



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:52 PM GMT

PDB ID : 5BW7
Title : Crystal structure of nonfucosylated Fc Y296W mutant complexed with bis-glycosylated soluble form of Fc gamma receptor IIIa
Authors : Isoda, Y.; Yagi, H.; Satoh, T.; Shibata-Koyama, M.; Masuda, K.; Satoh, M.; Kato, K.; Iida, S.
Deposited on : 2015-06-06
Resolution : 3.00 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-20026982
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-20026982

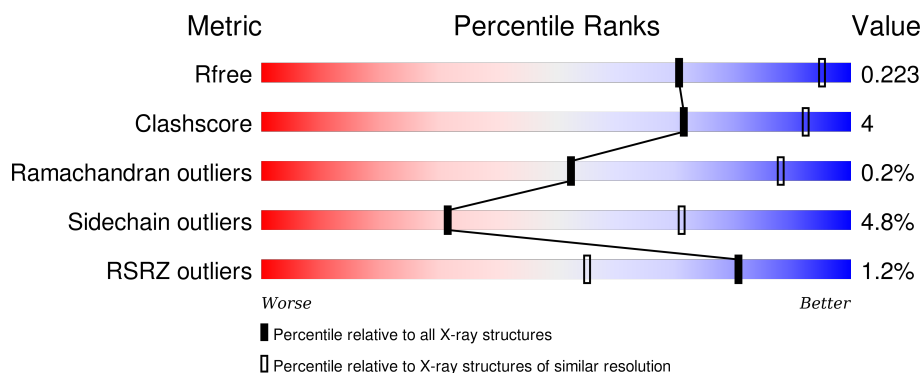
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	223	
1	B	223	
2	C	179	

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
6	GAL	A	1008	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5042 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	212	Total	C	N	O	S	0	0	0
			1695	1080	285	324	6			
1	B	215	Total	C	N	O	S	0	0	0
			1714	1093	288	327	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	TRP	TYR	engineered mutation	UNP P01857
B	296	TRP	TYR	engineered mutation	UNP P01857

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	155	Total	C	N	O	S	0	0	0
			1268	810	218	236	4			

There are 10 discrepancies between the modelled and reference sequences:

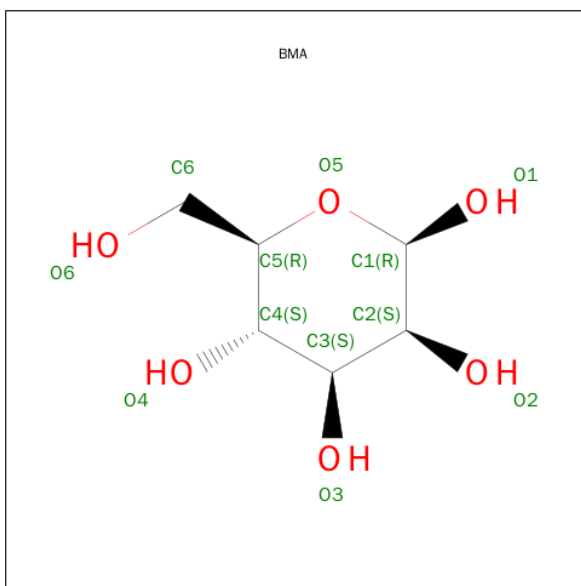
Chain	Residue	Modelled	Actual	Comment	Reference
C	38	GLN	ASN	engineered mutation	UNP P08637
C	74	GLN	ASN	engineered mutation	UNP P08637
C	158	VAL	PHE	engineered mutation	UNP P08637
C	169	GLN	ASN	engineered mutation	UNP P08637
C	176	HIS	-	expression tag	UNP P08637
C	177	HIS	-	expression tag	UNP P08637
C	178	HIS	-	expression tag	UNP P08637
C	179	HIS	-	expression tag	UNP P08637
C	180	HIS	-	expression tag	UNP P08637
C	181	HIS	-	expression tag	UNP P08637

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



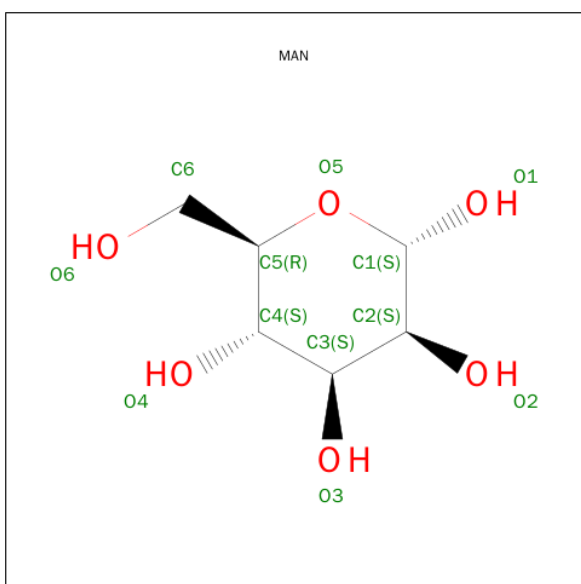
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1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

