



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:03 AM UTC

PDB ID : 2VLC / pdb_00002vlc
Title : Crystal structure of Natural Cinnamomin (Isoform III)
Authors : Azzi, A.; Wang, T.; Zhu, D.-W.; Zou, Y.-S.; Liu, W.-Y.; Lin, S.-X.
Deposited on : 2008-01-11
Resolution : 2.95 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 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

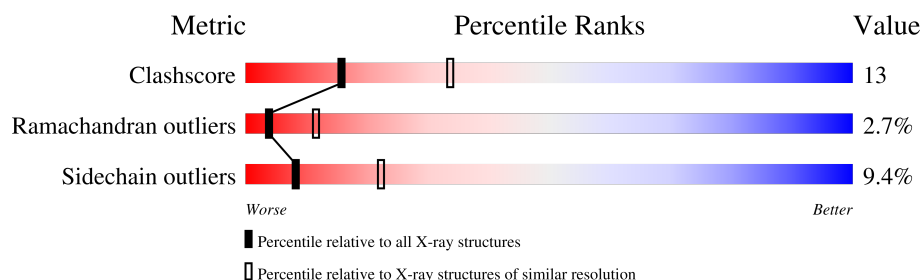
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	570	64% 22% . 9%
1	B	570	59% 25% 5% . 9%
2	C	2	50% 50%
2	D	2	50% 50%
2	E	2	50% 50%
2	F	2	100%
2	G	2	100%
2	H	2	100%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	C	1	X	-	-	-
2	NAG	C	2	X	-	-	-
2	NAG	D	1	X	-	-	-
2	NAG	D	2	X	-	-	-
2	NAG	E	1	X	-	-	-
2	NAG	E	2	X	-	-	-
2	NAG	F	1	X	-	-	-
2	NAG	F	2	X	-	-	-
2	NAG	G	1	X	-	-	-
2	NAG	G	2	X	-	-	-
2	NAG	H	1	X	-	-	-
2	NAG	H	2	X	-	-	-
4	XYP	B	601	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8406 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 Ribosome-inactivating protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	4	0	0
			4036	2529	713	773	21			
1	B	518	Total	C	N	O	S	5	0	0
			4038	2529	713	775	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	183	SER	THR	conflict	UNP Q94BW3
A	307	ARG	ASP	conflict	UNP Q94BW3
B	183	SER	THR	conflict	UNP Q94BW3
B	307	ARG	ASP	conflict	UNP Q94BW3

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



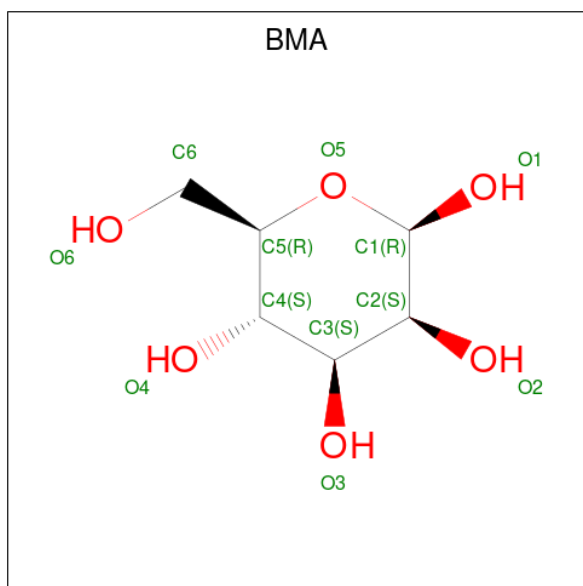
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

Continued on next page...

Continued from previous page...

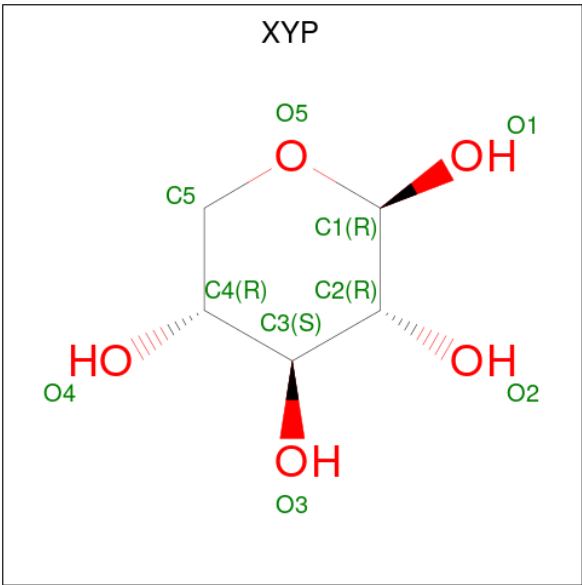
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is beta-D-mannopyranose (CCD ID: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is beta-D-xylopyranose (CCD ID: XYP) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	5	5		
4	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 5 is water.

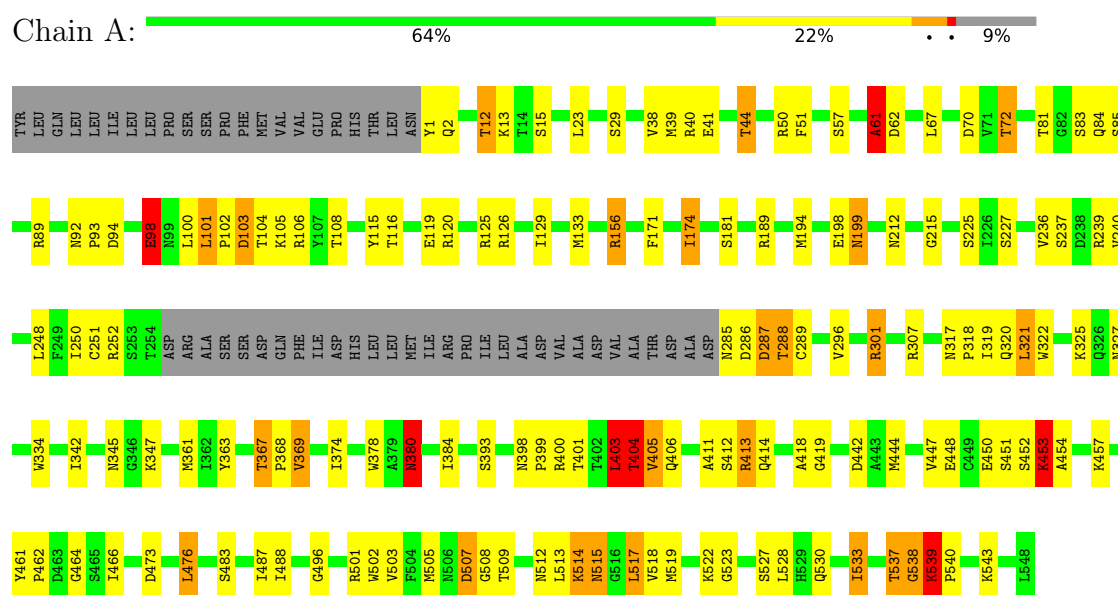
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total	O	0	0
			70	70		
5	B	50	Total	O	0	0
			50	50		

3 Residue-property plots

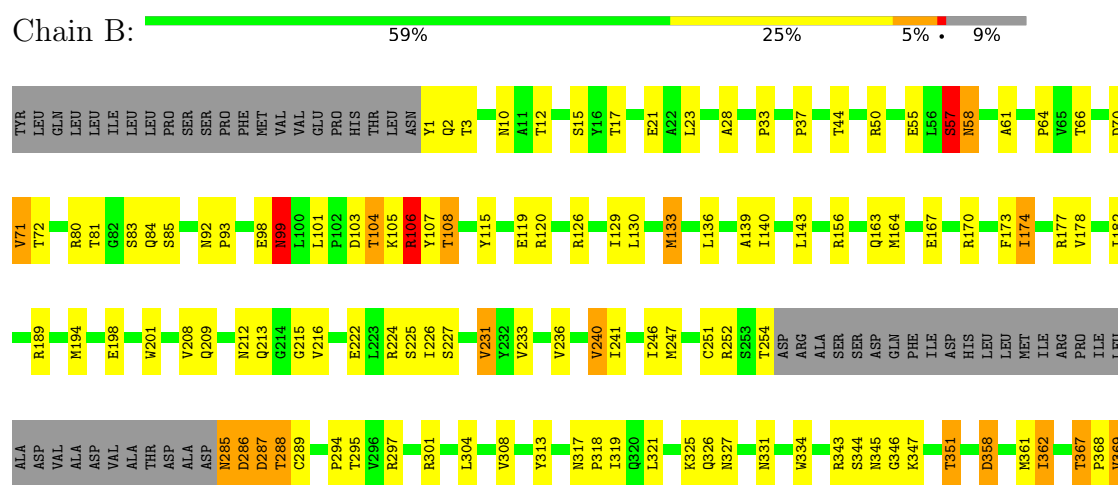
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

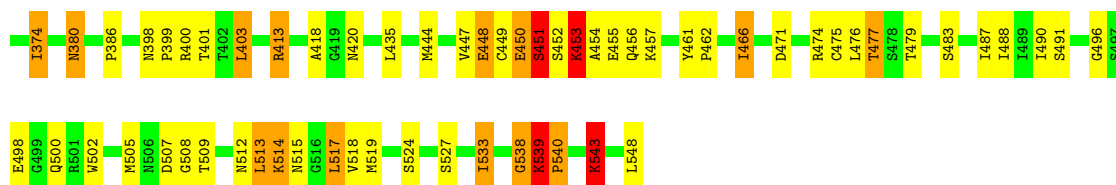
Note EDS was not executed.

