



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2024 – 12:37 PM EDT

PDB ID : 5U6S
Title : Crystal structure of UDP-glucosyltransferase, UGT74F2, with UDP and 2-bromobenzoic acid
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Deposited on : 2016-12-08
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

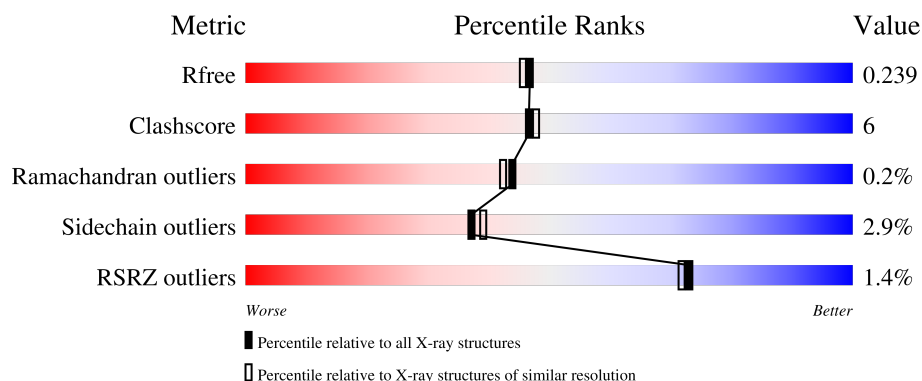
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	449	<div> <div> <div></div> <div>86%</div> <div>12%</div> <div>..</div> </div> <div> <div></div> <div>2%</div> <div></div> <div></div> </div> </div>
1	B	449	<div> <div> <div></div> <div>85%</div> <div>12%</div> <div>..</div> </div> <div> <div></div> <div>2%</div> <div></div> <div></div> </div> </div>
2	C	2	<div> <div>100%</div> </div>
2	D	2	<div> <div>100%</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7361 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.

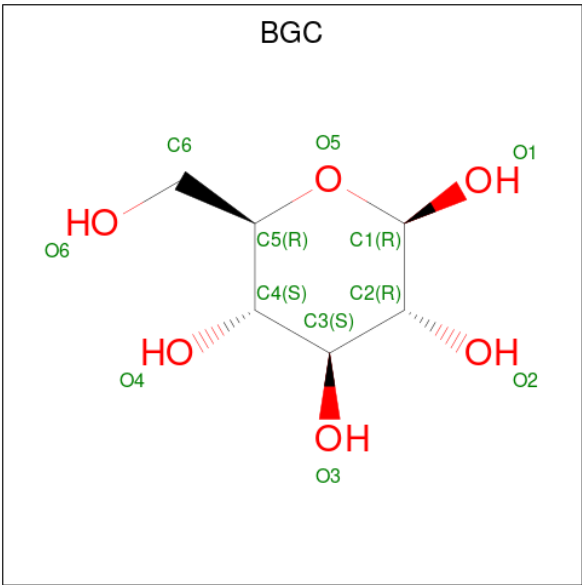
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3537	2277	572	672	16			
1	B	444	Total	C	N	O	S	0	0	0
			3537	2277	572	672	16			

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



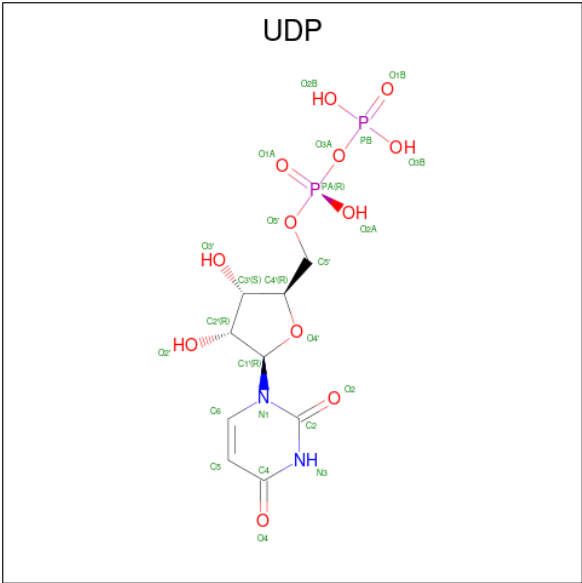
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			22	12	10			
2	D	2	Total	C	O	0	0	0
			22	12	10			

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



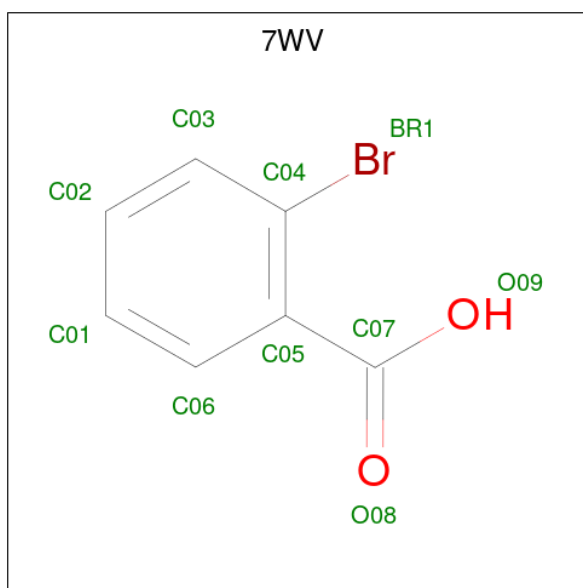
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

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



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

- 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		

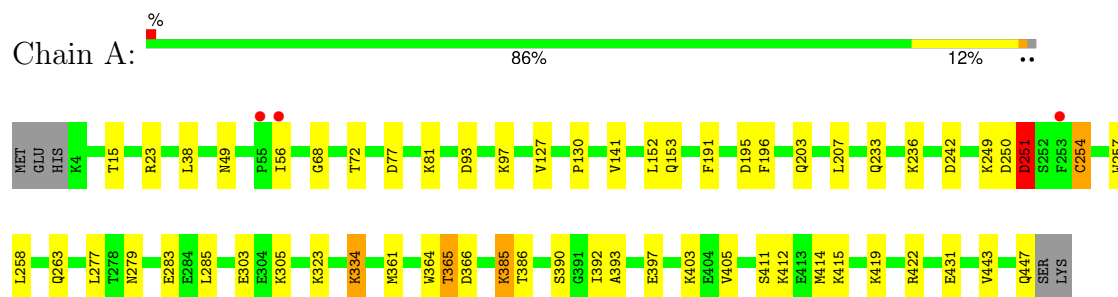
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	93	Total	O	0	0
			93	93		
6	B	58	Total	O	0	0
			58	58		

