WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 12:19 PM EST

PDB ID : 4WK0

Title : Metal Ion and Ligand Binding of Integrin

Authors : Xia, W.; Springer, T.A.

Deposited on : 2014-10-01

Resolution : 1.78 Å(reported)

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

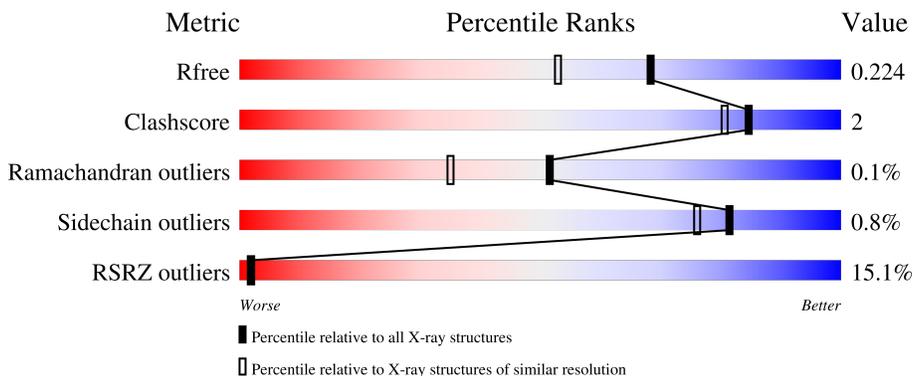|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.78 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.
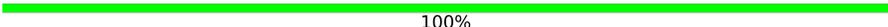
Metric	Percentile Ranks	Value
Rfree		0.224
Clashscore		2
Ramachandran outliers		0.1%
Sidechain outliers		0.8%
RSRZ outliers		15.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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 <=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	452	10% / 95%
2	B	445	20% / 89% / 7%
3	C	3	67% / 33%
4	D	6	33% / 67%
5	E	2	100%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	H	2	-	-	-	X
7	NAG	B	508	-	-	-	X
7	NAG	B	509	-	-	-	X

2　Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 14311 atoms, of which 6699 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Integrin alpha-5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	449	Total 6576	C 2160	H 3184	N 554	O 670	S 8	0	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	451	VAL	ILE	engineered mutation	UNP P08648

- Molecule 2 is a protein called Integrin beta-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	427	Total 6590	C 2080	H 3269	N 562	O 655	S 24	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	195	THR	SER	conflict	UNP P05556

- Molecule 3 is a protein called ARG-GLY-ASP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	3	Total 42	C 12	H 19	N 6	O 5	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
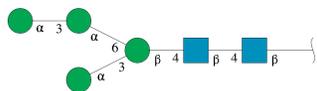
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	6	Total 136	C 40	H 64	N 2	O 30	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	2	Total 54	C 16	H 26	N 2	O 10	0	0	0
5	F	2	Total 55	C 16	H 27	N 2	O 10	0	0	0
5	G	2	Total 55	C 16	H 27	N 2	O 10	0	0	0
5	H	2	Total 55	C 16	H 27	N 2	O 10	0	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total 4	Ca 4	0	0
6	B	2	Total 2	Ca 2	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total 1	Mg 1	0	0

- Molecule 9 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	383	Total 383	O 383	0	0
9	B	239	Total 239	O 239	0	0
9	C	7	Total 7	O 7	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.
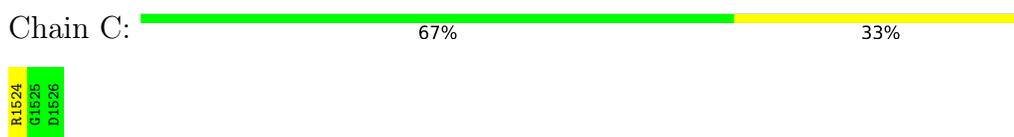
- Molecule 1: Integrin alpha-5
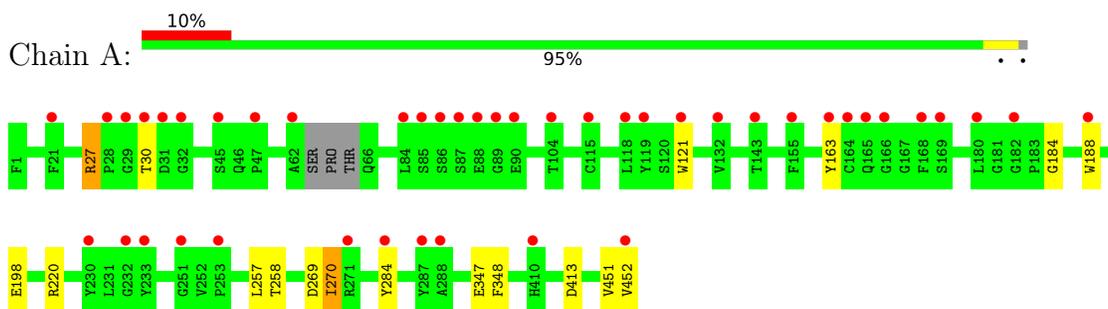
- Molecule 2: Integrin beta-1
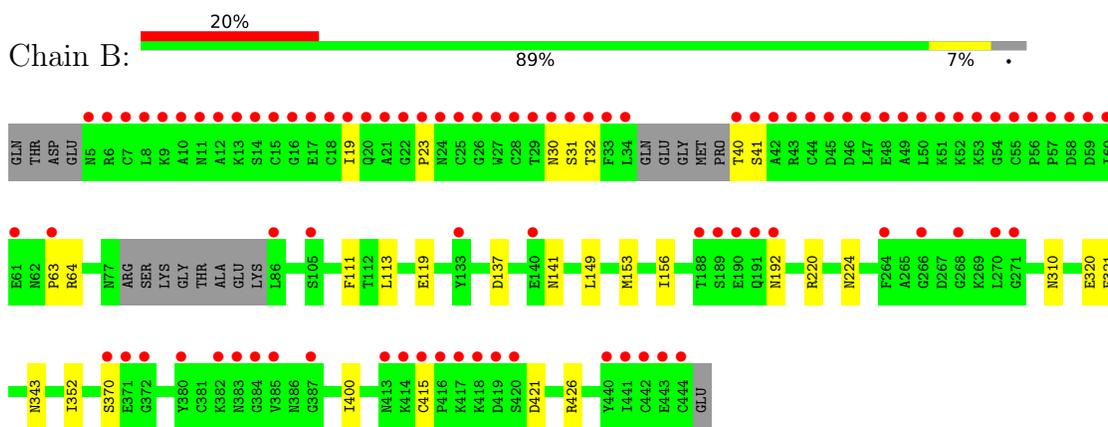
- Molecule 3: ARG-GLY-ASP