• Molecule 1: Ribosome-inactivating protein



• Molecule 1: Ribosome-inactivating protein





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

Chain C: 50% 50%



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

Chain D: 50% 50%



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

Chain E: 50% 50%



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

Chain F: 100%



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

Chain G: 100%



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

Chain H: 100%

MAG1
MAG2

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.39Å 126.33Å 161.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.00 – 2.95	Depositor
% Data completeness (in resolution range)	98.9 (17.00-2.95)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.238 , 0.309	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8406	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, XYP

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	1.21	8/4122 (0.2%)	1.22	30/5610 (0.5%)
1	B	1.13	9/4124 (0.2%)	1.37	26/5612 (0.5%)
All	All	1.17	17/8246 (0.2%)	1.30	56/11222 (0.5%)

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	A	0	9
1	B	0	6
All	All	0	15

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	PRO	N-CD	-41.17	0.90	1.47
1	B	358	ASP	CG-OD2	28.71	1.79	1.25
1	A	462	PRO	N-CD	-16.56	1.24	1.47
1	B	462	PRO	CB-CG	-15.85	0.70	1.49
1	A	462	PRO	CB-CG	-14.89	0.75	1.49
1	B	368	PRO	CB-CG	-10.00	0.99	1.49
1	A	368	PRO	CB-CG	-9.81	1.00	1.49
1	B	368	PRO	N-CD	-8.64	1.35	1.47
1	B	539	LYS	CA-C	8.52	1.63	1.52
1	A	374	ILE	CA-CB	6.61	1.62	1.54
1	A	539	LYS	CA-C	5.87	1.60	1.52
1	B	479	THR	CA-CB	5.82	1.62	1.53
1	B	509	THR	CA-CB	5.46	1.62	1.53
1	B	374	ILE	CA-CB	5.38	1.60	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	ILE	CA-CB	5.08	1.60	1.55
1	B	490	ILE	CA-CB	5.02	1.60	1.54
1	A	369	VAL	N-CA	5.01	1.52	1.46

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	358	ASP	CB-CG-OD2	-40.74	24.69	118.40
1	B	462	PRO	CA-N-CD	-15.91	89.73	112.00
1	B	451	SER	N-CA-C	-14.57	93.31	112.68
1	B	368	PRO	CA-N-CD	-14.17	92.16	112.00
1	B	368	PRO	N-CD-CG	11.04	119.77	103.20
1	A	367	THR	CA-C-N	-10.81	108.72	119.64
1	A	367	THR	C-N-CA	-10.81	108.72	119.64
1	B	358	ASP	OD1-CG-OD2	-10.09	98.68	122.90
1	B	462	PRO	CA-CB-CG	9.27	122.11	104.50
1	A	462	PRO	CA-N-CD	-8.79	99.70	112.00
1	A	403	LEU	CA-C-N	8.50	137.78	121.54
1	A	403	LEU	C-N-CA	8.50	137.78	121.54
1	B	539	LYS	N-CA-C	8.47	128.52	109.81
1	A	286	ASP	N-CA-C	8.07	121.66	107.61
1	B	367	THR	CA-C-N	-7.49	112.07	119.64
1	B	367	THR	C-N-CA	-7.49	112.07	119.64
1	A	405	VAL	N-CA-CB	6.87	118.21	110.72
1	B	540	PRO	N-CA-C	6.86	122.56	113.57
1	A	98	GLU	CA-C-N	6.72	133.28	123.13
1	A	98	GLU	C-N-CA	6.72	133.28	123.13
1	B	368	PRO	CA-CB-CG	6.45	116.75	104.50
1	B	461	TYR	CA-C-N	6.38	126.07	119.56
1	B	461	TYR	C-N-CA	6.38	126.07	119.56
1	A	380	ASN	CB-CA-C	-6.32	96.99	110.32
1	A	101	LEU	CA-C-N	-6.13	114.45	120.52
1	A	101	LEU	C-N-CA	-6.13	114.45	120.52
1	B	502	TRP	CA-C-N	-6.12	114.48	122.99
1	B	502	TRP	C-N-CA	-6.12	114.48	122.99
1	A	404	THR	N-CA-CB	5.87	120.41	110.49
1	A	461	TYR	CA-C-N	5.80	125.47	119.56
1	A	461	TYR	C-N-CA	5.80	125.47	119.56
1	A	540	PRO	N-CA-C	5.73	122.12	113.81
1	B	287	ASP	N-CA-C	5.73	123.00	110.80
1	A	368	PRO	CA-CB-CG	-5.71	93.66	104.50
1	B	453	LYS	N-CA-C	5.70	122.94	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	TYR	N-CA-C	5.67	117.91	110.08
1	A	502	TRP	CA-C-N	-5.63	115.17	122.99
1	A	502	TRP	C-N-CA	-5.63	115.17	122.99
1	A	539	LYS	N-CA-C	5.62	122.24	109.81
1	B	543	LYS	CD-CE-NZ	-5.54	94.16	111.90
1	A	403	LEU	O-C-N	-5.54	115.84	122.65
1	B	57	SER	CA-C-N	5.52	132.08	121.54
1	B	57	SER	C-N-CA	5.52	132.08	121.54
1	A	404	THR	CB-CA-C	5.44	121.25	110.42
1	A	368	PRO	N-CD-CG	5.30	111.14	103.20
1	A	156	ARG	N-CA-C	-5.29	105.41	111.07
1	B	285	ASN	CA-C-N	5.26	131.17	121.70
1	B	285	ASN	C-N-CA	5.26	131.17	121.70
1	B	343	ARG	N-CA-C	5.22	117.41	108.90
1	A	345	ASN	CB-CA-C	-5.18	110.18	117.23
1	A	199	ASN	N-CA-C	5.16	116.91	111.28
1	B	351	THR	CB-CA-C	-5.15	99.99	109.46
1	A	462	PRO	CB-CG-CD	5.14	122.54	106.10
1	A	473	ASP	N-CA-C	-5.09	107.12	113.38
1	A	380	ASN	CA-CB-CG	-5.03	107.57	112.60
1	B	108	THR	CB-CA-C	5.01	119.27	109.35

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	367	THR	Peptide
1	A	403	LEU	Peptide
1	A	450	GLU	Peptide
1	A	453	LYS	Peptide
1	A	537	THR	Peptide
1	A	539	LYS	Peptide
1	A	57	SER	Peptide
1	A	61	ALA	Peptide
1	A	98	GLU	Peptide
1	B	358	ASP	Sidechain
1	B	450	GLU	Peptide
1	B	453	LYS	Peptide
1	B	539	LYS	Peptide
1	B	57	SER	Peptide
1	B	61	ALA	Peptide

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	4036	0	3954	100	0
1	B	4038	0	3954	117	0
2	C	28	0	17	0	0
2	D	28	0	25	0	0
2	E	28	0	24	4	0
2	F	28	0	21	4	0
2	G	28	0	24	2	0
2	H	28	0	25	2	0
3	A	12	0	9	0	0
3	B	12	0	11	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
5	A	70	0	0	2	0
5	B	50	0	0	4	0
All	All	8406	0	8064	217	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 13.

