



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:12 AM UTC

PDB ID : 2HHU / pdb_00002hhu
Title : C:O6-methyl-guanine in the polymerase postinsertion site (-1 basepair position)
Authors : Warren, J.J.; Forsberg, L.J.; Beese, L.S.
Deposited on : 2006-06-28
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

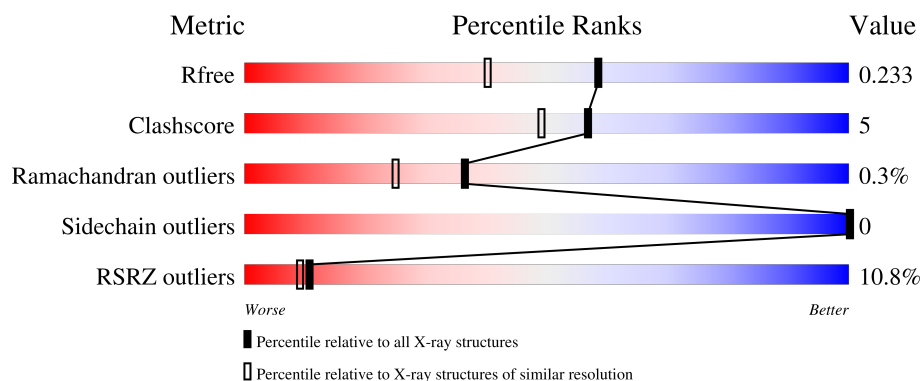
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	B	11	36% 64% 36%
2	C	16	31% 50% 31% 19%
3	A	580	10% 87% 13%
4	D	2	100%
4	E	2	100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5650 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(*GP*CP*GP*AP*TP*CP*AP*GP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	11	Total	C	N	O	P	0	0	0
			220	105	42	63	10			

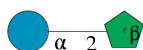
- Molecule 2 is a DNA chain called 5'-D(*GP*TP*AP*CP*(6OG)P*GP*GP*CP*TP*GP*AP*TP*CP*GP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	13	Total	C	N	O	P	0	0	0
			266	127	51	76	12			

- Molecule 3 is a protein called DNA Polymerase I.

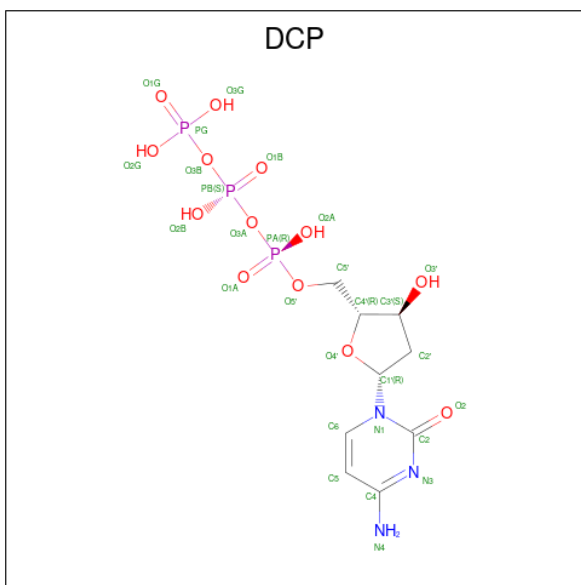
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	580	Total	C	N	O	S	0	0	0
			4650	2956	807	870	17			

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



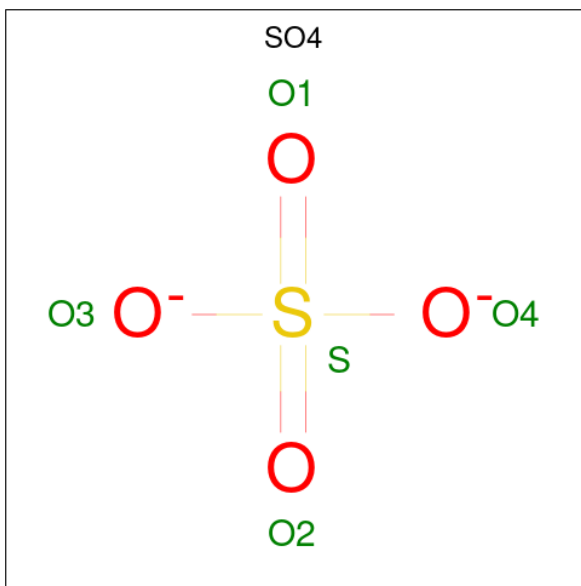
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	D	2	Total	C	O	0	0	0
			23	12	11			
4	E	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (CCD ID: DCP) (formula: C₉H₁₆N₃O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

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

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		

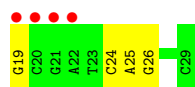
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	13	Total	O	0	0
			13	13		
8	C	15	Total	O	0	0
			15	15		
8	A	391	Total	O	0	0
			391	391		

