



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:11 AM UTC

PDB ID : 4JNT / pdb_00004jnt
Title : Crystal structure of the ectodomain of Bovine viral diarrhea virus 1 E2 envelope protein
Authors : Li, Y.; Wang, J.; Modis, Y.
Deposited on : 2013-03-15
Resolution : 4.09 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:

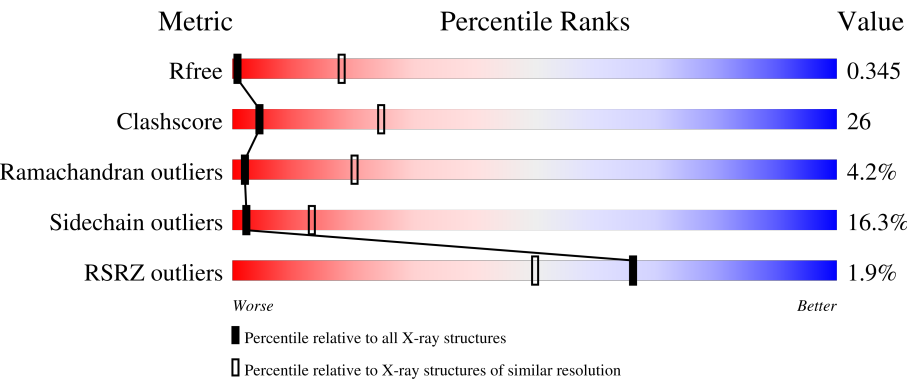
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 4.09 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	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	338	3% 46% 39% 10% . .
1	B	338	% 44% 42% 9% . .
2	C	2	100%
2	D	2	100%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	G	2	 100%
2	H	2	 50% 50%
2	I	2	 50% 50%
2	J	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	I	2	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5380 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 Envelope glycoprotein E2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2578	1639	432	481	26			
1	B	324	Total	C	N	O	S	0	0	0
			2578	1639	432	481	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	788	ASP	ASN	variant	UNP P19711
B	788	ASP	ASN	variant	UNP P19711

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

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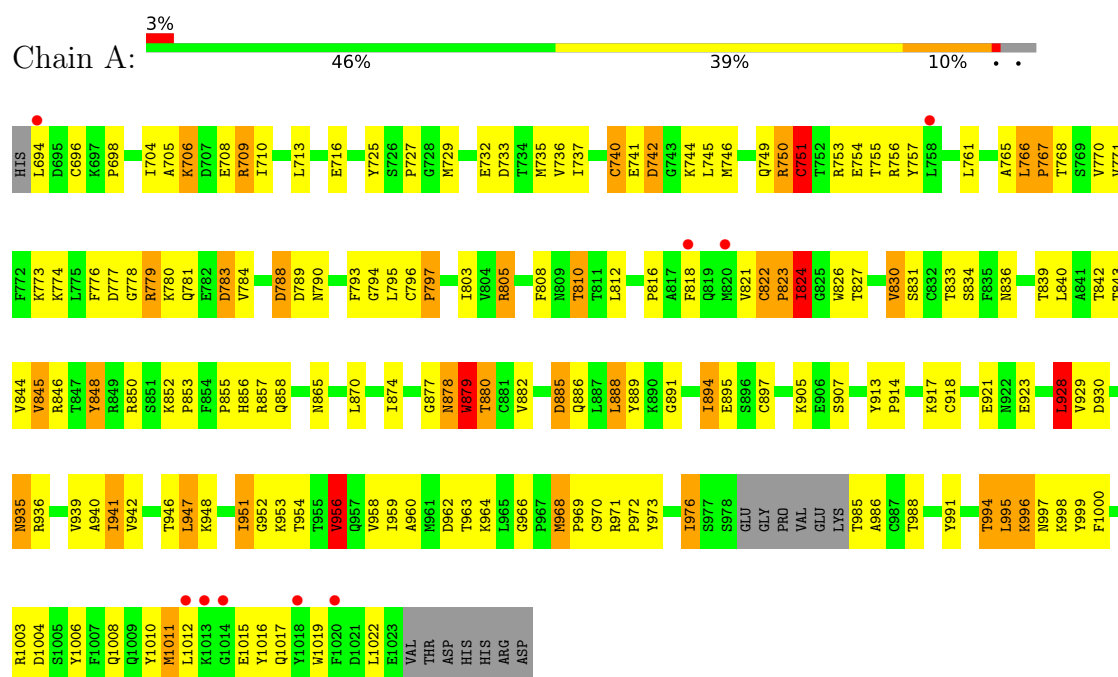
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

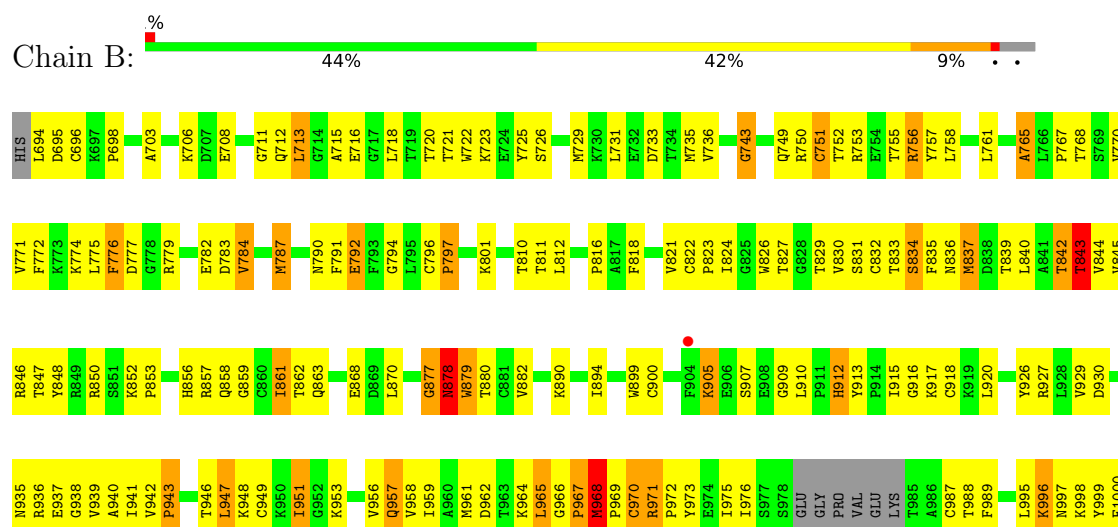
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: Envelope glycoprotein E2



• Molecule 1: Envelope glycoprotein E2





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

Chain C: 100%

MAG1
MAG2

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

Chain D: 100%

MAG1
MAG2

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

Chain E: 50% 50%

MAG1
MAG2

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

Chain F: 100%

MAG1
MAG2

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

Chain G: 100%

MAG1
MAG2

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

Chain H: 50% 50%

MAG1
MAG2

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

Chain I:  50% 50%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	155.63Å 67.89Å 139.41Å 90.00° 121.89° 90.00°	Depositor
Resolution (Å)	48.57 – 4.09 48.57 – 4.09	Depositor EDS
% Data completeness (in resolution range)	97.9 (48.57-4.09) 99.4 (48.57-4.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.321 , 0.376 0.279 , 0.345	Depositor DCC
R_{free} test set	780 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	66.1	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 124.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.138 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	5380	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.80	0/2639	1.08	10/3567 (0.3%)
1	B	0.81	1/2639 (0.0%)	1.12	9/3567 (0.3%)
All	All	0.80	1/5278 (0.0%)	1.10	19/7134 (0.3%)

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	2
1	B	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	877	GLY	C-O	-6.05	1.19	1.24

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	843	THR	N-CA-C	7.28	120.26	108.76
1	A	879	TRP	N-CA-C	6.49	124.62	110.80
1	A	956	VAL	CB-CA-C	-6.46	101.85	111.80
1	A	968	MET	N-CA-C	-6.46	101.63	109.83
1	A	822	CYS	CA-C-N	5.91	127.23	119.84
1	A	822	CYS	C-N-CA	5.91	127.23	119.84
1	A	880	THR	CB-CA-C	-5.91	101.19	110.94
1	B	879	TRP	N-CA-C	5.90	123.36	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	751	CYS	N-CA-C	-5.81	98.42	110.80
1	A	1012	LEU	N-CA-C	5.61	118.98	107.37
1	A	843	THR	N-CA-C	5.56	117.55	108.76
1	B	905	LYS	N-CA-C	-5.53	106.58	113.55
1	A	783	ASP	N-CA-C	5.47	116.28	108.74
1	B	756	ARG	N-CA-C	5.37	117.84	109.52
1	B	863	GLN	N-CA-C	5.33	116.72	107.93
1	B	861	ILE	CB-CA-C	-5.23	104.33	111.33
1	B	718	LEU	N-CA-C	5.19	117.22	108.96
1	B	715	ALA	N-CA-C	-5.18	103.55	110.55
1	B	743	GLY	N-CA-C	-5.08	108.00	114.85

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1011	MET	Peptide
1	A	986	ALA	Peptide
1	B	1010	TYR	Peptide
1	B	968	MET	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	2578	0	2519	142	0
1	B	2578	0	2522	137	0
2	C	28	0	25	1	0
2	D	28	0	25	0	0
2	E	28	0	25	6	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	1	0
2	I	28	0	25	7	0
2	J	28	0	25	0	0
All	All	5380	0	5241	280	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 26.

