wwPDB X-ray Structure Validation Summary Report (i)

Nov 10, 2024 – 08:27 PM EST

PDB ID	:	1DDX
Title	:	CRYSTAL STRUCTURE OF A MIXTURE OF ARACHIDONIC ACID AND PROSTAGLANDIN BOUND TO THE CYCLOOXYGENASE ACTIVE SITE OF COX-2: PROSTAGLANDIN STRUCTURE
Authors	:	Kiefer, J.R.; Pawlitz, J.L.; Moreland, K.T.; Stegeman, R.A.; Gierse, J.K.; Stevens, A.M.; Goodwin, D.C.; Rowlinson, S.W.; Marnett, L.J.; Stallings, W.C.; Kurumbail, R.G.
Deposited on	:	1999-11-11
Resolution	:	3.00 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 (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 (i)) were used in the production of this report:

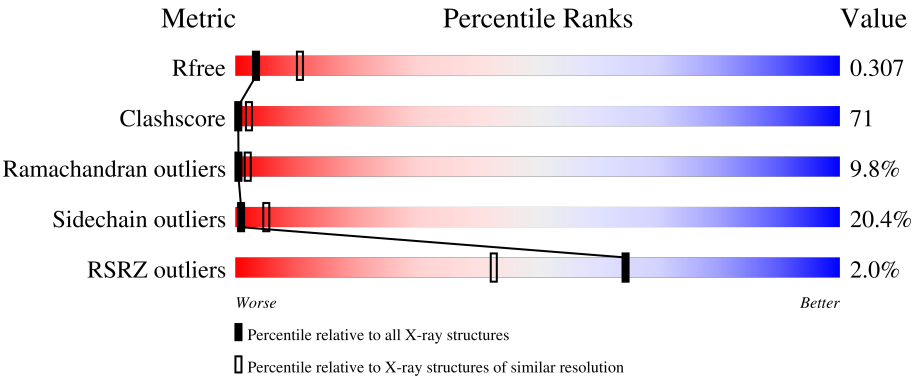
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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	552	19% 59% 21%
1	B	552	2% 19% 59% 20%
1	C	552	3% 20% 57% 22%

Continued on next page...

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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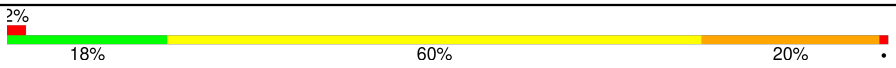
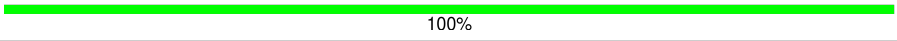
Mol	Chain	Length	Quality of chain
1	D	552	
2	E	2	
2	F	2	
2	G	2	
2	H	2	

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
5	PGX	A	701	-	-	X	-
5	PGX	B	1701	-	-	X	-
5	PGX	C	2701	-	-	X	-
5	PGX	D	3701	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 18477 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.

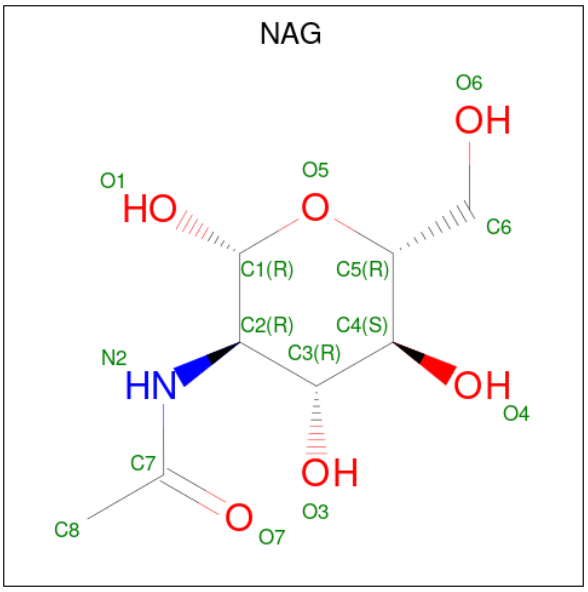
- Molecule 1 is a protein called PROTEIN (PROSTAGLANDIN H2 SYNTHASE-2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4475	2885	750	815	25			
1	B	552	Total	C	N	O	S	0	0	0
			4475	2885	750	815	25			
1	C	552	Total	C	N	O	S	0	0	0
			4475	2885	750	815	25			
1	D	552	Total	C	N	O	S	0	0	0
			4475	2885	750	815	25			

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

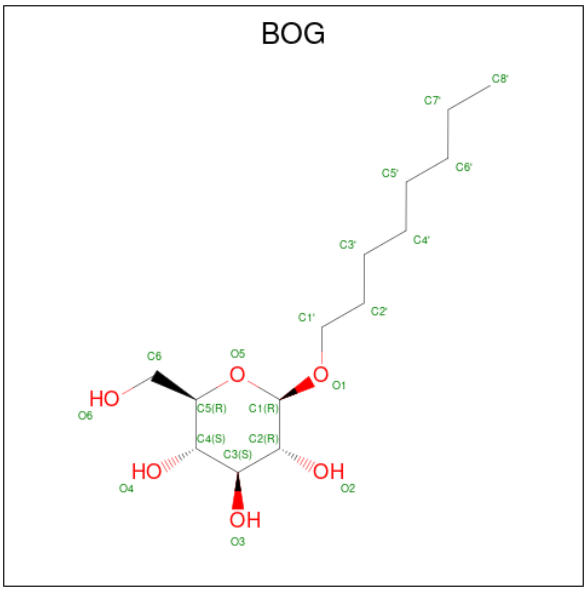
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



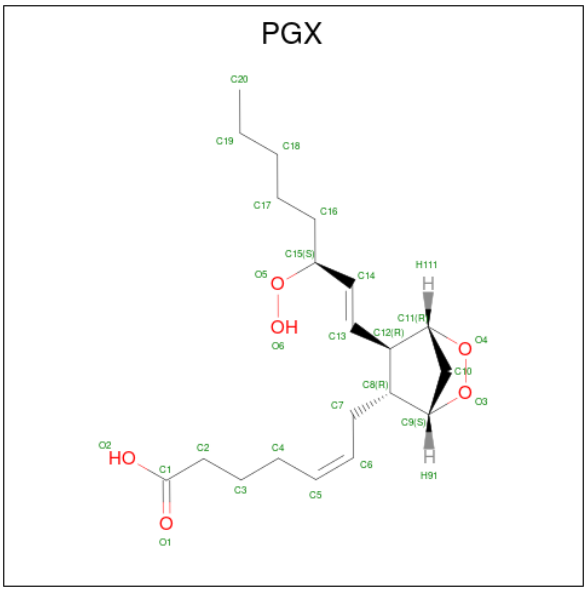
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 20 14 6	0	0
4	B	1	Total C O 20 14 6	0	0
4	C	1	Total C O 20 14 6	0	0
4	D	1	Total C O 20 14 6	0	0

- Molecule 5 is 7-[6-(3-HYDROPEROXY-OCT-1-ENYL)-2,3-DIOXA-BICYCLO[2.2.1]HEPT -5-YL]-HEPT-5-ENOIC ACID (three-letter code: PGX) (formula: $C_{20}H_{32}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 25 20 5	0	0
5	B	1	Total C O 25 20 5	0	0
5	C	1	Total C O 25 20 5	0	0
5	D	1	Total C O 25 20 5	0	0

- Molecule 6 is water.

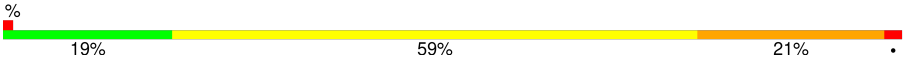
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	45	Total O 45 45	0	0
6	B	39	Total O 39 39	0	0
6	C	46	Total O 46 46	0	0
6	D	43	Total O 43 43	0	0

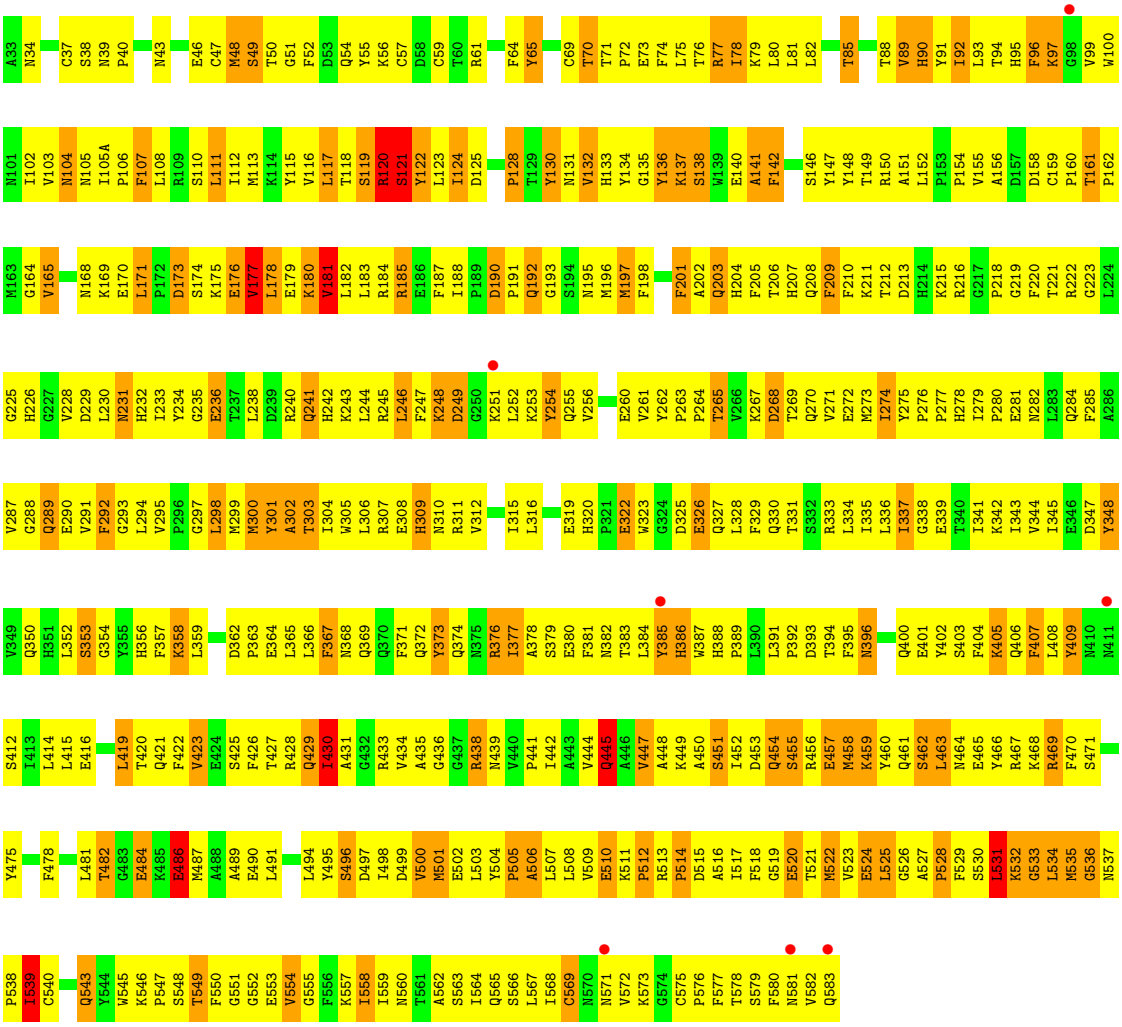
3 Residue-property plots (i)

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: PROTEIN (PROSTAGLANDIN H2 SYNTHASE-2)

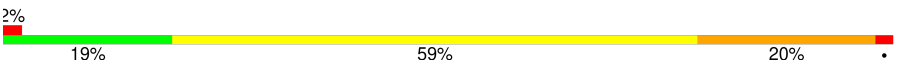
Chain A:

