Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2024 – 10:45 AM EDT

PDB ID	:	1N47
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:

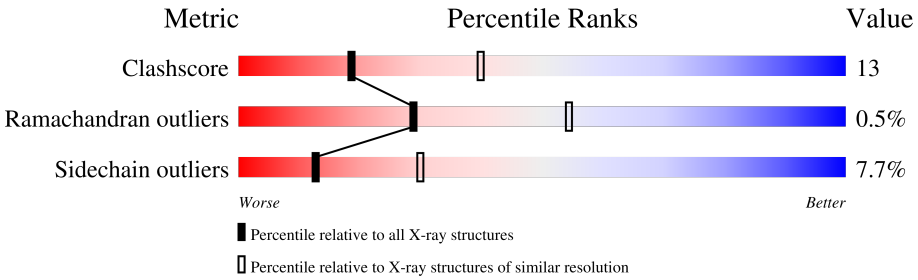
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	233	71% 27% .
1	B	233	76% 21% .
1	C	233	76% 21% .
1	D	233	73% 24% .
2	E	3	100%
2	F	3	100%
2	G	3	100%
2	H	3	100%

2 Entry composition

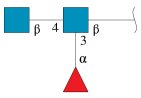
There are 7 unique types of molecules in this entry. The entry contains 7293 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: CA) (formula: Ca).

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

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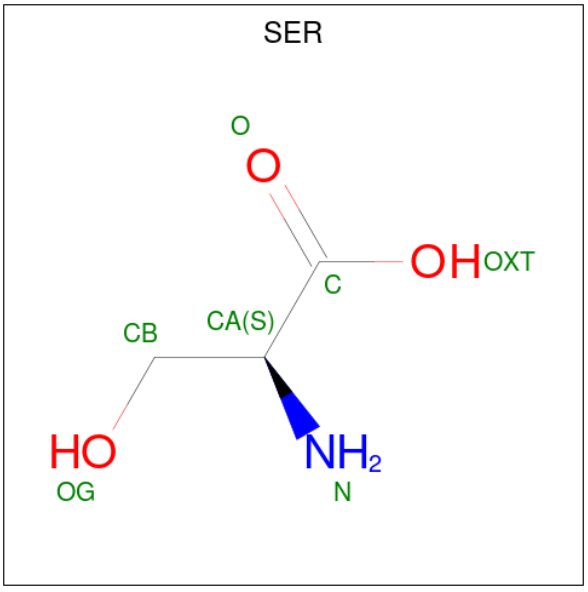
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 5 is SERINE (three-letter code: SER) (formula: $C_3H_7NO_3$).



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

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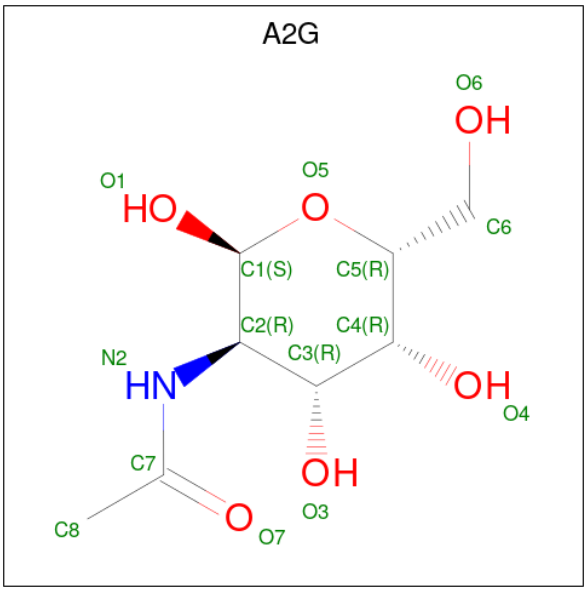
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O 7 3 1 3	0	0
5	D	1	Total C N O 7 3 1 3	0	0

- Molecule 6 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is water.

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

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

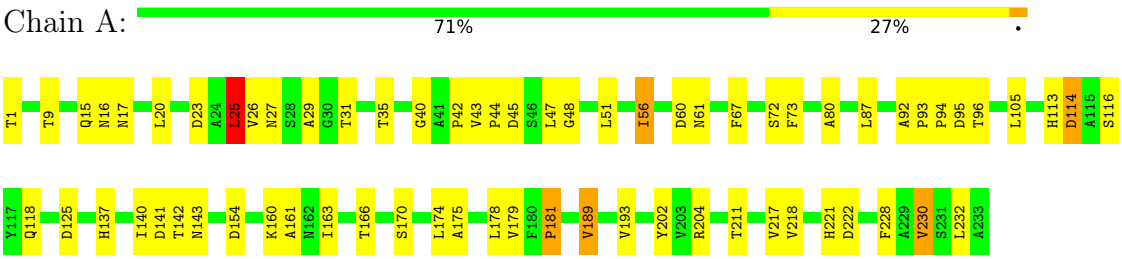
3 Residue-property plots (i)

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.

