wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2021 – 03:17 PM EDT

PDB ID	:	1D9K
Title	:	CRYSTAL STRUCTURE OF COMPLEX BETWEEN D10 TCR AND PMHC I-AK/CA
Authors	:	Reinherz, E.L.; Tan, K.; Tang, L.; Kern, P.; Liu, J.-H.; Xiong, Y.; Hussey, R.E.; Smolyar, A.; Hare, B.; Zhang, R.; Joachimiak, A.; Chang, H.-C.; Wagner, G.; Wang, J.-H.
Deposited on	:	1999-10-28
Resolution	:	3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

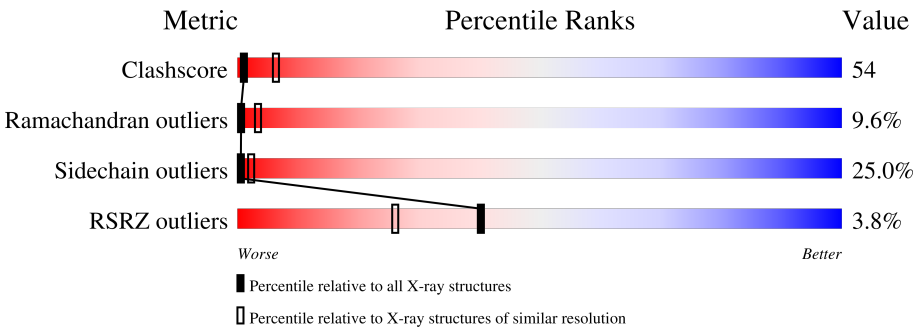
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	110	.% 26% 45% 26% .
1	E	110	.% 32% 49% 16% .
2	B	112	30% 44% 22% .
2	F	112	3% 29% 50% 18% .
3	C	183	.% 36% 51% 13% .
3	G	183	3% 21% 58% 19% .
4	D	188	6% 26% 57% 17% .

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Mol	Chain	Length	Quality of chain
4	H	188	10% 10% 56% 31% •
5	P	16	6% 38% 38% 25%
5	Q	16	12% 19% 50% 25% 6%
6	I	2	50% 50%
6	J	2	50% 50%
6	K	2	50% 50%
6	L	2	100%

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
6	NAG	I	1	X	-	-	-
6	NAG	J	1	X	-	-	X
6	NDG	J	2	-	-	-	X
6	NAG	K	1	X	-	-	-
6	NDG	K	2	-	-	-	X
6	NAG	L	1	-	-	-	X
6	NDG	L	2	-	-	-	X
7	NAG	C	201	X	-	-	X
7	NAG	G	201	X	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9962 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 T-CELL RECEPTOR D10 (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	110	877	563	145	167	2	0	0	0
1	E	110	877	563	145	167	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	SER	CYS	engineered mutation	GB 5724764
E	115	SER	CYS	engineered mutation	GB 5724764

- Molecule 2 is a protein called T-CELL RECEPTOR D10 (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	112	854	528	155	168	3	0	0	0
2	F	112	854	528	155	168	3	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	116B	GLY	GLU	SEE REMARK 999	GB 1791255
B	116C	SER	ASP	SEE REMARK 999	GB 1791255
F	116B	GLY	GLU	SEE REMARK 999	GB 1791255
F	116C	SER	ASP	SEE REMARK 999	GB 1791255

- Molecule 3 is a protein called MHC I-AK A CHAIN (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	183	1485	959	237	286	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	183	1485	959	237	286	3	0	0	0

- Molecule 4 is a protein called MHC I-AK B CHAIN (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	188	1575	991	287	291	6	0	0	0
			Total	C	N	O	S			
4	H	188	1575	991	287	291	6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	2	GLY	ASN	conflict	UNP P06343
H	2	GLY	ASN	conflict	UNP P06343

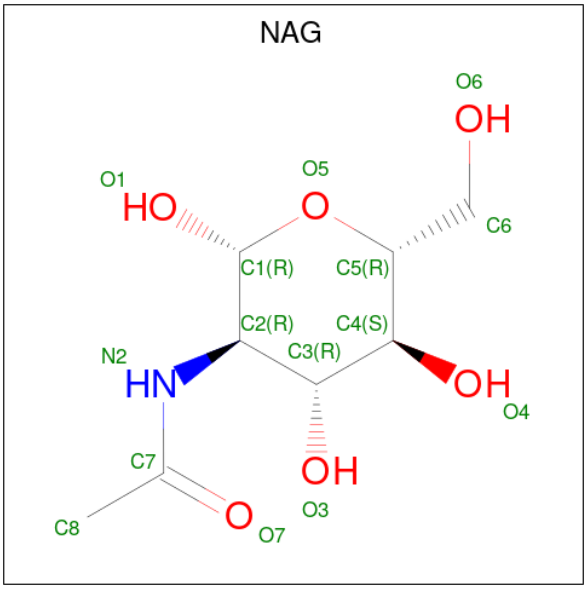
- Molecule 5 is a protein called CONALBUMIN PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	P	16	120	71	23	26	0	0	0
			Total	C	N	O			
5	Q	16	120	71	23	26	0	0	0

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	I	2	28	16	2	10	0	0	0
			Total	C	N	O			
6	J	2	28	16	2	10	0	0	0
			Total	C	N	O			
6	K	2	28	16	2	10	0	0	0
			Total	C	N	O			
6	L	2	28	16	2	10	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



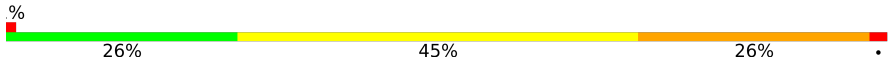
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	C	1	14	8	1	5	0	0
			Total	C	N	O		
7	G	1	14	8	1	5	0	0

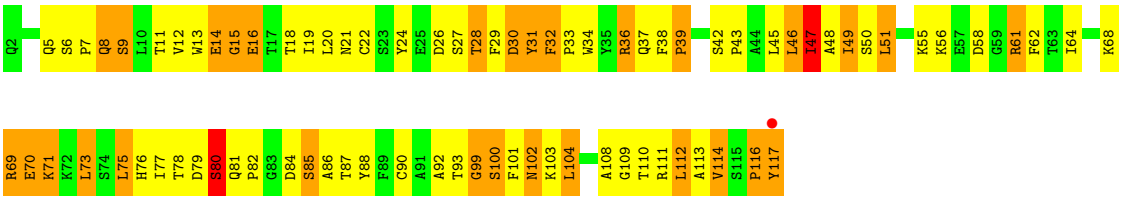
3 Residue-property plots (i)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

• Molecule 1: T-CELL RECEPTOR D10 (ALPHA CHAIN)

