



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:47 PM UTC

PDB ID : 1U4B / pdb_00001u4b
Title : Extension of an adenine-8oxoguanine mismatch
Authors : Hsu, G.W.; Ober, M.; Carell, T.; Beese, L.S.
Deposited on : 2004-07-23
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

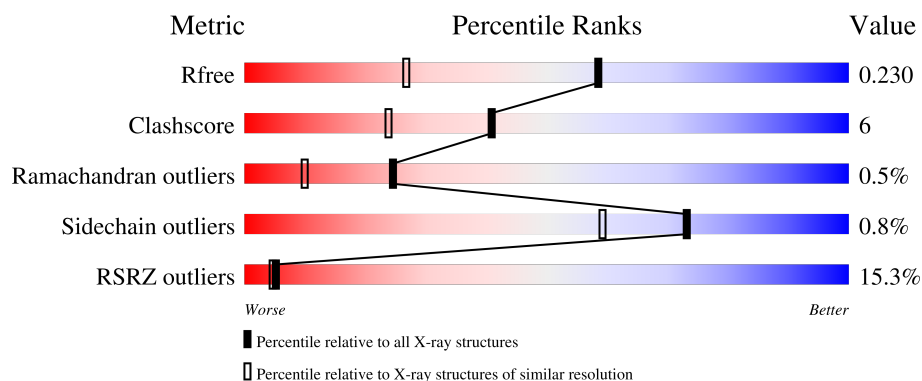
1 Overall quality at a glance

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	13	31% 23% 54% 23%
2	C	15	40% 33% 53% 13%
3	A	580	14% 86% 14%
4	D	2	100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5755 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	10	Total	C	N	O	P	0	0	0
			202	98	37	58	9			

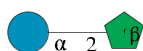
- Molecule 2 is a DNA chain called DNA template strand with 8-oxoguanine.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	13	Total	C	N	O	P	0	0	0
			268	127	53	76	12			

- Molecule 3 is a protein called DNA polymerase I.

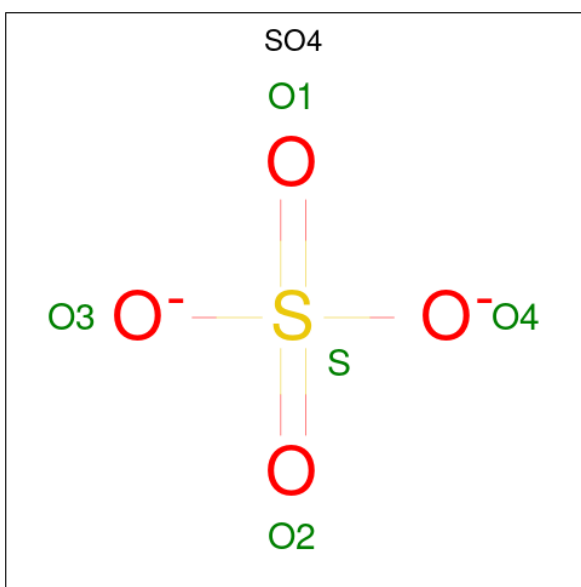
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	580	Total	C	N	O	S	0	0	0
			4650	2956	807	870	17			

- 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			

- 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	23	Total	O	0	0
			23	23		
7	C	39	Total	O	0	0
			39	39		
7	A	529	Total	O	0	0
			529	529		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.31Å 93.49Å 106.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.75 – 1.60 40.75 – 1.60	Depositor EDS
% Data completeness (in resolution range)	93.8 (40.75-1.60) 93.8 (40.75-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.45Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.213 , 0.227 0.216 , 0.230	Depositor DCC
R_{free} test set	5417 reflections (4.23%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 40.5	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	5755	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 4.39% 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, GLC, MG, SO4, 8OG

