WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Mar 5, 2024 – 01:55 pm GMT

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PDB ID	:	8AWK
Title	:	Structure of recombinant human beta-glucocerebrosidase in complex with D-carbaxylosyl chloride
Authors	:	Rowland, R.J.; Davies, G.J.
Deposited on	:	2022-08-30
Resolution	:	1.58 Å(reported)

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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 1.58 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.
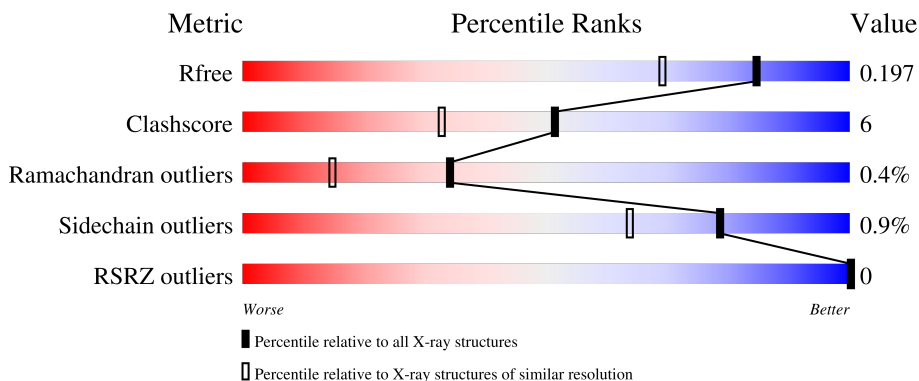
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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	AAA	497	91% 9%
2	AaA	4	75% 25%

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
4	EDO	AAA	513	-	-	X	-

2　Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 9182 atoms, of which 4310 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 Lysosomal acid glucosylceramidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	497	8234	2657	4096	718	747	16	222	25	0

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	AaA	4	100	28	50	2	20	11	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
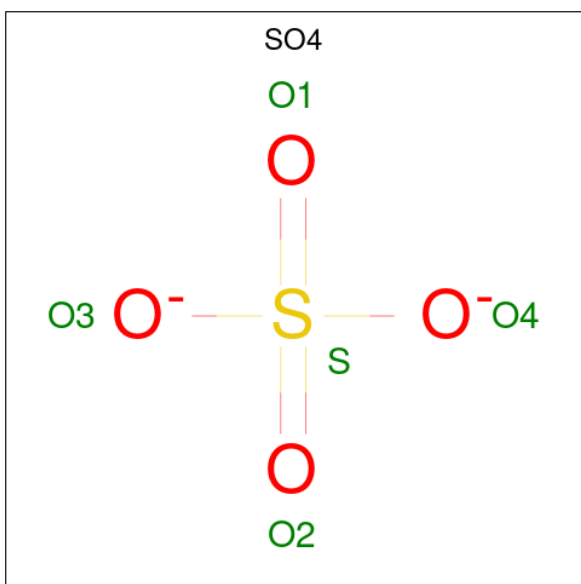
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	O	S	0	0
			5	4	1		
3	AAA	1	Total	O	S	0	0
			5	4	1		
3	AAA	1	Total	O	S	0	0
			5	4	1		

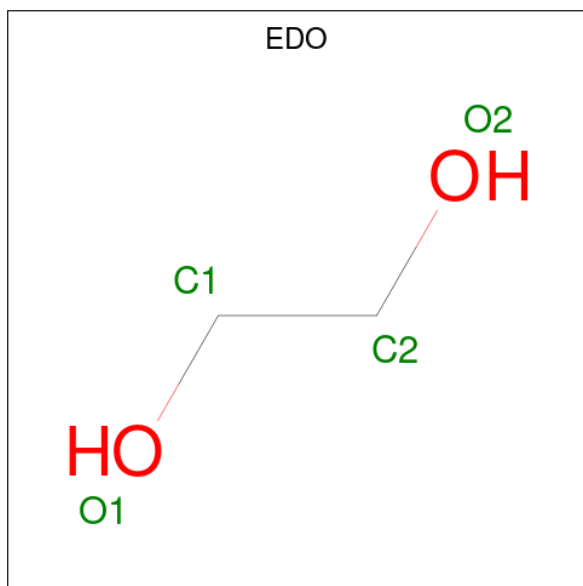- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

