



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:57 PM UTC

PDB ID : 2HHS / pdb_00002hhs
Title : O6-methyl:C pair in the polymerase-10 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
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

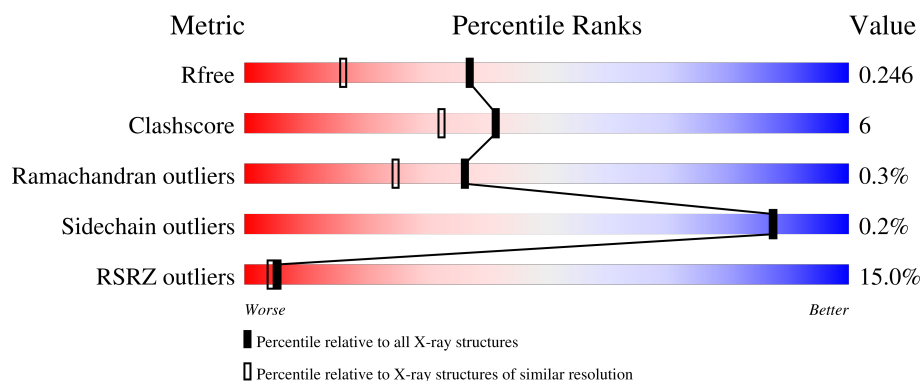
1 Overall quality at a glance

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	13	38% 62% 38%
2	C	14	50% 43% 57%
3	A	580	14% 86% 14%
4	D	2	50% 50%
4	E	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FRU	D	2	X	-	-	-
4	FRU	E	2	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5579 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*AP*TP*(6OG)P*CP*GP*AP*GP*TP*CP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	13	Total	C	N	O	P	0	0	0
			268	128	53	75	12			

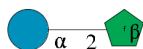
- Molecule 2 is a DNA chain called 5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*GP*CP*AP*TP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	14	Total	C	N	O	P	0	0	0
			281	135	51	82	13			

- 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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

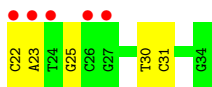
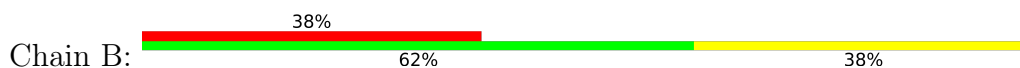
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	11	Total	O	0	0
			11	11		
7	C	19	Total	O	0	0
			19	19		
7	A	288	Total	O	0	0
			288	288		

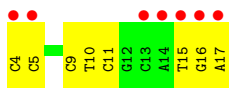
3 Residue-property plots

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.

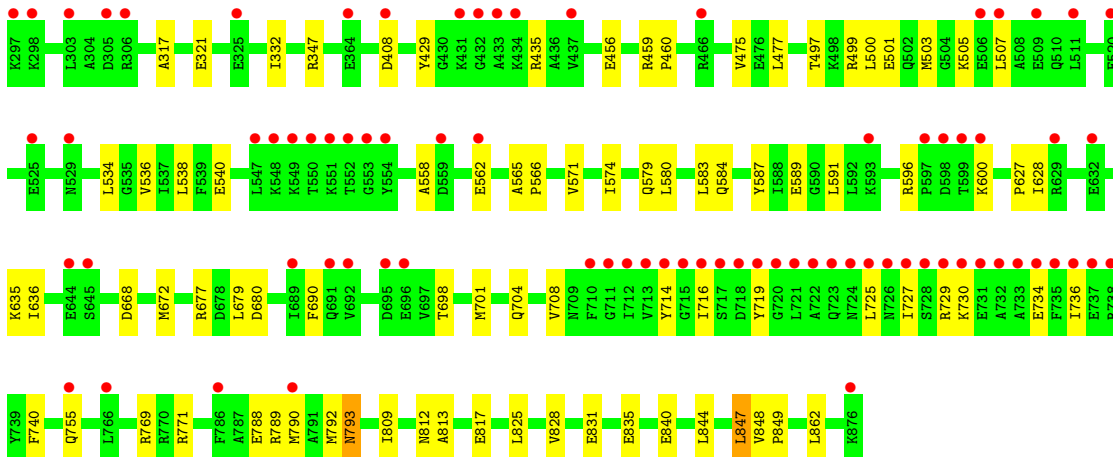
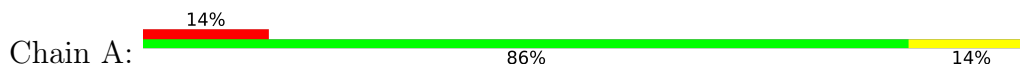
- Molecule 1: 5'-D(*CP*AP*TP*(6OG)P*CP*GP*AP*GP*TP*CP*AP*GP*G)-3'



