



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:15 AM UTC

PDB ID : 1NK4 / pdb_00001nk4
Title : GUANINE-GUANINE MISMATCH AT THE POLYMERASE ACTIVE SITE
Authors : Johnson, S.J.; Beese, L.S.
Deposited on : 2003-01-02
Resolution : 1.60 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

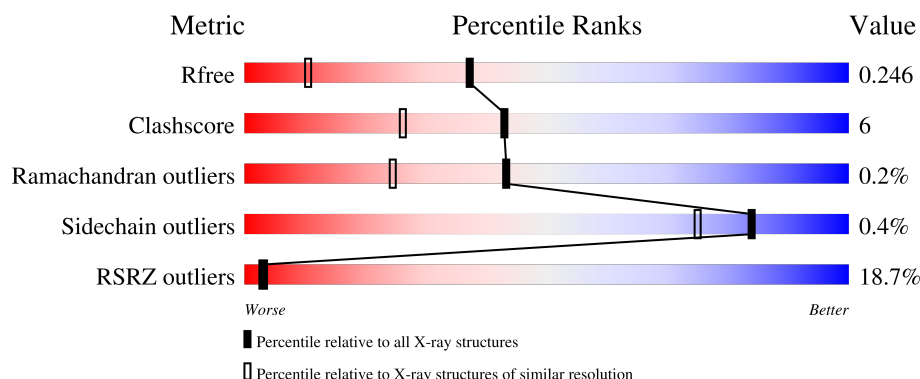
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	9	44% 67% 33%
2	C	16	25% 38% 25% 38%
3	A	580	18% 85% 14%
4	D	2	100%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5589 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	9	Total	C	N	O	P	0	0	0
			185	88	38	51	8			

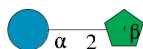
- Molecule 2 is a DNA chain called DNA TEMPLATE STRAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	0	0	0
			205	97	38	60	10			

- Molecule 3 is a protein called DNA POLYMERASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	580	Total	C	N	O	S	0	2	0
			4670	2967	813	873	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 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		
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		

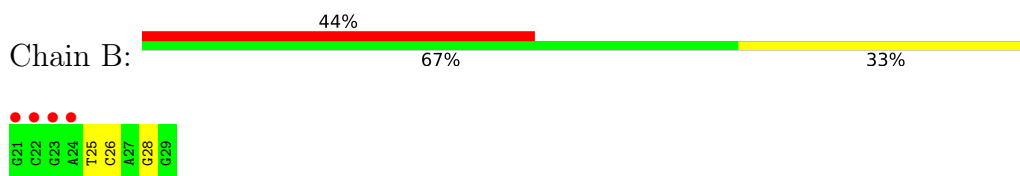
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	11	Total	O	0	0
			11	11		
7	C	17	Total	O	0	0
			17	17		
7	A	457	Total	O	0	0
			457	457		

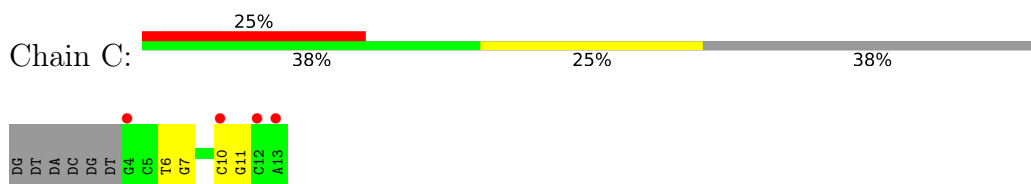
3 Residue-property plots

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.

