



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 02:45 PM BST

PDB ID : 5V2J
Title : Crystal structure of UDP-glucosyltransferase, UGT74F2 (T15S), with UDP and 2-bromobenzoic acid
Authors : George Thompson, A.M.; Iancu, C.V.; Dean, J.V.; Choe, J.
Deposited on : 2017-03-04
Resolution : 1.80 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 : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

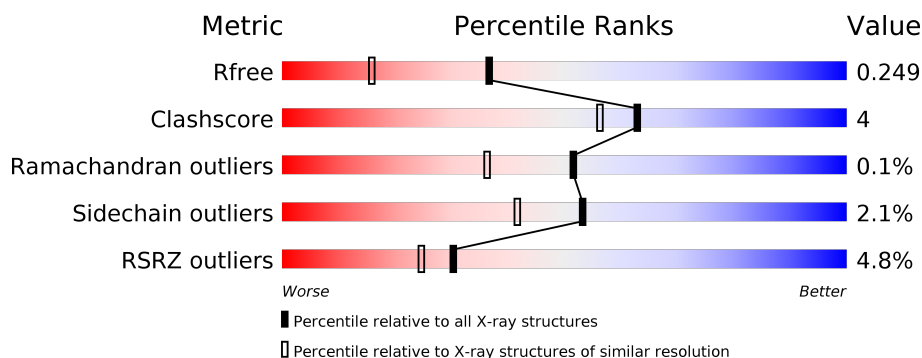
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	449	<div> <div>4%</div> <div>87%</div> <div>11%</div> <div>..</div> </div>
1	B	449	<div> <div>6%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
2	C	2	<div> <div>100%</div> </div>
2	D	2	<div> <div>50%</div> <div>50%</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7379 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 UDP-glycosyltransferase 74F2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3536	2276	572	672	16			
1	B	444	Total	C	N	O	S	0	0	0
			3536	2276	572	672	16			

There are 2 discrepancies between the modelled and reference sequences:

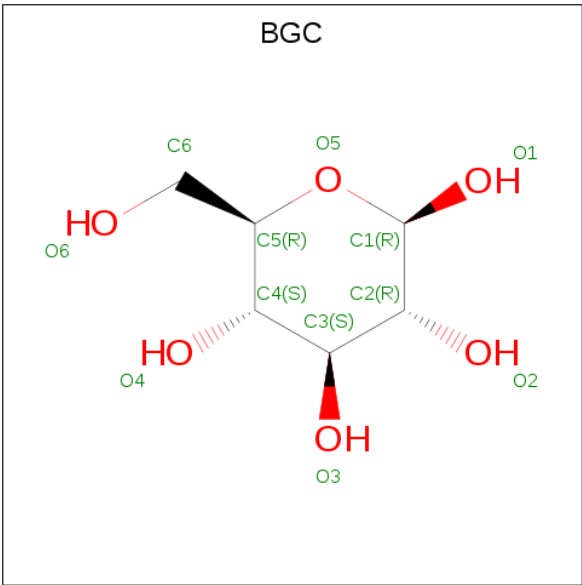
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	SER	THR	engineered mutation	UNP O22822
B	15	SER	THR	engineered mutation	UNP O22822

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



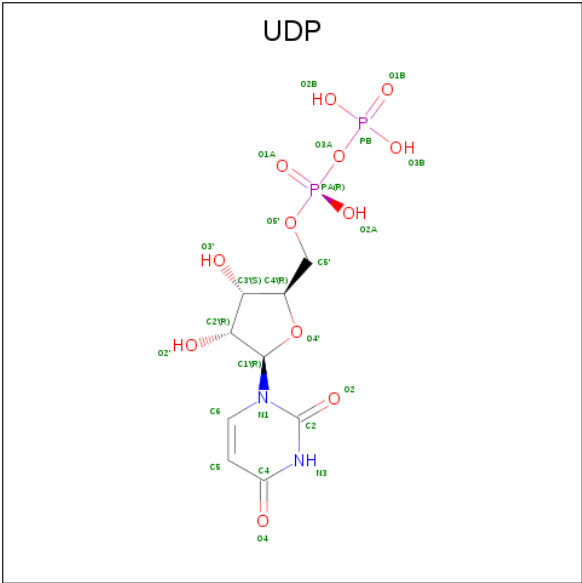
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			22	12	10			
2	D	2	Total	C	O	0	0	0
			22	12	10			

- Molecule 3 is beta-D-glucopyranose (three-letter code: BGC) (formula: C₆H₁₂O₆).

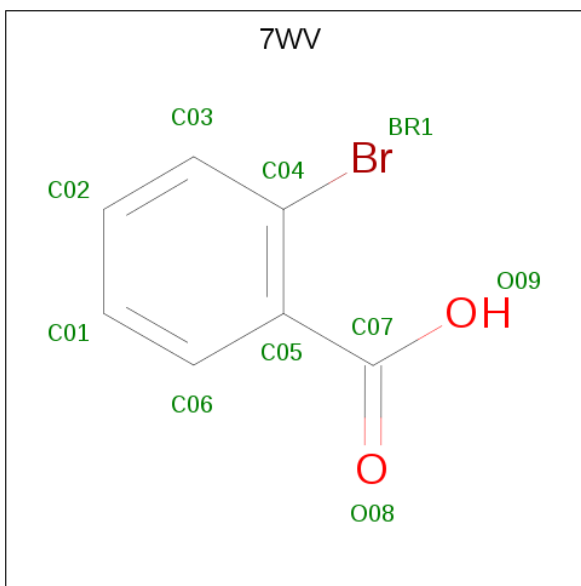


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



- Molecule 5 is 2-bromobenzoic acid (three-letter code: 7WV) (formula: $C_7H_5BrO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Br	C	O	0	0
			10	1	7	2		
5	B	1	Total	Br	C	O	0	0
			10	1	7	2		

