



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 28, 2025 – 01:45 PM JST

PDB ID : 9JR4 / pdb\_00009jr4  
Title : Crystal structure of RaTG13 receptor-binding domain complexed with squirrel ACE2  
Authors : Lan, J.; Nan, X.  
Deposited on : 2024-09-29  
Resolution : 2.76 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>.

---

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

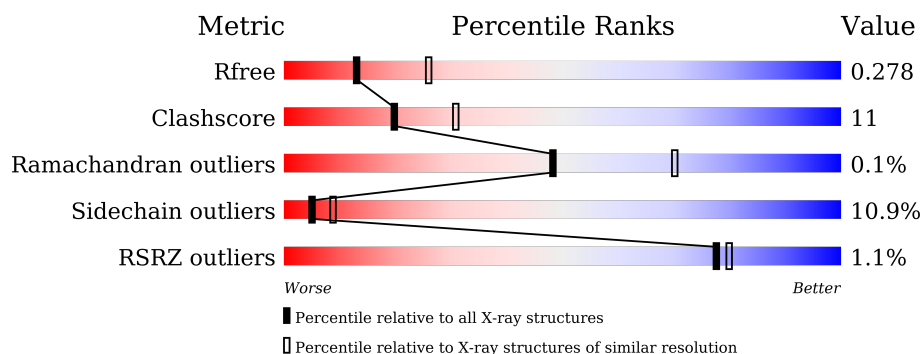
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.76 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))
$R_{free}$	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

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  $\leq 5\%$ . 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	B	597	<div> <div></div> <div>66% 29% . .</div> </div>
2	E	198	<div> <div></div> <div>68% 29% .</div> </div>
3	A	5	<div> <div></div> <div>60% 40%</div> </div>
4	C	2	<div> <div></div> <div>100%</div> </div>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6557 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.

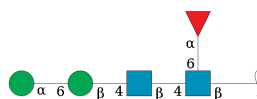
- Molecule 1 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	588	Total	C	N	O	S	0	0	0
			4819	3075	813	901	30			

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	198	Total	C	N	O	S	0	0	0
			1576	1012	264	292	8			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	5	Total	C	N	O	0	0	0
			60	34	2	24			

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

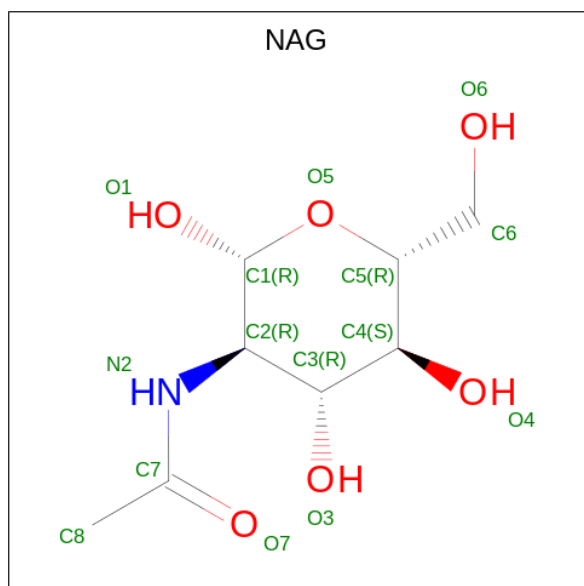


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	1	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Zn 1 1	0	0

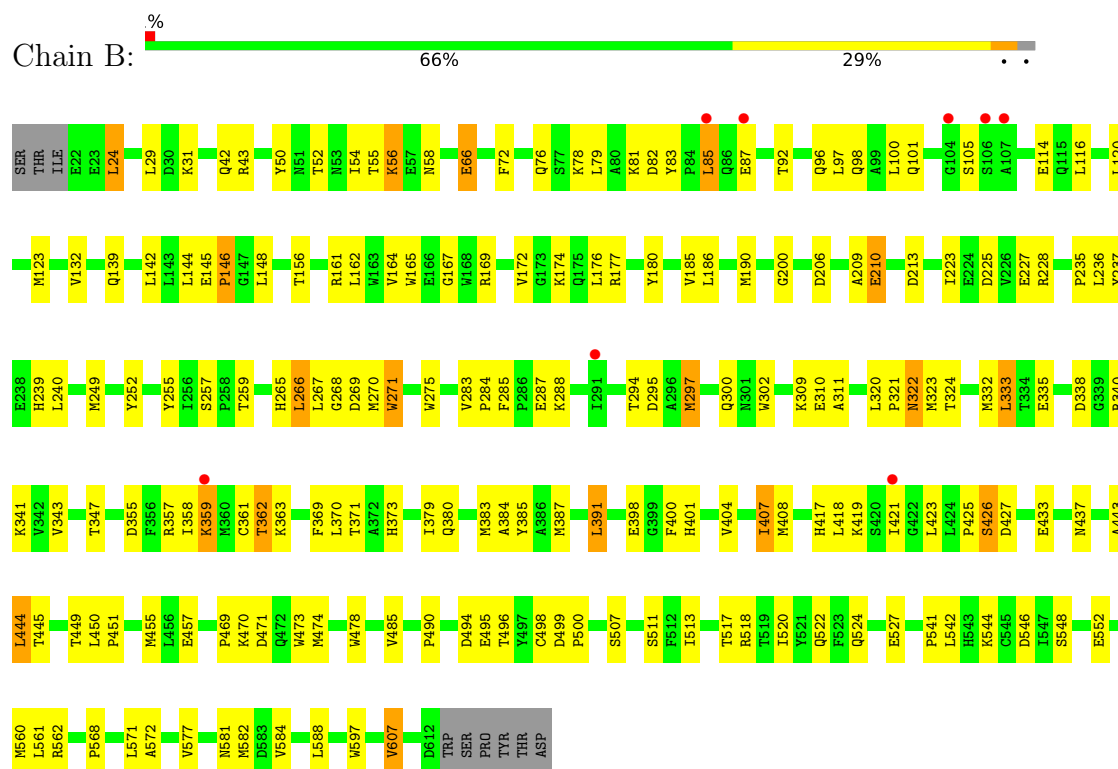
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	13	Total 13	O 13	0	0
8	E	3	Total 3	O 3	0	0