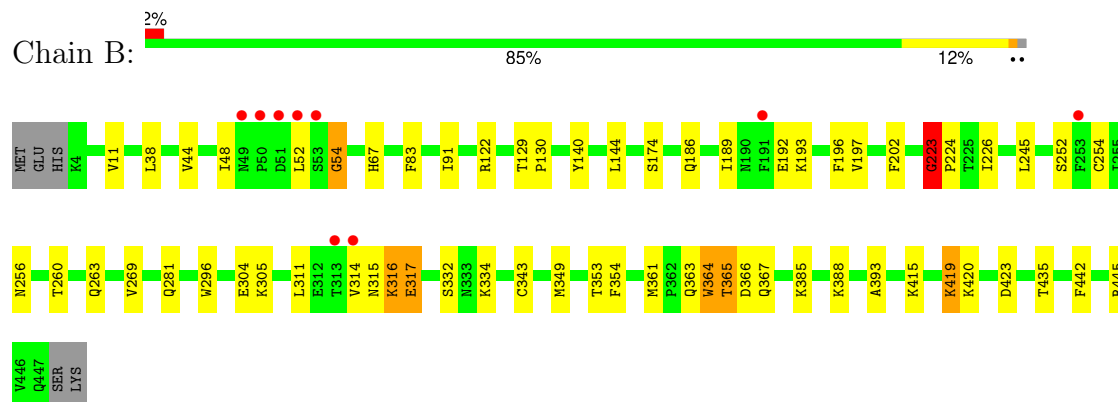
3 Residue-property plots

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

• Molecule 1: 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	65.15Å 87.25Å 162.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.54 – 2.00 37.54 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (37.54-2.00) 98.3 (37.54-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.00Å)	Xtriage
Refinement program	PHENIX (dev_2481: ???)	Depositor
R, R_{free}	0.184 , 0.238 0.185 , 0.239	Depositor DCC
R_{free} test set	3228 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7361	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.46	0/3626	0.59	0/4923
1	B	0.45	1/3626 (0.0%)	0.60	2/4923 (0.0%)
All	All	0.45	1/7252 (0.0%)	0.59	2/9846 (0.0%)

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	2
1	B	0	4
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	343	CYS	CB-SG	-5.44	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	GLY	C-N-CD	-6.69	105.89	120.60
1	B	38	LEU	CB-CG-CD2	-5.09	102.35	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	251	ASP	Peptide
1	A	364	TRP	Peptide
1	B	223	GLY	Peptide
1	B	316	LYS	Peptide
1	B	364	TRP	Peptide
1	B	54	GLY	Peptide

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	3537	0	3472	40	0
1	B	3537	0	3472	38	0
2	C	22	0	19	1	0
2	D	22	0	19	0	0
3	A	11	0	9	1	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	93	0	0	3	0
6	B	58	0	0	0	0
All	All	7361	0	7023	79	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 6.