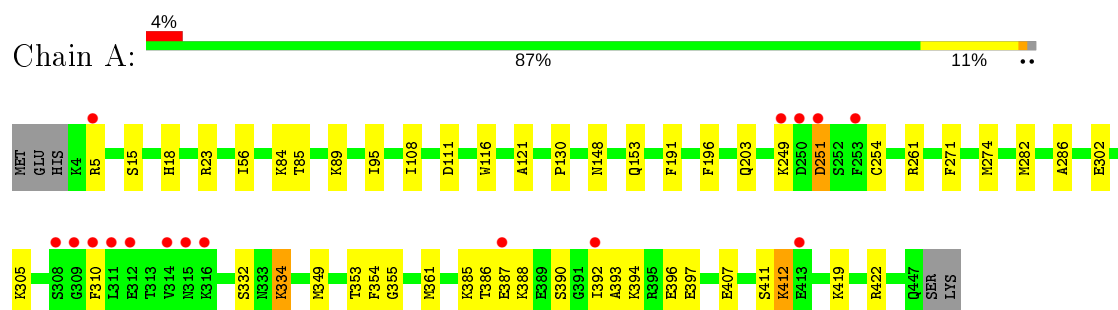
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	110	Total	O	0	0
			110	110		
6	B	61	Total	O	0	0
			61	61		

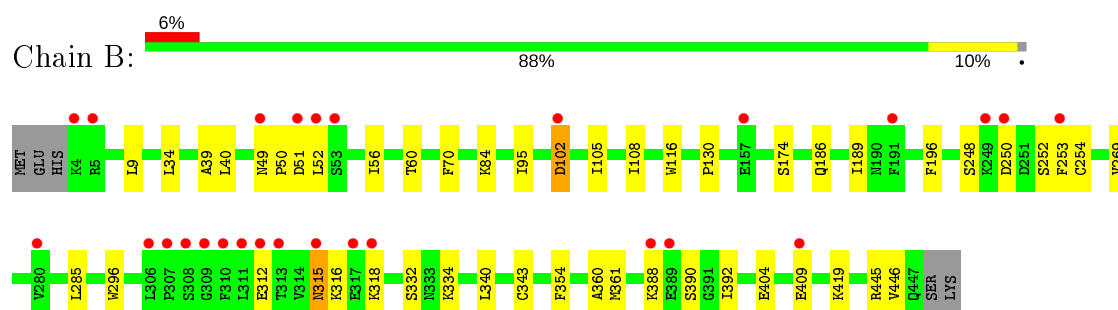
3 Residue-property plots [i](#)

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.

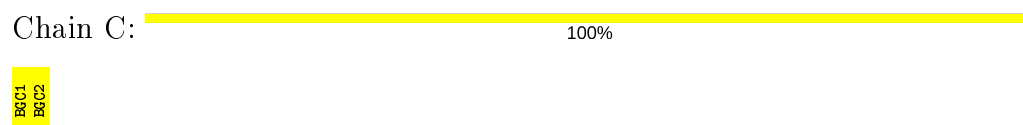
- Molecule 1: UDP-glycosyltransferase 74F2



- Molecule 1: UDP-glycosyltransferase 74F2



- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.22Å 87.41Å 162.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.21 – 1.80 42.21 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.21-1.80) 97.3 (42.21-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 1.76Å)	Xtriage
Refinement program	PHENIX (dev_2666: ???)	Depositor
R, R_{free}	0.202 , 0.249 0.202 , 0.249	Depositor DCC
R_{free} test set	4465 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7379	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 4.09% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, UDP, 7WV

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	0.45	0/3625	0.56	0/4921
1	B	0.40	0/3625	0.54	0/4921
All	All	0.42	0/7250	0.55	0/9842

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	251	ASP	Peptide
1	B	316	LYS	Peptide
1	B	51	ASP	Peptide

