



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:56 PM EDT

PDB ID : 6OPA / pdb_00006opa
Title : Crystal structure of bovine Fab NC-Cow1 in complex with HIV-1 BG505
SOSIP.664, and human Fabs 35022 and PGT128
Authors : Stanfield, R.L.; Wilson, I.A.
Deposited on : 2019-04-24
Resolution : 4.08 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

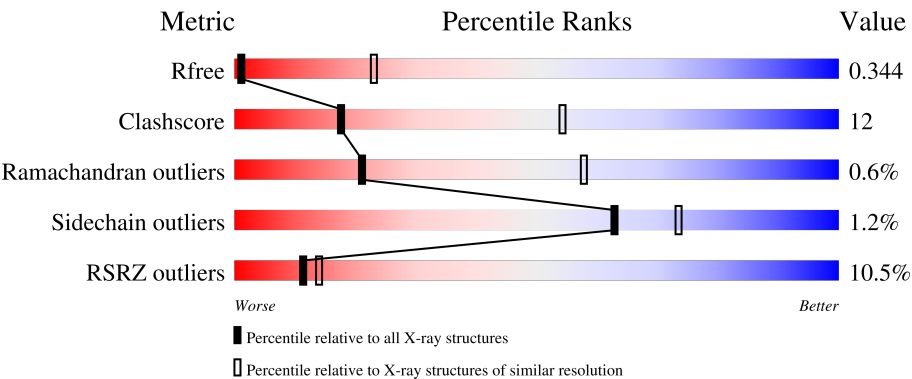
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.08 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))
R_{free}	180053	1200 (4.36-3.80)
Clashscore	190562	1249 (4.36-3.80)
Ramachandran outliers	187476	1169 (4.36-3.80)
Sidechain outliers	187428	1158 (4.36-3.80)
RSRZ outliers	180081	1199 (4.36-3.80)

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	215.24Å 215.24Å 438.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.76 – 4.08 48.76 – 4.08	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.76-4.08) 98.5 (48.76-4.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.22	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 4.14Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.332 , 0.343 0.336 , 0.344	Depositor DCC
R_{free} test set	1559 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	169.9	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 179.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	10798	wwPDB-VP
Average B, all atoms (Å ²)	214.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

3 Model quality [i](#)

3.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, 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	G	0.24	0/3429	0.61	2/4653 (0.0%)
2	B	0.17	0/1044	0.37	0/1415
3	F	0.19	0/1043	0.54	0/1416
4	I	0.19	0/860	0.55	0/1175
5	J	0.13	0/763	0.33	0/1040
6	K	0.22	0/1061	0.58	0/1455
7	R	0.17	0/822	0.38	0/1120
8	S	0.16	0/1331	0.41	0/1806
All	All	0.20	0/10353	0.51	2/14080 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	74	CYS	CA-C-N	5.63	128.99	121.23
1	G	74	CYS	C-N-CA	5.63	128.99	121.23

There are no chirality outliers.

There are no planarity outliers.

3.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3360	0	3306	135	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1026	0	1001	29	1
3	F	1015	0	985	31	0
4	I	836	0	785	24	0
5	J	746	0	721	8	0
6	K	1028	0	990	27	0
7	R	807	0	756	12	0
8	S	1302	0	1235	31	0
9	A	83	0	70	6	0
10	C	28	0	25	0	0
10	L	28	0	25	0	0
11	D	39	0	34	0	0
11	E	39	0	34	1	0
11	Q	39	0	34	0	0
12	H	50	0	43	3	0
12	N	50	0	43	0	0
13	M	61	0	52	0	0
13	O	61	0	52	0	0
13	P	61	0	52	1	0
13	U	61	0	52	0	0
14	T	50	0	43	0	0
15	B	28	0	26	2	0
All	All	10798	0	10364	262	1

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 12.

