



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 08:29 AM BST

PDB ID : 5JVZ
Title : Crystal structure of flurbiprofen bound to S121P murine COX-2 mutant
Authors : Malkowski, M.G.; Orlando, B.J.
Deposited on : 2016-05-11
Resolution : 2.62 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

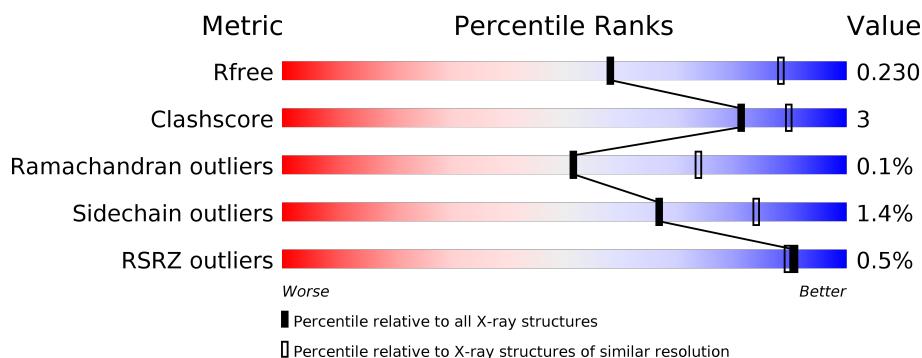
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	552	<div> <div style="width: 93%;"></div> <div style="width: 7%;"></div> </div> <div>93% 7%</div>
1	B	552	<div> <div style="width: 93%;"></div> <div style="width: 6%;"></div> </div> <div>93% 6%</div>
2	C	3	<div> <div style="width: 33%;"></div> <div style="width: 67%;"></div> </div> <div>33% 67%</div>
3	D	2	<div> <div style="width: 50%;"></div> <div style="width: 50%;"></div> </div> <div>50% 50%</div>

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
8	AKR	A	610	-	-	X	-
8	AKR	A	611	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 9431 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	6	2	0
			4457	2882	741	809	25			
1	B	551	Total	C	N	O	S	0	1	0
			4442	2871	743	803	25			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	HIS	-	expression tag	UNP Q05769
A	34	HIS	-	expression tag	UNP Q05769
A	122	PRO	SER	engineered mutation	UNP Q05769
B	33	HIS	-	expression tag	UNP Q05769
B	34	HIS	-	expression tag	UNP Q05769
B	122	PRO	SER	engineered mutation	UNP Q05769

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



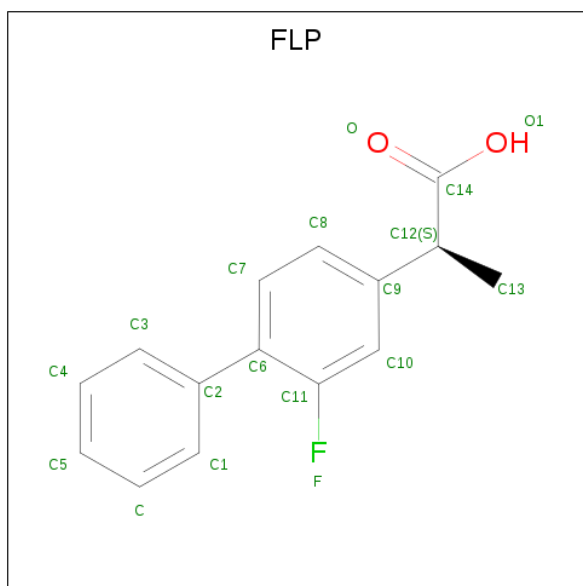
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



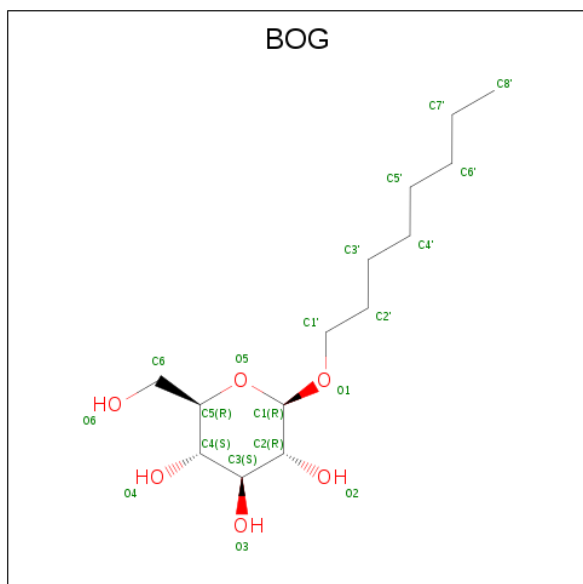
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is FLURBIPROFEN (three-letter code: FLP) (formula: $C_{15}H_{13}FO_2$).



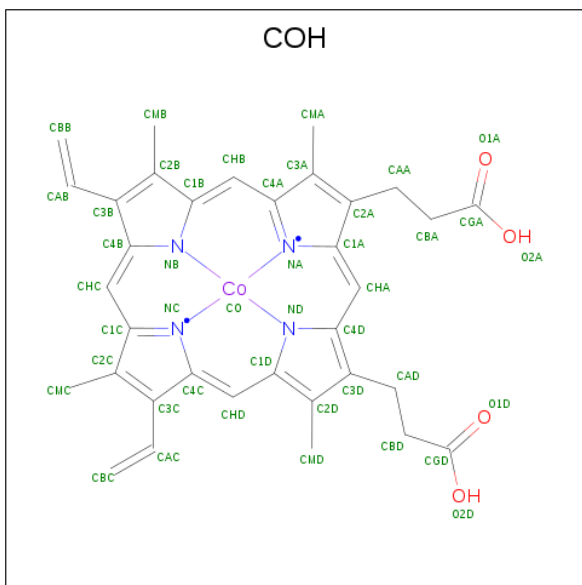
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	O	0	0
			18	15	1	2		
4	B	1	Total	C	F	O	0	0
			18	15	1	2		

- Molecule 5 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



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

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



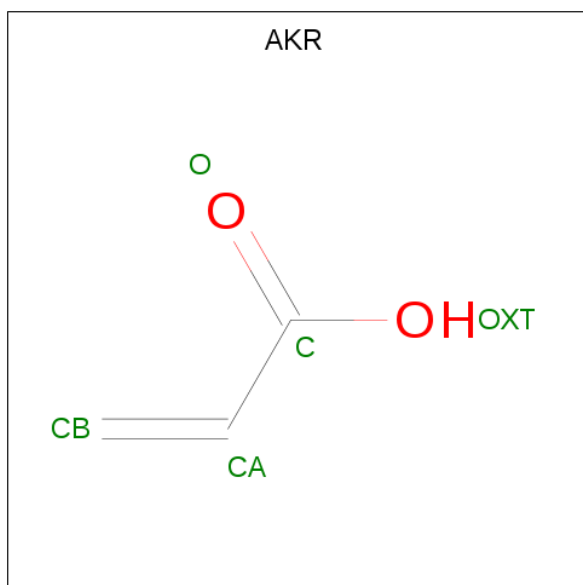
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Co	N	O	0	0
			43	34	1	4	4		
6	B	1	Total	C	Co	N	O	0	0
			43	34	1	4	4		

