



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:52 PM UTC

PDB ID : 1VSG / pdb_00001vsg
Title : 2.9 ANGSTROMS RESOLUTION STRUCTURE OF THE N-TERMINAL
DOMAIN OF A VARIANT SURFACE GLYCOPROTEIN FROM TRY-
PANOSOMA BRUCEI
Authors : Freymann, D.; Down, J.; Wiley, D.C.
Deposited on : 1990-10-22
Resolution : 2.90 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

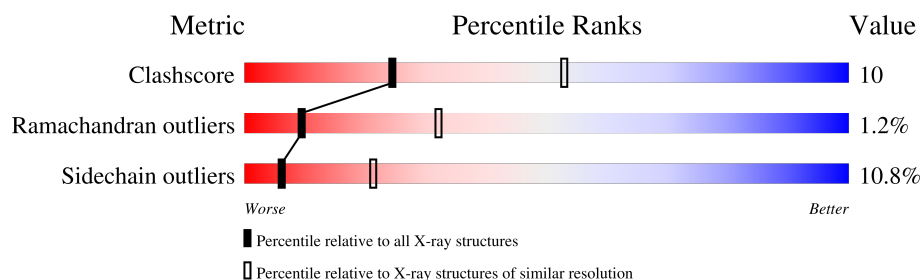
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	364	
1	B	364	
2	C	3	
3	D	3	

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	MAN	D	3	X	-	-	-

2 Entry composition [i](#)

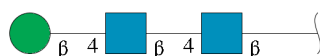
There are 4 unique types of molecules in this entry. The entry contains 5508 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 VARIANT SURFACE GLYCOPROTEIN MITAT 1.2.

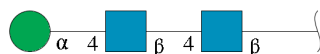
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2706	1684	472	540	10			
1	B	362	Total	C	N	O	S	0	0	0
			2706	1684	472	540	10			

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	10	Total	O	0	0
			10	10		

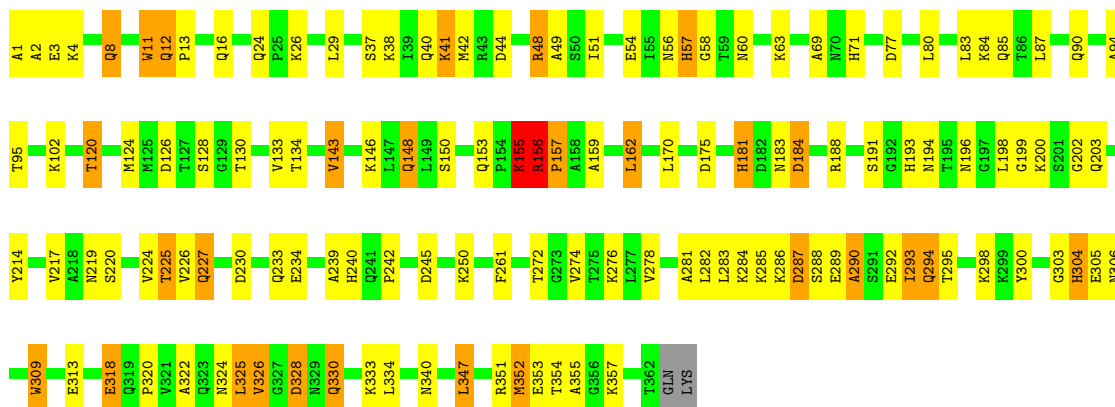
3 Residue-property plots

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.

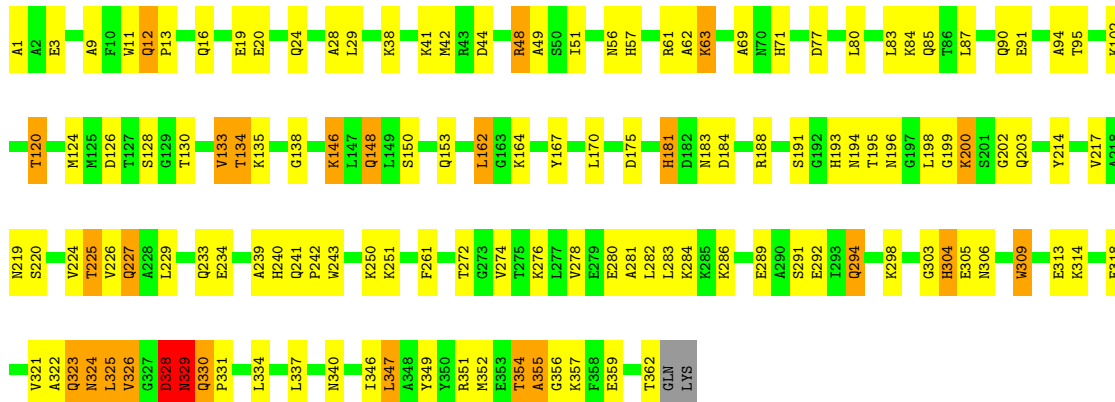
• Molecule 1: VARIANT SURFACE GLYCOPROTEIN MITAT 1.2