All (262) 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:G:350:ARG:HH22	1:G:396:ILE:HA	1.38	0.87
1:G:54:CYS:SG	2:B:571:TRP:CD2	2.73	0.81
1:G:473:GLY:HA3	8:S:130:PHE:HA	1.63	0.78
4:I:47:ILE:HG22	4:I:48:ILE:HG12	1.64	0.78
1:G:281:ALA:O	8:S:129:ARG:HD3	1.87	0.74
1:G:74:CYS:SG	2:B:571:TRP:HB3	2.28	0.73
5:J:35:TRP:HB2	5:J:48:ILE:HB	1.69	0.73
6:K:2:PRO:HA	6:K:25:SER:O	1.89	0.72
1:G:491:ILE:O	2:B:585:ARG:NH2	2.23	0.72
1:G:121:LYS:HA	1:G:202:THR:HA	1.72	0.71
4:I:83:GLU:HG3	4:I:105:SER:HA	1.71	0.71
4:I:35:TRP:HB2	4:I:48:ILE:HB	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:426:MET:HG3	1:G:427:TRP:HD1	1.55	0.70
8:S:39:GLN:HB2	8:S:45:LEU:HD23	1.76	0.68
1:G:192:ARG:HH22	12:H:1:NAG:H2	1.58	0.67
6:K:70:ALA:HB3	6:K:79:PHE:HB2	1.75	0.67
6:K:33:ASN:HA	6:K:100:LEU:HG	1.77	0.67
4:I:93:HIS:CE1	9:A:3:BMA:H4	2.30	0.66
1:G:220:PRO:HB3	2:B:578:ALA:HB1	1.76	0.66
1:G:254:VAL:HG11	1:G:261:LEU:HB2	1.78	0.65
1:G:94:ASN:HA	1:G:236:THR:HG22	1.78	0.65
1:G:230:ASP:HB3	1:G:233:PHE:HB2	1.78	0.65
1:G:424:ILE:HD11	1:G:434:MET:HE2	1.77	0.65
3:F:47:TRP:CD2	4:I:95(A):GLY:HA3	2.32	0.65
1:G:361:PHE:HE1	1:G:468:PHE:HD2	1.44	0.64
6:K:67:LEU:HD11	6:K:80:LEU:HD11	1.80	0.64
1:G:101:VAL:HG13	1:G:479:TRP:HB2	1.80	0.63
1:G:70:ALA:O	1:G:73:ALA:HB2	1.99	0.62
3:F:12:LYS:HG3	3:F:18:VAL:HB	1.81	0.62
1:G:130:GLN:HG3	11:E:1:NAG:H83	1.80	0.62
1:G:338:TRP:CE2	1:G:390:LEU:HD22	2.34	0.62
1:G:104:MET:O	1:G:108:ILE:HG12	2.00	0.62
1:G:54:CYS:SG	2:B:571:TRP:CE3	2.93	0.61
1:G:283:ASN:ND2	8:S:129:ARG:HB2	2.14	0.61
9:A:2:NAG:H3	9:A:2:NAG:H83	1.82	0.61
1:G:270:VAL:HG12	1:G:289:ASN:H	1.63	0.61
3:F:31:PHE:HB3	3:F:98:ARG:HD3	1.83	0.61
1:G:473:GLY:CA	8:S:130:PHE:HA	2.30	0.61
1:G:292:VAL:HB	1:G:449:ILE:CG2	2.31	0.60
1:G:476:ARG:HA	1:G:479:TRP:CD1	2.37	0.59
1:G:254:VAL:HG21	1:G:262:ASN:HB2	1.84	0.59
1:G:36:VAL:HG12	2:B:610:TRP:HE3	1.68	0.59
3:F:12:LYS:HE3	3:F:17:SER:O	2.03	0.58
15:B:802:NAG:H3	15:B:802:NAG:H83	1.85	0.58
6:K:31:ALA:HB1	6:K:33:ASN:HD22	1.68	0.58
8:S:66:ARG:NH2	8:S:82(B):GLY:O	2.37	0.58
3:F:47:TRP:CE3	4:I:95(A):GLY:HA3	2.38	0.57
1:G:292:VAL:HB	1:G:449:ILE:HG23	1.87	0.57
1:G:295:ASN:O	1:G:331:CYS:HA	2.05	0.56
1:G:343:GLY:O	1:G:347:LYS:HG2	2.05	0.56
3:F:51:ILE:HD13	3:F:71:THR:HG23	1.87	0.56
5:J:46:LEU:HD22	6:K:101:ASP:HA	1.87	0.56
15:B:801:NAG:H83	15:B:801:NAG:H3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:90:TYR:O	6:K:106:GLY:HA2	2.05	0.56
1:G:55:ALA:HB3	1:G:216:HIS:HB2	1.88	0.56
3:F:100(B):SER:OG	4:I:50:GLU:OE2	2.24	0.56
1:G:371:VAL:O	8:S:135:ARG:NH2	2.39	0.56
1:G:363:ASN:HD21	1:G:388:SER:HB3	1.71	0.55
1:G:70:ALA:HB3	1:G:213:ILE:HD11	1.88	0.55
1:G:37:THR:HG22	2:B:605:CYS:HA	1.89	0.55
13:P:1:NAG:H83	13:P:1:NAG:H3	1.88	0.55
3:F:2:GLY:HA2	3:F:26:GLY:HA3	1.88	0.54
1:G:304:ARG:HD3	1:G:318:TYR:CD1	2.43	0.54
1:G:261:LEU:HD11	1:G:374:HIS:CE1	2.42	0.54
1:G:269:GLU:OE1	1:G:351:LYS:NZ	2.40	0.54
1:G:426:MET:HG3	1:G:427:TRP:CD1	2.38	0.54
3:F:51:ILE:HG13	3:F:57:LYS:HG2	1.90	0.54
1:G:198:THR:HG22	12:H:1:NAG:H61	1.89	0.54
1:G:258:GLN:H	1:G:472:GLY:HA3	1.72	0.54
1:G:368:ASP:HB2	1:G:371:VAL:HG12	1.88	0.54
4:I:62:PHE:CE1	4:I:75:ILE:HG23	2.43	0.54
1:G:301:ASN:HB3	1:G:323:ILE:O	2.08	0.53
4:I:93:HIS:NE2	9:A:3:BMA:H4	2.23	0.53
8:S:108:TYR:CD1	8:S:127:GLY:HA2	2.44	0.53
8:S:129:ARG:HH12	8:S:138:GLY:HA2	1.74	0.53
6:K:51:LEU:HB3	6:K:57:THR:HG23	1.91	0.53
4:I:62:PHE:HE1	4:I:75:ILE:HG23	1.74	0.53
8:S:130:PHE:CZ	8:S:135:ARG:HG2	2.43	0.53
1:G:364:SER:HB2	8:S:135:ARG:HD2	1.91	0.52
7:R:2:TYR:HE2	7:R:4:LEU:HD23	1.75	0.52
1:G:201:ILE:HD11	1:G:435:TYR:HB2	1.92	0.52
1:G:427:TRP:CZ3	1:G:431:GLY:HA3	2.45	0.52
1:G:456:ARG:HG2	1:G:468:PHE:HE1	1.74	0.52
4:I:37:GLN:HB2	4:I:47:ILE:HD11	1.90	0.52
8:S:18:LEU:HD22	8:S:161:VAL:HG11	1.92	0.52
1:G:55:ALA:HB1	1:G:77:THR:HG22	1.90	0.52
1:G:93:PHE:HB2	1:G:233:PHE:HZ	1.74	0.52
7:R:106(A):LEU:HD22	7:R:107:GLY:H	1.74	0.52
1:G:175:LEU:HB2	1:G:320:THR:HB	1.92	0.52
8:S:113:ARG:NH1	8:S:117:GLN:OE1	2.43	0.52
2:B:606:THR:HG21	2:B:646:LEU:HD22	1.92	0.52
6:K:40:PRO:O	6:K:42:GLY:N	2.43	0.52
2:B:523:LEU:H	2:B:540:GLN:HG3	1.75	0.51
1:G:478:ASN:O	1:G:481:SER:OG	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:92:ASP:C	7:R:94:SER:H	2.19	0.51
3:F:31:PHE:HB3	3:F:98:ARG:CD	2.41	0.51
1:G:456:ARG:HG2	1:G:468:PHE:CE1	2.46	0.51
1:G:36:VAL:CG2	2:B:646:LEU:HD21	2.41	0.51
1:G:42:VAL:HA	2:B:537:LEU:HD22	1.92	0.51
1:G:386:ASN:HB3	1:G:417:PRO:HD2	1.93	0.51
1:G:455:THR:HG21	8:S:129:ARG:HE	1.74	0.51
2:B:621:GLU:O	2:B:625:ASN:HB3	2.11	0.51
3:F:98:ARG:NE	9:A:1:NAG:O6	2.43	0.50
1:G:36:VAL:HG12	2:B:610:TRP:CE3	2.47	0.50
1:G:90:THR:HA	1:G:239:CYS:O	2.12	0.50
1:G:182:VAL:HG11	1:G:194:ILE:HD13	1.92	0.50
1:G:258:GLN:CG	1:G:470:PRO:HB2	2.41	0.50
1:G:391:PHE:CD2	1:G:470:PRO:HG3	2.46	0.50
6:K:31:ALA:HB1	6:K:33:ASN:ND2	2.26	0.50
1:G:240:PRO:HG3	3:F:72(D):PRO:HG2	1.92	0.50
8:S:18:LEU:HD21	8:S:161:VAL:HG21	1.94	0.50
1:G:366:GLY:HA3	8:S:135:ARG:HA	1.94	0.50
1:G:361:PHE:CE1	1:G:468:PHE:HD2	2.29	0.49
1:G:384:TYR:HE2	1:G:421:LYS:HD3	1.77	0.49
8:S:129:ARG:NH1	8:S:138:GLY:HA2	2.26	0.49
1:G:258:GLN:HG2	1:G:470:PRO:HB2	1.92	0.49
7:R:94:SER:HB3	7:R:95(B):ASN:HB3	1.94	0.49
1:G:261:LEU:HD11	1:G:374:HIS:HE1	1.76	0.49
5:J:34:SER:HB3	6:K:100(J):TRP:HB3	1.95	0.49
3:F:35:ASN:O	3:F:92:CYS:HA	2.11	0.49
1:G:67:ASN:HB3	1:G:71:THR:HG23	1.95	0.49
6:K:51:LEU:HD23	6:K:69:LEU:HB3	1.94	0.49
8:S:87:SER:HA	8:S:161:VAL:O	2.12	0.49
2:B:644:GLY:O	2:B:647:GLU:HG2	2.12	0.48
1:G:161:MET:HE2	1:G:309:ILE:HB	1.95	0.48
1:G:381:GLU:HG2	1:G:439:ILE:HG12	1.95	0.48
2:B:546:SER:OG	2:B:547:GLY:N	2.46	0.48
4:I:2:SER:OG	4:I:3:VAL:N	2.46	0.48
7:R:4:LEU:HB2	7:R:99:GLY:HA2	1.95	0.48
3:F:30:ASN:O	3:F:53:TYR:HB2	2.13	0.48
1:G:298:ARG:HG3	1:G:420:ILE:HD11	1.95	0.48
