



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 01:12 AM BST

PDB ID : 3IJE
Title : Crystal structure of the complete integrin α V β 3 ectodomain plus an Alpha/beta transmembrane fragment
Authors : Xiong, J.-P.; Mahalingham, B.; Rui, X.; Hyman, B.T.; Goodman, S.L.; Arnaout, M.A.
Deposited on : 2009-08-04
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

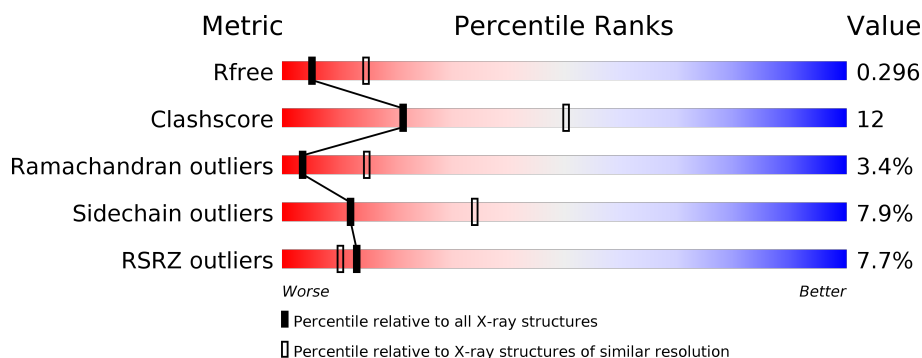
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	967	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>23%</div> <div>• •</div> </div> </div>
2	B	695	<div> <div>9%</div> <div> <div></div> <div>70%</div> <div>26%</div> <div>•</div> </div> </div>
3	C	5	<div> <div>40%</div> <div>60%</div> </div>
4	D	2	<div> <div>50%</div> <div>50%</div> </div>
4	F	2	<div> <div>50%</div> <div>50%</div> </div>
4	G	2	<div> <div>100%</div> </div>

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	2	-	-	X	-
6	BMA	J	3	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 13087 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.

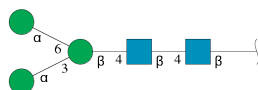
- Molecule 1 is a protein called Integrin alpha-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	938	Total	C	N	O	S	0	0	0
			7300	4628	1236	1400	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	695	Total	C	N	O	S	0	0	0
			5332	3276	909	1077	70			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
3	C	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



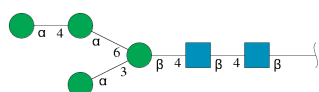
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-alpha-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	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



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

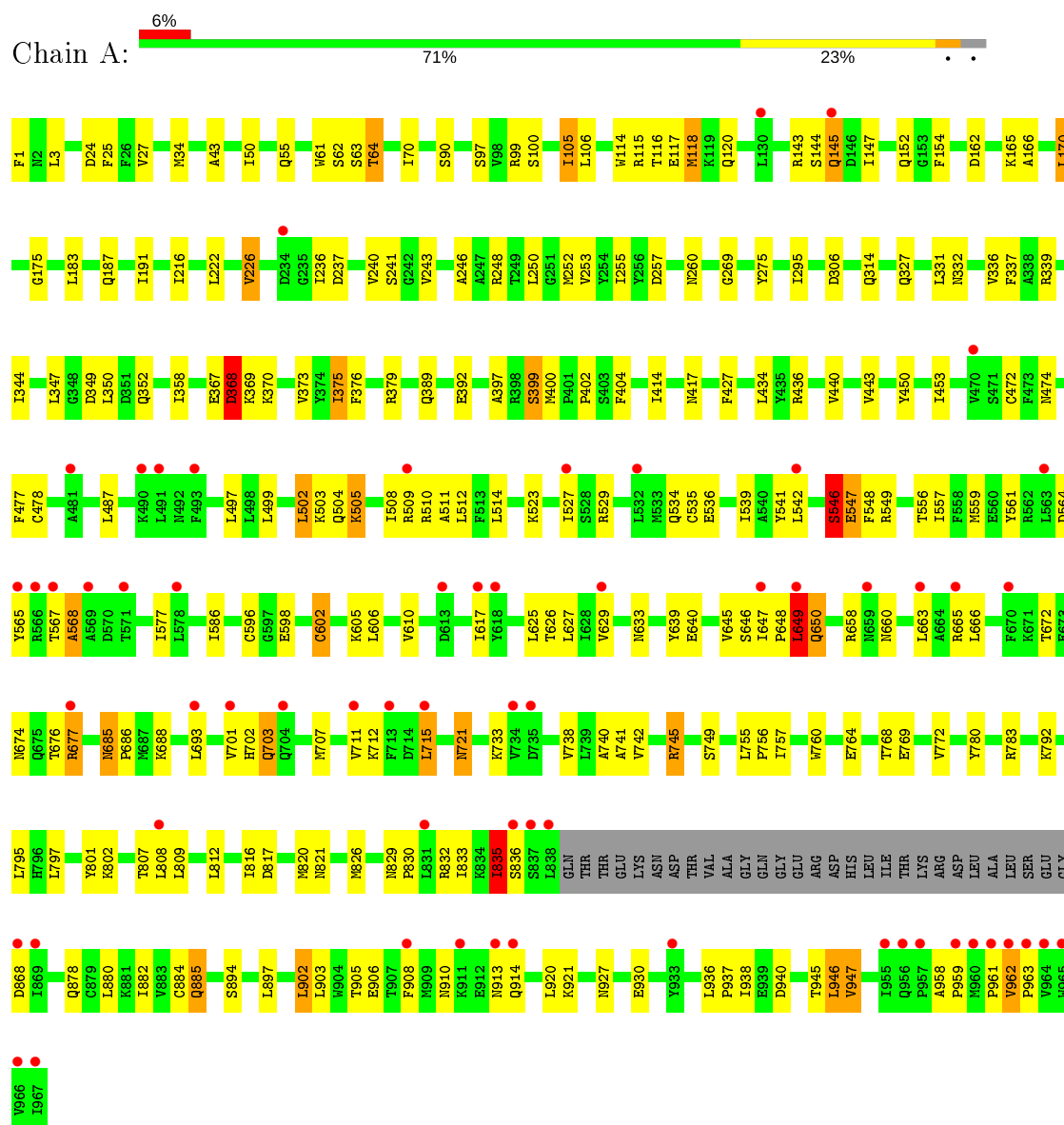
- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Ca	0	0
			1	1		
8	A	5	Total	Ca	0	0
			5	5		

3 Residue-property plots

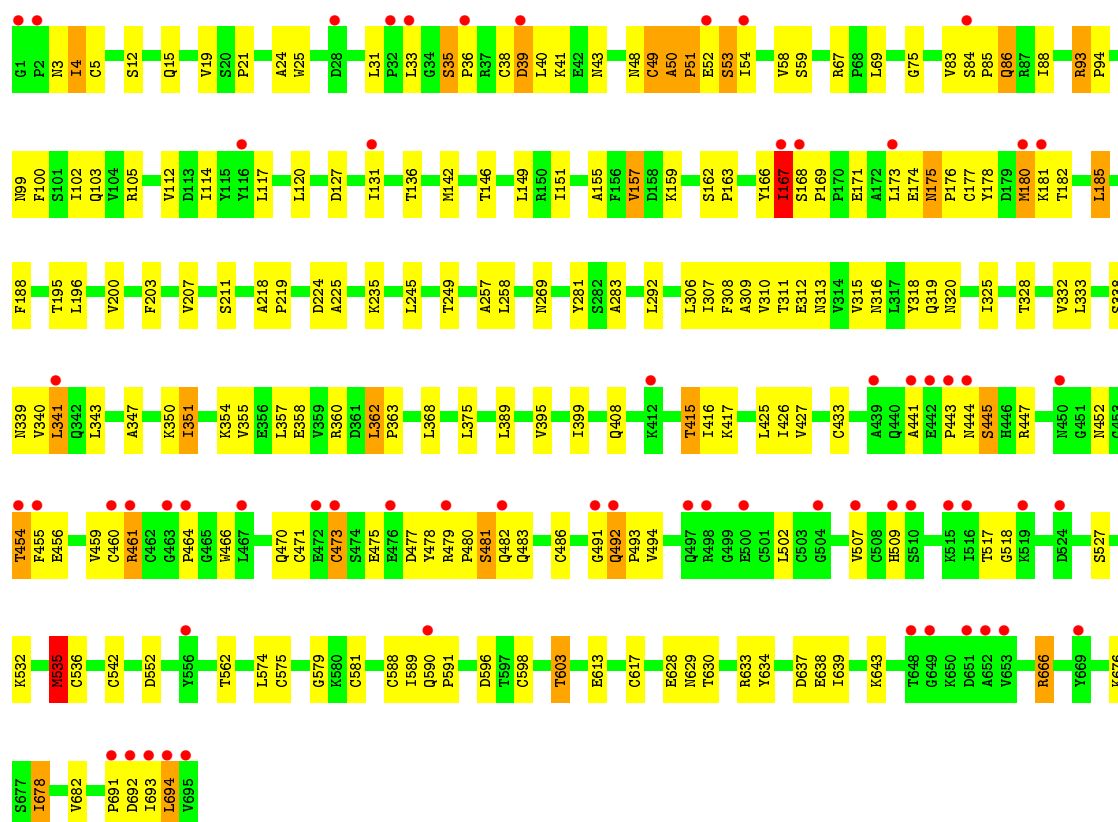
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 40% 60%



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

Chain D: 50% 50%



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

Chain F: 50% 50%



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

Chain G:  100%

GLG1
GLG2

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

Chain H:  50% 50%

GLG1
GLG2

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

Chain I:  100%

GLG1
GLG2

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

Chain K:  100%

GLG1
GLG2

- Molecule 5: alpha-D-mannopyranose-(1-4)-alpha-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:  33% 67%

GLG1
GLG2
MAN3
MAN4
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 J:  33% 67%

GLG1
GLG2
MAN3

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

Chain L:  100%

MAG1
MAG2
B/M3

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.87Å 129.87Å 305.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90 64.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.90) 92.7 (64.94-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019, CNS	Depositor
R, R_{free}	0.244 , 0.285 0.244 , 0.296	Depositor DCC
R_{free} test set	2924 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	82.4	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13087	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.33	0/7462	0.54	0/10123
2	B	0.35	0/5429	0.54	0/7344
All	All	0.34	0/12891	0.54	0/17467

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	546	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7300	0	7126	164	0
2	B	5332	0	5071	139	0
3	C	61	0	52	7	0
4	D	28	0	25	0	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	H	28	0	25	2	0
4	I	28	0	25	0	0
4	K	28	0	25	0	0
5	E	72	0	61	0	0
6	J	39	0	34	0	0
6	L	39	0	34	0	0
7	A	28	0	26	0	0
7	B	42	0	39	5	0
8	A	5	0	0	0	0
8	B	1	0	0	0	0
All	All	13087	0	12593	306	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 12.

