Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 11:43 AM BST

PDB ID	:	5IKR
Title	:	The Structure of Mefenamic Acid Bound to Human Cyclooxygenase-2
Authors	:	Orlando, B.J.; Malkowski, M.G.
Deposited on	:	2016-03-03
Resolution	:	2.34 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 ⓘ symbol.

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

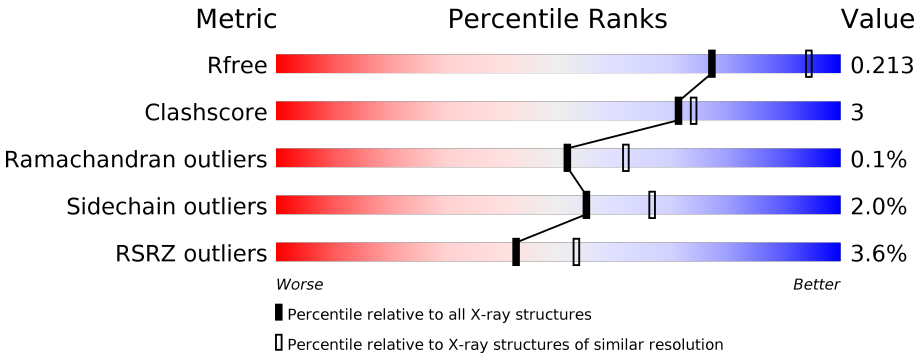
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.34 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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 on 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	551	2% 94% 5%
1	B	551	5% 93% 6%
2	C	3	33% 67%
2	D	3	33% 67%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	D	2	-	-	X	-
6	BOG	A	609	-	-	-	X

2 Entry composition

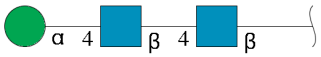
There are 8 unique types of molecules in this entry. The entry contains 18781 atoms, of which 9037 are hydrogens and 0 are deuteriums.

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.

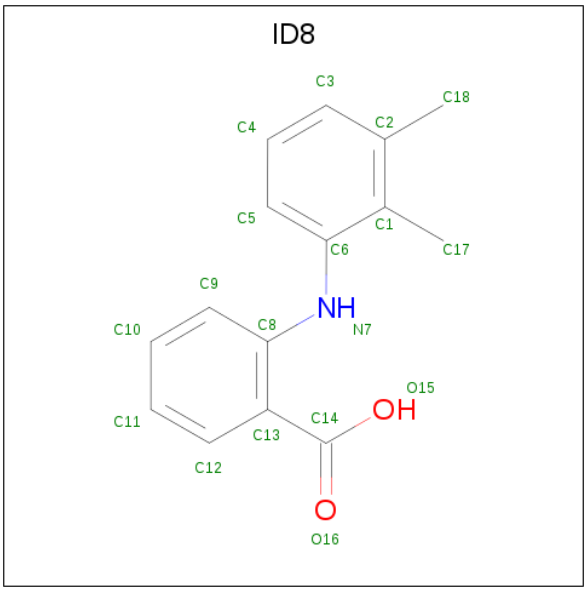
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	551	Total	C	H	N	O	S	77	0	0
			8825	2883	4355	755	806	26			
1	B	551	Total	C	H	N	O	S	243	0	0
			8826	2883	4356	755	806	26			

- Molecule 2 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.



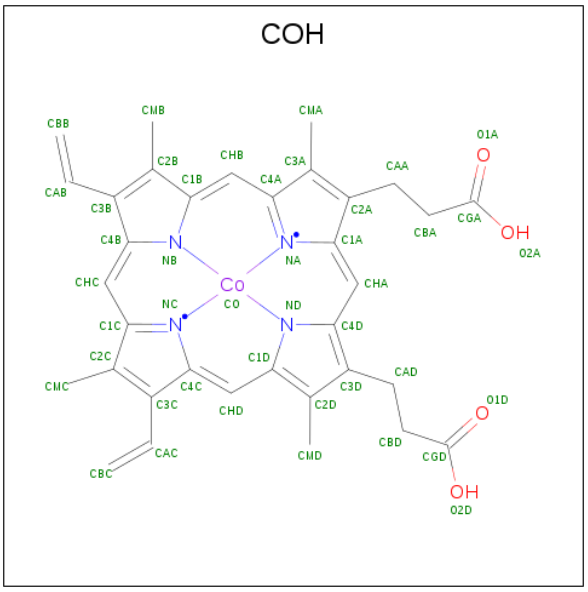
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	3	Total	C	H	N	O	0	0	0
			78	22	39	2	15			
2	D	3	Total	C	H	N	O	0	0	0
			78	22	39	2	15			

- Molecule 3 is 2-[(2,3-DIMETHYLPHENYL)AMINO]BENZOIC ACID (three-letter code: ID8) (formula: $C_{15}H_{15}NO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			32	15	14	1	2		
3	B	1	Total	C	H	N	O	0	0
			32	15	14	1	2		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING CO (three-letter code: COH) (formula: $C_{34}H_{32}CoN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Co	H	N	O	0	0
			73	34	1	30	4	4		

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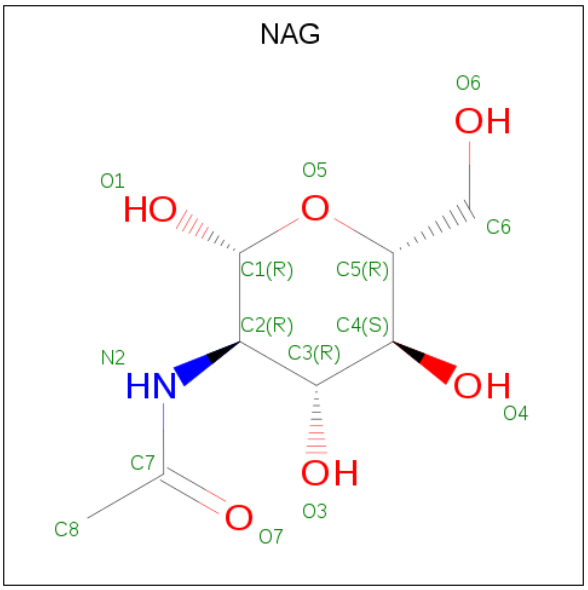
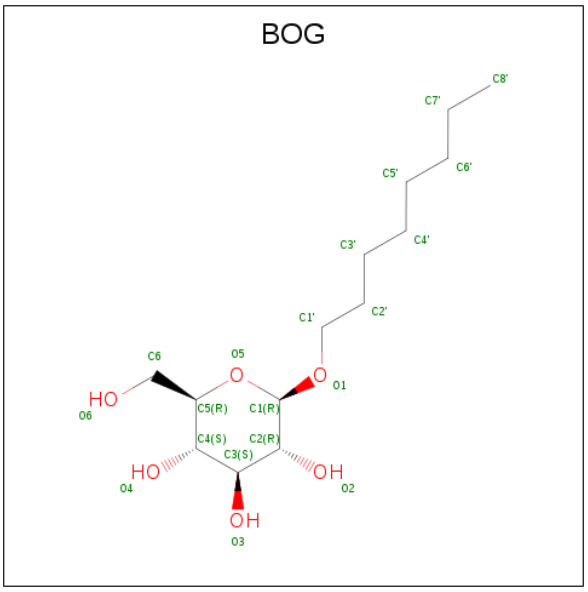
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	Co	H	N	O	0	0
			73	34	1	30	4	4		

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



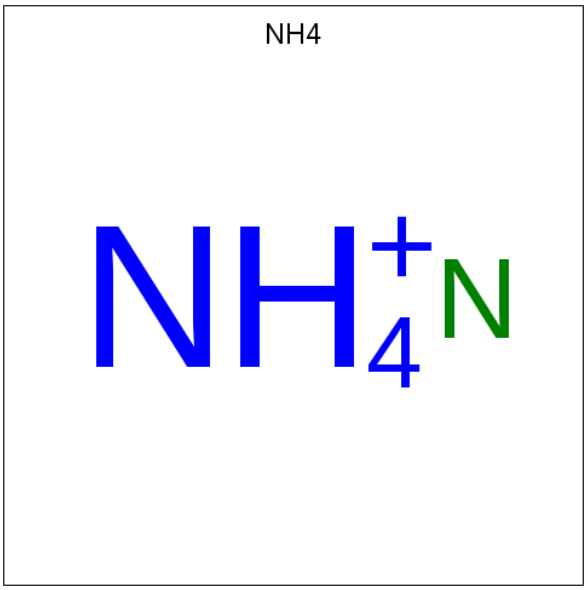
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O		0	0
			28	8	14	1	5			
5	B	1	Total	C	H	N	O		0	0
			28	8	14	1	5			

- Molecule 6 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			48	14	28	6		
6	A	1	Total	C	H	O	0	0
			48	14	28	6		
6	A	1	Total	C	H	O	0	0
			48	14	28	6		
6	B	1	Total	C	H	O	0	0
			48	14	28	6		

- Molecule 7 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total H N 5 4 1	0	0
7	A	1	Total H N 5 4 1	0	0
7	A	1	Total H N 5 4 1	0	0
7	B	1	Total H N 5 4 1	0	0
7	B	1	Total H N 5 4 1	0	0

- Molecule 8 is water.

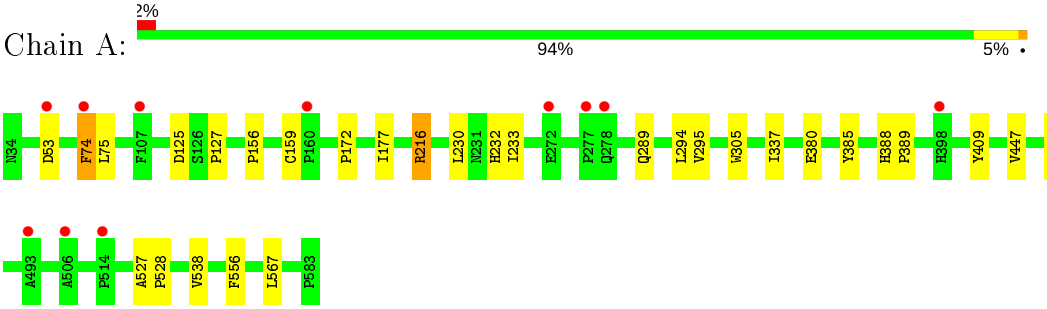
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	285	Total O 285 285	0	0
8	B	206	Total O 206 206	0	0

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.

