



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:35 PM UTC

PDB ID : 4MMX / pdb_00004mmx
Title : Integrin AlphaVBeta3 ectodomain bound to the tenth domain of Fibronectin
Authors : van Agthoven, J.; Xiong, J.; Arnaout, M.A.
Deposited on : 2013-09-09
Resolution : 3.32 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

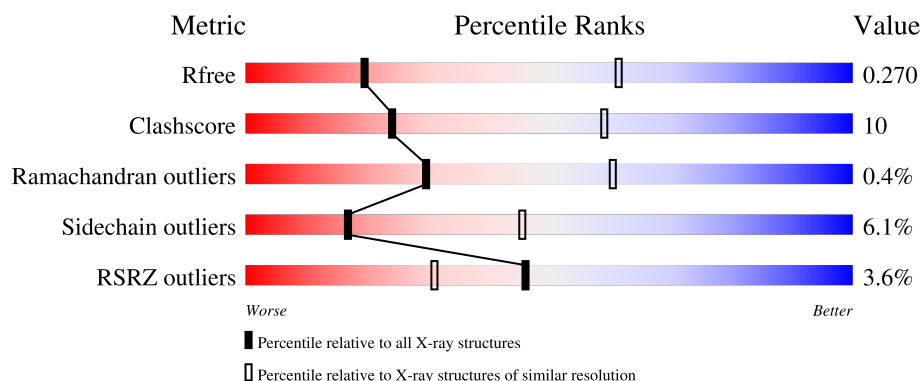
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 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.



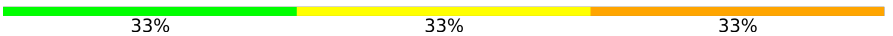
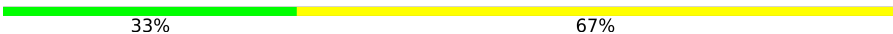
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

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	959	0% 70% 24% • •
2	B	692	5% 76% 21% •
3	C	98	14% 52% 36% 7% 5%
4	D	4	50% 50%
4	G	4	50% 50%

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Mol	Chain	Length	Quality of chain
5	E	2	 50%50%
5	H	2	 100%
5	I	2	 50%50%
5	K	2	 50%50%
6	F	6	 33%33%33%
7	J	3	 67%33%
7	L	3	 33%67%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 13626 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	924	Total	C	N	O	S	0	0	0
			7196	4556	1221	1384	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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	93	Total	C	N	O	0	0	0
			694	438	115	141			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1510	GLY	-	expression tag	UNP P02751
C	1511	LYS	-	expression tag	UNP P02751
C	1512	LYS	-	expression tag	UNP P02751
C	1513	GLY	-	expression tag	UNP P02751
C	1514	LYS	-	expression tag	UNP P02751

- Molecule 4 is an oligosaccharide called 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.



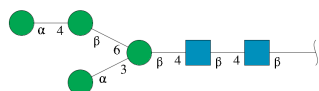
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	G	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



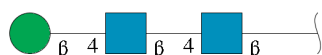
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 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
6	F	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 7 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
7	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

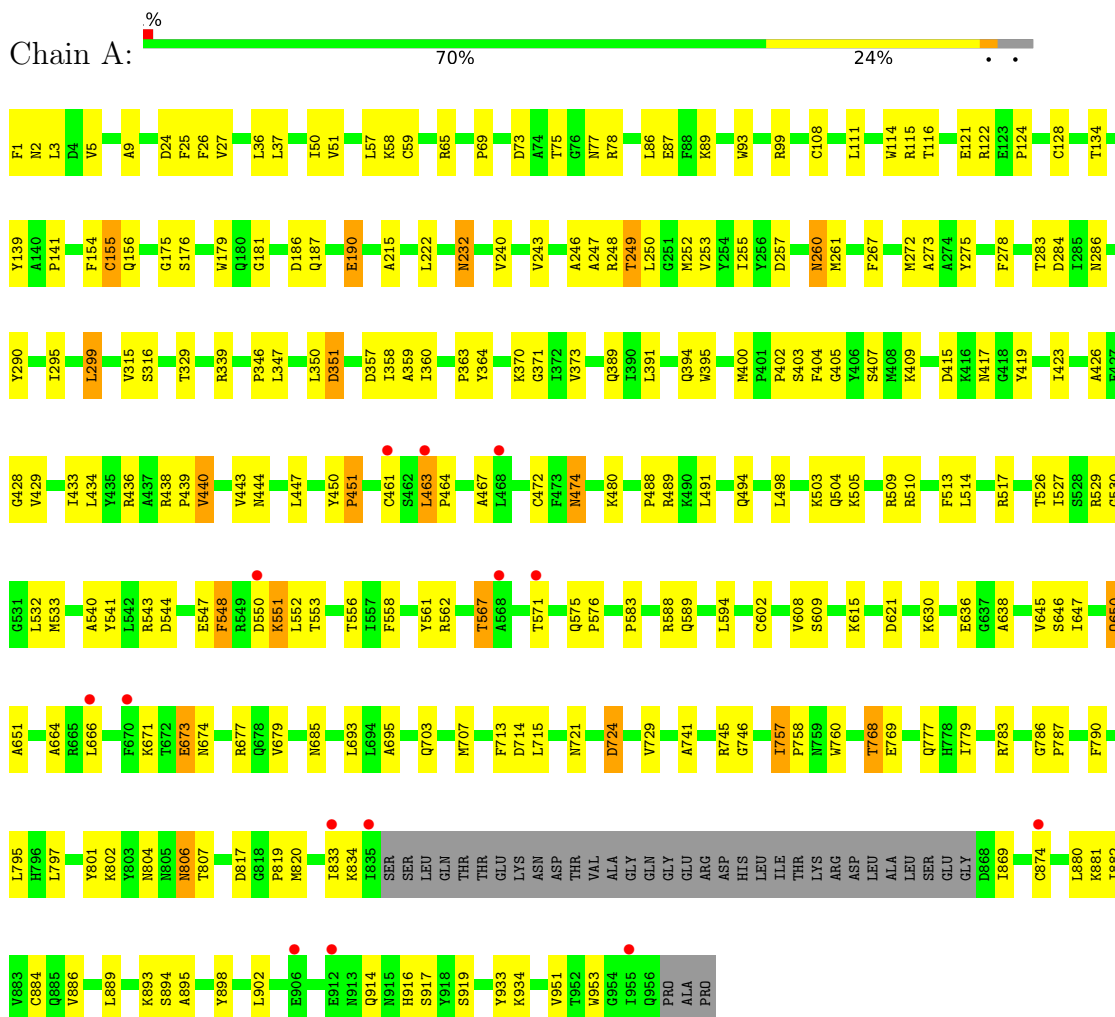
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	2	Total	O	0	0
			2	2		

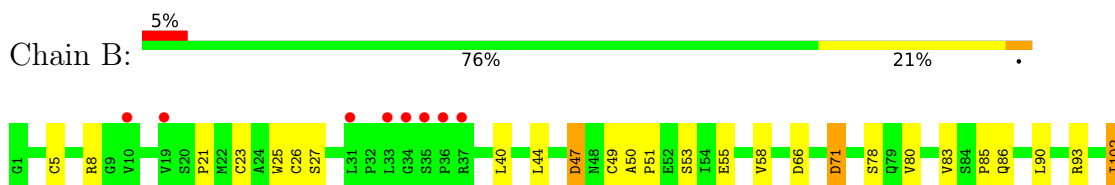
3 Residue-property plots

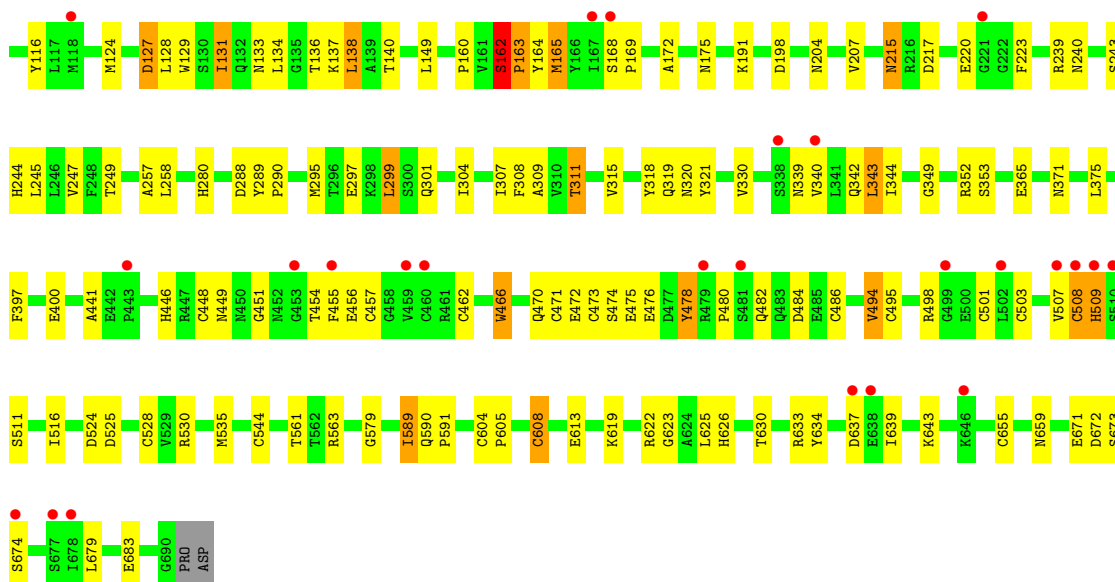
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Integrin alpha-V

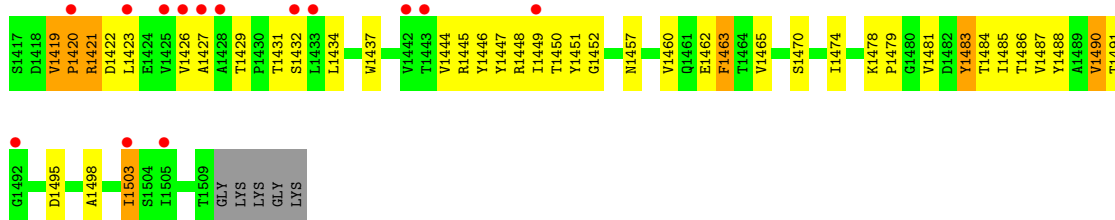


• Molecule 2: Integrin beta-3





- Molecule 3: Fibronectin



- Molecule 4: 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



- Molecule 4: 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



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 50% 50%



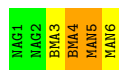
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 50% 50%



- Molecule 6: 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 F: 33% 33% 33%



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 67% 33%



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.86Å 129.86Å 305.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.51 – 3.32 42.51 – 3.32	Depositor EDS
% Data completeness (in resolution range)	88.0 (42.51-3.32) 87.9 (42.51-3.32)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 3.32Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.220 , 0.269 0.220 , 0.270	Depositor DCC
R_{free} test set	1943 reflections (2.89%)	wwPDB-VP
Wilson B-factor (Å ²)	86.7	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13626	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: MAN, MN, BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.15	0/7352	0.36	0/9967
2	B	0.15	0/5390	0.43	0/7289
3	C	0.17	0/710	0.45	0/975
All	All	0.15	0/13452	0.40	0/18231

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
2	B	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	162	SER	Peptide
2	B	475	GLU	Peptide
2	B	78	SER	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	7196	0	7013	153	0
2	B	5294	0	5024	95	0
3	C	694	0	688	28	0
4	D	50	0	43	0	0
4	G	50	0	43	0	0
5	E	28	0	25	0	0
5	H	28	0	25	0	0
5	I	28	0	25	0	0
5	K	28	0	25	1	0
6	F	72	0	61	2	0
7	J	39	0	34	0	0
7	L	39	0	34	0	0
8	A	42	0	39	1	0
8	B	28	0	26	2	0
9	A	5	0	0	0	0
9	B	3	0	0	0	0
10	B	2	0	0	0	0
All	All	13626	0	13105	267	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 10.

