



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 10:48 AM EST

PDB ID : 6NAJ
Title : Integrin AlphaVBeta3 ectodomain bound to Hr10 variant of the 10th domain of Fibronectin.
Authors : van Agthoven, J.; Arnaout, M.A.
Deposited on : 2018-12-05
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

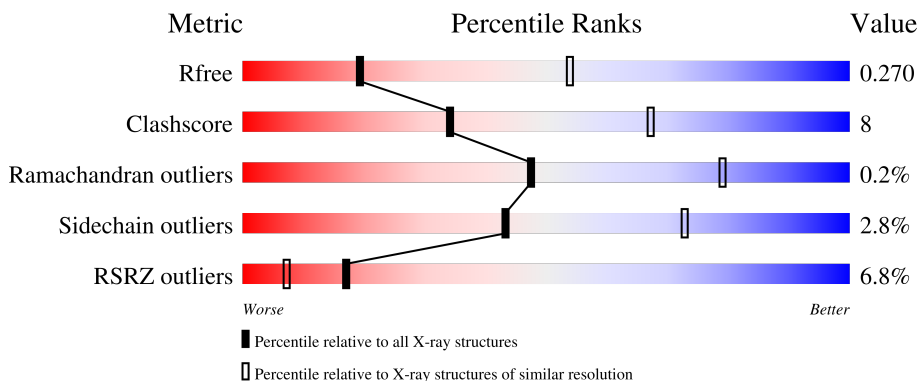
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.




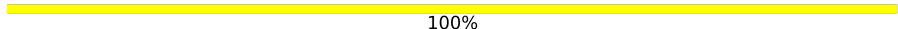

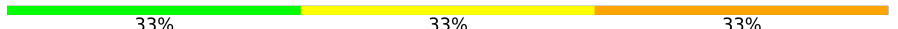
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	954	 2% 77% 18%
2	B	690	 10% 78% 21%
3	C	90	 36% 70% 26%
4	D	2	 100%
4	F	2	 50% 50%

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Mol	Chain	Length	Quality of chain
4	G	2	 100%
4	H	2	 50% 50%
4	J	2	 100%
5	E	6	 50% 17% 33%
6	I	3	 33% 33% 33%

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	NAG	F	2	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13500 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 Integrin alpha-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	920	7163	4535	1216	1377	35	0	0	0

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	690	5294	3250	904	1070	70	0	0	0

- Molecule 3 is a protein called Fibronectin, HR10 variant.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	90	680	433	110	137	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

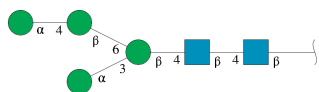
Chain	Residue	Modelled	Actual	Comment	Reference
C	1492	PRO	GLY	conflict	UNP P02751
C	?	-	SER	deletion	UNP P02751
C	1496	TRP	PRO	conflict	UNP P02751
C	1497	ASN	ALA	conflict	UNP P02751
C	1498	GLU	SER	conflict	UNP P02751
C	1499	GLY	SER	conflict	UNP P02751
C	1500	GLY	LYS	conflict	UNP P02751

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



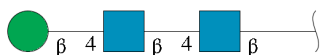
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	5	Total	Mn	0	0
			5	5		
8	B	3	Total	Mn	0	0
			3	3		

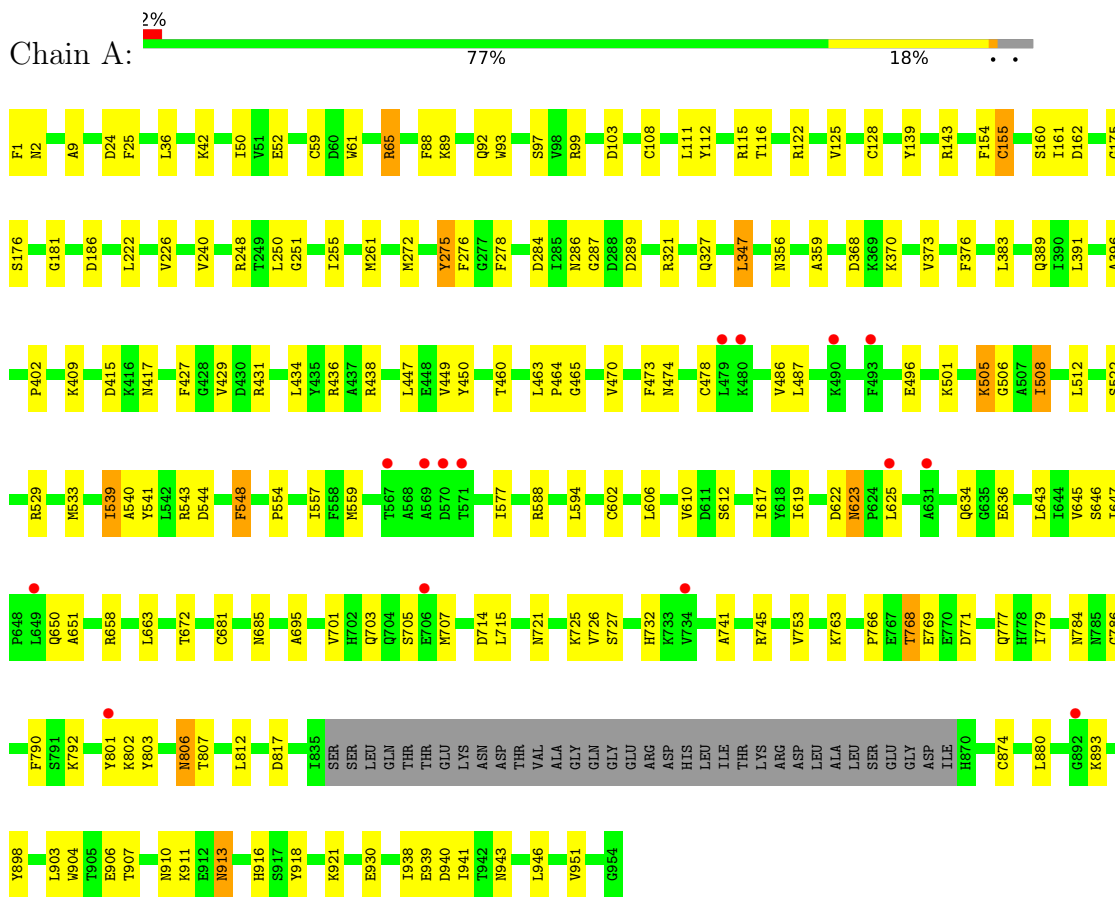
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	2	Total O 2 2	0	0
9	B	3	Total O 3 3	0	0
9	C	1	Total O 1 1	0	0

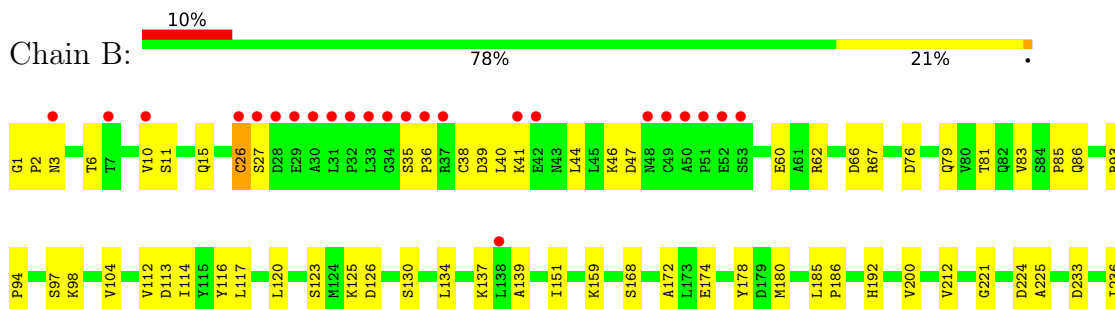
3 Residue-property plots [i](#)

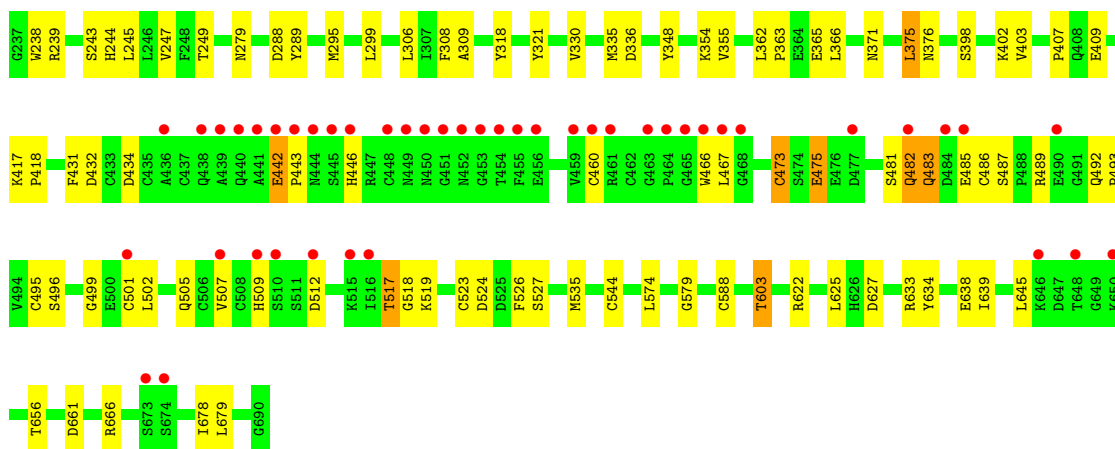
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

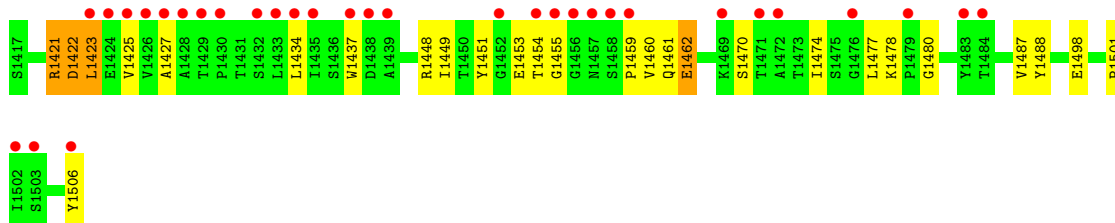


- Molecule 2: Integrin beta-3





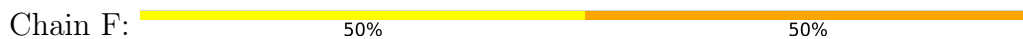
- Molecule 3: Fibronectin, HR10 variant



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



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



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




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

Chain H:  50% 50%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

- Molecule 5: alpha-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 17% 33%

MAG1
MAG2
BMA4
MAM5
MAM6

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 33% 33%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.71Å 129.71Å 308.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.62 – 3.10 49.62 – 3.10	Depositor EDS
% Data completeness (in resolution range)	90.9 (49.62-3.10) 90.9 (49.62-3.10)	Depositor EDS
R_{merge}	9.70	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.76 (at 3.12Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.238 , 0.268 0.239 , 0.270	Depositor DCC
R_{free} test set	2459 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	59.5	Xtrriage
Anisotropy	0.143	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	13500	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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: HRG, MN, MAN, NAG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/7319	0.50	0/9922
2	B	0.25	0/5390	0.51	0/7289
3	C	0.28	0/685	0.57	1/943 (0.1%)
All	All	0.25	0/13394	0.50	1/18154 (0.0%)

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	1
2	B	0	5
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1423	LEU	CA-CB-CG	5.88	128.82	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	539	ILE	Peptide
2	B	442	GLU	Peptide
2	B	481	SER	Peptide
2	B	482	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	B	496	SER	Peptide
2	B	76	ASP	Peptide

5.2 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	A	7163	0	6982	109	0
2	B	5294	0	5024	94	0
3	C	680	0	659	17	0
4	D	28	0	25	0	0
4	F	28	0	25	3	0
4	G	28	0	25	1	0
4	H	28	0	25	0	0
4	J	28	0	25	0	0
5	E	72	0	61	1	0
6	I	39	0	34	1	0
7	A	70	0	65	1	0
7	B	28	0	26	1	0
8	A	5	0	0	0	0
8	B	3	0	0	0	0
9	A	2	0	0	0	0
9	B	3	0	0	0	0
9	C	1	0	0	0	0
All	All	13500	0	12976	221	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 8.

