



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 07:03 PM EDT

PDB ID : 6A5E / pdb_00006a5e
Title : Crystal structure of plant peptide RALF23 in complex with FER and LLG2
Authors : Xiao, Y.; Chai, J.
Deposited on : 2018-06-23
Resolution : 2.77 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

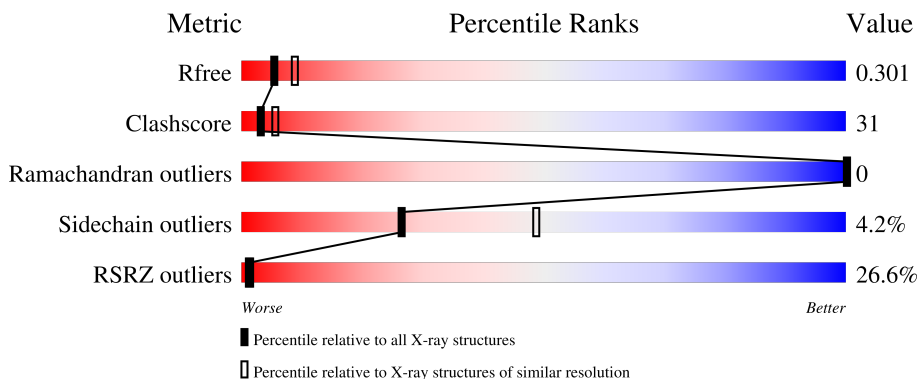
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 $\leq 5\%$. 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	396	
1	B	396	
2	C	84	
2	D	84	
3	E	15	

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Mol	Chain	Length	Quality of chain
3	F	15	
4	G	2	
4	H	2	
4	I	2	
4	J	2	

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	B	1004	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7564 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 Receptor-like protein kinase FERONIA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	375	2924	1871	466	577	10	0	0	0
1	B	375	2924	1871	466	577	10	0	0	0

- Molecule 2 is a protein called GPI-anchored protein LLG2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	84	650	408	105	127	10	0	0	0
2	D	84	650	408	105	127	10	0	0	0

- Molecule 3 is a protein called RALF23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	15	124	78	25	20	1	0	0	0
3	F	15	124	78	25	20	1	0	0	0

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



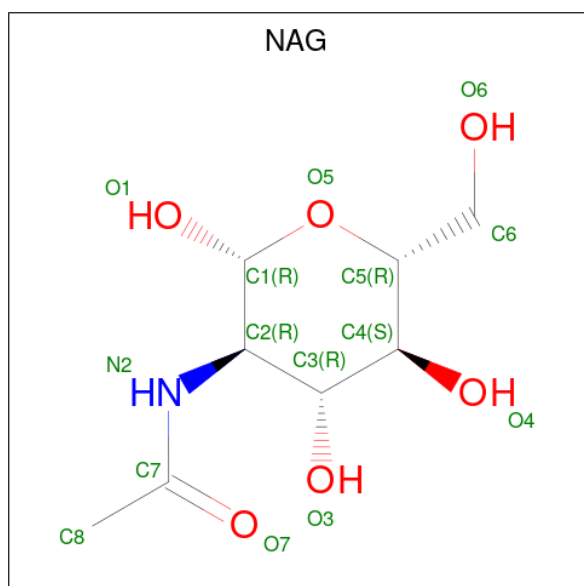
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	G	2	28	16	2	10	0	0	0

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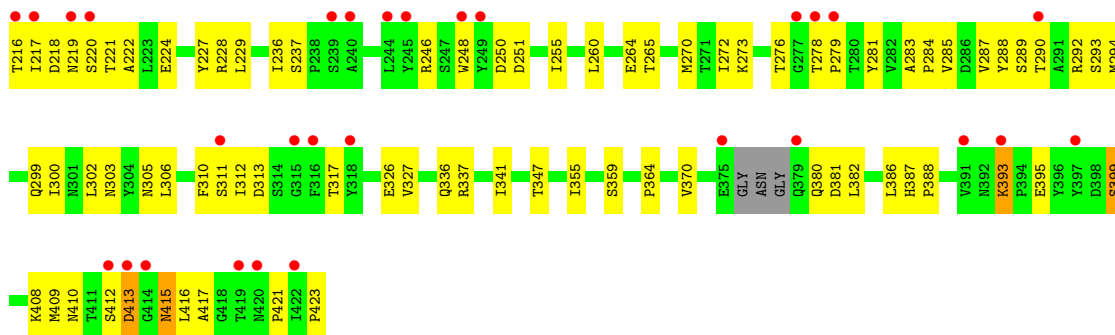
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	H	2	Total 28	C 16	N 2	O 10	0	0	0
4	I	2	Total 28	C 16	N 2	O 10	0	0	0
4	J	2	Total 28	C 16	N 2	O 10	0	0	0

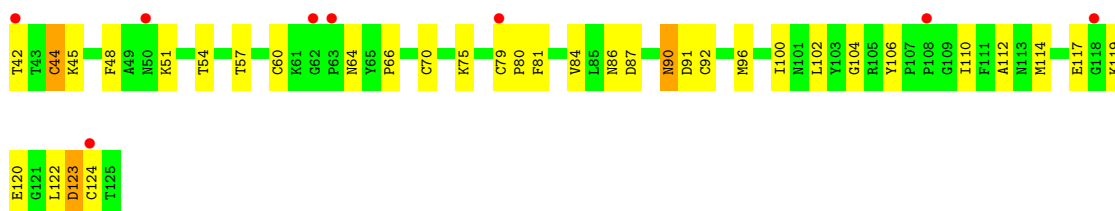
- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



