



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 08:28 PM EDT

PDB ID : 2WR9
Title : CRYSTAL STRUCTURE OF BURKHOLDERIA CENOCEPACIA LECTIN (BCLA) COMPLEXED WITH AMAN1-3MAN DISACCHARIDE
Authors : Lameignere, E.; Shiao, T.C.; Roy, R.; Wimmerova, M.; Dubreuil, F.; Varrot, A.; Imberty, A.
Deposited on : 2009-09-01
Resolution : 1.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 1.20.1
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

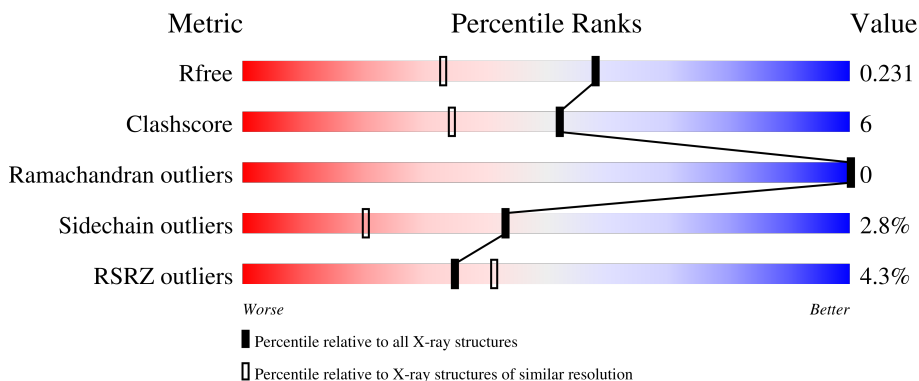
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	128	 2% 84% 9% 7%
1	B	128	 9% 82% 13% 5%
1	C	128	 3% 80% 13% 5%
1	D	128	 2% 88% 9% 5%
2	E	2	 100%

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Mol	Chain	Length	Quality of chain
2	F	2	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4293 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 LECTIN.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
1	A	119	917	575	159	183	0	2	0
1	B	123	939	586	167	186	0	0	0
1	C	121	927	580	165	182	0	0	0
1	D	124	946	590	168	188	0	0	0

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	O			
2	E	2	23	11	0	0	0
2	F	2	23	11	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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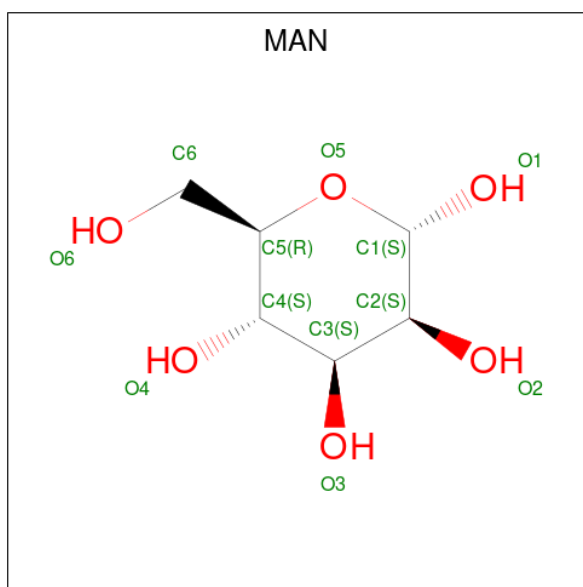
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Ca	0	0
			2	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 12 6 6	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	111	Total O 111 111	0	0
6	B	112	Total O 112 112	0	0
6	C	121	Total O 121 121	0	0
6	D	119	Total O 119 119	0	0

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.96Å 48.97Å 76.26Å 90.00° 98.89° 90.00°	Depositor
Resolution (Å)	75.38 – 1.75 75.34 – 1.75	Depositor EDS
% Data completeness (in resolution range)	97.7 (75.38-1.75) 97.7 (75.34-1.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.75Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.176 , 0.225 0.180 , 0.231	Depositor DCC
R_{free} test set	2120 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtrriage
Anisotropy	0.147	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4293	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5378e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MAN, CA, SO4

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	0/942	0.81	1/1274 (0.1%)
1	B	0.81	0/961	0.83	1/1302 (0.1%)
1	C	0.80	0/949	0.88	2/1286 (0.2%)
1	D	0.79	0/968	0.85	1/1312 (0.1%)
All	All	0.79	0/3820	0.85	5/5174 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	ASP	CB-CG-OD1	5.95	123.65	118.30
1	C	9	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	C	9	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	115	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	54	ARG	NE-CZ-NH2	-5.17	117.72	120.30

There are no chirality outliers.