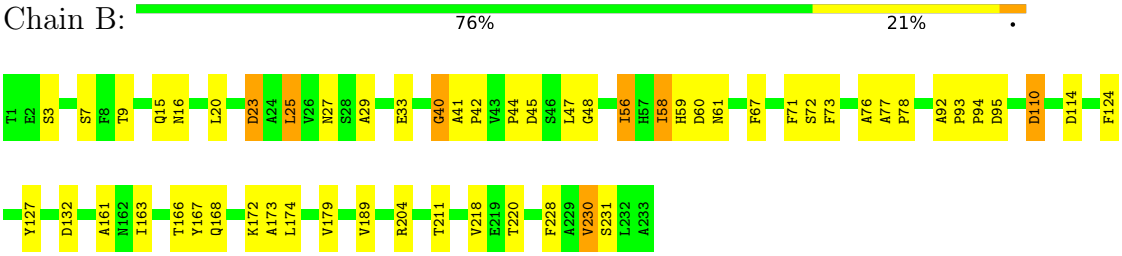
• Molecule 1: Isolectin B4

Chain A:



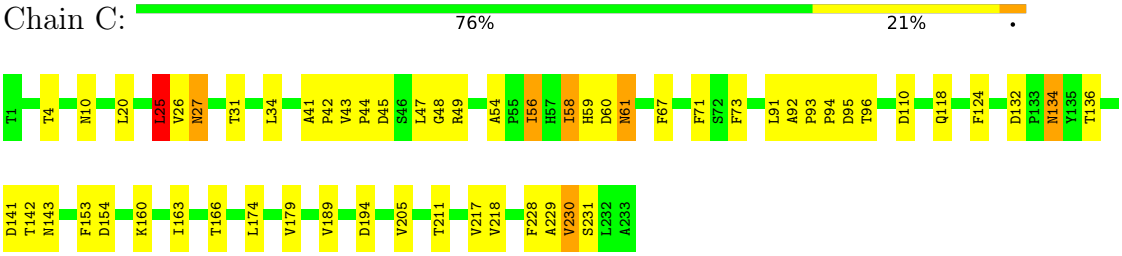
• Molecule 1: Isolectin B4

Chain B:



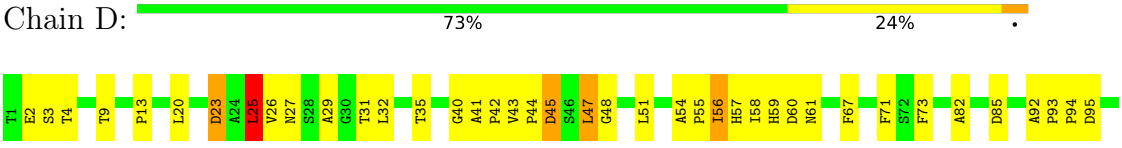
• Molecule 1: Isolectin B4

Chain C:



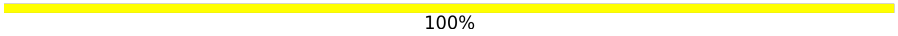
• Molecule 1: Isolectin B4

Chain D:



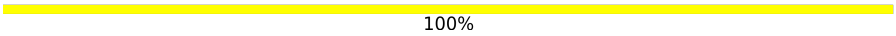
• Molecule 2: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



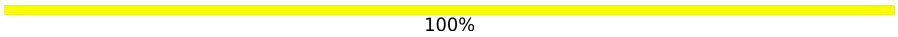
• Molecule 2: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



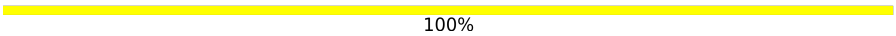
• Molecule 2: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• 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:



4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, FUC, A2G, MN

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	0.62	0/1791	0.93	8/2455 (0.3%)
1	B	0.65	0/1791	0.93	6/2455 (0.2%)
1	C	0.67	0/1791	0.94	9/2455 (0.4%)
1	D	0.66	0/1791	0.94	7/2455 (0.3%)
All	All	0.65	0/7164	0.93	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(^{o})	Ideal(^{o})
1	B	114	ASP	CB-CG-OD2	7.78	125.30	118.30
1	C	110	ASP	CB-CG-OD2	7.74	125.27	118.30
1	D	85	ASP	CB-CG-OD2	7.26	124.83	118.30
1	B	95	ASP	CB-CG-OD2	6.51	124.16	118.30
1	C	25	LEU	CA-CB-CG	6.50	130.26	115.30
1	C	141	ASP	CB-CG-OD2	6.45	124.11	118.30
1	A	95	ASP	CB-CG-OD2	6.45	124.10	118.30
1	B	23	ASP	CB-CG-OD2	6.43	124.09	118.30
1	D	23	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	114	ASP	CB-CG-OD2	6.37	124.03	118.30
1	C	45	ASP	CB-CG-OD2	6.25	123.93	118.30
1	C	154	ASP	CB-CG-OD2	6.05	123.75	118.30
1	D	114	ASP	CB-CG-OD2	5.88	123.59	118.30
1	D	45	ASP	CB-CG-OD2	5.84	123.56	118.30
1	B	40	GLY	N-CA-C	-5.82	98.55	113.10
1	A	189	VAL	CB-CA-C	-5.59	100.78	111.40
1	A	23	ASP	CB-CG-OD2	5.53	123.27	118.30
1	A	25	LEU	CA-CB-CG	5.52	127.99	115.30
1	B	110	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	141	ASP	CB-CG-OD2	5.50	123.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	40	GLY	N-CA-C	-5.46	99.46	113.10
1	C	95	ASP	CB-CG-OD2	5.45	123.21	118.30
1	C	194	ASP	CB-CG-OD2	5.42	123.17	118.30
1	D	154	ASP	CB-CG-OD2	5.37	123.13	118.30
1	D	25	LEU	CA-CB-CG	5.24	127.36	115.30
1	D	95	ASP	CB-CG-OD2	5.23	123.00	118.30
1	C	132	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	27	ASN	CB-CA-C	-5.19	100.03	110.40
1	A	154	ASP	CB-CG-OD2	5.13	122.91	118.30
1	B	132	ASP	CB-CG-OD2	5.05	122.84	118.30

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	1748	0	1679	47	0
1	B	1748	0	1679	43	0
1	C	1748	0	1679	47	0
1	D	1748	0	1679	52	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	186	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 13.

All (186) 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: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:C:59:HIS:HD2	1:C:61:ASN:N	1.84	0.70
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:179:VAL:C	1:A:181:PRO:HD3	2.15	0.67
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:25:LEU:C	1:D:25:LEU:HD23	2.15	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:D:56:ILE:HD12	1:D:56:ILE:C	2.16	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: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
1:D:60:ASP:O	1:D:61:ASN:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:SER:HA	1:B:161:ALA:O	2.04	0.57
1:C:134:ASN:HD22	1:C:134:ASN:C	2.06	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: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:D:43:VAL:HG13	1:D:44:PRO:HD2	1.89	0.53
1:D:172:LYS:HZ1	1:D:192:ARG:HH21	1.55	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:125:ASP:HB3	1:A:137:HIS:CE1	2.46	0.51
1:A:25:LEU:HD23	1:A:25:LEU:C	2.31	0.51
1:D:25:LEU:HD23	1:D:26:VAL:N	2.26	0.51
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:C:25:LEU:C	1:C:25:LEU:HD23	2.33	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:B:124:PHE:CZ	1:B:163:ILE:CD1	2.94	0.49
1:D:25:LEU:C	1:D:25:LEU:CD2	2.81	0.48
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:72:SER:HA	1:A:161:ALA:O	2.15	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:B:127:TYR:HH	5:B:306:SER:N	2.12	0.47
1:C:4:THR:HB	1:C:230:VAL:HG23	1.96	0.47
1:A:87:LEU:HD12	1:A:87:LEU:C	2.35	0.47
1:C:217:VAL:O	1:C:217:VAL:HG12	2.14	0.47
1:B:174:LEU:C	1:B:174:LEU:HD23	2.36	0.46
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: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:B:228:PHE:CD2	1:B:228:PHE:C	2.88	0.46
1:D:228:PHE:CZ	1:D:230:VAL:HG13	2.51	0.45
1:B:172:LYS:HZ3	1:B:172:LYS:HB2	1.81	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:D:2:GLU:CD	1:D:57:HIS:HD1	2.20	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: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
1:C:93:PRO:HA	1:C:94:PRO:HD3	1.92	0.44
1:D:59:HIS:CD2	1:D:59:HIS:C	2.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ASN:C	1:C:134:ASN:ND2	2.71	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:B:25:LEU:C	1:B:25:LEU:HD23	2.39	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: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:B:110:ASP:C	1:B:110:ASP:OD2	2.58	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: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:172:LYS:HB2	1:B:172:LYS:NZ	2.35	0.42
1:B:211:THR:HB	1:B:218:VAL:HG23	2.02	0.41
1:D:135:TYR:O	1:D:136:THR:C	2.58	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:A:73:PHE:CD1	1:A:73:PHE:C	2.94	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: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: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: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:CG1	2.50	0.40
1:C:67:PHE:HB3	1:C:230:VAL:HG13	2.01	0.40
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: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:B:44:PRO:O	1:B:45:ASP:HB2	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	231/233 (99%)	208 (90%)	22 (10%)	1 (0%)	34	60
1	B	231/233 (99%)	214 (93%)	15 (6%)	2 (1%)	17	40
1	C	231/233 (99%)	215 (93%)	15 (6%)	1 (0%)	34	60
1	D	231/233 (99%)	217 (94%)	13 (6%)	1 (0%)	34	60
All	All	924/932 (99%)	854 (92%)	65 (7%)	5 (0%)	29	54

