



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:37 PM UTC

PDB ID : 1ZIW / pdb_00001ziw
Title : Human Toll-like Receptor 3 extracellular domain structure
Authors : Wilson, I.A.; Choe, J.
Deposited on : 2005-04-27
Resolution : 2.10 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

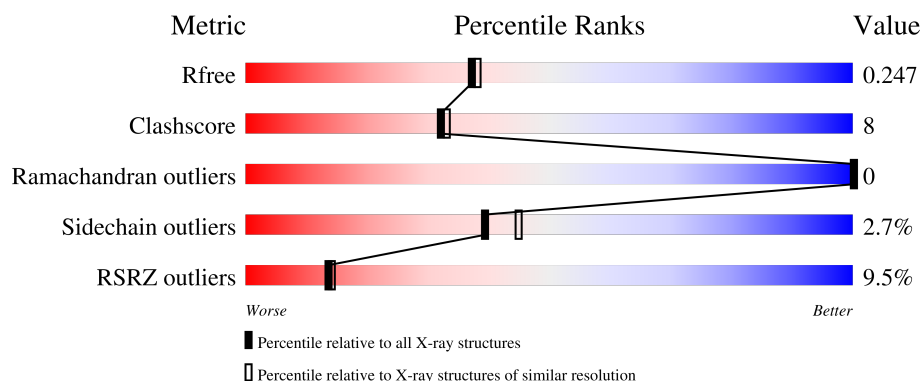
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	680	9% 78% 13% 8%
2	B	2	50% 50%
2	C	2	100%
2	D	2	100%
2	E	2	100%

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	1	X	-	-	-
3	NAG	A	7	X	-	-	-
5	GOL	A	782	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5628 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 Toll-like receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	629	5052	3232	856	948	16	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

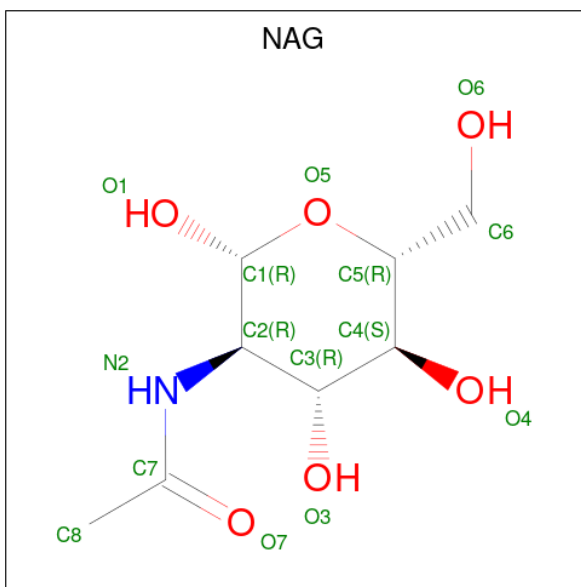
Chain	Residue	Modelled	Actual	Comment	Reference
A	701	HIS	-	expression tag	UNP O15455
A	702	HIS	-	expression tag	UNP O15455
A	703	HIS	-	expression tag	UNP O15455
A	704	HIS	-	expression tag	UNP O15455
A	705	HIS	-	expression tag	UNP O15455
A	706	HIS	-	expression tag	UNP O15455

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



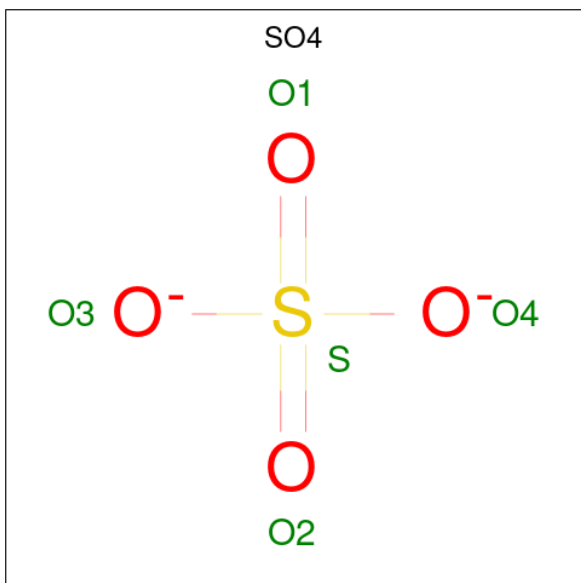
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	28	16	2	10	0	0	0
2	C	2	28	16	2	10	0	0	0
2	D	2	28	16	2	10	0	0	0
2	E	2	28	16	2	10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



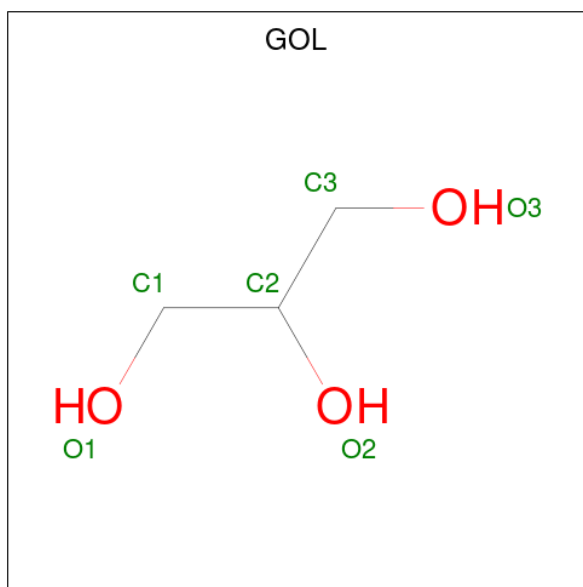
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0

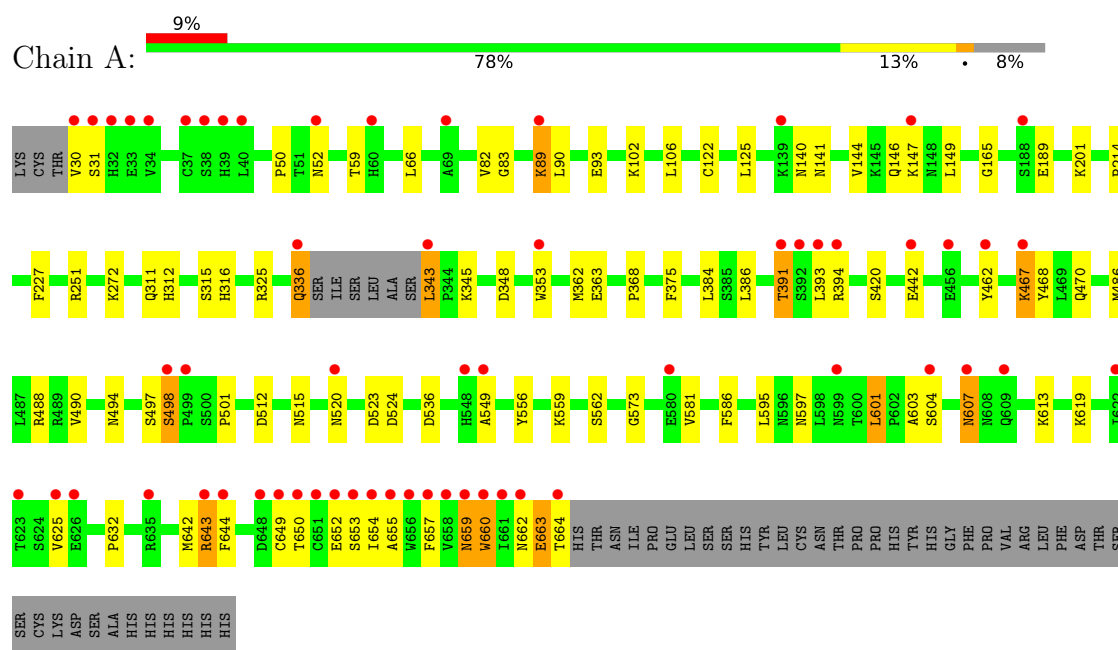
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	362	Total O 362 362	0	0

