



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:42 AM EDT

PDB ID : 4ILD / pdb_00004ild
Title : Crystal structure of truncated Bovine viral diarrhea virus 1 E2 envelope protein
Authors : Modis, Y.; Li, Y.; Wang, J.
Deposited on : 2012-12-30
Resolution : 3.27 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:

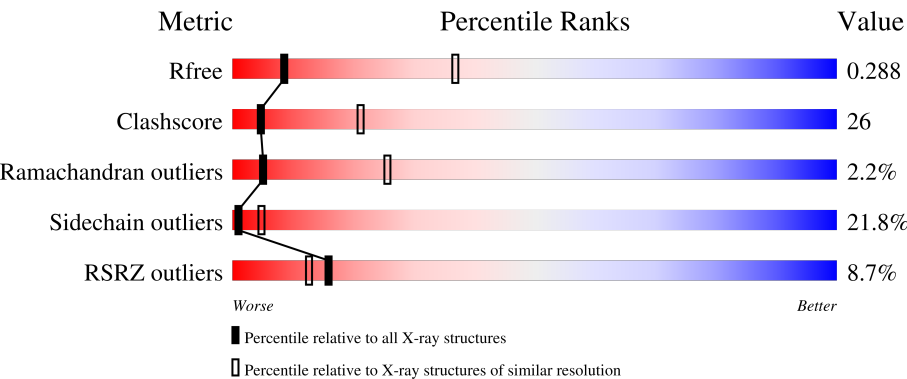
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.27 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.



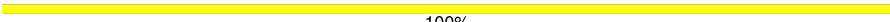
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)

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	253	4% 49% 35% 8% 7%
1	B	253	12% 42% 38% 12% 6%
2	C	2	100%
2	D	2	100%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	G	2	 50% 50%
2	H	2	 100%
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
4	IUM	B	2410	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3974 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	235	Total	C	N	O	S	0	0	0
			1858	1180	310	348	20			
1	B	237	Total	C	N	O	S	0	0	0
			1876	1191	313	352	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	778	LEU	-	expression tag	UNP P19711
A	779	LEU	-	expression tag	UNP P19711
A	780	GLU	-	expression tag	UNP P19711
A	788	ASP	ASN	conflict	UNP P19711
B	778	LEU	-	expression tag	UNP P19711
B	779	LEU	-	expression tag	UNP P19711
B	780	GLU	-	expression tag	UNP P19711
B	788	ASP	ASN	conflict	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			

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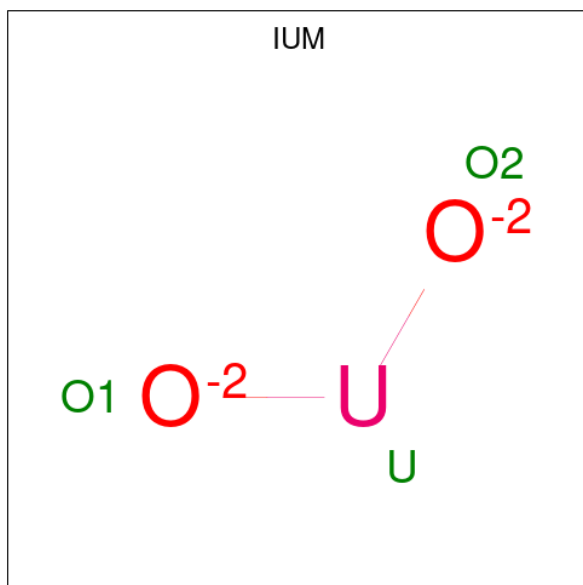
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Ca	0	0
			3	3		
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is URANYL (VI) ION (CCD ID: IUM) (formula: O₂U).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	U	0	0
			3	2	1		
4	B	1	Total	O	U	0	0
			3	2	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	U	0	0
			3	2	1		
4	B	1	Total	O	U	0	0
			3	2	1		

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:  100%

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:  50% 50%

MAG1
MAG2

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

Chain H:  100%

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	136.72Å 54.45Å 95.92Å 90.00° 92.23° 90.00°	Depositor
Resolution (Å)	47.97 – 3.27 47.97 – 3.27	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.97-3.27) 99.5 (47.97-3.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.246 , 0.289 0.246 , 0.288	Depositor DCC
R_{free} test set	556 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	3974	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IUM, CA, 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	0.75	1/1904 (0.1%)	1.01	8/2577 (0.3%)
1	B	0.69	1/1922 (0.1%)	1.04	7/2600 (0.3%)
All	All	0.72	2/3826 (0.1%)	1.02	15/5177 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	987	CYS	N-CA	6.27	1.53	1.45
1	B	882	VAL	CA-C	-5.05	1.49	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	986	ALA	N-CA-C	7.42	119.72	109.18
1	B	905	LYS	N-CA-C	-7.34	97.77	109.59
1	B	882	VAL	N-CA-C	-6.98	100.13	107.60
1	A	988	THR	N-CA-C	6.67	119.21	109.07
1	A	840	LEU	N-CA-C	-6.43	105.38	112.72
1	A	880	THR	N-CA-C	-6.34	105.47	113.72
1	B	798	CYS	N-CA-C	6.31	117.93	107.20
1	B	971	ARG	N-CA-C	-5.83	102.25	110.29
1	A	839	THR	N-CA-C	-5.72	101.55	110.42
1	A	988	THR	CB-CA-C	-5.56	98.50	110.45
1	B	873	CYS	CB-CA-C	-5.46	99.55	110.42
1	B	958	VAL	N-CA-C	5.30	115.35	108.35
1	B	949	CYS	N-CA-C	-5.29	101.67	109.86
1	A	958	VAL	N-CA-C	5.23	115.25	108.35
1	A	830	VAL	N-CA-C	-5.01	101.20	108.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1858	0	1792	80	2
1	B	1876	0	1816	123	1
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	1	0
2	H	28	0	25	0	0
2	I	28	0	25	3	0
2	J	28	0	25	0	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
4	B	12	0	0	2	1
All	All	3974	0	3808	201	2