There are no planarity outliers.

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	917	0	873	5	0
1	B	939	0	895	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	927	0	885	18	0
1	D	946	0	902	8	0
2	E	23	0	18	0	0
2	F	23	0	18	0	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	B	20	0	0	0	0
4	C	10	0	0	0	0
4	D	5	0	0	0	0
5	C	12	0	10	1	0
6	A	111	0	0	1	0
6	B	112	0	0	3	0
6	C	121	0	0	5	0
6	D	119	0	0	3	0
All	All	4293	0	3601	41	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 6.

All (41) 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:C:128:GLY:HA2	6:D:309:HOH:O	1.36	1.25
1:B:13:PHE:HE2	1:B:106:VAL:CG2	2.01	0.73
1:B:13:PHE:CE2	1:B:106:VAL:CG2	2.84	0.60
1:B:13:PHE:CE2	1:B:106:VAL:HG22	2.38	0.59
1:B:13:PHE:HE2	1:B:106:VAL:HG22	1.70	0.56
6:B:391:HOH:O	1:C:78:LYS:HE3	2.07	0.55
1:C:75:VAL:HG21	1:C:110:ASP:HB3	1.88	0.55
1:D:32:GLN:NE2	6:D:303:HOH:O	2.40	0.54
1:C:71:PHE:HZ	1:C:123:LEU:HD21	1.73	0.53
1:C:38:PHE:HB2	1:C:70:ARG:CG	2.38	0.53
1:C:8:ASN:C	1:C:8:ASN:HD22	2.12	0.53
1:C:38:PHE:HB2	1:C:70:ARG:HG3	1.89	0.53
1:B:18:ASN:ND2	6:B:301:HOH:O	2.34	0.53
1:C:24:ILE:HG21	1:D:24:ILE:HG21	1.91	0.52
1:B:70:ARG:NH1	1:B:72:GLU:OE2	2.36	0.51
1:C:75:VAL:HG21	1:C:110:ASP:CB	2.41	0.50
1:B:93:LYS:HD3	1:B:97:SER:OG	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:PHE:HE2	1:D:106:VAL:CG2	2.25	0.50
1:B:95:ASP:HB2	1:C:78:LYS:HD3	1.94	0.48
1:A:24:ILE:HG21	1:B:24:ILE:HG21	1.96	0.47
1:C:54:ARG:HG3	6:C:353:HOH:O	2.13	0.47
1:A:11:GLY:N	6:A:302:HOH:O	2.39	0.47
1:A:39:ILE:HD12	1:A:46:ALA:CB	2.45	0.47
1:B:32:GLN:NE2	6:B:306:HOH:O	2.47	0.46
1:A:107:VAL:HB	1:A:116:TYR:O	2.16	0.46
1:D:70:ARG:NH2	6:D:306:HOH:O	2.49	0.46
1:C:8:ASN:C	1:C:8:ASN:ND2	2.69	0.45
1:C:107:VAL:HB	1:C:116:TYR:O	2.16	0.45
1:C:39:ILE:HD13	1:C:63:ASN:O	2.17	0.45
1:C:9:ARG:NH2	1:D:92:LYS:O	2.50	0.45
1:C:37:LEU:C	1:C:37:LEU:HD23	2.37	0.45
1:D:13:PHE:CE2	1:D:106:VAL:CG2	3.00	0.44
6:C:330:HOH:O	1:D:128:GLY:HA2	2.17	0.43
1:C:11:GLY:HA2	6:C:309:HOH:O	2.18	0.43
1:B:75:VAL:HG21	1:B:110:ASP:CB	2.49	0.43
1:A:71:PHE:HZ	1:A:123:LEU:HD21	1.83	0.42
1:D:16:PRO:HA	1:D:17:PRO:HD3	1.99	0.41
1:B:75:VAL:HG21	1:B:110:ASP:HB2	2.02	0.41
1:B:112:HIS:N	1:B:112:HIS:ND1	2.69	0.41
1:C:53:THR:O	6:C:302:HOH:O	2.22	0.41
5:C:201:MAN:O1	6:C:301:HOH:O	2.20	0.40