All (221) 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)
2:B:375:LEU:HD13	2:B:633:ARG:HD2	1.66	0.78
1:A:619:ILE:HG23	1:A:703:GLN:HG3	1.67	0.77
2:B:114:ILE:HG22	2:B:245:LEU:HB2	1.69	0.74
2:B:67:ARG:HH21	2:B:86:GLN:HG2	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:GLU:HA	2:B:186:PRO:HG3	1.72	0.72
3:C:1453:GLU:HG3	3:C:1459:PRO:HD2	1.69	0.72
2:B:151:ILE:HD11	2:B:200:VAL:HA	1.72	0.72
1:A:725:LYS:HG3	1:A:726:VAL:HG13	1.70	0.72
2:B:39:ASP:HB3	2:B:44:LEU:HB2	1.73	0.70
1:A:938:ILE:HG13	1:A:939:GLU:H	1.59	0.68
2:B:366:LEU:HB3	2:B:403:VAL:HG12	1.78	0.66
1:A:9:ALA:HB3	1:A:434:LEU:HB3	1.77	0.66
1:A:753:VAL:HB	1:A:951:VAL:HG12	1.78	0.66
3:C:1422:ASP:HB3	3:C:1437:TRP:HA	1.78	0.65
1:A:99:ARG:HD2	1:A:162:ASP:HA	1.79	0.65
1:A:478:CYS:HB3	1:A:533:MET:HG2	1.78	0.64
1:A:779:ILE:HD12	1:A:898:TYR:HD1	1.64	0.62
1:A:1:PHE:HA	1:A:389:GLN:HB2	1.81	0.62
4:G:1:NAG:H61	4:G:2:NAG:H61	1.81	0.61
1:A:181:GLY:HA3	1:A:222:LEU:HB3	1.83	0.61
3:C:1449:ILE:HG13	3:C:1487:VAL:HG22	1.82	0.60
1:A:904:TRP:CD1	1:A:907:THR:HG23	2.36	0.60
1:A:24:ASP:HA	1:A:409:LYS:HG2	1.82	0.60
1:A:741:ALA:H	1:A:786:GLY:HA3	1.67	0.60
3:C:1437:TRP:O	3:C:1470:SER:OG	2.19	0.60
2:B:517:THR:OG1	2:B:518:GLY:N	2.35	0.59
1:A:913:ASN:HB3	1:A:918:TYR:HE2	1.69	0.58
1:A:623:ASN:OD1	1:A:623:ASN:N	2.37	0.58
1:A:240:VAL:HG22	1:A:255:ILE:HG12	1.83	0.58
4:F:1:NAG:H83	4:F:1:NAG:H3	1.86	0.57
1:A:250:LEU:HD12	1:A:272:MET:HG2	1.86	0.57
1:A:617:ILE:HD11	1:A:625:LEU:HD23	1.85	0.57
2:B:483:GLN:O	2:B:485:GLU:N	2.37	0.57
2:B:11:SER:HB2	2:B:519:LYS:HE3	1.86	0.57
2:B:499:GLY:HA3	2:B:509:HIS:H	1.70	0.57
1:A:122:ARG:N	2:B:168:SER:OG	2.35	0.57
1:A:321:ARG:HH21	1:A:327:GLN:HB2	1.68	0.57
2:B:125:LYS:HA	2:B:212:VAL:HG21	1.86	0.57
2:B:159:LYS:NZ	2:B:224:ASP:OD2	2.37	0.57
1:A:438:ARG:HH21	1:A:577:ILE:HB	1.69	0.57
2:B:10:VAL:HG22	2:B:38:CYS:HB3	1.87	0.56
2:B:638:GLU:HB2	2:B:678:ILE:HG22	1.87	0.56
1:A:557:ILE:N	1:A:588:ARG:O	2.35	0.56
1:A:606:LEU:HB2	1:A:727:SER:HB3	1.88	0.56
2:B:83:VAL:HG22	2:B:104:VAL:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:467:LEU:HB3	2:B:505:GLN:HG2	1.88	0.56
1:A:24:ASP:OD1	1:A:25:PHE:N	2.38	0.56
2:B:112:VAL:HG22	2:B:243:SER:HB3	1.88	0.56
2:B:407:PRO:HB2	2:B:409:GLU:HG3	1.88	0.56
1:A:753:VAL:HG11	1:A:903:LEU:HD22	1.87	0.55
1:A:645:VAL:HG22	1:A:715:LEU:HD22	1.88	0.55
3:C:1448:ARG:NH1	3:C:1498:GLU:OE2	2.40	0.55
7:A:1002:NAG:H83	7:A:1002:NAG:H3	1.88	0.55
2:B:134:LEU:HD12	2:B:137:LYS:HD2	1.87	0.55
1:A:93:TRP:CD1	1:A:111:LEU:HD12	2.42	0.55
1:A:921:LYS:HE2	1:A:946:LEU:HD22	1.87	0.55
1:A:940:ASP:O	1:A:941:ILE:HG13	2.06	0.55
1:A:763:LYS:HB2	1:A:766:PRO:HB3	1.88	0.55
2:B:239:ARG:O	2:B:244:HIS:NE2	2.20	0.55
2:B:489:ARG:HB3	2:B:492:GLN:HG3	1.89	0.54
1:A:450:TYR:HB2	1:A:474:ASN:HB2	1.90	0.54
6:I:2:NAG:H3	6:I:2:NAG:H83	1.89	0.54
2:B:126:ASP:OD1	2:B:126:ASP:N	2.40	0.53
3:C:1448:ARG:HB3	3:C:1488:TYR:HB2	1.91	0.53
2:B:574:LEU:H	2:B:574:LEU:HD23	1.74	0.53
1:A:939:GLU:O	1:A:940:ASP:HB2	2.08	0.53
4:F:1:NAG:H61	4:F:2:NAG:N2	2.24	0.53
1:A:508:ILE:HD12	1:A:548:PHE:HB2	1.91	0.53
2:B:2:PRO:HA	2:B:6:THR:HB	1.91	0.53
2:B:502:LEU:HD21	2:B:507:VAL:HB	1.90	0.53
2:B:139:ALA:HB2	2:B:200:VAL:HG11	1.92	0.52
1:A:501:LYS:NZ	2:B:512:ASP:OD2	2.40	0.52
2:B:35:SER:N	2:B:36:PRO:HD3	2.25	0.52
2:B:308:PHE:HB2	2:B:330:VAL:HG12	1.91	0.52
1:A:802:LYS:HG2	1:A:807:THR:HA	1.91	0.52
2:B:233:ASP:N	2:B:233:ASP:OD1	2.41	0.52
1:A:768:THR:HB	1:A:771:ASP:H	1.75	0.52
2:B:130:SER:OG	2:B:336:ASP:O	2.28	0.52
1:A:643:LEU:HB3	1:A:681:CYS:HB2	1.93	0.51
2:B:362:LEU:HD12	2:B:363:PRO:HD2	1.92	0.51
1:A:792:LYS:HB2	1:A:930:GLU:HB2	1.92	0.51
2:B:36:PRO:HB3	2:B:47:ASP:HB3	1.93	0.50
3:C:1421:ARG:HD3	3:C:1421:ARG:H	1.76	0.50
1:A:817:ASP:HB2	1:A:898:TYR:HE2	1.77	0.50
2:B:15:GLN:N	2:B:15:GLN:OE1	2.44	0.50
2:B:117:LEU:HD11	2:B:225:ALA:HB1	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:ASN:HB2	2:B:398:SER:OG	2.13	0.49
2:B:579:GLY:HA3	2:B:588:CYS:HA	1.94	0.49
1:A:612:SER:OG	1:A:732:HIS:NE2	2.35	0.49
2:B:486:CYS:SG	2:B:495:CYS:HB2	2.52	0.48
1:A:284:ASP:OD2	1:A:289:ASP:N	2.44	0.48
2:B:295:MET:O	2:B:299:LEU:HB2	2.14	0.48
1:A:769:GLU:HG3	1:A:812:LEU:HD11	1.95	0.48
1:A:36:LEU:HB2	1:A:59:CYS:HB2	1.96	0.48
1:A:806:ASN:HB2	1:A:907:THR:HG22	1.95	0.48
1:A:745:ARG:HE	2:B:603:THR:HG21	1.78	0.47
2:B:249:THR:HG22	2:B:309:ALA:HB3	1.96	0.47
1:A:647:ILE:HD12	1:A:651:ALA:HB3	1.96	0.47
3:C:1451:TYR:CE1	3:C:1461:GLN:HB3	2.48	0.47
3:C:1488:TYR:CE2	3:C:1501:PRO:HB3	2.48	0.47
1:A:115:ARG:O	1:A:116:THR:OG1	2.31	0.47
1:A:286:ASN:OD1	1:A:286:ASN:N	2.47	0.47
1:A:449:VAL:HG21	1:A:557:ILE:HD13	1.97	0.47
2:B:46:LYS:HD2	2:B:46:LYS:HA	1.69	0.47
2:B:66:ASP:HB3	2:B:85:PRO:HB3	1.96	0.47
2:B:365:GLU:HG3	2:B:407:PRO:HG3	1.97	0.47
1:A:248:ARG:HD3	7:B:702:NAG:O7	2.15	0.47
1:A:650:GLN:O	1:A:701:VAL:HA	2.14	0.47
3:C:1427:ALA:HB3	3:C:1434:LEU:HD12	1.97	0.47
2:B:627:ASP:N	2:B:627:ASP:OD1	2.47	0.47
1:A:447:LEU:HD21	1:A:557:ILE:HG22	1.97	0.47
1:A:473:PHE:CZ	1:A:540:ALA:HB1	2.50	0.47
1:A:470:VAL:HG11	1:A:541:TYR:HD2	1.79	0.46
1:A:251:GLY:HA3	1:A:276:PHE:HB3	1.97	0.46
2:B:288:ASP:OD1	2:B:289:TYR:N	2.47	0.46
2:B:467:LEU:H	2:B:473:CYS:HB2	1.79	0.46
2:B:639:ILE:HG12	2:B:679:LEU:HB2	1.97	0.46
1:A:463:LEU:HD23	1:A:465:GLY:H	1.80	0.46
2:B:104:VAL:HG21	2:B:355:VAL:HG11	1.97	0.46
1:A:154:PHE:O	1:A:175:GLY:HA3	2.15	0.46
1:A:474:ASN:HA	1:A:539:ILE:HG22	1.96	0.46
1:A:904:TRP:HD1	1:A:907:THR:HG23	1.77	0.46
2:B:113:ASP:OD1	2:B:113:ASP:N	2.49	0.46
2:B:656:THR:HG22	2:B:666:ARG:HG2	1.98	0.46
2:B:93:ARG:HB2	2:B:94:PRO:HD2	1.98	0.46
1:A:284:ASP:OD1	1:A:287:GLY:N	2.49	0.46
1:A:658:ARG:NH2	2:B:527:SER:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:475:GLU:H	2:B:475:GLU:HG3	1.55	0.46
2:B:622:ARG:HH12	2:B:661:ASP:CG	2.19	0.46
2:B:97:SER:HB3	2:B:402:LYS:HG3	1.97	0.45
1:A:373:VAL:HB	1:A:391:LEU:HB2	1.98	0.45
1:A:904:TRP:CD1	1:A:906:GLU:HB3	2.52	0.45
2:B:403:VAL:HG11	2:B:431:PHE:HE1	1.82	0.45
2:B:524:ASP:O	2:B:544:CYS:HA	2.17	0.45
2:B:417:LYS:NZ	2:B:418:PRO:O	2.47	0.45
1:A:42:LYS:HA	1:A:52:GLU:HB3	1.99	0.44
1:A:806:ASN:HB2	1:A:907:THR:CG2	2.47	0.44
2:B:39:ASP:OD1	2:B:40:LEU:N	2.49	0.44
1:A:155:CYS:HB2	1:A:176:SER:OG	2.16	0.44
1:A:803:TYR:O	1:A:806:ASN:ND2	2.51	0.44
2:B:236:ILE:HD11	2:B:238:TRP:CD1	2.51	0.44
1:A:65:ARG:HD3	1:A:65:ARG:HA	1.87	0.44
5:E:4:BMA:H4	5:E:5:MAN:H2	1.70	0.44
1:A:893:LYS:HD2	1:A:893:LYS:HA	1.78	0.44
1:A:61:TRP:HZ2	1:A:436:ARG:HH11	1.64	0.44
2:B:625:LEU:HD11	2:B:634:TYR:HD2	1.81	0.44
2:B:236:ILE:HD11	2:B:238:TRP:CE2	2.53	0.43
1:A:284:ASP:O	1:A:356:ASN:HB2	2.18	0.43
2:B:26:CYS:HB2	2:B:44:LEU:HD21	2.01	0.43
1:A:396:ALA:O	1:A:402:PRO:HG3	2.17	0.43
1:A:512:LEU:HB2	1:A:541:TYR:CE1	2.52	0.43
1:A:602:CYS:HA	1:A:636:GLU:OE1	2.18	0.43
1:A:779:ILE:HD12	1:A:898:TYR:CD1	2.48	0.43
2:B:3:ASN:HB2	2:B:40:LEU:HD21	1.99	0.43
2:B:517:THR:HG23	2:B:523:CYS:HB3	2.00	0.43
1:A:97:SER:HB3	1:A:161:ILE:HG12	2.00	0.43
1:A:275:TYR:HD2	1:A:278:PHE:HB2	1.84	0.43
1:A:496:GLU:OE1	1:A:522:SER:OG	2.27	0.43
1:A:705:SER:O	1:A:707:MET:HG2	2.18	0.43
2:B:83:VAL:O	2:B:86:GLN:NE2	2.51	0.43
2:B:180:MET:O	3:C:1448:ARG:NH2	2.42	0.43
2:B:442:GLU:HB3	2:B:446:HIS:CD2	2.54	0.43
1:A:112:TYR:OH	1:A:143:ARG:NH1	2.51	0.43
1:A:663:LEU:HB2	1:A:695:ALA:HA	2.00	0.43
2:B:192:HIS:O	2:B:279:ASN:HB3	2.18	0.43
1:A:376:PHE:HB3	1:A:383:LEU:HD11	2.00	0.43
2:B:221:GLY:HA3	2:B:289:TYR:HE2	1.84	0.43
2:B:318:TYR:HA	2:B:321:TYR:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:GLN:O	2:B:81:THR:HG22	2.19	0.43
1:A:88:PHE:CE1	1:A:122:ARG:HG2	2.54	0.42
1:A:784:ASN:HB2	1:A:790:PHE:HE1	1.85	0.42
2:B:487:SER:HB3	2:B:493:PRO:O	2.19	0.42
2:B:185:LEU:H	2:B:185:LEU:HD23	1.84	0.42
1:A:368:ASP:HB2	1:A:370:LYS:HG3	2.02	0.42
1:A:910:ASN:OD1	1:A:911:LYS:N	2.48	0.42
2:B:26:CYS:SG	2:B:27:SER:N	2.91	0.42
2:B:98:LYS:HD3	2:B:98:LYS:HA	1.86	0.42
1:A:160:SER:HB2	1:A:226:VAL:HG22	2.00	0.42
1:A:417:ASN:HA	1:A:486:VAL:HB	2.01	0.42
2:B:40:LEU:HD22	2:B:40:LEU:H	1.85	0.42
3:C:1425:VAL:HG11	3:C:1506:TYR:CD2	2.54	0.42
1:A:125:VAL:HG11	1:A:143:ARG:HB2	2.02	0.42
1:A:487:LEU:HD11	1:A:529:ARG:HE	1.84	0.42
1:A:721:ASN:O	1:A:725:LYS:HE2	2.20	0.42
2:B:172:ALA:HB2	2:B:178:TYR:HB2	2.02	0.42
2:B:354:LYS:HE2	2:B:354:LYS:HB3	1.88	0.42
1:A:777:GLN:HG2	1:A:779:ILE:HD11	2.01	0.42
2:B:245:LEU:HD11	2:B:348:TYR:CD1	2.55	0.42
3:C:1422:ASP:CB	3:C:1437:TRP:HA	2.49	0.41
2:B:1:GLY:HA3	2:B:2:PRO:HD3	1.93	0.41
2:B:60:GLU:HB3	2:B:62:ARG:HG3	2.02	0.41
2:B:116:TYR:HA	2:B:247:VAL:HG13	2.02	0.41
2:B:245:LEU:HD11	2:B:348:TYR:HD1	1.85	0.41
1:A:559:MET:HB3	1:A:559:MET:HE2	1.97	0.41
1:A:554:PRO:HG3	1:A:685:ASN:ND2	2.36	0.41
2:B:120:LEU:HD23	2:B:120:LEU:HA	1.88	0.41
1:A:50:ILE:HD12	1:A:89:LYS:HB3	2.01	0.41
2:B:645:LEU:HD12	2:B:645:LEU:HA	1.90	0.41
3:C:1478:LYS:O	3:C:1480:GLY:N	2.53	0.41
1:A:108:CYS:HA	1:A:128:CYS:HA	2.01	0.41
2:B:526:PHE:HA	2:B:535:MET:SD	2.61	0.41
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.90	0.41
1:A:347:LEU:HD21	1:A:359:ALA:HB2	2.03	0.41
1:A:610:VAL:HG21	1:A:715:LEU:HD12	2.03	0.41
1:A:646:SER:OG	1:A:714:ASP:HB2	2.21	0.41
2:B:299:LEU:HD21	2:B:306:LEU:HB2	2.01	0.41
2:B:434:ASP:N	2:B:434:ASP:OD1	2.53	0.41
3:C:1449:ILE:O	3:C:1462:GLU:HA	2.21	0.41
1:A:505:LYS:HG2	1:A:506:GLY:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LYS:HG3	1:A:92:GLN:OE1	2.20	0.40
3:C:1454:THR:OG1	3:C:1455:GLY:N	2.55	0.40
1:A:460:THR:HB	4:F:1:NAG:H62	2.02	0.40
1:A:463:LEU:HG	1:A:464:PRO:HD2	2.03	0.40
2:B:66:ASP:N	2:B:66:ASP:OD1	2.55	0.40
2:B:432:ASP:OD1	2:B:432:ASP:N	2.51	0.40
3:C:1451:TYR:CE1	3:C:1474:ILE:HD11	2.56	0.40
1:A:139:TYR:OH	1:A:186:ASP:OD2	2.30	0.40
1:A:801:TYR:HB2	1:A:880:LEU:HB2	2.04	0.40
1:A:2:ASN:OD1	1:A:2:ASN:N	2.52	0.40
1:A:61:TRP:CH2	1:A:415:ASP:HB3	2.57	0.40
1:A:429:VAL:HG23	1:A:431:ARG:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	916/954 (96%)	857 (94%)	59 (6%)	0	100	100
2	B	688/690 (100%)	607 (88%)	77 (11%)	4 (1%)	25	59
3	C	87/90 (97%)	72 (83%)	15 (17%)	0	100	100
All	All	1691/1734 (98%)	1536 (91%)	151 (9%)	4 (0%)	47	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	473	CYS
2	B	482	GLN
2	B	483	GLN
2	B	443	PRO

