



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:26 AM UTC

PDB ID : 2VS4 / pdb\_00002vs4  
Title : THE BINDING OF UDP-GALACTOSE BY AN ACTIVE SITE MUTANT OF alpha-1,3 GALACTOSYLTRANSFERASE (alpha3GT)  
Authors : Tumbale, P.; Jamaluddin, H.; Thiyagarajan, N.; Brew, K.; Acharya, K.R.  
Deposited on : 2008-04-18  
Resolution : 1.77 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](mailto: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>.

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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

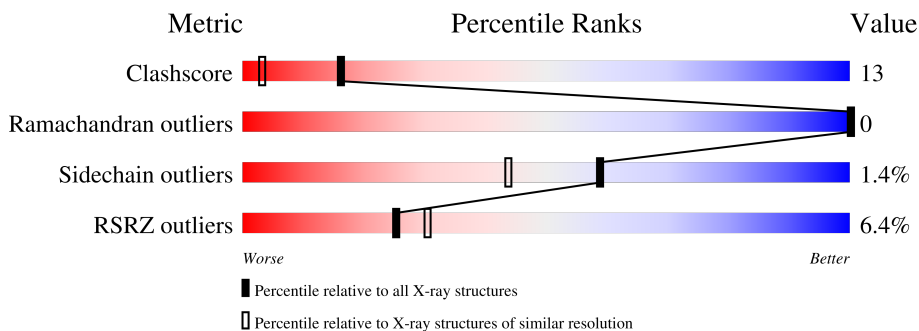
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

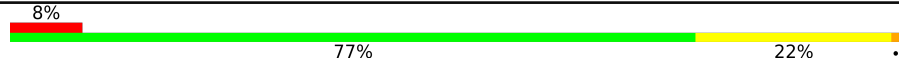

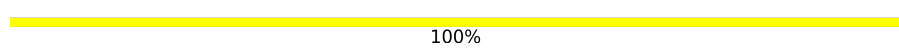
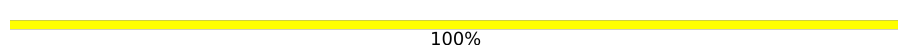
The reported resolution of this entry is 1.77 Å.

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))
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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  $\geq 3$ , 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	289	 8% 77% 22%
1	B	289	 5% 78% 19%
2	C	2	 100%
2	D	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NDG	C	1	X	-	-	-
2	NDG	D	1	X	-	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6170 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 N-ACETYLLACTOSAMINIDE ALPHA-1,3-GALACTOSYL TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	2400	1568	396	424	12	0	4	0
1	B	288	2400	1568	396	424	12	0	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	316	GLU	ASP	engineered mutation	UNP P14769
B	316	GLU	ASP	engineered mutation	UNP P14769

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

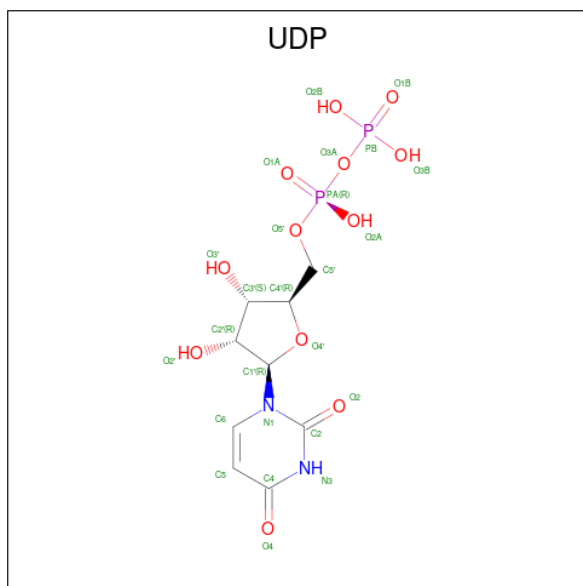


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	26	14	1	11	0	0	0
2	D	2	26	14	1	11	0	0	0

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

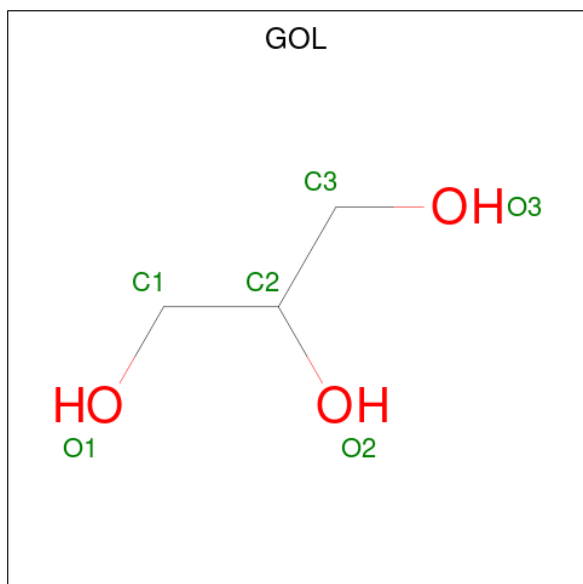
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		

- Molecule 4 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula:  $C_9H_{14}N_2O_{12}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
4	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
5	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

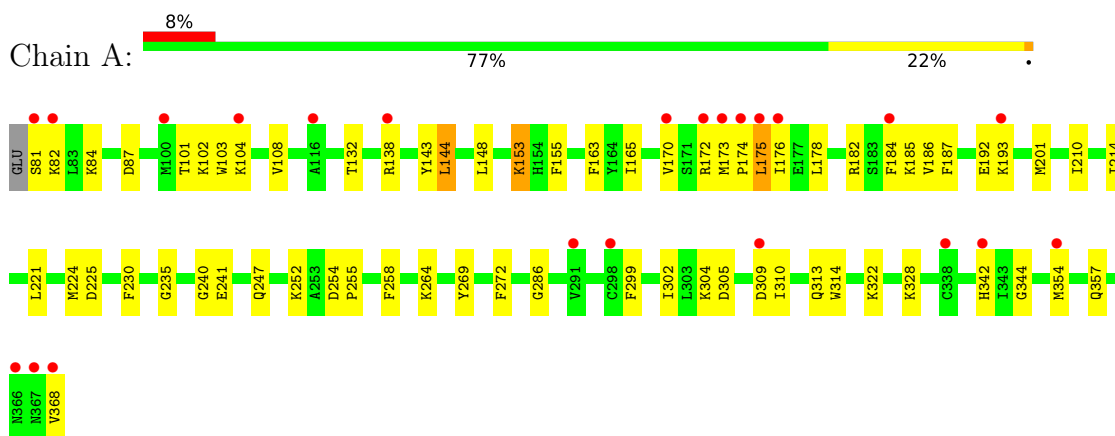
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	622	Total	O	0	0
			622	622		
6	B	632	Total	O	0	0
			632	632		