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



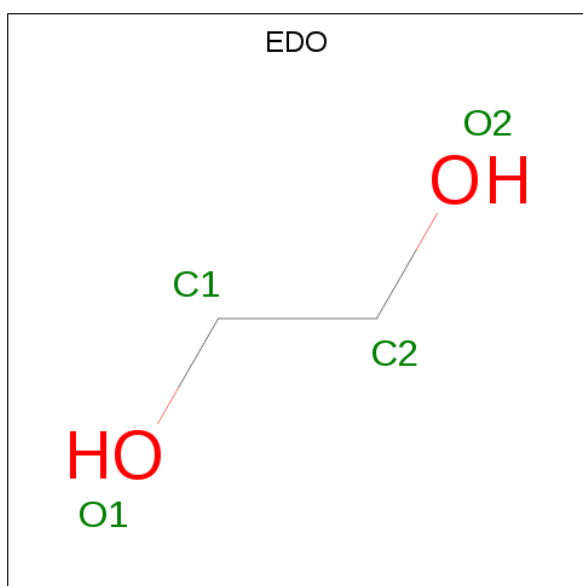
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is ACRYLIC ACID (three-letter code: AKR) (formula: $C_3H_4O_2$).



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

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

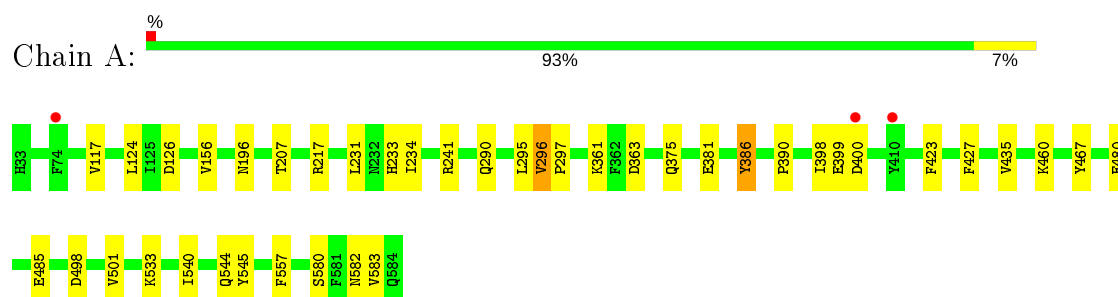
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	123	Total	O	0	0
			123	123		
10	B	100	Total	O	0	0
			100	100		

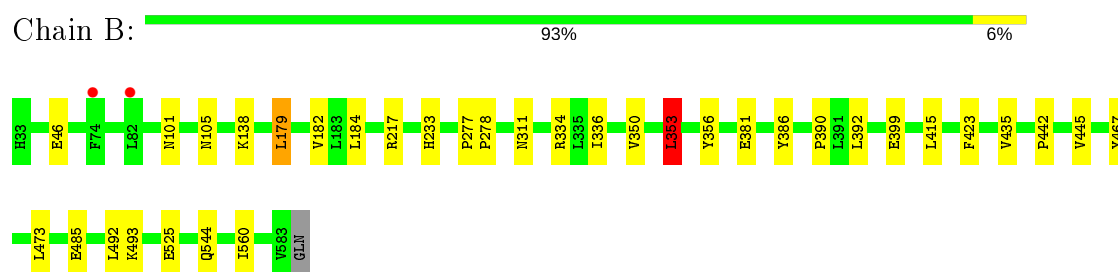
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Prostaglandin G/H synthase 2



- Molecule 1: Prostaglandin G/H synthase 2



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	119.92Å 131.59Å 179.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.62 30.00 – 2.62	Depositor EDS
% Data completeness (in resolution range)	94.1 (30.00-2.62) 88.9 (30.00-2.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.182 , 0.229 0.184 , 0.230	Depositor DCC
R_{free} test set	2061 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9431	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: BMA, NAG, FLP, EDO, AKR, COH, 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	0.23	0/4593	0.39	0/6237
1	B	0.23	0/4575	0.40	1/6211 (0.0%)
All	All	0.23	0/9168	0.39	1/12448 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	353	LEU	CA-CB-CG	5.41	127.74	115.30

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	4457	0	4306	24	0
1	B	4442	0	4293	20	0
2	C	39	0	34	1	0
3	D	28	0	25	1	0
4	A	18	0	12	0	0
4	B	18	0	12	1	0
5	A	40	0	56	2	0
6	A	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	43	0	30	4	0
7	A	28	0	26	0	0
7	B	28	0	26	0	0
8	A	10	0	6	4	0
8	B	10	0	6	1	0
9	B	4	0	6	1	0
10	A	123	0	0	0	0
10	B	100	0	0	1	0
All	All	9431	0	8868	47	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.

The worst 5 of 47 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)
6:A:603:COH:HBC1	6:A:603:COH:HHD	1.68	0.75
6:A:603:COH:HBB1	6:A:603:COH:HMB1	1.68	0.73
1:B:350:VAL:HA	1:B:353:LEU:HD22	1.74	0.70
6:B:602:COH:HHC	6:B:602:COH:HBB1	1.76	0.66
1:A:241:ARG:HH11	8:A:610:AKR:HA1	1.61	0.64

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	552/552 (100%)	533 (97%)	19 (3%)	0	100	100
1	B	550/552 (100%)	532 (97%)	17 (3%)	1 (0%)	47	69
All	All	1102/1104 (100%)	1065 (97%)	36 (3%)	1 (0%)	51	74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	399	GLU

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	483/494 (98%)	476 (99%)	7 (1%)	67	84
1	B	480/494 (97%)	474 (99%)	6 (1%)	69	85
All	All	963/988 (98%)	950 (99%)	13 (1%)	67	85

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	485	GLU
1	A	557	PHE
1	B	353	LEU
1	A	423	PHE
1	B	233	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	GLN
1	B	401	GLN
1	B	582	ASN

5.3.3 RNA [i](#)

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 ⓘ

5 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	0.26	0	17,19,21	0.53	0
2	NAG	C	2	2	14,14,15	0.50	0	17,19,21	0.46	0
2	BMA	C	3	2	11,11,12	0.75	0	15,15,17	1.15	1 (6%)
3	NAG	D	1	1,3	14,14,15	0.33	0	17,19,21	0.43	0
3	NAG	D	2	3	14,14,15	0.31	0	17,19,21	0.37	0

