



# Full wwPDB X-ray Structure Validation Report i

Nov 16, 2023 – 01:12 AM JST

PDB ID : 6KDK  
Title : HIV-1 reverse transcriptase with Q151M/Y115F/F116Y:DNA:dCTP ternary complex  
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Deposited on : 2019-07-02  
Resolution : 2.56 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>  
with specific help available everywhere you see the i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) i) 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 : 2.36  
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) : 2.36



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Mol	Chain	Length	Quality of chain
4	G	2	<div style="width: 50%;">50%</div> <div style="width: 50%;">50%</div>

## 2 Entry composition [\(i\)](#)

There are 8 unique types of molecules in this entry. The entry contains 17528 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 HIV-1 reverse transcriptase p66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	553	4498	2911	750	829	8	0	0	0
1	C	553	4498	2911	750	829	8	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP D3XFN5
A	0	VAL	-	expression tag	UNP D3XFN5
A	115	PHE	TYR	engineered mutation	UNP D3XFN5
A	116	TYR	PHE	engineered mutation	UNP D3XFN5
A	151	MET	GLN	engineered mutation	UNP D3XFN5
A	162	SER	CYS	engineered mutation	UNP D3XFN5
A	280	SER	CYS	engineered mutation	UNP D3XFN5
C	-1	MET	-	expression tag	UNP D3XFN5
C	0	VAL	-	expression tag	UNP D3XFN5
C	115	PHE	TYR	engineered mutation	UNP D3XFN5
C	116	TYR	PHE	engineered mutation	UNP D3XFN5
C	151	MET	GLN	engineered mutation	UNP D3XFN5
C	162	SER	CYS	engineered mutation	UNP D3XFN5
C	280	SER	CYS	engineered mutation	UNP D3XFN5

- Molecule 2 is a protein called HIV-1 RT p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	406	3347	2178	557	606	6	0	0	0
2	D	406	3347	2178	557	606	6	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	expression tag	UNP P12497
B	-14	ALA	-	expression tag	UNP P12497
B	-13	HIS	-	expression tag	UNP P12497
B	-12	HIS	-	expression tag	UNP P12497
B	-11	HIS	-	expression tag	UNP P12497
B	-10	HIS	-	expression tag	UNP P12497
B	-9	HIS	-	expression tag	UNP P12497
B	-8	HIS	-	expression tag	UNP P12497
B	-7	ALA	-	expression tag	UNP P12497
B	-6	LEU	-	expression tag	UNP P12497
B	-5	GLU	-	expression tag	UNP P12497
B	-4	VAL	-	expression tag	UNP P12497
B	-3	LEU	-	expression tag	UNP P12497
B	-2	PHE	-	expression tag	UNP P12497
B	-1	GLN	-	expression tag	UNP P12497
B	0	GLY	-	expression tag	UNP P12497
B	162	SER	CYS	engineered mutation	UNP P12497
B	280	SER	CYS	engineered mutation	UNP P12497
D	-15	MET	-	expression tag	UNP P12497
D	-14	ALA	-	expression tag	UNP P12497
D	-13	HIS	-	expression tag	UNP P12497
D	-12	HIS	-	expression tag	UNP P12497
D	-11	HIS	-	expression tag	UNP P12497
D	-10	HIS	-	expression tag	UNP P12497
D	-9	HIS	-	expression tag	UNP P12497
D	-8	HIS	-	expression tag	UNP P12497
D	-7	ALA	-	expression tag	UNP P12497
D	-6	LEU	-	expression tag	UNP P12497
D	-5	GLU	-	expression tag	UNP P12497
D	-4	VAL	-	expression tag	UNP P12497
D	-3	LEU	-	expression tag	UNP P12497
D	-2	PHE	-	expression tag	UNP P12497
D	-1	GLN	-	expression tag	UNP P12497
D	0	GLY	-	expression tag	UNP P12497
D	162	SER	CYS	engineered mutation	UNP P12497
D	280	SER	CYS	engineered mutation	UNP P12497

- Molecule 3 is a DNA chain called DNA/RNA (38-MER).

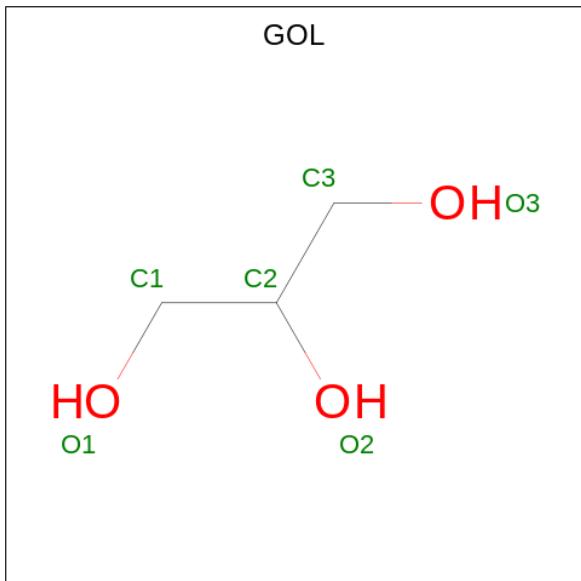
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	35	Total	C	N	O	P	0	0	0
			721	340	130	216	35			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	C	1	Total Mg 1 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	64	Total O 64 64	0	0
8	B	33	Total O 33 33	0	0
8	E	30	Total O 30 30	0	0
8	C	50	Total O 50 50	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	40	Total O 40 40	0	0
8	F	15	Total O 15 15	0	0





GLC1  
FR12

## 4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	284.85Å 284.85Å 95.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.74 – 2.56 48.74 – 2.56	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.74-2.56) 100.0 (48.74-2.56)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	1.25 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
$R$ , $R_{free}$	0.190 , 0.234 0.190 , 0.234	Depositor DCC
$R_{free}$ test set	4730 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.9	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 57.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17528	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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