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

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain E: 100%

NAG1 NAG2

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain F: 100%

NAG1 NAG2

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain G: 50%   50%

NAG1 NAG2

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain H: 50%   50%

NAG1 NAG2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.06Å 117.07Å 167.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.90 – 1.78 47.94 – 1.78	Depositor EDS
% Data completeness (in resolution range)	98.2 (47.90-1.78) 98.2 (47.94-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 1.78Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1760)	Depositor
R, R_{free}	0.186 , 0.223 0.192 , 0.224	Depositor DCC
R_{free} test set	1997 reflections (1.76%)	wwPDB-VP
Wilson B-factor (Å^2)	28.3	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 54.1	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14311	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NAG, CA, MAN, MG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.38	0/3492	0.56	0/4760
2	B	0.35	0/3377	0.52	0/4559
3	C	0.33	0/22	0.57	0/27
All	All	0.36	0/6891	0.54	0/9346

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 ⓘ

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	3392	3184	3194	13	0
2	B	3321	3269	3270	17	0
3	C	23	19	19	1	0
4	D	72	64	61	1	0
5	E	28	26	25	0	0
5	F	28	27	25	0	0
5	G	28	27	25	0	0
5	H	28	27	25	0	0
6	A	4	0	0	0	0
6	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	28	28	26	0	0
7	B	28	28	26	0	0
8	B	1	0	0	0	0
9	A	383	0	0	3	0
9	B	239	0	0	0	0
9	C	7	0	0	1	0
All	All	7612	6699	6696	31	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 (31) 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)
2:B:30:ASN:ND2	2:B:32:THR:OG1	1.62	1.28
1:A:451:VAL:O	1:A:452:VAL:HG22	1.89	0.72
1:A:27:ARG:HH22	1:A:30:THR:HG22	1.61	0.66
1:A:258:THR:HG21	9:A:938:HOH:O	2.00	0.62
2:B:40:THR:OG1	2:B:41:SER:N	2.36	0.57
3:C:1524:ARG:N	9:C:1604:HOH:O	2.40	0.54
2:B:149:LEU:O	2:B:153:MET:HG2	2.07	0.54
2:B:320:GLU:HG3	2:B:321:PHE:CD1	2.43	0.53
2:B:141:ASN:ND2	2:B:343:ASN:O	2.43	0.52
2:B:30:ASN:ND2	2:B:32:THR:CB	2.69	0.51
2:B:30:ASN:O	2:B:31:SER:OG	2.23	0.51
1:A:257:LEU:O	1:A:258:THR:OG1	2.23	0.49
1:A:198:GLU:OE1	9:A:867:HOH:O	2.21	0.47
1:A:27:ARG:HH12	1:A:30:THR:HG22	1.80	0.47
1:A:27:ARG:NH2	1:A:30:THR:HG22	2.29	0.46
2:B:119:GLU:HA	2:B:400:ILE:HG23	1.97	0.46
1:A:184:GLY:HA2	1:A:188:TRP:CD1	2.50	0.45
1:A:347:GLU:HG2	1:A:348:PHE:CD2	2.51	0.45
1:A:220:ARG:NH2	4:D:4:MAN:O2	2.50	0.45
2:B:23:PRO:O	2:B:64:ARG:NH2	2.49	0.44
2:B:156:ILE:CD1	2:B:352:ILE:HD12	2.48	0.43
2:B:137:ASP:OD1	2:B:137:ASP:N	2.51	0.43
2:B:111:PHE:CE2	2:B:113:LEU:HD13	2.54	0.42
2:B:19:ILE:HD12	2:B:63:PRO:HD2	2.01	0.42
1:A:163:TYR:O	1:A:184:GLY:HA3	2.20	0.41
1:A:30:THR:N	9:A:891:HOH:O	2.53	0.41
2:B:30:ASN:ND2	2:B:32:THR:CG2	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:ASN:OD1	2:B:426:ARG:NH1	2.47	0.41
2:B:370:SER:OG	2:B:421:ASP:OD2	2.26	0.41
2:B:192:ASN:O	2:B:220:ARG:NH1	2.50	0.41
1:A:269:ASP:O	1:A:270:ILE:HG22	2.20	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	447/452 (99%)	430 (96%)	16 (4%)	1 (0%)	47	32
2	B	421/445 (95%)	405 (96%)	16 (4%)	0	100	100
3	C	1/3 (33%)	1 (100%)	0	0	100	100
All	All	869/900 (97%)	836 (96%)	32 (4%)	1 (0%)	51	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	ILE

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	357/358 (100%)	353 (99%)	4 (1%)	73	65
2	B	380/395 (96%)	378 (100%)	2 (0%)	88	86
3	C	2/2 (100%)	2 (100%)	0	100	100
All	All	739/755 (98%)	733 (99%)	6 (1%)	81	76

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

Mol	Chain	Res	Type
1	A	27	ARG
1	A	121	TRP
1	A	284	TYR
1	A	413	ASP
2	B	224	ASN
2	B	415	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	GLN
2	B	30	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 ⓘ

14 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
4	NAG	D	1	4,1	14,14,15	0.42	0	17,19,21	0.54	0
4	NAG	D	2	4	14,14,15	0.32	0	17,19,21	0.59	0
4	BMA	D	3	4	11,11,12	0.96	1 (9%)	15,15,17	0.93	1 (6%)
4	MAN	D	4	4	11,11,12	0.79	0	15,15,17	0.95	0
4	MAN	D	5	4	11,11,12	0.89	1 (9%)	15,15,17	0.97	1 (6%)
4	MAN	D	6	4	11,11,12	0.81	1 (9%)	15,15,17	0.93	0
5	NAG	E	1	1,5	14,14,15	0.38	0	17,19,21	0.39	0
5	NAG	E	2	5	14,14,15	0.20	0	17,19,21	0.54	0
5	NAG	F	1	1,5	14,14,15	0.46	0	17,19,21	0.56	0
5	NAG	F	2	5	14,14,15	0.41	0	17,19,21	0.37	0
5	NAG	G	1	5,2	14,14,15	0.83	1 (7%)	17,19,21	0.60	0
5	NAG	G	2	5	14,14,15	0.28	0	17,19,21	0.46	0
5	NAG	H	1	5,2	14,14,15	0.61	1 (7%)	17,19,21	0.59	0
5	NAG	H	2	5	14,14,15	0.31	0	17,19,21	0.44	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
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
4	MAN	D	6	4	-	2/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	NAG	G	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	NAG	H	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	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)
5	G	1	NAG	O5-C1	-2.75	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3	BMA	O5-C1	-2.58	1.39	1.43
4	D	5	MAN	O5-C1	-2.21	1.40	1.43
5	H	1	NAG	O5-C1	-2.11	1.40	1.43
4	D	6	MAN	O5-C1	-2.11	1.40	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	3	BMA	C1-C2-C3	-2.28	106.86	109.67
4	D	5	MAN	C1-O5-C5	2.25	115.24	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

| Mol	Chain	Res	Type	Atoms
5	G	2	NAG	O5-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
4	D	6	MAN	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
4	D	6	MAN	C4-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	4	MAN	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.

