Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 03:54 PM EDT

PDB ID : 5JW1
Title : Crystal structure of Celecoxib bound to S121P murine COX-2 mutant
Authors : Malkowski, M.G.; Orlando, B.J.
Deposited on : 2016-05-11
Resolution : 2.82 Å(reported)

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

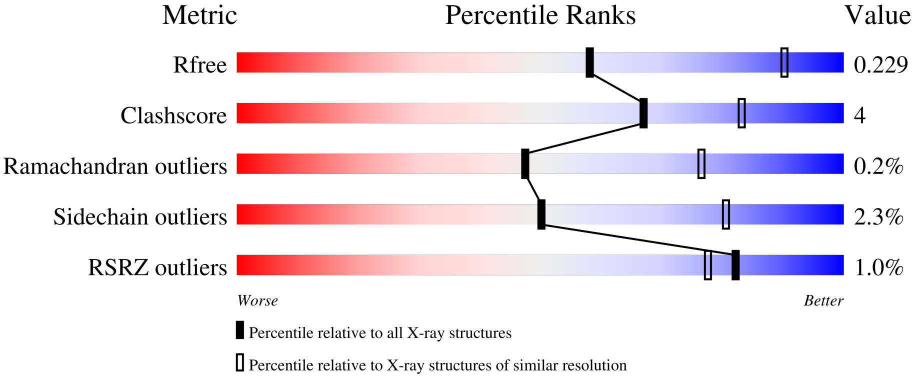
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

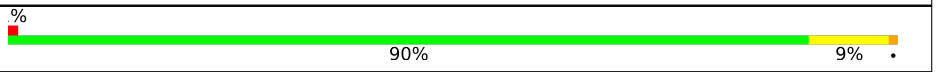
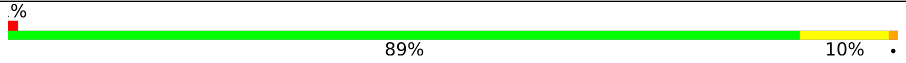
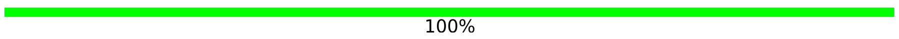
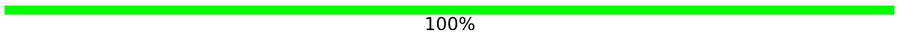
The reported resolution of this entry is 2.82 Å.

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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	552	
1	B	552	
2	C	2	
2	D	2	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9168 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.

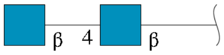
- Molecule 1 is a protein called Prostaglandin G/H synthase 2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	552	Total C N O S 4448 2876 738 809 25	0	1	0
1	B	551	Total C N O S 4435 2869 738 803 25	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

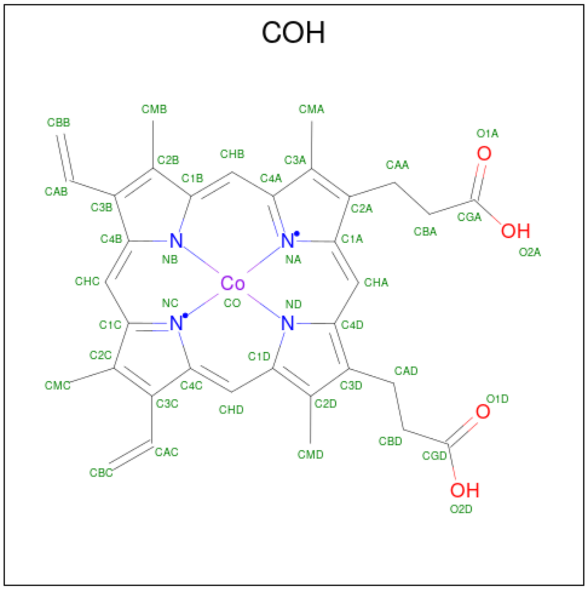
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	HIS	-	expression tag	UNP Q05769
A	34	HIS	-	expression tag	UNP Q05769
A	122	PRO	SER	engineered mutation	UNP Q05769
B	33	HIS	-	expression tag	UNP Q05769
B	34	HIS	-	expression tag	UNP Q05769
B	122	PRO	SER	engineered mutation	UNP Q05769

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



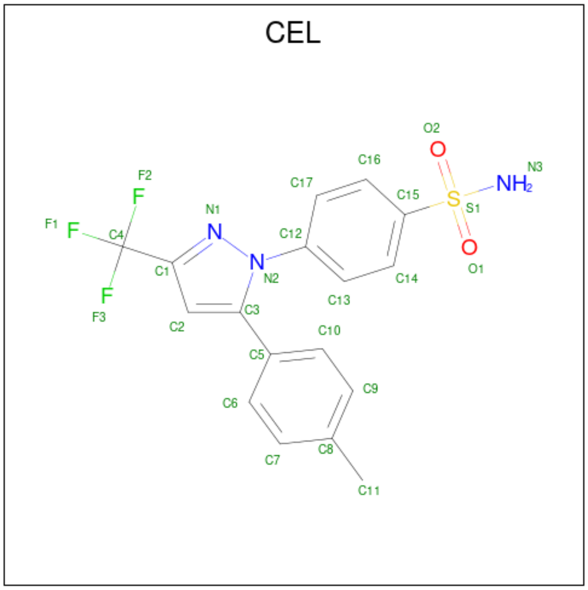
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	C	2	Total C N O 28 16 2 10	0	0	0
2	D	2	Total C N O 28 16 2 10	0	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING CO (three-letter code: COH) (formula: $C_{34}H_{32}CoN_4O_4$).



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

- Molecule 4 is 4-[5-(4-METHYLPHENYL)-3-(TRIFLUOROMETHYL)-1H-PYRAZOL-1-YL]BENZENESULFONAMIDE (three-letter code: CEL) (formula: $C_{17}H_{14}F_3N_3O_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
4	A	1	26	17	3	3	2	1	0	0

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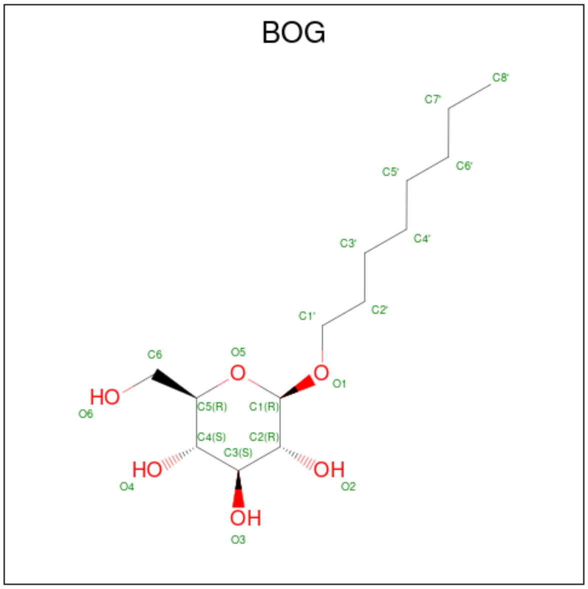
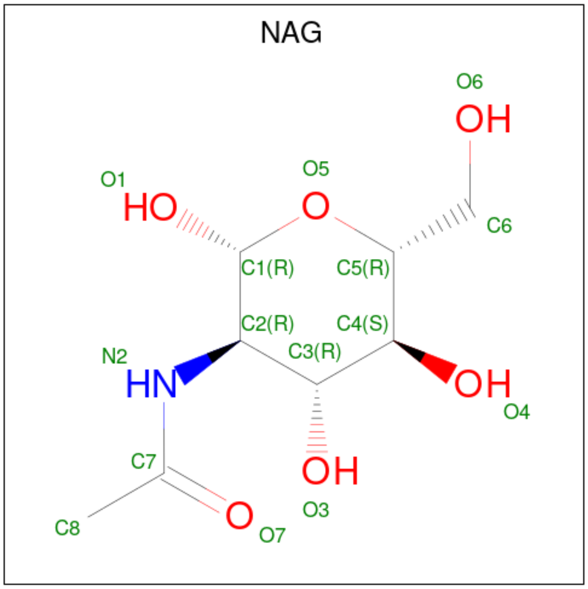
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
4	B	1	26	17	3	3	2	1	0	0

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



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is water.

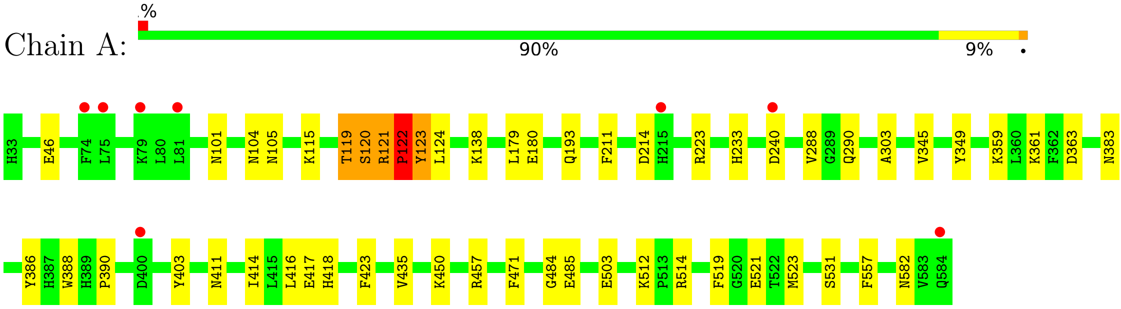
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	5	Total O 5 5	0	0
7	B	10	Total O 10 10	0	0

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.