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 (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	184/184 (100%)	169 (92%)	15 (8%)	11	26
1	B	184/184 (100%)	171 (93%)	13 (7%)	14	34
1	C	184/184 (100%)	170 (92%)	14 (8%)	13	30
1	D	184/184 (100%)	170 (92%)	14 (8%)	13	30
All	All	736/736 (100%)	680 (92%)	56 (8%)	13	30

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	16	ASN
1	A	20	LEU
1	A	25	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	181	PRO
1	A	189	VAL
1	A	230	VAL
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
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	10	ASN
1	C	20	LEU
1	C	25	LEU
1	C	47	LEU
1	C	56	ILE
1	C	58	ILE
1	C	96	THR
1	C	134	ASN
1	C	166	THR
1	C	174	LEU
1	C	179	VAL
1	C	189	VAL
1	C	230	VAL
1	C	231	SER

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Mol	Chain	Res	Type
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	166	THR
1	D	174	LEU
1	D	179	VAL
1	D	189	VAL
1	D	192	ARG
1	D	230	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	27	ASN
1	A	113	HIS
1	A	221	HIS
1	B	16	ASN
1	B	59	HIS
1	B	221	HIS
1	C	16	ASN
1	C	59	HIS
1	C	134	ASN
1	C	221	HIS
1	D	10	ASN
1	D	16	ASN
1	D	59	HIS
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 (i)

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

5.5 Carbohydrates (i)

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	1,2	14,14,15	0.70	0	17,19,21	1.11	1 (5%)
2	FUC	E	2	2	10,10,11	0.62	0	14,14,16	1.61	3 (21%)
2	NAG	E	3	2	14,14,15	0.43	0	17,19,21	1.13	2 (11%)
2	NAG	F	1	1,2	14,14,15	0.67	0	17,19,21	1.77	3 (17%)
2	FUC	F	2	2	10,10,11	0.85	0	14,14,16	1.07	1 (7%)
2	NAG	F	3	2	14,14,15	0.57	0	17,19,21	1.28	2 (11%)
2	NAG	G	1	1,2	14,14,15	0.69	0	17,19,21	1.77	2 (11%)
2	FUC	G	2	2	10,10,11	0.65	0	14,14,16	1.25	3 (21%)
2	NAG	G	3	2	14,14,15	0.66	0	17,19,21	1.59	3 (17%)
2	NAG	H	1	1,2	14,14,15	0.73	0	17,19,21	1.54	3 (17%)
2	FUC	H	2	2	10,10,11	0.67	0	14,14,16	1.77	4 (28%)
2	NAG	H	3	2	14,14,15	0.51	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	1,2	-	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	1,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,2	-	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	1,2	-	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 (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1	NAG	C1-O5-C5	5.78	120.03	112.19
2	F	1	NAG	O5-C5-C6	4.80	114.72	107.20
2	G	3	NAG	C2-N2-C7	-4.46	116.55	122.90
2	F	1	NAG	O5-C1-C2	-3.81	105.27	111.29
2	E	2	FUC	C6-C5-C4	-3.62	106.39	113.07
2	H	3	NAG	C1-O5-C5	3.60	117.06	112.19
2	E	1	NAG	C2-N2-C7	-3.58	117.81	122.90
2	G	1	NAG	C2-N2-C7	-3.52	117.89	122.90
2	H	2	FUC	O5-C1-C2	3.33	115.91	110.77
2	H	1	NAG	C1-O5-C5	3.09	116.38	112.19
2	E	2	FUC	O5-C5-C4	2.95	114.82	109.52
2	F	3	NAG	C1-O5-C5	2.86	116.06	112.19
2	E	3	NAG	C1-O5-C5	2.78	115.96	112.19
2	H	1	NAG	C3-C4-C5	-2.64	105.53	110.24
2	H	2	FUC	C1-C2-C3	2.58	112.84	109.67
2	H	1	NAG	O3-C3-C4	-2.58	104.39	110.35
2	G	2	FUC	C3-C4-C5	2.53	113.71	109.77
2	H	3	NAG	C4-C3-C2	-2.53	107.32	111.02
2	F	1	NAG	C1-O5-C5	-2.52	108.78	112.19
2	E	2	FUC	C1-O5-C5	2.45	118.33	112.78
2	G	2	FUC	C6-C5-C4	-2.35	108.72	113.07
2	F	3	NAG	O5-C5-C6	2.32	110.84	107.20
2	G	2	FUC	O5-C5-C4	2.21	113.49	109.52
2	G	3	NAG	C4-C3-C2	-2.14	107.88	111.02
2	H	2	FUC	O5-C5-C4	2.08	113.25	109.52
2	H	2	FUC	C2-C3-C4	2.06	114.45	110.89
2	E	3	NAG	O5-C5-C6	2.05	110.42	107.20
2	G	3	NAG	C1-C2-N2	-2.05	106.99	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2	FUC	C2-C3-C4	-2.05	107.36	110.89
2	H	3	NAG	O4-C4-C5	2.04	114.36	109.30

