wwPDB X-ray Structure Validation Summary Report (i)

Jun 24, 2024 – 06:54 AM EDT

PDB ID	:	6DFX
Title	:	human diabetogenic TCR T1D3 in complex with DQ8-p8E9E peptide
Authors	:	Wang, Y.; Dai, S.
Deposited on	:	2018-05-15
Resolution	:	2.03 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

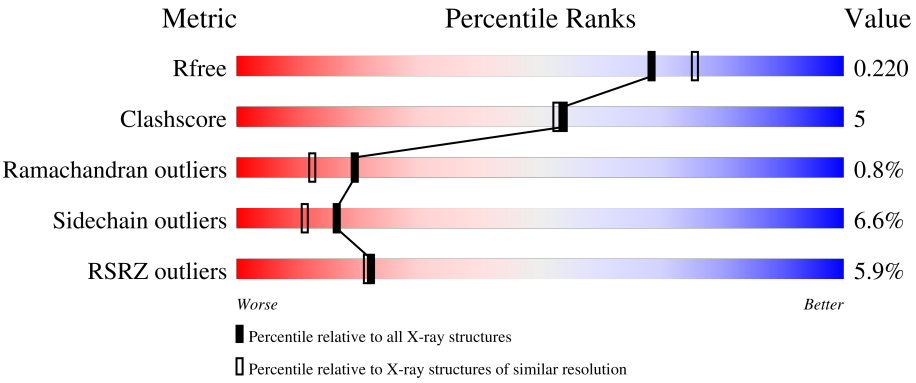
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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))
R_{free}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	188	81% 13%
1	D	188	85% 10%
2	B	221	9% 71% 16% 10%
2	E	221	8% 67% 19% 10%
3	G	207	9% 71% 16% 5% 6%

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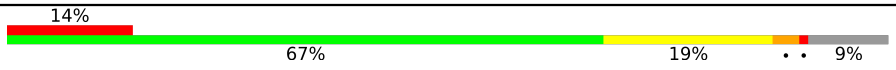
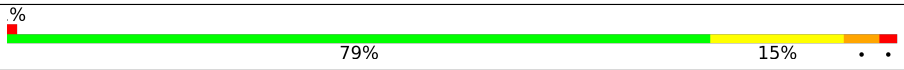
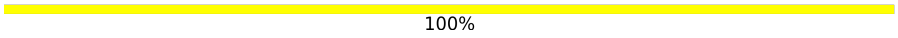
Mol	Chain	Length	Quality of chain
3	I	207	
4	H	238	
4	J	238	
5	C	2	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 13693 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 MHC class II HLA-DQ-alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1455	937	239	276	3			
1	D	180	Total	C	N	O	S	0	0	0
			1455	937	239	276	3			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	CYS	ILE	conflict	UNP Q30069
A	182	GLY	-	expression tag	UNP Q30069
A	183	GLY	-	expression tag	UNP Q30069
A	184	LEU	-	expression tag	UNP Q30069
A	185	VAL	-	expression tag	UNP Q30069
A	186	PRO	-	expression tag	UNP Q30069
A	187	ARG	-	expression tag	UNP Q30069
D	72	CYS	ILE	conflict	UNP Q30069
D	182	GLY	-	expression tag	UNP Q30069
D	183	GLY	-	expression tag	UNP Q30069
D	184	LEU	-	expression tag	UNP Q30069
D	185	VAL	-	expression tag	UNP Q30069
D	186	PRO	-	expression tag	UNP Q30069
D	187	ARG	-	expression tag	UNP Q30069