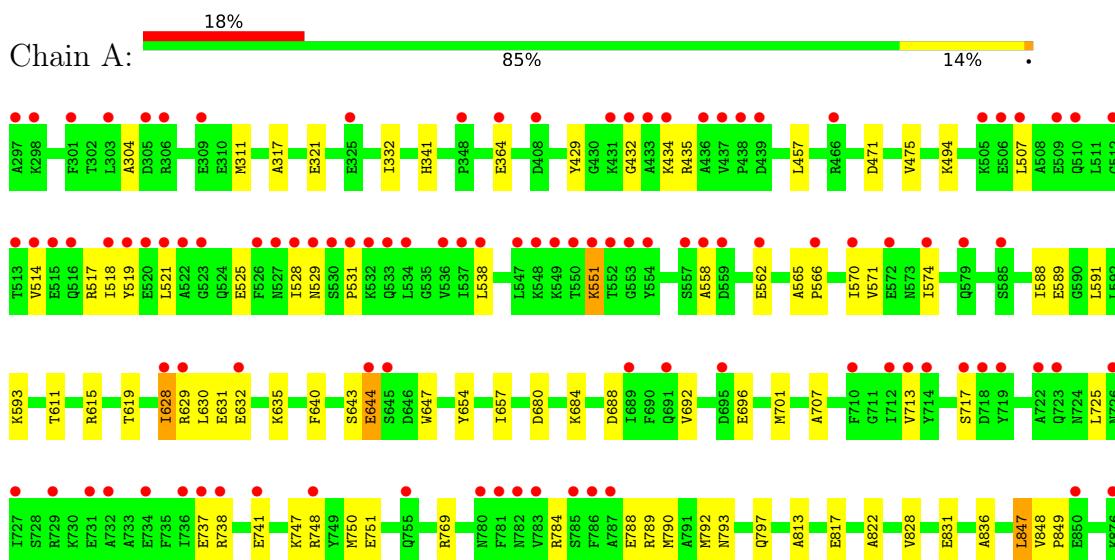
- Molecule 1: DNA PRIMER STRAND



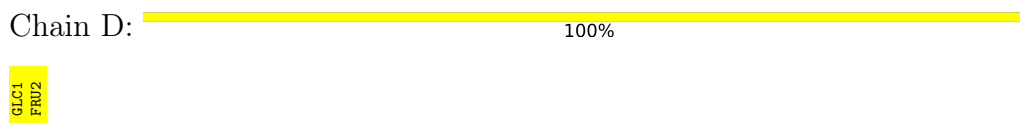
- Molecule 2: DNA TEMPLATE STRAND



- Molecule 3: DNA POLYMERASE I



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.89Å 93.67Å 105.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.60 – 1.60 25.60 – 1.60	Depositor EDS
% Data completeness (in resolution range)	84.0 (25.60-1.60) 90.2 (25.60-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 1.60Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.246 0.222 , 0.246	Depositor DCC
R_{free} test set	4845 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 38.2	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	5589	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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, GLC, MG, FRU

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	0.26	0/208	0.63	0/320
2	C	0.28	0/229	0.64	0/351
3	A	0.34	0/4754	0.85	10/6424 (0.2%)
All	All	0.34	0/5191	0.83	10/7095 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	321	GLU	N-CA-C	7.44	120.52	109.59
3	A	680	ASP	N-CA-C	-7.26	98.69	109.15
3	A	475	VAL	N-CA-C	7.03	117.82	110.72
3	A	793	ASN	N-CA-C	6.58	119.78	111.69
3	A	317	ALA	N-CA-C	-6.07	99.38	109.46
3	A	538	LEU	N-CA-C	5.90	117.51	111.14
3	A	769	ARG	N-CA-C	-5.55	102.67	110.50
3	A	332	ILE	N-CA-C	-5.53	99.91	107.99
3	A	457	LEU	N-CA-C	5.28	119.44	112.89
3	A	847	LEU	N-CA-C	5.18	116.74	111.14