All (79) 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:A:390:SER:HB2	1:A:392:ILE:HD12	1.57	0.87
1:B:281:GLN:HE22	1:B:393:ALA:H	1.23	0.82
1:A:23:ARG:HE	1:A:56:ILE:HG21	1.51	0.75
1:A:385:LYS:H	1:A:385:LYS:HD2	1.56	0.70
1:A:23:ARG:NH1	1:A:242:ASP:OD1	2.25	0.69
1:A:263:GLN:HB2	1:A:334:LYS:HE2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:LYS:O	1:B:419:LYS:HE2	1.95	0.66
1:B:363:GLN:H	1:B:367:GLN:HE21	1.45	0.64
1:A:279:ASN:O	1:A:283:GLU:HG2	1.98	0.64
1:A:93:ASP:OD1	1:A:97:LYS:NZ	2.31	0.63
1:B:314:VAL:HG13	1:B:316:LYS:HD3	1.80	0.63
1:B:365:THR:HG23	1:B:366:ASP:H	1.64	0.62
1:B:364:TRP:H	1:B:367:GLN:NE2	1.99	0.61
1:A:303:GLU:OE2	1:A:323:LYS:NZ	2.34	0.60
1:A:365:THR:HG23	1:A:366:ASP:H	1.67	0.59
1:A:23:ARG:NE	1:A:56:ILE:HG21	2.18	0.59
1:B:186:GLN:HG2	1:B:189:ILE:HD13	1.85	0.59
1:B:202:PHE:CD1	1:B:224:PRO:HD3	2.38	0.58
1:B:269:VAL:HG13	1:B:296:TRP:HA	1.85	0.58
1:A:233:GLN:O	1:A:236:LYS:NZ	2.28	0.57
1:A:431:GLU:OE1	1:A:431:GLU:N	2.33	0.55
1:B:304:GLU:OE1	1:B:305:LYS:HG2	2.06	0.55
1:A:15:THR:HG22	2:C:2:BGC:H3	1.87	0.55
1:A:38:LEU:HB2	1:A:56:ILE:HD11	1.89	0.54
1:A:81:LYS:N	1:A:81:LYS:HD3	2.24	0.52
1:A:386:THR:HG22	1:A:393:ALA:HB2	1.90	0.52
1:B:11:VAL:HG11	1:B:91:ILE:HD11	1.92	0.52
1:B:415:LYS:CE	1:B:419:LYS:HZ2	2.21	0.52
1:A:251:ASP:HB3	1:A:254:CYS:HB3	1.92	0.51
1:A:385:LYS:HB2	1:A:397:GLU:HG2	1.93	0.50
1:B:67:HIS:CD2	1:B:67:HIS:C	2.84	0.50
1:B:224:PRO:HB2	1:B:226:ILE:HG12	1.92	0.50
1:B:363:GLN:H	1:B:367:GLN:NE2	2.10	0.50
1:A:411:SER:O	1:A:415:LYS:HG3	2.13	0.49
1:A:443:VAL:O	1:A:447:GLN:HG2	2.13	0.48
3:A:501:BGC:H6C2	6:A:633:HOH:O	2.14	0.48
1:A:412:LYS:N	1:A:412:LYS:HD2	2.29	0.47
1:B:332:SER:HB3	1:B:354:PHE:CE1	2.49	0.47
1:A:77:ASP:HB2	6:A:669:HOH:O	2.15	0.46
1:B:223:GLY:O	1:B:435:THR:HG21	2.15	0.46
1:A:263:GLN:CB	1:A:334:LYS:HE2	2.45	0.45
1:B:122:ARG:NH2	1:B:193:LYS:HB3	2.32	0.45
1:B:130:PRO:HD2	1:B:196:PHE:O	2.17	0.45
1:A:68:GLY:HA3	1:A:72:THR:HG21	1.98	0.45
1:B:316:LYS:HA	1:B:316:LYS:HD2	1.56	0.45
1:B:52:LEU:HD13	1:B:54:GLY:N	2.32	0.45
1:B:263:GLN:HB2	1:B:334:LYS:HZ3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:MET:HE3	1:A:361:MET:HB2	1.61	0.44
1:A:385:LYS:HD3	1:A:397:GLU:OE2	2.18	0.44
1:B:140:TYR:CE2	1:B:144:LEU:HD11	2.52	0.44
1:B:311:LEU:O	1:B:314:VAL:HG12	2.17	0.44
1:A:249:LYS:HE2	1:A:249:LYS:HB3	1.44	0.44
1:A:385:LYS:HD2	1:A:385:LYS:N	2.28	0.43
1:B:44:VAL:O	1:B:48:ILE:HG12	2.18	0.43
1:A:152:LEU:HD12	1:A:152:LEU:HA	1.80	0.43
1:B:314:VAL:HG11	1:B:316:LYS:HZ3	1.82	0.43
1:B:361:MET:HE3	1:B:361:MET:HB2	1.91	0.43
1:B:315:ASN:O	1:B:317:GLU:N	2.50	0.43
1:B:129:THR:HG21	1:B:442:PHE:HE1	1.83	0.43
1:A:49:ASN:ND2	6:A:604:HOH:O	2.51	0.43
1:A:23:ARG:HD2	1:A:56:ILE:HD13	2.00	0.42
1:A:257:TRP:CE3	1:A:258:LEU:HD23	2.55	0.42
1:A:130:PRO:HD2	1:A:196:PHE:O	2.19	0.42
1:A:141:VAL:HG13	1:A:152:LEU:HD21	2.02	0.42
1:B:349:MET:O	1:B:353:THR:HG23	2.20	0.42
1:A:207:LEU:HD23	1:A:207:LEU:HA	1.91	0.42
1:B:314:VAL:CG1	1:B:316:LYS:HD3	2.49	0.42
1:B:314:VAL:HG22	1:B:316:LYS:HD3	2.02	0.41
1:A:277:LEU:O	1:A:305:LYS:HD2	2.20	0.41
1:A:415:LYS:O	1:A:419:LYS:HG2	2.21	0.41
1:B:130:PRO:HG2	1:B:197:VAL:HG22	2.03	0.41
1:B:365:THR:HG23	1:B:366:ASP:N	2.34	0.41
1:B:48:ILE:HD13	1:B:245:LEU:HD23	2.03	0.40
1:B:256:ASN:O	1:B:260:THR:HG23	2.21	0.40
1:A:249:LYS:HB3	1:A:251:ASP:OD2	2.21	0.40
1:B:419:LYS:HD3	1:B:419:LYS:HA	1.89	0.40
1:A:405:VAL:HG22	1:A:414:MET:CE	2.52	0.40
1:A:127:VAL:HG13	1:A:195:ASP:CG	2.42	0.40
1:B:52:LEU:HD13	1:B:52:LEU:C	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/449 (98%)	428 (97%)	13 (3%)	1 (0%)	44	42
1	B	442/449 (98%)	423 (96%)	18 (4%)	1 (0%)	44	42
All	All	884/898 (98%)	851 (96%)	31 (4%)	2 (0%)	44	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	THR
1	B	365	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	396/401 (99%)	385 (97%)	11 (3%)	38	40
1	B	396/401 (99%)	384 (97%)	12 (3%)	36	37
All	All	792/802 (99%)	769 (97%)	23 (3%)	37	39

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	191	PHE
1	A	203	GLN
1	A	250	ASP
1	A	251	ASP
1	A	254	CYS
1	A	285	LEU
1	A	334	LYS
1	A	385	LYS
1	A	403	LYS

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Mol	Chain	Res	Type
1	A	422	ARG
1	B	83	PHE
1	B	174	SER
1	B	192	GLU
1	B	252	SER
1	B	254	CYS
1	B	317	GLU
1	B	385	LYS
1	B	388	LYS
1	B	419	LYS
1	B	420	LYS
1	B	423	ASP
1	B	445	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	67	HIS
1	B	256	ASN
1	B	279	ASN
1	B	281	GLN
1	B	367	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	BGC	C	1	2,1	11,11,12	0.96	0	15,15,17	1.06	1 (6%)
2	BGC	C	2	2	11,11,12	0.48	0	15,15,17	0.86	0
2	BGC	D	1	2,1	11,11,12	0.90	0	15,15,17	1.09	1 (6%)
2	BGC	D	2	2	11,11,12	0.61	0	15,15,17	1.28	3 (20%)

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	2,1	-	0/2/19/22	0/1/1/1
2	BGC	C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	D	1	2,1	-	2/2/19/22	0/1/1/1
2	BGC	D	2	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	BGC	C2-C3-C4	2.95	116.06	110.86
2	C	1	BGC	C3-C4-C5	2.70	115.14	110.23
2	D	2	BGC	C3-C4-C5	2.58	114.90	110.23
2	D	1	BGC	O5-C5-C6	2.30	112.13	107.66
2	D	2	BGC	C1-O5-C5	-2.02	109.48	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

