



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 10:42 AM BST

PDB ID : 6EJJ
Title : Structure of a glycosyltransferase / state 2
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Deposited on : 2017-09-21
Resolution : 2.70 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

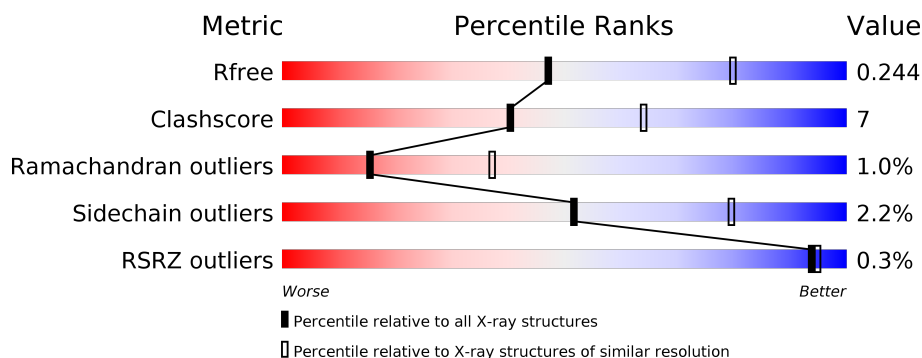
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	373	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>• •</div> </div> </div>
1	B	373	<div> <div></div> <div>77%</div> <div>18%</div> <div>• •</div> </div>
2	C	3	<div> <div></div> <div>67%</div> <div>33%</div> </div>
2	D	3	<div> <div></div> <div>67%</div> <div>33%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6034 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 WlaC protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	0	0
			2914	1886	486	529	13			
1	B	360	Total	C	N	O	S	0	0	0
			2914	1886	486	529	13			

There are 30 discrepancies between the modelled and reference sequences:

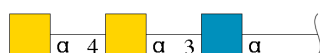
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O86151
A	2	MET	-	expression tag	UNP O86151
A	361	LEU	-	expression tag	UNP O86151
A	362	GLY	-	expression tag	UNP O86151
A	363	SER	-	expression tag	UNP O86151
A	364	HIS	-	expression tag	UNP O86151
A	365	HIS	-	expression tag	UNP O86151
A	366	HIS	-	expression tag	UNP O86151
A	367	HIS	-	expression tag	UNP O86151
A	368	HIS	-	expression tag	UNP O86151
A	369	HIS	-	expression tag	UNP O86151
A	370	HIS	-	expression tag	UNP O86151
A	371	HIS	-	expression tag	UNP O86151
A	372	HIS	-	expression tag	UNP O86151
A	373	HIS	-	expression tag	UNP O86151
B	1	MET	-	initiating methionine	UNP O86151
B	2	MET	-	expression tag	UNP O86151
B	361	LEU	-	expression tag	UNP O86151
B	362	GLY	-	expression tag	UNP O86151
B	363	SER	-	expression tag	UNP O86151
B	364	HIS	-	expression tag	UNP O86151
B	365	HIS	-	expression tag	UNP O86151
B	366	HIS	-	expression tag	UNP O86151
B	367	HIS	-	expression tag	UNP O86151
B	368	HIS	-	expression tag	UNP O86151

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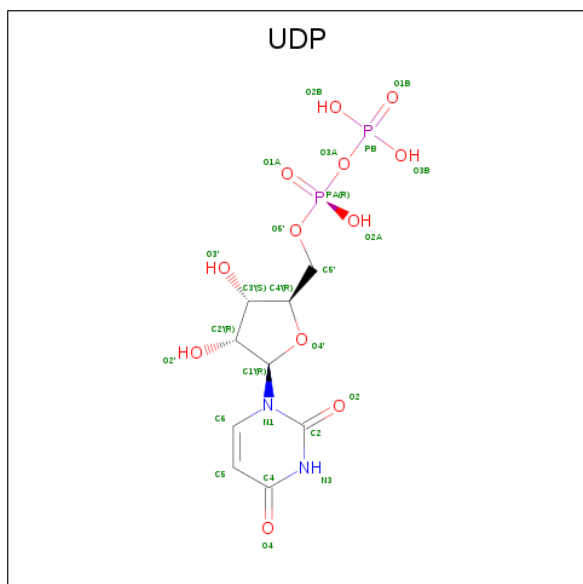
Chain	Residue	Modelled	Actual	Comment	Reference
B	369	HIS	-	expression tag	UNP O86151
B	370	HIS	-	expression tag	UNP O86151
B	371	HIS	-	expression tag	UNP O86151
B	372	HIS	-	expression tag	UNP O86151
B	373	HIS	-	expression tag	UNP O86151

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			42	24	3	15			
2	D	3	Total	C	N	O	0	0	0
			42	24	3	15			

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



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

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

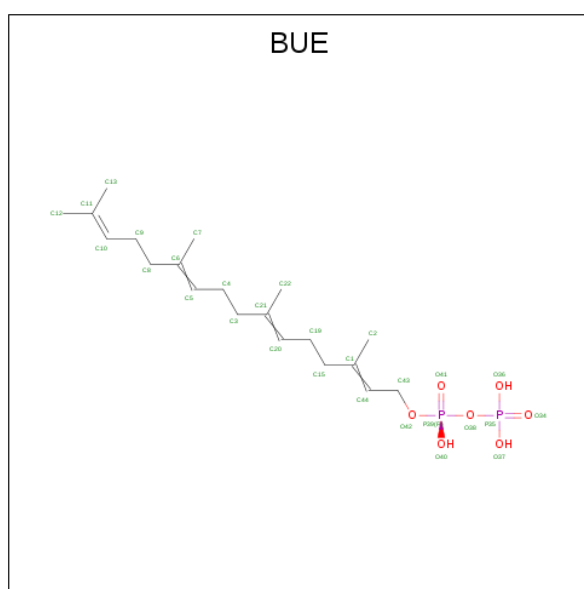
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Na	0	0
			2	2		
4	A	2	Total	Na	0	0
			2	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is NerylNeryl pyrophosphate (three-letter code: BUE) (formula: C₂₀H₃₆O₇P₂).

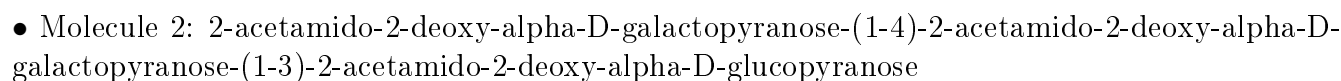


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	P	0	0
			11	2	7	2		
6	B	1	Total	C	O	P	0	0
			11	2	7	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	25	Total 25	O 25	0	0
7	B	20	Total 20	O 20	0	0

- Molecule 1: WlaC protein



Chain D:

67%

33%

HD01
A202
A203

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.51Å 125.78Å 71.01Å 90.00° 90.28° 90.00°	Depositor
Resolution (Å)	29.81 – 2.70 29.81 – 2.36	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.81-2.70) 78.2 (29.81-2.36)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.36Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.206 , 0.244 0.207 , 0.244	Depositor DCC
R_{free} test set	1724 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 16.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.119 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6034	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% 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, CL, NA, NDG, A2G, BUE

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	0.31	0/2968	0.50	0/3992
1	B	0.31	0/2968	0.50	0/3992
All	All	0.31	0/5936	0.50	0/7984