Chain A: 

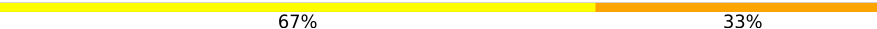


• Molecule 1: VARIANT SURFACE GLYCOPROTEIN MITAT 1.2

Chain B: 



• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 



- Molecule 3: α -D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  67% 33%



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	95.50Å 97.50Å 123.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5508	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

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, 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	1.10	10/2745 (0.4%)	1.80	65/3713 (1.8%)
1	B	1.12	11/2745 (0.4%)	1.79	58/3713 (1.6%)
All	All	1.11	21/5490 (0.4%)	1.80	123/7426 (1.7%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	VAL	CA-CB	7.98	1.65	1.53
1	B	19	GLU	C-O	7.83	1.34	1.24
1	B	57	HIS	CD2-NE2	-7.40	1.29	1.37
1	A	193	HIS	CD2-NE2	-6.86	1.30	1.37
1	B	241	GLN	CA-CB	-6.83	1.45	1.53
1	B	9	ALA	C-O	6.75	1.32	1.24
1	B	181	HIS	CD2-NE2	-6.71	1.30	1.37
1	B	193	HIS	CD2-NE2	-6.69	1.30	1.37
1	A	181	HIS	CD2-NE2	-6.31	1.30	1.37
1	B	71	HIS	CD2-NE2	-6.06	1.31	1.37
1	B	240	HIS	CD2-NE2	-5.98	1.31	1.37
1	A	240	HIS	CD2-NE2	-5.94	1.31	1.37
1	B	304	HIS	CD2-NE2	-5.89	1.31	1.37
1	A	71	HIS	CD2-NE2	-5.78	1.31	1.37
1	A	304	HIS	CD2-NE2	-5.65	1.31	1.37
1	B	181	HIS	CG-ND1	-5.46	1.32	1.38
1	A	240	HIS	CG-ND1	-5.30	1.32	1.38
1	A	57	HIS	CD2-NE2	-5.12	1.32	1.37
1	A	193	HIS	CG-ND1	-5.06	1.32	1.38
1	B	57	HIS	CG-ND1	-5.04	1.32	1.38
1	A	71	HIS	CG-ND1	-5.03	1.32	1.38

