



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 25, 2022 – 01:52 pm BST

PDB ID : 7P8I  
Title : Receptor-binding domain (RBD) of the spike protein of the bat coronavirus RaTG13 virus in complex with the extracellular domain of human angiotensin-converting enzyme 2 (ACE2) - Crystal form 1  
Authors : Scietti, L.; Castelli, M.; Faravelli, S.; Clementi, N.; Mancini, N.; Forneris, F.  
Deposited on : 2021-07-22  
Resolution : 4.50 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

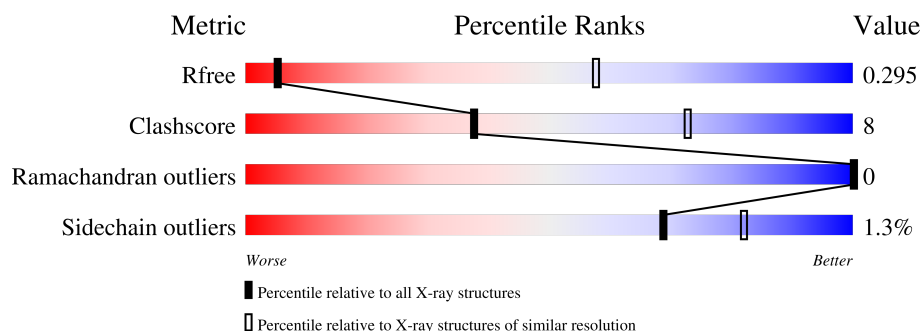
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.50 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.






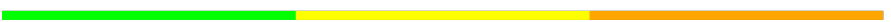

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	602	80% 19% ..
1	C	602	85% 14% .
2	B	233	62% 20% 17%
2	D	233	62% 21% 17%
3	E	2	50% 50%
3	H	2	50% 50%
3	J	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	K	2	 100%
4	F	3	 100%
4	G	3	 100%
4	I	3	 33%33%33%
4	L	3	 100%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13101 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 Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	0	0
			4863	3109	806	919	29			
1	C	596	Total	C	N	O	S	0	0	0
			4864	3112	805	918	29			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLY	-	expression tag	UNP Q9BYF1
A	18	SER	-	expression tag	UNP Q9BYF1
A	616	ALA	-	expression tag	UNP Q9BYF1
A	617	ALA	-	expression tag	UNP Q9BYF1
A	618	ALA	-	expression tag	UNP Q9BYF1
C	17	GLY	-	expression tag	UNP Q9BYF1
C	18	SER	-	expression tag	UNP Q9BYF1
C	616	ALA	-	expression tag	UNP Q9BYF1
C	617	ALA	-	expression tag	UNP Q9BYF1
C	618	ALA	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	193	Total	C	N	O	S	0	0	0
			1532	985	253	286	8			
2	D	193	Total	C	N	O	S	0	0	0
			1532	985	253	286	8			

There are 20 discrepancies between the modelled and reference sequences:

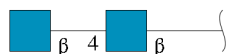
Chain	Residue	Modelled	Actual	Comment	Reference
B	317	GLY	-	expression tag	UNP A0A6B9WHD3
B	318	SER	-	expression tag	UNP A0A6B9WHD3

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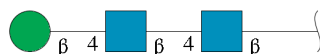
Chain	Residue	Modelled	Actual	Comment	Reference
B	542	ALA	-	expression tag	UNP A0A6B9WHD3
B	543	ALA	-	expression tag	UNP A0A6B9WHD3
B	544	HIS	-	expression tag	UNP A0A6B9WHD3
B	545	HIS	-	expression tag	UNP A0A6B9WHD3
B	546	HIS	-	expression tag	UNP A0A6B9WHD3
B	547	HIS	-	expression tag	UNP A0A6B9WHD3
B	548	HIS	-	expression tag	UNP A0A6B9WHD3
B	549	HIS	-	expression tag	UNP A0A6B9WHD3
D	317	GLY	-	expression tag	UNP A0A6B9WHD3
D	318	SER	-	expression tag	UNP A0A6B9WHD3
D	542	ALA	-	expression tag	UNP A0A6B9WHD3
D	543	ALA	-	expression tag	UNP A0A6B9WHD3
D	544	HIS	-	expression tag	UNP A0A6B9WHD3
D	545	HIS	-	expression tag	UNP A0A6B9WHD3
D	546	HIS	-	expression tag	UNP A0A6B9WHD3
D	547	HIS	-	expression tag	UNP A0A6B9WHD3
D	548	HIS	-	expression tag	UNP A0A6B9WHD3
D	549	HIS	-	expression tag	UNP A0A6B9WHD3

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



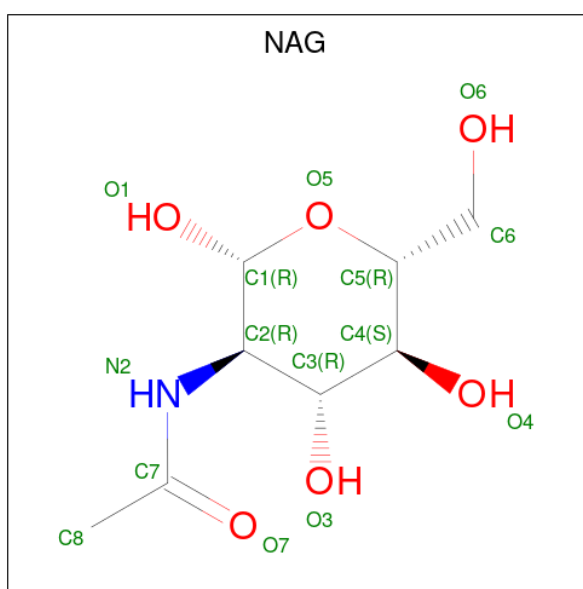
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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
4	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

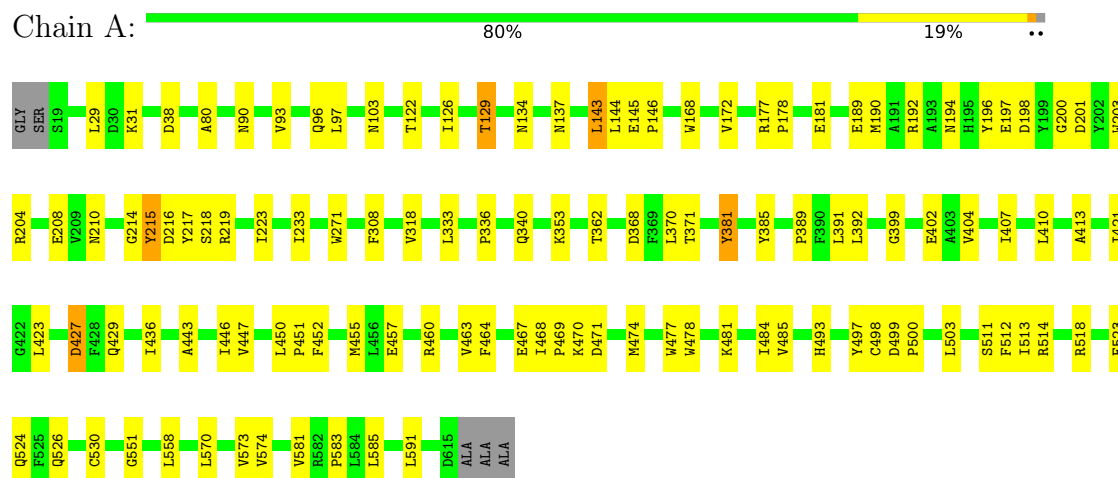


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

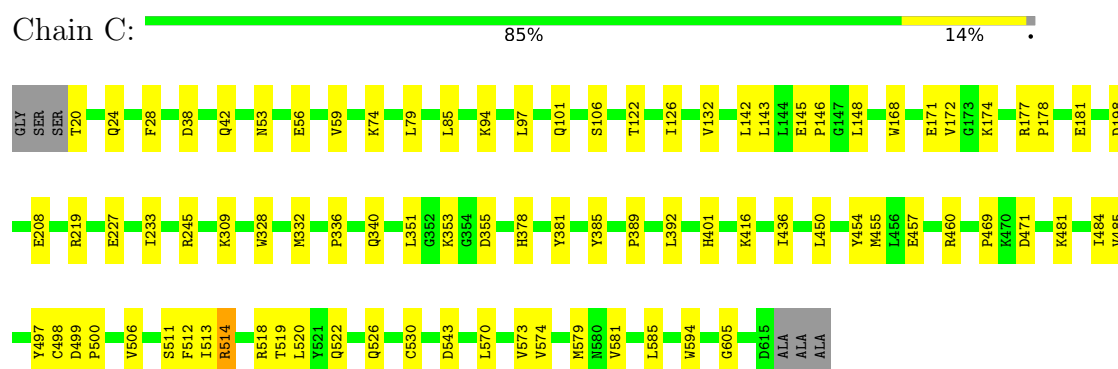
### 3 Residue-property plots

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. 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. 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: Processed angiotensin-converting enzyme 2



#### • Molecule 1: Processed angiotensin-converting enzyme 2



#### • Molecule 2: Spike glycoprotein



HIS  
HIS  
HIS  
HIS  
HIS

• Molecule 2: Spike glycoprotein

Chain D:  62% 21% 17%

GLY SER ARG VAL GLN PRO THR ASP SER ILE VAL ARG PHE PRO ASN ILE THR N334 F338 F342 N343 V353 N354 R355 F377 G381 T393 N394 D398 I402 T403 E406 V407 R408 Q409 I410 Q414 T415 I418 A419 M422 Y423 T430 G431 I434 A435

V436 N437 S438 I441 N448 R457 K458 A459 Q474 A475 G476 S477 K478 P479 C480 G485 L486 N487 C488 F497 G502 H505 Q506 P507 Y508 R509 F515 E516 L517 L518 A522 G526 PRO LYS SER THR ASN LEU VAL LYS ASN LYS CYS VAL ASN PHE ALA