All (217) 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)
5:B:743:HOH:O	2:H:2:NAG:O7	1.56	1.21
1:A:380:ASN:ND2	1:A:513:LEU:HD11	1.55	1.18
1:A:61:ALA:HB1	1:A:62:ASP:HA	1.44	1.00
1:B:251:CYS:HB2	1:B:288:THR:O	1.61	0.98
1:A:380:ASN:CG	1:A:380:ASN:O	2.08	0.96
1:A:251:CYS:HB2	1:A:288:THR:O	1.67	0.94
1:A:517:LEU:HD23	1:A:533:ILE:HG23	1.58	0.85
1:A:194:MET:O	1:A:198:GLU:HG3	1.80	0.82
1:A:380:ASN:CG	1:A:513:LEU:HD11	2.05	0.81
1:B:225:SER:O	1:B:227:SER:O	1.99	0.81
1:B:477:THR:HB	1:B:500:GLN:HG2	1.61	0.81
1:B:380:ASN:OD1	2:H:1:NAG:O6	1.97	0.81
1:B:254:THR:HA	5:B:737:HOH:O	1.81	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ALA:CB	1:A:62:ASP:HA	2.11	0.80
1:B:515:ASN:HB3	1:B:517:LEU:H	1.48	0.79
1:B:453:LYS:HE3	1:B:457:LYS:HE3	1.65	0.78
1:B:488:ILE:HD13	1:B:519:MET:HE3	1.64	0.78
1:A:517:LEU:HD23	1:A:533:ILE:CG2	2.15	0.77
1:A:380:ASN:OD1	1:A:501:ARG:NH1	2.17	0.76
1:B:98:GLU:O	1:B:99:ASN:HB2	1.85	0.76
1:A:513:LEU:O	1:A:514:LYS:CB	2.34	0.74
1:A:453:LYS:HB2	1:A:454:ALA:HA	1.68	0.74
1:A:505:MET:HA	1:A:505:MET:HE2	1.69	0.74
1:A:515:ASN:HB3	1:A:517:LEU:H	1.53	0.73
1:B:420:ASN:OD1	2:F:1:NAG:C1	2.36	0.73
1:B:285:ASN:CG	1:B:285:ASN:O	2.32	0.73
1:B:513:LEU:O	1:B:514:LYS:HB3	1.87	0.72
1:B:449:CYS:O	1:B:450:GLU:HB3	1.88	0.72
1:B:513:LEU:O	1:B:514:LYS:CB	2.37	0.72
1:A:453:LYS:HD2	1:A:457:LYS:HG2	1.72	0.71
1:A:398:ASN:O	1:A:401:THR:HG23	1.90	0.71
1:A:174:ILE:HD13	1:A:194:MET:HE3	1.72	0.71
1:A:451:SER:O	1:A:453:LYS:HG2	1.91	0.70
1:B:12:THR:HG23	1:B:15:SER:H	1.56	0.70
1:A:508:GLY:HA3	1:A:543:LYS:HE3	1.75	0.68
1:A:287:ASP:O	1:A:289:CYS:N	2.27	0.68
1:B:133:MET:HE3	1:B:182:ILE:HG12	1.74	0.68
1:B:451:SER:O	1:B:453:LYS:HG2	1.93	0.68
1:A:380:ASN:ND2	1:A:513:LEU:CD1	2.47	0.67
1:B:453:LYS:HE3	1:B:457:LYS:CE	2.25	0.67
1:B:28:ALA:HB1	5:B:712:HOH:O	1.93	0.67
1:B:119:GLU:OE2	1:B:126:ARG:HG3	1.94	0.67
1:A:488:ILE:HD13	1:A:519:MET:HE3	1.76	0.66
1:A:85:SER:H	1:A:105:LYS:HB3	1.59	0.66
1:B:287:ASP:O	1:B:289:CYS:N	2.29	0.66
1:A:442:ASP:OD2	1:B:538:GLY:HA2	1.96	0.66
1:A:133:MET:HE2	1:A:133:MET:HA	1.77	0.66
1:B:174:ILE:HD13	1:B:194:MET:HE3	1.79	0.65
1:B:285:ASN:CA	1:B:286:ASP:HB2	2.27	0.64
1:A:513:LEU:O	1:A:514:LYS:HB3	1.97	0.64
1:A:285:ASN:CG	1:A:285:ASN:O	2.42	0.63
1:A:453:LYS:HD2	1:A:457:LYS:CG	2.27	0.63
1:B:285:ASN:HA	1:B:286:ASP:HB2	1.79	0.62
1:A:70:ASP:OD1	1:A:72:THR:HB	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLN:HA	1:A:105:LYS:CB	2.31	0.61
1:A:84:GLN:HA	1:A:105:LYS:HB3	1.80	0.61
1:B:10:ASN:OD1	2:G:1:NAG:O4	2.19	0.61
1:A:321:LEU:HD13	1:A:403:LEU:HD21	1.83	0.60
1:B:477:THR:CG2	1:B:491:SER:HB3	2.32	0.60
1:A:119:GLU:OE2	1:A:126:ARG:HG3	2.01	0.60
1:B:101:LEU:O	1:B:104:THR:HG22	2.02	0.60
1:B:33:PRO:HG2	1:B:247:MET:HE1	1.84	0.59
1:A:451:SER:O	1:A:453:LYS:CG	2.51	0.59
1:A:513:LEU:HD22	2:E:1:NAG:H61	1.85	0.59
1:A:512:ASN:HB3	1:A:515:ASN:HB2	1.85	0.58
1:B:453:LYS:HD2	1:B:457:LYS:HG3	1.84	0.58
1:A:81:THR:HG23	1:A:81:THR:O	2.03	0.58
1:A:503:VAL:HG12	1:A:505:MET:HE3	1.86	0.58
1:B:471:ASP:CG	1:B:474:ARG:HD3	2.29	0.58
1:A:515:ASN:HB3	1:A:517:LEU:HB2	1.85	0.57
1:B:216:VAL:HG12	1:B:294:PRO:HG2	1.86	0.57
1:A:101:LEU:O	1:A:104:THR:HG22	2.05	0.57
1:B:101:LEU:O	1:B:104:THR:CG2	2.53	0.57
1:A:12:THR:HG23	1:A:15:SER:H	1.70	0.56
1:A:50:ARG:O	1:A:50:ARG:HG3	2.05	0.56
1:A:380:ASN:O	1:A:380:ASN:OD1	2.23	0.56
1:B:295:THR:O	2:F:1:NAG:H2	2.05	0.56
1:A:404:THR:HG22	1:A:406:GLN:HG2	1.88	0.56
1:A:466:ILE:HB	1:A:476:LEU:HB2	1.88	0.56
1:B:477:THR:HG21	1:B:491:SER:HB3	1.87	0.56
1:A:380:ASN:ND2	1:A:380:ASN:O	2.39	0.56
1:A:380:ASN:OD1	1:A:380:ASN:C	2.40	0.56
1:B:136:LEU:O	1:B:140:ILE:HG13	2.06	0.55
1:A:347:LYS:HB3	1:A:363:TYR:O	2.06	0.55
1:B:170:ARG:HD3	1:B:201:TRP:CD2	2.42	0.55
1:A:51:PHE:CD2	1:A:100:LEU:HD13	2.41	0.55
1:A:287:ASP:O	1:A:288:THR:C	2.50	0.54
1:A:537:THR:C	1:A:538:GLY:O	2.49	0.54
1:B:215:GLY:HA3	1:B:236:VAL:HG22	1.88	0.54
1:B:466:ILE:HB	1:B:476:LEU:HB2	1.90	0.54
1:B:50:ARG:O	1:B:71:VAL:HG23	2.09	0.54
1:A:225:SER:O	1:A:227:SER:O	2.26	0.53
1:B:55:GLU:HG2	1:B:64:PRO:HG2	1.91	0.52
1:B:285:ASN:O	1:B:285:ASN:ND2	2.41	0.52
1:B:517:LEU:HD23	1:B:533:ILE:HG23	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:VAL:HG22	1:B:418:ALA:HB3	1.90	0.52
1:B:453:LYS:CB	1:B:456:GLN:HB2	2.40	0.52
1:B:105:LYS:HE3	1:B:107:TYR:HB2	1.90	0.52
1:A:378:TRP:CE3	2:E:1:NAG:H3	2.44	0.52
1:B:399:PRO:O	1:B:400:ARG:HB2	2.09	0.52
1:A:319:ILE:HG22	1:A:403:LEU:HD12	1.92	0.51
1:A:444:MET:HE2	1:A:476:LEU:HD21	1.91	0.51
1:B:515:ASN:HB3	1:B:517:LEU:HB2	1.93	0.51
1:B:543:LYS:HE2	1:B:543:LYS:HA	1.92	0.51
1:B:285:ASN:N	1:B:286:ASP:HB2	2.25	0.51
1:B:222:GLU:OE2	1:B:224:ARG:NH2	2.44	0.51
1:B:539:LYS:HB2	1:B:540:PRO:HD3	1.93	0.51
1:B:231:VAL:HG21	1:B:548:LEU:HD11	1.93	0.51
1:B:508:GLY:HA3	1:B:543:LYS:NZ	2.26	0.51
1:A:307:ARG:HD2	1:A:322:TRP:CG	2.47	0.50