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	2914	0	2992	48	0
1	B	2914	0	2992	42	0
2	C	42	0	34	1	0
2	D	42	0	34	1	0
3	A	25	0	11	1	0
3	B	25	0	11	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	1	0
6	A	11	0	0	1	0
6	B	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	25	0	0	0	0
7	B	20	0	0	2	0
All	All	6034	0	6074	87	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (87) 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:169:HIS:HA	1:B:343:ILE:HD11	1.54	0.88
1:A:149:SER:HB3	1:A:290:ASN:HD21	1.43	0.82
1:A:169:HIS:HA	1:A:343:ILE:HD11	1.64	0.78
1:B:271:THR:N	3:B:401:UDP:O1A	2.18	0.76
1:A:196:LYS:NZ	1:A:267:GLU:OE1	2.21	0.73
1:B:196:LYS:NZ	1:B:267:GLU:OE1	2.21	0.70
1:A:320:VAL:HG13	1:A:327:ARG:HB2	1.77	0.66
1:A:195:ASN:HD21	1:A:266:VAL:H	1.43	0.64
1:A:34:VAL:HG22	1:A:52:VAL:HB	1.80	0.63
1:A:80:ARG:NH1	1:A:107:ILE:O	2.30	0.60
1:A:149:SER:HB3	1:A:290:ASN:ND2	2.15	0.59
1:A:9:ILE:O	1:A:38:LYS:HA	2.03	0.58
1:A:271:THR:N	3:A:401:UDP:O2A	2.33	0.56
1:B:198:PRO:HG2	1:B:230:LEU:HD11	1.89	0.55
1:A:248:GLU:HB2	1:B:61:ARG:NH1	2.23	0.54
1:A:267:GLU:HB2	1:A:288:TYR:CD1	2.43	0.53
1:A:72:ARG:NH2	6:A:408:BUE:O40	2.41	0.53
1:B:9:ILE:O	1:B:38:LYS:HA	2.08	0.53
1:A:198:PRO:HG2	1:A:230:LEU:HD11	1.91	0.52
1:A:219:VAL:HG12	1:A:242:ASP:HB2	1.92	0.51
1:A:45:PHE:O	1:B:61:ARG:NH2	2.44	0.51
1:A:99:ASN:O	1:A:103:ILE:HG12	2.10	0.50
1:B:80:ARG:NH1	1:B:107:ILE:O	2.42	0.50
1:B:109:LEU:O	7:B:501:HOH:O	2.19	0.50
1:A:22:VAL:HG13	1:A:48:LEU:HD13	1.93	0.50
1:B:144:SER:HB2	1:B:164:LEU:HD12	1.94	0.50
1:B:20:VAL:HG13	1:B:167:PRO:HD2	1.94	0.49
1:A:311:ILE:O	1:A:315:LYS:HG3	2.12	0.49
1:B:62:PHE:HE2	1:B:72:ARG:HH21	1.60	0.49
1:A:29:CYS:HA	1:A:34:VAL:HG13	1.95	0.49
1:A:12:LEU:HA	1:A:18:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:VAL:O	1:B:267:GLU:HG2	2.14	0.48
1:B:291:GLY:O	1:B:293:LYS:N	2.47	0.48
1:A:187:LEU:HD13	1:A:189:ILE:HD11	1.95	0.48
1:B:351:LEU:O	1:B:355:VAL:HG13	2.14	0.48
1:A:61:ARG:HD2	1:B:54:VAL:HG23	1.96	0.47
1:B:133:ARG:HD3	1:B:154:TYR:HE1	1.79	0.47
1:B:252:ALA:O	1:B:256:LYS:HD3	2.14	0.47
1:A:266:VAL:O	1:A:267:GLU:HG2	2.15	0.47
1:B:217:LYS:HE3	1:B:217:LYS:HB2	1.73	0.47
1:A:199:VAL:O	1:A:203:LYS:HG3	2.13	0.47
1:A:7:PHE:HB3	1:A:21:LEU:HD11	1.96	0.47
1:A:351:LEU:O	1:A:355:VAL:HG13	2.15	0.46
1:B:38:LYS:O	1:B:56:SER:HA	2.16	0.46
1:A:4:LYS:HB3	1:A:4:LYS:HE2	1.78	0.45
1:A:284:ILE:HG12	1:A:303:LEU:HB2	1.99	0.45
1:B:314:ALA:O	1:B:318:GLU:HG3	2.16	0.45
1:B:151:LYS:O	1:B:155:GLU:HB2	2.16	0.45
1:A:314:ALA:O	1:A:318:GLU:HG3	2.17	0.45
1:B:176:PHE:CE2	1:B:335:LYS:HB3	2.51	0.45
1:A:261:CYS:HA	1:A:284:ILE:O	2.17	0.45
1:B:191:ARG:NH1	7:B:506:HOH:O	2.50	0.45
1:A:160:ARG:NE	1:A:356:GLU:OE1	2.49	0.45
1:A:233:LYS:HA	1:A:236:SER:HB3	1.99	0.44
1:A:49:GLU:O	1:A:52:VAL:HG13	2.17	0.44
1:A:6:SER:HB2	1:A:91:PHE:CD1	2.53	0.44
1:B:182:LYS:NZ	1:B:279:PHE:O	2.35	0.44
1:A:348:GLU:O	1:A:352:LYS:HG3	2.17	0.44
1:B:7:PHE:HB3	1:B:21:LEU:HD11	1.98	0.44
1:A:13:ASN:O	1:A:15:GLY:N	2.48	0.44
1:A:176:PHE:CZ	1:A:335:LYS:HB3	2.52	0.44
1:B:317:LEU:HD12	1:B:317:LEU:HA	1.82	0.44
1:B:65:LEU:HA	1:B:68:LYS:HD2	2.00	0.44
2:C:1:NDG:H8C1	2:C:1:NDG:H2	1.76	0.44
1:B:199:VAL:O	1:B:203:LYS:HG3	2.19	0.43
1:B:345:ASN:OD1	1:B:346:ILE:HG13	2.19	0.43
1:B:348:GLU:O	1:B:352:LYS:HG3	2.19	0.43
1:B:201:PHE:O	1:B:205:ILE:HG13	2.19	0.43
2:D:1:NDG:H2	2:D:1:NDG:H8C1	1.73	0.43
1:A:204:ALA:O	1:A:208:LEU:HD13	2.19	0.43
1:B:188:PHE:HD1	1:B:220:ILE:HG23	1.84	0.43
1:A:317:LEU:HD12	1:A:317:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:HIS:O	1:B:146:LEU:HD12	2.19	0.42
1:B:121:GLU:HG3	1:B:153:TYR:CE2	2.54	0.42
1:A:63:ASP:HB3	1:B:43:GLU:HG3	2.01	0.42
1:A:20:VAL:HG13	1:A:167:PRO:HD2	2.01	0.42
1:A:6:SER:HB2	1:A:91:PHE:HD1	1.84	0.42
1:A:59:GLN:NE2	1:B:56:SER:OG	2.53	0.41
1:B:176:PHE:HE2	1:B:335:LYS:HB3	1.83	0.41
1:A:201:PHE:O	1:A:205:ILE:HG13	2.20	0.41
1:B:254:TYR:HE1	1:B:260:LEU:HD13	1.86	0.41
1:A:38:LYS:HE3	1:A:56:SER:OG	2.20	0.41
1:A:118:HIS:HB3	5:A:404:CL:CL	2.57	0.41
1:A:201:PHE:CE2	1:A:205:ILE:HD11	2.55	0.41
1:B:267:GLU:HB2	1:B:288:TYR:CD1	2.56	0.40
1:B:358:LYS:HE3	1:B:358:LYS:HB2	1.66	0.40
1:B:254:TYR:HB3	1:B:279:PHE:CG	2.57	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	358/373 (96%)	344 (96%)	10 (3%)	4 (1%)	14	34
1	B	358/373 (96%)	345 (96%)	10 (3%)	3 (1%)	19	43
All	All	716/746 (96%)	689 (96%)	20 (3%)	7 (1%)	15	37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	ASP
1	A	290	ASN
1	A	292	ALA

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Mol	Chain	Res	Type
1	B	292	ALA
1	B	177	ASP
1	B	180	PHE
1	A	291	GLY

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	324/336 (96%)	318 (98%)	6 (2%)	57	82
1	B	324/336 (96%)	316 (98%)	8 (2%)	47	76
All	All	648/672 (96%)	634 (98%)	14 (2%)	52	79

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	CYS
1	A	52	VAL
1	A	121	GLU
1	A	177	ASP
1	A	287	SER
1	A	307	CYS
1	B	56	SER
1	B	63	ASP
1	B	177	ASP
1	B	225	GLU
1	B	227	ARG
1	B	307	CYS
1	B	329	GLU
1	B	345	ASN

