Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2021 – 10:52 AM JST

PDB ID	:	7E9L
Title	:	Crystal Structure of POMGNT2 in complex with UDP and mono-mannosyl peptide (379Man short peptide)
Authors	:	Kuwabara, N.
Deposited on	:	2021-03-04
Resolution	:	2.10 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 following versions of software and data (see references ⓘ) were used in the production of this report:

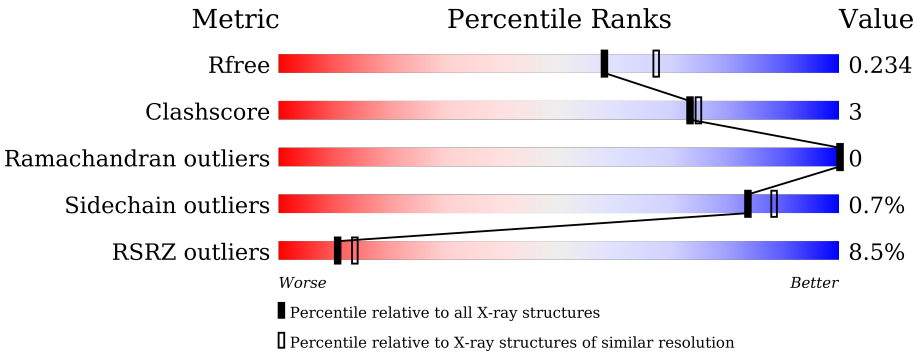
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	539	2% 89% 8%
1	B	539	15% 85% 11%
2	C	14	79% 21%
3	D	2	100%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 9056 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 Protein O-linked-mannose beta-1,4-N-acetylglucosaminyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	1	0
			4216	2730	722	743	21			
1	B	515	Total	C	N	O	S	0	1	0
			4113	2667	698	727	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	GLY	-	expression tag	UNP Q5NDF2
A	43	ALA	-	expression tag	UNP Q5NDF2
A	44	PRO	-	expression tag	UNP Q5NDF2
B	42	GLY	-	expression tag	UNP Q5NDF2
B	43	ALA	-	expression tag	UNP Q5NDF2
B	44	PRO	-	expression tag	UNP Q5NDF2

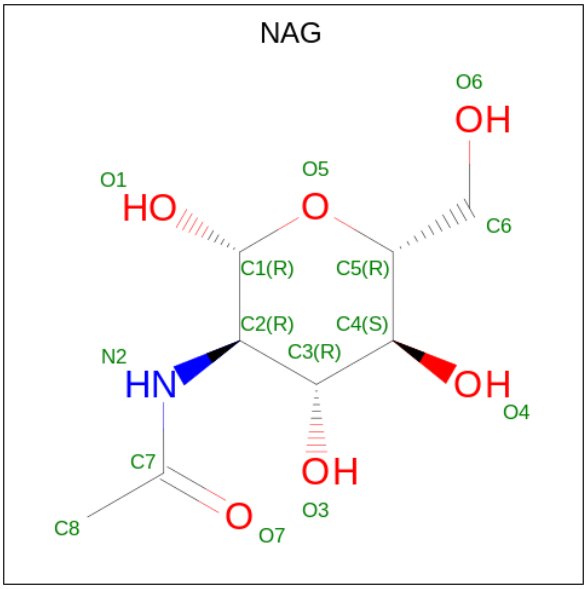
- Molecule 2 is a protein called mono-mannosyl peptide (379Man short peptide).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	14	Total	C	N	O	0	0	1
			95	59	18	18			

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

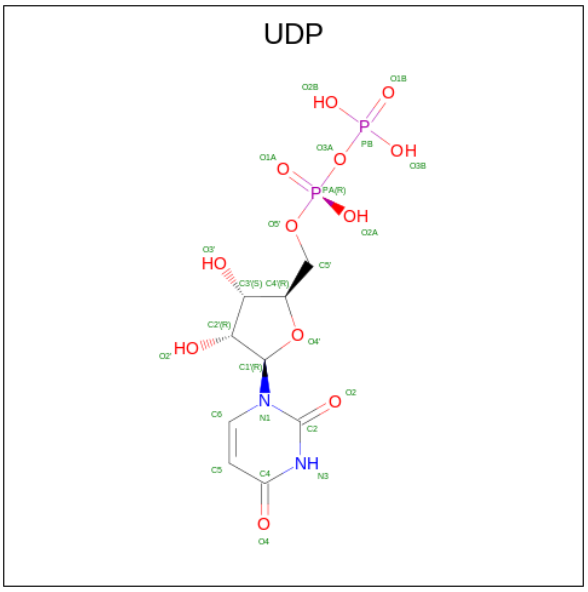
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



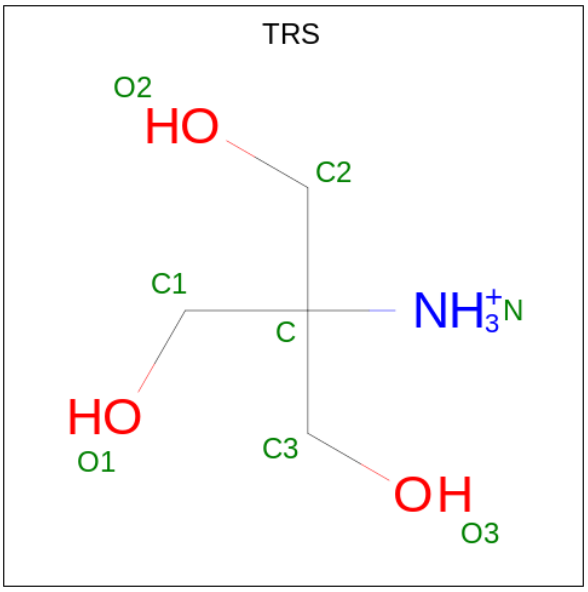
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).



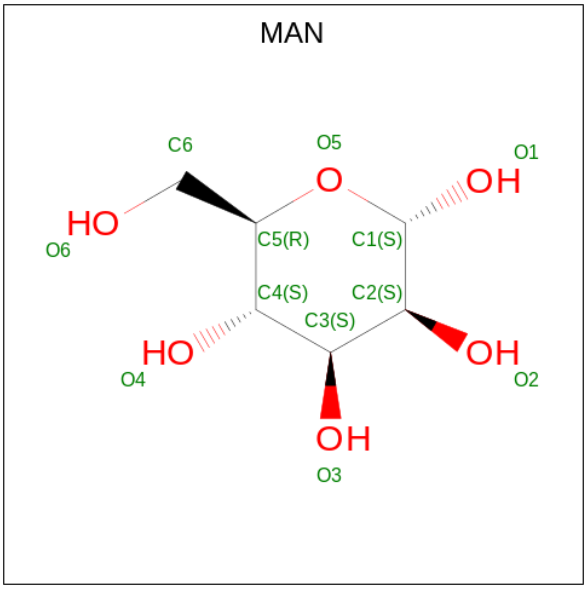
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
5	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 7 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 11 6 5	0	0

- Molecule 8 is water.

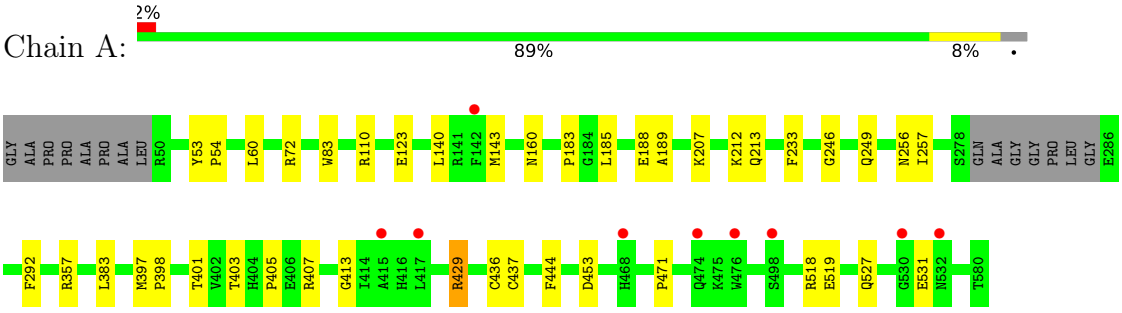
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	283	Total O 283 283	0	0
8	B	173	Total O 173 173	0	0
8	C	9	Total O 9 9	0	0

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.