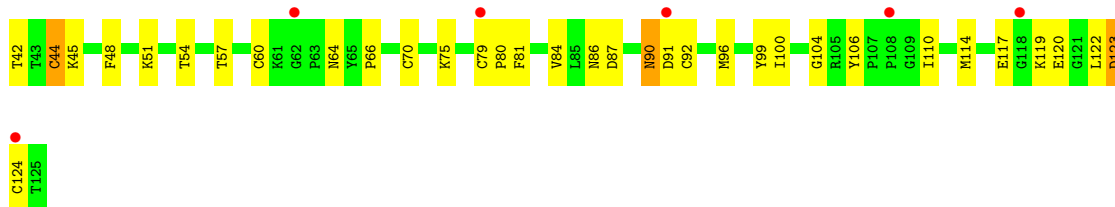
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	Total 14	C 8	N 1	O 5	0	0
5	C	1	Total 14	C 8	N 1	O 5	0	0
5	D	1	Total 14	C 8	N 1	O 5	0	0
5	B	1	Total 14	C 8	N 1	O 5	0	0



- Molecule 2: GPI-anchored protein LLG2



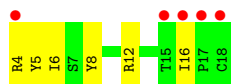
- Molecule 2: GPI-anchored protein LLG2



- Molecule 3: RALF23



- Molecule 3: RALF23



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

Chain G:  100%

MAG1
MAG2

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

Chain H:  100%


MAG1
MAG2

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

Chain I:  100%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.31Å 62.36Å 97.48Å 105.72° 91.30° 108.48°	Depositor
Resolution (Å)	42.61 – 2.77 42.61 – 2.77	Depositor EDS
% Data completeness (in resolution range)	96.5 (42.61-2.77) 96.5 (42.61-2.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.77Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.233 , 0.285 0.266 , 0.301	Depositor DCC
R_{free} test set	1674 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtrriage
Anisotropy	0.307	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7564	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.27% 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: 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	0.96	3/3002 (0.1%)	0.99	19/4106 (0.5%)
1	B	0.96	3/3002 (0.1%)	0.99	19/4106 (0.5%)
2	C	1.01	3/665 (0.5%)	1.05	6/898 (0.7%)
2	D	1.01	3/665 (0.5%)	1.05	6/898 (0.7%)
3	E	0.71	0/126	1.02	1/169 (0.6%)
3	F	0.71	0/126	1.01	1/169 (0.6%)
All	All	0.96	12/7586 (0.2%)	1.00	52/10346 (0.5%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	92	CYS	CB-SG	-9.25	1.50	1.81
2	D	92	CYS	CB-SG	-9.25	1.50	1.81
2	D	44	CYS	CB-SG	-8.39	1.53	1.81
2	C	44	CYS	CB-SG	-8.38	1.53	1.81
1	A	393	LYS	C-O	-7.45	1.20	1.23

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	92	CYS	CA-CB-SG	12.62	143.42	114.40
2	C	92	CYS	CA-CB-SG	12.59	143.36	114.40
2	C	92	CYS	N-CA-C	9.85	121.77	111.14
2	D	92	CYS	N-CA-C	9.83	121.76	111.14
2	C	123	ASP	N-CA-C	7.89	119.51	111.07

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	2924	0	2793	200	0
1	B	2924	0	2793	198	0
2	C	650	0	606	31	0
2	D	650	0	606	29	0
3	E	124	0	127	11	0
3	F	124	0	127	6	0
4	G	28	0	25	2	0
4	H	28	0	25	1	0
4	I	28	0	25	1	0
4	J	28	0	25	2	0
5	A	14	0	13	3	0
5	B	14	0	13	3	0
5	C	14	0	13	0	0
5	D	14	0	13	0	0
All	All	7564	0	7204	456	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 31.

The worst 5 of 456 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:305:ASN:HD21	4:J:1:NAG:C1	1.07	1.60
1:A:305:ASN:HD21	4:G:1:NAG:C1	1.07	1.58
1:A:123:LEU:HD23	1:A:184:TYR:CZ	1.53	1.43
1:B:123:LEU:HD23	1:B:184:TYR:CZ	1.53	1.40
1:A:222:ALA:H	1:A:410:ASN:ND2	1.18	1.38

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	363/396 (92%)	348 (96%)	15 (4%)	0	100	100
1	B	363/396 (92%)	348 (96%)	15 (4%)	0	100	100
2	C	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	D	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
3	E	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
3	F	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
All	All	916/990 (92%)	874 (95%)	42 (5%)	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	329/344 (96%)	313 (95%)	16 (5%)	22	43
1	B	329/344 (96%)	313 (95%)	16 (5%)	22	43
2	C	72/72 (100%)	71 (99%)	1 (1%)	59	75
2	D	72/72 (100%)	71 (99%)	1 (1%)	59	75
3	E	13/13 (100%)	12 (92%)	1 (8%)	12	22
3	F	13/13 (100%)	13 (100%)	0	100	100
All	All	828/858 (96%)	793 (96%)	35 (4%)	26	49

