



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2016 – 06:14 PM EST

PDB ID : 5LFU
Title : Myelin-associated glycoprotein (MAG) glycosylated and lysine-methylated full extracellular domain
Authors : Pronker, M.F.; Janssen, B.J.C.
Deposited on : 2016-07-04
Resolution : 4.30 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

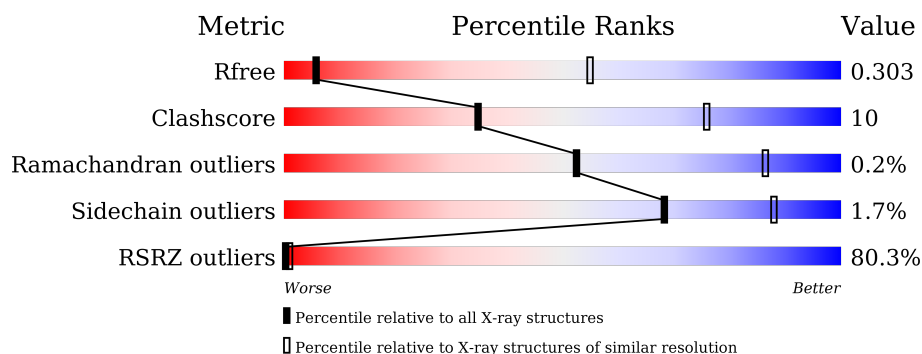
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 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	1059 (5.00-3.60)
Clashscore	102246	1166 (5.00-3.60)
Ramachandran outliers	100387	1106 (5.00-3.60)
Sidechain outliers	100360	1089 (5.00-3.60)
RSRZ outliers	91569	1062 (5.00-3.60)

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	500	

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	NAG	A	602	-	-	-	X
3	NAG	A	603	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	608	-	-	-	X
3	NAG	A	610	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3942 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.

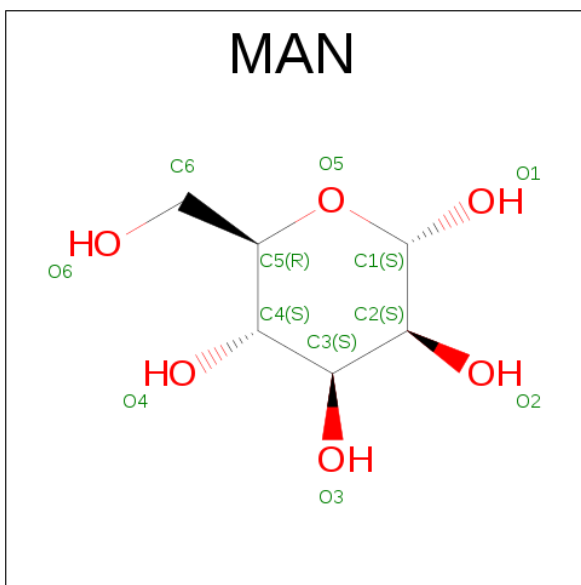
- Molecule 1 is a protein called Myelin-associated glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3776	2397	630	729	20			

There are 11 discrepancies between the modelled and reference sequences:

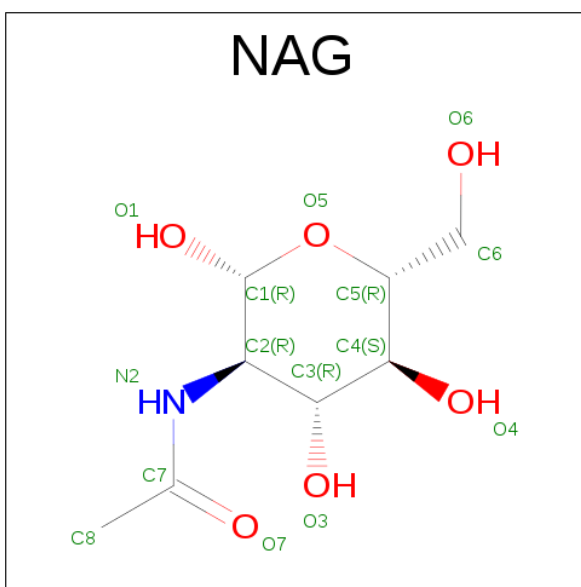
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	-	expression tag	UNP P20917
A	19	SER	-	expression tag	UNP P20917
A	509	ALA	-	expression tag	UNP P20917
A	510	ALA	-	expression tag	UNP P20917
A	511	ALA	-	expression tag	UNP P20917
A	512	HIS	-	expression tag	UNP P20917
A	513	HIS	-	expression tag	UNP P20917
A	514	HIS	-	expression tag	UNP P20917
A	515	HIS	-	expression tag	UNP P20917
A	516	HIS	-	expression tag	UNP P20917
A	517	HIS	-	expression tag	UNP P20917

