



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 12:01 AM EDT

PDB ID : 1NJW / pdb_00001njw
Title : GUANINE-THYMINE MISMATCH AT THE POLYMERASE ACTIVE SITE
Authors : Johnson, S.J.; Beese, L.S.
Deposited on : 2003-01-02
Resolution : 1.90 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

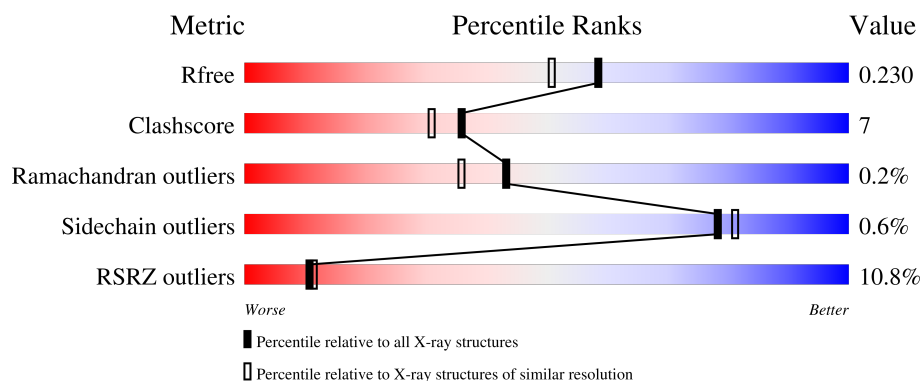
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	 45% 55%
2	C	15	 27% 47% 33% 20%
3	A	580	 11% 83% 16%
4	D	2	 100%
4	E	2	 100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5610 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
			226	107	46	63	10			

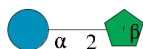
- Molecule 2 is a DNA chain called DNA TEMPLATE STRAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	P	0	0	0
			244	116	43	73	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 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	13	Total	O	0	0
			13	13		
7	C	19	Total	O	0	0
			19	19		
7	A	396	Total	O	0	0
			396	396		

● Molecule 1: DNA PRIMER STRAND

G19	C20	G21	A22	T23	C24		G28	G29
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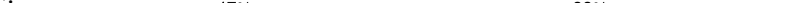
Chain C: 

Diagram illustrating the 16-bit register structure, showing fields DA, DC, DG, T4, C5, G6, C7, T8, G13, C14, and A15. The T8 field is highlighted in yellow, and the G13, C14, and A15 fields are highlighted in green.

Chain A:

