



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 03:02 AM EST

PDB ID : 8DVL  
Title : Crystal structure of LRP6 E3E4 in complex with disulfide constrained peptide E3.18  
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Deposited on : 2022-07-29  
Resolution : 2.50 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.

The types of validation reports are described at

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

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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 : 2.36  
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) : 2.36

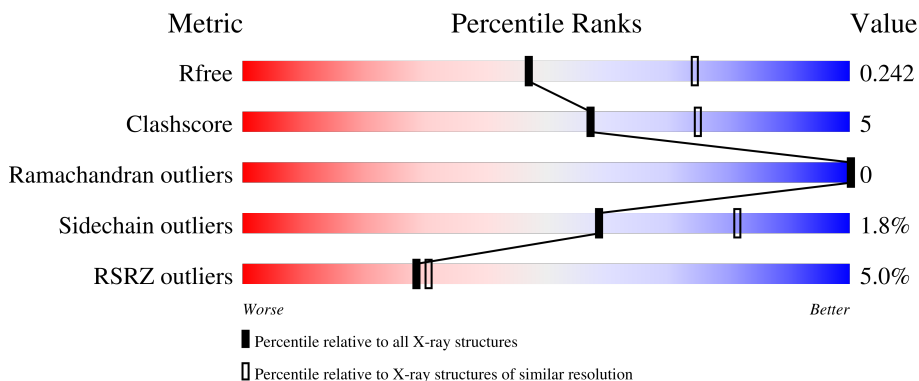
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	633	 5% 82% 15%
2	B	32	 6% 34% 9% 56%
3	C	3	 33% 67%
4	D	3	 67% 33%
5	E	6	 50% 50%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
3	FUC	C	2	-	-	-	X
3	NAG	C	3	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5197 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 Low-density lipoprotein receptor-related protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	610	4874	3055	864	930	25	0	2	0

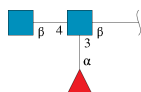
There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	630	SER	-	expression tag	UNP O75581
A	1062	ILE	VAL	variant	UNP O75581
A	1254	GLY	-	expression tag	UNP O75581
A	1255	ASN	-	expression tag	UNP O75581
A	1256	SER	-	expression tag	UNP O75581
A	1257	HIS	-	expression tag	UNP O75581
A	1258	HIS	-	expression tag	UNP O75581
A	1259	HIS	-	expression tag	UNP O75581
A	1260	HIS	-	expression tag	UNP O75581
A	1261	HIS	-	expression tag	UNP O75581
A	1262	HIS	-	expression tag	UNP O75581

- Molecule 2 is a protein called E3.18 Disulfide constrained peptide.

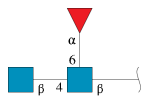
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	14	102	63	21	16	2	0	0	0

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



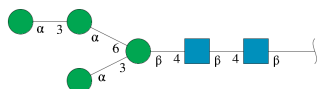
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	3	38	22	2	14	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	3	38	22	2	14	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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
			Total	C	N	O			
5	E	6	72	40	2	30	0	0	0

- Molecule 6 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>).

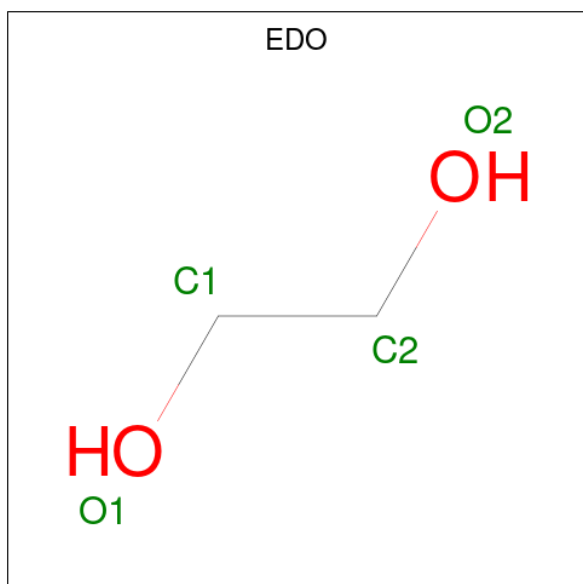


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

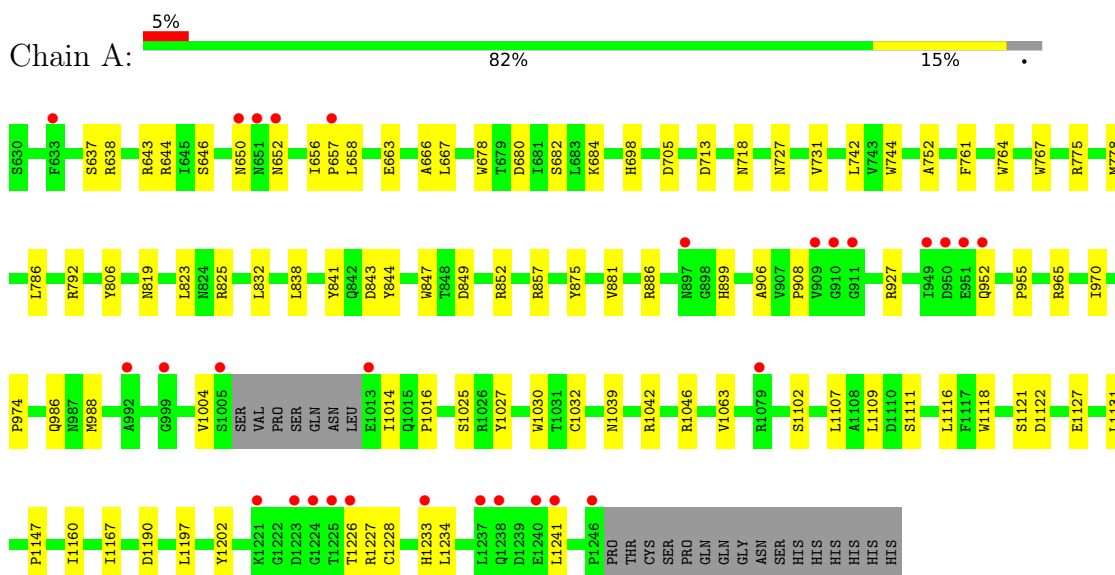
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	14	Total O 14 14	0	0

