



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2022 – 01:02 pm GMT

PDB ID : 6FCS
Title : The X-ray Structure of Lytic Transglycosylase Slt inactive mutant E503Q from *Pseudomonas aeruginosa* in complex with NAG-NAMpentapeptide-NAG-NAMpentapeptide
Authors : Batuecas, M.T.; Dominguez-Gil, T.; Hermoso, J.A.
Deposited on : 2017-12-21
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

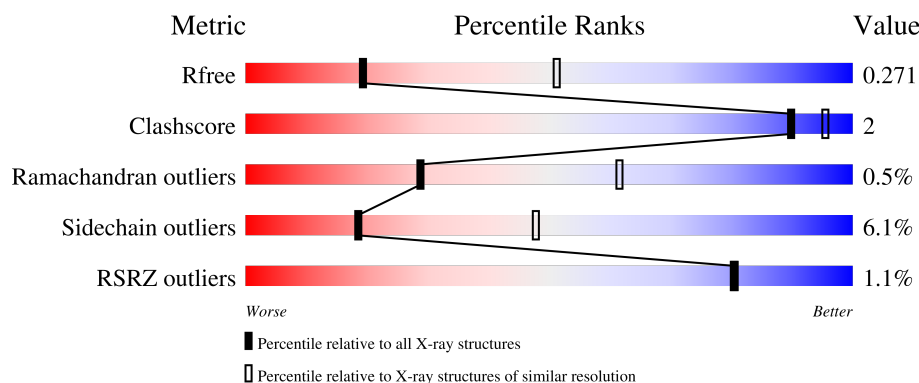
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	613	 91% 8%
2	B	5	 80% 20%
3	C	4	 100%
4	D	4	 50% 50%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5210 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 Soluble lytic murein transglycosylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	613	Total	C	N	O	S	0	1	0
			4977	3157	914	895	11			

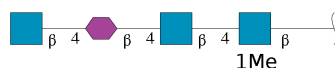
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	503	GLN	GLU	engineered mutation	UNP A0A069QJX4

- Molecule 2 is a protein (with D amino acids) called ALA-DGL-API-DAL-DAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	5	Total	C	N	O	0	0	0
			36	21	6	9			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-methyl 2-acetamido-2-deoxy-beta-D-glucopyranoside.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	4	Total	C	N	O	0	0	0
			62	36	4	22			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-3-O-[(2R)-1-amino-1-oxopropan-2-yl]-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-methyl 2-acetamido-3-O-[(1R)-1-carboxyethyl]-2-deoxy-beta-D-glucopyranoside.

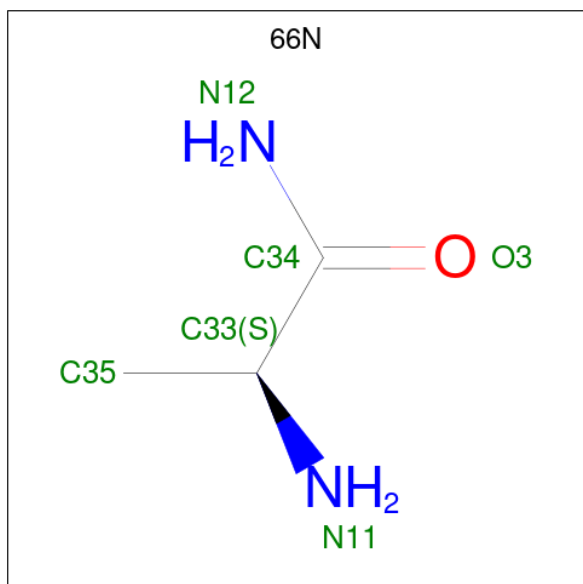
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	4	Total	C	N	O	0	0	0
			67	39	5	23			

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is L-alaninamide (three-letter code: 66N) (formula: $C_3H_8N_2O$).