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	185	0	102	3	0
2	C	205	0	113	5	0
3	A	4670	0	4717	57	0
4	D	23	0	21	0	0
5	A	20	0	0	0	0
6	A	1	0	0	0	0
7	A	457	0	0	3	0
7	B	11	0	0	0	0
7	C	17	0	0	0	0
All	All	5589	0	4953	62	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 (62) 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:494:LYS:HE2	3:A:643:SER:HA	1.67	0.76
3:A:507:LEU:HD12	3:A:588:ILE:HD12	1.76	0.68
3:A:789:ARG:HA	3:A:792:MET:HE3	1.77	0.67
3:A:518:ILE:HD13	3:A:574:ILE:HD13	1.77	0.66
3:A:692:VAL:HG21	3:A:701:MET:HE1	1.78	0.65
3:A:615[B]:ARG:NH2	3:A:797[B]:GLN:HG3	2.17	0.60
3:A:828:VAL:HB	3:A:831:GLU:HG2	1.83	0.60
3:A:784:ARG:O	3:A:788:GLU:HG3	2.02	0.59
3:A:494:LYS:CE	3:A:643:SER:HA	2.33	0.58
3:A:847:LEU:C	3:A:847:LEU:HD23	2.29	0.57
3:A:507:LEU:HD12	3:A:588:ILE:CD1	2.35	0.57
3:A:813:ALA:O	3:A:817:GLU:HG3	2.04	0.57
2:C:6:DT:H5''	3:A:611:THR:HG22	1.87	0.57
3:A:750:MET:SD	3:A:792:MET:HB3	2.45	0.56
3:A:629:ARG:NH1	3:A:630:LEU:HG	2.22	0.55
3:A:551:LYS:NZ	3:A:551:LYS:HB2	2.21	0.55
3:A:494:LYS:HE2	3:A:643:SER:CA	2.38	0.52
3:A:632:GLU:HG3	7:A:3551:HOH:O	2.09	0.52
3:A:570:ILE:O	3:A:574:ILE:HG12	2.10	0.52
3:A:788:GLU:O	3:A:792:MET:HG3	2.10	0.51
3:A:519:TYR:CD1	3:A:525:GLU:HA	2.46	0.51
2:C:10:DC:H2''	2:C:11:DG:H5'	1.93	0.51
3:A:738:ARG:HD2	3:A:741:GLU:OE1	2.10	0.51
3:A:747:LYS:O	3:A:751:GLU:HG3	2.11	0.51
3:A:429:TYR:O	3:A:435:ARG:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:471:ASP:HB3	7:A:3638:HOH:O	2.13	0.49
3:A:589:GLU:O	3:A:593:LYS:HG3	2.13	0.48
3:A:713:VAL:O	3:A:797[B]:GLN:NE2	2.47	0.48
