



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 6, 2023 – 10:12 am BST

PDB ID : 7NWV
Title : Structure of recombinant human beta-glucocerebrosidase in complex with BODIPY Tagged Cyclophellitol activity based probe
Authors : Rowland, R.J.; Davies, G.J.
Deposited on : 2021-03-17
Resolution : 1.86 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

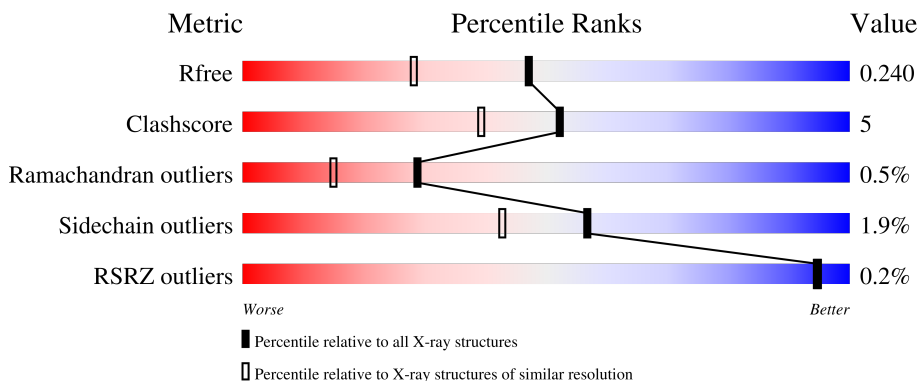
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	AAA	497	 88% 12%
1	BBB	497	 89% 11%
2	AdA	3	 67% 33%
2	BdB	3	 100%

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
6	EDO	BBB	505	-	-	X	-

2 Entry composition [i](#)

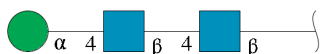
There are 8 unique types of molecules in this entry. The entry contains 17234 atoms, of which 8189 are hydrogens and 0 are deuteriums.

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.

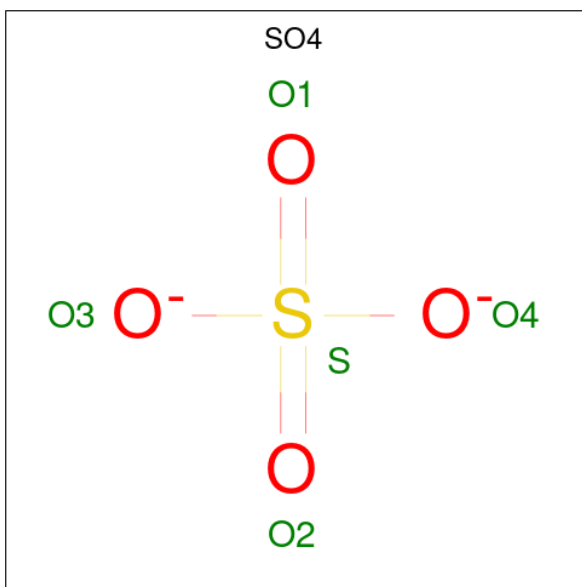
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	AAA	497	7830	2542	3882	676	714	16	203	4	0
1	BBB	497	7875	2551	3906	685	717	16	206	7	0

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



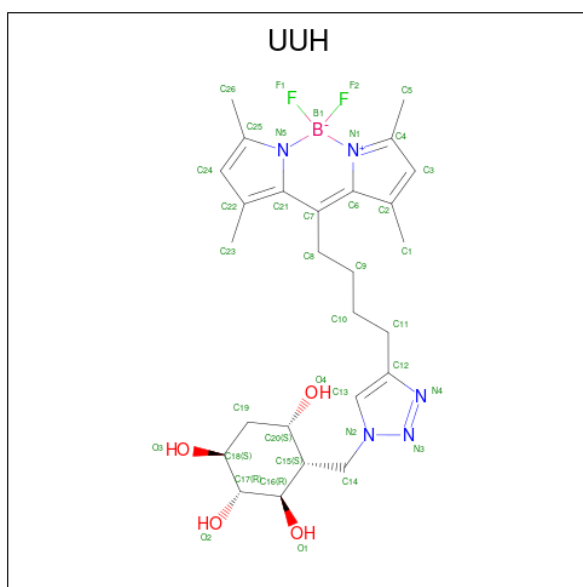
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	AdA	3	76	22	37	2	15	8	0	0
2	BdB	3	76	22	37	2	15	8	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total O S 5 4 1	0	0
3	AAA	1	Total O S 5 4 1	0	0
3	AAA	1	Total O S 5 4 1	0	0
3	BBB	1	Total O S 5 4 1	0	0
3	BBB	1	Total O S 5 4 1	0	0
3	BBB	1	Total O S 5 4 1	0	0
3	BBB	1	Total O S 5 4 1	0	0
3	BBB	1	Total O S 5 4 1	0	0

- Molecule 4 is (1 {S},2 {R},3 {R},4 {S},5 {S})-4-[[4-[4-[2,2-bis(fluoranyl)-4,6,10,12-tetramethyl-3-aza-1-azonia-2-boranuidatricyclo[7.3.0.0[^]{3,7}]dodeca-1(12),4,6,8,10-pentaen-8-yl]butyl]-1,2,3-triazol-1-yl]methyl]cyclohexane-1,2,3,5-tetrol (three-letter code: UUH) (formula: C₂₆H₃₆BF₂N₅O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	B	C	F	H	N		
4	AAA	1	73	1	26	2	35	5	4	0
4	BBB	1	Total	C	H	N	O			
			31	10	14	3	4			

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



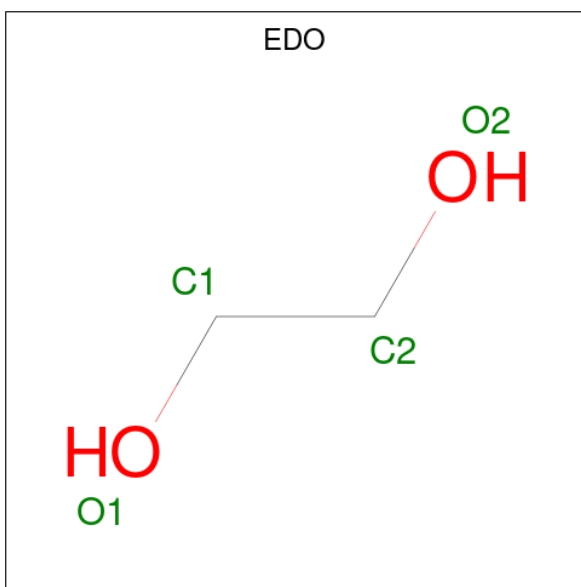
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
5	AAA	1	28	8	14	1	5	3	0