1:B:453:LYS:HB3	1:B:456:GLN:HB2	1.93	0.50
1:A:411:ALA:HB1	1:A:496:GLY:O	2.12	0.50
1:A:508:GLY:HA3	1:A:543:LYS:CE	2.42	0.49
1:A:380:ASN:HD22	1:A:503:VAL:HG21	1.77	0.49
1:A:393:SER:OG	1:A:414:GLN:HG2	2.12	0.49
1:B:313:TYR:OH	1:B:331:ASN:HA	2.12	0.49
1:A:380:ASN:HB3	2:E:1:NAG:O3	2.13	0.49
1:A:126:ARG:NH1	1:A:199:ASN:OD1	2.46	0.49
1:A:129:ILE:HG23	1:A:156:ARG:CZ	2.43	0.49
1:B:50:ARG:C	1:B:71:VAL:HG23	2.38	0.49
1:B:115:TYR:CD2	1:B:126:ARG:HD3	2.48	0.49
1:A:453:LYS:HB2	1:A:454:ALA:CA	2.41	0.48
1:A:307:ARG:HD2	1:A:322:TRP:CB	2.43	0.48
1:B:297:ARG:H	1:B:420:ASN:ND2	2.12	0.48
1:A:116:THR:O	1:A:120:ARG:HB2	2.14	0.48
1:A:399:PRO:O	1:A:400:ARG:HB2	2.14	0.48
1:B:92:ASN:O	1:B:93:PRO:C	2.55	0.48
1:B:233:VAL:HG11	1:B:241:ILE:HD11	1.95	0.48
1:B:163:GLN:O	1:B:167:GLU:HB2	2.14	0.48
1:A:101:LEU:O	1:A:104:THR:CG2	2.60	0.48
1:B:81:THR:HG23	1:B:81:THR:O	2.14	0.48
1:B:471:ASP:OD2	1:B:474:ARG:HD3	2.13	0.48
1:A:29:SER:HB3	1:A:40:ARG:HG2	1.96	0.48
1:A:171:PHE:HB2	1:A:174:ILE:HG23	1.96	0.48
1:A:212:ASN:OD1	1:A:212:ASN:C	2.57	0.48
1:A:518:VAL:HG12	1:A:519:MET:O	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:THR:O	1:B:80:ARG:N	2.39	0.47
1:A:115:TYR:CD2	1:A:126:ARG:HD3	2.48	0.47
1:B:163:GLN:HE21	1:B:198:GLU:CD	2.22	0.47
1:B:347:LYS:HB3	1:B:362:ILE:HD12	1.96	0.47
1:B:453:LYS:CD	1:B:457:LYS:HG3	2.44	0.47
1:B:133:MET:HE3	1:B:182:ILE:CG1	2.42	0.47
1:A:92:ASN:O	1:A:93:PRO:C	2.57	0.46
1:B:129:ILE:HG23	1:B:156:ARG:CZ	2.45	0.46
1:B:475:CYS:O	1:B:477:THR:HG22	2.16	0.46
1:B:374:ILE:O	1:B:386:PRO:HD2	2.16	0.46
1:B:57:SER:HA	1:B:58:ASN:HB2	1.96	0.46
1:B:85:SER:H	1:B:105:LYS:HB3	1.80	0.46
1:B:139:ALA:O	1:B:143:LEU:HG	2.15	0.46
1:B:170:ARG:HD3	1:B:201:TRP:CE2	2.49	0.46
1:B:507:ASP:O	1:B:543:LYS:HE3	2.16	0.46
1:B:345:ASN:HB3	1:B:346:GLY:H	1.60	0.46
1:B:84:GLN:HA	1:B:105:LYS:CB	2.45	0.46
1:B:50:ARG:HH21	1:B:70:ASP:CG	2.24	0.46
1:B:512:ASN:HB3	1:B:515:ASN:HB2	1.98	0.46
1:A:301:ARG:NH2	1:A:413:ARG:HG3	2.31	0.45
1:A:507:ASP:HB3	1:A:509:THR:HG23	1.97	0.45
1:A:513:LEU:O	1:A:514:LYS:HB2	2.12	0.45
1:A:325:LYS:C	1:A:327:ASN:H	2.24	0.45
1:A:404:THR:CG2	1:A:406:GLN:HG2	2.46	0.45
1:B:84:GLN:HA	1:B:105:LYS:HB2	1.98	0.45
1:B:208:VAL:HG22	1:B:236:VAL:HG12	1.98	0.45
1:B:413:ARG:HB2	1:B:496:GLY:O	2.17	0.45
1:A:307:ARG:HD3	1:A:320:GLN:HE21	1.81	0.44
1:A:378:TRP:CZ2	1:A:384:ILE:HG21	2.52	0.44
1:A:322:TRP:HH2	5:A:762:HOH:O	2.00	0.44
1:B:498:GLU:H	1:B:498:GLU:CD	2.25	0.44
1:A:522:LYS:HE2	1:A:530:GLN:OE1	2.17	0.44
1:B:130:LEU:HD22	1:B:189:ARG:NH2	2.32	0.44
1:B:301:ARG:HD2	1:B:413:ARG:HA	1.99	0.44
1:A:41:GLU:O	1:A:44:THR:HB	2.18	0.44
1:A:102:PRO:C	1:A:103:ASP:CG	2.86	0.44
1:A:296:VAL:HG21	1:A:418:ALA:HB1	2.00	0.44
1:A:378:TRP:CD2	2:E:1:NAG:H3	2.53	0.44
1:B:325:LYS:C	1:B:327:ASN:H	2.26	0.44
1:B:435:LEU:HD22	1:B:448:GLU:HA	2.00	0.44
1:B:453:LYS:O	1:B:455:GLU:N	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:MET:HE2	1:B:476:LEU:HD21	2.00	0.43
1:A:38:VAL:HG22	1:A:39:MET:N	2.33	0.43
1:A:537:THR:O	1:A:538:GLY:O	2.36	0.43
1:B:334:TRP:CZ3	1:B:344:SER:HB2	2.54	0.43
1:B:476:LEU:HD12	1:B:476:LEU:HA	1.72	0.43
1:A:464:GLY:HA3	1:A:501:ARG:HG2	2.01	0.43
1:B:37:PRO:HB3	5:B:712:HOH:O	2.16	0.43
1:A:413:ARG:HB2	1:A:496:GLY:O	2.18	0.43
1:B:420:ASN:OD1	2:F:1:NAG:C2	2.66	0.43
1:B:216:VAL:CG1	1:B:294:PRO:HG2	2.48	0.43
1:A:84:GLN:HA	1:A:105:LYS:HB2	1.99	0.42
1:A:215:GLY:HA3	1:A:236:VAL:HG22	2.01	0.42
1:B:362:ILE:HD13	1:B:362:ILE:HA	1.95	0.42
1:A:29:SER:HB3	1:A:40:ARG:CG	2.49	0.42
1:B:17:THR:O	1:B:21:GLU:HB2	2.18	0.42
1:B:308:VAL:HA	1:B:319:ILE:HD13	2.00	0.42
1:B:321:LEU:HD13	1:B:403:LEU:HD11	2.00	0.42
1:B:252:ARG:O	1:B:288:THR:HG22	2.20	0.42
1:B:420:ASN:OD1	2:F:1:NAG:N2	2.52	0.42
1:A:412:SER:C	1:A:414:GLN:N	2.76	0.42
1:B:173:PHE:O	1:B:177:ARG:HG2	2.20	0.42
1:B:488:ILE:HD11	1:B:533:ILE:HG12	2.00	0.42
1:B:533:ILE:HD13	1:B:533:ILE:HA	1.82	0.42
1:B:517:LEU:HD23	1:B:533:ILE:CG2	2.50	0.42
1:B:380:ASN:HB2	1:B:513:LEU:HD21	2.00	0.41
1:B:477:THR:HG23	1:B:491:SER:HB3	2.02	0.41
1:A:61:ALA:HB1	1:A:62:ASP:CA	2.32	0.41
1:B:398:ASN:O	1:B:401:THR:HG23	2.19	0.41
1:B:317:ASN:HA	1:B:318:PRO:HD3	1.95	0.41
1:B:164:MET:HE3	1:B:178:VAL:HG13	2.03	0.41
1:B:212:ASN:OD1	1:B:212:ASN:C	2.64	0.41
1:B:304:LEU:HB2	1:B:321:LEU:HG	2.02	0.41
1:A:334:TRP:CE3	1:A:342:ILE:HG22	2.56	0.41
1:B:10:ASN:HD21	2:G:2:NAG:C7	2.34	0.41
1:B:319:ILE:HD11	1:B:362:ILE:HG12	2.03	0.40
1:A:317:ASN:HA	1:A:318:PRO:HD3	1.84	0.40
1:A:453:LYS:HD2	1:A:457:LYS:HG3	2.03	0.40
1:B:106:ARG:HG3	1:B:106:ARG:HH11	1.86	0.40
1:B:240:VAL:HG21	1:B:548:LEU:HD13	2.02	0.40
1:A:419:GLY:HA3	5:A:701:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	514/570 (90%)	467 (91%)	33 (6%)	14 (3%)	4	11
1	B	514/570 (90%)	469 (91%)	31 (6%)	14 (3%)	4	11
All	All	1028/1140 (90%)	936 (91%)	64 (6%)	28 (3%)	4	11