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



- Molecule 3: DNA polymerase I



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



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

Chain E: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.25Å 93.51Å 105.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.2 (50.00-1.80) 92.2 (50.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.60Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.240 (Not available) , 0.246	Depositor DCC
R_{free} test set	4462 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.744	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 33.1	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	5579	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, FRU, GLC, MG, 6OG

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	0.28	0/274	0.64	0/419
2	C	0.30	0/314	0.69	0/482
3	A	0.34	0/4734	0.85	12/6398 (0.2%)
All	All	0.34	0/5322	0.83	12/7299 (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	7.15	117.94	110.72
3	A	321	GLU	N-CA-C	6.94	119.87	109.25
3	A	680	ASP	N-CA-C	-6.73	99.45	109.15
3	A	769	ARG	N-CA-C	-6.12	101.42	110.48
3	A	538	LEU	N-CA-C	5.86	117.47	111.14
3	A	332	ILE	N-CA-C	-5.83	98.74	107.37
3	A	862	LEU	N-CA-C	-5.72	100.38	109.59
3	A	317	ALA	N-CA-C	-5.62	100.12	109.46
3	A	847	LEU	N-CA-C	5.43	117.00	111.14
3	A	793	ASN	N-CA-C	5.41	118.34	111.69
3	A	347	ARG	N-CA-C	-5.07	103.64	109.93
3	A	571	VAL	N-CA-C	5.02	115.24	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	268	0	149	5	0
2	C	281	0	159	11	0
3	A	4650	0	4695	52	0
4	D	23	0	21	1	0
4	E	23	0	21	3	0
5	A	15	0	0	0	0
6	A	1	0	0	0	0
7	A	288	0	0	1	0
7	B	11	0	0	0	0
7	C	19	0	0	0	0
All	All	5579	0	5045	66	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (66) 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:790:MET:HE3	3:A:790:MET:HA	1.50	0.94
3:A:789:ARG:HA	3:A:792:MET:HE3	1.56	0.85
3:A:771:ARG:NH1	3:A:790:MET:HE2	1.92	0.84
2:C:10:DT:H2''	2:C:11:DC:H5'	1.66	0.77
3:A:840:GLU:O	3:A:844:LEU:HD23	1.94	0.67
2:C:15:DT:H2''	2:C:16:DG:C8	2.30	0.67
2:C:10:DT:H2''	2:C:11:DC:C5'	2.25	0.66
3:A:459:ARG:HB3	3:A:460:PRO:HD3	1.78	0.65
2:C:4:DC:H2'	2:C:5:DC:C6	2.32	0.65
3:A:456:GLU:HG2	7:A:2650:HOH:O	1.95	0.65
3:A:719:TYR:CZ	3:A:729:ARG:HD3	2.34	0.63
3:A:579:GLN:O	3:A:583:LEU:HD13	1.98	0.63
3:A:790:MET:HA	3:A:790:MET:CE	2.27	0.60
3:A:847:LEU:C	3:A:847:LEU:HD23	2.26	0.60