All (280) 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:B:890:LYS:HE3	2:I:2:NAG:O3	1.51	1.10
1:B:1009:GLN:O	1:B:1011:MET:SD	2.19	0.99
1:B:796:CYS:HB2	1:B:816:PRO:O	1.66	0.96
1:A:939:VAL:HG11	1:A:969:PRO:HD3	1.49	0.94
1:A:741:GLU:OE2	1:A:746:MET:SD	2.30	0.90
1:B:735:MET:HE1	1:B:751:CYS:SG	2.13	0.89
1:B:890:LYS:NZ	2:I:2:NAG:H4	1.90	0.86
1:B:947:LEU:HD12	1:B:948:LYS:N	1.95	0.81
1:A:878:ASN:O	1:A:880:THR:N	2.12	0.81
1:A:947:LEU:HD12	1:A:948:LYS:N	1.95	0.81
1:A:727:PRO:O	1:A:742:ASP:O	1.99	0.80
1:A:963:THR:O	1:A:997:ASN:ND2	2.16	0.79
1:A:750:ARG:HG3	1:A:750:ARG:O	1.82	0.79
1:A:952:GLY:O	1:A:971:ARG:NH2	2.16	0.78
1:B:878:ASN:O	1:B:880:THR:N	2.17	0.78
1:B:761:LEU:HB2	1:B:770:VAL:HG12	1.66	0.77
1:B:797:PRO:CG	1:B:845:VAL:HG21	2.16	0.75
1:B:836:ASN:O	1:B:839:THR:O	2.05	0.74
1:B:890:LYS:HZ1	2:I:2:NAG:H4	1.52	0.74
1:B:890:LYS:CE	2:I:2:NAG:O3	2.34	0.74
1:A:797:PRO:HG2	1:A:845:VAL:HG21	1.71	0.73
1:A:951:ILE:HG13	1:A:956:VAL:HG21	1.71	0.73
1:B:877:GLY:O	1:B:878:ASN:C	2.31	0.72
1:B:890:LYS:HZ2	2:I:2:NAG:C4	2.02	0.72
1:A:836:ASN:O	1:A:839:THR:O	2.08	0.71
1:A:741:GLU:N	1:A:741:GLU:OE1	2.23	0.71
1:A:968:MET:HG3	1:A:1000:PHE:CE1	2.26	0.71
1:B:1006:TYR:CE1	1:B:1022:LEU:HD23	2.26	0.70
1:B:708:GLU:HG3	1:B:772:PHE:CD2	2.27	0.69
1:A:960:ALA:HB2	1:A:995:LEU:HD23	1.73	0.69
1:B:837:MET:SD	1:B:837:MET:N	2.63	0.69
1:B:942:VAL:HB	1:B:943:PRO:CD	2.24	0.68
1:A:694:LEU:O	1:A:745:LEU:HG	1.93	0.68
1:B:890:LYS:NZ	2:I:2:NAG:C4	2.56	0.68
1:B:967:PRO:O	1:B:968:MET:HB2	1.94	0.68
1:A:1006:TYR:CE1	1:A:1022:LEU:HD23	2.30	0.67
1:B:787:MET:HE3	1:B:848:TYR:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:787:MET:HE3	1:B:848:TYR:CB	2.25	0.67
1:A:923:GLU:HG2	2:E:1:NAG:C7	2.25	0.67
1:A:796:CYS:HB2	1:A:816:PRO:O	1.96	0.66
1:A:939:VAL:CG1	1:A:969:PRO:HD3	2.22	0.65
1:B:711:GLY:HA3	1:B:716:GLU:OE2	1.97	0.65
1:B:968:MET:HG3	1:B:1000:PHE:CD1	2.31	0.65
1:B:736:VAL:HG23	1:B:749:GLN:HA	1.79	0.65
1:A:740:CYS:C	1:A:741:GLU:OE1	2.40	0.64
1:B:797:PRO:HG2	1:B:845:VAL:HG21	1.79	0.64
1:B:832:CYS:HB2	1:B:845:VAL:HG22	1.78	0.63
1:A:850:ARG:NE	1:A:852:LYS:O	2.32	0.63
1:B:951:ILE:HD11	1:B:956:VAL:HG21	1.81	0.62
1:B:833:THR:HA	1:B:844:VAL:HA	1.81	0.62
1:B:703:ALA:O	1:B:758:LEU:HD12	2.00	0.61
1:B:756:ARG:HB2	1:B:776:PHE:HE2	1.65	0.61
1:A:877:GLY:O	1:A:878:ASN:C	2.42	0.61
1:B:999:TYR:CE2	1:B:1010:TYR:CE2	2.88	0.61
1:A:833:THR:HA	1:A:844:VAL:HA	1.82	0.61
1:A:994:THR:HG23	1:A:995:LEU:N	2.14	0.61
1:B:942:VAL:HB	1:B:943:PRO:HD2	1.83	0.61
1:A:966:GLY:O	1:A:998:LYS:HA	2.00	0.61
1:A:1004:ASP:HB2	1:A:1011:MET:HE2	1.83	0.60
1:B:735:MET:HE1	1:B:751:CYS:HG	1.66	0.60
1:A:960:ALA:HB2	1:A:995:LEU:CD2	2.31	0.60
1:B:938:GLY:O	1:B:961:MET:HB3	2.02	0.60
1:A:725:TYR:HA	1:A:729:MET:HE3	1.83	0.60
1:B:787:MET:HB3	1:B:791:PHE:CB	2.32	0.59
1:B:935:ASN:OD1	1:B:940:ALA:HB2	2.02	0.59
1:B:696:CYS:SG	1:B:725:TYR:HE1	2.24	0.59
1:A:698:PRO:HA	1:A:725:TYR:CD2	2.38	0.59
1:A:951:ILE:HG13	1:A:956:VAL:CG2	2.32	0.58
1:A:923:GLU:HG2	2:E:1:NAG:O7	2.03	0.58
1:A:750:ARG:O	1:A:751:CYS:HB2	2.04	0.58
1:A:939:VAL:HG22	1:A:958:VAL:CG2	2.32	0.58
1:B:907:SER:HA	1:B:913:TYR:CD2	2.38	0.58
1:B:910:LEU:HD13	1:B:915:ILE:HG21	1.86	0.58
1:A:706:LYS:O	1:A:757:TYR:HE1	1.85	0.58
1:A:823:PRO:O	1:A:826:TRP:HB2	2.04	0.57
1:B:824:ILE:HG13	1:B:856:HIS:HA	1.85	0.57
1:B:890:LYS:HE3	2:I:2:NAG:HO3	1.69	0.57
1:A:997:ASN:C	1:A:998:LYS:HD3	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:783:ASP:O	1:A:784:VAL:HG13	2.04	0.57
1:A:856:HIS:O	1:A:857:ARG:HG2	2.04	0.57
1:B:835:PHE:HD1	1:B:842:THR:HG22	1.70	0.57
1:B:794:GLY:HA3	1:B:818:PHE:CZ	2.40	0.57
1:A:879:TRP:HE3	1:A:879:TRP:O	1.87	0.57
1:A:951:ILE:CG1	1:A:956:VAL:HG21	2.34	0.57
1:A:824:ILE:HG12	1:A:856:HIS:HA	1.87	0.56
1:B:787:MET:HB3	1:B:791:PHE:CG	2.41	0.56
1:B:826:TRP:O	1:B:853:PRO:HA	2.06	0.56
1:A:897:CYS:SG	1:A:914:PRO:HB3	2.46	0.56
1:A:821:VAL:HG11	1:A:879:TRP:CZ2	2.41	0.55
1:A:895:GLU:OE2	1:A:905:LYS:NZ	2.37	0.55
1:B:850:ARG:NE	1:B:852:LYS:O	2.39	0.55
1:A:755:THR:HB	1:A:778:GLY:HA3	1.87	0.55
1:A:777:ASP:O	1:A:779:ARG:NH2	2.40	0.55
1:A:756:ARG:CG	1:A:776:PHE:HE2	2.20	0.54
1:A:999:TYR:CD2	1:A:1010:TYR:CE2	2.95	0.54
1:A:935:ASN:HA	1:A:940:ALA:HA	1.89	0.54
1:A:740:CYS:HA	1:A:744:LYS:O	2.08	0.54
1:B:877:GLY:O	1:B:878:ASN:O	2.26	0.54
1:A:971:ARG:HG3	1:A:972:PRO:HD2	1.89	0.54
1:A:856:HIS:C	1:A:857:ARG:CG	2.81	0.53
1:A:1003:ARG:HG3	1:A:1010:TYR:CE1	2.44	0.53
1:A:877:GLY:O	1:A:878:ASN:O	2.26	0.53
1:B:790:ASN:O	1:B:792:GLU:OE1	2.27	0.53
1:A:793:PHE:CZ	1:A:795:LEU:HD12	2.45	0.52
1:A:808:PHE:CE1	1:A:826:TRP:HD1	2.27	0.52
1:B:720:THR:HG21	1:B:731:LEU:HD22	1.92	0.52
1:A:797:PRO:CG	1:A:845:VAL:HG21	2.38	0.51
1:A:709:ARG:O	1:A:716:GLU:HB3	2.10	0.51
1:B:939:VAL:HG11	1:B:968:MET:O	2.09	0.51
1:B:995:LEU:O	1:B:996:LYS:C	2.53	0.51
1:A:750:ARG:O	1:A:750:ARG:CG	2.56	0.51
1:B:971:ARG:HG3	1:B:972:PRO:HD2	1.92	0.51
1:A:985:THR:HG22	1:A:988:THR:OG1	2.10	0.51
1:B:735:MET:CE	1:B:751:CYS:HG	2.24	0.51
1:B:735:MET:CE	1:B:751:CYS:SG	2.94	0.51
1:A:708:GLU:O	1:A:709:ARG:C	2.52	0.51
1:B:753:ARG:HA	1:B:779:ARG:O	2.11	0.51
1:B:783:ASP:OD1	1:B:846:ARG:HG3	2.11	0.51
1:B:878:ASN:ND2	2:H:1:NAG:H83	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:966:GLY:O	1:B:998:LYS:HA	2.10	0.51
1:A:923:GLU:HG2	2:E:1:NAG:N2	2.26	0.51
1:A:995:LEU:O	1:A:996:LYS:C	2.54	0.51
1:B:706:LYS:HA	1:B:756:ARG:HD3	1.92	0.51
1:B:782:GLU:CD	1:B:844:VAL:HG13	2.36	0.51
1:B:949:CYS:HB2	1:B:971:ARG:O	2.11	0.50
1:A:750:ARG:O	1:A:751:CYS:CB	2.58	0.50
1:A:753:ARG:HB3	1:A:780:LYS:HD3	1.93	0.50
1:B:723:LYS:HB3	1:B:729:MET:HE3	1.93	0.50
1:A:735:MET:O	1:A:736:VAL:HG23	2.11	0.50
1:B:767:PRO:O	1:B:770:VAL:HG13	2.12	0.50
1:B:961:MET:HE2	1:B:962:ASP:HB3	1.93	0.50
1:A:976:ILE:HG23	1:A:991:TYR:CE1	2.47	0.49
1:B:787:MET:HE3	1:B:848:TYR:HB2	1.94	0.49
1:B:861:ILE:O	1:B:877:GLY:HA2	2.12	0.49
1:B:987:CYS:HB3	1:B:1022:LEU:CD1	2.42	0.49
1:A:826:TRP:O	1:A:853:PRO:HA	2.12	0.49
1:A:725:TYR:HA	1:A:729:MET:CE	2.42	0.49
1:B:965:LEU:C	1:B:965:LEU:HD12	2.37	0.49
1:B:999:TYR:CE2	1:B:1010:TYR:CZ	3.00	0.49
1:A:732:GLU:OE2	1:A:750:ARG:NH2	2.45	0.49
1:B:912:HIS:CD2	1:B:915:ILE:HD12	2.48	0.49
1:A:803:ILE:HD12	1:A:833:THR:HG21	1.94	0.49
1:A:780:LYS:HG2	1:A:781:GLN:HG3	1.94	0.49
1:B:940:ALA:O	1:B:958:VAL:HG23	2.13	0.49
1:A:788:ASP:OD1	1:A:789:ASP:N	2.46	0.48
1:B:696:CYS:SG	1:B:725:TYR:CE1	3.06	0.48
1:B:951:ILE:CD1	1:B:956:VAL:HG21	2.43	0.48
1:A:745:LEU:HD12	1:A:745:LEU:O	2.13	0.48
1:A:1004:ASP:HB3	1:A:1011:MET:SD	2.54	0.48
1:B:703:ALA:HB1	1:B:720:THR:OG1	2.12	0.48
1:B:1006:TYR:CZ	1:B:1022:LEU:HD23	2.48	0.48
2:C:1:NAG:O3	2:C:2:NAG:O5	2.24	0.48
1:B:752:THR:HG23	1:B:779:ARG:NH2	2.29	0.48
1:A:947:LEU:HD12	1:A:947:LEU:C	2.37	0.48
1:B:843:THR:HG22	1:B:844:VAL:N	2.29	0.48
1:A:704:ILE:HG22	1:A:705:ALA:N	2.28	0.48
1:B:755:THR:OG1	1:B:777:ASP:HA	2.14	0.48
1:B:756:ARG:HB2	1:B:776:PHE:CE2	2.47	0.48
1:B:999:TYR:HB3	1:B:1012:LEU:HD21	1.96	0.47
1:B:899:TRP:CD2	1:B:900:CYS:SG	3.08	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:797:PRO:CD	1:B:845:VAL:HG21	2.44	0.47
1:A:783:ASP:HB2	1:A:846:ARG:HA	1.96	0.47
1:A:889:TYR:CE1	1:A:894:ILE:HD11	2.49	0.47
1:A:698:PRO:HA	1:A:725:TYR:CG	2.50	0.47
1:A:753:ARG:HA	1:A:779:ARG:O	2.15	0.47
1:B:782:GLU:OE2	1:B:844:VAL:HG13	2.15	0.47
1:A:803:ILE:HG21	1:A:805:ARG:NH2	2.30	0.47
1:B:823:PRO:O	1:B:826:TRP:HB2	2.15	0.47
1:A:754:GLU:O	1:A:776:PHE:CZ	2.67	0.47
1:A:923:GLU:CD	2:E:1:NAG:HN2	2.23	0.47
1:B:844:VAL:HG22	1:B:846:ARG:N	2.31	0.46
1:B:939:VAL:CG1	1:B:968:MET:O	2.64	0.46
1:B:947:LEU:O	1:B:958:VAL:HG12	2.15	0.46
1:A:935:ASN:OD1	1:A:935:ASN:C	2.58	0.46
1:A:755:THR:HB	1:A:778:GLY:N	2.31	0.46
1:A:824:ILE:CG1	1:A:856:HIS:HA	2.45	0.46
1:A:856:HIS:C	1:A:857:ARG:HG2	2.40	0.46
1:A:706:LYS:O	1:A:757:TYR:CE1	2.67	0.46
1:B:834:SER:N	1:B:843:THR:O	2.49	0.46
1:B:969:PRO:O	1:B:970:CYS:CB	2.64	0.46
1:A:963:THR:O	1:A:963:THR:HG22	2.16	0.46
1:A:870:LEU:O	1:A:886:GLN:HG2	2.16	0.45
1:A:939:VAL:O	1:A:939:VAL:HG13	2.15	0.45
1:B:703:ALA:HB2	1:B:722:TRP:HA	1.97	0.45
1:A:755:THR:HB	1:A:778:GLY:CA	2.46	0.45
1:A:888:LEU:CD2	1:A:928:LEU:HD22	2.47	0.45
1:A:968:MET:HE1	1:A:995:LEU:HD22	1.98	0.45
1:B:775:LEU:N	1:B:775:LEU:HD23	2.29	0.45
1:A:877:GLY:C	1:A:878:ASN:O	2.58	0.45
1:A:895:GLU:HB2	1:A:921:GLU:HG3	1.98	0.45
1:A:946:THR:CG2	1:A:959:ILE:HD13	2.47	0.45
1:B:751:CYS:SG	1:B:752:THR:N	2.89	0.45
1:B:821:VAL:O	1:B:880:THR:HG21	2.17	0.45
1:B:783:ASP:O	1:B:784:VAL:HB	2.16	0.45
1:A:761:LEU:HB2	1:A:770:VAL:HG12	1.98	0.45
1:A:968:MET:HG3	1:A:1000:PHE:CZ	2.52	0.45
1:A:889:TYR:CE2	1:A:891:GLY:HA2	2.51	0.45
1:A:923:GLU:CG	2:E:1:NAG:N2	2.80	0.45
1:B:1004:ASP:OD2	1:B:1020:PHE:HB2	2.16	0.45
1:A:696:CYS:SG	1:A:725:TYR:HE1	2.40	0.45
1:A:783:ASP:OD2	1:A:846:ARG:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:941:ILE:HG21	1:A:956:VAL:HG11	1.99	0.45
1:A:1006:TYR:CZ	1:A:1022:LEU:HD23	2.51	0.44
1:B:733:ASP:OD2	1:B:756:ARG:NH1	2.50	0.44
1:A:917:LYS:C	1:A:918:CYS:SG	3.00	0.44
1:B:916:GLY:O	1:B:930:ASP:O	2.35	0.44
1:A:929:VAL:HG22	1:A:930:ASP:HB2	1.98	0.44
1:B:761:LEU:HD11	1:B:765:ALA:HB3	1.98	0.44
1:B:965:LEU:C	1:B:965:LEU:CD1	2.90	0.44
1:A:939:VAL:HG22	1:A:958:VAL:HG21	2.00	0.44
1:B:968:MET:HE2	1:B:1000:PHE:CE1	2.52	0.44
1:A:840:LEU:HD22	1:A:840:LEU:N	2.33	0.44
1:A:704:ILE:CG2	1:A:705:ALA:N	2.81	0.44
1:B:750:ARG:O	1:B:751:CYS:CB	2.66	0.44
1:B:832:CYS:N	1:B:844:VAL:HG23	2.33	0.43
1:A:733:ASP:C	1:A:733:ASP:OD1	2.61	0.43
1:A:821:VAL:O	1:A:822:CYS:C	2.61	0.43
1:B:844:VAL:HG22	1:B:846:ARG:H	1.83	0.43
1:B:758:LEU:O	1:B:772:PHE:HA	2.19	0.43
1:A:810:THR:HG21	1:A:826:TRP:CD1	2.54	0.43
1:A:929:VAL:HG13	1:A:930:ASP:N	2.33	0.43
1:B:845:VAL:HG23	1:B:846:ARG:N	2.34	0.43
1:A:757:TYR:CE2	1:A:774:LYS:HE2	2.53	0.43
1:A:794:GLY:HA3	1:A:818:PHE:CE1	2.53	0.43
1:B:917:LYS:C	1:B:918:CYS:SG	3.01	0.43
1:B:947:LEU:HD12	1:B:947:LEU:C	2.42	0.43
1:B:968:MET:HE2	1:B:1000:PHE:CZ	2.54	0.43
1:B:794:GLY:HA3	1:B:818:PHE:CE2	2.53	0.43
1:B:844:VAL:HG22	1:B:845:VAL:N	2.34	0.43
1:B:972:PRO:HG2	1:B:975:ILE:HD11	2.01	0.43
1:A:709:ARG:NH1	1:A:710:ILE:O	2.52	0.42
1:B:698:PRO:HA	1:B:725:TYR:CG	2.54	0.42
1:B:857:ARG:O	1:B:859:GLY:N	2.52	0.42
1:A:741:GLU:OE2	1:A:746:MET:CG	2.68	0.42
1:A:923:GLU:CG	2:E:1:NAG:HN2	2.33	0.42
1:B:695:ASP:HB3	1:B:743:GLY:O	2.19	0.42
1:A:940:ALA:O	1:A:958:VAL:HG23	2.20	0.42
1:B:946:THR:HG23	1:B:959:ILE:HD13	2.02	0.42
1:A:951:ILE:O	1:A:952:GLY:C	2.62	0.42
1:B:943:PRO:O	1:B:957:GLN:OE1	2.38	0.42
1:B:824:ILE:CG1	1:B:856:HIS:HA	2.49	0.42
1:A:749:GLN:OE1	1:A:776:PHE:HD1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:PRO:HB2	1:A:826:TRP:HB2	2.02	0.41
1:B:821:VAL:O	1:B:822:CYS:C	2.63	0.41
1:A:736:VAL:CG1	1:A:737:ILE:N	2.83	0.41
1:A:803:ILE:HD12	1:A:833:THR:CG2	2.49	0.41
1:A:973:TYR:CD1	1:A:973:TYR:C	2.98	0.41
1:B:810:THR:HG21	1:B:826:TRP:CD1	2.55	0.41
1:B:909:GLY:O	1:B:951:ILE:HG21	2.21	0.41
1:B:823:PRO:O	1:B:824:ILE:C	2.63	0.41
1:B:835:PHE:HZ	1:B:840:LEU:HD12	1.86	0.41
1:A:894:ILE:CG2	1:A:895:GLU:N	2.83	0.41
1:B:868:GLU:OE1	1:B:926:TYR:CE1	2.74	0.41
1:B:713:LEU:HD23	1:B:713:LEU:O	2.21	0.41
1:B:843:THR:HG22	1:B:844:VAL:H	1.85	0.41
1:A:1017:GLN:NE2	1:A:1019:TRP:CZ2	2.88	0.41
1:B:784:VAL:HA	1:B:847:THR:O	2.20	0.41
1:B:920:LEU:CD1	1:B:927:ARG:HD2	2.51	0.41
1:A:767:PRO:O	1:A:770:VAL:HG13	2.20	0.41
1:A:907:SER:HA	1:A:913:TYR:HB2	2.03	0.41
1:A:733:ASP:OD1	1:A:736:VAL:N	2.53	0.41
1:A:879:TRP:CE3	1:A:879:TRP:C	2.99	0.41
1:B:787:MET:HB3	1:B:791:PHE:HB2	2.03	0.41
1:B:835:PHE:CD1	1:B:842:THR:HG22	2.53	0.41
1:B:840:LEU:N	1:B:840:LEU:HD22	2.36	0.41
1:A:755:THR:N	1:A:778:GLY:HA3	2.36	0.41
1:A:947:LEU:HD12	1:A:948:LYS:C	2.46	0.40
1:B:761:LEU:CD1	1:B:765:ALA:HB3	2.51	0.40
1:B:877:GLY:C	1:B:878:ASN:O	2.63	0.40
1:A:888:LEU:HD21	1:A:928:LEU:HD22	2.04	0.40
1:A:1015:GLU:HB3	1:A:1016:TYR:CE1	2.56	0.40
1:B:733:ASP:OD1	1:B:733:ASP:C	2.63	0.40
1:A:781:GLN:N	1:A:781:GLN:OE1	2.54	0.40
1:A:968:MET:CB	1:A:1000:PHE:CE1	3.03	0.40
1:A:966:GLY:O	1:A:999:TYR:CD1	2.75	0.40
1:B:969:PRO:O	1:B:970:CYS:HB3	2.22	0.40
1:A:766:LEU:HD11	1:A:768:THR:OG1	2.21	0.40
1:A:830:VAL:HG13	1:A:848:TYR:HB2	2.03	0.40
1:B:757:TYR:HD1	1:B:774:LYS:HA	1.86	0.40
1:B:829:THR:HA	1:B:848:TYR: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	320/338 (95%)	274 (86%)	32 (10%)	14 (4%)	2	20
1	B	320/338 (95%)	274 (86%)	33 (10%)	13 (4%)	2	20
All	All	640/676 (95%)	548 (86%)	65 (10%)	27 (4%)	2	20