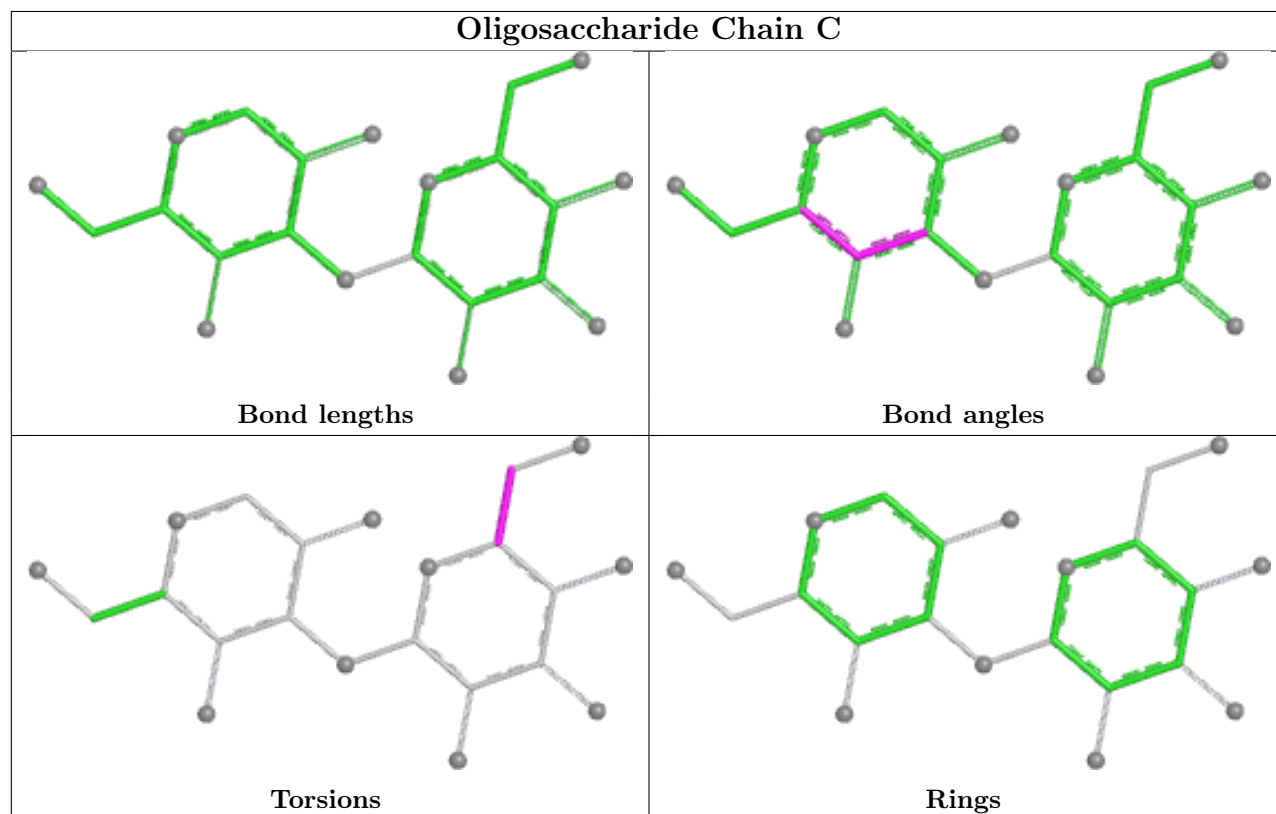
Mol	Chain	Res	Type	Atoms
2	D	2	BGC	C4-C5-C6-O6
2	D	2	BGC	O5-C5-C6-O6
2	D	1	BGC	O5-C5-C6-O6
2	C	2	BGC	C4-C5-C6-O6
2	C	2	BGC	O5-C5-C6-O6
2	D	1	BGC	C4-C5-C6-O6