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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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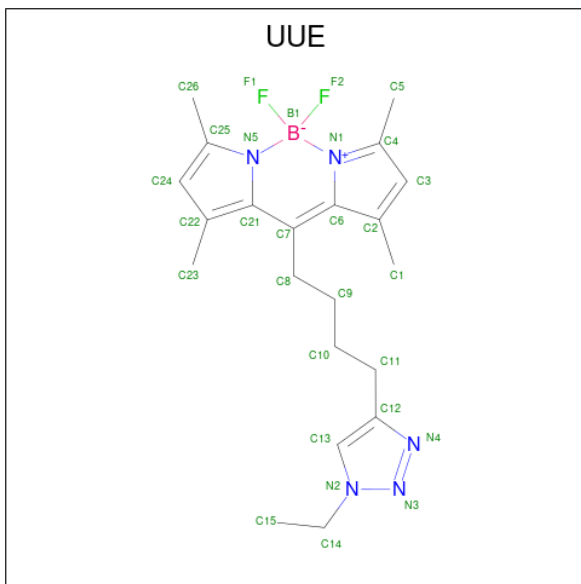
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	AAA	1	Total 10	C 2	H 6	O 2	1	0
6	AAA	1	Total 10	C 2	H 6	O 2	1	0
6	AAA	1	Total 10	C 2	H 6	O 2	1	0
6	AAA	1	Total 10	C 2	H 6	O 2	1	0
6	AAA	1	Total 10	C 2	H 6	O 2	1	0
6	AAA	1	Total 10	C 2	H 6	O 2	1	0
6	AAA	1	Total 10	C 2	H 6	O 2	1	0
6	AAA	1	Total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

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

- Molecule 7 is 8-[4-(1-ethyl-1,2,3-triazol-4-yl)butyl]-2,2-bis(fluoranyl)-4,6,10,12-tetramethyl-3-aza-1-azonia-2-boranidatricyclo[7.3.0.0[^]{3,7}]dodeca-1(12),4,6,8,10-pentaene (three-letter code: UUE) (formula: C₂₁H₂₈BF₂N₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
7	AAA	1	Total	B	C	F	H	N	1	0
			55	1	21	2	26	5		

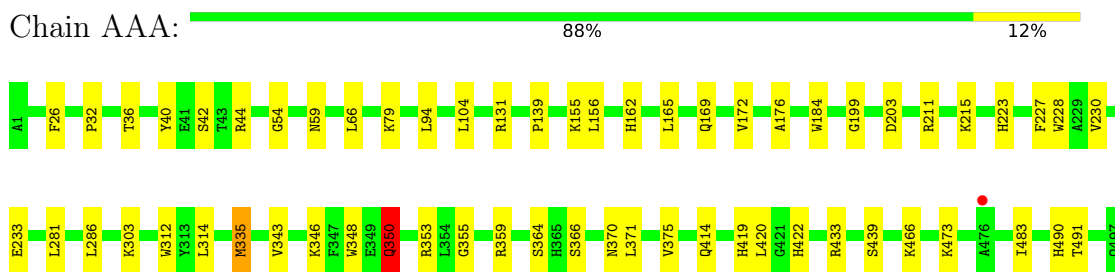
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	408	Total	O	0	0
			408	408		
8	BBB	336	Total	O	0	0
			336	336		

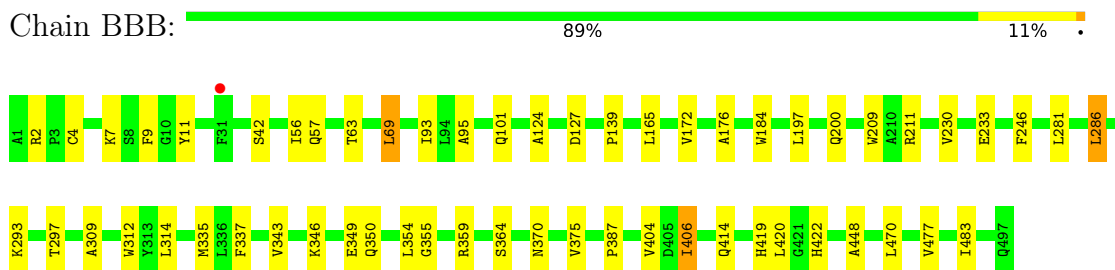
3 Residue-property plots [i](#)

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.

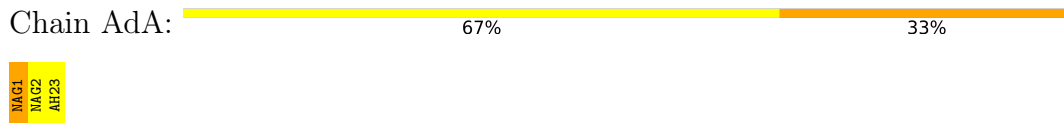
- Molecule 1: Lysosomal acid glucosylceramidase



- Molecule 1: Lysosomal acid glucosylceramidase



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.96Å 158.42Å 68.24Å 90.00° 102.15° 90.00°	Depositor
Resolution (Å)	66.80 – 1.86 79.21 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.9 (66.80-1.86) 100.0 (79.21-1.86)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 1.86Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.177 , 0.232 0.187 , 0.240	Depositor DCC
R_{free} test set	4665 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtrriage
Anisotropy	0.074	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17234	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.44% 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: EDO, AH2, SO4, NAG, UUE, UUH

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	0.70	0/4067	0.85	1/5547 (0.0%)
1	BBB	0.69	0/4087	0.82	0/5575
All	All	0.70	0/8154	0.83	1/11122 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	350	GLN	CB-CA-C	6.44	123.28	110.40

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	AAA	3948	3882	3853	47	1
1	BBB	3969	3906	3869	32	1
2	AdA	39	37	24	0	1
2	BdB	39	37	24	0	0
3	AAA	15	0	0	0	0
3	BBB	25	0	0	0	0
4	AAA	38	35	0	2	0
4	BBB	17	14	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AAA	14	14	13	0	0
5	BBB	28	28	26	1	0
6	AAA	92	138	138	13	0
6	BBB	48	72	72	7	0
7	AAA	29	26	0	2	0
8	AAA	408	0	0	13	0
8	BBB	336	0	0	6	0
All	All	9045	8189	8019	88	2

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 5.

The worst 5 of 88 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)
6:AAA:626:EDO:H11	8:AAA:929:HOH:O	1.68	0.92
6:AAA:626:EDO:C1	8:AAA:929:HOH:O	2.26	0.81
1:BBB:343[B]:VAL:HG11	1:BBB:359:ARG:HG2	1.62	0.80
1:AAA:169:GLN:HG2	8:AAA:780:HOH:O	1.81	0.78
1:BBB:7:LYS:HE3	1:BBB:9:PHE:CZ	2.22	0.74

All (2) 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:AdA:1:NAG:HO3[1_455]	1.20	0.40
1:BBB:63:THR:H	1:BBB:200:GLN:HE21[1_554]	1.30	0.30

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	AAA	499/497 (100%)	483 (97%)	14 (3%)	2 (0%)	34	19
1	BBB	502/497 (101%)	483 (96%)	16 (3%)	3 (1%)	25	12
All	All	1001/994 (101%)	966 (96%)	30 (3%)	5 (0%)	29	15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	233	GLU
1	AAA	281	LEU
1	BBB	124	ALA
1	BBB	233	GLU
1	BBB	281	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	AAA	423/424 (100%)	417 (99%)	6 (1%)	67	55
1	BBB	425/424 (100%)	414 (97%)	11 (3%)	46	30
All	All	848/848 (100%)	831 (98%)	17 (2%)	57	40