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

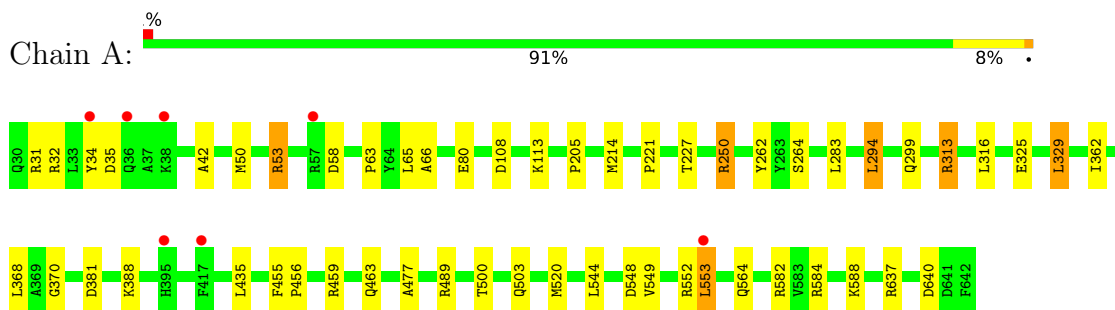
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	53	Total	O	0	0
			53	53		
7	B	1	Total	O	0	0
			1	1		

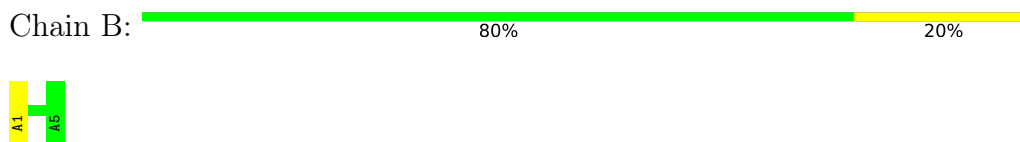
3 Residue-property plots

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.

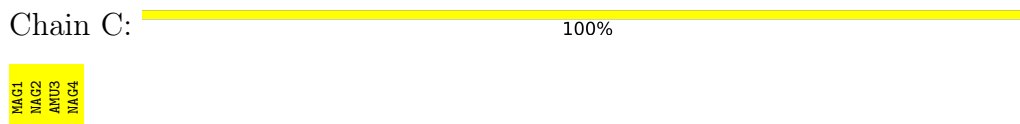
- Molecule 1: Soluble lytic murein transglycosylase



- Molecule 2: ALA-DGL-API-DAL-DAL



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-beta-muramic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-methyl 2-acetamido-2-deoxy-beta-D-glucopyranoside



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-3-O-[(2R)-1-amino-1-oxopropan-2-yl]-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-methyl 2-acetamido-3-O-[(1R)-1-carboxyethyl]-2-deoxy-beta-D-glucopyranoside



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	166.87Å 166.87Å 54.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	144.52 – 2.90 48.17 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (144.52-2.90) 100.0 (48.17-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.193 , 0.269 0.201 , 0.271	Depositor DCC
R_{free} test set	972 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	70.2	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5210	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: ACT, NM6, 66N, AMV, API, NAG, AMU, DAL, MAG, DGL

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	0.41	0/5104	0.70	0/6920
2	B	1.04	0/4	1.09	0/4
All	All	0.42	0/5108	0.70	0/6924

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4977	0	4909	17	0
2	B	36	0	32	1	0
3	C	62	0	56	0	0
4	D	67	0	50	2	0
5	A	8	0	6	0	0
6	A	6	0	0	0	0
7	A	53	0	0	4	2
7	B	1	0	0	0	0
All	All	5210	0	5053	18	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 2.

All (18) 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:66:ALA:N	7:A:801:HOH:O	2.06	0.89
1:A:63:PRO:C	7:A:801:HOH:O	2.23	0.75
1:A:294:LEU:HD13	1:A:316:LEU:HD23	1.79	0.64
1:A:500:THR:HG22	1:A:520:MET:HG2	1.83	0.61
1:A:313:ARG:HG2	1:A:329:LEU:HD11	1.82	0.59
1:A:503:GLN:NE2	4:D:1:AMV:O6	2.42	0.53
1:A:500:THR:HG22	1:A:520:MET:CG	2.39	0.52
1:A:50:MET:SD	1:A:53:ARG:NH1	2.85	0.50
1:A:370:GLY:HA2	1:A:388:LYS:HD2	1.97	0.46
1:A:564:GLN:HE21	1:A:584:ARG:NH2	2.14	0.45
1:A:549:VAL:O	1:A:553:LEU:HD23	2.16	0.45
1:A:582:ARG:NH1	2:B:1:ALA:O	2.51	0.43
1:A:65:LEU:N	7:A:801:HOH:O	2.51	0.43
4:D:1:AMV:H112	4:D:2:NAG:H62	2.01	0.42
1:A:250:ARG:NH2	7:A:804:HOH:O	2.51	0.42
1:A:455:PHE:HB3	1:A:456:PRO:HD3	2.02	0.41
1:A:227:THR:HB	1:A:262:TYR:CE2	2.55	0.41
1:A:381:ASP:OD2	1:A:637:ARG:NH2	2.54	0.41