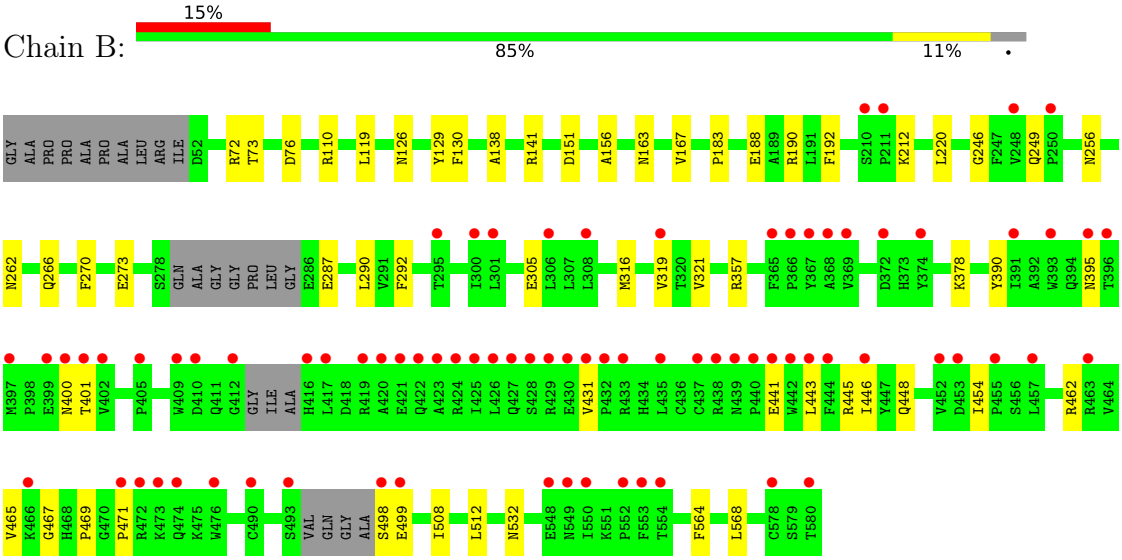
• Molecule 1: Protein O-linked-mannose beta-1,4-N-acetylglucosaminyltransferase 2

Chain A:



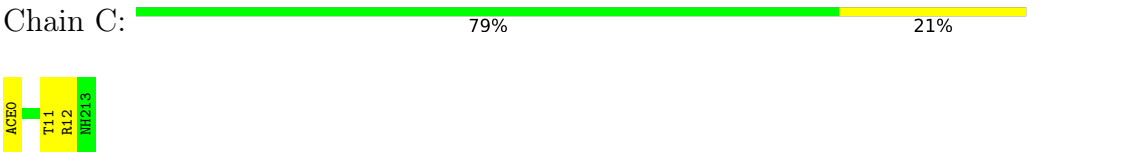
• Molecule 1: Protein O-linked-mannose beta-1,4-N-acetylglucosaminyltransferase 2

Chain B:



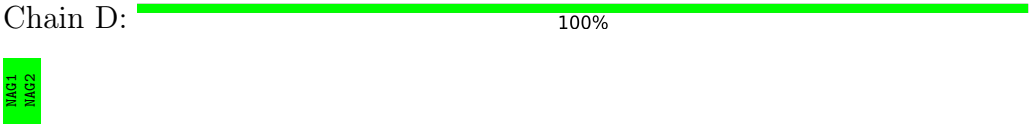
• Molecule 2: mono-mannosyl peptide (379Man short peptide)

Chain C:



• Molecule 3: 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	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.39Å 104.44Å 126.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.29 – 2.10 48.29 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.29-2.10) 99.7 (48.29-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.185 , 0.234 0.185 , 0.234	Depositor DCC
R_{free} test set	3481 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	37.2	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9056	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, ACE, TRS, NH2, UDP, MAN

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	0.44	0/4338	0.57	0/5910
1	B	0.37	0/4232	0.53	0/5769
2	C	0.32	0/94	0.61	0/130
All	All	0.41	0/8664	0.55	0/11809

There are no bond length outliers.

There are no bond angle outliers.

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	4216	0	4143	25	0
1	B	4113	0	4008	35	0
2	C	95	0	98	2	0
3	D	28	0	25	0	0
4	A	28	0	26	0	0
4	B	42	0	39	0	0
5	A	25	0	11	0	0
5	B	25	0	11	0	0
6	A	8	0	12	0	0
7	C	11	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	283	0	0	2	0
8	B	173	0	0	0	0
8	C	9	0	0	0	0
All	All	9056	0	8383	56	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (56) 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:119:LEU:HG	1:B:130:PHE:HB2	1.56	0.85
1:B:395:ASN:HD21	1:B:400:ASN:HB2	1.42	0.81
1:A:140:LEU:HA	1:A:143:MET:HE2	1.67	0.76
1:A:256[A]:ASN:OD1	1:B:110:ARG:NH1	2.23	0.71
1:B:151:ASP:OD2	1:B:190:ARG:NH1	2.27	0.68
1:A:403:THR:HG23	1:A:444:PHE:CE1	2.29	0.67
1:A:357:ARG:O	1:A:471:PRO:HB3	1.96	0.66
1:A:403:THR:HG22	1:A:405:PRO:HD3	1.79	0.64
8:A:742:HOH:O	2:C:0:ACE:H3	1.98	0.63
1:B:270:PHE:O	1:B:273:GLU:HG3	2.00	0.61
1:B:290:LEU:HD11	1:B:321:VAL:HB	1.85	0.59
1:A:183:PRO:HD2	1:B:183:PRO:HD2	1.85	0.58
1:B:188:GLU:O	1:B:212:LYS:HE2	2.06	0.55
1:A:527:GLN:NE2	1:A:531:GLU:O	2.30	0.55
1:A:397:MET:HE1	1:A:453:ASP:HB2	1.88	0.55
1:A:110:ARG:NH1	1:B:256[A]:ASN:OD1	2.40	0.54
1:B:305:GLU:HG2	1:B:454:ILE:HD12	1.89	0.54
1:A:429:ARG:HD3	8:A:971:HOH:O	2.07	0.54
1:A:403:THR:HG23	1:A:444:PHE:CZ	2.43	0.54
1:A:246:GLY:HA2	1:A:249:GLN:O	2.10	0.52
1:A:518:ARG:NH2	1:A:519:GLU:OE2	2.42	0.52
1:B:508:ILE:HB	1:B:512:LEU:HD23	1.93	0.51
1:B:287:GLU:HG2	1:B:316:MET:SD	2.50	0.51
1:A:407:ARG:O	1:A:413:GLY:HA3	2.11	0.51
1:B:126:ASN:HA	1:B:129:TYR:CE2	2.46	0.51
1:A:185:LEU:HD22	1:A:189:ALA:HB2	1.94	0.50
1:B:290:LEU:HA	1:B:319:VAL:HG23	1.94	0.49
1:B:357:ARG:O	1:B:471:PRO:HB3	2.12	0.49
1:A:257:ILE:HG21	1:A:383:LEU:HD11	1.95	0.49
1:A:60:LEU:HD13	1:A:83:TRP:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:GLY:HA2	1:B:249:GLN:O	2.12	0.49
1:B:401:THR:OG1	1:B:448:GLN:NE2	2.46	0.49
1:B:443:LEU:HA	1:B:446:ILE:HG22	1.95	0.48
1:B:138:ALA:O	1:B:141:ARG:HG2	2.14	0.48
1:B:445:ARG:O	1:B:448:GLN:HG3	2.13	0.48
1:B:431:VAL:HG13	1:B:441:GLU:HG3	1.94	0.47
1:B:465:VAL:HG11	1:B:469:PRO:HG3	1.97	0.46
1:A:53:TYR:HB3	1:A:54:PRO:HD3	1.98	0.46
1:B:378:LYS:HB2	1:B:390:TYR:CZ	2.51	0.45
1:B:462:ARG:NH1	1:B:467:GLY:O	2.34	0.45
1:B:564:PHE:HB2	1:B:568:LEU:HB2	1.99	0.45
1:B:498:SER:OG	1:B:499:GLU:N	2.49	0.44
1:B:192:PHE:CD2	1:B:220:LEU:HD11	2.52	0.44
1:A:72:ARG:NE	1:B:76:ASP:OD2	2.50	0.44
1:A:233:PHE:HZ	1:B:183:PRO:HG3	1.82	0.44
1:A:188:GLU:O	1:A:212:LYS:HE2	2.18	0.43
1:B:192:PHE:CE2	1:B:220:LEU:HD11	2.54	0.43
1:A:398:PRO:O	1:A:401:THR:HG22	2.18	0.43
1:B:119:LEU:HD22	1:B:156:ALA:HA	2.01	0.42
1:B:163:ASN:O	1:B:167:VAL:HG23	2.19	0.42
1:A:403:THR:CG2	1:A:444:PHE:CZ	3.02	0.42
1:B:532:ASN:ND2	2:C:11:THR:OG1	2.46	0.41
1:B:262:ASN:O	1:B:266:GLN:HG2	2.19	0.41
1:A:207:LYS:HE2	1:A:213:GLN:OE1	2.21	0.41
1:B:72:ARG:HG3	1:B:73:THR:HG23	2.02	0.41
1:A:436:CYS:HA	1:A:437:CYS:HA	1.79	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	521/539 (97%)	511 (98%)	10 (2%)	0	100	100
1	B	508/539 (94%)	498 (98%)	10 (2%)	0	100	100
2	C	12/14 (86%)	12 (100%)	0	0	100	100
All	All	1041/1092 (95%)	1021 (98%)	20 (2%)	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	452/467 (97%)	448 (99%)	4 (1%)	78	84
1	B	438/467 (94%)	437 (100%)	1 (0%)	93	96
2	C	11/11 (100%)	10 (91%)	1 (9%)	9	6
All	All	901/945 (95%)	895 (99%)	6 (1%)	84	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
1	A	160	ASN
1	A	292	PHE
1	A	429	ARG
1	B	292	PHE
2	C	12	ARG

