



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 03:16 PM EDT

PDB ID : 1FV3
Title : THE HC FRAGMENT OF TETANUS TOXIN COMPLEXED WITH AN ANALOGUE OF ITS GANGLIOSIDE RECEPTOR GT1B
Authors : Fotinou, C.; Emsley, P.; Black, I.; Ando, H.; Ishida, H.; Kiso, M.; Sinha, K.A.; Fairweather, N.F.; Isaacs, N.W.
Deposited on : 2000-09-18
Resolution : 2.30 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 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

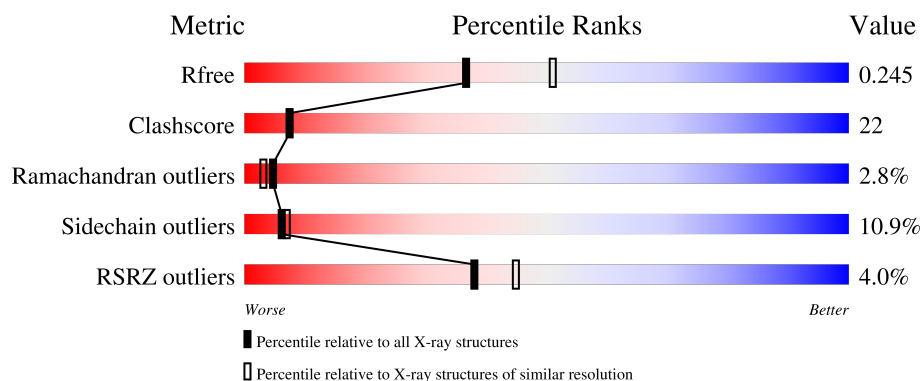
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	472	<div> <div>5%</div> <div> <div></div> <div>49%</div> <div>38%</div> <div>7%</div> <div>• •</div> </div> </div>
1	B	472	<div> <div>3%</div> <div> <div></div> <div>61%</div> <div>28%</div> <div>6%</div> <div>• •</div> </div> </div>
2	C	7	<div> <div>29%</div> <div>71%</div> </div>
2	D	7	<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
3	CEQ	A	8[A]	-	X	-	-
3	CEQ	B	8[A]	-	X	-	X
3	CEQ	B	8[B]	-	-	-	X
4	PO4	B	301	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7786 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 TETANUS TOXIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	1	0
			3652	2336	612	694	10			
1	B	451	Total	C	N	O	S	0	0	0
			3648	2334	611	693	10			

There are 42 discrepancies between the modelled and reference sequences:

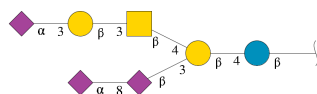
Chain	Residue	Modelled	Actual	Comment	Reference
A	844	MET	-	SEE REMARK 999	? P04958
A	845	GLY	-	SEE REMARK 999	? P04958
A	846	SER	-	SEE REMARK 999	? P04958
A	847	SER	-	SEE REMARK 999	? P04958
A	848	HIS	-	SEE REMARK 999	? P04958
A	849	HIS	-	SEE REMARK 999	? P04958
A	850	HIS	-	SEE REMARK 999	? P04958
A	851	HIS	-	SEE REMARK 999	? P04958
A	852	HIS	-	SEE REMARK 999	? P04958
A	853	HIS	-	SEE REMARK 999	? P04958
A	854	SER	-	SEE REMARK 999	? P04958
A	855	SER	-	SEE REMARK 999	? P04958
A	856	GLY	-	SEE REMARK 999	? P04958
A	857	LEU	-	SEE REMARK 999	? P04958
A	858	VAL	-	SEE REMARK 999	? P04958
A	859	PRO	-	SEE REMARK 999	? P04958
A	860	ARG	-	SEE REMARK 999	? P04958
A	861	GLY	-	SEE REMARK 999	? P04958
A	862	SER	-	SEE REMARK 999	? P04958
A	863	HIS	-	SEE REMARK 999	? P04958
A	864	MET	-	SEE REMARK 999	? P04958
B	844	MET	-	SEE REMARK 999	? P04958
B	845	GLY	-	SEE REMARK 999	? P04958
B	846	SER	-	SEE REMARK 999	? P04958
B	847	SER	-	SEE REMARK 999	? P04958