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	420	LEU
1	BBB	483	ILE
1	BBB	69	LEU
1	BBB	211	ARG
1	BBB	286	LEU

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	AdA	1	2,1	14,14,15	0.83	0	17,19,21	0.90	1 (5%)
2	NAG	AdA	2	2	14,14,15	0.73	0	17,19,21	1.25	1 (5%)
2	AH2	AdA	3	2	11,11,11	0.29	0	15,15,15	1.19	2 (13%)
2	NAG	BdB	1	2,1	14,14,15	0.85	0	17,19,21	1.12	1 (5%)
2	NAG	BdB	2	2	14,14,15	0.35	0	17,19,21	1.01	1 (5%)
2	AH2	BdB	3	2	11,11,11	0.48	0	15,15,15	1.85	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	AdA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	AdA	2	2	-	0/6/23/26	0/1/1/1
2	AH2	AdA	3	2	-	2/2/19/19	0/1/1/1
2	NAG	BdB	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	BdB	2	2	-	0/6/23/26	0/1/1/1
2	AH2	BdB	3	2	-	0/2/19/19	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BdB	3	AH2	C1-O5-C5	5.59	119.77	112.19
2	AdA	2	NAG	C1-O5-C5	3.50	116.93	112.19
2	BdB	1	NAG	C4-C3-C2	-3.22	106.30	111.02
2	BdB	2	NAG	C4-C3-C2	-2.88	106.79	111.02
2	AdA	3	AH2	C1-O5-C5	2.59	115.70	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

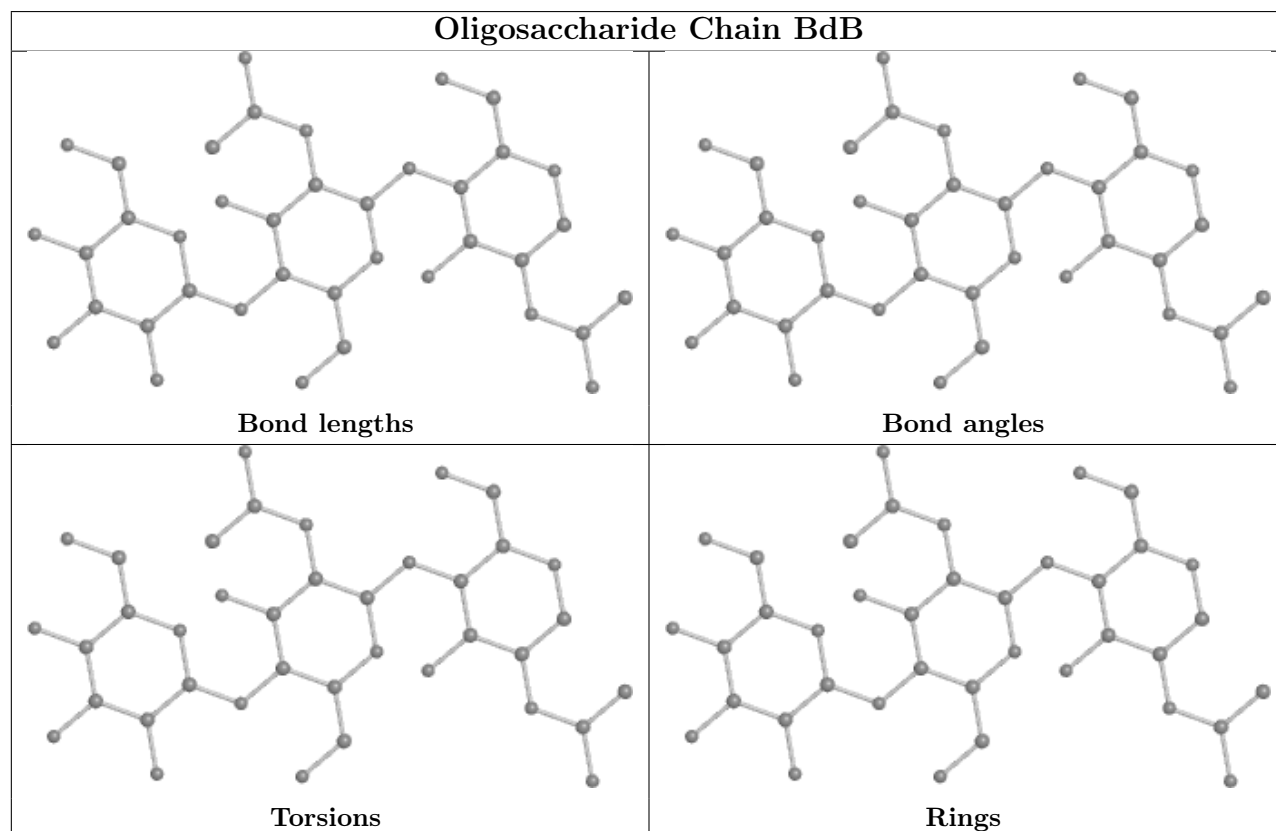
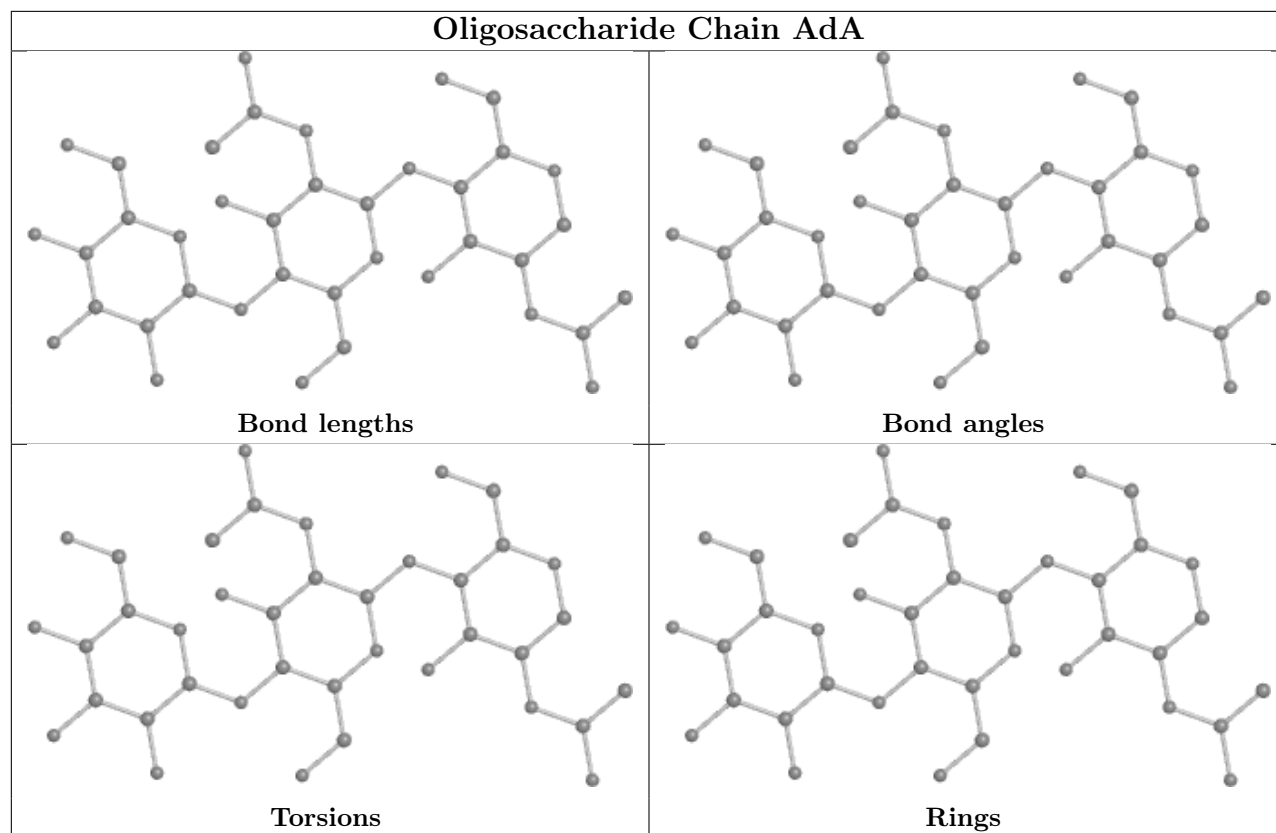
Mol	Chain	Res	Type	Atoms
2	AdA	3	AH2	O5-C5-C6-O6
2	AdA	3	AH2	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AdA	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.