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

Mol	Chain	Res	Type
1	A	400	ASN
1	B	296	GLN
1	B	448	GLN

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

2 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	$\#\|Z\| > 2$
3	NAG	D	1	3,1	14,14,15	0.40	0	17,19,21	0.38	0
3	NAG	D	2	3	14,14,15	0.46	0	17,19,21	0.44	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
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	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
3	D	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6

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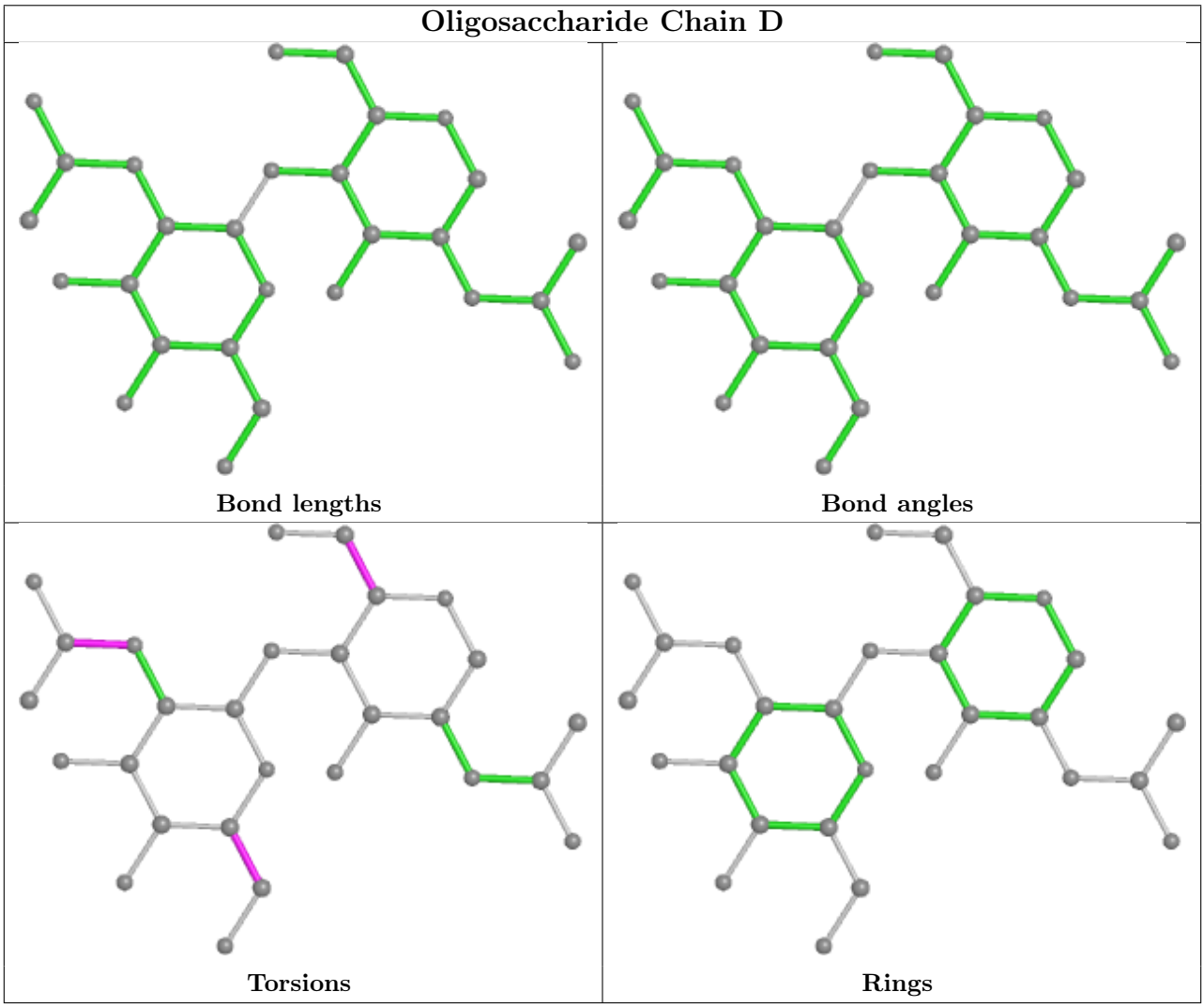
Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2