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	BMA	O2-C2-C3	-2.84	104.44	110.14

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

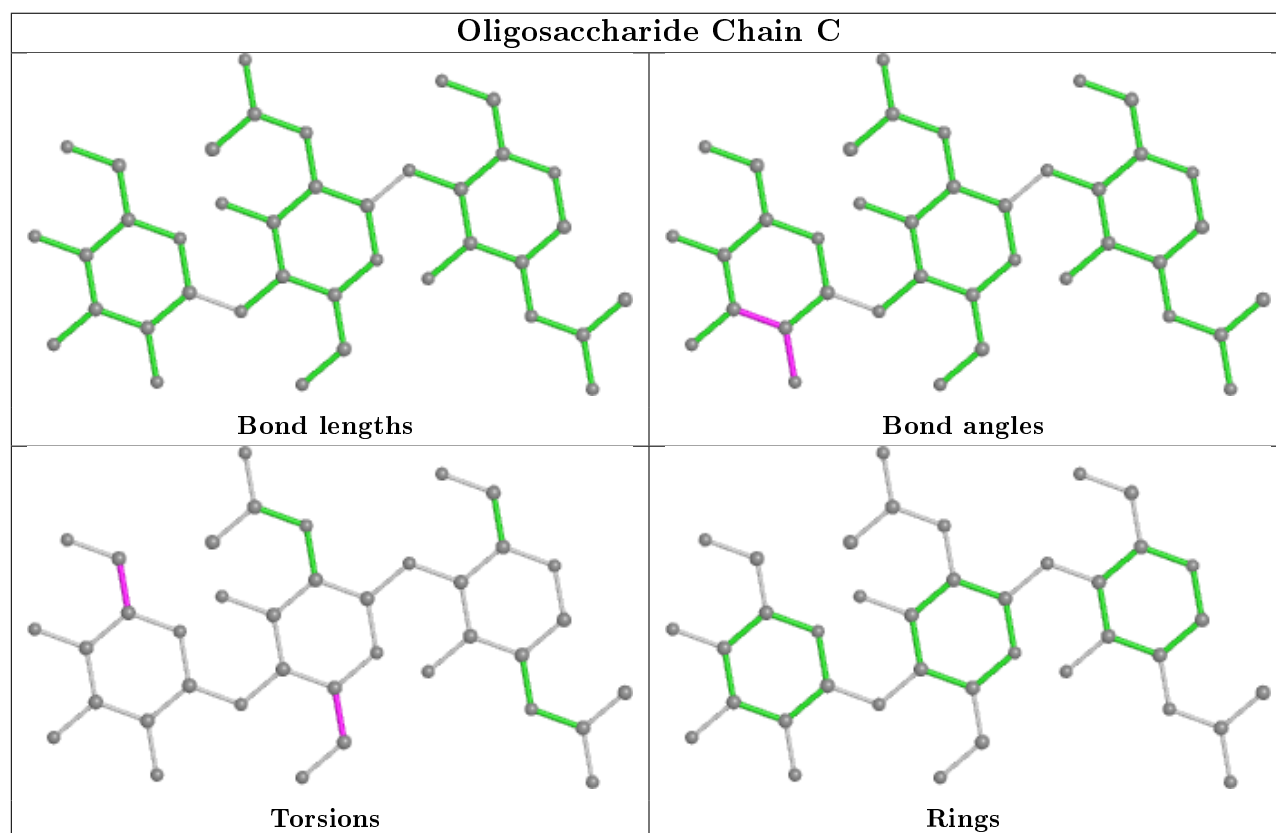
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6

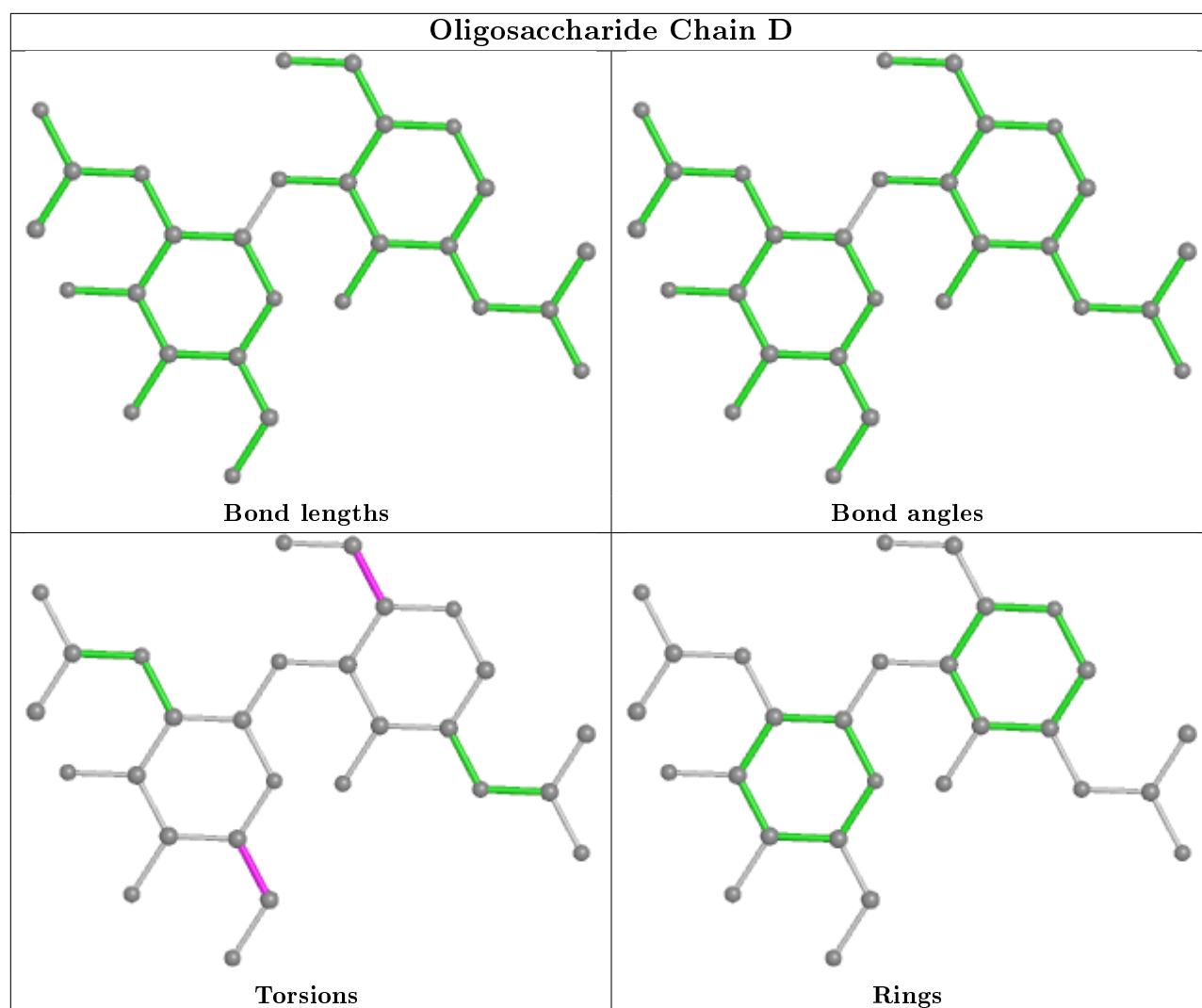
There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

