wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 12:58 AM EDT

PDB ID : 6XKG
Title : Crystal structure of 3-O-Sulfotransferase isoform 3 in complex with 8mer oligosaccharide with 6S sulfation
Authors : Pedersen, L.C.; Liu, J.; Wander, R.
Deposited on : 2020-06-26
Resolution : 1.55 Å(reported)

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

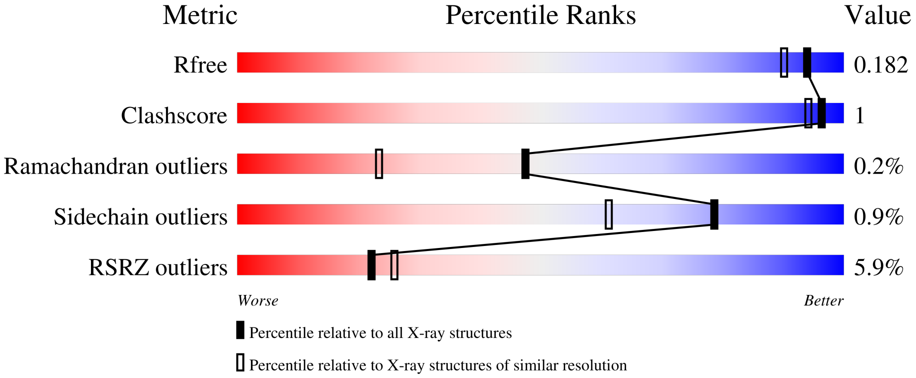
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

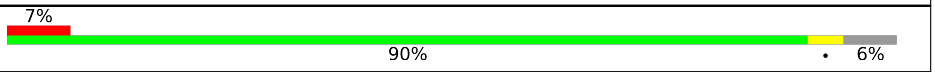
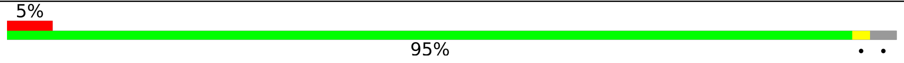
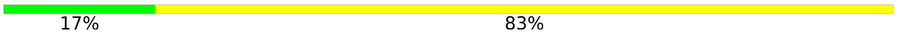
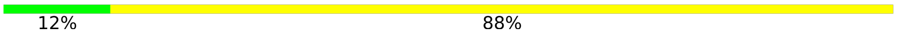
The reported resolution of this entry is 1.55 Å.

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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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	A	273	 7% 90% • 6%
1	B	273	 5% 95% • •
2	D	6	 17% 83%
3	E	8	 12% 88%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5338 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.

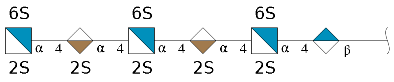
- Molecule 1 is a protein called Heparan sulfate glucosamine 3-O-sulfotransferase 3A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	266	Total 2208	C 1416	N 394	O 391	S 7	0	10	0
1	A	257	Total 2098	C 1348	N 374	O 369	S 7	0	4	0

There are 10 discrepancies between the modelled and reference sequences:

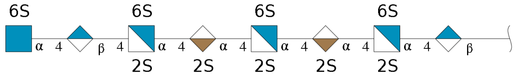
Chain	Residue	Modelled	Actual	Comment	Reference
B	134	GLY	-	expression tag	UNP Q9Y663
B	135	SER	-	expression tag	UNP Q9Y663
B	136	PRO	-	expression tag	UNP Q9Y663
B	137	ASN	-	expression tag	UNP Q9Y663
B	138	SER	-	expression tag	UNP Q9Y663
A	134	GLY	-	expression tag	UNP Q9Y663
A	135	SER	-	expression tag	UNP Q9Y663
A	136	PRO	-	expression tag	UNP Q9Y663
A	137	ASN	-	expression tag	UNP Q9Y663
A	138	SER	-	expression tag	UNP Q9Y663

- Molecule 2 is an oligosaccharide called 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid.



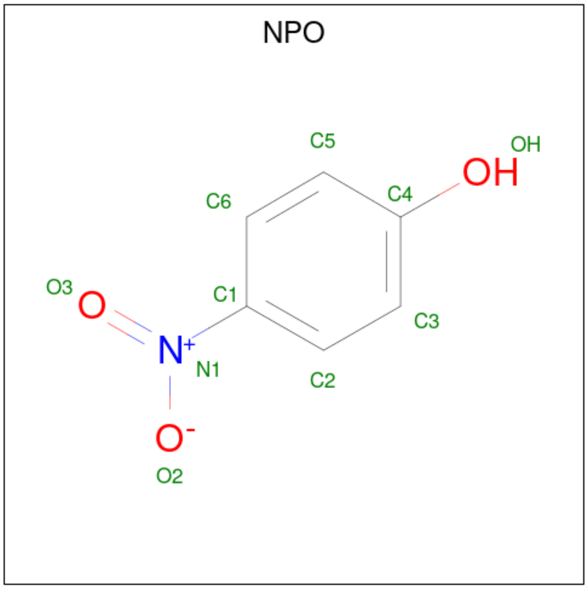
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	6	Total 101	C 36	N 3	O 54	S 8	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid.



