



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 02:03 AM BST

PDB ID : 6U7E
Title : HCoV-229E RBD Class III in complex with human APN
Authors : Tomlinson, A.C.A.; Li, Z.; Rini, J.M.
Deposited on : 2019-09-02
Resolution : 3.00 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

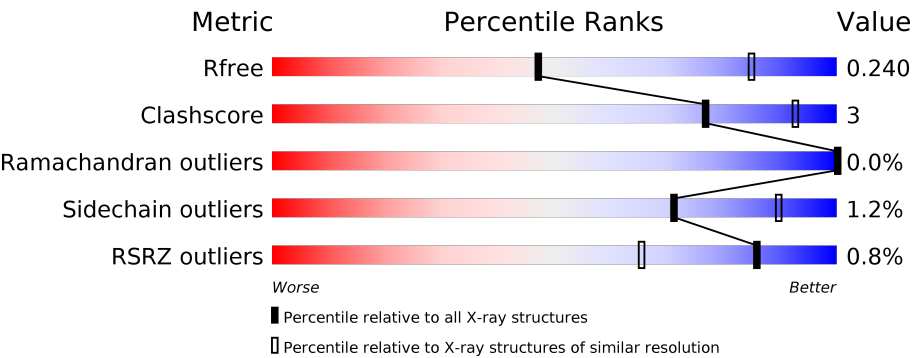
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



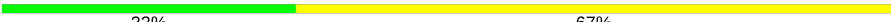

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	906	<div><div></div><div>92%7%</div></div>
1	B	906	<div><div></div><div>92%7%</div></div>
2	C	145	<div><div>2%</div><div>67%8%25%</div></div>
2	D	145	<div><div>5%</div><div>72%8%19%</div></div>
3	E	2	<div><div></div><div>50%50%</div></div>
3	H	2	<div><div></div><div>100%</div></div>

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Mol	Chain	Length	Quality of chain
4	F	3	 33% 67%
4	G	3	 67% 33%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16543 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 Aminopeptidase N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	900	Total	C	N	O	S	0	0	0
			7264	4632	1225	1383	24			
1	B	900	Total	C	N	O	S	0	0	0
			7264	4632	1225	1383	24			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	GLY	-	expression tag	UNP P15144
A	63	GLY	-	expression tag	UNP P15144
A	64	ARG	-	expression tag	UNP P15144
A	65	PRO	-	expression tag	UNP P15144
B	62	GLY	-	expression tag	UNP P15144
B	63	GLY	-	expression tag	UNP P15144
B	64	ARG	-	expression tag	UNP P15144
B	65	PRO	-	expression tag	UNP P15144

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	109	Total	C	N	O	S	0	0	0
			819	528	137	147	7			
2	D	117	Total	C	N	O	S	0	0	0
			887	575	148	156	8			

- 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			

- 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			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

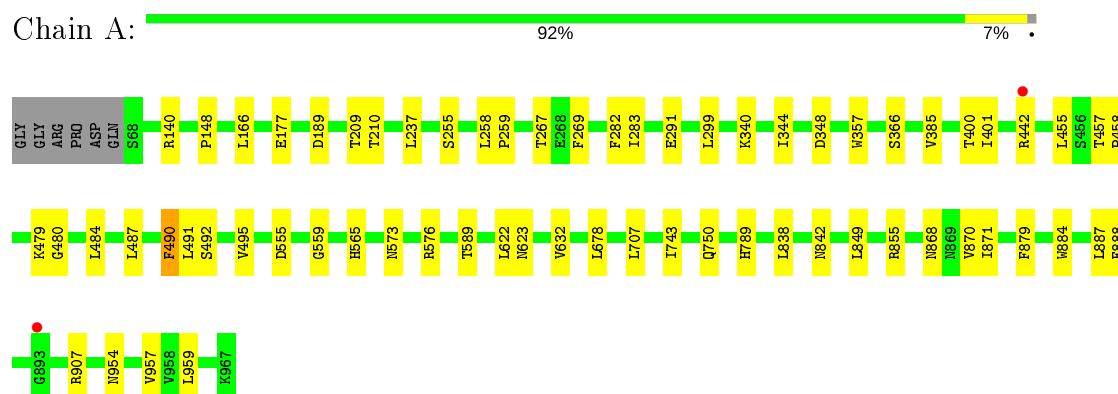
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total 3	O 3	0	0
7	B	2	Total 2	O 2	0	0

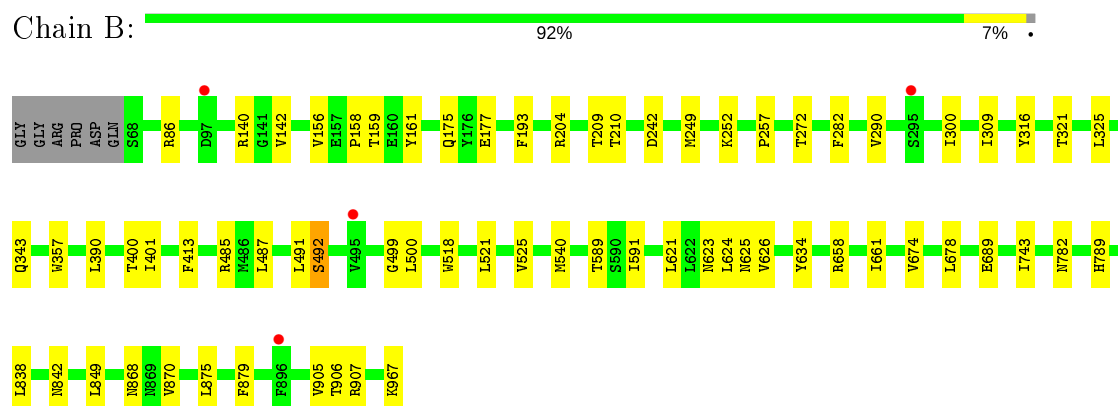
3 Residue-property plots [i](#)

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.