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



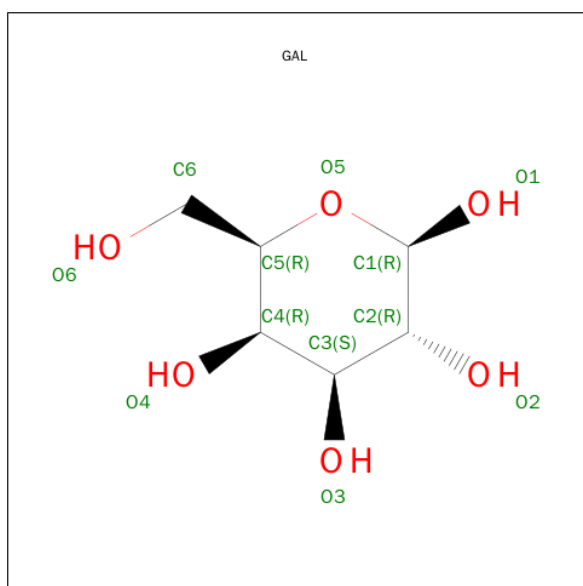
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



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

- Molecule 6 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: C₆H₁₂O₆).

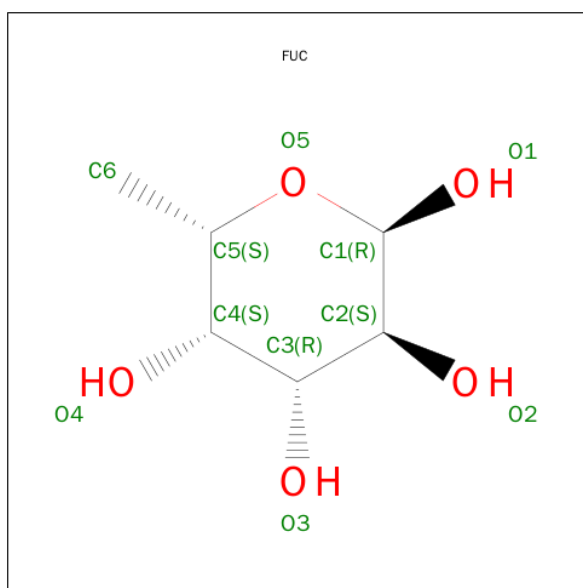


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



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

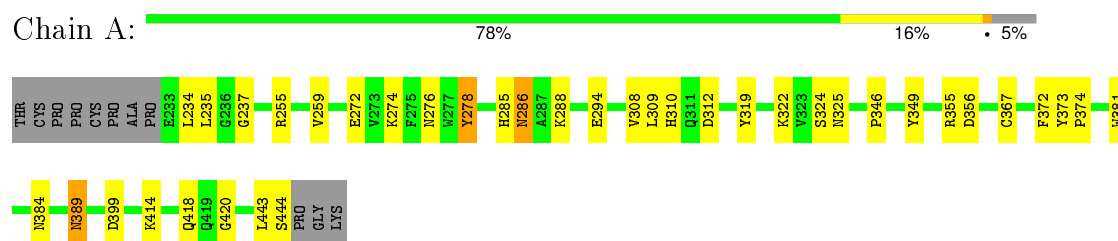
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	8	Total	O	0	0
			8	8		
9	B	13	Total	O	0	0
			13	13		
9	C	5	Total	O	0	0
			5	5		

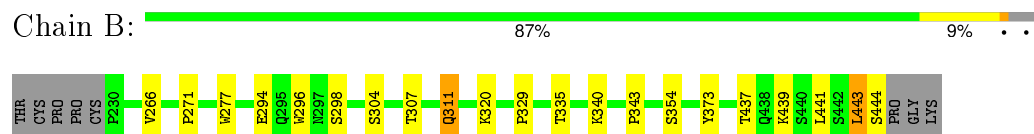
3 Residue-property plots

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 ($RSRZ > 2$). 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.