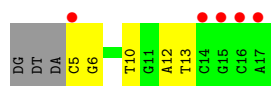
3 Residue-property plots

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

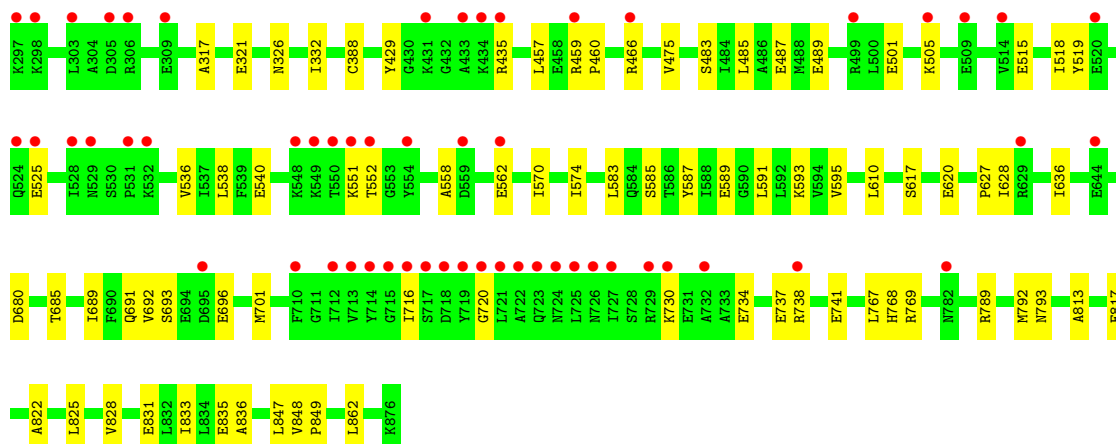
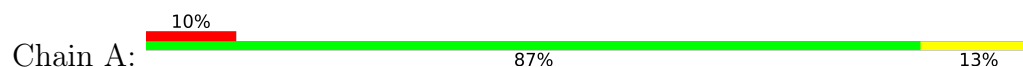
- Molecule 1: 5'-D(*GP*CP*GP*AP*TP*CP*AP*GP*CP*CP*C)-3'



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



- Molecule 3: DNA Polymerase I



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



GLC1
FRU2

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

Chain E:

100%

GLC1
FRU2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.80Å 93.42Å 105.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.2 (50.00-1.80) 94.5 (50.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 1.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.203 , 0.232 0.205 , 0.233	Depositor DCC
R_{free} test set	3928 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	18.1	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5650	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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: MG, GLC, DCP, FRU, 6OG, SO4

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	0.27	0/246	0.62	0/377
2	C	0.29	0/271	0.65	0/414
3	A	0.34	0/4734	0.84	12/6398 (0.2%)
All	All	0.33	0/5251	0.82	12/7189 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	475	VAL	N-CA-C	7.43	118.22	110.72
3	A	680	ASP	N-CA-C	-7.21	98.77	109.15
3	A	321	GLU	N-CA-C	6.73	119.55	109.25
3	A	769	ARG	N-CA-C	-6.47	101.37	110.50
3	A	585	SER	N-CA-C	5.93	117.55	111.14
3	A	847	LEU	N-CA-C	5.78	117.39	111.14
3	A	317	ALA	N-CA-C	-5.74	99.93	109.46
3	A	538	LEU	N-CA-C	5.68	117.27	111.14
3	A	862	LEU	N-CA-C	-5.28	101.10	109.59
3	A	332	ILE	N-CA-C	-5.22	99.73	107.51
3	A	617	SER	N-CA-C	-5.04	101.71	109.52
3	A	793	ASN	N-CA-C	5.00	117.84	111.69

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	220	0	124	4	0
2	C	266	0	149	4	0
3	A	4650	0	4695	41	0
4	D	23	0	21	0	0
4	E	23	0	21	0	0
5	A	28	0	12	0	0
6	A	20	0	0	0	0
7	A	1	0	0	0	0
8	A	391	0	0	2	0
8	B	13	0	0	0	0
8	C	15	0	0	0	0
All	All	5650	0	5022	47	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 5.