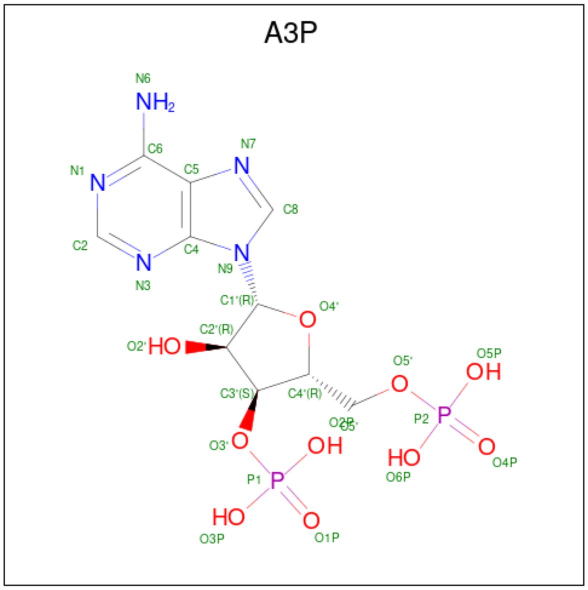
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	E	8	Total C N O S 137 51 4 72 10	0	1	0

- Molecule 4 is P-NITROPHENOL (three-letter code: NPO) (formula: $C_6H_5NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 10 6 1 3	0	0
4	A	1	Total C N O 10 6 1 3	0	0

- Molecule 5 is ADENOSINE-3'-5'-DIPHOSPHATE (three-letter code: A3P) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

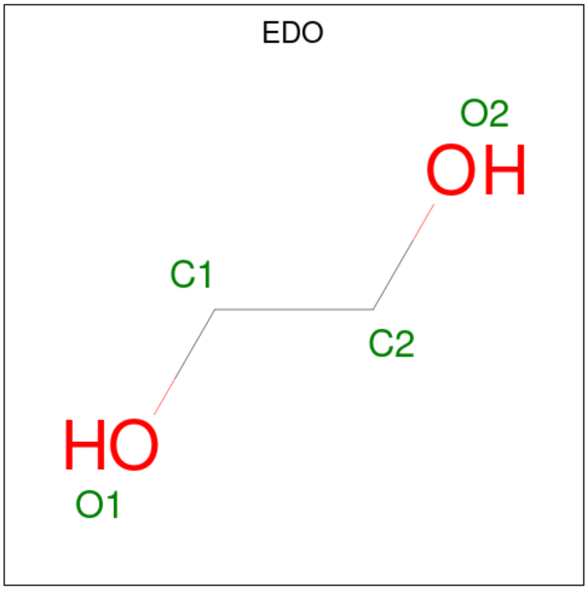


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O P 27 10 5 10 2	0	0
5	A	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Na 1 1	0	0
6	A	1	Total Na 1 1	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 8 is water.

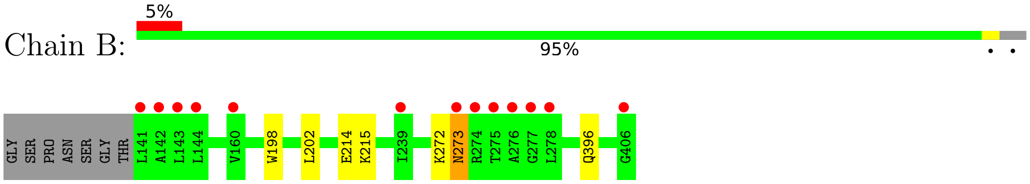
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	372	Total O 374 374	0	2
8	A	315	Total O 318 318	0	3

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.

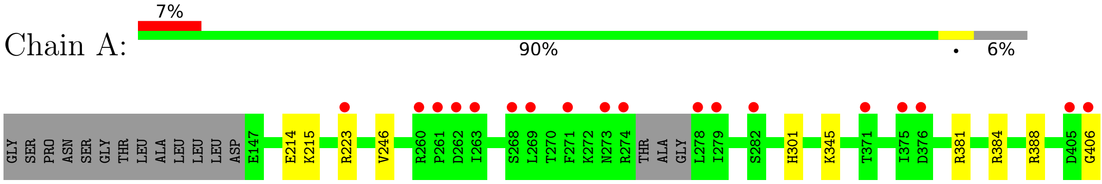
- Molecule 1: Heparan sulfate glucosamine 3-O-sulfotransferase 3A1

Chain B:



- Molecule 1: Heparan sulfate glucosamine 3-O-sulfotransferase 3A1

Chain A:



- Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid

Chain D:

- Molecule 3: 2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid

Chain E:

4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	133.76Å 65.01Å 92.23Å 90.00° 124.73° 90.00°	Depositor
Resolution (Å)	32.86 – 1.55 32.86 – 1.55	Depositor EDS
% Data completeness (in resolution range)	96.5 (32.86-1.55) 88.8 (32.86-1.55)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.05 (at 1.55Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.164 , 0.183 0.163 , 0.182	Depositor DCC
R_{free} test set	2000 reflections (2.19%)	wwPDB-VP
Wilson B-factor (Å^2)	16.8	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.9	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	0.97	EDS
Total number of atoms	5338	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% 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: SGN, IDS, NPO, BDP, EDO, NGY, A3P, NA

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	0.45	0/2152	0.64	0/2903
1	B	0.45	0/2263	0.65	0/3057
All	All	0.45	0/4415	0.65	0/5960

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	2098	0	2079	6	0
1	B	2208	0	2182	3	0
2	D	101	0	35	0	0
3	E	137	0	46	0	0
4	A	10	0	4	0	0
4	B	10	0	4	0	0
5	A	27	0	11	0	0
5	B	27	0	11	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	18	0	24	0	0
8	A	318	0	0	3	0
8	B	374	0	0	1	0
All	All	5338	0	4408	9	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 1.

The worst 5 of 9 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:301:HIS:ND1	8:A:602:HOH:O	2.32	0.60
1:A:388:ARG:NH1	1:A:406:GLY:O	2.41	0.51
1:A:381:ARG:NH2	8:A:604:HOH:O	2.44	0.51
1:A:246:VAL:HG21	1:A:384:ARG:HG2	1.92	0.50
1:B:198:TRP:CH2	1:B:202:LEU:HD11	2.48	0.48

There are no symmetry-related clashes.

