



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 04:11 AM BST

PDB ID : 2Y73
Title : THE NATIVE STRUCTURES OF SOLUBLE HUMAN PRIMARY AMINE
OXIDASE AOC3
Authors : Elovaara, H.; Kidron, H.; Parkash, V.; Nymalm, Y.; Bligt, E.; Ollikka, P.;
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Deposited on : 2011-01-28
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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 : 2.13.1
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) : 2.13.1

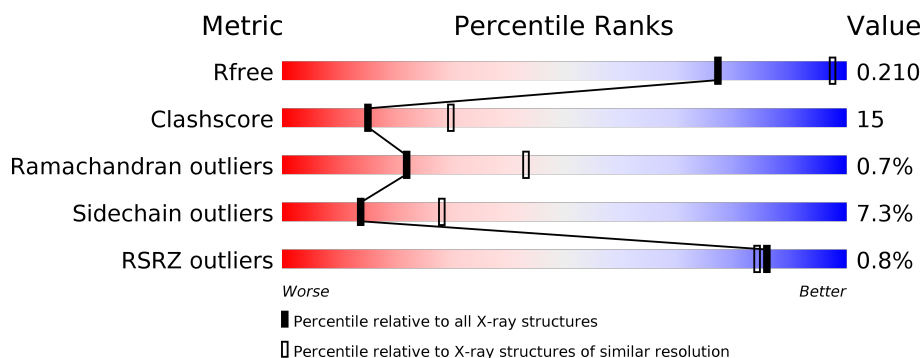
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	763	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>23%</div> <div>• 8%</div> </div> </div>
1	B	763	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>22%</div> <div>• • 8%</div> </div> </div>
2	C	3	<div> <div></div> <div>67%</div> <div>33%</div> </div>
2	E	3	<div> <div></div> <div>33%</div> <div>67%</div> </div>
3	D	2	<div> <div></div> <div>50%</div> <div>50%</div> </div>
3	F	2	<div> <div></div> <div>100%</div> </div>

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
6	IMD	A	804	-	-	X	-
7	NAG	A	813	-	-	-	X
7	NAG	B	813	-	-	-	X
8	FMT	A	815	-	-	X	-

2 Entry composition [i](#)

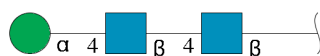
There are 9 unique types of molecules in this entry. The entry contains 11675 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MEMBRANE PRIMARY AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	705	Total	C	N	O	S	0	0	0
			5560	3570	957	1013	20			
1	B	701	Total	C	N	O	S	0	0	0
			5527	3551	950	1007	19			

- Molecule 2 is an oligosaccharide called alpha-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
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 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
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

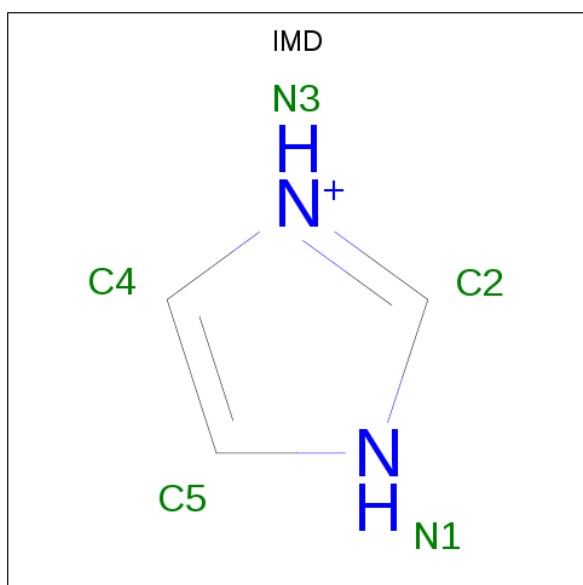
- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cu 1 1	0	0
4	A	1	Total Cu 1 1	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Ca 2 2	0	0
5	A	2	Total Ca 2 2	0	0

- Molecule 6 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



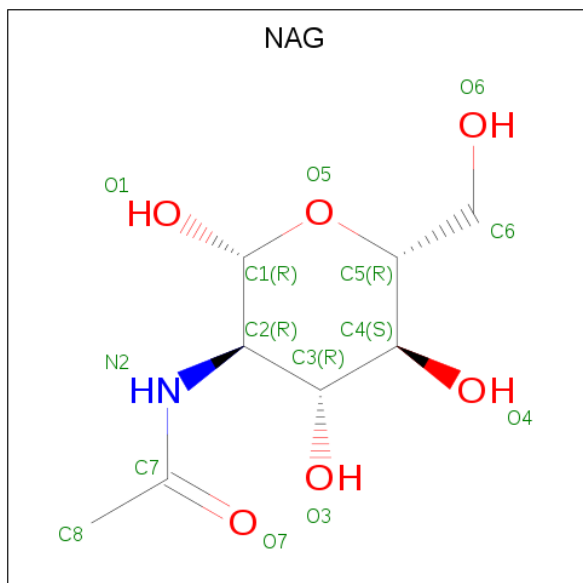
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N 5 3 2	0	0
6	A	1	Total C N 5 3 2	0	0
6	A	1	Total C N 5 3 2	0	0
6	A	1	Total C N 5 3 2	0	0
6	B	1	Total C N 5 3 2	0	0
6	B	1	Total C N 5 3 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	N	0	0
			5	3	2		
6	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