- Molecule 2 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



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

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



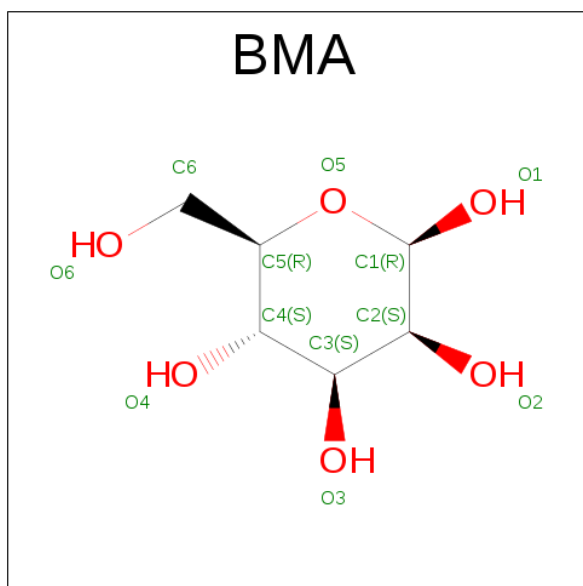
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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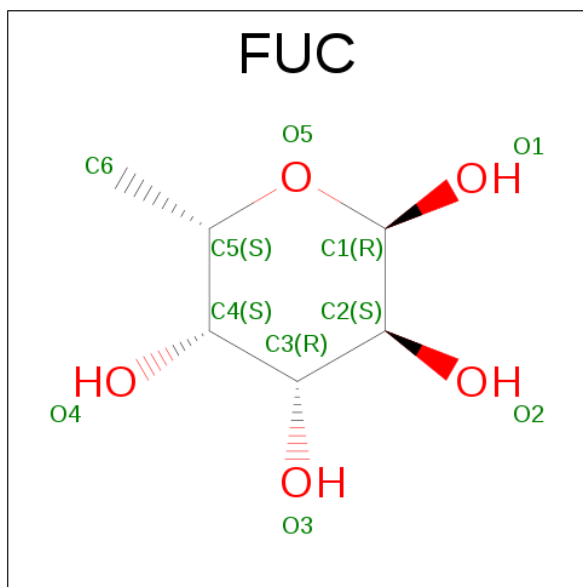
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- 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		