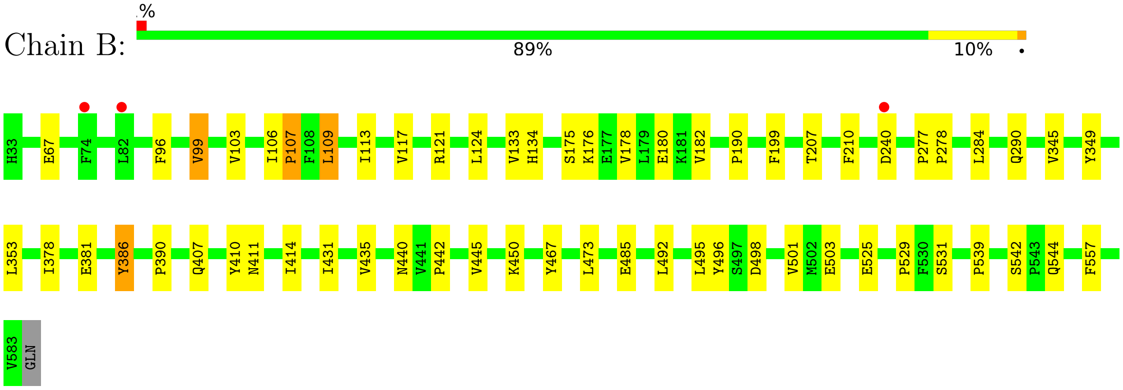
- Molecule 1: Prostaglandin G/H synthase 2

Chain A:



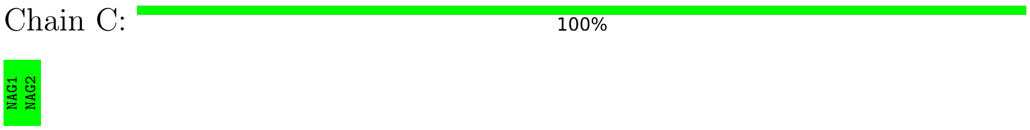
- Molecule 1: Prostaglandin G/H synthase 2

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 D:


NAG1
NAG2

4 Data and refinement statistics

Property	**Value**	**Source**
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	120.36Å 132.20Å 180.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.82 30.09 – 2.82	Depositor EDS
% Data completeness (in resolution range)	93.1 (30.00-2.82) 89.1 (30.09-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 2.80Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.189 , 0.226 0.194 , 0.229	Depositor DCC
R_{free} test set	1726 reflections (5.31%)	wwPDB-VP
Wilson B-factor (Å^2)	48.6	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 14.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9168	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: COH, NAG, BOG, CEL

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	0.29	0/4581	0.42	2/6222 (0.0%)
1	B	0.30	1/4568 (0.0%)	0.42	1/6203 (0.0%)
All	All	0.30	1/9149 (0.0%)	0.42	3/12425 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	107	PRO	N-CD	5.04	1.54	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	121	ARG	C-N-CD	6.67	142.42	128.40
1	B	106	ILE	C-N-CD	5.42	139.79	128.40
1	A	122	PRO	CA-N-CD	-5.30	104.09	111.50

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	4448	0	4291	32	0
1	B	4435	0	4274	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	28	0	25	0	0
2	D	28	0	25	0	0
3	A	43	0	30	4	0
3	B	43	0	30	3	0
4	A	26	0	14	1	0
4	B	26	0	14	0	0
5	A	20	0	28	1	0
6	A	28	0	26	2	0
6	B	28	0	26	2	0
7	A	5	0	0	0	0
7	B	10	0	0	0	0
All	All	9168	0	8783	69	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 (69) 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:A:115:LYS:O	1:A:119:THR:OG1	1.95	0.84
3:A:601:COH:HBB1	3:A:601:COH:HMB1	1.68	0.75
1:B:96:PHE:HB3	1:B:99:VAL:CG1	2.18	0.74
3:A:601:COH:HHD	3:A:601:COH:HBC1	1.79	0.65
1:B:414:ILE:HG12	6:B:606:NAG:H82	1.78	0.65
1:B:121:ARG:HD3	1:B:529:PRO:HG3	1.79	0.64
3:B:601:COH:HBB1	3:B:601:COH:HHC	1.80	0.63
1:A:120:SER:OG	1:A:121:ARG:N	2.32	0.63
1:A:122:PRO:HD2	1:A:123:TYR:H	1.65	0.61
3:B:601:COH:HHD	3:B:601:COH:HBC1	1.82	0.61
1:A:104:ASN:HB3	1:A:359:LYS:HD3	1.83	0.61
1:A:414:ILE:HA	6:A:607:NAG:H82	1.84	0.60
1:A:101:ASN:O	1:A:105:ASN:ND2	2.34	0.59
1:A:124:LEU:HD13	1:A:471:PHE:HD1	1.69	0.58
1:A:124:LEU:HD13	1:A:471:PHE:CD1	2.40	0.57
1:A:211:PHE:HB3	3:A:601:COH:HBD1	1.87	0.56
1:B:176:LYS:NZ	1:B:180:GLU:OE2	2.38	0.55
1:B:96:PHE:O	1:B:99:VAL:HG13	2.07	0.55
1:B:473:LEU:HD21	1:B:525:GLU:HG3	1.88	0.54
1:A:514:ARG:HH21	1:A:521:GLU:HG3	1.73	0.54
1:B:390:PRO:HB3	1:B:440:ASN:HB3	1.90	0.53
1:A:122:PRO:HG2	1:A:123:TYR:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:SER:OG	1:B:450:LYS:NZ	2.44	0.51
1:B:381:GLU:HG2	1:B:467:TYR:CE2	2.46	0.51
1:B:411:ASN:HB3	1:B:414:ILE:HG13	1.92	0.50
1:A:484:GLY:HA3	1:A:512:LYS:HD3	1.94	0.50
1:A:179:LEU:HD22	1:A:450:LYS:HB2	1.93	0.49
1:B:96:PHE:HB3	1:B:99:VAL:HG11	1.95	0.49
1:B:539:PRO:O	1:B:542:SER:OG	2.25	0.48
1:A:214:ASP:HB2	1:A:223:ARG:HG3	1.96	0.48
1:B:442:PRO:HG2	1:B:445:VAL:HG22	1.95	0.47
1:A:361:LYS:HE2	1:A:363:ASP:HB2	1.96	0.47
1:A:138:LYS:HE2	1:B:544:GLN:O	2.14	0.47
1:A:383:ASN:OD1	3:A:601:COH:HAD2	2.14	0.47
1:B:407:GLN:O	1:B:411:ASN:ND2	2.49	0.46
1:A:193:GLN:O	1:A:582[B]:ASN:ND2	2.49	0.46
1:A:288:VAL:HG11	1:A:303:ALA:HB1	1.96	0.46
1:A:388:TRP:HZ2	4:A:602:CEL:H112	1.80	0.46
1:B:345:VAL:HA	1:B:349:TYR:HB3	1.98	0.45
1:A:46:GLU:OE1	1:A:138:LYS:NZ	2.47	0.45
1:B:190:PRO:HB2	1:B:431:ILE:HD13	1.99	0.44
1:B:67:GLU:HB3	6:B:603:NAG:H82	1.99	0.44
1:B:178:VAL:HG22	1:B:495:LEU:HD13	1.98	0.44
1:A:345:VAL:HA	1:A:349:TYR:HB3	1.99	0.44
1:A:180:GLU:HB3	5:A:603:BOG:H4'2	2.00	0.44
1:A:122:PRO:HG2	1:A:123:TYR:CD2	2.53	0.44
1:B:496:TYR:HE1	1:B:503:GLU:HG3	1.83	0.43
1:A:411:ASN:HB3	1:A:414:ILE:HG13	2.00	0.43
1:B:498:ASP:HB3	1:B:501:VAL:HG22	2.00	0.43
1:B:277:PRO:HA	1:B:278:PRO:HD3	1.91	0.43
1:B:210:PHE:HB2	1:B:378:ILE:HG13	2.01	0.43
1:B:390:PRO:HB2	1:B:435:VAL:HA	2.00	0.42
1:B:96:PHE:CB	1:B:99:VAL:CG1	2.94	0.42
1:B:199:PHE:CZ	1:B:353:LEU:HD13	2.55	0.42
1:B:284:LEU:HD23	1:B:284:LEU:HA	1.93	0.42
1:A:122:PRO:CD	1:A:123:TYR:H	2.31	0.42
1:B:121:ARG:HB3	1:B:124:LEU:HD12	2.02	0.42
1:A:414:ILE:HG12	6:A:607:NAG:H82	2.01	0.42
1:B:103:VAL:HG13	1:B:109:LEU:HD13	2.02	0.42
1:A:403:TYR:OH	1:A:418:HIS:NE2	2.45	0.42
1:B:207:THR:HG21	1:B:386:TYR:CE2	2.56	0.41
1:A:124:LEU:HD23	1:A:124:LEU:HA	1.91	0.41
1:A:519:PHE:HB3	1:A:523:MET:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:VAL:HG13	1:B:134:HIS:CD2	2.56	0.41
1:A:390:PRO:HB2	1:A:435:VAL:HA	2.03	0.41
1:A:457:ARG:NH2	1:A:503:GLU:OE1	2.42	0.41
1:B:182:VAL:HG21	1:B:492:LEU:HD21	2.01	0.41
3:B:601:COH:HBC1	3:B:601:COH:CHD	2.49	0.40
1:B:113:ILE:O	1:B:117:VAL:HG23	2.22	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	551/552 (100%)	528 (96%)	21 (4%)	2 (0%)	34	64
1	B	550/552 (100%)	526 (96%)	24 (4%)	0	100	100
All	All	1101/1104 (100%)	1054 (96%)	45 (4%)	2 (0%)	47	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	SER
1	A	122	PRO

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	482/494 (98%)	470 (98%)	12 (2%)	47	78
1	B	477/494 (97%)	467 (98%)	10 (2%)	53	82
All	All	959/988 (97%)	937 (98%)	22 (2%)	50	80

