



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:26 PM UTC

PDB ID : 6U7G / pdb_00006u7g
Title : HCoV-229E RBD Class V in complex with human APN
Authors : Tomlinson, A.; Li, Z.; Rini, J.M.
Deposited on : 2019-09-02
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

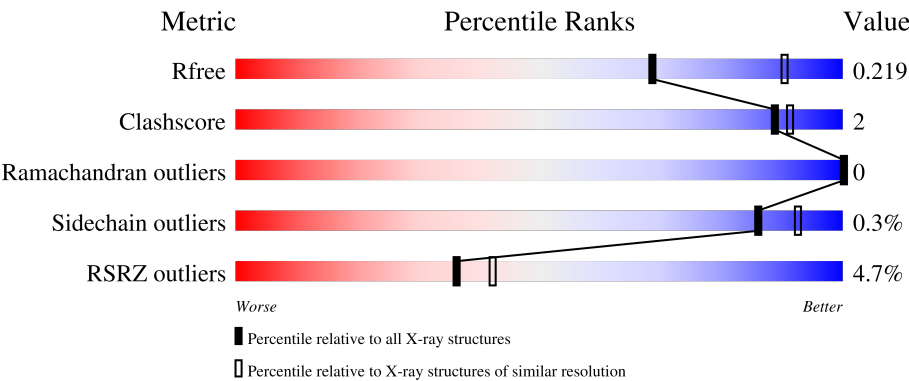
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	906	2% 95% 2% 1% 1%
1	B	906	2% 95% 2% 1% 1%
2	C	145	19% 78% 1% 1% 18%
2	D	145	18% 68% 8% 1% 23%
3	E	2	100%

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Mol	Chain	Length	Quality of chain
3	F	2	 50%50%
3	G	2	 100%
3	H	2	 50%50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 33302 atoms, of which 15945 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	898	Total	C	H	N	O	S	0	0	0
			14262	4623	7012	1223	1380	24			
1	B	899	Total	C	H	N	O	S	0	0	0
			14297	4634	7030	1225	1384	24			

There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Spike protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	119	Total	C	H	N	O	S	0	0	0
			1759	579	857	155	159	9			
2	D	111	Total	C	H	N	O	S	0	0	0
			1650	537	809	146	150	8			

There are 16 discrepancies between the modelled and reference sequences:

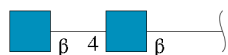
Chain	Residue	Modelled	Actual	Comment	Reference
C	289	GLY	-	cloning artifact	UNP H1AG31
C	290	GLY	-	cloning artifact	UNP H1AG31
C	291	ARG	-	cloning artifact	UNP H1AG31
C	292	PRO	-	cloning artifact	UNP H1AG31

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Chain	Residue	Modelled	Actual	Comment	Reference
C	300	MET	THR	conflict	UNP H1AG31
C	412	THR	SER	conflict	UNP H1AG31
C	422	GLY	VAL	conflict	UNP H1AG31
C	428	GLN	LYS	conflict	UNP H1AG31
D	289	GLY	-	cloning artifact	UNP H1AG31
D	290	GLY	-	cloning artifact	UNP H1AG31
D	291	ARG	-	cloning artifact	UNP H1AG31
D	292	PRO	-	cloning artifact	UNP H1AG31
D	300	MET	THR	conflict	UNP H1AG31
D	412	THR	SER	conflict	UNP H1AG31
D	422	GLY	VAL	conflict	UNP H1AG31
D	428	GLN	LYS	conflict	UNP H1AG31

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

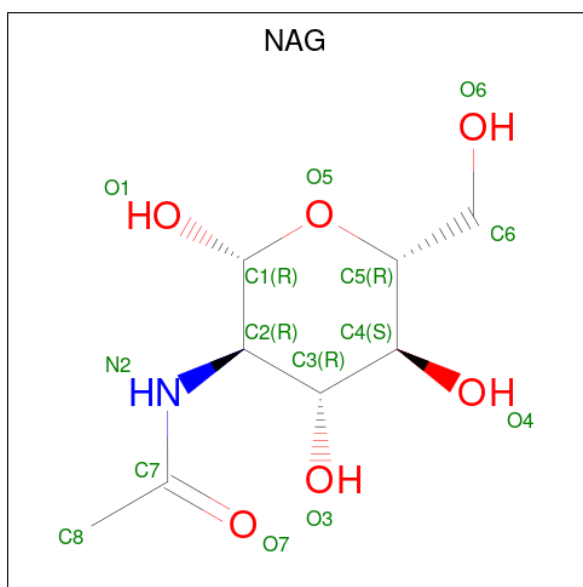


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	H	N	O	0	0
			56	16	28	2	10		
3	F	2	Total	C	H	N	O	0	0
			56	16	28	2	10		
3	G	2	Total	C	H	N	O	0	0
			56	16	28	2	10		
3	H	2	Total	C	N	O		0	0
			28	16	2	10			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	A	1	Total	C	N	O		0	0
			14	8	1	5			
5	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	B	1	Total	C	N	O		0	0
			14	8	1	5			
5	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

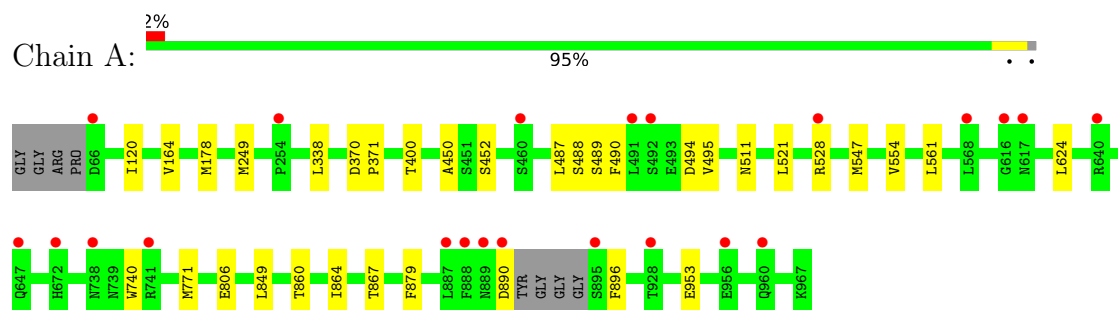
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	403	Total 403	O 403	0	0
6	B	350	Total 350	O 350	0	0
6	C	36	Total 36	O 36	0	0
6	D	12	Total 12	O 12	0	0

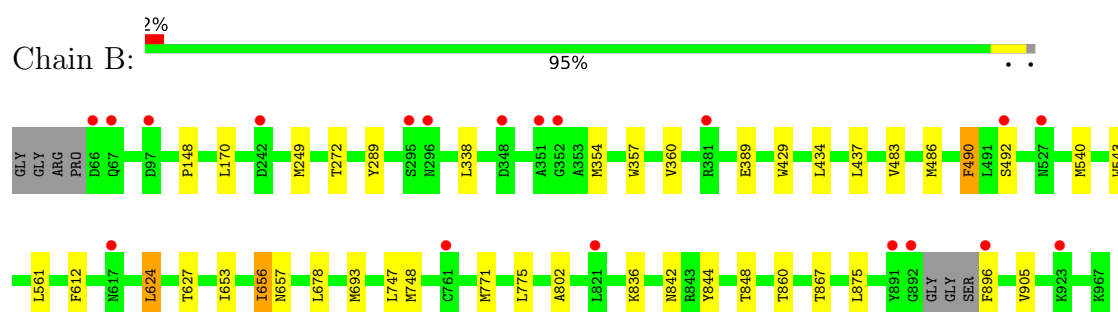
3 Residue-property plots [i](#)

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.

