



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:05 AM UTC

PDB ID : 6NAJ / pdb_00006naj
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	:	4-5-2 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

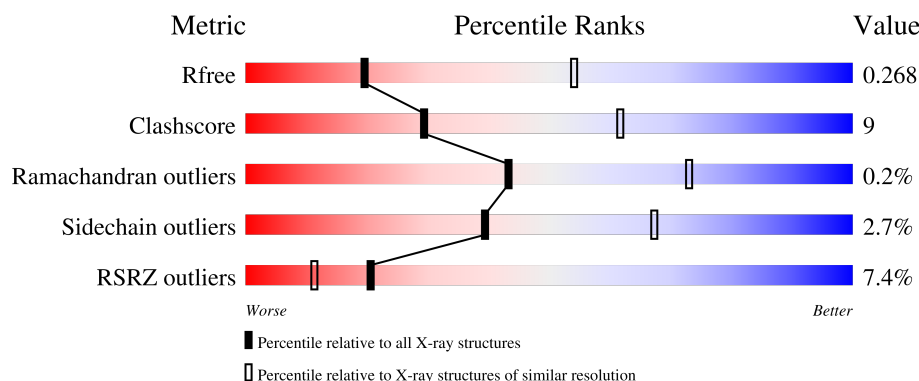
1 Overall quality at a glance

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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	4% 76% 19% • •
2	B	690	10% 77% 22% •
3	C	90	16% 69% 27% •
4	D	2	100%
4	F	2	50% 50%

Continued on next page...

Continued from previous page...

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%

2 Entry composition

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
1	A	920	Total	C	N	O	S	0	0	0
			7163	4535	1216	1377	35			

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

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

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

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

There are 7 discrepancies between the modelled and reference sequences:

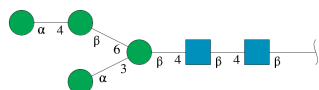
Chain	Residue	Modelled	Actual	Comment	Reference
C	1492	PRO	GLY	conflict	UNP P02751
C	?	-	SER	deletion	UNP P02751
C	1496	TRP	PRO	conflict	UNP P02751
C	1497	ASN	ALA	conflict	UNP P02751
C	1498	GLU	SER	conflict	UNP P02751
C	1499	GLY	SER	conflict	UNP P02751
C	1500	GLY	LYS	conflict	UNP P02751

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



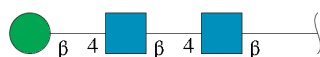
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).



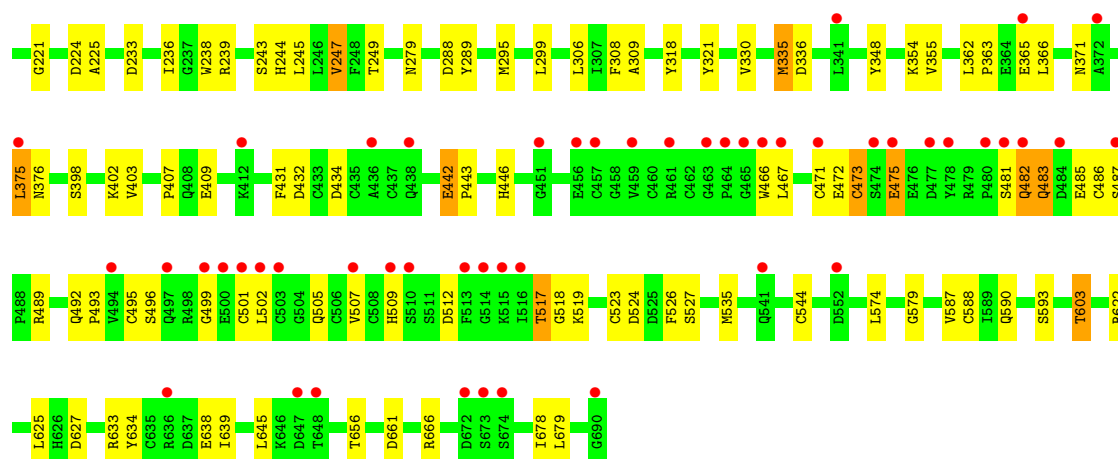
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

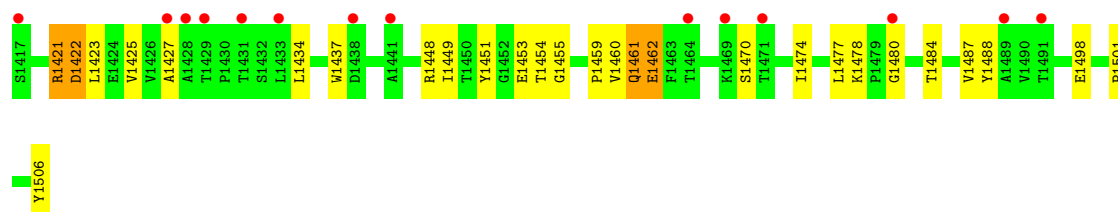
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	5	Total	Mn	0	0
			5	5		
8	B	3	Total	Mn	0	0
			3	3		

- Molecule 9 is water.

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



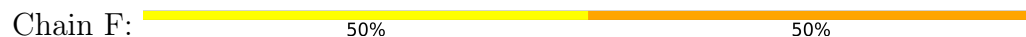
• Molecule 3: Fibronectin, HR10 variant



• 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

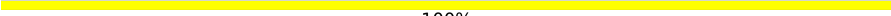


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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%

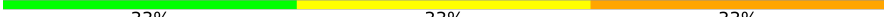
MAG1
MAG2

- 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
MAN5
MAN6

- 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) 90.8 (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)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.238 , 0.268 0.238 , 0.268	Depositor DCC
R_{free} test set	2459 reflections (4.45%)	wwPDB-VP
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
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

Xtriage'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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HRG, BMA, MAN, MN, 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	0.10	0/7319	0.33	0/9922
2	B	0.12	0/5390	0.38	2/7289 (0.0%)
3	C	0.15	0/685	0.43	0/943
All	All	0.11	0/13394	0.36	2/18154 (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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	471	CYS	CA-C-N	6.36	133.69	121.54
2	B	471	CYS	C-N-CA	6.36	133.69	121.54

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	B	482	GLN	Peptide
2	B	496	SER	Peptide
2	B	76	ASP	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	7163	0	6982	112	0
2	B	5294	0	5024	98	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	228	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 9.

All (228) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:ARG:HH21	2:B:86:GLN:HG2	1.52	0.74
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
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

Continued on next page...

Continued from previous page...

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:517:THR:OG1	2:B:518:GLY:N	2.35	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
1:A:496:GLU:OE1	1:A:522:SER:OG	2.27	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
2:B:622:ARG:HH12	2:B:661:ASP:CG	2.19	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:820:MET:HE2	1:A:886:VAL:HG22	1.96	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: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:158:ASP:HB3	2:B:187:MET:HE1	1.97	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:475:GLU:H	2:B:475:GLU:HG3	1.55	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
1:A:768:THR:C	1:A:770:GLU:H	2.24	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:210:THR:HG23	1:A:261:MET:HE3	1.98	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
1:A:115:ARG:O	1:A:116:THR:OG1	2.31	0.43
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:70:SER:OG	2:B:80:VAL:O	2.36	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
2:B:590:GLN:O	2:B:593:SER:OG	2.37	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:472:GLU:O	2:B:473:CYS:C	2.64	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:335:MET:HE3	2:B:335:MET:HB3	1.76	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:426:ALA:C	1:A:428:GLY:H	2.29	0.41
1:A:505:LYS:HG2	1:A:506:GLY:N	2.36	0.41
1:A:89:LYS:HG3	1:A:92:GLN:OE1	2.20	0.40
1:A:870:HIS:HE2	1:A:917:SER:HG	1.61	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: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: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
2:B:483:GLN:C	2:B:485:GLU:H	2.30	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	916/954 (96%)	857 (94%)	59 (6%)	0	100	100
2	B	688/690 (100%)	607 (88%)	77 (11%)	4 (1%)	21	52
3	C	87/90 (97%)	72 (83%)	15 (17%)	0	100	100
All	All	1691/1734 (98%)	1536 (91%)	151 (9%)	4 (0%)	43	73

