



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 10:45 AM BST

PDB ID : 2HVV
Title : ddCTP:O6MeG pair in the polymerase active site (0 position)
Authors : Warren, J.J.; Forsberg, L.J.; Beese, L.S.
Deposited on : 2006-07-28
Resolution : 2.49 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

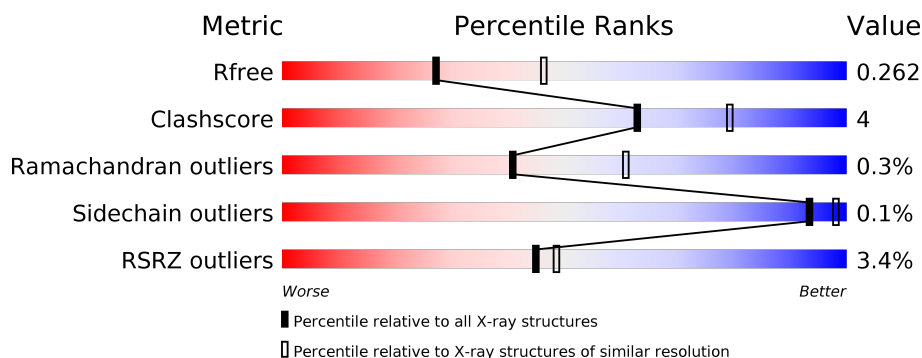
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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.



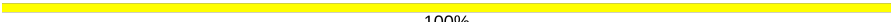

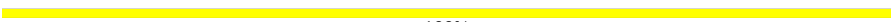
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	B	9	<div> <div>56%</div> <div>22%</div> <div>22%</div> </div>
1	E	9	<div> <div>33%</div> <div>22%</div> <div>44%</div> </div>
2	C	13	<div> <div>62%</div> <div>23%</div> <div>15%</div> </div>
2	F	13	<div> <div>46%</div> <div>23%</div> <div>15%</div> <div>15%</div> </div>
3	A	580	<div> <div>7%</div> <div>87%</div> <div>13%</div> </div>
3	D	580	<div> <div>93%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
4	G	2	 100%
4	H	2	 100%
4	I	2	 100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10548 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 DNA chain called 5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(DDG))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	9	Total	C	N	O	P	0	0	0
			177	86	31	52	8			
1	E	9	Total	C	N	O	P	0	0	0
			177	86	31	52	8			

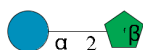
- Molecule 2 is a DNA chain called 5'-D(*CP*A*TP*(6OG)P*CP*GP*AP*GP*TP*CP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	P	0	0	0
			228	109	45	64	10			
2	F	11	Total	C	N	O	P	0	0	0
			228	109	45	64	10			

- Molecule 3 is a protein called DNA Polymerase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	580	Total	C	N	O	S	0	0	0
			4652	2958	808	869	17			
3	D	580	Total	C	N	O	S	0	1	0
			4658	2962	808	871	17			

- Molecule 4 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	G	2	Total	C	O	0	0	0
			23	12	11			

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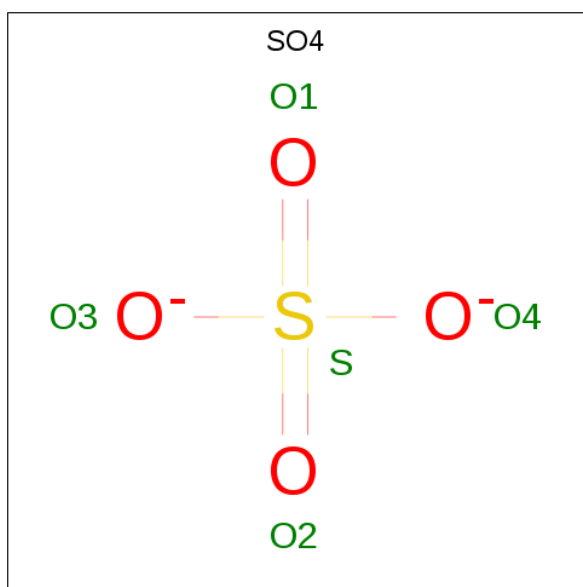
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	H	2	Total	C	O	0	0	0
			23	12	11			
4	I	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

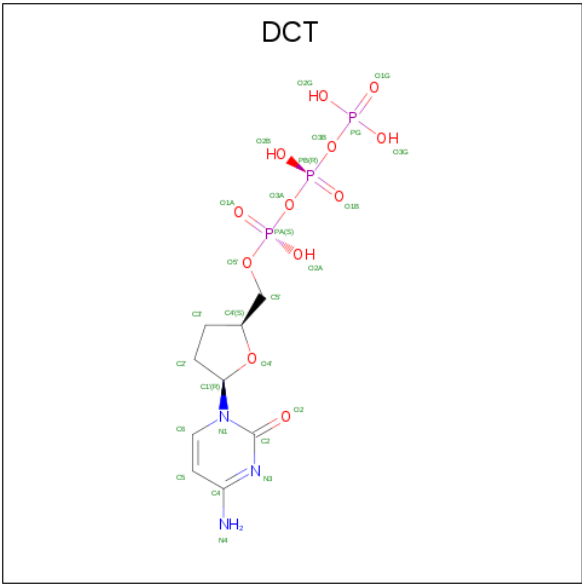
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mn	0	0
			1	1		
5	D	1	Total	Mn	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 2',3'-DIDEOXYCYTIDINE 5'-TRIPHOSPHATE (three-letter code: DCT) (formula: C₉H₁₆N₃O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	9	3	12	3		
7	D	1	Total	C	N	O	P	0	0
			27	9	3	12	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	5	Total	O	0	0
			5	5		
8	C	11	Total	O	0	0
			11	11		
8	E	10	Total	O	0	0
			10	10		
8	F	16	Total	O	0	0
			16	16		
8	A	86	Total	O	0	0
			86	86		
8	D	150	Total	O	0	0
			150	150		

3 Residue-property plots [i](#)


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

- Molecule 1: 5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(DDG))-3'

Chain B: 



- Molecule 1: 5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(DDG))-3'

Chain E: 



- Molecule 2: 5'-D(*CP*A*TP*(6OG)P*CP*GP*AP*GP*TP*CP*AP*GP*G)-3'

Chain C: 




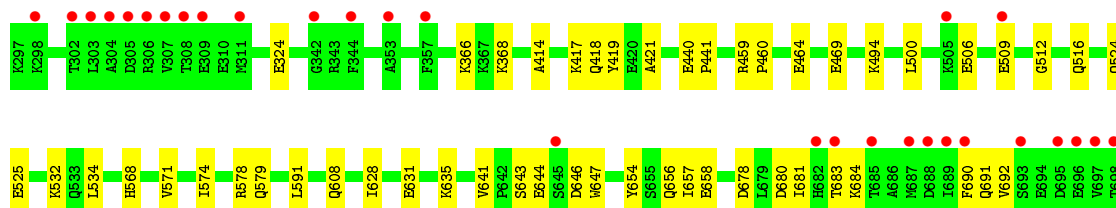
- Molecule 2: 5'-D(*CP*A*TP*(6OG)P*CP*GP*AP*GP*TP*CP*AP*GP*G)-3'

Chain F: 



- Molecule 3: DNA Polymerase I

Chain A: 



- Molecule 3: DNA Polymerase I

Chain D: 93% 7%



- Molecule 4: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain G: 100%



- Molecule 4: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain H: 100%



- Molecule 4: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain I:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.06Å 109.39Å 151.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.30 – 2.49 47.28 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.30-2.49) 98.8 (47.28-2.49)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.201 , 0.262 0.201 , 0.262	Depositor DCC
R_{free} test set	2765 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10548	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: 6OG, GLC, SO4, FRU, MN, DCT, DDG

