



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 29, 2022 – 12:07 am GMT

PDB ID : 2VLC
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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (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) : 2.31.3

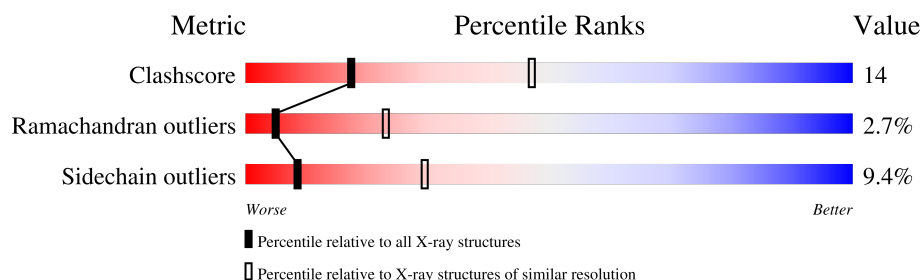
1 Overall quality at a glance

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	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)

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	
1	B	570	
2	C	2	
2	D	2	
2	E	2	
2	G	2	
2	H	2	
3	F	3	

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	YYQ	C	2	X	-	-	-
2	RTV	D	1	X	-	-	-
2	YYQ	D	2	X	-	-	-
2	YYQ	E	2	X	-	-	-
2	RTV	G	1	X	-	-	-
2	YYQ	G	2	X	-	-	-
2	RTV	H	1	X	-	-	-
2	YYQ	H	2	X	-	-	-
3	YYQ	F	2	X	-	X	-
3	BMA	F	3	-	-	X	-

2 Entry composition

There are 7 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.

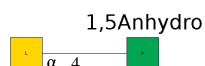
- Molecule 1 is a protein called TYPE 2 RIBOSOME-INACTIVATING PROTEIN CINNAMOMIN III.

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- α -L-galactopyranose-(1-4)-2-(acetylamino)-1,5-anhydro-2-deoxy-D-mannitol.

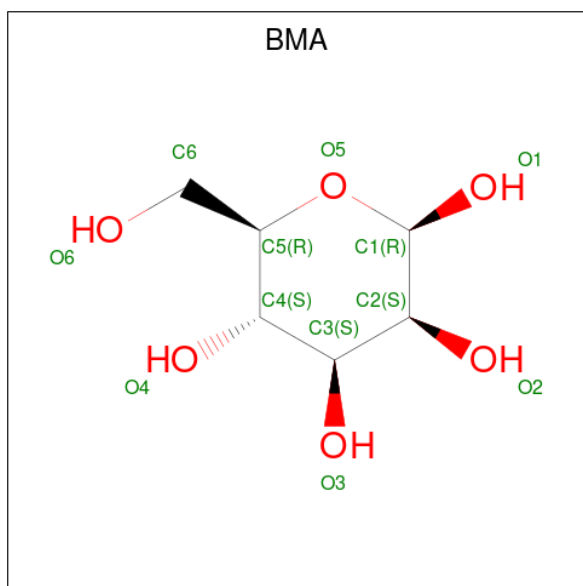


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(4-4)-2-acetamido-2-deoxy-alpha-L-galactopyranose-(1-4)-2-(acetylamino)-1,5-anhydro-2-deoxy-D-mannitol.

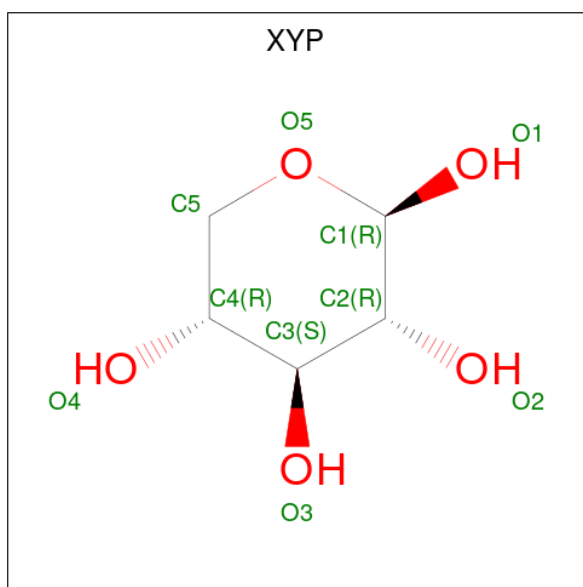
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	3	Total	C	N	O	0	0	0
			40	22	2	16			

- Molecule 4 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



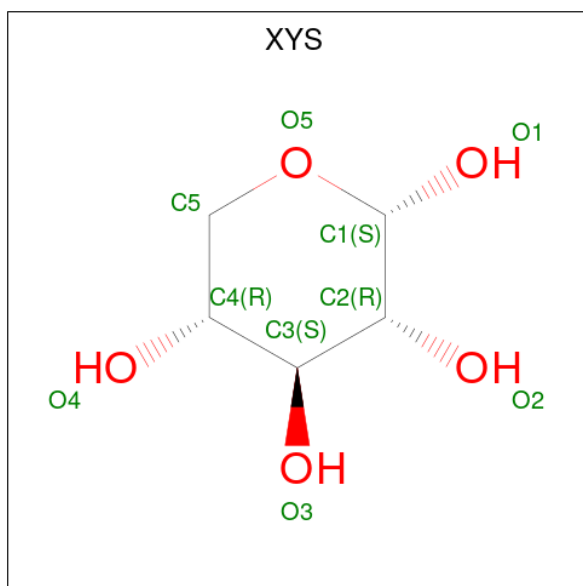
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 5 is beta-D-xylopyranose (three-letter code: XYP) (formula: $C_5H_{10}O_5$).



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

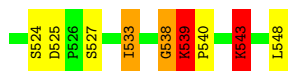
- Molecule 6 is alpha-D-xylopyranose (three-letter code: XYS) (formula: $C_5H_{10}O_5$).



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

- Molecule 7 is water.