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

Mol	Chain	Res	Type
1	A	59	GLN
1	A	195	ASN
1	A	213	GLN
1	A	249	ASN
1	A	290	ASN
1	A	325	ASN
1	B	13	ASN
1	B	67	HIS
1	B	290	ASN
1	B	359	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 ⓘ

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NDG	C	1	2,6	14,14,15	2.70	7 (50%)	17,19,21	2.02	7 (41%)
2	A2G	C	2	2	14,14,15	1.96	5 (35%)	17,19,21	1.37	2 (11%)
2	A2G	C	3	2	14,14,15	2.75	7 (50%)	17,19,21	1.32	3 (17%)
2	NDG	D	1	2,6	14,14,15	2.67	6 (42%)	17,19,21	2.15	6 (35%)
2	A2G	D	2	2	14,14,15	2.02	6 (42%)	17,19,21	1.65	3 (17%)
2	A2G	D	3	2	14,14,15	2.80	7 (50%)	17,19,21	1.61	2 (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
2	NDG	C	1	2,6	-	2/6/23/26	0/1/1/1
2	A2G	C	2	2	-	2/6/23/26	0/1/1/1
2	A2G	C	3	2	-	2/6/23/26	0/1/1/1
2	NDG	D	1	2,6	-	2/6/23/26	0/1/1/1
2	A2G	D	2	2	-	0/6/23/26	0/1/1/1
2	A2G	D	3	2	-	1/6/23/26	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	A2G	O5-C5	5.64	1.54	1.43
2	D	3	A2G	O5-C5	5.53	1.54	1.43
2	C	1	NDG	O5-C5	5.52	1.54	1.43
2	D	1	NDG	O5-C5	5.47	1.54	1.43
2	D	3	A2G	C2-N2	4.75	1.54	1.46
2	C	3	A2G	C2-N2	4.24	1.53	1.46
2	C	1	NDG	C2-N2	4.23	1.53	1.46
2	D	1	NDG	C2-N2	4.21	1.53	1.46
2	D	3	A2G	C7-N2	3.97	1.48	1.34
2	C	2	A2G	C7-N2	3.84	1.47	1.34
2	C	3	A2G	C7-N2	3.76	1.47	1.34
2	D	2	A2G	C7-N2	3.75	1.47	1.34
2	D	1	NDG	C7-N2	3.58	1.46	1.34
2	C	1	NDG	C7-N2	3.55	1.46	1.34
2	C	2	A2G	O5-C1	3.50	1.49	1.43
2	D	2	A2G	O5-C1	3.48	1.49	1.43
2	C	3	A2G	C6-C5	-3.25	1.40	1.51
2	D	1	NDG	O3-C3	3.19	1.50	1.43
2	D	3	A2G	C6-C5	-3.16	1.41	1.51
2	D	1	NDG	C6-C5	-3.15	1.41	1.51
2	C	1	NDG	O3-C3	3.05	1.50	1.43
2	C	3	A2G	C3-C2	-2.82	1.46	1.52
2	C	1	NDG	C6-C5	-2.80	1.42	1.51
2	D	3	A2G	O5-C1	2.73	1.48	1.43
2	C	3	A2G	O5-C1	2.57	1.47	1.43
2	D	3	A2G	C3-C2	-2.56	1.47	1.52
2	C	2	A2G	O5-C5	2.46	1.48	1.43
2	D	2	A2G	O5-C5	2.45	1.48	1.43
2	D	2	A2G	C2-N2	2.45	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NDG	C3-C2	-2.26	1.47	1.52
2	C	2	A2G	C3-C2	-2.25	1.47	1.52
2	D	3	A2G	O3-C3	2.20	1.48	1.43
2	C	1	NDG	O7-C7	-2.17	1.18	1.23
2	C	3	A2G	O3-C3	2.14	1.48	1.43
2	C	2	A2G	C2-N2	2.10	1.49	1.46
2	D	1	NDG	O7-C7	-2.08	1.18	1.23
2	D	2	A2G	O7-C7	-2.08	1.18	1.23
2	D	2	A2G	C8-C7	2.04	1.54	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	A2G	C1-O5-C5	4.17	117.84	112.19
2	D	1	NDG	C3-C4-C5	4.13	117.61	110.24
2	C	1	NDG	C3-C4-C5	3.78	116.98	110.24
2	D	1	NDG	O3-C3-C4	-3.66	101.88	110.35
2	C	1	NDG	O3-C3-C4	-3.30	102.72	110.35
2	D	1	NDG	C4-C3-C2	3.18	115.68	111.02
2	C	1	NDG	O3-C3-C2	-3.11	103.02	109.47
2	D	1	NDG	O3-C3-C2	-2.98	103.30	109.47
2	D	2	A2G	C8-C7-N2	2.95	121.09	116.10
2	D	2	A2G	C2-N2-C7	-2.93	118.73	122.90
2	C	2	A2G	C2-N2-C7	-2.87	118.82	122.90
2	D	1	NDG	C2-N2-C7	-2.71	119.04	122.90
2	C	1	NDG	C8-C7-N2	2.63	120.55	116.10
2	C	1	NDG	C4-C3-C2	2.58	114.80	111.02
2	D	3	A2G	C8-C7-N2	2.55	120.41	116.10
2	D	1	NDG	C8-C7-N2	2.51	120.34	116.10
2	C	1	NDG	C2-N2-C7	-2.45	119.42	122.90
2	C	2	A2G	O5-C1-C2	-2.17	107.86	111.29
2	C	1	NDG	O5-C5-C6	2.16	110.59	107.20
2	D	2	A2G	O5-C1-C2	-2.15	107.89	111.29
2	C	3	A2G	C1-O5-C5	2.11	115.05	112.19
2	C	3	A2G	C8-C7-N2	2.04	119.56	116.10
2	C	3	A2G	C2-N2-C7	-2.04	120.00	122.90