There are no chirality outliers.

All (12) torsion outliers are listed below:

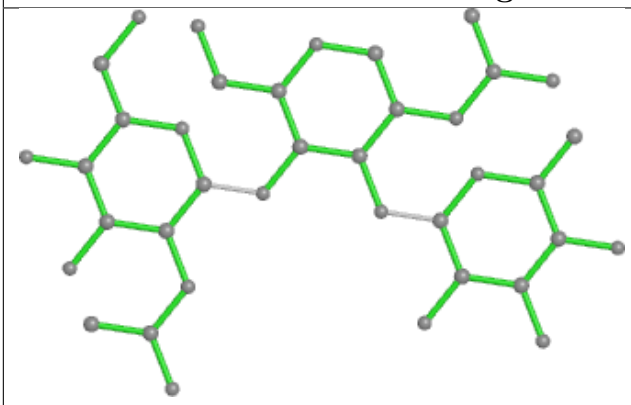
Mol	Chain	Res	Type	Atoms
2	E	3	NAG	C4-C5-C6-O6
2	E	3	NAG	O5-C5-C6-O6
2	H	3	NAG	C4-C5-C6-O6
2	H	3	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	G	3	NAG	C8-C7-N2-C2
2	F	1	NAG	O5-C5-C6-O6
2	G	3	NAG	O7-C7-N2-C2
2	H	3	NAG	C8-C7-N2-C2
2	H	3	NAG	O7-C7-N2-C2

There are no ring outliers.

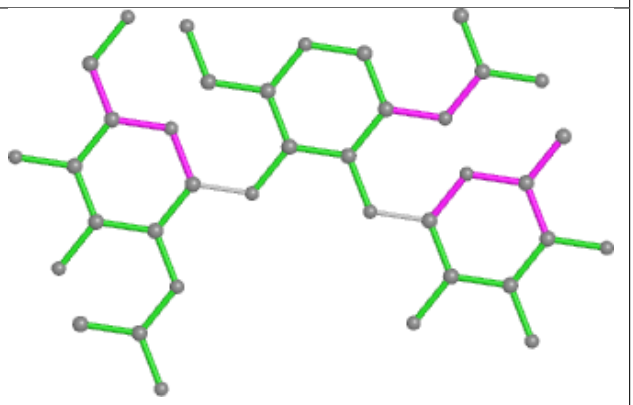
No monomer is involved in short contacts.