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)
7:A:824:HOH:O	7:A:842:HOH:O[6_655]	1.17	1.03
7:A:805:HOH:O	7:A:828:HOH:O[6_654]	1.91	0.29

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	612/613 (100%)	594 (97%)	15 (2%)	3 (0%)	29 61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ALA
1	A	477	ALA
1	A	205	PRO

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	508/507 (100%)	477 (94%)	31 (6%)	18 48

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	A	32	ARG
1	A	34	TYR
1	A	35	ASP
1	A	53	ARG
1	A	58	ASP
1	A	80	GLU
1	A	108	ASP
1	A	113	LYS
1	A	214	MET
1	A	221	PRO
1	A	250	ARG
1	A	264	SER
1	A	283	LEU
1	A	294	LEU
1	A	299	GLN
1	A	313	ARG
1	A	325	GLU

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Mol	Chain	Res	Type
1	A	329	LEU
1	A	362	ILE
1	A	368	LEU
1	A	435	LEU
1	A	459	ARG
1	A	463	GLN
1	A	489	ARG
1	A	544	LEU
1	A	548	ASP
1	A	552	ARG
1	A	553	LEU
1	A	588	LYS
1	A	640	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	GLN
1	A	503	GLN
1	A	564	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	$\# Z > 2$
2	API	B	3	2	6,11,12	0.76	0	2,13,15	1.28	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
2	API	B	3	2	-	3/7/12/14	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	API	C1-C2-C3-C4
2	B	3	API	N2-C2-C3-C4
2	B	3	API	C3-C4-C5-C6

There are no ring outliers.

No monomer is involved in short contacts.

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
3	MAG	C	1	3	16,16,16	1.88	5 (31%)	22,22,22	2.25	6 (27%)
3	NAG	C	2	3	14,14,15	1.18	2 (14%)	17,19,21	1.44	3 (17%)
3	AMU	C	3	3,6	17,18,20	1.03	2 (11%)	21,24,28	2.13	8 (38%)
3	NAG	C	4	3	14,14,15	0.83	0	17,19,21	1.57	3 (17%)
4	AMV	D	1	2,4	19,20,21	1.54	2 (10%)	22,27,29	1.73	6 (27%)
4	NAG	D	2	4	14,14,15	1.14	2 (14%)	17,19,21	1.46	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NM6	D	3	4	19,19,20	1.70	2 (10%)	22,26,28	1.86	6 (27%)
4	NAG	D	4	4	14,14,15	0.72	0	17,19,21	1.17	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
3	MAG	C	1	3	-	4/8/28/28	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	AMU	C	3	3,6	-	2/10/29/34	0/1/1/1
3	NAG	C	4	3	-	3/6/23/26	0/1/1/1
4	AMV	D	1	2,4	-	2/12/34/36	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NM6	D	3	4	-	1/14/31/34	0/1/1/1
4	NAG	D	4	4	-	2/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3	NM6	C3C-N3A	5.88	1.47	1.32
3	C	1	MAG	C7-N2	4.35	1.49	1.34
4	D	1	AMV	C7-N2	4.06	1.48	1.34
3	C	2	NAG	C1-C2	3.21	1.57	1.52
3	C	1	MAG	O1-C1	2.92	1.45	1.40
3	C	1	MAG	C2-N2	2.82	1.50	1.45
4	D	2	NAG	C1-C2	2.76	1.56	1.52
4	D	2	NAG	O5-C1	-2.60	1.39	1.43
4	D	1	AMV	O1-C1	2.46	1.44	1.40
4	D	3	NM6	C4-C5	2.34	1.58	1.53
3	C	1	MAG	C1-C2	2.27	1.56	1.53
3	C	3	AMU	C11-C9	2.22	1.56	1.51
3	C	1	MAG	O5-C1	2.12	1.47	1.41
3	C	2	NAG	O5-C1	-2.07	1.40	1.43
3	C	3	AMU	C4-C5	2.01	1.57	1.53