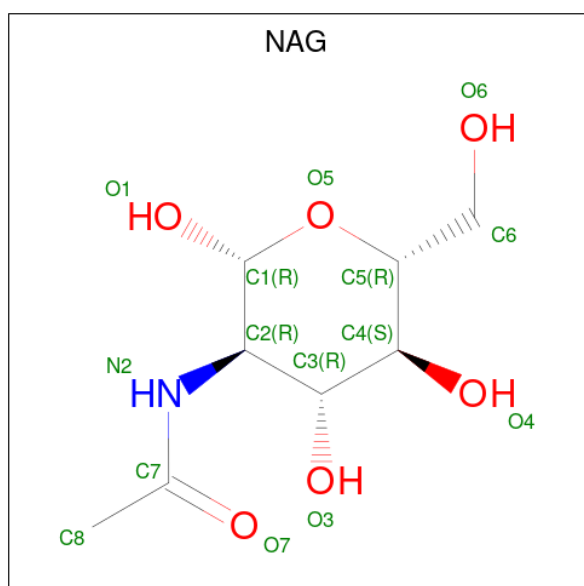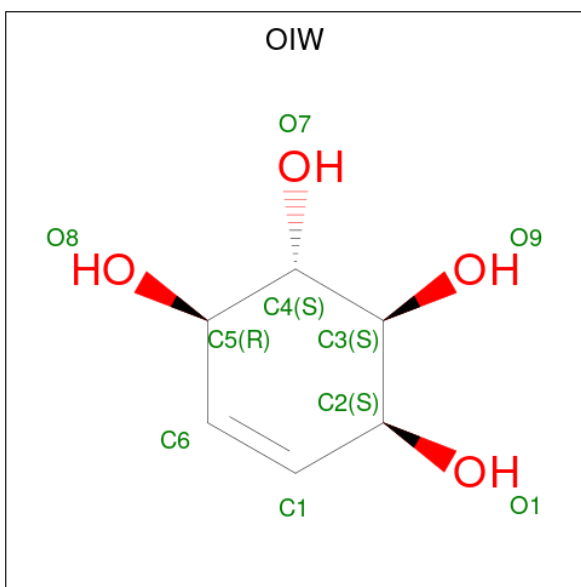| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	AAA	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
5	AAA	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

- Molecule 6 is (2 {S},3 {S},4 {R})-cyclohex-5-ene-1,2,3,4-tetrol (three-letter code: OIW) (formula: $C_6H_{10}O_4$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	AAA	1	Total	C	H	O	2	0
			19	6	10	3		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	1	Total	Na	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	547	Total	O	0	0
			547	547		

3 Residue-property plots ⓘ

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: Lysosomal acid glucosylceramidase

Chain AAA:
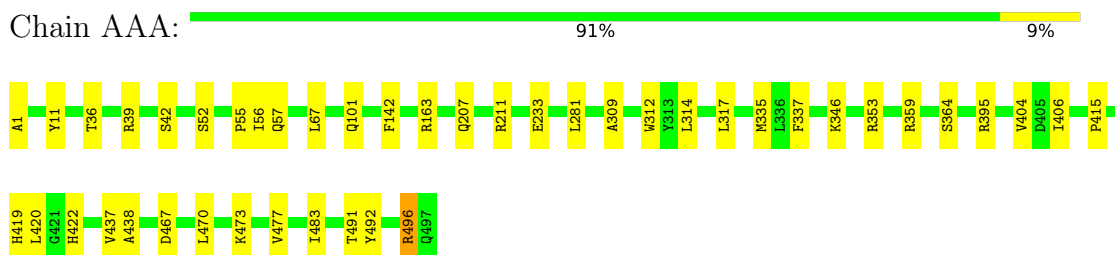
• Molecule 2: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AaA:
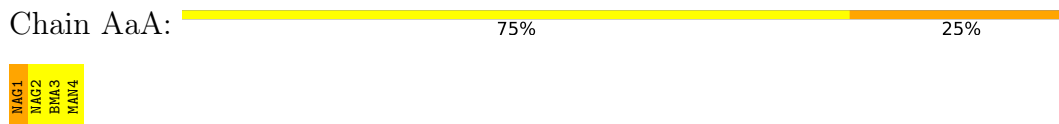
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.28Å 76.47Å 68.47Å 90.00° 102.05° 90.00°	Depositor
Resolution (Å)	52.16 – 1.58 52.10 – 1.58	Depositor EDS
% Data completeness (in resolution range)	99.9 (52.16-1.58) 100.0 (52.10-1.58)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.151 , 0.185 0.165 , 0.197	Depositor DCC
R_{free} test set	3644 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	17.3	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 47.2	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	9182	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: MAN, SO4, NA, EDO, BMA, OIW, NAG

