



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 28, 2023 – 06:27 pm GMT

PDB ID : 1E05  
Title : PLASMA ALPHA ANTITHROMBIN-III  
Authors : McCoy, A.J.; Skinner, R.; Abrahams, J.-P.; Pei, X.Y.; Carrell, R.W.  
Deposited on : 2000-03-09  
Resolution : 2.62 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](mailto: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>.

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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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

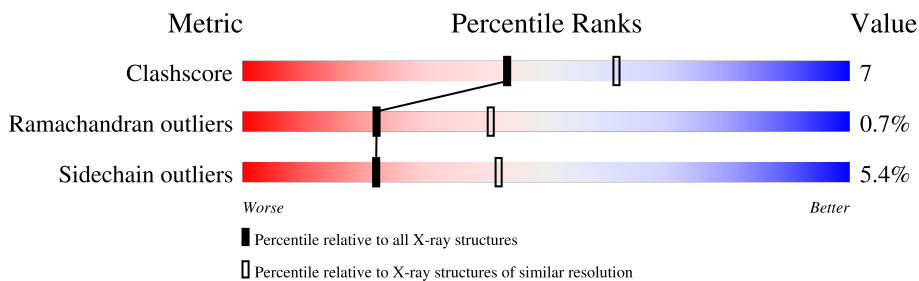
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.62 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	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)

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  $\geq 3$ , 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	I	432	
1	L	432	
2	A	2	
2	C	2	
3	B	3	
4	D	8	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GUP	D	3	X	-	-	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6903 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-III.

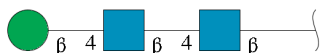
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	I	417	Total 3274	C 2088	N 553	O 617	S 16	0	0	0
1	L	417	Total 3261	C 2082	N 542	O 619	S 18	0	0	0

- 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	A	2	Total 28	C 16	N 2	O 10	0	0	0
2	C	2	Total 28	C 16	N 2	O 10	0	0	0

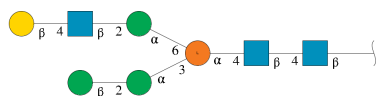
- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	B	3	Total 39	C 22	N 2	O 15	0	0	0

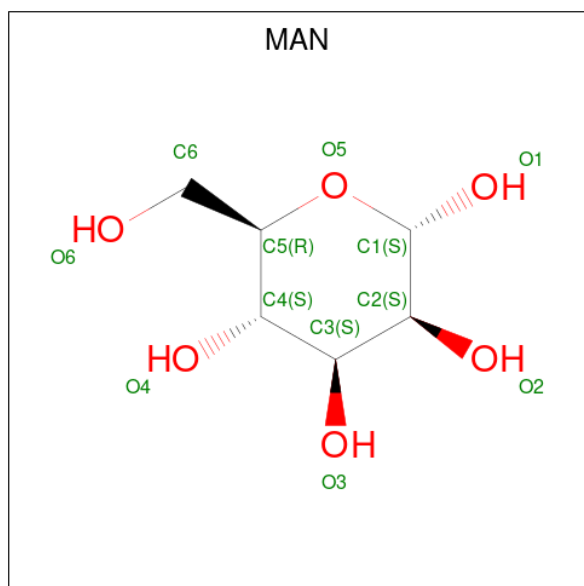
- Molecule 4 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]alpha-L-gulopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucop

yanose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
4	D	8	97	54	3	40	0	0	0

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



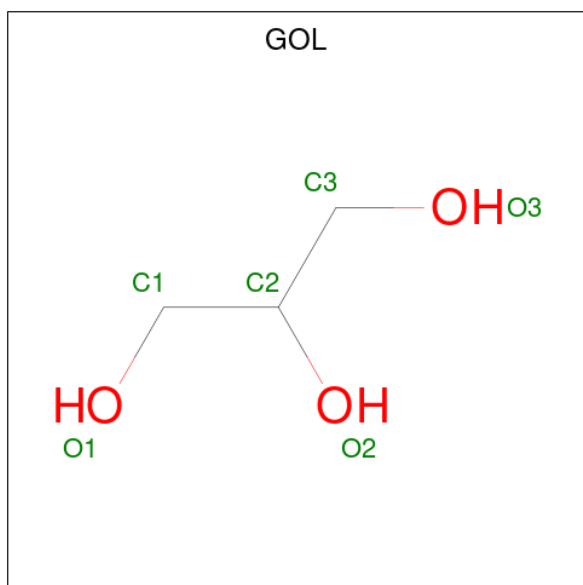
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	I	1	11	6	5	0	0
5	L	1	11	6	5	0	0
5	L	1	11	6	5	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