All (47) 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)
2:C:12:DA:H2''	2:C:13:DT:H5'	1.62	0.80
3:A:692:VAL:HG21	3:A:701:MET:HE1	1.65	0.78
3:A:813:ALA:O	3:A:817:GLU:HG3	1.89	0.71
3:A:518:ILE:HD13	3:A:574:ILE:HD13	1.72	0.69
3:A:789:ARG:HA	3:A:792:MET:HE3	1.75	0.68
1:B:24:DC:OP1	3:A:552:THR:HG22	1.93	0.68
2:C:12:DA:H2''	2:C:13:DT:C5'	2.24	0.67
3:A:459:ARG:HH12	3:A:466:ARG:NH2	1.94	0.64
1:B:25:DA:H2''	1:B:26:DG:H5'	1.81	0.63
2:C:5:DC:O4'	3:A:720:GLY:HA3	2.01	0.60
3:A:459:ARG:HH12	3:A:466:ARG:CZ	2.14	0.60
3:A:551:LYS:HB3	3:A:551:LYS:NZ	2.16	0.60
3:A:691:GLN:HG3	3:A:738:ARG:HH21	1.68	0.58
3:A:459:ARG:HB3	3:A:460:PRO:HD3	1.85	0.58
3:A:558:ALA:O	3:A:562:GLU:HG3	2.05	0.55
3:A:610:LEU:HD23	3:A:610:LEU:C	2.32	0.55
3:A:730:LYS:O	3:A:734:GLU:HG3	2.07	0.54
3:A:591:LEU:O	3:A:595:VAL:HG23	2.08	0.53
3:A:501:GLU:O	3:A:505:LYS:HG3	2.09	0.52
1:B:19:DG:H2'	1:B:19:DG:N3	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:519:TYR:CD1	3:A:525:GLU:HA	2.45	0.51
3:A:833:ILE:N	3:A:833:ILE:HD12	2.27	0.50
3:A:583:LEU:HD22	3:A:636:ILE:HD11	1.93	0.50
1:B:25:DA:H2''	1:B:26:DG:C5'	2.42	0.50
3:A:536:VAL:O	3:A:540:GLU:HB2	2.12	0.49
3:A:692:VAL:HB	3:A:696:GLU:HB2	1.95	0.47
3:A:483:SER:O	3:A:487:GLU:HG3	2.14	0.47
3:A:737:GLU:O	3:A:741:GLU:HG3	2.14	0.47
3:A:589:GLU:O	3:A:593:LYS:HG3	2.15	0.47
2:C:10:DT:H4'	8:A:3228:HOH:O	2.14	0.46
3:A:570:ILE:O	3:A:574:ILE:HG12	2.15	0.46
3:A:457:LEU:C	3:A:460:PRO:HD2	2.41	0.46
3:A:828:VAL:HB	3:A:831:GLU:CG	2.45	0.46
3:A:515:GLU:HG2	3:A:519:TYR:CE2	2.51	0.46
3:A:685:THR:O	3:A:689:ILE:HG12	2.18	0.44
3:A:587:TYR:CE2	3:A:627:PRO:HD3	2.53	0.43
3:A:767:LEU:O	3:A:768:HIS:HB2	2.18	0.43
3:A:822:ALA:CB	3:A:836:ALA:HB2	2.48	0.43
3:A:848:VAL:HB	3:A:849:PRO:HD3	1.99	0.43
3:A:551:LYS:HB3	3:A:551:LYS:HZ3	1.80	0.42
3:A:825:LEU:HD11	3:A:835:GLU:HB3	2.02	0.42
3:A:326:ASN:HD22	3:A:620:GLU:CD	2.26	0.42
3:A:429:TYR:O	3:A:435:ARG:HA	2.20	0.41
3:A:388:CYS:SG	8:A:3262:HOH:O	2.38	0.41
3:A:457:LEU:O	3:A:460:PRO:HD2	2.22	0.40
3:A:485:LEU:O	3:A:489:GLU:HG3	2.22	0.40
3:A:693:SER:OG	3:A:696:GLU:HG3	2.21	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%)	562 (97%)	14 (2%)	2 (0%)	36 25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	628	ILE
3	A	716	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	495/497 (100%)	495 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	468	ASN
3	A	470	GLN
3	A	510	GLN
3	A	524	GLN
3	A	624	GLN
3	A	656	GLN
3	A	752	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	6OG	C	6	2,1	22,25,26	1.79	2 (9%)	31,36,39	3.00	6 (19%)

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	6OG	C	6	2,1	-	2/9/23/24	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	6	6OG	O6-C6	-6.03	1.25	1.35
2	C	6	6OG	C6-N1	5.03	1.39	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	6OG	O6-C6-C5	10.64	130.00	117.17
2	C	6	6OG	C5-C6-N1	-9.28	111.07	123.49
2	C	6	6OG	C2-N1-C6	6.79	125.41	115.96
2	C	6	6OG	C4-C5-C6	3.38	118.54	115.22
2	C	6	6OG	C6-C5-N7	-2.60	130.77	133.82
2	C	6	6OG	C-O6-C6	2.40	119.45	117.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	6	6OG	N1-C6-O6-C
2	C	6	6OG	C5-C6-O6-C

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GLC	D	1	4	11,11,12	3.29	4 (36%)	15,15,17	1.49	2 (13%)
4	FRU	D	2	4	11,12,12	1.47	1 (9%)	10,18,18	0.83	0
4	GLC	E	1	4	11,11,12	3.31	4 (36%)	15,15,17	1.52	2 (13%)
4	FRU	E	2	4	11,12,12	1.50	1 (9%)	10,18,18	0.71	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	D	1	4	-	0/2/19/22	0/1/1/1
4	FRU	D	2	4	-	0/5/24/24	0/1/1/1
4	GLC	E	1	4	-	1/2/19/22	0/1/1/1
4	FRU	E	2	4	-	1/5/24/24	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	GLC	C2-C3	9.64	1.67	1.52
4	D	1	GLC	C2-C3	9.61	1.67	1.52
4	E	2	FRU	O2-C2	4.22	1.48	1.40
4	D	2	FRU	O2-C2	4.17	1.47	1.40
4	E	1	GLC	O5-C1	2.91	1.48	1.43
4	E	1	GLC	O5-C5	2.77	1.48	1.43
4	D	1	GLC	O5-C5	2.76	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	GLC	O5-C1	2.69	1.48	1.43
4	D	1	GLC	C4-C5	2.40	1.58	1.53
4	E	1	GLC	C4-C5	2.17	1.57	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	GLC	C1-O5-C5	4.10	117.68	112.19
4	E	1	GLC	C1-O5-C5	3.98	117.52	112.19
4	E	1	GLC	C1-C2-C3	-2.91	105.41	109.64
4	D	1	GLC	C1-C2-C3	-2.50	106.01	109.64

There are no chirality outliers.