HIS  
HIS  
HIS  
HIS  
HIS

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 50%

NAG1  
NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50% 50%

NAG1  
NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%

NAG1  
NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

NAG1  
NAG2

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

Chain F:  100%



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

Chain G:  100%



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

Chain I:  33% 33% 33%



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

Chain L:  100%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.56Å 131.21Å 115.72Å 90.00° 99.77° 90.00°	Depositor
Resolution (Å)	61.96 – 4.50 61.96 – 4.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (61.96-4.50) 99.1 (61.96-4.50)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 4.46Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.278 , 0.294 0.278 , 0.295	Depositor DCC
$R_{free}$ test set	706 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	164.7	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.77	EDS
Total number of atoms	13101	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	191.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.33	0/4999	0.55	0/6792
1	C	0.27	0/5001	0.44	0/6795
2	B	0.31	0/1576	0.53	0/2145
2	D	0.29	0/1576	0.49	0/2145
All	All	0.30	0/13152	0.50	0/17877

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	4863	0	4632	83	1
1	C	4864	0	4634	52	0
2	B	1532	0	1452	31	0
2	D	1532	0	1451	34	0
3	E	28	0	25	0	0
3	H	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
4	F	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	39	0	34	0	0
4	I	39	0	34	3	0
4	L	39	0	34	0	0
5	C	14	0	13	0	0
5	D	28	0	26	2	1
All	All	13101	0	12444	197	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (197) 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:402:GLU:HB2	1:A:518:ARG:HD2	1.31	1.06
2:B:339:GLY:HA3	4:I:1:NAG:H81	1.59	0.82
1:A:190:MET:SD	1:A:194:ASN:ND2	2.54	0.81
2:D:406:GLU:HB3	2:D:418:ILE:HG13	1.62	0.79
1:A:514:ARG:O	1:A:518:ARG:HG3	1.85	0.77
1:A:455:MET:HE3	1:A:485:VAL:HG23	1.70	0.73
1:A:192:ARG:HA	1:A:196:TYR:O	1.90	0.72
2:D:418:ILE:HD13	2:D:422:ASN:HD22	1.53	0.71
1:C:520:LEU:HD22	1:C:579:MET:HE2	1.76	0.68
1:C:142:LEU:HD22	1:C:146:PRO:HB2	1.76	0.67
2:B:339:GLY:CA	4:I:1:NAG:H81	2.25	0.67
2:B:358:ILE:HB	2:B:395:VAL:HG13	1.76	0.67
2:B:416:GLY:H	2:B:419:ALA:HB3	1.62	0.65
1:A:208:GLU:OE2	1:A:210:ASN:HB2	1.98	0.63
1:A:402:GLU:HB2	1:A:518:ARG:CD	2.19	0.61
1:A:216:ASP:O	1:A:217:TYR:HD1	1.83	0.61
1:A:455:MET:CE	1:A:485:VAL:HG23	2.30	0.61
1:C:177:ARG:HD3	1:C:498:CYS:HB2	1.83	0.61
1:A:198:ASP:HB2	1:A:464:PHE:HB3	1.83	0.61
1:C:208:GLU:OE1	1:C:219:ARG:NH1	2.33	0.61
2:B:403:THR:HG23	2:B:495:TYR:CZ	2.37	0.60
1:C:455:MET:HE1	1:C:481:LYS:HA	1.84	0.60
2:B:418:ILE:HD13	2:B:422:ASN:HD22	1.66	0.59
1:A:90:ASN:HB3	1:A:93:VAL:HG22	1.85	0.59
1:A:446:ILE:HD13	1:A:523:PHE:HZ	1.68	0.59
2:B:480:CYS:SG	2:B:481:ASN:N	2.75	0.59
2:B:365:TYR:CE1	2:B:368:LEU:HD22	2.37	0.59
1:A:216:ASP:O	1:A:217:TYR:CD1	2.55	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:MET:CE	1:C:485:VAL:HG23	2.34	0.58
1:A:399:GLY:CA	1:A:518:ARG:HG2	2.34	0.57
1:A:573:VAL:HG13	1:A:574:VAL:HG13	1.86	0.57
2:B:405:ASP:N	2:B:504:GLY:O	2.37	0.57
2:D:393:THR:HA	2:D:522:ALA:HA	1.85	0.57
1:C:511:SER:O	1:C:514:ARG:HD3	2.04	0.57
1:A:203:TRP:HH2	1:A:460:ARG:NH2	2.02	0.57
1:C:573:VAL:HG13	1:C:574:VAL:HG13	1.85	0.57
2:D:403:THR:HB	2:D:505:HIS:HA	1.87	0.57
2:D:415:THR:HA	2:D:419:ALA:HB3	1.87	0.56
2:B:339:GLY:C	2:B:341:VAL:N	2.54	0.56
1:C:520:LEU:HD21	1:C:581:VAL:HG22	1.87	0.56
1:A:511:SER:OG	1:A:514:ARG:NH2	2.29	0.55
1:A:389:PRO:HG2	1:A:392:LEU:HD22	1.86	0.55
2:D:381:GLY:HA3	2:D:430:THR:HG23	1.90	0.54
2:B:395:VAL:HG12	2:B:524:VAL:HG21	1.90	0.54
1:C:455:MET:HE3	1:C:485:VAL:HG23	1.90	0.54
1:C:519:THR:O	1:C:522:GLN:HG2	2.07	0.54
1:C:460:ARG:NH2	1:C:506:VAL:HA	2.23	0.54
2:D:448:ASN:HB3	2:D:497:PHE:HB2	1.90	0.54
2:B:404:GLY:O	2:B:407:VAL:HG12	2.08	0.54
1:C:132:VAL:HG12	1:C:171:GLU:HG3	1.89	0.54
1:A:402:GLU:CB	1:A:518:ARG:HD2	2.22	0.53
2:D:474:GLN:HG2	2:D:480:CYS:SG	2.48	0.53
1:A:524:GLN:HG3	1:A:583:PRO:HG2	1.89	0.53
1:C:168:TRP:O	1:C:172:VAL:HG22	2.08	0.53
2:D:409:GLN:OE1	2:D:418:ILE:N	2.40	0.53
1:C:38:ASP:HA	1:C:353:LYS:HE3	1.90	0.53
1:C:85:LEU:HD11	1:C:94:LYS:HG3	1.91	0.53
1:A:336:PRO:HB2	1:A:340:GLN:HB3	1.91	0.52
2:B:393:THR:HB	2:B:522:ALA:H	1.73	0.52
1:A:201:ASP:HB3	1:A:219:ARG:HH21	1.74	0.52
2:B:384:PRO:HA	2:B:387:LEU:HG	1.91	0.52
1:A:399:GLY:HA2	1:A:518:ARG:HG2	1.92	0.52
1:C:389:PRO:HG2	1:C:392:LEU:HD22	1.92	0.52
1:A:399:GLY:O	1:A:518:ARG:HG2	2.10	0.51
1:A:526:GLN:NE2	1:A:530:CYS:SG	2.83	0.51
2:D:476:GLY:H	2:D:487:ASN:HB3	1.74	0.51
2:D:394:ASN:HB3	2:D:516:GLU:HB3	1.92	0.51
1:C:581:VAL:HG12	1:C:585:LEU:HG	1.93	0.51
1:C:460:ARG:HH21	1:C:506:VAL:HA	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ILE:HA	1:A:129:THR:HG22	1.92	0.50
1:A:177:ARG:HB3	1:A:178:PRO:HD3	1.92	0.50
2:D:343:ASN:HB2	5:D:601:NAG:N2	2.26	0.50
2:D:402:ILE:HB	2:D:406:GLU:HB2	1.94	0.50
1:A:381:TYR:CD1	1:A:558:LEU:HD22	2.46	0.50
1:C:177:ARG:HB3	1:C:178:PRO:HD3	1.93	0.50
1:A:455:MET:SD	1:A:481:LYS:HA	2.52	0.50
1:A:404:VAL:O	1:A:407:ILE:HG12	2.12	0.50