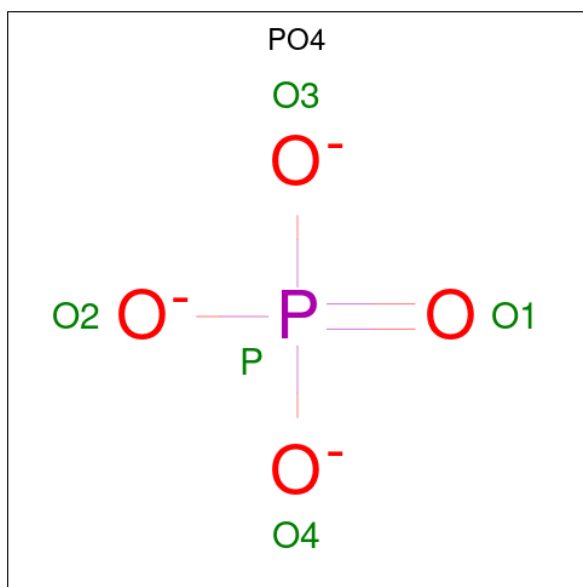
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	I	1	Total 14	C 8	N 1	O 5	0	0
6	I	1	Total 14	C 8	N 1	O 5	0	0
6	L	1	Total 14	C 8	N 1	O 5	0	0
6	L	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	1	Total C O 6 3 3	0	0
7	L	1	Total C O 6 3 3	0	0

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total O P 5 4 1	0	0

- Molecule 9 is water.


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	I	46	Total O 46 46	0	0
9	L	24	Total O 24 24	0	0

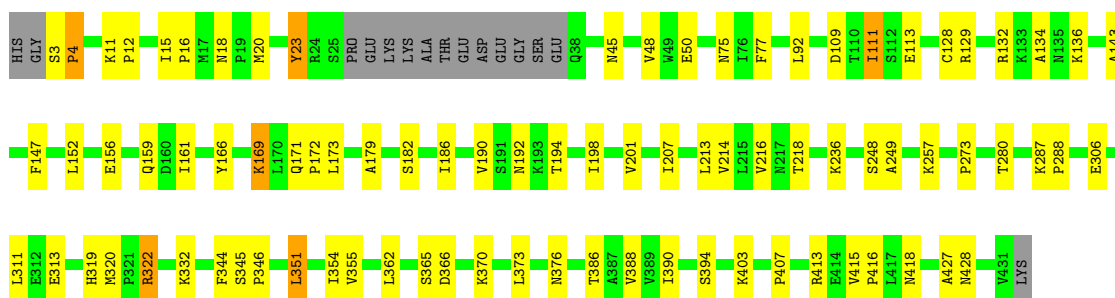
### 3 Residue-property plots

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. 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. 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.


Note EDS was not executed.

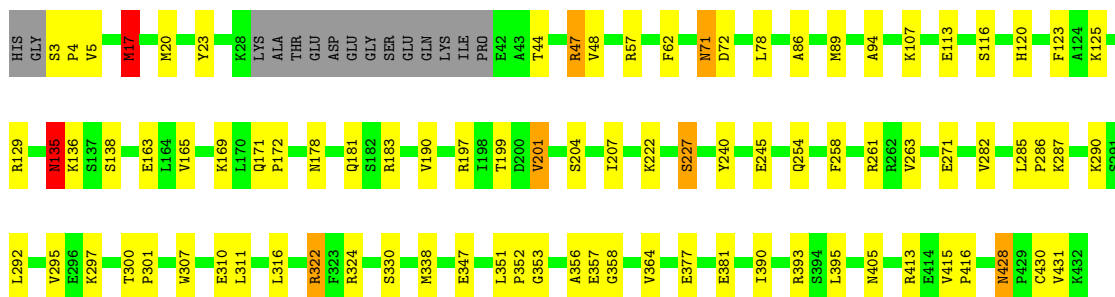
- Molecule 1: ANTITHROMBIN-III

Chain I: 