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 ⓘ

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%)	762 (98%)	18 (2%)	44	70
2	B	612/612 (100%)	598 (98%)	14 (2%)	44	70
3	C	74/74 (100%)	66 (89%)	8 (11%)	6	25
All	All	1466/1495 (98%)	1426 (97%)	40 (3%)	39	67

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	155	CYS
1	A	243	VAL
1	A	275	TYR
1	A	347	LEU
1	A	427	PHE
1	A	508	ILE
1	A	544	ASP
1	A	594	LEU
1	A	623	ASN
1	A	634	GLN
1	A	654	ILE
1	A	672	THR
1	A	768	THR
1	A	806	ASN
1	A	874	CYS
1	A	913	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	916	HIS
2	B	26	CYS
2	B	107	VAL
2	B	123	SER
2	B	193	VAL
2	B	247	VAL
2	B	335	MET
2	B	375	LEU
2	B	376	ASN
2	B	466	TRP
2	B	475	GLU
2	B	501	CYS
2	B	517	THR
2	B	587	VAL
2	B	603	THR
3	C	1421	ARG
3	C	1422	ASP
3	C	1423	LEU
3	C	1460	VAL
3	C	1461	GLN
3	C	1462	GLU
3	C	1477	LEU
3	C	1484	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	A	314	GLN
1	A	327	GLN
1	A	521	HIS
1	A	716	GLN
1	A	718	GLN
1	A	762	HIS
1	A	784	ASN
1	A	913	ASN
1	A	915	ASN
2	B	339	ASN
2	B	449	ASN
2	B	590	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	0.80	0	6,12,14	0.45	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	-	5/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) 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
3	C	1493	HRG	C-CA-CB-CG'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

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	4,1	14,14,15	0.31	0	17,19,21	0.41	0
4	NAG	D	2	4	14,14,15	0.24	0	17,19,21	0.45	0
5	NAG	E	1	1,5	14,14,15	0.26	0	17,19,21	0.39	0
5	NAG	E	2	5	14,14,15	0.23	0	17,19,21	0.41	0
5	BMA	E	3	5	11,11,12	0.69	0	15,15,17	0.81	0
5	BMA	E	4	5	11,11,12	1.21	1 (9%)	15,15,17	1.03	1 (6%)
5	MAN	E	5	5	11,11,12	0.93	1 (9%)	15,15,17	0.81	1 (6%)
5	MAN	E	6	5	11,11,12	0.65	0	15,15,17	1.03	2 (13%)
4	NAG	F	1	4,1	14,14,15	0.46	0	17,19,21	1.42	3 (17%)
4	NAG	F	2	4	14,14,15	0.24	0	17,19,21	0.41	0
4	NAG	G	1	4,1	14,14,15	0.40	0	17,19,21	0.70	1 (5%)
4	NAG	G	2	4	14,14,15	0.77	1 (7%)	17,19,21	0.95	1 (5%)
4	NAG	H	1	4,2	14,14,15	0.31	0	17,19,21	0.53	0
4	NAG	H	2	4	14,14,15	0.89	2 (14%)	17,19,21	0.91	1 (5%)
6	NAG	I	1	6,2	14,14,15	0.20	0	17,19,21	0.48	0
6	NAG	I	2	6	14,14,15	0.66	1 (7%)	17,19,21	1.42	3 (17%)
6	BMA	I	3	6	11,11,12	0.79	0	15,15,17	1.05	1 (6%)
4	NAG	J	1	4,2	14,14,15	0.60	1 (7%)	17,19,21	1.37	1 (5%)
4	NAG	J	2	4	14,14,15	0.24	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	4,1	-	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	4,1	-	6/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	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	4,2	-	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	6,2	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	4/6/23/26	0/1/1/1
6	BMA	I	3	6	-	1/2/19/22	0/1/1/1
4	NAG	J	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	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	2.47	1.47	1.43
5	E	4	BMA	C4-C5	2.32	1.58	1.53
5	E	5	MAN	O5-C1	-2.32	1.39	1.43
6	I	2	NAG	C1-C2	2.19	1.55	1.52
4	G	2	NAG	O5-C1	2.17	1.47	1.43
4	H	2	NAG	C1-C2	2.14	1.55	1.52
4	J	1	NAG	O5-C1	2.11	1.47	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1	NAG	C1-O5-C5	4.91	118.77	112.19
4	F	1	NAG	C2-N2-C7	4.62	129.09	122.90
4	J	2	NAG	C1-O5-C5	4.56	118.30	112.19
6	I	2	NAG	C2-N2-C7	4.49	128.92	122.90
4	G	2	NAG	C1-O5-C5	3.67	117.11	112.19
4	H	2	NAG	C1-O5-C5	3.47	116.83	112.19
6	I	3	BMA	C1-O5-C5	2.72	115.83	112.19
5	E	6	MAN	C1-O5-C5	2.55	115.60	112.19
5	E	6	MAN	O2-C2-C3	-2.24	105.51	110.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	C1-C2-N2	2.21	113.92	110.43
4	G	1	NAG	C1-O5-C5	2.15	115.07	112.19
5	E	5	MAN	O2-C2-C3	-2.15	105.70	110.15
4	F	1	NAG	C1-O5-C5	2.08	114.97	112.19
6	I	2	NAG	C1-C2-N2	2.04	113.65	110.43
5	E	4	BMA	C3-C4-C5	2.04	113.92	110.23
6	I	2	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (31) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

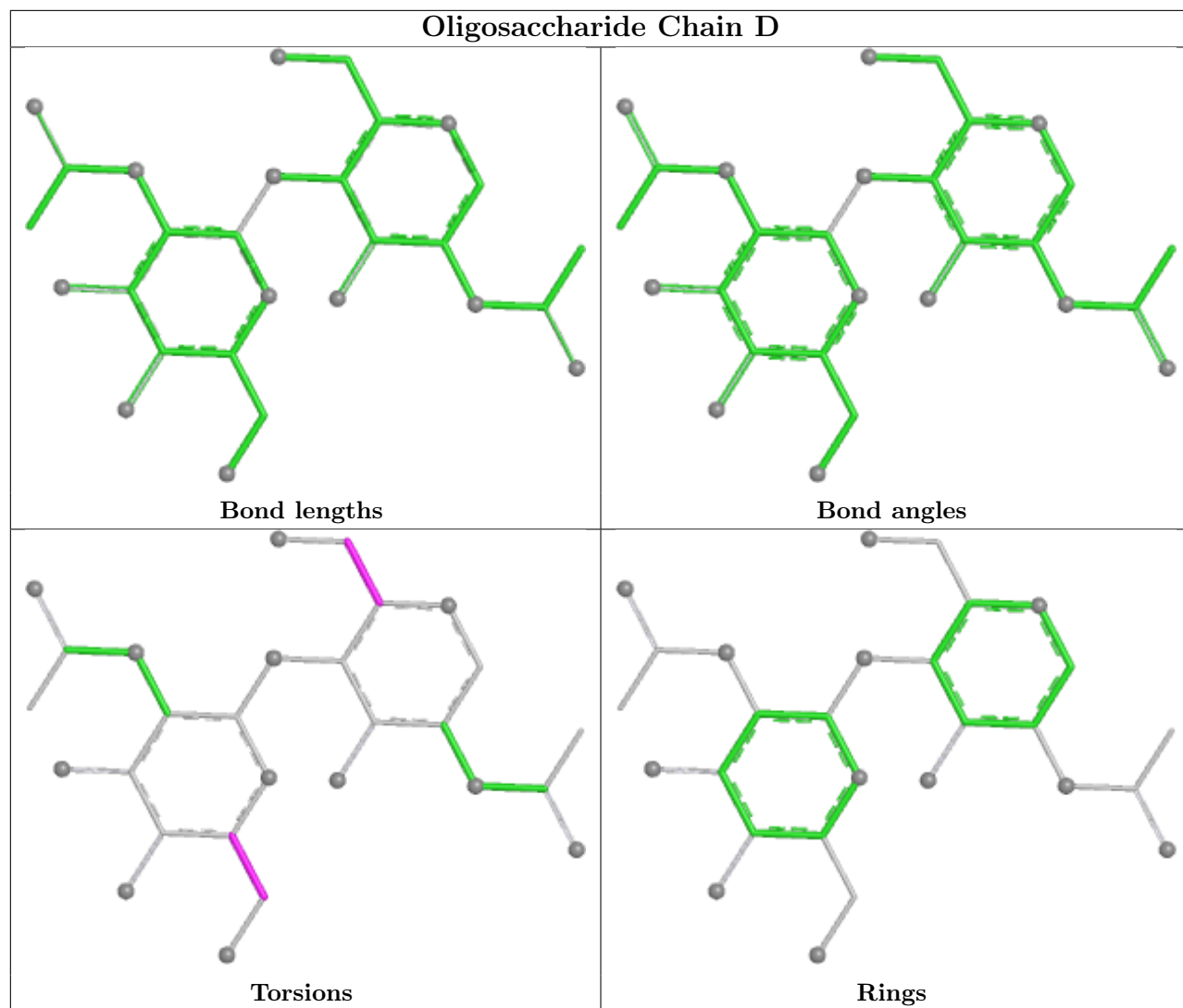
Mol	Chain	Res	Type	Atoms
6	I	1	NAG	O5-C5-C6-O6