All (267) 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)
3:C:1421:ARG:HG2	3:C:1422:ASP:H	1.38	0.87
1:A:488:PRO:HG2	1:A:567:THR:HG22	1.60	0.82
2:B:134:LEU:O	2:B:138:LEU:N	2.13	0.76
1:A:551:LYS:HB3	1:A:553:THR:H	1.49	0.76
1:A:504:GLN:HG2	1:A:509:ARG:HG3	1.67	0.75
1:A:351:ASP:OD1	1:A:351:ASP:N	2.16	0.75
2:B:590:GLN:HG2	2:B:591:PRO:HD2	1.69	0.74
2:B:27:SER:HB2	2:B:53:SER:HB3	1.68	0.73
1:A:480:LYS:HB2	1:A:533:MET:HG2	1.73	0.71
2:B:623:GLY:HA2	2:B:626:HIS:HB3	1.74	0.69
1:A:741:ALA:H	1:A:786:GLY:HA3	1.56	0.69
1:A:187:GLN:HB2	1:A:190:GLU:HB2	1.74	0.69
3:C:1421:ARG:HB2	3:C:1503:ILE:HD12	1.74	0.69
2:B:448:CYS:SG	2:B:449:ASN:ND2	2.62	0.68
1:A:556:THR:HG22	1:A:589:GLN:HG2	1.74	0.68
1:A:769:GLU:HG2	1:A:902:LEU:HD11	1.75	0.68
1:A:779:ILE:HD12	1:A:898:TYR:HD1	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:SER:O	2:B:164:TYR:N	2.28	0.67
2:B:133:ASN:O	2:B:204:ASN:ND2	2.27	0.67
2:B:168:SER:HB2	2:B:169:PRO:HD2	1.75	0.67
2:B:473:CYS:SG	2:B:474:SER:N	2.58	0.67
2:B:446:HIS:HA	2:B:451:GLY:HA2	1.77	0.66
2:B:498:ARG:O	2:B:508:CYS:HB3	1.95	0.66
1:A:503:LYS:HG3	1:A:510:ARG:HD3	1.77	0.66
1:A:609:SER:HB3	1:A:630:LYS:HB3	1.76	0.66
1:A:395:TRP:HE1	1:A:433:ILE:HD11	1.61	0.66
3:C:1451:TYR:HB3	3:C:1485:ILE:HG23	1.77	0.66
1:A:402:PRO:HA	1:A:428:GLY:HA3	1.78	0.65
2:B:124:MET:HA	2:B:127:ASP:OD2	1.98	0.64
1:A:347:LEU:HD11	1:A:357:ASP:HB2	1.79	0.64
1:A:450:TYR:HB3	1:A:451:PRO:HD2	1.79	0.63
1:A:474:ASN:OD1	1:A:474:ASN:N	2.31	0.63
1:A:463:LEU:HA	1:A:467:ALA:HB2	1.80	0.63
2:B:579:GLY:HA2	2:B:589:ILE:HG13	1.79	0.63
1:A:371:GLY:HA3	1:A:404:PHE:HB3	1.80	0.63
1:A:505:LYS:HB3	2:B:509:HIS:CD2	2.32	0.63
1:A:544:ASP:HB3	1:A:547:GLU:HG3	1.82	0.62
1:A:802:LYS:HG2	1:A:807:THR:HA	1.82	0.62
1:A:240:VAL:HG22	1:A:255:ILE:HG12	1.80	0.62
2:B:622:ARG:HH22	2:B:659:ASN:HD22	1.48	0.62
1:A:707:MET:HE2	1:A:934:LYS:H	1.65	0.61
3:C:1448:ARG:HB2	3:C:1488:TYR:HB2	1.82	0.61
1:A:1:PHE:HA	1:A:389:GLN:HB2	1.83	0.61
2:B:71:ASP:OD1	2:B:71:ASP:N	2.32	0.61
1:A:621:ASP:HB2	1:A:787:PRO:HB3	1.81	0.61
3:C:1448:ARG:NH2	3:C:1462:GLU:OE1	2.28	0.61
2:B:8:ARG:NH2	2:B:544:CYS:SG	2.74	0.61
1:A:181:GLY:HA3	1:A:222:LEU:HB3	1.83	0.60
2:B:498:ARG:HD3	2:B:516:ILE:HD13	1.83	0.60
1:A:438:ARG:NE	1:A:575:GLN:O	2.27	0.59
1:A:914:GLN:O	1:A:953:TRP:NE1	2.35	0.59
2:B:129:TRP:HZ3	2:B:339:ASN:HD21	1.50	0.59
2:B:83:VAL:O	2:B:86:GLN:NE2	2.35	0.59
1:A:73:ASP:OD1	1:A:75:THR:OG1	2.19	0.59
1:A:250:LEU:HD12	1:A:272:MET:HG2	1.85	0.59
1:A:347:LEU:HD23	1:A:359:ALA:HB2	1.84	0.59
1:A:768:THR:HG23	1:A:834:LYS:HB2	1.85	0.59
1:A:249:THR:HG23	1:A:273:ALA:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:ASN:O	3:C:1495:ASP:HB3	2.04	0.58
1:A:77:ASN:HB3	1:A:87:GLU:HG3	1.85	0.58
1:A:552:LEU:HD21	1:A:594:LEU:HD22	1.86	0.57
2:B:639:ILE:HG12	2:B:679:LEU:HD23	1.86	0.56
1:A:215:ALA:HB3	3:C:1445:ARG:HD3	1.88	0.56
1:A:447:LEU:O	1:A:588:ARG:NE	2.36	0.56
1:A:646:SER:HB2	1:A:714:ASP:HB2	1.87	0.56
1:A:395:TRP:HB3	1:A:429:VAL:HG11	1.86	0.56
1:A:50:ILE:HD12	1:A:89:LYS:HB2	1.88	0.56
3:C:1437:TRP:O	3:C:1470:SER:OG	2.24	0.56
1:A:645:VAL:HB	1:A:679:VAL:HB	1.88	0.55
1:A:284:ASP:OD2	1:A:290:TYR:N	2.39	0.55
1:A:436:ARG:HH12	1:A:571:THR:HB	1.70	0.55
1:A:664:ALA:HB3	1:A:695:ALA:HB2	1.87	0.55
3:C:1429:THR:OG1	3:C:1431:THR:O	2.23	0.55
1:A:801:TYR:HB2	1:A:880:LEU:HB2	1.86	0.55
3:C:1426:VAL:HB	3:C:1434:LEU:HD23	1.87	0.54
3:C:1478:LYS:HE3	3:C:1479:PRO:HD2	1.88	0.54
1:A:232:ASN:OD1	1:A:232:ASN:N	2.37	0.54
1:A:78:ARG:HB3	1:A:86:LEU:HB3	1.89	0.54
1:A:373:VAL:HB	1:A:391:LEU:HB2	1.88	0.54
2:B:643:LYS:HA	2:B:683:GLU:HG2	1.90	0.54
1:A:347:LEU:HD13	1:A:350:LEU:HB2	1.90	0.54
1:A:513:PHE:HA	1:A:540:ALA:HA	1.90	0.54
2:B:164:TYR:O	2:B:215:ASN:HB2	2.09	0.53
2:B:243:SER:OG	2:B:352:ARG:NH1	2.41	0.53
2:B:134:LEU:O	2:B:137:LYS:N	2.42	0.53
2:B:25:TRP:HB3	2:B:55:GLU:HB2	1.91	0.53
1:A:494:GLN:HB2	1:A:562:ARG:HB3	1.90	0.52
1:A:464:PRO:HD2	1:A:467:ALA:HA	1.92	0.52
3:C:1419:VAL:HG22	3:C:1420:PRO:HD2	1.92	0.52
3:C:1420:PRO:O	3:C:1421:ARG:HB3	2.09	0.52
2:B:561:THR:HG22	2:B:563:ARG:H	1.74	0.52
1:A:155:CYS:HB2	1:A:176:SER:OG	2.09	0.51
3:C:1450:THR:O	3:C:1486:THR:N	2.38	0.51
2:B:239:ARG:O	2:B:244:HIS:NE2	2.43	0.51
2:B:339:ASN:CG	2:B:340:VAL:H	2.19	0.51
1:A:402:PRO:HB3	1:A:429:VAL:HG13	1.92	0.51
1:A:589:GLN:OE1	1:A:685:ASN:ND2	2.43	0.51
2:B:530:ARG:HG2	2:B:535:MET:HA	1.91	0.51
1:A:820:MET:HG3	1:A:886:VAL:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:HG	1:A:350:LEU:HD21	1.93	0.50
2:B:509:HIS:ND1	2:B:509:HIS:N	2.59	0.50
1:A:489:ARG:H	1:A:489:ARG:HD3	1.77	0.50
1:A:804:ASN:O	1:A:806:ASN:ND2	2.45	0.50
1:A:819:PRO:HD3	1:A:893:LYS:HE3	1.93	0.50
2:B:441:ALA:HB1	2:B:455:PHE:HE2	1.77	0.50
1:A:2:ASN:OD1	1:A:2:ASN:N	2.44	0.50
1:A:423:ILE:HG12	1:A:434:LEU:HD23	1.93	0.49
2:B:319:GLN:HA	2:B:330:VAL:HG21	1.94	0.49
2:B:480:PRO:C	2:B:482:GLN:H	2.19	0.49
1:A:498:LEU:HB2	1:A:558:PHE:HB3	1.93	0.49
1:A:498:LEU:HD23	1:A:558:PHE:HD2	1.76	0.49
1:A:783:ARG:HG3	1:A:894:SER:HB3	1.94	0.49
1:A:439:PRO:HD2	1:A:576:PRO:HA	1.94	0.49
1:A:671:LYS:NZ	1:A:673:GLU:OE1	2.39	0.49
2:B:613:GLU:HG2	2:B:625:LEU:HB2	1.93	0.49
3:C:1419:VAL:HG13	3:C:1420:PRO:O	2.13	0.49
2:B:23:CYS:HA	2:B:40:LEU:HB3	1.94	0.49
2:B:288:ASP:OD1	2:B:289:TYR:N	2.38	0.49
1:A:9:ALA:HB3	1:A:434:LEU:HB3	1.95	0.48
1:A:415:ASP:OD2	1:A:417:ASN:ND2	2.46	0.48
1:A:114:TRP:CE2	1:A:116:THR:HA	2.48	0.48
1:A:602:CYS:HA	1:A:636:GLU:OE1	2.13	0.48
2:B:494:VAL:HG12	2:B:501:CYS:HB2	1.94	0.48
1:A:154:PHE:HD2	2:B:163:PRO:HB3	1.78	0.48
1:A:510:ARG:HH12	1:A:553:THR:HB	1.79	0.48
1:A:24:ASP:OD1	1:A:25:PHE:N	2.42	0.48
1:A:404:PHE:HE1	1:A:433:ILE:HD12	1.79	0.48
1:A:405:GLY:C	1:A:407:SER:H	2.22	0.48
2:B:340:VAL:HA	2:B:343:LEU:HD23	1.95	0.48
1:A:179:TRP:HZ2	2:B:163:PRO:HB2	1.78	0.48
2:B:245:LEU:HD22	2:B:307:ILE:HD11	1.96	0.48
2:B:509:HIS:C	2:B:511:SER:H	2.21	0.48
1:A:543:ARG:NH1	1:A:547:GLU:OE1	2.46	0.47
1:A:674:ASN:HD22	8:A:1002:NAG:H61	1.78	0.47
2:B:136:THR:H	2:B:204:ASN:HD21	1.60	0.47
2:B:671:GLU:HG3	2:B:672:ASP:H	1.79	0.47
1:A:139:TYR:OH	1:A:186:ASP:OD2	2.25	0.47
1:A:248:ARG:NH1	1:A:272:MET:SD	2.87	0.47
1:A:529:ARG:HG2	1:A:530:GLY:H	1.79	0.47
2:B:5:CYS:SG	2:B:40:LEU:HD23	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:HIS:HB2	2:B:304:ILE:HA	1.95	0.47
1:A:243:VAL:HG22	1:A:246:ALA:HB2	1.96	0.47
2:B:311:THR:O	2:B:315:VAL:HG23	2.14	0.47
1:A:869:ILE:HA	1:A:917:SER:HB2	1.96	0.47
2:B:400:GLU:HB2	5:K:1:NAG:H83	1.96	0.47
1:A:472:CYS:HA	1:A:541:TYR:HA	1.97	0.47
1:A:666:LEU:HD11	1:A:693:LEU:HD13	1.97	0.47
2:B:295:MET:O	2:B:299:LEU:HB2	2.15	0.47
2:B:318:TYR:HA	2:B:321:TYR:HB2	1.97	0.47
1:A:57:LEU:HA	1:A:69:PRO:HA	1.96	0.46
2:B:50:ALA:N	2:B:51:PRO:HD3	2.30	0.46
2:B:21:PRO:O	2:B:93:ARG:NH1	2.49	0.46
2:B:249:THR:HG22	2:B:309:ALA:HB3	1.97	0.46
2:B:375:LEU:HD21	2:B:630:THR:HG22	1.97	0.46
3:C:1452:GLY:HA3	3:C:1460:VAL:HG12	1.97	0.46
1:A:505:LYS:HD2	2:B:509:HIS:HD2	1.80	0.46
1:A:510:ARG:HG2	1:A:548:PHE:CD2	2.51	0.46
1:A:124:PRO:HB2	1:A:156:GLN:HG2	1.96	0.46
6:F:4:BMA:H3	6:F:5:MAN:H5	1.98	0.46
1:A:638:ALA:HA	1:A:721:ASN:HD21	1.79	0.46
1:A:36:LEU:HB2	1:A:59:CYS:HB2	1.96	0.46
2:B:673:SER:O	2:B:674:SER:OG	2.29	0.46
1:A:248:ARG:HG3	1:A:250:LEU:HD13	1.97	0.46
1:A:154:PHE:CD2	2:B:163:PRO:HB3	2.51	0.46
3:C:1421:ARG:HG2	3:C:1422:ASP:N	2.18	0.46
1:A:415:ASP:OD1	1:A:415:ASP:N	2.46	0.46
1:A:419:TYR:OH	1:A:439:PRO:O	2.30	0.45
2:B:604:CYS:HB2	2:B:605:PRO:HD2	1.98	0.45
1:A:419:TYR:CE1	1:A:439:PRO:HA	2.52	0.45
3:C:1420:PRO:O	3:C:1421:ARG:CB	2.64	0.45
3:C:1444:VAL:HA	3:C:1491:THR:HG22	1.99	0.45
1:A:139:TYR:CZ	1:A:141:PRO:HG3	2.51	0.45
2:B:66:ASP:HB3	2:B:85:PRO:HB3	1.98	0.45
1:A:346:PRO:HA	1:A:358:ILE:HG13	1.98	0.45
6:F:3:BMA:H62	6:F:4:BMA:H2	1.47	0.45
1:A:247:ALA:HB2	1:A:252:MET:HE3	1.98	0.45
1:A:295:ILE:HB	1:A:316:SER:HB3	1.99	0.45
1:A:464:PRO:O	1:A:517:ARG:NH2	2.50	0.45
1:A:24:ASP:HA	1:A:409:LYS:HG2	1.98	0.44
1:A:253:VAL:HB	1:A:267:PHE:HB2	1.98	0.44
1:A:757:ILE:HG23	1:A:760:TRP:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1446:TYR:CZ	3:C:1490:VAL:HG11	2.52	0.44
3:C:1449:ILE:O	3:C:1462:GLU:HA	2.17	0.44
1:A:757:ILE:HD12	1:A:758:PRO:HD2	1.98	0.44
2:B:47:ASP:N	2:B:47:ASP:OD1	2.49	0.44
2:B:456:GLU:HG2	2:B:457:CYS:H	1.81	0.44
1:A:820:MET:HE3	1:A:895:ALA:HB1	1.98	0.44
2:B:482:GLN:HB3	2:B:484:ASP:H	1.82	0.44
1:A:363:PRO:HA	1:A:404:PHE:O	2.17	0.44
1:A:797:LEU:HB3	1:A:882:ILE:HB	1.99	0.44
1:A:745:ARG:NH2	2:B:591:PRO:HB2	2.33	0.44
1:A:790:PHE:CZ	1:A:889:LEU:HB2	2.53	0.44
1:A:550:ASP:O	1:A:551:LYS:NZ	2.47	0.44
1:A:561:TYR:OH	1:A:583:PRO:O	2.20	0.44
1:A:115:ARG:O	1:A:115:ARG:HG2	2.18	0.43
1:A:299:LEU:HD21	2:B:257:ALA:HB3	1.99	0.43
3:C:1490:VAL:HG23	3:C:1498:ALA:HB1	1.98	0.43
1:A:248:ARG:O	1:A:249:THR:HG22	2.19	0.43
1:A:257:ASP:HB3	1:A:260:ASN:O	2.18	0.43
1:A:444:ASN:HB3	1:A:480:LYS:HB3	2.01	0.43
1:A:248:ARG:CZ	8:B:702:NAG:H2	2.48	0.43
2:B:136:THR:O	2:B:140:THR:HG23	2.18	0.43
2:B:524:ASP:OD1	2:B:525:ASP:N	2.52	0.43
1:A:339:ARG:HD2	1:A:364:TYR:CD2	2.53	0.43
1:A:795:LEU:HB3	1:A:884:CYS:HB2	2.00	0.43
2:B:375:LEU:HD22	2:B:633:ARG:HG2	1.99	0.43
2:B:608:CYS:HB3	2:B:655:CYS:HB3	1.86	0.43
1:A:286:ASN:OD1	1:A:286:ASN:N	2.51	0.43
1:A:645:VAL:HG22	1:A:715:LEU:HD22	2.00	0.43
2:B:619:LYS:HD3	2:B:619:LYS:HA	1.82	0.43
1:A:450:TYR:O	1:A:451:PRO:C	2.61	0.43
2:B:240:ASN:OD1	2:B:240:ASN:N	2.50	0.43
2:B:320:ASN:ND2	8:B:702:NAG:O7	2.45	0.43
1:A:797:LEU:HD23	1:A:882:ILE:HD12	2.01	0.43
2:B:308:PHE:HB2	2:B:330:VAL:HG22	2.00	0.43
1:A:154:PHE:O	1:A:175:GLY:HA3	2.18	0.42
1:A:315:VAL:HG21	1:A:360:ILE:HD13	2.00	0.42
1:A:514:LEU:HA	1:A:541:TYR:CD1	2.54	0.42
1:A:746:GLY:HA2	1:A:779:ILE:O	2.19	0.42
1:A:651:ALA:O	1:A:677:ARG:NH1	2.38	0.42
1:A:400:MET:HE2	1:A:400:MET:HB3	1.92	0.42
1:A:403:SER:O	1:A:426:ALA:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:LEU:O	2:B:131:ILE:HG22	2.19	0.42
1:A:65:ARG:HA	1:A:65:ARG:HD3	1.91	0.42
2:B:172:ALA:HA	2:B:175:ASN:O	2.18	0.42
2:B:462:CYS:SG	2:B:466:TRP:HB3	2.60	0.42
1:A:370:LYS:HD3	1:A:394:GLN:HA	2.01	0.42
1:A:514:LEU:HA	1:A:541:TYR:HD1	1.84	0.42
1:A:724:ASP:N	1:A:724:ASP:OD1	2.51	0.42
2:B:297:GLU:O	2:B:301:GLN:HG2	2.20	0.42
2:B:476:GLU:C	2:B:478:TYR:H	2.26	0.42
1:A:108:CYS:HA	1:A:128:CYS:HA	2.00	0.42
1:A:647:ILE:HG22	1:A:713:PHE:CE2	2.55	0.42
2:B:191:LYS:HE2	2:B:280:HIS:NE2	2.35	0.42
2:B:441:ALA:HB1	2:B:455:PHE:CE2	2.53	0.42
1:A:650:GLN:CD	1:A:650:GLN:H	2.26	0.42
2:B:365:GLU:OE1	2:B:365:GLU:N	2.53	0.42
2:B:486:CYS:HB3	2:B:495:CYS:HB3	2.02	0.42
1:A:551:LYS:HA	1:A:551:LYS:HD3	1.58	0.41
1:A:777:GLN:HG2	1:A:779:ILE:HD11	2.02	0.41
2:B:160:PRO:C	2:B:165:MET:HE2	2.45	0.41
1:A:278:PHE:CD1	2:B:258:LEU:HD13	2.55	0.41
2:B:349:GLY:O	2:B:353:SER:OG	2.25	0.41
2:B:470:GLN:O	2:B:471:CYS:SG	2.78	0.41
1:A:650:GLN:HG2	1:A:703:GLN:C	2.45	0.41
3:C:1447:TYR:HB2	3:C:1465:VAL:HG23	2.02	0.41
1:A:438:ARG:O	1:A:440:VAL:HG23	2.21	0.41
1:A:26:PHE:HB2	1:A:37:LEU:HG	2.03	0.41
1:A:741:ALA:H	1:A:786:GLY:CA	2.28	0.41
1:A:121:GLU:HG3	1:A:122:ARG:H	1.86	0.41
1:A:93:TRP:CD1	1:A:111:LEU:HD22	2.55	0.41
2:B:102:ILE:HG23	2:B:397:PHE:HB2	2.02	0.41
2:B:249:THR:HA	2:B:309:ALA:O	2.21	0.41
2:B:473:CYS:HA	2:B:503:CYS:HB2	2.03	0.41
3:C:1463:PHE:HD1	3:C:1463:PHE:HA	1.68	0.41
1:A:869:ILE:HD11	1:A:919:SER:HB3	2.01	0.40
2:B:223:PHE:HB3	2:B:290:PRO:HG2	2.02	0.40
2:B:634:TYR:HD1	2:B:634:TYR:HA	1.76	0.40
3:C:1432:SER:OG	3:C:1474:ILE:O	2.28	0.40
2:B:160:PRO:O	2:B:165:MET:HE2	2.21	0.40
3:C:1448:ARG:O	3:C:1488:TYR:N	2.33	0.40
1:A:463:LEU:N	1:A:464:PRO:HD3	2.37	0.40
1:A:491:LEU:O	1:A:526:THR:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1483:TYR:HD1	3:C:1483:TYR:HA	1.74	0.40
1:A:272:MET:SD	2:B:320:ASN:HB3	2.61	0.40
2:B:27:SER:OG	2:B:457:CYS:SG	2.71	0.40
3:C:1427:ALA:H	3:C:1434:LEU:HB3	1.87	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	920/959 (96%)	862 (94%)	56 (6%)	2 (0%)	43	72
2	B	688/692 (99%)	607 (88%)	78 (11%)	3 (0%)	30	60
3	C	91/98 (93%)	80 (88%)	9 (10%)	2 (2%)	5	27
All	All	1699/1749 (97%)	1549 (91%)	143 (8%)	7 (0%)	30	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	451	PRO
3	C	1421	ARG
2	B	162	SER
2	B	163	PRO
2	B	49	CYS
3	C	1420	PRO
1	A	440	VAL