1:G:192:ARG:HH12	12:H:1:NAG:C7	2.26	0.47
1:G:503:ARG:NH1	2:B:653:GLN:OE1	2.46	0.47
1:G:258:GLN:HB3	1:G:259:LEU:HD23	1.96	0.47
1:G:298:ARG:HG3	1:G:420:ILE:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:283:ASN:OD1	8:S:129:ARG:HD2	2.14	0.47
6:K:29:THR:OG1	6:K:73:THR:HA	2.15	0.47
3:F:96:LEU:HG	3:F:97:LEU:HG	1.97	0.47
8:S:113:ARG:O	8:S:117:GLN:HG2	2.15	0.47
3:F:24:THR:O	3:F:75:THR:HA	2.15	0.46
3:F:29:PHE:CE2	3:F:52(A):PRO:HB3	2.49	0.46
9:A:3:BMA:H61	9:A:4:MAN:H2	1.47	0.46
1:G:371:VAL:HG11	8:S:133:TYR:HB3	1.95	0.46
1:G:425:ASN:HB3	1:G:428:GLN:HB3	1.97	0.46
1:G:96:TRP:CE3	1:G:480:ARG:HD3	2.50	0.46
1:G:325:ASP:HA	6:K:100(B):TYR:O	2.15	0.46
1:G:307:ILE:HD11	1:G:317:PHE:HD2	1.80	0.46
1:G:68:VAL:HG21	1:G:208:VAL:HG12	1.97	0.46
1:G:111:LEU:HD11	2:B:571:TRP:CZ2	2.51	0.46
7:R:31:GLY:HA2	7:R:66:ARG:NE	2.31	0.46
1:G:134:VAL:HG23	1:G:154:LEU:O	2.16	0.46
6:K:98:GLU:O	6:K:100(B):TYR:HB3	2.15	0.46
1:G:325:ASP:HB3	1:G:327:ARG:HG3	1.98	0.46
4:I:27:ASN:HA	4:I:27(C):CYS:O	2.16	0.45
5:J:98:PHE:HB2	6:K:45:LEU:O	2.17	0.45
1:G:67:ASN:O	1:G:71:THR:OG1	2.32	0.45
1:G:161:MET:HG2	1:G:309:ILE:HG22	1.98	0.45
4:I:18:SER:HA	4:I:75:ILE:O	2.17	0.45
1:G:335:LYS:HB2	1:G:412:ASP:O	2.17	0.45
7:R:28:VAL:HG13	7:R:33:VAL:HG21	1.96	0.45
1:G:231:LYS:HD2	1:G:267:GLU:HB3	1.98	0.45
1:G:289:ASN:OD1	1:G:290:THR:N	2.50	0.45
1:G:360:ARG:HG2	1:G:467:THR:HG22	1.98	0.45
7:R:47:ILE:HG22	7:R:48:ILE:HG12	1.99	0.45
4:I:35:TRP:CD2	4:I:73:LEU:HB2	2.52	0.45
1:G:240:PRO:HG3	3:F:72(D):PRO:CG	2.47	0.44
1:G:494:LEU:HD23	1:G:494:LEU:HA	1.72	0.44
3:F:94:LYS:HD3	3:F:102:LEU:HB2	2.00	0.44
6:K:36:TRP:CD2	6:K:80:LEU:HD22	2.52	0.44
8:S:30:ASN:ND2	8:S:30:ASN:O	2.48	0.44
3:F:56:ASP:OD2	9:A:4:MAN:O4	2.23	0.44
8:S:6:GLU:OE1	8:S:6:GLU:N	2.50	0.44
1:G:270:VAL:HG22	1:G:348:GLN:HG3	1.99	0.44
1:G:368:ASP:OD1	8:S:134:CYS:HB2	2.18	0.44
4:I:35:TRP:CE2	4:I:73:LEU:HB2	2.53	0.44
5:J:49:TYR:HB2	6:K:100(J):TRP:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:80:MET:HE3	3:F:80:MET:HB3	1.88	0.44
1:G:50:THR:HG21	1:G:223:PHE:HD2	1.82	0.44
1:G:183:GLN:HB3	1:G:191:TYR:CZ	2.52	0.44
1:G:184:ILE:HG13	1:G:185:ASN:H	1.82	0.44
2:B:534:SER:HA	2:B:537:LEU:HG	1.99	0.44
4:I:35:TRP:CZ3	4:I:88:CYS:HB3	2.53	0.44
8:S:94:THR:OG1	8:S:154:ALA:HB3	2.18	0.44
1:G:370:GLU:HG3	8:S:133:TYR:CE1	2.52	0.44
1:G:56:SER:O	1:G:76:PRO:HA	2.17	0.44
2:B:642:ILE:O	2:B:646:LEU:HG	2.18	0.44
7:R:83:GLU:HA	7:R:104:LEU:O	2.18	0.44
1:G:162:THR:HG22	1:G:169:LYS:HE2	1.99	0.43
1:G:193:LEU:HD23	1:G:423:ILE:HD11	2.00	0.43
1:G:384:TYR:CE2	1:G:421:LYS:HB2	2.53	0.43
3:F:17:SER:HB3	3:F:82(A):ARG:HG2	1.99	0.43
3:F:35:ASN:OD1	3:F:50:TRP:HB3	2.18	0.43
6:K:20:LEU:HD11	6:K:109:VAL:HG21	2.00	0.43
1:G:361:PHE:CD1	1:G:468:PHE:HB2	2.52	0.43
1:G:494:LEU:HD21	2:B:593:LEU:HD11	2.01	0.43
4:I:79:ARG:O	4:I:106:VAL:HG21	2.18	0.43
1:G:260:LEU:HD12	1:G:451:GLY:HA3	2.01	0.43
3:F:87:THR:HG23	3:F:110:THR:HA	2.00	0.43
1:G:101:VAL:HG11	1:G:480:ARG:HG3	2.00	0.43
3:F:47:TRP:CZ2	3:F:49:GLY:HA2	2.54	0.43
5:J:38:GLN:NE2	5:J:44:PRO:HG3	2.34	0.43
1:G:116:LEU:HD23	1:G:116:LEU:HA	1.80	0.43
6:K:73:THR:OG1	6:K:74:PRO:HD3	2.19	0.43
8:S:38:ARG:NH2	8:S:46:GLN:OE1	2.48	0.43
1:G:460:SER:OG	1:G:461:THR:N	2.51	0.43
4:I:34:SER:HB3	4:I:91:TYR:CE1	2.53	0.43
4:I:84:THR:OG1	4:I:85:THR:N	2.48	0.43
1:G:421:LYS:HG2	1:G:423:ILE:O	2.19	0.43
4:I:34:SER:HB3	4:I:91:TYR:HE1	1.83	0.43
1:G:286:VAL:HB	1:G:452:LEU:HB2	2.01	0.43
2:B:570:VAL:HA	2:B:573:ILE:HD12	2.00	0.43
8:S:117:GLN:HG3	8:S:118:TYR:CD2	2.53	0.43
6:K:33:ASN:OD1	6:K:100:LEU:HD11	2.19	0.42
7:R:106(A):LEU:HD13	7:R:107:GLY:N	2.34	0.42
1:G:334:SER:HA	1:G:413:SER:HB3	2.00	0.42
1:G:299:PRO:HA	1:G:442:VAL:HG13	2.00	0.42
3:F:100(E):LEU:HD12	3:F:100(F):PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:95:PHE:CD1	6:K:100(K):VAL:HG22	2.55	0.42
6:K:97:GLY:HA2	6:K:100(J):TRP:CZ2	2.54	0.42
2:B:542:ARG:C	2:B:544:LEU:H	2.27	0.42
4:I:27(C):CYS:HA	4:I:28:CYS:HA	1.52	0.42
8:S:100:ASN:HD21	8:S:149:GLU:CD	2.27	0.42
1:G:363:ASN:HD21	1:G:388:SER:CB	2.32	0.42
5:J:39:HIS:HB2	5:J:42:LYS:HD3	2.01	0.42
1:G:264:SER:O	1:G:287:GLN:NE2	2.36	0.42
1:G:439:ILE:HB	1:G:443:ILE:HD11	2.02	0.42
1:G:54:CYS:SG	2:B:571:TRP:CE2	3.12	0.42
1:G:346:VAL:HG21	1:G:395:TRP:HB2	2.01	0.42
1:G:67:ASN:ND2	1:G:211:GLU:HG3	2.35	0.42
1:G:238:PRO:HB3	3:F:72(F):THR:O	2.19	0.42
1:G:432:GLN:HG3	1:G:433:ALA:H	1.85	0.42
2:B:592:LEU:HD23	2:B:595:ILE:HD11	2.01	0.42
1:G:172:VAL:HG21	1:G:307:ILE:HD12	2.02	0.42
6:K:90:TYR:HE2	6:K:109:VAL:HB	1.85	0.42
4:I:92:THR:OG1	4:I:93:HIS:N	2.52	0.41
2:B:587:LEU:HD23	2:B:587:LEU:HA	1.90	0.41
2:B:593:LEU:HD23	2:B:601:LYS:HA	2.01	0.41
1:G:297:THR:HG22	1:G:444:ARG:HG3	2.03	0.41
7:R:38:LEU:O	7:R:84:ALA:HB1	2.20	0.41
1:G:368:ASP:OD2	8:S:113:ARG:NH1	2.44	0.41
3:F:47:TRP:CH2	3:F:49:GLY:HA2	2.55	0.41
5:J:54:ARG:NH1	5:J:62:PHE:O	2.54	0.41
1:G:286:VAL:O	1:G:451:GLY:HA2	2.21	0.41
1:G:299:PRO:HD3	1:G:329:ALA:HA	2.01	0.41
3:F:28:ARG:NH2	3:F:72(B):GLU:OE2	2.49	0.41
7:R:39:ILE:HG12	7:R:84:ALA:HB2	2.03	0.41
1:G:75:VAL:HG11	2:B:548:ILE:O	2.21	0.41
1:G:257:THR:OG1	1:G:375:SER:OG	2.31	0.41
1:G:341:THR:O	1:G:345:VAL:HG23	2.21	0.41
6:K:22:CYS:HB3	6:K:78:VAL:HB	2.03	0.41
6:K:23:ALA:HA	6:K:77:LEU:HD23	2.02	0.41
1:G:498:PRO:HB3	2:B:610:TRP:CD2	2.57	0.40
1:G:87:GLU:O	1:G:89:VAL:HG23	2.21	0.40
1:G:231:LYS:HE2	1:G:267:GLU:HG2	2.03	0.40
1:G:259:LEU:HB3	1:G:452:LEU:HD23	2.02	0.40
1:G:374:HIS:HB3	1:G:385:CYS:HB2	2.03	0.40
2:B:661:LEU:H	2:B:661:LEU:HG	1.81	0.40
3:F:12:LYS:O	3:F:111:VAL:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:101:ASP:OD1	6:K:102:LEU:N	2.54	0.40
8:S:22:CYS:HB2	8:S:36:TRP:CZ2	2.57	0.40
4:I:16:GLY:HA2	4:I:77:ASP:OD1	2.21	0.40
3:F:72(F):THR:OG1	3:F:72(G):SER:N	2.46	0.40

