



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 11, 2022 – 12:18 PM EDT

PDB ID : 7N3T  
Title : TrkA ECD complex with designed miniprotein ligand  
Authors : Jude, K.M.; Cao, L.; Garcia, K.C.  
Deposited on : 2021-06-01  
Resolution : 1.84 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](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.

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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) : 1.13  
EDS : 2.27  
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) : 2.27

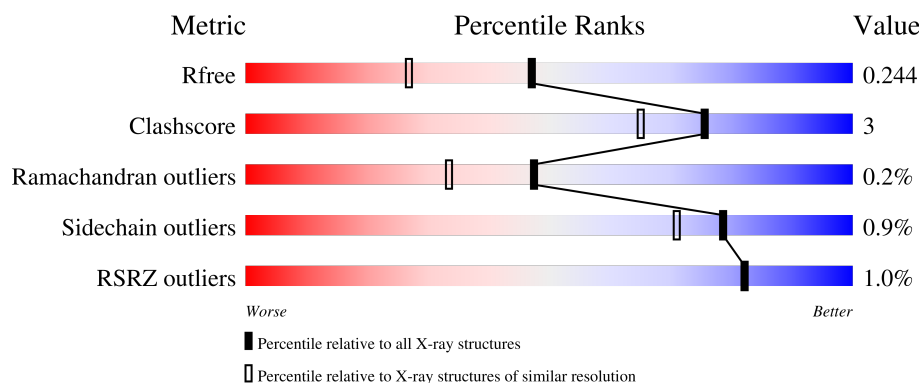
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.84 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	359	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>89%</span> <span>7%</span> <span>.</span> </div> </div>
1	B	359	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>89%</span> <span>7%</span> <span>.</span> </div> </div>
2	C	81	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>69%</span> <span>5%</span> <span>26%</span> </div> </div>
2	D	81	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>65%</span> <span>7%</span> <span>27%</span> </div> </div>
3	E	3	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>67%</span> <span>33%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
4	F	2	

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6886 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 High affinity nerve growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2665	1666	480	502	17			
1	B	346	Total	C	N	O	S	0	1	0
			2658	1662	478	500	18			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	SER	-	expression tag	UNP P04629
A	263	LEU	VAL	conflict	UNP P04629
A	383	ALA	-	expression tag	UNP P04629
A	384	ALA	-	expression tag	UNP P04629
A	385	ALA	-	expression tag	UNP P04629
A	386	HIS	-	expression tag	UNP P04629
A	387	HIS	-	expression tag	UNP P04629
A	388	HIS	-	expression tag	UNP P04629
A	389	HIS	-	expression tag	UNP P04629
A	390	HIS	-	expression tag	UNP P04629
A	391	HIS	-	expression tag	UNP P04629
A	392	HIS	-	expression tag	UNP P04629
A	393	HIS	-	expression tag	UNP P04629
B	35	SER	-	expression tag	UNP P04629
B	263	LEU	VAL	conflict	UNP P04629
B	383	ALA	-	expression tag	UNP P04629
B	384	ALA	-	expression tag	UNP P04629
B	385	ALA	-	expression tag	UNP P04629
B	386	HIS	-	expression tag	UNP P04629
B	387	HIS	-	expression tag	UNP P04629
B	388	HIS	-	expression tag	UNP P04629
B	389	HIS	-	expression tag	UNP P04629
B	390	HIS	-	expression tag	UNP P04629
B	391	HIS	-	expression tag	UNP P04629
B	392	HIS	-	expression tag	UNP P04629

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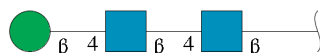
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Chain	Residue	Modelled	Actual	Comment	Reference
B	393	HIS	-	expression tag	UNP P04629

- Molecule 2 is a protein called Designed TrkA-binding miniprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	60	Total	C	N	O	0	1	0
			482	304	91	87			
2	D	59	Total	C	N	O	0	0	0
			470	297	89	84			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 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
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- 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	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	126	Total	O	0	1
			127	127		
8	B	120	Total	O	0	1
			121	121		

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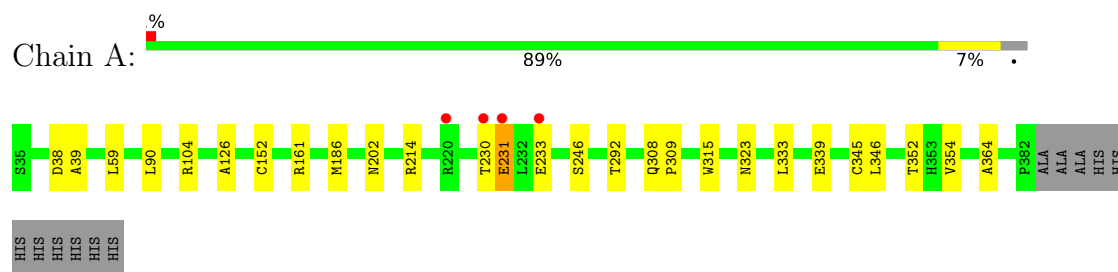
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	7	Total	O	0	0
			7	7		
8	D	7	Total	O	0	0
			7	7		