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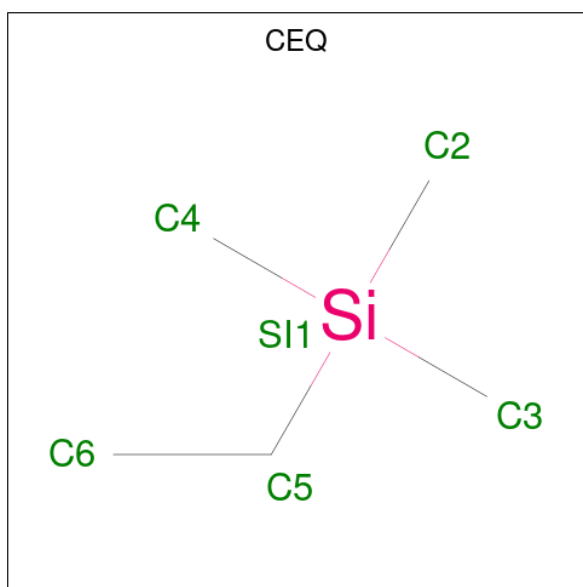
Chain	Residue	Modelled	Actual	Comment	Reference
B	848	HIS	-	SEE REMARK 999	? P04958
B	849	HIS	-	SEE REMARK 999	? P04958
B	850	HIS	-	SEE REMARK 999	? P04958
B	851	HIS	-	SEE REMARK 999	? P04958
B	852	HIS	-	SEE REMARK 999	? P04958
B	853	HIS	-	SEE REMARK 999	? P04958
B	854	SER	-	SEE REMARK 999	? P04958
B	855	SER	-	SEE REMARK 999	? P04958
B	856	GLY	-	SEE REMARK 999	? P04958
B	857	LEU	-	SEE REMARK 999	? P04958
B	858	VAL	-	SEE REMARK 999	? P04958
B	859	PRO	-	SEE REMARK 999	? P04958
B	860	ARG	-	SEE REMARK 999	? P04958
B	861	GLY	-	SEE REMARK 999	? P04958
B	862	SER	-	SEE REMARK 999	? P04958
B	863	HIS	-	SEE REMARK 999	? P04958
B	864	MET	-	SEE REMARK 999	? P04958

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-beta-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



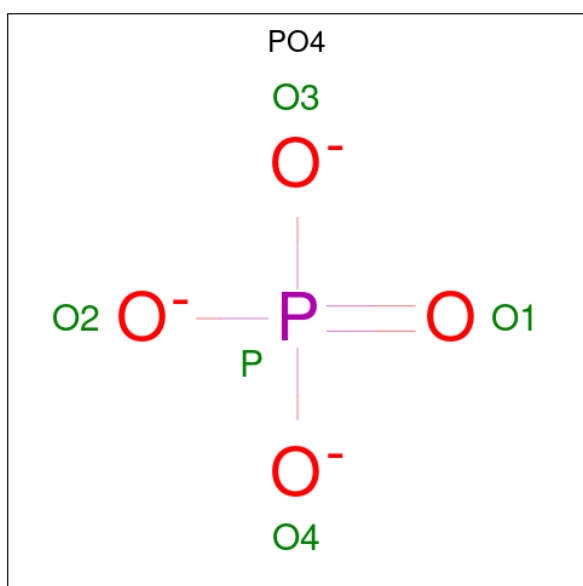
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	0	0	0
			108	59	4	45			
2	D	7	Total	C	N	O	0	0	0
			108	59	4	45			

- Molecule 3 is ETHYL-TRIMETHYL-SILANE (three-letter code: CEQ) (formula: C₅H₁₄Si).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	Si	0	1
			12	10	2		
3	B	1	Total	C	Si	0	1
			12	10	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		