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	A	257/273 (94%)	252 (98%)	5 (2%)	0	100	100
1	B	274/273 (100%)	265 (97%)	8 (3%)	1 (0%)	34	14
All	All	531/546 (97%)	517 (97%)	13 (2%)	1 (0%)	47	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	273	ASN

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	A	220/236 (93%)	218 (99%)	2 (1%)	78	61
1	B	230/236 (98%)	228 (99%)	2 (1%)	78	61
All	All	450/472 (95%)	446 (99%)	4 (1%)	78	61

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

Mol	Chain	Res	Type
1	B	214	GLU
1	B	215	LYS
1	A	214	GLU
1	A	215	LYS

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 ⓘ

15 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	BDP	D	1	2,4	12,12,13	0.78	0	14,17,19	0.83	0
2	SGN	D	2	2	18,19,20	1.02	2 (11%)	22,29,31	0.85	1 (4%)
2	IDS	D	3	2	16,16,17	0.82	0	17,24,26	1.11	1 (5%)
2	SGN	D	4	2	18,19,20	0.83	0	22,29,31	1.12	1 (4%)
2	IDS	D	5	2	16,16,17	0.91	1 (6%)	17,24,26	0.92	0
2	SGN	D	6	2	18,19,20	0.91	0	22,29,31	1.18	2 (9%)
3	BDP	E	1	3,4	12,12,13	0.69	0	14,17,19	0.63	0
3	SGN	E	2	3,6	18,19,20	0.95	1 (5%)	22,29,31	1.15	2 (9%)
3	IDS	E	3	3,6	16,16,17	0.91	0	17,24,26	1.39	2 (11%)
3	SGN	E	4	3	18,19,20	0.98	1 (5%)	22,29,31	1.22	1 (4%)
3	IDS	E	5	3	16,16,17	0.83	0	17,24,26	1.27	1 (5%)
3	SGN	E	6[A]	-	18,19,20	0.98	1 (5%)	22,29,31	1.32	3 (13%)
3	SGN	E	6[B]	-	18,19,20	0.92	1 (5%)	22,29,31	1.13	2 (9%)
3	BDP	E	7	3	12,12,13	0.90	0	14,17,19	1.10	2 (14%)
3	NGY	E	8	3	18,18,19	0.61	0	22,26,28	0.77	1 (4%)

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	BDP	D	1	2,4	-	0/4/21/24	0/1/1/1
2	SGN	D	2	2	-	0/11/28/31	0/1/1/1
2	IDS	D	3	2	-	0/9/26/29	0/1/1/1
2	SGN	D	4	2	-	1/11/28/31	0/1/1/1
2	IDS	D	5	2	-	0/9/26/29	0/1/1/1
2	SGN	D	6	2	-	3/11/28/31	0/1/1/1
3	BDP	E	1	3,4	-	0/4/21/24	0/1/1/1
3	SGN	E	2	3,6	-	0/11/28/31	0/1/1/1
3	IDS	E	3	3,6	-	0/9/26/29	0/1/1/1
3	SGN	E	4	3	-	0/11/28/31	0/1/1/1
3	IDS	E	5	3	-	3/9/26/29	0/1/1/1
3	SGN	E	6[A]	-	-	1/11/28/31	0/1/1/1
3	SGN	E	6[B]	-	-	3/11/28/31	0/1/1/1
3	BDP	E	7	3	-	0/4/21/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NGY	E	8	3	-	0/10/27/30	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	SGN	O1S-S1	2.93	1.45	1.42
3	E	2	SGN	O1S-S1	2.77	1.45	1.42
2	D	2	SGN	O1S-S1	2.31	1.44	1.42
3	E	6[A]	SGN	C2-N2	-2.22	1.44	1.47
3	E	6[B]	SGN	C2-N2	-2.22	1.44	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4	SGN	O1S-S1-O2S	-4.46	109.62	120.16
3	E	4	SGN	O1S-S1-O2S	-4.44	109.66	120.16
2	D	6	SGN	O1S-S1-O2S	-4.29	110.03	120.16
3	E	3	IDS	C2-O2-S	4.27	123.48	117.91
3	E	5	IDS	C2-O2-S	3.99	123.11	117.91