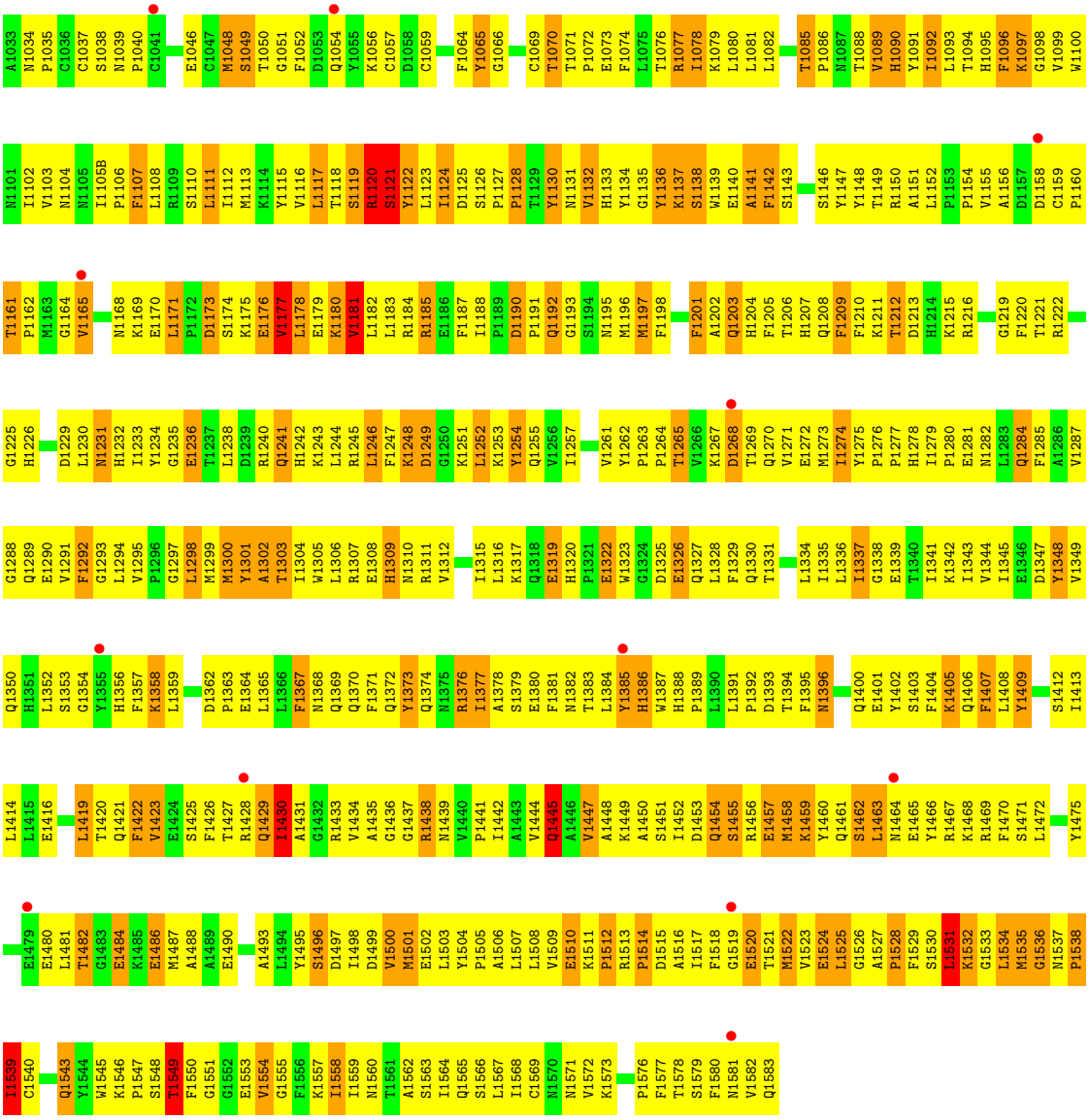




• Molecule 1: PROTEIN (PROSTAGLANDIN H2 SYNTHASE-2)

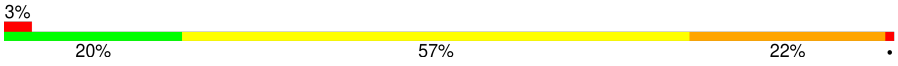
Chain B:

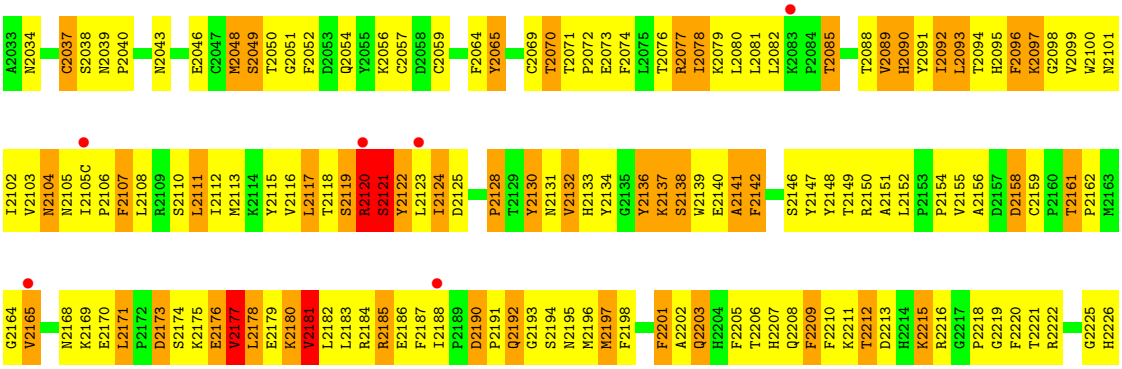


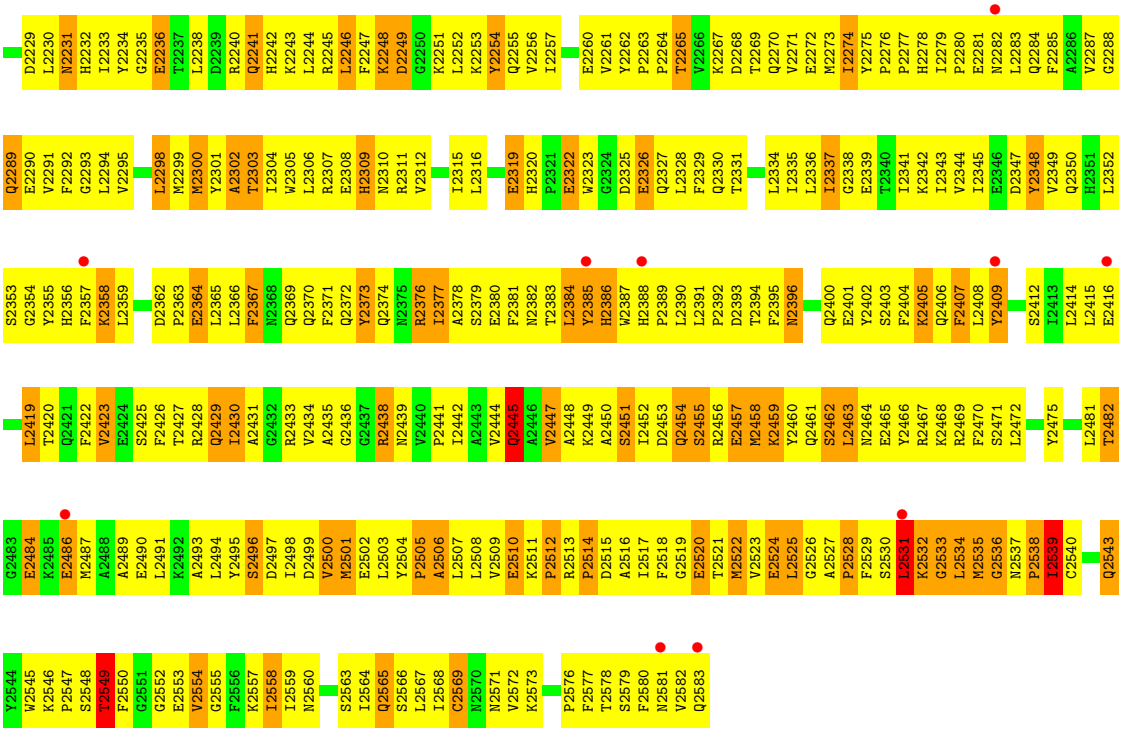


• Molecule 1: PROTEIN (PROSTAGLANDIN H2 SYNTHASE-2)

Chain C:

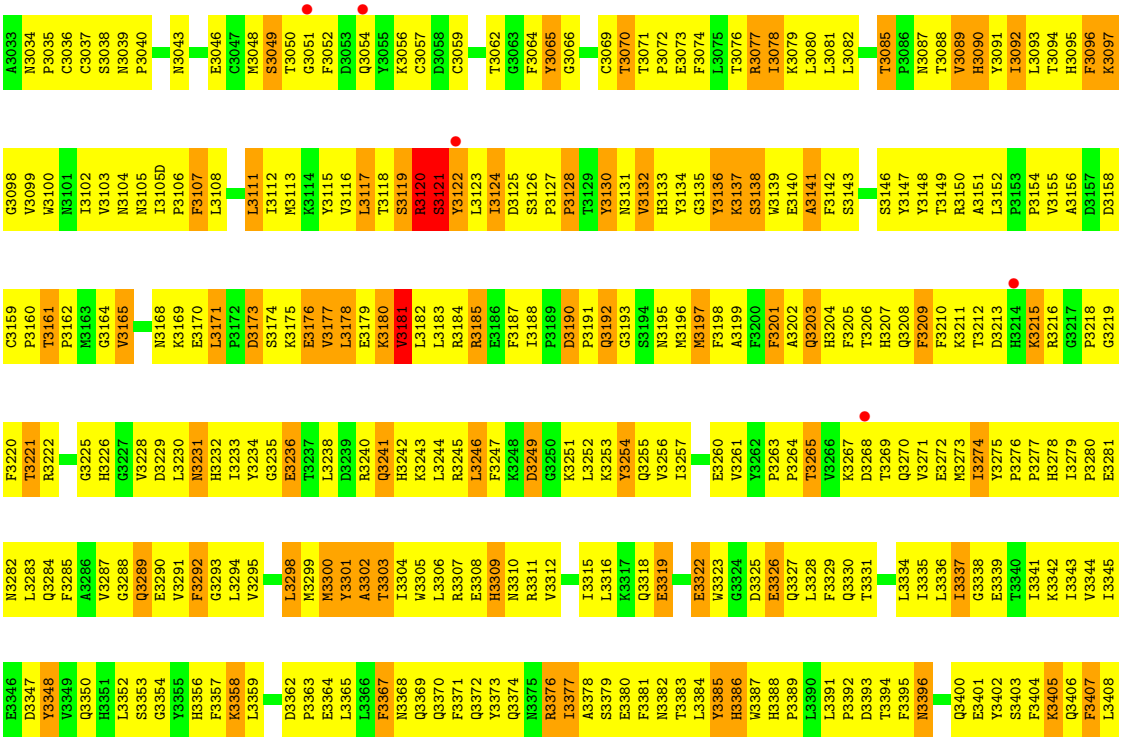


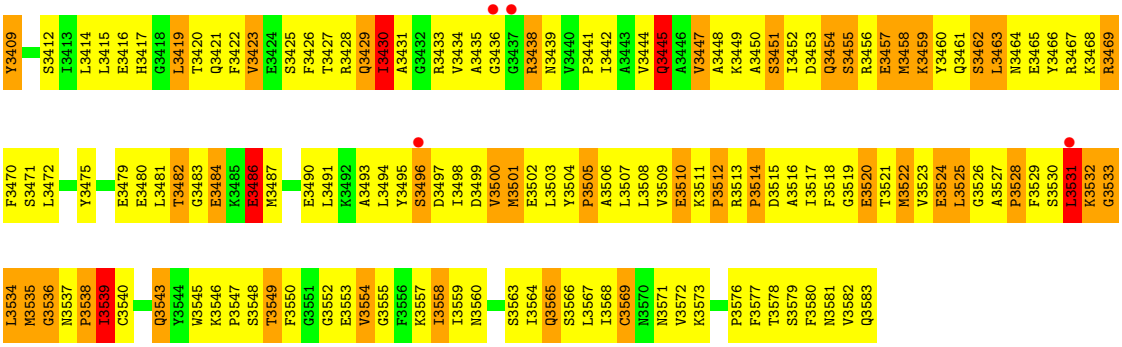




• Molecule 1: PROTEIN (PROSTAGLANDIN H2 SYNTHASE-2)

Chain D:





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

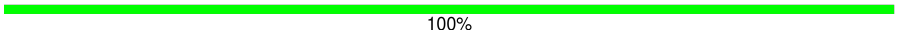
Chain E:

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

Chain F:

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

Chain G:



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

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	180.24Å 134.80Å 122.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	76.1 (20.00-3.00) 75.7 (20.00-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 3.00Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.267 , 0.324 0.252 , 0.307	Depositor DCC
R_{free} test set	4324 reflections (9.44%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.915	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 55.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	18477	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.3521e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: NAG, PGX, BOG

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	0/4602	0.65	0/6239
1	B	0.45	0/4602	0.65	0/6239
1	C	0.45	0/4602	0.65	0/6239
1	D	0.46	0/4602	0.64	0/6239
All	All	0.45	0/18408	0.64	0/24956

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	4475	0	4373	650	0
1	B	4475	0	4373	653	0
1	C	4475	0	4373	663	0
1	D	4475	0	4373	668	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
3	A	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	26	0	0
3	C	28	0	26	0	0
3	D	28	0	26	0	0
4	A	20	0	28	0	0
4	B	20	0	28	0	0
4	C	20	0	28	0	0
4	D	20	0	28	1	0
5	A	25	0	30	9	0
5	B	25	0	30	13	0
5	C	25	0	30	14	0
5	D	25	0	30	11	0
6	A	45	0	0	14	0
6	B	39	0	0	12	0
6	C	46	0	0	20	0
6	D	43	0	0	15	0
All	All	18477	0	17928	2579	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 71.