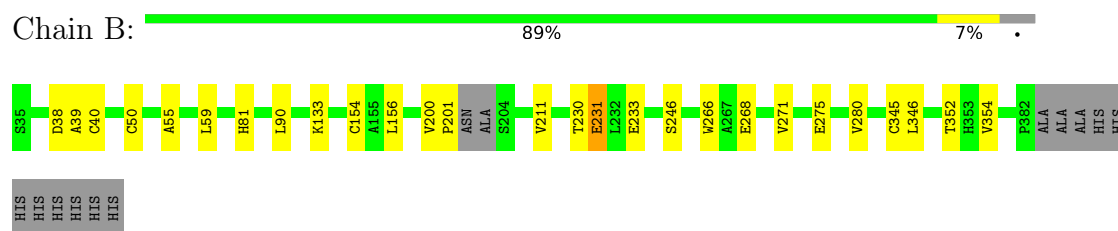
### 3 Residue-property plots [i](#)

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.

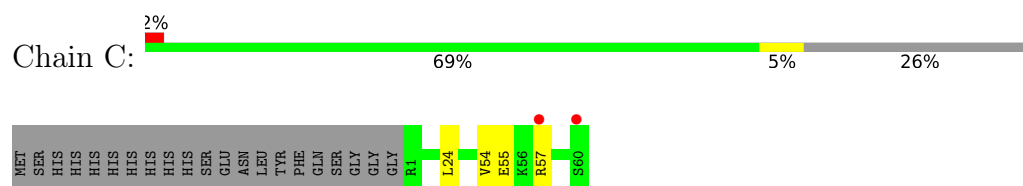
- Molecule 1: High affinity nerve growth factor receptor



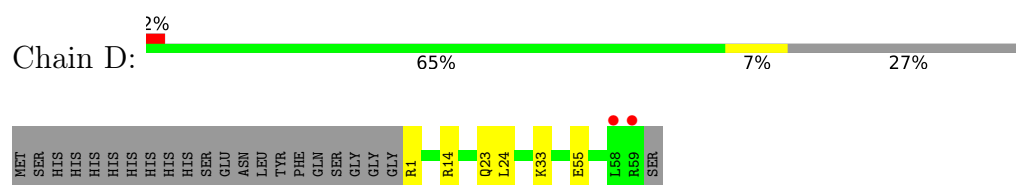
- Molecule 1: High affinity nerve growth factor receptor



- Molecule 2: Designed TrkA-binding miniprotein



- Molecule 2: Designed TrkA-binding miniprotein



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





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

Chain F:  50% 50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.20Å 205.69Å 72.57Å 90.00° 106.42° 90.00°	Depositor
Resolution (Å)	41.36 – 1.84 41.36 – 1.84	Depositor EDS
% Data completeness (in resolution range)	96.2 (41.36-1.84) 82.4 (41.36-1.84)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.10 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122+SVN	Depositor
R, $R_{free}$	0.214 , 0.242 0.213 , 0.244	Depositor DCC
$R_{free}$ test set	2487 reflections (2.49%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 39.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.116 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6886	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, NAG, BMA, SO4

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	0.57	0/2726	0.72	0/3714
1	B	0.56	0/2718	0.71	0/3701
2	C	0.55	0/487	0.66	0/648
2	D	0.54	0/472	0.66	0/628
All	All	0.56	0/6403	0.71	0/8691

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
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	345	CYS	Peptide
1	B	345	CYS	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2665	0	2583	20	0
1	B	2658	0	2573	15	0
2	C	482	0	511	5	0
2	D	470	0	498	2	0
3	E	39	0	34	0	0
4	F	28	0	25	0	0
5	A	84	0	78	1	0
5	B	112	0	104	3	0
6	A	20	0	30	4	0
6	B	16	0	24	0	0
7	A	25	0	0	0	0
7	B	25	0	0	0	0
8	A	127	0	0	1	0
8	B	121	0	0	2	0
8	C	7	0	0	0	0
8	D	7	0	0	0	0
All	All	6886	0	6460	41	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 3.