All (306) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:HD11	1:A:350:LEU:HD11	1.58	0.85
2:B:249:THR:HG22	2:B:309:ALA:HB3	1.59	0.82
2:B:281:TYR:CE1	2:B:283:ALA:HB3	2.14	0.82
1:A:639:TYR:H	1:A:721:ASN:HD21	1.30	0.80
1:A:546:SER:O	1:A:547:GLU:HB2	1.82	0.77
1:A:958:ALA:HB1	1:A:959:PRO:HD2	1.65	0.77
2:B:169:PRO:HG2	2:B:173:LEU:HD23	1.65	0.77
1:A:821:ASN:HD21	4:H:1:NAG:C1	1.98	0.76
1:A:3:LEU:CD1	1:A:350:LEU:HD11	2.15	0.76
1:A:772:VAL:HG21	1:A:833:ILE:HD13	1.70	0.74
2:B:579:GLY:HA2	2:B:589:ILE:HD13	1.71	0.73
2:B:375:LEU:HD13	2:B:633:ARG:HD2	1.70	0.73
1:A:443:VAL:HG21	1:A:561:TYR:CE1	2.23	0.72
1:A:596:CYS:HG	1:A:602:CYS:HG	0.80	0.72
1:A:617:ILE:HD13	1:A:701:VAL:HG11	1.70	0.71
2:B:454:THR:HG23	2:B:461:ARG:O	1.91	0.71
2:B:589:ILE:HG22	2:B:591:PRO:HD3	1.71	0.71
2:B:574:LEU:HD11	2:B:581:CYS:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:CYS:HB3	2:B:38:CYS:SG	2.33	0.69
2:B:292:LEU:HD22	2:B:325:ILE:HD11	1.75	0.68
1:A:499:LEU:HD23	1:A:557:ILE:HD12	1.77	0.67
2:B:333:LEU:HD11	2:B:340:VAL:HG22	1.77	0.67
2:B:479:ARG:O	2:B:481:SER:N	2.28	0.66
1:A:116:THR:HG21	1:A:147:ILE:HD13	1.78	0.66
2:B:320:ASN:OD1	7:B:3320:NAG:H82	1.96	0.66
2:B:355:VAL:HG12	2:B:389:LEU:CD1	2.26	0.66
2:B:454:THR:O	2:B:460:CYS:HB2	1.96	0.65
1:A:885:GLN:N	1:A:885:GLN:HE21	1.95	0.65
2:B:362:LEU:HD23	2:B:363:PRO:HD2	1.79	0.65
2:B:589:ILE:HG23	2:B:590:GLN:H	1.62	0.64
1:A:368:ASP:O	1:A:370:LYS:N	2.31	0.63
1:A:527:ILE:HG22	1:A:534:GLN:HB3	1.79	0.63
1:A:147:ILE:O	1:A:147:ILE:HD12	1.97	0.63
1:A:617:ILE:HD11	1:A:625:LEU:HD22	1.81	0.63
1:A:314:GLN:HE21	1:A:332:ASN:HD21	1.45	0.63
1:A:443:VAL:HG21	1:A:561:TYR:HE1	1.63	0.62
1:A:116:THR:CG2	1:A:118:MET:SD	2.87	0.62
1:A:27:VAL:HG13	1:A:34:MET:HE2	1.81	0.62
2:B:588:CYS:HG	2:B:598:CYS:HG	0.70	0.62
3:C:2:NAG:H82	3:C:4:MAN:H62	1.82	0.62
1:A:236:ILE:HD12	1:A:237:ASP:H	1.65	0.61
1:A:807:THR:O	1:A:807:THR:HG22	2.00	0.61
2:B:149:LEU:HD21	2:B:151:ILE:HG23	1.83	0.61
2:B:50:ALA:O	2:B:54:ILE:HG23	2.00	0.61
1:A:768:THR:HB	1:A:835:ILE:HD12	1.82	0.61
2:B:613:GLU:O	2:B:617:CYS:HB2	2.00	0.61
1:A:769:GLU:HG2	1:A:812:LEU:HD11	1.82	0.60
1:A:248:ARG:HD2	7:B:3320:NAG:H81	1.83	0.60
2:B:281:TYR:CZ	2:B:283:ALA:HB3	2.36	0.60
2:B:589:ILE:CG2	2:B:590:GLN:H	2.14	0.60
2:B:180:MET:O	2:B:182:THR:HG22	2.00	0.60
2:B:332:VAL:O	2:B:343:LEU:HD21	2.02	0.60
2:B:316:ASN:HB3	7:B:3320:NAG:H83	1.84	0.60
2:B:589:ILE:CG2	2:B:590:GLN:N	2.65	0.60
1:A:610:VAL:HG11	1:A:715:LEU:HD21	1.85	0.59
2:B:218:ALA:HB3	2:B:219:PRO:HD3	1.84	0.59
1:A:546:SER:O	1:A:547:GLU:CB	2.51	0.59
1:A:508:ILE:HD11	2:B:475:GLU:O	2.02	0.59
2:B:502:LEU:HD13	2:B:507:VAL:CG2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:ARG:HG3	2:B:603:THR:HG21	1.84	0.59
2:B:694:LEU:HD23	2:B:694:LEU:O	2.03	0.59
1:A:187:GLN:O	1:A:191:ILE:HD12	2.03	0.58
1:A:672:THR:HG23	1:A:676:THR:O	2.03	0.58
1:A:627:LEU:HD12	1:A:627:LEU:O	2.03	0.58
2:B:355:VAL:HG12	2:B:389:LEU:HD11	1.85	0.58
1:A:755:LEU:HD11	1:A:908:PHE:HB3	1.86	0.58
1:A:70:ILE:HD13	1:A:105:ILE:HD11	1.86	0.58
1:A:165:LYS:O	1:A:166:ALA:HB3	2.04	0.57
1:A:666:LEU:HD21	1:A:693:LEU:HD23	1.86	0.57
2:B:51:PRO:O	2:B:53:SER:N	2.37	0.57
1:A:721:ASN:HD22	1:A:721:ASN:N	2.02	0.57
1:A:936:LEU:HD22	1:A:937:PRO:HD2	1.85	0.57
1:A:567:THR:HG23	1:A:567:THR:O	2.05	0.56
2:B:169:PRO:CG	2:B:173:LEU:HD23	2.35	0.56
2:B:24:ALA:O	2:B:38:CYS:HA	2.05	0.56
1:A:685:ASN:HB3	1:A:686:PRO:CD	2.36	0.56
1:A:816:ILE:HG23	1:A:820:MET:HE3	1.87	0.56
1:A:116:THR:HG22	1:A:118:MET:H	1.68	0.56
1:A:170:LEU:HD13	1:A:226:VAL:HG22	1.87	0.56
2:B:441:ALA:HB1	2:B:456:GLU:CB	2.35	0.56
1:A:24:ASP:OD2	1:A:25:PHE:N	2.38	0.56
2:B:39:ASP:O	2:B:40:LEU:HD22	2.06	0.56
1:A:61:TRP:O	1:A:63:SER:N	2.39	0.56
2:B:159:LYS:NZ	2:B:224:ASP:OD1	2.39	0.56
1:A:502:LEU:HD12	2:B:509:HIS:CD2	2.41	0.56
1:A:3:LEU:H	1:A:389:GLN:HE22	1.53	0.55
1:A:757:ILE:O	1:A:757:ILE:HG23	2.04	0.55
1:A:936:LEU:HD13	1:A:937:PRO:HD2	1.89	0.55
1:A:3:LEU:HD13	1:A:350:LEU:HD21	1.88	0.55
2:B:149:LEU:HD23	2:B:149:LEU:C	2.27	0.55
1:A:332:ASN:N	1:A:332:ASN:HD22	2.02	0.55
2:B:112:VAL:HG11	2:B:142:MET:CE	2.38	0.54
2:B:173:LEU:O	2:B:173:LEU:HD12	2.06	0.54
2:B:50:ALA:HB3	2:B:51:PRO:HD3	1.89	0.54
1:A:946:LEU:HD23	1:A:946:LEU:H	1.73	0.54
2:B:83:VAL:O	2:B:86:GLN:NE2	2.36	0.54
1:A:816:ILE:HG23	1:A:820:MET:CE	2.37	0.54
2:B:15:GLN:O	2:B:19:VAL:HG23	2.07	0.54
1:A:936:LEU:HD13	1:A:937:PRO:CD	2.38	0.54
1:A:547:GLU:CD	2:B:477:ASP:HA	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:VAL:O	2:B:157:VAL:HG12	2.09	0.53
1:A:547:GLU:O	1:A:548:PHE:C	2.43	0.53
1:A:792:LYS:HB2	1:A:930:GLU:HB2	1.90	0.53
2:B:441:ALA:CB	2:B:456:GLU:HB2	2.39	0.53
2:B:491:GLY:O	2:B:492:GLN:HB2	2.09	0.53
1:A:648:PRO:HG3	1:A:711:VAL:HG22	1.90	0.53
1:A:795:LEU:HB3	1:A:884:CYS:HB2	1.90	0.53
1:A:154:PHE:O	1:A:175:GLY:HA3	2.08	0.53
1:A:414:ILE:HG21	1:A:434:LEU:HD21	1.91	0.53
2:B:308:PHE:CE2	2:B:328:THR:HG21	2.44	0.53
1:A:617:ILE:HD11	1:A:625:LEU:CD2	2.39	0.52
2:B:131:ILE:HG22	2:B:207:VAL:HG21	1.91	0.52
1:A:314:GLN:HE21	1:A:332:ASN:ND2	2.06	0.52
1:A:755:LEU:O	1:A:757:ILE:N	2.43	0.52
2:B:637:ASP:O	2:B:639:ILE:HD12	2.09	0.52
1:A:347:LEU:CD1	1:A:375:ILE:HD13	2.37	0.52
1:A:510:ARG:O	1:A:542:LEU:HD12	2.10	0.52
1:A:347:LEU:HD13	1:A:350:LEU:HD22	1.91	0.52
2:B:375:LEU:HD21	2:B:630:THR:HG22	1.91	0.52
2:B:459:VAL:HG22	2:B:460:CYS:N	2.25	0.52
1:A:165:LYS:O	1:A:236:ILE:HD11	2.09	0.52
1:A:246:ALA:HB1	1:A:252:MET:HE3	1.92	0.52
1:A:400:MET:HE1	1:A:427:PHE:CE1	2.44	0.52
1:A:453:ILE:HD11	1:A:639:TYR:CE2	2.45	0.52
2:B:441:ALA:HB1	2:B:456:GLU:HB3	1.92	0.52
2:B:693:ILE:O	2:B:693:ILE:HG23	2.10	0.52
1:A:222:LEU:HA	1:A:243:VAL:HG22	1.92	0.51
2:B:166:TYR:CD2	2:B:173:LEU:HD21	2.45	0.51
1:A:100:SER:HB2	1:A:105:ILE:HG22	1.91	0.51
1:A:903:LEU:HD21	1:A:908:PHE:CD1	2.45	0.51
1:A:880:LEU:C	1:A:880:LEU:HD23	2.30	0.51
1:A:246:ALA:HB1	1:A:252:MET:CE	2.41	0.51
2:B:112:VAL:HG12	2:B:146:THR:HG21	1.93	0.51
1:A:769:GLU:HG2	1:A:902:LEU:HD21	1.92	0.51
1:A:903:LEU:HD23	1:A:903:LEU:C	2.31	0.51
1:A:43:ALA:HB3	1:A:55:GLN:HG2	1.92	0.51
2:B:112:VAL:CG1	2:B:146:THR:HG21	2.41	0.51
2:B:185:LEU:HD11	2:B:211:SER:O	2.11	0.51
2:B:3:ASN:O	2:B:5:CYS:N	2.43	0.50
1:A:116:THR:HG22	1:A:117:GLU:N	2.25	0.50
1:A:946:LEU:HD23	1:A:946:LEU:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:VAL:HG11	2:B:318:TYR:CD1	2.46	0.50
2:B:33:LEU:HD21	2:B:470:GLN:HE21	1.76	0.50
1:A:625:LEU:HD12	1:A:626:THR:N	2.28	0.49
2:B:333:LEU:CD1	2:B:340:VAL:HG22	2.40	0.49
1:A:243:VAL:HG12	1:A:246:ALA:HB2	1.94	0.49
2:B:3:ASN:HB3	2:B:4:ILE:HD12	1.94	0.49
1:A:253:VAL:HG21	1:A:295:ILE:HD13	1.93	0.49
2:B:40:LEU:HD23	2:B:43:ASN:HD22	1.78	0.49
2:B:39:ASP:OD1	2:B:40:LEU:N	2.43	0.49
1:A:514:LEU:HD23	1:A:539:ILE:HD13	1.95	0.49
2:B:99:ASN:HD22	7:B:3099:NAG:H61	1.78	0.49
2:B:535:MET:SD	2:B:536:CYS:N	2.78	0.48
1:A:472:CYS:HA	1:A:541:TYR:HA	1.94	0.48
2:B:177:CYS:HB3	2:B:182:THR:HG23	1.94	0.48
1:A:183:LEU:HD13	1:A:222:LEU:HG	1.95	0.48
1:A:809:LEU:HG	1:A:920:LEU:HD13	1.95	0.48
1:A:936:LEU:HD13	1:A:937:PRO:N	2.29	0.48
2:B:117:LEU:HD21	2:B:225:ALA:HB1	1.95	0.48
2:B:40:LEU:HD23	2:B:43:ASN:ND2	2.27	0.48
2:B:456:GLU:O	2:B:459:VAL:O	2.32	0.48
2:B:574:LEU:HD13	2:B:575:CYS:N	2.29	0.48
1:A:645:VAL:O	1:A:645:VAL:HG13	2.13	0.48
2:B:67:ARG:N	2:B:86:GLN:OE1	2.47	0.48
1:A:1:PHE:HA	1:A:389:GLN:HB2	1.94	0.47
1:A:567:THR:O	1:A:568:ALA:HB2	2.14	0.47
1:A:70:ILE:HD13	1:A:105:ILE:CD1	2.45	0.47
2:B:21:PRO:HA	2:B:93:ARG:HD2	1.96	0.47
1:A:499:LEU:CD2	1:A:557:ILE:HD12	2.45	0.47
2:B:175:ASN:OD1	2:B:175:ASN:N	2.47	0.47
2:B:455:PHE:O	2:B:456:GLU:HB3	2.13	0.47
2:B:375:LEU:HD21	2:B:630:THR:CG2	2.43	0.47
1:A:514:LEU:CD2	1:A:539:ILE:HD13	2.44	0.47
2:B:307:ILE:HD13	2:B:347:ALA:CB	2.45	0.47
2:B:166:TYR:HD2	2:B:173:LEU:HD21	1.78	0.47
2:B:195:THR:HG22	2:B:235:LYS:O	2.15	0.47
2:B:88:ILE:CG2	2:B:427:VAL:HG22	2.44	0.47
3:C:2:NAG:H82	3:C:4:MAN:C6	2.46	0.47
1:A:397:ALA:HB2	1:A:402:PRO:HD3	1.97	0.46
1:A:400:MET:HE1	1:A:427:PHE:CZ	2.49	0.46
2:B:517:THR:HG22	2:B:518:GLY:H	1.79	0.46
1:A:596:CYS:CB	1:A:602:CYS:HG	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:VAL:HG13	1:A:34:MET:CE	2.45	0.46
2:B:332:VAL:HG13	2:B:332:VAL:O	2.15	0.46
1:A:257:ASP:O	1:A:260:ASN:O	2.34	0.46
1:A:927:ASN:HD21	1:A:940:ASP:HB3	1.81	0.46
1:A:962:VAL:N	1:A:963:PRO:CD	2.78	0.46
2:B:362:LEU:HD11	2:B:368:LEU:HD13	1.97	0.46
2:B:93:ARG:HD3	2:B:94:PRO:HD2	1.97	0.46
1:A:685:ASN:C	1:A:685:ASN:HD22	2.19	0.46
3:C:2:NAG:O3	3:C:3:BMA:C2	2.63	0.46
1:A:649:LEU:HD12	1:A:677:ARG:HB3	1.97	0.46
2:B:249:THR:HG22	2:B:309:ALA:CB	2.38	0.46
2:B:312:GLU:O	2:B:315:VAL:HG12	2.15	0.46
2:B:360:ARG:HB2	2:B:415:THR:HG23	1.98	0.46
1:A:738:VAL:HG23	1:A:936:LEU:HD12	1.98	0.46
2:B:389:LEU:HD23	2:B:633:ARG:HH12	1.81	0.45
2:B:426:ILE:HD12	2:B:426:ILE:N	2.31	0.45
2:B:114:ILE:HB	2:B:151:ILE:HG22	1.98	0.45
2:B:39:ASP:C	2:B:40:LEU:HD22	2.37	0.45
1:A:170:LEU:HD13	1:A:226:VAL:CG2	2.47	0.45
2:B:25:TRP:HZ2	2:B:459:VAL:HG11	1.80	0.45
2:B:84:SER:HB3	2:B:85:PRO:HD3	1.98	0.45
1:A:821:ASN:ND2	4:H:1:NAG:C1	2.74	0.45
2:B:339:ASN:O	2:B:343:LEU:HD13	2.17	0.45
2:B:445:SER:OG	7:B:3452:NAG:H82	2.16	0.45
1:A:144:SER:OG	1:A:152:GLN:NE2	2.50	0.45
1:A:511:ALA:O	1:A:512:LEU:HD23	2.17	0.45
1:A:100:SER:CB	1:A:105:ILE:HG22	2.47	0.45
2:B:441:ALA:HB1	2:B:456:GLU:HB2	1.99	0.45
1:A:546:SER:O	1:A:546:SER:OG	2.28	0.45
1:A:253:VAL:HG21	1:A:295:ILE:CD1	2.47	0.44
1:A:610:VAL:HG12	1:A:629:VAL:HG22	2.00	0.44
2:B:355:VAL:HG11	2:B:395:VAL:HG21	1.98	0.44
2:B:103:GLN:OE1	2:B:103:GLN:N	2.51	0.44
1:A:797:LEU:HD23	1:A:882:ILE:HD12	1.99	0.44
1:A:504:GLN:HE22	1:A:509:ARG:HB3	1.81	0.44
2:B:306:LEU:O	2:B:328:THR:HG23	2.17	0.44
2:B:666:ARG:O	2:B:682:VAL:HG12	2.18	0.44
2:B:180:MET:O	2:B:182:THR:N	2.50	0.44
1:A:250:LEU:HD22	1:A:269:GLY:O	2.18	0.44
1:A:477:PHE:HD2	1:A:497:LEU:HD21	1.82	0.44
1:A:559:MET:HE1	1:A:586:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:ALA:O	1:A:742:VAL:HG23	2.17	0.44
1:A:757:ILE:HG23	1:A:760:TRP:CB	2.48	0.44
2:B:166:TYR:O	2:B:167:ILE:C	2.56	0.44
1:A:116:THR:HG22	1:A:118:MET:SD	2.57	0.44
1:A:757:ILE:HG23	1:A:760:TRP:HB3	2.00	0.44
1:A:962:VAL:O	1:A:962:VAL:HG12	2.18	0.44
2:B:441:ALA:HB2	2:B:456:GLU:HB2	2.00	0.44
1:A:885:GLN:H	1:A:885:GLN:HE21	1.63	0.43
2:B:69:LEU:HB3	2:B:105:ARG:HE	1.83	0.43
1:A:183:LEU:HD21	1:A:241:SER:HB2	2.00	0.43
1:A:165:LYS:O	1:A:166:ALA:CB	2.66	0.43
1:A:243:VAL:CG1	1:A:246:ALA:HB2	2.49	0.43
1:A:253:VAL:CG2	1:A:295:ILE:HD13	2.48	0.43
1:A:640:GLU:N	1:A:685:ASN:O	2.52	0.43
1:A:660:ASN:ND2	1:A:663:LEU:HD13	2.32	0.43
2:B:638:GLU:HB2	2:B:678:ILE:HG22	2.00	0.43
1:A:375:ILE:HD12	1:A:376:PHE:N	2.33	0.43
1:A:477:PHE:CD2	1:A:497:LEU:HD21	2.54	0.43
1:A:50:ILE:HG23	1:A:90:SER:HA	2.01	0.43
2:B:100:PHE:CE1	2:B:399:ILE:HD12	2.54	0.43
2:B:88:ILE:HG23	2:B:427:VAL:HG22	2.00	0.43
1:A:502:LEU:HD21	1:A:556:THR:OG1	2.19	0.43
2:B:58:VAL:HG12	2:B:59:SER:O	2.18	0.43
1:A:647:ILE:HD12	1:A:647:ILE:C	2.39	0.42
2:B:83:VAL:HG13	2:B:102:ILE:HD11	2.00	0.42
1:A:945:THR:HG22	1:A:946:LEU:N	2.35	0.42
2:B:136:THR:HA	2:B:200:VAL:HG11	1.99	0.42
2:B:311:THR:OG1	2:B:313:ASN:ND2	2.52	0.42
1:A:236:ILE:HD12	1:A:237:ASP:N	2.32	0.42
3:C:2:NAG:C3	3:C:3:BMA:H2	2.50	0.42
1:A:27:VAL:HG22	1:A:34:MET:HE2	2.01	0.42
1:A:757:ILE:O	1:A:757:ILE:CG2	2.66	0.42
2:B:157:VAL:HG23	2:B:188:PHE:CZ	2.54	0.42
1:A:336:VAL:HG12	1:A:337:PHE:CD2	2.55	0.42
1:A:648:PRO:O	1:A:650:GLN:N	2.52	0.42
1:A:50:ILE:HG23	1:A:90:SER:CA	2.49	0.42
2:B:162:SER:HB3	2:B:167:ILE:HG23	2.02	0.42
1:A:344:ILE:HG22	1:A:358:ILE:HD11	2.00	0.42
1:A:702:HIS:O	1:A:703:GLN:C	2.58	0.42
1:A:801:TYR:CD2	1:A:802:LYS:HG3	2.55	0.42
3:C:2:NAG:O3	3:C:3:BMA:H2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:358:GLU:N	2:B:417:LYS:O	2.45	0.42
1:A:114:TRP:CE3	1:A:143:ARG:HD2	2.55	0.42
1:A:240:VAL:HG22	1:A:255:ILE:HG12	2.01	0.42
2:B:257:ALA:O	2:B:258:LEU:HB2	2.19	0.42
2:B:48:ASN:O	2:B:49:CYS:C	2.58	0.42
1:A:672:THR:O	1:A:672:THR:HG22	2.20	0.41
1:A:835:ILE:HG22	1:A:836:SER:N	2.34	0.41
1:A:905:THR:O	1:A:906:GLU:C	2.58	0.41
2:B:310:VAL:HG11	2:B:318:TYR:CG	2.55	0.41
2:B:102:ILE:HD12	2:B:425:LEU:HB2	2.02	0.41
1:A:936:LEU:O	1:A:938:ILE:HG23	2.20	0.41
2:B:492:GLN:N	2:B:493:PRO:HD2	2.36	0.41
1:A:780:TYR:CZ	1:A:947:VAL:HG13	2.55	0.41
1:A:829:ASN:N	1:A:830:PRO:HD3	2.36	0.41
2:B:203:PHE:O	2:B:207:VAL:HG12	2.21	0.41
2:B:50:ALA:O	2:B:51:PRO:O	2.38	0.41
2:B:630:THR:HB	2:B:634:TYR:CD1	2.56	0.41
1:A:685:ASN:HB3	1:A:686:PRO:HD3	2.02	0.41
2:B:245:LEU:CD2	2:B:351:ILE:HD11	2.50	0.41
2:B:589:ILE:HG22	2:B:590:GLN:N	2.36	0.41
1:A:145:GLN:C	1:A:147:ILE:HG23	2.40	0.41
1:A:826:MET:HE2	1:A:880:LEU:HG	2.02	0.41
2:B:48:ASN:O	2:B:50:ALA:HB2	2.20	0.41
2:B:552:ASP:HA	2:B:562:THR:OG1	2.20	0.41
2:B:94:PRO:HD3	2:B:433:CYS:HB3	2.02	0.41
2:B:12:SER:HB3	2:B:461:ARG:HH21	1.86	0.41
2:B:682:VAL:HG13	2:B:682:VAL:O	2.20	0.41
1:A:349:ASP:O	1:A:352:GLN:NE2	2.47	0.41
2:B:399:ILE:HD13	2:B:416:ILE:HD13	2.02	0.41
1:A:373:VAL:HG23	1:A:404:PHE:CE2	2.56	0.41
1:A:440:VAL:HG22	1:A:577:ILE:CG2	2.50	0.41
2:B:340:VAL:O	2:B:341:LEU:C	2.59	0.41
1:A:63:SER:O	1:A:64:THR:C	2.60	0.40
1:A:306:ASP:N	1:A:306:ASP:OD1	2.48	0.40
1:A:332:ASN:N	1:A:332:ASN:ND2	2.69	0.40
2:B:35:SER:HB3	2:B:36:PRO:HD3	2.03	0.40
2:B:502:LEU:HD13	2:B:507:VAL:HG23	2.03	0.40
2:B:173:LEU:HD13	2:B:178:TYR:CE1	2.56	0.40
3:C:2:NAG:HO3	3:C:3:BMA:C2	2.33	0.40
1:A:801:TYR:CD2	1:A:826:MET:HE1	2.56	0.40
3:C:2:NAG:C3	3:C:3:BMA:C2	3.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:LEU:HG	2:B:155:ALA:HB1	2.03	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	934/967 (97%)	843 (90%)	68 (7%)	23 (2%)	5	21
2	B	693/695 (100%)	579 (84%)	82 (12%)	32 (5%)	2	9
All	All	1627/1662 (98%)	1422 (87%)	150 (9%)	55 (3%)	3	15

