



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:02 AM BST

PDB ID : 1MOM
Title : CRYSTAL STRUCTURE OF MOMORDIN, A TYPE I RIBOSOME INACTIVATING PROTEIN FROM THE SEEDS OF MOMORDICA CHARANTIA
Authors : Husain, J.; Tickle, I.J.; Wood, S.P.
Deposited on : 1994-03-04
Resolution : 2.16 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)
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) : 2.13.1

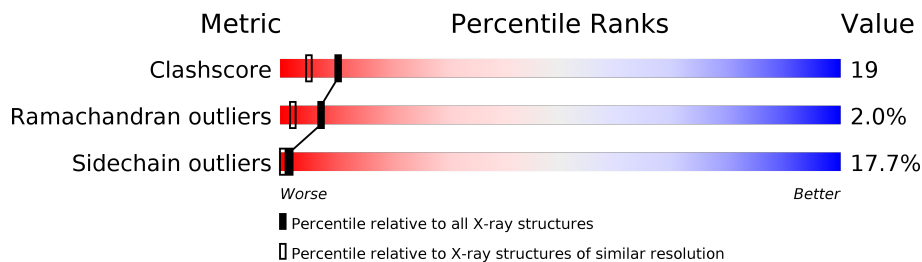
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	246	
2	B	2	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2158 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.

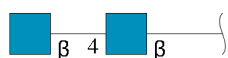
- Molecule 1 is a protein called MOMORDIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	246	1933	1234	335	361	3	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	LEU	VAL	conflict	UNP P16094

- 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 water.

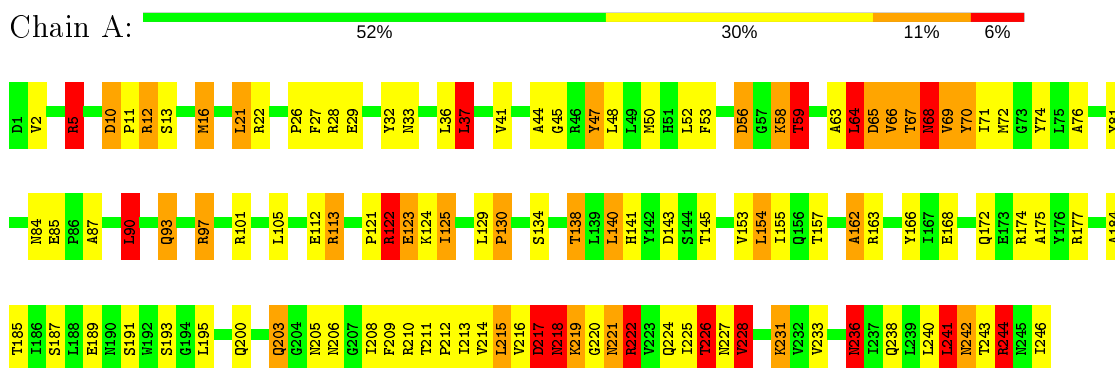
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	197	Total	O	0	0
			197	197		

3 Residue-property plots [i](#)

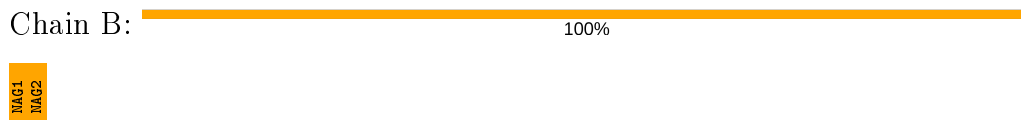
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: MOMORDIN



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



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	131.17Å 131.17Å 40.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.16	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.16)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, RESTRAIN, X-PLOR	Depositor
R, R_{free}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2158	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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:
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	A	0.98	0/1969	2.19	73/2675 (2.7%)