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	170	LEU
1	B	201	SER
1	B	276	THR
1	A	208	MET
1	A	205	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	234	ASN
1	B	379	GLN
1	B	410	ASN
1	B	387	HIS
1	B	305	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	$\# Z > 2$
4	NAG	G	1	4	14,14,15	0.34	0	17,19,21	0.62	0
4	NAG	G	2	4	14,14,15	0.47	0	17,19,21	1.19	1 (5%)
4	NAG	H	1	4,1	14,14,15	0.83	0	17,19,21	2.62	5 (29%)
4	NAG	H	2	4	14,14,15	1.00	0	17,19,21	1.95	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	I	1	4,1	14,14,15	0.83	0	17,19,21	2.62	5 (29%)
4	NAG	I	2	4	14,14,15	1.00	0	17,19,21	1.95	6 (35%)
4	NAG	J	1	4	14,14,15	0.33	0	17,19,21	0.62	0
4	NAG	J	2	4	14,14,15	0.47	0	17,19,21	1.19	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	H	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	H	2	4	-	4/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	I	2	4	-	4/6/23/26	0/1/1/1
4	NAG	J	1	4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	NAG	C4-C3-C2	-5.59	102.82	111.02
4	H	1	NAG	C4-C3-C2	-5.58	102.84	111.02
4	H	1	NAG	C1-O5-C5	5.52	119.59	112.19
4	I	1	NAG	C1-O5-C5	5.51	119.57	112.19
4	H	1	NAG	O4-C4-C5	5.03	121.72	109.32

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

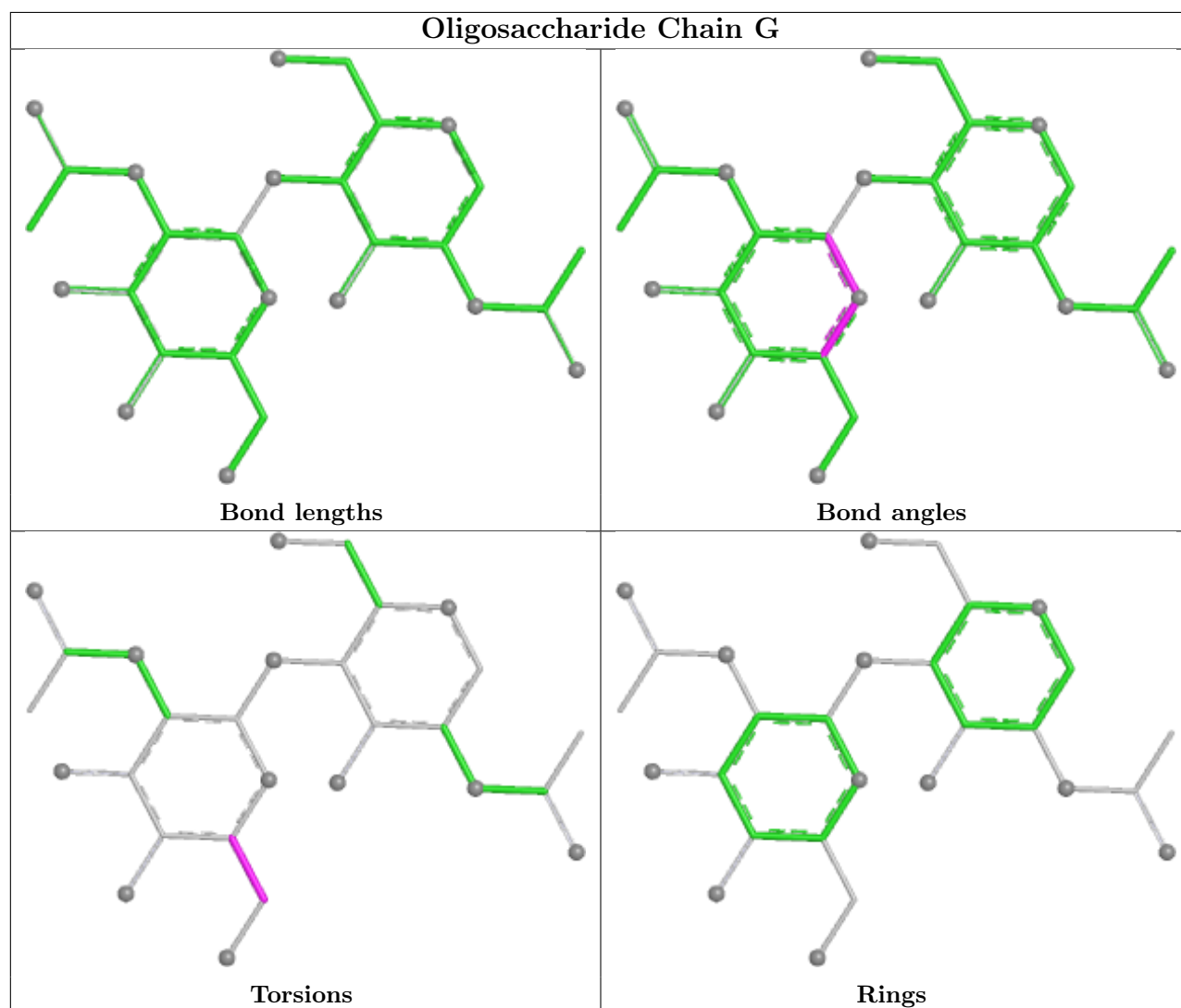
Mol	Chain	Res	Type	Atoms
4	J	2	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6

