



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:50 AM UTC

PDB ID : 8DVN / pdb_00008dvn
Title : Crystal structure of LRP6 E3E4 in complex with disulfide constrained peptide E3.10
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Deposited on : 2022-07-29
Resolution : 2.53 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

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)
Xtriage (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

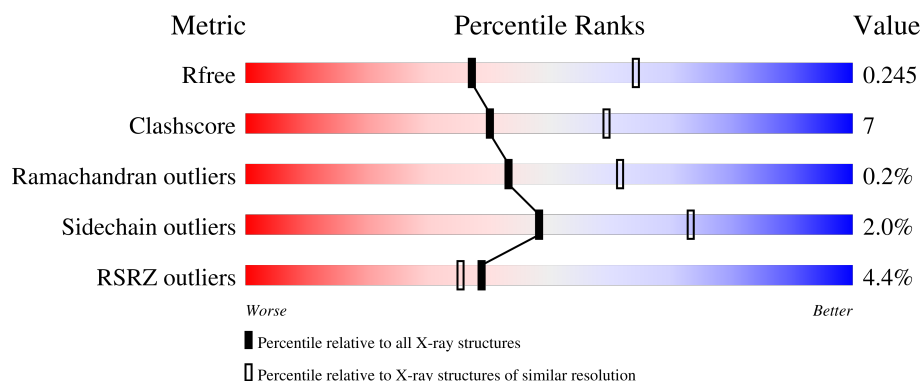
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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 ≥ 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	4% 79% 17% .
2	B	32	16% 78% 19% .
3	C	3	33% 67%
4	D	3	33% 67%
5	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
6	F	2	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5273 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
1	A	612	Total	C	N	O	S	0	0	0
			4876	3057	862	932	25			

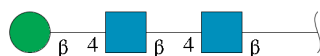
There are 11 discrepancies between the modelled and reference sequences:

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 E3.10 Disulfide constrained peptide.

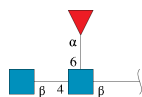
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	32	Total	C	N	O	S	0	0	0
			237	145	41	44	7			

- 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.



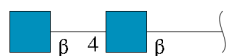
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



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

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

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



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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	4	Total	Ca	0	0
			4	4		

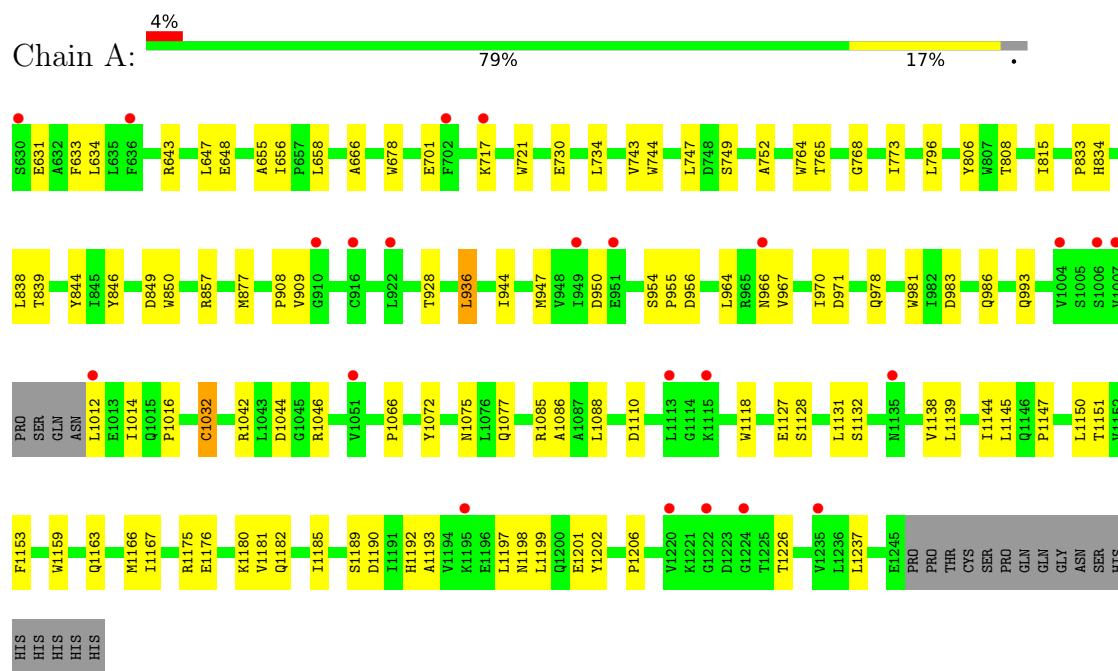
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	8	Total	O	0	0
			8	8		
9	B	1	Total	O	0	0
			1	1		

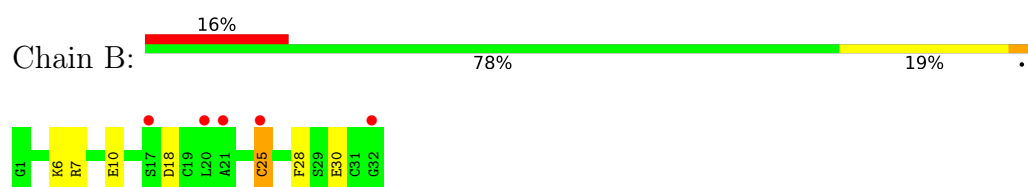
3 Residue-property plots [i](#)

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: E3.10 Disulfide constrained peptide



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

Chain D:  33% 67%


MAG1
MAG2
FUC3

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

Chain E:  50% 50%


MAG1
MAG2

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

Chain F:  50% 50%


MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.10Å 116.78Å 127.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.33 – 2.53 44.33 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.33-2.53) 87.5 (44.33-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.34 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.20rc3-4406_final	Depositor
R, R_{free}	0.209 , 0.246 0.208 , 0.245	Depositor DCC
R_{free} test set	1995 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5273	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, CA, BMA, FUC, OCS

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	0.49	0/4967	0.52	0/6737
2	B	0.26	0/240	0.61	0/318
All	All	0.48	0/5207	0.52	0/7055

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1032	OCS	Mainchain

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	4876	0	4748	66	0
2	B	237	0	223	2	0
3	C	39	0	34	0	0
4	D	38	0	34	0	0
5	E	28	0	25	0	0
6	F	28	0	25	0	0
7	A	14	0	13	0	0
8	A	4	0	0	0	0
9	A	8	0	0	0	0
9	B	1	0	0	0	0
All	All	5273	0	5102	68	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 7.

