



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 4, 2022 – 10:04 pm BST

PDB ID : 7O2S
Title : Crystal structure of a tetrameric form of Carbonic anhydrase from Schistosoma mansoni
Authors : Ferraroni, M.; Angeli, A.
Deposited on : 2021-03-31
Resolution : 2.28 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

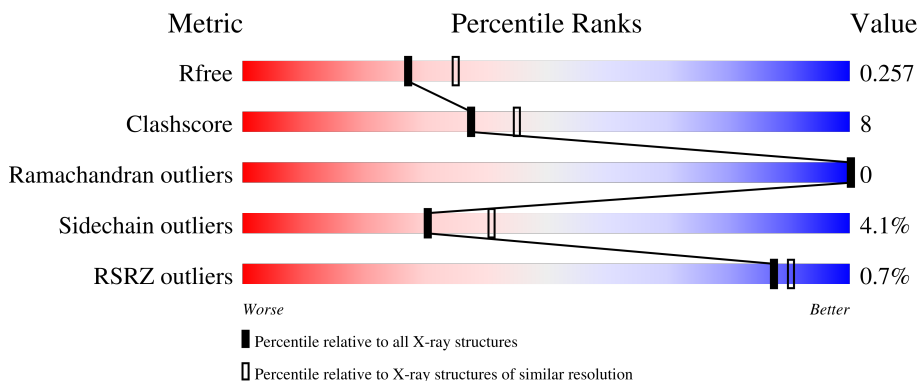
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

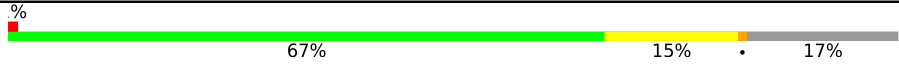
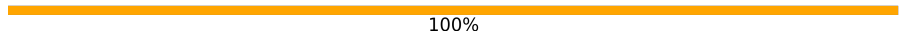
The reported resolution of this entry is 2.28 Å.