3:A:771:ARG:HH12	3:A:790:MET:HE2	1.68	0.59
3:A:587:TYR:HB3	3:A:636:ILE:HD13	1.86	0.56
3:A:587:TYR:CB	3:A:636:ILE:HD13	2.36	0.56
3:A:690:PHE:CG	3:A:701:MET:HE2	2.41	0.56
3:A:534:LEU:HD11	3:A:574:ILE:HD13	1.87	0.55
1:B:23:DA:H61	2:C:15:DT:H3	1.54	0.55
3:A:714:TYR:HD2	3:A:793:ASN:ND2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:501:GLU:O	3:A:505:LYS:HG3	2.09	0.53
1:B:22:DC:H42	2:C:16:DG:H1	1.57	0.52
3:A:840:GLU:O	3:A:844:LEU:CD2	2.59	0.51
3:A:755:GLN:NE2	4:E:2:FRU:H3	2.25	0.51
2:C:9:DC:H2'	2:C:10:DT:H72	1.92	0.50
3:A:690:PHE:CB	3:A:701:MET:HE2	2.41	0.50
3:A:825:LEU:HD11	3:A:835:GLU:HB3	1.94	0.50
3:A:677:ARG:HB2	3:A:679:LEU:HG	1.93	0.50
2:C:4:DC:H2'	2:C:5:DC:H6	1.75	0.50
3:A:584:GLN:O	3:A:589:GLU:HG3	2.12	0.49
3:A:500:LEU:HD11	3:A:591:LEU:HD23	1.94	0.48
2:C:16:DG:H2''	2:C:17:DA:C8	2.48	0.48
2:C:10:DT:H2'	2:C:11:DC:C6	2.49	0.48
3:A:503:MET:HE1	3:A:635:LYS:C	2.40	0.47
3:A:730:LYS:O	3:A:734:GLU:HG3	2.14	0.47
3:A:729:ARG:HG2	3:A:729:ARG:HH11	1.78	0.47
3:A:408:ASP:HB2	4:D:2:FRU:O1	2.15	0.46
3:A:704:GLN:O	3:A:708:VAL:HG23	2.16	0.46
3:A:565:ALA:N	3:A:566:PRO:HD2	2.31	0.46
3:A:499:ARG:O	3:A:503:MET:HG3	2.16	0.46
3:A:536:VAL:O	3:A:540:GLU:HB2	2.16	0.45
3:A:755:GLN:CD	4:E:2:FRU:H3	2.41	0.45
3:A:788:GLU:OE1	4:E:1:GLC:H4	2.17	0.44
2:C:15:DT:H2''	2:C:16:DG:N7	2.32	0.44
3:A:828:VAL:HB	3:A:831:GLU:CG	2.47	0.44
3:A:848:VAL:HB	3:A:849:PRO:HD3	1.99	0.44
3:A:668:ASP:O	3:A:672:MET:HG3	2.18	0.44
3:A:503:MET:HE1	3:A:635:LYS:O	2.17	0.44
3:A:790:MET:HE3	3:A:790:MET:CA	2.34	0.44
3:A:497:THR:O	3:A:501:GLU:HG3	2.18	0.44
3:A:587:TYR:CE2	3:A:627:PRO:HD3	2.53	0.43
3:A:477:LEU:HD12	3:A:809:ILE:HD12	2.01	0.43
3:A:596:ARG:O	3:A:600:LYS:N	2.51	0.42
3:A:429:TYR:O	3:A:435:ARG:HA	2.19	0.42
1:B:30:DT:H2''	1:B:31:DC:C5'	2.50	0.41
3:A:698:THR:OG1	3:A:701:MET:HG3	2.21	0.41
3:A:719:TYR:CE2	3:A:729:ARG:HD3	2.55	0.41
1:B:22:DC:H2''	1:B:23:DA:H8	1.85	0.41
3:A:736:ILE:HG22	3:A:740:PHE:CE2	2.55	0.41
3:A:725:LEU:O	3:A:727:ILE:HG23	2.21	0.41
1:B:30:DT:H2''	1:B:31:DC:O5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:507:LEU:CD1	3:A:580:LEU:HD22	2.51	0.40
3:A:558:ALA:O	3:A:562:GLU:HG3	2.22	0.40
3:A:729:ARG:HG2	3:A:729:ARG:NH1	2.37	0.40
3:A:813:ALA:O	3:A:817:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	560 (97%)	16 (3%)	2 (0%)	36 25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	716	ILE
3	A	628	ILE