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<b>Atom-1</b>	<b>Atom-2</b>	<b>Interatomic distance (Å)</b>	<b>Clash overlap (Å)</b>
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.46	0.51
1:A:331:LYS:NZ	1:C:297:GLU:OE2	2.33	0.51
2:B:353:LYS:HD2	2:B:427:TYR:OH	2.11	0.51
2:D:319:TYR:OH	2:D:385:LYS:HE2	2.10	0.50
3:F:1:DC:H2'	3:F:2:OMC:C6	2.46	0.50
1:C:78:ARG:O	1:C:82:LYS:HG3	2.11	0.50
2:B:252:TRP:CD1	2:B:295:LEU:HD11	2.46	0.50
1:C:450:THR:O	1:C:451:LYS:HB2	2.11	0.50
1:A:542:ILE:HD12	1:A:542:ILE:H	1.77	0.50
2:D:183:TYR:CE2	2:D:184:MET:HG3	2.47	0.50
1:A:331:LYS:NZ	1:A:364:ASP:OD2	2.44	0.50
2:B:168:LEU:O	2:B:172:ARG:HG3	2.11	0.50
1:C:457:TYR:CE2	1:C:484:LEU:HD22	2.43	0.49
1:A:135:ILE:O	1:A:137:ASN:N	2.42	0.49
2:B:64:LYS:HE2	2:B:69:THR:O	2.13	0.49
2:B:303:LEU:O	2:B:307:ARG:HG3	2.12	0.49
1:C:450:THR:HG23	1:C:452:LEU:H	1.78	0.49
1:A:458:VAL:HG12	2:B:286:THR:HG21	1.94	0.49
1:A:438:GLU:OE2	1:A:459:THR:HG21	2.13	0.49
2:D:297:GLU:HA	2:D:300:GLU:HG2	1.93	0.49
1:A:538:ALA:O	1:A:540:LYS:HG2	2.12	0.49
1:A:393:ILE:O	1:A:414:TRP:HZ3	1.95	0.48
3:E:10:DC:H2"	3:E:11:DG:C8	2.48	0.48
2:D:66:LYS:NZ	2:D:232:TYR:CE2	2.71	0.48
2:D:421:PRO:O	2:D:424:LYS:HB2	2.12	0.48
1:A:135:ILE:O	1:A:135:ILE:CG2	2.52	0.48
1:C:491:LEU:HB3	1:C:529:GLU:HG3	1.94	0.48
1:A:41:MET:HB3	1:A:46:LYS:HB2	1.95	0.48
2:B:5:ILE:HG22	2:B:6:GLU:H	1.78	0.48
2:D:66:LYS:HZ1	2:D:232:TYR:HD2	0.64	0.48
1:C:40:GLU:OE2	1:C:44:GLU:HG3	2.13	0.48
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.96	0.48
2:D:297:GLU:HA	2:D:300:GLU:CG	2.44	0.48
1:A:58:THR:HG21	1:A:77:PHE:CD1	2.49	0.48
2:B:199:ARG:NH1	2:B:233:GLU:OE2	2.47	0.48
1:A:248:GLU:HG2	1:A:307:ARG:NH2	2.29	0.48
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.49	0.47
2:B:199:ARG:O	2:B:202:ILE:HB	2.14	0.47
2:B:312:GLU:HB3	2:B:313:PRO:HD2	1.95	0.47
2:B:103:LYS:NZ	2:B:190:GLY:O	2.42	0.47
2:B:266:TRP:HH2	2:B:426:TRP:CZ2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:ASP:OD1	2:B:322:SER:OG	2.32	0.47
1:A:69:THR:O	1:A:69:THR:HG22	2.14	0.47
3:E:23:DC:H2"	3:E:24:DG:C8	2.49	0.47
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.96	0.47
1:A:23:GLN:OE1	1:A:59:PRO:HA	2.15	0.47
1:C:184:MET:HG2	3:F:33:DG:H2"	1.96	0.47
2:D:356:ARG:HB3	2:D:367:GLN:HG2	1.96	0.47
2:B:203:GLU:HA	2:B:206:ARG:CG	2.44	0.47
2:B:298:GLU:HA	2:B:301:LEU:HB2	1.96	0.47
2:D:64:LYS:HD3	2:D:69:THR:C	2.35	0.47
1:A:283:LEU:O	1:A:286:THR:OG1	2.31	0.47
1:C:221:HIS:NE2	1:C:223:LYS:HE2	2.29	0.47
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.50	0.46
1:A:139:THR:HG23	1:A:140:PRO:HD2	1.97	0.46
2:D:297:GLU:HA	2:D:300:GLU:OE2	2.15	0.46
1:A:3:SER:HB3	1:A:5:ILE:HG22	1.97	0.46
2:B:21:VAL:HG11	4:G:2:FRU:H11	1.97	0.46
2:B:422:LEU:N	2:B:422:LEU:CD2	2.73	0.46
2:B:103:LYS:HZ1	2:B:179:VAL:N	2.14	0.46
1:A:66:LYS:N	1:A:66:LYS:HD3	2.30	0.46
1:A:406:TRP:CZ2	2:B:420:PRO:HG3	2.50	0.46
1:A:500:GLN:H	1:A:500:GLN:NE2	2.14	0.46
2:B:208:HIS:HE1	2:B:212:TRP:HE1	1.64	0.46
1:C:63:ILE:HG12	1:C:74:LEU:HD11	1.97	0.46
1:C:393:ILE:O	1:C:414:TRP:HZ3	1.99	0.46
2:B:17:ASP:O	2:B:83:ARG:HD3	2.16	0.46
2:B:199:ARG:HA	2:B:202:ILE:CD1	2.42	0.46
2:B:356:ARG:HH11	2:B:357:MET:HA	1.77	0.46
2:B:203:GLU:HA	2:B:206:ARG:CD	2.46	0.45
2:B:297:GLU:HG2	2:B:298:GLU:OE1	2.15	0.45
1:C:51:GLY:N	1:C:53:GLU:OE1	2.38	0.45
7:C:602:GOL:H11	2:D:394:GLN:CB	2.42	0.45
1:A:265:ASN:OD1	1:A:353:LYS:HE3	2.17	0.45
2:D:46:LYS:HD3	2:D:116:PHE:HB3	1.98	0.45
1:C:52:PRO:O	1:C:54:ASN:N	2.50	0.45
1:C:237:ASP:OD2	1:C:237:ASP:N	2.38	0.45
1:C:298:GLU:H	1:C:298:GLU:CD	2.20	0.45
2:D:64:LYS:CD	2:D:69:THR:C	2.85	0.44
1:C:114:ALA:HB1	1:C:160:PHE:CE2	2.53	0.44
1:A:79:GLU:HA	1:A:82:LYS:HZ3	1.82	0.44
2:B:276:VAL:O	2:B:280:SER:OG	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:GLU:OE1	2:B:308:GLU:HA	2.16	0.44
2:B:308:GLU:O	2:B:311:LYS:HB2	2.18	0.44
1:A:30:LYS:NZ	1:A:62:ALA:O	2.33	0.44
2:B:426:TRP:O	2:B:427:TYR:HD2	2.01	0.44
1:A:219:LYS:HB2	1:A:219:LYS:HE3	1.73	0.44
1:A:520:GLN:HA	1:A:523:GLU:HG2	1.99	0.44
1:C:524:GLN:O	1:C:528:LYS:HG2	2.18	0.44
2:D:344:GLU:HG2	2:D:345:PRO:HD2	1.99	0.44
1:A:60:VAL:HB	1:A:75:VAL:HG22	2.00	0.44
2:D:232:TYR:CD1	2:D:234:LEU:HD21	2.53	0.44
8:A:703:HOH:O	2:B:394:GLN:HB3	2.18	0.43
2:B:356:ARG:O	2:B:357:MET:SD	2.76	0.43
2:B:365:VAL:HG11	2:B:401:TRP:HB2	2.00	0.43
1:A:467:VAL:HG22	1:A:484:LEU:HD11	2.00	0.43
1:C:199:ARG:O	1:C:203:GLU:HG2	2.18	0.43
2:D:66:LYS:HE2	2:D:66:LYS:HB2	1.84	0.43
3:F:2:OMC:HM22	3:F:3:DC:O4'	2.18	0.43
2:D:277:ARG:HD3	2:D:277:ARG:HA	1.77	0.43
2:D:356:ARG:HG3	2:D:356:ARG:HH11	1.83	0.43
1:C:320:ASP:OD2	1:C:322:SER:HB3	2.19	0.43
2:B:263:LYS:HA	2:B:423:VAL:HG11	2.01	0.43
2:B:208:HIS:O	2:B:211:ARG:HB3	2.18	0.43
1:A:23:GLN:OE1	1:A:60:VAL:HG12	2.19	0.42
1:A:550:LYS:HD3	1:A:550:LYS:HA	1.83	0.42
1:A:37:ILE:O	1:A:41:MET:HG3	2.19	0.42
1:A:246:LEU:HD11	1:A:310:LEU:CD1	2.49	0.42
2:D:89:GLU:CD	2:D:89:GLU:H	2.23	0.42
2:D:38:CYS:HB3	2:D:47:ILE:HD11	2.02	0.42
1:A:28:GLU:OE2	1:A:28:GLU:N	2.51	0.42
1:C:539:HIS:C	1:C:540:LYS:HD2	2.40	0.42
1:C:22:LYS:N	1:C:22:LYS:HD2	2.35	0.42
2:D:64:LYS:CD	2:D:69:THR:O	2.66	0.42
1:A:451:LYS:HG3	1:A:471:ASP:HA	2.02	0.41
3:E:2:OMC:HM23	3:E:2:OMC:H1'	1.91	0.41
3:F:23:DC:H2"	3:F:24:DG:C8	2.56	0.41
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.19	0.41
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.56	0.41
3:F:23:DC:OP2	8:F:101:HOH:O	2.21	0.41
2:B:66:LYS:H	2:B:407:GLN:HE22	1.68	0.41
2:B:194:GLU:CD	2:B:195:ILE:H	2.24	0.41
1:A:65:LYS:HB2	1:A:70:LYS:O	2.21	0.41

