Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 11:21 AM JST

PDB ID	:	5Z1X
Title	:	Crystal Structure of Laccase from Cerrena sp. RSD1
Authors	:	Lee, C.C.; Wu, M.H.; Ho, T.H.; Wang, A.H.J.
Deposited on	:	2017-12-28
Resolution	:	1.38 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 (i) 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 (1)) were used in the production of this report:

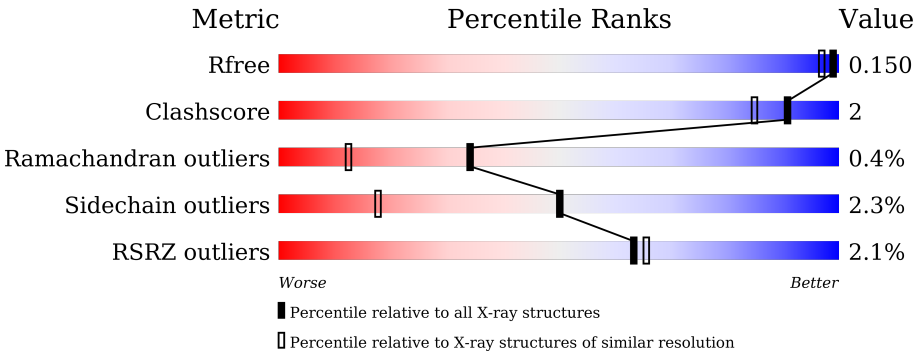
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.38 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	2907 (1.40-1.36)
Clashscore	141614	3037 (1.40-1.36)
Ramachandran outliers	138981	2970 (1.40-1.36)
Sidechain outliers	138945	2969 (1.40-1.36)
RSRZ outliers	127900	2846 (1.40-1.36)

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 <=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	495	2% 95% 5%
1	B	495	2% 95% .
2	C	2	50% 50%
2	D	2	50% 50%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 9234 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.

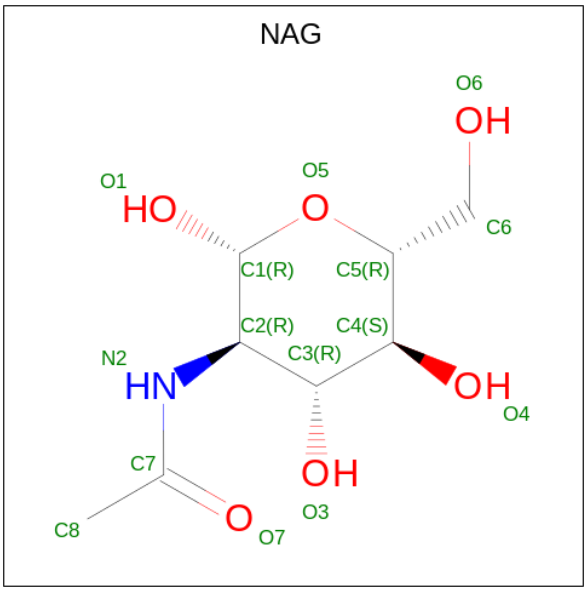
- Molecule 1 is a protein called Laccase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3744	2378	646	713	7			
1	B	495	Total	C	N	O	S	0	0	0
			3744	2378	646	713	7			

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

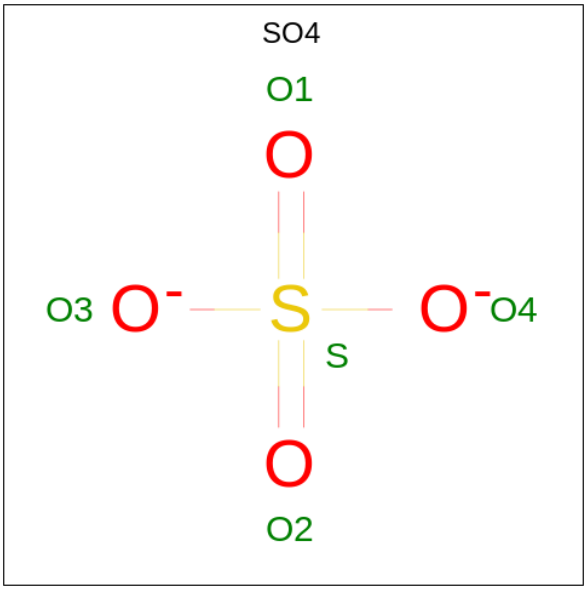
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