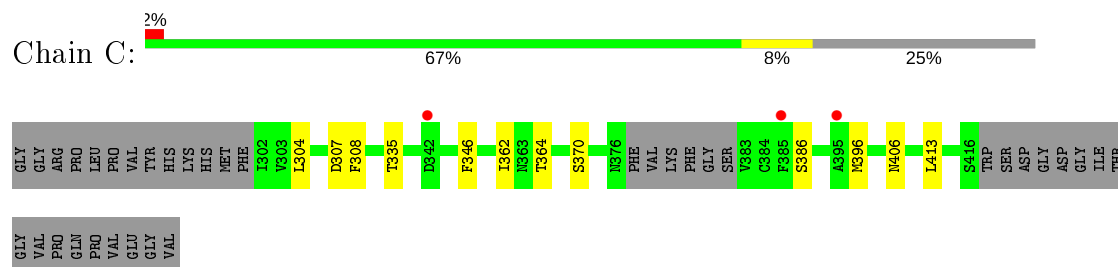
• Molecule 1: Aminopeptidase N



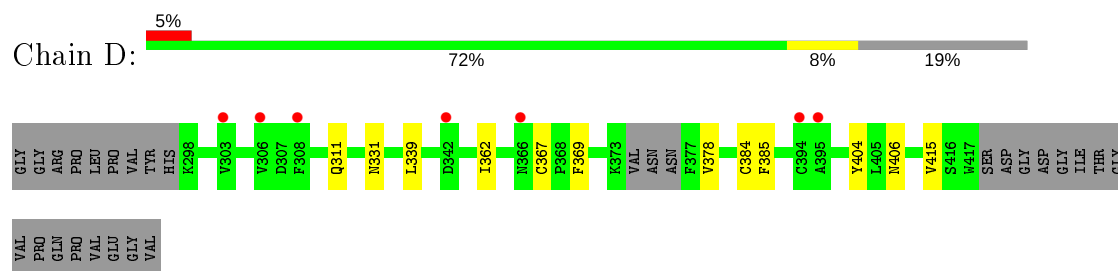
• Molecule 1: Aminopeptidase N



• Molecule 2: Spike glycoprotein



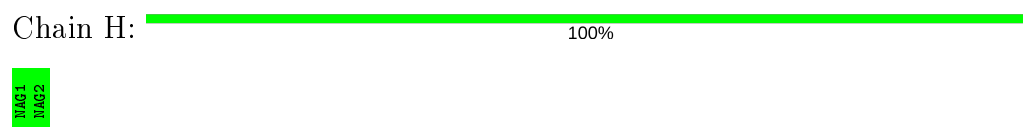
- Molecule 2: Spike glycoprotein



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



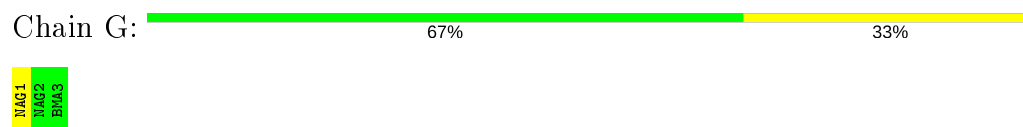
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.32Å 98.52Å 153.62Å 90.00° 104.44° 90.00°	Depositor
Resolution (Å)	48.09 – 3.00 48.09 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.09-3.00) 99.9 (48.09-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.16rc1_3535	Depositor
R, R_{free}	0.203 , 0.244 0.203 , 0.240	Depositor DCC
R_{free} test set	3189 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	84.2	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16543	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: ZN, BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/7452	0.41	0/10149
1	B	0.27	0/7452	0.43	0/10149
2	C	0.27	0/838	0.48	0/1140
2	D	0.26	0/910	0.45	0/1235
All	All	0.26	0/16652	0.42	0/22673

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	7264	0	7028	37	0
1	B	7264	0	7028	45	0
2	C	819	0	795	9	0
2	D	887	0	858	7	0
3	E	28	0	25	0	0
3	H	28	0	25	0	0
4	F	39	0	34	0	0
4	G	39	0	34	1	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
6	A	56	0	52	0	0
6	B	56	0	52	7	0
6	C	28	0	26	2	0
6	D	28	0	26	0	0
7	A	3	0	0	0	0
7	B	2	0	0	0	0
All	All	16543	0	15983	98	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 3.

