



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:38 AM UTC

PDB ID : 4RRX / pdb_00004rrx
Title : Crystal Structure of Apo Murine V89W Cyclooxygenase-2 Complexed with Lumiracoxib
Authors : Xu, S.; Blobaum, A.L.; Banerjee, S.; Marnett, L.J.
Deposited on : 2014-11-06
Resolution : 2.78 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

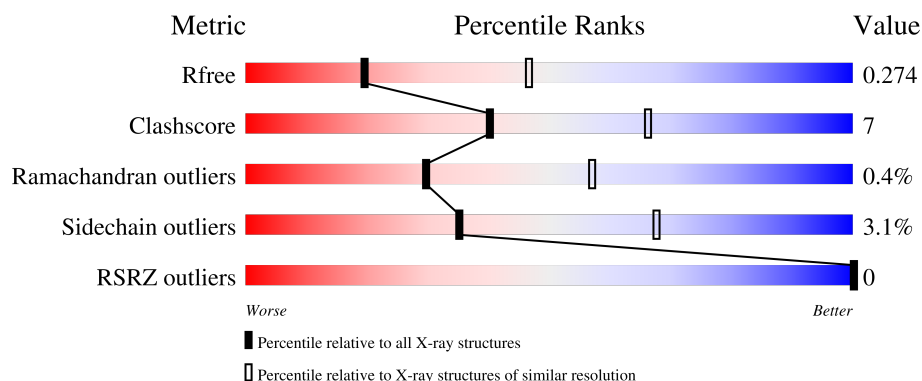
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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 $\leq 5\%$. 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	587	 76% 17% • 6%
1	B	587	 77% 16% •• 6%
2	C	2	 50% 50%
2	D	2	 50% 50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9409 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	0	3	0
			4506	2905	757	819	25			
1	B	552	Total	C	N	O	S	0	2	0
			4498	2900	754	819	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	TRP	VAL	engineered mutation	UNP Q05769
B	89	TRP	VAL	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.



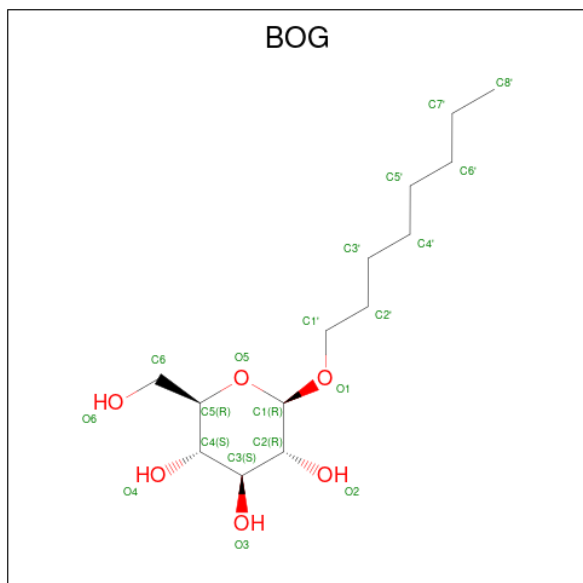
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



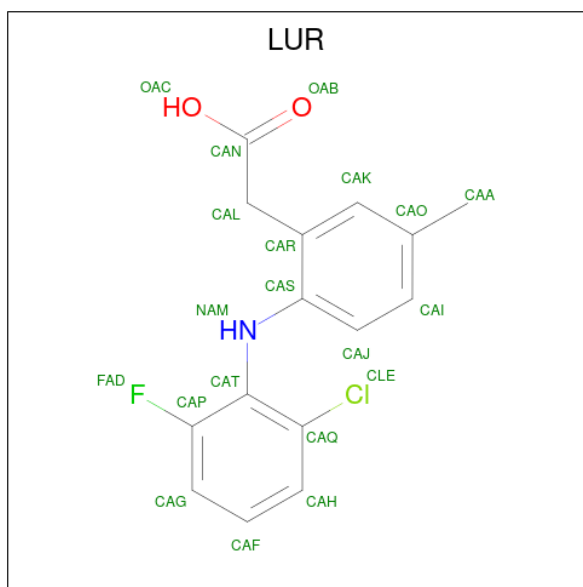
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



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

- Molecule 5 is {2-[(2-chloro-6-fluorophenyl)amino]-5-methylphenyl}acetic acid (CCD ID: LUR) (formula: C₁₅H₁₃ClFNO₂).



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

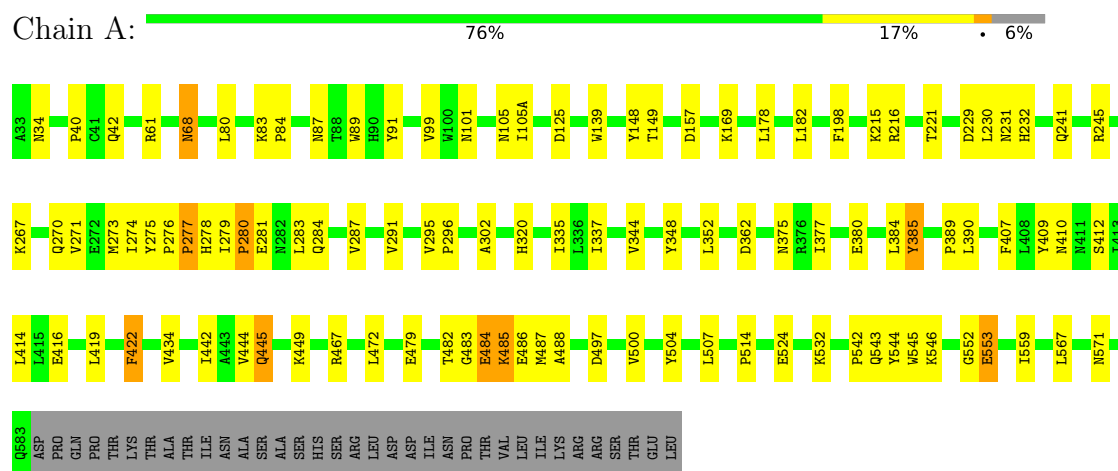
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	101	Total	O	0	0
			101	101		
6	B	112	Total	O	0	0
			112	112		