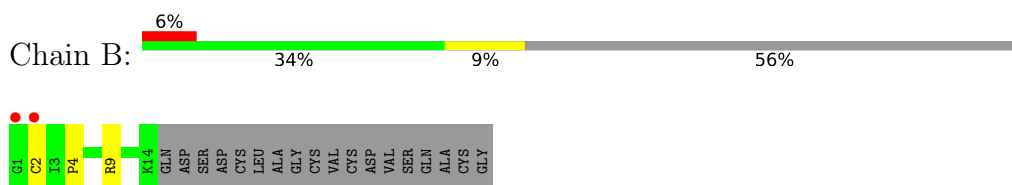
### 3 Residue-property plots [i](#)

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: Low-density lipoprotein receptor-related protein 6



- Molecule 2: E3.18 Disulfide constrained peptide



- Molecule 3: alpha-L-fucopyranose-(1-3)-[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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

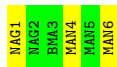






- Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.91Å 73.83Å 87.19Å 90.00° 96.58° 90.00°	Depositor
Resolution (Å)	45.58 – 2.50 45.58 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.8 (45.58-2.50) 88.7 (45.58-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 2.48Å)	Xtrriage
Refinement program	PHENIX 1.20rc3-4406_final	Depositor
R, $R_{free}$	0.197 , 0.245 0.195 , 0.242	Depositor DCC
$R_{free}$ test set	1949 reflections (7.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.7	Xtrriage
Anisotropy	0.440	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5197	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% 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, BMA, OCS, FUC, MAN, CA, 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	0.32	0/4969	0.58	0/6739
2	B	0.36	0/102	0.63	0/136
All	All	0.32	0/5071	0.58	0/6875

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	4874	0	4745	49	0
2	B	102	0	116	2	0
3	C	38	0	34	0	0
4	D	38	0	34	1	0
5	E	72	0	61	1	0
6	A	28	0	26	0	0
7	A	3	0	0	0	0
8	A	28	0	41	0	0
9	A	14	0	0	0	0
All	All	5197	0	5057	50	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.