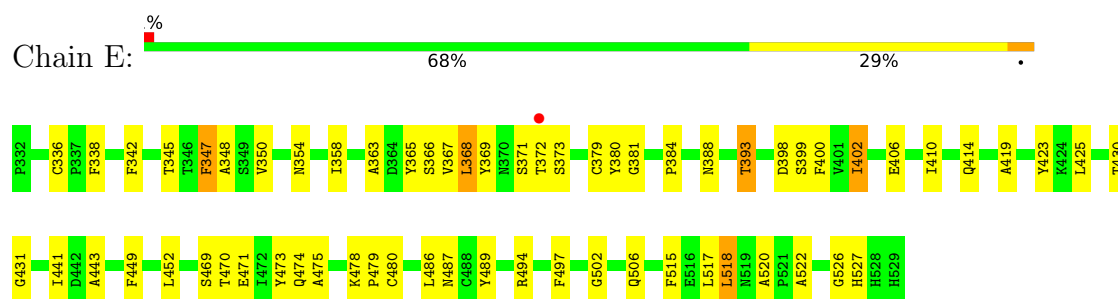
### 3 Residue-property plots

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: Angiotensin-converting enzyme



#### • Molecule 2: Spike glycoprotein



#### • Molecule 3: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:  60% 40%

MAG1  
MAG2  
BGL3  
MAN4  
FUC5

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

Chain C:  100%

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.99Å 168.99Å 86.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.22 – 2.76 28.22 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.4 (28.22-2.76) 99.3 (28.22-2.76)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 2.76Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, $R_{free}$	0.211 , 0.278 0.226 , 0.278	Depositor DCC
$R_{free}$ test set	1614 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.6	Xtriage
Anisotropy	0.698	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 64.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6557	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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

### 5.1 Standard geometry

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

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	B	0.40	0/4950	0.61	0/6712
2	E	0.41	0/1624	0.61	0/2211
All	All	0.40	0/6574	0.61	0/8923

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	B	0	1
2	E	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	423	LEU	Peptide
2	E	358	ILE	Peptide

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4819	0	4629	117	0
2	E	1576	0	1488	33	0
3	A	60	0	52	0	0
4	C	28	0	25	0	0
5	B	1	0	0	0	0
6	B	42	0	39	2	0
6	E	14	0	13	0	0
7	B	1	0	0	0	0
8	B	13	0	0	7	0
8	E	3	0	0	0	0
All	All	6557	0	6246	145	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 11.