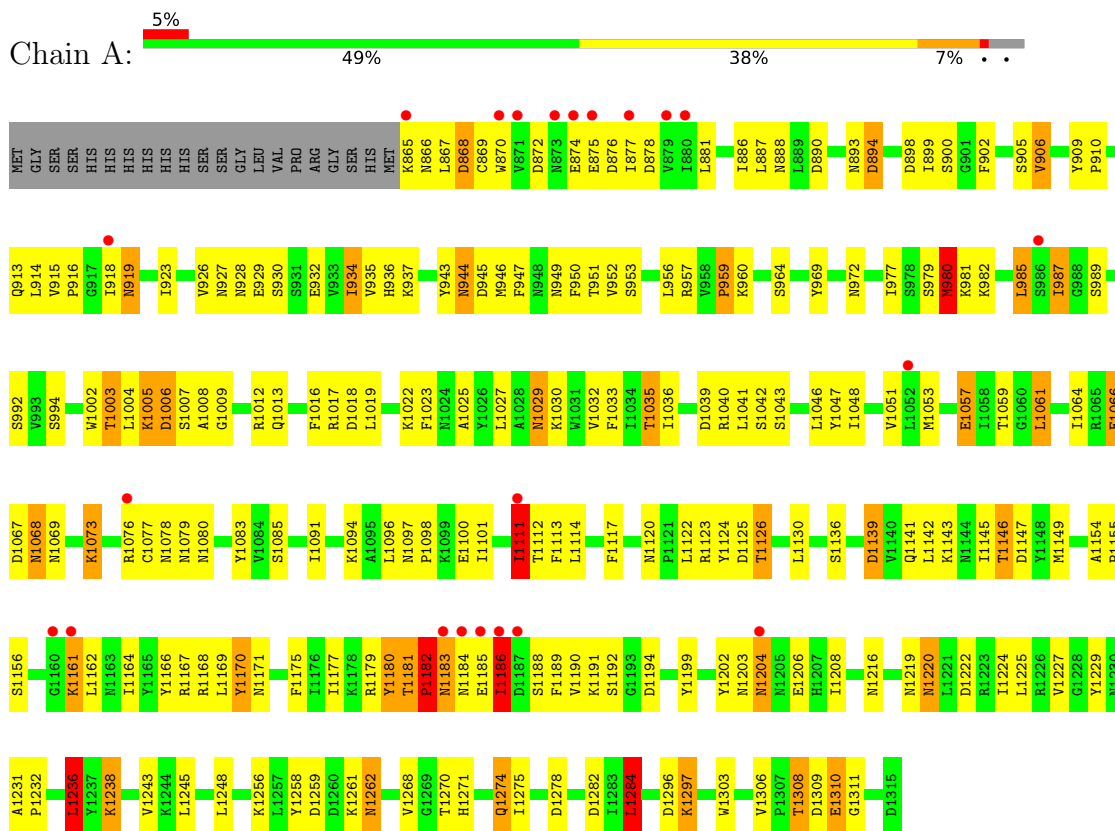
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	87	Total 87	O 87	0	0
5	B	154	Total 154	O 154	0	0

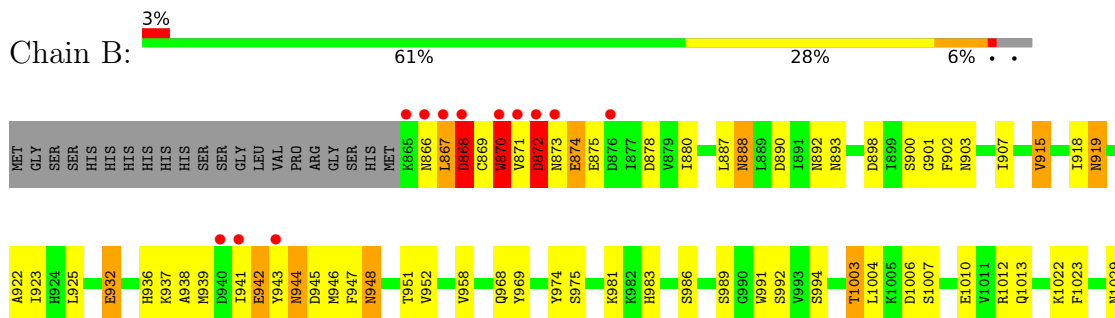
3 Residue-property plots [i](#)

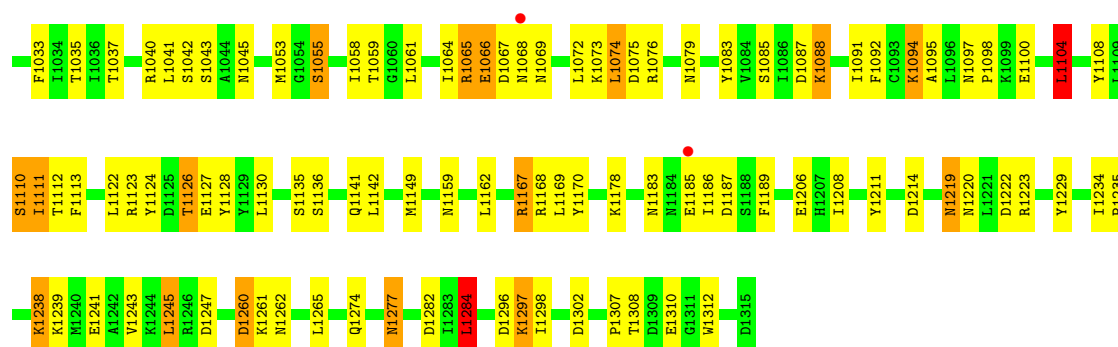
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: TETANUS TOXIN HEAVY CHAIN