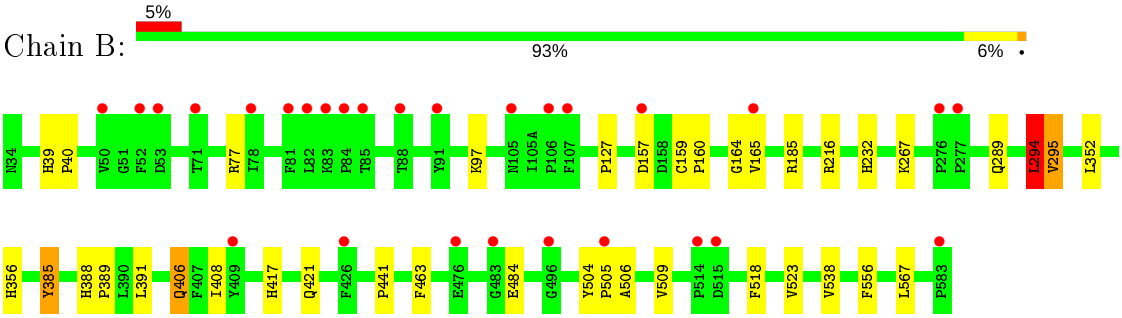
• Molecule 1: Prostaglandin G/H synthase 2

Chain A:



• Molecule 1: Prostaglandin G/H synthase 2

Chain B:



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

Chain C:

• Molecule 2: 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	127.67Å 149.69Å 188.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.34 19.99 – 2.34	Depositor EDS
% Data completeness (in resolution range)	95.4 (20.00-2.34) 95.4 (19.99-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.21 (at 2.35Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.185 , 0.211 0.190 , 0.213	Depositor DCC
R_{free} test set	3580 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 53.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18781	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: NAG, ID8, NH4, COH, MAN, BOG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.25	0/4602	0.40	0/6241
1	B	0.30	0/4602	0.41	1/6241 (0.0%)
All	All	0.28	0/9204	0.40	1/12482 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	294	LEU	CA-CB-CG	5.07	126.96	115.30

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	4470	4355	4353	20	0
1	B	4470	4356	4353	33	0
2	C	39	39	34	5	0
2	D	39	39	34	7	0
3	A	18	14	14	2	0
3	B	18	14	14	6	0
4	A	43	30	30	2	0
4	B	43	30	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	14	14	13	0	0
5	B	14	14	12	0	0
6	A	60	84	84	2	0
6	B	20	28	28	1	0
7	A	3	12	0	0	0
7	B	2	8	0	0	0
8	A	285	0	0	1	0
8	B	206	0	0	2	0
All	All	9744	9037	8999	62	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 3.

All (62) 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:216:ARG:HH11	2:D:2:NAG:H83	1.28	0.97
1:B:216:ARG:HH11	2:D:2:NAG:C8	1.83	0.90
1:B:216:ARG:NH1	2:D:2:NAG:H83	1.91	0.85
1:A:216:ARG:HD3	2:C:2:NAG:H81	1.63	0.80
1:A:216:ARG:HH11	2:C:2:NAG:H83	1.54	0.73
1:B:216:ARG:NH2	8:B:701:HOH:O	2.13	0.70
1:B:216:ARG:HD3	2:D:2:NAG:H81	1.77	0.67
4:B:603:COH:HHC	4:B:603:COH:HBB1	1.78	0.65
4:A:602:COH:HBB1	4:A:602:COH:HHC	1.79	0.64
1:B:185:ARG:NH1	8:B:704:HOH:O	2.34	0.59
1:B:160:PRO:HG2	1:B:165:VAL:HA	1.85	0.59
4:B:603:COH:HMC1	4:B:603:COH:HBC1	1.86	0.58
4:A:602:COH:HMC1	4:A:602:COH:HBC1	1.86	0.57
1:B:160:PRO:CG	1:B:165:VAL:HG12	2.35	0.56
1:B:216:ARG:HD3	2:D:2:NAG:C8	2.38	0.53
1:B:388:HIS:N	1:B:389:PRO:HD2	2.25	0.51
1:B:159:CYS:HB3	1:B:164:GLY:O	2.11	0.49
3:B:602:ID8:C5	3:B:602:ID8:H9	2.43	0.49
1:A:216:ARG:HH11	2:C:2:NAG:C8	2.26	0.48
1:B:523:VAL:HG13	3:B:602:ID8:C4	2.43	0.48
1:B:294:LEU:HD22	1:B:408:ILE:HG23	1.96	0.48
1:B:216:ARG:HH11	2:D:2:NAG:H81	1.76	0.48
1:B:391:LEU:HB2	1:B:441:PRO:HG2	1.95	0.47
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.96	0.47
1:A:216:ARG:CD	2:C:2:NAG:H81	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ASP:OD1	1:A:53:ASP:N	2.48	0.47
1:B:160:PRO:HG2	1:B:165:VAL:HG12	1.96	0.46
1:B:160:PRO:HG3	1:B:165:VAL:HG12	1.97	0.45
3:A:601:ID8:H9	3:A:601:ID8:C5	2.46	0.45
1:A:125:ASP:OD2	8:A:701:HOH:O	2.21	0.45
1:B:352:LEU:HD11	1:B:518:PHE:CE2	2.52	0.44
4:B:603:COH:HMA2	4:B:603:COH:HBA2	2.00	0.44
1:B:216:ARG:NH1	2:D:2:NAG:C8	2.63	0.44
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.99	0.44
1:A:567:LEU:HA	6:A:609:BOG:H8'1	1.98	0.44
1:B:417:HIS:HB3	1:B:421:GLN:HG2	2.01	0.43
1:A:294:LEU:HA	1:A:409:TYR:CE1	2.53	0.43
1:B:506:ALA:HA	1:B:509:VAL:HG22	2.01	0.43
1:B:567:LEU:HA	6:B:601:BOG:H8'1	2.00	0.43
1:A:388:HIS:CE1	1:A:447:VAL:HG11	2.53	0.43
1:B:39:HIS:N	1:B:40:PRO:HD3	2.33	0.43
6:A:609:BOG:H1	6:A:609:BOG:H2'1	1.91	0.43
1:B:523:VAL:HG13	3:B:602:ID8:H4	2.01	0.43
1:A:388:HIS:N	1:A:389:PRO:CD	2.82	0.42
1:A:484:GLU:HG2	1:A:485:LYS:H	1.84	0.42
3:B:602:ID8:C9	3:B:602:ID8:C5	2.96	0.42
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.55	0.42
3:B:602:ID8:C9	3:B:602:ID8:H5	2.50	0.42
1:B:463:PHE:CD1	1:B:506:ALA:HB3	2.56	0.41
1:A:216:ARG:HD3	2:C:2:NAG:C8	2.41	0.41
1:A:127:PRO:HB2	1:B:538:VAL:HG23	2.03	0.41
1:B:294:LEU:HD13	1:B:295:VAL:HG13	2.02	0.41
1:A:538:VAL:HG23	1:B:127:PRO:HG2	2.02	0.41
1:B:160:PRO:HG2	1:B:164:GLY:O	2.21	0.41
1:B:97:LYS:HG3	1:B:356:HIS:CE1	2.56	0.41
1:B:406:GLN:HE21	1:B:406:GLN:HB3	1.77	0.41
1:A:230:LEU:HG	1:A:337:ILE:HG12	2.03	0.41
1:A:156:PRO:HG2	1:A:159:CYS:SG	2.61	0.40
1:A:172:PRO:HG2	1:A:177:ILE:HD11	2.03	0.40
1:A:233:ILE:HD13	1:A:305:TRP:HB3	2.04	0.40
3:A:601:ID8:C9	3:A:601:ID8:C5	2.96	0.40
1:B:385:TYR:CE1	3:B:602:ID8:H12	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	549/551 (100%)	533 (97%)	15 (3%)	1 (0%)	47 55
1	B	549/551 (100%)	530 (96%)	19 (4%)	0	100 100
All	All	1098/1102 (100%)	1063 (97%)	34 (3%)	1 (0%)	51 62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	PHE

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	490/490 (100%)	481 (98%)	9 (2%)	59 70
1	B	490/490 (100%)	479 (98%)	11 (2%)	52 63
All	All	980/980 (100%)	960 (98%)	20 (2%)	55 66

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	PHE
1	A	75	LEU
1	A	216	ARG
1	A	232	HIS
1	A	289	GLN

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Mol	Chain	Res	Type
1	A	295	VAL
1	A	385	TYR
1	A	484	GLU
1	A	556	PHE
1	B	77	ARG
1	B	157	ASP
1	B	232	HIS
1	B	267	LYS
1	B	289	GLN
1	B	294	LEU
1	B	295	VAL
1	B	385	TYR
1	B	406	GLN
1	B	484	GLU
1	B	556	PHE

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	1,2	14,14,15	0.34	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	C	2	2	14,14,15	0.35	0	17,19,21	0.61	0
2	MAN	C	3	2	11,11,12	0.99	1 (9%)	15,15,17	1.56	2 (13%)
2	NAG	D	1	1,2	14,14,15	0.29	0	17,19,21	0.51	0
2	NAG	D	2	2	14,14,15	0.29	0	17,19,21	0.57	0
2	MAN	D	3	2	11,11,12	0.97	1 (9%)	15,15,17	1.43	2 (13%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	MAN	C1-C2	2.61	1.58	1.52
2	D	3	MAN	C1-C2	2.31	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	MAN	C1-O5-C5	4.21	117.90	112.19
2	D	3	MAN	C1-O5-C5	3.90	117.47	112.19
2	C	3	MAN	O2-C2-C3	-3.24	103.65	110.14
2	D	3	MAN	O2-C2-C3	-3.01	104.10	110.14