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	ASP
1	A	288	THR
1	A	404	THR
1	A	514	LYS
1	A	538	GLY
1	A	539	LYS
1	B	58	ASN
1	B	99	ASN
1	B	286	ASP
1	B	288	THR
1	B	453	LYS
1	B	454	ALA
1	B	514	LYS
1	B	539	LYS
1	A	61	ALA
1	A	413	ARG
1	B	413	ARG
1	B	538	GLY
1	A	507	ASP
1	A	523	GLY
1	B	452	SER
1	A	106	ARG
1	A	301	ARG
1	A	453	LYS
1	B	106	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	326	GLN
1	A	369	VAL
1	B	369	VAL

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	A	446/496 (90%)	407 (91%)	39 (9%)	9	25
1	B	446/496 (90%)	401 (90%)	45 (10%)	7	20
All	All	892/992 (90%)	808 (91%)	84 (9%)	8	22

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	TYR
1	A	2	GLN
1	A	12	THR
1	A	13	LYS
1	A	23	LEU
1	A	44	THR
1	A	67	LEU
1	A	72	THR
1	A	83	SER
1	A	89	ARG
1	A	94	ASP
1	A	98	GLU
1	A	103	ASP
1	A	108	THR
1	A	125	ARG
1	A	174	ILE
1	A	181	SER
1	A	189	ARG
1	A	237	SER
1	A	239	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	240	VAL
1	A	248	LEU
1	A	252	ARG
1	A	321	LEU
1	A	361	MET
1	A	380	ASN
1	A	404	THR
1	A	405	VAL
1	A	447	VAL
1	A	448	GLU
1	A	452	SER
1	A	476	LEU
1	A	483	SER
1	A	487	ILE
1	A	515	ASN
1	A	517	LEU
1	A	527	SER
1	A	528	LEU
1	A	533	ILE
1	B	1	TYR
1	B	2	GLN
1	B	3	THR
1	B	23	LEU
1	B	44	THR
1	B	57	SER
1	B	71	VAL
1	B	72	THR
1	B	83	SER
1	B	99	ASN
1	B	103	ASP
1	B	104	THR
1	B	106	ARG
1	B	108	THR
1	B	120	ARG
1	B	133	MET
1	B	174	ILE
1	B	209	GLN
1	B	213	GLN
1	B	226	ILE
1	B	231	VAL
1	B	240	VAL
1	B	246	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	351	THR
1	B	361	MET
1	B	362	ILE
1	B	367	THR
1	B	369	VAL
1	B	380	ASN
1	B	403	LEU
1	B	447	VAL
1	B	448	GLU
1	B	451	SER
1	B	466	ILE
1	B	477	THR
1	B	483	SER
1	B	487	ILE
1	B	505	MET
1	B	513	LEU
1	B	517	LEU
1	B	518	VAL
1	B	524	SER
1	B	527	SER
1	B	533	ILE
1	B	543	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	314	ASN
1	A	317	ASN
1	B	213	GLN
1	B	326	GLN
1	B	385	ASN
1	B	529	HIS
1	B	530	GLN

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 ⓘ

12 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	C	1	1,2	14,14,15	0.80	0	17,19,21	2.24	7 (41%)
2	NAG	C	2	2	14,14,15	2.47	6 (42%)	17,19,21	7.14	11 (64%)
2	NAG	D	1	2	14,14,15	0.66	0	17,19,21	1.88	2 (11%)
2	NAG	D	2	2	14,14,15	1.29	1 (7%)	17,19,21	2.83	5 (29%)
2	NAG	E	1	1,2	14,14,15	0.83	0	17,19,21	3.19	5 (29%)
2	NAG	E	2	2	14,14,15	2.48	2 (14%)	17,19,21	2.81	7 (41%)
2	NAG	F	1	1,2	14,14,15	0.50	0	17,19,21	2.37	7 (41%)
2	NAG	F	2	2	14,14,15	2.56	1 (7%)	17,19,21	3.02	5 (29%)
2	NAG	G	1	2	14,14,15	0.68	0	17,19,21	1.30	2 (11%)
2	NAG	G	2	2	14,14,15	0.81	1 (7%)	17,19,21	10.80	6 (35%)
2	NAG	H	1	1,2	14,14,15	1.03	1 (7%)	17,19,21	2.17	4 (23%)
2	NAG	H	2	2	14,14,15	1.24	2 (14%)	17,19,21	1.95	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	C	1	1,2	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	C	2	2	3/3/5/7	5/6/23/26	0/1/1/1
2	NAG	D	1	2	2/2/5/7	3/6/23/26	0/1/1/1
2	NAG	D	2	2	1/1/5/7	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	1/1/5/7	5/6/23/26	1/1/1/1
2	NAG	E	2	2	1/1/5/7	5/6/23/26	0/1/1/1
2	NAG	F	1	1,2	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	F	2	2	4/4/5/7	2/6/23/26	0/1/1/1
2	NAG	G	1	2	2/2/5/7	5/6/23/26	0/1/1/1
2	NAG	G	2	2	4/4/5/7	5/6/23/26	0/1/1/1
2	NAG	H	1	1,2	2/2/5/7	3/6/23/26	0/1/1/1
2	NAG	H	2	2	4/4/5/7	4/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	NAG	O3-C3	-9.16	1.20	1.43
2	E	2	NAG	O3-C3	-8.29	1.22	1.43
2	C	2	NAG	O6-C6	4.90	1.63	1.42
2	C	2	NAG	O3-C3	-4.05	1.32	1.43
2	D	2	NAG	O3-C3	4.01	1.52	1.43
2	C	2	NAG	C8-C7	3.50	1.57	1.50
2	E	2	NAG	C1-C2	3.29	1.56	1.52
2	C	2	NAG	C1-C2	3.08	1.56	1.52
2	C	2	NAG	O5-C5	2.89	1.49	1.43
2	H	2	NAG	O5-C5	2.83	1.48	1.43
2	H	2	NAG	C4-C5	2.43	1.58	1.53
2	H	1	NAG	C4-C3	2.27	1.58	1.52
2	G	2	NAG	O3-C3	2.23	1.48	1.43
2	C	2	NAG	C4-C5	2.03	1.57	1.53

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NAG	C8-C7-N2	26.21	159.59	116.12
2	C	2	NAG	O3-C3-C2	25.01	161.35	109.40
2	G	2	NAG	O7-C7-N2	-24.18	79.26	121.98
2	G	2	NAG	O7-C7-C8	-23.36	80.46	122.05
2	G	2	NAG	O3-C3-C2	11.41	133.09	109.40
2	C	2	NAG	O3-C3-C4	-9.55	87.86	110.38
2	E	1	NAG	C4-C3-C2	-7.98	99.32	111.02
2	F	2	NAG	O6-C6-C5	7.83	137.99	111.33
2	E	1	NAG	C1-C2-N2	7.71	122.59	110.43
2	C	2	NAG	C1-O5-C5	7.37	122.06	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	O3-C3-C2	6.38	122.65	109.40
2	F	1	NAG	C2-N2-C7	6.19	131.19	122.90
2	D	1	NAG	C1-O5-C5	6.11	120.38	112.19
2	D	2	NAG	O3-C3-C4	5.78	124.00	110.38
2	C	2	NAG	O5-C5-C6	5.73	118.81	107.66
2	F	2	NAG	O3-C3-C2	5.72	121.28	109.40
2	E	2	NAG	C1-O5-C5	5.55	119.62	112.19
2	D	2	NAG	O4-C4-C5	5.49	122.85	109.32
2	H	1	NAG	O3-C3-C4	5.42	123.16	110.38
2	C	1	NAG	C4-C3-C2	5.39	118.92	111.02
2	F	2	NAG	O3-C3-C4	5.09	122.37	110.38
2	E	2	NAG	C1-C2-N2	5.08	118.44	110.43
2	E	2	NAG	O3-C3-C2	4.78	119.32	109.40
2	E	2	NAG	O4-C4-C5	4.71	120.92	109.32
2	E	1	NAG	O5-C1-C2	-4.62	104.15	111.29
2	H	2	NAG	O5-C1-C2	-4.58	104.20	111.29
2	F	2	NAG	O4-C4-C5	4.46	120.31	109.32
2	D	2	NAG	O4-C4-C3	4.39	120.72	110.38
2	H	1	NAG	O4-C4-C3	4.21	120.30	110.38
2	H	2	NAG	O5-C5-C6	4.11	115.67	107.66
2	G	2	NAG	O3-C3-C4	-3.81	101.39	110.38
2	E	1	NAG	O4-C4-C5	3.69	118.41	109.32
2	F	1	NAG	C4-C3-C2	3.59	116.28	111.02
2	C	2	NAG	O6-C6-C5	-3.56	99.22	111.33
2	C	1	NAG	C2-N2-C7	3.51	127.61	122.90
2	H	1	NAG	C1-C2-N2	3.44	115.85	110.43
2	G	1	NAG	C1-O5-C5	3.22	116.51	112.19
2	E	2	NAG	O3-C3-C4	3.16	117.81	110.38
2	F	1	NAG	C1-C2-N2	-3.05	105.62	110.43
2	C	2	NAG	O4-C4-C3	2.98	117.39	110.38
2	D	2	NAG	C2-N2-C7	2.93	126.83	122.90
2	C	2	NAG	C2-N2-C7	2.91	126.79	122.90
2	H	1	NAG	O6-C6-C5	-2.83	101.71	111.33
2	E	2	NAG	O5-C5-C4	2.82	117.70	110.83
2	D	1	NAG	C1-C2-N2	2.66	114.63	110.43
2	G	1	NAG	C2-N2-C7	2.65	126.45	122.90
2	H	2	NAG	C2-N2-C7	-2.65	119.35	122.90
2	C	1	NAG	O5-C1-C2	-2.63	107.22	111.29
2	E	2	NAG	C2-N2-C7	2.62	126.41	122.90
2	H	2	NAG	O4-C4-C5	2.52	115.54	109.32
2	F	1	NAG	C3-C4-C5	2.52	114.81	110.23
2	F	1	NAG	O4-C4-C3	-2.48	104.53	110.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	O7-C7-C8	2.48	126.47	122.05
2	C	2	NAG	O5-C5-C4	2.44	116.76	110.83
2	E	1	NAG	C3-C4-C5	-2.43	105.83	110.23
2	C	1	NAG	O4-C4-C5	2.40	115.23	109.32
2	C	2	NAG	O5-C1-C2	-2.38	107.62	111.29
2	F	2	NAG	O5-C1-C2	-2.34	107.66	111.29
2	F	1	NAG	C8-C7-N2	2.32	119.96	116.12
2	C	2	NAG	C1-C2-N2	2.22	113.92	110.43
2	G	2	NAG	C1-O5-C5	2.20	115.13	112.19
2	F	1	NAG	C1-O5-C5	2.16	115.08	112.19
2	C	1	NAG	O3-C3-C2	-2.16	104.92	109.40
2	C	1	NAG	O5-C5-C4	2.12	115.98	110.83
2	C	1	NAG	C1-O5-C5	2.00	114.87	112.19

