wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 06:34 PM GMT

PDB ID	:	1BHG
Title	:	HUMAN BETA-GLUCURONIDASE AT 2.6 A RESOLUTION
Authors	:	Jain, S.; Drendel, W.B.
Deposited on	:	1996-03-04
Resolution	:	2.53 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i)) were used in the production of this report:

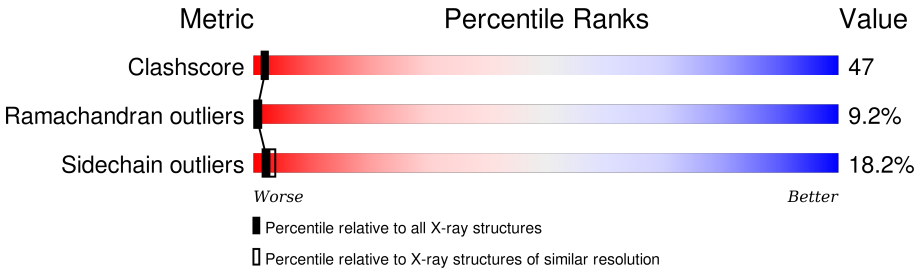
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.53 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))
Clashscore	102246	4968 (2.54-2.50)
Ramachandran outliers	100387	4873 (2.54-2.50)
Sidechain outliers	100360	4875 (2.54-2.50)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	613	32% 49% 16% •
1	B	613	29% 51% 18% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10190 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 BETA-GLUCURONIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4990	3216	848	911	15			
1	B	611	Total	C	N	O	S	0	0	0
			4990	3216	848	911	15			

- Molecule 2 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	9	Total	C	N	O	0	0
			105	58	2	45		
2	B	9	Total	C	N	O	0	0
			105	58	2	45		

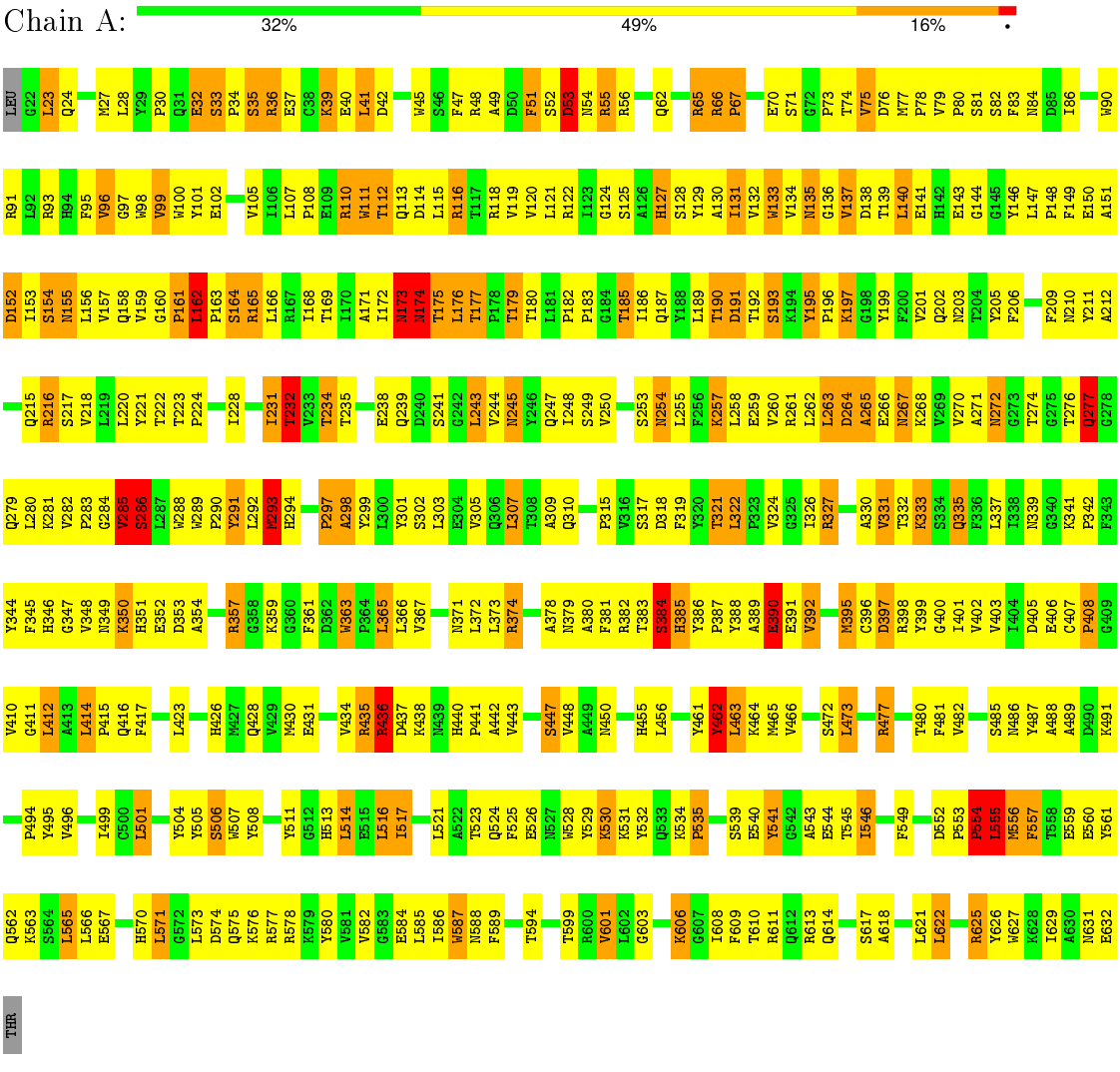
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

