



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:22 AM UTC

PDB ID : 1N47 / pdb_00001n47
Title : Isolectin B4 from Vicia villosa in complex with the Tn antigen
Authors : Babino, A.; Tello, D.; Rojas, A.; Bay, S.; Osinaga, E.; Alzari, P.M.
Deposited on : 2002-10-30
Resolution : 2.70 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

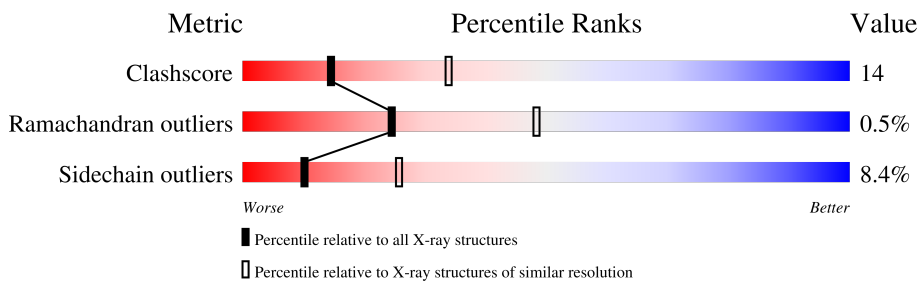
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	233	
1	B	233	
1	C	233	
1	D	233	
2	E	3	
2	F	3	
2	G	3	
2	H	3	

2 Entry composition

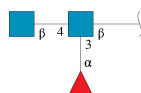
There are 7 unique types of molecules in this entry. The entry contains 7293 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Isolectin B4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1748	1113	286	347	2			
1	B	233	Total	C	N	O	S	0	0	0
			1748	1113	286	347	2			
1	C	233	Total	C	N	O	S	0	0	0
			1748	1113	286	347	2			
1	D	233	Total	C	N	O	S	0	0	0
			1748	1113	286	347	2			

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	F	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	G	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	H	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

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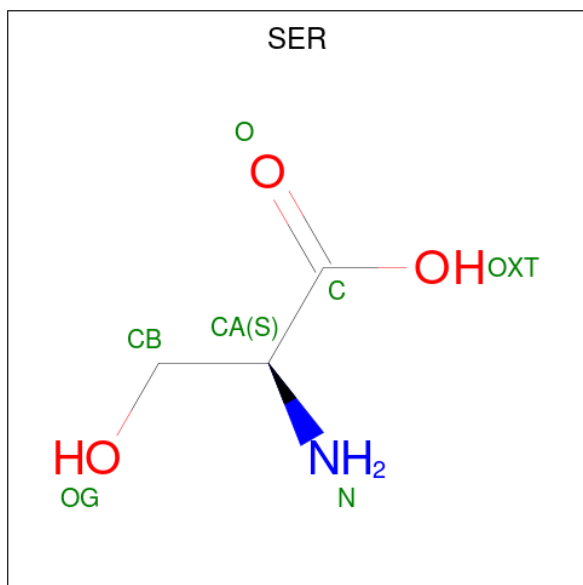
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		
4	B	1	Total	Mn	0	0
			1	1		
4	C	1	Total	Mn	0	0
			1	1		
4	D	1	Total	Mn	0	0
			1	1		

- Molecule 5 is SERINE (CCD ID: SER) (formula: C₃H₇NO₃).



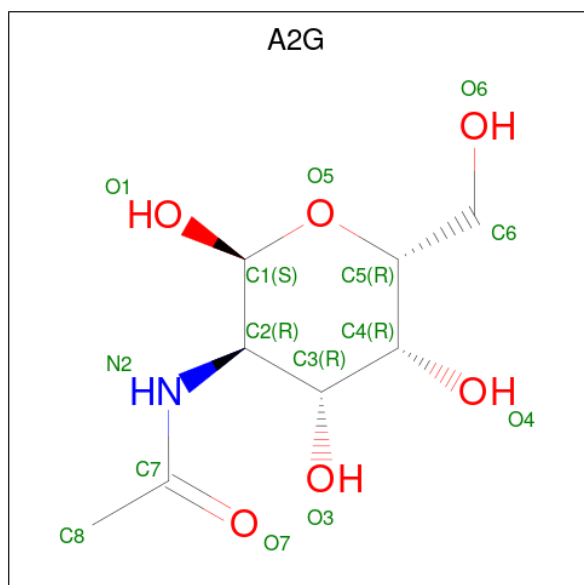
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			7	3	1	3		
5	B	1	Total	C	N	O	0	0
			7	3	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			7	3	1	3		
5	D	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 6 is 2-acetamido-2-deoxy- α -D-galactopyranose (CCD ID: A2G) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	9	Total	O	0	0
			9	9		
7	B	14	Total	O	0	0
			14	14		
7	C	18	Total	O	0	0
			18	18		

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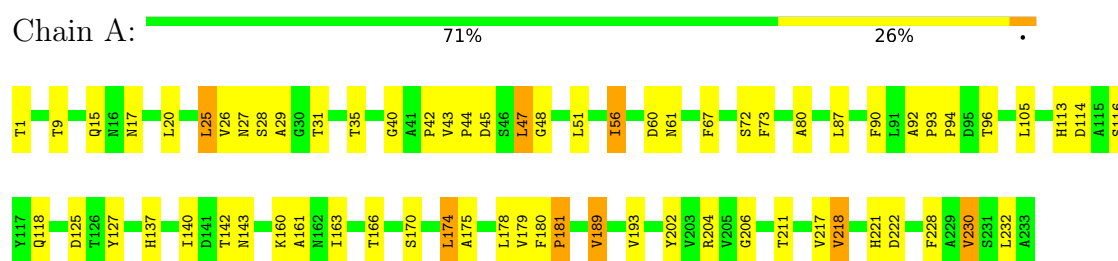
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	16	Total	O	0	0
			16	16		

3 Residue-property plots

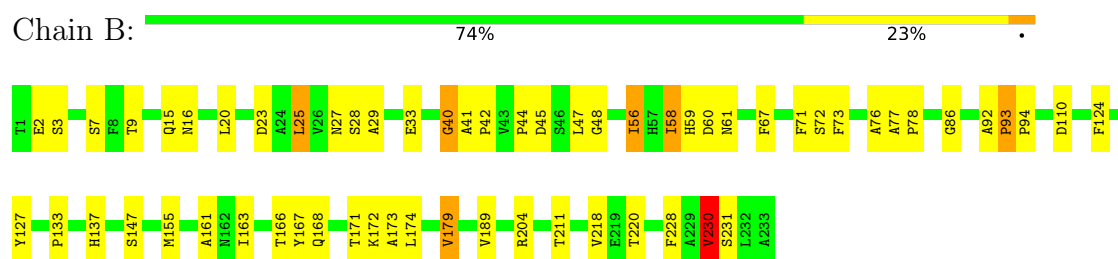
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