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2

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

All (2) ring outliers are listed below:

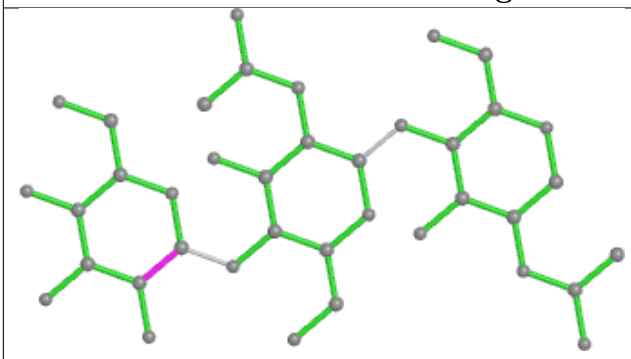
Mol	Chain	Res	Type	Atoms
2	C	3	MAN	C1-C2-C3-C4-C5-O5
2	D	3	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 12 short contacts:

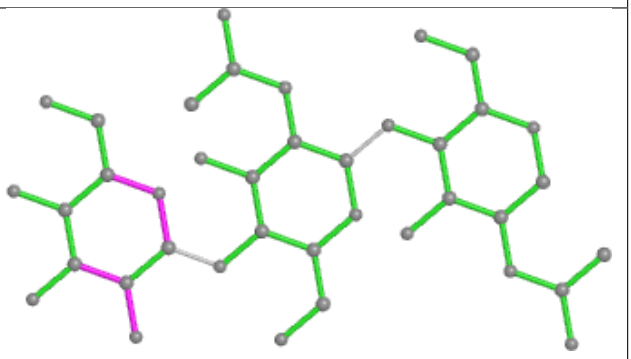
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	5	0
2	D	2	NAG	7	0

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

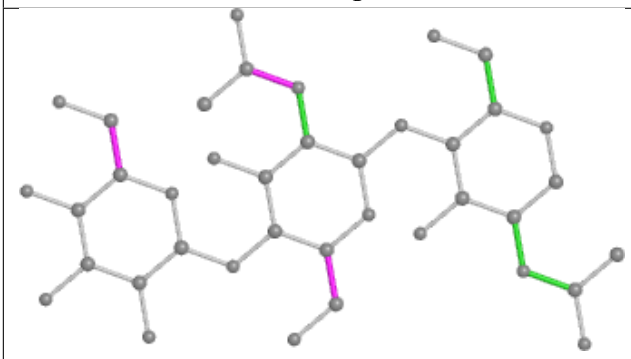
Oligosaccharide Chain C



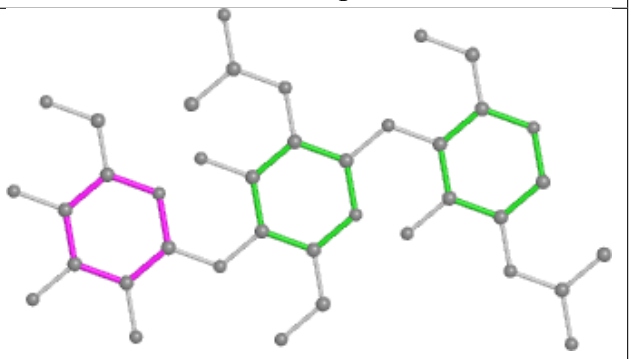
Bond lengths



Bond angles

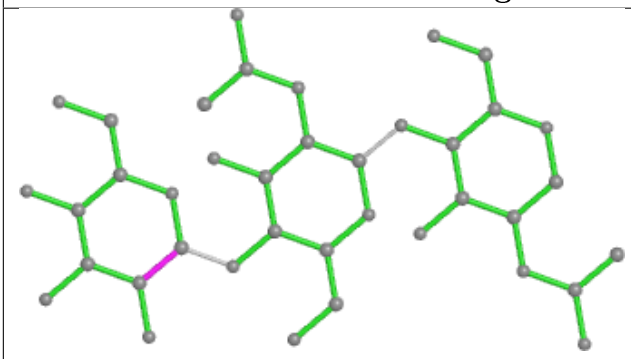


Torsions

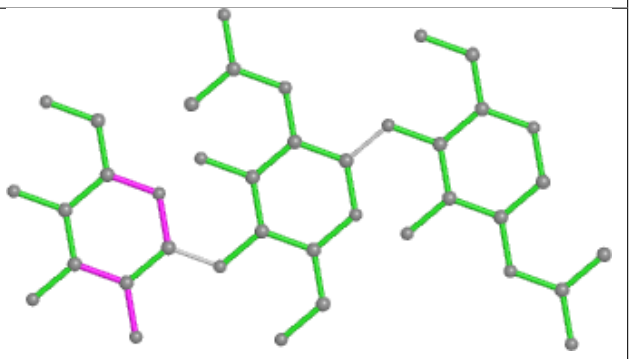


Rings

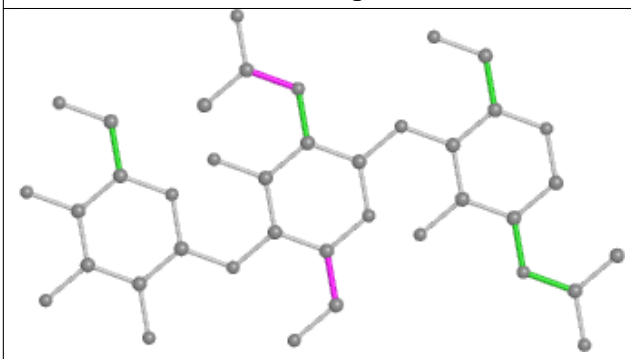
Oligosaccharide Chain D



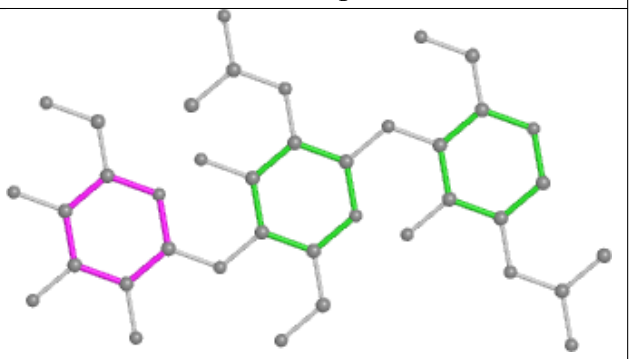
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 5 are modelled with single atom - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	BOG	A	609	-	20,20,20	1.15	2 (10%)	25,25,25	1.05	1 (4%)
3	ID8	B	602	-	17,19,19	1.81	3 (17%)	22,26,26	1.44	2 (9%)
4	COH	A	602	1	31,50,50	5.46	23 (74%)	23,82,82	4.67	7 (30%)
6	BOG	A	608	-	20,20,20	1.19	1 (5%)	25,25,25	0.78	0
5	NAG	B	607	1	14,14,15	0.20	0	17,19,21	0.44	0
5	NAG	A	606	1	14,14,15	0.21	0	17,19,21	0.48	0
3	ID8	A	601	-	17,19,19	1.98	5 (29%)	22,26,26	1.10	2 (9%)
6	BOG	A	607	-	20,20,20	1.18	2 (10%)	25,25,25	0.82	0
4	COH	B	603	1	31,50,50	5.46	23 (74%)	23,82,82	4.45	5 (21%)
6	BOG	B	601	-	20,20,20	1.16	1 (5%)	25,25,25	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BOG	A	609	-	-	6/11/31/31	0/1/1/1
3	ID8	B	602	-	-	0/4/8/8	0/2/2/2
4	COH	A	602	1	-	2/8/94/94	-
6	BOG	A	608	-	-	3/11/31/31	0/1/1/1
5	NAG	B	607	1	-	0/6/23/26	0/1/1/1
5	NAG	A	606	1	-	0/6/23/26	0/1/1/1
3	ID8	A	601	-	-	0/4/8/8	0/2/2/2
6	BOG	A	607	-	-	5/11/31/31	0/1/1/1
4	COH	B	603	1	-	3/8/94/94	-
6	BOG	B	601	-	-	5/11/31/31	0/1/1/1