All (68) 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:964:LEU:HD11	1:A:967:VAL:CG2	1.79	1.12
1:A:964:LEU:HD11	1:A:967:VAL:HG23	1.17	1.06
1:A:964:LEU:CD1	1:A:967:VAL:HG23	2.00	0.91
1:A:964:LEU:CD1	1:A:967:VAL:CG2	2.58	0.81
1:A:1206:PRO:HB2	1:A:1226:THR:HG22	1.66	0.77
1:A:833:PRO:HD2	1:A:849:ASP:OD2	1.96	0.66
1:A:808:THR:HG22	1:A:815:ILE:HG12	1.77	0.65
1:A:749:SER:HB2	1:A:768:GLY:H	1.64	0.60
1:A:839:THR:HG22	1:A:846:TYR:HB2	1.84	0.60
1:A:717:LYS:HD2	1:A:734:LEU:HD12	1.85	0.59
1:A:1072:TYR:CZ	1:A:1131:LEU:HD12	2.37	0.59
1:A:1042:ARG:HG3	1:A:1046:ARG:O	2.06	0.56
1:A:1167:ILE:HG22	1:A:1181:VAL:HB	1.86	0.56
1:A:744:TRP:CG	1:A:955:PRO:HG3	2.41	0.55
1:A:1175:ARG:HG3	1:A:1176:GLU:HG2	1.89	0.54
1:A:765:THR:HG22	1:A:773:ILE:HG12	1.91	0.53
1:A:1144:ILE:HG22	1:A:1147:PRO:HD3	1.91	0.53
1:A:634:LEU:HB2	1:A:647:LEU:HD11	1.91	0.51
1:A:1166:MET:HE2	1:A:1180:LYS:HD3	1.93	0.51
1:A:950:ASP:OD1	1:A:950:ASP:C	2.54	0.51
1:A:1085:ARG:NH2	1:A:1132:SER:HA	2.25	0.50
1:A:966:ASN:O	1:A:983:ASP:HA	2.12	0.49
1:A:970:ILE:HG12	1:A:1190:ASP:HB3	1.94	0.49
1:A:1072:TYR:OH	1:A:1131:LEU:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:ILE:HG22	1:A:658:LEU:HG	1.94	0.48
1:A:1182:GLN:HB3	1:A:1185:ILE:HD11	1.96	0.47
1:A:743:VAL:HG12	1:A:747:LEU:HD22	1.96	0.47
1:A:1085:ARG:HG2	1:A:1086:ALA:N	2.29	0.47
1:A:908:PRO:HA	1:A:909:VAL:HA	1.68	0.47
1:A:1044:ASP:OD1	1:A:1044:ASP:C	2.58	0.47
1:A:666:ALA:O	1:A:678:TRP:HA	2.15	0.46
1:A:631:GLU:HB3	1:A:633:PHE:CE1	2.50	0.46
1:A:1110:ASP:OD1	1:A:1110:ASP:C	2.59	0.46
1:A:950:ASP:OD2	1:A:954:SER:OG	2.30	0.46
1:A:643:ARG:NH1	1:A:655:ALA:HB2	2.30	0.45
1:A:844:TYR:HB3	1:A:857:ARG:HG3	1.99	0.45
1:A:1128:SER:HB2	1:A:1139:LEU:HD11	1.98	0.45
1:A:834:HIS:ND1	1:A:850:TRP:HB2	2.32	0.45
1:A:978:GLN:NE2	1:A:993:GLN:OE1	2.50	0.45
1:A:1118:TRP:CE2	1:A:1127:GLU:HB2	2.52	0.44
1:A:964:LEU:HD11	1:A:967:VAL:HG21	1.86	0.44
1:A:944:ILE:HD11	1:A:967:VAL:HG21	1.99	0.44
1:A:721:TRP:CE2	1:A:730:GLU:HB2	2.53	0.44
1:A:1075:ASN:HD21	1:A:1077:GLN:HE21	1.66	0.44
1:A:850:TRP:CZ2	1:A:877:MET:HE1	2.53	0.44
1:A:796:LEU:HD12	1:A:796:LEU:HA	1.84	0.43
1:A:806:TYR:HB3	1:A:838:LEU:HD21	2.00	0.43
1:A:971:ASP:OD1	1:A:1192:HIS:NE2	2.51	0.43
2:B:6:LYS:O	2:B:10:GLU:HG3	2.18	0.43
1:A:1127:GLU:HG2	1:A:1138:VAL:HG22	2.00	0.43
1:A:631:GLU:HB3	1:A:633:PHE:HE1	1.84	0.43
1:A:1066:PRO:HA	1:A:1088:LEU:HD11	2.00	0.42
1:A:1145:LEU:HB2	1:A:1163:GLN:HB3	2.01	0.42
1:A:752:ALA:O	1:A:764:TRP:HA	2.18	0.42
1:A:956:ASP:OD1	1:A:956:ASP:N	2.51	0.42
1:A:1153:PHE:HD1	1:A:1193:ALA:HB1	1.84	0.42
1:A:947:MET:HE3	1:A:947:MET:HB2	1.87	0.42
1:A:1085:ARG:HH22	1:A:1132:SER:HA	1.85	0.41
1:A:1198:ASN:ND2	1:A:1201:GLU:OE2	2.53	0.41
2:B:28:PHE:CE1	2:B:30:GLU:HB2	2.55	0.41
1:A:1150:LEU:HD23	1:A:1159:TRP:HB3	2.01	0.41
1:A:936:LEU:HB2	1:A:947:MET:HG3	2.01	0.41
1:A:1197:LEU:HD11	1:A:1202:TYR:HB2	2.01	0.41
1:A:967:VAL:HG22	1:A:981:TRP:CD1	2.56	0.41
1:A:744:TRP:CD1	1:A:955:PRO:HG3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1014:ILE:HD12	1:A:1016:PRO:HD3	2.03	0.40
1:A:1012:LEU:HD12	1:A:1012:LEU:HA	1.92	0.40
1:A:1237:LEU:HD23	1:A:1237:LEU:HA	1.87	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%)	579 (95%)	28 (5%)	0	100	100
2	B	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	3	4
All	All	637/665 (96%)	606 (95%)	30 (5%)	1 (0%)	43	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	25	CYS