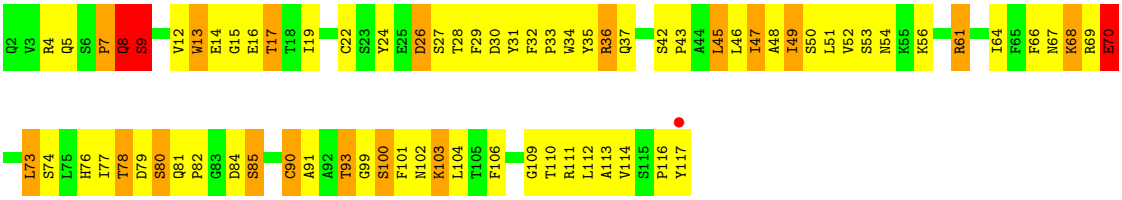
Chain A:





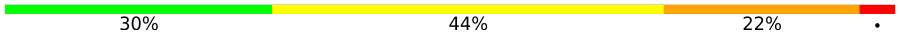
• Molecule 1: T-CELL RECEPTOR D10 (ALPHA CHAIN)

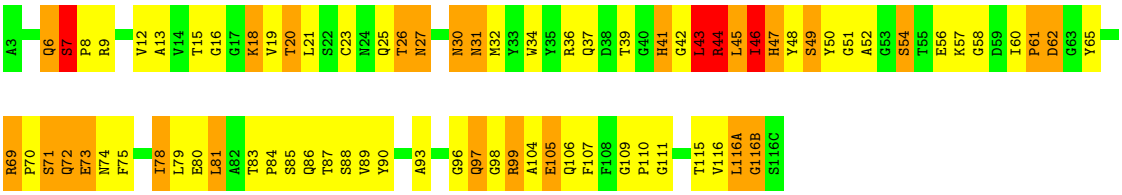
Chain E:



• Molecule 2: T-CELL RECEPTOR D10 (BETA CHAIN)

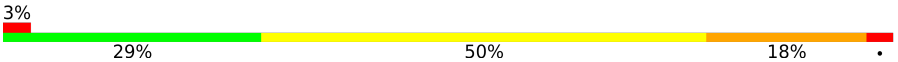
Chain B:

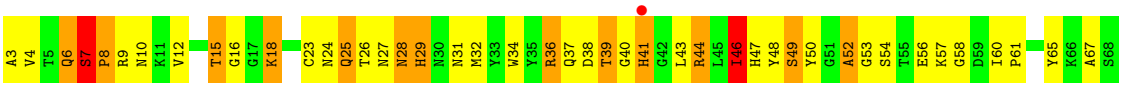


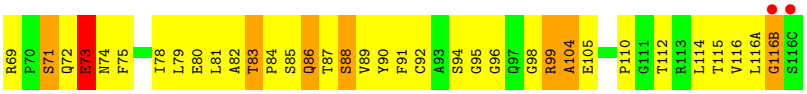


• Molecule 2: T-CELL RECEPTOR D10 (BETA CHAIN)

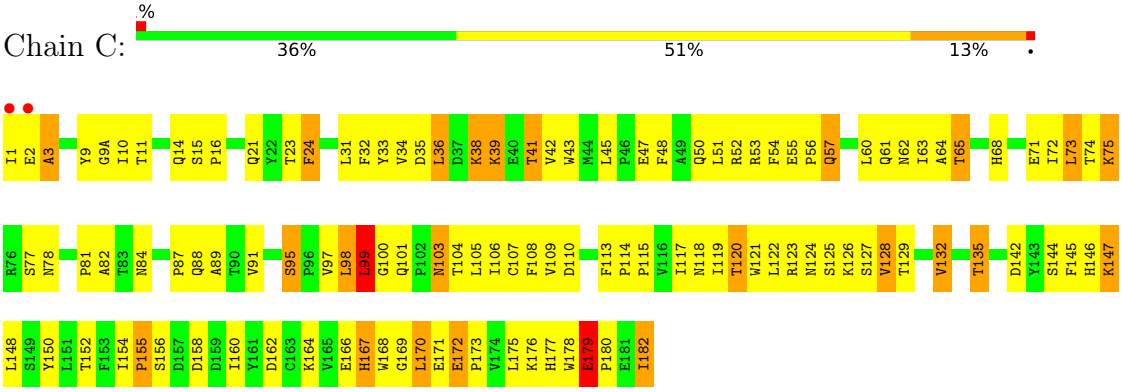
Chain F:



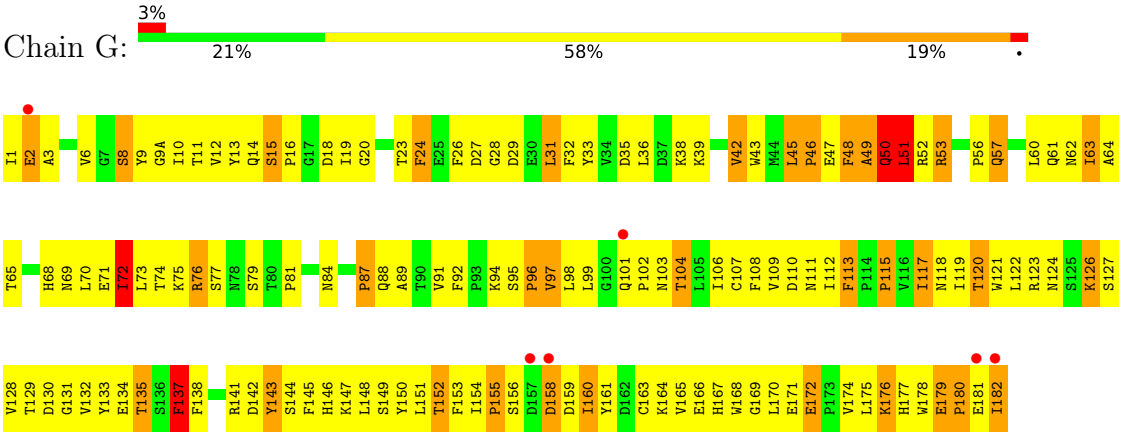




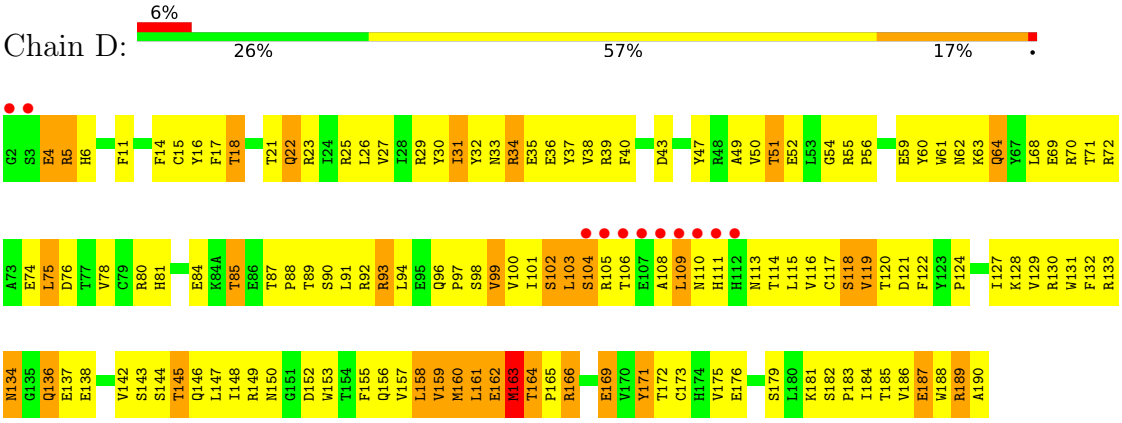
• Molecule 3: MHC I-AK A CHAIN (ALPHA CHAIN)



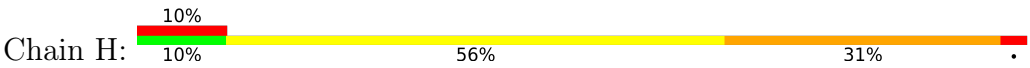
• Molecule 3: MHC I-AK A CHAIN (ALPHA CHAIN)

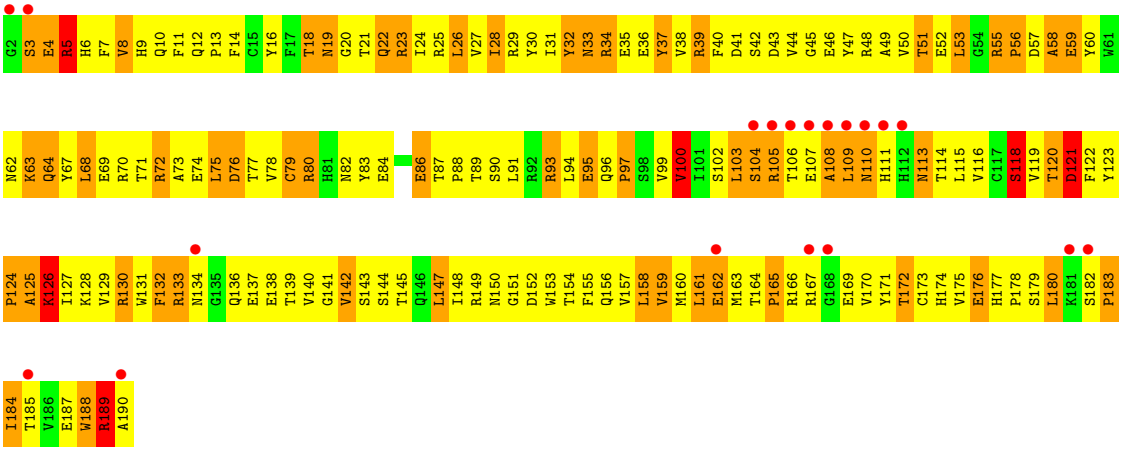


• Molecule 4: MHC I-AK B CHAIN (BETA CHAIN)



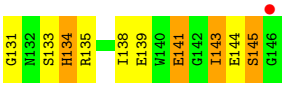
• Molecule 4: MHC I-AK B CHAIN (BETA CHAIN)





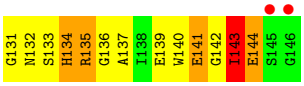
• Molecule 5: CONALBUMIN PEPTIDE

Chain P:



• Molecule 5: CONALBUMIN PEPTIDE

Chain Q:



• Molecule 6: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 6: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

• Molecule 6: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

• Molecule 6: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	97.60Å 345.30Å 97.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 15.02 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.2 (15.00-3.20) 91.4 (15.02-3.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 3.19Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.247 , 0.293 0.266 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.840	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 74.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	9962	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: NDG, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.61	0/901	0.88	3/1220 (0.2%)
1	E	0.57	0/901	0.88	3/1220 (0.2%)
2	B	0.54	0/873	0.92	5/1181 (0.4%)
2	F	0.44	1/873 (0.1%)	0.80	2/1181 (0.2%)
3	C	0.29	0/1530	0.56	0/2087
3	G	0.31	0/1530	0.56	0/2087
4	D	0.30	0/1615	0.58	0/2191
4	H	0.33	0/1615	0.56	0/2191
5	P	0.40	0/122	0.66	0/161
5	Q	0.37	0/122	0.88	0/161
All	All	0.41	1/10082 (0.0%)	0.69	13/13680 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	53	GLY	CA-C	5.04	1.59	1.51

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	52	ALA	O-C-N	-8.58	108.62	123.20
2	B	43	LEU	O-C-N	-7.59	110.56	122.70
2	B	47	HIS	CB-CA-C	-7.36	95.67	110.40
2	B	44	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	A	70	GLU	N-CA-C	-6.87	92.45	111.00

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	877	0	848	95	0
1	E	877	0	848	99	0
2	B	854	0	813	101	0
2	F	854	0	813	93	0
3	C	1485	0	1413	120	0
3	G	1485	0	1413	206	0
4	D	1575	0	1518	151	0
4	H	1575	0	1517	259	0
5	P	120	0	102	15	0
5	Q	120	0	102	38	0
6	I	28	0	24	3	0
6	J	28	0	24	0	0
6	K	28	0	24	0	0
6	L	28	0	24	4	0
7	C	14	0	13	0	0
7	G	14	0	13	0	0
All	All	9962	0	9509	1043	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 54.