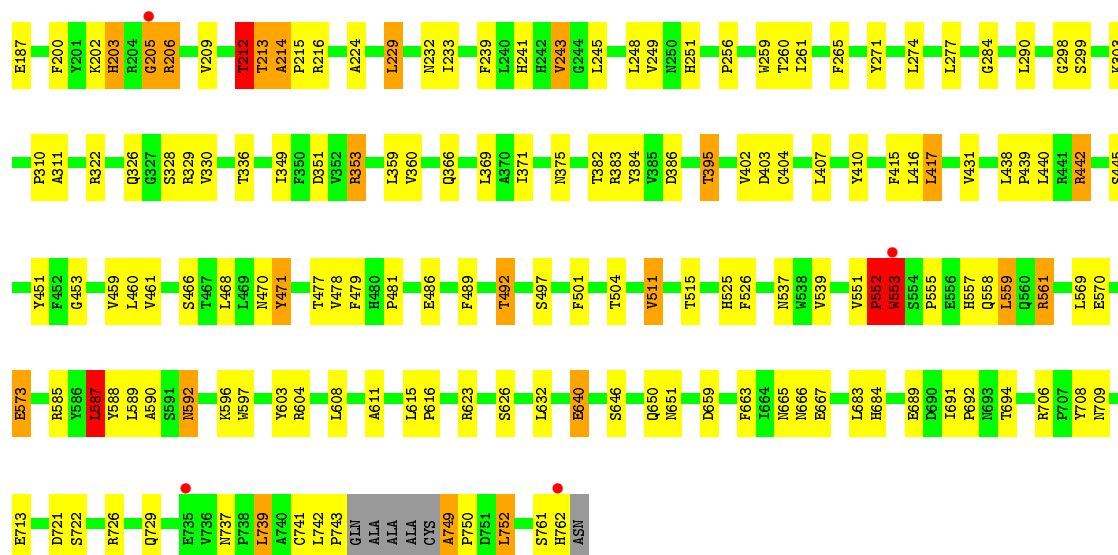
- Molecule 8 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			3	1	2		
8	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	191	Total	O	0	0
			191	191		
9	B	155	Total	O	0	0
			155	155		



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

Chain C:  67% 33%



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

Chain E:  33% 67%



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

Chain D:  50% 50%



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

Chain F:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	225.75Å 225.75Å 216.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.93 – 2.60 19.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.93-2.60) 100.0 (19.93-2.60)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.56 (at 2.59Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.175 , 0.213 0.173 , 0.210	Depositor DCC
R_{free} test set	4978 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11675	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: NAG, IMD, CA, TPQ, FMT, CU, MAN

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	0.76	4/5721 (0.1%)	0.87	9/7800 (0.1%)
1	B	0.80	7/5688 (0.1%)	0.82	5/7757 (0.1%)
All	All	0.78	11/11409 (0.1%)	0.85	14/15557 (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	1
1	B	0	7
All	All	0	8

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	552	PRO	C-N	-19.80	0.88	1.34
1	B	553	TRP	C-N	-11.17	1.08	1.34
1	B	741	CYS	CA-CB	-10.79	1.30	1.53
1	B	95	CYS	CB-SG	-7.89	1.68	1.82
1	A	137	ASN	CG-ND2	7.80	1.52	1.32

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	SER	N-CA-CB	-14.32	89.03	110.50
1	A	329	ARG	NE-CZ-NH2	-9.39	115.61	120.30
1	B	229	LEU	CA-CB-CG	-9.35	93.80	115.30
1	A	56	GLN	N-CA-C	7.77	131.98	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	587	LEU	CA-CB-CG	-7.31	98.49	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	THR	Peptide
1	B	203	HIS	Peptide
1	B	205	GLY	Peptide
1	B	213	THR	Peptide
1	B	94	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5560	0	5307	179	0
1	B	5527	0	5264	174	0
2	C	39	0	33	2	0
2	E	39	0	34	2	0
3	D	28	0	25	1	0
3	F	28	0	25	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	20	0	20	6	0
6	B	20	0	20	5	0
7	A	28	0	26	3	0
7	B	28	0	26	2	0
8	A	6	0	2	4	0
9	A	191	0	0	5	0
9	B	155	0	0	2	0
All	All	11675	0	10782	331	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 15.

The worst 5 of 331 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:206:ARG:N	1:A:206:ARG:HD2	1.52	1.13
1:B:58:GLN:HG3	1:B:59:LEU:H	1.15	1.11
1:A:201:TYR:O	1:A:202:LYS:HG2	1.50	1.09
1:B:214:ALA:CB	1:B:215:PRO:HD2	1.90	1.01
1:B:212:THR:HG21	1:B:216:ARG:NH2	1.76	1.01

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	700/763 (92%)	656 (94%)	37 (5%)	7 (1%)	15	32
1	B	696/763 (91%)	653 (94%)	40 (6%)	3 (0%)	34	57
All	All	1396/1526 (92%)	1309 (94%)	77 (6%)	10 (1%)	22	43

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	ALA
1	A	744	GLN
1	A	745	ALA
1	A	746	ALA
1	B	58	GLN

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	585/634 (92%)	541 (92%)	44 (8%)	13	27
1	B	581/634 (92%)	540 (93%)	41 (7%)	14	29
All	All	1166/1268 (92%)	1081 (93%)	85 (7%)	14	28

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	635	THR
1	B	103	LEU
1	B	646	SER
1	A	695	VAL
1	A	762	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	77	GLN
1	B	174	GLN
1	B	699	ASN
1	B	94	ASN
1	A	276	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	TPQ	B	471	1,4	13,14,15	3.59	7 (53%)	15,19,21	1.40	3 (20%)
1	TPQ	A	471	1,4	13,14,15	3.70	7 (53%)	15,19,21	1.33	2 (13%)

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	TPQ	B	471	1,4	-	5/5/22/24	0/1/1/1
1	TPQ	A	471	1,4	-	5/5/22/24	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	TPQ	C1-C2	-7.56	1.37	1.49
1	B	471	TPQ	C1-C2	-6.57	1.39	1.49
1	A	471	TPQ	O5-C5	5.79	1.40	1.24
1	B	471	TPQ	O5-C5	5.72	1.39	1.24
1	B	471	TPQ	O2-C2	5.69	1.39	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	471	TPQ	C4-C3-C2	2.70	123.29	120.30
1	A	471	TPQ	CB-C1-C2	2.54	123.12	118.57
1	A	471	TPQ	CB-CA-C	2.47	116.11	111.47
1	B	471	TPQ	CB-C1-C2	2.40	122.86	118.57
1	B	471	TPQ	C3-C4-C5	-2.39	118.79	121.26