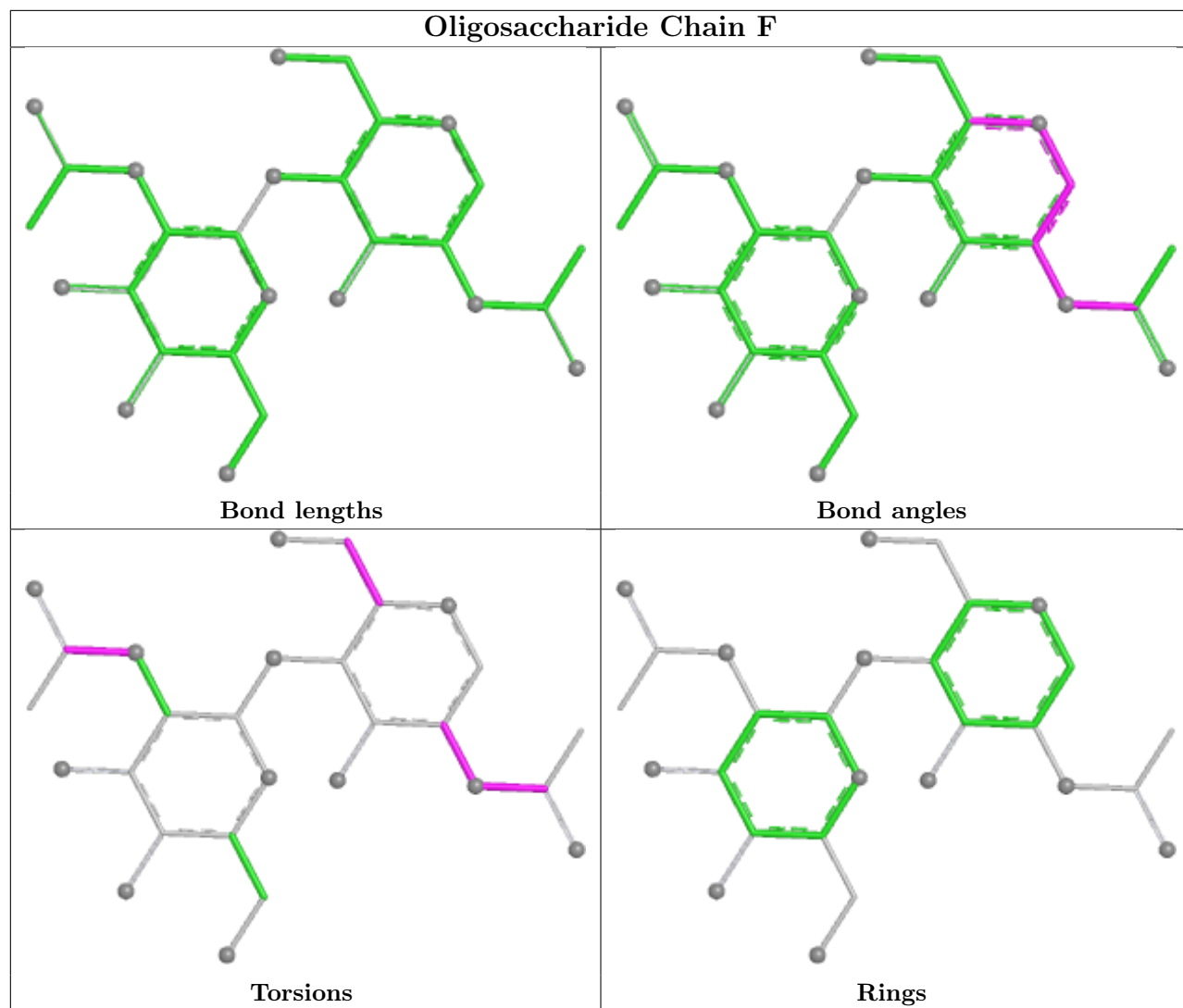
There are no ring outliers.

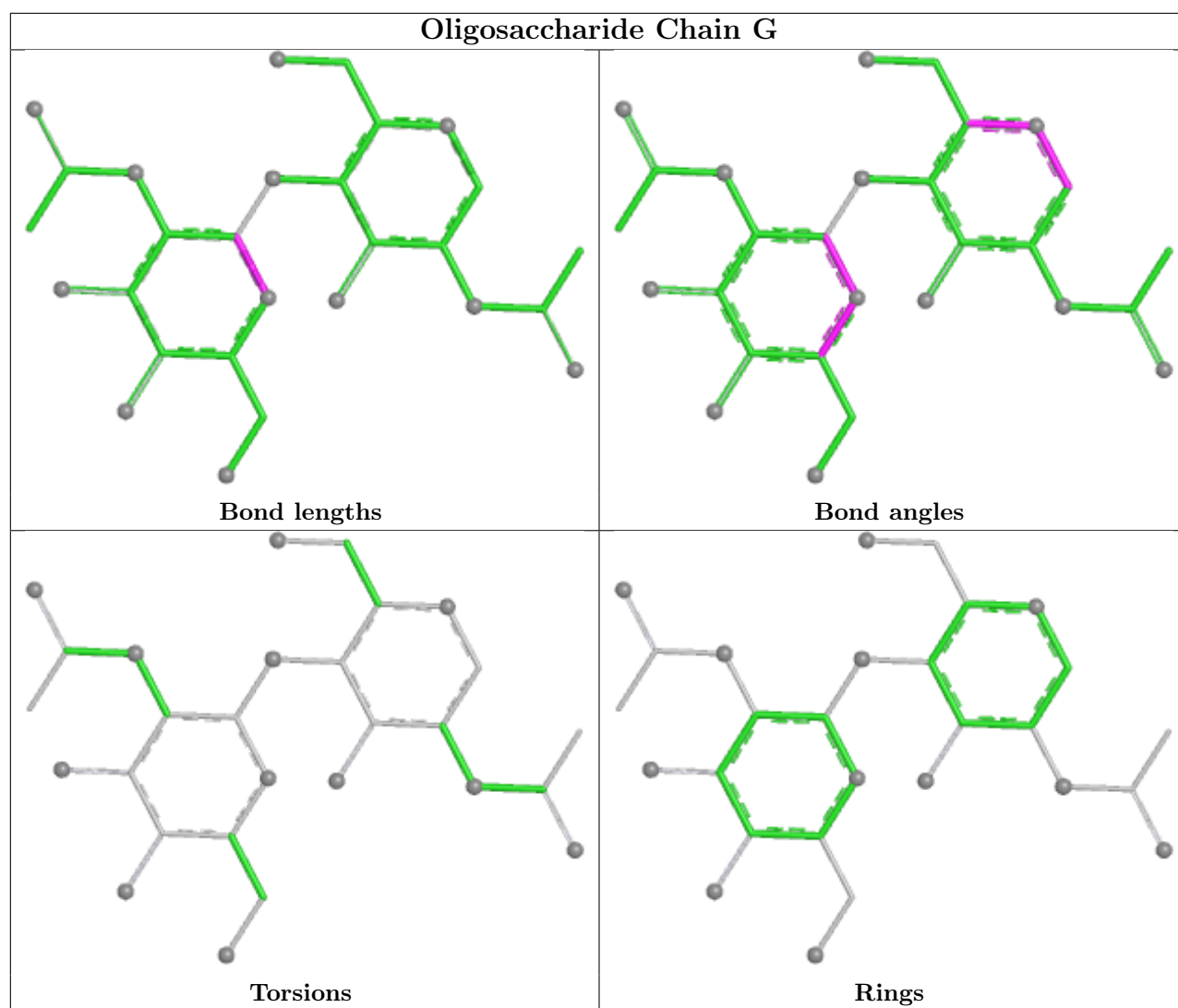
7 monomers are involved in 6 short contacts:

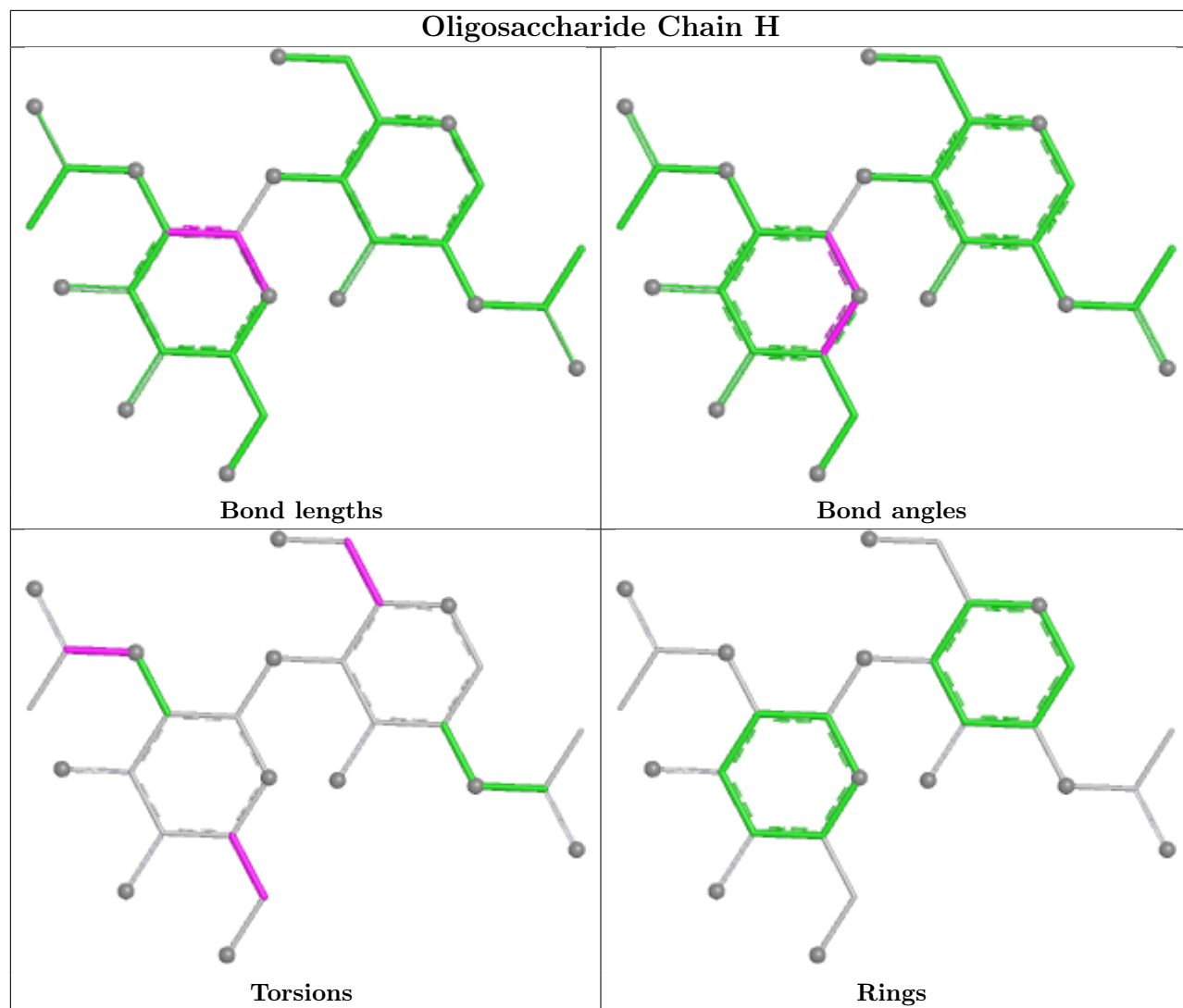
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	NAG	1	0
4	G	1	NAG	1	0
6	I	2	NAG	1	0
5	E	4	BMA	1	0
4	G	2	NAG	1	0
4	F	1	NAG	3	0
5	E	5	MAN	1	0

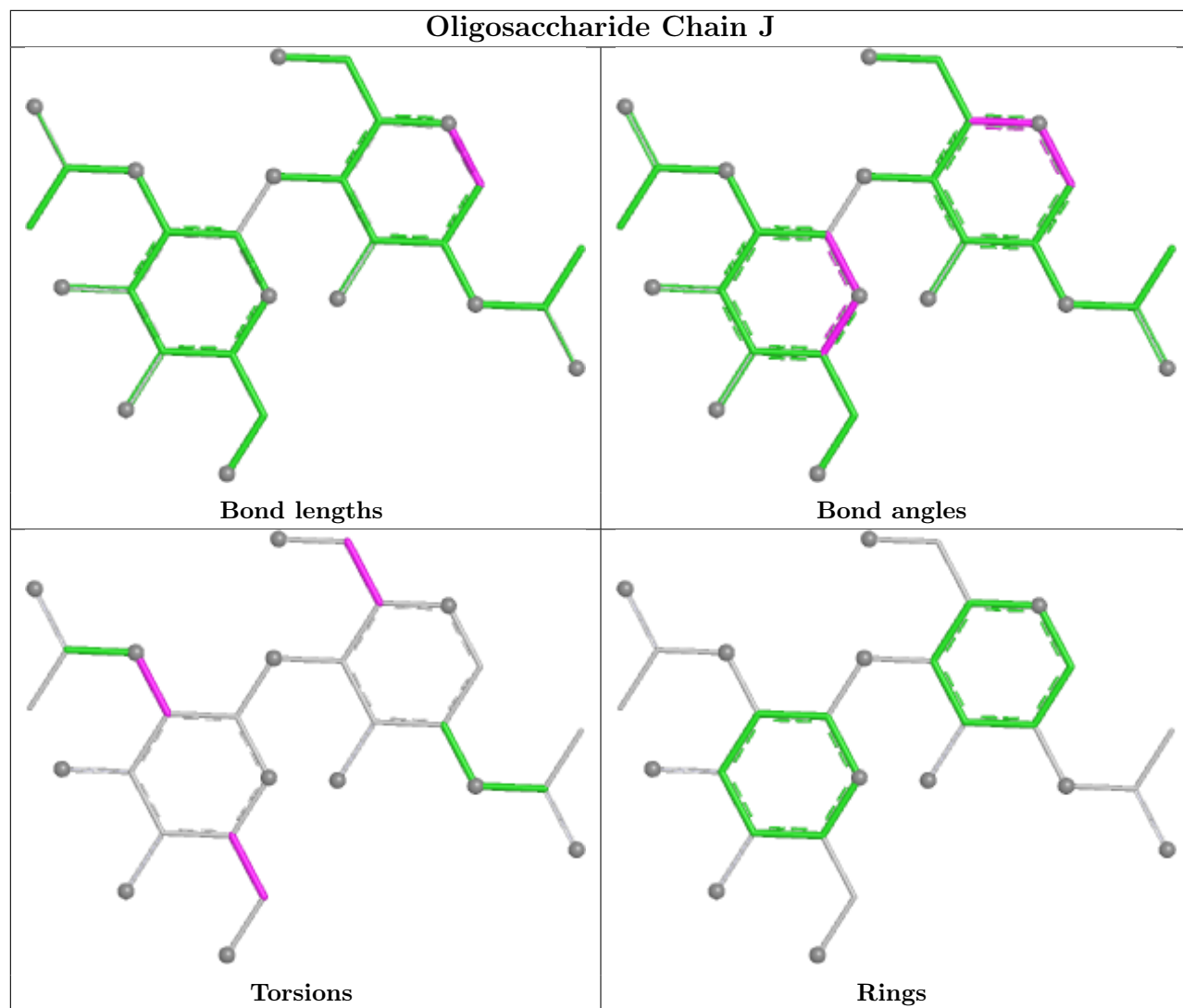
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