- Molecule 2 is a protein called MHC class II antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	200	Total	C	N	O	S	0	0	0
			1623	1025	283	307	8			
2	E	199	Total	C	N	O	S	0	0	0
			1610	1018	277	307	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-27	VAL	-	expression tag	UNP U3PYM0
B	-26	GLU	-	expression tag	UNP U3PYM0
B	-25	GLU	-	expression tag	UNP U3PYM0
B	-24	LEU	-	expression tag	UNP U3PYM0
B	-23	TYR	-	expression tag	UNP U3PYM0
B	-22	LEU	-	expression tag	UNP U3PYM0
B	-21	VAL	-	expression tag	UNP U3PYM0
B	-20	ALA	-	expression tag	UNP U3PYM0
B	-19	GLY	-	expression tag	UNP U3PYM0
B	-18	GLU	-	expression tag	UNP U3PYM0
B	-17	GLU	-	expression tag	UNP U3PYM0
B	-16	GLY	-	expression tag	UNP U3PYM0
B	-15	CYS	-	expression tag	UNP U3PYM0
B	-14	GLY	-	expression tag	UNP U3PYM0
B	-13	GLY	-	expression tag	UNP U3PYM0
B	-12	GLY	-	expression tag	UNP U3PYM0
B	-11	GLY	-	expression tag	UNP U3PYM0
B	-10	SER	-	expression tag	UNP U3PYM0
B	-9	LEU	-	expression tag	UNP U3PYM0
B	-4	VAL	-	expression tag	UNP U3PYM0
B	-3	GLY	-	expression tag	UNP U3PYM0
B	-2	GLY	-	expression tag	UNP U3PYM0
B	-1	SER	-	expression tag	UNP U3PYM0
B	0	GLY	-	expression tag	UNP U3PYM0
B	1	GLY	-	expression tag	UNP U3PYM0
B	2	GLY	-	expression tag	UNP U3PYM0
B	192	GLY	-	expression tag	UNP U3PYM0
B	193	GLY	-	expression tag	UNP U3PYM0
B	194	LEU	-	expression tag	UNP U3PYM0
B	195	VAL	-	expression tag	UNP U3PYM0
B	196	PRO	-	expression tag	UNP U3PYM0
B	197	ARG	-	expression tag	UNP U3PYM0
E	-27	VAL	-	expression tag	UNP U3PYM0
E	-26	GLU	-	expression tag	UNP U3PYM0
E	-25	GLU	-	expression tag	UNP U3PYM0
E	-24	LEU	-	expression tag	UNP U3PYM0
E	-23	TYR	-	expression tag	UNP U3PYM0
E	-22	LEU	-	expression tag	UNP U3PYM0
E	-21	VAL	-	expression tag	UNP U3PYM0
E	-20	ALA	-	expression tag	UNP U3PYM0
E	-19	GLY	-	expression tag	UNP U3PYM0
E	-18	GLU	-	expression tag	UNP U3PYM0
E	-17	GLU	-	expression tag	UNP U3PYM0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-16	GLY	-	expression tag	UNP U3PYM0
E	-15	CYS	-	expression tag	UNP U3PYM0
E	-14	GLY	-	expression tag	UNP U3PYM0
E	-13	GLY	-	expression tag	UNP U3PYM0
E	-12	GLY	-	expression tag	UNP U3PYM0
E	-11	GLY	-	expression tag	UNP U3PYM0
E	-10	SER	-	expression tag	UNP U3PYM0
E	-9	LEU	-	expression tag	UNP U3PYM0
E	-4	VAL	-	expression tag	UNP U3PYM0
E	-3	GLY	-	expression tag	UNP U3PYM0
E	-2	GLY	-	expression tag	UNP U3PYM0
E	-1	SER	-	expression tag	UNP U3PYM0
E	0	GLY	-	expression tag	UNP U3PYM0
E	1	GLY	-	expression tag	UNP U3PYM0
E	2	GLY	-	expression tag	UNP U3PYM0
E	192	GLY	-	expression tag	UNP U3PYM0
E	193	GLY	-	expression tag	UNP U3PYM0
E	194	LEU	-	expression tag	UNP U3PYM0
E	195	VAL	-	expression tag	UNP U3PYM0
E	196	PRO	-	expression tag	UNP U3PYM0
E	197	ARG	-	expression tag	UNP U3PYM0

- Molecule 3 is a protein called T1D3 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	194	Total	C	N	O	S	0	0	0
			1506	928	264	306	8			
3	I	188	Total	C	N	O	S	0	0	0
			1453	899	253	293	8			

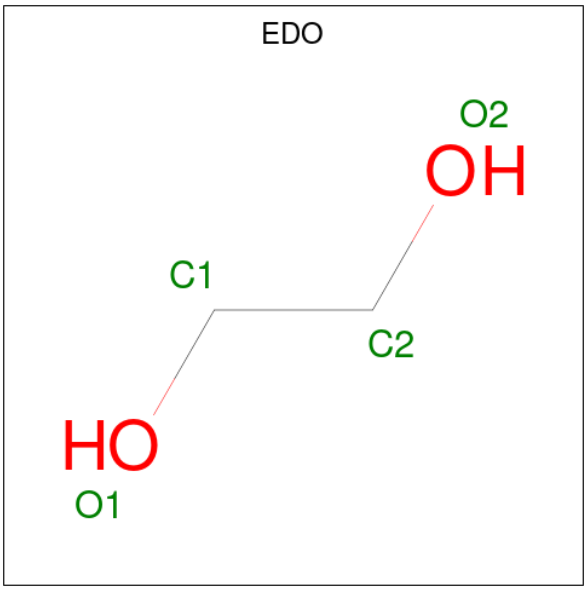
- Molecule 4 is a protein called T1D3 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	237	Total	C	N	O	S	0	0	0
			1885	1187	331	360	7			
4	J	237	Total	C	N	O	S	0	0	0
			1885	1187	331	360	7			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