All (50) 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:1042:ARG:NH2	1:A:1046:ARG:HE	1.89	0.71
1:A:1063:VAL:CG2	1:A:1109:LEU:HD23	2.22	0.69
1:A:1014:ILE:HG22	1:A:1016:PRO:HD3	1.81	0.61
1:A:1063:VAL:HG23	1:A:1109:LEU:HD23	1.83	0.61
1:A:1197:LEU:HD11	1:A:1202:TYR:HB2	1.82	0.61
1:A:1042:ARG:HH22	1:A:1046:ARG:HE	1.51	0.57
1:A:637:SER:HB3	1:A:667:LEU:HD21	1.89	0.54
1:A:1121:SER:HA	1:A:1147:PRO:HD2	1.90	0.53
1:A:650:ASN:N	1:A:650:ASN:OD1	2.39	0.53
4:D:1:NAG:HN2	5:E:1:NAG:H81	1.74	0.53
1:A:638:ARG:HH11	1:A:643[A]:ARG:HH12	1.57	0.53
1:A:1228:CYS:SG	1:A:1241:LEU:HD23	2.49	0.52
1:A:646:SER:HB3	1:A:652:ASN:HB3	1.91	0.52
1:A:841:TYR:HB2	1:A:881:VAL:HG21	1.91	0.52
1:A:666:ALA:O	1:A:678:TRP:HA	2.10	0.52
1:A:1107:LEU:HD23	1:A:1118:TRP:HB3	1.93	0.51
1:A:1160:ILE:HG22	1:A:1167:ILE:HG12	1.92	0.50
1:A:744:TRP:CE2	1:A:955:PRO:HD3	2.46	0.50
1:A:1102:SER:HB3	1:A:1122:ASP:HB2	1.93	0.49
1:A:752:ALA:O	1:A:764:TRP:HA	2.14	0.48
1:A:775:ARG:HB2	1:A:786:LEU:HD13	1.95	0.48
1:A:899:HIS:HB2	1:A:927:ARG:HD3	1.96	0.48
1:A:638:ARG:NH1	1:A:643[A]:ARG:HH12	2.10	0.48
1:A:849:ASP:HB3	1:A:852:ARG:HB2	1.96	0.47
1:A:1025:SER:HB3	1:A:1027:TYR:CE2	2.49	0.47
1:A:727:ASN:HD21	2:B:9:ARG:HH12	1.63	0.47
1:A:778:MET:HB2	1:A:906:ALA:O	2.14	0.47
1:A:988:MET:HG2	1:A:1004:VAL:HG23	1.96	0.47
1:A:819:ASN:HD21	1:A:823:LEU:HB2	1.80	0.47
1:A:1118:TRP:CE2	1:A:1127:GLU:HB2	2.51	0.46
1:A:1116:LEU:HB2	1:A:1131:LEU:HD23	1.97	0.46
1:A:761:PHE:CE1	1:A:908:PRO:HG3	2.50	0.46
1:A:974:PRO:HB2	1:A:1197:LEU:HB2	1.97	0.46
1:A:767:TRP:CE2	1:A:792:ARG:HB3	2.52	0.45
1:A:644:ARG:HE	1:A:652:ASN:HD21	1.65	0.45
1:A:832:LEU:HD21	1:A:847:TRP:CE2	2.52	0.45
1:A:1233:HIS:CD2	1:A:1234:LEU:HD22	2.51	0.45
1:A:806:TYR:HB3	1:A:838:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:TYR:CD1	2:B:4:PRO:HG2	2.52	0.44
1:A:965:ARG:HG3	1:A:986:GLN:NE2	2.32	0.44
1:A:1030:TRP:CE2	1:A:1039:ASN:HB3	2.53	0.43
1:A:713:ASP:HB3	1:A:718:ASN:HB2	2.01	0.43
1:A:970:ILE:HG12	1:A:1190:ASP:HB3	2.00	0.42
1:A:844:TYR:HB3	1:A:857:ARG:HG3	2.01	0.42
1:A:663:GLU:O	1:A:680:ASP:HA	2.20	0.42
1:A:988:MET:SD	1:A:1004:VAL:HG23	2.61	0.40
1:A:731:VAL:HB	1:A:742:LEU:HD11	2.03	0.40
1:A:656:ILE:HA	1:A:657:PRO:HD3	1.97	0.40
1:A:656:ILE:HG22	1:A:658:LEU:HD13	2.03	0.40
1:A:684:LYS:HD3	1:A:705:ASP:HA	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	607/633 (96%)	585 (96%)	22 (4%)	0	100	100
2	B	12/32 (38%)	12 (100%)	0	0	100	100
All	All	619/665 (93%)	597 (96%)	22 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	532/553 (96%)	523 (98%)	9 (2%)	60	82
2	B	12/26 (46%)	11 (92%)	1 (8%)	11	22
All	All	544/579 (94%)	534 (98%)	10 (2%)	59	81

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	682	SER
1	A	698	HIS
1	A	825	ARG
1	A	843	ASP
1	A	886	ARG
1	A	952	GLN
1	A	1111	SER
1	A	1226	THR
1	A	1227	ARG
2	B	2	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	652	ASN
1	A	653	ASN
1	A	870	GLN
1	A	1200	GLN
1	A	1204	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	OCS	A	1032	1	7,8,9	0.92	0	6,11,13	1.69	1 (16%)

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
1	OCS	A	1032	1	-	1/4/7/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1032	OCS	OD2-SG-CB	2.80	110.20	105.74

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1032	OCS	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	1	3,1	14,14,15	0.98	1 (7%)	17,19,21	0.90	1 (5%)
3	FUC	C	2	3	10,10,11	1.08	0	14,14,16	0.99	0
3	NAG	C	3	3	14,14,15	0.82	1 (7%)	17,19,21	0.57	0
4	NAG	D	1	4,1	14,14,15	0.40	0	17,19,21	0.38	0
4	NAG	D	2	4	14,14,15	0.35	0	17,19,21	0.36	0
4	FUC	D	3	4	10,10,11	0.80	0	14,14,16	1.03	0
5	NAG	E	1	1,5	14,14,15	0.47	0	17,19,21	0.43	0
5	NAG	E	2	5	14,14,15	0.28	0	17,19,21	0.39	0
5	BMA	E	3	5	11,11,12	0.53	0	15,15,17	1.09	0
5	MAN	E	4	5	11,11,12	0.94	1 (9%)	15,15,17	0.93	0
5	MAN	E	5	5	11,11,12	0.87	0	15,15,17	0.91	0
5	MAN	E	6	5	11,11,12	0.87	0	15,15,17	0.98	1 (6%)

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	C	1	3,1	-	4/6/23/26	0/1/1/1
3	FUC	C	2	3	-	-	0/1/1/1
3	NAG	C	3	3	-	2/6/23/26	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	FUC	D	3	4	-	-	0/1/1/1
5	NAG	E	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	2/2/19/22	0/1/1/1
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1
5	MAN	E	5	5	-	2/2/19/22	0/1/1/1
5	MAN	E	6	5	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	O5-C1	-3.53	1.38	1.43
3	C	3	NAG	O5-C1	-2.38	1.39	1.43
5	E	4	MAN	C2-C3	2.02	1.55	1.52

All (2) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	C	1	NAG	C3-C4-C5	2.07	113.94	110.24
5	E	6	MAN	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

