Full wwPDB X-ray Structure Validation Report (i)

Oct 1, 2023 – 02:16 PM EDT

PDB ID	:	4OTY
Title	:	Crystal structure of lumiracoxib bound to the apo-mouse-cyclooxygenase-2
Authors	:	Xu, S.; Windsor, M.A.; Banerjee, S.; Marnett, L.J.
Deposited on	:	2014-02-14
Resolution	:	2.35 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

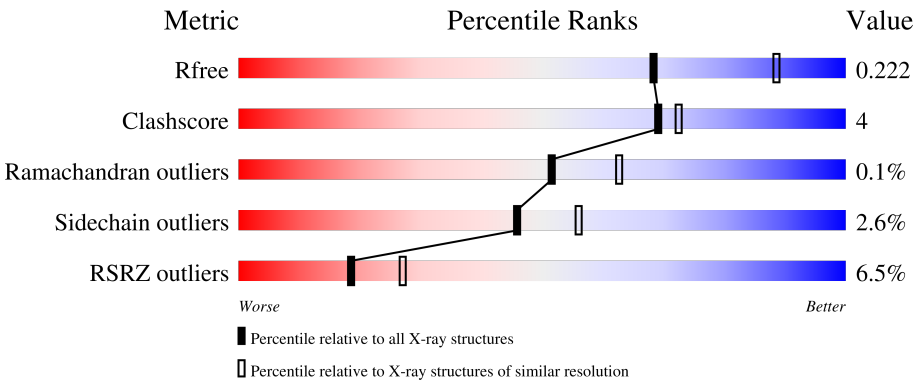
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	587	6% 86% 8% • 6%
1	B	587	6% 82% 11% • 6%
2	C	2	50% 50%
2	D	2	50% 50%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9418 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

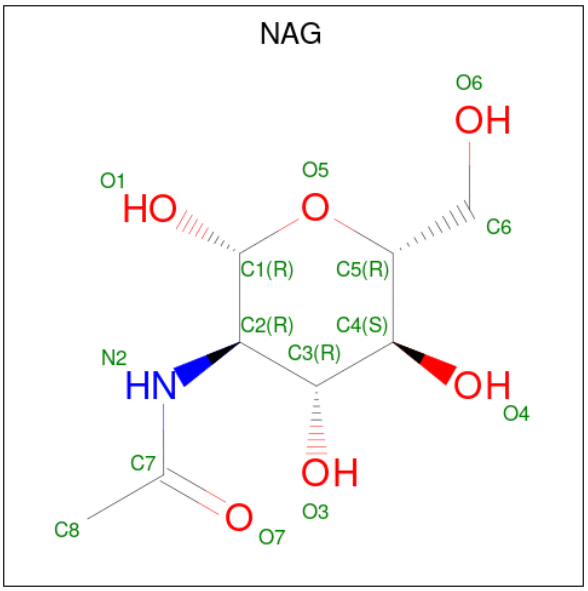
- Molecule 1 is a protein called Prostaglandin G/H synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	552	4474	2885	750	814	25	0	0	0
1	B	551	4465	2880	748	812	25	0	0	0

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

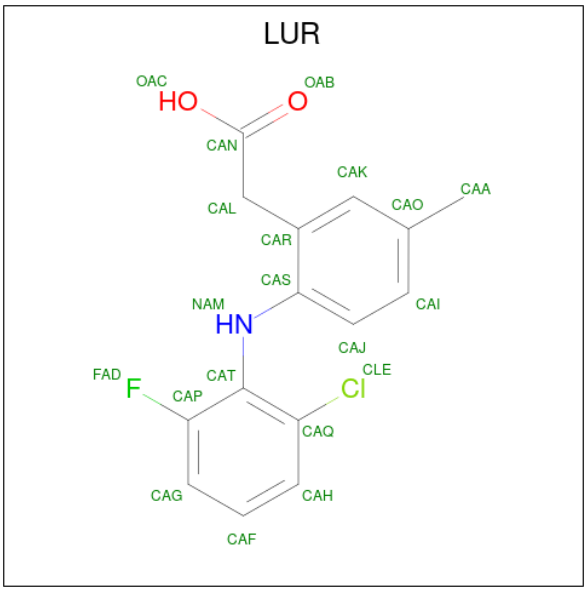
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0
2	D	2	28	16	2	10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



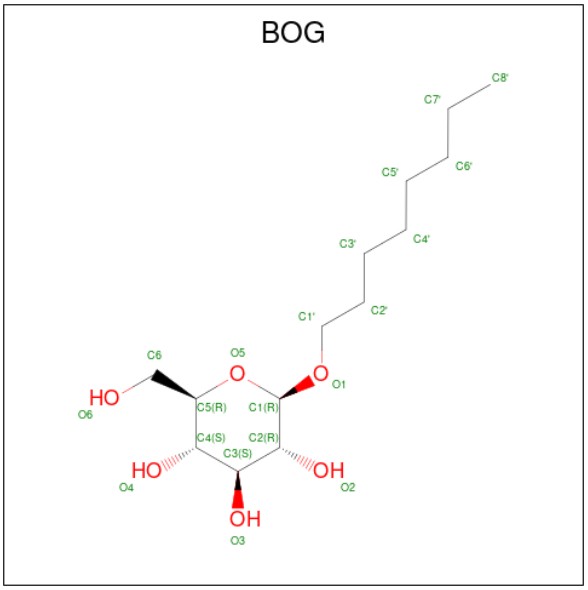
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
			Total	C	N	O		
3	B	1	14	8	1	5	0	0
			Total	C	N	O		
3	B	1	14	8	1	5	0	0

- Molecule 4 is {2-[(2-chloro-6-fluorophenyl)amino]-5-methylphenyl}acetic acid (three-letter code: LUR) (formula: $C_{15}H_{13}ClFNO_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	F	N	O		
4	A	1	20	15	1	1	1	2	0	0
4	B	1	20	15	1	1	1	2	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	B	1	20	14	6	0	0

- Molecule 6 is water.