- Molecule 1: ANTITHROMBIN-III

Chain L: 



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

Chain A: 



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

Chain C: 



MAG1  
MAG2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

100%

MAG1  
MAG2  
BMA3

- Molecule 4: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]alpha-L-gulopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

12%

62%

25%

MAG1  
MAG2  
GUP3  
MAN4  
MAG5  
GAL6  
MAN7  
BMA8

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.41Å 98.31Å 90.41Å 90.00° 103.32° 90.00°	Depositor
Resolution (Å)	20.00 – 2.62	Depositor
% Data completeness (in resolution range)	72.0 (20.00-2.62)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.196 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6903	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

## 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: GAL, PO4, GOL, MAN, BMA, GUP, 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	0.39	0/3340	1.02	4/4519 (0.1%)
1	L	0.37	0/3326	0.99	5/4500 (0.1%)
All	All	0.38	0/6666	1.00	9/9019 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	2
1	L	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	322	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	L	17	MET	CA-CB-CG	7.00	125.20	113.30
1	L	322	ARG	CD-NE-CZ	6.86	133.21	123.60
1	I	413	ARG	CD-NE-CZ	6.39	132.54	123.60
1	I	351	LEU	CA-CB-CG	6.15	129.45	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	113	GLU	Mainchain

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Mol	Chain	Res	Type	Group
1	I	166	TYR	Mainchain
1	L	107	LYS	Mainchain

## 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	3274	0	3213	47	0
1	L	3261	0	3207	42	0
2	A	28	0	25	2	0
2	C	28	0	25	0	0
3	B	39	0	34	0	0
4	D	97	0	79	1	0
5	I	11	0	10	1	0
5	L	22	0	20	1	0
6	I	28	0	26	0	0
6	L	28	0	26	1	0
7	I	6	0	8	0	0
7	L	6	0	8	1	0
8	L	5	0	0	0	0
9	I	46	0	0	0	0
9	L	24	0	0	0	0
All	All	6903	0	6681	91	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 7.

The worst 5 of 91 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:75:ASN:HD21	1:I:428:ASN:H	1.21	0.88
1:I:16:PRO:HD2	1:I:161:ILE:HD11	1.57	0.84
1:I:75:ASN:ND2	1:I:427:ALA:H	1.77	0.83
1:I:75:ASN:HD22	1:I:427:ALA:H	1.30	0.80
1:I:319:HIS:HB2	1:I:403:LYS:HA	1.66	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%)	388 (94%)	22 (5%)	3 (1%)	22	41
1	L	413/432 (96%)	374 (91%)	36 (9%)	3 (1%)	22	41
All	All	826/864 (96%)	762 (92%)	58 (7%)	6 (1%)	22	41

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	4	PRO
1	L	245	GLU
1	L	136	LYS
1	L	263	VAL
1	I	407	PRO

### 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	I	354/383 (92%)	338 (96%)	16 (4%)	27	50
1	L	355/383 (93%)	333 (94%)	22 (6%)	18	35
All	All	709/766 (93%)	671 (95%)	38 (5%)	22	42

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	285	LEU
1	L	405	ASN
1	L	297	LYS
1	L	347	GLU
1	L	431	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	418	ASN
1	L	405	ASN
1	L	120	HIS
1	L	336	GLN
1	L	71	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](#)