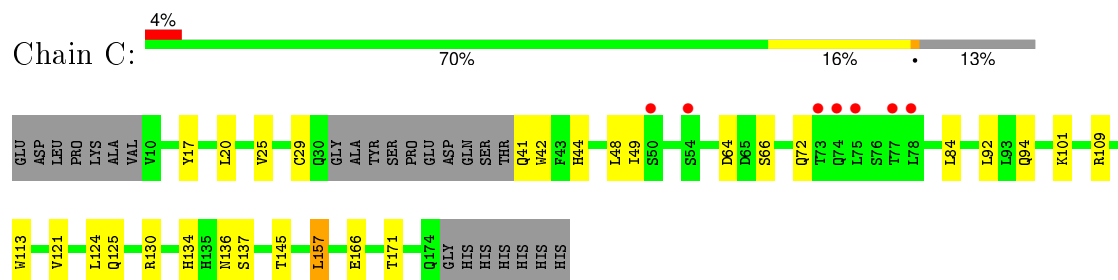
- Molecule 1: Ig gamma-1 chain C region



- Molecule 1: Ig gamma-1 chain C region



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	77.27Å 77.27Å 350.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 19.95 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-3.00) 98.6 (19.95-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.11 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.204 , 0.250 0.213 , 0.223	Depositor DCC
R_{free} test set	1081 reflections (5.16%)	DCC
Wilson B-factor (Å ²)	65.3	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 21.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 22015 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5042	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CL, GAL, FUC, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.58	0/1742	0.74	0/2374
1	B	0.62	0/1763	0.74	0/2404
2	C	0.59	0/1302	0.73	0/1766
All	All	0.59	0/4807	0.74	0/6544

There are no bond length outliers.

There are no bond angle outliers.

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	1695	0	1662	22	0
1	B	1714	0	1682	10	0
2	C	1268	0	1220	14	0
3	A	56	0	49	0	0
3	B	56	0	50	0	0
3	C	84	0	73	2	0
4	A	11	0	8	0	0
4	B	11	0	8	0	0
4	C	22	0	17	0	0
5	A	22	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	22	0	18	0	0
5	C	33	0	28	0	0
6	A	11	0	10	0	0
7	A	1	0	0	0	0
8	C	10	0	10	0	0
9	A	8	0	0	0	1
9	B	13	0	0	0	0
9	C	5	0	0	0	0
All	All	5042	0	4853	42	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 4.

All (42) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:64:ASP:OD1	3:C:1009:NAG:O6	2.04	0.76
1:A:309:LEU:HB2	1:A:312:ASP:OD2	1.94	0.67
1:A:309:LEU:HD12	1:A:312:ASP:OD2	1.95	0.66
2:C:29:CYS:HB2	2:C:42:TRP:CZ2	2.34	0.63
1:A:285:HIS:O	1:A:286:ASN:ND2	2.29	0.61
1:B:277:TRP:HE1	1:B:304:SER:HG	1.56	0.54
2:C:42:TRP:HB2	2:C:49:ILE:CD1	2.39	0.53
1:A:356:ASP:OD2	1:B:439:LYS:HE3	2.11	0.51
2:C:157:LEU:HD13	3:C:1001:NAG:H83	1.92	0.51
1:A:443:LEU:HD12	1:A:444:SER:H	1.75	0.51
2:C:20:LEU:HD13	2:C:92:LEU:HB2	1.93	0.51
2:C:42:TRP:HB2	2:C:49:ILE:HD11	1.94	0.50
1:A:373:TYR:CG	1:A:374:PRO:HA	2.47	0.49
1:B:343:PRO:HA	1:B:373:TYR:O	2.13	0.49
2:C:125:GLN:OE1	2:C:130:ARG:NH1	2.45	0.49
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.48	0.49
1:A:389:ASN:N	1:A:389:ASN:OD1	2.47	0.48
1:A:276:ASN:HB2	1:A:322:LYS:HB3	1.96	0.48
2:C:94:GLN:OE1	2:C:109:ARG:NH1	2.47	0.47
1:A:308:VAL:HG22	1:A:319:TYR:CE1	2.50	0.46
1:A:384:ASN:HD22	1:A:384:ASN:N	2.13	0.46
1:B:320:LYS:HG3	1:B:335:THR:HG22	1.97	0.46
1:A:276:ASN:HB3	1:A:278:TYR:HE2	1.82	0.45
2:C:66:SER:HA	2:C:84:LEU:O	2.17	0.45
1:A:349:TYR:HB3	1:B:354:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:VAL:CG1	1:B:271:PRO:HA	2.47	0.44
1:A:237:GLY:HA2	2:C:134:HIS:CD2	2.53	0.44
1:A:346:PRO:HB3	1:A:372:PHE:HB3	2.00	0.43
1:A:272:GLU:O	1:A:325:ASN:ND2	2.51	0.43
2:C:124:LEU:HD12	2:C:124:LEU:N	2.33	0.43
2:C:41:GLN:N	2:C:72:GLN:O	2.52	0.43
1:A:418:GLN:C	1:A:420:GLY:N	2.73	0.42
1:A:310:HIS:H	1:A:310:HIS:CD2	2.37	0.42
1:B:329:PRO:HB3	2:C:113:TRP:CD2	2.55	0.42
1:A:255:ARG:O	1:A:310:HIS:CE1	2.73	0.41
2:C:121:VAL:HG21	2:C:136:ASN:HA	2.02	0.41
1:B:443:LEU:HD23	1:B:444:SER:N	2.35	0.41
1:A:259:VAL:HG23	1:A:308:VAL:HG21	2.03	0.41
1:A:274:LYS:HB3	1:A:324:SER:HB2	2.02	0.41
1:B:311:GLN:H	1:B:311:GLN:NE2	2.19	0.41
1:A:384:ASN:ND2	1:A:384:ASN:N	2.68	0.40
1:B:294:GLU:OE2	1:B:298:SER:HA	2.21	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)
9:A:1101:HOH:O	9:A:1104:HOH:O[6_544]	1.60	0.60

