Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 11:58 PM EDT

PDB ID	:	3HS5 / pdb_00003hs5
Title	:	X-ray crystal structure of arachidonic 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	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

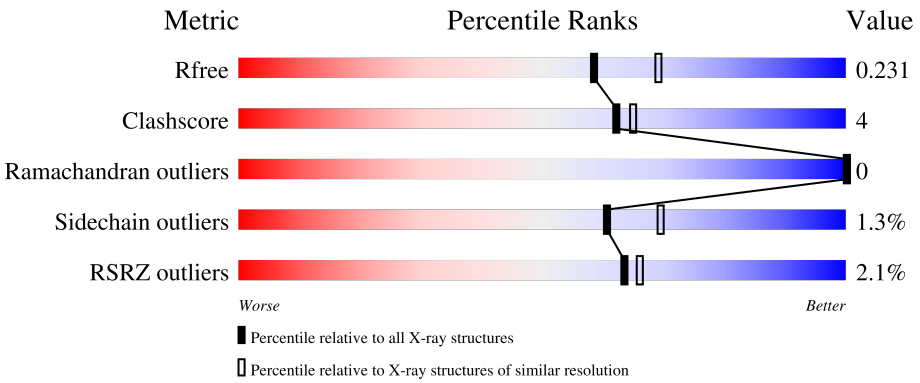
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	2%, 87%, 6%, 7%
1	B	591	2%, 86%, 6%, •, 7%
2	C	2	100%
2	E	2	100%
2	F	2	50%, 50%

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Mol	Chain	Length	Quality of chain
3	D	3	67% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACD	A	1[A]	-	-	X	-
4	ACD	B	1	-	-	X	-
5	AKR	A	2	-	-	X	-
6	COH	A	619	X	-	-	-
6	COH	B	619	X	-	-	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 10230 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.

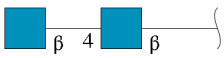
- Molecule 1 is a protein called Prostaglandin G/H synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	552	4468	2889	743	811	25	0	4	0
1	B	551	4454	2880	743	806	25	0	4	0

There are 14 discrepancies between the modelled and reference sequences:

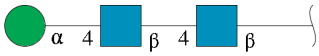
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	HIS	-	expression tag	UNP Q05769
A	30	HIS	-	expression tag	UNP Q05769
A	31	HIS	-	expression tag	UNP Q05769
A	32	HIS	-	expression tag	UNP Q05769
A	33	HIS	-	expression tag	UNP Q05769
A	34	HIS	-	expression tag	UNP Q05769
A	594	ALA	ASN	engineered mutation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



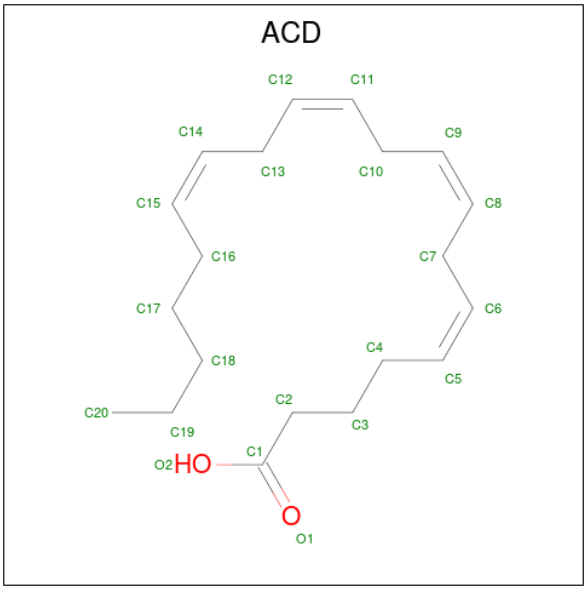
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0
			Total	C	N	O			
2	E	2	28	16	2	10	0	0	0
			Total	C	N	O			
2	F	2	28	16	2	10	0	0	0

- 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.



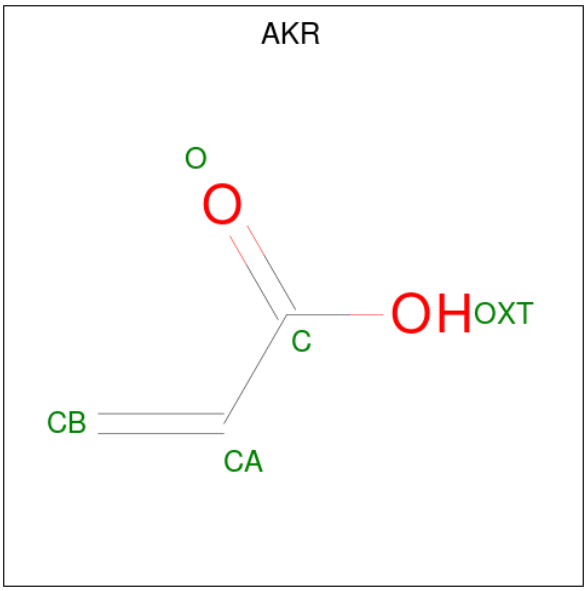
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	3	39	22	2	15	0	0	0

- Molecule 4 is ARACHIDONIC ACID (CCD ID: ACD) (formula: $C_{20}H_{32}O_2$).



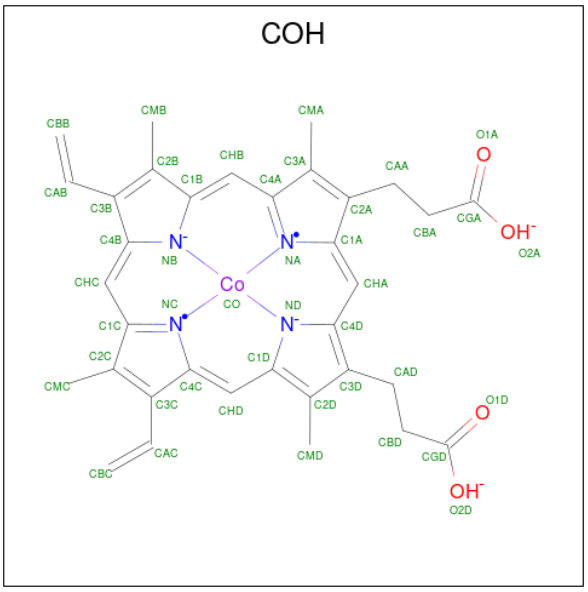
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	44	40	4	0	1
			Total	C	O		
4	B	1	22	20	2	0	0

- Molecule 5 is ACRYLIC ACID (CCD ID: AKR) (formula: $C_3H_4O_2$).



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

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING CO (CCD ID: COH) (formula: $C_{34}H_{32}CoN_4O_4$).



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

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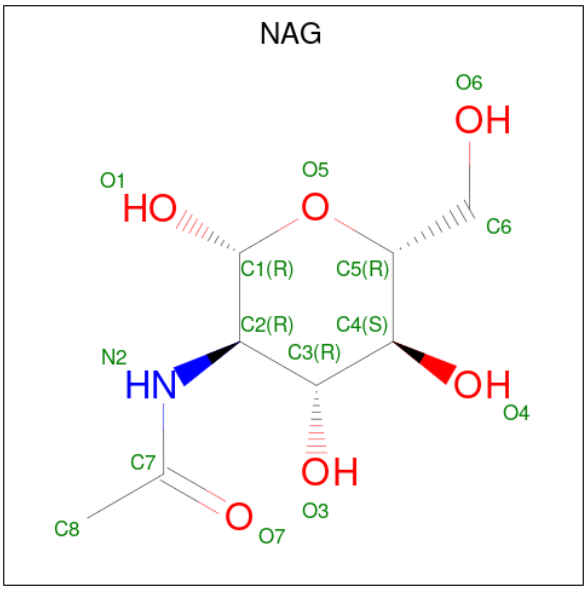
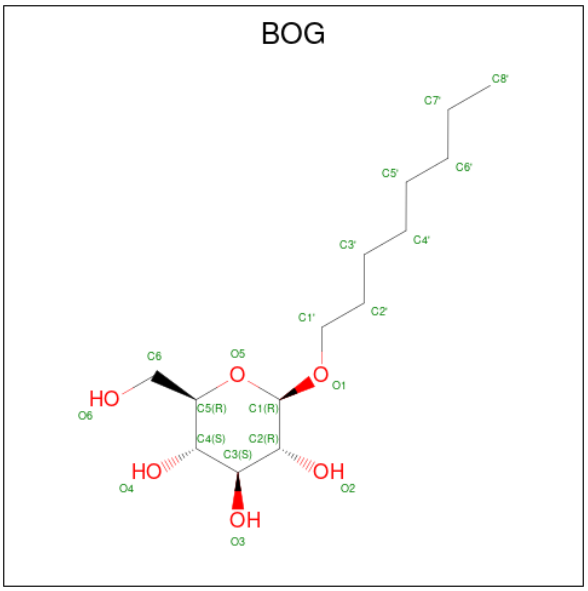
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Co	N	O		
6	B	1	43	34	1	4	4	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



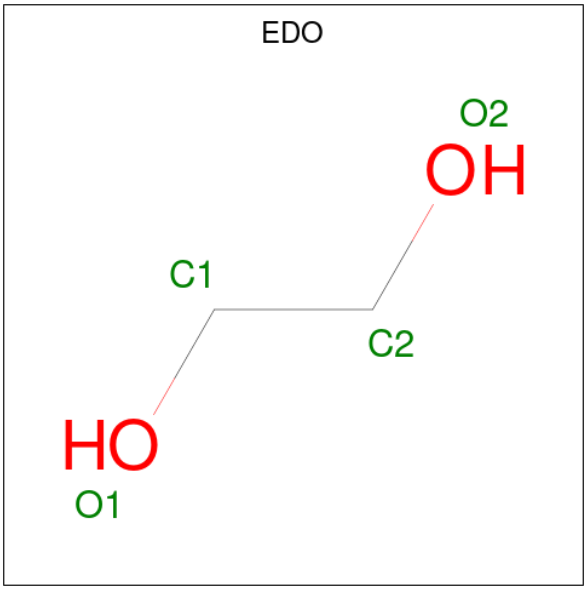
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O			
7	A	1	14	8	1	5		0	0
7	B	1	14	8	1	5		0	0

- Molecule 8 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



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

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 10 is water.

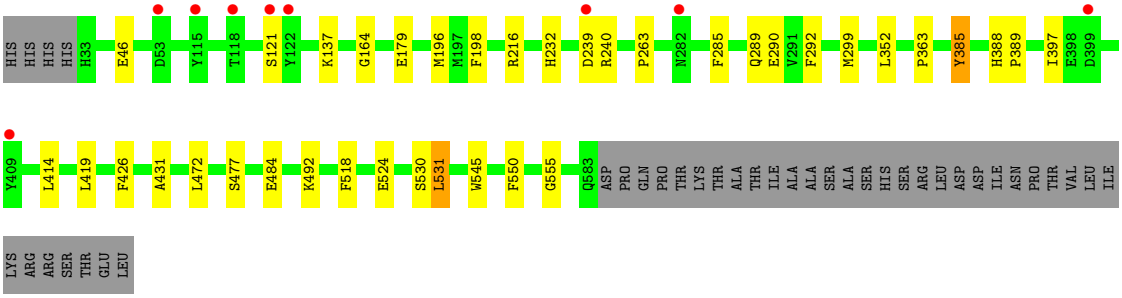
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	471	471	471	0	0
			Total	O		
10	B	436	436	436	0	0

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.

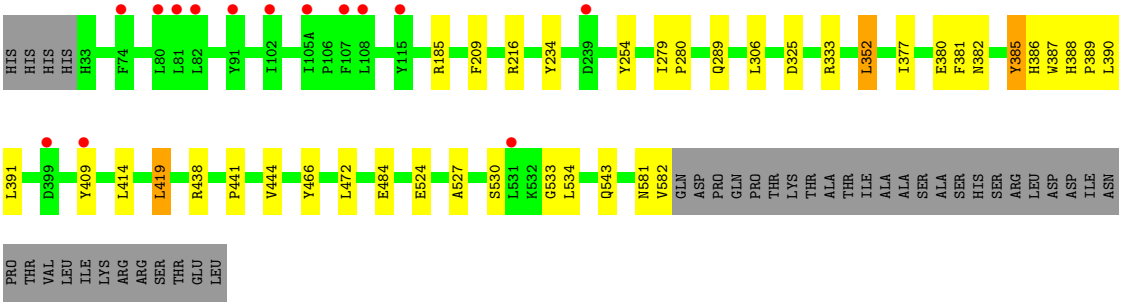
• Molecule 1: Prostaglandin G/H synthase 2

Chain A:



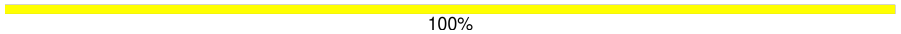
• Molecule 1: Prostaglandin G/H synthase 2

Chain B:

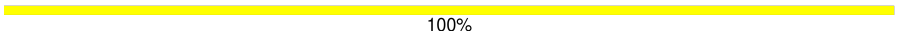


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



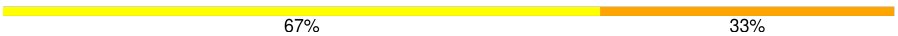
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 

• 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: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	119.98Å 132.55Å 180.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.10) 99.6 (20.00-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.169 , 0.210 0.198 , 0.231	Depositor DCC
R_{free} test set	4175 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10230	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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 (i)

5.1 Standard geometry (i)

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

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	0.55	1/4610 (0.0%)	0.80	0/6259
1	B	0.54	0/4594	0.80	0/6238
All	All	0.54	1/9204 (0.0%)	0.80	0/12497

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	GLY	C-N	-5.62	1.27	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4468	0	4321	39	0
1	B	4454	0	4291	31	0
2	C	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	2	0
3	D	39	0	34	4	0
4	A	44	0	62	18	0
4	B	22	0	31	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	10	0	6	4	0
6	A	43	0	30	0	0
6	B	43	0	30	1	0
7	A	14	0	13	0	0
7	B	14	0	13	0	0
8	A	20	0	28	1	0
8	B	20	0	28	0	0
9	A	16	0	24	0	0
9	B	32	0	48	3	0
10	A	471	0	0	1	0
10	B	436	0	0	1	0
All	All	10230	0	9034	76	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.