5.3.2 Protein sidechains [i](#)

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%)	494 (100%)	1 (0%)	87 87

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

Mol	Chain	Res	Type
3	A	812	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	341	HIS
3	A	405	GLN
3	A	524	GLN
3	A	576	HIS
3	A	579	GLN
3	A	624	GLN
3	A	755	GLN
3	A	768	HIS
3	A	793	ASN
3	A	797	GLN
3	A	867	HIS

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	$\# Z > 2$
1	6OG	B	25	1,2	22,25,26	1.83	2 (9%)	31,36,39	2.82	5 (16%)

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	6OG	B	25	1,2	-	0/9/23/24	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	25	6OG	O6-C6	-6.16	1.25	1.35
1	B	25	6OG	C6-N1	5.43	1.40	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	6OG	C5-C6-N1	-9.16	111.24	123.49
1	B	25	6OG	O6-C6-C5	8.87	127.87	117.17
1	B	25	6OG	C2-N1-C6	6.68	125.25	115.96
1	B	25	6OG	C4-C5-C6	3.78	118.93	115.22
1	B	25	6OG	C6-C5-N7	-3.01	130.29	133.82

There are no chirality outliers.

There are no torsion outliers.

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	3.35	4 (36%)	15,15,17	1.52	2 (13%)
4	FRU	D	2	4	11,12,12	1.52	2 (18%)	10,18,18	1.04	1 (10%)
4	GLC	E	1	4	11,11,12	3.26	4 (36%)	15,15,17	1.55	3 (20%)
4	FRU	E	2	4	11,12,12	1.72	3 (27%)	10,18,18	3.41	2 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLC	D	1	4	-	0/2/19/22	0/1/1/1
4	FRU	D	2	4	2/2/4/4	0/5/24/24	0/1/1/1
4	GLC	E	1	4	-	0/2/19/22	0/1/1/1
4	FRU	E	2	4	2/2/4/4	2/5/24/24	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	GLC	C2-C3	9.80	1.67	1.52
4	E	1	GLC	C2-C3	9.45	1.67	1.52
4	E	2	FRU	C1-C2	3.98	1.61	1.52
4	D	2	FRU	O2-C2	3.97	1.47	1.40
4	E	1	GLC	O5-C1	2.90	1.48	1.43
4	D	1	GLC	O5-C1	2.79	1.48	1.43
4	D	1	GLC	O5-C5	2.67	1.48	1.43
4	E	2	FRU	O2-C2	2.58	1.45	1.40
4	E	1	GLC	O5-C5	2.45	1.48	1.43
4	E	1	GLC	C4-C5	2.45	1.58	1.53
4	D	1	GLC	C4-C5	2.35	1.58	1.53
4	D	2	FRU	C1-C2	2.32	1.57	1.52
4	E	2	FRU	C4-C5	2.01	1.58	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2	FRU	O2-C2-O5	10.08	128.67	109.33
4	D	1	GLC	C1-O5-C5	3.80	117.28	112.19
4	E	1	GLC	C1-O5-C5	3.75	117.21	112.19
4	E	1	GLC	C1-C2-C3	-3.23	104.95	109.64
4	D	1	GLC	C1-C2-C3	-3.06	105.19	109.64
4	E	2	FRU	O1-C1-C2	3.05	118.41	111.67
4	D	2	FRU	O2-C2-O5	-2.28	104.94	109.33
4	E	1	GLC	O3-C3-C2	-2.07	105.82	110.05

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	2	FRU	C4

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Mol	Chain	Res	Type	Atom
4	D	2	FRU	C3
4	E	2	FRU	C5
4	E	2	FRU	C2

All (2) torsion outliers are listed below:

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

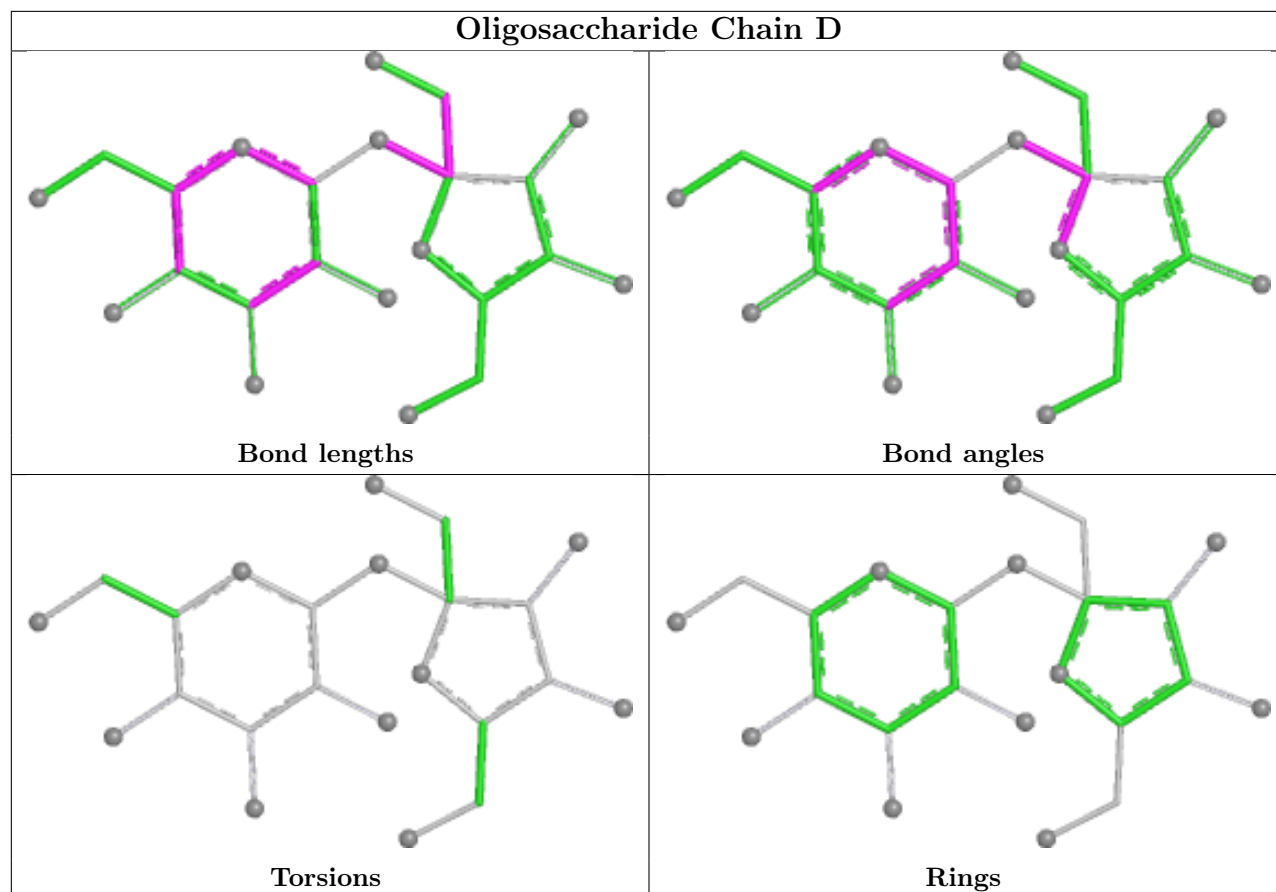
There are no ring outliers.