All (26) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	NAG	C2
2	C	2	NAG	C5
2	C	2	NAG	C3
2	C	2	NAG	C2
2	D	1	NAG	C3
2	D	1	NAG	C2
2	D	2	NAG	C3
2	E	1	NAG	C2
2	E	2	NAG	C5
2	F	1	NAG	C2
2	F	2	NAG	C5
2	F	2	NAG	C4
2	F	2	NAG	C3
2	F	2	NAG	C2
2	G	1	NAG	C5
2	G	1	NAG	C2
2	G	2	NAG	C5
2	G	2	NAG	C4
2	G	2	NAG	C3
2	G	2	NAG	C2
2	H	1	NAG	C5
2	H	1	NAG	C4
2	H	2	NAG	C4
2	H	2	NAG	C3
2	H	2	NAG	C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
2	H	2	NAG	C2

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C3-C2-N2-C7
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	E	1	NAG	C1-C2-N2-C7
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C3-C2-N2-C7
2	E	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	G	1	NAG	C1-C2-N2-C7
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C3-C2-N2-C7
2	G	2	NAG	O7-C7-N2-C2
2	H	1	NAG	C1-C2-N2-C7
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	G	2	NAG	C8-C7-N2-C2
2	G	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	H	1	NAG	C3-C2-N2-C7
2	H	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7
2	F	1	NAG	C3-C2-N2-C7
2	G	1	NAG	C4-C5-C6-O6

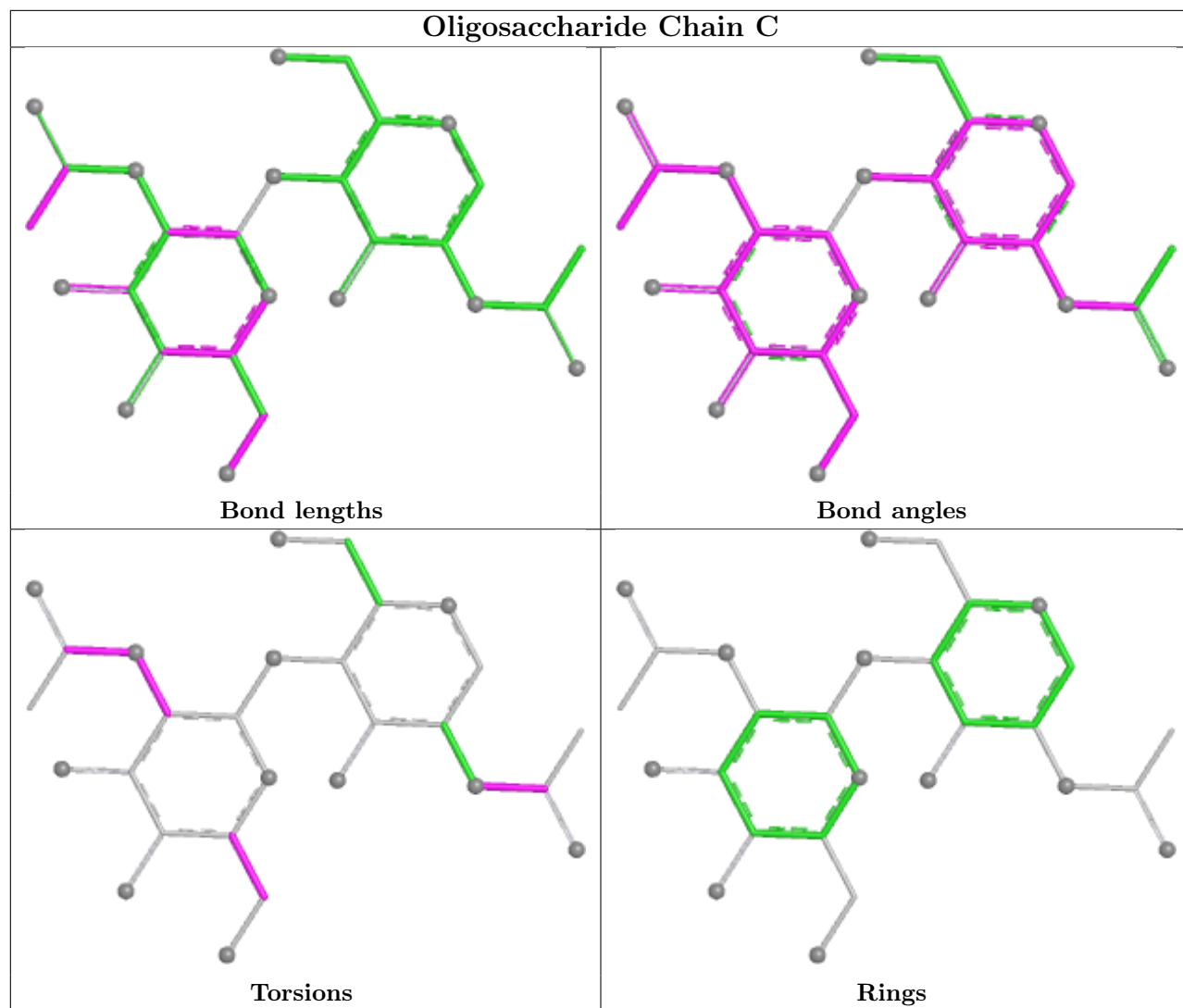
All (1) ring outliers are listed below:

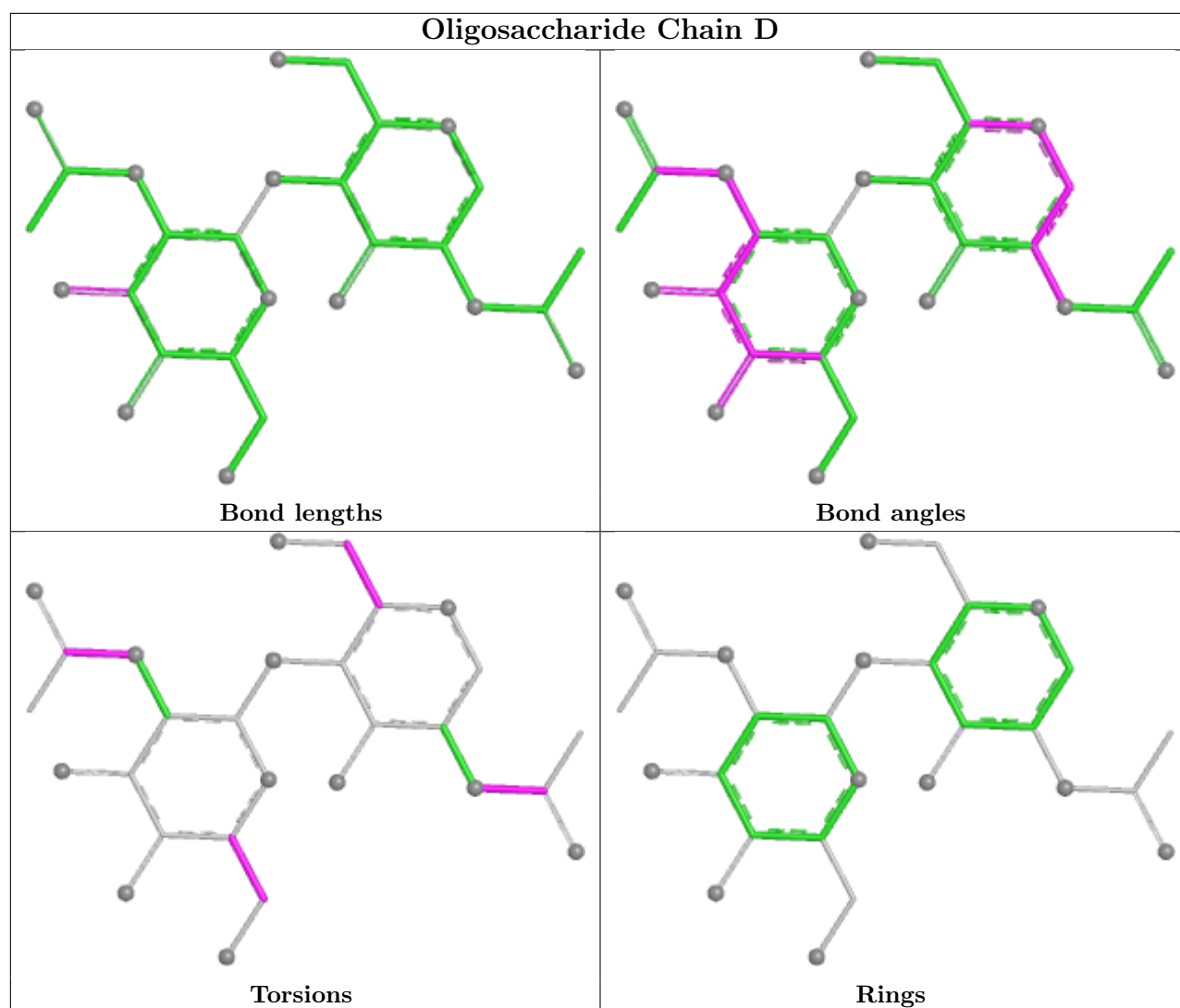
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C1-C2-C3-C4-C5-O5