3 Residue-property plots

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.

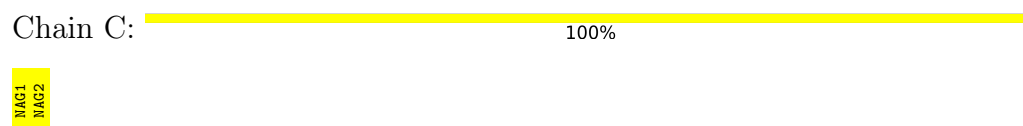
- Molecule 1: Toll-like receptor 3



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



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



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

Chain D:  100%

MAG1
MAG2

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

Chain E:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	138.50Å 155.12Å 119.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.10) 99.6 (20.00-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.2.0013	Depositor
R, R_{free}	0.208 , 0.248 0.207 , 0.247	Depositor DCC
R_{free} test set	3795 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5628	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, 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	0.90	3/5152 (0.1%)	0.95	8/6987 (0.1%)

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	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	549	ALA	CA-CB	7.37	1.66	1.53
1	A	467	LYS	CE-NZ	5.15	1.64	1.49
1	A	581	VAL	CA-CB	5.07	1.61	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	643	ARG	N-CA-C	7.08	125.87	110.80
1	A	655	ALA	N-CA-C	6.86	121.40	112.89
1	A	393	LEU	N-CA-C	-6.17	98.31	108.49
1	A	467	LYS	CD-CE-NZ	5.98	131.02	111.90
1	A	607	ASN	N-CA-C	5.78	118.36	111.71
1	A	601	LEU	CA-C-N	-5.52	114.29	120.14
1	A	601	LEU	C-N-CA	-5.52	114.29	120.14
1	A	650	THR	N-CA-C	5.26	117.53	109.95

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	391	THR	Peptide
1	A	498	SER	Peptide
1	A	654	ILE	Peptide

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	5052	0	5081	79	1
2	B	28	0	25	2	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
3	A	56	0	52	2	0
4	A	10	0	0	0	0
5	A	36	0	47	7	0
6	A	362	0	0	26	1
All	All	5628	0	5280	84	2

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 8.

All (84) 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:524:ASP:HB3	6:A:1070:HOH:O	1.14	1.30
1:A:442:GLU:OE1	1:A:467:LYS:HE2	1.43	1.17
5:A:780:GOL:O3	6:A:1125:HOH:O	1.77	1.02
1:A:523:ASP:HB3	6:A:1103:HOH:O	1.61	1.01
1:A:644:PHE:N	6:A:1055:HOH:O	1.75	0.97
1:A:315:SER:O	1:A:353:TRP:CZ3	2.18	0.97
1:A:315:SER:O	1:A:353:TRP:HZ3	1.47	0.96
1:A:556:TYR:O	1:A:559:LYS:HE2	1.68	0.94
1:A:362:MET:HE3	1:A:386:LEU:CD2	2.03	0.89
1:A:394:ARG:HB2	6:A:1076:HOH:O	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:SER:HB2	6:A:797:HOH:O	1.76	0.84
1:A:362:MET:CE	1:A:386:LEU:HD21	2.09	0.83
1:A:512:ASP:OD2	5:A:782:GOL:H31	1.81	0.81
1:A:562:SER:HB3	6:A:1098:HOH:O	1.84	0.78
1:A:348:ASP:OD2	6:A:1112:HOH:O	2.03	0.77
1:A:336:GLN:O	1:A:343:LEU:HD12	1.84	0.77
1:A:362:MET:CE	1:A:386:LEU:CD2	2.62	0.76
1:A:442:GLU:CD	1:A:467:LYS:HE2	2.14	0.72
1:A:573:GLY:C	6:A:1130:HOH:O	2.33	0.71
1:A:660:TRP:HE3	1:A:664:THR:HA	1.59	0.68
6:A:971:HOH:O	2:B:2:NAG:O6	2.12	0.67
1:A:520:ASN:HB3	6:A:1054:HOH:O	1.97	0.64
1:A:660:TRP:CE3	1:A:664:THR:HA	2.35	0.61
1:A:597:ASN:N	6:A:1130:HOH:O	2.27	0.60
1:A:343:LEU:HD23	1:A:368:PRO:HG3	1.82	0.60
1:A:325:ARG:CZ	6:A:1096:HOH:O	2.49	0.59
1:A:595:LEU:N	1:A:595:LEU:HD12	2.19	0.58
1:A:607:ASN:ND2	1:A:632:PRO:HG3	2.18	0.58
1:A:251:ARG:NH2	6:A:1013:HOH:O	2.37	0.57
1:A:659:ASN:OD1	1:A:659:ASN:N	2.35	0.57
1:A:442:GLU:OE1	1:A:467:LYS:CE	2.36	0.57
1:A:363:GLU:CD	6:A:924:HOH:O	2.47	0.56
1:A:90:LEU:HD11	1:A:106:LEU:HD11	1.86	0.56
1:A:362:MET:HE2	1:A:386:LEU:HD21	1.87	0.56
1:A:59:THR:HA	1:A:83:GLY:O	2.06	0.56
1:A:442:GLU:CD	1:A:467:LYS:CE	2.79	0.56
1:A:147:LYS:HE3	6:A:992:HOH:O	2.05	0.55
1:A:523:ASP:HB2	1:A:559:LYS:HE3	1.87	0.54
1:A:315:SER:O	1:A:353:TRP:CH2	2.59	0.54
1:A:362:MET:HE1	1:A:375:PHE:CZ	2.43	0.53
5:A:778:GOL:O3	6:A:1049:HOH:O	0.53	0.53
1:A:660:TRP:CE3	1:A:664:THR:HG22	2.43	0.53
1:A:603:ALA:O	1:A:604:SER:HB2	2.09	0.53
1:A:523:ASP:CB	6:A:1103:HOH:O	2.34	0.53
1:A:189:GLU:CD	6:A:841:HOH:O	2.51	0.52
1:A:343:LEU:HD11	1:A:391:THR:HG21	1.91	0.52
1:A:497:SER:HB2	1:A:501:PRO:HD3	1.91	0.52
1:A:362:MET:HE2	1:A:384:LEU:HD11	1.93	0.51
6:A:793:HOH:O	2:B:1:NAG:H82	2.11	0.50
1:A:536:ASP:OD2	5:A:782:GOL:O3	2.22	0.50
1:A:146:GLN:HB3	1:A:149:LEU:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:ASP:OD2	5:A:782:GOL:C3	2.58	0.48
1:A:102:LYS:HE2	3:A:1:NAG:O7	2.14	0.48
1:A:586:PHE:HB2	6:A:1085:HOH:O	2.14	0.48
1:A:362:MET:HE3	1:A:386:LEU:HD23	1.91	0.48
1:A:643:ARG:O	1:A:663:GLU:O	2.32	0.47
1:A:93:GLU:HG3	6:A:949:HOH:O	2.15	0.47
1:A:660:TRP:CD1	1:A:660:TRP:N	2.82	0.47
1:A:30:VAL:CG1	6:A:1026:HOH:O	2.63	0.47
1:A:660:TRP:HE3	1:A:664:THR:CA	2.27	0.47
1:A:30:VAL:HG11	6:A:1026:HOH:O	2.14	0.46
1:A:201:LYS:HG3	1:A:227:PHE:CE2	2.50	0.46
1:A:316:HIS:HA	1:A:353:TRP:CZ3	2.50	0.46
1:A:66:LEU:HD11	1:A:82:VAL:HG21	1.98	0.46
1:A:604:SER:HA	1:A:607:ASN:ND2	2.31	0.46
1:A:89:LYS:HB2	6:A:1036:HOH:O	2.15	0.45
1:A:102:LYS:HE2	3:A:1:NAG:C7	2.46	0.45
1:A:442:GLU:HA	1:A:467:LYS:HG2	1.98	0.45
1:A:140:ASN:O	1:A:165:GLY:HA2	2.17	0.44
1:A:470:GLN:HG3	1:A:494:ASN:OD1	2.18	0.44
1:A:488:ARG:NH1	1:A:515:ASN:ND2	2.66	0.44
1:A:362:MET:HE1	1:A:375:PHE:HZ	1.84	0.42
1:A:50:PRO:HB2	1:A:52:ASN:HB2	2.01	0.42
1:A:462:TYR:CD1	1:A:486:MET:HG3	2.53	0.42
1:A:625:VAL:HG21	1:A:642:MET:HE1	2.01	0.42
1:A:619:LYS:HG2	1:A:644:PHE:HB2	2.01	0.41
1:A:141:ASN:HB3	1:A:144:VAL:HB	2.01	0.41
1:A:312:HIS:CE1	1:A:345:LYS:HD3	2.55	0.41
1:A:122:CYS:HB3	1:A:125:LEU:HG	2.02	0.41
1:A:468:TYR:HA	1:A:490:VAL:O	2.20	0.41
1:A:536:ASP:CG	5:A:782:GOL:HO3	2.24	0.41
5:A:778:GOL:O2	6:A:1117:HOH:O	2.21	0.41
1:A:613:LYS:HA	1:A:613:LYS:HD2	1.95	0.40
1:A:601:LEU:HD23	1:A:601:LEU:HA	1.89	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:LYS:NZ	1:A:467:LYS:NZ[4_555]	1.07	1.13
6:A:841:HOH:O	6:A:841:HOH:O[3_555]	1.84	0.36