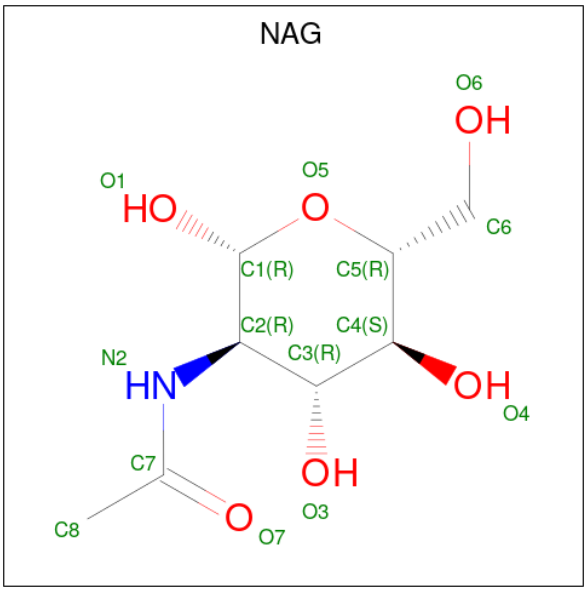
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	C	2	Total C N O 28 16 2 10	0	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	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
7	D	1	Total C N O 14 8 1 5	0	0

- Molecule 8 is water.

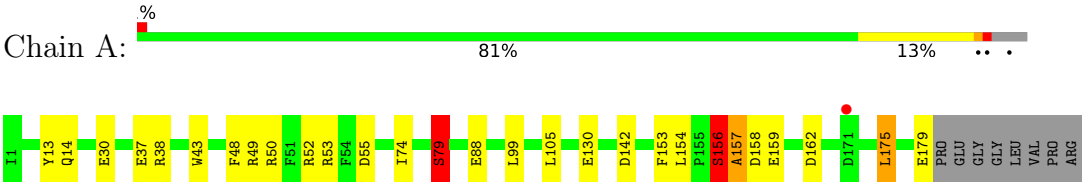
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	116	Total O 116 116	0	0
8	B	146	Total O 146 146	0	0
8	D	96	Total O 96 96	0	0
8	E	84	Total O 84 84	0	0
8	G	57	Total O 57 57	0	0
8	H	131	Total O 131 131	0	0
8	I	46	Total O 46 46	0	0
8	J	99	Total O 99 99	0	0

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.

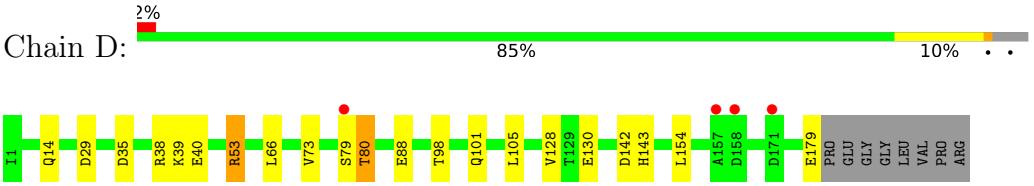
• Molecule 1: MHC class II HLA-DQ-alpha chain

Chain A:



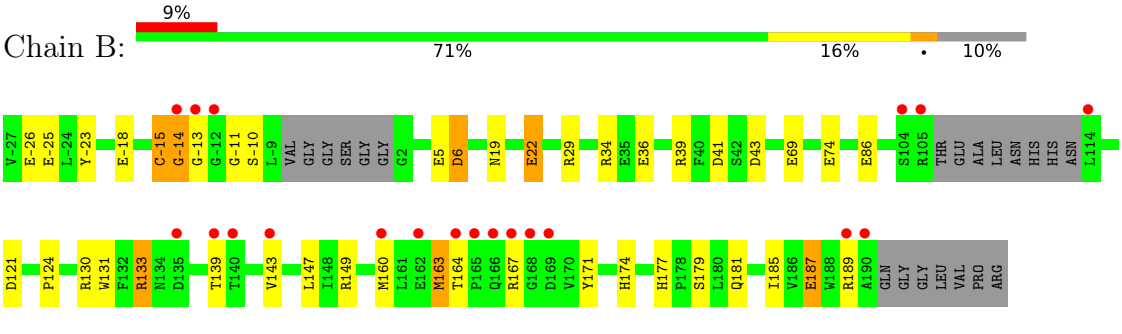
• Molecule 1: MHC class II HLA-DQ-alpha chain

Chain D:



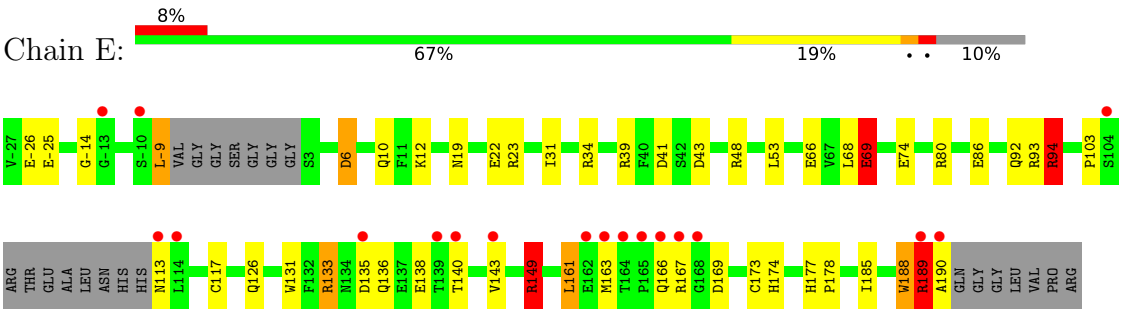
• Molecule 2: MHC class II antigen

Chain B:



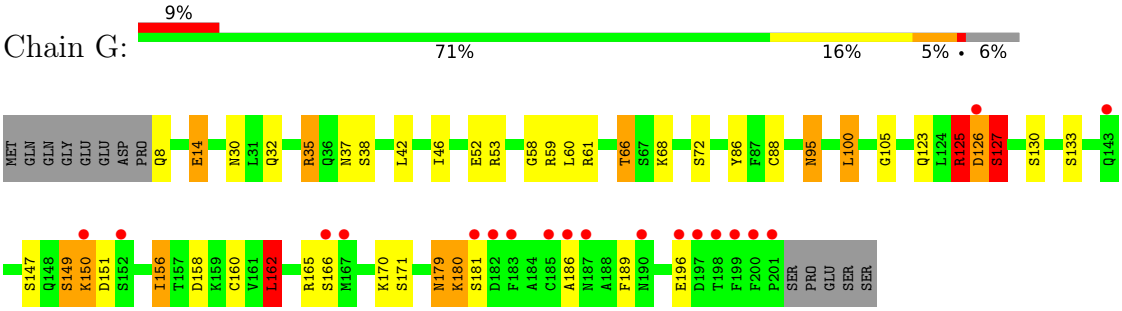
• Molecule 2: MHC class II antigen

Chain E:



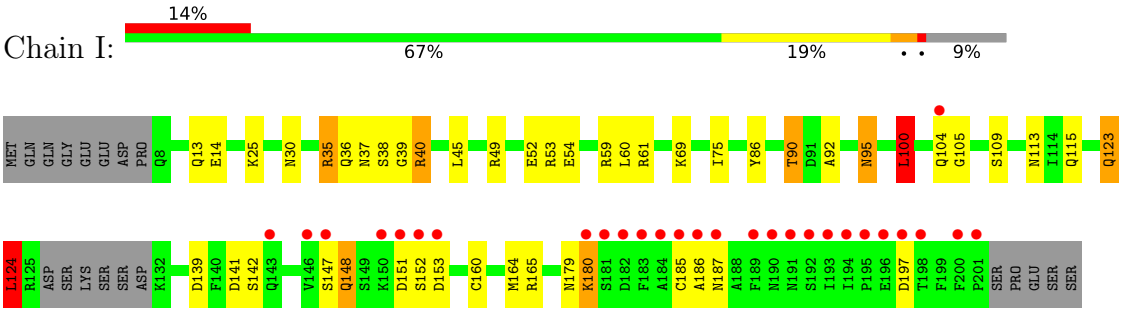
• Molecule 3: T1D3 alpha chain

Chain G:



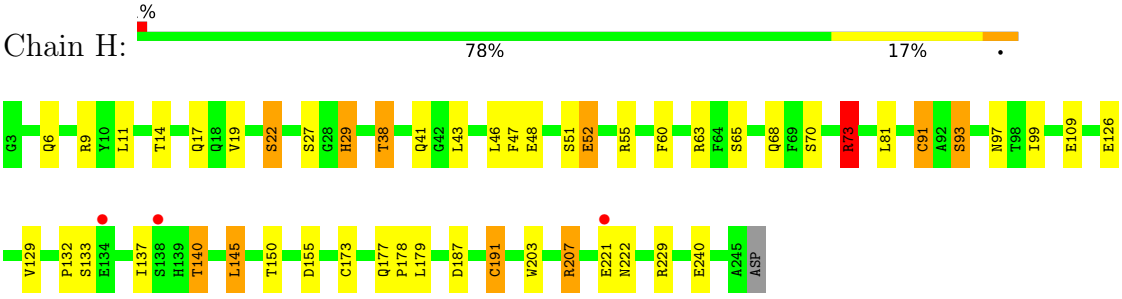
• Molecule 3: T1D3 alpha chain

Chain I:



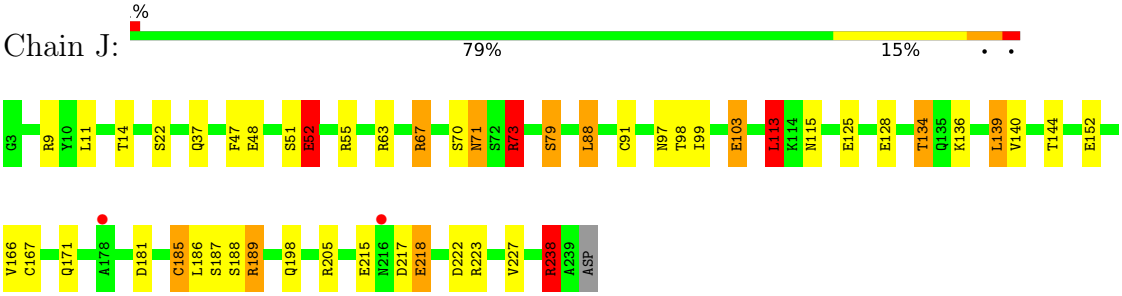
• Molecule 4: T1D3 beta chain

Chain H:



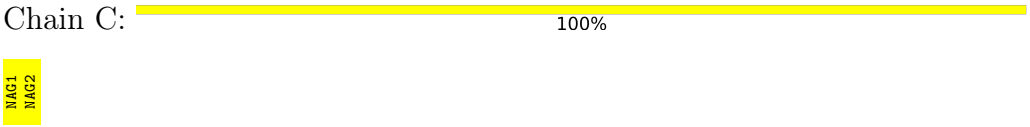
• Molecule 4: T1D3 beta chain

Chain J:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	111.70Å 88.90Å 116.78Å 90.00° 104.26° 90.00°	Depositor
Resolution (Å)	50.01 – 2.03 47.74 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.01-2.03) 99.2 (47.74-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.181 , 0.217 0.188 , 0.220	Depositor DCC
R_{free} test set	7241 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	40.5	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13693	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.62% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, 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	1.46	13/1498 (0.9%)	1.23	11/2044 (0.5%)
1	D	1.30	3/1498 (0.2%)	1.16	3/2044 (0.1%)
2	B	1.53	16/1660 (1.0%)	1.35	18/2257 (0.8%)
2	E	1.45	11/1647 (0.7%)	1.46	25/2242 (1.1%)
3	G	1.41	11/1531 (0.7%)	1.32	14/2068 (0.7%)
3	I	1.25	6/1477 (0.4%)	1.31	17/1997 (0.9%)
4	H	1.49	13/1937 (0.7%)	1.29	18/2635 (0.7%)
4	J	1.43	14/1937 (0.7%)	1.27	23/2635 (0.9%)
All	All	1.42	87/13185 (0.7%)	1.30	129/17922 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	6
3	G	0	3
3	I	0	2
All	All	0	11

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	103	GLU	CD-OE1	13.44	1.40	1.25
4	H	126	GLU	CD-OE2	13.20	1.40	1.25
2	B	74	GLU	CD-OE1	11.38	1.38	1.25
2	E	74	GLU	CD-OE2	9.76	1.36	1.25
4	H	191	CYS	CB-SG	-9.71	1.65	1.82

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	149	ARG	NE-CZ-NH1	-15.50	112.55	120.30
3	I	165	ARG	NE-CZ-NH2	14.08	127.34	120.30
2	E	149	ARG	NE-CZ-NH2	13.92	127.26	120.30
2	E	34	ARG	NE-CZ-NH2	-12.97	113.81	120.30
3	G	61	ARG	NE-CZ-NH1	11.07	125.84	120.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	-14	GLY	Peptide
2	E	149	ARG	Sidechain
2	E	167	ARG	Peptide
2	E	188	TRP	Peptide
2	E	94	ARG	Sidechain

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	1455	0	1392	9	0
1	D	1455	0	1392	11	0
2	B	1623	0	1568	16	0
2	E	1610	0	1547	25	0
3	G	1506	0	1450	20	0
3	I	1453	0	1392	22	0
4	H	1885	0	1785	27	0
4	J	1885	0	1786	24	0
5	C	28	0	25	0	0
6	A	4	0	6	0	0
7	D	14	0	13	0	0
8	A	116	0	0	0	0
8	B	146	0	0	1	0
8	D	96	0	0	1	0
8	E	84	0	0	2	0
8	G	57	0	0	0	0
8	H	131	0	0	4	0
8	I	46	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	99	0	0	1	0
All	All	13693	0	12356	132	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 5.