5.3.2 Protein sidechains [i](#)

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	780/809 (96%)	757 (97%)	23 (3%)	42 72
2	B	612/612 (100%)	600 (98%)	12 (2%)	55 80
3	C	74/74 (100%)	68 (92%)	6 (8%)	11 39
All	All	1466/1495 (98%)	1425 (97%)	41 (3%)	43 73

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	103	ASP
1	A	155	CYS
1	A	261	MET
1	A	275	TYR
1	A	347	LEU
1	A	427	PHE
1	A	505	LYS
1	A	508	ILE
1	A	543	ARG
1	A	544	ASP
1	A	548	PHE
1	A	594	LEU
1	A	622	ASP
1	A	623	ASN
1	A	634	GLN
1	A	672	THR
1	A	768	THR
1	A	806	ASN
1	A	874	CYS
1	A	913	ASN
1	A	916	HIS
1	A	943	ASN
2	B	26	CYS
2	B	41	LYS
2	B	123	SER

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Mol	Chain	Res	Type
2	B	335	MET
2	B	375	LEU
2	B	376	ASN
2	B	460	CYS
2	B	466	TRP
2	B	475	GLU
2	B	501	CYS
2	B	517	THR
2	B	603	THR
3	C	1421	ARG
3	C	1422	ASP
3	C	1423	LEU
3	C	1460	VAL
3	C	1462	GLU
3	C	1477	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
3	HRG	C	1493	3	10,11,12	0.75	0	6,12,14	0.46	0

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
3	HRG	C	1493	3	-	4/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1493	HRG	O-C-CA-CB
3	C	1493	HRG	NH1-CZ-NE-CD
3	C	1493	HRG	NH2-CZ-NE-CD
3	C	1493	HRG	CD-CG-CG'-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

