



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2024 – 11:01 PM EDT

PDB ID : 1MZ5
Title : Trypanosoma rangeli sialidase
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Deposited on : 2002-10-05
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

<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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

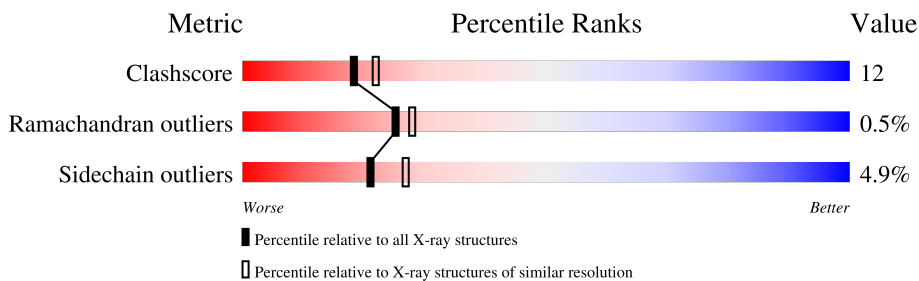
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	638	 77% 16% • •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5203 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 sialidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	622	4768	3012	837	903	16	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	177	VAL	ILE	conflict	UNP O44049

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



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

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

- Molecule 3 is water.

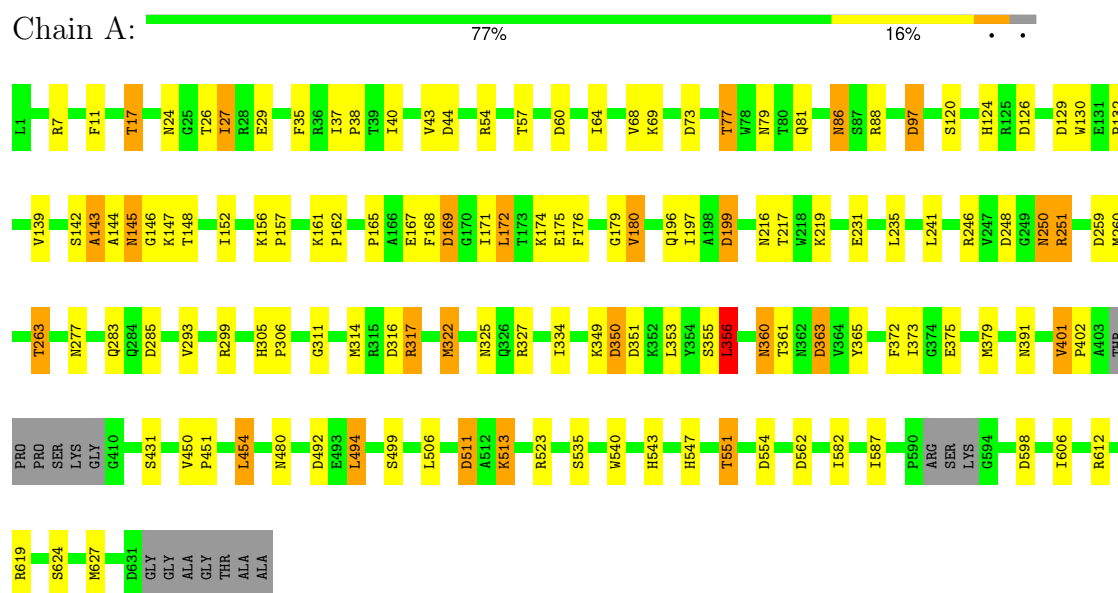
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	365	Total	O	0	0
			365	365		

3 Residue-property plots

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. 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. 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: sialidase



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.15Å 93.41Å 105.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20	Depositor
% Data completeness (in resolution range)	99.5 (15.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.180 , 0.237	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5203	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: NAG

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	0.77	1/4874 (0.0%)	1.00	23/6628 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	322	MET	SD-CE	-5.61	1.46	1.77

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	350	ASP	CB-CG-OD2	7.68	125.21	118.30
1	A	492	ASP	CB-CG-OD2	7.65	125.19	118.30
1	A	251	ARG	NE-CZ-NH1	-7.61	116.50	120.30
1	A	562	ASP	CB-CG-OD2	7.41	124.97	118.30
1	A	129	ASP	CB-CG-OD2	7.33	124.90	118.30
1	A	248	ASP	CB-CG-OD2	7.12	124.71	118.30
1	A	60	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	506	LEU	CB-CG-CD1	-6.42	100.08	111.00
1	A	169	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	7	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	511	ASP	N-CA-CB	-6.06	99.69	110.60
1	A	351	ASP	CB-CG-OD2	5.94	123.64	118.30
1	A	126	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	363	ASP	CB-CG-OD2	5.61	123.34	118.30
1	A	494	LEU	CA-CB-CG	5.58	128.13	115.30
1	A	199	ASP	CB-CG-OD2	5.39	123.16	118.30
1	A	97	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	511	ASP	CB-CA-C	-5.37	99.66	110.40
1	A	598	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	317	ARG	NE-CZ-NH2	-5.30	117.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	LEU	CB-CG-CD2	5.24	119.91	111.00
1	A	251	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	A	454	LEU	CB-CG-CD1	5.18	119.80	111.00

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	4768	0	4658	114	0
2	A	70	0	65	3	0
3	A	365	0	0	10	2
All	All	5203	0	4723	114	2

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 12.