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	533/553 (96%)	525 (98%)	8 (2%)	57	79
2	B	26/26 (100%)	23 (88%)	3 (12%)	5	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	559/579 (96%)	548 (98%)	11 (2%)	48 73

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	648	GLU
1	A	701	GLU
1	A	928	THR
1	A	936	LEU
1	A	986	GLN
1	A	1151	THR
1	A	1189	SER
1	A	1199	LEU
2	B	7	ARG
2	B	18	ASP
2	B	25	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	864	GLN
1	A	945	ASN
1	A	1065	ASN
1	A	1077	GLN
1	A	1164	GLN
1	A	1200	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	6,8,9	3.43	2 (33%)	7,11,13	1.29	1 (14%)

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	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1032	OCS	OD3-SG	6.15	1.62	1.45
1	A	1032	OCS	CB-CA	-5.07	1.49	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1032	OCS	OD1-SG-CB	2.09	109.88	106.76

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

10 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	0.55	0	17,19,21	2.43	5 (29%)
3	NAG	C	2	3	14,14,15	0.50	0	17,19,21	1.34	2 (11%)
3	BMA	C	3	3	11,11,12	0.24	0	15,15,17	0.79	0
4	NAG	D	1	1,4	14,14,15	0.51	0	17,19,21	2.19	6 (35%)
4	NAG	D	2	4	14,14,15	0.31	0	17,19,21	1.19	1 (5%)
4	FUC	D	3	4	10,10,11	0.39	0	14,14,16	0.55	0
5	NAG	E	1	1,5	14,14,15	0.50	0	17,19,21	1.73	4 (23%)
5	NAG	E	2	5	14,14,15	0.50	0	17,19,21	0.93	0
6	NAG	F	1	1,6	14,14,15	0.53	0	17,19,21	1.25	2 (11%)
6	NAG	F	2	6	14,14,15	0.37	0	17,19,21	0.46	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	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	1/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	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	-	4/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
6	NAG	F	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C4-C3-C2	-6.99	100.77	111.02
4	D	1	NAG	C4-C3-C2	-4.94	103.77	111.02
3	C	1	NAG	C2-N2-C7	-4.30	117.14	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	NAG	O5-C1-C2	-4.18	104.83	111.29
3	C	1	NAG	C1-O5-C5	3.89	117.40	112.19
4	D	1	NAG	C3-C4-C5	-3.58	103.73	110.23
4	D	2	NAG	C1-O5-C5	3.31	116.62	112.19
4	D	1	NAG	C1-O5-C5	-3.17	107.94	112.19
5	E	1	NAG	C2-N2-C7	3.07	127.01	122.90
4	D	1	NAG	O5-C5-C6	2.99	113.48	107.66
4	D	1	NAG	C2-N2-C7	-2.98	118.91	122.90
5	E	1	NAG	C1-C2-N2	2.77	114.79	110.43
6	F	1	NAG	C2-N2-C7	-2.70	119.28	122.90
3	C	2	NAG	C1-O5-C5	2.53	115.58	112.19
3	C	2	NAG	C4-C3-C2	2.47	114.64	111.02
5	E	1	NAG	O3-C3-C2	-2.35	104.51	109.40
3	C	1	NAG	O4-C4-C5	2.30	114.99	109.32
4	D	1	NAG	O4-C4-C3	2.24	115.66	110.38
3	C	1	NAG	O4-C4-C3	2.22	115.62	110.38
6	F	1	NAG	C4-C3-C2	-2.07	107.99	111.02

There are no chirality outliers.