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	0/226	0.67	0/347
2	C	0.29	0/274	0.68	0/419
3	A	0.33	0/4734	0.83	12/6398 (0.2%)
All	All	0.33	0/5234	0.81	12/7164 (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	7.47	118.27	110.72
3	A	321	GLU	N-CA-C	6.98	119.85	109.59
3	A	680	ASP	N-CA-C	-6.58	98.47	108.67
3	A	620	GLU	CB-CA-C	-6.42	106.64	111.20
3	A	769	ARG	N-CA-C	-5.79	102.33	110.50
3	A	847	LEU	N-CA-C	5.55	117.14	111.14
3	A	317	ALA	N-CA-C	-5.43	100.44	109.46
3	A	715	GLY	N-CA-C	-5.29	100.64	113.18
3	A	862	LEU	N-CA-C	-5.26	101.11	109.59
3	A	793	ASN	N-CA-C	5.18	118.06	111.69
3	A	332	ILE	N-CA-C	-5.15	99.83	107.51
3	A	716	ILE	N-CA-C	5.05	116.91	109.63

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	202	0	115	7	0
2	C	268	0	147	7	0
3	A	4650	0	4701	53	0
4	D	23	0	21	0	0
5	A	20	0	0	0	0
6	A	1	0	0	0	0
7	A	529	0	0	3	0
7	B	23	0	0	0	0
7	C	39	0	0	0	0
All	All	5755	0	4984	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:843:ARG:HH11	3:A:843:ARG:HB3	1.45	0.80
2:C:10:DG:H2''	2:C:11:DT:H5'	1.64	0.79
1:B:22:DA:H2''	1:B:23:DC:C5'	2.17	0.74
3:A:692:VAL:HG21	3:A:701:MET:HE1	1.71	0.73
3:A:632:GLU:H	3:A:632:GLU:CD	1.97	0.72
3:A:820:LEU:HD21	3:A:843:ARG:NH1	2.10	0.67
3:A:349:GLU:H	3:A:349:GLU:CD	2.05	0.65
1:B:22:DA:H2''	1:B:23:DC:H5'	1.80	0.62
3:A:518:ILE:HD13	3:A:574:ILE:HD13	1.82	0.62
1:B:22:DA:H2''	1:B:23:DC:H5''	1.81	0.62
2:C:10:DG:H2''	2:C:11:DT:C5'	2.29	0.62
3:A:692:VAL:HB	3:A:696:GLU:HB2	1.81	0.61
2:C:13:DA:H2''	2:C:14:DG:C8	2.38	0.59
3:A:820:LEU:HD21	3:A:843:ARG:HH12	1.67	0.58
3:A:827:GLN:NE2	3:A:829:HIS:H	2.02	0.58
3:A:503:MET:HE1	3:A:636:ILE:HD13	1.86	0.57
3:A:843:ARG:HH11	3:A:843:ARG:CB	2.14	0.56
3:A:813:ALA:O	3:A:817:GLU:HG3	2.05	0.56
3:A:730:LYS:O	3:A:734:GLU:HG3	2.05	0.55
1:B:25:DC:H2''	1:B:26:DG:H5'	1.88	0.55
3:A:308:THR:OG1	3:A:311:MET:HE3	2.07	0.55
3:A:503:MET:CE	3:A:636:ILE:HD13	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:693:SER:OG	3:A:696:GLU:HG3	2.07	0.53
3:A:550:THR:HG23	3:A:555:SER:HA	1.91	0.53
3:A:347:ARG:HB3	3:A:349:GLU:OE2	2.09	0.53
3:A:549:LYS:HG3	3:A:553:GLY:O	2.09	0.52
3:A:519:TYR:CD1	3:A:525:GLU:HA	2.44	0.52
3:A:536:VAL:O	3:A:540:GLU:HB2	2.10	0.51
3:A:827:GLN:HE21	3:A:827:GLN:C	2.18	0.51
3:A:728:SER:OG	3:A:730:LYS:HG2	2.10	0.50
2:C:13:DA:H2''	2:C:14:DG:N7	2.27	0.50
3:A:789:ARG:HA	3:A:792:MET:HE3	1.94	0.49
3:A:632:GLU:CD	3:A:632:GLU:N	2.70	0.49
3:A:565:ALA:N	3:A:566:PRO:HD2	2.28	0.49
3:A:459:ARG:HB2	3:A:459:ARG:NH1	2.29	0.48
1:B:22:DA:C2'	1:B:23:DC:H5''	2.41	0.48
3:A:355:PRO:HB2	3:A:356:GLN:OE1	2.15	0.47
3:A:848:VAL:HB	3:A:849:PRO:HD3	1.95	0.47
3:A:579:GLN:NE2	3:A:630:LEU:HD13	2.31	0.45
3:A:435:ARG:O	3:A:436:ALA:HB2	2.17	0.45
3:A:527:ASN:HD21	3:A:529:ASN:HB2	1.82	0.45
1:B:24:DT:OP1	3:A:552:THR:HG22	2.17	0.44
1:B:28:DT:H2'	1:B:29:DA:C8	2.53	0.44
2:C:12:DC:H2'	2:C:13:DA:C8	2.52	0.44
3:A:689:ILE:O	3:A:738:ARG:NH1	2.50	0.44
3:A:833:ILE:N	3:A:833:ILE:HD12	2.32	0.44
3:A:516:GLN:NE2	3:A:516:GLN:HA	2.33	0.44
3:A:677:ARG:HB2	3:A:679:LEU:HG	1.98	0.44
3:A:558:ALA:O	3:A:562:GLU:HG3	2.17	0.43
3:A:610:LEU:HD23	3:A:610:LEU:C	2.44	0.43
3:A:693:SER:HG	3:A:696:GLU:HG3	1.84	0.43
3:A:816:LYS:HE3	7:A:3569:HOH:O	2.18	0.43
2:C:9:DA:H2''	2:C:10:DG:C8	2.53	0.43
3:A:822:ALA:CB	3:A:836:ALA:HB2	2.49	0.43
3:A:515:GLU:HG2	3:A:519:TYR:CE2	2.54	0.42
3:A:820:LEU:HD11	3:A:843:ARG:HH12	1.85	0.42
2:C:3:DC:H6	2:C:3:DC:H2'	1.65	0.42
3:A:429:TYR:O	3:A:435:ARG:HA	2.20	0.41
3:A:692:VAL:CG2	3:A:701:MET:HE1	2.45	0.41
3:A:356:GLN:OE1	3:A:356:GLN:N	2.54	0.41
3:A:514:VAL:O	3:A:518:ILE:HG13	2.21	0.41
3:A:418:GLN:HA	7:A:2575:HOH:O	2.20	0.40
3:A:685:THR:O	3:A:689:ILE:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:596:ARG:HA	3:A:597:PRO:HD3	1.96	0.40
3:A:828:VAL:HB	3:A:831:GLU:CG	2.52	0.40
3:A:730:LYS:HE3	7:A:3421:HOH:O	2.20	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%)	562 (97%)	13 (2%)	3 (0%)	24 10

