



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 02:03 PM UTC

PDB ID : 1AZX / pdb_00001azx
Title : ANTITHROMBIN/PENTASACCHARIDE COMPLEX
Authors : Jin, L.; Abrahams, J.P.; Skinner, R.; Petitou, M.; Pike, R.N.; Carrell, R.W.
Deposited on : 1997-11-23
Resolution : 2.90 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

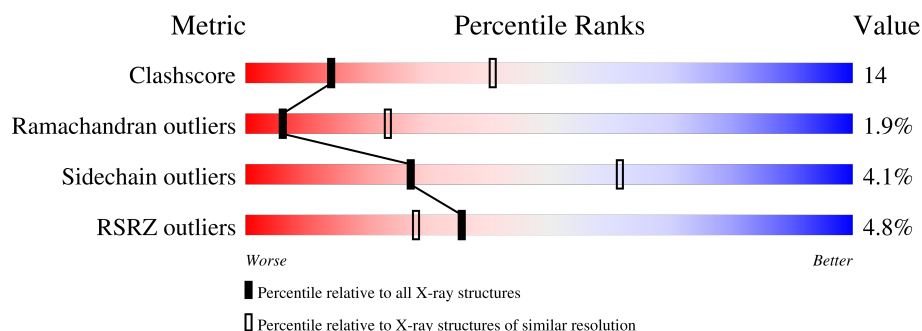
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	I	432	6% 64% 29% • •
1	L	432	4% 62% 31% • •
2	A	5	60% 40%
2	B	5	40% 60%

2 Entry composition [i](#)

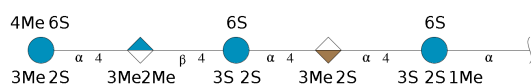
There are 3 unique types of molecules in this entry. The entry contains 6881 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ANTITHROMBIN.

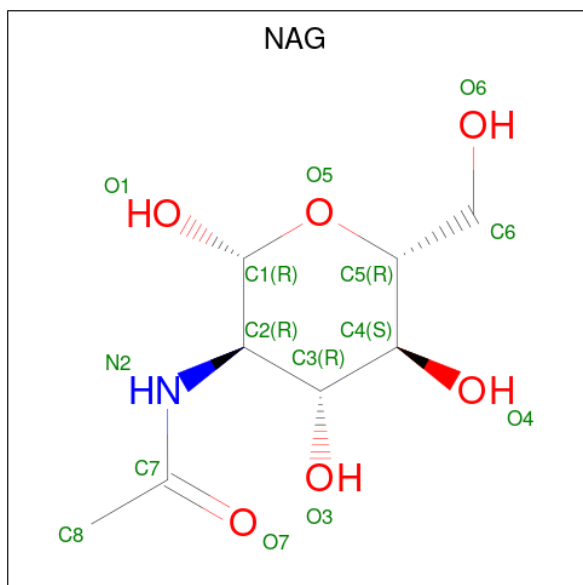
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	417	Total	C	N	O	S	0	0	0
			3328	2121	562	627	18			
1	L	414	Total	C	N	O	S	0	0	0
			3311	2111	559	623	18			

- Molecule 2 is an oligosaccharide called 3,4-di-O-methyl-2,6-di-O-sulfo-alpha-D-glucopyranoside-(1-4)-2,3-di-O-methyl-beta-D-glucopyranuronic acid-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-3-O-methyl-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2,3,6-tri-O-sulfo-alpha-D-glucopyranoside.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	5	Total	C	O	S	0	0	0
			100	36	55	9			
2	B	5	Total	C	O	S	0	0	0
			100	36	55	9			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		

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.