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	COH	C4D-ND	10.26	1.39	1.34
4	A	602	COH	C4D-ND	9.93	1.39	1.34
4	B	603	COH	C1D-ND	9.69	1.39	1.34
4	A	602	COH	C1D-ND	9.43	1.39	1.34
4	A	602	COH	CHA-C1A	-8.95	1.37	1.53
4	A	602	COH	C4B-NB	8.73	1.39	1.34
4	B	603	COH	CHA-C1A	-8.57	1.38	1.53
4	A	602	COH	CHB-C4A	-8.53	1.38	1.53
4	B	603	COH	CHB-C4A	-8.52	1.38	1.53
4	B	603	COH	CHC-C1C	-8.46	1.38	1.53
4	B	603	COH	CHD-C4C	-8.43	1.38	1.53
4	A	602	COH	CHD-C4C	-8.40	1.38	1.53
4	A	602	COH	CHC-C1C	-8.26	1.39	1.53
4	B	603	COH	C4B-NB	8.23	1.38	1.34
4	A	602	COH	C1B-NB	8.01	1.38	1.34
4	B	603	COH	C1B-NB	7.85	1.38	1.34
4	B	603	COH	C3D-C2D	5.71	1.54	1.37
4	A	602	COH	C3D-C2D	5.64	1.54	1.37
4	A	602	COH	C1D-C2D	5.45	1.45	1.38
4	A	602	COH	CHA-C4D	-5.44	1.37	1.51
4	B	603	COH	C1D-C2D	5.33	1.45	1.38
4	B	603	COH	C1B-C2B	5.31	1.45	1.38
4	A	602	COH	C1B-C2B	5.31	1.45	1.38
4	B	603	COH	C4D-C3D	5.21	1.45	1.38
4	B	603	COH	CHC-C4B	-5.19	1.38	1.51
4	B	603	COH	CHA-C4D	-5.17	1.38	1.51
4	B	603	COH	CHB-C1B	-5.12	1.38	1.51
4	A	602	COH	CHD-C1D	-5.12	1.38	1.51
4	A	602	COH	CHB-C1B	-5.10	1.38	1.51
4	A	602	COH	CHC-C4B	-5.10	1.38	1.51
4	B	603	COH	CHD-C1D	-5.05	1.38	1.51
4	A	602	COH	C4D-C3D	5.03	1.45	1.38
3	B	602	ID8	C13-C14	4.62	1.51	1.47
4	A	602	COH	C3B-C2B	-4.11	1.34	1.40
4	B	603	COH	C3B-C2B	-4.01	1.34	1.40
4	B	603	COH	C3B-CAB	4.00	1.56	1.47
4	A	602	COH	C3B-CAB	3.86	1.55	1.47
4	A	602	COH	C4C-C3C	-3.49	1.45	1.51
4	B	603	COH	C4C-C3C	-3.36	1.45	1.51
3	A	601	ID8	C13-C14	3.29	1.50	1.47
4	B	603	COH	CAA-C2A	3.20	1.55	1.51
4	B	603	COH	CMC-C2C	3.03	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	COH	CMC-C2C	2.96	1.55	1.50
6	A	608	BOG	O5-C1	2.96	1.49	1.41
6	A	607	BOG	O5-C1	2.91	1.49	1.41
4	B	603	COH	CMA-C3A	2.87	1.55	1.50
6	B	601	BOG	O5-C1	2.78	1.48	1.41
4	A	602	COH	CAA-C2A	2.75	1.55	1.51
6	A	609	BOG	O5-C1	2.68	1.48	1.41
4	A	602	COH	CMA-C3A	2.62	1.54	1.50
4	A	602	COH	CAD-C3D	2.60	1.55	1.52
3	A	601	ID8	C9-C8	-2.56	1.35	1.39
4	B	603	COH	CAD-C3D	2.53	1.55	1.52
3	A	601	ID8	C8-N7	-2.42	1.33	1.39
3	A	601	ID8	C6-N7	-2.35	1.33	1.39
3	A	601	ID8	C3-C2	-2.14	1.35	1.39
3	B	602	ID8	C8-N7	-2.10	1.34	1.39
6	A	607	BOG	O2-C2	2.05	1.47	1.43
3	B	602	ID8	C6-N7	-2.01	1.34	1.39
6	A	609	BOG	O2-C2	2.01	1.47	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	602	COH	CHA-C1A-NA	11.24	126.67	110.12
4	A	602	COH	CHC-C1C-NC	11.01	126.33	110.12
4	B	603	COH	CHC-C1C-NC	10.93	126.21	110.12
4	B	603	COH	CHA-C1A-NA	10.60	125.72	110.12
4	A	602	COH	CHD-C4C-NC	10.57	125.68	110.12
4	A	602	COH	CHB-C4A-NA	10.25	125.20	110.12
4	B	603	COH	CHB-C4A-NA	10.03	124.88	110.12
4	B	603	COH	CHD-C4C-NC	10.00	124.83	110.12
3	B	602	ID8	C12-C13-C14	-3.89	114.40	120.20
6	A	609	BOG	C1-O5-C5	-3.14	107.52	113.69
4	A	602	COH	CBA-CAA-C2A	-3.00	109.04	114.35
3	A	601	ID8	C12-C13-C14	-2.78	116.07	120.20
4	A	602	COH	C4B-C3B-C2B	2.16	107.73	104.41
3	B	602	ID8	C5-C6-C1	-2.11	118.24	121.22
3	A	601	ID8	C6-N7-C8	2.02	131.73	125.36
4	B	603	COH	C4B-C3B-C2B	2.02	107.50	104.41
4	A	602	COH	CBD-CAD-C3D	-2.01	108.77	112.49

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	609	BOG	C2'-C1'-O1-C1
6	A	608	BOG	C2'-C1'-O1-C1
4	B	603	COH	C3A-C2A-CAA-CBA
6	A	607	BOG	O5-C5-C6-O6
6	A	607	BOG	C4-C5-C6-O6
6	A	609	BOG	O5-C5-C6-O6
6	B	601	BOG	C4-C5-C6-O6
6	A	609	BOG	C4-C5-C6-O6
4	B	603	COH	C2A-CAA-CBA-CGA
6	B	601	BOG	O1-C1'-C2'-C3'
6	B	601	BOG	O5-C5-C6-O6
6	A	607	BOG	C4'-C5'-C6'-C7'
6	A	607	BOG	C2'-C1'-O1-C1
6	A	607	BOG	C3'-C4'-C5'-C6'
6	A	609	BOG	O1-C1'-C2'-C3'
6	B	601	BOG	C2'-C1'-O1-C1
4	A	602	COH	C1A-C2A-CAA-CBA
4	B	603	COH	C1A-C2A-CAA-CBA
6	A	609	BOG	C3'-C4'-C5'-C6'
6	B	601	BOG	C2'-C3'-C4'-C5'
6	A	609	BOG	C1'-C2'-C3'-C4'
4	A	602	COH	C3A-C2A-CAA-CBA
6	A	608	BOG	C3'-C4'-C5'-C6'
6	A	608	BOG	C5'-C6'-C7'-C8'

There are no ring outliers.

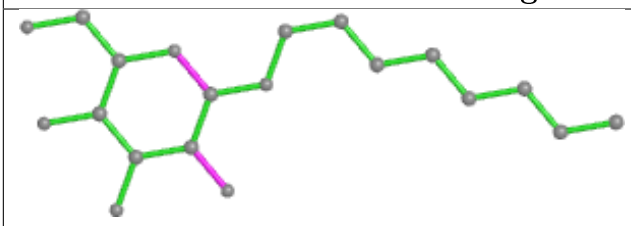
6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	609	BOG	2	0
3	B	602	ID8	6	0
4	A	602	COH	2	0
3	A	601	ID8	2	0
4	B	603	COH	3	0
6	B	601	BOG	1	0

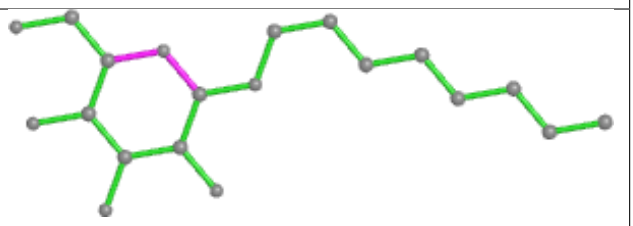
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