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Mol	Chain	Res	Type
1	C	278	GLN
1	C	334	GLN
1	C	547	GLN
2	D	137	ASN
2	D	182	GLN
2	D	242	GLN
2	D	407	GLN
2	D	418	ASN

### 5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OMC	F	2	3	19,22,23	3.37	8 (42%)	26,31,34	0.75	0
3	OMC	F	4	3	19,22,23	3.38	8 (42%)	26,31,34	0.74	0
3	OMC	E	2	3	19,22,23	3.38	8 (42%)	26,31,34	0.73	0
3	OMC	E	4	3	19,22,23	3.32	8 (42%)	26,31,34	0.68	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	F	2	3	-	0/9/27/28	0/2/2/2
3	OMC	F	4	3	-	0/9/27/28	0/2/2/2
3	OMC	E	2	3	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	E	4	3	-	0/9/27/28	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	OMC	C6-C5	6.57	1.50	1.35
3	F	4	OMC	C2-N3	6.55	1.49	1.36
3	E	2	OMC	C6-C5	6.54	1.50	1.35
3	E	2	OMC	C2-N3	6.40	1.49	1.36
3	F	4	OMC	C6-C5	6.39	1.49	1.35
3	E	4	OMC	C2-N3	6.37	1.49	1.36
3	F	2	OMC	C2-N3	6.36	1.49	1.36
3	E	4	OMC	C6-C5	6.34	1.49	1.35
3	E	2	OMC	C4-N3	6.25	1.47	1.34
3	F	4	OMC	C4-N3	6.24	1.47	1.34
3	F	2	OMC	C4-N3	6.17	1.46	1.34
3	E	4	OMC	C4-N3	6.13	1.46	1.34
3	F	2	OMC	C4-N4	6.02	1.48	1.33
3	E	2	OMC	C4-N4	5.98	1.48	1.33
3	F	4	OMC	C4-N4	5.96	1.48	1.33
3	E	4	OMC	C4-N4	5.91	1.47	1.33
3	F	4	OMC	C2-N1	5.08	1.51	1.40
3	E	2	OMC	C2-N1	4.99	1.50	1.40
3	E	4	OMC	C2-N1	4.93	1.50	1.40
3	F	2	OMC	C2-N1	4.79	1.50	1.40
3	E	2	OMC	C6-N1	4.06	1.47	1.38
3	F	2	OMC	C6-N1	4.05	1.47	1.38
3	E	4	OMC	C6-N1	3.90	1.47	1.38
3	F	4	OMC	C6-N1	3.90	1.47	1.38
3	F	2	OMC	O2-C2	-3.01	1.18	1.23
3	F	4	OMC	O2-C2	-2.96	1.18	1.23
3	E	4	OMC	O2-C2	-2.93	1.18	1.23
3	E	2	OMC	O2-C2	-2.91	1.18	1.23
3	F	2	OMC	C5-C4	2.79	1.49	1.42
3	E	2	OMC	C5-C4	2.76	1.49	1.42
3	E	4	OMC	C5-C4	2.70	1.49	1.42
3	F	4	OMC	C5-C4	2.69	1.49	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	OMC	2	0
3	F	4	OMC	2	0
3	E	2	OMC	1	0
3	E	4	OMC	1	0