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	751	CYS
1	A	797	PRO
1	A	858	GLN
1	A	879	TRP
1	A	996	LYS
1	B	765	ALA
1	B	797	PRO
1	B	858	GLN
1	B	879	TRP
1	B	968	MET
1	B	970	CYS
1	B	973	TYR
1	A	765	ALA
1	A	885	ASP
1	A	928	LEU
1	B	751	CYS
1	B	784	VAL
1	B	996	LYS
1	A	878	ASN
1	B	967	PRO
1	A	709	ARG
1	A	810	THR
1	B	878	ASN
1	B	943	PRO
1	A	1008	GLN

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Mol	Chain	Res	Type
1	A	824	ILE
1	A	855	PRO

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	285/298 (96%)	239 (84%)	46 (16%)	2	13
1	B	285/298 (96%)	238 (84%)	47 (16%)	2	13
All	All	570/596 (96%)	477 (84%)	93 (16%)	2	13

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	706	LYS
1	A	713	LEU
1	A	740	CYS
1	A	742	ASP
1	A	750	ARG
1	A	766	LEU
1	A	767	PRO
1	A	771	VAL
1	A	773	LYS
1	A	779	ARG
1	A	788	ASP
1	A	790	ASN
1	A	805	ARG
1	A	812	LEU
1	A	823	PRO
1	A	824	ILE
1	A	827	THR
1	A	830	VAL
1	A	831	SER
1	A	834	SER
1	A	842	THR

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Mol	Chain	Res	Type
1	A	845	VAL
1	A	848	TYR
1	A	865	ASN
1	A	874	ILE
1	A	879	TRP
1	A	882	VAL
1	A	885	ASP
1	A	888	LEU
1	A	894	ILE
1	A	928	LEU
1	A	935	ASN
1	A	936	ARG
1	A	941	ILE
1	A	942	VAL
1	A	947	LEU
1	A	951	ILE
1	A	953	LYS
1	A	954	THR
1	A	956	VAL
1	A	962	ASP
1	A	964	LYS
1	A	970	CYS
1	A	976	ILE
1	A	994	THR
1	A	995	LEU
1	B	694	LEU
1	B	712	GLN
1	B	713	LEU
1	B	721	THR
1	B	726	SER
1	B	768	THR
1	B	771	VAL
1	B	776	PHE
1	B	787	MET
1	B	792	GLU
1	B	801	LYS
1	B	811	THR
1	B	812	LEU
1	B	827	THR
1	B	830	VAL
1	B	831	SER
1	B	834	SER