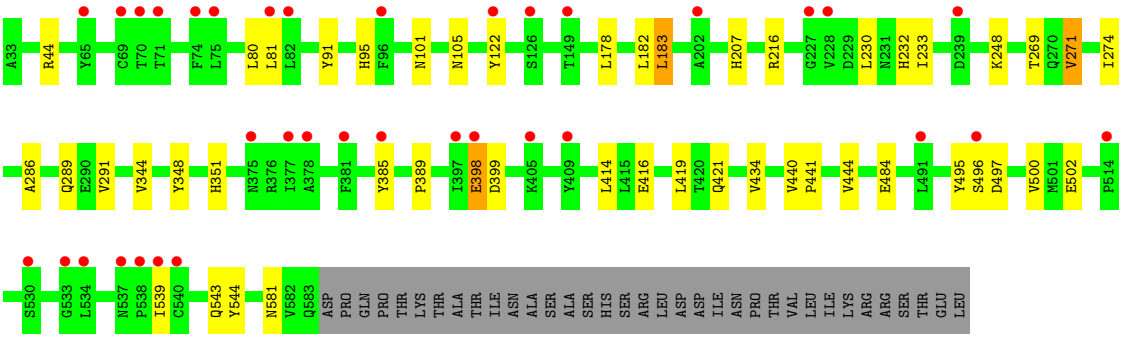
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	152	152	152	0	0
6	B	155	155	155	0	0

3 Residue-property plots (i)

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

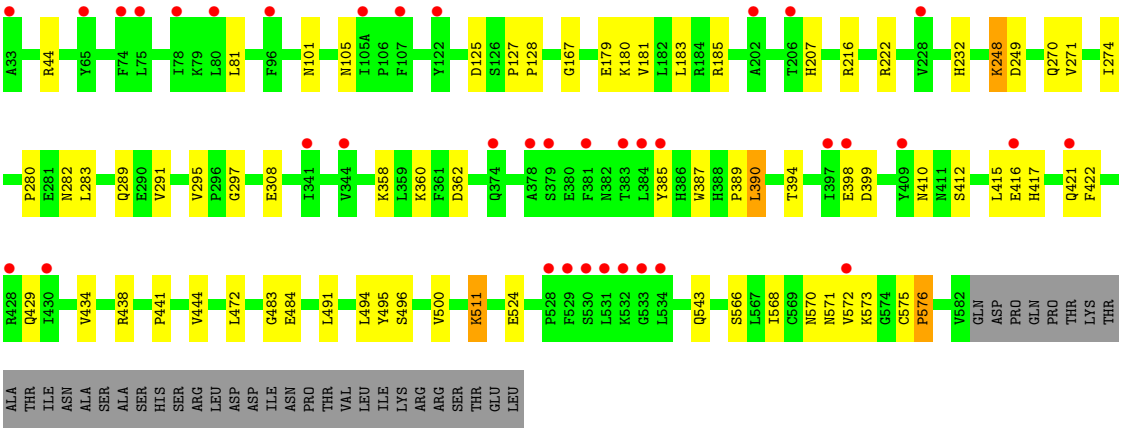
• Molecule 1: Prostaglandin G/H synthase 2

Chain A:



• Molecule 1: Prostaglandin G/H synthase 2

Chain B:



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

Chain C:

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

Chain 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	122.66Å 133.17Å 181.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.12 – 2.35 43.12 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.12-2.35) 99.6 (43.12-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.37Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.180 , 0.221 0.188 , 0.222	Depositor DCC
R_{free} test set	1876 reflections (3.05%)	wwPDB-VP
Wilson B-factor (Å^2)	48.8	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9418	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BOG, NAG, LUR

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	0.42	0/4601	0.42	1/6239 (0.0%)
1	B	0.43	2/4592 (0.0%)	0.43	2/6227 (0.0%)
All	All	0.42	2/9193 (0.0%)	0.42	3/12466 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	576	PRO	N-CD	5.39	1.55	1.47
1	B	128	PRO	N-CD	5.05	1.54	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	440	VAL	C-N-CD	5.66	140.28	128.40
1	B	511	LYS	C-N-CD	5.63	140.23	128.40
1	B	127	PRO	C-N-CD	5.49	139.94	128.40

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	4474	0	4373	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4465	0	4364	41	0
2	C	28	0	25	1	0
2	D	28	0	25	1	0
3	A	28	0	26	0	0
3	B	28	0	26	1	0
4	A	20	0	12	0	0
4	B	20	0	12	0	0
5	B	20	0	27	1	0
6	A	152	0	0	0	0
6	B	155	0	0	3	0
All	All	9418	0	8890	66	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 (66) 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:398:GLU:OE1	1:B:399:ASP:OD1	1.91	0.87
1:B:398:GLU:OE1	1:B:399:ASP:CG	2.15	0.84
1:B:568:ILE:HG23	1:B:572:VAL:HG21	1.62	0.81
1:A:398:GLU:HG3	1:A:421:GLN:CD	2.04	0.77
1:B:185:ARG:NH1	1:B:438:ARG:HG2	2.04	0.72
1:A:398:GLU:HG3	1:A:421:GLN:OE1	1.95	0.66
1:A:216:ARG:NH1	2:C:2:NAG:O7	2.29	0.65
1:B:568:ILE:HG23	1:B:572:VAL:CG2	2.27	0.64
1:B:398:GLU:HG3	1:B:421:GLN:HE22	1.64	0.63
1:B:101:ASN:O	1:B:105:ASN:ND2	2.30	0.62
1:B:216:ARG:NH1	2:D:2:NAG:O7	2.33	0.61
1:A:495:TYR:O	1:A:496:SER:HB2	2.03	0.58
1:A:389:PRO:HB2	1:A:434:VAL:HA	1.85	0.57
1:B:248:LYS:HE3	1:B:249:ASP:H	1.70	0.57
1:B:389:PRO:HB2	1:B:434:VAL:HA	1.86	0.56
1:A:398:GLU:HG3	1:A:421:GLN:CG	2.35	0.56
1:A:399:ASP:N	1:A:399:ASP:OD1	2.37	0.56
1:B:495:TYR:O	1:B:496:SER:HB2	2.06	0.55
1:B:398:GLU:HG3	1:B:421:GLN:NE2	2.23	0.54
1:B:572:VAL:HG11	1:B:576:PRO:HG3	1.90	0.53
1:B:44:ARG:NH2	1:B:125:ASP:OD1	2.40	0.53
1:B:179:GLU:O	1:B:185:ARG:NH2	2.41	0.53
1:A:101:ASN:O	1:A:105:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:THR:O	1:B:429:GLN:NE2	2.41	0.52
1:B:483:GLY:HA3	1:B:511:LYS:HD2	1.91	0.52
1:B:566:SER:O	1:B:570:ASN:HB2	2.10	0.52
1:A:274:ILE:HD12	1:A:291:VAL:HG12	1.92	0.51
1:A:441:PRO:HG2	1:A:444:VAL:HG22	1.93	0.50
1:B:360:LYS:HE2	1:B:362:ASP:HB2	1.93	0.50
1:B:295:VAL:HG12	1:B:297:GLY:H	1.77	0.50
1:A:497:ASP:HB3	1:A:500:VAL:HG23	1.93	0.50
1:B:222:ARG:NH1	6:B:857:HOH:O	2.43	0.50
1:B:410:ASN:OD1	1:B:412:SER:OG	2.24	0.49
1:B:183:LEU:O	1:B:185:ARG:NH1	2.43	0.49
1:B:416:GLU:OE1	3:B:703:NAG:O6	2.29	0.49
1:A:351:HIS:CE1	1:A:581:ASN:HB3	2.48	0.49
1:B:417:HIS:O	1:B:421:GLN:HG3	2.13	0.49
1:B:472:LEU:HD21	1:B:524:GLU:HG3	1.94	0.49
1:B:572:VAL:HG11	1:B:576:PRO:CG	2.43	0.48
1:B:572:VAL:HB	1:B:576:PRO:HD2	1.94	0.48
1:A:91:TYR:O	1:A:95:HIS:ND1	2.43	0.48
1:A:539:ILE:HA	1:A:544:TYR:HB3	1.97	0.47
1:B:572:VAL:CG1	1:B:576:PRO:CD	2.93	0.46
1:A:495:TYR:HE2	1:A:502:GLU:HG3	1.81	0.46
1:A:271:VAL:HG22	1:A:286:ALA:HB1	1.98	0.45
5:B:706:BOG:H5'1	5:B:706:BOG:H2'1	1.68	0.45
1:B:167:GLY:HA3	1:B:500:VAL:HG21	1.99	0.44
1:B:280:PRO:HG2	1:B:283:LEU:HD12	2.00	0.44
1:A:269:THR:HB	1:A:271:VAL:HG13	1.99	0.44
1:B:283:LEU:HD21	1:B:415:LEU:HD12	2.00	0.43
1:A:414:LEU:HD11	1:A:419:LEU:HD23	1.99	0.43
1:B:472:LEU:HD11	1:B:524:GLU:HB2	2.00	0.43
1:A:543:GLN:HB2	6:B:807:HOH:O	2.17	0.43
1:B:387:TRP:O	1:B:390:LEU:HB2	2.18	0.43
1:A:344:VAL:O	1:A:348:TYR:HB3	2.19	0.42
1:A:344:VAL:HA	1:A:348:TYR:HB3	2.00	0.42
1:B:274:ILE:HD12	1:B:291:VAL:HG12	2.01	0.42
1:B:573:LYS:C	1:B:575:CYS:H	2.22	0.41
1:B:180:LYS:HD2	1:B:494:LEU:HD11	2.02	0.41
1:B:308:GLU:HB2	1:B:571:ASN:HD21	1.84	0.41
1:A:178:LEU:HG	1:A:183:LEU:HD13	2.02	0.41
1:B:181:VAL:HG21	1:B:491:LEU:HD21	2.02	0.41
1:A:230:LEU:HG	1:A:233:ILE:HD12	2.02	0.41
1:A:178:LEU:HA	1:A:182:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:PRO:HG2	1:B:444:VAL:HG22	2.02	0.40
1:B:543:GLN:HB2	6:B:815:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/587 (94%)	534 (97%)	15 (3%)	1 (0%)	47	56
1	B	549/587 (94%)	532 (97%)	17 (3%)	0	100	100
All	All	1099/1174 (94%)	1066 (97%)	32 (3%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	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	493/525 (94%)	480 (97%)	13 (3%)	46	56
1	B	492/525 (94%)	479 (97%)	13 (3%)	46	56
All	All	985/1050 (94%)	959 (97%)	26 (3%)	46	56

