



wwPDB X-ray Structure Validation Summary Report

Oct 11, 2023 – 08:41 AM EDT

PDB ID : 7JJN
Title : Eubacterium rectale Amy13B (EUR_01860)
Authors : Koropatkin, N.M.; Cockburn, D.W.; Cerqueira, F.M.
Deposited on : 2020-07-27
Resolution : 2.25 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 : 2.35.1
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) : 2.35.1

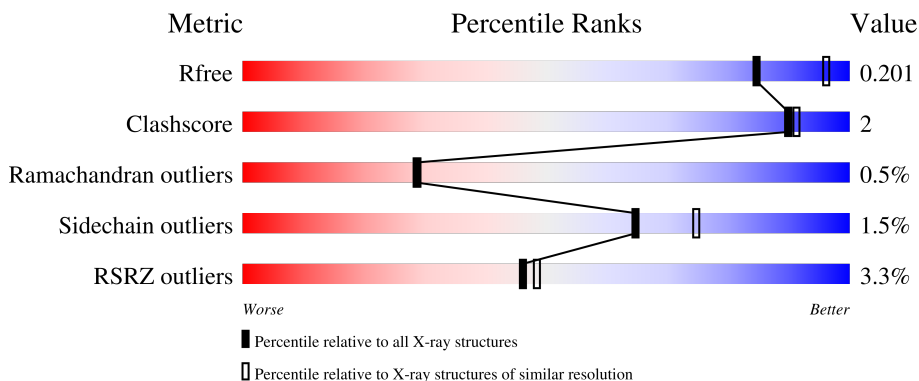
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

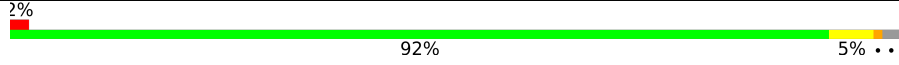
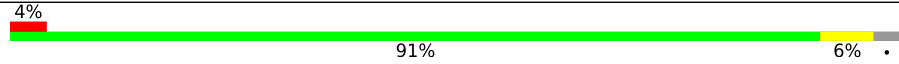
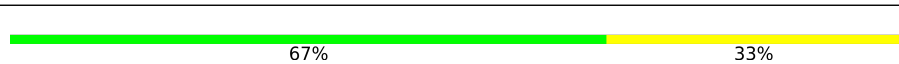
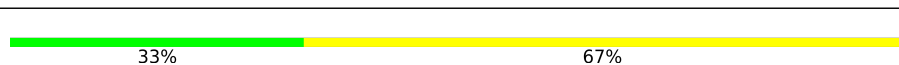
The reported resolution of this entry is 2.25 Å.

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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	526	 2% 92% 5% ..
1	B	526	 4% 91% 6% .
2	D	3	 67% 33%
2	E	3	 33% 67%

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 8787 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.

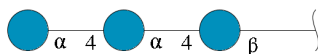
- Molecule 1 is a protein called Glycosidases.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	514	4089	2577	661	827	24	0	0	0
1	B	509	4055	2557	655	819	24	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	ALA	ASP	engineered mutation	UNP D6E1Y4
A	543	ALA	LYS	engineered mutation	UNP D6E1Y4
A	544	ALA	LYS	engineered mutation	UNP D6E1Y4
A	565	GLU	-	expression tag	UNP D6E1Y4
A	566	ASN	-	expression tag	UNP D6E1Y4
A	567	LEU	-	expression tag	UNP D6E1Y4
A	568	TYR	-	expression tag	UNP D6E1Y4
B	265	ALA	ASP	engineered mutation	UNP D6E1Y4
B	543	ALA	LYS	engineered mutation	UNP D6E1Y4
B	544	ALA	LYS	engineered mutation	UNP D6E1Y4
B	565	GLU	-	expression tag	UNP D6E1Y4
B	566	ASN	-	expression tag	UNP D6E1Y4
B	567	LEU	-	expression tag	UNP D6E1Y4
B	568	TYR	-	expression tag	UNP D6E1Y4

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	3	Total	C	O	0	0	0
			34	18	16			
2	E	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	286	Total	O	0	0
			286	286		
7	B	257	Total	O	0	0
			257	257		