15 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	A	1	1,2	14,14,15	1.25	1 (7%)	17,19,21	1.05	2 (11%)
2	NAG	A	2	2	14,14,15	1.15	1 (7%)	17,19,21	1.36	2 (11%)
3	NAG	B	1	1,3	14,14,15	1.35	2 (14%)	17,19,21	2.39	5 (29%)
3	NAG	B	2	3	14,14,15	1.25	1 (7%)	17,19,21	1.11	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BMA	B	3	3	11,11,12	0.67	0	15,15,17	1.19	2 (13%)
2	NAG	C	1	1,2	14,14,15	1.26	1 (7%)	17,19,21	0.77	0
2	NAG	C	2	2	14,14,15	1.20	1 (7%)	17,19,21	1.36	3 (17%)
4	NAG	D	1	1,4	14,14,15	1.24	1 (7%)	17,19,21	1.13	1 (5%)
4	NAG	D	2	4	14,14,15	1.25	1 (7%)	17,19,21	1.59	2 (11%)
4	GUP	D	3	4	11,11,12	0.81	0	15,15,17	2.48	4 (26%)
4	MAN	D	4	4	11,11,12	1.44	1 (9%)	15,15,17	3.28	5 (33%)
4	NAG	D	5	4	14,14,15	1.47	3 (21%)	17,19,21	2.14	6 (35%)
4	GAL	D	6	4	11,11,12	3.31	3 (27%)	15,15,17	1.76	4 (26%)
4	MAN	D	7	4	11,11,12	0.98	1 (9%)	15,15,17	2.10	3 (20%)
4	BMA	D	8	4	11,11,12	0.76	0	15,15,17	1.03	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
2	NAG	A	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	4/6/23/26	0/1/1/1
3	NAG	B	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1
3	BMA	B	3	3	-	0/2/19/22	0/1/1/1
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	5/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	GUP	D	3	4	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	1/1/1/1
4	NAG	D	5	4	-	2/6/23/26	0/1/1/1
4	GAL	D	6	4	-	2/2/19/22	0/1/1/1
4	MAN	D	7	4	-	2/2/19/22	0/1/1/1
4	BMA	D	8	4	-	2/2/19/22	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	6	GAL	C2-C3	-9.95	1.37	1.52
4	D	4	MAN	O2-C2	-4.02	1.34	1.43
4	D	5	NAG	O7-C7	-3.85	1.14	1.23
2	C	2	NAG	O7-C7	-3.84	1.14	1.23
4	D	2	NAG	O7-C7	-3.77	1.14	1.23

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	4	MAN	O2-C2-C3	7.79	125.74	110.14
4	D	7	MAN	C1-O5-C5	6.55	121.07	112.19
4	D	4	MAN	O2-C2-C1	6.43	122.31	109.15
3	B	1	NAG	C1-O5-C5	6.40	120.87	112.19
4	D	3	GUP	O5-C5-C6	5.51	115.84	107.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	3	GUP	C5

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	3	GUP	O5-C5-C6-O6
2	A	2	NAG	O5-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
3	B	2	NAG	O5-C5-C6-O6
2	A	2	NAG	C4-C5-C6-O6

All (1) ring outliers are listed below:

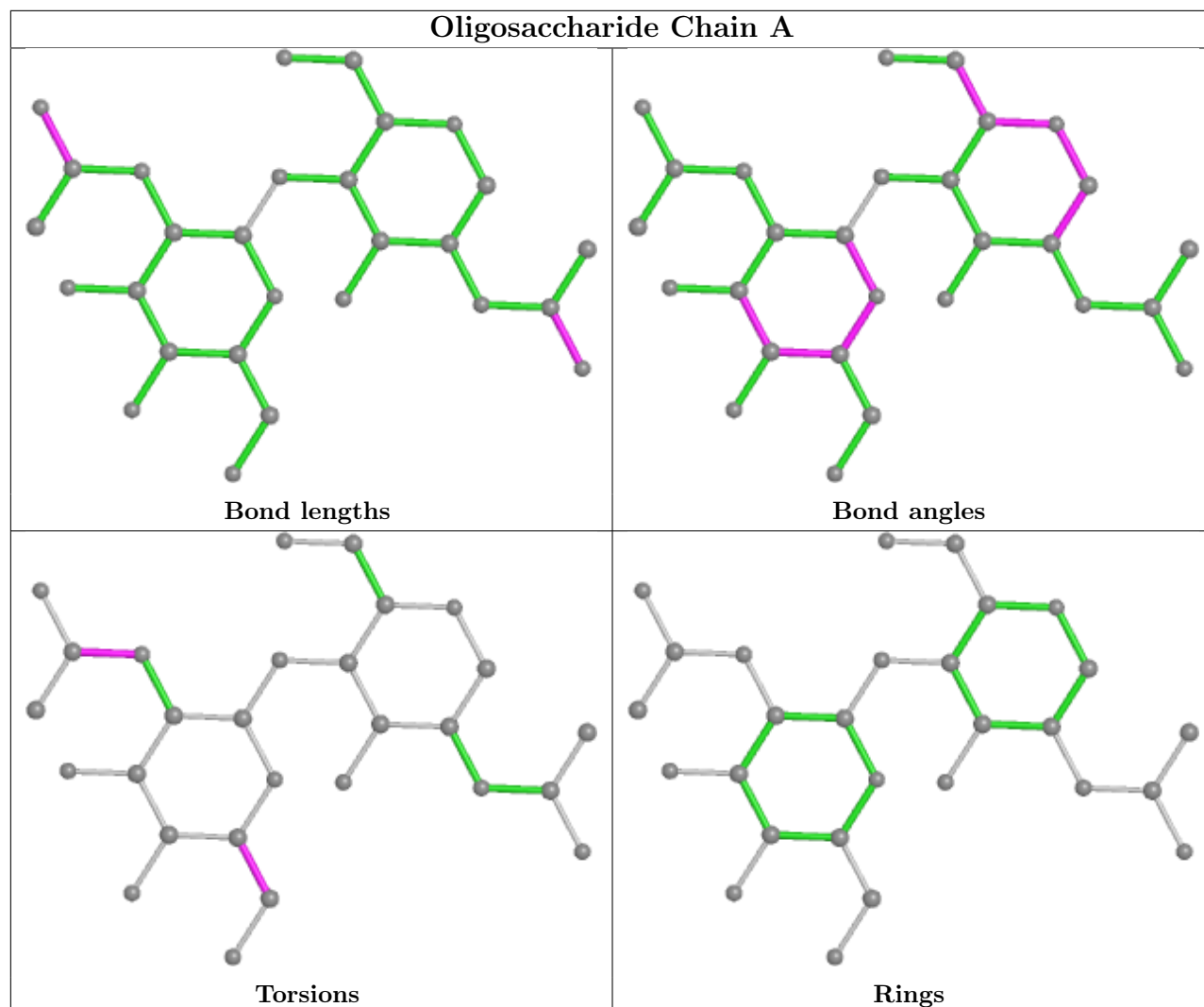
Mol	Chain	Res	Type	Atoms
4	D	4	MAN	C1-C2-C3-C4-C5-O5