## 5.5 Carbohydrates [\(i\)](#)

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GLC	G	1	4	11,11,12	0.56	0	15,15,17	0.83	1 (6%)
4	FRU	G	2	4	11,12,12	0.56	0	10,18,18	0.54	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
4	GLC	G	1	4	-	0/2/19/22	0/1/1/1
4	FRU	G	2	4	-	1/5/24/24	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	G	1	GLC	C1-O5-C5	2.21	115.19	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

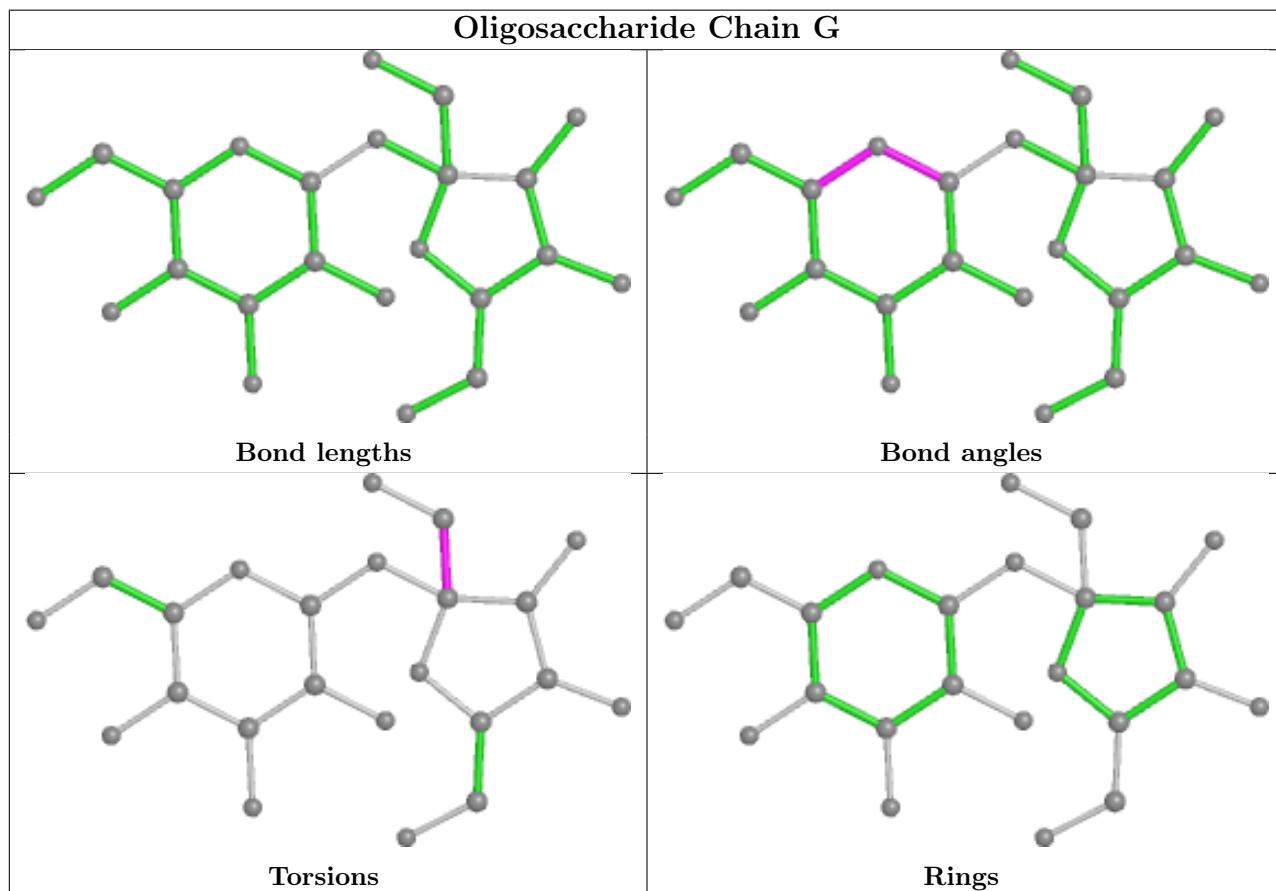
Mol	Chain	Res	Type	Atoms
4	G	2	FRU	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	FRU	1	0
4	G	1	GLC	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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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$
7	GOL	B	702	-	5,5,5	0.86	0	5,5,5	1.01	0
7	GOL	B	701	-	5,5,5	0.90	0	5,5,5	0.99	0
5	DCP	C	601	6	25,29,29	3.74	14 (56%)	37,45,45	0.95	2 (5%)
5	DCP	A	601	6	25,29,29	3.72	14 (56%)	37,45,45	0.97	2 (5%)
7	GOL	D	501	-	5,5,5	0.88	0	5,5,5	1.00	0
7	GOL	C	602	-	5,5,5	0.89	0	5,5,5	0.87	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
7	GOL	B	702	-	-	2/4/4/4	-
7	GOL	B	701	-	-	2/4/4/4	-
5	DCP	C	601	6	-	5/22/34/34	0/2/2/2
5	DCP	A	601	6	-	5/22/34/34	0/2/2/2
7	GOL	D	501	-	-	0/4/4/4	-
7	GOL	C	602	-	-	2/4/4/4	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	601	DCP	O4'-C4'	7.69	1.62	1.45
5	A	601	DCP	O4'-C4'	7.55	1.61	1.45
5	C	601	DCP	C2-N3	6.98	1.50	1.36
5	A	601	DCP	C2-N3	6.83	1.50	1.36
5	A	601	DCP	C6-C5	6.79	1.50	1.35
5	C	601	DCP	C6-C5	6.77	1.50	1.35
5	A	601	DCP	C3'-C4'	-6.45	1.35	1.53
5	C	601	DCP	C3'-C4'	-6.40	1.35	1.53
5	A	601	DCP	C4-N4	5.92	1.47	1.33
5	C	601	DCP	C4-N4	5.90	1.47	1.33
5	C	601	DCP	C4-N3	5.61	1.45	1.34
5	A	601	DCP	C4-N3	5.49	1.45	1.34
5	A	601	DCP	O4'-C1'	-5.18	1.30	1.42
5	C	601	DCP	O4'-C1'	-5.10	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	601	DCP	C2-N1	4.37	1.49	1.40
5	A	601	DCP	C2-N1	4.19	1.49	1.40
5	A	601	DCP	C6-N1	3.44	1.46	1.38
5	C	601	DCP	C6-N1	3.37	1.46	1.38
5	C	601	DCP	PA-O5'	2.47	1.69	1.59
5	C	601	DCP	C5-C4	2.44	1.48	1.42
5	A	601	DCP	PA-O5'	2.43	1.69	1.59
5	A	601	DCP	C5-C4	2.42	1.48	1.42
5	C	601	DCP	O3'-C3'	2.37	1.48	1.43
5	A	601	DCP	O3'-C3'	2.37	1.48	1.43
5	A	601	DCP	C2'-C1'	2.36	1.59	1.52
5	C	601	DCP	C2'-C1'	2.35	1.58	1.52
5	C	601	DCP	O2-C2	-2.18	1.19	1.23
5	A	601	DCP	O2-C2	-2.13	1.19	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	DCP	C2'-C1'-N1	-2.93	107.03	113.77
5	A	601	DCP	PB-O3B-PG	-2.34	124.79	132.83
5	C	601	DCP	PB-O3B-PG	-2.32	124.86	132.83
5	C	601	DCP	C2'-C1'-N1	-2.17	108.78	113.77