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



- Molecule 2: 2-acetamido-2-deoxy-alpha-L-galactopyranose-(1-4)-2-(acetylamino)-1,5-anhydro-2-deoxy-D-mannitol

Chain C: 50% 50%



- Molecule 2: 2-acetamido-2-deoxy-alpha-L-galactopyranose-(1-4)-2-(acetylamino)-1,5-anhydro-2-deoxy-D-mannitol

Chain D: 50% 50%



- Molecule 2: 2-acetamido-2-deoxy-alpha-L-galactopyranose-(1-4)-2-(acetylamino)-1,5-anhydro-2-deoxy-D-mannitol

Chain E: 50% 50%



- Molecule 2: 2-acetamido-2-deoxy-alpha-L-galactopyranose-(1-4)-2-(acetylamino)-1,5-anhydro-2-deoxy-D-mannitol

Chain G: 100%



- Molecule 2: 2-acetamido-2-deoxy-alpha-L-galactopyranose-(1-4)-2-(acetylamino)-1,5-anhydro-2-deoxy-D-mannitol

Chain H: 100%



- Molecule 3: beta-D-mannopyranose-(4-4)-2-acetamido-2-deoxy-alpha-L-galactopyranose-(1-4)-2-(acetylamino)-1,5-anhydro-2-deoxy-D-mannitol

Chain F: 100%



4 Data and refinement statistics

Xtrriage (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.	Xtrriage
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: XYP, RTV, XYS, YYQ, BMA

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	1.05	4/4122 (0.1%)	0.91	13/5610 (0.2%)
1	B	0.89	4/4124 (0.1%)	1.71	15/5612 (0.3%)
All	All	0.98	8/8246 (0.1%)	1.37	28/11222 (0.2%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	PRO	N-CD	-41.24	0.90	1.47
1	B	358	ASP	CG-OD2	23.72	1.79	1.25
1	A	462	PRO	N-CD	-16.64	1.24	1.47
1	B	462	PRO	CB-CG	-15.91	0.70	1.50
1	A	462	PRO	CB-CG	-14.95	0.75	1.50
1	B	368	PRO	CB-CG	-10.06	0.99	1.50
1	A	368	PRO	CB-CG	-9.87	1.00	1.50
1	B	368	PRO	N-CD	-8.71	1.35	1.47

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	358	ASP	CB-CG-OD2	-104.02	24.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	462	PRO	CA-N-CD	-15.55	89.73	111.50
1	B	368	PRO	CA-N-CD	-13.82	92.16	111.50
1	B	358	ASP	OD1-CG-OD2	-12.96	98.68	123.30
1	B	368	PRO	N-CD-CG	11.04	119.77	103.20
1	B	462	PRO	CA-CB-CG	9.11	122.11	104.80
1	A	462	PRO	CA-N-CD	-8.43	99.70	111.50
1	B	130	LEU	CA-CB-CG	7.92	133.52	115.30
1	B	543	LYS	CD-CE-NZ	-7.62	94.16	111.70
1	A	367	THR	C-N-CD	7.32	143.76	128.40
1	B	461	TYR	C-N-CD	7.09	143.29	128.40
1	A	380	ASN	CB-CA-C	-6.70	96.99	110.40
1	A	50	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	B	451	SER	N-CA-C	-6.55	93.31	111.00
1	B	539	LYS	N-CA-C	6.49	128.52	111.00
1	A	403	LEU	C-N-CA	6.43	137.78	121.70
1	B	368	PRO	CA-CB-CG	6.29	116.75	104.80
1	A	23	LEU	CB-CG-CD2	-6.04	100.72	111.00
1	B	177	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	413	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	A	368	PRO	CA-CB-CG	-5.44	93.66	104.00
1	A	396	SER	N-CA-CB	-5.40	102.40	110.50
1	A	404	THR	N-CA-CB	5.32	120.41	110.30
1	A	368	PRO	N-CD-CG	5.30	111.14	103.20
1	B	505	MET	CG-SD-CE	5.27	108.63	100.20
1	A	50	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	B	525	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	408	ASP	CB-CG-OD1	5.06	122.86	118.30

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

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Mol	Chain	Res	Type	Group
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	92	0
1	B	4038	0	3954	110	0
2	C	28	0	0	6	0
2	D	28	0	0	0	0
2	E	28	0	0	3	0
2	G	28	0	0	2	0
2	H	28	0	0	3	0
3	F	40	0	11	16	0
4	A	12	0	9	4	0
5	A	10	0	0	2	0
6	B	10	0	10	2	0
7	A	70	0	0	2	0
7	B	50	0	0	4	0
All	All	8406	0	7938	224	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.