All (76) 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	4:B:1:ACD:H191	1.21	1.12
1:A:531:LEU:HB2	4:A:1[A]:ACD:H201	1.24	1.10
1:A:531:LEU:HB2	4:A:1[A]:ACD:C20	1.92	0.99
1:A:530[B]:SER:OG	4:A:1[B]:ACD:C3	2.13	0.96
4:A:1[B]:ACD:H132	4:A:1[B]:ACD:H9	1.51	0.92
1:A:531:LEU:CB	4:A:1[A]:ACD:H201	2.01	0.89
1:A:530[B]:SER:OG	4:A:1[B]:ACD:H31	1.76	0.85
1:B:533:GLY:HA3	4:B:1:ACD:C19	2.06	0.84
1:A:216:ARG:HH11	3:D:2:NAG:H83	1.48	0.78
1:A:216:ARG:NH1	3:D:2:NAG:H83	1.99	0.78
1:A:492:LYS:HD3	5:A:2:AKR:HA1	1.65	0.77
1:A:263:PRO:HG2	1:A:299:MET:HE1	1.67	0.77
4:A:1[B]:ACD:H132	4:A:1[B]:ACD:C9	2.15	0.77
1:B:381:PHE:HE2	4:B:1:ACD:H203	1.51	0.76
1:A:530[B]:SER:OG	4:A:1[B]:ACD:H32	1.86	0.74
1:B:216:ARG:HG2	2:F:2:NAG:H81	1.69	0.73
1:A:385:TYR:OH	4:A:1[A]:ACD:H31	1.89	0.71
1:B:534:LEU:HG	4:B:1:ACD:H172	1.75	0.68
1:A:477:SER:HB2	5:A:2:AKR:HB2	1.77	0.65
4:A:1[B]:ACD:H9	4:A:1[B]:ACD:C13	2.26	0.64
1:B:414:LEU:HD11	1:B:419:LEU:HD22	1.80	0.64
1:B:325:ASP:HB3	9:B:10:EDO:H12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530[A]:SER:HB2	4:A:1[A]:ACD:H42	1.78	0.64
1:A:531:LEU:HG	4:A:1[A]:ACD:H201	1.81	0.63
1:B:185:ARG:NH1	1:B:438:ARG:HG2	2.14	0.61
1:A:531:LEU:CG	4:A:1[A]:ACD:H201	2.29	0.61
4:A:1[B]:ACD:C9	4:A:1[B]:ACD:C13	2.75	0.61
1:A:531:LEU:HB2	4:A:1[A]:ACD:C19	2.30	0.61
1:A:46:GLU:OE1	10:A:1337:HOH:O	2.17	0.58
1:B:234:TYR:CE2	1:B:333:ARG:HG3	2.40	0.56
1:A:216:ARG:HG2	3:D:2:NAG:H81	1.89	0.55
1:A:137:LYS:HE2	1:B:543:GLN:O	2.07	0.54
1:A:414:LEU:HD11	1:A:419:LEU:HD12	1.89	0.53
4:B:1:ACD:H6	4:B:1:ACD:H11	1.91	0.52
1:A:216:ARG:HH11	3:D:2:NAG:C8	2.22	0.51
1:B:216:ARG:HH11	2:F:2:NAG:H83	1.76	0.51
1:B:377:ILE:CD1	4:B:1:ACD:H201	2.41	0.50
1:B:382:ASN:O	1:B:386:HIS:HD2	1.94	0.49
1:B:472:LEU:HD21	1:B:524:GLU:HG3	1.96	0.48
1:A:472:LEU:HD21	1:A:524:GLU:HG3	1.95	0.48
1:B:381:PHE:CE2	4:B:1:ACD:H203	2.41	0.48
1:B:530[B]:SER:OG	4:B:1:ACD:H102	2.13	0.47
4:A:1[A]:ACD:H41	4:A:1[A]:ACD:H71	1.56	0.47
1:A:530[A]:SER:OG	4:A:1[A]:ACD:H22	2.15	0.47
1:A:530[A]:SER:OG	4:A:1[A]:ACD:O1	2.32	0.47
1:B:391:LEU:HD21	6:B:619:COH:HHC	1.97	0.46
1:A:285:PHE:CD2	1:A:299:MET:HE2	2.51	0.46
1:B:385:TYR:OH	4:B:1:ACD:H131	2.16	0.46
1:A:196:MET:CE	1:A:431:ALA:HB2	2.47	0.45
1:A:240:ARG:HH11	5:A:3:AKR:CA	2.29	0.45
1:B:382:ASN:O	1:B:386:HIS:CD2	2.70	0.45
1:A:492:LYS:CD	5:A:2:AKR:HA1	2.40	0.44
1:B:306:LEU:C	1:B:306:LEU:HD23	2.42	0.44
1:A:179:GLU:HB3	8:A:703:BOG:H4'2	1.99	0.43
1:A:397:ILE:HD11	1:A:426:PHE:CE1	2.54	0.43
9:B:9:EDO:H11	10:B:1428:HOH:O	2.19	0.43
1:A:363:PRO:HG2	1:A:545:TRP:CD2	2.54	0.42
1:B:581:ASN:O	1:B:582:VAL:HB	2.19	0.42
1:B:527:ALA:HB2	4:B:1:ACD:H21	2.00	0.42
1:A:232:HIS:HB2	1:A:292:PHE:CE2	2.54	0.42
1:B:441:PRO:HG2	1:B:444:VAL:HG22	2.02	0.42
1:B:209:PHE:CZ	4:B:1:ACD:H182	2.54	0.42
1:B:352:LEU:HB3	4:B:1:ACD:H5	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388[A]:HIS:N	1:B:389:PRO:CD	2.83	0.41
1:A:196:MET:HE2	1:A:431:ALA:HB2	2.02	0.41
1:A:240:ARG:NH2	1:A:290:GLU:HG3	2.36	0.41
1:B:387:TRP:O	1:B:390:LEU:HB2	2.21	0.41
1:A:388[B]:HIS:HB2	1:A:389:PRO:HD3	2.03	0.41
1:B:279:ILE:HA	1:B:280:PRO:HD3	1.93	0.41
1:B:380:GLU:HG2	1:B:466:TYR:CE2	2.55	0.41
1:A:352:LEU:HD22	1:A:518:PHE:CE2	2.56	0.40
1:B:254:TYR:CE2	9:B:3:EDO:H21	2.57	0.40
1:A:46:GLU:OE1	1:A:137:LYS:NZ	2.54	0.40
1:A:198:PHE:CZ	1:A:352:LEU:HD21	2.57	0.40
1:A:550:PHE:O	1:A:555:GLY:HA3	2.21	0.40
1:B:209:PHE:CE2	4:B:1:ACD:H182	2.56	0.40

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	554/591 (94%)	545 (98%)	9 (2%)	0	100	100
1	B	553/591 (94%)	539 (98%)	14 (2%)	0	100	100
All	All	1107/1182 (94%)	1084 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	485/529 (92%)	479 (99%)	6 (1%)	63	72
1	B	480/529 (91%)	474 (99%)	6 (1%)	61	69
All	All	965/1058 (91%)	953 (99%)	12 (1%)	61	72

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	A	239	ASP
1	A	289	GLN
1	A	385	TYR
1	A	484	GLU
1	A	531	LEU
1	B	289	GLN
1	B	352	LEU
1	B	385	TYR
1	B	409	TYR
1	B	419	LEU
1	B	484	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	214	HIS
1	A	241	GLN
1	A	318	GLN
1	A	396	ASN
1	A	421	GLN
1	A	461	GLN
1	A	560	ASN
1	A	571	ASN
1	B	39	ASN
1	B	571	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	2,1	14,14,15	0.84	0	17,19,21	1.58	3 (17%)
2	NAG	C	2	2	14,14,15	0.47	0	17,19,21	1.05	2 (11%)
3	NAG	D	1	3,1	14,14,15	0.59	0	17,19,21	1.26	2 (11%)
3	NAG	D	2	3	14,14,15	0.50	0	17,19,21	0.98	1 (5%)
3	MAN	D	3	3	11,11,12	0.48	0	15,15,17	2.34	2 (13%)
2	NAG	E	1	2,1	14,14,15	0.59	0	17,19,21	0.73	1 (5%)
2	NAG	E	2	2	14,14,15	0.65	0	17,19,21	1.12	2 (11%)
2	NAG	F	1	2,1	14,14,15	0.50	0	17,19,21	1.10	1 (5%)
2	NAG	F	2	2	14,14,15	0.54	0	17,19,21	1.15	1 (5%)

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	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	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	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	1	2,1	-	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.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	3	MAN	C1-O5-C5	7.67	122.47	112.19
2	C	1	NAG	C3-C4-C5	-4.30	102.44	110.23
3	D	1	NAG	C1-O5-C5	4.05	117.61	112.19
2	F	1	NAG	C1-O5-C5	3.79	117.27	112.19
2	F	2	NAG	C4-C3-C2	3.02	115.45	111.02
3	D	3	MAN	C3-C4-C5	2.77	115.26	110.23
3	D	1	NAG	C2-N2-C7	-2.77	119.19	122.90
2	C	1	NAG	O5-C5-C6	2.58	112.69	107.66
2	E	2	NAG	O5-C1-C2	2.55	115.24	111.29
2	C	2	NAG	C4-C3-C2	2.51	114.70	111.02
3	D	2	NAG	C4-C3-C2	2.28	114.36	111.02
2	E	2	NAG	C1-C2-N2	-2.26	106.87	110.43
2	C	1	NAG	O4-C4-C5	2.20	114.73	109.32
2	C	2	NAG	C3-C4-C5	2.14	114.10	110.23
2	E	1	NAG	C4-C3-C2	2.12	114.13	111.02

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
3	D	3	MAN	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
3	D	2	NAG	C8-C7-N2-C2
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
3	D	3	MAN	C4-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	E	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6

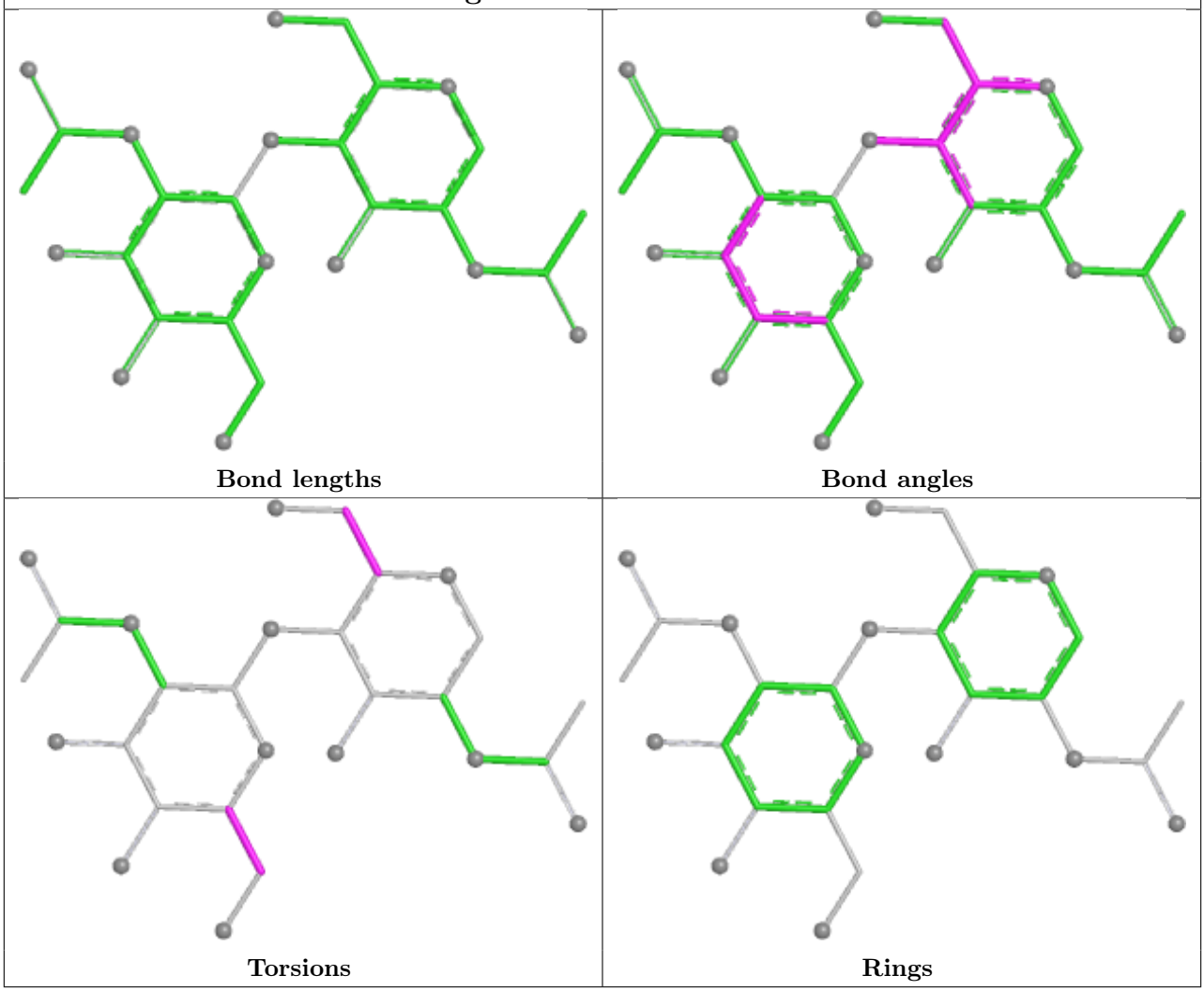
There are no ring outliers.