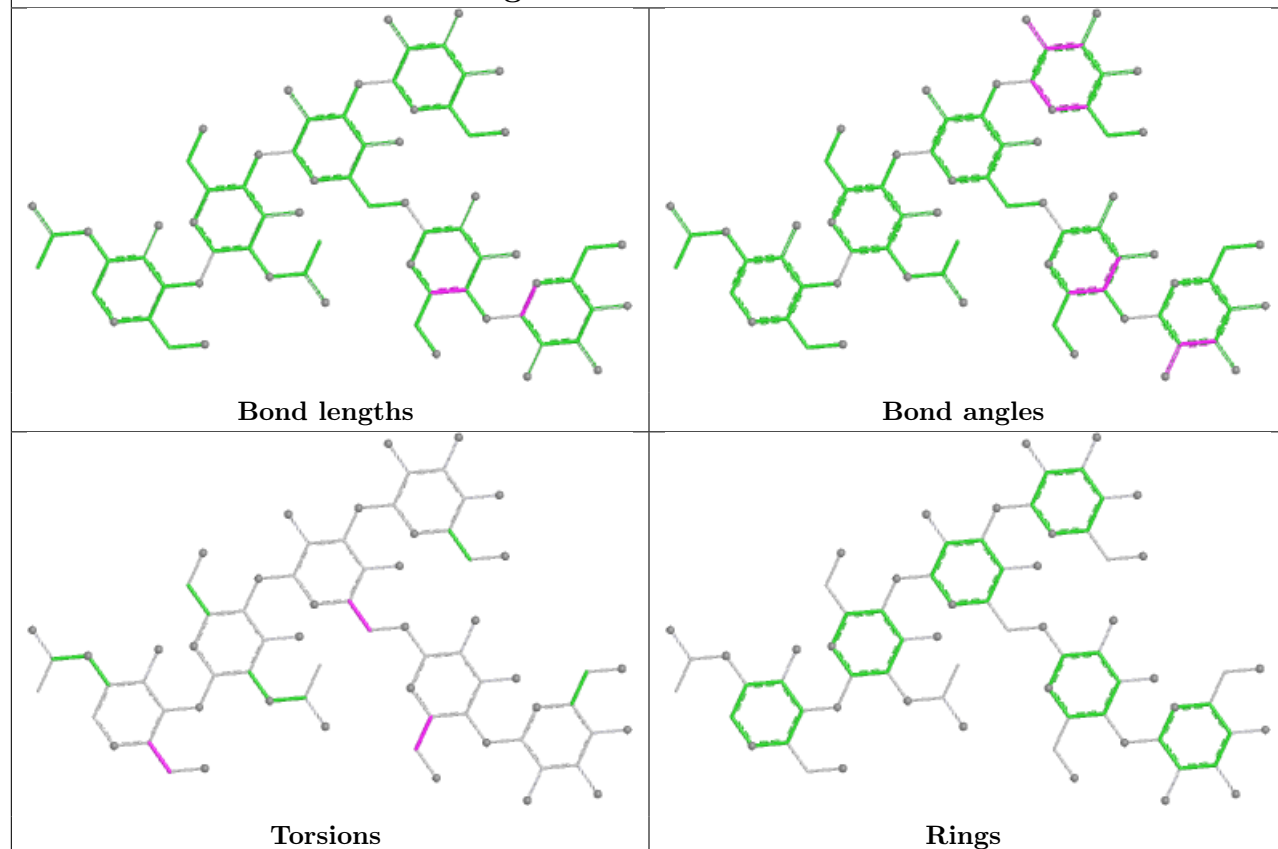




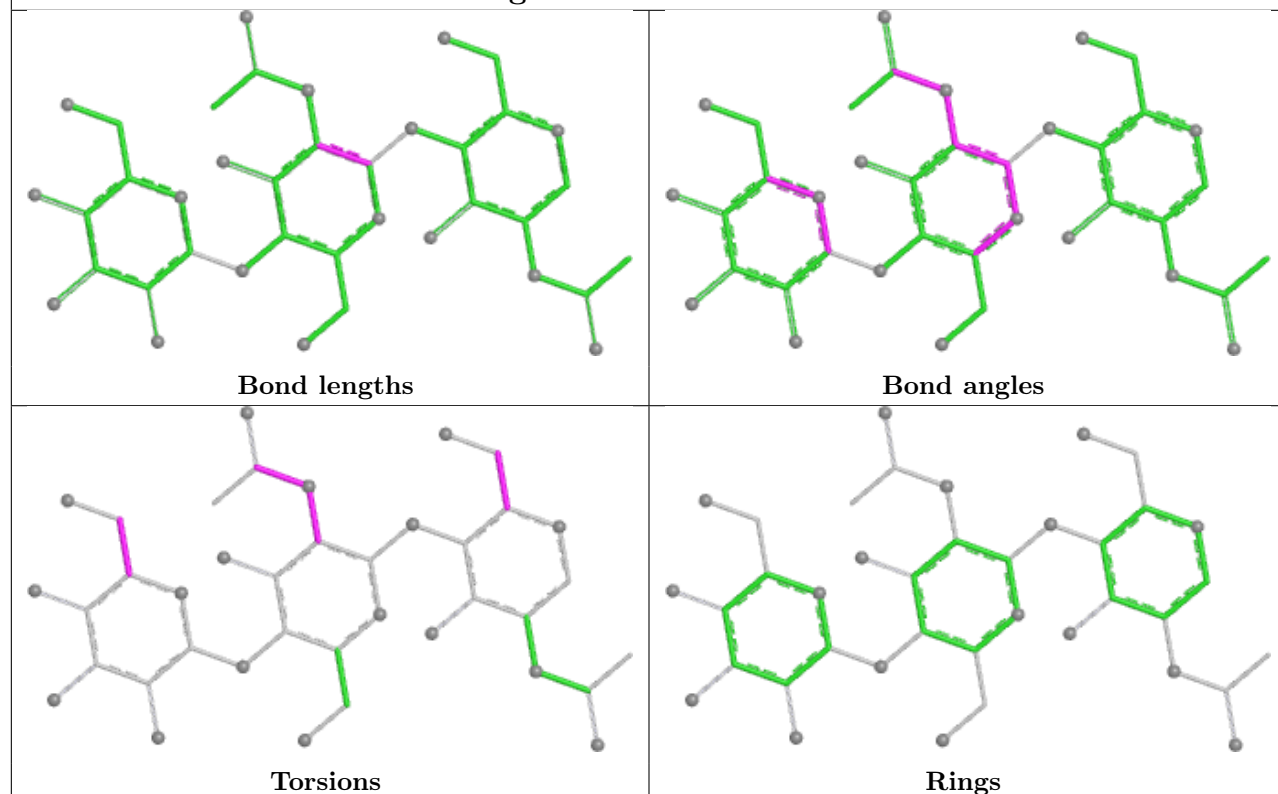




Oligosaccharide Chain E



Oligosaccharide Chain I



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	1005	1	14,14,15	0.19	0	17,19,21	0.44	0
7	NAG	A	1004	1	14,14,15	0.26	0	17,19,21	0.46	0
7	NAG	A	1002	1	14,14,15	0.47	0	17,19,21	1.33	2 (11%)
7	NAG	A	1003	1	14,14,15	0.24	0	17,19,21	0.49	0
7	NAG	A	1001	1	14,14,15	0.83	1 (7%)	17,19,21	1.29	1 (5%)
7	NAG	B	701	2	14,14,15	0.64	0	17,19,21	0.86	1 (5%)
7	NAG	B	702	2	14,14,15	0.21	0	17,19,21	0.49	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	1005	1	-	3/6/23/26	0/1/1/1
7	NAG	A	1004	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1002	1	-	4/6/23/26	0/1/1/1
7	NAG	A	1003	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1001	1	-	2/6/23/26	0/1/1/1
7	NAG	B	701	2	-	2/6/23/26	0/1/1/1
7	NAG	B	702	2	-	2/6/23/26	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	2.95	1.48	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1001	NAG	C1-O5-C5	5.08	119.00	112.19
7	A	1002	NAG	C2-N2-C7	4.61	129.08	122.90
7	B	701	NAG	C1-O5-C5	3.30	116.61	112.19
7	A	1002	NAG	C1-C2-N2	2.16	113.84	110.43

There are no chirality outliers.