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ARG	CD-NE-CZ	30.31	166.03	123.60
1	A	122	ARG	CD-NE-CZ	17.47	148.06	123.60
1	A	113	ARG	NE-CZ-NH1	16.71	128.65	120.30
1	A	244	ARG	NE-CZ-NH1	14.27	127.44	120.30
1	A	174	ARG	NE-CZ-NH2	14.05	127.33	120.30
1	A	12	ARG	CD-NE-CZ	11.94	140.31	123.60
1	A	22	ARG	NE-CZ-NH1	-10.37	115.12	120.30
1	A	70	TYR	CB-CG-CD2	10.28	127.17	121.00
1	A	5	ARG	NE-CZ-NH2	-9.95	115.33	120.30
1	A	113	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	A	72	MET	CG-SD-CE	8.70	114.12	100.20
1	A	22	ARG	NE-CZ-NH2	8.66	124.63	120.30
1	A	47	TYR	CB-CG-CD2	-8.42	115.95	121.00
1	A	154	LEU	CA-CB-CG	8.12	133.98	115.30
1	A	64	LEU	CB-CG-CD2	-8.09	97.25	111.00
1	A	12	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	A	5	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	A	74	TYR	CB-CG-CD1	-7.91	116.25	121.00
1	A	28	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	209	PHE	CA-CB-CG	7.83	132.68	113.90
1	A	177	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	A	143	ASP	CB-CG-OD2	7.78	125.30	118.30
1	A	177	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	226	THR	N-CA-CB	-7.42	96.20	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	TYR	CB-CG-CD1	7.16	125.30	121.00
1	A	90	LEU	CB-CA-C	7.09	123.67	110.20
1	A	163	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	10	ASP	CB-CA-C	6.78	123.96	110.40
1	A	85	GLU	CB-CA-C	-6.52	97.36	110.40
1	A	236	ASN	CB-CG-OD1	-6.44	108.72	121.60
1	A	222	ARG	CD-NE-CZ	6.40	132.56	123.60
1	A	64	LEU	N-CA-CB	-6.38	97.63	110.40
1	A	210	ARG	NE-CZ-NH1	-6.35	117.13	120.30
1	A	228	VAL	N-CA-CB	-6.32	97.59	111.50
1	A	241	LEU	CA-CB-CG	6.25	129.67	115.30
1	A	218	ASN	C-N-CA	6.25	137.31	121.70
1	A	85	GLU	CA-CB-CG	6.23	127.11	113.40
1	A	63	ALA	N-CA-CB	6.17	118.74	110.10
1	A	64	LEU	CD1-CG-CD2	6.14	128.92	110.50
1	A	65	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	143	ASP	OD1-CG-OD2	-6.08	111.76	123.30
1	A	222	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	68	ASN	O-C-N	5.96	132.24	122.70
1	A	130	PRO	O-C-N	-5.85	113.33	122.70
1	A	141	HIS	N-CA-CB	5.85	121.13	110.60
1	A	162	ALA	CB-CA-C	5.79	118.78	110.10
1	A	59	THR	C-N-CA	5.79	136.17	121.70
1	A	64	LEU	CA-CB-CG	-5.64	102.32	115.30
1	A	70	TYR	CG-CD1-CE1	5.49	125.69	121.30
1	A	81	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	A	209	PHE	CB-CG-CD2	-5.44	116.99	120.80
1	A	122	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	37	LEU	CB-CA-C	5.37	120.40	110.20
1	A	47	TYR	CD1-CE1-CZ	-5.35	114.98	119.80
1	A	50	MET	CA-CB-CG	5.32	122.35	113.30
1	A	123	GLU	CG-CD-OE1	-5.30	107.70	118.30
1	A	65	ASP	C-N-CA	5.29	134.92	121.70
1	A	101	ARG	CA-CB-CG	5.28	125.01	113.40
1	A	12	ARG	CG-CD-NE	5.23	122.78	111.80
1	A	244	ARG	NH1-CZ-NH2	-5.23	113.65	119.40
1	A	219	LYS	N-CA-CB	5.22	120.00	110.60
1	A	209	PHE	CB-CG-CD1	5.20	124.44	120.80
1	A	193	SER	CB-CA-C	5.18	119.95	110.10
1	A	59	THR	CB-CA-C	-5.15	97.70	111.60
1	A	28	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
1	A	64	LEU	CB-CG-CD1	-5.14	102.26	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	A	56	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	A	162	ALA	O-C-N	-5.10	114.55	122.70
1	A	66	VAL	N-CA-CB	-5.09	100.30	111.50
1	A	97	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	16	MET	CA-CB-CG	5.03	121.84	113.30
1	A	130	PRO	C-N-CA	5.01	134.22	121.70

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	A	1933	0	1969	73	1
2	B	28	0	25	2	0
3	A	197	0	0	11	3
All	All	2158	0	1994	74	3

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 19.