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H
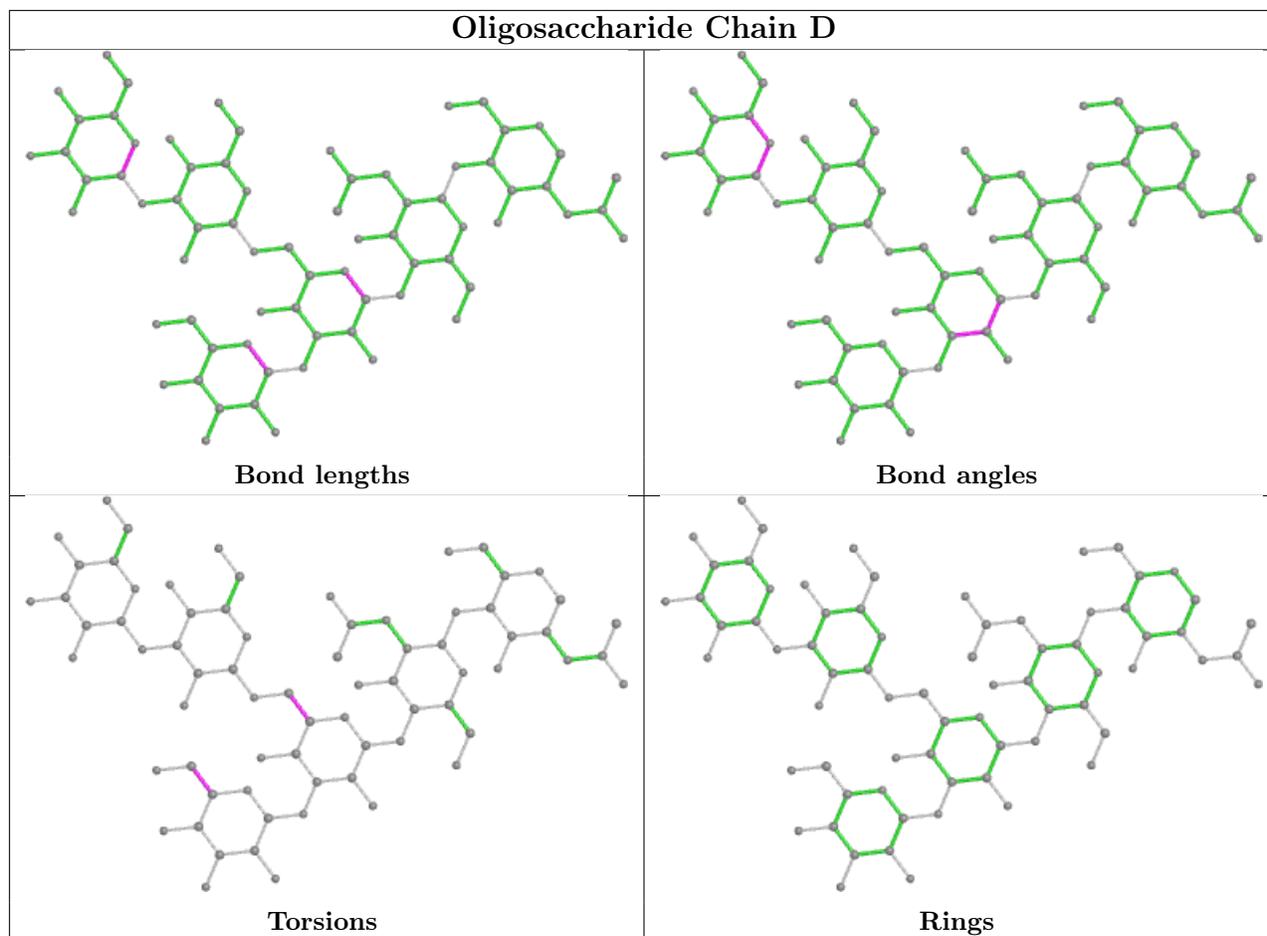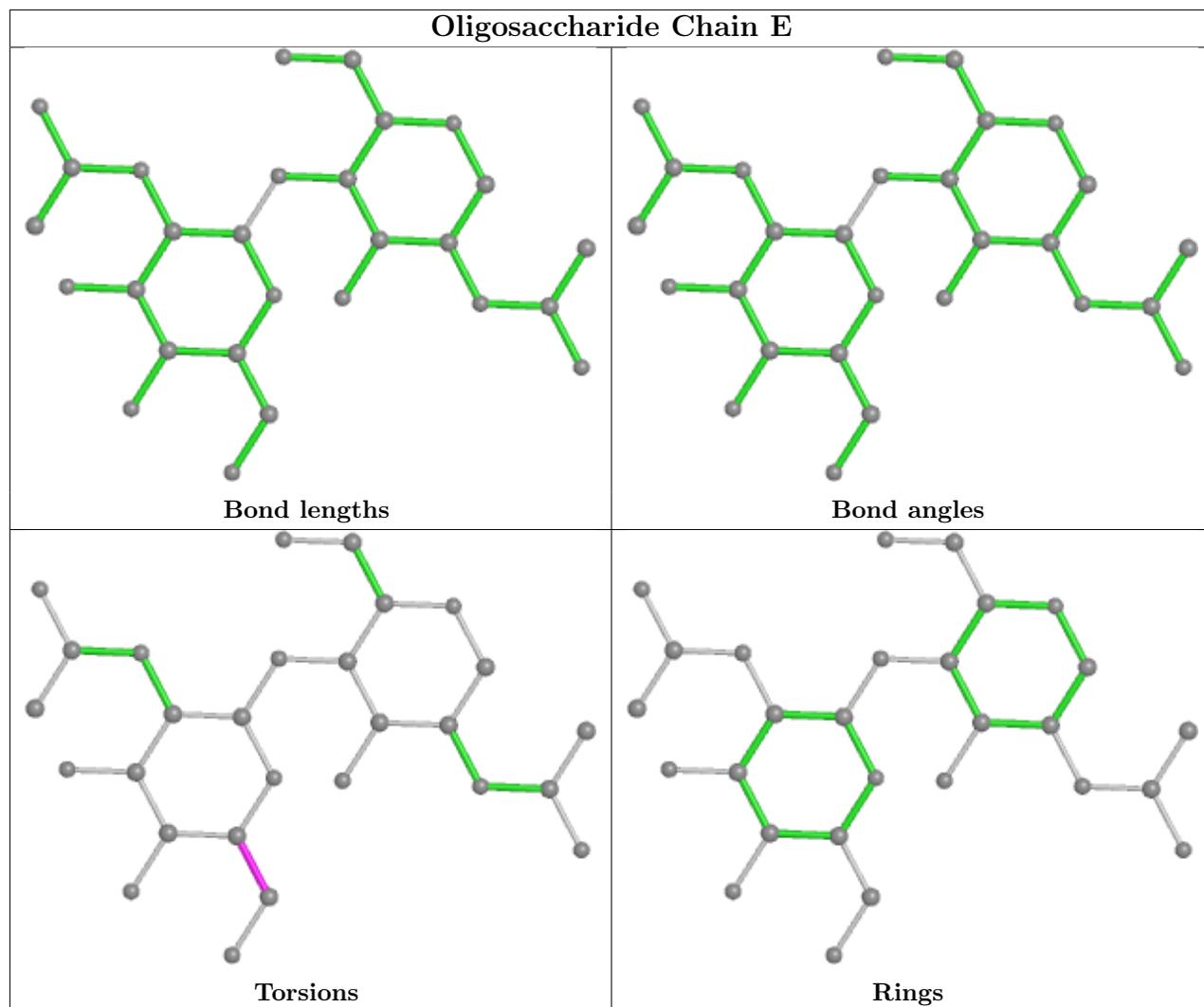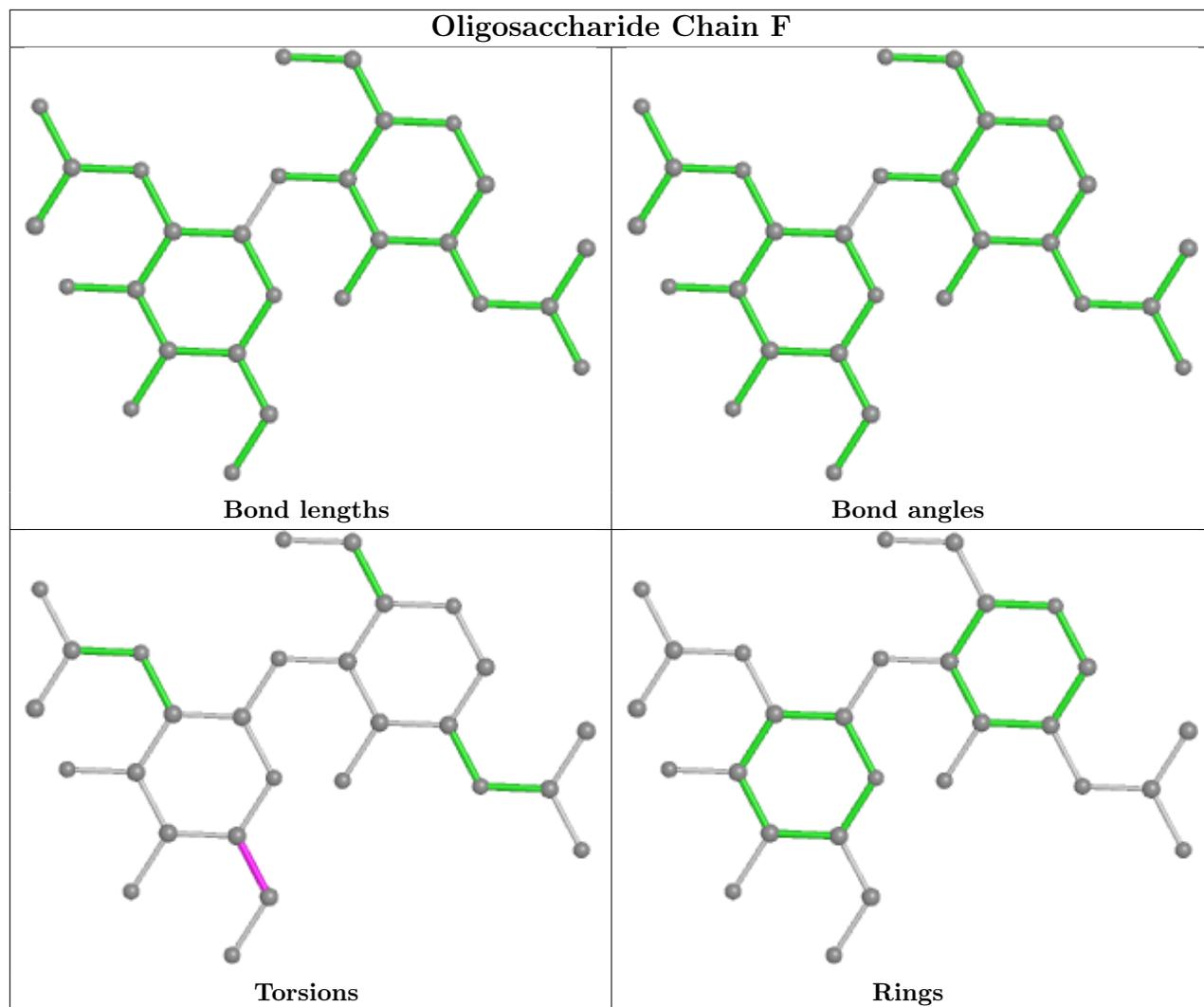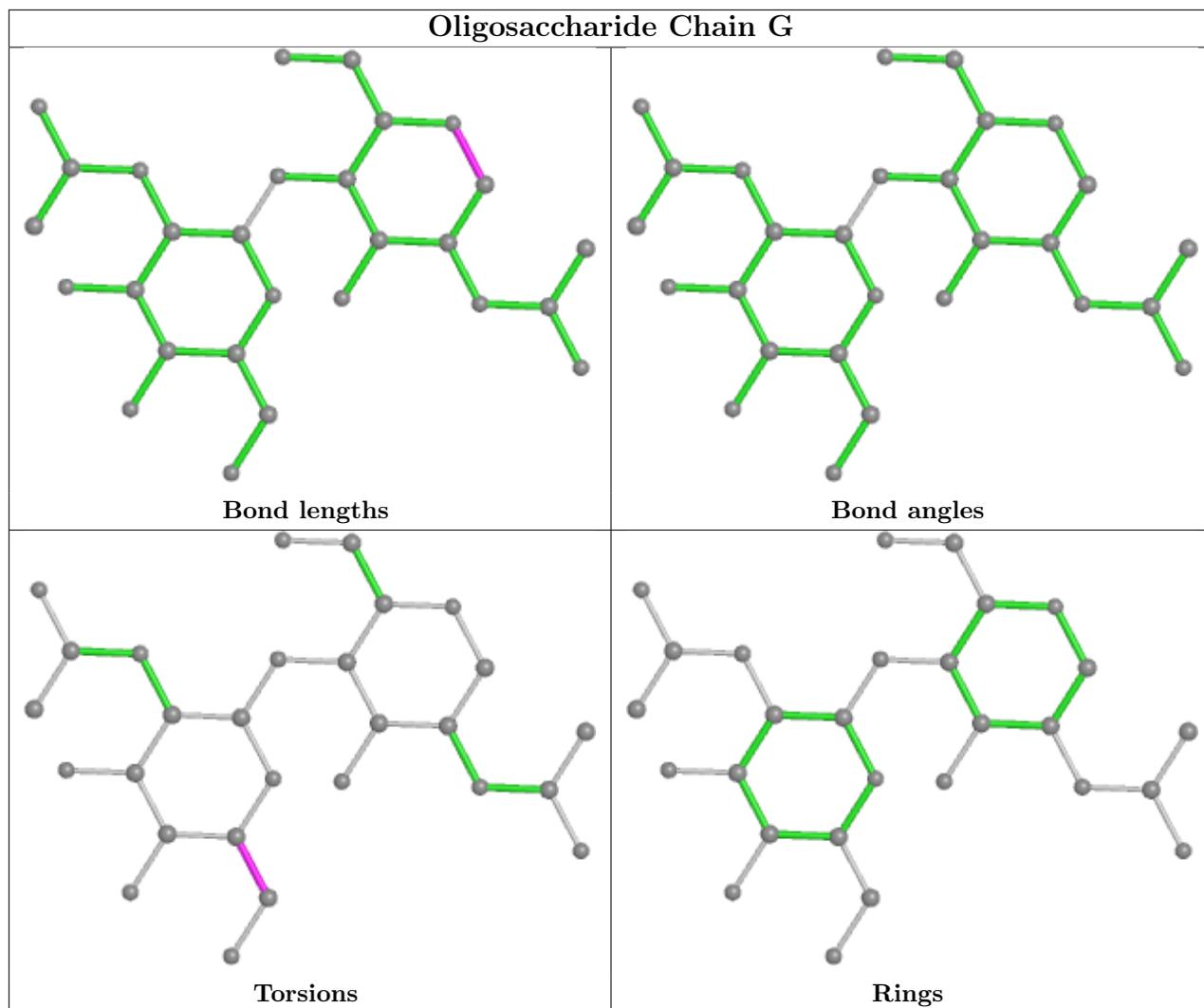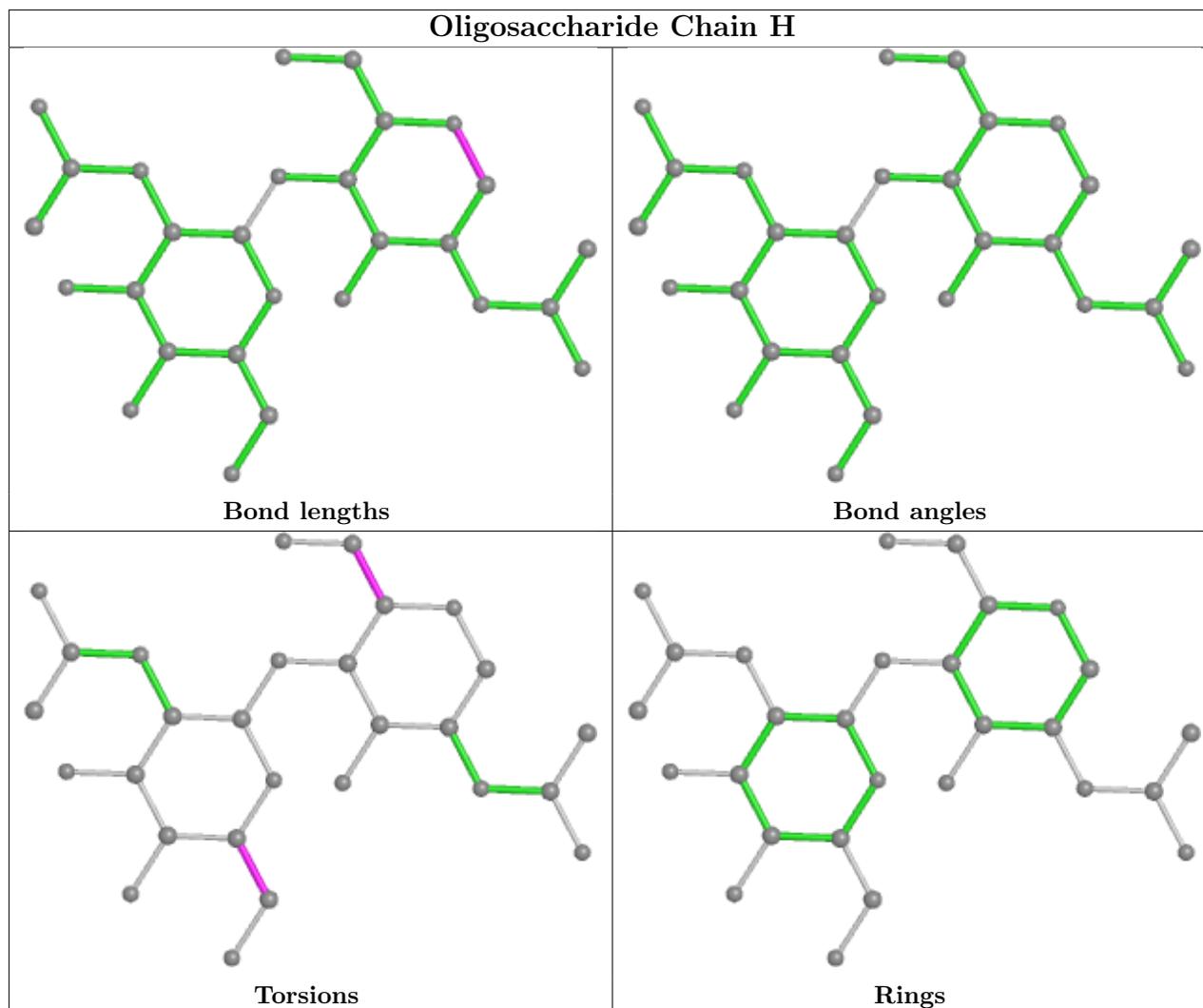
5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 7 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	#$|Z| > 2$
7	NAG	B	508	2	14,14,15	0.17	0	17,19,21	0.51	0
7	NAG	A	516	1	14,14,15	0.16	0	17,19,21	0.43	0
7	NAG	B	509	2	14,14,15	0.40	0	17,19,21	0.78	1 (5%)