The worst 5 of 132 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)
3:G:126:ASP:HA	3:G:127:SER:HB2	1.24	1.09
3:G:126:ASP:HB3	4:H:129:VAL:O	1.69	0.92
4:J:51:SER:O	4:J:52:GLU:HB2	1.70	0.90
3:G:126:ASP:HA	3:G:127:SER:CB	2.08	0.83
2:E:189:ARG:HB3	2:E:190:ALA:HB3	1.59	0.82

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	178/188 (95%)	169 (95%)	8 (4%)	1 (1%)	25 18
1	D	178/188 (95%)	173 (97%)	5 (3%)	0	100 100
2	B	194/221 (88%)	187 (96%)	6 (3%)	1 (0%)	29 22
2	E	193/221 (87%)	182 (94%)	9 (5%)	2 (1%)	15 9
3	G	192/207 (93%)	174 (91%)	12 (6%)	6 (3%)	4 1
3	I	184/207 (89%)	176 (96%)	5 (3%)	3 (2%)	9 4
4	H	235/238 (99%)	228 (97%)	7 (3%)	0	100 100
4	J	235/238 (99%)	226 (96%)	9 (4%)	0	100 100
All	All	1589/1708 (93%)	1515 (95%)	61 (4%)	13 (1%)	19 12

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	ALA
3	G	127	SER
3	G	149	SER
3	G	150	LYS
3	I	180	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	165/171 (96%)	157 (95%)	8 (5%)	25 21
1	D	165/171 (96%)	157 (95%)	8 (5%)	25 21
2	B	178/192 (93%)	169 (95%)	9 (5%)	24 19
2	E	177/192 (92%)	161 (91%)	16 (9%)	9 5
3	G	171/183 (93%)	154 (90%)	17 (10%)	8 4
3	I	163/183 (89%)	150 (92%)	13 (8%)	12 7
4	H	207/208 (100%)	197 (95%)	10 (5%)	25 21
4	J	207/208 (100%)	193 (93%)	14 (7%)	16 10
All	All	1433/1508 (95%)	1338 (93%)	95 (7%)	16 11

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	196	GLU
3	I	95	ASN
4	H	27	SER
4	H	81	LEU
3	I	123	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
3	I	36	GLN
4	J	77	ASN
3	I	37	ASN
3	I	113	ASN
4	J	216	ASN

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)

2 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	$\#\|Z\| > 2$
5	NAG	C	1	5,1	14,14,15	1.07	1 (7%)	17,19,21	1.53	6 (35%)
5	NAG	C	2	5	14,14,15	1.61	5 (35%)	17,19,21	2.32	9 (52%)

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	NAG	C	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	2/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2	NAG	O4-C4	2.94	1.49	1.43
5	C	2	NAG	C2-N2	2.84	1.51	1.46
5	C	2	NAG	C1-C2	2.38	1.55	1.52
5	C	2	NAG	C4-C5	2.10	1.57	1.53
5	C	1	NAG	C1-C2	2.06	1.55	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	2	NAG	C8-C7-N2	4.50	123.73	116.10
5	C	2	NAG	C4-C3-C2	3.50	116.14	111.02
5	C	2	NAG	O7-C7-C8	-3.09	116.32	122.06
5	C	1	NAG	O5-C1-C2	-3.02	106.52	111.29
5	C	2	NAG	O5-C5-C6	-2.74	102.91	107.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