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	625/680 (92%)	578 (92%)	47 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	586/634 (92%)	570 (97%)	16 (3%)	39	45

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	LYS
1	A	214	PRO
1	A	272	LYS
1	A	311	GLN
1	A	336	GLN
1	A	343	LEU
1	A	420	SER
1	A	498	SER
1	A	649	CYS
1	A	652	GLU
1	A	653	SER
1	A	657	PHE
1	A	659	ASN

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Mol	Chain	Res	Type
1	A	660	TRP
1	A	662	ASN
1	A	663	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	60	HIS
1	A	70	ASN
1	A	108	HIS
1	A	129	HIS
1	A	148	ASN
1	A	208	GLN
1	A	515	ASN
1	A	563	HIS
1	A	607	ASN
1	A	609	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](#)

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

5.5 Carbohydrates [i](#)

8 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
2	NAG	B	1	2,1	14,14,15	0.60	0	17,19,21	1.25	2 (11%)
2	NAG	B	2	2	14,14,15	0.59	0	17,19,21	0.90	0
2	NAG	C	1	2,1	14,14,15	0.86	1 (7%)	17,19,21	1.10	1 (5%)
2	NAG	C	2	2	14,14,15	0.68	0	17,19,21	1.21	1 (5%)
2	NAG	D	1	2,1	14,14,15	0.94	1 (7%)	17,19,21	1.79	4 (23%)
2	NAG	D	2	2	14,14,15	0.63	0	17,19,21	2.73	3 (17%)
2	NAG	E	1	2,1	14,14,15	0.68	0	17,19,21	2.21	4 (23%)
2	NAG	E	2	2	14,14,15	0.61	0	17,19,21	1.34	2 (11%)

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
2	NAG	B	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	C1-C2	2.16	1.55	1.52
2	D	1	NAG	C1-C2	2.14	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C1-O5-C5	9.94	125.51	112.19
2	E	1	NAG	C1-O5-C5	6.72	121.19	112.19
2	E	2	NAG	C4-C3-C2	4.17	117.12	111.02
2	D	1	NAG	C1-O5-C5	4.08	117.65	112.19
2	D	1	NAG	C2-N2-C7	-3.48	118.23	122.90
2	E	1	NAG	C2-N2-C7	-3.38	118.37	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	3.34	116.66	112.19
2	D	2	NAG	C3-C4-C5	-3.17	104.48	110.23
2	E	1	NAG	O5-C1-C2	-3.00	106.66	111.29
2	D	1	NAG	O5-C1-C2	-2.95	106.72	111.29
2	B	1	NAG	O4-C4-C3	-2.66	104.10	110.38
2	D	1	NAG	O6-C6-C5	-2.64	102.35	111.33
2	B	1	NAG	O5-C1-C2	-2.64	107.21	111.29
2	D	2	NAG	O5-C1-C2	2.58	115.28	111.29
2	E	1	NAG	C6-C5-C4	-2.52	106.83	113.02
2	E	2	NAG	C3-C4-C5	2.37	114.54	110.23
2	C	1	NAG	O7-C7-C8	-2.09	118.34	122.05

There are no chirality outliers.

