



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:32 PM UTC

PDB ID : 6EZS / pdb_00006ezs
Title : Crystal structure of GH20 Exo beta-N-Acetylglucosaminidase from *Vibrio harveyi* in complex with N-acetylglucosamine
Authors : Porfetye, A.T.; Meekrathok, P.; Burger, M.; Vetter, I.R.; Suginta, W.
Deposited on : 2017-11-16
Resolution : 2.50 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

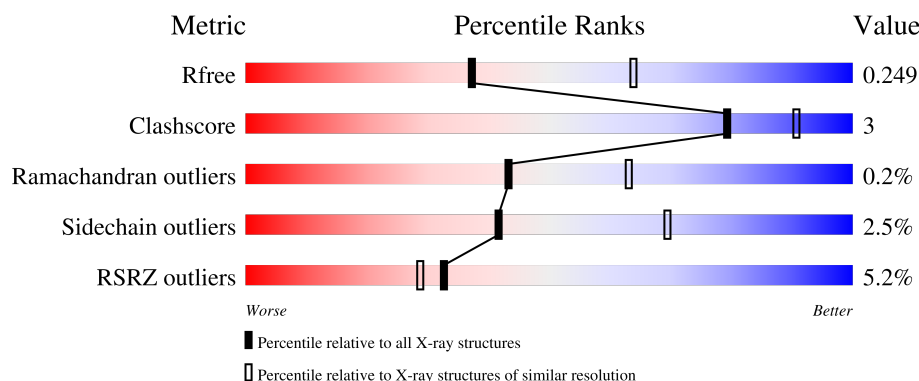
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	652	5% 88% 9% ..
1	B	652	5% 91% 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
3	MLI	A	702	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11254 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.

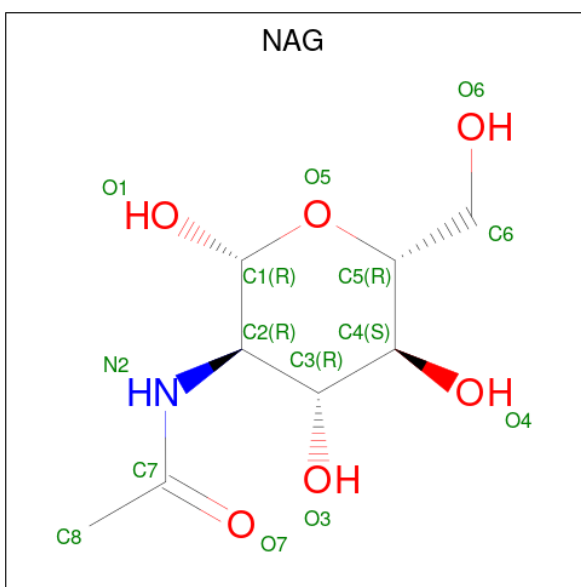
- Molecule 1 is a protein called Beta-N-acetylglucosaminidase Nag2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	639	Total	C	N	O	S	0	3	0
			5161	3285	880	974	22			
1	B	639	Total	C	N	O	S	0	3	0
			5164	3287	882	973	22			

There are 20 discrepancies between the modelled and reference sequences:

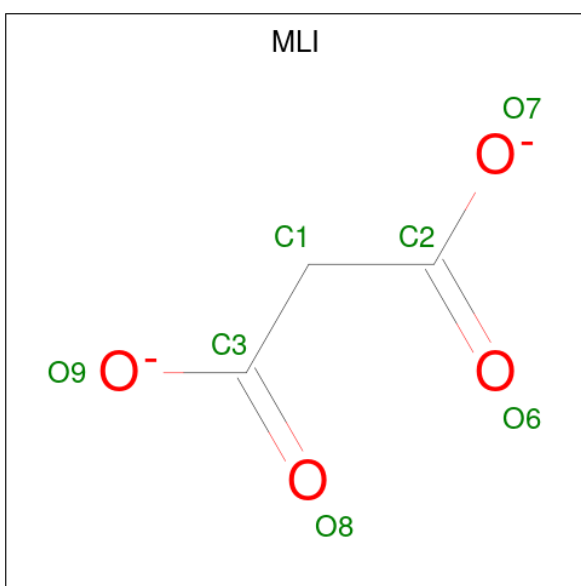
Chain	Residue	Modelled	Actual	Comment	Reference
A	643	ARG	-	expression tag	UNP D9ISE0
A	644	SER	-	expression tag	UNP D9ISE0
A	645	ARG	-	expression tag	UNP D9ISE0
A	646	SER	-	expression tag	UNP D9ISE0
A	647	HIS	-	expression tag	UNP D9ISE0
A	648	HIS	-	expression tag	UNP D9ISE0
A	649	HIS	-	expression tag	UNP D9ISE0
A	650	HIS	-	expression tag	UNP D9ISE0
A	651	HIS	-	expression tag	UNP D9ISE0
A	652	HIS	-	expression tag	UNP D9ISE0
B	643	ARG	-	expression tag	UNP D9ISE0
B	644	SER	-	expression tag	UNP D9ISE0
B	645	ARG	-	expression tag	UNP D9ISE0
B	646	SER	-	expression tag	UNP D9ISE0
B	647	HIS	-	expression tag	UNP D9ISE0
B	648	HIS	-	expression tag	UNP D9ISE0
B	649	HIS	-	expression tag	UNP D9ISE0
B	650	HIS	-	expression tag	UNP D9ISE0
B	651	HIS	-	expression tag	UNP D9ISE0
B	652	HIS	-	expression tag	UNP D9ISE0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	3	4		
3	B	1	Total	C	O	0	0
			7	3	4		

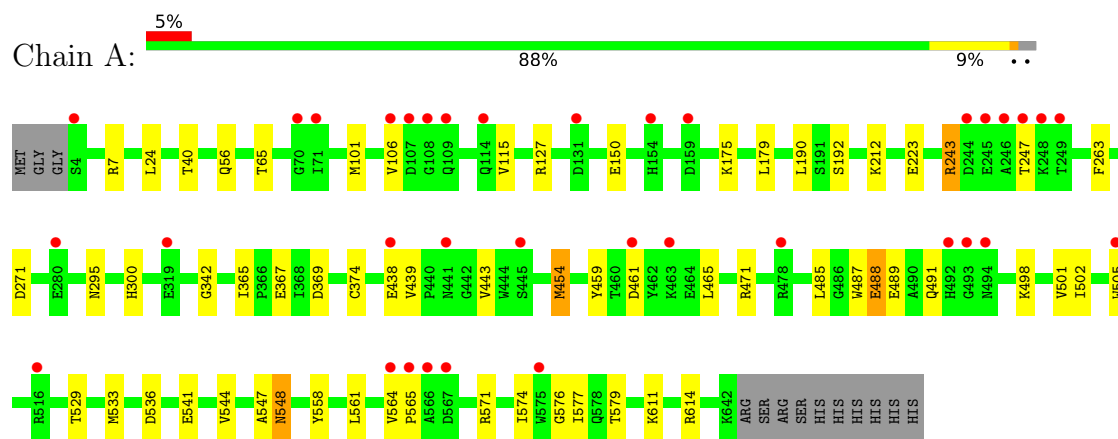
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	419	Total 419	O 419	0	0
4	B	466	Total 466	O 466	0	0

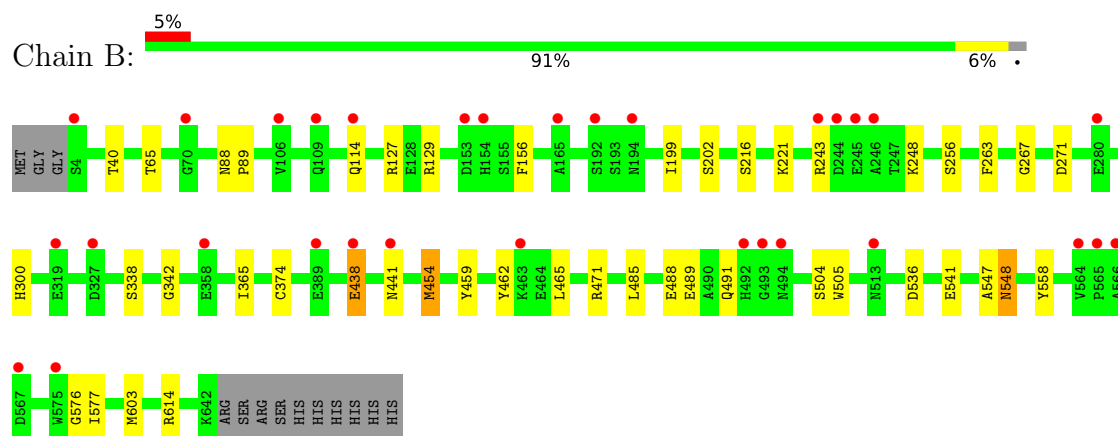
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Beta-N-acetylglucosaminidase Nag2