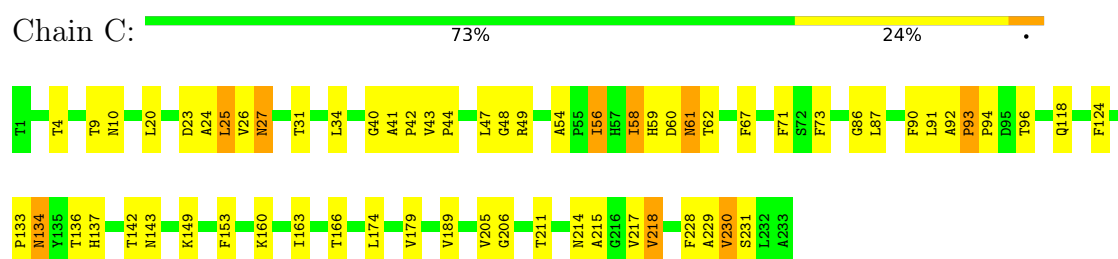
• Molecule 1: Isolectin B4



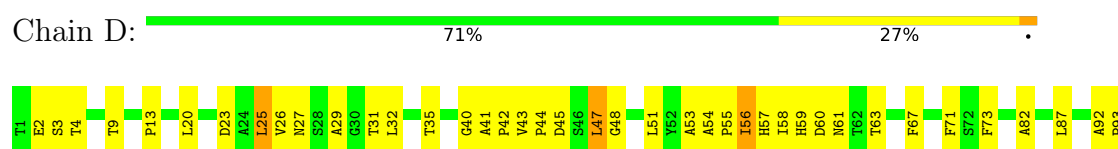
• Molecule 1: Isolectin B4

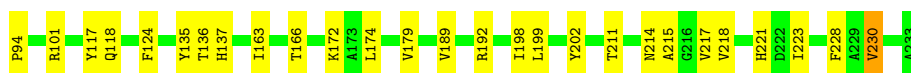


• Molecule 1: Isolectin B4



• Molecule 1: Isolectin B4





- Molecule 2: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%



- Molecule 2: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  33% 67%



- Molecule 2: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%



- Molecule 2: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	85.51Å 85.51Å 153.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	99.9 (20.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.188 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7293	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: MN, FUC, A2G, NAG, CA

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	0.79	0/1791	1.18	9/2455 (0.4%)
1	B	0.83	0/1791	1.19	9/2455 (0.4%)
1	C	0.85	0/1791	1.21	9/2455 (0.4%)
1	D	0.83	0/1791	1.17	3/2455 (0.1%)
All	All	0.83	0/7164	1.19	30/9820 (0.3%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	GLY	N-CA-C	7.03	119.59	110.45
1	B	28	SER	N-CA-C	-6.70	104.98	113.02
1	B	40	GLY	N-CA-C	-6.17	98.55	113.18
1	A	218	VAL	N-CA-C	6.00	117.35	108.65
1	D	137	HIS	N-CA-C	5.97	117.93	108.79
1	B	93	PRO	O-C-N	5.81	123.98	121.31
1	A	40	GLY	N-CA-C	-5.79	99.46	113.18
1	A	189	VAL	CB-CA-C	-5.78	100.78	111.18
1	C	137	HIS	N-CA-C	5.75	117.53	108.96
1	C	27	ASN	N-CA-C	5.74	117.95	110.43
1	A	218	VAL	N-CA-CB	-5.64	103.95	112.35
1	A	90	PHE	N-CA-C	5.62	117.33	108.96
1	C	90	PHE	N-CA-C	5.59	117.57	109.07
1	C	133	PRO	N-CA-C	-5.56	103.11	111.57
1	C	93	PRO	O-C-N	5.52	123.85	121.31
1	B	86	GLY	N-CA-C	5.49	117.94	111.63
1	B	147	SER	N-CA-C	5.49	117.37	110.24
1	A	180	PHE	CA-C-N	5.45	126.66	119.84
1	A	180	PHE	C-N-CA	5.45	126.66	119.84
1	A	28	SER	N-CA-C	-5.44	106.60	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	VAL	CB-CA-C	-5.41	102.33	110.55
1	D	53	ALA	N-CA-C	5.35	117.11	111.28
1	B	133	PRO	N-CA-C	-5.33	103.42	111.41
1	B	137	HIS	N-CA-C	5.28	116.86	108.79
1	B	179	VAL	N-CA-C	5.23	116.01	108.48
1	C	218	VAL	N-CA-C	5.17	115.10	107.75
1	C	40	GLY	N-CA-C	-5.15	100.97	113.18
1	C	86	GLY	N-CA-C	5.07	117.46	111.63
1	D	198	ILE	CB-CA-C	-5.06	106.63	111.44
1	A	206	GLY	N-CA-C	5.01	117.35	110.69

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	1748	0	1679	50	0
1	B	1748	0	1679	45	0
1	C	1748	0	1679	50	0
1	D	1748	0	1679	56	0
2	E	38	0	34	0	0
2	F	38	0	34	0	0
2	G	38	0	34	0	0
2	H	38	0	34	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	7	0	3	0	0
5	B	7	0	3	1	0
5	C	7	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	7	0	3	0	0
6	A	14	0	12	0	0
6	B	14	0	12	0	0
6	C	14	0	12	0	0
6	D	14	0	12	0	0
7	A	9	0	0	0	0
7	B	14	0	0	0	0
7	C	18	0	0	0	0
7	D	16	0	0	1	0
All	All	7293	0	6912	198	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 14.