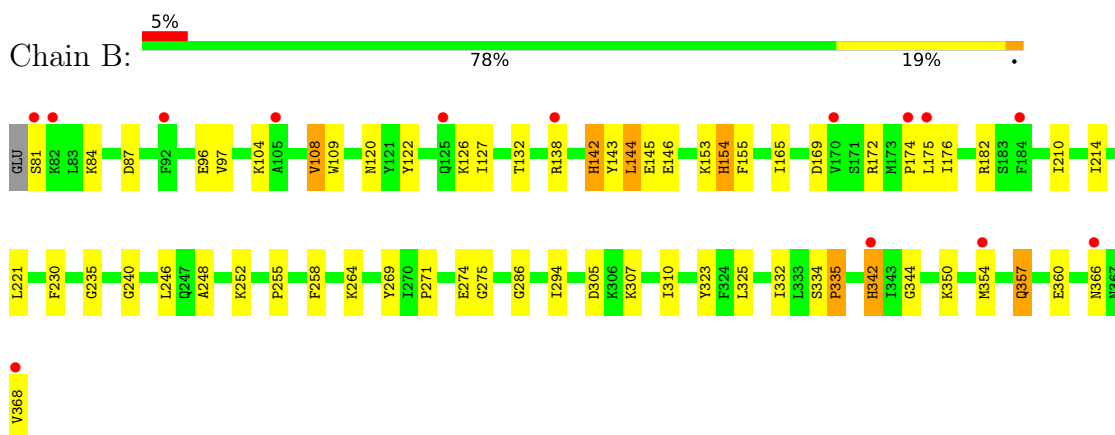
### 3 Residue-property plots [i](#)

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: N-ACETYLLACTOSAMINIDE ALPHA-1,3-GALACTOSYLTRANSFERAS E



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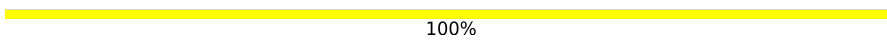


- Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucofuranose



- Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucofuranose

Chain D:



100%

NDG1  
GAL2

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.25Å 94.63Å 94.69Å 90.00° 98.90° 90.00°	Depositor
Resolution (Å)	32.50 – 1.77 32.50 – 1.77	Depositor EDS
% Data completeness (in resolution range)	91.3 (32.50-1.77) 91.4 (32.50-1.77)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 1.77Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.263 , 0.278 0.269 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.2	Xtrriage
Anisotropy	0.463	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 32.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6170	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6731e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, GAL, UDP, MN, NDG

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	0.56	2/2473 (0.1%)	0.92	10/3349 (0.3%)
1	B	0.43	1/2473 (0.0%)	0.93	11/3349 (0.3%)
All	All	0.50	3/4946 (0.1%)	0.92	21/6698 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	GLN	C-O	-15.03	1.06	1.24
1	A	247	GLN	CD-OE1	-9.51	1.05	1.23
1	B	342[B]	HIS	C-O	-6.47	1.15	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	GLY	N-CA-C	8.84	123.39	112.79
1	B	235	GLY	N-CA-C	8.65	123.18	112.79
1	A	108	VAL	N-CA-C	6.41	117.65	107.98
1	B	248	ALA	N-CA-C	6.31	118.96	111.33
1	A	153	LYS	N-CA-C	6.30	119.44	111.69
1	B	350	LYS	N-CA-C	5.98	117.88	111.36
1	B	344	GLY	N-CA-C	-5.97	103.41	112.84
1	A	143	TYR	N-CA-C	5.92	122.08	114.56
1	B	154	HIS	N-CA-C	5.56	121.48	114.31
1	B	108	VAL	N-CA-C	5.52	116.32	107.98
1	A	272	PHE	N-CA-C	-5.46	102.19	110.28
1	B	357	GLN	N-CA-C	-5.46	101.63	110.32
1	B	144	LEU	N-CA-C	5.46	116.91	111.07
1	A	155	PHE	N-CA-C	5.45	117.12	108.67
1	B	143	TYR	N-CA-C	5.44	121.46	114.56
1	B	155	PHE	N-CA-C	5.37	116.99	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	MET	N-CA-C	5.30	117.73	109.52
1	A	144	LEU	N-CA-C	5.20	116.63	111.07
1	A	344	GLY	N-CA-C	-5.19	104.64	112.84
1	B	142	HIS	N-CA-C	5.16	116.99	111.36
1	A	225	ASP	N-CA-C	-5.11	103.78	110.53

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	2400	0	2355	72	0
1	B	2400	0	2356	55	0
2	C	26	0	20	0	0
2	D	26	0	20	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	25	0	11	0	0
4	B	25	0	11	0	0
5	A	6	0	7	0	0
5	B	6	0	7	1	0
6	A	622	0	0	38	3
6	B	632	0	0	32	2
All	All	6170	0	4787	127	5

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 13.