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	3536	0	3470	32	0
1	B	3536	0	3470	29	0
2	C	22	0	19	0	0
2	D	22	0	19	1	0
3	A	11	0	9	0	0
3	B	11	0	10	0	0
4	A	25	0	11	0	0
4	B	25	0	11	0	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
6	A	110	0	0	0	0
6	B	61	0	0	0	0
All	All	7379	0	7019	61	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (61) 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:340:LEU:HD21	1:B:361:MET:HE2	1.69	0.74
1:A:396:GLU:N	1:A:396:GLU:OE2	2.24	0.70
1:A:407:GLU:O	1:A:412:LYS:NZ	2.26	0.69
1:A:148:ASN:HD21	1:A:153:GLN:HE22	1.43	0.66
1:B:409:GLU:H	1:B:409:GLU:CD	1.98	0.66
1:A:85:THR:O	1:A:89:LYS:HD3	1.97	0.64
1:B:95:ILE:HA	1:B:105:ILE:HD12	1.81	0.63
1:A:390:SER:HB2	1:A:392:ILE:HD12	1.82	0.60
1:B:186:GLN:HG2	1:B:189:ILE:HD12	1.83	0.60
1:A:18:HIS:HD2	1:A:111:ASP:OD2	1.84	0.59
1:B:340:LEU:HD21	1:B:361:MET:CE	2.31	0.58
1:B:315:ASN:HD21	1:B:318:LYS:HB2	1.69	0.58
1:B:250:ASP:HB3	1:B:253:PHE:HB3	1.86	0.58
1:B:250:ASP:HB3	1:B:253:PHE:HD2	1.71	0.55
1:A:261:ARG:O	1:A:334:LYS:NZ	2.39	0.55
1:A:355:GLY:HA3	1:A:419:LYS:HD3	1.89	0.55
1:B:269:VAL:HG13	1:B:296:TRP:HA	1.89	0.54
1:A:23:ARG:HH22	1:A:56:ILE:HB	1.73	0.54
1:B:315:ASN:ND2	1:B:318:LYS:HB2	2.23	0.54
1:A:386:THR:HG22	1:A:393:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ASP:HB3	1:B:253:PHE:CD2	2.43	0.53
1:A:251:ASP:HB3	1:A:254:CYS:HB3	1.92	0.52
1:A:385:LYS:O	1:A:397:GLU:HG2	2.10	0.52
1:A:387:GLU:OE1	1:A:394:LYS:HD2	2.10	0.51
1:A:271:PHE:HZ	1:A:361:MET:HE3	1.75	0.51
1:A:95:ILE:HD11	1:A:108:ILE:HD11	1.92	0.51
1:B:340:LEU:C	1:B:340:LEU:HD23	2.31	0.51
1:B:343:CYS:SG	1:B:360:ALA:HB1	2.51	0.50
1:B:312:GLU:N	1:B:312:GLU:OE1	2.45	0.50
1:A:108:ILE:HD12	1:A:121:ALA:HB2	1.92	0.50
1:A:18:HIS:CD2	1:A:111:ASP:OD2	2.64	0.49
1:A:23:ARG:NH2	1:A:56:ILE:HB	2.26	0.49
1:B:70:PHE:CE2	2:D:1:BGC:H4	2.49	0.47
1:A:148:ASN:HD21	1:A:153:GLN:NE2	2.10	0.47
1:B:130:PRO:HD2	1:B:196:PHE:O	2.14	0.47
1:B:49:ASN:HA	1:B:50:PRO:HD3	1.79	0.47
1:A:286:ALA:HB1	1:A:310:PHE:CE1	2.50	0.46
1:B:34:LEU:HD21	1:B:446:VAL:HG11	1.98	0.46
1:B:95:ILE:HD11	1:B:108:ILE:HD11	1.98	0.46
1:B:102:ASP:N	1:B:102:ASP:OD1	2.50	0.45
1:A:302:GLU:OE2	1:A:305:LYS:NZ	2.41	0.45
1:A:15:SER:HB2	1:A:274:MET:HE1	1.99	0.44
1:A:271:PHE:HZ	1:A:361:MET:CE	2.30	0.44
1:A:84:LYS:HG3	1:A:116:TRP:CG	2.53	0.43
1:A:282:MET:HG3	1:A:305:LYS:HB2	2.00	0.43
1:A:130:PRO:HD2	1:A:196:PHE:O	2.18	0.43
1:A:388:LYS:HG2	1:A:388:LYS:H	1.64	0.43
1:A:332:SER:HB3	1:A:354:PHE:CE1	2.54	0.42
1:B:52:LEU:HD13	1:B:56:ILE:HG21	2.01	0.42
1:B:269:VAL:HG13	1:B:296:TRP:CD1	2.54	0.42
1:B:390:SER:HB2	1:B:392:ILE:HG12	2.01	0.42
1:B:332:SER:HB3	1:B:354:PHE:CE1	2.55	0.42
1:B:269:VAL:HG23	1:B:340:LEU:HD22	2.02	0.42
1:B:84:LYS:HE3	1:B:116:TRP:HB3	2.02	0.41
1:A:353:THR:O	1:A:422:ARG:HB2	2.19	0.41
1:B:419:LYS:HE2	1:B:419:LYS:HB2	1.87	0.41
1:A:385:LYS:H	1:A:397:GLU:CD	2.24	0.41
1:B:9:LEU:HD11	1:B:39:ALA:HB2	2.03	0.41
1:B:40:LEU:O	1:B:60:THR:HA	2.22	0.40
1:A:349:MET:O	1:A:353:THR:HG23	2.21	0.40
1:A:396:GLU:H	1:A:396:GLU:CD	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/449 (98%)	430 (97%)	12 (3%)	0	100	100
1	B	442/449 (98%)	427 (97%)	14 (3%)	1 (0%)	47	33
All	All	884/898 (98%)	857 (97%)	26 (3%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	315	ASN

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	396/401 (99%)	389 (98%)	7 (2%)	59	48
1	B	396/401 (99%)	386 (98%)	10 (2%)	47	34
All	All	792/802 (99%)	775 (98%)	17 (2%)	53	42

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	191	PHE

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Mol	Chain	Res	Type
1	A	203	GLN
1	A	249	LYS
1	A	334	LYS
1	A	411	SER
1	A	412	LYS
1	B	102	ASP
1	B	174	SER
1	B	248	SER
1	B	252	SER
1	B	254	CYS
1	B	285	LEU
1	B	334	LYS
1	B	388	LYS
1	B	404	GLU
1	B	445	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	24	GLN
1	A	153	GLN
1	A	281	GLN
1	A	327	GLN
1	B	46	ASN
1	B	49	ASN
1	B	148	ASN
1	B	210	ASN
1	B	315	ASN
1	B	370	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	BGC	C	1	1,2	11,11,12	0.97	0	15,15,17	1.36	3 (20%)
2	BGC	C	2	2	11,11,12	0.54	0	15,15,17	1.23	1 (6%)
2	BGC	D	1	1,2	11,11,12	0.98	0	15,15,17	1.33	2 (13%)
2	BGC	D	2	2	11,11,12	0.35	0	15,15,17	0.98	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	BGC	C	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	D	1	1,2	-	0/2/19/22	0/1/1/1
2	BGC	D	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	BGC	C1-C2-C3	-3.25	105.67	109.67
2	D	1	BGC	O5-C5-C6	3.11	112.08	107.20
2	C	1	BGC	O2-C2-C3	-2.52	105.09	110.14
2	D	1	BGC	O2-C2-C1	2.43	114.12	109.15
2	C	1	BGC	C6-C5-C4	-2.23	107.77	113.00
2	C	1	BGC	O5-C5-C6	2.02	110.38	107.20

There are no chirality outliers.