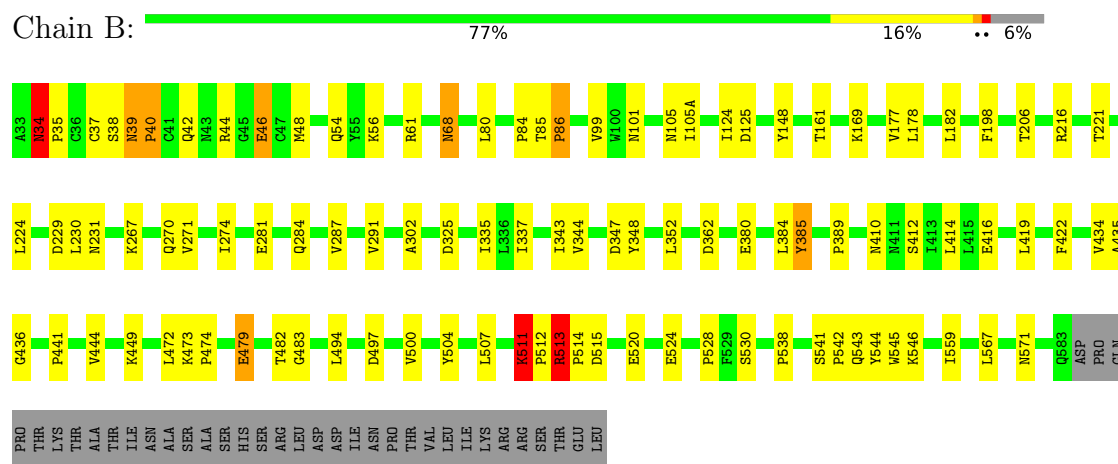
3 Residue-property plots

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





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

Chain D:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	180.99Å 132.43Å 120.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.25 – 2.78 45.25 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.25-2.78) 72.0 (45.25-2.78)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.91 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.249 , 0.277 0.253 , 0.274	Depositor DCC
R_{free} test set	1091 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 20.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9409	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.38% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BOG, 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	0.55	5/4638 (0.1%)	0.78	9/6289 (0.1%)
1	B	0.58	4/4627 (0.1%)	0.83	14/6275 (0.2%)
All	All	0.56	9/9265 (0.1%)	0.81	23/12564 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	34	ASN	C-N	6.53	1.40	1.33
1	A	552	GLY	C-O	-5.73	1.17	1.23
1	A	279	ILE	C-N	5.34	1.40	1.33
1	A	275	TYR	C-N	5.32	1.39	1.33
1	B	86	PRO	N-CD	5.27	1.55	1.47
1	B	84	PRO	N-CD	5.20	1.55	1.47
1	A	280	PRO	N-CD	5.12	1.54	1.47
1	A	277	PRO	N-CD	5.04	1.54	1.47
1	B	40	PRO	N-CD	5.01	1.54	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	TYR	CA-C-N	-6.63	113.55	120.38
1	A	275	TYR	C-N-CA	-6.63	113.55	120.38
1	B	34	ASN	CA-C-N	-6.61	113.11	120.45
1	B	34	ASN	C-N-CA	-6.61	113.11	120.45
1	B	511	LYS	CA-C-N	-6.53	113.05	119.78
1	B	511	LYS	C-N-CA	-6.53	113.05	119.78
1	A	279	ILE	CA-C-N	-5.85	113.56	120.11
1	A	279	ILE	C-N-CA	-5.85	113.56	120.11
1	A	105(A)	ILE	CA-C-N	5.69	126.95	119.84
1	A	105(A)	ILE	C-N-CA	5.69	126.95	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	ASN	CA-C-N	-5.64	113.21	119.19
1	B	39	ASN	C-N-CA	-5.64	113.21	119.19
1	B	105(A)	ILE	CA-C-N	5.60	126.84	119.84
1	B	105(A)	ILE	C-N-CA	5.60	126.84	119.84
1	A	486	GLU	N-CA-C	5.27	116.88	111.03
1	A	362	ASP	CA-C-N	5.24	124.91	119.56
1	A	362	ASP	C-N-CA	5.24	124.91	119.56
1	B	362	ASP	CA-C-N	5.18	124.84	119.56
1	B	362	ASP	C-N-CA	5.18	124.84	119.56
1	B	513	ARG	CA-C-N	-5.17	113.38	119.84
1	B	513	ARG	C-N-CA	-5.17	113.38	119.84
1	B	161	THR	CA-C-N	-5.00	113.59	119.84
1	B	161	THR	C-N-CA	-5.00	113.59	119.84

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	4506	0	4397	65	0
1	B	4498	0	4384	60	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	0	0
4	A	20	0	28	5	0
4	B	20	0	28	0	0
5	A	20	0	12	1	0
5	B	20	0	12	2	0
6	A	101	0	0	8	0
6	B	112	0	0	8	0
All	All	9409	0	8963	120	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 7.