The worst 5 of 2579 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:D:3312:VAL:HA	1:D:3315:ILE:HD12	1.33	1.09
1:A:312:VAL:HA	1:A:315:ILE:HD12	1.33	1.08
1:B:1312:VAL:HA	1:B:1315:ILE:HD12	1.36	1.07
1:B:1301:TYR:HA	1:B:1304:ILE:HD12	1.37	1.07
1:A:99:VAL:HA	1:A:102:ILE:HD12	1.37	1.06

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	550/552 (100%)	374 (68%)	124 (22%)	52 (10%)	0 2
1	B	550/552 (100%)	379 (69%)	119 (22%)	52 (10%)	0 2
1	C	550/552 (100%)	372 (68%)	120 (22%)	58 (10%)	0 2
1	D	550/552 (100%)	376 (68%)	121 (22%)	53 (10%)	0 2
All	All	2200/2208 (100%)	1501 (68%)	484 (22%)	215 (10%)	0 2

5 of 215 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	A	122	TYR
1	A	176	GLU
1	A	180	LYS
1	A	348	TYR

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	493/493 (100%)	391 (79%)	102 (21%)	1 5
1	B	493/493 (100%)	391 (79%)	102 (21%)	1 5
1	C	493/493 (100%)	393 (80%)	100 (20%)	1 5
1	D	493/493 (100%)	394 (80%)	99 (20%)	1 5
All	All	1972/1972 (100%)	1569 (80%)	403 (20%)	1 5

5 of 403 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2165	VAL
1	C	2482	THR
1	D	3543	GLN
1	C	2190	ASP
1	C	2322	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1571	ASN
1	D	3560	ASN
1	C	2396	ASN
1	D	3464	ASN
1	D	3374	GLN

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)

8 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	E	1	1,2	14,14,15	0.67	0	17,19,21	0.68	0
2	NAG	E	2	2	14,14,15	0.80	0	17,19,21	0.51	0
2	NAG	F	1	1,2	14,14,15	0.88	0	17,19,21	0.75	1 (5%)
2	NAG	F	2	2	14,14,15	0.93	0	17,19,21	0.53	0
2	NAG	G	1	1,2	14,14,15	0.67	0	17,19,21	0.71	0
2	NAG	G	2	2	14,14,15	0.80	0	17,19,21	0.52	0
2	NAG	H	1	1,2	14,14,15	0.76	0	17,19,21	0.70	0
2	NAG	H	2	2	14,14,15	0.85	0	17,19,21	0.57	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	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1	NAG	C2-N2-C7	-2.08	120.11	122.90

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

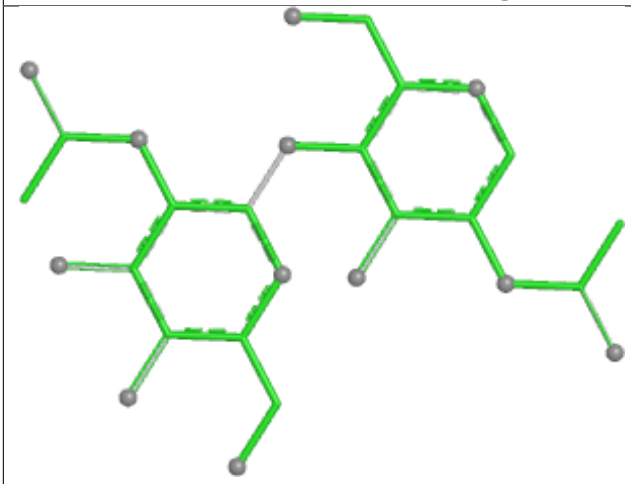
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C1-C2-N2-C7
2	F	2	NAG	C1-C2-N2-C7
2	G	2	NAG	C1-C2-N2-C7
2	H	2	NAG	C1-C2-N2-C7
2	F	2	NAG	C3-C2-N2-C7

There are no ring outliers.

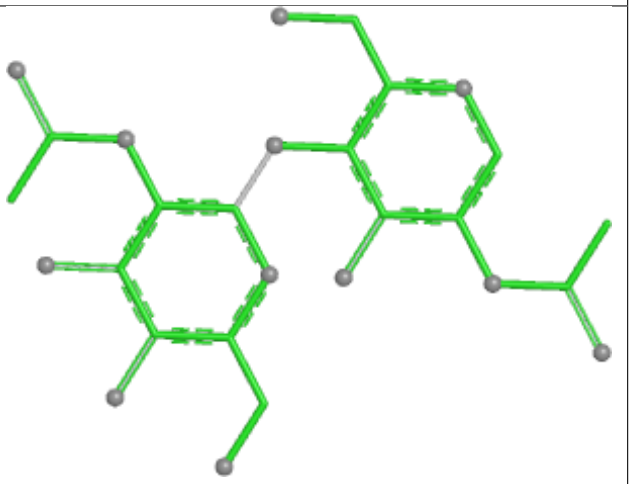
No monomer is involved in short contacts.

