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	303	VAL	3.3
1	C	329	PRO	3.2
1	C	291	PRO	3.1
1	C	288	LYS	3.1
1	C	295	GLN	3.1
1	C	301	ARG	3.0
1	C	240	VAL	3.0
1	A	443	LEU	3.0
1	C	293	GLU	2.9
1	A	418	GLN	2.9
1	C	275	PHE	2.9
1	C	355	ARG	2.9
1	C	305	VAL	2.9
1	C	269	GLU	2.8
1	C	271	PRO	2.8
1	C	282	VAL	2.6
1	C	322	LYS	2.6
1	A	422	VAL	2.5
1	C	283	GLU	2.4
1	A	359	THR	2.3
1	C	420	GLY	2.3
1	C	284	VAL	2.3
1	A	362	GLN	2.2
1	C	264	VAL	2.2
1	C	260	THR	2.1
1	A	354	CYS	2.1
1	A	417	TRP	2.1
1	C	327	ALA	2.0
1	C	256	THR	2.0
1	C	386	GLN	2.0
1	C	321	CYS	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
4	GAL	C	507	11/12	0.91	0.15	-0.18	63,67,84,85	0
2	NAG	C	505	14/15	0.86	0.20	-0.21	76,87,91,99	0
2	NAG	A	501	14/15	0.95	0.10	-0.98	36,40,49,50	0
2	NAG	A	502	14/15	0.97	0.10	-1.46	31,36,45,47	0
2	NAG	A	505	14/15	0.97	0.11	-1.51	35,39,48,50	0
4	GAL	A	507	11/12	0.94	0.11	-1.98	33,38,43,53	0
2	NAG	C	502	14/15	0.83	0.13	-2.03	87,121,126,128	0
2	NAG	C	501	14/15	0.72	0.19	-	107,123,137,137	0
2	NAG	C	509	14/15	0.70	0.26	-	109,116,121,128	0
2	NAG	A	509	14/15	0.77	0.20	-	85,91,99,103	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
4	GAL	C	507	11/12	0.91	0.15	-0.18	63,67,84,85	0
2	NAG	C	505	14/15	0.86	0.20	-0.21	76,87,91,99	0
2	NAG	A	501	14/15	0.95	0.10	-0.98	36,40,49,50	0
2	NAG	A	502	14/15	0.97	0.10	-1.46	31,36,45,47	0
2	NAG	A	505	14/15	0.97	0.11	-1.51	35,39,48,50	0
4	GAL	A	507	11/12	0.94	0.11	-1.98	33,38,43,53	0
2	NAG	C	502	14/15	0.83	0.13	-2.03	87,121,126,128	0
2	NAG	A	509	14/15	0.77	0.20	-	85,91,99,103	0
2	NAG	C	509	14/15	0.70	0.26	-	109,116,121,128	0
3	BMA	C	506	11/12	0.72	0.24	-	95,113,119,129	0
3	BMA	A	506	11/12	0.90	0.12	-	59,66,83,85	0
5	FUC	C	508	10/11	0.72	0.40	-	121,132,138,141	0
3	BMA	A	504	11/12	0.95	0.09	-	38,40,47,53	0
3	BMA	C	504	11/12	0.84	0.14	-	85,96,101,108	0
2	NAG	C	501	14/15	0.72	0.19	-	107,123,137,137	0
3	BMA	A	503	11/12	0.94	0.11	-	36,42,53,55	0
3	BMA	C	503	11/12	0.78	0.16	-	88,106,112,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	FUC	A	508	10/11	0.93	0.07	-	37,46,49,51	0

6.5 Other polymers (i)

There are no such residues in this entry.