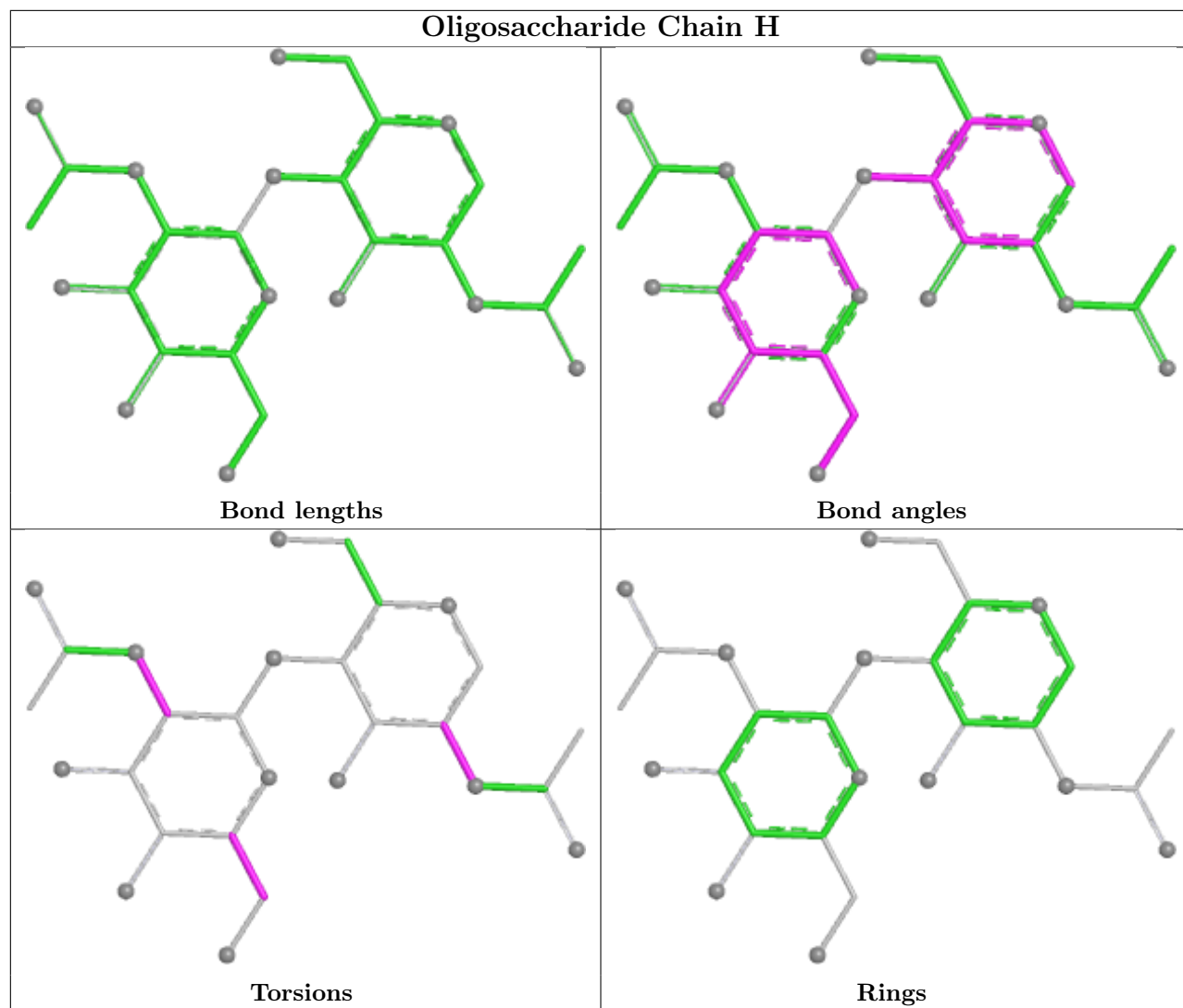
There are no ring outliers.