Chain I:

Chain L:

4% 62% 31%

HIS
GLY
SER
PRO
V5
C8
K11
P12
M103
R13
E104
D14
I15
P16
M17
N18
P19
W20
C21
T22
Y23
R24
S25
PRO
GLU
LYS
LYS
ALA
THR
GLU
ASP
GLU
GLY
SER
SER
GLU
GLN
K39
I40
P41
R46
P47
V48
W49
K53
F62
L66
K70
D74
F77
A86
F87
A98
H89
T90
K91
SER
L92
G93
A94
C95
H96
M103
R103
E104
D109
K114
T115
S116
D117
Q118
I119
H120
F123
A124
C128
R129
L130
Y131
R132
K133
A134
M135
K136
S142
A143
R144
M145
L146
F147
G148
D149
L152
T153
F154
M155
Y158
V165
Y166
L170
Q171
P172
L173
S181
I198
T199
D200
P203
A206
E209
L210
T211
V212
L213
N217
K226
S227
K228
F229
S230
P231
E232
K236
F239
S246
C247
Y253
K257
R261
R262
V263
V269
L272
K275
V282
L283
L284
L285
P286
K287
P288
E289
K290
S291
L292
V296
E298
K297
E298
L304
W307
L308
L311
E312
E313
M314
M315
L316
V317
R322
F323
R324
L326
Q336
K337
M338
G339
L340
V341
D342
L351
P352
V355
A356
E357
C358
R359
D360
V364
S365
D366
K370
A371
F372
L373
E374
V375
M376
E377
A382
V389
I390
A391
N396
P397



- Molecule 2: 3,4-di-O-methyl-2,6-di-O-sulfo-alpha-D-glucopyranose-(1-4)-2,3-di-O-methyl-beta-D-glucopyranuronic acid-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-3-O-methyl-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2,3,6-tri-O-sulfo-alpha-D-glucopyranoside

Chain A: 60% 40%



- Molecule 2: 3,4-di-O-methyl-2,6-di-O-sulfo-alpha-D-glucopyranose-(1-4)-2,3-di-O-methyl-beta-D-glucopyranuronic acid-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-3-O-methyl-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2,3,6-tri-O-sulfo-alpha-D-glucopyranoside

Chain B: 40% 60%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.44Å 86.97Å 97.22Å 90.00° 108.88° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.2 (30.00-2.90) 94.4 (30.00-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.01 (at 2.90Å)	Xtriage
Refinement program	TNT 5D	Depositor
R, R_{free}	0.195 , 0.280 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 85.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6881	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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: GU6, Z9L, Z9H, GU1, Z9K, NAG

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	I	0.40	0/3394	0.88	3/4582 (0.1%)
1	L	0.42	0/3376	0.90	12/4557 (0.3%)
All	All	0.41	0/6770	0.89	15/9139 (0.2%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	322	ARG	N-CA-C	-6.92	97.94	108.67
1	L	287	LYS	CA-C-N	6.80	128.34	119.84
1	L	287	LYS	C-N-CA	6.80	128.34	119.84
1	L	226	LYS	N-CA-C	-6.11	104.70	111.36
1	I	88	ALA	N-CA-C	-5.97	104.90	111.82

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	I	3328	0	3333	93	0
1	L	3311	0	3323	94	0
2	A	100	0	16	4	0
2	B	100	0	16	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	14	0	13	5	0
3	L	28	0	26	3	0
All	All	6881	0	6727	191	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 14.

The worst 5 of 191 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:I:356:ALA:O	3:I:501:NAG:H81	1.60	1.01
1:L:129:ARG:HD3	1:L:417:LEU:HD21	1.56	0.87
1:L:20:MET:HA	3:L:501:NAG:H61	1.55	0.87
1:I:17:MET:HB2	1:I:120:HIS:HE1	1.39	0.86
1:I:144:ASN:HB3	1:I:217:ASN:HA	1.67	0.77

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	I	413/432 (96%)	367 (89%)	36 (9%)	10 (2%)	4	18
1	L	410/432 (95%)	377 (92%)	27 (7%)	6 (2%)	8	28
All	All	823/864 (95%)	744 (90%)	63 (8%)	16 (2%)	6	23

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	4	PRO
1	I	200	ASP

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Mol	Chain	Res	Type
1	I	359	ARG
1	L	404	ALA
1	L	288	PRO

5.3.2 Protein sidechains ⓘ

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	I	370/383 (97%)	357 (96%)	13 (4%)	32	66
1	L	368/383 (96%)	351 (95%)	17 (5%)	24	57
All	All	738/766 (96%)	708 (96%)	30 (4%)	27	61