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	B	0.73	0/173	1.55	4/264 (1.5%)
1	E	0.82	0/173	1.62	7/264 (2.7%)
2	C	0.80	0/229	1.38	2/350 (0.6%)
2	F	0.95	0/229	1.50	2/350 (0.6%)
3	A	0.37	0/4736	0.56	0/6400
3	D	0.44	0/4745	0.61	0/6412
All	All	0.45	0/10285	0.71	15/14040 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	11	DG	O4'-C1'-N9	-8.81	101.83	108.00
1	B	27	DT	O4'-C4'-C3'	-8.50	100.90	106.00
1	E	28	DC	O4'-C4'-C3'	-7.86	101.28	106.00
1	B	25	DA	O4'-C4'-C3'	-7.85	101.29	106.00
1	E	21	DC	O4'-C4'-C3'	-7.00	101.70	104.50
1	E	27	DT	O4'-C4'-C3'	-6.76	101.80	104.50
2	C	11	DG	O4'-C1'-N9	-6.34	103.56	108.00
1	B	26	DC	O4'-C1'-N1	6.21	112.35	108.00
2	C	12	DG	O4'-C1'-N9	6.09	112.26	108.00
1	E	21	DC	P-O3'-C3'	5.91	126.79	119.70
1	E	21	DC	O4'-C1'-N1	5.64	111.95	108.00
2	F	9	DC	O4'-C1'-N1	5.31	111.72	108.00
1	E	26	DC	O4'-C1'-N1	5.11	111.58	108.00
1	E	22	DC	O4'-C1'-N1	-5.07	104.45	108.00
1	B	27	DT	O4'-C1'-N1	5.07	111.55	108.00

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	B	177	0	103	2	0
1	E	177	0	103	4	0
2	C	228	0	127	0	0
2	F	228	0	127	3	0
3	A	4652	0	4707	49	0
3	D	4658	0	4713	29	0
4	G	23	0	21	0	0
4	H	23	0	21	3	0
4	I	23	0	21	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	15	0	0	0	0
6	D	10	0	0	0	0
7	A	27	0	12	7	0
7	D	27	0	12	6	0
8	A	86	0	0	5	0
8	B	5	0	0	0	0
8	C	11	0	0	0	0
8	D	150	0	0	4	0
8	E	10	0	0	0	0
8	F	16	0	0	1	0
All	All	10548	0	9967	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 4.

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)
3:A:830:ASP:OD2	7:A:883:DCT:H5"	1.77	0.85
3:D:867:HIS:HB2	3:D:875:ALA:O	1.81	0.80
3:A:658:GLU:OE2	7:A:883:DCT:H2"	1.85	0.77
3:A:789:ARG:HG2	3:A:792:MET:HE3	1.67	0.77
3:A:608:GLN:O	8:A:88:HOH:O	2.10	0.69
4:H:1:GLC:C1	4:H:2:FRU:O1	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:853:GLU:HG2	3:A:862:LEU:O	1.96	0.64
3:D:843:ARG:HD2	8:D:196:HOH:O	1.97	0.64
3:A:506:GLU:O	3:A:509:GLU:HG2	1.99	0.62
3:A:830:ASP:OD2	7:A:883:DCT:C5'	2.47	0.61
3:D:676:ARG:NH1	8:D:230:HOH:O	2.29	0.61
3:D:656:GLN:HA	7:D:881:DCT:O1B	2.00	0.61
3:A:324:GLU:OE1	8:A:201:HOH:O	2.16	0.60
3:A:421:ALA:O	8:A:51:HOH:O	2.16	0.60
3:D:767:LEU:HD12	3:D:802:ASP:HB3	1.83	0.59
3:A:469:GLU:O	4:H:2:FRU:H61	2.05	0.57
1:B:25:DA:H5''	3:A:578:ARG:NH2	2.19	0.57
3:D:658:GLU:CD	7:D:881:DCT:H2''	2.25	0.57
3:A:440:GLU:HB3	3:A:441:PRO:HD3	1.87	0.56
3:A:524:GLN:HG2	3:A:525:GLU:N	2.20	0.56
3:A:631:GLU:OE2	3:A:635:LYS:HE3	2.06	0.55
3:D:754:VAL:HG13	3:D:776:ILE:HD11	1.91	0.53
3:D:656:GLN:HA	7:D:881:DCT:PB	2.49	0.52
3:A:709:ASN:O	3:A:713:VAL:HG13	2.10	0.52
3:D:848:VAL:HB	3:D:849:PRO:HD3	1.92	0.52
3:A:512:GLY:O	3:A:516:GLN:HG2	2.11	0.51
3:A:754:VAL:HG12	3:A:758:LYS:HE2	1.92	0.51
3:A:680:ASP:HB3	3:A:683:THR:HB	1.92	0.51
3:A:532:LYS:NZ	8:A:268:HOH:O	2.15	0.50
3:A:658:GLU:HB2	3:A:710:TYR:CE1	2.45	0.50
1:E:21:DC:H2'	1:E:22:DC:C6	2.46	0.50
3:A:417:LYS:NZ	3:A:464:GLU:OE2	2.31	0.50
3:A:681:ILE:HA	3:A:684:LYS:HB3	1.94	0.50
3:A:767:LEU:HG	3:A:802:ASP:HB3	1.92	0.50
3:A:658:GLU:HB2	3:A:710:TYR:HE1	1.76	0.49
7:D:881:DCT:O2A	8:D:77:HOH:O	2.19	0.49
3:A:500:LEU:HD21	3:A:591:LEU:HD23	1.94	0.49
3:D:828:VAL:HB	3:D:831:GLU:HG2	1.94	0.48
3:D:646:ASP:O	3:D:838:LYS:HG3	2.13	0.48
3:A:644:GLU:HB2	3:A:647:TRP:CG	2.49	0.48
3:D:484:ILE:O	3:D:488:MET:HG3	2.14	0.48
2:F:3:6OG:H2	7:D:881:DCT:HN41	1.78	0.48
1:B:29:DDG:H2''	7:A:883:DCT:O4'	2.14	0.47
3:D:712:ILE:HA	3:D:716:ILE:HG22	1.96	0.47
3:A:579:GLN:HB2	8:A:162:HOH:O	2.14	0.47
3:A:417:LYS:O	3:A:418:GLN:HB2	2.14	0.47
3:A:656:GLN:HA	7:A:883:DCT:O1B	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:690:PHE:C	3:A:692:VAL:H	2.18	0.47
2:F:9:DC:H2''	2:F:10:DA:C8	2.50	0.46
3:D:642:PRO:HD3	3:D:870:SER:O	2.16	0.46
3:A:789:ARG:HA	3:A:792:MET:HE3	1.99	0.45
3:A:459:ARG:HB3	3:A:460:PRO:HD3	1.99	0.45
3:A:712:ILE:HA	3:A:716:ILE:HG22	1.98	0.45
3:D:780:ASN:OD1	3:D:782:ASN:N	2.50	0.44
3:A:641:VAL:HG12	3:A:871:THR:HG22	2.00	0.44
1:E:28:DC:H2'	1:E:29:DDG:H8	1.98	0.44
3:D:656:GLN:HG2	3:D:682:HIS:CD2	2.53	0.44
3:D:718:ASP:OD2	3:D:719:TYR:N	2.51	0.44
3:D:831:GLU:O	3:D:832:LEU:HD23	2.18	0.44
3:D:423:ARG:HG2	3:D:423:ARG:HH11	1.82	0.43
3:D:598:ALA:HB3	8:D:107:HOH:O	2.17	0.43
3:A:804:ILE:HD12	3:A:830:ASP:HA	1.99	0.43
3:D:446:HIS:O	3:D:450:LYS:HG3	2.18	0.43
3:D:591:LEU:HA	3:D:591:LEU:HD12	1.90	0.43
3:A:690:PHE:O	3:A:692:VAL:N	2.52	0.43
3:A:494:LYS:HD3	3:A:643:SER:HA	2.00	0.42
3:A:768:HIS:NE2	4:H:1:GLC:H5	2.34	0.42
3:A:830:ASP:OD2	7:A:883:DCT:O2A	2.36	0.42
3:A:366:LYS:O	3:A:368:LYS:HD2	2.19	0.42
3:A:702:ARG:O	3:A:706:LYS:HB2	2.19	0.42
2:F:2:DT:O5'	8:F:135:HOH:O	1.99	0.42
3:A:658:GLU:CD	7:A:883:DCT:H2''	2.40	0.42
3:A:534:LEU:HD11	3:A:574:ILE:HD13	2.00	0.42
3:D:614:GLY:HA3	3:D:769:ARG:CD	2.49	0.42
3:D:847:LEU:HD23	3:D:847:LEU:C	2.40	0.42
3:A:414:ALA:HB1	3:A:419:TYR:HB3	2.00	0.42
3:A:654:TYR:HB3	3:A:657:ILE:HB	2.02	0.41
3:A:680:ASP:O	3:A:684:LYS:N	2.52	0.41
1:E:28:DC:H5''	3:D:628:ILE:HG22	2.02	0.41
3:A:568:HIS:O	3:A:571:VAL:HG22	2.21	0.41
3:A:646:ASP:O	3:A:838:LYS:HB2	2.21	0.41
3:A:799:SER:O	3:A:803:ILE:HG13	2.21	0.41
3:D:511:LEU:HA	3:D:511:LEU:HD23	1.75	0.41
3:D:746:VAL:O	3:D:750:MET:HG2	2.20	0.41
1:E:29:DDG:H2''	7:D:881:DCT:O4'	2.21	0.41
3:D:671:LEU:HA	3:D:671:LEU:HD12	1.92	0.40
3:D:475:VAL:HG12	3:D:476:GLU:HG3	2.03	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	
3	A	578/580 (100%)	543 (94%)	32 (6%)	3 (0%)	29	48
3	D	579/580 (100%)	564 (97%)	14 (2%)	1 (0%)	47	68
All	All	1157/1160 (100%)	1107 (96%)	46 (4%)	4 (0%)	41	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	628	ILE
3	A	678	ASP
3	A	691	GLN
3	A	628	ILE