2 monomers are involved in 6 short contacts:

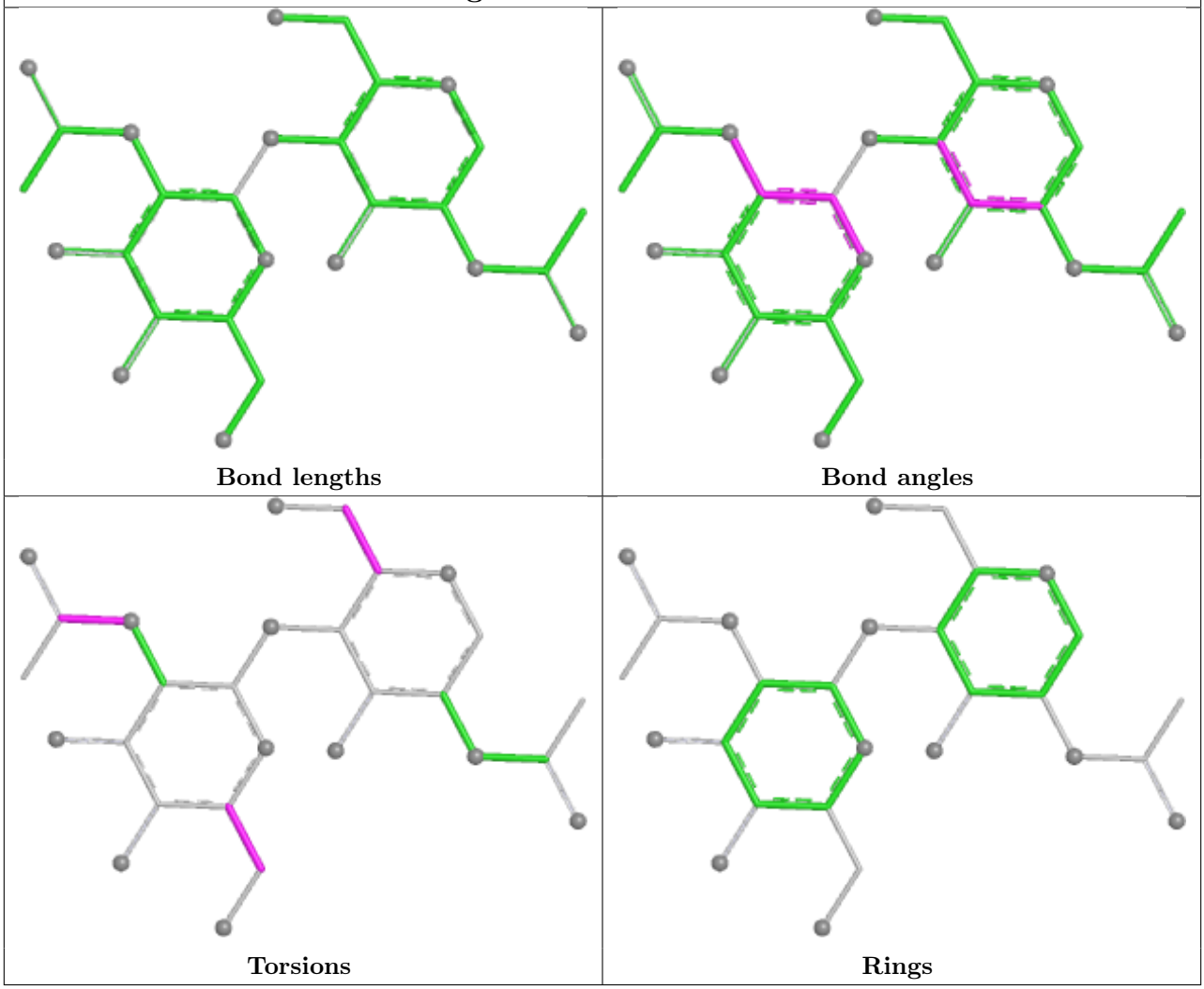
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	NAG	2	0
3	D	2	NAG	4	0