All (98) 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:257:PRO:HD3	6:B:5010:NAG:H61	1.66	0.76
1:B:249:MET:HG2	1:B:272:THR:HG22	1.73	0.70
1:B:300:ILE:HD12	1:B:321:THR:HG22	1.76	0.67
1:B:316:TYR:HB2	6:B:5006:NAG:H81	1.75	0.67
1:A:258:LEU:HD12	1:A:259:PRO:HD2	1.77	0.67
2:C:364:THR:HG21	2:C:370:SER:HA	1.77	0.65
1:A:283:ILE:HD13	1:A:344:ILE:HD13	1.83	0.60
1:A:291:GLU:OE1	1:A:299:LEU:HD11	2.02	0.59
2:C:307:ASP:OD1	2:C:308:PHE:N	2.36	0.59
1:A:622:LEU:HB2	1:A:632:VAL:HG11	1.83	0.58
2:C:335:THR:HG21	6:C:2002:NAG:H62	1.86	0.58
1:B:591:ILE:CG2	1:B:624:LEU:HD12	2.35	0.56
1:B:674:VAL:HB	1:B:678:LEU:HD23	1.88	0.55
1:A:589:THR:O	1:A:623:ASN:N	2.40	0.55
1:A:838:LEU:HD23	1:B:870:VAL:HG22	1.88	0.55
1:A:348:ASP:OD2	1:A:855:ARG:NH1	2.41	0.54
1:B:499:GLY:HA3	1:B:521:LEU:HD23	1.89	0.54
1:B:621:LEU:HD23	1:B:634:TYR:OH	2.07	0.54
1:B:591:ILE:HG22	1:B:624:LEU:HD12	1.89	0.54
1:B:487:LEU:HD22	1:B:540:MET:HE2	1.90	0.54
1:A:870:VAL:HG22	1:B:838:LEU:HD23	1.89	0.54
1:A:140:ARG:NH2	1:A:177:GLU:OE1	2.43	0.52
1:B:316:TYR:HB2	6:B:5006:NAG:C8	2.40	0.52
1:B:838:LEU:HD11	1:B:875:LEU:HD13	1.92	0.51
2:C:362:ILE:HG23	2:C:362:ILE:O	2.10	0.51
1:B:842:ASN:CA	1:B:875:LEU:HD21	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:364:THR:HG22	2:C:396:MET:CE	2.40	0.51
1:B:325:LEU:HD13	1:B:390:LEU:HD13	1.93	0.51
1:A:887:LEU:HD23	1:A:887:LEU:O	2.11	0.51
1:A:400:THR:HG22	1:A:401:ILE:H	1.76	0.50
1:A:487:LEU:HD12	1:A:490:PHE:CE2	2.48	0.49
1:A:884:TRP:O	1:A:888:PHE:N	2.45	0.49
1:A:868:ASN:OD1	1:A:907:ARG:NH2	2.45	0.49
1:A:189:ASP:N	1:A:189:ASP:OD1	2.32	0.49
1:A:849:LEU:HD11	1:A:879:PHE:HZ	1.78	0.49
1:B:842:ASN:HA	1:B:875:LEU:HD21	1.94	0.49
1:B:316:TYR:N	6:B:5006:NAG:H82	2.28	0.48
1:B:209:THR:OG1	1:B:210:THR:N	2.46	0.48
2:C:335:THR:CG2	6:C:2002:NAG:H62	2.43	0.48
1:A:457:THR:HG22	1:A:458:PRO:HD2	1.96	0.48
1:B:290:VAL:HG13	1:B:309:ILE:HG23	1.95	0.48
1:B:487:LEU:HD22	1:B:540:MET:CE	2.44	0.47
1:A:255:SER:OG	1:A:267:THR:OG1	2.25	0.47
2:C:304:LEU:HD22	2:C:413:LEU:HD12	1.95	0.47
1:A:480:GLY:O	1:A:484:LEU:HD23	2.14	0.47
6:B:5006:NAG:O4	2:D:404:TYR:HB3	2.14	0.47
1:A:209:THR:OG1	1:A:210:THR:N	2.47	0.46
1:A:954:ASN:HA	1:A:957:VAL:HG12	1.97	0.46
1:B:868:ASN:OD1	1:B:907:ARG:NH2	2.48	0.46
1:B:400:THR:HG22	1:B:401:ILE:N	2.31	0.46
2:D:331:ASN:O	2:D:339:LEU:HD22	2.16	0.46
1:B:159:THR:HG1	1:B:161:TYR:HD2	1.61	0.46
2:D:362:ILE:O	2:D:362:ILE:HG23	2.16	0.45
1:A:555:ASP:O	1:A:559:GLY:N	2.49	0.45
1:B:621:LEU:HD11	1:B:661:ILE:HD11	1.98	0.45
1:B:485:ARG:NH2	1:B:626:VAL:O	2.48	0.45
1:B:491:LEU:O	1:B:492:SER:CB	2.64	0.45
1:B:142:VAL:HG23	1:B:175:GLN:HB2	1.99	0.45
2:D:311:GLN:N	2:D:311:GLN:OE1	2.50	0.45
1:B:413:PHE:CZ	1:B:500:LEU:HD11	2.52	0.44
2:C:364:THR:HG22	2:C:396:MET:HE2	1.98	0.44
1:A:870:VAL:HG13	1:A:871:ILE:CD1	2.48	0.44
1:B:242:ASP:N	1:B:242:ASP:OD1	2.51	0.44
1:B:413:PHE:HZ	1:B:500:LEU:HD11	1.83	0.44
1:A:491:LEU:O	1:A:492:SER:HB2	2.18	0.44
6:B:5002:NAG:O3	6:B:5002:NAG:O7	2.34	0.44
1:A:455:LEU:HD13	1:A:479:LYS:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:LEU:HD23	1:B:625:ASN:N	2.33	0.43
1:B:658:ARG:NH1	1:B:689:GLU:OE1	2.48	0.43
1:A:400:THR:HG22	1:A:401:ILE:N	2.32	0.43
1:A:707:LEU:HD13	1:A:907:ARG:HB3	2.00	0.43
1:A:743:ILE:HD13	1:A:789:HIS:CE1	2.54	0.43
6:B:5010:NAG:H83	6:B:5010:NAG:H2	1.68	0.43
1:B:487:LEU:HB2	1:B:540:MET:HE2	1.99	0.43
2:D:369:PHE:CE1	2:D:378:VAL:HG13	2.54	0.43
1:A:678:LEU:HD23	1:A:678:LEU:C	2.38	0.43
1:B:300:ILE:HD12	1:B:321:THR:CG2	2.46	0.43
1:B:743:ILE:HD13	1:B:789:HIS:CE1	2.54	0.42
1:A:237:LEU:HD12	1:A:269:PHE:CE1	2.55	0.42
1:A:887:LEU:HD23	1:A:887:LEU:C	2.40	0.42
1:A:366:SER:HB3	1:A:385:VAL:HG11	2.02	0.41
1:A:491:LEU:O	1:A:495:VAL:HB	2.20	0.41
1:A:743:ILE:HD12	1:A:750:GLN:OE1	2.20	0.41
1:B:849:LEU:HD11	1:B:879:PHE:CZ	2.55	0.41
1:B:156:VAL:HG12	1:B:158:PRO:HD2	2.02	0.41
1:B:589:THR:O	1:B:623:ASN:N	2.52	0.41
1:B:86:ARG:NH1	4:G:1:NAG:O7	2.54	0.41
1:A:870:VAL:HG13	1:A:871:ILE:HD12	2.01	0.41
1:B:905:VAL:HG13	1:B:906:THR:HG23	2.02	0.41
1:B:252:LYS:O	1:B:252:LYS:HG3	2.21	0.41
1:B:400:THR:HG22	1:B:401:ILE:H	1.85	0.41
2:D:385:PHE:CE1	2:D:415:VAL:HG21	2.56	0.40
2:D:384:CYS:O	2:D:415:VAL:HG23	2.21	0.40
1:A:148:PRO:HG2	1:A:166:LEU:HD13	2.03	0.40
1:B:491:LEU:HD22	1:B:525:VAL:HG22	2.02	0.40
2:C:364:THR:HG22	2:C:396:MET:HE1	2.04	0.40
1:A:959:LEU:HD23	1:A:959:LEU:O	2.22	0.40
1:B:140:ARG:NH2	1:B:177:GLU:OE1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	898/906 (99%)	869 (97%)	29 (3%)	0	100	100
1	B	898/906 (99%)	866 (96%)	31 (4%)	1 (0%)	51	85
2	C	105/145 (72%)	98 (93%)	7 (7%)	0	100	100
2	D	113/145 (78%)	103 (91%)	10 (9%)	0	100	100
All	All	2014/2102 (96%)	1936 (96%)	77 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	492	SER

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	798/802 (100%)	789 (99%)	9 (1%)	73	90
1	B	798/802 (100%)	790 (99%)	8 (1%)	76	91
2	C	90/121 (74%)	87 (97%)	3 (3%)	38	73
2	D	96/121 (79%)	94 (98%)	2 (2%)	53	82
All	All	1782/1846 (96%)	1760 (99%)	22 (1%)	71	90

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	282	PHE
1	A	340	LYS
1	A	357	TRP
1	A	442	ARG
1	A	490	PHE
1	A	565	HIS
1	A	573	ASN

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Mol	Chain	Res	Type
1	A	576	ARG
1	A	842	ASN
1	B	193	PHE
1	B	204	ARG
1	B	282	PHE
1	B	343	GLN
1	B	357	TRP
1	B	518	TRP
1	B	782	ASN
1	B	967	LYS
2	C	346	PHE
2	C	386	SER
2	C	406	ASN
2	D	367	CYS
2	D	406	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	HIS