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	SER
1	A	505	LYS
1	A	547	GLU
1	A	568	ALA
1	A	703	GLN
1	A	741	ALA
1	A	961	PRO
2	B	39	ASP
2	B	51	PRO
2	B	52	GLU
2	B	167	ILE
2	B	168	SER
2	B	181	LYS
2	B	473	CYS
2	B	478	TYR
2	B	480	PRO
2	B	481	SER

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Mol	Chain	Res	Type
2	B	492	GLN
1	A	64	THR
1	A	368	ASP
1	A	369	LYS
1	A	546	SER
1	A	707	MET
1	A	835	ILE
1	A	914	GLN
2	B	35	SER
2	B	49	CYS
2	B	53	SER
2	B	196	LEU
2	B	444	ASN
2	B	535	MET
1	A	503	LYS
1	A	674	ASN
1	A	808	LEU
2	B	50	ALA
2	B	482	GLN
2	B	527	SER
1	A	399	SER
1	A	529	ARG
1	A	649	LEU
2	B	4	ILE
2	B	443	PRO
2	B	532	LYS
1	A	910	ASN
2	B	41	LYS
2	B	157	VAL
2	B	445	SER
1	A	756	PRO
2	B	464	PRO
2	B	691	PRO
2	B	163	PRO
2	B	176	PRO
1	A	962	VAL
2	B	75	GLY
2	B	494	VAL

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	797/821 (97%)	727 (91%)	70 (9%)	10	30
2	B	617/617 (100%)	575 (93%)	42 (7%)	16	42
All	All	1414/1438 (98%)	1302 (92%)	112 (8%)	12	34

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	SER
1	A	99	ARG
1	A	105	ILE
1	A	106	LEU
1	A	115	ARG
1	A	118	MET
1	A	120	GLN
1	A	145	GLN
1	A	162	ASP
1	A	170	LEU
1	A	216	ILE
1	A	226	VAL
1	A	275	TYR
1	A	327	GLN
1	A	331	LEU
1	A	339	ARG
1	A	367	GLU
1	A	368	ASP
1	A	375	ILE
1	A	379	ARG
1	A	392	GLU
1	A	399	SER
1	A	417	ASN
1	A	436	ARG
1	A	450	TYR
1	A	474	ASN
1	A	478	CYS

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Mol	Chain	Res	Type
1	A	487	LEU
1	A	502	LEU
1	A	505	LYS
1	A	523	LYS
1	A	535	CYS
1	A	536	GLU
1	A	549	ARG
1	A	564	ASP
1	A	565	TYR
1	A	598	GLU
1	A	602	CYS
1	A	605	LYS
1	A	606	LEU
1	A	633	ASN
1	A	646	SER
1	A	649	LEU
1	A	650	GLN
1	A	658	ARG
1	A	665	ARG
1	A	677	ARG
1	A	685	ASN
1	A	688	LYS
1	A	712	LYS
1	A	715	LEU
1	A	721	ASN
1	A	733	LYS
1	A	745	ARG
1	A	749	SER
1	A	764	GLU
1	A	783	ARG
1	A	817	ASP
1	A	832	ARG
1	A	835	ILE
1	A	868	ASP
1	A	878	GLN
1	A	885	GLN
1	A	894	SER
1	A	897	LEU
1	A	902	LEU
1	A	913	ASN
1	A	921	LYS
1	A	946	LEU

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Mol	Chain	Res	Type
1	A	947	VAL
2	B	31	LEU
2	B	86	GLN
2	B	93	ARG
2	B	127	ASP
2	B	167	ILE
2	B	171	GLU
2	B	174	GLU
2	B	175	ASN
2	B	180	MET
2	B	185	LEU
2	B	269	ASN
2	B	319	GLN
2	B	338	SER
2	B	341	LEU
2	B	350	LYS
2	B	351	ILE
2	B	354	LYS
2	B	357	LEU
2	B	362	LEU
2	B	408	GLN
2	B	415	THR
2	B	447	ARG
2	B	452	ASN
2	B	454	THR
2	B	461	ARG
2	B	466	TRP
2	B	471	CYS
2	B	473	CYS
2	B	483	GLN
2	B	486	CYS
2	B	535	MET
2	B	542	CYS
2	B	596	ASP
2	B	603	THR
2	B	628	GLU
2	B	629	ASN
2	B	643	LYS
2	B	666	ARG
2	B	676	LYS
2	B	678	ILE
2	B	692	ASP

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Mol	Chain	Res	Type
2	B	694	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	152	GLN
1	A	187	GLN
1	A	205	ASN
1	A	332	ASN
1	A	389	GLN
1	A	394	GLN
1	A	456	GLN
1	A	492	ASN
1	A	504	GLN
1	A	580	GLN
1	A	614	GLN
1	A	623	ASN
1	A	633	ASN
1	A	650	GLN
1	A	685	ASN
1	A	704	GLN
1	A	721	ASN
1	A	732	HIS
1	A	784	ASN
1	A	796	HIS
1	A	885	GLN
1	A	927	ASN
1	A	956	GLN
2	B	43	ASN
2	B	240	ASN
2	B	244	HIS
2	B	269	ASN
2	B	301	GLN
2	B	303	ASN
2	B	313	ASN
2	B	342	GLN
2	B	376	ASN
2	B	408	GLN
2	B	450	ASN
2	B	470	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