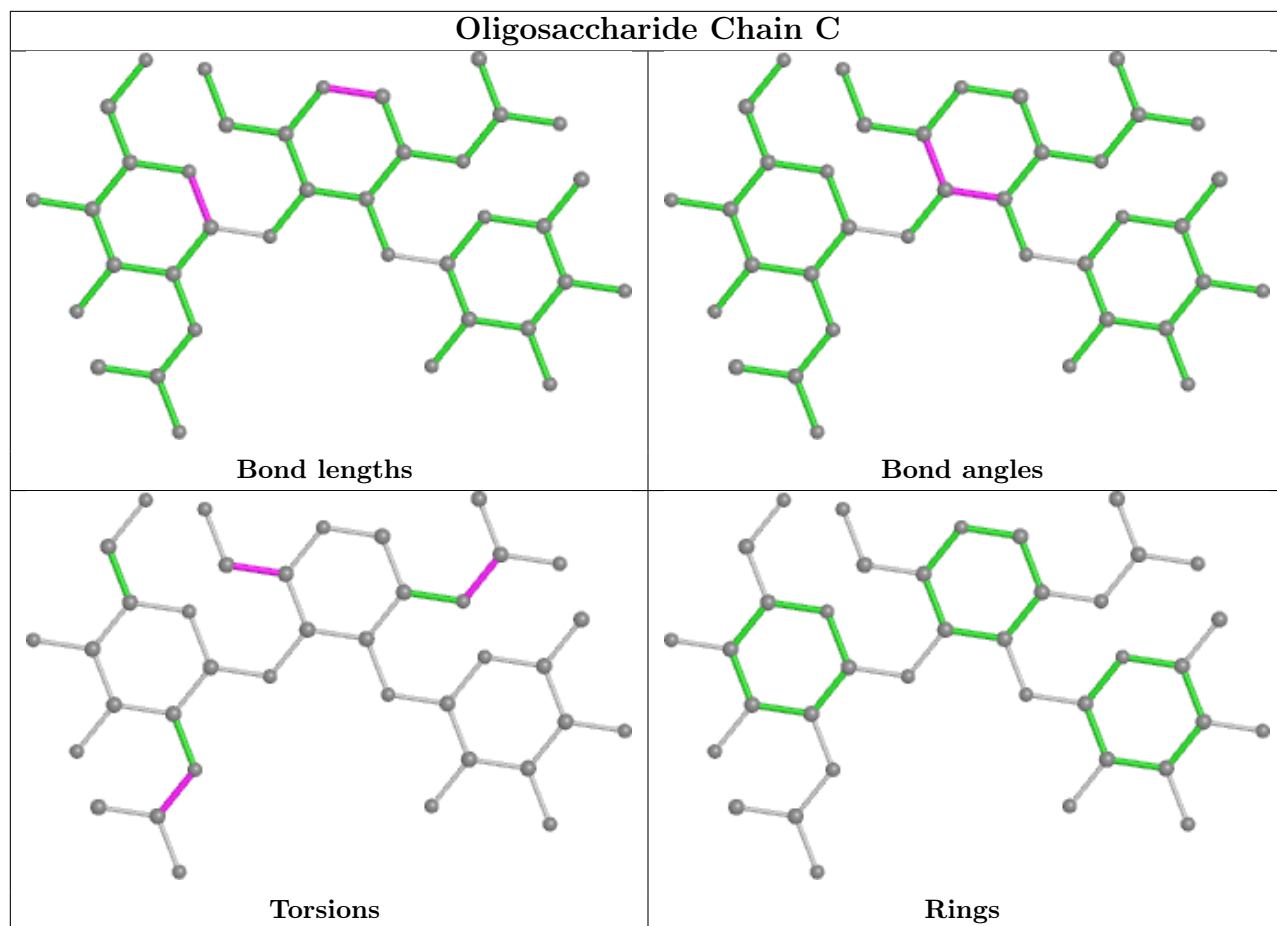
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C4-C5-C6-O6
5	E	5	MAN	C4-C5-C6-O6
5	E	6	MAN	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
5	E	3	BMA	C4-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	3	NAG	C8-C7-N2-C2
3	C	3	NAG	O7-C7-N2-C2
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
5	E	5	MAN	O5-C5-C6-O6
5	E	6	MAN	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6