All (120) 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:206:THR:HG21	1:B:385:TYR:CZ	1.71	1.25
1:B:206:THR:HG21	1:B:385:TYR:CE1	1.87	1.07
1:A:553:GLU:HG3	6:A:882:HOH:O	1.72	0.89
1:B:206:THR:CG2	1:B:385:TYR:CZ	2.57	0.88
1:A:442:ILE:O	1:A:445:GLN:HG2	1.74	0.86
1:B:267:LYS:O	1:B:270:GLN:NE2	2.25	0.69
1:B:567:LEU:O	1:B:571:ASN:ND2	2.25	0.69
1:A:479:GLU:O	1:A:483:GLY:N	2.26	0.66
1:B:216:ARG:NH1	2:D:2:NAG:O7	2.29	0.66
1:B:229:ASP:OD1	1:B:231:ASN:ND2	2.28	0.66
1:A:87:ASN:HD22	4:A:705:BOG:H61	1.61	0.66
1:A:567:LEU:O	1:A:571:ASN:ND2	2.30	0.64
1:A:229:ASP:OD1	1:A:231:ASN:ND2	2.28	0.64
1:A:276:PRO:O	1:A:278:HIS:N	2.32	0.63
4:A:705:BOG:H62	6:A:839:HOH:O	1.99	0.63
1:A:87:ASN:ND2	4:A:705:BOG:H61	2.14	0.62
1:A:484:GLU:OE2	1:A:487:MET:N	2.29	0.61
1:B:101:ASN:O	1:B:105:ASN:ND2	2.34	0.61
1:A:280:PRO:O	1:A:284:GLN:HG3	2.01	0.60
1:B:198:PHE:HZ	1:B:352:LEU:HD23	1.67	0.60
1:B:344:VAL:HA	1:B:348:TYR:HB3	1.83	0.60
1:A:216:ARG:NH1	2:C:2:NAG:O7	2.35	0.59
1:A:344:VAL:HA	1:A:348:TYR:HB3	1.84	0.59
1:A:280:PRO:HD2	1:A:283:LEU:HD12	1.83	0.59
1:A:198:PHE:HZ	1:A:352:LEU:HD23	1.67	0.59
1:A:482:THR:HB	1:A:484:GLU:OE1	2.03	0.59
1:B:206:THR:CG2	1:B:385:TYR:OH	2.51	0.59
1:A:276:PRO:C	1:A:278:HIS:H	2.12	0.57
1:A:335:ILE:HA	1:A:559:ILE:HD11	1.86	0.57
1:A:125:ASP:OD1	1:B:543:GLN:NE2	2.35	0.57
1:A:68:ASN:ND2	6:A:811:HOH:O	2.38	0.55
1:A:543:GLN:NE2	1:B:125:ASP:OD1	2.34	0.55
1:A:389:PRO:HB2	1:A:434:VAL:HA	1.90	0.54
1:B:178:LEU:HD22	1:B:449:LYS:HB2	1.89	0.54
1:B:35:PRO:HG3	1:B:54:GLN:O	2.08	0.54
1:A:414:LEU:HD11	1:A:419:LEU:HD23	1.89	0.53
1:A:198:PHE:CZ	1:A:352:LEU:HD23	2.43	0.53
1:A:34:ASN:ND2	6:A:814:HOH:O	2.41	0.53
1:B:436:GLY:HA2	1:B:512:PRO:HD3	1.92	0.52
1:B:206:THR:HG21	1:B:385:TYR:OH	2.04	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:LEU:HD11	1:B:419:LEU:HD23	1.91	0.52
1:B:56:LYS:NZ	6:B:839:HOH:O	2.43	0.52
1:B:34:ASN:HB2	1:B:37:CYS:SG	2.50	0.52
1:A:230:LEU:HD13	1:A:337:ILE:HG12	1.92	0.51
1:B:435:ALA:HB2	6:B:887:HOH:O	2.09	0.51
1:B:44:ARG:NH1	6:B:806:HOH:O	2.44	0.51
1:B:514:PRO:O	1:B:515:ASP:HB2	2.11	0.51
1:A:542:PRO:O	1:B:61:ARG:NH2	2.37	0.51
1:B:389:PRO:HB2	1:B:434:VAL:HA	1.92	0.51
1:A:385:TYR:OH	5:A:706:LUR:OAB	2.20	0.50
1:B:385:TYR:OH	5:B:706:LUR:OAB	2.21	0.50
1:B:343:ILE:O	1:B:347:ASP:HB2	2.12	0.49
1:B:198:PHE:CZ	1:B:352:LEU:HD23	2.47	0.49
1:B:40:PRO:O	1:B:42:GLN:NE2	2.42	0.49
1:A:83:LYS:HD2	1:A:84:PRO:HD2	1.93	0.48
1:A:274:ILE:HD12	1:A:291:VAL:HG12	1.95	0.48
1:B:538:PRO:O	1:B:541:SER:OG	2.21	0.48
1:A:61:ARG:NH2	1:B:542:PRO:O	2.41	0.48
1:B:178:LEU:HA	1:B:182:LEU:HD12	1.94	0.48
1:A:276:PRO:HD3	1:A:409:TYR:CD1	2.47	0.48
1:A:504:TYR:HA	1:A:507:LEU:HD12	1.94	0.48
1:A:380:GLU:O	1:A:384:LEU:HG	2.14	0.48
1:B:230:LEU:HD13	1:B:337:ILE:HG12	1.95	0.48
1:B:335:ILE:HA	1:B:559:ILE:HD11	1.95	0.48
1:B:39:ASN:ND2	6:B:897:HOH:O	2.47	0.47
1:A:87:ASN:CB	4:A:705:BOG:H61	2.44	0.47
1:A:287:VAL:HG11	1:A:302:ALA:HB1	1.95	0.47
1:A:444:VAL:O	1:A:444:VAL:HG23	2.13	0.47
1:B:472:LEU:HD21	1:B:524:GLU:HG3	1.95	0.47
1:B:497:ASP:HB3	1:B:500:VAL:HG23	1.97	0.47
1:A:375:ASN:OD1	1:A:532:LYS:HG3	2.15	0.47
1:A:101:ASN:O	1:A:105:ASN:ND2	2.49	0.46
1:B:274:ILE:HD12	1:B:291:VAL:HG12	1.96	0.46
1:B:513:ARG:NH2	1:B:520:GLU:HG3	2.30	0.46
1:A:91:TYR:CD2	4:A:705:BOG:H4'1	2.50	0.46
1:B:224:LEU:O	6:B:888:HOH:O	2.21	0.46
1:B:34:ASN:CB	1:B:37:CYS:SG	3.04	0.46
1:B:325:ASP:OD2	6:B:833:HOH:O	2.21	0.45
1:B:504:TYR:HA	1:B:507:LEU:HD12	1.99	0.44
1:B:68:ASN:OD1	1:B:68:ASN:N	2.50	0.44
1:B:530:SER:OG	5:B:706:LUR:OAC	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:THR:HG22	1:A:377:ILE:O	2.17	0.44
1:A:497:ASP:HB3	1:A:500:VAL:HG23	2.00	0.44
1:A:40:PRO:O	1:A:42:GLN:NE2	2.47	0.44
1:A:178:LEU:HD22	1:A:449:LYS:HB2	1.99	0.44
1:A:148:TYR:CZ	1:A:221:THR:HB	2.53	0.43
1:A:241:GLN:OE1	6:A:864:HOH:O	2.21	0.43
1:A:296:PRO:HD2	1:A:407:PHE:CE2	2.52	0.43
1:A:84:PRO:HG2	1:A:89:TRP:NE1	2.33	0.43
1:A:178:LEU:HA	1:A:182:LEU:HD12	2.01	0.43
1:A:267:LYS:HE3	1:A:267:LYS:HB2	1.85	0.43
1:A:472:LEU:HD21	1:A:524:GLU:HG3	1.99	0.43
1:A:267:LYS:O	1:A:270:GLN:NE2	2.49	0.43
1:B:473:LYS:HA	1:B:474:PRO:HD3	1.92	0.43
1:A:320:HIS:HE1	1:B:48:MET:HE3	1.84	0.42
1:B:124:ILE:HD11	1:B:528:PRO:HB2	2.02	0.42
1:A:482:THR:OG1	1:A:488:ALA:HB2	2.19	0.42
1:B:380:GLU:O	1:B:384:LEU:HG	2.19	0.42
1:B:148:TYR:CZ	1:B:221:THR:HB	2.54	0.42
1:B:287:VAL:HG11	1:B:302:ALA:HB1	2.00	0.42
1:B:410:ASN:OD1	1:B:412:SER:OG	2.36	0.42
1:A:230:LEU:HA	1:A:232:HIS:CE1	2.53	0.42
1:A:295:VAL:HA	1:A:296:PRO:HD3	1.95	0.42
1:B:544:TYR:O	1:B:546:LYS:N	2.52	0.42
1:B:284:GLN:NE2	6:B:906:HOH:O	2.53	0.41
1:A:157:ASP:OD2	6:A:818:HOH:O	2.21	0.41
1:B:177:VAL:HG22	1:B:494:LEU:HD13	2.02	0.41
1:B:441:PRO:HG2	1:B:444:VAL:HG22	2.02	0.41
1:B:479:GLU:O	1:B:483:GLY:N	2.49	0.41
1:A:245:ARG:O	6:A:821:HOH:O	2.21	0.41
1:A:484:GLU:HG2	1:A:485:LYS:N	2.35	0.41
1:A:414:LEU:HA	1:A:422:PHE:CE1	2.55	0.41
1:A:544:TYR:O	1:A:546:LYS:N	2.52	0.41
1:A:390:LEU:HD23	1:A:390:LEU:HA	1.93	0.41
1:A:273:MET:N	6:A:835:HOH:O	2.33	0.40
1:B:482:THR:C	1:B:511:LYS:HB2	2.46	0.40
1:A:410:ASN:OD1	1:A:412:SER:OG	2.39	0.40
1:B:46:GLU:OE2	6:B:801:HOH:O	2.22	0.40
1:A:467:ARG:HB3	1:A:472:LEU:HB2	2.03	0.40
1:A:139:TRP:CZ2	1:B:229:ASP:HB3	2.56	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	553/587 (94%)	531 (96%)	19 (3%)	3 (0%)	24	52
1	B	552/587 (94%)	526 (95%)	25 (4%)	1 (0%)	43	70
All	All	1105/1174 (94%)	1057 (96%)	44 (4%)	4 (0%)	30	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	PRO
1	A	514	PRO
1	A	545	TRP
1	B	545	TRP

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	496/525 (94%)	482 (97%)	14 (3%)	38	70
1	B	495/525 (94%)	478 (97%)	17 (3%)	32	65
All	All	991/1050 (94%)	960 (97%)	31 (3%)	35	68

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	80	LEU

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Mol	Chain	Res	Type
1	A	99	VAL
1	A	169	LYS
1	A	215	LYS
1	A	271	VAL
1	A	281	GLU
1	A	385	TYR
1	A	416	GLU
1	A	422	PHE
1	A	445	GLN
1	A	484	GLU
1	A	485	LYS
1	A	553	GLU
1	B	34	ASN
1	B	38	SER
1	B	46	GLU
1	B	68	ASN
1	B	80	LEU
1	B	85	THR
1	B	86	PRO
1	B	99	VAL
1	B	169	LYS
1	B	271	VAL
1	B	281	GLU
1	B	385	TYR
1	B	416	GLU
1	B	422	PHE
1	B	479	GLU
1	B	511	LYS
1	B	513	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	95	HIS
1	A	241	GLN
1	A	560	ASN
1	B	34	ASN
1	B	39	ASN
1	B	204	HIS
1	B	370	GLN
1	B	560	ASN

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	1,2	14,14,15	0.35	0	17,19,21	0.41	0
2	NAG	C	2	2	14,14,15	0.33	0	17,19,21	0.40	0
2	NAG	D	1	1,2	14,14,15	0.32	0	17,19,21	0.44	0
2	NAG	D	2	2	14,14,15	0.28	0	17,19,21	0.42	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	NAG	D	1	1,2	-	2/6/23/26	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 (6) torsion outliers are listed below:

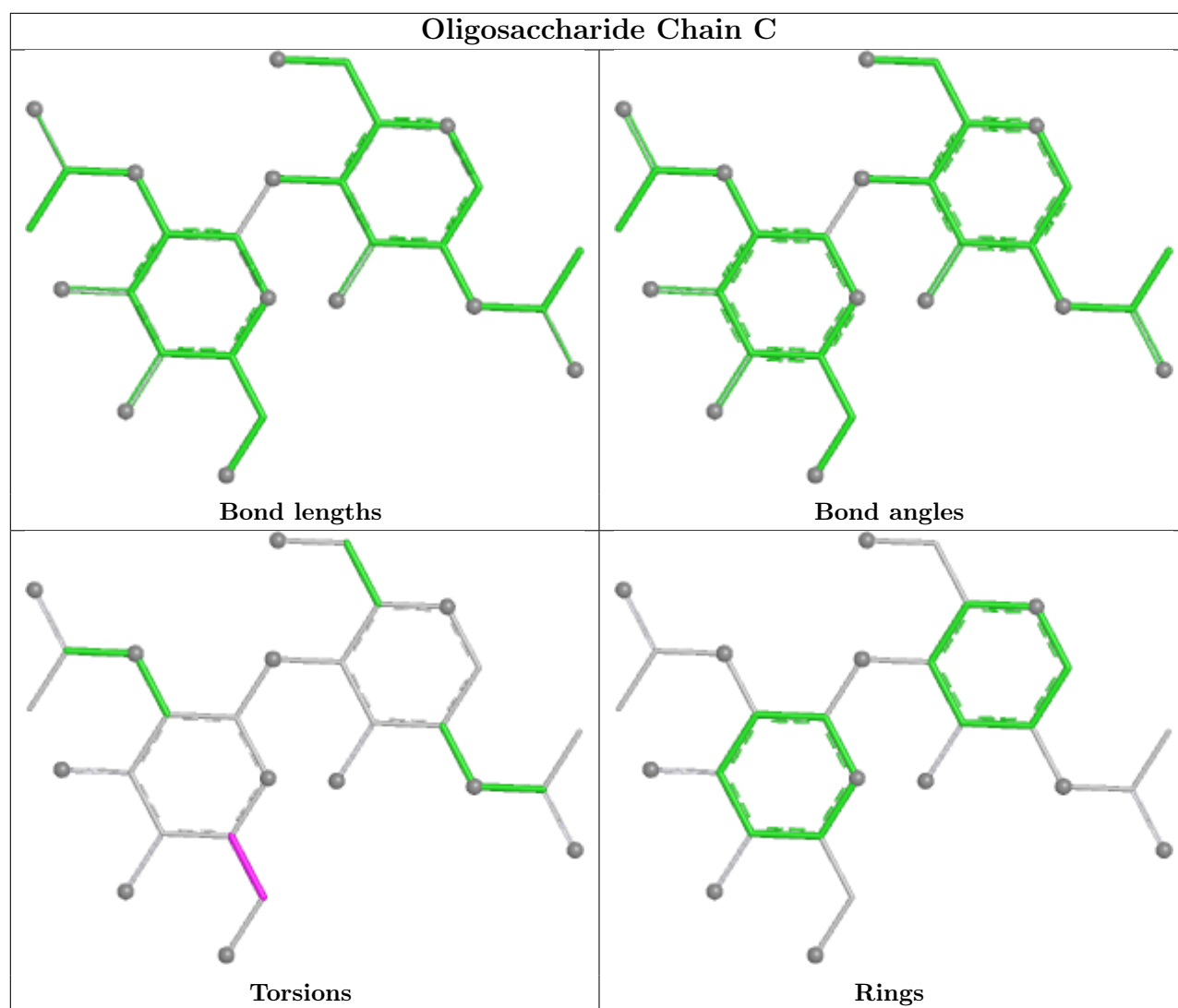
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6

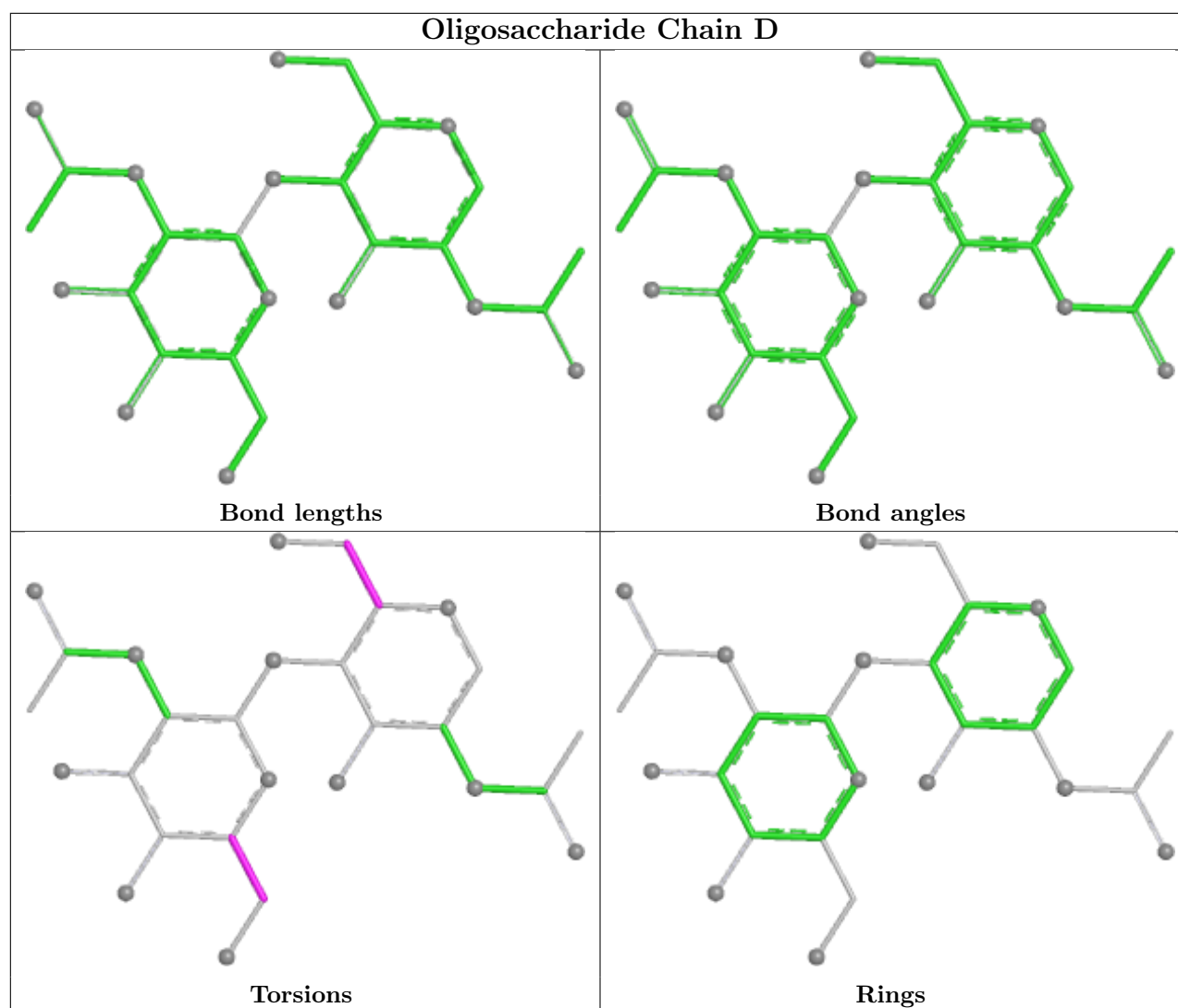
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	1	0
2	C	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 [i](#)

8 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	B	704	1	14,14,15	0.32	0	17,19,21	0.47	0
4	BOG	A	705	-	20,20,20	0.36	0	25,25,25	0.99	1 (4%)
3	NAG	B	701	1	14,14,15	0.26	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BOG	B	705	-	20,20,20	1.04	1 (5%)	25,25,25	1.10	3 (12%)
3	NAG	A	704	1	14,14,15	0.30	0	17,19,21	0.43	0
5	LUR	B	706	-	21,21,21	2.80	6 (28%)	28,29,29	1.35	3 (10%)
3	NAG	A	701	1	14,14,15	0.34	0	17,19,21	0.51	0
5	LUR	A	706	-	21,21,21	2.80	6 (28%)	28,29,29	1.36	4 (14%)