1:C:245:ARG:NH1	1:C:605:GLY:O	2.31	0.49
2:D:353:TRP:HZ3	2:D:355:ARG:HH11	1.59	0.49
2:D:486:LEU:HD12	2:D:487:ASN:N	2.27	0.49
1:A:443:ALA:O	1:A:447:VAL:HG12	2.12	0.49
2:B:497:PHE:CD2	2:B:507:PRO:HG3	2.47	0.49
1:A:436:ILE:HD11	1:A:591:LEU:HA	1.93	0.49
1:C:353:LYS:HB3	2:D:505:HIS:HE2	1.77	0.49
1:A:134:ASN:ND2	1:A:137:ASN:OD1	2.46	0.49
2:B:377:PHE:HD1	2:B:434:ILE:HG12	1.78	0.49
1:C:526:GLN:NE2	1:C:530:CYS:SG	2.84	0.49
1:A:144:LEU:HD21	1:A:271:TRP:HH2	1.77	0.49
1:A:455:MET:HE1	1:A:481:LYS:HA	1.94	0.49
1:A:38:ASP:HA	1:A:353:LYS:HE2	1.95	0.49
1:A:455:MET:CE	1:A:484:ILE:HB	2.42	0.49
2:B:473:TYR:HE2	2:B:475:ALA:HB2	1.78	0.48
1:C:74:LYS:HE3	1:C:106:SER:HB3	1.94	0.48
1:C:455:MET:HE2	1:C:484:ILE:HB	1.96	0.48
1:A:168:TRP:O	1:A:172:VAL:HG22	2.13	0.48
2:B:350:VAL:HG22	2:B:422:ASN:HB3	1.95	0.48
1:A:421:ILE:HD12	1:A:423:LEU:H	1.78	0.48
1:A:455:MET:HE2	1:A:484:ILE:HB	1.95	0.48
2:B:393:THR:O	2:B:522:ALA:HB3	2.14	0.48
1:A:204:ARG:HH12	1:A:223:ILE:HD11	1.78	0.48
1:C:436:ILE:HD13	1:C:594:TRP:CD1	2.49	0.47
1:C:457:GLU:HG2	1:C:512:PHE:HB3	1.94	0.47
2:D:342:PHE:HB2	5:D:601:NAG:C8	2.44	0.47
2:D:438:SER:HB2	2:D:441:ILE:HB	1.96	0.47
1:A:233:ILE:HD13	1:A:450:LEU:HD13	1.96	0.47
1:A:308:PHE:HE2	1:A:362:THR:HG21	1.80	0.47
2:D:409:GLN:HB3	2:D:419:ALA:HB2	1.97	0.47
1:A:177:ARG:HD3	1:A:498:CYS:SG	2.55	0.47
1:A:333:LEU:O	1:A:362:THR:HG22	2.14	0.47
1:C:336:PRO:HG2	1:C:340:GLN:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ASP:HB2	1:A:429:GLN:HG2	1.97	0.47
1:C:450:LEU:HD21	1:C:519:THR:HG21	1.97	0.47
2:D:457:ARG:NH1	2:D:459:ALA:O	2.48	0.47
1:A:470:LYS:HG3	1:A:471:ASP:N	2.30	0.46
1:A:493:HIS:CD2	1:A:497:TYR:CD2	3.03	0.46
2:D:393:THR:HG21	2:D:518:LEU:HB2	1.96	0.46
1:C:332:MET:HE3	1:C:336:PRO:HD3	1.96	0.46
1:C:378:HIS:CE1	1:C:401:HIS:HB3	2.51	0.46
2:B:395:VAL:HB	2:B:515:PHE:CE1	2.50	0.46
1:C:145:GLU:HB2	1:C:146:PRO:HD3	1.98	0.46
1:A:581:VAL:HG12	1:A:585:LEU:HG	1.97	0.45
1:C:351:LEU:HB2	1:C:355:ASP:HB3	1.97	0.45
1:A:97:LEU:HA	1:A:97:LEU:HD23	1.66	0.45
2:B:502:GLY:O	2:B:506:GLN:HG3	2.16	0.45
1:C:174:LYS:HE2	1:C:497:TYR:HE1	1.80	0.45
2:B:368:LEU:HA	2:B:371:SER:HB2	1.99	0.45
2:D:355:ARG:HG2	2:D:398:ASP:OD1	2.15	0.45
1:A:197:GLU:HB2	1:A:201:ASP:OD2	2.16	0.45
1:A:200:GLY:O	1:A:204:ARG:HG2	2.16	0.45
1:C:457:GLU:HG3	1:C:513:ILE:HB	1.98	0.45
1:A:103:ASN:HB2	1:A:194:ASN:OD1	2.17	0.45
1:A:477:TRP:CD2	1:A:500:PRO:HG3	2.52	0.45
1:A:469:PRO:HB2	1:A:471:ASP:OD1	2.16	0.45
1:C:177:ARG:O	1:C:181:GLU:HG3	2.17	0.45
2:D:338:PHE:HE2	2:D:342:PHE:HE2	1.65	0.45
1:A:80:ALA:HB1	1:A:97:LEU:HD22	2.00	0.44
1:A:452:PHE:HZ	1:A:503:LEU:HD22	1.82	0.44
2:D:377:PHE:HD1	2:D:434:ILE:HG12	1.82	0.44
1:A:177:ARG:O	1:A:181:GLU:HG3	2.18	0.44
1:A:514:ARG:HG3	1:A:518:ARG:HE	1.83	0.44
2:B:438:SER:HB2	2:B:441:ILE:HB	2.00	0.44
1:A:467:GLU:O	1:A:467:GLU:HG2	2.17	0.43
1:C:97:LEU:O	1:C:101:GLN:HG3	2.18	0.43
2:D:485:GLY:H	2:D:488:CYS:HB2	1.83	0.43
2:D:502:GLY:O	2:D:506:GLN:HG3	2.18	0.43
1:A:143:LEU:H	1:A:143:LEU:HD23	1.84	0.43
1:A:410:LEU:HD23	1:A:410:LEU:HA	1.83	0.43
1:A:451:PRO:HB2	1:A:485:VAL:HG13	2.00	0.43
1:A:478:TRP:CZ3	1:A:481:LYS:HG2	2.53	0.43
2:B:394:ASN:ND2	2:B:516:GLU:HB3	2.33	0.43
2:B:436:TRP:CZ2	2:B:509:ARG:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:GLU:HA	1:C:59:VAL:HG12	2.00	0.43
1:C:499:ASP:N	1:C:500:PRO:HD2	2.34	0.43
2:D:436:TRP:CZ2	2:D:509:ARG:HD2	2.53	0.43
1:A:463:VAL:HG23	1:A:468:ILE:HD12	2.00	0.43
1:C:469:PRO:HB2	1:C:471:ASP:OD1	2.18	0.43
1:A:450:LEU:HB2	1:A:451:PRO:HD3	2.01	0.43
1:A:134:ASN:HB3	1:A:137:ASN:OD1	2.19	0.43
1:A:318:VAL:O	1:A:551:GLY:HA3	2.19	0.43
1:A:474:MET:HE1	1:A:499:ASP:HB2	2.01	0.43
2:B:343:ASN:ND2	4:I:1:NAG:H61	2.34	0.43
1:A:218:SER:OG	1:A:219:ARG:N	2.52	0.43
1:A:457:GLU:HG2	1:A:512:PHE:HB3	2.01	0.43
2:D:497:PHE:CG	2:D:507:PRO:HG3	2.54	0.43
2:B:377:PHE:CD1	2:B:434:ILE:HG12	2.54	0.42
1:C:416:LYS:HE3	1:C:543:ASP:HB3	2.00	0.42
1:C:353:LYS:O	2:D:505:HIS:NE2	2.52	0.42
2:D:410:ILE:HD12	2:D:423:TYR:HD2	1.83	0.42
1:A:31:LYS:HD2	2:B:489:TYR:CD1	2.55	0.42
2:B:339:GLY:HA2	2:B:342:PHE:HD2	1.84	0.42
1:A:368:ASP:HA	1:A:371:THR:OG1	2.20	0.42
1:A:399:GLY:HA2	1:A:518:ARG:CG	2.50	0.42
2:B:404:GLY:HA2	2:B:508:TYR:CD2	2.54	0.42
1:C:28:PHE:HE1	1:C:79:LEU:HD23	1.83	0.42
1:C:570:LEU:O	1:C:574:VAL:HG22	2.20	0.42
2:D:478:LYS:HE3	2:D:486:LEU:HD11	2.02	0.42
1:A:122:THR:O	1:A:126:ILE:HG12	2.19	0.42
1:C:177:ARG:NH2	1:C:181:GLU:OE2	2.53	0.42
1:A:29:LEU:HD13	1:A:96:GLN:OE1	2.19	0.41
2:D:406:GLU:H	2:D:406:GLU:HG2	1.21	0.41
1:A:570:LEU:O	1:A:574:VAL:HG22	2.20	0.41
1:A:391:LEU:HD12	1:A:391:LEU:H	1.85	0.41
1:A:145:GLU:HA	1:A:146:PRO:HA	1.93	0.41
1:A:214:GLY:C	1:A:215:TYR:CD1	2.94	0.41
1:C:122:THR:O	1:C:126:ILE:HG12	2.21	0.41
1:A:452:PHE:CZ	1:A:503:LEU:HD22	2.55	0.41
1:C:309:LYS:HD2	1:C:328:TRP:CH2	2.56	0.41
2:B:497:PHE:CG	2:B:507:PRO:HG3	2.56	0.41
1:C:233:ILE:HD13	1:C:450:LEU:HD13	2.03	0.41
2:D:431:GLY:HA2	2:D:515:PHE:CD2	2.56	0.41
1:A:370:LEU:HD21	1:A:413:ALA:HB2	2.04	0.40
1:A:457:GLU:HG3	1:A:513:ILE:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:THR:O	1:C:24:GLN:HG3	2.21	0.40
1:C:38:ASP:O	1:C:42:GLN:HG2	2.22	0.40
2:D:408:ARG:NH1	2:D:414:GLN:HB2	2.36	0.40
1:C:53:ASN:OD1	1:C:340:GLN:HG3	2.22	0.40
1:C:227:GLU:HG2	1:C:454:TYR:OH	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:OE2	5:D:602:NAG:O3[2_554]	2.10	0.10