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	784/813 (96%)	742 (95%)	42 (5%)	20	48
2	B	612/614 (100%)	574 (94%)	38 (6%)	16	45
3	C	78/81 (96%)	68 (87%)	10 (13%)	4	18
All	All	1474/1508 (98%)	1384 (94%)	90 (6%)	17	45

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	27	VAL
1	A	51	VAL
1	A	58	LYS
1	A	99	ARG
1	A	134	THR
1	A	155	CYS
1	A	190	GLU
1	A	232	ASN
1	A	249	THR
1	A	260	ASN
1	A	261	MET
1	A	275	TYR
1	A	283	THR
1	A	299	LEU
1	A	329	THR
1	A	351	ASP
1	A	443	VAL
1	A	461	CYS
1	A	463	LEU
1	A	474	ASN
1	A	527	ILE
1	A	532	LEU
1	A	548	PHE
1	A	551	LYS
1	A	567	THR
1	A	608	VAL
1	A	615	LYS
1	A	650	GLN
1	A	673	GLU

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Mol	Chain	Res	Type
1	A	724	ASP
1	A	729	VAL
1	A	757	ILE
1	A	768	THR
1	A	806	ASN
1	A	817	ASP
1	A	833	ILE
1	A	874	CYS
1	A	881	LYS
1	A	916	HIS
1	A	933	TYR
1	A	951	VAL
2	B	26	CYS
2	B	44	LEU
2	B	47	ASP
2	B	58	VAL
2	B	71	ASP
2	B	80	VAL
2	B	90	LEU
2	B	102	ILE
2	B	116	TYR
2	B	127	ASP
2	B	131	ILE
2	B	138	LEU
2	B	149	LEU
2	B	165	MET
2	B	198	ASP
2	B	207	VAL
2	B	215	ASN
2	B	217	ASP
2	B	220	GLU
2	B	247	VAL
2	B	299	LEU
2	B	311	THR
2	B	342	GLN
2	B	343	LEU
2	B	344	ILE
2	B	371	ASN
2	B	454	THR
2	B	466	TRP
2	B	472	GLU
2	B	478	TYR