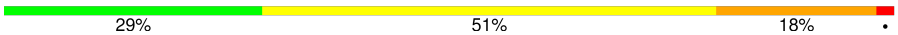
- Molecule 1: BETA-GLUCURONIDASE

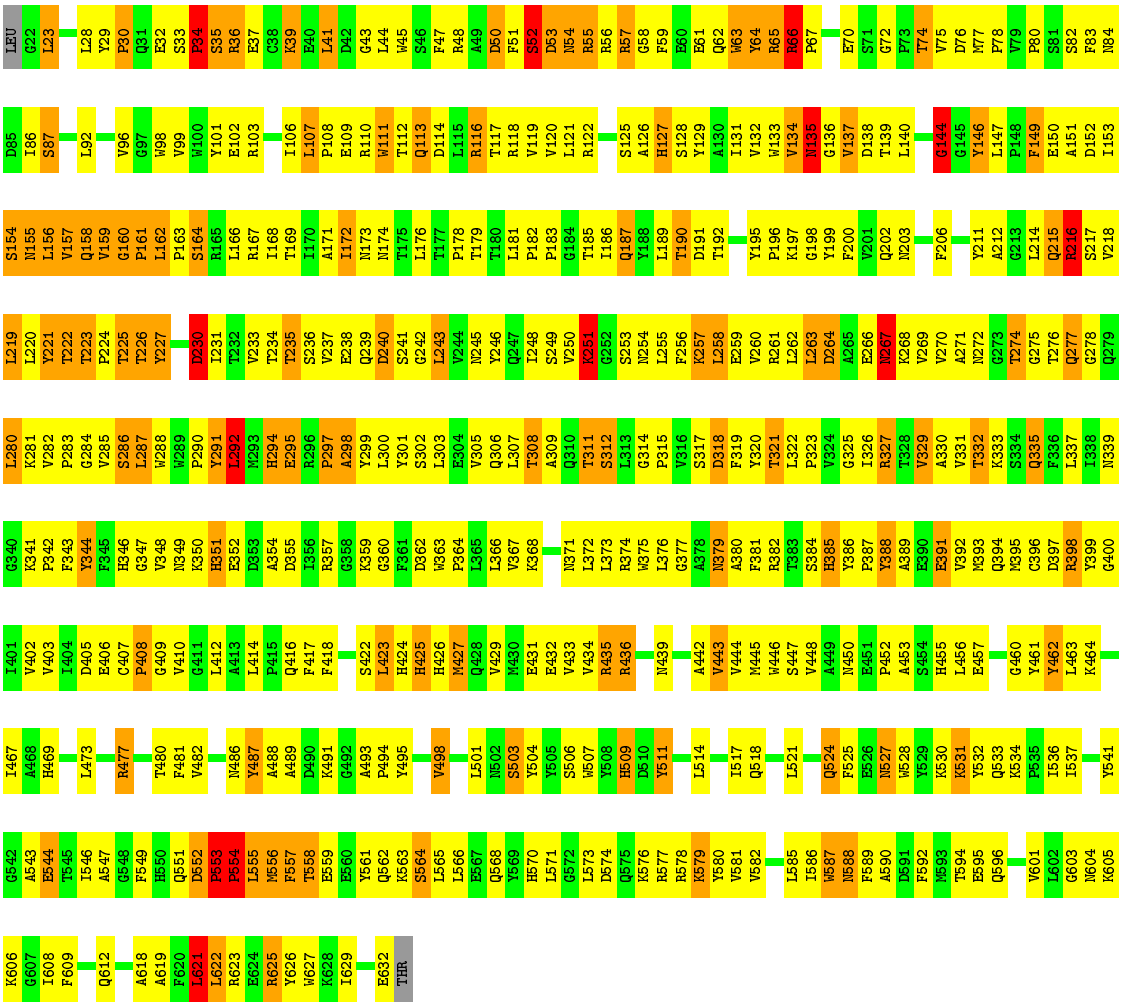
Chain A:



- Molecule 1: BETA-GLUCURONIDASE

Chain B:




LEU G22 L23 L28 Y29 P30 Q31 E32 S33 P34 S35 R36 E37 C38 K39 E40 L41 D42 G43 L44 W45 S46 F47 R48 A49 D50 F51 S52 D53 N54 R55 R56 R57 G58 F59 E60 E61 Q62 W63 Y64 R65 R66 P67 E70 S71 G72 P73 T74 V75 D76 M77 P78 V79 P80 S81 S82 F83 N84
D85 I86 S87 L92 V96 G97 W98 V99 W100 Y101 E102 R103 I106 L107 P108 E109 R110 W111 T112 Q113 D114 L115 R116 T117 R118 V119 V120 L121 R122 S125 A126 H127 S128 Y129 A130 I131 V132 W133 V134 N135 G136 V137 D138 T139 L140 G144 G145 Y146 L147 P148 F149 E150 A151 D152 I153
S154 N155 L156 V157 Q158 V159 G160 P161 L162 P163 S164 R165 L166 R167 I168 T169 I170 A171 I172 N173 N174 T175 L176 T177 P178 T179 T180 L181 P182 P183 G184 T185 I186 Q187 Y188 L189 T190 D191 T192 Y195 P196 K197 G198 Y199 F200 V201 Q202 N203 F206 Y211 A212 G213 L214 Q215 R216 S217 V218
L219 L220 Y221 T222 T223 P224 T225 T226 Y227 D230 I231 T232 Y233 T234 T235 S236 V237 E238 Q239 D240 S241 G242 L243 V244 N245 Y246 Q247 I248 S249 V250 K251 C252 S253 N254 L255 F256 K257 L258 E259 V260 R261 L262 D264 A265 E266 N267 K268 V269 V270 A271 N272 G273 T274 G275 T276 Q277 G278 Q279
L280 K281 V282 P283 G284 V285 S286 L287 W288 W289 P290 Y291 L292 M293 H294 E295 R296 P297 A298 Y299 L300 Y301 S302 L303 E304 V305 Q306 L307 T308 A309 Q310 T311 S312 L313 G314 P315 V316 S317 D318 F319 Y320 T321 L322 P323 V324 G325 I326 R327 T328 V329 A330 V331 T332 K333 S334 Q335 F336 L337 I338 N339
G340 K341 P342 F343 Y344 F345 H346 G347 V348 N349 K350 H351 E352 D353 A354 D355 I356 R357 G358 K359 G360 F361 D362 W363 P364 L365 I366 V367 K368 N371 I372 I373 R374 W375 L376 G377 A378 N379 A380 F381 R382 T383 S384 H385 Y386 P387 Y388 A389 E390 E391 V392 N393 Q394 M395 C396 D397 R398 Y399 G400
I401 V402 V403 I404 D405 E406 C407 P408 G409 V410 G411 L412 A413 L414 P415 Q416 F417 F418 S422 L423 H424 H425 H426 M427 Q428 V429 M430 E431 E432 V433 V434 R435 R436 N439 A442 V443 V444 M445 W446 S447 V448 A449 N450 E451 P452 A453 S454 H455 L456 E457 G460 Y461 Y462 L463 K464
I467 A468 H469 L473 R477 T480 F481 V482 N486 Y487 A488 A489 D490 K491 G492 A493 P494 Y495 V498 L501 N502 S503 Y504 Y505 S506 W507 Y508 H509 D510 Y511 L514 I517 Q518 L521 Q524 F525 E526 N527 W528 Y529 K530 K531 Y532 Q533 K534 P535 I536 I537 Y541
G542 A543 E544 T545 I546 A547 G548 F549 H550 Q551 D552 P553 P554 L555 M556 F557 T558 E559 E560 Y561 Q562 K563 S564 L565 L566 E567 Q568 Y569 H570 L571 G572 L573 D574 Q575 K576 R577 R578 K579 Y580 V581 V582 L585 I586 W587 N588 F589 A590 D591 F592 K593 T594 E595 Q596 V601 L602 G603 N604 K605
K606 G607 I608 F609 Q612 A618 A619 F620 L621 L622 R623 E624 R625 Y626 W627 K628 I629 E632 THR