All (17) torsion outliers are listed below:

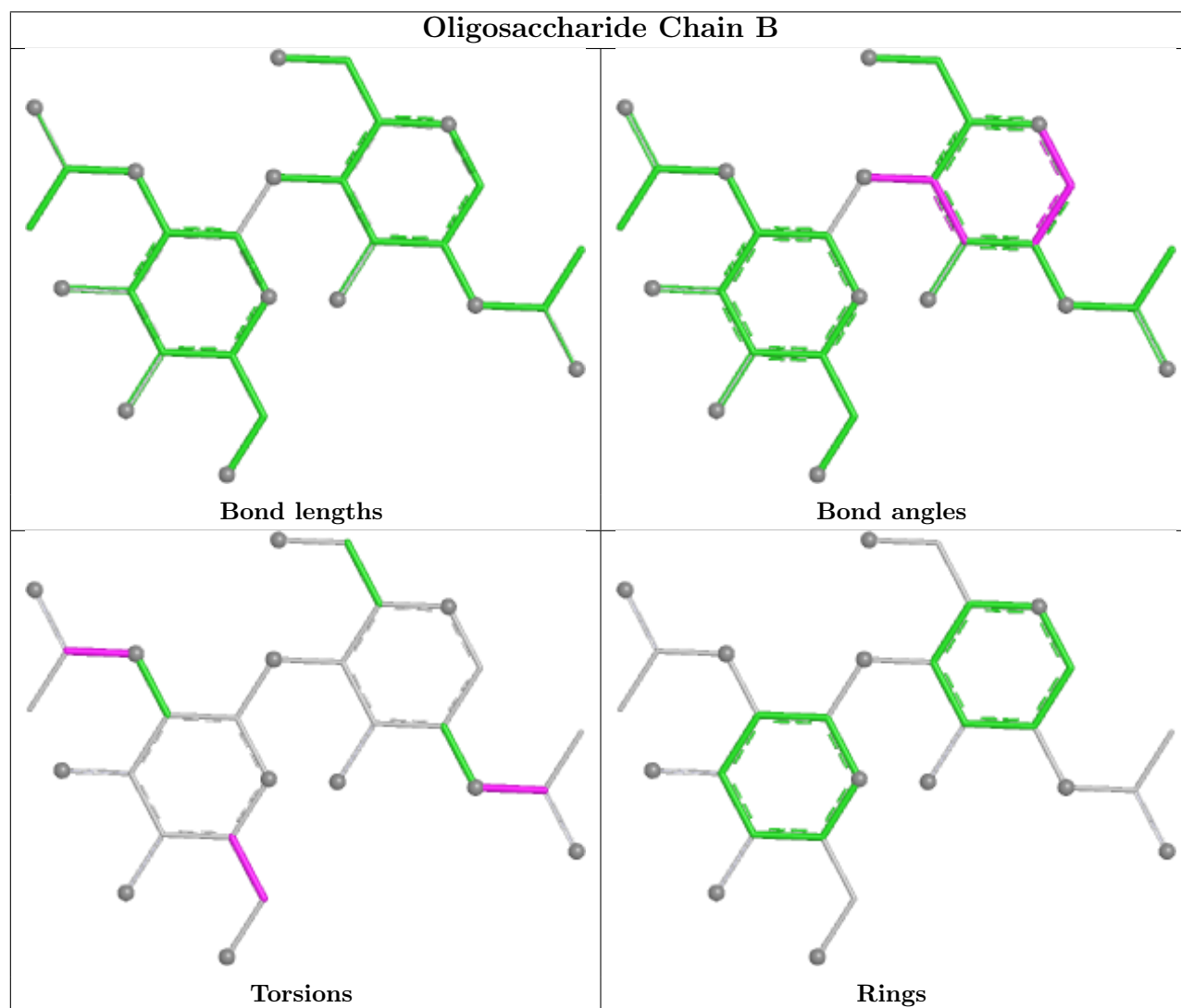
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	C	1	NAG	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	B	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C4-C5-C6-O6

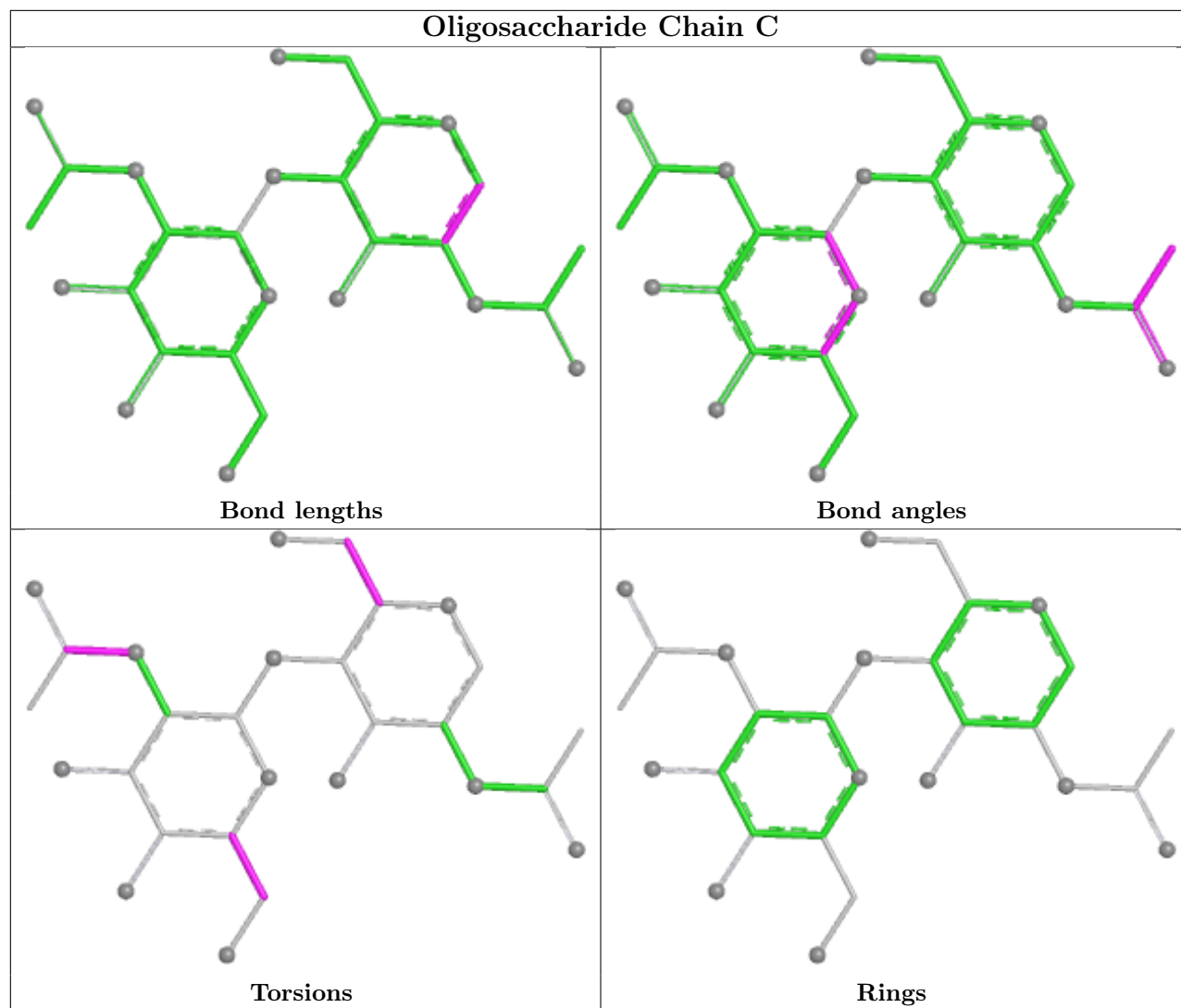
There are no ring outliers.