All (145) 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:B:332:MET:SD	1:B:359:LYS:NZ	2.33	1.00
1:B:268:GLY:HA3	8:B:807:HOH:O	1.64	0.96
1:B:98:GLN:HG3	8:B:806:HOH:O	1.68	0.91
1:B:165:TRP:HA	1:B:270:MET:HE1	1.55	0.87
1:B:169:ARG:HH22	1:B:270:MET:HE2	1.46	0.81
1:B:494:ASP:OD1	1:B:496:THR:HG22	1.83	0.79
1:B:116:LEU:HD13	1:B:186:LEU:HB2	1.78	0.66
1:B:338:ASP:HB2	1:B:340:ARG:HB2	1.78	0.66
1:B:225:ASP:OD2	1:B:581:ASN:ND2	2.28	0.64
1:B:548:SER:HB2	6:B:702:NAG:H82	1.79	0.64
1:B:83:TYR:OH	2:E:487:ASN:OD1	2.14	0.64
1:B:340:ARG:HD3	6:B:703:NAG:H82	1.80	0.63
1:B:265:HIS:ND1	1:B:490:PRO:HG3	2.13	0.63
2:E:381:GLY:HA3	2:E:430:THR:HG22	1.81	0.61
1:B:209:ALA:HB1	1:B:568:PRO:HB3	1.83	0.60
1:B:200:GLY:HA3	8:B:812:HOH:O	2.02	0.58
1:B:333:LEU:O	1:B:362:THR:HG22	2.03	0.58
1:B:169:ARG:NH2	1:B:270:MET:HE2	2.17	0.58
2:E:366:SER:HA	2:E:369:TYR:CZ	2.37	0.58
1:B:387:MET:HA	1:B:387:MET:HE2	1.84	0.58
1:B:24:LEU:HD13	2:E:487:ASN:ND2	2.19	0.57
1:B:132:VAL:HG21	1:B:167:GLY:HA3	1.85	0.57
1:B:239:HIS:CE1	1:B:607:VAL:HG11	2.39	0.57
1:B:284:PRO:HD2	1:B:437:ASN:OD1	2.04	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:ILE:HD11	1:B:522:GLN:O	2.05	0.56
1:B:85:LEU:CD2	8:B:806:HOH:O	2.53	0.56
1:B:400:PHE:HE2	1:B:560:MET:HE1	1.71	0.56
1:B:400:PHE:CE2	1:B:560:MET:HE1	2.42	0.55
2:E:449:PHE:O	2:E:494:ARG:HD3	2.08	0.54
1:B:469:PRO:HB2	1:B:471:ASP:OD1	2.07	0.54
1:B:324:THR:HG23	1:B:383:MET:HE2	1.88	0.54
1:B:474:MET:HA	1:B:474:MET:HE2	1.90	0.54
2:E:410:ILE:HG23	2:E:425:LEU:HD11	1.89	0.53
1:B:24:LEU:HD21	2:E:475:ALA:HB3	1.90	0.53
1:B:225:ASP:CG	1:B:581:ASN:HD21	2.15	0.53
1:B:148:LEU:HD22	1:B:164:VAL:HG13	1.90	0.53
1:B:355:ASP:OD1	1:B:355:ASP:C	2.51	0.53
1:B:357:ARG:HG2	8:B:803:HOH:O	2.09	0.53
1:B:457:GLU:HG3	1:B:513:ILE:HB	1.92	0.52
2:E:380:TYR:O	2:E:430:THR:HA	2.10	0.52
1:B:541:PRO:HG2	1:B:544:LYS:HE2	1.91	0.52
1:B:252:TYR:HB3	1:B:255:TYR:HD2	1.76	0.51
1:B:180:TYR:OH	8:B:801:HOH:O	2.14	0.51
1:B:52:THR:O	1:B:340:ARG:HD2	2.11	0.50
2:E:347:PHE:CE2	2:E:399:SER:HB2	2.47	0.50
1:B:560:MET:CE	1:B:572:ALA:HB1	2.41	0.50
1:B:284:PRO:HB3	1:B:597:TRP:CH2	2.47	0.50
1:B:335:GLU:HB2	1:B:361:CYS:SG	2.52	0.50
1:B:474:MET:HE1	1:B:500:PRO:HD2	1.94	0.50
1:B:43:ARG:HD2	1:B:66:GLU:OE2	2.12	0.50
2:E:379:CYS:SG	2:E:384:PRO:HG3	2.51	0.50
1:B:235:PRO:HD2	8:B:804:HOH:O	2.12	0.49
1:B:520:ILE:O	1:B:524:GLN:HG3	2.11	0.49
1:B:359:LYS:C	1:B:359:LYS:HE3	2.36	0.49
1:B:284:PRO:HB2	1:B:285:PHE:CD1	2.48	0.49
1:B:527:GLU:HA	1:B:542:LEU:HD11	1.95	0.49
1:B:132:VAL:HG12	1:B:148:LEU:HD11	1.95	0.48
1:B:288:LYS:HD3	1:B:433:GLU:OE2	2.13	0.48
1:B:237:TYR:CD1	1:B:451:PRO:HG2	2.49	0.48
1:B:560:MET:HB2	1:B:560:MET:HE2	1.50	0.48
2:E:452:LEU:HD11	2:E:494:ARG:NH1	2.28	0.48
1:B:31:LYS:HD2	2:E:489:TYR:CD1	2.48	0.48
1:B:369:PHE:CD1	1:B:370:LEU:HD23	2.49	0.47
2:E:402:ILE:HG13	2:E:406:GLU:OE2	2.14	0.47
1:B:50:TYR:CE1	1:B:54:ILE:HG23	2.49	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:HIS:HB2	1:B:546:ASP:OD2	2.14	0.47
1:B:560:MET:HE2	1:B:572:ALA:HB1	1.96	0.47
2:E:354:ASN:O	2:E:398:ASP:HA	2.15	0.47
2:E:517:LEU:HD12	2:E:517:LEU:HA	1.72	0.47
1:B:419:LYS:HE3	1:B:426:SER:HA	1.96	0.47
1:B:320:LEU:HB3	1:B:321:PRO:HD2	1.96	0.47
1:B:206:ASP:CG	1:B:398:GLU:HG2	2.40	0.47
2:E:473:TYR:CE2	2:E:475:ALA:HB2	2.50	0.46