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	471	TPQ	C-CA-CB-C1
1	B	471	TPQ	O-C-CA-CB
1	A	471	TPQ	C-CA-CB-C1
1	A	471	TPQ	O-C-CA-CB
1	A	471	TPQ	C2-C1-CB-CA

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	471	TPQ	2	0
1	A	471	TPQ	2	0

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
2	NAG	C	1	1,2	14,14,15	2.00	5 (35%)	17,19,21	1.84	6 (35%)
2	NAG	C	2	2	14,14,15	2.29	5 (35%)	17,19,21	1.82	5 (29%)
2	MAN	C	3	2	11,11,12	1.86	3 (27%)	15,15,17	2.13	6 (40%)
3	NAG	D	1	1,3	14,14,15	2.20	5 (35%)	17,19,21	1.53	4 (23%)
3	NAG	D	2	3	14,14,15	2.09	4 (28%)	17,19,21	1.41	3 (17%)
2	NAG	E	1	1,2	14,14,15	2.01	5 (35%)	17,19,21	1.49	3 (17%)
2	NAG	E	2	2	14,14,15	2.05	5 (35%)	17,19,21	2.37	4 (23%)
2	MAN	E	3	2	11,11,12	1.73	2 (18%)	15,15,17	2.39	6 (40%)
3	NAG	F	1	1,3	14,14,15	2.01	5 (35%)	17,19,21	2.07	5 (29%)
3	NAG	F	2	3	14,14,15	2.19	5 (35%)	17,19,21	2.23	5 (29%)

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	C	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	MAN	C	3	2	-	2/2/19/22	1/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	MAN	E	3	2	-	2/2/19/22	1/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	O5-C5	5.41	1.54	1.43
2	E	1	NAG	C3-C2	-4.65	1.42	1.52
3	F	2	NAG	O5-C5	4.65	1.52	1.43
3	D	2	NAG	O5-C5	4.63	1.52	1.43
2	E	2	NAG	O5-C5	4.47	1.52	1.43

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C2-N2-C7	-6.72	113.33	122.90
3	F	1	NAG	C4-C3-C2	4.92	118.23	111.02
2	E	3	MAN	C1-C2-C3	-4.60	104.01	109.67
2	E	2	NAG	C4-C3-C2	4.36	117.40	111.02
2	E	3	MAN	O2-C2-C1	4.31	117.98	109.15

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	NAG	O7-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O7-C7-N2-C2

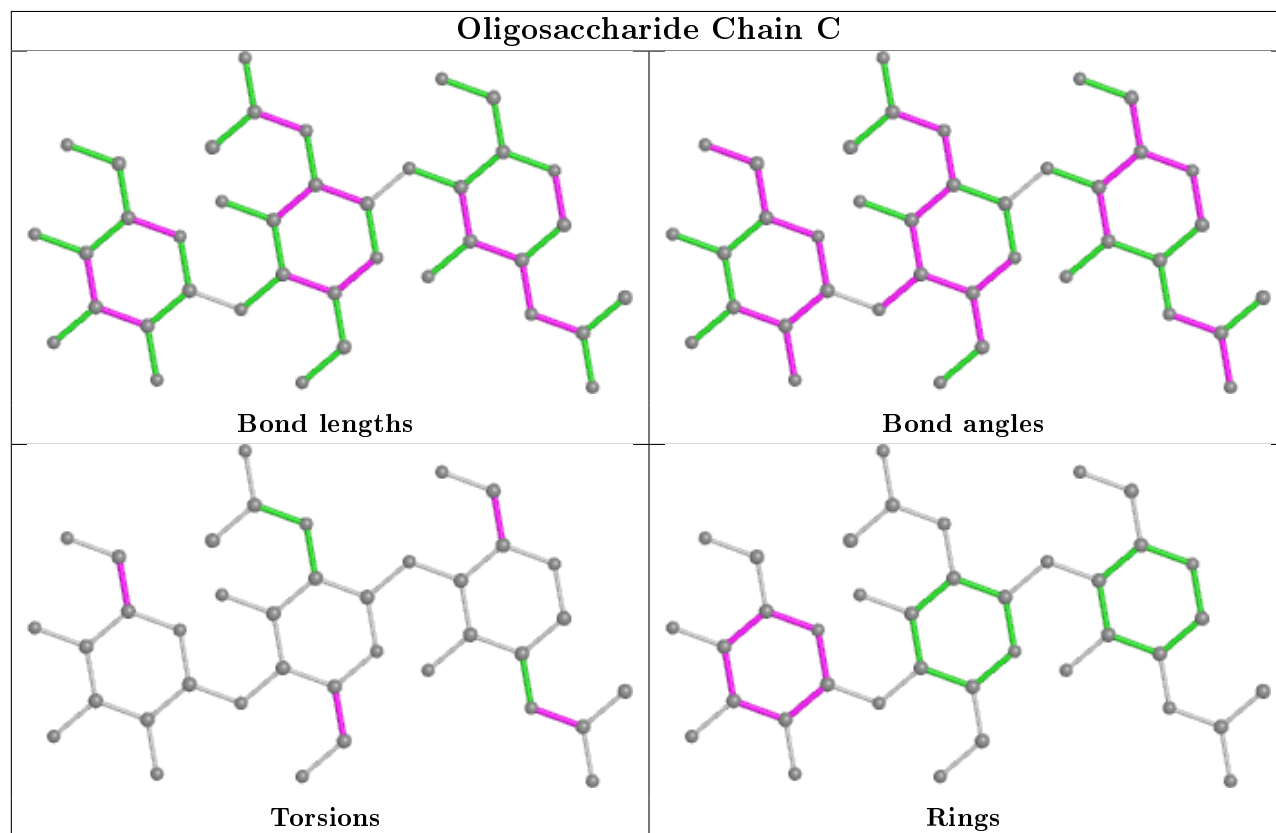
All (2) ring outliers are listed below:

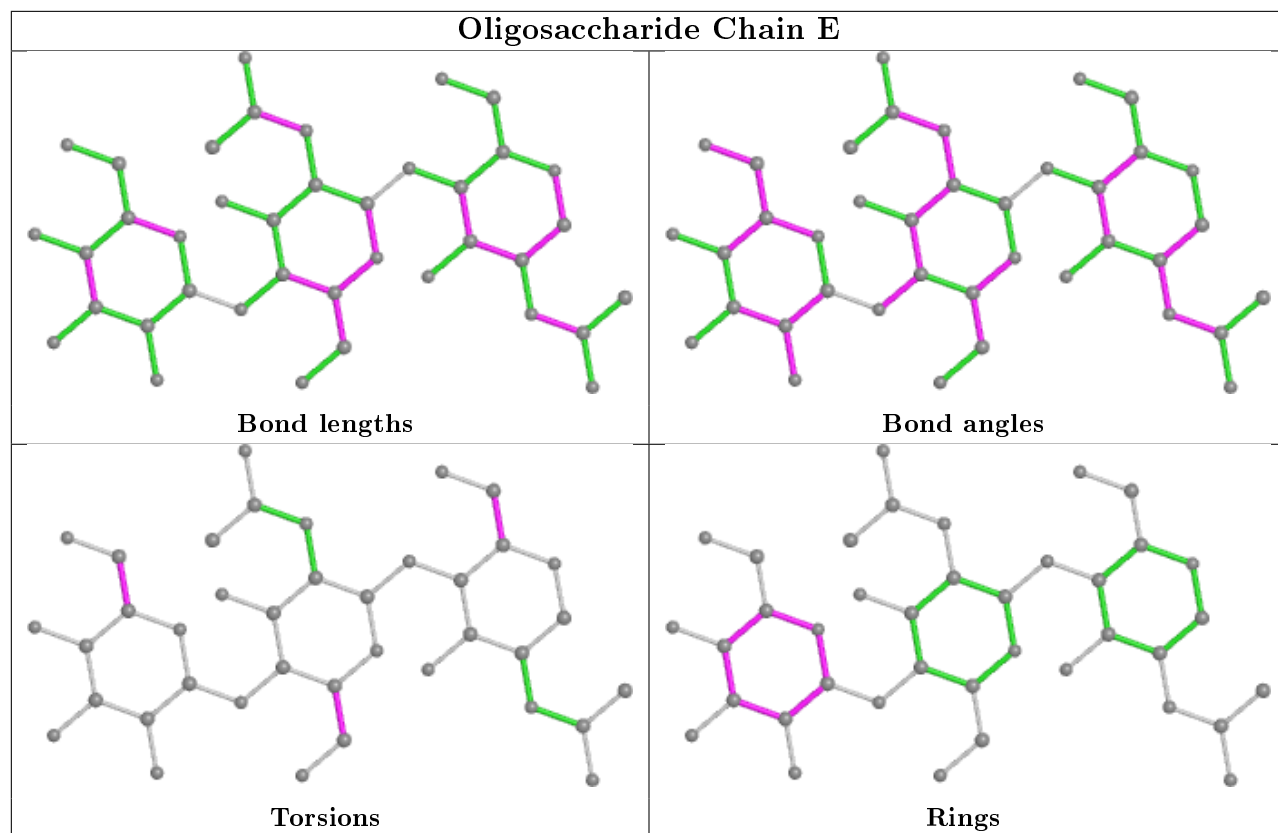
Mol	Chain	Res	Type	Atoms
2	C	3	MAN	C1-C2-C3-C4-C5-O5
2	E	3	MAN	C1-C2-C3-C4-C5-O5

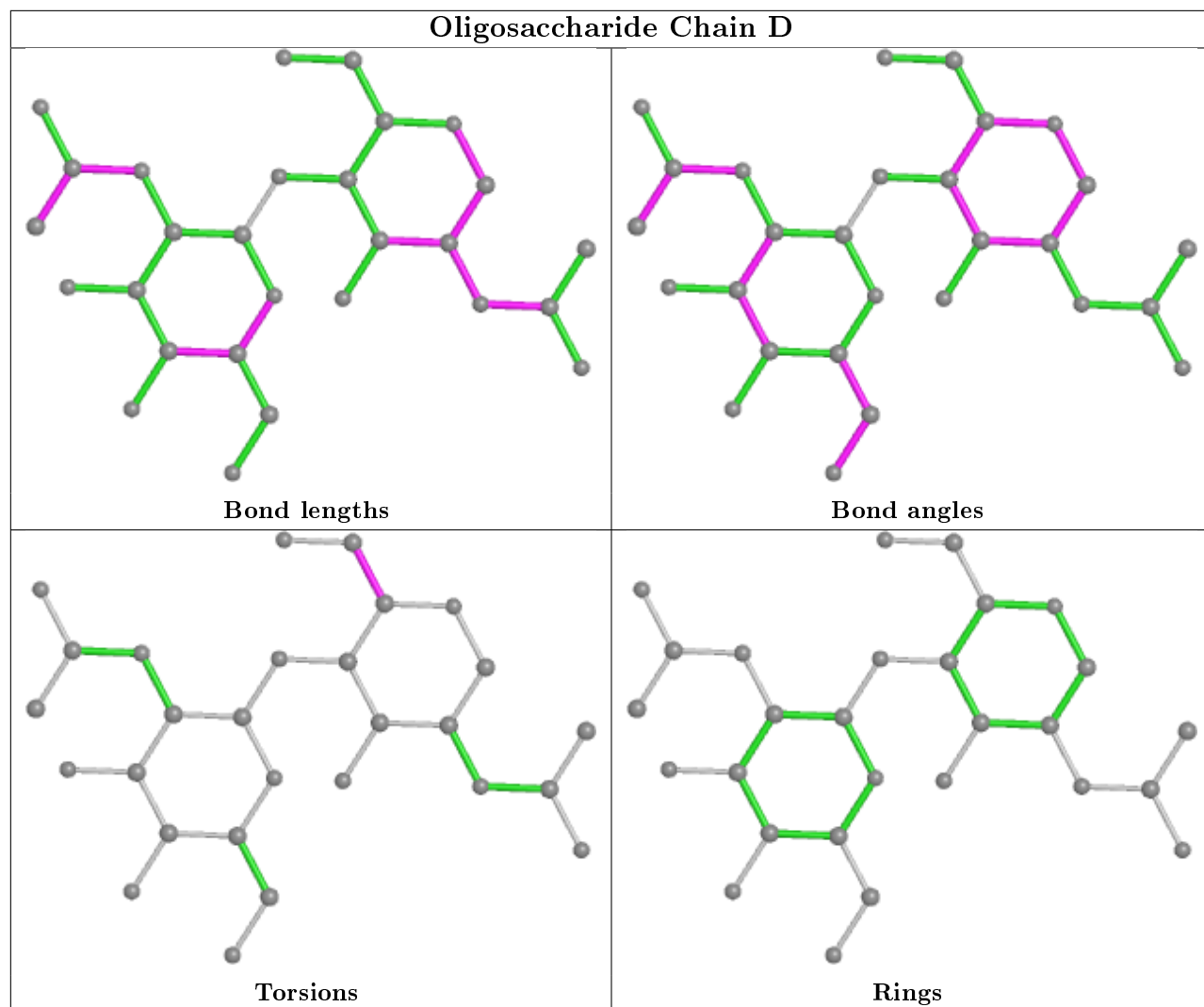
4 monomers are involved in 5 short contacts:

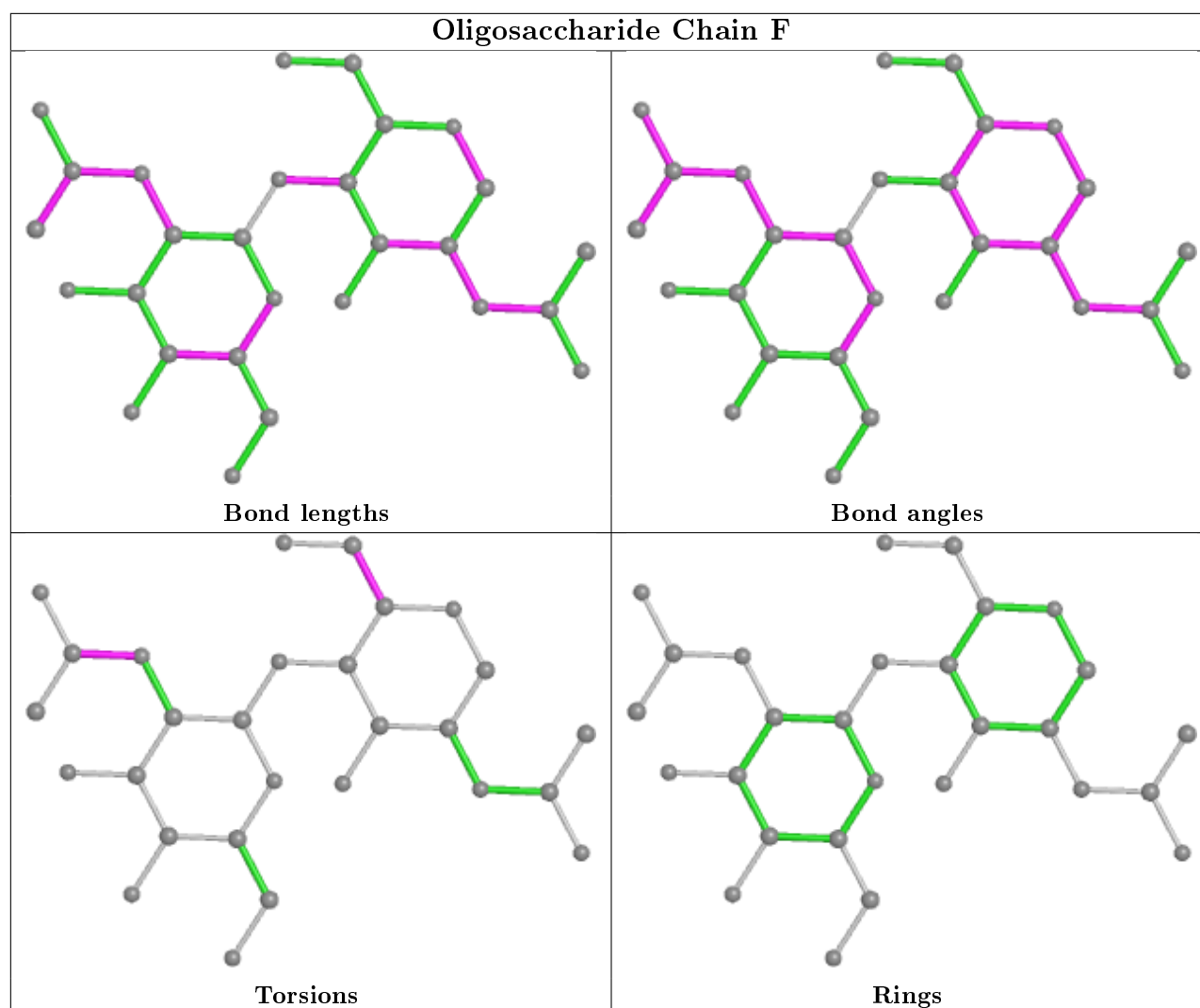
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	2	0
2	E	1	NAG	2	0
3	D	1	NAG	1	0
2	E	2	NAG	1	0