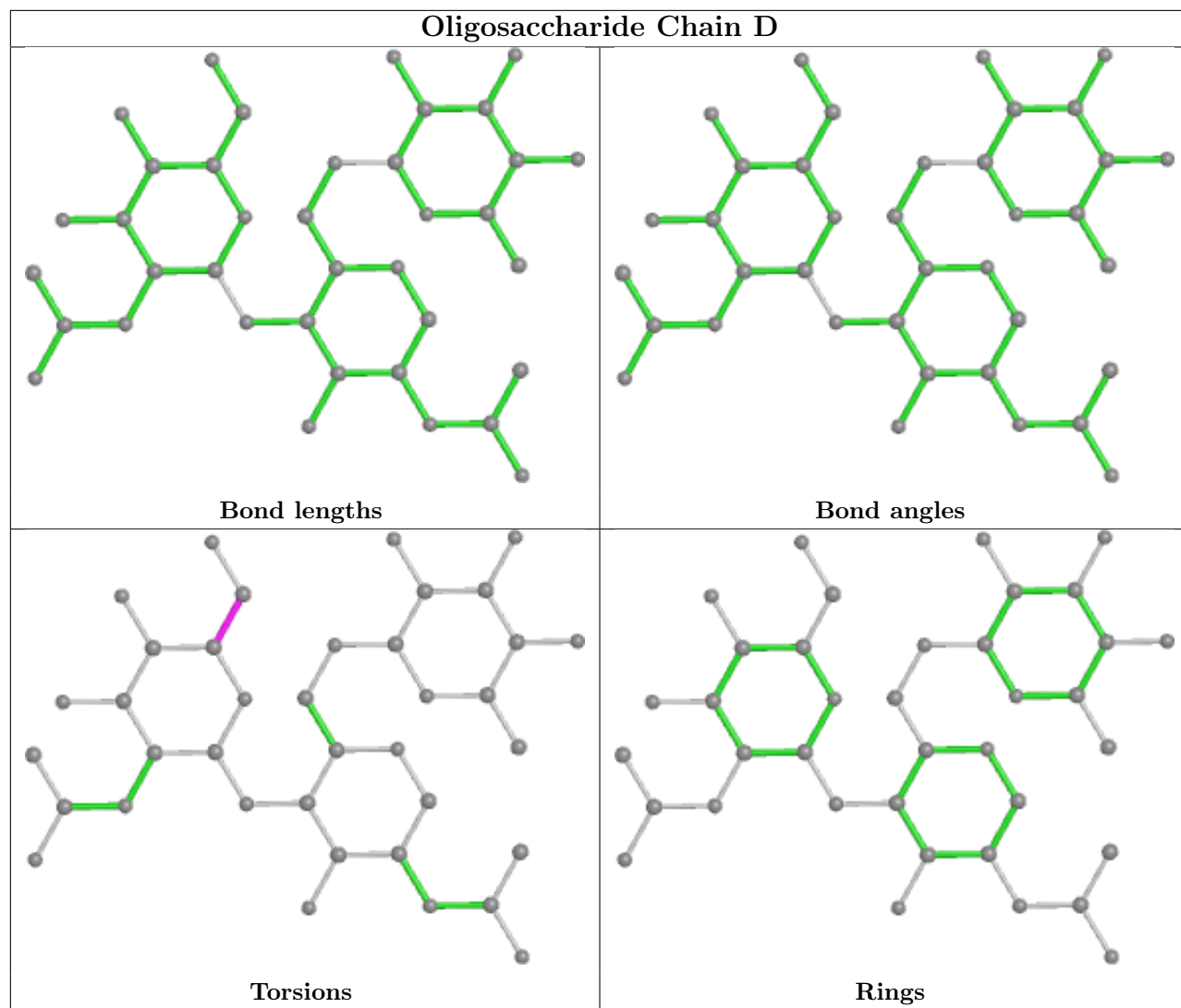
There are no ring outliers.

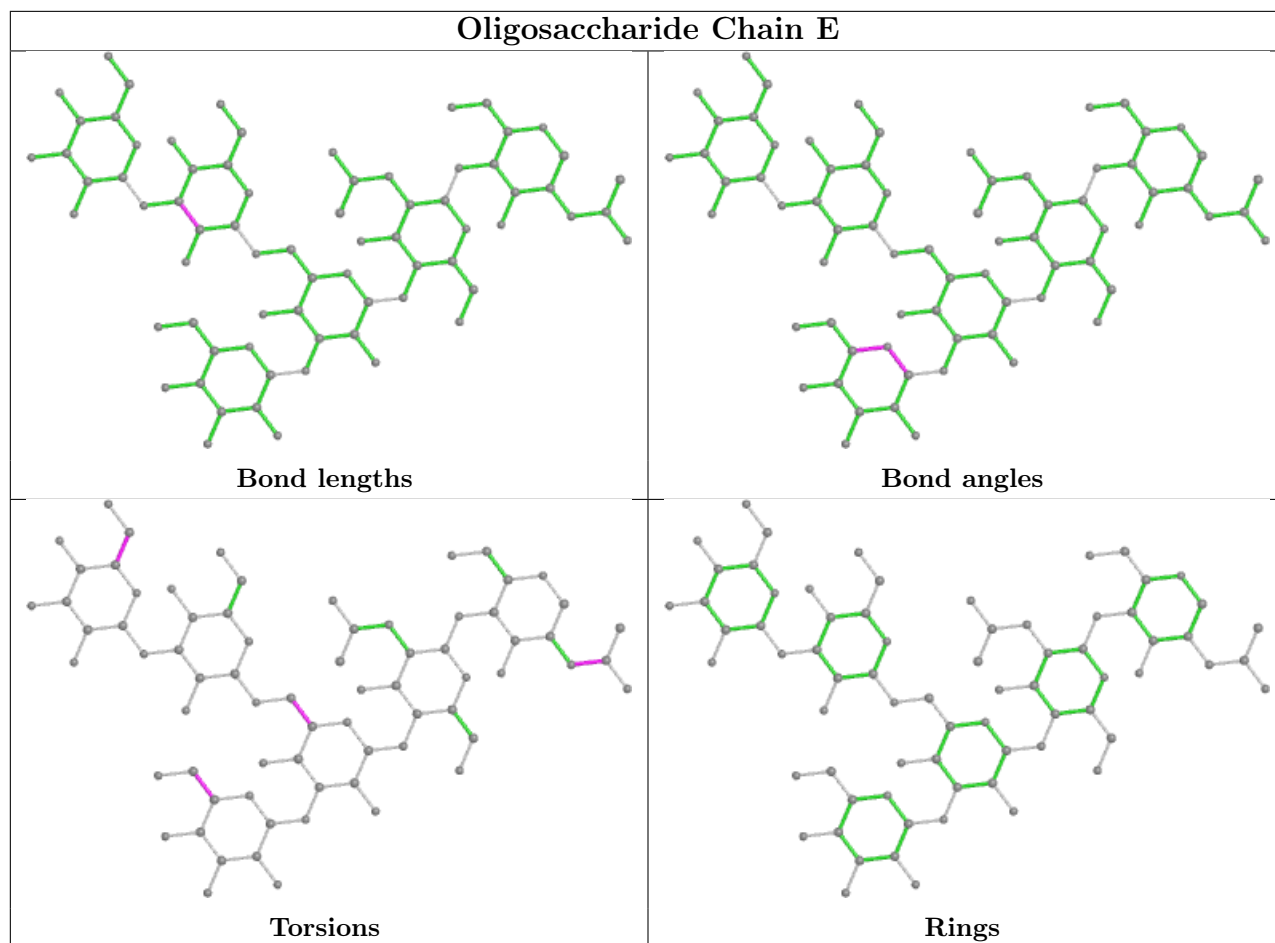
2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0
5	E	1	NAG	1	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.







## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
8	EDO	A	1306	-	3,3,3	0.47	0	2,2,2	0.33	0
8	EDO	A	1308	-	3,3,3	0.48	0	2,2,2	0.21	0
8	EDO	A	1307	-	3,3,3	0.44	0	2,2,2	0.40	0
6	NAG	A	1302	1	14,14,15	0.23	0	17,19,21	0.71	1 (5%)
6	NAG	A	1301	1	14,14,15	0.21	0	17,19,21	0.61	0
8	EDO	A	1309	7	3,3,3	0.48	0	2,2,2	0.20	0
8	EDO	A	1311	-	3,3,3	0.46	0	2,2,2	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	EDO	A	1310	-	3,3,3	0.45	0	2,2,2	0.53	0
8	EDO	A	1312	-	3,3,3	0.49	0	2,2,2	0.31	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
8	EDO	A	1306	-	-	0/1/1/1	-
8	EDO	A	1308	-	-	0/1/1/1	-
8	EDO	A	1307	-	-	0/1/1/1	-
6	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
6	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
8	EDO	A	1309	7	-	0/1/1/1	-
8	EDO	A	1311	-	-	0/1/1/1	-
8	EDO	A	1310	-	-	0/1/1/1	-
8	EDO	A	1312	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1302	NAG	C1-O5-C5	2.34	115.37	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1302	NAG	C8-C7-N2-C2
6	A	1302	NAG	O7-C7-N2-C2
6	A	1302	NAG	O5-C5-C6-O6
6	A	1302	NAG	C4-C5-C6-O6
6	A	1301	NAG	C3-C2-N2-C7

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

### 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<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	609/633 (96%)	0.26	29 (4%) 30 32	35, 58, 92, 133	0
2	B	14/32 (43%)	0.66	2 (14%) 2 2	55, 73, 103, 113	0
All	All	623/665 (93%)	0.27	31 (4%) 28 30	35, 58, 93, 133	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1241	LEU	4.7
1	A	951	GLU	4.4
1	A	909	VAL	4.1
1	A	952	GLN	4.1
1	A	1225	THR	3.9
2	B	2	CYS	3.7
1	A	651	ASN	3.6
1	A	652	ASN	3.4
1	A	911	GLY	3.4
1	A	1246	PRO	3.3
1	A	1223	ASP	3.3
1	A	1226	THR	3.1
1	A	1013	GLU	3.0
1	A	1224	GLY	2.8
1	A	1238	GLN	2.8
1	A	1233	HIS	2.8
1	A	949	ILE	2.7
1	A	1240	GLU	2.6
1	A	992	ALA	2.6
1	A	999	GLY	2.5
1	A	1237	LEU	2.5
1	A	650	ASN	2.4
1	A	657	PRO	2.4
1	A	633	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1221	LYS	2.3
1	A	1079	ARG	2.2
2	B	1	GLY	2.2
1	A	897	ASN	2.2
1	A	1005	SER	2.1
1	A	910	GLY	2.1
1	A	950	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	OCS	A	1032	9/10	0.98	0.16	44,51,59,66	0