1:B:320:LEU:HB3	1:B:380:GLN:OE1	2.15	0.46
1:B:269:ASP:OD1	1:B:271:TRP:O	2.33	0.46
1:B:55:THR:HB	1:B:58:ASN:H	1.79	0.46
1:B:96:GLN:HB3	1:B:391:LEU:HD12	1.97	0.46
1:B:223:ILE:O	1:B:227:GLU:HG3	2.15	0.46
1:B:407:ILE:HG22	1:B:408:MET:SD	2.56	0.45
1:B:546:ASP:OD1	1:B:548:SER:OG	2.34	0.45
1:B:297:MET:HE3	1:B:302:TRP:CE3	2.51	0.45
1:B:517:THR:HG22	1:B:582:MET:SD	2.56	0.45
1:B:240:LEU:HD22	1:B:443:ALA:HB1	1.99	0.45
1:B:249:MET:HE3	1:B:249:MET:HB2	1.78	0.45
1:B:322:ASN:OD1	1:B:322:ASN:N	2.42	0.45
2:E:474:GLN:CD	2:E:479:PRO:HA	2.42	0.45
1:B:297:MET:HB3	1:B:302:TRP:HB2	1.98	0.45
1:B:369:PHE:HD1	1:B:370:LEU:HD23	1.81	0.45
1:B:341:LYS:HD3	1:B:341:LYS:HA	1.62	0.44
2:E:469:SER:HB3	2:E:471:GLU:HG3	1.99	0.44
1:B:169:ARG:HH21	1:B:169:ARG:HG3	1.81	0.44
1:B:210:GLU:O	1:B:210:GLU:HG3	2.16	0.44
1:B:72:PHE:O	1:B:76:GLN:HG2	2.18	0.44
1:B:225:ASP:OD1	1:B:228:ARG:NH1	2.51	0.44
2:E:419:ALA:HA	2:E:423:TYR:O	2.17	0.44
2:E:431:GLY:HA2	2:E:515:PHE:HD2	1.82	0.44
1:B:185:VAL:HG23	1:B:186:LEU:HG	2.00	0.43
1:B:92:THR:O	1:B:96:GLN:HG3	2.18	0.43
1:B:302:TRP:CH2	1:B:310:GLU:HG3	2.53	0.43
1:B:470:LYS:HA	1:B:473:TRP:CD1	2.53	0.43
1:B:270:MET:O	1:B:270:MET:HG3	2.16	0.43
1:B:275:TRP:HB2	1:B:444:LEU:O	2.18	0.43
1:B:478:TRP:CE3	1:B:478:TRP:HA	2.52	0.43
2:E:388:ASN:HA	2:E:526:GLY:HA3	2.00	0.43
1:B:78:LYS:HA	1:B:81:LYS:HD2	2.00	0.43
1:B:265:HIS:CD2	1:B:266:LEU:HD13	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:PRO:C	1:B:427:ASP:H	2.27	0.42
1:B:101:GLN:O	1:B:105:SER:OG	2.29	0.42
1:B:499:ASP:N	1:B:500:PRO:HD2	2.33	0.42
2:E:518:LEU:O	2:E:520:ALA:N	2.48	0.42
2:E:366:SER:HA	2:E:369:TYR:CE1	2.55	0.42
1:B:309:LYS:HD3	1:B:309:LYS:HA	1.83	0.42
1:B:81:LYS:NZ	1:B:105:SER:HB3	2.34	0.42
1:B:237:TYR:CG	1:B:451:PRO:HG2	2.54	0.42
1:B:379:ILE:CG2	1:B:383:MET:HE3	2.49	0.42
2:E:443:ALA:HB2	2:E:497:PHE:HB3	2.01	0.42
1:B:300:GLN:HB3	1:B:302:TRP:CD1	2.54	0.42
1:B:552:GLU:H	1:B:552:GLU:CD	2.28	0.42
2:E:365:TYR:O	2:E:368:LEU:HB2	2.20	0.42
1:B:24:LEU:HD11	2:E:475:ALA:C	2.45	0.41
1:B:56:LYS:HE2	1:B:56:LYS:HB2	1.85	0.41
1:B:123:MET:HE3	1:B:507:SER:O	2.19	0.41
1:B:457:GLU:OE1	1:B:457:GLU:HA	2.20	0.41
1:B:560:MET:SD	1:B:561:LEU:HD23	2.59	0.41
2:E:336:CYS:SG	2:E:363:ALA:HB2	2.60	0.41
2:E:338:PHE:O	2:E:342:PHE:HD2	2.02	0.41
1:B:79:LEU:O	1:B:82:ASP:HB2	2.20	0.41
1:B:162:LEU:HD23	1:B:162:LEU:C	2.46	0.41
1:B:177:ARG:HB2	1:B:498:CYS:HB2	2.01	0.41
1:B:311:ALA:HA	1:B:373:HIS:NE2	2.36	0.41
1:B:174:LYS:HG2	1:B:496:THR:O	2.21	0.41
2:E:486:LEU:H	2:E:486:LEU:HD22	1.84	0.41
1:B:24:LEU:HD23	1:B:24:LEU:O	2.21	0.41
2:E:350:VAL:HG21	2:E:402:ILE:HD13	2.03	0.41
1:B:161:ARG:NH2	1:B:267:LEU:O	2.53	0.41
1:B:300:GLN:HB3	1:B:302:TRP:HD1	1.86	0.41
1:B:323:MET:HA	1:B:383:MET:HE1	2.02	0.41
1:B:384:ALA:O	1:B:562:ARG:HA	2.21	0.41
1:B:450:LEU:HB2	1:B:451:PRO:HD3	2.02	0.41
1:B:177:ARG:NH2	1:B:495:GLU:O	2.54	0.40
2:E:348:ALA:O	2:E:400:PHE:HA	2.21	0.40
1:B:520:ILE:HD12	1:B:520:ILE:N	2.36	0.40
2:E:393:THR:HA	2:E:522:ALA:HA	2.04	0.40
2:E:502:GLY:O	2:E:506:GLN:HG3	2.21	0.40
1:B:145:GLU:HB3	1:B:146:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	586/597 (98%)	555 (95%)	30 (5%)	1 (0%)	44	63
2	E	196/198 (99%)	179 (91%)	17 (9%)	0	100	100
All	All	782/795 (98%)	734 (94%)	47 (6%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	146	PRO