• Molecule 1: TETANUS TOXIN HEAVY CHAIN





- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-beta-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain C: 29% 71%

BGC1
GAL2
GAL3
GAL4
SIA5
SLB6
SLA7

- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-beta-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain D: 100%

BGC1
GAL2
GAL3
GAL4
SIA5
SLB6
SLA7

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.31Å 53.07Å 118.28Å 90.00° 89.78° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.3 (30.00-2.30) 96.5 (29.93-2.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.237 , 0.306 0.228 , 0.245	Depositor DCC
R_{free} test set	1543 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å ²)	13.5	Xtriage
Anisotropy	0.848	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.13$	Xtriage
Estimated twinning fraction	0.220 for h,-k,-l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	7786	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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: NGA, SIA, SLB, CEQ, BGC, GAL, PO4

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	0/3740	1.07	20/5076 (0.4%)
1	B	0.94	1/3731 (0.0%)	1.13	19/5064 (0.4%)
All	All	0.85	1/7471 (0.0%)	1.10	39/10140 (0.4%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1229	TYR	CD2-CE2	-5.04	1.31	1.39

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1075	ASP	CB-CG-OD2	9.21	126.59	118.30
1	B	1222	ASP	CB-CG-OD2	8.71	126.14	118.30
1	B	1087	ASP	CB-CG-OD2	7.70	125.23	118.30
1	B	1104	LEU	CB-CG-CD1	-7.20	98.77	111.00
1	B	1282	ASP	CB-CG-OD2	6.92	124.53	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1182	PRO	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	3652	0	3592	170	0
1	B	3648	0	3588	150	1
2	C	108	0	88	8	0
2	D	108	0	88	7	0
3	A	12	0	0	0	0
3	B	12	0	0	0	0
4	B	5	0	0	2	0
5	A	87	0	0	4	0
5	B	154	0	0	2	0
All	All	7786	0	7356	331	1

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 22.

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:1145:ILE:H	1:A:1145:ILE:HD12	1.14	1.07
1:A:985:LEU:HD22	1:A:985:LEU:O	1.54	1.06
1:B:1064:ILE:HG22	1:B:1064:ILE:O	1.68	0.93
1:B:1111:ILE:HD12	1:B:1112:THR:H	1.33	0.92
1:B:1124:TYR:O	1:B:1126:THR:HG22	1.72	0.88

All (1) 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:B:873:ASN:O	1:B:1127:GLU:OE1[1_565]	2.17	0.03

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	450/472 (95%)	399 (89%)	38 (8%)	13 (3%)	4	3
1	B	449/472 (95%)	396 (88%)	41 (9%)	12 (3%)	5	3
All	All	899/944 (95%)	795 (88%)	79 (9%)	25 (3%)	5	3

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	929	GLU
1	A	1025	ALA
1	A	1182	PRO
1	B	870	TRP
1	B	1066	GLU

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	408/425 (96%)	350 (86%)	58 (14%)	3	3
1	B	407/425 (96%)	375 (92%)	32 (8%)	12	15
All	All	815/850 (96%)	725 (89%)	90 (11%)	6	7

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1310	GLU

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Mol	Chain	Res	Type
1	B	1059	THR
1	B	867	LEU
1	B	944	ASN
1	B	1088	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1068	ASN
1	B	1216	ASN
1	B	1293	HIS
1	B	1220	ASN
1	B	1078	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