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	601	DCP	PB-O3B-PG-O2G
7	B	701	GOL	O1-C1-C2-C3
7	B	702	GOL	O1-C1-C2-C3
7	C	602	GOL	O1-C1-C2-O2
7	C	602	GOL	O1-C1-C2-C3
7	B	701	GOL	O1-C1-C2-O2
7	B	702	GOL	O1-C1-C2-O2
5	A	601	DCP	PB-O3B-PG-O1G
5	C	601	DCP	PA-O3A-PB-O2B
5	C	601	DCP	PB-O3B-PG-O1G
5	A	601	DCP	PB-O3B-PG-O2G
5	A	601	DCP	PB-O3B-PG-O3G
5	C	601	DCP	PB-O3B-PG-O3G
5	A	601	DCP	PB-O3A-PA-O1A
5	A	601	DCP	PA-O3A-PB-O1B

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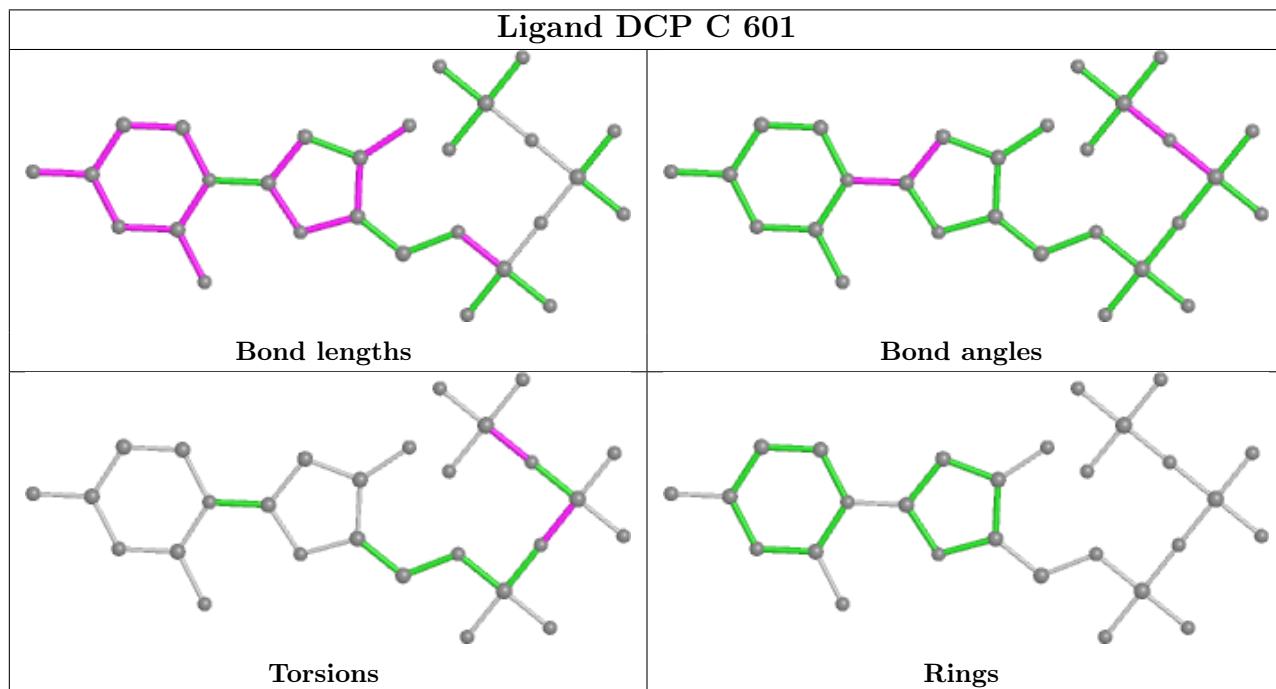
Mol	Chain	Res	Type	Atoms
5	C	601	DCP	PA-O3A-PB-O1B