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	THR
1	A	123	TYR
1	A	233	HIS
1	A	240	ASP
1	A	290	GLN
1	A	386	TYR
1	A	416	LEU
1	A	417	GLU
1	A	423	PHE
1	A	485	GLU
1	A	531	SER
1	A	557	PHE
1	B	99	VAL
1	B	107	PRO
1	B	109	LEU
1	B	240	ASP
1	B	290	GLN
1	B	386	TYR
1	B	410	TYR
1	B	485	GLU
1	B	531	SER
1	B	557	PHE

Sometimes 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 ⓘ

4 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	0.39	0	17,19,21	0.45	0
2	NAG	C	2	2	14,14,15	0.31	0	17,19,21	0.52	0
2	NAG	D	1	2,1	14,14,15	0.34	0	17,19,21	0.47	0
2	NAG	D	2	2	14,14,15	0.32	0	17,19,21	0.41	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	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

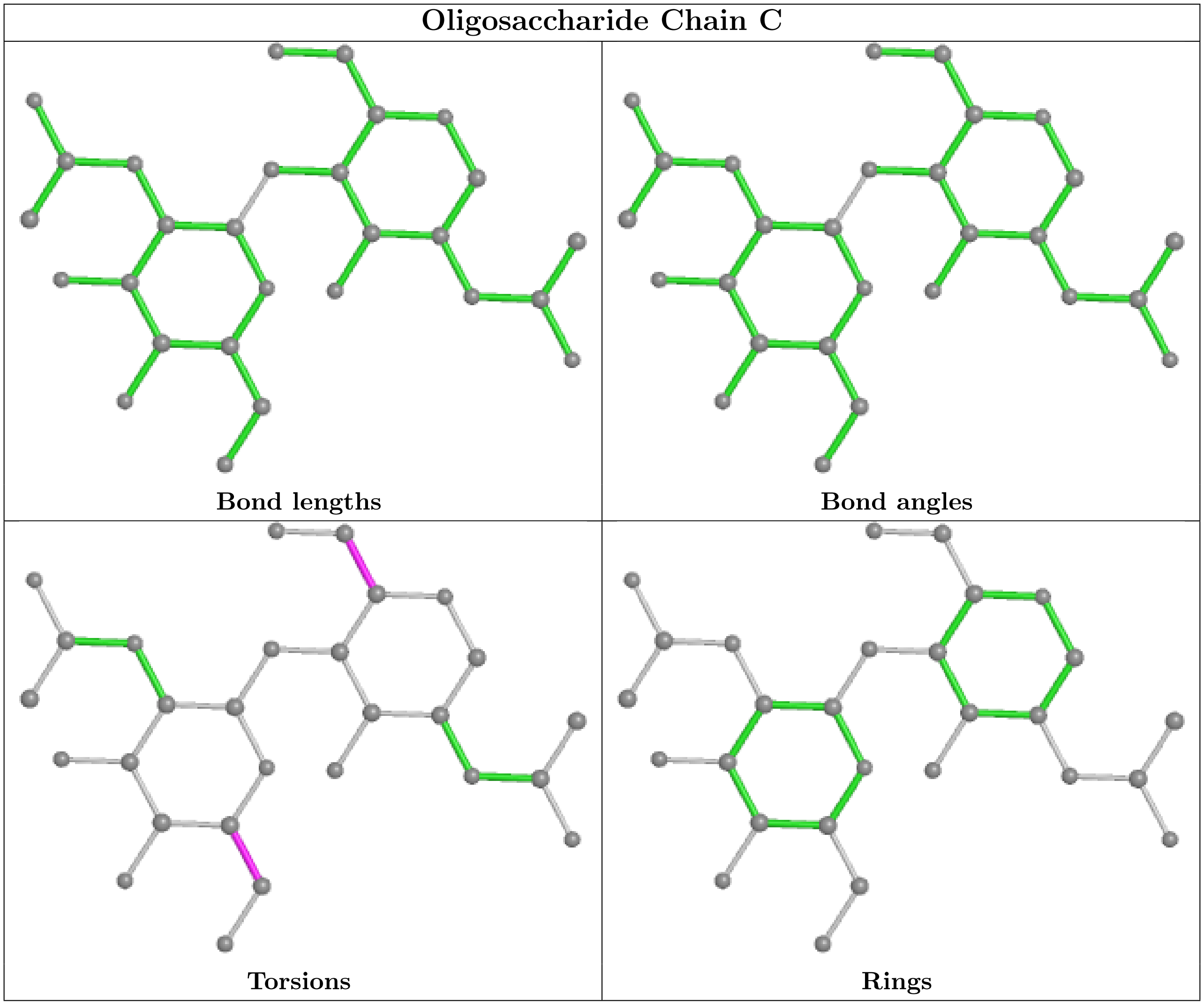
All (7) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

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



Oligosaccharide Chain C

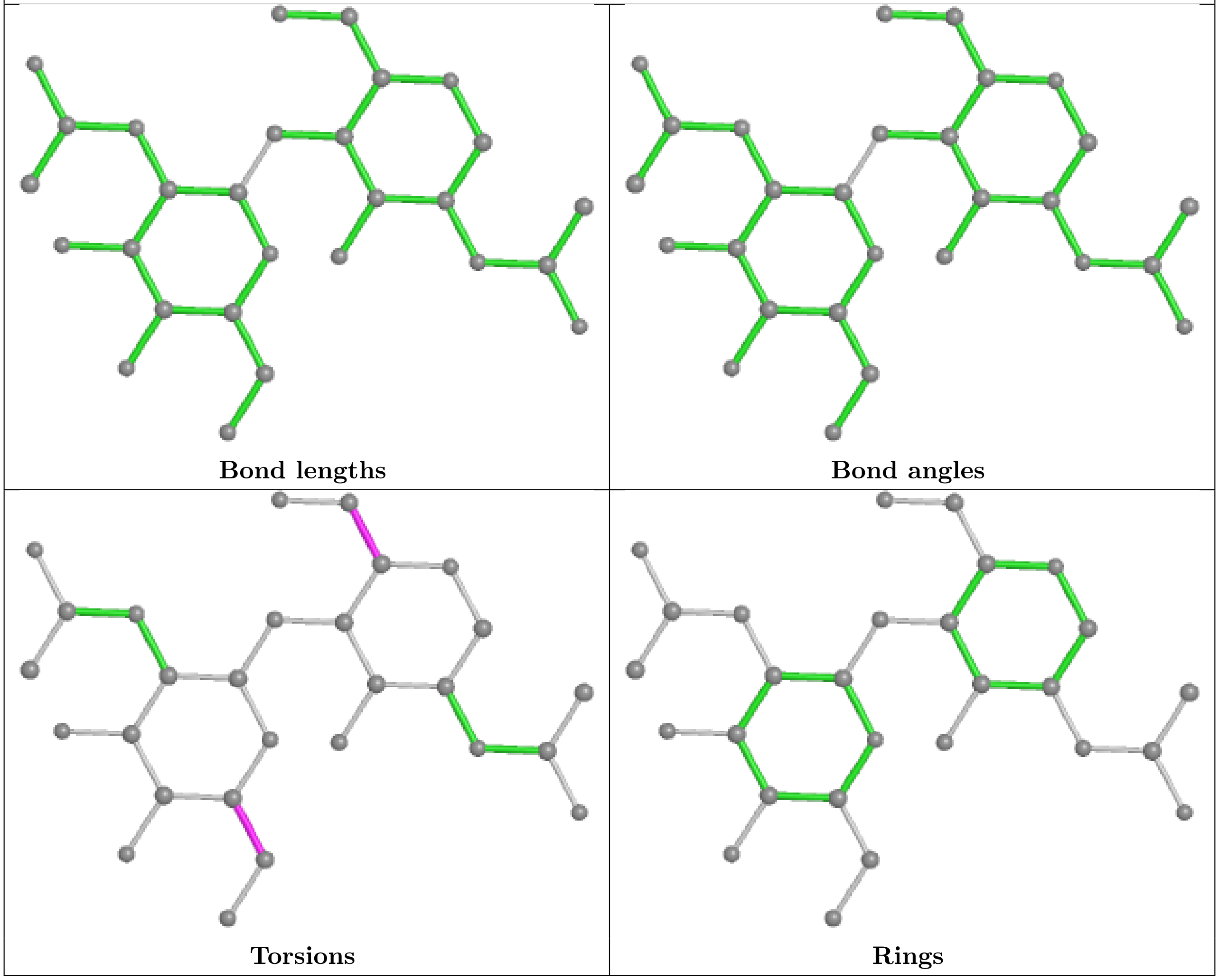
Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D



Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	A	604	1	14,14,15	0.29	0	17,19,21	0.51	0
4	CEL	A	602	-	25,28,28	1.25	4 (16%)	31,43,43	2.69	10 (32%)
3	COH	B	601	-	40,50,50	1.91	9 (22%)	38,82,82	2.87	12 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	CEL	B	602	-	25,28,28	1.26	3 (12%)	31,43,43	2.63	9 (29%)
6	NAG	B	603	1	14,14,15	0.20	0	17,19,21	0.46	0
5	BOG	A	603	-	20,20,20	0.91	1 (5%)	25,25,25	0.89	1 (4%)
6	NAG	A	607	1	14,14,15	0.28	0	17,19,21	0.35	0
6	NAG	B	606	1	14,14,15	0.29	0	17,19,21	0.37	0
3	COH	A	601	-	40,50,50	1.88	8 (20%)	38,82,82	3.26	15 (39%)