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 ⓘ

10 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	0.52	0	17,19,21	0.81	1 (5%)
3	NAG	E	2	3	14,14,15	0.36	0	17,19,21	0.81	0
4	NAG	F	1	1,4	14,14,15	0.41	0	17,19,21	0.85	1 (5%)
4	NAG	F	2	4	14,14,15	0.49	0	17,19,21	1.76	4 (23%)
4	BMA	F	3	4	11,11,12	0.30	0	15,15,17	0.77	0
4	NAG	G	1	1,4	14,14,15	0.37	0	17,19,21	0.92	0
4	NAG	G	2	4	14,14,15	0.36	0	17,19,21	0.75	0
4	BMA	G	3	4	11,11,12	0.29	0	15,15,17	0.71	0
3	NAG	H	1	1,3	14,14,15	0.34	0	17,19,21	0.63	0
3	NAG	H	2	3	14,14,15	0.30	0	17,19,21	0.73	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	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	2	NAG	C3-C4-C5	4.01	117.40	110.24
4	F	2	NAG	C4-C3-C2	3.40	116.00	111.02
4	F	2	NAG	O5-C1-C2	-3.17	106.29	111.29
4	F	2	NAG	C1-O5-C5	-2.78	108.43	112.19
4	F	1	NAG	O5-C1-C2	-2.37	107.55	111.29
3	E	1	NAG	O5-C1-C2	-2.19	107.83	111.29

There are no chirality outliers.

All (19) torsion outliers are listed below:

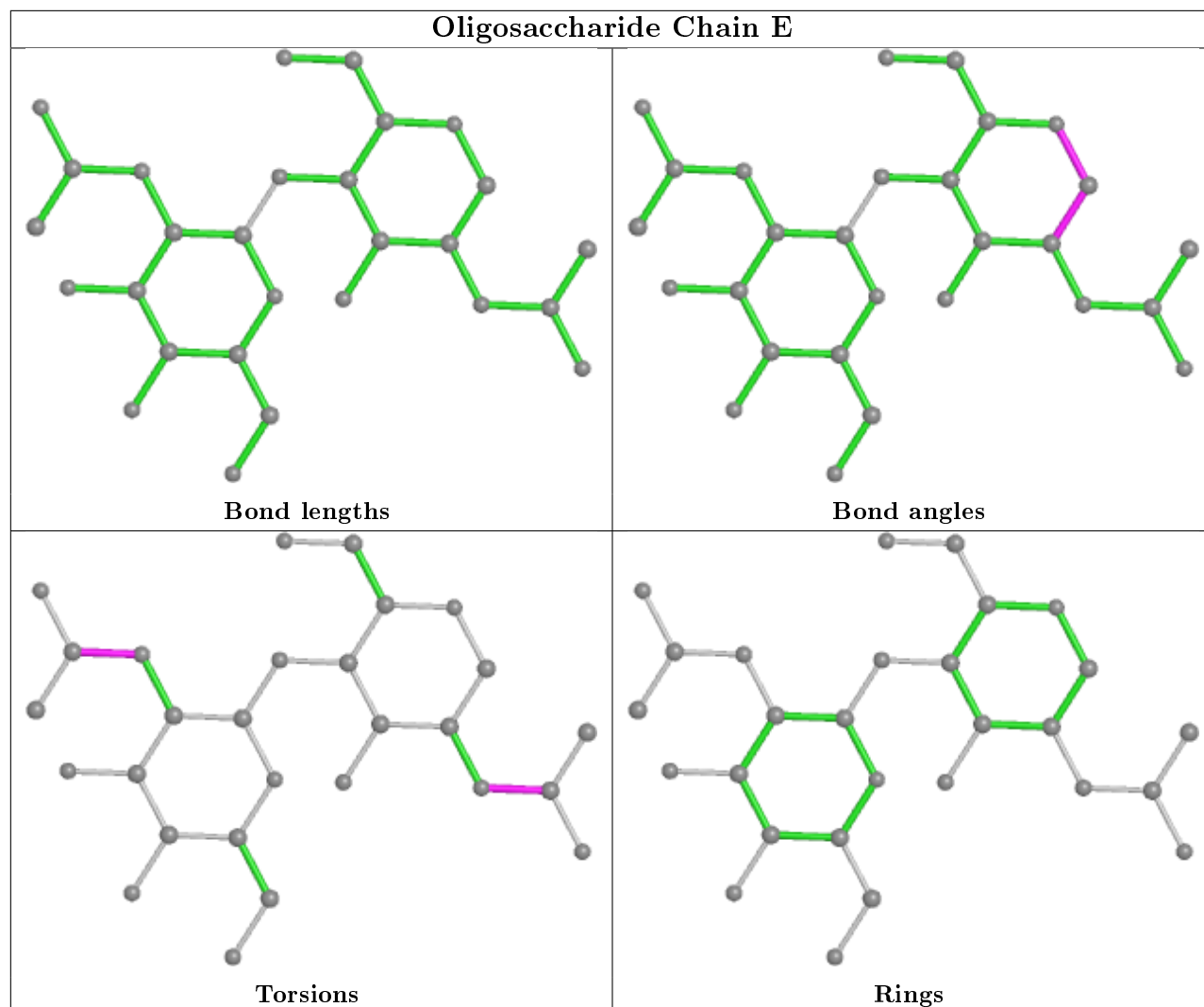
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
3	H	2	NAG	O5-C5-C6-O6
4	G	1	NAG	C8-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	H	2	NAG	C4-C5-C6-O6
4	G	1	NAG	O7-C7-N2-C2
4	G	3	BMA	C4-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6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