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	324	ASN	CA-CB-CG	16.49	129.09	112.60
1	A	340	ASN	CA-CB-CG	10.05	122.65	112.60
1	B	20	GLU	O-C-N	10.00	136.56	122.36
1	B	340	ASN	CA-CB-CG	8.91	121.51	112.60
1	A	153	GLN	OE1-CD-NE2	-7.99	114.61	122.60
1	B	153	GLN	OE1-CD-NE2	-7.85	114.75	122.60
1	A	170	LEU	CA-C-O	7.82	131.27	121.58
1	B	329	ASN	OD1-CG-ND2	-7.79	114.81	122.60
1	A	330	GLN	CA-C-N	7.51	127.52	119.78
1	A	330	GLN	C-N-CA	7.51	127.52	119.78
1	A	77	ASP	CA-CB-CG	7.48	120.08	112.60
1	B	324	ASN	OD1-CG-ND2	-7.42	115.18	122.60
1	A	56	ASN	OD1-CG-ND2	-7.35	115.25	122.60
1	B	57	HIS	CA-CB-CG	7.29	121.09	113.80
1	A	324	ASN	CB-CG-ND2	7.28	127.32	116.40
1	A	183	ASN	OD1-CG-ND2	-7.27	115.33	122.60
1	B	183	ASN	OD1-CG-ND2	-7.11	115.49	122.60
1	B	57	HIS	ND1-CG-CD2	7.10	113.20	106.10
1	A	230	ASP	CA-CB-CG	6.95	119.55	112.60
1	A	196	ASN	CA-CB-CG	6.84	119.44	112.60
1	A	12	GLN	OE1-CD-NE2	-6.77	115.83	122.60
1	B	305	GLU	CB-CG-CD	6.76	124.10	112.60
1	B	323	GLN	OE1-CD-NE2	-6.76	115.84	122.60
1	A	225	THR	CA-CB-OG1	-6.76	99.46	109.60
1	A	330	GLN	CG-CD-NE2	6.74	126.51	116.40
1	B	234	GLU	CA-CB-CG	6.73	127.57	114.10
1	A	234	GLU	CA-CB-CG	6.73	127.55	114.10
1	A	8	GLN	CG-CD-NE2	6.72	126.48	116.40
1	B	294	GLN	CA-CB-CG	6.67	127.44	114.10
1	B	57	HIS	CB-CG-CD2	-6.66	122.54	131.20
1	A	48	ARG	NE-CZ-NH1	-6.64	114.86	121.50
1	A	294	GLN	CA-CB-CG	6.63	127.36	114.10
1	B	95	THR	CA-CB-OG1	-6.62	99.67	109.60
1	A	305	GLU	CB-CG-CD	6.59	123.81	112.60
1	B	9	ALA	O-C-N	6.57	131.53	122.46
1	B	330	GLN	OE1-CD-NE2	-6.56	116.04	122.60
1	A	306	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	B	150	SER	CA-C-N	6.47	126.85	119.93
1	B	150	SER	C-N-CA	6.47	126.85	119.93
1	B	175	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	48	ARG	NE-CZ-NH2	6.44	125.00	119.20
1	B	217	VAL	N-CA-CB	-6.43	103.79	111.90
1	B	153	GLN	CG-CD-NE2	6.43	126.05	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	GLU	CA-C-O	-6.33	112.20	119.60
1	B	126	ASP	CA-CB-CG	6.33	118.93	112.60
1	B	77	ASP	CA-CB-CG	6.32	118.92	112.60
1	B	196	ASN	CA-CB-CG	6.27	118.87	112.60
1	A	95	THR	CA-CB-OG1	-6.26	100.21	109.60
1	B	225	THR	CA-CB-OG1	-6.25	100.22	109.60
1	A	183	ASN	CA-CB-CG	6.24	118.83	112.60
1	A	153	GLN	CG-CD-NE2	6.23	125.75	116.40
1	A	217	VAL	N-CA-CB	-6.22	104.06	111.90
1	A	294	GLN	OE1-CD-NE2	-6.20	116.40	122.60
1	A	175	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	324	ASN	OD1-CG-ND2	-6.17	116.43	122.60
1	B	184	ASP	CA-CB-CG	6.11	118.71	112.60
1	B	346	ILE	N-CA-C	-6.10	104.57	110.42
1	A	230	ASP	N-CA-C	6.06	120.54	113.20
1	A	156	ARG	N-CA-C	-6.06	102.15	109.72
1	B	340	ASN	CB-CG-ND2	6.05	125.48	116.40
1	B	309	TRP	CG-CD2-CE3	6.04	139.94	133.90
1	B	134	THR	CA-CB-OG1	-6.01	100.58	109.60
1	A	294	GLN	CG-CD-NE2	5.92	125.27	116.40
1	A	126	ASP	CA-CB-CG	5.91	118.51	112.60
1	B	329	ASN	CB-CG-ND2	5.90	125.25	116.40
1	A	328	ASP	CA-CB-CG	5.88	118.47	112.60
1	B	48	ARG	NE-CZ-NH1	-5.82	115.68	121.50
1	A	354	THR	CA-CB-OG1	-5.81	100.88	109.60
1	A	12	GLN	CG-CD-NE2	5.80	125.10	116.40
1	B	12	GLN	OE1-CD-NE2	-5.77	116.83	122.60
1	B	340	ASN	OD1-CG-ND2	-5.77	116.83	122.60
1	A	227	GLN	OE1-CD-NE2	-5.76	116.84	122.60
1	A	150	SER	CA-C-N	5.75	126.08	119.93
1	A	150	SER	C-N-CA	5.75	126.08	119.93
1	A	57	HIS	N-CA-C	5.71	118.52	110.23
1	B	227	GLN	OE1-CD-NE2	-5.70	116.90	122.60
1	A	290	ALA	N-CA-C	5.70	119.75	112.34
1	B	324	ASN	CB-CG-ND2	5.66	124.90	116.40
1	A	272	THR	CA-CB-OG1	-5.64	101.13	109.60
1	B	272	THR	CA-CB-OG1	-5.64	101.14	109.60
1	B	354	THR	CA-CB-OG1	-5.59	101.22	109.60
1	B	306	ASN	OD1-CG-ND2	-5.58	117.02	122.60
1	A	143	VAL	CA-C-N	5.49	126.35	119.98
1	A	143	VAL	C-N-CA	5.49	126.35	119.98
1	A	102	LYS	CB-CG-CD	5.46	123.86	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	TRP	CG-CD2-CE3	5.43	139.33	133.90
1	A	54	GLU	CB-CA-C	-5.43	102.54	110.95
1	B	102	LYS	CB-CG-CD	5.42	123.77	111.30
1	A	155	LYS	CA-CB-CG	5.41	124.91	114.10
1	B	57	HIS	CG-CD2-NE2	-5.41	101.80	107.20
1	A	324	ASN	CA-CB-CG	5.39	118.00	112.60
1	B	11	TRP	CE2-CD2-CG	-5.39	100.73	107.20
1	B	328	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	156	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	B	355	ALA	CA-C-N	5.37	125.90	119.94
1	B	355	ALA	C-N-CA	5.37	125.90	119.94
1	A	245	ASP	N-CA-C	5.35	116.80	111.07
1	B	48	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	A	11	TRP	CE2-CD2-CG	-5.34	100.79	107.20
1	B	153	GLN	CB-CA-C	5.33	117.13	108.87
1	B	183	ASN	CA-CB-CG	5.29	117.89	112.60
1	B	95	THR	CA-CB-CG2	5.25	119.43	110.50
1	A	95	THR	CA-CB-CG2	5.25	119.42	110.50
1	A	340	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	B	294	GLN	CG-CD-NE2	5.22	124.24	116.40
1	A	184	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	198	LEU	N-CA-C	5.20	119.25	113.01
1	A	11	TRP	CB-CG-CD1	-5.17	119.15	126.90
1	A	8	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	B	193	HIS	CB-CG-CD2	-5.16	124.50	131.20
1	B	12	GLN	CG-CD-NE2	5.13	124.10	116.40
1	A	198	LEU	N-CA-C	5.12	119.15	113.01
1	B	227	GLN	CG-CD-NE2	5.12	124.07	116.40
1	A	40	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	A	293	ILE	CA-C-N	5.11	127.37	120.38
1	A	293	ILE	C-N-CA	5.11	127.37	120.38
1	A	340	ASN	CB-CG-ND2	5.10	124.05	116.40
1	A	293	ILE	N-CA-C	-5.09	105.75	110.53
1	B	134	THR	N-CA-CB	-5.09	101.79	111.00
1	B	11	TRP	CG-CD2-CE3	5.07	138.97	133.90
1	A	309	TRP	CG-CD2-CE3	5.06	138.96	133.90
1	A	295	THR	CA-CB-OG1	-5.01	102.08	109.60
1	A	170	LEU	CD1-CG-CD2	-5.01	99.78	110.80