All (127) 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:334:SER:HB2	6:B:697:HOH:O	1.46	1.13
1:B:335:PRO:HD2	6:B:697:HOH:O	1.58	1.03
1:B:145:GLU:HG3	6:B:892:HOH:O	1.69	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ILE:HG21	1:A:173:MET:HE1	1.57	0.86
1:B:368:VAL:HA	6:B:512:HOH:O	1.75	0.85
1:B:342[B]:HIS:ND1	6:B:501:HOH:O	2.01	0.85
1:B:360:GLU:CD	6:B:513:HOH:O	2.20	0.84
1:B:368:VAL:HG12	6:B:584:HOH:O	1.77	0.83
1:B:120:ASN:HB2	6:B:722:HOH:O	1.80	0.80
1:A:176:ILE:HA	6:A:521:HOH:O	1.82	0.79
1:A:172:ARG:NH2	6:A:502:HOH:O	2.14	0.78
1:B:252:LYS:HD2	6:B:869:HOH:O	1.83	0.78
1:A:101:THR:O	6:A:501:HOH:O	2.01	0.78
1:A:153:LYS:HD3	6:A:584:HOH:O	1.86	0.74
1:A:254:ASP:HB3	6:A:793:HOH:O	1.86	0.74
1:A:132:THR:HG23	1:A:221:LEU:HD11	1.71	0.73
1:A:82:LYS:NZ	1:A:84:LYS:HD3	2.04	0.73
1:A:165:ILE:CG2	1:A:173:MET:HE1	2.21	0.71
1:A:175:LEU:HD23	1:B:175:LEU:HD11	1.73	0.70
1:B:146:GLU:OE1	6:B:502:HOH:O	2.09	0.70
1:B:81:SER:N	6:B:506:HOH:O	2.24	0.70
1:A:104:LYS:N	6:A:501:HOH:O	1.96	0.68
1:B:342[B]:HIS:CE1	6:B:501:HOH:O	2.44	0.68
1:A:252:LYS:HD2	6:A:942:HOH:O	1.94	0.68
1:A:193:LYS:HD3	6:A:1010:HOH:O	1.94	0.67
1:B:210:ILE:HA	1:B:214:ILE:HB	1.75	0.67
1:B:104:LYS:HB3	6:B:667:HOH:O	1.98	0.64
1:B:271:PRO:HG2	1:B:274:GLU:HG3	1.80	0.64
1:A:368:VAL:HG12	6:A:832:HOH:O	1.96	0.63
1:A:255:PRO:HA	1:A:258:PHE:CD1	2.33	0.63
1:A:304:LYS:CE	6:A:531:HOH:O	2.47	0.62
1:A:193:LYS:HE3	6:A:876:HOH:O	2.01	0.60
1:B:109:TRP:CH2	6:B:697:HOH:O	2.51	0.60
1:B:108:VAL:O	1:B:334:SER:HB3	2.01	0.60
1:A:104:LYS:CA	6:A:501:HOH:O	2.47	0.59
1:B:81:SER:HB2	6:B:879:HOH:O	2.03	0.59
1:A:304:LYS:HE3	6:A:540:HOH:O	2.03	0.59
1:A:313:GLN:HG2	1:A:314:TRP:CD1	2.38	0.58
1:A:185:LYS:HG2	1:A:187:PHE:CE1	2.39	0.58
1:A:174:PRO:CA	6:A:517:HOH:O	2.51	0.57
1:A:252:LYS:NZ	6:A:514:HOH:O	2.38	0.57
1:B:230:PHE:HA	1:B:354[B]:MET:HG2	1.87	0.56
1:A:84:LYS:O	1:A:87:ASP:HB2	2.06	0.56
1:A:174:PRO:HA	6:A:517:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:TRP:CZ2	6:B:697:HOH:O	2.58	0.56
1:B:142:HIS:HD2	6:B:861:HOH:O	1.88	0.56
1:A:313:GLN:HG3	6:A:678:HOH:O	2.05	0.55
1:A:342[A]:HIS:CG	6:A:644:HOH:O	2.58	0.55
1:B:368:VAL:HG21	6:B:794:HOH:O	2.06	0.55
1:A:175:LEU:N	6:A:517:HOH:O	2.39	0.55
1:B:255:PRO:HA	1:B:258:PHE:CD1	2.42	0.54
1:A:309:ASP:CB	6:A:577:HOH:O	2.56	0.54
1:B:138:ARG:NH1	6:B:511:HOH:O	2.41	0.54
1:A:210:ILE:HA	1:A:214:ILE:HB	1.88	0.54
1:A:176:ILE:N	6:A:521:HOH:O	2.40	0.53
1:B:153:LYS:HE3	1:B:154:HIS:CE1	2.44	0.53
1:A:102:LYS:HE3	6:A:932:HOH:O	2.08	0.53
1:A:104:LYS:HA	6:A:501:HOH:O	2.07	0.52
1:B:138:ARG:HH11	1:B:138:ARG:HG3	1.75	0.52
1:A:170:VAL:O	1:A:173:MET:HB3	2.10	0.52
1:B:172:ARG:NH2	6:B:516:HOH:O	2.43	0.52
1:A:148:LEU:HD11	1:A:165:ILE:HD13	1.92	0.50
1:A:81:SER:O	1:A:82:LYS:HB3	2.11	0.50
1:A:230:PHE:HA	1:A:354[A]:MET:HG2	1.94	0.50
1:A:138:ARG:NE	6:A:525:HOH:O	2.45	0.49
1:B:335:PRO:CD	6:B:697:HOH:O	2.35	0.49
1:A:368:VAL:OXT	1:A:368:VAL:HG22	2.12	0.49
1:B:307:LYS:HE2	6:B:748:HOH:O	2.12	0.49
5:B:404:GOL:H12	6:B:836:HOH:O	2.12	0.49
1:A:309:ASP:HB2	6:A:577:HOH:O	2.11	0.49
1:B:109:TRP:CZ3	6:B:697:HOH:O	2.64	0.49
1:B:255:PRO:HA	1:B:258:PHE:CE1	2.48	0.49
1:B:96:GLU:HG2	1:B:97:VAL:HG13	1.95	0.48
1:B:144:LEU:HD23	1:B:174:PRO:HD2	1.94	0.48
1:B:305:ASP:HB3	1:B:310:ILE:O	2.14	0.48
1:A:322:LYS:HE2	6:A:859:HOH:O	2.13	0.48
1:A:173:MET:HE3	1:A:186:VAL:CG2	2.44	0.47
1:B:176:ILE:C	1:B:176:ILE:HD12	2.40	0.46
1:B:126:LYS:CE	6:B:520:HOH:O	2.63	0.46
1:A:304:LYS:NZ	6:A:531:HOH:O	2.48	0.46
1:A:82:LYS:HZ1	1:A:84:LYS:HD3	1.79	0.46
1:B:334:SER:CB	6:B:697:HOH:O	2.28	0.46
1:A:138:ARG:HD3	1:A:138:ARG:HA	1.79	0.45
1:A:82:LYS:HE2	1:A:84:LYS:CG	2.47	0.45
1:B:165:ILE:HD12	1:B:165:ILE:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:LYS:HG2	1:B:269:TYR:CZ	2.52	0.45
1:A:304:LYS:CE	6:A:540:HOH:O	2.64	0.45
1:A:309:ASP:CG	6:A:577:HOH:O	2.60	0.45
1:A:144:LEU:HD23	1:A:174:PRO:HD2	1.99	0.45
1:B:252:LYS:CD	6:B:869:HOH:O	2.54	0.44
1:B:132:THR:HG23	1:B:221:LEU:HD11	1.99	0.44
1:B:169:ASP:HB3	1:B:172:ARG:HD3	1.99	0.44
1:B:145:GLU:CG	6:B:892:HOH:O	2.47	0.44
1:A:201:MET:HE1	6:A:882:HOH:O	2.18	0.44
1:A:305:ASP:HB3	1:A:310:ILE:O	2.18	0.43
1:B:240:GLY:O	1:B:286:GLY:HA2	2.18	0.43
1:A:163:PHE:HB2	1:A:184[A]:PHE:HD2	1.83	0.43
1:A:103:TRP:O	1:A:104:LYS:HB2	2.17	0.43
1:A:174:PRO:C	6:A:517:HOH:O	2.61	0.43
1:A:103:TRP:CE2	1:A:328:LYS:HB3	2.52	0.43
1:A:304:LYS:CD	6:A:531:HOH:O	2.66	0.43
1:A:342[A]:HIS:CD2	6:A:644:HOH:O	2.72	0.43
1:B:122:TYR:CD2	1:B:127:ILE:HD13	2.54	0.42
1:A:264:LYS:HA	1:A:269:TYR:CG	2.53	0.42
1:A:304:LYS:HE2	6:A:531:HOH:O	2.17	0.42
1:A:82:LYS:HZ3	1:A:84:LYS:HD3	1.83	0.42
1:A:192:GLU:CD	1:A:201:MET:HG3	2.45	0.42
1:A:82:LYS:CE	1:A:84:LYS:HD3	2.49	0.42
1:B:275:GLY:HA2	1:B:325:LEU:HD13	2.02	0.42
1:A:138:ARG:NH2	6:A:537:HOH:O	2.51	0.42
1:A:255:PRO:HA	1:A:258:PHE:CE1	2.54	0.42
1:B:175:LEU:N	6:B:529:HOH:O	2.53	0.41
1:B:126:LYS:NZ	6:B:520:HOH:O	2.45	0.41
1:B:252:LYS:HE2	6:B:567:HOH:O	2.19	0.41
1:B:174:PRO:CA	6:B:529:HOH:O	2.68	0.41
1:B:294:ILE:HG12	1:B:323:TYR:CE1	2.56	0.41
1:B:84:LYS:O	1:B:87:ASP:HB2	2.20	0.41
1:A:299:PHE:HA	1:A:302:ILE:HD12	2.01	0.41
1:A:82:LYS:HE2	1:A:84:LYS:HG2	2.02	0.41
1:A:175:LEU:C	6:A:521:HOH:O	2.63	0.41
1:B:176:ILE:H	1:B:176:ILE:HG13	1.73	0.41
1:A:241:GLU:O	1:A:286:GLY:HA3	2.21	0.41
1:A:101:THR:C	6:A:501:HOH:O	2.57	0.40
1:A:240:GLY:O	1:A:286:GLY:HA2	2.20	0.40
1:A:176:ILE:CA	6:A:521:HOH:O	2.51	0.40
1:A:178:LEU:HD11	1:A:184[A]:PHE:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:LEU:HG	1:B:332:ILE:CG2	2.51	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:540:HOH:O	6:A:554:HOH:O[1_455]	1.91	0.29
6:A:1038:HOH:O	6:A:1056:HOH:O[1_655]	2.10	0.10
6:A:508:HOH:O	6:A:655:HOH:O[2_646]	2.11	0.09
6:B:803:HOH:O	6:B:854:HOH:O[2_555]	2.17	0.03
6:B:773:HOH:O	6:B:874:HOH:O[2_545]	2.18	0.02