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	517/527 (98%)	458 (89%)	59 (11%)	4	7
2	E	170/170 (100%)	154 (91%)	16 (9%)	7	13
All	All	687/697 (99%)	612 (89%)	75 (11%)	5	9

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	24	LEU
1	B	29	LEU
1	B	42	GLN
1	B	56	LYS
1	B	66	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	85	LEU
1	B	87	GLU
1	B	97	LEU
1	B	100	LEU
1	B	114	GLU
1	B	120	LEU
1	B	139	GLN
1	B	142	LEU
1	B	144	LEU
1	B	156	THR
1	B	172	VAL
1	B	176	LEU
1	B	190	MET
1	B	210	GLU
1	B	213	ASP
1	B	236	LEU
1	B	257	SER
1	B	259	THR
1	B	266	LEU
1	B	271	TRP
1	B	283	VAL
1	B	287	GLU
1	B	294	THR
1	B	295	ASP
1	B	297	MET
1	B	322	ASN
1	B	333	LEU
1	B	343	VAL
1	B	347	THR
1	B	358	ILE
1	B	359	LYS
1	B	362	THR
1	B	363	LYS
1	B	371	THR
1	B	385	TYR
1	B	391	LEU
1	B	401	HIS
1	B	404	VAL
1	B	407	ILE
1	B	418	LEU
1	B	421	ILE
1	B	426	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	444	LEU
1	B	445	THR
1	B	449	THR
1	B	455	MET
1	B	485	VAL
1	B	511	SER
1	B	518	ARG
1	B	571	LEU
1	B	577	VAL
1	B	584	VAL
1	B	588	LEU
1	B	607	VAL
2	E	345	THR
2	E	347	PHE
2	E	367	VAL
2	E	368	LEU
2	E	371	SER
2	E	372	THR
2	E	373	SER
2	E	393	THR
2	E	402	ILE
2	E	414	GLN
2	E	441	ILE
2	E	470	THR
2	E	478	LYS
2	E	480	CYS
2	E	518	LEU
2	E	527	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	42	GLN
1	B	49	ASN
1	B	63	ASN
1	B	76	GLN
1	B	101	GLN
1	B	604	ASN
2	E	414	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 ⓘ

7 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	A	1	3,1	14,14,15	0.61	0	17,19,21	0.52	0
3	NAG	A	2	3	14,14,15	0.33	0	17,19,21	0.45	0
3	BMA	A	3	3	11,11,12	1.57	3 (27%)	15,15,17	1.21	2 (13%)
3	MAN	A	4	3	11,11,12	1.83	3 (27%)	15,15,17	1.21	1 (6%)
3	FUC	A	5	3	10,10,11	0.95	0	14,14,16	0.97	0
4	NAG	C	1	2,4	14,14,15	0.81	1 (7%)	17,19,21	1.04	1 (5%)
4	NAG	C	2	4	14,14,15	1.56	2 (14%)	17,19,21	1.07	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
3	NAG	A	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	A	2	3	-	0/6/23/26	0/1/1/1
3	BMA	A	3	3	-	0/2/19/22	0/1/1/1
3	MAN	A	4	3	-	0/2/19/22	0/1/1/1
3	FUC	A	5	3	-	-	0/1/1/1
4	NAG	C	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2	NAG	O5-C1	4.69	1.51	1.43
3	A	4	MAN	C2-C3	3.46	1.57	1.52
4	C	2	NAG	C1-C2	3.32	1.57	1.52
3	A	4	MAN	C1-C2	3.12	1.59	1.52
3	A	3	BMA	C4-C5	3.00	1.59	1.53
3	A	4	MAN	C4-C3	2.70	1.59	1.52
3	A	3	BMA	O5-C5	2.56	1.48	1.43
3	A	3	BMA	C4-C3	2.23	1.58	1.52
4	C	1	NAG	O5-C1	-2.17	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2	NAG	C1-O5-C5	4.05	117.67	112.19
3	A	3	BMA	O2-C2-C3	-2.60	104.94	110.14
3	A	4	MAN	O2-C2-C1	2.41	114.09	109.15
3	A	3	BMA	O5-C1-C2	-2.32	107.18	110.77
4	C	1	NAG	C1-O5-C5	2.25	115.24	112.19

There are no chirality outliers.