All (16) torsion outliers are listed below:

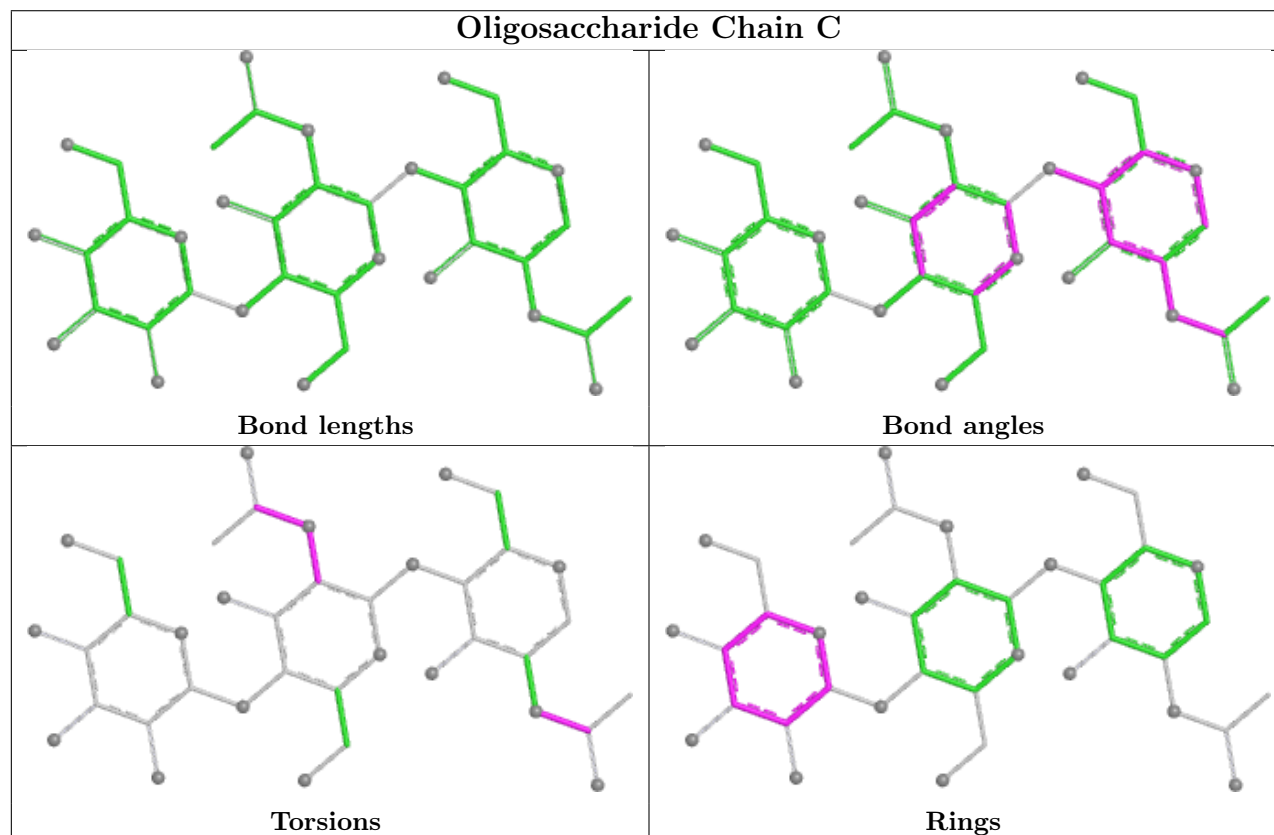
Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C1-C2-N2-C7
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
6	F	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
3	C	2	NAG	C3-C2-N2-C7
3	C	1	NAG	O7-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
5	E	1	NAG	C3-C2-N2-C7
5	E	1	NAG	C8-C7-N2-C2

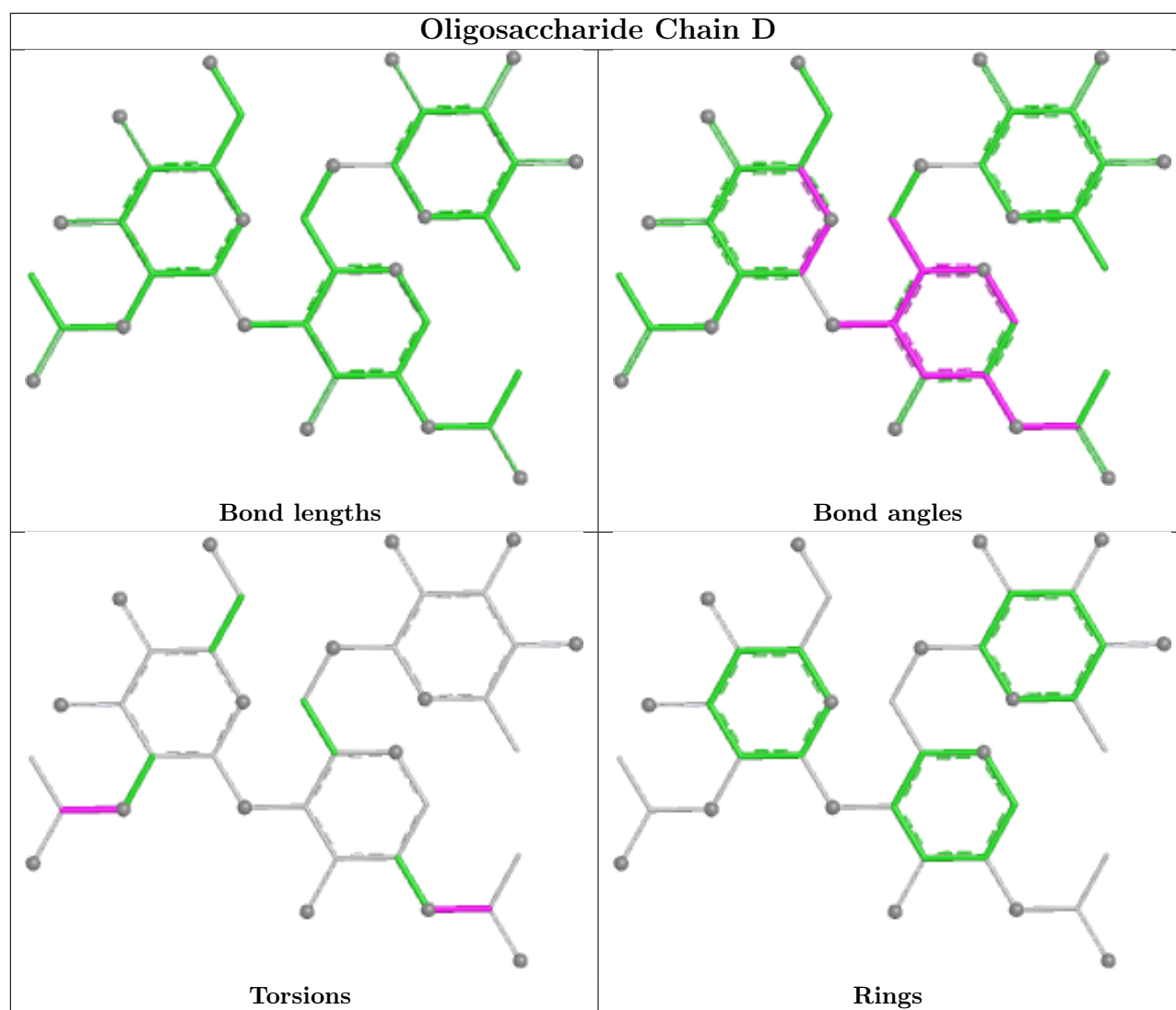
All (1) ring outliers are listed below:

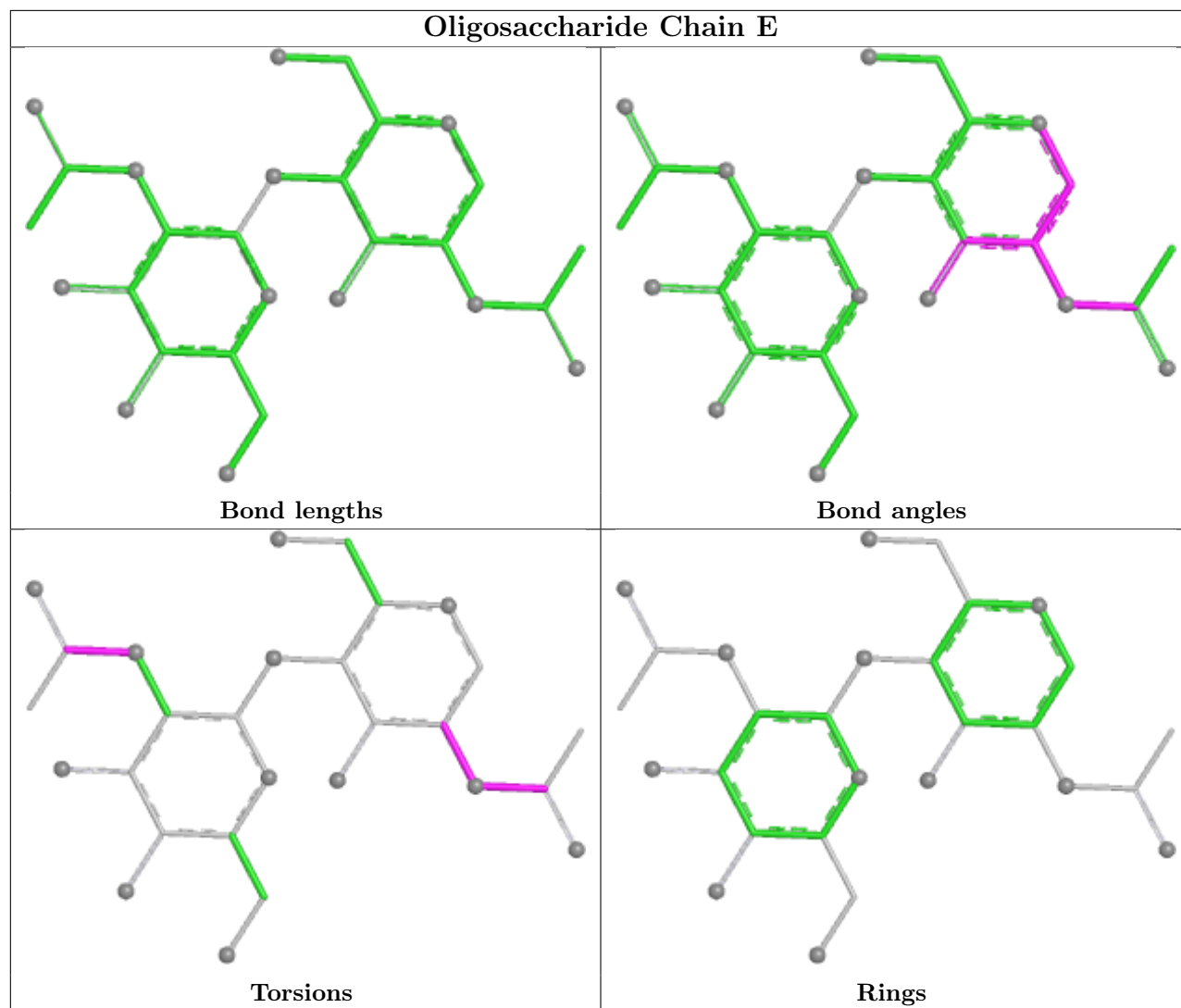
Mol	Chain	Res	Type	Atoms
3	C	3	BMA	C1-C2-C3-C4-C5-O5