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	431	LYS
3	A	551	LYS
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	495/495 (100%)	491 (99%)	4 (1%)	73 59

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	303	LEU
3	A	356	GLN
3	A	827	GLN
3	A	843	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	405	GLN
3	A	516	GLN
3	A	527	ASN
3	A	579	GLN
3	A	584	GLN
3	A	723	GLN
3	A	724	ASN
3	A	752	ASN
3	A	827	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	$\# Z > 2$
2	8OG	C	6	2,1	22,25,26	2.45	8 (36%)	26,37,40	2.10	6 (23%)

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	8OG	C	6	2,1	-	2/7/21/22	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	6	8OG	C8-N9	-6.08	1.30	1.40
2	C	6	8OG	C5-C4	5.25	1.44	1.37
2	C	6	8OG	C8-N7	-4.69	1.29	1.38
2	C	6	8OG	C2-N3	3.49	1.41	1.33
2	C	6	8OG	C4-N3	3.20	1.41	1.34
2	C	6	8OG	C2-N1	2.28	1.43	1.37
2	C	6	8OG	C1'-N9	2.23	1.50	1.47
2	C	6	8OG	C6-N1	2.19	1.42	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	8OG	N9-C4-N3	6.46	134.21	126.13
2	C	6	8OG	N7-C8-N9	4.40	111.51	106.61
2	C	6	8OG	C2-N3-C4	4.22	119.58	112.30
2	C	6	8OG	O6-C6-C5	-2.76	120.60	127.26
2	C	6	8OG	C5-C6-N1	2.61	119.30	112.13
2	C	6	8OG	C2-N1-C6	-2.36	120.84	125.11

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	6	8OG	O4'-C1'-N9-C8
2	C	6	8OG	O4'-C1'-N9-C4

There are no ring outliers.

No monomer is involved in short contacts.