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	210/223 (94%)	198 (94%)	12 (6%)	0	100	100
1	B	213/223 (96%)	206 (97%)	6 (3%)	1 (0%)	34	76
2	C	151/179 (84%)	139 (92%)	12 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	574/625 (92%)	543 (95%)	30 (5%)	1 (0%)	52 88

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	441	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	197/206 (96%)	187 (95%)	10 (5%)	29 69
1	B	199/206 (97%)	193 (97%)	6 (3%)	48 83
2	C	142/162 (88%)	132 (93%)	10 (7%)	19 55
All	All	538/574 (94%)	512 (95%)	26 (5%)	31 71

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	LEU
1	A	235	LEU
1	A	278	TYR
1	A	286	ASN
1	A	288	LYS
1	A	294	GLU
1	A	355	ARG
1	A	389	ASN
1	A	399	ASP
1	A	414	LYS
1	B	296	TRP
1	B	307	THR
1	B	311	GLN
1	B	340	LYS
1	B	437	THR

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Mol	Chain	Res	Type
1	B	443	LEU
2	C	17	TYR
2	C	25	VAL
2	C	44	HIS
2	C	48	LEU
2	C	101	LYS
2	C	137	SER
2	C	145	THR
2	C	157	LEU
2	C	166	GLU
2	C	171	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	HIS
1	A	384	ASN
1	A	421	ASN
1	B	311	GLN
1	B	325	ASN
1	B	421	ASN
1	B	438	GLN
2	C	15	GLN
2	C	119	HIS
2	C	134	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