R770	R771	R779	R780	R781	R782	R783	R784	R785	R786	R787	R788	R789	R790	R791	R792	R793	G798	N812	A813	E817	E818	R819	A822	H823	L824	L825	L826	A836	P837	K838	L847	V848	P849	L862	D874	A875	K876	S845	D846	Y854	I657	D680	I689	F690	Q691	M701	A707	G711	I712	V713	Y714	G715	I716	S717	D718	Y719	G720	L721	A722	G723	N724	L725	N726	I727	S728	R729	K730	E731	A732	A733	E734	F735	I736	E737	R738	Y739	F740	E741	G747	R748	Y749	M750	I753	K758	S845	D846	Y854	I657	D680	I689	F690	Q691	M701	A707	G711	I712	V713	Y714	G715	I716	S717	D718	Y719	G720	L721	A722	G723	N724	L725	N726	I727	S728	R729	K730	E731	A732	A733	E734	F735	I736	E737	R738	Y739	F740	E741	G747	R748	Y749	M750	I753	K758	S845	D846	Y854	I657	D680	I689	F690	Q691	M701	A707	G711	I712	V713	Y714	G715	I716	S717	D718	Y719	G720	L721	A722	G723	N724	L725	N726	I727	S728	R729	K730	E731	A732	A733	E734	F735	I736	E737	R738	Y739	F740	E741	G747	R748	Y749	M750	I753	K758	S845	D846	Y854	I657	D680	I689	F690	Q691	M701	A707	G711	I712	V713	Y714	G715	I716	S717	D718	Y719	G720	L721	A722	G723	N724	L725	N726	I727	S728	R729	K730	E731	A732	A733	E734	F735	I736	E737	R738	Y739	F740	E741	G747	R748	Y749	M750	I753	K758	S845	D846	Y854	I657	D680	I689	F690	Q691	M701	A707	G711	I712	V713	Y714	G715	I716	S717	D718	Y719	G720	L721	A722	G723	N724	L725	N726	I727	S728	R729	K730	E731	A732	A733	E734	F735	I736	E737	R738	Y739	F740	E741	G747	R748	Y749	M750	I753	K758	S845	D846	Y854	I657	D680	I689	F690	Q691	M701	A707	G711	I712	V713	Y714	G715	I716	S717	D718	Y719	G720	L721	A722	G723	N724	L725	N726	I727	S728	R729	K730	E731	A732	A733	E734	F735	I736	E737	R738	Y739	F740	E741	G747	R748	Y749	M750	I753	K758	S845	D846	Y854	I657	D680	I689	F690	Q691	M701	A707	G711	I712	V713	Y714	G715	I716	S717	D718	Y719	G720	L721	A722	G723	N724	L725	N726	I727	S728	R729	K730	E731	A732	A733	E734	F735	I736	E737	R738	Y739	F740	E741	G747	R748	Y749	M750	I753	K758	S845	D846	Y854	I657	D680	I689	F690	Q691	M701	A707	G711	I712	V713	Y714	G715	I716	S717	D718	Y719	G720	L721	A722	G723	N724	L725	N726	I727	S728	R729	K730	E731	A732	A733	E734	F735	I736	E737	R738	Y739	F740	E741	G747	R748	Y749	M750	I753	K758	S845	D846	Y854	I657	D680	I689	F690	Q691	M701	A707	G711	I712	V713	Y714	G715	I716	S717	D718	Y719	G720	L721	A722	G723	N724	L725	N726	I727	S728	R729	K730	E731	A732	A733	E734	F735	I736	E737	R738	Y739	F740	E741	G747	R748	Y749	M750	I753	K758	S845	D846	Y854	I657	D680	I689	F690	Q691	M701	A707	G711	I712	V713	Y714	G715	I716	S717	D718	Y719	G720	L721	A722	G723	N724	L725	N726	I727	S728	R729	K730	E731	A732	A733	E734	F735	I736	E737	R738	Y739	F740	E741	G747	R748
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Chain D: 100%

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	87.95Å 93.69Å 104.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.48 – 1.90 32.48 – 1.90	Depositor EDS
% Data completeness (in resolution range)	90.9 (32.48-1.90) 90.9 (32.48-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.209 , 0.240 0.203 , 0.230	Depositor DCC
R_{free} test set	3116 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.6	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	0.94	EDS
Total number of atoms	5610	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: SO4, FRU, MG, 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	0/254	0.73	0/391
2	C	0.32	0/272	0.68	0/417
3	A	0.39	1/4734 (0.0%)	0.86	15/6398 (0.2%)
All	All	0.38	1/5260 (0.0%)	0.84	15/7206 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	750	MET	SD-CE	-5.33	1.66	1.79

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	680	ASP	N-CA-C	-7.16	98.85	109.15
3	A	321	GLU	N-CA-C	6.58	119.26	109.59
3	A	793	ASN	N-CA-C	6.45	119.63	111.69
3	A	317	ALA	N-CA-C	-6.16	99.24	109.46
3	A	862	LEU	N-CA-C	-6.11	99.75	109.59

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	226	0	124	5	0
2	C	244	0	136	5	0
3	A	4650	0	4698	67	0
4	D	23	0	21	2	0
4	E	23	0	21	0	0
5	A	15	0	0	0	0
6	A	1	0	0	0	0
7	A	396	0	0	5	0
7	B	13	0	0	0	0
7	C	19	0	0	0	0
All	All	5610	0	5000	74	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 7.

The worst 5 of 74 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:771:ARG:HH22	3:A:790:MET:HE3	1.30	0.97
3:A:771:ARG:NH2	3:A:790:MET:HE3	1.84	0.93
3:A:499:ARG:HG3	3:A:503:MET:HE2	1.73	0.71
1:B:23:DT:H2''	1:B:24:DC:H5'	1.72	0.71
2:C:7:DC:H2''	2:C:8:DT:H5'	1.73	0.69

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%)	17 (3%)	1 (0%)	43 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	495/496 (100%)	492 (99%)	3 (1%)	78 81