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	B	704	1	-	2/6/23/26	0/1/1/1
4	BOG	A	705	-	-	8/11/31/31	0/1/1/1
3	NAG	B	701	1	-	4/6/23/26	0/1/1/1
4	BOG	B	705	-	-	5/11/31/31	0/1/1/1
3	NAG	A	704	1	-	2/6/23/26	0/1/1/1
5	LUR	B	706	-	-	3/8/8/8	0/2/2/2
3	NAG	A	701	1	-	4/6/23/26	0/1/1/1
5	LUR	A	706	-	-	1/8/8/8	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	706	LUR	CAT-CAP	6.97	1.48	1.38
5	B	706	LUR	CAT-CAP	6.95	1.48	1.38
5	B	706	LUR	CAS-CAR	6.90	1.48	1.40
5	A	706	LUR	CAS-CAR	6.89	1.48	1.40
5	B	706	LUR	CAT-CAQ	5.95	1.48	1.40
5	A	706	LUR	CAT-CAQ	5.92	1.48	1.40
5	A	706	LUR	OAB-CAN	3.43	1.33	1.22
5	B	706	LUR	OAB-CAN	3.41	1.33	1.22
5	B	706	LUR	CAQ-CLE	2.68	1.80	1.73
5	A	706	LUR	CAQ-CLE	2.65	1.79	1.73
5	B	706	LUR	OAC-CAN	-2.65	1.22	1.30
5	A	706	LUR	OAC-CAN	-2.60	1.22	1.30
4	B	705	BOG	O2-C2	-2.39	1.37	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	705	BOG	C1-O5-C5	-2.99	107.89	113.72
5	A	706	LUR	FAD-CAP-CAT	2.97	120.72	117.64
5	B	706	LUR	FAD-CAP-CAT	2.96	120.71	117.64
4	B	705	BOG	C1'-O1-C1	2.88	118.60	113.68
5	A	706	LUR	CAG-CAP-CAT	-2.70	118.96	122.83
5	B	706	LUR	CAG-CAP-CAT	-2.66	119.02	122.83
4	A	705	BOG	C1-C2-C3	-2.48	104.80	110.01
4	B	705	BOG	O1-C1-C2	2.17	111.58	108.27
5	B	706	LUR	CAI-CAO-CAK	2.10	121.05	117.96
5	A	706	LUR	CAI-CAO-CAK	2.08	121.03	117.96
5	A	706	LUR	CAR-CAK-CAO	-2.05	119.69	122.06

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	705	BOG	C2-C1-O1-C1'
4	B	705	BOG	C2-C1-O1-C1'
5	B	706	LUR	CAN-CAL-CAR-CAS
4	B	705	BOG	O5-C5-C6-O6
4	A	705	BOG	O5-C1-O1-C1'
4	A	705	BOG	O5-C5-C6-O6
3	B	701	NAG	O5-C5-C6-O6
4	B	705	BOG	C4-C5-C6-O6
5	A	706	LUR	CAN-CAL-CAR-CAS
3	A	701	NAG	O5-C5-C6-O6
4	B	705	BOG	O5-C1-O1-C1'
4	A	705	BOG	C2'-C1'-O1-C1
4	B	705	BOG	C2'-C3'-C4'-C5'
3	B	701	NAG	C4-C5-C6-O6
4	A	705	BOG	C4-C5-C6-O6
4	A	705	BOG	C4'-C5'-C6'-C7'
3	A	704	NAG	C4-C5-C6-O6
4	A	705	BOG	C1'-C2'-C3'-C4'
3	A	701	NAG	C4-C5-C6-O6
3	A	704	NAG	O5-C5-C6-O6
3	B	704	NAG	C4-C5-C6-O6
3	A	701	NAG	C3-C2-N2-C7
3	B	701	NAG	C3-C2-N2-C7
3	A	701	NAG	C1-C2-N2-C7
3	B	701	NAG	C1-C2-N2-C7
5	B	706	LUR	CAN-CAL-CAR-CAK
5	B	706	LUR	CAP-CAT-NAM-CAS

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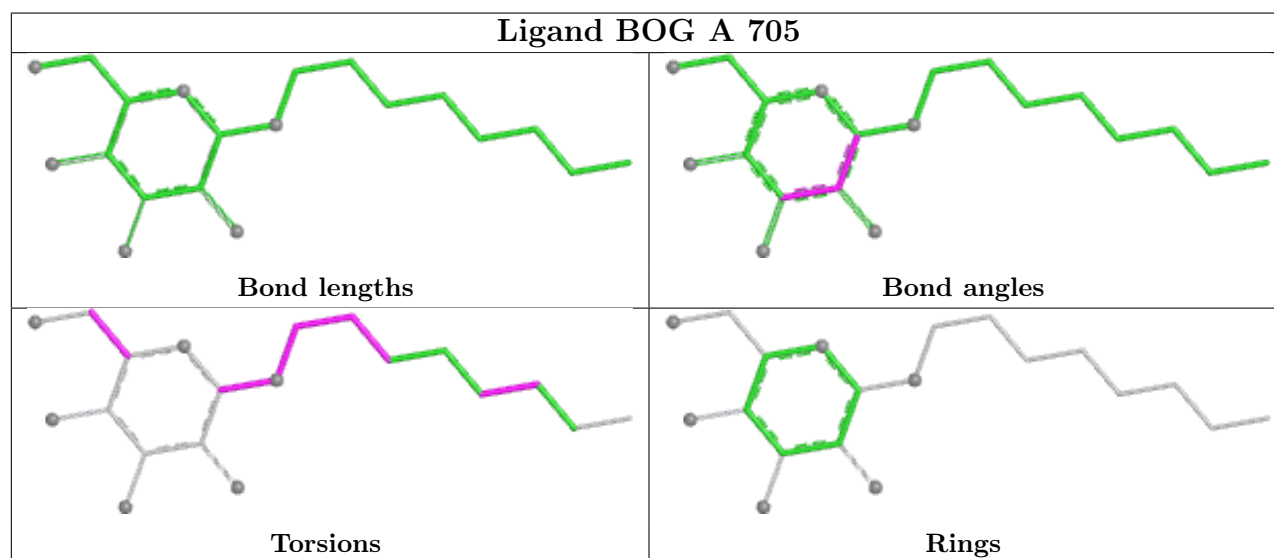
Mol	Chain	Res	Type	Atoms
4	A	705	BOG	O1-C1'-C2'-C3'
3	B	704	NAG	O5-C5-C6-O6