7	NAG	A	511	1	14,14,15	0.37	0	17,19,21	0.51	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
7	NAG	B	508	2	-	2/6/23/26	0/1/1/1
7	NAG	A	516	1	-	0/6/23/26	0/1/1/1
7	NAG	B	509	2	-	2/6/23/26	0/1/1/1
7	NAG	A	511	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	509	NAG	C1-O5-C5	2.82	116.01	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	509	NAG	O5-C5-C6-O6
7	B	509	NAG	C4-C5-C6-O6
7	B	508	NAG	C4-C5-C6-O6
7	A	511	NAG	C4-C5-C6-O6
7	A	511	NAG	O5-C5-C6-O6
7	B	508	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	449/452 (99%)	0.60	44 (9%)	7	7	20, 32, 70, 132	0
2	B	427/445 (95%)	1.51	89 (20%)	1	0	21, 40, 124, 173	0
3	C	3/3 (100%)	0.45	0	100	100	48, 48, 55, 71	0
All	All	879/900 (97%)	1.04	133 (15%)	2	2	20, 35, 107, 173	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	33	PHE	17.4
2	B	34	LEU	17.1
2	B	47	LEU	16.1
2	B	31	SER	14.1
2	B	50	LEU	14.0
2	B	415	CYS	12.3
2	B	8	LEU	12.2
2	B	28	CYS	11.2
2	B	60	ILE	11.1
2	B	49	ALA	10.9
2	B	30	ASN	10.7
2	B	19	ILE	10.7
2	B	32	THR	10.7
2	B	56	PRO	10.6
2	B	55	CYS	10.2
2	B	42	ALA	9.9
2	B	52	LYS	9.8
2	B	5	ASN	9.8
2	B	29	THR	9.7
2	B	7	CYS	9.5
2	B	51	LYS	9.5
2	B	27	TRP	9.5
2	B	44	CYS	9.1