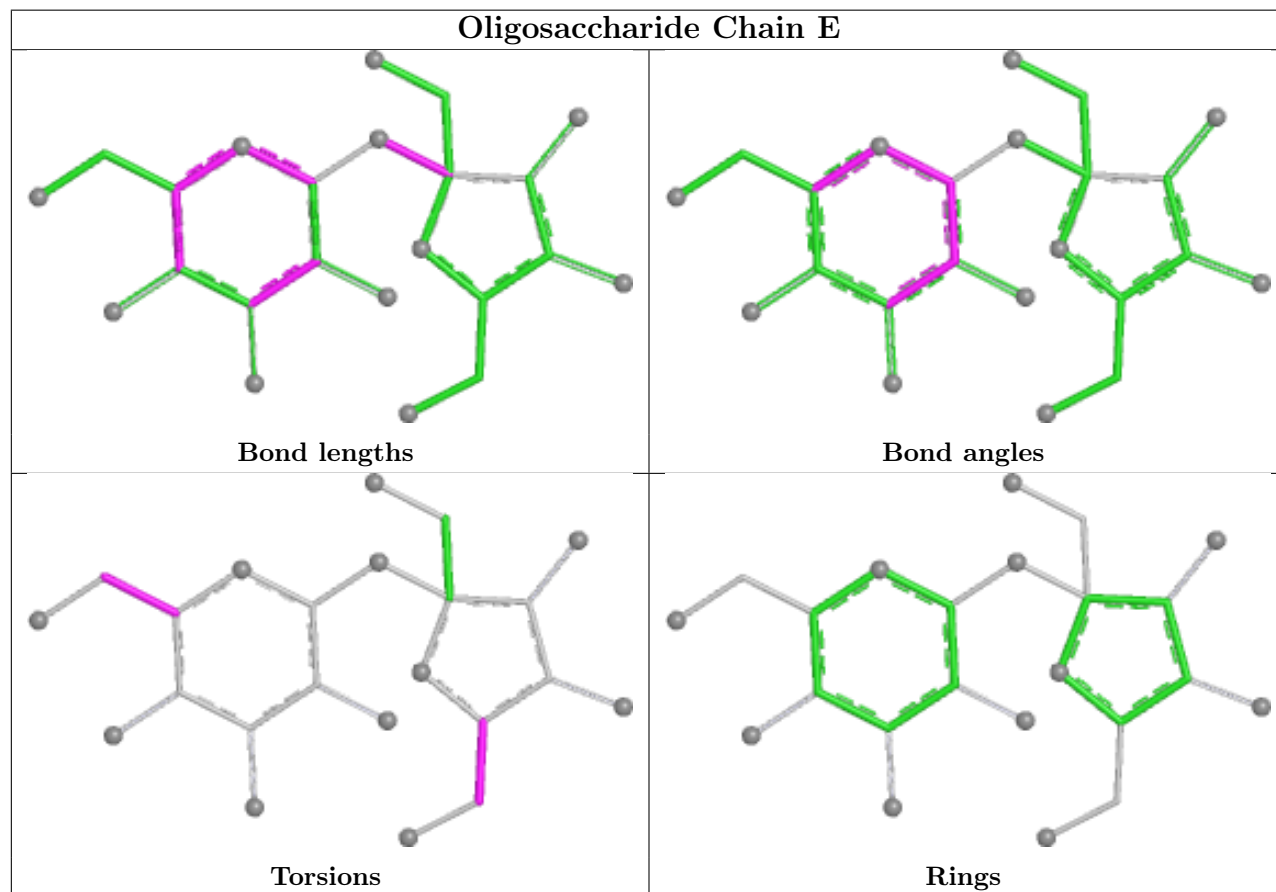
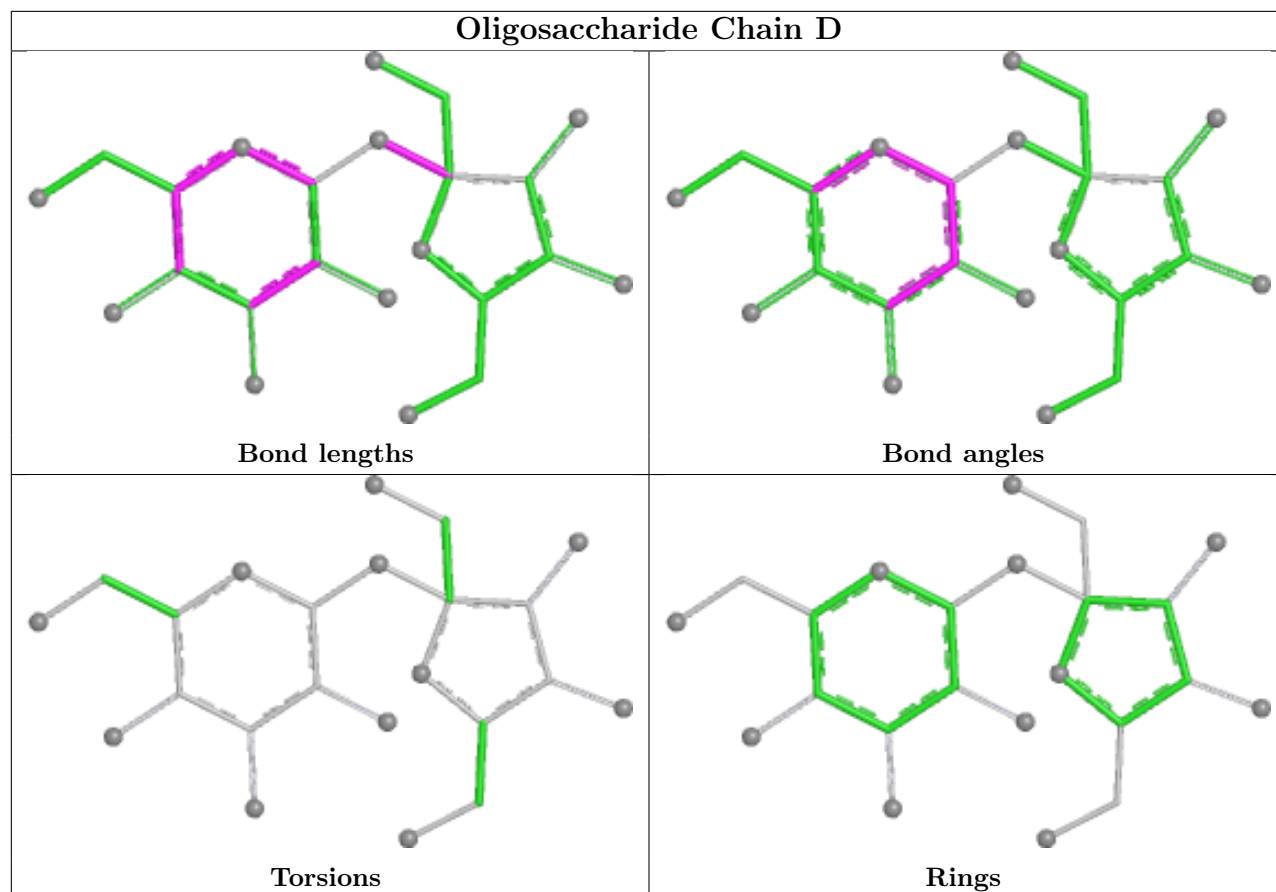
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	GLC	C4-C5-C6-O6
4	E	2	FRU	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	912	-	4,4,4	0.36	0	6,6,6	0.08	0
6	SO4	A	913	-	4,4,4	0.38	0	6,6,6	0.07	0
5	DCP	A	113	-	28,29,29	1.60	7 (25%)	41,45,45	1.38	4 (9%)
6	SO4	A	910	-	4,4,4	0.36	0	6,6,6	0.08	0
6	SO4	A	911	-	4,4,4	0.38	0	6,6,6	0.08	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
5	DCP	A	113	-	-	1/22/34/34	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	113	DCP	C4-N3	3.61	1.41	1.34
5	A	113	DCP	PB-O3B	3.20	1.63	1.59
5	A	113	DCP	O4'-C1'	2.56	1.48	1.42
5	A	113	DCP	C6-C5	2.43	1.40	1.35
5	A	113	DCP	C2-N3	2.42	1.41	1.36
5	A	113	DCP	PB-O3A	2.40	1.62	1.59
5	A	113	DCP	PA-O3A	2.15	1.61	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	113	DCP	O3A-PB-O1B	-4.36	97.60	110.70
5	A	113	DCP	O2B-PB-O3B	3.77	117.47	107.27
5	A	113	DCP	O2B-PB-O3A	-3.77	97.08	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	113	DCP	O2B-PB-O1B	2.71	125.04	112.44