All (41) 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:A:59:LEU:HD21	1:A:90:LEU:HD11	1.63	0.79
1:A:364:ALA:HB3	6:A:406:EDO:H12	1.74	0.69
2:C:24:LEU:HD13	2:C:55:GLU:HG3	1.73	0.68
1:B:59:LEU:HD21	1:B:90:LEU:HD11	1.75	0.68
2:D:24:LEU:HD13	2:D:55:GLU:HG3	1.81	0.62
1:A:231:GLU:HG3	1:A:233:GLU:HG3	1.82	0.62
2:D:14:ARG:HB2	2:D:23:GLN:HG2	1.88	0.56
1:B:50[B]:CYS:SG	1:B:55:ALA:HB2	2.46	0.56
1:B:38:ASP:OD1	1:B:39:ALA:N	2.40	0.55
1:A:161:ARG:NH2	8:A:501:HOH:O	2.31	0.54
1:A:38:ASP:OD1	1:A:39:ALA:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:CYS:SG	1:B:50[B]:CYS:HB2	2.51	0.50
1:A:214:ARG:HD3	1:A:246:SER:OG	2.12	0.49
1:A:352:THR:OG1	1:A:354:VAL:HG22	2.14	0.48
1:A:308:GLN:HA	1:A:309:PRO:C	2.34	0.48
1:A:339:GLU:HB3	5:A:409:NAG:H82	1.96	0.48
1:A:292:THR:HB	2:C:57:ARG:HH12	1.79	0.47
1:B:211:VAL:HG11	1:B:280:VAL:HG11	1.97	0.46
1:A:315:TRP:CZ2	1:A:346:LEU:HB2	2.52	0.46
2:C:24:LEU:CD1	2:C:55:GLU:HG3	2.45	0.45
1:B:133:LYS:NZ	1:B:268:GLU:OE2	2.49	0.45
1:B:154:CYS:HB3	1:B:271:VAL:HG22	1.99	0.45
1:A:292:THR:HB	2:C:57:ARG:NH1	2.32	0.45
1:A:333:LEU:HD23	6:A:408:EDO:H11	1.98	0.45
5:B:402:NAG:N2	8:B:502:HOH:O	2.22	0.44
1:A:352:THR:HG22	5:B:402:NAG:H83	2.00	0.44
1:B:346:LEU:HD12	1:B:346:LEU:HA	1.89	0.44
1:B:246:SER:OG	8:B:501:HOH:O	2.22	0.43
1:A:352:THR:HG22	5:B:402:NAG:C8	2.49	0.43
1:A:364:ALA:CB	6:A:406:EDO:H12	2.48	0.42
1:A:152:CYS:HB3	1:A:186:MET:SD	2.59	0.42
1:B:200:VAL:HB	1:B:201:PRO:HD2	2.01	0.42
2:C:24:LEU:HD11	2:C:54:VAL:HG12	2.01	0.42
1:B:266:TRP:HZ3	1:B:268:GLU:HG2	1.85	0.41
1:A:230:THR:O	1:A:231:GLU:C	2.58	0.41
1:B:352:THR:OG1	1:B:354:VAL:HG22	2.19	0.41
1:B:230:THR:O	1:B:231:GLU:C	2.59	0.41
1:A:333:LEU:CD2	6:A:408:EDO:H11	2.50	0.41
1:B:156:LEU:HD23	1:B:156:LEU:HA	1.92	0.41
1:B:231:GLU:HG3	1:B:233:GLU:HG3	2.03	0.41
1:A:104:ARG:HG2	1:A:126:ALA:HB3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	346/359 (96%)	336 (97%)	9 (3%)	1 (0%)	41	27
1	B	343/359 (96%)	333 (97%)	9 (3%)	1 (0%)	41	27
2	C	59/81 (73%)	58 (98%)	1 (2%)	0	100	100
2	D	57/81 (70%)	56 (98%)	1 (2%)	0	100	100
All	All	805/880 (92%)	783 (97%)	20 (2%)	2 (0%)	47	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	GLU
1	B	231	GLU

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	294/302 (97%)	292 (99%)	2 (1%)	84	78
1	B	294/302 (97%)	292 (99%)	2 (1%)	84	78
2	C	49/71 (69%)	49 (100%)	0	100	100
2	D	47/71 (66%)	45 (96%)	2 (4%)	29	12
All	All	684/746 (92%)	678 (99%)	6 (1%)	78	71

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	A	323	ASN
1	B	81	HIS
1	B	275	GLU
2	D	1	ARG
2	D	33	LYS



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

5 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	$\# Z  > 2$
3	NAG	E	1	3,1	14,14,15	0.44	0	17,19,21	0.66	0
3	NAG	E	2	3	14,14,15	0.42	0	17,19,21	0.46	0
3	BMA	E	3	3	11,11,12	1.44	2 (18%)	15,15,17	1.01	0
4	NAG	F	1	4,1	14,14,15	0.72	1 (7%)	17,19,21	0.54	0
4	NAG	F	2	4	14,14,15	0.41	0	17,19,21	0.61	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
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	3	BMA	C1-C2	2.70	1.58	1.52
3	E	3	BMA	C4-C5	2.68	1.58	1.53
4	F	1	NAG	O5-C1	2.06	1.47	1.43

There are no bond angle outliers.