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	538	LEU
3	A	623	LEU
3	A	812	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	529	ASN
3	A	691	GLN
3	A	704	GLN
3	A	854	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	3.31	4 (36%)	15,15,17	1.49	2 (13%)
4	FRU	D	2	4	11,12,12	1.33	1 (9%)	10,18,18	0.81	0
4	GLC	E	1	4	11,11,12	3.24	4 (36%)	15,15,17	1.51	2 (13%)
4	FRU	E	2	4	11,12,12	1.61	1 (9%)	10,18,18	0.69	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	-	0/2/19/22	0/1/1/1
4	FRU	E	2	4	-	0/5/24/24	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	GLC	C2-C3	9.70	1.67	1.52
4	E	1	GLC	C2-C3	9.36	1.66	1.52
4	E	2	FRU	O2-C2	4.48	1.48	1.40
4	D	2	FRU	O2-C2	3.64	1.47	1.40
4	D	1	GLC	O5-C5	2.85	1.49	1.43

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	4.07	117.63	112.19
4	E	1	GLC	C1-C2-C3	-2.81	105.55	109.64
4	D	1	GLC	C1-C2-C3	-2.74	105.66	109.64

There are no chirality outliers.

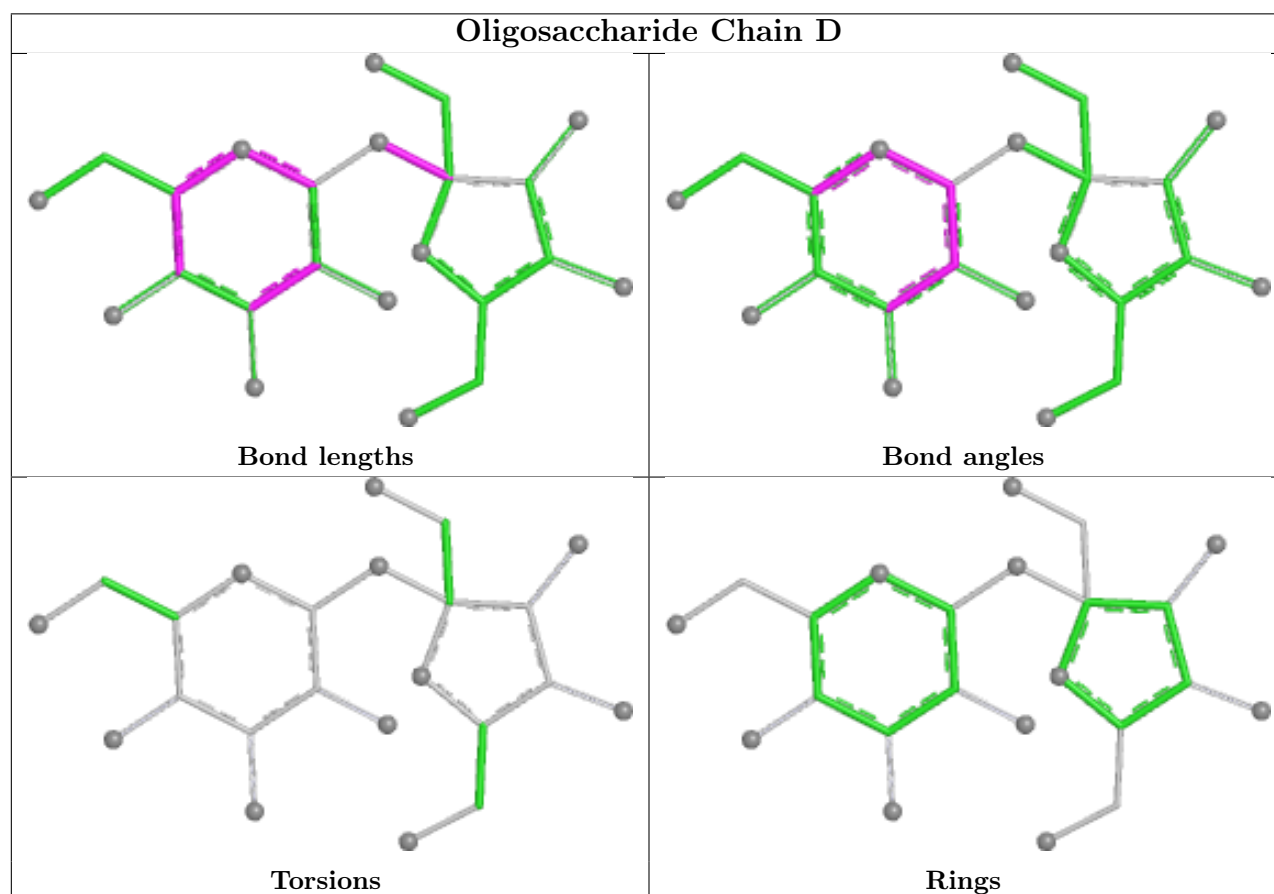
There are no torsion outliers.