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	AAA	0.67	0/4257	0.80	1/5797 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	496	ARG	NE-CZ-NH2	-5.10	117.75	120.30

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	AAA	4138	4096	4054	46	1
2	AaA	50	50	43	0	1
3	AAA	15	0	0	1	0
4	AAA	84	126	126	9	0
5	AAA	28	28	26	1	0
6	AAA	9	10	0	0	0
7	AAA	1	0	0	0	0
8	AAA	547	0	0	8	0
All	All	4872	4310	4249	47	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 6.

The worst 5 of 47 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:AAA:404[A]:VAL:HG11	1:AAA:406[A]:ILE:HD11	1.56	0.87
1:AAA:317[B]:LEU:C	1:AAA:317[B]:LEU:HD23	2.01	0.79
1:AAA:142:PHE:O	1:AAA:211[B]:ARG:NH1	2.15	0.78
1:AAA:404[A]:VAL:CG1	1:AAA:406[A]:ILE:CD1	2.62	0.77
1:AAA:395[B]:ARG:NH1	8:AAA:601:HOH:O	2.18	0.76

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:AAA:473:LYS:HZ3	2:AaA:1:NAG:HO3[1_455]	0.98	0.62

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	AAA	519/497 (104%)	506 (98%)	11 (2%)	2 (0%)	34	15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	233	GLU
1	AAA	281	LEU

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	AAA	448/424 (106%)	444 (99%)	4 (1%)	78	64

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	312	TRP
1	AAA	335	MET
1	AAA	415	PRO
1	AAA	420	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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	AaA	1	2,1	14,14,15	0.84	0	17,19,21	1.17	2 (11%)
2	NAG	AaA	2	2	14,14,15	0.46	0	17,19,21	1.64	2 (11%)
2	BMA	AaA	3	2	11,11,12	0.45	0	15,15,17	1.29	1 (6%)
2	MAN	AaA	4	2	11,11,12	0.71	0	15,15,17	1.33	2 (13%)

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	AaA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	AaA	2	2	-	0/6/23/26	0/1/1/1
2	BMA	AaA	3	2	-	0/2/19/22	0/1/1/1
2	MAN	AaA	4	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AaA	2	NAG	C1-O5-C5	5.20	119.24	112.19
2	AaA	4	MAN	C1-C2-C3	3.87	114.42	109.67
2	AaA	3	BMA	C1-O5-C5	3.32	116.68	112.19
2	AaA	2	NAG	C3-C4-C5	2.54	114.78	110.24
2	AaA	4	MAN	C2-C3-C4	2.27	114.82	110.89