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)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	603	1	14,14,15	0.40	0	17,19,21	0.60	0
6	TRS	A	604	-	7,7,7	0.34	0	9,9,9	0.69	0
4	NAG	A	602	1	14,14,15	0.37	0	17,19,21	0.56	0
4	NAG	A	601	1	14,14,15	0.18	0	17,19,21	0.64	0
5	UDP	B	604	-	20,26,26	0.98	1 (5%)	25,40,40	1.22	4 (16%)
4	NAG	B	601	1	14,14,15	0.28	0	17,19,21	0.65	0
5	UDP	A	603	-	20,26,26	1.10	1 (5%)	25,40,40	1.13	2 (8%)
4	NAG	B	602	1	14,14,15	0.35	0	17,19,21	0.65	0
7	MAN	C	101	2	11,11,12	1.24	1 (9%)	15,15,17	1.14	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
4	NAG	B	603	1	-	0/6/23/26	0/1/1/1
6	TRS	A	604	-	-	0/9/9/9	-
4	NAG	A	602	1	-	0/6/23/26	0/1/1/1
4	NAG	A	601	1	-	3/6/23/26	0/1/1/1
5	UDP	B	604	-	-	3/14/32/32	0/2/2/2
4	NAG	B	601	1	-	3/6/23/26	0/1/1/1
5	UDP	A	603	-	-	0/14/32/32	0/2/2/2
4	NAG	B	602	1	-	2/6/23/26	0/1/1/1
7	MAN	C	101	2	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	604	UDP	C4-N3	3.23	1.38	1.33
5	A	603	UDP	C4-N3	3.18	1.38	1.33
7	C	101	MAN	C4-C3	2.96	1.59	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	604	UDP	C5-C4-N3	-3.88	114.77	123.31
5	A	603	UDP	C5-C4-N3	-3.82	114.91	123.31
7	C	101	MAN	C1-O5-C5	2.98	116.22	112.19
5	B	604	UDP	O3B-PB-O2B	2.44	116.94	107.64
5	B	604	UDP	O3B-PB-O3A	2.30	112.33	104.64
7	C	101	MAN	O2-C2-C3	-2.20	105.73	110.14
5	A	603	UDP	O3B-PB-O3A	2.17	111.90	104.64
5	B	604	UDP	PA-O3A-PB	-2.07	125.73	132.83

There are no chirality outliers.

All (11) torsion outliers are listed below:

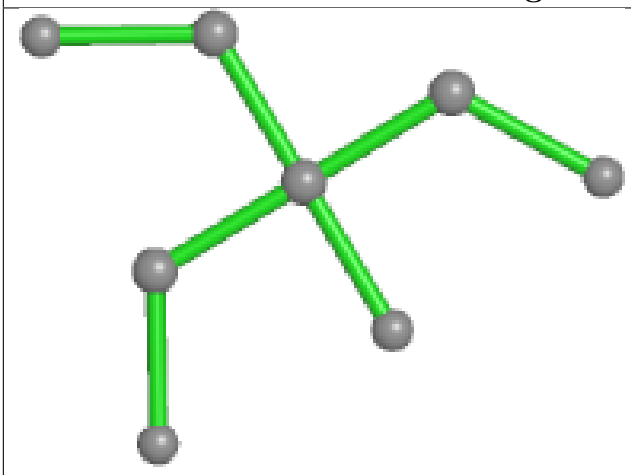
Mol	Chain	Res	Type	Atoms
5	B	604	UDP	C2'-C1'-N1-C6
5	B	604	UDP	O4'-C1'-N1-C6
4	B	602	NAG	O5-C5-C6-O6
4	A	601	NAG	O5-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6
4	B	602	NAG	C4-C5-C6-O6
4	B	601	NAG	C4-C5-C6-O6
4	B	601	NAG	O5-C5-C6-O6
5	B	604	UDP	PB-O3A-PA-O2A
4	A	601	NAG	C3-C2-N2-C7
4	B	601	NAG	C3-C2-N2-C7

There are no ring outliers.

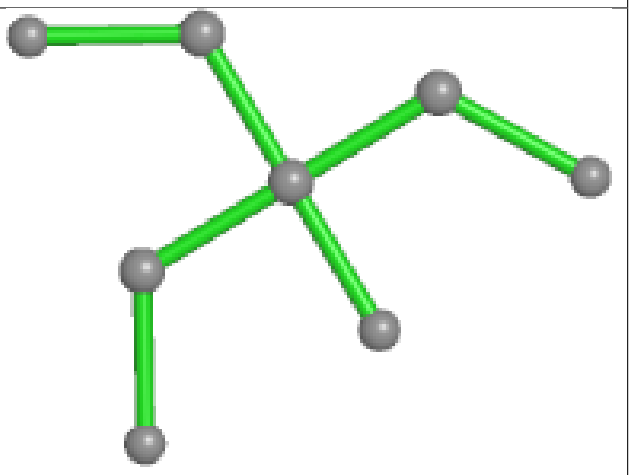
No monomer is involved in short contacts.