All (114) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ASP:OD1	1:A:263:THR:HG22	1.55	1.05
1:A:24:ASN:OD1	1:A:26:THR:HG22	1.56	1.05
1:A:250:ASN:HD22	1:A:251:ARG:H	1.09	0.98
1:A:259:ASP:OD1	1:A:263:THR:CG2	2.18	0.92
1:A:360:ASN:HD21	1:A:363:ASP:H	1.14	0.90
1:A:543:HIS:HD2	3:A:821:HOH:O	1.57	0.88
1:A:401:VAL:HG12	1:A:402:PRO:HD2	1.56	0.87
1:A:17:THR:CG2	1:A:29:GLU:OE2	2.23	0.86
1:A:391:ASN:CB	3:A:995:HOH:O	2.25	0.84
1:A:143:ALA:CB	1:A:148:THR:HA	2.10	0.82
1:A:587:ILE:HD13	1:A:606:ILE:HD12	1.62	0.79
1:A:77:THR:HG22	3:A:925:HOH:O	1.87	0.73
1:A:241:LEU:HD11	1:A:260:MET:HE1	1.70	0.73
1:A:305:HIS:HD2	1:A:306:PRO:O	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ASN:C	1:A:360:ASN:HD22	1.92	0.71
1:A:73:ASP:OD2	1:A:77:THR:HB	1.89	0.71
1:A:143:ALA:HB2	1:A:148:THR:HA	1.73	0.70
1:A:624:SER:HB2	1:A:627:MET:HE3	1.72	0.70
1:A:241:LEU:HD11	1:A:260:MET:CE	2.23	0.68
1:A:360:ASN:HD21	1:A:363:ASP:N	1.88	0.68
1:A:86:ASN:C	1:A:86:ASN:HD22	1.99	0.66
1:A:360:ASN:HD22	1:A:361:THR:N	1.93	0.66
1:A:250:ASN:HD22	1:A:251:ARG:N	1.88	0.66
1:A:322:MET:HE3	1:A:379:MET:HG2	1.78	0.66
1:A:355:SER:HB2	1:A:372:PHE:CE1	2.31	0.65
1:A:360:ASN:ND2	1:A:363:ASP:H	1.91	0.65
1:A:246:ARG:HG3	1:A:285:ASP:HB3	1.78	0.64
1:A:431:SER:OG	2:A:654:NAG:H81	1.98	0.64
1:A:551:THR:HG21	3:A:813:HOH:O	1.98	0.63
1:A:349:LYS:NZ	1:A:350:ASP:OD2	2.29	0.62
1:A:360:ASN:C	1:A:360:ASN:ND2	2.52	0.62
1:A:317:ARG:HD2	3:A:776:HOH:O	1.99	0.62
1:A:373:ILE:HD13	1:A:373:ILE:N	2.15	0.61
1:A:250:ASN:ND2	1:A:251:ARG:H	1.88	0.60
1:A:17:THR:HG22	1:A:29:GLU:OE2	2.02	0.60
1:A:196:GLN:NE2	1:A:231:GLU:H	2.00	0.60
1:A:511:ASP:OD2	1:A:511:ASP:N	2.31	0.60
1:A:612:ARG:HD2	3:A:813:HOH:O	2.01	0.59
1:A:401:VAL:CG1	1:A:402:PRO:HD2	2.31	0.59
1:A:551:THR:HG23	1:A:612:ARG:HD3	1.84	0.59
1:A:334:ILE:HD12	1:A:372:PHE:HZ	1.67	0.59
1:A:27:ILE:HD12	1:A:27:ILE:C	2.24	0.58
1:A:167:GLU:CB	3:A:913:HOH:O	2.52	0.57
1:A:587:ILE:HG21	1:A:606:ILE:HD11	1.86	0.57
1:A:305:HIS:CD2	1:A:306:PRO:HD2	2.40	0.56
1:A:277:ASN:ND2	1:A:283:GLN:H	2.03	0.56
1:A:587:ILE:CD1	1:A:606:ILE:HD12	2.36	0.55
1:A:124:HIS:HD2	1:A:175:GLU:OE2	1.89	0.54
1:A:334:ILE:HD12	1:A:372:PHE:CZ	2.43	0.54
1:A:624:SER:HB2	1:A:627:MET:CE	2.37	0.54
1:A:139:VAL:HG22	1:A:152:ILE:HG12	1.90	0.53
1:A:167:GLU:HA	1:A:171:ILE:O	2.08	0.53
1:A:587:ILE:HD13	1:A:606:ILE:CD1	2.34	0.53
1:A:355:SER:HB2	1:A:372:PHE:CZ	2.46	0.52
1:A:551:THR:HG22	1:A:551:THR:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:ILE:HG12	1:A:606:ILE:HD13	1.92	0.51