3:A:631:GLU:O	3:A:635:LYS:HG3	2.12	0.48
3:A:591:LEU:HD21	3:A:640:PHE:CZ	2.49	0.48
3:A:304:ALA:CB	3:A:311:MET:HE1	2.44	0.48
3:A:432:GLY:C	3:A:434:LYS:H	2.21	0.47
3:A:565:ALA:HB3	3:A:566:PRO:HD3	1.97	0.47
3:A:848:VAL:HB	3:A:849:PRO:HD3	1.96	0.47
1:B:25:DT:H2''	1:B:26:DC:H5'	1.97	0.46
3:A:692:VAL:HB	3:A:696:GLU:HB2	1.97	0.46
3:A:790:MET:HE2	3:A:790:MET:HA	1.98	0.46
3:A:565:ALA:HA	3:A:571:VAL:HB	1.97	0.46
1:B:25:DT:H2''	1:B:26:DC:C5'	2.46	0.45
3:A:341:HIS:HE1	7:A:3442:HOH:O	2.00	0.45
1:B:28:DG:H5''	3:A:628:ILE:HG22	1.99	0.45
3:A:517:ARG:CZ	3:A:521:LEU:HD21	2.47	0.45
3:A:615[B]:ARG:HH11	3:A:615[B]:ARG:HG2	1.82	0.44
2:C:10:DC:H2'	2:C:11:DG:C8	2.51	0.44
3:A:822:ALA:CB	3:A:836:ALA:HB2	2.47	0.44
3:A:558:ALA:O	3:A:562:GLU:HG3	2.18	0.43
3:A:529:ASN:O	3:A:531:PRO:HD3	2.18	0.43
3:A:615[B]:ARG:CZ	3:A:797[B]:GLN:HG3	2.48	0.43
3:A:789:ARG:CA	3:A:792:MET:HE3	2.48	0.43
3:A:717:SER:HB3	3:A:789:ARG:CZ	2.49	0.43
3:A:518:ILE:HD12	3:A:528:ILE:HD13	2.02	0.42
3:A:644:GLU:HB2	3:A:647:TRP:CD1	2.55	0.42
3:A:707:ALA:CB	3:A:725:LEU:HD21	2.49	0.42
3:A:514:VAL:O	3:A:518:ILE:HG13	2.19	0.42
3:A:517:ARG:NH2	3:A:521:LEU:HD21	2.35	0.41
3:A:748:ARG:HH11	3:A:748:ARG:HG3	1.86	0.41
3:A:364:GLU:O	3:A:364:GLU:HG3	2.20	0.41
3:A:654:TYR:HB3	3:A:657:ILE:HB	2.03	0.40
2:C:7:DG:H3'	3:A:619:THR:HG22	2.02	0.40
2:C:10:DC:H2''	2:C:11:DG:C5'	2.52	0.40
3:A:684:LYS:HE3	3:A:688:ASP:OD2	2.22	0.40
3:A:737:GLU:O	3:A:741:GLU:HG3	2.22	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	580/580 (100%)	563 (97%)	16 (3%)	1 (0%)	43	24