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





5.6 Ligand geometry ⓘ

15 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	FLP	A	601	-	16,19,19	1.45	1 (6%)	22,26,26	0.90	2 (9%)
8	AKR	A	611	-	1,4,4	0.93	0	0,4,4	0.00	-
6	COH	A	603	-	31,50,50	5.50	22 (70%)	23,82,82	4.50	10 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	EDO	B	607	-	3,3,3	0.46	0	2,2,2	0.23	0
4	FLP	B	601	-	16,19,19	1.47	1 (6%)	22,26,26	1.02	2 (9%)
6	COH	B	602	-	31,50,50	5.51	22 (70%)	23,82,82	4.56	9 (39%)
5	BOG	A	604	-	20,20,20	0.90	1 (5%)	25,25,25	0.90	1 (4%)
8	AKR	B	608	-	1,4,4	0.93	0	0,4,4	0.00	-
7	NAG	B	606	1	14,14,15	0.24	0	17,19,21	0.41	0
5	BOG	A	602	-	20,20,20	0.92	1 (5%)	25,25,25	0.86	0
8	AKR	A	610	-	1,4,4	0.92	0	0,4,4	0.00	-
7	NAG	B	603	1	14,14,15	0.28	0	17,19,21	0.45	0
7	NAG	A	605	1	14,14,15	0.29	0	17,19,21	0.52	0
7	NAG	A	609	1	14,14,15	0.30	0	17,19,21	0.45	0
8	AKR	B	609	-	1,4,4	0.91	0	0,4,4	0.00	-

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	FLP	A	601	-	-	0/8/12/12	0/2/2/2
8	AKR	A	611	-	-	0/0/2/2	-
6	COH	A	603	-	-	2/8/94/94	-
9	EDO	B	607	-	-	0/1/1/1	-
4	FLP	B	601	-	-	0/8/12/12	0/2/2/2
6	COH	B	602	-	-	2/8/94/94	-
5	BOG	A	604	-	-	4/11/31/31	0/1/1/1
8	AKR	B	608	-	-	0/0/2/2	-
7	NAG	B	606	1	-	0/6/23/26	0/1/1/1
5	BOG	A	602	-	-	5/11/31/31	0/1/1/1
8	AKR	A	610	-	-	0/0/2/2	-
7	NAG	B	603	1	-	2/6/23/26	0/1/1/1
7	NAG	A	605	1	-	2/6/23/26	0/1/1/1
7	NAG	A	609	1	-	0/6/23/26	0/1/1/1
8	AKR	B	609	-	-	0/0/2/2	-

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	COH	C1D-ND	10.48	1.39	1.34
6	A	603	COH	C4D-ND	10.38	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	602	COH	C4D-ND	10.10	1.39	1.34
6	B	602	COH	C1D-ND	9.83	1.39	1.34
6	A	603	COH	CHA-C1A	-8.87	1.38	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	602	COH	CHC-C1C-NC	10.88	126.14	110.12
6	A	603	COH	CHC-C1C-NC	10.84	126.08	110.12
6	B	602	COH	CHA-C1A-NA	10.52	125.60	110.12
6	B	602	COH	CHB-C4A-NA	10.11	124.99	110.12
6	A	603	COH	CHB-C4A-NA	10.08	124.96	110.12

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	605	NAG	O5-C5-C6-O6
7	B	603	NAG	O5-C5-C6-O6
7	A	605	NAG	C4-C5-C6-O6
7	B	603	NAG	C4-C5-C6-O6
6	B	602	COH	C2A-CAA-CBA-CGA

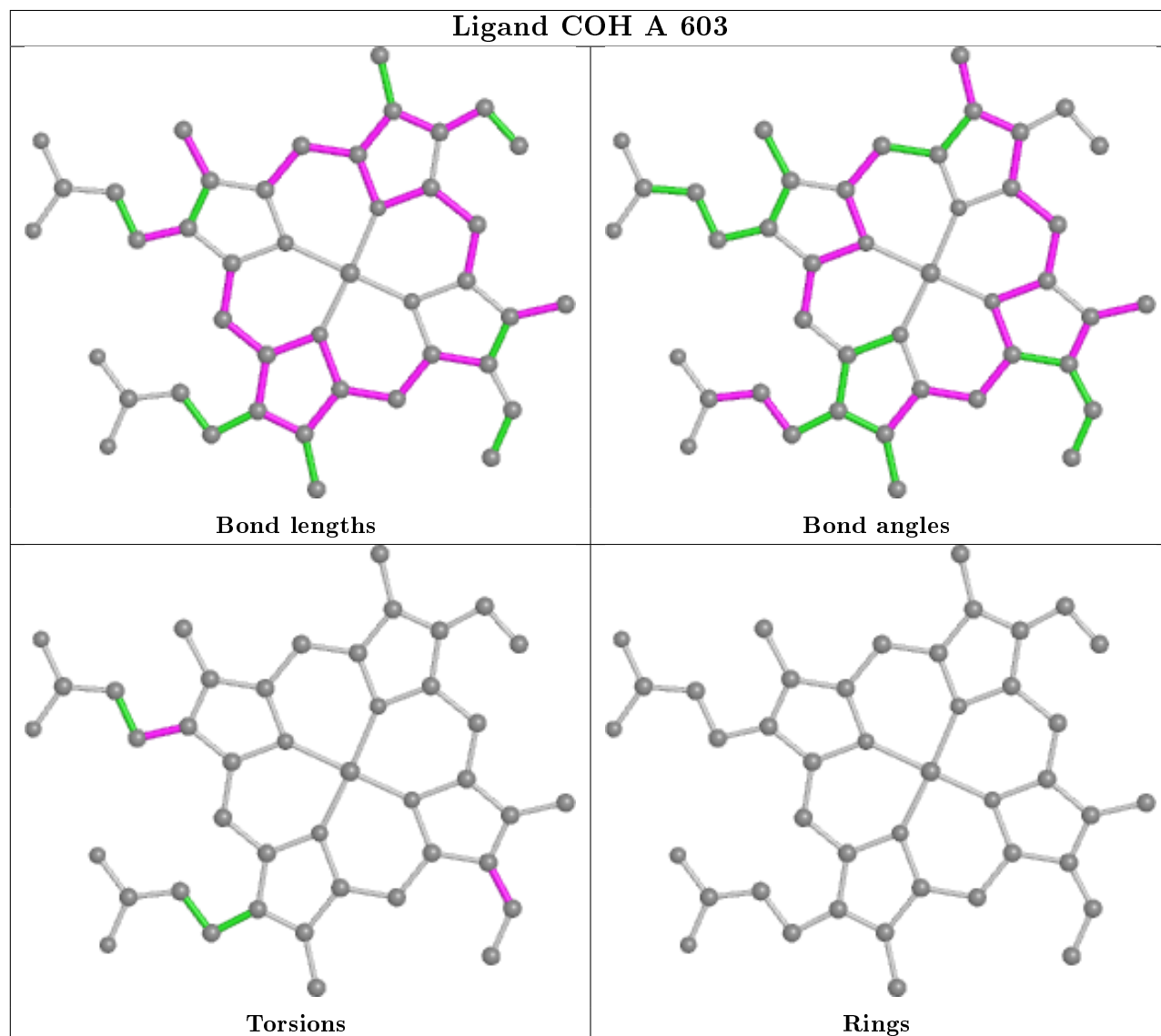
There are no ring outliers.