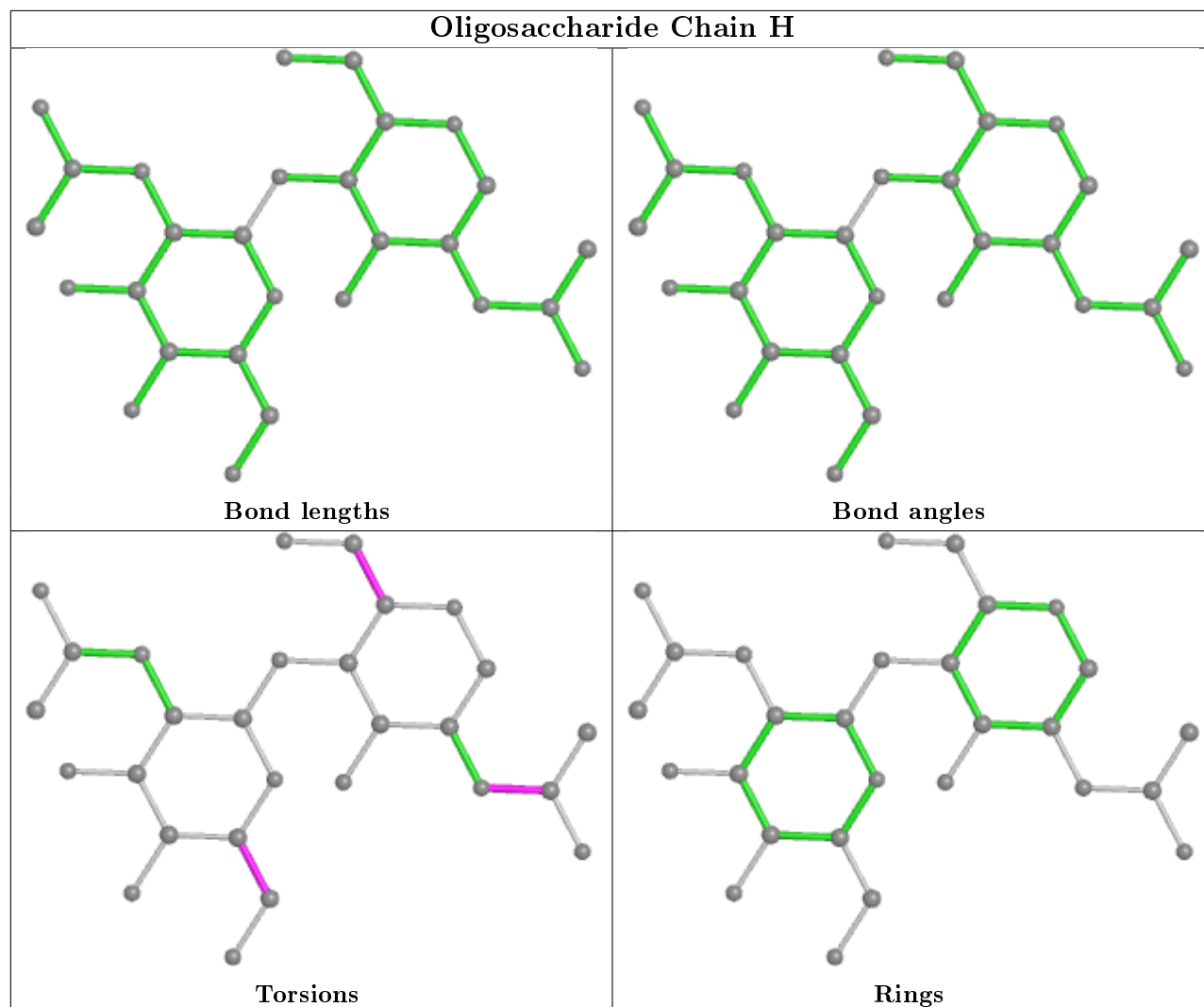
There are no ring outliers.

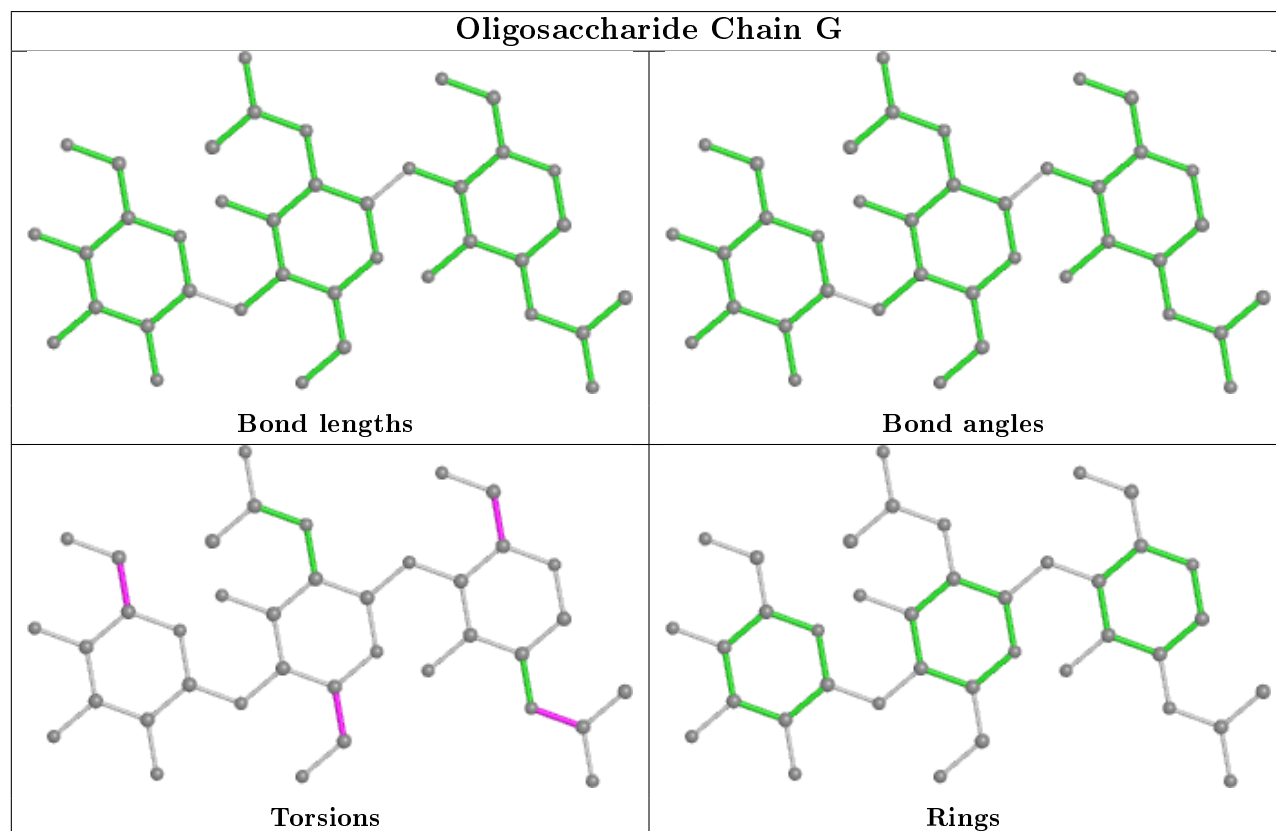
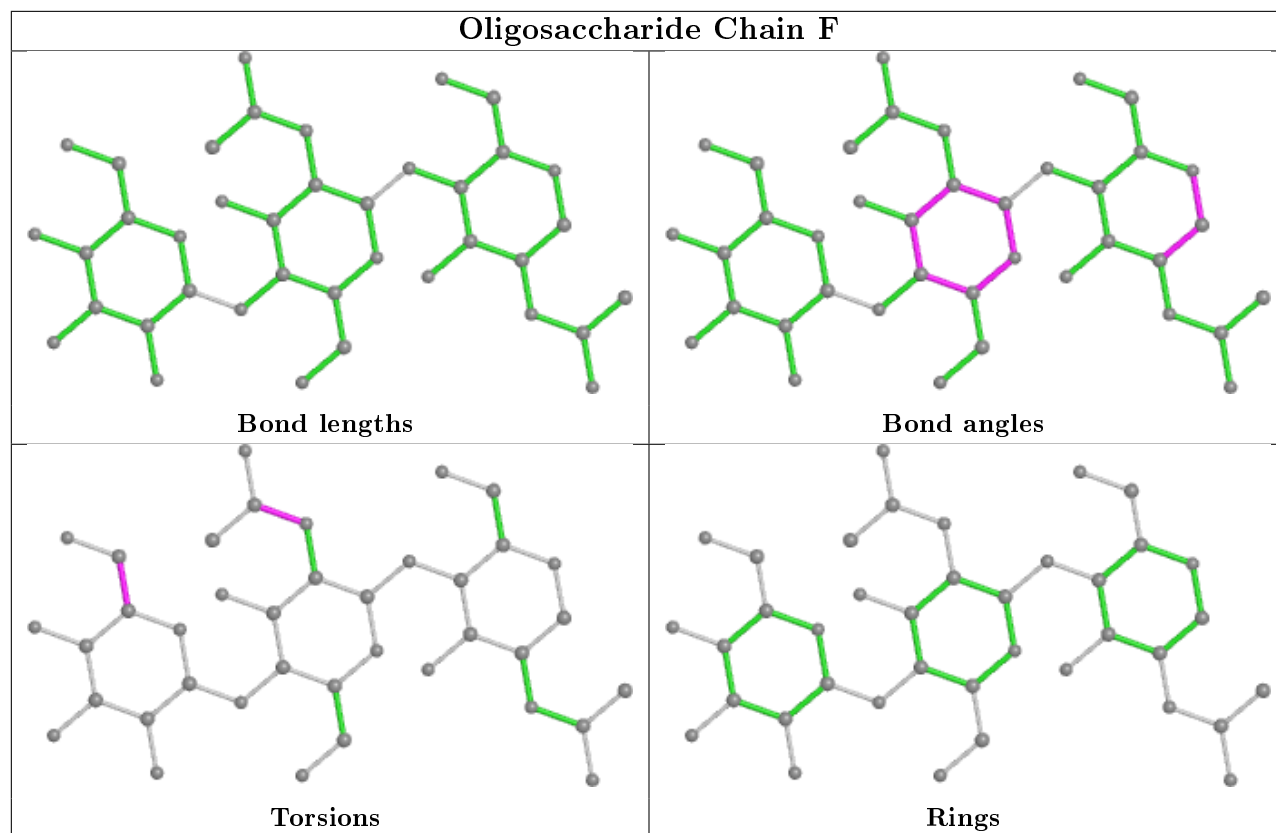
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	1	0