All (1) 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)
2:B:579:ARG:NH2	2:B:581:LEU:CA[3_455]	2.12	0.08

3.3 Torsion angles [i](#)

3.3.1 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	G	415/475 (87%)	390 (94%)	22 (5%)	3 (1%)	18	55
2	B	125/153 (82%)	114 (91%)	9 (7%)	2 (2%)	7	38
3	F	128/240 (53%)	124 (97%)	3 (2%)	1 (1%)	16	52
4	I	108/216 (50%)	102 (94%)	6 (6%)	0	100	100
5	J	100/211 (47%)	94 (94%)	6 (6%)	0	100	100
6	K	130/239 (54%)	119 (92%)	10 (8%)	1 (1%)	16	52
7	R	110/216 (51%)	103 (94%)	6 (6%)	1 (1%)	14	49
8	S	166/272 (61%)	159 (96%)	7 (4%)	0	100	100
All	All	1282/2022 (63%)	1205 (94%)	69 (5%)	8 (1%)	21	58

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	73	ALA

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Mol	Chain	Res	Type
2	B	549	VAL
2	B	602	LEU
1	G	427	TRP
6	K	41	PRO
7	R	93	ASP
1	G	431	GLY
3	F	8	GLY

3.3.2 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	G	381/422 (90%)	376 (99%)	5 (1%)	61	72
2	B	111/129 (86%)	105 (95%)	6 (5%)	20	44
3	F	108/203 (53%)	108 (100%)	0	100	100
4	I	96/189 (51%)	96 (100%)	0	100	100
5	J	83/177 (47%)	83 (100%)	0	100	100
6	K	110/203 (54%)	110 (100%)	0	100	100
7	R	92/184 (50%)	91 (99%)	1 (1%)	65	74
8	S	148/238 (62%)	146 (99%)	2 (1%)	59	71
All	All	1129/1745 (65%)	1115 (99%)	14 (1%)	63	73

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	36	VAL
1	G	165	LEU
1	G	258	GLN
1	G	259	LEU
1	G	270	VAL
2	B	551	GLN
2	B	570	VAL
2	B	583	VAL

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Mol	Chain	Res	Type
2	B	584	GLU
2	B	660	LEU
2	B	661	LEU
7	R	93	ASP
8	S	27	SER
8	S	116	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	67	ASN
1	G	185	ASN
1	G	293	GLN
1	G	330	HIS
1	G	374	HIS
1	G	425	ASN
2	B	658	GLN
3	F	3	GLN
5	J	38	GLN
6	K	39	GLN
6	K	60	ASN
8	S	39	GLN
8	S	60	ASN
8	S	73	ASN
8	S	97	GLN

3.3.3 RNA ⓘ

There are no RNA molecules in this entry.

3.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

3.5 Carbohydrates ⓘ

Of 52 monosaccharides modelled in this entry, zero was used for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