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

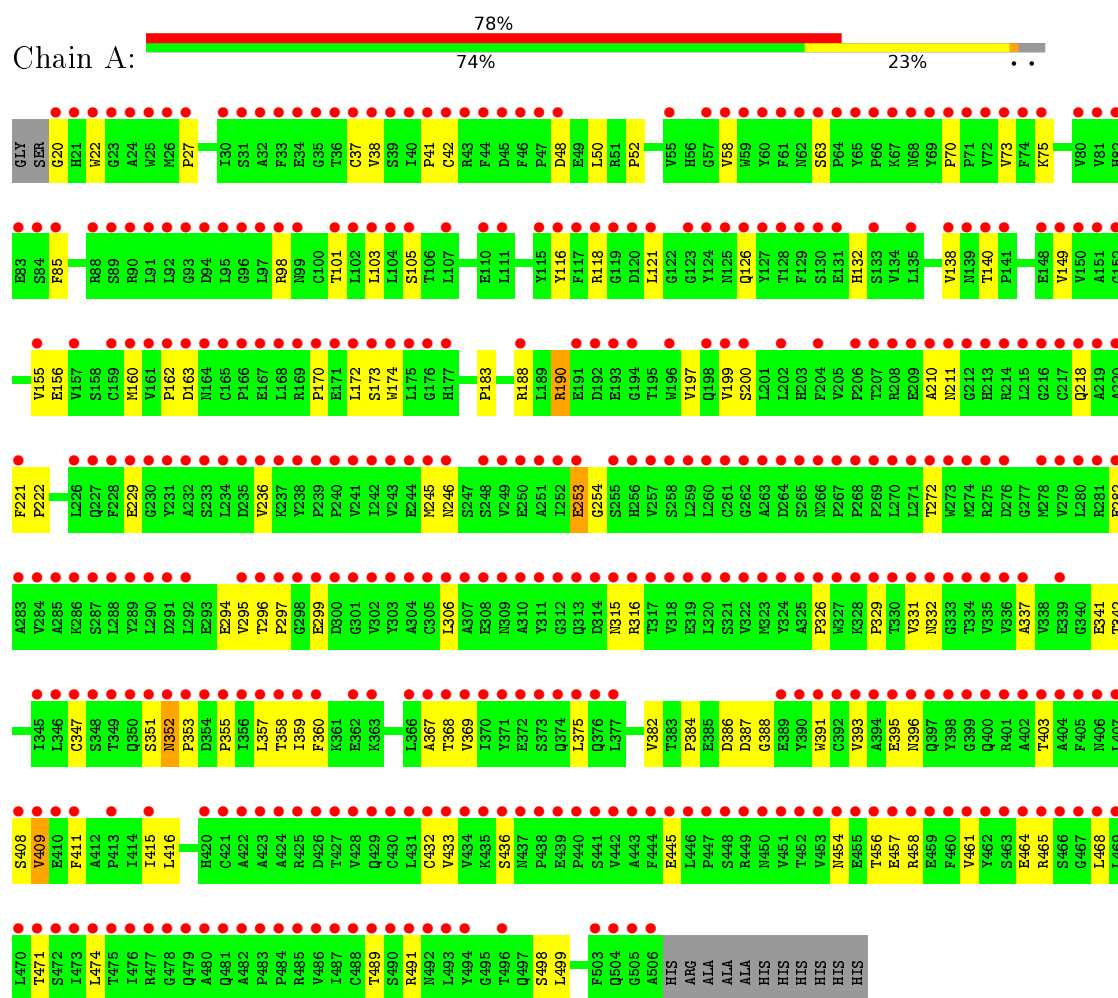


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		

3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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: Myelin-associated glycoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	101.24Å 101.24Å 687.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	114.58 – 4.30 114.58 – 4.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (114.58-4.30) 91.0 (114.58-4.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 4.30Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.285 , 0.295 0.291 , 0.303	Depositor DCC
R_{free} test set	682 reflections (4.86%)	DCC
Wilson B-factor (Å ²)	237.8	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 592.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3942	wwPDB-VP
Average B, all atoms (Å ²)	420.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: FUC, 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	0.37	0/3872	0.57	1/5297 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	468	LEU	CA-CB-CG	5.35	127.60	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3776	0	3655	76	1
2	A	33	0	30	2	0
3	A	112	0	100	3	0
4	A	11	0	8	1	0
5	A	10	0	10	0	0
All	All	3942	0	3803	77	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 10.