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	2706	0	2702	58	0
1	B	2706	0	2702	58	0
2	C	39	0	34	2	0
3	D	39	0	34	2	0
4	A	8	0	0	0	0
4	B	10	0	0	0	0
All	All	5508	0	5472	109	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 10.

All (109) 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:322:ALA:HB3	1:A:325:LEU:HD22	1.53	0.89
1:B:322:ALA:HB3	1:B:325:LEU:HD22	1.62	0.82
1:A:2:ALA:O	1:A:4:LYS:HG2	1.85	0.76
1:A:42:MET:HE2	2:C:1:NAG:H82	1.65	0.76
1:B:42:MET:HE2	3:D:1:NAG:H82	1.68	0.75
1:B:162:LEU:HD13	1:B:250:LYS:HD3	1.74	0.69
1:A:326:VAL:HG13	1:A:330:GLN:HB2	1.75	0.68
1:A:159:ALA:HB1	1:A:162:LEU:O	1.96	0.65
1:A:3:GLU:HG2	1:A:191:SER:OG	1.97	0.65
1:A:289:GLU:O	1:A:292:GLU:HG2	1.97	0.64
1:B:356:GLY:O	1:B:359:GLU:HG2	1.98	0.64
1:A:352:MET:SD	1:B:63:LYS:HG2	2.38	0.64
1:A:1:ALA:O	1:A:181:HIS:HB3	1.99	0.62
1:A:3:GLU:HG2	1:A:191:SER:CB	2.29	0.62
1:B:146:LYS:O	1:B:148:GLN:HG3	1.98	0.62
1:B:331:PRO:O	1:B:337:LEU:HD21	2.00	0.61
1:B:38:LYS:HD2	1:B:261:PHE:HB3	1.82	0.61
1:A:3:GLU:HG2	1:A:191:SER:HB3	1.83	0.59
1:A:38:LYS:HD2	1:A:261:PHE:HB3	1.83	0.59
1:B:56:ASN:O	1:B:62:ALA:HB2	2.04	0.58
1:B:289:GLU:O	1:B:292:GLU:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ARG:HD3	1:B:334:LEU:O	2.05	0.56
1:B:138:GLY:HA3	1:B:146:LYS:HD2	1.85	0.56
1:A:309:TRP:O	1:A:313:GLU:HG3	2.08	0.54
1:B:309:TRP:O	1:B:313:GLU:HG3	2.08	0.54
1:A:347:LEU:O	1:A:351:ARG:HG3	2.08	0.54
1:B:314:LYS:O	1:B:318:GLU:HG2	2.06	0.54
1:A:188:ARG:NH2	1:B:200:LYS:HA	2.23	0.54
1:B:120:THR:HG22	1:B:130:THR:O	2.09	0.53
1:A:48:ARG:HD3	1:A:334:LEU:O	2.08	0.52
1:A:200:LYS:HA	1:B:188:ARG:NH2	2.24	0.52
1:A:155:LYS:HD2	1:A:157:PRO:HB3	1.91	0.51
1:A:352:MET:O	1:A:355:ALA:HB3	2.11	0.51
1:A:41:LYS:HB2	2:C:1:NAG:H83	1.92	0.51
1:B:278:VAL:HG22	1:B:282:LEU:HD12	1.91	0.51
1:B:325:LEU:HD21	1:B:349:TYR:CD1	2.45	0.51
1:A:278:VAL:HG22	1:A:282:LEU:HD12	1.92	0.51
1:B:84:LYS:HE3	1:B:85:GLN:HE21	1.76	0.50
1:A:203:GLN:HB2	1:A:219:ASN:HB2	1.93	0.50
1:A:120:THR:HG22	1:A:130:THR:O	2.12	0.50
1:A:146:LYS:O	1:A:148:GLN:HG3	2.10	0.50
1:B:281:ALA:O	1:B:284:LYS:HG2	2.13	0.49
1:B:44:ASP:HB3	1:B:48:ARG:NH1	2.27	0.49
1:B:162:LEU:HG	1:B:167:TYR:CE1	2.48	0.49
1:A:285:LYS:HD3	1:A:288:SER:OG	2.13	0.49
1:B:203:GLN:HB2	1:B:219:ASN:HB2	1.95	0.49
1:B:347:LEU:O	1:B:351:ARG:HG3	2.13	0.49
1:A:44:ASP:HB3	1:A:48:ARG:NH1	2.28	0.48
1:A:51:ILE:HG13	1:A:347:LEU:HG	1.96	0.48
1:A:188:ARG:HH21	1:B:200:LYS:HA	1.79	0.48
1:A:281:ALA:O	1:A:284:LYS:HG3	2.14	0.48
1:A:4:LYS:HE3	1:A:184:ASP:HA	1.96	0.48
1:B:3:GLU:HG2	1:B:191:SER:HB3	1.94	0.48