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 (201) 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:976:ILE:HD11	1:B:991:TYR:CZ	1.22	1.69
1:B:976:ILE:CD1	1:B:991:TYR:CE1	1.94	1.50
1:B:976:ILE:CD1	1:B:991:TYR:CZ	1.96	1.48
1:B:976:ILE:HD11	1:B:991:TYR:CE1	1.59	1.27
1:B:976:ILE:HD12	1:B:991:TYR:CE1	1.71	1.18
1:B:951:ILE:HG23	1:B:956:VAL:HG11	1.30	1.14
1:B:951:ILE:CG2	1:B:956:VAL:HG11	1.78	1.11
1:B:976:ILE:HD11	1:B:991:TYR:CE2	1.88	1.08
1:B:791:PHE:O	1:B:857:ARG:NH2	1.93	1.02
1:A:923:GLU:OE2	1:A:927:ARG:NH2	1.96	0.98
1:B:849:ARG:NH1	1:B:851:SER:HB2	1.80	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:850:ARG:NH2	1:B:852:LYS:O	2.01	0.93
1:A:935:ASN:ND2	1:A:961:MET:SD	2.42	0.92
1:B:790:ASN:O	1:B:790:ASN:ND2	2.06	0.88
1:B:877:GLY:HA3	1:B:880:THR:HG23	1.55	0.88
1:B:968:MET:HE3	1:B:1000:PHE:CE1	2.09	0.87
1:B:983:GLU:N	1:B:983:GLU:OE1	2.09	0.85
1:B:976:ILE:HD12	1:B:991:TYR:HE1	1.43	0.84
1:A:994:THR:N	1:A:1015:GLU:O	2.10	0.84
1:B:850:ARG:HG3	1:B:854:PHE:HE1	1.43	0.83
2:I:2:NAG:C8	2:I:2:NAG:H3	2.10	0.82
1:A:987:CYS:SG	1:B:987:CYS:O	2.38	0.82
1:B:974:GLU:OE1	4:B:2410:IUM:O2	1.97	0.82
1:B:951:ILE:HG22	1:B:956:VAL:HG11	1.62	0.81
1:A:906:GLU:OE2	1:A:953:LYS:NZ	2.14	0.80
1:B:857:ARG:HH11	1:B:857:ARG:HG3	1.45	0.80
1:B:849:ARG:CZ	1:B:851:SER:HB2	2.10	0.80
1:B:850:ARG:HG3	1:B:854:PHE:CE1	2.16	0.80
1:A:939:VAL:HG11	1:A:969:PRO:HD3	1.63	0.79
1:B:976:ILE:CD1	1:B:991:TYR:OH	2.30	0.79
1:B:976:ILE:CG1	1:B:991:TYR:CE1	2.65	0.79
1:B:962:ASP:OD2	1:B:964:LYS:HG3	1.83	0.78
2:I:2:NAG:H3	2:I:2:NAG:H83	1.64	0.78
1:B:787:MET:HG3	1:B:791:PHE:CD2	2.19	0.78
1:A:994:THR:OG1	1:A:1000:PHE:CE2	2.38	0.77
1:A:877:GLY:O	1:A:880:THR:OG1	2.07	0.73
1:B:951:ILE:HD12	1:B:952:GLY:H	1.52	0.73
1:B:805:ARG:N	1:B:805:ARG:HD3	2.05	0.71
1:B:889:TYR:HA	1:B:927:ARG:HD3	1.72	0.71
1:B:908:GLU:OE2	4:B:2411:IUM:U	1.69	0.71
1:B:791:PHE:CD1	1:B:792:GLU:N	2.58	0.71
1:B:877:GLY:CA	1:B:880:THR:HG23	2.21	0.70
1:A:939:VAL:CG1	1:A:969:PRO:HD3	2.22	0.70
1:B:822:CYS:CB	1:B:877:GLY:HA2	2.20	0.70
1:B:951:ILE:HD12	1:B:952:GLY:N	2.06	0.69
1:B:809:ASN:HD22	2:G:1:NAG:H83	1.56	0.68
1:B:976:ILE:HG13	1:B:991:TYR:CD1	2.28	0.68
1:B:788:ASP:OD1	1:B:789:ASP:N	2.28	0.67
1:A:835:PHE:CE1	1:A:836:ASN:O	2.48	0.66
1:B:962:ASP:OD2	1:B:964:LYS:CG	2.44	0.66
1:B:933:SER:OG	1:B:935:ASN:N	2.28	0.65
1:B:975:ILE:HD12	1:B:975:ILE:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:LEU:HD22	1:A:1022:LEU:N	2.12	0.65
1:A:919:LYS:NZ	1:A:920:LEU:O	2.30	0.64
1:B:889:TYR:OH	1:B:894:ILE:HD11	1.97	0.63
1:B:946:THR:HG22	1:B:959:ILE:HD13	1.82	0.62
1:B:945:GLY:HA3	1:B:957:GLN:HG2	1.81	0.62
1:B:907:SER:HB2	1:B:913:TYR:CD1	2.34	0.62
1:B:968:MET:CE	1:B:1000:PHE:CE1	2.82	0.62
1:B:1009:GLN:HG3	1:B:1011:MET:HE3	1.83	0.61
1:B:822:CYS:HB2	1:B:877:GLY:HA2	1.84	0.60
1:B:937:GLU:HA	1:B:937:GLU:OE1	2.00	0.59
1:A:889:TYR:CZ	1:A:894:ILE:HD11	2.37	0.59
1:B:1005:SER:O	1:B:1008:GLN:NE2	2.35	0.59
1:A:930:ASP:OD2	1:A:932:THR:HG23	2.03	0.59
1:A:904:PHE:HD1	1:A:954:THR:HG21	1.68	0.58
1:B:857:ARG:HG3	1:B:857:ARG:NH1	2.17	0.58
1:B:994:THR:N	1:B:1015:GLU:O	2.35	0.58
1:B:1011:MET:HA	1:B:1011:MET:HE2	1.84	0.58
1:A:840:LEU:HD22	1:A:840:LEU:N	2.19	0.57
1:A:850:ARG:NE	1:A:852:LYS:O	2.34	0.57
1:A:923:GLU:CD	1:A:927:ARG:HH21	2.05	0.57
1:A:836:ASN:HB3	1:A:839:THR:O	2.05	0.56
1:A:899:TRP:CD2	1:A:915:ILE:HD13	2.40	0.56
1:A:939:VAL:HG21	1:A:995:LEU:CD2	2.35	0.56
1:A:1013:LYS:HD3	1:B:1006:TYR:CE1	2.41	0.55
1:B:879:TRP:O	1:B:879:TRP:HE3	1.89	0.55
1:B:875:LEU:HB2	1:B:882:VAL:CG2	2.37	0.55
1:A:840:LEU:N	1:A:840:LEU:CD2	2.69	0.55
1:B:917:LYS:HB3	1:B:926:TYR:HB3	1.87	0.55
1:B:950:LYS:CD	1:B:971:ARG:NH2	2.70	0.54
1:A:829:THR:HG22	1:A:849:ARG:HG2	1.88	0.54
1:B:976:ILE:HD12	1:B:991:TYR:CZ	2.06	0.53
1:B:907:SER:O	1:B:907:SER:OG	2.19	0.53
1:A:894:ILE:HG23	1:A:918:CYS:HB3	1.89	0.53
1:B:850:ARG:CG	1:B:854:PHE:CE1	2.91	0.53
1:B:873:CYS:HB3	1:B:881:CYS:HA	1.90	0.53
1:A:939:VAL:CG2	1:A:995:LEU:CD2	2.87	0.52
1:B:1022:LEU:HD12	1:B:1022:LEU:N	2.24	0.52
1:B:968:MET:HE3	1:B:1000:PHE:HE1	1.67	0.52
1:B:822:CYS:HB3	1:B:877:GLY:HA2	1.90	0.52
1:B:976:ILE:CG1	1:B:991:TYR:CD1	2.92	0.52
1:B:976:ILE:HG13	1:B:976:ILE:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:789:ASP:HA	1:B:850:ARG:NH1	2.25	0.52
1:B:976:ILE:HG13	1:B:991:TYR:CE1	2.39	0.52
1:A:946:THR:HG23	1:A:959:ILE:HD13	1.91	0.51
1:A:1013:LYS:HD3	1:B:1006:TYR:CZ	2.46	0.51
1:B:885:ASP:N	1:B:885:ASP:OD1	2.43	0.51
1:A:1006:TYR:CZ	1:B:1013:LYS:HG2	2.46	0.51
1:B:787:MET:HE3	1:B:848:TYR:HB3	1.92	0.51
1:B:910:LEU:HD23	1:B:951:ILE:HD11	1.91	0.51
1:B:951:ILE:HG22	1:B:956:VAL:CG1	2.37	0.51
1:A:858:GLN:CG	1:A:859:GLY:H	2.23	0.51
1:B:950:LYS:HD2	1:B:971:ARG:NH2	2.26	0.51
1:B:963:THR:O	1:B:997:ASN:ND2	2.43	0.50
1:B:879:TRP:O	1:B:879:TRP:CE3	2.66	0.49
1:A:994:THR:HG22	1:A:995:LEU:O	2.12	0.49
1:A:810:THR:OG1	1:A:821:VAL:O	2.29	0.49
1:B:907:SER:HB2	1:B:913:TYR:HB2	1.95	0.49
1:B:972:PRO:HD3	1:B:1000:PHE:CG	2.48	0.49
1:B:798:CYS:C	1:B:800:ALA:N	2.70	0.48
1:B:911:PRO:HG3	1:B:936:ARG:NH2	2.27	0.48
1:B:803:ILE:HD12	1:B:803:ILE:C	2.39	0.48
1:A:810:THR:OG1	1:A:810:THR:O	2.32	0.48
1:A:994:THR:OG1	1:A:1000:PHE:HE2	1.95	0.48
1:A:839:THR:C	1:A:840:LEU:HD22	2.39	0.47
1:A:988:THR:O	1:A:1021:ASP:N	2.44	0.47
1:B:1006:TYR:HD1	1:B:1007:PHE:CD1	2.32	0.47
1:B:996:LYS:O	1:B:997:ASN:HB2	2.14	0.47
1:A:818:PHE:CE1	1:A:830:VAL:HG21	2.50	0.47
1:A:959:ILE:HD12	1:A:960:ALA:H	1.79	0.47
1:A:960:ALA:HB2	1:A:995:LEU:HG	1.97	0.46
1:A:1003:ARG:NH1	1:A:1009:GLN:HA	2.30	0.46
1:B:1007:PHE:CD1	1:B:1007:PHE:N	2.81	0.46
2:I:2:NAG:C1	2:I:2:NAG:H82	2.46	0.46
1:B:923:GLU:CD	1:B:927:ARG:HH12	2.23	0.46
1:B:805:ARG:N	1:B:805:ARG:CD	2.78	0.46
1:B:968:MET:HG2	1:B:998:LYS:HB3	1.98	0.46
1:B:966:GLY:O	1:B:998:LYS:HA	2.16	0.46
1:B:973:TYR:CD1	1:B:973:TYR:C	2.93	0.46
1:A:818:PHE:CE2	1:A:830:VAL:HG11	2.51	0.46
1:A:904:PHE:CD1	1:A:954:THR:HG21	2.50	0.46
1:A:972:PRO:CG	1:A:975:ILE:HD11	2.46	0.46
1:B:791:PHE:HD1	1:B:792:GLU:N	2.10	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:968:MET:CE	1:B:1000:PHE:CZ	2.99	0.46
1:A:1015:GLU:C	1:A:1016:TYR:CD1	2.94	0.45
1:A:987:CYS:SG	1:B:987:CYS:C	3.00	0.45
1:A:1016:TYR:CD1	1:A:1016:TYR:N	2.82	0.45
1:B:989:PHE:CD2	1:B:1018:TYR:HD2	2.35	0.45
1:B:803:ILE:HD11	1:B:805:ARG:CZ	2.46	0.45
1:A:879:TRP:HE3	1:A:879:TRP:O	2.00	0.45
1:A:1013:LYS:HE2	1:A:1018:TYR:OH	2.16	0.45
1:B:870:LEU:HB3	1:B:887:LEU:HD13	1.98	0.45
1:B:930:ASP:OD2	1:B:932:THR:HG23	2.17	0.45
1:A:956:VAL:HG12	1:A:957:GLN:N	2.31	0.45
1:A:994:THR:HG23	1:A:995:LEU:N	2.32	0.44
1:B:940:ALA:O	1:B:958:VAL:HG23	2.17	0.44
1:A:956:VAL:HG12	1:A:957:GLN:H	1.83	0.44
1:B:791:PHE:CD1	1:B:791:PHE:C	2.95	0.44
1:A:1013:LYS:HB3	1:A:1013:LYS:HE3	1.68	0.44
1:B:1007:PHE:N	1:B:1007:PHE:HD1	2.16	0.44
1:A:946:THR:CG2	1:A:959:ILE:HD13	2.48	0.44
1:A:1022:LEU:N	1:A:1022:LEU:CD2	2.80	0.44
1:B:917:LYS:CB	1:B:926:TYR:HB3	2.47	0.44
1:B:954:THR:O	1:B:956:VAL:HG12	2.18	0.43
1:B:972:PRO:HD3	1:B:1000:PHE:HB3	1.99	0.43
1:B:857:ARG:HH11	1:B:857:ARG:CG	2.25	0.43
1:B:965:LEU:HA	1:B:997:ASN:O	2.18	0.43
1:A:855:PRO:O	1:A:857:ARG:HG3	2.18	0.43
1:A:1011:MET:HE1	1:A:1020:PHE:HD2	1.83	0.43
1:A:1007:PHE:CD1	1:A:1007:PHE:N	2.86	0.43
1:B:1006:TYR:C	1:B:1006:TYR:CD1	2.96	0.43
1:B:1006:TYR:CD1	1:B:1007:PHE:CD1	3.06	0.43
1:A:796:CYS:SG	1:A:802:PRO:HB3	2.58	0.43
1:B:803:ILE:HD12	1:B:803:ILE:O	2.19	0.43
1:A:939:VAL:HG22	1:A:958:VAL:CG2	2.49	0.43
1:A:1004:ASP:O	1:A:1008:GLN:HA	2.19	0.43
1:A:797:PRO:O	1:A:799:ASP:N	2.51	0.42
1:A:994:THR:HG21	1:A:998:LYS:O	2.19	0.42
1:B:973:TYR:O	1:B:973:TYR:HD1	2.03	0.42
1:B:787:MET:CG	1:B:791:PHE:CD2	2.98	0.42
1:A:825:GLY:HA2	1:A:853:PRO:HB3	2.01	0.42
1:A:994:THR:CG2	1:A:995:LEU:N	2.82	0.42
1:A:966:GLY:O	1:A:998:LYS:HA	2.19	0.42
1:B:950:LYS:HD3	1:B:971:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:CYS:HA	1:A:918:CYS:HA	2.01	0.42
1:A:939:VAL:CG2	1:A:995:LEU:HD21	2.49	0.42
1:B:794:GLY:HA3	1:B:818:PHE:CZ	2.54	0.42
1:A:835:PHE:CD1	1:A:836:ASN:N	2.88	0.42
1:A:910:LEU:CD2	1:A:951:ILE:HG21	2.50	0.42
1:A:878:ASN:OD1	1:A:878:ASN:N	2.43	0.42
1:A:878:ASN:O	1:A:879:TRP:CD1	2.73	0.42
1:B:880:THR:O	1:B:880:THR:OG1	2.26	0.42
1:B:945:GLY:HA2	1:B:959:ILE:HG12	2.01	0.42
1:A:791:PHE:CZ	1:A:793:PHE:O	2.73	0.41
1:A:951:ILE:HG12	1:A:956:VAL:HG21	2.02	0.41
1:A:1004:ASP:HB2	1:A:1011:MET:HE2	2.01	0.41
1:B:785:VAL:HG12	1:B:848:TYR:HA	2.03	0.41
1:A:787:MET:HE3	1:A:850:ARG:HB2	2.02	0.41
1:B:857:ARG:NH1	1:B:857:ARG:CG	2.83	0.41
1:A:939:VAL:HG23	1:A:995:LEU:HD21	2.03	0.41
1:A:1011:MET:HE3	1:A:1011:MET:HB2	1.80	0.40
1:A:895:GLU:OE1	1:A:896:SER:HB3	2.21	0.40
1:A:976:ILE:HG12	1:A:991:TYR:CE1	2.56	0.40
1:B:906:GLU:O	1:B:913:TYR:HE1	2.04	0.40
1:B:916:GLY:O	1:B:929:VAL:HG13	2.21	0.40
1:B:920:LEU:HD12	1:B:923:GLU:OE2	2.20	0.40
1:B:994:THR:HG22	1:B:995:LEU:O	2.21	0.40
1:A:818:PHE:CZ	1:A:830:VAL:HG21	2.56	0.40
1:B:819:GLN:HG2	1:B:821:VAL:HG12	2.02	0.40
1:B:894:ILE:HD12	1:B:894:ILE:N	2.36	0.40