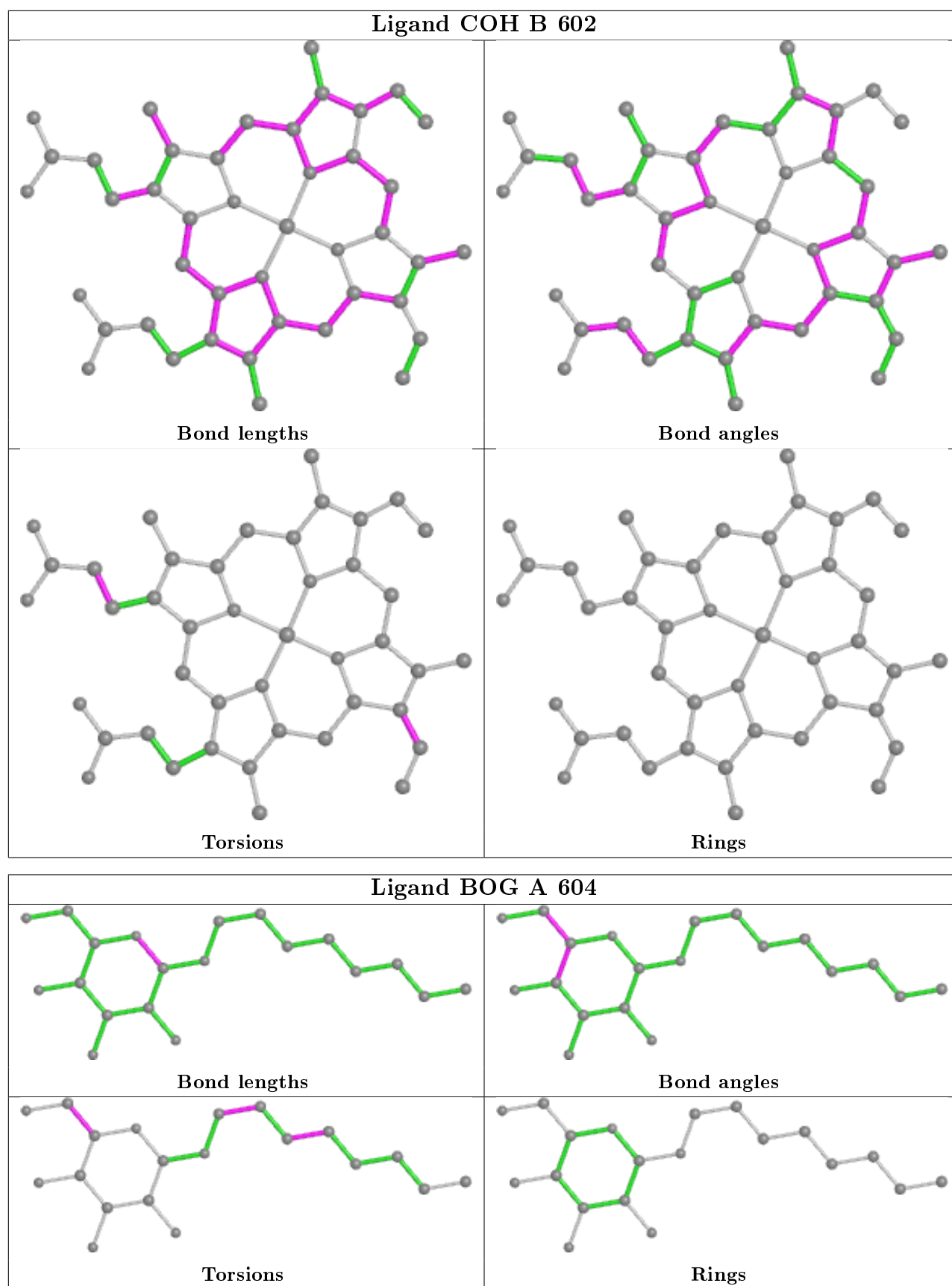
8 monomers are involved in 16 short contacts:

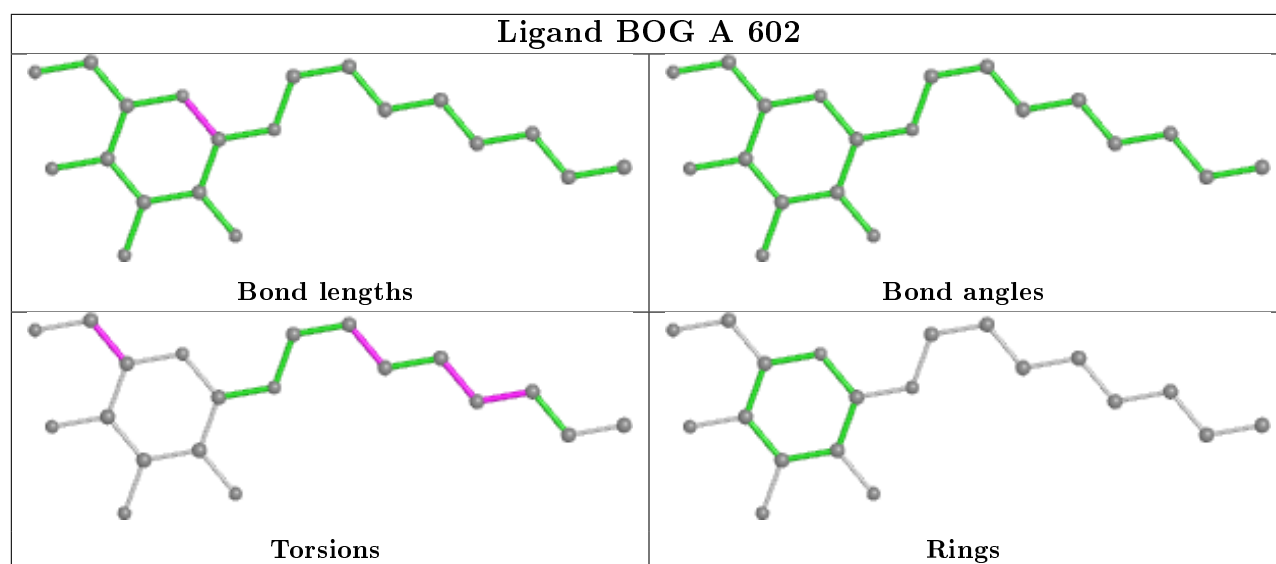
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	611	AKR	2	0
6	A	603	COH	3	0
9	B	607	EDO	1	0
4	B	601	FLP	1	0
6	B	602	COH	4	0
5	A	602	BOG	2	0
8	A	610	AKR	2	0
8	B	609	AKR	1	0

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 than 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.







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	552/552 (100%)	-0.41	3 (0%) 91 89	28, 37, 52, 74	0
1	B	551/552 (99%)	-0.48	2 (0%) 92 91	28, 38, 56, 79	0
All	All	1103/1104 (99%)	-0.44	5 (0%) 91 89	28, 37, 54, 79	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	82	LEU	3.5
1	A	400	ASP	3.1
1	A	74	PHE	3.0
1	B	74	PHE	2.4
1	A	410	TYR	2.2

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

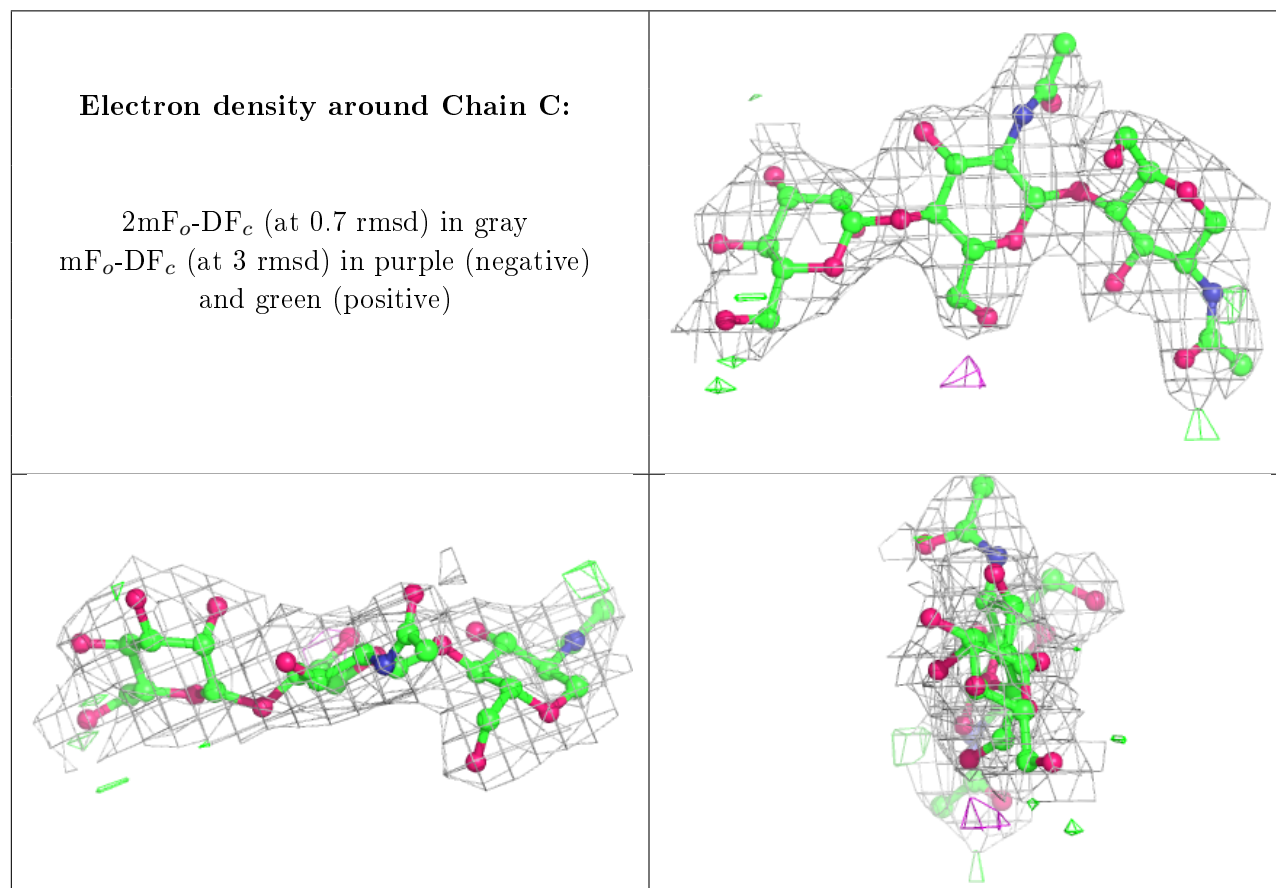
There are no non-standard protein/DNA/RNA residues in this entry.

