



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 02:35 PM BST

PDB ID : 5M2K
Title : Crystal structure of vancomycin-Zn(II) complex
Authors : Zarkan, A.; Macklyne, H.-R.; Chirgadze, D.Y.; Bond, A.D.; Hesketh, A.R.;
Hong, H.-J.
Deposited on : 2016-10-13
Resolution : 1.00 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

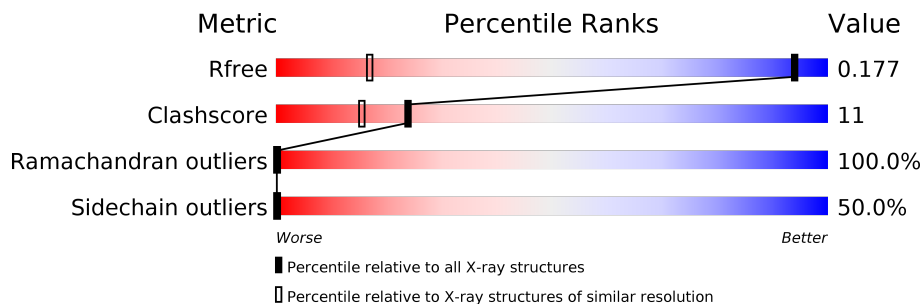
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.00 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	1050 (1.06-0.94)
Clashscore	141614	1117 (1.06-0.94)
Ramachandran outliers	138981	1043 (1.06-0.94)
Sidechain outliers	138945	1045 (1.06-0.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	7	57% (Green), 29% (Yellow), 14% (Red)
1	B	7	71% (Green), 29% (Yellow)
2	C	2	50% (Green), 50% (Yellow)
2	D	2	50% (Green), 50% (Yellow)

2 Entry composition i

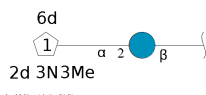
There are 5 unique types of molecules in this entry. The entry contains 274 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 vancomycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	Cl	N				O
1	A	7	80	53	2	8	17	0	0	0
1	B	7	80	53	2	8	17	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	21	13	1	7	0	0	0
2	D	2	21	13	1	7	0	0	0

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



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Zn 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	26	Total O 26 26	0	0
5	B	37	Total O 37 37	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. 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. 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: vancomycin

Chain A: 



- Molecule 1: vancomycin

Chain B: 



- Molecule 2: vancosamine-(1-2)-beta-D-glucopyranose

Chain C: 



- Molecule 2: vancosamine-(1-2)-beta-D-glucopyranose

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	35.90Å 35.90Å 55.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.13 – 1.00 27.13 – 1.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (27.13-1.00) 99.5 (27.13-1.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.27 (at 1.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.097 , 0.104 0.171 , 0.177	Depositor DCC
R_{free} test set	1440 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	4.5	Xtrriage
Anisotropy	0.047	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 79.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.489 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	274	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.04% 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: ZN, BGC, GHP, RER, EDO, OMZ, MLU, 3FG, OMY

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	3.53	1/7 (14.3%)	2.21	0/8
1	B	3.06	1/7 (14.3%)	1.59	0/8
All	All	3.31	2/14 (14.3%)	1.93	0/16

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3	ASN	CA-CB	6.02	1.68	1.53
1	A	3	ASN	CA-CB	5.54	1.67	1.53

There are no bond angle outliers.

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	80	0	47	2	2
1	B	80	0	47	1	0
2	C	21	0	22	0	0
2	D	21	0	22	0	0
3	A	4	0	6	1	0
3	B	4	0	6	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	26	0	0	2	3
5	B	37	0	0	1	1
All	All	274	0	150	4	4

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 11.

All (4) 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:3:ASN:HD22	1:A:4:GHP:H	1.24	0.83
1:A:7:3FG:O	5:A:201:HOH:O	1.98	0.81
1:B:7:3FG:OXT	5:B:201:HOH:O	2.00	0.79
3:A:103:EDO:H22	5:A:202:HOH:O	2.08	0.53

All (4) 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)
5:B:215:HOH:O	5:B:227:HOH:O[6_445]	1.35	0.85
5:A:202:HOH:O	5:A:212:HOH:O[3_555]	1.78	0.42
1:A:7:3FG:OXT	5:A:202:HOH:O[2_555]	1.90	0.30
1:A:1:MLU:CN	5:A:216:HOH:O[9_444]	2.16	0.04