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Mol	Chain	Res	Type
1	B	837	MET
1	B	842	THR
1	B	843	THR
1	B	862	THR
1	B	870	LEU
1	B	878	ASN
1	B	882	VAL
1	B	894	ILE
1	B	905	LYS
1	B	912	HIS
1	B	929	VAL
1	B	936	ARG
1	B	937	GLU
1	B	941	ILE
1	B	947	LEU
1	B	951	ILE
1	B	953	LYS
1	B	957	GLN
1	B	964	LYS
1	B	965	LEU
1	B	968	MET
1	B	971	ARG
1	B	976	ILE
1	B	988	THR
1	B	989	PHE
1	B	997	ASN
1	B	1012	LEU
1	B	1015	GLU
1	B	1022	LEU
1	B	1023	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	712	GLN
1	A	749	GLN
1	A	762	HIS
1	B	871	HIS
1	B	912	HIS

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 ⓘ

16 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	2,1	14,14,15	0.71	0	17,19,21	2.41	5 (29%)
2	NAG	C	2	2	14,14,15	0.76	0	17,19,21	1.76	4 (23%)
2	NAG	D	1	2,1	14,14,15	0.58	0	17,19,21	1.80	5 (29%)
2	NAG	D	2	2	14,14,15	0.84	1 (7%)	17,19,21	1.19	1 (5%)
2	NAG	E	1	2,1	14,14,15	0.50	0	17,19,21	1.73	6 (35%)
2	NAG	E	2	2	14,14,15	0.61	0	17,19,21	1.61	2 (11%)
2	NAG	F	1	2,1	14,14,15	0.55	0	17,19,21	1.82	3 (17%)
2	NAG	F	2	2	14,14,15	0.86	1 (7%)	17,19,21	1.82	2 (11%)
2	NAG	G	1	2,1	14,14,15	0.54	0	17,19,21	3.42	8 (47%)
2	NAG	G	2	2	14,14,15	0.65	0	17,19,21	1.15	2 (11%)
2	NAG	H	1	2,1	14,14,15	0.96	0	17,19,21	3.20	10 (58%)
2	NAG	H	2	2	14,14,15	0.79	0	17,19,21	2.34	4 (23%)
2	NAG	I	1	2,1	14,14,15	0.49	0	17,19,21	1.73	6 (35%)
2	NAG	I	2	2	14,14,15	0.59	0	17,19,21	1.60	2 (11%)
2	NAG	J	1	2,1	14,14,15	0.45	0	17,19,21	2.14	6 (35%)
2	NAG	J	2	2	14,14,15	0.63	0	17,19,21	1.56	2 (11%)

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	2,1	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	J	2	2	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	C1-C2	2.61	1.55	1.52
2	F	2	NAG	C1-C2	2.45	1.55	1.52

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	NAG	C1-O5-C5	8.66	123.80	112.19
2	H	2	NAG	C1-O5-C5	6.84	121.36	112.19
2	H	1	NAG	O5-C1-C2	-6.70	100.92	111.29
2	C	1	NAG	C1-O5-C5	6.59	121.02	112.19
2	G	1	NAG	C4-C3-C2	-6.50	101.50	111.02
2	G	1	NAG	C1-C2-N2	6.04	119.95	110.43
2	H	1	NAG	C1-O5-C5	5.64	119.74	112.19
2	J	2	NAG	C1-O5-C5	5.26	119.23	112.19
2	F	2	NAG	C1-O5-C5	5.03	118.93	112.19
2	E	2	NAG	C1-O5-C5	4.82	118.64	112.19
2	I	2	NAG	C1-O5-C5	4.78	118.59	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	NAG	C8-C7-N2	4.62	123.77	116.12
2	C	2	NAG	C4-C3-C2	4.59	117.75	111.02
2	H	2	NAG	C1-C2-N2	4.46	117.46	110.43
2	F	1	NAG	C4-C3-C2	-4.23	104.81	111.02
2	H	1	NAG	O4-C4-C3	4.20	120.27	110.38
2	F	2	NAG	O5-C1-C2	3.96	117.42	111.29
2	H	1	NAG	O7-C7-C8	-3.96	115.00	122.05
2	H	1	NAG	O5-C5-C6	3.80	115.05	107.66
2	J	1	NAG	C1-O5-C5	3.70	117.15	112.19
2	H	1	NAG	C8-C7-N2	3.64	122.16	116.12
2	D	1	NAG	C8-C7-N2	3.53	121.97	116.12
2	J	1	NAG	O5-C1-C2	-3.38	106.06	111.29
2	D	1	NAG	C1-O5-C5	3.26	116.55	112.19
2	F	1	NAG	C8-C7-N2	3.24	121.49	116.12
2	D	1	NAG	O5-C1-C2	-3.20	106.33	111.29
2	G	1	NAG	C8-C7-N2	3.19	121.41	116.12
2	C	1	NAG	C3-C4-C5	3.18	115.99	110.23
2	C	1	NAG	O3-C3-C4	3.18	117.86	110.38
2	G	1	NAG	O7-C7-C8	-3.17	116.41	122.05
2	J	1	NAG	O7-C7-C8	-3.10	116.53	122.05
2	E	2	NAG	O5-C1-C2	3.02	115.97	111.29
2	I	2	NAG	O5-C1-C2	3.02	115.96	111.29
2	H	1	NAG	C1-C2-N2	2.99	115.14	110.43
2	I	1	NAG	O5-C1-C2	2.89	115.77	111.29
2	C	1	NAG	C8-C7-N2	2.89	120.90	116.12
2	C	2	NAG	C2-N2-C7	2.88	126.75	122.90
2	E	1	NAG	O5-C1-C2	2.86	115.72	111.29
2	G	1	NAG	O3-C3-C2	2.85	115.33	109.40
2	H	1	NAG	C3-C4-C5	-2.84	105.09	110.23
2	C	1	NAG	C4-C3-C2	-2.82	106.89	111.02
2	I	1	NAG	C1-O5-C5	2.77	115.90	112.19
2	E	1	NAG	C1-O5-C5	2.77	115.89	112.19
2	H	2	NAG	C2-N2-C7	2.69	126.50	122.90
2	J	1	NAG	C2-N2-C7	2.67	126.48	122.90
2	D	1	NAG	O7-C7-C8	-2.61	117.40	122.05
2	G	1	NAG	O4-C4-C5	2.51	115.50	109.32
2	J	1	NAG	C4-C3-C2	-2.44	107.44	111.02
2	C	2	NAG	O7-C7-C8	-2.42	117.75	122.05
2	H	1	NAG	O5-C5-C4	2.40	116.66	110.83
2	H	1	NAG	C4-C3-C2	-2.37	107.55	111.02
2	J	2	NAG	O5-C1-C2	2.30	114.85	111.29
2	I	1	NAG	O5-C5-C4	-2.28	105.28	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	O5-C5-C4	-2.27	105.30	110.83
2	G	2	NAG	O5-C1-C2	2.24	114.76	111.29
2	D	2	NAG	C1-C2-N2	2.24	113.96	110.43
2	I	1	NAG	C2-N2-C7	2.23	125.89	122.90
2	C	2	NAG	C1-O5-C5	2.22	115.16	112.19
2	E	1	NAG	C2-N2-C7	2.22	125.87	122.90
2	D	1	NAG	C3-C4-C5	-2.19	106.25	110.23
2	H	2	NAG	O5-C1-C2	-2.19	107.90	111.29
2	E	1	NAG	C8-C7-N2	2.19	119.74	116.12
2	I	1	NAG	C8-C7-N2	2.14	119.67	116.12
2	G	1	NAG	O5-C5-C4	2.13	116.01	110.83
2	E	1	NAG	C3-C4-C5	-2.11	106.40	110.23
2	I	1	NAG	C3-C4-C5	-2.09	106.44	110.23
2	F	1	NAG	O4-C4-C3	2.08	115.27	110.38
2	G	2	NAG	O5-C5-C4	-2.05	105.84	110.83

There are no chirality outliers.

All (39) torsion outliers are listed below:

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

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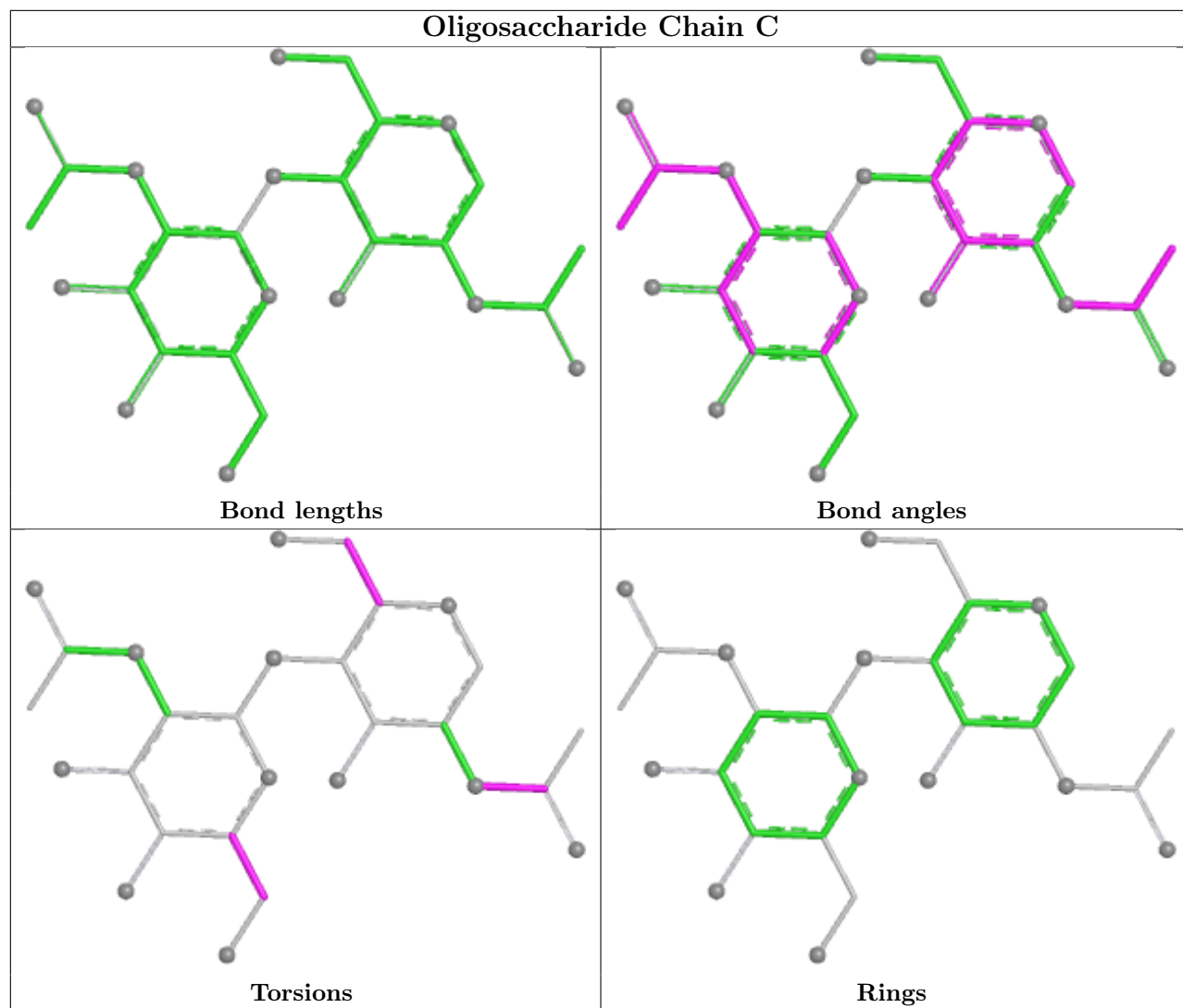
Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	I	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6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