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NDG	C8-C7-N2-C2

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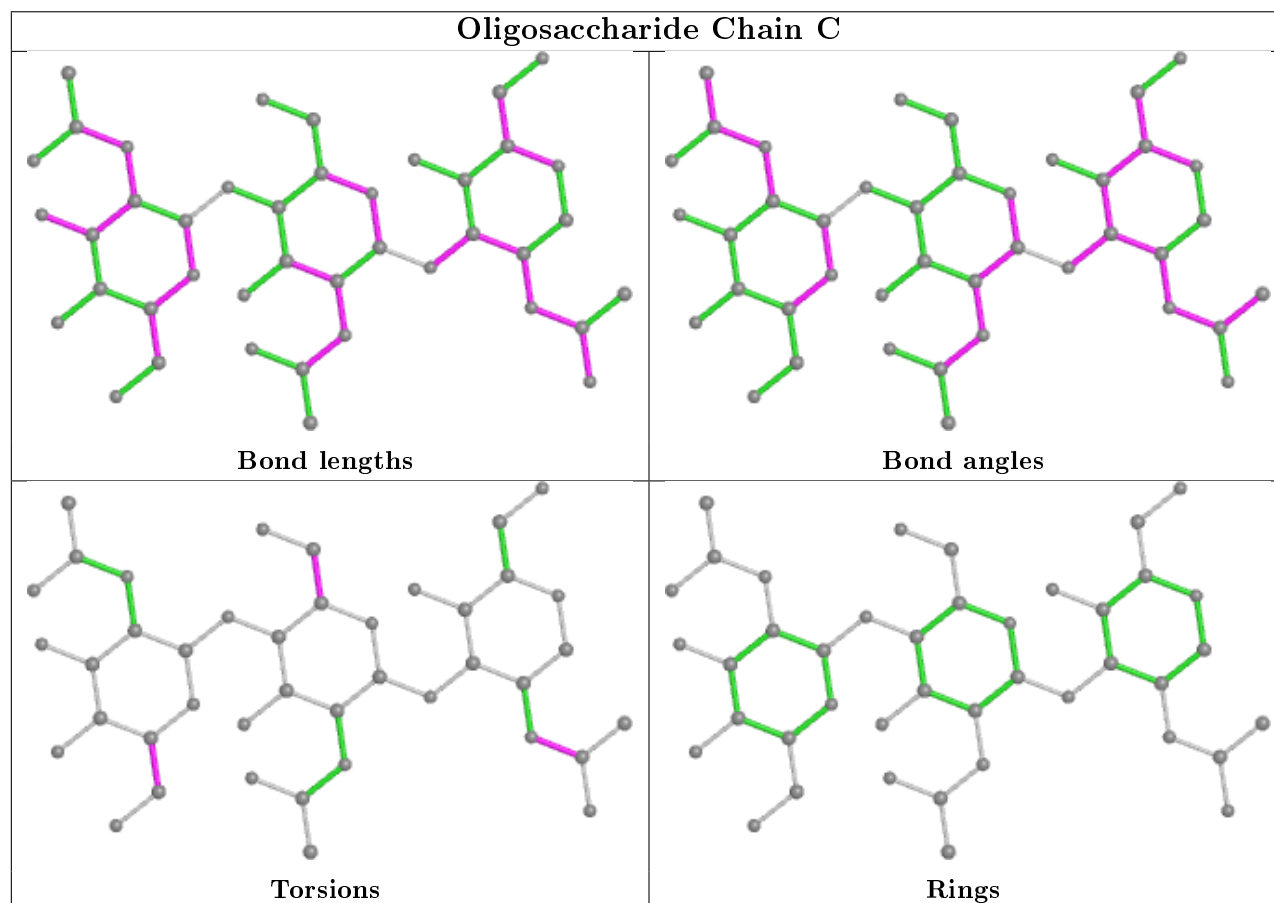
Mol	Chain	Res	Type	Atoms
2	D	1	NDG	O7-C7-N2-C2
2	C	1	NDG	C8-C7-N2-C2
2	C	1	NDG	O7-C7-N2-C2
2	C	2	A2G	O5-C5-C6-O6
2	D	3	A2G	O5-C5-C6-O6
2	C	3	A2G	C4-C5-C6-O6
2	C	2	A2G	C4-C5-C6-O6
2	C	3	A2G	O5-C5-C6-O6

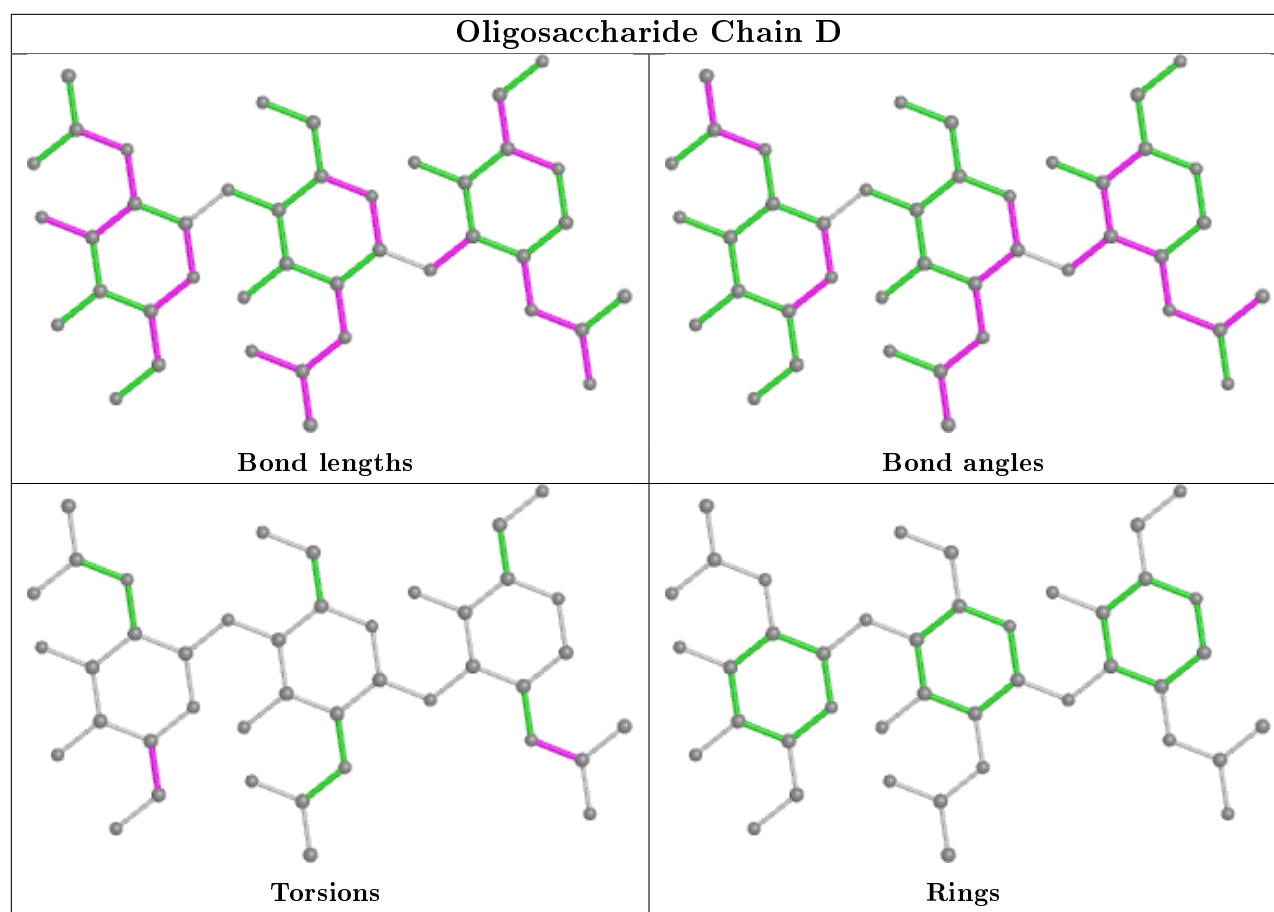
There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	UDP	A	401	-	20,26,26	1.51	4 (20%)	25,40,40	1.13	2 (8%)
6	BUE	A	408	2,4	8,10,28	2.43	2 (25%)	12,15,37	1.44	3 (25%)
3	UDP	B	401	4	20,26,26	1.58	5 (25%)	25,40,40	1.02	1 (4%)
6	BUE	B	407	2,4	8,10,28	1.83	2 (25%)	12,15,37	1.59	3 (25%)

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	UDP	A	401	-	-	5/14/32/32	0/2/2/2
6	BUE	A	408	2,4	-	4/10/10/31	-
3	UDP	B	401	4	-	6/14/32/32	0/2/2/2
6	BUE	B	407	2,4	-	6/10/10/31	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	408	BUE	P35-O34	5.51	1.68	1.50
3	B	401	UDP	C2'-C1'	-3.64	1.48	1.53
6	B	407	BUE	P35-O36	3.62	1.68	1.54
3	A	401	UDP	O4'-C1'	3.45	1.45	1.41
3	B	401	UDP	O4'-C1'	3.38	1.45	1.41
3	A	401	UDP	C2'-C1'	-3.08	1.49	1.53
3	A	401	UDP	C3'-C2'	-2.68	1.46	1.53
3	B	401	UDP	C3'-C2'	-2.65	1.46	1.53
3	B	401	UDP	C4-N3	2.23	1.36	1.33
6	A	408	BUE	P35-O36	-2.08	1.46	1.54
6	B	407	BUE	P35-O37	-2.05	1.46	1.54
3	A	401	UDP	C3'-C4'	-2.03	1.47	1.53
3	B	401	UDP	C3'-C4'	-2.00	1.47	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	407	BUE	O37-P35-O34	-3.22	98.07	110.68
3	A	401	UDP	PA-O3A-PB	-2.94	122.75	132.83
6	A	408	BUE	O40-P39-O41	-2.76	98.62	112.24
6	B	407	BUE	O40-P39-O41	-2.65	99.12	112.24
6	B	407	BUE	O36-P35-O38	2.60	113.35	104.64
3	B	401	UDP	PA-O3A-PB	-2.53	124.13	132.83
6	A	408	BUE	O37-P35-O36	-2.52	98.01	107.64
3	A	401	UDP	C3'-C2'-C1'	2.29	104.43	100.98
6	A	408	BUE	O37-P35-O38	2.29	112.31	104.64

There are no chirality outliers.