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.18Å 82.76Å 85.86Å 90.00° 92.86° 90.00°	Depositor
Resolution (Å)	38.07 – 2.25 38.07 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.07-2.25) 99.0 (38.07-2.25)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.162 , 0.198 0.169 , 0.201	Depositor DCC
R_{free} test set	2783 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.005 for l,k,-h 0.019 for -h,-l,-k 0.008 for -h,l,k 0.011 for k,h,-l 0.008 for -k,-h,-l 0.005 for l,h,k 0.009 for k,l,h 0.011 for -l,-h,k 0.007 for -k,-l,h 0.032 for h,-k,-l 0.018 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8787	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 5.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, BGC, GLC, CA, GOL, EDO

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	0.40	0/4186	0.59	1/5679 (0.0%)
1	B	0.39	0/4149	0.57	0/5626
All	All	0.40	0/8335	0.58	1/11305 (0.0%)

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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	211	ASN	CB-CA-C	-5.57	99.26	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	478	ARG	Sidechain
1	A	505	ARG	Sidechain
1	B	478	ARG	Sidechain

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	4089	0	3830	13	0
1	B	4055	0	3793	15	0
2	D	34	0	30	0	0
2	E	34	0	30	0	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
4	A	6	0	8	2	0
4	B	6	0	8	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	286	0	0	0	0
7	B	257	0	0	1	0
All	All	8787	0	7711	28	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 2.

The worst 5 of 28 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:486:ARG:HH22	4:A:602:GOL:H31	1.45	0.81
1:B:106:ASP:OD1	1:B:158:ARG:NH1	2.19	0.75
1:A:486:ARG:HH22	4:A:602:GOL:C3	2.06	0.68
1:B:122:MET:HE3	1:B:132:ILE:HD13	1.78	0.65
1:A:387:ASN:HA	1:A:390:GLU:OE1	1.98	0.64

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	512/526 (97%)	488 (95%)	21 (4%)	3 (1%)	25	25
1	B	503/526 (96%)	480 (95%)	21 (4%)	2 (0%)	34	37
All	All	1015/1052 (96%)	968 (95%)	42 (4%)	5 (0%)	29	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	272	ASN
1	A	212	THR
1	A	192	ALA
1	A	193	GLU
1	B	211	ASN

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	440/448 (98%)	431 (98%)	9 (2%)	55	64
1	B	436/448 (97%)	432 (99%)	4 (1%)	78	86
All	All	876/896 (98%)	863 (98%)	13 (2%)	65	75

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	522	GLU

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Mol	Chain	Res	Type
1	A	525	VAL
1	B	451	GLU
1	B	140	LYS
1	B	351	LEU

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	217	GLN
1	B	62	GLN
1	B	217	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](#)

6 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	D	1	2	12,12,12	0.41	0	17,17,17	0.55	0
2	GLC	D	2	2	11,11,12	0.37	0	15,15,17	0.76	0
2	GLC	D	3	2	11,11,12	0.32	0	15,15,17	1.21	2 (13%)
2	BGC	E	1	2	12,12,12	0.40	0	17,17,17	0.71	0
2	GLC	E	2	2	11,11,12	0.42	0	15,15,17	0.76	1 (6%)
2	GLC	E	3	2	11,11,12	0.34	0	15,15,17	1.52	3 (20%)

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	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	3	2	-	2/2/19/22	0/1/1/1
2	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1
2	GLC	E	3	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	GLC	C1-O5-C5	4.13	117.79	112.19
2	D	3	GLC	C1-O5-C5	2.60	115.71	112.19
2	E	3	GLC	C3-C4-C5	2.31	114.36	110.24
2	E	3	GLC	C6-C5-C4	-2.18	107.90	113.00
2	E	2	GLC	O5-C1-C2	-2.15	107.46	110.77

There are no chirality outliers.

