



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 06:02 PM UTC

PDB ID : 6DFX / pdb\_00006dfx  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

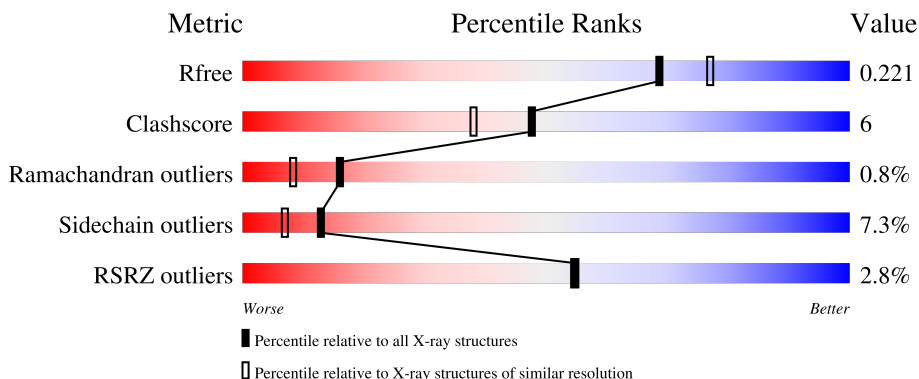
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.03 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.



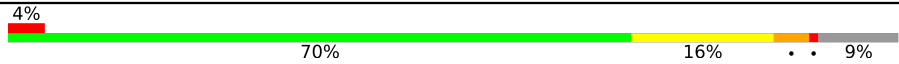

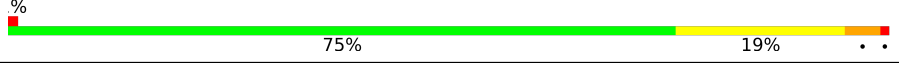
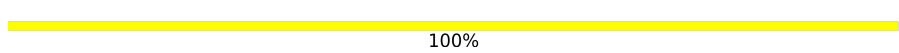
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	 2% 74% 18% . . .
1	D	188	 % 77% 17% . .
2	B	221	 4% 65% 22% . 10%
2	E	221	 3% 63% 22% . . 10%
3	G	207	 4% 61% 25% 6% . 6%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	I	207	 <p>4% 70% 16% • • 9%</p>
4	H	238	 <p>2% 73% 22% 5%</p>
4	J	238	 <p>% 75% 19% • •</p>
5	C	2	 <p>100%</p>

## 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
			Total	C	N	O	S			
1	A	180	1455	937	239	276	3	0	0	0
1	D	180	1455	937	239	276	3	0	0	0

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
			Total	C	N	O	S			
2	B	200	1623	1025	283	307	8	0	0	0
2	E	199	1610	1018	277	307	8	0	0	0

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

*Continued on next page...*

Continued from previous page...

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

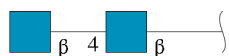
- Molecule 3 is a protein called T1D3 alpha chain.

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

- Molecule 4 is a protein called T1D3 beta chain.

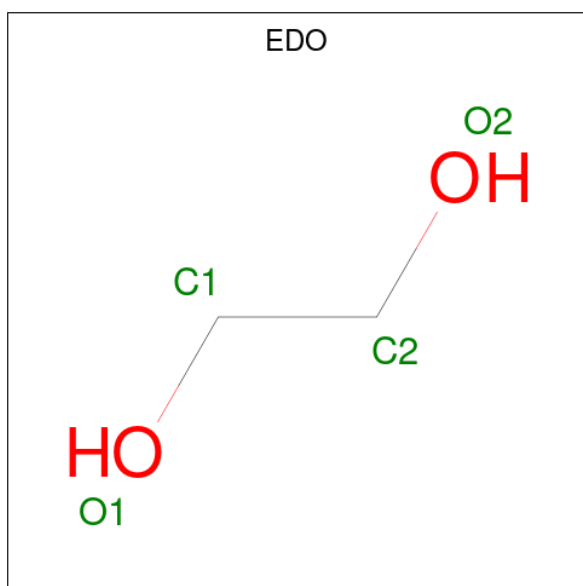
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	237	1885	1187	331	360	7	0	0	0
4	J	237	1885	1187	331	360	7	0	0	0