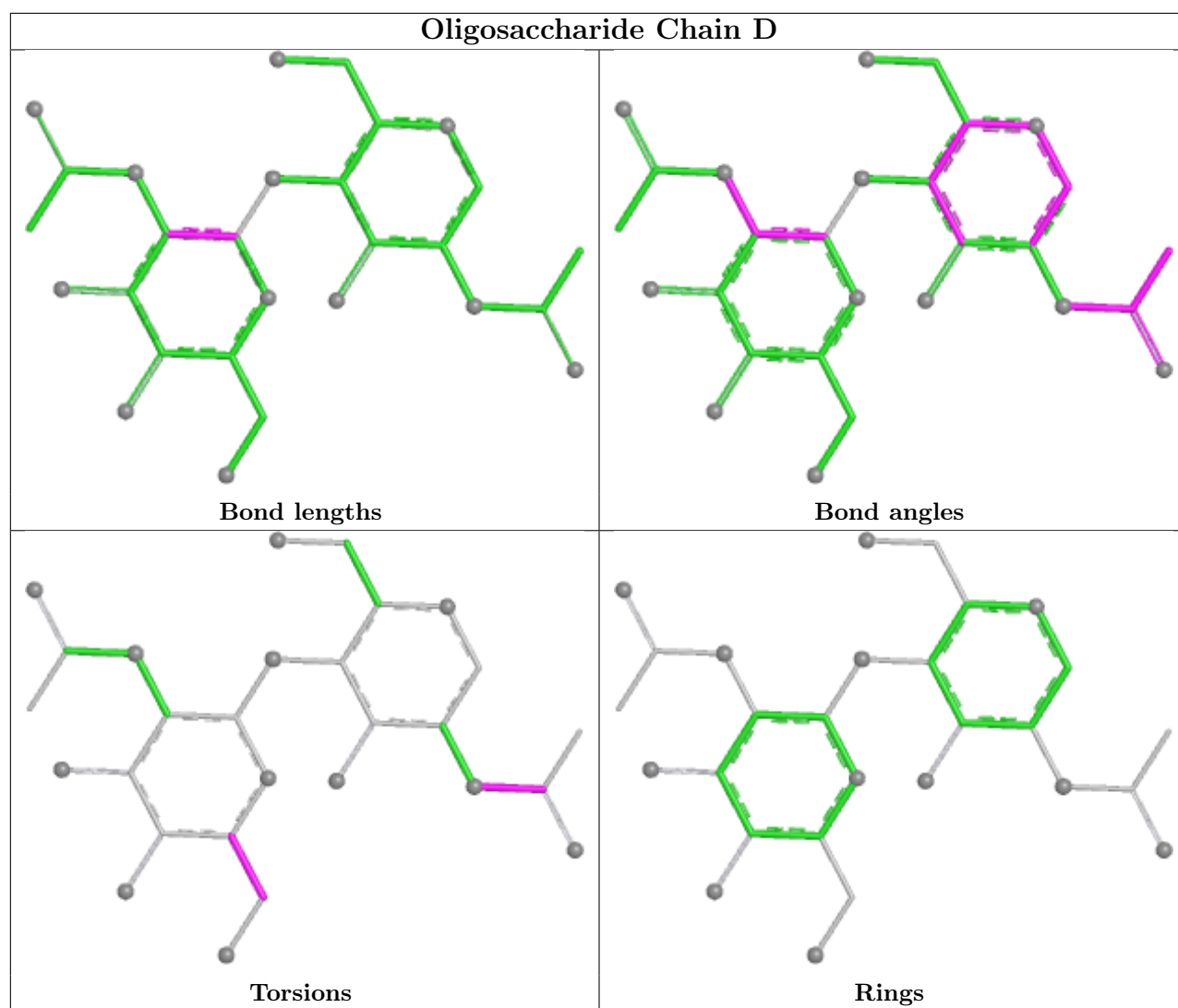
There are no ring outliers.

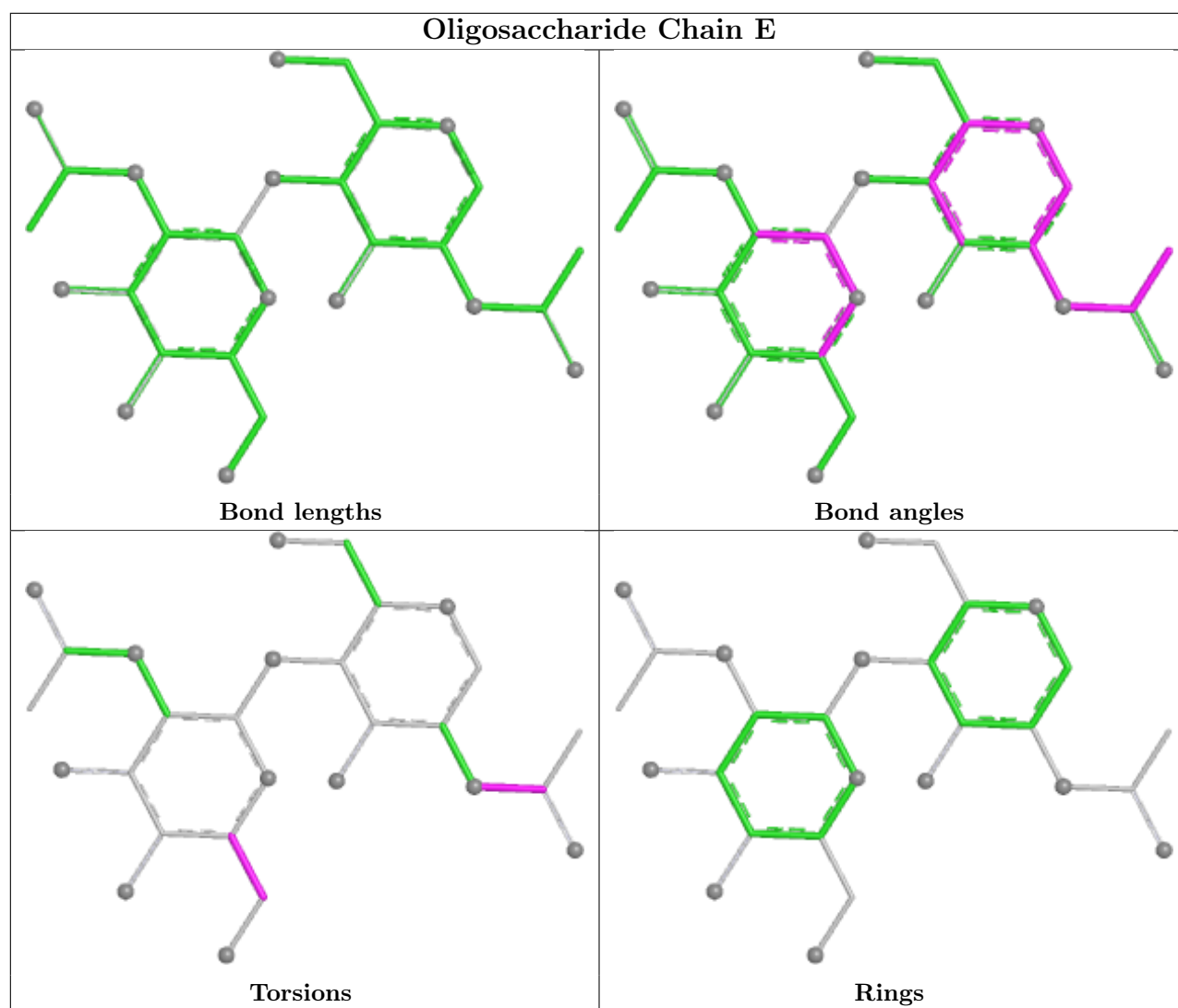
5 monomers are involved in 15 short contacts:

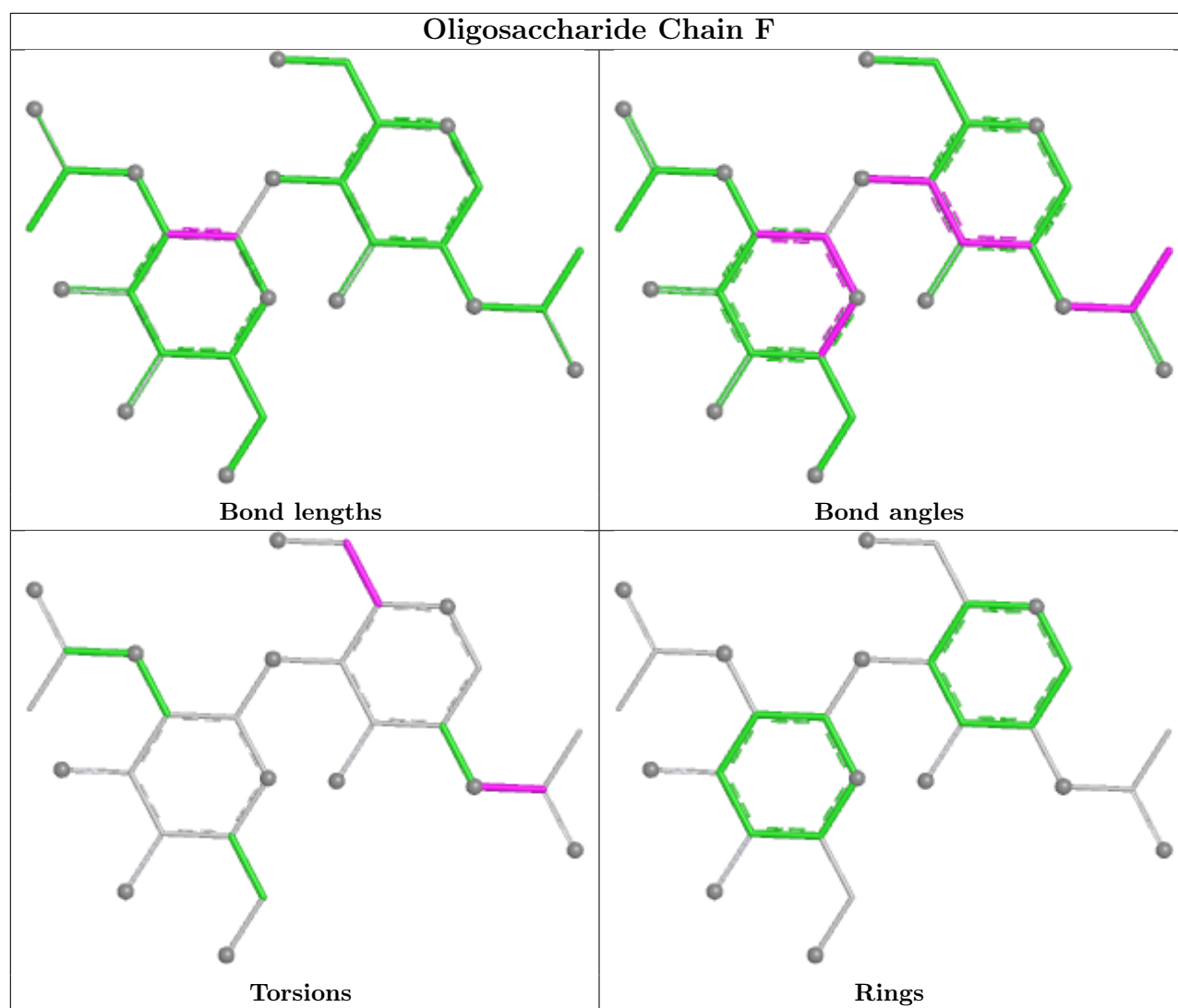
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	2	NAG	7	0
2	E	1	NAG	6	0
2	H	1	NAG	1	0
2	C	2	NAG	1	0
2	C	1	NAG	1	0

