Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:20 PM GMT

PDB ID	:	3WWG
Title	:	Crystal structure of the N-glycan-deficient variant N448A of isopullulanase complexed with isopanose
Authors	:	Miyazaki, T.; Yashiro, H.; Nishikawa, A.; Tonozuka, T.
Deposited on	:	2014-06-17
Resolution	:	2.20 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:

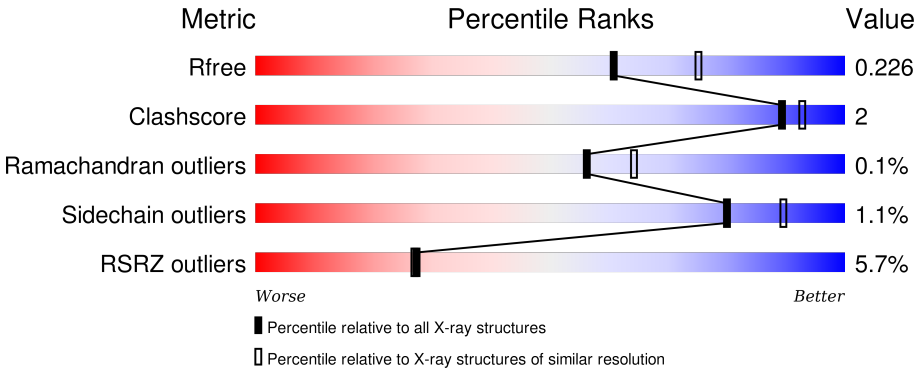
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	549	4% 92% 5%
1	B	549	6% 92% 7%
1	C	549	6% 92% 6%
1	D	549	7% 92% 6%

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
2	NAG	A	1001	-	-	-	X
2	NAG	A	1004	-	-	-	X
2	NAG	A	1005	-	-	-	X
2	NAG	A	1008	-	-	-	X
2	NAG	B	1001	-	-	-	X
2	NAG	B	1003	-	-	-	X
2	NAG	B	1004	-	-	-	X
2	NAG	B	1007	-	-	-	X
2	NAG	C	1002	-	-	-	X
2	NAG	C	1006	-	-	-	X
2	NAG	D	1001	-	-	-	X
2	NAG	D	1005	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17816 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.

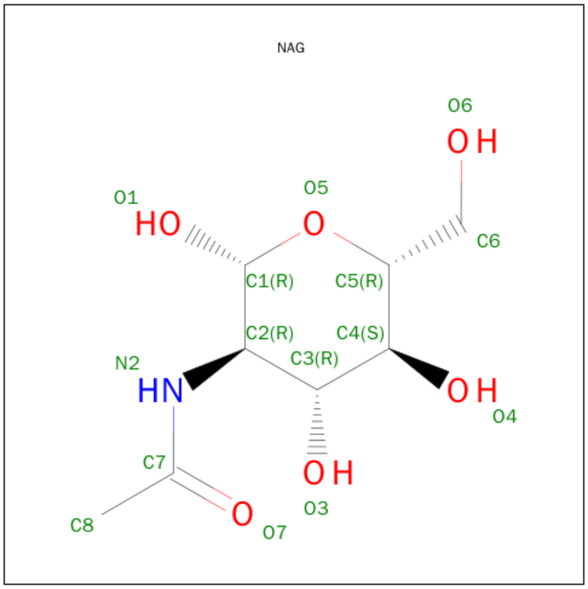
- Molecule 1 is a protein called Isopullulanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4148	2625	692	820	11			
1	B	542	Total	C	N	O	S	0	1	0
			4194	2650	699	834	11			
1	C	541	Total	C	N	O	S	0	0	0
			4186	2647	698	830	11			
1	D	540	Total	C	N	O	S	0	0	0
			4171	2633	697	830	11			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ARG	-	EXPRESSION TAG	UNP O00105
A	17	GLU	-	EXPRESSION TAG	UNP O00105
A	18	PHE	-	EXPRESSION TAG	UNP O00105
A	19	MET	-	EXPRESSION TAG	UNP O00105
A	448	ALA	ASN	ENGINEERED MUTATION	UNP O00105
B	16	ARG	-	EXPRESSION TAG	UNP O00105
B	17	GLU	-	EXPRESSION TAG	UNP O00105
B	18	PHE	-	EXPRESSION TAG	UNP O00105
B	19	MET	-	EXPRESSION TAG	UNP O00105
B	448	ALA	ASN	ENGINEERED MUTATION	UNP O00105
C	16	ARG	-	EXPRESSION TAG	UNP O00105
C	17	GLU	-	EXPRESSION TAG	UNP O00105
C	18	PHE	-	EXPRESSION TAG	UNP O00105
C	19	MET	-	EXPRESSION TAG	UNP O00105
C	448	ALA	ASN	ENGINEERED MUTATION	UNP O00105
D	16	ARG	-	EXPRESSION TAG	UNP O00105
D	17	GLU	-	EXPRESSION TAG	UNP O00105
D	18	PHE	-	EXPRESSION TAG	UNP O00105
D	19	MET	-	EXPRESSION TAG	UNP O00105
D	448	ALA	ASN	ENGINEERED MUTATION	UNP O00105