5.6 Ligand geometry

49 ligands 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
6	EDO	AAA	629	-	3,3,3	0.09	0	2,2,2	0.19	0
6	EDO	AAA	627	-	3,3,3	0.12	0	2,2,2	0.19	0
6	EDO	AAA	609	-	3,3,3	0.18	0	2,2,2	0.32	0
6	EDO	AAA	606	-	3,3,3	0.18	0	2,2,2	0.25	0
6	EDO	AAA	620	-	3,3,3	0.37	0	2,2,2	0.15	0
5	NAG	BBB	514	1	14,14,15	0.78	0	17,19,21	1.42	3 (17%)
3	SO4	BBB	501	-	4,4,4	0.46	0	6,6,6	0.35	0
6	EDO	AAA	607	-	3,3,3	0.25	0	2,2,2	0.49	0
6	EDO	BBB	507	-	3,3,3	0.33	0	2,2,2	0.34	0
6	EDO	BBB	511	-	3,3,3	0.16	0	2,2,2	0.26	0
6	EDO	BBB	512	-	3,3,3	0.25	0	2,2,2	0.57	0
6	EDO	BBB	519	-	3,3,3	0.09	0	2,2,2	0.33	0
5	NAG	AAA	604	1	14,14,15	0.58	0	17,19,21	1.58	4 (23%)
6	EDO	AAA	628	-	3,3,3	0.07	0	2,2,2	0.20	0
6	EDO	AAA	613	-	3,3,3	0.05	0	2,2,2	0.20	0
3	SO4	BBB	513	-	4,4,4	0.28	0	6,6,6	0.07	0
6	EDO	BBB	508	-	3,3,3	0.15	0	2,2,2	0.29	0
6	EDO	BBB	518	-	3,3,3	0.14	0	2,2,2	0.20	0
6	EDO	AAA	611	-	3,3,3	0.40	0	2,2,2	0.72	0
6	EDO	AAA	618	-	3,3,3	0.11	0	2,2,2	0.05	0
6	EDO	BBB	520	-	3,3,3	0.15	0	2,2,2	0.28	0
6	EDO	AAA	626	-	3,3,3	0.22	0	2,2,2	0.60	0
7	UUE	AAA	624	-	30,32,32	0.88	1 (3%)	32,49,49	1.21	4 (12%)
6	EDO	AAA	608	-	3,3,3	0.26	0	2,2,2	0.57	0
6	EDO	AAA	605	-	3,3,3	0.45	0	2,2,2	0.18	0
6	EDO	AAA	612	-	3,3,3	0.77	0	2,2,2	0.78	0
6	EDO	BBB	510	-	3,3,3	0.14	0	2,2,2	0.24	0
6	EDO	AAA	615	-	3,3,3	0.07	0	2,2,2	0.22	0
6	EDO	AAA	621	-	3,3,3	0.11	0	2,2,2	0.37	0
6	EDO	BBB	505	-	3,3,3	0.23	0	2,2,2	0.56	0
3	SO4	AAA	610	-	4,4,4	0.28	0	6,6,6	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	AAA	603	-	4,4,4	0.40	0	6,6,6	0.25	0
3	SO4	BBB	517	-	4,4,4	0.33	0	6,6,6	0.10	0
5	NAG	BBB	504	1	14,14,15	0.65	0	17,19,21	1.44	2 (11%)
6	EDO	BBB	515	-	3,3,3	0.22	0	2,2,2	0.50	0
6	EDO	AAA	625	-	3,3,3	0.14	0	2,2,2	0.11	0
6	EDO	AAA	617	-	3,3,3	0.11	0	2,2,2	0.09	0
3	SO4	BBB	516	-	4,4,4	0.30	0	6,6,6	0.13	0
6	EDO	BBB	509	-	3,3,3	0.12	0	2,2,2	0.12	0
4	UUH	AAA	602	1	39,42,42	0.74	1 (2%)	43,65,65	1.40	6 (13%)
6	EDO	AAA	623	-	3,3,3	0.07	0	2,2,2	0.06	0
6	EDO	AAA	622	-	3,3,3	0.20	0	2,2,2	0.34	0
4	UUH	BBB	502	1	17,18,42	0.79	0	18,26,65	0.87	0
3	SO4	BBB	503	-	4,4,4	0.40	0	6,6,6	0.20	0
6	EDO	AAA	616	-	3,3,3	0.24	0	2,2,2	0.65	0
6	EDO	BBB	506	-	3,3,3	0.09	0	2,2,2	0.15	0
6	EDO	AAA	619	-	3,3,3	0.27	0	2,2,2	0.35	0
3	SO4	AAA	601	-	4,4,4	0.45	0	6,6,6	0.22	0
6	EDO	AAA	614	-	3,3,3	0.15	0	2,2,2	0.13	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
6	EDO	AAA	629	-	-	1/1/1/1	-
6	EDO	AAA	627	-	-	0/1/1/1	-
6	EDO	AAA	609	-	-	0/1/1/1	-
6	EDO	AAA	606	-	-	0/1/1/1	-
6	EDO	AAA	620	-	-	0/1/1/1	-
5	NAG	BBB	514	1	-	2/6/23/26	0/1/1/1
6	EDO	AAA	607	-	-	0/1/1/1	-
6	EDO	BBB	507	-	-	1/1/1/1	-
6	EDO	BBB	511	-	-	1/1/1/1	-
6	EDO	BBB	512	-	-	1/1/1/1	-
6	EDO	BBB	519	-	-	1/1/1/1	-
5	NAG	AAA	604	1	-	2/6/23/26	0/1/1/1
6	EDO	AAA	628	-	-	1/1/1/1	-
6	EDO	AAA	613	-	-	1/1/1/1	-
6	EDO	BBB	508	-	-	1/1/1/1	-
6	EDO	BBB	518	-	-	0/1/1/1	-
6	EDO	AAA	611	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	AAA	618	-	-	0/1/1/1	-
6	EDO	BBB	520	-	-	1/1/1/1	-
6	EDO	AAA	626	-	-	1/1/1/1	-
7	UUE	AAA	624	-	-	0/9/45/45	0/4/4/4
6	EDO	AAA	608	-	-	0/1/1/1	-
6	EDO	AAA	605	-	-	1/1/1/1	-
6	EDO	AAA	612	-	-	1/1/1/1	-
6	EDO	BBB	510	-	-	1/1/1/1	-
6	EDO	AAA	615	-	-	1/1/1/1	-
6	EDO	AAA	621	-	-	0/1/1/1	-
6	EDO	BBB	505	-	-	0/1/1/1	-
5	NAG	BBB	504	1	-	0/6/23/26	0/1/1/1
6	EDO	BBB	515	-	-	1/1/1/1	-
6	EDO	AAA	625	-	-	0/1/1/1	-
6	EDO	AAA	617	-	-	1/1/1/1	-
6	EDO	BBB	509	-	-	0/1/1/1	-
4	UUH	AAA	602	1	-	3/11/67/67	0/5/5/5
6	EDO	AAA	623	-	-	0/1/1/1	-
6	EDO	AAA	622	-	-	0/1/1/1	-
4	UUH	BBB	502	1	-	0/4/24/67	0/2/2/5
6	EDO	AAA	616	-	-	1/1/1/1	-
6	EDO	BBB	506	-	-	1/1/1/1	-
6	EDO	AAA	619	-	-	0/1/1/1	-
6	EDO	AAA	614	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AAA	602	UUH	C12-N4	2.17	1.36	1.34
7	AAA	624	UUE	C6-N1	-2.15	1.37	1.40