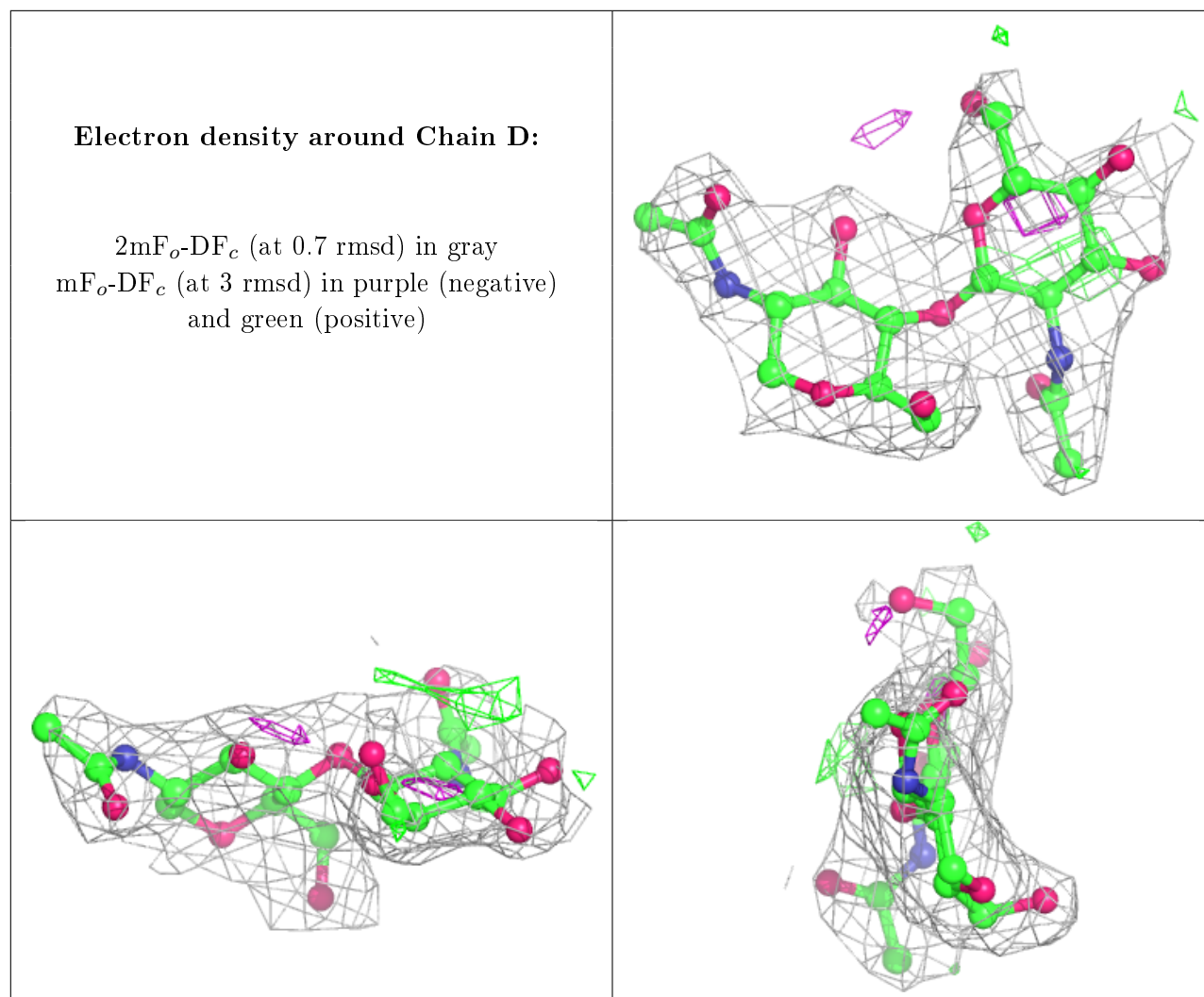
6.3 Carbohydrates [i](#)

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
3	NAG	D	2	14/15	0.84	0.33	39,69,76,77	0
2	BMA	C	3	11/12	0.87	0.23	70,76,84,90	0
2	NAG	C	2	14/15	0.94	0.26	47,52,61,77	0
3	NAG	D	1	14/15	0.96	0.21	25,32,39,40	0
2	NAG	C	1	14/15	0.96	0.15	19,31,41,43	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.





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	COH	A	603	43/43	0.76	0.32	52,96,105,147	0
5	BOG	A	602	20/20	0.82	0.38	47,79,94,96	0
6	COH	B	602	43/43	0.83	0.29	49,85,109,111	0
8	AKR	B	609	5/5	0.87	0.29	55,57,61,61	0
7	NAG	B	603	14/15	0.88	0.25	45,64,74,82	0
7	NAG	A	609	14/15	0.89	0.24	45,53,62,66	0
7	NAG	B	606	14/15	0.89	0.28	61,68,77,79	0
7	NAG	A	605	14/15	0.90	0.28	43,55,64,67	0
8	AKR	B	608	5/5	0.91	0.22	58,59,63,66	0

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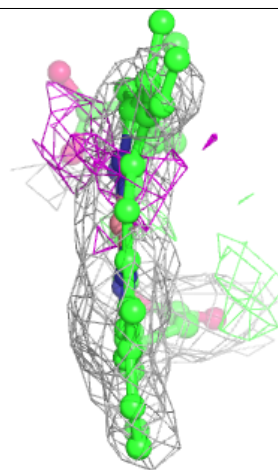
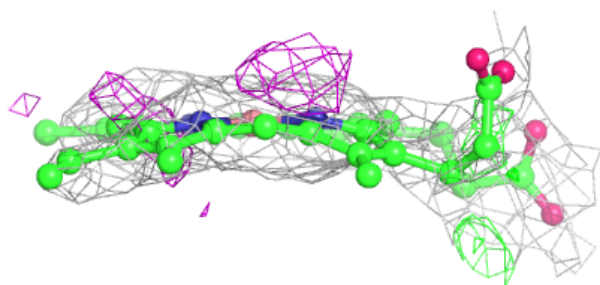
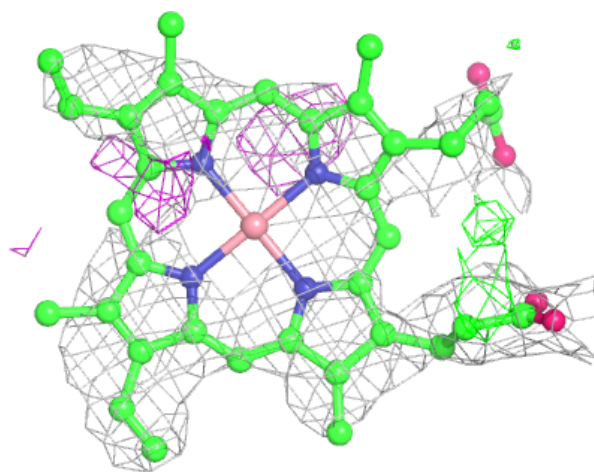
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	AKR	A	610	5/5	0.92	0.36	51,55,60,67	0
4	FLP	A	601	18/18	0.95	0.14	25,31,47,57	0
9	EDO	B	607	4/4	0.95	0.28	31,33,34,37	0
8	AKR	A	611	5/5	0.95	0.32	53,56,60,61	0
5	BOG	A	604	20/20	0.95	0.14	35,51,70,73	0
4	FLP	B	601	18/18	0.96	0.14	24,38,52,63	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.