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	80	LEU
1	A	81	LEU
1	A	122	TYR
1	A	183	LEU
1	A	207	HIS
1	A	232	HIS
1	A	248	LYS
1	A	271	VAL
1	A	289	GLN
1	A	385	TYR
1	A	416	GLU
1	A	484	GLU
1	B	81	LEU
1	B	207	HIS
1	B	232	HIS
1	B	248	LYS
1	B	270	GLN
1	B	271	VAL
1	B	282	ASN
1	B	289	GLN
1	B	358	LYS
1	B	385	TYR
1	B	390	LEU
1	B	422	PHE
1	B	484	GLU

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

Mol	Chain	Res	Type
1	B	255	GLN
1	B	421	GLN
1	B	461	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	0.31	0	17,19,21	0.51	0
2	NAG	C	2	2	14,14,15	0.35	0	17,19,21	0.41	0
2	NAG	D	1	2,1	14,14,15	0.37	0	17,19,21	0.51	0
2	NAG	D	2	2	14,14,15	0.30	0	17,19,21	0.40	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	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

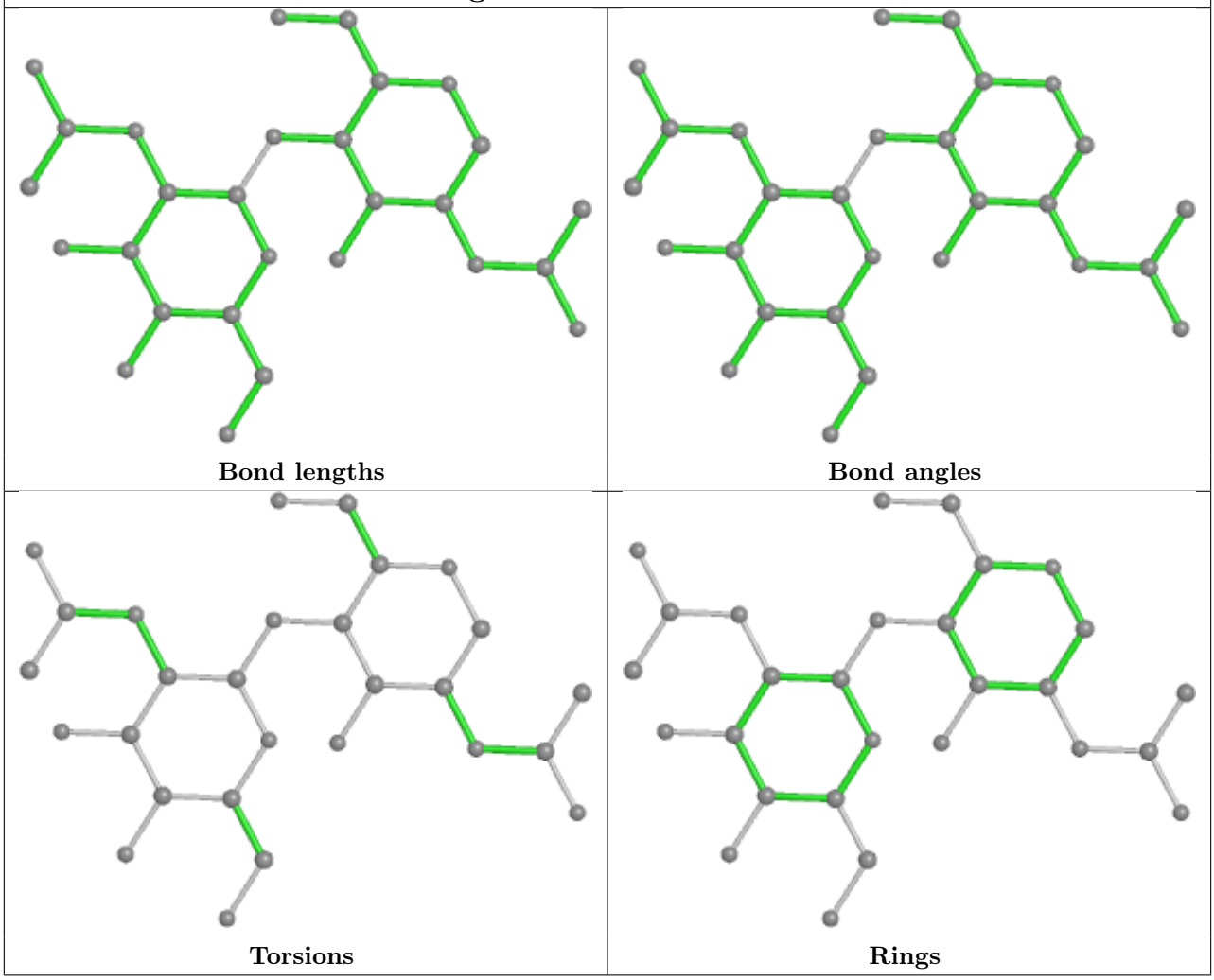
There are no ring outliers.