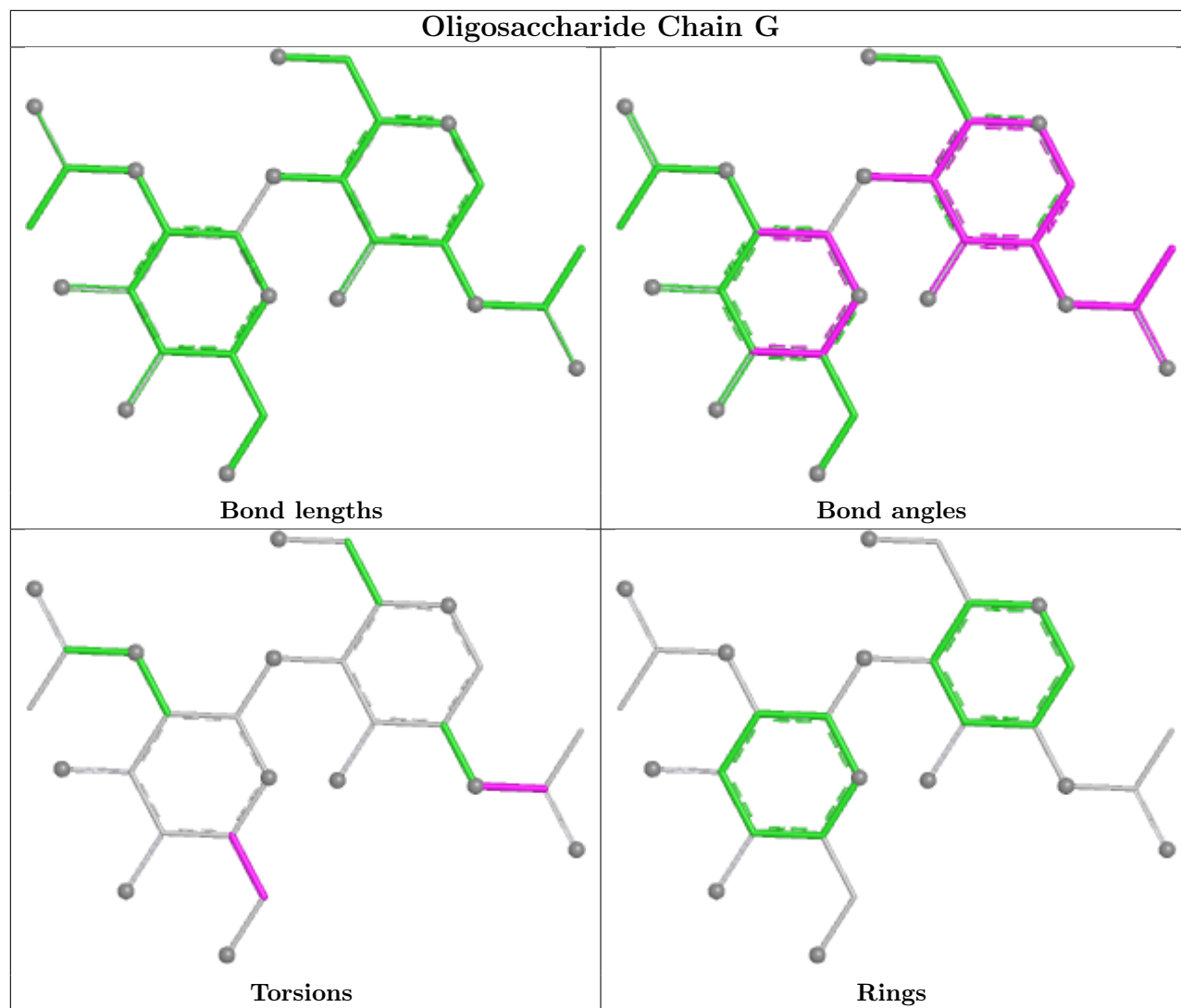
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