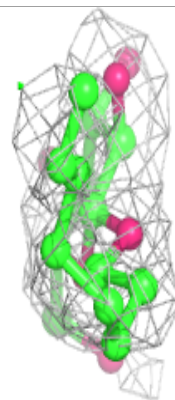
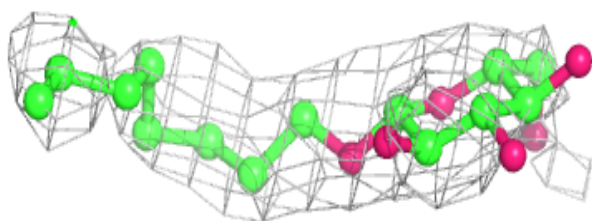
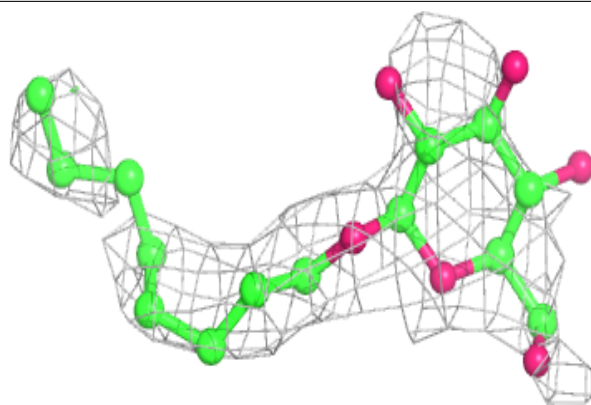
Electron density around COH A 603:

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



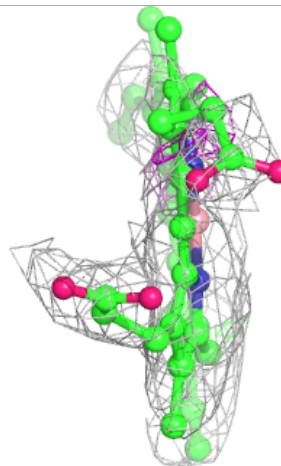
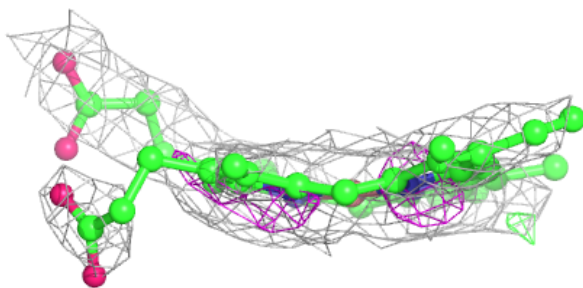
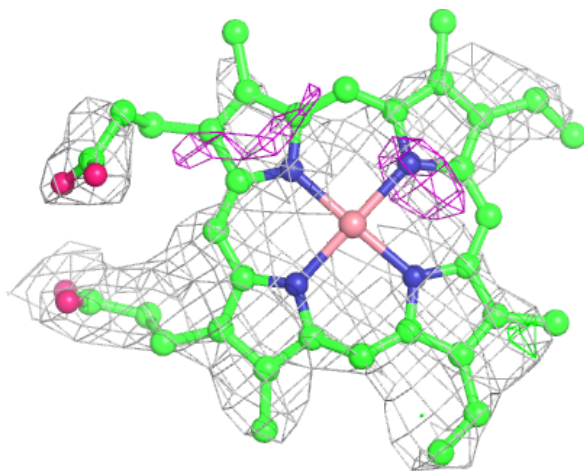
Electron density around BOG A 602:

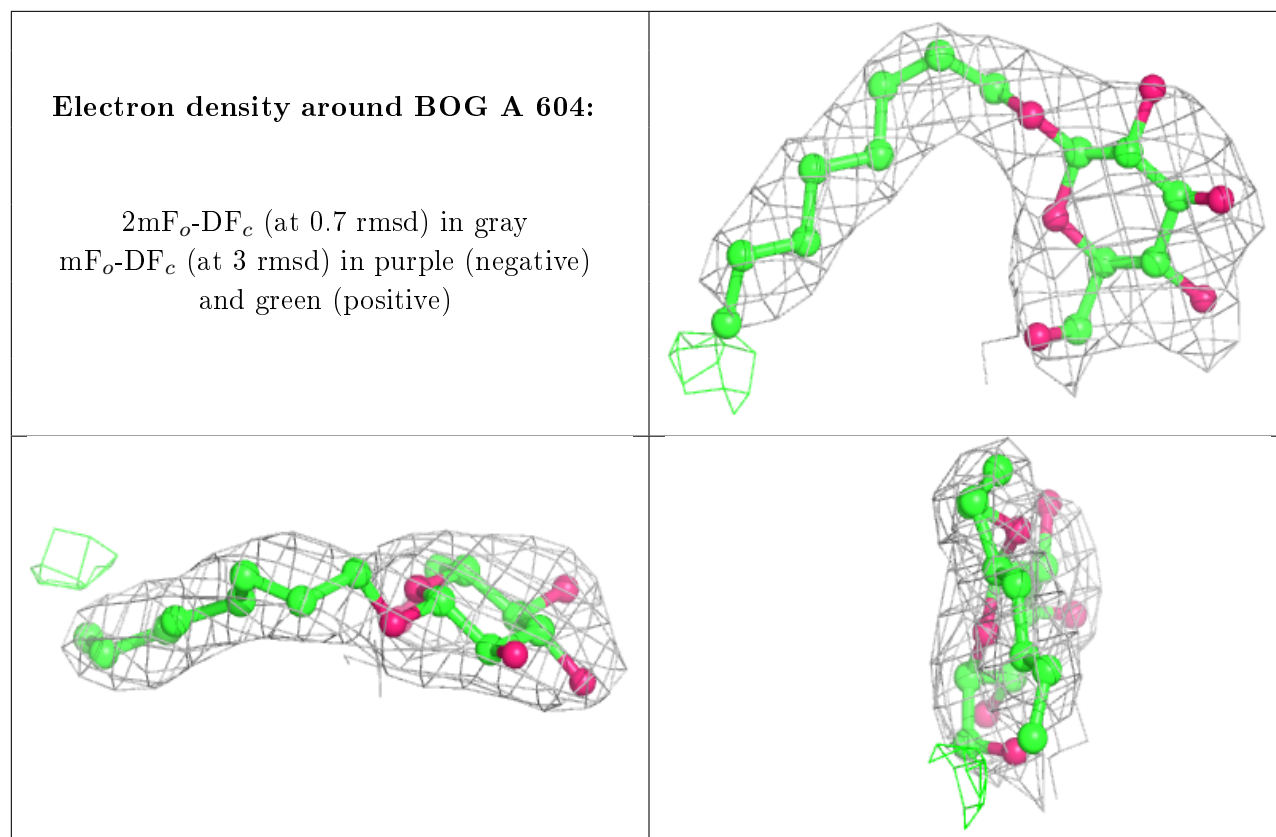
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around COH B 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.