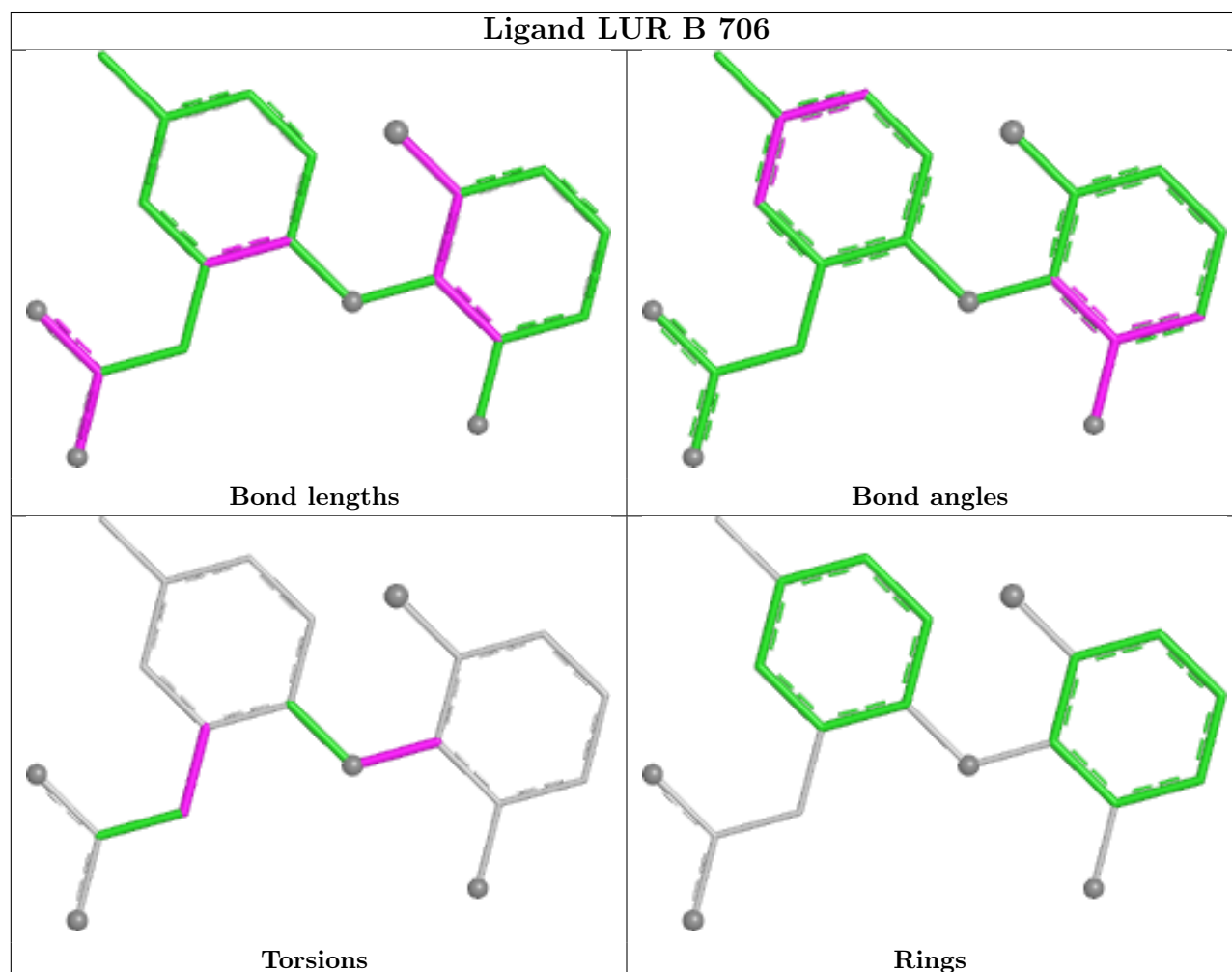
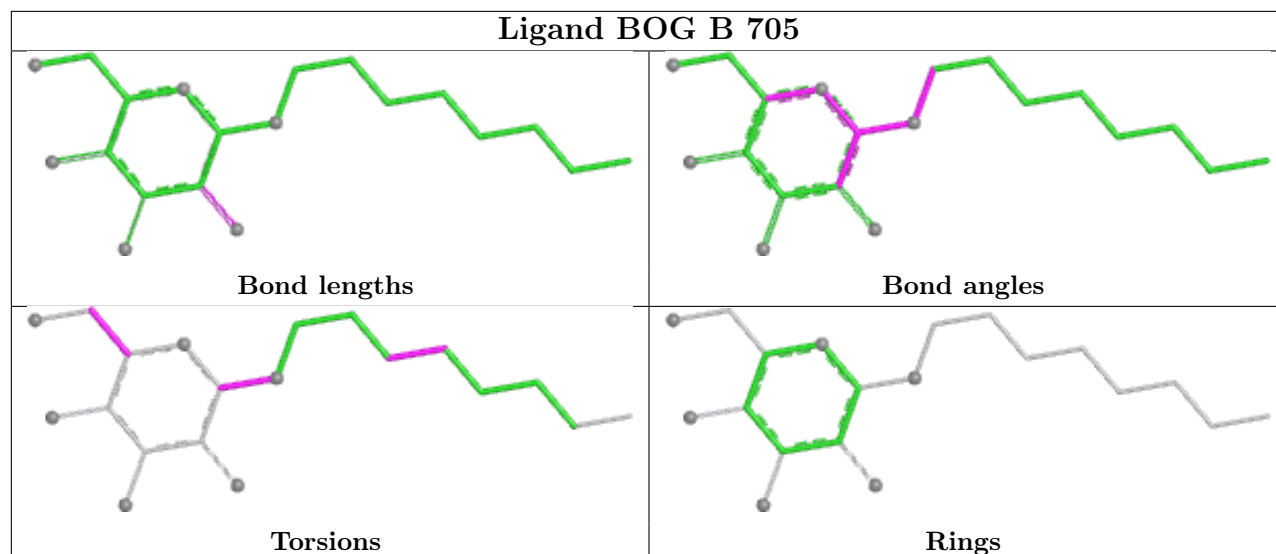
There are no ring outliers.

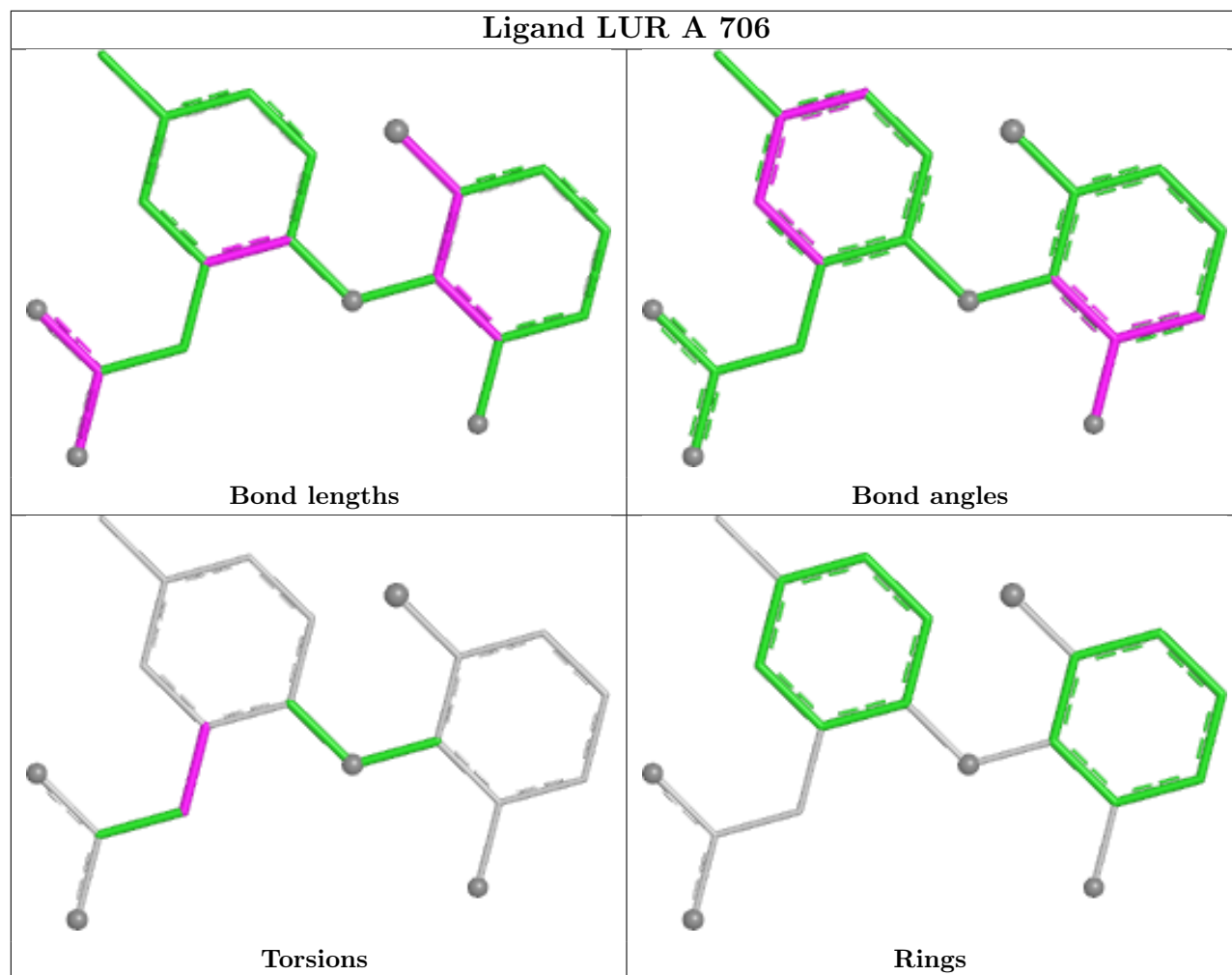
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	705	BOG	5	0
5	B	706	LUR	2	0
5	A	706	LUR	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	552/587 (94%)	-0.88	0 100 100	21, 45, 66, 79	3 (0%)
1	B	552/587 (94%)	-0.80	0 100 100	24, 46, 72, 96	2 (0%)
All	All	1104/1174 (94%)	-0.84	0 100 100	21, 45, 69, 96	5 (0%)

There are no RSRZ outliers to report.