• Molecule 1: Beta-N-acetylglucosaminidase Nag2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.25Å 129.63Å 100.00Å 90.00° 114.36° 90.00°	Depositor
Resolution (Å)	48.02 – 2.50 48.02 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.02-2.50) 99.6 (48.02-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.200 , 0.248 0.205 , 0.249	Depositor DCC
R_{free} test set	3648 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11254	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.6025e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NAG, MLI

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	0.63	0/5307	0.85	2/7216 (0.0%)
1	B	0.64	0/5307	0.83	2/7215 (0.0%)
All	All	0.63	0/10614	0.84	4/14431 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	488	GLU	N-CA-C	6.87	120.55	111.75
1	A	342	GLY	N-CA-C	6.66	119.11	110.45
1	B	342	GLY	N-CA-C	5.56	118.09	110.58
1	B	267	GLY	N-CA-C	5.06	118.97	111.18

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	5161	0	5000	34	0
1	B	5164	0	5006	22	0
2	A	15	0	15	0	0
2	B	15	0	15	0	0
3	A	7	0	2	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	7	0	2	0	0
4	A	419	0	0	5	0
4	B	466	0	0	4	0
All	All	11254	0	10040	56	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 3.

All (56) 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:40:THR:HG22	1:B:65:THR:HG22	1.70	0.74
1:A:536:ASP:HB3	1:A:541:GLU:HG3	1.84	0.58
1:A:485:LEU:HD22	1:A:501:VAL:HB	1.86	0.57
1:A:7:ARG:HD2	4:A:1074:HOH:O	2.05	0.56
1:B:454:MET:HE1	1:B:462:TYR:CG	2.40	0.56
1:A:243:ARG:NH1	4:A:802:HOH:O	2.30	0.56
1:B:489:GLU:HG2	4:B:1032:HOH:O	2.07	0.55
1:B:536:ASP:HB3	1:B:541:GLU:HG3	1.90	0.53
1:A:558:TYR:O	1:A:614:ARG:NH2	2.42	0.52
1:A:40:THR:HG22	1:A:65:THR:HG22	1.92	0.52
1:A:547:ALA:O	1:A:548:ASN:HB2	2.10	0.51
1:B:547:ALA:O	1:B:548:ASN:HB2	2.11	0.50
1:B:576:GLY:C	1:B:577:ILE:HD12	2.35	0.50
1:B:271:ASP:HA	1:B:300:HIS:HB3	1.94	0.49
1:B:454:MET:HE1	1:B:462:TYR:CD1	2.48	0.49
1:A:454:MET:HE2	1:A:459:TYR:HB2	1.93	0.48
1:B:558:TYR:O	1:B:614:ARG:NH2	2.47	0.48
1:B:256:SER:HB2	4:B:1102:HOH:O	2.14	0.47
1:A:488:GLU:HA	1:A:502:ILE:HG23	1.96	0.47
1:B:603:MET:HA	1:B:603:MET:HE2	1.98	0.46
1:B:488:GLU:CG	1:B:504:SER:HA	2.46	0.45
1:B:454:MET:HG3	1:B:459:TYR:HB2	1.98	0.45
1:A:488:GLU:HA	1:A:502:ILE:CG2	2.46	0.45
1:A:101:MET:HA	1:A:115:VAL:HG23	1.99	0.45
1:B:505:TRP:C	1:B:505:TRP:CD1	2.95	0.44
1:B:114:GLN:HE21	1:B:338:SER:HB3	1.83	0.44
1:B:438[B]:GLU:HB2	1:B:489:GLU:HG3	1.99	0.44
1:B:127:ARG:HD2	4:B:1180:HOH:O	2.18	0.44
1:A:471:ARG:NH2	4:A:814:HOH:O	2.51	0.43
1:A:439:VAL:HB	1:A:443:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ILE:HG21	1:A:485:LEU:HD12	2.00	0.43
1:A:295:ASN:HD22	3:A:702:MLI:C1	2.32	0.43
1:A:498:LYS:HA	1:A:498:LYS:HD3	1.81	0.43
1:B:471:ARG:NH2	4:B:805:HOH:O	2.46	0.43
1:A:561:LEU:HD11	1:A:574:ILE:HG21	2.00	0.43
1:A:263:PHE:CD2	1:A:577:ILE:HD13	2.54	0.42
1:A:295:ASN:ND2	3:A:702:MLI:H12	2.34	0.42
1:B:156:PHE:HB2	1:B:216:SER:O	2.20	0.42
1:B:263:PHE:CD2	1:B:577:ILE:HD13	2.54	0.42
1:A:505:TRP:CD1	1:A:505:TRP:C	2.98	0.42
1:A:565:PRO:O	1:A:571:ARG:NH1	2.51	0.42
1:A:24:LEU:C	1:A:24:LEU:HD23	2.45	0.42
1:B:365:ILE:HG21	1:B:485:LEU:HD12	2.02	0.42
1:A:40:THR:HG23	4:A:874:HOH:O	2.20	0.41
1:A:529:THR:HB	1:A:579:THR:HA	2.02	0.41
1:A:40:THR:CG2	1:A:65:THR:HG22	2.50	0.41
1:A:295:ASN:HD22	3:A:702:MLI:H12	1.85	0.41
1:A:367:GLU:OE2	1:A:369:ASP:OD1	2.39	0.41
1:A:271:ASP:HA	1:A:300:HIS:HB3	2.02	0.41
1:A:127:ARG:HD2	4:A:1165:HOH:O	2.21	0.41
1:A:576:GLY:C	1:A:577:ILE:HD12	2.45	0.41
1:A:179:LEU:HD22	1:A:190:LEU:HB2	2.03	0.41
1:B:88:ASN:HB3	1:B:89:PRO:CD	2.50	0.41
1:A:533:MET:HA	1:A:544:VAL:O	2.21	0.41
1:A:212:LYS:HB2	1:A:223:GLU:HB2	2.03	0.40
1:A:487:TRP:HB3	1:A:505:TRP:HZ3	1.86	0.40