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

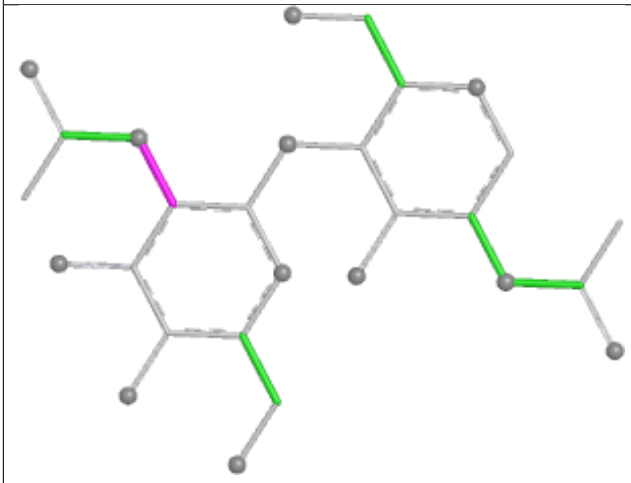
Oligosaccharide Chain E



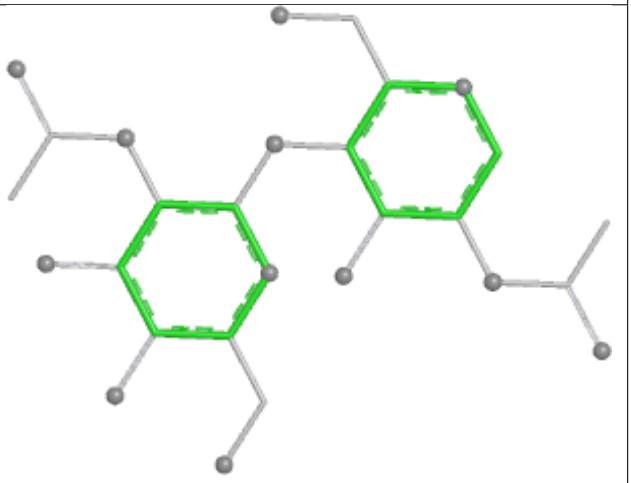
Bond lengths



Bond angles

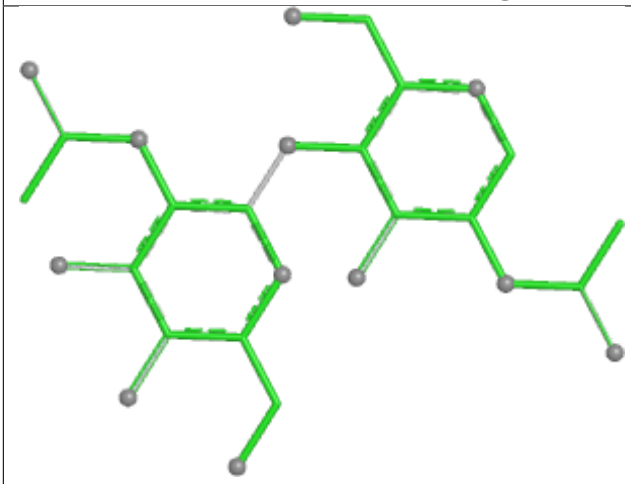


Torsions

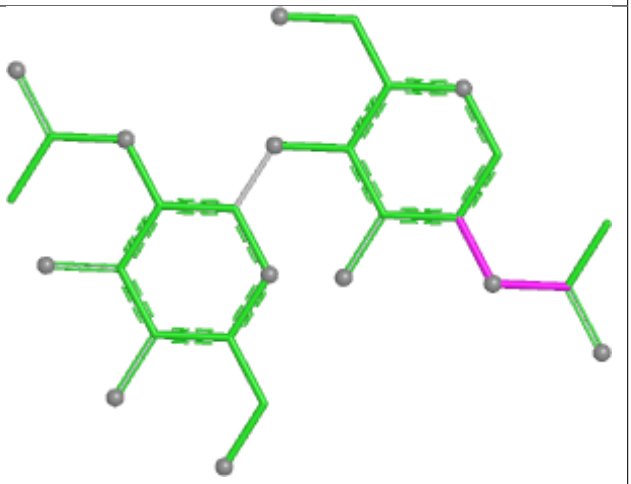


Rings

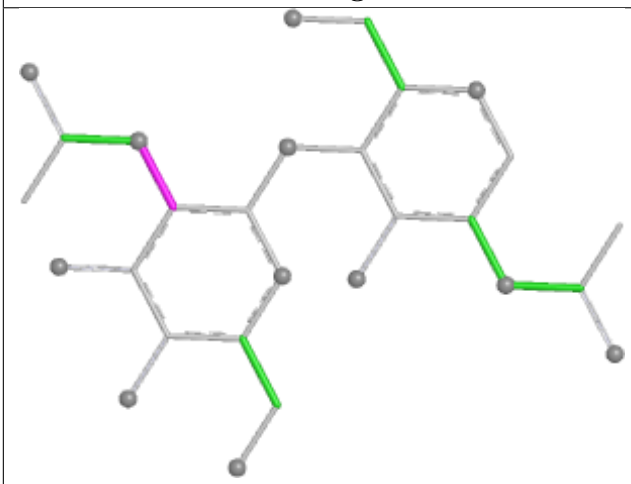
Oligosaccharide Chain F



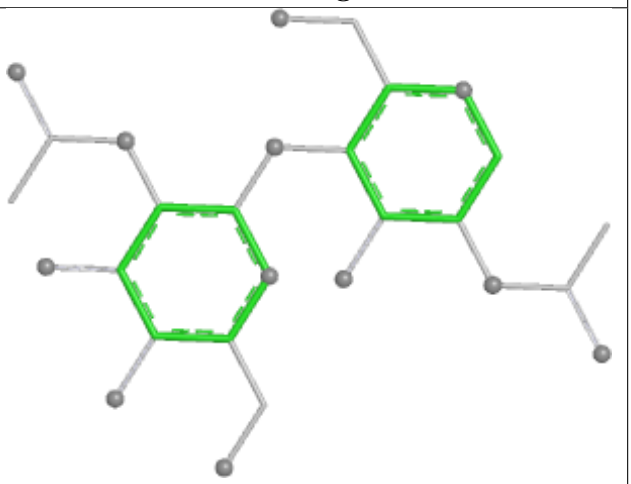
Bond lengths



Bond angles

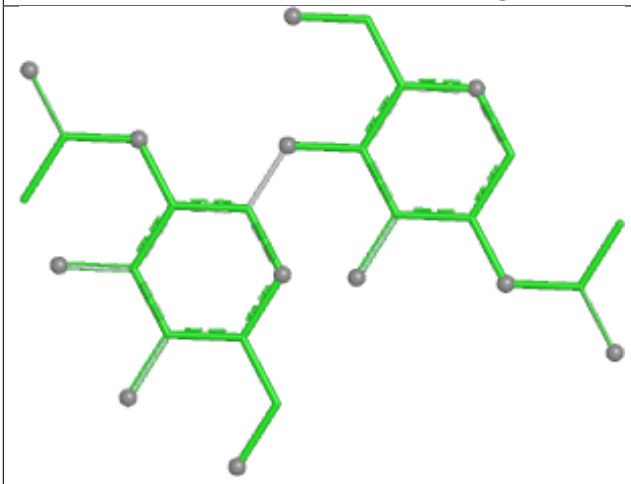


Torsions

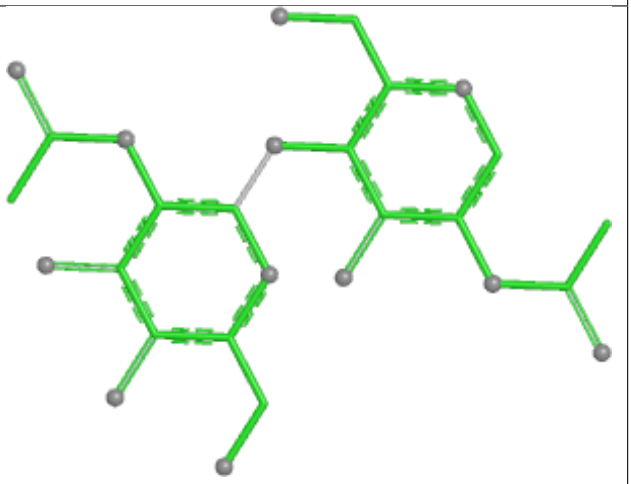


Rings

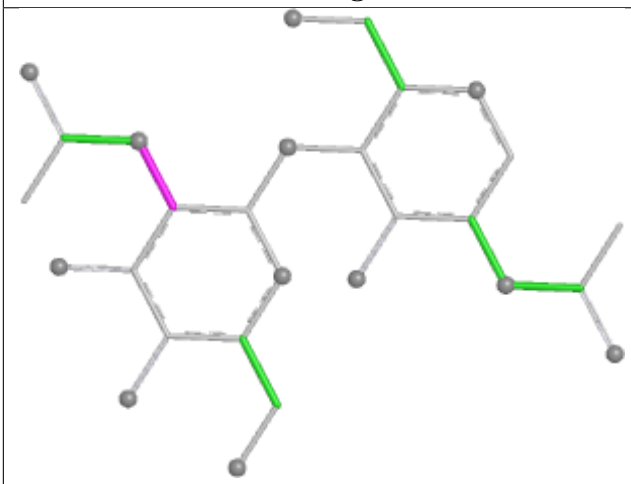
Oligosaccharide Chain G



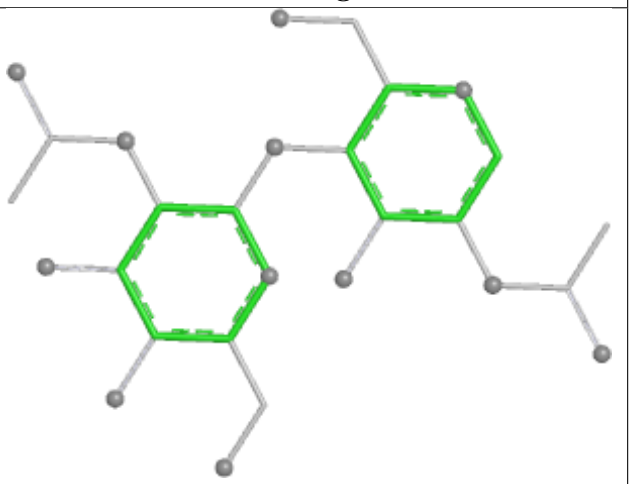
Bond lengths



Bond angles

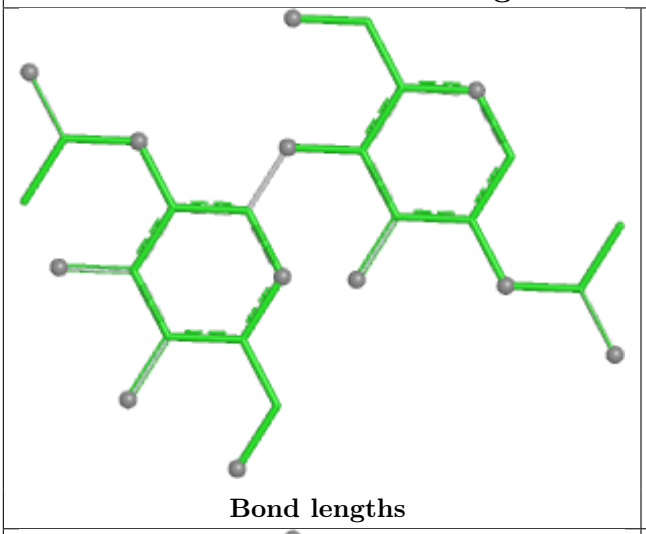


Torsions

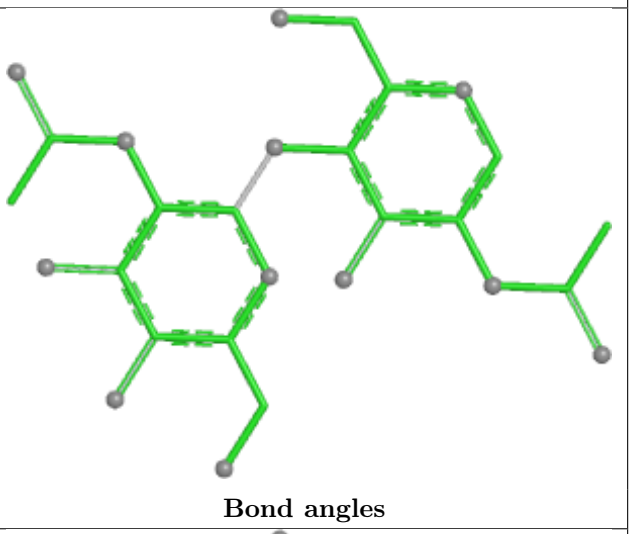


Rings

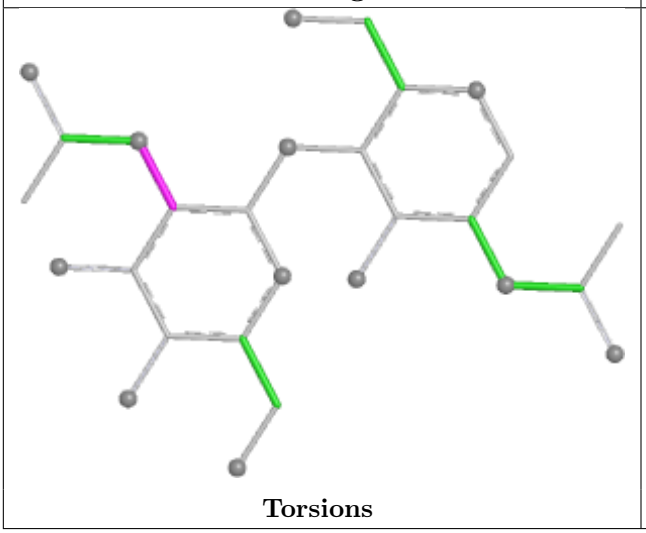
Oligosaccharide Chain H



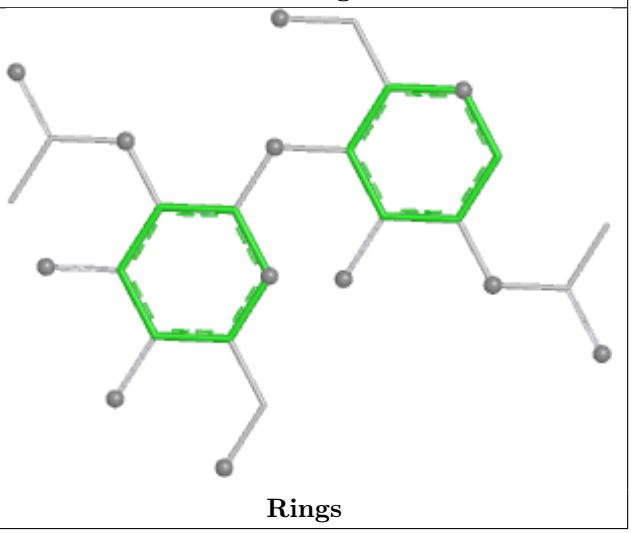
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

16 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	$\#\|Z\| > 2$
3	NAG	A	681	1	14,14,15	0.73	0	17,19,21	0.70	0
3	NAG	A	671	1	14,14,15	0.71	0	17,19,21	1.12	2 (11%)
5	PGX	C	2701	-	24,26,27	1.47	1 (4%)	25,33,34	1.50	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PGX	A	701	-	24,26,27	1.51	3 (12%)	25,33,34	1.52	1 (4%)
4	BOG	D	3702	-	20,20,20	0.89	2 (10%)	25,25,25	0.59	0
5	PGX	D	3701	-	24,26,27	1.50	1 (4%)	25,33,34	1.52	1 (4%)
5	PGX	B	1701	-	24,26,27	1.52	2 (8%)	25,33,34	1.51	1 (4%)
4	BOG	B	1702	-	20,20,20	0.87	2 (10%)	25,25,25	0.62	0
3	NAG	D	3671	1	14,14,15	0.61	0	17,19,21	1.00	2 (11%)
3	NAG	B	1681	1	14,14,15	0.69	0	17,19,21	0.65	0
4	BOG	A	702	-	20,20,20	0.90	2 (10%)	25,25,25	0.61	0
3	NAG	B	1671	1	14,14,15	0.57	0	17,19,21	0.89	1 (5%)
3	NAG	C	2671	1	14,14,15	0.72	0	17,19,21	1.07	1 (5%)
4	BOG	C	2702	-	20,20,20	0.97	2 (10%)	25,25,25	0.60	0
3	NAG	D	3681	1	14,14,15	0.62	0	17,19,21	0.51	0
3	NAG	C	2681	1	14,14,15	0.72	0	17,19,21	0.63	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	681	1	-	2/6/23/26	0/1/1/1
3	NAG	A	671	1	-	2/6/23/26	0/1/1/1
5	PGX	C	2701	-	-	11/19/40/42	0/2/2/2
5	PGX	A	701	-	-	11/19/40/42	0/2/2/2
4	BOG	D	3702	-	-	2/11/31/31	0/1/1/1
5	PGX	D	3701	-	-	11/19/40/42	0/2/2/2
5	PGX	B	1701	-	-	11/19/40/42	0/2/2/2
4	BOG	B	1702	-	-	2/11/31/31	0/1/1/1
3	NAG	D	3671	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1681	1	-	3/6/23/26	0/1/1/1
4	BOG	A	702	-	-	2/11/31/31	0/1/1/1
3	NAG	B	1671	1	-	2/6/23/26	0/1/1/1
3	NAG	C	2671	1	-	2/6/23/26	0/1/1/1
4	BOG	C	2702	-	-	2/11/31/31	0/1/1/1
3	NAG	D	3681	1	-	3/6/23/26	0/1/1/1
3	NAG	C	2681	1	-	2/6/23/26	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1701	PGX	O4-O3	-5.68	1.24	1.46
5	D	3701	PGX	O4-O3	-5.64	1.24	1.46
5	C	2701	PGX	O4-O3	-5.63	1.24	1.46
5	A	701	PGX	O4-O3	-5.56	1.24	1.46
4	C	2702	BOG	O1-C1	2.91	1.45	1.40

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	3701	PGX	C11-C10-C9	-6.37	85.67	103.67
5	A	701	PGX	C11-C10-C9	-6.30	85.86	103.67
5	B	1701	PGX	C11-C10-C9	-6.27	85.95	103.67
5	C	2701	PGX	C11-C10-C9	-6.25	85.99	103.67
3	A	671	NAG	C2-N2-C7	-2.84	119.09	122.90

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	701	PGX	C6-C7-C8-C9
5	A	701	PGX	C6-C7-C8-C12
5	A	701	PGX	C8-C12-C13-C14
5	A	701	PGX	C11-C12-C13-C14
5	A	701	PGX	C14-C15-C16-C17

There are no ring outliers.