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Mol	Chain	Res	Type
2	B	494	VAL
2	B	507	VAL
2	B	508	CYS
2	B	509	HIS
2	B	528	CYS
2	B	589	ILE
2	B	608	CYS
2	B	637	ASP
3	C	1419	VAL
3	C	1423	LEU
3	C	1457	ASN
3	C	1463	PHE
3	C	1481	VAL
3	C	1483	TYR
3	C	1484	THR
3	C	1487	VAL
3	C	1490	VAL
3	C	1503	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	131	GLN
1	A	314	GLN
1	A	589	GLN
1	A	685	ASN
1	A	785	ASN
2	B	14	GLN
2	B	133	ASN
2	B	272	GLN
2	B	339	ASN
2	B	408	GLN
2	B	505	GLN
2	B	509	HIS
2	B	541	GLN
2	B	629	ASN
2	B	654	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

28 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	0.39	0	17,19,21	0.45	0
4	NAG	D	2	4	14,14,15	0.23	0	17,19,21	0.49	0
4	BMA	D	3	4	11,11,12	0.90	0	15,15,17	1.04	1 (6%)
4	MAN	D	4	4	11,11,12	0.68	0	15,15,17	1.03	2 (13%)
5	NAG	E	1	1,5	14,14,15	1.22	1 (7%)	17,19,21	1.75	4 (23%)
5	NAG	E	2	5	14,14,15	0.21	0	17,19,21	0.39	0
6	NAG	F	1	6,1	14,14,15	0.35	0	17,19,21	0.42	0
6	NAG	F	2	6	14,14,15	0.23	0	17,19,21	0.49	0
6	BMA	F	3	6	11,11,12	0.66	0	15,15,17	0.74	0
6	BMA	F	4	6	11,11,12	1.19	2 (18%)	15,15,17	1.07	1 (6%)
6	MAN	F	5	6	11,11,12	1.01	1 (9%)	15,15,17	1.49	4 (26%)
6	MAN	F	6	6	11,11,12	0.78	0	15,15,17	0.94	2 (13%)
4	NAG	G	1	1,4	14,14,15	0.24	0	17,19,21	0.47	0
4	NAG	G	2	4	14,14,15	0.27	0	17,19,21	0.39	0
4	BMA	G	3	4	11,11,12	0.72	0	15,15,17	0.86	1 (6%)
4	MAN	G	4	4	11,11,12	0.58	0	15,15,17	1.01	2 (13%)
5	NAG	H	1	1,5	14,14,15	0.30	0	17,19,21	0.36	0
5	NAG	H	2	5	14,14,15	0.26	0	17,19,21	0.40	0
5	NAG	I	1	1,5	14,14,15	0.39	0	17,19,21	0.37	0
5	NAG	I	2	5	14,14,15	0.65	0	17,19,21	0.90	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	J	1	1,7	14,14,15	0.27	0	17,19,21	0.47	0
7	NAG	J	2	7	14,14,15	0.42	0	17,19,21	0.49	0
7	BMA	J	3	7	11,11,12	0.95	1 (9%)	15,15,17	1.30	2 (13%)
5	NAG	K	1	2,5	14,14,15	0.48	0	17,19,21	0.96	1 (5%)
5	NAG	K	2	5	14,14,15	0.38	0	17,19,21	1.08	2 (11%)
7	NAG	L	1	7,2	14,14,15	0.23	0	17,19,21	0.42	0
7	NAG	L	2	7	14,14,15	0.78	1 (7%)	17,19,21	1.22	1 (5%)
7	BMA	L	3	7	11,11,12	0.83	0	15,15,17	1.12	1 (6%)

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	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	6/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
6	NAG	F	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
6	BMA	F	3	6	-	1/2/19/22	0/1/1/1
6	BMA	F	4	6	-	1/2/19/22	0/1/1/1
6	MAN	F	5	6	-	0/2/19/22	0/1/1/1
6	MAN	F	6	6	-	0/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	1/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
5	NAG	H	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
7	NAG	J	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
7	BMA	J	3	7	-	0/2/19/22	0/1/1/1
5	NAG	K	1	2,5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
7	NAG	L	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	L	2	7	-	1/6/23/26	0/1/1/1
7	BMA	L	3	7	-	1/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1	NAG	O5-C1	-4.36	1.36	1.43
6	F	5	MAN	C1-C2	2.77	1.58	1.52
7	L	2	NAG	O5-C1	2.73	1.48	1.43
7	J	3	BMA	C1-C2	2.39	1.57	1.52
6	F	4	BMA	C4-C5	2.34	1.58	1.53
6	F	4	BMA	O5-C5	2.15	1.47	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	NAG	C2-N2-C7	4.77	129.29	122.90
7	L	2	NAG	C1-O5-C5	4.71	118.50	112.19
5	E	1	NAG	C3-C4-C5	3.54	116.66	110.23
5	K	2	NAG	C1-O5-C5	3.46	116.82	112.19
5	I	2	NAG	C1-O5-C5	3.45	116.81	112.19
6	F	5	MAN	C1-O5-C5	3.12	116.36	112.19
5	K	1	NAG	C1-O5-C5	3.03	116.25	112.19
7	L	3	BMA	C1-O5-C5	2.97	116.16	112.19
6	F	5	MAN	C1-C2-C3	2.85	113.79	109.64
4	D	4	MAN	C1-O5-C5	2.83	115.98	112.19
6	F	4	BMA	C1-O5-C5	2.77	115.90	112.19
4	G	4	MAN	C1-O5-C5	2.61	115.68	112.19
7	J	3	BMA	C1-O5-C5	2.59	115.66	112.19
4	D	3	BMA	O3-C3-C2	2.55	115.25	110.05
5	E	1	NAG	C4-C3-C2	2.48	114.65	111.02
5	E	1	NAG	C1-C2-N2	2.47	114.33	110.43
6	F	5	MAN	O2-C2-C3	-2.46	105.05	110.15
4	G	3	BMA	O2-C2-C3	-2.43	105.11	110.15
4	G	4	MAN	O2-C2-C3	-2.23	105.54	110.15
7	J	3	BMA	C1-C2-C3	2.22	112.88	109.64
6	F	6	MAN	O2-C2-C3	-2.13	105.74	110.15
5	K	2	NAG	C3-C4-C5	2.09	114.02	110.23
4	D	4	MAN	O2-C2-C3	-2.07	105.86	110.15
6	F	6	MAN	C1-O5-C5	2.06	114.95	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	5	MAN	O5-C1-C2	2.03	115.62	110.79

There are no chirality outliers.

All (34) torsion outliers are listed below:

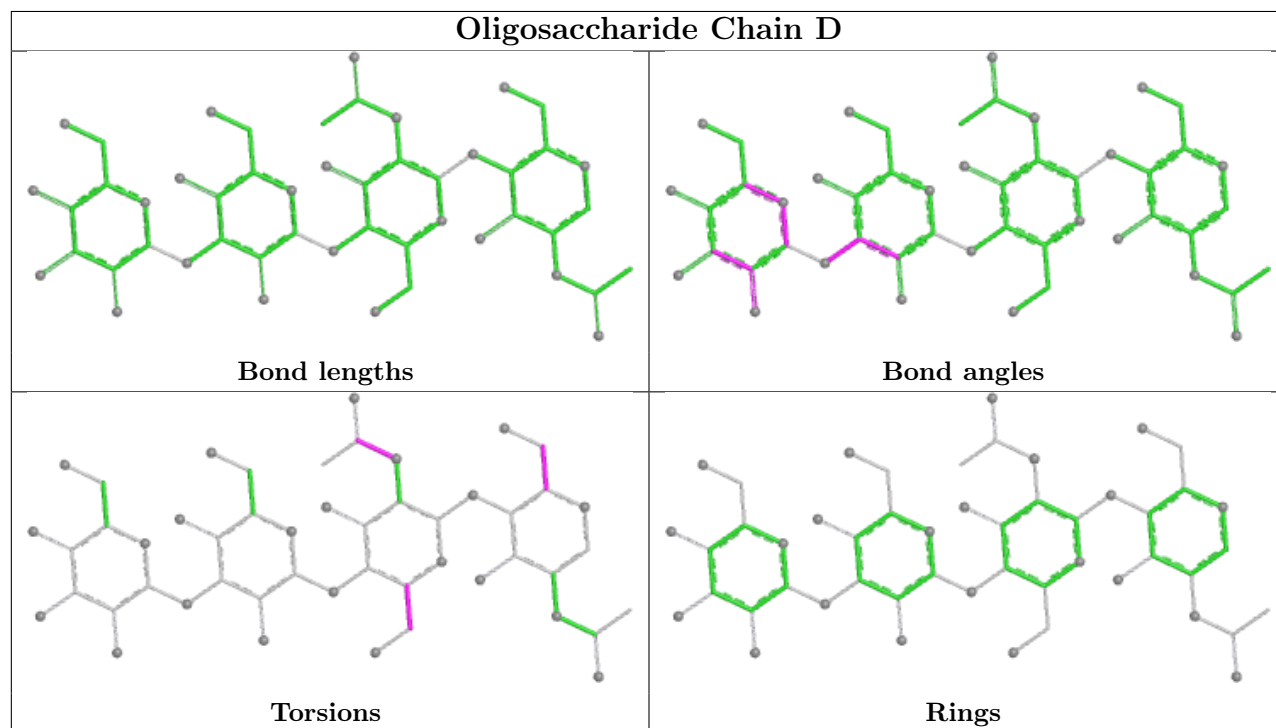
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
7	L	1	NAG	O5-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
7	L	1	NAG	C4-C5-C6-O6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

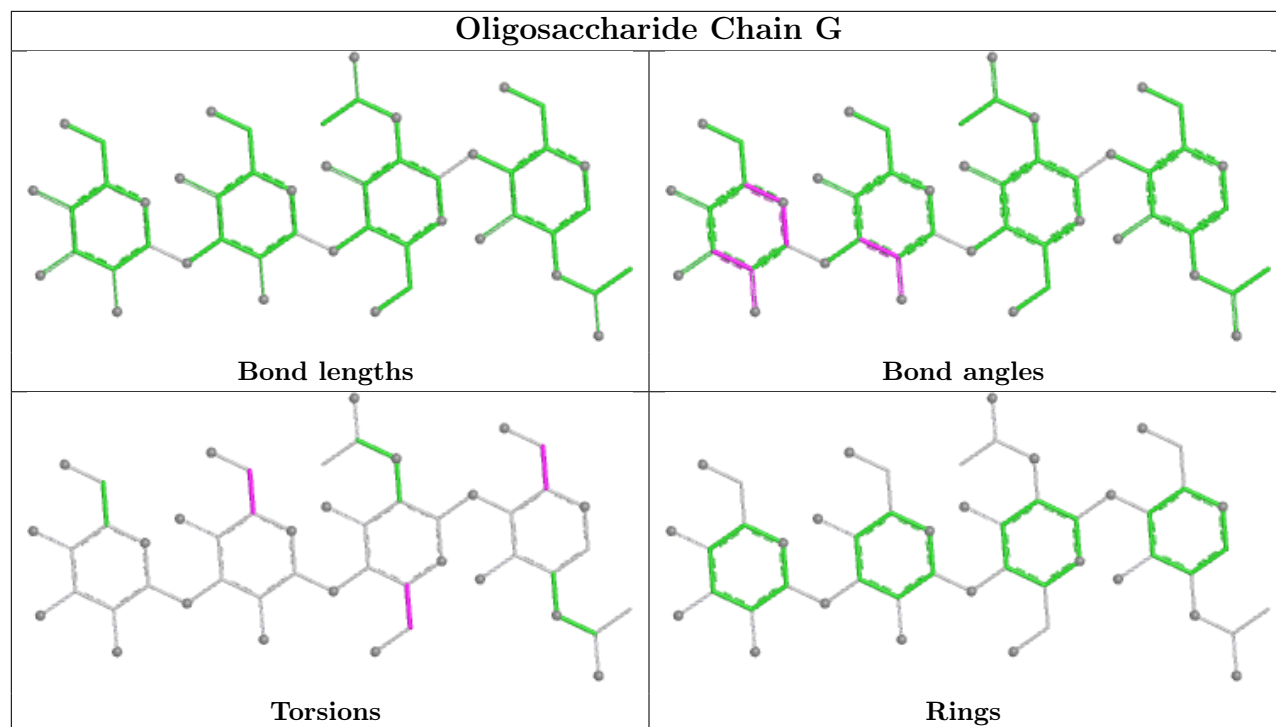
There are no ring outliers.