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

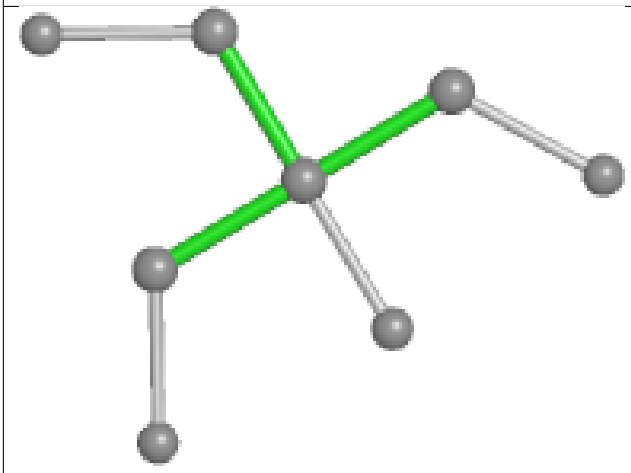
Ligand TRS A 604



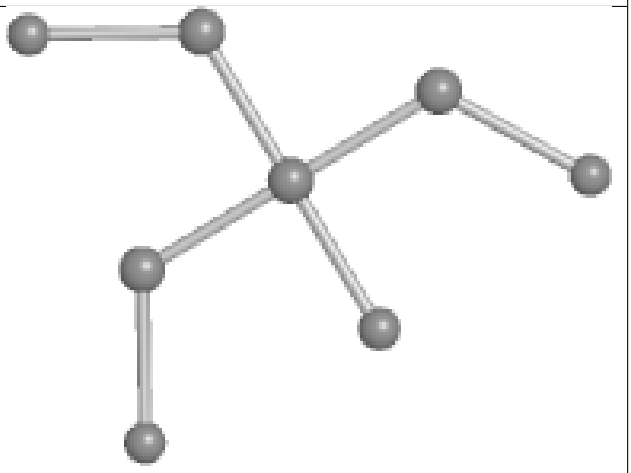
Bond lengths



Bond angles

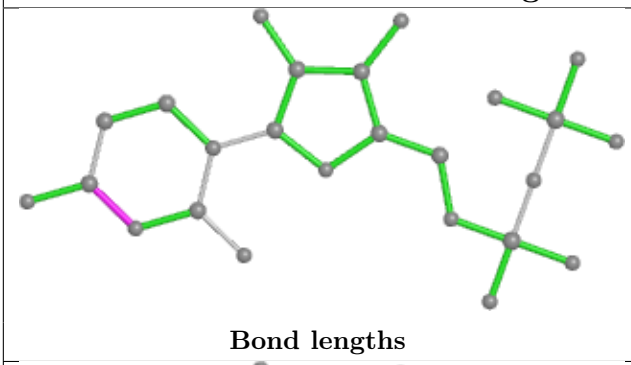


Torsions

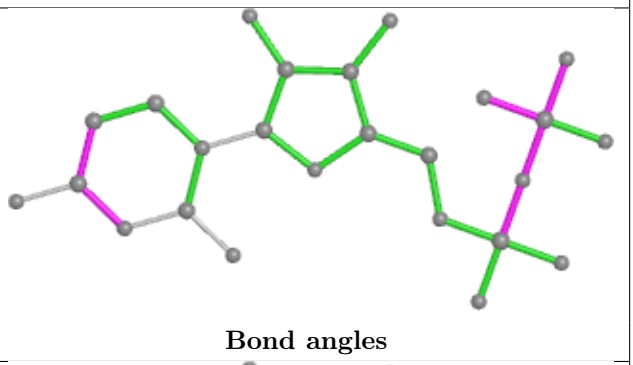


Rings

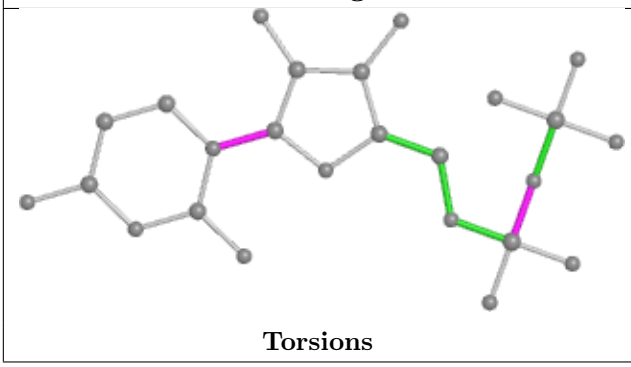
Ligand UDP B 604



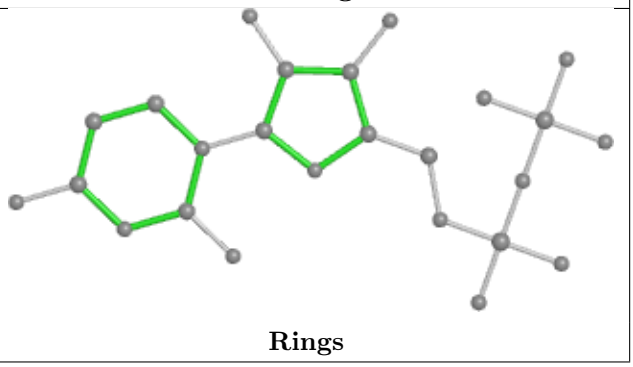
Bond lengths



Bond angles

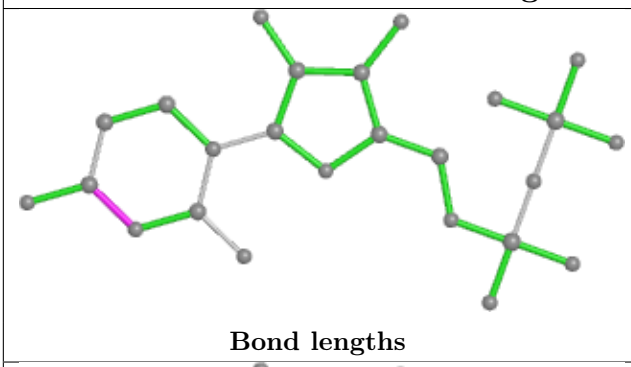


Torsions

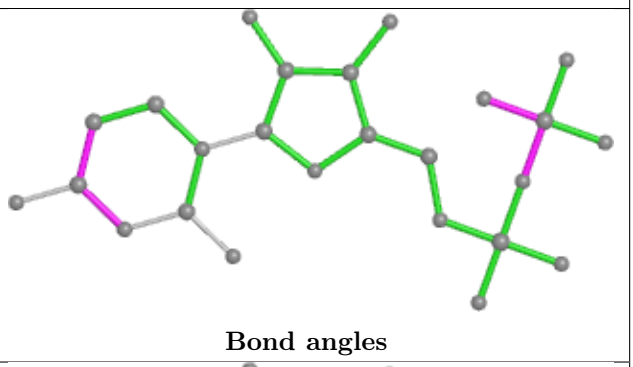


Rings

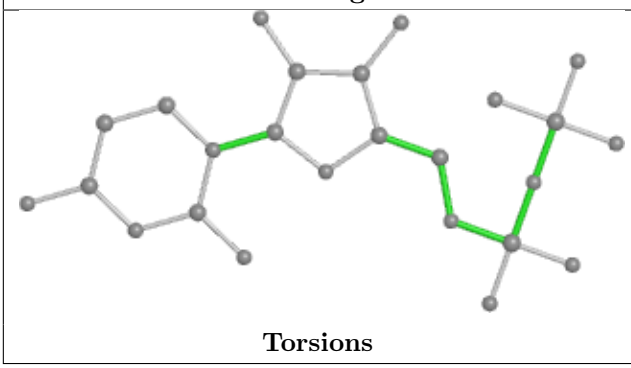
Ligand UDP A 603



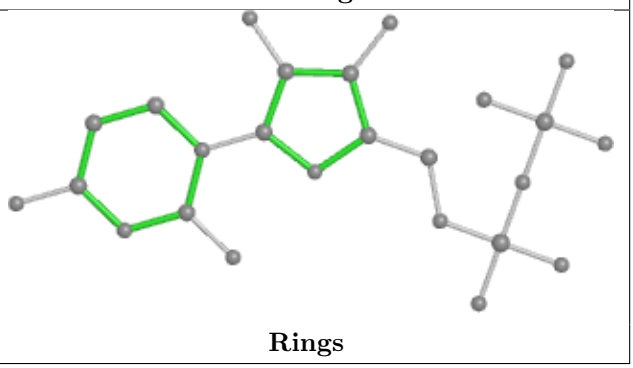
Bond lengths



Bond angles

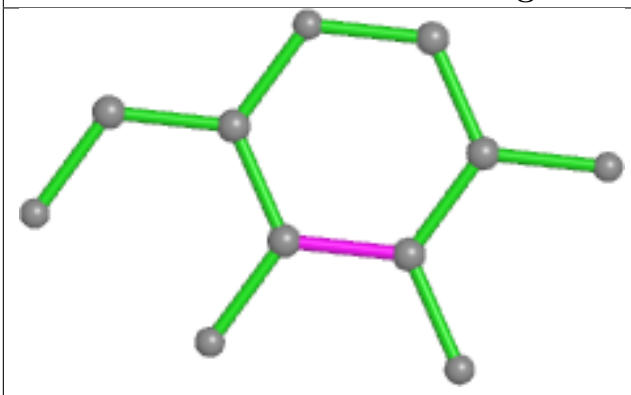


Torsions

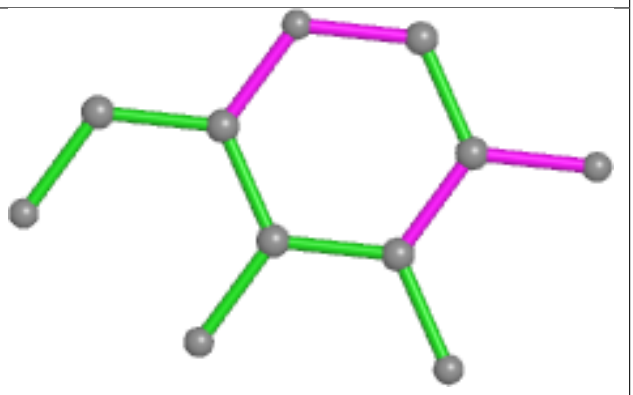


Rings

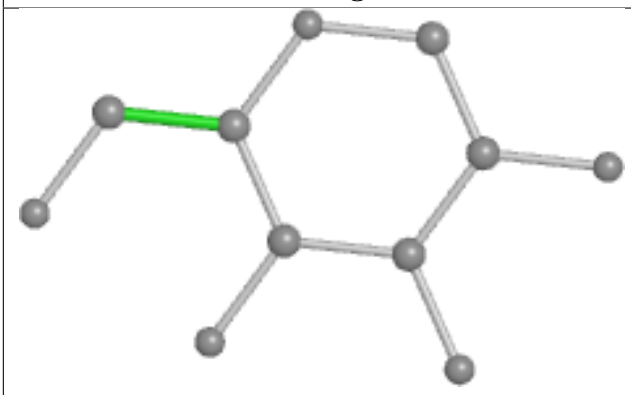
Ligand MAN C 101



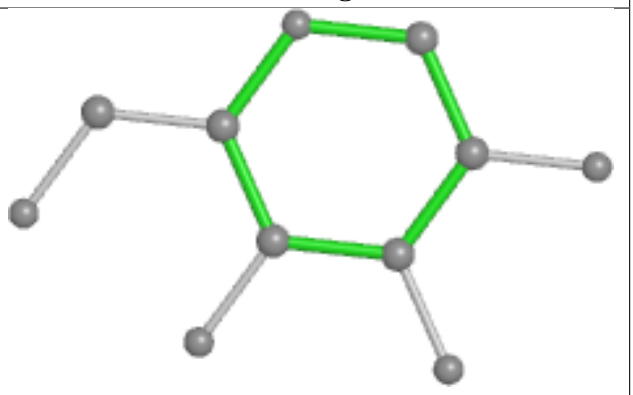
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	524/539 (97%)	0.00	9 (1%) 70 74	24, 38, 64, 111	0
1	B	515/539 (95%)	0.66	80 (15%) 2 2	26, 52, 110, 139	0
2	C	12/14 (85%)	0.28	0 100 100	34, 42, 81, 107	0
All	All	1051/1092 (96%)	0.33	89 (8%) 10 13	24, 43, 102, 139	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	401	THR	7.9
1	B	396	THR	6.8
1	B	423	ALA	6.5
1	B	425	ILE	6.4
1	B	420	ALA	6.3
1	B	368	ALA	5.0
1	B	437	CYS	4.5
1	B	432	PRO	4.3
1	B	393	TRP	4.2
1	B	366	PRO	4.2
1	B	439	ASN	4.2
1	B	367	TYR	4.1
1	B	400	ASN	4.0
1	B	426	LEU	4.0