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](#)

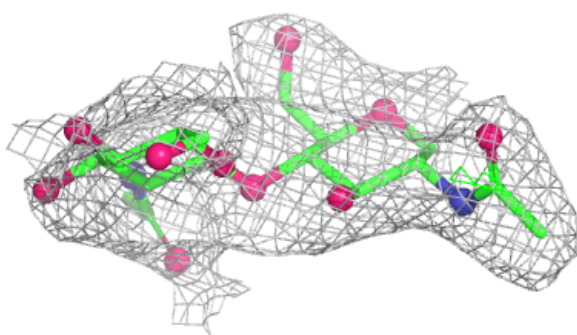
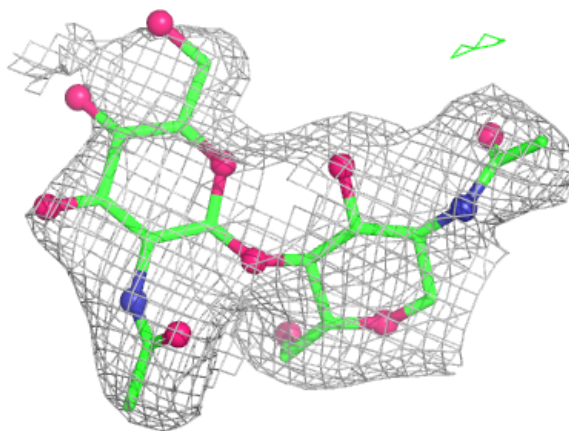
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists 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	D	2	14/15	0.97	0.08	51,59,64,65	0
2	NAG	C	2	14/15	0.98	0.06	52,59,69,71	0
2	NAG	C	1	14/15	0.98	0.05	16,23,33,45	0
2	NAG	D	1	14/15	0.99	0.04	15,22,28,38	0

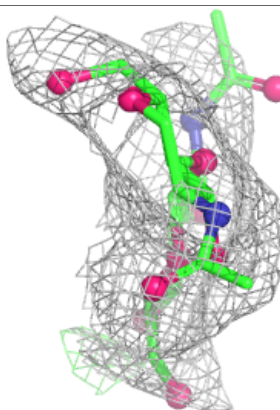
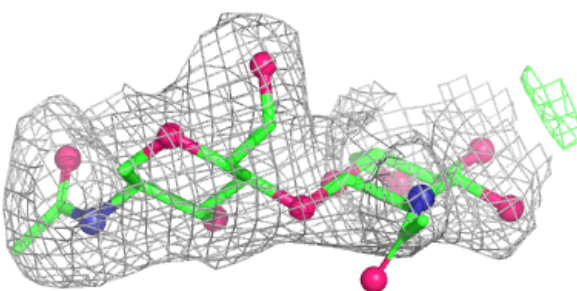
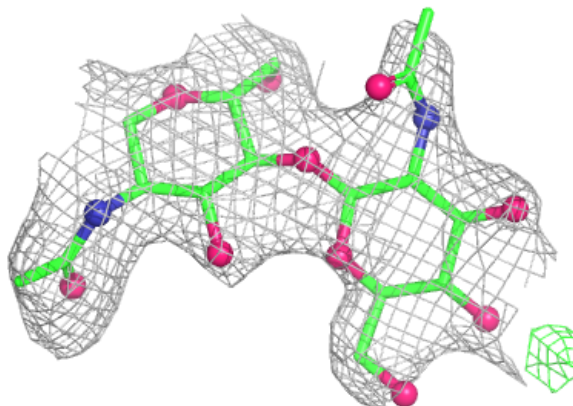
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

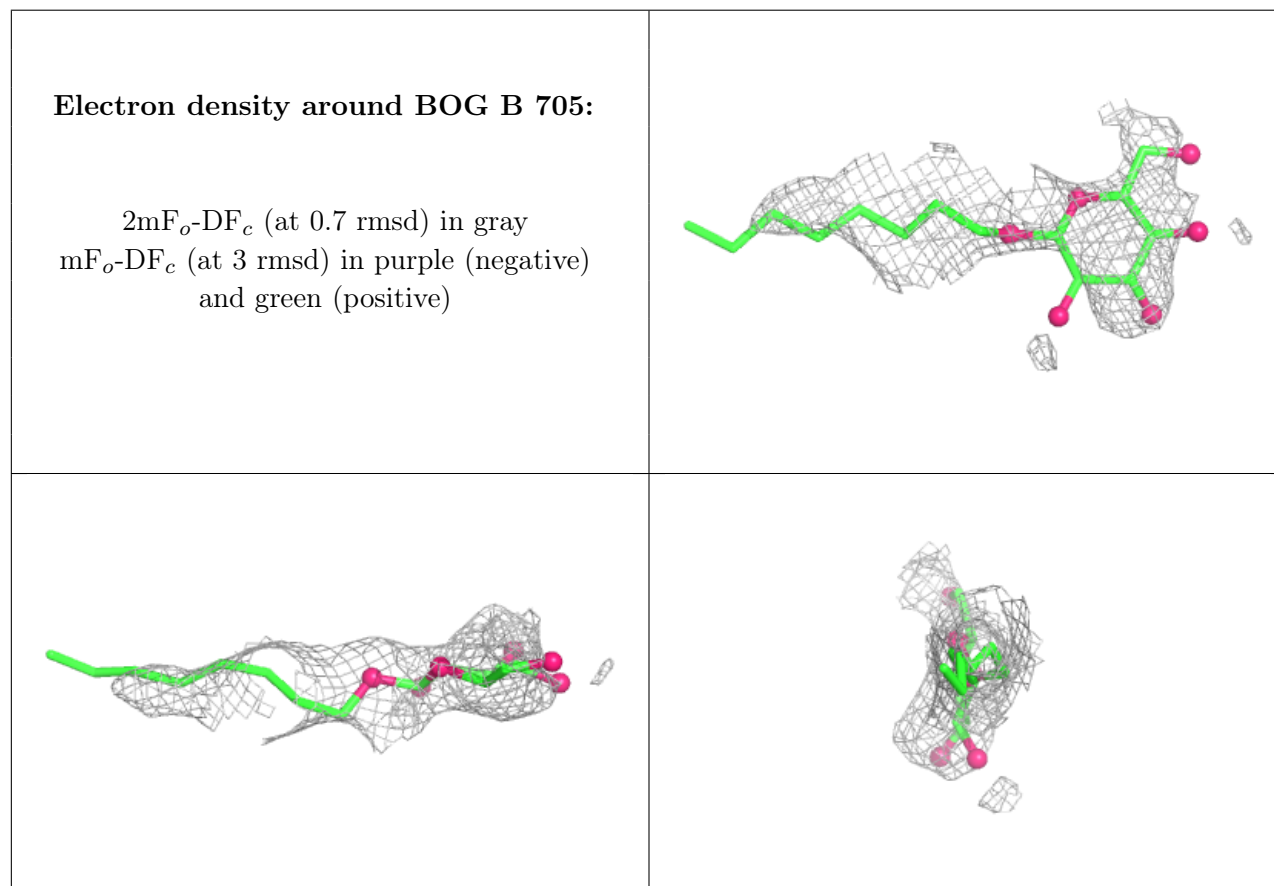


6.4 Ligands ⓘ

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.