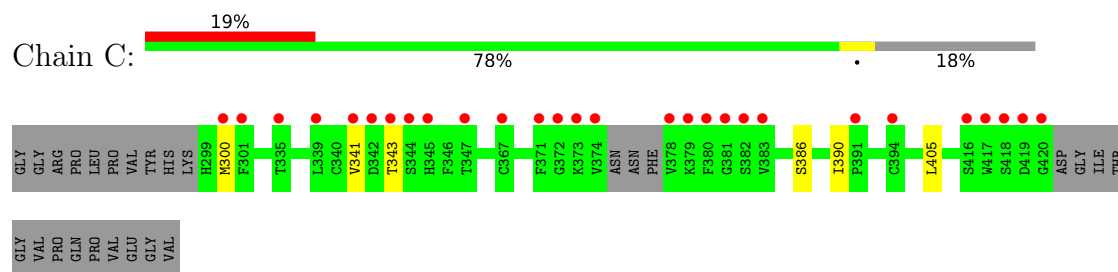
• Molecule 1: Aminopeptidase N



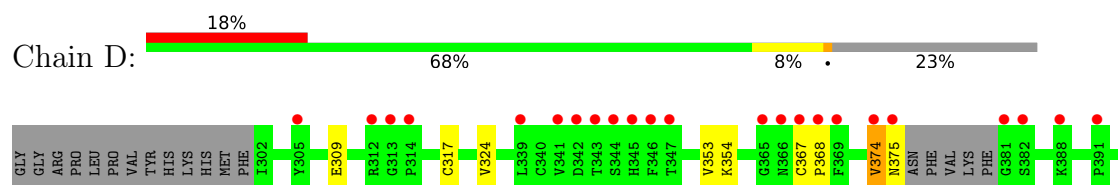
• Molecule 1: Aminopeptidase N

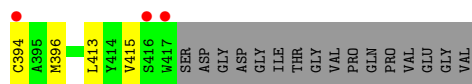


• Molecule 2: Spike protein



• Molecule 2: Spike protein





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

Chain E:  100%



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

Chain F:  50% 50%



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

Chain G:  100%



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

Chain H:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.56Å 98.68Å 147.53Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	45.61 – 2.35 45.61 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.0 (45.61-2.35) 96.1 (45.61-2.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.16rc1_3535	Depositor
R, R_{free}	0.179 , 0.218 0.180 , 0.219	Depositor DCC
R_{free} test set	5552 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.7	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	0.94	EDS
Total number of atoms	33302	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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, 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	0.27	2/7436 (0.0%)	0.37	2/10127 (0.0%)
1	B	0.32	3/7454 (0.0%)	0.44	2/10151 (0.0%)
2	C	0.22	0/925	0.45	0/1257
2	D	0.30	0/861	0.47	0/1171
All	All	0.30	5/16676 (0.0%)	0.41	4/22706 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	371	PRO	C-O	-6.83	1.15	1.24
1	A	370	ASP	C-O	-5.67	1.17	1.24
1	B	653	ILE	C-O	-5.32	1.17	1.24
1	B	657	ASN	C-O	-5.13	1.17	1.24
1	B	656	ILE	C-O	-5.05	1.18	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	627	THR	N-CA-C	-5.90	104.97	111.82
1	A	490	PHE	CB-CA-C	5.87	120.17	110.90
1	B	490	PHE	CA-CB-CG	5.36	119.16	113.80
1	A	490	PHE	CA-CB-CG	5.07	118.87	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7250	7012	7011	24	0
1	B	7267	7030	7028	23	0
2	C	902	857	857	4	0
2	D	841	809	811	10	0
3	E	28	28	25	0	0
3	F	28	28	25	2	0
3	G	28	28	25	0	0
3	H	28	0	24	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	70	55	65	1	0
5	B	56	42	52	1	0
5	C	28	28	26	0	0
5	D	28	28	26	0	0
6	A	403	0	0	2	0
6	B	350	0	0	0	0
6	C	36	0	0	0	0
6	D	12	0	0	0	0
All	All	17357	15945	15975	61	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 2.