2 monomers are involved in 2 short contacts:

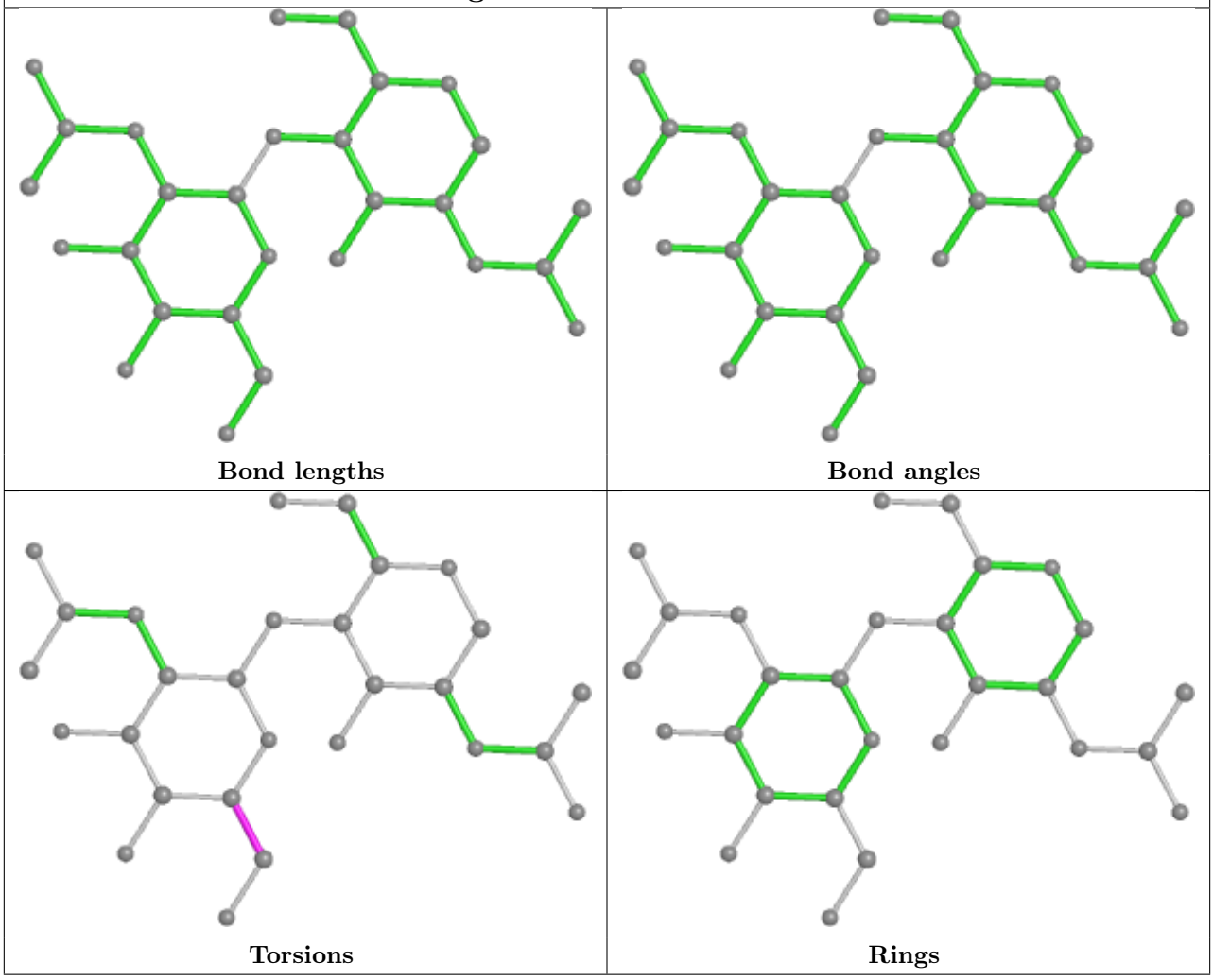
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0
2	D	2	NAG	1	0

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

Oligosaccharide Chain C



Oligosaccharide Chain D



5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
3	NAG	A	703	1	14,14,15	0.34	0	17,19,21	0.51	0
3	NAG	B	704	1	14,14,15	0.31	0	17,19,21	0.43	0
3	NAG	A	704	1	14,14,15	0.34	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	BOG	B	706	-	20,20,20	1.35	3 (15%)	25,25,25	1.17	2 (8%)
3	NAG	B	703	1	14,14,15	0.30	0	17,19,21	0.50	0
4	LUR	A	705	-	21,21,21	2.87	4 (19%)	28,29,29	1.41	3 (10%)
4	LUR	B	705	-	21,21,21	2.91	4 (19%)	28,29,29	1.41	2 (7%)

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
3	NAG	A	703	1	-	1/6/23/26	0/1/1/1
3	NAG	B	704	1	-	2/6/23/26	0/1/1/1
3	NAG	A	704	1	-	2/6/23/26	0/1/1/1
5	BOG	B	706	-	-	7/11/31/31	0/1/1/1
3	NAG	B	703	1	-	1/6/23/26	0/1/1/1
4	LUR	A	705	-	-	0/8/8/8	0/2/2/2
4	LUR	B	705	-	-	0/8/8/8	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	705	LUR	CAT-CAP	9.16	1.48	1.38
4	A	705	LUR	CAT-CAP	8.99	1.48	1.38
4	A	705	LUR	CAS-CAR	6.81	1.48	1.40
4	B	705	LUR	CAS-CAR	6.78	1.48	1.40
4	B	705	LUR	CAT-CAQ	5.78	1.48	1.40
4	A	705	LUR	CAT-CAQ	5.59	1.48	1.40
5	B	706	BOG	O2-C2	-2.77	1.36	1.43
4	B	705	LUR	CAQ-CLE	2.61	1.79	1.73
4	A	705	LUR	CAQ-CLE	2.57	1.79	1.73
5	B	706	BOG	O5-C5	-2.32	1.38	1.44
5	B	706	BOG	O5-C1	-2.01	1.36	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	705	LUR	CAG-CAP-CAT	-3.61	118.81	122.88
4	A	705	LUR	CAG-CAP-CAT	-3.45	118.99	122.88
4	B	705	LUR	FAD-CAP-CAT	3.27	120.52	117.70
4	A	705	LUR	FAD-CAP-CAT	3.07	120.34	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	706	BOG	O5-C1-O1	-2.71	103.56	109.97
5	B	706	BOG	C1'-O1-C1	2.66	118.26	113.84
4	A	705	LUR	CAR-CAK-CAO	-2.02	119.70	122.04

