



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 15, 2024 – 08:20 AM JST

PDB ID : 5XWU
Title : Crystal structure of PTPdelta Ig1-Ig3 in complex with SALM2 LRR-Ig
Authors : Goto-Ito, S.; Yamagata, A.; Sato, Y.; Fukai, S.
Deposited on : 2017-06-30
Resolution : 3.16 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

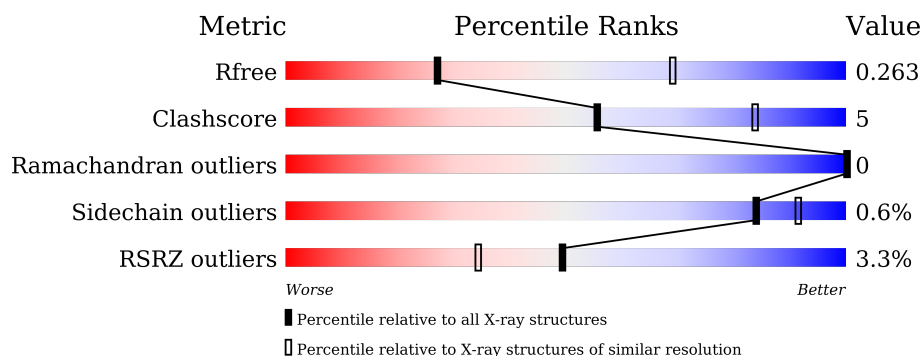
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2168 (3.20-3.12)
Clashscore	180529	2333 (3.20-3.12)
Ramachandran outliers	177936	2266 (3.20-3.12)
Sidechain outliers	177891	2265 (3.20-3.12)
RSRZ outliers	164620	2169 (3.20-3.12)

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	313	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>6%</div> </div> </div>
1	C	313	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>6%</div> </div> </div>
2	B	365	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>6%</div> </div> </div>
2	D	365	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>7%</div> </div> </div>
3	E	2	<div> <div></div> <div>100%</div> </div>
3	F	2	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	2	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9973 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-type tyrosine-protein phosphatase delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2259	1403	405	438	13			
1	C	294	Total	C	N	O	S	0	0	0
			2268	1408	406	441	13			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	LEU	-	expression tag	UNP Q64487
A	23	MET	-	expression tag	UNP Q64487
A	24	GLY	-	expression tag	UNP Q64487
A	25	CYS	-	expression tag	UNP Q64487
A	26	VAL	-	expression tag	UNP Q64487
A	329	HIS	-	expression tag	UNP Q64487
A	330	HIS	-	expression tag	UNP Q64487
A	331	HIS	-	expression tag	UNP Q64487
A	332	HIS	-	expression tag	UNP Q64487
A	333	HIS	-	expression tag	UNP Q64487
A	334	HIS	-	expression tag	UNP Q64487
C	22	LEU	-	expression tag	UNP Q64487
C	23	MET	-	expression tag	UNP Q64487
C	24	GLY	-	expression tag	UNP Q64487
C	25	CYS	-	expression tag	UNP Q64487
C	26	VAL	-	expression tag	UNP Q64487
C	329	HIS	-	expression tag	UNP Q64487
C	330	HIS	-	expression tag	UNP Q64487
C	331	HIS	-	expression tag	UNP Q64487
C	332	HIS	-	expression tag	UNP Q64487
C	333	HIS	-	expression tag	UNP Q64487
C	334	HIS	-	expression tag	UNP Q64487

- Molecule 2 is a protein called Leucine-rich repeat and fibronectin type III domain-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	343	Total	C	N	O	S	0	0	0
			2651	1658	487	491	15			
2	D	340	Total	C	N	O	S	0	0	0
			2631	1643	484	489	15			

There are 12 discrepancies between the modelled and reference sequences:

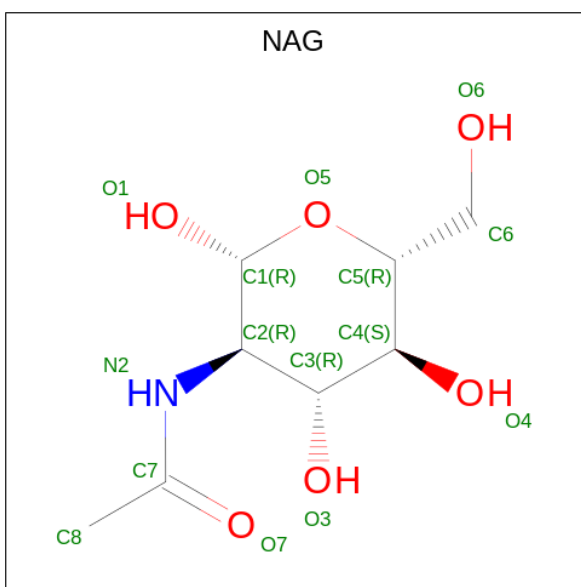
Chain	Residue	Modelled	Actual	Comment	Reference
B	391	HIS	-	expression tag	UNP Q2WF71
B	392	HIS	-	expression tag	UNP Q2WF71
B	393	HIS	-	expression tag	UNP Q2WF71
B	394	HIS	-	expression tag	UNP Q2WF71
B	395	HIS	-	expression tag	UNP Q2WF71
B	396	HIS	-	expression tag	UNP Q2WF71
D	391	HIS	-	expression tag	UNP Q2WF71
D	392	HIS	-	expression tag	UNP Q2WF71
D	393	HIS	-	expression tag	UNP Q2WF71
D	394	HIS	-	expression tag	UNP Q2WF71
D	395	HIS	-	expression tag	UNP Q2WF71
D	396	HIS	-	expression tag	UNP Q2WF71

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



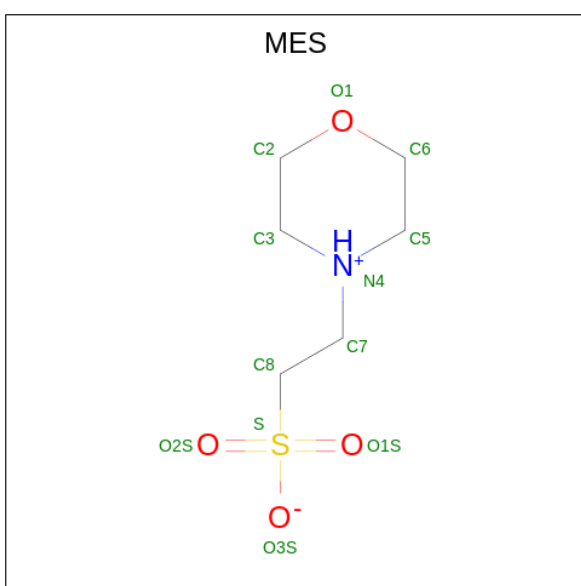
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).