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	NAG	A	604	1	-	2/6/23/26	0/1/1/1
4	CEL	A	602	-	-	0/12/20/20	0/3/3/3
3	COH	B	601	-	-	4/12/94/94	-
4	CEL	B	602	-	-	0/12/20/20	0/3/3/3
6	NAG	B	603	1	-	0/6/23/26	0/1/1/1
5	BOG	A	603	-	-	5/11/31/31	0/1/1/1
6	NAG	A	607	1	-	2/6/23/26	0/1/1/1
6	NAG	B	606	1	-	0/6/23/26	0/1/1/1
3	COH	A	601	-	-	5/12/94/94	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	COH	C3D-C2D	5.48	1.53	1.37
3	B	601	COH	C3D-C2D	5.44	1.53	1.37
3	B	601	COH	C3B-C2B	-4.73	1.33	1.40
3	A	601	COH	C3B-CAB	3.98	1.55	1.47
3	A	601	COH	C3B-C2B	-3.79	1.35	1.40
3	B	601	COH	C3B-CAB	3.70	1.55	1.47
4	B	602	CEL	C3-N2	-3.39	1.36	1.40
4	A	602	CEL	C3-N2	-3.23	1.36	1.40
3	A	601	COH	CAC-C3C	3.02	1.55	1.47
3	B	601	COH	CAC-C3C	2.99	1.55	1.47
3	B	601	COH	CMA-C3A	2.82	1.55	1.50
3	A	601	COH	CMA-C3A	2.75	1.55	1.50
5	A	603	BOG	O5-C1	2.69	1.48	1.41
3	A	601	COH	CMC-C2C	2.61	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	COH	CAA-C2A	2.58	1.55	1.51
3	B	601	COH	C3B-C4B	2.49	1.46	1.40
3	B	601	COH	CMC-C2C	2.46	1.54	1.50
3	A	601	COH	CAA-C2A	2.42	1.55	1.51
3	A	601	COH	C3B-C4B	2.18	1.46	1.40
4	B	602	CEL	S1-N3	2.10	1.64	1.60
4	A	602	CEL	C2-C1	-2.07	1.36	1.39
4	B	602	CEL	C13-C12	-2.06	1.39	1.41
4	A	602	CEL	S1-N3	2.05	1.64	1.60
3	B	601	COH	CO-ND	2.03	2.09	1.97
4	A	602	CEL	C13-C12	-2.02	1.39	1.41

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	602	CEL	O1-S1-O2	-10.53	101.44	118.76
4	B	602	CEL	O1-S1-O2	-10.53	101.45	118.76
3	A	601	COH	CHC-C1C-NC	9.14	126.44	121.29
3	B	601	COH	CHC-C1C-NC	8.03	125.82	121.29
3	A	601	COH	CHA-C1A-NA	7.93	125.76	121.29
3	B	601	COH	CHA-C1A-NA	7.69	125.62	121.29
3	A	601	COH	CHB-C4A-NA	6.70	125.06	121.29
3	A	601	COH	CHA-C4D-ND	6.37	127.07	122.40
3	A	601	COH	CHD-C4C-NC	5.89	124.61	121.29
3	B	601	COH	CHD-C4C-NC	5.54	124.41	121.29
4	A	602	CEL	C4-C1-N1	5.54	126.23	119.72
4	B	602	CEL	C4-C1-N1	5.34	126.00	119.72
3	B	601	COH	CHB-C4A-NA	5.25	124.25	121.29
3	A	601	COH	CHD-C1D-ND	5.13	126.17	122.40
3	B	601	COH	CHA-C4D-ND	4.90	126.00	122.40
3	B	601	COH	CHB-C1B-NB	4.76	125.89	122.40
4	A	602	CEL	O1-S1-C15	4.30	112.15	107.35
3	A	601	COH	CHB-C1B-NB	4.24	125.51	122.40
3	B	601	COH	CHD-C1D-ND	4.20	125.48	122.40
3	A	601	COH	CHC-C4B-NB	3.98	125.32	122.40
4	B	602	CEL	O1-S1-C15	3.85	111.65	107.35
4	A	602	CEL	O2-S1-C15	3.31	111.05	107.35
4	B	602	CEL	O2-S1-C15	3.27	111.00	107.35
3	A	601	COH	C1A-CHA-C4D	3.25	127.45	118.67
4	B	602	CEL	C2-C1-N1	-3.12	106.90	111.41
3	A	601	COH	C2A-C1A-NA	-3.10	107.97	114.81
3	B	601	COH	C2A-C1A-NA	-3.00	108.18	114.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	COH	C4C-CHD-C1D	2.98	126.72	118.67
3	A	601	COH	C1C-CHC-C4B	2.91	126.54	118.67
3	A	601	COH	CBD-CAD-C3D	-2.91	107.70	112.60
4	A	602	CEL	C2-C1-N1	-2.90	107.20	111.41
3	B	601	COH	C1A-CHA-C4D	2.88	126.47	118.67
3	B	601	COH	C1C-CHC-C4B	2.84	126.36	118.67
4	A	602	CEL	O1-S1-N3	2.82	111.55	107.36
3	B	601	COH	C4C-CHD-C1D	2.58	125.65	118.67
4	A	602	CEL	C16-C17-C12	-2.56	119.65	121.79
4	B	602	CEL	O1-S1-N3	2.50	111.07	107.36
4	B	602	CEL	C16-C17-C12	-2.47	119.73	121.79
3	B	601	COH	CHC-C4B-NB	2.43	124.18	122.40
3	A	601	COH	CMB-C2B-C3B	2.32	129.01	124.68
4	B	602	CEL	O2-S1-N3	2.32	110.80	107.36
4	A	602	CEL	F2-C4-C1	-2.25	108.62	112.47
4	A	602	CEL	O2-S1-N3	2.22	110.65	107.36
5	A	603	BOG	C6-C5-C4	-2.15	107.97	113.00
3	A	601	COH	C4A-CHB-C1B	2.12	124.40	118.67
4	A	602	CEL	C13-C12-C17	2.07	119.38	116.27
4	B	602	CEL	C13-C12-C17	2.02	119.30	116.27

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	607	NAG	O5-C5-C6-O6
6	A	607	NAG	C4-C5-C6-O6
6	A	604	NAG	C4-C5-C6-O6
3	A	601	COH	C3D-CAD-CBD-CGD
5	A	603	BOG	C2-C1-O1-C1'
6	A	604	NAG	O5-C5-C6-O6
5	A	603	BOG	O5-C1-O1-C1'
3	A	601	COH	C2A-CAA-CBA-CGA
3	A	601	COH	C4C-C3C-CAC-CBC
3	B	601	COH	C4C-C3C-CAC-CBC
5	A	603	BOG	C2'-C1'-O1-C1
5	A	603	BOG	C4-C5-C6-O6
3	B	601	COH	C3D-CAD-CBD-CGD
3	B	601	COH	CAA-CBA-CGA-O2A
3	B	601	COH	CAA-CBA-CGA-O1A
5	A	603	BOG	O5-C5-C6-O6
3	A	601	COH	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
3	A	601	COH	CAA-CBA-CGA-O2A

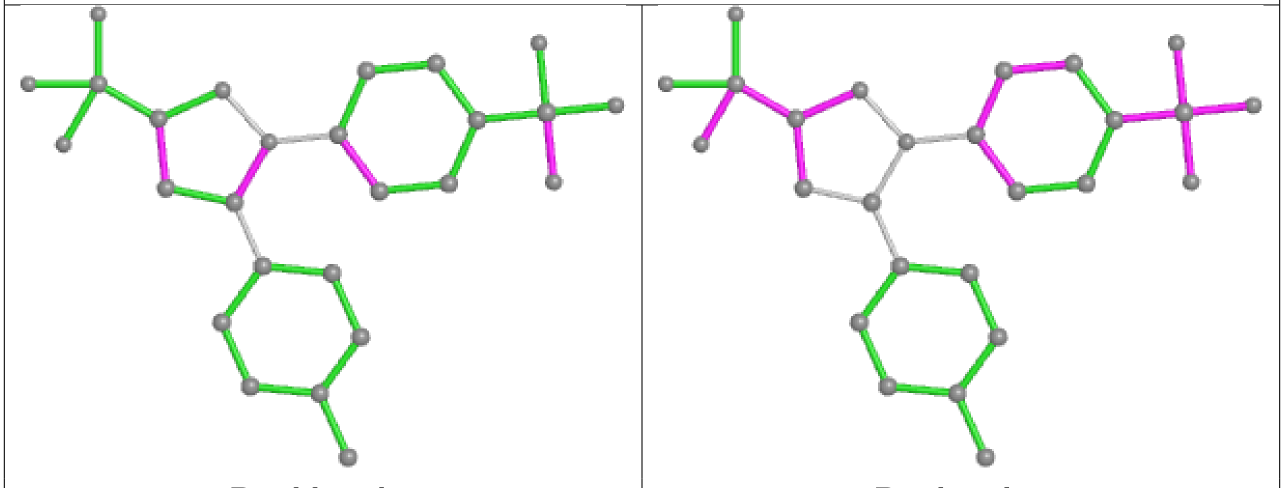
There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	CEL	1	0
3	B	601	COH	3	0
6	B	603	NAG	1	0
5	A	603	BOG	1	0
6	A	607	NAG	2	0
6	B	606	NAG	1	0
3	A	601	COH	4	0