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	706	BOG	C2-C1-O1-C1'
5	B	706	BOG	O5-C1-O1-C1'
3	B	704	NAG	O5-C5-C6-O6
3	A	704	NAG	O5-C5-C6-O6
3	B	704	NAG	C4-C5-C6-O6
3	A	704	NAG	C4-C5-C6-O6
5	B	706	BOG	O1-C1'-C2'-C3'
5	B	706	BOG	C4'-C5'-C6'-C7'
5	B	706	BOG	C2'-C1'-O1-C1
5	B	706	BOG	C5'-C6'-C7'-C8'
5	B	706	BOG	C1'-C2'-C3'-C4'
3	B	703	NAG	C4-C5-C6-O6
3	A	703	NAG	C4-C5-C6-O6

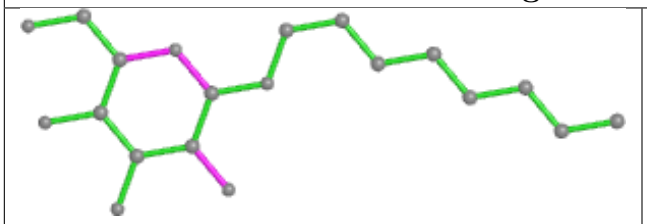
There are no ring outliers.

2 monomers are involved in 2 short contacts:

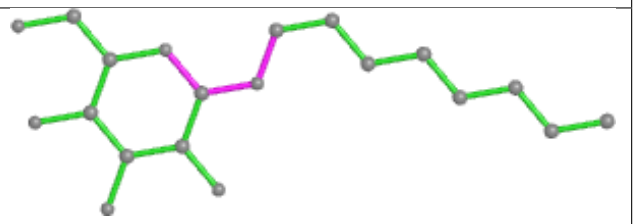
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	706	BOG	1	0
3	B	703	NAG	1	0