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	3.24	4 (36%)	15,15,17	1.51	2 (13%)
4	FRU	D	2	4	11,12,12	1.39	1 (9%)	10,18,18	0.79	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	9.47	1.67	1.52
4	D	2	FRU	O2-C2	3.96	1.47	1.40
4	D	1	GLC	O5-C1	2.74	1.48	1.43
4	D	1	GLC	O5-C5	2.59	1.48	1.43
4	D	1	GLC	C4-C5	2.26	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	4.07	117.65	112.19
4	D	1	GLC	C1-C2-C3	-2.81	105.55	109.64

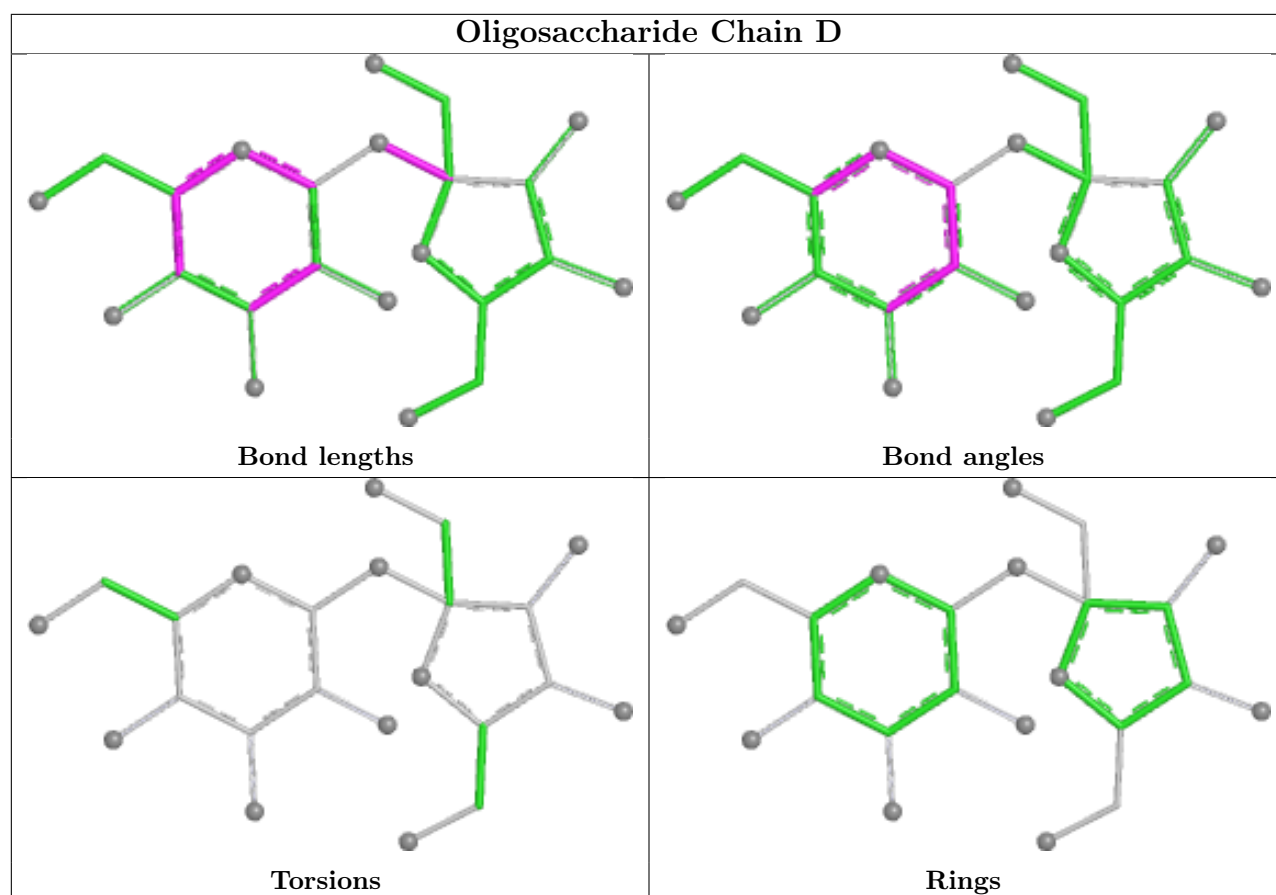
There are no chirality outliers.

