wwPDB X-ray Structure Validation Summary Report (i)

Aug 4, 2026 – 12:28 AM EDT

PDB ID	:	3HS6 / pdb_00003hs6
Title	:	X-ray crystal structure of eicosapentaenoic acid bound to the cyclooxygenase channel of cyclooxygenase-2
Authors	:	Vecchio, A.J.; Simmons, D.M.; Malkowski, M.G.
Deposited on	:	2009-06-10
Resolution	:	2.40 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:

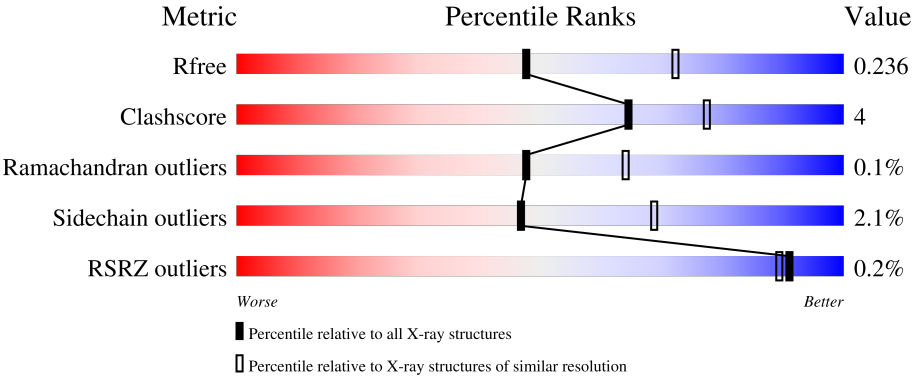
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	591	86% 7% • 7%
1	B	591	84% 8% 7%
2	C	2	50% 50%
2	F	2	100%
3	D	3	100%

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Mol	Chain	Length	Quality of chain
4	E	2	50% 50%

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
2	NAG	C	1	X	-	-	-
5	EPA	B	1	-	-	X	-
6	AKR	A	2	-	-	X	-
6	AKR	B	2	-	-	X	-
7	COH	A	619	X	-	-	-
7	COH	B	619	X	-	-	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 9765 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.

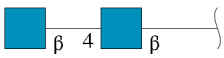
- Molecule 1 is a protein called Prostaglandin G/H synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	3	0
			4463	2882	743	813	25			
1	B	551	Total	C	N	O	S	0	3	0
			4442	2868	742	807	25			

There are 14 discrepancies between the modelled and reference sequences:

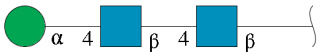
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	HIS	-	expression tag	UNP Q05769
A	30	HIS	-	expression tag	UNP Q05769
A	31	HIS	-	expression tag	UNP Q05769
A	32	HIS	-	expression tag	UNP Q05769
A	33	HIS	-	expression tag	UNP Q05769
A	34	HIS	-	expression tag	UNP Q05769
A	594	ALA	ASN	engineered mutation	UNP Q05769
B	29	HIS	-	expression tag	UNP Q05769
B	30	HIS	-	expression tag	UNP Q05769
B	31	HIS	-	expression tag	UNP Q05769
B	32	HIS	-	expression tag	UNP Q05769
B	33	HIS	-	expression tag	UNP Q05769
B	34	HIS	-	expression tag	UNP Q05769
B	594	ALA	ASN	engineered mutation	UNP Q05769

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



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

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



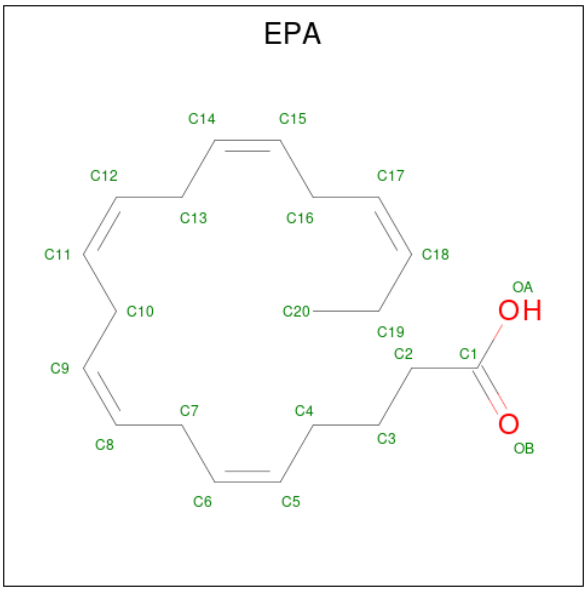
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	D	3	Total C N O 39 22 2 15	0	0	0

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



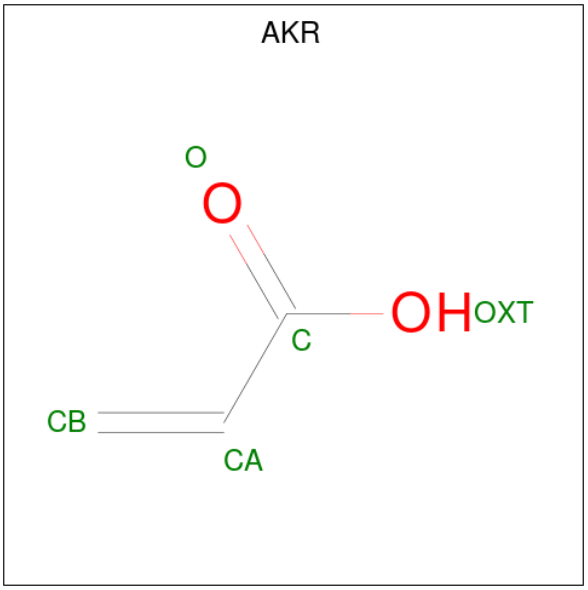
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	E	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 is 5,8,11,14,17-EICOSAPENTAENOIC ACID (CCD ID: EPA) (formula: $C_{20}H_{30}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 22 20 2	0	0
5	B	1	Total C O 22 20 2	0	0

- Molecule 6 is ACRYLIC ACID (CCD ID: AKR) (formula: $C_3H_4O_2$).



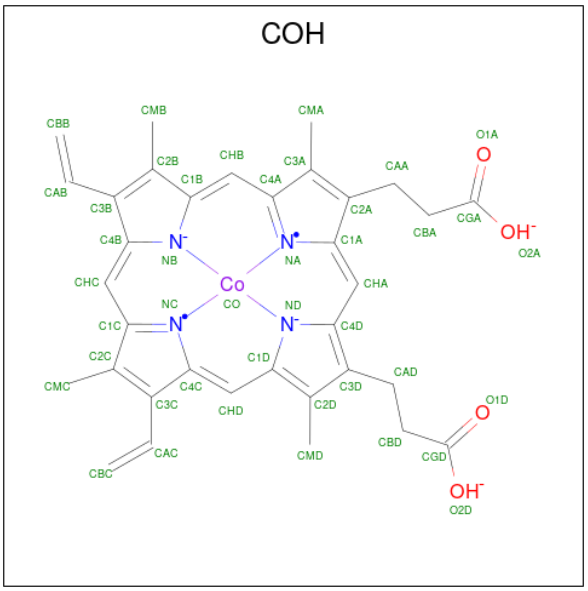
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 5 3 2	0	0
6	A	1	Total C O 5 3 2	0	0

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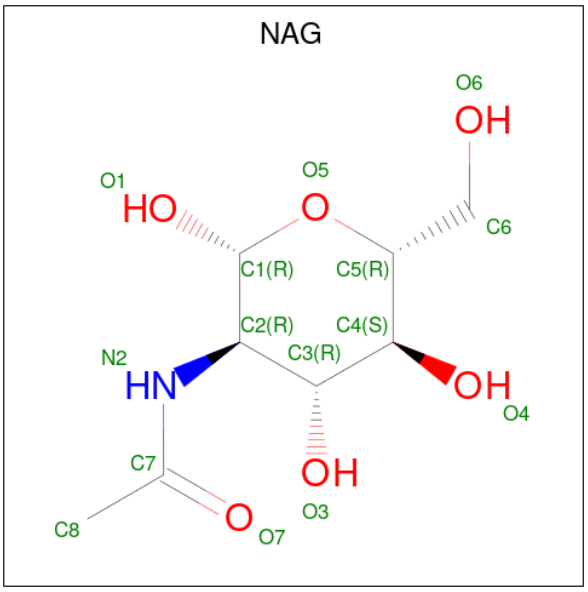
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 5 3 2	0	0
6	B	1	Total C O 5 3 2	0	0

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING CO (CCD ID: COH) (formula: $C_{34}H_{32}CoN_4O_4$).



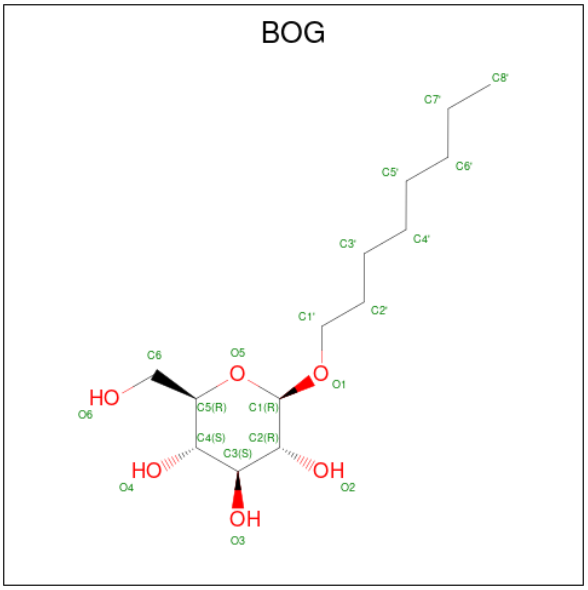
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C Co N O 43 34 1 4 4	0	0
7	B	1	Total C Co N O 43 34 1 4 4	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



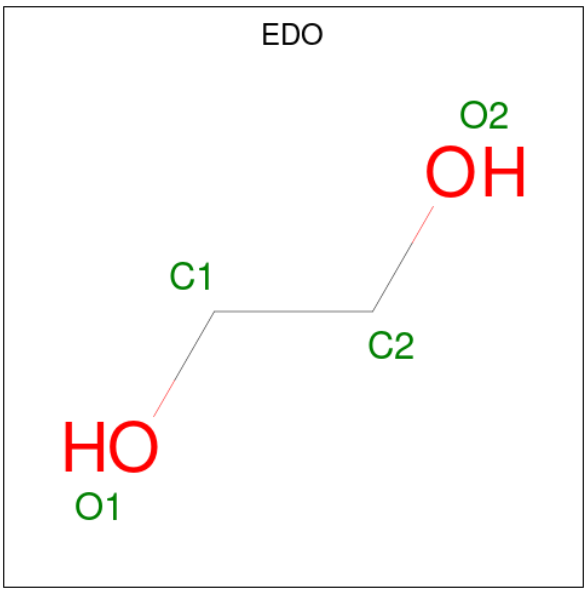
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 14 8 1 5	0	0
8	B	1	Total C N O 14 8 1 5	0	0

- Molecule 9 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



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

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	258	Total O 258 258	0	0
11	B	229	Total O 229 229	0	0