19 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	$\# Z > 2$
4	NAG	D	1	1,4	14,14,15	0.32	0	17,19,21	0.39	0
4	NAG	D	2	4	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	E	1	1,5	14,14,15	0.27	0	17,19,21	0.37	0
5	NAG	E	2	5	14,14,15	0.23	0	17,19,21	0.39	0
5	BMA	E	3	5	11,11,12	0.71	0	15,15,17	0.84	0
5	BMA	E	4	5	11,11,12	1.24	2 (18%)	15,15,17	1.08	1 (6%)
5	MAN	E	5	5	11,11,12	0.96	1 (9%)	15,15,17	0.87	1 (6%)
5	MAN	E	6	5	11,11,12	0.67	0	15,15,17	1.10	2 (13%)
4	NAG	F	1	1,4	14,14,15	0.44	0	17,19,21	1.34	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	F	2	4	14,14,15	0.24	0	17,19,21	0.39	0
4	NAG	G	1	1,4	14,14,15	0.37	0	17,19,21	0.69	1 (5%)
4	NAG	G	2	4	14,14,15	0.77	1 (7%)	17,19,21	0.93	1 (5%)
4	NAG	H	1	2,4	14,14,15	0.32	0	17,19,21	0.51	0
4	NAG	H	2	4	14,14,15	0.89	1 (7%)	17,19,21	0.89	1 (5%)
6	NAG	I	1	2,6	14,14,15	0.20	0	17,19,21	0.46	0
6	NAG	I	2	6	14,14,15	0.61	1 (7%)	17,19,21	1.35	1 (5%)
6	BMA	I	3	6	11,11,12	0.80	0	15,15,17	1.14	1 (6%)
4	NAG	J	1	2,4	14,14,15	0.63	1 (7%)	17,19,21	1.36	1 (5%)
4	NAG	J	2	4	14,14,15	0.23	0	17,19,21	1.28	1 (5%)

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. ^{1,2} means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
5	NAG	E	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	1/2/19/22	0/1/1/1
5	BMA	E	4	5	-	1/2/19/22	0/1/1/1
5	MAN	E	5	5	-	0/2/19/22	0/1/1/1
5	MAN	E	6	5	-	0/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	5/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	NAG	H	1	2,4	-	1/6/23/26	0/1/1/1
4	NAG	H	2	4	-	4/6/23/26	0/1/1/1
6	NAG	I	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	3/6/23/26	0/1/1/1
6	BMA	I	3	6	-	1/2/19/22	0/1/1/1
4	NAG	J	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	3/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2	NAG	O5-C1	2.59	1.47	1.43
5	E	5	MAN	O5-C1	-2.45	1.39	1.43
5	E	4	BMA	C4-C5	2.34	1.58	1.53
4	G	2	NAG	O5-C1	2.27	1.47	1.43
4	J	1	NAG	O5-C1	2.21	1.47	1.43
5	E	4	BMA	O5-C1	-2.04	1.40	1.43
6	I	2	NAG	C1-C2	2.00	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1	NAG	C1-O5-C5	4.85	118.77	112.19
4	J	2	NAG	C1-O5-C5	4.51	118.30	112.19
4	F	1	NAG	C2-N2-C7	4.34	129.09	122.90
6	I	2	NAG	C2-N2-C7	4.23	128.92	122.90
4	G	2	NAG	C1-O5-C5	3.63	117.11	112.19
4	H	2	NAG	C1-O5-C5	3.42	116.83	112.19
6	I	3	BMA	C1-O5-C5	2.69	115.83	112.19
5	E	6	MAN	C1-O5-C5	2.51	115.60	112.19
5	E	6	MAN	O2-C2-C3	-2.31	105.51	110.14
5	E	5	MAN	O2-C2-C3	-2.22	105.70	110.14
4	G	1	NAG	C1-O5-C5	2.12	115.07	112.19
5	E	4	BMA	C3-C4-C5	2.07	113.92	110.24
4	F	1	NAG	C1-O5-C5	2.05	114.97	112.19
4	F	1	NAG	C1-C2-N2	2.01	113.92	110.49

There are no chirality outliers.

All (30) torsion outliers are listed below:

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

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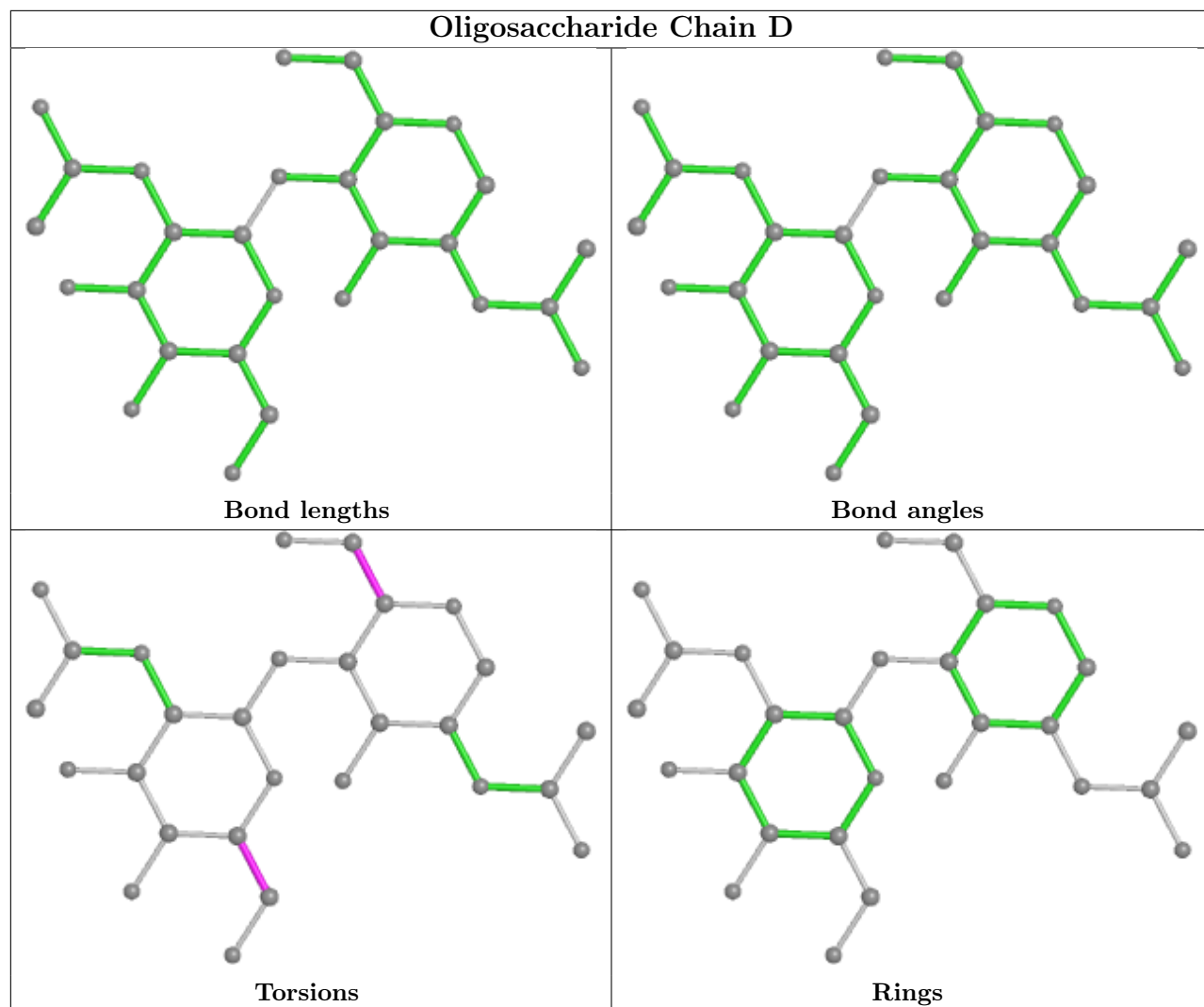
Mol	Chain	Res	Type	Atoms
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
4	D	1	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6
6	I	3	BMA	O5-C5-C6-O6
4	J	2	NAG	C1-C2-N2-C7
5	E	1	NAG	O5-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
5	E	4	BMA	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	F	1	NAG	C3-C2-N2-C7
4	J	2	NAG	C3-C2-N2-C7
6	I	2	NAG	C3-C2-N2-C7
6	I	1	NAG	O5-C5-C6-O6

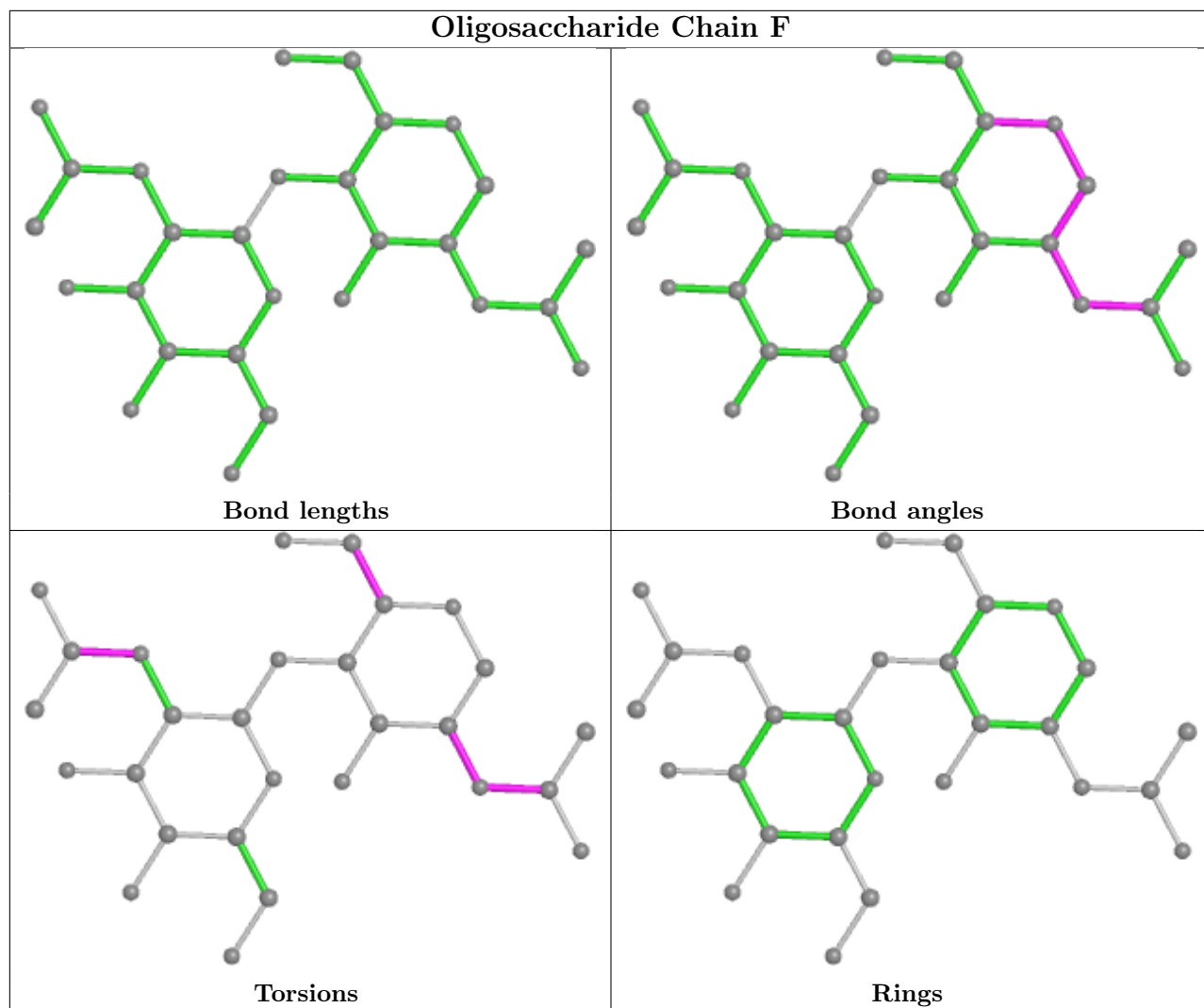
There are no ring outliers.