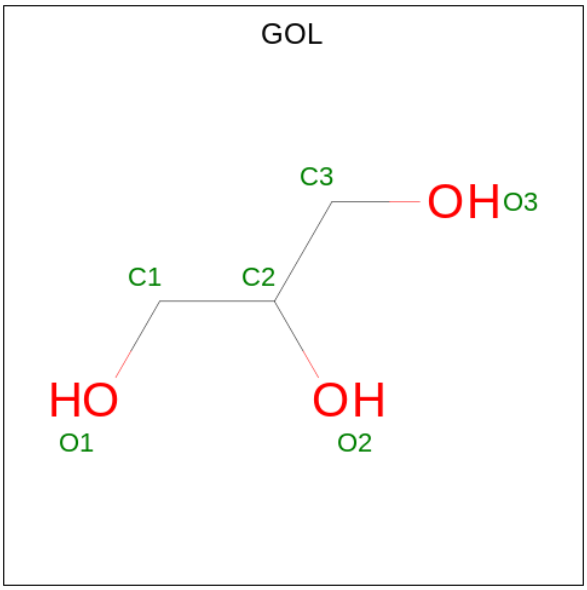
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

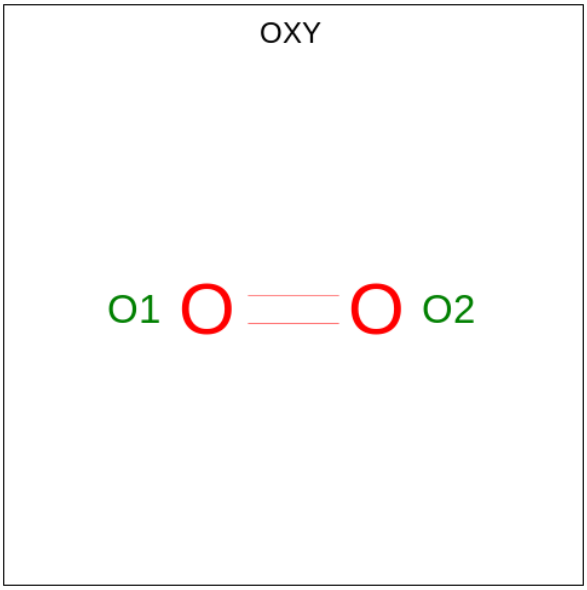
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	4	Total Cu 4 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	4	Total Cu 4 4	0	0

- Molecule 7 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 2 2	0	0
7	B	1	Total O 2 2	0	0

- Molecule 8 is water.

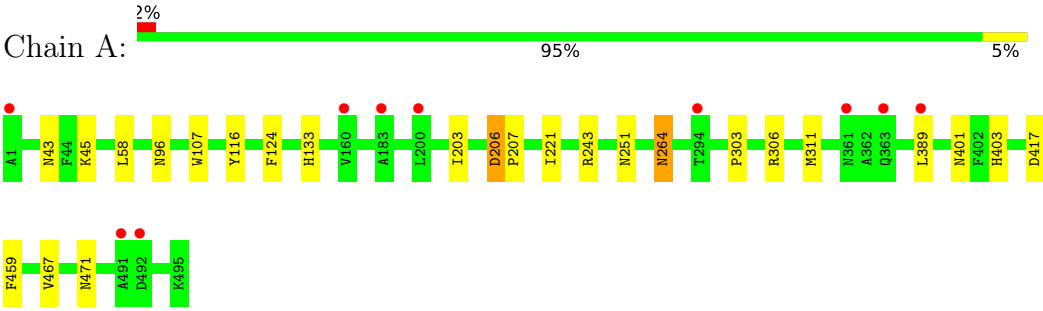
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	843	Total O 843 843	0	0
8	B	753	Total O 753 753	0	0

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.

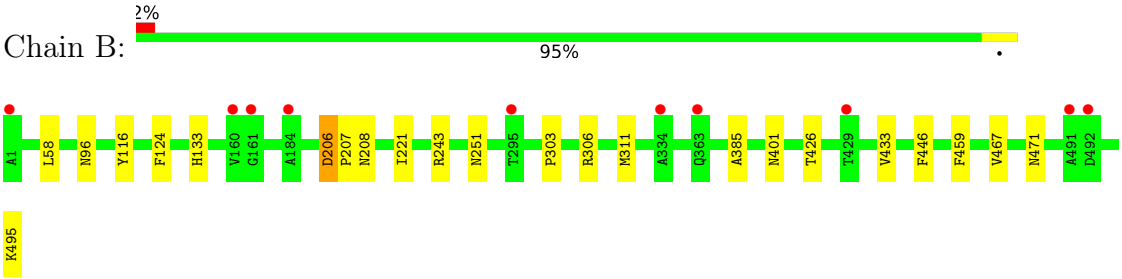
• Molecule 1: Laccase

Chain A:



• Molecule 1: Laccase

Chain B:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.63Å 88.80Å 147.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.38 26.66 – 1.38	Depositor EDS
% Data completeness (in resolution range)	98.6 (25.00-1.38) 98.6 (26.66-1.38)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.19 (at 1.38Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.126 , 0.149 0.126 , 0.150	Depositor DCC
R_{free} test set	11421 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	14.1	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 43.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	9234	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CU, GOL, NAG, OXY, 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	0.27	0/3848	0.56	0/5283
1	B	0.27	0/3848	0.55	0/5283
All	All	0.27	0/7696	0.56	0/10566

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	3744	0	3617	13	0
1	B	3744	0	3617	12	0
2	C	28	0	25	0	0
2	D	28	0	25	2	0
3	A	14	0	13	1	0
3	B	14	0	13	1	0
4	A	15	0	0	0	0
4	B	15	0	0	0	0
5	A	12	0	16	0	0
5	B	12	0	16	0	0
6	A	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	4	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
8	A	843	0	0	2	0
8	B	753	0	0	4	0
All	All	9234	0	7342	25	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.

All (25) 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:B:495:LYS:C	8:B:604:HOH:O	1.65	1.28
1:B:311:MET:SD	8:B:1334:HOH:O	2.50	0.69
1:A:264:ASN:H	1:A:264:ASN:HD22	1.42	0.68
1:A:401:ASN:ND2	8:A:601:HOH:O	2.33	0.61
1:B:401:ASN:ND2	8:B:601:HOH:O	2.35	0.59
1:B:306:ARG:NH2	8:B:602:HOH:O	2.39	0.56
1:A:306:ARG:NH2	8:A:603:HOH:O	2.39	0.55
1:B:206:ASP:HB3	1:B:207:PRO:CD	2.42	0.49
1:B:467:VAL:HB	3:B:503:NAG:H82	1.96	0.48
1:A:207:PRO:HA	1:A:264:ASN:HD21	1.79	0.48
1:A:206:ASP:HB3	1:A:207:PRO:CD	2.44	0.47
1:A:303:PRO:O	1:A:306:ARG:NH2	2.49	0.46
1:A:467:VAL:HB	3:A:503:NAG:H82	1.97	0.46
1:A:133:HIS:CD2	1:A:221:ILE:HB	2.52	0.45
1:A:43:ASN:ND2	1:A:45:LYS:HE3	2.32	0.44
1:B:133:HIS:CD2	1:B:221:ILE:HB	2.53	0.44
1:B:206:ASP:HB3	1:B:207:PRO:HD3	2.00	0.44
1:B:385:ALA:CB	2:D:1:NAG:H82	2.48	0.43
1:B:385:ALA:HB1	2:D:1:NAG:H82	2.01	0.42
1:B:426:THR:HA	1:B:433:VAL:HG21	2.02	0.42
1:A:107:TRP:CE3	1:A:203:ILE:HG22	2.55	0.42
1:B:303:PRO:O	1:B:306:ARG:NH2	2.53	0.42
1:A:306:ARG:NE	1:A:417:ASP:O	2.53	0.41
1:A:311:MET:O	1:A:403:HIS:HE1	2.04	0.41
1:A:206:ASP:HB3	1:A:207:PRO:HD3	2.02	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	493/495 (100%)	483 (98%)	8 (2%)	2 (0%)	34 12
1	B	493/495 (100%)	483 (98%)	8 (2%)	2 (0%)	34 12
All	All	986/990 (100%)	966 (98%)	16 (2%)	4 (0%)	34 12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ASP
1	B	206	ASP
1	A	58	LEU
1	B	58	LEU

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	406/406 (100%)	396 (98%)	10 (2%)	47 14
1	B	406/406 (100%)	397 (98%)	9 (2%)	52 19
All	All	812/812 (100%)	793 (98%)	19 (2%)	50 18