All (198) 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:D:73:PHE:HE2	1:D:163:ILE:HD11	1.07	1.17
1:C:73:PHE:HE2	1:C:163:ILE:HD11	1.11	1.13
1:A:179:VAL:HG12	1:A:181:PRO:HD3	1.37	1.05
1:D:73:PHE:CE2	1:D:163:ILE:HD11	1.92	1.03
1:D:67:PHE:HB3	1:D:230:VAL:HG12	1.36	1.03
1:A:163:ILE:CD1	1:A:178:LEU:HD13	1.90	1.00
1:B:59:HIS:HD2	1:B:61:ASN:H	1.07	0.97
1:B:67:PHE:HB3	1:B:230:VAL:HG12	1.47	0.97
1:C:73:PHE:CE2	1:C:163:ILE:HD11	1.99	0.96
1:A:228:PHE:CE2	1:A:230:VAL:HG22	2.00	0.96
1:B:73:PHE:HE2	1:B:163:ILE:HD11	1.28	0.96
1:C:59:HIS:HD2	1:C:61:ASN:H	1.01	0.94
1:A:228:PHE:HE2	1:A:230:VAL:HG22	1.31	0.93
1:D:59:HIS:HD2	1:D:61:ASN:H	1.20	0.89
1:A:113:HIS:HE1	1:A:142:THR:O	1.56	0.88
1:B:59:HIS:CD2	1:B:61:ASN:H	1.94	0.85
1:A:56:ILE:HD13	1:A:230:VAL:HG21	1.59	0.83
1:A:228:PHE:HE2	1:A:230:VAL:CG2	1.92	0.83
1:A:179:VAL:HG12	1:A:181:PRO:CD	2.09	0.82
1:C:71:PHE:CE1	1:C:163:ILE:HD12	2.15	0.82
1:B:27:ASN:HB3	1:B:29:ALA:H	1.45	0.82
1:A:163:ILE:HD11	1:A:178:LEU:HD13	1.62	0.82
1:A:163:ILE:HD13	1:A:178:LEU:HD13	1.62	0.81
1:C:42:PRO:HB2	1:C:218:VAL:HG22	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:HIS:CD2	1:C:61:ASN:H	1.93	0.79
1:B:124:PHE:CZ	1:B:163:ILE:HD13	2.18	0.78
1:A:67:PHE:HB3	1:A:230:VAL:HG13	1.66	0.77
1:B:71:PHE:CE1	1:B:163:ILE:HD12	2.21	0.75
1:D:71:PHE:CE1	1:D:163:ILE:HD12	2.21	0.75
1:C:211:THR:HB	1:C:218:VAL:HG23	1.69	0.75
1:D:56:ILE:HD13	1:D:230:VAL:HG21	1.69	0.74
1:A:179:VAL:C	1:A:181:PRO:HD3	2.15	0.72
1:B:94:PRO:HA	1:B:204:ARG:HG3	1.71	0.72
1:C:56:ILE:CD1	1:C:230:VAL:HG11	2.20	0.71
1:D:67:PHE:CB	1:D:230:VAL:HG12	2.16	0.71
1:C:60:ASP:O	1:C:61:ASN:HB2	1.89	0.71
1:C:124:PHE:CZ	1:C:163:ILE:HD13	2.25	0.71
1:C:228:PHE:HE2	1:C:230:VAL:HG22	1.55	0.71
1:D:25:LEU:C	1:D:25:LEU:HD23	2.15	0.71
1:C:59:HIS:HD2	1:C:61:ASN:N	1.84	0.70
1:D:56:ILE:C	1:D:56:ILE:HD12	2.16	0.68
1:A:15:GLN:HG3	1:A:17:ASN:OD1	1.93	0.68
1:D:42:PRO:HB2	1:D:218:VAL:HG22	1.74	0.68
1:C:56:ILE:HD13	1:C:230:VAL:HG21	1.76	0.68
1:A:27:ASN:HB3	1:A:29:ALA:H	1.60	0.67
1:C:56:ILE:HD13	1:C:230:VAL:HG11	1.77	0.66
1:B:73:PHE:CE2	1:B:163:ILE:HD11	2.20	0.66
1:D:56:ILE:HD12	1:D:57:HIS:N	2.11	0.65
1:B:76:ALA:N	1:B:220:THR:OG1	2.23	0.64
1:D:4:THR:HB	1:D:230:VAL:CG2	2.27	0.64
1:A:163:ILE:HD13	1:A:178:LEU:CD1	2.28	0.63
1:B:67:PHE:HB3	1:B:230:VAL:CG1	2.25	0.63
1:C:134:ASN:HD22	1:C:134:ASN:C	2.06	0.62
1:B:56:ILE:HD13	1:B:230:VAL:HG21	1.80	0.62
1:B:67:PHE:CB	1:B:230:VAL:HG12	2.28	0.62
1:C:228:PHE:CE2	1:C:230:VAL:HG22	2.35	0.61
1:C:27:ASN:HB2	1:C:31:THR:H	1.65	0.61
1:D:47:LEU:HD22	1:D:48:GLY:N	2.16	0.61
1:A:25:LEU:HD23	1:A:26:VAL:N	2.15	0.61
1:D:59:HIS:CD2	1:D:61:ASN:H	2.10	0.60
1:A:142:THR:O	1:A:143:ASN:HB2	2.01	0.60
1:B:58:ILE:HD13	1:B:58:ILE:O	2.02	0.59
1:A:179:VAL:O	1:A:181:PRO:HD3	2.02	0.59
1:D:73:PHE:CE2	1:D:163:ILE:CD1	2.78	0.59
1:C:73:PHE:HE2	1:C:163:ILE:CD1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:ASP:O	1:D:61:ASN:HB2	2.03	0.58
1:B:72:SER:HA	1:B:161:ALA:O	2.04	0.57
1:A:113:HIS:CE1	1:A:142:THR:O	2.46	0.57
1:D:172:LYS:NZ	1:D:192:ARG:HH21	2.03	0.57
1:D:73:PHE:HE2	1:D:163:ILE:CD1	1.99	0.56
1:C:42:PRO:HB2	1:C:218:VAL:CG2	2.34	0.56
1:A:94:PRO:HA	1:A:204:ARG:HG3	1.88	0.56
1:A:25:LEU:HD23	1:A:25:LEU:C	2.31	0.55
1:A:35:THR:OG1	1:A:221:HIS:HD2	1.88	0.55
1:A:217:VAL:HG12	1:A:217:VAL:O	2.06	0.55
1:B:73:PHE:HE2	1:B:163:ILE:CD1	2.12	0.55
1:D:211:THR:HB	1:D:218:VAL:HG23	1.89	0.55
1:D:27:ASN:HB3	1:D:29:ALA:H	1.71	0.55
1:C:25:LEU:C	1:C:25:LEU:HD23	2.33	0.54
1:D:43:VAL:HG13	1:D:44:PRO:HD2	1.89	0.53
1:D:25:LEU:C	1:D:25:LEU:CD2	2.81	0.53
1:D:67:PHE:HB3	1:D:230:VAL:CG1	2.24	0.53
1:C:73:PHE:CE2	1:C:163:ILE:CD1	2.83	0.52
1:B:60:ASP:O	1:B:61:ASN:HB2	2.09	0.52
1:C:136:THR:HG22	1:C:153:PHE:CE1	2.45	0.52
1:C:43:VAL:CG1	1:C:44:PRO:HD2	2.40	0.52
1:D:23:ASP:HB2	1:D:47:LEU:O	2.09	0.51
1:C:4:THR:HB	1:C:230:VAL:CG2	2.41	0.51
1:A:60:ASP:O	1:A:61:ASN:HB2	2.08	0.51
1:A:87:LEU:HD12	1:A:87:LEU:C	2.35	0.51
1:B:174:LEU:C	1:B:174:LEU:HD23	2.36	0.51
1:A:125:ASP:HB3	1:A:137:HIS:CE1	2.46	0.51
1:B:172:LYS:HZ3	1:B:172:LYS:HB2	1.74	0.51
1:D:25:LEU:HD23	1:D:26:VAL:N	2.26	0.51
1:B:228:PHE:CD2	1:B:228:PHE:C	2.88	0.50
1:C:56:ILE:HD11	1:C:58:ILE:HG12	1.93	0.50
1:B:47:LEU:HD23	1:B:48:GLY:N	2.26	0.50
1:C:56:ILE:HD11	1:C:230:VAL:HG11	1.92	0.50
1:B:92:ALA:HB1	1:B:93:PRO:CD	2.42	0.50
1:A:93:PRO:HD3	1:A:118:GLN:O	2.11	0.49
1:A:113:HIS:CE1	1:A:143:ASN:HB2	2.47	0.49
1:D:2:GLU:CD	1:D:57:HIS:HD1	2.20	0.49