23 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	1001	1,3	14,14,15	0.76	1 (7%)	15,19,21	1.11	1 (6%)
3	NAG	A	1002	3,4	14,14,15	1.11	1 (7%)	15,19,21	1.72	3 (20%)
5	MAN	A	1004	3,4	11,11,12	0.69	0	15,15,17	1.41	3 (20%)
3	NAG	A	1005	5	14,14,15	0.66	0	15,19,21	1.98	4 (26%)
5	MAN	A	1006	3,4	11,11,12	0.65	0	15,15,17	1.53	1 (6%)
3	NAG	A	1007	5,6	14,14,15	0.79	0	15,19,21	1.38	2 (13%)
6	GAL	A	1008	3	11,11,12	0.67	0	15,15,17	1.18	0
3	NAG	B	1001	1,3	14,14,15	0.58	0	15,19,21	1.94	4 (26%)
3	NAG	B	1002	3,4	14,14,15	0.56	0	15,19,21	1.33	3 (20%)
5	MAN	B	1004	3,4	11,11,12	0.68	0	15,15,17	1.12	1 (6%)
3	NAG	B	1005	5	14,14,15	0.57	0	15,19,21	0.99	1 (6%)
5	MAN	B	1006	3,4	11,11,12	0.68	0	15,15,17	1.12	0
3	NAG	B	1007	5	14,14,15	0.61	0	15,19,21	0.98	0
3	NAG	C	1001	8,3,2	14,14,15	0.82	0	15,19,21	2.75	5 (33%)
3	NAG	C	1002	3,4	14,14,15	0.53	0	15,19,21	1.26	2 (13%)
5	MAN	C	1004	4	11,11,12	0.73	0	15,15,17	1.73	4 (26%)
5	MAN	C	1005	3,4	11,11,12	0.56	0	15,15,17	1.70	3 (20%)
3	NAG	C	1006	5	14,14,15	0.68	0	15,19,21	2.01	4 (26%)
8	FUC	C	1007	3	10,10,11	0.63	0	13,14,16	1.26	1 (7%)
3	NAG	C	1008	3,2	14,14,15	0.56	0	15,19,21	1.40	1 (6%)
3	NAG	C	1009	3,4	14,14,15	0.47	0	15,19,21	1.13	1 (6%)
5	MAN	C	1011	3,4	11,11,12	0.49	0	15,15,17	1.14	1 (6%)
3	NAG	C	1012	5	14,14,15	0.77	1 (7%)	15,19,21	2.77	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	1001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1002	3,4	-	0/6/23/26	0/1/1/1
5	MAN	A	1004	3,4	-	0/2/19/22	0/1/1/1
3	NAG	A	1005	5	-	0/6/23/26	0/1/1/1
5	MAN	A	1006	3,4	-	0/2/19/22	0/1/1/1
3	NAG	A	1007	5,6	-	0/6/23/26	0/1/1/1
6	GAL	A	1008	3	-	0/2/19/22	0/1/1/1
3	NAG	B	1001	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1002	3,4	-	0/6/23/26	0/1/1/1
5	MAN	B	1004	3,4	-	0/2/19/22	0/1/1/1
3	NAG	B	1005	5	-	0/6/23/26	0/1/1/1
5	MAN	B	1006	3,4	-	0/2/19/22	0/1/1/1
3	NAG	B	1007	5	-	0/6/23/26	0/1/1/1
3	NAG	C	1001	8,3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	1002	3,4	-	0/6/23/26	0/1/1/1
5	MAN	C	1004	4	-	0/2/19/22	0/1/1/1
5	MAN	C	1005	3,4	-	0/2/19/22	0/1/1/1
3	NAG	C	1006	5	-	0/6/23/26	0/1/1/1
8	FUC	C	1007	3	-	0/0/17/20	0/1/1/1
3	NAG	C	1008	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	1009	3,4	-	0/6/23/26	0/1/1/1
5	MAN	C	1011	3,4	-	0/2/19/22	0/1/1/1
3	NAG	C	1012	5	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	NAG	O5-C1	-2.71	1.39	1.43
3	A	1001	NAG	O5-C1	-2.09	1.40	1.43
3	C	1012	NAG	C1-C2	2.22	1.55	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	NAG	O3-C3-C2	-4.37	100.03	109.37
5	C	1005	MAN	C1-C2-C3	-3.54	105.27	109.55
3	C	1001	NAG	O7-C7-C8	-3.52	115.59	122.07
3	B	1002	NAG	O6-C6-C5	-3.28	100.36	111.30
3	B	1001	NAG	O7-C7-C8	-2.93	116.68	122.07
3	C	1002	NAG	C3-C4-C5	-2.86	105.12	110.23
3	A	1005	NAG	O7-C7-C8	-2.84	116.84	122.07
3	A	1002	NAG	C4-C3-C2	-2.66	107.20	111.34
3	A	1007	NAG	O4-C4-C3	-2.53	104.64	110.36
5	A	1004	MAN	O2-C2-C3	-2.41	105.32	110.19
5	A	1004	MAN	O5-C1-C2	-2.39	107.08	110.89
5	A	1004	MAN	C2-C3-C4	-2.39	106.88	111.05
3	C	1002	NAG	O4-C4-C3	-2.36	105.03	110.36
3	A	1005	NAG	O5-C5-C4	-2.36	106.23	110.13
3	B	1002	NAG	O3-C3-C4	-2.33	105.11	110.36
3	B	1001	NAG	C4-C3-C2	-2.32	107.74	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1012	NAG	O7-C7-C8	-2.29	117.85	122.07
3	C	1006	NAG	O5-C5-C4	-2.11	106.65	110.13
3	C	1001	NAG	O6-C6-C5	-2.09	104.33	111.30
3	C	1006	NAG	O7-C7-C8	-2.02	118.35	122.07
3	B	1001	NAG	O7-C7-N2	2.09	126.11	121.84
3	B	1005	NAG	O5-C5-C6	2.16	111.97	107.34
5	C	1004	MAN	O5-C5-C6	2.17	111.99	107.34
3	B	1002	NAG	O5-C5-C4	2.18	113.74	110.13
3	A	1001	NAG	C1-O5-C5	2.21	115.39	112.14