## 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	286/289 (99%)	276 (96%)	10 (4%)	0	100	100
1	B	286/289 (99%)	280 (98%)	6 (2%)	0	100	100
All	All	572/578 (99%)	556 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	259/260 (100%)	256 (99%)	3 (1%)	63	49
1	B	259/260 (100%)	255 (98%)	4 (2%)	57	41
All	All	518/520 (100%)	511 (99%)	7 (1%)	59	44

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	LEU
1	A	182	ARG
1	A	357	GLN
1	B	182	ARG
1	B	335	PRO
1	B	357	GLN
1	B	366	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	293	ASN
1	A	296	GLN
1	A	313	GLN
1	A	357	GLN
1	B	120	ASN
1	B	290	GLN
1	B	296	GLN
1	B	313	GLN
1	B	357	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	NDG	C	1	2	15,15,15	2.06	3 (20%)	21,21,21	1.26	2 (9%)
2	GAL	C	2	2	11,11,12	1.69	2 (18%)	15,15,17	1.32	3 (20%)
2	NDG	D	1	2	15,15,15	2.03	3 (20%)	21,21,21	1.34	2 (9%)
2	GAL	D	2	2	11,11,12	1.70	2 (18%)	15,15,17	1.37	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDG	C	1	2	1/1/6/7	0/6/26/26	0/1/1/1
2	GAL	C	2	2	-	0/2/19/22	0/1/1/1
2	NDG	D	1	2	1/1/6/7	0/6/26/26	0/1/1/1
2	GAL	D	2	2	-	0/2/19/22	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NDG	C8-C7	-6.05	1.38	1.50
2	C	1	NDG	C8-C7	-5.99	1.38	1.50
2	D	2	GAL	O5-C5	-3.57	1.36	1.43
2	C	2	GAL	O5-C5	-3.40	1.36	1.43
2	D	1	NDG	O3-C3	-3.31	1.34	1.43
2	C	1	NDG	O3-C3	-3.26	1.34	1.43
2	C	2	GAL	C4-C5	2.89	1.59	1.53
2	D	2	GAL	C4-C5	2.81	1.59	1.53
2	C	1	NDG	C1-C2	-2.39	1.50	1.52
2	D	1	NDG	O7-C7	-2.05	1.18	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NDG	O5-C5-C6	3.14	114.22	106.44
2	D	1	NDG	O5-C5-C6	2.92	113.67	106.44
2	D	2	GAL	O2-C2-C1	2.77	115.56	109.22
2	D	1	NDG	O5-C1-C2	2.63	112.16	109.52
2	C	2	GAL	O2-C2-C1	2.61	115.20	109.22
2	D	2	GAL	C1-O5-C5	2.60	115.67	112.19
2	C	2	GAL	C1-O5-C5	2.47	115.49	112.19
2	C	1	NDG	O5-C1-C2	2.32	111.85	109.52
2	C	2	GAL	O4-C4-C5	2.08	114.44	109.32

All (2) chirality outliers are listed below:

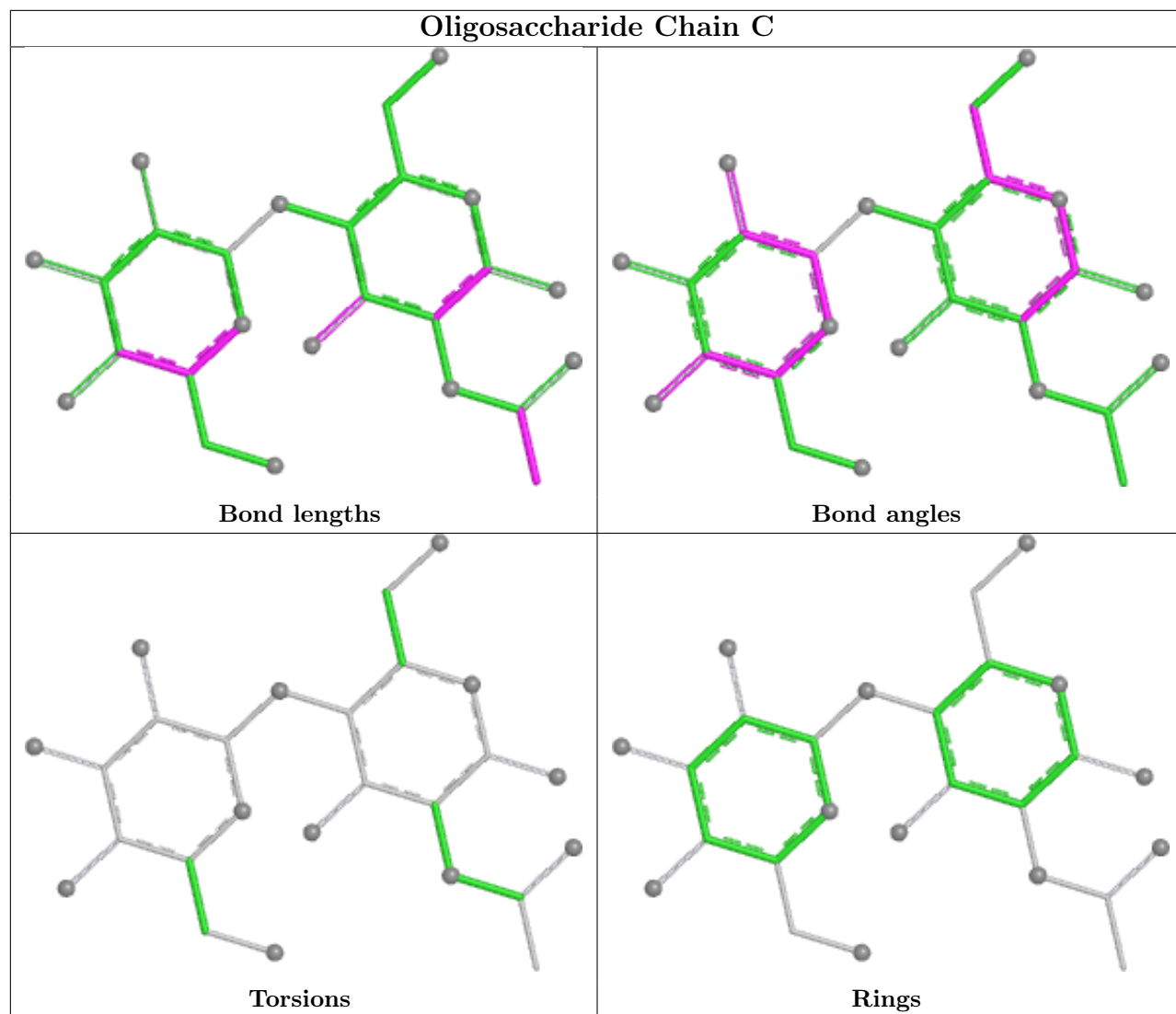
Mol	Chain	Res	Type	Atom
2	C	1	NDG	C1
2	D	1	NDG	C1