All (77) 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:63:SER:HB2	1:A:70:PRO:HB3	1.55	0.86
1:A:382:VAL:HG11	1:A:409:VAL:HG11	1.61	0.80
1:A:20:GLY:N	1:A:48:ASP:OD2	2.17	0.78
1:A:52:PRO:HG2	1:A:121:LEU:HB2	1.67	0.76
1:A:48:ASP:OD1	1:A:98:ARG:NH2	2.19	0.76
1:A:272:THR:HG22	1:A:282:GLU:HG3	1.71	0.73
1:A:436:SER:O	1:A:465:ARG:NH1	2.21	0.72
1:A:27:PRO:HG3	1:A:41:PRO:HG2	1.71	0.72
1:A:149:VAL:HG13	1:A:155:VAL:HG21	1.79	0.63
1:A:387:ASP:OD2	1:A:408:SER:HA	1.99	0.63
1:A:357:LEU:HD11	1:A:375:LEU:HB3	1.81	0.62
1:A:190:ARG:HD3	1:A:190:ARG:H	1.65	0.61
1:A:332:ASN:HB3	3:A:610:NAG:H82	1.83	0.59
1:A:352:ASN:N	1:A:352:ASN:OD1	2.35	0.59
1:A:163:ASP:OD2	1:A:188:ARG:NH2	2.33	0.59
1:A:162:PRO:HA	1:A:197:VAL:HG22	1.86	0.57
1:A:138:VAL:HG22	1:A:140:THR:H	1.70	0.56
1:A:329:PRO:HG2	1:A:403:THR:HB	1.88	0.56
1:A:461:VAL:HG12	1:A:474:LEU:HA	1.88	0.56
1:A:218:GLN:HG3	1:A:229:GLU:HG2	1.88	0.56
1:A:489:THR:HG22	1:A:498:SER:HB3	1.87	0.56
1:A:253:GLU:HA	1:A:295:VAL:HB	1.89	0.55
1:A:331:VAL:HG22	1:A:347:CYS:HA	1.89	0.55
1:A:306:LEU:HD13	1:A:315:ASN:HB3	1.90	0.52
1:A:210:ALA:HB3	1:A:236:VAL:HG11	1.91	0.52
1:A:351:SER:HB3	1:A:355:PRO:HG3	1.92	0.52
1:A:369:VAL:HB	1:A:375:LEU:HD13	1.92	0.52
1:A:415:ILE:HD13	1:A:499:LEU:HB3	1.90	0.51
1:A:41:PRO:HA	1:A:101:THR:HG22	1.92	0.51
1:A:42:CYS:H	1:A:101:THR:HG22	1.74	0.51
1:A:174:TRP:CD1	1:A:183:PRO:HB3	2.46	0.51
1:A:116:TYR:CD1	1:A:132:HIS:HB3	2.46	0.50
1:A:254:GLY:HA2	1:A:294:GLU:HA	1.94	0.49
1:A:170:PRO:HB3	1:A:221:PHE:CE2	2.48	0.49
1:A:358:THR:HG22	1:A:368:THR:HA	1.95	0.49
1:A:37:CYS:HA	1:A:105:SER:HA	1.95	0.49
1:A:149:VAL:HB	1:A:236:VAL:HA	1.94	0.49
1:A:357:LEU:HG	1:A:369:VAL:HG12	1.95	0.48
1:A:456:THR:OG1	1:A:457:GLU:N	2.46	0.48
1:A:332:ASN:HB3	3:A:610:NAG:N2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ASP:OD1	1:A:388:GLY:N	2.47	0.48
1:A:384:PRO:HA	1:A:411:PHE:CE1	2.49	0.47
1:A:416:LEU:HB2	1:A:433:VAL:HG23	1.95	0.47
1:A:326:PRO:HB3	1:A:351:SER:HB2	1.96	0.47
1:A:353:PRO:HG2	1:A:396:ASN:HD21	1.79	0.47
1:A:73:VAL:HG22	1:A:85:PHE:CE2	2.50	0.47
1:A:50:LEU:HD13	1:A:121:LEU:HD13	1.97	0.47
1:A:170:PRO:HB3	1:A:221:PHE:HE2	1.81	0.46
1:A:454:ASN:H	1:A:458:ARG:HD2	1.81	0.46
1:A:353:PRO:HG2	1:A:396:ASN:ND2	2.31	0.46
1:A:433:VAL:HG12	1:A:471:THR:HA	1.96	0.46
1:A:173:SER:HB2	1:A:218:GLN:HB3	1.98	0.45
1:A:464:GLU:OE1	1:A:465:ARG:N	2.49	0.45
1:A:337:ALA:HB1	1:A:341:GLU:OE2	2.16	0.45
1:A:359:ILE:HG12	1:A:367:ALA:HB3	1.98	0.45
1:A:50:LEU:HD12	1:A:50:LEU:O	2.16	0.45
1:A:393:VAL:HG22	1:A:395:GLU:HG3	1.99	0.44
1:A:245:MET:HB3	1:A:316:ARG:HH11	1.83	0.43
1:A:387:ASP:CG	1:A:408:SER:HA	2.38	0.43
1:A:22:TRP:N	2:A:601:MAN:O2	2.50	0.43
1:A:211:ASN:HB2	1:A:236:VAL:HG12	2.01	0.43
1:A:38:VAL:O	1:A:103:LEU:HA	2.18	0.43
4:A:604:BMA:H61	2:A:606:MAN:H2	1.44	0.43
1:A:297:PRO:HG3	1:A:352:ASN:HD21	1.84	0.43
1:A:118:ARG:NH1	1:A:126:GLN:HB2	2.34	0.42
1:A:382:VAL:HG13	1:A:386:ASP:HB2	2.01	0.42
1:A:172:LEU:HD13	1:A:200:SER:HB2	2.02	0.42
1:A:296:THR:OG1	1:A:299:GLU:HG2	2.19	0.42
1:A:58:VAL:HG11	1:A:75:LYS:HE2	2.02	0.42
1:A:489:THR:HG22	1:A:498:SER:CB	2.49	0.42
1:A:341:GLU:HG2	1:A:342:THR:H	1.85	0.41
1:A:160:MET:HG2	1:A:199:VAL:HG13	2.01	0.41
1:A:332:ASN:HB3	3:A:610:NAG:C8	2.50	0.41
1:A:454:ASN:N	1:A:458:ARG:HD2	2.36	0.40
1:A:156:GLU:O	1:A:156:GLU:HG3	2.21	0.40
1:A:218:GLN:HG3	1:A:229:GLU:CG	2.51	0.40
1:A:360:PHE:CE1	1:A:391:TRP:HB2	2.56	0.40

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:75:LYS:NZ	1:A:445:GLU:OE2[6_644]	2.08	0.12

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	485/500 (97%)	441 (91%)	43 (9%)	1 (0%)	52 86

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	PRO

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	422/431 (98%)	415 (98%)	7 (2%)	68 88

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	ARG
1	A	246	ASN
1	A	253	GLU
1	A	352	ASN
1	A	409	VAL

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Mol	Chain	Res	Type
1	A	432	CYS
1	A	491	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