1:D:228:PHE:CE2	1:D:230:VAL:HG13	2.48	0.49
1:C:142:THR:O	1:C:143:ASN:HB2	2.13	0.49
1:C:134:ASN:C	1:C:134:ASN:ND2	2.71	0.49
1:B:124:PHE:CZ	1:B:163:ILE:CD1	2.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:LYS:HZ1	1:D:192:ARG:HH21	1.60	0.49
1:C:92:ALA:HB1	1:C:93:PRO:CD	2.42	0.48
1:A:47:LEU:HD23	1:A:48:GLY:N	2.28	0.48
1:B:67:PHE:CB	1:B:230:VAL:CG1	2.89	0.48
1:D:59:HIS:CD2	1:D:59:HIS:C	2.91	0.48
1:B:168:GLN:HE22	1:C:160:LYS:NZ	2.11	0.47
1:A:174:LEU:HD23	1:A:175:ALA:N	2.30	0.47
1:D:59:HIS:HE1	1:D:199:LEU:O	1.98	0.47
1:D:67:PHE:CB	1:D:230:VAL:CG1	2.89	0.47
1:C:48:GLY:O	1:C:49:ARG:HG2	2.14	0.47
1:B:25:LEU:C	1:B:25:LEU:HD23	2.39	0.47
1:A:72:SER:HA	1:A:161:ALA:O	2.15	0.47
1:B:127:TYR:HH	5:B:306:SER:N	2.13	0.47
1:D:94:PRO:HD3	1:D:202:TYR:O	2.14	0.47
1:B:56:ILE:HD13	1:B:230:VAL:HG11	1.96	0.47
1:C:4:THR:HB	1:C:230:VAL:HG23	1.96	0.47
1:C:217:VAL:O	1:C:217:VAL:HG12	2.14	0.47
1:A:27:ASN:HD22	1:A:31:THR:HB	1.79	0.46
1:C:91:LEU:HG	1:C:205:VAL:HG12	1.97	0.46
1:D:82:ALA:HB1	1:D:217:VAL:HG22	1.98	0.46
1:D:135:TYR:O	1:D:136:THR:C	2.58	0.46
1:C:54:ALA:HB2	1:D:54:ALA:HB2	1.97	0.46
1:C:43:VAL:HG13	1:C:44:PRO:HD2	1.98	0.46
1:A:73:PHE:C	1:A:73:PHE:CD1	2.94	0.46
1:B:110:ASP:C	1:B:110:ASP:OD2	2.58	0.46
1:D:228:PHE:CZ	1:D:230:VAL:HG13	2.51	0.45
1:D:27:ASN:HB2	1:D:31:THR:H	1.82	0.45
1:B:124:PHE:CE1	1:B:163:ILE:HD13	2.50	0.45
1:B:171:THR:C	1:B:172:LYS:HZ3	2.25	0.45
1:B:228:PHE:HE2	1:B:230:VAL:HG22	1.83	0.44
1:B:42:PRO:HB2	1:B:218:VAL:HG13	1.98	0.44
1:C:41:ALA:HA	1:C:42:PRO:HD3	1.85	0.44
1:D:13:PRO:HA	1:D:26:VAL:HB	1.99	0.44
1:A:179:VAL:O	1:A:181:PRO:CD	2.64	0.44
1:B:77:ALA:HA	1:B:78:PRO:HD2	1.82	0.44
1:D:4:THR:HB	1:D:230:VAL:HG23	1.99	0.44
1:A:92:ALA:HB1	1:A:93:PRO:HD2	1.99	0.44
1:B:155:MET:HE3	1:B:155:MET:HB3	1.67	0.44
1:C:58:ILE:HD11	1:C:67:PHE:CD2	2.53	0.44
1:C:60:ASP:O	1:C:61:ASN:CB	2.61	0.44
1:A:44:PRO:O	1:A:45:ASP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ASP:O	1:C:24:ALA:C	2.59	0.44
1:C:93:PRO:HA	1:C:94:PRO:HD3	1.92	0.44
1:C:87:LEU:C	1:C:87:LEU:HD12	2.43	0.43
1:D:47:LEU:CD2	1:D:48:GLY:N	2.80	0.43
1:B:59:HIS:HD2	1:B:61:ASN:N	1.92	0.43
1:D:92:ALA:HB1	1:D:93:PRO:HD2	2.01	0.43
1:A:114:ASP:OD2	1:A:116:SER:OG	2.36	0.43
1:B:27:ASN:OD1	1:B:33:GLU:OE2	2.37	0.43
1:A:193:VAL:O	1:A:193:VAL:HG13	2.18	0.43
1:D:124:PHE:CZ	1:D:163:ILE:HD13	2.54	0.43
1:A:202:TYR:CG	1:B:16:ASN:HB2	2.54	0.42
1:A:1:THR:HA	1:A:232:LEU:O	2.19	0.42
1:A:56:ILE:CD1	1:A:230:VAL:HG11	2.49	0.42
1:D:32:LEU:HB3	1:D:223:ILE:HB	2.01	0.42
1:D:214:ASN:O	1:D:215:ALA:C	2.62	0.42
1:A:31:THR:CG2	1:A:222:ASP:HB3	2.50	0.42
1:A:211:THR:HB	1:A:218:VAL:HG23	2.02	0.42
1:D:2:GLU:OE1	1:D:57:HIS:ND1	2.44	0.42
1:D:43:VAL:CG1	1:D:44:PRO:HD2	2.50	0.42
1:C:214:ASN:O	1:C:215:ALA:C	2.63	0.42
1:D:101:ARG:HB2	7:D:409:HOH:O	2.19	0.42
1:B:93:PRO:HA	1:B:94:PRO:HD3	1.94	0.42
1:B:211:THR:HB	1:B:218:VAL:HG23	2.02	0.41
1:D:35:THR:OG1	1:D:221:HIS:HD2	2.03	0.41
1:A:92:ALA:HB1	1:A:93:PRO:CD	2.51	0.41
1:D:47:LEU:HD22	1:D:47:LEU:C	2.46	0.41
1:B:92:ALA:HB1	1:B:93:PRO:HD2	2.02	0.41
1:D:60:ASP:O	1:D:61:ASN:CB	2.69	0.41
1:D:117:TYR:O	1:D:118:GLN:C	2.62	0.41
1:B:41:ALA:HA	1:B:42:PRO:HD3	1.91	0.41
1:D:41:ALA:HA	1:D:42:PRO:HD3	1.91	0.41
1:C:93:PRO:HD3	1:C:118:GLN:O	2.21	0.41
1:A:47:LEU:HD23	1:A:47:LEU:C	2.46	0.41
1:D:44:PRO:O	1:D:45:ASP:HB2	2.20	0.41
1:A:42:PRO:HB2	1:A:218:VAL:HG22	2.03	0.41
1:A:25:LEU:HD23	1:A:26:VAL:C	2.46	0.40
1:B:127:TYR:CD1	1:B:127:TYR:C	2.99	0.40
1:D:93:PRO:HD3	1:D:118:GLN:O	2.20	0.40
1:C:34:LEU:O	1:C:48:GLY:HA3	2.21	0.40
1:C:67:PHE:HB3	1:C:230:VAL:HG13	2.01	0.40
1:C:67:PHE:HB3	1:C:230:VAL:CG1	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ALA:HB1	1:C:93:PRO:HD2	2.04	0.40
1:D:54:ALA:HA	1:D:55:PRO:HD3	1.98	0.40
1:A:127:TYR:CD1	1:A:127:TYR:C	2.99	0.40
1:B:167:TYR:HA	1:B:173:ALA:O	2.22	0.40
1:C:25:LEU:HD23	1:C:26:VAL:N	2.35	0.40
1:A:43:VAL:HA	1:A:44:PRO:HD3	1.87	0.40
1:A:93:PRO:HA	1:A:94:PRO:HD3	1.92	0.40
1:C:4:THR:O	1:C:229:ALA:HA	2.22	0.40
1:D:87:LEU:HD12	1:D:87:LEU:C	2.45	0.40
1:B:44:PRO:O	1:B:45:ASP:HB2	2.22	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	231/233 (99%)	208 (90%)	22 (10%)	1 (0%)	30	54
1	B	231/233 (99%)	214 (93%)	15 (6%)	2 (1%)	14	35
1	C	231/233 (99%)	215 (93%)	15 (6%)	1 (0%)	30	54
1	D	231/233 (99%)	217 (94%)	13 (6%)	1 (0%)	30	54
All	All	924/932 (99%)	854 (92%)	65 (7%)	5 (0%)	24	48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	ALA
1	C	61	ASN
1	B	15	GLN
1	B	40	GLY
1	D	40	GLY

