



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 01:13 PM BST

PDB ID : 1THG
Title : 1.8 ANGSTROMS REFINED STRUCTURE OF THE LIPASE FROM
GEOTRICHUM CANDIDUM
Authors : Schrag, J.D.; Cygler, M.
Deposited on : 1992-07-28
Resolution : 1.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

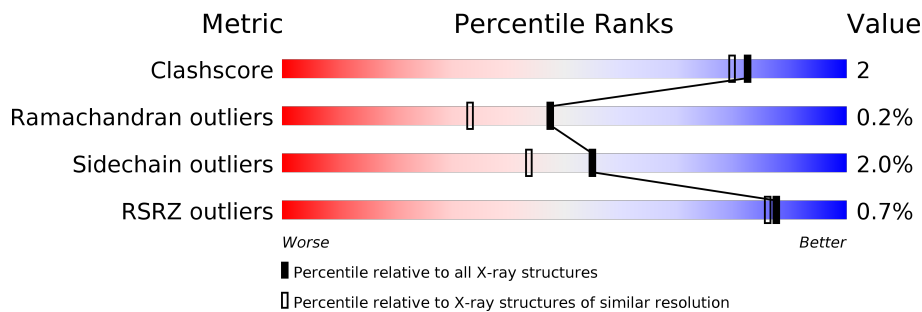
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on 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	544	
2	B	2	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 4694 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 Lipase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	544	4295	2742	719	818	16	0	17	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PCA	-	expression tag	UNP P22394
A	4	THR	ARG	conflict	UNP P22394
A	5	ALA	PRO	conflict	UNP P22394
A	6	VAL	SER	conflict	UNP P22394

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



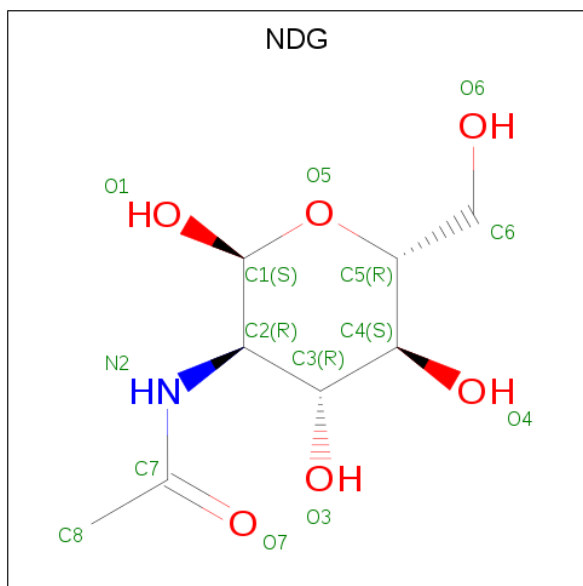
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	28	16	2	10	0	0	0

- 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	14	8	1	5	0	0

- Molecule 4 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0

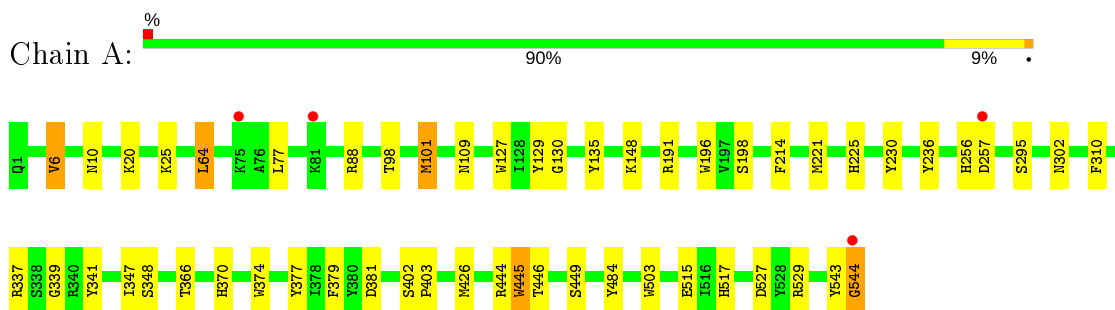
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	343	Total 343	O 343	0	0