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AAA	602	UUH	C2-C6-N1	-3.94	104.36	107.68
5	BBB	504	NAG	C1-O5-C5	3.93	117.51	112.19
7	AAA	624	UUE	C6-N1-C4	3.63	111.35	108.17
4	AAA	602	UUH	C6-N1-C4	3.62	111.34	108.17
5	BBB	514	NAG	O5-C1-C2	3.49	116.80	111.29

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

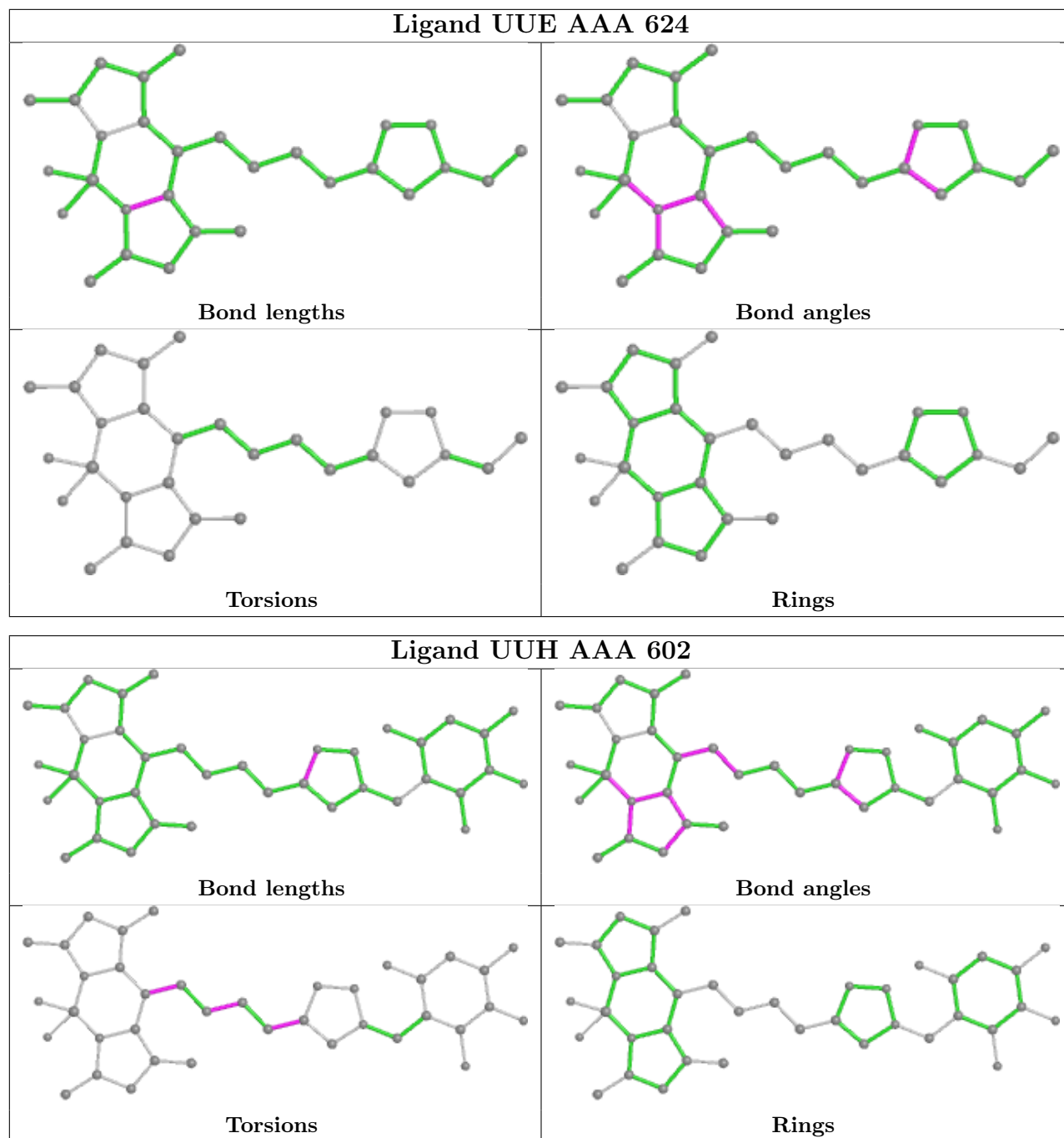
Mol	Chain	Res	Type	Atoms
4	AAA	602	UUH	C10-C11-C12-N4
5	AAA	604	NAG	C8-C7-N2-C2
5	AAA	604	NAG	O7-C7-N2-C2
6	BBB	507	EDO	O1-C1-C2-O2
6	BBB	510	EDO	O1-C1-C2-O2