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	
3	A	495/496 (100%)	494 (100%)	1 (0%)	93	98
3	D	496/496 (100%)	496 (100%)	0	100	100
All	All	991/992 (100%)	990 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	827	GLN

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

Mol	Chain	Res	Type
3	A	576	HIS
3	A	759	GLN
3	D	867	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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$
1	DDG	B	29	1,2	17,23,24	1.31	2 (11%)	15,33,36	2.75	3 (20%)
1	DDG	E	29	1,2	17,23,24	1.24	1 (5%)	15,33,36	2.64	4 (26%)
2	6OG	F	3	2	18,25,26	1.60	2 (11%)	20,36,39	2.73	6 (30%)
2	6OG	C	3	2	18,25,26	1.60	1 (5%)	20,36,39	2.89	5 (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
1	DDG	B	29	1,2	-	0/3/18/19	0/3/3/3
1	DDG	E	29	1,2	-	0/3/18/19	0/3/3/3
2	6OG	F	3	2	-	2/5/23/24	0/3/3/3
2	6OG	C	3	2	-	2/5/23/24	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	6OG	C6-N1	5.62	1.41	1.31
2	F	3	6OG	C6-N1	5.47	1.41	1.31
1	B	29	DDG	C6-N1	3.87	1.39	1.33
1	E	29	DDG	C6-N1	3.86	1.39	1.33
1	B	29	DDG	C8-N7	-2.36	1.30	1.34
2	F	3	6OG	C8-N7	-2.35	1.30	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	DDG	C5-C6-N1	-8.21	112.20	123.43
2	C	3	6OG	O6-C6-C5	8.14	127.64	116.01
1	E	29	DDG	C5-C6-N1	-7.39	113.33	123.43
2	F	3	6OG	O6-C6-C5	6.98	125.99	116.01
2	F	3	6OG	C5-C6-N1	-6.16	111.53	123.26
2	C	3	6OG	C5-C6-N1	-6.14	111.57	123.26
2	C	3	6OG	C2-N1-C6	6.10	125.88	116.08
2	F	3	6OG	C2-N1-C6	5.72	125.27	116.08
1	E	29	DDG	C6-N1-C2	5.08	124.01	115.93
1	B	29	DDG	C6-N1-C2	5.02	123.90	115.93
2	C	3	6OG	N3-C2-N1	-3.52	122.53	127.22
1	E	29	DDG	N3-C2-N1	-2.96	123.28	127.22
1	B	29	DDG	C2-N3-C4	-2.91	112.03	115.36
2	F	3	6OG	N3-C2-N1	-2.85	123.42	127.22
2	F	3	6OG	C2-N3-C4	-2.59	112.40	115.36
2	F	3	6OG	O6-C6-N1	2.49	122.48	119.03
1	E	29	DDG	C6-C5-C4	-2.48	118.42	120.80
2	C	3	6OG	C2-N3-C4	-2.27	112.77	115.36

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	6OG	C3'-C4'-C5'-O5'
2	C	3	6OG	O4'-C4'-C5'-O5'
2	F	3	6OG	C3'-C4'-C5'-O5'
2	F	3	6OG	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	29	DDG	1	0
1	E	29	DDG	2	0
2	F	3	6OG	1	0

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$
4	GLC	G	1	4	11,11,12	0.94	0	15,15,17	1.37	2 (13%)
4	FRU	G	2	4	11,12,12	1.22	1 (9%)	10,18,18	0.79	0
4	GLC	H	1	4	11,11,12	0.50	0	15,15,17	1.59	4 (26%)
4	FRU	H	2	4	11,12,12	1.94	2 (18%)	10,18,18	1.23	1 (10%)
4	GLC	I	1	4	11,11,12	1.03	1 (9%)	15,15,17	0.71	0
4	FRU	I	2	4	11,12,12	1.25	1 (9%)	10,18,18	0.80	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	-	0/5/24/24	0/1/1/1
4	GLC	H	1	4	-	2/2/19/22	0/1/1/1
4	FRU	H	2	4	-	1/5/24/24	0/1/1/1
4	GLC	I	1	4	-	2/2/19/22	0/1/1/1
4	FRU	I	2	4	-	3/5/24/24	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2	FRU	O5-C2	4.34	1.50	1.43
4	H	2	FRU	O2-C2	4.10	1.47	1.40
4	I	2	FRU	O2-C2	3.31	1.46	1.40
4	G	2	FRU	O2-C2	2.95	1.45	1.40
4	I	1	GLC	O5-C1	2.18	1.47	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	GLC	C6-C5-C4	-3.13	105.67	113.00
4	G	1	GLC	O5-C5-C6	3.10	112.06	107.20
4	G	1	GLC	C1-C2-C3	3.09	113.46	109.67
4	H	1	GLC	C3-C4-C5	2.76	115.16	110.24
4	H	2	FRU	O5-C5-C6	2.72	116.43	108.85
4	H	1	GLC	O5-C5-C4	2.60	117.16	110.83
4	H	1	GLC	O5-C1-C2	-2.14	107.47	110.77

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	2	FRU	O1-C1-C2-O2
4	H	1	GLC	O5-C5-C6-O6
4	H	1	GLC	C4-C5-C6-O6
4	I	2	FRU	O1-C1-C2-C3
4	I	1	GLC	O5-C5-C6-O6
4	I	1	GLC	C4-C5-C6-O6
4	H	2	FRU	O1-C1-C2-C3
4	I	2	FRU	O1-C1-C2-O5