There are no chirality outliers.

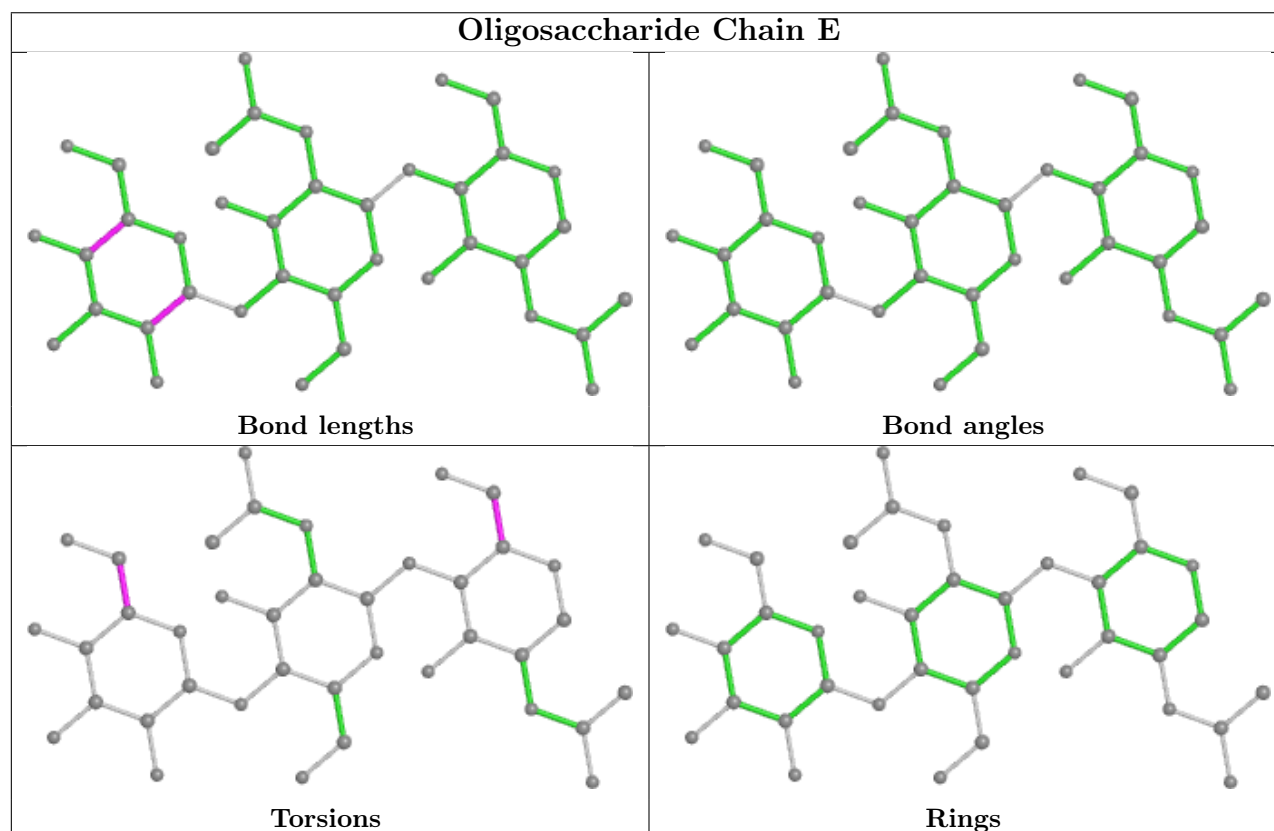
All (4) torsion outliers are listed below:

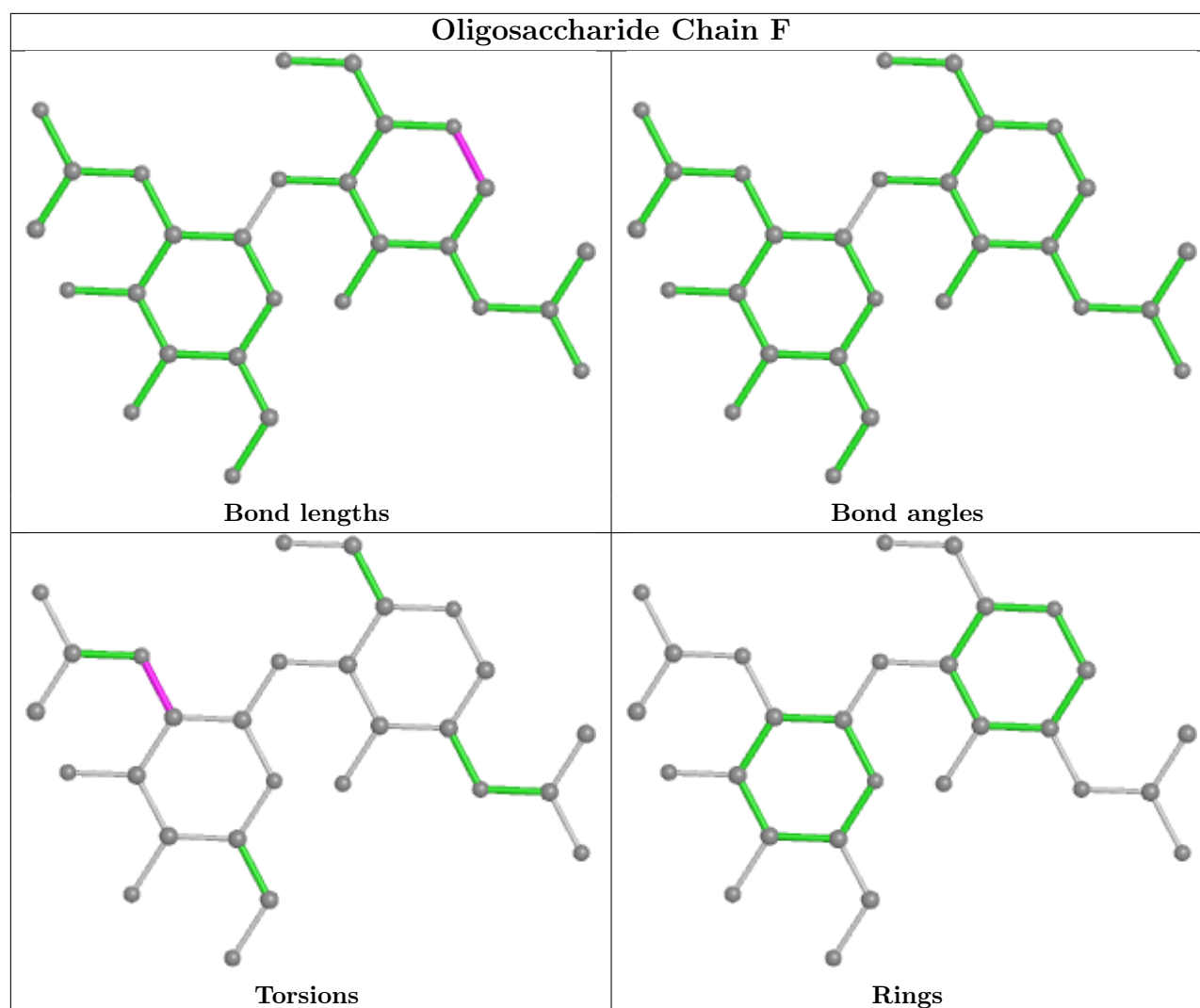
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
4	F	2	NAG	C3-C2-N2-C7

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](#)