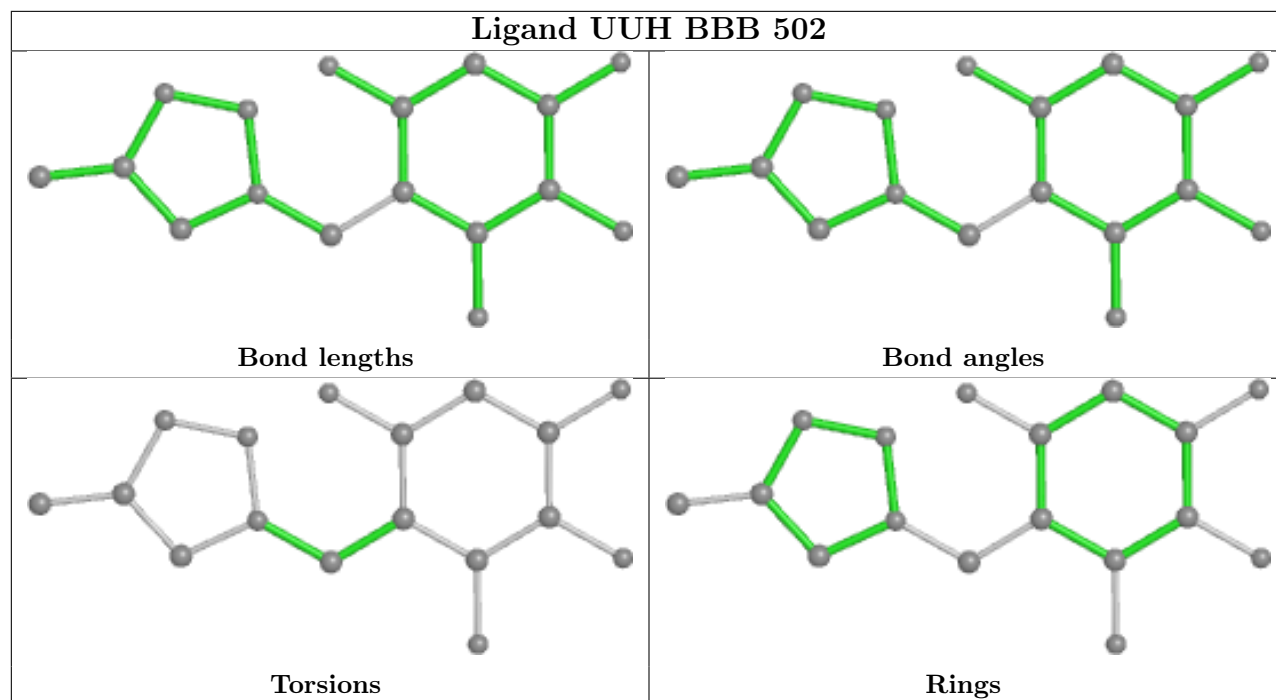
There are no ring outliers.

14 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	AAA	609	EDO	1	0
6	AAA	606	EDO	1	0
5	BBB	514	NAG	1	0
6	BBB	512	EDO	2	0
6	BBB	508	EDO	1	0
6	AAA	611	EDO	1	0
6	AAA	626	EDO	3	0
7	AAA	624	UUE	2	0
6	AAA	605	EDO	1	0
6	AAA	615	EDO	1	0
6	AAA	621	EDO	3	0
6	BBB	505	EDO	4	0
4	AAA	602	UUH	2	0
6	AAA	616	EDO	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 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 than 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.





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	AAA	497/497 (100%)	-0.32	1 (0%) 95 94	15, 21, 37, 50	0
1	BBB	497/497 (100%)	-0.34	1 (0%) 95 94	17, 25, 39, 66	0
All	All	994/994 (100%)	-0.33	2 (0%) 95 94	15, 23, 38, 66	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	31	PHE	2.1
1	AAA	476	ALA	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.

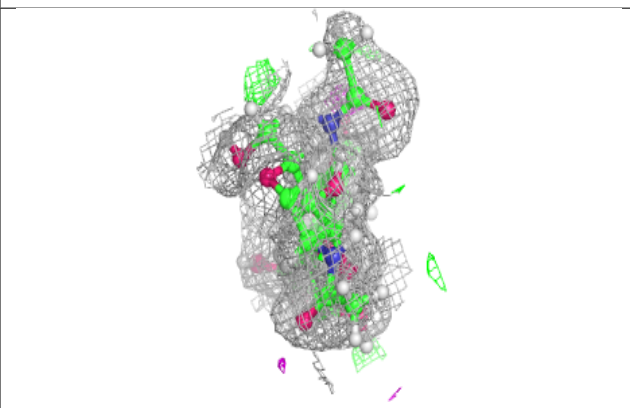
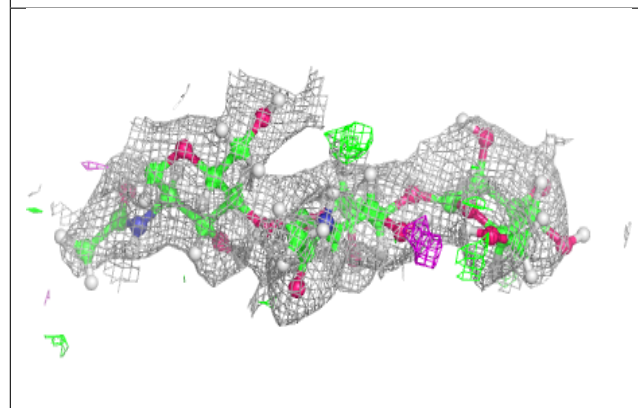
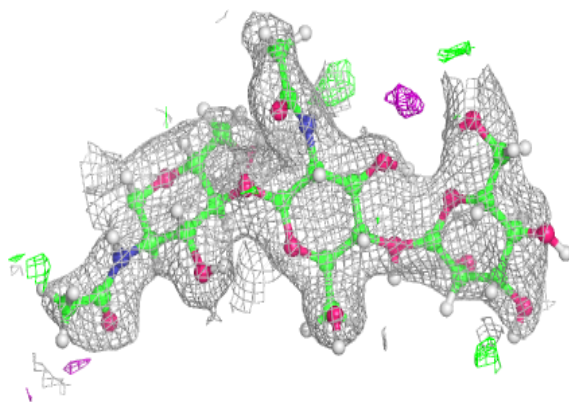
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AH2	BdB	3	11/11	0.74	0.21	55,66,73,73	4
2	AH2	AdA	3	11/11	0.78	0.14	49,61,63,65	4
2	NAG	BdB	1	14/15	0.92	0.13	30,34,37,38	2
2	NAG	BdB	2	14/15	0.92	0.11	36,41,42,49	2
2	NAG	AdA	2	14/15	0.92	0.10	33,36,46,51	2
2	NAG	AdA	1	14/15	0.95	0.07	24,27,29,29	2