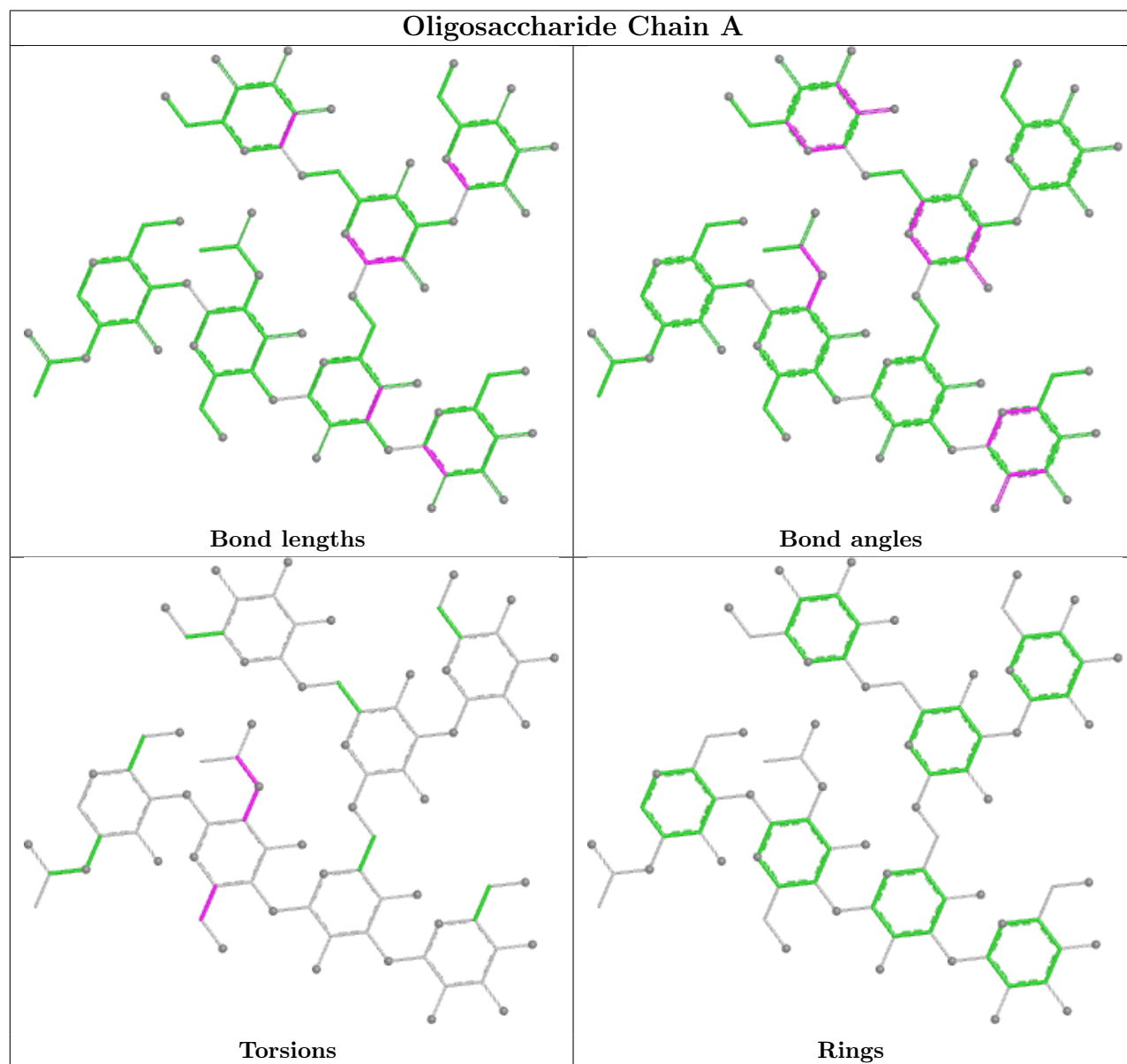
There are no chirality outliers.

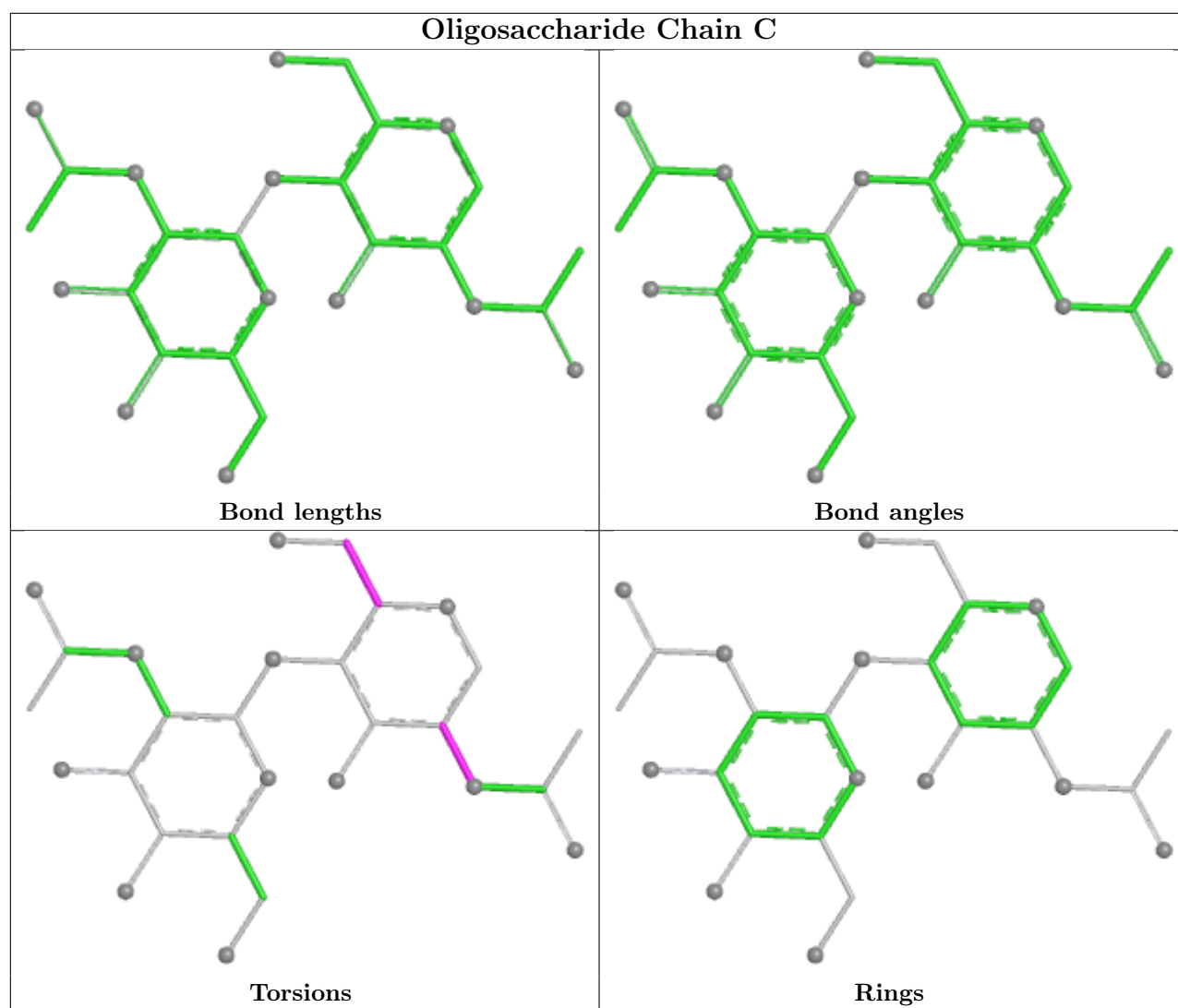
There are no torsion outliers.

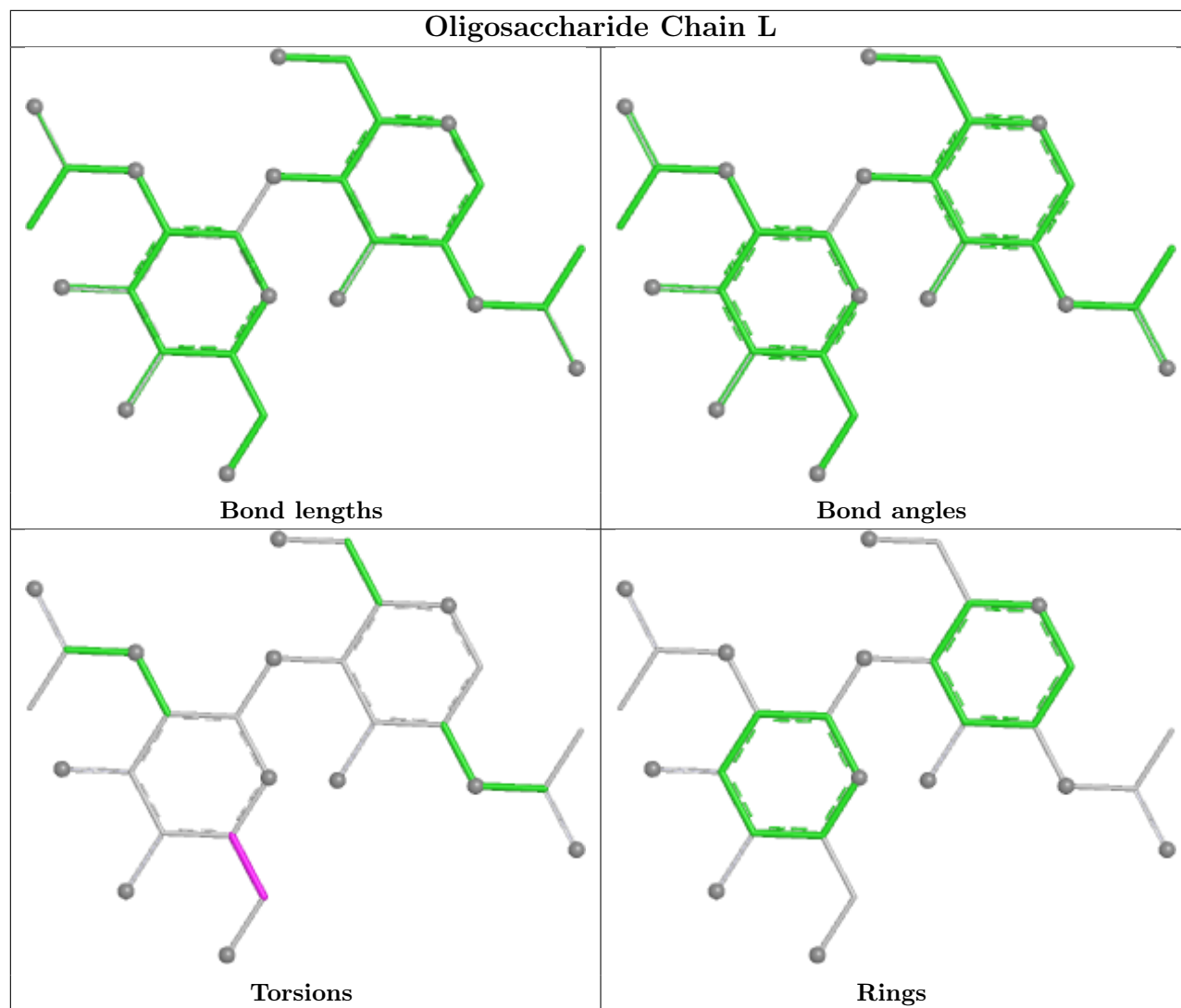
There are no ring outliers.