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

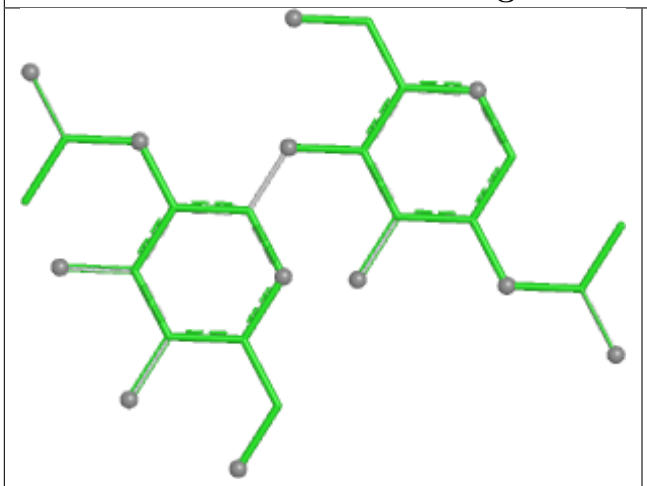
Oligosaccharide Chain C



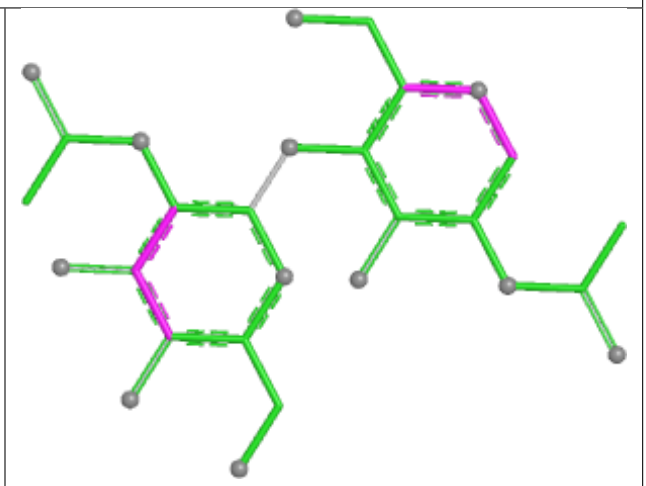
Oligosaccharide Chain E



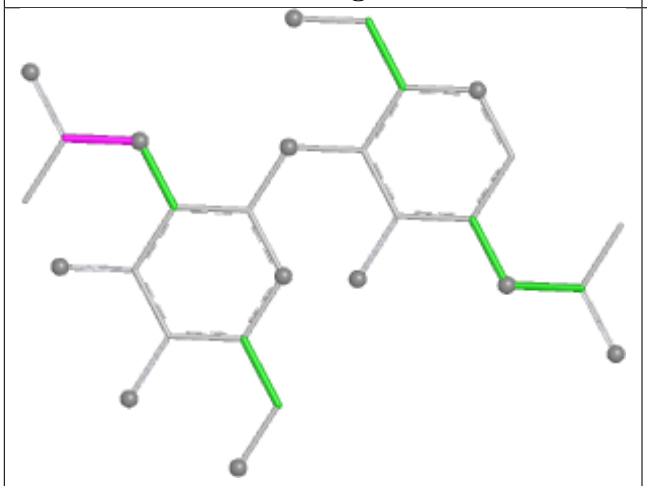
Oligosaccharide Chain F



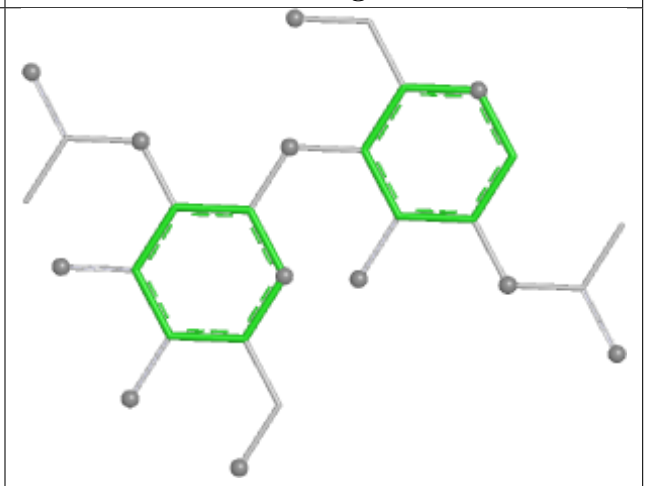
Bond lengths



Bond angles

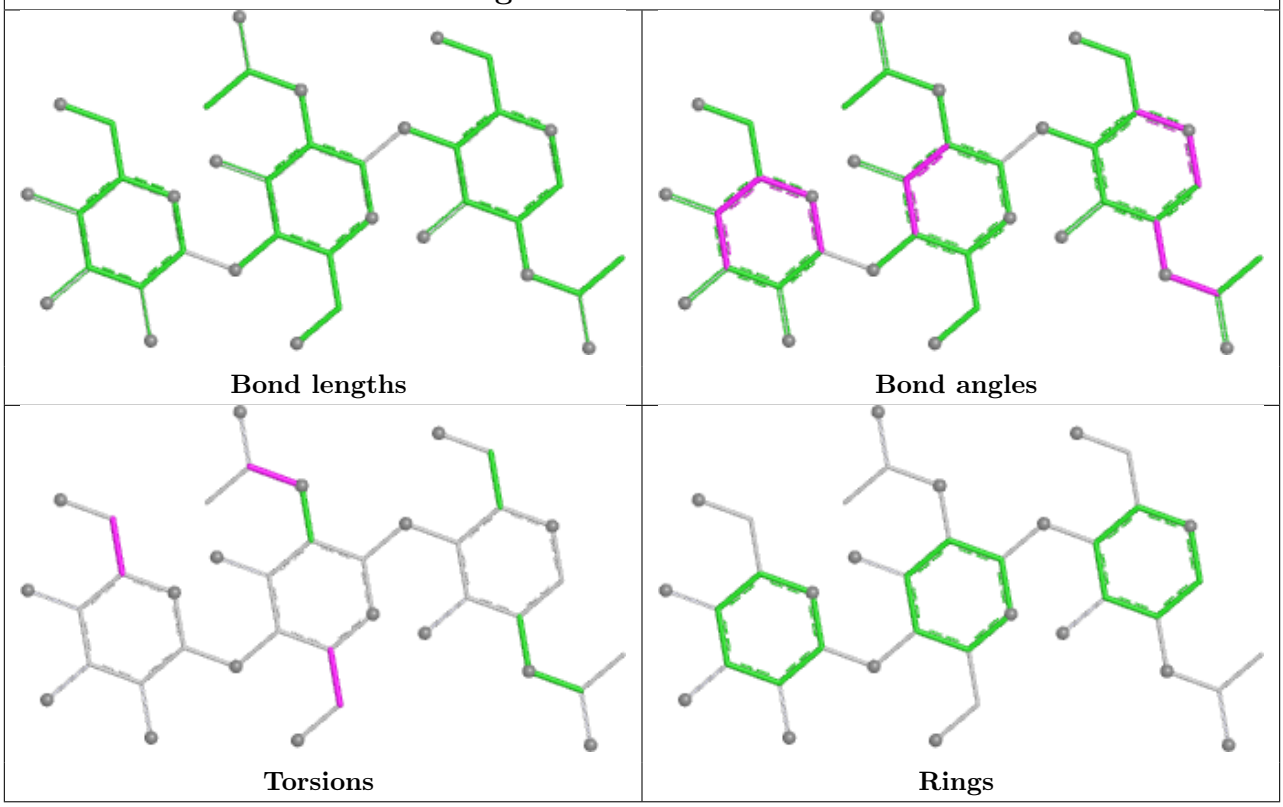


Torsions



Rings

Oligosaccharide Chain D



5.6 Ligand geometry (i)

23 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	$\#\|Z\| > 2$
4	ACD	A	1[B]	-	21,21,21	0.47	0	21,21,21	0.79	0
9	EDO	A	4	-	3,3,3	0.47	0	2,2,2	0.35	0
6	COH	A	619	1	50,50,50	1.72	11 (22%)	66,82,82	1.53	10 (15%)
9	EDO	B	11	-	3,3,3	0.36	0	2,2,2	0.40	0
6	COH	B	619	1	50,50,50	1.68	10 (20%)	66,82,82	1.51	10 (15%)
8	BOG	A	703	8	20,20,20	0.48	0	25,25,25	0.62	0
9	EDO	B	7	-	3,3,3	0.43	0	2,2,2	0.35	0
4	ACD	B	1	-	21,21,21	0.52	0	21,21,21	0.68	0
5	AKR	A	2	-	4,4,4	2.02	2 (50%)	4,4,4	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	EDO	B	9	-	3,3,3	0.42	0	2,2,2	0.52	0
9	EDO	A	620	-	3,3,3	0.48	0	2,2,2	0.24	0
9	EDO	B	10	-	3,3,3	0.45	0	2,2,2	0.24	0
9	EDO	B	6	-	3,3,3	0.43	0	2,2,2	0.53	0
9	EDO	B	2	-	3,3,3	0.46	0	2,2,2	0.30	0
9	EDO	B	8	-	3,3,3	0.41	0	2,2,2	0.36	0
9	EDO	A	5	-	3,3,3	0.47	0	2,2,2	0.36	0
7	NAG	A	681	1	14,14,15	0.55	0	17,19,21	0.86	0
9	EDO	B	3	-	3,3,3	0.38	0	2,2,2	0.24	0
9	EDO	A	12	-	3,3,3	0.46	0	2,2,2	0.34	0
4	ACD	A	1[A]	-	21,21,21	0.48	0	21,21,21	0.74	0
8	BOG	B	703	8	20,20,20	0.40	0	25,25,25	0.71	0
5	AKR	A	3	-	4,4,4	1.99	2 (50%)	4,4,4	0.92	0
7	NAG	B	681	1	14,14,15	0.47	0	17,19,21	0.92	1 (5%)

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
4	ACD	A	1[B]	-	-	10/19/19/19	-
9	EDO	A	4	-	-	0/1/1/1	-
6	COH	A	619	1	1/1/3/9	9/14/54/54	-
9	EDO	B	11	-	-	0/1/1/1	-
6	COH	B	619	1	1/1/3/9	3/14/54/54	-
8	BOG	A	703	8	-	5/11/31/31	0/1/1/1
9	EDO	B	7	-	-	1/1/1/1	-
4	ACD	B	1	-	-	8/19/19/19	-
5	AKR	A	2	-	-	0/2/2/2	-
9	EDO	B	9	-	-	1/1/1/1	-
9	EDO	A	620	-	-	0/1/1/1	-
9	EDO	B	10	-	-	1/1/1/1	-
9	EDO	B	6	-	-	0/1/1/1	-
9	EDO	B	2	-	-	1/1/1/1	-
9	EDO	B	8	-	-	0/1/1/1	-
9	EDO	A	5	-	-	1/1/1/1	-
7	NAG	A	681	1	-	0/6/23/26	0/1/1/1
9	EDO	B	3	-	-	0/1/1/1	-
9	EDO	A	12	-	-	0/1/1/1	-
4	ACD	A	1[A]	-	-	11/19/19/19	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BOG	B	703	8	-	3/11/31/31	0/1/1/1
5	AKR	A	3	-	-	0/2/2/2	-
7	NAG	B	681	1	-	1/6/23/26	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	619	COH	C3D-C2D	5.90	1.54	1.38
6	A	619	COH	C3D-C2D	5.80	1.54	1.38
6	A	619	COH	CO-NA	4.79	2.13	1.96
6	B	619	COH	CO-NA	4.07	2.11	1.96
6	A	619	COH	CO-NB	4.03	2.11	1.96
6	B	619	COH	CO-NB	3.61	2.10	1.96
6	B	619	COH	CO-ND	3.51	2.09	1.96
6	A	619	COH	CO-ND	3.47	2.09	1.96
6	B	619	COH	CAC-C3C	2.94	1.55	1.47
6	A	619	COH	CAB-C3B	2.88	1.55	1.47
6	B	619	COH	CAB-C3B	2.85	1.55	1.47
6	A	619	COH	CAC-C3C	2.80	1.54	1.47
6	B	619	COH	CO-NC	2.74	2.06	1.96
5	A	2	AKR	CA-C	-2.72	1.39	1.46
5	A	3	AKR	CA-C	-2.63	1.39	1.46
6	A	619	COH	CO-NC	2.49	2.05	1.96
6	B	619	COH	CMA-C3A	2.31	1.55	1.50
6	A	619	COH	CMA-C3A	2.20	1.55	1.50
6	B	619	COH	CMB-C2B	2.19	1.55	1.50
6	A	619	COH	CMC-C2C	2.18	1.55	1.50
6	B	619	COH	CMC-C2C	2.15	1.55	1.50
6	A	619	COH	CMB-C2B	2.14	1.55	1.50
5	A	2	AKR	OXT-C	-2.14	1.25	1.30
6	A	619	COH	CMD-C2D	2.05	1.55	1.50
5	A	3	AKR	OXT-C	-2.05	1.25	1.30

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	619	COH	C4D-ND-C1D	4.83	112.22	105.11
6	A	619	COH	C4D-ND-C1D	4.80	112.18	105.11
6	A	619	COH	C2B-C1B-NB	-4.10	107.69	110.88
6	B	619	COH	C2B-C1B-NB	-3.92	107.83	110.88
6	A	619	COH	C2C-C1C-NC	-3.68	107.13	110.96
6	B	619	COH	C2C-C1C-NC	-3.65	107.17	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	619	COH	C4C-NC-C1C	3.03	108.97	105.12
6	A	619	COH	C3A-C4A-NA	-3.01	107.83	110.96
6	B	619	COH	C4C-NC-C1C	2.99	108.93	105.12
6	B	619	COH	C3A-C4A-NA	-2.89	107.95	110.96
6	B	619	COH	C3D-C4D-ND	-2.86	108.19	110.73
6	A	619	COH	C3D-C4D-ND	-2.75	108.28	110.73
6	B	619	COH	C1A-NA-C4A	2.50	108.30	105.12
6	A	619	COH	C3C-C2C-C1C	2.49	108.28	106.41
6	B	619	COH	C3C-C2C-C1C	2.46	108.26	106.41
6	A	619	COH	C1A-NA-C4A	2.46	108.24	105.12
6	B	619	COH	C4B-NB-C1B	2.38	108.63	105.11
6	A	619	COH	C4B-NB-C1B	2.33	108.55	105.11
6	B	619	COH	C2A-C1A-NA	-2.10	108.00	110.57
6	A	619	COH	C2A-C1A-NA	-2.09	108.01	110.57
7	B	681	NAG	C1-O5-C5	2.05	114.93	112.19

All (2) chirality outliers are listed below:

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

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	619	COH	C2B-C3B-CAB-CBB
4	A	1[B]	ACD	C1-C2-C3-C4
8	A	703	BOG	O1-C1'-C2'-C3'
4	A	1[A]	ACD	C17-C18-C19-C20
6	B	619	COH	C2A-CAA-CBA-CGA
8	B	703	BOG	C4'-C5'-C6'-C7'
4	B	1	ACD	C16-C17-C18-C19
9	B	10	EDO	O1-C1-C2-O2
4	A	1[A]	ACD	C16-C17-C18-C19
4	B	1	ACD	C15-C16-C17-C18
6	A	619	COH	C2B-C3B-CAB-CBB
6	A	619	COH	C2C-C3C-CAC-CBC
8	A	703	BOG	C2'-C3'-C4'-C5'
6	A	619	COH	C1A-C2A-CAA-CBA
9	A	5	EDO	O1-C1-C2-O2
9	B	7	EDO	O1-C1-C2-O2
4	A	1[B]	ACD	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
4	A	1[B]	ACD	C17-C18-C19-C20
6	A	619	COH	C2A-CAA-CBA-CGA
6	A	619	COH	C3A-C2A-CAA-CBA
4	A	1[A]	ACD	C11-C10-C9-C8
4	A	1[A]	ACD	C9-C10-C11-C12
4	A	1[A]	ACD	C11-C12-C13-C14
4	A	1[A]	ACD	C12-C13-C14-C15
4	A	1[B]	ACD	C6-C7-C8-C9
4	A	1[B]	ACD	C9-C10-C11-C12
4	A	1[B]	ACD	C11-C12-C13-C14
4	A	1[B]	ACD	C12-C13-C14-C15
4	B	1	ACD	C9-C10-C11-C12
4	B	1	ACD	C12-C13-C14-C15
4	B	1	ACD	C17-C18-C19-C20
4	B	1	ACD	C1-C2-C3-C4
7	B	681	NAG	C4-C5-C6-O6
6	A	619	COH	C4C-C3C-CAC-CBC
6	B	619	COH	C4B-C3B-CAB-CBB
8	A	703	BOG	C5'-C6'-C7'-C8'
8	A	703	BOG	C3'-C4'-C5'-C6'
8	B	703	BOG	O5-C1-O1-C1'
6	A	619	COH	C4B-C3B-CAB-CBB
8	B	703	BOG	C1'-C2'-C3'-C4'
4	A	1[B]	ACD	O2-C1-C2-C3
4	A	1[A]	ACD	C6-C7-C8-C9
4	B	1	ACD	C11-C12-C13-C14
4	A	1[B]	ACD	O1-C1-C2-C3
4	A	1[A]	ACD	C14-C15-C16-C17
6	A	619	COH	CAA-CBA-CGA-O2A
8	A	703	BOG	C1'-C2'-C3'-C4'
9	B	9	EDO	O1-C1-C2-O2
4	A	1[B]	ACD	C14-C15-C16-C17
6	A	619	COH	CAA-CBA-CGA-O1A
4	A	1[A]	ACD	C1-C2-C3-C4
4	B	1	ACD	C14-C15-C16-C17
4	A	1[A]	ACD	O1-C1-C2-C3
9	B	2	EDO	O1-C1-C2-O2
4	A	1[A]	ACD	O2-C1-C2-C3

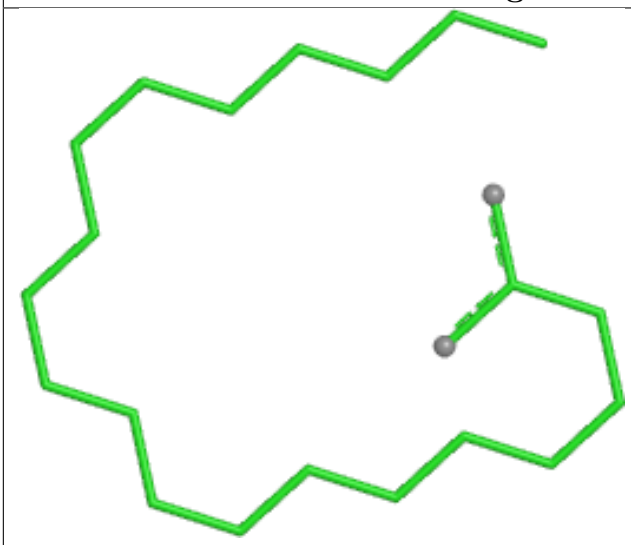
There are no ring outliers.