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	MAG	C1-O5-C5	7.57	128.54	113.69
3	C	3	AMU	O5-C1-C2	-4.69	103.88	111.29
4	D	3	NM6	O3-C3-C2	4.39	119.14	108.85
3	C	4	NAG	C4-C3-C2	3.94	116.79	111.02
4	D	1	AMV	C3-C2-N2	3.82	117.26	110.91
4	D	3	NM6	O5-C1-C2	-3.54	105.70	111.29
4	D	1	AMV	O1-C1-C2	3.46	113.44	108.14
3	C	3	AMU	O3-C3-C4	3.39	116.29	107.28
3	C	2	NAG	O5-C1-C2	-3.37	105.97	111.29
3	C	3	AMU	C2-N2-C7	3.34	127.66	122.90
3	C	4	NAG	C2-N2-C7	3.25	127.53	122.90
3	C	1	MAG	C1-C2-N2	3.07	116.29	111.00
3	C	3	AMU	C3-C2-N2	2.90	115.95	110.58
4	D	4	NAG	C2-N2-C7	2.89	127.02	122.90
4	D	2	NAG	O5-C5-C4	-2.88	103.83	110.83
4	D	3	NM6	C1-C2-C3	-2.79	105.19	109.17
4	D	1	AMV	O5-C5-C6	2.73	113.23	106.44
4	D	1	AMV	O5-C1-C2	-2.63	105.44	110.58
3	C	3	AMU	O4-C4-C5	-2.61	102.80	109.30
3	C	1	MAG	CM-O1-C1	2.61	117.30	113.27
4	D	1	AMV	C2-N2-C7	-2.43	117.26	123.18
4	D	4	NAG	C1-O5-C5	2.39	115.43	112.19
3	C	1	MAG	O3-C3-C2	-2.38	104.86	109.66
3	C	1	MAG	O5-C5-C6	2.35	112.29	106.44
4	D	3	NM6	O3-C3-C4	2.33	113.49	107.28
3	C	1	MAG	O7-C7-C8	-2.33	117.72	122.06
3	C	3	AMU	C4-C3-C2	2.31	115.21	111.18
3	C	2	NAG	C1-O5-C5	2.28	115.29	112.19
3	C	2	NAG	O3-C3-C2	-2.28	104.75	109.47
3	C	3	AMU	C6-C5-C4	2.12	117.98	113.00
4	D	2	NAG	O7-C7-C8	-2.12	118.12	122.06
3	C	3	AMU	C1-O5-C5	-2.12	109.33	112.19
4	D	2	NAG	C1-O5-C5	2.11	115.06	112.19
4	D	2	NAG	C2-N2-C7	2.10	125.89	122.90
4	D	3	NM6	O3B-C3C-N3A	-2.06	119.42	123.00
4	D	3	NM6	O4-C4-C5	2.05	114.39	109.30
3	C	4	NAG	O7-C7-C8	-2.03	118.29	122.06
4	D	1	AMV	O5-C1-O1	2.03	115.67	110.97

There are no chirality outliers.