All (61) 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:624:LEU:HD21	3:F:1:NAG:H82	1.65	0.78
5:A:5010:NAG:O3	5:A:5010:NAG:H82	1.86	0.74
2:D:396:MET:HE2	2:D:413:LEU:HD12	1.78	0.65
1:B:747:LEU:HD23	1:B:748:MET:CE	2.28	0.63
1:B:656:ILE:HG12	1:B:693:MET:HE1	1.82	0.61
2:D:309:GLU:HB2	2:D:324:VAL:HG22	1.84	0.60
1:B:842:ASN:HA	1:B:875:LEU:HD21	1.83	0.59
1:A:164:VAL:HG21	1:A:178:MET:HE2	1.83	0.59
1:A:554:VAL:HG22	1:A:561:LEU:HD22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:ASP:N	1:A:890:ASP:OD1	2.39	0.55
2:C:341:VAL:HG22	2:C:343:THR:OG1	2.06	0.55
2:D:394:CYS:SG	2:D:415:VAL:HB	2.47	0.55
1:A:450:ALA:O	1:A:547:MET:HE1	2.09	0.53
1:A:120:ILE:HG21	1:A:178:MET:HE3	1.91	0.53
2:C:300:MET:HE2	2:C:343:THR:HG23	1.91	0.53
1:B:624:LEU:HD22	3:H:1:NAG:H82	1.90	0.52
1:B:354:MET:O	1:B:360:VAL:HG13	2.10	0.52
1:A:554:VAL:HG22	1:A:561:LEU:CD2	2.40	0.51
2:D:367:CYS:CB	2:D:394:CYS:SG	2.99	0.50
1:A:740:TRP:CE2	1:A:771:MET:HE2	2.48	0.49
2:D:367:CYS:SG	2:D:368:PRO:HD2	2.53	0.48
2:C:386:SER:HB3	2:C:390:ILE:HD11	1.95	0.48
1:A:452:SER:HB3	1:A:547:MET:HE3	1.96	0.48
1:B:844:TYR:O	1:B:848:THR:HG23	2.14	0.47
1:B:747:LEU:HD23	1:B:748:MET:HE3	1.95	0.47
1:B:561:LEU:HD11	1:B:612:PHE:CE2	2.49	0.47
1:A:860:THR:HG22	1:A:896:PHE:CE1	2.51	0.46
1:A:864:ILE:O	1:A:867:THR:HG22	2.15	0.46
1:B:867:THR:HG21	1:B:905:VAL:HA	1.99	0.45
1:B:437:LEU:HD11	1:B:693:MET:HG2	1.98	0.45
2:D:353:VAL:HG22	2:D:354:LYS:N	2.32	0.45
1:B:148:PRO:HD2	1:B:170:LEU:HD23	1.98	0.45
1:B:771:MET:SD	1:B:775:LEU:HD12	2.57	0.45
2:D:396:MET:CE	2:D:413:LEU:HD12	2.47	0.45
1:A:249:MET:HE1	1:A:338:LEU:HG	1.98	0.44
1:A:494:ASP:OD1	1:A:528:ARG:NH2	2.48	0.44
1:B:249:MET:HG2	1:B:272:THR:HG22	1.99	0.44
1:A:806:GLU:OE1	6:A:5101:HOH:O	2.20	0.44
1:A:864:ILE:HA	1:A:867:THR:HG22	2.00	0.44
1:B:483:VAL:HG13	1:B:540:MET:HE1	1.99	0.44
1:A:860:THR:HG23	6:A:5212:HOH:O	2.17	0.44
1:B:486:MET:HE1	1:B:543:TRP:CD2	2.53	0.43
1:B:678:LEU:HB2	5:B:5009:NAG:H82	2.01	0.43
1:B:434:LEU:HD11	1:B:748:MET:HE1	2.00	0.43
1:B:860:THR:HG23	1:B:896:PHE:CD1	2.53	0.43
1:A:487:LEU:HD21	1:A:521:LEU:CD1	2.49	0.43
2:D:374:VAL:O	2:D:375:ASN:HB3	2.19	0.42
1:B:360:VAL:HG11	1:B:389:GLU:HB3	2.02	0.42
1:B:429:TRP:CD2	1:B:747:LEU:HD22	2.54	0.42
1:A:495:VAL:HG22	1:A:528:ARG:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:367:CYS:HB2	2:D:394:CYS:SG	2.60	0.42
1:A:488:SER:O	1:A:488:SER:OG	2.37	0.42
1:A:120:ILE:HG21	1:A:178:MET:CE	2.50	0.41
1:A:849:LEU:HD11	1:A:879:PHE:CZ	2.56	0.41
1:A:860:THR:HG22	1:A:896:PHE:CD1	2.56	0.41
1:A:624:LEU:CD2	3:F:1:NAG:H82	2.42	0.41
1:B:338:LEU:HD11	1:B:357:TRP:CD1	2.55	0.41
1:A:400:THR:O	1:A:511:ASN:HA	2.20	0.40
1:B:802:ALA:O	1:B:836:LYS:HD2	2.21	0.40
2:C:405:LEU:HD12	2:C:405:LEU:HA	1.90	0.40
1:B:289:TYR:CZ	2:D:317:CYS:HB2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	894/906 (99%)	875 (98%)	19 (2%)	0	100	100
1	B	895/906 (99%)	876 (98%)	19 (2%)	0	100	100
2	C	115/145 (79%)	108 (94%)	7 (6%)	0	100	100
2	D	107/145 (74%)	104 (97%)	3 (3%)	0	100	100
All	All	2011/2102 (96%)	1963 (98%)	48 (2%)	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	797/802 (99%)	795 (100%)	2 (0%)	86	92
1	B	799/802 (100%)	796 (100%)	3 (0%)	84	91
2	C	97/123 (79%)	97 (100%)	0	100	100
2	D	92/123 (75%)	91 (99%)	1 (1%)	65	79
All	All	1785/1850 (96%)	1779 (100%)	6 (0%)	86	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	489	SER
1	A	953	GLU
1	B	490	PHE
1	B	492	SER
1	B	624	LEU
2	D	374	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	HIS
1	A	596	GLN
1	A	643	GLN
1	A	732	HIS
1	A	883	ASN
1	B	146	GLN
1	B	202	ASN
1	B	510	GLN
1	B	650	HIS
1	B	881	GLN
1	B	883	ASN
1	B	939	GLN
1	B	965	ASN
2	C	401	ASN
2	C	409	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 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	0.21	0	17,19,21	0.45	0
3	NAG	E	2	3	14,14,15	0.19	0	17,19,21	0.46	0
3	NAG	F	1	1,3	14,14,15	0.16	0	17,19,21	0.49	0
3	NAG	F	2	3	14,14,15	0.23	0	17,19,21	0.40	0
3	NAG	G	1	1,3	14,14,15	0.25	0	17,19,21	0.40	0
3	NAG	G	2	3	14,14,15	0.25	0	17,19,21	0.39	0
3	NAG	H	1	1,3	14,14,15	2.23	4 (28%)	17,19,21	2.03	7 (41%)
3	NAG	H	2	3	14,14,15	1.22	1 (7%)	17,19,21	1.75	6 (35%)

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	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	NAG	O5-C1	-4.50	1.36	1.43
3	H	1	NAG	C1-C2	3.92	1.57	1.52
3	H	1	NAG	O5-C5	-3.34	1.36	1.43
3	H	2	NAG	O5-C1	-3.16	1.38	1.43
3	H	1	NAG	O7-C7	-2.22	1.18	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	O3-C3-C4	-4.08	100.76	110.38
3	H	2	NAG	C2-N2-C7	-3.41	118.33	122.90
3	H	1	NAG	O4-C4-C3	-3.34	102.50	110.38
3	H	2	NAG	O5-C1-C2	-3.14	106.44	111.29
3	H	2	NAG	C4-C3-C2	-2.95	106.70	111.02
3	H	1	NAG	C2-N2-C7	-2.69	119.29	122.90
3	H	1	NAG	O3-C3-C2	-2.54	104.12	109.40
3	H	1	NAG	C1-C2-N2	-2.45	106.58	110.43
3	H	1	NAG	C4-C3-C2	-2.44	107.44	111.02
3	H	2	NAG	C3-C4-C5	-2.38	105.91	110.23
3	H	2	NAG	O5-C5-C4	-2.16	105.56	110.83
3	H	1	NAG	O5-C5-C6	-2.10	103.58	107.66
3	H	2	NAG	C1-O5-C5	2.07	114.96	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6