10 monomers are involved in 40 short contacts:

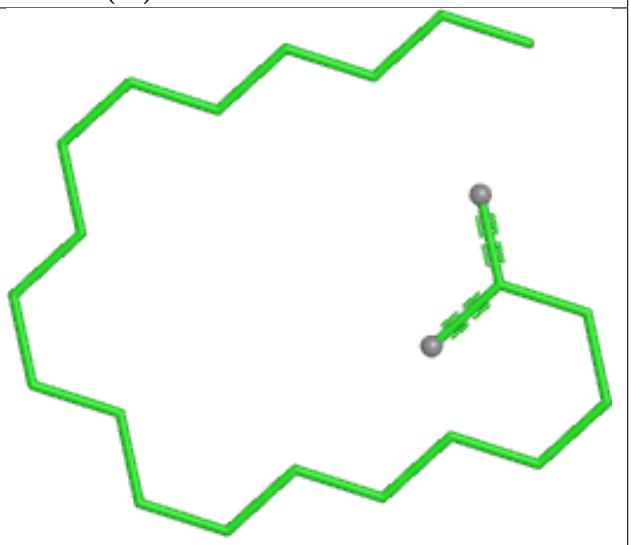
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1[B]	ACD	7	0
6	B	619	COH	1	0
8	A	703	BOG	1	0
4	B	1	ACD	13	0
5	A	2	AKR	3	0
9	B	9	EDO	1	0
9	B	10	EDO	1	0
9	B	3	EDO	1	0
4	A	1[A]	ACD	11	0
5	A	3	AKR	1	0

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

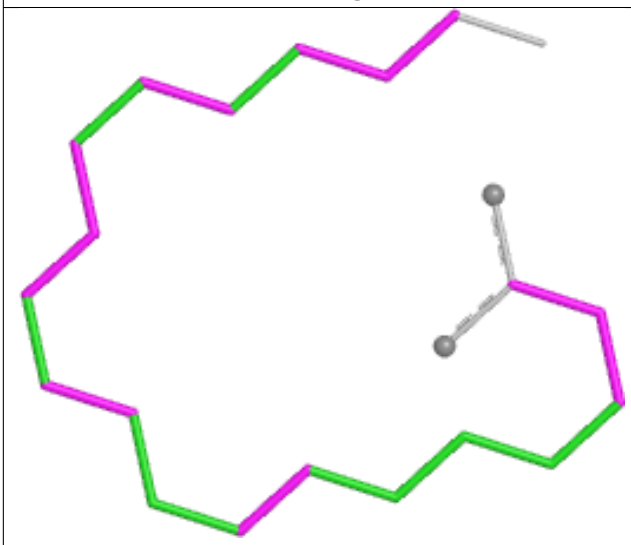
Ligand ACD A 1 (B)