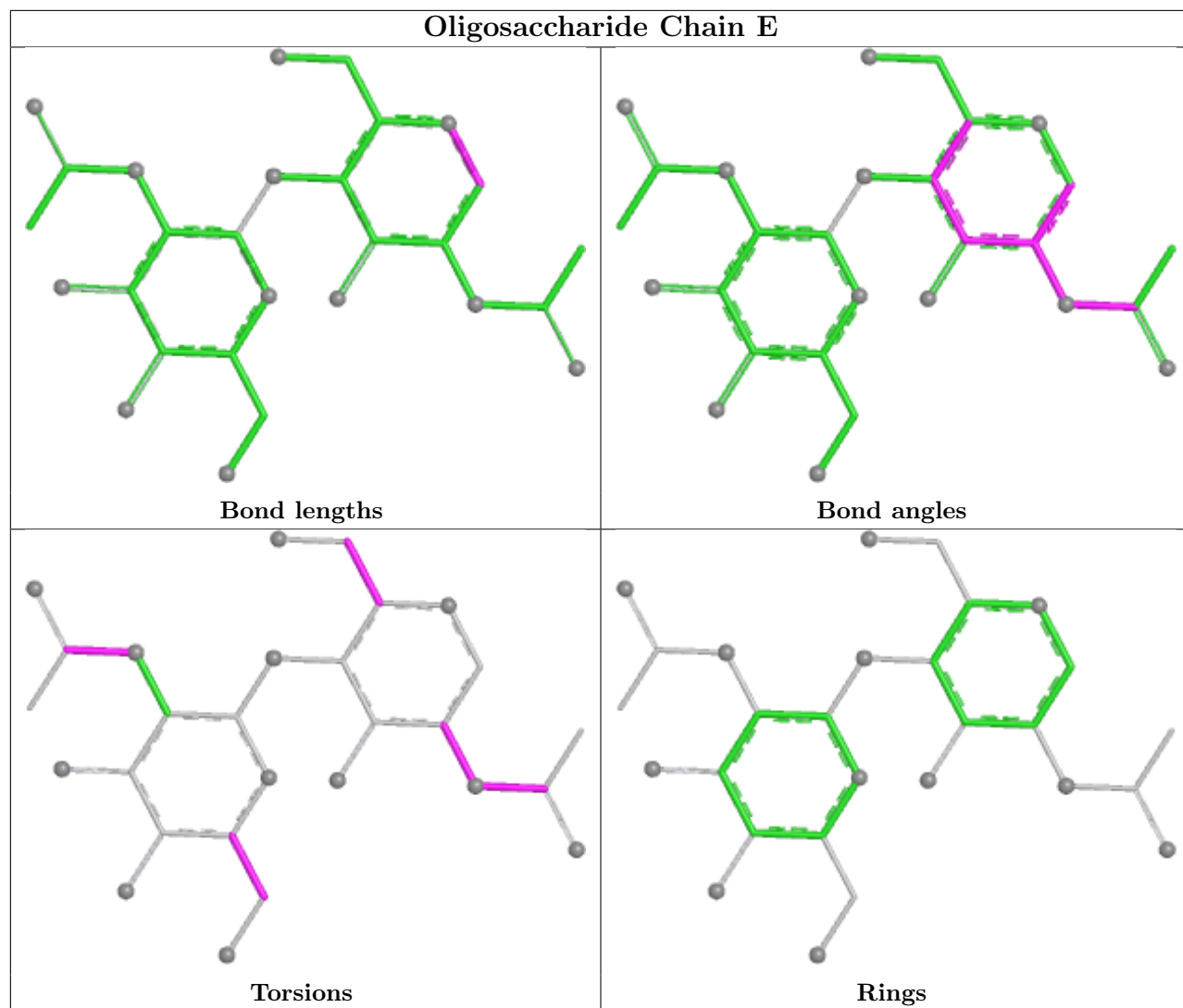
4 monomers are involved in 3 short contacts:

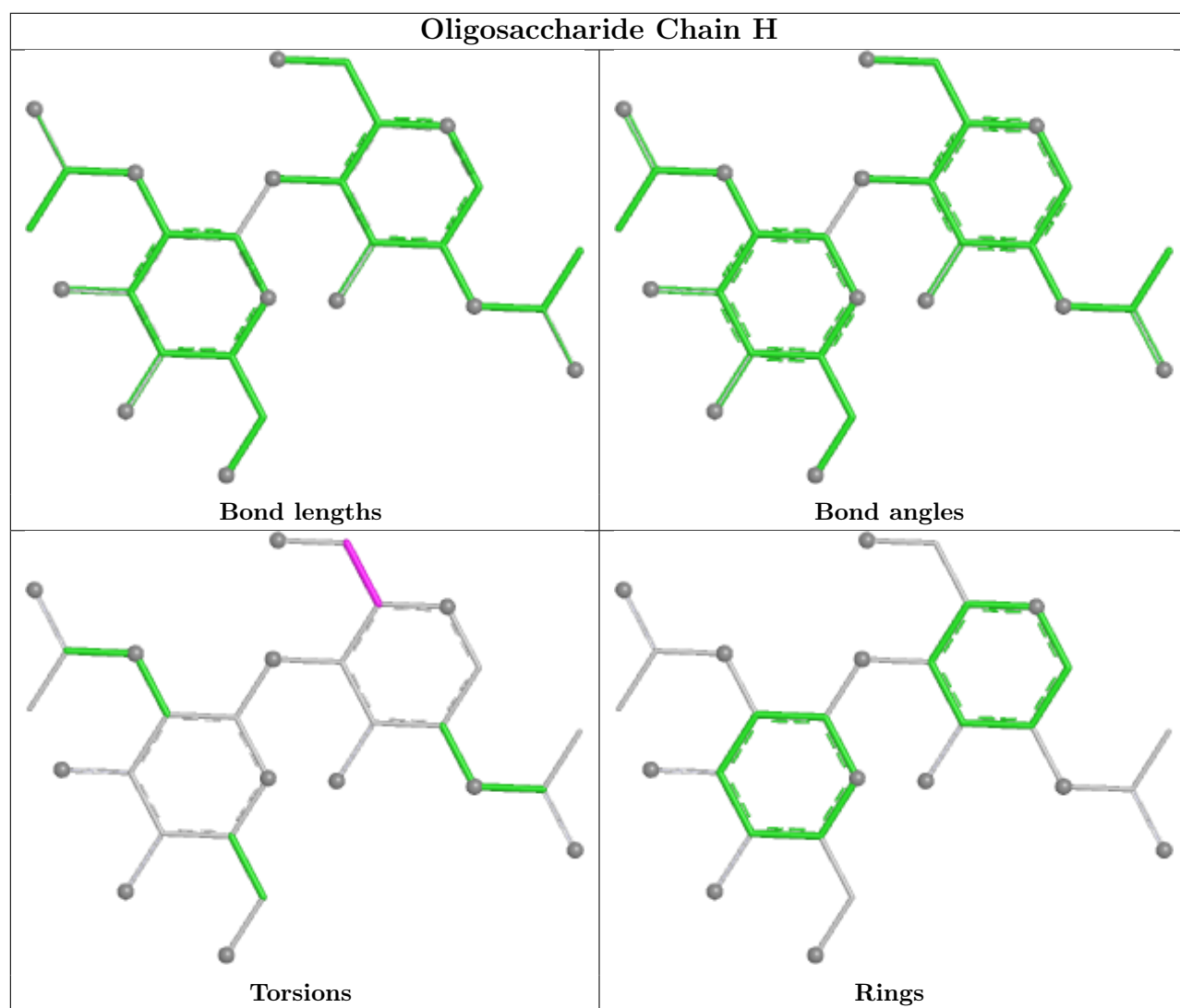
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	3	BMA	1	0
6	F	5	MAN	1	0
5	K	1	NAG	1	0
6	F	4	BMA	2	0

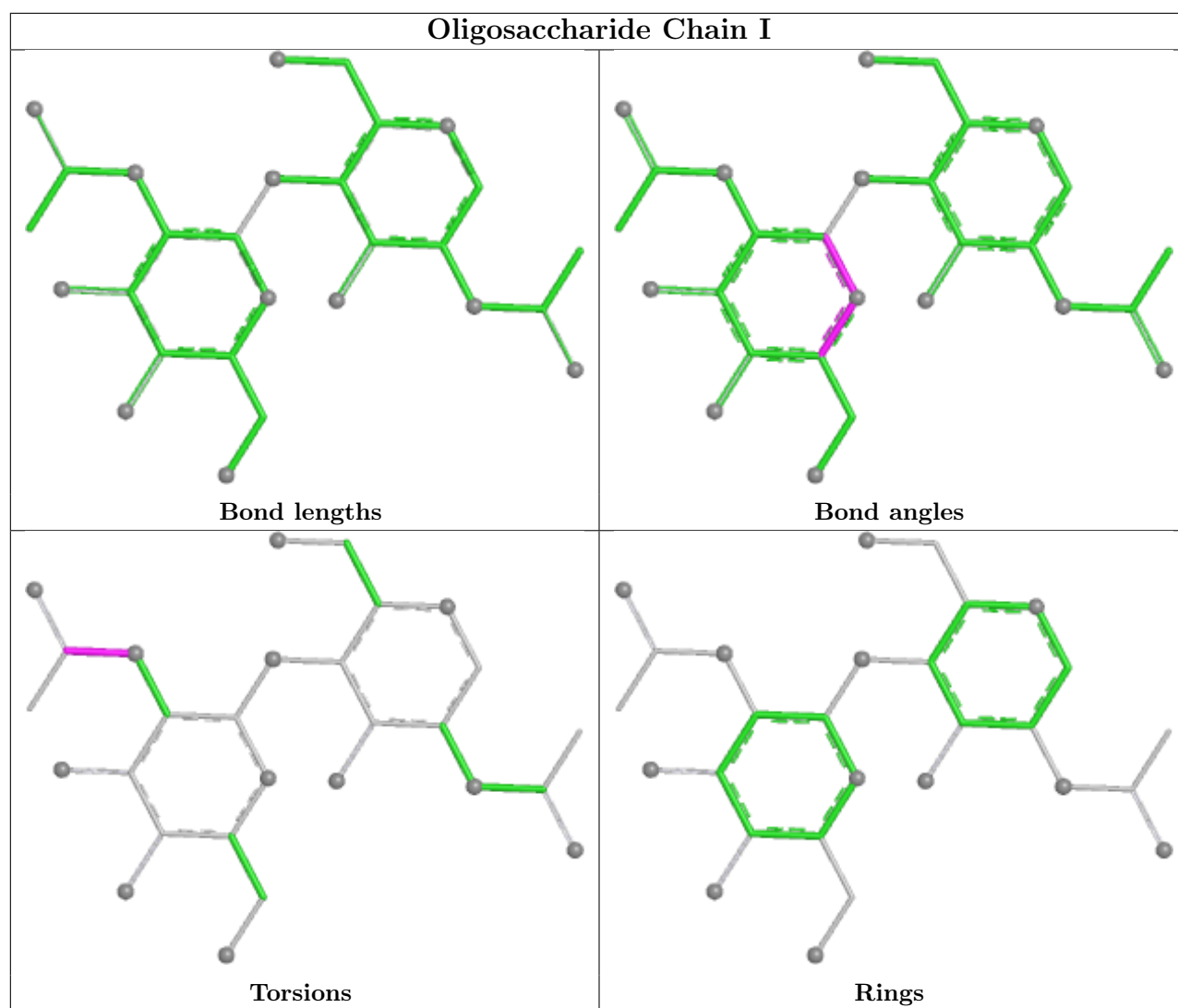
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