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







5.6 Ligand geometry

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	A	5007	1	14,14,15	0.41	0	17,19,21	1.07	1 (5%)
6	NAG	A	5003	1	14,14,15	0.44	0	17,19,21	0.78	0
6	NAG	B	5010	1	14,14,15	0.88	0	17,19,21	1.87	4 (23%)
6	NAG	C	2001	2	14,14,15	0.51	0	17,19,21	1.16	2 (11%)
6	NAG	A	5002	1	14,14,15	0.55	0	17,19,21	0.92	1 (5%)
6	NAG	C	2002	2	14,14,15	0.30	0	17,19,21	0.64	0
6	NAG	B	5006	1	14,14,15	0.36	0	17,19,21	0.70	0
6	NAG	B	5009	1	14,14,15	0.36	0	17,19,21	0.73	0
6	NAG	A	5004	1	14,14,15	0.54	0	17,19,21	0.90	1 (5%)
6	NAG	D	2001	2	14,14,15	0.29	0	17,19,21	0.62	0
6	NAG	D	2002	2	14,14,15	0.28	0	17,19,21	0.75	0
6	NAG	B	5002	1	14,14,15	0.19	0	17,19,21	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	5007	1	-	4/6/23/26	0/1/1/1
6	NAG	A	5003	1	-	2/6/23/26	0/1/1/1
6	NAG	B	5010	1	-	4/6/23/26	0/1/1/1
6	NAG	C	2001	2	-	4/6/23/26	0/1/1/1
6	NAG	A	5002	1	-	0/6/23/26	0/1/1/1
6	NAG	C	2002	2	-	0/6/23/26	0/1/1/1
6	NAG	B	5006	1	-	0/6/23/26	0/1/1/1
6	NAG	B	5009	1	-	4/6/23/26	0/1/1/1
6	NAG	A	5004	1	-	4/6/23/26	0/1/1/1
6	NAG	D	2001	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	D	2002	2	-	3/6/23/26	0/1/1/1
6	NAG	B	5002	1	-	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(°)
6	B	5010	NAG	C2-N2-C7	-4.21	116.90	122.90
6	B	5010	NAG	O5-C1-C2	-3.56	105.67	111.29
6	B	5010	NAG	C1-O5-C5	-3.46	107.50	112.19
6	C	2001	NAG	C2-N2-C7	-2.78	118.94	122.90
6	A	5007	NAG	O5-C1-C2	-2.75	106.94	111.29
6	B	5010	NAG	C1-C2-N2	-2.35	106.48	110.49
6	A	5002	NAG	C4-C3-C2	-2.34	107.58	111.02
6	C	2001	NAG	C4-C3-C2	-2.29	107.67	111.02
6	A	5004	NAG	O5-C5-C6	2.16	110.59	107.20