1:A:26:THR:HG21	2:A:652:NAG:C1	2.41	0.51
1:A:17:THR:HG23	1:A:29:GLU:OE2	2.05	0.51
1:A:142:SER:O	1:A:143:ALA:HB2	2.10	0.50
1:A:37:ILE:HG21	1:A:97:ASP:HA	1.92	0.50
1:A:511:ASP:O	1:A:513:LYS:HE2	2.12	0.50
1:A:353:LEU:HG	1:A:372:PHE:HD1	1.76	0.49
1:A:401:VAL:HG12	1:A:402:PRO:CD	2.37	0.49
1:A:547:HIS:HE1	3:A:801:HOH:O	1.95	0.49
1:A:165:PRO:HG2	1:A:168:PHE:CE2	2.49	0.48
1:A:322:MET:HE3	1:A:379:MET:CG	2.43	0.48
1:A:17:THR:CG2	1:A:29:GLU:HB3	2.43	0.48
1:A:619:ARG:NH1	3:A:871:HOH:O	2.42	0.48
1:A:311:GLY:O	1:A:314:MET:HG2	2.14	0.48
1:A:322:MET:HE3	1:A:379:MET:CE	2.44	0.48
1:A:17:THR:HG21	1:A:29:GLU:HB3	1.96	0.48
1:A:38:PRO:CB	1:A:356:LEU:HD13	2.44	0.47
1:A:86:ASN:HD21	1:A:88:ARG:HD3	1.78	0.47
1:A:523:ARG:HA	1:A:540:TRP:CZ2	2.50	0.47
1:A:322:MET:CE	1:A:379:MET:HB3	2.45	0.47
1:A:587:ILE:CD1	1:A:606:ILE:CD1	2.93	0.47
1:A:86:ASN:ND2	1:A:88:ARG:H	2.13	0.46
1:A:174:LYS:HG2	1:A:175:GLU:HG3	1.97	0.46
1:A:293:VAL:O	1:A:299:ARG:HD2	2.15	0.46
1:A:355:SER:CB	1:A:372:PHE:CZ	2.98	0.46
1:A:27:ILE:O	1:A:27:ILE:HG13	2.16	0.46
1:A:86:ASN:C	1:A:86:ASN:ND2	2.69	0.45
1:A:124:HIS:CD2	1:A:175:GLU:OE2	2.67	0.45
1:A:285:ASP:OD1	1:A:305:HIS:HE1	1.99	0.45
1:A:401:VAL:HG11	3:A:871:HOH:O	2.15	0.45
1:A:11:PHE:HB3	1:A:35:PHE:CG	2.52	0.45
1:A:235:LEU:HD12	1:A:235:LEU:C	2.37	0.45
1:A:68:VAL:CG2	1:A:81:GLN:HB2	2.47	0.45
1:A:144:ALA:O	1:A:146:GLY:N	2.50	0.45
1:A:480:ASN:OD1	1:A:582:ILE:HG13	2.17	0.44
1:A:172:LEU:H	1:A:172:LEU:HG	1.53	0.44
1:A:431:SER:OG	2:A:654:NAG:C8	2.65	0.44
1:A:143:ALA:HB1	1:A:148:THR:HA	1.98	0.44
1:A:179:GLY:O	1:A:180:VAL:HB	2.17	0.44
1:A:54:ARG:HG2	1:A:64:ILE:HG12	1.99	0.43
1:A:216:ASN:HD22	1:A:217:THR:HG23	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ASN:HD21	1:A:283:GLN:H	1.65	0.43
1:A:372:PHE:HB3	1:A:375:GLU:HB2	2.01	0.43
1:A:624:SER:CB	1:A:627:MET:CE	2.96	0.43
1:A:43:VAL:O	1:A:44:ASP:C	2.57	0.43
1:A:130:TRP:CZ2	1:A:132:PRO:HG3	2.54	0.43
1:A:168:PHE:O	1:A:169:ASP:C	2.56	0.42
1:A:322:MET:HE1	1:A:379:MET:HB3	2.00	0.42
1:A:450:VAL:HB	1:A:451:PRO:HD2	2.02	0.42
1:A:86:ASN:HD22	1:A:88:ARG:H	1.65	0.42
1:A:176:PHE:HB2	1:A:197:ILE:HD13	2.02	0.41
1:A:241:LEU:HD11	1:A:260:MET:HE3	2.01	0.41
1:A:40:ILE:HG23	1:A:40:ILE:O	2.21	0.41
1:A:285:ASP:OD1	1:A:305:HIS:CE1	2.74	0.41
1:A:316:ASP:OD1	1:A:317:ARG:HG3	2.21	0.41
1:A:69:LYS:HA	1:A:79:ASN:O	2.22	0.40
1:A:161:LYS:N	1:A:162:PRO:CD	2.84	0.40
1:A:156:LYS:HA	1:A:157:PRO:HD3	1.91	0.40
1:A:199:ASP:C	1:A:199:ASP:OD1	2.59	0.40