All (2) 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)
1:A:1023:GLU:OE1	4:B:2410:IUM:O2[2_555]	1.67	0.53
1:A:792:GLU:OE2	1:B:805:ARG:NH1[4_545]	2.08	0.12

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	231/253 (91%)	200 (87%)	28 (12%)	3 (1%)	9	35
1	B	233/253 (92%)	195 (84%)	31 (13%)	7 (3%)	3	20
All	All	464/506 (92%)	395 (85%)	59 (13%)	10 (2%)	5	25

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	911	PRO
1	A	797	PRO
1	A	1014	GLY
1	B	799	ASP
1	B	809	ASN
1	B	884	GLY
1	B	914	PRO
1	A	945	GLY
1	B	855	PRO
1	B	853	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	208/225 (92%)	170 (82%)	38 (18%)	2	7
1	B	210/225 (93%)	157 (75%)	53 (25%)	0	2
All	All	418/450 (93%)	327 (78%)	91 (22%)	1	5

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	789	ASP
1	A	798	CYS

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Mol	Chain	Res	Type
1	A	799	ASP
1	A	811	THR
1	A	813	LEU
1	A	821	VAL
1	A	830	VAL
1	A	833	THR
1	A	838	ASP
1	A	840	LEU
1	A	844	VAL
1	A	846	ARG
1	A	856	HIS
1	A	861	ILE
1	A	870	LEU
1	A	878	ASN
1	A	903	GLN
1	A	915	ILE
1	A	920	LEU
1	A	927	ARG
1	A	929	VAL
1	A	930	ASP
1	A	933	SER
1	A	936	ARG
1	A	941	ILE
1	A	947	LEU
1	A	948	LYS
1	A	953	LYS
1	A	954	THR
1	A	971	ARG
1	A	976	ILE
1	A	978	SER
1	A	985	THR
1	A	994	THR
1	A	995	LEU
1	A	1012	LEU
1	A	1013	LYS
1	A	1022	LEU
1	B	785	VAL
1	B	787	MET
1	B	790	ASN
1	B	792	GLU
1	B	803	ILE
1	B	804	VAL

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Mol	Chain	Res	Type
1	B	805	ARG
1	B	810	THR
1	B	811	THR
1	B	813	LEU
1	B	821	VAL
1	B	831	SER
1	B	833	THR
1	B	840	LEU
1	B	843	THR
1	B	844	VAL
1	B	845	VAL
1	B	850	ARG
1	B	852	LYS
1	B	857	ARG
1	B	872	ASN
1	B	873	CYS
1	B	880	THR
1	B	888	LEU
1	B	890	LYS
1	B	895	GLU
1	B	900	CYS
1	B	912	HIS
1	B	915	ILE
1	B	917	LYS
1	B	923	GLU
1	B	924	THR
1	B	929	VAL
1	B	931	SER
1	B	937	GLU
1	B	939	VAL
1	B	942	VAL
1	B	944	GLN
1	B	946	THR
1	B	947	LEU
1	B	949	CYS
1	B	951	ILE
1	B	954	THR
1	B	956	VAL
1	B	958	VAL
1	B	965	LEU
1	B	970	CYS
1	B	975	ILE

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Mol	Chain	Res	Type
1	B	983	GLU
1	B	985	THR
1	B	994	THR
1	B	1007	PHE
1	B	1022	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	836	ASN
1	B	790	ASN
1	B	836	ASN
1	B	856	HIS
1	B	871	HIS
1	B	872	ASN
1	B	886	GLN
1	B	1009	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	0.49	0	17,19,21	1.96	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	2	2	14,14,15	0.74	0	17,19,21	1.36	1 (5%)
2	NAG	D	1	2,1	14,14,15	0.64	0	17,19,21	2.46	8 (47%)
2	NAG	D	2	2	14,14,15	0.80	0	17,19,21	1.16	2 (11%)
2	NAG	E	1	2,1	14,14,15	0.49	0	17,19,21	1.73	6 (35%)
2	NAG	E	2	2	14,14,15	0.60	0	17,19,21	1.61	2 (11%)
2	NAG	F	1	2,1	14,14,15	0.60	0	17,19,21	1.51	3 (17%)
2	NAG	F	2	2	14,14,15	0.44	0	17,19,21	2.55	2 (11%)
2	NAG	G	1	2,1	14,14,15	0.47	0	17,19,21	2.76	8 (47%)
2	NAG	G	2	2	14,14,15	0.40	0	17,19,21	2.43	3 (17%)
2	NAG	H	1	2,1	14,14,15	0.48	0	17,19,21	1.74	5 (29%)
2	NAG	H	2	2	14,14,15	0.75	0	17,19,21	1.21	2 (11%)
2	NAG	I	1	2,1	14,14,15	0.61	0	17,19,21	2.05	4 (23%)
2	NAG	I	2	2	14,14,15	0.58	0	17,19,21	1.51	2 (11%)
2	NAG	J	1	2,1	14,14,15	0.56	0	17,19,21	1.70	5 (29%)
2	NAG	J	2	2	14,14,15	0.49	0	17,19,21	2.60	3 (17%)

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	-	0/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	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	-	2/6/23/26	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	-	3/6/23/26	0/1/1/1
2	NAG	H	2	2	-	1/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	I	2	2	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	J	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	2	NAG	C1-O5-C5	9.73	125.22	112.19
2	F	2	NAG	C1-O5-C5	9.49	124.91	112.19
2	G	2	NAG	C1-O5-C5	8.22	123.21	112.19
2	I	1	NAG	C4-C3-C2	5.60	119.22	111.02
2	D	1	NAG	C1-O5-C5	5.52	119.58	112.19
2	G	1	NAG	C1-O5-C5	5.33	119.33	112.19
2	C	1	NAG	C1-O5-C5	5.32	119.31	112.19
2	G	1	NAG	C1-C2-N2	5.31	118.80	110.43
2	D	1	NAG	O5-C1-C2	-4.91	103.69	111.29
2	E	2	NAG	C1-O5-C5	4.81	118.63	112.19
2	G	1	NAG	C8-C7-N2	4.42	123.45	116.12
2	H	1	NAG	C1-O5-C5	4.28	117.92	112.19
2	I	2	NAG	O5-C1-C2	-3.91	105.25	111.29
2	G	2	NAG	C4-C3-C2	-3.80	105.46	111.02
2	C	2	NAG	C1-O5-C5	3.73	117.19	112.19
2	I	1	NAG	C1-C2-N2	-3.59	104.77	110.43
2	D	1	NAG	C8-C7-N2	3.52	121.96	116.12
2	G	1	NAG	C2-N2-C7	3.40	127.46	122.90
2	F	1	NAG	C8-C7-N2	3.37	121.71	116.12
2	C	1	NAG	C8-C7-N2	3.32	121.62	116.12
2	I	2	NAG	C4-C3-C2	3.31	115.88	111.02
2	F	2	NAG	O5-C1-C2	3.28	116.37	111.29
2	J	1	NAG	C8-C7-N2	3.13	121.31	116.12
2	H	1	NAG	O5-C1-C2	-3.09	106.51	111.29
2	D	1	NAG	C4-C3-C2	3.03	115.47	111.02
2	H	1	NAG	C8-C7-N2	3.03	121.14	116.12
2	E	2	NAG	O5-C1-C2	3.03	115.97	111.29
2	G	1	NAG	O5-C1-C2	-2.99	106.67	111.29
2	D	2	NAG	C4-C3-C2	2.96	115.36	111.02
2	G	1	NAG	O7-C7-C8	-2.95	116.80	122.05
2	I	1	NAG	O5-C1-C2	-2.93	106.76	111.29
2	E	1	NAG	O5-C1-C2	2.89	115.77	111.29
2	J	1	NAG	C3-C4-C5	-2.85	105.07	110.23
2	E	1	NAG	C1-O5-C5	2.79	115.92	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NAG	O5-C5-C4	2.77	117.56	110.83
2	J	1	NAG	C1-O5-C5	2.70	115.80	112.19
2	F	1	NAG	C2-N2-C7	2.63	126.43	122.90
2	F	1	NAG	O7-C7-C8	-2.56	117.50	122.05
2	G	1	NAG	C3-C4-C5	2.53	114.83	110.23
2	H	2	NAG	C3-C4-C5	-2.51	105.68	110.23
2	C	1	NAG	O7-C7-C8	-2.50	117.61	122.05
2	C	1	NAG	C4-C3-C2	-2.49	107.36	111.02
2	D	1	NAG	O7-C7-C8	-2.47	117.66	122.05
2	J	1	NAG	O7-C7-C8	-2.46	117.68	122.05
2	D	1	NAG	C2-N2-C7	2.41	126.13	122.90
2	J	2	NAG	O5-C5-C4	2.35	116.55	110.83
2	D	1	NAG	C3-C4-C5	2.33	114.46	110.23
2	D	2	NAG	O5-C5-C4	-2.33	105.17	110.83
2	E	1	NAG	O5-C5-C4	-2.30	105.24	110.83
2	J	2	NAG	O5-C1-C2	2.30	114.84	111.29
2	H	1	NAG	O7-C7-C8	-2.29	117.98	122.05
2	J	1	NAG	C2-N2-C7	2.27	125.95	122.90
2	H	2	NAG	O5-C5-C4	-2.27	105.30	110.83
2	E	1	NAG	C2-N2-C7	2.25	125.92	122.90
2	H	1	NAG	C2-N2-C7	2.20	125.85	122.90
2	G	1	NAG	C4-C3-C2	-2.16	107.86	111.02
2	E	1	NAG	C8-C7-N2	2.15	119.69	116.12
2	E	1	NAG	C3-C4-C5	-2.11	106.41	110.23
2	I	1	NAG	C2-N2-C7	2.08	125.69	122.90
2	D	1	NAG	C1-C2-N2	2.07	113.69	110.43
2	C	1	NAG	C2-N2-C7	2.06	125.66	122.90

There are no chirality outliers.