1	B	431	VAL	3.9
1	A	468	HIS	3.9
1	B	446	ILE	3.9
1	B	405	PRO	3.8
1	B	429	ARG	3.7
1	B	548	GLU	3.7
1	B	453	ASP	3.7
1	B	440	PRO	3.7
1	B	471	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	463	ARG	3.6
1	B	452	VAL	3.6
1	B	365	PHE	3.5
1	B	402	VAL	3.5
1	B	399	GLU	3.4
1	B	438	ARG	3.4
1	B	474	GLN	3.4
1	B	211	PRO	3.3
1	B	417	LEU	3.3
1	B	412	GLY	3.3
1	B	300	ILE	3.3
1	B	409	TRP	3.2
1	B	442	TRP	3.2
1	B	473	LYS	3.2
1	B	427	GLN	3.1
1	B	395	ASN	3.1
1	B	433	ARG	3.1
1	B	308	LEU	3.1
1	B	457	LEU	3.1
1	B	369	VAL	3.0
1	B	428	SER	3.0
1	A	532	ASN	3.0
1	B	578	CYS	2.9
1	B	444	PHE	2.9
1	B	552	PRO	2.9
1	B	248	VAL	2.8
1	B	422	GLN	2.7
1	A	474	GLN	2.7
1	B	493	SER	2.7
1	B	498	SER	2.7
1	B	419	ARG	2.7
1	B	499	GLU	2.6
1	A	476	TRP	2.6
1	B	391	ILE	2.6
1	B	430	GLU	2.6
1	A	142	PHE	2.5
1	B	210	SER	2.5
1	B	319	VAL	2.5
1	B	476	TRP	2.5
1	B	397	MET	2.4
1	B	374	TYR	2.4
1	B	554	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	498	SER	2.4
1	B	443	LEU	2.4
1	B	250	PRO	2.4
1	B	455	PRO	2.4
1	B	306	LEU	2.3
1	B	550	ILE	2.3
1	B	435	LEU	2.3
1	B	472	ARG	2.3
1	B	372	ASP	2.3
1	A	530	GLY	2.3
1	B	553	PHE	2.3
1	B	441	GLU	2.2
1	A	415	ALA	2.2
1	B	421	GLU	2.2
1	B	490	CYS	2.1
1	B	424	ARG	2.1
1	B	295	THR	2.1
1	B	580	THR	2.1
1	B	410	ASP	2.1
1	A	417	LEU	2.1
1	B	416	HIS	2.1
1	B	466	LYS	2.1
1	B	301	LEU	2.0
1	B	549	ASN	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.

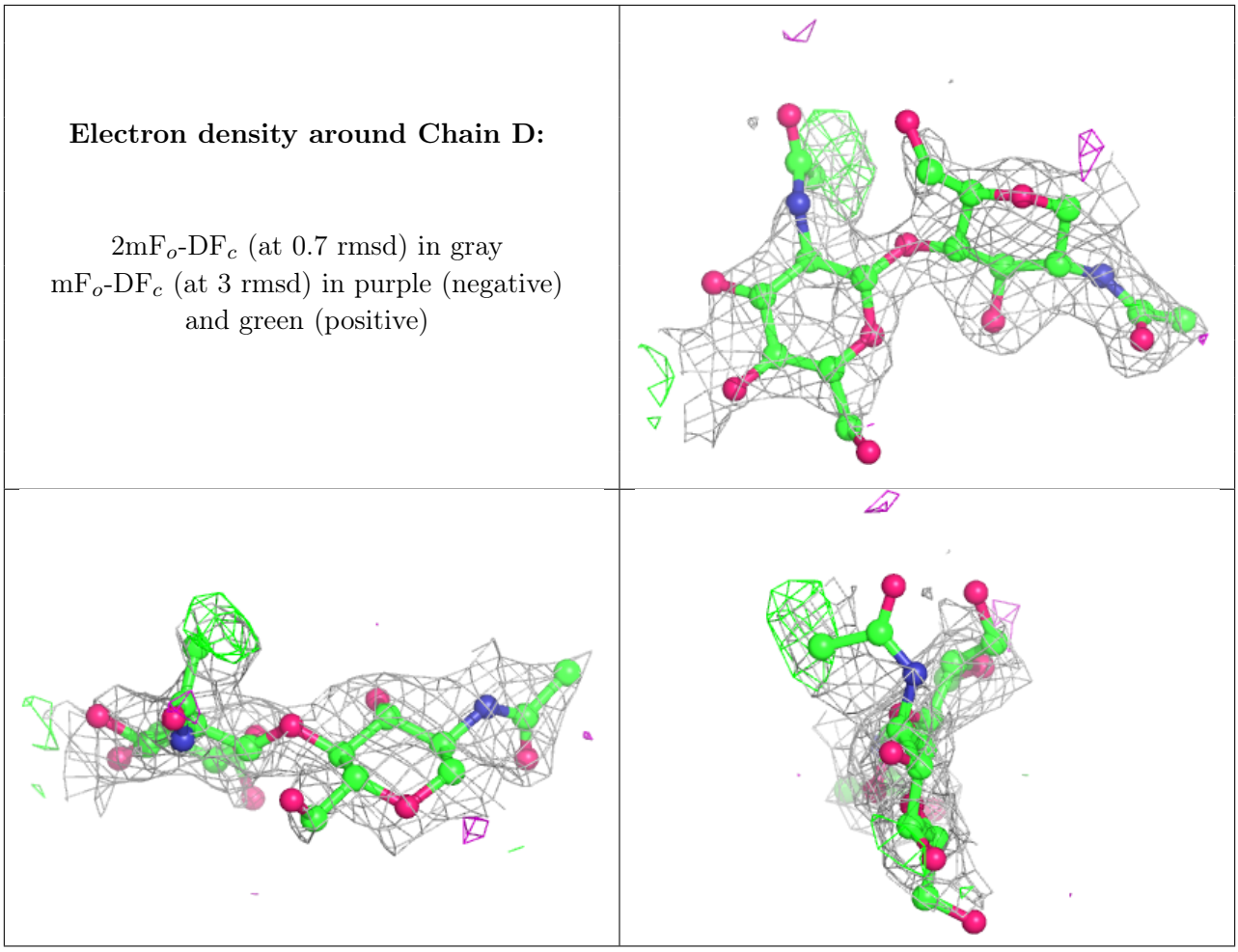
6.3 Carbohydrates (i)