3 monomers are involved in 4 short contacts:

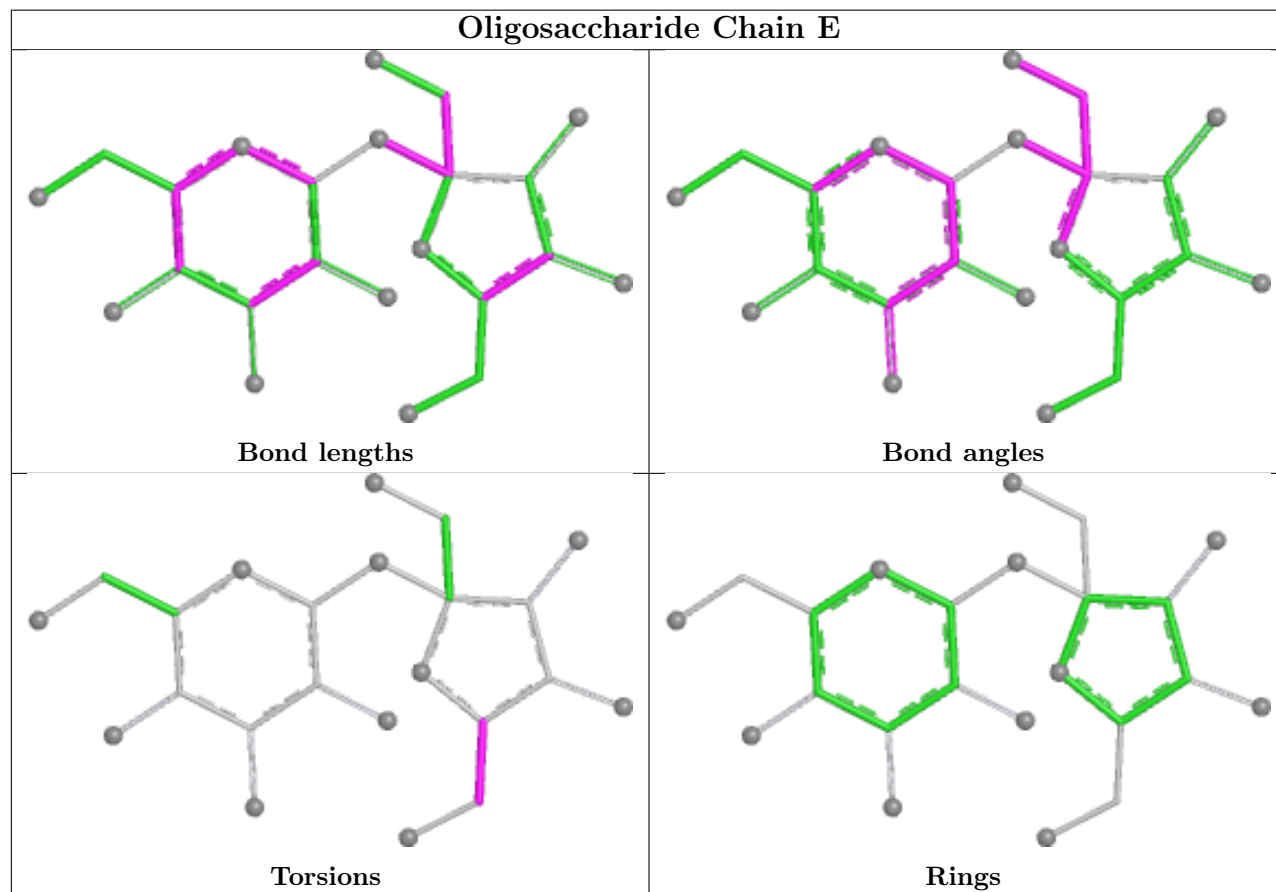
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	FRU	2	0
4	D	2	FRU	1	0
4	E	1	GLC	1	0