All (21) torsion outliers are listed below:

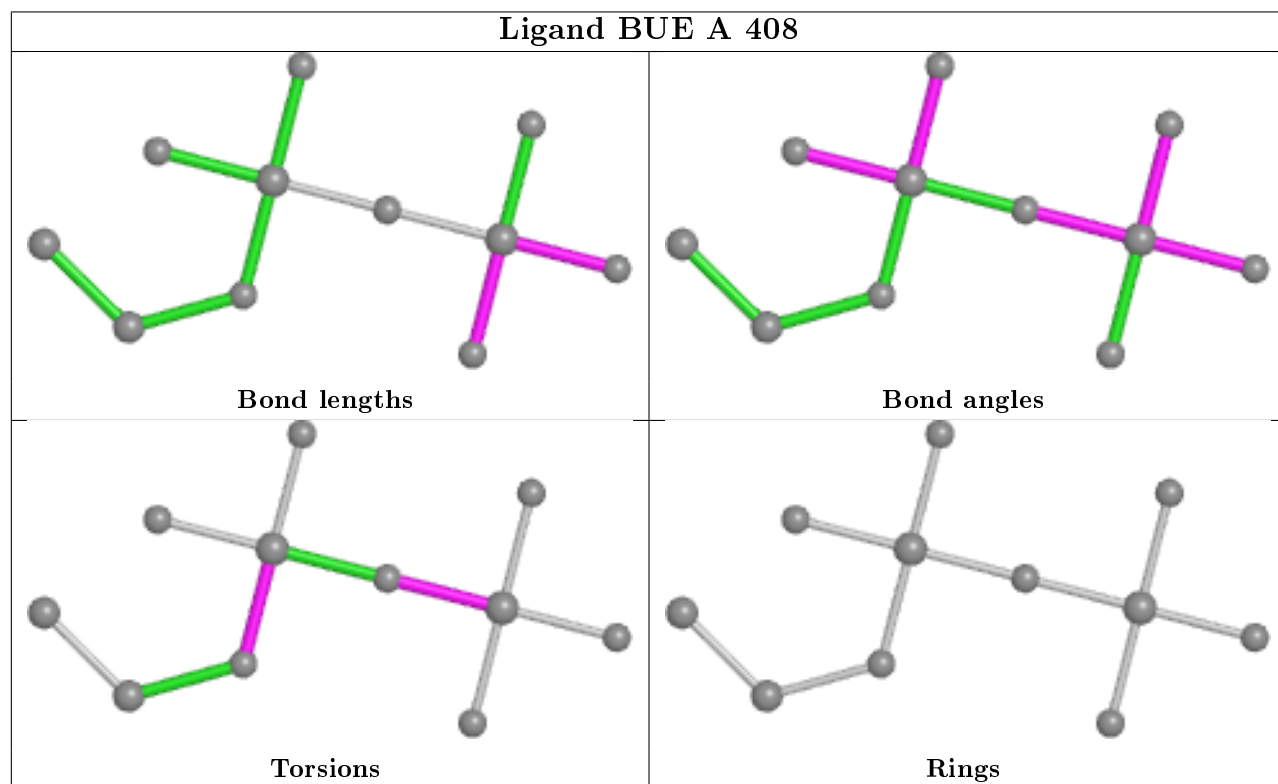
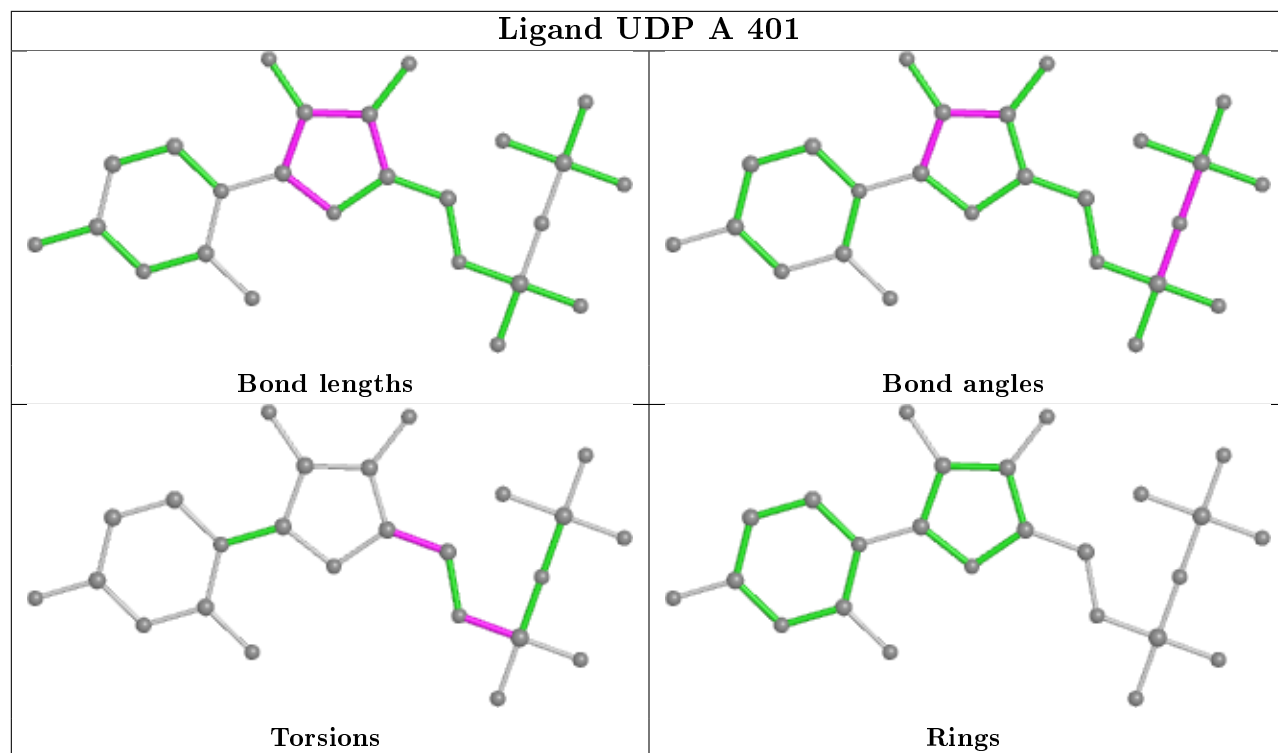
Mol	Chain	Res	Type	Atoms
3	A	401	UDP	C5'-O5'-PA-O1A
3	A	401	UDP	C5'-O5'-PA-O2A
6	B	407	BUE	C43-O42-P39-O40
6	B	407	BUE	C43-O42-P39-O41
6	A	408	BUE	C43-O42-P39-O40
6	A	408	BUE	C43-O42-P39-O41
3	B	401	UDP	C5'-O5'-PA-O1A
3	B	401	UDP	C5'-O5'-PA-O2A
3	B	401	UDP	PB-O3A-PA-O5'
3	A	401	UDP	C3'-C4'-C5'-O5'
3	A	401	UDP	O4'-C4'-C5'-O5'
3	B	401	UDP	C3'-C4'-C5'-O5'
3	B	401	UDP	O4'-C4'-C5'-O5'
6	A	408	BUE	P39-O38-P35-O36
3	A	401	UDP	C5'-O5'-PA-O3A
6	B	407	BUE	P39-O38-P35-O36
6	B	407	BUE	P39-O38-P35-O37
6	B	407	BUE	C43-O42-P39-O38
6	A	408	BUE	C43-O42-P39-O38
3	B	401	UDP	C5'-O5'-PA-O3A
6	B	407	BUE	P35-O38-P39-O41