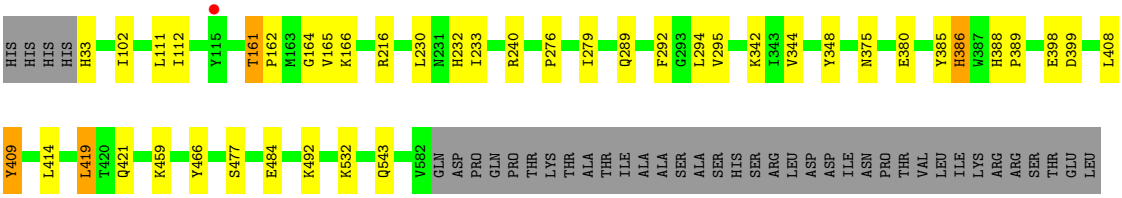
3 Residue-property plots (i)

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: Prostaglandin G/H synthase 2

Chain A:

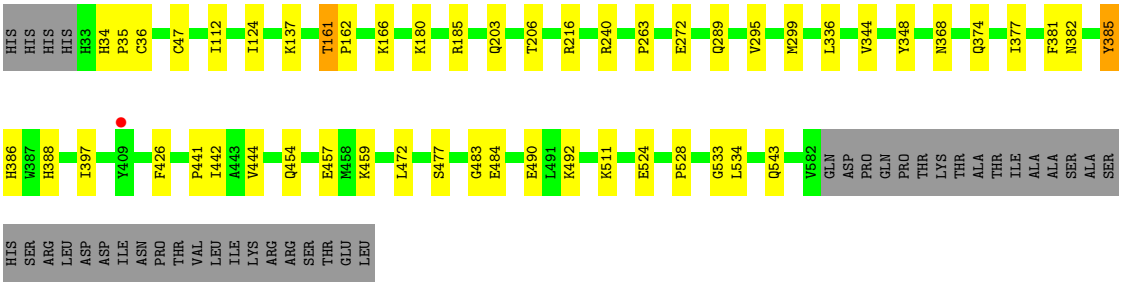




• Molecule 1: Prostaglandin G/H synthase 2

Chain B:





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

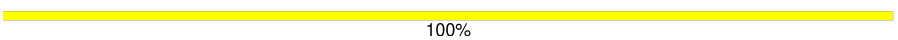
Chain C:





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

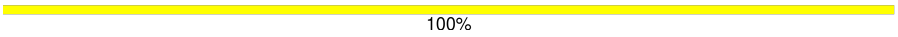
Chain F:





• Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:





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

Chain E:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	121.85Å 132.34Å 180.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.40 19.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.95-2.40) 99.7 (19.95-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.176 , 0.223 0.188 , 0.236	Depositor DCC
R_{free} test set	2889 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9765	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AKR, COH, MAN, BOG, NAG, NDG, EDO, EPA

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	0.54	1/4600 (0.0%)	0.82	2/6249 (0.0%)
1	B	0.55	2/4578 (0.0%)	0.82	0/6218
All	All	0.55	3/9178 (0.0%)	0.82	2/12467 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	GLN	CD-OE1	5.30	1.33	1.23
1	A	375	ASN	CG-OD1	5.28	1.33	1.23
1	B	374	GLN	CD-OE1	5.08	1.33	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	386	HIS	CB-CG-CD2	-6.49	122.77	131.20
1	A	386	HIS	CB-CG-ND1	5.55	131.03	122.70

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	4463	0	4295	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4442	0	4263	43	0
2	C	28	0	25	0	0
2	F	28	0	25	1	0
3	D	39	0	34	3	0
4	E	28	0	24	0	0
5	A	22	0	29	0	0
5	B	22	0	29	9	0
6	A	10	0	6	5	0
6	B	10	0	6	5	0
7	A	43	0	30	0	0
7	B	43	0	30	0	0
8	A	14	0	13	0	0
8	B	14	0	13	0	0
9	A	20	0	28	0	0
9	B	20	0	28	5	0
10	A	20	0	30	2	0
10	B	12	0	18	2	0
11	A	258	0	0	3	0
11	B	229	0	0	1	0
All	All	9765	0	8926	70	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 4.

The worst 5 of 70 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:GLY:HA3	5:B:1:EPA:H181	1.44	0.99
1:A:477:SER:HB2	6:A:2:AKR:HA1	1.51	0.93
1:B:477:SER:HB2	6:B:2:AKR:HA1	1.51	0.90
1:A:216:ARG:HH11	3:D:2:NAG:H83	1.43	0.81
1:B:185:ARG:CZ	9:B:703:BOG:H4'2	2.11	0.81

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	552/591 (93%)	537 (97%)	13 (2%)	2 (0%)	30 43
1	B	552/591 (93%)	537 (97%)	15 (3%)	0	100 100
All	All	1104/1182 (93%)	1074 (97%)	28 (2%)	2 (0%)	48 58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	409[A]	TYR
1	A	409[B]	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	484/529 (92%)	472 (98%)	12 (2%)	42 64
1	B	477/529 (90%)	468 (98%)	9 (2%)	50 71
All	All	961/1058 (91%)	940 (98%)	21 (2%)	47 67

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	289	GLN
1	B	368	ASN
1	B	484	GLU
1	B	385	TYR

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Mol	Chain	Res	Type
1	B	336	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	168	ASN
1	B	278	HIS
1	B	571	ASN
1	B	400	GLN
1	A	375	ASN

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)

9 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	1,2	14,14,15	0.59	0	17,19,21	1.19	1 (5%)
2	NAG	C	2	2	14,14,15	0.46	0	17,19,21	1.13	1 (5%)
3	NAG	D	1	1,3	14,14,15	0.56	0	17,19,21	1.11	1 (5%)
3	NAG	D	2	3	14,14,15	0.59	0	17,19,21	0.91	0
3	MAN	D	3	3	11,11,12	0.52	0	15,15,17	1.38	2 (13%)
4	NAG	E	1	1,4	14,14,15	0.59	0	17,19,21	0.98	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NDG	E	2	4	14,14,15	0.68	0	17,19,21	0.97	0
2	NAG	F	1	1,2	14,14,15	0.61	0	17,19,21	0.98	1 (5%)
2	NAG	F	2	2	14,14,15	0.54	0	17,19,21	0.76	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	2/2/5/7	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1
3	MAN	D	3	3	-	2/2/19/22	1/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NDG	E	2	4	-	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

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	3	MAN	C1-O5-C5	4.32	117.97	112.19
3	D	1	NAG	C1-O5-C5	3.89	117.40	112.19
2	F	1	NAG	C1-O5-C5	3.55	116.94	112.19
2	C	1	NAG	C1-O5-C5	3.16	116.43	112.19
4	E	1	NAG	C1-O5-C5	2.43	115.44	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	NAG	C1
2	C	1	NAG	C5

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	F	2	NAG	O7-C7-N2-C2
3	D	3	MAN	C4-C5-C6-O6
3	D	3	MAN	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

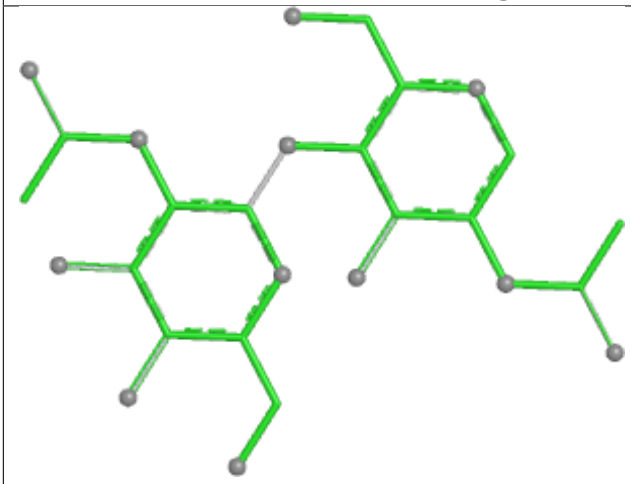
Mol	Chain	Res	Type	Atoms
3	D	3	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 4 short contacts:

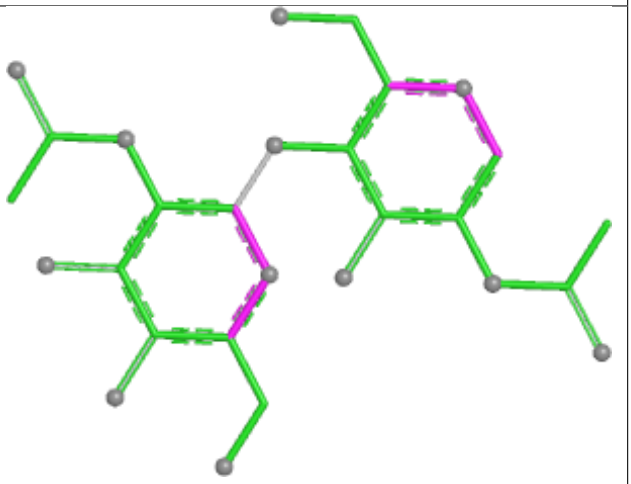
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	NAG	3	0
2	F	2	NAG	1	0