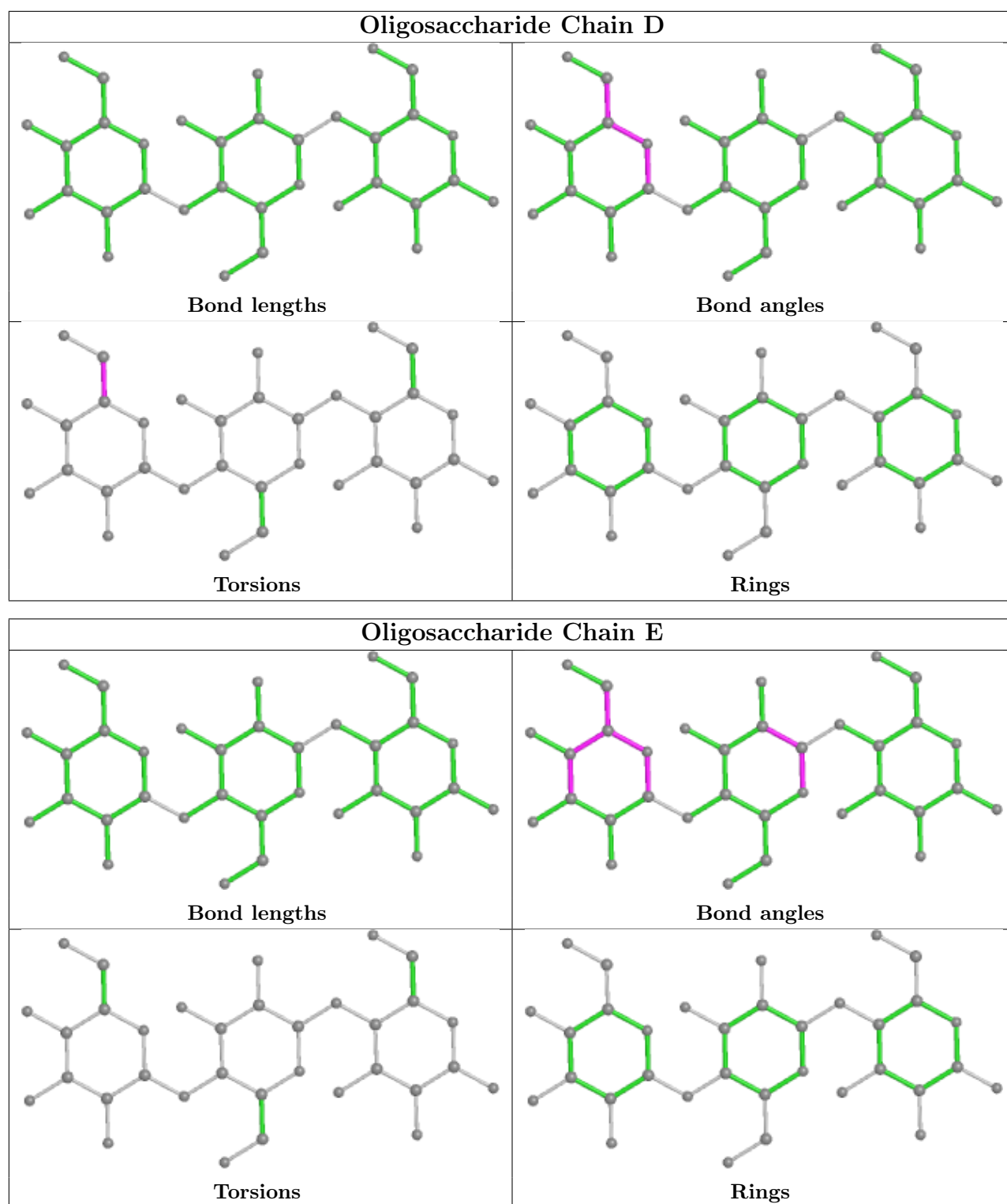
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	GLC	O5-C5-C6-O6
2	D	3	GLC	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
6	SO4	B	604	-	4,4,4	0.39	0	6,6,6	0.19	0
3	EDO	B	601	-	3,3,3	0.45	0	2,2,2	0.43	0
4	GOL	A	602	-	5,5,5	0.39	0	5,5,5	0.63	0
4	GOL	B	602	-	5,5,5	0.34	0	5,5,5	0.59	0
3	EDO	A	601	-	3,3,3	0.41	0	2,2,2	0.46	0
6	SO4	A	604	-	4,4,4	0.35	0	6,6,6	0.14	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	602	-	-	3/4/4/4	-
3	EDO	A	601	-	-	1/1/1/1	-
3	EDO	B	601	-	-	1/1/1/1	-
4	GOL	B	602	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	GOL	C1-C2-C3-O3
4	B	602	GOL	O1-C1-C2-C3
4	A	602	GOL	O1-C1-C2-C3
4	A	602	GOL	O2-C2-C3-O3
4	B	602	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	GOL	2	0
4	B	602	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	514/526 (97%)	-0.19	11 (2%) 63 66	23, 32, 49, 79	0
1	B	509/526 (96%)	-0.01	23 (4%) 33 36	24, 34, 61, 78	0
All	All	1023/1052 (97%)	-0.10	34 (3%) 46 48	23, 33, 56, 79	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	222	ASN	4.8
1	B	437	ALA	4.4
1	B	438	LYS	4.0
1	B	386	ASP	4.0
1	B	436	LYS	3.9

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.