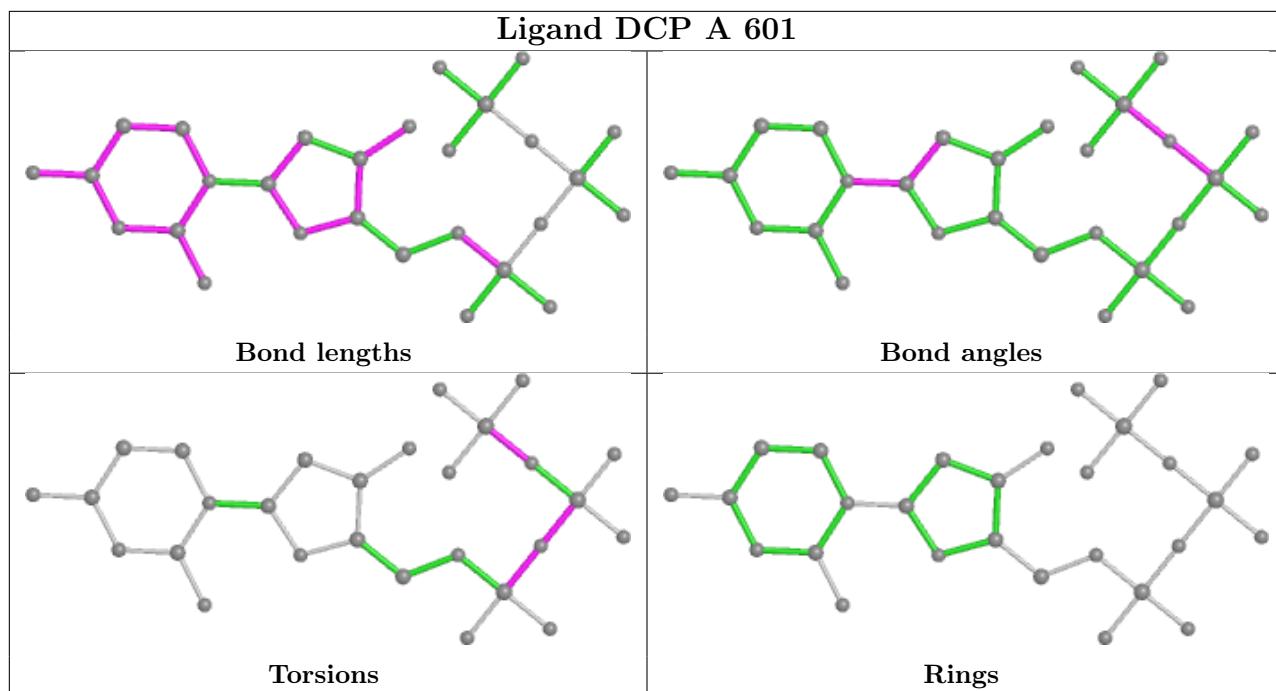
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	DCP	1	0
7	C	602	GOL	2	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	553/557 (99%)	0.52	36 (6%) 18 23	39, 64, 101, 141	0
1	C	553/557 (99%)	0.73	58 (10%) 6 9	39, 67, 106, 165	0
2	B	406/444 (91%)	0.97	59 (14%) 2 3	40, 79, 123, 139	0
2	D	406/444 (91%)	0.49	30 (7%) 14 19	34, 60, 96, 116	0
3	E	33/38 (86%)	0.02	0 100 100	40, 64, 94, 128	0
3	F	36/38 (94%)	0.19	1 (2%) 53 62	43, 72, 125, 146	0
All	All	1987/2078 (95%)	0.65	184 (9%) 8 12	34, 66, 113, 165	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	PRO	9.3
2	B	88	TRP	8.7
2	D	360	ALA	7.8
1	C	69	THR	7.7
1	C	136	ASN	7.3
1	C	137	ASN	7.3
2	B	212	TRP	6.8
1	C	133	PRO	6.7
1	A	27	THR	6.7
2	B	427	TYR	6.6
2	B	360	ALA	6.5
1	A	140	PRO	6.3
1	A	28	GLU	6.3
1	A	69	THR	6.3
1	C	135	ILE	6.3
2	D	361	HIS	6.3
1	C	140	PRO	6.3
1	C	139	THR	6.2
2	B	92	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
1	C	141	GLY	6.1
1	A	137	ASN	6.1
2	D	359	GLY	6.1
1	C	553	SER	6.0
2	B	301	LEU	6.0
1	C	31	ILE	5.9
2	B	94	ILE	5.8
2	B	357	MET	5.8
2	B	91	GLN	5.6
2	B	213	GLY	5.4
2	B	361	HIS	5.4
2	D	231	GLY	5.4
2	B	93	GLY	5.3
2	B	359	GLY	5.3
2	D	212	TRP	5.3
2	B	67	ASP	5.3
1	C	50	ILE	5.3
2	B	297	GLU	5.2
1	C	34	LEU	5.2
1	C	452	LEU	5.2
2	D	232	TYR	5.2
1	C	132	ILE	5.1
1	A	134	SER	5.1
2	B	232	TYR	5.1
1	C	71	TRP	5.0
2	D	68	SER	5.0
2	B	90	VAL	5.0
1	A	141	GLY	5.0
1	C	449	GLU	4.9
2	B	423	VAL	4.8
2	B	299	ALA	4.8
2	B	295	LEU	4.7
1	A	135	ILE	4.7
1	A	138	GLU	4.6
2	B	231	GLY	4.6
2	D	67	ASP	4.6
1	A	66	LYS	4.6
1	A	24	TRP	4.5
1	A	67	ASP	4.5
2	B	362	THR	4.5
1	A	139	THR	4.4
1	A	33	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	136	ASN	4.4
1	C	28	GLU	4.3
1	C	68	SER	4.3
1	A	142	ILE	4.3
1	A	25	PRO	4.3
2	B	89	GLU	4.3
2	B	87	PHE	4.2
1	C	54	ASN	4.1
1	C	138	GLU	4.1
1	C	26	LEU	4.1
1	C	448	ARG	4.1
1	C	67	ASP	4.0
2	B	7	THR	3.9
1	A	541	GLY	3.9
1	A	68	SER	3.9
1	C	32	LYS	3.9
1	A	64	LYS	3.8
1	C	35	VAL	3.8
2	B	68	SER	3.8
1	C	52	PRO	3.8
2	B	252	TRP	3.8
1	C	33	ALA	3.7
2	B	211	ARG	3.7
2	D	69	THR	3.7
1	C	550	LYS	3.7
1	A	61	PHE	3.7
2	B	6	GLU	3.6
1	A	63	ILE	3.6
1	C	469	LEU	3.6
2	B	248	GLU	3.5
2	D	357	MET	3.5
2	D	5	ILE	3.5
2	B	209	LEU	3.5
2	B	66	LYS	3.4
2	D	166	LYS	3.4
2	B	10	VAL	3.3
1	C	142	ILE	3.3
2	B	95	PRO	3.3
2	D	358	LYS	3.2
1	C	552	VAL	3.2
2	B	251	SER	3.2
1	C	51	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	39	THR	3.1
1	A	413	GLU	3.1
1	C	104	LYS	3.1
2	B	5	ILE	3.1
2	B	422	LEU	3.1
2	D	425	LEU	3.0
1	C	66	LYS	3.0
2	D	174	GLN	3.0
1	C	551	LEU	3.0
2	B	178	ILE	3.0
2	B	195	ILE	2.9
1	C	49	LYS	2.9
2	B	168	LEU	2.9
2	D	283	LEU	2.9
2	D	211	ARG	2.9
2	B	177	ASP	2.9
2	D	421	PRO	2.9
1	A	132	ILE	2.9
1	A	36	GLU	2.8
2	D	66	LYS	2.8
1	A	30	LYS	2.8
2	B	279	LEU	2.8
1	C	144	TYR	2.8
2	D	172	ARG	2.8
2	B	250	ASP	2.8
2	B	161	GLN	2.8
1	C	37	ILE	2.7
1	C	143	ARG	2.7
1	A	29	GLU	2.7
1	C	131	THR	2.7
2	B	245	VAL	2.7
2	D	177	ASP	2.7
1	C	30	LYS	2.6
1	C	70	LYS	2.6
1	C	457	TYR	2.6
1	C	447	ASN	2.6
1	C	468	PRO	2.5
2	B	305	GLU	2.5
2	B	85	GLN	2.5
1	C	194	GLU	2.5
3	F	18	DT	2.5
2	B	9	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	70	LYS	2.5
1	C	55	PRO	2.5
2	B	196	GLY	2.4
1	A	346	PHE	2.4
1	C	450	THR	2.4
2	B	249	LYS	2.4
2	D	90	VAL	2.4
2	B	104	LYS	2.4
2	B	202	ILE	2.4
2	D	420	PRO	2.4
2	B	210	LEU	2.3
2	B	304	ALA	2.3
1	C	134	SER	2.3
2	D	93	GLY	2.3
1	C	128	THR	2.3
1	A	62	ALA	2.2
2	D	362	THR	2.2
2	D	95	PRO	2.2
1	C	177	ASP	2.2
1	C	470	THR	2.2
1	A	237	ASP	2.2
2	B	424	LYS	2.1
1	C	60	VAL	2.1
1	A	71	TRP	2.1
1	A	402	TRP	2.1
1	C	24	TRP	2.1
2	B	180	ILE	2.1
2	B	260	LEU	2.1
2	D	209	LEU	2.1
1	A	65	LYS	2.1
1	C	538	ALA	2.1
2	D	284	ARG	2.1
2	B	293	VAL	2.1
1	A	32	LYS	2.1
2	D	178	ILE	2.0
2	D	427	TYR	2.0
2	B	277	ARG	2.0
1	C	63	ILE	2.0
1	C	64	LYS	2.0