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	116	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	124	PHE
1	A	243	ARG
1	A	251	ASN
1	A	264	ASN
1	A	389	LEU
1	A	446	PHE
1	A	459	PHE
1	A	471	ASN
1	B	96	ASN
1	B	116	TYR
1	B	124	PHE
1	B	208	ASN
1	B	243	ARG
1	B	251	ASN
1	B	446	PHE
1	B	459	PHE
1	B	471	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	47	ASN
1	A	70	GLN
1	A	84	GLN
1	A	96	ASN
1	A	115	GLN
1	A	158	GLN
1	A	227	ASN
1	A	251	ASN
1	A	252	GLN
1	A	264	ASN
1	A	301	GLN
1	A	401	ASN
1	A	403	HIS
1	A	471	ASN
1	A	481	ASN
1	B	43	ASN
1	B	70	GLN
1	B	84	GLN
1	B	96	ASN
1	B	115	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	158	GLN
1	B	208	ASN
1	B	227	ASN
1	B	237	GLN
1	B	251	ASN
1	B	252	GLN
1	B	301	GLN
1	B	401	ASN
1	B	403	HIS
1	B	471	ASN
1	B	481	ASN
1	B	482	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

6 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	NAG	D	1	1,2	14,14,15	0.48	0	17,19,21	0.93	1 (5%)
3	NAG	A	503	1	14,14,15	0.52	0	17,19,21	0.83	0
2	NAG	D	2	2	14,14,15	0.51	0	17,19,21	0.69	0
2	NAG	C	2	2	14,14,15	0.55	0	17,19,21	0.65	0
3	NAG	B	503	1	14,14,15	0.46	0	17,19,21	1.01	1 (5%)
2	NAG	C	1	1,2	14,14,15	0.49	0	17,19,21	0.91	1 (5%)

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	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
3	NAG	A	503	1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
3	NAG	B	503	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	503	NAG	C1-O5-C5	3.09	116.38	112.19
2	D	1	NAG	C1-O5-C5	2.97	116.21	112.19
2	C	1	NAG	C1-O5-C5	2.74	115.91	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	2	0
3	A	503	NAG	1	0
3	B	503	NAG	1	0

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	NAG	C	1	1,2	14,14,15	0.49	0	17,19,21	0.91	1 (5%)
2	NAG	C	2	2	14,14,15	0.55	0	17,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	D	1	1,2	14,14,15	0.48	0	17,19,21	0.93	1 (5%)
2	NAG	D	2	2	14,14,15	0.51	0	17,19,21	0.69	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	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	NAG	C1-O5-C5	2.97	116.21	112.19
2	C	1	NAG	C1-O5-C5	2.74	115.91	112.19

There are no chirality outliers.

There are no torsion outliers.

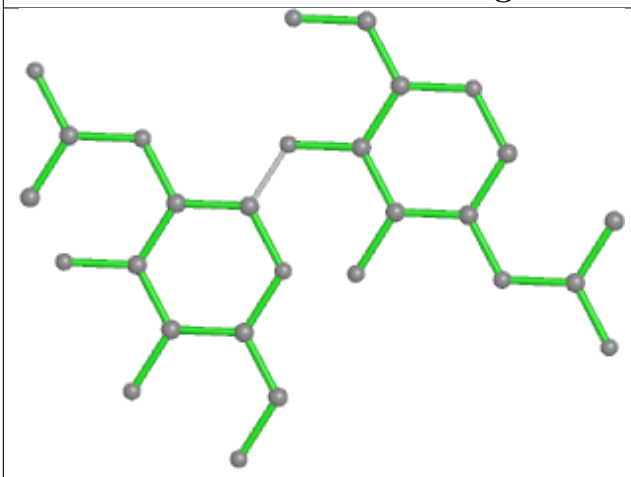
There are no ring outliers.

1 monomer is involved in 2 short contacts:

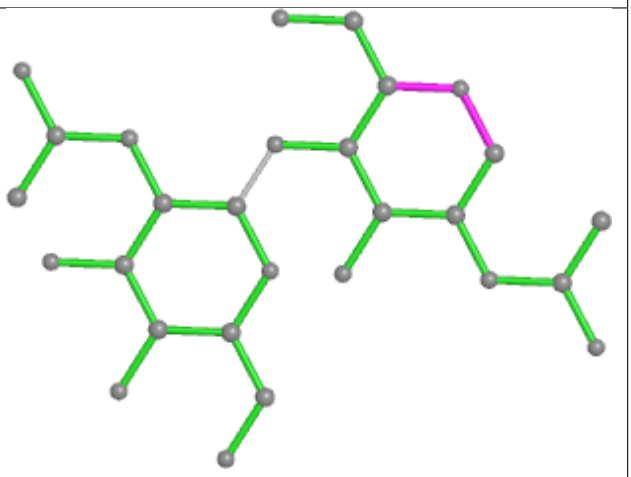
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	2	0