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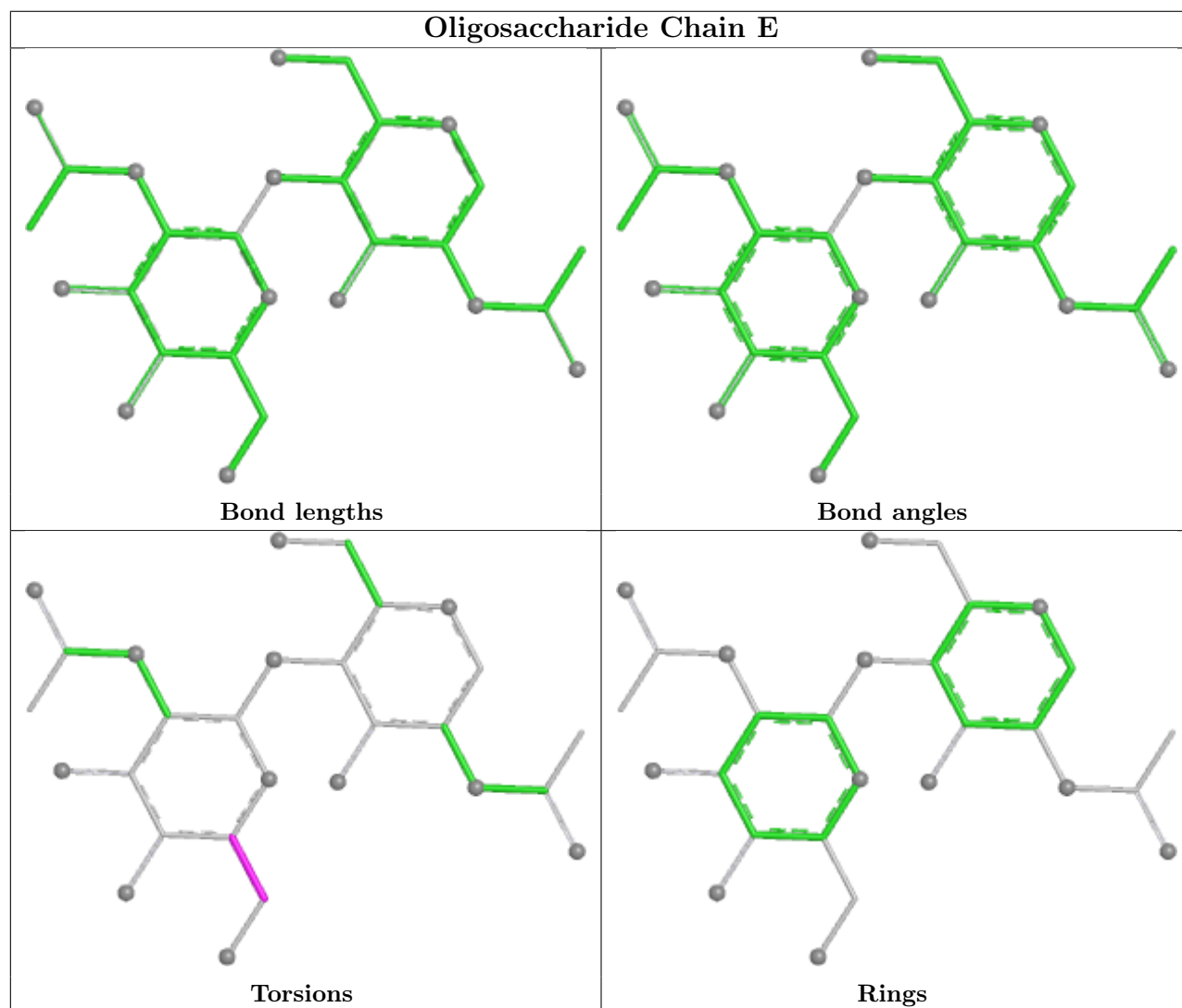
Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6

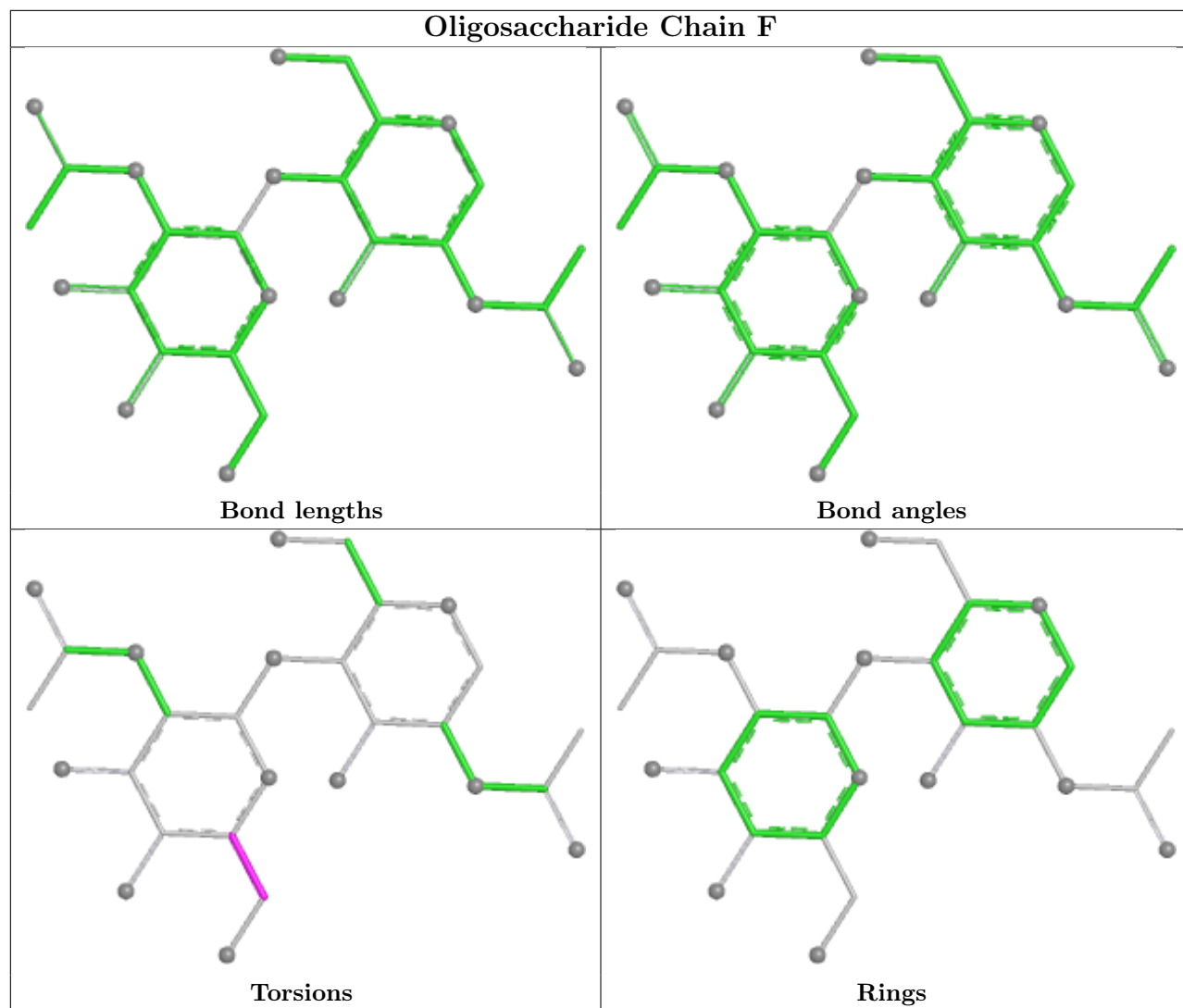
There are no ring outliers.