5	B	1004	MAN	O2-C2-C1	2.28	113.80	109.23
5	C	1005	MAN	O5-C5-C4	2.33	113.99	110.13
3	C	1009	NAG	O5-C5-C6	2.40	112.48	107.34
3	C	1012	NAG	O5-C5-C4	2.49	114.25	110.13
5	C	1004	MAN	O2-C2-C1	2.80	114.83	109.23
8	C	1007	FUC	O5-C5-C6	2.80	111.30	106.28
5	C	1004	MAN	C3-C4-C5	2.81	115.24	110.23
5	C	1004	MAN	C2-C3-C4	2.99	116.27	111.05
3	C	1001	NAG	O3-C3-C2	3.12	116.04	109.37
3	C	1008	NAG	C1-O5-C5	3.20	116.84	112.14
3	A	1007	NAG	C8-C7-N2	3.25	122.33	116.10
3	A	1002	NAG	O3-C3-C4	3.27	117.73	110.36
5	C	1005	MAN	C1-O5-C5	3.35	117.07	112.14
5	C	1011	MAN	C1-O5-C5	3.55	117.36	112.14
3	C	1006	NAG	C2-N2-C7	4.15	128.50	123.11
3	C	1001	NAG	O7-C7-N2	4.30	130.61	121.84
3	A	1005	NAG	C2-N2-C7	4.39	128.82	123.11
3	A	1005	NAG	C8-C7-N2	4.41	124.54	116.10
5	A	1006	MAN	C1-O5-C5	4.53	118.81	112.14
3	C	1006	NAG	C1-O5-C5	4.54	118.82	112.14
3	C	1012	NAG	C2-N2-C7	5.25	129.93	123.11
3	B	1001	NAG	C1-O5-C5	5.55	120.30	112.14
3	C	1001	NAG	C2-N2-C7	7.25	132.53	123.11
3	C	1012	NAG	C1-O5-C5	8.09	124.04	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1001	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1009	NAG	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 1 is monoatomic - leaving 27 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	1001	1,3	14,14,15	0.76	1 (7%)	15,19,21	1.11	1 (6%)
3	NAG	A	1002	3,4	14,14,15	1.11	1 (7%)	15,19,21	1.72	3 (20%)
4	BMA	A	1003	3,5	11,11,12	0.44	0	15,15,17	1.25	1 (6%)
5	MAN	A	1004	3,4	11,11,12	0.69	0	15,15,17	1.41	3 (20%)
3	NAG	A	1005	5	14,14,15	0.66	0	15,19,21	1.98	4 (26%)
5	MAN	A	1006	3,4	11,11,12	0.65	0	15,15,17	1.53	1 (6%)
3	NAG	A	1007	5,6	14,14,15	0.79	0	15,19,21	1.38	2 (13%)
6	GAL	A	1008	3	11,11,12	0.67	0	15,15,17	1.18	0
3	NAG	B	1001	1,3	14,14,15	0.58	0	15,19,21	1.94	4 (26%)
3	NAG	B	1002	3,4	14,14,15	0.56	0	15,19,21	1.33	3 (20%)
4	BMA	B	1003	3,5	11,11,12	0.68	0	15,15,17	1.28	2 (13%)
5	MAN	B	1004	3,4	11,11,12	0.68	0	15,15,17	1.12	1 (6%)
3	NAG	B	1005	5	14,14,15	0.57	0	15,19,21	0.99	1 (6%)
5	MAN	B	1006	3,4	11,11,12	0.68	0	15,15,17	1.12	0
3	NAG	B	1007	5	14,14,15	0.61	0	15,19,21	0.98	0
3	NAG	C	1001	8,3,2	14,14,15	0.82	0	15,19,21	2.75	5 (33%)
3	NAG	C	1002	3,4	14,14,15	0.53	0	15,19,21	1.26	2 (13%)
4	BMA	C	1003	3,5	11,11,12	0.60	0	15,15,17	1.27	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	C	1004	4	11,11,12	0.73	0	15,15,17	1.73	4 (26%)
5	MAN	C	1005	3,4	11,11,12	0.56	0	15,15,17	1.70	3 (20%)
3	NAG	C	1006	5	14,14,15	0.68	0	15,19,21	2.01	4 (26%)
8	FUC	C	1007	3	10,10,11	0.63	0	13,14,16	1.26	1 (7%)
3	NAG	C	1008	3,2	14,14,15	0.56	0	15,19,21	1.40	1 (6%)
3	NAG	C	1009	3,4	14,14,15	0.47	0	15,19,21	1.13	1 (6%)
4	BMA	C	1010	3,5	11,11,12	0.82	0	15,15,17	2.90	4 (26%)
5	MAN	C	1011	3,4	11,11,12	0.49	0	15,15,17	1.14	1 (6%)
3	NAG	C	1012	5	14,14,15	0.77	1 (7%)	15,19,21	2.77	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	1001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1002	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	1003	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	1004	3,4	-	0/2/19/22	0/1/1/1
3	NAG	A	1005	5	-	0/6/23/26	0/1/1/1
5	MAN	A	1006	3,4	-	0/2/19/22	0/1/1/1
3	NAG	A	1007	5,6	-	0/6/23/26	0/1/1/1
6	GAL	A	1008	3	-	0/2/19/22	0/1/1/1
3	NAG	B	1001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1002	3,4	-	0/6/23/26	0/1/1/1
4	BMA	B	1003	3,5	-	0/2/19/22	0/1/1/1
5	MAN	B	1004	3,4	-	0/2/19/22	0/1/1/1
3	NAG	B	1005	5	-	0/6/23/26	0/1/1/1
5	MAN	B	1006	3,4	-	0/2/19/22	0/1/1/1
3	NAG	B	1007	5	-	0/6/23/26	0/1/1/1
3	NAG	C	1001	8,3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	1002	3,4	-	0/6/23/26	0/1/1/1