- 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	
			Total	C	N				O
5	C	2	28	16	2	10	0	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	4	2	2	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

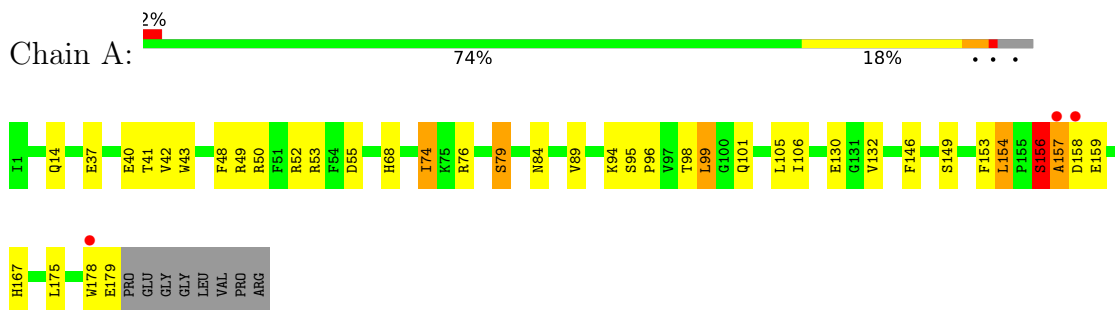
- Molecule 8 is water.

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

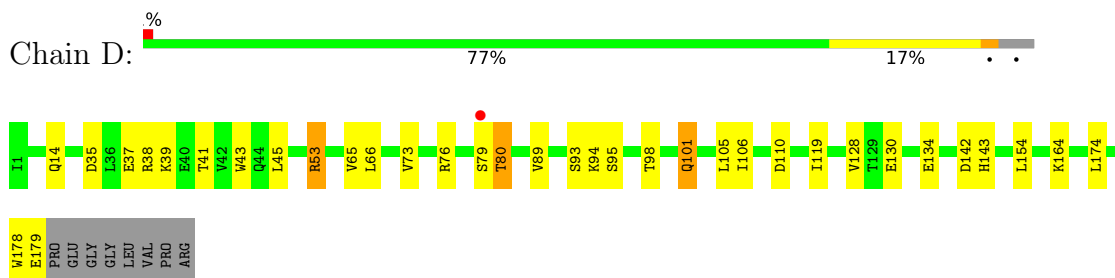
### 3 Residue-property plots [i](#)

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.

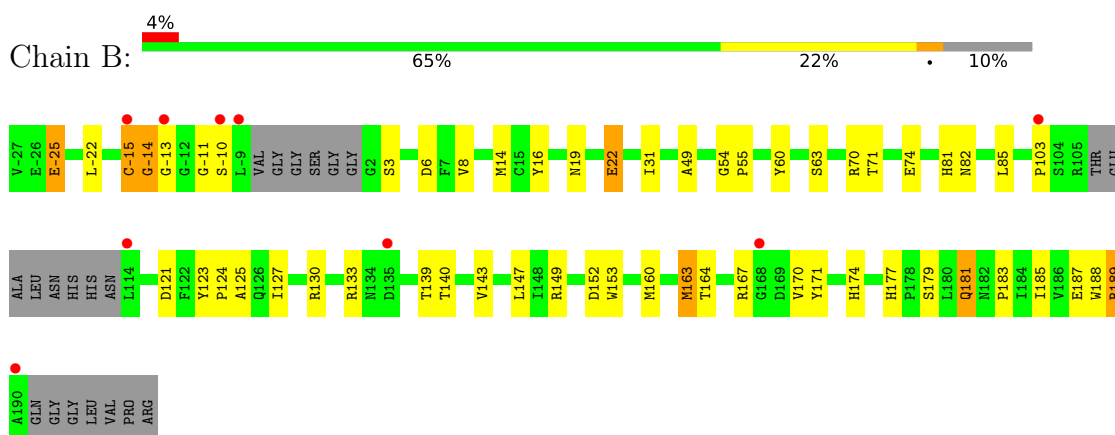
- Molecule 1: MHC class II HLA-DQ-alpha chain