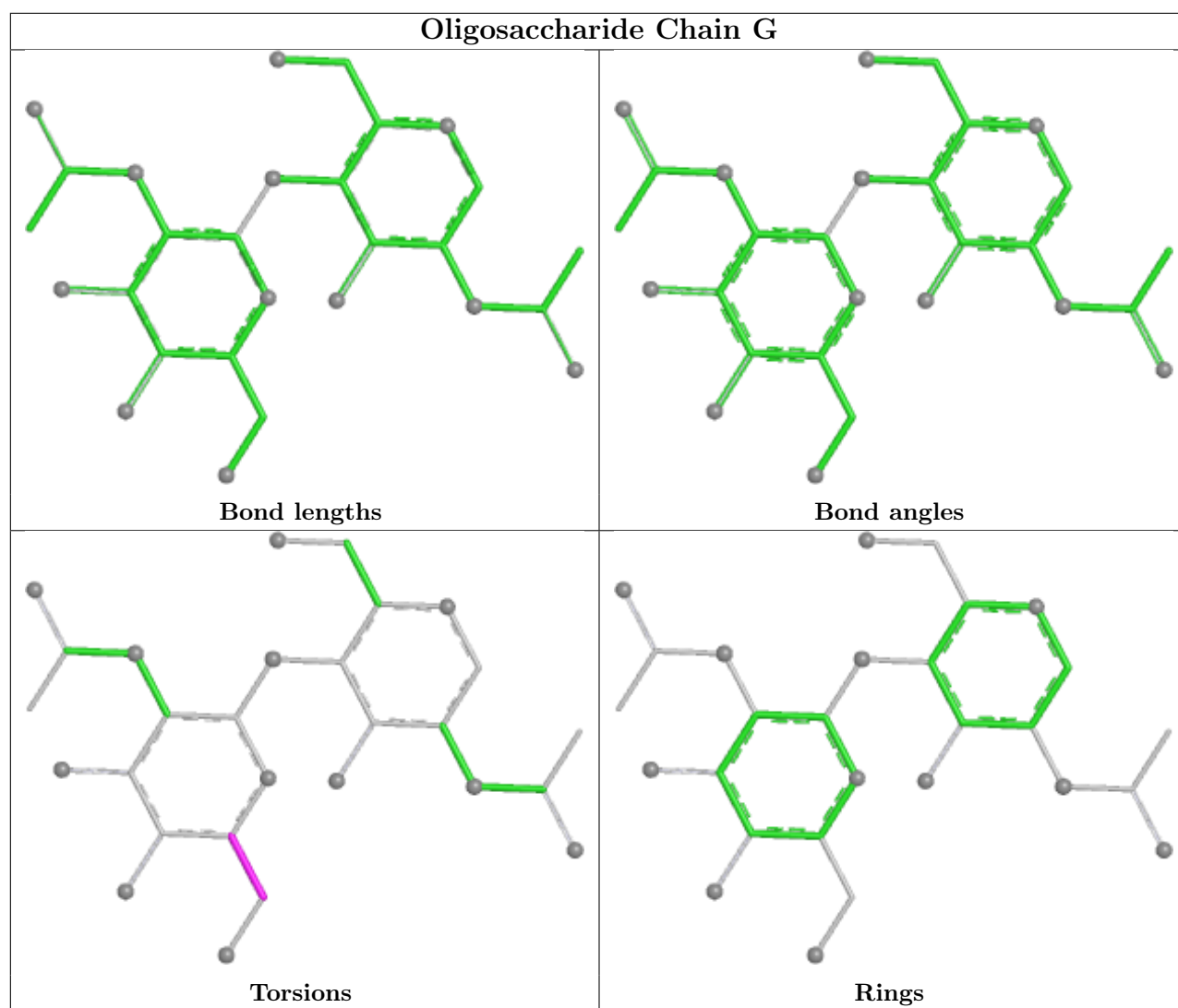
2 monomers are involved in 3 short contacts:

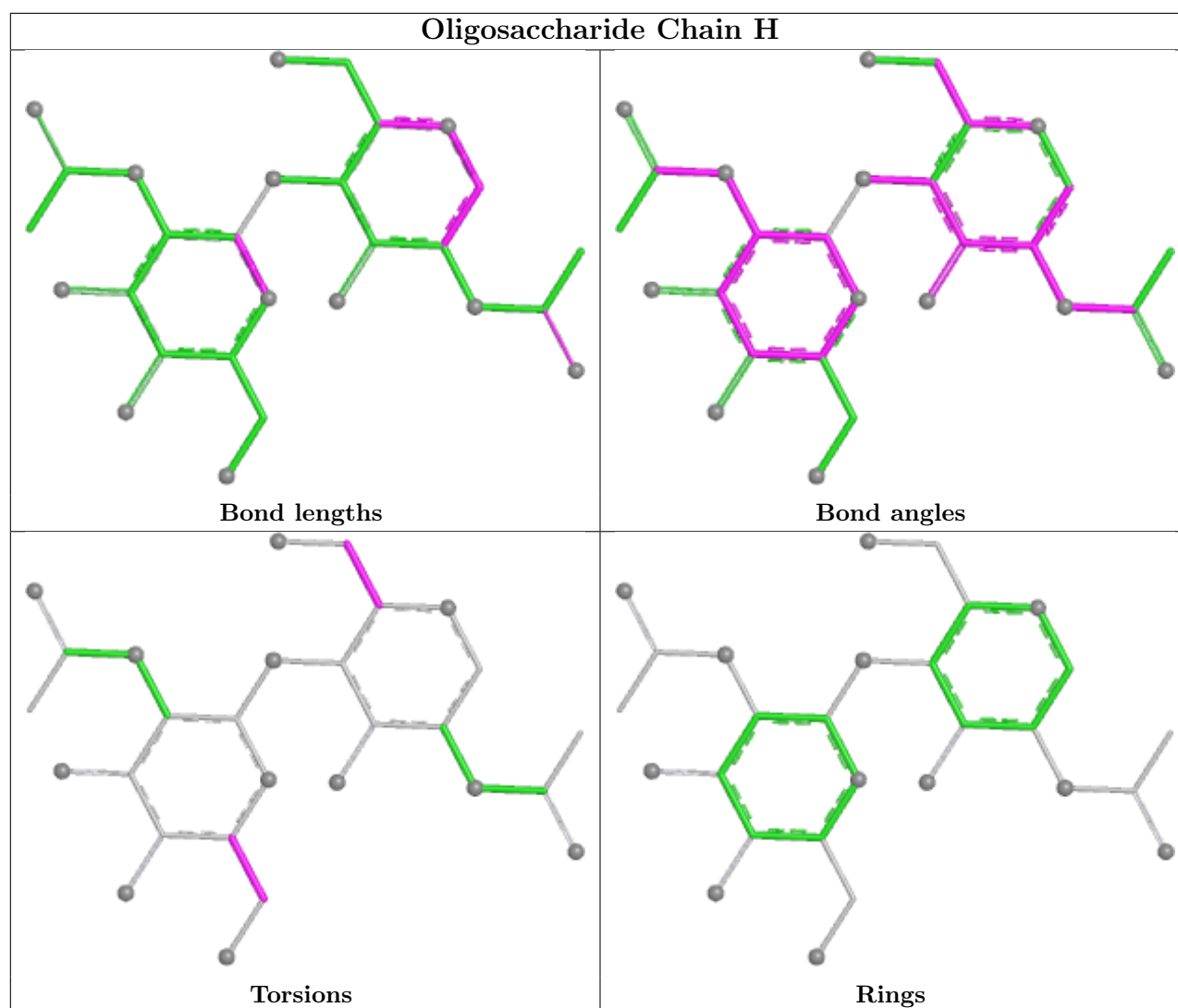
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	1	0
3	F	1	NAG	2	0