## 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	595/602 (99%)	580 (98%)	15 (2%)	0	100	100
1	C	594/602 (99%)	581 (98%)	13 (2%)	0	100	100
2	B	191/233 (82%)	173 (91%)	18 (9%)	0	100	100
2	D	191/233 (82%)	175 (92%)	16 (8%)	0	100	100
All	All	1571/1670 (94%)	1509 (96%)	62 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	526/528 (100%)	520 (99%)	6 (1%)	73	85
1	C	526/528 (100%)	519 (99%)	7 (1%)	69	82
2	B	165/202 (82%)	160 (97%)	5 (3%)	41	63
2	D	165/202 (82%)	165 (100%)	0	100	100
All	All	1382/1460 (95%)	1364 (99%)	18 (1%)	69	82

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	THR
1	A	143	LEU
1	A	215	TYR
1	A	381	TYR
1	A	385	TYR
1	A	427	ASP
2	B	336	CYS
2	B	338	PHE
2	B	343	ASN
2	B	370	ASN
2	B	487	ASN
1	C	143	LEU
1	C	148	LEU
1	C	198	ASP
1	C	381	TYR
1	C	385	TYR
1	C	514	ARG
1	C	518	ARG

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

### 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 ⓘ

20 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	E	1	1,3	14,14,15	0.25	0	17,19,21	0.45	0
3	NAG	E	2	3	14,14,15	0.61	0	17,19,21	1.11	1 (5%)
4	NAG	F	1	4,1	14,14,15	0.29	0	17,19,21	0.43	0
4	NAG	F	2	4	14,14,15	0.20	0	17,19,21	0.37	0
4	BMA	F	3	4	11,11,12	0.62	0	15,15,17	0.78	0
4	NAG	G	1	4,1	14,14,15	0.20	0	17,19,21	0.53	0
4	NAG	G	2	4	14,14,15	0.27	0	17,19,21	0.45	0
4	BMA	G	3	4	11,11,12	0.64	0	15,15,17	0.82	0
3	NAG	H	1	1,3	14,14,15	0.68	0	17,19,21	1.98	4 (23%)
3	NAG	H	2	3	14,14,15	0.32	0	17,19,21	0.71	0
4	NAG	I	1	4,2	14,14,15	0.65	1 (7%)	17,19,21	1.99	2 (11%)
4	NAG	I	2	4	14,14,15	0.32	0	17,19,21	0.90	1 (5%)
4	BMA	I	3	4	11,11,12	0.45	0	15,15,17	0.77	0
3	NAG	J	1	1,3	14,14,15	0.29	0	17,19,21	0.70	1 (5%)
3	NAG	J	2	3	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	K	1	1,3	14,14,15	0.17	0	17,19,21	0.43	0
3	NAG	K	2	3	14,14,15	0.25	0	17,19,21	0.39	0
4	NAG	L	1	4,1	14,14,15	0.16	0	17,19,21	0.37	0
4	NAG	L	2	4	14,14,15	0.25	0	17,19,21	0.47	0
4	BMA	L	3	4	11,11,12	0.58	0	15,15,17	0.82	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	2/6/23/26	0/1/1/1

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1	NAG	C1-C2	2.20	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	NAG	C1-O5-C5	6.59	121.11	112.19
3	H	1	NAG	O5-C1-C2	-4.47	104.23	111.29
3	H	1	NAG	C1-O5-C5	4.38	118.13	112.19
3	H	1	NAG	C3-C4-C5	-4.32	102.53	110.24
3	E	2	NAG	C1-O5-C5	4.18	117.86	112.19
4	I	1	NAG	C2-N2-C7	2.90	127.03	122.90
4	I	2	NAG	C1-O5-C5	2.55	115.65	112.19
3	J	1	NAG	C1-O5-C5	2.34	115.37	112.19
3	H	1	NAG	O4-C4-C3	2.28	115.63	110.35

There are no chirality outliers.

All (26) torsion outliers are listed below:

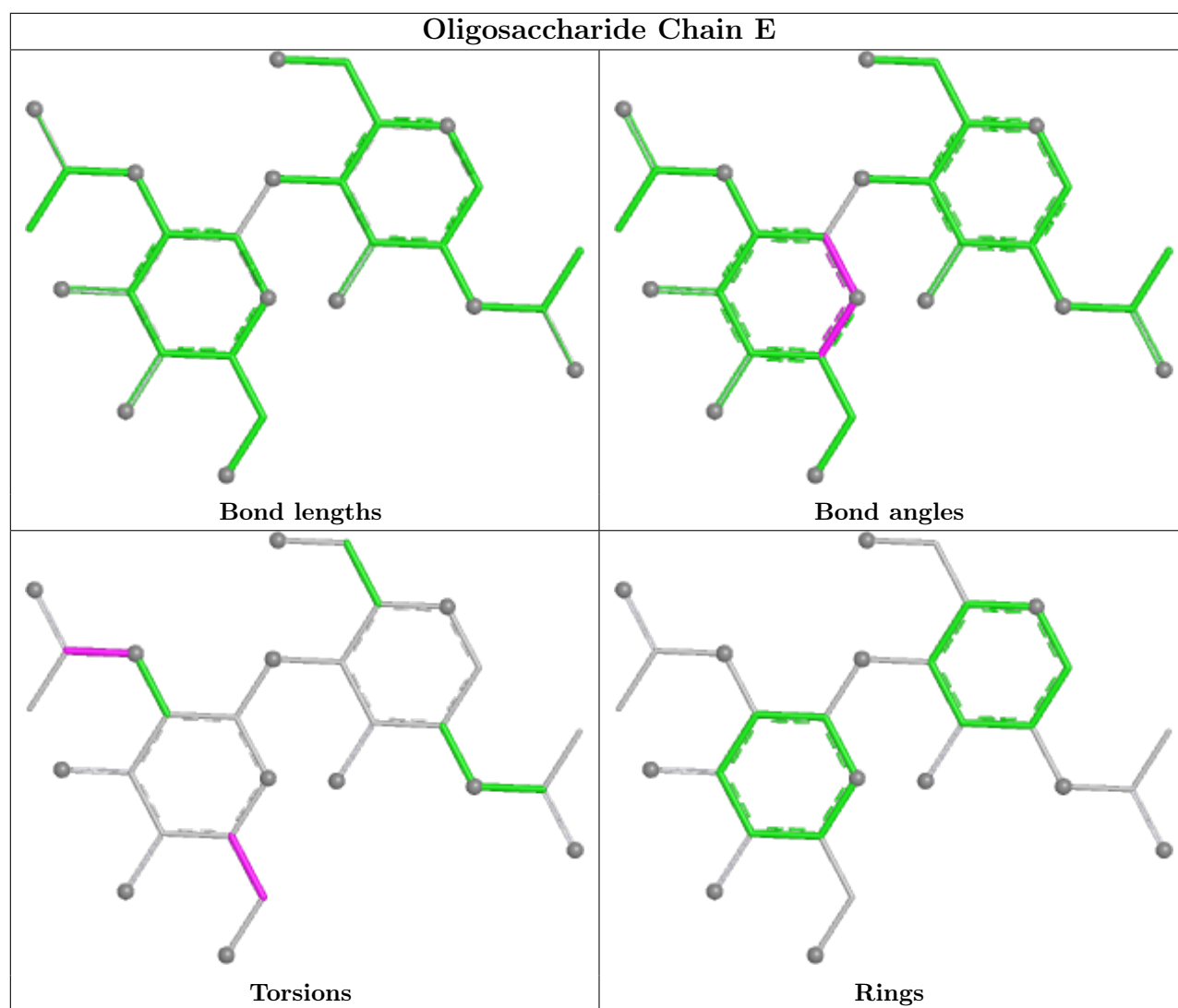
Mol	Chain	Res	Type	Atoms
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
4	I	1	NAG	C1-C2-N2-C7
4	L	1	NAG	C4-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
4	L	1	NAG	C8-C7-N2-C2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

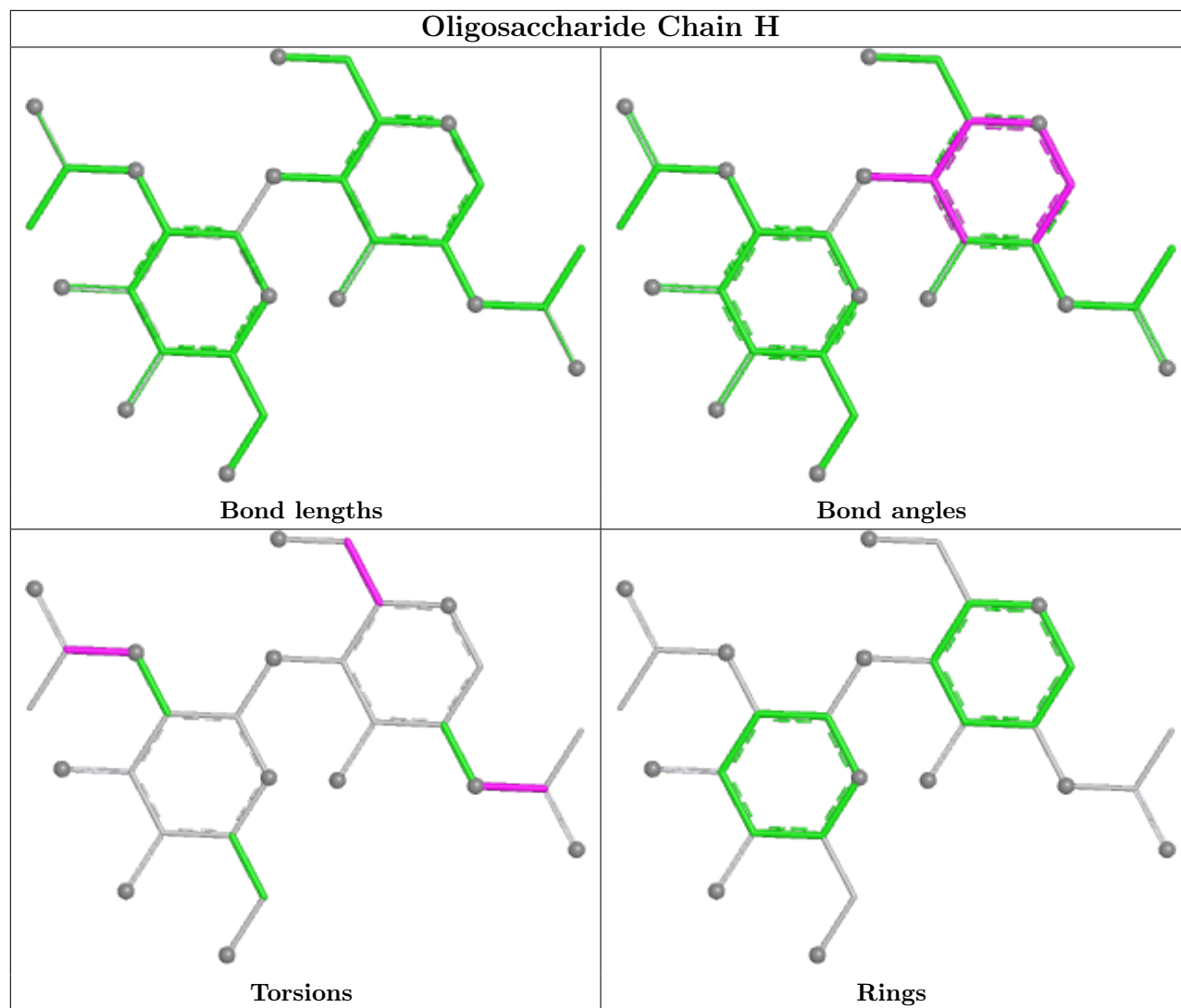
There are no ring outliers.