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

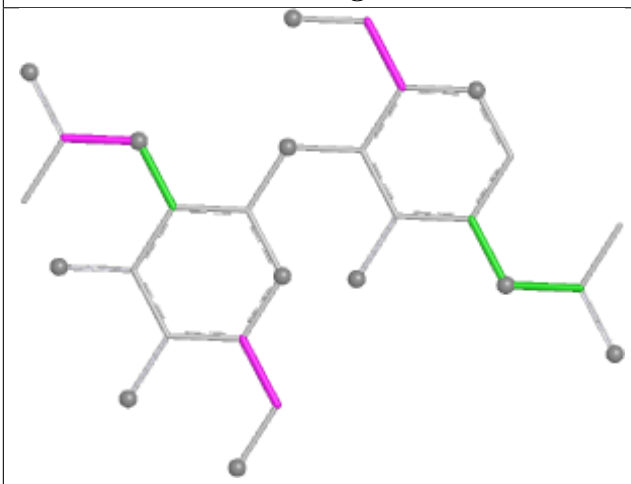
Oligosaccharide Chain C



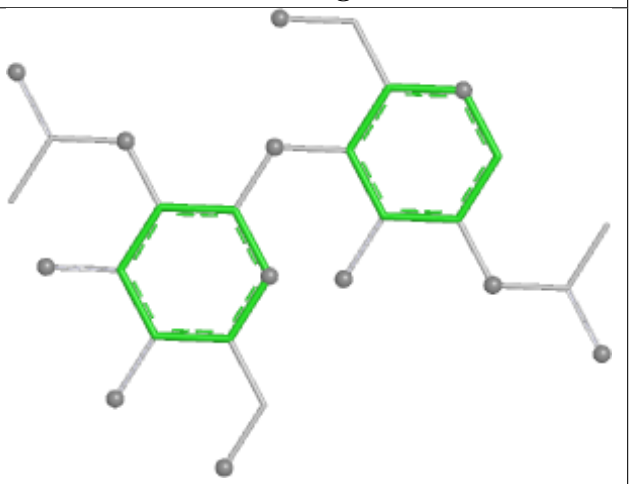
Bond lengths



Bond angles

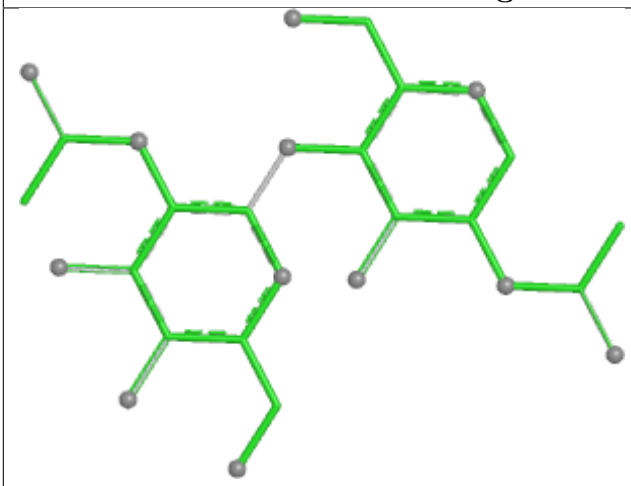


Torsions

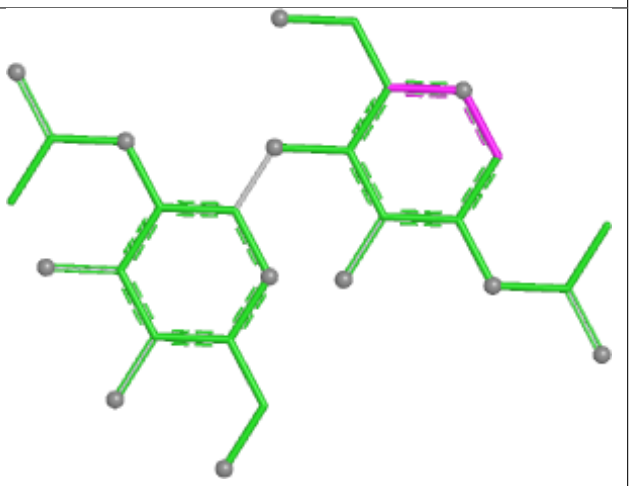


Rings

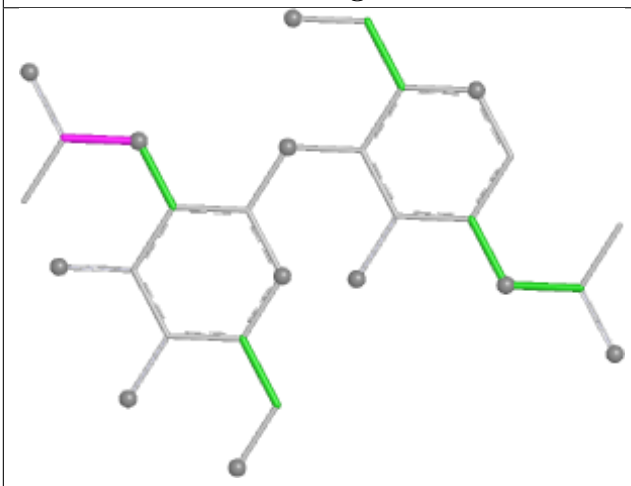
Oligosaccharide Chain F



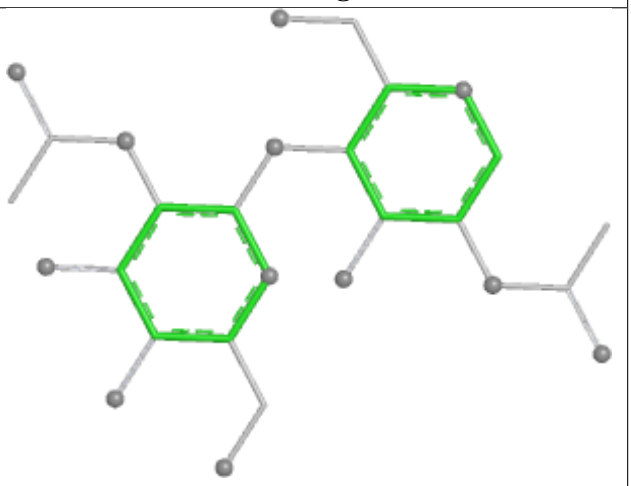
Bond lengths



Bond angles

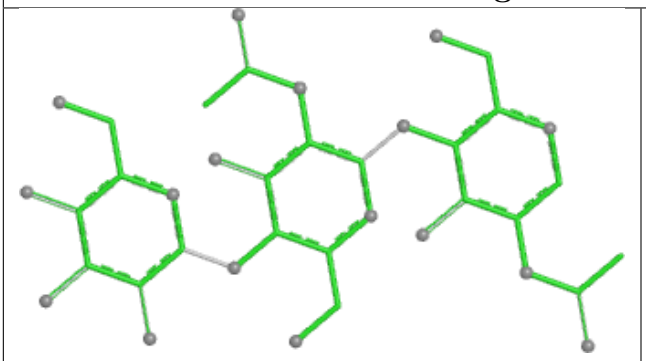


Torsions

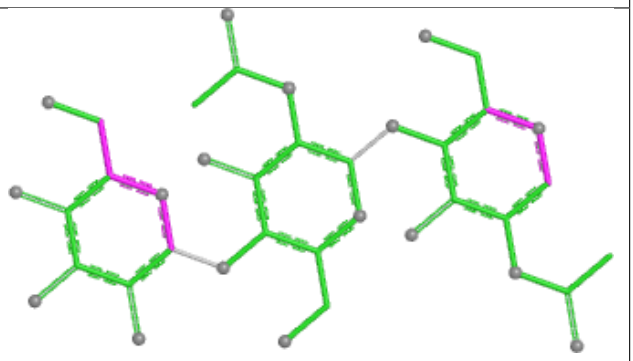


Rings

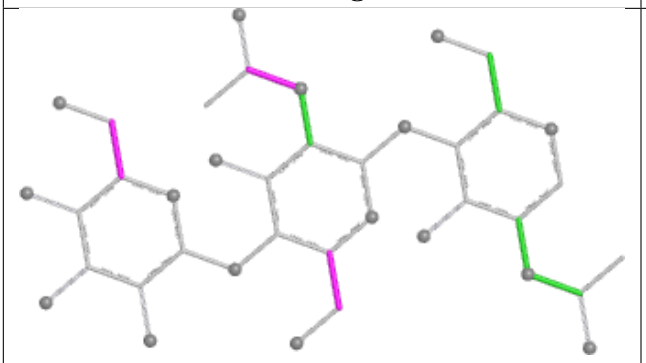
Oligosaccharide Chain D



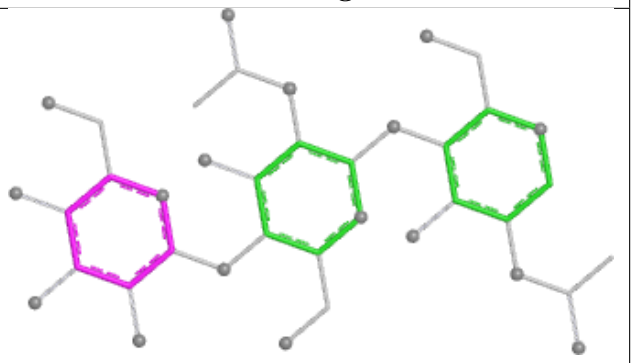
Bond lengths



Bond angles

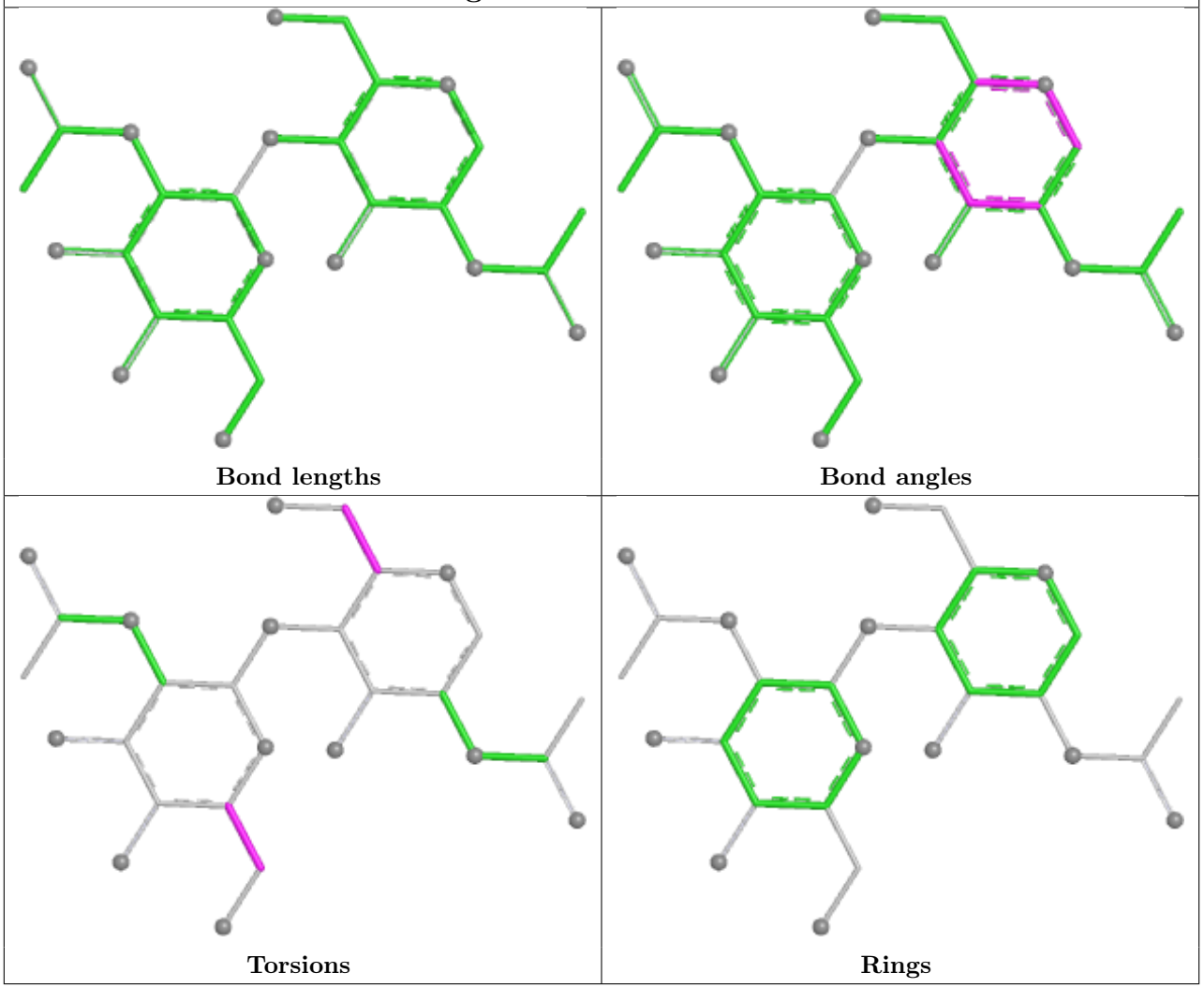


Torsions



Rings

Oligosaccharide Chain E



5.6 Ligand geometry (i)

20 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	AKR	A	2	-	4,4,4	1.97	2 (50%)	4,4,4	1.26	1 (25%)
8	NAG	B	681	1	14,14,15	0.56	0	17,19,21	0.73	0
8	NAG	A	681	1	14,14,15	0.59	0	17,19,21	1.10	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	BOG	A	703	9	20,20,20	0.45	0	25,25,25	0.69	0
10	EDO	B	620	-	3,3,3	0.50	0	2,2,2	0.29	0
10	EDO	B	621	-	3,3,3	0.32	0	2,2,2	0.56	0
5	EPA	A	1	-	21,21,21	0.50	0	21,21,21	0.85	1 (4%)
10	EDO	A	4	-	3,3,3	0.41	0	2,2,2	0.46	0
5	EPA	B	1	-	21,21,21	0.49	0	21,21,21	0.80	0
6	AKR	B	2	-	4,4,4	1.96	1 (25%)	4,4,4	1.08	0
7	COH	A	619	1	50,50,50	1.75	10 (20%)	66,82,82	1.60	10 (15%)
6	AKR	B	3	-	4,4,4	2.01	2 (50%)	4,4,4	0.82	0
6	AKR	A	3	-	4,4,4	1.96	3 (75%)	4,4,4	0.84	0
9	BOG	B	703	9	20,20,20	0.53	1 (5%)	25,25,25	0.67	0
10	EDO	A	8	-	3,3,3	0.41	0	2,2,2	0.46	0
10	EDO	A	5	-	3,3,3	0.42	0	2,2,2	0.43	0
10	EDO	B	7	-	3,3,3	0.33	0	2,2,2	0.52	0
10	EDO	A	6	-	3,3,3	0.46	0	2,2,2	0.43	0
10	EDO	A	620	-	3,3,3	0.49	0	2,2,2	0.29	0
7	COH	B	619	1	50,50,50	1.79	10 (20%)	66,82,82	1.57	11 (16%)