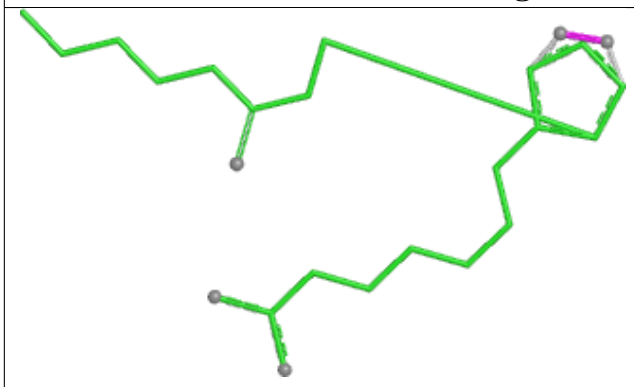
5 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2701	PGX	14	0
5	A	701	PGX	9	0
4	D	3702	BOG	1	0
5	D	3701	PGX	11	0
5	B	1701	PGX	13	0

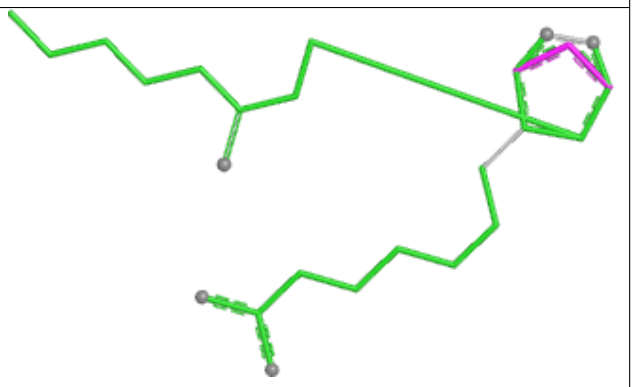
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