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	184/184 (100%)	168 (91%)	16 (9%)	9	24
1	B	184/184 (100%)	170 (92%)	14 (8%)	12	30
1	C	184/184 (100%)	167 (91%)	17 (9%)	8	22
1	D	184/184 (100%)	170 (92%)	14 (8%)	12	30
All	All	736/736 (100%)	675 (92%)	61 (8%)	10	26

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	20	LEU
1	A	25	LEU
1	A	47	LEU
1	A	51	LEU
1	A	56	ILE
1	A	96	THR
1	A	105	LEU
1	A	140	ILE
1	A	160	LYS
1	A	166	THR
1	A	170	SER
1	A	174	LEU
1	A	181	PRO
1	A	189	VAL
1	A	230	VAL
1	B	2	GLU
1	B	3	SER
1	B	7	SER
1	B	9	THR
1	B	20	LEU
1	B	23	ASP
1	B	25	LEU
1	B	56	ILE

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Mol	Chain	Res	Type
1	B	58	ILE
1	B	166	THR
1	B	179	VAL
1	B	189	VAL
1	B	230	VAL
1	B	231	SER
1	C	9	THR
1	C	10	ASN
1	C	20	LEU
1	C	25	LEU
1	C	47	LEU
1	C	56	ILE
1	C	58	ILE
1	C	62	THR
1	C	96	THR
1	C	134	ASN
1	C	149	LYS
1	C	166	THR
1	C	174	LEU
1	C	179	VAL
1	C	189	VAL
1	C	230	VAL
1	C	231	SER
1	D	3	SER
1	D	9	THR
1	D	20	LEU
1	D	25	LEU
1	D	47	LEU
1	D	51	LEU
1	D	56	ILE
1	D	58	ILE
1	D	63	THR
1	D	166	THR
1	D	174	LEU
1	D	179	VAL
1	D	189	VAL
1	D	230	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN

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Mol	Chain	Res	Type
1	A	113	HIS
1	A	118	GLN
1	A	129	ASN
1	A	168	GLN
1	A	221	HIS
1	B	16	ASN
1	B	59	HIS
1	B	113	HIS
1	B	221	HIS
1	C	16	ASN
1	C	59	HIS
1	C	113	HIS
1	C	118	GLN
1	C	134	ASN
1	C	143	ASN
1	C	221	HIS
1	D	10	ASN
1	D	16	ASN
1	D	59	HIS
1	D	162	ASN
1	D	214	ASN
1	D	221	HIS

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 ⓘ

12 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	E	1	2,1	14,14,15	0.68	0	17,19,21	1.15	1 (5%)
2	FUC	E	2	2	10,10,11	0.61	0	14,14,16	1.58	3 (21%)
2	NAG	E	3	2	14,14,15	0.43	0	17,19,21	1.08	1 (5%)
2	NAG	F	1	2,1	14,14,15	0.66	0	17,19,21	1.61	3 (17%)
2	FUC	F	2	2	10,10,11	0.83	0	14,14,16	1.05	0
2	NAG	F	3	2	14,14,15	0.56	0	17,19,21	1.23	2 (11%)
2	NAG	G	1	2,1	14,14,15	0.66	0	17,19,21	1.81	2 (11%)
2	FUC	G	2	2	10,10,11	0.64	0	14,14,16	1.24	3 (21%)
2	NAG	G	3	2	14,14,15	0.65	0	17,19,21	1.61	3 (17%)
2	NAG	H	1	2,1	14,14,15	0.71	0	17,19,21	1.50	3 (17%)
2	FUC	H	2	2	10,10,11	0.66	0	14,14,16	1.56	4 (28%)
2	NAG	H	3	2	14,14,15	0.52	0	17,19,21	1.45	3 (17%)