All (40) torsion outliers are listed below:

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

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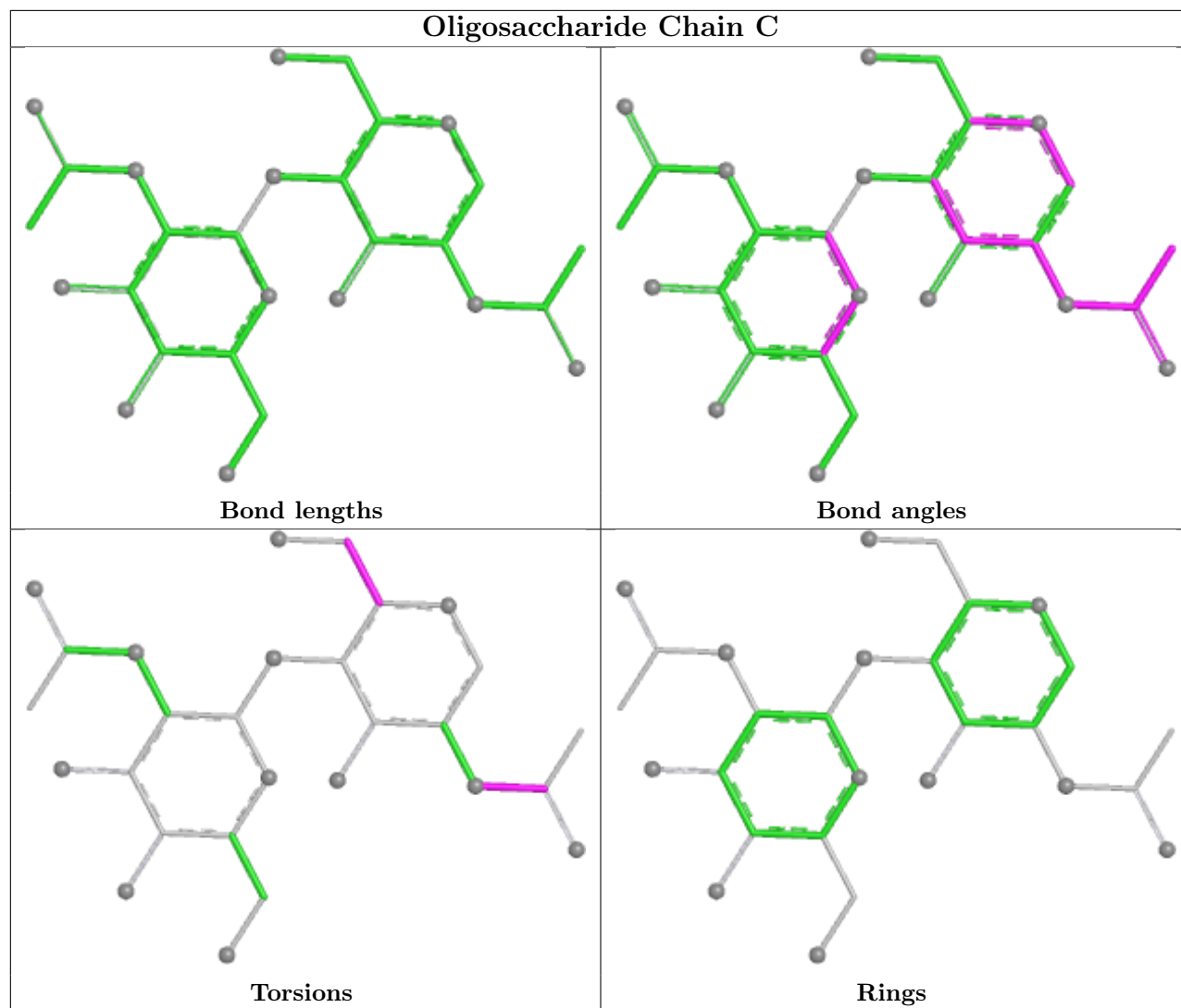
Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C4-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2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

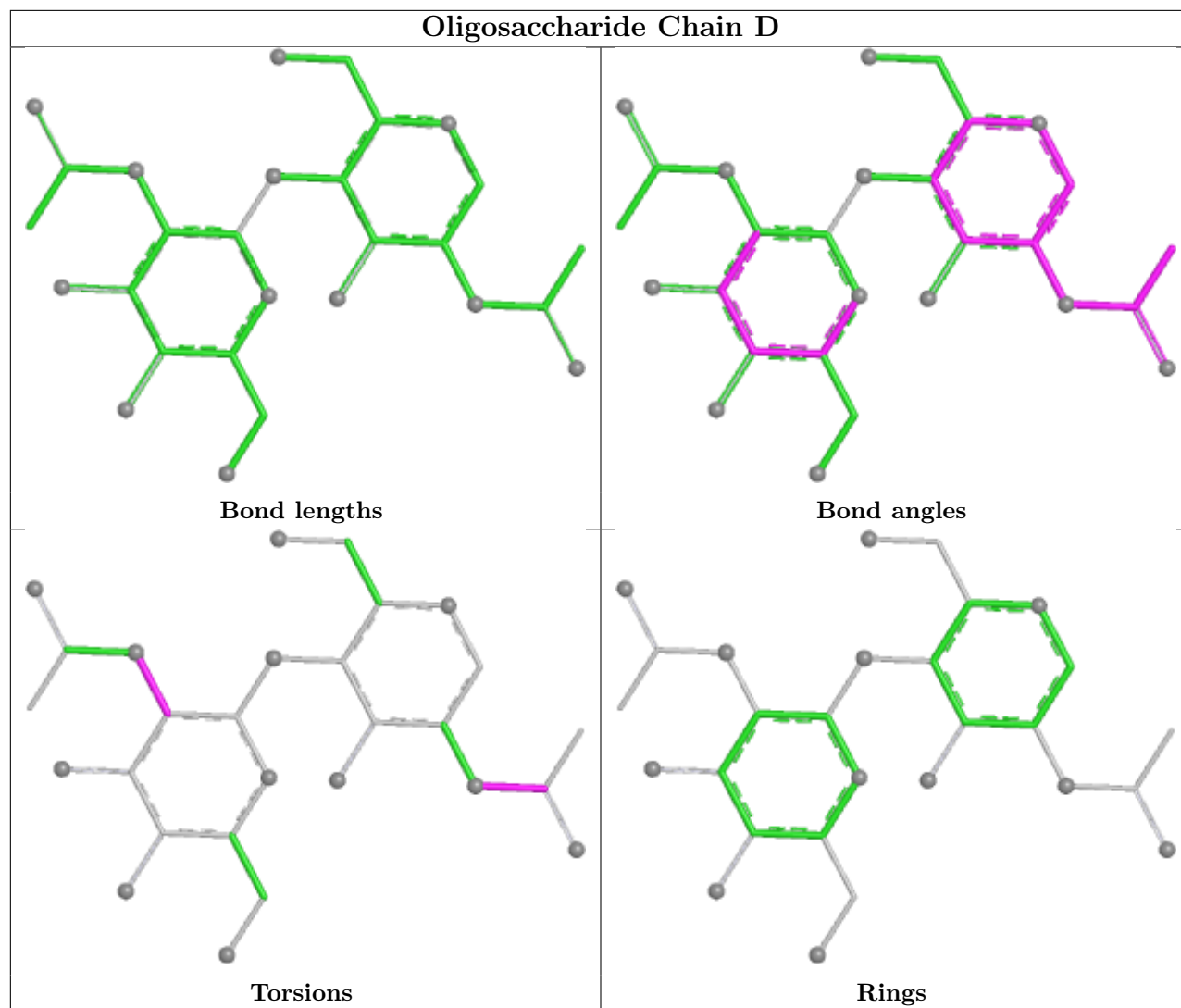
There are no ring outliers.