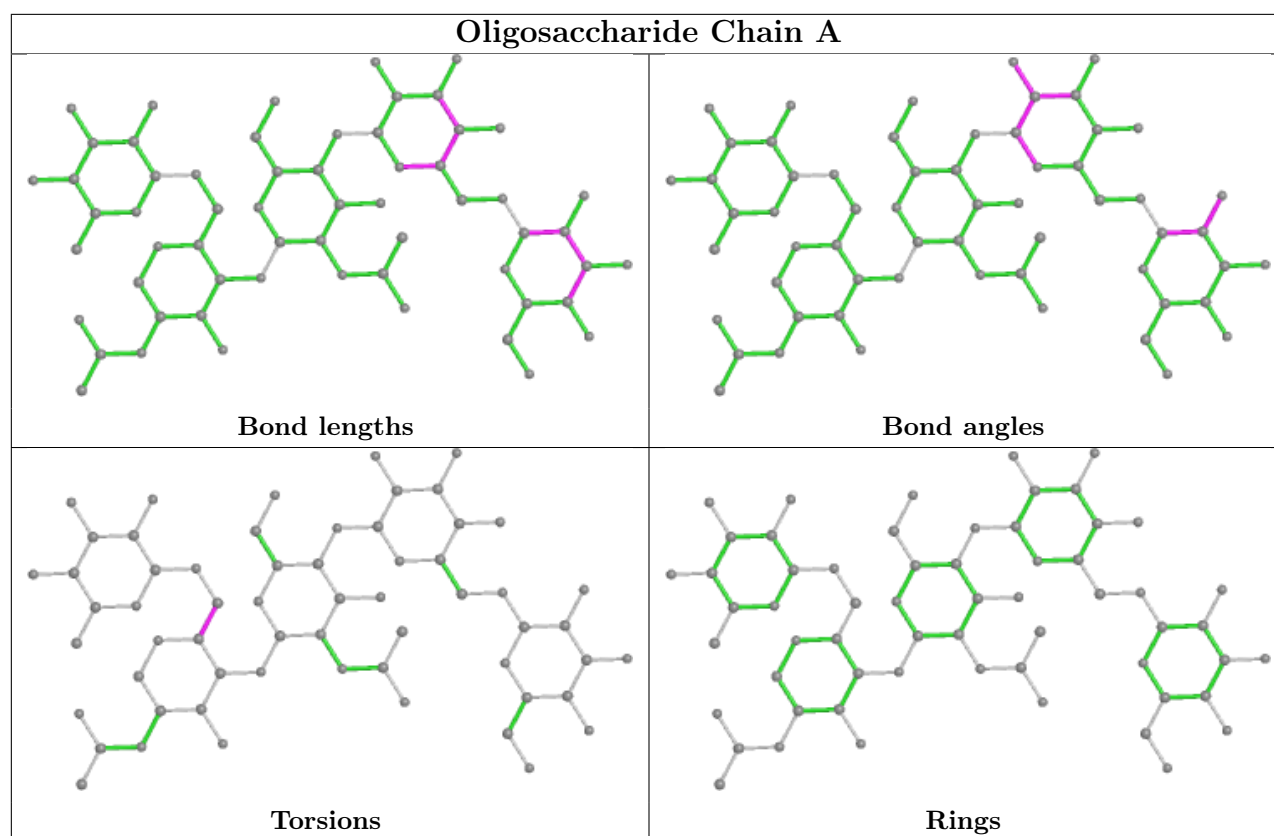
All (4) torsion outliers are listed below:

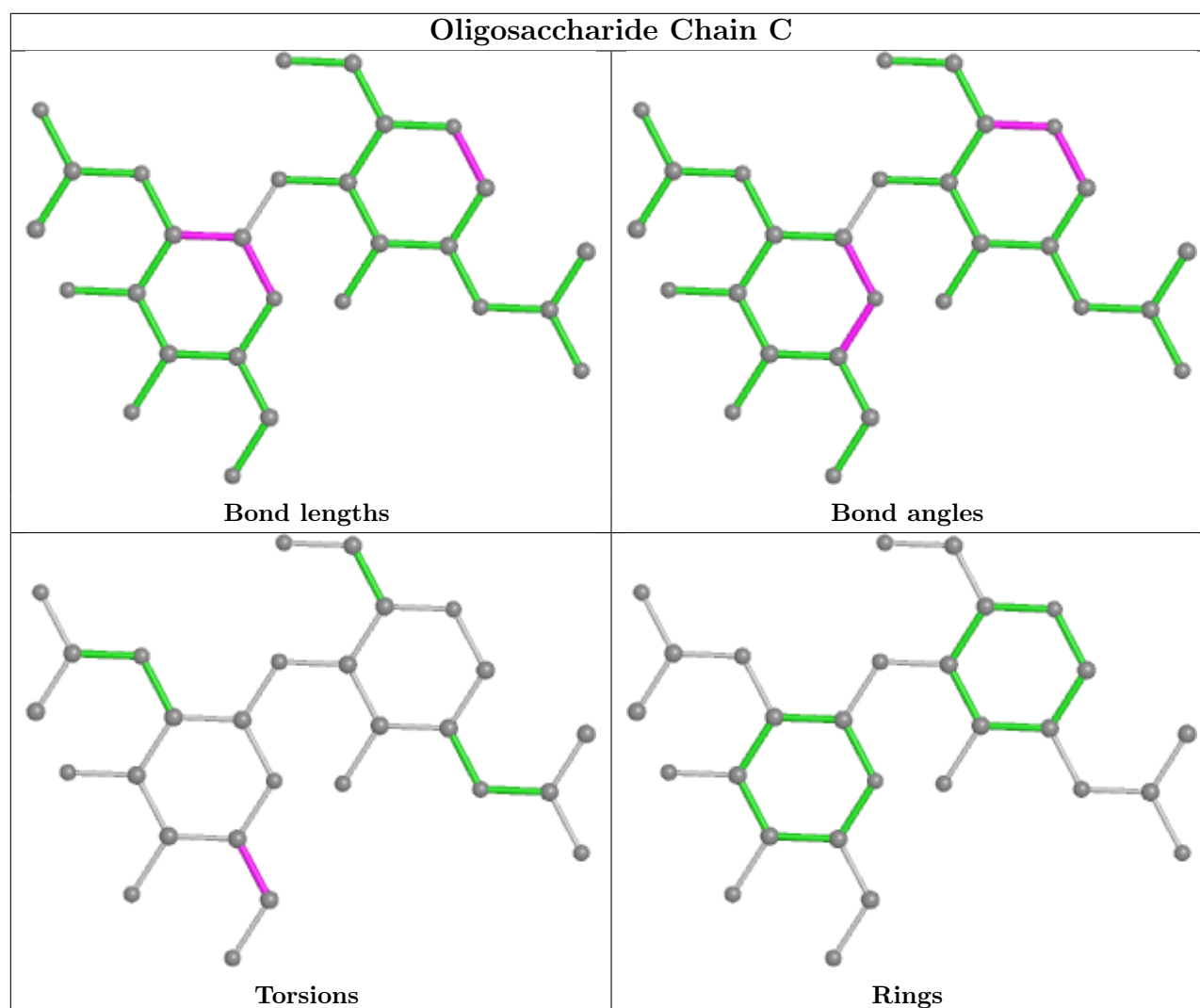
Mol	Chain	Res	Type	Atoms
4	C	2	NAG	O5-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6
3	A	1	NAG	C4-C5-C6-O6
3	A	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z  > 2$
6	NAG	B	703	1	14,14,15	0.80	1 (7%)	17,19,21	0.70	0
6	NAG	B	704	1	14,14,15	0.52	0	17,19,21	0.69	0
6	NAG	E	601	2	14,14,15	0.26	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	B	702	1	14,14,15	0.74	1 (7%)	17,19,21	0.78	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
6	NAG	B	703	1	-	2/6/23/26	0/1/1/1
6	NAG	B	704	1	-	2/6/23/26	0/1/1/1
6	NAG	E	601	2	-	4/6/23/26	0/1/1/1
6	NAG	B	702	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	703	NAG	O5-C1	2.87	1.48	1.43
6	B	702	NAG	O5-C1	2.20	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	702	NAG	C1-O5-C5	2.76	115.93	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	702	NAG	C4-C5-C6-O6
6	B	703	NAG	C4-C5-C6-O6
6	E	601	NAG	C4-C5-C6-O6
6	B	702	NAG	O5-C5-C6-O6
6	B	703	NAG	O5-C5-C6-O6
6	E	601	NAG	C8-C7-N2-C2
6	E	601	NAG	O7-C7-N2-C2
6	E	601	NAG	O5-C5-C6-O6
6	B	704	NAG	O5-C5-C6-O6
6	B	704	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	703	NAG	1	0
6	B	702	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	588/597 (98%)	-0.18	8 (1%) 73 75	63, 81, 119, 188	0
2	E	198/198 (100%)	-0.20	1 (0%) 87 89	66, 76, 110, 133	0
All	All	786/795 (98%)	-0.18	9 (1%) 77 80	63, 79, 116, 188	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	421	ILE	3.8
1	B	107	ALA	3.6
1	B	291	ILE	3.2
1	B	106	SER	2.5
1	B	87	GLU	2.4
1	B	359	LYS	2.2
2	E	372	THR	2.2
1	B	85	LEU	2.2
1	B	104	GLY	2.1