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

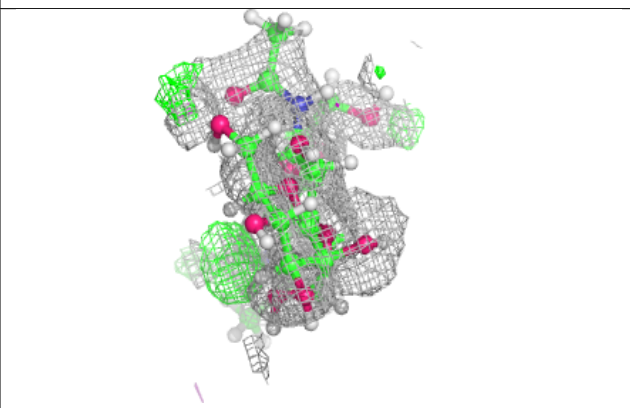
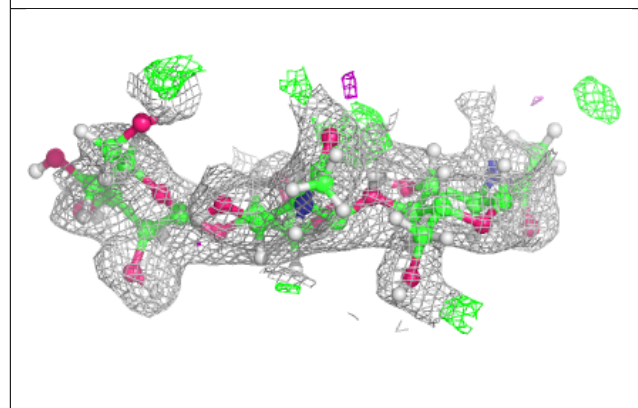
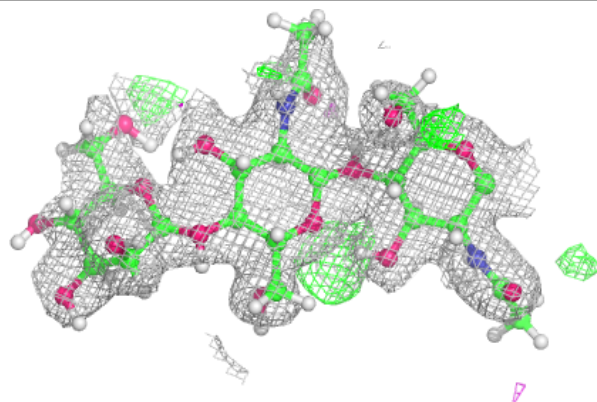
Electron density around Chain AdA:

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



Electron density around Chain BdB:

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



6.4 Ligands [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.

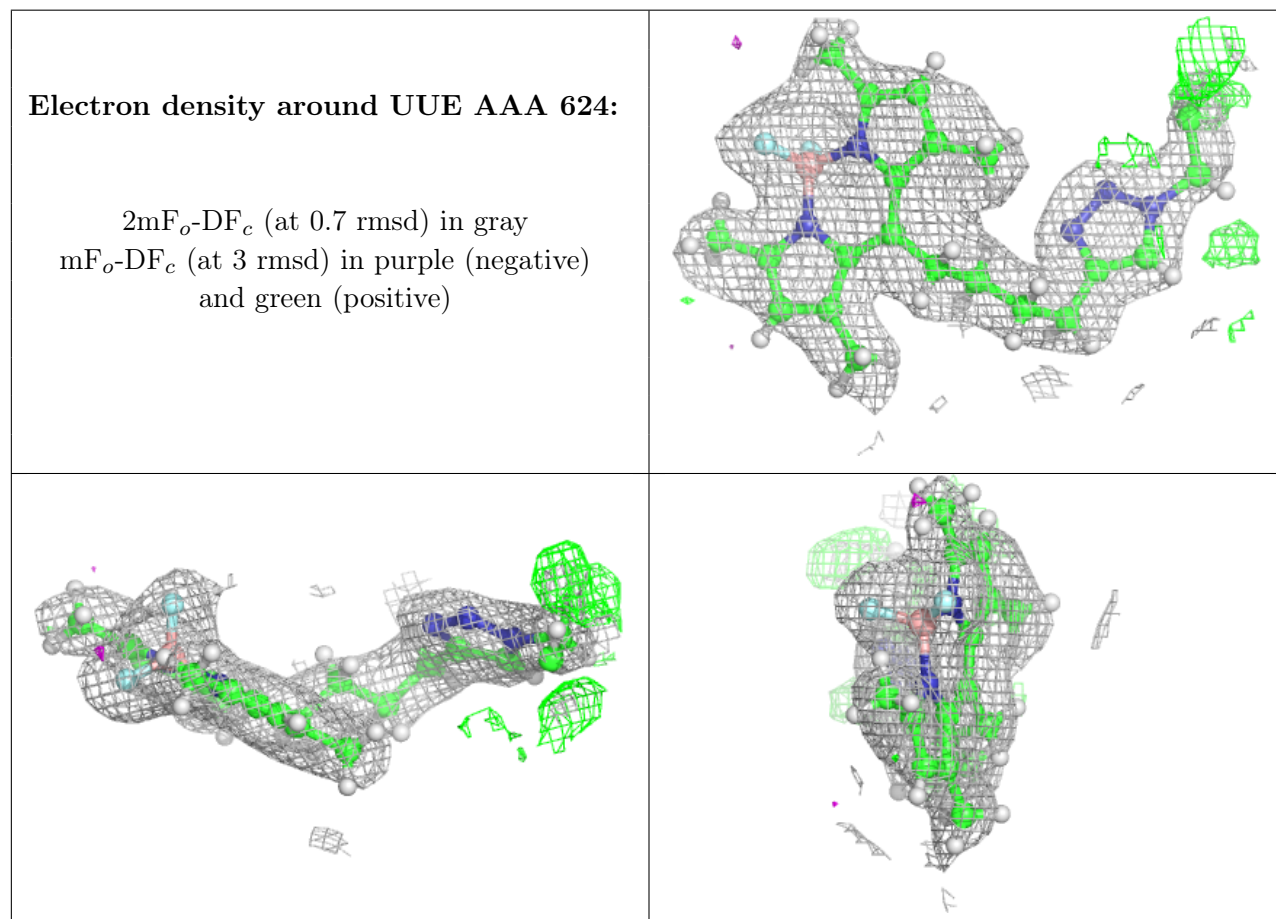
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	BBB	514	14/15	0.40	0.27	58,72,79,82	3
5	NAG	AAA	604	14/15	0.56	0.22	52,63,69,70	3
6	EDO	AAA	622	4/4	0.62	0.17	45,52,53,54	1
6	EDO	AAA	628	4/4	0.66	0.18	64,64,65,65	1
6	EDO	AAA	625	4/4	0.67	0.13	49,52,57,57	1
6	EDO	AAA	612	4/4	0.68	0.31	37,44,45,45	1
6	EDO	AAA	611	4/4	0.68	0.24	47,48,48,49	1
6	EDO	AAA	629	4/4	0.68	0.12	56,58,60,61	1
6	EDO	BBB	512	4/4	0.71	0.18	47,53,56,56	1
6	EDO	BBB	507	4/4	0.72	0.18	45,48,50,50	1
5	NAG	BBB	504	14/15	0.72	0.18	60,71,75,80	3
6	EDO	BBB	515	4/4	0.73	0.28	43,49,51,51	1
3	SO4	BBB	513	5/5	0.74	0.21	71,72,80,88	0
6	EDO	AAA	626	4/4	0.76	0.19	46,48,51,53	1
6	EDO	AAA	607	4/4	0.77	0.17	39,48,49,49	1
6	EDO	AAA	627	4/4	0.78	0.14	50,51,52,52	1
6	EDO	AAA	609	4/4	0.78	0.14	53,53,54,55	1
6	EDO	AAA	616	4/4	0.81	0.16	38,39,41,42	1
6	EDO	BBB	511	4/4	0.82	0.13	53,57,62,63	1
6	EDO	BBB	505	4/4	0.83	0.12	38,42,43,43	1
6	EDO	BBB	519	4/4	0.83	0.22	42,50,55,57	1
6	EDO	AAA	615	4/4	0.85	0.14	53,54,56,56	1
6	EDO	AAA	613	4/4	0.85	0.11	38,41,46,47	1
6	EDO	AAA	623	4/4	0.86	0.19	53,56,58,58	1
6	EDO	BBB	506	4/4	0.87	0.12	45,50,58,61	1
6	EDO	AAA	618	4/4	0.87	0.14	48,52,55,55	1
6	EDO	AAA	608	4/4	0.88	0.13	27,31,34,35	1
3	SO4	AAA	610	5/5	0.88	0.12	48,56,56,56	0
6	EDO	AAA	614	4/4	0.88	0.10	44,46,47,48	1
3	SO4	BBB	517	5/5	0.88	0.20	67,69,72,76	0
6	EDO	BBB	520	4/4	0.88	0.11	55,58,62,62	1
7	UUE	AAA	624	29/29	0.89	0.12	27,33,36,40	1
6	EDO	AAA	605	4/4	0.91	0.17	29,34,41,42	1
6	EDO	BBB	510	4/4	0.91	0.09	45,46,46,47	1
6	EDO	AAA	606	4/4	0.91	0.20	35,37,39,39	1
3	SO4	BBB	516	5/5	0.91	0.23	49,59,61,71	0
6	EDO	BBB	509	4/4	0.92	0.12	48,50,52,53	1