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

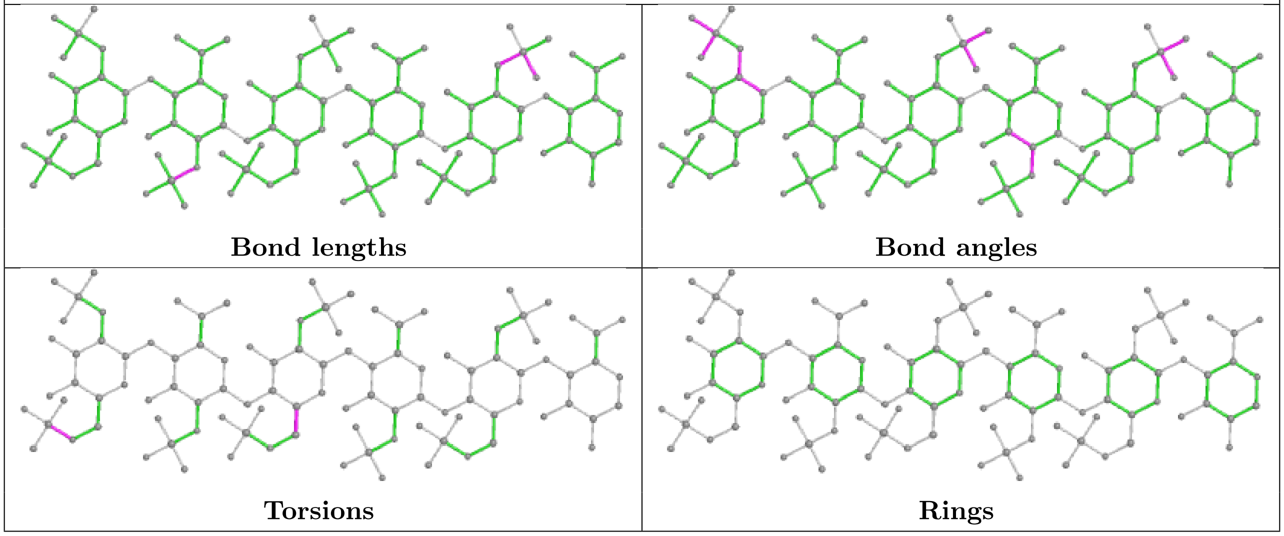
Mol	Chain	Res	Type	Atoms
2	D	6	SGN	C6-O6-S2-O4S
3	E	5	IDS	C2-O2-S-O1S
3	E	5	IDS	C2-O2-S-O2S
3	E	5	IDS	C2-O2-S-O3S
3	E	6[B]	SGN	O5-C5-C6-O6

There are no ring outliers.

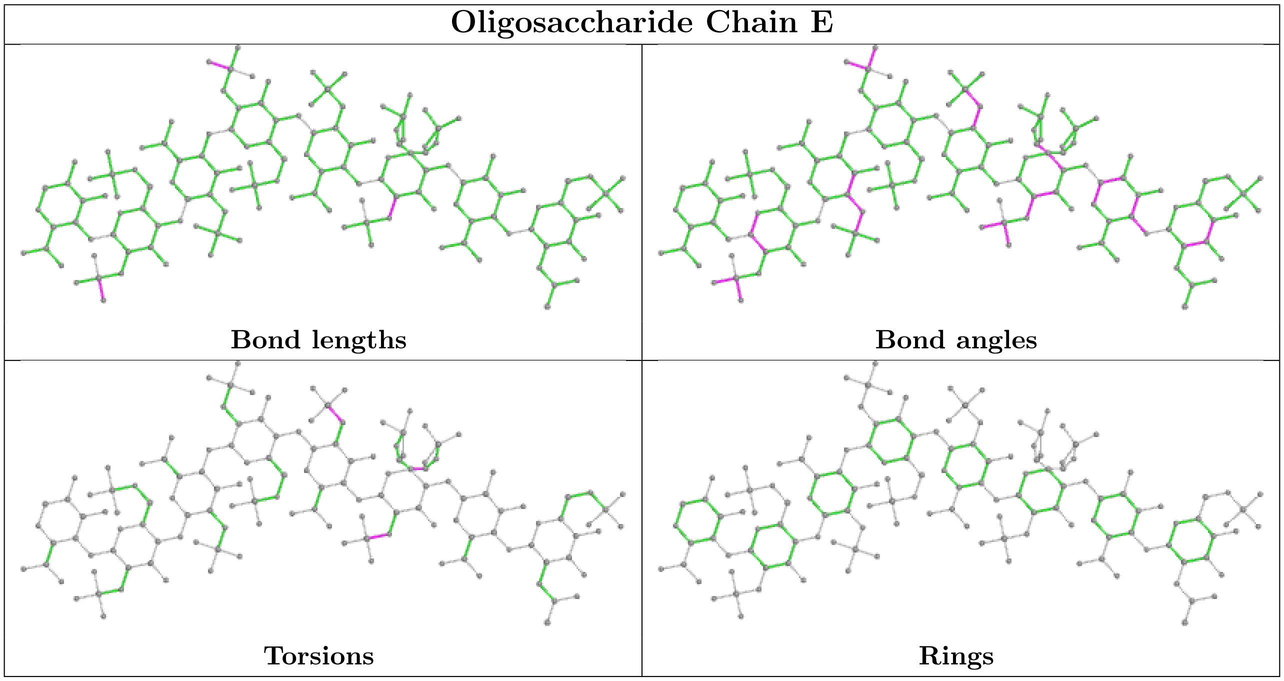
No monomer is involved in short contacts.

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

Oligosaccharide Chain D



Oligosaccharide Chain E



5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	EDO	B	506	-	2,2,3	0.50	0	1,1,2	0.33	0
7	EDO	B	504	-	3,3,3	0.49	0	2,2,2	0.39	0
7	EDO	B	505	-	3,3,3	0.43	0	2,2,2	0.61	0
4	NPO	A	501	2	9,10,10	0.60	0	11,13,13	1.75	3 (27%)
5	A3P	B	502	-	26,29,29	0.80	0	31,45,45	1.01	1 (3%)
5	A3P	A	502	-	26,29,29	0.74	0	31,45,45	0.91	1 (3%)
7	EDO	B	508	-	3,3,3	0.49	0	2,2,2	0.41	0
7	EDO	A	504	-	3,3,3	0.51	0	2,2,2	0.28	0
7	EDO	A	505	-	3,3,3	0.36	0	2,2,2	0.70	0
7	EDO	B	507	-	2,2,3	0.39	0	1,1,2	0.00	0
4	NPO	B	501	3	9,10,10	0.34	0	11,13,13	0.99	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
7	EDO	B	504	-	-	0/1/1/1	-
7	EDO	B	505	-	-	1/1/1/1	-
4	NPO	A	501	2	-	0/2/4/4	0/1/1/1
5	A3P	B	502	-	-	2/11/31/31	0/3/3/3
5	A3P	A	502	-	-	2/11/31/31	0/3/3/3
7	EDO	B	508	-	-	0/1/1/1	-
7	EDO	A	504	-	-	0/1/1/1	-
7	EDO	A	505	-	-	0/1/1/1	-
4	NPO	B	501	3	-	0/2/4/4	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	NPO	C2-C1-N1	-3.31	116.89	119.38
4	A	501	NPO	C6-C1-C2	2.43	123.87	119.86
5	A	502	A3P	C5-C6-N6	2.13	123.59	120.35
4	A	501	NPO	C5-C6-C1	-2.05	117.23	120.08
5	B	502	A3P	C5-C6-N6	2.04	123.46	120.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