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	118/128 (92%)	115 (98%)	3 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	121/128 (94%)	118 (98%)	3 (2%)	0	100	100
1	C	119/128 (93%)	117 (98%)	2 (2%)	0	100	100
1	D	122/128 (95%)	119 (98%)	3 (2%)	0	100	100
All	All	480/512 (94%)	469 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	97/104 (93%)	94 (97%)	3 (3%)	40	17
1	B	100/104 (96%)	95 (95%)	5 (5%)	24	6
1	C	98/104 (94%)	97 (99%)	1 (1%)	76	63
1	D	101/104 (97%)	99 (98%)	2 (2%)	55	34
All	All	396/416 (95%)	385 (97%)	11 (3%)	43	20

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	54	ARG
1	A	92	LYS
1	B	9	ARG
1	B	14	SER
1	B	74	SER
1	B	112	HIS
1	B	114	SER
1	C	8	ASN
1	D	9	ARG
1	D	43	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	B	32	GLN
1	C	8	ASN
1	C	32	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](#)

4 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	MAN	E	1	2	12,12,12	0.63	0	17,17,17	2.00	3 (17%)
2	MAN	E	2	3,2	11,11,12	0.70	0	15,15,17	1.28	2 (13%)
2	MAN	F	1	2	12,12,12	0.73	0	17,17,17	1.65	4 (23%)
2	MAN	F	2	3,2	11,11,12	0.73	0	15,15,17	0.84	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	MAN	E	1	2	-	0/2/22/22	0/1/1/1
2	MAN	E	2	3,2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	F	1	2	-	0/2/22/22	0/1/1/1
2	MAN	F	2	3,2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	MAN	O1-C1-O5	5.59	127.02	110.41
2	F	1	MAN	O1-C1-O5	-3.78	99.20	110.41
2	E	2	MAN	O4-C4-C5	3.13	117.03	109.32
2	F	1	MAN	C1-O5-C5	3.05	119.56	113.65
2	E	1	MAN	O5-C1-C2	2.95	115.48	110.30
2	E	1	MAN	C1-C2-C3	-2.88	104.48	110.36
2	E	2	MAN	C1-O5-C5	2.25	115.21	112.19
2	F	1	MAN	C4-C3-C2	-2.07	107.19	110.83
2	F	1	MAN	O3-C3-C2	-2.06	105.53	110.38