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	46	ARG
1	L	375	VAL
1	L	228	LYS
1	L	402	PHE
1	L	313	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	127	ASN
1	L	268	GLN
1	L	418	ASN
1	L	336	GLN
1	L	396	ASN

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 ⓘ

10 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	Z9L	A	1	2	25,25,25	1.07	0	34,39,39	0.92	1 (2%)
2	Z9K	A	2	2	17,17,18	1.27	2 (11%)	17,25,27	1.17	1 (5%)
2	GU6	A	3	2	23,23,24	1.29	4 (17%)	28,36,38	1.10	1 (3%)
2	GU1	A	4	2	14,14,15	0.92	0	15,19,21	0.94	1 (6%)
2	Z9H	A	5	2	21,21,22	1.05	1 (4%)	26,31,33	1.15	1 (3%)
2	Z9L	B	1	2	25,25,25	1.02	0	34,39,39	0.96	1 (2%)
2	Z9K	B	2	2	17,17,18	1.32	2 (11%)	17,25,27	1.22	3 (17%)
2	GU6	B	3	2	23,23,24	1.19	3 (13%)	28,36,38	1.18	2 (7%)
2	GU1	B	4	2	14,14,15	0.78	0	15,19,21	0.94	1 (6%)
2	Z9H	B	5	2	21,21,22	1.12	1 (4%)	26,31,33	1.04	1 (3%)

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	Z9L	A	1	2	-	8/18/38/38	0/1/1/1
2	Z9K	A	2	2	-	0/11/28/31	0/1/1/1
2	GU6	A	3	2	-	9/16/33/36	0/1/1/1
2	GU1	A	4	2	-	3/8/25/28	0/1/1/1
2	Z9H	A	5	2	-	5/15/32/35	0/1/1/1
2	Z9L	B	1	2	-	6/18/38/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Z9K	B	2	2	-	0/11/28/31	0/1/1/1
2	GU6	B	3	2	-	8/16/33/36	0/1/1/1
2	GU1	B	4	2	-	2/8/25/28	0/1/1/1
2	Z9H	B	5	2	-	5/15/32/35	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	Z9H	O2-C2	-3.35	1.42	1.47
2	B	2	Z9K	O2-C2	-3.28	1.42	1.47
2	A	5	Z9H	O2-C2	-2.91	1.43	1.47
2	B	3	GU6	O2-C2	-2.86	1.43	1.47
2	A	2	Z9K	C1-C2	2.72	1.56	1.51

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5	Z9H	O2-C2-C3	3.76	110.81	106.65
2	A	3	GU6	O2-C2-C3	3.49	110.52	106.65
2	B	3	GU6	O2-C2-C3	2.95	109.92	106.65
2	B	5	Z9H	O2-C2-C3	2.75	109.70	106.65
2	A	2	Z9K	O2-C2-C3	2.69	109.63	106.65

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	Z9L	C6-O6-S1-O7
2	A	1	Z9L	C6-O6-S1-O11
2	A	3	GU6	C1-C2-O2-S2
2	A	3	GU6	C6-O6-S6-O19
2	A	3	GU6	C6-O6-S6-O20

There are no ring outliers.

5 monomers are involved in 9 short contacts:

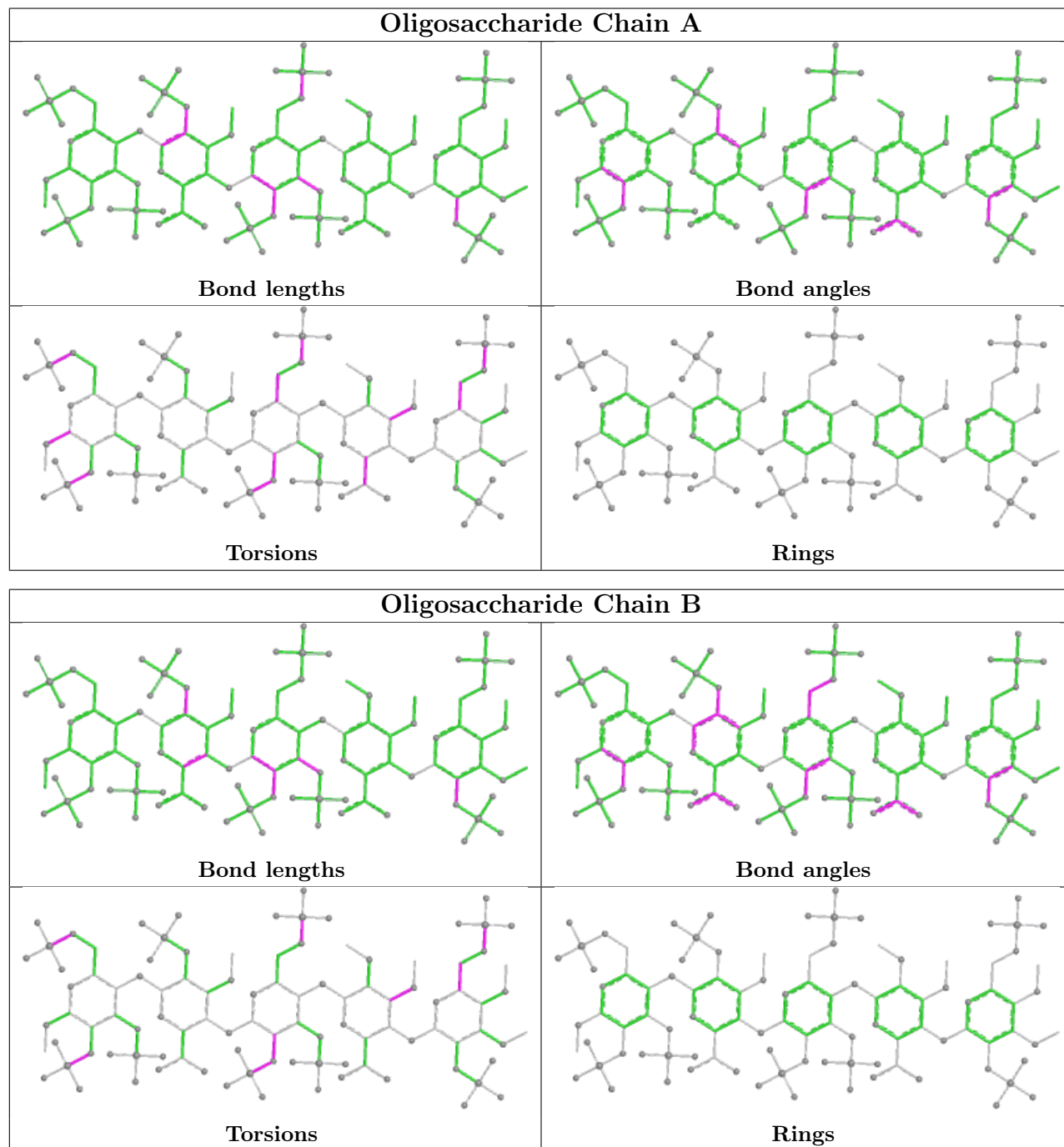
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4	GU1	2	0
2	B	3	GU6	4	0
2	B	4	GU1	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3	GU6	2	0
2	B	2	Z9K	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

3 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	L	502	1	14,14,15	0.86	0	17,19,21	1.67	4 (23%)
3	NAG	I	501	1	14,14,15	0.87	0	17,19,21	1.67	4 (23%)
3	NAG	L	501	1	14,14,15	0.86	0	17,19,21	1.68	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	L	502	1	-	2/6/23/26	0/1/1/1
3	NAG	I	501	1	-	2/6/23/26	0/1/1/1
3	NAG	L	501	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	501	NAG	O5-C1-C2	-3.45	105.96	111.29
3	I	501	NAG	O5-C1-C2	-3.43	105.99	111.29
3	L	502	NAG	O5-C1-C2	-3.41	106.02	111.29
3	L	502	NAG	C1-O5-C5	3.06	116.28	112.19
3	I	501	NAG	C1-O5-C5	3.05	116.28	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	501	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	I	501	NAG	O7-C7-N2-C2
3	L	501	NAG	C8-C7-N2-C2
3	L	501	NAG	O7-C7-N2-C2
3	L	502	NAG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	501	NAG	5	0
3	L	501	NAG	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	I	417/432 (96%)	0.28	24 (5%) 29 22	2, 35, 78, 114	0
1	L	414/432 (95%)	0.11	16 (3%) 43 35	2, 27, 70, 97	0
All	All	831/864 (96%)	0.19	40 (4%) 35 28	2, 32, 74, 114	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	2	GLY	5.1
1	I	223	GLY	5.1
1	I	3	SER	4.8
1	I	25	SER	4.8
1	L	397	PRO	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.