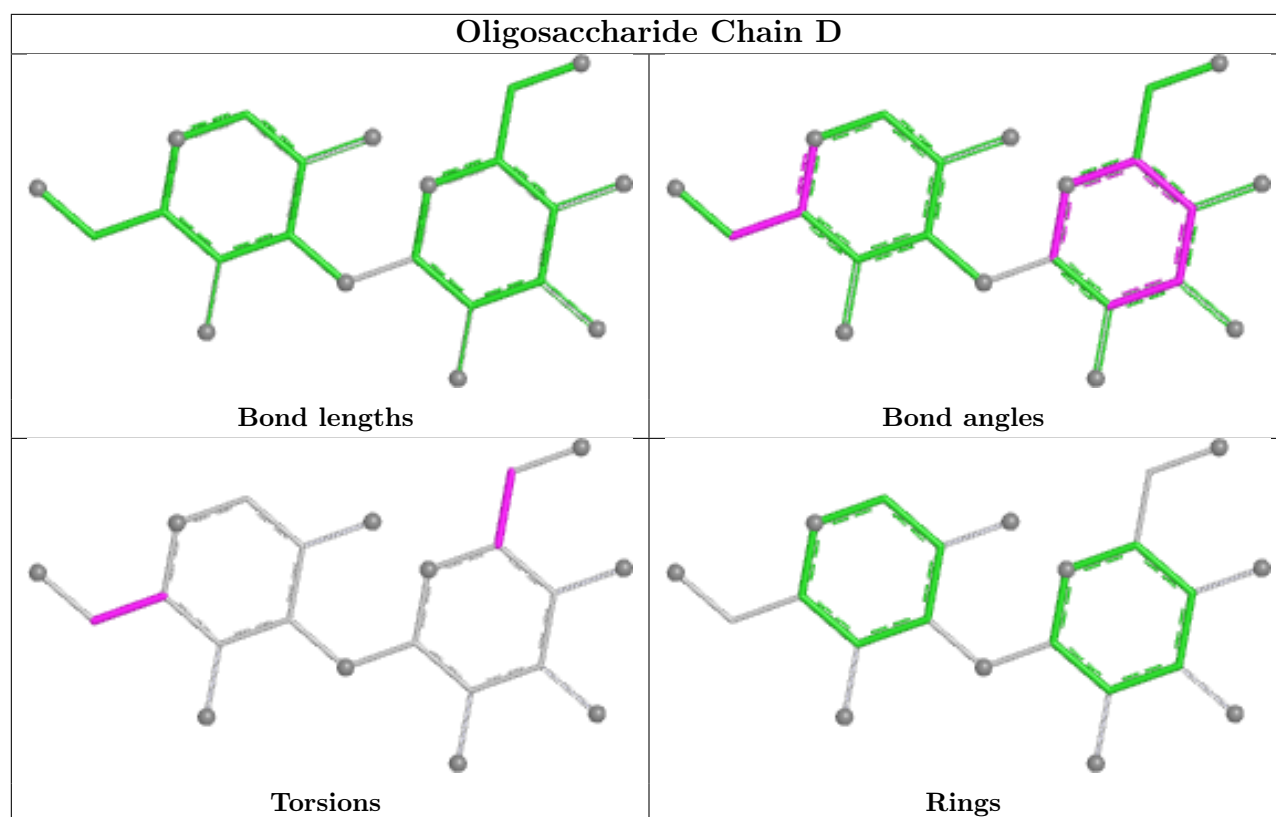
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	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	A	503	-	25,26,26	3.03	13 (52%)	38,40,40	1.54	9 (23%)
5	7WV	B	504	-	10,10,10	2.13	2 (20%)	13,13,13	1.50	2 (15%)
3	BGC	B	501	1	11,11,12	1.20	1 (9%)	15,15,17	1.19	1 (6%)
4	UDP	B	503	-	25,26,26	3.00	13 (52%)	38,40,40	1.46	7 (18%)
3	BGC	A	501	1	11,11,12	1.19	0	15,15,17	1.75	3 (20%)
5	7WV	A	504	-	10,10,10	1.78	2 (20%)	13,13,13	1.31	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	UDP	A	503	-	-	3/16/32/32	0/2/2/2
5	7WV	B	504	-	-	0/4/4/4	0/1/1/1
3	BGC	B	501	1	-	0/2/19/22	0/1/1/1
4	UDP	B	503	-	-	3/16/32/32	0/2/2/2
3	BGC	A	501	1	-	1/2/19/22	0/1/1/1
5	7WV	A	504	-	-	2/4/4/4	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	UDP	C6-C5	6.01	1.49	1.35
4	B	503	UDP	C6-C5	5.79	1.48	1.35
4	A	503	UDP	C3'-C4'	-5.72	1.38	1.53
4	B	503	UDP	C3'-C4'	-5.58	1.38	1.53
4	B	503	UDP	O4'-C4'	5.43	1.57	1.45
4	A	503	UDP	O4'-C4'	5.39	1.57	1.45
5	B	504	7WV	BR1-C04	5.08	2.01	1.89
4	B	503	UDP	C2-N1	4.86	1.46	1.38
4	A	503	UDP	C2-N3	4.55	1.45	1.38
4	A	503	UDP	C2-N1	4.30	1.45	1.38
4	B	503	UDP	C2-N3	4.22	1.45	1.38
4	B	503	UDP	C4-N3	4.12	1.45	1.38
5	A	504	7WV	BR1-C04	3.95	1.98	1.89
4	A	503	UDP	O4'-C1'	-3.93	1.32	1.42
4	A	503	UDP	C4-N3	3.87	1.45	1.38
4	B	503	UDP	PA-O3A	3.78	1.63	1.59
5	B	504	7WV	C05-C07	3.65	1.57	1.49
4	A	503	UDP	PA-O3A	3.59	1.63	1.59
4	B	503	UDP	O4'-C1'	-3.54	1.33	1.42
5	A	504	7WV	C05-C07	3.32	1.56	1.49
4	A	503	UDP	O2-C2	-3.23	1.17	1.23
4	B	503	UDP	O2-C2	-3.18	1.17	1.23
4	A	503	UDP	C6-N1	2.94	1.45	1.38
4	B	503	UDP	C6-N1	2.93	1.45	1.38
4	A	503	UDP	O3'-C3'	2.92	1.50	1.43
4	B	503	UDP	O3'-C3'	2.66	1.49	1.43
4	A	503	UDP	O4-C4	-2.42	1.19	1.24
4	B	503	UDP	O4-C4	-2.39	1.19	1.24
4	B	503	UDP	C5-C4	2.23	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	UDP	C5-C4	2.20	1.48	1.43
3	B	501	BGC	C6-C5	2.15	1.59	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	BGC	C1-O5-C5	4.53	118.25	112.19
3	B	501	BGC	C1-C2-C3	3.56	114.82	109.64
5	A	504	7WV	O08-C07-C05	-3.44	113.77	121.97
4	A	503	UDP	C4-N3-C2	-3.37	122.44	126.61
4	B	503	UDP	C2'-C3'-C4'	3.27	108.93	102.61
4	B	503	UDP	C5-C4-N3	3.10	119.14	114.80
4	B	503	UDP	C4-N3-C2	-3.00	122.89	126.61
5	B	504	7WV	C04-C05-C07	2.98	127.24	124.34
4	B	503	UDP	O4-C4-C5	-2.83	120.28	125.16
5	B	504	7WV	O08-C07-C05	-2.83	115.22	121.97
4	A	503	UDP	C2'-C3'-C4'	2.83	108.08	102.61
4	B	503	UDP	O3A-PA-O1A	-2.82	102.23	110.70
4	A	503	UDP	C5-C4-N3	2.80	118.71	114.80
4	A	503	UDP	O4-C4-C5	-2.56	120.75	125.16
4	A	503	UDP	O4'-C1'-N1	-2.44	102.84	108.36
3	A	501	BGC	O5-C5-C6	-2.41	102.97	107.66
4	A	503	UDP	N3-C2-N1	2.41	118.03	114.89
3	A	501	BGC	C1-C2-C3	2.40	113.14	109.64
4	A	503	UDP	O2A-PA-O3A	2.39	113.74	107.27
4	B	503	UDP	O4'-C1'-N1	-2.21	103.36	108.36
4	A	503	UDP	O2-C2-N1	-2.17	119.97	122.80
4	A	503	UDP	O3A-PA-O1A	-2.04	104.56	110.70
4	B	503	UDP	O3B-PB-O2B	2.01	115.32	107.80

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	UDP	PB-O3A-PA-O5'
4	B	503	UDP	C3'-C4'-C5'-O5'
4	A	503	UDP	PB-O3A-PA-O5'
4	B	503	UDP	O4'-C4'-C5'-O5'
4	A	503	UDP	C3'-C4'-C5'-O5'
3	A	501	BGC	C4-C5-C6-O6
5	A	504	7WV	C04-C05-C07-O08
5	A	504	7WV	C04-C05-C07-O09