1:B:164:LYS:HE3	1:B:251:LYS:HZ2	1.78	0.48
1:A:84:LYS:HE3	1:A:85:GLN:HE21	1.78	0.47
1:A:200:LYS:NZ	1:B:195:THR:O	2.47	0.47
1:B:1:ALA:O	1:B:181:HIS:HB3	2.14	0.47
1:A:12:GLN:O	1:A:16:GLN:HG3	2.15	0.47
1:B:181:HIS:NE2	1:B:224:VAL:HG22	2.29	0.46
1:A:156:ARG:H	1:A:156:ARG:HH21	1.64	0.46
1:A:353:GLU:O	1:A:357:LYS:HG2	2.16	0.46
1:B:51:ILE:HG13	1:B:347:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:TYR:CE1	1:B:226:VAL:HB	2.50	0.46
1:B:294:GLN:HG2	1:B:304:HIS:CD2	2.50	0.46
1:B:298:LYS:HA	1:B:303:GLY:H	1.81	0.46
1:A:199:GLY:HA3	1:A:202:GLY:O	2.16	0.46
1:B:199:GLY:HA3	1:B:202:GLY:O	2.15	0.46
1:A:330:GLN:HE21	1:A:330:GLN:HA	1.80	0.46
1:B:291:SER:O	1:B:294:GLN:HB3	2.16	0.46
1:A:294:GLN:HG2	1:A:304:HIS:CD2	2.50	0.45
1:B:325:LEU:HD11	1:B:349:TYR:CD2	2.50	0.45
1:A:162:LEU:HD13	1:A:250:LYS:HD3	1.99	0.45
1:A:318:GLU:O	1:A:333:LYS:HG2	2.17	0.45
1:B:326:VAL:O	1:B:330:GLN:HB2	2.17	0.45
1:A:200:LYS:HA	1:B:188:ARG:HH21	1.82	0.45
1:A:298:LYS:HA	1:A:303:GLY:H	1.82	0.44
1:B:3:GLU:HG2	1:B:191:SER:CB	2.48	0.44
1:B:214:TYR:CZ	1:B:226:VAL:HB	2.53	0.44
1:A:26:LYS:HD2	1:A:155:LYS:HG2	2.00	0.44
1:B:328:ASP:O	1:B:330:GLN:N	2.50	0.44
1:B:354:THR:HA	1:B:357:LYS:HD2	1.99	0.44
1:A:214:TYR:CE1	1:A:226:VAL:HB	2.53	0.43
1:B:41:LYS:HB2	3:D:1:NAG:H83	1.99	0.43
1:A:60:ASN:HB3	1:A:300:TYR:HD2	1.83	0.43
1:B:83:LEU:HA	1:B:87:LEU:HB2	1.99	0.43
1:A:124:MET:HB3	1:A:133:VAL:HG22	2.00	0.43
1:B:194:ASN:HB3	1:B:202:GLY:C	2.43	0.43
1:B:229:LEU:HD13	1:B:243:TRP:CE3	2.53	0.43
1:A:83:LEU:HA	1:A:87:LEU:HB2	1.99	0.43
1:B:49:ALA:HB3	1:B:69:ALA:HB2	2.00	0.43
1:B:24:GLN:HE21	1:B:94:ALA:HB1	1.84	0.42
1:B:323:GLN:NE2	1:B:328:ASP:O	2.52	0.42
1:A:11:TRP:HZ2	1:A:133:VAL:HG11	1.85	0.42
1:B:12:GLN:O	1:B:16:GLN:HG3	2.18	0.42
1:B:24:GLN:NE2	1:B:94:ALA:HB1	2.34	0.42
1:A:286:LYS:O	1:A:287:ASP:HB2	2.20	0.42
1:B:124:MET:HB3	1:B:133:VAL:CG2	2.50	0.41
1:A:37:SER:O	1:A:41:LYS:HG3	2.20	0.41
1:B:28:ALA:HA	1:B:91:GLU:OE1	2.20	0.41
1:A:1:ALA:O	1:A:181:HIS:CB	2.67	0.41
1:A:290:ALA:HA	1:A:293:ILE:HG12	2.03	0.41
1:A:24:GLN:HE21	1:A:94:ALA:HB1	1.86	0.41
1:B:280:GLU:HB2	1:B:286:LYS:NZ	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:HIS:NE2	1:A:224:VAL:HG22	2.34	0.41
1:A:214:TYR:CZ	1:A:226:VAL:HB	2.55	0.41
1:A:194:ASN:HB3	1:A:202:GLY:C	2.46	0.41
1:A:49:ALA:HB3	1:A:69:ALA:HB2	2.02	0.40
1:B:194:ASN:HB3	1:B:202:GLY:O	2.21	0.40
1:A:58:GLY:HA2	1:B:355:ALA: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	360/364 (99%)	323 (90%)	32 (9%)	5 (1%)	9	30
1	B	360/364 (99%)	324 (90%)	32 (9%)	4 (1%)	11	36
All	All	720/728 (99%)	647 (90%)	64 (9%)	9 (1%)	9	32

