Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 05:15 AM EDT

PDB ID	:	1VSG
Title	:	2.9 ANGSTROMS RESOLUTION STRUCTURE OF THE N-TERMINAL DOMAIN OF A VARIANT SURFACE GLYCOPROTEIN FROM TRYPANOSOMA 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:

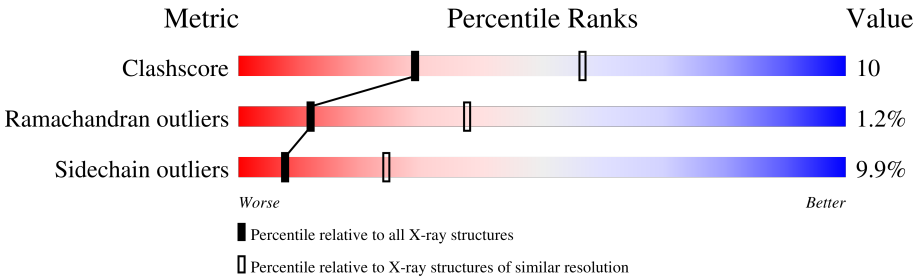
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.90 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	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	364	68% 26%
1	B	364	67% 28%
2	C	3	67% 33%
3	D	3	67% 33%

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)

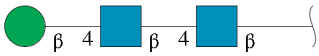
There are 4 unique types of molecules in this entry. The entry contains 5508 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

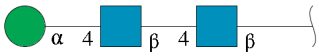
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2706	1684	472	540	10			
1	B	362	Total	C	N	O	S	0	0	0
			2706	1684	472	540	10			

- 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 10 10	0	0

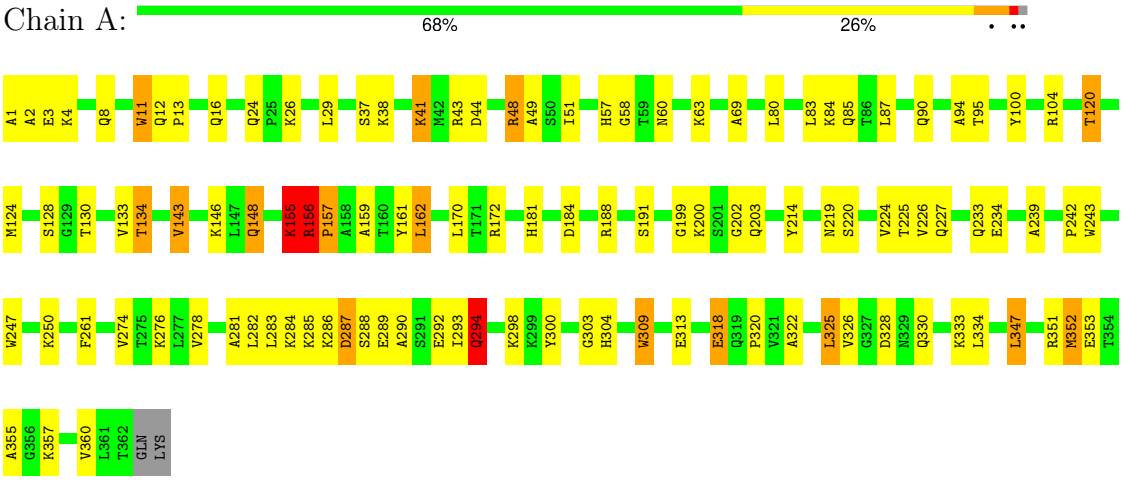
3 Residue-property plots (i)

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. 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.

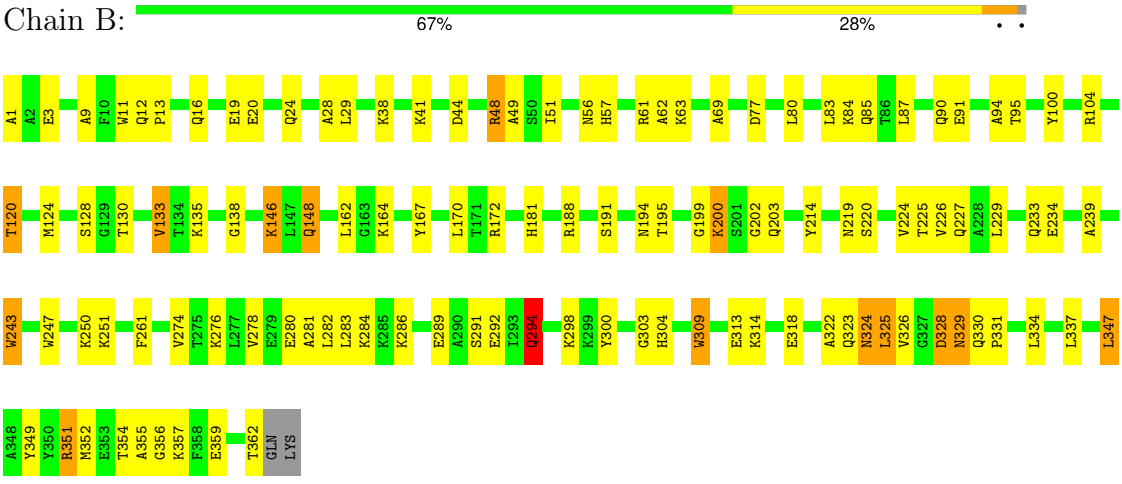
• Molecule 1: VARIANT SURFACE GLYCOPROTEIN MITAT 1.2