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	497/496 (100%)	495 (100%)	2 (0%)	84	75

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	551	LYS
3	A	644	GLU

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	524	GLN
3	A	529	ASN
3	A	576	HIS

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Mol	Chain	Res	Type
3	A	704	GLN
3	A	752	ASN
3	A	768	HIS
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	3.31	4 (36%)	15,15,17	1.50	2 (13%)
4	FRU	D	2	4	11,12,12	1.40	1 (9%)	10,18,18	0.81	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	9.66	1.67	1.52
4	D	2	FRU	O2-C2	3.92	1.47	1.40
4	D	1	GLC	O5-C1	2.90	1.48	1.43
4	D	1	GLC	O5-C5	2.74	1.48	1.43
4	D	1	GLC	C4-C5	2.24	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	4.01	117.56	112.19
4	D	1	GLC	C1-C2-C3	-2.81	105.55	109.64

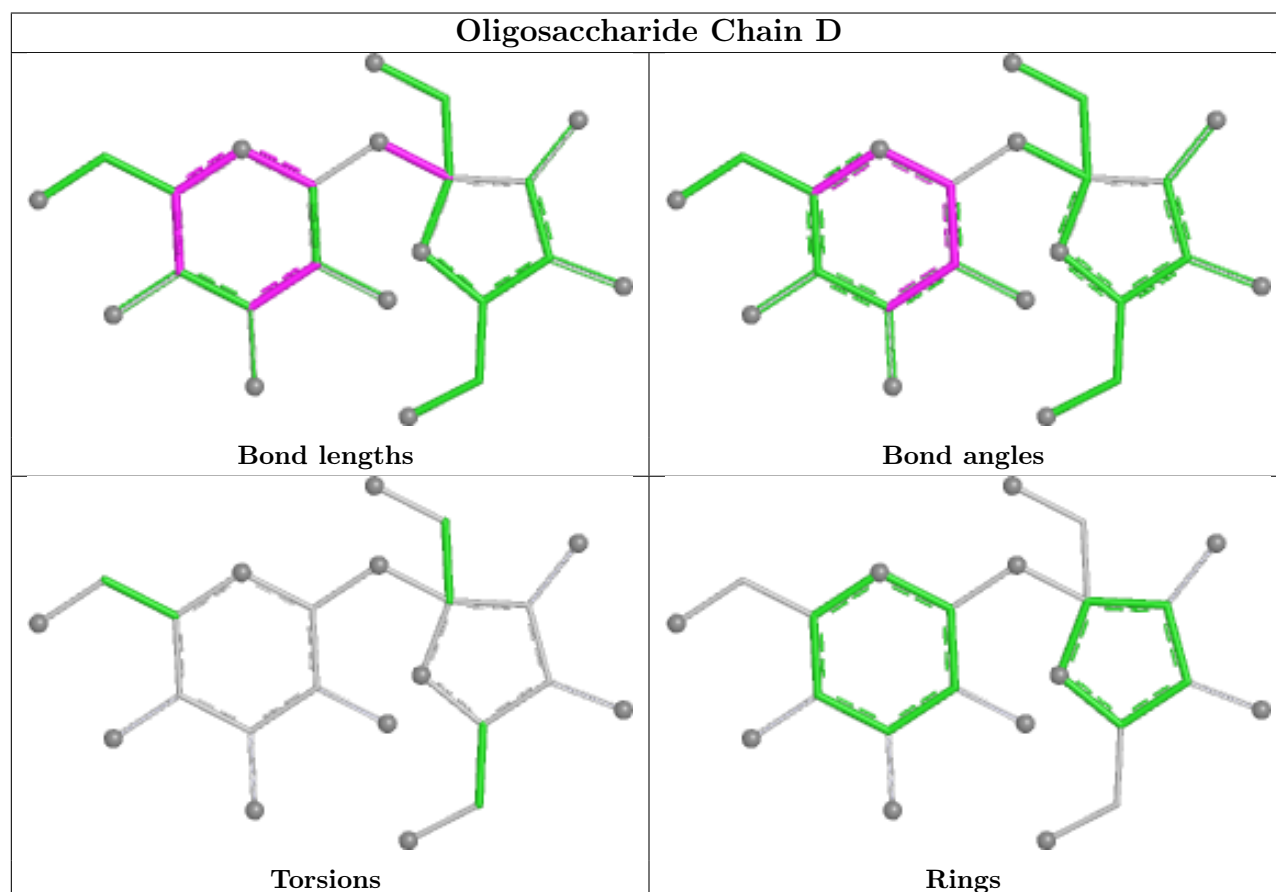
There are no chirality outliers.