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









5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	$\# Z > 2$
5	NAG	A	5010	1	14,14,15	0.28	0	17,19,21	0.51	0
5	NAG	A	5002	1	14,14,15	0.29	0	17,19,21	0.40	0
5	NAG	A	5005	1	14,14,15	0.29	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	5009	1	14,14,15	1.46	2 (14%)	17,19,21	2.09	4 (23%)
5	NAG	B	5005	1	14,14,15	0.24	0	17,19,21	0.40	0
5	NAG	C	2001	2	14,14,15	0.34	0	17,19,21	0.48	0
5	NAG	B	5006	1	14,14,15	0.16	0	17,19,21	0.47	0
5	NAG	C	2002	2	14,14,15	0.33	0	17,19,21	0.54	0
5	NAG	D	501	2	14,14,15	0.27	0	17,19,21	0.54	0
5	NAG	D	502	2	14,14,15	0.58	0	17,19,21	1.48	1 (5%)
5	NAG	B	5002	1	14,14,15	0.21	0	17,19,21	0.43	0
5	NAG	A	5006	1	14,14,15	1.75	4 (28%)	17,19,21	1.74	5 (29%)
5	NAG	A	5007	1	14,14,15	0.21	0	17,19,21	0.42	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	A	5010	1	-	2/6/23/26	0/1/1/1
5	NAG	A	5002	1	-	2/6/23/26	0/1/1/1
5	NAG	A	5005	1	-	0/6/23/26	0/1/1/1
5	NAG	B	5009	1	-	0/6/23/26	0/1/1/1
5	NAG	B	5005	1	-	0/6/23/26	0/1/1/1
5	NAG	C	2001	2	-	0/6/23/26	0/1/1/1
5	NAG	B	5006	1	-	0/6/23/26	0/1/1/1
5	NAG	C	2002	2	-	0/6/23/26	0/1/1/1
5	NAG	D	501	2	-	2/6/23/26	0/1/1/1
5	NAG	D	502	2	-	2/6/23/26	0/1/1/1
5	NAG	B	5002	1	-	2/6/23/26	0/1/1/1
5	NAG	A	5006	1	-	0/6/23/26	0/1/1/1
5	NAG	A	5007	1	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5006	NAG	O5-C5	-3.08	1.37	1.43
5	A	5006	NAG	O7-C7	-2.86	1.16	1.23
5	B	5009	NAG	O5-C1	-2.42	1.39	1.43
5	B	5009	NAG	O5-C5	-2.31	1.38	1.43
5	A	5006	NAG	C2-N2	-2.21	1.42	1.46
5	A	5006	NAG	O5-C1	-2.03	1.40	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	502	NAG	C1-O5-C5	5.70	119.82	112.19
5	B	5009	NAG	O5-C1-C2	-5.53	102.73	111.29
5	B	5009	NAG	C1-C2-N2	3.58	116.08	110.43
5	B	5009	NAG	C2-N2-C7	-3.26	118.53	122.90
5	A	5006	NAG	C3-C4-C5	-3.14	104.54	110.23
5	A	5006	NAG	C8-C7-N2	2.98	121.06	116.12
5	A	5006	NAG	C1-O5-C5	2.64	115.73	112.19
5	A	5006	NAG	O4-C4-C5	-2.35	103.53	109.32
5	B	5009	NAG	O6-C6-C5	-2.26	103.63	111.33
5	A	5006	NAG	O7-C7-C8	-2.06	118.39	122.05

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	502	NAG	O5-C5-C6-O6
5	D	502	NAG	C4-C5-C6-O6
5	A	5010	NAG	C8-C7-N2-C2
5	A	5010	NAG	O7-C7-N2-C2
5	A	5002	NAG	O5-C5-C6-O6
5	A	5002	NAG	C4-C5-C6-O6
5	B	5002	NAG	C4-C5-C6-O6
5	B	5002	NAG	O5-C5-C6-O6
5	D	501	NAG	C4-C5-C6-O6
5	D	501	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	5010	NAG	1	0
5	B	5009	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	898/906 (99%)	-0.19	22 (2%) 59 66	19, 36, 65, 93	0
1	B	899/906 (99%)	-0.14	19 (2%) 63 68	18, 38, 66, 86	0
2	C	119/145 (82%)	1.08	28 (23%) 2 1	30, 57, 107, 127	0
2	D	111/145 (76%)	1.30	26 (23%) 2 1	41, 71, 105, 129	0
All	All	2027/2102 (96%)	-0.02	95 (4%) 36 42	18, 39, 76, 129	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	380	PHE	6.8
2	C	344	SER	6.6
1	B	892	GLY	6.2
2	C	342	ASP	6.2
2	C	379	LYS	6.1
2	C	378	VAL	5.9
2	D	369	PHE	5.7
1	A	66	ASP	5.6
1	B	352	GLY	4.7
2	D	341	VAL	4.6
2	D	342	ASP	4.5
2	C	343	THR	4.4
2	D	374	VAL	4.4
2	C	391	PRO	4.2
2	D	313	GLY	4.1
2	D	345	HIS	4.0
1	B	492	SER	4.0
1	A	890	ASP	3.8
2	D	417	TRP	3.8
2	D	375	ASN	3.7
1	A	895	SER	3.7