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

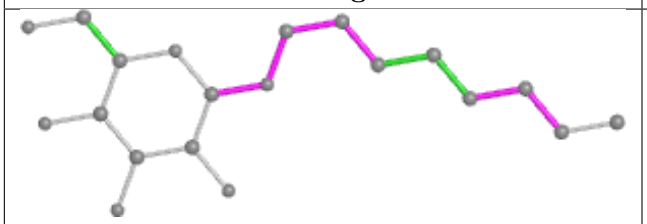
Ligand BOG B 706



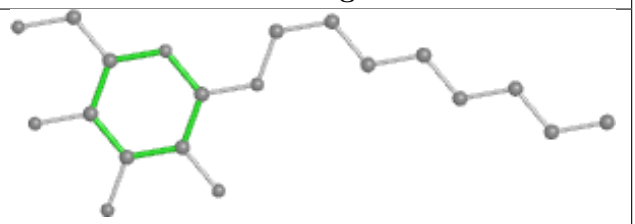
Bond lengths



Bond angles

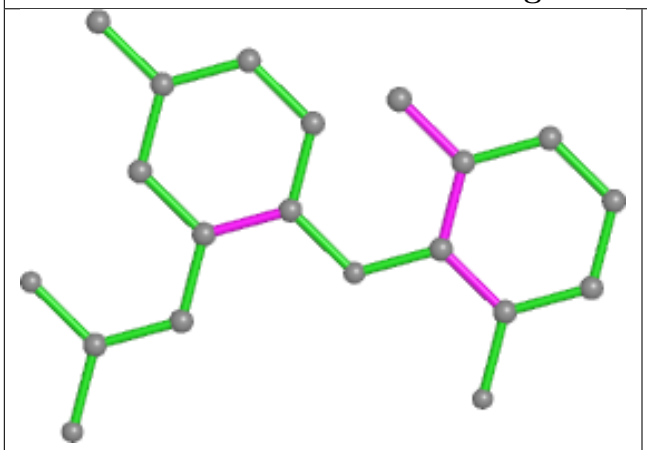


Torsions

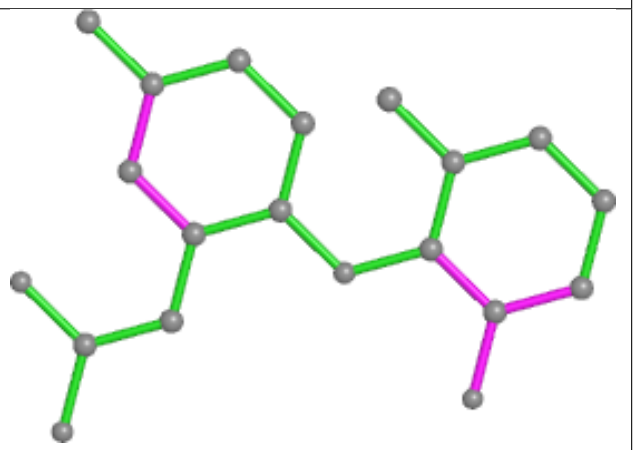


Rings

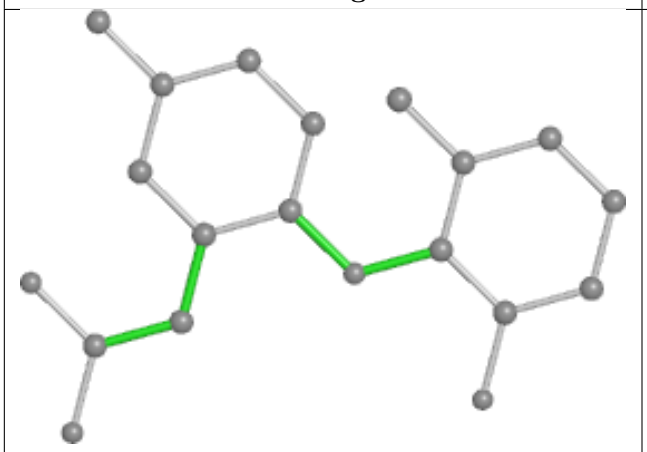
Ligand LUR A 705



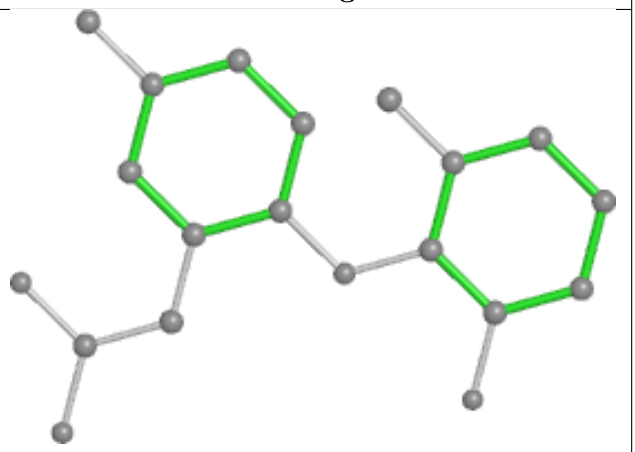
Bond lengths



Bond angles

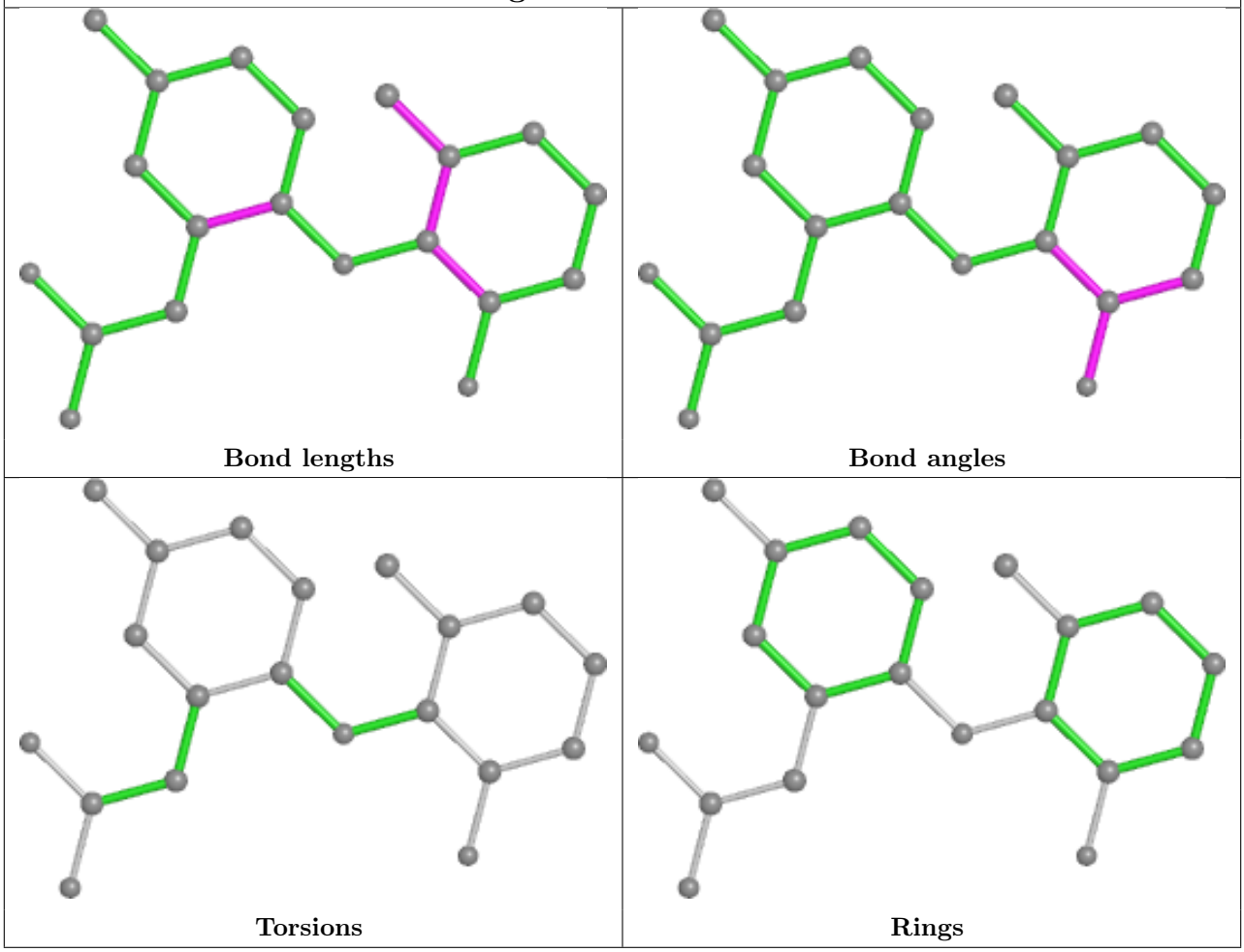


Torsions



Rings

Ligand LUR B 705



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	552/587 (94%)	0.20	35 (6%)	20	29	32, 51, 79, 124	0
1	B	551/587 (93%)	0.22	37 (6%)	17	26	35, 55, 86, 123	0
All	All	1103/1174 (93%)	0.21	72 (6%)	18	27	32, 54, 83, 124	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	74	PHE	4.4
1	A	74	PHE	4.2
1	A	65	TYR	4.0
1	B	533	GLY	3.6
1	A	82	LEU	3.4
1	A	81	LEU	3.4
1	A	533	GLY	3.2
1	B	397	ILE	3.1
1	B	96	PHE	3.1
1	B	107	PHE	3.1
1	B	381	PHE	3.1
1	B	378	ALA	3.1
1	B	202	ALA	3.0
1	A	530	SER	2.9
1	B	341	ILE	2.9
1	B	398	GLU	2.9
1	A	397	ILE	2.9
1	B	531	LEU	2.9
1	A	385	TYR	2.8
1	B	122	TYR	2.8
1	A	491	LEU	2.8
1	A	377	ILE	2.8
1	A	228	VAL	2.7
1	B	529	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	344	VAL	2.7
1	B	206	THR	2.7
1	B	409	TYR	2.7
1	B	572	VAL	2.7
1	B	75	LEU	2.6
1	A	539	ILE	2.5
1	B	430	ILE	2.5
1	A	534	LEU	2.5
1	A	378	ALA	2.5
1	A	96	PHE	2.4
1	B	530	SER	2.4
1	A	75	LEU	2.4
1	A	381	PHE	2.4
1	B	105(A)	ILE	2.4
1	A	375	ASN	2.4
1	A	398	GLU	2.4
1	B	385	TYR	2.3
1	B	384	LEU	2.3
1	B	416	GLU	2.3
1	A	202	ALA	2.3
1	A	540	CYS	2.3
1	B	228	VAL	2.3
1	A	514	PRO	2.3
1	A	227	GLY	2.2
1	B	374	GLN	2.2
1	B	379	SER	2.2
1	A	122	TYR	2.2
1	A	71	THR	2.2
1	A	126	SER	2.2
1	A	537	ASN	2.2
1	B	33	ALA	2.2
1	B	78	ILE	2.2
1	B	383	THR	2.2
1	A	405	LYS	2.1
1	A	538	PRO	2.1
1	B	421	GLN	2.1
1	B	532	LYS	2.1
1	B	534	LEU	2.1
1	A	239	ASP	2.1
1	A	69	CYS	2.1
1	A	70	THR	2.1
1	A	149	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	65	TYR	2.1
1	B	528	PRO	2.1
1	B	428	ARG	2.0
1	A	496	SER	2.0
1	A	409	TYR	2.0
1	B	80	LEU	2.0