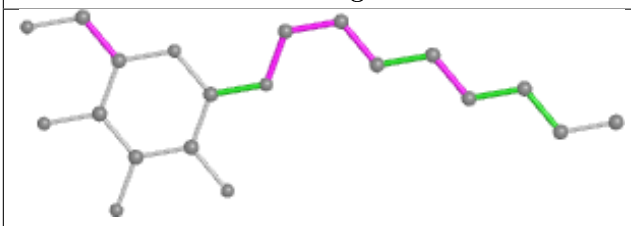
Ligand BOG A 609



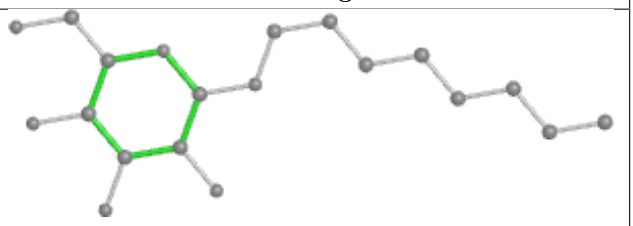
Bond lengths



Bond angles

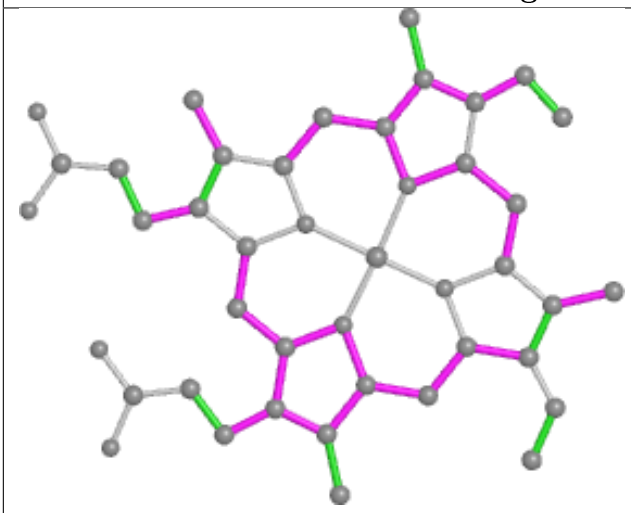


Torsions

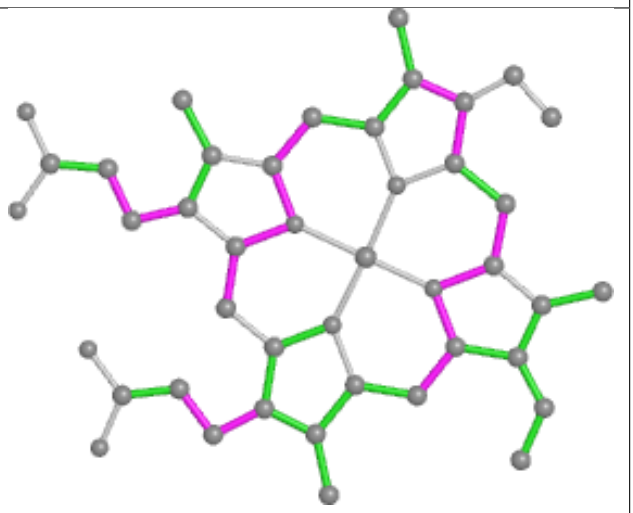


Rings

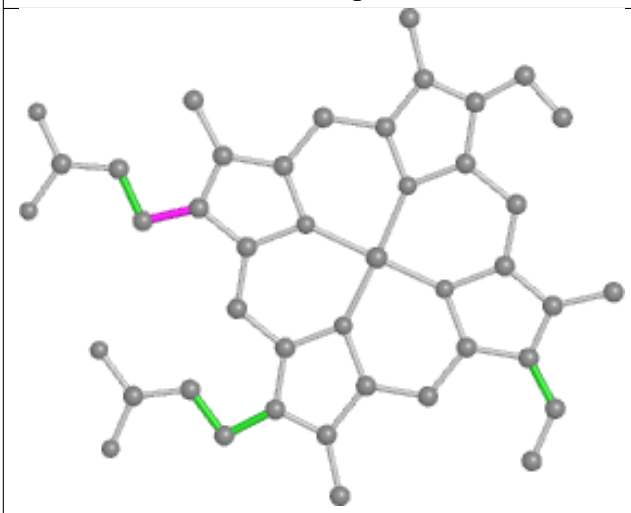
Ligand COH A 602



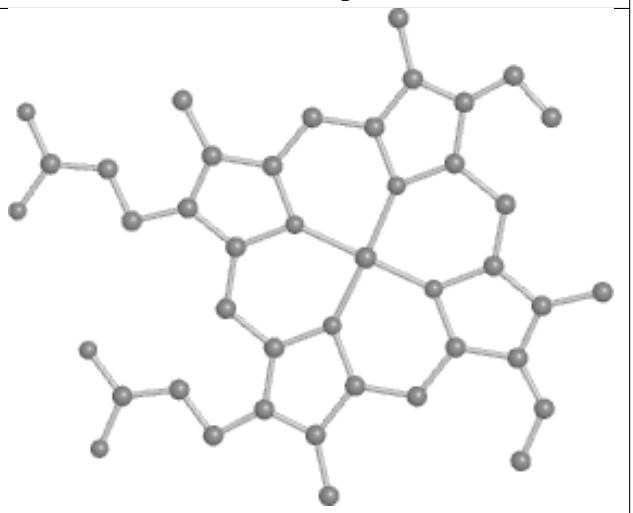
Bond lengths



Bond angles

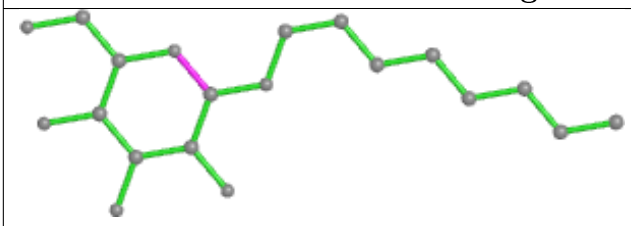


Torsions

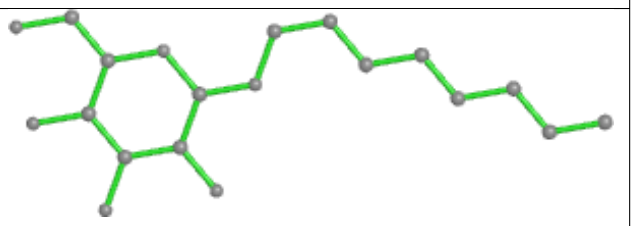


Rings

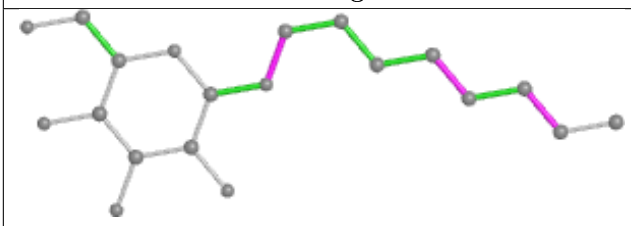
Ligand BOG A 608



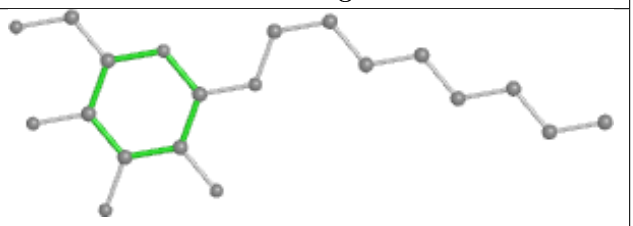
Bond lengths



Bond angles

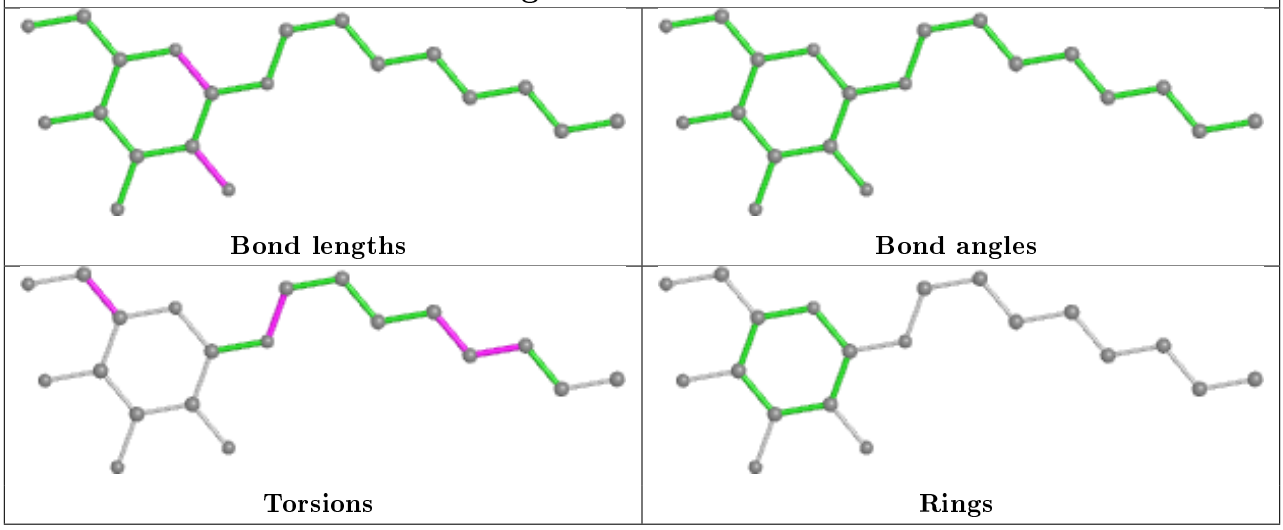


Torsions

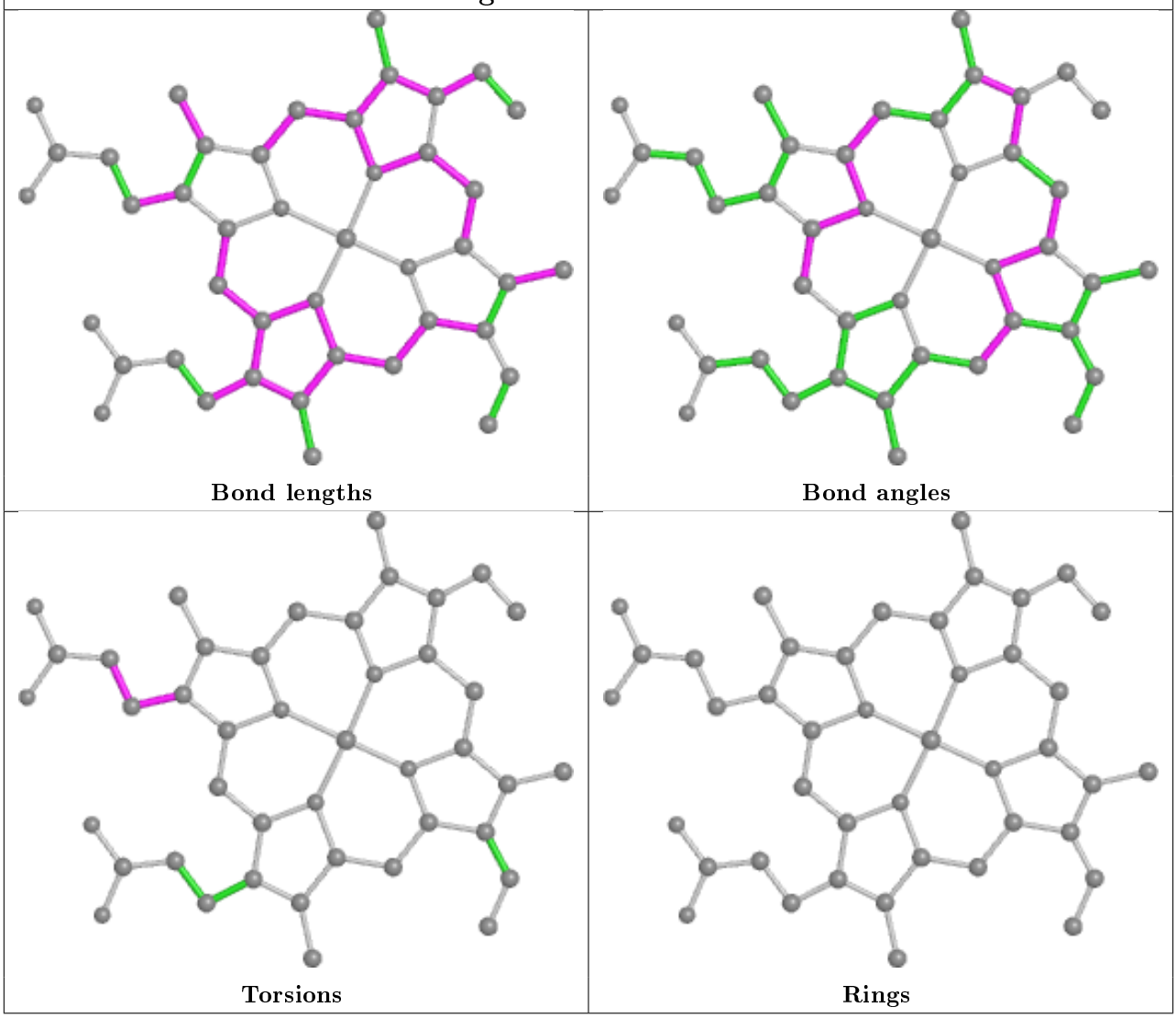


Rings

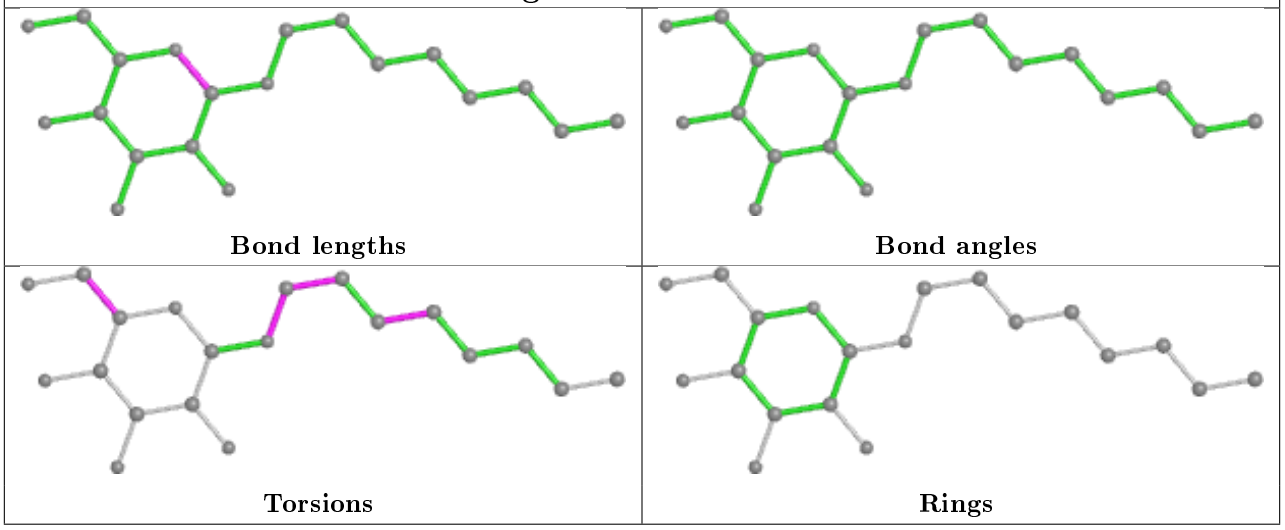
Ligand BOG A 607



Ligand COH B 603



Ligand BOG B 601



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	551/551 (100%)	-0.10	12 (2%)	62	71	14, 34, 58, 83	9 (1%)
1	B	551/551 (100%)	0.18	28 (5%)	28	39	18, 48, 78, 94	25 (4%)