All (14) 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	A	1001	NAG	C4-C5-C6-O6
7	B	702	NAG	C4-C5-C6-O6
7	B	701	NAG	O5-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	C4-C5-C6-O6
7	A	1003	NAG	O5-C5-C6-O6
7	A	1005	NAG	O5-C5-C6-O6
7	A	1002	NAG	C1-C2-N2-C7
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%)	0.24	42 (4%) 37 20	22, 56, 111, 148	0
2	B	690/690 (100%)	0.76	70 (10%) 12 6	29, 77, 159, 204	2 (0%)
3	C	89/90 (98%)	1.13	14 (15%) 5 2	57, 110, 144, 159	0
All	All	1699/1734 (97%)	0.50	126 (7%) 20 11	22, 67, 141, 204	2 (0%)

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	509	HIS	6.4
2	B	510	SER	6.1
1	A	538	LEU	5.3
2	B	507	VAL	5.0
2	B	516	ILE	4.9
2	B	36	PRO	4.6
2	B	31	LEU	4.5
1	A	940	ASP	4.4
2	B	35	SER	4.3
1	A	508	ILE	4.1
2	B	33	LEU	4.0
1	A	954	GLY	3.9
2	B	341	LEU	3.9
2	B	7	THR	3.9
2	B	501	CYS	3.8
2	B	4	ILE	3.7
2	B	515	LYS	3.7
1	A	892	GLY	3.6
1	A	909	MET	3.6
2	B	480	PRO	3.5
1	A	801	TYR	3.4
2	B	500	GLU	3.2
2	B	478	TYR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	463	GLY	3.2
2	B	513	PHE	3.2
1	A	480	LYS	3.2
1	A	416	LYS	3.1
2	B	690	GLY	3.1
2	B	673	SER	3.0
1	A	411	ALA	3.0
2	B	466	TRP	3.0
1	A	835	ILE	2.9
3	C	1428	ALA	2.9
2	B	10	VAL	2.9
2	B	502	LEU	2.9
1	A	532	LEU	2.9
1	A	547	GLU	2.9
2	B	457	CYS	2.9
2	B	636	ARG	2.9
2	B	482	GLN	2.8
3	C	1427	ALA	2.8
2	B	464	PRO	2.8
1	A	670	PHE	2.8
1	A	652	ASP	2.7
2	B	552	ASP	2.7
1	A	567	THR	2.7
2	B	55	GLU	2.7
2	B	467	LEU	2.7
1	A	306	ASP	2.7
2	B	494	VAL	2.7
1	A	490	LYS	2.7
2	B	474	SER	2.7
1	A	467	ALA	2.7
3	C	1441	ALA	2.6
2	B	459	VAL	2.6
2	B	1	GLY	2.6
2	B	41	LYS	2.6
2	B	9	GLY	2.5
1	A	552	LEU	2.5
3	C	1433	LEU	2.5
2	B	647	ASP	2.5
2	B	375	LEU	2.5
2	B	438	GLN	2.5
1	A	703	GLN	2.5
1	A	539	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	649	LEU	2.4
1	A	771	ASP	2.4
1	A	481	ALA	2.4
2	B	484	ASP	2.4
1	A	479	LEU	2.4
1	A	706	GLU	2.4
2	B	94	PRO	2.3
1	A	167	ASP	2.3
2	B	499	GLY	2.3
2	B	514	GLY	2.3
3	C	1431	THR	2.3
2	B	475	GLU	2.3
2	B	173	LEU	2.3
2	B	541	GLN	2.3
1	A	655	GLY	2.2
2	B	436	ALA	2.2
3	C	1469	LYS	2.2
2	B	456	GLU	2.2
1	A	873	GLY	2.2
2	B	451	GLY	2.2
3	C	1464	THR	2.2
3	C	1491	THR	2.2
3	C	1417	SER	2.2
1	A	938	ILE	2.2
2	B	365	GLU	2.2
1	A	444	ASN	2.2
2	B	372	ALA	2.2
1	A	893	LYS	2.2
3	C	1438	ASP	2.2
2	B	37	ARG	2.2
1	A	629	VAL	2.2
2	B	54	ILE	2.2
2	B	2	PRO	2.2
1	A	625	LEU	2.1
2	B	497	GLN	2.1
1	A	396	ALA	2.1
2	B	648	THR	2.1
3	C	1429	THR	2.1
2	B	481	SER	2.1
2	B	471	CYS	2.1
2	B	503	CYS	2.1
1	A	939	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	674	SER	2.1
2	B	25	TRP	2.1
2	B	412	LYS	2.1
1	A	874	CYS	2.1
2	B	672	ASP	2.1
2	B	78	SER	2.1
2	B	487	SER	2.1
1	A	505	LYS	2.1
2	B	50	ALA	2.1
1	A	506	GLY	2.1
1	A	260	ASN	2.0
2	B	477	ASP	2.0
2	B	465	GLY	2.0
2	B	461	ARG	2.0
2	B	162	SER	2.0
3	C	1471	THR	2.0
3	C	1489	ALA	2.0
3	C	1480	GLY	2.0
1	A	502	LEU	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	0.89	0.15	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.

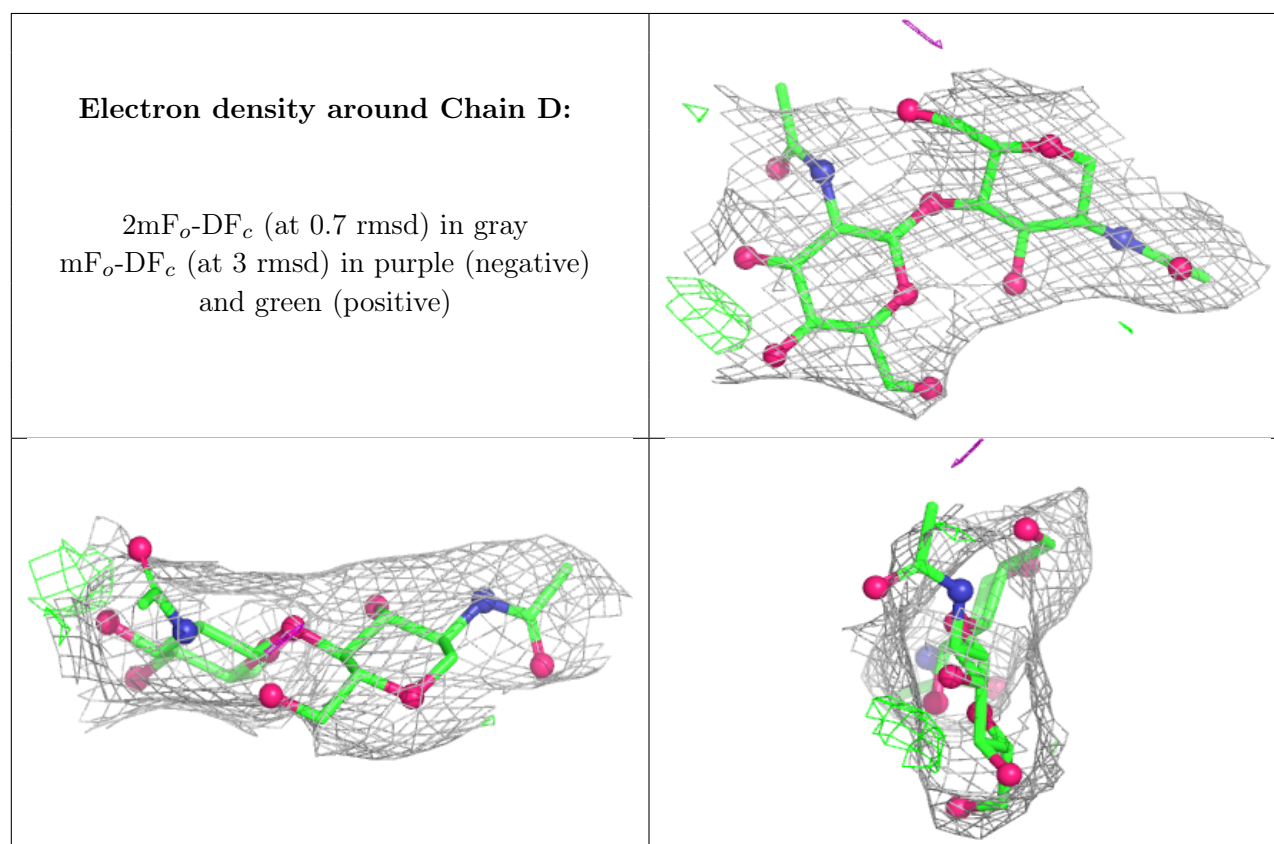
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	J	2	14/15	0.35	0.16	66,117,129,133	0
4	NAG	G	2	14/15	0.48	0.18	65,94,122,126	0
4	NAG	F	2	14/15	0.48	0.17	82,111,123,127	0