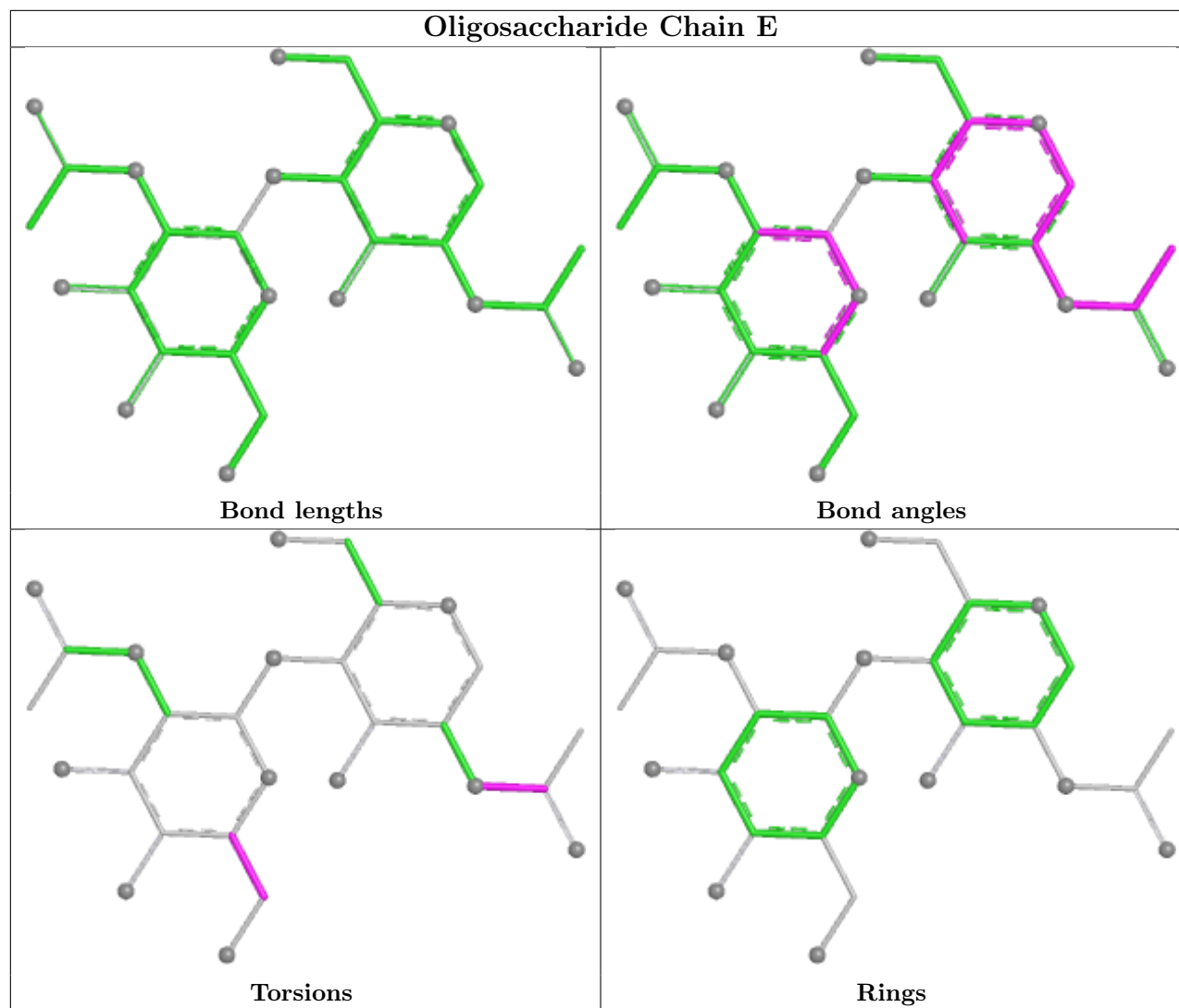
2 monomers are involved in 4 short contacts:

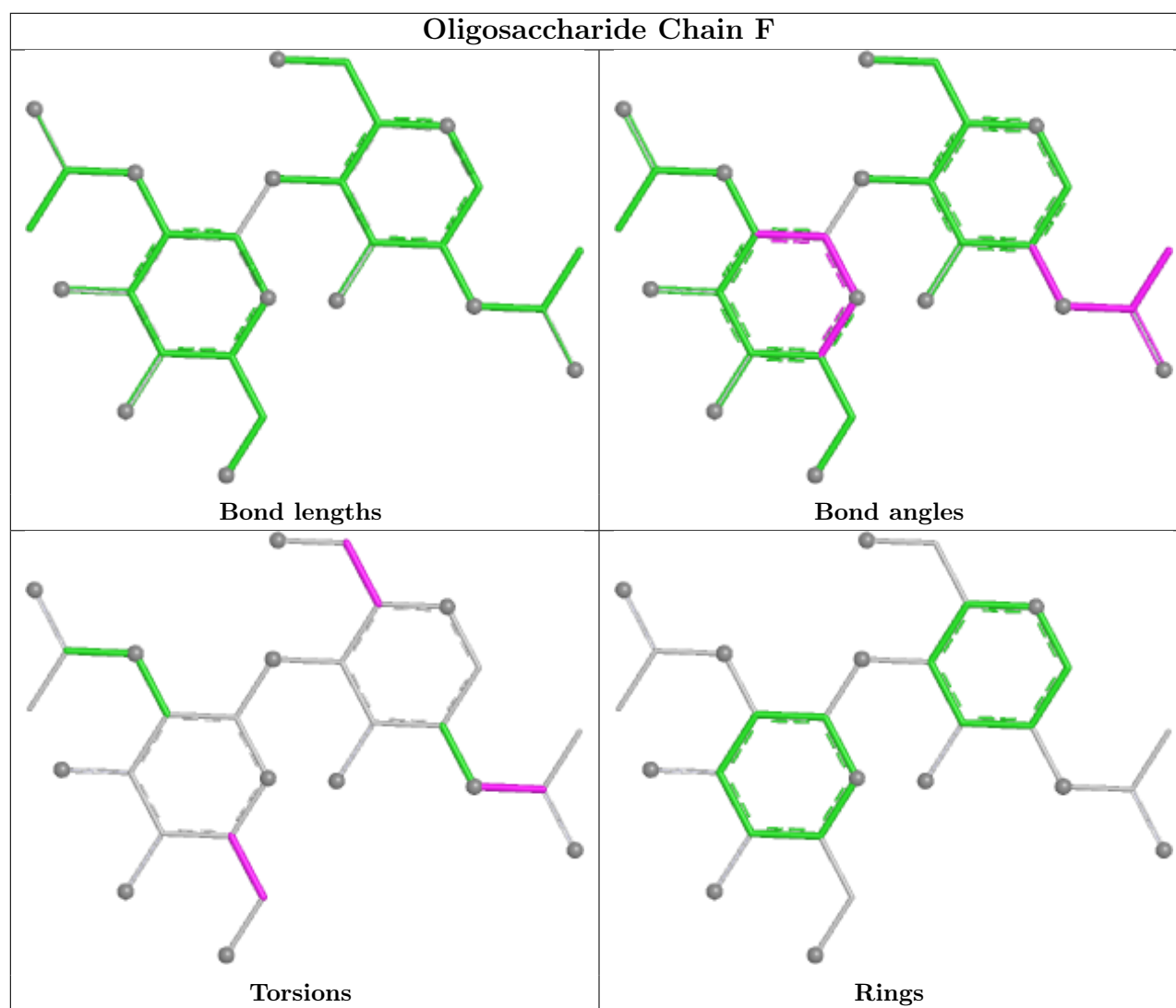
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	1	0
2	I	2	NAG	3	0

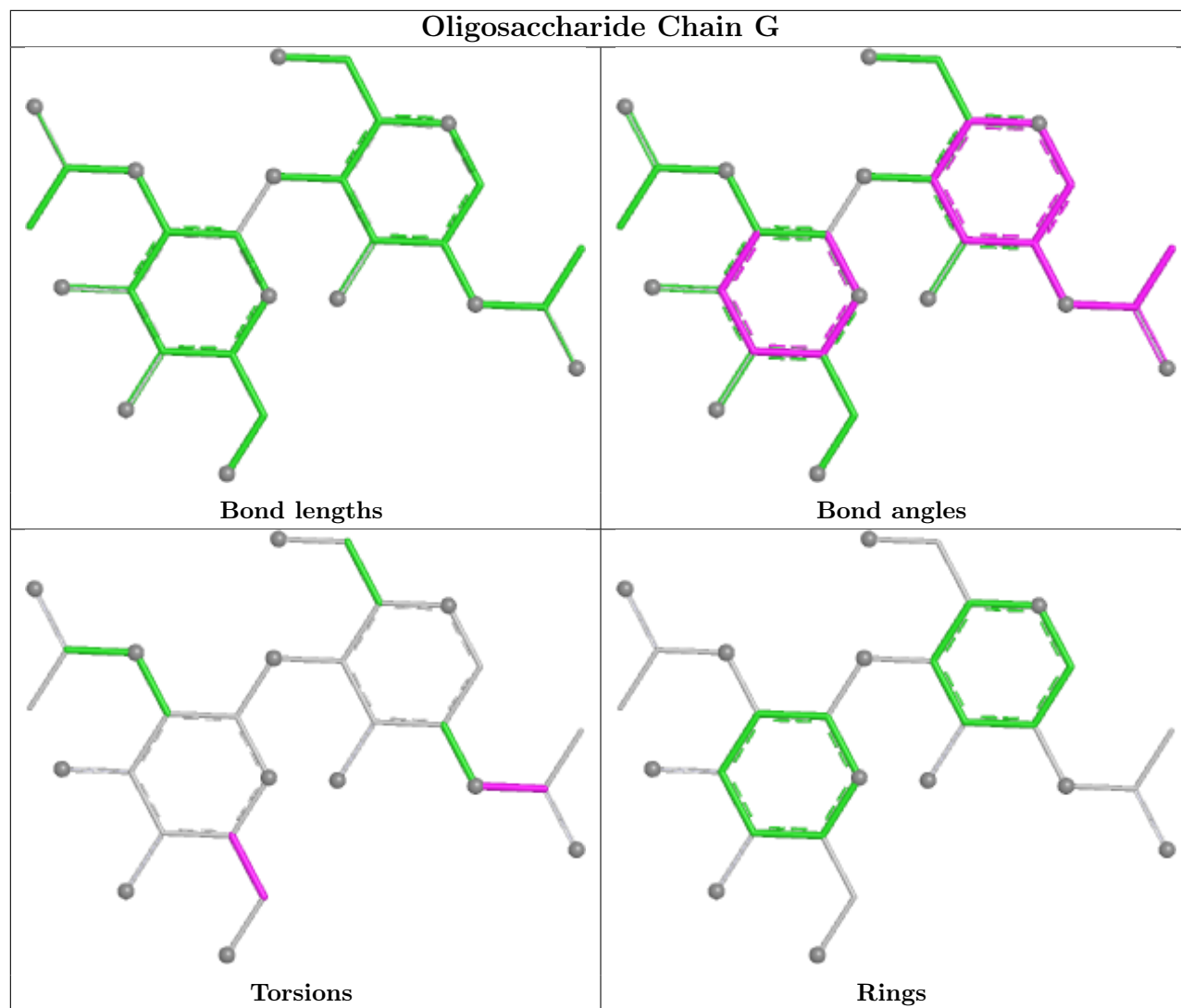
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