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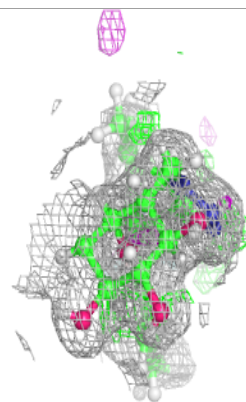
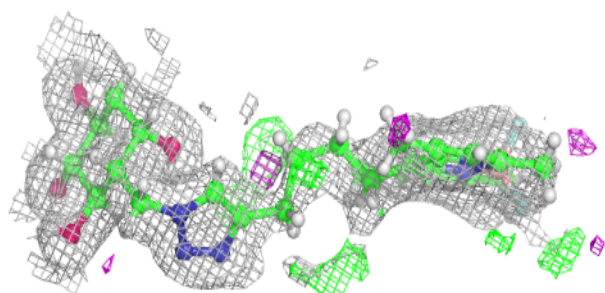
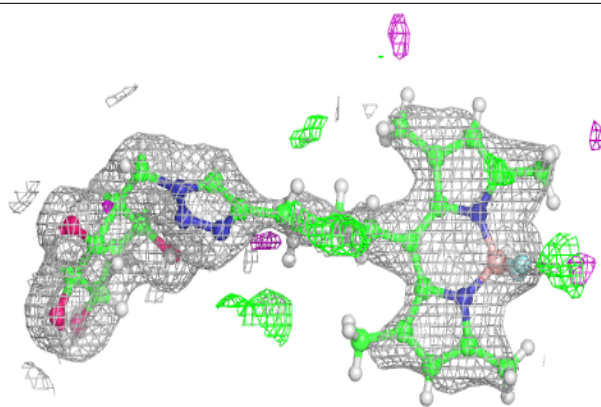
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	EDO	AAA	619	4/4	0.92	0.24	24,33,43,43	1
6	EDO	BBB	518	4/4	0.93	0.13	37,41,42,43	1
6	EDO	BBB	508	4/4	0.93	0.28	35,44,49,49	1
6	EDO	AAA	621	4/4	0.94	0.34	38,42,47,47	1
4	UUH	AAA	602	38/38	0.94	0.14	15,47,57,64	4
6	EDO	AAA	617	4/4	0.94	0.20	30,41,51,55	1
6	EDO	AAA	620	4/4	0.95	0.11	23,24,25,26	1
4	UUH	BBB	502	17/38	0.96	0.11	17,19,34,37	4
3	SO4	AAA	603	5/5	0.97	0.08	33,34,36,37	0
3	SO4	BBB	501	5/5	0.98	0.09	24,26,27,31	0
3	SO4	BBB	503	5/5	0.98	0.09	39,42,42,44	0
3	SO4	AAA	601	5/5	0.99	0.09	23,26,27,29	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.

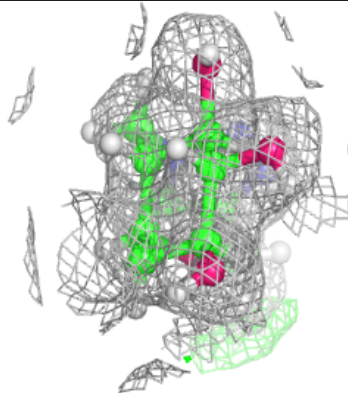
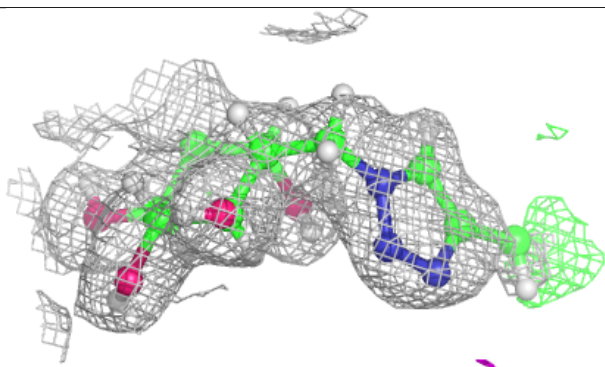
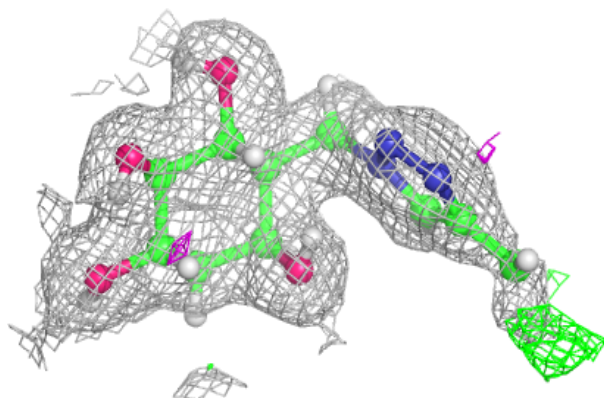


Electron density around UUH AAA 602:

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

**Electron density around UUH BBB 502:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.