



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:37 PM UTC

PDB ID : 1NK0 / pdb_00001nk0
Title : ADENINE-GUANINE MISMATCH AT THE POLYMERASE ACTIVE SITE
Authors : Johnson, S.J.; Beese, L.S.
Deposited on : 2003-01-02
Resolution : 1.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

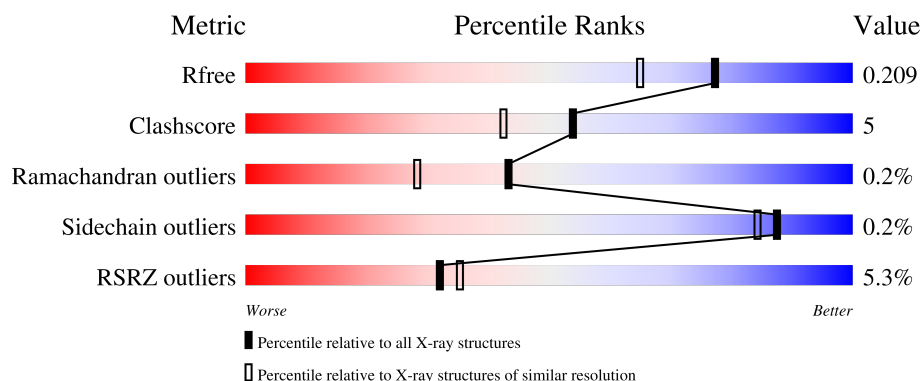
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	9% 82% 18%
2	C	15	20% 33% 47% 20%
3	A	580	5% 85% 15%
4	D	2	100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5829 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 DNA PRIMER STRAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	11	Total	C	N	O	P	0	0	0
			224	107	46	61	10			

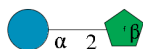
- Molecule 2 is a DNA chain called DNA TEMPLATE STRAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	P	0	0	0
			242	116	43	72	11			

- 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			

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is SULFATE ION (CCD ID: 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		

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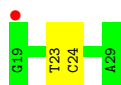
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	23	Total	O	0	0
			23	23		
7	C	47	Total	O	0	0
			47	47		
7	A	588	Total	O	0	0
			588	588		

● Molecule 1: DNA PRIMER STRAND



Category	Number of Genes
DG	0
DT	0
DA	0
C3	10
G4	1
T5	1
G6	1
C7	1
T8	1
C12	10
G13	1
C14	10

L847	N700	A297
V848	M701	K298
P849	A707	L303
Q854	W719	A304
L862	Q723	D305
K876	M724	T308
	L725	E309
	K730	M311
	E734	A317
	F737	E321
	R738	H328
	E741	I332
	K747	Q356
	M750	G432
	E751	A433
	M752	K434
	I753	R435
	L767	A436
	H768	V437
	R769	E440
	M780	P441
	F781	V475
	R784	E478
	E788	T497
	R789	K498
	M792	R499
	N793	L500
	G798	E501
	D802	Q502
	A813	M503
	E817	E506
	E818	L507
	R819	A508
	A822	E509
	H823	Q510
	L824	L511
	L825	V514
	E835	I518
	A836	V519
		E520
		E525
		Q533

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	88.12Å 93.61Å 104.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.32 – 1.70 28.32 – 1.70	Depositor EDS
% Data completeness (in resolution range)	92.8 (28.32-1.70) 96.0 (28.32-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 1.70Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.189 , 0.209 0.189 , 0.209	Depositor DCC
R_{free} test set	4513 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	15.9	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5829	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: FRU, MES, SO4, GLC

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	0/252	0.65	0/387
2	C	0.27	0/270	0.67	0/415
3	A	0.49	9/4734 (0.2%)	0.86	18/6398 (0.3%)
All	All	0.47	9/5256 (0.2%)	0.84	18/7200 (0.2%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	823	HIS	ND1-CE1	5.27	1.37	1.32
3	A	328	HIS	ND1-CE1	5.27	1.37	1.32
3	A	356	GLN	CD-OE1	5.13	1.33	1.23
3	A	510	GLN	CD-OE1	5.12	1.33	1.23
3	A	533	GLN	CD-OE1	5.12	1.33	1.23