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



- Molecule 2: MHC class II antigen

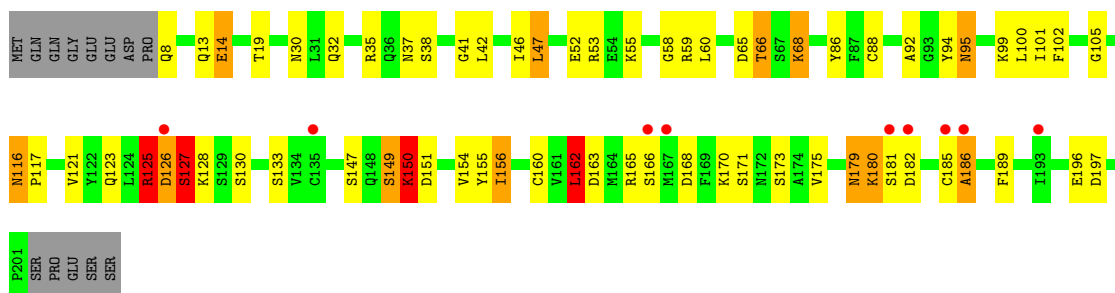


- Molecule 2: MHC class II antigen

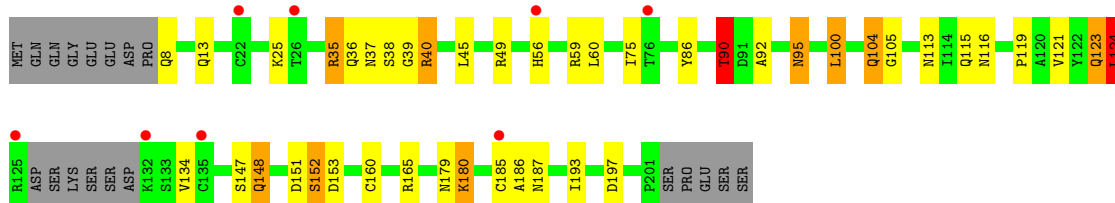




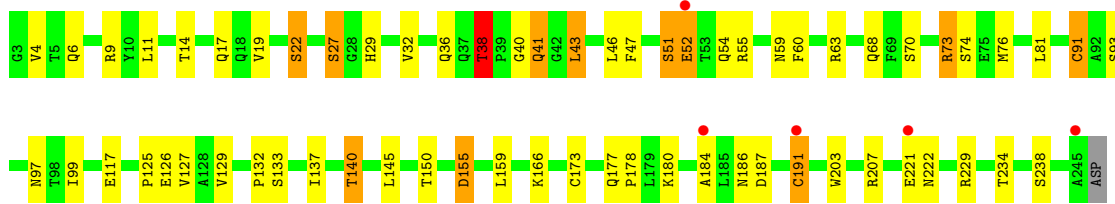
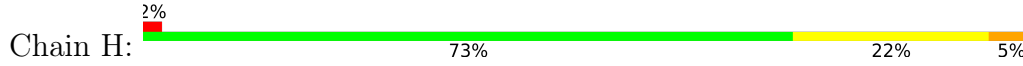
• Molecule 3: T1D3 alpha chain