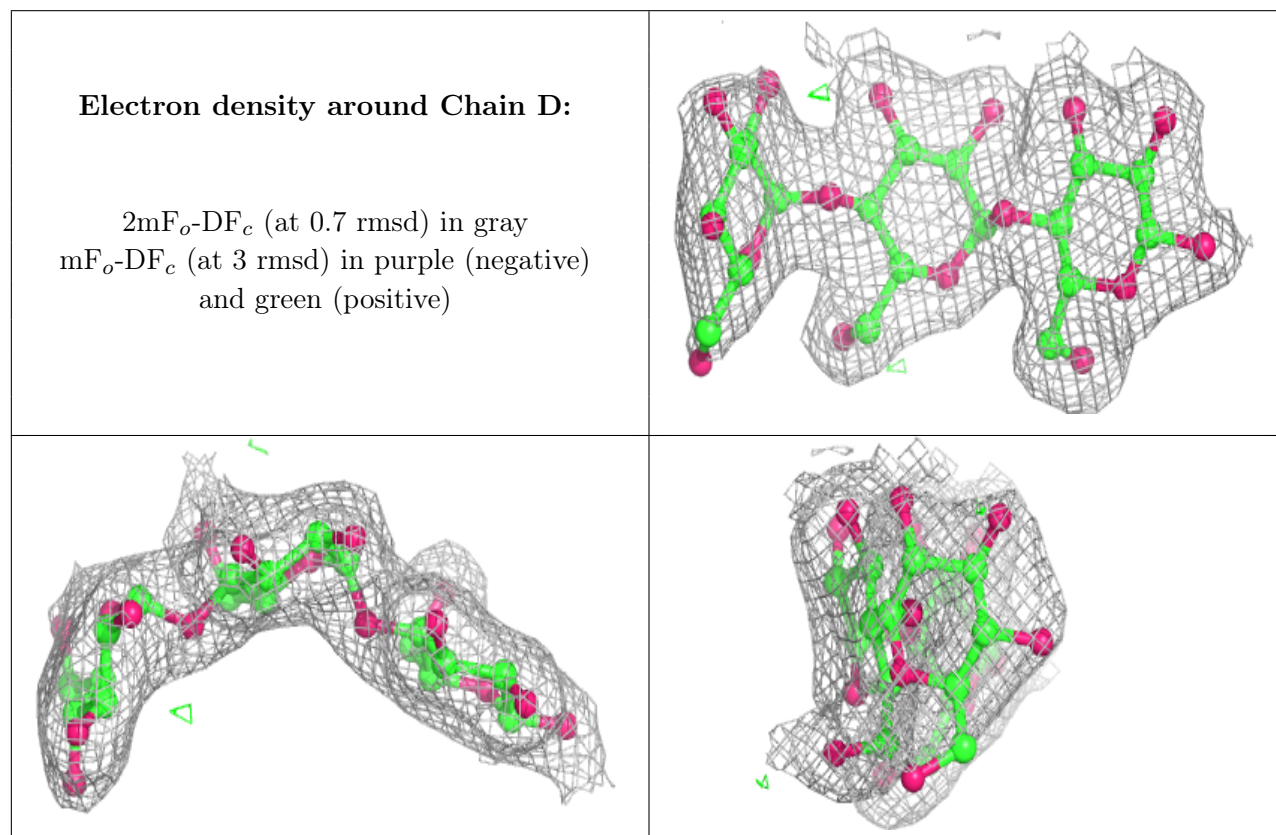
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	E	3	11/12	0.91	0.15	51,55,58,59	0
2	GLC	D	3	11/12	0.92	0.20	48,55,58,58	0
2	GLC	E	2	11/12	0.95	0.11	33,35,37,42	0
2	GLC	D	2	11/12	0.96	0.08	30,32,34,38	0
2	BGC	E	1	12/12	0.96	0.14	27,29,32,32	0