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}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	A	332	 67% 15% 17%
2	D	2	 100%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2301 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 protein called Carbonic anhydrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	2218	1417	376	418	7	0	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP A0A3Q0KSG2
A	-7	GLU	-	expression tag	UNP A0A3Q0KSG2
A	-6	THR	-	expression tag	UNP A0A3Q0KSG2
A	-5	ASP	-	expression tag	UNP A0A3Q0KSG2
A	-4	THR	-	expression tag	UNP A0A3Q0KSG2
A	-3	LEU	-	expression tag	UNP A0A3Q0KSG2
A	-2	LEU	-	expression tag	UNP A0A3Q0KSG2
A	-1	LEU	-	expression tag	UNP A0A3Q0KSG2
A	0	TRP	-	expression tag	UNP A0A3Q0KSG2
A	1	VAL	-	expression tag	UNP A0A3Q0KSG2
A	2	LEU	-	expression tag	UNP A0A3Q0KSG2
A	3	LEU	-	expression tag	UNP A0A3Q0KSG2
A	4	LEU	-	expression tag	UNP A0A3Q0KSG2
A	5	TRP	-	expression tag	UNP A0A3Q0KSG2
A	6	VAL	-	expression tag	UNP A0A3Q0KSG2
A	7	PRO	-	expression tag	UNP A0A3Q0KSG2
A	8	GLY	-	expression tag	UNP A0A3Q0KSG2
A	9	SER	-	expression tag	UNP A0A3Q0KSG2
A	10	THR	-	expression tag	UNP A0A3Q0KSG2
A	11	GLY	-	expression tag	UNP A0A3Q0KSG2
A	12	ASP	-	expression tag	UNP A0A3Q0KSG2
A	13	ALA	-	expression tag	UNP A0A3Q0KSG2
A	14	ALA	-	expression tag	UNP A0A3Q0KSG2
A	15	GLN	-	expression tag	UNP A0A3Q0KSG2
A	16	PRO	-	expression tag	UNP A0A3Q0KSG2
A	17	ALA	-	expression tag	UNP A0A3Q0KSG2
A	18	ARG	-	expression tag	UNP A0A3Q0KSG2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ARG	-	expression tag	UNP A0A3Q0KSG2
A	20	ALA	-	expression tag	UNP A0A3Q0KSG2
A	299	ARG	-	expression tag	UNP A0A3Q0KSG2
A	300	GLY	-	expression tag	UNP A0A3Q0KSG2
A	301	GLY	-	expression tag	UNP A0A3Q0KSG2
A	302	PRO	-	expression tag	UNP A0A3Q0KSG2
A	303	GLU	-	expression tag	UNP A0A3Q0KSG2
A	304	GLN	-	expression tag	UNP A0A3Q0KSG2
A	305	LYS	-	expression tag	UNP A0A3Q0KSG2
A	306	LEU	-	expression tag	UNP A0A3Q0KSG2
A	307	ILE	-	expression tag	UNP A0A3Q0KSG2
A	308	SER	-	expression tag	UNP A0A3Q0KSG2
A	309	GLU	-	expression tag	UNP A0A3Q0KSG2
A	310	GLU	-	expression tag	UNP A0A3Q0KSG2
A	311	ASP	-	expression tag	UNP A0A3Q0KSG2
A	312	LEU	-	expression tag	UNP A0A3Q0KSG2
A	313	ASN	-	expression tag	UNP A0A3Q0KSG2
A	314	SER	-	expression tag	UNP A0A3Q0KSG2
A	315	ALA	-	expression tag	UNP A0A3Q0KSG2
A	316	VAL	-	expression tag	UNP A0A3Q0KSG2
A	317	ASP	-	expression tag	UNP A0A3Q0KSG2
A	318	HIS	-	expression tag	UNP A0A3Q0KSG2
A	319	HIS	-	expression tag	UNP A0A3Q0KSG2
A	320	HIS	-	expression tag	UNP A0A3Q0KSG2
A	321	HIS	-	expression tag	UNP A0A3Q0KSG2
A	322	HIS	-	expression tag	UNP A0A3Q0KSG2
A	323	HIS	-	expression tag	UNP A0A3Q0KSG2

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	2	28	16	2	10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	13	8	1	4	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	6	6	6	0	0

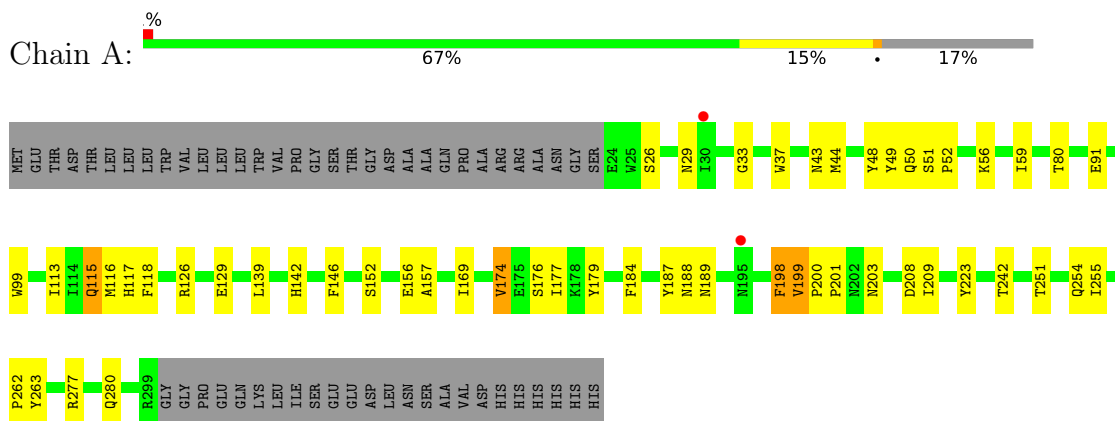
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	36	36	36	0	0