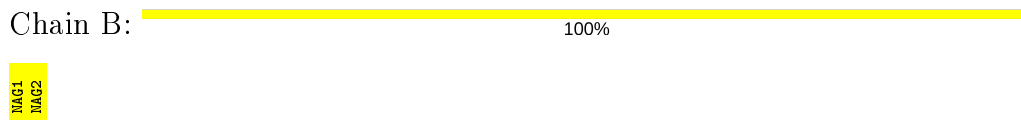
3 Residue-property plots [i](#)

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: Lipase 2



- 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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.40 Å 84.00 Å 56.00 Å 90.00° 100.10° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.80 15.44 – 1.78	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.80) 62.5 (15.44-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 1.78 Å)	Xtrriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.157 , (Not available) 0.148 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.1	Xtrriage
Anisotropy	0.358	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 64.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4694	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.96% 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: PCA, NAG, NDG

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	0.67	0/4454	1.19	30/6057 (0.5%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	543	TYR	CA-C-N	-9.46	97.28	116.20
1	A	374	TRP	CD1-CG-CD2	8.34	112.97	106.30
1	A	445	TRP	CD1-CG-CD2	7.42	112.24	106.30
1	A	445	TRP	CE2-CD2-CG	-7.26	101.49	107.30
1	A	374	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	A	529	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	A	196	TRP	CD1-CG-CD2	6.72	111.68	106.30
1	A	196	TRP	CE2-CD2-CG	-6.61	102.01	107.30
1	A	444	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	A	529	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	88	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	337	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	A	127	TRP	CD1-CG-CD2	5.88	111.00	106.30
1	A	543	TYR	O-C-N	5.82	133.10	123.20
1	A	445	TRP	CG-CD2-CE3	5.67	139.00	133.90
1	A	129	TYR	CB-CG-CD2	-5.59	117.64	121.00
1	A	444	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	191	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	527	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	445	TRP	CB-CG-CD1	-5.43	119.94	127.00
1	A	544	GLY	N-CA-C	-5.43	99.52	113.10
1	A	503	TRP	CD1-CG-CD2	5.40	110.62	106.30
1	A	127	TRP	CE2-CD2-CG	-5.31	103.05	107.30
1	A	236	TYR	CB-CG-CD2	-5.29	117.82	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	A	101	MET	CA-CB-CG	5.14	122.05	113.30
1	A	484	TYR	CB-CG-CD2	-5.11	117.94	121.00
1	A	196	TRP	CB-CG-CD1	-5.08	120.40	127.00
1	A	374	TRP	CG-CD1-NE1	-5.06	105.04	110.10
1	A	257	ASP	CB-CG-OD1	5.01	122.81	118.30

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	4295	0	4132	20	0
2	B	28	0	25	0	0
3	A	14	0	13	0	0
4	A	14	0	12	3	0
5	A	343	0	0	2	0
All	All	4694	0	4182	21	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 2.