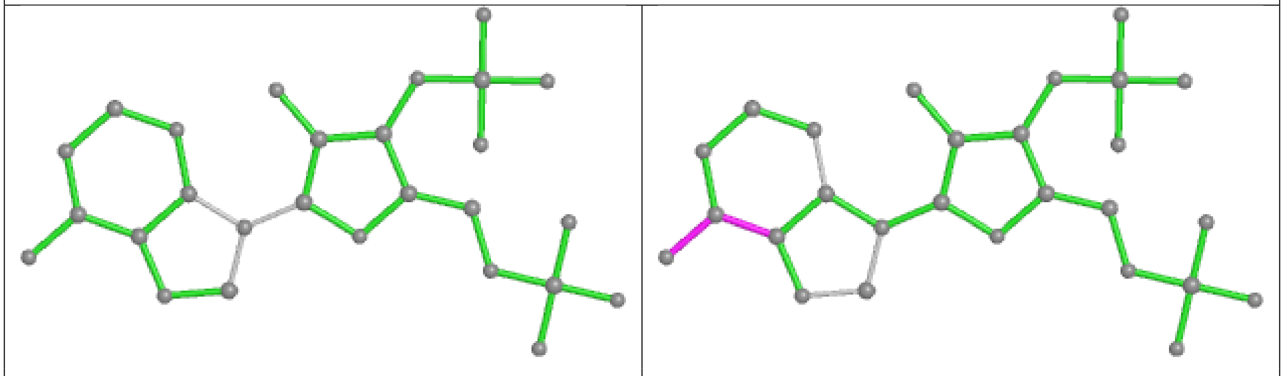
Mol	Chain	Res	Type	Atoms
5	B	502	A3P	C2'-C3'-O3'-P1
5	A	502	A3P	C2'-C3'-O3'-P1
5	B	502	A3P	C4'-C3'-O3'-P1
5	A	502	A3P	C4'-C3'-O3'-P1
7	B	505	EDO	O1-C1-C2-O2

There are no ring outliers.

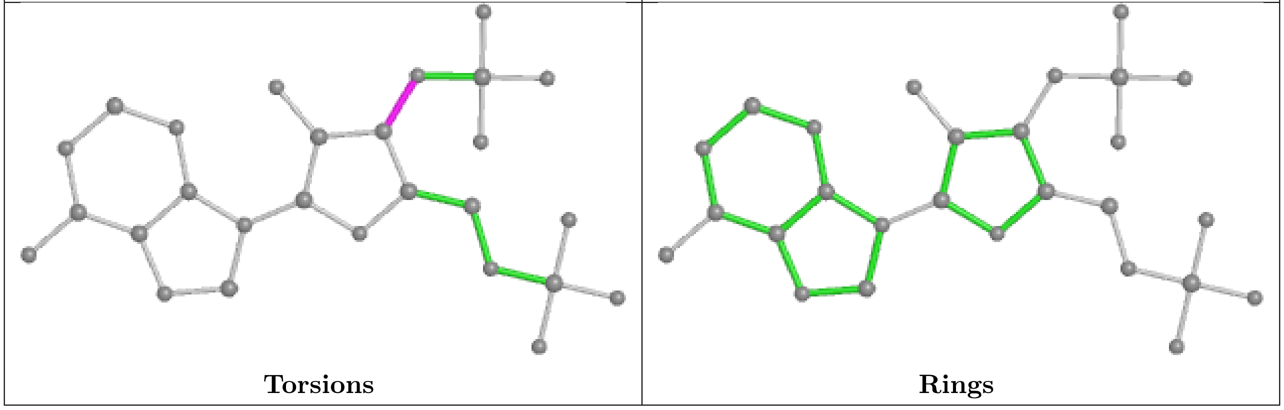
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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 A3P B 502