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

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

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

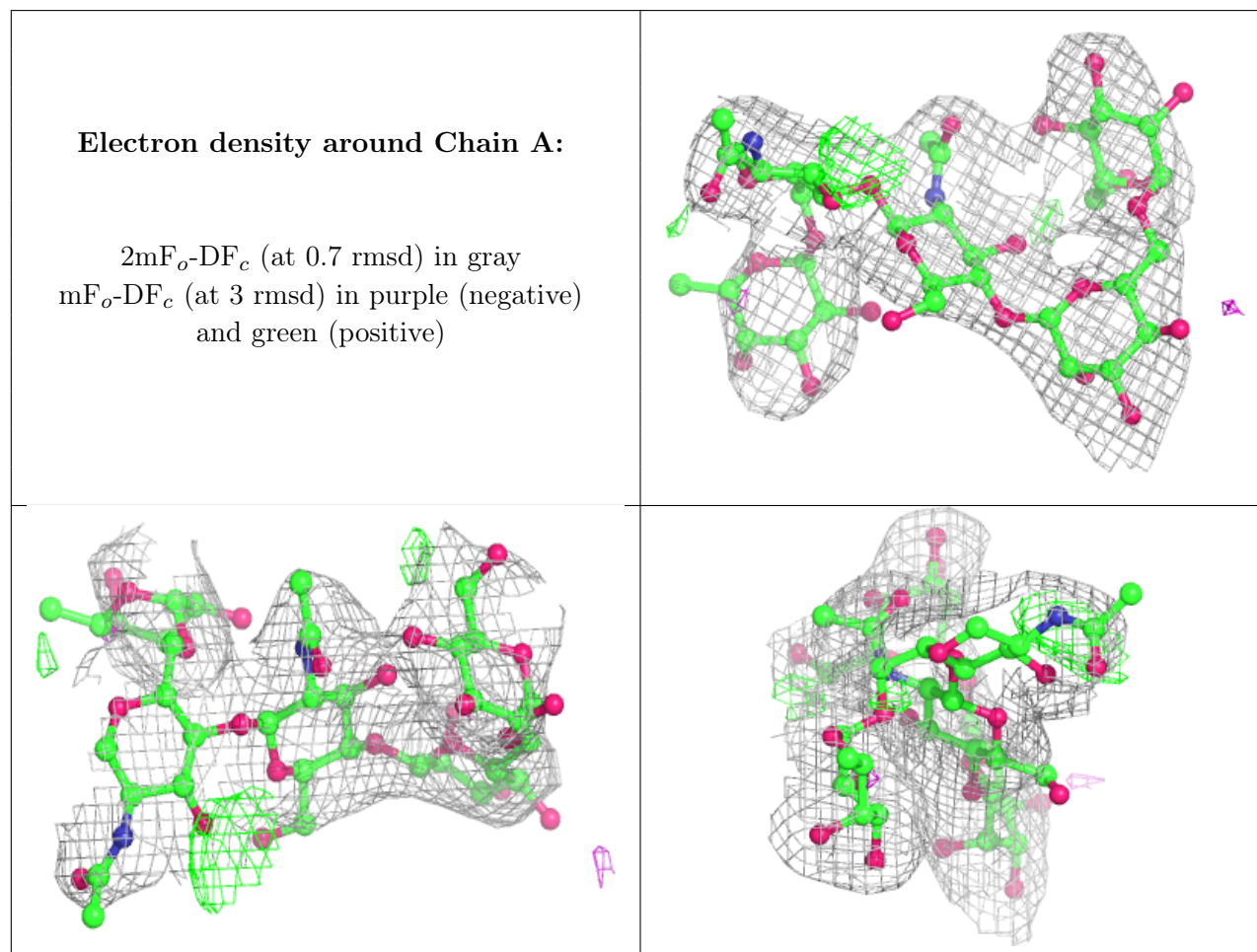
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	1	14/15	-	-	90,105,117,124	0