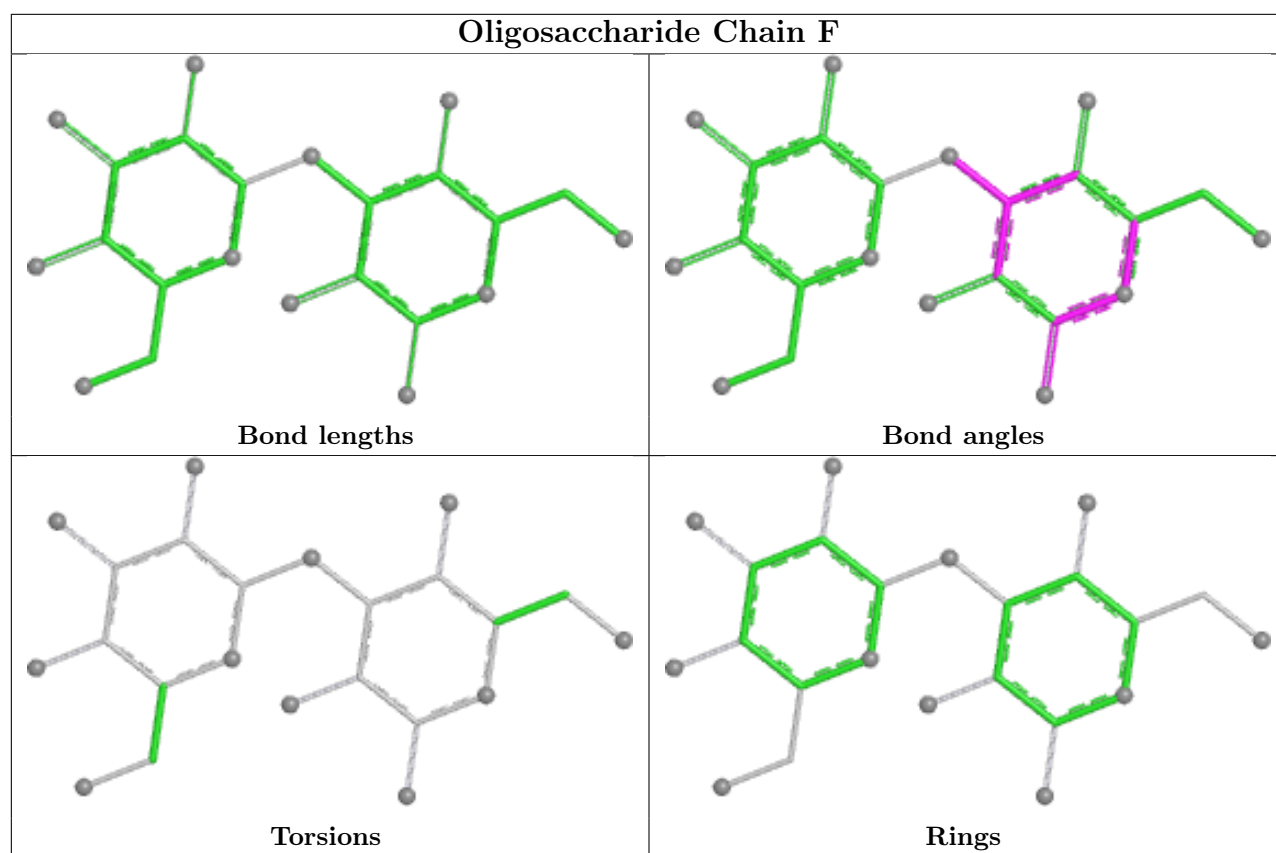
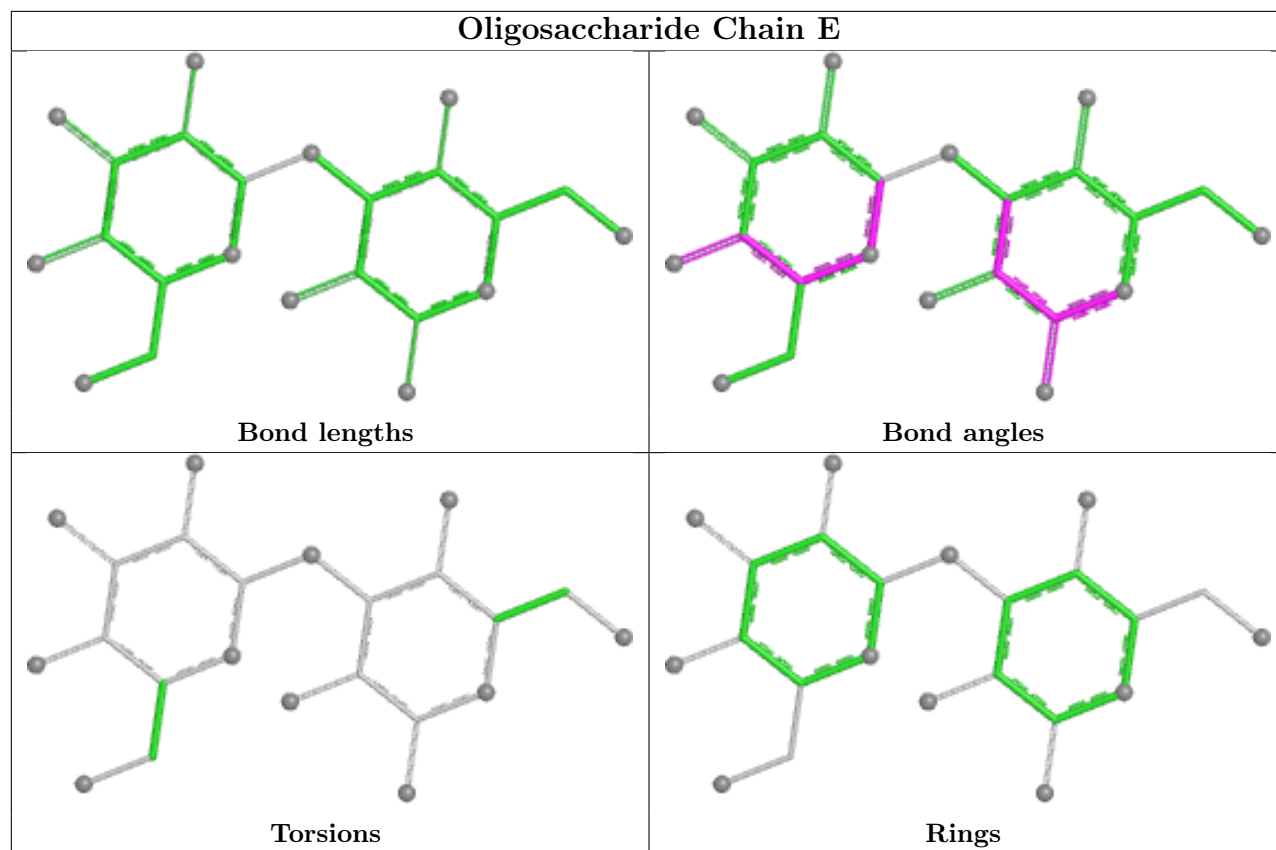
There are no chirality outliers.