14 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	BGC	C	1	3,2	12,12,12	1.65	1 (8%)	17,17,17	3.06	5 (29%)
2	GAL	C	2	2	11,11,12	1.87	2 (18%)	15,15,17	3.04	6 (40%)
2	NGA	C	3	2	14,14,15	1.25	1 (7%)	17,19,21	1.68	4 (23%)
2	GAL	C	4	2	11,11,12	0.79	0	15,15,17	1.52	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SIA	C	5	2	20,20,21	5.39	3 (15%)	24,28,31	2.26	6 (25%)
2	SLB	C	6	2	20,20,21	1.52	2 (10%)	24,28,31	2.30	10 (41%)
2	SIA	C	7	2	20,20,21	4.35	1 (5%)	24,28,31	2.21	5 (20%)
2	BGC	D	1	3,2	12,12,12	1.47	1 (8%)	17,17,17	2.19	4 (23%)
2	GAL	D	2	2	11,11,12	1.83	2 (18%)	15,15,17	4.41	5 (33%)
2	NGA	D	3	2	14,14,15	1.30	1 (7%)	17,19,21	2.02	5 (29%)
2	GAL	D	4	2	11,11,12	1.67	3 (27%)	15,15,17	2.30	2 (13%)
2	SIA	D	5	2	20,20,21	5.18	3 (15%)	24,28,31	2.37	9 (37%)
2	SLB	D	6	2	20,20,21	1.72	3 (15%)	24,28,31	2.93	13 (54%)
2	SIA	D	7	2	20,20,21	5.36	4 (20%)	24,28,31	2.13	7 (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	BGC	C	1	3,2	-	0/2/22/22	0/1/1/1
2	GAL	C	2	2	-	1/2/19/22	0/1/1/1
2	NGA	C	3	2	-	4/6/23/26	0/1/1/1
2	GAL	C	4	2	-	2/2/19/22	0/1/1/1
2	SIA	C	5	2	-	8/18/34/38	0/1/1/1
2	SLB	C	6	2	-	7/18/34/38	0/1/1/1
2	SIA	C	7	2	-	0/18/34/38	0/1/1/1
2	BGC	D	1	3,2	-	0/2/22/22	0/1/1/1
2	GAL	D	2	2	-	2/2/19/22	0/1/1/1
2	NGA	D	3	2	-	2/6/23/26	0/1/1/1
2	GAL	D	4	2	-	2/2/19/22	0/1/1/1
2	SIA	D	5	2	-	7/18/34/38	0/1/1/1
2	SLB	D	6	2	-	7/18/34/38	0/1/1/1
2	SIA	D	7	2	-	7/18/34/38	0/1/1/1

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	5	SIA	C2-C1	-23.69	1.31	1.52
2	D	7	SIA	C2-C1	-23.34	1.31	1.52
2	D	5	SIA	C2-C1	-22.68	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	7	SIA	C2-C1	-19.13	1.35	1.52
2	D	6	SLB	C2-C1	-5.91	1.47	1.52

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GAL	O3-C3-C4	12.33	138.87	110.35
2	D	2	GAL	O4-C4-C3	-8.01	91.83	110.35
2	C	1	BGC	O4-C4-C3	-7.94	91.99	110.35
2	C	1	BGC	O4-C4-C5	7.92	128.97	109.30
2	D	4	GAL	O3-C3-C4	7.59	127.90	110.35

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

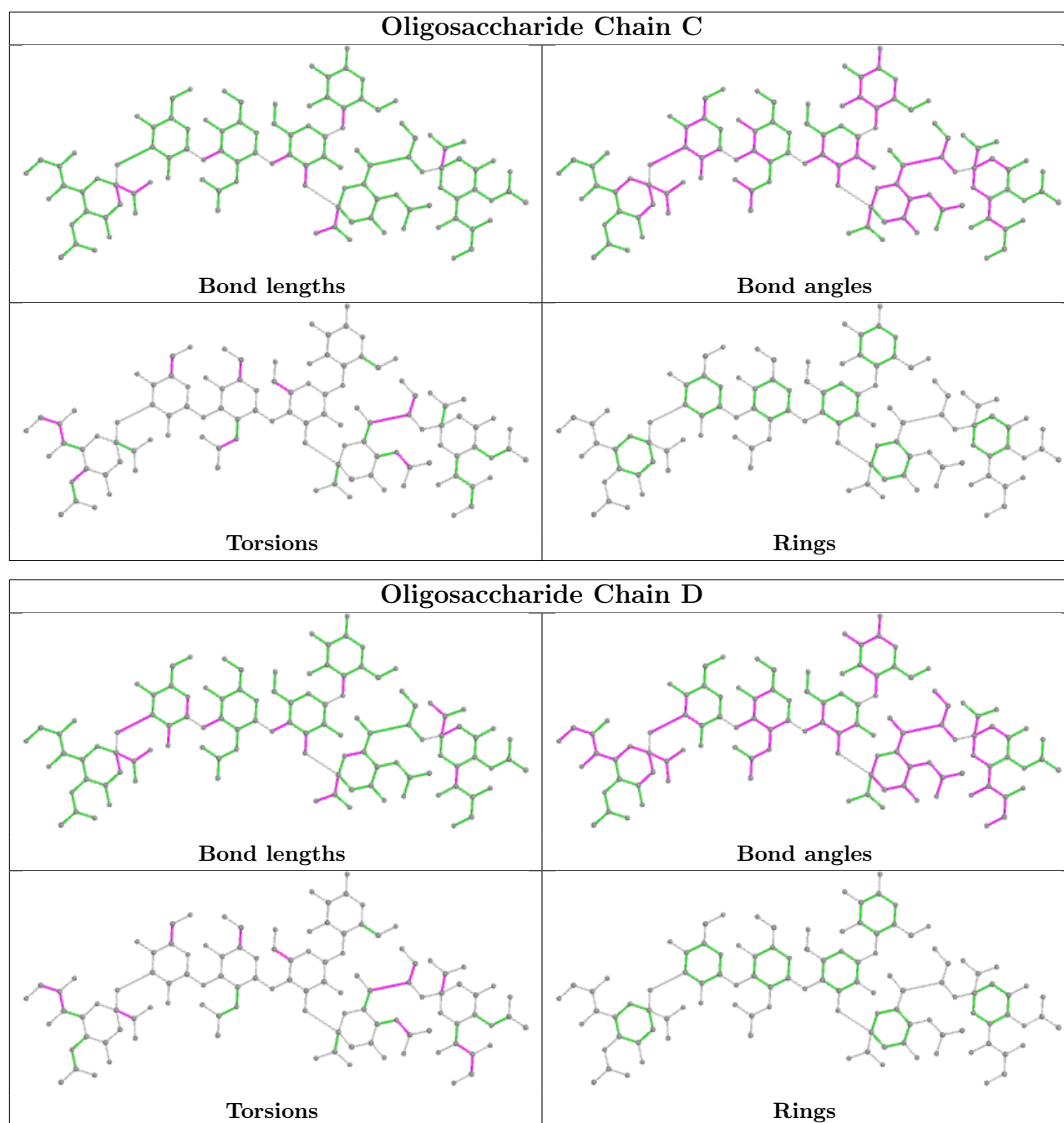
Mol	Chain	Res	Type	Atoms
2	C	5	SIA	C6-C7-C8-C9
2	C	5	SIA	O7-C7-C8-C9
2	C	5	SIA	O8-C8-C9-O9
2	C	6	SLB	C11-C10-N5-C5
2	C	6	SLB	O10-C10-N5-C5