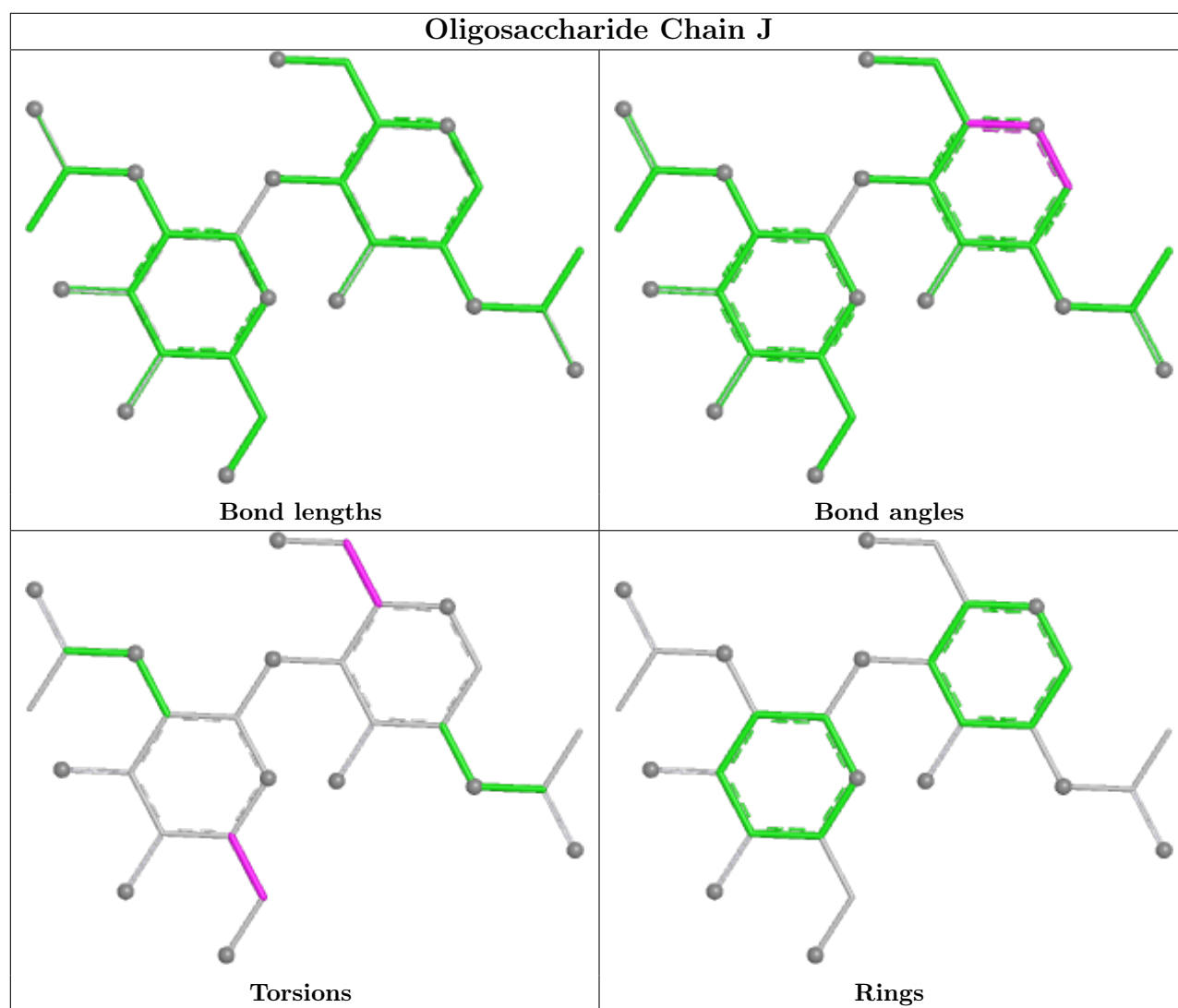
1 monomer is involved in 3 short contacts:

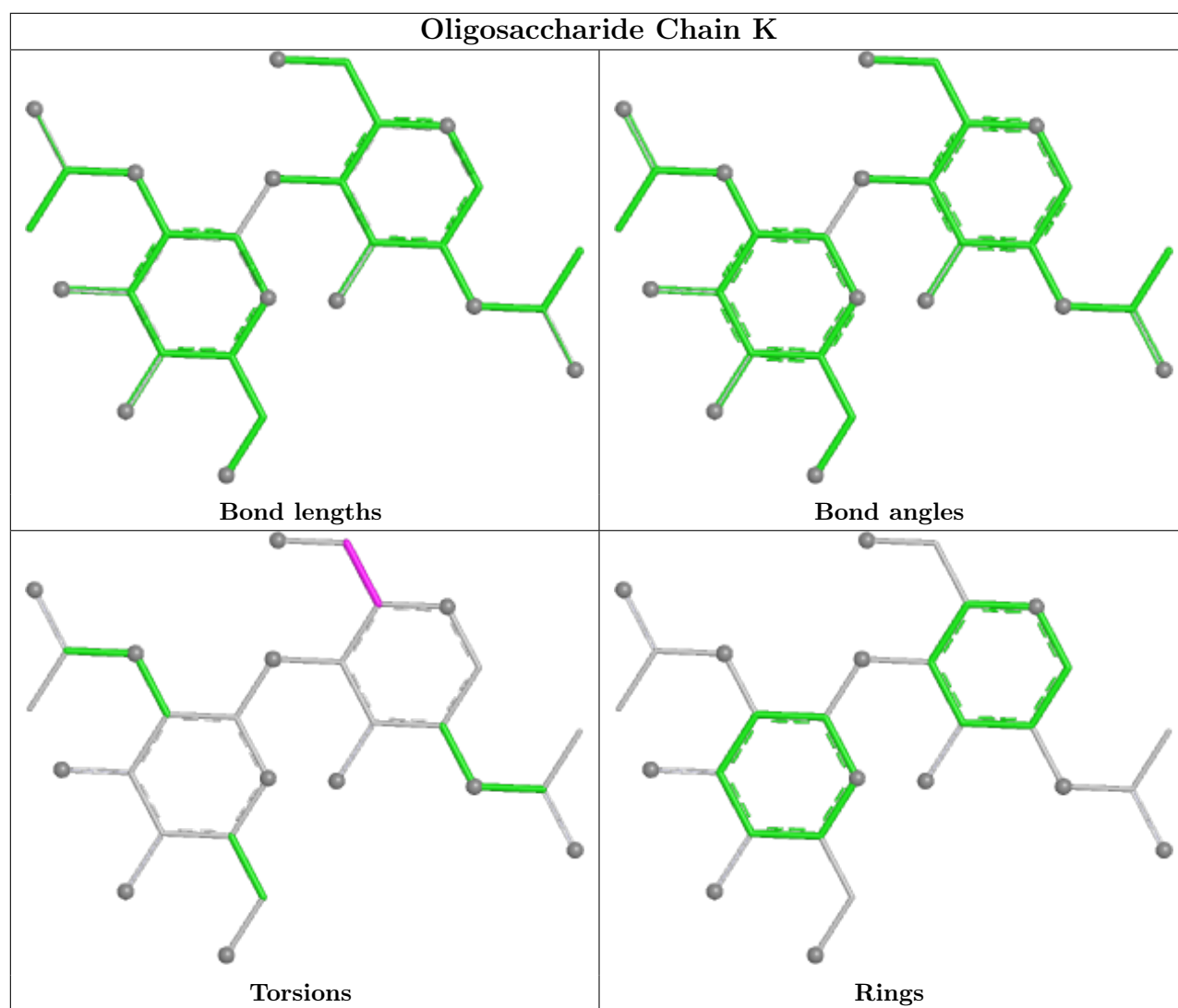
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	3	0