- Molecule 2 is SUGAR (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	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	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0

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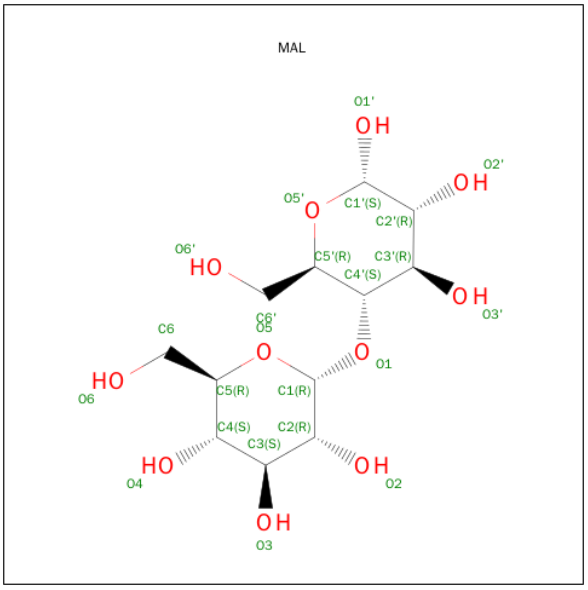
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	C	1	Total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

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total C O 23 12 11	0	0

- Molecule 4 is SUGAR (MALTOSE) (three-letter code: MAL) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 23 12 11	0	0

- Molecule 5 is water.

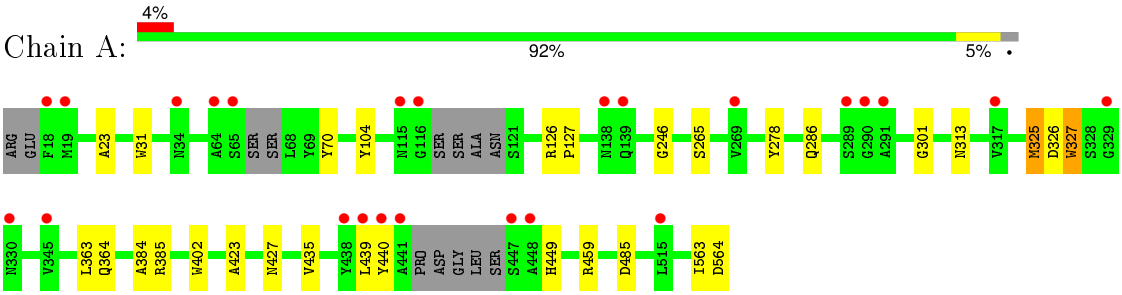
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	182	Total O 182 182	0	0
5	B	175	Total O 175 175	0	0
5	C	137	Total O 137 137	0	0
5	D	129	Total O 129 129	0	0

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.

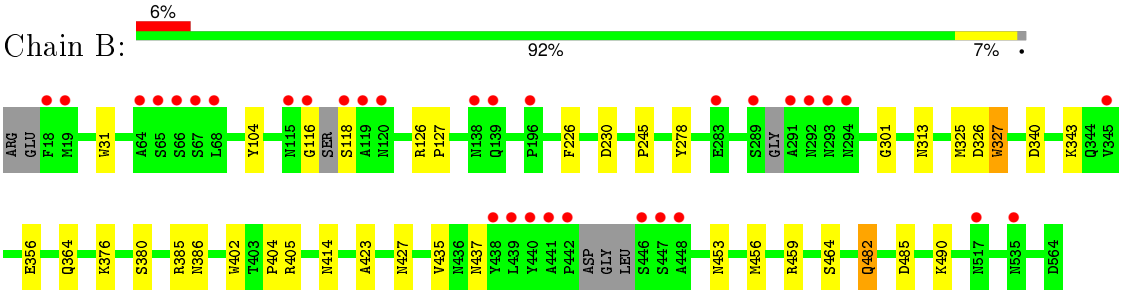
- Molecule 1: Isopullulanase

Chain A:



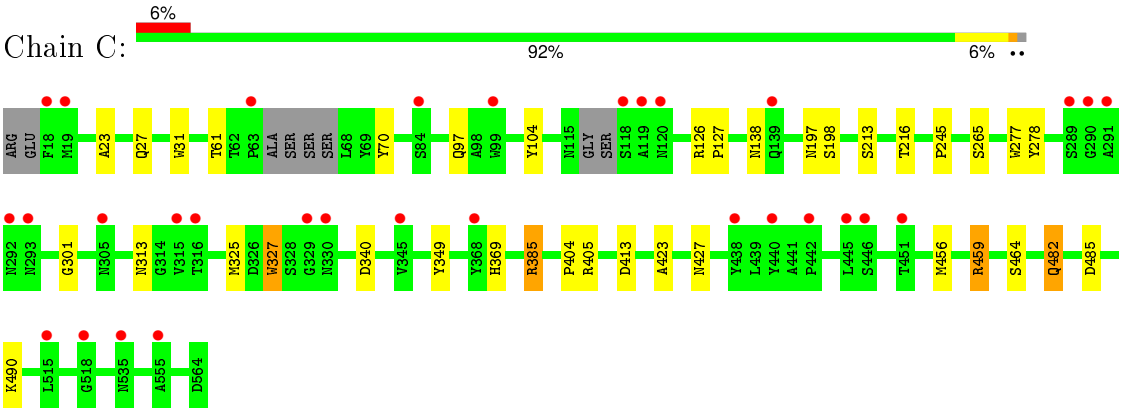
- Molecule 1: Isopullulanase

Chain B:



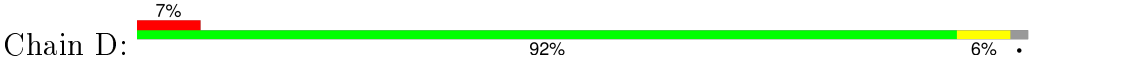
- Molecule 1: Isopullulanase

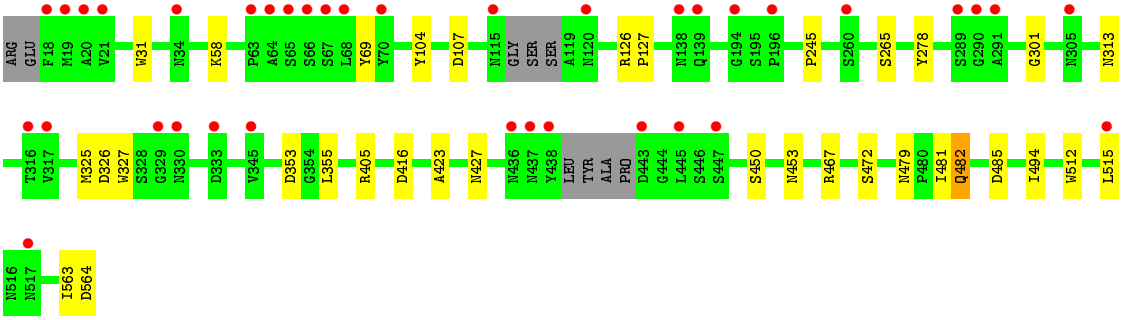
Chain C:



- Molecule 1: Isopullulanase

Chain D:




ARG GLU F18 M19 A20 V21 W31 N34 K58 P63 A64 S65 S66 S67 L68 Y69 Y70 Y104 D107 N115 GLY SER SER A119 N120 R126 P127 N138 Q139 G194 S195 P196 P245 S260 S265 Y278 S289 G290 A291 G301 N305 N313
T316 V317 M325 D326 W327 S328 G329 N330 D333 V345 D353 G354 L355 R405 D416 A423 N427 N436 N437 Y438 LEU TYR ALA PRO D443 G444 L445 S446 S447 S450 N453 R467 S472 N479 P480 I481 Q482 D485 I494 W512 L515
N516 N517 I563 D564

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.40Å 108.10Å 116.00Å 90.00° 103.90° 90.00°	Depositor
Resolution (Å)	34.04 – 2.20 34.04 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.4 (34.04-2.20) 97.4 (34.04-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.26 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.183 , 0.224 0.191 , 0.226	Depositor DCC
R_{free} test set	5738 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 33.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 114129 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17816	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.06% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GLC, BGC, NAG, MAL

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	0.39	0/4259	0.59	0/5825
1	B	0.39	0/4309	0.60	0/5894
1	C	0.37	0/4299	0.58	0/5882
1	D	0.37	0/4282	0.57	0/5857
All	All	0.38	0/17149	0.58	0/23458

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

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	4148	0	3895	17	0
1	B	4194	0	3938	22	0
1	C	4186	0	3931	20	0
1	D	4171	0	3915	21	0
2	A	112	0	104	0	0
2	B	98	0	91	1	0
2	C	126	0	117	0	0
2	D	112	0	104	1	0
3	B	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	23	0	22	0	0
5	A	182	0	0	2	0
5	B	175	0	0	0	0
5	C	137	0	0	0	0
5	D	129	0	0	0	0
All	All	17816	0	16138	79	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 2.