## 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.

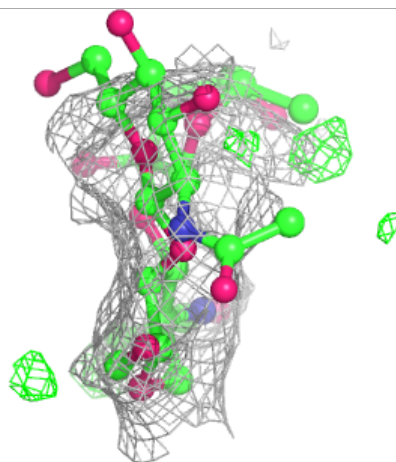
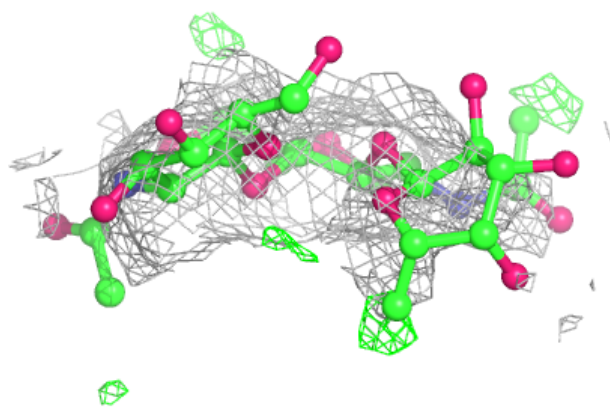
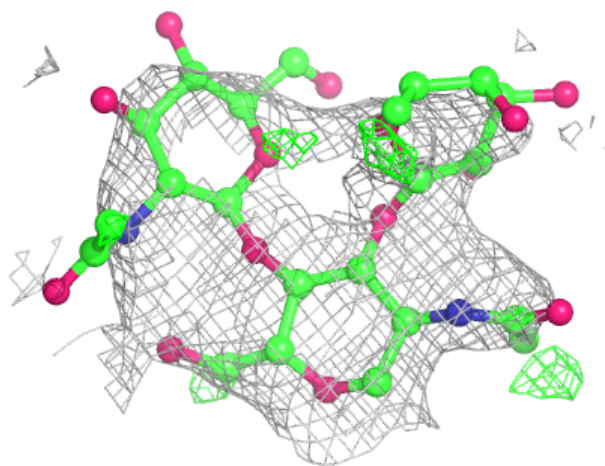
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	FUC	C	2	10/11	0.67	0.61	124,132,136,137	0
3	NAG	C	1	14/15	0.77	0.34	110,116,128,128	0
5	MAN	E	6	11/12	0.77	0.31	88,97,101,102	0
4	NAG	D	2	14/15	0.80	0.40	84,98,100,103	0
3	NAG	C	3	14/15	0.80	0.52	119,130,135,138	0
5	MAN	E	5	11/12	0.81	0.22	81,86,93,94	0
4	NAG	D	1	14/15	0.83	0.17	72,83,90,91	0
5	MAN	E	4	11/12	0.83	0.27	80,89,97,98	0
5	BMA	E	3	11/12	0.89	0.17	81,89,97,97	0
4	FUC	D	3	10/11	0.91	0.23	75,82,89,90	0
5	NAG	E	2	14/15	0.92	0.11	63,71,78,80	0
5	NAG	E	1	14/15	0.96	0.13	54,61,69,69	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.



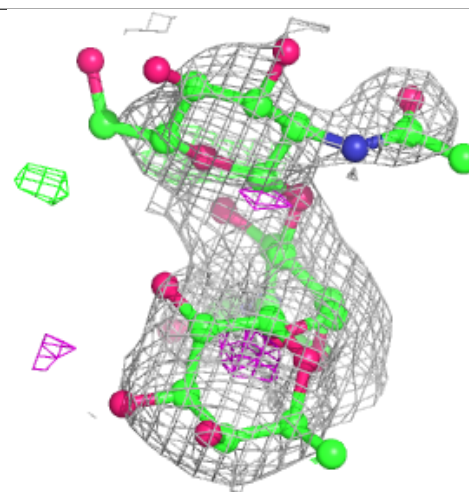
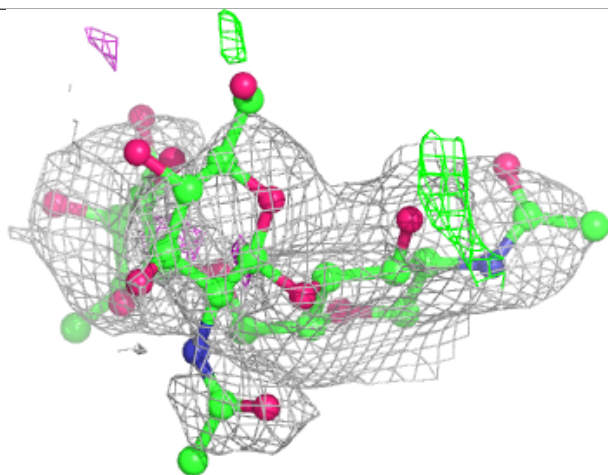
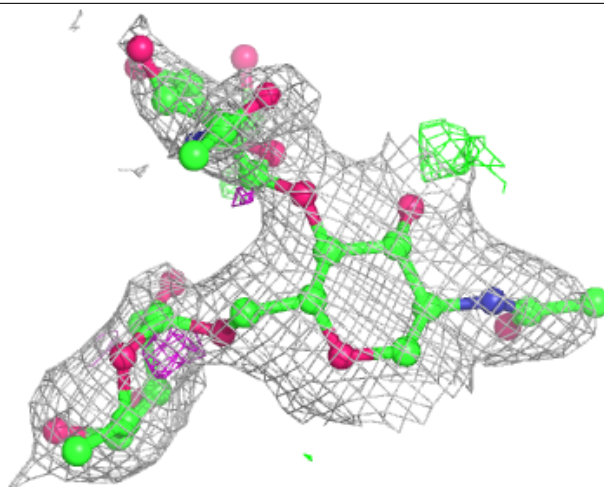
**Electron density around Chain C:**