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

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

6.3 Carbohydrates (i)

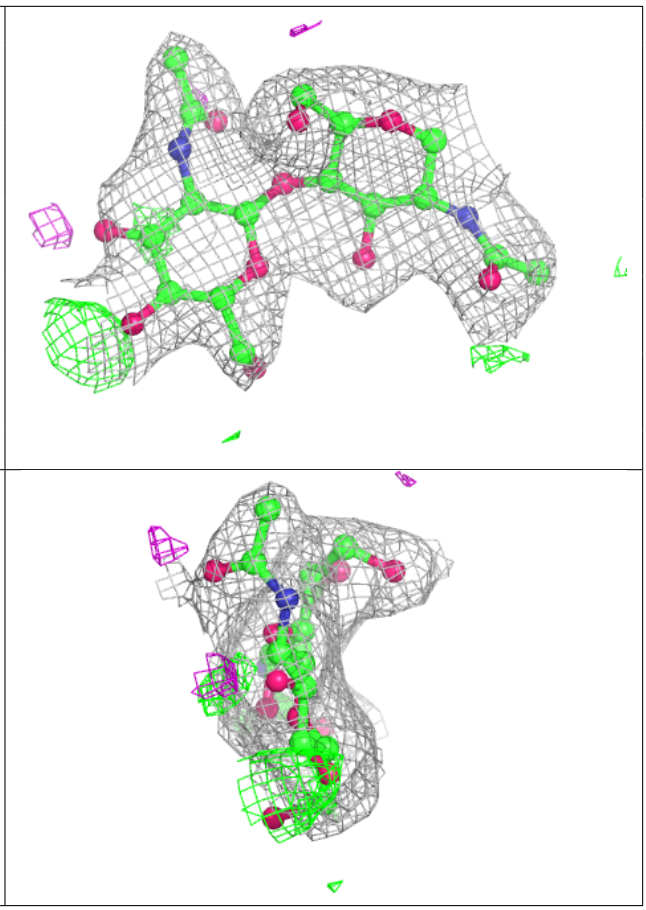
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

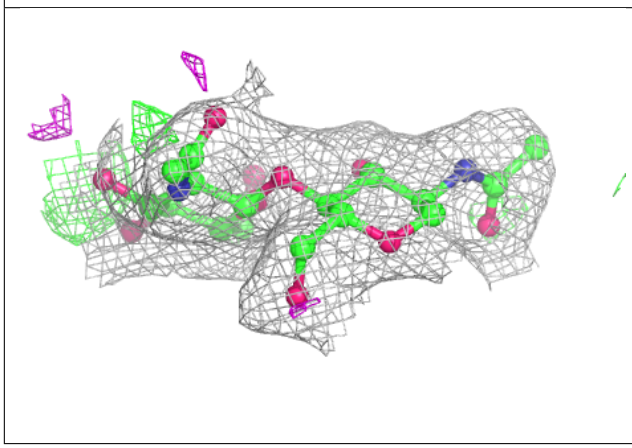
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	C	2	14/15	0.80	0.23	42,84,91,98	0
2	NAG	D	2	14/15	0.90	0.16	51,67,83,87	0
2	NAG	D	1	14/15	0.96	0.10	37,46,50,57	0
2	NAG	C	1	14/15	0.97	0.08	31,42,51,64	0

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:

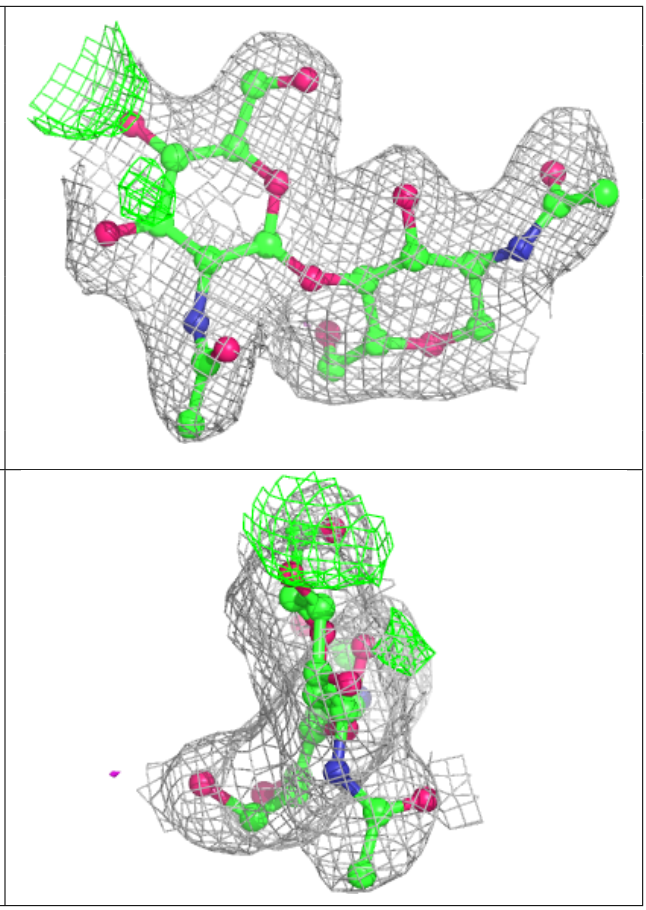
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





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 (i)

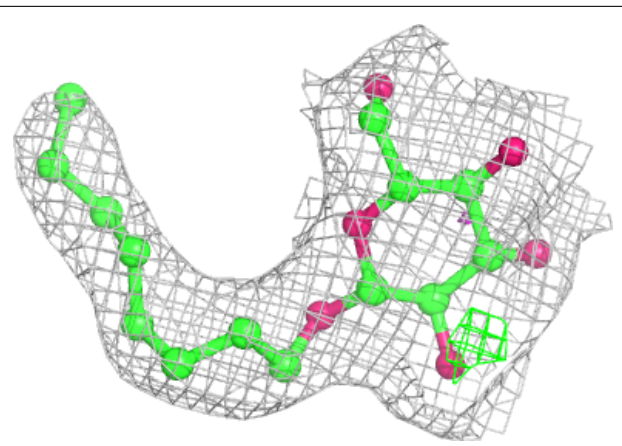
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

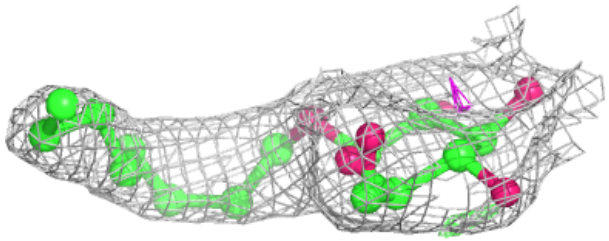
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	B	703	14/15	0.85	0.30	81,96,104,114	0
3	NAG	A	704	14/15	0.89	0.20	74,91,98,104	0
5	BOG	B	706	20/20	0.89	0.21	65,80,89,90	0
3	NAG	A	703	14/15	0.90	0.17	69,79,89,95	0
3	NAG	B	704	14/15	0.92	0.14	68,82,92,99	0
4	LUR	B	705	20/20	0.94	0.19	42,56,64,87	0
4	LUR	A	705	20/20	0.96	0.20	38,52,64,75	0