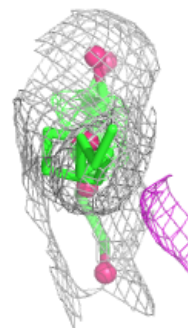
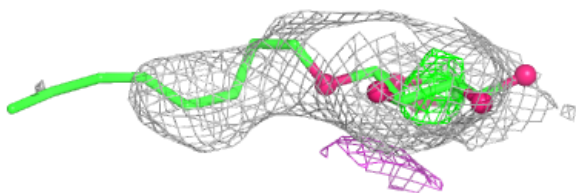
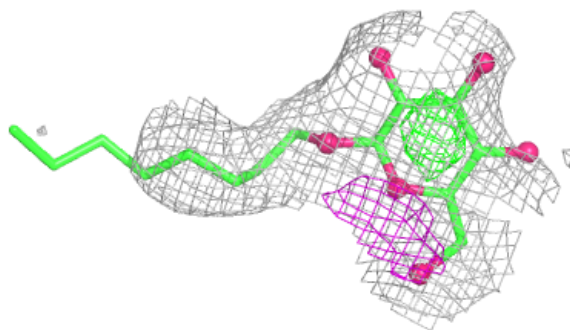
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	704	14/15	0.96	0.07	45,53,58,61	0
3	NAG	B	701	14/15	0.96	0.07	44,67,75,76	0
3	NAG	B	704	14/15	0.96	0.08	41,51,65,67	0
4	BOG	B	705	20/20	0.96	0.10	74,90,100,102	0
4	BOG	A	705	20/20	0.97	0.08	74,89,96,100	0
3	NAG	A	701	14/15	0.97	0.06	44,51,65,66	0
5	LUR	A	706	20/20	0.98	0.05	1,6,19,37	0
5	LUR	B	706	20/20	0.98	0.07	22,27,39,52	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.

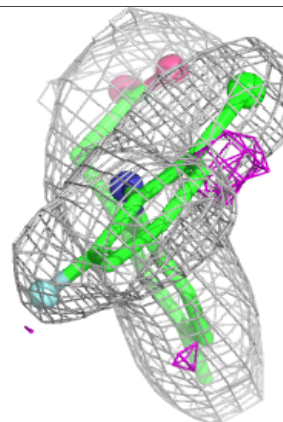
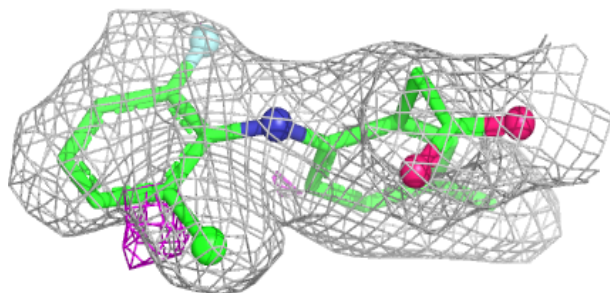
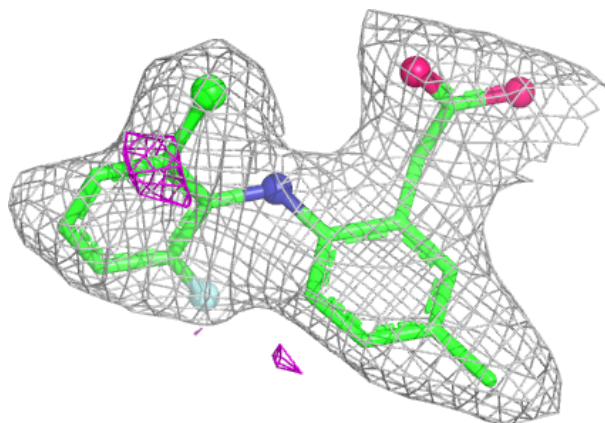


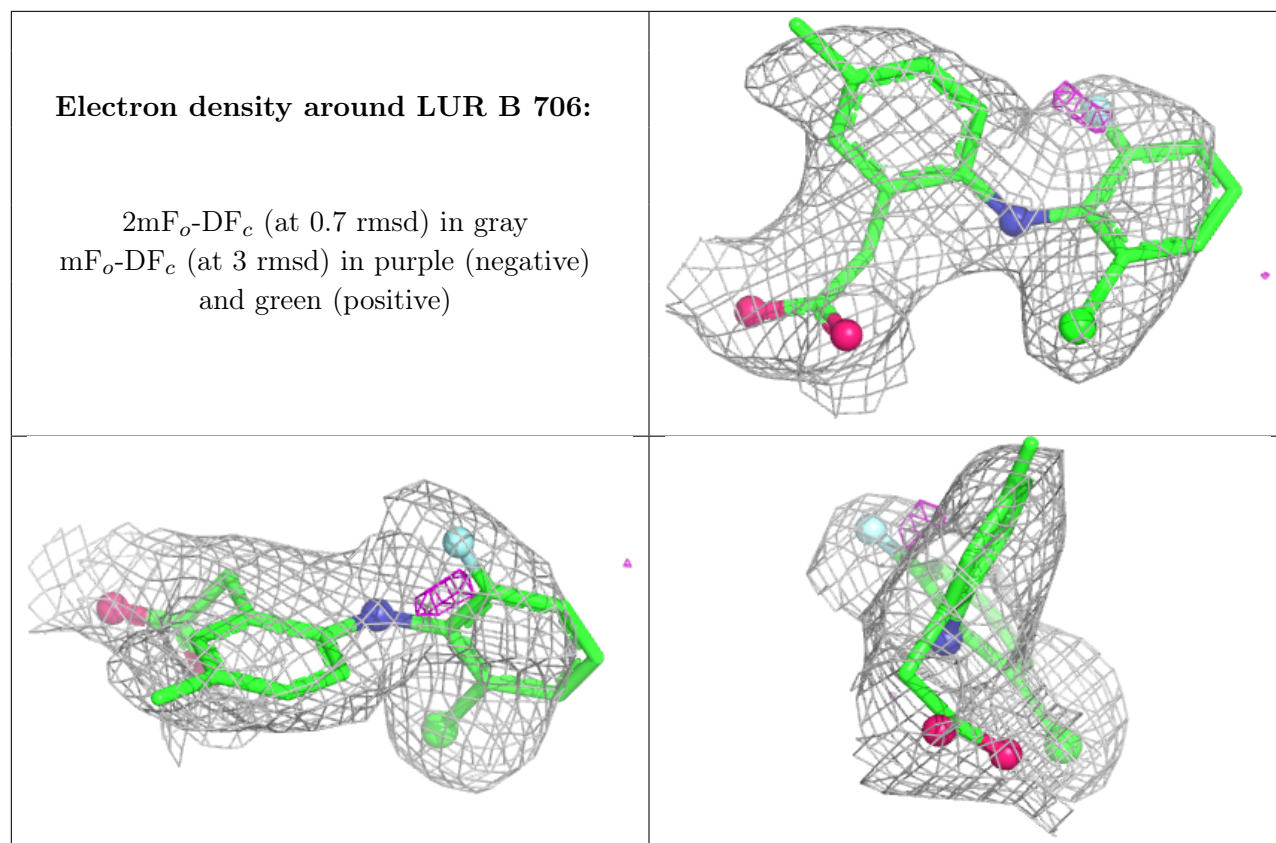
Electron density around BOG A 705:

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

**Electron density around LUR A 706:**

$2mF_o-DF_c$ (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.