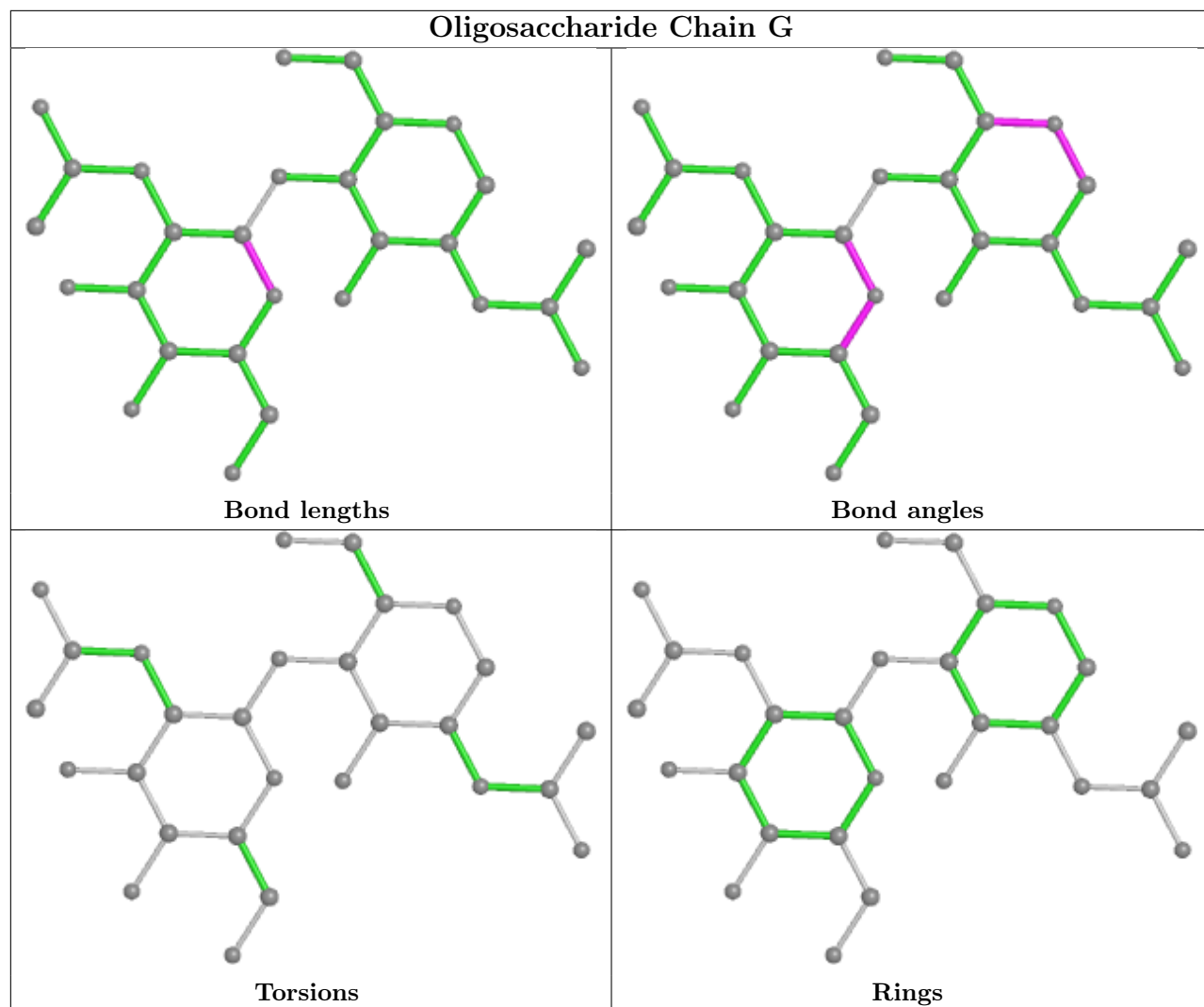
7 monomers are involved in 6 short contacts:

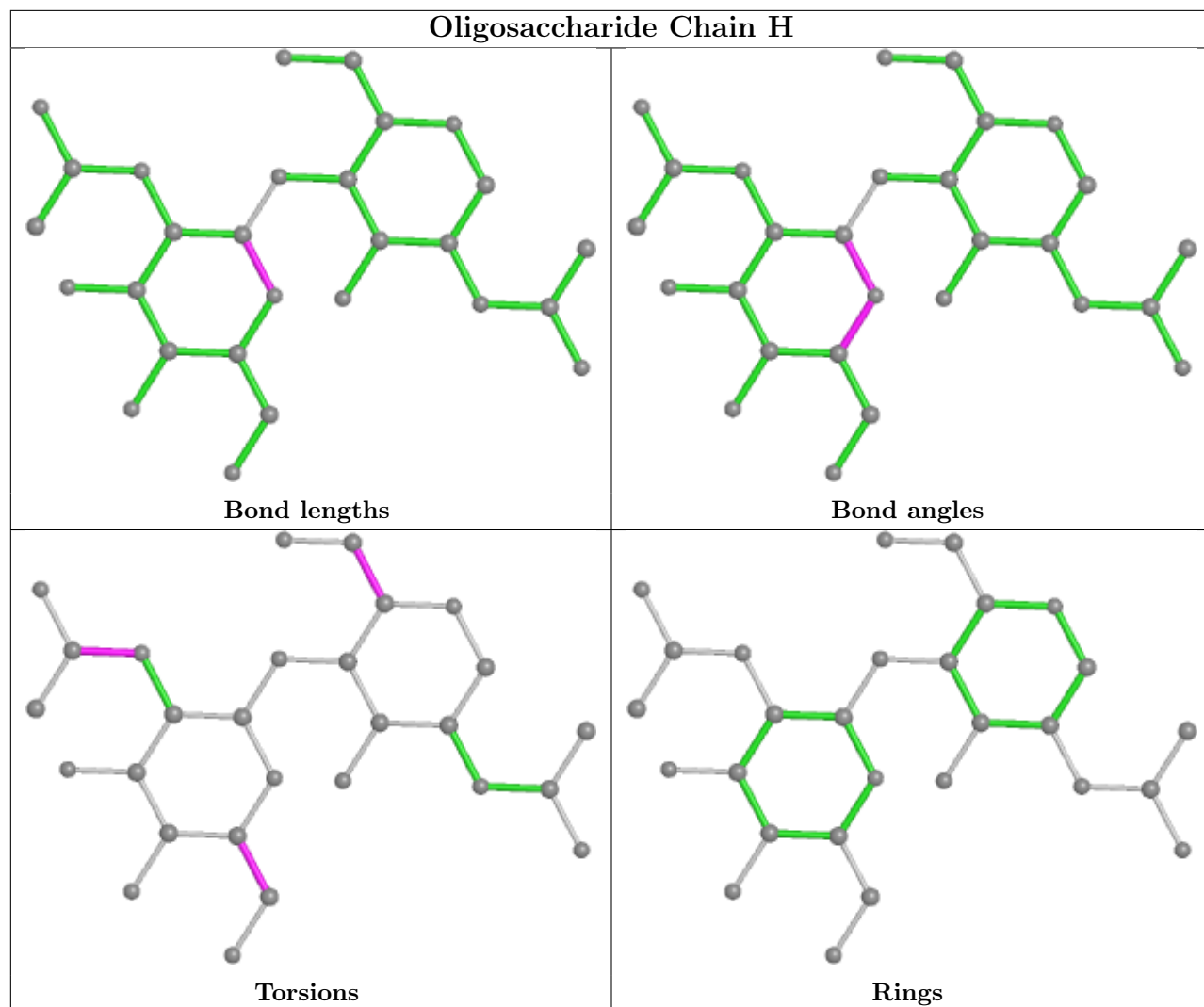
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	3	0
4	G	2	NAG	1	0
5	E	5	MAN	1	0
4	F	2	NAG	1	0
4	G	1	NAG	1	0
6	I	2	NAG	1	0
5	E	4	BMA	1	0

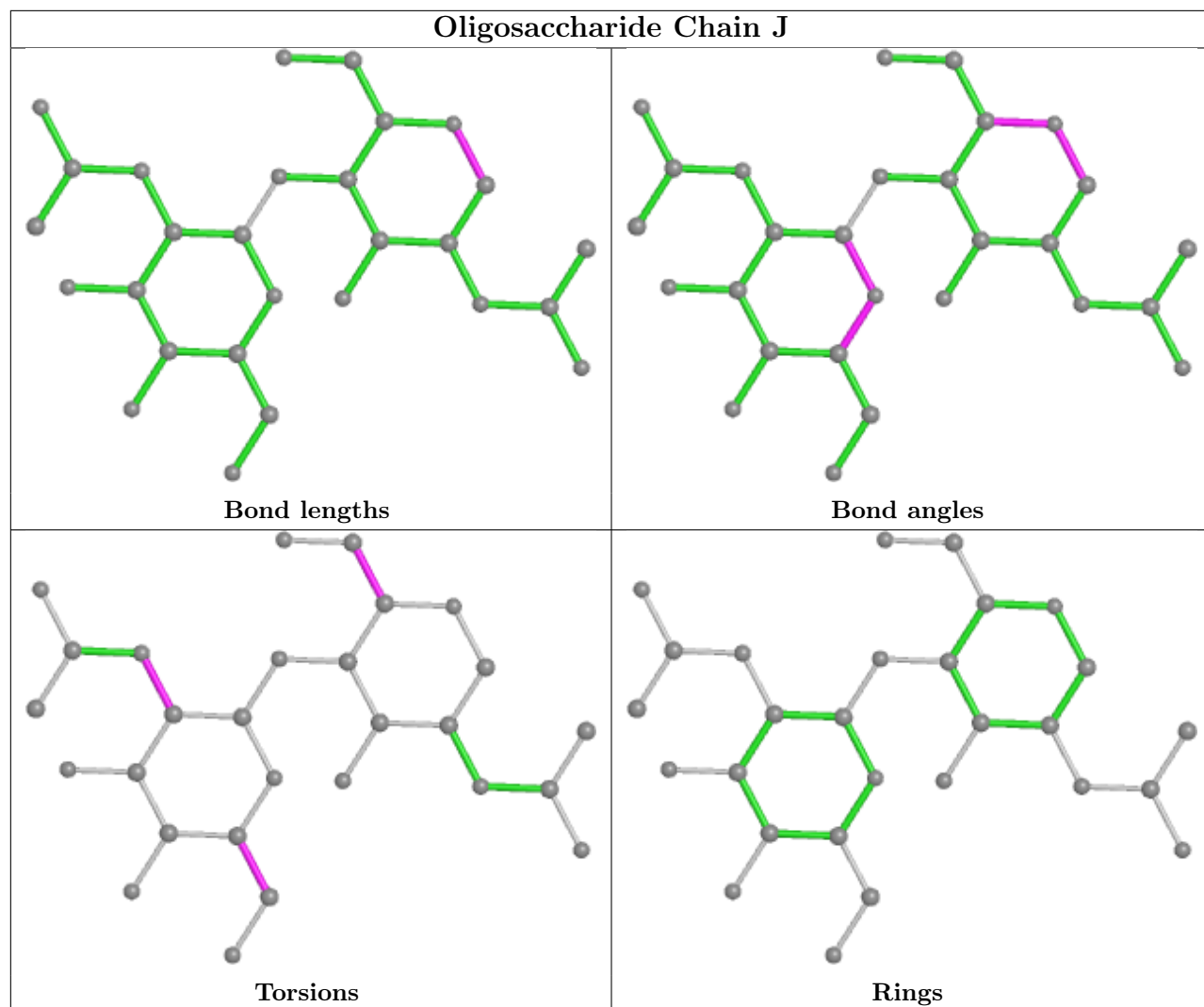
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