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

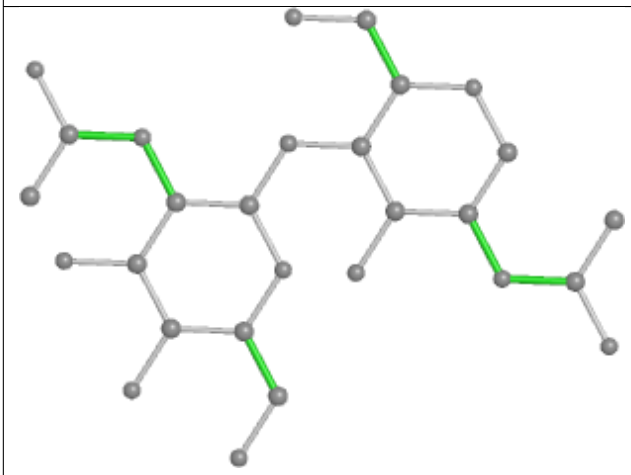
Oligosaccharide Chain C



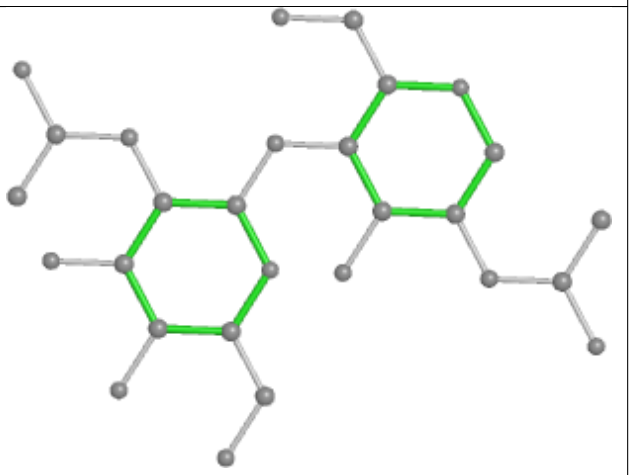
Bond lengths



Bond angles

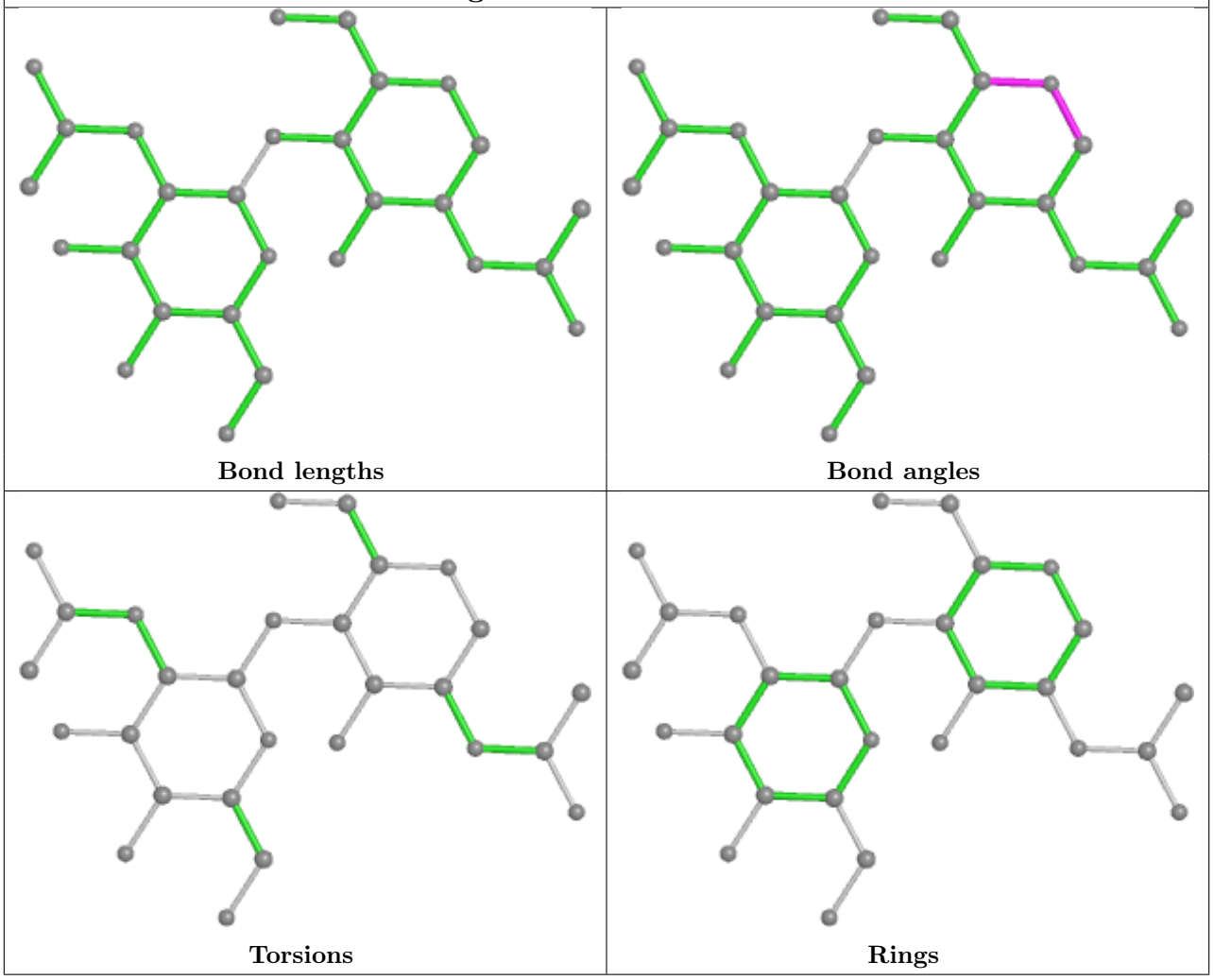


Torsions



Rings

Oligosaccharide Chain D



5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 8 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
7	OXY	A	513	6	1,1,1	0.21	0	-		
3	NAG	A	503	1	14,14,15	0.52	0	17,19,21	0.83	0
4	SO4	B	506	-	4,4,4	0.33	0	6,6,6	0.05	0
5	GOL	B	507	-	5,5,5	0.27	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	B	504	-	4,4,4	0.32	0	6,6,6	0.09	0
4	SO4	A	504	-	4,4,4	0.32	0	6,6,6	0.06	0
7	OXY	B	513	6	1,1,1	0.06	0	-		
4	SO4	A	505	-	4,4,4	0.35	0	6,6,6	0.10	0
4	SO4	B	505	-	4,4,4	0.33	0	6,6,6	0.05	0
5	GOL	A	507	-	5,5,5	0.27	0	5,5,5	0.35	0
5	GOL	A	508	-	5,5,5	0.31	0	5,5,5	0.37	0
3	NAG	B	503	1	14,14,15	0.46	0	17,19,21	1.01	1 (5%)
4	SO4	A	506	-	4,4,4	0.33	0	6,6,6	0.08	0
5	GOL	B	508	-	5,5,5	0.29	0	5,5,5	0.28	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
3	NAG	A	503	1	-	0/6/23/26	0/1/1/1