All (79) 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:B:405:ARG:H	1:B:482:GLN:HE21	1.38	0.72
1:B:386:ASN:HD22	1:B:414:ASN:HD22	1.37	0.69
1:D:325:MET:HE3	1:D:355:LEU:HD22	1.74	0.68
1:C:404:PRO:HB2	1:C:456:MET:HE3	1.75	0.67
1:B:386:ASN:ND2	1:B:414:ASN:HD22	1.94	0.66
1:D:127:PRO:HB3	1:D:416:ASP:OD2	2.00	0.61
1:C:197:ASN:ND2	1:C:213:SER:O	2.29	0.60
1:A:286:GLN:HG3	5:A:1134:HOH:O	2.04	0.57
1:C:301:GLY:HA3	1:C:327:TRP:CE2	2.39	0.56
1:D:325:MET:CE	1:D:355:LEU:HD22	2.36	0.55
1:D:450:SER:O	1:D:515:LEU:HA	2.06	0.55
1:B:453:ASN:HD22	1:B:456:MET:HE2	1.71	0.55
1:D:479:ASN:HD22	1:D:512:TRP:HE1	1.56	0.54
1:D:405:ARG:H	1:D:482:GLN:HE21	1.56	0.53
1:D:416:ASP:HB2	1:D:467:ARG:NH2	2.24	0.52
1:B:453:ASN:HD22	1:B:456:MET:CE	2.23	0.52
1:D:325:MET:HG2	1:D:326:ASP:N	2.25	0.52
1:C:459:ARG:HA	1:C:485:ASP:O	2.10	0.51
1:C:405:ARG:H	1:C:482:GLN:HE21	1.57	0.51
1:B:325:MET:O	1:B:326[B]:ASP:CG	2.49	0.51
1:B:301:GLY:HA3	1:B:327:TRP:CE2	2.46	0.50
1:D:563:ILE:O	1:D:564:ASP:HB2	2.12	0.49
1:C:198:SER:HB3	1:C:216:THR:HB	1.95	0.49
1:D:31:TRP:CZ3	1:D:245:PRO:HB3	2.47	0.49
1:B:116:GLY:O	1:B:118:SER:N	2.47	0.48
1:C:404:PRO:HB2	1:C:456:MET:CE	2.43	0.48
1:B:126:ARG:HA	1:B:127:PRO:C	2.33	0.48
1:A:325:MET:HG2	1:A:326:ASP:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:SER:HA	1:C:490:LYS:O	2.15	0.47
1:A:364:GLN:HA	1:A:385:ARG:O	2.14	0.47
1:D:301:GLY:HA3	1:D:327:TRP:CE2	2.50	0.47
1:C:31:TRP:CZ3	1:C:245:PRO:HB3	2.49	0.47
1:A:423:ALA:H	1:A:427:ASN:HD22	1.62	0.46
1:A:31:TRP:CD1	1:A:246:GLY:HA2	2.50	0.46
1:B:402:TRP:CZ2	1:B:435:VAL:HG21	2.51	0.45
1:A:23:ALA:HB2	1:A:70:TYR:CG	2.51	0.45
1:B:404:PRO:HD3	1:B:437:ASN:HD21	1.82	0.45
1:A:23:ALA:HB2	1:A:70:TYR:CD2	2.52	0.45
1:B:459:ARG:HA	1:B:485:ASP:O	2.16	0.45
1:A:402:TRP:CE2	1:A:435:VAL:HG21	2.52	0.45
1:A:449:HIS:HD2	5:A:1138:HOH:O	2.00	0.44
1:D:265:SER:HA	1:D:313:ASN:O	2.17	0.44
1:B:226:PHE:O	1:B:230:ASP:HB3	2.17	0.44
1:B:380:SER:HB2	2:B:1004:NAG:H82	1.97	0.44
1:D:58:LYS:HB3	1:D:69:TYR:HB3	1.99	0.44
1:C:423:ALA:H	1:C:427:ASN:ND2	2.15	0.44
1:C:97:GLN:HE22	1:C:369:HIS:CD2	2.35	0.44
1:D:325:MET:O	1:D:326:ASP:CG	2.55	0.44
1:A:126:ARG:HA	1:A:127:PRO:C	2.38	0.44
1:B:386:ASN:HD22	1:B:414:ASN:ND2	2.09	0.43
1:C:485:ASP:OD2	1:D:485:ASP:OD2	2.36	0.43
1:D:453:ASN:HA	2:D:1005:NAG:H82	1.99	0.43
1:C:126:ARG:HA	1:C:127:PRO:C	2.39	0.43
1:A:363:LEU:O	1:A:384:ALA:HA	2.19	0.43
1:D:423:ALA:H	1:D:427:ASN:HD22	1.65	0.43
1:D:325:MET:HE3	1:D:355:LEU:HB3	2.00	0.42
1:A:301:GLY:HA3	1:A:327:TRP:CE2	2.53	0.42
1:A:439:LEU:HD22	1:A:440:TYR:CZ	2.53	0.42
1:C:277:TRP:CD1	1:C:349:TYR:HB3	2.54	0.42
1:C:27:GLN:OE1	1:C:61:THR:HG21	2.19	0.42
1:B:31:TRP:CZ3	1:B:245:PRO:HB3	2.54	0.42
1:C:385:ARG:HA	1:C:413:ASP:O	2.19	0.42
1:B:356:GLU:OE2	1:B:376:LYS:NZ	2.48	0.42
1:C:23:ALA:HB2	1:C:70:TYR:CG	2.55	0.42
1:A:459:ARG:HA	1:A:485:ASP:O	2.19	0.42
1:A:563:ILE:O	1:A:564:ASP:HB2	2.19	0.42
1:B:464:SER:HA	1:B:490:LYS:O	2.20	0.42
1:D:481:ILE:HG22	1:D:512:TRP:CH2	2.56	0.41
1:B:423:ALA:H	1:B:427:ASN:ND2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ALA:H	1:A:427:ASN:ND2	2.17	0.41
1:B:364:GLN:HA	1:B:385:ARG:O	2.21	0.41
1:A:265:SER:HA	1:A:313:ASN:O	2.21	0.41
1:B:405:ARG:N	1:B:482:GLN:HE21	2.13	0.41
1:D:472:SER:HB3	1:D:494:ILE:HG23	2.02	0.41
1:D:126:ARG:HA	1:D:127:PRO:C	2.41	0.40
1:C:423:ALA:H	1:C:427:ASN:HD22	1.68	0.40
1:C:265:SER:HA	1:C:313:ASN:O	2.21	0.40
1:B:313:ASN:HA	1:B:340:ASP:O	2.20	0.40
1:C:313:ASN:HA	1:C:340:ASP:O	2.22	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	528/549 (96%)	501 (95%)	27 (5%)	0	100	100
1	B	535/549 (97%)	507 (95%)	28 (5%)	0	100	100
1	C	535/549 (97%)	504 (94%)	31 (6%)	0	100	100
1	D	534/549 (97%)	497 (93%)	35 (7%)	2 (0%)	39	42
All	All	2132/2196 (97%)	2009 (94%)	121 (6%)	2 (0%)	56	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	107	ASP
1	D	353	ASP