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	640/652 (98%)	631 (99%)	8 (1%)	1 (0%)	43 63
1	B	640/652 (98%)	630 (98%)	9 (1%)	1 (0%)	43 63
All	All	1280/1304 (98%)	1261 (98%)	17 (1%)	2 (0%)	43 63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	548	ASN
1	A	548	ASN

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	559/567 (99%)	542 (97%)	17 (3%)	36 64
1	B	559/567 (99%)	546 (98%)	13 (2%)	44 72
All	All	1118/1134 (99%)	1088 (97%)	30 (3%)	42 67

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	106	VAL
1	A	150	GLU
1	A	175	LYS
1	A	192	SER
1	A	243	ARG
1	A	247	THR
1	A	374	CYS
1	A	438[A]	GLU
1	A	438[B]	GLU
1	A	454	MET
1	A	461	ASP
1	A	465	LEU
1	A	489	GLU

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Mol	Chain	Res	Type
1	A	491	GLN
1	A	564	VAL
1	A	611	LYS
1	B	129	ARG
1	B	199	ILE
1	B	202	SER
1	B	221	LYS
1	B	243	ARG
1	B	248	LYS
1	B	374	CYS
1	B	438[A]	GLU
1	B	438[B]	GLU
1	B	441	ASN
1	B	454	MET
1	B	465	LEU
1	B	491	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	56	GLN
1	A	161	GLN
1	A	359	GLN
1	A	441	ASN
1	A	636	ASN
1	B	114	GLN
1	B	161	GLN
1	B	183	GLN
1	B	339	GLN
1	B	383	HIS
1	B	441	ASN
1	B	494	ASN
1	B	527	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
3	MLI	B	702	-	6,6,6	1.11	0	7,7,7	0.76	0
3	MLI	A	702	-	6,6,6	1.19	0	7,7,7	0.92	0
2	NAG	A	701	-	15,15,15	0.81	1 (6%)	21,21,21	2.33	4 (19%)
2	NAG	B	701	-	15,15,15	0.62	0	21,21,21	1.25	4 (19%)