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Mol	Chain	Res	Type	RSRZ
2	B	57	PRO	8.9
2	B	54	GLY	8.7
2	B	6	ARG	8.3
2	B	12	ALA	8.0
2	B	9	LYS	7.9
2	B	53	LYS	7.4
2	B	13	LYS	7.3
2	B	416	PRO	7.2
2	B	15	CYS	7.1
2	B	442	CYS	7.0
1	A	29	GLY	6.8
2	B	45	ASP	6.7
2	B	418	LYS	6.7
2	B	21	ALA	6.5
1	A	32	GLY	6.5
2	B	43	ARG	6.4
2	B	190	GLU	6.4
1	A	85	SER	6.3
2	B	11	ASN	6.3
2	B	417	LYS	6.2
2	B	59	ASP	6.1
2	B	22	GLY	5.9
2	B	48	GLU	5.9
2	B	385	VAL	5.8
2	B	41	SER	5.7
1	A	84	LEU	5.7
2	B	10	ALA	5.6
2	B	24	ASN	5.5
2	B	419	ASP	5.5
2	B	188	THR	5.4
2	B	16	GLY	5.3
2	B	384	GLY	5.1
2	B	40	THR	5.0
2	B	20	GLN	5.0
2	B	383	ASN	5.0
1	A	86	SER	5.0
2	B	413	ASN	4.9
2	B	26	GLY	4.8
2	B	414	LYS	4.8
1	A	168	PHE	4.8
2	B	18	CYS	4.6
2	B	46	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	25	CYS	4.5
1	A	28	PRO	4.0
1	A	62	ALA	4.0
2	B	189	SER	3.9
1	A	30	THR	3.9
2	B	58	ASP	3.9
1	A	287	TYR	3.8
1	A	271	ARG	3.8
1	A	233	TYR	3.8
1	A	452	VAL	3.8
2	B	371	GLU	3.7
1	A	155[A]	PHE	3.7
2	B	420	SER	3.7
2	B	14	SER	3.6
2	B	270	LEU	3.6
2	B	61	GLU	3.6
2	B	444	CYS	3.5
2	B	441	ILE	3.5
2	B	372	GLY	3.5
1	A	31	ASP	3.5
2	B	192	ASN	3.4
2	B	23	PRO	3.4
1	A	121	TRP	3.3
2	B	86	LEU	3.2
2	B	17	GLU	3.1
1	A	288	ALA	3.1
2	B	440	TYR	3.0
1	A	88	GLU	3.0
2	B	105	SER	2.9
1	A	163	TYR	2.9
1	A	284	TYR	2.8
1	A	164	CYS	2.8
2	B	382	LYS	2.8
2	B	264	PHE	2.8
1	A	166	GLY	2.8
1	A	90	GLU	2.7
2	B	380	TYR	2.7
1	A	232	GLY	2.7
2	B	443	GLU	2.7
1	A	410	HIS	2.6
2	B	133	TYR	2.5
1	A	143	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	119	TYR	2.5
2	B	140	GLU	2.5
1	A	104	THR	2.5
1	A	87	SER	2.5
1	A	21	PHE	2.5
1	A	230	TYR	2.4
1	A	115	CYS	2.4
1	A	132	VAL	2.4
1	A	169	SER	2.4
1	A	89	GLY	2.3
2	B	266	GLY	2.3
1	A	188	TRP	2.3
2	B	370	SER	2.3
2	B	191	GLN	2.2
2	B	271	GLY	2.2
1	A	118	LEU	2.2
1	A	180	LEU	2.2
1	A	253	PRO	2.2
2	B	63	PRO	2.2
1	A	45	SER	2.1
1	A	182	GLY	2.1
1	A	165	GLN	2.1
2	B	268	GLY	2.1
2	B	387	GLY	2.1
1	A	47	PRO	2.0
1	A	251	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.
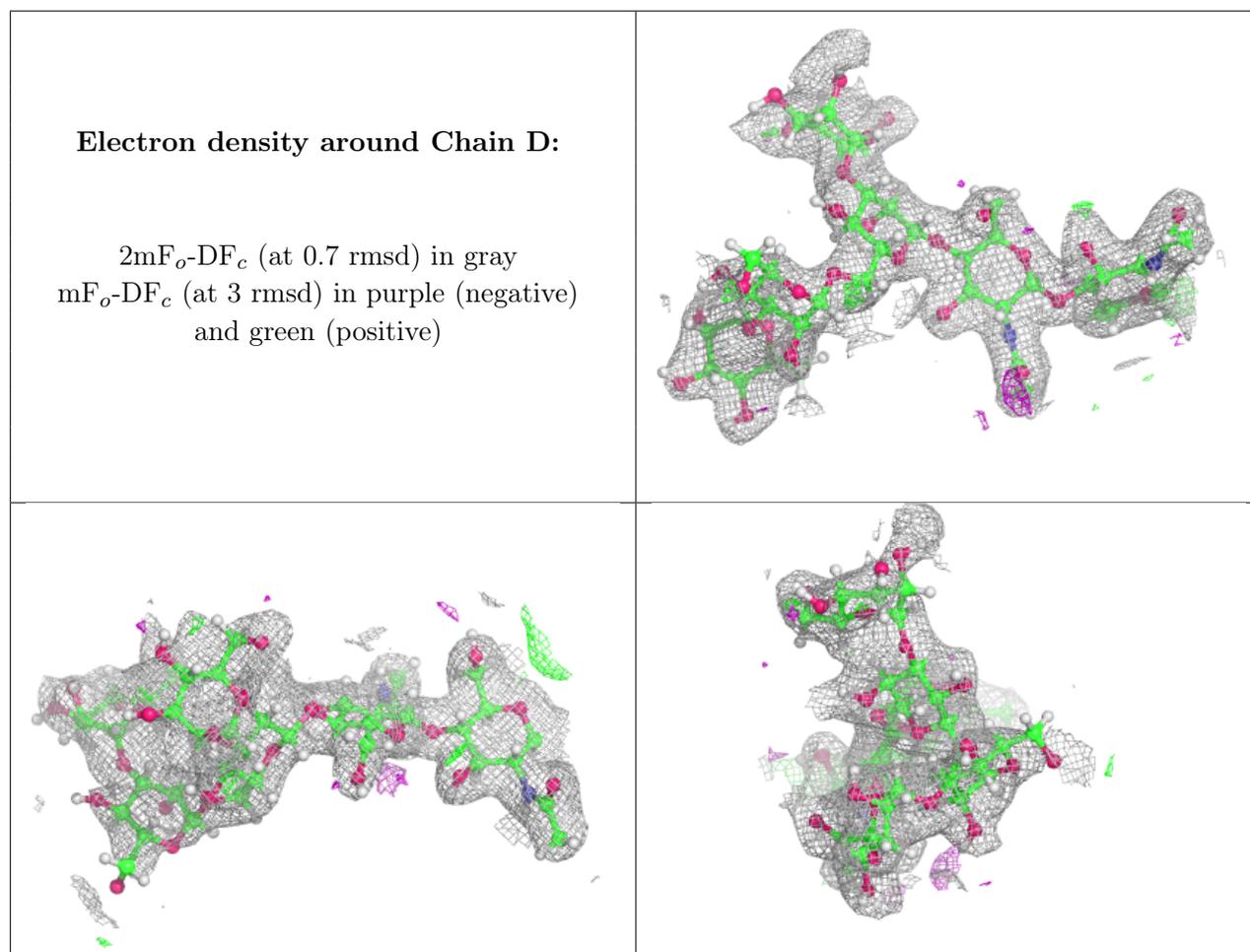
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	G	2	14/15	0.68	0.35	91,121,150,158	0
5	NAG	H	2	14/15	0.68	0.49	94,117,139,140	0