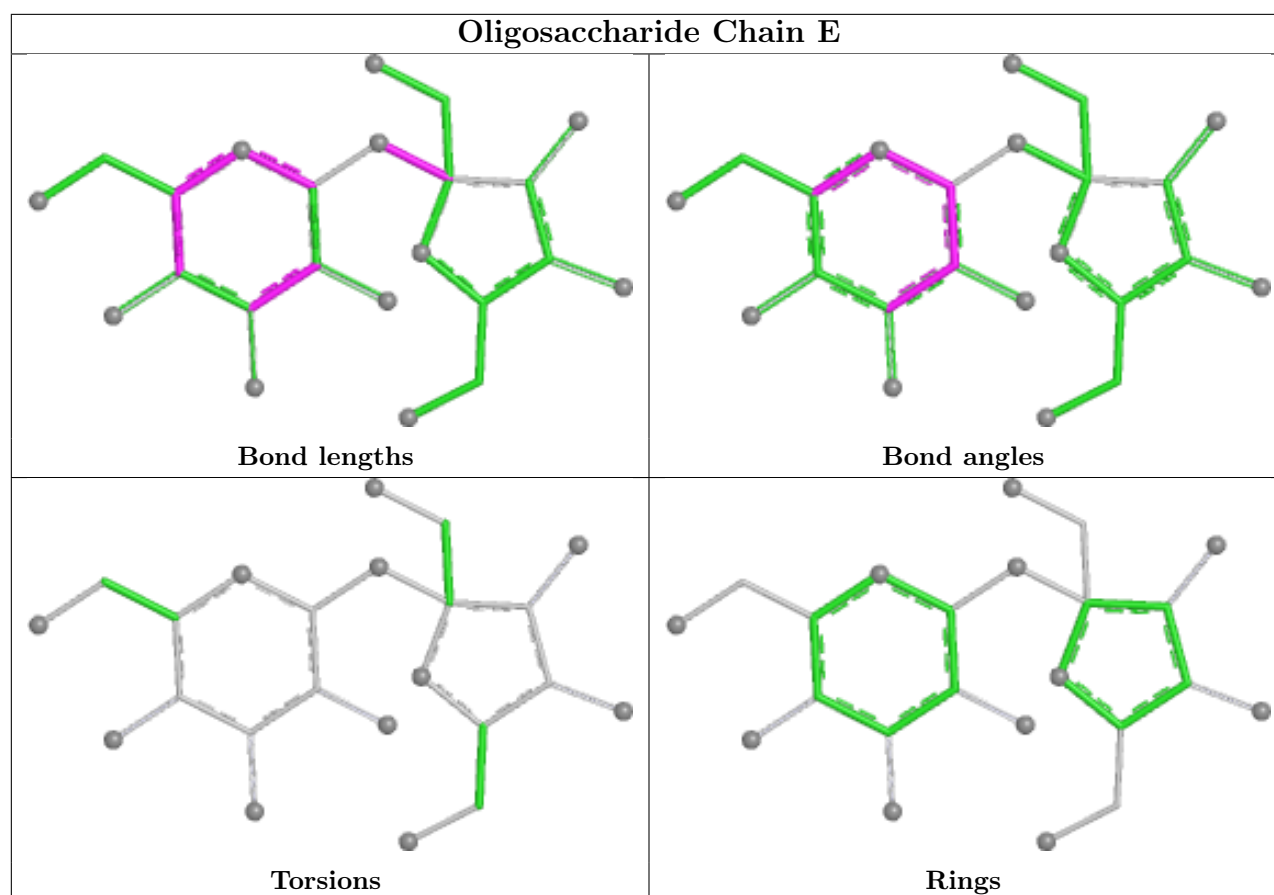
There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

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





5.6 Ligand geometry [i](#)

Of 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	905	-	4,4,4	0.37	0	6,6,6	0.09	0
5	SO4	A	903	-	4,4,4	0.34	0	6,6,6	0.13	0
5	SO4	A	904	-	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

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.75	0 100 100	32, 39, 62, 63	0
2	C	12/15 (80%)	1.40	4 (33%) 1 1	32, 42, 73, 77	0
3	A	580/580 (100%)	0.56	61 (10%) 11 12	15, 26, 46, 51	0
All	All	603/606 (99%)	0.58	65 (10%) 11 11	15, 26, 47, 77	0

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	297	ALA	5.5
3	A	781	PHE	4.5
3	A	738	ARG	4.4
3	A	719	TYR	4.2
3	A	733	ALA	4.1

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.