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

Oligosaccharide Chain D



Oligosaccharide Chain E



5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z > 2$
5	SO4	A	911	-	4,4,4	0.35	0	6,6,6	0.07	0
5	SO4	A	912	-	4,4,4	0.35	0	6,6,6	0.11	0
5	SO4	A	910	-	4,4,4	0.36	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	12/13 (92%)	1.06	5 (41%) 0 0	26, 31, 70, 72	0
2	C	14/14 (100%)	1.96	7 (50%) 0 0	24, 40, 71, 72	0
3	A	580/580 (100%)	0.70	79 (13%) 7 5	17, 27, 51, 63	0
All	All	606/607 (99%)	0.73	91 (15%) 5 4	17, 27, 53, 72	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	716	ILE	12.8
3	A	714	TYR	7.8
3	A	719	TYR	7.5
3	A	713	VAL	6.6
3	A	559	ASP	6.4
3	A	715	GLY	6.2
3	A	717	SER	6.1
2	C	17	DA	5.9
3	A	712	ILE	5.3
3	A	720	GLY	5.2
3	A	552	THR	5.1
3	A	723	GLN	4.6
3	A	433	ALA	4.6
3	A	730	LYS	4.5
3	A	718	ASP	4.5
3	A	732	ALA	4.5
3	A	721	LEU	4.5
2	C	16	DG	4.3
3	A	876	LYS	4.3
3	A	728	SER	4.3
3	A	722	ALA	4.2
3	A	689	ILE	4.0
3	A	729	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
3	A	554	TYR	3.8
3	A	727	ILE	3.8
3	A	297	LYS	3.8
1	B	22	DC	3.8
3	A	305	ASP	3.6
3	A	551	LYS	3.6
3	A	431	LYS	3.6
3	A	735	PHE	3.6
3	A	529	ASN	3.3
3	A	434	LYS	3.3
3	A	629	ARG	3.3
3	A	733	ALA	3.3
3	A	550	THR	3.3
3	A	509	GLU	3.2
3	A	520	GLU	3.2
2	C	5	DC	3.1
1	B	23	DA	3.1
3	A	710	PHE	3.1
3	A	736	ILE	3.0
3	A	734	GLU	3.0
2	C	4	DC	3.0
3	A	506	GLU	3.0
3	A	726	ASN	3.0
2	C	15	DT	2.9
3	A	691	GLN	2.9
3	A	553	GLY	2.8
3	A	599	THR	2.8
3	A	738	ARG	2.8
3	A	598	ASP	2.8
3	A	731	GLU	2.7
3	A	737	GLU	2.7
3	A	692	VAL	2.7
3	A	364	GLU	2.7
3	A	711	GLY	2.6
1	B	24	DT	2.6
3	A	755	GLN	2.5
3	A	525	GLU	2.4
2	C	13	DC	2.4
3	A	306	ARG	2.4
2	C	14	DA	2.4
3	A	695	ASP	2.4
3	A	593	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
3	A	507	LEU	2.3
3	A	644	GLU	2.3
1	B	27	DG	2.3
3	A	725	LEU	2.3
3	A	786	PHE	2.3
3	A	724	ASN	2.3
3	A	549	LYS	2.3
3	A	562	GLU	2.3
1	B	26	DC	2.3
3	A	511	LEU	2.3
3	A	298	LYS	2.3
3	A	696	GLU	2.2
3	A	790	MET	2.2
3	A	547	LEU	2.2
3	A	432	GLY	2.2
3	A	632	GLU	2.2
3	A	437	VAL	2.2
3	A	408	ASP	2.2
3	A	766	LEU	2.2
3	A	600	LYS	2.2
3	A	645	SER	2.1
3	A	303	LEU	2.1
3	A	548	LYS	2.1
3	A	325	GLU	2.1
3	A	597	PRO	2.0
3	A	466	ARG	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, 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
1	6OG	B	25	23/24	0.72	0.20	57,59,70,71	0