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
2	AaA	1	NAG	0	1

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 AaA

Bond lengths

Bond angles

Torsions

Rings
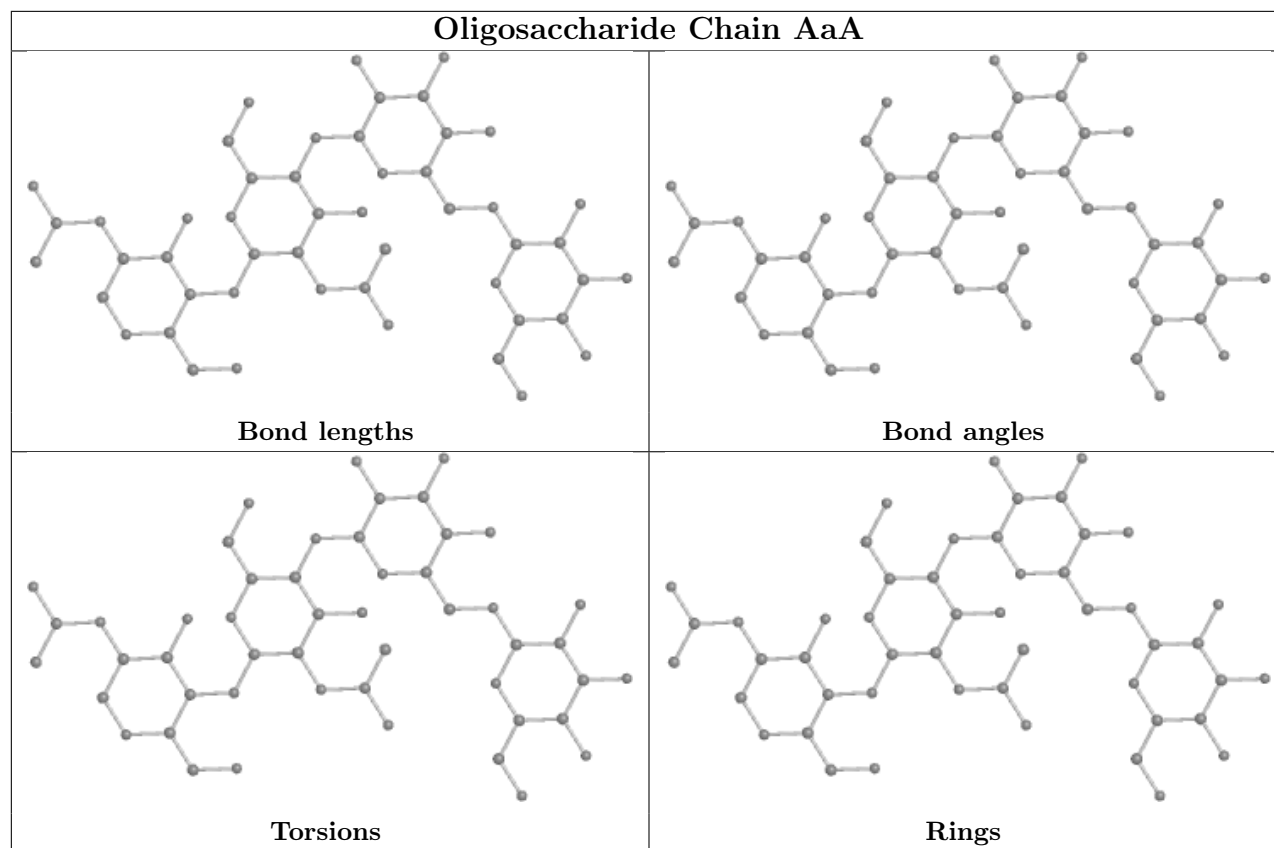
5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 1 is monoatomic - leaving 27 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	$\#|Z| > 2$
5	NAG	AAA	517	1	14,14,15	1.03	1 (7%)	17,19,21	1.01	1 (5%)
4	EDO	AAA	525	-	3,3,3	0.20	0	2,2,2	0.36	0
4	EDO	AAA	519	-	3,3,3	0.34	0	2,2,2	0.20	0
4	EDO	AAA	524	-	3,3,3	0.06	0	2,2,2	0.15	0
3	SO4	AAA	501	-	4,4,4	0.52	0	6,6,6	0.25	0
4	EDO	AAA	511	-	3,3,3	0.22	0	2,2,2	0.25	0
3	SO4	AAA	506	-	4,4,4	0.37	0	6,6,6	0.09	0
4	EDO	AAA	503	-	3,3,3	0.18	0	2,2,2	0.11	0
4	EDO	AAA	513	-	3,3,3	0.41	0	2,2,2	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	EDO	AAA	520	-	3,3,3	0.23	0	2,2,2	0.16	0
3	SO4	AAA	502	-	4,4,4	0.38	0	6,6,6	0.23	0
4	EDO	AAA	508	-	3,3,3	0.22	0	2,2,2	0.26	0
4	EDO	AAA	512	-	3,3,3	0.21	0	2,2,2	0.21	0
4	EDO	AAA	526	-	3,3,3	0.12	0	2,2,2	0.45	0
4	EDO	AAA	507	-	3,3,3	0.05	0	2,2,2	0.04	0
4	EDO	AAA	521	-	3,3,3	0.08	0	2,2,2	0.27	0
4	EDO	AAA	522	-	3,3,3	0.24	0	2,2,2	0.36	0
4	EDO	AAA	509	-	3,3,3	0.05	0	2,2,2	0.08	0
5	NAG	AAA	505	1	14,14,15	0.75	0	17,19,21	1.84	5 (29%)
4	EDO	AAA	510	-	3,3,3	0.24	0	2,2,2	0.13	0
4	EDO	AAA	518	-	3,3,3	0.22	0	2,2,2	0.04	0
4	EDO	AAA	514	-	3,3,3	0.44	0	2,2,2	0.20	0