13 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	MAN	A	601	1	11,11,12	1.53	2 (18%)	15,15,17	1.81	2 (13%)
3	NAG	A	602	1,3	14,14,15	0.67	1 (7%)	15,19,21	0.61	0
3	NAG	A	603	3,4	14,14,15	0.33	0	15,19,21	0.45	0
4	BMA	A	604	3,2	11,11,12	1.53	2 (18%)	15,15,17	1.55	3 (20%)
2	MAN	A	605	4	11,11,12	1.10	1 (9%)	15,15,17	0.99	1 (6%)
2	MAN	A	606	4	11,11,12	1.55	2 (18%)	15,15,17	1.46	1 (6%)
3	NAG	A	607	1	14,14,15	0.77	1 (7%)	15,19,21	0.81	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	608	1	14,14,15	0.78	1 (7%)	15,19,21	0.64	1 (6%)
3	NAG	A	609	1	14,14,15	0.52	0	15,19,21	0.38	0
3	NAG	A	610	1,5	14,14,15	2.16	1 (7%)	15,19,21	0.66	0
5	FUC	A	611	3	10,10,11	0.28	0	13,14,16	0.84	0
3	NAG	A	612	1,3	14,14,15	0.84	1 (7%)	15,19,21	1.09	2 (13%)
3	NAG	A	613	3	14,14,15	0.90	1 (7%)	15,19,21	0.73	1 (6%)

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	MAN	A	601	1	-	0/2/19/22	0/1/1/1
3	NAG	A	602	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	603	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	604	3,2	-	0/2/19/22	0/1/1/1
2	MAN	A	605	4	-	0/2/19/22	0/1/1/1
2	MAN	A	606	4	-	0/2/19/22	0/1/1/1
3	NAG	A	607	1	-	0/6/23/26	0/1/1/1
3	NAG	A	608	1	-	0/6/23/26	0/1/1/1
3	NAG	A	609	1	-	0/6/23/26	0/1/1/1
3	NAG	A	610	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	FUC	A	611	3	-	0/0/17/20	0/1/1/1
3	NAG	A	612	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	613	3	-	0/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	NAG	O5-C1	-2.31	1.40	1.43
2	A	605	MAN	C4-C5	2.04	1.57	1.53
3	A	608	NAG	C1-C2	2.13	1.55	1.52
2	A	606	MAN	C1-C2	2.18	1.57	1.52
3	A	607	NAG	C1-C2	2.61	1.56	1.52
3	A	612	NAG	O5-C1	2.63	1.48	1.43
3	A	613	NAG	C1-C2	2.69	1.56	1.52
4	A	604	BMA	C4-C3	2.89	1.60	1.52
2	A	601	MAN	C4-C5	2.92	1.59	1.53
4	A	604	BMA	C2-C3	2.99	1.56	1.52
2	A	601	MAN	O5-C5	3.46	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	606	MAN	C2-C3	3.90	1.57	1.52
3	A	610	NAG	C1-C2	8.03	1.63	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	608	NAG	C1-O5-C5	2.08	115.20	112.14
2	A	605	MAN	C1-O5-C5	2.30	115.52	112.14
3	A	607	NAG	C1-O5-C5	2.39	115.65	112.14
3	A	613	NAG	C1-O5-C5	2.48	115.78	112.14
3	A	612	NAG	C1-O5-C5	2.56	115.90	112.14
3	A	612	NAG	O4-C4-C5	2.77	116.51	109.23
2	A	601	MAN	O5-C5-C4	2.99	115.08	110.13
4	A	604	BMA	C1-C2-C3	3.17	113.39	109.55
4	A	604	BMA	C2-C3-C4	3.17	116.58	111.05
4	A	604	BMA	C3-C4-C5	3.17	115.89	110.23
2	A	606	MAN	C1-O5-C5	4.33	118.51	112.14
2	A	601	MAN	C1-O5-C5	5.32	119.96	112.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	610	NAG	C1

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
2	A	601	MAN	1	0
4	A	604	BMA	1	0
2	A	606	MAN	1	0
3	A	610	NAG	3	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, 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	487/500 (97%)	5.89	391 (80%) 0 1	347, 422, 477, 567	0

All (391) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	CYS	32.4
1	A	262	GLY	23.9
1	A	261	CYS	23.8
1	A	326	PRO	23.4
1	A	506	ALA	23.4
1	A	325	ALA	22.8
1	A	237	LYS	22.1
1	A	287	SER	22.0
1	A	322	VAL	21.9
1	A	395	GLU	21.8
1	A	323	MET	21.6
1	A	314	ASP	21.6
1	A	169	ARG	19.6
1	A	351	SER	19.4
1	A	170	PRO	19.2
1	A	307	ALA	18.9
1	A	327	TRP	17.8
1	A	321	SER	17.7
1	A	264	ASP	17.2
1	A	423	ALA	17.2
1	A	316	ARG	17.0
1	A	505	GLY	16.9
1	A	485	ARG	16.6
1	A	324	TYR	16.0
1	A	308	GLU	16.0
1	A	304	ALA	15.7
1	A	240	PRO	15.6