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| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	D	5	11/12	0.74	0.25	71,96,112,119	0
4	MAN	D	6	11/12	0.76	0.33	94,114,134,143	0
4	MAN	D	4	11/12	0.84	0.38	75,101,128,128	0
4	BMA	D	3	11/12	0.85	0.19	62,75,91,93	0
5	NAG	F	2	14/15	0.88	0.39	57,84,107,127	0
5	NAG	G	1	14/15	0.88	0.11	55,77,95,97	0
5	NAG	E	2	14/15	0.92	0.30	67,89,113,117	0
5	NAG	H	1	14/15	0.93	0.36	53,78,93,94	0
5	NAG	E	1	14/15	0.94	0.14	37,51,70,76	0
5	NAG	F	1	14/15	0.95	0.16	29,44,60,65	0
4	NAG	D	2	14/15	0.95	0.11	29,44,63,75	0
4	NAG	D	1	14/15	0.97	0.06	27,36,40,46	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.
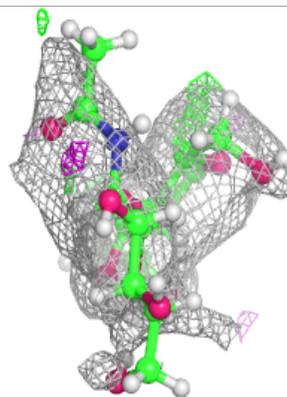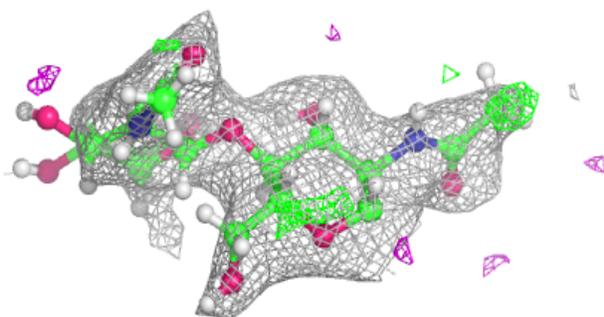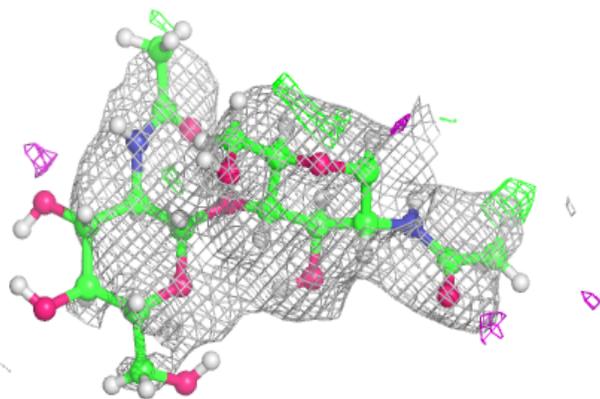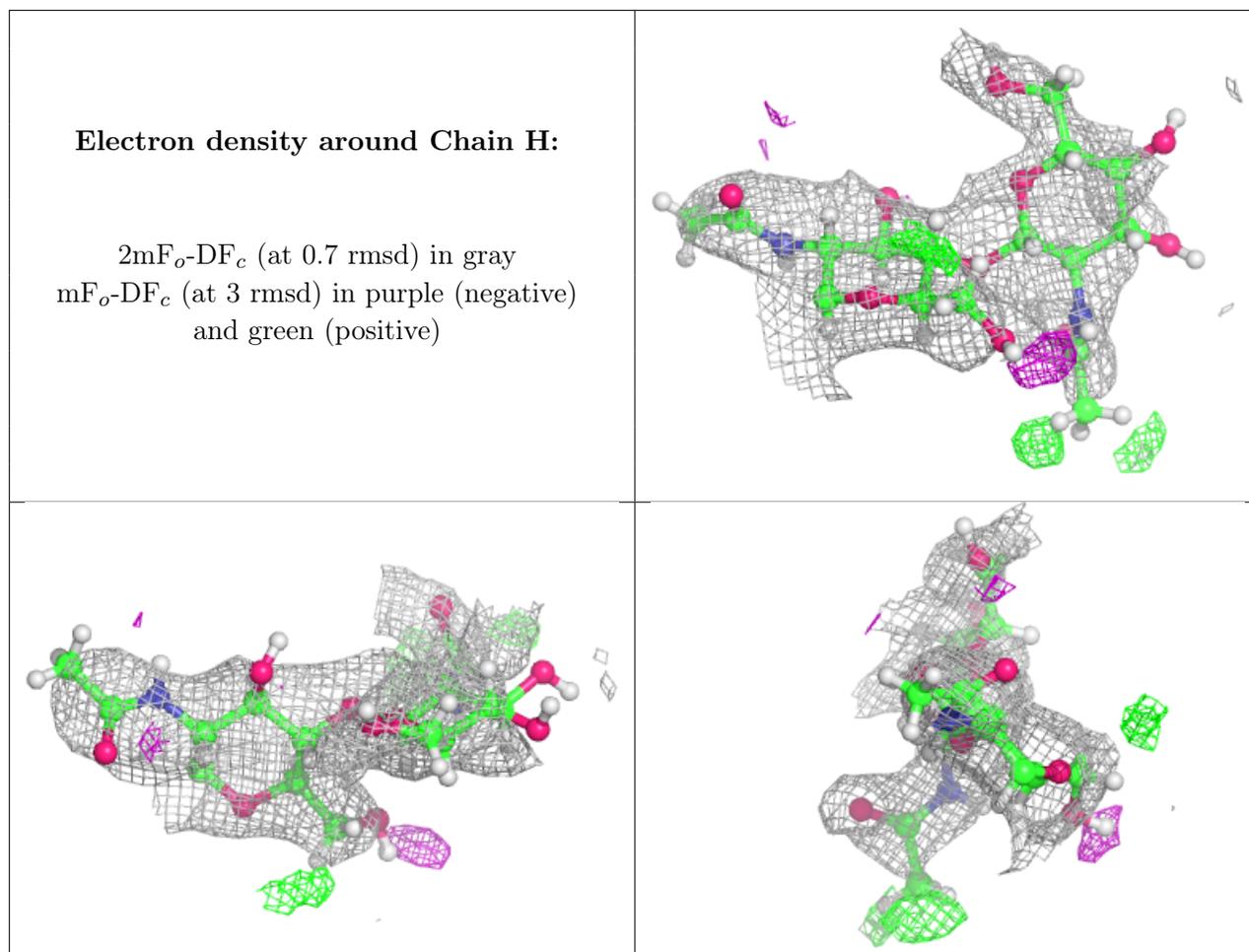