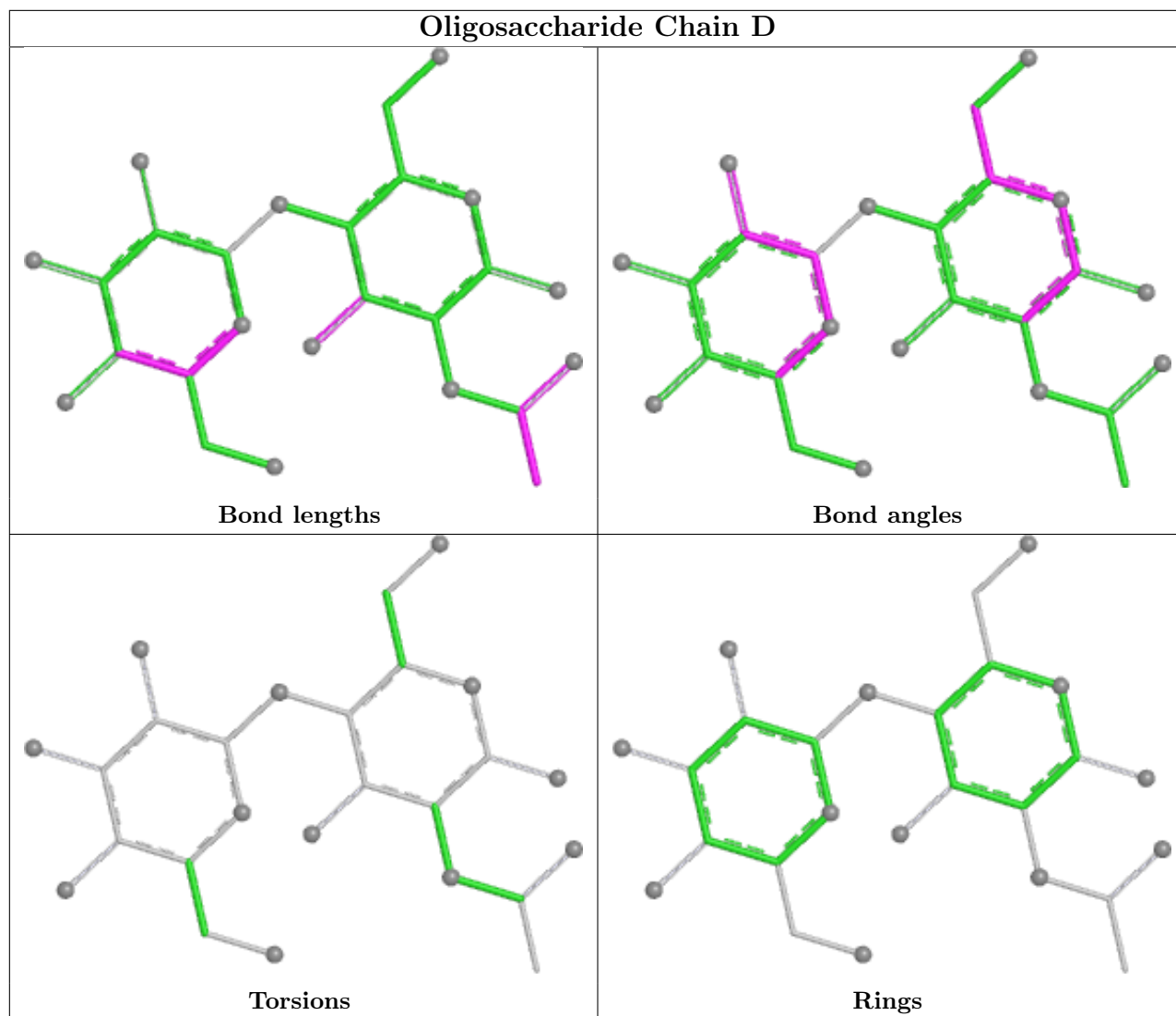
There are no torsion outliers.

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.





## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	UDP	B	402	3	25,26,26	3.05	12 (48%)	38,40,40	1.28	5 (13%)
5	GOL	A	404	-	5,5,5	1.17	0	5,5,5	0.90	0
5	GOL	B	404	-	5,5,5	1.36	0	5,5,5	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	UDP	A	402	3	25,26,26	3.04	10 (40%)	38,40,40	1.29	6 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	UDP	B	402	3	-	1/16/32/32	0/2/2/2
5	GOL	A	404	-	-	0/4/4/4	-
5	GOL	B	404	-	-	2/4/4/4	-
4	UDP	A	402	3	-	1/16/32/32	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	UDP	PB-O2B	-7.75	1.26	1.54
4	A	402	UDP	PB-O2B	-7.47	1.27	1.54
4	B	402	UDP	O2-C2	-5.37	1.13	1.23
4	A	402	UDP	O2-C2	-5.37	1.13	1.23
4	A	402	UDP	PB-O3B	-5.32	1.35	1.54
4	B	402	UDP	PB-O3B	-5.09	1.35	1.54
4	A	402	UDP	PB-O1B	-4.89	1.35	1.50
4	B	402	UDP	PB-O1B	-4.78	1.35	1.50
4	A	402	UDP	PA-O1A	-4.74	1.34	1.50
4	B	402	UDP	PA-O1A	-4.46	1.35	1.50
4	A	402	UDP	PA-O3A	-3.81	1.55	1.59
4	A	402	UDP	C2-N1	3.80	1.44	1.38
4	B	402	UDP	PA-O3A	-3.61	1.55	1.59
4	B	402	UDP	C2-N1	3.56	1.44	1.38
4	B	402	UDP	PA-O2A	-3.40	1.39	1.55
4	A	402	UDP	PA-O2A	-3.31	1.40	1.55
4	B	402	UDP	O4'-C4'	-2.69	1.39	1.45
4	A	402	UDP	C1'-N1	2.62	1.55	1.47
4	B	402	UDP	C1'-N1	2.55	1.54	1.47
4	A	402	UDP	O4'-C4'	-2.30	1.39	1.45
4	B	402	UDP	C3'-C2'	-2.19	1.47	1.53
4	B	402	UDP	C6-C5	2.07	1.39	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	402	UDP	O2A-PA-O3A	2.56	114.20	107.27
4	B	402	UDP	O2A-PA-O3A	2.48	113.98	107.27
4	A	402	UDP	C5-C6-N1	2.37	125.68	121.84
4	A	402	UDP	C6-C5-C4	-2.35	116.53	119.53
4	B	402	UDP	C5-C6-N1	2.30	125.58	121.84
4	B	402	UDP	O4-C4-C5	-2.28	121.23	125.16
4	A	402	UDP	O4-C4-C5	-2.26	121.27	125.16
4	B	402	UDP	C6-C5-C4	-2.25	116.65	119.53
4	A	402	UDP	O4'-C1'-N1	2.22	113.38	108.36
4	B	402	UDP	O4'-C1'-N1	2.13	113.18	108.36
4	A	402	UDP	C5-C4-N3	2.02	117.63	114.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