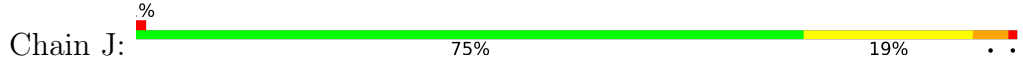
• Molecule 3: T1D3 alpha chain

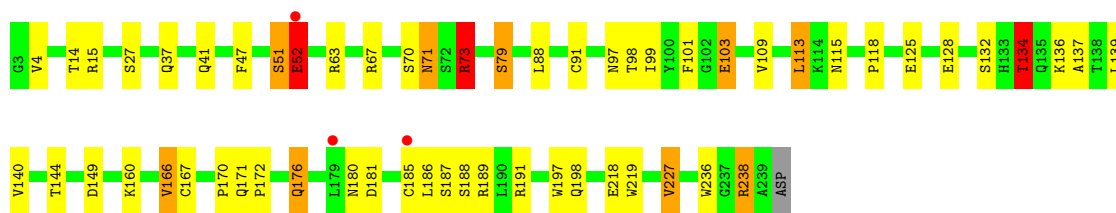


• Molecule 4: T1D3 beta chain

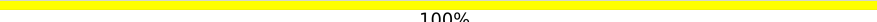


• Molecule 4: T1D3 beta chain





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

Chain C:  100%

MAG1  
MAG2

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.70Å 88.90Å 116.78Å 90.00° 104.26° 90.00°	Depositor
Resolution (Å)	50.01 – 2.03 50.01 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.01-2.03) 99.4 (50.01-2.03)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.03Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.181 , 0.217 0.189 , 0.221	Depositor DCC
$R_{free}$ test set	7241 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.5	Xtrriage
Anisotropy	0.133	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.016 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13693	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: NAG, EDO

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	1.81	26/1498 (1.7%)	1.35	5/2044 (0.2%)
1	D	1.69	17/1498 (1.1%)	1.31	6/2044 (0.3%)
2	B	1.83	29/1660 (1.7%)	1.44	16/2257 (0.7%)
2	E	1.72	22/1647 (1.3%)	1.52	24/2242 (1.1%)
3	G	1.76	27/1531 (1.8%)	1.48	18/2068 (0.9%)
3	I	1.57	8/1477 (0.5%)	1.40	12/1997 (0.6%)
4	H	1.78	32/1937 (1.7%)	1.45	24/2635 (0.9%)
4	J	1.69	23/1937 (1.2%)	1.41	20/2635 (0.8%)
All	All	1.74	184/13185 (1.4%)	1.42	125/17922 (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 184 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	126	ASP	N-CA	10.20	1.59	1.46
2	B	189	ARG	CA-C	9.85	1.64	1.52
4	J	70	SER	C-O	-8.87	1.12	1.24
2	B	-10	SER	N-CA	8.72	1.56	1.46
3	I	40	ARG	C-O	-8.71	1.14	1.23

The worst 5 of 125 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	164	THR	CB-CA-C	10.30	120.83	110.33
4	H	140	THR	N-CA-C	-9.28	96.51	110.14
3	I	165	ARG	NE-CZ-NH2	9.05	127.34	119.20
2	E	149	ARG	NE-CZ-NH2	8.96	127.26	119.20
2	E	149	ARG	NE-CZ-NH1	-8.95	112.55	121.50

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	17	0
2	E	1610	0	1547	25	0
3	G	1506	0	1450	24	0
3	I	1453	0	1392	23	0
4	H	1885	0	1785	28	0
4	J	1885	0	1786	25	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

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	99	0	0	1	0
All	All	13693	0	12356	140	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 6.

The worst 5 of 140 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%)	21	12
1	D	178/188 (95%)	173 (97%)	5 (3%)	0	100	100
2	B	194/221 (88%)	187 (96%)	6 (3%)	1 (0%)	24	17
2	E	193/221 (87%)	182 (94%)	9 (5%)	2 (1%)	12	5
3	G	192/207 (93%)	174 (91%)	12 (6%)	6 (3%)	3	0
3	I	184/207 (89%)	176 (96%)	5 (3%)	3 (2%)	7	2
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%)	16	8