There are no torsion outliers.

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

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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
4	SO4	B	209	-	4,4,4	0.23	0	6,6,6	0.66	0
4	SO4	B	207	-	4,4,4	0.23	0	6,6,6	0.13	0
4	SO4	B	206	-	4,4,4	0.30	0	6,6,6	0.53	0
4	SO4	D	205	-	4,4,4	0.39	0	6,6,6	0.23	0
4	SO4	B	208	-	4,4,4	0.27	0	6,6,6	0.52	0
4	SO4	C	204	-	4,4,4	0.29	0	6,6,6	0.20	0
5	MAN	C	201	3	12,12,12	0.75	0	17,17,17	2.17	4 (23%)
4	SO4	C	205	-	4,4,4	0.25	0	6,6,6	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	C	201	3	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	201	MAN	O1-C1-O5	5.46	126.63	110.41
5	C	201	MAN	C1-O5-C5	-4.33	105.27	113.65
5	C	201	MAN	O5-C1-C2	3.08	115.71	110.30
5	C	201	MAN	C1-C2-C3	-3.00	104.24	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	201	MAN	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	119/128 (92%)	0.02	3 (2%) 57 63	6, 14, 26, 36	1 (0%)
1	B	123/128 (96%)	0.20	11 (8%) 9 12	5, 13, 31, 35	1 (0%)
1	C	121/128 (94%)	0.11	4 (3%) 46 53	6, 14, 28, 34	2 (1%)
1	D	124/128 (96%)	-0.04	3 (2%) 59 65	6, 12, 26, 30	2 (1%)
All	All	487/512 (95%)	0.07	21 (4%) 35 41	5, 13, 29, 36	6 (1%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	ALA	5.0
1	D	128	GLY	4.1
1	B	11	GLY	3.6
1	B	114	SER	3.5
1	B	8	ASN	3.5
1	A	10	ALA	3.4
1	B	9	ARG	3.4
1	C	9	ARG	3.4
1	B	112	HIS	3.2
1	C	8	ASN	3.1
1	C	94	SER	3.1
1	A	11	GLY	2.9
1	D	43	GLN	2.9
1	A	128[A]	GLY	2.8
1	B	111	GLY	2.5
1	C	11	GLY	2.4
1	B	95	ASP	2.4
1	B	94	SER	2.4
1	D	9	ARG	2.3
1	B	7	SER	2.2
1	B	12	GLU	2.1