33 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	$\# Z  > 2$
5	NAG	A	403	1	14,14,15	0.43	0	17,19,21	0.58	0
5	NAG	A	402	1	14,14,15	0.57	0	17,19,21	0.53	0
7	SO4	B	413	-	4,4,4	0.25	0	6,6,6	0.55	0
5	NAG	B	403	1	14,14,15	0.26	0	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	405	1	14,14,15	0.39	0	17,19,21	0.78	1 (5%)
7	SO4	B	415	-	4,4,4	0.20	0	6,6,6	0.45	0
7	SO4	A	412	-	4,4,4	0.19	0	6,6,6	0.32	0
5	NAG	A	404	1	14,14,15	0.80	1 (7%)	17,19,21	0.57	0
7	SO4	B	414	-	4,4,4	0.14	0	6,6,6	0.48	0
5	NAG	A	401	1	14,14,15	0.40	0	17,19,21	0.52	0
6	EDO	A	408	-	3,3,3	0.55	0	2,2,2	0.46	0
5	NAG	B	402	1	14,14,15	0.56	0	17,19,21	0.74	0
6	EDO	A	410	-	3,3,3	0.60	0	2,2,2	0.43	0
5	NAG	A	409	1	14,14,15	1.06	2 (14%)	17,19,21	0.74	1 (5%)
7	SO4	B	417	-	4,4,4	0.20	0	6,6,6	0.85	0
6	EDO	A	406	-	3,3,3	0.49	0	2,2,2	0.16	0
7	SO4	A	414	-	4,4,4	0.14	0	6,6,6	0.23	0
5	NAG	B	404	1	14,14,15	0.68	0	17,19,21	0.46	0
6	EDO	B	407	-	3,3,3	0.43	0	2,2,2	1.05	0
6	EDO	B	410	-	3,3,3	0.52	0	2,2,2	0.73	0
5	NAG	B	408	1	14,14,15	0.31	0	17,19,21	0.39	0
5	NAG	B	405	1	14,14,15	0.32	0	17,19,21	0.69	1 (5%)
7	SO4	A	416	-	4,4,4	0.19	0	6,6,6	0.55	0
6	EDO	B	406	-	3,3,3	0.94	0	2,2,2	0.17	0
6	EDO	B	412	-	3,3,3	0.23	0	2,2,2	0.93	0
7	SO4	A	415	-	4,4,4	0.26	0	6,6,6	0.77	0
7	SO4	A	413	-	4,4,4	0.38	0	6,6,6	0.35	0
5	NAG	B	409	1	14,14,15	0.75	1 (7%)	17,19,21	0.62	0
5	NAG	B	411	1	14,14,15	0.22	0	17,19,21	0.62	0
6	EDO	A	407	-	3,3,3	0.42	0	2,2,2	0.84	0
6	EDO	A	411	-	3,3,3	0.57	0	2,2,2	0.21	0
7	SO4	B	416	-	4,4,4	0.13	0	6,6,6	0.35	0
5	NAG	B	401	1	14,14,15	0.49	0	17,19,21	0.57	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
5	NAG	A	403	1	-	0/6/23/26	0/1/1/1
5	NAG	A	402	1	-	0/6/23/26	0/1/1/1
5	NAG	B	403	1	-	0/6/23/26	0/1/1/1
5	NAG	A	405	1	-	0/6/23/26	0/1/1/1
5	NAG	A	404	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	401	1	-	0/6/23/26	0/1/1/1
6	EDO	A	408	-	-	0/1/1/1	-
5	NAG	B	402	1	-	0/6/23/26	0/1/1/1
6	EDO	A	410	-	-	0/1/1/1	-
5	NAG	A	409	1	-	0/6/23/26	0/1/1/1
6	EDO	A	406	-	-	0/1/1/1	-
5	NAG	B	404	1	-	2/6/23/26	0/1/1/1
6	EDO	B	407	-	-	1/1/1/1	-
6	EDO	B	410	-	-	0/1/1/1	-
5	NAG	B	408	1	-	0/6/23/26	0/1/1/1
5	NAG	B	405	1	-	2/6/23/26	0/1/1/1
6	EDO	B	406	-	-	0/1/1/1	-
6	EDO	B	412	-	-	0/1/1/1	-
5	NAG	B	409	1	-	0/6/23/26	0/1/1/1
5	NAG	B	411	1	-	0/6/23/26	0/1/1/1
6	EDO	A	407	-	-	1/1/1/1	-
6	EDO	A	411	-	-	0/1/1/1	-
5	NAG	B	401	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	409	NAG	C1-C2	3.12	1.57	1.52
5	A	404	NAG	O5-C1	2.55	1.47	1.43
5	A	409	NAG	O5-C1	2.30	1.47	1.43
5	B	409	NAG	O5-C1	2.13	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	405	NAG	C1-O5-C5	2.58	115.69	112.19
5	A	409	NAG	C1-O5-C5	2.21	115.19	112.19
5	B	405	NAG	C1-O5-C5	2.02	114.94	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	404	NAG	O5-C5-C6-O6
5	B	404	NAG	C4-C5-C6-O6
5	B	405	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	405	NAG	O5-C5-C6-O6
6	B	407	EDO	O1-C1-C2-O2
6	A	407	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	408	EDO	2	0
5	B	402	NAG	3	0
5	A	409	NAG	1	0
6	A	406	EDO	2	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 [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	348/359 (96%)	-0.15	4 (1%) 80 80	24, 39, 59, 88	0
1	B	346/359 (96%)	-0.17	0 100 100	24, 38, 55, 85	0
2	C	60/81 (74%)	0.10	2 (3%) 46 43	30, 46, 79, 94	0
2	D	59/81 (72%)	0.14	2 (3%) 45 41	31, 47, 70, 76	0
All	All	813/880 (92%)	-0.12	8 (0%) 82 82	24, 39, 63, 94	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	60	SER	3.9
1	A	230	THR	2.8
2	C	57	ARG	2.7
2	D	58	LEU	2.4
2	D	59	ARG	2.4
1	A	220	ARG	2.1
1	A	231	GLU	2.1
1	A	233	GLU	2.0