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	913	-	4,4,4	0.38	0	6,6,6	0.09	0
5	SO4	A	910	-	4,4,4	0.36	0	6,6,6	0.05	0
5	SO4	A	911	-	4,4,4	0.36	0	6,6,6	0.09	0
5	SO4	A	912	-	4,4,4	0.36	0	6,6,6	0.09	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

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	10/13 (76%)	1.50	4 (40%) 1 0	12, 22, 60, 64	0
2	C	12/15 (80%)	2.05	6 (50%) 0 0	10, 25, 69, 74	0
3	A	580/580 (100%)	0.64	82 (14%) 6 6	8, 16, 34, 41	0
All	All	602/608 (99%)	0.68	92 (15%) 5 5	8, 16, 35, 74	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	433	ALA	9.3
3	A	431	LYS	6.6
1	B	20	DT	6.2
2	C	15	DG	6.1
3	A	549	LYS	6.1
3	A	297	ALA	6.0
3	A	550	THR	5.6
2	C	13	DA	5.4
3	A	531	PRO	5.2
3	A	559	ASP	5.1
2	C	14	DG	5.1
3	A	434	LYS	5.1
3	A	552	THR	5.0
3	A	551	LYS	4.7
3	A	298	ALA	4.6
3	A	530	SER	4.3
2	C	12	DC	4.2
3	A	547	LEU	4.1
1	B	21	DG	4.1
3	A	511	LEU	3.9
3	A	432	GLY	3.9
3	A	876	LYS	3.8
3	A	435	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
3	A	520	GLU	3.7
3	A	554	TYR	3.7
3	A	719	TYR	3.6
3	A	526	PHE	3.5
3	A	553	GLY	3.5
3	A	562	GLU	3.4
3	A	529	ASN	3.4
3	A	528	ILE	3.4
3	A	738	ARG	3.2
3	A	437	VAL	3.2
3	A	519	TYR	3.2
3	A	632	GLU	3.2
3	A	303	LEU	3.2
3	A	514	VAL	3.2
3	A	309	GLU	3.1
3	A	532	LYS	3.1
3	A	305	ASP	3.1
3	A	843	ARG	3.1
3	A	522	ALA	3.0
3	A	726	ASN	3.0
1	B	22	DA	3.0
3	A	356	GLN	3.0
3	A	516	GLN	2.9
3	A	505	LYS	2.9
3	A	730	LYS	2.9
3	A	507	LEU	2.9
3	A	546	VAL	2.9
3	A	306	ARG	2.8
3	A	523	GLY	2.8
3	A	534	LEU	2.8
3	A	748	ARG	2.8
3	A	695	ASP	2.8
3	A	436	ALA	2.7
3	A	629	ARG	2.7
3	A	518	ILE	2.7
1	B	23	DC	2.7
3	A	729	ARG	2.7
3	A	593	LYS	2.6
3	A	525	GLU	2.6
3	A	459	ARG	2.6
3	A	502	GLN	2.6
3	A	430	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
3	A	533	GLN	2.5
3	A	548	LYS	2.5
3	A	325	GLU	2.5
3	A	506	GLU	2.5
3	A	572	GLU	2.5
3	A	521	LEU	2.4
3	A	524	GLN	2.4
3	A	535	GLY	2.3
3	A	509	GLU	2.3
3	A	466	ARG	2.3
3	A	723	GLN	2.3
3	A	472	ARG	2.3
3	A	512	GLY	2.3
3	A	737	GLU	2.3
3	A	579	GLN	2.2
3	A	710	PHE	2.2
2	C	10	DG	2.2
3	A	636	ILE	2.2
3	A	558	ALA	2.2
2	C	11	DT	2.2
3	A	350	THR	2.2
3	A	755	GLN	2.1
3	A	560	VAL	2.1
3	A	566	PRO	2.1
3	A	536	VAL	2.1
3	A	527	ASN	2.1
3	A	364	GLU	2.1

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.