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

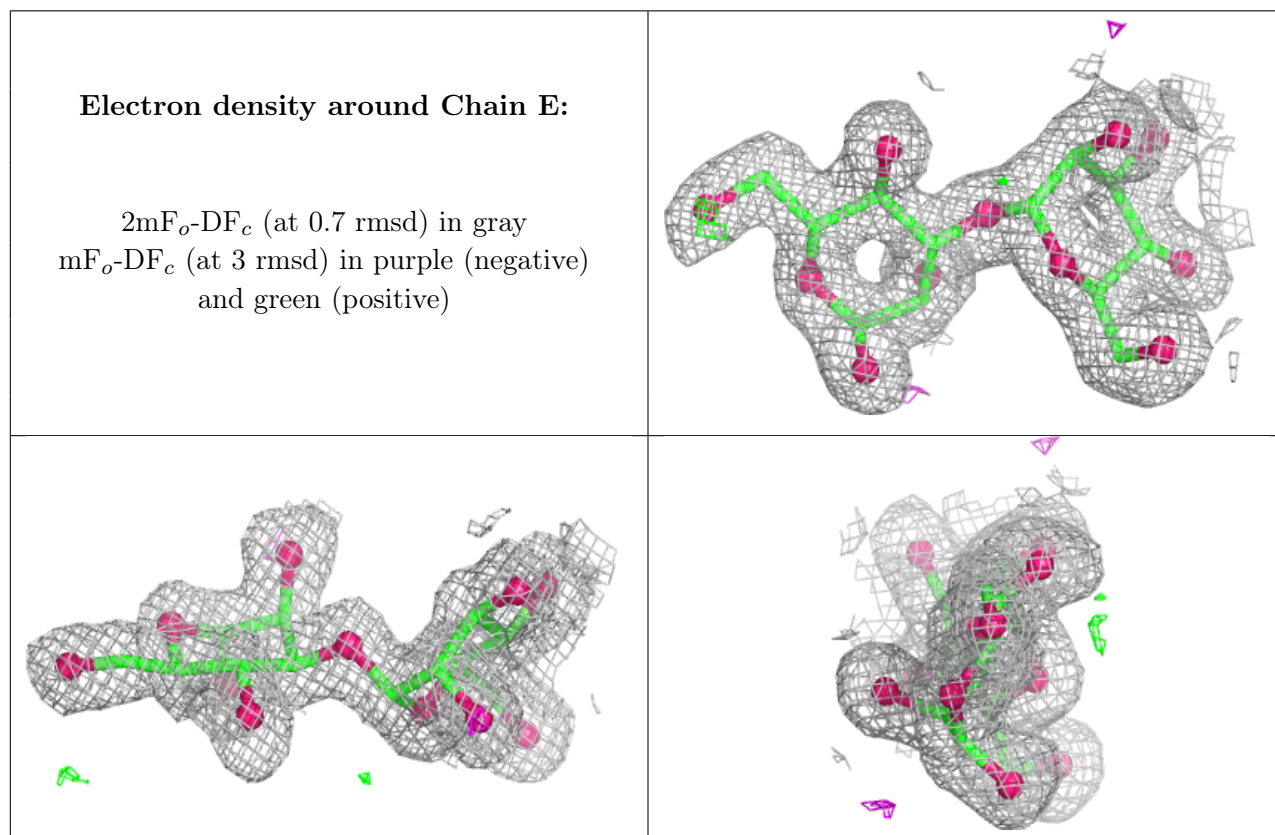
There are no non-standard protein/DNA/RNA residues in this entry.