All (224) 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)
7:B:743:HOH:O	2:H:2:YYQ:O7	1.56	1.21
1:A:380:ASN:ND2	1:A:513:LEU:HD11	1.55	1.18
3:F:2:YYQ:C4	3:F:3:BMA:O6	1.96	1.12
3:F:2:YYQ:C5	3:F:3:BMA:O6	2.03	1.07
4:A:601:BMA:O3	2:C:2:YYQ:C2	2.03	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ALA:HB1	1:A:62:ASP:HA	1.44	1.00
3:F:2:YYQ:C6	3:F:3:BMA:HO6	1.76	0.98
1:B:251:CYS:HB2	1:B:288:THR:O	1.61	0.98
1:A:251:CYS:HB2	1:A:288:THR:O	1.67	0.94
3:F:2:YYQ:C6	3:F:3:BMA:O6	2.14	0.93
3:F:2:YYQ:C1	3:F:3:BMA:O6	2.17	0.92
5:A:602:XYP:O1	2:C:2:YYQ:O3	1.86	0.92
1:A:380:ASN:CG	1:A:380:ASN:O	2.08	0.91
3:F:2:YYQ:C1	3:F:3:BMA:C6	2.53	0.86
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
3:F:3:BMA:O6	3:F:3:BMA:O4	1.92	0.81
1:B:380:ASN:OD1	2:H:1:RTV:O6	1.97	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:254:THR:HA	7:B:737:HOH:O	1.81	0.80
1:A:61:ALA:CB	1:A:62:ASP:HA	2.11	0.80
3:F:2:YYQ:C1	3:F:3:BMA:H62	2.13	0.79
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:A:517:LEU:HD23	1:A:533:ILE:CG2	2.15	0.77
1:A:380:ASN:CG	1:A:513:LEU:HD11	2.05	0.76
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
4:A:601:BMA:O3	2:C:2:YYQ:N2	2.21	0.74
1:A:515:ASN:HB3	1:A:517:LEU:H	1.53	0.73
1:B:420:ASN:OD1	3:F:1:RTV:C1	2.36	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: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:B:285:ASN:CG	1:B:285:ASN:O	2.32	0.68
1:A:287:ASP:O	1:A:289:CYS:N	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:LYS:HE3	1:B:457:LYS:CE	2.25	0.67
1:B:28:ALA:HB1	7:B:712:HOH:O	1.93	0.67
1:B:119:GLU:OE2	1:B:126:ARG:HG3	1.94	0.67
2:E:2:YYQ:O3	2:E:2:YYQ:C7	2.43	0.67
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: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
2:H:1:RTV:N2	2:H:2:YYQ:O4	2.30	0.64
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
3:F:2:YYQ:O5	3:F:3:BMA:O6	2.17	0.62
1:A:70:ASP:OD1	1:A:72:THR:HB	2.00	0.61
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:RTV: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:A:451:SER:O	1:A:453:LYS:CG	2.51	0.59
1:A:285:ASN:CG	1:A:285:ASN:O	2.42	0.58
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: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:B:488:ILE:HD13	1:B:519:MET:HE2	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:PHE:CD2	1:A:100:LEU:HD13	2.41	0.55
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:471:ASP:CG	1:B:474:ARG:HD3	2.29	0.53
1:B:285:ASN:O	1:B:285:ASN:ND2	2.41	0.53
1:A:488:ILE:HD13	1:A:519:MET:HE3	1.91	0.53
1:B:55:GLU:HG2	1:B:64:PRO:HG2	1.91	0.52
1:B:517:LEU:HD23	1:B:533:ILE:HG23	1.92	0.52
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:380:ASN:OD1	1:A:380:ASN:C	2.40	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: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
3:F:2:YYQ:O6	3:F:3:BMA:O6	2.26	0.50
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:A:537:THR:C	1:A:538:GLY:O	2.49	0.49
1:A:287:ASP:O	1:A:288:THR:C	2.50	0.49
1:B:313:TYR:OH	1:B:331:ASN:HA	2.12	0.49
1:A:380:ASN:HB3	2:E:1:RTV: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:488:ILE:HG21	1:B:519:MET:HE3	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1:RTV:O3	2:E:1:RTV:O5	2.29	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: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:518:VAL:HG12	1:A:519:MET:O	2.13	0.47
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: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: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
6:B:602:XYS:O3	3:F:2:YYQ:O3	2.30	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:A:133:MET:HA	1:A:133:MET:CE	2.45	0.46
5:A:602:XYP:O1	2:C:2:YYQ:C3	2.61	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: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
3:F:1:RTV:O4	3:F:3:BMA:H62	2.17	0.45
4:A:601:BMA:C4	2:C:2:YYQ:C2	2.94	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:B:136:LEU:HD22	1:B:164:MET:HE1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:602:XYS:HO3	3:F:2:YYQ:C3	2.25	0.44
1:A:322:TRP:HH2	7:A:762:HOH:O	2.00	0.44
1:A:522:LYS:HE2	1:A:530:GLN:OE1	2.17	0.44
1:B:50:ARG:C	1:B:71:VAL:HG23	2.38	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:296:VAL:HG21	1:A:418:ALA:HB1	2.00	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
1:B:92:ASN:O	1:B:93:PRO:C	2.55	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	7:B:712:HOH:O	2.16	0.43
1:A:212:ASN:OD1	1:A:212:ASN:C	2.57	0.43
1:A:413:ARG:HB2	1:A:496:GLY:O	2.18	0.43
4:A:601:BMA:C3	2:C:2:YYQ:C2	2.95	0.43
1:B:420:ASN:OD1	3:F:1:RTV:C2	2.66	0.43
1:B:216:VAL:CG1	1:B:294:PRO:HG2	2.48	0.43
1:B:163:GLN:HE21	1:B:198:GLU:CD	2.22	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:133:MET:HE2	1:B:182:ILE:HG12	2.00	0.42
1:B:252:ARG:O	1:B:288:THR:HG22	2.20	0.42
1:B:420:ASN:OD1	3:F:1:RTV:N2	2.52	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:A:92:ASN:O	1:A:93:PRO:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:50:ARG:HH21	1:B:70:ASP:CG	2.24	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:YYQ:C7	2.34	0.41
1:B:319:ILE:HD11	1:B:362:ILE:HG12	2.03	0.40
1:A:505:MET:HA	1:A:505:MET:HE2	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:325:LYS:C	1:A:327:ASN:H	2.24	0.40
1:A:419:GLY:HA3	7:A:701:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	514/570 (90%)	467 (91%)	33 (6%)	14 (3%)	5	23
1	B	514/570 (90%)	469 (91%)	31 (6%)	14 (3%)	5	23
All	All	1028/1140 (90%)	936 (91%)	64 (6%)	28 (3%)	5	23

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

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Mol	Chain	Res	Type
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
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%)	406 (91%)	40 (9%)	9	32
1	B	446/496 (90%)	402 (90%)	44 (10%)	8	27
All	All	892/992 (90%)	808 (91%)	84 (9%)	8	29

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	67	LEU
1	A	72	THR
1	A	80	ARG
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
1	A	240	VAL
1	A	248	LEU
1	A	252	ARG
1	A	321	LEU
1	A	361	MET
1	A	366	ARG
1	A	377	PHE
1	A	380	ASN
1	A	405	VAL
1	A	447	VAL
1	A	448	GLU
1	A	452	SER
1	A	483	SER
1	A	487	ILE
1	A	501	ARG
1	A	515	ASN
1	A	527	SER
1	A	528	LEU
1	A	533	ILE
1	A	539	LYS
1	B	1	TYR
1	B	2	GLN
1	B	3	THR

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Mol	Chain	Res	Type
1	B	44	THR
1	B	57	SER
1	B	71	VAL
1	B	72	THR
1	B	83	SER
1	B	89	ARG
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	202	SER
1	B	209	GLN
1	B	213	GLN
1	B	226	ILE
1	B	240	VAL
1	B	253	SER
1	B	351	THR
1	B	361	MET
1	B	362	ILE
1	B	367	THR
1	B	377	PHE
1	B	380	ASN
1	B	400	ARG
1	B	403	LEU
1	B	447	VAL
1	B	448	GLU
1	B	451	SER
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	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 (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	GLN
1	B	213	GLN
1	B	285	ASN
1	B	380	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 ⓘ