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	321	GLU	N-CA-C	7.47	120.68	109.25
3	A	793	ASN	N-CA-C	7.28	120.65	111.69
3	A	680	ASP	N-CA-C	-7.23	98.74	109.15
3	A	332	ILE	N-CA-C	-6.45	98.57	107.99
3	A	328	HIS	CB-CG-CD2	-6.40	122.89	131.20

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	224	0	124	2	0
2	C	242	0	137	7	0
3	A	4650	0	4698	42	0
4	D	23	0	21	0	0
5	A	12	0	13	0	0
6	A	20	0	0	0	0
7	A	588	0	0	2	0
7	B	23	0	0	0	0
7	C	47	0	0	0	0
All	All	5829	0	4993	50	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.

The worst 5 of 50 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:546:VAL:HG11	3:A:549:LYS:NZ	1.99	0.78
3:A:789:ARG:HA	3:A:792:MET:HE3	1.69	0.74
3:A:692:VAL:HG21	3:A:701:MET:HE1	1.72	0.70
3:A:497:THR:O	3:A:501:GLU:HG3	1.95	0.67
3:A:546:VAL:HG11	3:A:549:LYS:HZ2	1.58	0.66

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%)	15 (3%)	1 (0%)	43 28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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%)	87 84

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

Mol	Chain	Res	Type
3	A	435	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	524	GLN
3	A	529	ASN
3	A	768	HIS
3	A	797	GLN
3	A	821	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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	D	1	4	11,11,12	3.18	4 (36%)	15,15,17	1.50	2 (13%)
4	FRU	D	2	4	11,12,12	1.58	1 (9%)	10,18,18	0.70	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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	GLC	C2-C3	9.24	1.66	1.52
4	D	2	FRU	O2-C2	4.37	1.48	1.40
4	D	1	GLC	O5-C5	2.74	1.48	1.43
4	D	1	GLC	O5-C1	2.55	1.48	1.43
4	D	1	GLC	C4-C5	2.22	1.57	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	GLC	C1-O5-C5	4.15	117.75	112.19
4	D	1	GLC	C1-C2-C3	-2.71	105.70	109.64