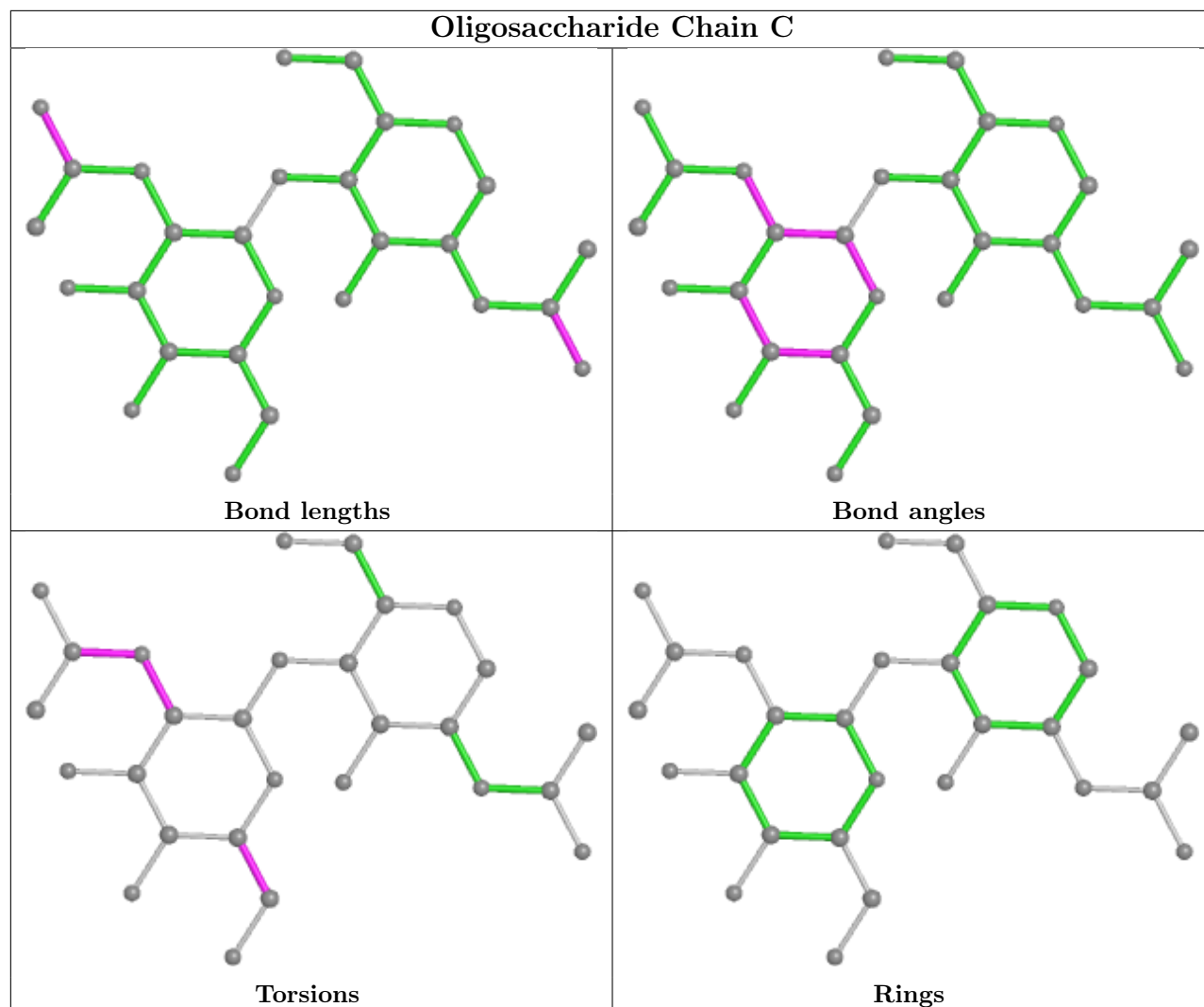
3 monomers are involved in 3 short contacts:

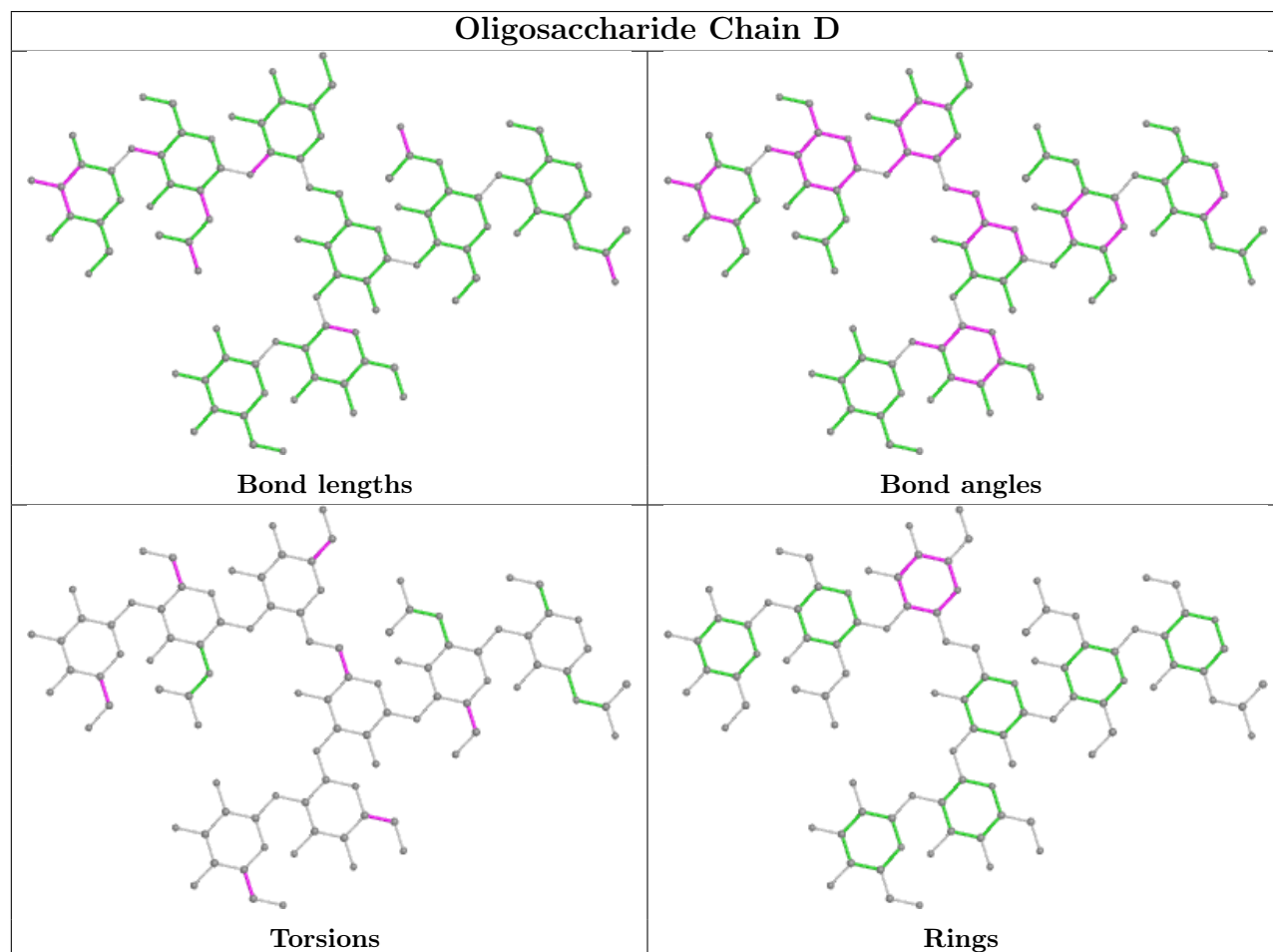
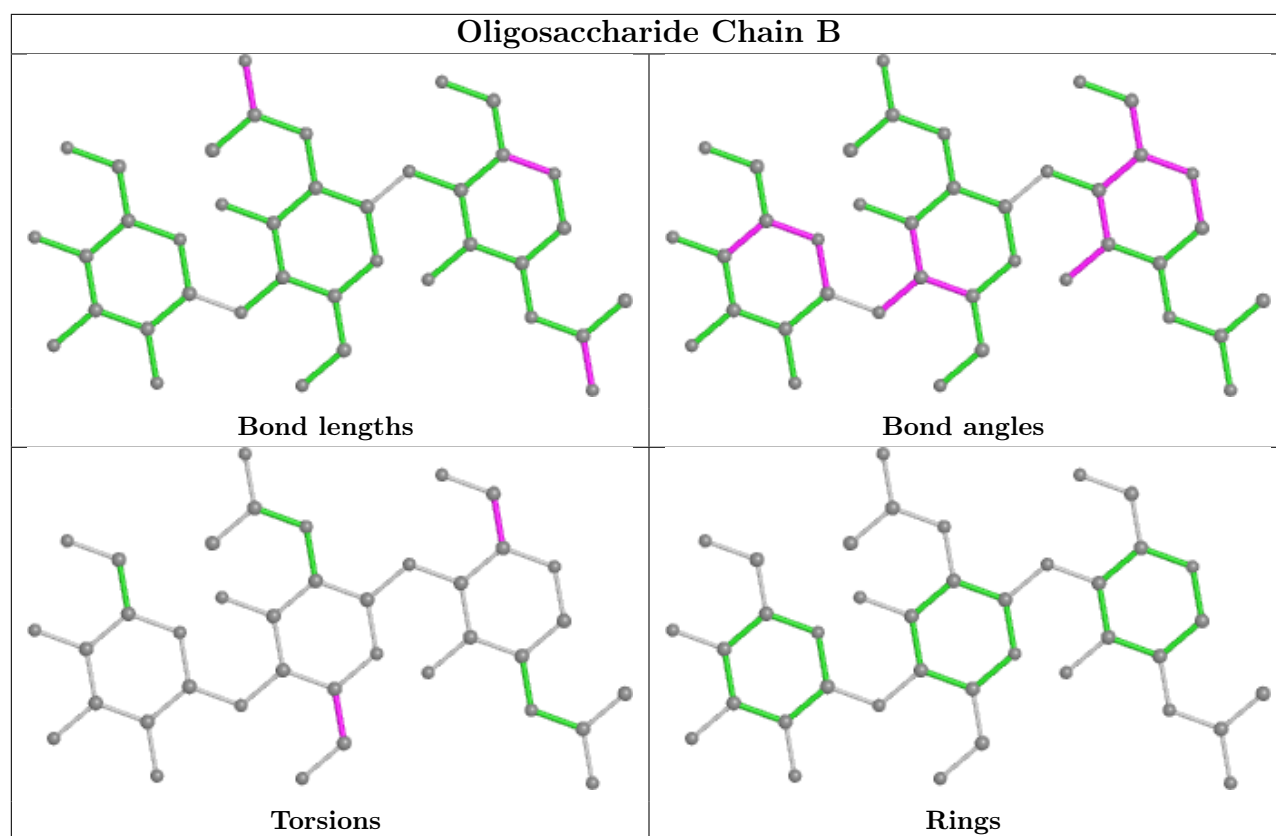
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2	NAG	2	0
4	D	2	NAG	1	0
4	D	1	NAG	1	0