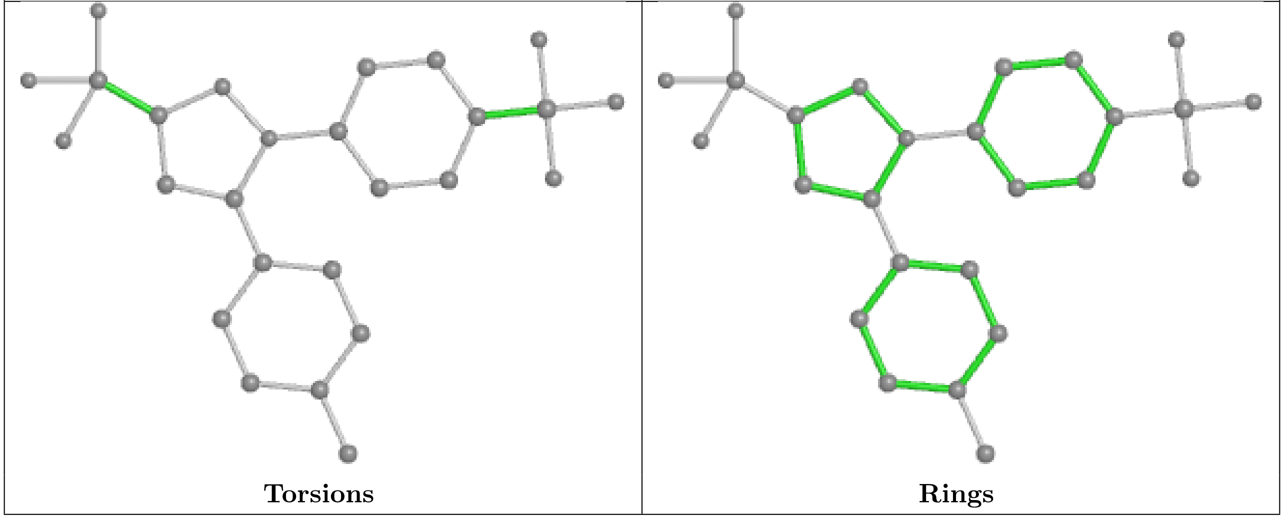
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 CEL A 602