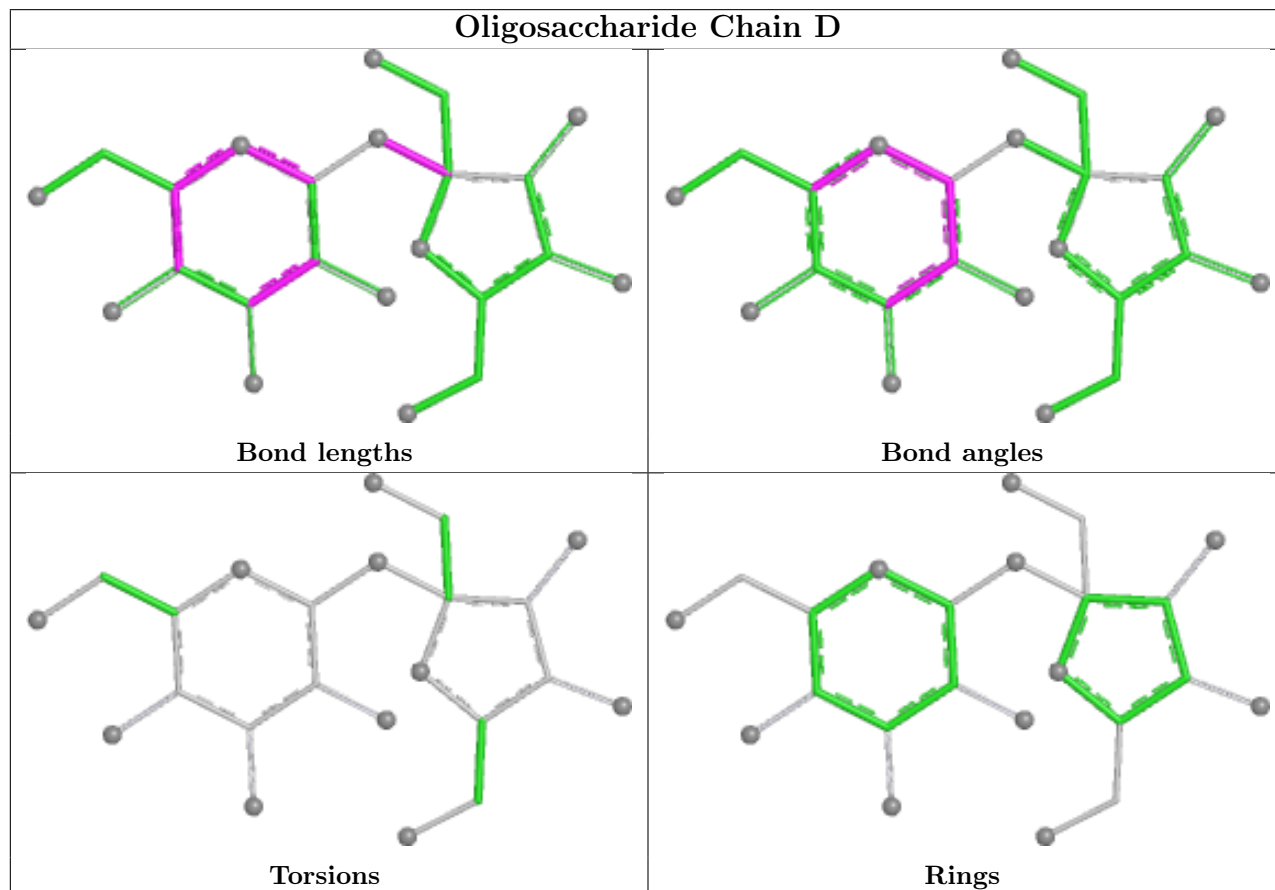
There are no chirality outliers.

There are no torsion outliers.

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 [i](#)

5 ligands 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	$\# Z > 2$
6	SO4	A	5	-	4,4,4	0.35	0	6,6,6	0.11	0
6	SO4	A	4	-	4,4,4	0.37	0	6,6,6	0.08	0
5	MES	A	2	-	12,12,12	1.44	3 (25%)	15,16,16	0.72	0
6	SO4	A	6	-	4,4,4	0.40	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	A	3	-	4,4,4	0.35	0	6,6,6	0.07	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	MES	A	2	-	-	0/6/14/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2	MES	C3-N4	2.65	1.54	1.46
5	A	2	MES	C5-N4	2.43	1.53	1.46
5	A	2	MES	C7-N4	2.39	1.52	1.47

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	11/11 (100%)	0.42	1 (9%) 15 15	14, 20, 49, 55	0
2	C	12/15 (80%)	0.71	3 (25%) 2 1	15, 20, 55, 62	0
3	A	580/580 (100%)	0.16	28 (4%) 35 39	9, 17, 32, 42	0
All	All	603/606 (99%)	0.17	32 (5%) 32 35	9, 17, 33, 62	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	297	ALA	7.4
3	A	433	ALA	4.0
3	A	551	LYS	3.7
1	B	19	DG	3.5
2	C	3	DC	3.5