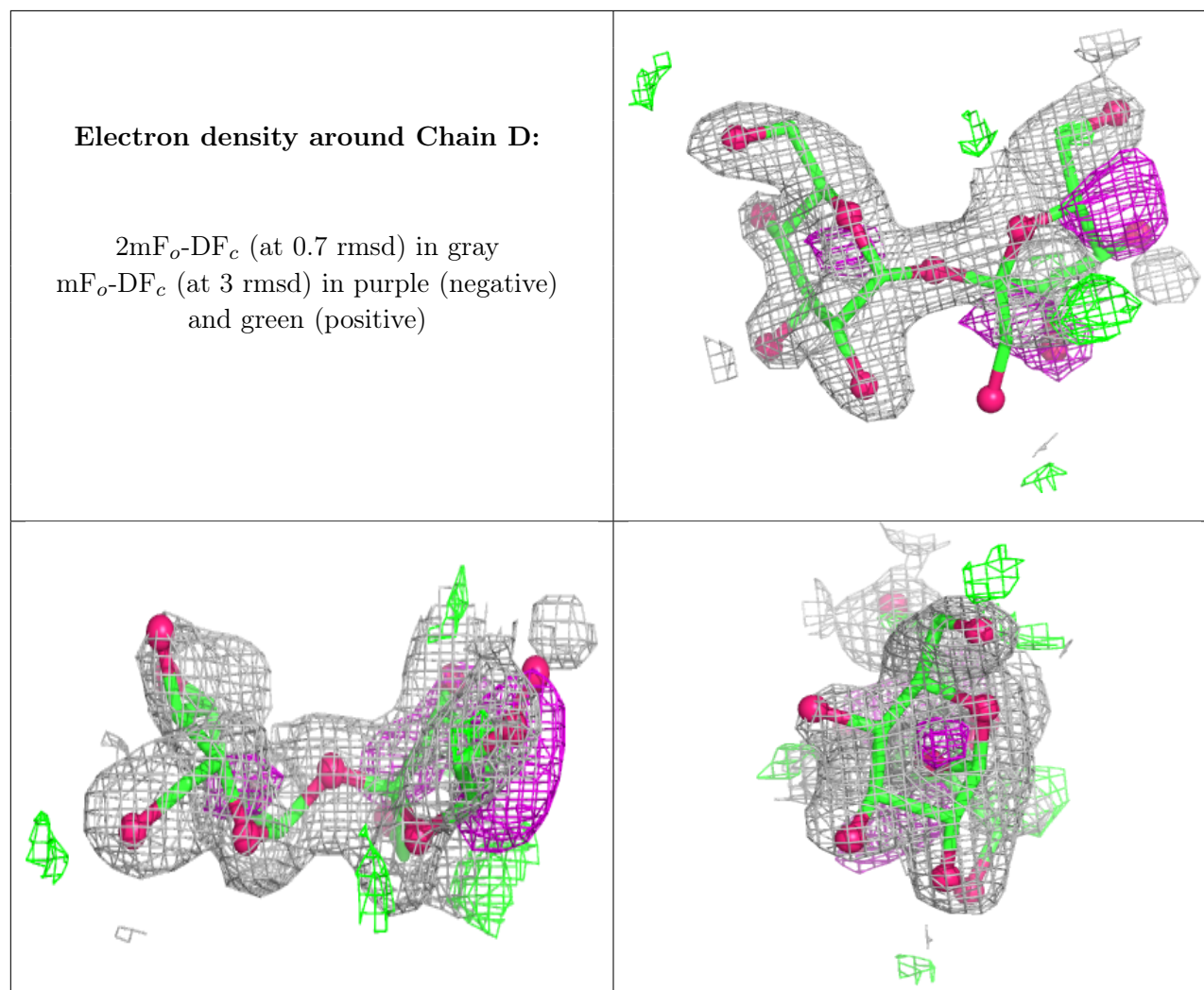
6.3 Carbohydrates [i](#)