29 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	$\# Z > 2$
3	NAG	C	1	1,3	14,14,15	0.63	0	17,19,21	1.25	2 (11%)
3	NAG	C	2	3	14,14,15	0.42	0	17,19,21	1.51	3 (17%)
3	BMA	C	3	3	11,11,12	0.51	0	15,15,17	2.55	2 (13%)
3	MAN	C	4	3	11,11,12	0.56	0	15,15,17	1.03	2 (13%)
3	MAN	C	5	3	11,11,12	0.60	0	15,15,17	1.06	1 (6%)
4	NAG	D	1	1,4	14,14,15	0.52	0	17,19,21	0.73	0
4	NAG	D	2	4	14,14,15	0.47	0	17,19,21	0.85	1 (5%)
5	NAG	E	1	1,5	14,14,15	0.55	0	17,19,21	1.20	2 (11%)
5	NAG	E	2	5	14,14,15	0.54	0	17,19,21	0.67	0
5	BMA	E	3	5	11,11,12	0.25	0	15,15,17	0.86	1 (6%)
5	MAN	E	4	5	11,11,12	0.62	0	15,15,17	1.22	1 (6%)
5	MAN	E	5	5	11,11,12	0.65	0	15,15,17	0.95	1 (6%)
5	MAN	E	6	5	11,11,12	0.63	0	15,15,17	0.78	0
4	NAG	F	1	1,4	14,14,15	0.58	0	17,19,21	1.27	1 (5%)
4	NAG	F	2	4	14,14,15	0.50	0	17,19,21	0.79	0
4	NAG	G	1	1,4	14,14,15	0.65	0	17,19,21	1.43	2 (11%)
4	NAG	G	2	4	14,14,15	0.69	0	17,19,21	0.96	1 (5%)
4	NAG	H	1	4	14,14,15	0.68	0	17,19,21	1.65	2 (11%)
4	NAG	H	2	4	14,14,15	0.68	0	17,19,21	1.00	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	I	1	1,4	14,14,15	0.68	0	17,19,21	1.25	1 (5%)
4	NAG	I	2	4	14,14,15	0.51	0	17,19,21	1.23	1 (5%)
6	NAG	J	1	1,6	14,14,15	0.50	0	17,19,21	0.99	2 (11%)
6	NAG	J	2	6	14,14,15	0.68	0	17,19,21	1.20	1 (5%)
6	BMA	J	3	6	11,11,12	0.32	0	15,15,17	0.68	0
4	NAG	K	1	2,4	14,14,15	0.47	0	17,19,21	1.91	2 (11%)
4	NAG	K	2	4	14,14,15	0.52	0	17,19,21	1.39	2 (11%)
6	NAG	L	1	2,6	14,14,15	0.51	0	17,19,21	1.10	2 (11%)
6	NAG	L	2	6	14,14,15	0.57	0	17,19,21	1.25	2 (11%)
6	BMA	L	3	6	11,11,12	0.45	0	15,15,17	0.88	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
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	1/2/19/22	0/1/1/1
3	MAN	C	5	3	-	2/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
5	NAG	E	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	2/2/19/22	0/1/1/1
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1
5	MAN	E	5	5	-	2/2/19/22	0/1/1/1
5	MAN	E	6	5	-	2/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	H	1	4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	3/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
6	NAG	J	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	6/6/23/26	0/1/1/1
6	BMA	J	3	6	-	2/2/19/22	0/1/1/1
4	NAG	K	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	K	2	4	-	4/6/23/26	0/1/1/1
6	NAG	L	1	2,6	-	4/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1
6	BMA	L	3	6	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	BMA	C1-O5-C5	7.77	122.72	112.19
4	K	1	NAG	C1-O5-C5	5.58	119.76	112.19
3	C	3	BMA	C1-C2-C3	4.84	115.61	109.67
4	G	1	NAG	C4-C3-C2	4.49	117.59	111.02
4	H	1	NAG	C3-C4-C5	4.39	118.07	110.24
4	K	1	NAG	O4-C4-C5	4.25	119.85	109.30
4	I	2	NAG	C1-O5-C5	4.14	117.81	112.19
4	I	1	NAG	C4-C3-C2	4.08	117.00	111.02
4	K	2	NAG	C1-O5-C5	3.84	117.40	112.19
6	J	2	NAG	C4-C3-C2	3.79	116.57	111.02
4	H	1	NAG	O5-C1-C2	-3.56	105.67	111.29
4	F	1	NAG	C4-C3-C2	3.45	116.07	111.02
6	L	1	NAG	O5-C1-C2	-3.40	105.91	111.29
6	L	2	NAG	C4-C3-C2	3.31	115.87	111.02
3	C	2	NAG	O4-C4-C3	3.14	117.61	110.35
3	C	5	MAN	C1-C2-C3	3.09	113.46	109.67
3	C	2	NAG	C1-O5-C5	3.00	116.26	112.19
3	C	4	MAN	C1-O5-C5	2.89	116.11	112.19
3	C	2	NAG	O3-C3-C2	-2.83	103.62	109.47
3	C	1	NAG	C1-O5-C5	2.83	116.02	112.19
4	H	2	NAG	C4-C3-C2	2.75	115.05	111.02
5	E	4	MAN	O4-C4-C3	-2.71	104.09	110.35
4	G	2	NAG	C4-C3-C2	2.58	114.81	111.02
5	E	3	BMA	O5-C5-C6	2.56	111.22	107.20
5	E	1	NAG	O5-C1-C2	-2.54	107.28	111.29
4	G	1	NAG	C3-C4-C5	2.52	114.74	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	5	MAN	C1-C2-C3	2.50	112.73	109.67
4	K	2	NAG	O5-C5-C6	2.42	111.00	107.20
6	L	2	NAG	O5-C5-C6	2.41	110.98	107.20
5	E	1	NAG	O5-C5-C6	2.38	110.94	107.20
6	L	1	NAG	C1-O5-C5	2.27	115.27	112.19
6	J	1	NAG	O5-C1-C2	-2.22	107.78	111.29
6	L	3	BMA	O5-C5-C6	2.12	110.53	107.20
4	D	2	NAG	C1-O5-C5	2.11	115.05	112.19
3	C	4	MAN	C1-C2-C3	2.07	112.21	109.67
3	C	1	NAG	O4-C4-C5	-2.05	104.20	109.30
6	J	1	NAG	C4-C3-C2	-2.01	108.08	111.02

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	2	NAG	C8-C7-N2-C2
6	L	2	NAG	O7-C7-N2-C2
4	K	2	NAG	C8-C7-N2-C2
4	K	2	NAG	O7-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
6	J	1	NAG	C8-C7-N2-C2
6	J	1	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
6	L	1	NAG	C8-C7-N2-C2
6	L	1	NAG	O7-C7-N2-C2
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
6	J	2	NAG	C8-C7-N2-C2
6	J	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	F	1	NAG	C3-C2-N2-C7
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	I	1	NAG	O5-C5-C6-O6

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

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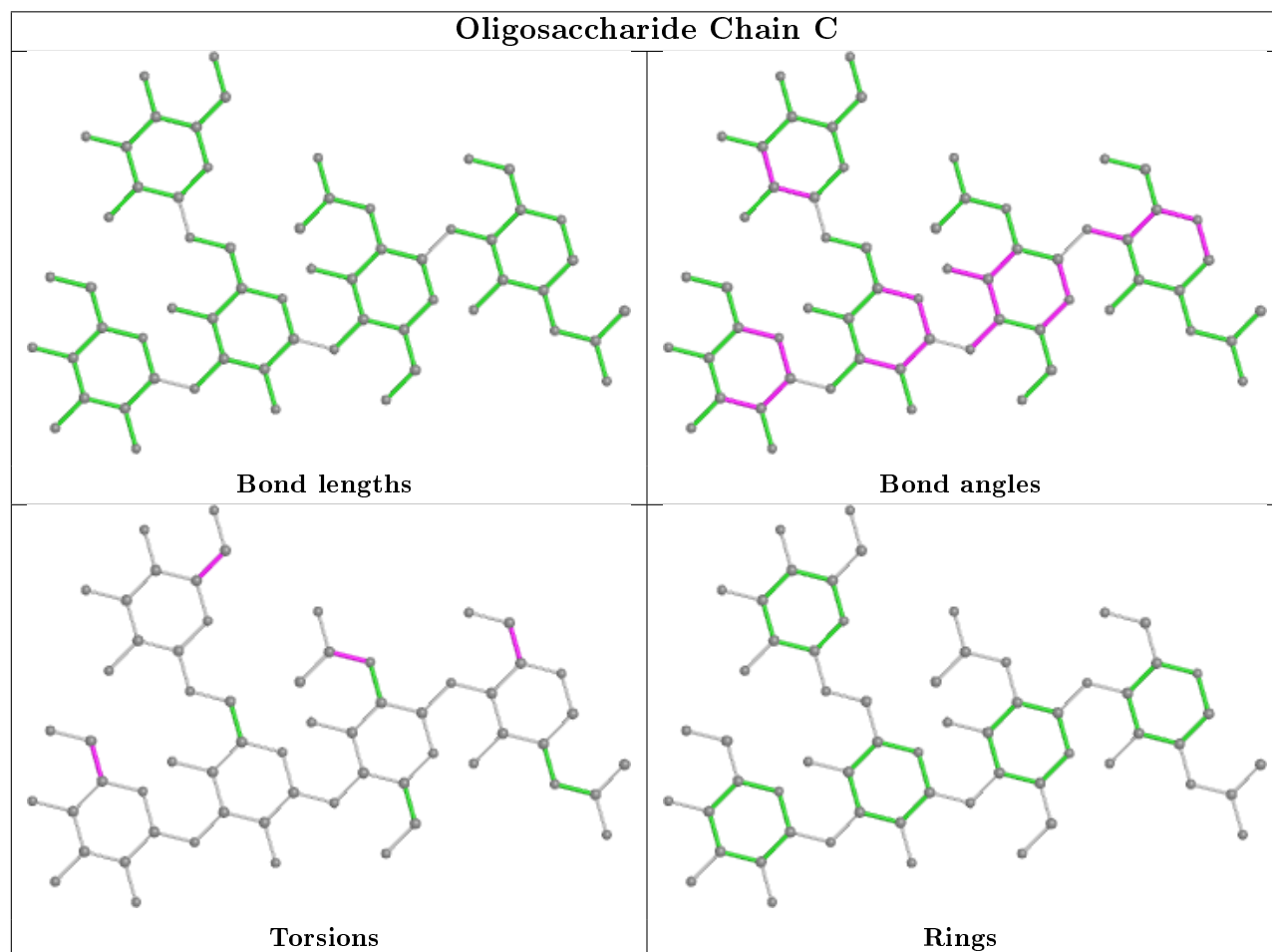
Mol	Chain	Res	Type	Atoms
6	J	2	NAG	O5-C5-C6-O6

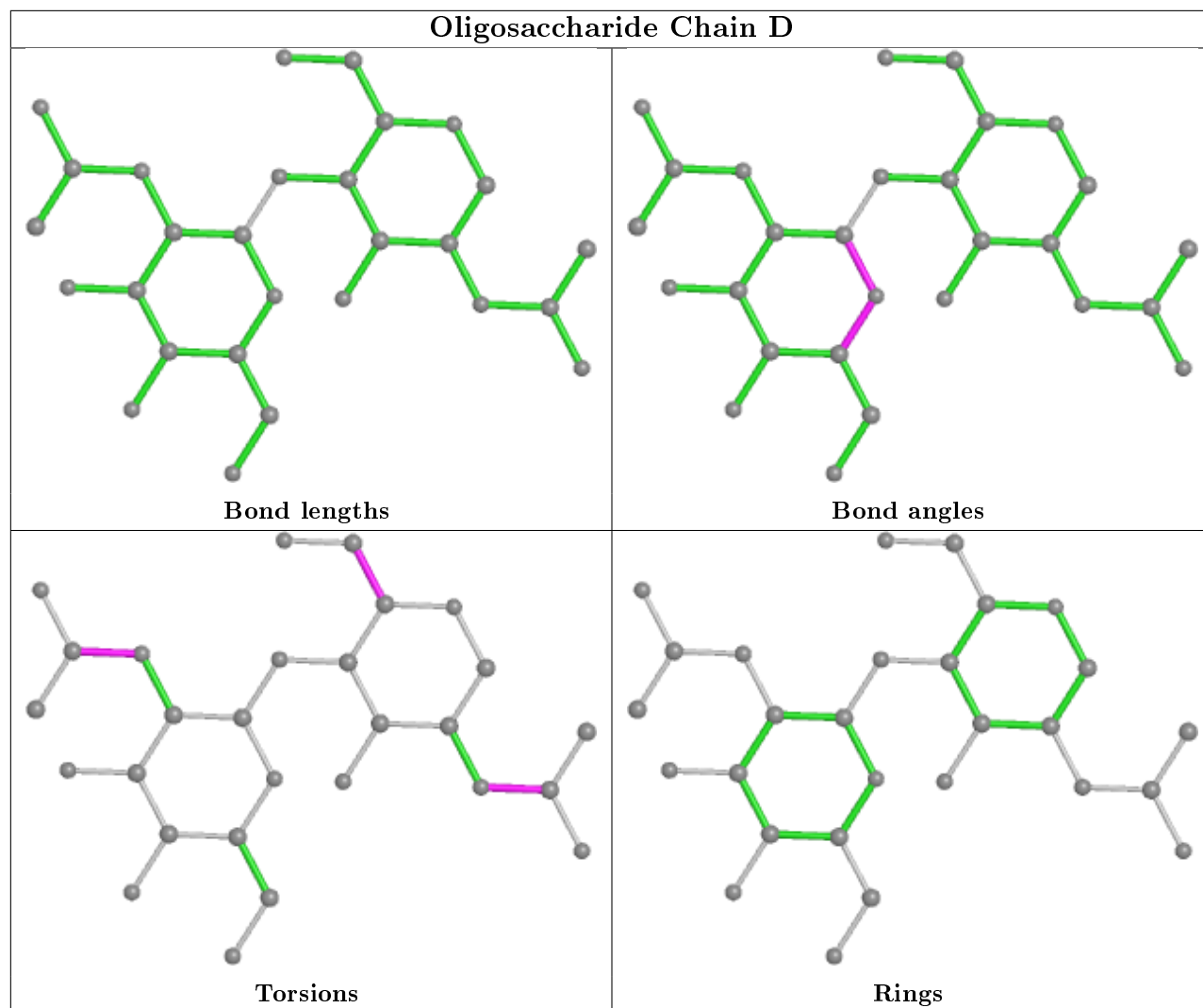
There are no ring outliers.