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	ASP
1	B	329	ASN
1	A	157	PRO
1	B	239	ALA
1	A	239	ALA
1	A	8	GLN
1	A	274	VAL
1	B	328	ASP
1	B	274	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	277/279 (99%)	248 (90%)	29 (10%)	6	22
1	B	277/279 (99%)	246 (89%)	31 (11%)	6	19
All	All	554/558 (99%)	494 (89%)	60 (11%)	6	21

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	PRO
1	A	29	LEU
1	A	41	LYS
1	A	57	HIS
1	A	63	LYS
1	A	80	LEU
1	A	90	GLN
1	A	120	THR
1	A	128	SER
1	A	134	THR
1	A	143	VAL
1	A	148	GLN
1	A	155	LYS
1	A	156	ARG
1	A	162	LEU
1	A	220	SER
1	A	225	THR
1	A	227	GLN
1	A	233	GLN
1	A	242	PRO
1	A	276	LYS
1	A	283	LEU
1	A	318	GLU
1	A	320	PRO
1	A	325	LEU
1	A	326	VAL
1	A	328	ASP

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Mol	Chain	Res	Type
1	A	347	LEU
1	A	352	MET
1	B	13	PRO
1	B	29	LEU
1	B	61	ARG
1	B	63	LYS
1	B	80	LEU
1	B	90	GLN
1	B	120	THR
1	B	128	SER
1	B	133	VAL
1	B	134	THR
1	B	135	LYS
1	B	146	LYS
1	B	148	GLN
1	B	162	LEU
1	B	170	LEU
1	B	200	LYS
1	B	220	SER
1	B	225	THR
1	B	227	GLN
1	B	233	GLN
1	B	242	PRO
1	B	276	LYS
1	B	283	LEU
1	B	321	VAL
1	B	324	ASN
1	B	325	LEU
1	B	326	VAL
1	B	329	ASN
1	B	347	LEU
1	B	352	MET
1	B	362	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	70	ASN
1	A	85	GLN
1	A	330	GLN
1	B	57	HIS