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

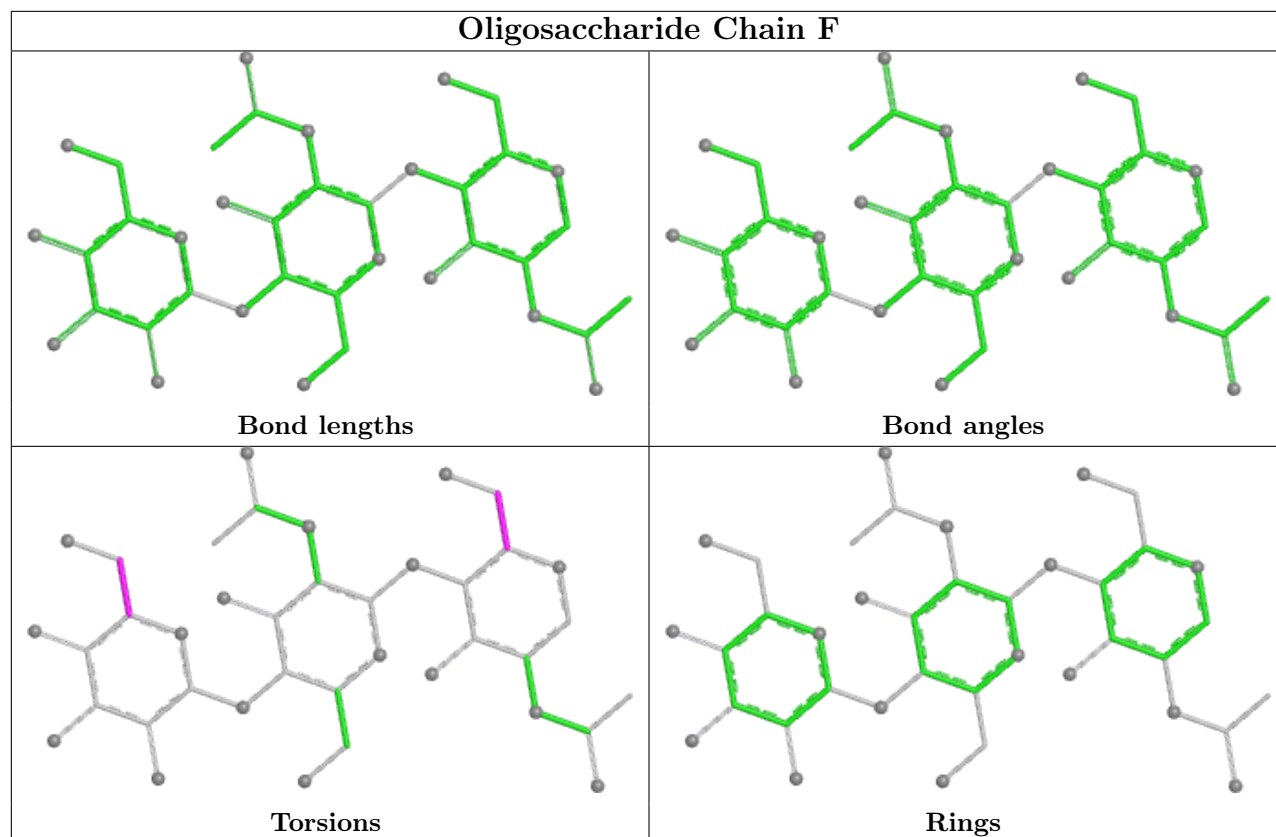




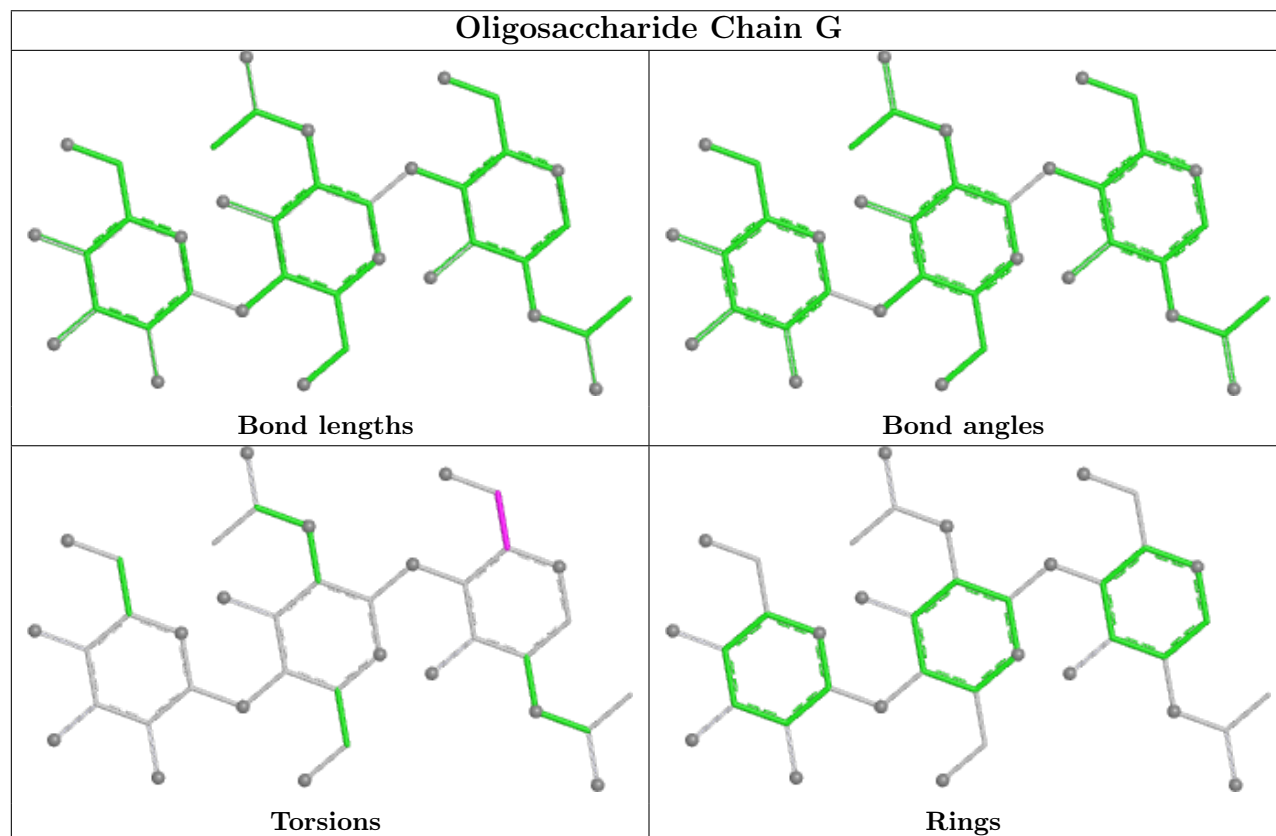


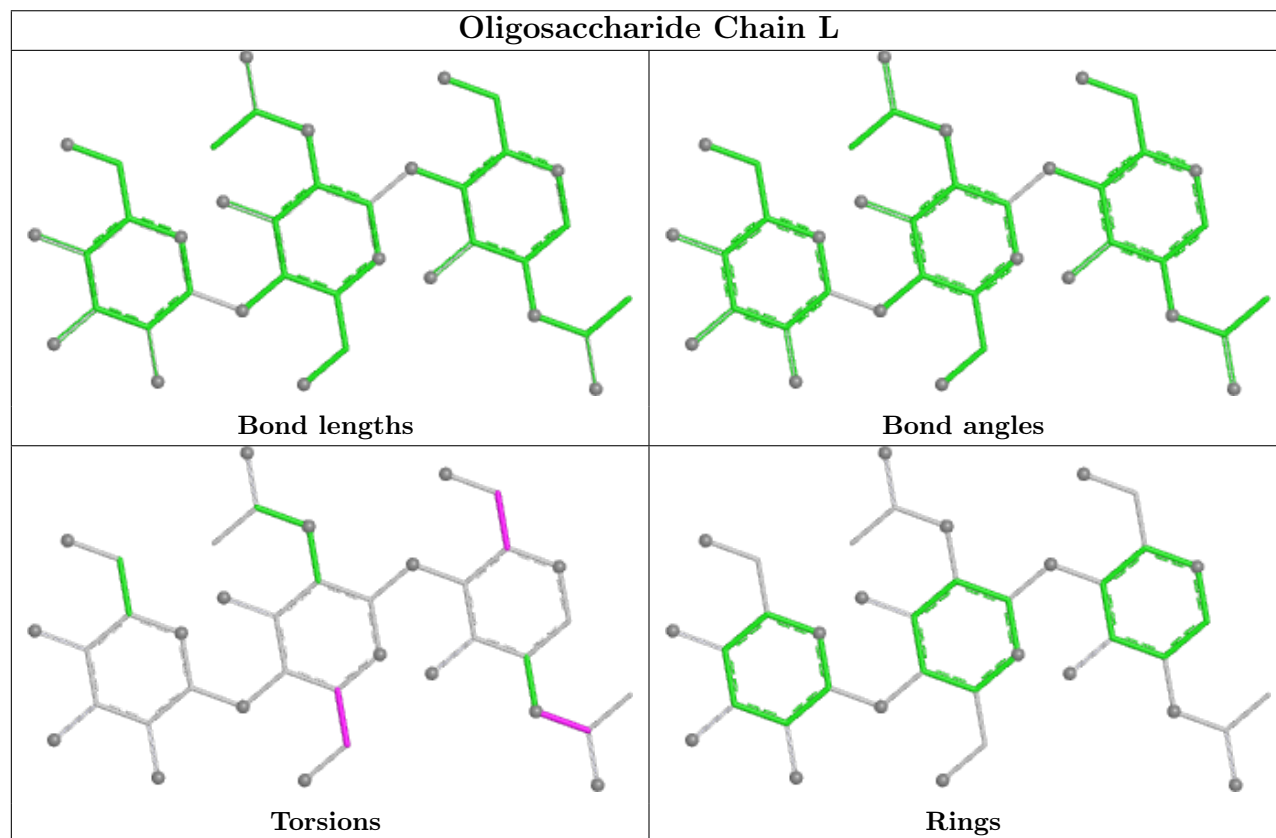
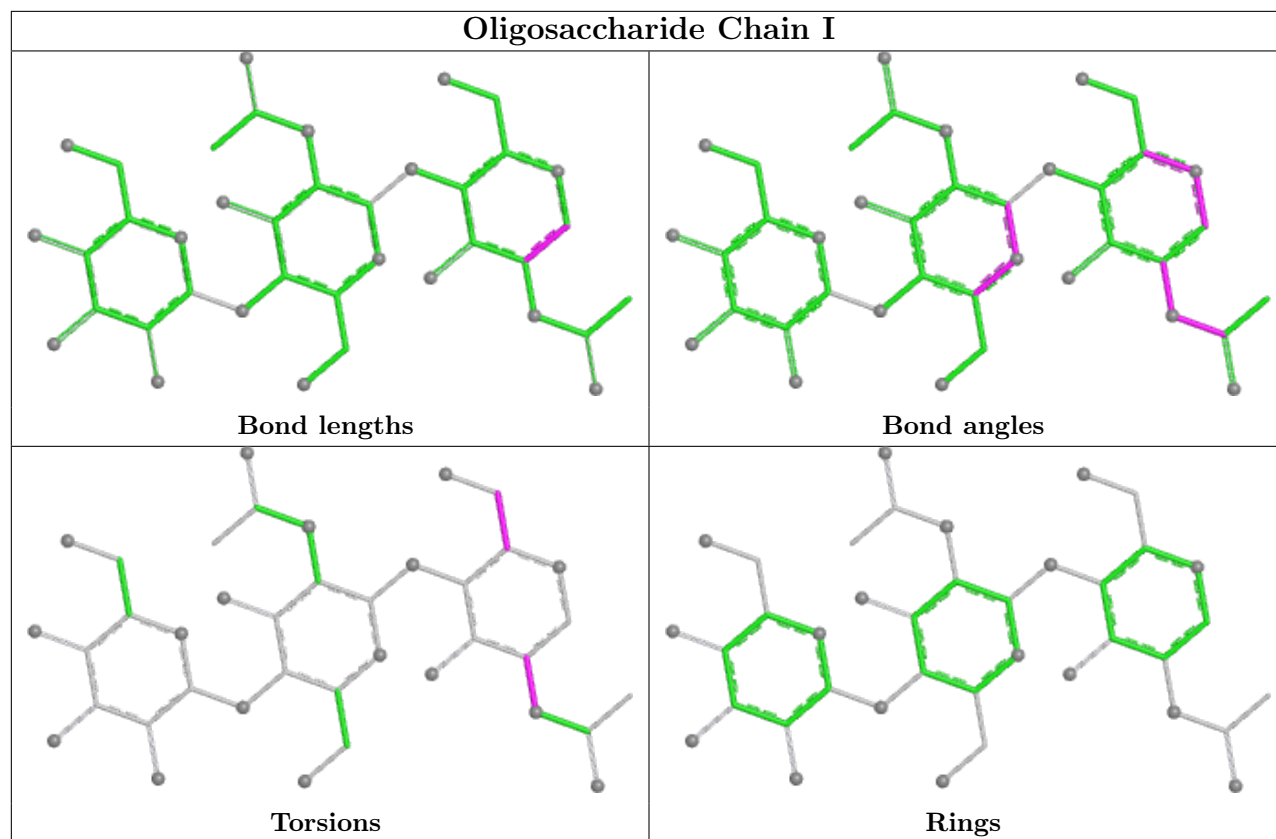