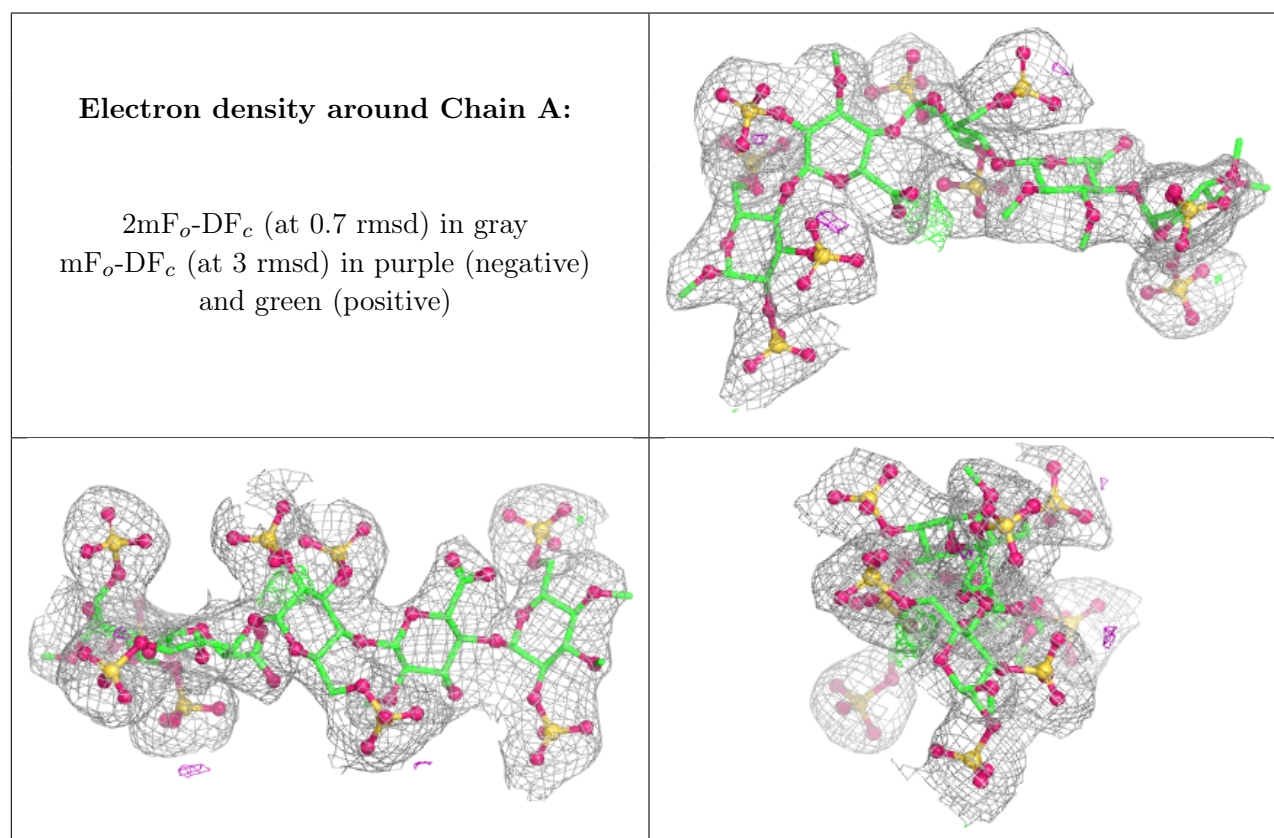
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	Z9L	A	1	25/25	-	-	41,51,52,55	0
2	Z9K	A	2	17/18	-	-	35,55,71,71	0
2	GU6	A	3	23/24	-	-	30,50,65,65	0
2	GU1	A	4	14/15	-	-	37,40,53,53	0
2	Z9H	A	5	21/22	-	-	27,41,56,62	0