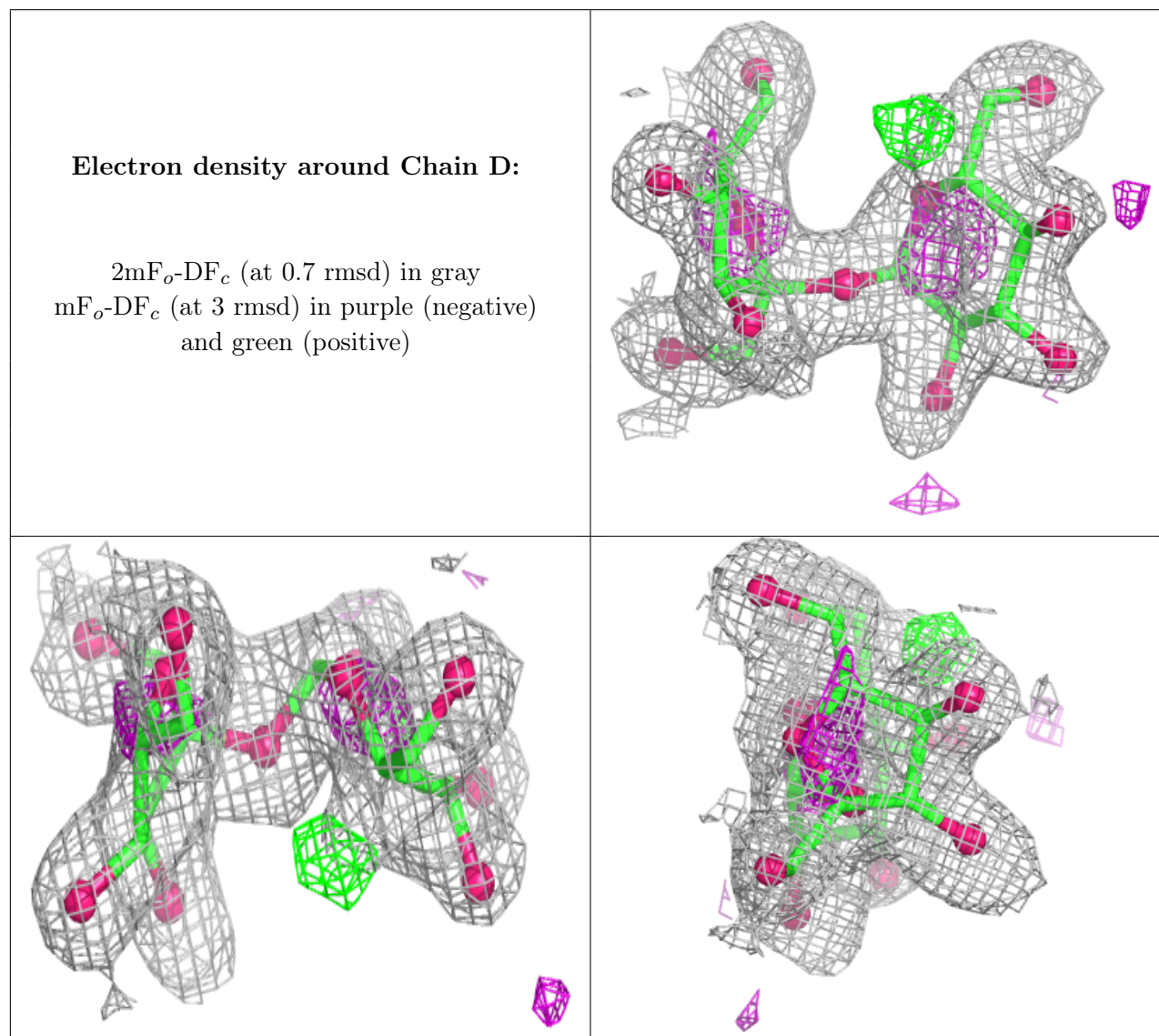
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GLC	E	1	11/12	0.73	0.15	49,50,50,50	0
4	FRU	E	2	12/12	0.73	0.16	50,51,51,51	0
4	GLC	D	1	11/12	0.79	0.13	37,37,38,38	0