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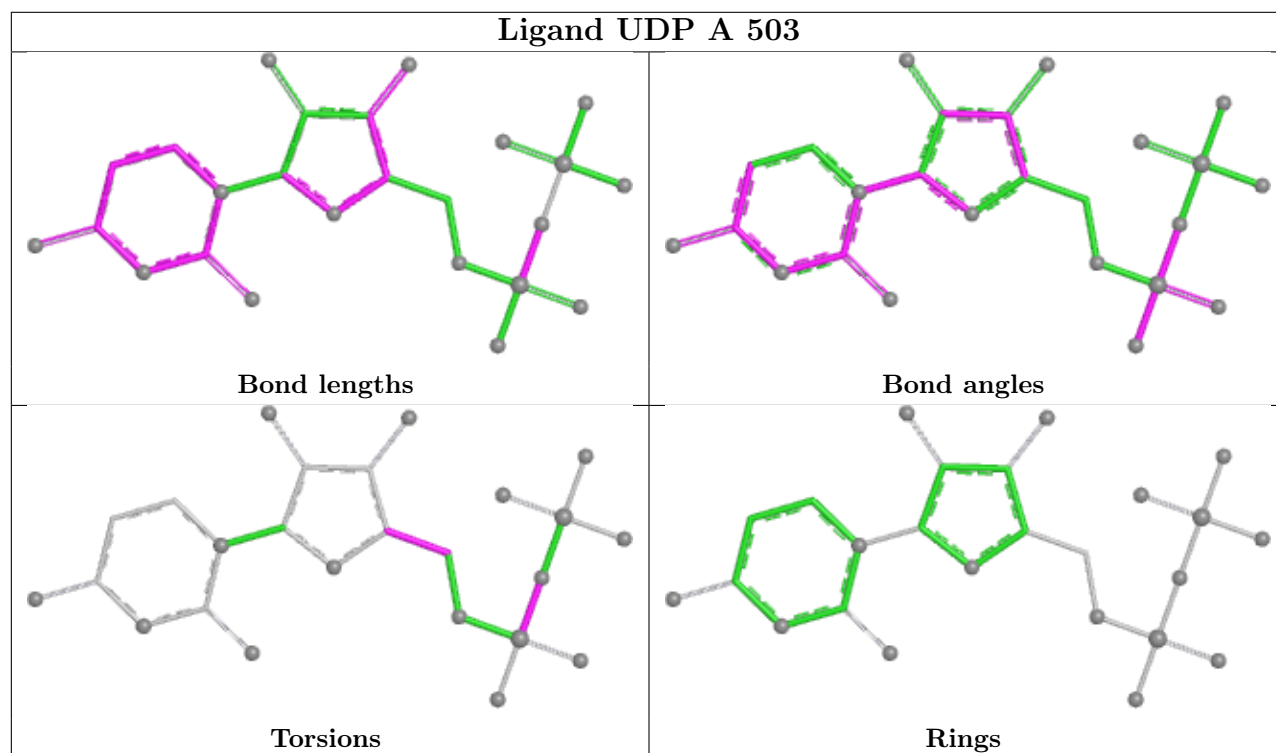
Mol	Chain	Res	Type	Atoms
4	A	503	UDP	O4'-C4'-C5'-O5'

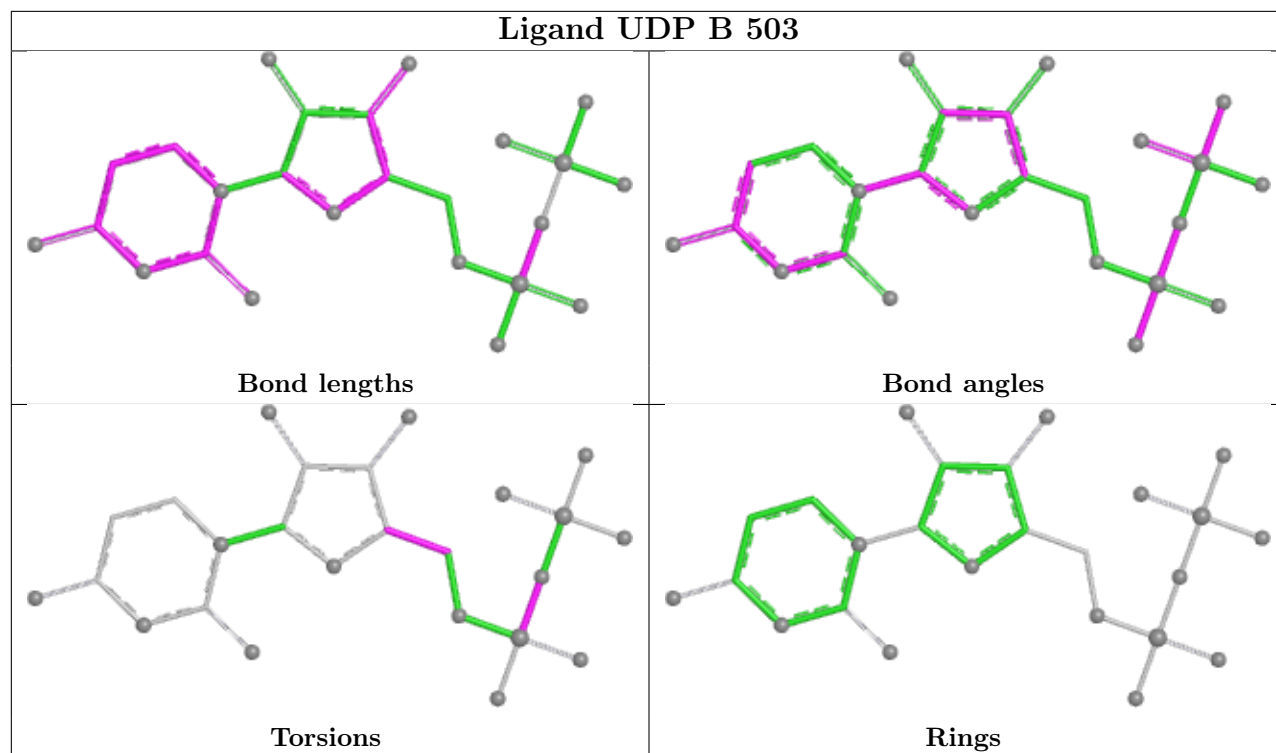
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	444/449 (98%)	-0.11	3 (0%) 84 83	22, 42, 78, 122	0
1	B	444/449 (98%)	0.02	9 (2%) 64 63	27, 45, 90, 130	0
All	All	888/898 (98%)	-0.04	12 (1%) 73 72	22, 44, 84, 130	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	52	LEU	3.7
1	B	191	PHE	2.9
1	B	50	PRO	2.8
1	B	53	SER	2.8
1	B	253	PHE	2.6
1	A	56	ILE	2.5
1	A	253	PHE	2.4
1	B	313	THR	2.4
1	B	49	ASN	2.3
1	A	55	PRO	2.2
1	B	314	VAL	2.1
1	B	51	ASP	2.1