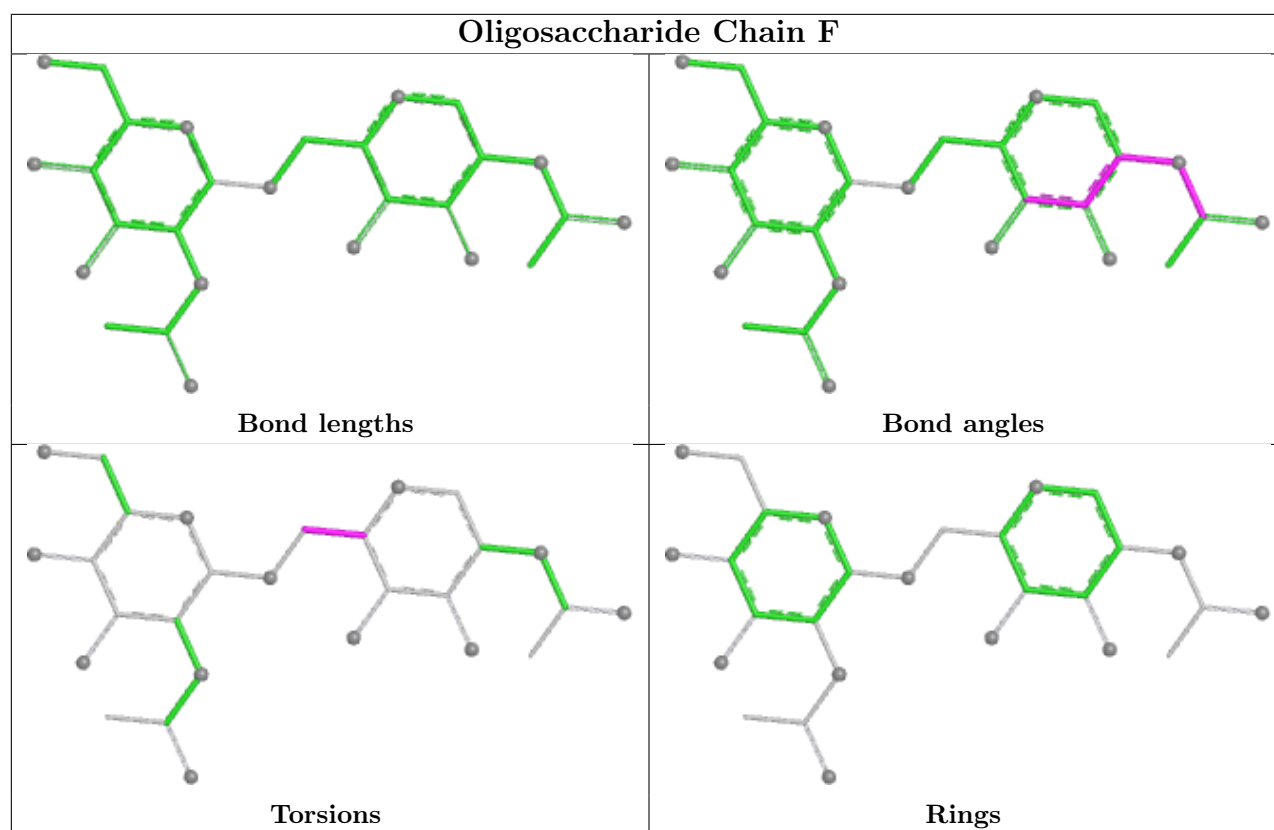
No monomer is involved in short contacts.

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](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\# Z > 2$
7	NAG	A	1301	1	14,14,15	0.43	0	17,19,21	0.69	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	A	1301	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1301	NAG	O5-C5-C6-O6
7	A	1301	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	611/633 (96%)	0.39	23 (3%) 44 40	53, 80, 129, 165	0
2	B	32/32 (100%)	1.01	5 (15%) 5 4	66, 112, 168, 179	0
All	All	643/665 (96%)	0.42	28 (4%) 39 35	53, 81, 135, 179	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1012	LEU	5.3
1	A	1007	VAL	4.5
1	A	951	GLU	4.4
2	B	20	LEU	3.7
1	A	949	ILE	3.6
2	B	17	SER	2.9
2	B	32	GLY	2.9
2	B	25	CYS	2.6
1	A	966	ASN	2.6
1	A	1051	VAL	2.6
1	A	1235	VAL	2.5
2	B	21	ALA	2.5
1	A	910	GLY	2.4
1	A	717	LYS	2.4
1	A	702	PHE	2.3
1	A	1195	LYS	2.3
1	A	1224	GLY	2.3
1	A	916	CYS	2.3
1	A	1006	SER	2.2
1	A	1135	ASN	2.2
1	A	1115	LYS	2.2
1	A	922	LEU	2.1
1	A	1113	LEU	2.1
1	A	636	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1220	VAL	2.0
1	A	1222	GLY	2.0
1	A	630	SER	2.0
1	A	1004	VAL	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	OCS	A	1032	9/10	0.94	0.11	67,83,94,108	0