All (16) torsion outliers are listed below:

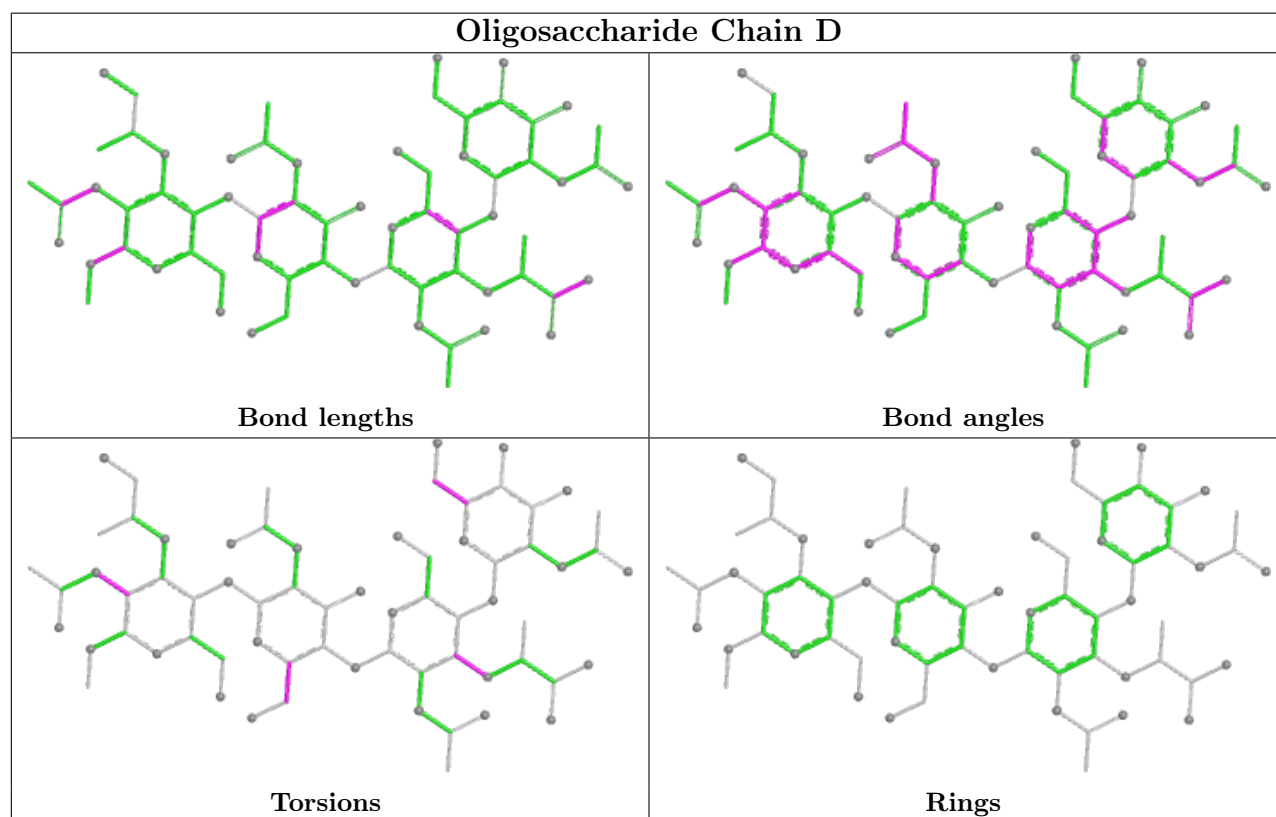
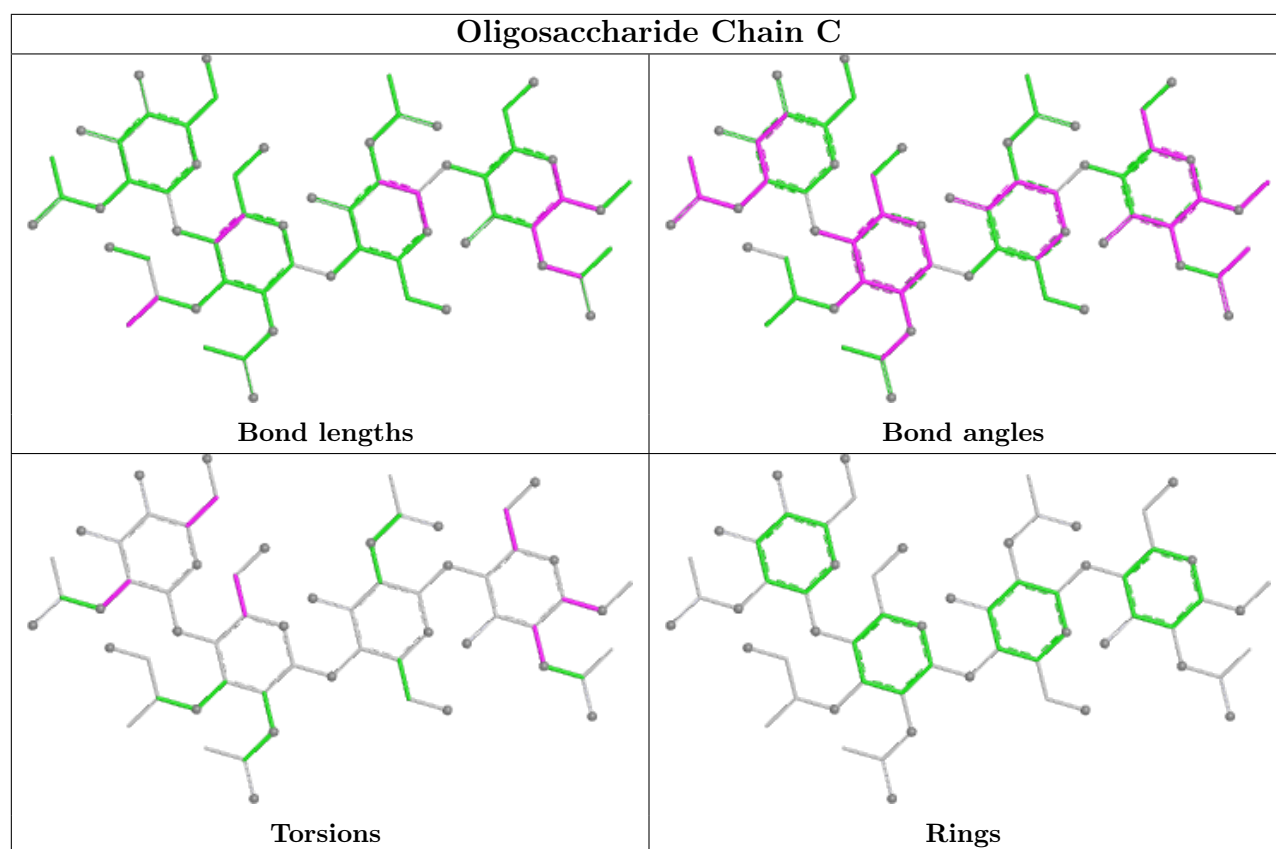
Mol	Chain	Res	Type	Atoms
3	C	1	MAG	O5-C1-O1-CM
4	D	3	NM6	C2-C3-O3-C3A
4	D	2	NAG	C4-C5-C6-O6
3	C	3	AMU	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
3	C	4	NAG	C4-C5-C6-O6
3	C	4	NAG	O5-C5-C6-O6
3	C	3	AMU	O5-C5-C6-O6
4	D	4	NAG	O5-C5-C6-O6
3	C	1	MAG	O5-C5-C6-O6
4	D	4	NAG	C4-C5-C6-O6
4	D	1	AMV	C3-C2-N2-C7
3	C	4	NAG	C3-C2-N2-C7
3	C	1	MAG	C3-C2-N2-C7
3	C	1	MAG	C1-C2-N2-C7
4	D	1	AMV	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	AMV	2	0
4	D	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