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	AKR	A	2	-	-	0/2/2/2	-
8	NAG	B	681	1	-	3/6/23/26	0/1/1/1
8	NAG	A	681	1	-	0/6/23/26	0/1/1/1
9	BOG	A	703	9	-	5/11/31/31	0/1/1/1
10	EDO	B	620	-	-	0/1/1/1	-
10	EDO	B	621	-	-	1/1/1/1	-
5	EPA	A	1	-	-	7/19/19/19	-
10	EDO	A	4	-	-	1/1/1/1	-
5	EPA	B	1	-	-	8/19/19/19	-
6	AKR	B	2	-	-	0/2/2/2	-
7	COH	A	619	1	1/1/3/9	6/14/54/54	-
6	AKR	B	3	-	-	0/2/2/2	-
6	AKR	A	3	-	-	0/2/2/2	-
9	BOG	B	703	9	-	6/11/31/31	0/1/1/1
10	EDO	A	8	-	-	1/1/1/1	-
10	EDO	A	5	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	EDO	B	7	-	-	1/1/1/1	-
10	EDO	A	6	-	-	1/1/1/1	-
10	EDO	A	620	-	-	0/1/1/1	-
7	COH	B	619	1	1/1/3/9	7/14/54/54	-

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	619	COH	C3D-C2D	5.88	1.54	1.38
7	A	619	COH	C3D-C2D	5.68	1.53	1.38
7	B	619	COH	CO-ND	4.84	2.15	1.96
7	A	619	COH	CO-ND	4.39	2.13	1.96
7	B	619	COH	CO-NC	4.31	2.12	1.96

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	619	COH	C4D-ND-C1D	4.89	112.32	105.11
7	A	619	COH	C4D-ND-C1D	4.80	112.19	105.11
7	A	619	COH	C2B-C1B-NB	-4.55	107.34	110.88
7	B	619	COH	C2B-C1B-NB	-4.47	107.41	110.88
7	A	619	COH	C2C-C1C-NC	-3.79	107.02	110.96

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	619	COH	NB
7	B	619	COH	NB

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1	EPA	C12-C13-C14-C15
9	B	703	BOG	O5-C1-O1-C1'
9	B	703	BOG	C4-C5-C6-O6
7	B	619	COH	C2A-CAA-CBA-CGA
9	B	703	BOG	O5-C5-C6-O6

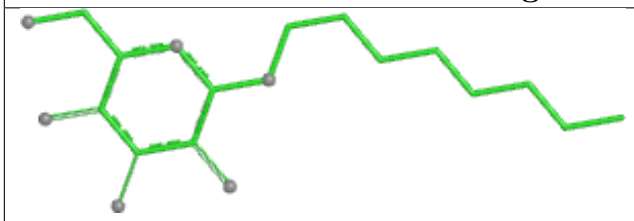
There are no ring outliers.

8 monomers are involved in 28 short contacts:

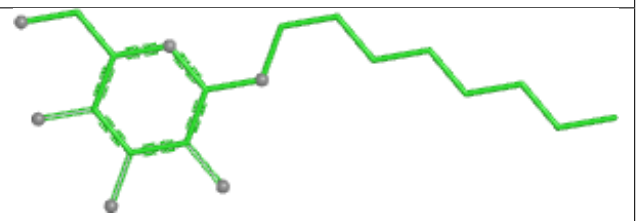
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2	AKR	4	0
10	A	4	EDO	2	0
5	B	1	EPA	9	0
6	B	2	AKR	4	0
6	B	3	AKR	1	0
6	A	3	AKR	1	0
9	B	703	BOG	5	0
10	B	7	EDO	2	0

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 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.