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 ⓘ

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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	B	812	1	14,14,15	2.11	4 (28%)	17,19,21	2.63	7 (41%)
6	IMD	A	814	-	3,5,5	0.43	0	4,5,5	0.51	0
7	NAG	A	813	1	14,14,15	2.13	5 (35%)	17,19,21	2.74	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	IMD	B	805	-	3,5,5	0.48	0	4,5,5	0.28	0
6	IMD	B	806	-	3,5,5	0.45	0	4,5,5	0.43	0
6	IMD	A	806	-	3,5,5	0.36	0	4,5,5	0.69	0
6	IMD	B	814	-	3,5,5	0.44	0	4,5,5	0.77	0
7	NAG	A	812	1	14,14,15	0.89	1 (7%)	17,19,21	2.72	5 (29%)
6	IMD	A	805	-	3,5,5	0.42	0	4,5,5	0.63	0
8	FMT	A	815	-	0,2,2	0.00	-	0,1,1	0.00	-
6	IMD	A	804	-	3,5,5	0.40	0	4,5,5	0.53	0
6	IMD	B	804	-	3,5,5	0.45	0	4,5,5	0.44	0
8	FMT	A	816	-	0,2,2	0.00	-	0,1,1	0.00	-
7	NAG	B	813	1	14,14,15	0.88	0	17,19,21	2.25	4 (23%)

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	B	812	1	-	2/6/23/26	0/1/1/1
6	IMD	A	814	-	-	-	0/1/1/1
7	NAG	A	813	1	-	3/6/23/26	0/1/1/1
6	IMD	B	805	-	-	-	0/1/1/1
6	IMD	B	806	-	-	-	0/1/1/1
6	IMD	A	806	-	-	-	0/1/1/1
6	IMD	B	814	-	-	-	0/1/1/1
7	NAG	A	812	1	-	2/6/23/26	0/1/1/1
6	IMD	A	805	-	-	-	0/1/1/1
7	NAG	B	813	1	-	1/6/23/26	0/1/1/1
6	IMD	A	804	-	-	-	0/1/1/1
6	IMD	B	804	-	-	-	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	812	NAG	C7-N2	4.96	1.51	1.34
7	A	813	NAG	C7-N2	4.75	1.50	1.34
7	A	813	NAG	O5-C5	4.09	1.51	1.43
7	B	812	NAG	O5-C5	3.52	1.50	1.43
7	A	813	NAG	C4-C3	-2.93	1.44	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	813	NAG	C1-O5-C5	8.37	123.53	112.19
7	A	812	NAG	O5-C1-C2	-6.72	100.68	111.29
7	B	812	NAG	C8-C7-N2	6.27	126.72	116.10
7	A	812	NAG	C1-O5-C5	6.04	120.38	112.19
7	B	813	NAG	C1-O5-C5	5.91	120.19	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	813	NAG	C8-C7-N2-C2
7	B	812	NAG	C8-C7-N2-C2
7	A	813	NAG	O7-C7-N2-C2
7	A	812	NAG	O5-C5-C6-O6
7	A	812	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	812	NAG	2	0
7	A	813	NAG	3	0
6	B	806	IMD	3	0
6	B	814	IMD	1	0
6	A	805	IMD	1	0
8	A	815	FMT	3	0
6	A	804	IMD	5	0
6	B	804	IMD	1	0
8	A	816	FMT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	553:TRP	C	554:SER	N	1.08
1	A	470:ASN	C	471:TPQ	N	1.04
1	B	552:PRO	C	553:TRP	N	0.88

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	704/763 (92%)	-0.90	4 (0%) 89 88	18, 33, 56, 101	0
1	B	700/763 (91%)	-0.86	7 (1%) 82 80	17, 35, 60, 104	0
All	All	1404/1526 (92%)	-0.88	11 (0%) 86 84	17, 34, 58, 104	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	57	SER	4.0
1	A	762	HIS	3.6
1	B	205	GLY	3.1
1	B	762	HIS	3.0
1	B	735	GLU	2.6

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.

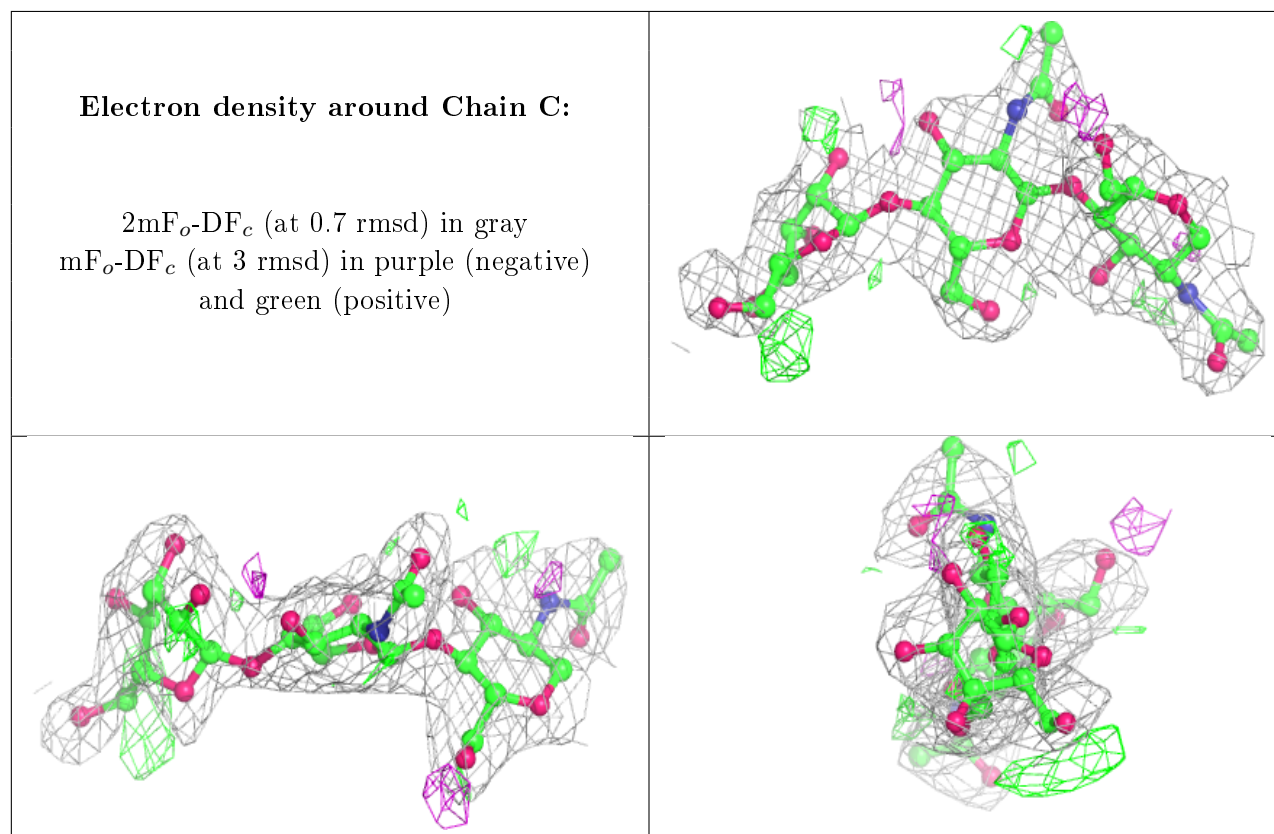
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPQ	A	471	14/15	0.97	0.09	26,39,44,46	0
1	TPQ	B	471	14/15	0.98	0.09	27,35,43,45	0