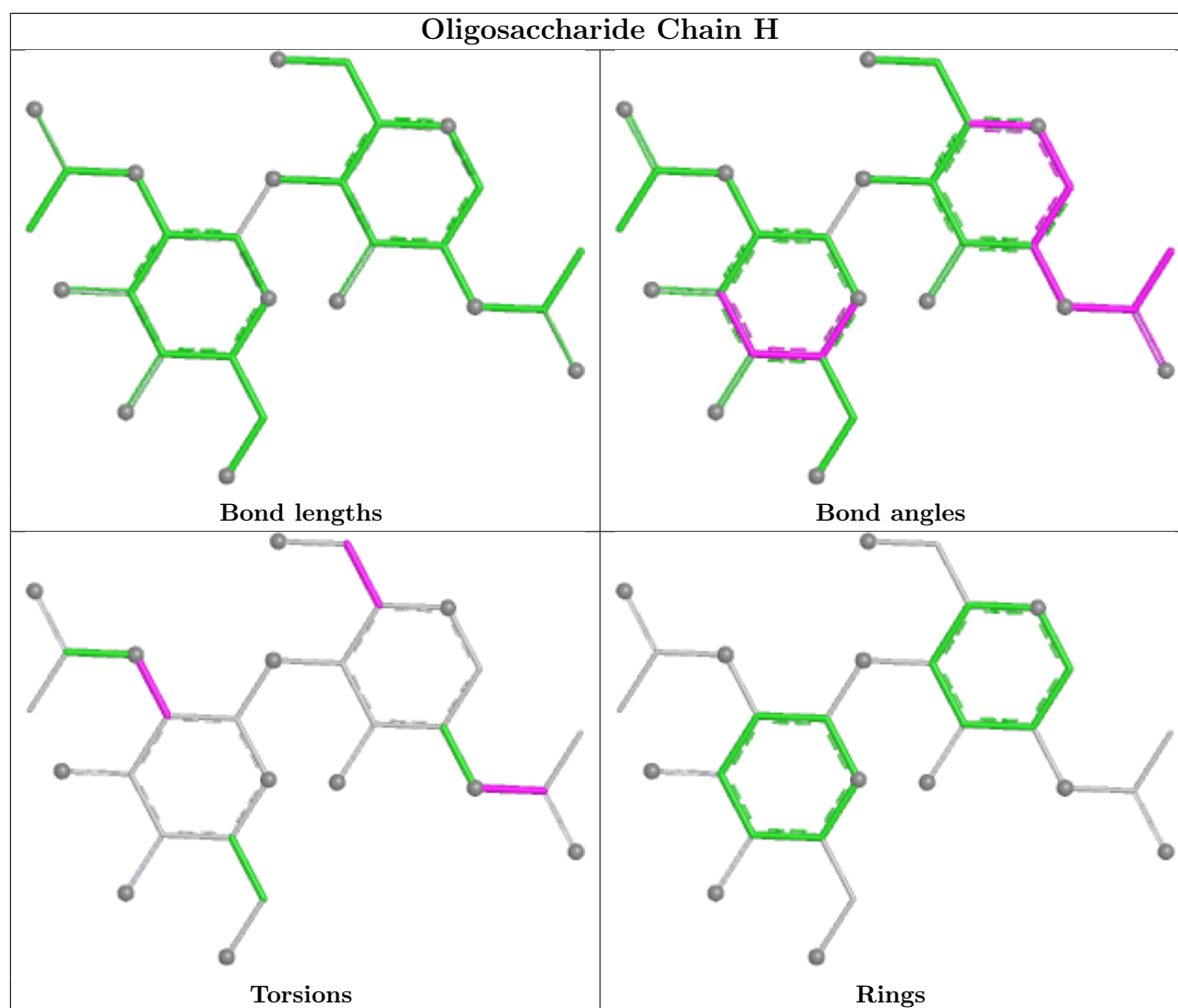


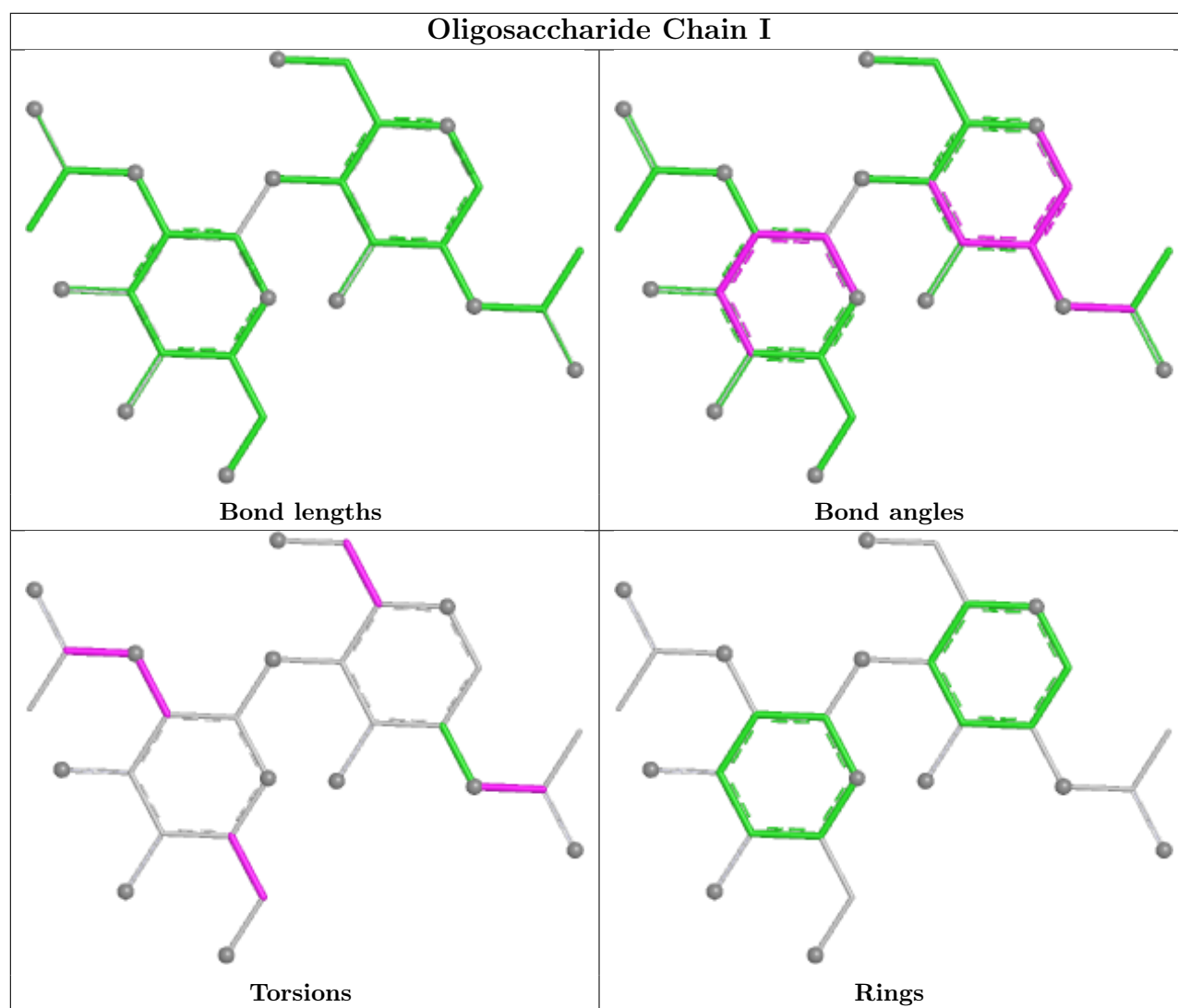


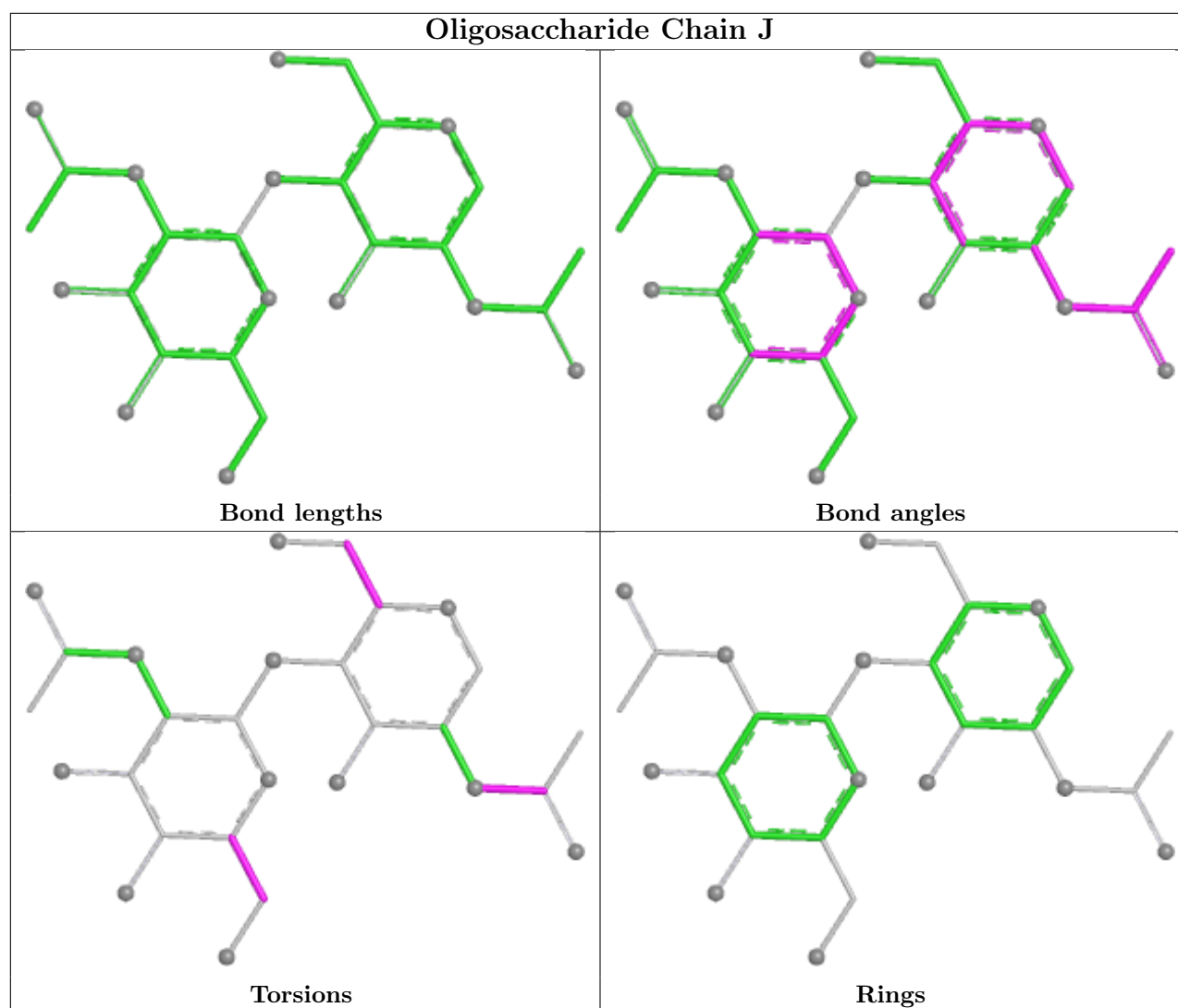












5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	IUM	B	2412	4	0,2,2	-	-	-		
4	IUM	B	2413	1	0,2,2	-	-	-		
4	IUM	B	2410	1	0,2,2	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	IUM	B	2411	1,4	0,2,2	-	-	-		