All (2) 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)
3:A:889:HOH:O	3:A:924:HOH:O[2_655]	2.16	0.04
3:A:857:HOH:O	3:A:926:HOH:O[2_654]	2.18	0.02

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	616/638 (97%)	580 (94%)	33 (5%)	3 (0%)	25 28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	ALA
1	A	145	ASN
1	A	180	VAL

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	510/530 (96%)	485 (95%)	25 (5%)	21	27

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	27	ILE
1	A	57	THR
1	A	77	THR
1	A	86	ASN
1	A	120	SER
1	A	145	ASN
1	A	147	LYS
1	A	172	LEU
1	A	219	LYS
1	A	250	ASN
1	A	263	THR
1	A	325	ASN
1	A	327	ARG
1	A	356	LEU
1	A	360	ASN
1	A	365	TYR
1	A	401	VAL
1	A	454	LEU
1	A	494	LEU
1	A	499	SER
1	A	513	LYS

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Mol	Chain	Res	Type
1	A	535	SER
1	A	551	THR
1	A	554	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	124	HIS
1	A	145	ASN
1	A	196	GLN
1	A	216	ASN
1	A	250	ASN
1	A	277	ASN
1	A	305	HIS
1	A	360	ASN
1	A	543	HIS
1	A	547	HIS
1	A	605	ASN
1	A	625	GLN

5.3.3 RNA [i](#)

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](#)

5 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	655	1	14,14,15	0.82	0	17,19,21	1.29	3 (17%)
2	NAG	A	652	1	14,14,15	0.55	0	17,19,21	1.60	5 (29%)
2	NAG	A	653	1	14,14,15	0.50	0	17,19,21	0.89	0
2	NAG	A	654	1	14,14,15	0.90	1 (7%)	17,19,21	1.97	4 (23%)
2	NAG	A	651	1	14,14,15	0.55	0	17,19,21	1.11	1 (5%)

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	655	1	-	3/6/23/26	0/1/1/1
2	NAG	A	652	1	-	3/6/23/26	0/1/1/1
2	NAG	A	653	1	-	0/6/23/26	0/1/1/1
2	NAG	A	654	1	-	4/6/23/26	0/1/1/1
2	NAG	A	651	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	654	NAG	O5-C1	-2.76	1.39	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	654	NAG	O5-C1-C2	-6.09	101.87	111.29
2	A	652	NAG	C4-C3-C2	-3.77	105.49	111.02
2	A	654	NAG	O5-C5-C6	-2.82	102.17	107.66
2	A	651	NAG	O5-C1-C2	-2.69	107.13	111.29
2	A	654	NAG	O6-C6-C5	-2.56	102.62	111.33
2	A	654	NAG	C4-C3-C2	2.54	114.74	111.02
2	A	655	NAG	O5-C5-C4	-2.30	105.22	110.83
2	A	652	NAG	O3-C3-C2	2.24	114.06	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	652	NAG	O5-C1-C2	-2.19	107.90	111.29
2	A	652	NAG	C1-C2-N2	2.15	113.82	110.43
2	A	655	NAG	O5-C5-C6	-2.05	103.67	107.66
2	A	652	NAG	C1-O5-C5	2.05	114.93	112.19
2	A	655	NAG	O6-C6-C5	-2.02	104.46	111.33

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	654	NAG	C1-C2-N2-C7
2	A	654	NAG	C8-C7-N2-C2
2	A	654	NAG	O7-C7-N2-C2
2	A	652	NAG	C4-C5-C6-O6
2	A	655	NAG	C8-C7-N2-C2
2	A	655	NAG	O7-C7-N2-C2
2	A	652	NAG	O5-C5-C6-O6
2	A	651	NAG	C8-C7-N2-C2
2	A	651	NAG	O7-C7-N2-C2
2	A	654	NAG	O5-C5-C6-O6
2	A	655	NAG	O5-C5-C6-O6
2	A	652	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	652	NAG	1	0
2	A	654	NAG	2	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.