There are no chirality outliers.

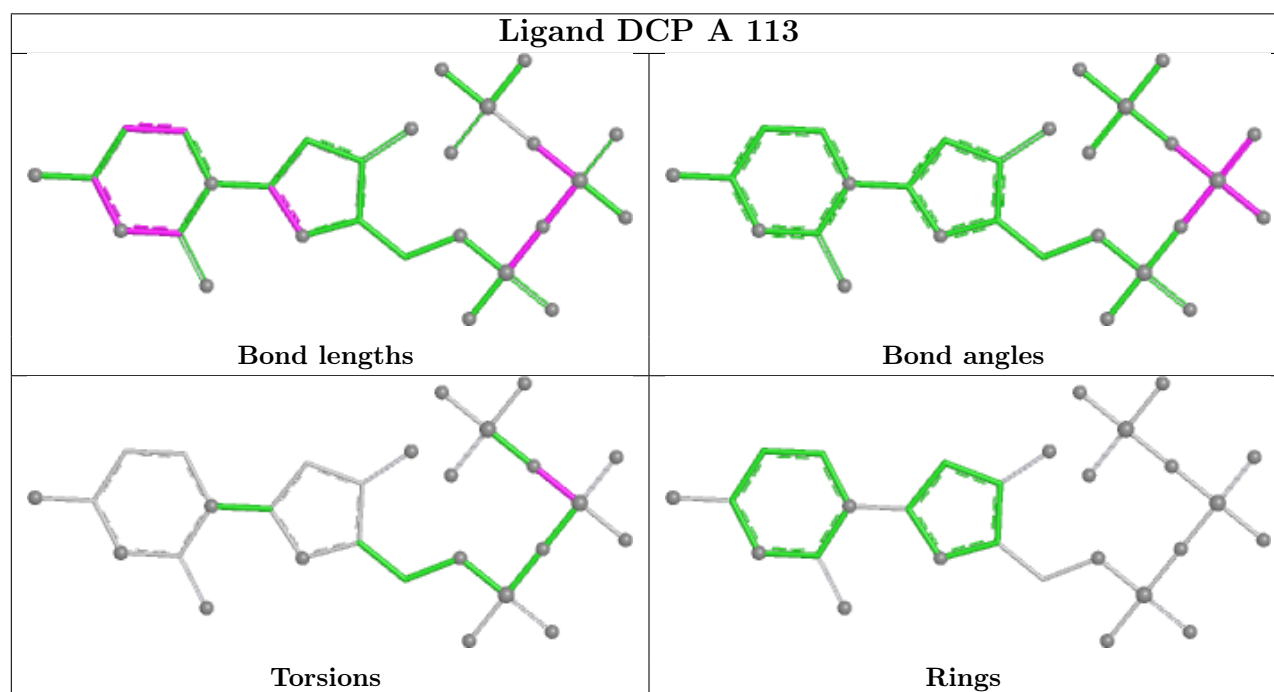
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	113	DCP	PG-O3B-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	11/11 (100%)	1.27	4 (36%) 1 0	18, 31, 63, 68	0
2	C	12/16 (75%)	1.45	5 (41%) 0 0	17, 33, 70, 75	0
3	A	580/580 (100%)	0.34	56 (9%) 13 11	10, 20, 40, 52	0
All	All	603/607 (99%)	0.38	65 (10%) 11 9	10, 20, 42, 75	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	719	TYR	7.1
1	B	19	DG	4.9
3	A	433	ALA	4.9
3	A	297	LYS	4.8
3	A	559	ASP	4.7
3	A	710	PHE	4.6
2	C	17	DA	4.5
3	A	552	THR	4.5
3	A	551	LYS	4.3
3	A	431	LYS	4.3
3	A	716	ILE	4.0
3	A	550	THR	3.9
3	A	714	TYR	3.6
3	A	729	ARG	3.6
3	A	554	TYR	3.5
3	A	730	LYS	3.5
3	A	717	SER	3.5
2	C	16	DC	3.5
3	A	309	GLU	3.4
3	A	720	GLY	3.3
3	A	434	LYS	3.2
3	A	549	LYS	3.1
3	A	738	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	15	DG	3.1
3	A	721	LEU	3.0
3	A	305	ASP	3.0
3	A	435	ARG	3.0
3	A	298	LYS	2.9
3	A	529	ASN	2.8
3	A	718	ASP	2.7
3	A	712	ILE	2.7
3	A	306	ARG	2.7
3	A	723	GLN	2.7
1	B	20	DC	2.7
3	A	531	PRO	2.7
3	A	499	ARG	2.5
3	A	509	GLU	2.5
3	A	732	ALA	2.5
3	A	514	VAL	2.4
3	A	562	GLU	2.4
2	C	5	DC	2.4
3	A	715	GLY	2.4
3	A	505	LYS	2.3
3	A	725	LEU	2.3
3	A	459	ARG	2.3
1	B	21	DG	2.3
1	B	22	DA	2.3
3	A	727	ILE	2.2
3	A	532	LYS	2.2
3	A	726	ASN	2.2
2	C	14	DC	2.2
3	A	629	ARG	2.2
3	A	644	GLU	2.1
3	A	303	LEU	2.1
3	A	520	GLU	2.1
3	A	524	GLN	2.1
3	A	722	ALA	2.1
3	A	528	ILE	2.1
3	A	695	ASP	2.1
3	A	548	LYS	2.0
3	A	724	ASN	2.0
3	A	782	ASN	2.0
3	A	525	GLU	2.0
3	A	466	ARG	2.0
3	A	713	VAL	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	6	23/24	0.90	0.11	22,30,34,35	0