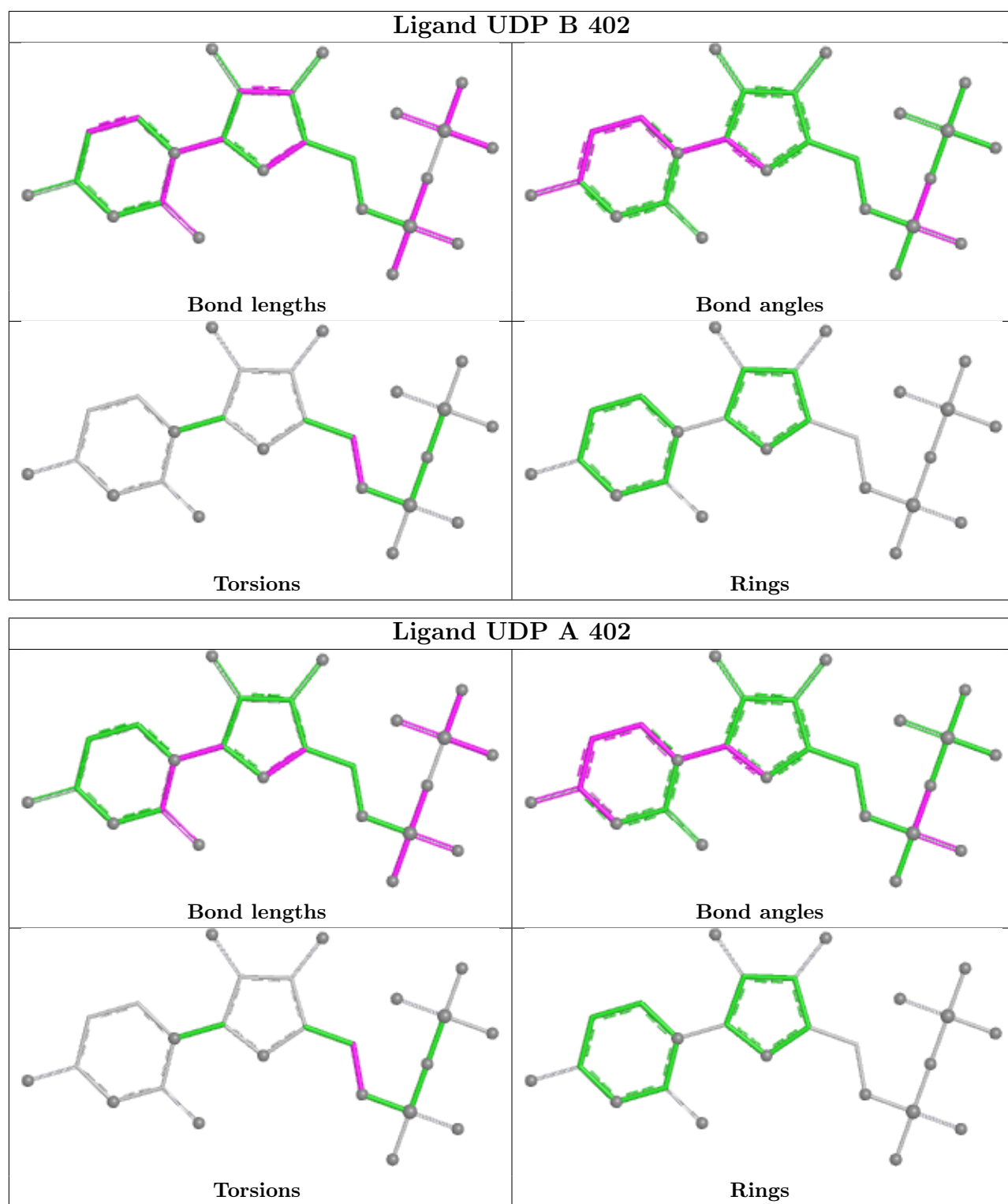
Mol	Chain	Res	Type	Atoms
5	B	404	GOL	C1-C2-C3-O3
5	B	404	GOL	O2-C2-C3-O3
4	B	402	UDP	C4'-C5'-O5'-PA
4	A	402	UDP	C4'-C5'-O5'-PA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	404	GOL	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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	288/289 (99%)	0.95	23 (7%) 18 21	5, 20, 23, 26	4 (1%)
1	B	288/289 (99%)	0.86	14 (4%) 35 41	5, 20, 22, 25	3 (1%)
All	All	576/578 (99%)	0.90	37 (6%) 25 30	5, 20, 23, 26	7 (1%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	354[B]	MET	18.5
1	A	354[A]	MET	18.4
1	A	184[A]	PHE	12.0
1	B	184[B]	PHE	8.5
1	A	100[A]	MET	8.5
1	B	342[B]	HIS	7.3
1	B	368	VAL	7.1
1	A	342[A]	HIS	7.0
1	A	368	VAL	6.7
1	A	81	SER	5.9
1	B	81	SER	5.4
1	A	175	LEU	5.3
1	B	174	PRO	5.2
1	A	174	PRO	4.8
1	B	175	LEU	4.2
1	B	170	VAL	3.8
1	A	82	LYS	3.7
1	A	173	MET	3.4
1	B	125	GLN	2.9
1	A	138	ARG	2.9
1	B	366	ASN	2.9
1	B	82	LYS	2.7
1	A	172	ARG	2.5
1	A	367	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	116	ALA	2.5
1	A	170	VAL	2.5
1	A	104	LYS	2.5
1	A	366	ASN	2.4
1	A	176	ILE	2.4
1	B	105	ALA	2.3
1	A	193	LYS	2.3
1	A	338	CYS	2.2
1	B	138	ARG	2.2
1	A	298	CYS	2.2
1	A	309	ASP	2.1
1	A	291	VAL	2.1
1	B	92	PHE	2.1