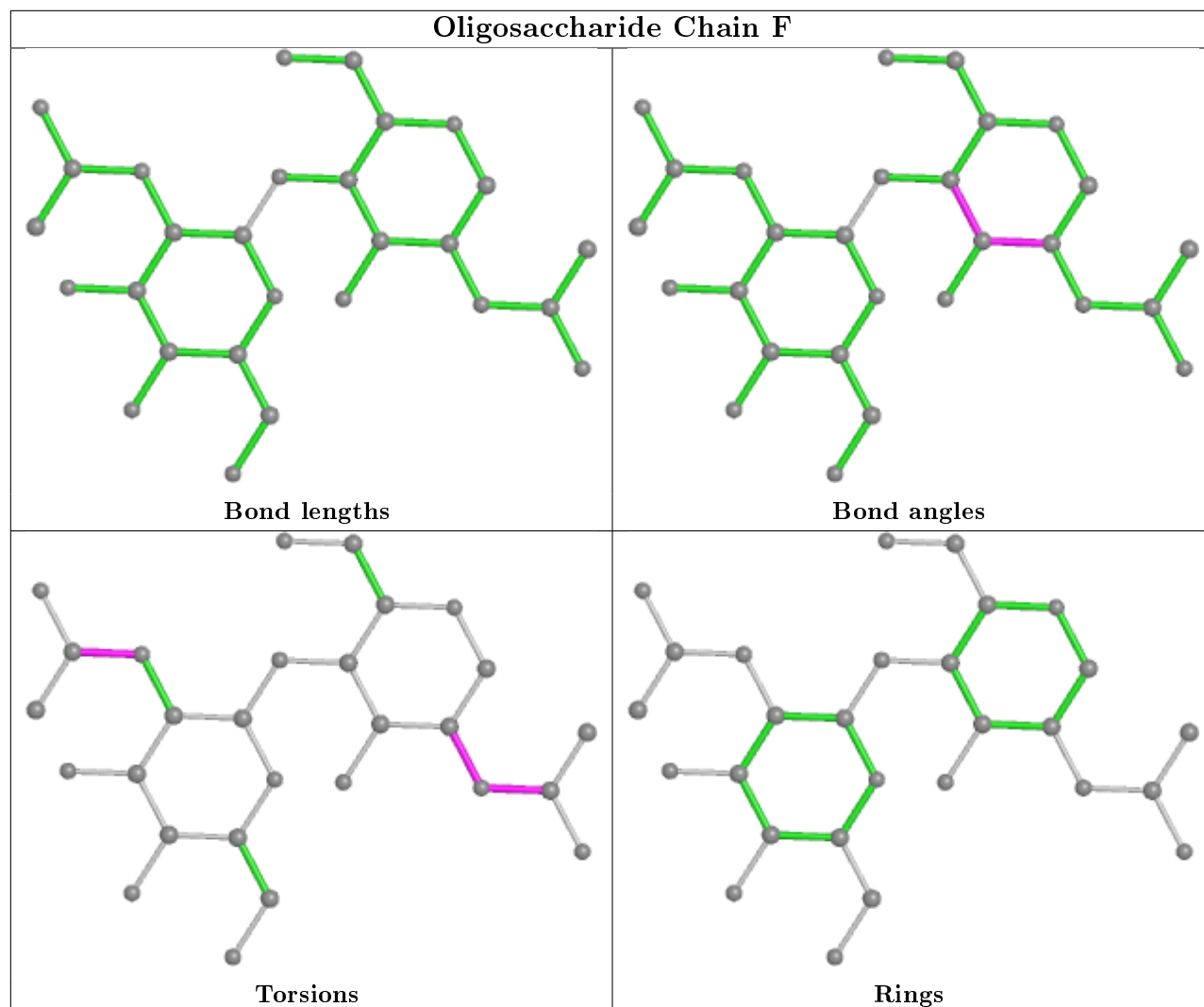
4 monomers are involved in 9 short contacts:

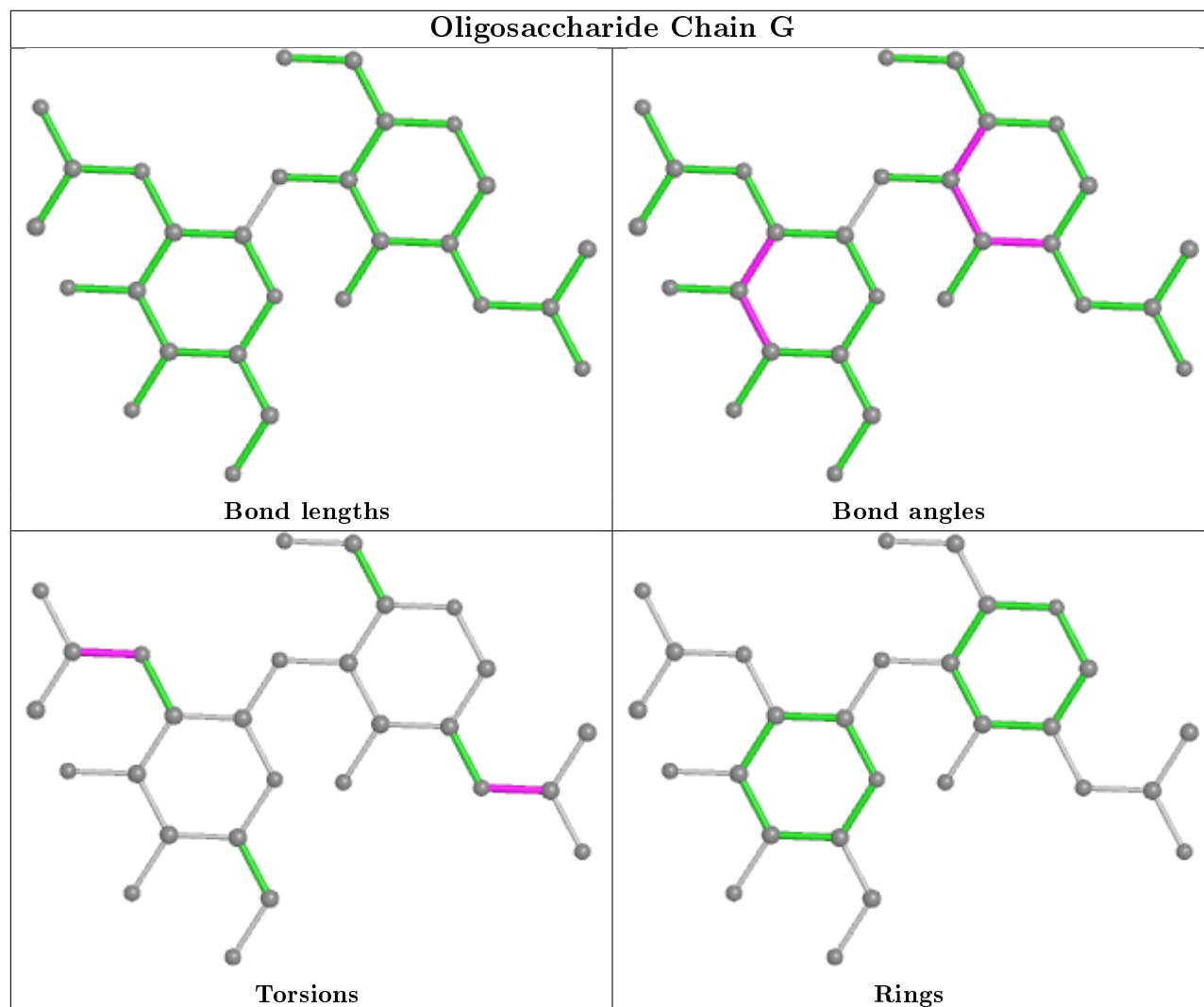
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	NAG	7	0
3	C	4	MAN	2	0
3	C	3	BMA	5	0
4	H	1	NAG	2	0

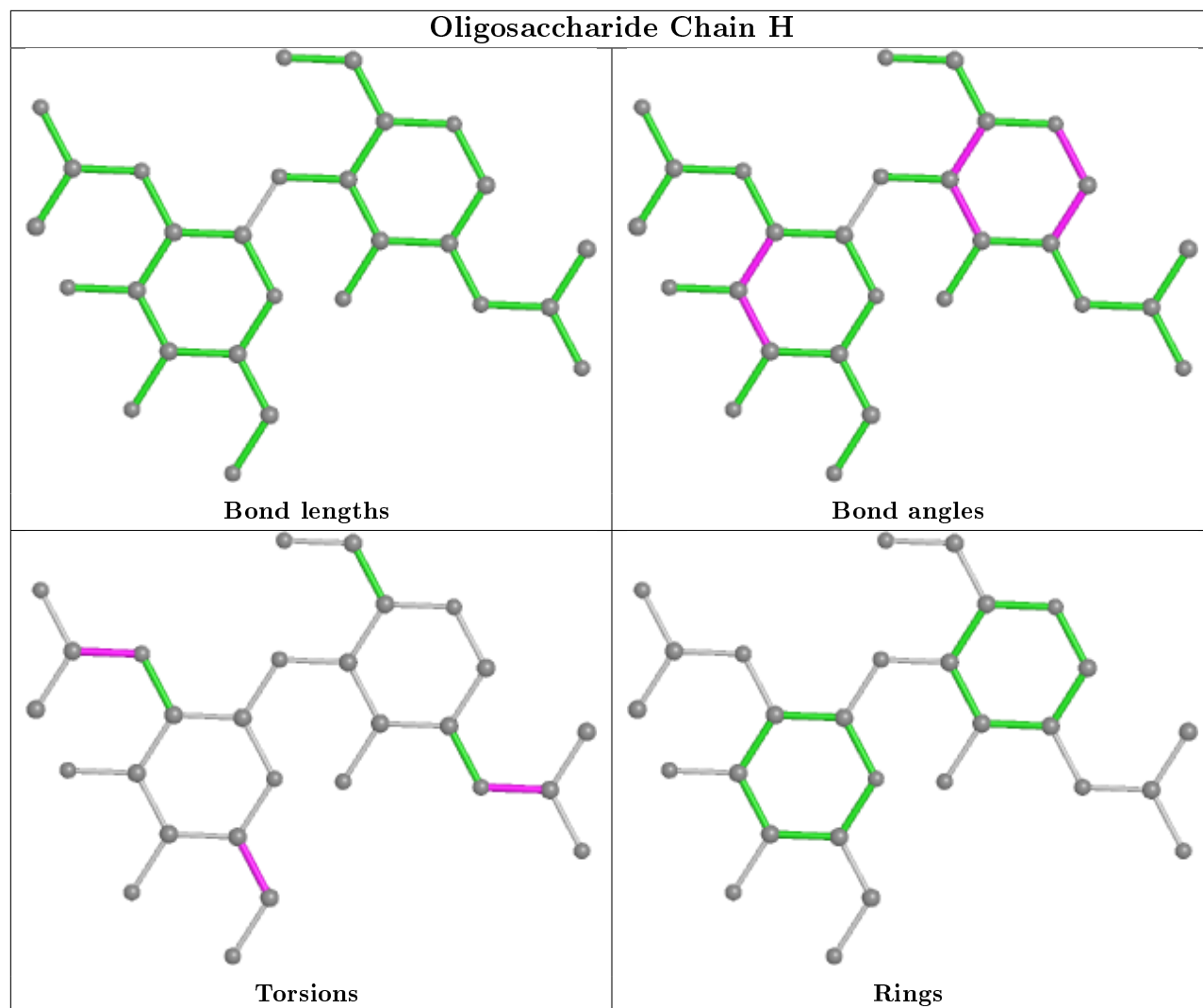
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