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	453/465 (97%)	449 (99%)	4 (1%)	84 92
1	B	461/465 (99%)	456 (99%)	5 (1%)	80 89
1	C	459/465 (99%)	451 (98%)	8 (2%)	68 81
1	D	458/465 (98%)	455 (99%)	3 (1%)	88 94
All	All	1831/1860 (98%)	1811 (99%)	20 (1%)	80 89

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	TYR
1	A	278	TYR
1	A	325	MET
1	A	327	TRP
1	B	104	TYR
1	B	278	TYR
1	B	327	TRP
1	B	343	LYS
1	B	482	GLN
1	C	104	TYR
1	C	138	ASN
1	C	278	TYR
1	C	325	MET
1	C	327	TRP
1	C	385	ARG
1	C	459	ARG
1	C	482	GLN
1	D	104	TYR
1	D	278	TYR
1	D	482	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	427	ASN
1	A	449	HIS
1	A	516	ASN
1	B	51	GLN
1	B	88	GLN
1	B	106	HIS
1	B	122	ASN
1	B	323	ASN
1	B	351	GLN
1	B	386	ASN
1	B	427	ASN
1	B	437	ASN
1	B	482	GLN
1	C	51	GLN
1	C	120	ASN
1	C	386	ASN
1	C	414	ASN
1	C	427	ASN
1	C	482	GLN
1	C	516	ASN
1	D	51	GLN
1	D	88	GLN
1	D	192	GLN
1	D	323	ASN
1	D	386	ASN
1	D	427	ASN
1	D	479	ASN
1	D	482	GLN
1	D	486	ASN

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

2 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	BGC	B	1008	3	12,12,12	0.47	0	17,17,17	0.79	0
3	GLC	B	1009	3	11,11,12	0.56	0	14,15,17	1.10	1 (7%)

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	BGC	B	1008	3	-	0/2/22/22	0/1/1/1
3	GLC	B	1009	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1009	GLC	C1-C2-C3	3.04	113.14	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