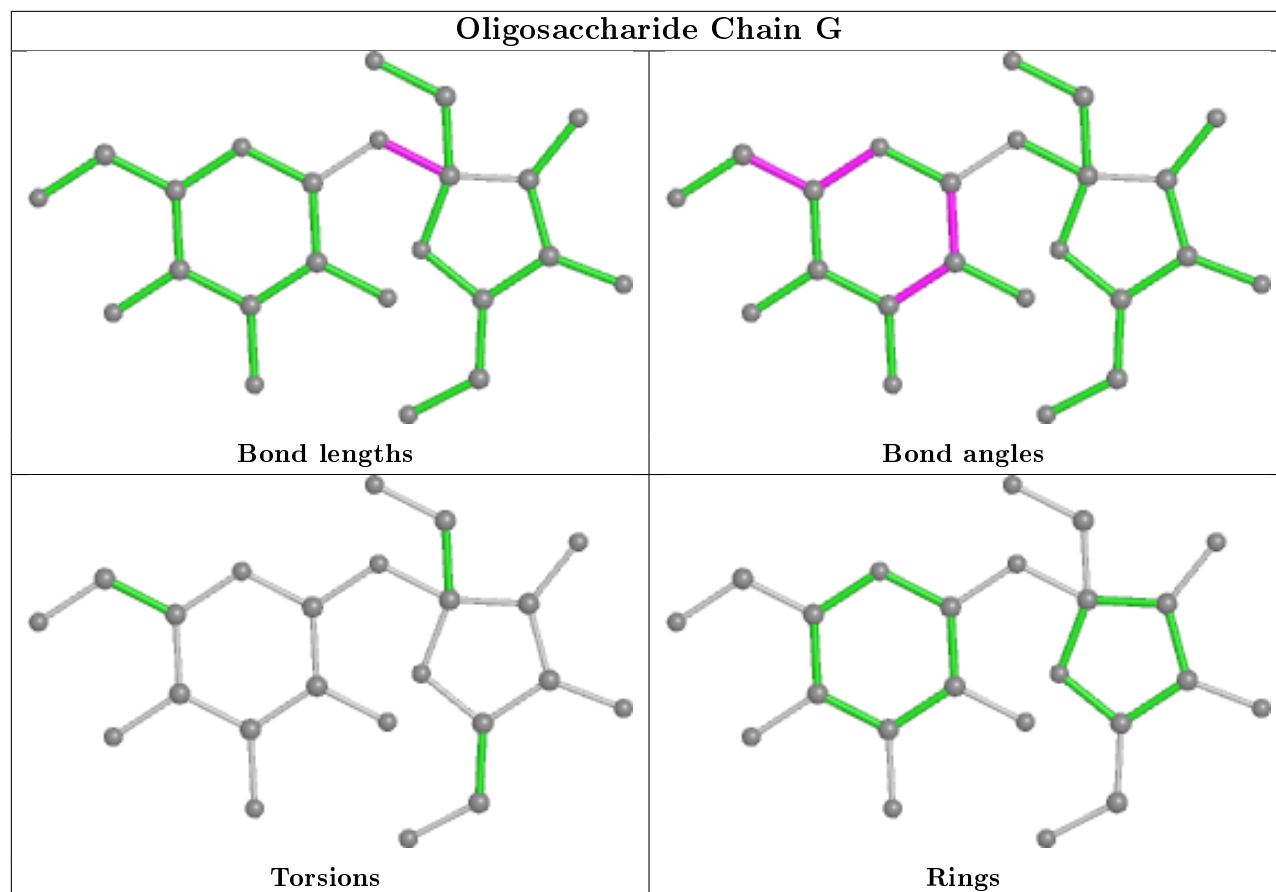
There are no ring outliers.

2 monomers are involved in 3 short contacts:

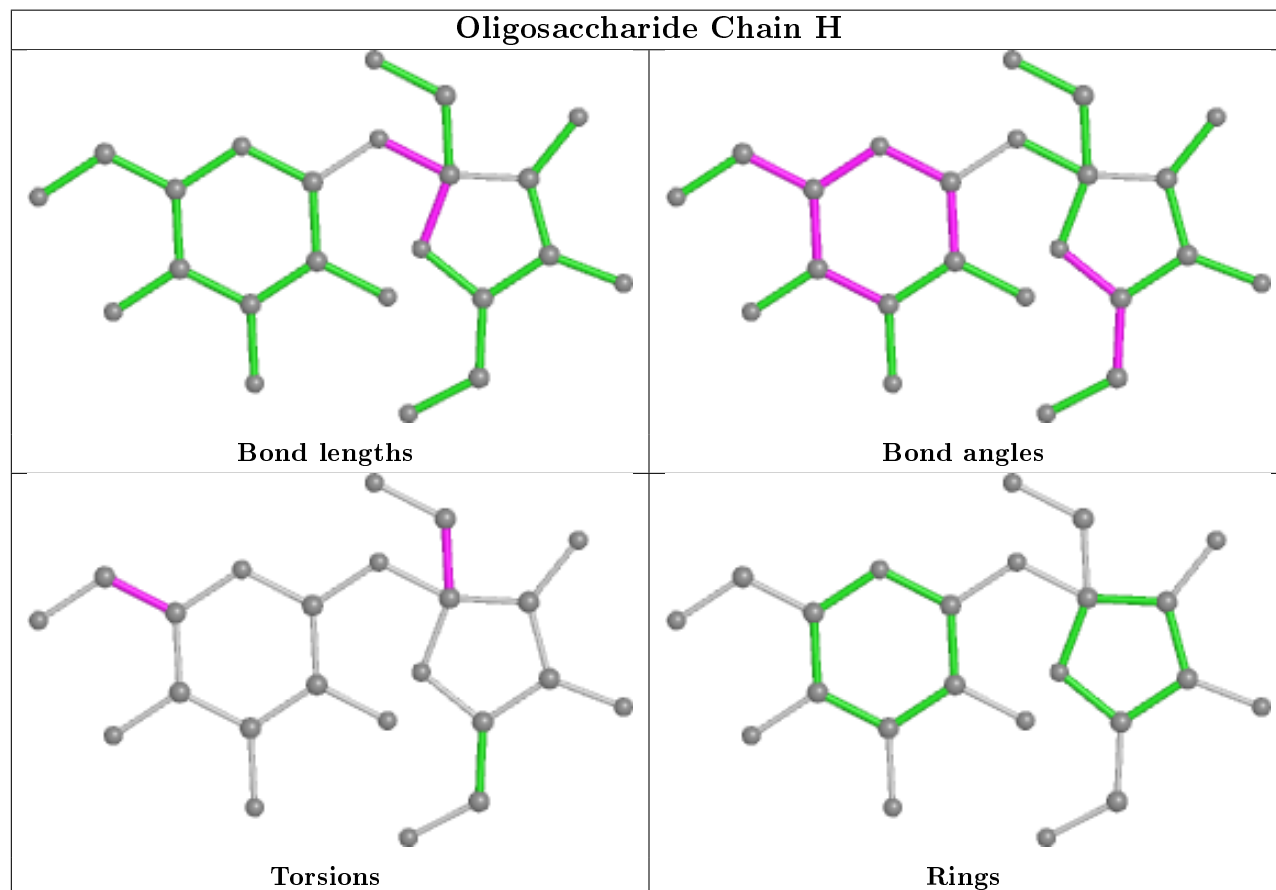
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	2	FRU	2	0
4	H	1	GLC	2	0