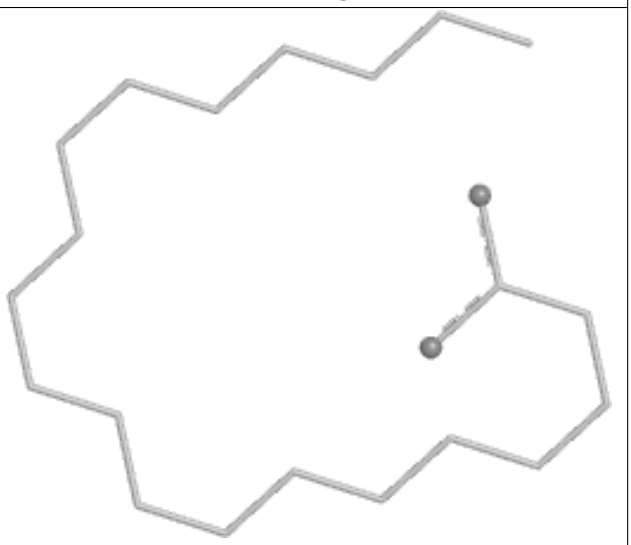
Bond lengths



Bond angles

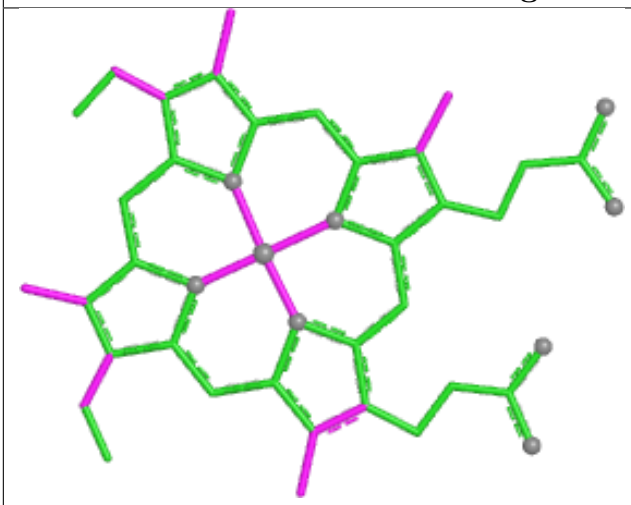


Torsions

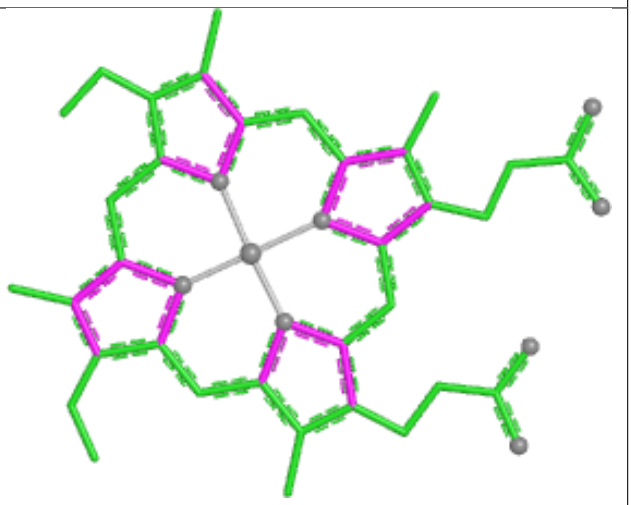


Rings

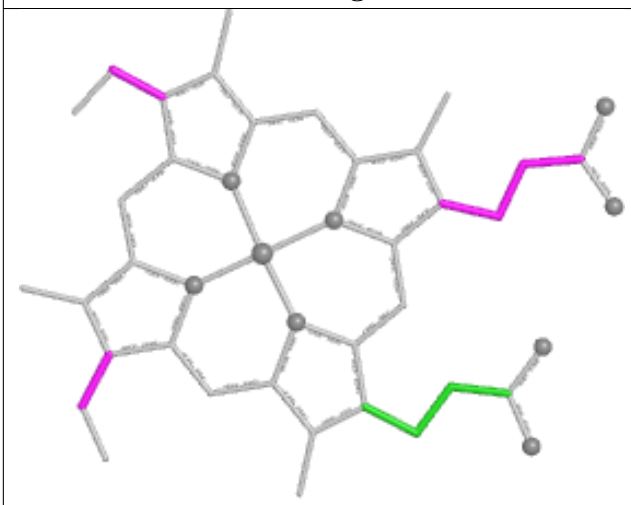
Ligand COH A 619



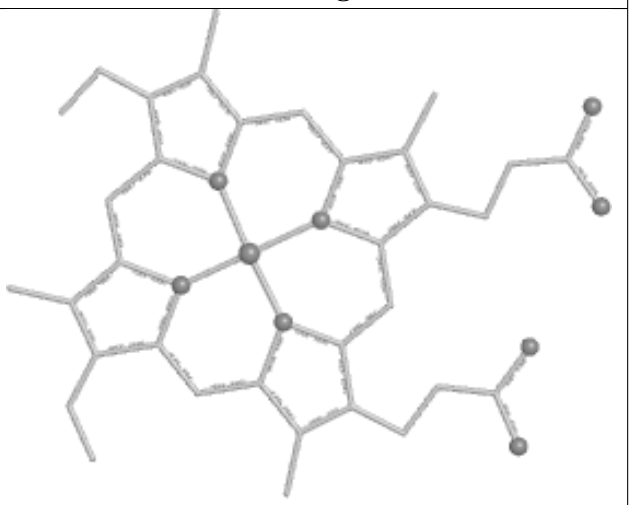
Bond lengths



Bond angles

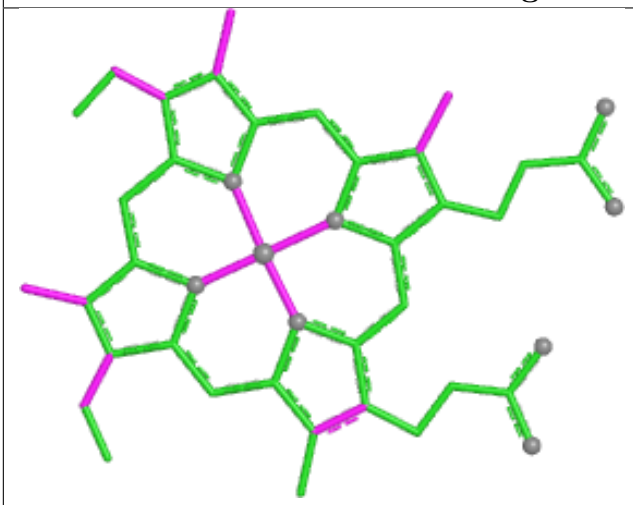


Torsions

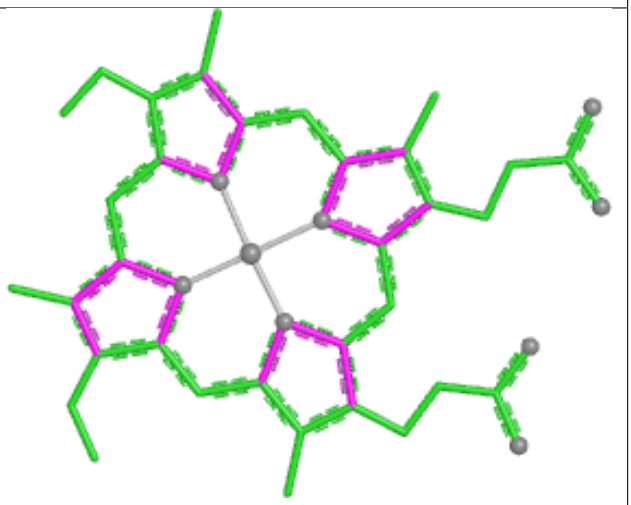


Rings

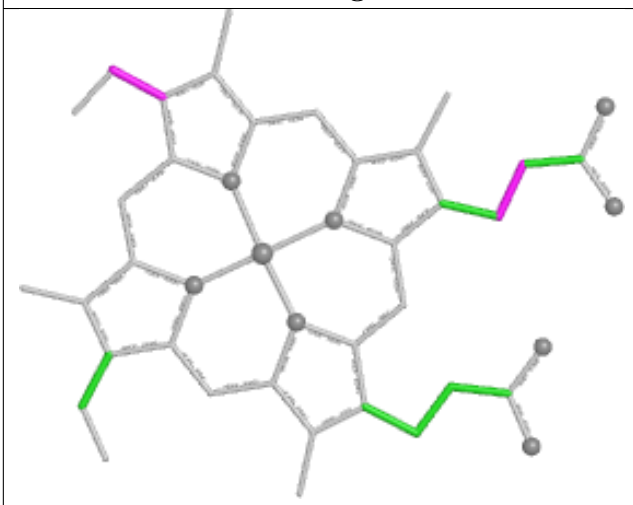
Ligand COH B 619



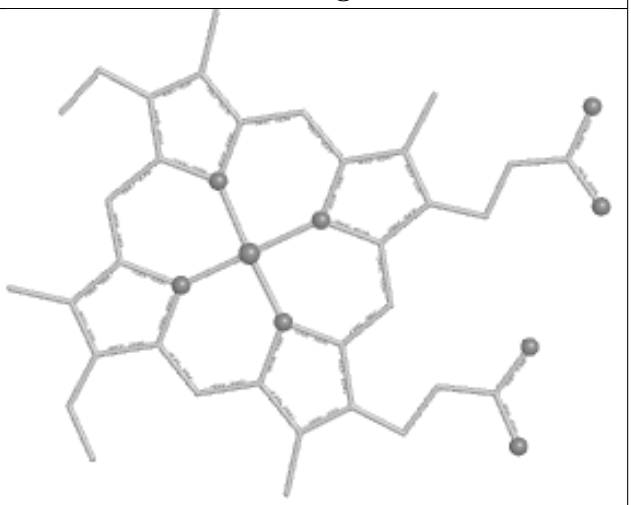
Bond lengths



Bond angles

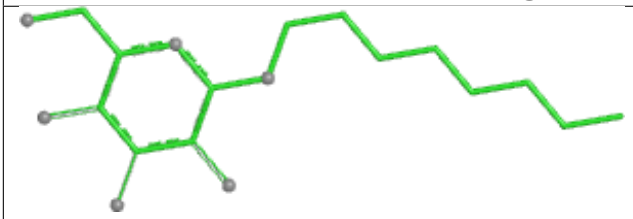


Torsions

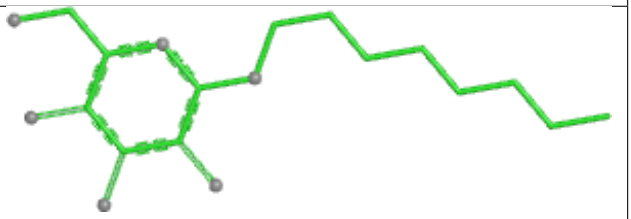


Rings

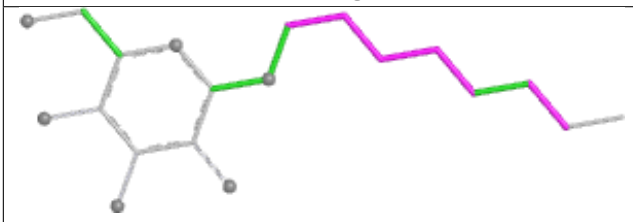
Ligand BOG A 703



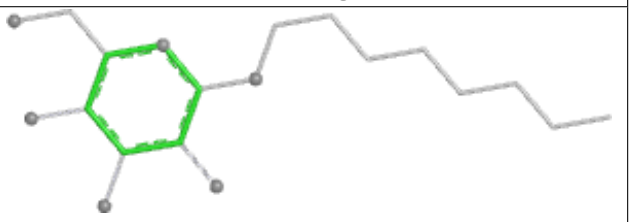
Bond lengths



Bond angles

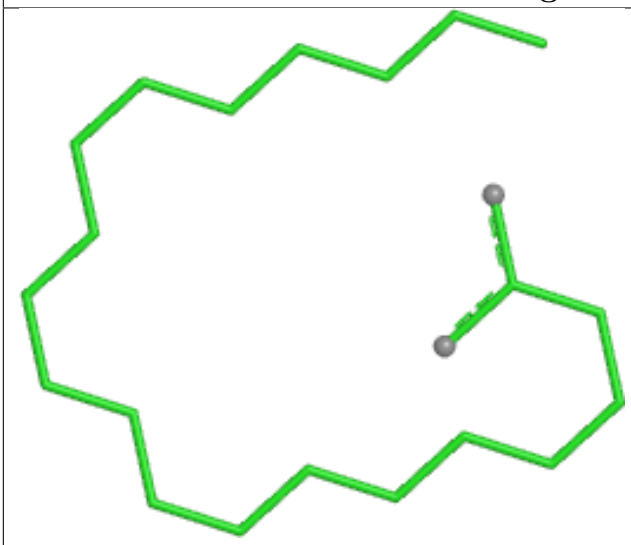


Torsions

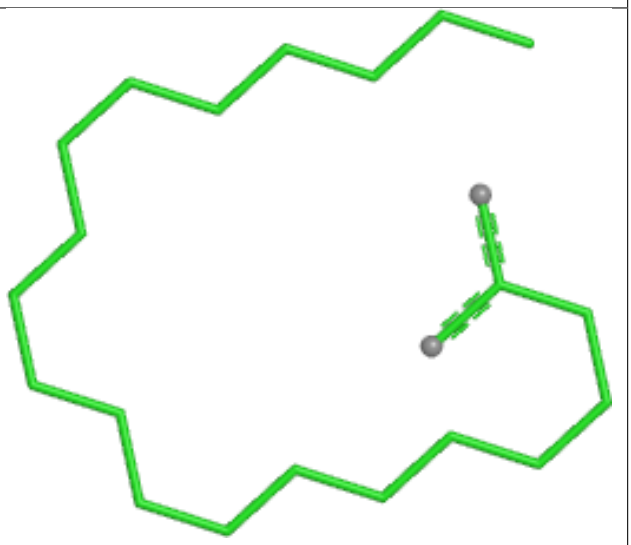


Rings

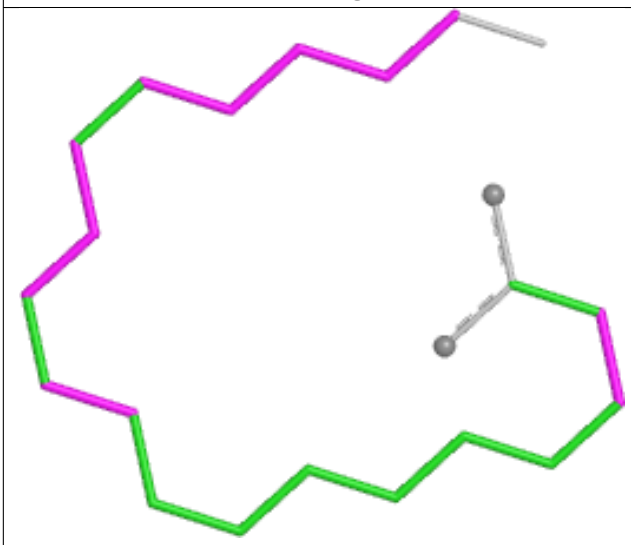
Ligand ACD B 1



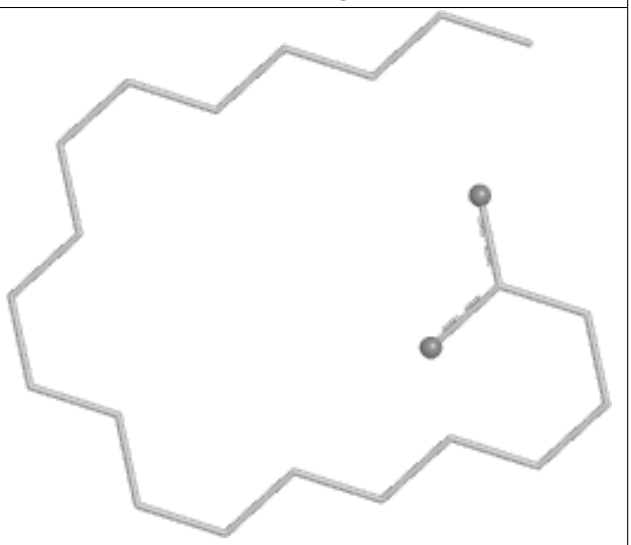
Bond lengths



Bond angles

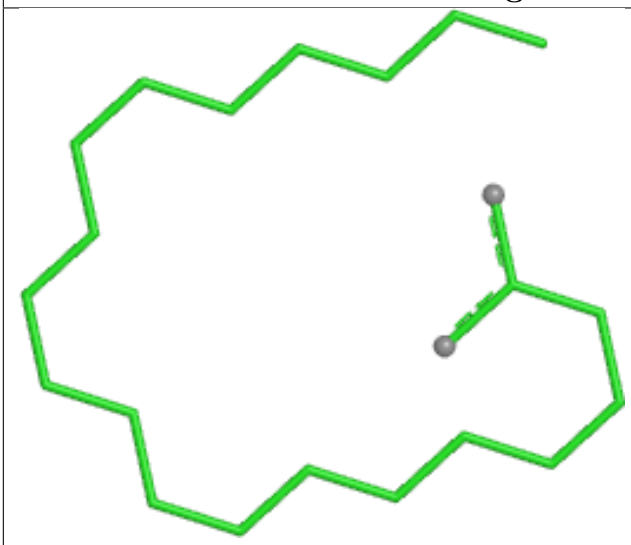


Torsions



Rings

Ligand ACD A 1 (A)



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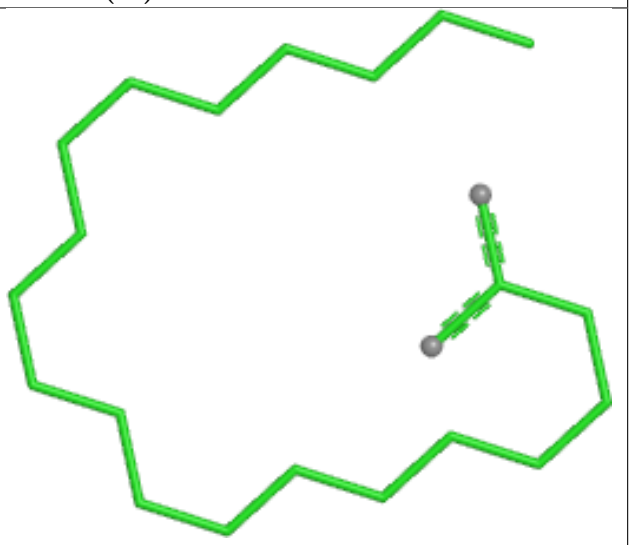
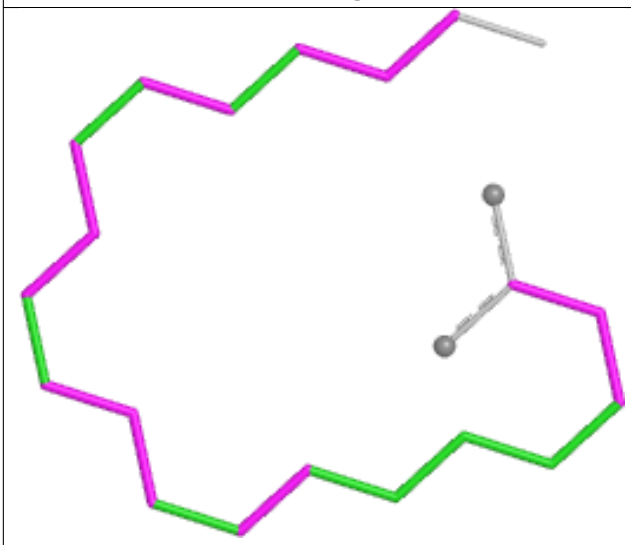


Bond angles



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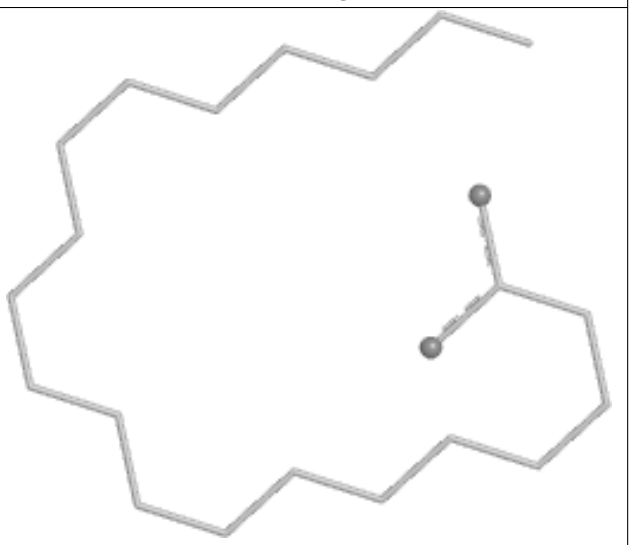
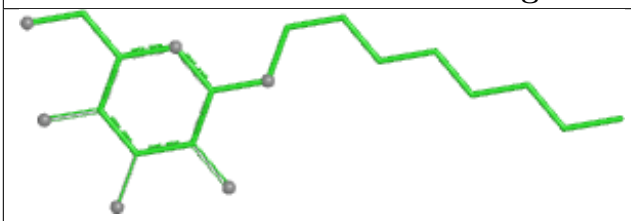


Rings

Ligand BOG B 703



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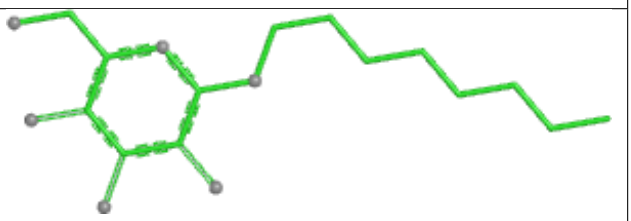
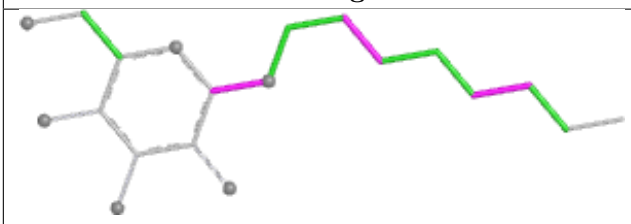


Bond angles



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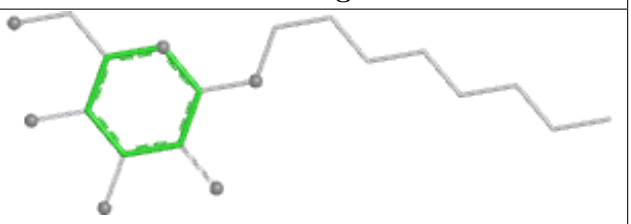


Rings

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	552/591 (93%)	-0.15	9 (1%)	70	73	15, 31, 50, 72	4 (0%)
1	B	551/591 (93%)	0.01	14 (2%)	58	61	15, 33, 57, 86	4 (0%)
All	All	1103/1182 (93%)	-0.07	23 (2%)	63	66	15, 32, 54, 86	8 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	TYR	3.4
1	B	82	LEU	3.1
1	B	115	TYR	3.1
1	A	121	SER	3.1
1	A	115	TYR	3.0
1	A	399	ASP	3.0
1	B	80	LEU	2.9
1	B	74	PHE	2.8
1	A	53	ASP	2.7
1	B	81	LEU	2.7
1	B	107	PHE	2.6
1	B	239	ASP	2.6
1	B	409	TYR	2.5
1	B	102	ILE	2.5
1	B	91	TYR	2.4
1	A	118	THR	2.4
1	A	282	ASN	2.3
1	A	239	ASP	2.3
1	B	105(A)	ILE	2.1
1	A	409	TYR	2.1
1	B	531	LEU	2.1
1	B	108	LEU	2.0
1	B	399	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

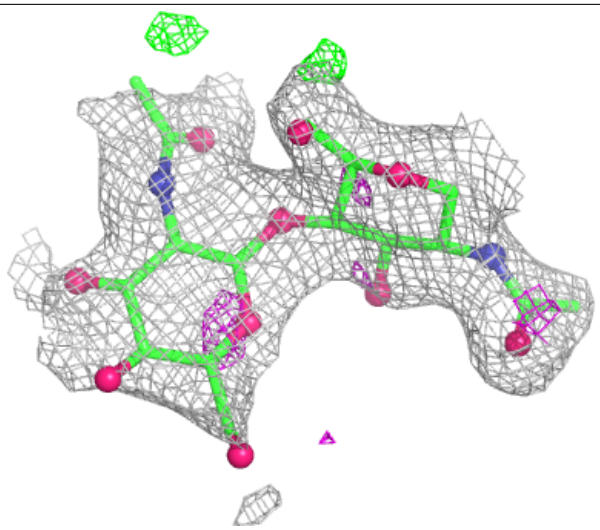
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