13 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	RTV	C	1	2	14,14,14	0.82	0	17,19,19	2.21	7 (41%)
2	YYQ	C	2	2,4	14,14,15	2.47	6 (42%)	17,19,21	7.24	11 (64%)
2	RTV	D	1	2	14,14,14	0.65	0	17,19,19	1.85	2 (11%)
2	YYQ	D	2	2	14,14,15	1.33	1 (7%)	17,19,21	2.84	5 (29%)
2	RTV	E	1	2	14,14,14	0.84	0	17,19,19	3.11	5 (29%)
2	YYQ	E	2	2	14,14,15	2.55	2 (14%)	17,19,21	2.75	7 (41%)
3	RTV	F	1	3	14,14,14	0.51	0	17,19,19	2.31	7 (41%)
3	YYQ	F	2	3	14,14,15	2.67	1 (7%)	17,19,21	3.02	5 (29%)
3	BMA	F	3	3	12,12,12	0.79	0	17,17,17	1.89	5 (29%)
2	RTV	G	1	2	14,14,14	0.66	0	17,19,19	1.28	2 (11%)
2	YYQ	G	2	2	14,14,15	0.81	1 (7%)	17,19,21	10.49	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	RTV	H	1	2	14,14,14	1.04	1 (7%)	17,19,19	2.17	4 (23%)
2	YYQ	H	2	2	14,14,15	1.23	2 (14%)	17,19,21	2.09	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	RTV	C	1	2	-	2/6/23/23	0/1/1/1
2	YYQ	C	2	2,4	1/1/5/7	4/6/23/26	0/1/1/1
2	RTV	D	1	2	1/1/5/6	3/6/23/23	0/1/1/1
2	YYQ	D	2	2	2/2/5/7	4/6/23/26	0/1/1/1
2	RTV	E	1	2	-	5/6/23/23	1/1/1/1
2	YYQ	E	2	2	2/2/5/7	5/6/23/26	0/1/1/1
3	RTV	F	1	3	-	4/6/23/23	0/1/1/1
3	YYQ	F	2	3	1/1/5/7	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/22/22	0/1/1/1
2	RTV	G	1	2	1/1/5/6	5/6/23/23	0/1/1/1
2	YYQ	G	2	2	1/1/5/7	5/6/23/26	0/1/1/1
2	RTV	H	1	2	3/3/5/6	3/6/23/23	0/1/1/1
2	YYQ	H	2	2	3/3/5/7	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)
3	F	2	YYQ	O3-C3	-9.64	1.20	1.43
2	E	2	YYQ	O3-C3	-8.72	1.22	1.43
2	C	2	YYQ	O6-C6	4.88	1.63	1.42
2	C	2	YYQ	O3-C3	-4.27	1.32	1.43
2	D	2	YYQ	O3-C3	4.21	1.52	1.43
2	C	2	YYQ	C8-C7	3.50	1.57	1.50
2	E	2	YYQ	C1-C2	3.00	1.56	1.52
2	C	2	YYQ	C1-C2	2.81	1.56	1.52
2	C	2	YYQ	O5-C5	2.77	1.49	1.43
2	H	2	YYQ	O5-C5	2.71	1.48	1.43
2	H	2	YYQ	C4-C5	2.46	1.58	1.53
2	G	2	YYQ	O3-C3	2.34	1.48	1.43
2	H	1	RTV	C3-C4	2.32	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	YYQ	C4-C5	2.05	1.57	1.53

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	YYQ	C8-C7-N2	25.69	159.59	116.10
2	C	2	YYQ	O3-C3-C2	25.07	161.35	109.47
2	G	2	YYQ	O7-C7-N2	-23.22	79.26	121.95
2	G	2	YYQ	O7-C7-C8	-22.40	80.46	122.06
2	G	2	YYQ	O3-C3-C2	11.42	133.09	109.47
2	C	2	YYQ	O3-C3-C4	-9.73	87.86	110.35
2	E	1	RTV	C4-C3-C2	-7.98	99.32	111.02
3	F	2	YYQ	O6-C6-C5	7.78	137.99	111.29
2	C	2	YYQ	O5-C5-C6	7.40	118.81	107.20
2	C	2	YYQ	C1-O5-C5	7.28	122.06	112.19
2	E	1	RTV	C1-C2-N2	7.08	122.59	110.49
2	D	2	YYQ	O3-C3-C2	6.37	122.65	109.47
2	D	1	RTV	C1-O5-C5	6.04	120.38	112.19
2	D	2	YYQ	O3-C3-C4	5.90	124.00	110.35
3	F	1	RTV	C2-N2-C7	5.82	131.19	122.90
3	F	2	YYQ	O3-C3-C2	5.71	121.28	109.47
2	H	1	RTV	O3-C3-C4	5.54	123.16	110.35
2	E	2	YYQ	C1-O5-C5	5.48	119.62	112.19
2	D	2	YYQ	O4-C4-C5	5.46	122.85	109.30
2	H	2	YYQ	O5-C5-C6	5.40	115.67	107.20
2	C	1	RTV	C4-C3-C2	5.39	118.92	111.02
3	F	2	YYQ	O3-C3-C4	5.20	122.37	110.35
2	E	2	YYQ	O3-C3-C2	4.76	119.32	109.47
2	E	2	YYQ	O4-C4-C5	4.68	120.92	109.30
2	E	2	YYQ	C1-C2-N2	4.66	118.44	110.49
2	E	1	RTV	O5-C1-C2	-4.52	104.15	111.29
2	D	2	YYQ	O4-C4-C3	4.49	120.72	110.35
2	H	2	YYQ	O5-C1-C2	-4.49	104.20	111.29
3	F	2	YYQ	O4-C4-C5	4.43	120.31	109.30
2	H	1	RTV	O4-C4-C3	4.30	120.30	110.35
3	F	3	BMA	O6-C6-C5	-4.02	97.51	111.29
2	G	2	YYQ	O3-C3-C4	-3.87	101.39	110.35
2	E	1	RTV	O4-C4-C5	3.67	118.41	109.30
3	F	1	RTV	C4-C3-C2	3.59	116.28	111.02
2	C	2	YYQ	O6-C6-C5	-3.52	99.22	111.29
2	C	1	RTV	C2-N2-C7	3.30	127.61	122.90
2	E	2	YYQ	O3-C3-C4	3.23	117.81	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	RTV	C1-O5-C5	3.18	116.51	112.19
3	F	3	BMA	O5-C5-C6	3.17	114.31	106.44
2	H	1	RTV	C1-C2-N2	3.14	115.85	110.49
3	F	3	BMA	O4-C4-C5	3.10	117.00	109.30
2	C	2	YYQ	O4-C4-C3	3.05	117.39	110.35
3	F	3	BMA	C3-C4-C5	-2.85	105.15	110.24
3	F	1	RTV	C1-C2-N2	-2.85	105.62	110.49
2	E	2	YYQ	O5-C5-C4	2.82	117.70	110.83
2	H	1	RTV	O6-C6-C5	-2.79	101.71	111.29
2	D	2	YYQ	C2-N2-C7	2.76	126.83	122.90
2	C	2	YYQ	C2-N2-C7	2.73	126.79	122.90
2	C	1	RTV	O5-C1-C2	-2.57	107.22	111.29
3	F	1	RTV	C3-C4-C5	2.56	114.81	110.24
3	F	1	RTV	O4-C4-C3	-2.52	104.53	110.35
2	H	2	YYQ	O4-C4-C5	2.51	115.54	109.30
2	G	1	RTV	C2-N2-C7	2.49	126.45	122.90
2	H	2	YYQ	C2-N2-C7	-2.49	119.35	122.90
2	E	1	RTV	C3-C4-C5	-2.47	105.83	110.24
2	E	2	YYQ	C2-N2-C7	2.47	126.41	122.90
2	C	2	YYQ	O5-C5-C4	2.44	116.76	110.83
2	D	1	RTV	C1-C2-N2	2.42	114.63	110.49
2	C	1	RTV	O4-C4-C5	2.39	115.23	109.30
2	C	2	YYQ	O7-C7-C8	2.37	126.47	122.06
2	C	2	YYQ	O5-C1-C2	-2.33	107.62	111.29
3	F	2	YYQ	O5-C1-C2	-2.30	107.66	111.29
3	F	1	RTV	C8-C7-N2	2.28	119.96	116.10
2	C	1	RTV	O3-C3-C2	-2.20	104.92	109.47
2	G	2	YYQ	C1-O5-C5	2.17	115.13	112.19
3	F	1	RTV	C1-O5-C5	2.13	115.08	112.19
3	F	3	BMA	C1-C2-C3	2.12	114.72	110.31
2	C	1	RTV	O5-C5-C4	2.12	115.98	110.83
2	C	1	RTV	O4-C4-C3	2.03	115.03	110.35
2	C	2	YYQ	C1-C2-N2	2.01	113.92	110.49
2	G	2	YYQ	O5-C5-C6	2.00	110.34	107.20