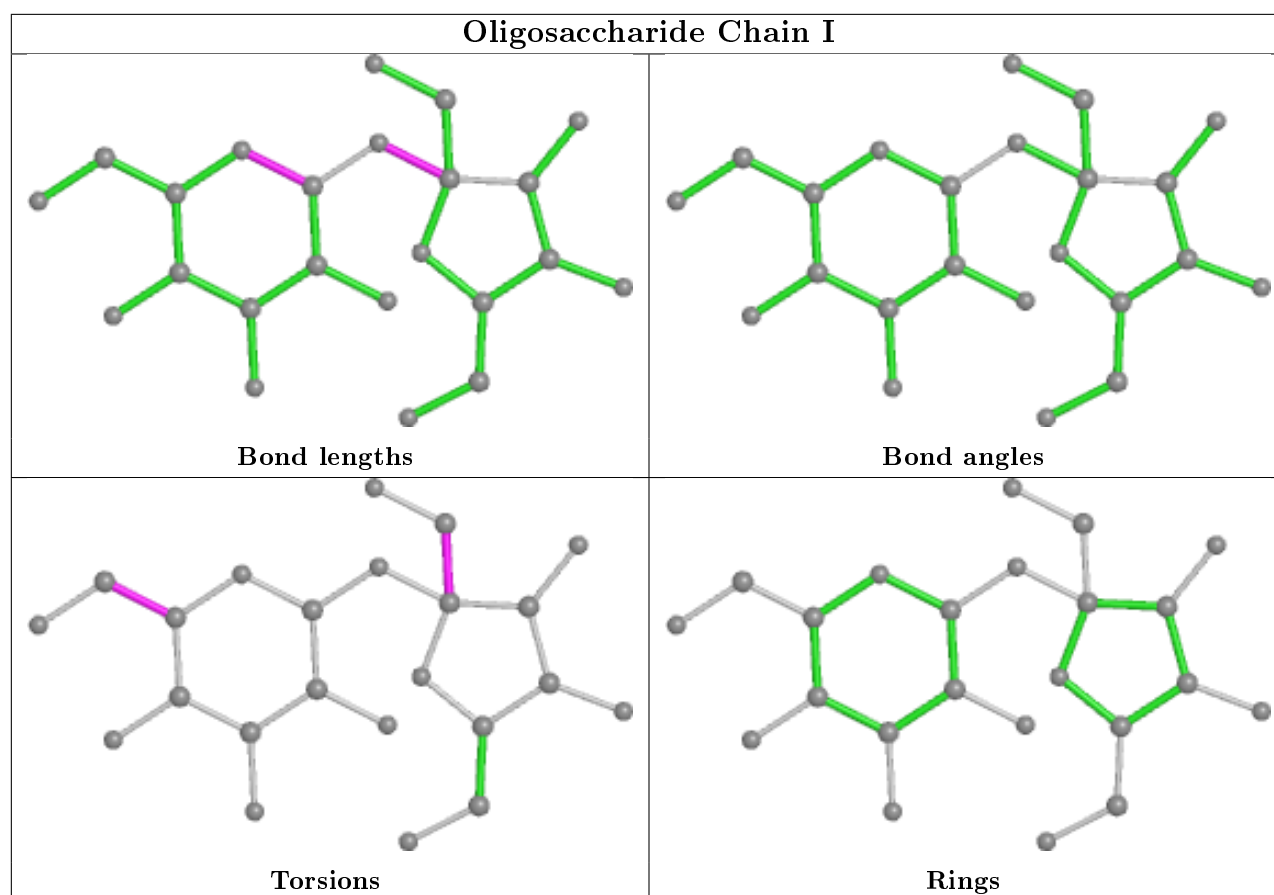
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain G



Oligosaccharide Chain H





5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\# Z > 2$
6	SO4	A	882	-	4,4,4	0.14	0	6,6,6	0.12	0
6	SO4	D	880	-	4,4,4	0.16	0	6,6,6	0.09	0
7	DCT	D	881	5	22,28,28	1.77	3 (13%)	26,43,43	1.45	3 (11%)
6	SO4	A	880	-	4,4,4	0.14	0	6,6,6	0.07	0
7	DCT	A	883	-	22,28,28	1.84	5 (22%)	26,43,43	1.58	5 (19%)
6	SO4	A	881	-	4,4,4	0.11	0	6,6,6	0.25	0
6	SO4	D	879	-	4,4,4	0.11	0	6,6,6	0.28	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	DCT	D	881	5	-	8/19/31/31	0/2/2/2
7	DCT	A	883	-	-	5/19/31/31	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	881	DCT	C6-N1	4.77	1.41	1.35
7	A	883	DCT	C6-N1	4.71	1.41	1.35
7	A	883	DCT	PG-O1G	4.10	1.63	1.50
7	D	881	DCT	C4-N3	3.69	1.41	1.35
7	D	881	DCT	PG-O1G	3.69	1.62	1.50
7	A	883	DCT	C4-N3	3.11	1.40	1.35
7	A	883	DCT	PG-O3G	2.14	1.63	1.54
7	A	883	DCT	O4'-C1'	2.10	1.47	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	883	DCT	C2-N3-C4	3.70	120.09	116.34
7	A	883	DCT	C2'-C1'-N1	-3.58	105.74	112.48
7	D	881	DCT	O2G-PG-O3B	3.17	115.25	104.64
7	D	881	DCT	C2-N3-C4	3.09	119.47	116.34
7	D	881	DCT	C2'-C1'-N1	-2.58	107.63	112.48
7	A	883	DCT	O2G-PG-O3B	2.45	112.86	104.64
7	A	883	DCT	PB-O3B-PG	-2.44	124.45	132.83
7	A	883	DCT	O4'-C4'-C5'	2.40	113.47	109.52

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	881	DCT	PB-O3B-PG-O2G
7	A	883	DCT	C5'-O5'-PA-O2A
7	A	883	DCT	PB-O3A-PA-O5'
7	D	881	DCT	O4'-C4'-C5'-O5'
7	D	881	DCT	PA-O3A-PB-O1B
7	A	883	DCT	C5'-O5'-PA-O3A