6.3 Carbohydrates ⓘ

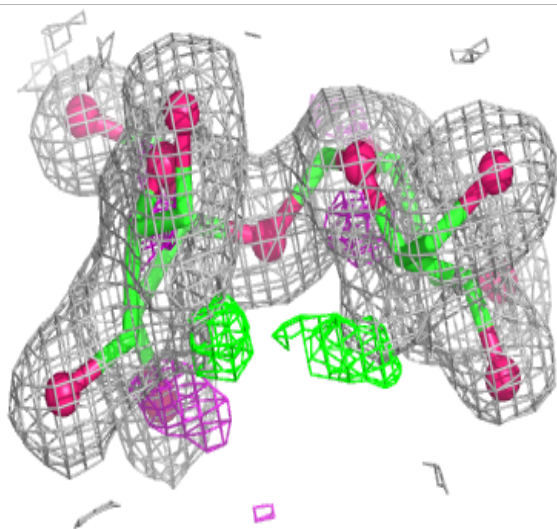
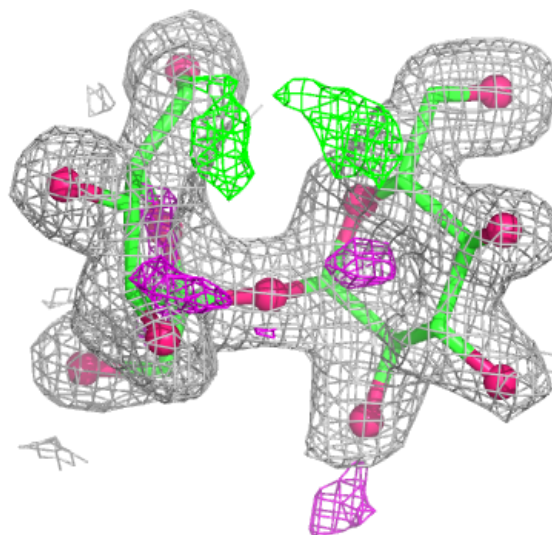
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

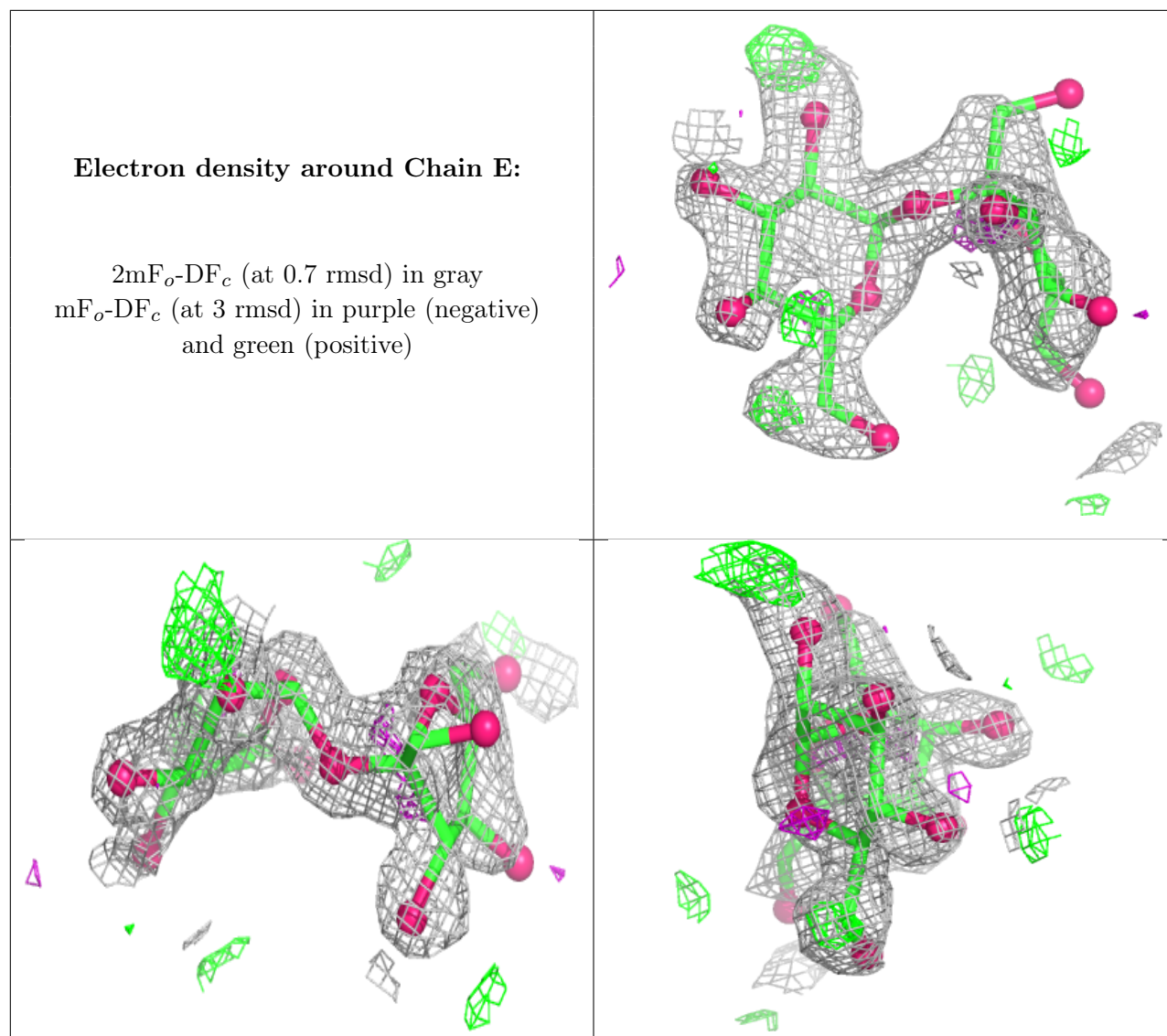
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GLC	E	1	11/12	0.68	0.18	48,51,51,52	0
4	FRU	E	2	12/12	0.73	0.17	53,56,57,59	0
4	GLC	D	1	11/12	0.86	0.11	25,31,33,35	0
4	FRU	D	2	12/12	0.89	0.11	21,27,29,29	0