Chain A:



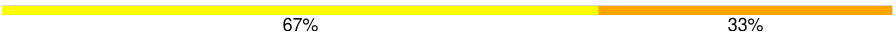
• Molecule 1: VARIANT SURFACE GLYCOPROTEIN MITAT 1.2

Chain B:



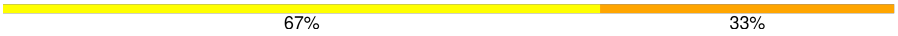
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

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: NAG, BMA, 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	0.87	1/2745 (0.0%)	1.44	30/3713 (0.8%)
1	B	0.86	1/2745 (0.0%)	1.41	28/3713 (0.8%)
All	All	0.87	2/5490 (0.0%)	1.42	58/7426 (0.8%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	19	GLU	C-O	5.76	1.34	1.23
1	A	143	VAL	CA-CB	5.08	1.65	1.54

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	48	ARG	NE-CZ-NH1	-10.88	114.86	120.30
1	B	11	TRP	CD1-CG-CD2	9.41	113.83	106.30
1	A	48	ARG	NE-CZ-NH2	9.40	125.00	120.30
1	B	48	ARG	NE-CZ-NH1	-9.23	115.68	120.30
1	A	11	TRP	CD1-CG-CD2	9.22	113.68	106.30
1	B	20	GLU	O-C-N	8.66	136.56	122.70
1	B	11	TRP	CE2-CD2-CG	-8.21	100.73	107.30
1	A	11	TRP	CE2-CD2-CG	-8.14	100.79	107.30
1	B	100	TYR	CB-CG-CD2	-8.08	116.15	121.00
1	B	309	TRP	CD1-CG-CD2	7.94	112.65	106.30
1	A	100	TYR	CB-CG-CD2	-7.85	116.29	121.00
1	A	309	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	A	243	TRP	CD1-CG-CD2	7.57	112.35	106.30
1	A	309	TRP	CE2-CD2-CG	-7.54	101.27	107.30
1	A	156	ARG	NE-CZ-NH2	7.47	124.03	120.30
1	B	48	ARG	NE-CZ-NH2	7.43	124.01	120.30
1	B	324	ASN	CA-CB-CG	7.13	129.09	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	309	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	A	243	TRP	CE2-CD2-CG	-6.90	101.78	107.30
1	B	243	TRP	CD1-CG-CD2	6.76	111.71	106.30
1	B	247	TRP	CE2-CD2-CG	-6.74	101.91	107.30
1	B	309	TRP	CG-CD2-CE3	6.71	139.94	133.90
1	A	247	TRP	CE2-CD2-CG	-6.67	101.97	107.30
1	B	234	GLU	CA-CB-CG	6.44	127.57	113.40
1	A	234	GLU	CA-CB-CG	6.43	127.55	113.40
1	B	294	GLN	CA-CB-CG	6.38	127.44	113.40
1	A	294	GLN	CA-CB-CG	6.34	127.36	113.40
1	B	243	TRP	CE2-CD2-CG	-6.31	102.25	107.30
1	A	11	TRP	CG-CD1-NE1	-6.24	103.86	110.10
1	B	104	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	A	134	THR	CA-CB-CG2	-6.19	103.73	112.40
1	B	11	TRP	CG-CD1-NE1	-6.14	103.96	110.10
1	B	300	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	A	11	TRP	CB-CG-CD1	-6.04	119.15	127.00
1	A	11	TRP	CG-CD2-CE3	6.04	139.33	133.90
1	A	170	LEU	CA-C-N	-5.86	104.31	117.20
1	A	43	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	B	309	TRP	CB-CG-CD1	-5.75	119.53	127.00
1	A	247	TRP	CD1-CG-CD2	5.74	110.89	106.30
1	A	243	TRP	CG-CD1-NE1	-5.70	104.40	110.10
1	B	11	TRP	CG-CD2-CE3	5.64	138.97	133.90
1	A	309	TRP	CG-CD2-CE3	5.63	138.96	133.90
1	B	172	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	B	11	TRP	CB-CG-CD1	-5.55	119.79	127.00
1	B	9	ALA	O-C-N	5.52	131.53	122.70
1	B	247	TRP	CD1-CG-CD2	5.34	110.58	106.30
1	B	77	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	351	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	A	170	LEU	CA-C-O	5.32	131.27	120.10
1	A	360	VAL	CA-CB-CG1	5.31	118.87	110.90
1	A	161	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	A	104	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	A	155	LYS	CA-CB-CG	5.23	124.91	113.40
1	A	172	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	A	172	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	B	57	HIS	CB-CA-C	-5.06	100.28	110.40
1	B	95	THR	CA-CB-CG2	5.02	119.43	112.40
1	A	95	THR	CA-CB-CG2	5.02	119.42	112.40