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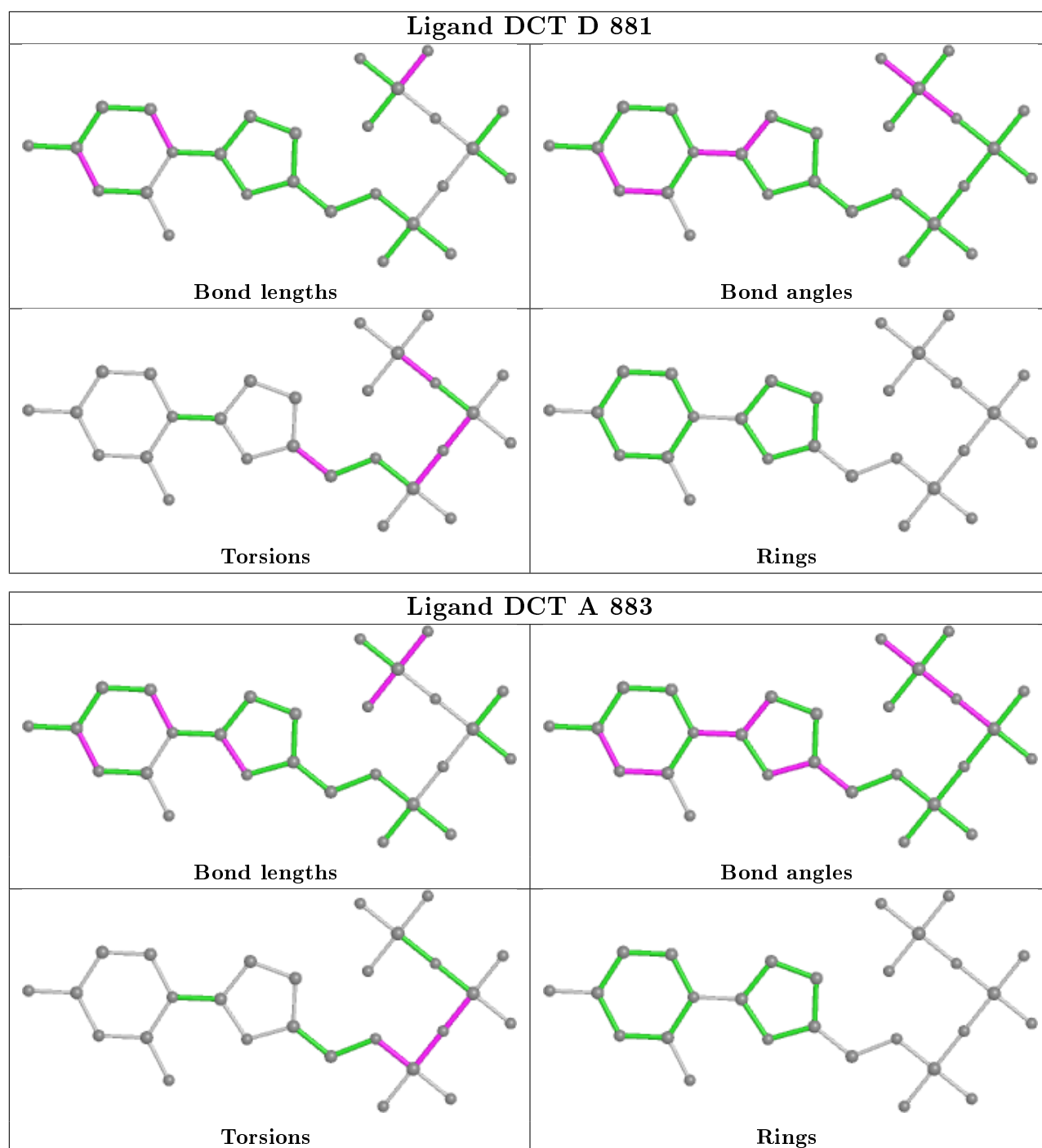
Mol	Chain	Res	Type	Atoms
7	D	881	DCT	PB-O3A-PA-O1A
7	A	883	DCT	C5'-O5'-PA-O1A
7	D	881	DCT	PA-O3A-PB-O2B
7	A	883	DCT	PA-O3A-PB-O2B
7	D	881	DCT	PB-O3A-PA-O2A
7	D	881	DCT	PB-O3B-PG-O1G
7	D	881	DCT	PB-O3B-PG-O3G

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	881	DCT	6	0
7	A	883	DCT	7	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	8/9 (88%)	-0.51	0 100 100	25, 27, 41, 46	0
1	E	8/9 (88%)	-0.72	0 100 100	15, 21, 31, 45	0
2	C	10/13 (76%)	-0.60	0 100 100	19, 24, 31, 62	0
2	F	10/13 (76%)	-0.61	0 100 100	9, 17, 25, 54	0
3	A	580/580 (100%)	0.28	40 (6%) 16 17	20, 37, 67, 91	0
3	D	580/580 (100%)	-0.23	1 (0%) 95 95	6, 21, 40, 52	0
All	All	1196/1204 (99%)	0.01	41 (3%) 45 48	6, 30, 54, 91	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	701	MET	6.1
3	A	688	ASP	5.7
3	A	687	MET	5.2
3	A	707	ALA	5.2
3	A	298	LYS	4.7
3	A	693	SER	4.2
3	A	698	THR	4.0
3	A	695	ASP	3.9
3	A	683	THR	3.8
3	A	696	GLU	3.6
3	A	697	VAL	3.3
3	A	685	THR	3.1
3	A	866	TYR	3.1
3	A	689	ILE	3.1
3	A	306	ARG	3.1
3	A	713	VAL	3.1
3	A	344	PHE	2.9
3	A	690	PHE	2.9
3	A	353	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
3	A	846	ARG	2.6
3	A	311	MET	2.5
3	A	645	SER	2.5
3	A	307	VAL	2.5
3	A	303	LEU	2.4
3	D	689	ILE	2.4
3	A	714	TYR	2.3
3	A	309	GLU	2.3
3	A	704	GLN	2.3
3	A	682	HIS	2.2
3	A	699	PRO	2.2
3	A	843	ARG	2.2
3	A	505	LYS	2.2
3	A	700	ASN	2.2
3	A	305	ASP	2.1
3	A	842	GLU	2.1
3	A	357	PHE	2.1
3	A	342	GLY	2.1
3	A	509	GLU	2.0
3	A	302	THR	2.0
3	A	304	ALA	2.0
3	A	308	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	6OG	C	3	23/24	0.89	0.17	37,44,49,49	0
2	6OG	F	3	23/24	0.95	0.13	25,29,40,41	0
1	DDG	B	29	21/22	0.97	0.13	14,15,22,24	0
1	DDG	E	29	21/22	0.99	0.12	12,13,14,15	0