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

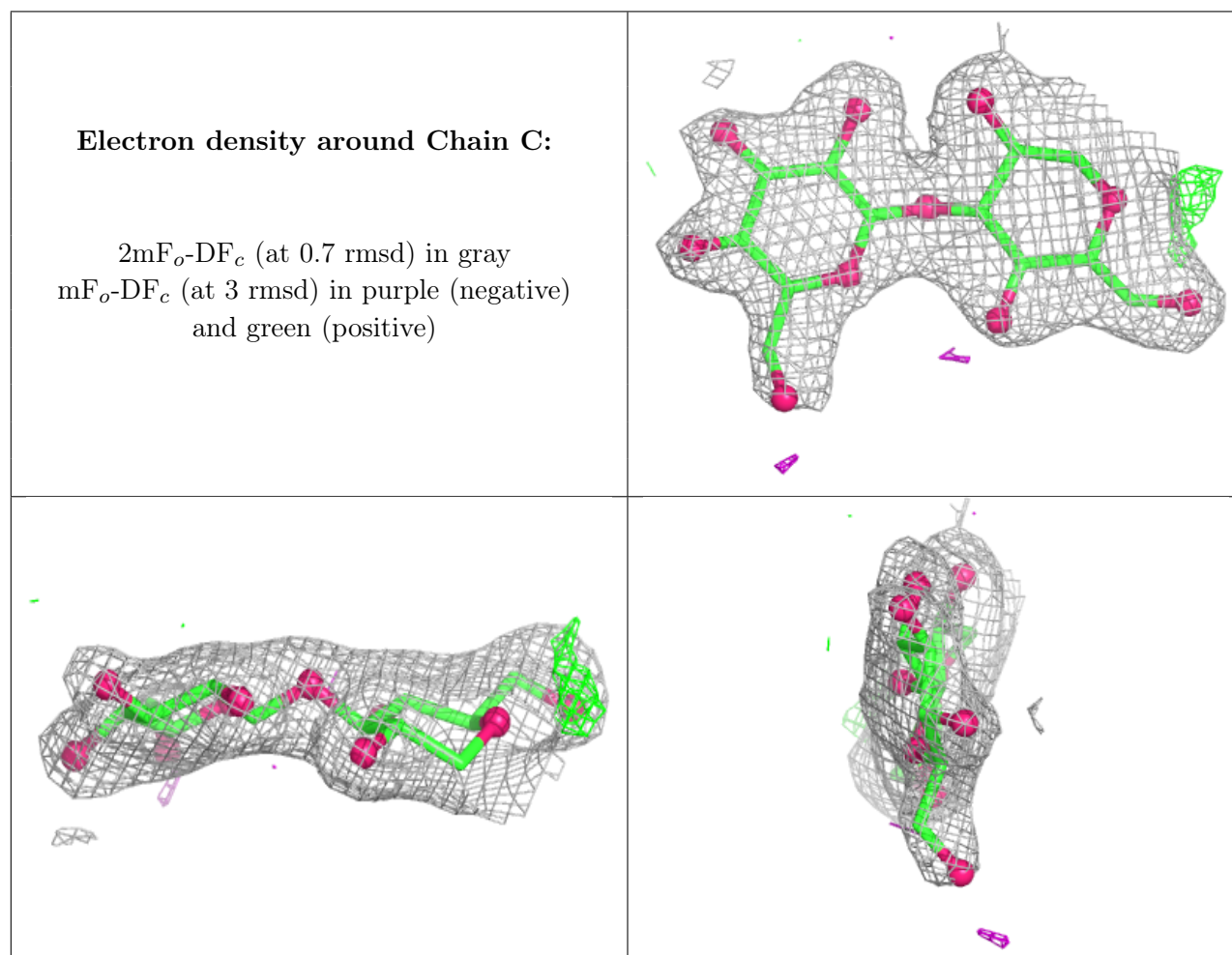
There are no non-standard protein/DNA/RNA residues in this entry.

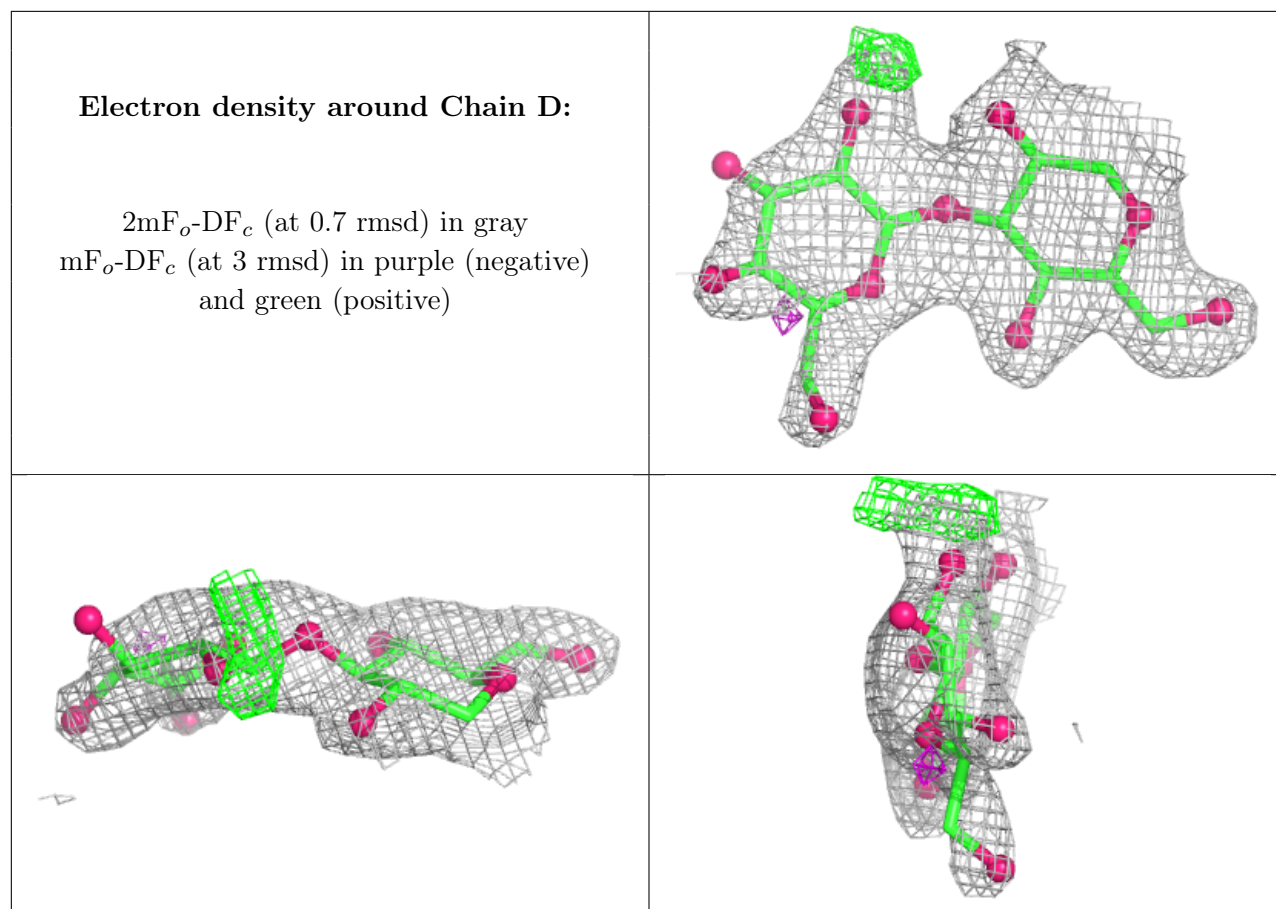
6.3 Carbohydrates [i](#)