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	2706	0	2702	56	0
1	B	2706	0	2702	56	0
2	C	39	0	34	1	0
3	D	39	0	34	1	0
4	A	8	0	0	0	0
4	B	10	0	0	0	0
All	All	5508	0	5472	105	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 (105) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:GLU:O	1:B:292:GLU:HG2	2.05	0.56
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: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:164:LYS:HE3	1:B:251:LYS:HZ2	1.80	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: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: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%)	11	36
1	B	360/364 (99%)	324 (90%)	32 (9%)	4 (1%)	14	42
All	All	720/728 (99%)	647 (90%)	64 (9%)	9 (1%)	12	37

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 (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	277/279 (99%)	248 (90%)	29 (10%)	7	21
1	B	277/279 (99%)	251 (91%)	26 (9%)	8	26
All	All	554/558 (99%)	499 (90%)	55 (10%)	8	24

All (55) 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	294	GLN
1	A	318	GLU
1	A	320	PRO
1	A	325	LEU
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	80	LEU
1	B	90	GLN
1	B	120	THR
1	B	128	SER
1	B	133	VAL
1	B	135	LYS
1	B	146	LYS
1	B	148	GLN
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	276	LYS
1	B	283	LEU
1	B	294	GLN
1	B	324	ASN
1	B	325	LEU
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 (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	85	GLN
1	A	153	GLN
1	A	221	GLN
1	A	227	GLN
1	A	330	GLN
1	B	85	GLN
1	B	323	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)

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	1,2	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	1,3	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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	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(^{o})	Ideal(^{o})
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

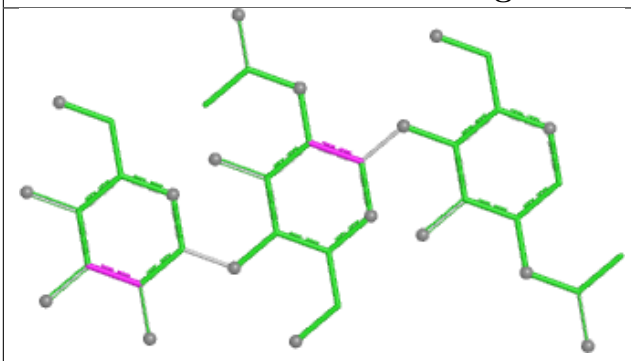
There are no ring outliers.

2 monomers are involved in 2 short contacts:

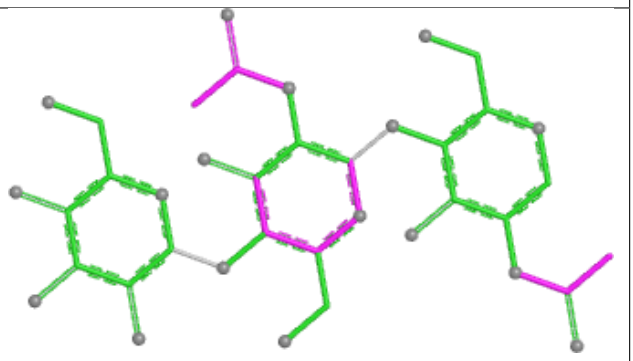
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	1	0
2	C	1	NAG	1	0