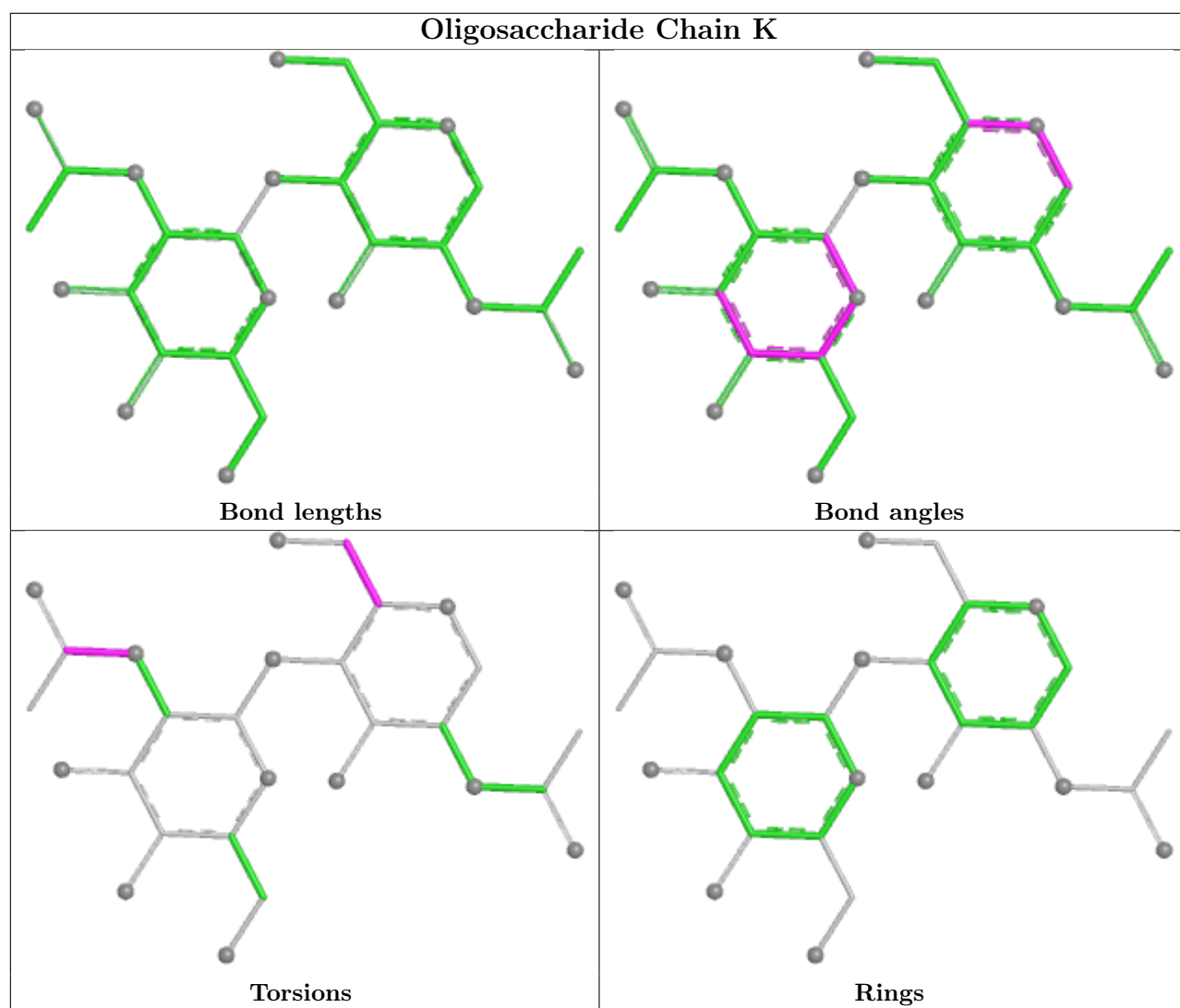




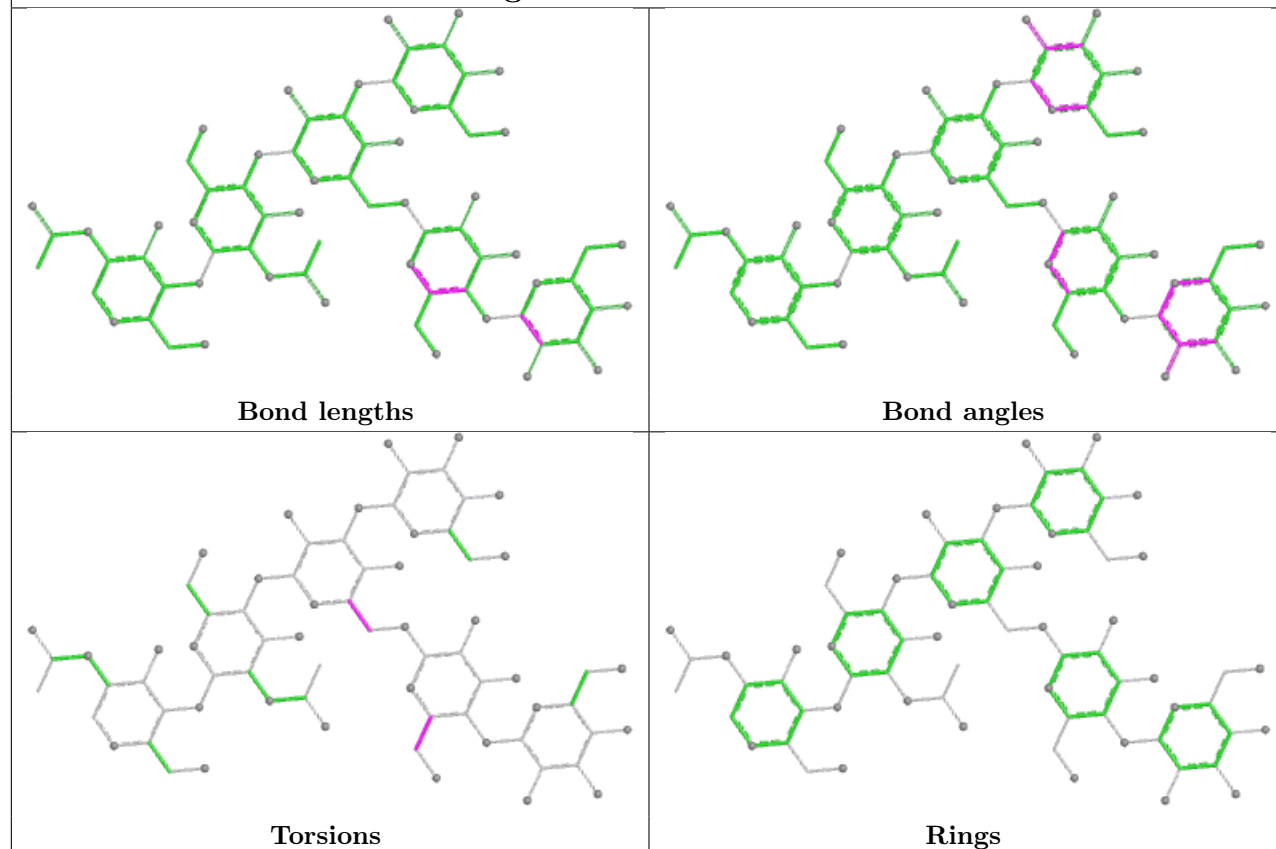




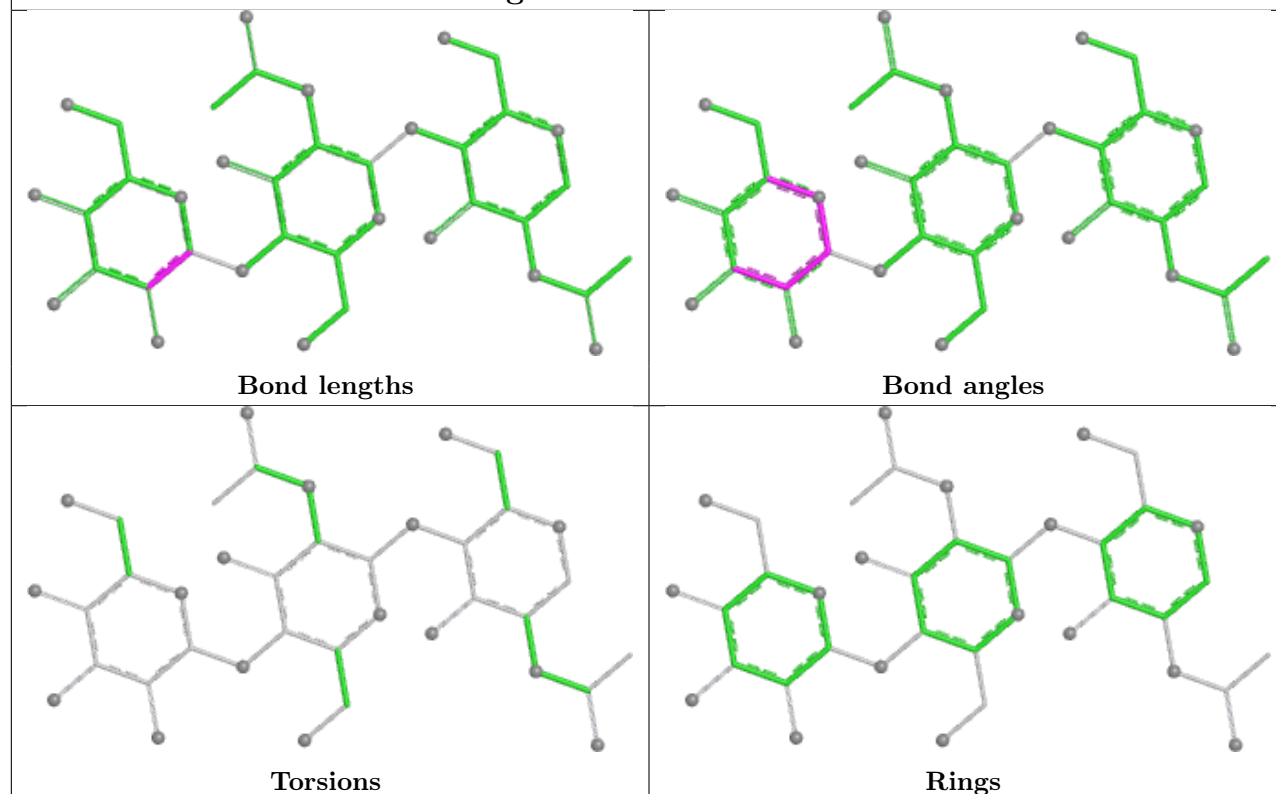


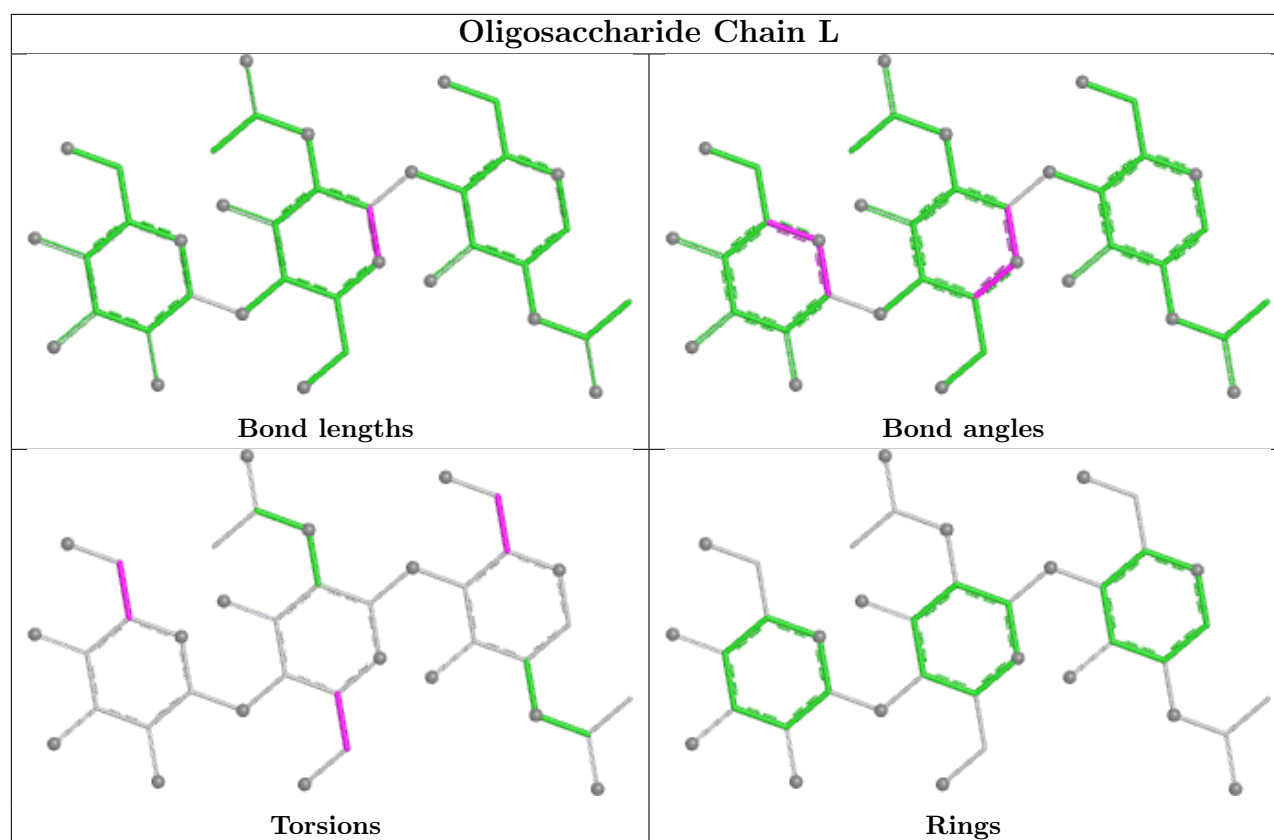


Oligosaccharide Chain F



Oligosaccharide Chain J





5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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	$\# Z > 2$
8	NAG	A	1001	1	14,14,15	0.27	0	17,19,21	0.46	0
8	NAG	B	701	2	14,14,15	0.76	1 (7%)	17,19,21	1.23	1 (5%)
8	NAG	A	1002	1	14,14,15	0.85	1 (7%)	17,19,21	1.22	1 (5%)
8	NAG	A	1003	1	14,14,15	0.27	0	17,19,21	0.53	0
8	NAG	B	702	2	14,14,15	0.35	0	17,19,21	0.62	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
8	NAG	A	1001	1	-	2/6/23/26	0/1/1/1
8	NAG	B	701	2	-	1/6/23/26	0/1/1/1
8	NAG	A	1002	1	-	1/6/23/26	0/1/1/1
8	NAG	A	1003	1	-	1/6/23/26	0/1/1/1
8	NAG	B	702	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1002	NAG	O5-C1	2.99	1.48	1.43
8	B	701	NAG	O5-C1	2.70	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	701	NAG	C1-O5-C5	4.84	118.68	112.19
8	A	1002	NAG	C1-O5-C5	4.80	118.62	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1001	NAG	O5-C5-C6-O6
8	A	1001	NAG	C4-C5-C6-O6
8	B	702	NAG	O5-C5-C6-O6
8	B	702	NAG	C4-C5-C6-O6
8	B	701	NAG	O5-C5-C6-O6
8	A	1002	NAG	C4-C5-C6-O6
8	A	1003	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1002	NAG	1	0
8	B	702	NAG	2	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	924/959 (96%)	-0.00	14 (1%)	72 53	48, 83, 135, 155	0
2	B	690/692 (99%)	0.31	33 (4%)	35 24	50, 96, 190, 224	1 (0%)
3	C	93/98 (94%)	1.03	14 (15%)	5 5	70, 186, 307, 319	0
All	All	1707/1749 (97%)	0.18	61 (3%)	46 31	48, 90, 187, 319	1 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1505	ILE	4.1
2	B	677	SER	3.9
1	A	550	ASP	3.9
3	C	1428	ALA	3.7
2	B	460	CYS	3.7
2	B	37	ARG	3.6
1	A	835	ILE	3.6
2	B	36	PRO	3.6
2	B	499	GLY	3.4
2	B	167	ILE	3.3
2	B	19	VAL	3.2
2	B	453	GLY	3.2
2	B	35	SER	3.1
2	B	674	SER	3.0
2	B	459	VAL	3.0
2	B	33	LEU	2.9
2	B	443	PRO	2.9
3	C	1426	VAL	2.9
1	A	571	THR	2.9
3	C	1432	SER	2.8
2	B	168	SER	2.8
3	C	1420	PRO	2.7
3	C	1425	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	463	LEU	2.7
3	C	1433	LEU	2.5
1	A	833	ILE	2.4
1	A	670	PHE	2.4
2	B	340	VAL	2.4
1	A	666	LEU	2.4
2	B	10	VAL	2.4
2	B	507	VAL	2.4
3	C	1503	ILE	2.4
2	B	455	PHE	2.3
2	B	509	HIS	2.3
2	B	637	ASP	2.3