## Oligosaccharide Chain F



## Oligosaccharide Chain G





## 5.6 Ligand geometry

3 ligands 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
5	NAG	D	602	2	14,14,15	1.27	1 (7%)	17,19,21	1.42	3 (17%)
5	NAG	D	601	2	14,14,15	0.81	1 (7%)	17,19,21	0.61	0
5	NAG	C	701	1	14,14,15	0.30	0	17,19,21	0.64	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
5	NAG	D	602	2	-	0/6/23/26	0/1/1/1
5	NAG	D	601	2	-	1/6/23/26	0/1/1/1
5	NAG	C	701	1	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	602	NAG	O5-C1	4.23	1.50	1.43
5	D	601	NAG	C1-C2	2.16	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	602	NAG	C1-O5-C5	4.87	118.79	112.19
5	D	602	NAG	C3-C4-C5	-2.03	106.62	110.24
5	D	602	NAG	O3-C3-C4	-2.00	105.72	110.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	701	NAG	O5-C5-C6-O6
5	C	701	NAG	C4-C5-C6-O6
5	D	601	NAG	O5-C5-C6-O6
5	C	701	NAG	C8-C7-N2-C2
5	C	701	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	602	NAG	0	1
5	D	601	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

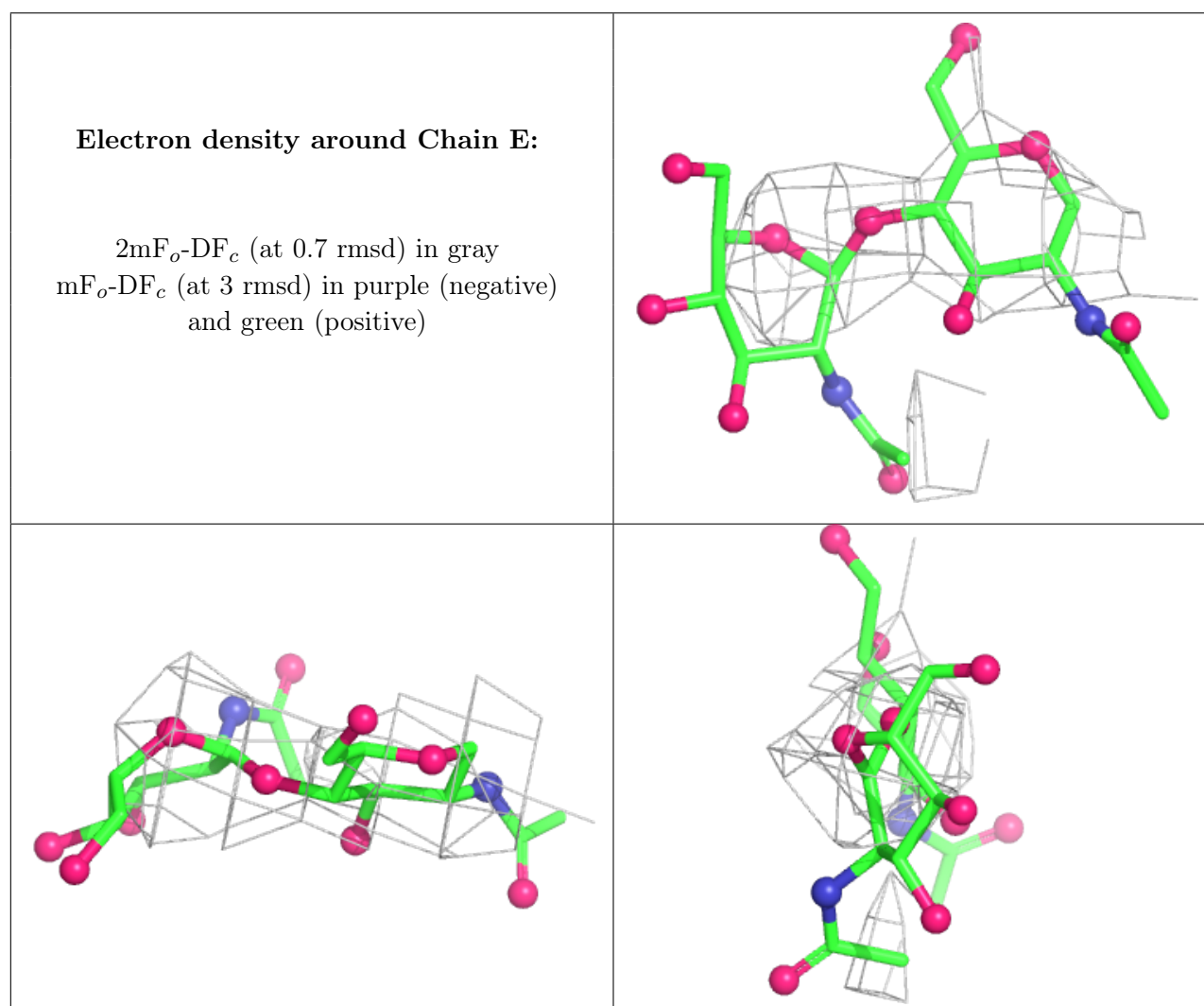
### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

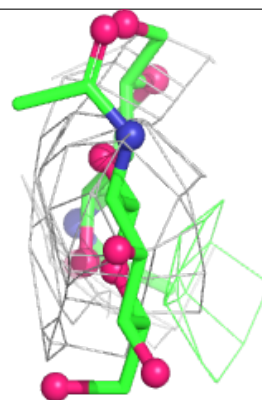
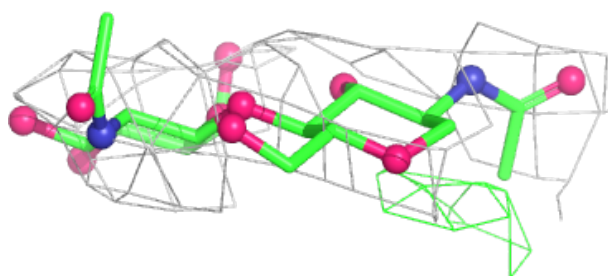
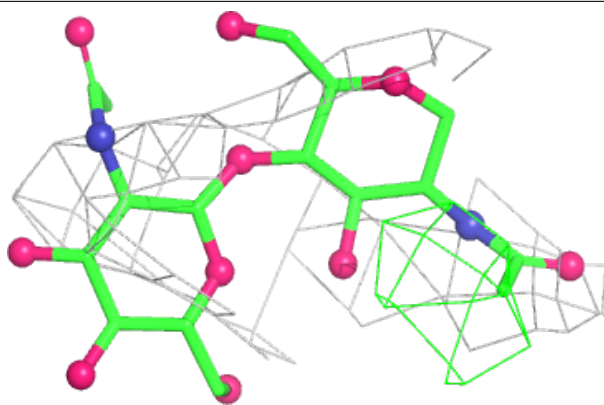
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

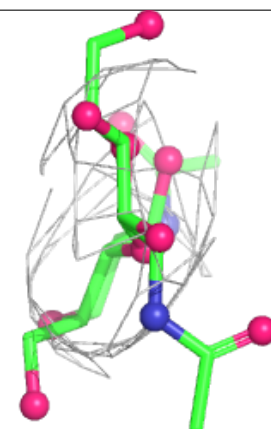
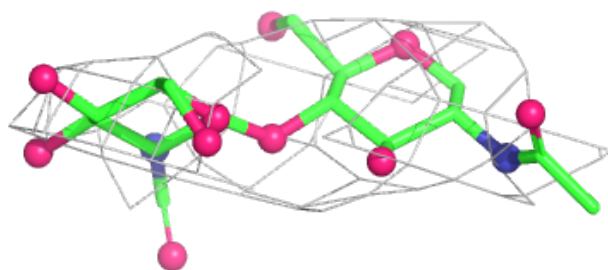
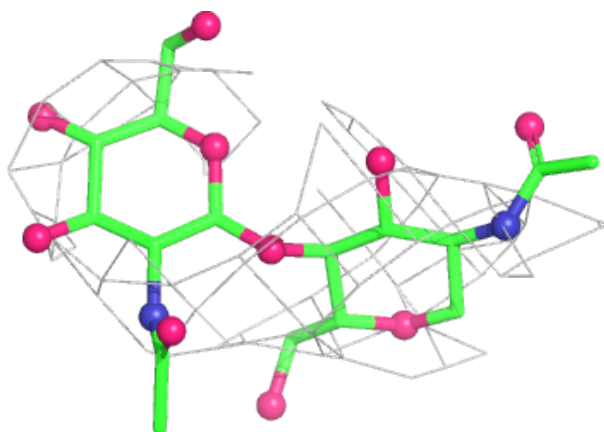