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

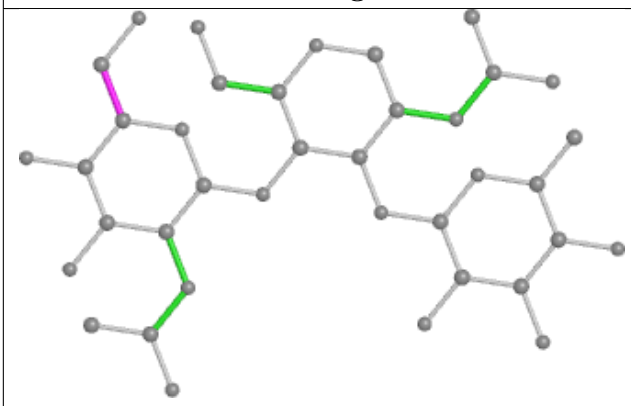
Oligosaccharide Chain E



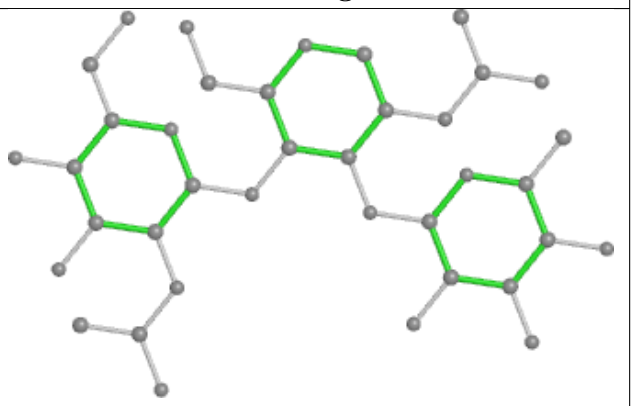
Bond lengths



Bond angles

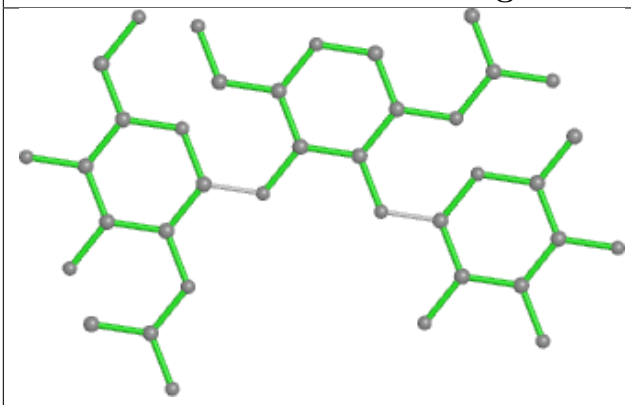


Torsions

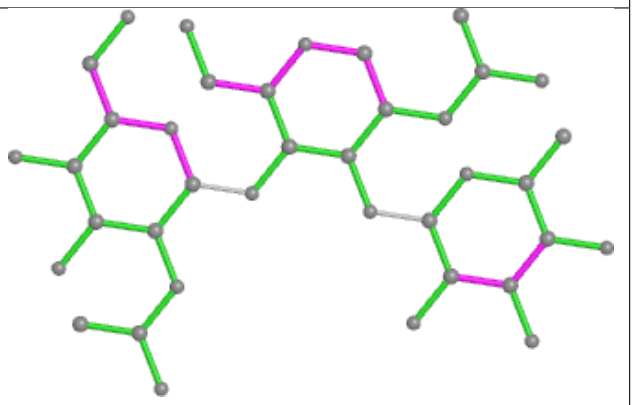


Rings

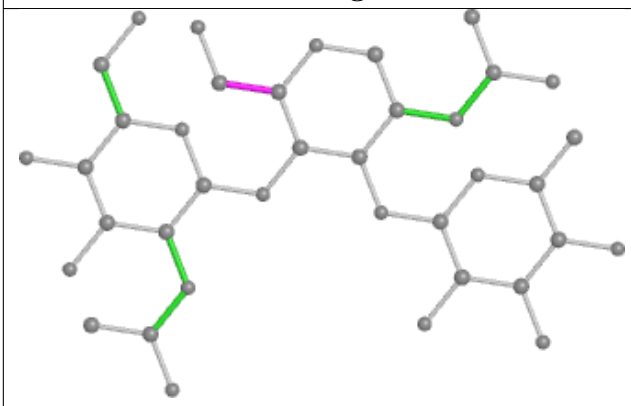
Oligosaccharide Chain F



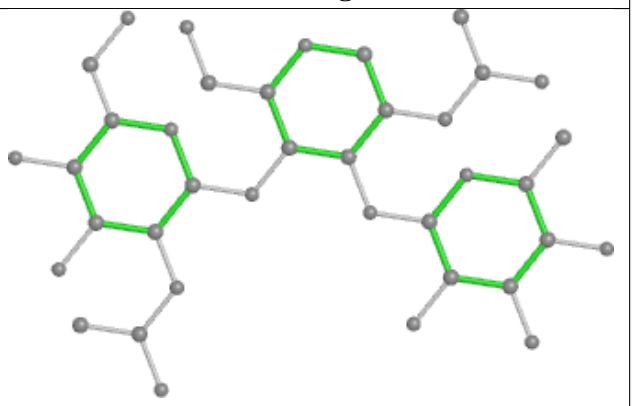
Bond lengths



Bond angles

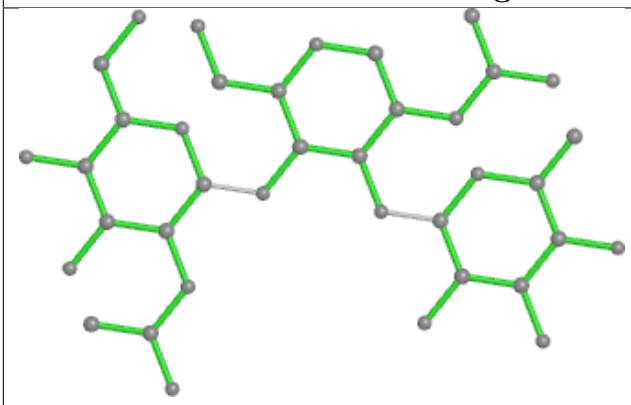


Torsions

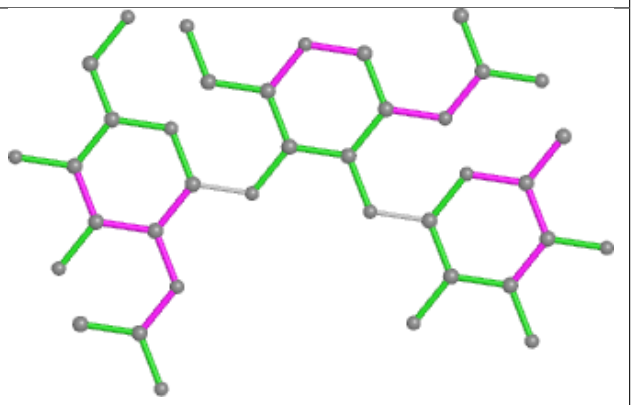


Rings

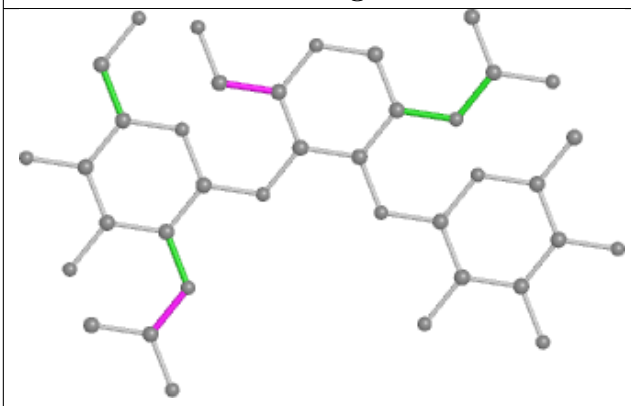
Oligosaccharide Chain G



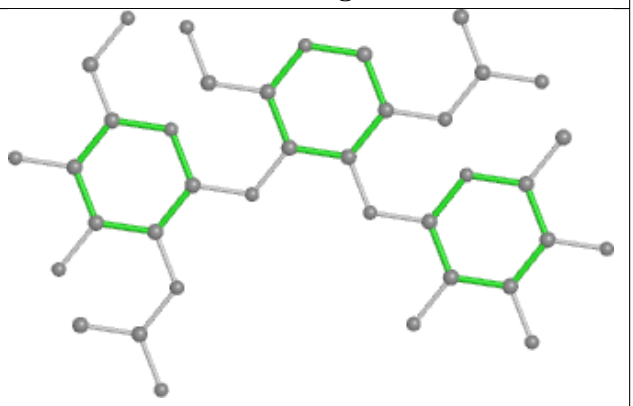
Bond lengths



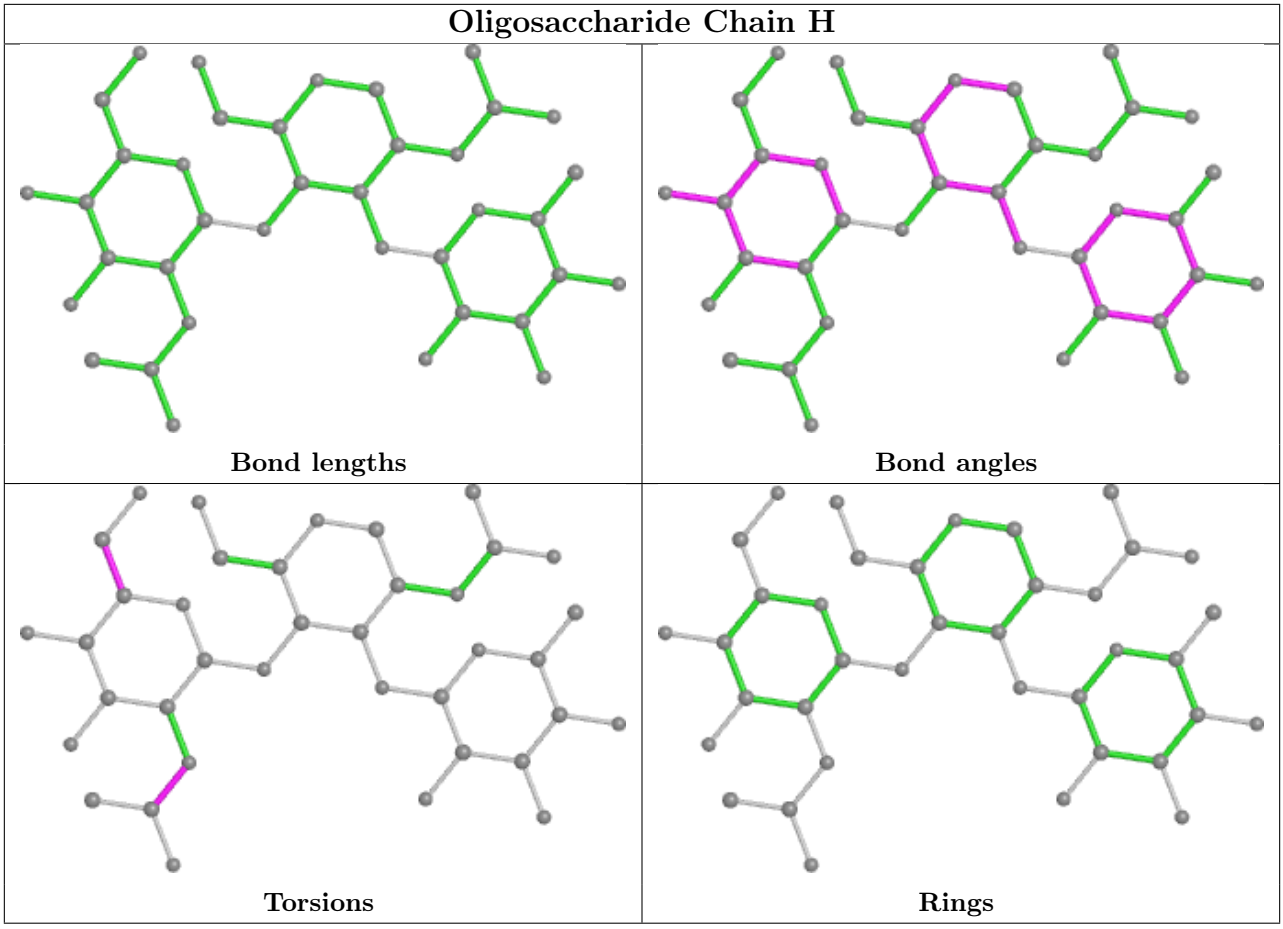
Bond angles



Torsions



Rings