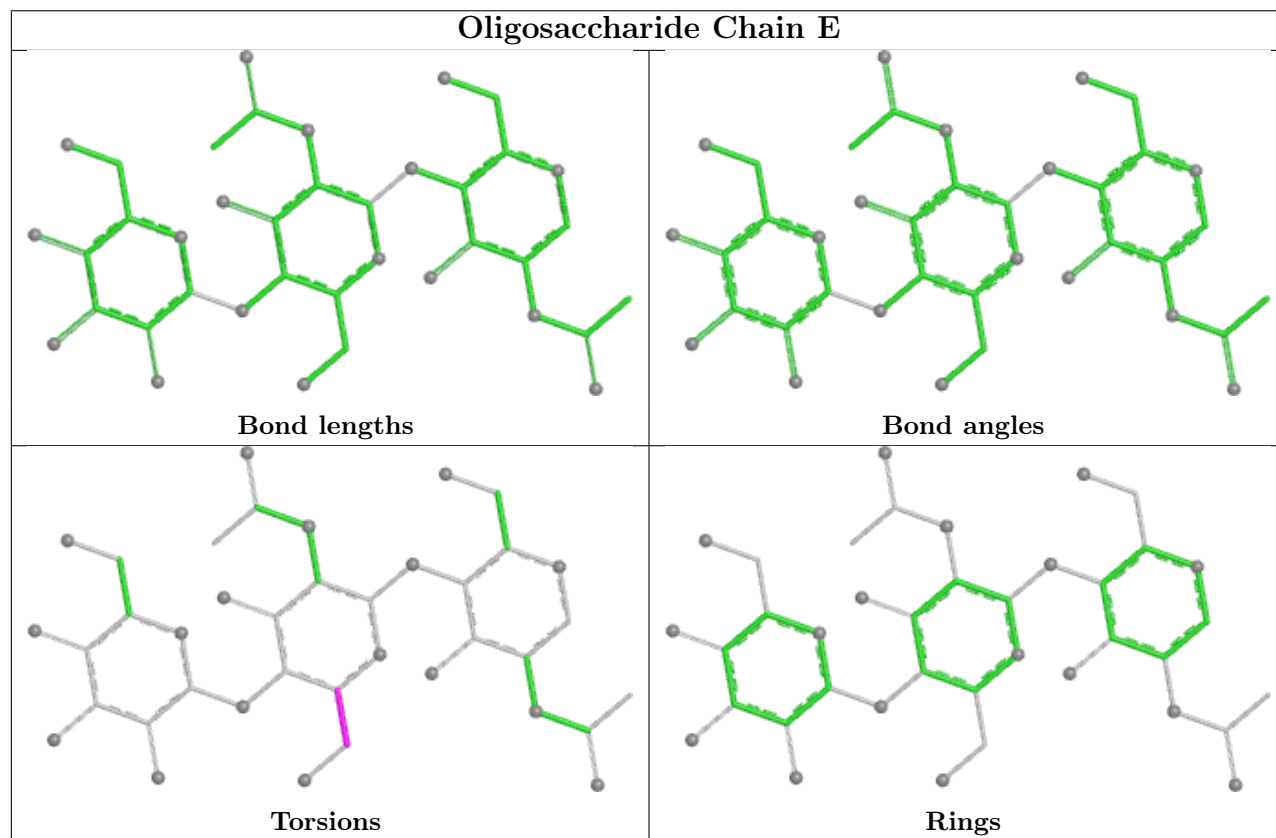
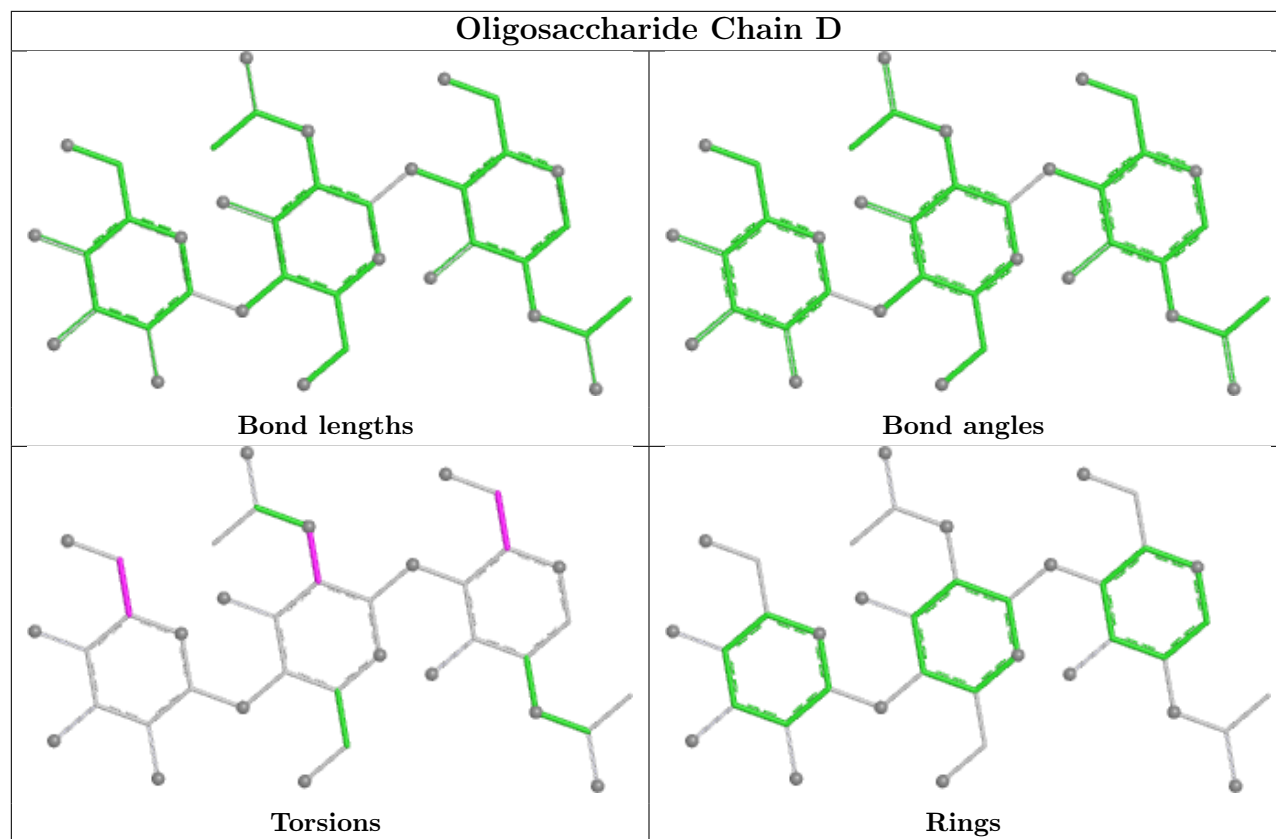
No monomer is involved in short contacts.

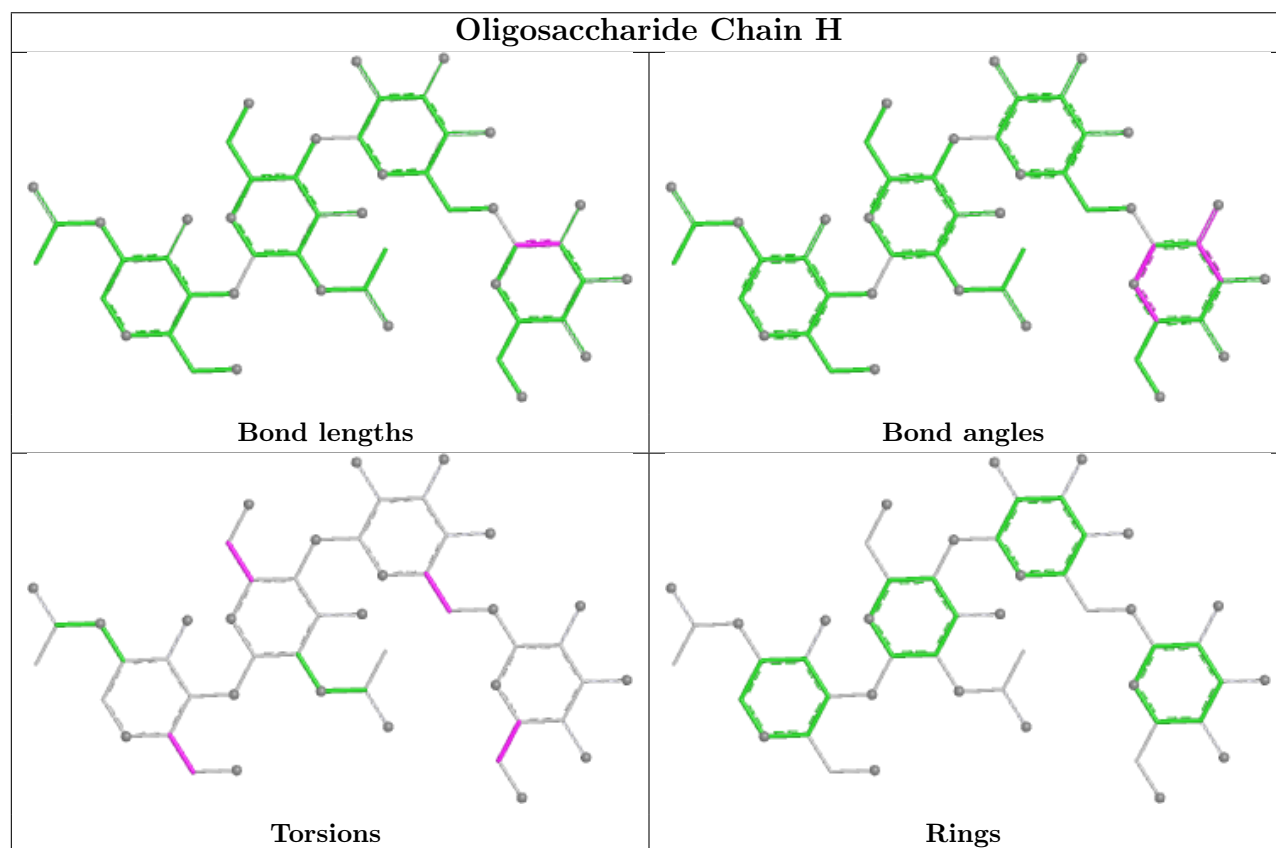
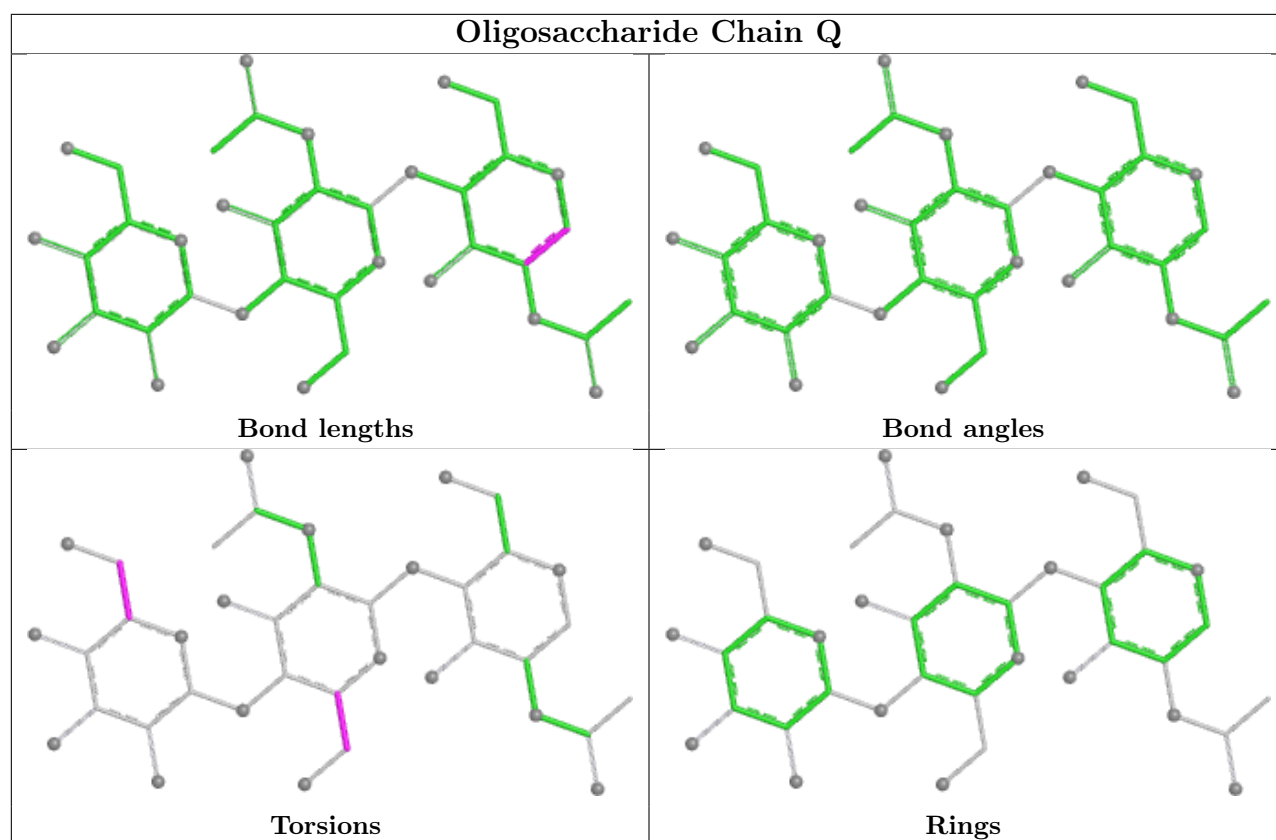
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