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	5010	NAG	C8-C7-N2-C2
6	B	5010	NAG	O7-C7-N2-C2
6	C	2001	NAG	C8-C7-N2-C2
6	C	2001	NAG	O7-C7-N2-C2
6	A	5004	NAG	C8-C7-N2-C2
6	A	5004	NAG	O7-C7-N2-C2
6	A	5007	NAG	C8-C7-N2-C2
6	C	2001	NAG	O5-C5-C6-O6
6	B	5010	NAG	O5-C5-C6-O6
6	A	5007	NAG	O7-C7-N2-C2
6	B	5010	NAG	C4-C5-C6-O6
6	B	5002	NAG	O5-C5-C6-O6
6	A	5004	NAG	O5-C5-C6-O6
6	A	5007	NAG	O5-C5-C6-O6
6	B	5002	NAG	C4-C5-C6-O6
6	A	5003	NAG	O5-C5-C6-O6
6	B	5002	NAG	C1-C2-N2-C7
6	A	5003	NAG	C4-C5-C6-O6
6	A	5004	NAG	C4-C5-C6-O6
6	D	2001	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	D	2001	NAG	C4-C5-C6-O6
6	B	5009	NAG	C8-C7-N2-C2
6	C	2001	NAG	C4-C5-C6-O6
6	B	5009	NAG	O7-C7-N2-C2
6	D	2002	NAG	C8-C7-N2-C2
6	B	5009	NAG	C4-C5-C6-O6
6	B	5009	NAG	O5-C5-C6-O6
6	D	2002	NAG	C4-C5-C6-O6
6	B	5002	NAG	C3-C2-N2-C7
6	D	2002	NAG	O7-C7-N2-C2
6	A	5007	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	5010	NAG	2	0
6	C	2002	NAG	2	0
6	B	5006	NAG	4	0
6	B	5002	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, 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	900/906 (99%)	-0.28	2 (0%) 95 87	54, 89, 131, 169	0
1	B	900/906 (99%)	-0.31	4 (0%) 92 79	58, 92, 126, 165	0
2	C	109/145 (75%)	0.00	3 (2%) 53 25	70, 108, 168, 222	0
2	D	117/145 (80%)	0.60	7 (5%) 21 7	100, 143, 192, 201	0
All	All	2026/2102 (96%)	-0.23	16 (0%) 86 65	54, 93, 144, 222	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	395	ALA	3.7
2	D	394	CYS	3.2
1	B	295	SER	3.0
2	C	342	ASP	3.0
1	B	896	PHE	3.0
2	C	385	PHE	2.8
1	B	495	VAL	2.5
1	A	893	GLY	2.4
2	D	395	ALA	2.4
2	D	308	PHE	2.3
1	B	97	ASP	2.2
2	D	306	VAL	2.2
1	A	442	ARG	2.2
2	D	342	ASP	2.1
2	D	366	ASN	2.1
2	D	303	VAL	2.0

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

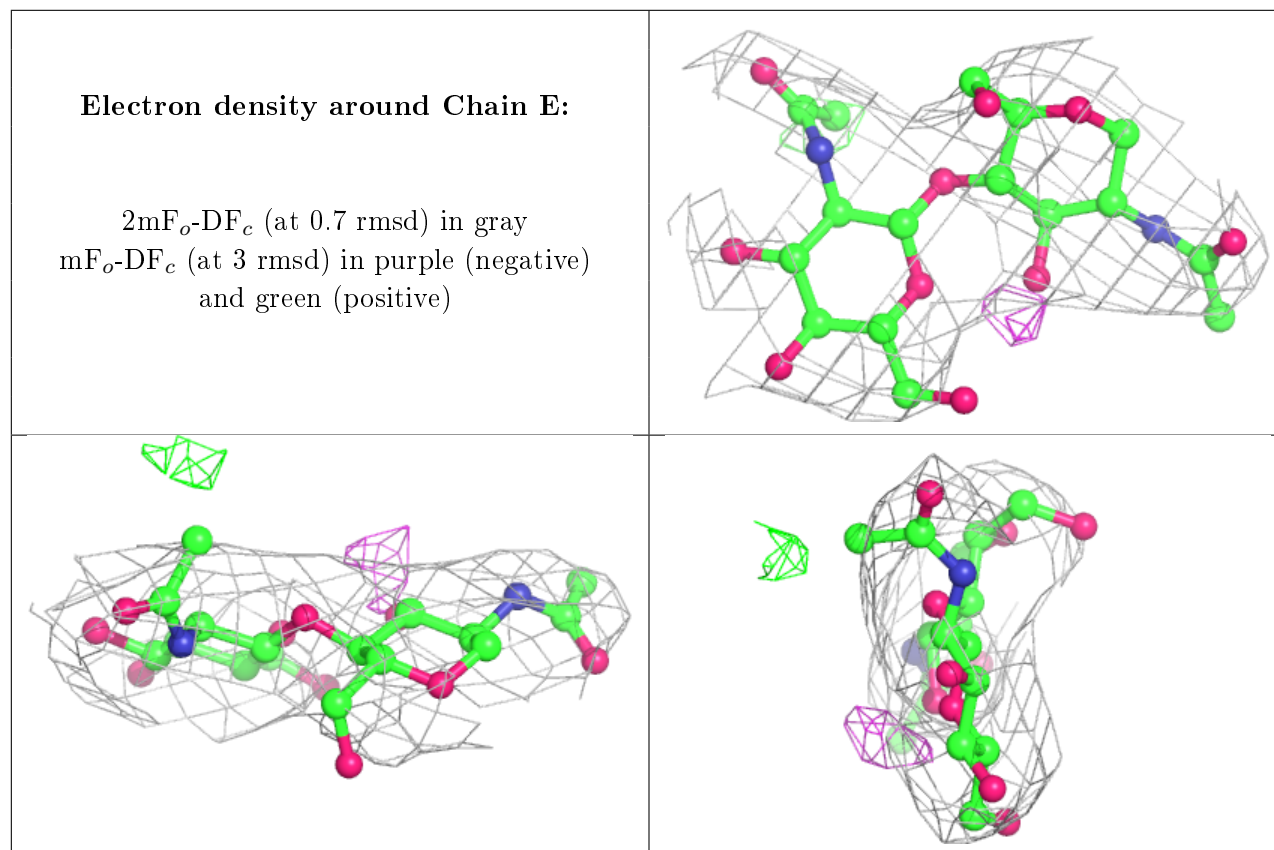
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.