3	C	1442	VAL	2.3
1	A	568	ALA	2.3
3	C	1423	LEU	2.3
1	A	906	GLU	2.3
1	A	955	ILE	2.3
3	C	1449	ILE	2.3
2	B	31	LEU	2.3
2	B	646	LYS	2.2
2	B	481	SER	2.2
1	A	461	CYS	2.2
2	B	638	GLU	2.2
2	B	508	CYS	2.2
2	B	678	ILE	2.2
3	C	1427	ALA	2.2
1	A	912	GLU	2.1
2	B	338	SER	2.1
2	B	502	LEU	2.1
3	C	1443	THR	2.1
2	B	34	GLY	2.1
2	B	118	MET	2.1
2	B	510	SER	2.1
1	A	468	LEU	2.1
2	B	221	GLY	2.1
1	A	874	CYS	2.0
3	C	1492	GLY	2.0
2	B	479	ARG	2.0

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

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

6.3 Carbohydrates

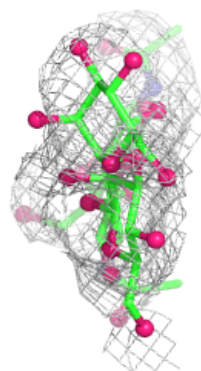
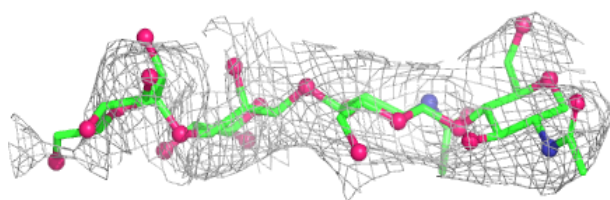
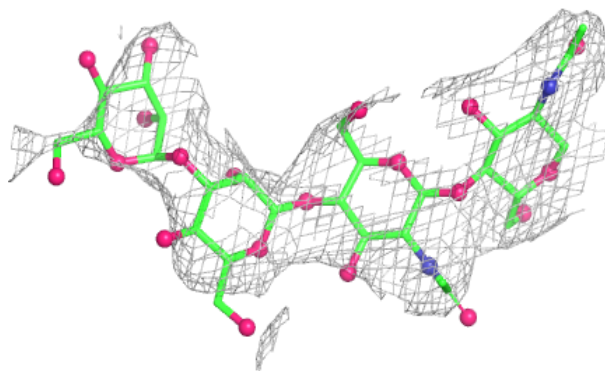
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	D	4	11/12	0.34	0.10	157,165,170,173	0
7	BMA	J	3	11/12	0.37	0.13	160,166,175,175	0
4	MAN	G	4	11/12	0.45	0.12	144,152,158,162	0
7	NAG	J	2	14/15	0.49	0.13	121,137,156,169	0
4	BMA	G	3	11/12	0.53	0.13	145,147,159,167	0
4	NAG	G	2	14/15	0.60	0.14	122,138,152,159	0
5	NAG	H	2	14/15	0.60	0.11	126,135,138,141	0
4	BMA	D	3	11/12	0.62	0.09	140,150,154,161	0
5	NAG	I	2	14/15	0.64	0.11	137,144,154,156	0
5	NAG	E	2	14/15	0.66	0.12	127,136,146,150	0
6	MAN	F	6	11/12	0.67	0.10	109,121,135,136	0
5	NAG	K	2	14/15	0.73	0.14	134,138,153,158	0
7	BMA	L	3	11/12	0.74	0.11	103,112,118,119	0
5	NAG	I	1	14/15	0.75	0.11	107,127,143,146	0
6	BMA	F	4	11/12	0.75	0.12	90,106,127,128	0
5	NAG	H	1	14/15	0.76	0.11	111,127,138,141	0
5	NAG	E	1	14/15	0.80	0.10	101,119,128,137	0
5	NAG	K	1	14/15	0.83	0.12	91,117,137,141	0
4	NAG	G	1	14/15	0.85	0.11	108,126,140,148	0
6	MAN	F	5	11/12	0.85	0.10	100,107,116,117	0
6	BMA	F	3	11/12	0.85	0.07	88,95,111,122	0
4	NAG	D	2	14/15	0.87	0.09	100,112,117,135	0
7	NAG	L	2	14/15	0.88	0.14	96,111,123,123	0
7	NAG	J	1	14/15	0.92	0.07	76,100,118,120	0
4	NAG	D	1	14/15	0.94	0.09	75,86,101,106	0
6	NAG	F	2	14/15	0.96	0.07	47,62,87,94	0
7	NAG	L	1	14/15	0.96	0.07	75,100,107,107	0
6	NAG	F	1	14/15	0.97	0.06	45,60,89,90	0

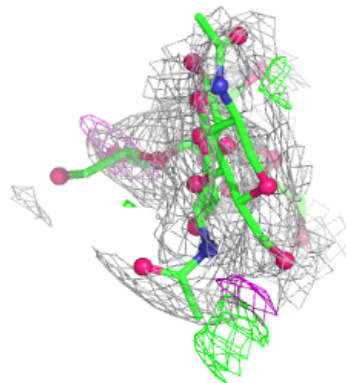
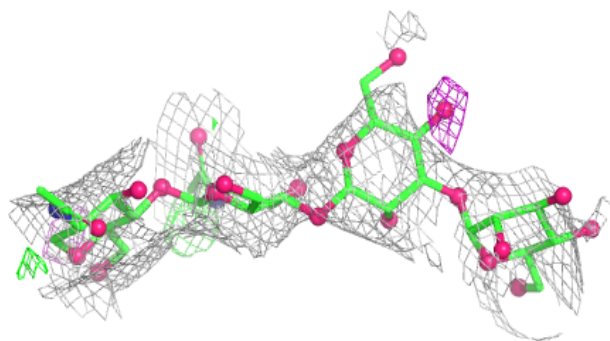
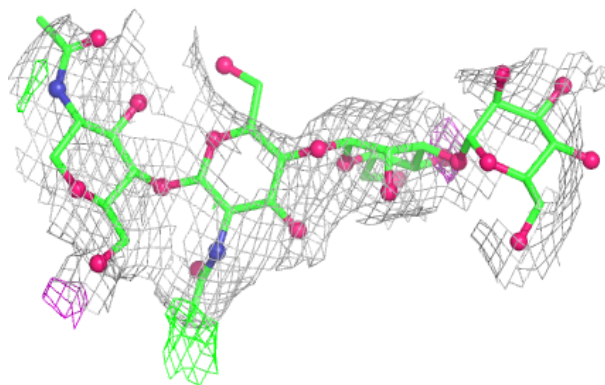
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

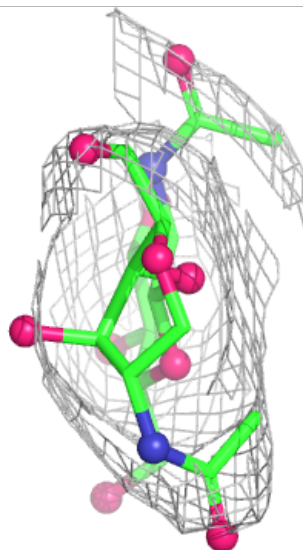
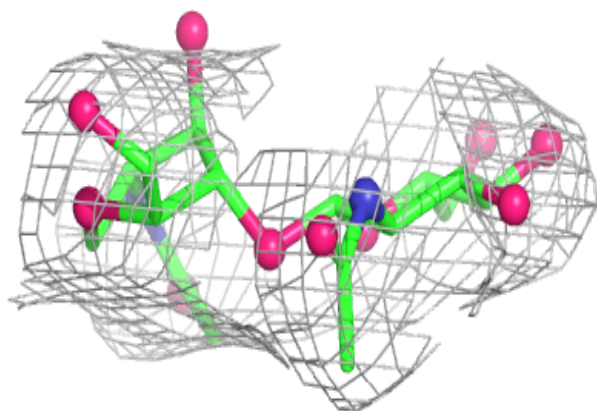
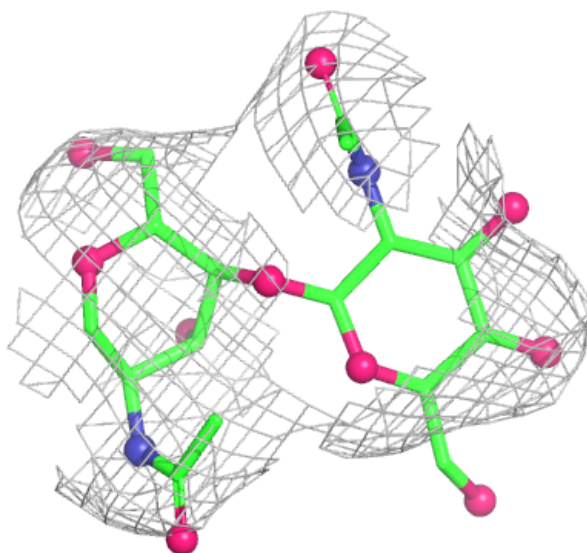
**Electron density around Chain G:**