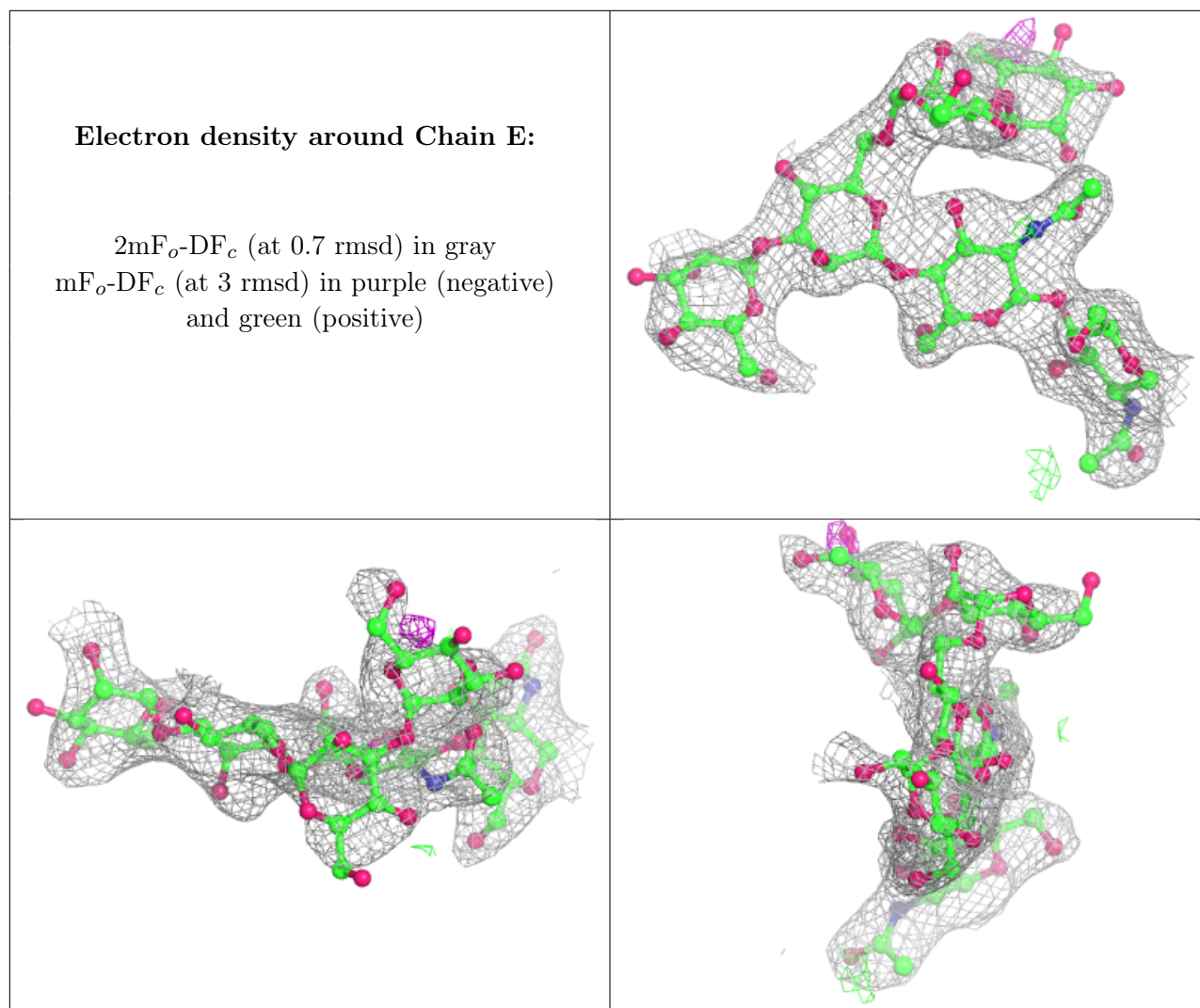
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain D:**

$2mF_o-DF_c$  (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, 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
7	CA	A	1303	1/1	0.54	0.15	84,84,84,84	0
8	EDO	A	1312	4/4	0.83	0.22	49,57,72,76	0
7	CA	A	1305	1/1	0.84	0.08	95,95,95,95	0
6	NAG	A	1302	14/15	0.84	0.18	66,81,84,85	0
6	NAG	A	1301	14/15	0.89	0.22	71,80,93,95	0
8	EDO	A	1311	4/4	0.92	0.14	55,65,65,67	0
7	CA	A	1304	1/1	0.93	0.20	86,86,86,86	0
8	EDO	A	1308	4/4	0.94	0.18	53,53,57,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	EDO	A	1309	4/4	0.95	0.15	41,44,45,49	0
8	EDO	A	1310	4/4	0.95	0.19	48,54,60,69	0
8	EDO	A	1307	4/4	0.95	0.24	52,55,58,67	0
8	EDO	A	1306	4/4	0.95	0.13	53,57,57,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.