33 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	1001	1	14,14,15	0.46	0	15,19,21	0.67	0
2	NAG	A	1002	1	14,14,15	0.44	0	15,19,21	1.24	2 (13%)
2	NAG	A	1003	1	14,14,15	0.57	0	15,19,21	0.96	1 (6%)
2	NAG	A	1004	1	14,14,15	0.38	0	15,19,21	0.96	1 (6%)
2	NAG	A	1005	1	14,14,15	0.52	0	15,19,21	0.94	0
2	NAG	A	1006	1	14,14,15	0.55	0	15,19,21	1.09	1 (6%)
2	NAG	A	1007	1	14,14,15	0.57	0	15,19,21	0.79	0
2	NAG	A	1008	1	14,14,15	0.54	0	15,19,21	2.21	4 (26%)
2	NAG	B	1001	1	14,14,15	0.61	0	15,19,21	1.22	1 (6%)
2	NAG	B	1002	1	14,14,15	0.59	0	15,19,21	1.45	3 (20%)
2	NAG	B	1003	1	14,14,15	0.59	0	15,19,21	1.10	1 (6%)
2	NAG	B	1004	1	14,14,15	0.51	0	15,19,21	1.24	1 (6%)
2	NAG	B	1005	1	14,14,15	0.56	0	15,19,21	1.12	1 (6%)
2	NAG	B	1006	1	14,14,15	0.55	0	15,19,21	0.83	0
2	NAG	B	1007	1	14,14,15	0.48	0	15,19,21	1.76	1 (6%)
2	NAG	C	1001	1	14,14,15	0.62	0	15,19,21	0.87	0
2	NAG	C	1002	1	14,14,15	0.46	0	15,19,21	1.33	1 (6%)
2	NAG	C	1003	1	14,14,15	0.56	0	15,19,21	0.70	0
2	NAG	C	1004	1	14,14,15	0.71	0	15,19,21	1.19	1 (6%)
2	NAG	C	1005	1	14,14,15	0.43	0	15,19,21	0.88	0
2	NAG	C	1006	1	14,14,15	0.47	0	15,19,21	1.35	1 (6%)
2	NAG	C	1007	1	14,14,15	0.55	0	15,19,21	1.07	1 (6%)
2	NAG	C	1008	1	14,14,15	0.47	0	15,19,21	1.40	2 (13%)
2	NAG	C	1009	1	14,14,15	0.44	0	15,19,21	1.99	2 (13%)
4	MAL	C	1010	-	24,24,24	0.49	0	35,35,35	0.90	2 (5%)
2	NAG	D	1001	1	14,14,15	0.55	0	15,19,21	1.07	0
2	NAG	D	1002	1	14,14,15	0.46	0	15,19,21	0.77	0
2	NAG	D	1003	1	14,14,15	0.53	0	15,19,21	1.16	1 (6%)
2	NAG	D	1004	1	14,14,15	0.48	0	15,19,21	1.03	1 (6%)
2	NAG	D	1005	1	14,14,15	0.38	0	15,19,21	1.56	3 (20%)
2	NAG	D	1006	1	14,14,15	0.52	0	15,19,21	0.99	0
2	NAG	D	1007	1	14,14,15	0.47	0	15,19,21	1.32	1 (6%)
2	NAG	D	1008	1	14,14,15	0.54	0	15,19,21	0.90	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	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1003	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1004	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1005	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1008	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1003	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1004	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1005	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1006	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1007	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1002	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1003	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1004	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1005	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1006	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1007	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1008	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1009	1	-	0/6/23/26	0/1/1/1
4	MAL	C	1010	-	-	0/8/48/48	0/2/2/2
2	NAG	D	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1002	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1003	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1004	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1005	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1006	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1007	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1008	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1008	NAG	C4-C3-C2	-2.60	107.18	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1009	NAG	C4-C3-C2	-2.36	107.56	111.23
2	B	1005	NAG	C4-C3-C2	-2.26	107.72	111.23
2	D	1008	NAG	O7-C7-C8	-2.23	117.97	122.06
2	B	1002	NAG	C4-C3-C2	-2.13	107.91	111.23
2	C	1007	NAG	O7-C7-C8	-2.11	118.18	122.06
2	C	1008	NAG	C6-C5-C4	-2.04	107.98	113.02
2	D	1005	NAG	C6-C5-C4	-2.02	108.04	113.02
2	A	1002	NAG	C8-C7-N2	2.02	119.98	116.11
2	A	1004	NAG	O5-C5-C6	2.26	112.24	107.35
2	D	1004	NAG	C1-O5-C5	2.28	115.14	112.25
2	A	1003	NAG	C1-O5-C5	2.32	115.20	112.25
2	D	1005	NAG	C3-C4-C5	2.34	114.28	110.20
4	C	1010	MAL	O5'-C5'-C4'	2.37	114.75	109.75
2	B	1002	NAG	C2-N2-C7	2.42	126.15	123.04
2	A	1006	NAG	C1-O5-C5	2.76	115.75	112.25
2	B	1001	NAG	C1-O5-C5	2.82	115.83	112.25
2	A	1008	NAG	C8-C7-N2	2.83	121.53	116.11
4	C	1010	MAL	C1'-O5'-C5'	2.85	118.73	113.47
2	B	1003	NAG	C1-O5-C5	3.00	116.06	112.25
2	D	1007	NAG	C1-O5-C5	3.08	116.16	112.25
2	C	1004	NAG	C1-O5-C5	3.24	116.36	112.25
2	B	1002	NAG	C8-C7-N2	3.29	122.39	116.11
2	A	1002	NAG	C1-O5-C5	3.56	116.76	112.25
2	C	1008	NAG	C1-O5-C5	3.69	116.93	112.25
2	D	1003	NAG	C1-O5-C5	3.78	117.05	112.25
2	B	1004	NAG	C1-O5-C5	3.79	117.06	112.25
2	C	1002	NAG	C1-O5-C5	4.13	117.49	112.25
2	C	1006	NAG	C1-O5-C5	4.19	117.56	112.25
2	D	1005	NAG	C1-O5-C5	4.24	117.63	112.25
2	A	1008	NAG	C2-N2-C7	4.28	128.53	123.04
2	A	1008	NAG	C1-O5-C5	5.47	119.19	112.25
2	B	1007	NAG	C1-O5-C5	6.00	119.86	112.25
2	C	1009	NAG	C1-O5-C5	6.79	120.87	112.25