The worst 5 of 1043 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:E:67:ASN:OD1	1:E:70:GLU:HB2	1.25	1.36
1:A:7:PRO:HB2	1:A:110:THR:HG21	1.20	1.17
3:C:179:GLU:H	3:C:180:PRO:CD	1.59	1.16
1:E:102:ASN:HA	2:F:104:ALA:HA	1.24	1.15
1:E:26:ASP:HB3	1:E:29:PHE:CD1	1.84	1.13

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	108/110 (98%)	80 (74%)	12 (11%)	16 (15%)	0	1
1	E	108/110 (98%)	82 (76%)	17 (16%)	9 (8%)	1	5
2	B	110/112 (98%)	77 (70%)	19 (17%)	14 (13%)	0	1
2	F	110/112 (98%)	79 (72%)	15 (14%)	16 (14%)	0	1
3	C	181/183 (99%)	161 (89%)	15 (8%)	5 (3%)	5	29
3	G	181/183 (99%)	133 (74%)	33 (18%)	15 (8%)	1	5
4	D	186/188 (99%)	145 (78%)	30 (16%)	11 (6%)	1	12
4	H	186/188 (99%)	129 (69%)	33 (18%)	24 (13%)	0	1
5	P	14/16 (88%)	12 (86%)	1 (7%)	1 (7%)	1	8
5	Q	14/16 (88%)	9 (64%)	1 (7%)	4 (29%)	0	0
All	All	1198/1218 (98%)	907 (76%)	176 (15%)	115 (10%)	0	3

5 of 115 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	14	GLU
1	A	68	LYS
1	A	71	LYS
1	A	103	LYS

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	96/96 (100%)	75 (78%)	21 (22%)	1	5
1	E	96/96 (100%)	72 (75%)	24 (25%)	0	2
2	B	91/91 (100%)	66 (72%)	25 (28%)	0	1
2	F	91/91 (100%)	72 (79%)	19 (21%)	1	6
3	C	166/166 (100%)	135 (81%)	31 (19%)	1	8
3	G	166/166 (100%)	126 (76%)	40 (24%)	0	3
4	D	174/174 (100%)	130 (75%)	44 (25%)	0	2
4	H	174/174 (100%)	119 (68%)	55 (32%)	0	0
5	P	11/11 (100%)	5 (46%)	6 (54%)	0	0
5	Q	11/11 (100%)	7 (64%)	4 (36%)	0	0
All	All	1076/1076 (100%)	807 (75%)	269 (25%)	0	2

5 of 269 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	76	ASP
4	H	103	LEU
4	H	176	GLU
4	D	120	THR
4	D	109	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	8	GLN
1	E	102	ASN
4	H	22	GLN
1	E	76	HIS
2	F	29	HIS

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)

8 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	$\#\|Z\| > 2$
6	NAG	I	1	3,6	14,14,15	0.60	0	17,19,21	0.63	0
6	NDG	I	2	6	14,14,15	0.64	0	17,19,21	0.63	1 (5%)
6	NAG	J	1	4,6	14,14,15	0.69	0	17,19,21	0.73	0
6	NDG	J	2	6	14,14,15	0.71	0	17,19,21	0.67	1 (5%)
6	NAG	K	1	3,6	14,14,15	0.79	0	17,19,21	0.73	0
6	NDG	K	2	6	14,14,15	0.68	0	17,19,21	0.78	1 (5%)
6	NAG	L	1	4,6	14,14,15	0.71	0	17,19,21	1.46	3 (17%)
6	NDG	L	2	6	14,14,15	0.79	0	17,19,21	0.94	2 (11%)

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	NAG	I	1	3,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NDG	I	2	6	-	2/6/23/26	0/1/1/1
6	NAG	J	1	4,6	1/1/5/7	2/6/23/26	0/1/1/1
6	NDG	J	2	6	-	1/6/23/26	0/1/1/1
6	NAG	K	1	3,6	1/1/5/7	2/6/23/26	0/1/1/1
6	NDG	K	2	6	-	2/6/23/26	0/1/1/1
6	NAG	L	1	4,6	-	2/6/23/26	0/1/1/1
6	NDG	L	2	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	1	NAG	C4-C3-C2	3.97	116.83	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	1	NAG	C3-C4-C5	3.25	116.04	110.24
6	L	2	NDG	C2-N2-C7	-2.39	119.50	122.90
6	L	2	NDG	C1-O5-C5	2.27	115.27	112.19
6	K	2	NDG	C1-O5-C5	2.08	115.02	112.19

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	I	1	NAG	C1
6	J	1	NAG	C1
6	K	1	NAG	C1

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	2	NDG	C1-C2-N2-C7
6	I	2	NDG	C4-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6
6	I	2	NDG	O5-C5-C6-O6

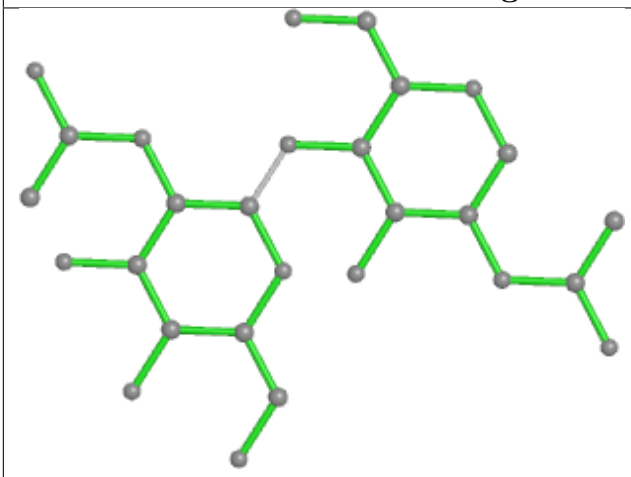
There are no ring outliers.

4 monomers are involved in 7 short contacts:

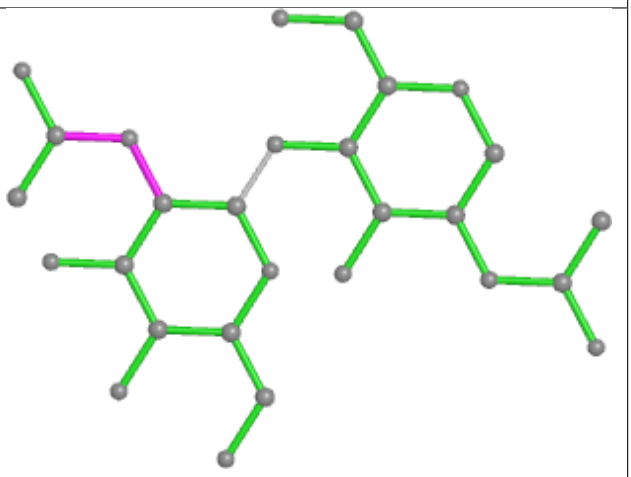
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	2	NDG	1	0
6	I	1	NAG	3	0
6	L	1	NAG	3	0
6	I	2	NDG	3	0