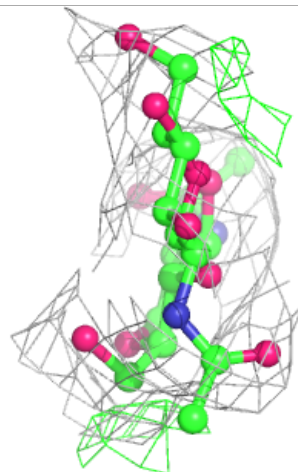
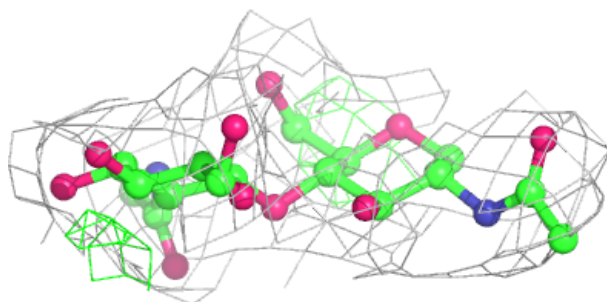
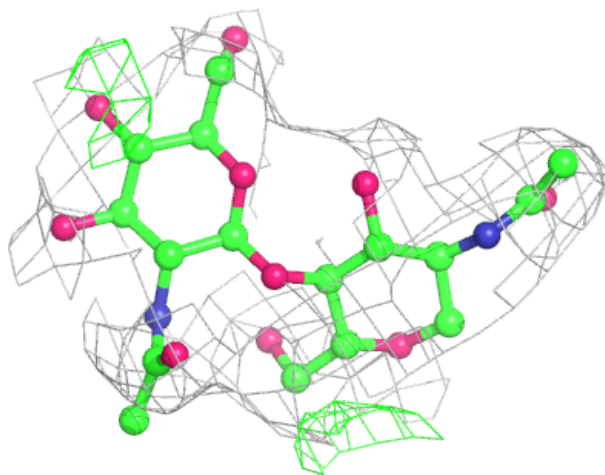
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	F	3	11/12	0.41	0.36	164,168,170,171	0
4	NAG	F	2	14/15	0.73	0.38	166,174,177,179	0
4	BMA	G	3	11/12	0.73	0.30	133,134,137,139	0
4	NAG	G	2	14/15	0.88	0.22	121,125,127,131	0
4	NAG	F	1	14/15	0.89	0.15	108,119,130,145	0
3	NAG	H	2	14/15	0.91	0.12	147,152,155,156	0
3	NAG	H	1	14/15	0.93	0.09	107,110,120,132	0
3	NAG	E	2	14/15	0.94	0.12	136,143,147,148	0
4	NAG	G	1	14/15	0.95	0.10	98,104,112,115	0
3	NAG	E	1	14/15	0.96	0.14	104,106,114,122	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.



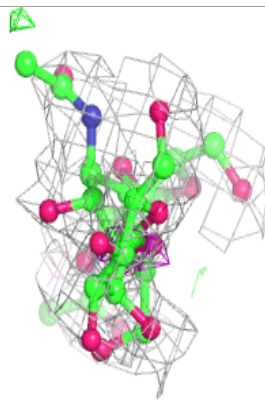
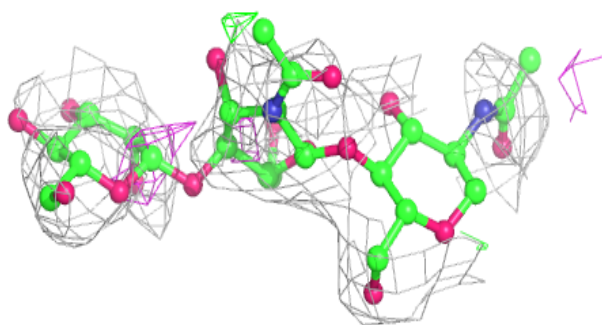
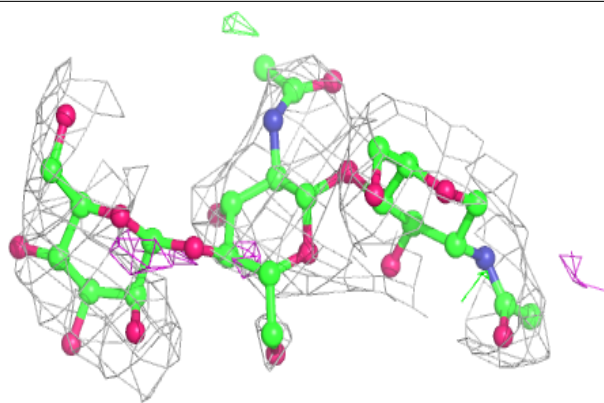
Electron density around Chain H:

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

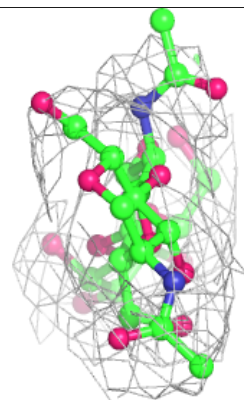
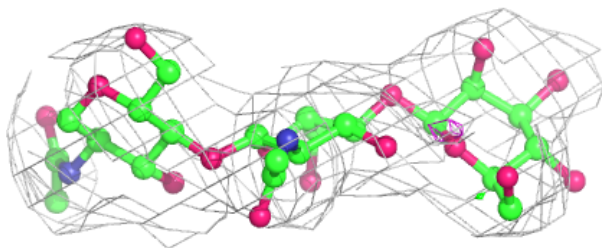
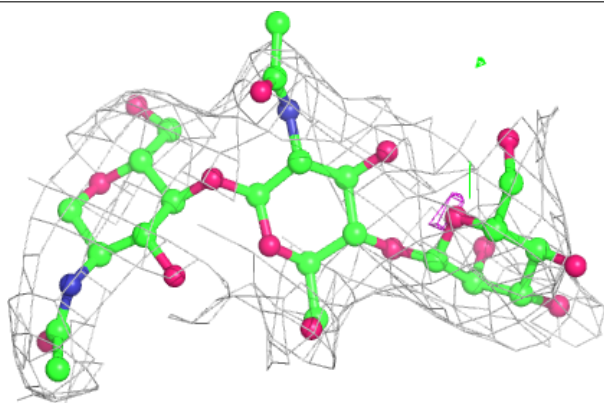


Electron density around Chain F:

$2mF_o-DF_c$ (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)



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, 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
6	NAG	D	2002	14/15	0.81	0.37	129,138,143,144	0
6	NAG	B	5010	14/15	0.85	0.17	144,151,155,156	0
6	NAG	A	5007	14/15	0.87	0.19	120,130,133,134	0
6	NAG	C	2002	14/15	0.90	0.23	93,111,121,123	0
6	NAG	A	5003	14/15	0.92	0.09	99,106,108,109	0
6	NAG	B	5009	14/15	0.93	0.13	118,123,127,127	0
6	NAG	B	5002	14/15	0.93	0.19	98,101,105,107	0
6	NAG	D	2001	14/15	0.93	0.36	144,148,153,154	0
6	NAG	C	2001	14/15	0.94	0.13	111,117,120,123	0
6	NAG	B	5006	14/15	0.94	0.17	106,117,123,125	0
6	NAG	A	5004	14/15	0.95	0.16	89,95,99,102	0
6	NAG	A	5002	14/15	0.97	0.13	73,75,80,84	0
5	ZN	A	5001	1/1	0.98	0.28	85,85,85,85	0
5	ZN	B	5001	1/1	0.98	0.25	81,81,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.