All (74) 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:221:ASN:HD22	1:A:221:ASN:H	1.26	0.82
1:A:221:ASN:ND2	1:A:221:ASN:H	1.78	0.79
1:A:175:ALA:O	3:A:508:HOH:O	2.01	0.77
1:A:214:VAL:HG22	1:A:224:GLN:HG2	1.69	0.74
1:A:241:LEU:HD13	1:A:246:ILE:HG12	1.71	0.73
1:A:166:TYR:H	1:A:236:ASN:ND2	1.86	0.72
1:A:2:VAL:HG13	3:A:429:HOH:O	1.90	0.69
1:A:208:ILE:HD11	2:B:1:NAG:H82	1.76	0.68
1:A:52:LEU:O	1:A:59:THR:HG22	2.01	0.61
1:A:244:ARG:O	1:A:244:ARG:HD3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PRO:HB3	1:A:172:GLN:HB3	1.83	0.59
1:A:121:PRO:HG2	1:A:124:LYS:HD3	1.85	0.59
1:A:58:LYS:HB3	1:A:140:LEU:HD21	1.85	0.58
1:A:168:GLU:O	1:A:172:GLN:HG3	2.03	0.58
1:A:222:ARG:HG2	1:A:222:ARG:HH11	1.69	0.58
1:A:65:ASP:OD1	1:A:67:THR:HB	2.04	0.58
1:A:53:PHE:CD2	1:A:59:THR:HG23	2.39	0.57
1:A:244:ARG:HH11	1:A:244:ARG:HA	1.69	0.57
1:A:87:ALA:HB1	3:A:585:HOH:O	2.04	0.57
1:A:220:GLY:HA2	3:A:521:HOH:O	2.04	0.57
1:A:216:VAL:HB	3:A:521:HOH:O	2.03	0.57
1:A:221:ASN:N	1:A:221:ASN:HD22	1.99	0.55
1:A:45:GLY:HA3	3:A:555:HOH:O	2.06	0.55
1:A:112:GLU:HB2	3:A:476:HOH:O	2.07	0.54
1:A:221:ASN:ND2	1:A:221:ASN:N	2.54	0.54
1:A:37:LEU:HB2	1:A:240:LEU:O	2.08	0.53
1:A:200:GLN:O	1:A:203:GLN:HG3	2.09	0.53
1:A:13:SER:HA	1:A:16:MET:CE	2.38	0.53
1:A:226:THR:CG2	1:A:227:ASN:HD22	2.22	0.52
1:A:44:ALA:HB1	3:A:545:HOH:O	2.09	0.52
1:A:184:ALA:HA	1:A:216:VAL:HG23	1.92	0.51
1:A:129:LEU:N	1:A:130:PRO:CD	2.73	0.51
1:A:185:THR:O	1:A:189:GLU:HG3	2.12	0.50
1:A:217:ASP:O	1:A:221:ASN:ND2	2.45	0.50
1:A:47:TYR:HA	1:A:64:LEU:O	2.11	0.49
1:A:242:ASN:HD22	1:A:244:ARG:H	1.61	0.49
1:A:26:PRO:HD2	1:A:66:VAL:HG13	1.95	0.49
1:A:200:GLN:OE1	1:A:243:THR:HG23	2.13	0.48
1:A:166:TYR:H	1:A:236:ASN:HD21	1.56	0.48
1:A:213:ILE:HG22	1:A:215:LEU:HD13	1.94	0.48
1:A:215:LEU:HD22	1:A:225:ILE:HG13	1.95	0.48
1:A:244:ARG:HA	1:A:244:ARG:NH1	2.28	0.48
1:A:187:SER:CB	1:A:216:VAL:HG22	2.43	0.47
1:A:228:VAL:HA	1:A:233:VAL:HG11	1.95	0.47
1:A:27:PHE:HB2	1:A:36:LEU:O	2.13	0.47
1:A:13:SER:HA	1:A:16:MET:HE3	1.94	0.47
1:A:205:ASN:O	1:A:206:ASN:HB2	2.15	0.47
1:A:5:ARG:HG2	1:A:5:ARG:NH1	2.30	0.46
1:A:122:ARG:HA	1:A:125:ILE:HG23	1.98	0.46
1:A:236:ASN:O	1:A:238:GLN:HG2	2.17	0.45
1:A:84:ASN:HB2	1:A:105:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ASN:HB2	1:A:70:TYR:CE1	2.52	0.44
1:A:90:LEU:O	1:A:93:GLN:HG3	2.17	0.44
1:A:65:ASP:HB3	1:A:68:ASN:HD21	1.82	0.44
1:A:231:LYS:CD	1:A:231:LYS:H	2.29	0.44
3:A:433:HOH:O	2:B:2:NAG:H82	2.17	0.44
1:A:187:SER:HB2	1:A:216:VAL:HG22	1.99	0.43
1:A:41:VAL:HG13	3:A:551:HOH:O	2.19	0.43
1:A:123:GLU:HG3	3:A:468:HOH:O	2.19	0.43
1:A:32:TYR:O	1:A:33:ASN:HB3	2.19	0.43
1:A:71:ILE:HD12	1:A:155:ILE:HG12	2.00	0.43
1:A:76:ALA:HB1	1:A:140:LEU:HD12	2.01	0.42
1:A:243:THR:HA	1:A:246:ILE:HD12	2.01	0.42
1:A:10:ASP:HB2	1:A:11:PRO:HD3	2.01	0.42
1:A:244:ARG:CA	1:A:244:ARG:HH11	2.32	0.42
1:A:5:ARG:HG2	1:A:5:ARG:HH11	1.84	0.42
1:A:125:ILE:HD11	1:A:153:VAL:CG2	2.49	0.42
1:A:65:ASP:HB3	1:A:68:ASN:ND2	2.35	0.42
1:A:211:THR:HA	1:A:212:PRO:HD3	1.74	0.42
1:A:68:ASN:ND2	1:A:70:TYR:H	2.17	0.42
1:A:153:VAL:O	1:A:157:THR:HG23	2.21	0.41
1:A:226:THR:HG22	1:A:227:ASN:HD22	1.86	0.41
1:A:21:LEU:HD13	1:A:162:ALA:CB	2.51	0.41
1:A:134:SER:O	1:A:138:THR:HG23	2.21	0.41