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

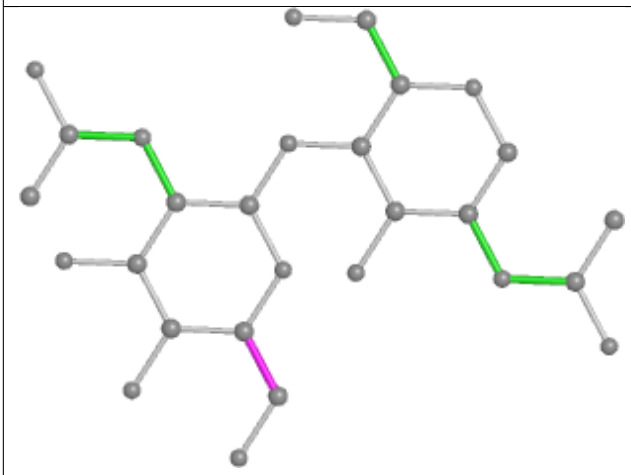
Oligosaccharide Chain I



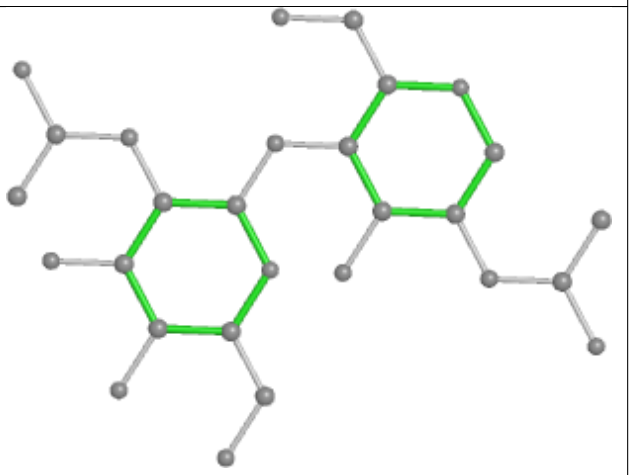
Bond lengths



Bond angles

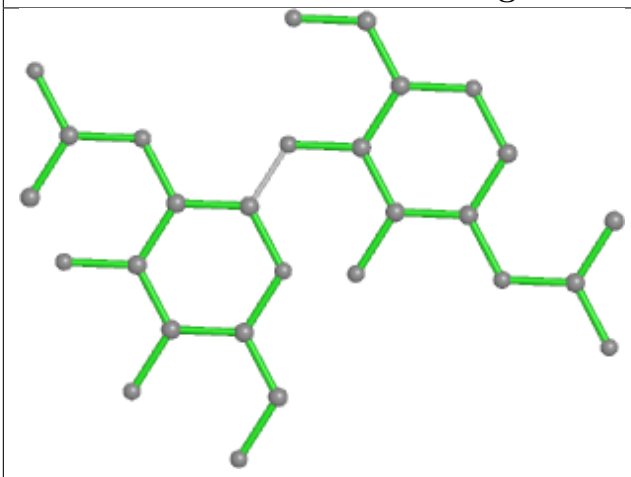


Torsions

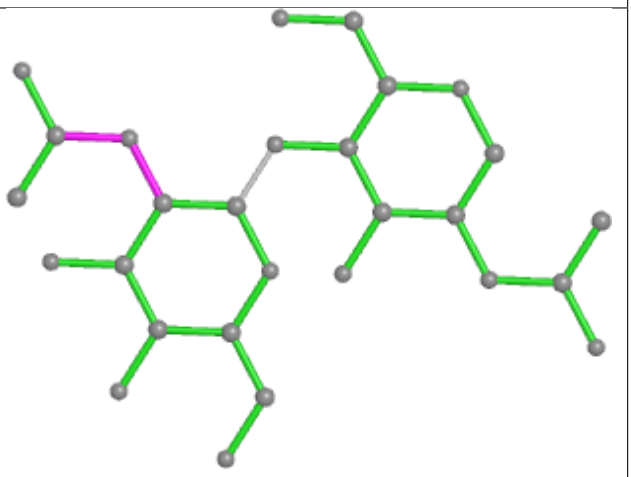


Rings

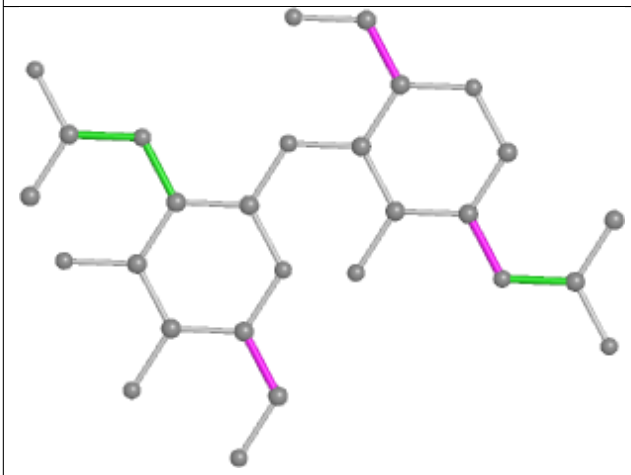
Oligosaccharide Chain J



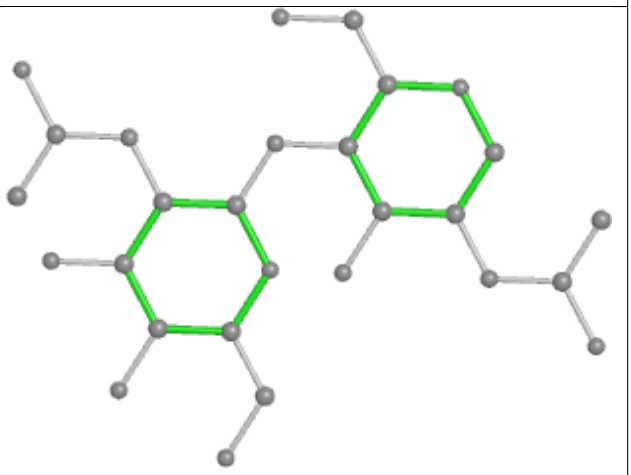
Bond lengths



Bond angles

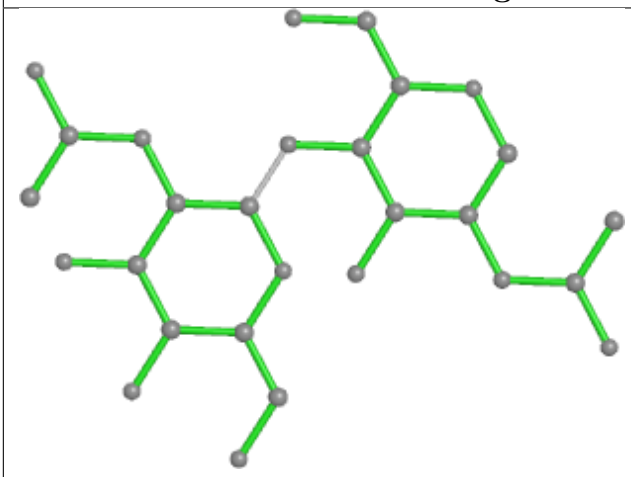


Torsions

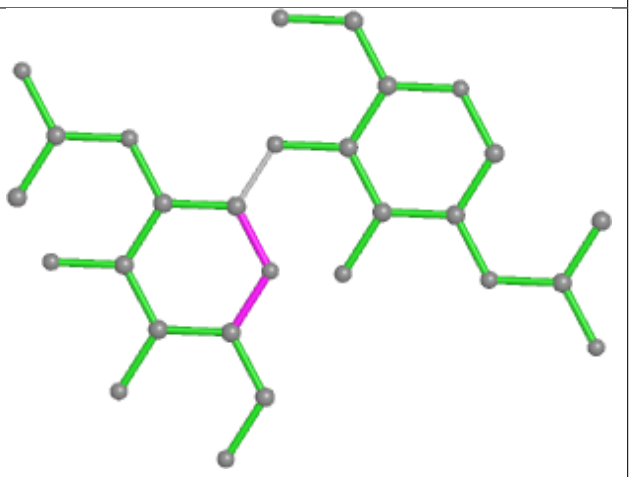


Rings

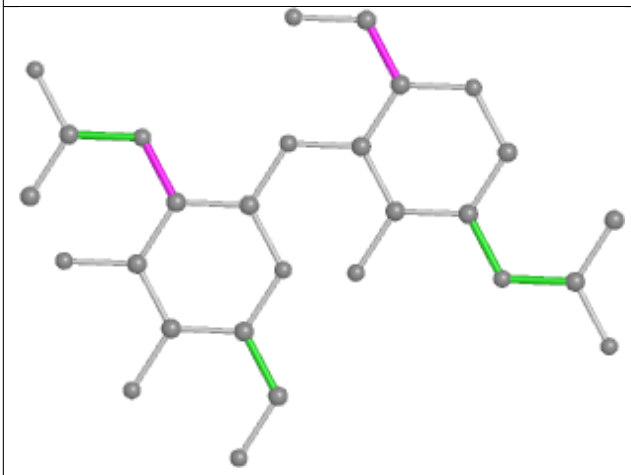
Oligosaccharide Chain K