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

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

## 6.3 Carbohydrates [i](#)

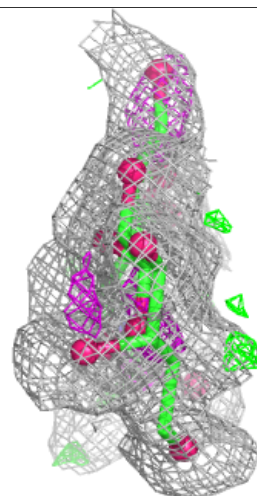
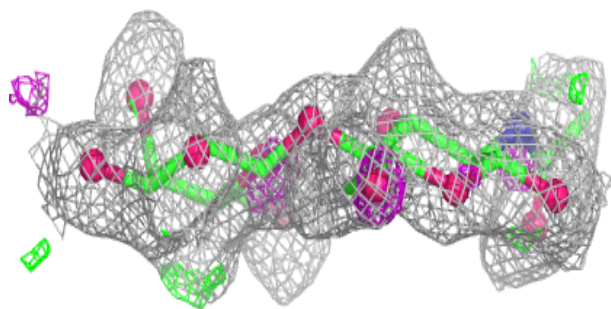
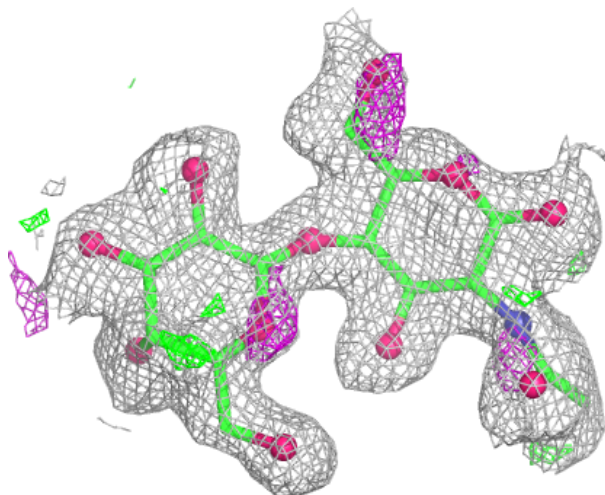
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

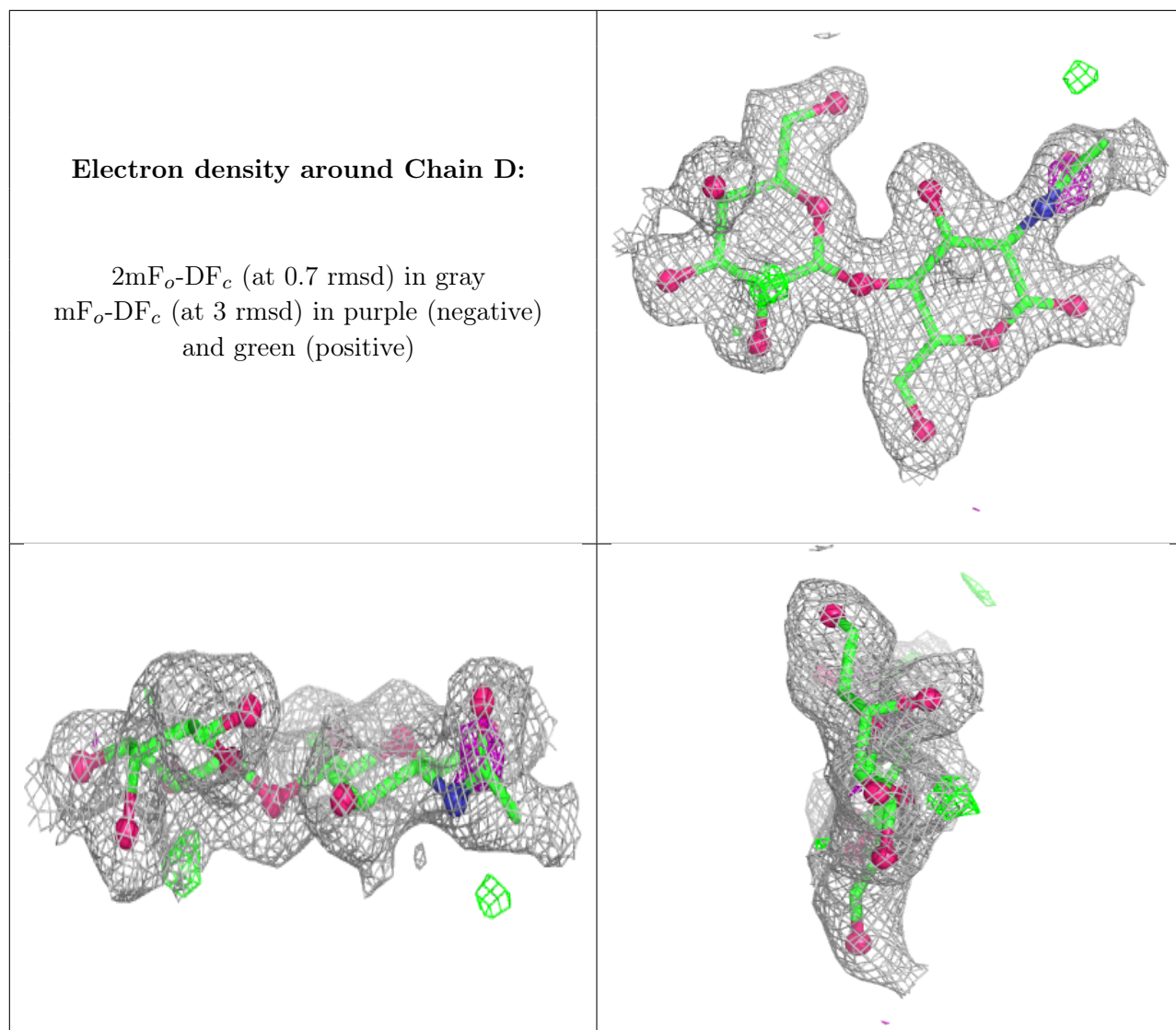
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NDG	C	1	15/15	0.81	0.12	20,22,25,25	0
2	GAL	C	2	11/12	0.86	0.10	20,22,23,24	0
2	GAL	D	2	11/12	0.86	0.11	19,21,22,23	0
2	NDG	D	1	15/15	0.88	0.10	21,23,25,25	0