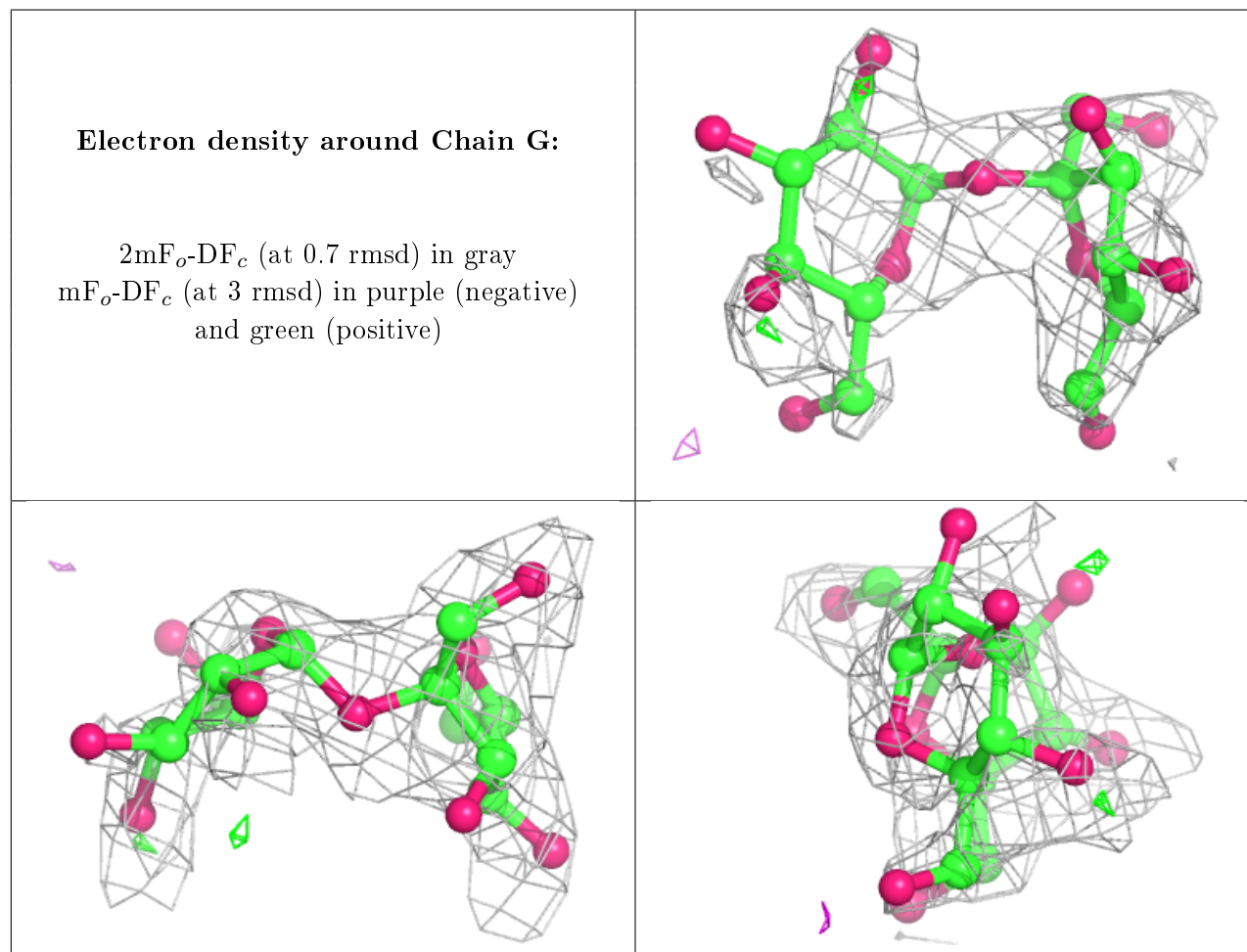
6.3 Carbohydrates ⓘ

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.

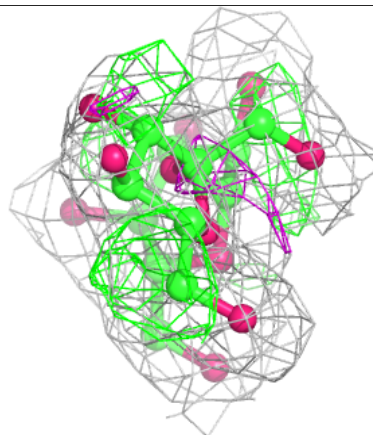
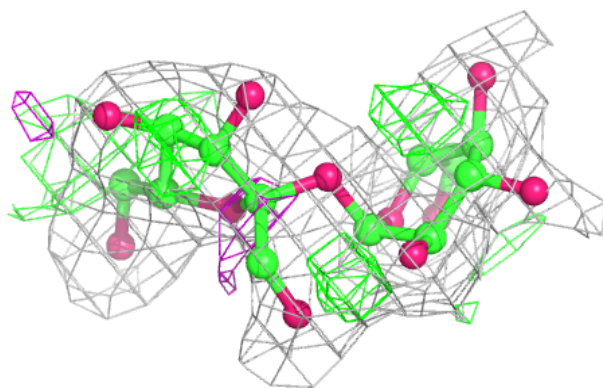
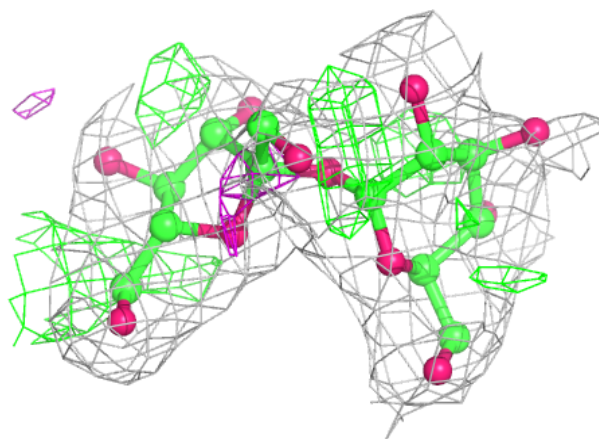
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GLC	G	1	11/12	0.68	0.34	90,91,91,91	0
4	FRU	H	2	12/12	0.71	0.27	39,45,45,46	0
4	FRU	G	2	12/12	0.81	0.23	88,89,90,90	0
4	GLC	H	1	11/12	0.85	0.24	44,45,46,47	0
4	FRU	I	2	12/12	0.86	0.18	52,53,53,54	0
4	GLC	I	1	11/12	0.87	0.27	51,53,53,53	0

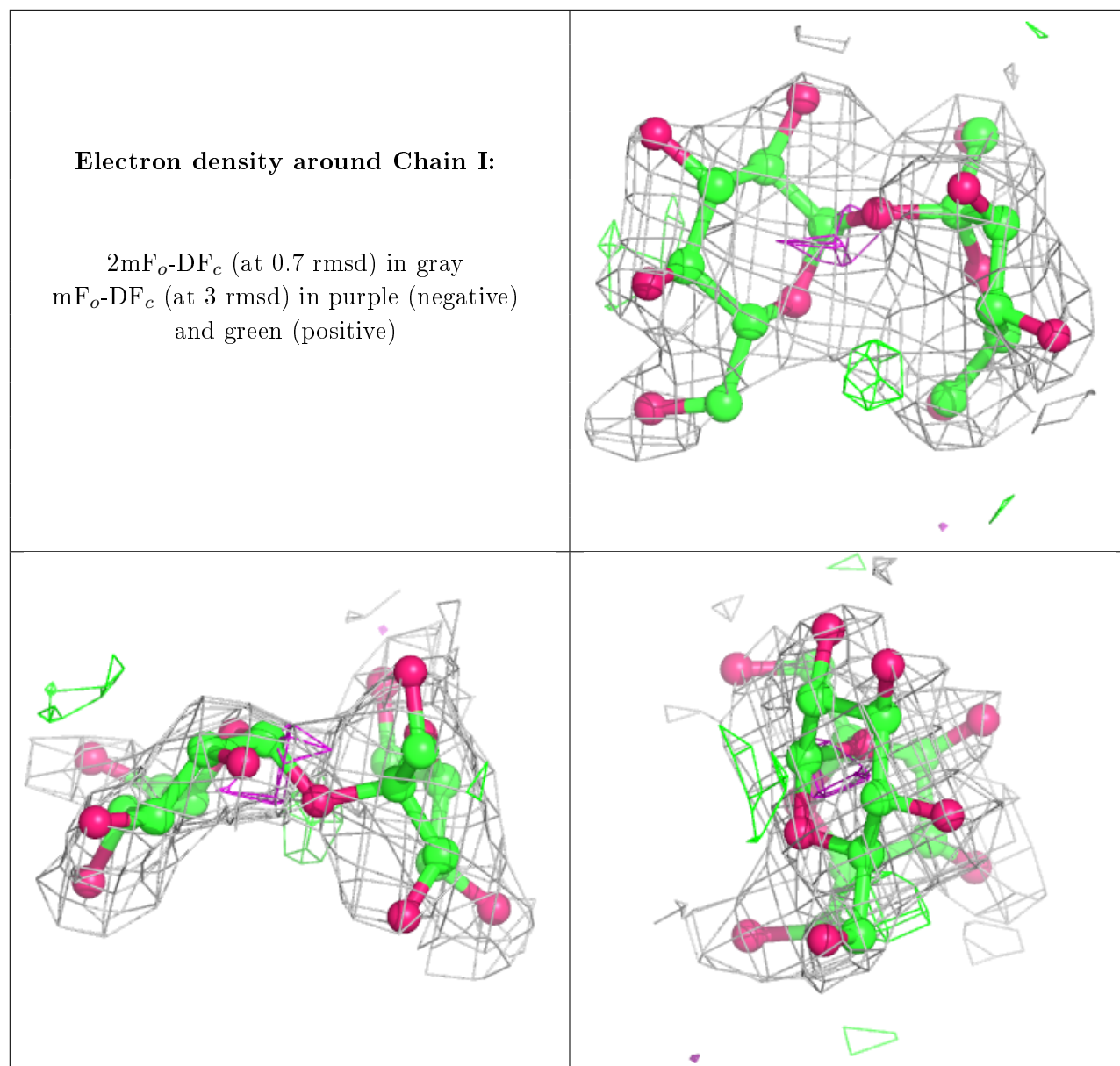
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain H:

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





6.4 Ligands ⓘ

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

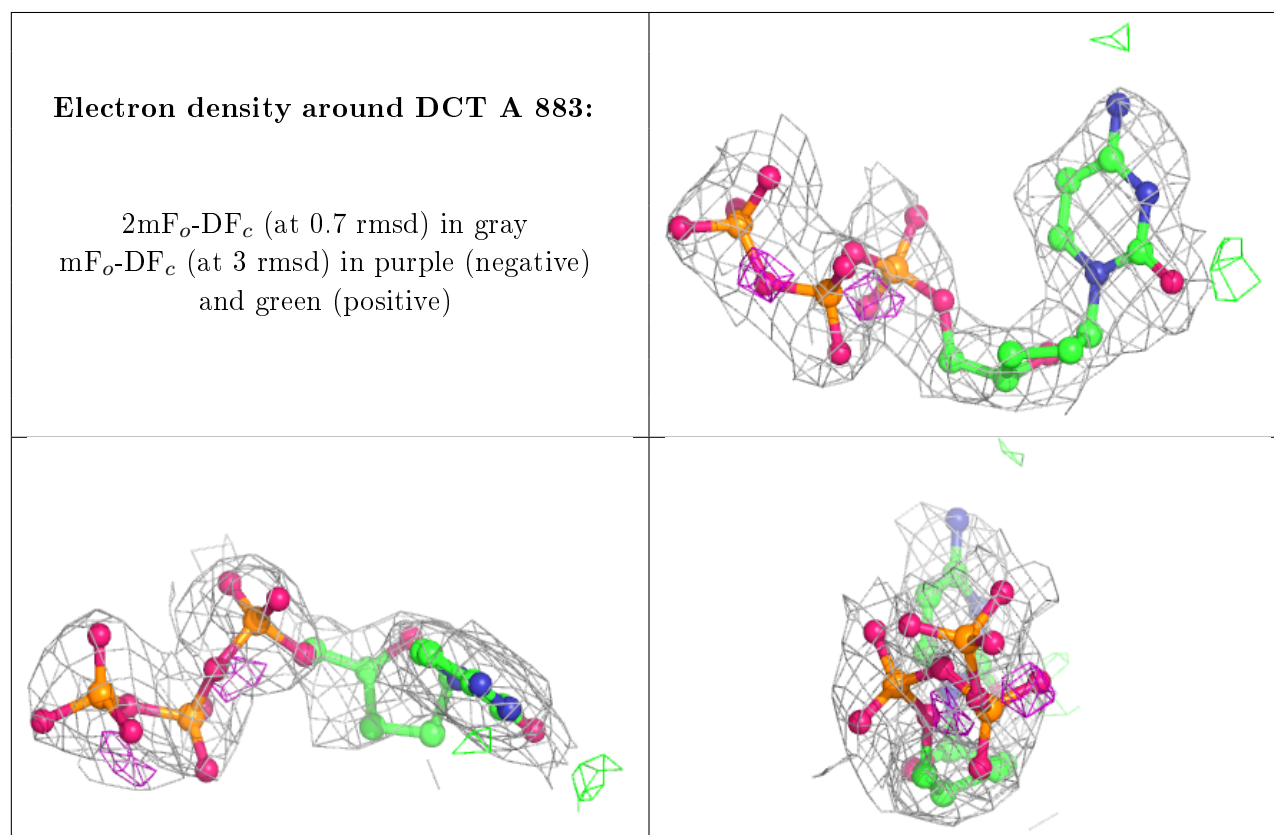
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	A	880	5/5	0.84	0.35	112,112,112,112	0
7	DCT	A	883	27/27	0.89	0.20	56,58,61,61	0
6	SO4	A	882	5/5	0.95	0.20	61,62,62,62	0
6	SO4	D	880	5/5	0.95	0.27	70,70,71,71	0
5	MN	A	879	1/1	0.96	0.04	64,64,64,64	0

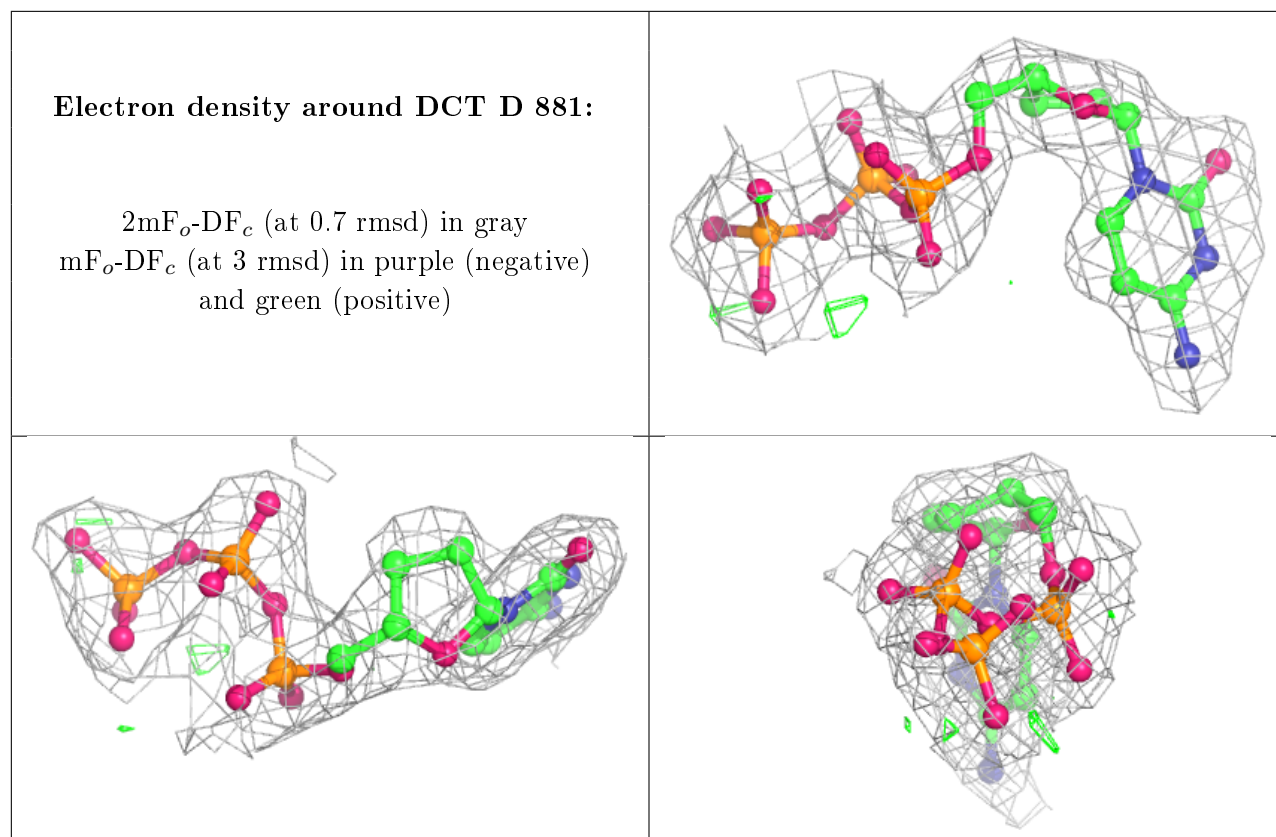
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	SO4	A	881	5/5	0.97	0.12	43,44,44,44	0
7	DCT	D	881	27/27	0.98	0.11	17,19,23,24	0
5	MN	D	878	1/1	0.98	0.09	23,23,23,23	0
6	SO4	D	879	5/5	0.98	0.12	29,30,30,31	0

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.