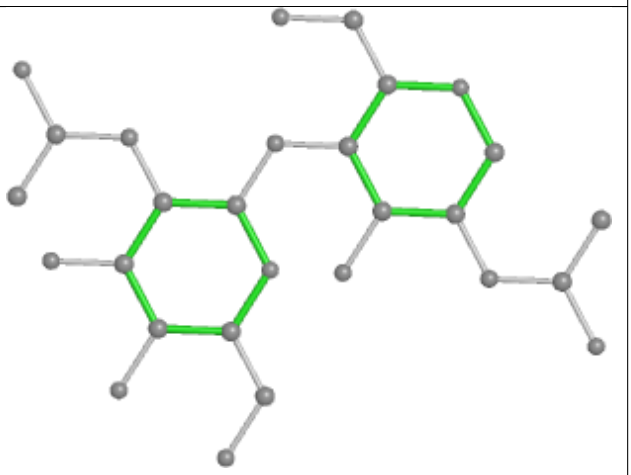
Bond lengths



Bond angles

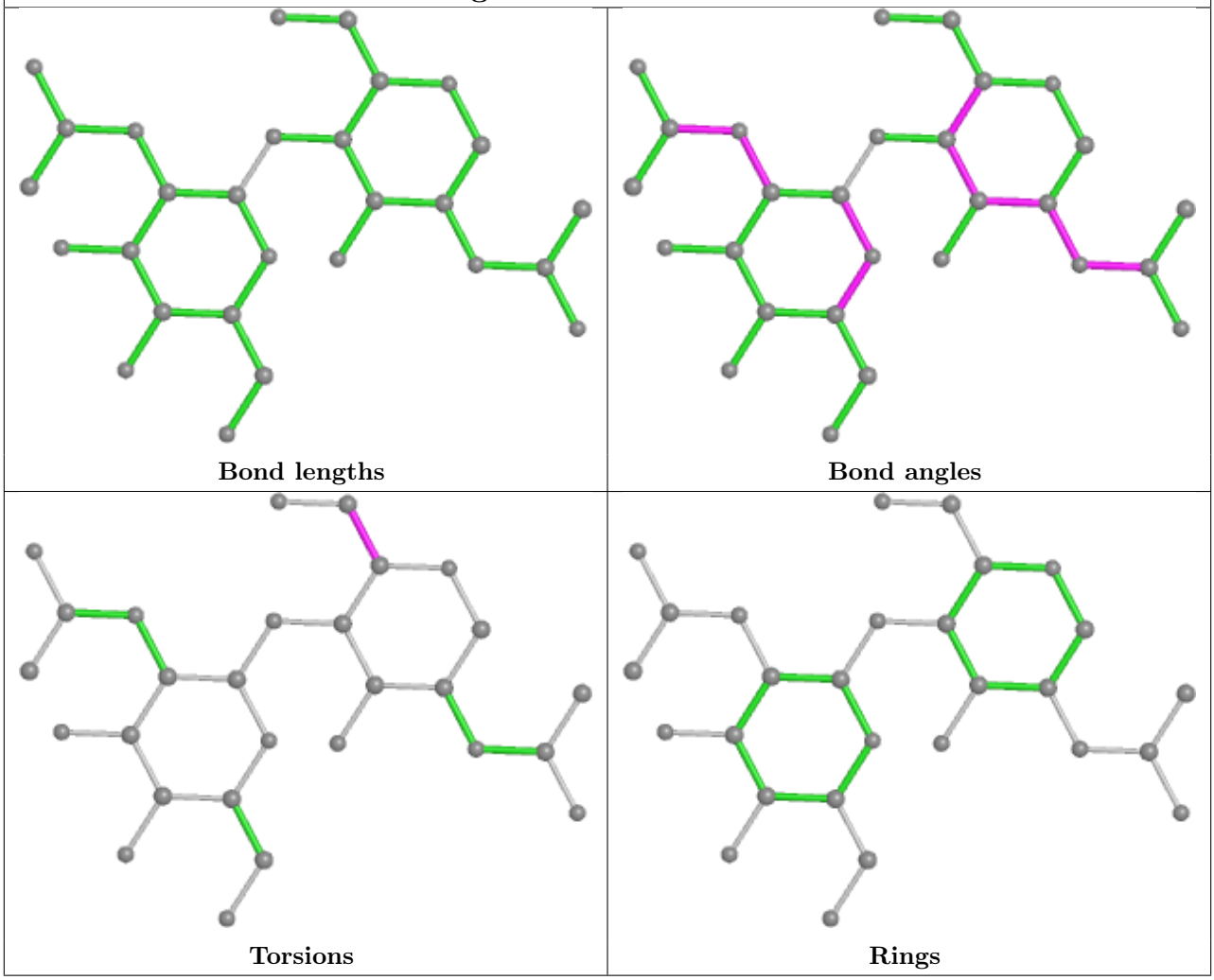


Torsions



Rings

Oligosaccharide Chain L



5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	C	201	3	14,14,15	0.64	0	17,19,21	0.78	1 (5%)
7	NAG	G	201	3	14,14,15	0.69	0	17,19,21	0.59	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	201	3	1/1/5/7	1/6/23/26	0/1/1/1
7	NAG	G	201	3	1/1/5/7	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	201	NAG	C2-N2-C7	-2.24	119.72	122.90
7	G	201	NAG	C2-N2-C7	-2.04	120.00	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	C	201	NAG	C1
7	G	201	NAG	C1