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:473:HOH:O	3:A:513:HOH:O[1_556]	2.02	0.18
1:A:56:ASP:OD1	3:A:488:HOH:O[2_765]	2.15	0.05
3:A:557:HOH:O	3:A:587:HOH:O[2_765]	2.19	0.01

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	244/246 (99%)	229 (94%)	10 (4%)	5 (2%)	7 2

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	ASP
1	A	236	ASN
1	A	219	LYS
1	A	218	ASN
1	A	69	VAL

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	209/209 (100%)	172 (82%)	37 (18%)	2 0

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	12	ARG
1	A	21	LEU
1	A	29	GLU
1	A	37	LEU
1	A	48	LEU
1	A	58	LYS
1	A	59	THR
1	A	64	LEU
1	A	67	THR
1	A	68	ASN
1	A	69	VAL
1	A	90	LEU
1	A	93	GLN

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Mol	Chain	Res	Type
1	A	97	ARG
1	A	113	ARG
1	A	122	ARG
1	A	125	ILE
1	A	138	THR
1	A	140	LEU
1	A	145	THR
1	A	154	LEU
1	A	191	SER
1	A	195	LEU
1	A	203	GLN
1	A	215	LEU
1	A	217	ASP
1	A	218	ASN
1	A	221	ASN
1	A	222	ARG
1	A	226	THR
1	A	228	VAL
1	A	231	LYS
1	A	236	ASN
1	A	241	LEU
1	A	242	ASN
1	A	244	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	33	ASN
1	A	68	ASN
1	A	110	ASN
1	A	169	GLN
1	A	170	GLN
1	A	172	GLN
1	A	218	ASN
1	A	221	ASN
1	A	236	ASN
1	A	238	GLN
1	A	242	ASN
1	A	245	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	B	1	1,2	14,14,15	1.33	2 (14%)	17,19,21	2.98	7 (41%)
2	NAG	B	2	2	14,14,15	1.38	1 (7%)	17,19,21	2.19	7 (41%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	O7-C7	-4.08	1.14	1.23
2	B	1	NAG	O7-C7	-2.83	1.16	1.23
2	B	1	NAG	C2-N2	2.48	1.50	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	1	NAG	C1-O5-C5	9.56	125.15	112.19
2	B	2	NAG	C1-O5-C5	4.51	118.30	112.19
2	B	1	NAG	O5-C1-C2	4.29	118.06	111.29
2	B	2	NAG	O5-C5-C6	3.76	113.09	107.20
2	B	1	NAG	O4-C4-C3	-3.16	103.03	110.35
2	B	2	NAG	C8-C7-N2	-3.14	110.78	116.10
2	B	2	NAG	C3-C4-C5	-2.95	104.97	110.24
2	B	1	NAG	C8-C7-N2	-2.69	111.55	116.10
2	B	2	NAG	O7-C7-N2	2.64	126.80	121.95
2	B	1	NAG	O4-C4-C5	2.54	115.61	109.30
2	B	1	NAG	O7-C7-C8	2.37	126.46	122.06
2	B	1	NAG	O3-C3-C4	-2.34	104.95	110.35
2	B	2	NAG	O3-C3-C2	2.22	114.06	109.47
2	B	2	NAG	O5-C1-C2	-2.19	107.83	111.29

There are no chirality outliers.