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Mol	Chain	Res	Type	RSRZ
1	A	258	SER	15.5
1	A	272	THR	15.5
1	A	349	THR	15.3
1	A	286	LYS	15.2
1	A	456	THR	14.7
1	A	394	ALA	14.7
1	A	306	LEU	14.6
1	A	317	THR	14.3
1	A	162	PRO	14.2
1	A	313	GLN	14.2
1	A	401	ARG	14.1
1	A	285	ALA	14.0
1	A	289	TYR	13.9
1	A	238	TYR	13.8
1	A	260	LEU	13.6
1	A	352	ASN	13.5
1	A	171	GLU	13.3
1	A	250	GLU	13.2
1	A	350	GLN	13.2
1	A	242	ILE	13.2
1	A	241	VAL	13.2
1	A	288	LEU	13.1
1	A	373	SER	12.6
1	A	273	TRP	12.5
1	A	374	GLN	12.4
1	A	328	LYS	12.2
1	A	263	ALA	12.2
1	A	301	GLY	12.2
1	A	149	VAL	12.0
1	A	449	ARG	12.0
1	A	34	GLU	12.0
1	A	251	ALA	11.9
1	A	392	CYS	11.8
1	A	393	VAL	11.8
1	A	445	GLU	11.7
1	A	172	LEU	11.1
1	A	477	ARG	11.1
1	A	448	SER	11.1
1	A	239	PRO	11.0
1	A	318	VAL	11.0
1	A	312	GLY	10.9
1	A	444	PHE	10.9

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Mol	Chain	Res	Type	RSRZ
1	A	208	ARG	10.8
1	A	274	MET	10.7
1	A	219	ALA	10.6
1	A	269	PRO	10.5
1	A	400	GLN	10.5
1	A	161	VAL	10.4
1	A	396	ASN	10.3
1	A	220	ALA	10.3
1	A	236	VAL	10.3
1	A	266	ASN	10.3
1	A	357	LEU	10.3
1	A	281	ARG	10.2
1	A	315	ASN	10.1
1	A	375	LEU	10.0
1	A	24	ALA	9.9
1	A	270	LEU	9.9
1	A	369	VAL	9.9
1	A	303	TYR	9.8
1	A	335	VAL	9.6
1	A	98	ARG	9.4
1	A	348	SER	9.4
1	A	139	ASN	9.3
1	A	424	ALA	9.3
1	A	356	ILE	9.3
1	A	302	VAL	9.2
1	A	271	LEU	9.0
1	A	168	LEU	9.0
1	A	484	PRO	9.0
1	A	150	VAL	8.8
1	A	244	GLU	8.8
1	A	36	THR	8.8
1	A	35	GLY	8.7
1	A	319	GLU	8.7
1	A	334	THR	8.6
1	A	297	PRO	8.6
1	A	422	ALA	8.5
1	A	39	SER	8.5
1	A	126	GLN	8.5
1	A	404	ALA	8.5
1	A	353	PRO	8.4
1	A	409	VAL	8.4
1	A	329	PRO	8.3