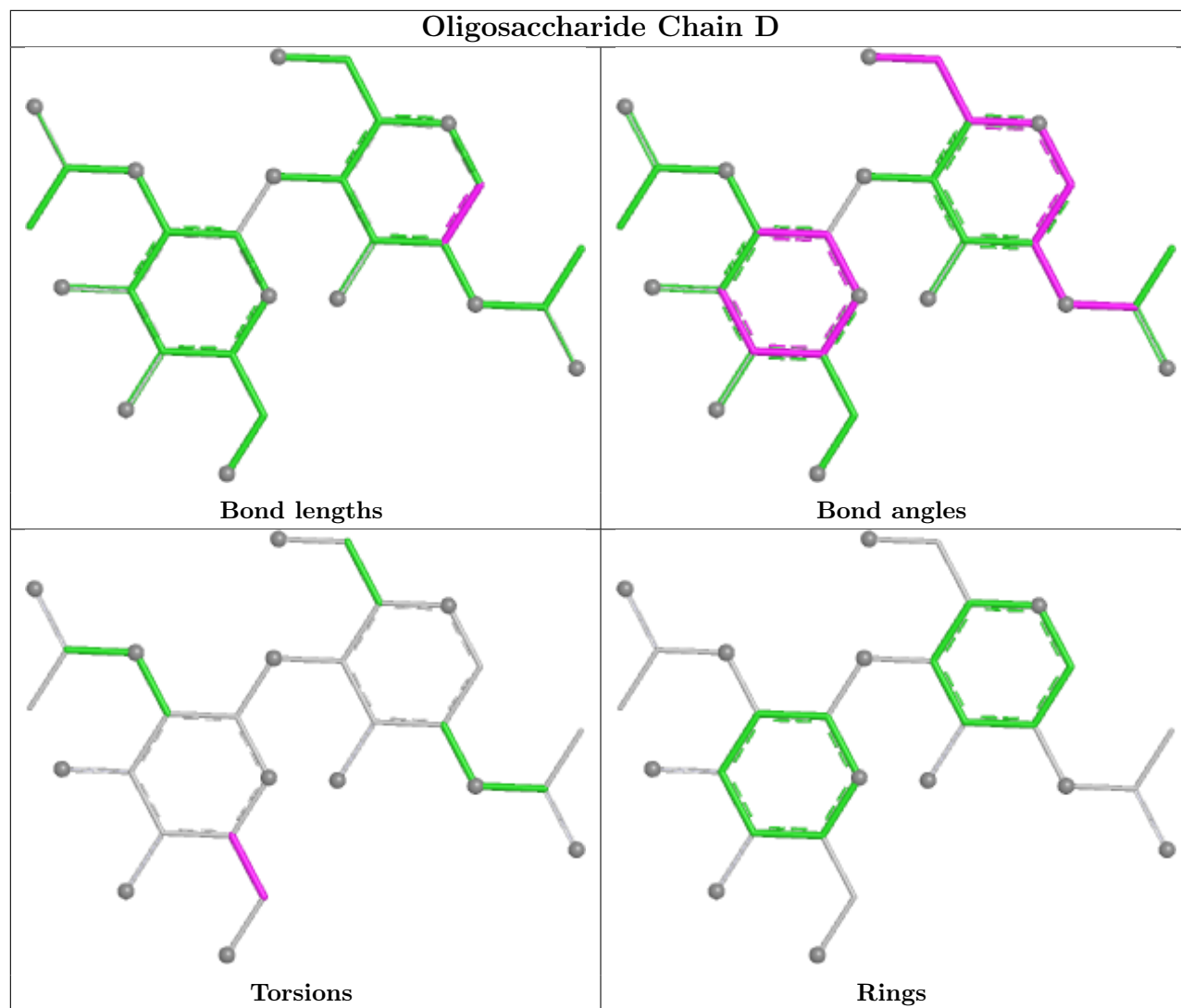
2 monomers are involved in 2 short contacts:

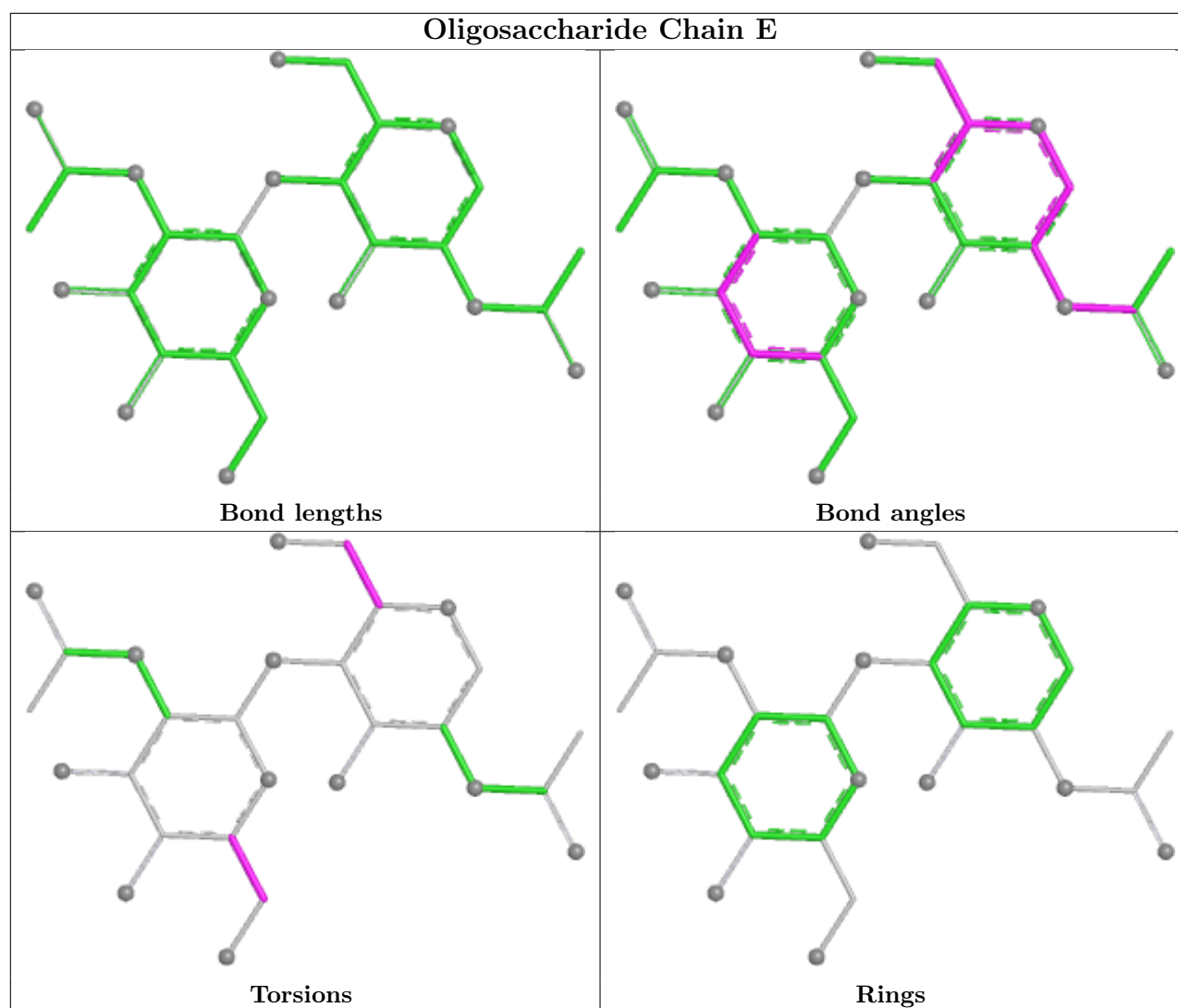
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	1	0
2	B	2	NAG	1	0