All (15) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	2	YYQ	C3
2	D	1	RTV	C3
2	D	2	YYQ	C5
2	D	2	YYQ	C2

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Mol	Chain	Res	Type	Atom
2	E	2	YYQ	C3
2	E	2	YYQ	C2
2	G	1	RTV	C5
2	G	2	YYQ	C4
2	H	1	RTV	C5
2	H	1	RTV	C4
2	H	1	RTV	C2
2	H	2	YYQ	C1
2	H	2	YYQ	C5
2	H	2	YYQ	C4
3	F	2	YYQ	C4

All (48) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	G	1	RTV	C1-C2-N2-C7
2	D	2	YYQ	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
2	E	2	YYQ	O5-C5-C6-O6
2	H	2	YYQ	O5-C5-C6-O6
2	G	2	YYQ	C4-C5-C6-O6
2	E	1	RTV	C4-C5-C6-O6
2	H	2	YYQ	C4-C5-C6-O6
2	D	2	YYQ	C4-C5-C6-O6
2	G	2	YYQ	C8-C7-N2-C2
2	G	1	RTV	O5-C5-C6-O6
2	G	2	YYQ	O5-C5-C6-O6
2	E	2	YYQ	C4-C5-C6-O6
2	D	1	RTV	O5-C5-C6-O6
3	F	1	RTV	C1-C2-N2-C7
2	C	2	YYQ	O5-C5-C6-O6
2	H	1	RTV	O5-C5-C6-O6
2	H	1	RTV	C1-C2-N2-C7
3	F	3	BMA	C4-C5-C6-O6
3	F	1	RTV	C3-C2-N2-C7
2	G	1	RTV	C4-C5-C6-O6

All (1) ring outliers are listed below:

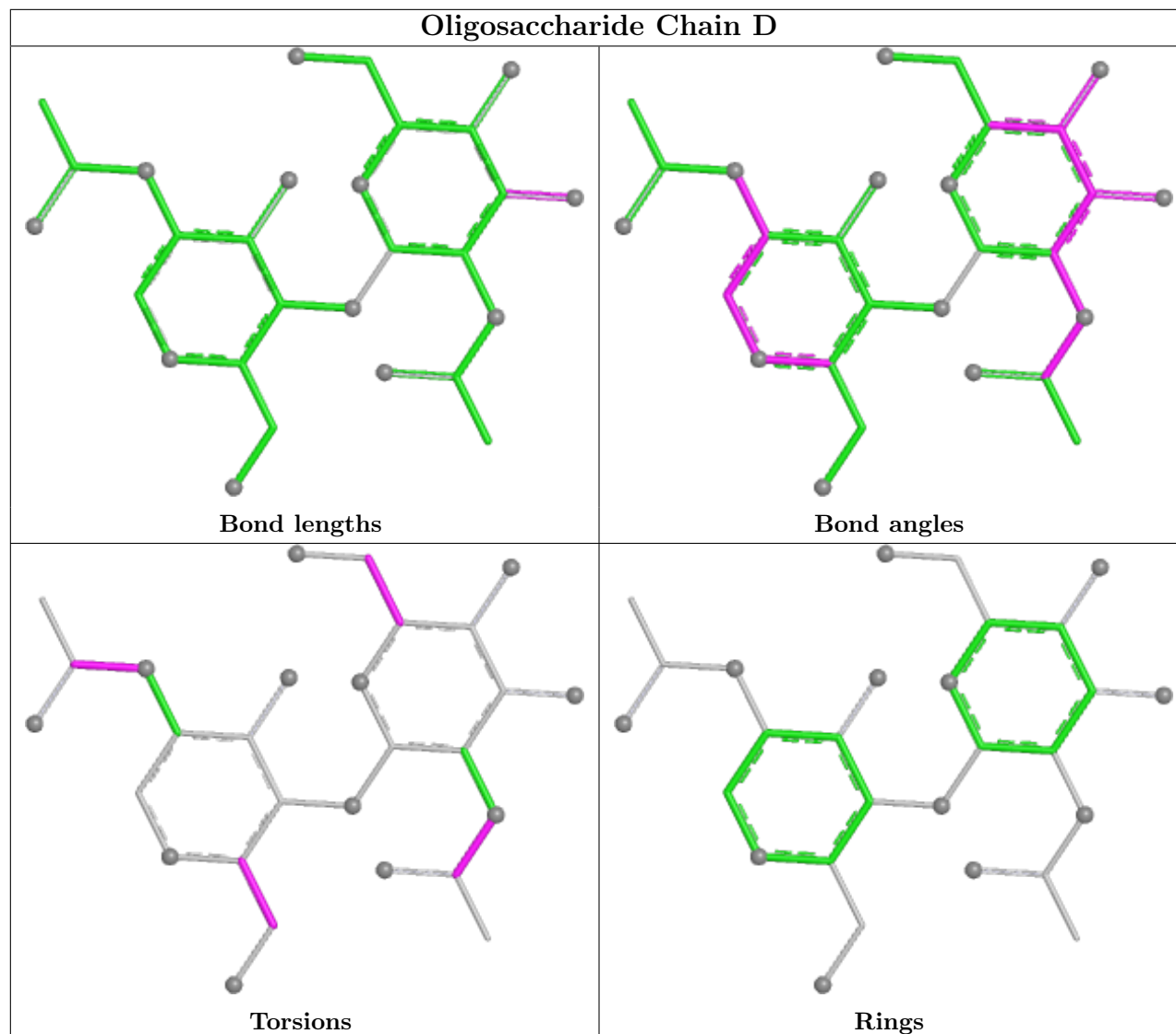
Mol	Chain	Res	Type	Atoms
2	E	1	RTV	C1-C2-C3-C4-C5-O5