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

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

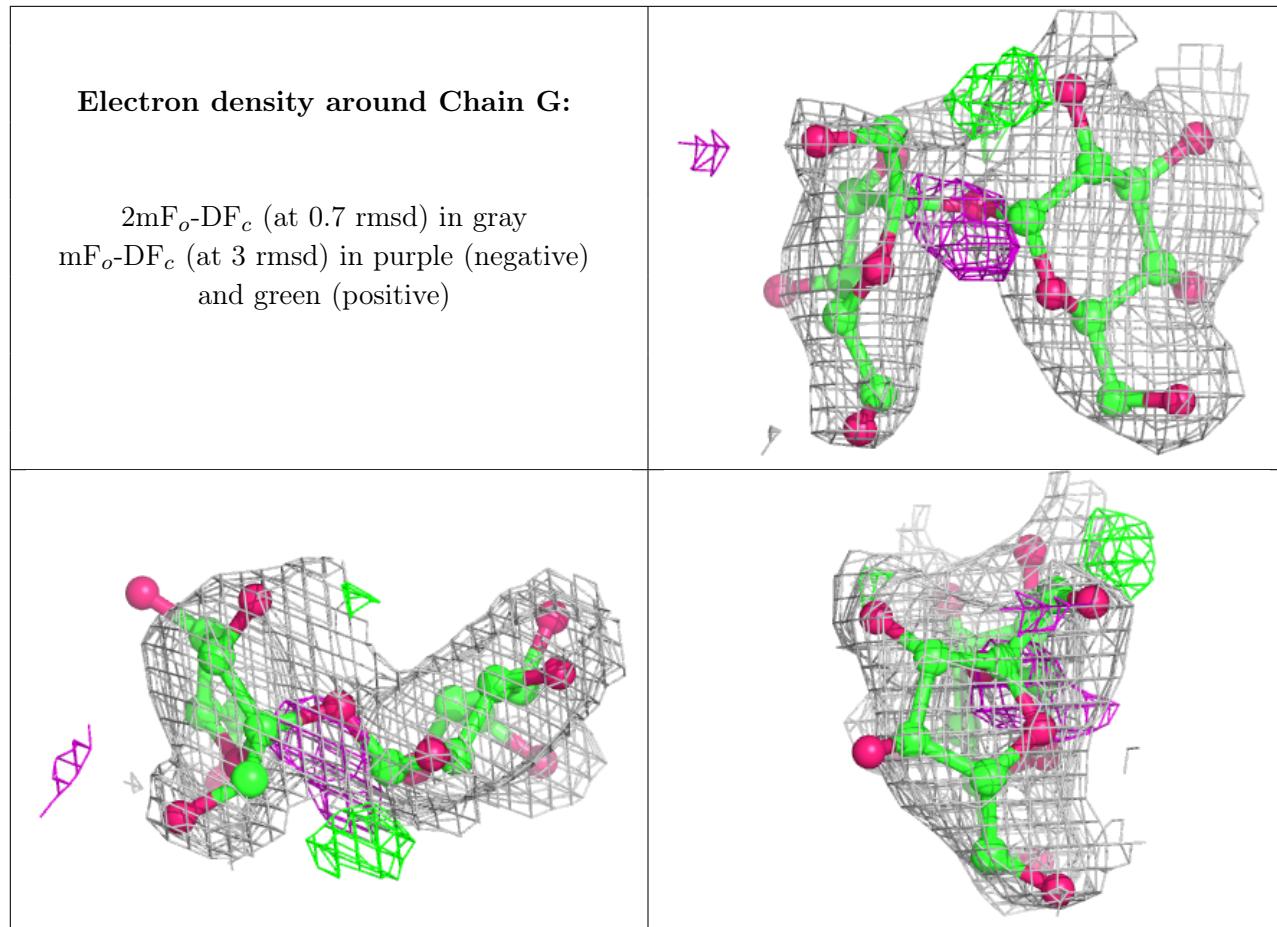
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	OMC	F	4	21/22	0.97	0.22	39,49,54,57	0
3	OMC	F	2	21/22	0.98	0.18	49,61,68,75	0
3	OMC	E	4	21/22	0.98	0.21	31,43,49,51	0
3	OMC	E	2	21/22	0.98	0.21	40,45,57,61	0