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](#)

12 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	$\# Z > 2$
4	SO4	A	777	-	4,4,4	0.25	0	6,6,6	0.35	0
5	GOL	A	779	-	5,5,5	0.53	0	5,5,5	0.80	0
3	NAG	A	7	1	14,14,15	0.74	0	17,19,21	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	A	778	-	5,5,5	1.51	1 (20%)	5,5,5	0.83	0
5	GOL	A	782	-	5,5,5	0.48	0	5,5,5	0.78	0
3	NAG	A	1	1	14,14,15	0.58	0	17,19,21	2.13	6 (35%)
3	NAG	A	4	1	14,14,15	0.43	0	17,19,21	2.64	5 (29%)
4	SO4	A	776	-	4,4,4	0.42	0	6,6,6	0.57	0
3	NAG	A	8	1	14,14,15	0.47	0	17,19,21	1.69	3 (17%)
5	GOL	A	783	-	5,5,5	0.53	0	5,5,5	0.47	0
5	GOL	A	780	-	5,5,5	0.48	0	5,5,5	0.41	0
5	GOL	A	781	-	5,5,5	0.42	0	5,5,5	0.40	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	GOL	A	779	-	-	3/4/4/4	-
3	NAG	A	7	1	1/1/5/7	2/6/23/26	0/1/1/1
5	GOL	A	778	-	-	2/4/4/4	-
5	GOL	A	782	-	-	2/4/4/4	-
3	NAG	A	1	1	1/1/5/7	5/6/23/26	0/1/1/1
3	NAG	A	4	1	-	3/6/23/26	0/1/1/1
3	NAG	A	8	1	-	2/6/23/26	0/1/1/1
5	GOL	A	783	-	-	4/4/4/4	-
5	GOL	A	780	-	-	4/4/4/4	-
5	GOL	A	781	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	778	GOL	O3-C3	-3.24	1.28	1.42

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4	NAG	C1-O5-C5	8.39	123.43	112.19
3	A	1	NAG	C1-O5-C5	4.10	117.68	112.19
3	A	1	NAG	C3-C4-C5	4.04	117.56	110.23
3	A	8	NAG	C1-O5-C5	3.79	117.27	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	NAG	C2-N2-C7	3.64	127.77	122.90
3	A	8	NAG	C3-C4-C5	3.49	116.56	110.23
3	A	4	NAG	C4-C3-C2	-3.43	105.99	111.02
3	A	1	NAG	C4-C3-C2	3.33	115.89	111.02
3	A	4	NAG	O5-C5-C4	3.02	118.18	110.83
3	A	4	NAG	C2-N2-C7	2.94	126.84	122.90
3	A	1	NAG	O5-C5-C4	2.28	116.38	110.83
3	A	8	NAG	O7-C7-C8	-2.15	118.22	122.05
3	A	1	NAG	C1-C2-N2	-2.05	107.20	110.43
3	A	4	NAG	O5-C1-C2	2.04	114.45	111.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1	NAG	C1
3	A	7	NAG	C1

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	NAG	C8-C7-N2-C2
3	A	1	NAG	O7-C7-N2-C2
5	A	778	GOL	C1-C2-C3-O3
5	A	779	GOL	C1-C2-C3-O3
5	A	780	GOL	O1-C1-C2-C3
5	A	780	GOL	C1-C2-C3-O3
5	A	782	GOL	O1-C1-C2-C3
5	A	783	GOL	O1-C1-C2-C3
5	A	783	GOL	C1-C2-C3-O3
3	A	8	NAG	C4-C5-C6-O6
3	A	8	NAG	O5-C5-C6-O6
3	A	1	NAG	C4-C5-C6-O6
3	A	4	NAG	C4-C5-C6-O6
3	A	1	NAG	O5-C5-C6-O6
5	A	780	GOL	O1-C1-C2-O2
5	A	782	GOL	O1-C1-C2-O2
5	A	781	GOL	C1-C2-C3-O3
5	A	778	GOL	O2-C2-C3-O3
5	A	780	GOL	O2-C2-C3-O3
5	A	783	GOL	O1-C1-C2-O2
5	A	783	GOL	O2-C2-C3-O3
5	A	779	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	4	NAG	C3-C2-N2-C7
3	A	4	NAG	O5-C5-C6-O6
3	A	7	NAG	C4-C5-C6-O6
3	A	1	NAG	C3-C2-N2-C7
5	A	781	GOL	O2-C2-C3-O3
3	A	7	NAG	O5-C5-C6-O6
5	A	779	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	778	GOL	2	0
5	A	782	GOL	4	0
3	A	1	NAG	2	0
5	A	780	GOL	1	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, 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	629/680 (92%)	0.69	60 (9%) 14 14	30, 40, 60, 87	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	656	TRP	9.9
1	A	649	CYS	9.3
1	A	664	THR	8.5
1	A	661	ILE	8.3
1	A	660	TRP	7.7
1	A	30	VAL	7.5
1	A	654	ILE	7.3
1	A	657	PHE	6.1
1	A	658	VAL	5.4
1	A	655	ALA	5.2
1	A	651	CYS	4.7
1	A	39	HIS	4.6
1	A	392	SER	4.6
1	A	32	HIS	4.3
1	A	467	LYS	4.2
1	A	648	ASP	4.1
1	A	650	THR	4.0
1	A	353	TRP	4.0
1	A	498	SER	3.9
1	A	499	PRO	3.8
1	A	652	GLU	3.8
1	A	38	SER	3.6
1	A	33	GLU	3.6
1	A	548	HIS	3.6
1	A	442	GLU	3.5
1	A	626	GLU	3.4
1	A	653	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	662	ASN	3.3
1	A	659	ASN	3.2
1	A	549	ALA	3.2
1	A	343	LEU	3.2
1	A	391	THR	3.0
1	A	599	ASN	3.0
1	A	60	HIS	3.0
1	A	31	SER	2.9
1	A	40	LEU	2.8
1	A	34	VAL	2.8
1	A	623	THR	2.8
1	A	462	TYR	2.7
1	A	147	LYS	2.6
1	A	336	GLN	2.6
1	A	609	GLN	2.6
1	A	625	VAL	2.6
1	A	607	ASN	2.6
1	A	139	LYS	2.5
1	A	394	ARG	2.5
1	A	635	ARG	2.5
1	A	393	LEU	2.4
1	A	644	PHE	2.4
1	A	37	CYS	2.4
1	A	643	ARG	2.3
1	A	188	SER	2.3
1	A	604	SER	2.3
1	A	69	ALA	2.3
1	A	52	ASN	2.1
1	A	580	GLU	2.1
1	A	89	LYS	2.1
1	A	456	GLU	2.0
1	A	520	ASN	2.0
1	A	622	ILE	2.0