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
2	B	1004	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1005	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, 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	536/549 (97%)	0.00	24 (4%)	37	36	17, 25, 45, 78	0
1	B	542/549 (98%)	0.06	32 (5%)	26	25	16, 26, 50, 72	0
1	C	541/549 (98%)	0.18	31 (5%)	27	27	18, 29, 53, 79	0
1	D	540/549 (98%)	0.30	37 (6%)	20	19	18, 30, 59, 83	0
All	All	2159/2196 (98%)	0.14	124 (5%)	27	27	16, 27, 53, 83	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	330	ASN	7.9
1	D	443	ASP	7.2
1	D	138	ASN	7.0
1	A	438	TYR	6.5
1	C	438	TYR	6.5
1	B	119	ALA	6.2
1	D	18	PHE	6.1
1	C	290	GLY	6.0
1	A	330	ASN	6.0
1	C	535	ASN	5.7
1	D	19	MET	5.7
1	A	290	GLY	5.5
1	A	441	ALA	5.4
1	B	118	SER	5.2
1	A	440	TYR	4.9
1	D	196	PRO	4.7
1	D	438	TYR	4.6
1	D	437	ASN	4.5
1	B	120	ASN	4.5
1	A	139	GLN	4.4
1	B	438	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	139	GLN	4.3
1	D	329	GLY	4.3
1	B	18	PHE	4.3
1	D	436	ASN	4.2
1	B	116	GLY	4.2
1	D	291	ALA	4.0
1	C	119	ALA	4.0
1	D	21	VAL	3.9
1	A	18	PHE	3.9
1	C	305	ASN	3.9
1	A	447	SER	3.8
1	C	329	GLY	3.8
1	C	291	ALA	3.8
1	A	291	ALA	3.8
1	D	68	LEU	3.8
1	C	139	GLN	3.8
1	B	115	ASN	3.7
1	D	65	SER	3.7
1	B	68	LEU	3.7
1	B	139	GLN	3.6
1	C	440	TYR	3.6
1	D	330	ASN	3.6
1	A	34	ASN	3.5
1	C	18	PHE	3.5
1	C	63	PRO	3.5
1	A	65	SER	3.5
1	D	66	SER	3.5
1	A	115	ASN	3.4
1	D	64	ALA	3.4
1	B	289	SER	3.4
1	C	118	SER	3.4
1	B	448	ALA	3.4
1	D	20	ALA	3.4
1	B	19	MET	3.3
1	B	293	ASN	3.3
1	B	138	ASN	3.2
1	D	289	SER	3.2
1	A	448	ALA	3.2
1	D	115	ASN	3.1
1	A	329	GLY	3.1
1	A	19	MET	3.1
1	C	515	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	34	ASN	3.0
1	B	345	VAL	3.0
1	B	67	SER	3.0
1	B	535	ASN	2.9
1	B	440	TYR	2.9
1	C	19	MET	2.9
1	D	63	PRO	2.8
1	B	65	SER	2.8
1	B	292	ASN	2.8
1	D	67	SER	2.7
1	B	517	ASN	2.7
1	C	289	SER	2.7
1	C	345	VAL	2.6
1	A	439	LEU	2.6
1	B	294	ASN	2.6
1	B	66	SER	2.5
1	A	289	SER	2.5
1	D	317	VAL	2.5
1	D	120	ASN	2.5
1	A	345	VAL	2.5
1	D	290	GLY	2.4
1	A	116	GLY	2.4
1	A	515	LEU	2.4
1	C	518	GLY	2.4
1	D	515	LEU	2.4
1	D	345	VAL	2.4
1	A	138	ASN	2.4
1	B	291	ALA	2.4
1	B	446	SER	2.4
1	B	64	ALA	2.3
1	B	447	SER	2.3
1	B	439	LEU	2.3
1	C	315	VAL	2.2
1	C	446	SER	2.2
1	D	333	ASP	2.2
1	D	447	SER	2.2
1	A	64	ALA	2.2
1	B	441	ALA	2.2
1	C	99	TRP	2.1
1	C	84	SER	2.1
1	D	316	THR	2.1
1	A	269	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	445	LEU	2.1
1	C	368	TYR	2.1
1	D	305	ASN	2.1
1	C	442	PRO	2.1
1	C	445	LEU	2.1
1	C	451	THR	2.1
1	D	70	TYR	2.1
1	C	293	ASN	2.1
1	B	283	GLU	2.1
1	B	196	PRO	2.1
1	A	317	VAL	2.1
1	C	316	THR	2.1
1	D	517	ASN	2.1
1	C	555	ALA	2.1
1	D	260	SER	2.1
1	C	120	ASN	2.0
1	C	292	ASN	2.0
1	D	194	GLY	2.0
1	B	442	PRO	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	BGC	B	1008	12/12	0.85	0.22	0.99	60,63,65,67	0
3	GLC	B	1009	11/12	0.65	0.27	-	66,71,74,75	0