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%)	158 (96%)	7 (4%)	26	20
1	D	165/171 (96%)	157 (95%)	8 (5%)	23	15
2	B	178/192 (93%)	167 (94%)	11 (6%)	16	9
2	E	177/192 (92%)	158 (89%)	19 (11%)	6	2
3	G	171/183 (93%)	152 (89%)	19 (11%)	6	1
3	I	163/183 (89%)	148 (91%)	15 (9%)	8	3
4	H	207/208 (100%)	198 (96%)	9 (4%)	26	19
4	J	207/208 (100%)	190 (92%)	17 (8%)	10	5
All	All	1433/1508 (95%)	1328 (93%)	105 (7%)	13	7

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	154	VAL
4	H	145	LEU
4	J	160	LYS
3	G	162	LEU
4	H	27	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
4	H	177	GLN
3	I	30	ASN
4	H	204	GLN
4	H	215	GLN
3	I	37	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	1.09	1 (7%)	17,19,21	1.56	6 (35%)
5	NAG	C	2	5	14,14,15	1.62	5 (35%)	17,19,21	2.33	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	C2-N2	2.96	1.51	1.46
5	C	2	NAG	O4-C4	2.81	1.49	1.43
5	C	2	NAG	C1-C2	2.61	1.55	1.52
5	C	1	NAG	C1-C2	2.26	1.55	1.52
5	C	2	NAG	C4-C5	2.08	1.57	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2	NAG	C8-C7-N2	4.59	123.73	116.12
5	C	2	NAG	C4-C3-C2	3.50	116.14	111.02
5	C	2	NAG	O7-C7-C8	-3.22	116.32	122.05
5	C	1	NAG	O5-C1-C2	-3.08	106.52	111.29
5	C	2	NAG	O5-C1-C2	2.78	115.60	111.29

There are no chirality outliers.

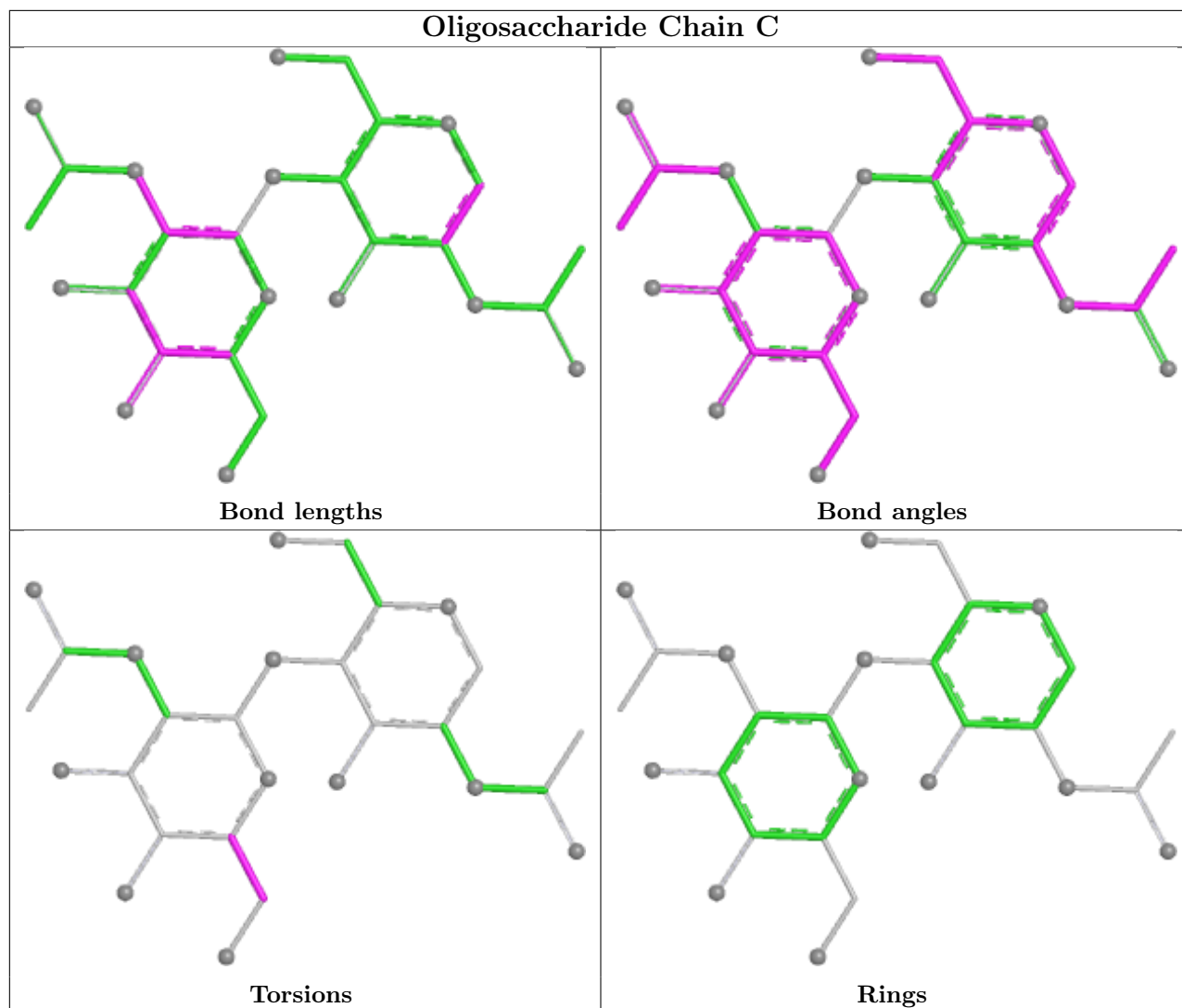
All (2) torsion outliers are listed below:

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.



## 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	2.69	5 (35%)	17,19,21	3.60	8 (47%)
6	EDO	A	203	-	3,3,3	0.79	0	2,2,2	0.47	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	5.80	1.64	1.52
7	D	201	NAG	O4-C4	4.77	1.54	1.43
7	D	201	NAG	O5-C5	4.69	1.52	1.43
7	D	201	NAG	C1-C2	3.10	1.56	1.52
7	D	201	NAG	C4-C3	2.39	1.58	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	201	NAG	C3-C4-C5	-7.12	97.31	110.23
7	D	201	NAG	O4-C4-C3	6.77	126.33	110.38
7	D	201	NAG	O5-C1-C2	-5.62	102.59	111.29
7	D	201	NAG	C1-C2-N2	-5.49	101.78	110.43
7	D	201	NAG	O3-C3-C4	4.50	120.97	110.38

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

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	180/188 (95%)	-0.18	3 (1%) 69 69	25, 40, 71, 82	0
1	D	180/188 (95%)	-0.09	1 (0%) 85 86	31, 44, 71, 87	0
2	B	200/221 (90%)	0.01	9 (4%) 38 37	26, 39, 86, 109	0
2	E	199/221 (90%)	0.06	7 (3%) 47 46	32, 45, 78, 96	0
3	G	194/207 (93%)	0.34	9 (4%) 37 36	28, 58, 89, 109	0
3	I	188/207 (90%)	0.50	8 (4%) 40 39	37, 59, 88, 100	0
4	H	237/238 (99%)	-0.10	5 (2%) 63 63	30, 42, 69, 77	0
4	J	237/238 (99%)	-0.08	3 (1%) 75 75	34, 44, 68, 79	0
All	All	1615/1708 (94%)	0.05	45 (2%) 55 54	25, 46, 80, 109	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	190	ALA	5.3
1	A	157	ALA	4.6
4	J	185	CYS	4.4
2	E	-9	LEU	4.2
2	E	190	ALA	3.8