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	1/7 (14%)	0	0	1 (100%)	0 0
1	B	1/7 (14%)	0	0	1 (100%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2/14 (14%)	0	0	2 (100%)	0 0

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	B	3	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	1/1 (100%)	0	1 (100%)	0 0
1	B	1/1 (100%)	1 (100%)	0	100 100
All	All	2/2 (100%)	1 (50%)	1 (50%)	0 0

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	GHP	B	5	1	10,11,12	1.60	2 (20%)	11,14,16	1.20	1 (9%)
1	MLU	A	1	1,4	7,8,9	1.04	0	6,9,11	0.65	0
1	GHP	A	4	1,2	10,11,12	1.79	3 (30%)	11,14,16	1.14	1 (9%)
1	MLU	B	1	1,4	7,8,9	1.14	1 (14%)	6,9,11	0.81	0
1	GHP	B	4	1,2	10,11,12	1.84	3 (30%)	11,14,16	1.13	0
1	OMZ	B	2	1	12,14,15	1.57	3 (25%)	17,19,21	1.27	3 (17%)
1	OMZ	A	2	1	12,14,15	1.53	3 (25%)	17,19,21	1.17	2 (11%)
1	OMY	A	6	1	12,14,15	1.52	2 (16%)	17,19,21	1.18	3 (17%)
1	3FG	B	7	1	9,13,13	1.79	3 (33%)	13,18,18	0.84	1 (7%)
1	GHP	A	5	1	10,11,12	1.55	3 (30%)	11,14,16	1.27	1 (9%)
1	3FG	A	7	1	9,13,13	1.69	2 (22%)	13,18,18	0.76	0
1	OMY	B	6	1	12,14,15	1.58	3 (25%)	17,19,21	1.18	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
1	GHP	B	5	1	-	0/4/6/8	0/1/1/1
1	MLU	A	1	1,4	-	0/5/8/10	-
1	GHP	A	4	1,2	-	2/4/6/8	0/1/1/1
1	MLU	B	1	1,4	-	1/5/8/10	-
1	GHP	B	4	1,2	-	2/4/6/8	0/1/1/1
1	OMZ	B	2	1	-	1/9/10/12	0/1/1/1
1	OMZ	A	2	1	-	1/9/10/12	0/1/1/1
1	OMY	A	6	1	-	1/9/10/12	0/1/1/1
1	3FG	B	7	1	-	1/4/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GHP	A	5	1	-	0/4/6/8	0/1/1/1
1	3FG	A	7	1	-	1/4/8/8	0/1/1/1
1	OMY	B	6	1	-	1/9/10/12	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	GHP	C1-CA	3.68	1.56	1.52
1	B	4	GHP	C1-CA	3.65	1.56	1.52
1	B	2	OMZ	CD1-CG	2.98	1.43	1.39
1	A	5	GHP	CA-C	2.91	1.57	1.51
1	B	5	GHP	CA-C	2.91	1.57	1.51
1	A	2	OMZ	CG-CB	2.85	1.56	1.51
1	A	7	3FG	CG1-CD1	2.71	1.43	1.39
1	B	5	GHP	C1-CA	2.59	1.55	1.52
1	B	4	GHP	C3-C2	2.58	1.43	1.38
1	B	6	OMY	OCZ-CZ	2.55	1.41	1.36
1	A	6	OMY	CD2-CE2	2.54	1.43	1.38
1	B	7	3FG	CG1-CD1	2.49	1.42	1.39
1	B	7	3FG	CG2-CD2	2.47	1.42	1.39
1	A	6	OMY	OCZ-CZ	2.44	1.41	1.36
1	B	6	OMY	CD2-CG	2.42	1.42	1.39
1	A	4	GHP	C3-C2	2.36	1.43	1.38
1	A	2	OMZ	CD1-CG	2.35	1.42	1.39
1	A	7	3FG	CZ-CD1	2.35	1.42	1.39
1	B	2	OMZ	CG-CB	2.30	1.55	1.51
1	A	4	GHP	CA-C	2.21	1.55	1.51
1	B	7	3FG	CZ-CD1	2.20	1.42	1.39
1	A	2	OMZ	CE2-CZ	2.13	1.43	1.39
1	B	1	MLU	CA-N	2.12	1.51	1.47
1	A	5	GHP	C6-C5	2.08	1.42	1.38
1	A	5	GHP	C2-C1	2.08	1.42	1.39
1	B	4	GHP	CA-C	2.05	1.55	1.51
1	B	6	OMY	CZ-CE1	2.04	1.41	1.39
1	B	2	OMZ	CD1-CE1	2.00	1.41	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	OMY	CG-CB-CA	-3.10	107.34	111.49
1	B	2	OMZ	CD1-CE1-CL	3.00	123.33	118.49
1	A	6	OMY	CG-CB-CA	-2.80	107.73	111.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	OMZ	CE2-CZ-CE1	2.37	120.85	118.55
1	A	2	OMZ	CD1-CE1-CL	2.36	122.30	118.49
1	A	4	GHP	C3-C2-C1	-2.24	118.94	121.20
1	B	6	OMY	CE2-CZ-CE1	2.16	120.65	118.55
1	A	6	OMY	CE2-CZ-CE1	2.15	120.63	118.55
1	B	2	OMZ	CD1-CE1-CZ	-2.12	119.69	120.91
1	A	5	GHP	C2-C1-CA	-2.10	117.27	120.65
1	A	2	OMZ	CZ-CE1-CL	-2.07	115.64	119.53
1	A	6	OMY	CD1-CE1-CZ	-2.05	119.72	120.91
1	B	5	GHP	C2-C1-CA	-2.04	117.36	120.65
1	B	7	3FG	CG2-CB-CG1	2.02	120.95	118.08