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, 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	0.80	0.14	60,72,85,86	0
2	BGC	D	1	11/12	0.92	0.08	38,42,56,59	0
2	BGC	C	1	11/12	0.92	0.08	34,46,58,60	0
2	BGC	C	2	11/12	0.94	0.07	48,60,73,75	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.





6.4 Ligands ⓘ

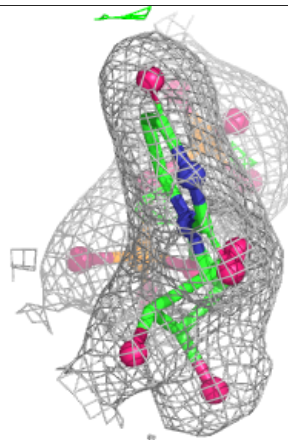
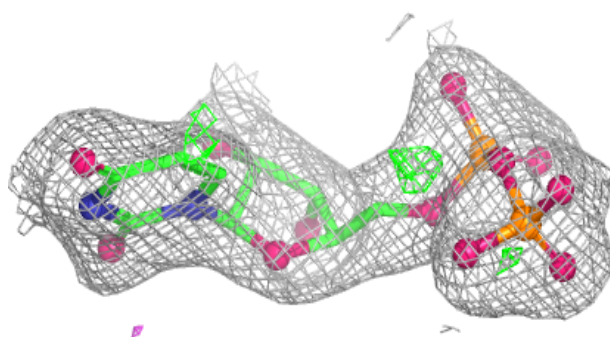
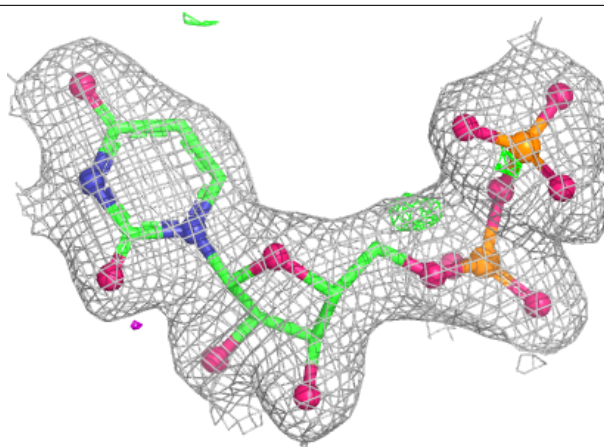
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	7WV	A	504	10/10	0.86	0.18	61,99,108,149	0
5	7WV	B	504	10/10	0.87	0.13	49,74,83,109	0
3	BGC	A	501	11/12	0.92	0.08	37,44,47,70	0
3	BGC	B	501	11/12	0.96	0.06	49,57,62,63	0
4	UDP	A	503	25/25	0.97	0.06	30,37,42,47	0
4	UDP	B	503	25/25	0.98	0.05	28,35,43,45	0

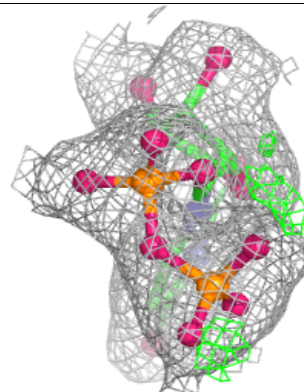
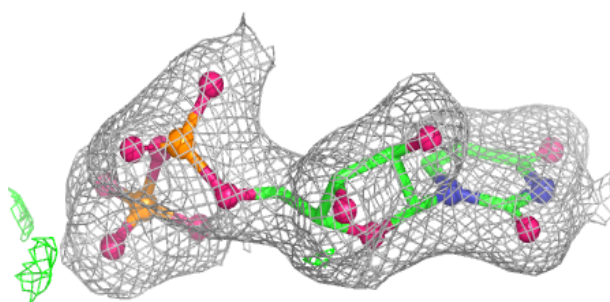
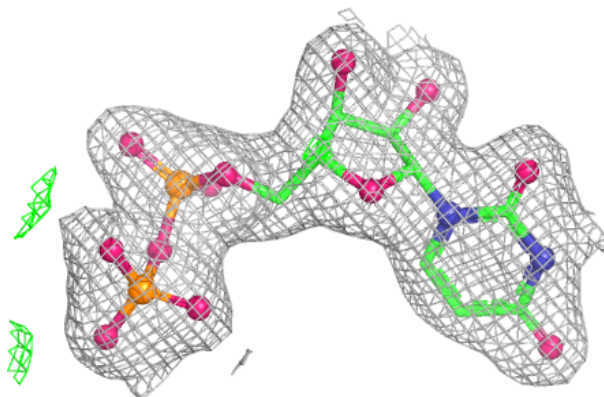
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UDP A 503:

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

**Electron density around UDP B 503:**

$2mF_o-DF_c$ (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.