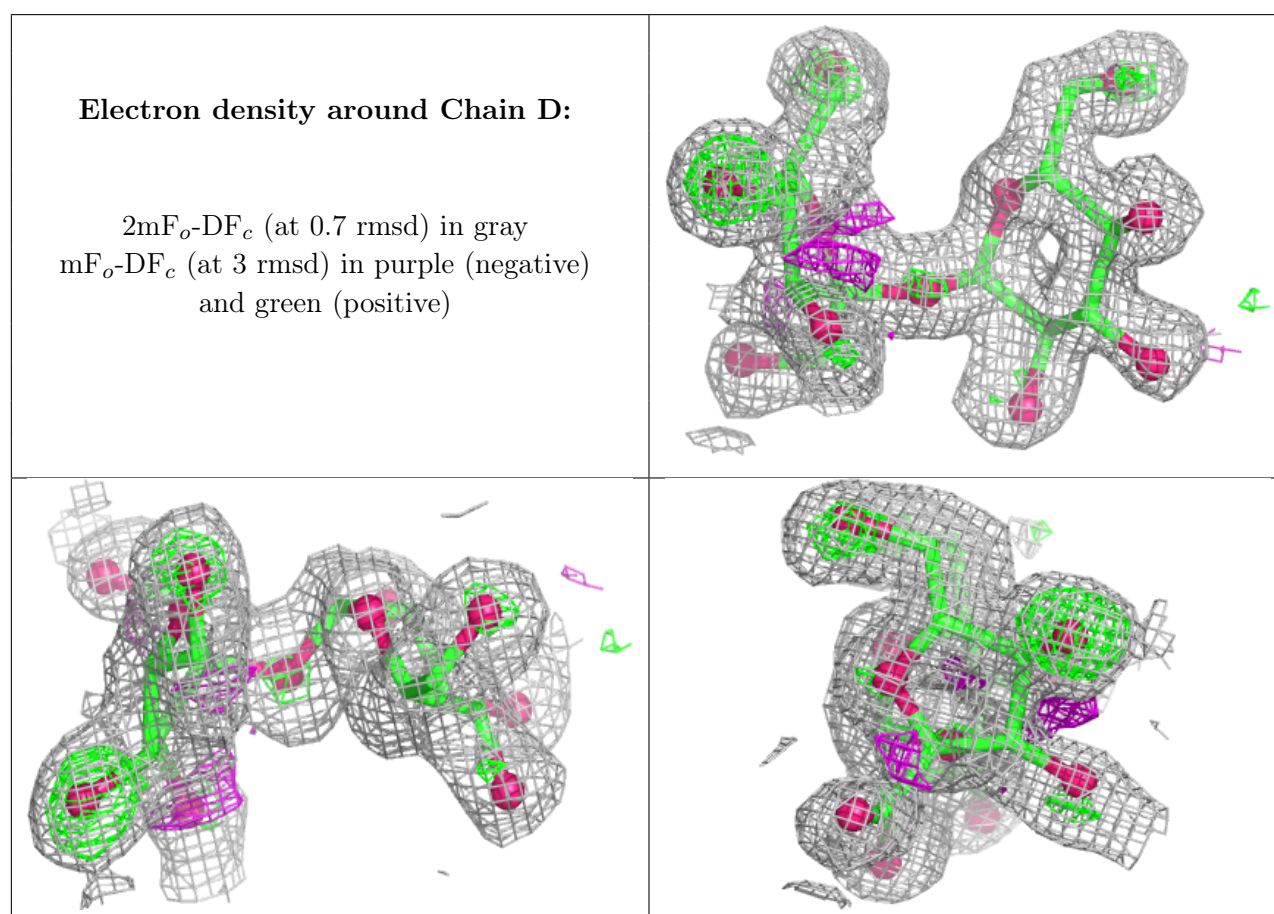
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	8OG	C	6	23/24	0.98	0.05	9,10,11,11	0

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(Å ²)	Q<0.9
4	FRU	D	2	12/12	0.79	0.25	44,44,45,45	0
4	GLC	D	1	11/12	0.80	0.20	45,45,45,45	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	913	5/5	0.85	0.12	53,54,54,54	0
5	SO4	A	912	5/5	0.86	0.15	36,36,36,36	0
5	SO4	A	910	5/5	0.88	0.13	48,48,48,48	0
5	SO4	A	911	5/5	0.97	0.11	22,22,22,22	0
6	MG	A	920	1/1	0.99	0.09	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.