6.3 Carbohydrates [i](#)

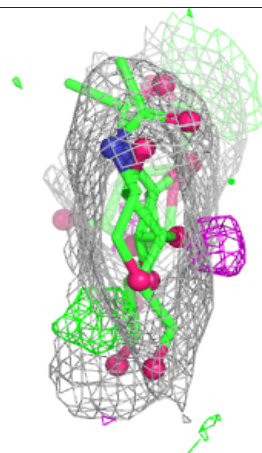
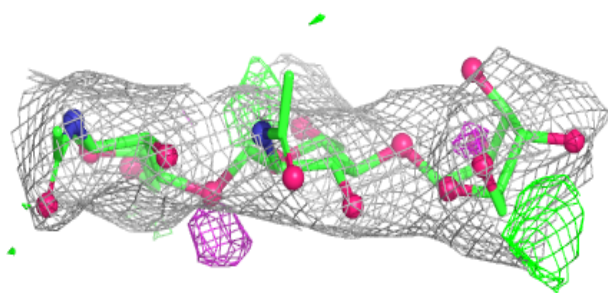
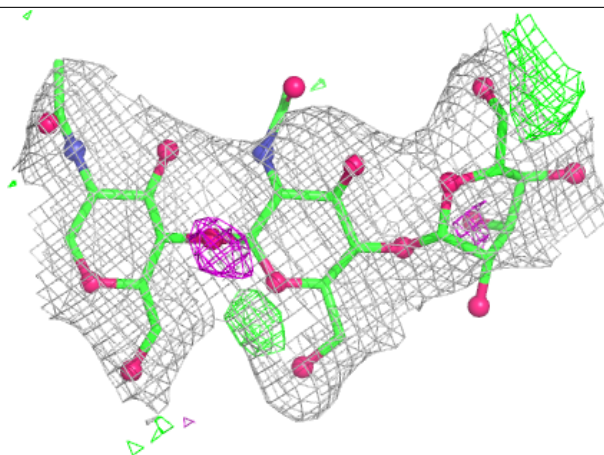
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	F	2	14/15	0.12	0.16	121,143,146,146	0
3	BMA	C	3	11/12	0.31	0.15	111,133,137,144	0
5	NAG	E	2	14/15	0.45	0.14	115,130,134,136	0
4	NAG	D	2	14/15	0.58	0.15	121,132,138,139	0
3	NAG	C	2	14/15	0.65	0.17	102,114,128,130	0
6	NAG	F	1	14/15	0.69	0.14	108,120,134,139	0
4	FUC	D	3	10/11	0.70	0.17	115,122,129,131	0
4	NAG	D	1	14/15	0.70	0.13	111,115,123,128	0
5	NAG	E	1	14/15	0.75	0.13	109,120,133,134	0
3	NAG	C	1	14/15	0.88	0.14	84,90,96,108	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.

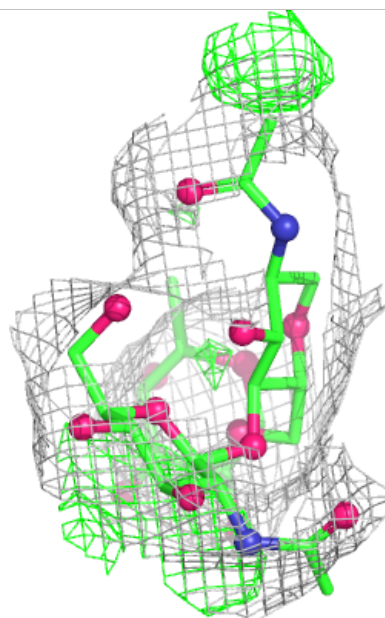
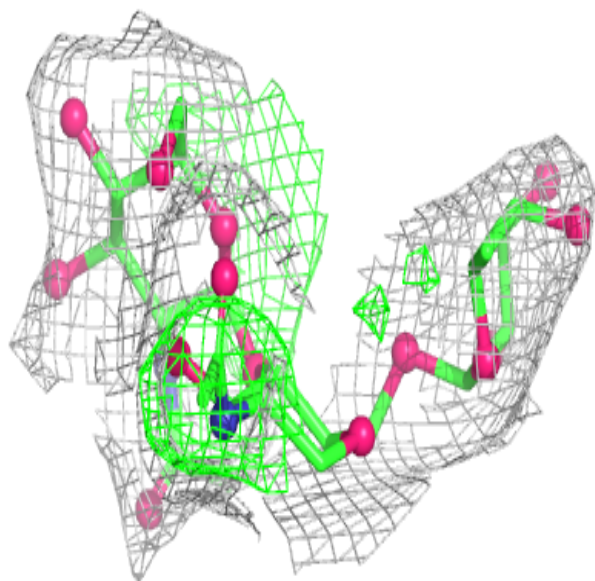
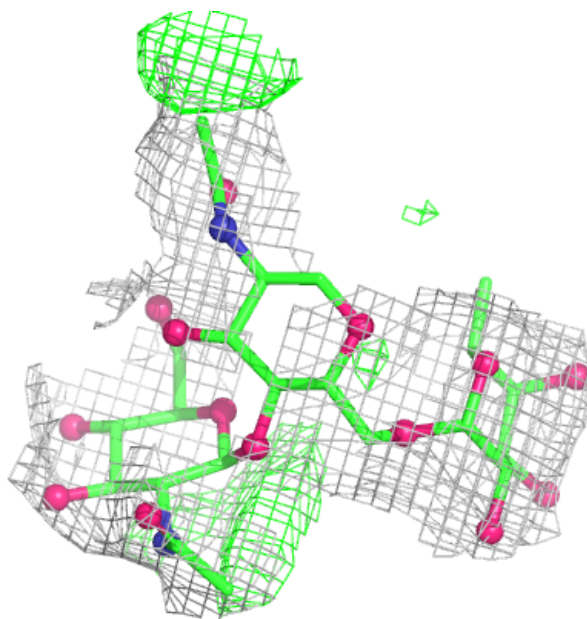
Electron density around Chain C:

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



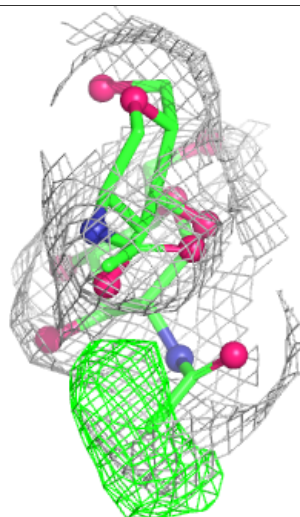
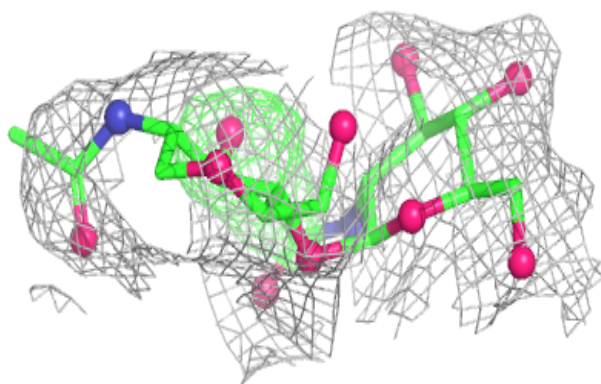
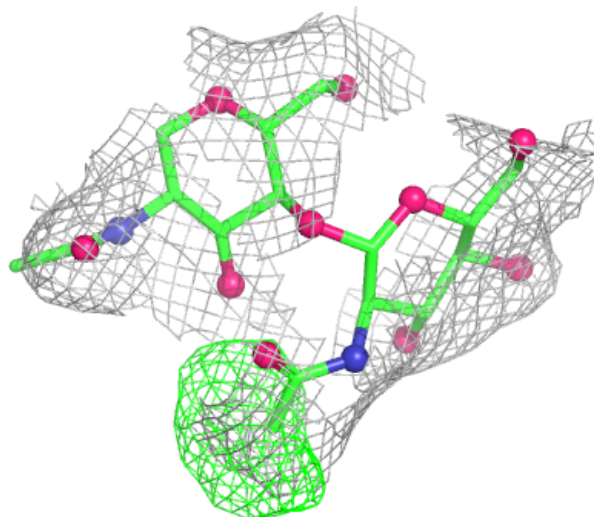
Electron density around Chain D:

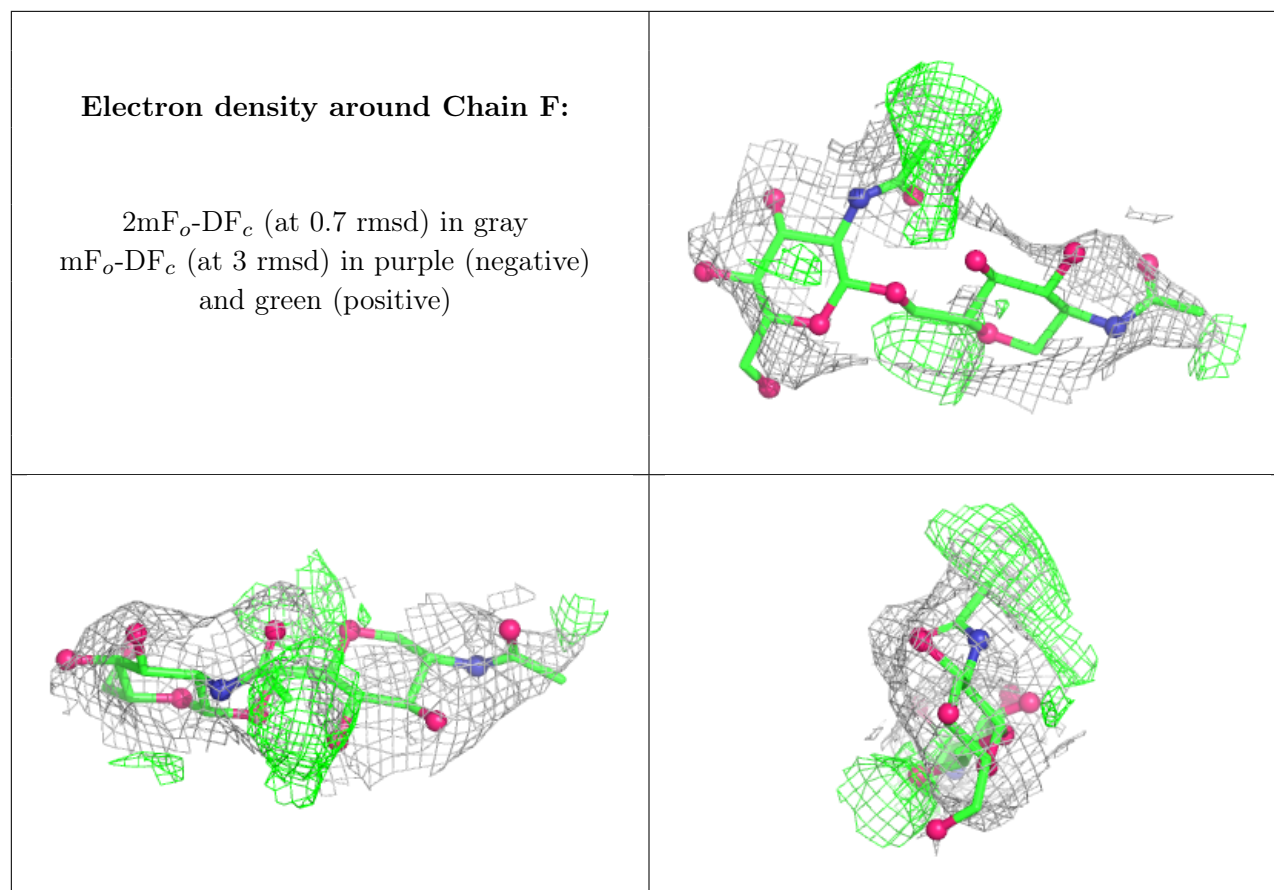
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain E:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	A	1301	14/15	0.33	0.18	117,134,139,142	0
8	CA	A	1304	1/1	0.81	0.14	90,90,90,90	0
8	CA	A	1302	1/1	0.91	0.10	81,81,81,81	0
8	CA	A	1305	1/1	0.95	0.08	81,81,81,81	0
8	CA	A	1303	1/1	0.97	0.06	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.