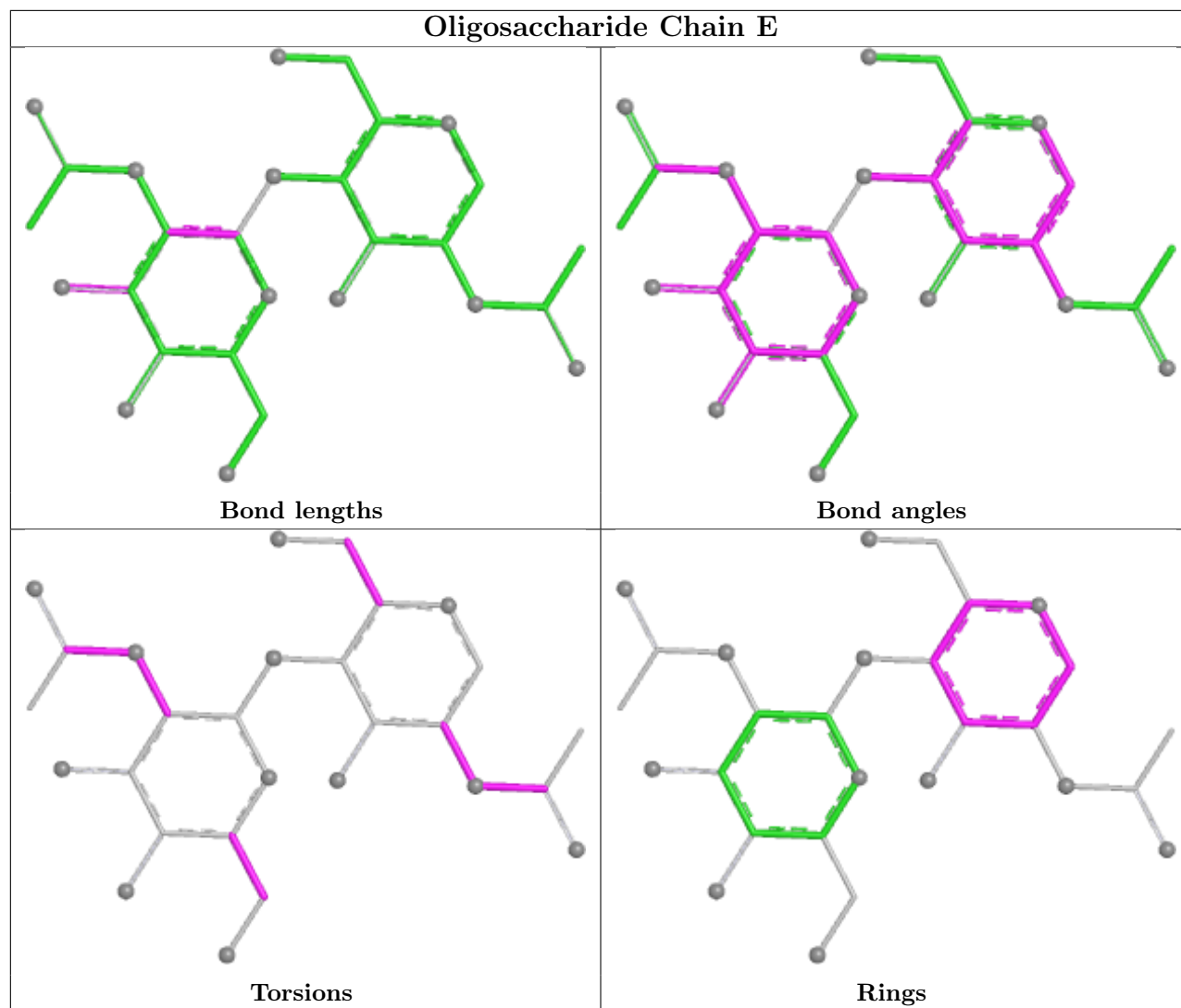
6 monomers are involved in 12 short contacts:

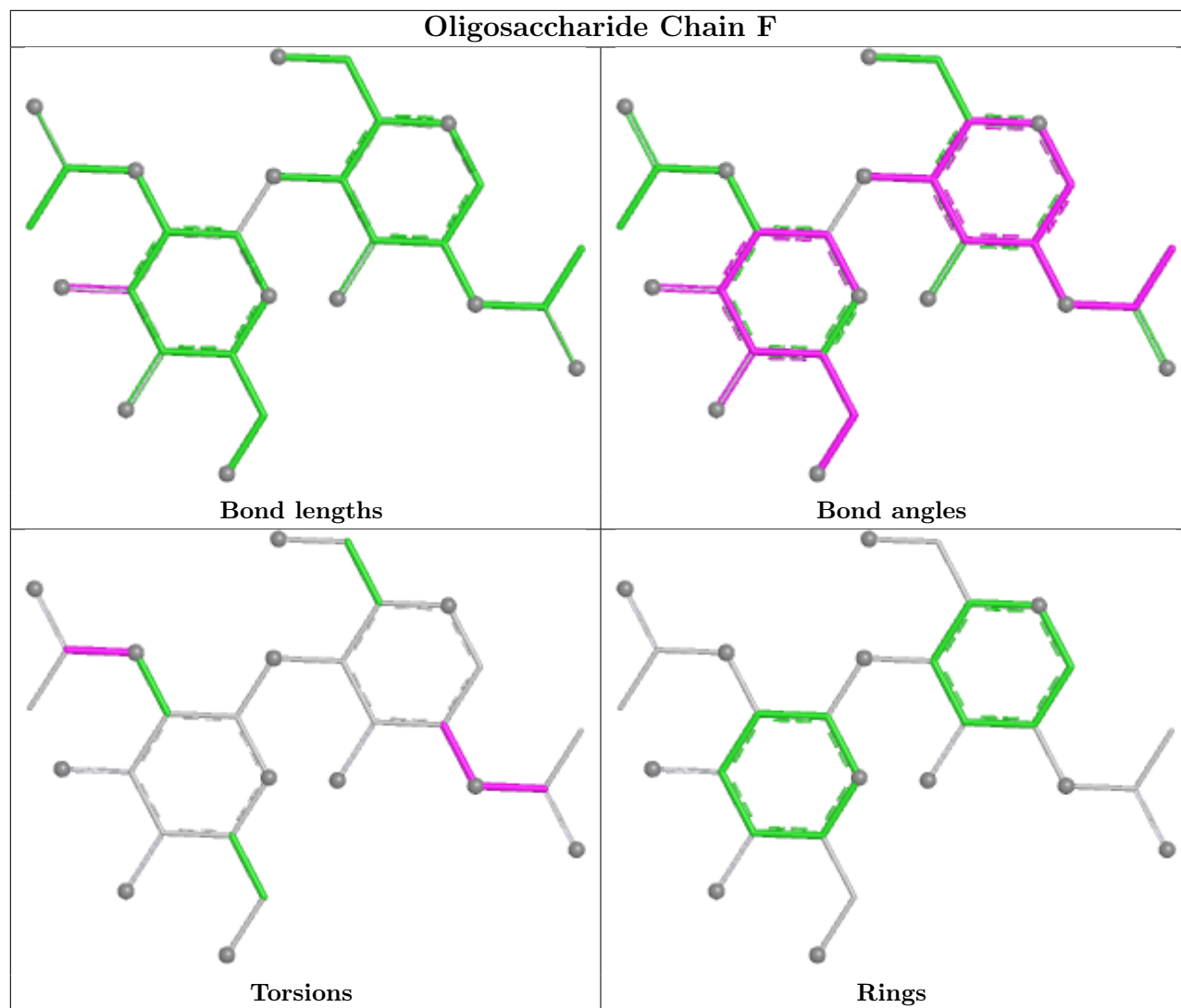
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2	NAG	1	0
2	H	1	NAG	1	0
2	F	1	NAG	4	0
2	G	2	NAG	1	0
2	G	1	NAG	1	0
2	E	1	NAG	4	0