4	BMA	C	1003	3,5	-	0/2/19/22	0/1/1/1
5	MAN	C	1004	4	-	0/2/19/22	0/1/1/1
5	MAN	C	1005	3,4	-	0/2/19/22	0/1/1/1
3	NAG	C	1006	5	-	0/6/23/26	0/1/1/1
8	FUC	C	1007	3	-	0/0/17/20	0/1/1/1
3	NAG	C	1008	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	1009	3,4	-	0/6/23/26	0/1/1/1
4	BMA	C	1010	3,5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	C	1011	3,4	-	0/2/19/22	0/1/1/1
3	NAG	C	1012	5	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	NAG	O5-C1	-2.71	1.39	1.43
3	A	1001	NAG	O5-C1	-2.09	1.40	1.43
3	C	1012	NAG	C1-C2	2.22	1.55	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	NAG	O3-C3-C2	-4.37	100.03	109.37
5	C	1005	MAN	C1-C2-C3	-3.54	105.27	109.55
3	C	1001	NAG	O7-C7-C8	-3.52	115.59	122.07
3	B	1002	NAG	O6-C6-C5	-3.28	100.36	111.30
3	B	1001	NAG	O7-C7-C8	-2.93	116.68	122.07
3	C	1002	NAG	C3-C4-C5	-2.86	105.12	110.23
3	A	1005	NAG	O7-C7-C8	-2.84	116.84	122.07
3	A	1002	NAG	C4-C3-C2	-2.66	107.20	111.34
3	A	1007	NAG	O4-C4-C3	-2.53	104.64	110.36
5	A	1004	MAN	O2-C2-C3	-2.41	105.32	110.19
5	A	1004	MAN	O5-C1-C2	-2.39	107.08	110.89
5	A	1004	MAN	C2-C3-C4	-2.39	106.88	111.05
3	C	1002	NAG	O4-C4-C3	-2.36	105.03	110.36
3	A	1005	NAG	O5-C5-C4	-2.36	106.23	110.13
3	B	1002	NAG	O3-C3-C4	-2.33	105.11	110.36
3	B	1001	NAG	C4-C3-C2	-2.32	107.74	111.34
3	C	1012	NAG	O7-C7-C8	-2.29	117.85	122.07
4	C	1003	BMA	O3-C3-C4	-2.16	105.49	110.36
3	C	1006	NAG	O5-C5-C4	-2.11	106.65	110.13
3	C	1001	NAG	O6-C6-C5	-2.09	104.33	111.30
3	C	1006	NAG	O7-C7-C8	-2.02	118.35	122.07
3	B	1001	NAG	O7-C7-N2	2.09	126.11	121.84
3	B	1005	NAG	O5-C5-C6	2.16	111.97	107.34
5	C	1004	MAN	O5-C5-C6	2.17	111.99	107.34
3	B	1002	NAG	O5-C5-C4	2.18	113.74	110.13
3	A	1001	NAG	C1-O5-C5	2.21	115.39	112.14
5	B	1004	MAN	O2-C2-C1	2.28	113.80	109.23
5	C	1005	MAN	O5-C5-C4	2.33	113.99	110.13
3	C	1009	NAG	O5-C5-C6	2.40	112.48	107.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1012	NAG	O5-C5-C4	2.49	114.25	110.13
4	C	1010	BMA	O3-C3-C2	2.64	114.84	110.01
4	C	1003	BMA	O5-C5-C6	2.71	113.14	107.34
4	B	1003	BMA	C1-O5-C5	2.76	116.21	112.14
4	B	1003	BMA	C1-C2-C3	2.77	112.91	109.55
5	C	1004	MAN	O2-C2-C1	2.80	114.83	109.23
8	C	1007	FUC	O5-C5-C6	2.80	111.30	106.28
5	C	1004	MAN	C3-C4-C5	2.81	115.24	110.23
5	C	1004	MAN	C2-C3-C4	2.99	116.27	111.05
4	A	1003	BMA	C1-C2-C3	3.08	113.29	109.55
3	C	1001	NAG	O3-C3-C2	3.12	116.04	109.37
3	C	1008	NAG	C1-O5-C5	3.20	116.84	112.14
3	A	1007	NAG	C8-C7-N2	3.25	122.33	116.10
3	A	1002	NAG	O3-C3-C4	3.27	117.73	110.36
5	C	1005	MAN	C1-O5-C5	3.35	117.07	112.14
5	C	1011	MAN	C1-O5-C5	3.55	117.36	112.14
3	C	1006	NAG	C2-N2-C7	4.15	128.50	123.11
4	C	1010	BMA	O5-C1-C2	4.17	117.57	110.89
3	C	1001	NAG	O7-C7-N2	4.30	130.61	121.84
3	A	1005	NAG	C2-N2-C7	4.39	128.82	123.11
3	A	1005	NAG	C8-C7-N2	4.41	124.54	116.10
5	A	1006	MAN	C1-O5-C5	4.53	118.81	112.14
3	C	1006	NAG	C1-O5-C5	4.54	118.82	112.14
3	C	1012	NAG	C2-N2-C7	5.25	129.93	123.11
3	B	1001	NAG	C1-O5-C5	5.55	120.30	112.14
4	C	1010	BMA	C1-O5-C5	5.58	120.34	112.14
3	C	1001	NAG	C2-N2-C7	7.25	132.53	123.11
4	C	1010	BMA	C1-C2-C3	7.80	119.00	109.55
3	C	1012	NAG	C1-O5-C5	8.09	124.04	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1001	NAG	1	0
3	C	1009	NAG	1	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	212/223 (95%)	-0.58	0	100 100	41, 62, 87, 121	0
1	B	215/223 (96%)	-0.73	0	100 100	42, 53, 75, 106	0
2	C	155/179 (86%)	-0.28	7 (4%)	37 15	46, 70, 125, 150	0
All	All	582/625 (93%)	-0.56	7 (1%)	81 55	41, 59, 110, 150	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	54	SER	4.1
2	C	74	GLN	3.6
2	C	75	LEU	3.4
2	C	78	LEU	2.4
2	C	77	THR	2.2
2	C	50	SER	2.1
2	C	73	THR	2.0