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

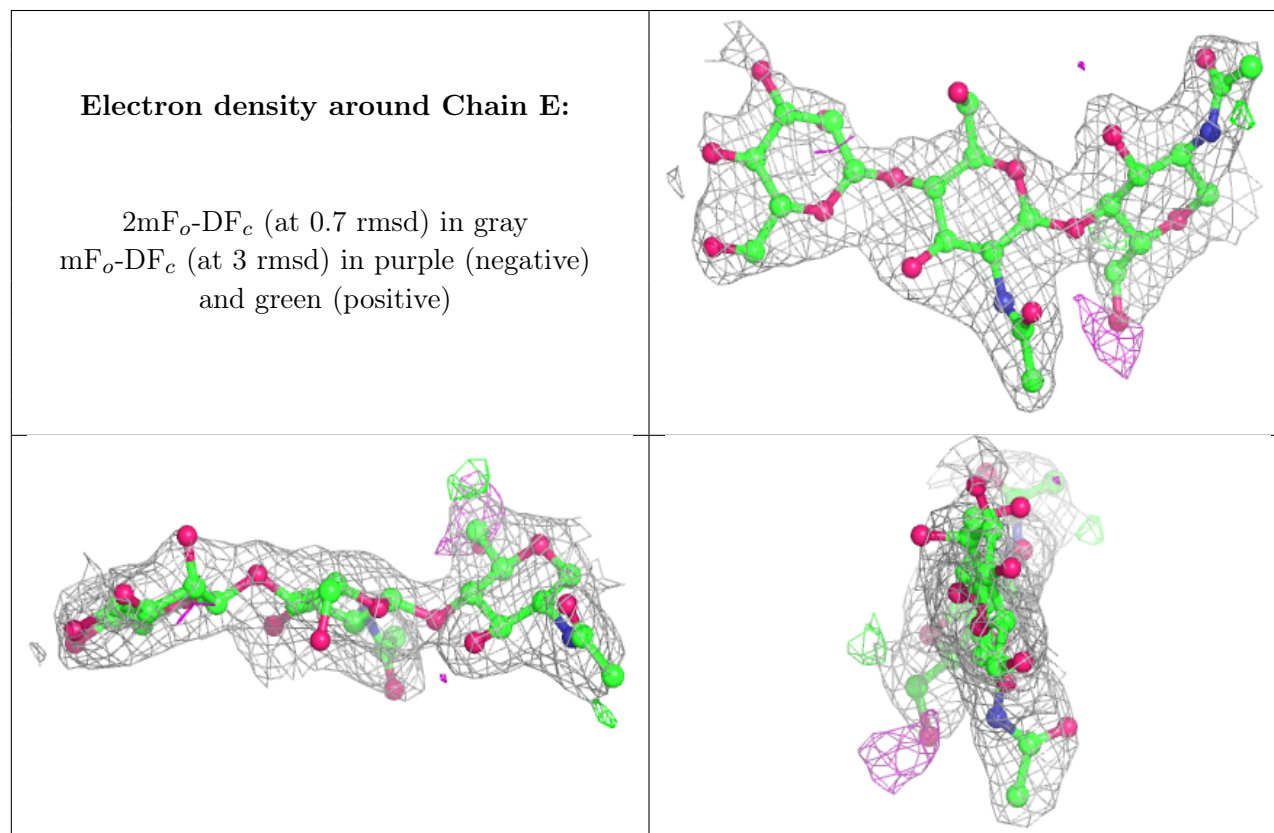
There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