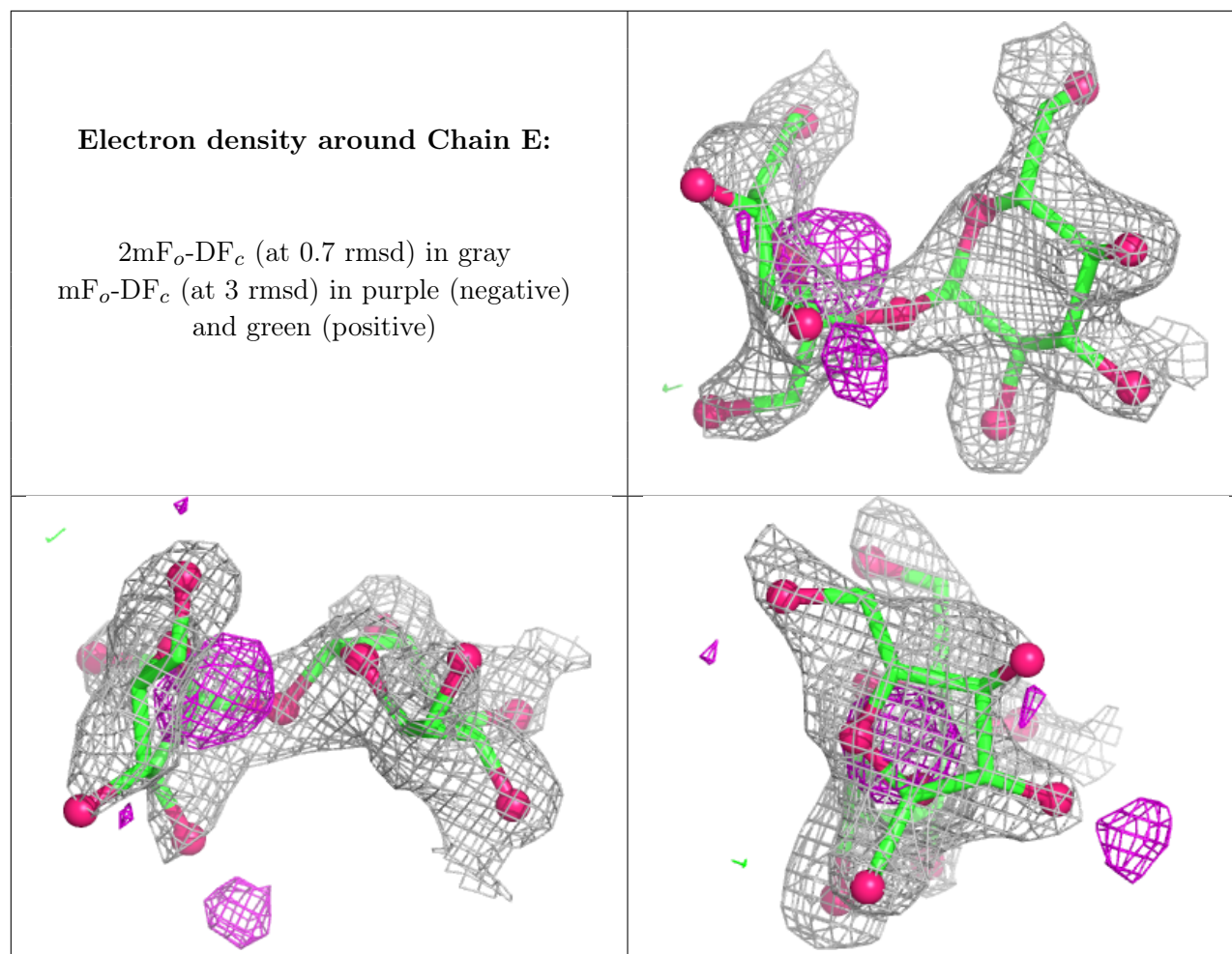
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FRU	D	2	12/12	0.85	0.12	34,35,36,36	0

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	905	5/5	0.77	0.13	77,77,77,77	0
5	SO4	A	904	5/5	0.90	0.09	58,58,58,58	0
5	SO4	A	903	5/5	0.92	0.12	47,47,47,47	0
6	MG	A	920	1/1	0.96	0.08	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.