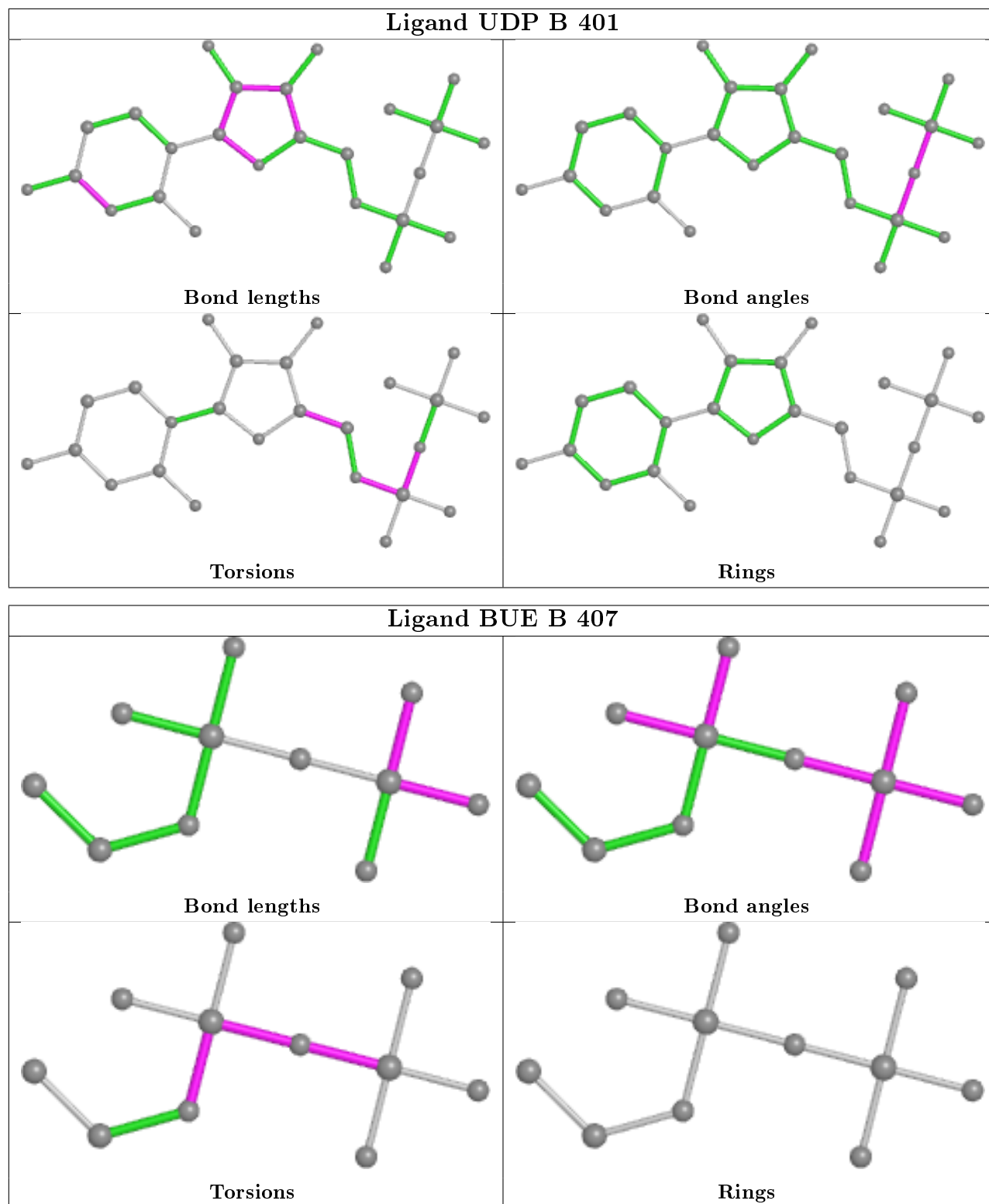
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	UDP	1	0
6	A	408	BUE	1	0
3	B	401	UDP	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	360/373 (96%)	-0.50	2 (0%) 89 91	34, 53, 75, 101	0
1	B	360/373 (96%)	-0.48	0 100 100	33, 53, 82, 108	0
All	All	720/746 (96%)	-0.49	2 (0%) 94 95	33, 53, 79, 108	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	177	ASP	3.0
1	A	58	GLU	2.3

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

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

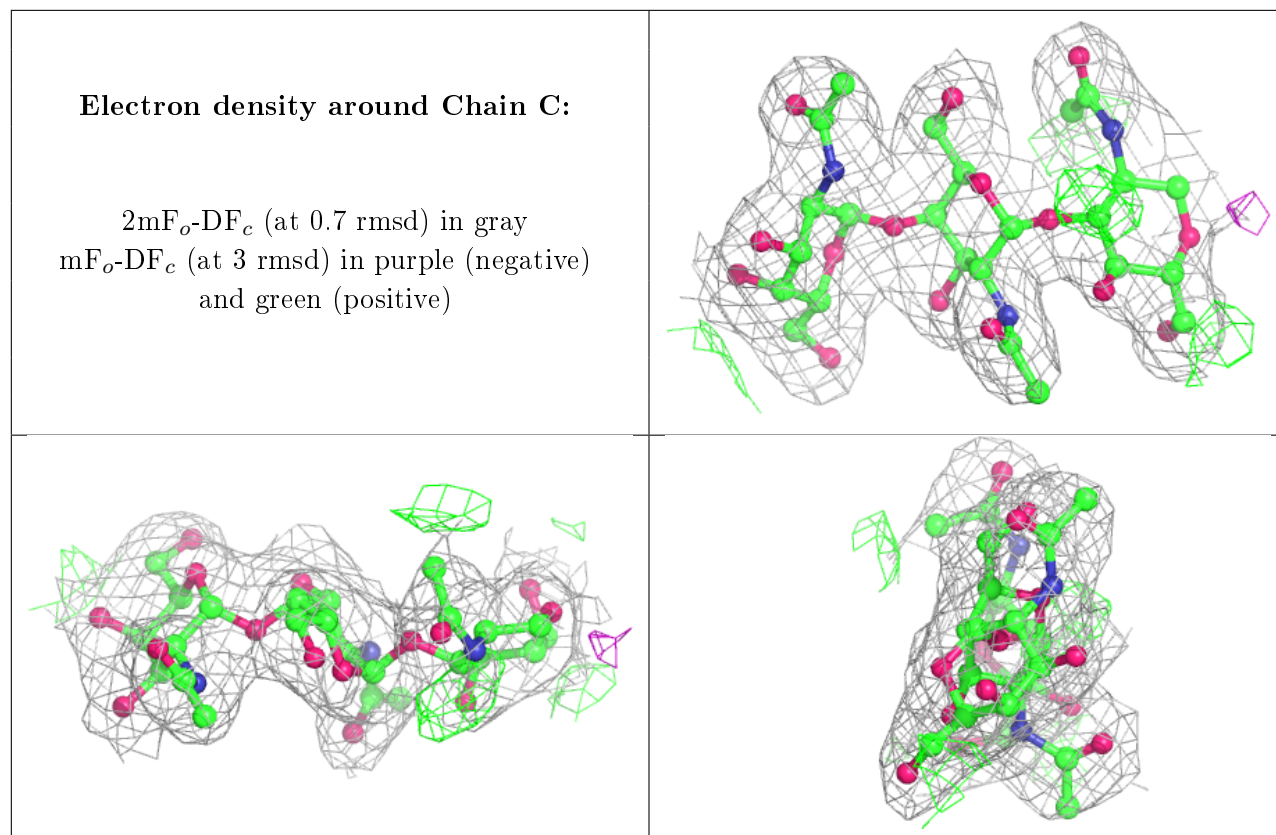
6.3 Carbohydrates [i](#)