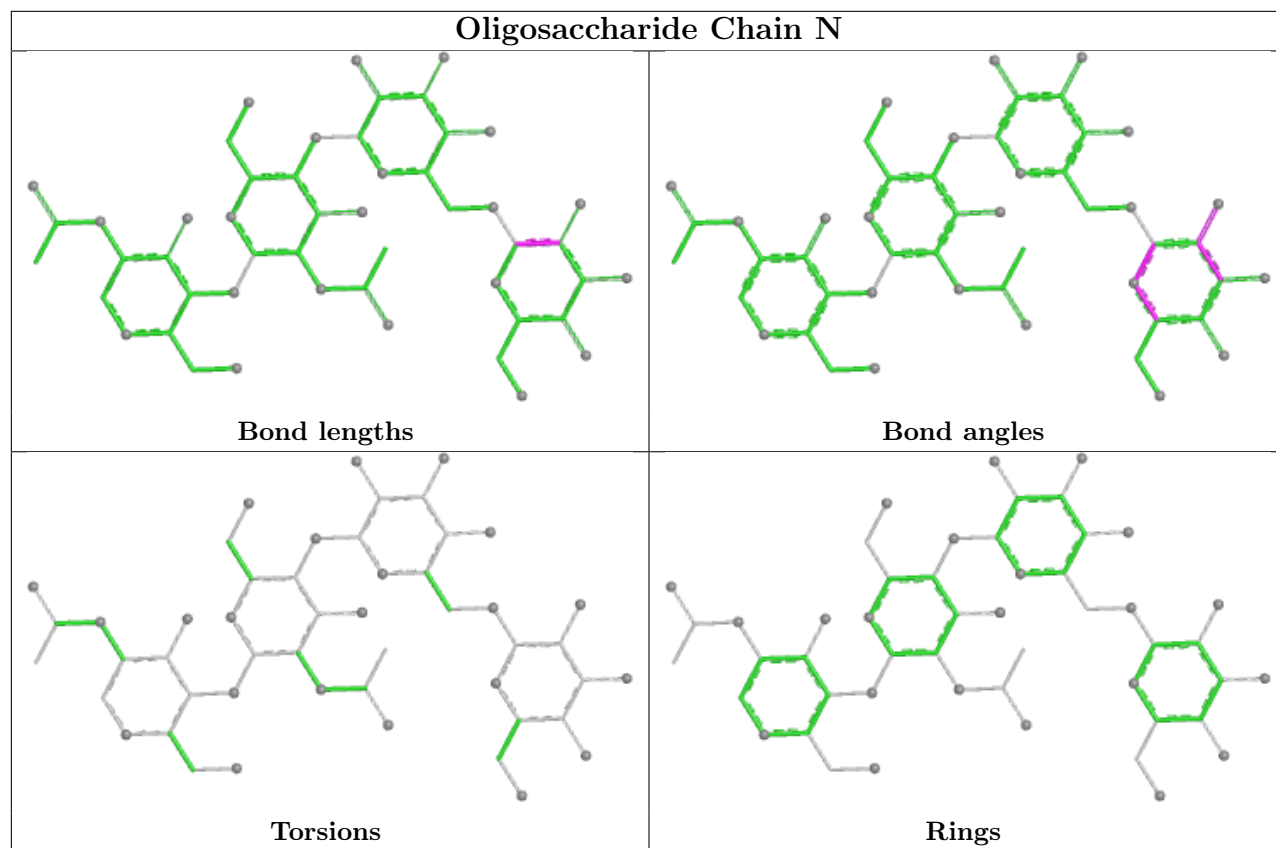


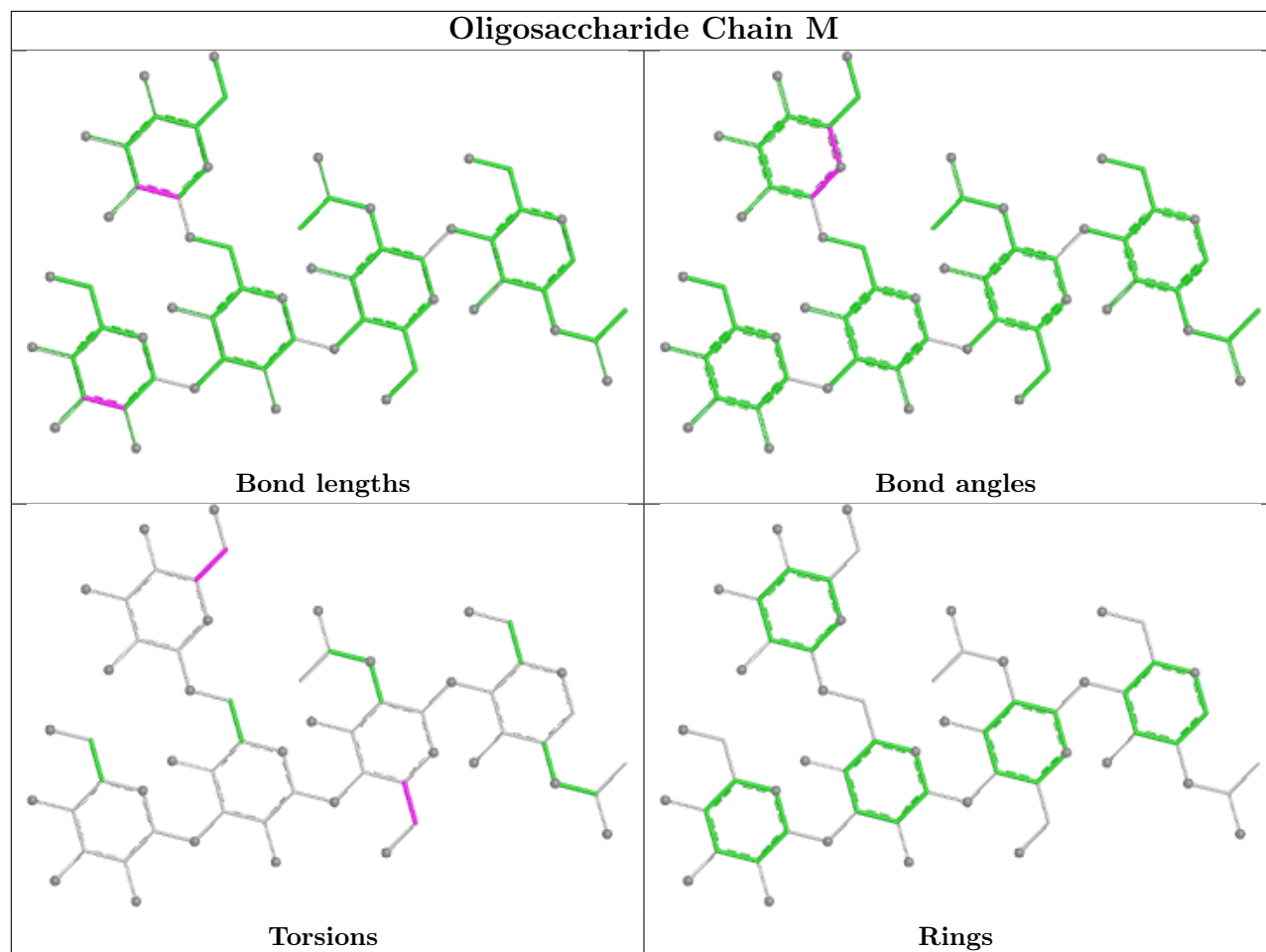


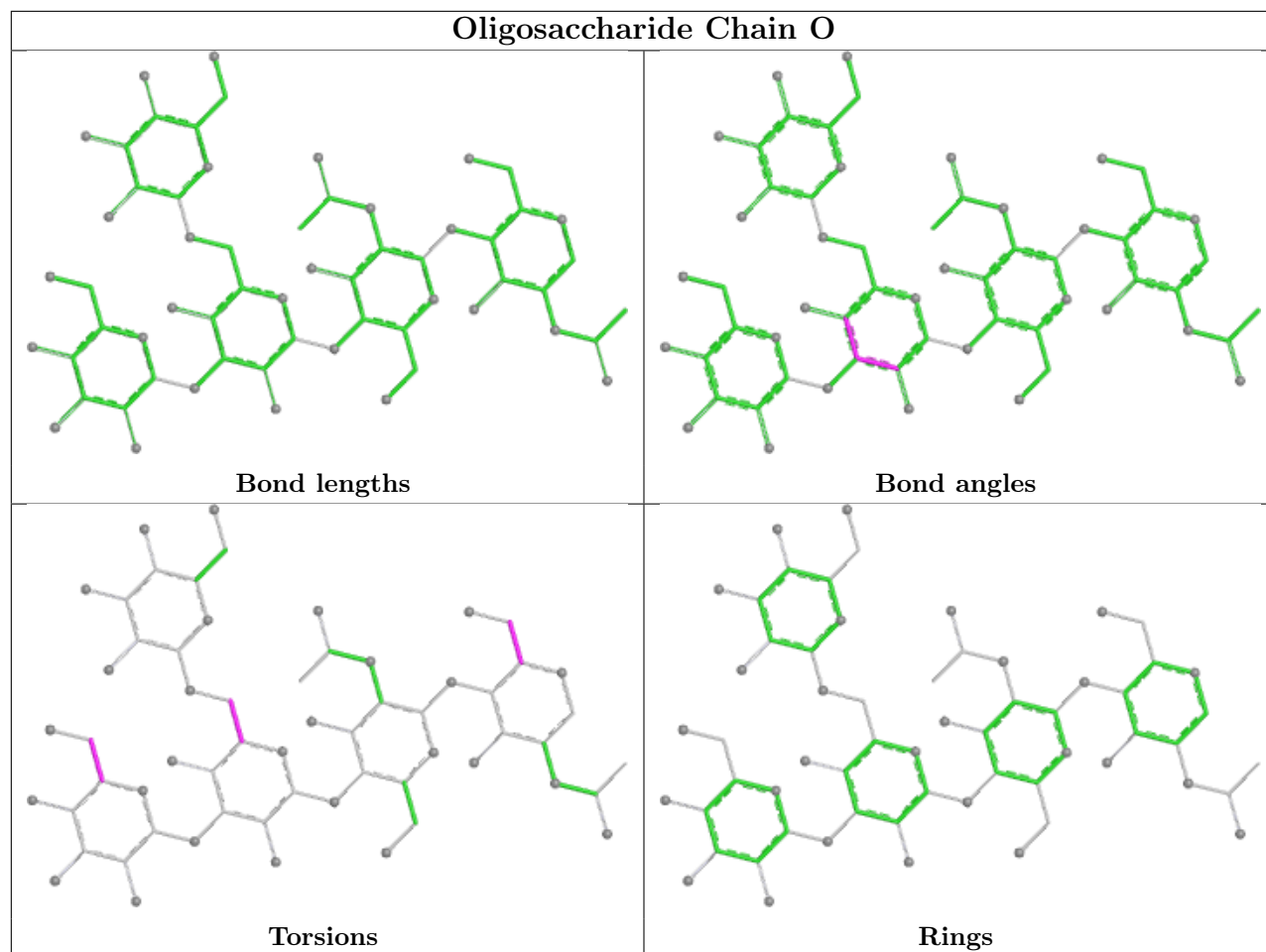


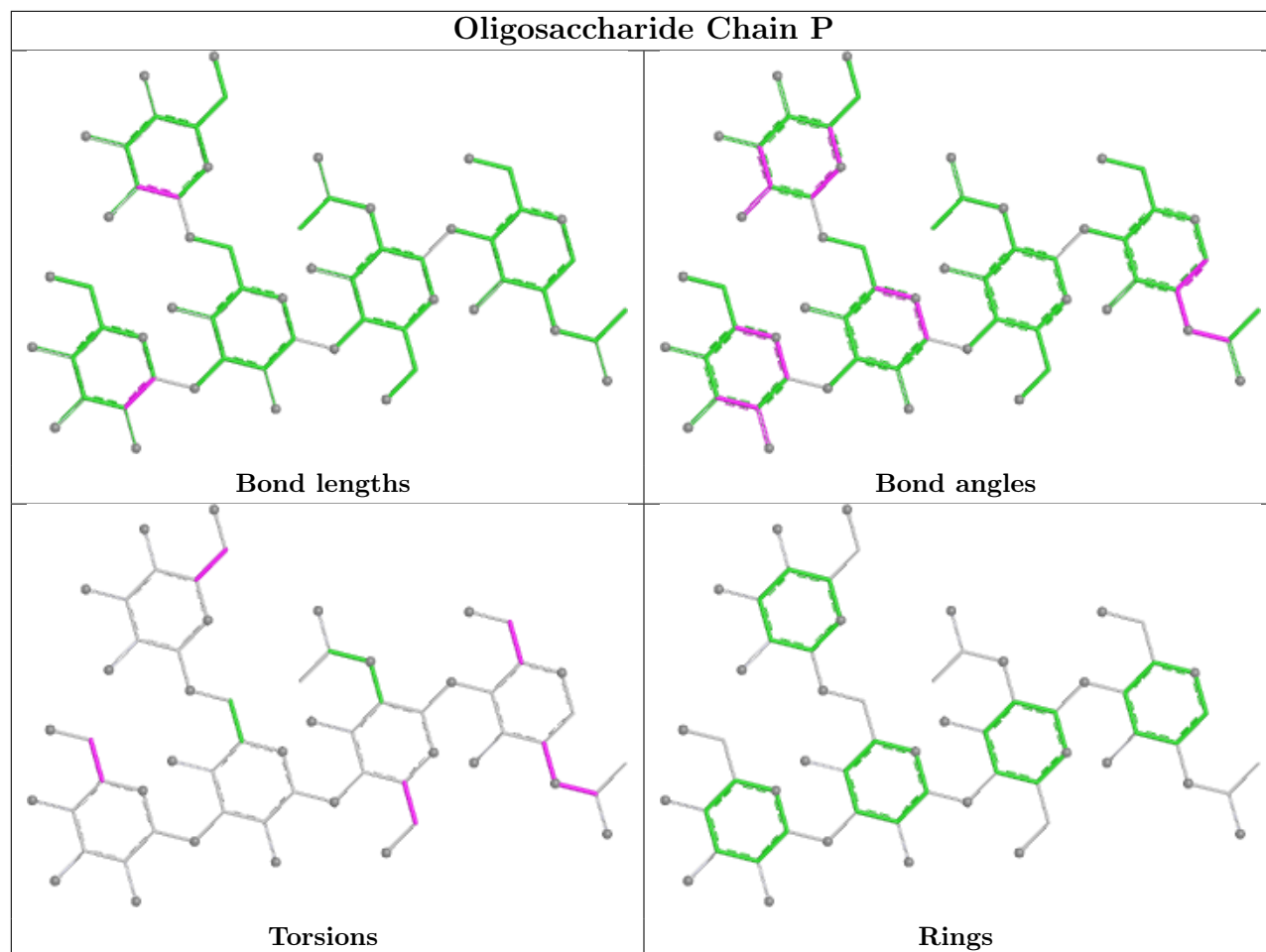


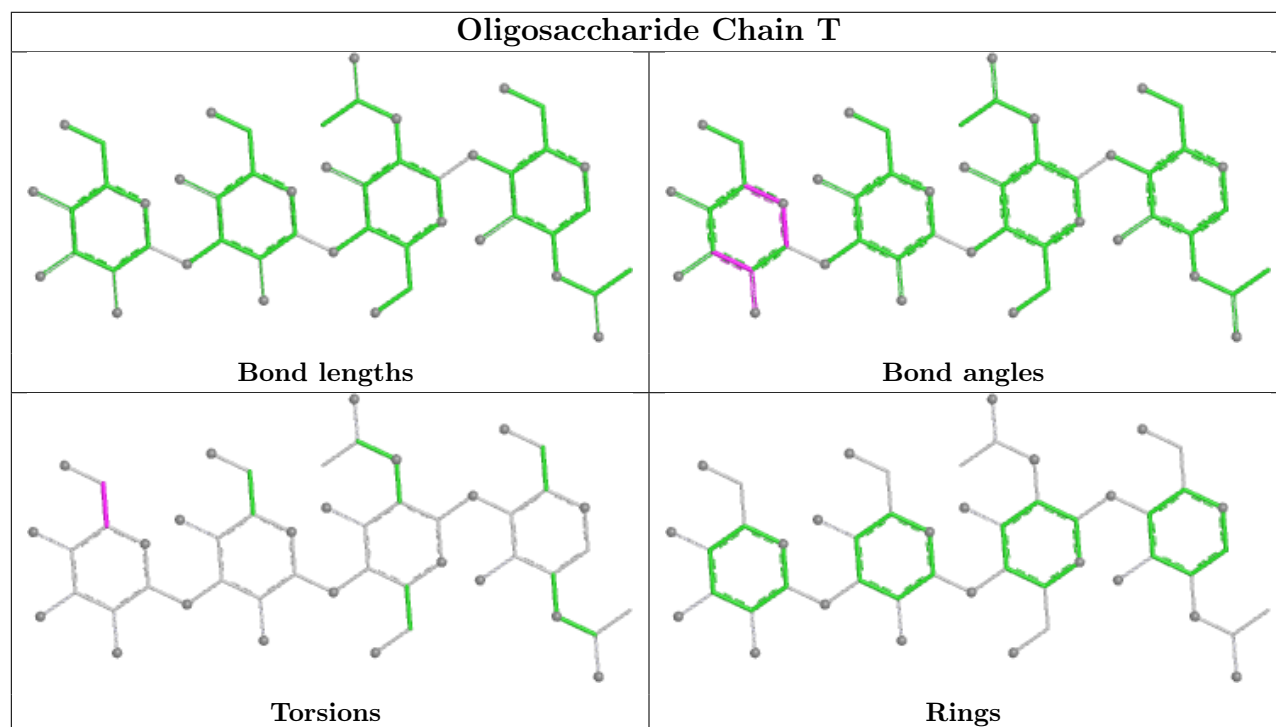
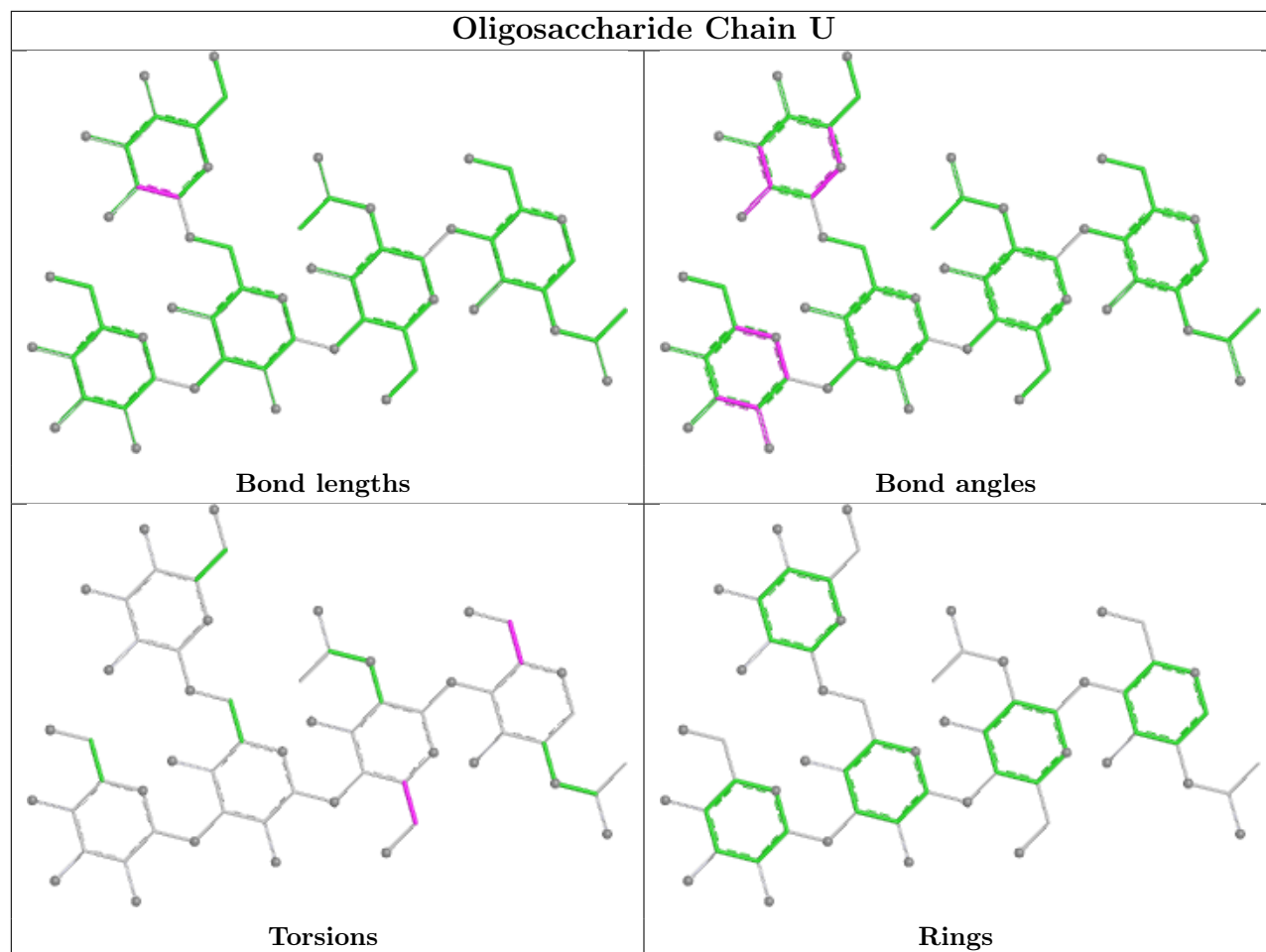












3.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

3.7 Other polymers [i](#)

There are no such residues in this entry.

3.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

4 Fit of model and data ⓘ

4.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	G	427/475 (89%)	1.04	55 (12%) 7 11	152, 184, 215, 243	0
2	B	129/153 (84%)	1.15	20 (15%) 5 9	158, 176, 213, 235	0
3	F	130/240 (54%)	0.77	9 (6%) 23 21	180, 211, 232, 237	0
4	I	110/216 (50%)	0.99	11 (10%) 12 15	187, 210, 222, 225	0
5	J	102/211 (48%)	0.49	5 (4%) 35 29	246, 283, 297, 298	0
6	K	132/239 (55%)	0.98	18 (13%) 7 10	224, 272, 298, 313	0
7	R	112/216 (51%)	0.56	7 (6%) 26 24	202, 216, 232, 236	0
8	S	168/272 (61%)	0.71	12 (7%) 22 21	179, 248, 270, 274	0
All	All	1310/2022 (64%)	0.89	137 (10%) 11 14	152, 208, 287, 313	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	K	52(E)	TYR	7.5
8	S	141	ASN	6.5
1	G	232	LYS	6.0
8	S	14	PRO	5.9
6	K	35(A)	TRP	5.4
1	G	58	ALA	4.9
3	F	46	GLU	4.9
1	G	397	SER	4.9
2	B	552	GLN	4.8
3	F	90	TYR	4.4
7	R	56	SER	4.3
8	S	124	ASP	4.3
3	F	72(A)	THR	4.2
1	G	430	ILE	4.0
8	S	142	TYR	4.0
1	G	272	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
6	K	19	SER	3.8
1	G	49	GLU	3.7
3	F	45	PRO	3.7
2	B	569	THR	3.6
6	K	52(D)	SER	3.5
8	S	143	ILE	3.4
1	G	465	THR	3.4
5	J	3	ALA	3.3
1	G	246	GLN	3.3
2	B	625	ASN	3.3
6	K	3	GLN	3.3
2	B	577	GLN	3.3
2	B	576	LEU	3.2
6	K	68	THR	3.2
1	G	442	VAL	3.2
4	I	87	TYR	3.1
1	G	426	MET	3.1
4	I	47	ILE	3.1
3	F	39	GLN	3.1
6	K	2	PRO	3.1
1	G	52	LEU	3.1
2	B	582	ALA	3.1
1	G	460	SER	3.0
3	F	68	ILE	3.0