There are no ring outliers.

12 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	6	SLB	2	0
2	D	5	SIA	1	0
2	D	6	SLB	4	0
2	C	4	GAL	1	0
2	C	2	GAL	2	0
2	D	4	GAL	1	0
2	C	3	NGA	2	0
2	D	7	SIA	4	0
2	D	1	BGC	1	0
2	D	2	GAL	1	0
2	C	5	SIA	3	0
2	D	3	NGA	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](#)

5 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	PO4	B	301	-	4,4,4	0.93	0	6,6,6	0.77	0
3	CEQ	A	8[B]	2	5,5,5	2.61	4 (80%)	7,7,7	1.05	1 (14%)
3	CEQ	B	8[A]	2	5,5,5	2.61	4 (80%)	7,7,7	1.00	1 (14%)
3	CEQ	A	8[A]	2	5,5,5	2.66	4 (80%)	7,7,7	1.08	1 (14%)
3	CEQ	B	8[B]	2	5,5,5	2.59	4 (80%)	7,7,7	0.76	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	CEQ	A	8[B]	2	-	0/3/3/3	-
3	CEQ	B	8[A]	2	-	1/3/3/3	-
3	CEQ	A	8[A]	2	-	1/3/3/3	-
3	CEQ	B	8[B]	2	-	1/3/3/3	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	8[A]	CEQ	SI1-C5	-3.72	1.78	1.87
3	B	8[B]	CEQ	SI1-C5	-3.60	1.79	1.87
3	A	8[B]	CEQ	SI1-C5	-3.54	1.79	1.87
3	B	8[A]	CEQ	SI1-C5	-3.49	1.79	1.87
3	A	8[A]	CEQ	SI1-C2	-2.82	1.78	1.87

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	8[A]	CEQ	SI1-C5-C6	-2.33	111.18	115.95
3	A	8[A]	CEQ	SI1-C5-C6	-2.19	111.45	115.95
3	A	8[B]	CEQ	SI1-C5-C6	-2.15	111.54	115.95

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	8[A]	CEQ	C6-C5-SI1-C3
3	B	8[A]	CEQ	C6-C5-SI1-C3
3	B	8[B]	CEQ	C6-C5-SI1-C3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	PO4	2	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	451/472 (95%)	0.13	22 (4%) 29 36	27, 37, 54, 68	0
1	B	451/472 (95%)	-0.12	14 (3%) 49 56	17, 29, 51, 71	0
All	All	902/944 (95%)	0.00	36 (3%) 38 45	17, 34, 54, 71	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	867	LEU	8.1
1	B	871	VAL	7.1
1	A	870	TRP	5.1
1	B	872	ASP	5.0
1	A	1183	ASN	4.6

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

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

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.