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

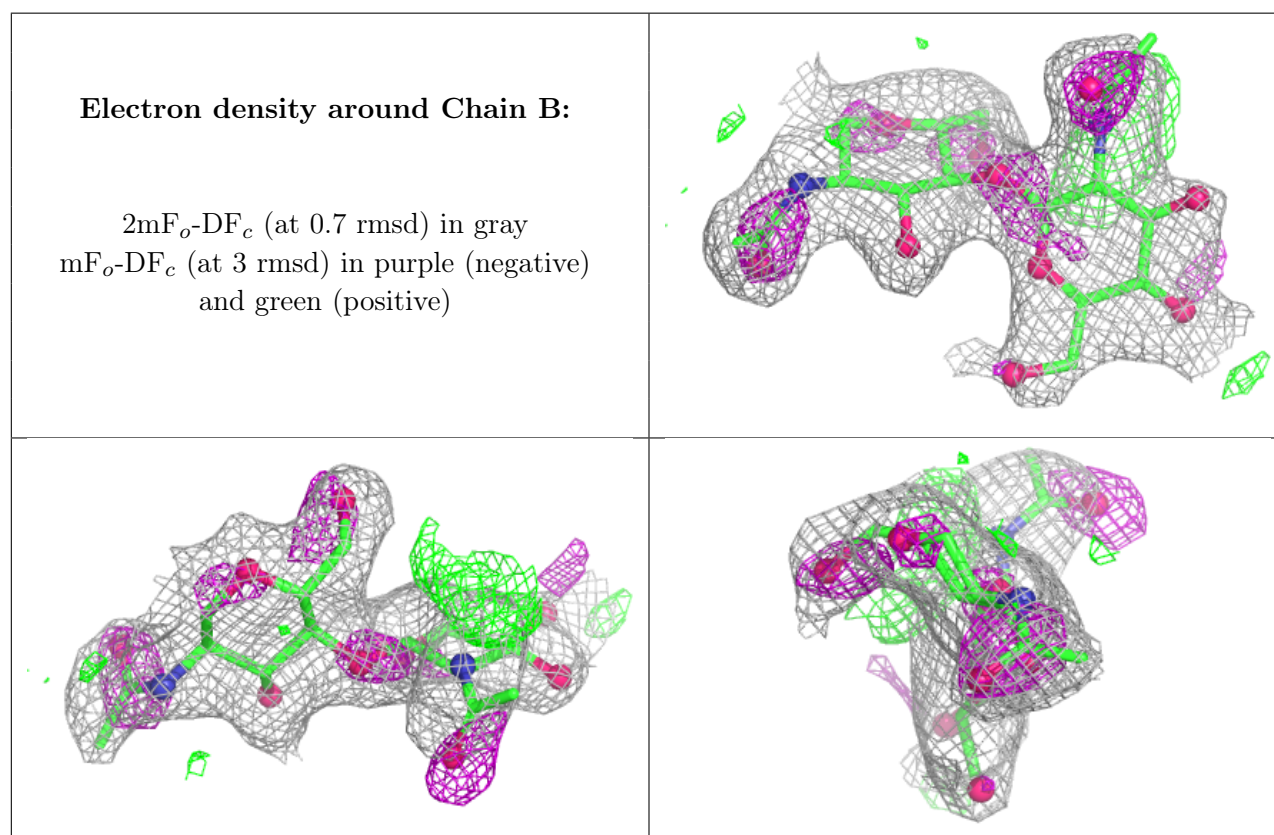
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

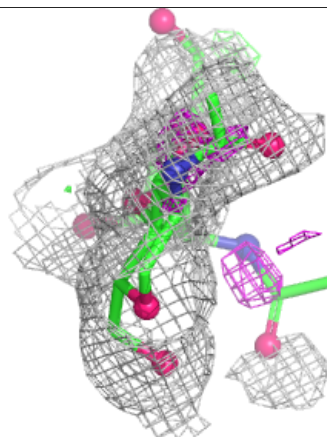
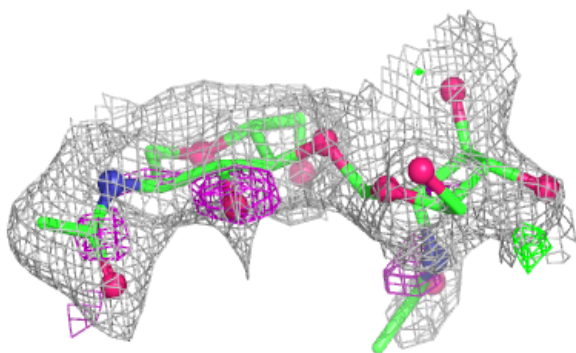
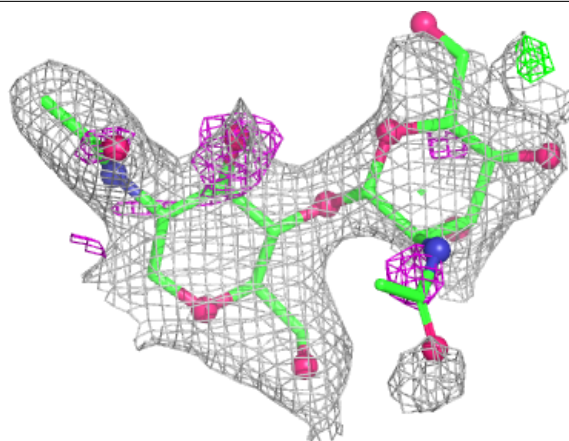
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	2	14/15	0.34	0.23	98,99,99,99	0
2	NAG	B	2	14/15	0.60	0.19	65,70,72,73	0
2	NAG	D	2	14/15	0.62	0.20	48,64,80,83	0
2	NAG	E	2	14/15	0.65	0.17	79,87,91,93	0
2	NAG	C	1	14/15	0.83	0.14	38,61,73,89	0
2	NAG	B	1	14/15	0.86	0.14	46,49,54,55	0
2	NAG	E	1	14/15	0.88	0.13	33,45,65,74	0
2	NAG	D	1	14/15	0.92	0.10	25,32,44,53	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.