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	1	MLU	O-C-CA-CB
1	A	6	OMY	O-C-CA-CB
1	B	6	OMY	O-C-CA-CB
1	B	7	3FG	C-CA-CB-CG2
1	A	7	3FG	C-CA-CB-CG2
1	A	4	GHP	C6-C1-CA-C
1	B	4	GHP	C6-C1-CA-C
1	B	2	OMZ	O-C-CA-CB
1	A	2	OMZ	O-C-CA-CB
1	A	4	GHP	C2-C1-CA-C
1	B	4	GHP	C2-C1-CA-C

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	MLU	0	1
1	A	4	GHP	1	0
1	B	7	3FG	1	0
1	A	7	3FG	1	1

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	BGC	C	1	1,2	11,11,12	1.08	0	15,15,17	0.44	0
2	RER	C	2	2	6,10,11	1.47	1 (16%)	6,15,17	0.57	0
2	BGC	D	1	1,2	11,11,12	0.95	0	15,15,17	0.57	0
2	RER	D	2	2	6,10,11	1.43	1 (16%)	6,15,17	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	BGC	C	1	1,2	-	0/2/19/22	0/1/1/1
2	RER	C	2	2	-	-	0/1/1/1
2	BGC	D	1	1,2	-	0/2/19/22	0/1/1/1
2	RER	D	2	2	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	RER	C5A-C5	3.24	1.59	1.51
2	D	2	RER	C5A-C5	3.24	1.59	1.51

There are no bond angle outliers.