Bond lengths

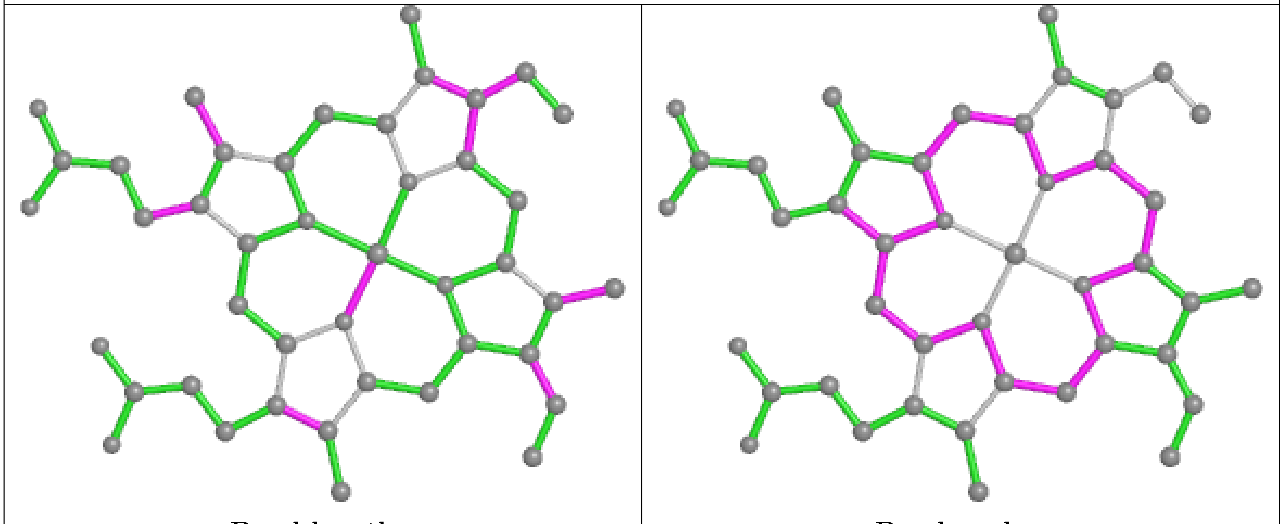
Bond angles



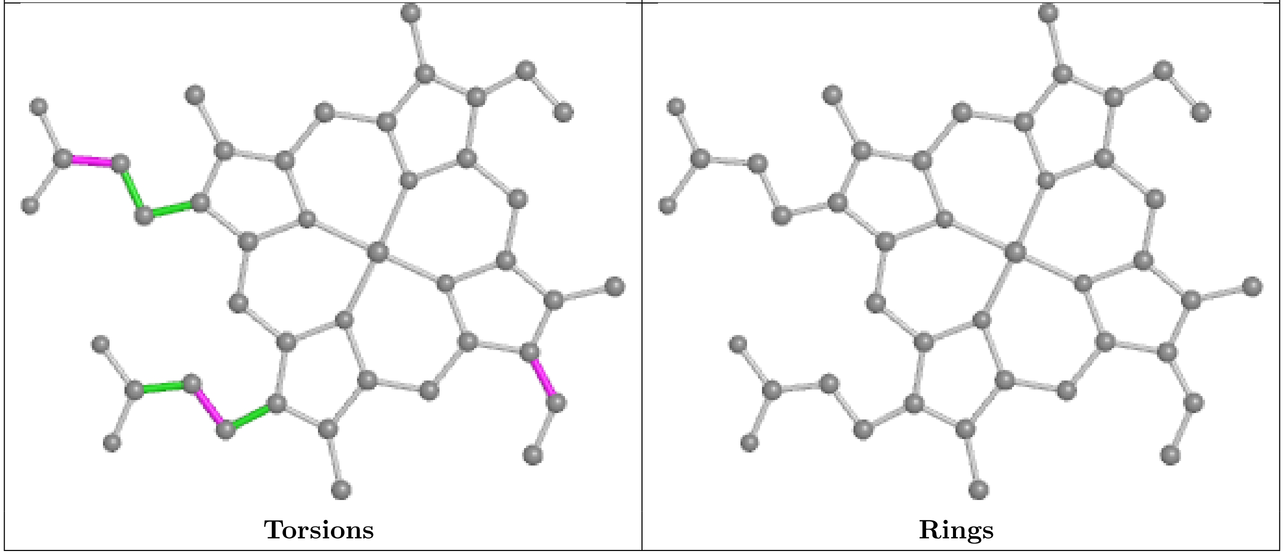
Torsions

Rings

Ligand COH B 601

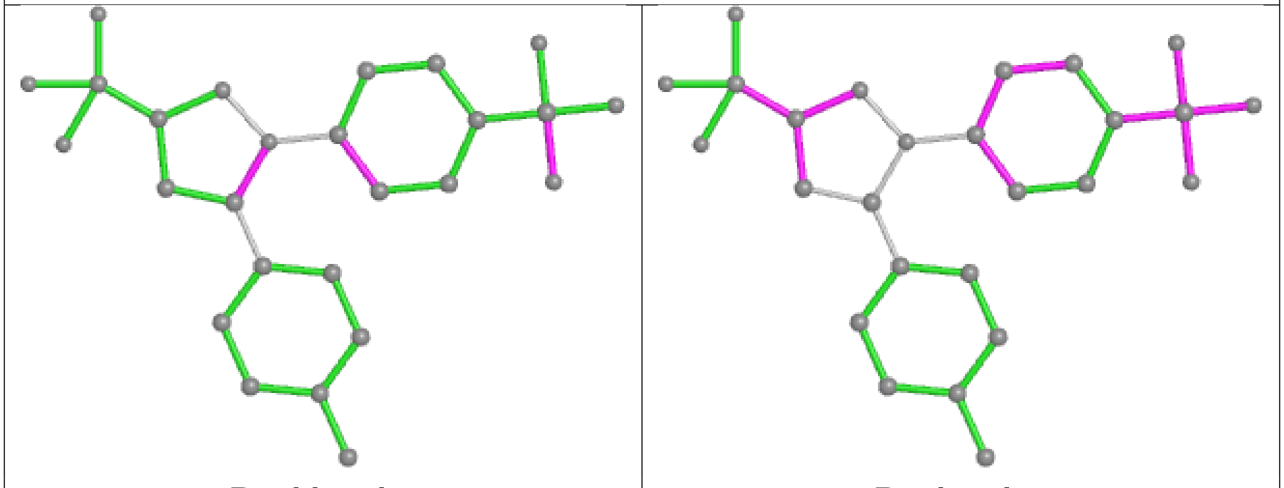


Bond lengths **Bond angles**



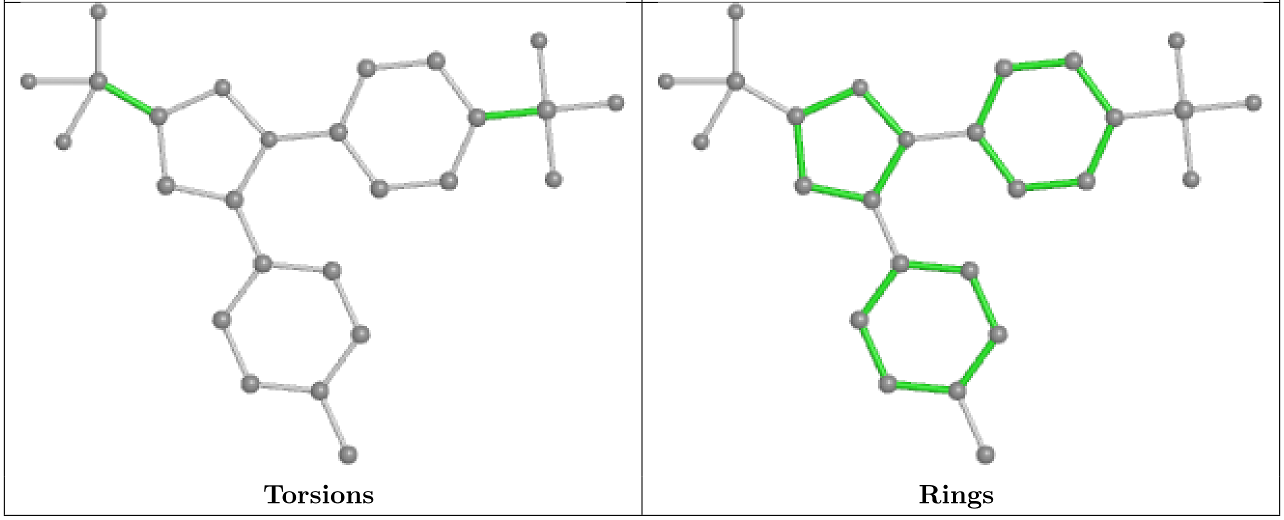
Torsions **Rings**

Ligand CEL B 602



Bond lengths

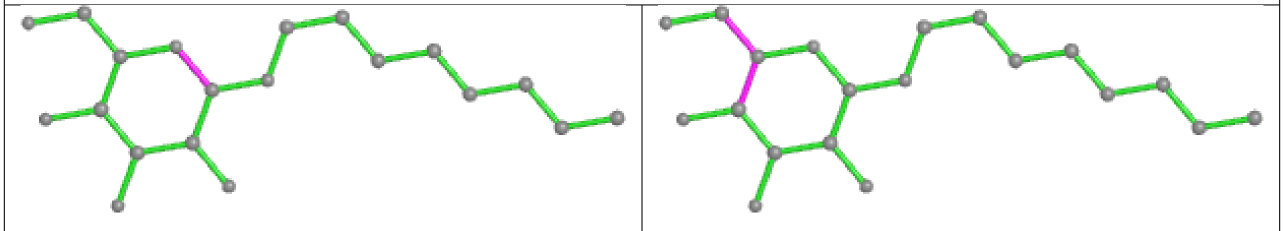
Bond angles



Torsions

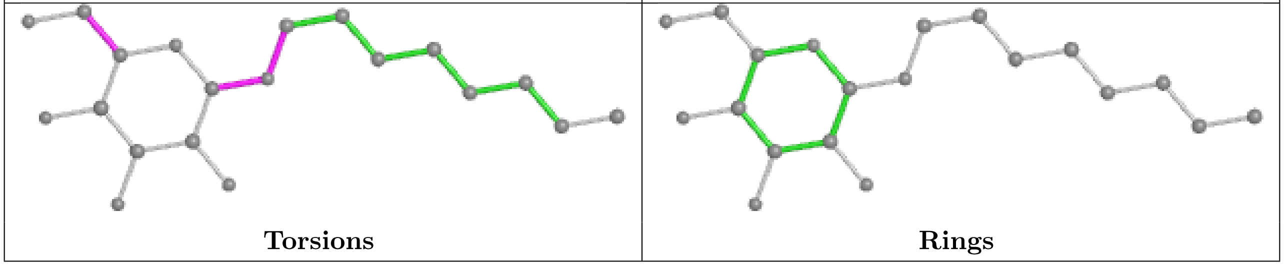
Rings

Ligand BOG A 603



Bond lengths

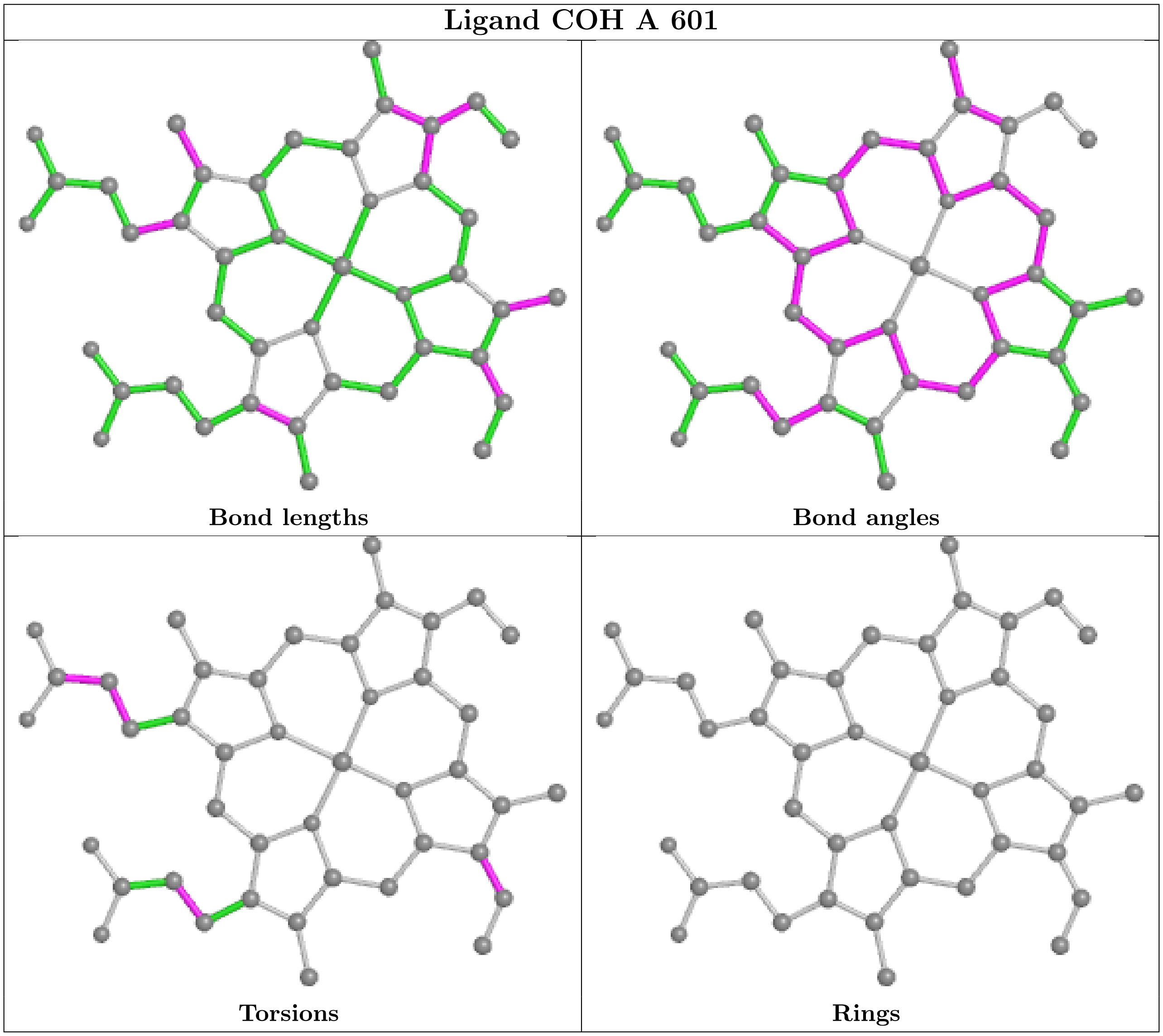
Bond angles



Torsions

Rings

Ligand COH A 601



Bond lengths

Bond angles

Torsions

Rings

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, 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%)	-0.32	8 (1%)	75	69	29, 40, 58, 81	0
1	B	551/552 (99%)	-0.37	3 (0%)	91	88	31, 40, 60, 95	0
All	All	1103/1104 (99%)	-0.34	11 (0%)	82	77	29, 40, 59, 95	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	PHE	3.8
1	B	74	PHE	3.2
1	B	82	LEU	2.9
1	A	75	LEU	2.9
1	A	79	LYS	2.4
1	A	584	GLN	2.3
1	A	81	LEU	2.3
1	A	400	ASP	2.1
1	A	240	ASP	2.1
1	A	215	HIS	2.1
1	B	240	ASP	2.0

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

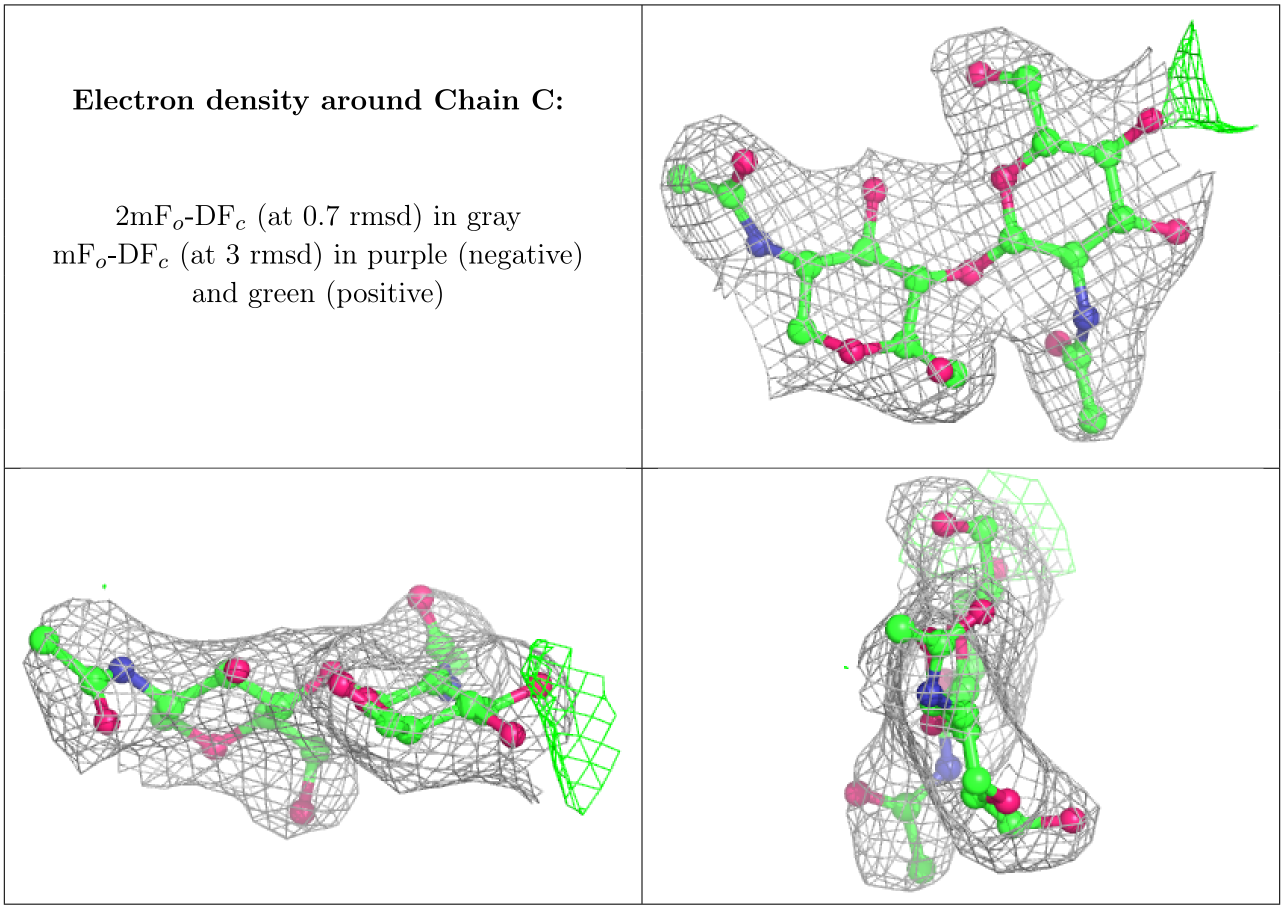
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