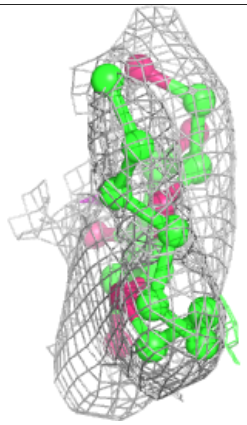
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BOG B 706:

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

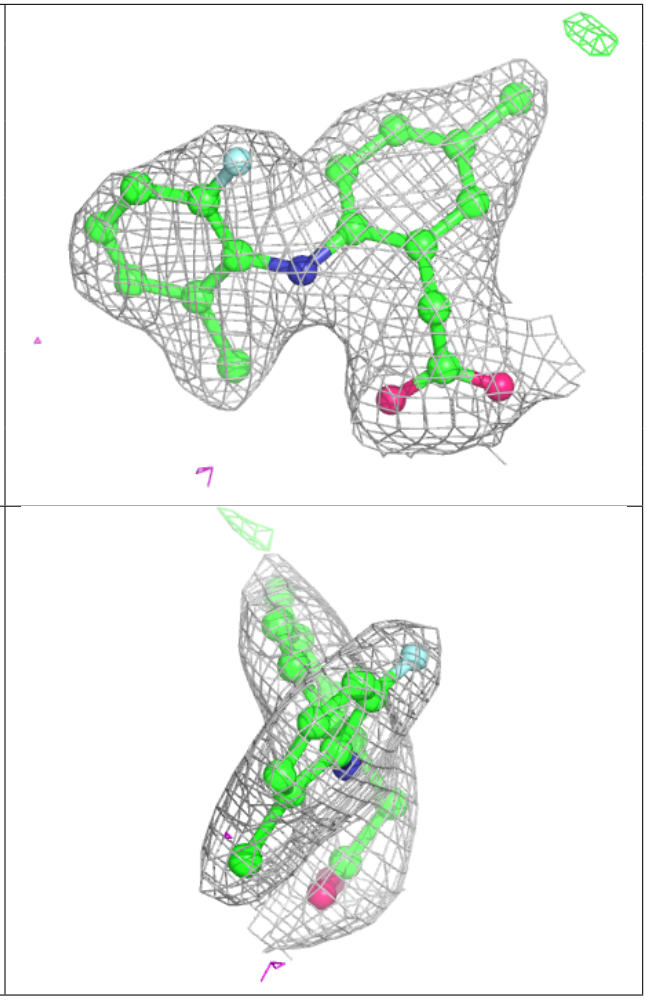






Electron density around LUR B 705:

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



Electron density around LUR A 705:

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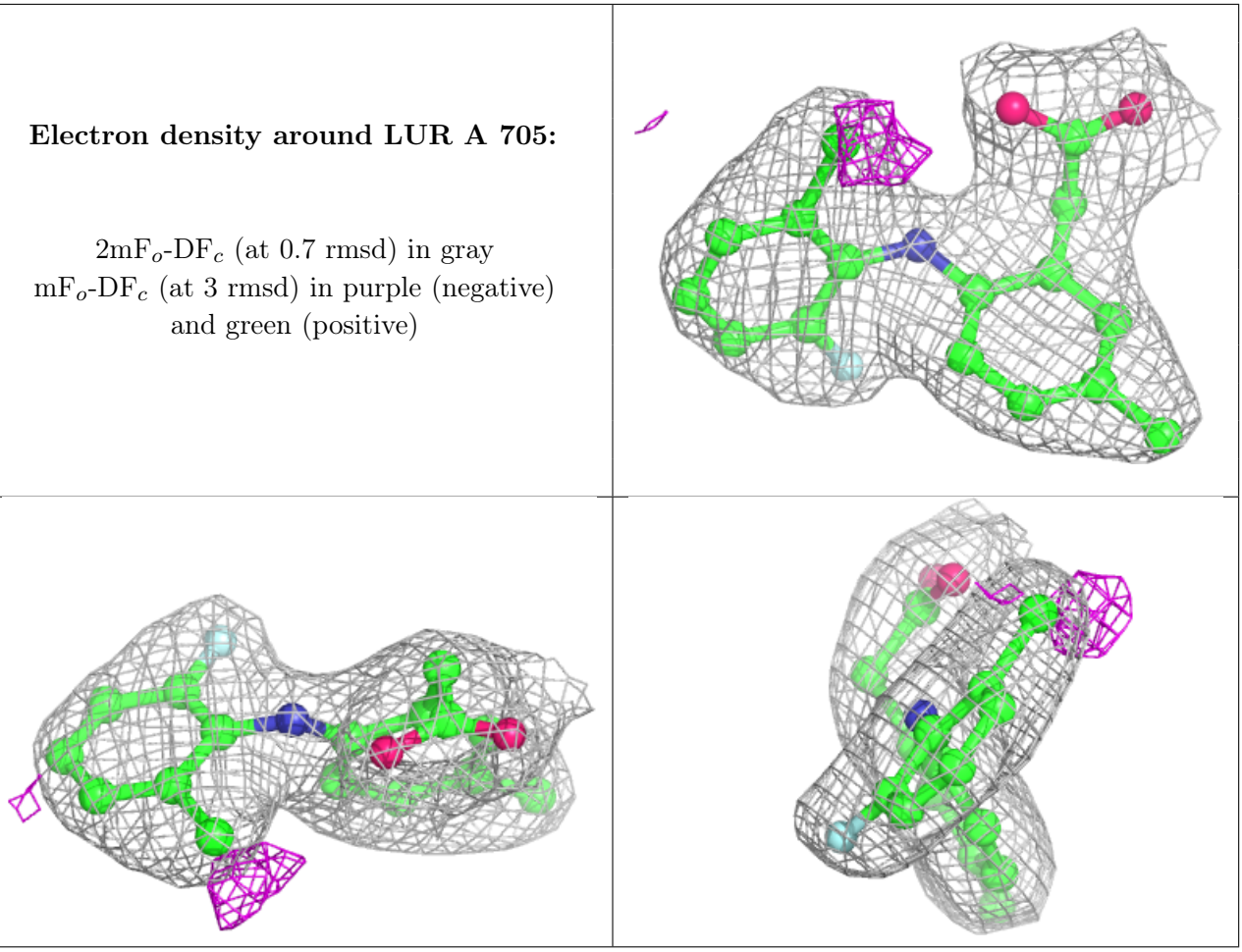
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.