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](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	910	-	4,4,4	0.35	0	6,6,6	0.11	0
5	SO4	A	911	-	4,4,4	0.36	0	6,6,6	0.08	0
5	SO4	A	912	-	4,4,4	0.37	0	6,6,6	0.08	0
5	SO4	A	913	-	4,4,4	0.41	0	6,6,6	0.11	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	9/9 (100%)	1.62	4 (44%) 0 0	27, 31, 57, 60	0
2	C	10/16 (62%)	1.83	4 (40%) 1 0	29, 40, 51, 56	0
3	A	580/580 (100%)	0.92	104 (17%) 3 3	9, 23, 43, 47	2 (0%)
All	All	599/605 (99%)	0.95	112 (18%) 3 3	9, 23, 44, 60	2 (0%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	433	ALA	9.4
3	A	297	ALA	6.9
3	A	550	THR	5.2
3	A	549	LYS	5.0
3	A	719	TYR	5.0
3	A	551	LYS	4.8
3	A	552	THR	4.6
3	A	723	GLN	4.6
3	A	559	ASP	4.5
3	A	523	GLY	4.2
3	A	531	PRO	4.1
3	A	526	PHE	4.1
3	A	553	GLY	4.0
3	A	734	GLU	3.9
3	A	507	LEU	3.9
3	A	782	ASN	3.9
3	A	691	GLN	3.9
3	A	530	SER	3.8
2	C	13	DA	3.8
3	A	431	LYS	3.7
3	A	729	ARG	3.6
1	B	21	DG	3.6
3	A	438	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
3	A	514	VAL	3.6
3	A	520	GLU	3.5
3	A	689	ILE	3.5
3	A	781	PHE	3.5
3	A	522	ALA	3.4
3	A	558	ALA	3.4
3	A	309	GLU	3.4
1	B	23	DG	3.4
3	A	512	GLY	3.4
3	A	714	TYR	3.4
3	A	437	VAL	3.3
3	A	466	ARG	3.2
3	A	510	GLN	3.2
3	A	554	TYR	3.1
3	A	532	LYS	3.1
3	A	306	ARG	3.1
3	A	305	ASP	3.1
3	A	574	ILE	3.1
3	A	528	ILE	3.0
3	A	562	GLU	3.0
3	A	519	TYR	3.0
3	A	557	SER	3.0
3	A	536	VAL	2.9
3	A	727	ILE	2.9
3	A	533	GLN	2.8
3	A	738	ARG	2.8
2	C	4	DG	2.8
3	A	726	ASN	2.8
3	A	629	ARG	2.8
3	A	695	ASP	2.8
3	A	566	PRO	2.8
3	A	748	ARG	2.8
3	A	741	GLU	2.8
3	A	783	VAL	2.7
3	A	432	GLY	2.7
3	A	527	ASN	2.7
3	A	521	LEU	2.7
3	A	301	PHE	2.6
3	A	434	LYS	2.6
2	C	12	DC	2.6
3	A	736	ILE	2.6
3	A	722	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
3	A	786	PHE	2.6
3	A	298	LYS	2.6
3	A	710	PHE	2.5
3	A	780	ASN	2.5
3	A	547	LEU	2.5
3	A	505	LYS	2.5
1	B	22	DC	2.5
3	A	538	LEU	2.5
3	A	537	ILE	2.5
3	A	645	SER	2.5
3	A	785	SER	2.4
3	A	787	ALA	2.4
3	A	408	ASP	2.4
3	A	348	PRO	2.3
3	A	513	THR	2.3
3	A	755	GLN	2.3
3	A	644	GLU	2.2
3	A	737	GLU	2.2
3	A	529	ASN	2.2
3	A	516	GLN	2.2
3	A	579	GLN	2.2
3	A	876	LYS	2.2
3	A	364	GLU	2.2
3	A	515	GLU	2.2
3	A	572	GLU	2.2
3	A	548	LYS	2.2
3	A	585	SER	2.2
3	A	509	GLU	2.2
1	B	24	DA	2.1
3	A	534	LEU	2.1
3	A	325	GLU	2.1
3	A	506	GLU	2.1
3	A	632	GLU	2.1
3	A	712	ILE	2.1
3	A	518	ILE	2.1
3	A	570	ILE	2.1
3	A	732	ALA	2.1
2	C	10	DC	2.1
3	A	713	VAL	2.0
3	A	718	ASP	2.0
3	A	303	LEU	2.0
3	A	731	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
3	A	850	GLU	2.0
3	A	628	ILE	2.0
3	A	436	ALA	2.0
3	A	439	ASP	2.0
3	A	717	SER	2.0