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Mol	Chain	Res	Type
1	B	85	GLN
1	B	221	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 ⓘ

6 monosaccharides 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	C	1	2,1	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
2	NAG	C	2	2	14,14,15	1.12	1 (7%)	17,19,21	1.50	4 (23%)
2	BMA	C	3	2	11,11,12	1.03	1 (9%)	15,15,17	0.95	0
3	NAG	D	1	3,1	14,14,15	0.71	1 (7%)	17,19,21	1.15	2 (11%)
3	NAG	D	2	3	14,14,15	0.98	0	17,19,21	1.47	4 (23%)
3	MAN	D	3	3	11,11,12	0.95	1 (9%)	15,15,17	0.92	0

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	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	C1-C2	2.39	1.55	1.52
3	D	1	NAG	C1-C2	2.02	1.55	1.52
3	D	3	MAN	C2-C3	2.02	1.55	1.52
2	C	3	BMA	C2-C3	2.02	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	O7-C7-C8	-2.76	117.15	122.05
2	C	2	NAG	C3-C4-C5	2.69	115.12	110.23
3	D	1	NAG	C1-O5-C5	2.62	115.69	112.19
2	C	2	NAG	O7-C7-C8	-2.50	117.61	122.05
2	C	2	NAG	C1-O5-C5	2.46	115.48	112.19
3	D	1	NAG	C8-C7-N2	2.45	120.18	116.12
3	D	2	NAG	C3-C4-C5	2.37	114.53	110.23
2	C	2	NAG	C8-C7-N2	2.37	120.05	116.12
2	C	1	NAG	C8-C7-N2	2.31	119.95	116.12
3	D	2	NAG	C1-O5-C5	2.24	115.19	112.19
3	D	2	NAG	C8-C7-N2	2.23	119.81	116.12

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	3	MAN	C1

All (2) torsion outliers are listed below:

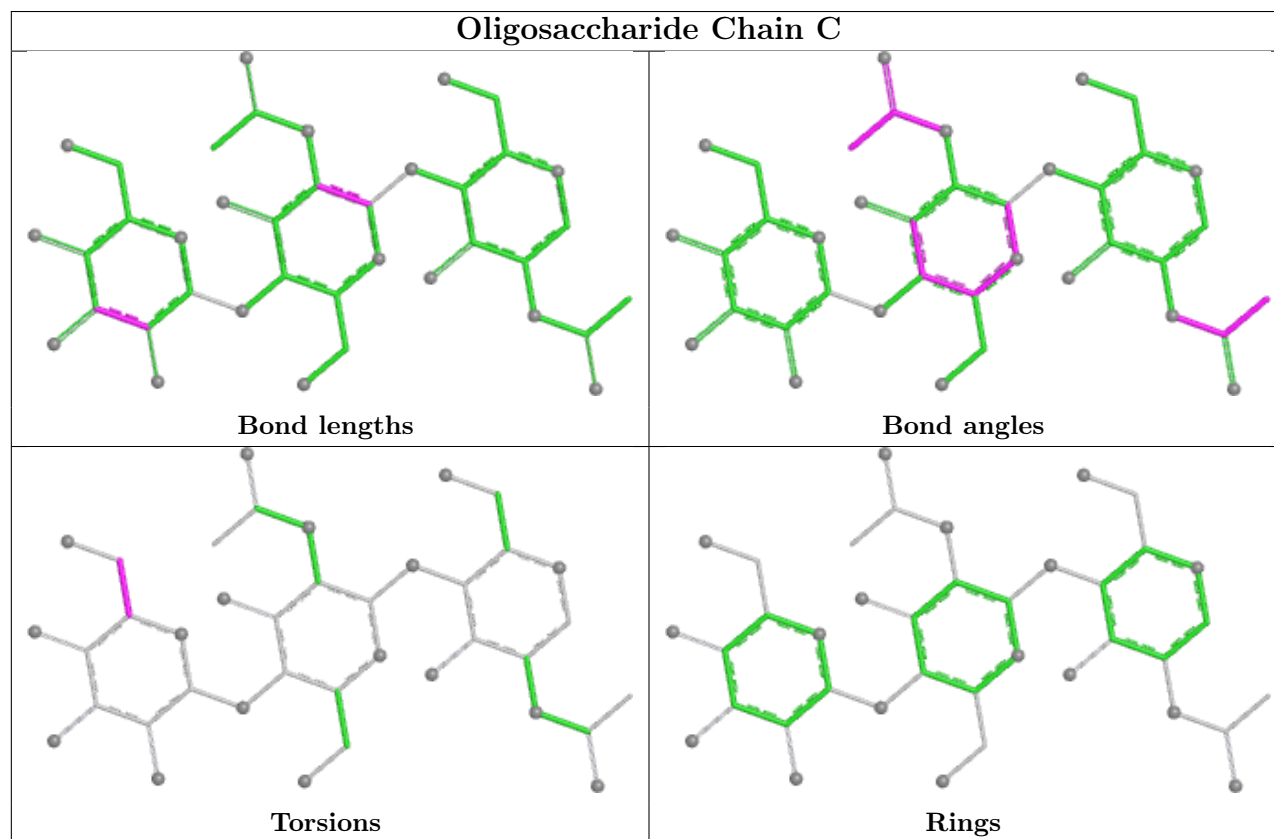
Mol	Chain	Res	Type	Atoms
3	D	3	MAN	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6