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

**Electron density around Chain C:**

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



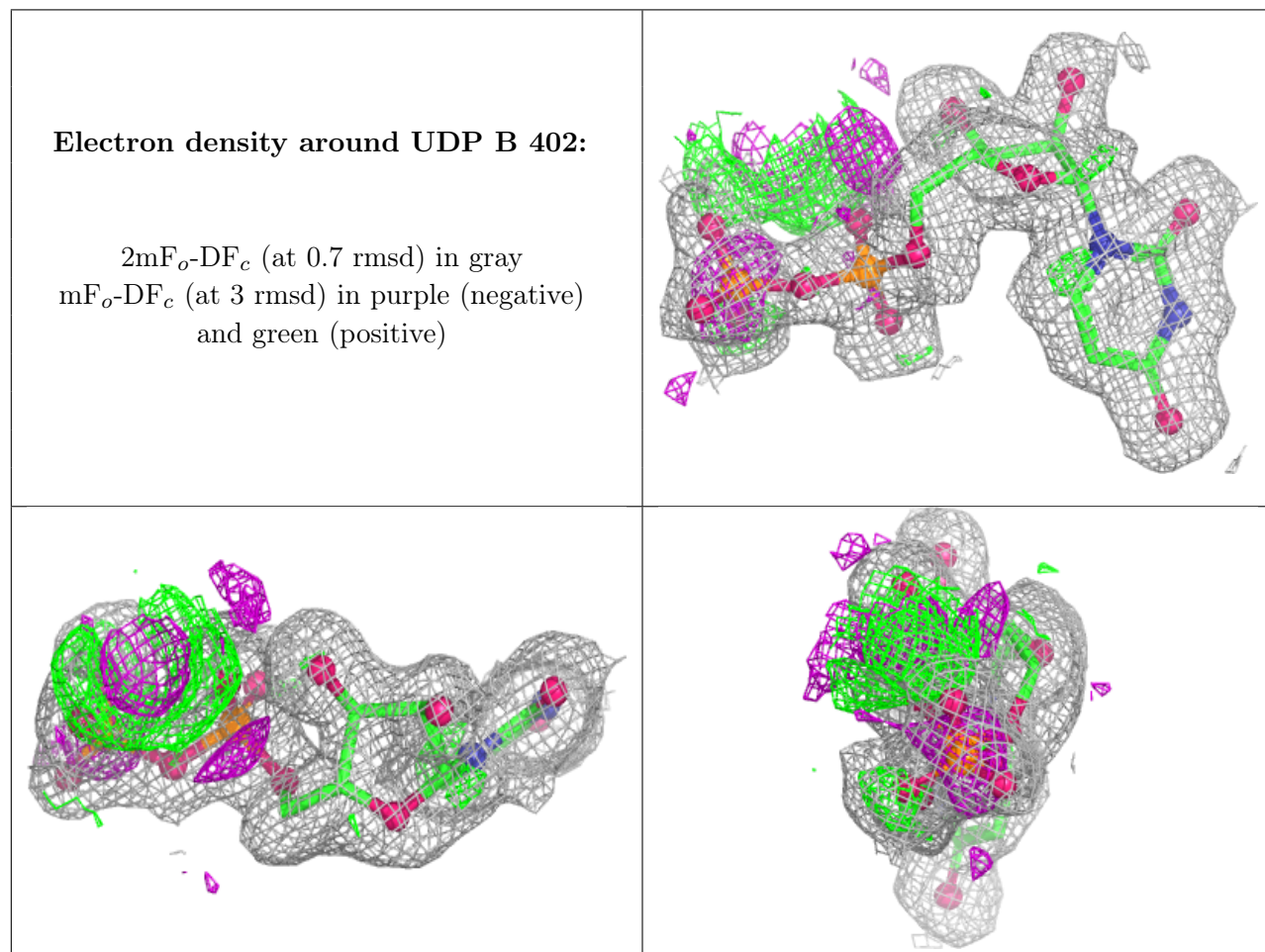


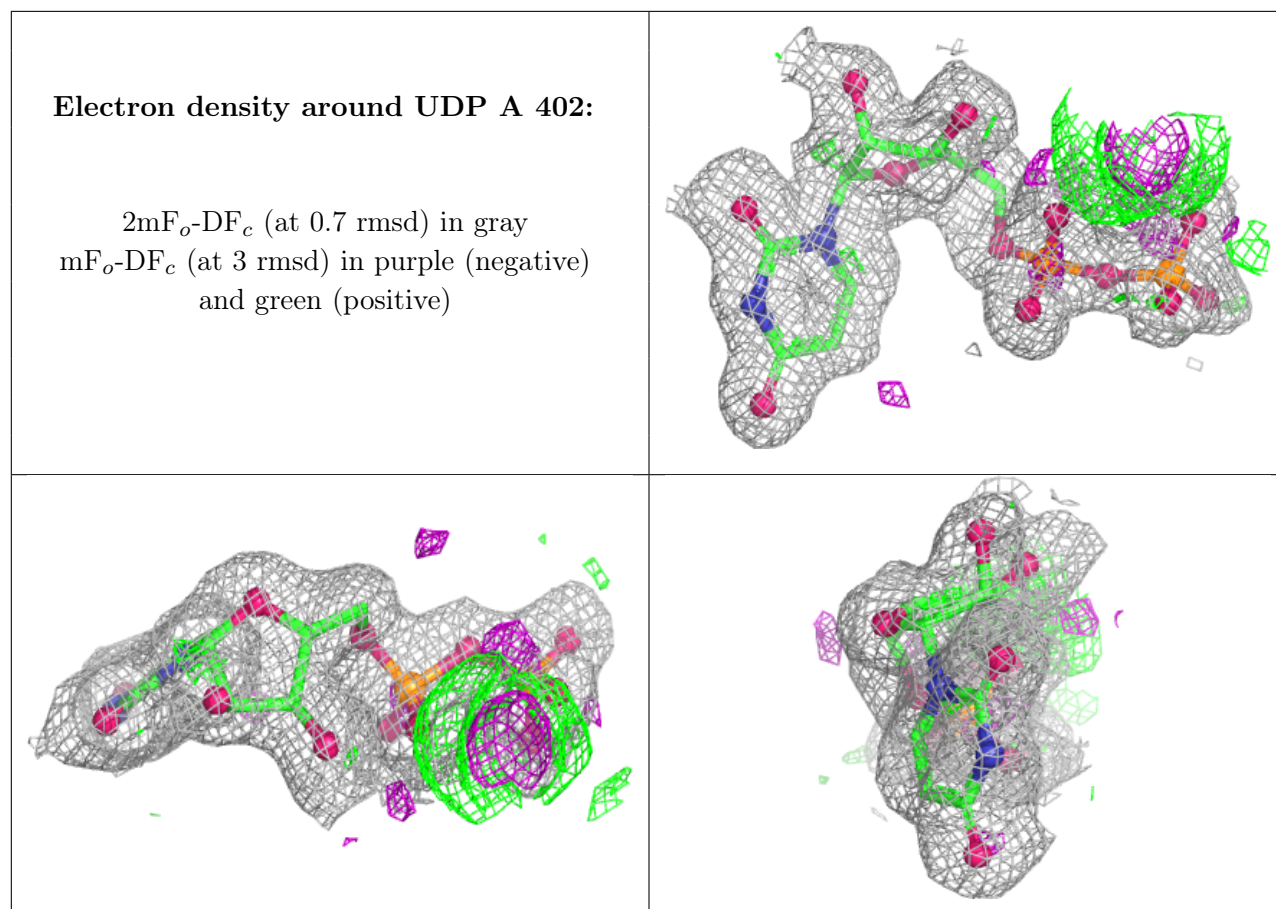
## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	GOL	B	404	6/6	0.76	0.24	23,23,23,25	0
5	GOL	A	404	6/6	0.84	0.13	21,23,25,26	0
3	MN	A	401	1/1	0.88	0.21	1,1,1,1	0
4	UDP	B	402	25/25	0.92	0.11	8,18,20,22	0
4	UDP	A	402	25/25	0.94	0.09	12,19,21,22	0
3	MN	B	401	1/1	0.99	0.19	1,1,1,1	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.