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

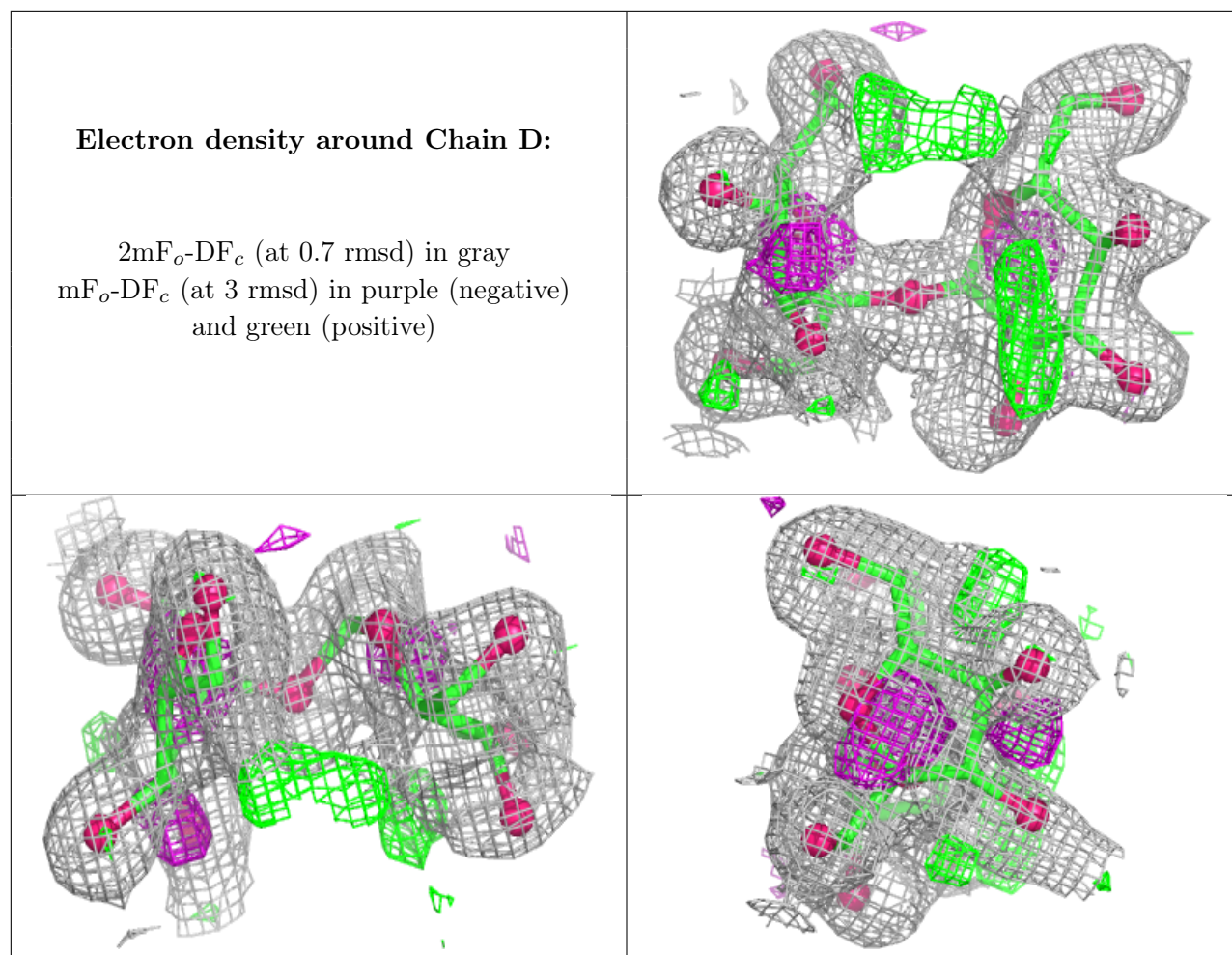
There are no non-standard protein/DNA/RNA residues in this entry.

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	D	1	11/12	0.68	0.17	42,42,43,43	0
4	FRU	D	2	12/12	0.76	0.16	40,41,41,42	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(Å ²)	Q<0.9
5	SO4	A	913	5/5	0.83	0.13	38,38,38,38	0
5	SO4	A	912	5/5	0.85	0.14	57,57,58,58	0
5	SO4	A	910	5/5	0.90	0.15	46,46,46,46	0
5	SO4	A	911	5/5	0.91	0.10	51,51,51,51	0
6	MG	A	920	1/1	0.97	0.07	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.