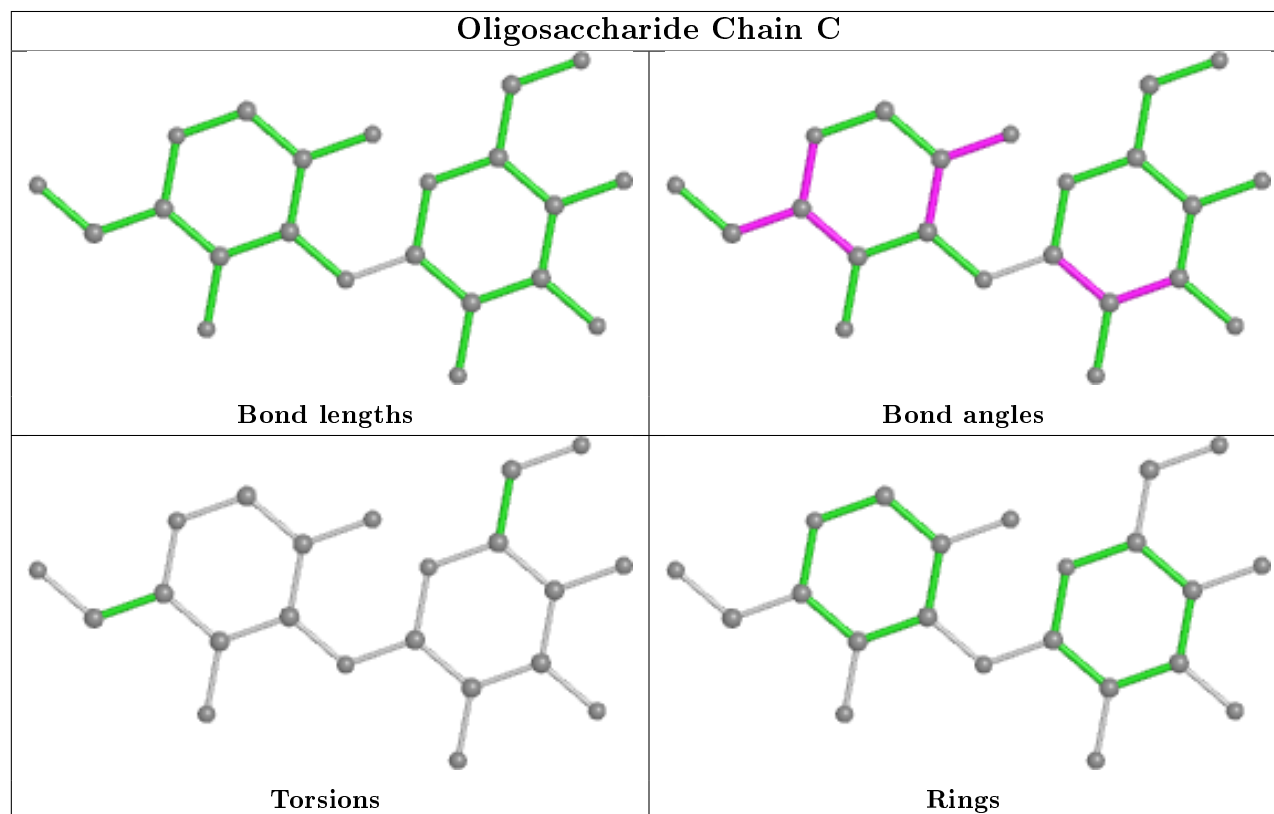
There are no torsion outliers.

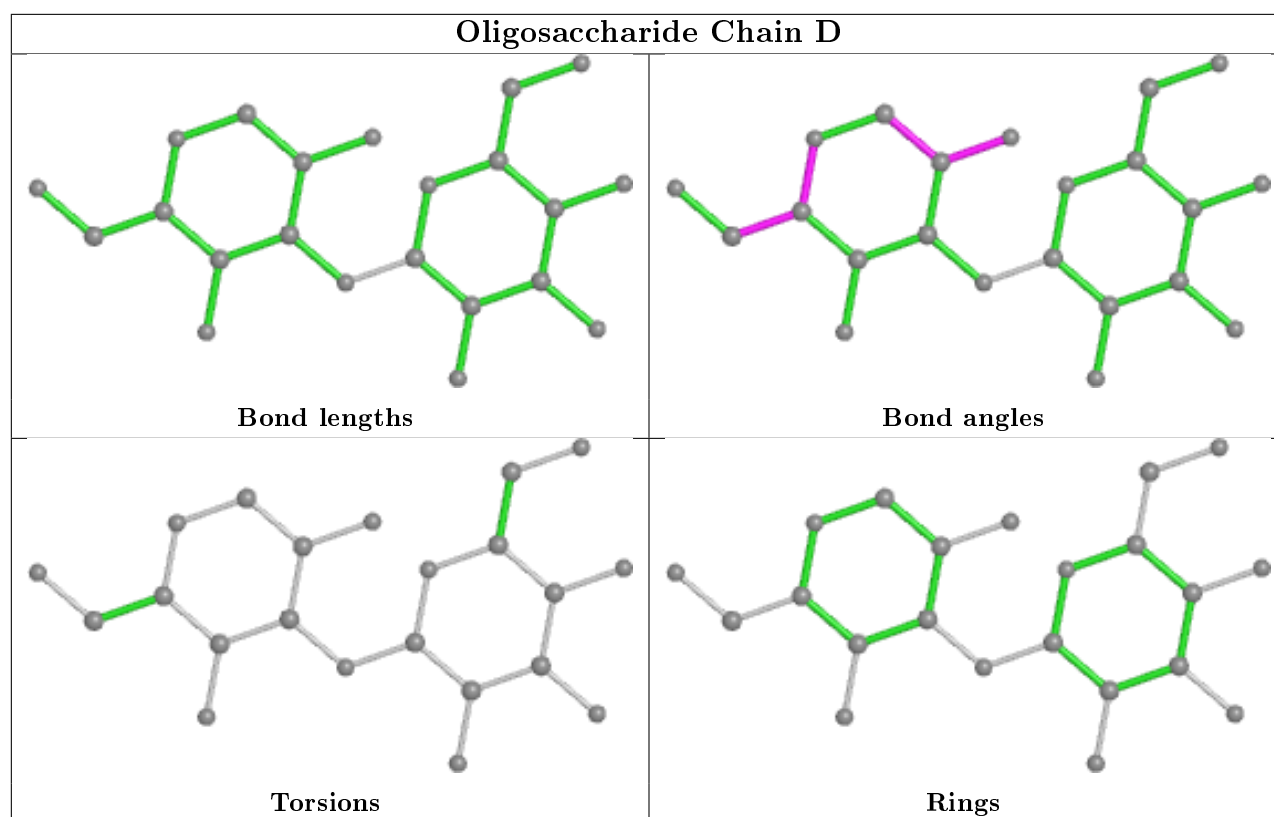
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	BGC	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](#)