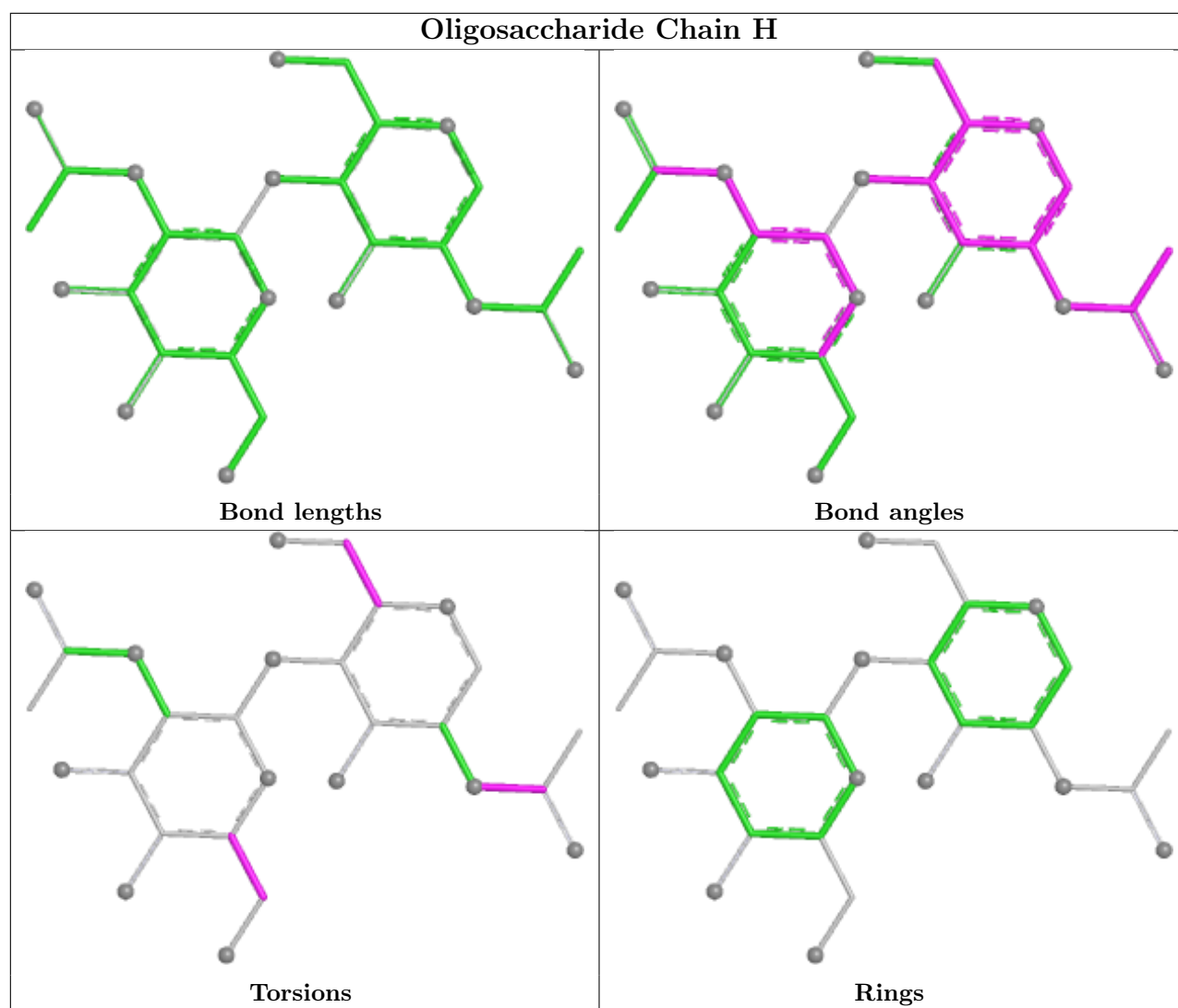


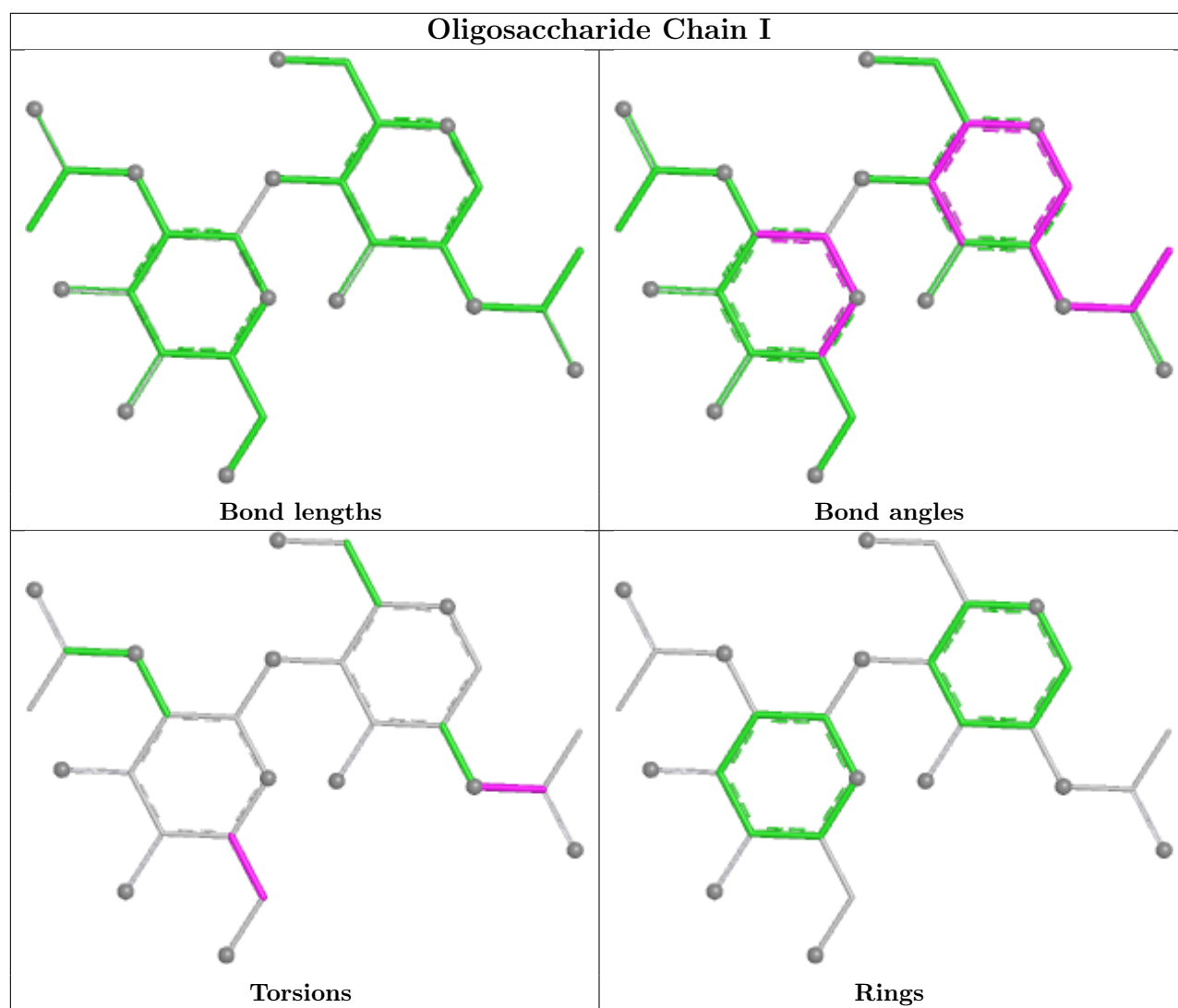


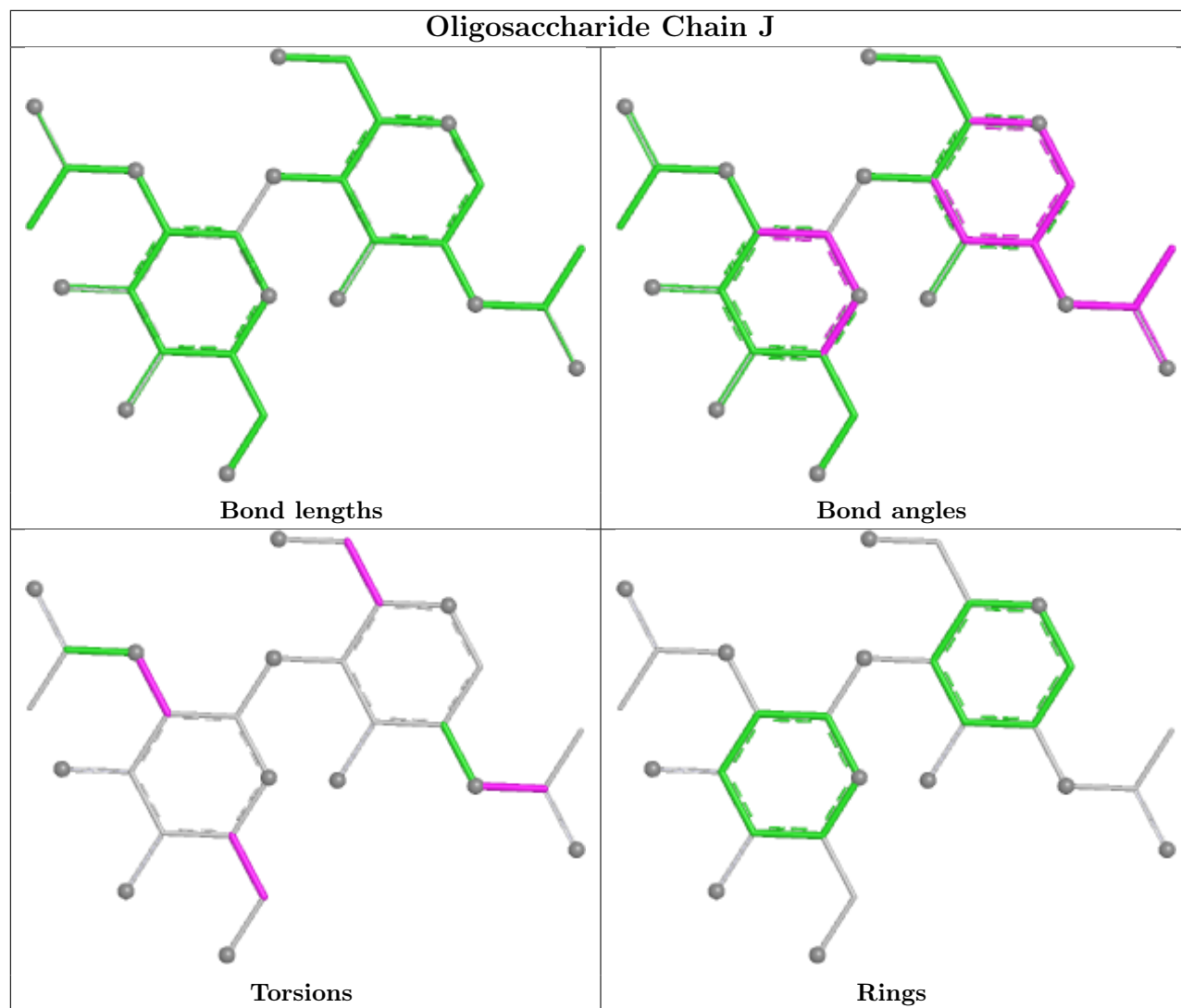












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A	324/338 (95%)	0.19	9 (2%)	55 41	63, 112, 172, 210	0
1	B	324/338 (95%)	0.19	3 (0%)	81 65	62, 108, 149, 177	0
All	All	648/676 (95%)	0.19	12 (1%)	66 50	62, 109, 162, 210	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	820	MET	4.4
1	A	1014	GLY	3.9
1	A	1013	LYS	3.2
1	B	1001	GLU	3.2
1	A	758	LEU	3.1
1	A	1018	TYR	2.6
1	A	1012	LEU	2.5
1	B	904	PHE	2.4
1	A	1020	PHE	2.4
1	B	1002	PRO	2.2
1	A	818	PHE	2.2
1	A	694	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

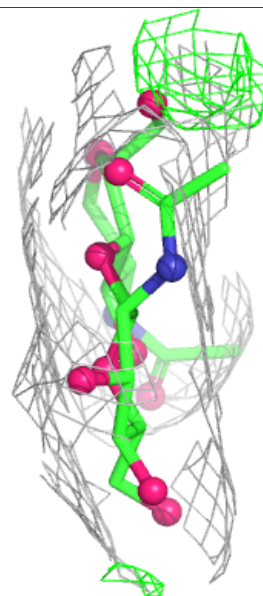
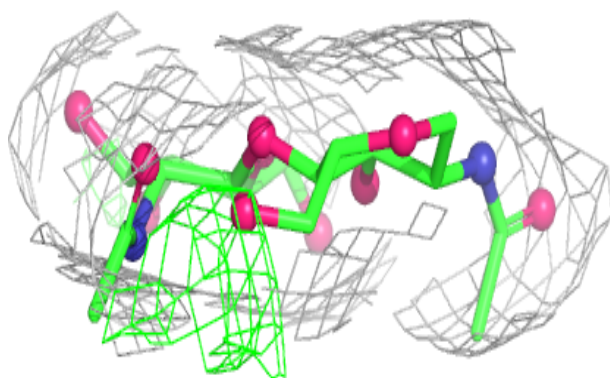
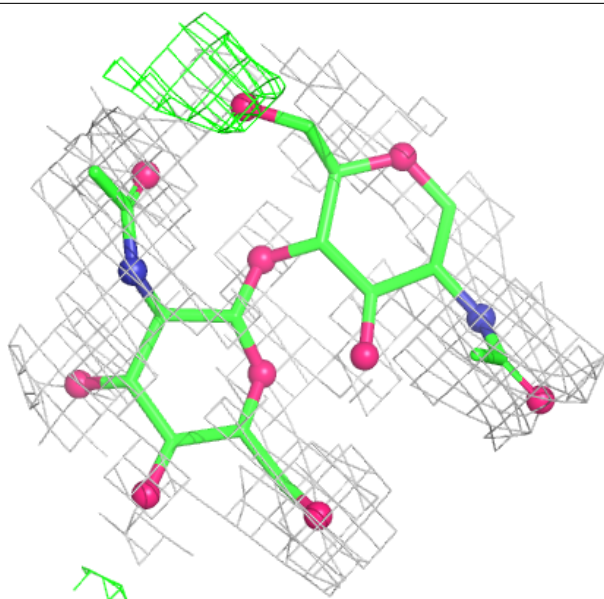
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	I	2	14/15	-0.04	0.17	136,143,145,146	0
2	NAG	F	2	14/15	0.19	0.13	137,202,231,236	0
2	NAG	H	2	14/15	0.22	0.17	112,181,230,239	0
2	NAG	E	2	14/15	0.31	0.16	136,143,145,146	0
2	NAG	D	2	14/15	0.57	0.12	99,162,186,198	0
2	NAG	J	2	14/15	0.61	0.11	136,200,227,240	0
2	NAG	E	1	14/15	0.63	0.13	92,105,118,130	0
2	NAG	I	1	14/15	0.71	0.14	92,105,118,130	0
2	NAG	G	2	14/15	0.73	0.12	140,225,283,337	0
2	NAG	J	1	14/15	0.77	0.11	119,171,232,241	0
2	NAG	G	1	14/15	0.78	0.14	97,177,229,235	0
2	NAG	F	1	14/15	0.80	0.08	129,201,215,223	0
2	NAG	C	2	14/15	0.87	0.11	71,117,157,163	0
2	NAG	D	1	14/15	0.89	0.13	128,169,206,223	0
2	NAG	H	1	14/15	0.90	0.10	101,159,192,206	0
2	NAG	C	1	14/15	0.93	0.09	59,73,92,97	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

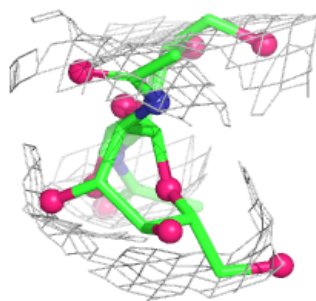
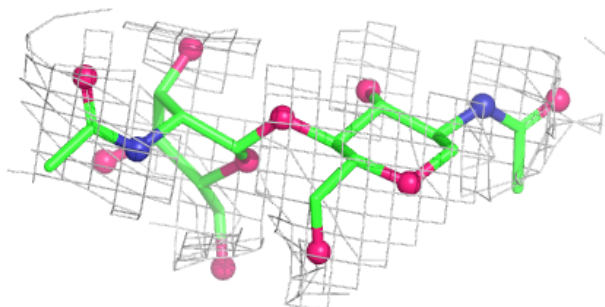
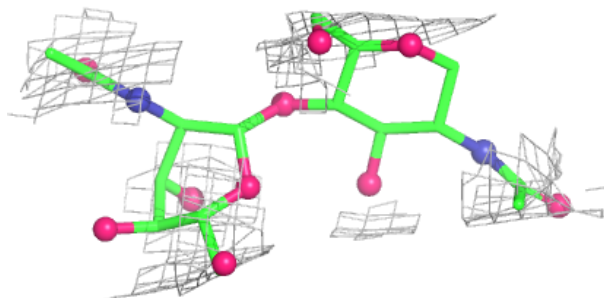
Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

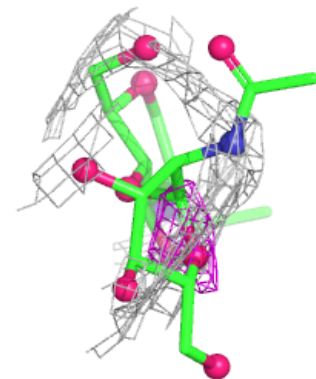
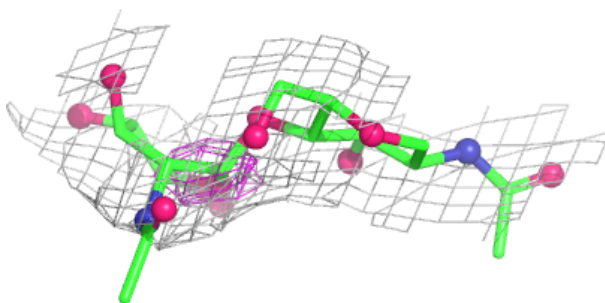
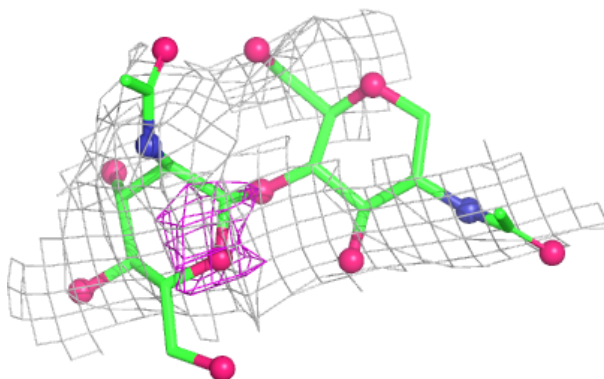


Electron density around Chain D:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