5	GOL	B	507	-	-	1/4/4/4	-
5	GOL	A	507	-	-	2/4/4/4	-
5	GOL	A	508	-	-	1/4/4/4	-
3	NAG	B	503	1	-	0/6/23/26	0/1/1/1
5	GOL	B	508	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	503	NAG	C1-O5-C5	3.09	116.38	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	507	GOL	C1-C2-C3-O3
5	A	507	GOL	O2-C2-C3-O3
5	A	508	GOL	C1-C2-C3-O3
5	B	507	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	NAG	1	0
3	B	503	NAG	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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	495/495 (100%)	-0.23	11 (2%)	62	64	9, 14, 21, 33	0
1	B	495/495 (100%)	-0.14	10 (2%)	65	68	10, 15, 24, 34	0
All	All	990/990 (100%)	-0.18	21 (2%)	63	65	9, 15, 23, 34	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	VAL	6.9
1	B	295	THR	4.8
1	A	363	GLN	4.6
1	B	1	ALA	4.2
1	A	1	ALA	4.1
1	A	492	ASP	3.6
1	B	363	GLN	3.4
1	B	492	ASP	3.3
1	A	389	LEU	3.1
1	A	160	VAL	3.1
1	B	491	ALA	3.0
1	B	184	ALA	2.8
1	A	491	ALA	2.5
1	B	161	GLY	2.4
1	B	429	THR	2.4
1	A	200	LEU	2.3
1	A	447	LEU	2.3
1	B	334	ALA	2.2
1	A	361	ASN	2.2
1	A	294	THR	2.2
1	A	183	ALA	2.0