6 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	UDP	B	503	-	20,26,26	3.60	8 (40%)	25,40,40	1.00	1 (4%)
3	BGC	B	501	1	11,11,12	1.26	0	15,15,17	1.34	1 (6%)
5	7WV	B	504	-	8,10,10	4.49	3 (37%)	9,13,13	1.70	3 (33%)
3	BGC	A	501	1	11,11,12	1.11	1 (9%)	15,15,17	2.19	4 (26%)
4	UDP	A	503	-	20,26,26	3.72	8 (40%)	25,40,40	1.26	3 (12%)
5	7WV	A	504	-	8,10,10	4.08	2 (25%)	9,13,13	1.14	1 (11%)

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	503	-	-	3/14/32/32	0/2/2/2
3	BGC	B	501	1	-	1/2/19/22	0/1/1/1
5	7WV	B	504	-	-	0/0/4/4	0/1/1/1
3	BGC	A	501	1	-	2/2/19/22	0/1/1/1
4	UDP	A	503	-	-	2/14/32/32	0/2/2/2
5	7WV	A	504	-	-	0/0/4/4	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	504	7WV	C05-C07	10.30	1.57	1.47
5	A	504	7WV	BR1-C04	8.27	2.08	1.89
4	A	503	UDP	C6-N1	8.17	1.45	1.35
5	A	504	7WV	C05-C07	7.88	1.55	1.47
4	B	503	UDP	C6-N1	7.29	1.44	1.35
5	B	504	7WV	BR1-C04	6.88	2.05	1.89
4	B	503	UDP	C4-N3	6.87	1.45	1.33
4	B	503	UDP	O4'-C4'	6.13	1.58	1.45
4	A	503	UDP	C4-N3	6.01	1.43	1.33
4	A	503	UDP	O4'-C1'	-5.96	1.32	1.41
4	A	503	UDP	O4'-C4'	5.95	1.58	1.45
4	A	503	UDP	C3'-C4'	-5.83	1.38	1.53
4	B	503	UDP	C3'-C4'	-5.69	1.38	1.53
4	A	503	UDP	C6-C5	5.64	1.50	1.38
4	B	503	UDP	O4'-C1'	-5.31	1.33	1.41
4	B	503	UDP	C6-C5	4.79	1.48	1.38
4	B	503	UDP	C2-N3	4.13	1.46	1.38
4	A	503	UDP	C2-N3	3.97	1.46	1.38
4	B	503	UDP	O3'-C3'	2.77	1.49	1.43
4	A	503	UDP	O3'-C3'	2.51	1.48	1.43
5	B	504	7WV	C05-C04	2.36	1.42	1.39
3	A	501	BGC	C6-C5	2.14	1.59	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	BGC	C1-O5-C5	5.24	119.30	112.19
3	A	501	BGC	C1-C2-C3	4.56	115.28	109.67
3	B	501	BGC	C1-C2-C3	4.12	114.73	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	504	7WV	C06-C05-C07	-3.44	115.08	120.20
4	A	503	UDP	C2'-C3'-C4'	3.30	109.06	102.64
4	B	503	UDP	C2'-C3'-C4'	3.22	108.90	102.64
5	B	504	7WV	BR1-C04-C05	2.76	123.87	120.55
5	A	504	7WV	C06-C05-C07	-2.54	116.42	120.20
4	A	503	UDP	C5-C4-N3	-2.51	117.79	123.31
4	A	503	UDP	O3A-PB-O1B	-2.37	98.04	111.19
3	A	501	BGC	O2-C2-C3	-2.19	105.76	110.14
5	B	504	7WV	BR1-C04-C03	-2.11	113.70	117.81
3	A	501	BGC	C6-C5-C4	-2.03	108.25	113.00

There are no chirality outliers.