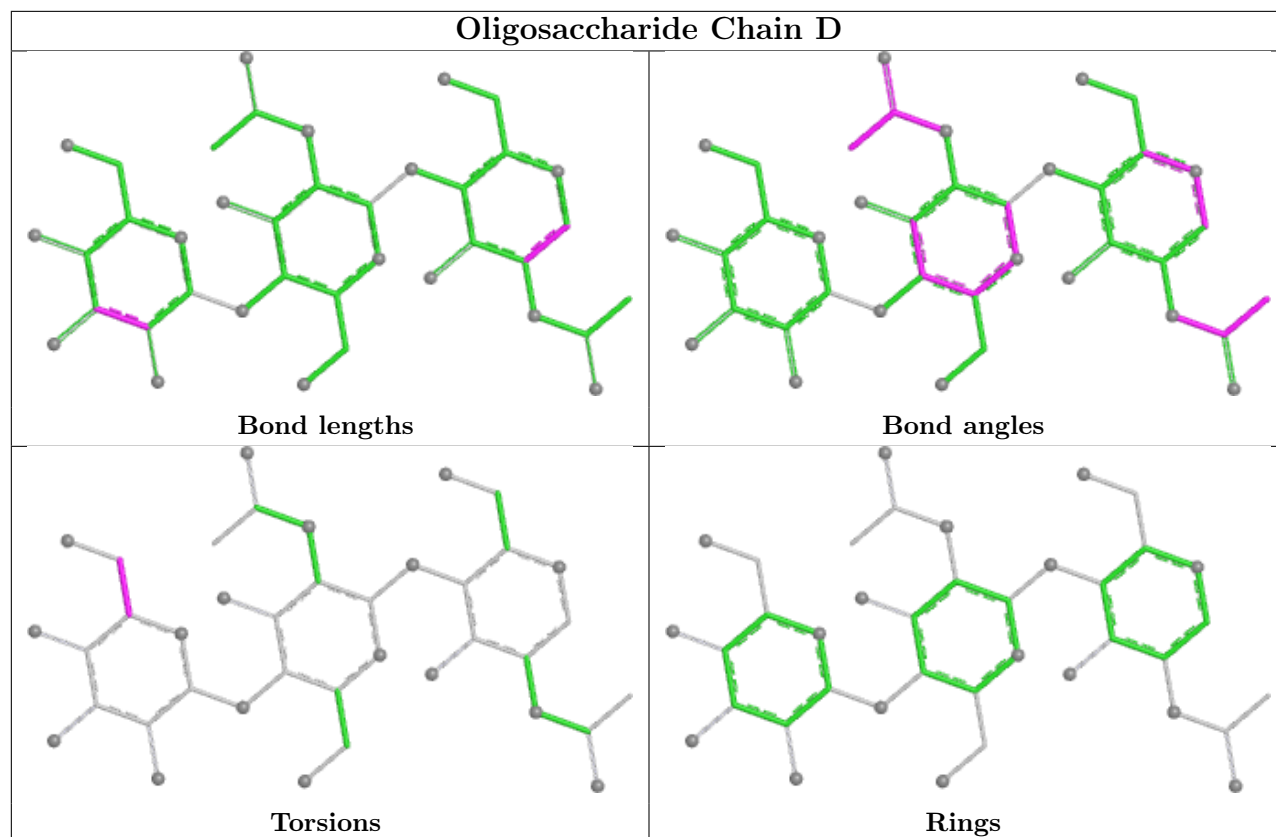
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	2	0
3	D	1	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





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 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.