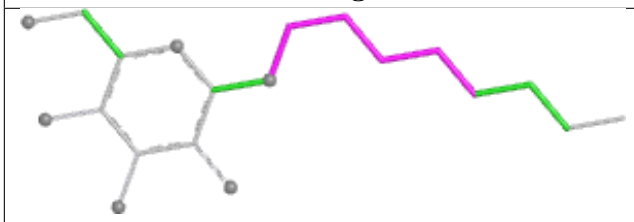
Ligand BOG A 703



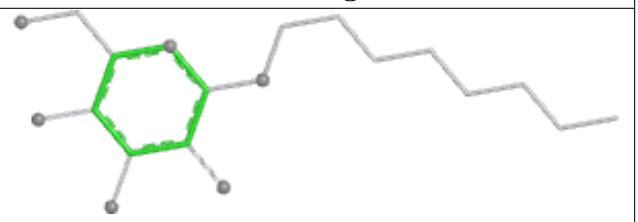
Bond lengths



Bond angles

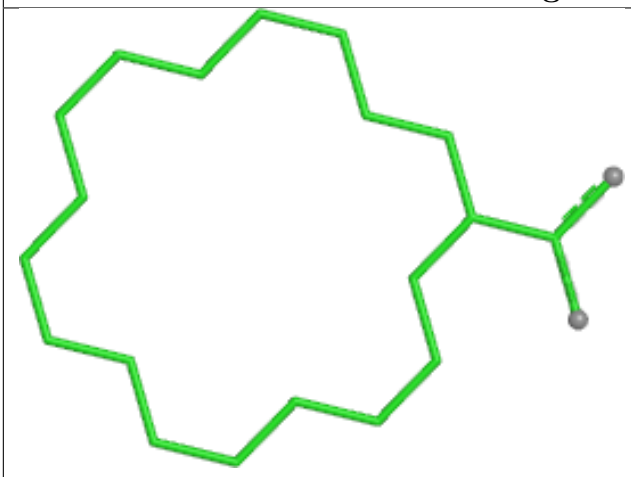


Torsions

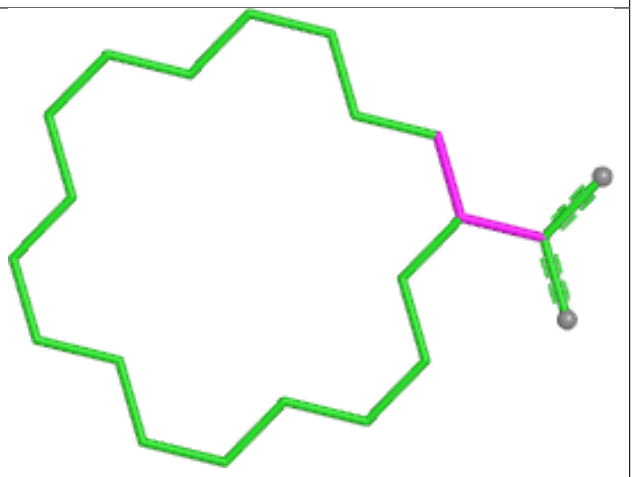


Rings

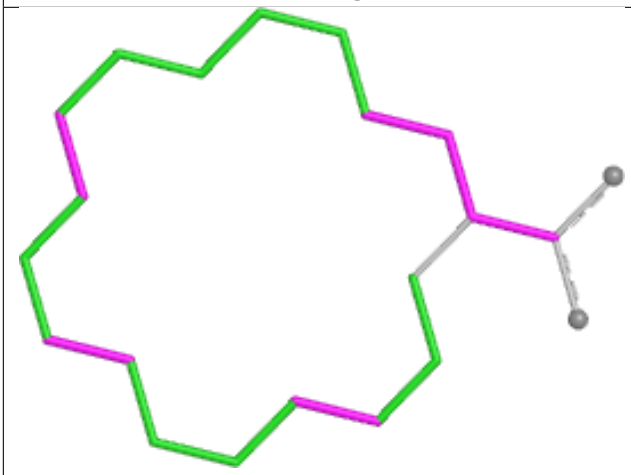
Ligand EPA A 1



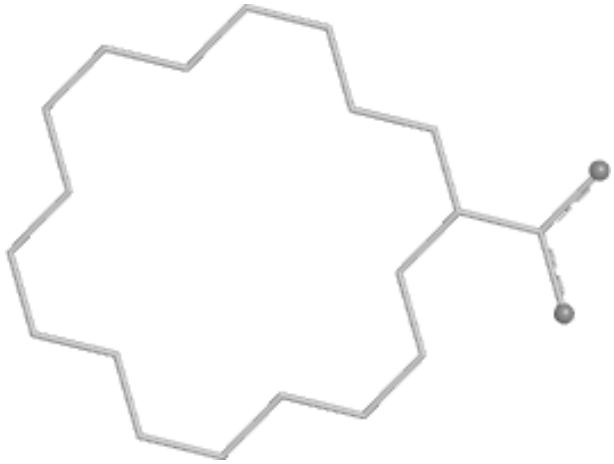
Bond lengths



Bond angles

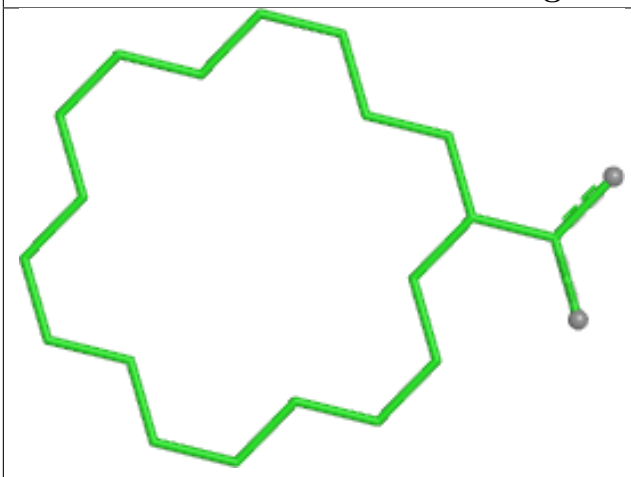


Torsions

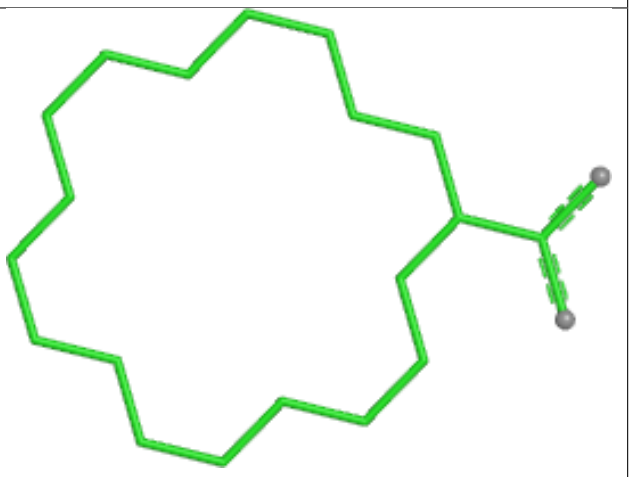


Rings

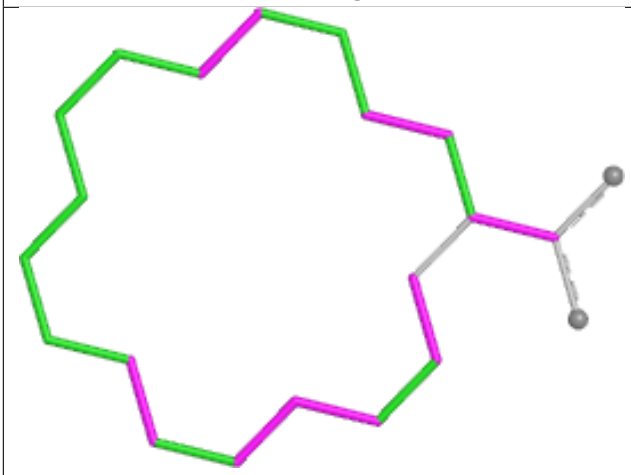
Ligand EPA B 1



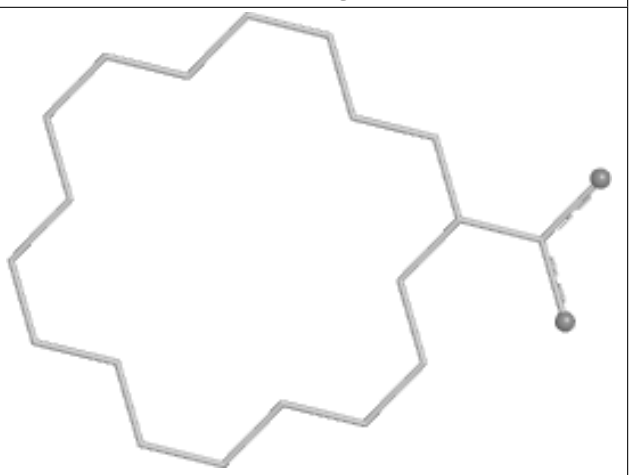
Bond lengths



Bond angles

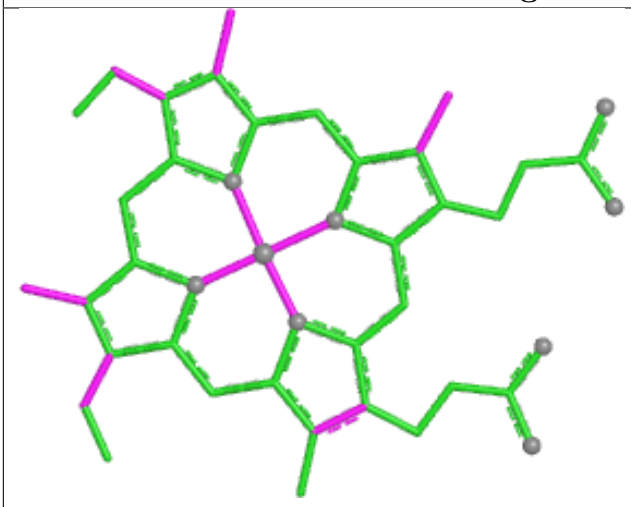


Torsions

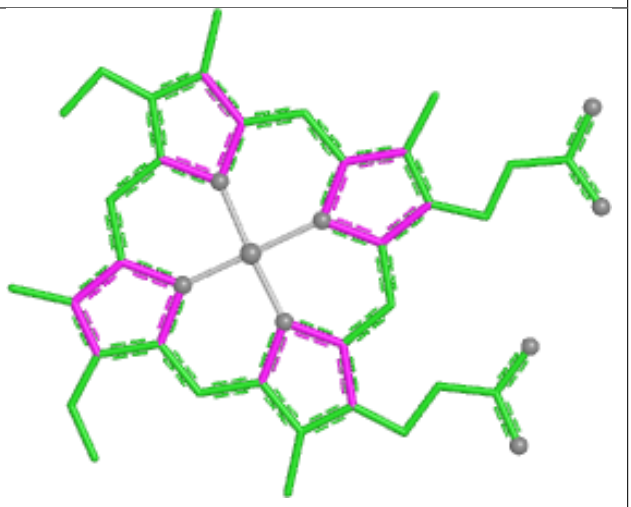


Rings

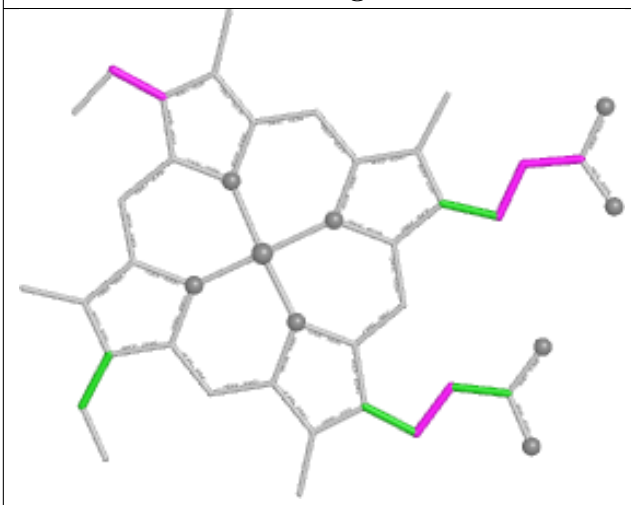
Ligand COH A 619



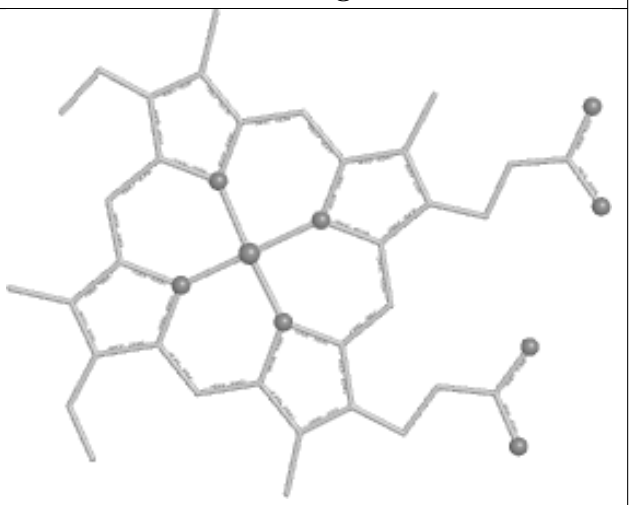
Bond lengths



Bond angles

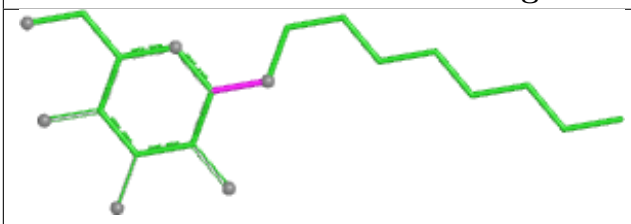


Torsions

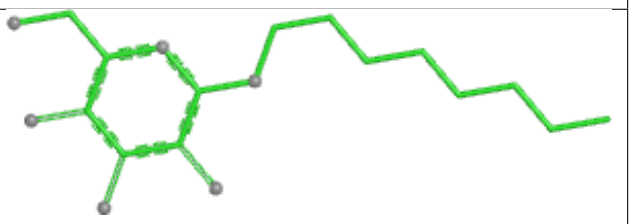


Rings

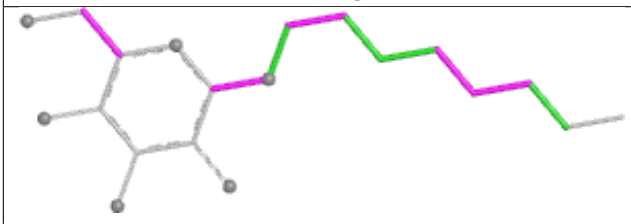
Ligand BOG B 703



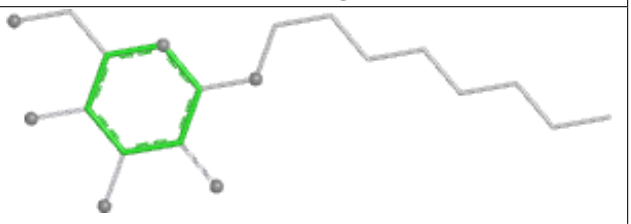
Bond lengths



Bond angles

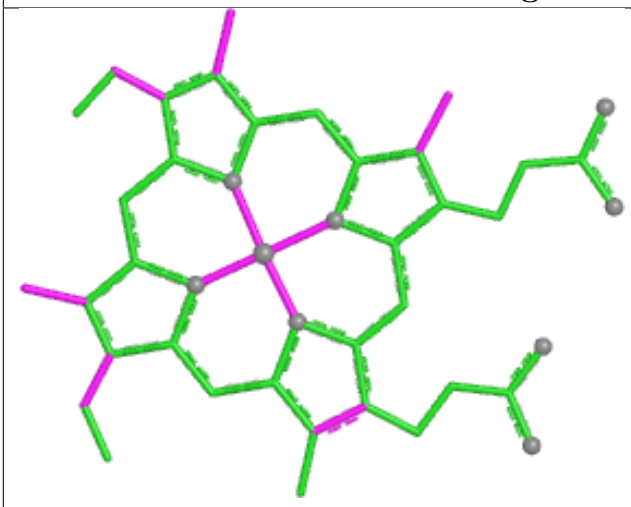


Torsions

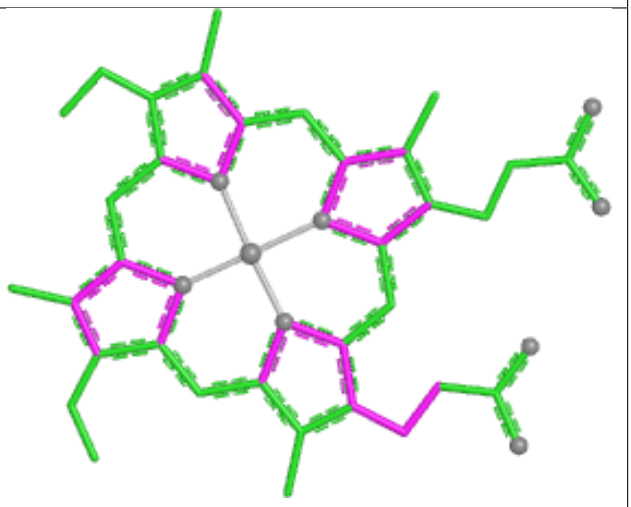


Rings

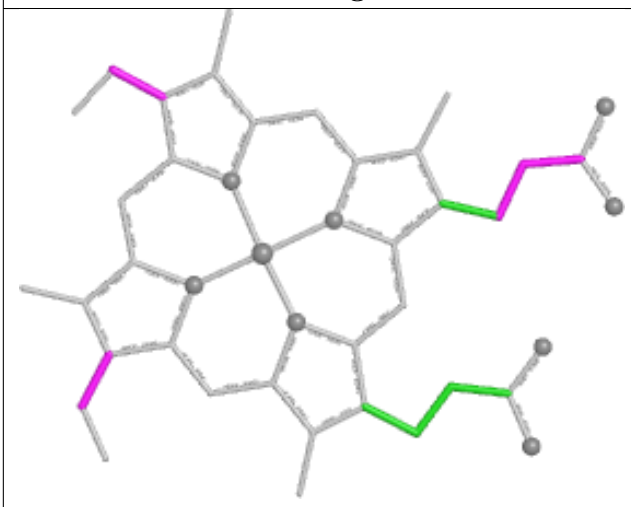
Ligand COH B 619



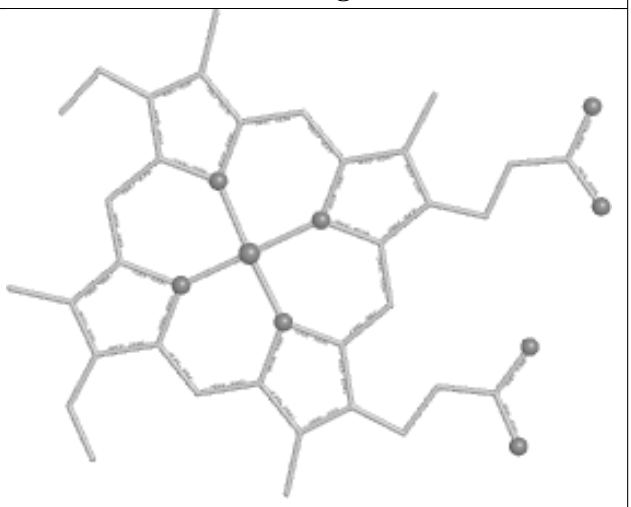
Bond lengths



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	551/591 (93%)	-0.42	1 (0%)	91	89	14, 33, 51, 58	3 (0%)
1	B	551/591 (93%)	-0.35	1 (0%)	91	89	14, 34, 53, 68	4 (0%)
All	All	1102/1182 (93%)	-0.39	2 (0%)	91	89	14, 33, 52, 68	7 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	409	TYR	2.3
1	A	115	TYR	2.2