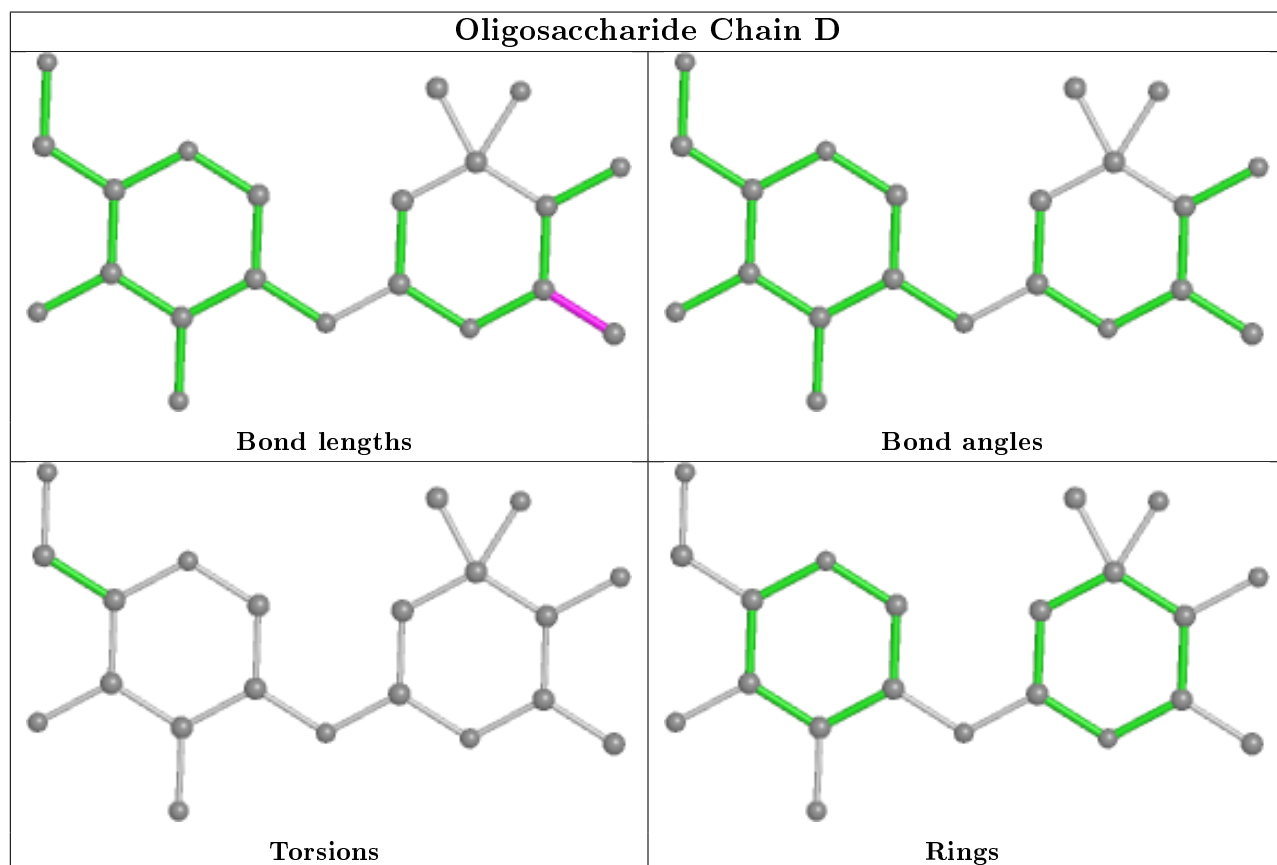
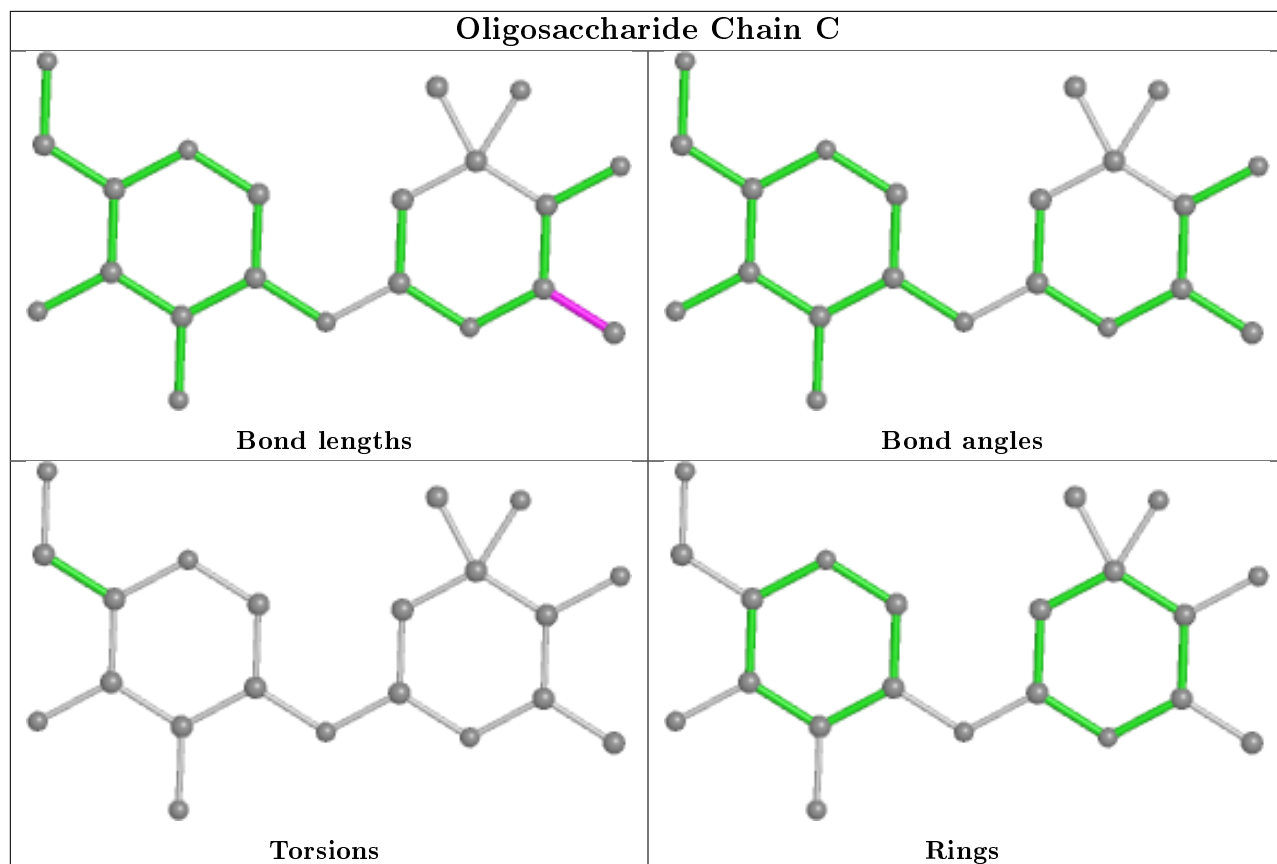
There are no chirality outliers.