All (21) 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:20:LYS:HE2	1:A:148[A]:LYS:HG2	1.65	0.77
1:A:366:THR:H	1:A:370:HIS:HD2	1.47	0.61
1:A:221:MET:O	1:A:225:HIS:HD2	1.92	0.53
1:A:6:VAL:HG13	4:A:996:NDG:H8C3	1.92	0.52
1:A:379[A]:PHE:CZ	1:A:426:MET:SD	3.03	0.52
1:A:515:GLU:OE2	1:A:517:HIS:HE1	1.92	0.51
1:A:339:GLY:HA2	1:A:341:TYR:CE1	2.49	0.48
1:A:101:MET:HE2	1:A:135:TYR:HE1	1.79	0.48
1:A:381:ASP:HB2	1:A:544:GLY:HA3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:SER:HA	1:A:403:PRO:C	2.34	0.47
1:A:64:LEU:HD21	1:A:302[B]:ASN:HA	1.97	0.46
1:A:25:LYS:HA	1:A:109:ASN:HD22	1.80	0.46
1:A:64:LEU:HD21	1:A:302[A]:ASN:HA	1.98	0.44
1:A:347:ILE:HG12	1:A:445:TRP:HB2	2.00	0.43
1:A:6:VAL:CG1	4:A:996:NDG:H8C3	2.48	0.43
1:A:20:LYS:HE2	1:A:148[B]:LYS:HG3	2.00	0.42
1:A:198:SER:HA	5:A:656:HOH:O	2.18	0.42
1:A:101:MET:CE	1:A:135:TYR:HE1	2.33	0.41
1:A:310:PHE:HE2	1:A:377:TYR:CE2	2.37	0.41
4:A:996:NDG:C8	5:A:649:HOH:O	2.69	0.40
1:A:348:SER:O	1:A:446:THR:HA	2.21	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
1	A	559/544 (103%)	537 (96%)	21 (4%)	1 (0%)	47 33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	GLY

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	467/451 (104%)	457 (98%)	10 (2%)	53 42

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	10	ASN
1	A	64	LEU
1	A	77	LEU
1	A	98	THR
1	A	214	PHE
1	A	256	HIS
1	A	295[A]	SER
1	A	295[B]	SER
1	A	449	SER

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

Mol	Chain	Res	Type
1	A	63	GLN
1	A	109	ASN
1	A	225	HIS
1	A	248	GLN
1	A	298	HIS
1	A	370	HIS
1	A	470	GLN
1	A	479	ASN
1	A	517	HIS
1	A	521	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](#)

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	$\# Z > 2$
1	PCA	A	1	1	7,8,9	0.85	0	9,10,12	0.78	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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1

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.

5.5 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	B	1	1,2	14,14,15	0.40	0	17,19,21	1.17	2 (11%)
2	NAG	B	2	2	14,14,15	0.56	0	17,19,21	1.04	1 (5%)

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	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C8-C7-N2	2.12	119.69	116.10
2	B	2	NAG	C1-O5-C5	2.07	114.99	112.19
2	B	1	NAG	C2-N2-C7	-2.06	119.97	122.90