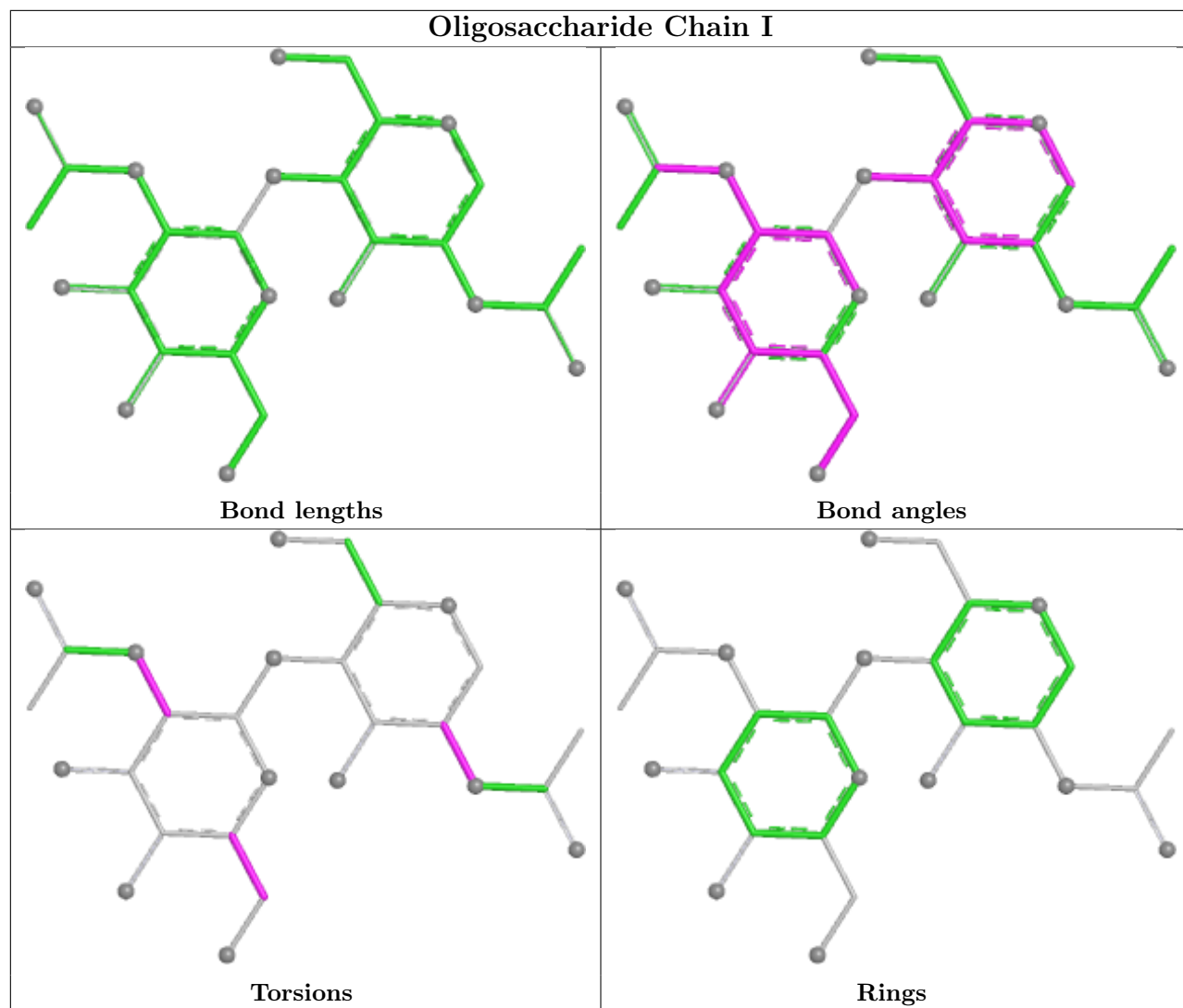
6 monomers are involved in 6 short contacts:

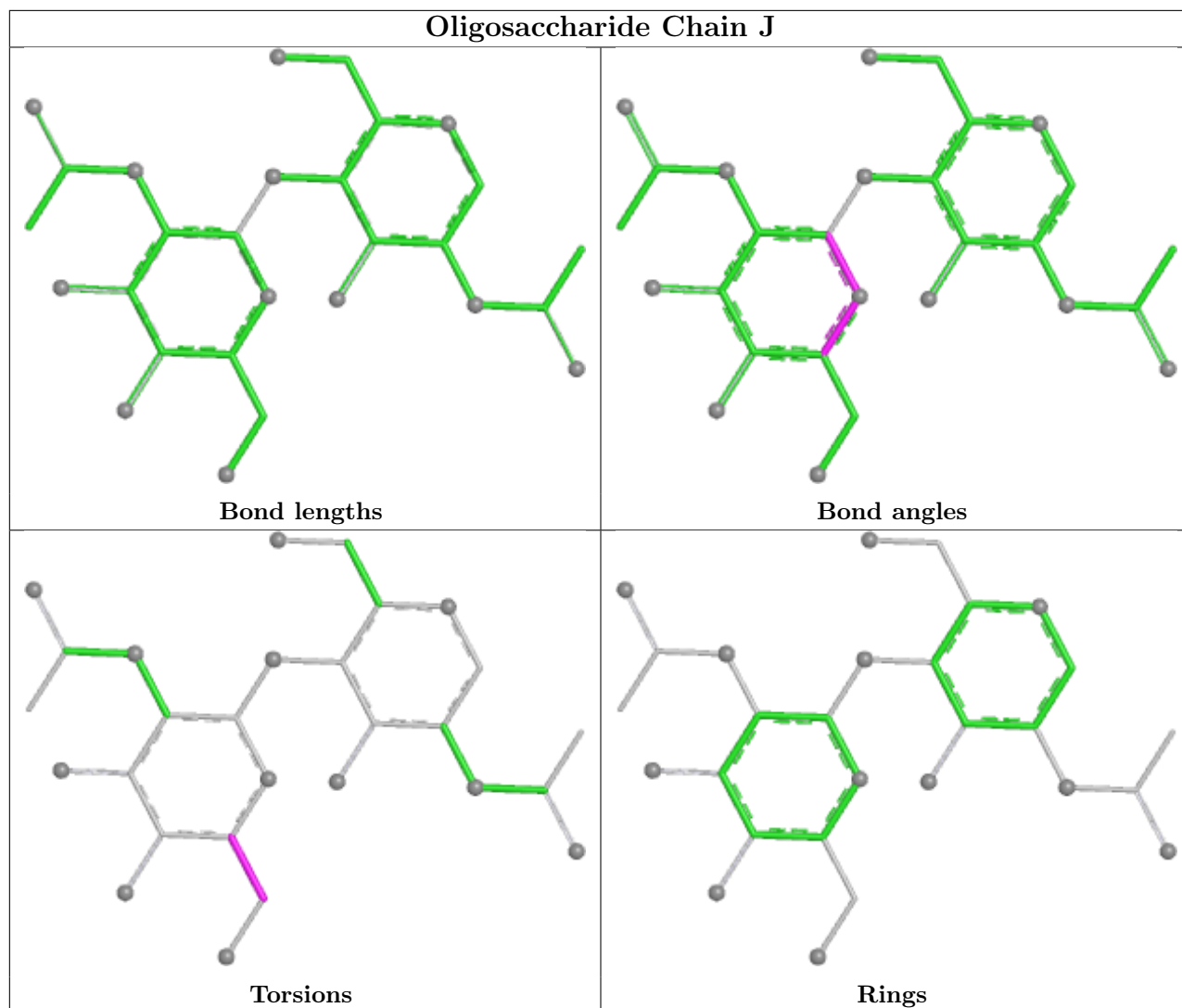
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	1	0
4	J	1	NAG	2	0
4	G	1	NAG	2	0
4	H	1	NAG	1	0
4	I	2	NAG	1	0
4	H	2	NAG	1	0