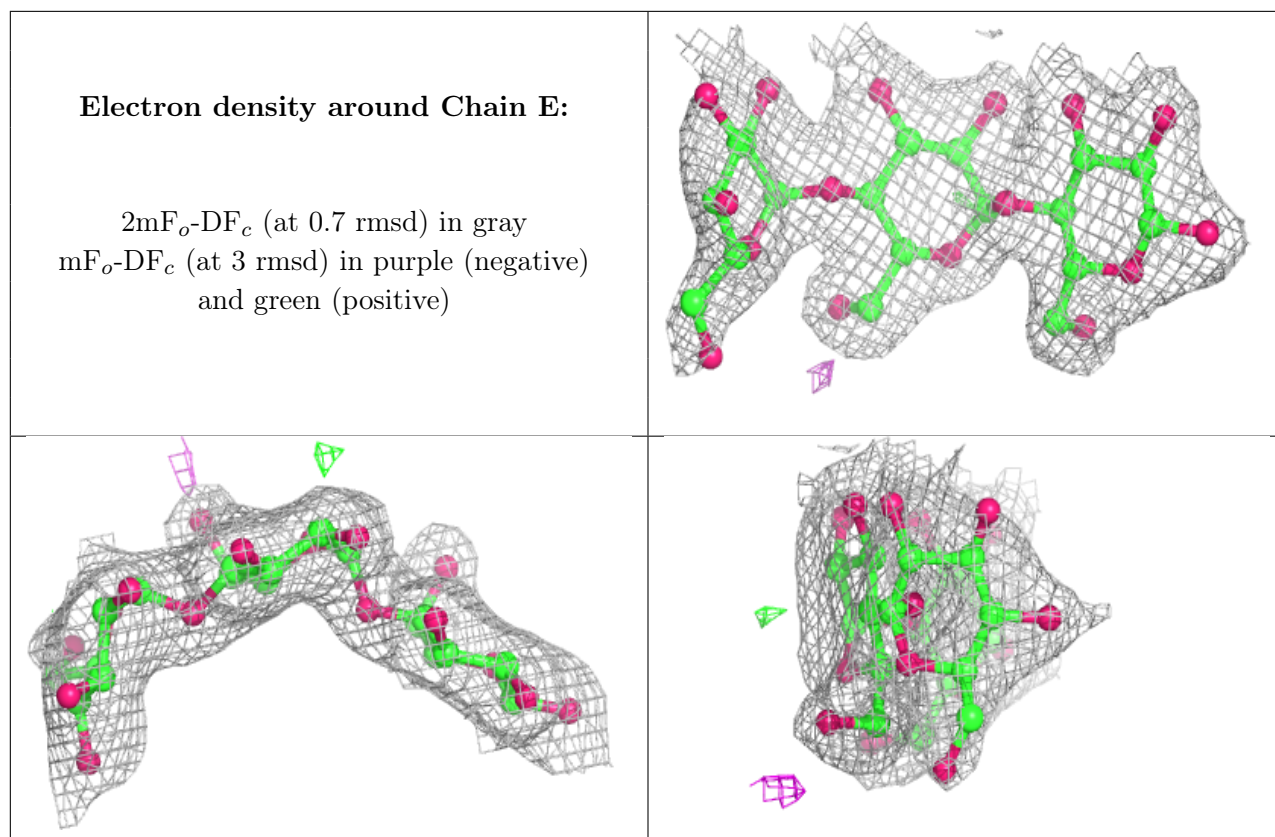
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BGC	D	1	12/12	0.98	0.12	24,28,29,30	0

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(Å ²)	Q<0.9
3	EDO	B	601	4/4	0.86	0.27	53,56,56,56	0
4	GOL	A	602	6/6	0.89	0.19	35,37,38,39	0
3	EDO	A	601	4/4	0.92	0.17	54,54,54,57	0
4	GOL	B	602	6/6	0.95	0.18	38,38,39,39	0
5	CA	A	603	1/1	0.96	0.03	37,37,37,37	0
5	CA	B	603	1/1	0.98	0.03	40,40,40,40	0
6	SO4	A	604	5/5	0.98	0.12	52,55,56,58	0
6	SO4	B	604	5/5	0.99	0.08	46,46,47,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.