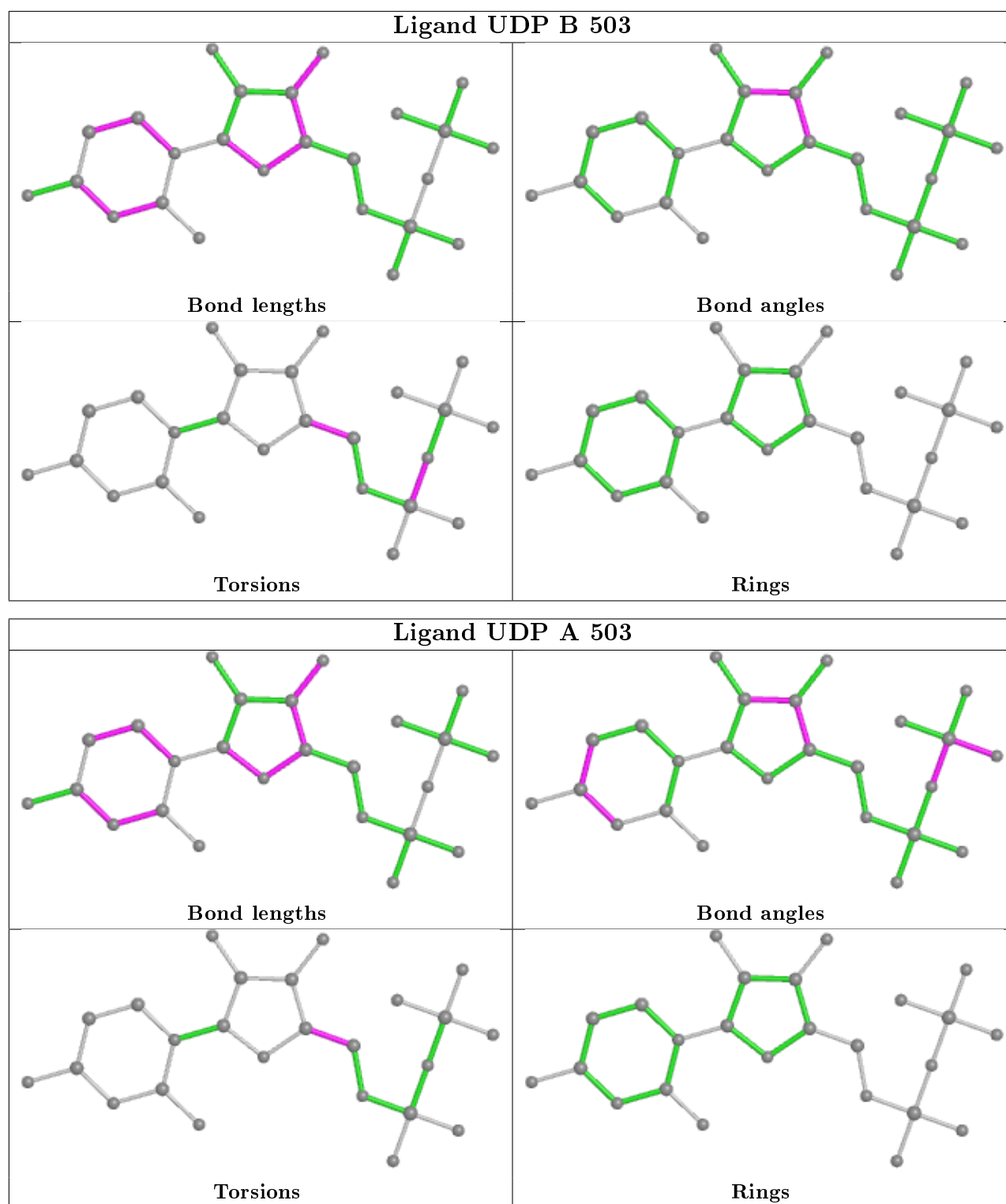
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	UDP	PB-O3A-PA-O5'
3	A	501	BGC	C4-C5-C6-O6
4	A	503	UDP	O4'-C4'-C5'-O5'
3	B	501	BGC	C4-C5-C6-O6
4	A	503	UDP	C3'-C4'-C5'-O5'
4	B	503	UDP	O4'-C4'-C5'-O5'
4	B	503	UDP	C3'-C4'-C5'-O5'
3	A	501	BGC	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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, 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	444/449 (98%)	-0.05	16 (3%) 42 37	21, 41, 86, 114	0
1	B	444/449 (98%)	0.10	27 (6%) 21 16	27, 46, 91, 124	0
All	All	888/898 (98%)	0.02	43 (4%) 30 25	21, 44, 88, 124	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	249	LYS	5.5
1	B	5	ARG	5.3
1	B	250	ASP	5.1
1	A	253	PHE	4.0
1	B	309	GLY	3.9
1	B	52	LEU	3.8
1	B	53	SER	3.7
1	B	253	PHE	3.5
1	B	317	GLU	3.4
1	B	308	SER	3.2
1	B	102	ASP	3.2
1	B	388	LYS	3.1
1	B	409	GLU	3.1
1	B	51	ASP	3.0
1	B	49	ASN	3.0
1	B	389	GLU	3.0
1	A	314	VAL	2.9
1	B	312	GLU	2.9
1	B	4	LYS	2.9
1	A	308	SER	2.8
1	B	315	ASN	2.8
1	A	309	GLY	2.8
1	A	316	LYS	2.7
1	A	310	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	5	ARG	2.5
1	B	318	LYS	2.5
1	B	310	PHE	2.5
1	B	311	LEU	2.5
1	A	312	GLU	2.5
1	B	157	GLU	2.5
1	B	191	PHE	2.4
1	A	315	ASN	2.3
1	A	392	ILE	2.3
1	A	387	GLU	2.2
1	B	313	THR	2.2
1	A	250	ASP	2.2
1	A	249	LYS	2.2
1	A	311	LEU	2.1
1	B	307	PRO	2.1
1	A	251	ASP	2.1
1	A	413	GLU	2.1
1	B	280	VAL	2.1
1	B	306	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