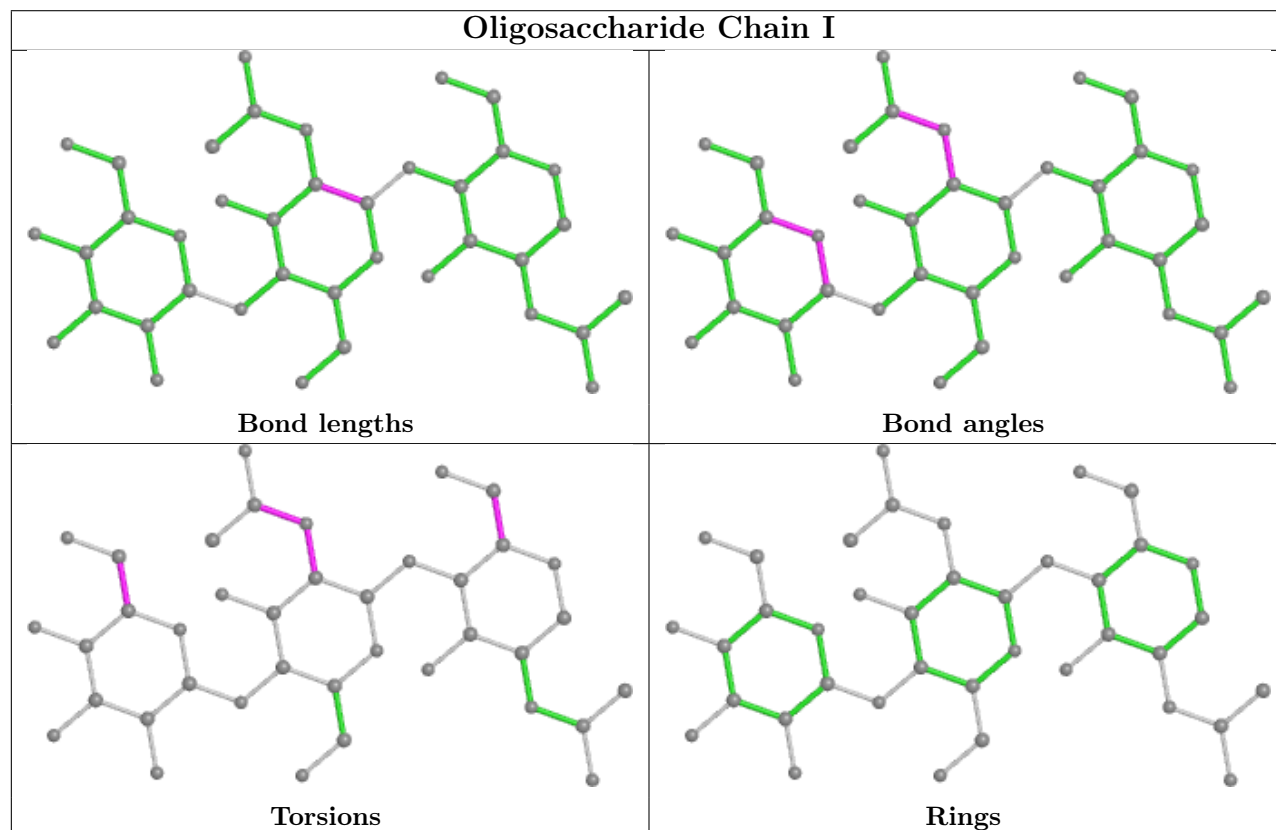
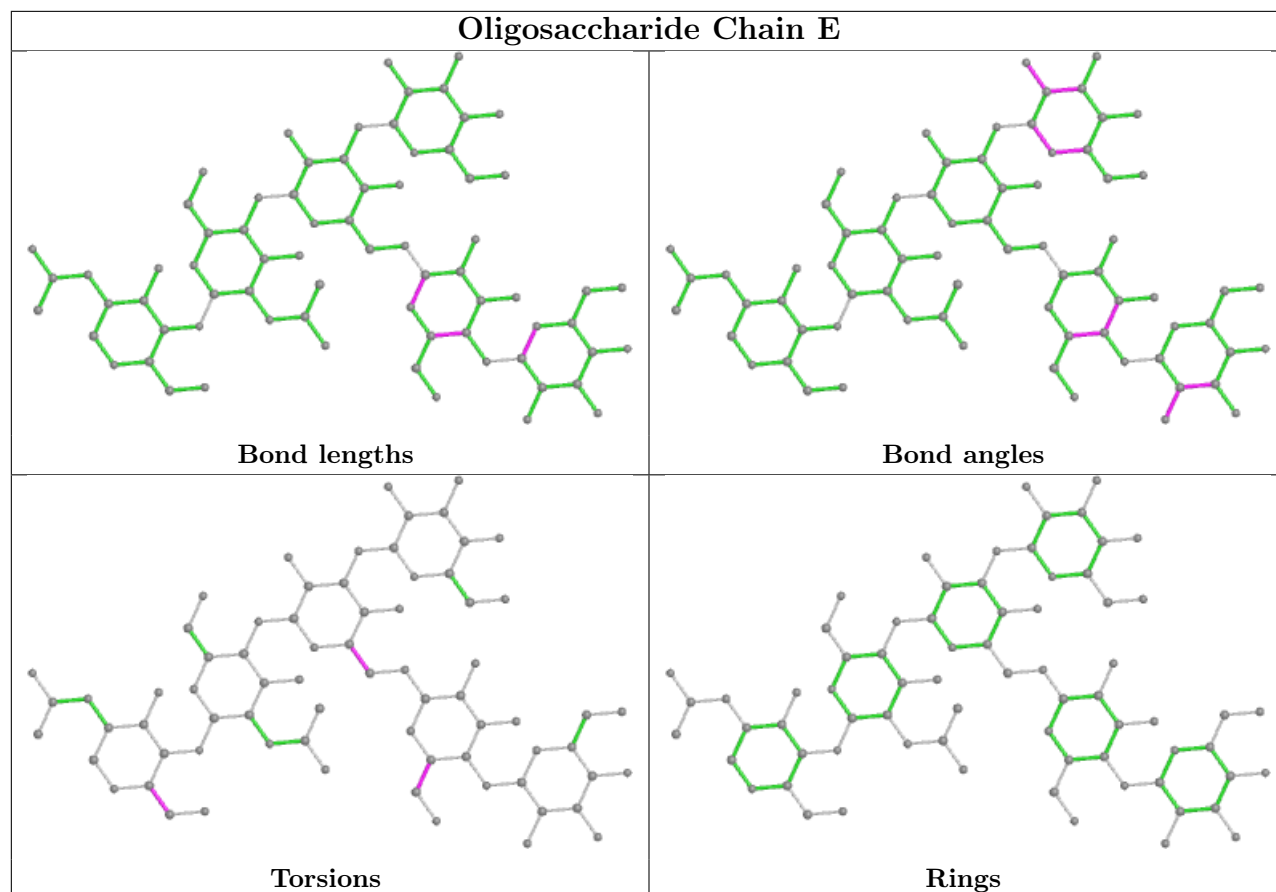












5.6 Ligand geometry

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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
7	NAG	A	1004	1	14,14,15	0.24	0	17,19,21	0.44	0
7	NAG	A	1002	1	14,14,15	0.44	0	17,19,21	1.25	1 (5%)
7	NAG	B	702	2	14,14,15	0.20	0	17,19,21	0.47	0
7	NAG	B	701	2	14,14,15	0.64	0	17,19,21	0.84	1 (5%)
7	NAG	A	1001	1	14,14,15	0.86	1 (7%)	17,19,21	1.27	1 (5%)
7	NAG	A	1005	1	14,14,15	0.19	0	17,19,21	0.42	0
7	NAG	A	1003	1	14,14,15	0.23	0	17,19,21	0.47	0