All	All	1102/1102 (100%)	0.04	40 (3%)	42	53	14, 39, 73, 94	34 (3%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	483	GLY	4.3
1	B	107	PHE	4.2
1	A	74	PHE	4.1
1	B	82	LEU	3.9
1	B	496	GLY	3.5
1	B	514	PRO	3.4
1	B	84	PRO	3.1
1	B	277	PRO	3.1
1	B	81	PHE	3.1
1	B	157	ASP	2.9
1	B	85	THR	2.9
1	A	277	PRO	2.8
1	B	106	PRO	2.8
1	B	91	TYR	2.8
1	B	276	PRO	2.7
1	B	583	PRO	2.7
1	A	107	PHE	2.6
1	A	278	GLN	2.6
1	B	53	ASP	2.5
1	A	493	ALA	2.5
1	A	53	ASP	2.4
1	A	160	PRO	2.3
1	A	514	PRO	2.3
1	B	409	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	52	PHE	2.3
1	B	88	THR	2.3
1	B	426	PHE	2.3
1	B	50	VAL	2.2
1	B	165	VAL	2.2
1	B	505	PRO	2.2
1	A	485	LYS	2.1
1	A	506	ALA	2.1
1	B	71	THR	2.1
1	B	78	ILE	2.1
1	A	398	HIS	2.1
1	A	272	GLU	2.1
1	B	476	GLU	2.1
1	B	515	ASP	2.0
1	B	105	ASN	2.0
1	B	83	LYS	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)

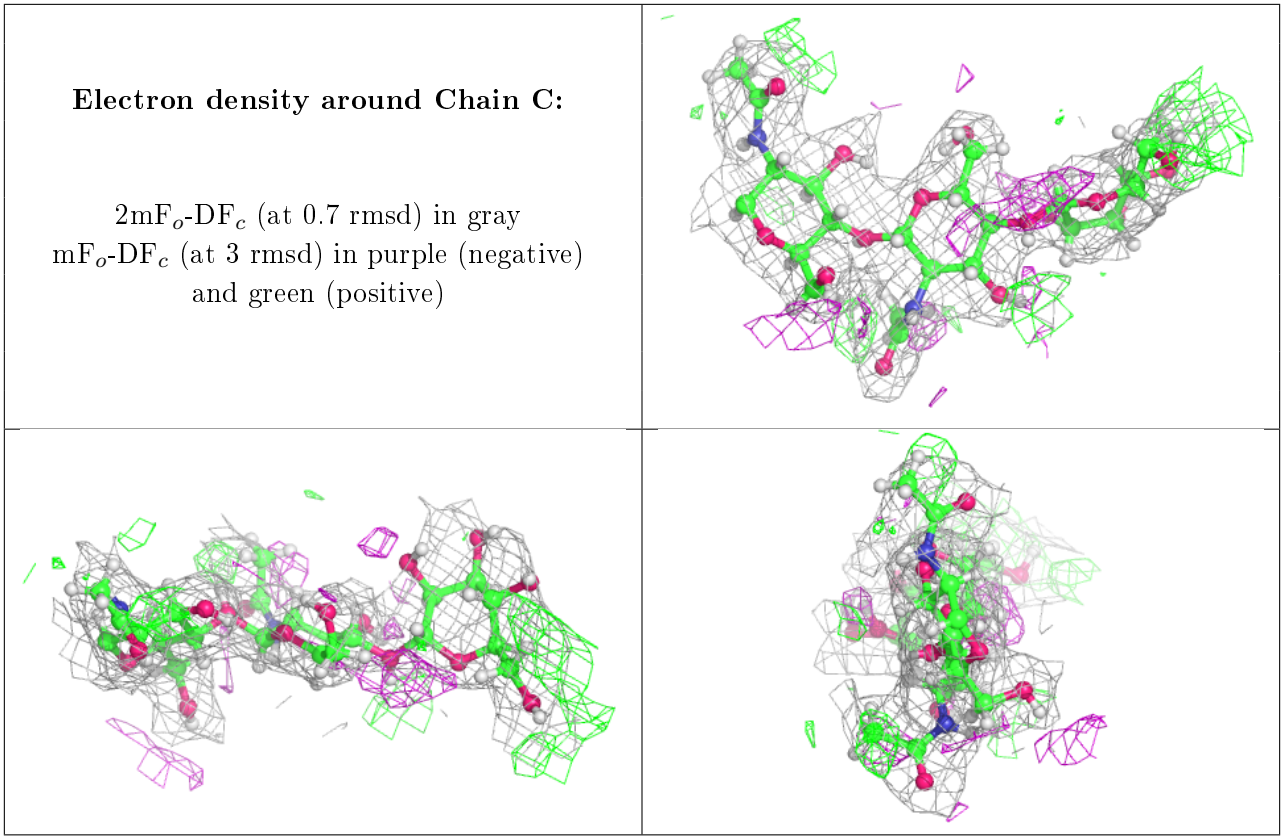
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