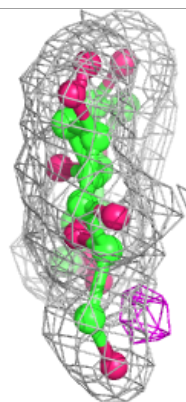
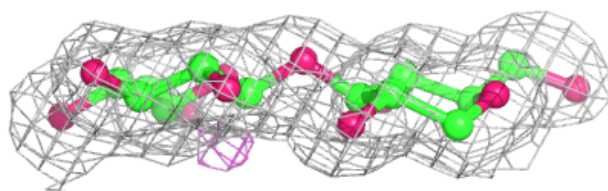
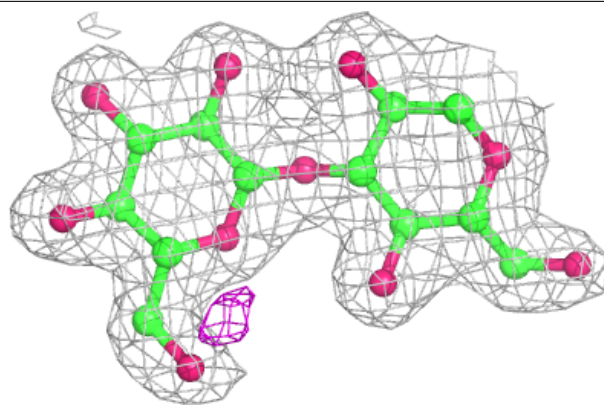
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BGC	D	2	11/12	0.92	0.08	39,45,49,51	0
2	BGC	C	1	11/12	0.95	0.10	24,29,35,46	0
2	BGC	D	1	11/12	0.97	0.06	31,36,45,47	0
2	BGC	C	2	11/12	0.97	0.08	24,30,37,38	0

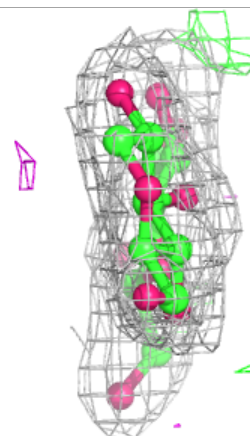
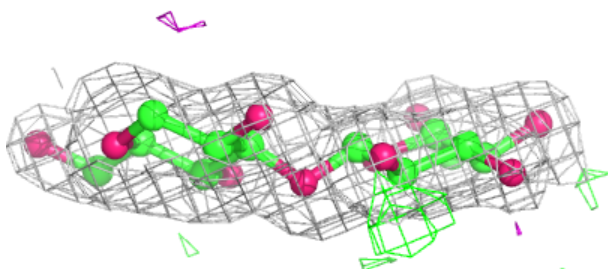
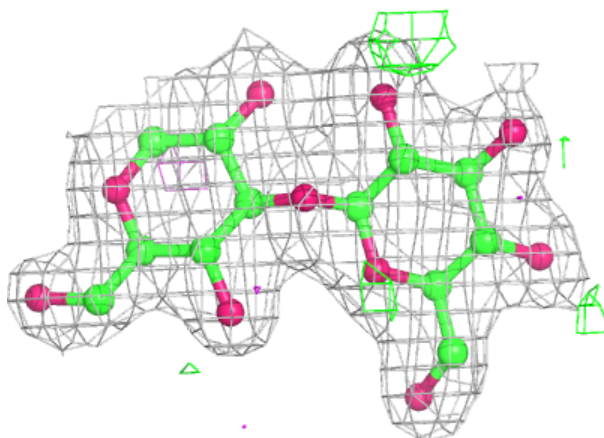
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