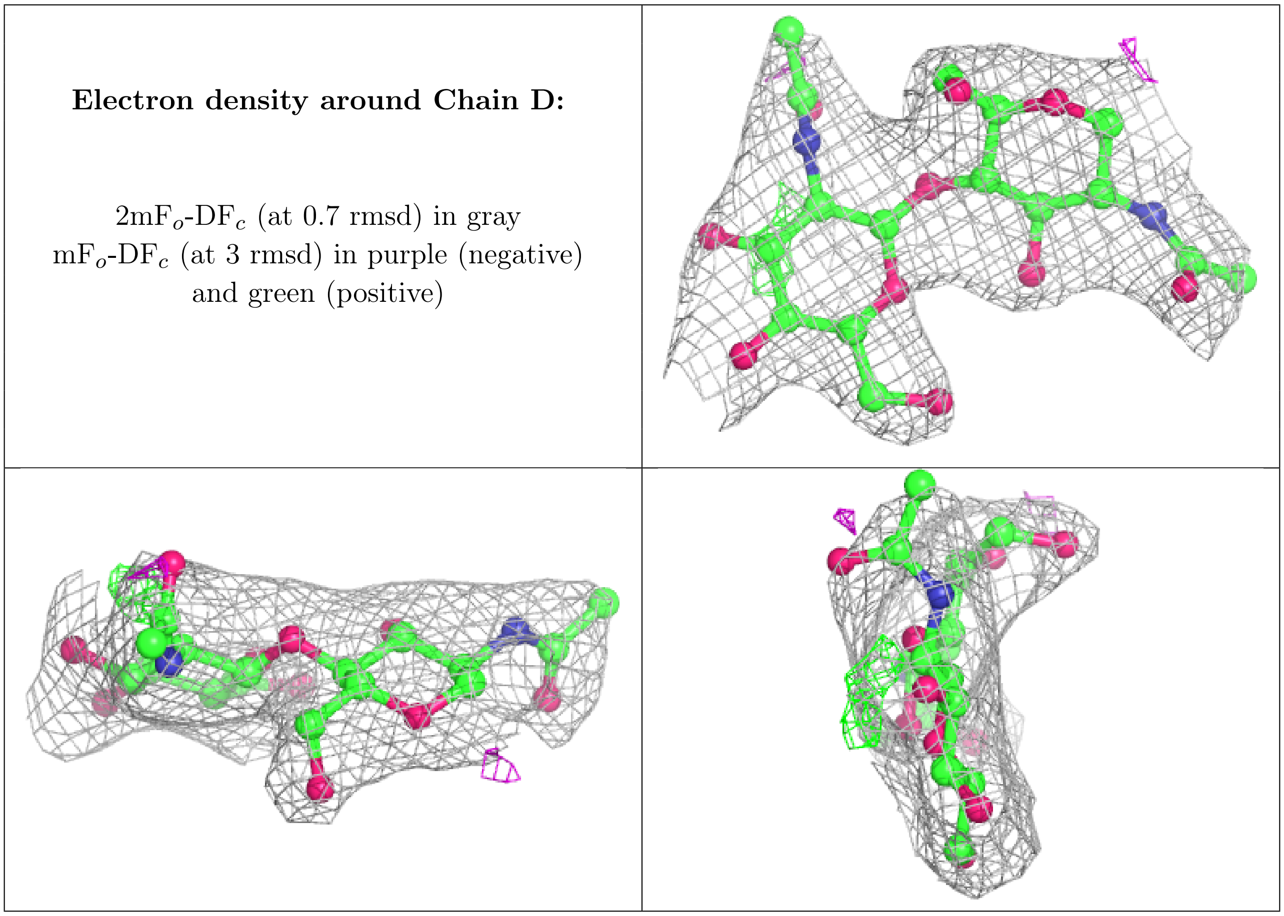
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	D	2	14/15	0.84	0.34	47,57,69,69	0
2	NAG	C	2	14/15	0.88	0.25	41,46,57,62	0
2	NAG	D	1	14/15	0.96	0.21	35,38,44,48	0
2	NAG	C	1	14/15	0.97	0.20	31,34,41,49	0

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 D:

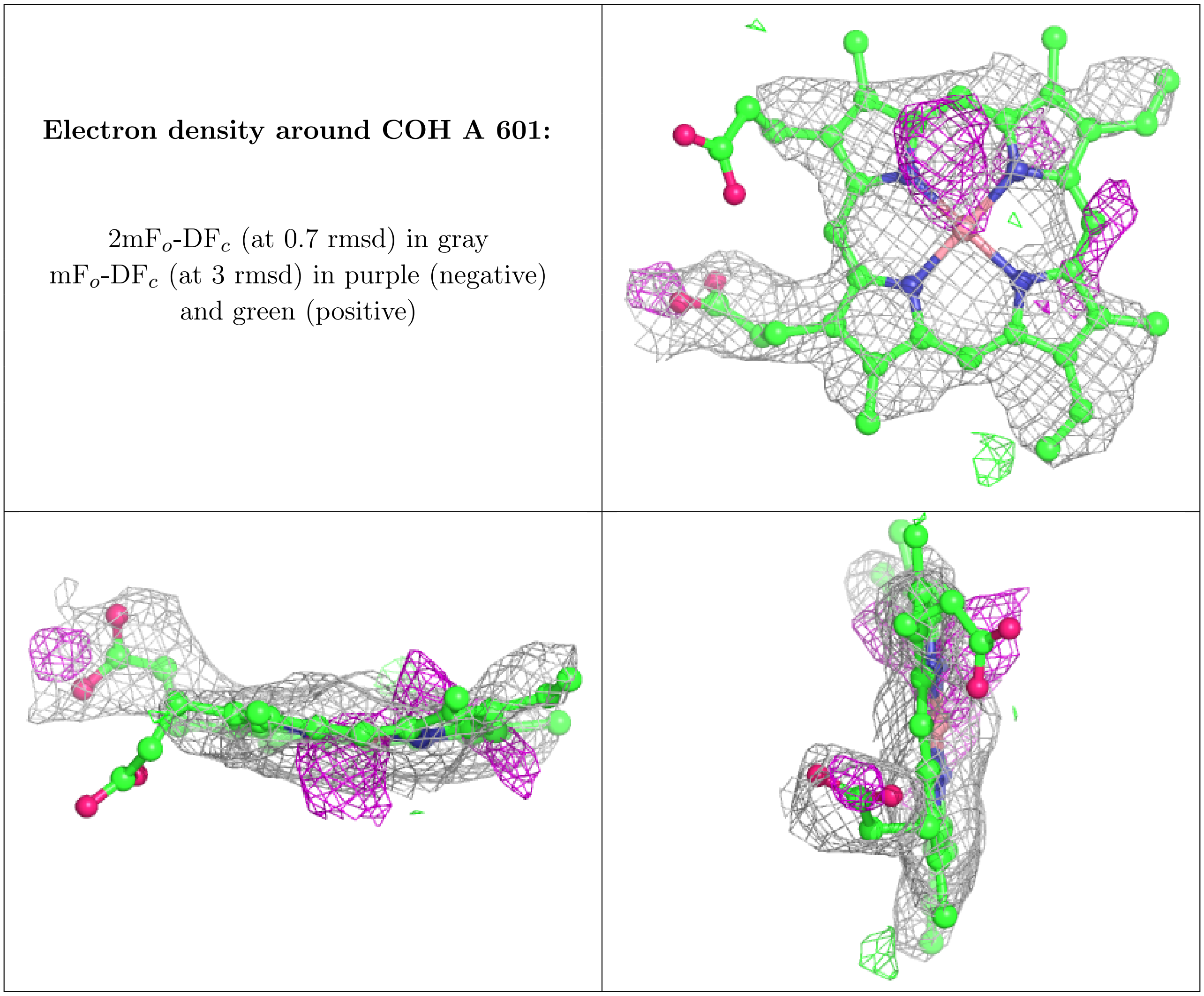
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.4 Ligands ⓘ

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	COH	A	601	43/43	0.83	0.31	50,87,105,109	0
3	COH	B	601	43/43	0.85	0.32	48,78,100,104	0
6	NAG	B	606	14/15	0.85	0.35	56,66,82,82	0
6	NAG	A	607	14/15	0.88	0.30	56,66,79,92	0
6	NAG	B	603	14/15	0.89	0.28	59,66,77,83	0
6	NAG	A	604	14/15	0.91	0.31	50,53,64,70	0
5	BOG	A	603	20/20	0.95	0.22	43,49,66,71	0
4	CEL	B	602	26/26	0.96	0.15	37,43,49,67	0
4	CEL	A	602	26/26	0.96	0.13	36,38,48,49	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.