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	201	NAG	C4-C5-C6-O6
7	G	201	NAG	O5-C5-C6-O6
7	C	201	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	110/110 (100%)	-0.43	1 (0%) 84 75	23, 43, 73, 96	0
1	E	110/110 (100%)	-0.35	1 (0%) 84 75	31, 52, 79, 94	0
2	B	112/112 (100%)	-0.41	0 100 100	29, 48, 69, 91	0
2	F	112/112 (100%)	-0.21	3 (2%) 54 39	28, 51, 81, 100	0
3	C	183/183 (100%)	-0.47	2 (1%) 80 69	20, 44, 86, 100	0
3	G	183/183 (100%)	0.06	6 (3%) 46 30	41, 84, 100, 100	0
4	D	188/188 (100%)	-0.16	11 (5%) 22 13	18, 48, 100, 100	0
4	H	188/188 (100%)	0.36	19 (10%) 7 4	49, 91, 100, 100	0
5	P	16/16 (100%)	0.23	1 (6%) 20 11	28, 48, 96, 100	0
5	Q	16/16 (100%)	0.46	2 (12%) 3 2	57, 73, 99, 100	0
All	All	1218/1218 (100%)	-0.15	46 (3%) 40 26	18, 58, 100, 100	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	112	HIS	5.4
4	D	111	HIS	5.4
4	H	111	HIS	5.2
4	H	107	GLU	5.2
4	H	2	GLY	5.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

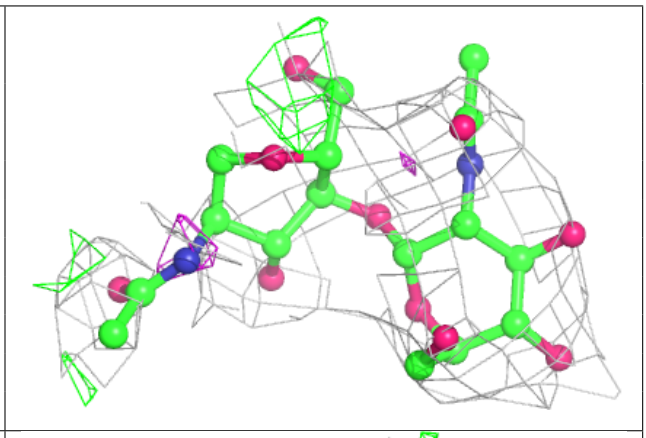
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

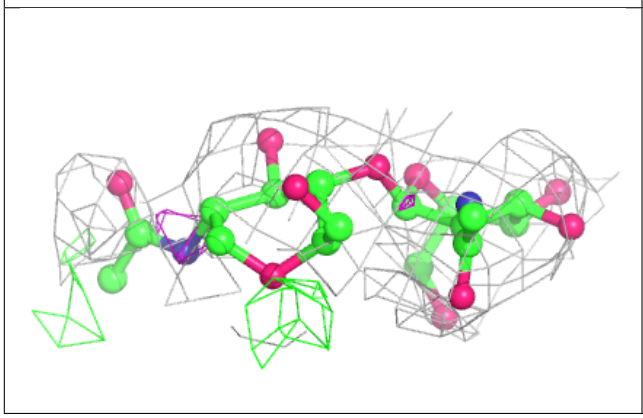
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	L	1	14/15	0.43	0.66	92,100,100,100	0
6	NDG	L	2	14/15	0.51	0.77	97,100,100,100	0
6	NDG	J	2	14/15	0.52	0.69	98,100,100,100	0
6	NAG	J	1	14/15	0.65	0.43	87,97,100,100	0
6	NDG	K	2	14/15	0.70	0.56	98,100,100,100	0
6	NAG	K	1	14/15	0.71	0.39	93,100,100,100	0
6	NAG	I	1	14/15	0.78	0.34	80,90,100,100	0
6	NDG	I	2	14/15	0.87	0.36	98,100,100,100	0

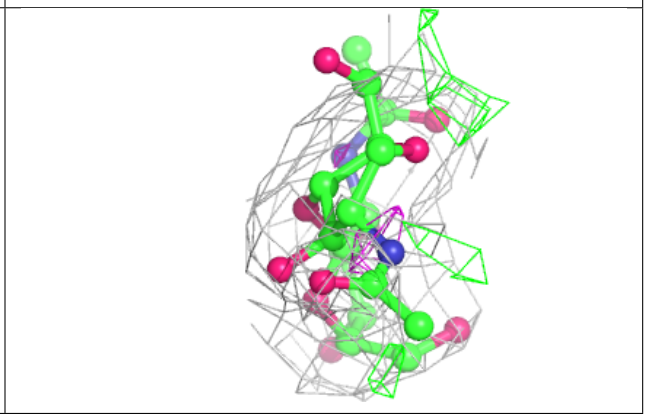
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