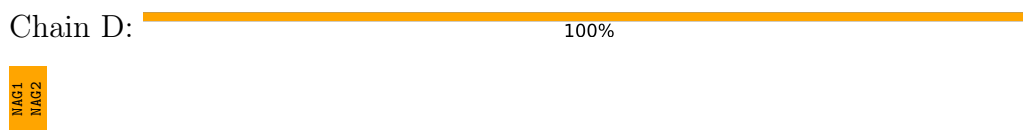
3 Residue-property plots [i](#)

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: Carbonic anhydrase



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	77.81Å 77.81Å 138.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.28 43.05 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-2.28) 99.5 (43.05-2.28)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.205 , 0.254 0.206 , 0.257	Depositor DCC
R_{free} test set	1003 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2301	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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: NAG, ZN

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	A	0.39	0/2278	0.78	1/3104 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ARG	CG-CD-NE	-5.90	99.41	111.80

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	A	2218	0	2130	33	0
2	D	28	0	25	1	0
3	A	13	0	11	1	0
4	A	6	0	0	0	0
5	A	36	0	0	1	0
All	All	2301	0	2166	34	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 8.

The worst 5 of 34 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)
1:A:115:GLN:NE2	1:A:117:HIS:HD1	1.62	0.98
1:A:115:GLN:HE22	1:A:117:HIS:HD1	0.96	0.94
1:A:199:VAL:HG12	1:A:262:PRO:HG3	1.57	0.86
1:A:91:GLU:OE2	1:A:115:GLN:HG3	1.97	0.64
1:A:48:TYR:HE1	1:A:49:TYR:CZ	2.17	0.62

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
1	A	274/332 (82%)	264 (96%)	10 (4%)	0	100 100

There are no Ramachandran outliers to report.

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
1	A	246/297 (83%)	236 (96%)	10 (4%)	30 41

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	A	255	ILE
1	A	263	TYR
1	A	174	VAL
1	A	176	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	115	GLN
1	A	188	ASN

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](#)

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	$\# Z > 2$
2	NAG	D	1	2,1	14,14,15	0.62	0	17,19,21	1.67	4 (23%)
2	NAG	D	2	2	14,14,15	1.01	1 (7%)	17,19,21	2.12	4 (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	NAG	D	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	C1-C2	2.26	1.55	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C4-C3-C2	5.29	118.77	111.02
2	D	1	NAG	C3-C4-C5	-4.28	102.60	110.24
2	D	2	NAG	C1-O5-C5	4.18	117.85	112.19
2	D	1	NAG	O5-C1-C2	-2.85	106.78	111.29
2	D	2	NAG	O5-C5-C6	2.63	111.33	107.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