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, 95^{th} 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	NAG	D	2	14/15	0.82	0.21	25,33,41,44	0
2	NAG	C	2	14/15	0.84	0.25	21,26,33,34	0
3	NAG	A	503	14/15	0.88	0.16	20,23,28,30	0
3	NAG	B	503	14/15	0.90	0.14	21,24,28,29	0
2	NAG	C	1	14/15	0.96	0.07	16,18,21,23	0
2	NAG	D	1	14/15	0.97	0.07	20,23,26,28	0

6.3 Carbohydrates (i)

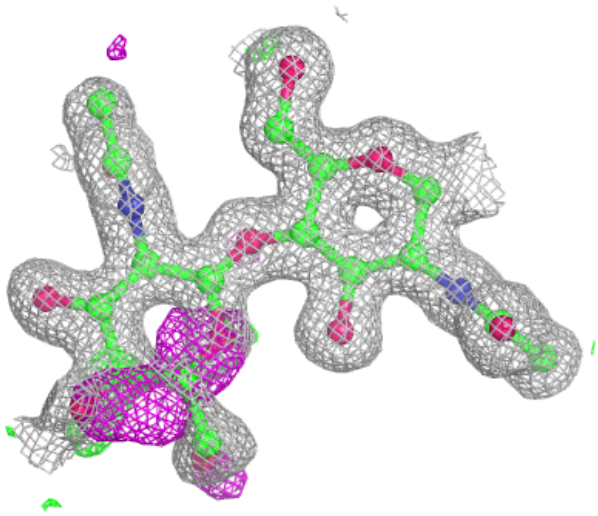
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

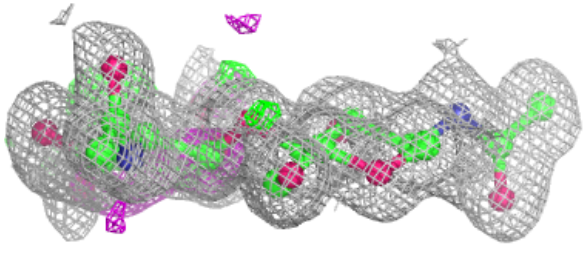
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	D	2	14/15	0.82	0.21	25,33,41,44	0
2	NAG	C	2	14/15	0.84	0.25	21,26,33,34	0
2	NAG	C	1	14/15	0.96	0.07	16,18,21,23	0
2	NAG	D	1	14/15	0.97	0.07	20,23,26,28	0

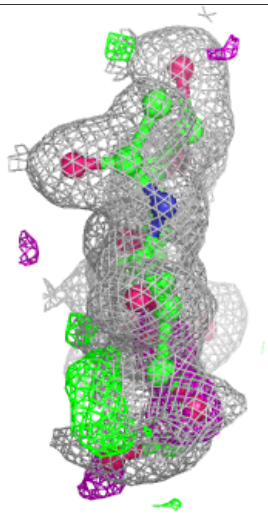
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