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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2410	IUM	1	1
4	B	2411	IUM	1	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

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	235/253 (92%)	0.55	11 (4%) 36 25	20, 36, 61, 83	0
1	B	237/253 (93%)	0.81	30 (12%) 8 7	19, 49, 87, 128	0
All	All	472/506 (93%)	0.68	41 (8%) 16 13	19, 43, 75, 128	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	944	GLN	4.7
1	A	987	CYS	4.3
1	B	985	THR	4.1
1	B	983	GLU	4.0
1	B	906	GLU	3.4
1	A	986	ALA	3.3
1	B	841	ALA	3.1
1	B	1022	LEU	2.8
1	B	834	SER	2.8
1	B	947	LEU	2.8
1	B	884	GLY	2.7
1	B	783	ASP	2.6
1	B	959	ILE	2.6
1	A	985	THR	2.6
1	B	840	LEU	2.5
1	B	858	GLN	2.5
1	B	784	VAL	2.5
1	B	943	PRO	2.4
1	B	837	MET	2.4
1	B	986	ALA	2.4
1	A	978	SER	2.4
1	A	963	THR	2.3
1	B	842	THR	2.3
1	B	799	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	835	PHE	2.3
1	B	942	VAL	2.3
1	B	1006	TYR	2.2
1	B	958	VAL	2.2
1	A	943	PRO	2.2
1	B	797	PRO	2.2
1	B	860	CYS	2.2
1	B	924	THR	2.2
1	A	1008	GLN	2.2
1	A	945	GLY	2.1
1	A	962	ASP	2.1
1	A	1011	MET	2.1
1	A	965	LEU	2.1
1	B	914	PRO	2.1
1	B	838	ASP	2.1
1	B	925	GLY	2.1
1	B	961	MET	2.0

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

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

6.3 Carbohydrates ⓘ

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.

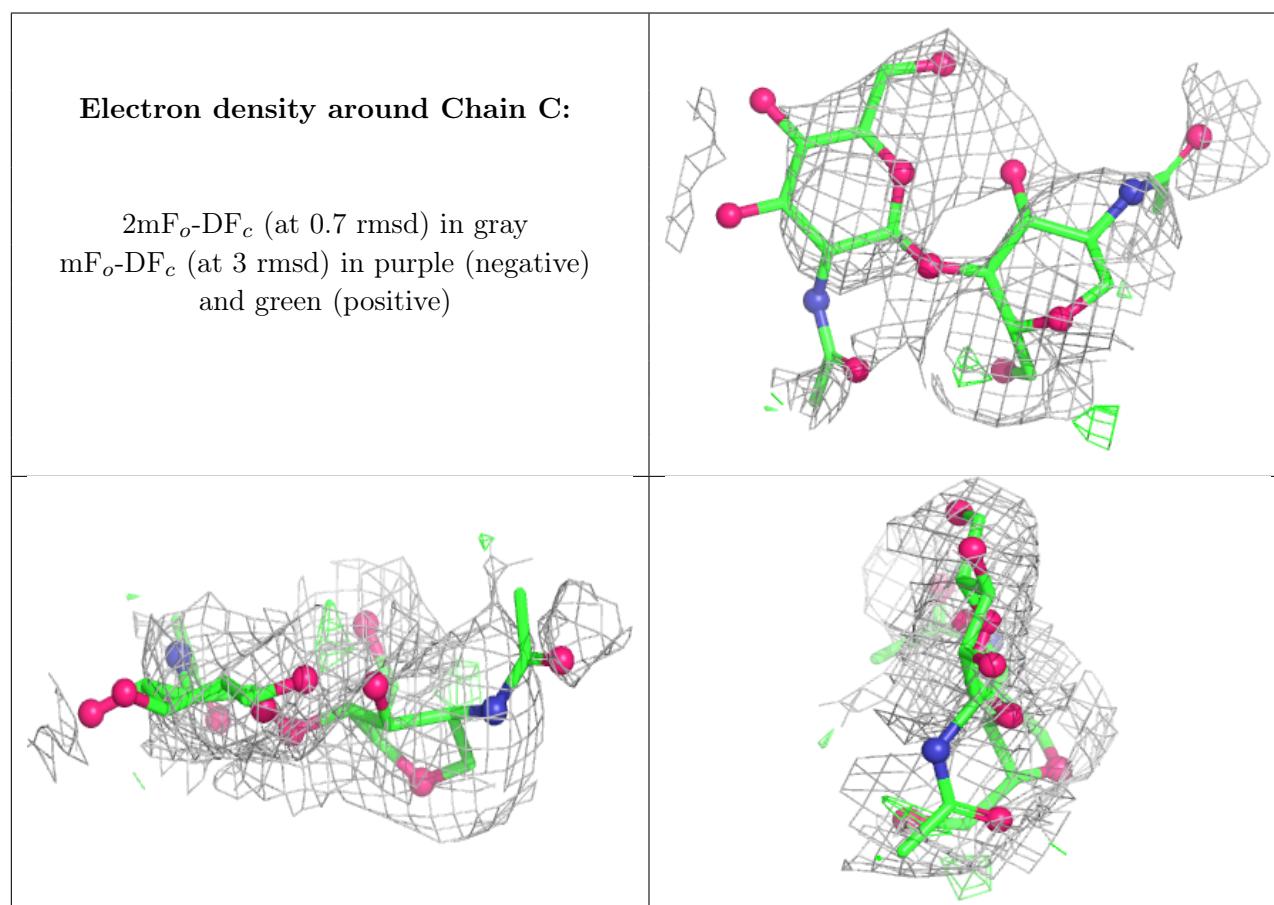
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	E	2	14/15	0.12	0.29	136,143,145,146	0
2	NAG	I	2	14/15	0.34	0.25	136,143,145,146	0
2	NAG	F	2	14/15	0.40	0.24	127,137,142,144	0
2	NAG	I	1	14/15	0.46	0.23	92,105,118,130	0
2	NAG	J	2	14/15	0.46	0.23	137,150,157,158	0
2	NAG	H	2	14/15	0.55	0.19	82,90,101,104	0
2	NAG	C	1	14/15	0.57	0.22	60,76,88,99	0
2	NAG	C	2	14/15	0.58	0.23	97,111,123,124	0
2	NAG	F	1	14/15	0.61	0.21	94,108,130,140	0
2	NAG	J	1	14/15	0.63	0.15	83,95,113,132	0
2	NAG	D	1	14/15	0.71	0.17	54,61,70,77	0

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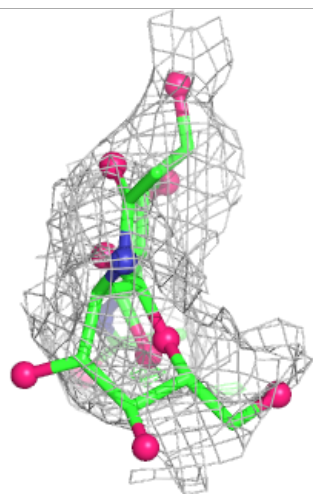
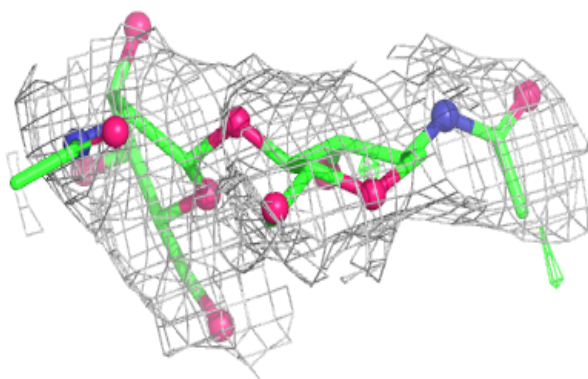
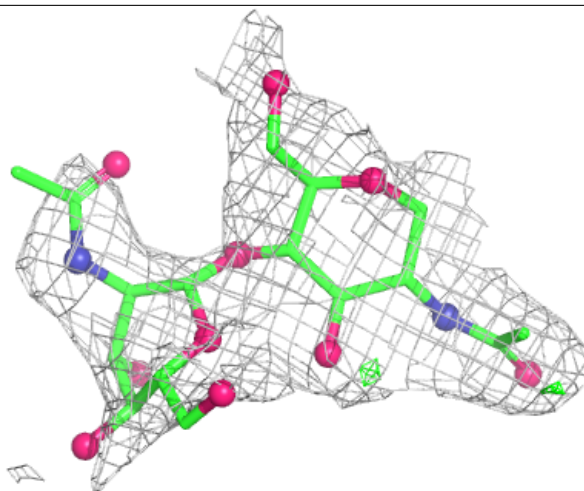
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	2	14/15	0.72	0.20	84,95,99,108	0
2	NAG	E	1	14/15	0.72	0.22	92,105,118,130	0
2	NAG	G	2	14/15	0.79	0.17	55,61,67,70	0
2	NAG	H	1	14/15	0.86	0.13	53,59,67,75	0
2	NAG	G	1	14/15	0.88	0.12	33,40,44,46	0

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.