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 [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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
3	EDO	A	103	-	3,3,3	0.35	0	2,2,2	0.27	0
3	EDO	B	104	-	3,3,3	0.37	0	2,2,2	0.21	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	EDO	A	103	-	-	0/1/1/1	-
3	EDO	B	104	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

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
3	A	103	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

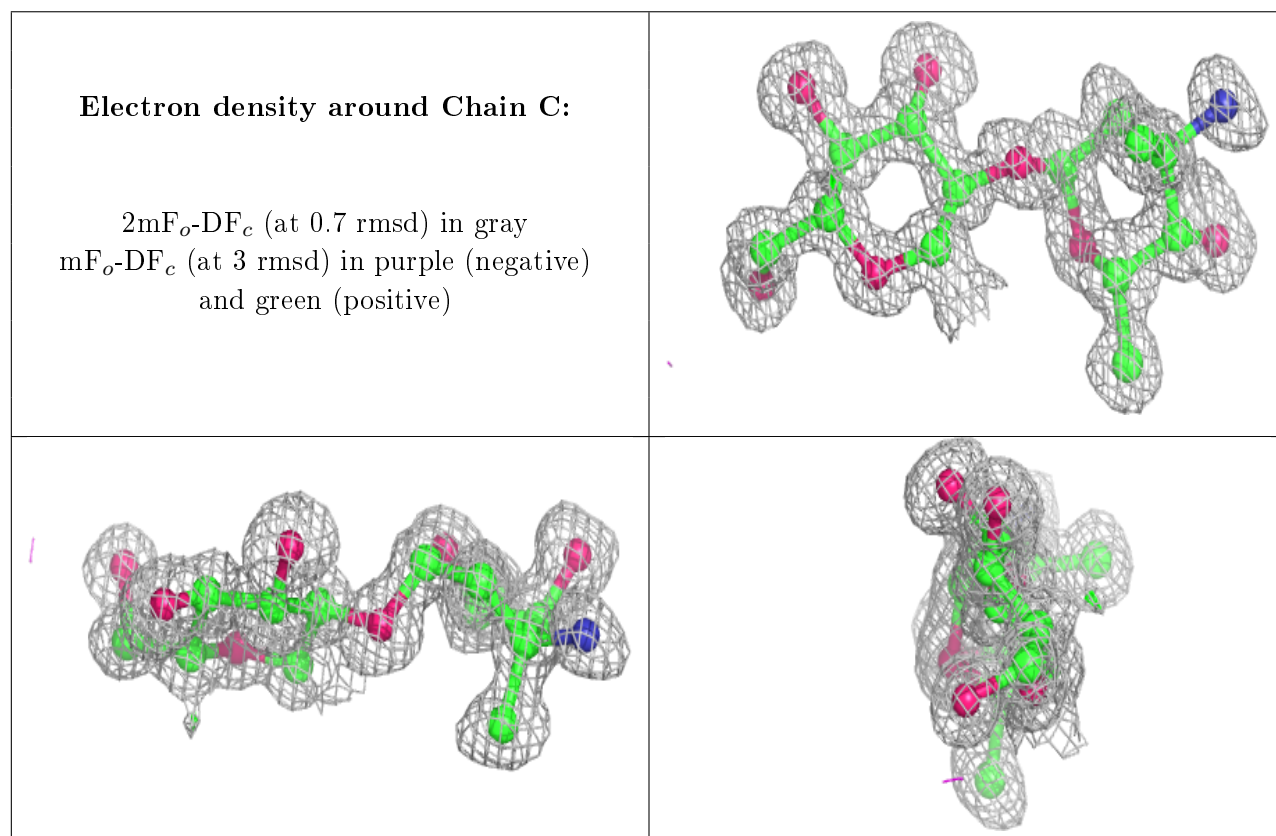
6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