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 [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	B	1004	1	14,14,15	0.42	0	17,19,21	1.16	2 (11%)
5	NAG	A	1004	1	14,14,15	0.43	0	17,19,21	1.16	2 (11%)
5	NAG	D	1001	2	14,14,15	0.53	0	17,19,21	0.65	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	202	2	14,14,15	0.53	0	17,19,21	0.65	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1004	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1004	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1001	2	-	2/6/23/26	0/1/1/1
5	NAG	C	202	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1004	NAG	C8-C7-N2	2.38	120.06	116.12
5	A	1004	NAG	C8-C7-N2	2.36	120.03	116.12
5	A	1004	NAG	C2-N2-C7	-2.16	120.01	122.90
5	B	1004	NAG	C2-N2-C7	-2.13	120.05	122.90
5	C	202	NAG	C1-O5-C5	2.12	115.02	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	202	NAG	O5-C5-C6-O6
5	D	1001	NAG	O5-C5-C6-O6
5	C	202	NAG	C4-C5-C6-O6
5	D	1001	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1004	NAG	3	0
5	A	1004	NAG	3	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	375/396 (94%)	1.37	102 (27%) 1 1	31, 69, 122, 147	0
1	B	375/396 (94%)	1.58	127 (33%) 1 0	31, 69, 122, 147	0
2	C	84/84 (100%)	0.83	8 (9%) 14 13	30, 52, 92, 97	0
2	D	84/84 (100%)	0.90	6 (7%) 22 22	30, 52, 92, 97	0
3	E	15/15 (100%)	1.36	4 (26%) 1 1	44, 61, 100, 115	0
3	F	15/15 (100%)	1.48	5 (33%) 1 0	44, 61, 100, 115	0
All	All	948/990 (95%)	1.36	252 (26%) 1 1	30, 64, 117, 147	0

The worst 5 of 252 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	179	ALA	5.3
1	B	71	SER	5.2
1	A	93	VAL	4.9
1	B	205	THR	4.8
1	A	76	ALA	4.6

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

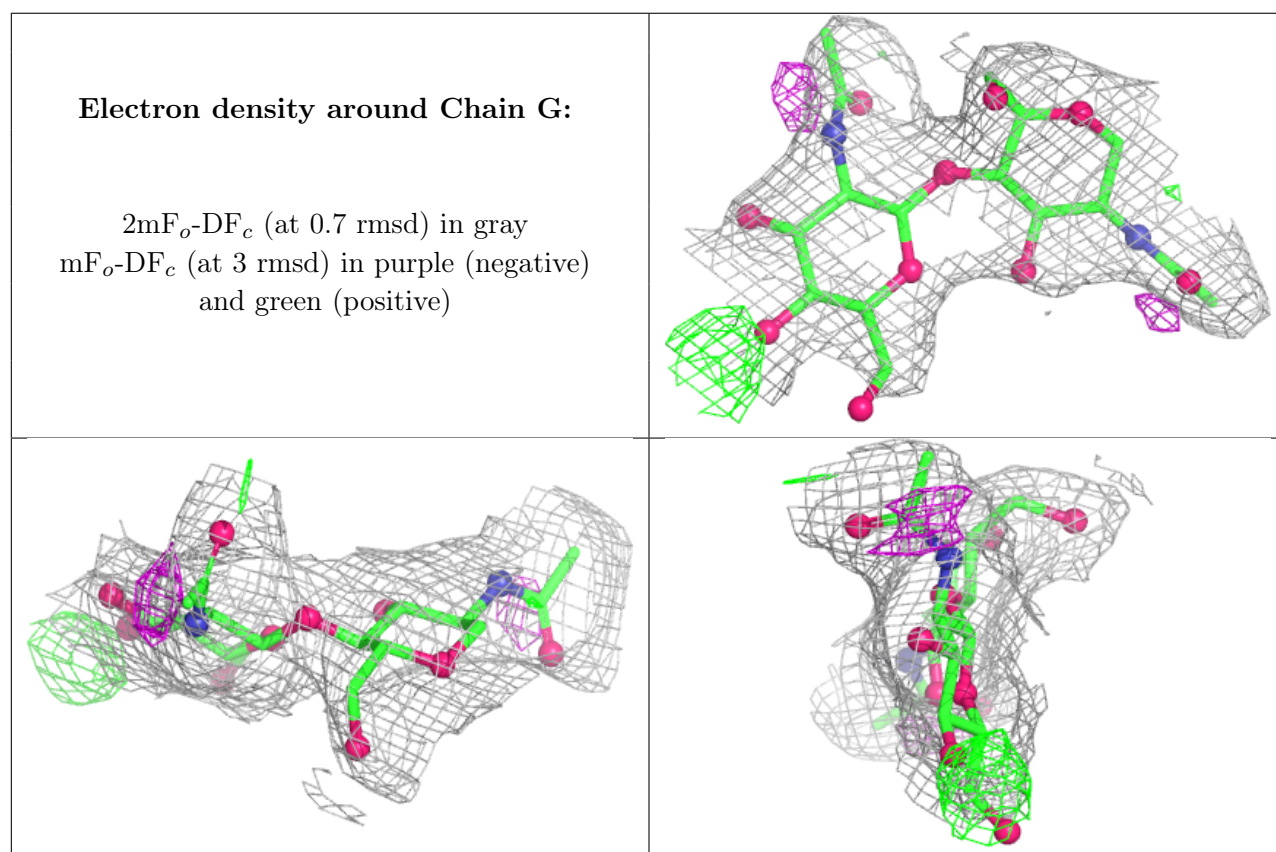
There are no non-standard protein/DNA/RNA residues in this entry.