4	EDO	AAA	515	-	3,3,3	0.05	0	2,2,2	0.27	0
6	OIW	AAA	527	1	9,9,10	1.04	0	9,12,14	1.67	1 (11%)
4	EDO	AAA	504	-	3,3,3	0.10	0	2,2,2	0.28	0
4	EDO	AAA	516	-	3,3,3	0.06	0	2,2,2	0.06	0
4	EDO	AAA	523	-	3,3,3	0.44	0	2,2,2	0.60	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	NAG	AAA	517	1	-	0/6/23/26	0/1/1/1
4	EDO	AAA	525	-	-	1/1/1/1	-
4	EDO	AAA	519	-	-	0/1/1/1	-
4	EDO	AAA	524	-	-	1/1/1/1	-
4	EDO	AAA	511	-	-	0/1/1/1	-
4	EDO	AAA	513	-	-	1/1/1/1	-
4	EDO	AAA	503	-	-	1/1/1/1	-
4	EDO	AAA	520	-	-	0/1/1/1	-
4	EDO	AAA	508	-	-	1/1/1/1	-
4	EDO	AAA	512	-	-	1/1/1/1	-
4	EDO	AAA	526	-	-	1/1/1/1	-
4	EDO	AAA	507	-	-	0/1/1/1	-
4	EDO	AAA	521	-	-	1/1/1/1	-
4	EDO	AAA	522	-	-	1/1/1/1	-
4	EDO	AAA	509	-	-	0/1/1/1	-
5	NAG	AAA	505	1	-	3/6/23/26	0/1/1/1
4	EDO	AAA	510	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	AAA	518	-	-	0/1/1/1	-
4	EDO	AAA	514	-	-	0/1/1/1	-
4	EDO	AAA	515	-	-	0/1/1/1	-
6	OIW	AAA	527	1	-	-	0/1/1/1
4	EDO	AAA	504	-	-	1/1/1/1	-
4	EDO	AAA	516	-	-	1/1/1/1	-
4	EDO	AAA	523	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AAA	517	NAG	C1-C2	2.07	1.55	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	AAA	505	NAG	C8-C7-N2	4.36	123.49	116.10
6	AAA	527	OIW	C3-C2-C1	-4.31	106.95	112.42
5	AAA	505	NAG	C2-N2-C7	3.11	127.33	122.90
5	AAA	517	NAG	O5-C5-C6	2.57	111.24	107.20
5	AAA	505	NAG	C1-O5-C5	2.53	115.61	112.19