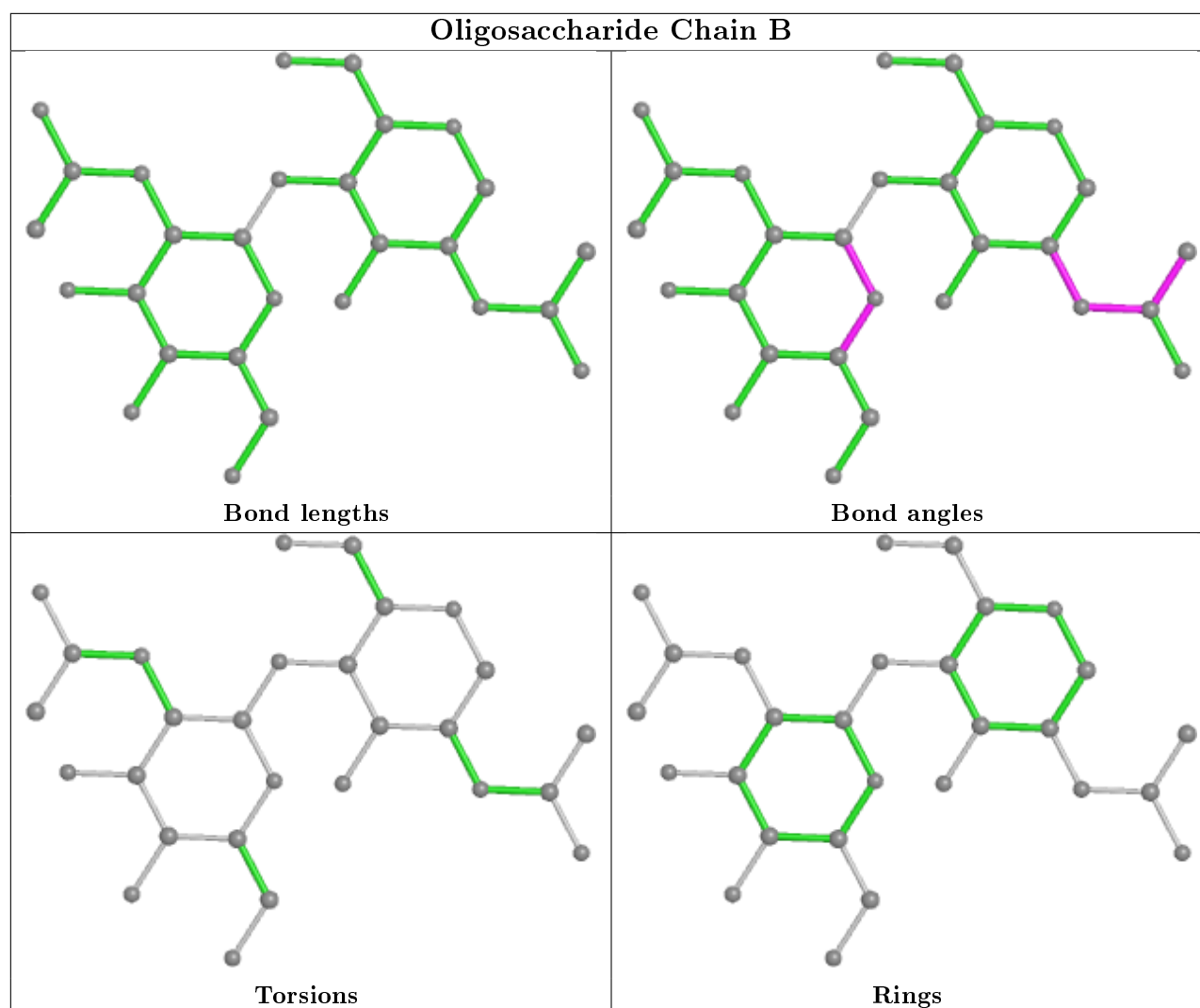
There are no chirality outliers.

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](#)

2 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	$\# Z > 2$
3	NAG	A	994	1	14,14,15	0.68	0	17,19,21	1.20	1 (5%)
4	NDG	A	996	1	14,14,15	0.76	0	17,19,21	1.56	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
3	NAG	A	994	1	-	2/6/23/26	0/1/1/1
4	NDG	A	996	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	996	NDG	O5-C1-C2	-3.20	106.24	111.29
4	A	996	NDG	C2-N2-C7	-2.46	119.41	122.90
4	A	996	NDG	O3-C3-C2	2.29	114.20	109.47
4	A	996	NDG	C6-C5-C4	-2.28	107.67	113.00
3	A	994	NAG	O5-C5-C6	2.15	110.58	107.20

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	996	NDG	C4-C5-C6-O6
4	A	996	NDG	O5-C5-C6-O6
3	A	994	NAG	C4-C5-C6-O6
3	A	994	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	996	NDG	3	0

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	A	543/544 (99%)	-0.72	4 (0%) 87 86	6, 15, 31, 50	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	544	GLY	7.9
1	A	81	LYS	2.7
1	A	75	LYS	2.2
1	A	257	ASP	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.