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

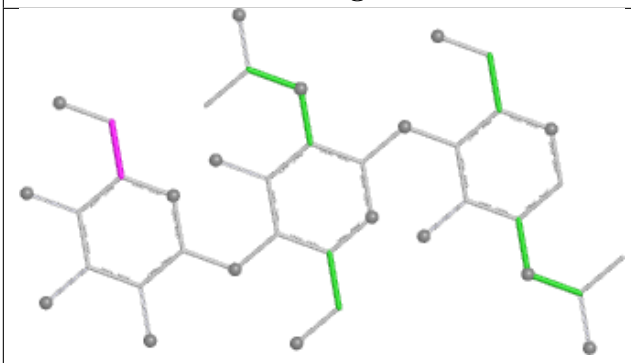
Oligosaccharide Chain C



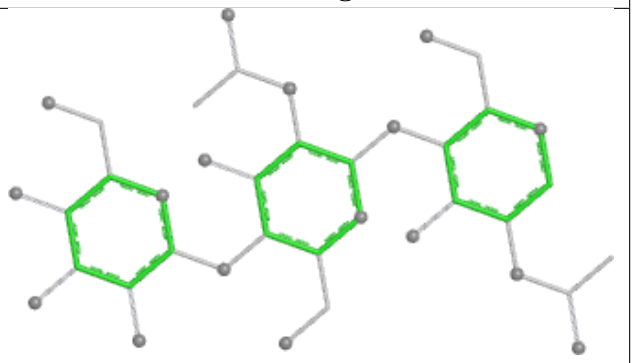
Bond lengths



Bond angles

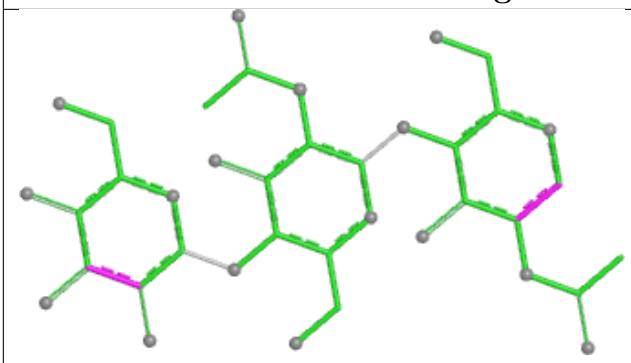


Torsions

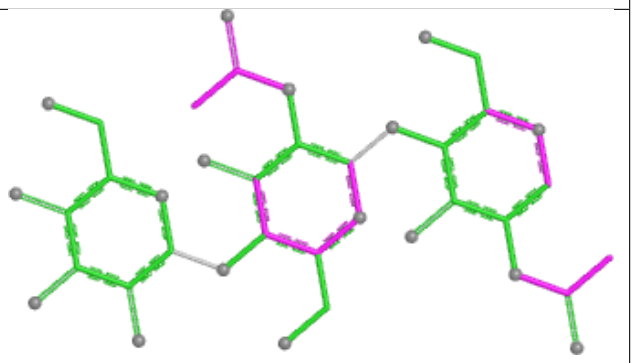


Rings

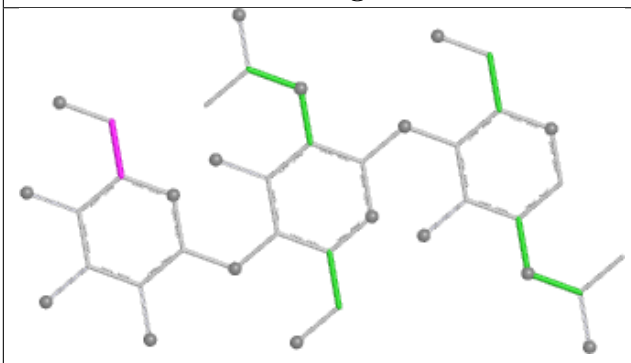
Oligosaccharide Chain D



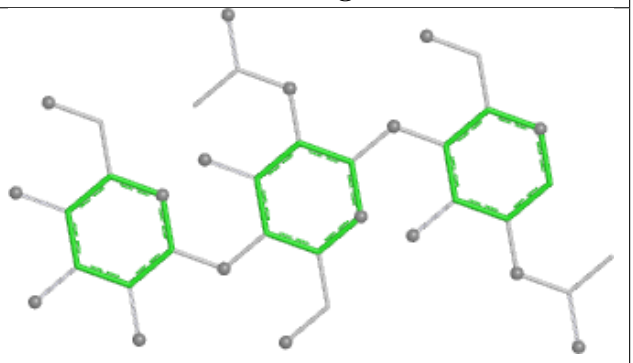
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

There are no ligands in this entry.

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

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.