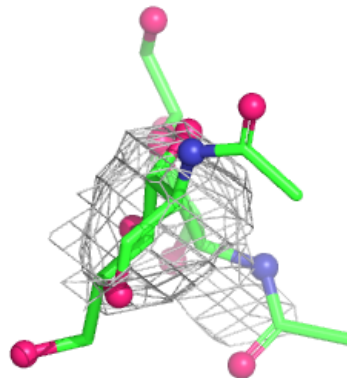
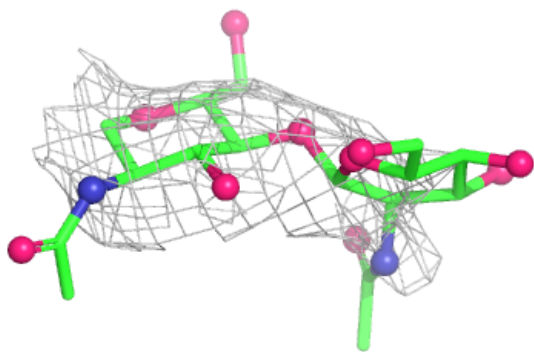
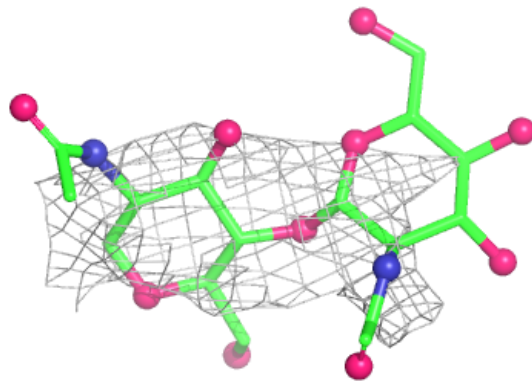
**Electron density around Chain E:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



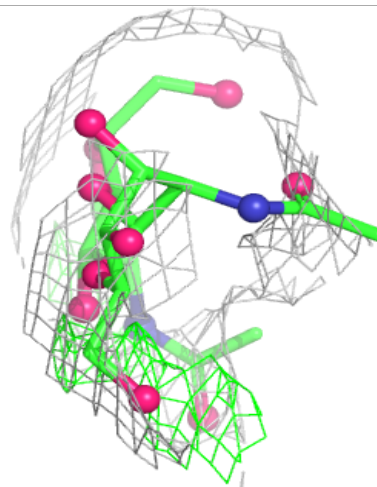
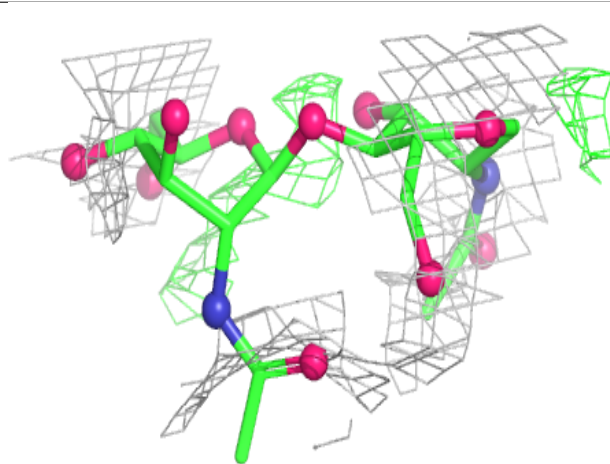
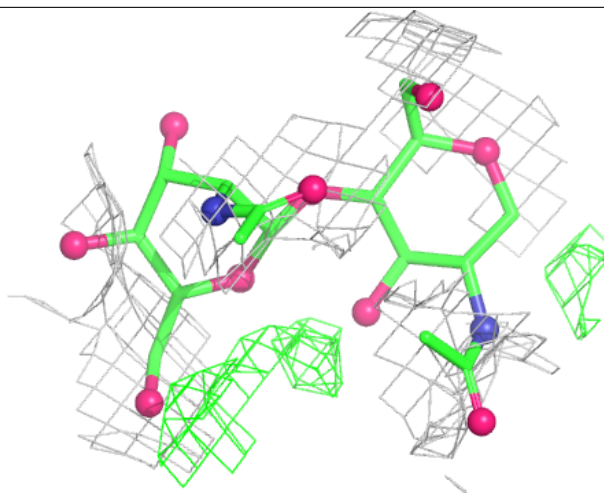
Electron density around Chain F:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



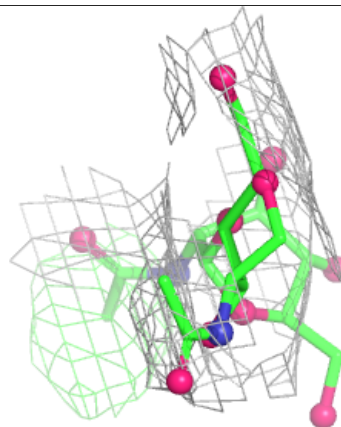
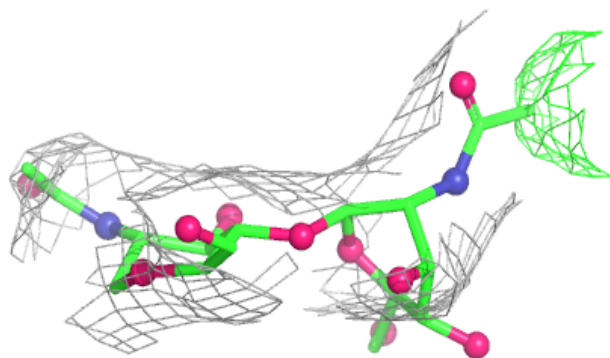
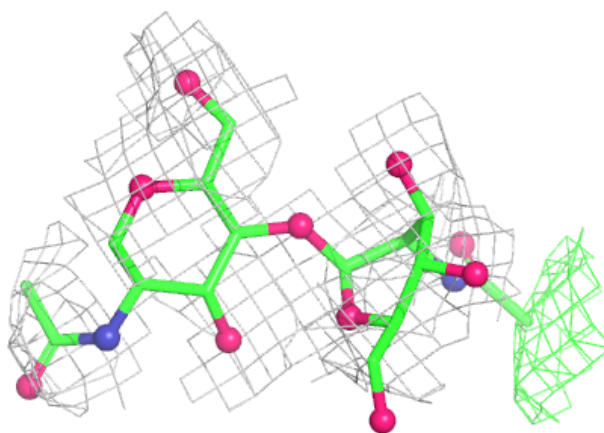
Electron density around Chain G:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

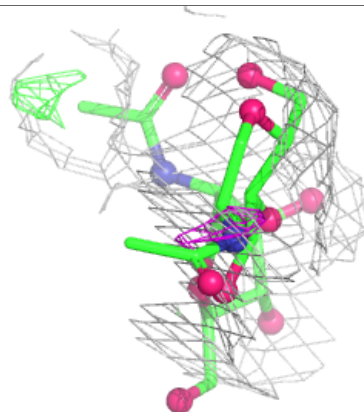
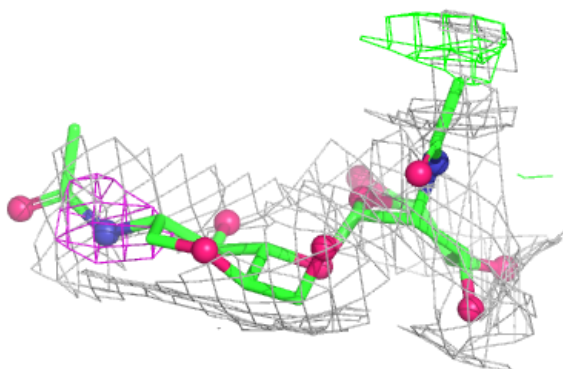
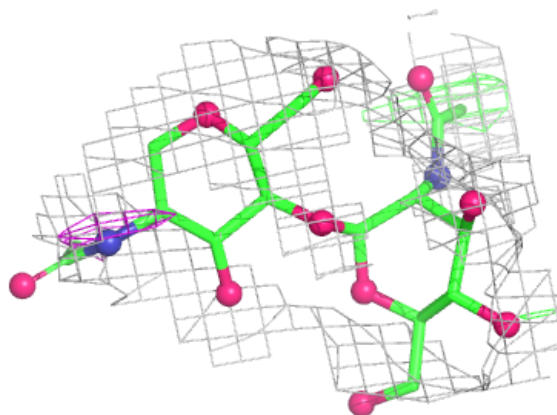


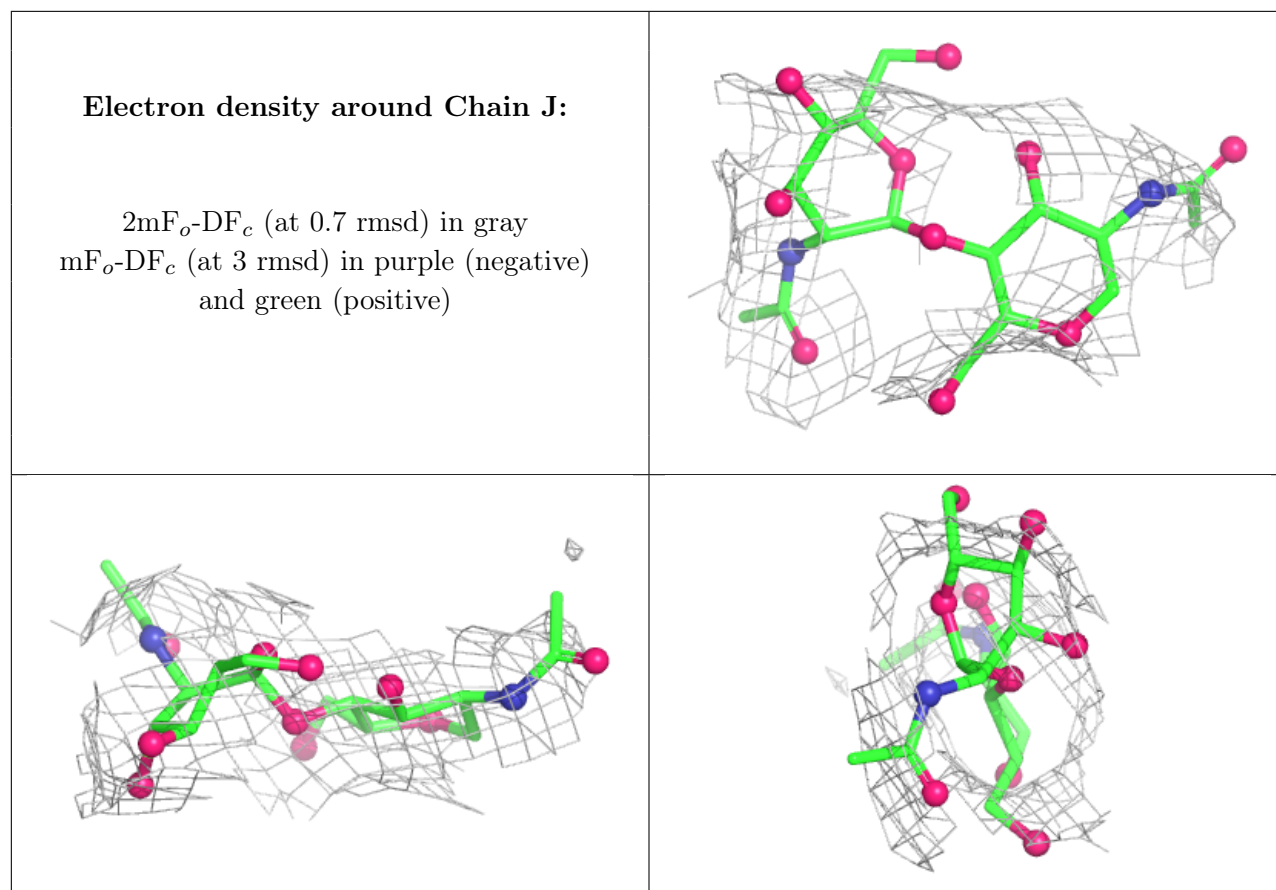
Electron density around Chain H:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain I:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.