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Mol	Chain	Res	Type	RSRZ
2	C	374	VAL	3.6
2	C	341	VAL	3.6
2	C	345	HIS	3.6
1	A	741	ARG	3.6
1	A	738	ASN	3.6
1	B	66	ASP	3.5
1	B	896	PHE	3.5
2	D	381	GLY	3.4
2	D	391	PRO	3.4
2	C	372	GLY	3.4
2	C	394	CYS	3.3
1	A	568	LEU	3.3
1	B	296	ASN	3.3
1	A	887	LEU	3.0
2	C	418	SER	3.0
1	A	889	ASN	3.0
2	D	339	LEU	2.9
2	D	346	PHE	2.9
1	A	928	THR	2.8
2	D	388	LYS	2.8
1	B	821	LEU	2.8
1	B	348	ASP	2.8
1	B	527	ASN	2.8
2	C	367	CYS	2.7
2	D	382	SER	2.7
2	D	344	SER	2.6
1	A	528	ARG	2.6
2	C	420	GLY	2.6
1	B	351	ALA	2.6
2	C	417	TRP	2.6
2	C	373	LYS	2.6
1	A	616	GLY	2.6
2	D	394	CYS	2.5
2	D	314	PRO	2.5
2	D	367	CYS	2.4
2	C	335	THR	2.4
2	D	347	THR	2.4
2	C	382	SER	2.4
2	D	416	SER	2.4
2	D	366	ASN	2.4
2	D	368	PRO	2.4
1	B	761	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	300	MET	2.4
1	B	381	ARG	2.4
2	D	312	ARG	2.4
2	C	381	GLY	2.3
2	D	343	THR	2.3
1	A	640	ARG	2.3
1	A	254	PRO	2.3
2	C	416	SER	2.3
1	B	891	TYR	2.3
1	B	295	SER	2.3
2	C	383	VAL	2.3
2	C	347	THR	2.3
1	B	242	ASP	2.2
1	A	460	SER	2.2
2	C	301	PHE	2.2
1	A	491	LEU	2.2
1	B	617	ASN	2.2
2	D	365	GLY	2.2
2	C	371	PHE	2.2
2	C	419	ASP	2.2
1	A	956	GLU	2.2
1	A	647	GLN	2.2
1	A	672	HIS	2.1
1	A	617	ASN	2.1
1	B	67	GLN	2.1
1	B	97	ASP	2.1
2	D	305	TYR	2.1
1	A	492	SER	2.0
1	A	888	PHE	2.0
1	B	923	LYS	2.0
1	A	960	GLN	2.0
2	C	339	LEU	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.

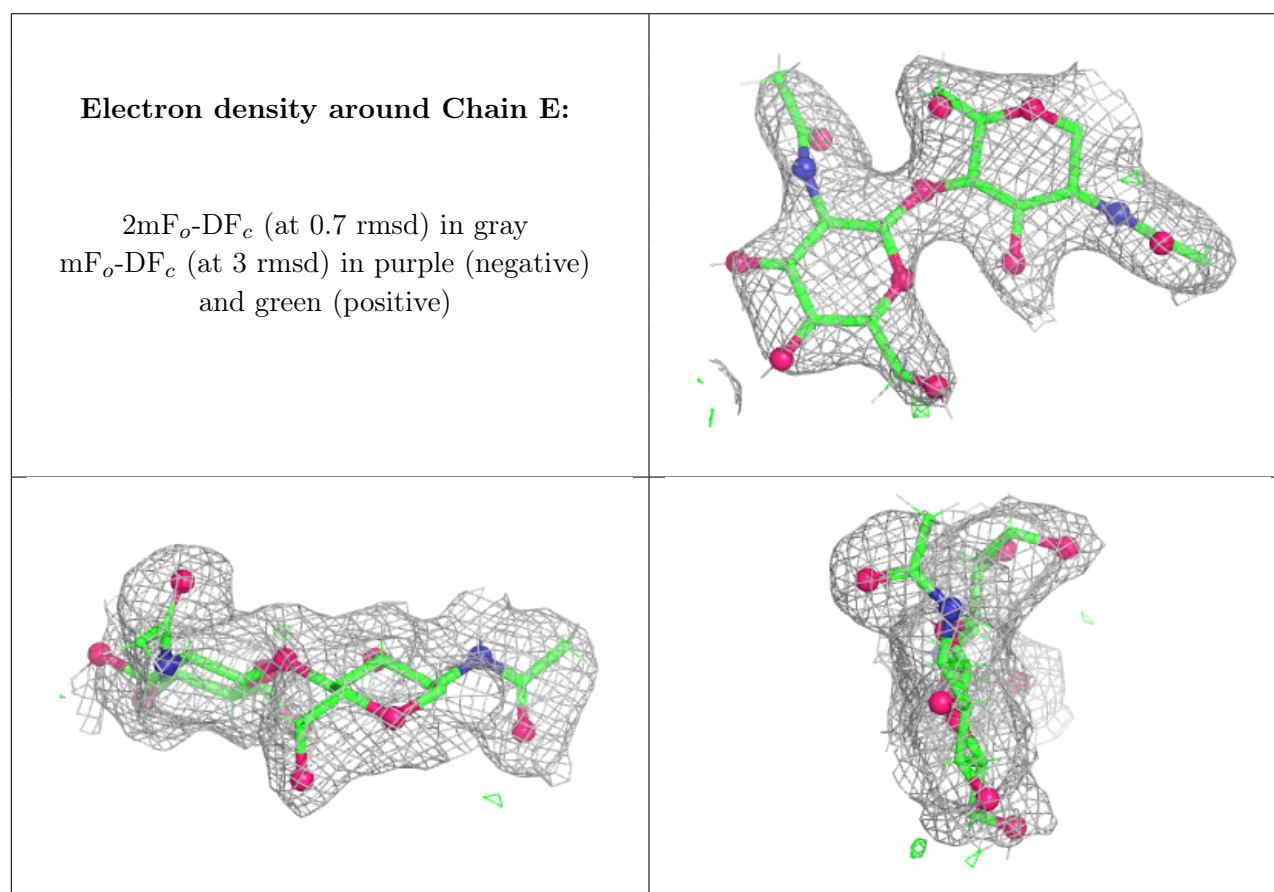
6.3 Carbohydrates [i](#)

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.

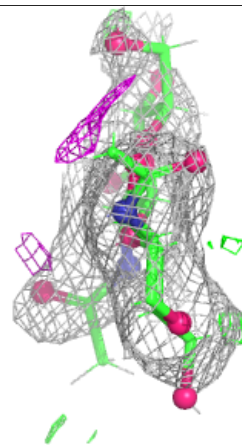
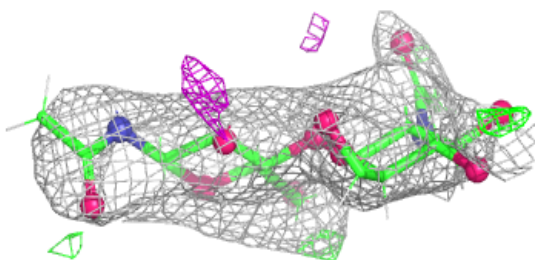
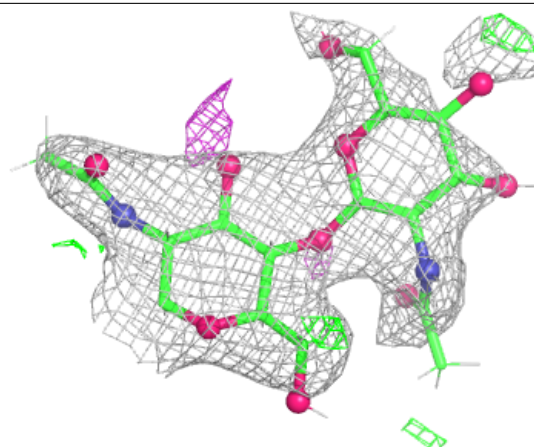
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	F	2	14/15	0.69	0.15	80,96,113,118	0
3	NAG	H	2	14/15	0.77	0.16	69,76,87,88	0
3	NAG	E	2	14/15	0.79	0.13	61,74,88,92	0
3	NAG	G	2	14/15	0.82	0.14	67,81,93,99	0
3	NAG	F	1	14/15	0.88	0.11	50,66,78,84	0
3	NAG	E	1	14/15	0.93	0.08	37,48,61,70	0
3	NAG	G	1	14/15	0.94	0.07	39,49,60,69	0
3	NAG	H	1	14/15	0.95	0.08	42,47,57,68	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.