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



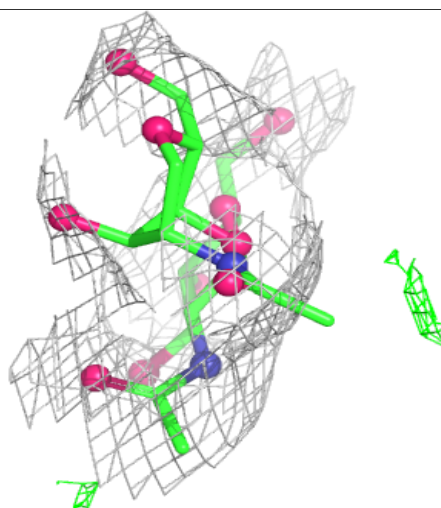
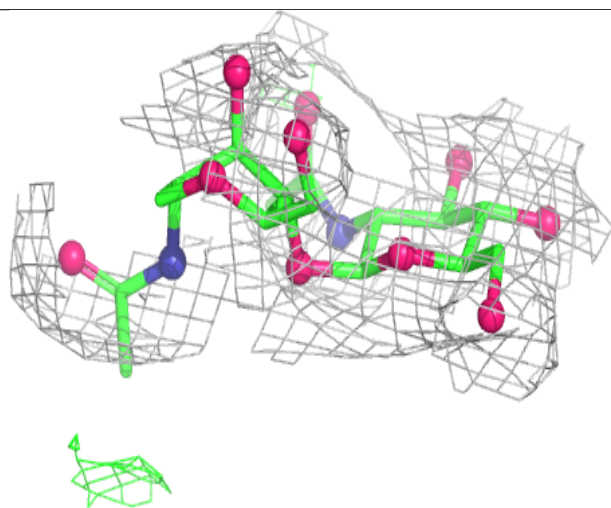
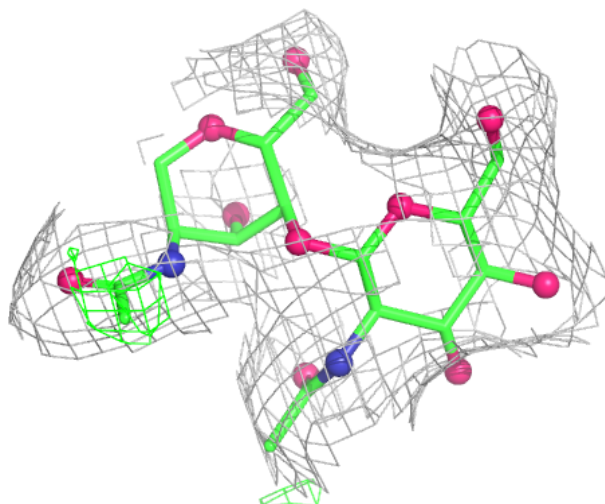
Electron density around Chain E:

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



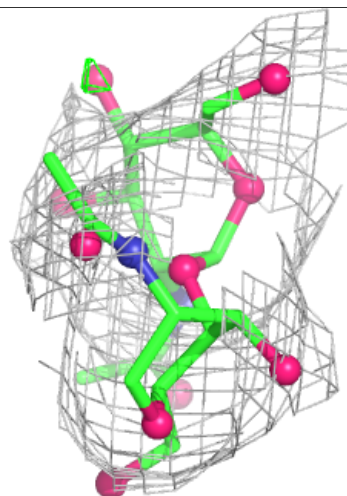
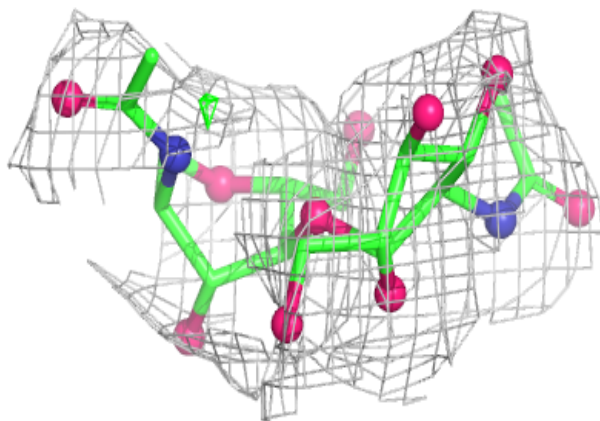
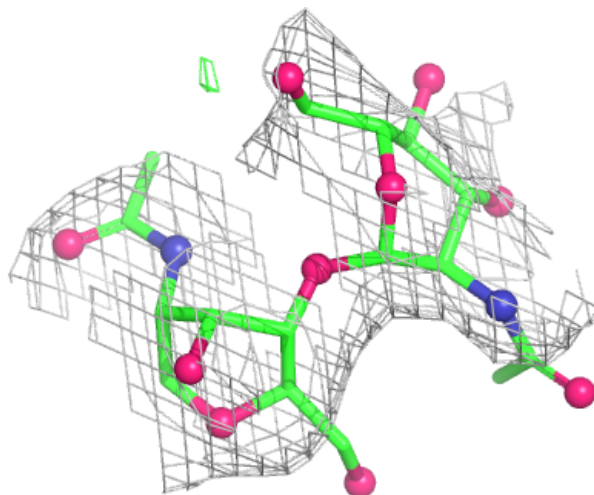
Electron density around Chain H:

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



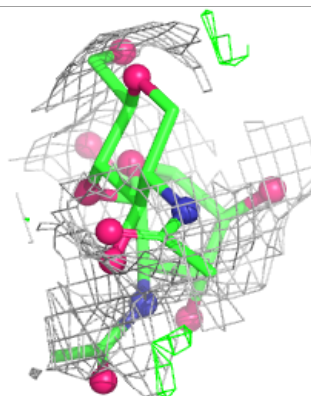
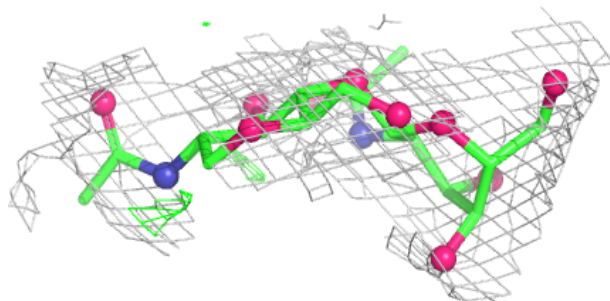
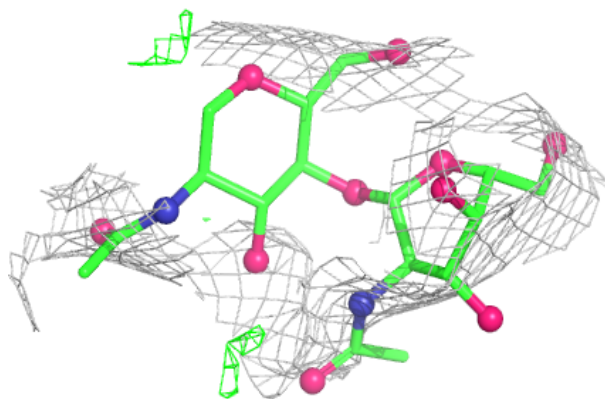
Electron density around Chain I:

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

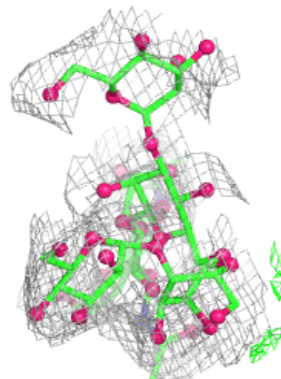
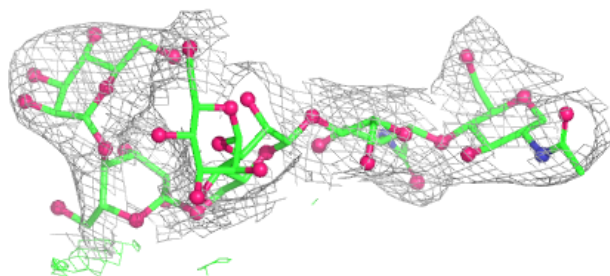
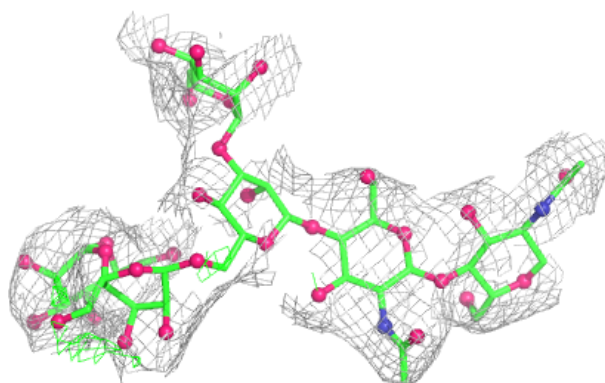


Electron density around Chain K:

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

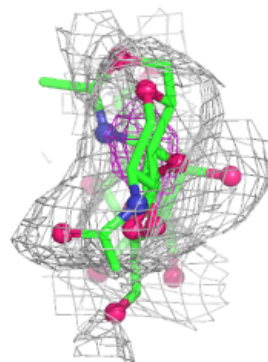
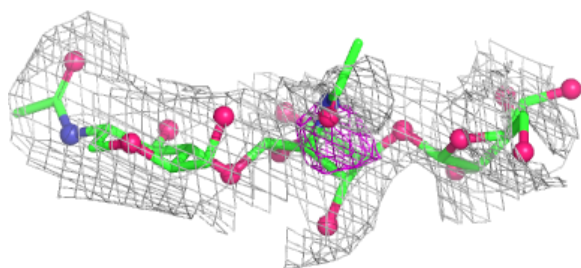
**Electron density around Chain F:**

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

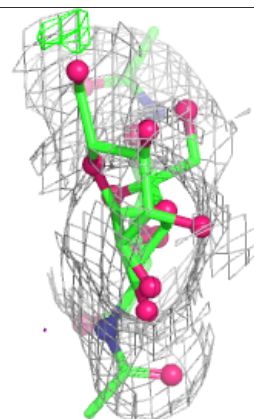
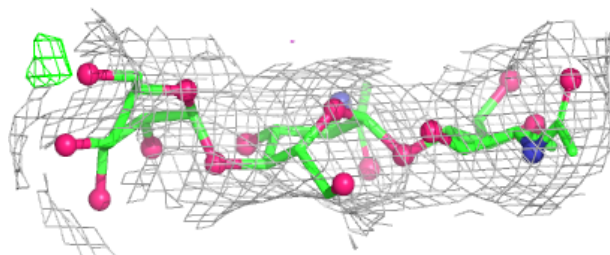
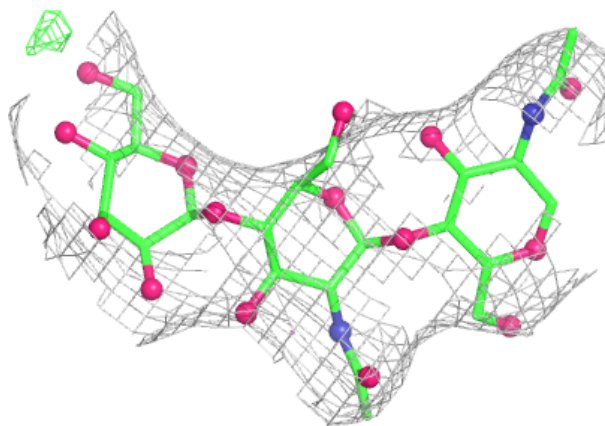


Electron density around Chain J:

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

**Electron density around Chain L:**

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
8	NAG	A	1002	14/15	0.58	0.11	164,180,187,187	0
8	NAG	A	1001	14/15	0.63	0.12	143,162,169,172	0
8	NAG	B	701	14/15	0.64	0.13	101,128,137,148	0
8	NAG	A	1003	14/15	0.77	0.11	93,108,117,120	0
8	NAG	B	702	14/15	0.87	0.09	80,95,106,114	0
9	MN	A	1004	1/1	0.93	0.08	96,96,96,96	0
9	MN	A	1005	1/1	0.95	0.06	84,84,84,84	0
9	MN	A	1006	1/1	0.97	0.09	119,119,119,119	0
9	MN	B	704	1/1	0.97	0.05	81,81,81,81	0
9	MN	A	1007	1/1	0.98	0.08	114,114,114,114	0
9	MN	A	1008	1/1	0.99	0.03	92,92,92,92	0
9	MN	B	703	1/1	1.00	0.02	57,57,57,57	0
9	MN	B	705	1/1	1.00	0.02	55,55,55,55	0

6.5 Other polymers

There are no such residues in this entry.