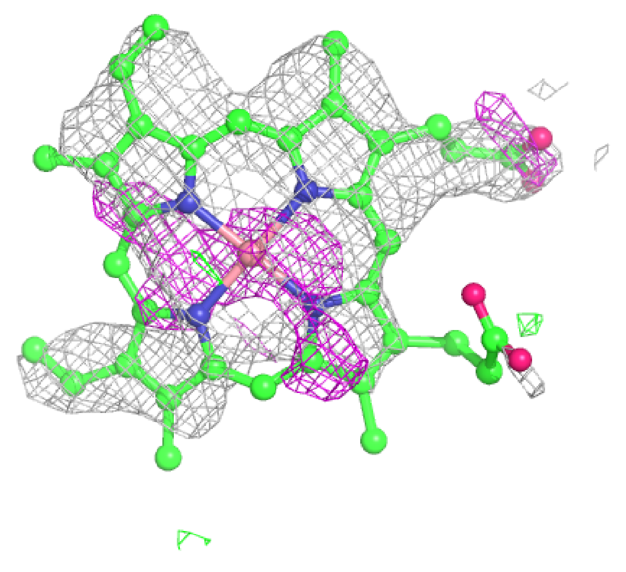


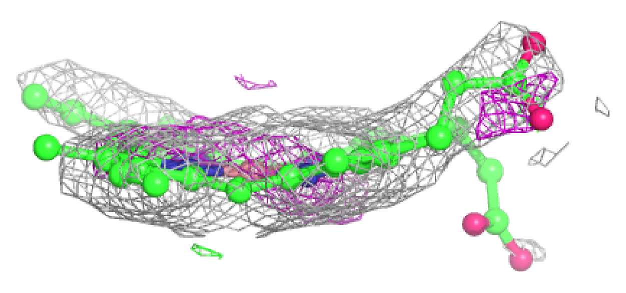
Electron density around COH A 601:

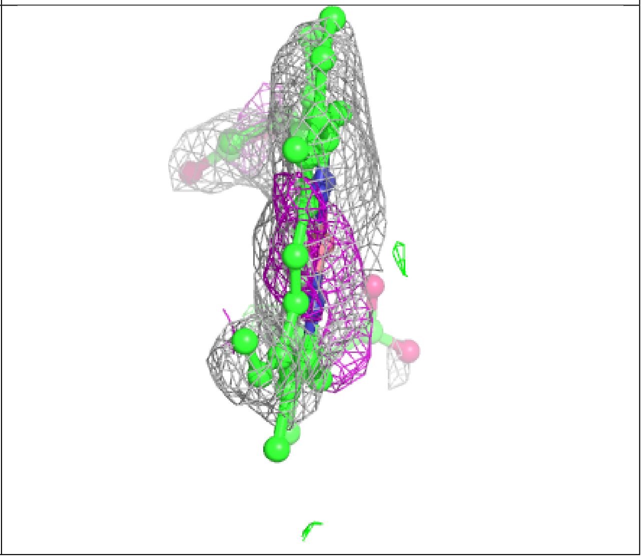
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around COH 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)

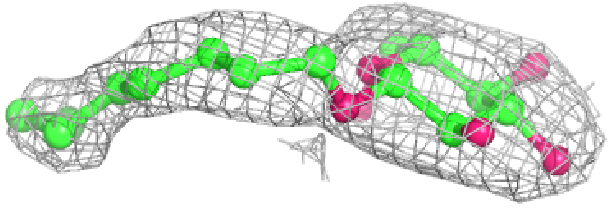


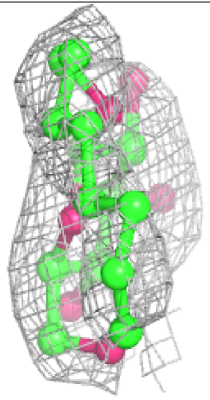




Electron density around BOG A 603:

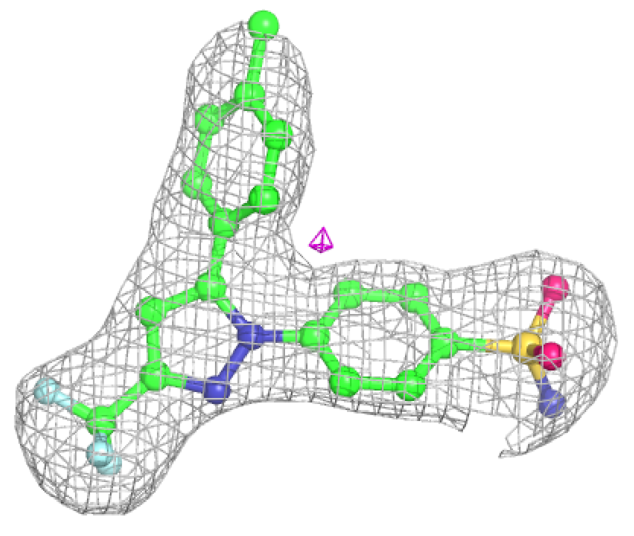
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

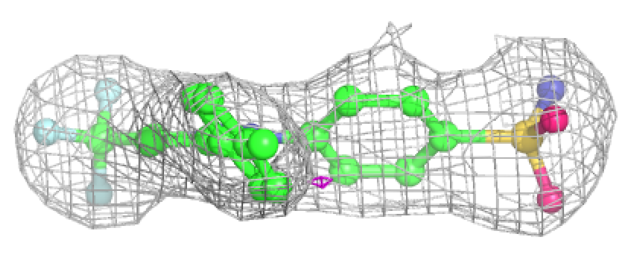


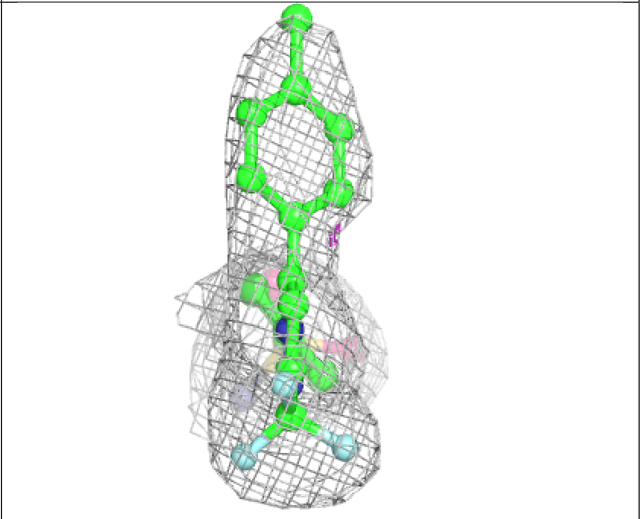


Electron density around CEL B 602:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

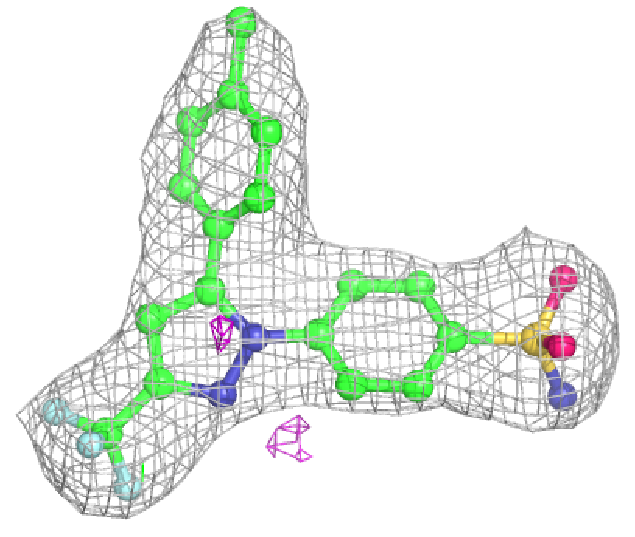


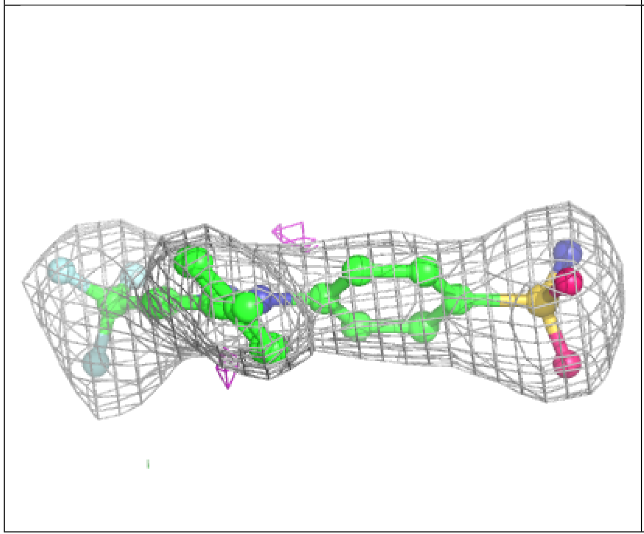


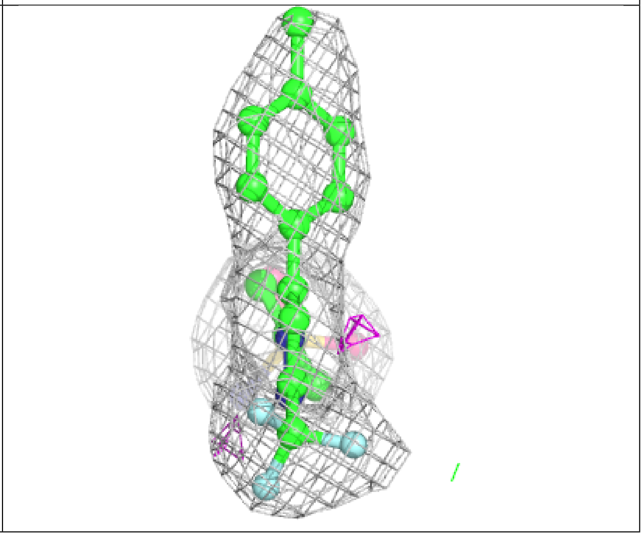


Electron density around CEL A 602:

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 ⓘ

There are no such residues in this entry.