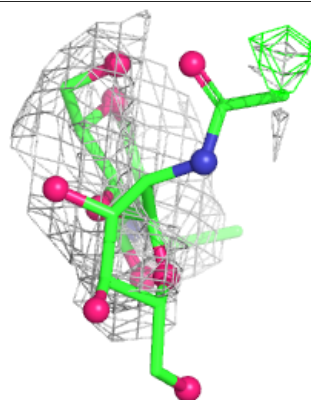
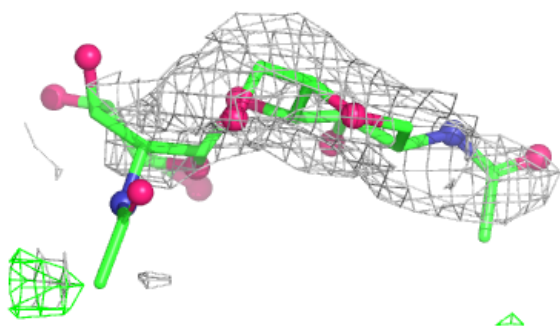
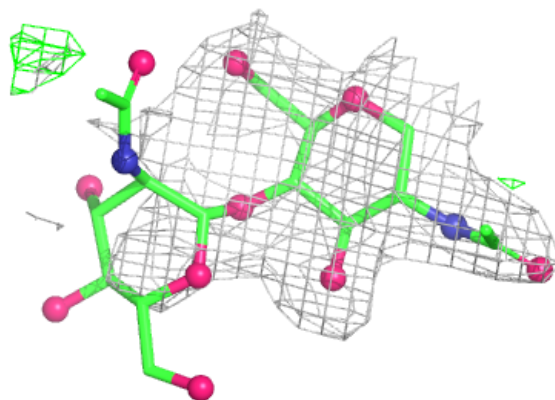
Electron density around Chain D:

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



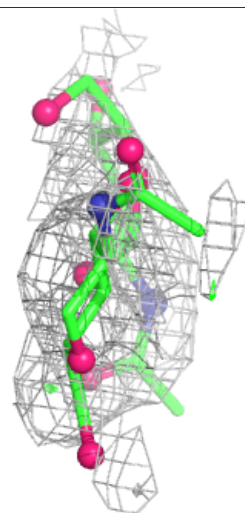
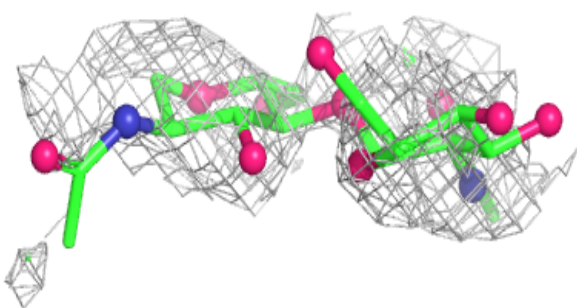
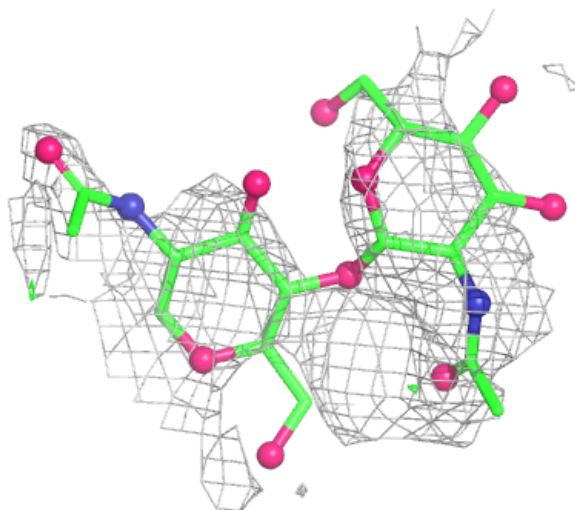
Electron density around Chain E:

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



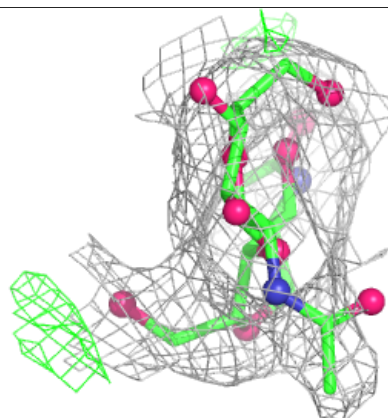
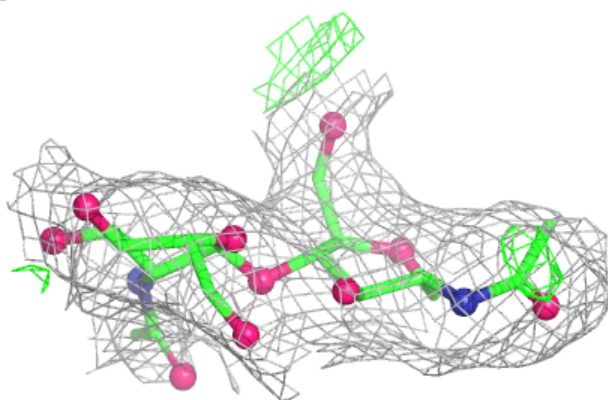
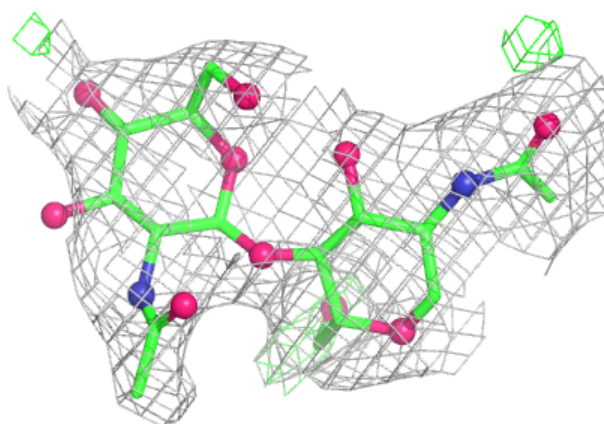
Electron density around Chain F:

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

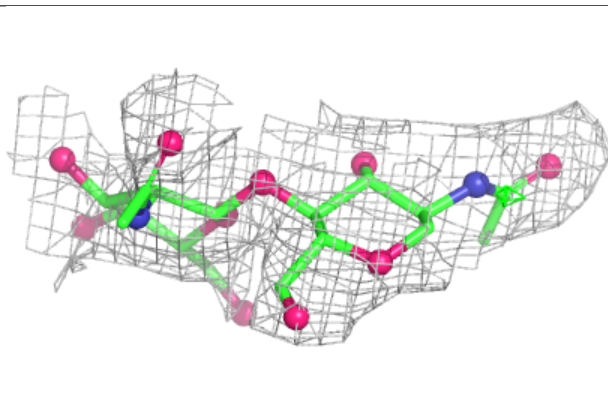
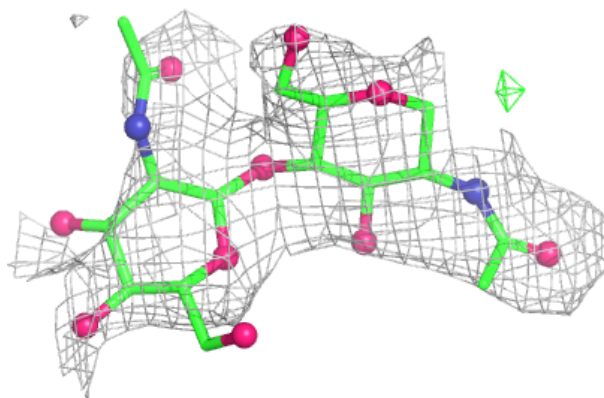


Electron density around Chain G:

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

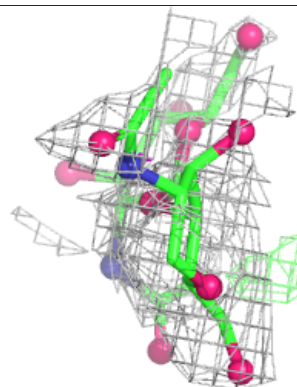
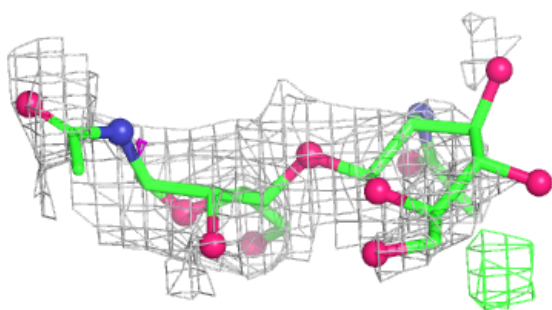
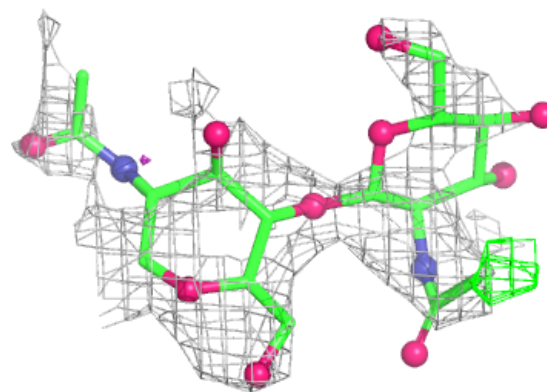
**Electron density around Chain H:**

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

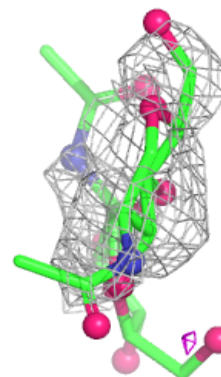
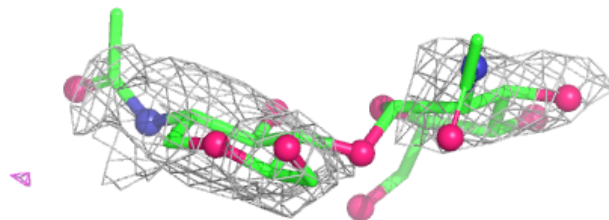
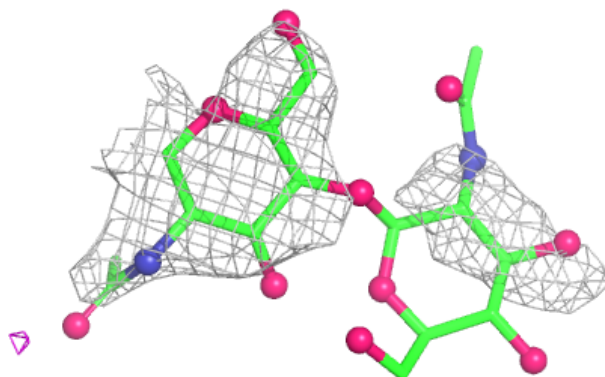


Electron density around Chain I:

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

**Electron density around Chain J:**

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



6.4 Ligands [i](#)

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
4	IUM	B	2413	3/3	0.75	0.23	63,63,65,116	3
3	CA	A	2410	1/1	0.91	0.07	14,14,14,14	0
3	CA	A	2411	1/1	0.94	0.06	30,30,30,30	0
3	CA	A	2409	1/1	0.94	0.08	41,41,41,41	0
4	IUM	B	2411	3/3	0.95	0.14	56,56,68,93	3
3	CA	B	2409	1/1	0.95	0.14	30,30,30,30	0
4	IUM	B	2412	3/3	0.97	0.10	60,60,72,80	3
4	IUM	B	2410	3/3	0.99	0.14	12,12,15,17	3

6.5 Other polymers [i](#)

There are no such residues in this entry.