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	ACT	A	701	-	1,3,3	1.19	0	0,3,3	-	-
5	ACT	A	702	-	1,3,3	1.64	0	0,3,3	-	-
6	66N	A	707	3	5,5,5	2.61	1 (20%)	6,6,6	1.17	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	66N	A	707	3	-	0/3/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	707	66N	C34-N12	5.61	1.47	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	707	66N	O3-C34-N12	-2.66	118.37	123.00

There are no chirality outliers.

There are no torsion outliers.

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 [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	613/613 (100%)	0.10	7 (1%) 80 80	50, 74, 102, 121	0
2	B	1/5 (20%)	-0.11	0 100 100	81, 81, 81, 81	0
All	All	614/618 (99%)	0.09	7 (1%) 80 80	50, 74, 102, 121	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	GLN	3.3
1	A	553	LEU	3.3
1	A	395	HIS	3.2
1	A	38	LYS	2.9
1	A	417	PHE	2.7
1	A	34	TYR	2.7
1	A	57	ARG	2.3

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.

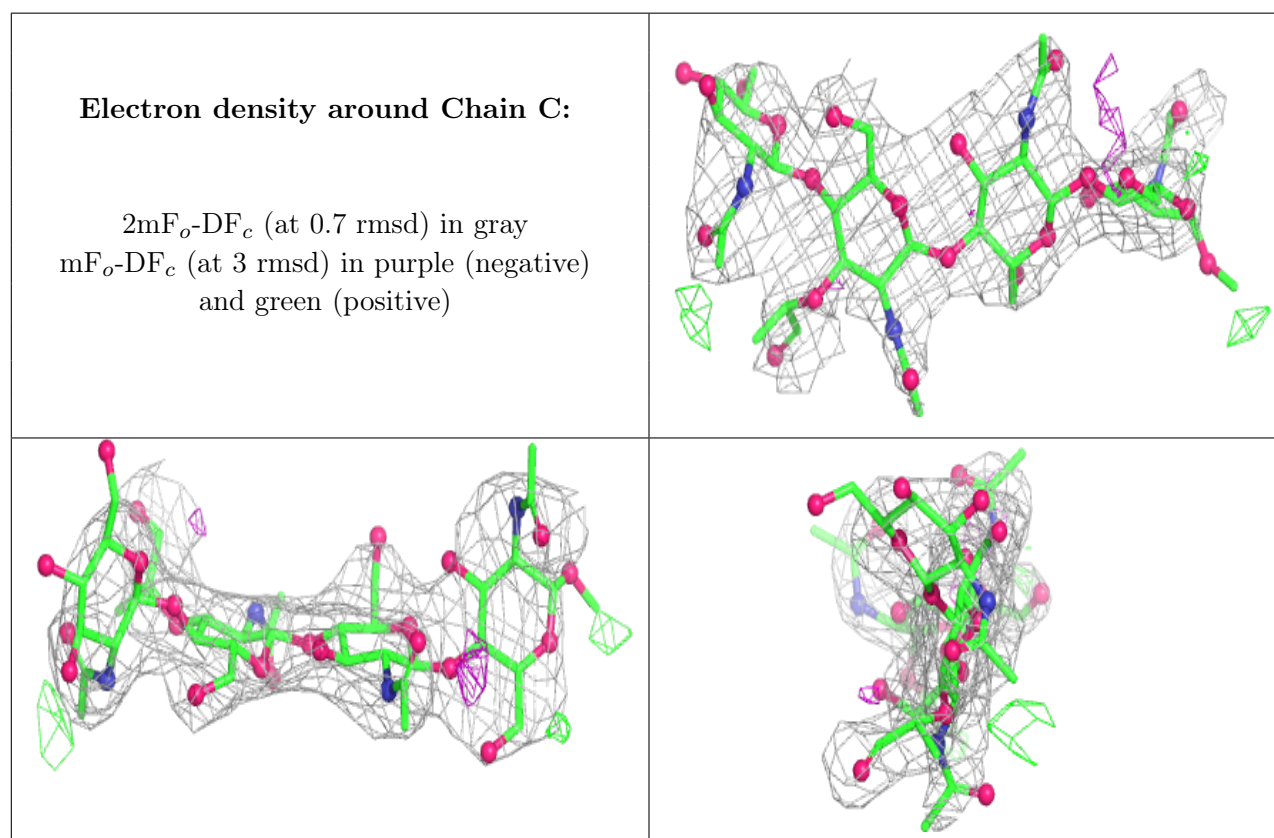
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DAL	B	5	6/6	0.78	0.39	118,122,122,123	0
2	API	B	3	12/13	0.83	0.30	104,106,110,112	0
2	DAL	B	4	5/6	0.84	0.39	118,122,125,127	0
2	DGL	B	2	8/10	0.85	0.25	90,100,102,104	0