## 6.3 Carbohydrates [\(i\)](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	FRU	G	2	12/12	0.81	0.22	86,103,105,110	0
4	GLC	G	1	11/12	0.92	0.19	61,70,82,88	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.



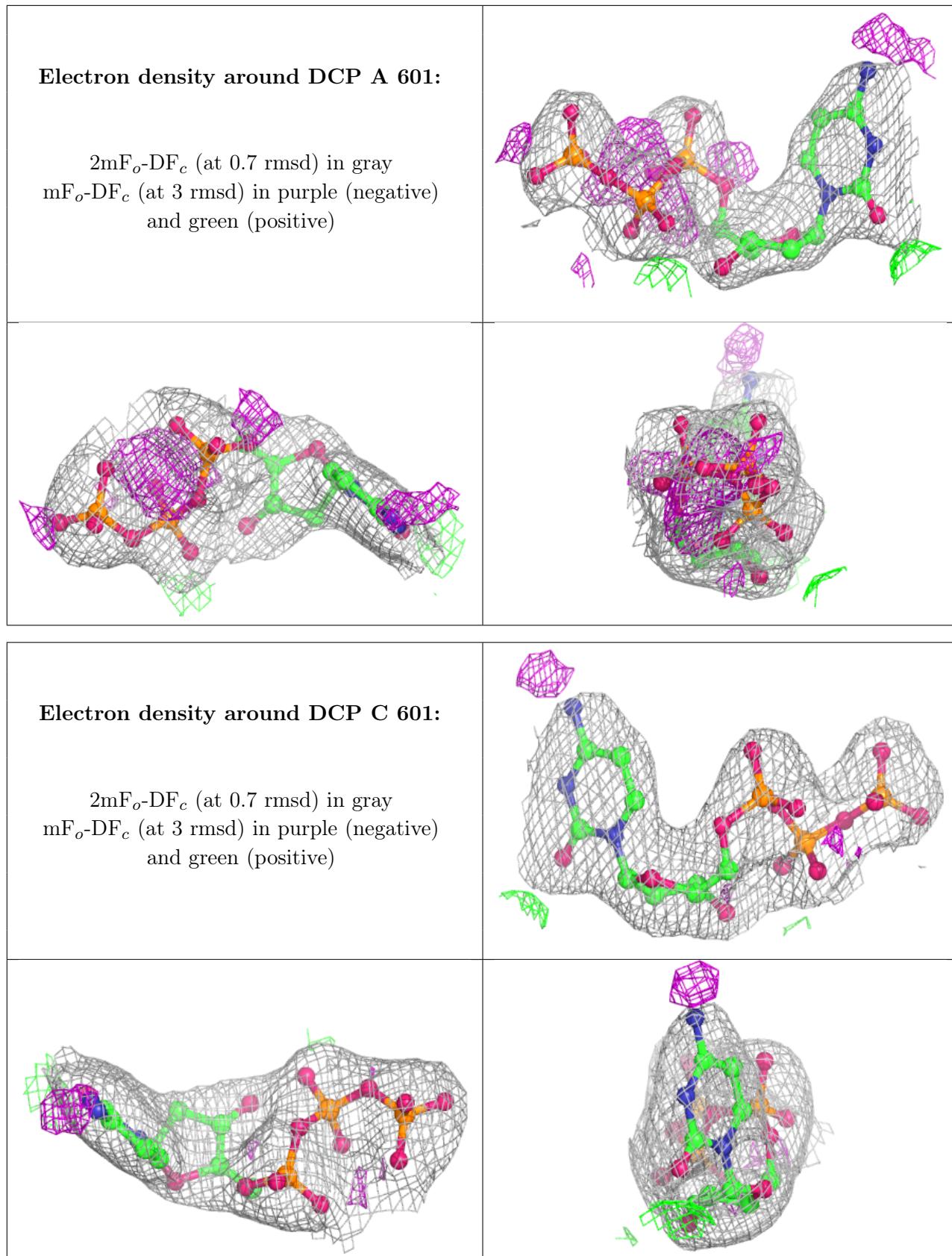
## 6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	GOL	B	701	6/6	0.79	0.26	72,74,78,79	0
6	MG	A	602	1/1	0.81	0.12	63,63,63,63	0
6	MG	C	603	1/1	0.84	0.08	58,58,58,58	0
7	GOL	C	602	6/6	0.93	0.20	58,60,64,66	0
5	DCP	A	601	28/28	0.94	0.16	53,60,72,83	0
5	DCP	C	601	28/28	0.94	0.15	49,62,81,85	0
7	GOL	B	702	6/6	0.95	0.31	52,57,61,69	0
7	GOL	D	501	6/6	0.95	0.26	54,55,56,57	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.