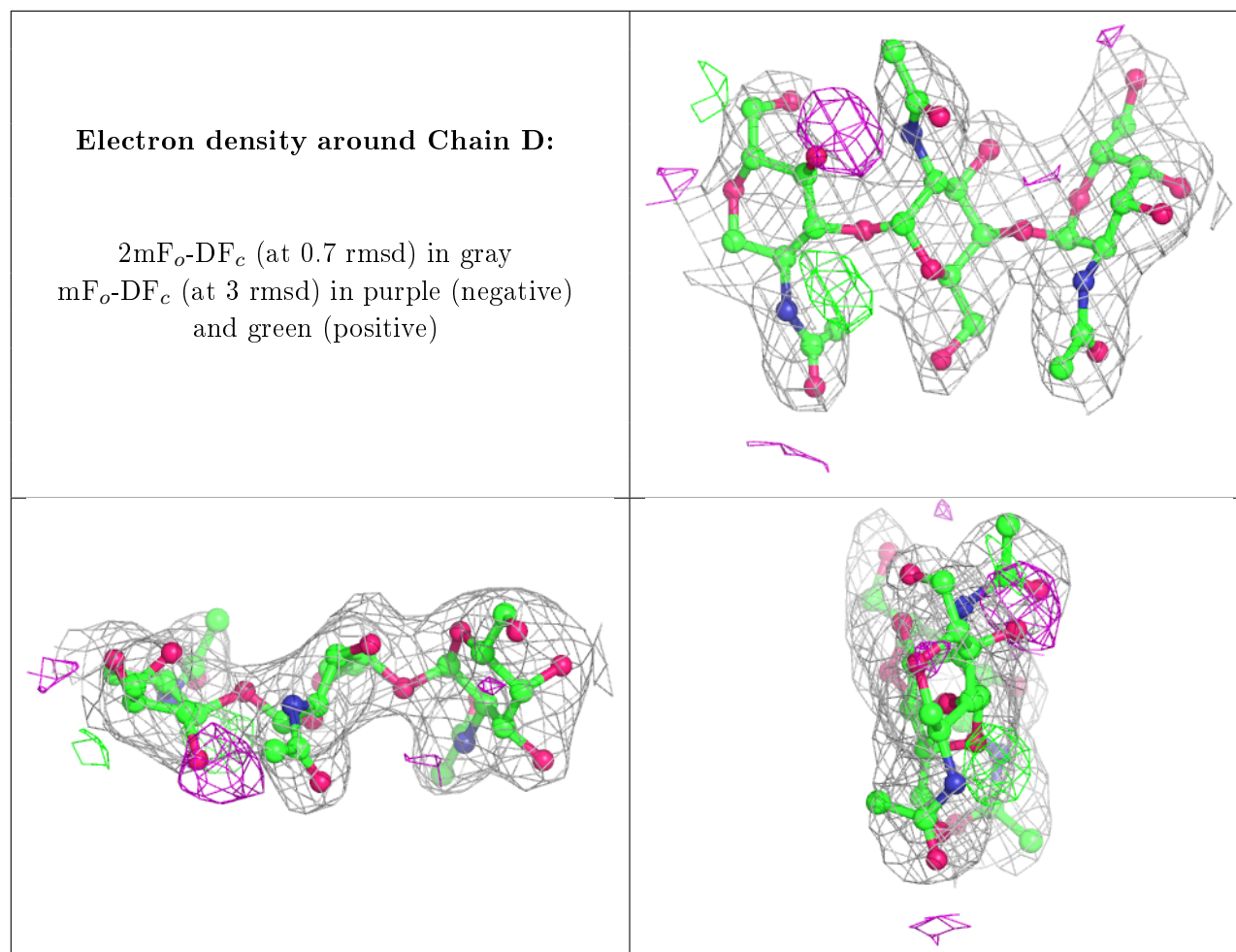
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NDG	C	1	14/15	0.87	0.13	63,67,70,70	0
2	NDG	D	1	14/15	0.88	0.17	65,68,72,72	0
2	A2G	C	2	14/15	0.96	0.14	55,58,61,63	0
2	A2G	D	3	14/15	0.97	0.13	55,56,58,60	0
2	A2G	C	3	14/15	0.97	0.13	46,50,55,58	0
2	A2G	D	2	14/15	0.98	0.12	58,60,63,64	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.





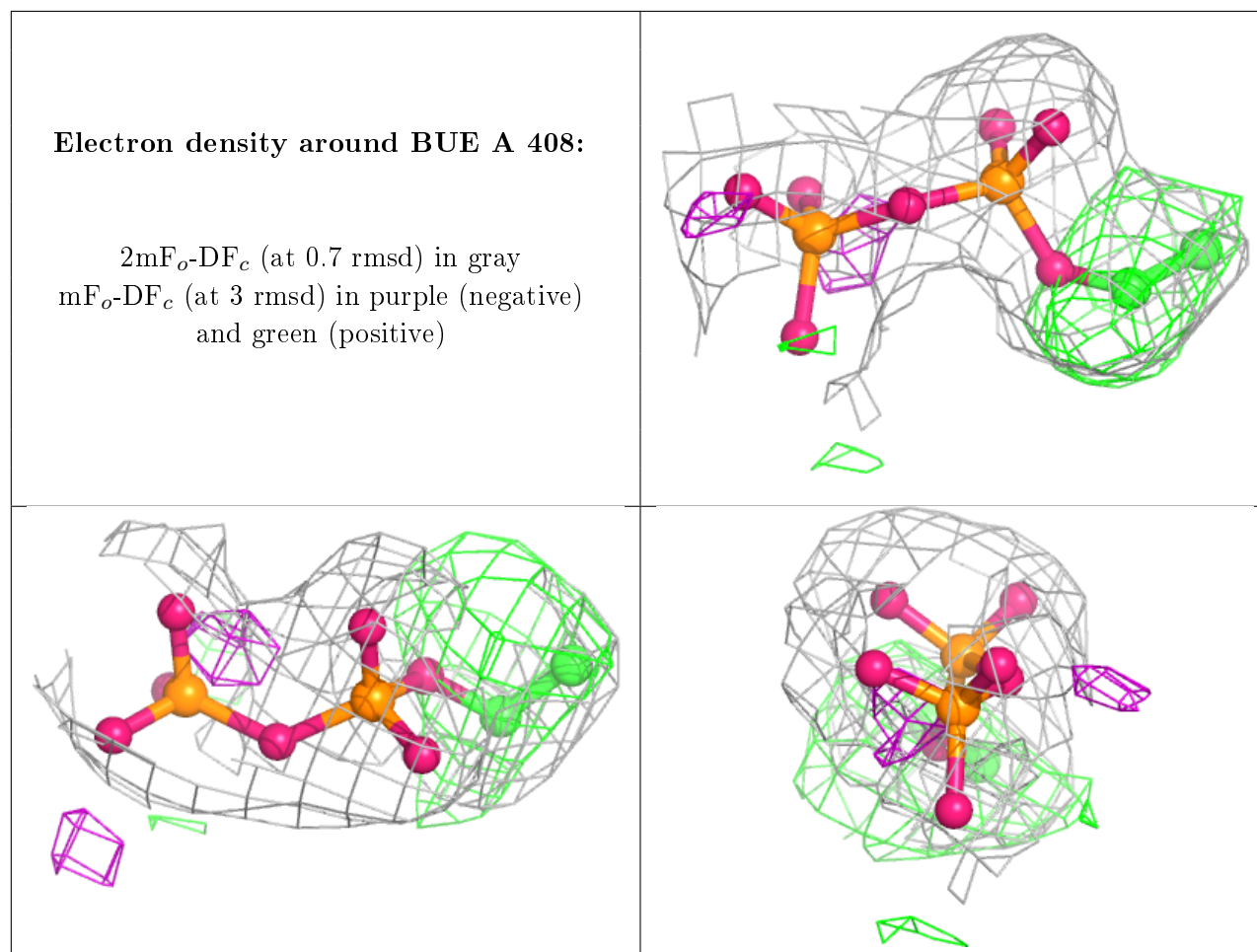
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	BUE	A	408	11/29	0.81	0.12	68,74,76,78	0
6	BUE	B	407	11/29	0.87	0.11	70,75,78,80	0
5	CL	A	404	1/1	0.91	0.07	82,82,82,82	0
4	NA	A	402	1/1	0.92	0.15	59,59,59,59	0
4	NA	A	403	1/1	0.93	0.06	58,58,58,58	0
4	NA	B	403	1/1	0.96	0.12	71,71,71,71	0
4	NA	B	402	1/1	0.97	0.21	53,53,53,53	0
3	UDP	B	401	25/25	0.98	0.13	48,49,50,50	0
3	UDP	A	401	25/25	0.98	0.13	43,47,51,53	0