Continued on next page...

Continued from previous page...

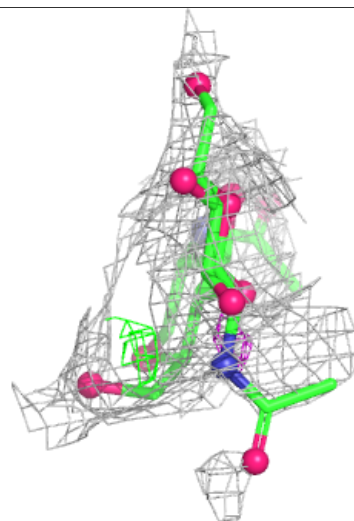
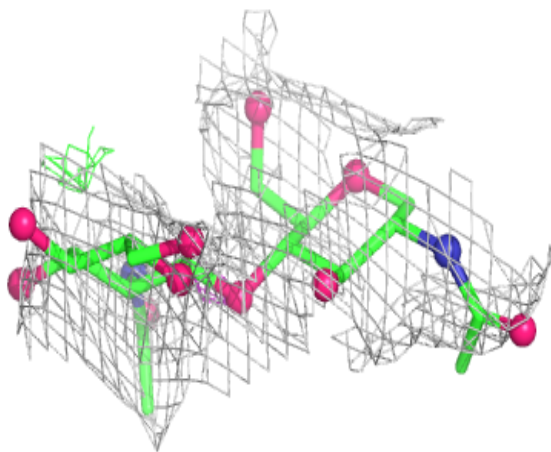
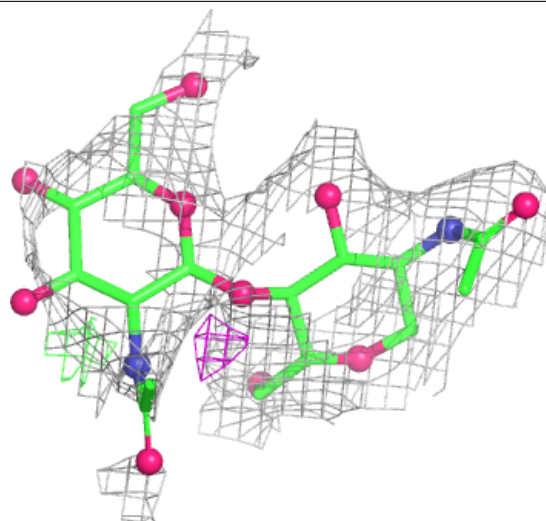
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	H	2	14/15	0.55	0.13	95,104,114,116	0
4	NAG	F	1	14/15	0.59	0.14	78,95,105,111	0
4	NAG	G	1	14/15	0.60	0.15	41,78,95,115	0
4	NAG	J	1	14/15	0.63	0.15	83,90,120,126	0
5	MAN	E	6	11/12	0.69	0.11	72,81,97,97	0
6	BMA	I	3	11/12	0.70	0.15	67,95,109,113	0
5	MAN	E	5	11/12	0.75	0.13	62,81,96,105	0
6	NAG	I	2	14/15	0.76	0.17	92,104,114,130	0
5	BMA	E	4	11/12	0.81	0.11	73,77,88,94	0
5	BMA	E	3	11/12	0.82	0.11	65,73,80,88	0
4	NAG	D	2	14/15	0.82	0.12	61,70,92,107	0
4	NAG	H	1	14/15	0.84	0.12	84,92,102,105	0
5	NAG	E	2	14/15	0.92	0.10	29,45,67,83	0
6	NAG	I	1	14/15	0.93	0.09	70,86,96,102	0
5	NAG	E	1	14/15	0.93	0.09	29,34,42,58	0
4	NAG	D	1	14/15	0.93	0.09	33,46,65,79	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.



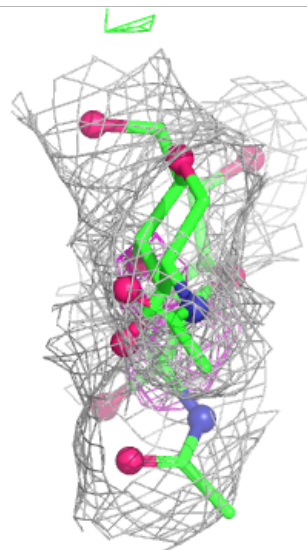
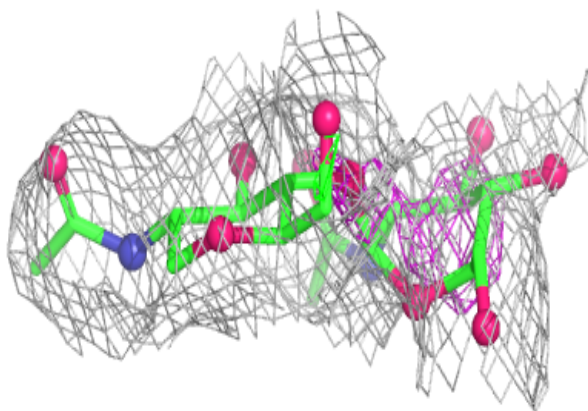
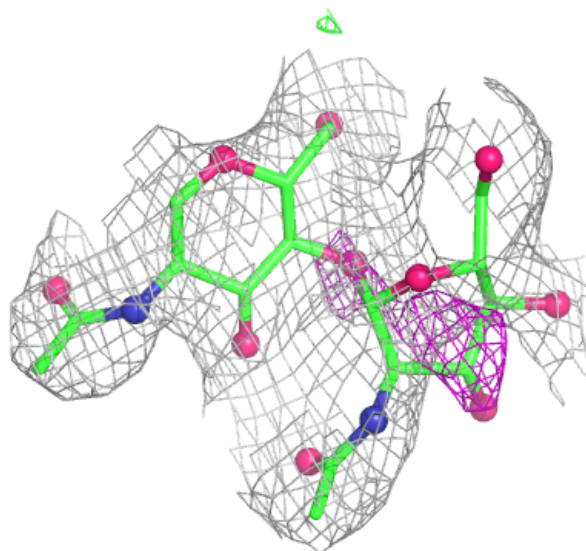
Electron density around Chain F:

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



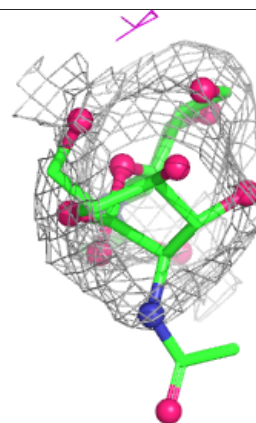
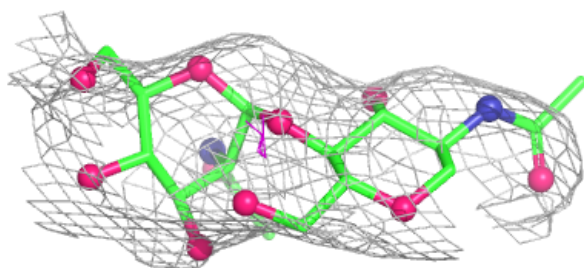
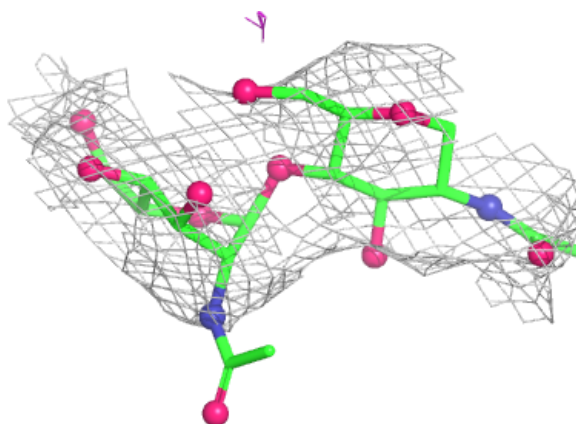
Electron density around Chain G:

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

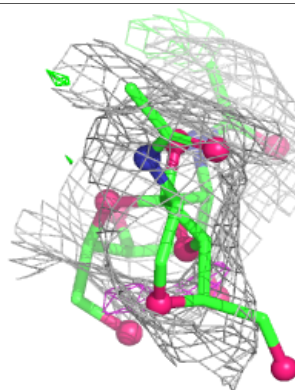
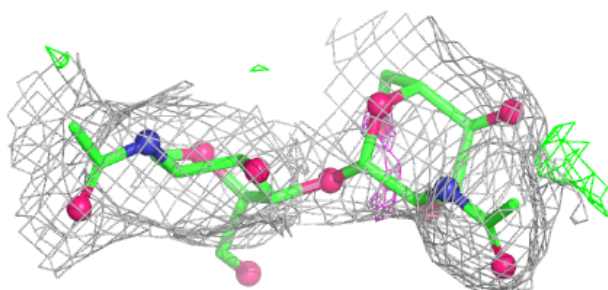
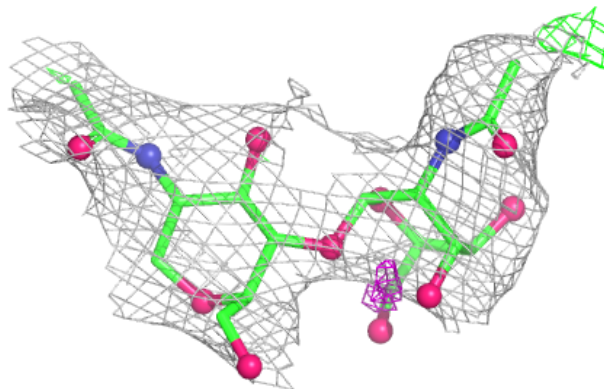


Electron density around Chain H:

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

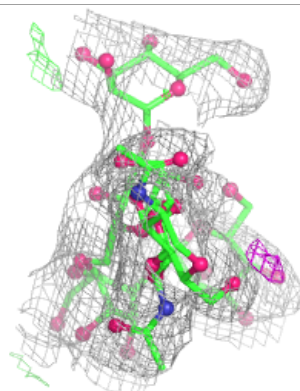
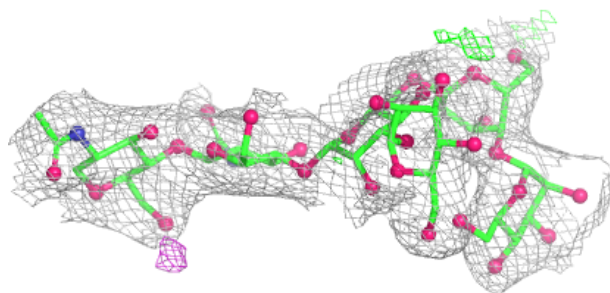
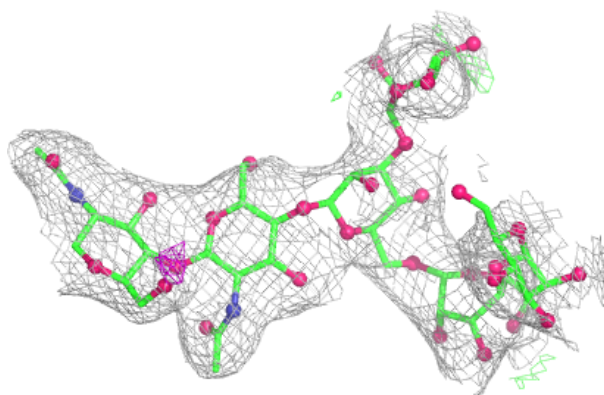
**Electron density around Chain J:**

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

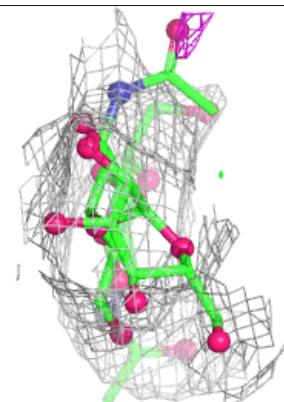
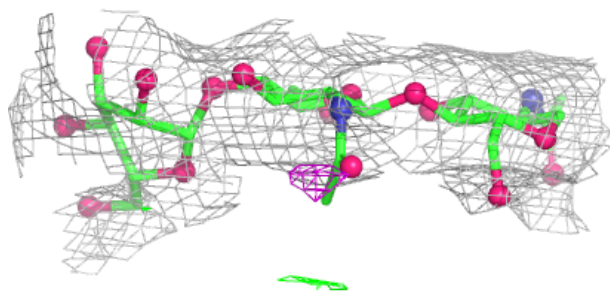
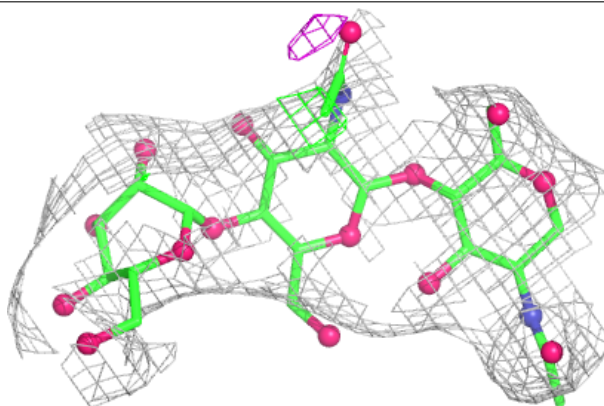


Electron density around Chain E:

$2mF_o-DF_c$ (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

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
7	NAG	A	1003	14/15	0.60	0.15	90,105,115,117	0
7	NAG	B	701	14/15	0.64	0.16	81,103,112,114	0
7	NAG	A	1001	14/15	0.69	0.17	67,80,93,97	0
7	NAG	A	1002	14/15	0.69	0.13	66,90,96,100	0
7	NAG	A	1004	14/15	0.70	0.15	60,79,92,106	0
7	NAG	B	702	14/15	0.75	0.14	62,85,95,100	0
7	NAG	A	1005	14/15	0.82	0.11	56,65,81,82	0
8	MN	A	1007	1/1	0.96	0.05	69,69,69,69	0
8	MN	A	1006	1/1	0.99	0.03	68,68,68,68	0
8	MN	A	1008	1/1	0.99	0.03	72,72,72,72	0
8	MN	A	1009	1/1	0.99	0.05	115,115,115,115	0
8	MN	A	1010	1/1	0.99	0.05	70,70,70,70	0
8	MN	B	704	1/1	0.99	0.04	70,70,70,70	0
8	MN	B	703	1/1	1.00	0.03	55,55,55,55	0
8	MN	B	705	1/1	1.00	0.02	51,51,51,51	0

6.5 Other polymers

There are no such residues in this entry.