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

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

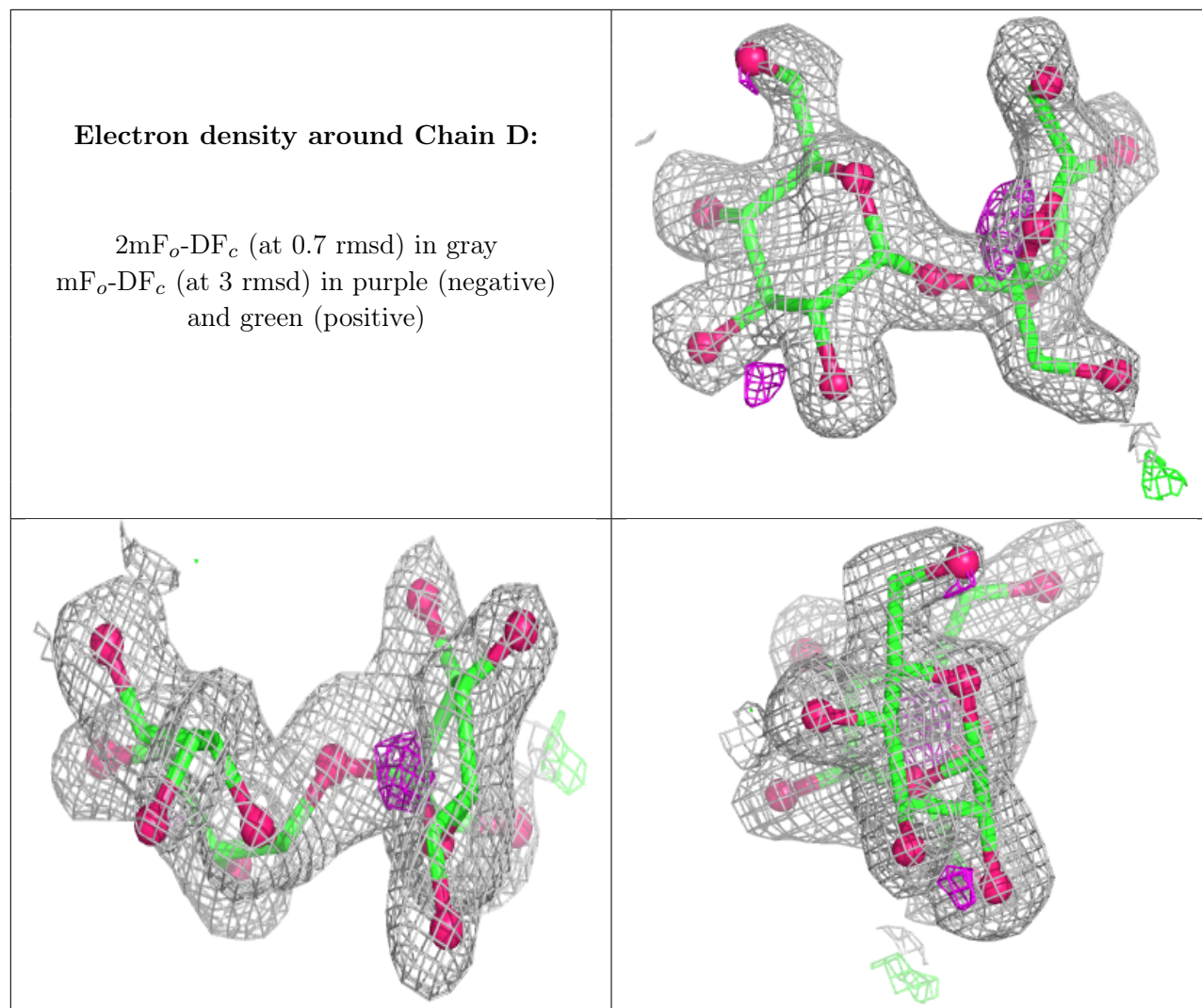
6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FRU	D	2	12/12	0.82	0.13	35,37,38,38	0
4	GLC	D	1	11/12	0.86	0.12	32,33,35,36	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	A	4	5/5	0.82	0.12	53,53,53,53	0
5	MES	A	2	12/12	0.83	0.15	32,33,36,36	0
6	SO4	A	6	5/5	0.89	0.17	24,25,25,26	0
6	SO4	A	5	5/5	0.92	0.11	36,37,38,38	0
6	SO4	A	3	5/5	0.94	0.08	39,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.