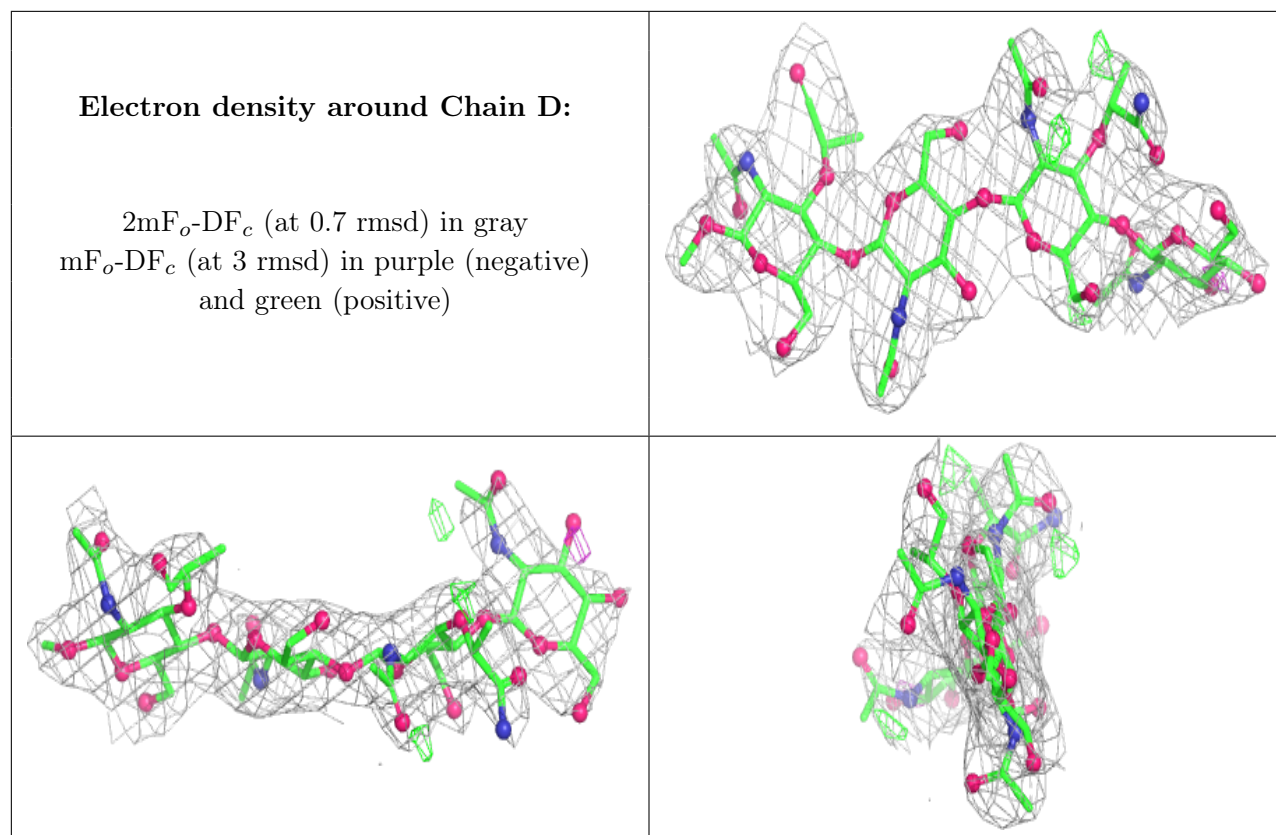
6.3 Carbohydrates [i](#)

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
3	MAG	C	1	16/16	0.80	0.32	104,119,124,124	0
3	AMU	C	3	18/20	0.85	0.28	97,115,123,125	0
3	NAG	C	2	14/15	0.86	0.27	98,110,116,117	0
3	NAG	C	4	14/15	0.86	0.21	107,119,123,127	0
4	NAG	D	4	14/15	0.88	0.27	88,100,108,108	0
4	NM6	D	3	19/20	0.94	0.16	76,81,89,89	0
4	AMV	D	1	20/21	0.95	0.18	67,72,79,79	0
4	NAG	D	2	14/15	0.95	0.21	63,65,70,74	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
6	66N	A	707	6/6	0.72	0.36	104,106,109,113	0
5	ACT	A	702	4/4	0.76	0.39	88,89,92,92	0
5	ACT	A	701	4/4	0.84	0.17	79,82,82,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.