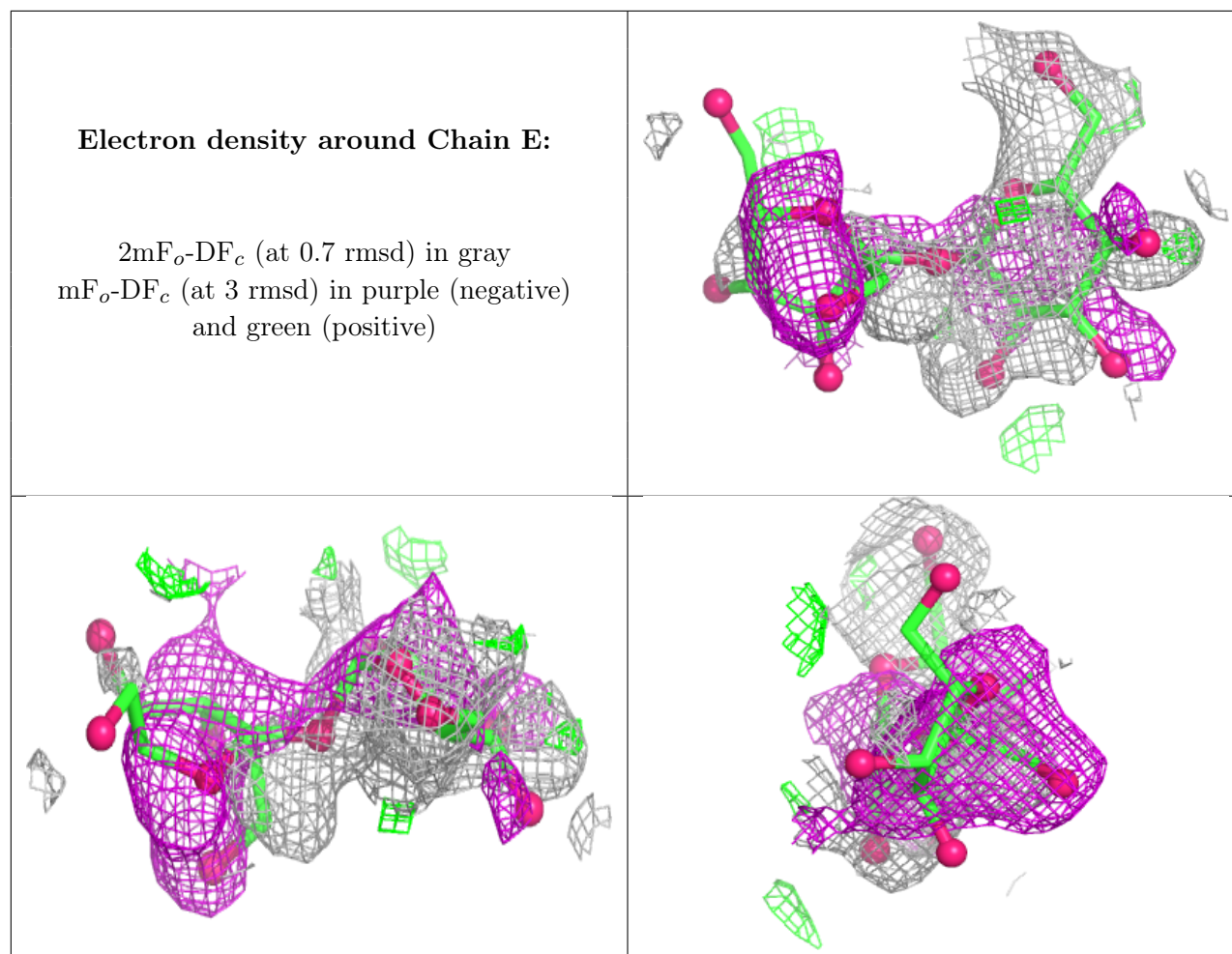
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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($\text{\AA}^2$)	Q<0.9
4	FRU	E	2	12/12	0.16	0.30	65,67,68,69	0
4	GLC	E	1	11/12	0.33	0.29	60,62,63,64	0
4	FRU	D	2	12/12	0.55	0.27	61,67,69,71	0
4	GLC	D	1	11/12	0.73	0.16	53,55,56,57	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, 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($\text{\AA}^2$)	Q<0.9
5	SO4	A	910	5/5	0.88	0.13	65,65,65,65	0
5	SO4	A	912	5/5	0.90	0.13	44,45,46,47	0
5	SO4	A	911	5/5	0.94	0.08	48,48,49,49	0
6	MG	A	920	1/1	0.96	0.18	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.