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	E	1	2,1	-	0/6/23/26	0/1/1/1
2	FUC	E	2	2	-	-	0/1/1/1
2	NAG	E	3	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	F	2	2	-	-	0/1/1/1
2	NAG	F	3	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	G	2	2	-	-	0/1/1/1
2	NAG	G	3	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	FUC	H	2	2	-	-	0/1/1/1
2	NAG	H	3	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	NAG	C1-O5-C5	5.85	120.03	112.19
2	G	3	NAG	C2-N2-C7	-4.74	116.55	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	O5-C1-C2	-3.89	105.27	111.29
2	E	1	NAG	C2-N2-C7	-3.80	117.81	122.90
2	G	1	NAG	C2-N2-C7	-3.74	117.89	122.90
2	E	2	FUC	C6-C5-C4	-3.66	106.39	113.08
2	H	3	NAG	C1-O5-C5	3.64	117.06	112.19
2	F	1	NAG	O5-C5-C6	3.63	114.72	107.66
2	H	1	NAG	C1-O5-C5	3.13	116.38	112.19
2	E	2	FUC	O5-C5-C4	2.93	114.82	109.55
2	F	3	NAG	C1-O5-C5	2.89	116.06	112.19
2	E	3	NAG	C1-O5-C5	2.82	115.96	112.19
2	H	1	NAG	C3-C4-C5	-2.60	105.53	110.23
2	G	2	FUC	C3-C4-C5	2.57	113.71	109.81
2	F	1	NAG	C1-O5-C5	-2.54	108.78	112.19
2	H	1	NAG	O3-C3-C4	-2.54	104.39	110.38
2	H	3	NAG	C4-C3-C2	-2.53	107.32	111.02
2	G	2	FUC	C6-C5-C4	-2.38	108.72	113.08
2	E	2	FUC	C1-O5-C5	2.27	118.33	112.97
2	H	2	FUC	C1-C2-C3	2.19	112.84	109.64
2	G	2	FUC	O5-C5-C4	2.19	113.49	109.55
2	G	3	NAG	C1-C2-N2	-2.18	106.99	110.43
2	H	2	FUC	O5-C1-C2	2.15	115.91	110.79
2	G	3	NAG	C4-C3-C2	-2.14	107.88	111.02
2	F	3	NAG	C2-N2-C7	-2.11	120.07	122.90
2	H	2	FUC	O5-C5-C4	2.06	113.25	109.55
2	H	3	NAG	O4-C4-C5	2.04	114.36	109.32
2	H	2	FUC	C2-C3-C4	2.04	114.45	110.86

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	3	NAG	C4-C5-C6-O6
2	E	3	NAG	O5-C5-C6-O6
2	H	3	NAG	C4-C5-C6-O6
2	H	3	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	G	3	NAG	C8-C7-N2-C2
2	F	1	NAG	O5-C5-C6-O6
2	G	3	NAG	O7-C7-N2-C2
2	H	3	NAG	C8-C7-N2-C2

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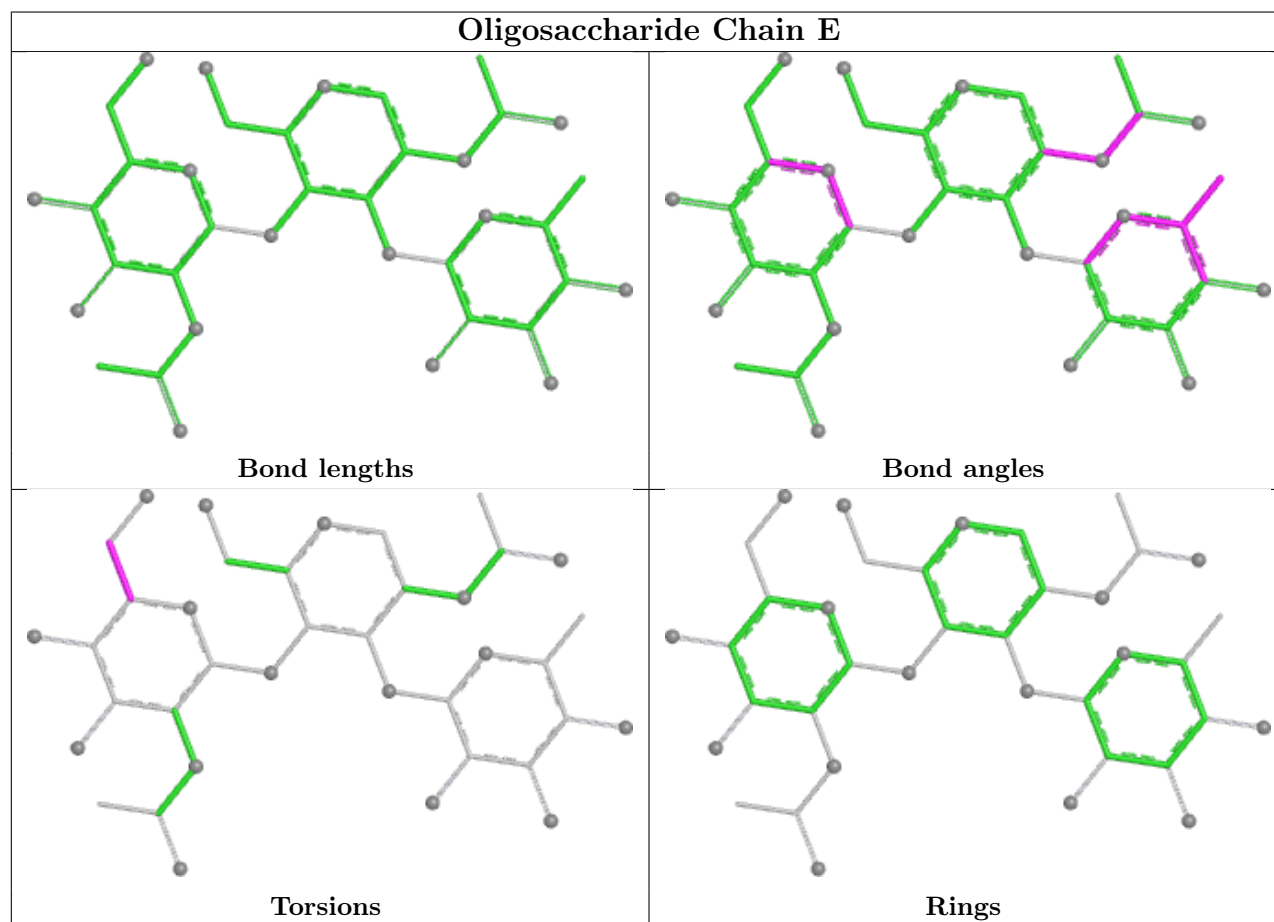
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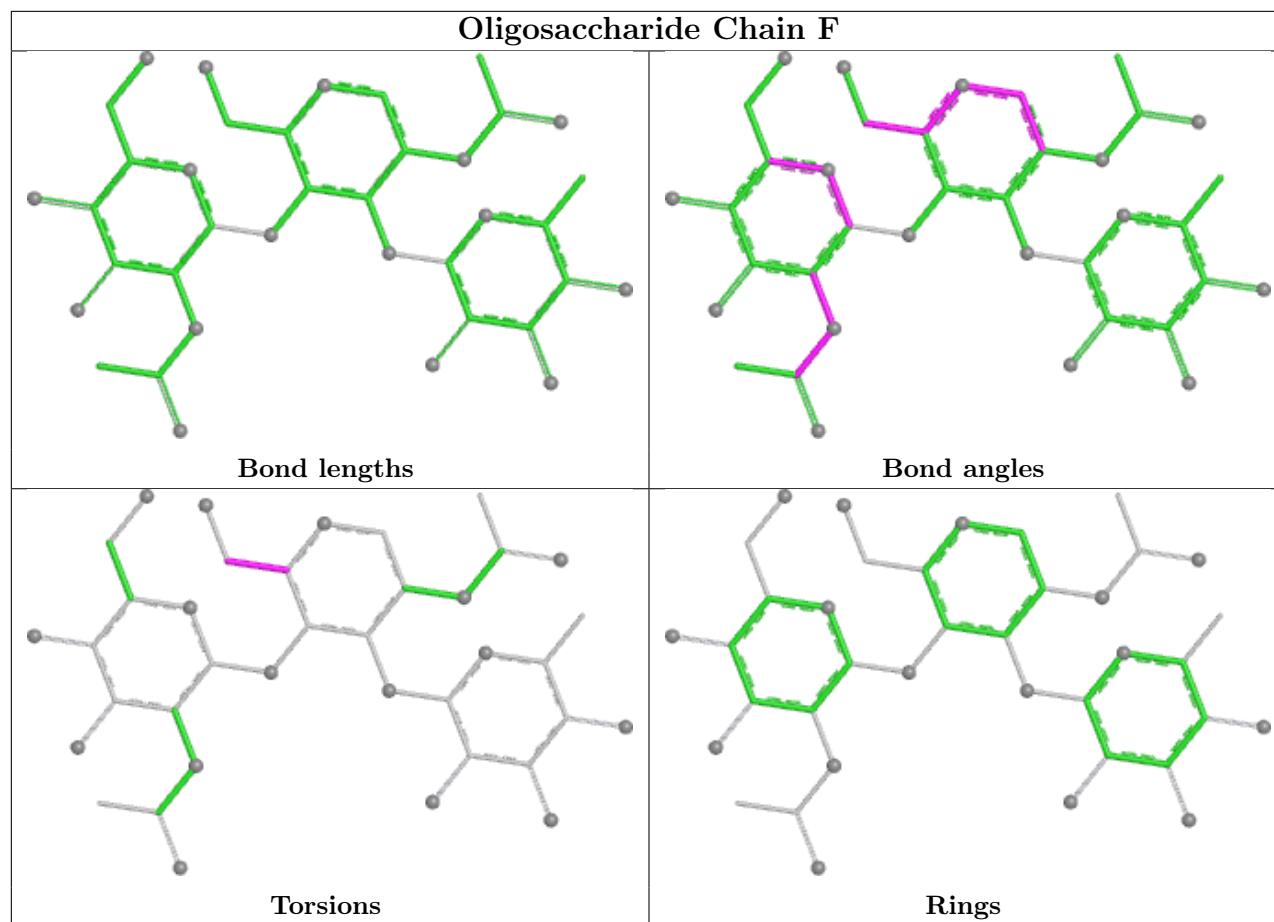
Mol	Chain	Res	Type	Atoms
2	H	3	NAG	O7-C7-N2-C2