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.

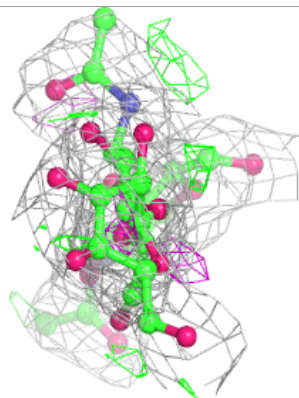
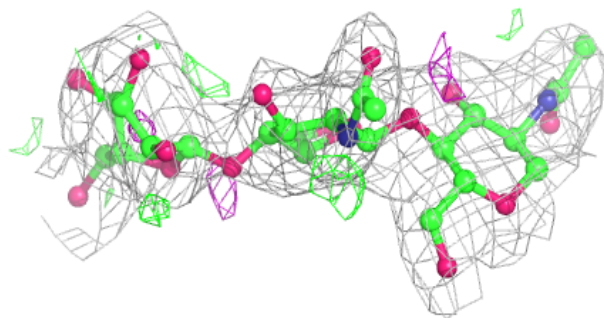
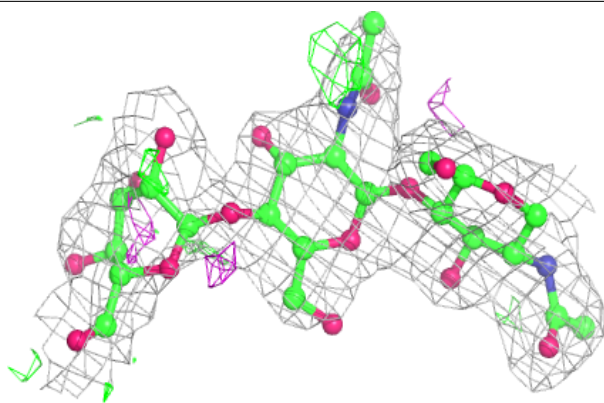
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MAN	E	3	11/12	0.74	0.34	59,84,97,102	0
2	MAN	C	3	11/12	0.81	0.34	80,96,105,111	0
3	NAG	D	2	14/15	0.86	0.41	67,92,102,109	0
3	NAG	F	2	14/15	0.86	0.43	66,96,105,105	0
2	NAG	E	2	14/15	0.87	0.20	48,72,82,88	0
2	NAG	C	2	14/15	0.92	0.18	48,65,76,93	0
3	NAG	D	1	14/15	0.93	0.21	59,74,83,87	0
3	NAG	F	1	14/15	0.93	0.23	57,68,81,92	0
2	NAG	C	1	14/15	0.96	0.11	32,38,47,53	0
2	NAG	E	1	14/15	0.96	0.08	35,44,56,61	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.



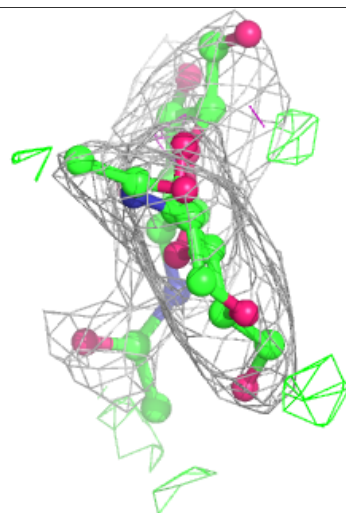
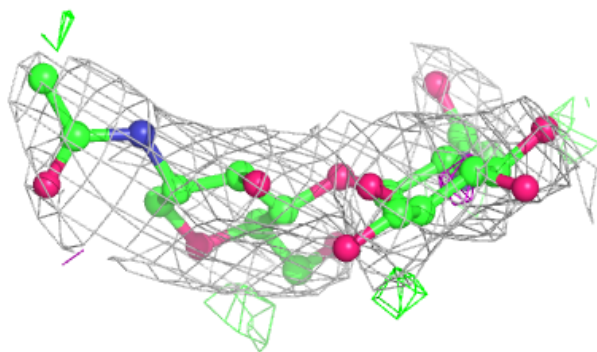
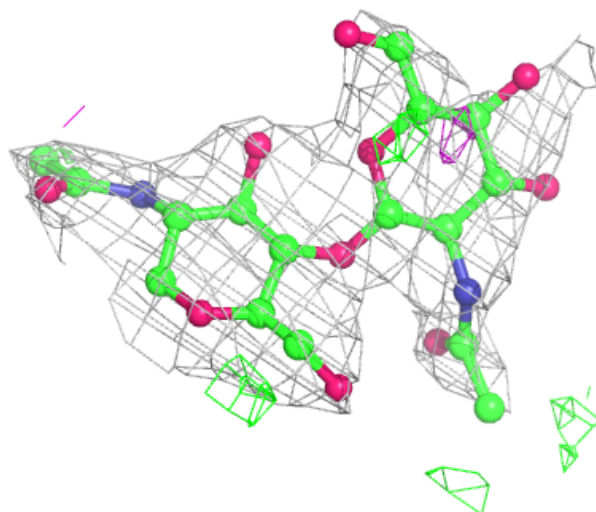
Electron density around Chain E:

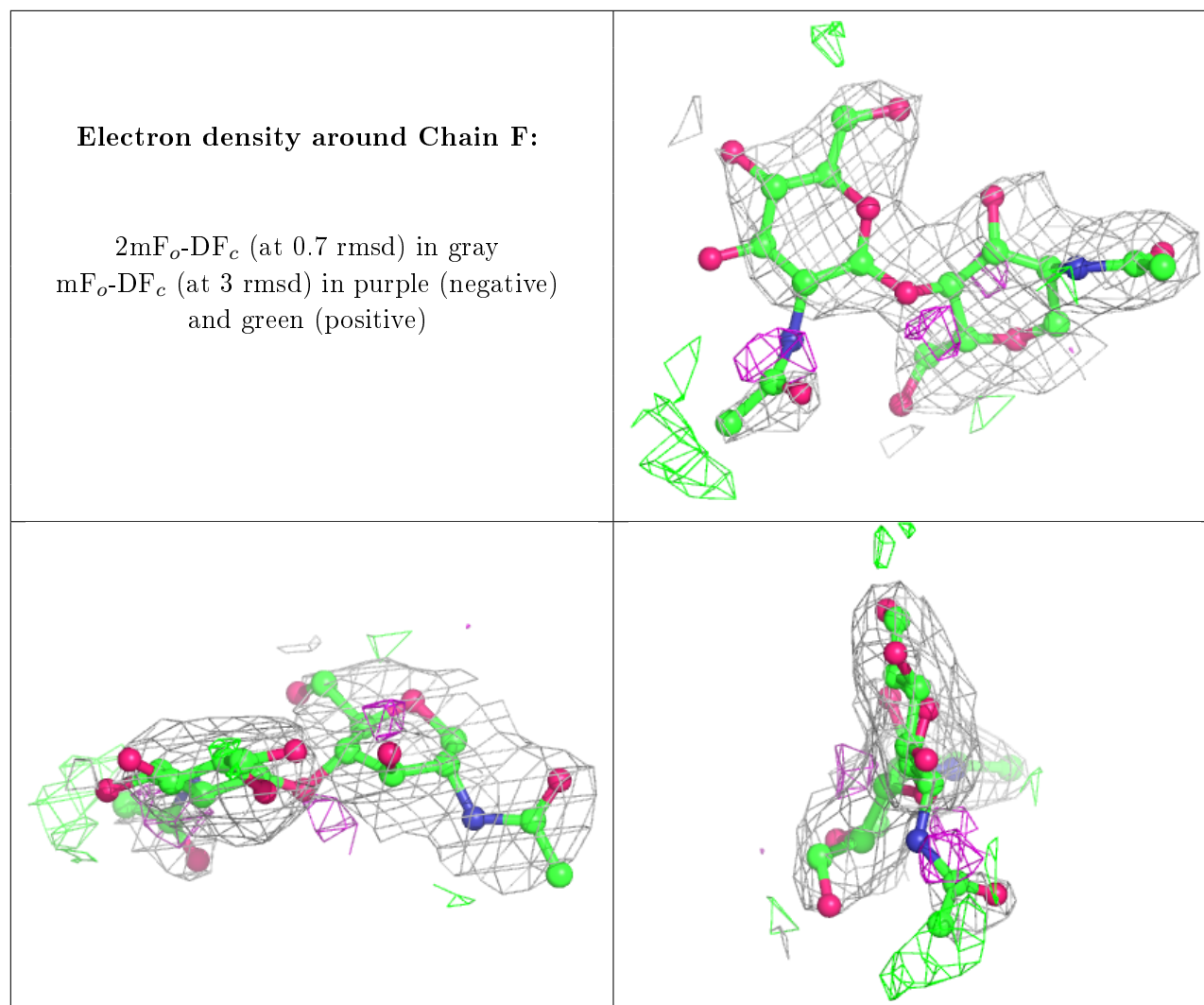
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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 ⓘ

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
7	NAG	B	813	14/15	0.76	0.43	77,78,78,79	0
7	NAG	B	812	14/15	0.77	0.34	52,85,100,105	0
7	NAG	A	813	14/15	0.79	0.42	72,88,95,98	0
7	NAG	A	812	14/15	0.87	0.32	77,78,78,79	0
6	IMD	B	805	5/5	0.94	0.22	49,55,60,66	0
8	FMT	A	816	3/3	0.95	0.14	38,38,43,50	0
6	IMD	A	814	5/5	0.97	0.16	58,60,66,69	0
6	IMD	A	804	5/5	0.98	0.10	49,52,55,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	IMD	A	806	5/5	0.98	0.10	23,27,32,33	0
8	FMT	A	815	3/3	0.99	0.07	34,34,35,39	0
6	IMD	B	806	5/5	0.99	0.08	43,43,48,48	0
5	CA	B	803	1/1	0.99	0.06	32,32,32,32	0
5	CA	B	802	1/1	0.99	0.09	29,29,29,29	0
6	IMD	B	804	5/5	0.99	0.11	24,24,28,28	0
6	IMD	B	814	5/5	0.99	0.07	30,32,32,34	0
5	CA	A	802	1/1	1.00	0.08	24,24,24,24	0
6	IMD	A	805	5/5	1.00	0.13	20,22,26,26	0
5	CA	A	803	1/1	1.00	0.05	29,29,29,29	0
4	CU	B	801	1/1	1.00	0.07	29,29,29,29	0
4	CU	A	801	1/1	1.00	0.06	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.