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	D	2	14/15	0.54	0.33	95,99,101,102	0
3	NAG	D	1	14/15	0.78	0.26	62,69,80,89	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands

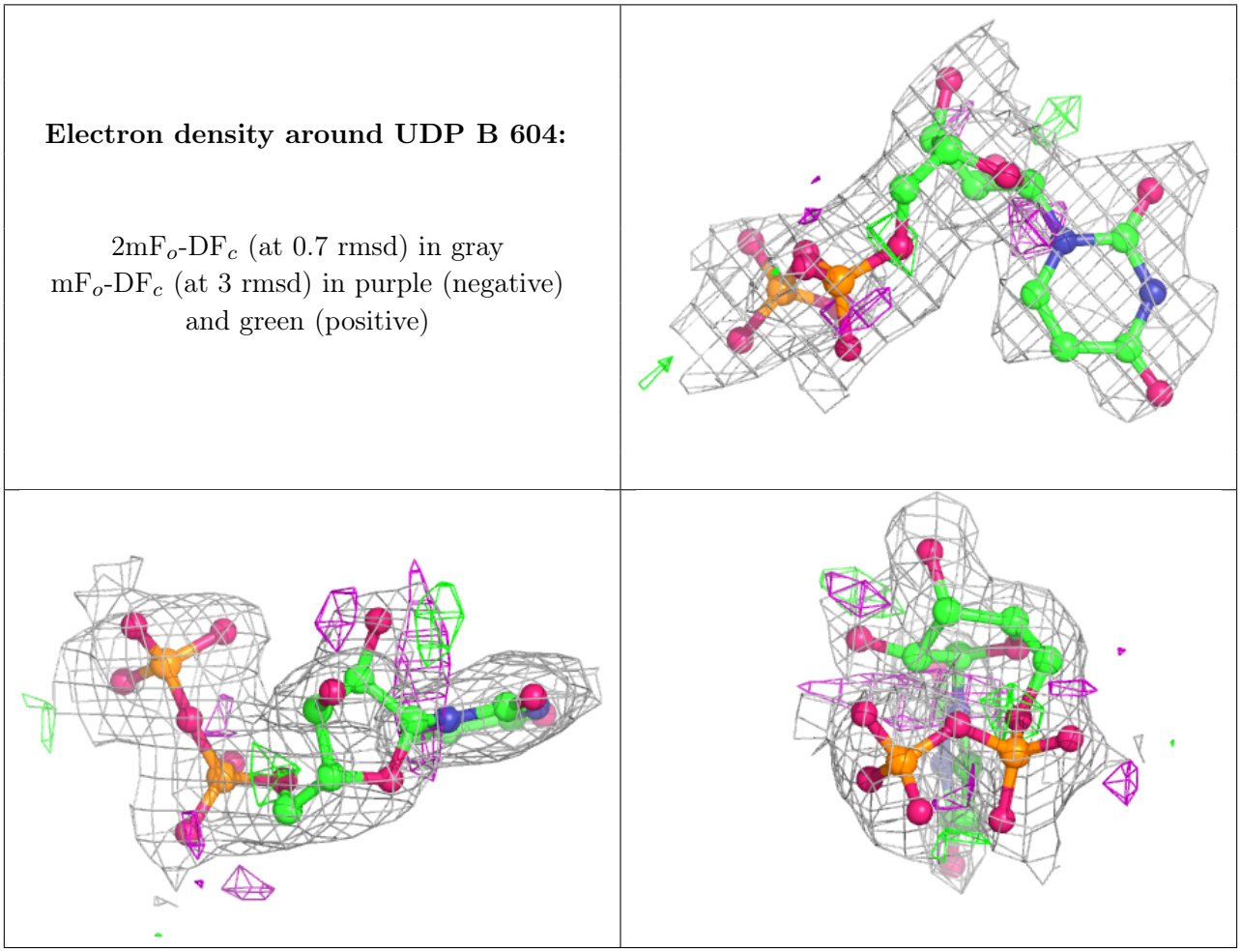
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	NAG	B	602	14/15	0.60	0.33	76,88,94,96	0
4	NAG	B	601	14/15	0.78	0.19	51,65,70,70	0
4	NAG	A	602	14/15	0.82	0.24	48,58,69,72	0
4	NAG	A	601	14/15	0.83	0.14	52,66,70,75	0
5	UDP	B	604	25/25	0.85	0.19	52,62,69,70	0
7	MAN	C	101	11/12	0.89	0.12	28,31,34,36	0
4	NAG	B	603	14/15	0.90	0.14	44,54,60,62	0
6	TRS	A	604	8/8	0.91	0.12	29,35,37,39	0
5	UDP	A	603	25/25	0.97	0.10	27,31,42,44	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.

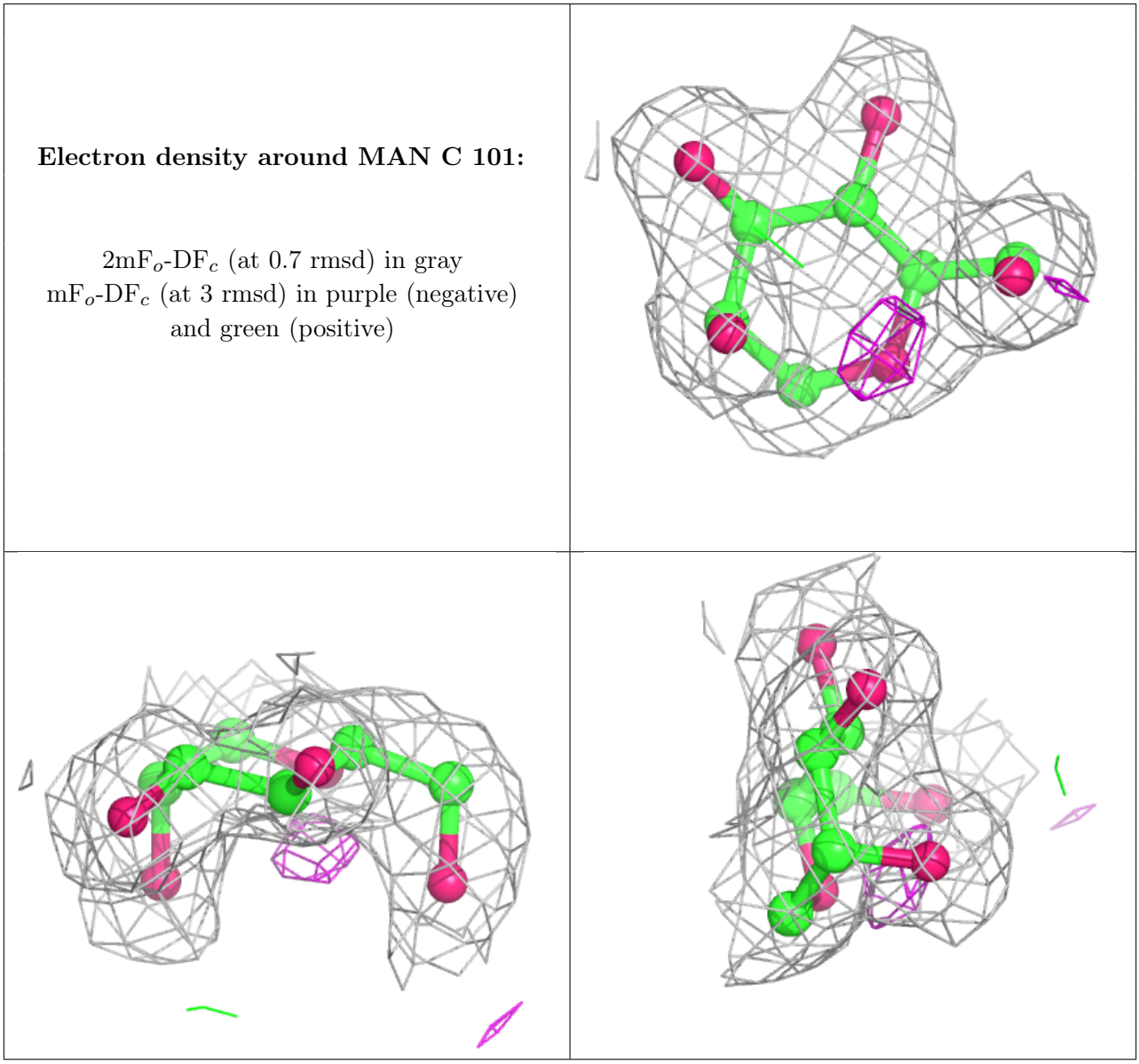
Electron density around UDP B 604:

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



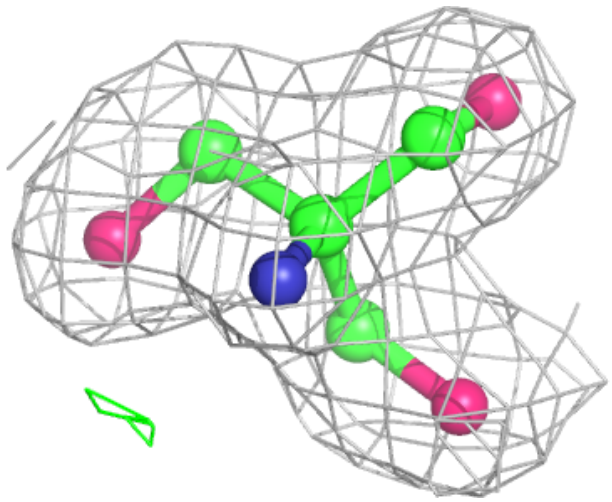
Electron density around MAN C 101:

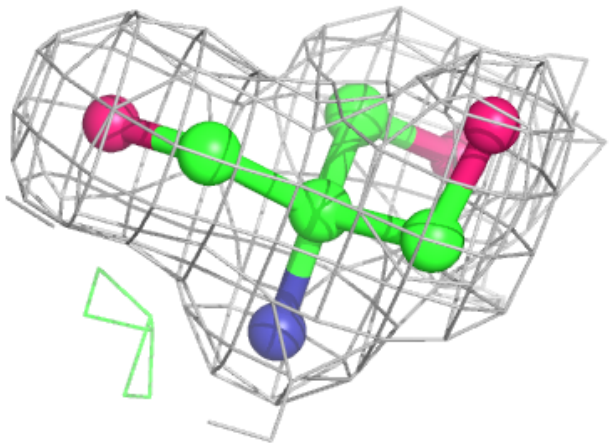
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

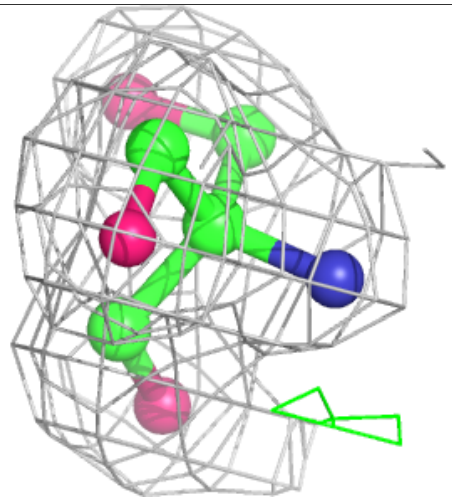


Electron density around TRS A 604:

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

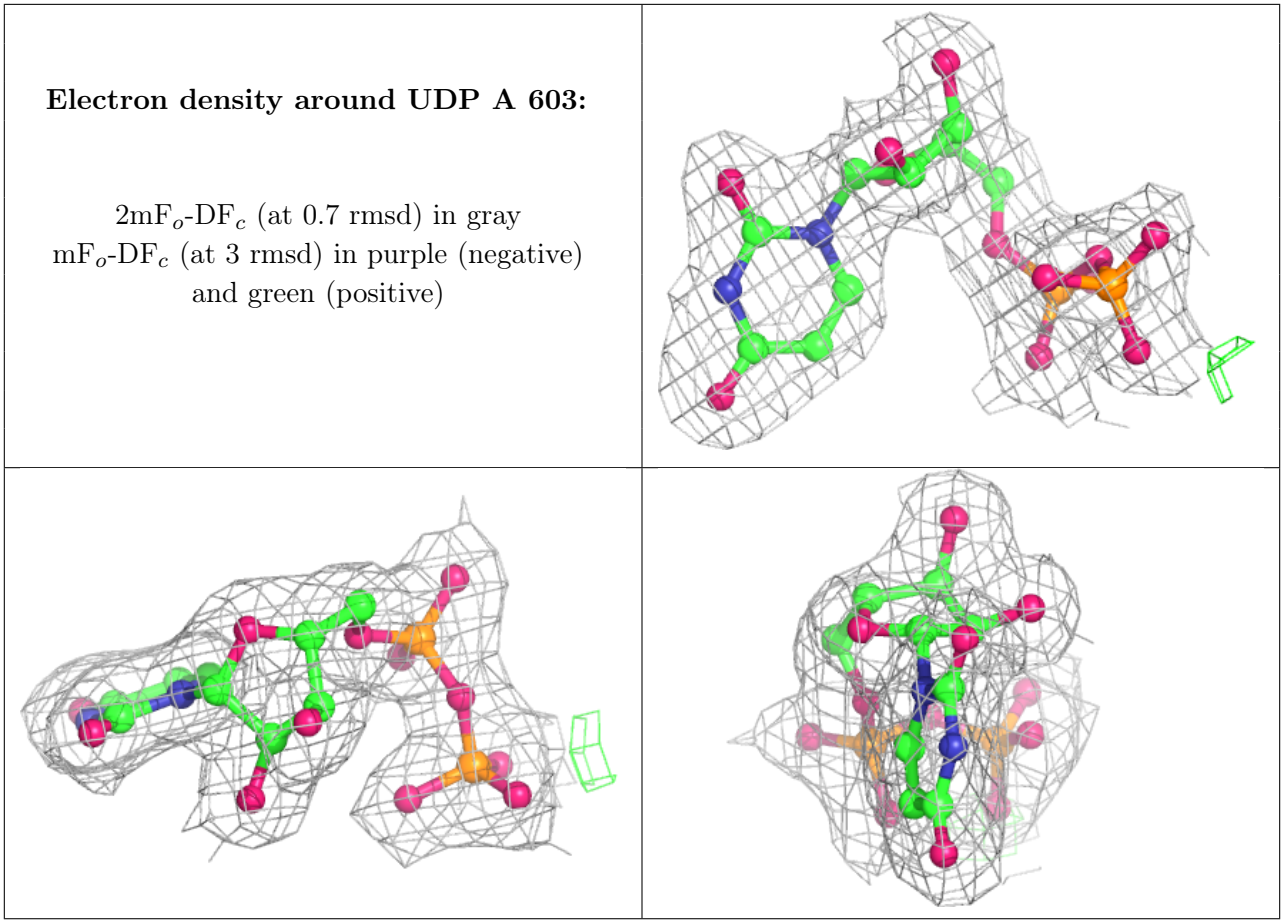






Electron density around UDP A 603:

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



6.5 Other polymers (i)

There are no such residues in this entry.