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	95.10Å 124.40Å 134.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.53	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.53)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.231 , 0.310	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10190	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.72	0/5139	0.97	13/7000 (0.2%)
1	B	0.74	0/5139	0.97	4/7000 (0.1%)
All	All	0.73	0/10278	0.97	17/14000 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	2
All	All	0	7

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	436	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	A	140	LEU	CA-CB-CG	8.29	134.36	115.30
1	A	216	ARG	NE-CZ-NH2	7.85	124.23	120.30
1	B	144	GLY	N-CA-C	6.86	130.26	113.10
1	B	23	LEU	CA-CB-CG	6.12	129.37	115.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	436	ARG	Sidechain
1	A	462	TYR	Sidechain
1	A	511	TYR	Sidechain
1	A	541	TYR	Sidechain

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	4990	0	4846	424	0
1	B	4990	0	4845	518	0
2	A	105	0	88	4	0
2	B	105	0	88	7	0
All	All	10190	0	9867	945	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 47.

The worst 5 of 945 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:118:ARG:HH21	1:B:153:ILE:HA	1.25	0.99
1:A:107:LEU:HG	1:A:156:LEU:HD21	1.42	0.99
1:A:156:LEU:HD11	1:A:166:LEU:HD13	1.43	0.99
1:B:146:TYR:HB3	1:B:216:ARG:HH22	1.30	0.97
1:B:162:LEU:HB2	1:B:163:PRO:HD3	1.48	0.94

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	609/613 (99%)	462 (76%)	99 (16%)	48 (8%)	1 1
1	B	609/613 (99%)	442 (73%)	103 (17%)	64 (10%)	1 0
All	All	1218/1226 (99%)	904 (74%)	202 (17%)	112 (9%)	1 0

5 of 112 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	SER
1	A	35	SER
1	A	52	SER
1	A	115	LEU
1	A	137	VAL

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	540/542 (100%)	445 (82%)	95 (18%)	2 3
1	B	540/542 (100%)	438 (81%)	102 (19%)	2 3
All	All	1080/1084 (100%)	883 (82%)	197 (18%)	2 3