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 D:

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



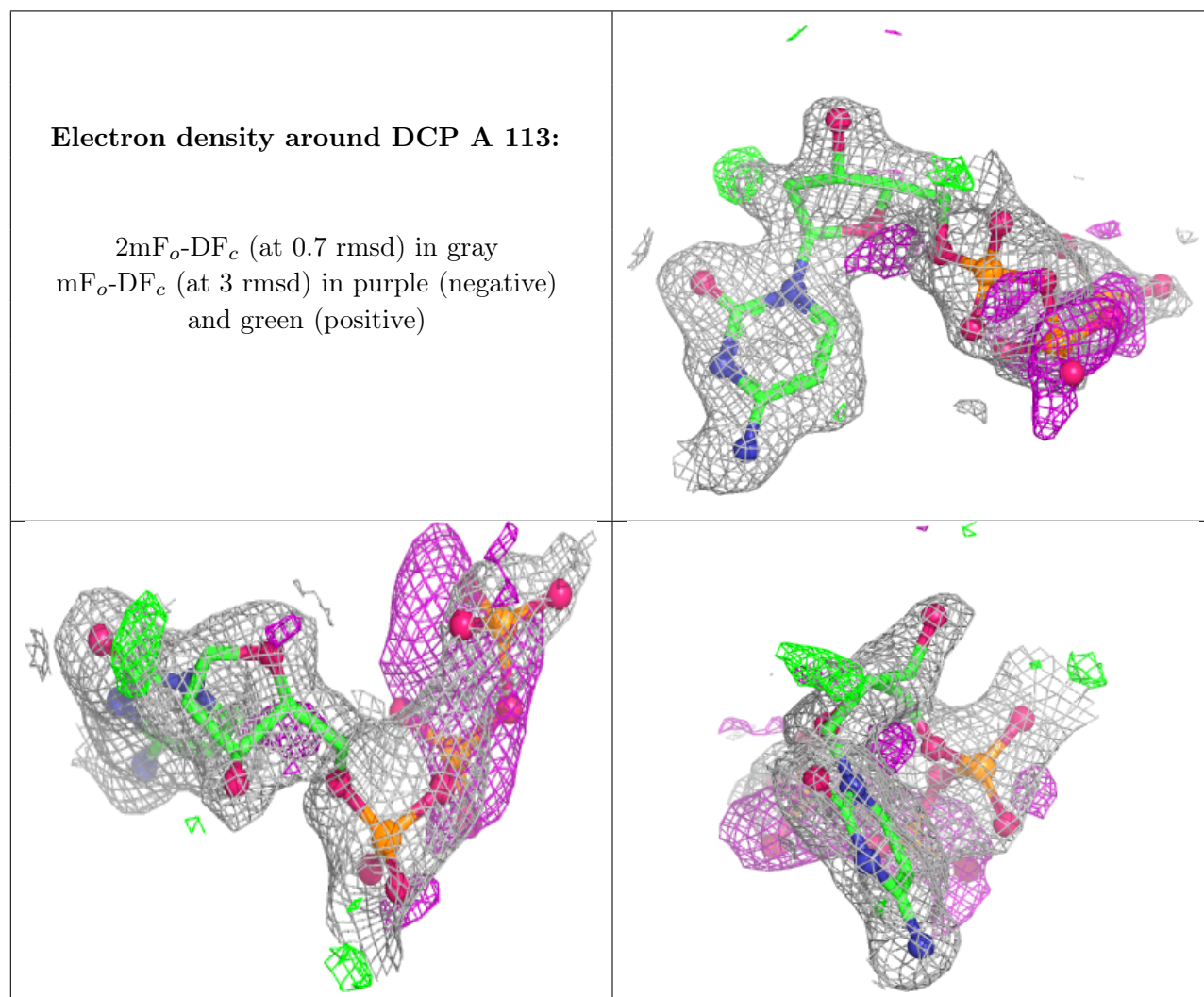


6.4 Ligands [i](#)

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	SO4	A	913	5/5	0.58	0.19	82,82,83,83	0
5	DCP	A	113	28/28	0.81	0.15	18,38,71,71	0
6	SO4	A	910	5/5	0.83	0.13	60,60,60,61	0
6	SO4	A	912	5/5	0.89	0.12	43,44,45,45	0
6	SO4	A	911	5/5	0.93	0.08	42,42,42,43	0
7	MG	A	920	1/1	0.99	0.08	29,29,29,29	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.