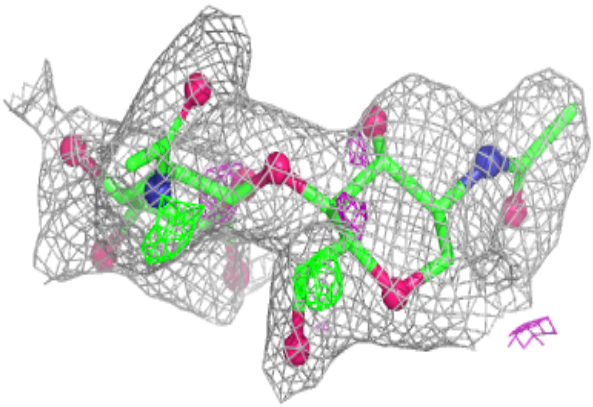
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	C	2	14/15	0.52	0.13	61,63,65,65	0
3	MAN	D	3	11/12	0.56	0.15	58,60,61,62	0
2	NAG	E	2	14/15	0.57	0.12	64,67,68,68	0
2	NAG	E	1	14/15	0.74	0.12	44,52,54,60	0
2	NAG	C	1	14/15	0.77	0.11	41,48,52,56	0
2	NAG	F	2	14/15	0.81	0.14	43,46,49,49	0
3	NAG	D	2	14/15	0.82	0.10	43,46,50,54	0
2	NAG	F	1	14/15	0.95	0.07	24,29,32,39	0
3	NAG	D	1	14/15	0.95	0.07	26,32,33,39	0

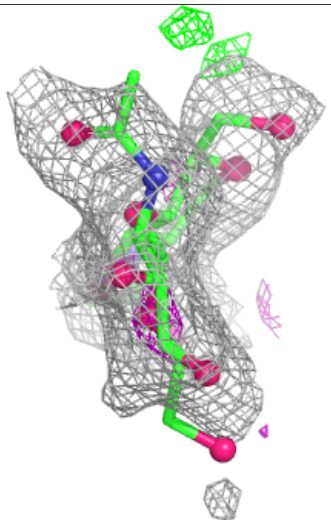
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

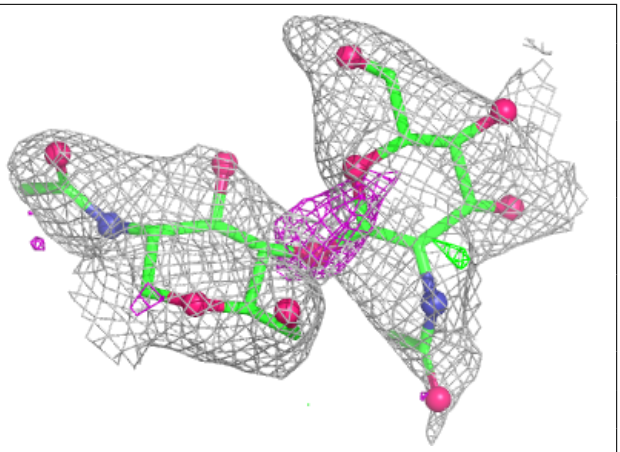


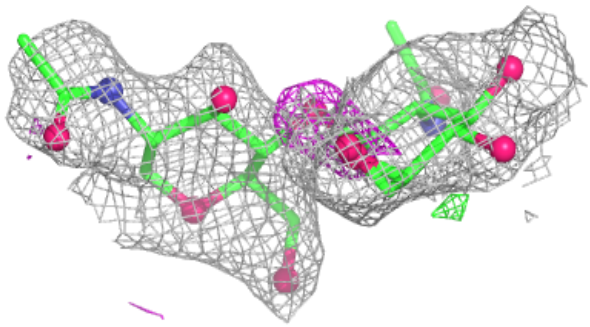


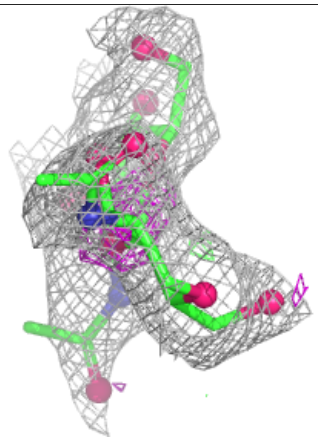


Electron density around Chain E:

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

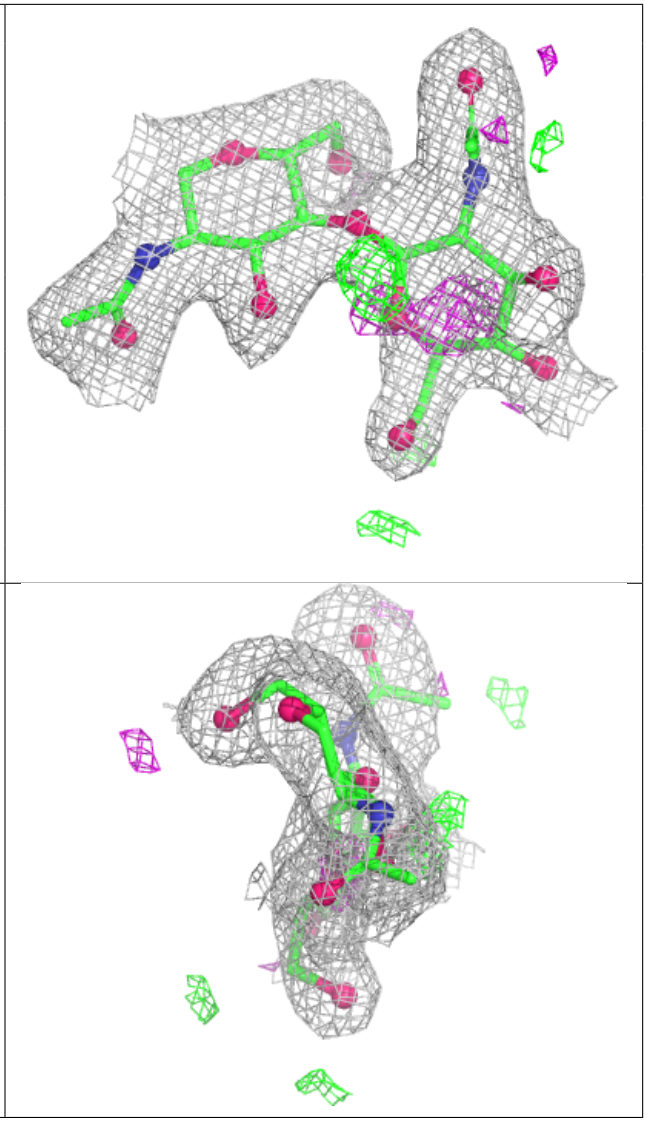






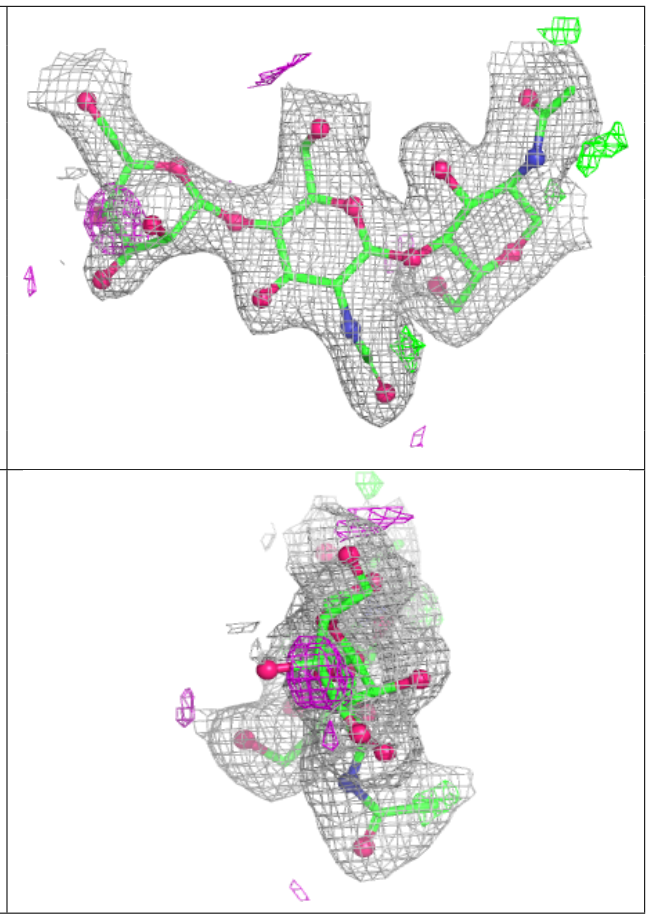
Electron density around Chain F:

$2mF_o$-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 D:

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



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	AKR	A	2	5/5	0.73	0.17	53,53,53,53	0
9	EDO	A	5	4/4	0.76	0.17	64,66,66,67	0
4	ACD	B	1	22/22	0.79	0.17	45,52,58,59	0
7	NAG	B	681	14/15	0.80	0.10	44,50,53,53	0
6	COH	A	619	43/43	0.80	0.18	74,77,82,83	0
9	EDO	B	7	4/4	0.80	0.18	67,67,67,68	0
5	AKR	A	3	5/5	0.82	0.14	51,51,51,51	0
9	EDO	A	620	4/4	0.82	0.16	41,41,42,42	0
9	EDO	B	2	4/4	0.83	0.17	49,50,50,51	0
6	COH	B	619	43/43	0.83	0.16	61,63,69,71	0
9	EDO	B	9	4/4	0.83	0.12	42,42,43,43	0
9	EDO	B	10	4/4	0.83	0.16	35,36,37,37	0

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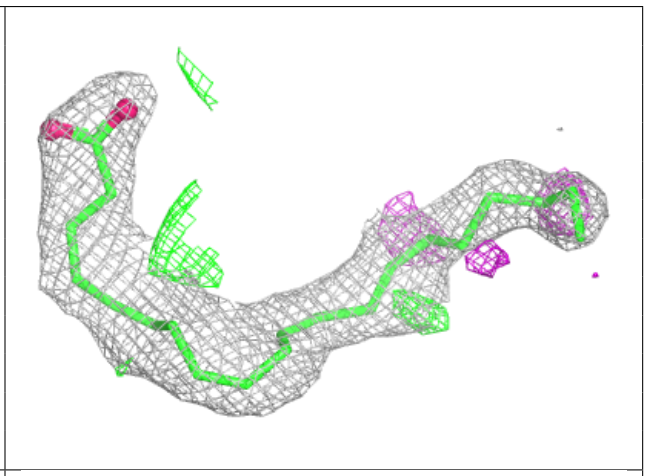
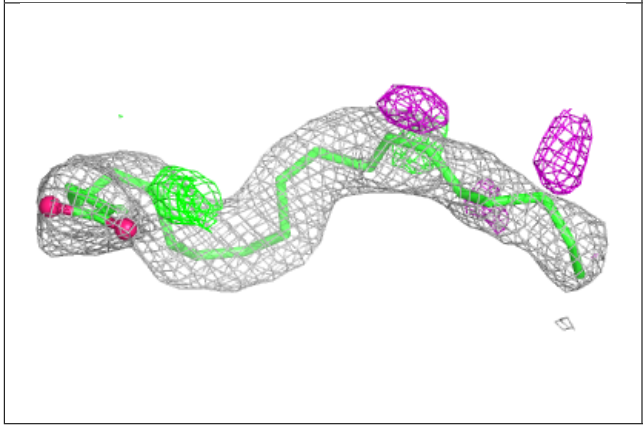
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	EDO	B	6	4/4	0.84	0.14	43,43,44,45	0
4	ACD	A	1[B]	22/22	0.86	0.12	50,51,53,53	22
4	ACD	A	1[A]	22/22	0.86	0.12	32,34,38,39	22
9	EDO	B	11	4/4	0.86	0.17	52,52,53,53	0
9	EDO	A	4	4/4	0.88	0.11	41,41,42,44	0
7	NAG	A	681	14/15	0.88	0.08	42,47,48,48	0
9	EDO	B	8	4/4	0.91	0.10	36,37,39,39	0
9	EDO	A	12	4/4	0.92	0.10	36,37,37,38	0
8	BOG	A	703	20/20	0.93	0.09	36,38,38,38	20
8	BOG	B	703	20/20	0.94	0.08	30,32,32,33	20
9	EDO	B	3	4/4	0.94	0.08	34,35,35,36	0

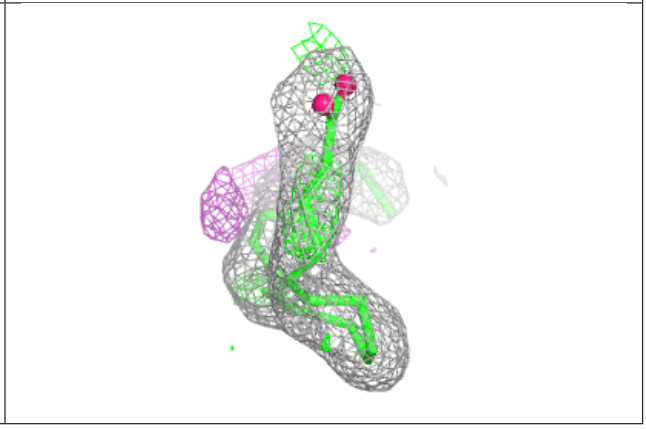
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACD 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)