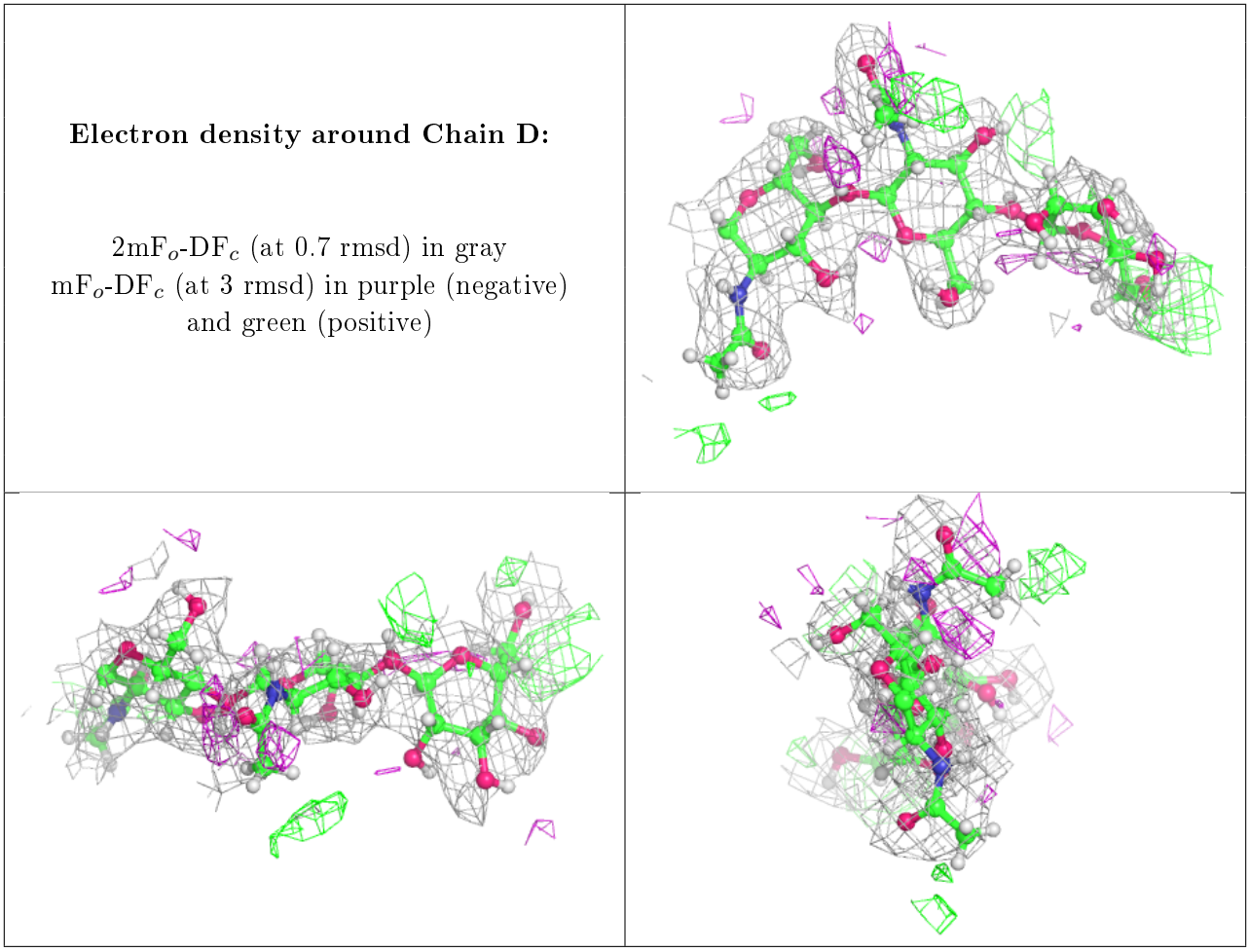
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	D	3	11/12	0.72	0.35	61,74,88,95	0
2	MAN	C	3	11/12	0.80	0.26	62,76,91,95	0
2	NAG	C	2	14/15	0.89	0.27	31,48,61,74	0
2	NAG	D	2	14/15	0.91	0.23	32,45,56,68	0
2	NAG	D	1	14/15	0.95	0.10	24,31,36,42	0
2	NAG	C	1	14/15	0.97	0.08	18,25,34,43	0

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)





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
6	BOG	B	601	20/20	0.60	0.40	32,113,149,154	0
6	BOG	A	609	20/20	0.63	0.45	30,134,181,187	0
6	BOG	A	607	20/20	0.68	0.25	38,103,134,204	0
7	NH4	A	611	1/1	0.79	0.20	35,43,43,43	0
6	BOG	A	608	20/20	0.82	0.19	38,100,124,124	0
7	NH4	B	609	1/1	0.89	0.23	48,58,58,58	0
5	NAG	B	607	14/15	0.89	0.24	54,71,86,86	0
5	NAG	A	606	14/15	0.90	0.20	33,47,57,59	0
4	COH	B	603	43/43	0.92	0.16	36,72,88,94	0
4	COH	A	602	43/43	0.92	0.16	24,50,73,79	0
7	NH4	A	610	1/1	0.93	0.27	24,29,29,29	0

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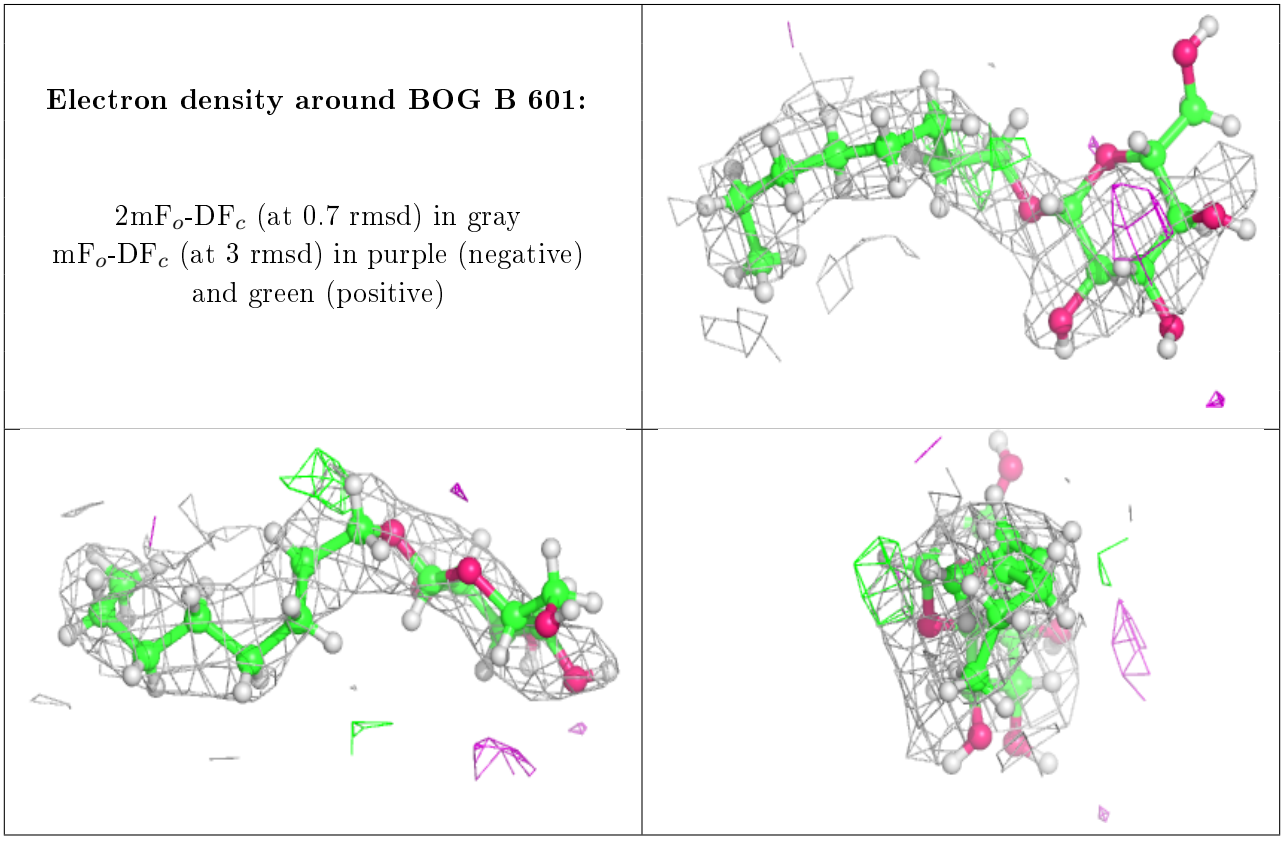
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NH4	A	612	1/1	0.93	0.21	32,39,39,39	0
7	NH4	B	608	1/1	0.93	0.29	27,33,33,33	0
3	ID8	B	602	18/18	0.96	0.11	30,37,45,47	0
3	ID8	A	601	18/18	0.97	0.09	14,22,28,29	0

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

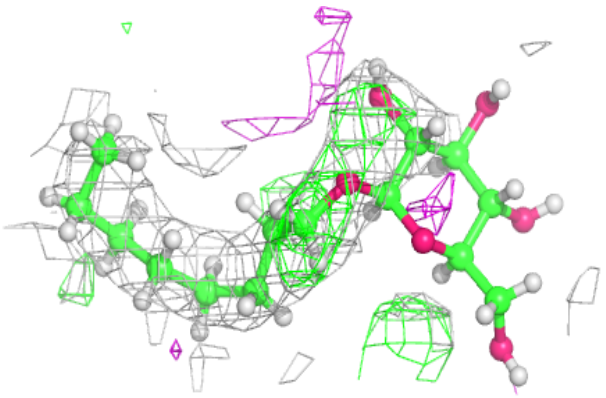
Electron density around BOG B 601:

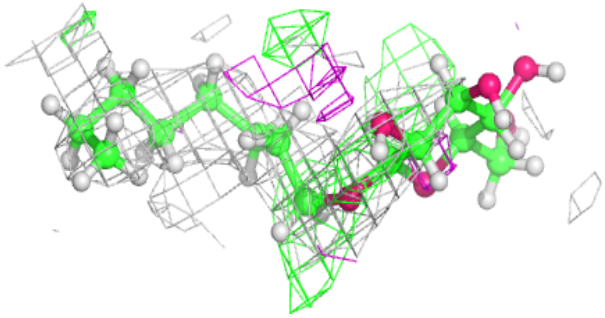
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

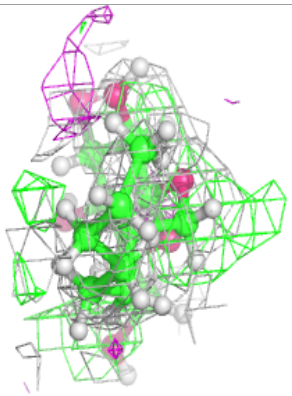


Electron density around BOG A 609:

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

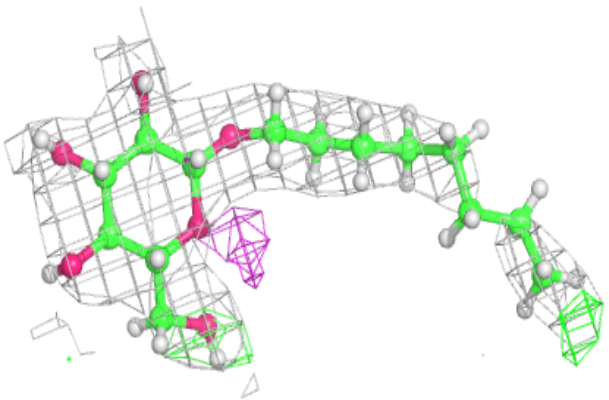


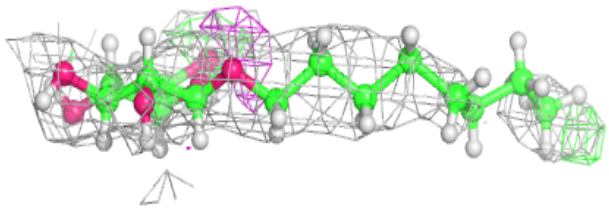


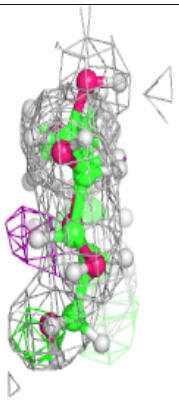


Electron density around BOG A 607:

$2mF_o$-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 608:

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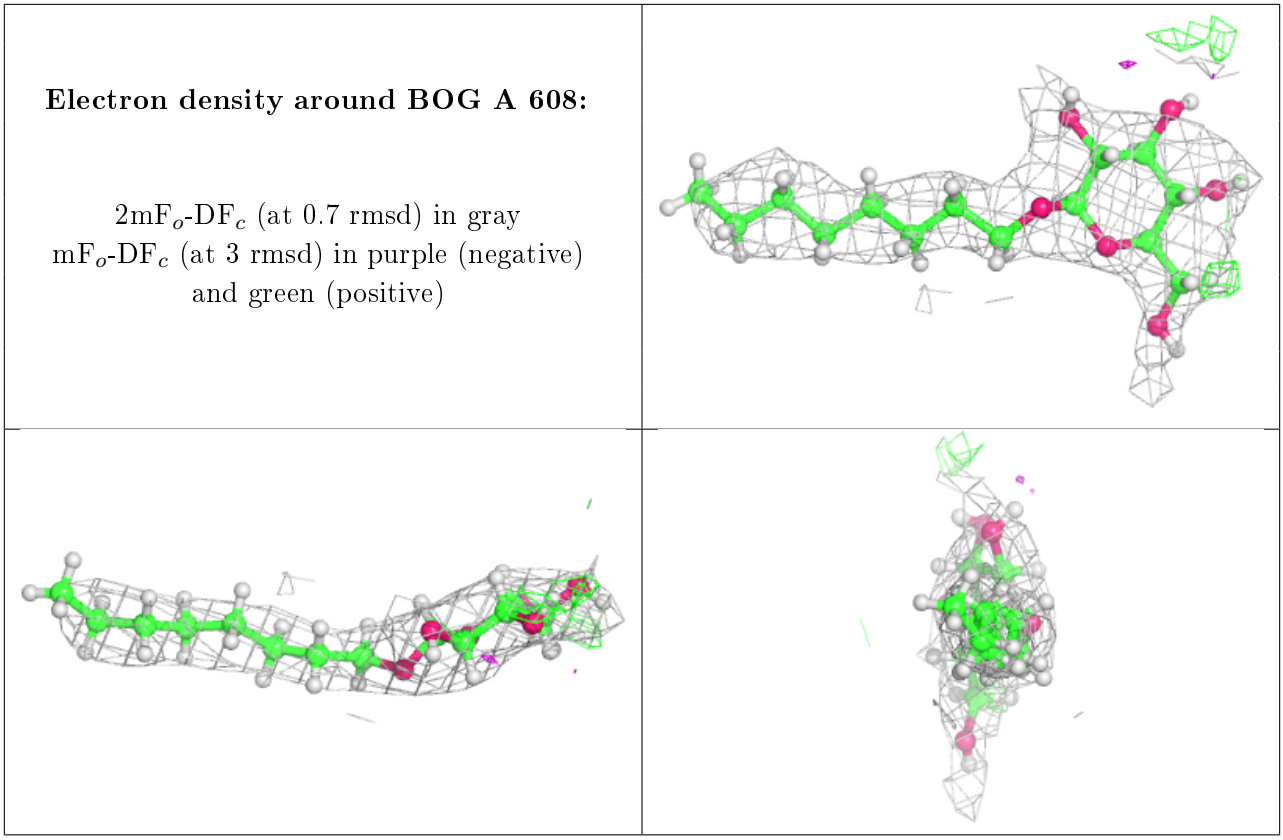
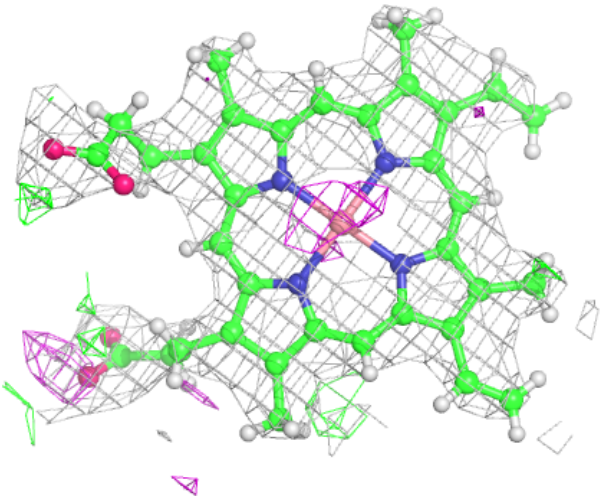
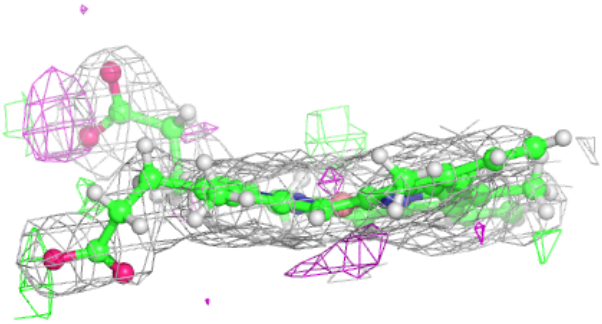
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around COH B 603:

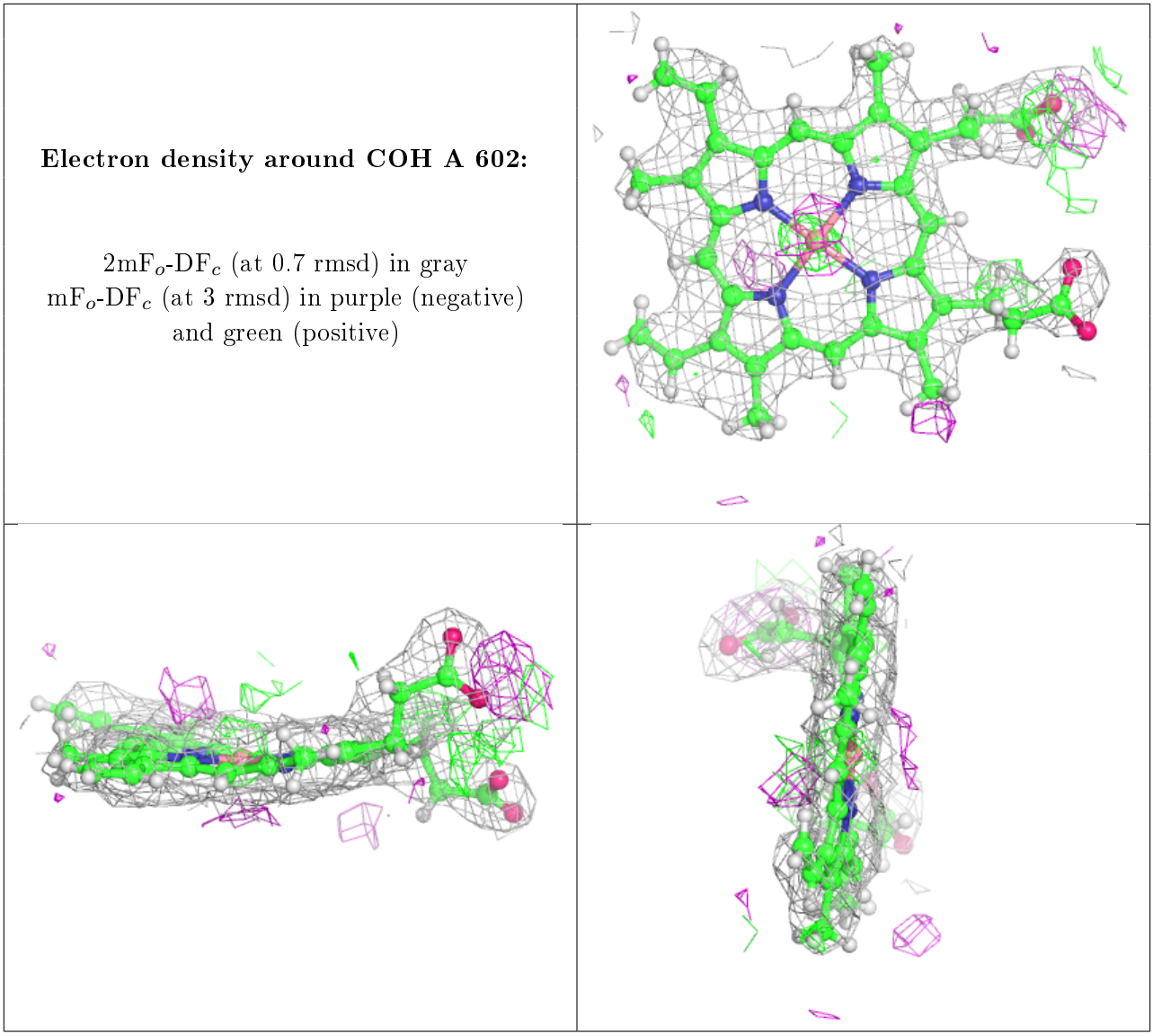
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around COH A 602:

$2mF_o$-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.