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	$\#\|Z\| > 2$
6	A2G	A	307	5	14,14,15	0.50	0	17,19,21	1.26	3 (17%)
6	A2G	B	307	5	14,14,15	0.39	0	17,19,21	1.86	4 (23%)
5	SER	A	306	6	5,6,6	1.07	1 (20%)	5,7,7	1.37	2 (40%)
5	SER	D	306	6	5,6,6	0.95	0	5,7,7	1.29	1 (20%)
5	SER	B	306	6	5,6,6	1.04	1 (20%)	5,7,7	1.40	2 (40%)
6	A2G	C	307	5	14,14,15	0.45	0	17,19,21	1.22	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	A2G	D	307	5	14,14,15	0.44	0	17,19,21	1.25	3 (17%)
5	SER	C	306	6	5,6,6	1.32	1 (20%)	5,7,7	1.37	1 (20%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	306	SER	OXT-C	-2.87	1.21	1.30
5	A	306	SER	OXT-C	-2.30	1.23	1.30
5	B	306	SER	OXT-C	-2.21	1.23	1.30

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	307	A2G	C1-C2-N2	-4.51	102.78	110.49
6	B	307	A2G	C1-O5-C5	3.87	117.44	112.19
6	D	307	A2G	C1-C2-N2	-2.91	105.51	110.49
6	C	307	A2G	C2-N2-C7	-2.67	119.10	122.90
6	C	307	A2G	C3-C4-C5	2.48	114.66	110.24
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	A	307	A2G	C1-C2-N2	-2.37	106.44	110.49
6	D	307	A2G	C1-O5-C5	2.31	115.32	112.19
6	C	307	A2G	C6-C5-C4	-2.17	107.92	113.00
5	A	306	SER	OXT-C-O	-2.16	119.19	124.09
6	B	307	A2G	C6-C5-C4	-2.10	108.08	113.00
6	A	307	A2G	C2-N2-C7	-2.08	119.94	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	306	SER	OXT-C-O	-2.08	119.37	124.09
5	B	306	SER	OXT-C-O	-2.07	119.39	124.09
5	A	306	SER	OXT-C-CA	2.07	120.44	113.38
6	D	307	A2G	O5-C5-C6	2.04	110.40	107.20
5	D	306	SER	OXT-C-CA	2.02	120.28	113.38
5	B	306	SER	OXT-C-CA	2.02	120.26	113.38

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.