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.

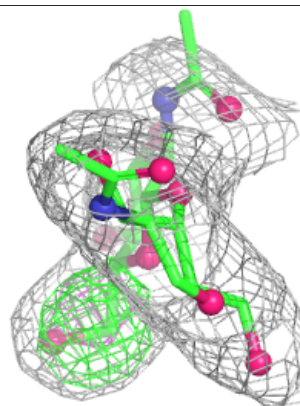
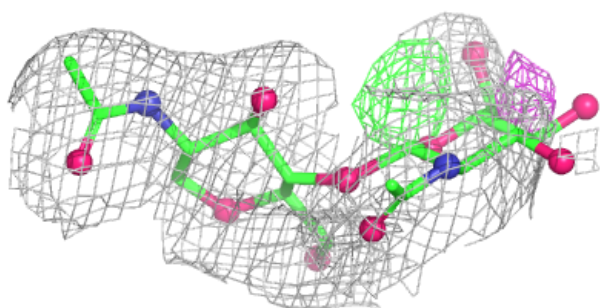
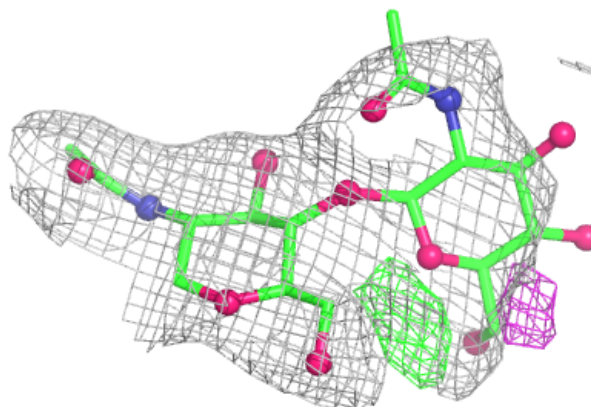
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	I	2	14/15	0.61	0.24	41,96,111,121	0
4	NAG	H	2	14/15	0.62	0.22	41,96,111,121	0
4	NAG	G	2	14/15	0.69	0.18	41,63,113,116	0
4	NAG	J	2	14/15	0.73	0.19	41,63,113,116	0
4	NAG	I	1	14/15	0.79	0.15	48,67,107,112	0
4	NAG	G	1	14/15	0.83	0.15	19,44,66,69	0
4	NAG	H	1	14/15	0.87	0.12	48,67,107,112	0
4	NAG	J	1	14/15	0.88	0.12	19,44,66,69	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.

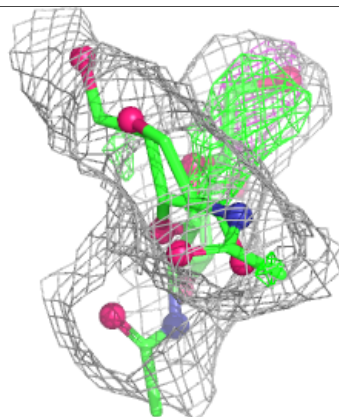
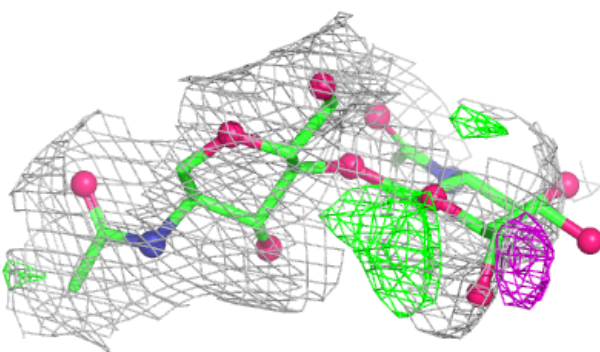
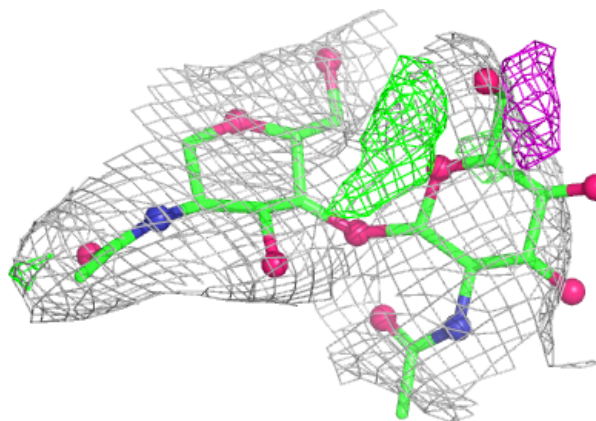