5 of 197 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	599	THR
1	B	76	ASP
1	B	544	GLU
1	A	606	LYS
1	B	39	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	570	HIS
1	B	158	GLN
1	B	524	GLN
1	B	127	HIS
1	B	187	GLN

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

18 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	$\#\|Z\| > 2$
2	NAG	A	651	1,2	14,14,15	0.83	1 (7%)	15,19,21	1.13	2 (13%)
2	NAG	A	652	2	14,14,15	0.56	0	15,19,21	0.63	0
2	BMA	A	653	2	11,11,12	0.39	0	14,15,17	1.16	2 (14%)
2	MAN	A	654	2	11,11,12	0.89	1 (9%)	14,15,17	0.74	0
2	MAN	A	655	2	11,11,12	0.58	0	14,15,17	0.59	0
2	MAN	A	656	2	11,11,12	0.64	0	14,15,17	1.77	2 (14%)
2	MAN	A	657	2	11,11,12	0.65	0	14,15,17	0.92	0
2	MAN	A	658	2	11,11,12	0.76	0	14,15,17	0.88	1 (7%)
2	MAN	A	659	2	11,11,12	0.49	0	14,15,17	1.03	1 (7%)
2	NAG	B	651	1,2	14,14,15	0.86	1 (7%)	15,19,21	0.48	0
2	NAG	B	652	2	14,14,15	0.57	0	15,19,21	0.72	0
2	BMA	B	653	2	11,11,12	0.68	0	14,15,17	0.88	0
2	MAN	B	654	2	11,11,12	0.54	0	14,15,17	1.34	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	B	655	2	11,11,12	0.36	0	14,15,17	0.85	1 (7%)
2	MAN	B	656	2	11,11,12	0.49	0	14,15,17	1.07	1 (7%)
2	MAN	B	657	2	11,11,12	0.56	0	14,15,17	1.11	1 (7%)
2	MAN	B	658	2	11,11,12	0.63	0	14,15,17	0.93	1 (7%)
2	MAN	B	659	2	11,11,12	0.61	0	14,15,17	0.74	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
2	NAG	A	651	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	652	2	-	0/6/23/26	0/1/1/1
2	BMA	A	653	2	-	0/2/19/22	0/1/1/1
2	MAN	A	654	2	-	0/2/19/22	0/1/1/1
2	MAN	A	655	2	-	0/2/19/22	0/1/1/1
2	MAN	A	656	2	-	0/2/19/22	0/1/1/1
2	MAN	A	657	2	-	0/2/19/22	0/1/1/1
2	MAN	A	658	2	-	0/2/19/22	0/1/1/1
2	MAN	A	659	2	-	0/2/19/22	1/1/1/1
2	NAG	B	651	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	652	2	-	0/6/23/26	0/1/1/1
2	BMA	B	653	2	-	0/2/19/22	0/1/1/1
2	MAN	B	654	2	-	0/2/19/22	0/1/1/1
2	MAN	B	655	2	-	0/2/19/22	0/1/1/1
2	MAN	B	656	2	-	0/2/19/22	0/1/1/1
2	MAN	B	657	2	-	0/2/19/22	0/1/1/1
2	MAN	B	658	2	-	0/2/19/22	0/1/1/1
2	MAN	B	659	2	-	0/2/19/22	1/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	654	MAN	C2-C3	2.10	1.55	1.52
2	B	651	NAG	C1-C2	2.22	1.55	1.52
2	A	651	NAG	C1-C2	2.46	1.55	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	653	BMA	C1-C2-C3	-2.79	106.24	109.54
2	A	651	NAG	C2-N2-C7	-2.49	119.83	123.04
2	A	653	BMA	O5-C1-C2	-2.36	107.03	110.86
2	B	654	MAN	C1-C2-C3	-2.16	106.99	109.54
2	A	658	MAN	C1-O5-C5	2.11	114.93	112.25

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	659	MAN	C1-C2-C3-C4-C5-O5
2	A	659	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	655	MAN	1	0
2	A	659	MAN	3	0
2	B	651	NAG	5	0
2	B	655	MAN	1	0
2	B	658	MAN	1	0

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.