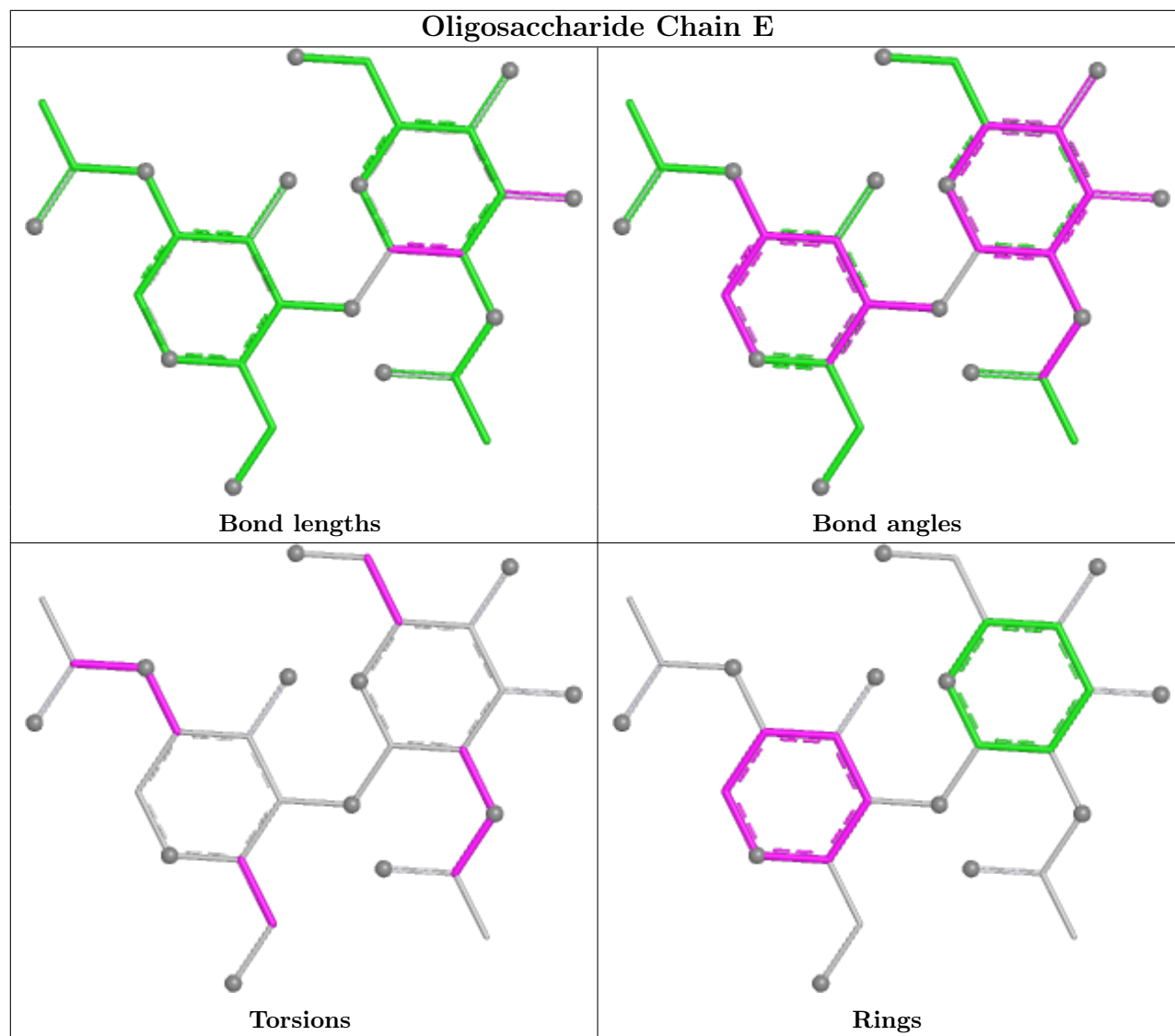
10 monomers are involved in 30 short contacts:

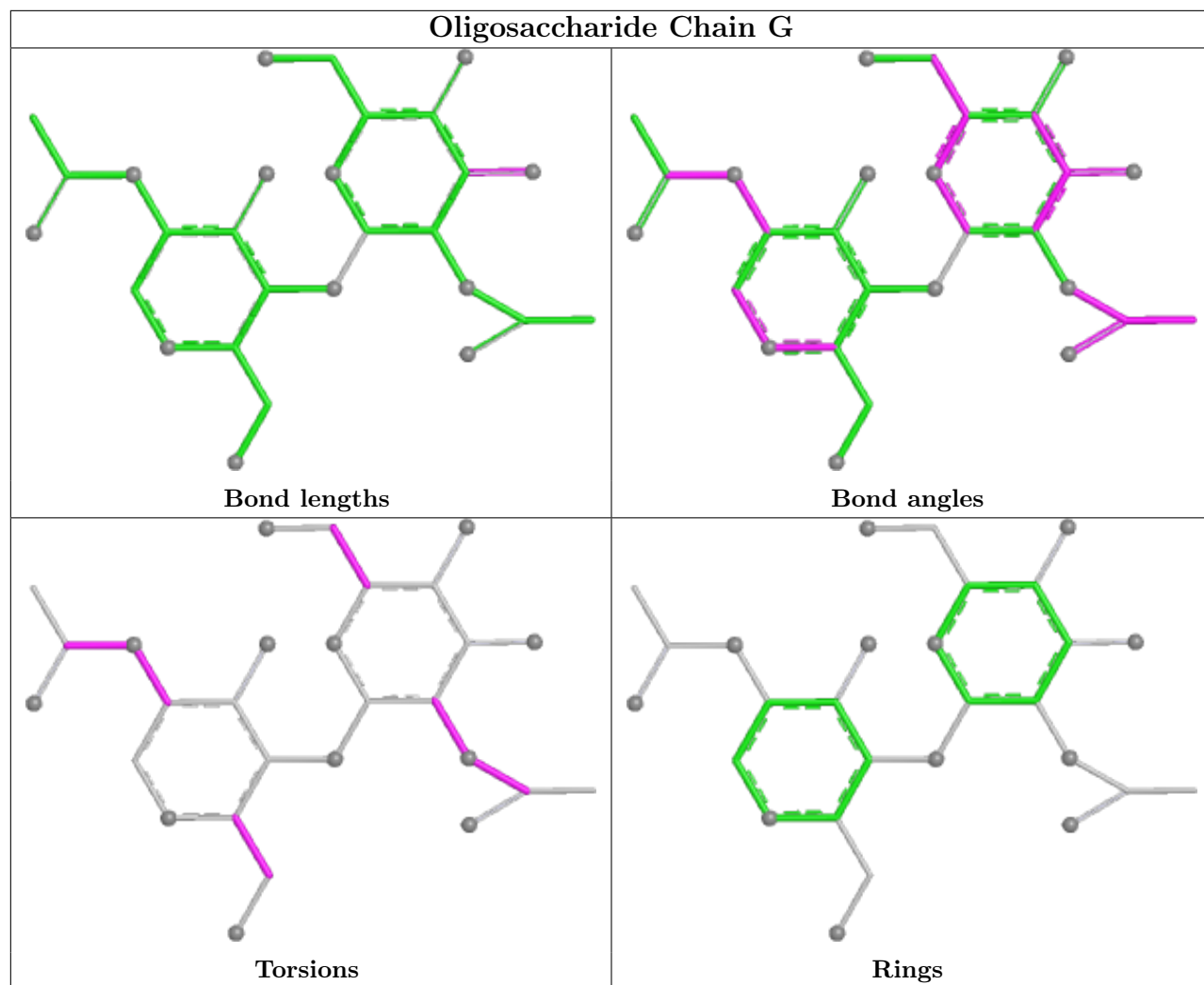
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	RTV	4	0
3	F	3	BMA	11	0
2	H	2	YYQ	2	0
2	C	2	YYQ	6	0
3	F	2	YYQ	11	0
2	E	2	YYQ	1	0
2	H	1	RTV	2	0
2	E	1	RTV	2	0
2	G	2	YYQ	1	0
2	G	1	RTV	1	0

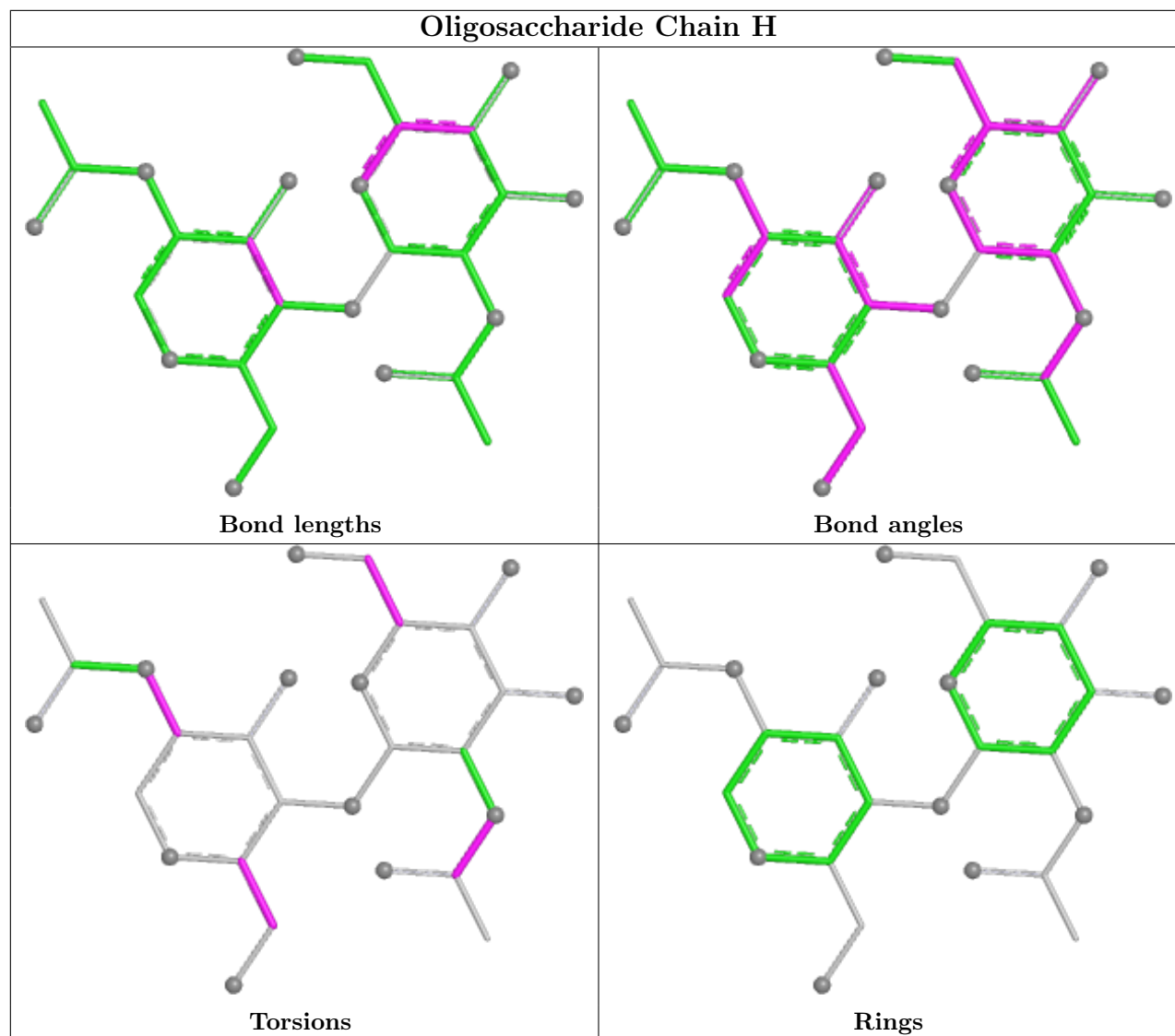
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