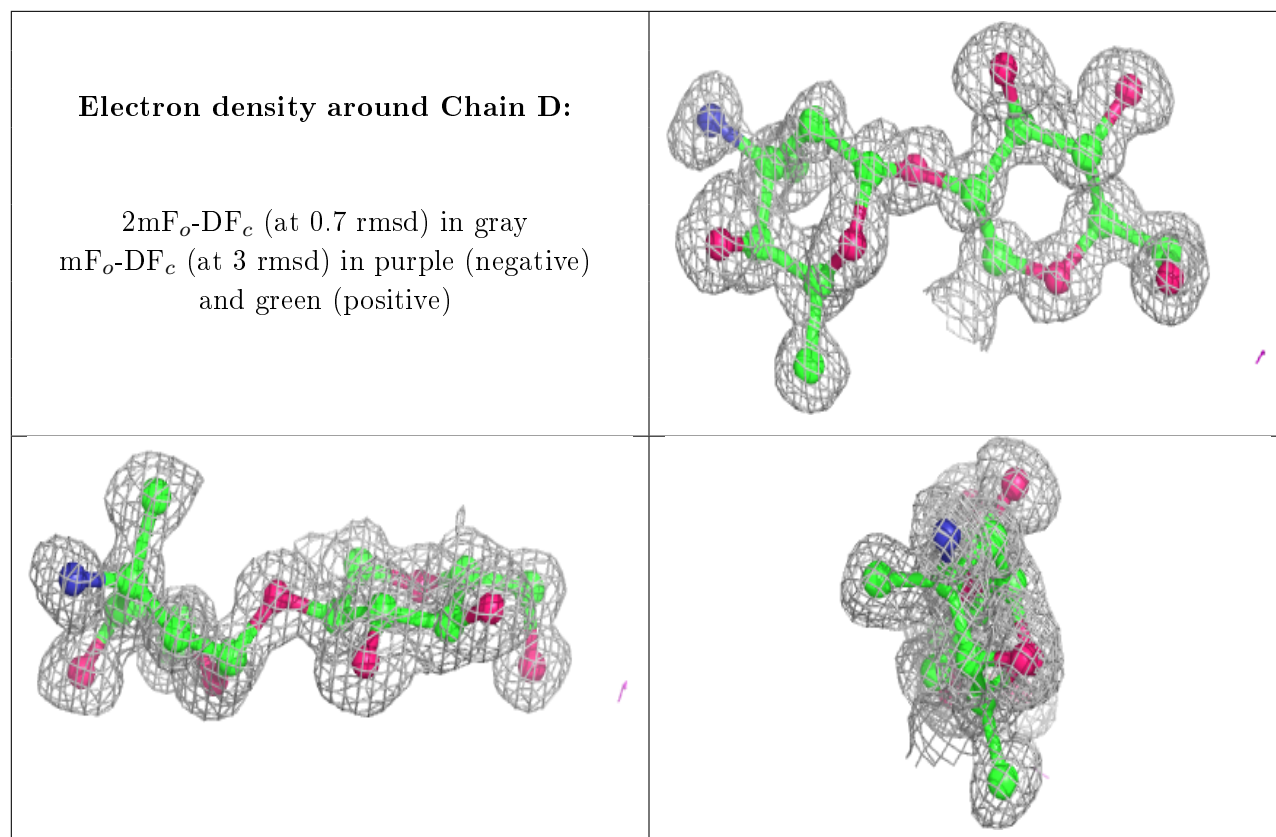
Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.