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	MLI	B	702	-	-	0/4/4/4	-
3	MLI	A	702	-	-	4/4/4/4	-
2	NAG	A	701	-	-	0/6/26/26	0/1/1/1
2	NAG	B	701	-	-	0/6/26/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	NAG	C1-C2	2.07	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	NAG	O5-C1-C2	-8.39	101.08	109.52
2	A	701	NAG	C1-C2-N2	-2.80	107.49	110.73
2	A	701	NAG	C1-C2-C3	2.77	114.32	110.54
2	B	701	NAG	C1-C2-N2	-2.52	107.81	110.73
2	B	701	NAG	C8-C7-N2	-2.32	112.26	116.12
2	B	701	NAG	O5-C1-C2	-2.25	107.26	109.52
2	B	701	NAG	C1-C2-C3	2.22	113.57	110.54
2	A	701	NAG	C8-C7-N2	-2.16	112.54	116.12

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	MLI	C3-C1-C2-O7
3	A	702	MLI	C3-C1-C2-O6
3	A	702	MLI	C2-C1-C3-O8
3	A	702	MLI	C2-C1-C3-O9

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	MLI	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	639/652 (98%)	0.44	35 (5%) 30 27	20, 34, 58, 97	3 (0%)
1	B	639/652 (98%)	0.46	31 (4%) 35 31	17, 33, 58, 97	3 (0%)
All	All	1278/1304 (98%)	0.45	66 (5%) 33 29	17, 34, 58, 97	6 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	ALA	6.2
1	A	564	VAL	5.3
1	B	493	GLY	4.7
1	A	565	PRO	4.2
1	A	567	ASP	4.0
1	A	108	GLY	3.9
1	A	566	ALA	3.8
1	A	493	GLY	3.5
1	A	492	HIS	3.4
1	B	565	PRO	3.3
1	B	154	HIS	3.2
1	A	441	ASN	3.2
1	A	114	GLN	3.1
1	A	4	SER	3.1
1	A	107	ASP	3.1
1	A	248	LYS	3.0
1	A	280	GLU	3.0
1	B	280	GLU	2.9
1	A	575	TRP	2.9
1	B	564	VAL	2.9
1	B	4	SER	2.8
1	B	566	ALA	2.8
1	B	245	GLU	2.8
1	B	109	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	389	GLU	2.8
1	A	249	THR	2.7
1	B	192	SER	2.7
1	A	247	THR	2.7
1	A	245	GLU	2.7
1	B	438[A]	GLU	2.7
1	A	106	VAL	2.7
1	A	319	GLU	2.6
1	B	575	TRP	2.6
1	A	154	HIS	2.6
1	A	445	SER	2.6
1	B	567	ASP	2.6
1	A	463	LYS	2.6
1	A	244	ASP	2.5
1	A	461	ASP	2.5
1	B	246	ALA	2.5
1	B	494	ASN	2.5
1	B	319	GLU	2.4
1	B	463	LYS	2.4
1	A	438[A]	GLU	2.4
1	B	492	HIS	2.4
1	B	441	ASN	2.4
1	B	114	GLN	2.3
1	B	358	GLU	2.3
1	A	505	TRP	2.3
1	A	159	ASP	2.3
1	B	70	GLY	2.3
1	B	153	ASP	2.3
1	B	327	ASP	2.3
1	A	516	ARG	2.2
1	B	165	ALA	2.2
1	A	71	ILE	2.2
1	B	243	ARG	2.2
1	A	70	GLY	2.2
1	B	194	ASN	2.2
1	B	244	ASP	2.2
1	B	513	ASN	2.1
1	A	478	ARG	2.1
1	A	109	GLN	2.1
1	A	131	ASP	2.1
1	A	494	ASN	2.0
1	B	106	VAL	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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
3	MLI	A	702	7/7	0.66	0.27	34,36,37,38	7
2	NAG	A	701	15/15	0.93	0.11	26,27,30,30	0
2	NAG	B	701	15/15	0.94	0.09	23,25,27,28	0
3	MLI	B	702	7/7	0.94	0.12	42,43,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.