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

10 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
7	GOL	L	901	-	5,5,5	0.73	0	5,5,5	0.57	0
5	MAN	L	844	-	11,11,12	0.86	0	15,15,17	0.99	1 (6%)
7	GOL	I	901	-	5,5,5	0.72	0	5,5,5	0.62	0
6	NAG	L	821	1	14,14,15	1.28	1 (7%)	17,19,21	1.43	2 (11%)
6	NAG	I	861	1	14,14,15	1.22	1 (7%)	17,19,21	1.40	2 (11%)
5	MAN	I	803	-	11,11,12	0.74	0	15,15,17	1.75	3 (20%)
6	NAG	L	801	1	14,14,15	1.24	1 (7%)	17,19,21	1.23	1 (5%)
8	PO4	L	501	-	4,4,4	0.96	0	6,6,6	0.65	0
6	NAG	I	821	1	14,14,15	1.30	1 (7%)	17,19,21	1.47	2 (11%)
5	MAN	L	843	-	11,11,12	0.89	1 (9%)	15,15,17	1.50	2 (13%)

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
7	GOL	L	901	-	-	1/4/4/4	-
5	MAN	L	844	-	-	2/2/19/22	1/1/1/1
7	GOL	I	901	-	-	2/4/4/4	-
6	NAG	L	821	1	-	3/6/23/26	0/1/1/1
6	NAG	I	861	1	-	0/6/23/26	0/1/1/1
5	MAN	I	803	-	-	2/2/19/22	0/1/1/1
6	NAG	L	801	1	-	3/6/23/26	0/1/1/1
6	NAG	I	821	1	-	1/6/23/26	0/1/1/1
5	MAN	L	843	-	-	1/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	801	NAG	O7-C7	-3.81	1.14	1.23
6	I	861	NAG	O7-C7	-3.76	1.14	1.23
6	I	821	NAG	O7-C7	-3.72	1.14	1.23
6	L	821	NAG	O7-C7	-3.71	1.14	1.23
5	L	843	MAN	O5-C1	-2.05	1.40	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	803	MAN	C1-C2-C3	-4.95	103.59	109.67
6	L	821	NAG	C3-C4-C5	4.61	118.46	110.24
6	I	821	NAG	C1-O5-C5	4.29	118.01	112.19
6	I	861	NAG	O5-C1-C2	-4.05	104.90	111.29
6	L	801	NAG	C1-O5-C5	3.57	117.03	112.19

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	901	GOL	C1-C2-C3-O3
5	I	803	MAN	O5-C5-C6-O6
5	I	803	MAN	C4-C5-C6-O6
6	L	801	NAG	O5-C5-C6-O6
6	L	801	NAG	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	844	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	901	GOL	1	0
5	L	844	MAN	1	0
6	L	821	NAG	1	0
5	I	803	MAN	1	0
5	L	843	MAN	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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.