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	AAA	505	NAG	C8-C7-N2-C2
5	AAA	505	NAG	O7-C7-N2-C2
4	AAA	525	EDO	O1-C1-C2-O2
4	AAA	503	EDO	O1-C1-C2-O2
4	AAA	522	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 11 short contacts:

| Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	501	SO4	1	0
4	AAA	513	EDO	5	0
4	AAA	520	EDO	1	0
4	AAA	526	EDO	2	0
5	AAA	505	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	523	EDO	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand OIW AAA 527

Bond lengths

Bond angles

Torsions

Rings
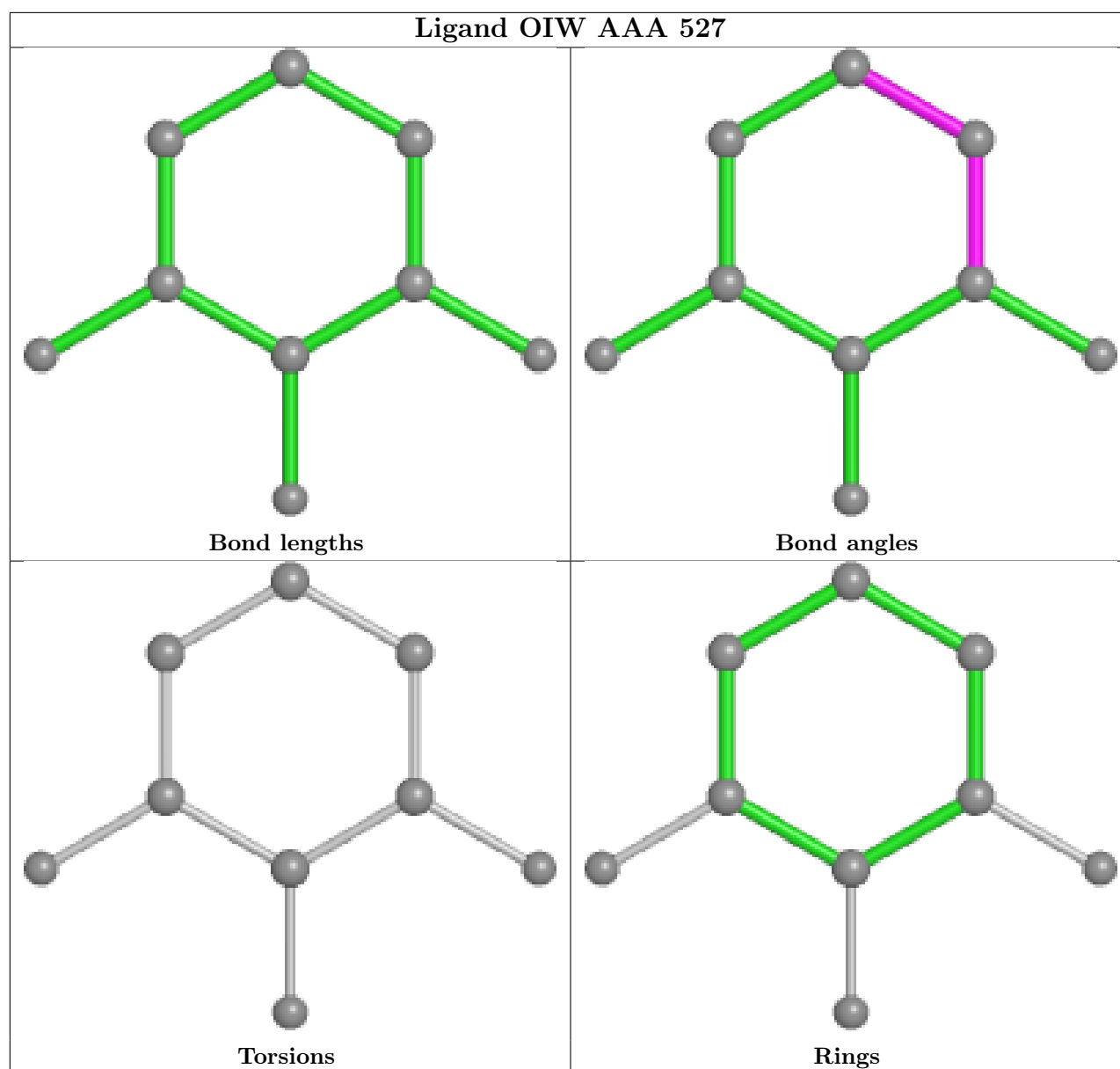
5.7 Other polymers ⓘ

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 ⓘ