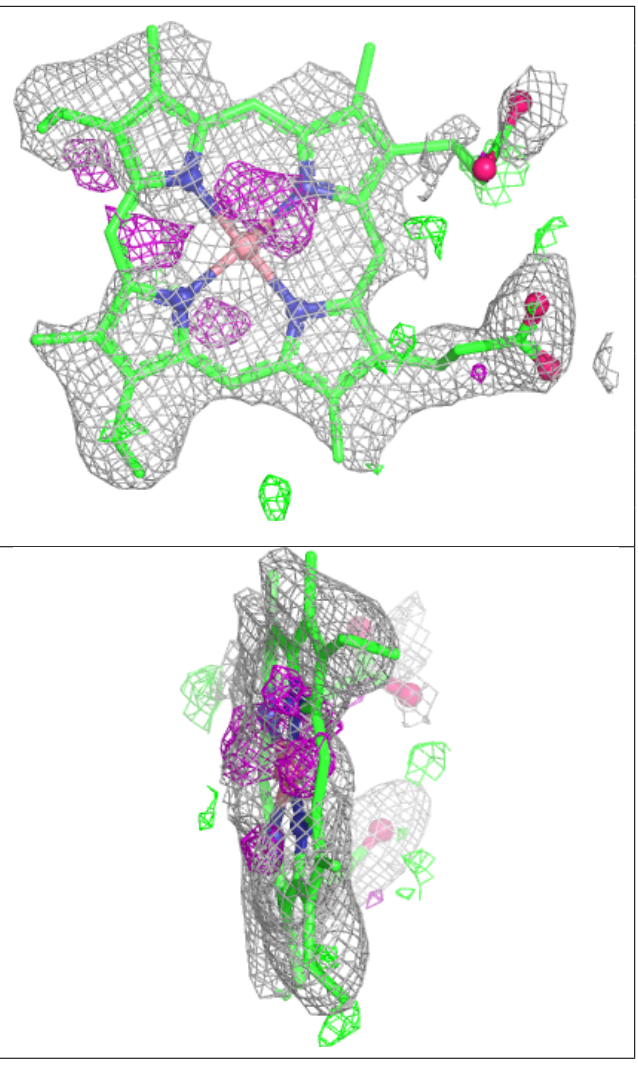






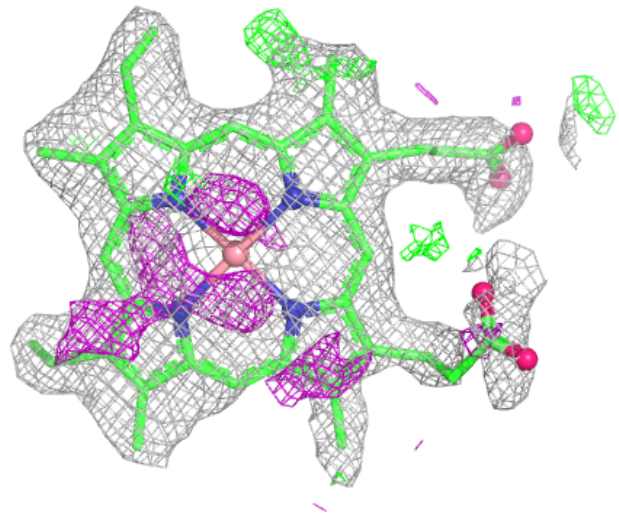
Electron density around COH A 619:

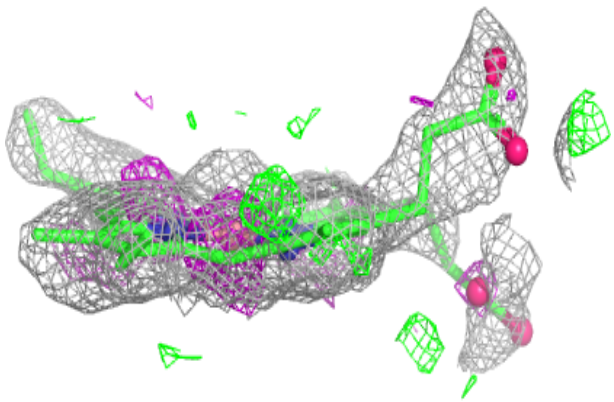
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

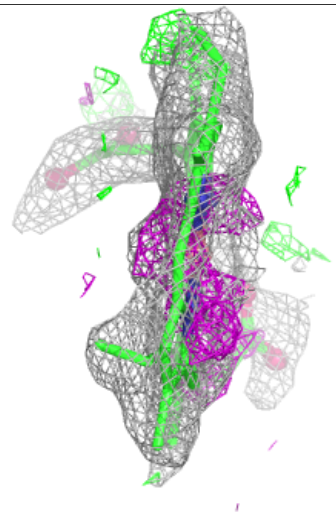


Electron density around COH B 619:

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

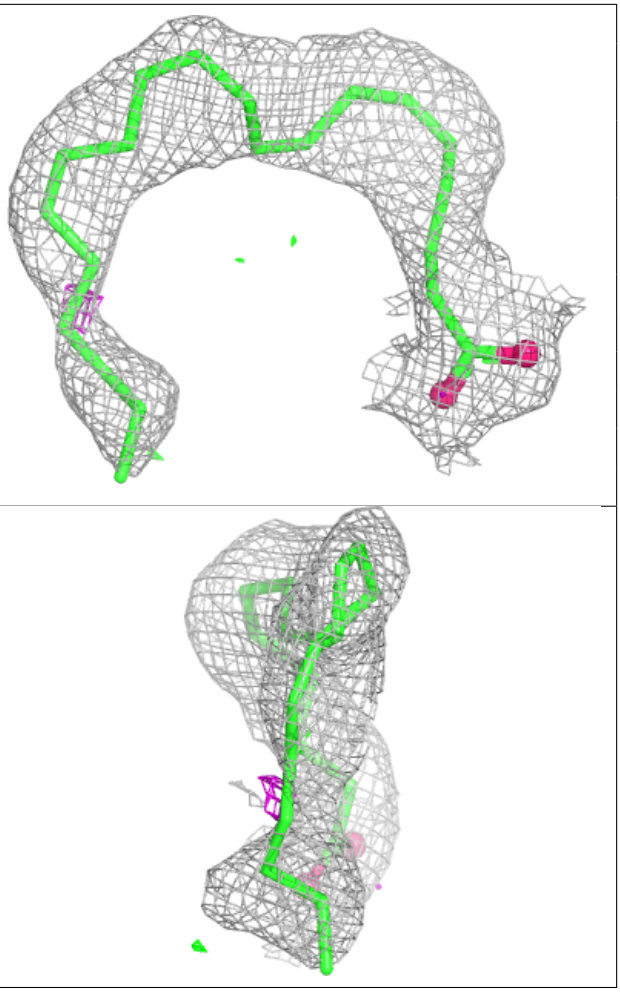


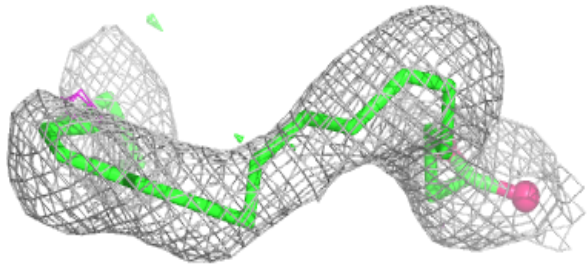




Electron density around ACD A 1 (B):

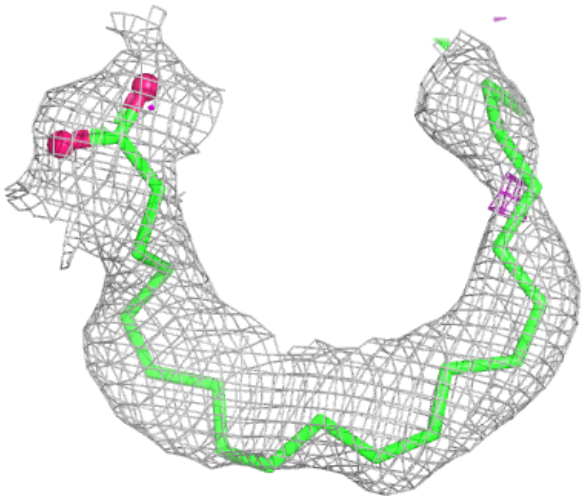
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

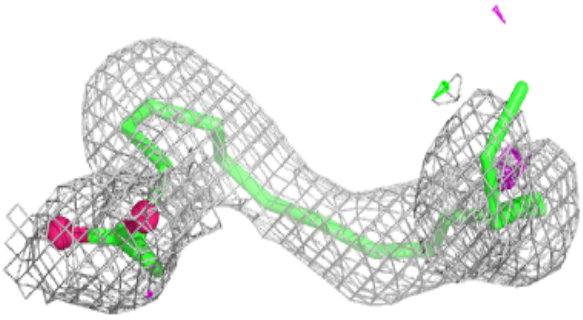


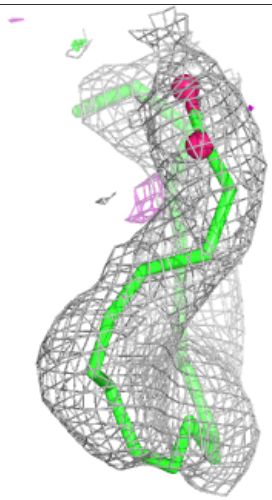


Electron density around ACD A 1 (A):

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

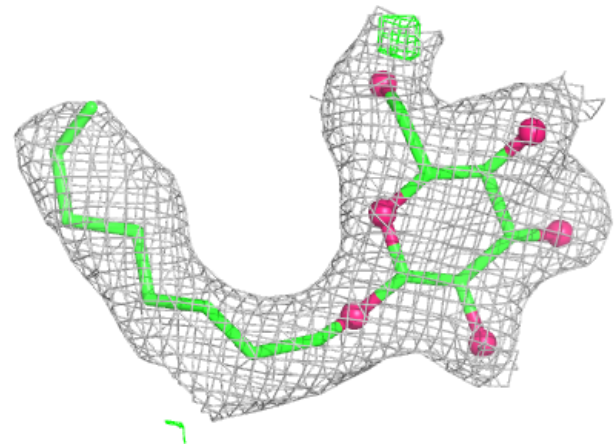


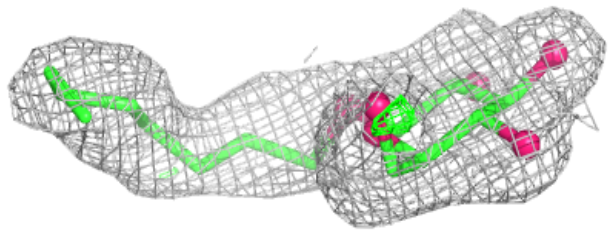


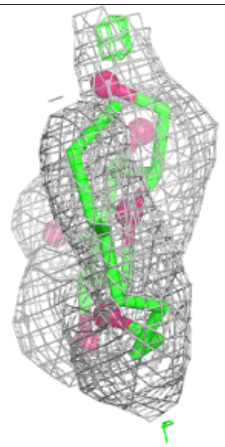


Electron density around BOG A 703:

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

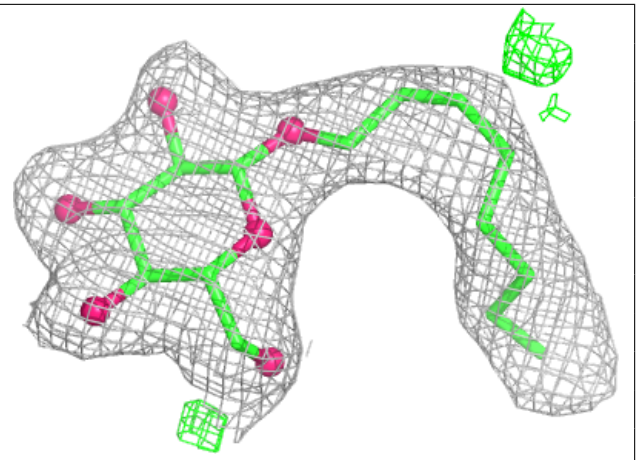


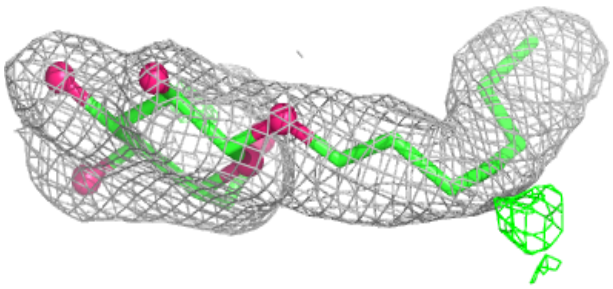


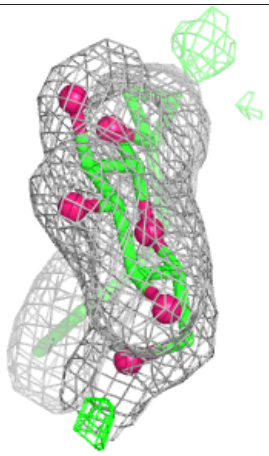


Electron density around BOG B 703:

$2mF_o$-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.