1	G	170	GLN	3.0
2	B	628	TRP	3.0
6	K	69	LEU	3.0
1	G	317	PHE	2.9
1	G	321(A)	ASP	2.9
1	G	252	LYS	2.9
1	G	323	ILE	2.9
6	K	110	THR	2.9
1	G	208	VAL	2.7
1	G	189	LYS	2.7
3	F	113	SER	2.7
6	K	20	LEU	2.7
2	B	578	ALA	2.7
7	R	97	VAL	2.7
4	I	27	ASN	2.7
4	I	62	PHE	2.7
1	G	379	GLY	2.6
8	S	1	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
3	F	100(B)	SER	2.6
6	K	74	PRO	2.6
5	J	86	TYR	2.6
1	G	125	LEU	2.5
5	J	56	SER	2.5
7	R	62	PHE	2.5
1	G	345	VAL	2.5
6	K	98	GLU	2.5
1	G	316	ALA	2.5
6	K	100	LEU	2.5
1	G	396	ILE	2.5
4	I	38	TRP	2.5
1	G	285	LEU	2.4
4	I	107	GLY	2.4
1	G	326	ILE	2.4
6	K	90	TYR	2.4
4	I	86	TYR	2.4
2	B	575	GLN	2.4
1	G	353	PHE	2.4
2	B	535	MET	2.4
8	S	102	LYS	2.4
7	R	2	TYR	2.4
2	B	619	LEU	2.4
8	S	31	ASP	2.4
1	G	419	ARG	2.4
1	G	224	ALA	2.3
2	B	526	ALA	2.3
1	G	264	SER	2.3
1	G	181	VAL	2.3
1	G	350	ARG	2.3
1	G	71	THR	2.3
6	K	25	SER	2.3
1	G	359	ILE	2.3
4	I	18	SER	2.3
6	K	64	LYS	2.3
1	G	307	ILE	2.3
1	G	389	GLY	2.3
1	G	171	LYS	2.3
1	G	464	THR	2.3
8	S	164	SER	2.3
1	G	68	VAL	2.3
3	F	69	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	462	ASN	2.2
2	B	662	ALA	2.2
1	G	376	PHE	2.2
1	G	180	ASP	2.2
4	I	37	GLN	2.2
1	G	128	THR	2.2
2	B	534	SER	2.2
2	B	550	GLN	2.2
8	S	64	LYS	2.2
6	K	14	ALA	2.2
1	G	162	THR	2.2
1	G	440	GLN	2.2
2	B	548	ILE	2.2
1	G	477	ASP	2.1
1	G	121	LYS	2.1
1	G	155	LYS	2.1
4	I	3	VAL	2.1
1	G	131	CYS	2.1
2	B	641	ILE	2.1
1	G	478	ASN	2.1
5	J	40	ALA	2.1
5	J	100	GLY	2.1
8	S	9	PRO	2.1
1	G	341	THR	2.1
4	I	11	VAL	2.1
1	G	169	LYS	2.1
6	K	81	LYS	2.1
2	B	623	TRP	2.1
7	R	109	PRO	2.1
7	R	18	ARG	2.1
2	B	537	LEU	2.1
2	B	571	TRP	2.1
7	R	106(A)	LEU	2.0
1	G	74	CYS	2.0
1	G	269	GLU	2.0
1	G	161	MET	2.0
8	S	30	ASN	2.0

4.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

SUGAR-RSR INFOmissingINFO

LIGAND-RSR INFOmissingINFO

4.3 Other polymers [i](#)

There are no such residues in this entry.