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
7	NAG	A	1004	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1002	1	-	3/6/23/26	0/1/1/1
7	NAG	B	702	2	-	2/6/23/26	0/1/1/1
7	NAG	B	701	2	-	2/6/23/26	0/1/1/1
7	NAG	A	1001	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1005	1	-	3/6/23/26	0/1/1/1
7	NAG	A	1003	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1001	NAG	O5-C1	3.08	1.48	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1001	NAG	C1-O5-C5	5.02	119.00	112.19
7	A	1002	NAG	C2-N2-C7	4.34	129.08	122.90
7	B	701	NAG	C1-O5-C5	3.26	116.61	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	702	NAG	O5-C5-C6-O6
7	A	1001	NAG	O5-C5-C6-O6
7	B	702	NAG	C4-C5-C6-O6
7	A	1001	NAG	C4-C5-C6-O6
7	A	1002	NAG	C8-C7-N2-C2
7	A	1002	NAG	O7-C7-N2-C2
7	A	1005	NAG	C8-C7-N2-C2
7	A	1005	NAG	O7-C7-N2-C2
7	B	701	NAG	O5-C5-C6-O6
7	B	701	NAG	C4-C5-C6-O6
7	A	1003	NAG	O5-C5-C6-O6
7	A	1005	NAG	O5-C5-C6-O6
7	A	1002	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1002	NAG	1	0
7	B	702	NAG	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	920/954 (96%)	-0.02	15 (1%) 72 51	22, 56, 111, 148	0
2	B	690/690 (100%)	0.41	69 (10%) 7 2	29, 77, 159, 204	2 (0%)
3	C	89/90 (98%)	1.67	32 (35%) 0 0	57, 110, 144, 159	0
All	All	1699/1734 (97%)	0.25	116 (6%) 17 7	22, 67, 141, 204	2 (0%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	36	PRO	8.1
3	C	1427	ALA	6.7
3	C	1428	ALA	6.2
2	B	35	SER	5.8
2	B	37	ARG	5.8
2	B	463	GLY	5.8
2	B	465	GLY	5.6
2	B	509	HIS	5.6
3	C	1458	SER	5.1
3	C	1433	LEU	5.0
2	B	510	SER	4.9
2	B	452	ASN	4.8
2	B	464	PRO	4.8
3	C	1456	GLY	4.6
2	B	443	PRO	4.5
2	B	451	GLY	4.5
2	B	446	HIS	4.5
3	C	1425	VAL	4.4
2	B	515	LYS	4.4
3	C	1471	THR	4.2
2	B	453	GLY	4.2
3	C	1434	LEU	4.2
2	B	438	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	444	ASN	4.0
2	B	455	PHE	3.9
2	B	674	SER	3.9
2	B	467	LEU	3.8
2	B	3	ASN	3.8
3	C	1430	PRO	3.8
2	B	456	GLU	3.7
2	B	51	PRO	3.7
3	C	1469	LYS	3.6
2	B	461	ARG	3.6
2	B	450	ASN	3.6
3	C	1432	SER	3.5
3	C	1439	ALA	3.5
3	C	1437	TRP	3.4
2	B	442	GLU	3.4
3	C	1455	GLY	3.4
2	B	28	ASP	3.4
2	B	52	GLU	3.4
2	B	468	GLY	3.3
2	B	485	GLU	3.3
1	A	625	LEU	3.2
2	B	507	VAL	3.2
1	A	649	LEU	3.2
2	B	673	SER	3.1
2	B	440	GLN	3.1
2	B	29	GLU	3.1
2	B	512	ASP	3.1
2	B	41	LYS	3.0
3	C	1459	PRO	3.0
2	B	516	ILE	3.0
3	C	1452	GLY	3.0
2	B	42	GLU	3.0
2	B	50	ALA	3.0
2	B	445	SER	2.9
2	B	484	ASP	2.9
1	A	490	LYS	2.9
3	C	1457	ASN	2.9
3	C	1479	PRO	2.9
2	B	441	ALA	2.9
3	C	1435	ILE	2.8
1	A	567	THR	2.8
2	B	7	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	479	LEU	2.8
1	A	480	LYS	2.7
2	B	460	CYS	2.7
2	B	646	LYS	2.7
2	B	34	GLY	2.7
2	B	454	THR	2.7
2	B	482	GLN	2.7
2	B	439	ALA	2.7
3	C	1484	THR	2.6
3	C	1472	ALA	2.6
2	B	53	SER	2.6
2	B	30	ALA	2.5
2	B	477	ASP	2.5
3	C	1429	THR	2.5
1	A	706	GLU	2.4
3	C	1424	GLU	2.4
2	B	648	THR	2.4
3	C	1454	THR	2.4
1	A	570	ASP	2.4
2	B	31	LEU	2.4
2	B	466	TRP	2.4
2	B	138	LEU	2.4
1	A	892	GLY	2.3
3	C	1483	TYR	2.3
2	B	448	CYS	2.3
3	C	1503	SER	2.3
3	C	1502	ILE	2.3
3	C	1438	ASP	2.3
1	A	734	VAL	2.3
2	B	501	CYS	2.3
3	C	1506	TYR	2.3
3	C	1426	VAL	2.2
2	B	27	SER	2.2
2	B	449	ASN	2.2
3	C	1423	LEU	2.2
2	B	33	LEU	2.2
1	A	493	PHE	2.2
2	B	49	CYS	2.2
1	A	571	THR	2.2
1	A	569	ALA	2.2
2	B	48	ASN	2.1
2	B	32	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	10	VAL	2.1
2	B	650	LYS	2.1
2	B	490	GLU	2.1
3	C	1476	GLY	2.1
2	B	436	ALA	2.1
2	B	459	VAL	2.1
1	A	801	TYR	2.0
1	A	631	ALA	2.0
2	B	26	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
3	HRG	C	1493	12/13	0.91	0.23	55,57,61,62	0

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.

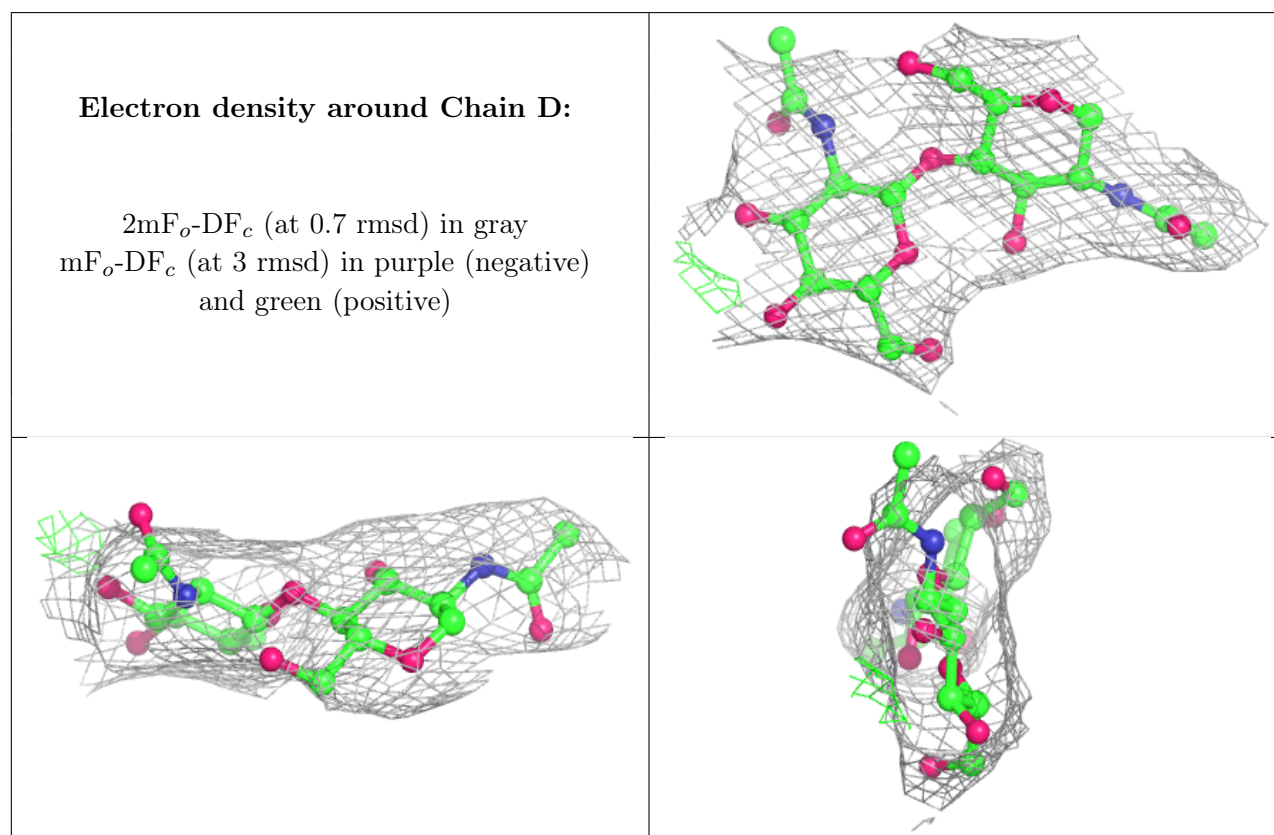
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	G	2	14/15	0.60	0.35	65,94,122,126	0
6	BMA	I	3	11/12	0.69	0.21	67,95,109,113	0
4	NAG	F	2	14/15	0.75	0.43	82,111,123,127	0
4	NAG	G	1	14/15	0.75	0.26	41,78,95,115	0
4	NAG	F	1	14/15	0.77	0.29	78,95,105,111	0
4	NAG	J	2	14/15	0.79	0.31	66,117,129,133	0
4	NAG	J	1	14/15	0.80	0.30	83,90,120,126	0
4	NAG	H	2	14/15	0.81	0.27	95,104,114,116	0
5	MAN	E	6	11/12	0.83	0.24	72,81,97,97	0
5	MAN	E	5	11/12	0.85	0.24	62,81,96,105	0
5	BMA	E	4	11/12	0.87	0.14	73,77,88,94	0
6	NAG	I	2	14/15	0.88	0.30	92,104,114,130	0
4	NAG	H	1	14/15	0.89	0.22	84,92,102,105	0

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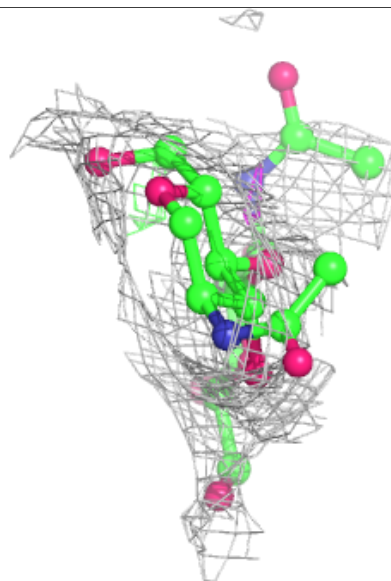
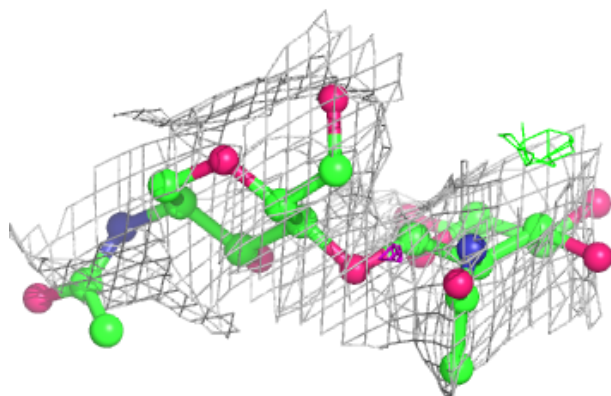
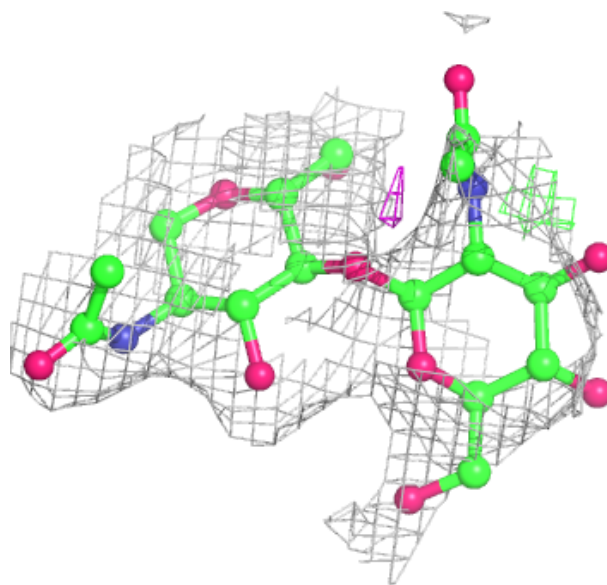
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	D	2	14/15	0.90	0.20	61,70,92,107	0
5	BMA	E	3	11/12	0.92	0.13	65,73,80,88	0
5	NAG	E	2	14/15	0.92	0.18	29,45,67,83	0
6	NAG	I	1	14/15	0.93	0.14	70,86,96,102	0
4	NAG	D	1	14/15	0.95	0.15	33,46,65,79	0
5	NAG	E	1	14/15	0.96	0.17	29,34,42,58	0