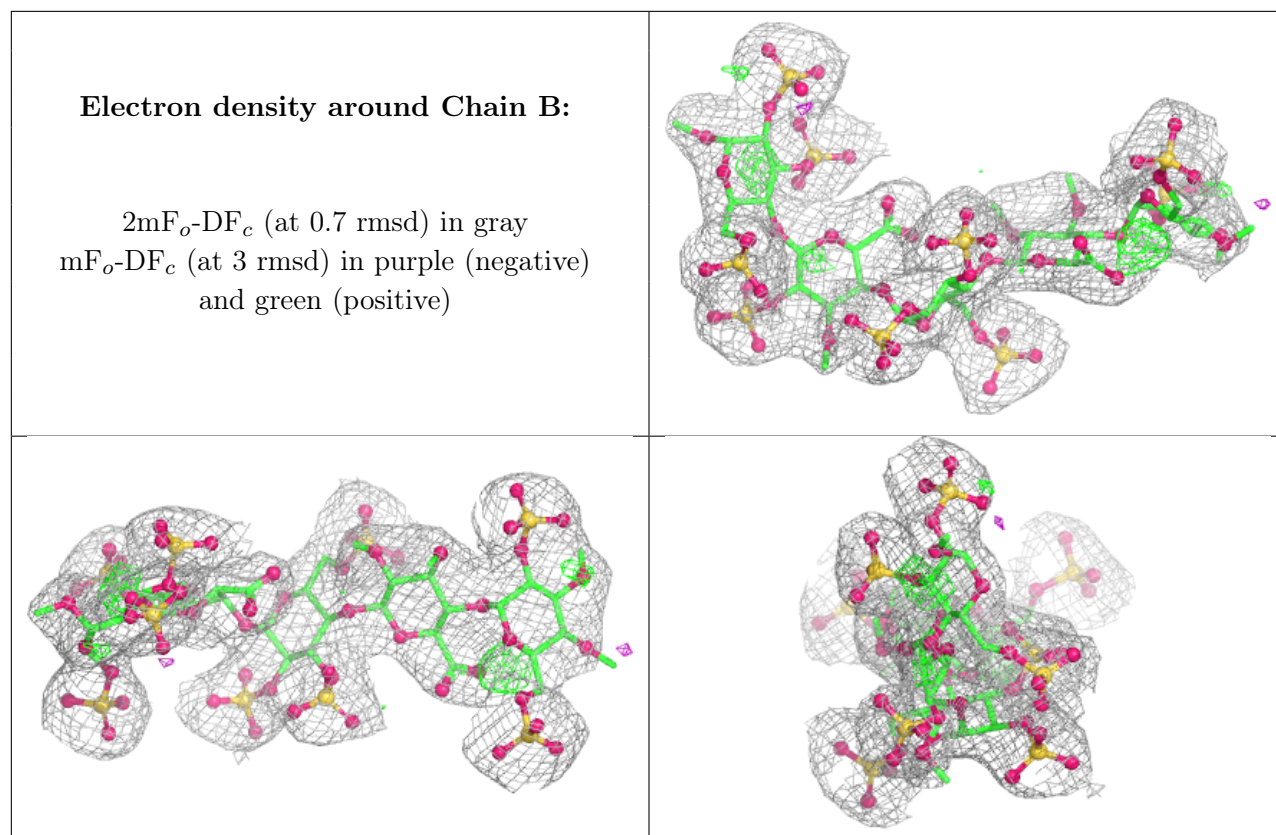
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	Z9L	B	1	25/25	-	-	21,30,44,44	0
2	Z9K	B	2	17/18	-	-	26,30,33,33	0
2	GU6	B	3	23/24	-	-	26,27,56,56	0
2	GU1	B	4	14/15	-	-	28,28,74,74	0
2	Z9H	B	5	21/22	-	-	36,38,45,67	0

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
3	NAG	L	501	14/15	0.45	0.24	30,60,78,82	0
3	NAG	L	502	14/15	0.47	0.19	30,60,78,82	0
3	NAG	I	501	14/15	0.67	0.14	35,55,55,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.