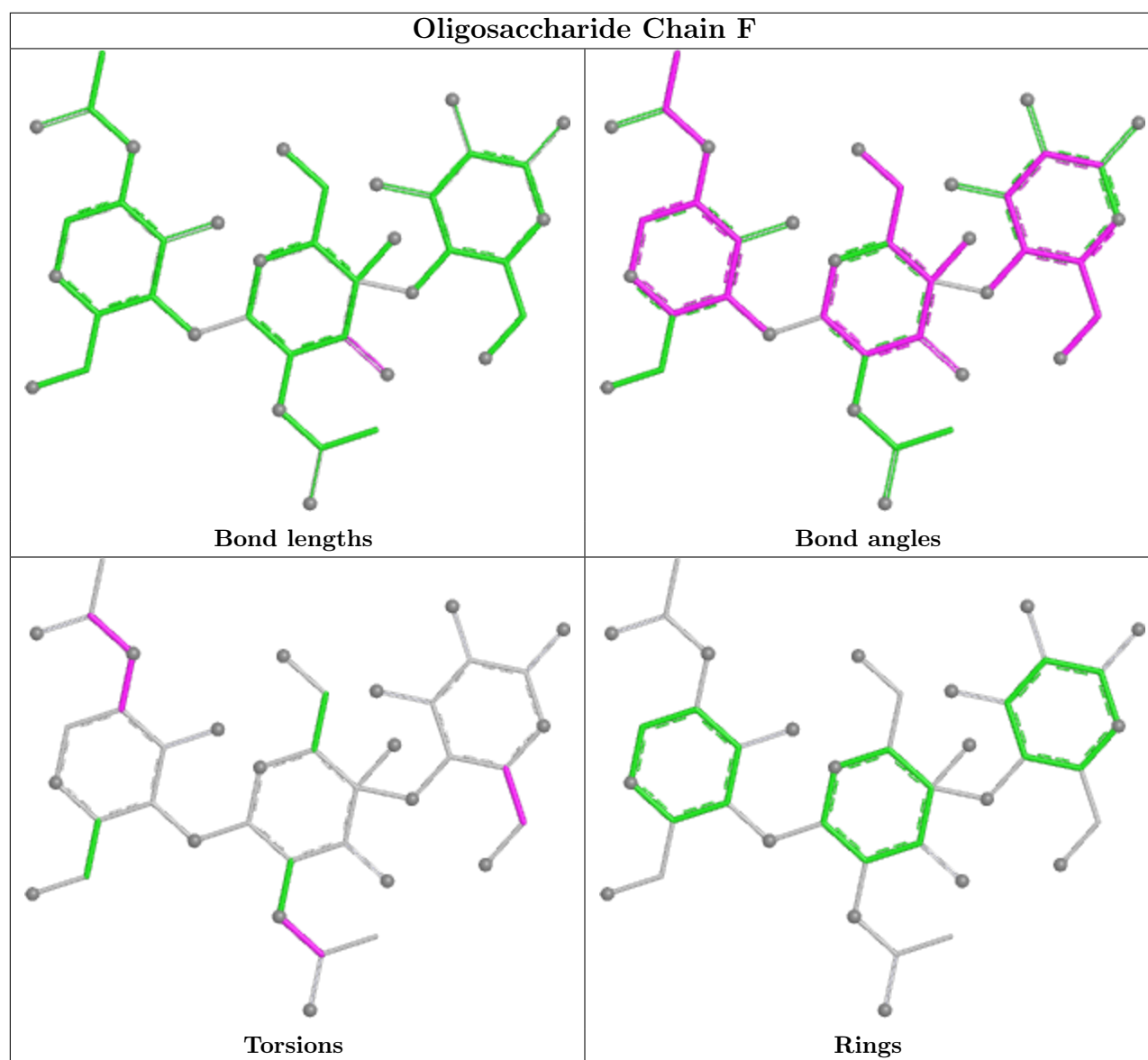
bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

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
6	XYS	B	602	-	10,10,10	1.38	1 (10%)	14,14,14	1.45	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	A	601	2	12,12,12	0.75	0	17,17,17	2.37	7 (41%)
5	XYP	A	602	-	10,10,10	1.41	1 (10%)	14,14,14	1.51	4 (28%)

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
6	XYS	B	602	-	-	-	0/1/1/1
4	BMA	A	601	2	-	2/2/22/22	0/1/1/1
5	XYP	A	602	-	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	XYP	O5-C1	-4.07	1.37	1.43
6	B	602	XYS	O5-C1	-3.78	1.37	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	BMA	O6-C6-C5	-4.51	95.82	111.29
4	A	601	BMA	C4-C3-C2	-4.44	103.08	110.82
4	A	601	BMA	O4-C4-C5	3.92	119.04	109.30
4	A	601	BMA	O5-C5-C4	-3.24	103.81	109.69
4	A	601	BMA	O4-C4-C3	3.19	117.73	110.35
6	B	602	XYS	O5-C5-C4	-2.89	106.30	110.77
4	A	601	BMA	C6-C5-C4	-2.73	106.61	113.00
5	A	602	XYP	C5-O5-C1	2.69	117.23	112.71
5	A	602	XYP	C5-C4-C3	-2.46	106.65	109.67
6	B	602	XYS	C1-C2-C3	-2.45	105.23	110.31
5	A	602	XYP	C4-C3-C2	-2.34	106.84	110.89
6	B	602	XYS	O3-C3-C2	-2.29	105.06	110.35
5	A	602	XYP	O5-C1-C2	2.25	112.77	109.43
4	A	601	BMA	C3-C4-C5	-2.09	106.52	110.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	BMA	C4-C5-C6-O6
4	A	601	BMA	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	602	XYS	2	0
4	A	601	BMA	4	0
5	A	602	XYP	2	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

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.