Electron density around Chain D:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around Chain E:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
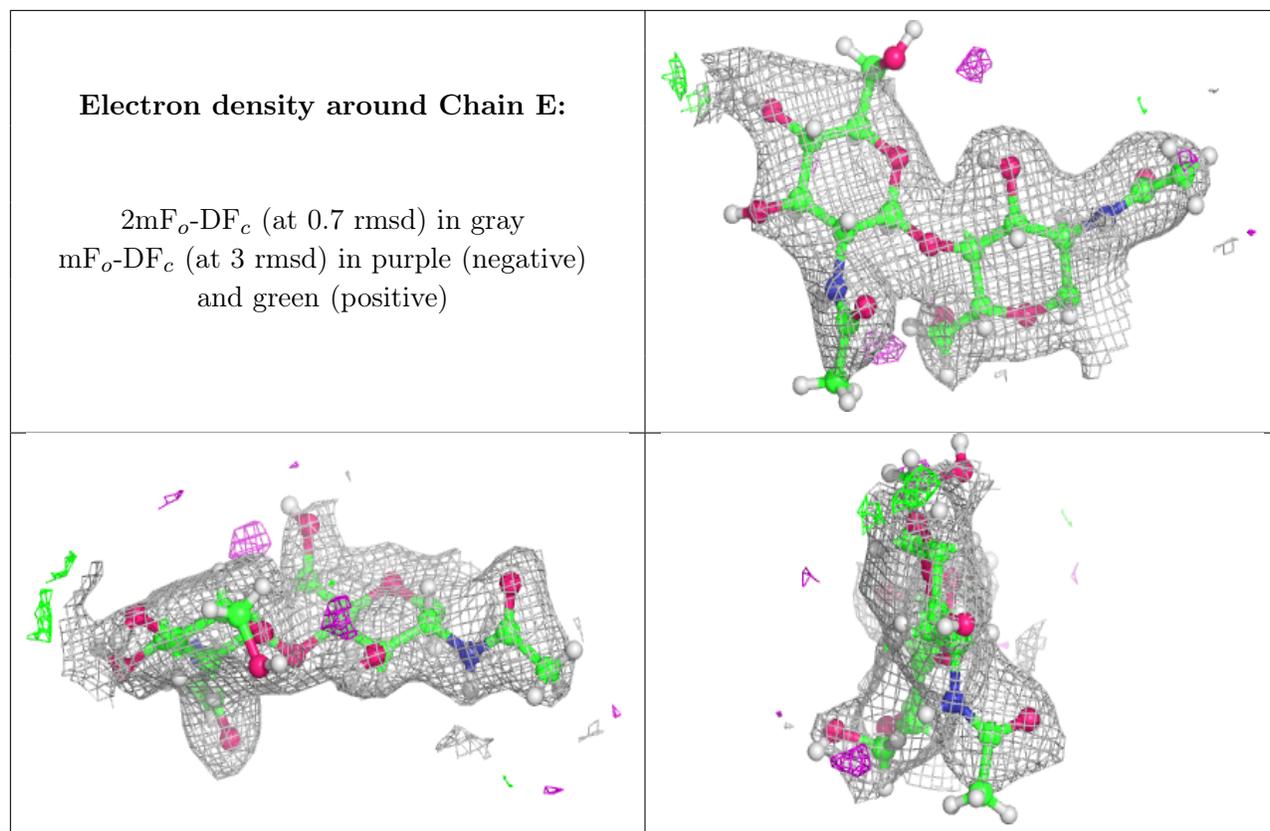
Electron density around Chain F:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
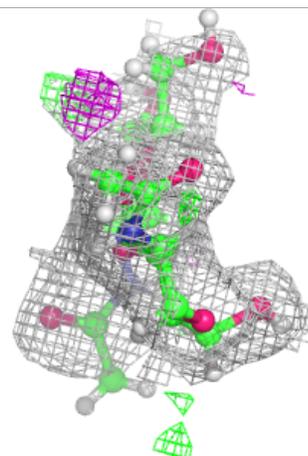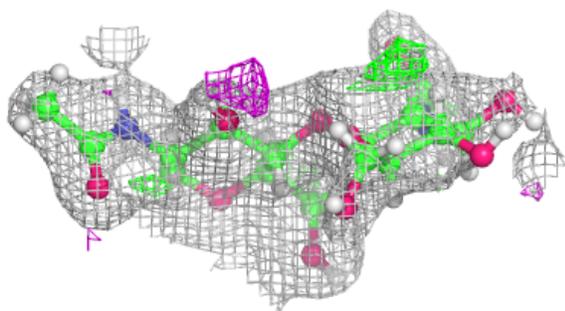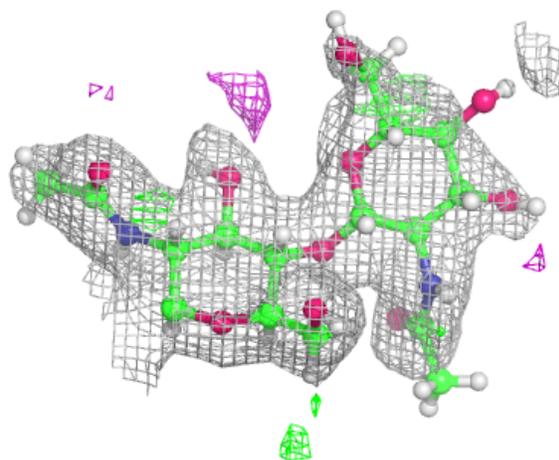
Electron density around Chain G:

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

Electron density around Chain H:

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

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	B	508	14/15	0.59	0.44	116,138,163,165	0
7	NAG	A	511	14/15	0.67	0.24	65,101,148,164	0
7	NAG	B	509	14/15	0.68	0.49	97,140,168,173	0
7	NAG	A	516	14/15	0.86	0.34	68,91,111,113	0
6	CA	A	503	1/1	0.94	0.34	68,68,68,68	0
6	CA	B	502	1/1	0.98	0.04	43,43,43,43	0
8	MG	B	501	1/1	0.98	0.10	26,26,26,26	0
6	CA	A	501	1/1	0.99	0.11	33,33,33,33	0
6	CA	A	504	1/1	0.99	0.21	45,45,45,45	0
6	CA	B	503	1/1	1.00	0.13	26,26,26,26	0
6	CA	A	502	1/1	1.00	0.15	31,31,31,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.