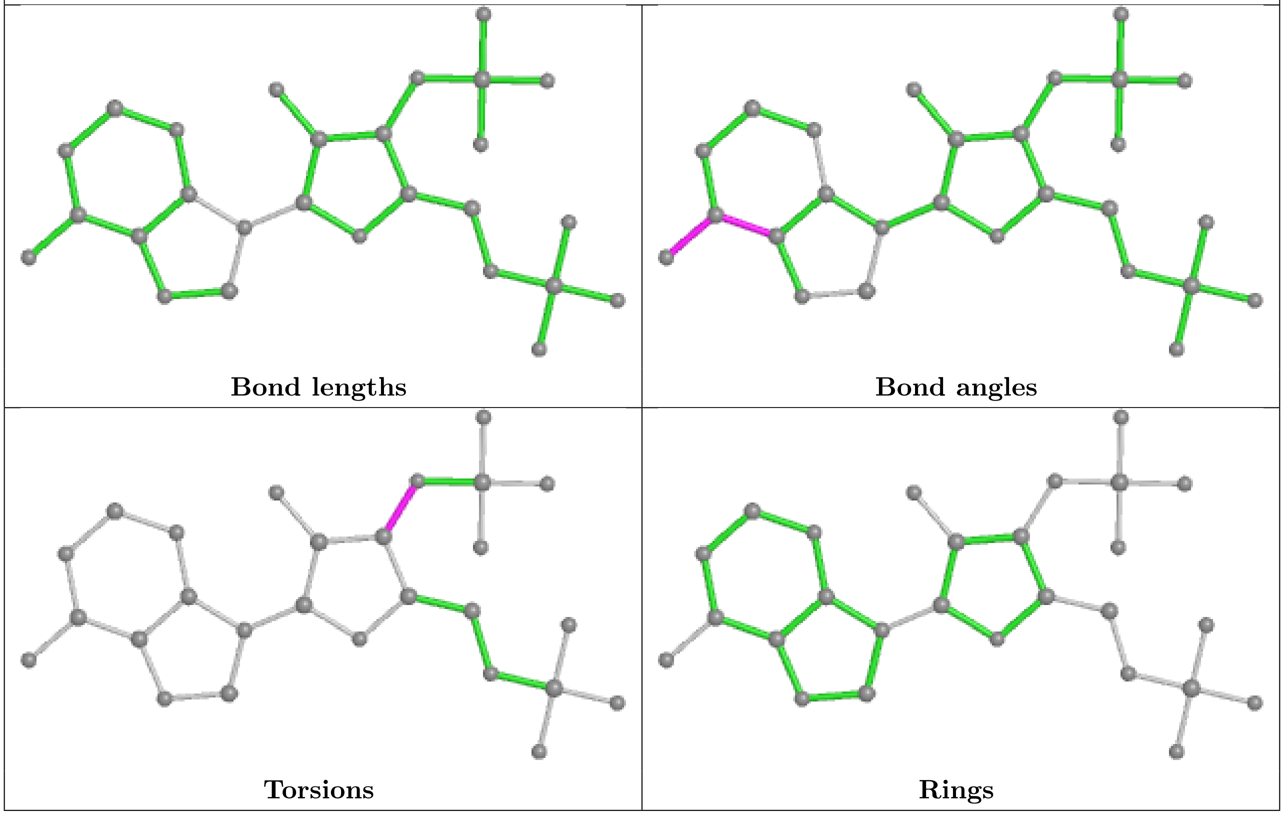


Bond lengths **Bond angles**



Torsions **Rings**

Ligand A3P A 502



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(Å^2)	Q<0.9
1	A	257/273 (94%)	0.15	18 (7%)	16	19	14, 22, 52, 80	0
1	B	266/273 (97%)	0.08	13 (4%)	29	34	12, 18, 35, 69	0
All	All	523/546 (95%)	0.12	31 (5%)	22	26	12, 20, 47, 80	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	141	LEU	6.1
1	B	143	LEU	6.0
1	B	142	ALA	5.4
1	B	278	LEU	5.3
1	B	275	THR	5.2

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(Å^2)	Q<0.9
2	SGN	D	6	19/20	0.77	0.23	48,62,73,77	0
2	IDS	D	5	16/17	0.85	0.13	36,52,69,72	0
3	BDP	E	1	12/13	0.91	0.08	18,24,29,34	0
3	BDP	E	7	12/13	0.91	0.10	23,27,35,47	0
2	SGN	D	4	19/20	0.94	0.08	25,30,46,46	0

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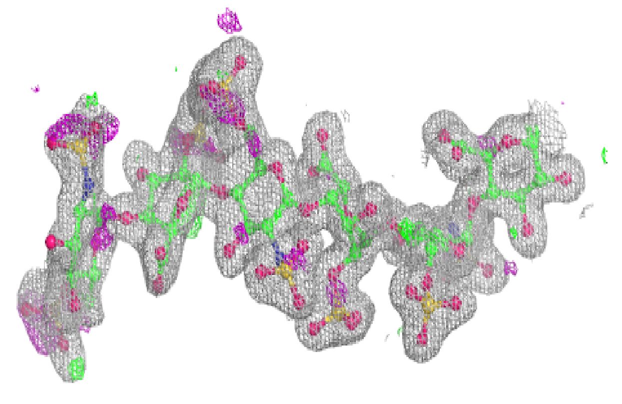
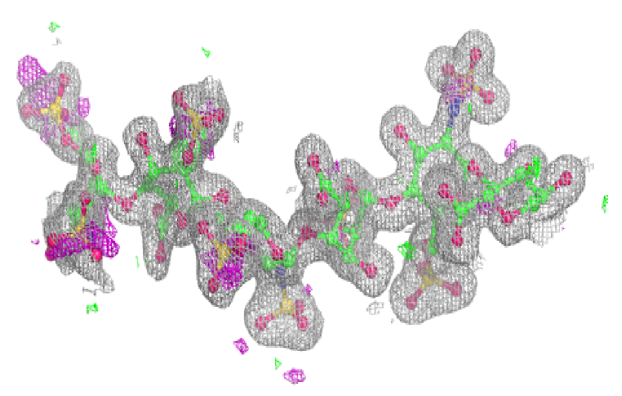
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NGY	E	8	18/19	0.94	0.09	23,27,37,40	0
3	SGN	E	6[B]	19/20	0.95	0.09	19,26,34,38	6
2	BDP	D	1	12/13	0.95	0.08	17,19,22,22	0
3	SGN	E	6[A]	19/20	0.95	0.09	19,25,32,34	6
3	IDS	E	3	16/17	0.96	0.07	15,18,27,29	0
2	IDS	D	3	16/17	0.97	0.06	20,24,28,29	0
3	SGN	E	2	19/20	0.98	0.06	15,19,36,42	0
2	SGN	D	2	19/20	0.98	0.07	16,18,28,30	0
3	SGN	E	4	19/20	0.98	0.07	13,15,27,31	0
3	IDS	E	5	16/17	0.98	0.06	14,18,23,23	0