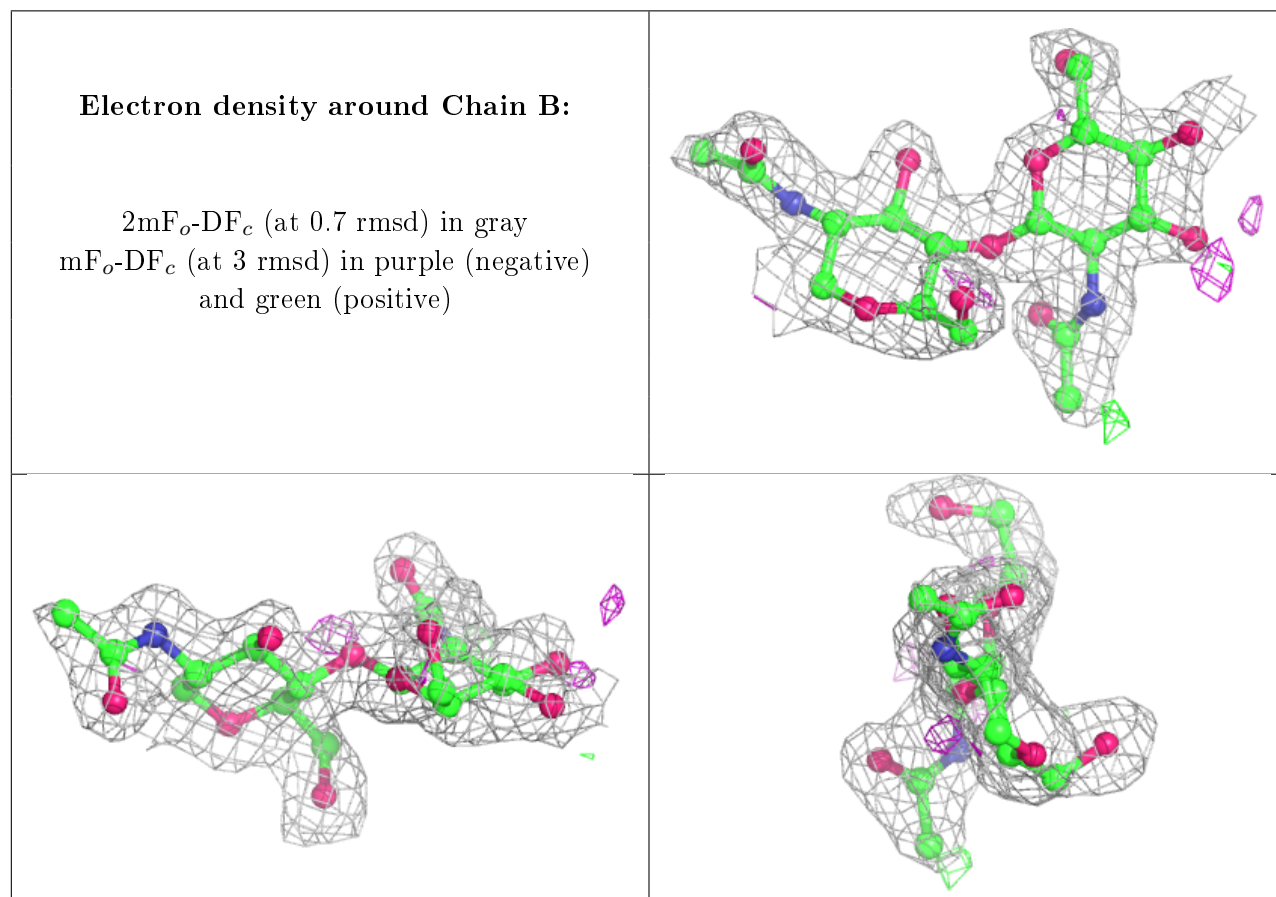
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PCA	A	1	8/9	0.96	0.06	21,22,25,28	0

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
2	NAG	B	2	14/15	0.78	0.24	39,42,44,45	0
2	NAG	B	1	14/15	0.93	0.12	33,36,37,38	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(\AA^2)	Q<0.9
4	NDG	A	996	14/15	0.79	0.28	37,43,46,48	0
3	NAG	A	994	14/15	0.83	0.37	42,45,48,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.