**Electron density around Chain H:**

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

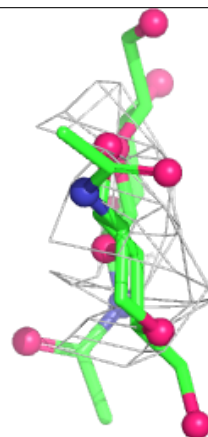
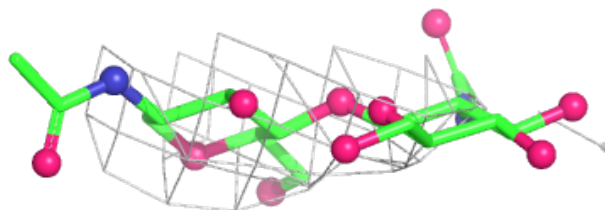
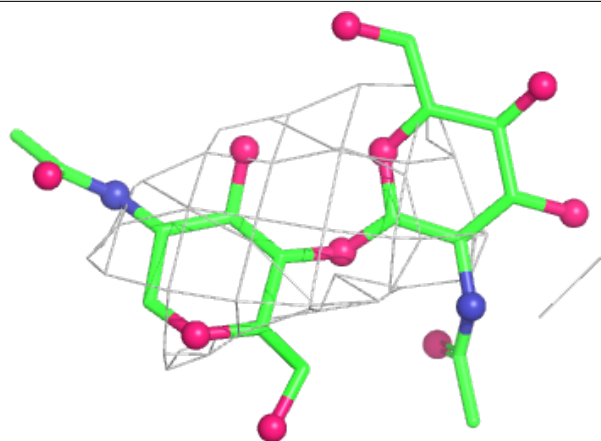
**Electron density around Chain J:**

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

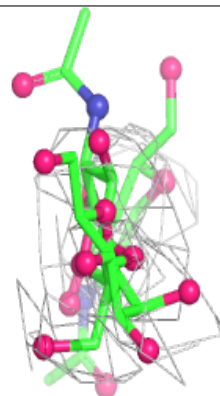
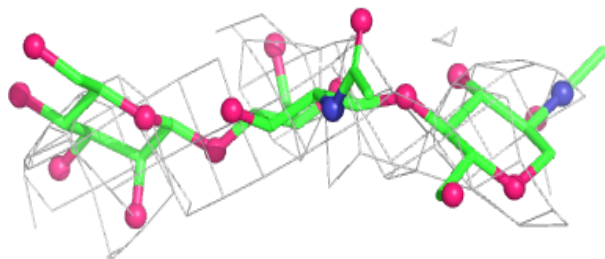
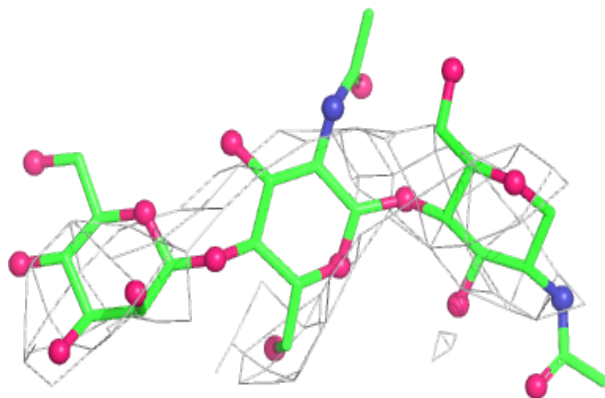


**Electron density around Chain K:**

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

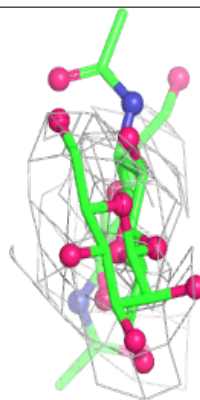
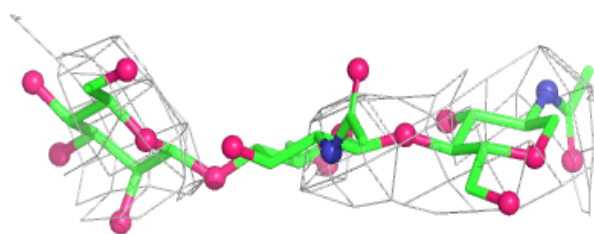
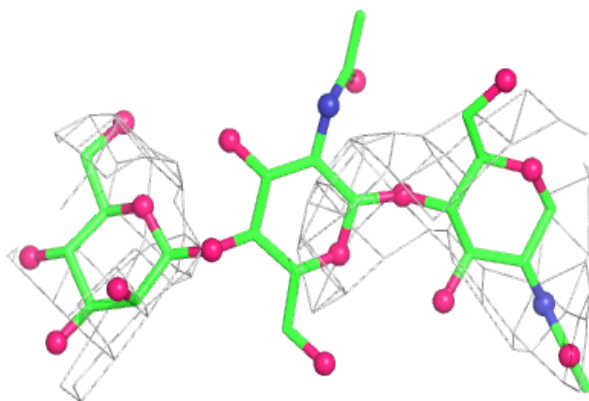
**Electron density around Chain F:**

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

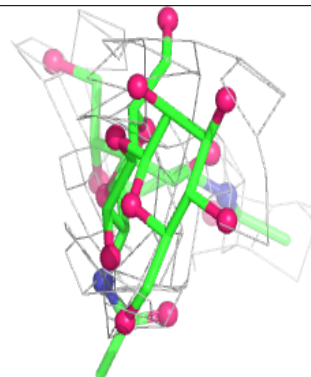
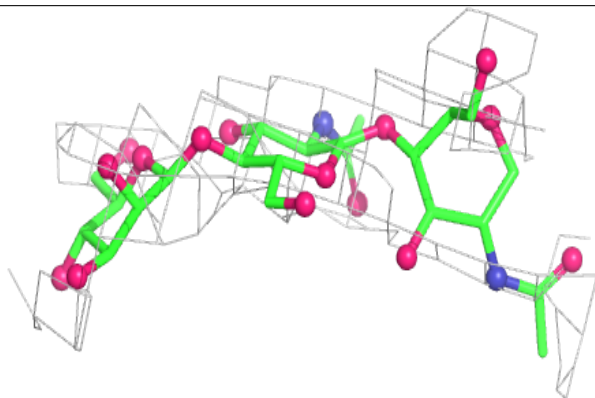
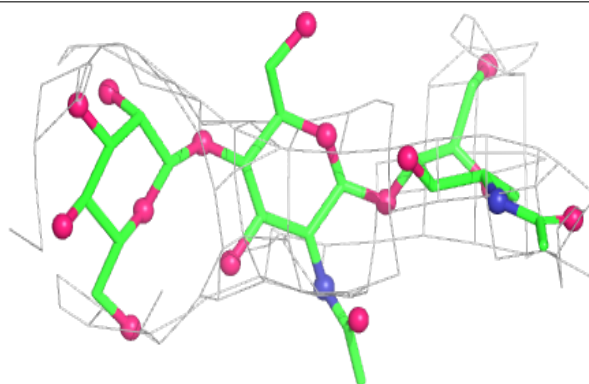


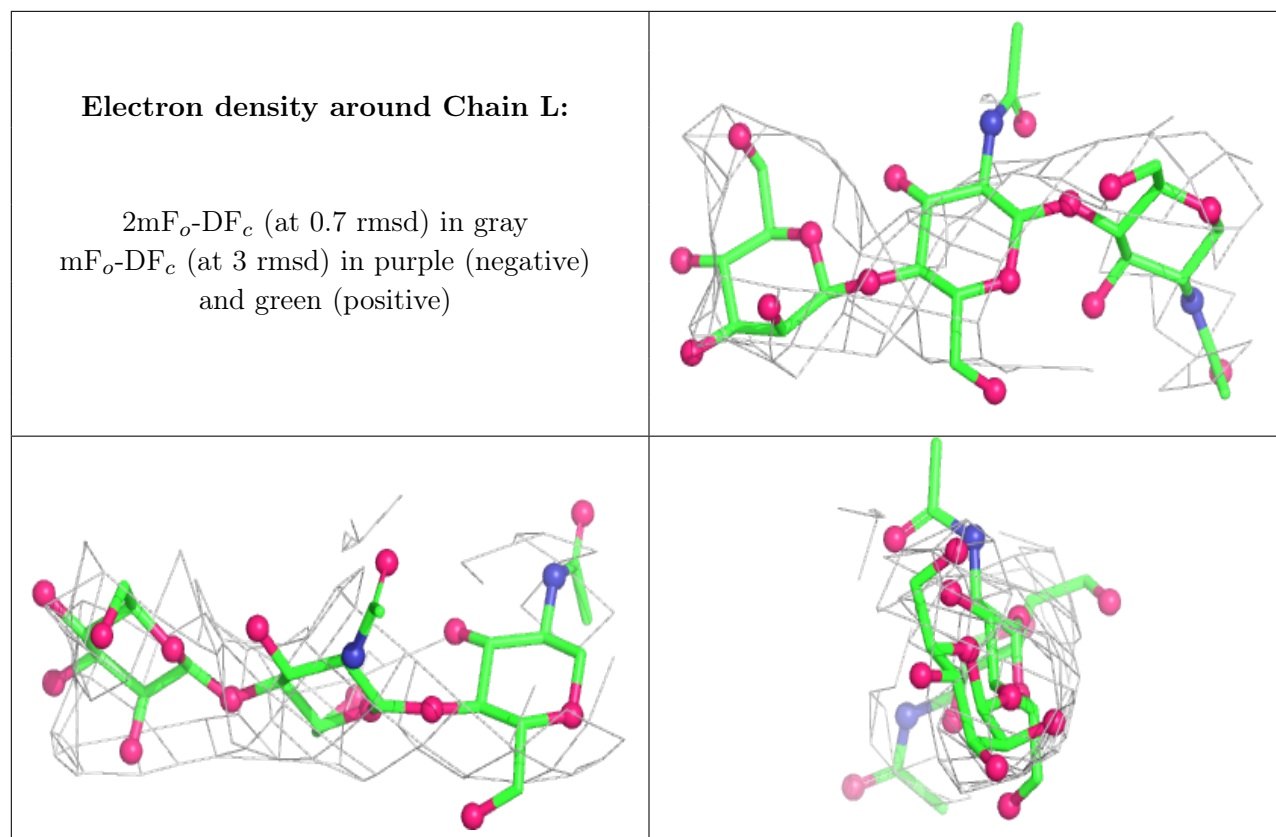
**Electron density around Chain G:**

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

**Electron density around Chain I:**

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





## 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.