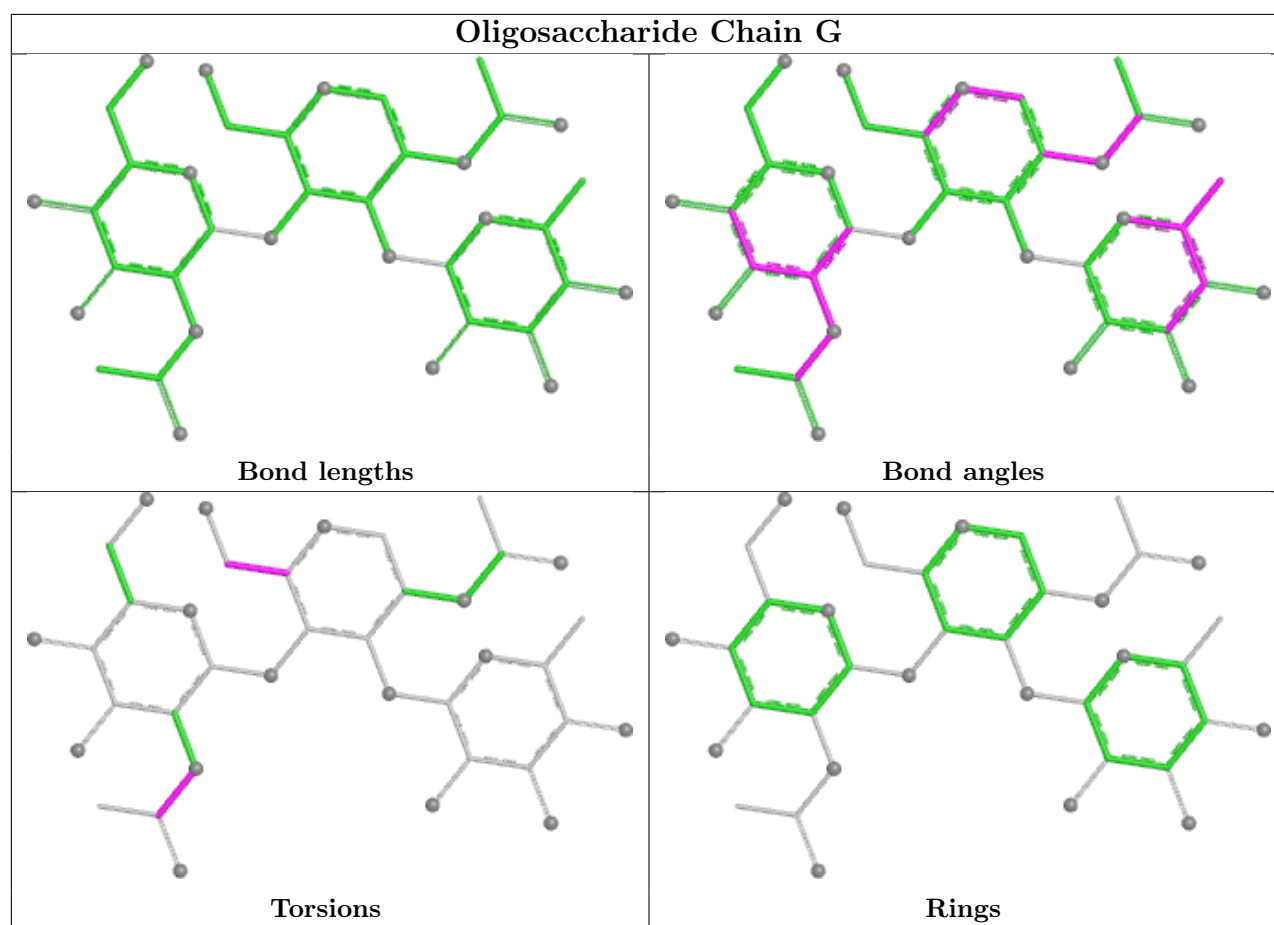
There are no ring outliers.