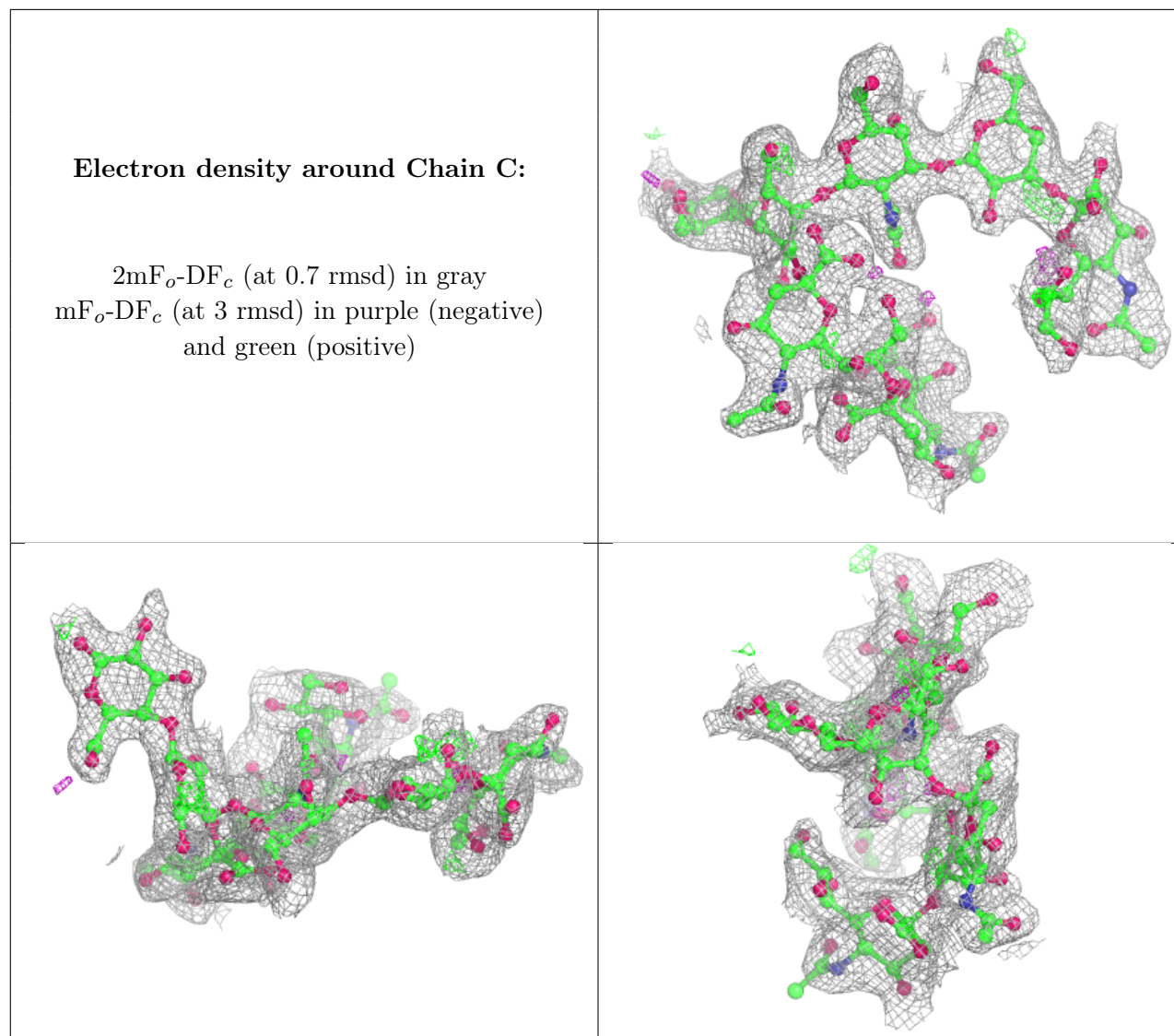
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SIA	C	5	20/21	0.76	0.21	58,64,67,67	0
2	SIA	D	5	20/21	0.78	0.20	59,62,68,69	0
2	NGA	C	3	14/15	0.84	0.15	50,51,53,53	0
2	SIA	D	7	20/21	0.85	0.17	44,50,60,63	0
2	GAL	C	4	11/12	0.87	0.18	46,50,53,55	0