6.4 Ligands (i)

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

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
2	NAG	B	1001	14/15	0.76	0.31	13.16	48,56,66,67	0
2	NAG	D	1001	14/15	0.70	0.28	10.23	61,63,65,66	0
2	NAG	B	1007	14/15	0.88	0.27	6.26	51,54,56,58	0
2	NAG	C	1002	14/15	0.92	0.22	6.21	34,37,40,41	0
2	NAG	B	1003	14/15	0.89	0.17	4.72	41,44,46,46	0
2	NAG	A	1001	14/15	0.80	0.18	4.56	43,44,47,48	0
2	NAG	C	1006	14/15	0.77	0.42	4.34	47,54,57,57	0
2	NAG	A	1008	14/15	0.83	0.37	3.47	46,50,53,54	0
2	NAG	D	1005	14/15	0.68	0.36	3.34	47,60,63,64	0
2	NAG	A	1005	14/15	0.84	0.29	2.65	41,44,47,48	0
2	NAG	B	1004	14/15	0.90	0.21	2.11	42,45,52,53	0
2	NAG	A	1004	14/15	0.88	0.21	2.10	41,46,48,49	0
2	NAG	C	1003	14/15	0.67	0.33	1.88	76,80,82,82	0
4	MAL	C	1010	23/23	0.85	0.23	1.84	43,48,52,52	0
2	NAG	C	1001	14/15	0.79	0.22	1.76	45,52,60,60	0
2	NAG	C	1005	14/15	0.86	0.22	1.74	45,51,55,56	0
2	NAG	D	1004	14/15	0.87	0.23	1.73	44,49,53,55	0
2	NAG	C	1004	14/15	0.86	0.21	1.71	39,44,46,47	0
2	NAG	A	1003	14/15	0.90	0.18	0.67	33,34,36,36	0
2	NAG	D	1008	14/15	0.94	0.10	-0.60	30,31,36,38	0
2	NAG	A	1006	14/15	0.97	0.11	-0.86	18,19,19,20	0
2	NAG	C	1007	14/15	0.98	0.11	-1.06	20,21,22,23	0
2	NAG	B	1005	14/15	0.98	0.10	-1.08	20,20,21,21	0
2	NAG	D	1006	14/15	0.97	0.09	-2.14	20,21,22,22	0
2	NAG	A	1007	14/15	0.93	0.22	-	31,33,38,40	0
2	NAG	B	1002	14/15	0.95	0.21	-	35,37,40,44	0
2	NAG	D	1002	14/15	0.94	0.24	-	38,42,45,47	0
2	NAG	C	1009	14/15	0.78	0.31	-	59,62,64,64	0
2	NAG	B	1006	14/15	0.89	0.21	-	32,36,39,43	0
2	NAG	C	1008	14/15	0.87	0.23	-	32,39,44,48	0
2	NAG	A	1002	14/15	0.94	0.20	-	37,40,41,42	0
2	NAG	D	1003	14/15	0.82	0.26	-	52,55,56,56	0
2	NAG	D	1007	14/15	0.89	0.19	-	31,38,41,44	0

6.5 Other polymers

There are no such residues in this entry.