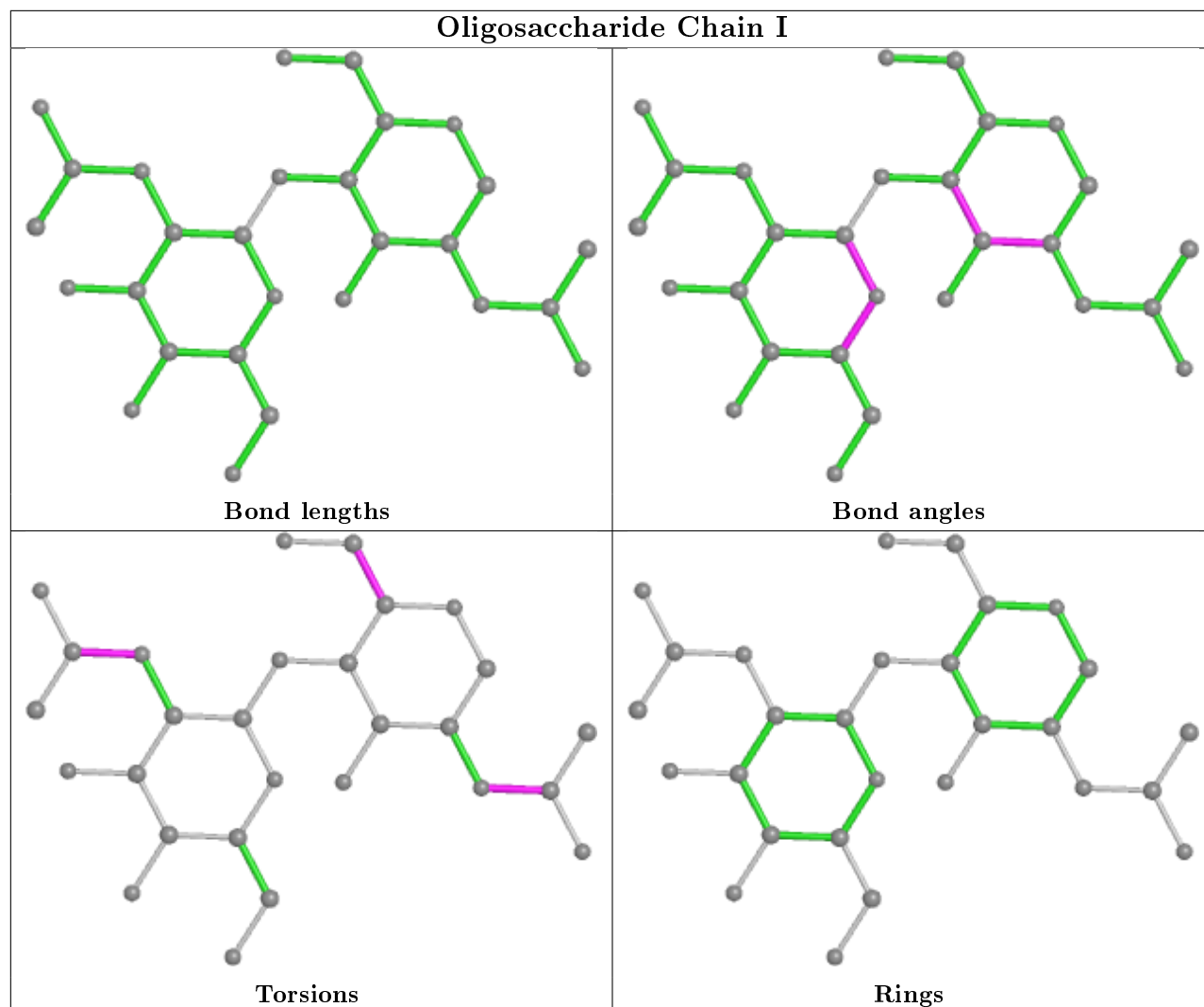


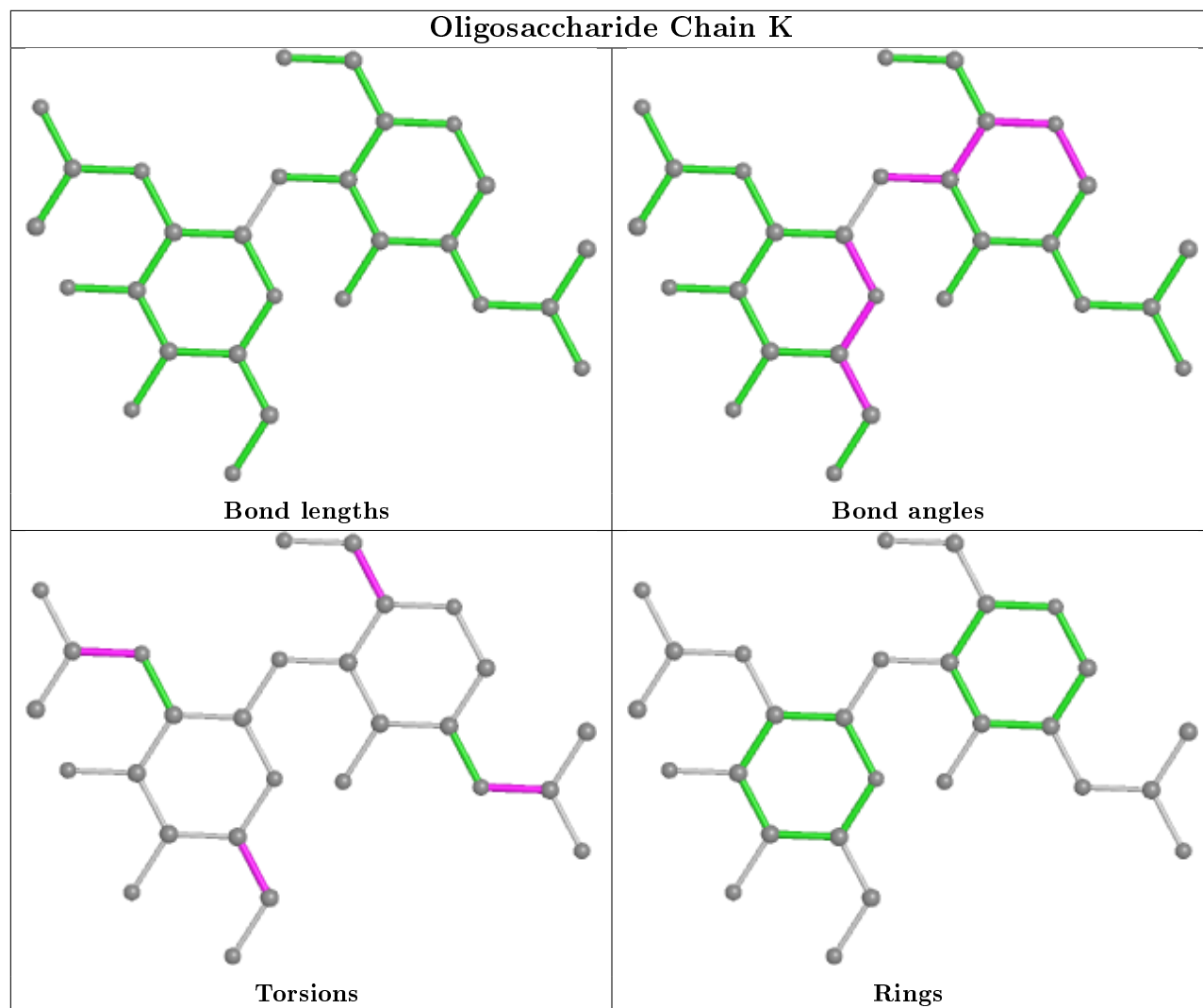


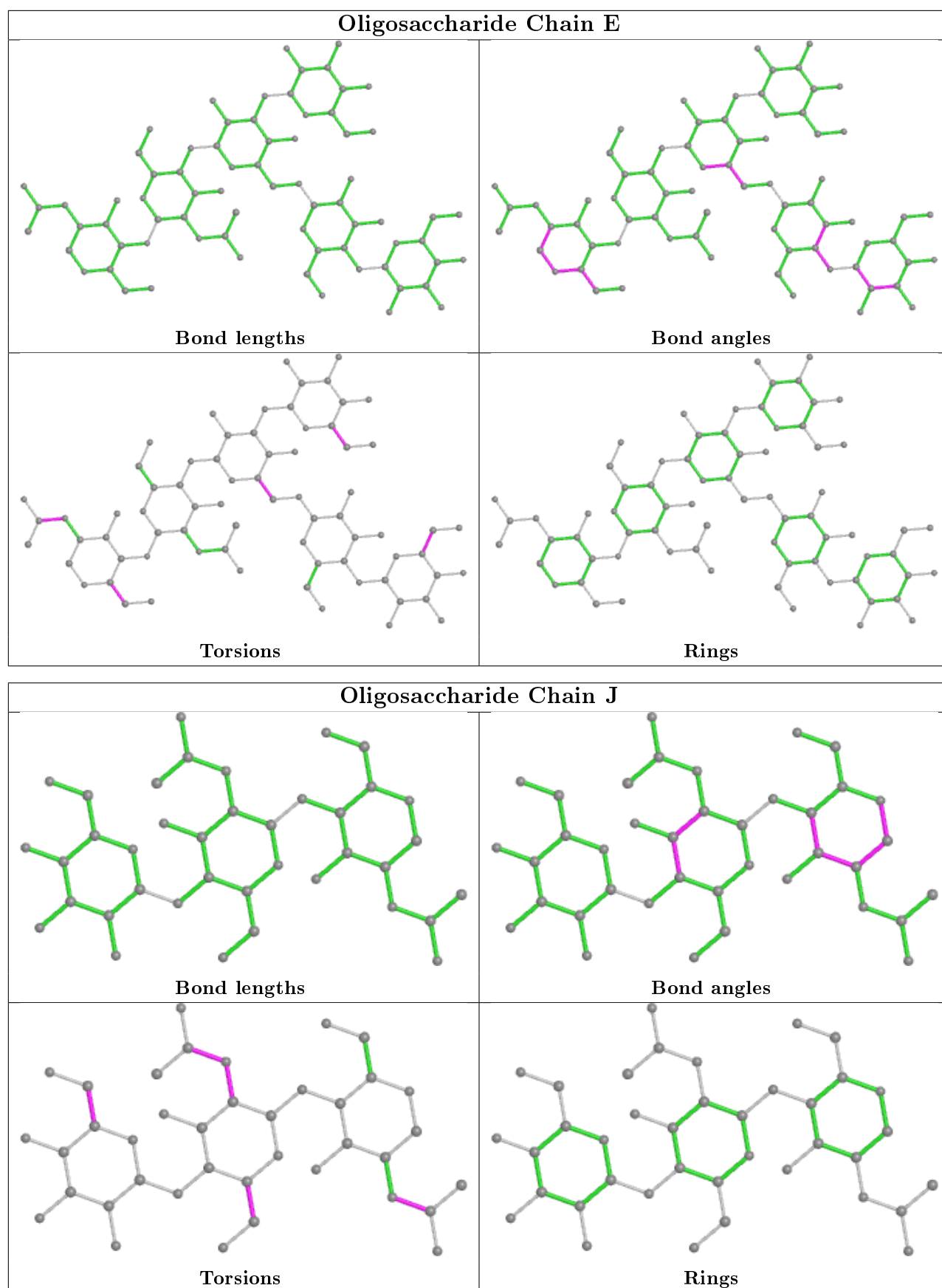


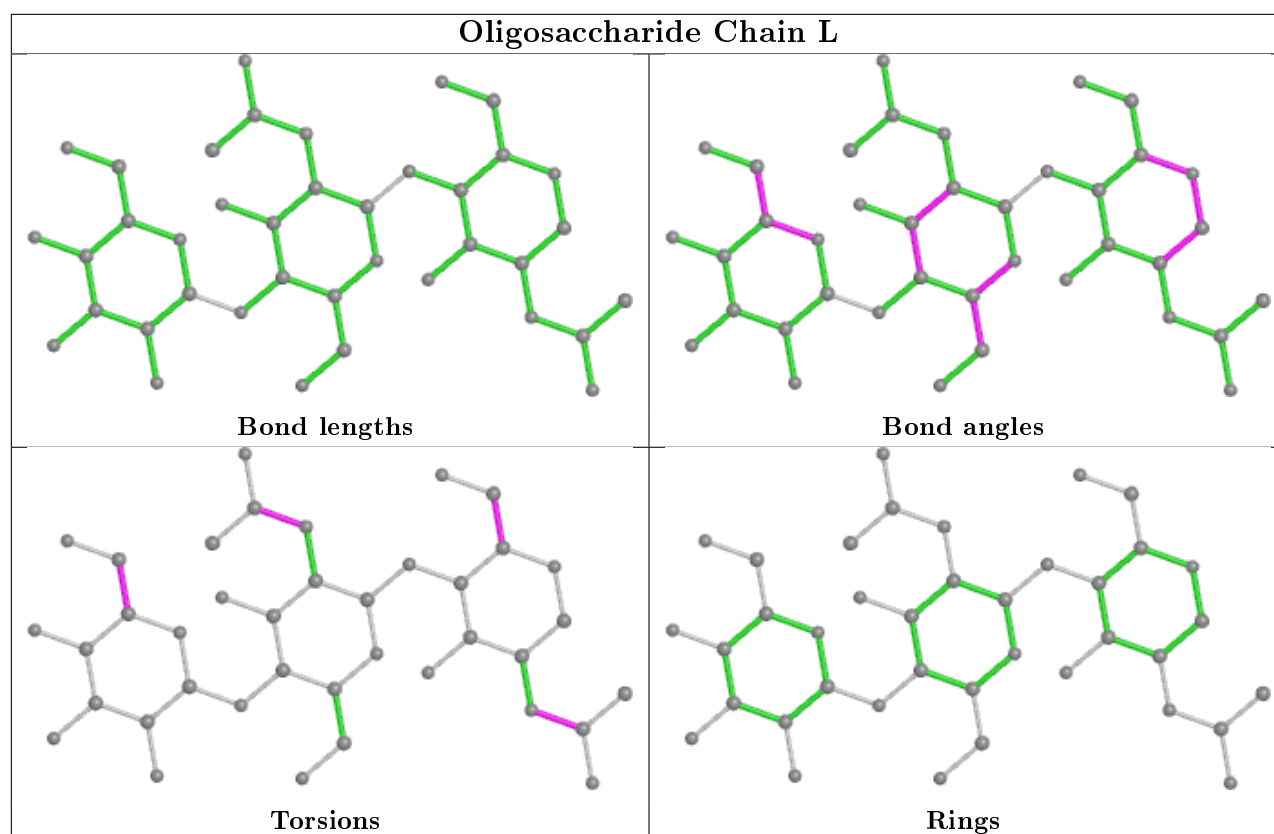












5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 6 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	$\# Z > 2$
7	NAG	A	2805	1	14,14,15	0.57	0	17,19,21	0.94	0
7	NAG	A	2524	1	14,14,15	0.44	0	17,19,21	1.02	2 (11%)
7	NAG	B	3099	2	14,14,15	0.49	0	17,19,21	1.33	2 (11%)
7	NAG	B	3320	2	14,14,15	0.68	0	17,19,21	1.71	4 (23%)
7	NAG	B	3452	2	14,14,15	0.62	0	17,19,21	0.84	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
7	NAG	A	2805	1	-	2/6/23/26	0/1/1/1
7	NAG	A	2524	1	-	3/6/23/26	0/1/1/1
7	NAG	B	3099	2	-	4/6/23/26	0/1/1/1
7	NAG	B	3320	2	-	4/6/23/26	0/1/1/1
7	NAG	B	3452	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	3320	NAG	C4-C3-C2	4.26	117.25	111.02
7	B	3320	NAG	O5-C5-C6	3.77	113.11	107.20
7	B	3099	NAG	C1-O5-C5	3.74	117.26	112.19
7	A	2524	NAG	C1-O5-C5	2.74	115.91	112.19
7	B	3452	NAG	C1-O5-C5	2.54	115.64	112.19
7	B	3099	NAG	O5-C5-C6	2.50	111.13	107.20
7	B	3320	NAG	C3-C4-C5	2.40	114.52	110.24
7	B	3320	NAG	C1-O5-C5	2.34	115.36	112.19
7	A	2524	NAG	C3-C4-C5	2.04	113.88	110.24