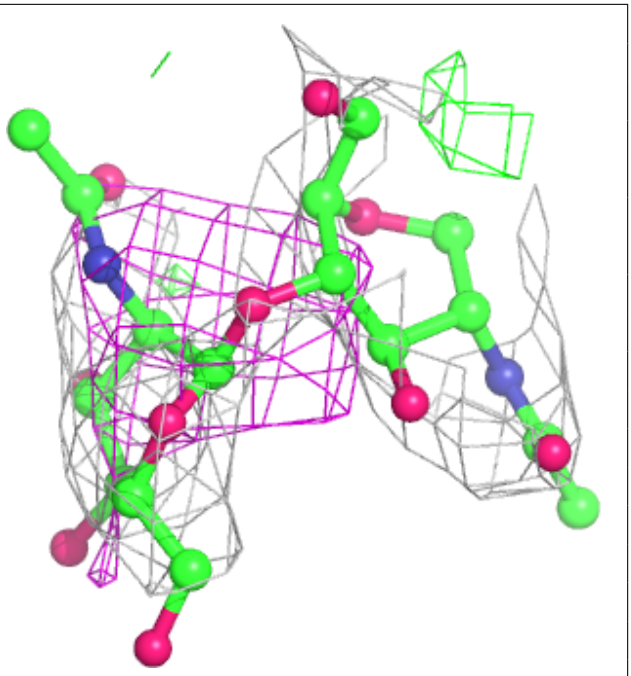


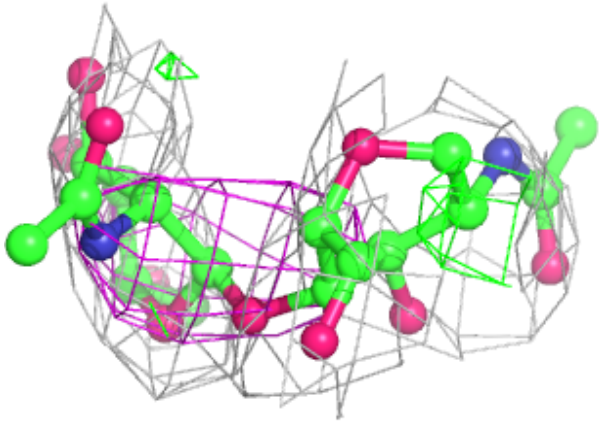


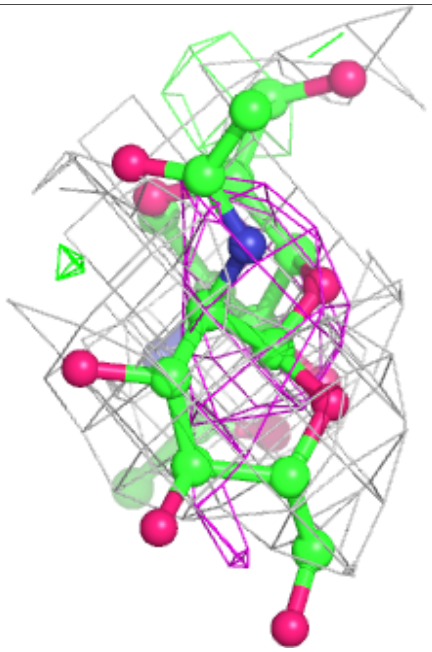


Electron density around Chain J:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

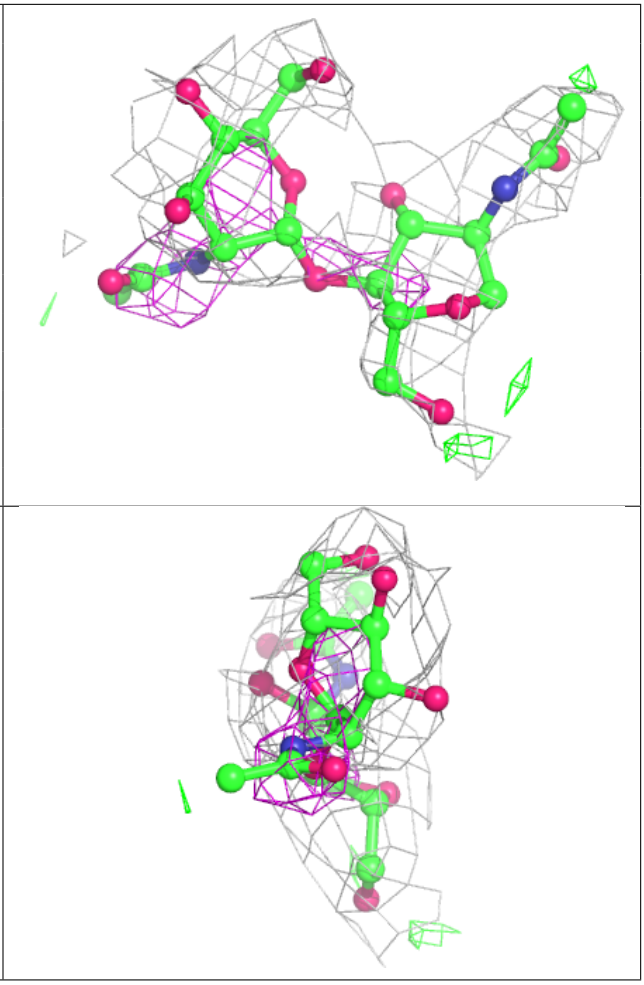






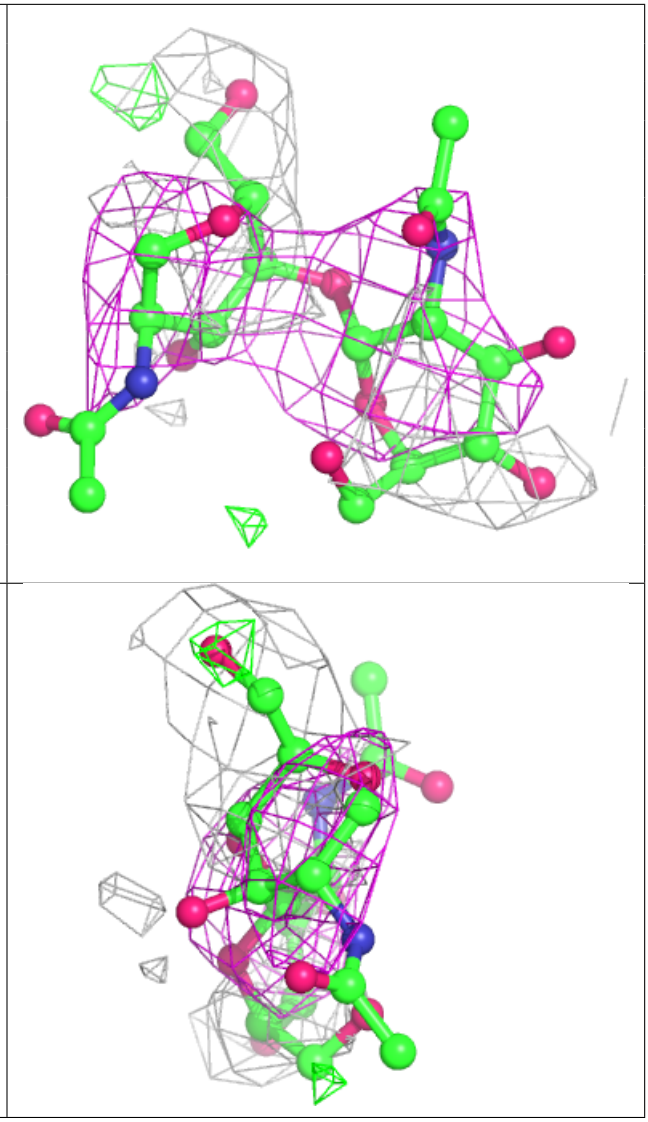
Electron density around Chain K:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain L:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	G	201	14/15	0.37	0.62	97,100,100,100	0
7	NAG	C	201	14/15	0.76	0.65	95,100,100,100	0

6.5 Other polymers (i)

There are no such residues in this entry.