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Mol	Chain	Res	Type	RSRZ
1	A	458	ARG	8.3
1	A	245	MET	8.3
1	A	129	PHE	8.2
1	A	235	ASP	8.2
1	A	459	GLU	8.2
1	A	311	TYR	8.1
1	A	33	PHE	8.1
1	A	403	THR	8.1
1	A	198	GLN	8.0
1	A	41	PRO	8.0
1	A	26	MET	7.9
1	A	478	GLY	7.9
1	A	300	ASP	7.8
1	A	199	VAL	7.7
1	A	429	GLN	7.7
1	A	446	LEU	7.7
1	A	354	ASP	7.7
1	A	164	ASN	7.6
1	A	90	ARG	7.6
1	A	60	TYR	7.6
1	A	193	GLU	7.6
1	A	347	CYS	7.6
1	A	218	GLN	7.5
1	A	290	LEU	7.5
1	A	232	ALA	7.4
1	A	397	GLN	7.4
1	A	231	TYR	7.4
1	A	23	GLY	7.4
1	A	148	GLU	7.3
1	A	163	ASP	7.3
1	A	246	ASN	7.3
1	A	440	PRO	7.3
1	A	228	PHE	7.2
1	A	428	VAL	7.2
1	A	40	ILE	7.1
1	A	93	GLY	7.1
1	A	452	THR	7.1
1	A	275	ARG	7.0
1	A	44	PHE	7.0
1	A	173	SER	7.0
1	A	167	GLU	6.9
1	A	320	LEU	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	124	TYR	6.9
1	A	25	TRP	6.8
1	A	117	PHE	6.8
1	A	299	GLU	6.8
1	A	259	LEU	6.8
1	A	355	PRO	6.8
1	A	268	PRO	6.8
1	A	265	SER	6.7
1	A	481	GLN	6.7
1	A	402	ALA	6.6
1	A	127	TYR	6.6
1	A	398	TYR	6.6
1	A	479	GLN	6.6
1	A	43	ARG	6.5
1	A	410	GLU	6.5
1	A	358	THR	6.5
1	A	91	LEU	6.4
1	A	80	VAL	6.4
1	A	119	GLY	6.4
1	A	81	VAL	6.3
1	A	457	GLU	6.3
1	A	118	ARG	6.3
1	A	249	VAL	6.3
1	A	96	GLY	6.2
1	A	209	GLU	6.2
1	A	331	VAL	6.2
1	A	104	LEU	6.0
1	A	207	THR	6.0
1	A	128	THR	5.9
1	A	216	GLY	5.9
1	A	368	THR	5.9
1	A	215	LEU	5.9
1	A	175	LEU	5.9
1	A	455	GLU	5.8
1	A	213	HIS	5.7
1	A	476	ILE	5.7
1	A	38	VAL	5.6
1	A	309	ASN	5.6
1	A	217	CYS	5.6
1	A	486	VAL	5.6
1	A	89	SER	5.6
1	A	330	THR	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	447	PRO	5.6
1	A	210	ALA	5.6
1	A	253	GLU	5.6
1	A	74	PHE	5.5
1	A	116	TYR	5.5
1	A	257	VAL	5.5
1	A	174	TRP	5.5
1	A	102	LEU	5.5
1	A	59	TRP	5.4
1	A	160	MET	5.4
1	A	97	LEU	5.4
1	A	462	TYR	5.4
1	A	61	PHE	5.3
1	A	92	LEU	5.3
1	A	376	GLN	5.3
1	A	442	VAL	5.3
1	A	291	ASP	5.2
1	A	151	ALA	5.2
1	A	62	ASN	5.2
1	A	125	ASN	5.2
1	A	206	PRO	5.2
1	A	32	ALA	5.2
1	A	133	SER	5.2
1	A	27	PRO	5.1
1	A	427	THR	5.1
1	A	95	LEU	5.1
1	A	88	ARG	5.1
1	A	491	ARG	5.1
1	A	370	ILE	5.1
1	A	504	GLN	5.0
1	A	336	VAL	5.0
1	A	461	VAL	5.0
1	A	42	CYS	5.0
1	A	64	PRO	5.0
1	A	230	GLY	5.0
1	A	58	VAL	4.9
1	A	282	GLU	4.9
1	A	252	ILE	4.9
1	A	46	PHE	4.9
1	A	211	ASN	4.9
1	A	75	LYS	4.8
1	A	425	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	69	TYR	4.7
1	A	73	VAL	4.7
1	A	450	ASN	4.7
1	A	166	PRO	4.7
1	A	176	GLY	4.7
1	A	221	PHE	4.7
1	A	71	PRO	4.6
1	A	439	GLU	4.6
1	A	267	PRO	4.6
1	A	405	PHE	4.6
1	A	475	THR	4.5
1	A	430	CYS	4.5
1	A	45	ASP	4.5
1	A	408	SER	4.5
1	A	372	GLU	4.5
1	A	487	ILE	4.5
1	A	140	THR	4.5
1	A	333	GLY	4.5
1	A	280	LEU	4.4
1	A	48	ASP	4.4
1	A	411	PHE	4.4
1	A	431	LEU	4.4
1	A	243	VAL	4.4
1	A	437	ASN	4.4
1	A	346	LEU	4.3
1	A	107	LEU	4.3
1	A	389	GLU	4.3
1	A	214	ARG	4.3
1	A	467	GLY	4.2
1	A	94	ASP	4.2
1	A	200	SER	4.2
1	A	474	LEU	4.2
1	A	103	LEU	4.2
1	A	37	CYS	4.2
1	A	63	SER	4.1