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, 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
4	NDG	E	2	14/15	0.48	0.16	69,72,73,73	0
2	NAG	C	2	14/15	0.60	0.14	64,67,68,68	0
3	MAN	D	3	11/12	0.64	0.14	60,62,63,63	0
4	NAG	E	1	14/15	0.76	0.12	52,57,60,65	0
2	NAG	C	1	14/15	0.86	0.10	45,51,54,59	0
2	NAG	F	2	14/15	0.88	0.10	43,46,48,48	0
3	NAG	D	2	14/15	0.89	0.09	46,48,52,56	0

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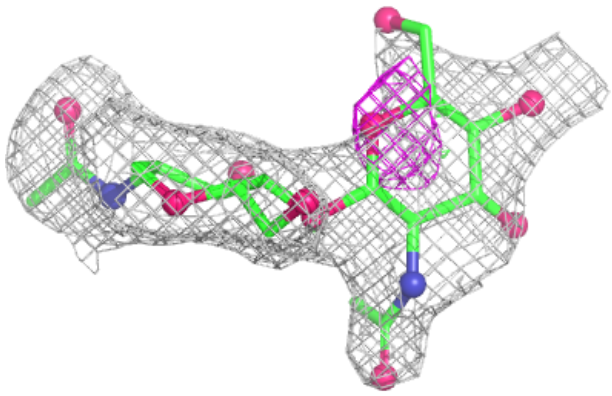
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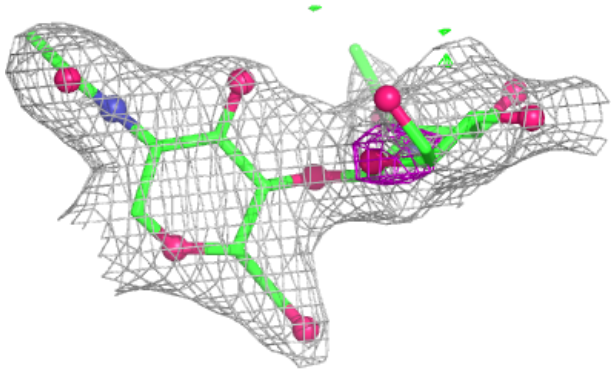
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	F	1	14/15	0.93	0.08	30,34,37,41	0
3	NAG	D	1	14/15	0.95	0.06	30,36,38,42	0

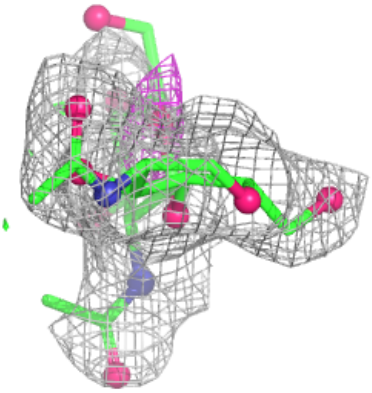
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

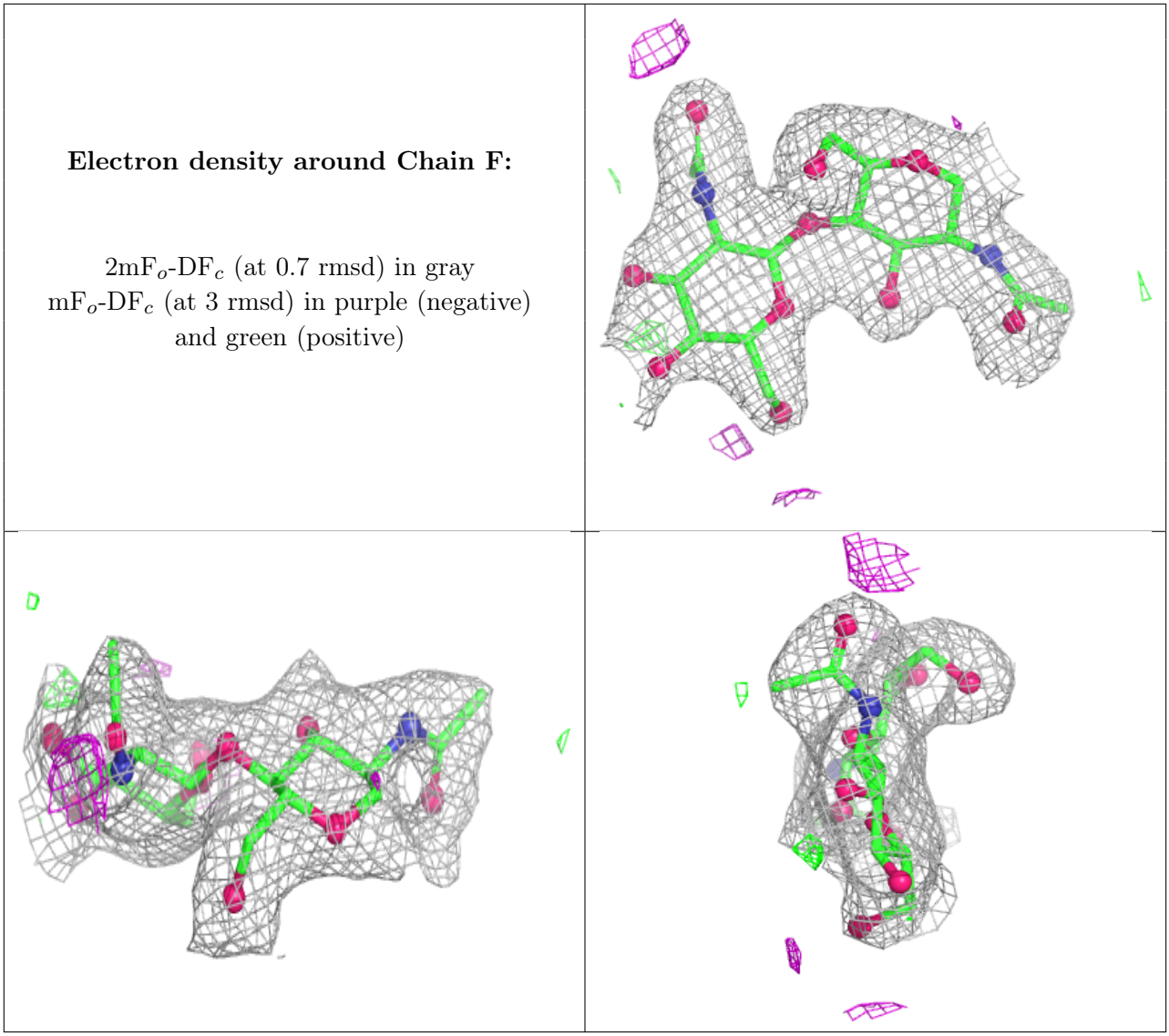






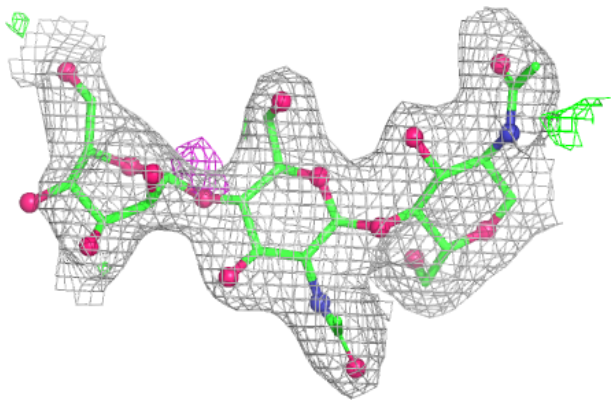
Electron density around Chain F:

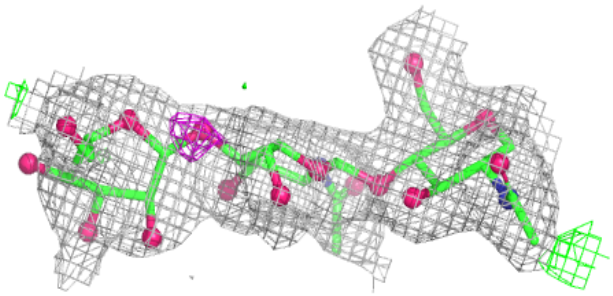
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

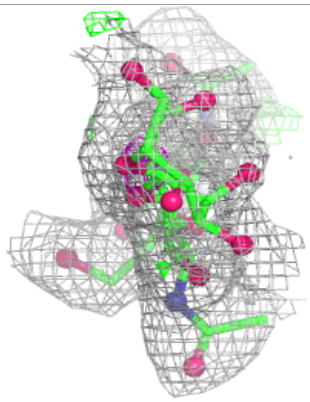


Electron density around Chain D:

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

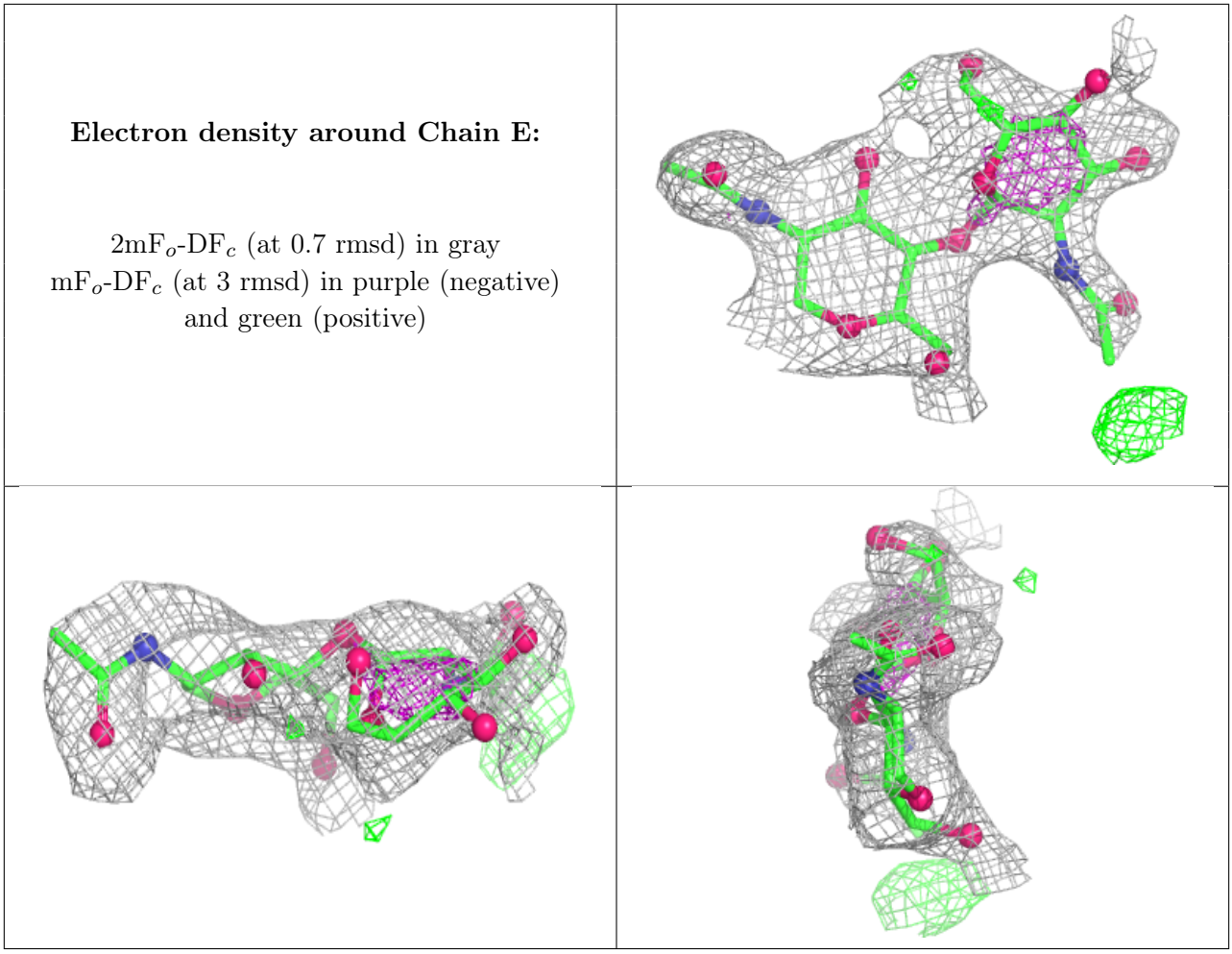






Electron density around Chain E:

$2mF_o$-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
10	EDO	A	6	4/4	0.66	0.23	58,58,58,58	0
6	AKR	B	2	5/5	0.77	0.19	65,65,66,66	0
7	COH	B	619	43/43	0.79	0.21	80,85,87,88	0
6	AKR	A	3	5/5	0.80	0.15	54,54,54,54	0
8	NAG	B	681	14/15	0.80	0.11	52,56,59,59	0
10	EDO	A	5	4/4	0.80	0.16	61,62,62,63	0
6	AKR	A	2	5/5	0.80	0.15	52,52,52,52	0
7	COH	A	619	43/43	0.81	0.20	92,94,96,97	0
8	NAG	A	681	14/15	0.83	0.11	48,52,54,55	0
6	AKR	B	3	5/5	0.86	0.16	63,63,63,63	0

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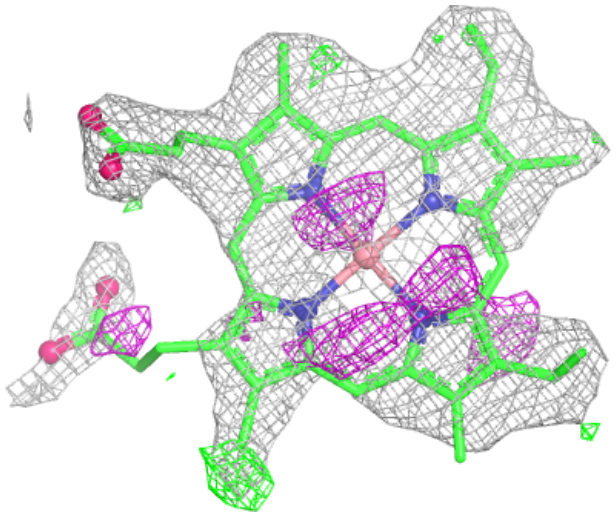
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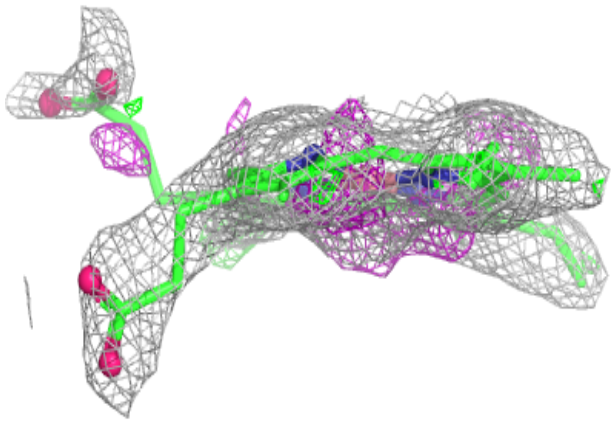
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EPA	B	1	22/22	0.87	0.14	42,45,50,52	0
10	EDO	A	4	4/4	0.88	0.10	38,39,41,41	0
5	EPA	A	1	22/22	0.90	0.11	41,43,48,49	0
10	EDO	A	8	4/4	0.91	0.10	39,39,41,42	0
10	EDO	A	620	4/4	0.92	0.10	36,36,37,37	0
10	EDO	B	620	4/4	0.92	0.10	34,35,36,36	0
10	EDO	B	621	4/4	0.92	0.09	33,33,34,34	0
10	EDO	B	7	4/4	0.93	0.08	39,39,39,40	0
9	BOG	A	703	20/20	0.96	0.07	22,23,27,27	20
9	BOG	B	703	20/20	0.96	0.07	36,37,37,37	20

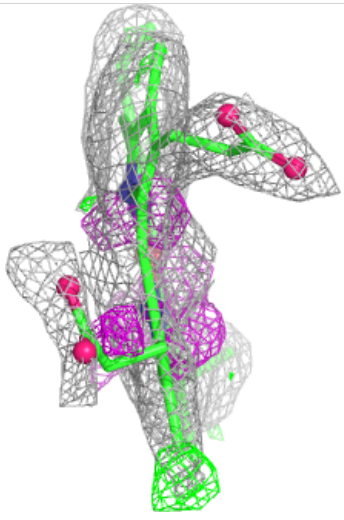
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COH B 619:

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

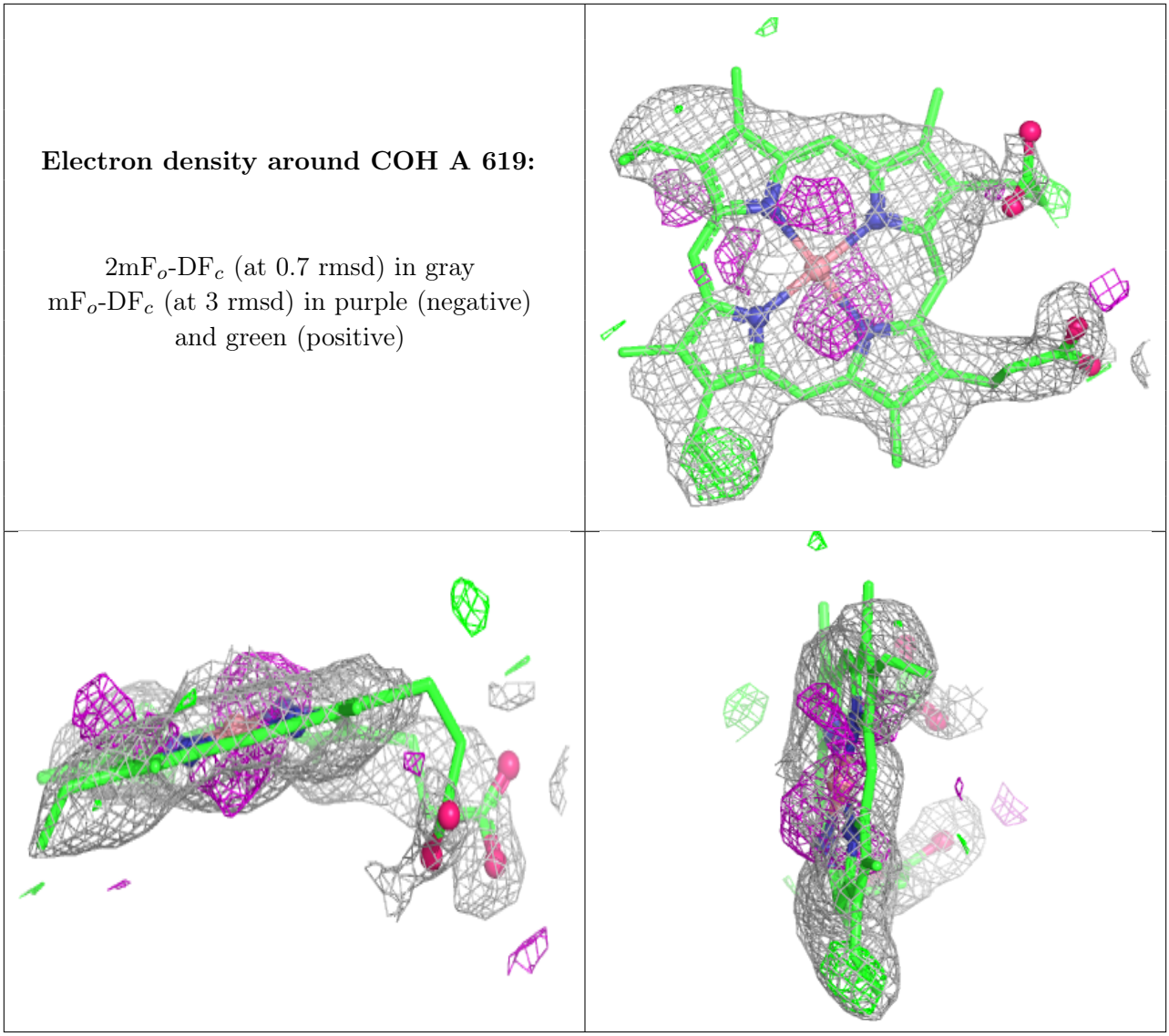






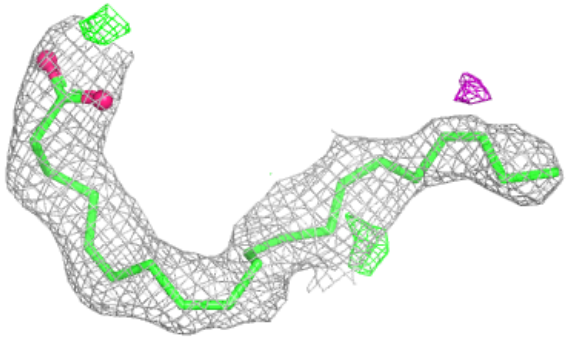
Electron density around COH A 619:

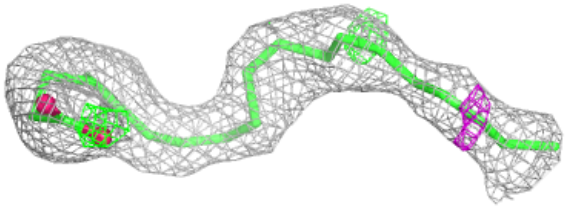
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

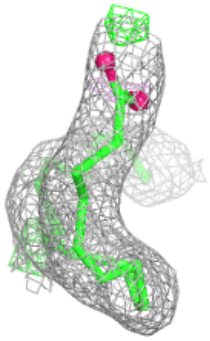


Electron density around EPA B 1:

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

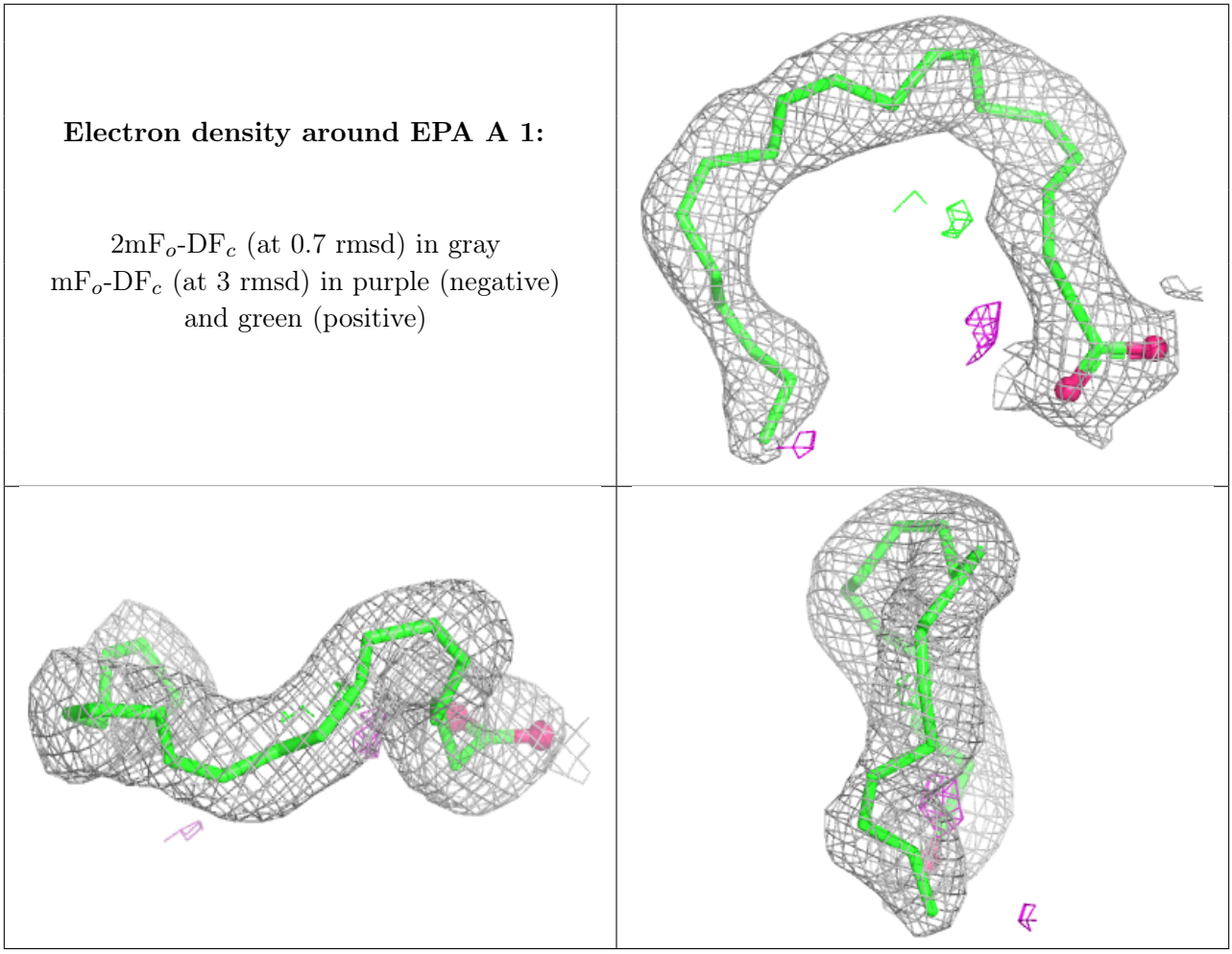






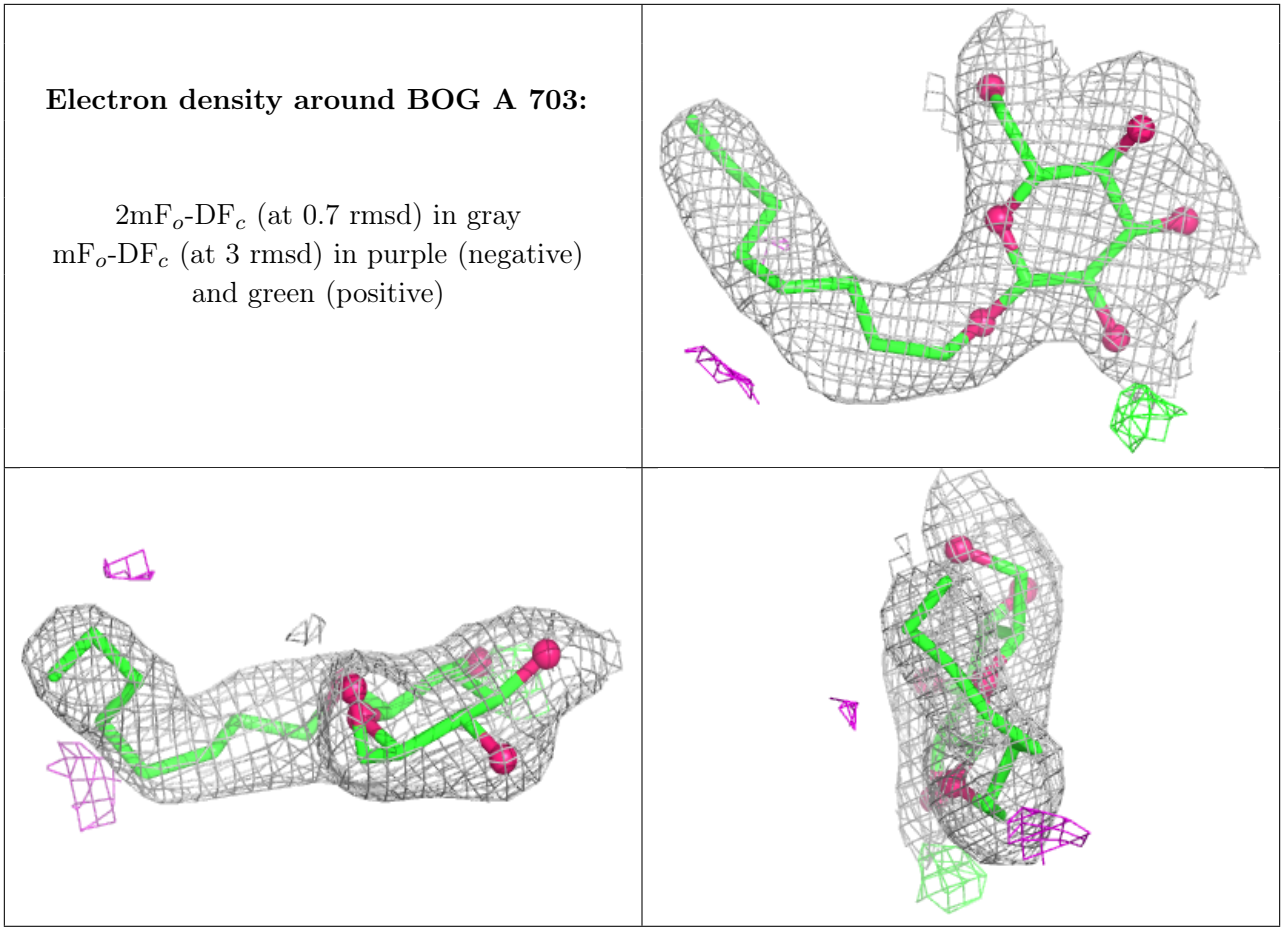
Electron density around EPA A 1:

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



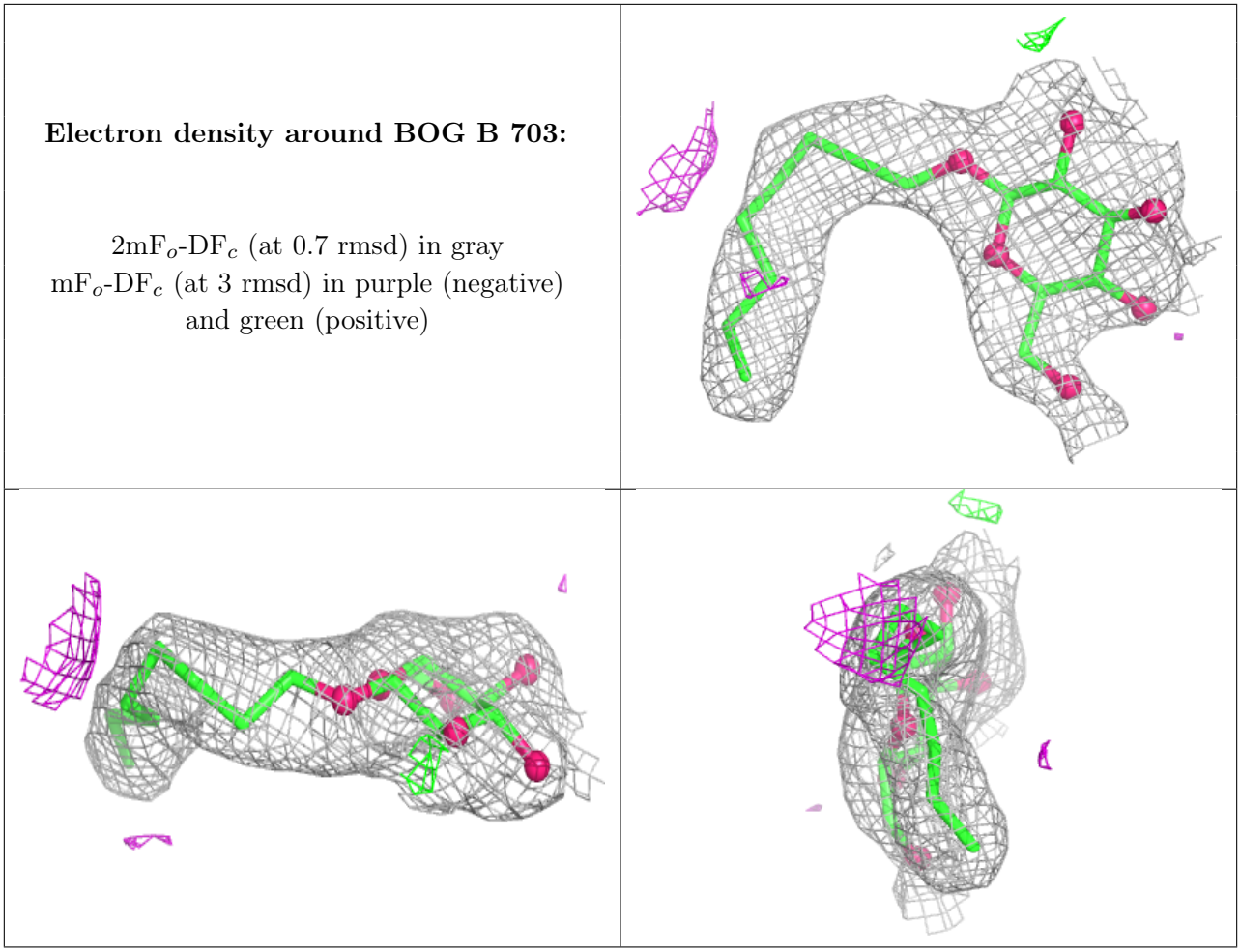
Electron density around BOG A 703:

$2mF_o$-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 B 703:

$2mF_o$-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.