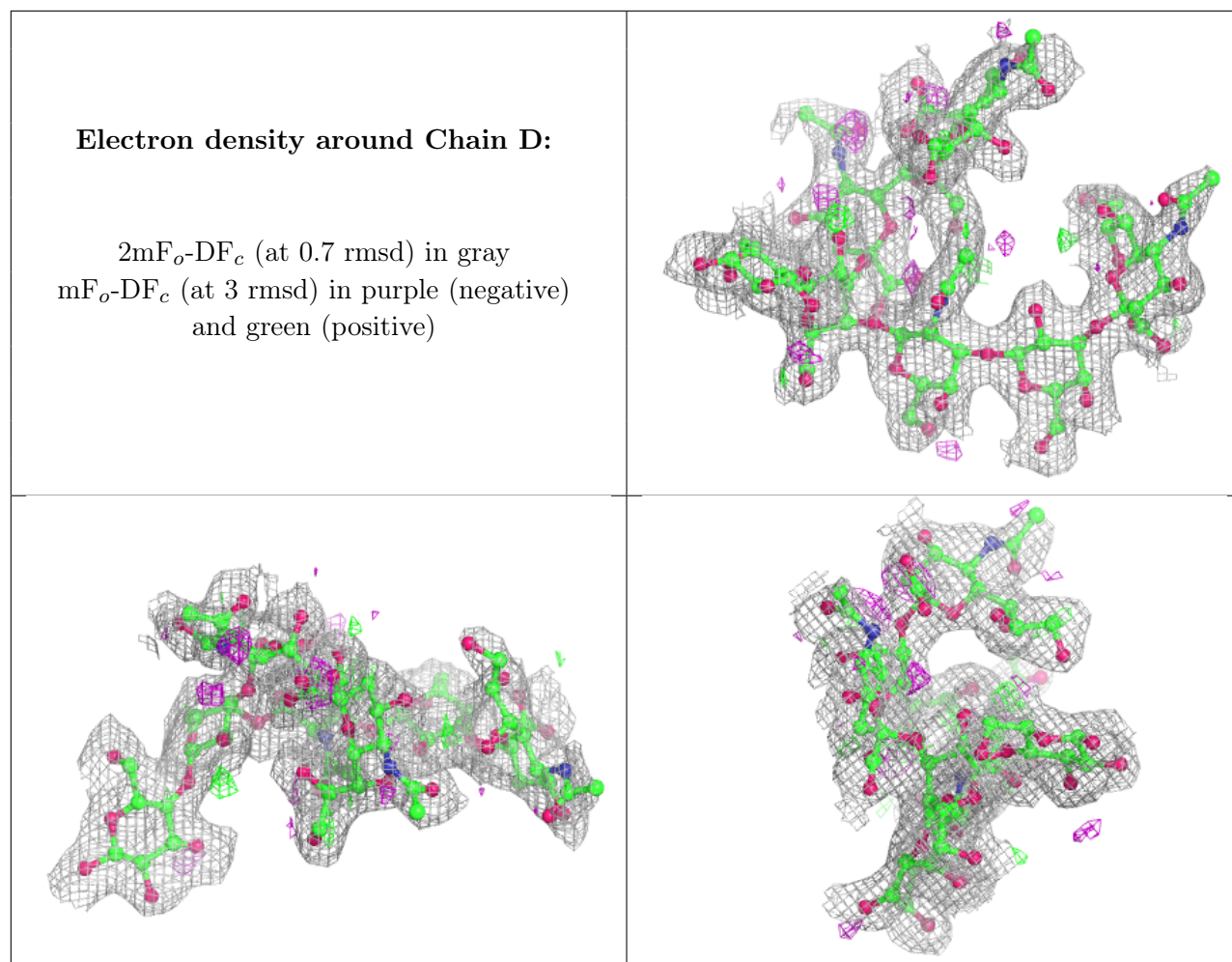
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SLB	D	6	20/21	0.88	0.15	42,49,57,58	0
2	SLB	C	6	20/21	0.88	0.15	47,54,63,65	0
2	SIA	C	7	20/21	0.89	0.16	44,56,65,65	0
2	GAL	D	2	11/12	0.90	0.13	41,44,45,47	0
2	BGC	D	1	12/12	0.90	0.11	39,51,57,61	0
2	BGC	C	1	12/12	0.92	0.15	47,54,61,62	0
2	GAL	C	2	11/12	0.92	0.12	45,48,52,58	0
2	NGA	D	3	14/15	0.94	0.12	36,39,42,43	0
2	GAL	D	4	11/12	0.97	0.08	34,37,40,46	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
3	CEQ	B	8[A]	6/6	0.65	0.56	71,75,76,76	6
3	CEQ	B	8[B]	6/6	0.65	0.56	64,65,65,65	6
3	CEQ	A	8[A]	6/6	0.82	0.39	72,76,76,76	6
3	CEQ	A	8[B]	6/6	0.82	0.39	66,68,68,68	6
4	PO4	B	301	5/5	0.97	0.09	58,60,60,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.