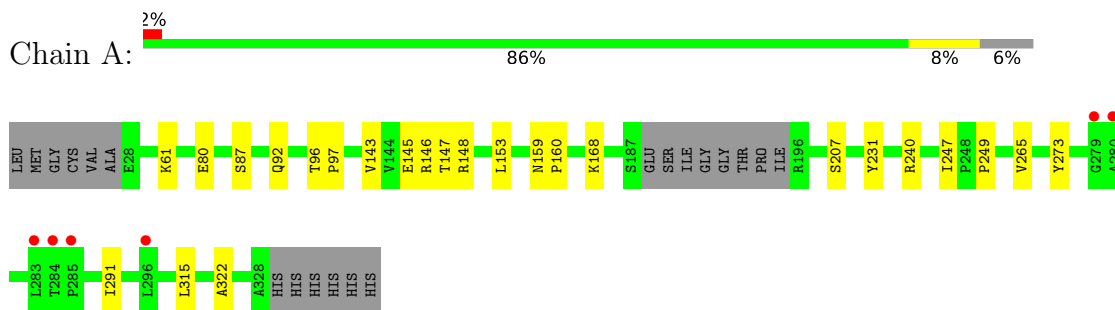


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

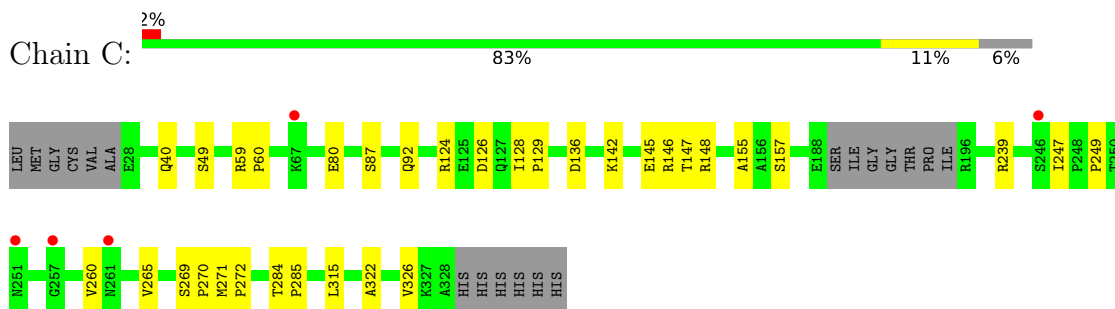
3 Residue-property plots [i](#)

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.

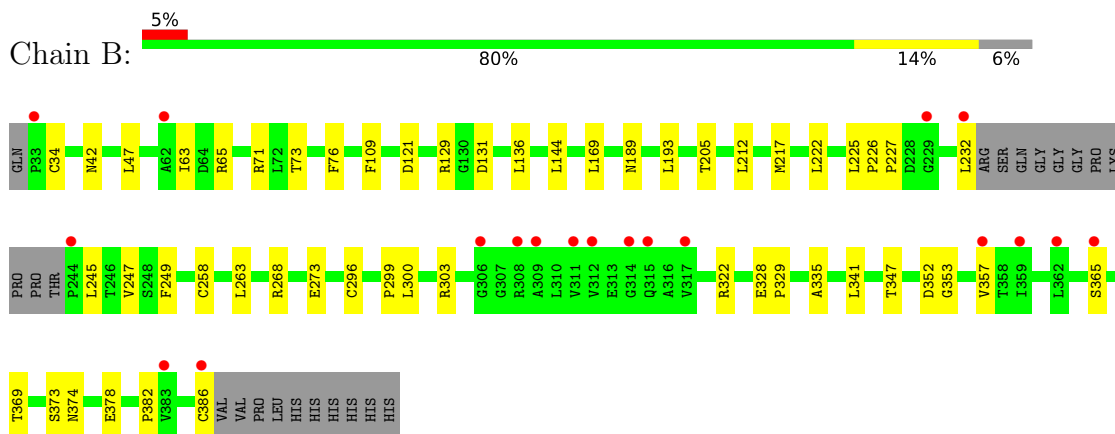
- Molecule 1: Receptor-type tyrosine-protein phosphatase delta



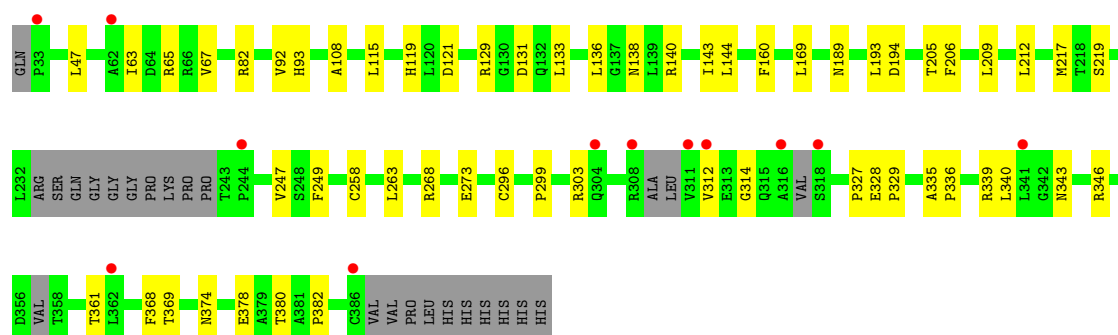
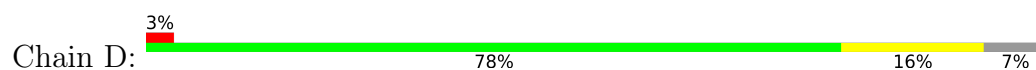
- Molecule 1: Receptor-type tyrosine-protein phosphatase delta