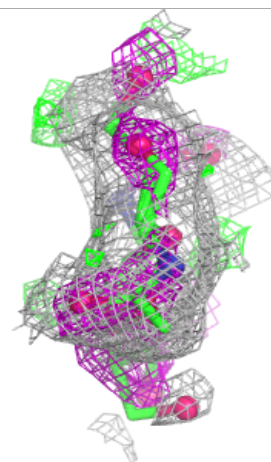
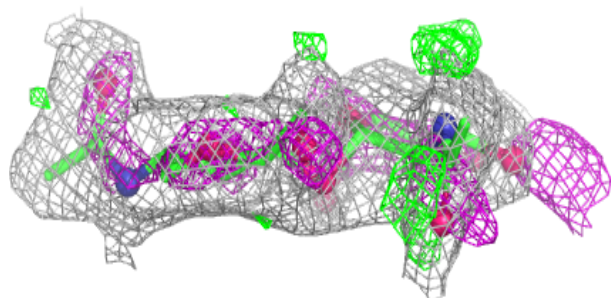
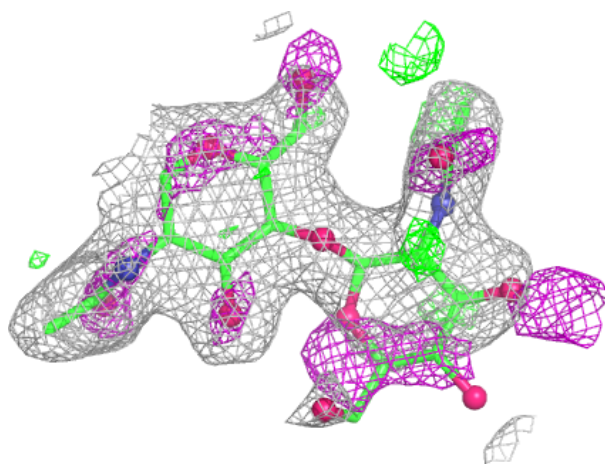
Electron density around Chain C:

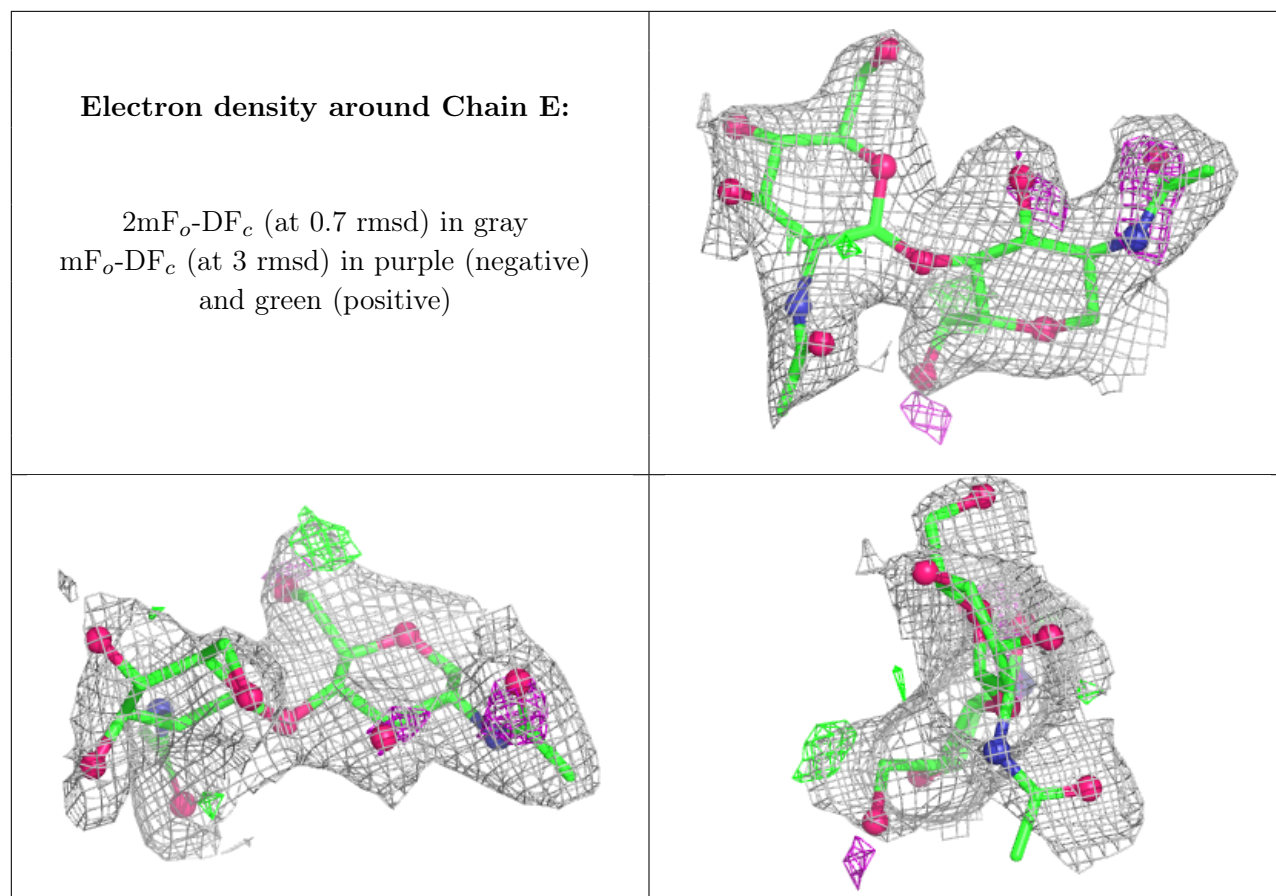
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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, 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
3	NAG	A	1	14/15	0.62	0.18	80,90,96,98	0
3	NAG	A	4	14/15	0.70	0.16	65,76,85,85	0
5	GOL	A	781	6/6	0.75	0.23	71,78,85,90	0
5	GOL	A	779	6/6	0.76	0.22	56,69,76,77	0
3	NAG	A	7	14/15	0.77	0.17	64,77,81,83	0
3	NAG	A	8	14/15	0.78	0.14	71,75,79,86	0
5	GOL	A	782	6/6	0.80	0.17	50,65,72,74	0
5	GOL	A	780	6/6	0.85	0.18	31,58,69,69	0
5	GOL	A	783	6/6	0.86	0.17	33,51,62,65	0
5	GOL	A	778	6/6	0.95	0.17	9,44,50,59	0
4	SO4	A	777	5/5	0.96	0.17	53,59,61,65	0
4	SO4	A	776	5/5	0.98	0.12	34,34,35,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.