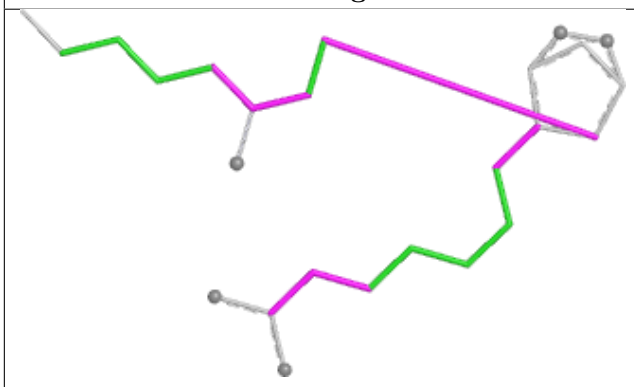
Ligand PGX C 2701



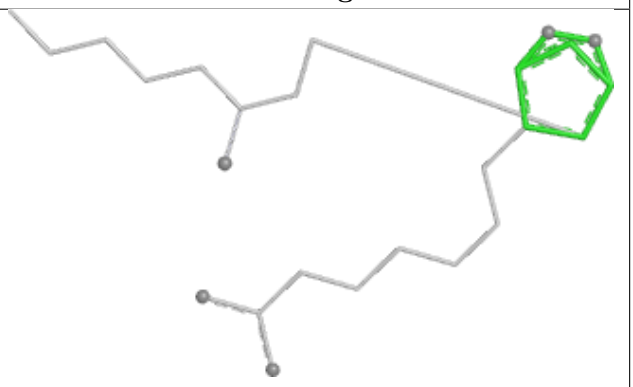
Bond lengths



Bond angles

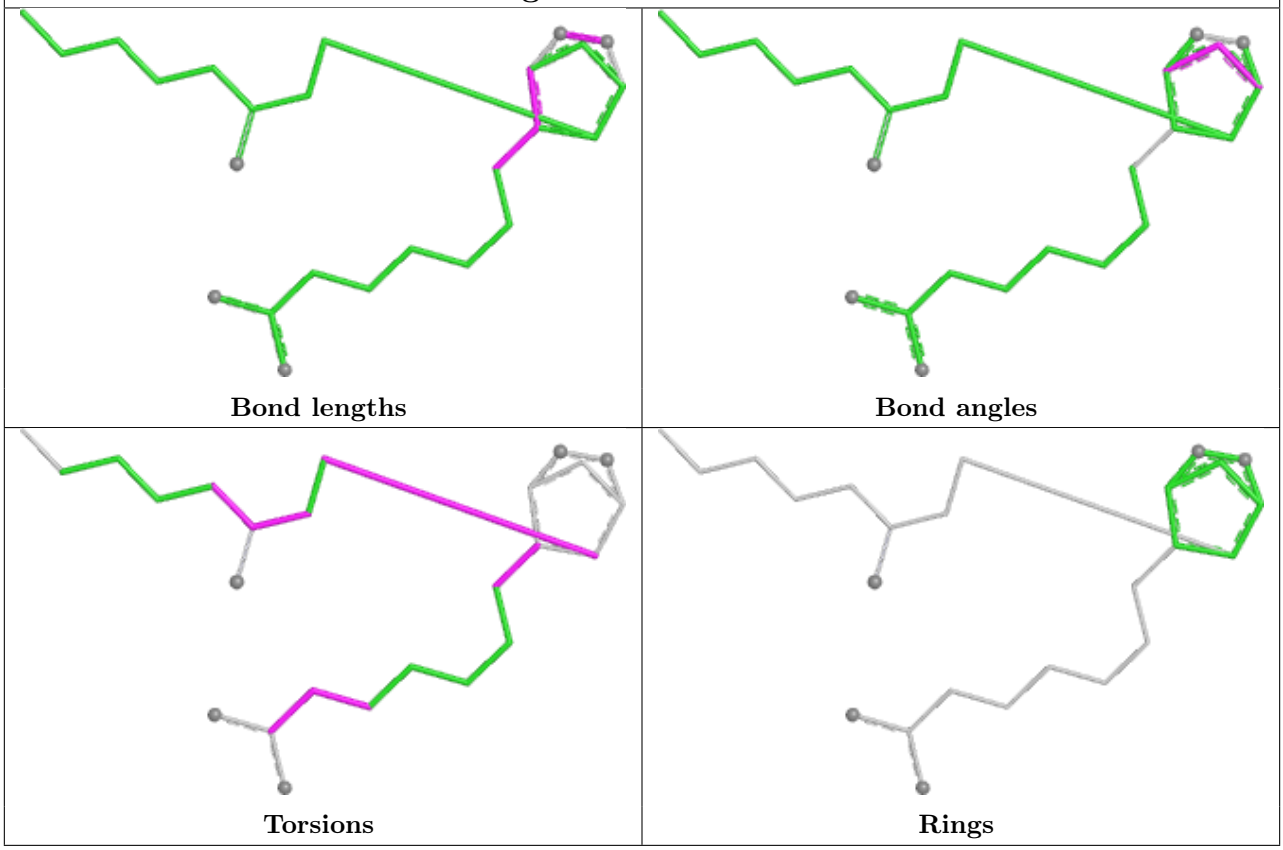


Torsions

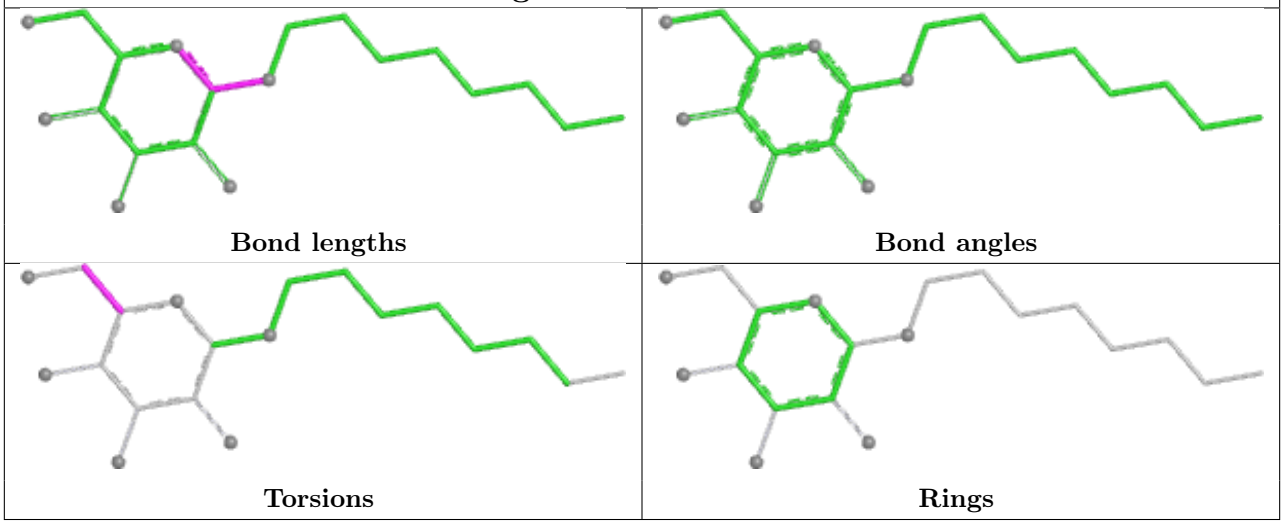


Rings

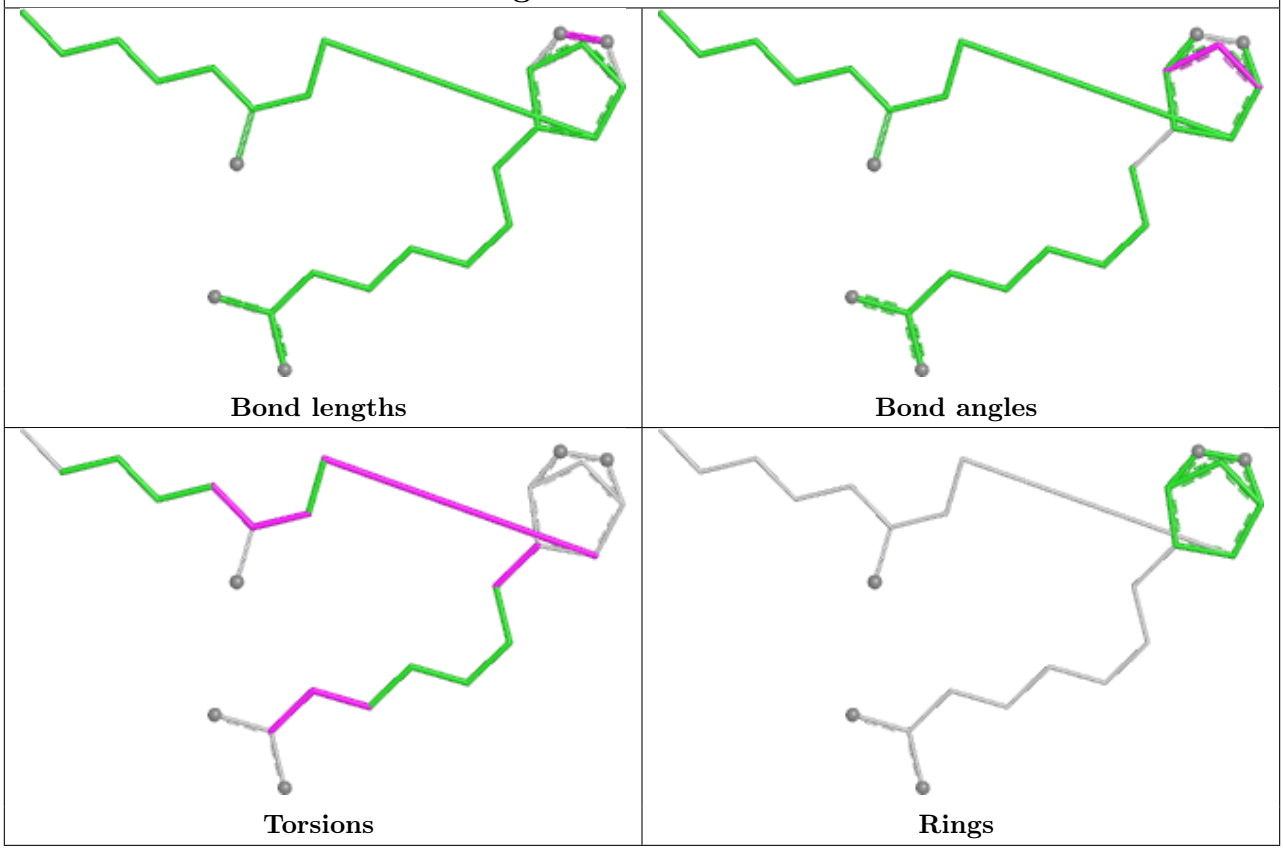
Ligand PGX A 701



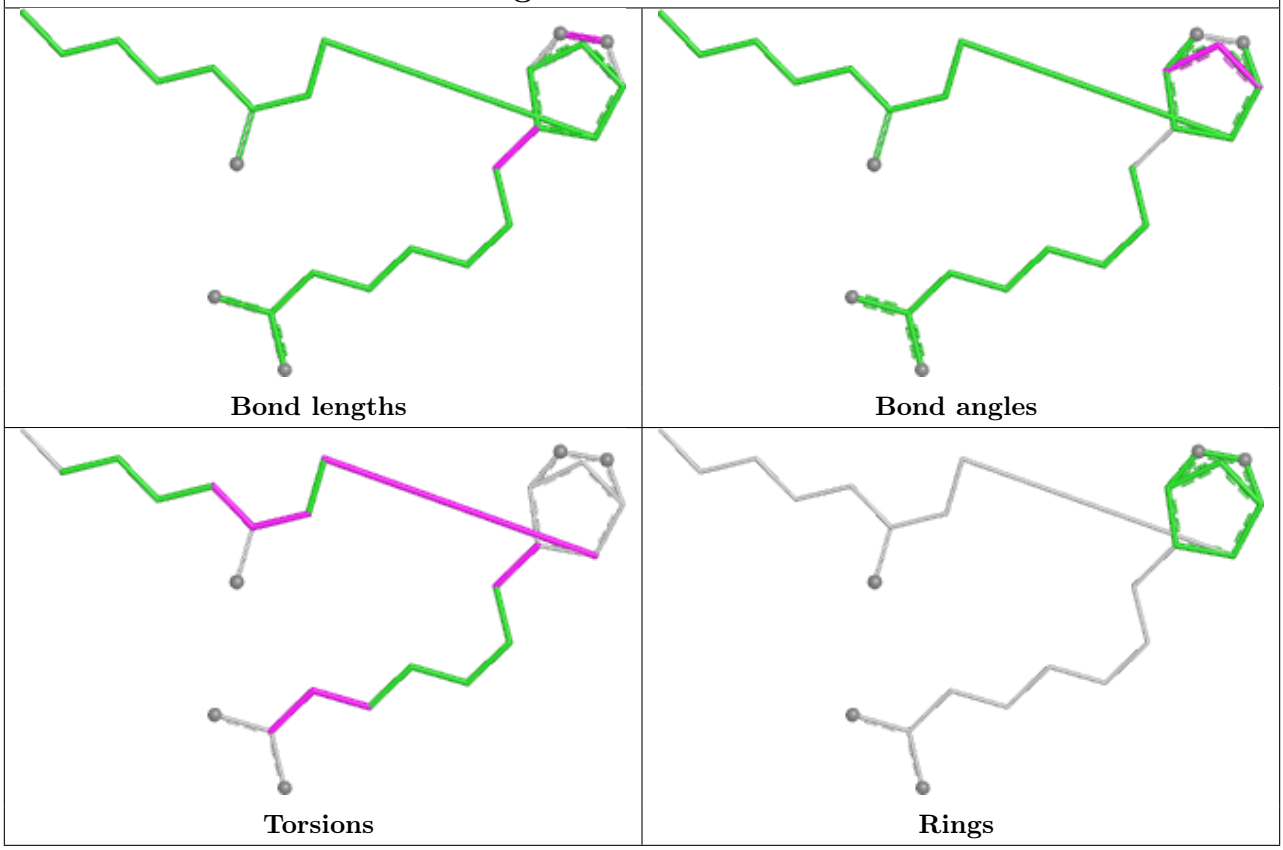
Ligand BOG D 3702



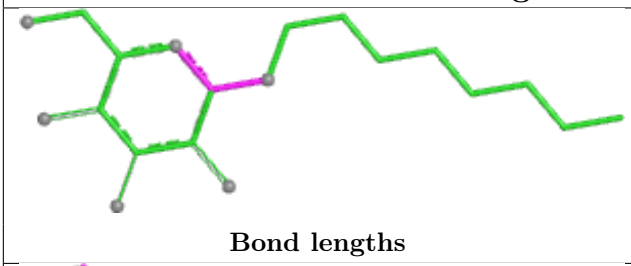
Ligand PGX D 3701



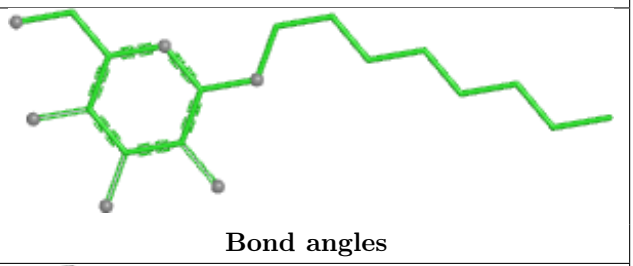
Ligand PGX B 1701



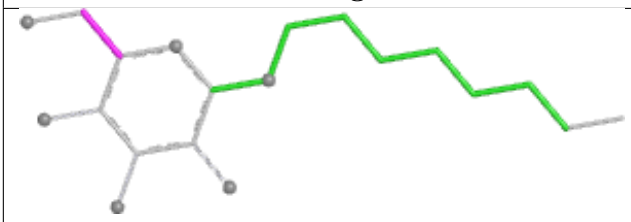
Ligand BOG B 1702



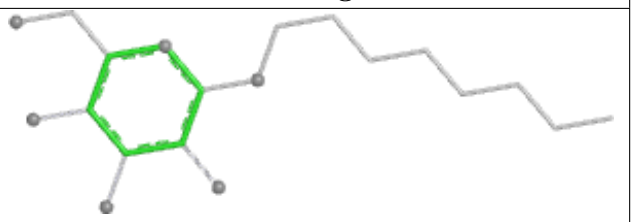
Bond lengths



Bond angles

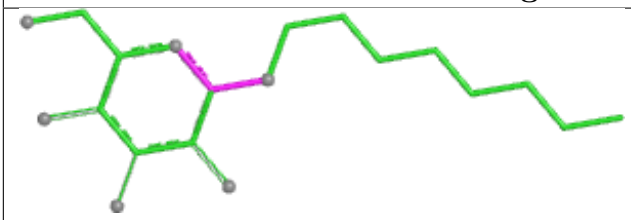


Torsions

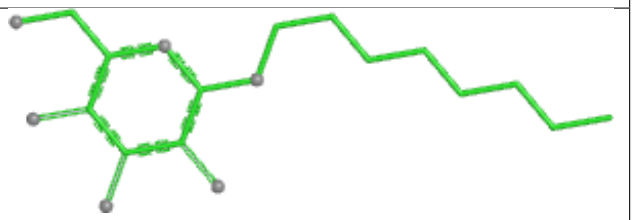


Rings

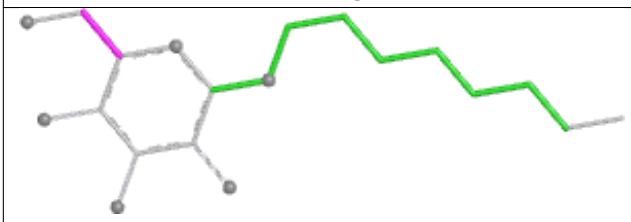
Ligand BOG A 702



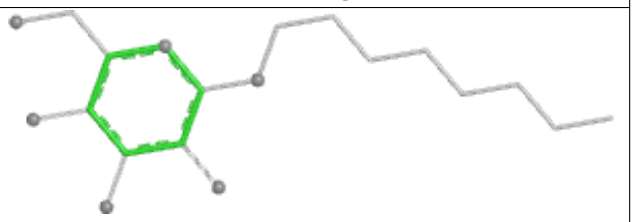
Bond lengths



Bond angles

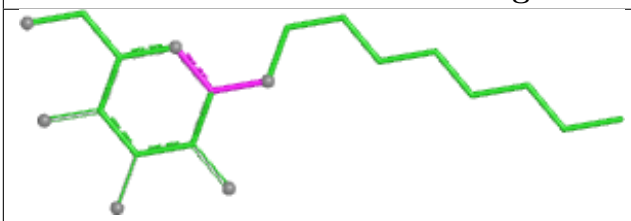


Torsions

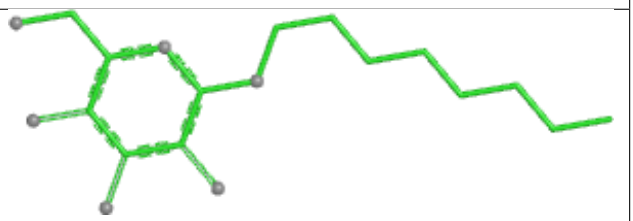


Rings

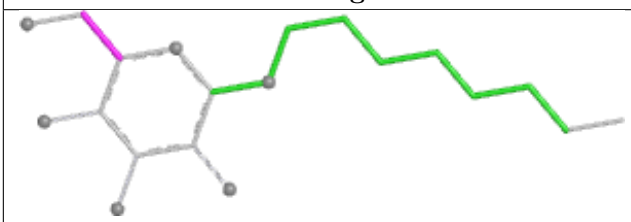
Ligand BOG C 2702



Bond lengths



Bond angles



Torsions

Rings

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	552/552 (100%)	0.26	7 (1%)	74	54	2, 25, 52, 71	0
1	B	552/552 (100%)	0.27	12 (2%)	62	40	3, 25, 51, 70	0
1	C	552/552 (100%)	0.29	16 (2%)	54	32	2, 25, 51, 70	0
1	D	552/552 (100%)	0.25	9 (1%)	70	49	3, 25, 51, 70	0
All	All	2208/2208 (100%)	0.27	44 (1%)	64	43	2, 25, 51, 71	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2486	GLU	3.8
1	D	3268	ASP	3.7
1	C	2357	PHE	2.9
1	B	1158	ASP	2.9
1	C	2531	LEU	2.8

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, 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	F	2	14/15	0.46	0.20	78,81,84,84	0
2	NAG	E	2	14/15	0.55	0.17	77,81,84,84	0

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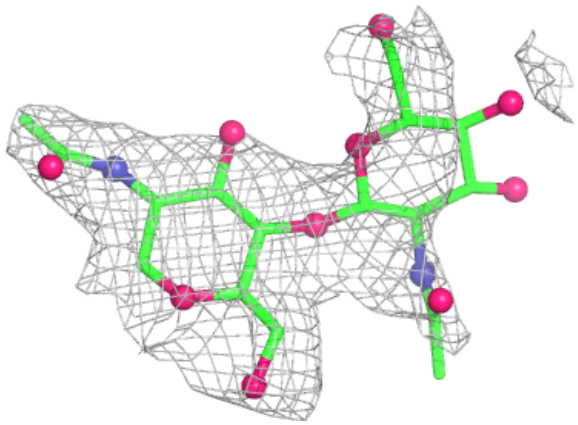
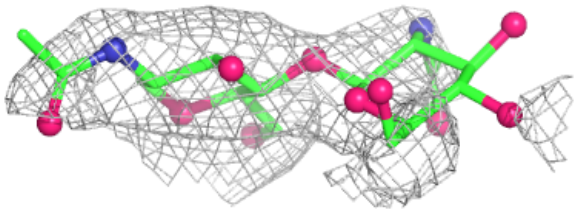
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	G	2	14/15	0.59	0.18	78,81,85,85	0
2	NAG	H	2	14/15	0.60	0.18	77,80,85,86	0
2	NAG	F	1	14/15	0.74	0.14	52,60,67,74	0
2	NAG	G	1	14/15	0.76	0.16	51,59,64,72	0
2	NAG	H	1	14/15	0.77	0.14	51,62,66,71	0
2	NAG	E	1	14/15	0.78	0.13	52,59,65,72	0

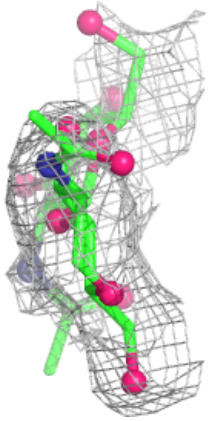
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

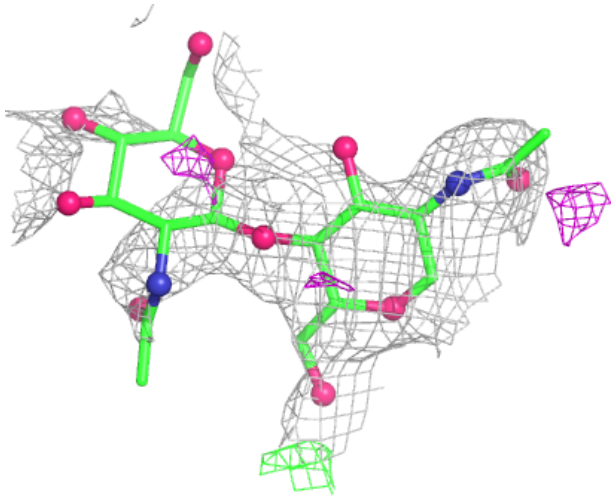


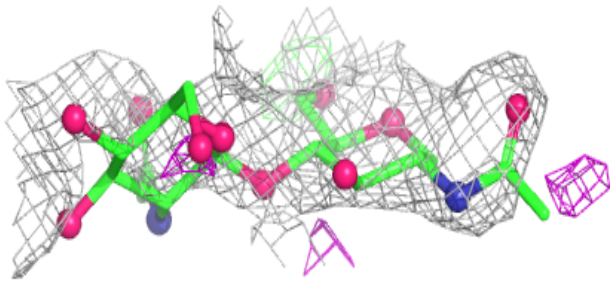


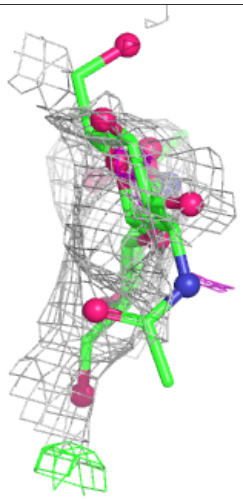


Electron density around Chain F:

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

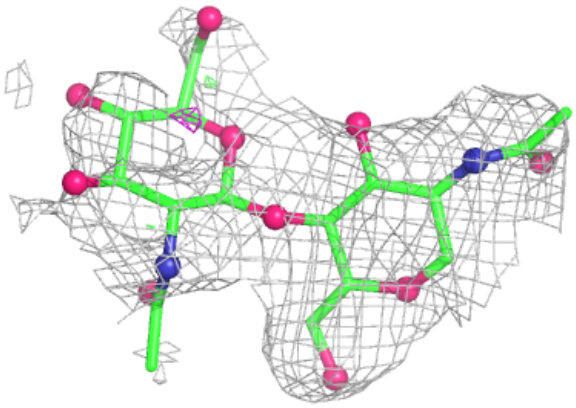


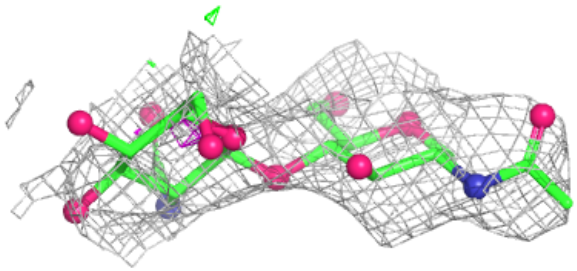


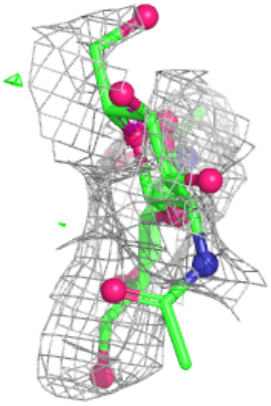


Electron density around Chain G:

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

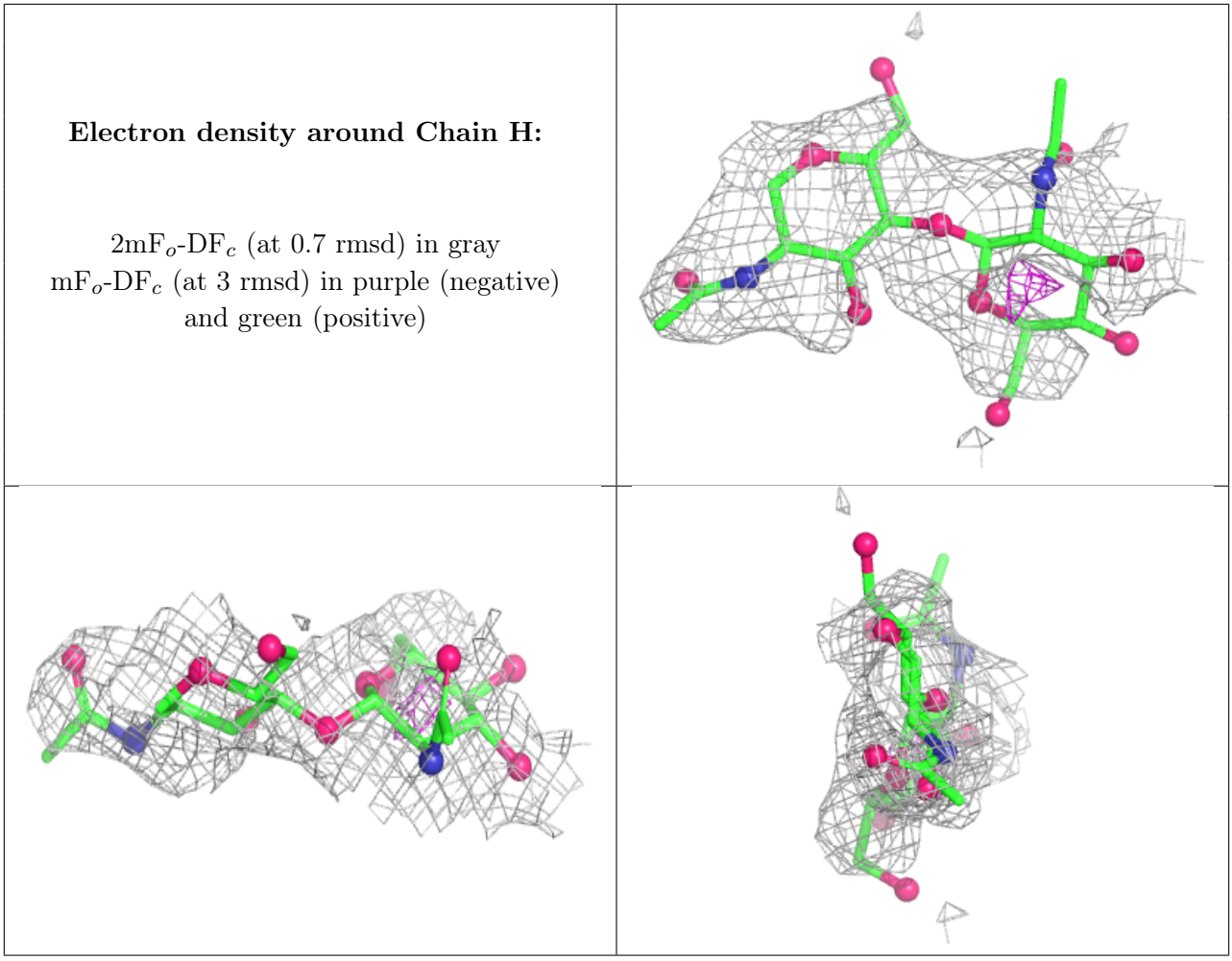






Electron density around Chain H:

$2mF_o$-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
3	NAG	C	2681	14/15	0.46	0.22	66,69,73,73	0
3	NAG	A	681	14/15	0.56	0.19	67,70,73,74	0
4	BOG	B	1702	20/20	0.64	0.19	50,54,59,59	0
4	BOG	A	702	20/20	0.65	0.19	54,58,62,65	0
3	NAG	B	1681	14/15	0.67	0.17	66,71,73,75	0
3	NAG	D	3681	14/15	0.67	0.15	66,70,72,73	0
4	BOG	C	2702	20/20	0.67	0.22	56,60,64,66	0
5	PGX	C	2701	25/26	0.68	0.33	75,79,84,84	0
5	PGX	A	701	25/26	0.69	0.35	73,78,86,87	0
5	PGX	D	3701	25/26	0.69	0.34	74,78,86,87	0

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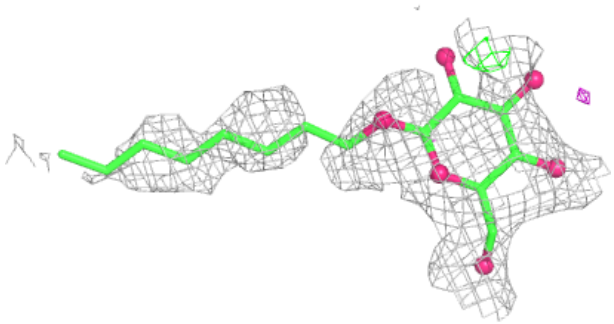
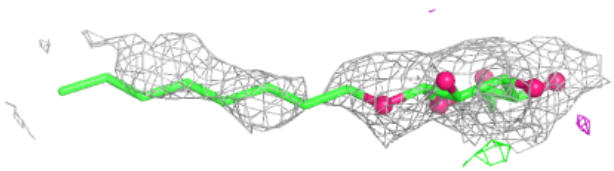
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BOG	D	3702	20/20	0.70	0.18	46,53,59,62	0
5	PGX	B	1701	25/26	0.73	0.34	72,78,84,85	0
3	NAG	B	1671	14/15	0.87	0.13	5,10,25,26	0
3	NAG	A	671	14/15	0.88	0.10	2,9,25,27	0
3	NAG	C	2671	14/15	0.88	0.12	7,10,25,28	0
3	NAG	D	3671	14/15	0.90	0.10	2,9,23,25	0

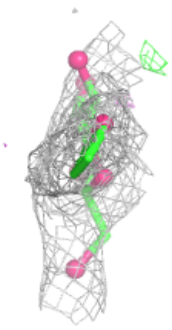
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BOG B 1702:

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

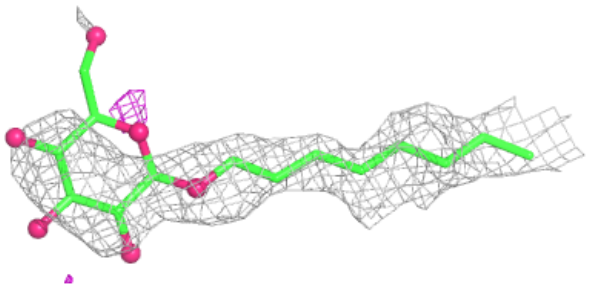


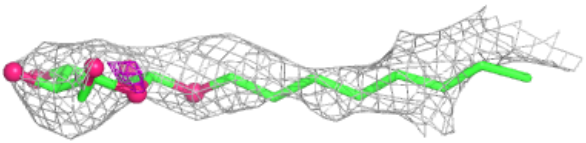


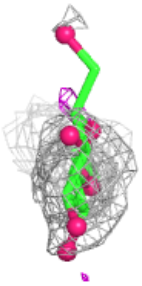


Electron density around BOG A 702:

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

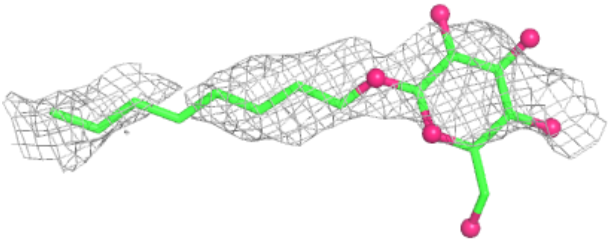


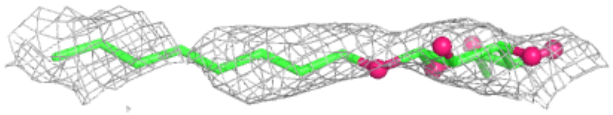


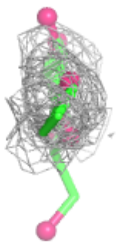


Electron density around BOG C 2702:

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

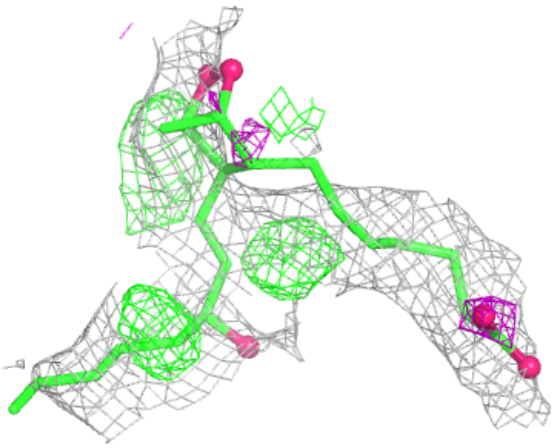


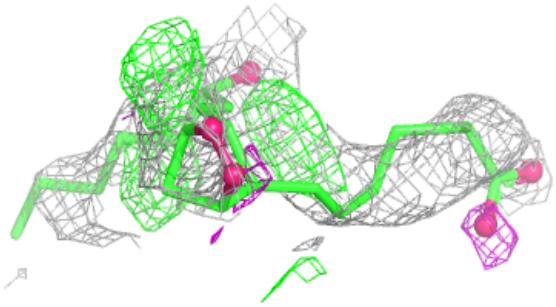


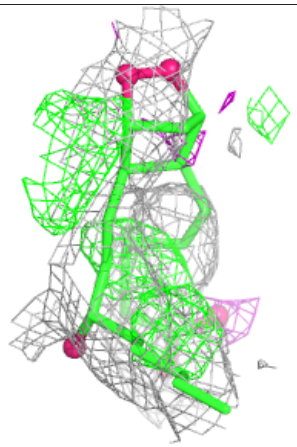


Electron density around PGX C 2701:

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

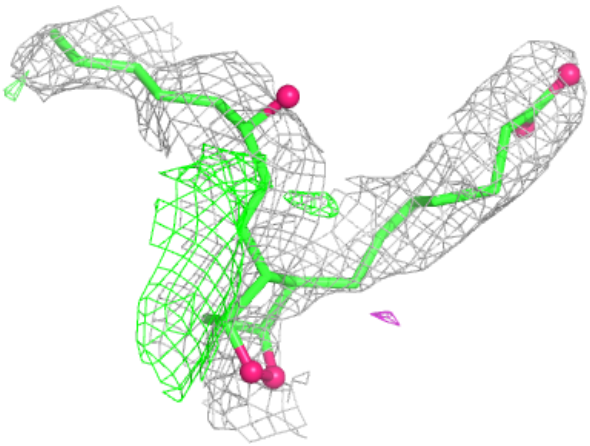


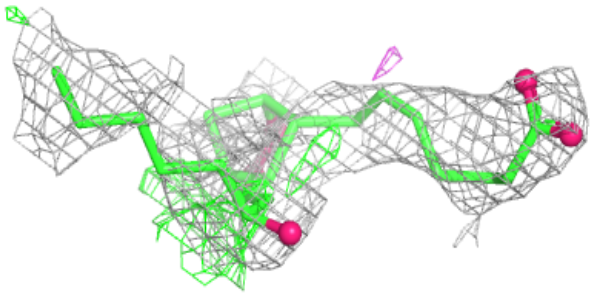


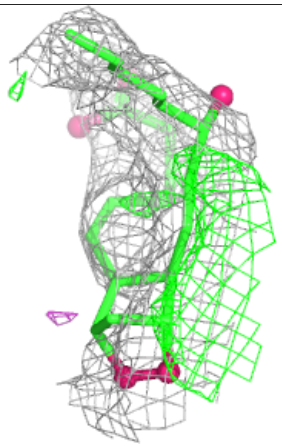


Electron density around PGX A 701:

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

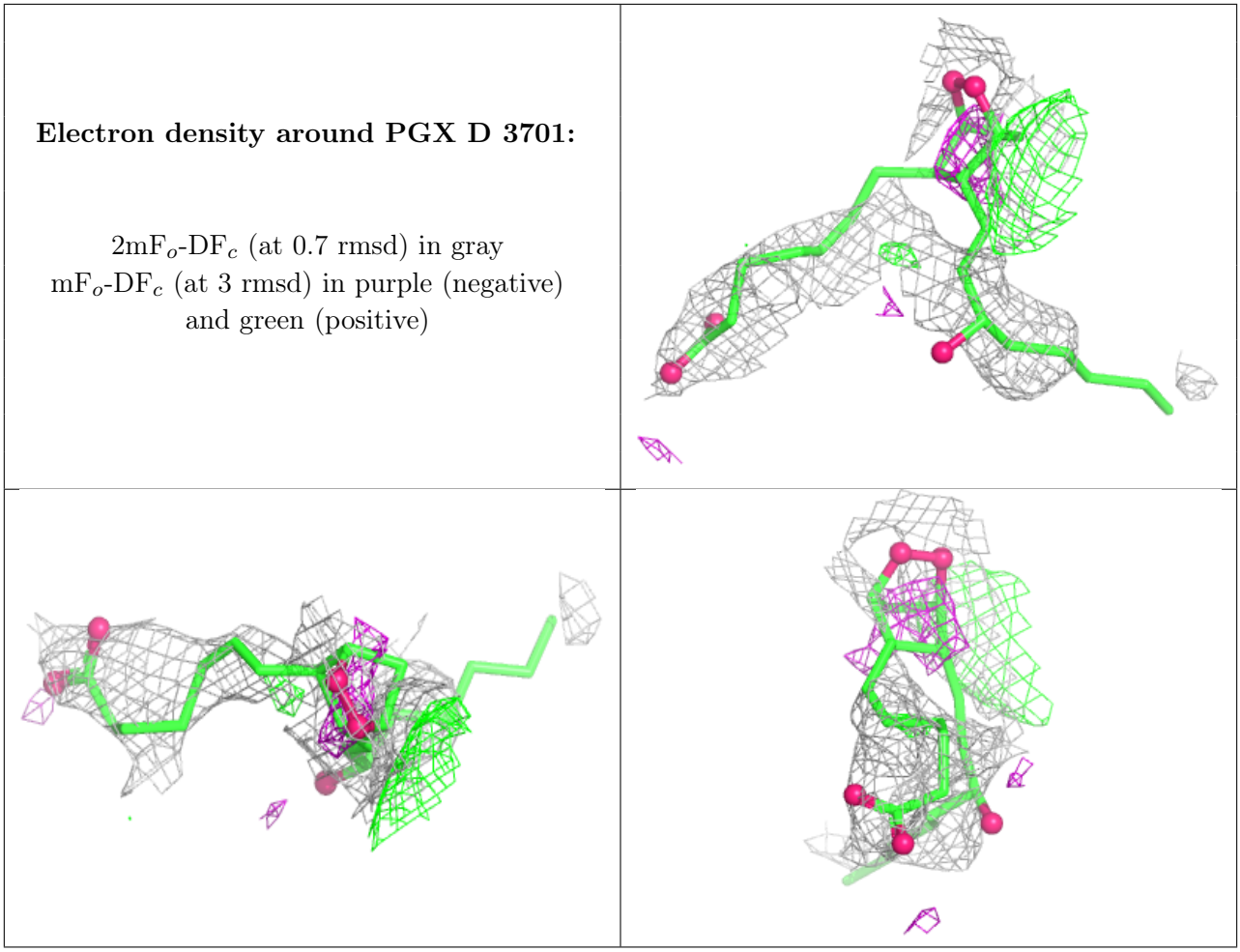






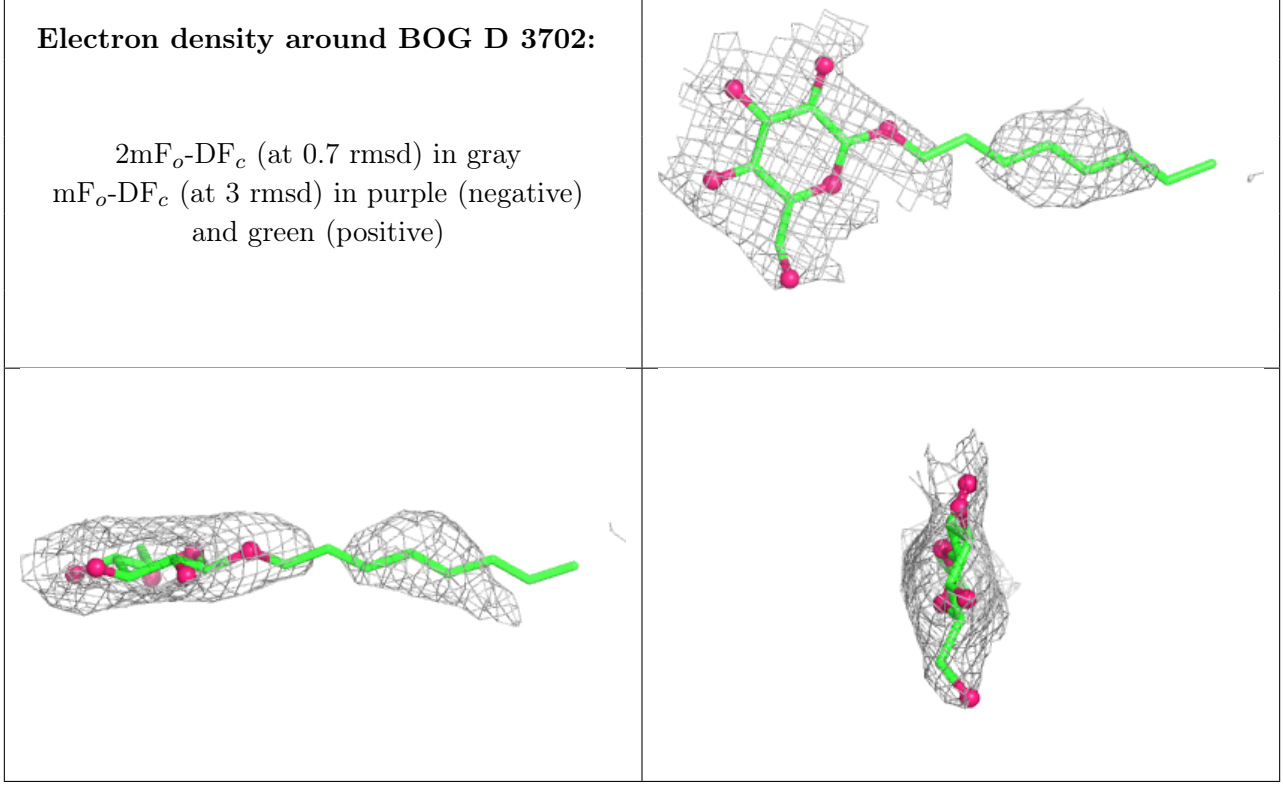
Electron density around PGX D 3701:

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



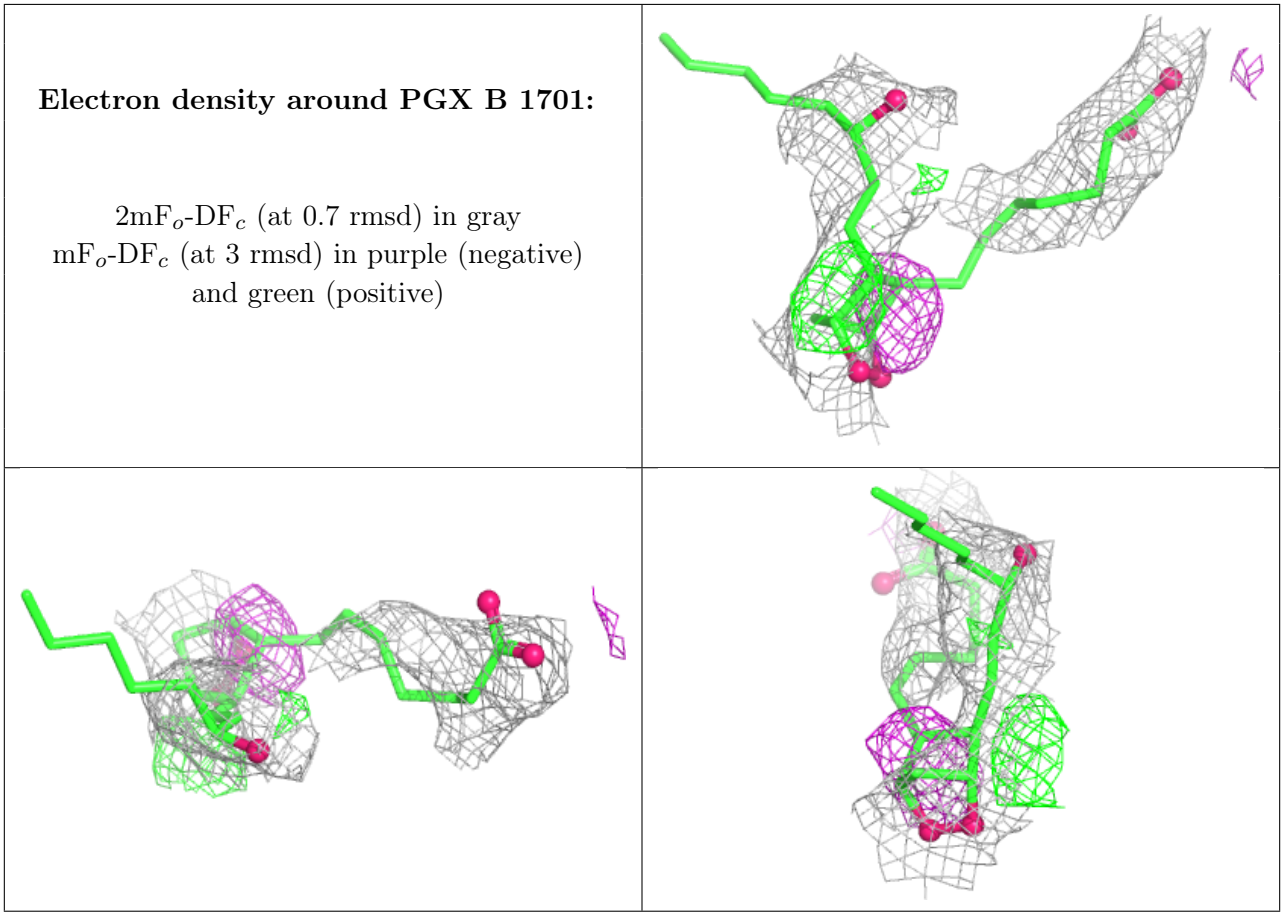
Electron density around BOG D 3702:

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



Electron density around PGX B 1701:

$2mF_o$-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.