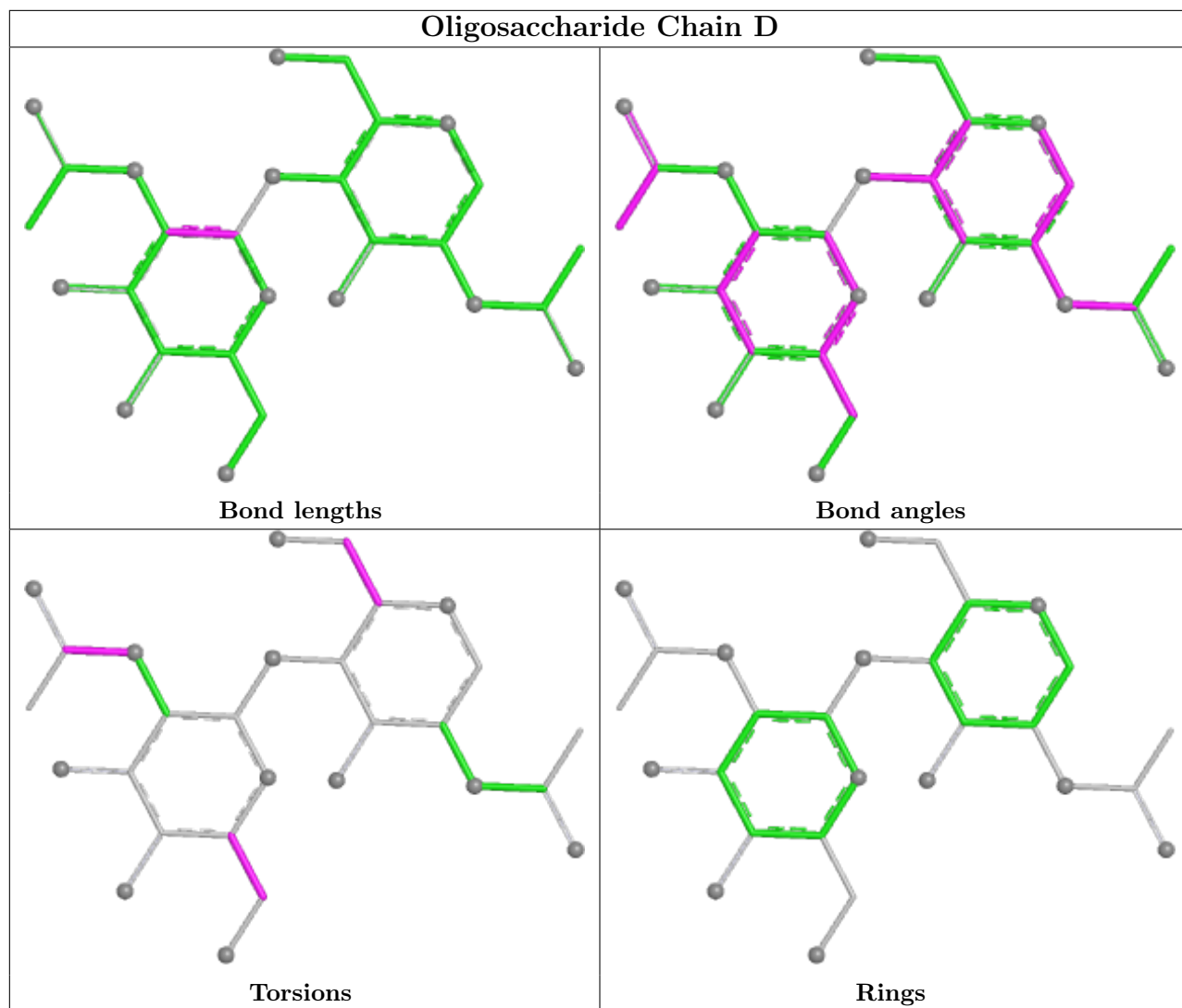
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	1	0
2	D	1	NAG	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 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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	$\# Z > 2$
3	NAG	A	401	1	13,13,15	0.84	1 (7%)	16,17,21	1.55	5 (31%)

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
3	NAG	A	401	1	-	4/6/19/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	NAG	C1-C2	2.06	1.53	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NAG	O5-C5-C6	3.04	111.97	107.20
3	A	401	NAG	C2-N2-C7	2.63	126.25	122.78
3	A	401	NAG	C8-C7-N2	2.44	120.23	116.10
3	A	401	NAG	C3-C4-C5	2.18	113.60	110.77
3	A	401	NAG	C3-C2-C1	2.18	111.50	109.50

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	NAG	O5-C5-C6-O6
3	A	401	NAG	C8-C7-N2-C2
3	A	401	NAG	O7-C7-N2-C2
3	A	401	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NAG	1	0

5.7 Other polymers [i](#)

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	A	276/332 (83%)	-0.21	2 (0%) 87 90	46, 62, 91, 130	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	30	ILE	2.3
1	A	195	ASN	2.3