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	3099	NAG	C8-C7-N2-C2
7	B	3099	NAG	O7-C7-N2-C2
7	B	3452	NAG	C8-C7-N2-C2
7	B	3452	NAG	O7-C7-N2-C2
7	A	2524	NAG	C8-C7-N2-C2
7	A	2524	NAG	O7-C7-N2-C2
7	B	3320	NAG	C8-C7-N2-C2
7	B	3320	NAG	O7-C7-N2-C2
7	B	3452	NAG	O5-C5-C6-O6
7	A	2805	NAG	C8-C7-N2-C2
7	B	3099	NAG	O5-C5-C6-O6
7	B	3452	NAG	C4-C5-C6-O6
7	A	2805	NAG	O7-C7-N2-C2
7	B	3099	NAG	C4-C5-C6-O6
7	B	3320	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	A	2524	NAG	C4-C5-C6-O6
7	B	3320	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	3099	NAG	1	0
7	B	3320	NAG	3	0
7	B	3452	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	938/967 (97%)	0.60	62 (6%) 18 14	42, 51, 60, 123	0
2	B	695/695 (100%)	0.66	63 (9%) 9 6	44, 51, 61, 94	0
All	All	1633/1662 (98%)	0.62	125 (7%) 13 10	42, 51, 60, 123	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	868	ASP	14.4
1	A	965	TRP	9.1
1	A	967	ILE	7.8
1	A	963	PRO	7.6
2	B	693	ILE	7.6
2	B	509	HIS	7.3
1	A	565	TYR	7.2
2	B	695	VAL	7.1
2	B	694	LEU	6.6
1	A	962	VAL	6.2
1	A	961	PRO	6.2
1	A	960	MET	6.2
1	A	869	ILE	6.0
1	A	964	VAL	6.0
2	B	510	SER	5.9
1	A	966	VAL	5.8
2	B	649	GLY	5.6
2	B	450	ASN	5.4
1	A	957	PRO	4.7
2	B	515	LYS	4.7
2	B	492	GLN	4.7
1	A	838	LEU	4.6
2	B	467	LEU	4.5
2	B	507	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	959	PRO	4.3
2	B	39	ASP	4.2
2	B	691	PRO	4.0
2	B	52	GLU	4.0
2	B	516	ILE	4.0
2	B	479	ARG	3.9
2	B	28	ASP	3.9
2	B	444	ASN	3.8
2	B	648	THR	3.8
2	B	441	ALA	3.7
2	B	472	GLU	3.6
1	A	913	ASN	3.6
2	B	460	CYS	3.5
1	A	837	SER	3.5
1	A	836	SER	3.3
2	B	692	ASP	3.3
2	B	504	GLY	3.3
2	B	653	VAL	3.3
1	A	234	ASP	3.2
1	A	527	ILE	3.2
2	B	652	ALA	3.2
2	B	669	TYR	3.1
1	A	571	THR	3.1
2	B	463	GLY	3.0
2	B	464	PRO	3.0
2	B	1	GLY	3.0
2	B	84	SER	3.0
1	A	567	THR	3.0
1	A	566	ARG	3.0
2	B	556	TYR	3.0
2	B	173	LEU	2.9
2	B	500	GLU	2.9
2	B	461	ARG	2.9
2	B	167	ILE	2.8
2	B	482	GLN	2.8
1	A	617	ILE	2.8
1	A	647	ILE	2.8
1	A	713	PHE	2.8
1	A	955	ILE	2.8
2	B	33	LEU	2.8
2	B	116	TYR	2.7
1	A	509	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	54	ILE	2.7
1	A	542	LEU	2.7
1	A	470	VAL	2.6
1	A	649	LEU	2.6
1	A	481	ALA	2.6
1	A	493	PHE	2.6
2	B	519	LYS	2.6
1	A	663	LEU	2.5
1	A	933	TYR	2.5
2	B	498	ARG	2.5
1	A	569	ALA	2.5
1	A	956	GLN	2.5
2	B	473	CYS	2.4
2	B	651	ASP	2.4
2	B	168	SER	2.4
2	B	341	LEU	2.4
2	B	476	GLU	2.3
2	B	443	PRO	2.3
1	A	704	GLN	2.3
1	A	711	VAL	2.3
1	A	734	VAL	2.3
1	A	715	LEU	2.3
2	B	439	ALA	2.3
1	A	618	TYR	2.3
2	B	497	GLN	2.2
2	B	524	ASP	2.2
2	B	2	PRO	2.2
2	B	491	GLY	2.2
2	B	180	MET	2.2
1	A	670	PHE	2.2
2	B	590	GLN	2.2
2	B	455	PHE	2.2
1	A	490	LYS	2.2
1	A	629	VAL	2.2
1	A	677	ARG	2.2
1	A	701	VAL	2.2
1	A	659	ASN	2.1
2	B	454	THR	2.1
1	A	130	LEU	2.1
1	A	578	LEU	2.1
1	A	532	LEU	2.1
1	A	491	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	831	LEU	2.1
1	A	735	ASP	2.1
2	B	32	PRO	2.1
1	A	808	LEU	2.1
2	B	412	LYS	2.1
1	A	145	GLN	2.1
2	B	442	GLU	2.1
1	A	908	PHE	2.1
1	A	613	ASP	2.0
1	A	665	ARG	2.0
1	A	563	LEU	2.0
1	A	911	LYS	2.0
1	A	693	LEU	2.0
2	B	181	LYS	2.0
1	A	914	GLN	2.0
2	B	36	PRO	2.0
2	B	131	ILE	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	NAG	H	2	14/15	0.63	0.34	110,111,111,111	0
3	MAN	C	4	11/12	0.74	0.30	104,105,105,105	0
6	BMA	J	3	11/12	0.76	0.40	105,106,106,107	0
4	NAG	G	2	14/15	0.79	0.35	91,93,93,94	0
4	NAG	I	2	14/15	0.80	0.35	92,93,94,94	0
4	NAG	K	1	14/15	0.80	0.20	71,76,78,80	0
4	NAG	K	2	14/15	0.80	0.19	83,85,86,86	0
5	MAN	E	5	11/12	0.80	0.28	97,98,98,98	0
6	NAG	J	2	14/15	0.81	0.36	98,101,102,104	0
3	BMA	C	3	11/12	0.81	0.25	97,100,102,103	0
4	NAG	D	2	14/15	0.81	0.28	85,87,88,88	0

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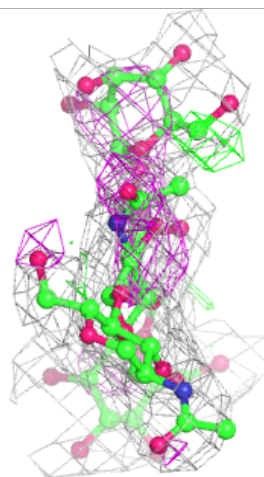
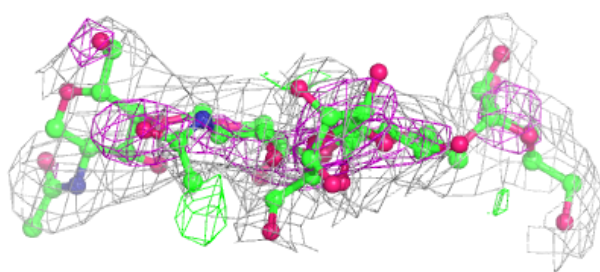
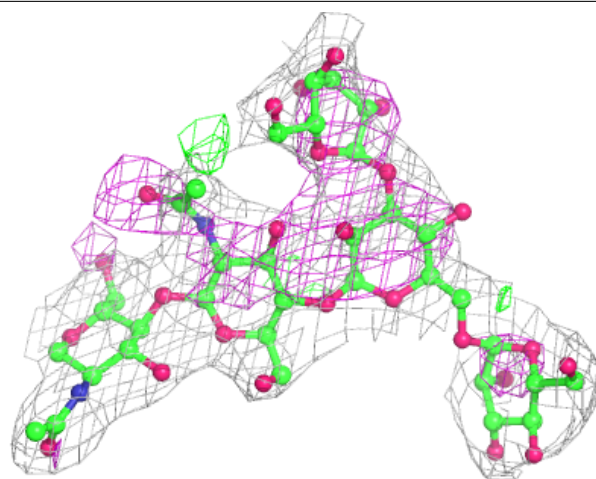
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	H	1	14/15	0.81	0.20	106,107,108,110	0
4	NAG	F	1	14/15	0.82	0.23	72,77,79,81	0
3	MAN	C	5	11/12	0.82	0.20	104,104,104,104	0
5	MAN	E	6	11/12	0.82	0.26	91,92,93,93	0
4	NAG	I	1	14/15	0.83	0.19	80,83,86,89	0
3	NAG	C	2	14/15	0.84	0.24	81,85,88,93	0
5	MAN	E	4	11/12	0.85	0.15	93,95,95,97	0
4	NAG	F	2	14/15	0.86	0.29	84,86,86,86	0
4	NAG	D	1	14/15	0.86	0.17	74,78,80,82	0
6	NAG	L	2	14/15	0.90	0.17	82,84,86,87	0
4	NAG	G	1	14/15	0.90	0.19	79,84,86,89	0
6	BMA	L	3	11/12	0.90	0.10	88,90,90,90	0
6	NAG	J	1	14/15	0.91	0.21	85,89,91,95	0
5	BMA	E	3	11/12	0.93	0.11	83,87,89,91	0
6	NAG	L	1	14/15	0.93	0.15	69,73,75,78	0
5	NAG	E	1	14/15	0.94	0.13	58,59,62,65	0
3	NAG	C	1	14/15	0.95	0.15	61,64,69,75	0
5	NAG	E	2	14/15	0.95	0.13	65,69,74,79	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.

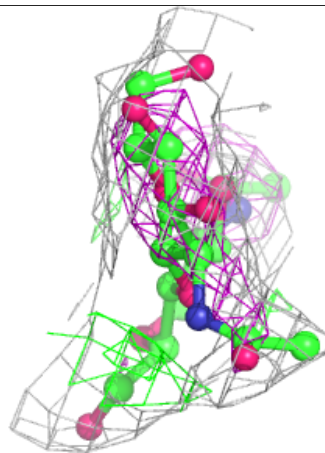
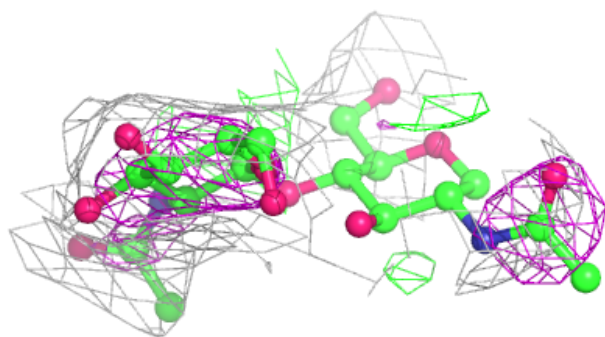
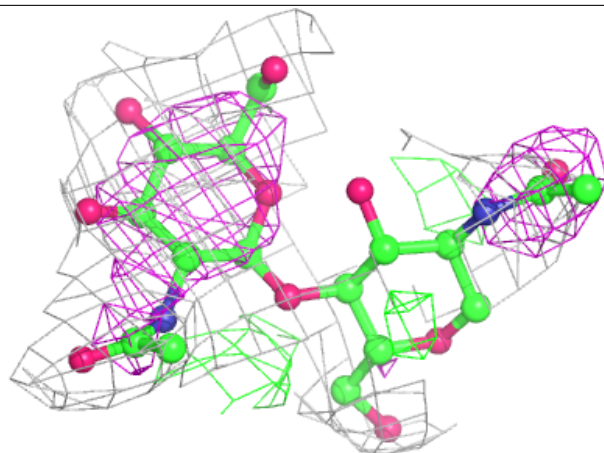
Electron density around Chain C:

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



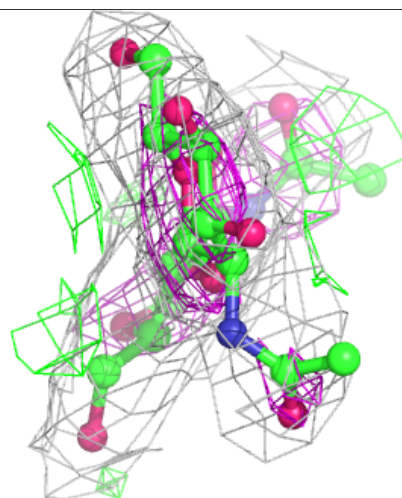
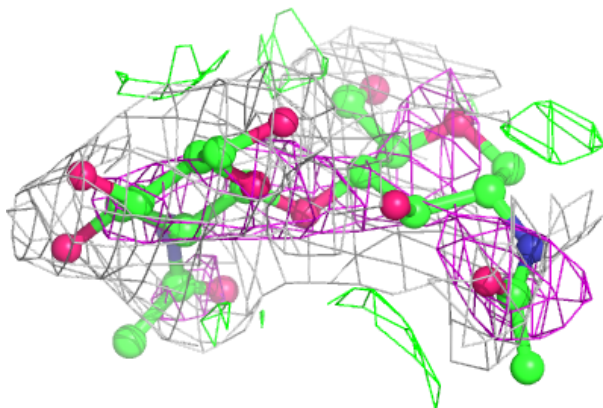
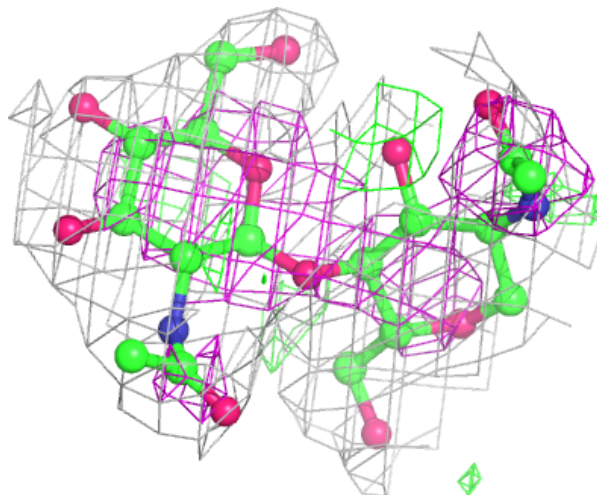
Electron density around Chain D:

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



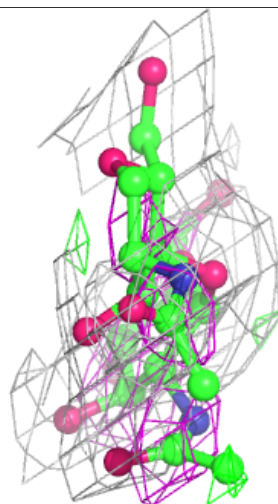
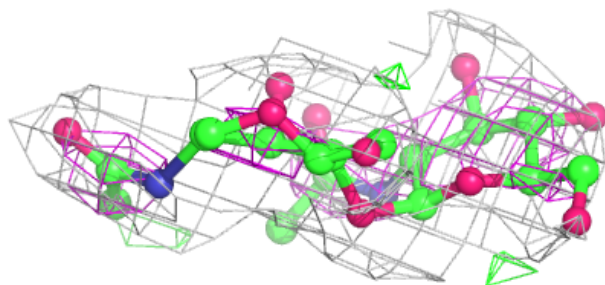
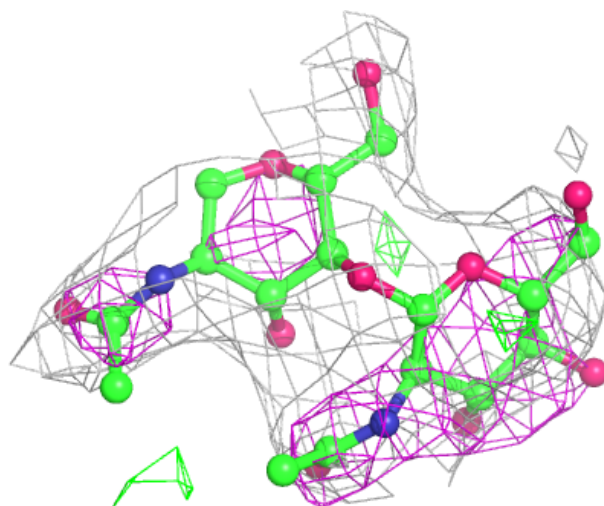
Electron density around Chain F:

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



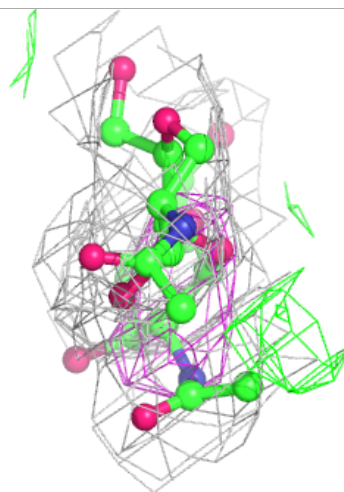
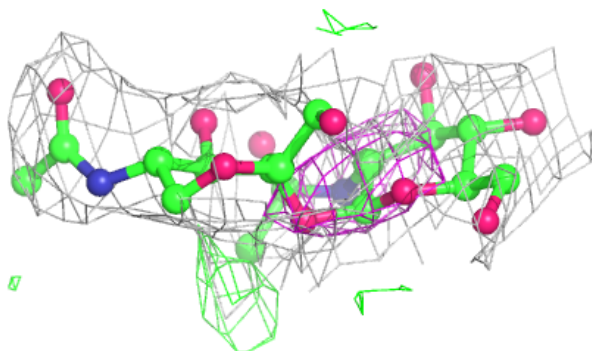
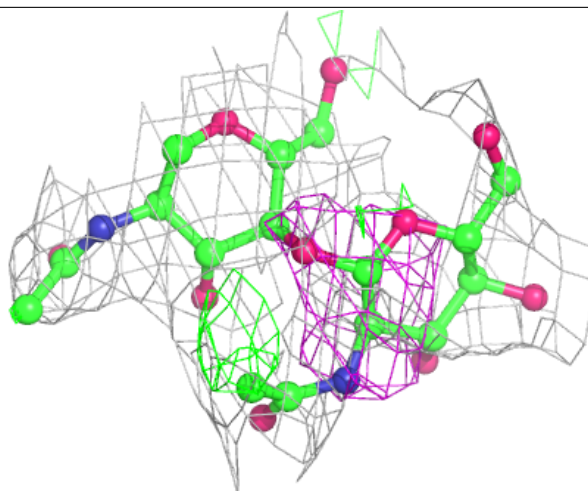
Electron density around Chain G:

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



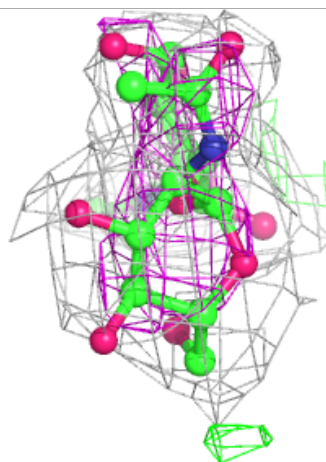
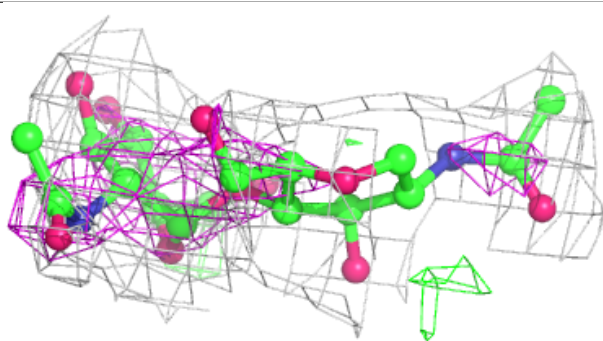
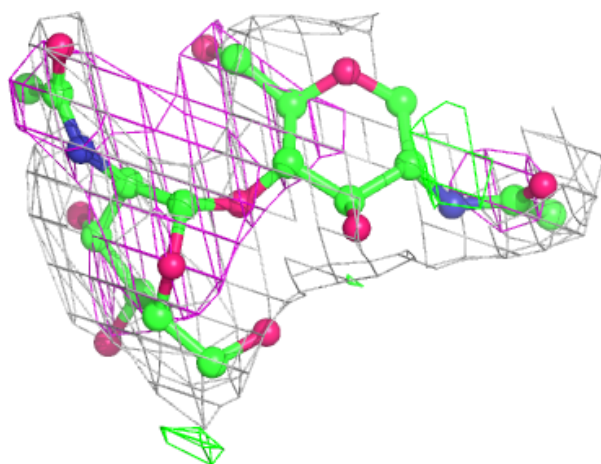
Electron density around Chain H:

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



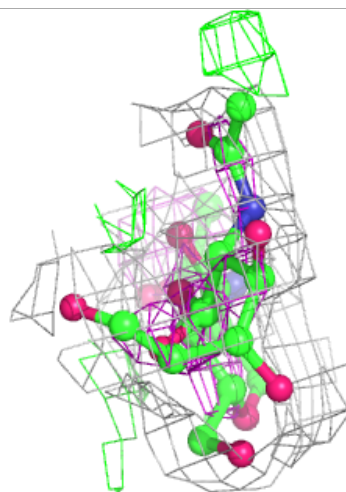
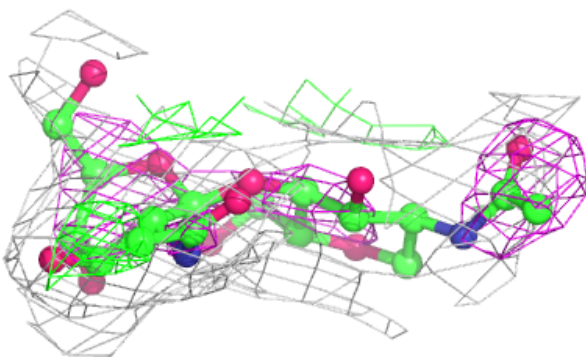
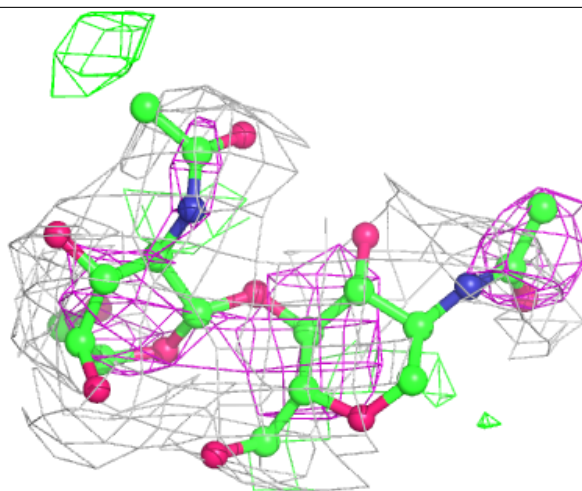
Electron density around Chain I:

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



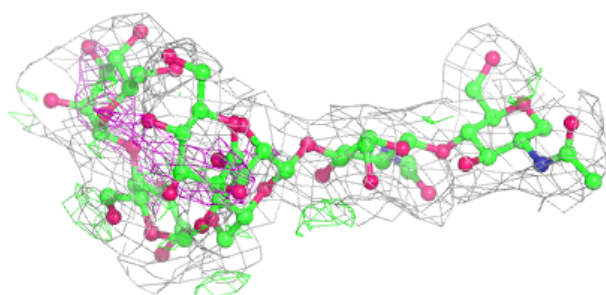
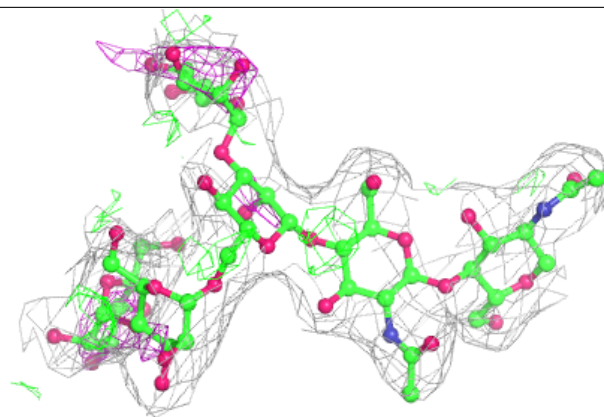
Electron density around Chain K:

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

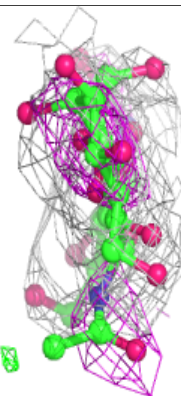
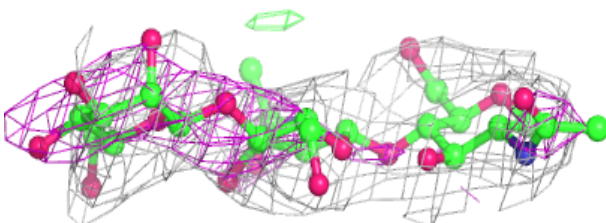
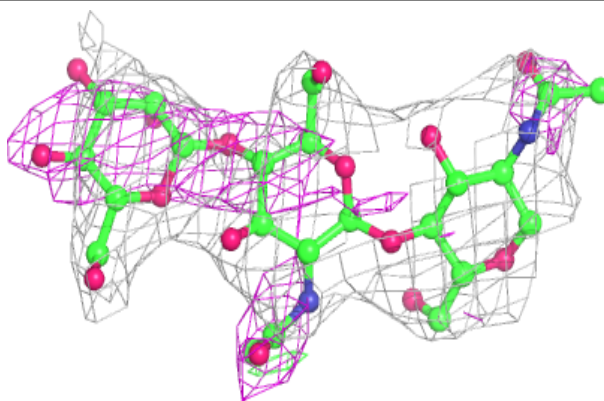


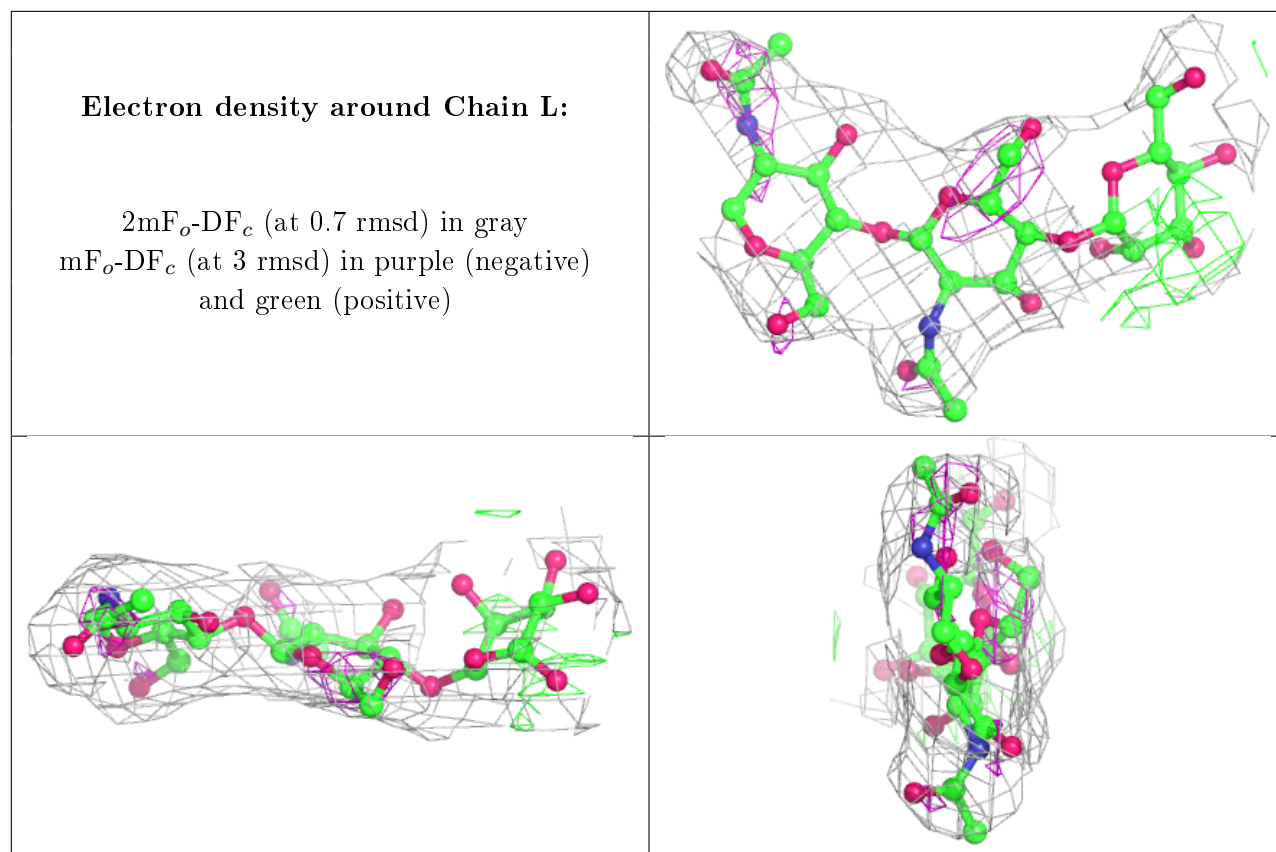
Electron density around Chain E:

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

**Electron density around Chain J:**

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	NAG	B	3452	14/15	0.58	0.35	86,90,91,91	0
7	NAG	A	2524	14/15	0.66	0.30	81,86,87,87	0
7	NAG	A	2805	14/15	0.72	0.34	74,79,79,80	0
7	NAG	B	3320	14/15	0.73	0.22	68,71,72,73	0
7	NAG	B	3099	14/15	0.78	0.37	74,79,80,81	0
8	CA	B	4002	1/1	0.91	0.17	55,55,55,55	0
8	CA	A	4005	1/1	0.92	0.21	46,46,46,46	0
8	CA	A	4004	1/1	0.92	0.16	78,78,78,78	0
8	CA	A	4007	1/1	0.93	0.26	34,34,34,34	0
8	CA	A	4008	1/1	0.94	0.22	32,32,32,32	0
8	CA	A	4006	1/1	0.96	0.28	59,59,59,59	0

6.5 Other polymers

There are no such residues in this entry.