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 F:

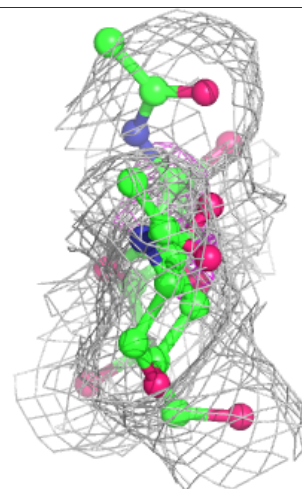
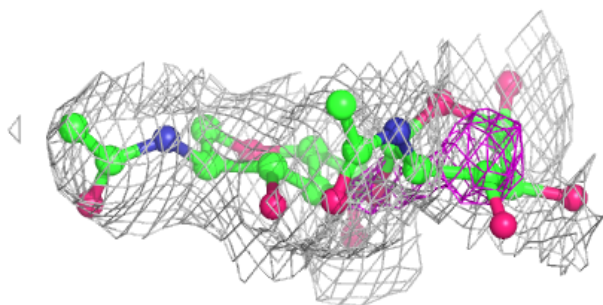
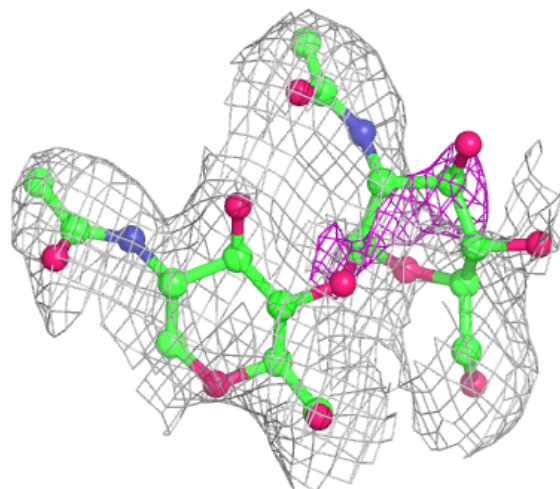
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

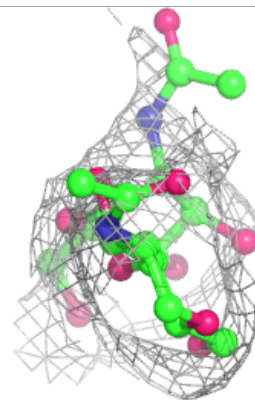
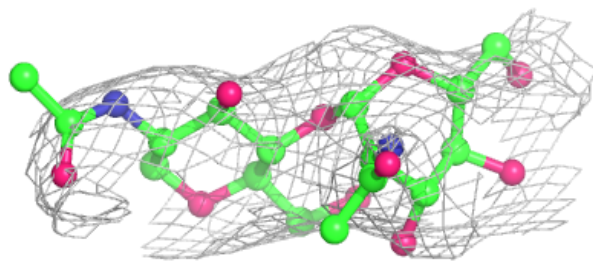
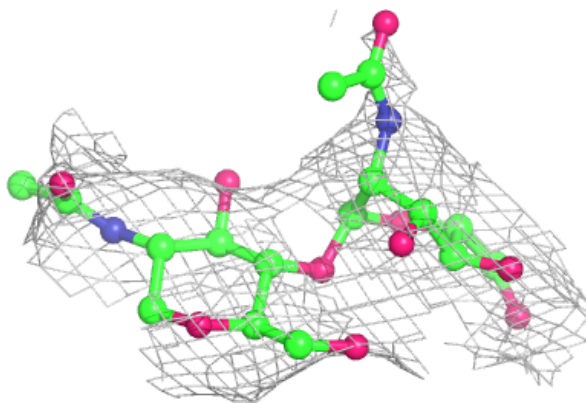
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

4

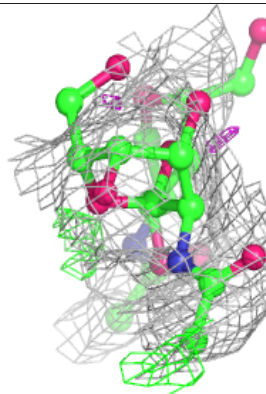
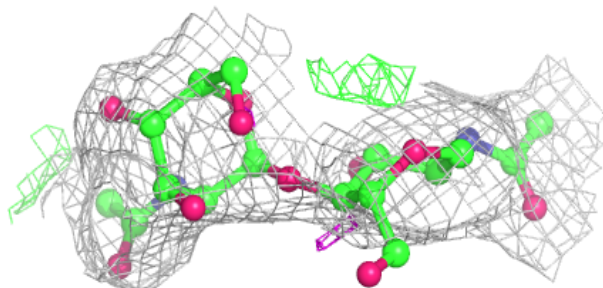
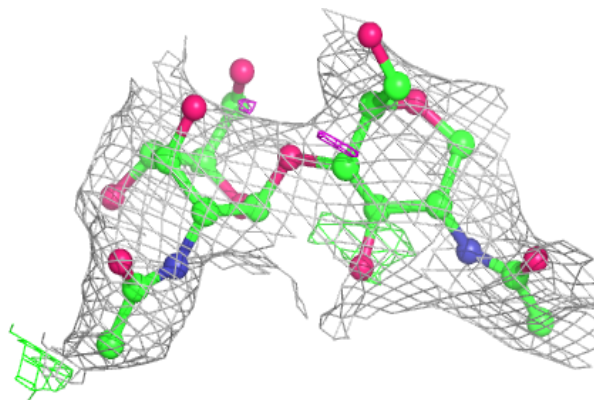


Electron density around Chain H:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

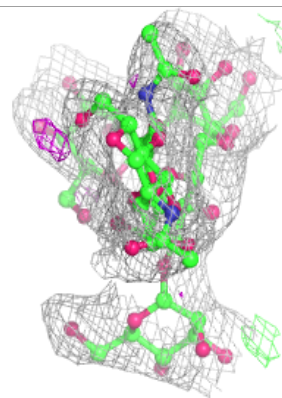
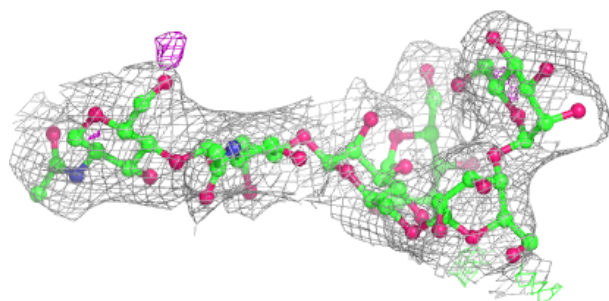
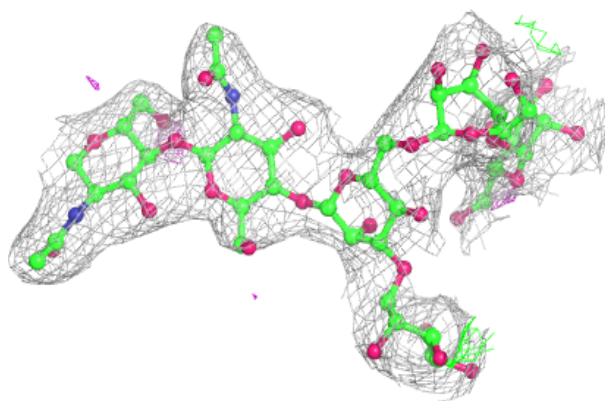
**Electron density around Chain J:**

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

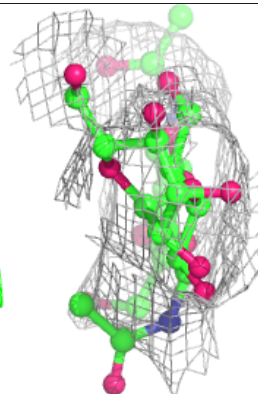
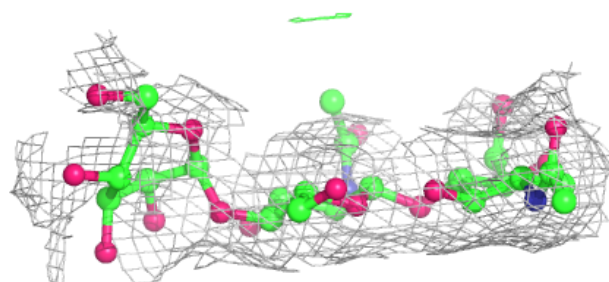
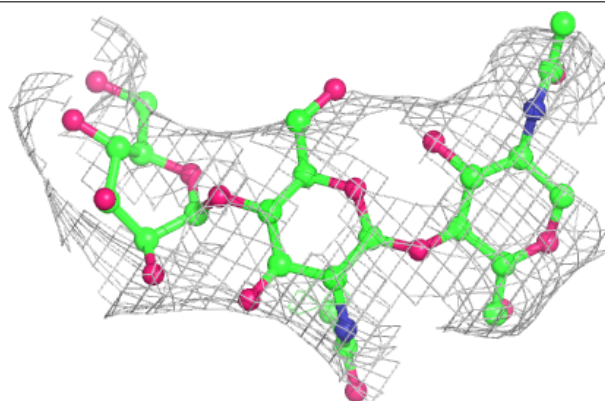


Electron density around Chain E:

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

**Electron density around Chain 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](#)

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(\AA^2)	Q<0.9
7	NAG	A	1003	14/15	0.76	0.35	90,105,115,117	0
7	NAG	B	701	14/15	0.77	0.38	81,103,112,114	0
7	NAG	A	1001	14/15	0.79	0.26	67,80,93,97	0
7	NAG	B	702	14/15	0.81	0.22	62,85,95,100	0
7	NAG	A	1002	14/15	0.82	0.19	66,90,96,100	0
7	NAG	A	1004	14/15	0.82	0.24	60,79,92,106	0
7	NAG	A	1005	14/15	0.88	0.19	56,65,81,82	0
8	MN	A	1009	1/1	0.92	0.17	115,115,115,115	0
8	MN	B	704	1/1	0.94	0.18	70,70,70,70	0
8	MN	A	1010	1/1	0.95	0.13	70,70,70,70	0
8	MN	A	1008	1/1	0.97	0.17	72,72,72,72	0
8	MN	A	1006	1/1	0.98	0.12	68,68,68,68	0
8	MN	A	1007	1/1	0.98	0.16	69,69,69,69	0
8	MN	B	703	1/1	0.99	0.20	55,55,55,55	0
8	MN	B	705	1/1	0.99	0.21	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.