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

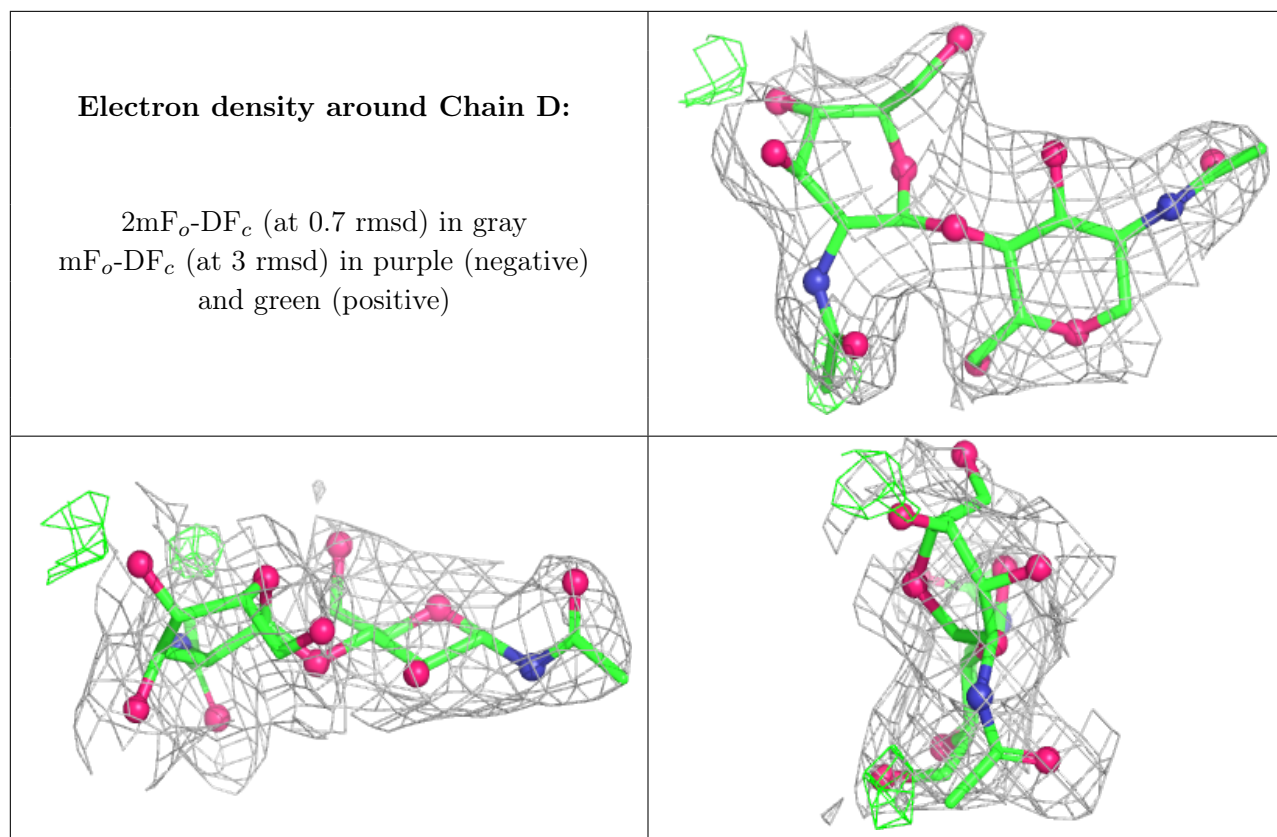
There are no non-standard protein/DNA/RNA residues in this entry.

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
2	NAG	D	2	14/15	0.76	0.22	81,111,120,122	0
2	NAG	D	1	14/15	0.96	0.12	62,90,100,100	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
3	NAG	A	401	13/15	0.84	0.20	87,97,116,121	0
4	ZN	A	406	1/1	0.95	0.10	103,103,103,103	1
4	ZN	A	404	1/1	0.96	0.21	80,80,80,80	1
4	ZN	A	407	1/1	0.96	0.09	103,103,103,103	1
4	ZN	A	403	1/1	0.98	0.10	85,85,85,85	0
4	ZN	A	402	1/1	0.99	0.15	60,60,60,60	0
4	ZN	A	405	1/1	0.99	0.10	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.