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

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

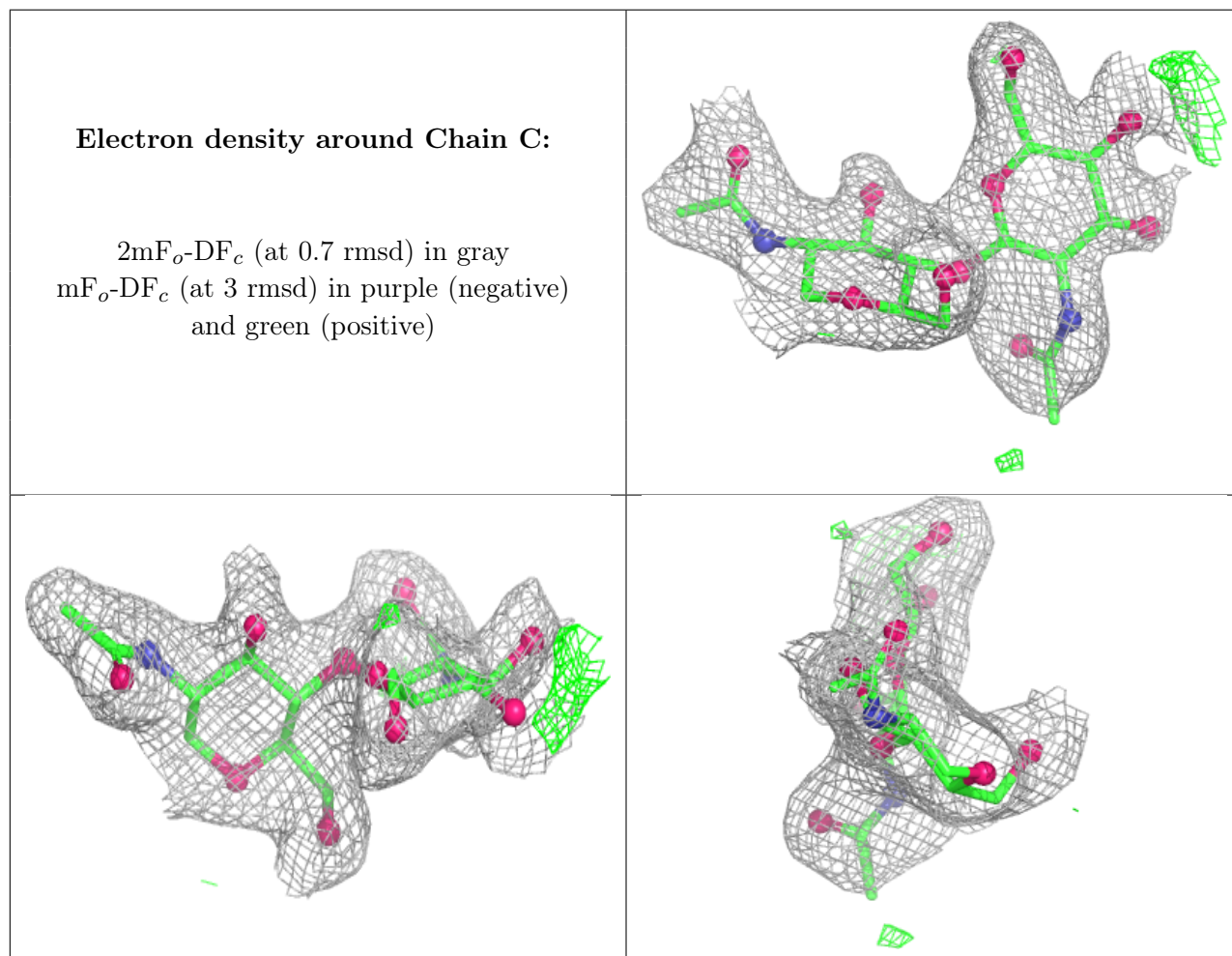
### 6.3 Carbohydrates [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	NAG	C	1	14/15	-	-	47,56,60,65	0
5	NAG	C	2	14/15	-	-	70,75,83,83	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	EDO	A	203	4/4	0.71	0.16	61,65,66,67	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	D	201	14/15	0.82	0.12	47,53,57,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.