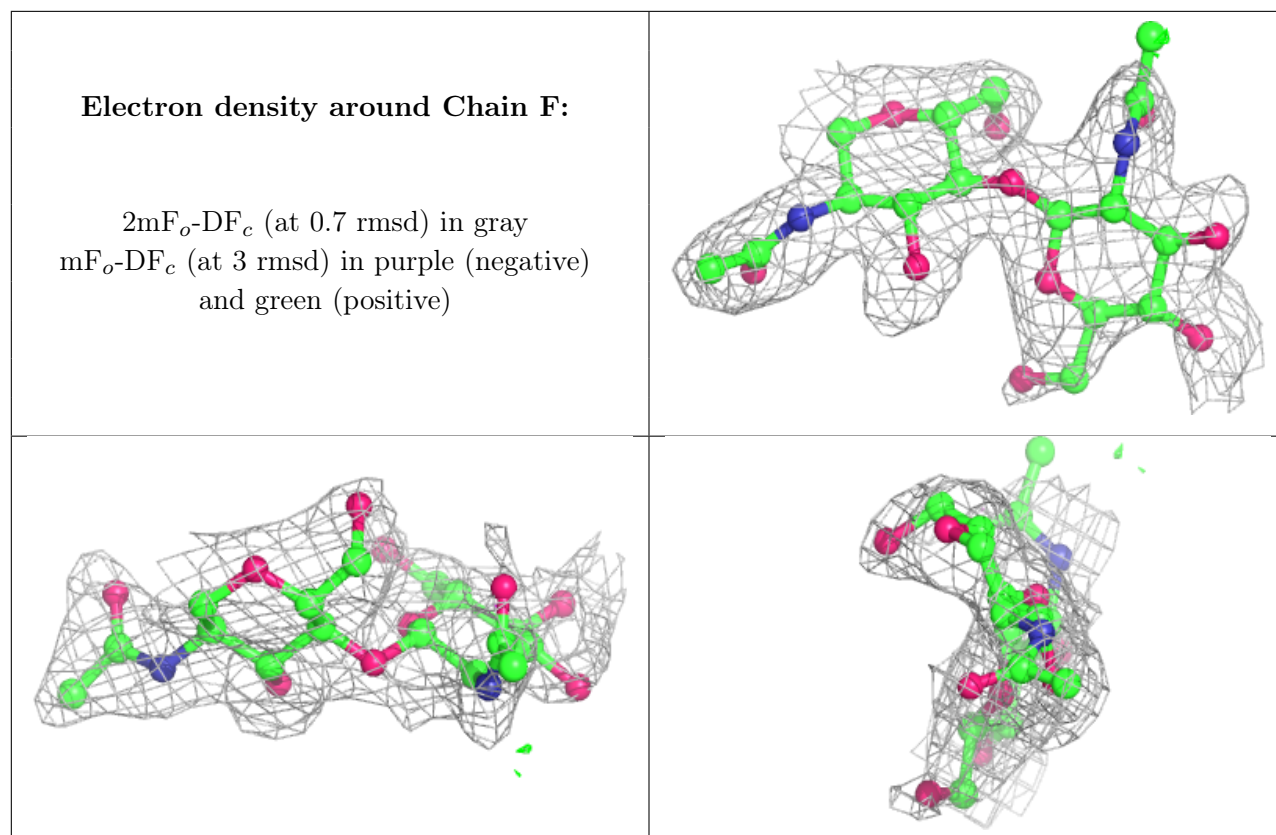
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BMA	E	3	11/12	0.62	0.21	86,95,101,101	0
4	NAG	F	2	14/15	0.79	0.25	67,75,81,84	0
3	NAG	E	2	14/15	0.84	0.18	60,76,91,92	0
4	NAG	F	1	14/15	0.91	0.14	43,50,57,66	0
3	NAG	E	1	14/15	0.92	0.15	49,52,62,68	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
5	NAG	B	408	14/15	0.72	0.30	78,84,89,90	0
5	NAG	B	411	14/15	0.72	0.35	73,81,89,89	0
5	NAG	B	405	14/15	0.77	0.19	51,61,70,71	0
5	NAG	B	409	14/15	0.86	0.14	65,71,76,78	0
5	NAG	A	405	14/15	0.86	0.15	60,71,75,85	0
6	EDO	B	410	4/4	0.86	0.14	46,50,56,56	0
5	NAG	A	409	14/15	0.87	0.26	54,66,78,84	0
7	SO4	A	416	5/5	0.88	0.13	34,45,48,51	5
5	NAG	B	401	14/15	0.90	0.13	34,42,48,53	0
5	NAG	B	403	14/15	0.90	0.14	49,56,61,66	0
6	EDO	B	407	4/4	0.90	0.15	39,42,46,47	0
5	NAG	A	401	14/15	0.90	0.20	54,67,76,87	0
7	SO4	A	415	5/5	0.90	0.17	32,33,36,45	5
5	NAG	A	402	14/15	0.90	0.15	51,59,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	EDO	A	407	4/4	0.91	0.16	36,38,41,43	0
6	EDO	B	406	4/4	0.91	0.13	31,36,43,45	0
5	NAG	A	404	14/15	0.91	0.10	40,46,51,52	0
5	NAG	B	404	14/15	0.92	0.21	58,69,74,79	0
7	SO4	A	414	5/5	0.93	0.12	53,55,64,64	5
5	NAG	B	402	14/15	0.93	0.11	31,37,42,43	0
6	EDO	B	412	4/4	0.93	0.21	41,44,49,58	0
6	EDO	A	408	4/4	0.94	0.15	34,41,41,45	0
5	NAG	A	403	14/15	0.94	0.12	30,33,42,43	0
6	EDO	A	411	4/4	0.95	0.24	42,46,48,50	0
6	EDO	A	410	4/4	0.95	0.29	44,45,47,52	0
7	SO4	B	417	5/5	0.95	0.13	32,32,38,43	5
7	SO4	B	416	5/5	0.96	0.12	59,66,70,72	0
7	SO4	B	415	5/5	0.96	0.09	43,43,47,48	5
7	SO4	B	413	5/5	0.98	0.10	49,53,64,67	0
6	EDO	A	406	4/4	0.98	0.11	33,35,38,40	0
7	SO4	A	412	5/5	0.99	0.06	46,54,60,70	0
7	SO4	A	413	5/5	0.99	0.08	41,51,51,55	0
7	SO4	B	414	5/5	0.99	0.11	40,43,43,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.