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, 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(Å²)	Q<0.9
1	AAA	497/497 (100%)	-0.54	0	100	100	12, 18, 27, 37	6 (1%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ
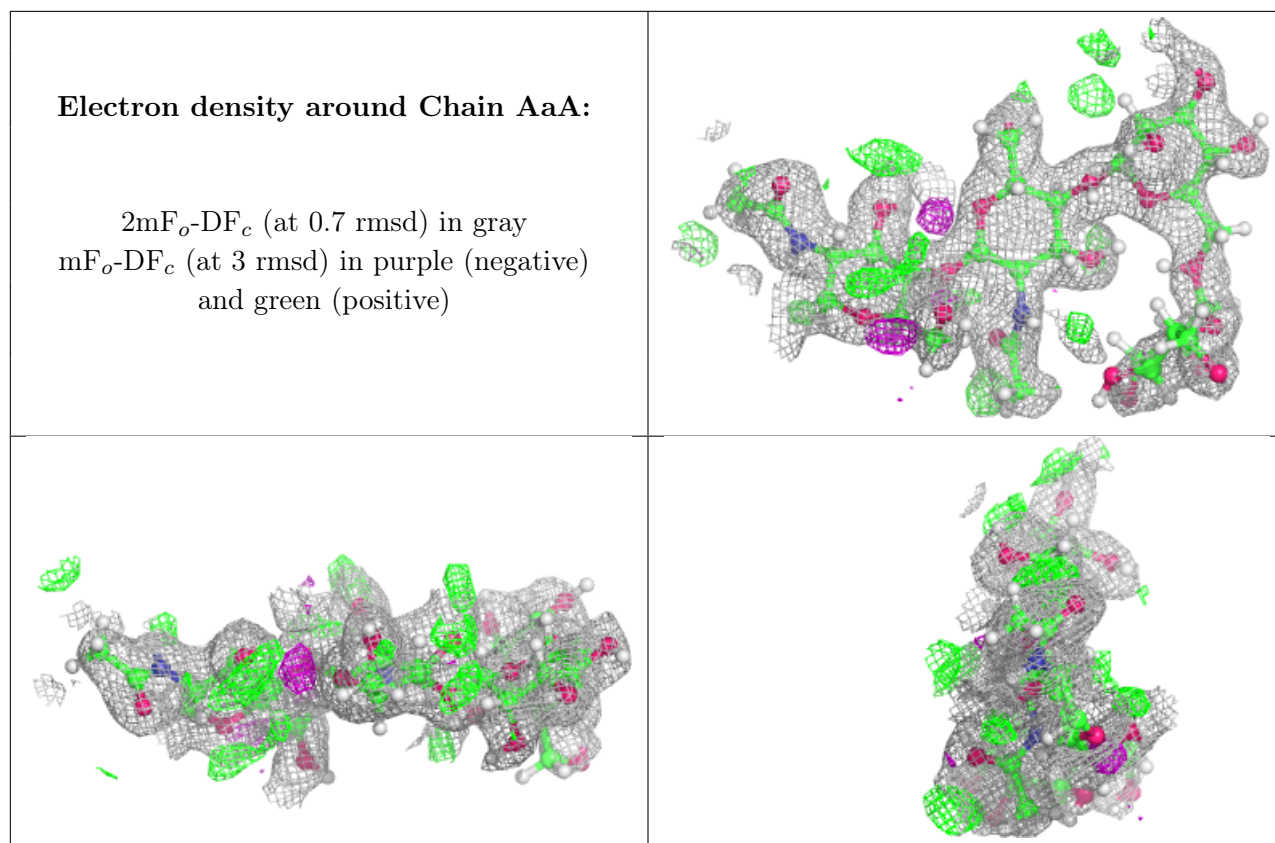
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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(Å²)	Q<0.9
2	MAN	AaA	4	11/12	0.64	0.24	71,76,79,80	4
2	BMA	AaA	3	11/12	0.77	0.23	57,62,67,68	3
2	NAG	AaA	2	14/15	0.87	0.11	29,37,42,47	2
2	NAG	AaA	1	14/15	0.90	0.11	24,30,33,36	4

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 AaA:

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

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.
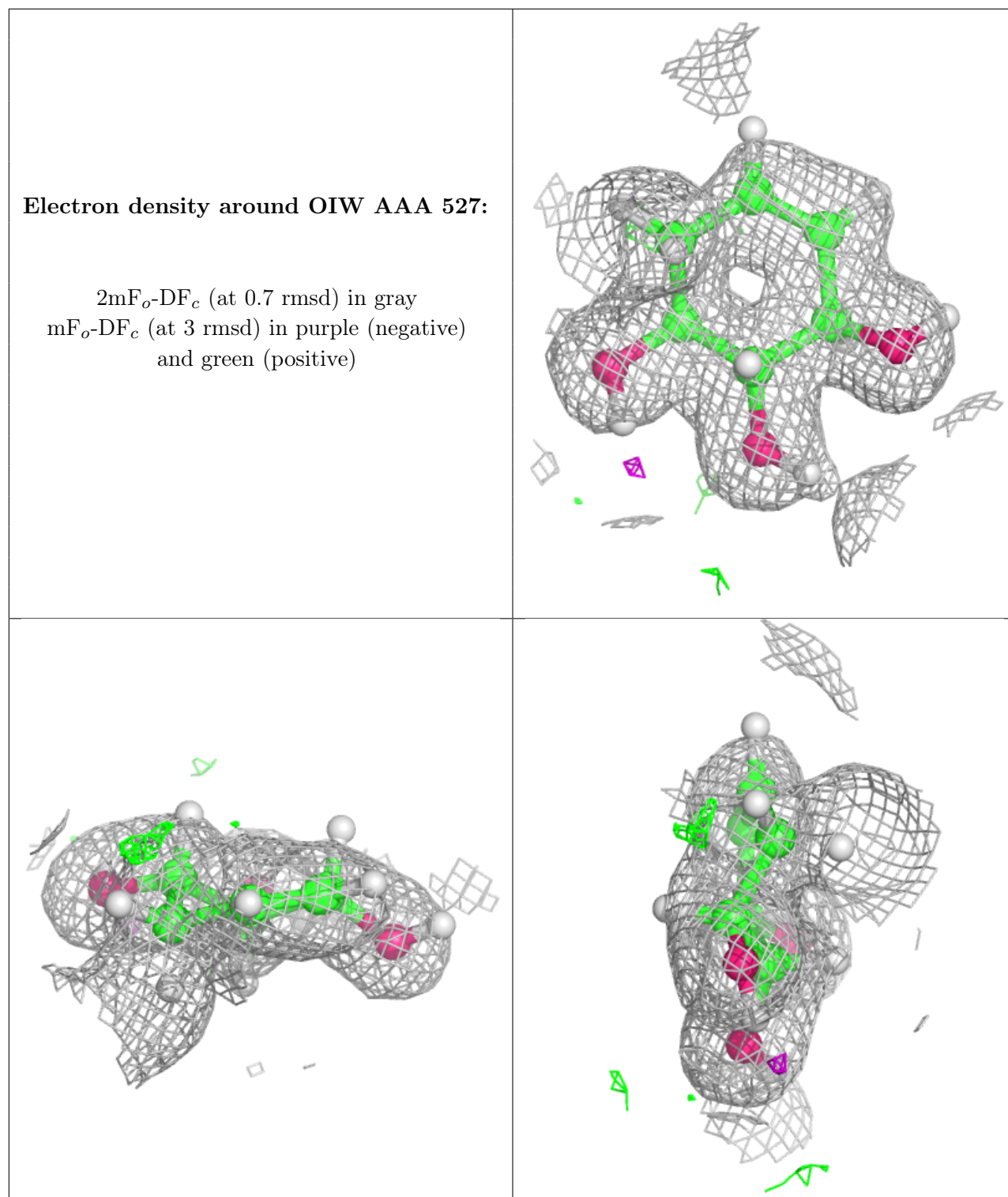
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
5	NAG	AAA	517	14/15	0.63	0.22	50,54,60,62	3
4	EDO	AAA	509	4/4	0.65	0.15	51,52,53,54	1
5	NAG	AAA	505	14/15	0.70	0.25	67,79,84,93	3
4	EDO	AAA	523	4/4	0.70	0.19	41,44,45,46	1
4	EDO	AAA	525	4/4	0.71	0.24	49,53,54,55	1
4	EDO	AAA	512	4/4	0.80	0.21	47,51,52,53	1
4	EDO	AAA	524	4/4	0.81	0.22	51,60,63,63	1
4	EDO	AAA	522	4/4	0.81	0.22	40,45,46,47	1
4	EDO	AAA	516	4/4	0.82	0.14	52,53,57,57	1
4	EDO	AAA	526	4/4	0.84	0.18	45,49,50,50	1
3	SO4	AAA	506	5/5	0.85	0.24	79,81,88,91	0
4	EDO	AAA	503	4/4	0.85	0.08	47,48,48,48	1
4	EDO	AAA	521	4/4	0.86	0.20	37,42,52,52	1
4	EDO	AAA	504	4/4	0.86	0.09	48,48,53,53	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	AAA	518	4/4	0.88	0.13	43,45,49,50	1
4	EDO	AAA	513	4/4	0.91	0.19	27,29,34,37	10
4	EDO	AAA	508	4/4	0.92	0.23	44,44,48,49	1
4	EDO	AAA	507	4/4	0.93	0.17	35,39,44,45	1
4	EDO	AAA	515	4/4	0.94	0.08	30,33,37,37	1
4	EDO	AAA	519	4/4	0.95	0.11	24,28,36,39	1
4	EDO	AAA	520	4/4	0.96	0.14	29,33,34,34	1
6	OIW	AAA	527	9/10	0.96	0.07	17,19,21,22	5
4	EDO	AAA	511	4/4	0.97	0.05	22,26,27,28	1
4	EDO	AAA	514	4/4	0.97	0.07	18,20,21,22	1
3	SO4	AAA	502	5/5	0.98	0.06	36,37,37,39	0
3	SO4	AAA	501	5/5	0.99	0.08	22,24,26,31	0
4	EDO	AAA	510	4/4	0.99	0.05	22,23,24,24	1
7	NA	AAA	528	1/1	0.99	0.06	17,17,17,17	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around OIW AAA 527:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.