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

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
6	GAL	A	1008	11/12	0.87	0.35	5.34	82,96,106,108	0
3	NAG	B	1001	14/15	0.97	0.12	-0.80	43,50,54,56	0
3	NAG	A	1007	14/15	0.94	0.17	-1.00	63,70,75,83	0
3	NAG	C	1001	14/15	0.96	0.12	-1.03	44,50,57,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	A	1001	14/15	0.98	0.15	-1.16	45,48,53,55	0
3	NAG	C	1008	14/15	0.92	0.14	-1.29	68,85,99,100	0
5	MAN	C	1011	11/12	0.84	0.55	-	131,152,160,162	0
5	MAN	C	1004	11/12	0.82	0.27	-	92,102,107,119	0
5	MAN	A	1004	11/12	0.95	0.27	-	70,88,101,116	0
3	NAG	A	1005	14/15	0.78	0.43	-	111,131,139,142	0
3	NAG	C	1006	14/15	0.87	0.28	-	112,131,136,144	0
3	NAG	B	1002	14/15	0.97	0.13	-	45,51,55,63	0
3	NAG	B	1005	14/15	0.85	0.35	-	97,112,117,121	0
3	NAG	C	1002	14/15	0.95	0.15	-	56,59,62,78	0
3	NAG	C	1009	14/15	0.91	0.25	-	84,102,112,124	0
5	MAN	C	1005	11/12	0.91	0.32	-	112,123,136,147	0
5	MAN	A	1006	11/12	0.94	0.21	-	57,62,66,69	0
5	MAN	B	1004	11/12	0.92	0.30	-	77,85,93,106	0
3	NAG	C	1012	14/15	0.71	0.52	-	130,144,152,154	0
3	NAG	B	1007	14/15	0.89	0.20	-	71,77,81,83	0
5	MAN	B	1006	11/12	0.95	0.13	-	61,70,75,75	0
3	NAG	A	1002	14/15	0.97	0.12	-	47,52,60,61	0
8	FUC	C	1007	10/11	0.93	0.39	-	77,91,95,95	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	GAL	A	1008	11/12	0.87	0.35	5.34	82,96,106,108	0
3	NAG	B	1001	14/15	0.97	0.12	-0.80	43,50,54,56	0
3	NAG	A	1007	14/15	0.94	0.17	-1.00	63,70,75,83	0
3	NAG	C	1001	14/15	0.96	0.12	-1.03	44,50,57,76	0
3	NAG	A	1001	14/15	0.98	0.15	-1.16	45,48,53,55	0
3	NAG	C	1008	14/15	0.92	0.14	-1.29	68,85,99,100	0
5	MAN	A	1006	11/12	0.94	0.21	-	57,62,66,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	MAN	B	1006	11/12	0.95	0.13	-	61,70,75,75	0
4	BMA	C	1003	11/12	0.92	0.16	-	72,100,111,114	0
5	MAN	C	1004	11/12	0.82	0.27	-	92,102,107,119	0
5	MAN	A	1004	11/12	0.95	0.27	-	70,88,101,116	0
3	NAG	A	1005	14/15	0.78	0.43	-	111,131,139,142	0
3	NAG	C	1006	14/15	0.87	0.28	-	112,131,136,144	0
3	NAG	B	1002	14/15	0.97	0.13	-	45,51,55,63	0
3	NAG	B	1005	14/15	0.85	0.35	-	97,112,117,121	0
3	NAG	C	1002	14/15	0.95	0.15	-	56,59,62,78	0
4	BMA	A	1003	11/12	0.97	0.17	-	57,60,73,79	0
4	BMA	C	1010	11/12	0.79	0.32	-	123,135,145,155	0
3	NAG	C	1009	14/15	0.91	0.25	-	84,102,112,124	0
5	MAN	C	1011	11/12	0.84	0.55	-	131,152,160,162	0
5	MAN	C	1005	11/12	0.91	0.32	-	112,123,136,147	0
7	CL	A	1009	1/1	0.93	0.14	-	64,64,64,64	0
5	MAN	B	1004	11/12	0.92	0.30	-	77,85,93,106	0
3	NAG	C	1012	14/15	0.71	0.52	-	130,144,152,154	0
4	BMA	B	1003	11/12	0.97	0.13	-	50,56,59,67	0
3	NAG	B	1007	14/15	0.89	0.20	-	71,77,81,83	0
3	NAG	A	1002	14/15	0.97	0.12	-	47,52,60,61	0
8	FUC	C	1007	10/11	0.93	0.39	-	77,91,95,95	0

6.5 Other polymers

There are no such residues in this entry.