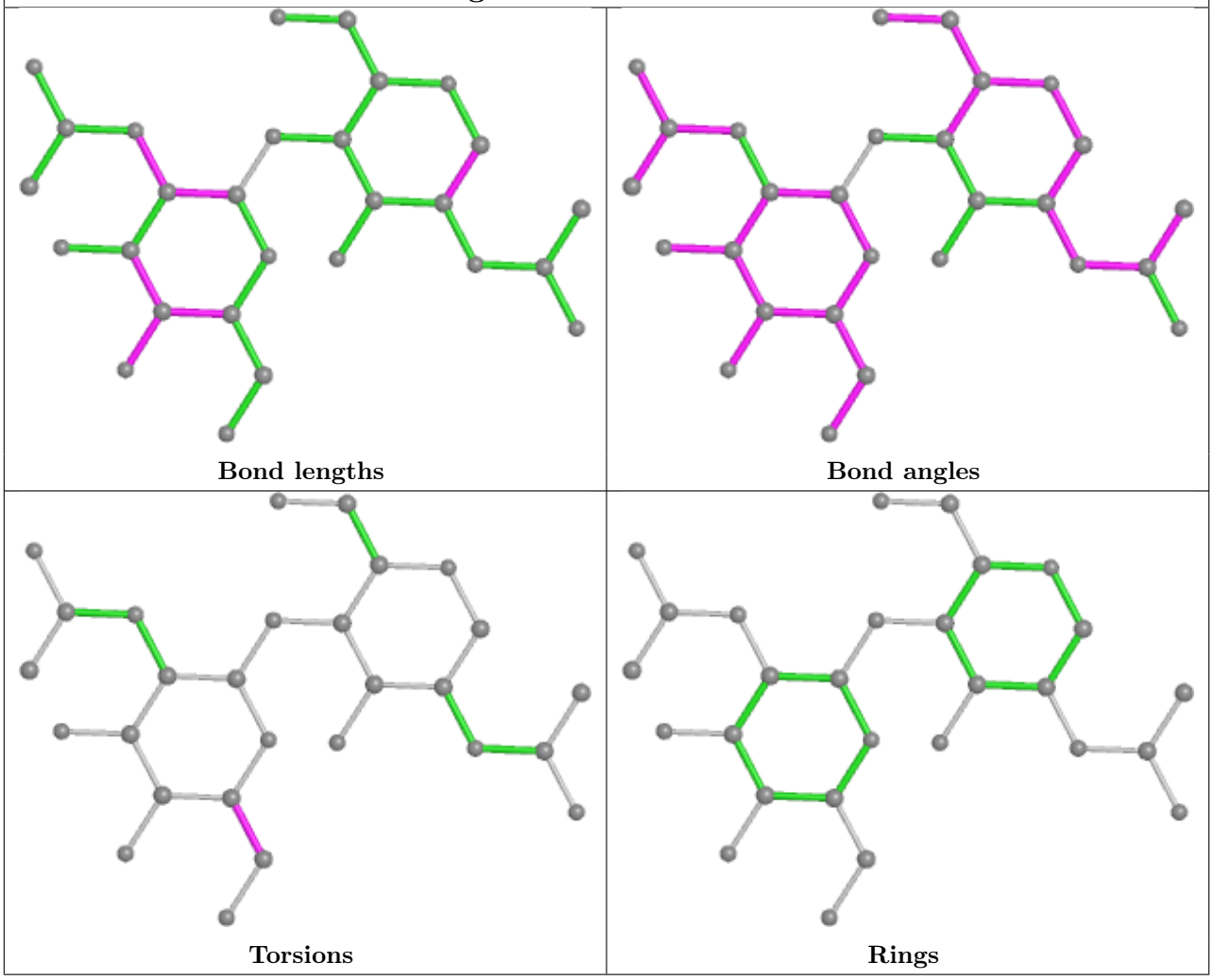
Mol	Chain	Res	Type	Atoms
5	C	2	NAG	O5-C5-C6-O6
5	C	2	NAG	C4-C5-C6-O6

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 C



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	D	201	1	14,14,15	2.67	5 (35%)	17,19,21	3.59	7 (41%)
6	EDO	A	203	-	3,3,3	0.82	0	2,2,2	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	D	201	1	-	0/6/23/26	0/1/1/1
6	EDO	A	203	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	201	NAG	C3-C2	5.73	1.64	1.52
7	D	201	NAG	O4-C4	5.01	1.54	1.43
7	D	201	NAG	O5-C5	4.51	1.52	1.43
7	D	201	NAG	C1-C2	2.83	1.56	1.52
7	D	201	NAG	C4-C3	2.44	1.58	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	201	NAG	C3-C4-C5	-7.25	97.31	110.24
7	D	201	NAG	O4-C4-C3	6.91	126.33	110.35
7	D	201	NAG	O5-C1-C2	-5.51	102.59	111.29
7	D	201	NAG	C1-C2-N2	-5.10	101.78	110.49
7	D	201	NAG	O3-C3-C4	4.59	120.97	110.35

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	203	EDO	O1-C1-C2-O2

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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	180/188 (95%)	0.04	1 (0%) 89 89	25, 40, 71, 82	0
1	D	180/188 (95%)	-0.06	4 (2%) 62 61	31, 44, 71, 87	0
2	B	200/221 (90%)	0.44	20 (10%) 7 6	26, 39, 86, 109	0
2	E	199/221 (90%)	0.20	18 (9%) 9 9	32, 45, 78, 96	0
3	G	194/207 (93%)	0.39	19 (9%) 7 7	28, 58, 89, 109	0
3	I	188/207 (90%)	0.56	28 (14%) 2 2	37, 59, 88, 100	0
4	H	237/238 (99%)	-0.18	3 (1%) 77 76	30, 42, 69, 77	0
4	J	237/238 (99%)	-0.00	2 (0%) 86 85	34, 44, 68, 79	0
All	All	1615/1708 (94%)	0.16	95 (5%) 22 21	25, 46, 80, 109	0