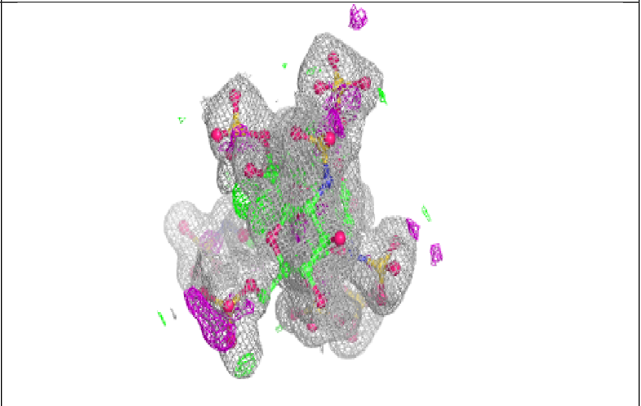
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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 E:

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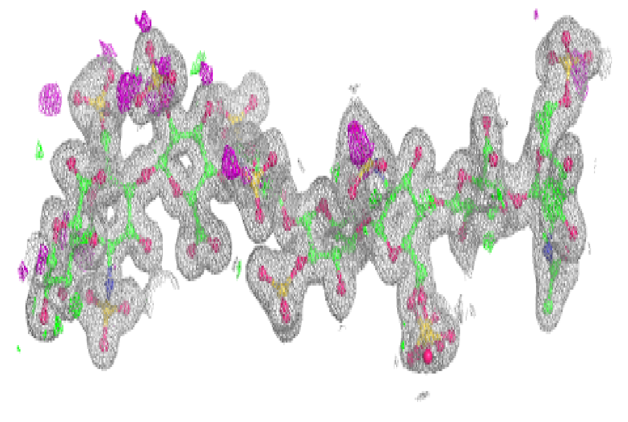
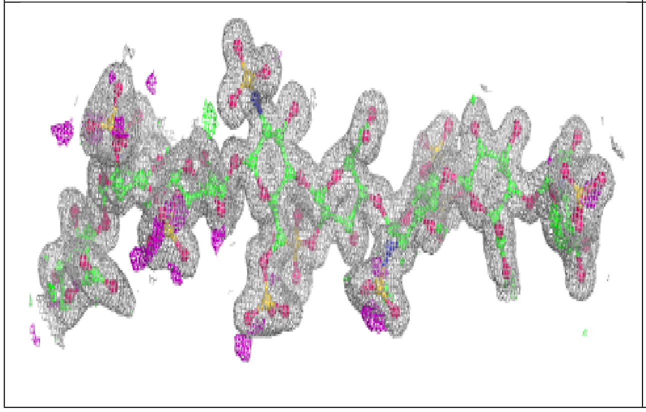
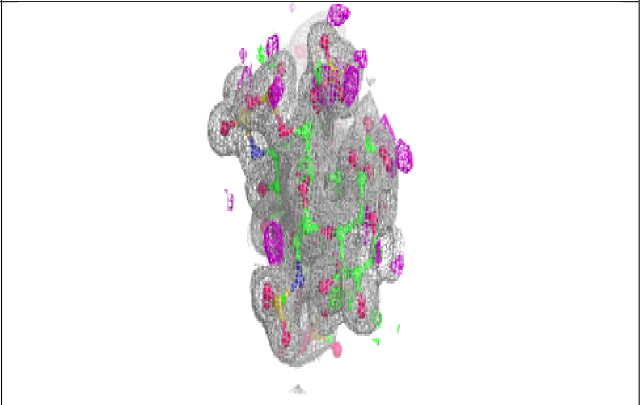
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)