*Continued on next page...*

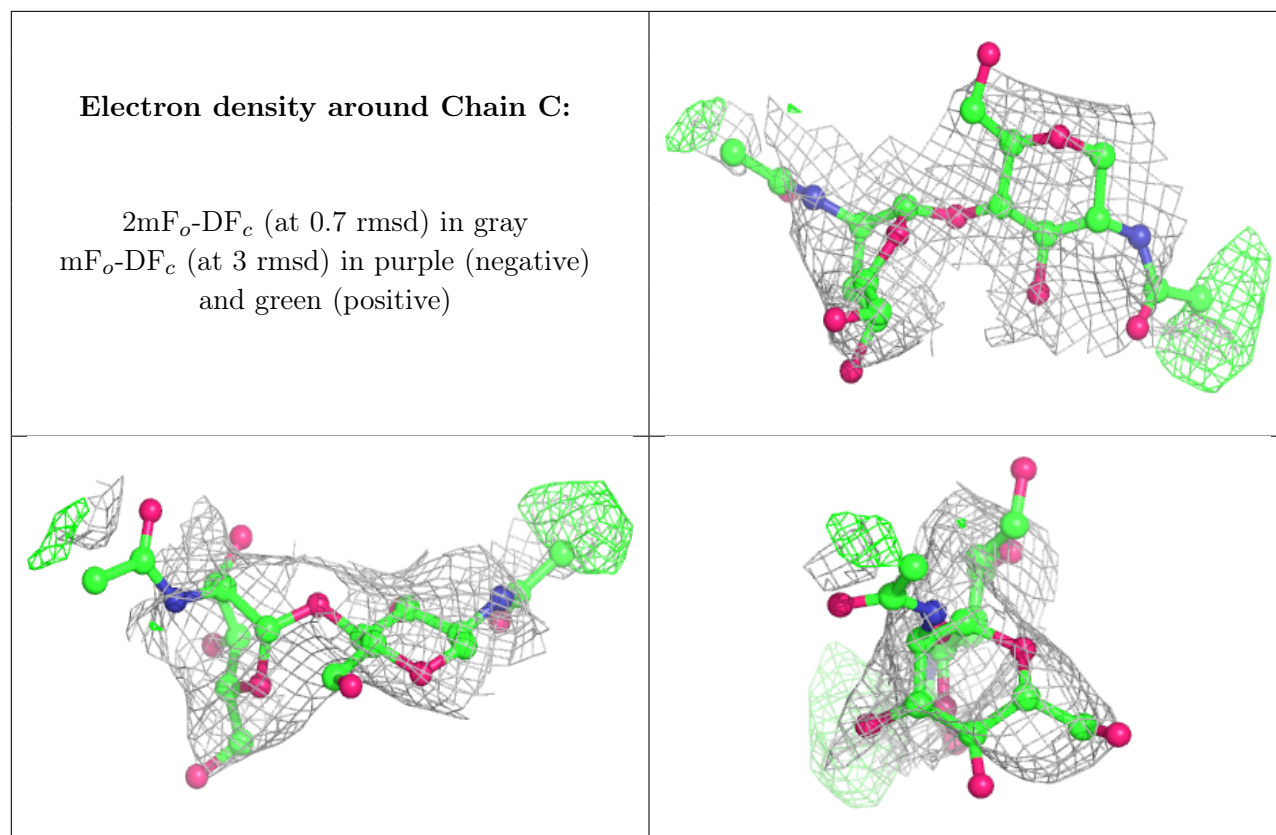
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	2	14/15	-	-	100,112,115,116	0
3	BMA	A	3	11/12	-	-	106,110,117,118	0
3	MAN	A	4	11/12	-	-	108,117,119,120	0
3	FUC	A	5	10/11	-	-	136,140,142,142	0
4	NAG	C	1	14/15	0.79	0.09	152,160,167,167	0
4	NAG	C	2	14/15	0.89	0.08	147,160,162,163	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.







## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CL	B	701	1/1	-	-	63,63,63,63	1
6	NAG	B	704	14/15	0.53	0.11	163,169,177,177	0
6	NAG	B	702	14/15	0.68	0.14	137,146,158,158	0
6	NAG	E	601	14/15	0.72	0.15	148,156,165,166	0
6	NAG	B	703	14/15	0.81	0.09	110,120,128,129	0
7	ZN	B	705	1/1	0.93	0.49	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.