The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	181	SER	8.5
2	E	-13	GLY	5.8
3	I	150	LYS	5.4
3	I	193	ILE	5.2
2	B	167	ARG	5.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

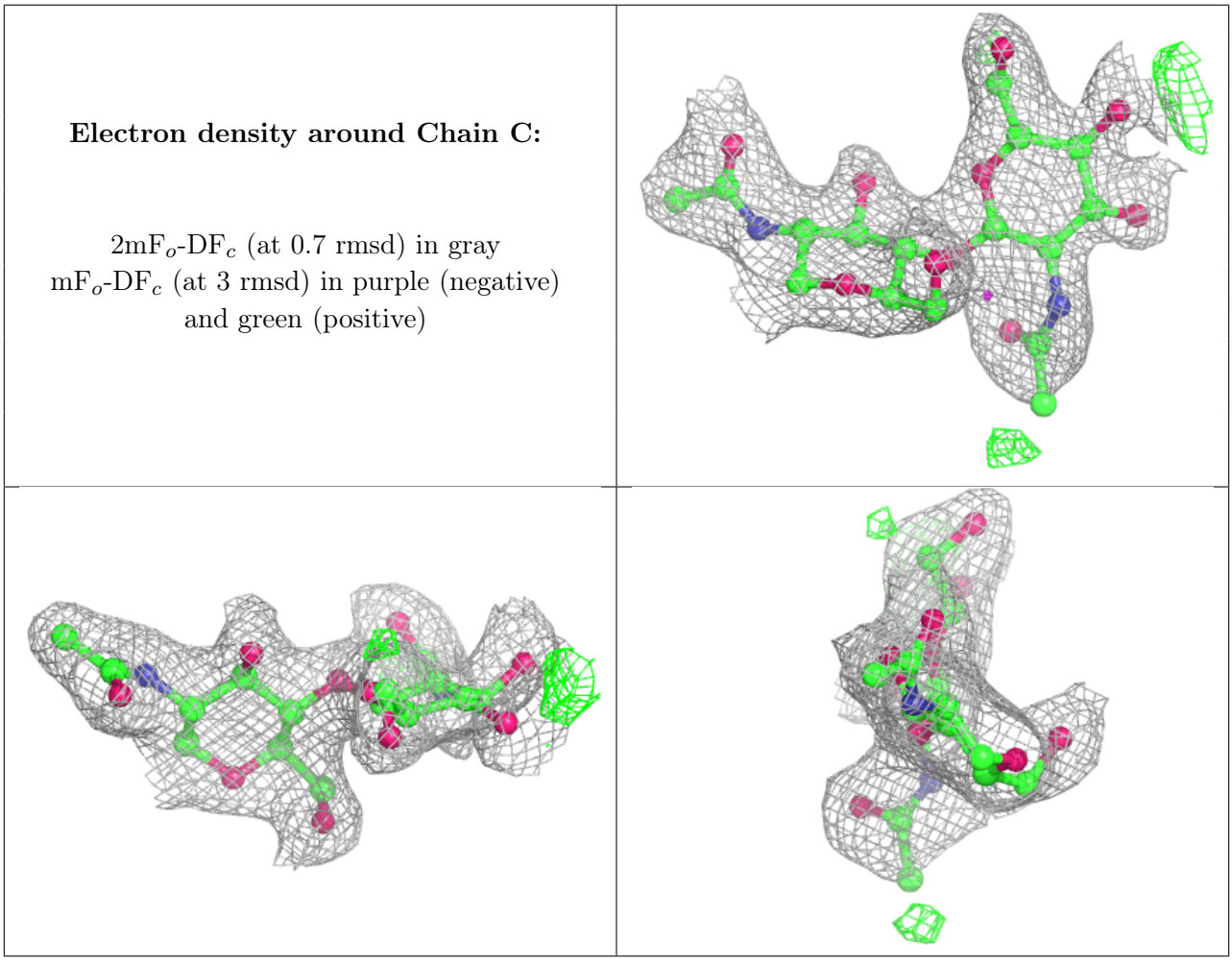
6.3 Carbohydrates

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, 95^{th} 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
5	NAG	C	2	14/15	0.78	0.27	70,75,83,83	0
5	NAG	C	1	14/15	0.92	0.17	47,56,60,65	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.



6.4 Ligands

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, 95^{th} 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	EDO	A	203	4/4	0.65	0.21	61,65,66,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	D	201	14/15	0.83	0.13	47,53,57,58	0

6.5 Other polymers (i)

There are no such residues in this entry.