All (1) torsion outliers are listed below:

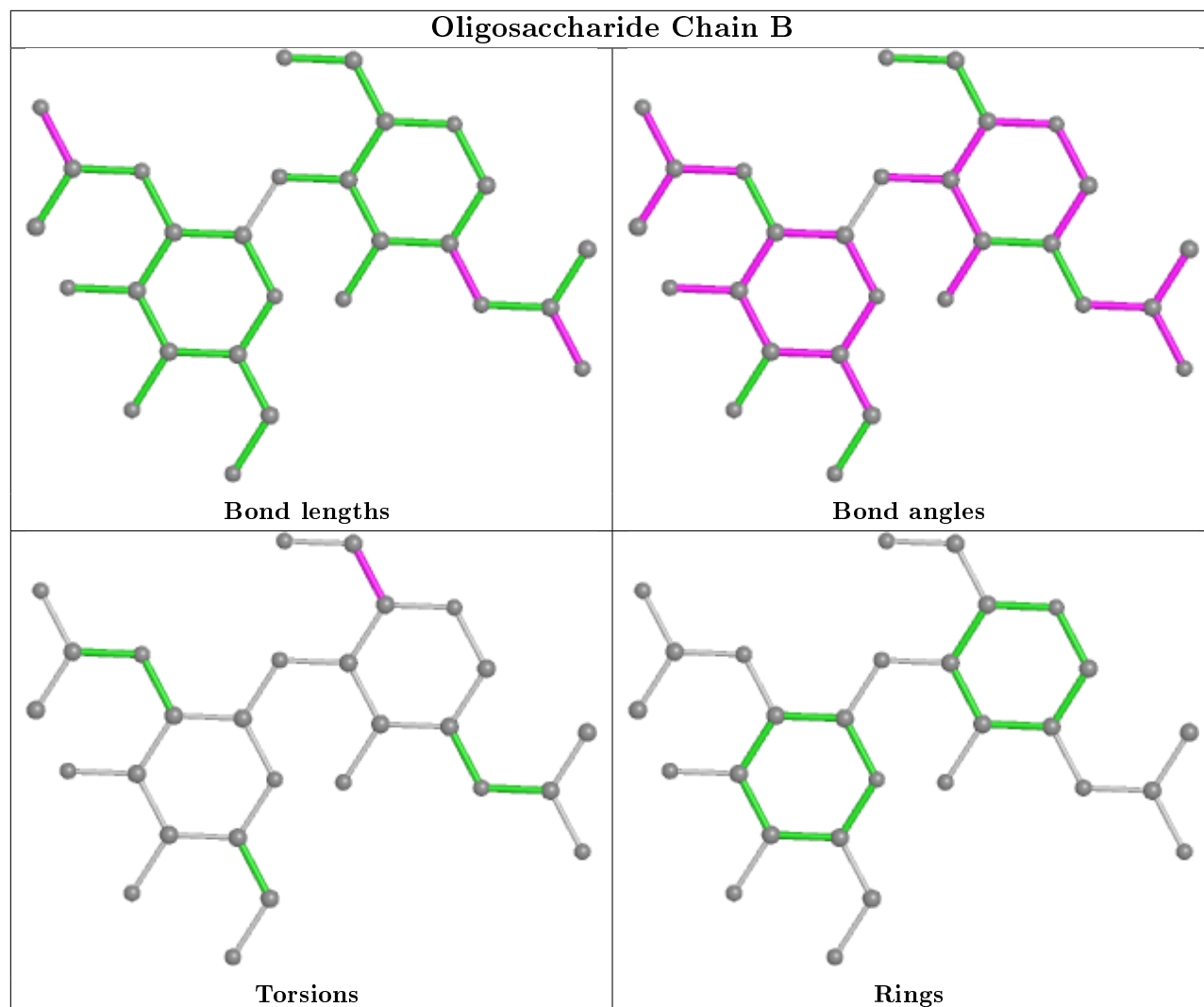
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	1	0
2	B	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](#)

There are no ligands in this entry.

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

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.