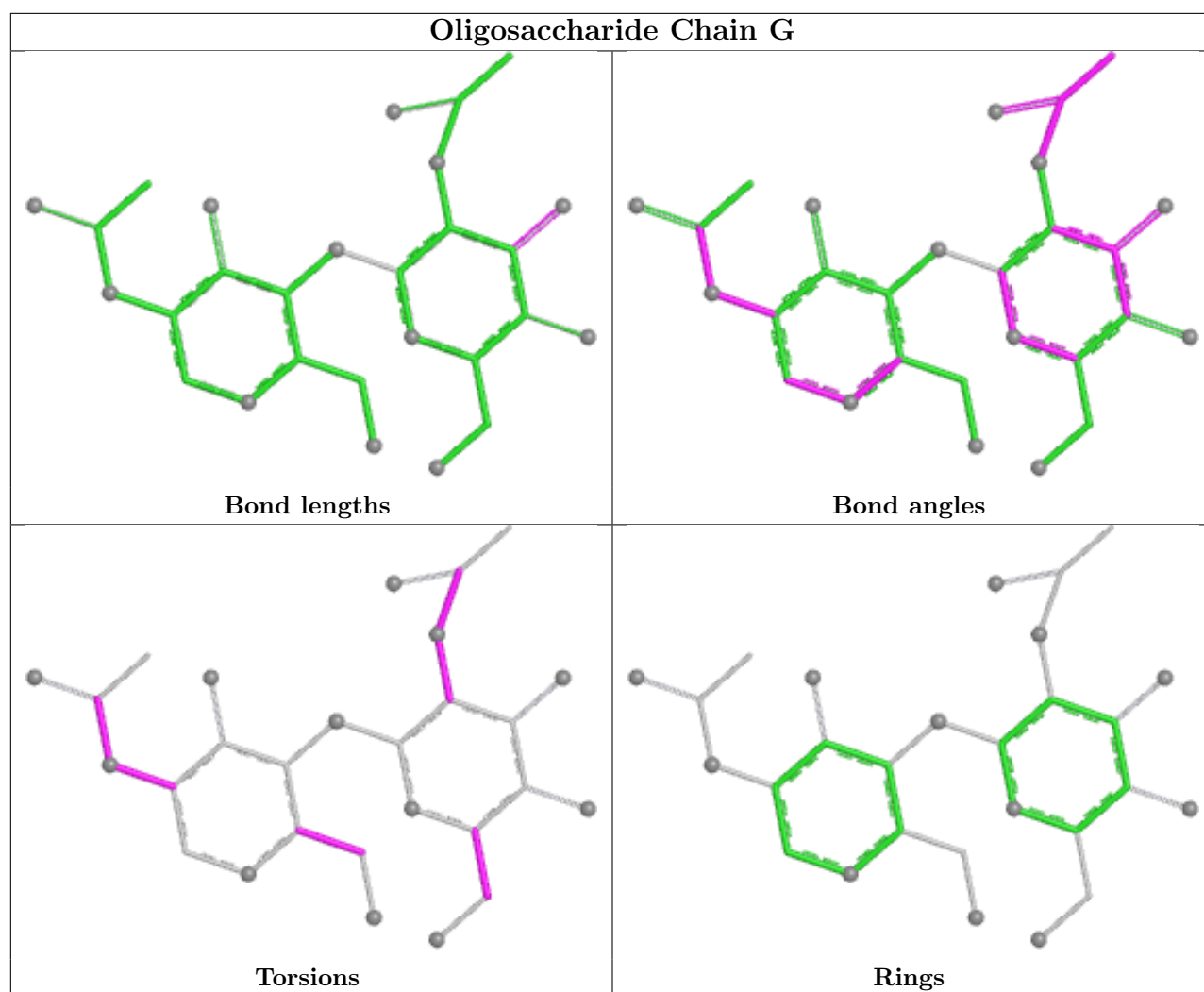
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

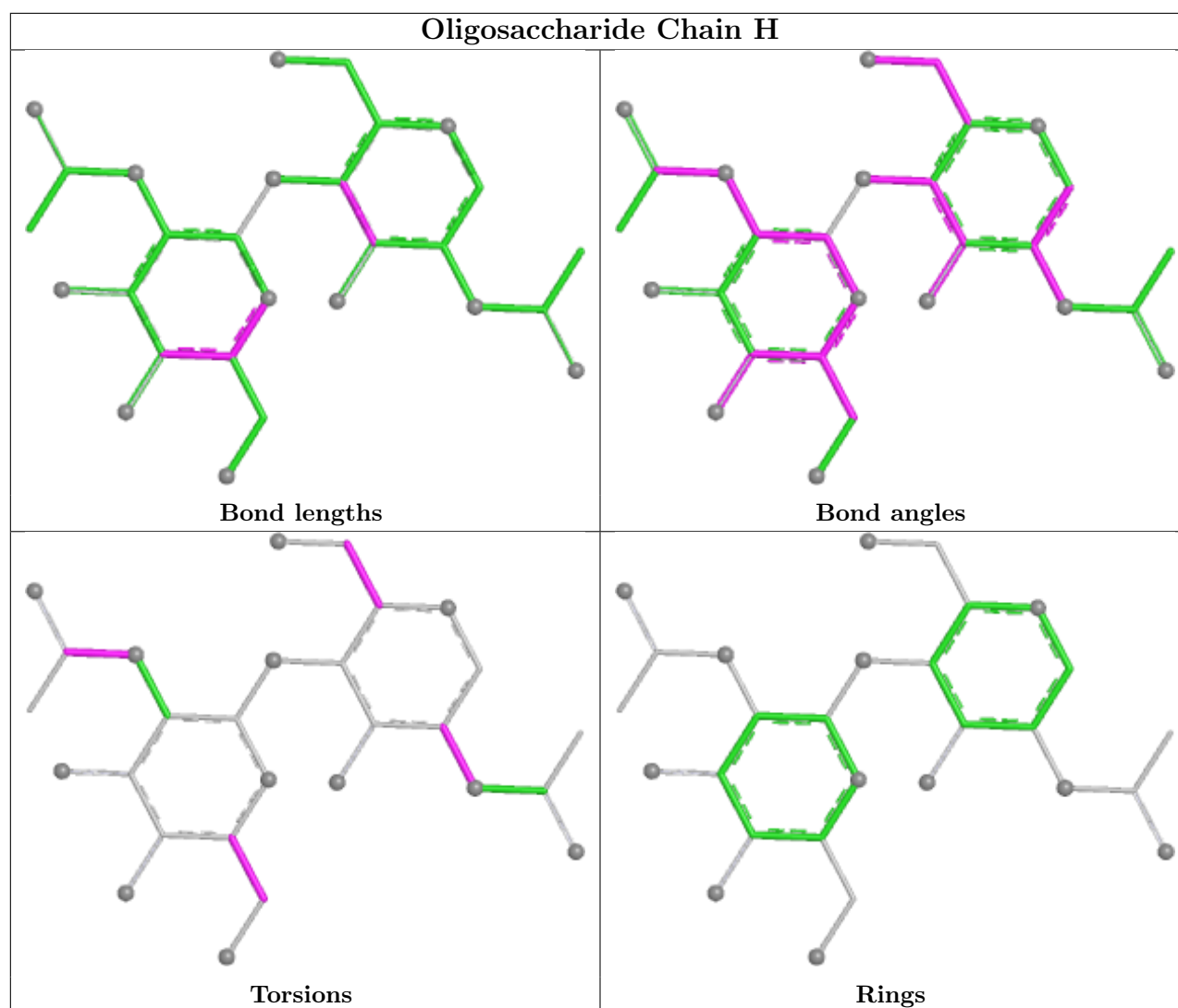












5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
4	XYP	B	601	-	10,10,10	1.23	1 (10%)	14,14,14	1.29	2 (14%)
4	XYP	A	602	-	10,10,10	1.24	1 (10%)	14,14,14	1.28	3 (21%)
3	BMA	B	602	-	12,12,12	0.79	0	17,17,17	1.88	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	A	601	-	12,12,12	0.75	0	17,17,17	2.36	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
4	XYP	B	601	-	1/1/4/4	-	0/1/1/1
4	XYP	A	602	-	-	-	0/1/1/1
3	BMA	B	602	-	-	2/2/22/22	0/1/1/1
3	BMA	A	601	-	-	2/2/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	XYP	O5-C1	-3.48	1.37	1.43
4	B	601	XYP	O5-C1	-3.24	1.37	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	BMA	O6-C6-C5	-4.55	95.82	111.33
3	A	601	BMA	C4-C3-C2	-4.42	103.08	110.83
3	B	602	BMA	O6-C6-C5	-4.06	97.51	111.33
3	A	601	BMA	O4-C4-C5	3.94	119.04	109.32
3	A	601	BMA	O5-C5-C4	-3.27	103.81	109.70
3	B	602	BMA	O5-C5-C6	3.18	114.31	106.44
3	A	601	BMA	O4-C4-C3	3.12	117.73	110.38
3	B	602	BMA	O4-C4-C5	3.12	117.00	109.32
3	B	602	BMA	C3-C4-C5	-2.80	105.15	110.23
3	A	601	BMA	C6-C5-C4	-2.61	106.61	113.02
4	B	601	XYP	C1-C2-C3	-2.51	105.23	110.36
4	A	602	XYP	C5-O5-C1	2.30	117.23	112.46
4	A	602	XYP	C4-C3-C2	-2.29	106.84	110.86
4	B	601	XYP	O3-C3-C2	-2.25	105.06	110.38
3	B	602	BMA	C1-C2-C3	2.14	114.72	110.36
4	A	602	XYP	C5-C4-C3	-2.06	106.65	109.64
3	A	601	BMA	C3-C4-C5	-2.05	106.52	110.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	601	XYP	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	BMA	O5-C5-C6-O6
3	A	601	BMA	C4-C5-C6-O6
3	B	602	BMA	C4-C5-C6-O6
3	A	601	BMA	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.