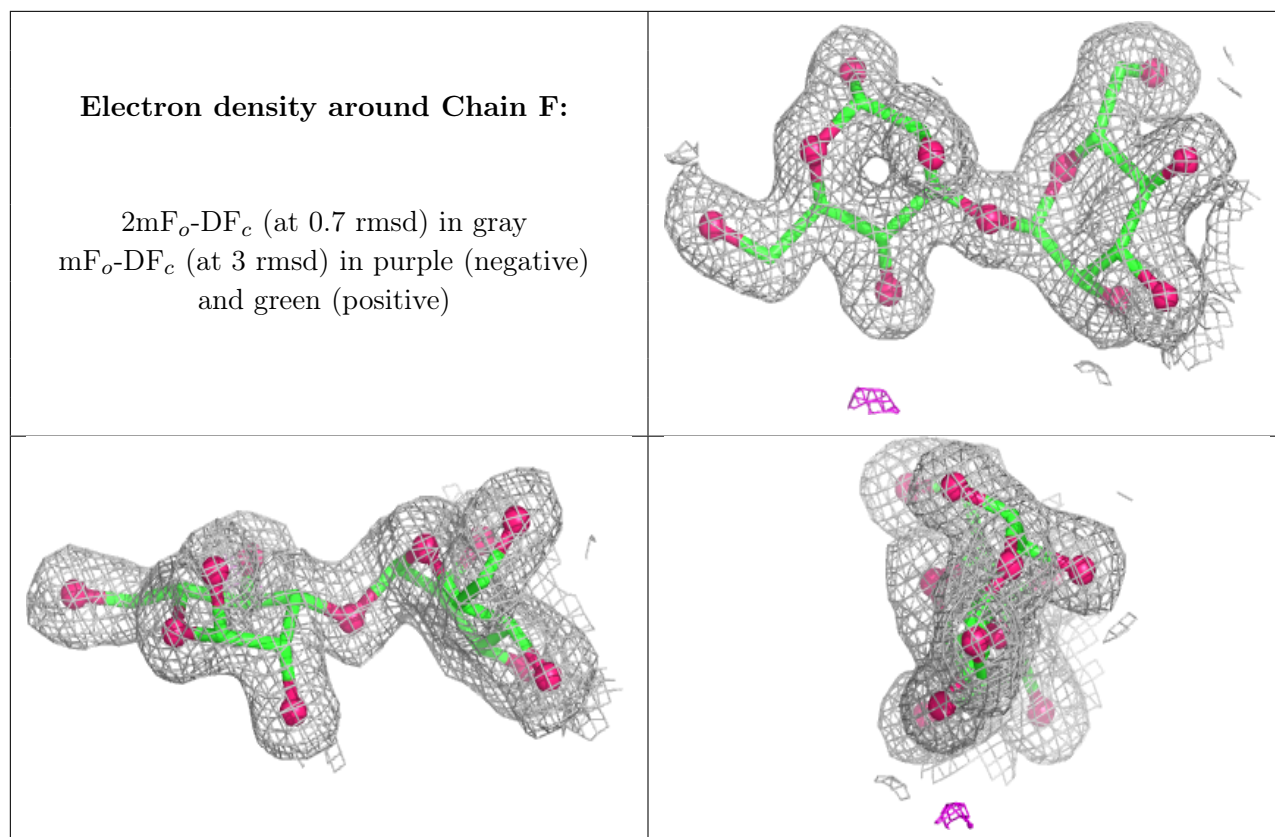
6.3 Carbohydrates [i](#)

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	MAN	E	1	12/12	0.94	0.11	12,15,17,18	0
2	MAN	E	2	11/12	0.97	0.09	10,12,14,15	0
2	MAN	F	1	12/12	0.97	0.10	8,14,16,16	0
2	MAN	F	2	11/12	0.98	0.07	8,11,12,13	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
5	MAN	C	201	12/12	0.87	0.16	22,26,29,30	0
4	SO4	B	207	5/5	0.95	0.14	41,41,43,43	0
4	SO4	C	204	5/5	0.95	0.12	46,47,48,49	0
4	SO4	B	206	5/5	0.95	0.13	34,36,39,39	0
3	CA	A	201	1/1	0.96	0.14	32,32,32,32	0
4	SO4	C	205	5/5	0.98	0.10	28,30,32,33	0
4	SO4	D	205	5/5	0.98	0.07	24,25,27,29	0
4	SO4	B	208	5/5	0.98	0.08	25,28,29,30	0
4	SO4	B	209	5/5	0.99	0.07	23,24,27,30	0
3	CA	D	204	1/1	0.99	0.05	7,7,7,7	0
3	CA	B	205	1/1	0.99	0.04	21,21,21,21	0
3	CA	C	202	1/1	0.99	0.04	19,19,19,19	0
3	CA	C	203	1/1	0.99	0.05	15,15,15,15	0
3	CA	B	204	1/1	1.00	0.07	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	B	203	1/1	1.00	0.06	7,7,7,7	0
3	CA	D	203	1/1	1.00	0.07	3,3,3,3	0

6.5 Other polymers [i](#)

There are no such residues in this entry.