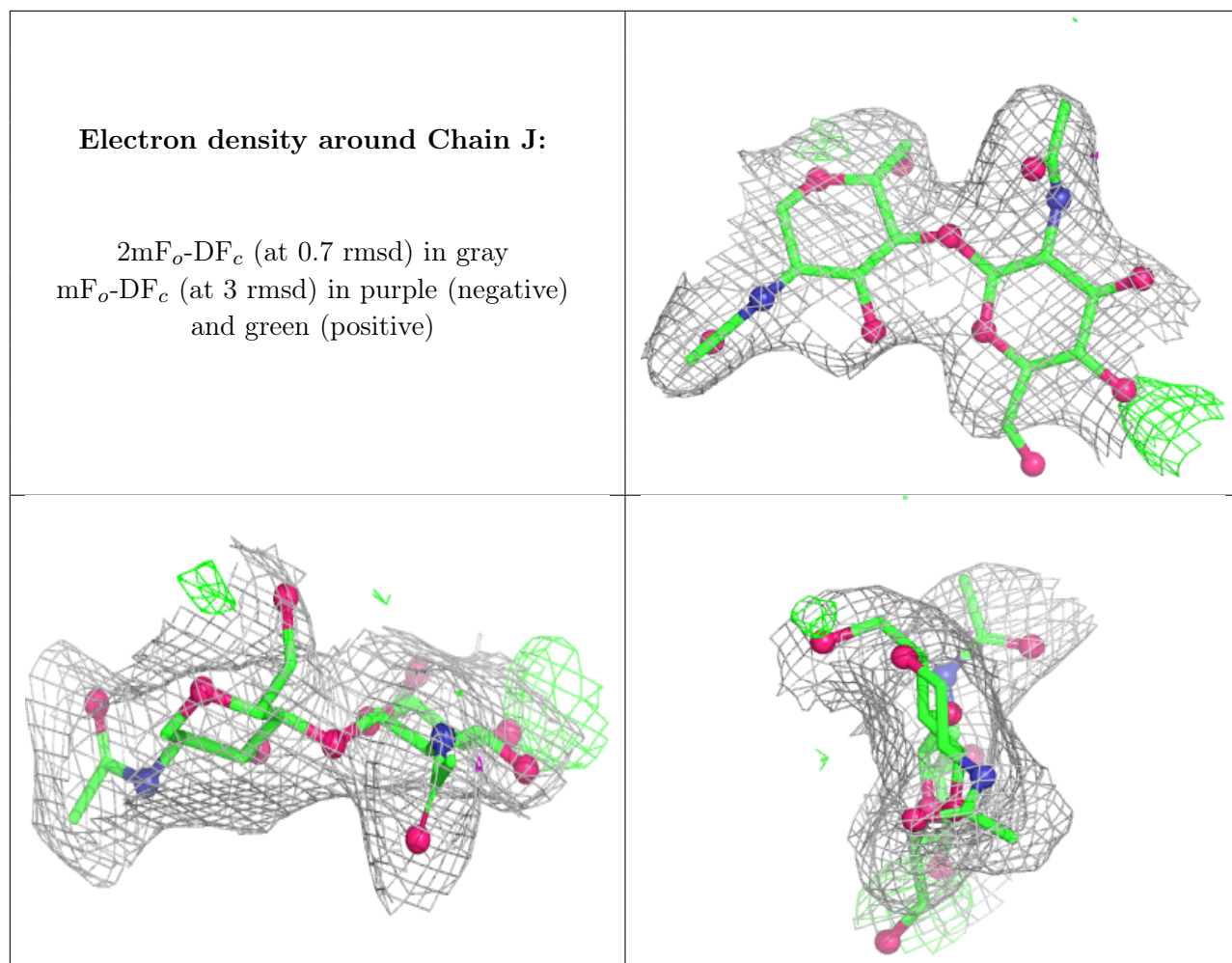
Electron density around Chain H:

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

**Electron density around Chain I:**

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





6.4 Ligands [i](#)

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
5	NAG	B	1004	14/15	0.52	0.41	20,20,20,20	0
5	NAG	A	1004	14/15	0.53	0.36	20,20,20,20	0
5	NAG	D	1001	14/15	0.71	0.20	67,107,148,151	0
5	NAG	C	202	14/15	0.71	0.21	67,107,148,151	0

6.5 Other polymers [i](#)

There are no such residues in this entry.