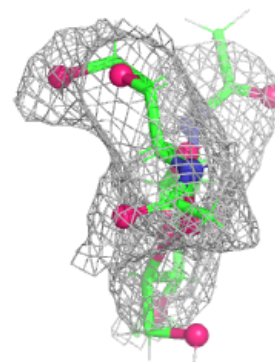
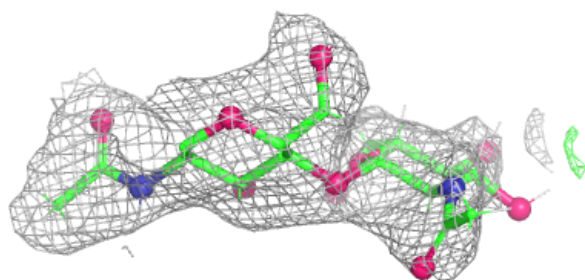
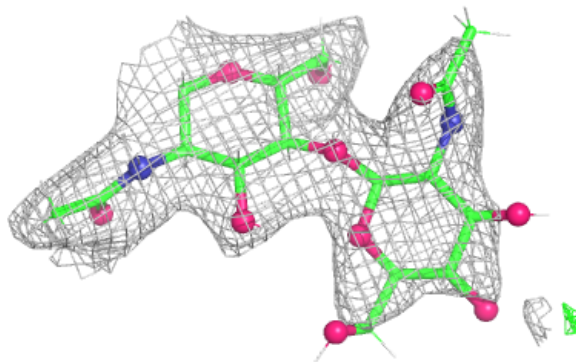
Electron density around Chain F:

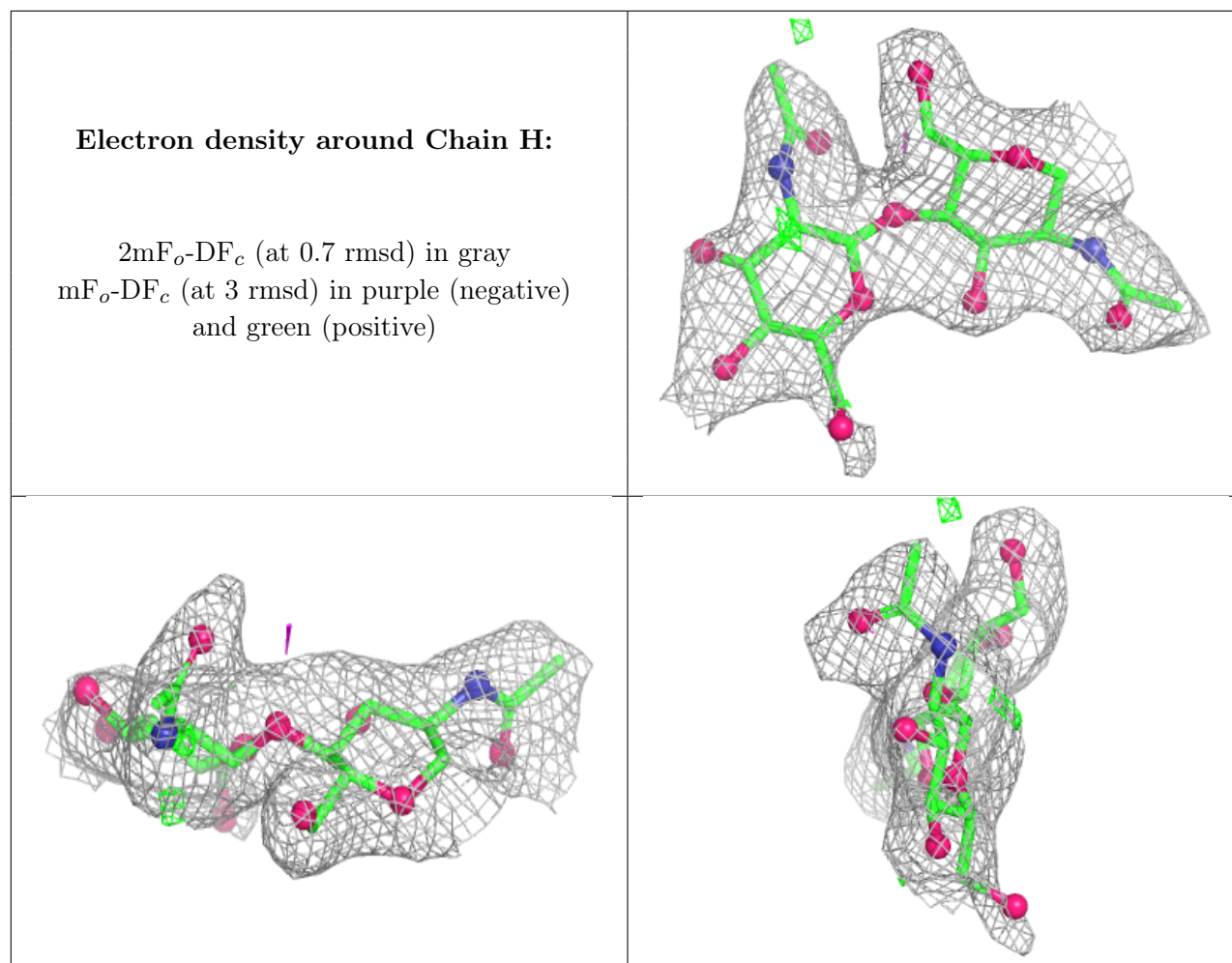
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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($\text{\AA}^2$)	Q<0.9
5	NAG	A	5010	14/15	0.67	0.20	70,85,102,104	0
5	NAG	D	502	14/15	0.71	0.18	84,87,102,104	0
5	NAG	A	5005	14/15	0.78	0.15	56,69,82,84	0
5	NAG	D	501	14/15	0.79	0.15	66,72,84,85	0
5	NAG	B	5005	14/15	0.80	0.15	73,89,103,124	0
5	NAG	B	5002	14/15	0.84	0.14	50,65,81,82	0
5	NAG	B	5009	14/15	0.84	0.15	52,64,70,72	0
5	NAG	A	5007	14/15	0.87	0.10	51,62,74,75	0
5	NAG	A	5006	14/15	0.89	0.11	37,41,48,51	0
5	NAG	C	2001	14/15	0.90	0.09	48,58,69,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	C	2002	14/15	0.90	0.10	44,53,60,64	0
5	NAG	B	5006	14/15	0.92	0.09	38,46,59,64	0
5	NAG	A	5002	14/15	0.92	0.08	29,39,48,53	0
4	ZN	A	5001	1/1	0.99	0.02	21,21,21,21	0
4	ZN	B	5001	1/1	1.00	0.03	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.