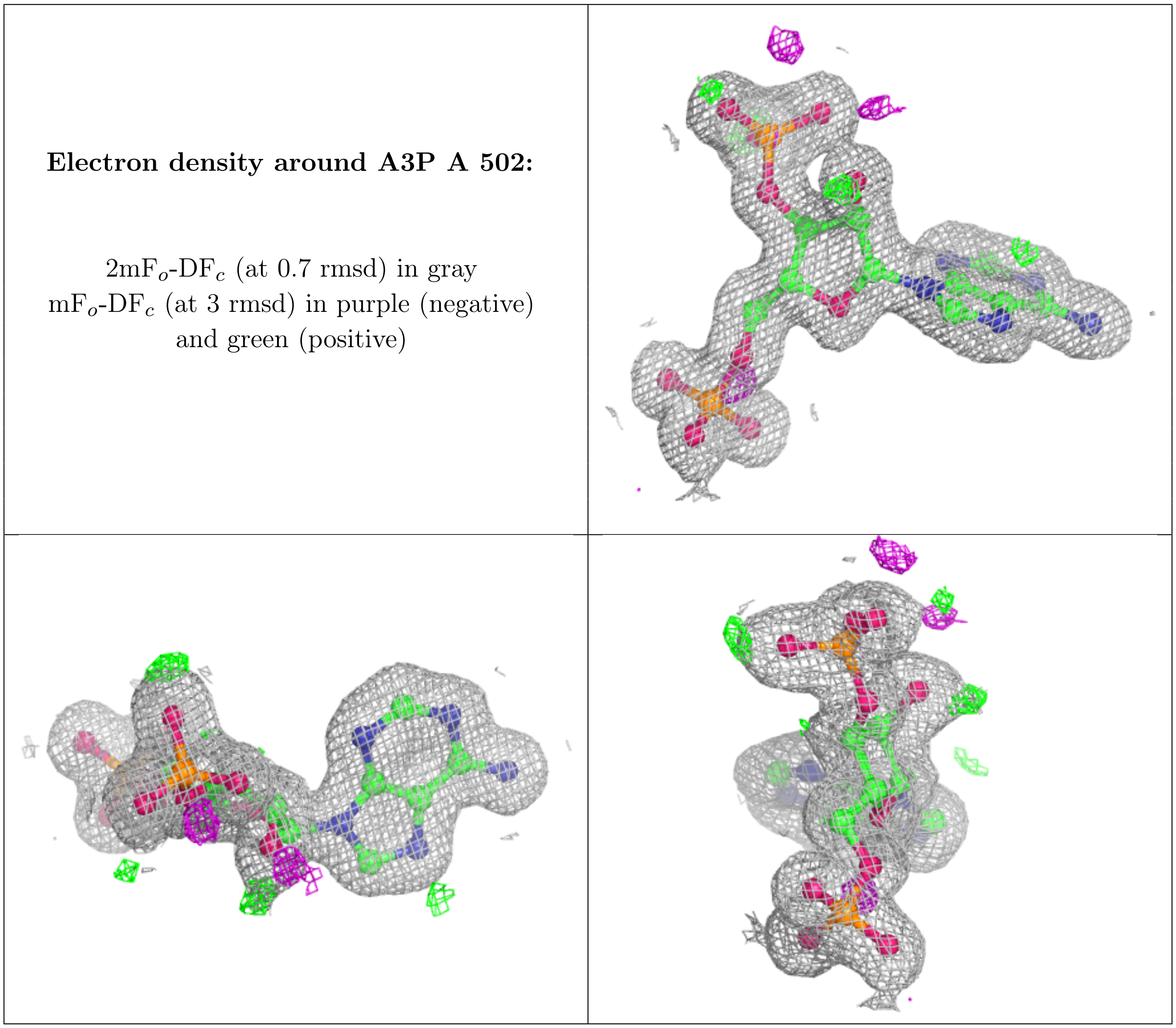


6.4 Ligands ⓘ

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, 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
7	EDO	B	506	3/4	0.64	0.19	29,29,32,35	0
7	EDO	B	508	4/4	0.82	0.29	27,44,44,47	0
6	NA	A	503	1/1	0.88	0.10	38,38,38,38	0
7	EDO	B	504	4/4	0.91	0.20	29,32,36,36	0
4	NPO	A	501	10/10	0.92	0.12	18,23,35,37	0
4	NPO	B	501	10/10	0.93	0.11	21,25,33,35	0
7	EDO	B	505	4/4	0.93	0.18	31,33,34,45	0
7	EDO	B	507	3/4	0.94	0.12	32,32,38,39	0
7	EDO	A	505	4/4	0.94	0.09	26,28,31,35	0
5	A3P	A	502	27/27	0.98	0.07	13,16,19,20	0
7	EDO	A	504	4/4	0.98	0.08	21,24,24,24	0
5	A3P	B	502	27/27	0.98	0.08	12,14,16,17	0
6	NA	B	503	1/1	0.99	0.06	19,19,19,19	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.

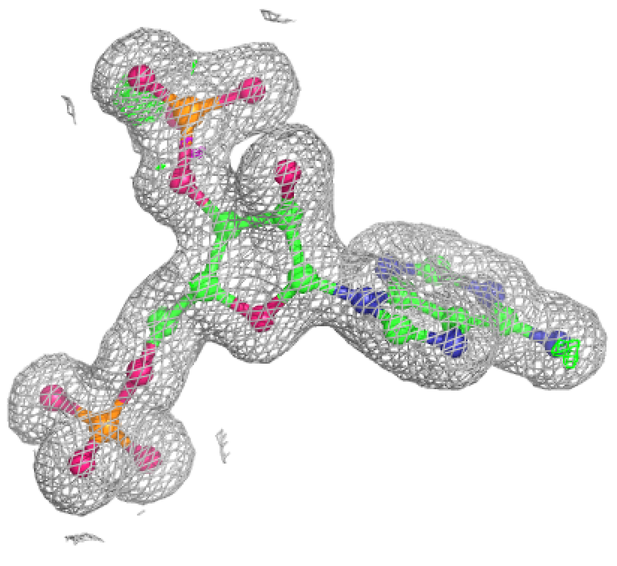


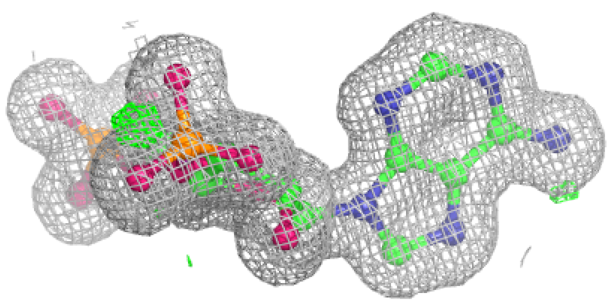
Electron density around A3P A 502:

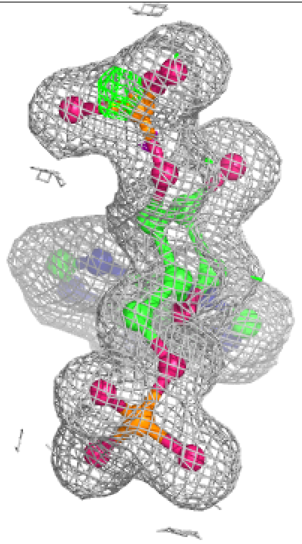
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around A3P B 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 ⓘ

There are no such residues in this entry.