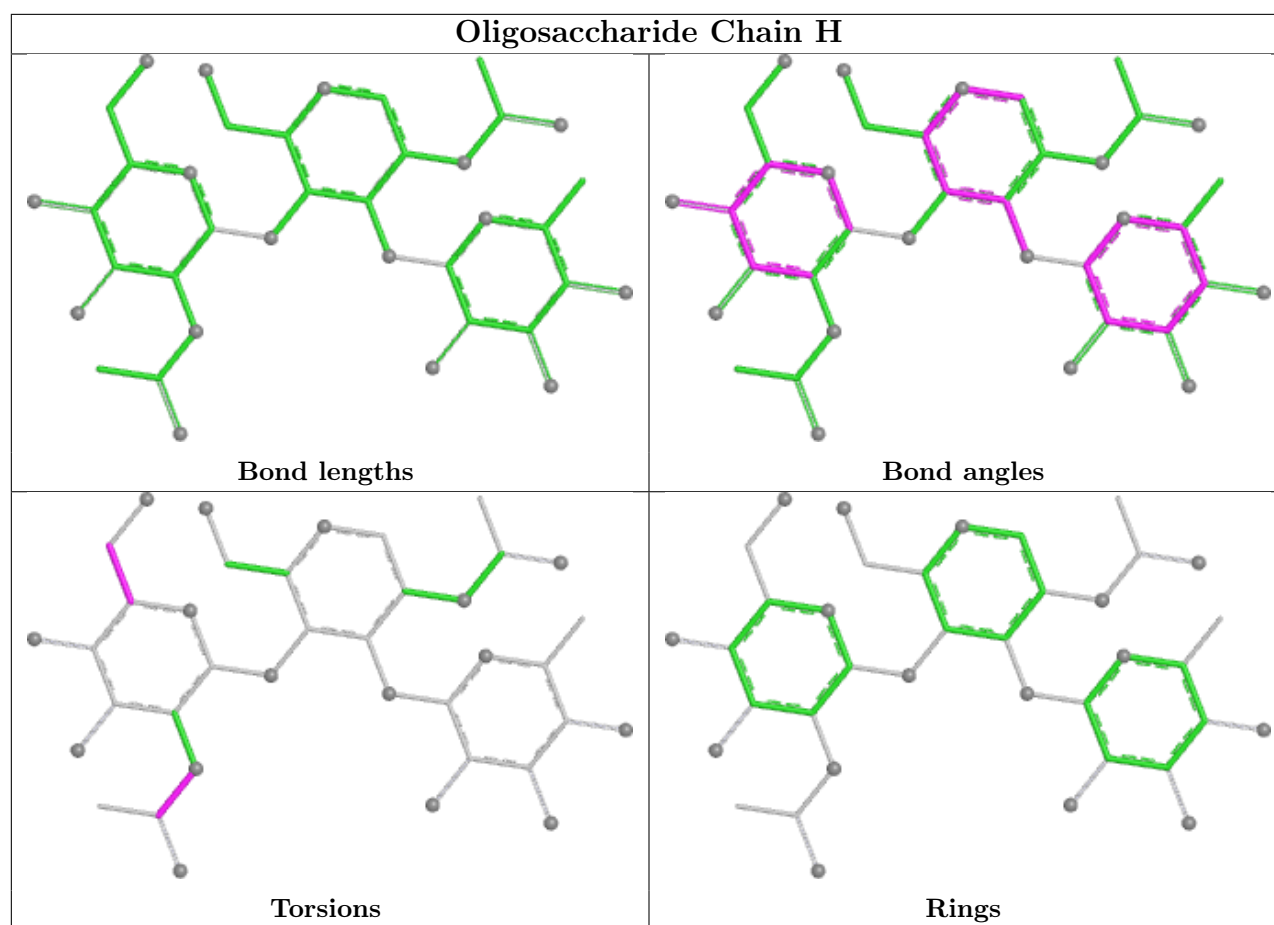
No monomer is involved in short contacts.

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](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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	$\# Z > 2$
5	SER	D	306	6	4,6,6	1.08	1 (25%)	2,7,7	1.23	0
6	A2G	D	307	5	14,14,15	0.44	0	17,19,21	1.24	2 (11%)
5	SER	A	306	6	4,6,6	1.23	1 (25%)	2,7,7	1.60	1 (50%)
6	A2G	B	307	5	14,14,15	0.39	0	17,19,21	1.92	4 (23%)
5	SER	B	306	6	4,6,6	1.18	1 (25%)	2,7,7	1.47	1 (50%)
6	A2G	C	307	5	14,14,15	0.44	0	17,19,21	1.24	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SER	C	306	6	4,6,6	1.53	1 (25%)	2,7,7	1.50	1 (50%)
6	A2G	A	307	5	14,14,15	0.50	0	17,19,21	1.29	3 (17%)

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
5	SER	D	306	6	-	0/6/6/6	-
6	A2G	D	307	5	-	2/6/23/26	0/1/1/1
5	SER	A	306	6	-	0/6/6/6	-
6	A2G	B	307	5	-	1/6/23/26	0/1/1/1
5	SER	B	306	6	-	2/6/6/6	-
6	A2G	C	307	5	-	2/6/23/26	0/1/1/1
5	SER	C	306	6	-	2/6/6/6	-
6	A2G	A	307	5	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	306	SER	OXT-C	-2.98	1.21	1.30
5	A	306	SER	OXT-C	-2.40	1.23	1.30
5	B	306	SER	OXT-C	-2.31	1.23	1.30
5	D	306	SER	OXT-C	-2.05	1.24	1.30

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	307	A2G	C1-C2-N2	-4.85	102.78	110.43
6	B	307	A2G	C1-O5-C5	3.92	117.44	112.19
6	D	307	A2G	C1-C2-N2	-3.12	105.51	110.43
6	C	307	A2G	C2-N2-C7	-2.83	119.10	122.90
6	A	307	A2G	C1-C2-N2	-2.53	106.44	110.43
6	C	307	A2G	C3-C4-C5	2.44	114.66	110.23
6	B	307	A2G	C4-C3-C2	-2.42	107.47	111.02
6	A	307	A2G	C4-C3-C2	-2.41	107.49	111.02
6	D	307	A2G	C1-O5-C5	2.34	115.32	112.19
6	A	307	A2G	C2-N2-C7	-2.21	119.94	122.90
5	A	306	SER	OXT-C-O	-2.15	119.19	124.08
6	C	307	A2G	C6-C5-C4	-2.08	107.92	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	306	SER	OXT-C-O	-2.07	119.37	124.08
5	B	306	SER	OXT-C-O	-2.07	119.39	124.08
6	B	307	A2G	C6-C5-C4	-2.01	108.08	113.02

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	306	SER	N-CA-CB-OG
5	C	306	SER	N-CA-CB-OG
6	C	307	A2G	C4-C5-C6-O6
6	C	307	A2G	O5-C5-C6-O6
5	B	306	SER	C-CA-CB-OG
6	D	307	A2G	C4-C5-C6-O6
6	D	307	A2G	O5-C5-C6-O6
6	B	307	A2G	C4-C5-C6-O6
5	C	306	SER	C-CA-CB-OG
6	A	307	A2G	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	306	SER	1	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.