1	A	465	ARG	4.1
1	A	473	ILE	4.1
1	A	292	LEU	4.1
1	A	363	LYS	4.1
1	A	435	LYS	4.0
1	A	434	VAL	4.0
1	A	483	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	55	VAL	4.0
1	A	407	LEU	3.9
1	A	72	VAL	3.9
1	A	345	ILE	3.9
1	A	194	GLY	3.9
1	A	234	LEU	3.9
1	A	466	SER	3.9
1	A	283	ALA	3.9
1	A	229	GLU	3.9
1	A	453	VAL	3.9
1	A	192	ASP	3.9
1	A	371	TYR	3.8
1	A	298	GLY	3.8
1	A	66	PRO	3.8
1	A	470	LEU	3.8
1	A	469	LEU	3.7
1	A	99	ASN	3.7
1	A	256	HIS	3.7
1	A	332	ASN	3.6
1	A	468	LEU	3.6
1	A	131	GLU	3.6
1	A	233	SER	3.6
1	A	441	SER	3.6
1	A	432	CYS	3.6
1	A	130	SER	3.6
1	A	471	THR	3.6
1	A	362	GLU	3.5
1	A	138	VAL	3.5
1	A	494	TYR	3.5
1	A	464	GLU	3.5
1	A	360	PHE	3.5
1	A	22	TRP	3.4
1	A	426	ASP	3.4
1	A	276	ASP	3.4
1	A	391	TRP	3.3
1	A	155	VAL	3.3
1	A	70	PRO	3.3
1	A	443	ALA	3.3
1	A	105	SER	3.3
1	A	115	TYR	3.3
1	A	337	ALA	3.3
1	A	496	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	482	ALA	3.3
1	A	226	LEU	3.3
1	A	284	VAL	3.3
1	A	177	HIS	3.2
1	A	279	VAL	3.2
1	A	202	LEU	3.2
1	A	359	ILE	3.1
1	A	188	ARG	3.1
1	A	503	PHE	3.1
1	A	67	LYS	3.1
1	A	480	ALA	3.1
1	A	204	PHE	3.0
1	A	451	VAL	3.0
1	A	454	ASN	3.0
1	A	20	GLY	3.0
1	A	420	HIS	3.0
1	A	310	ALA	3.0
1	A	21	HIS	3.0
1	A	84	SER	3.0
1	A	490	SER	3.0
1	A	31	SER	2.9
1	A	141	PRO	2.9
1	A	57	GLY	2.9
1	A	406	ASN	2.9
1	A	438	PRO	2.9
1	A	191	GLU	2.8
1	A	472	SER	2.8
1	A	399	GLY	2.8
1	A	85	PHE	2.8
1	A	120	ASP	2.8
1	A	295	VAL	2.8
1	A	413	PRO	2.7
1	A	227	GLN	2.7
1	A	83	GLU	2.7
1	A	212	GLY	2.7
1	A	415	ILE	2.6
1	A	68	ASN	2.6
1	A	47	PRO	2.6
1	A	493	LEU	2.6
1	A	460	PHE	2.6
1	A	296	THR	2.6
1	A	135	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	121	LEU	2.6
1	A	421	CYS	2.6
1	A	367	ALA	2.6
1	A	492	ASN	2.5
1	A	463	SER	2.5
1	A	436	SER	2.5
1	A	165	CYS	2.5
1	A	157	VAL	2.5
1	A	339	GLU	2.5
1	A	390	TYR	2.4
1	A	196	TRP	2.4
1	A	110	GLU	2.4
1	A	489	THR	2.4
1	A	65	TYR	2.3
1	A	82	HIS	2.3
1	A	111	LEU	2.3
1	A	101	THR	2.3
1	A	488	CYS	2.2
1	A	433	VAL	2.2
1	A	123	GLY	2.1
1	A	248	SER	2.1
1	A	159	CYS	2.1
1	A	366	LEU	2.1
1	A	278	MET	2.1
1	A	255	SER	2.1
1	A	152	GLY	2.1
1	A	30	ILE	2.1
1	A	377	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
3	NAG	A	603	14/15	0.88	2.27	3.18	296,360,390,420	0
3	NAG	A	602	14/15	0.96	1.87	1.07	275,341,386,392	0
3	NAG	A	608	14/15	0.05	1.34	-0.46	363,399,399,399	0
3	NAG	A	607	14/15	0.75	0.45	-	413,413,413,413	0
3	NAG	A	610	14/15	0.36	1.29	-	381,401,401,401	0
2	MAN	A	605	11/12	0.55	0.93	-	402,402,402,402	0
3	NAG	A	612	14/15	0.77	0.84	-	344,377,377,377	0
2	MAN	A	601	11/12	0.77	0.62	-	366,373,385,386	0
3	NAG	A	613	14/15	0.83	0.78	-	381,381,381,381	0
3	NAG	A	609	14/15	0.58	1.55	-	306,361,361,361	0
2	MAN	A	606	11/12	0.56	0.75	-	350,350,350,350	0
5	FUC	A	611	10/11	0.76	1.98	-	404,404,404,404	0
4	BMA	A	604	11/12	0.61	0.75	-	302,400,400,400	0

6.5 Other polymers

There are no such residues in this entry.