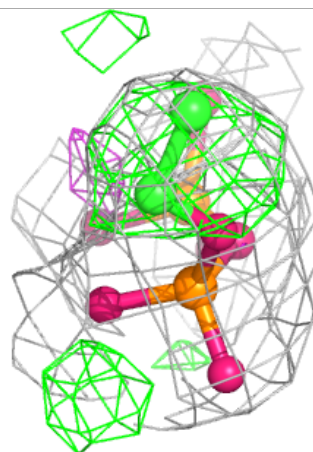
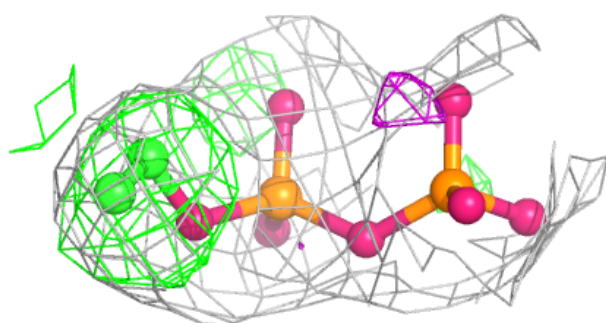
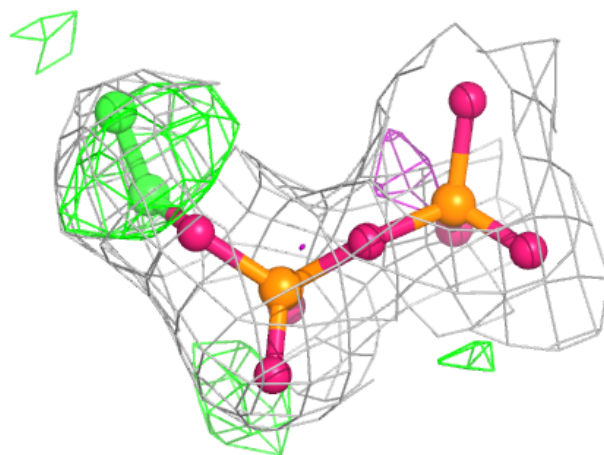
The following is a graphical depiction of the model fit to experimental electron density of all

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.

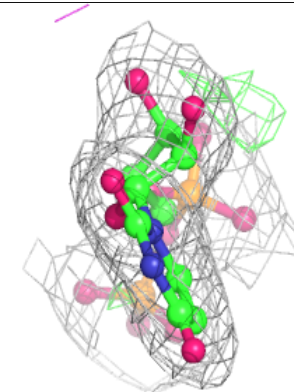
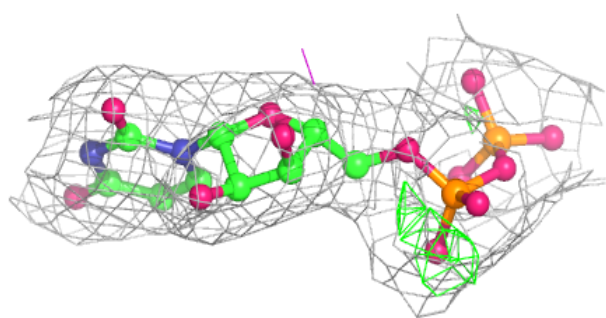
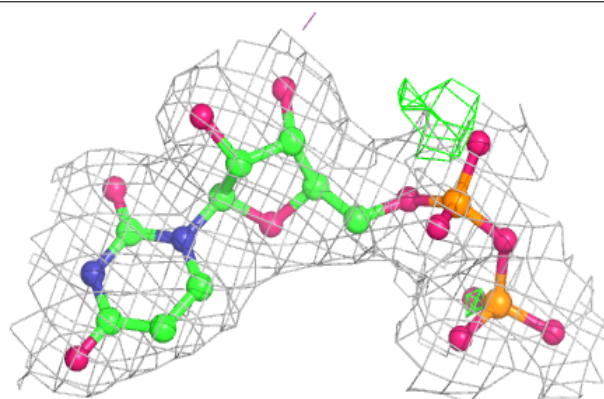


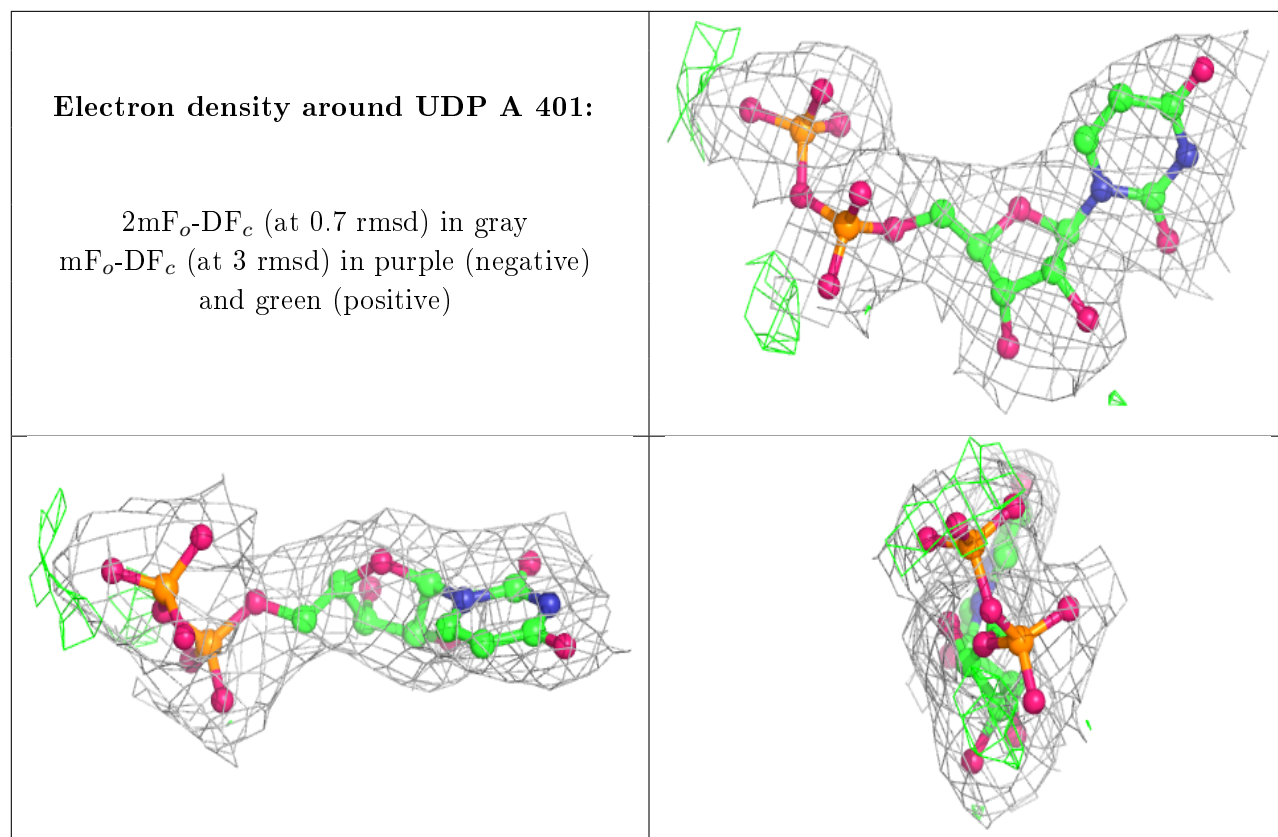
Electron density around BUE B 407:

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

**Electron density around UDP B 401:**

$2mF_o-DF_c$ (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.