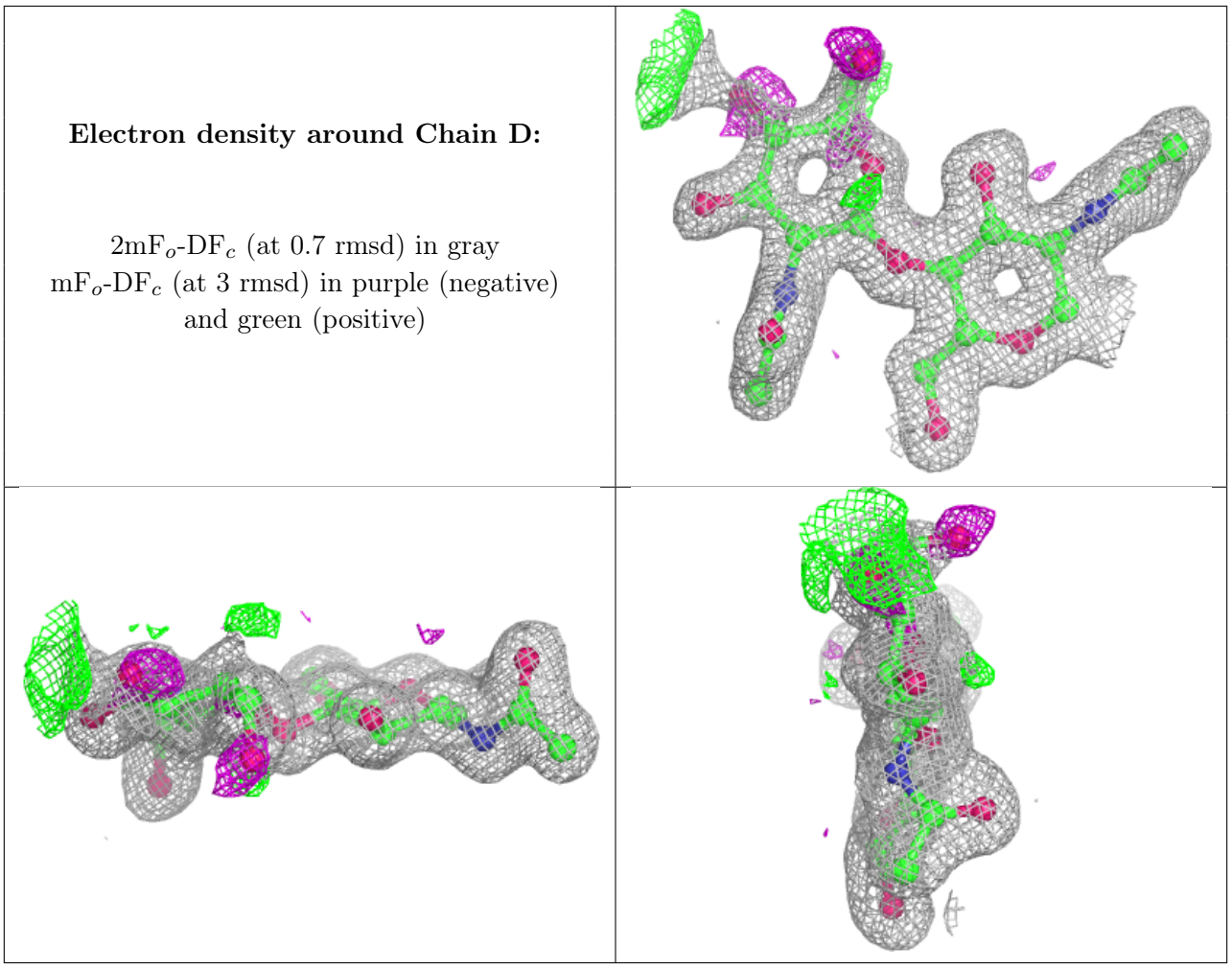






Electron density around Chain D:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.4 Ligands

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, 95^{th} 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
7	OXY	B	513	2/2	0.74	0.28	45,45,45,61	0
5	GOL	A	508	6/6	0.83	0.13	17,21,27,28	0
5	GOL	B	507	6/6	0.85	0.19	30,31,35,35	0
5	GOL	A	507	6/6	0.85	0.12	30,32,35,36	0
5	GOL	B	508	6/6	0.88	0.11	17,21,26,27	0
3	NAG	A	503	14/15	0.88	0.16	20,23,28,30	0
3	NAG	B	503	14/15	0.90	0.14	21,24,28,29	0
4	SO4	B	505	5/5	0.91	0.26	54,57,63,65	0
4	SO4	A	505	5/5	0.94	0.23	28,29,31,32	0
4	SO4	A	506	5/5	0.94	0.18	33,37,40,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	OXY	A	513	2/2	0.96	0.11	22,22,22,26	0
4	SO4	B	506	5/5	0.98	0.17	34,36,41,41	0
4	SO4	A	504	5/5	0.99	0.11	27,29,32,33	0
4	SO4	B	504	5/5	0.99	0.13	29,30,32,34	0
6	CU	A	511	1/1	1.00	0.02	13,13,13,13	0
6	CU	A	512	1/1	1.00	0.02	17,17,17,17	0
6	CU	B	509	1/1	1.00	0.01	12,12,12,12	0
6	CU	B	510	1/1	1.00	0.01	15,15,15,15	0
6	CU	B	511	1/1	1.00	0.03	14,14,14,14	0
6	CU	B	512	1/1	1.00	0.01	19,19,19,19	0
6	CU	A	509	1/1	1.00	0.01	12,12,12,12	0
6	CU	A	510	1/1	1.00	0.01	13,13,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.