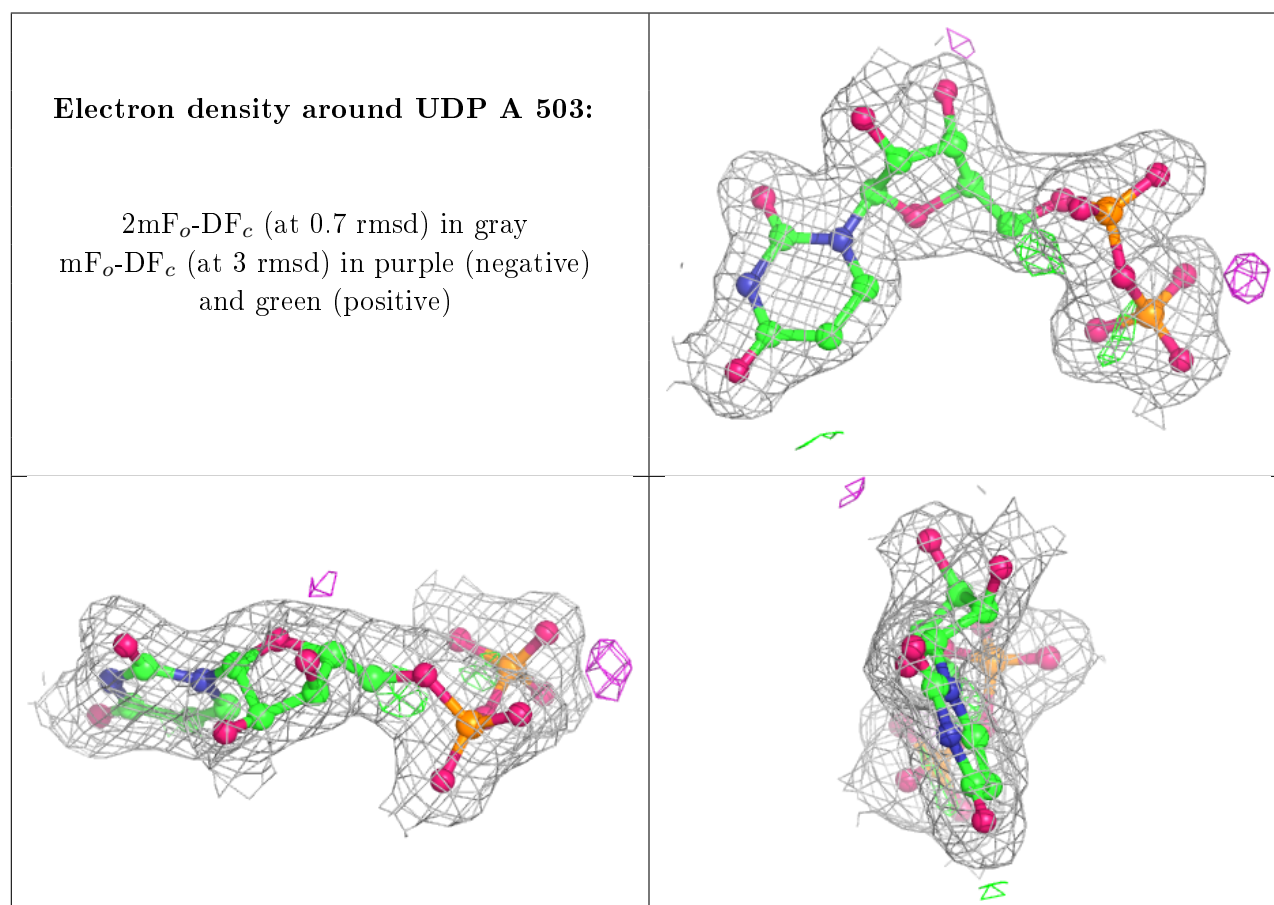


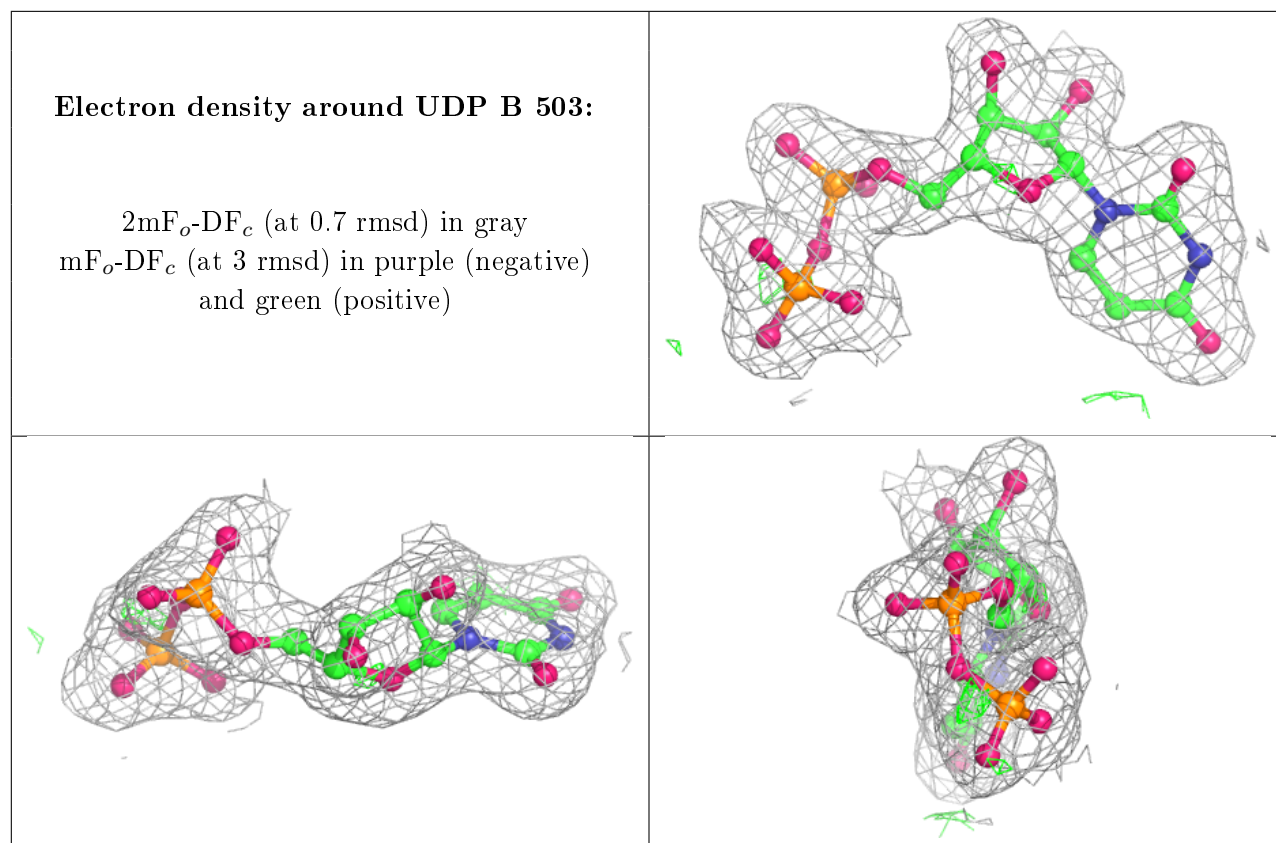
6.4 Ligands ⓘ

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	BGC	B	501	11/12	0.94	0.07	39,51,55,57	0
3	BGC	A	501	11/12	0.95	0.10	36,40,50,60	0
5	7WV	A	504	10/10	0.95	0.16	52,65,77,83	0
4	UDP	A	503	25/25	0.97	0.13	25,31,36,37	0
5	7WV	B	504	10/10	0.98	0.08	35,45,70,78	0
4	UDP	B	503	25/25	0.98	0.11	27,32,37,40	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.