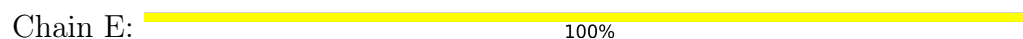
- Molecule 2: Leucine-rich repeat and fibronectin type III domain-containing protein 1



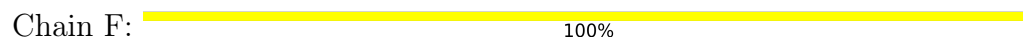
- Molecule 2: Leucine-rich repeat and fibronectin type III domain-containing protein 1



- 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 3: 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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.04Å 127.20Å 210.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.71 – 3.16 48.71 – 3.16	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.71-3.16) 98.6 (48.71-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.218 , 0.259 0.227 , 0.263	Depositor DCC
R_{free} test set	2072 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9973	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6165e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, MES

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	0.22	0/2301	0.40	0/3127
1	C	0.22	0/2310	0.41	0/3139
2	B	0.22	0/2699	0.41	0/3673
2	D	0.22	0/2676	0.41	0/3637
All	All	0.22	0/9986	0.41	0/13576

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	2259	0	2244	16	0
1	C	2268	0	2250	18	0
2	B	2651	0	2651	29	0
2	D	2631	0	2621	33	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	2	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	28	0	26	0	0
5	A	12	0	12	1	0
5	C	12	0	12	1	0
All	All	9973	0	9917	91	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 5.

The worst 5 of 91 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:145:GLU:OE1	1:A:148:ARG:NH1	2.24	0.70
1:C:124:ARG:NH1	1:C:126:ASP:OD2	2.25	0.70
1:C:249:PRO:HB2	1:C:322:ALA:HB2	1.77	0.66
1:C:40:GLN:NE2	1:C:49:SER:O	2.31	0.64
2:D:346:ARG:NH1	2:D:361:THR:OG1	2.31	0.64

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	289/313 (92%)	274 (95%)	15 (5%)	0	100	100
1	C	290/313 (93%)	273 (94%)	17 (6%)	0	100	100
2	B	339/365 (93%)	313 (92%)	26 (8%)	0	100	100
2	D	330/365 (90%)	303 (92%)	27 (8%)	0	100	100
All	All	1248/1356 (92%)	1163 (93%)	85 (7%)	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	253/269 (94%)	253 (100%)	0	100	100
1	C	254/269 (94%)	252 (99%)	2 (1%)	79	89
2	B	290/309 (94%)	288 (99%)	2 (1%)	81	90
2	D	288/309 (93%)	285 (99%)	3 (1%)	73	85
All	All	1085/1156 (94%)	1078 (99%)	7 (1%)	84	91

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	326	VAL
2	D	205	THR
2	D	380	THR
2	D	343	ASN
1	C	260	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	103	GLN
2	B	304	GLN
1	C	74	GLN

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 ⓘ

6 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	1.52	2 (14%)	17,19,21	1.24	2 (11%)
3	NAG	E	2	3	14,14,15	1.48	2 (14%)	17,19,21	1.10	1 (5%)
3	NAG	F	1	2,3	14,14,15	1.46	2 (14%)	17,19,21	1.10	1 (5%)
3	NAG	F	2	3	14,14,15	1.59	2 (14%)	17,19,21	1.25	2 (11%)
3	NAG	G	1	2,3	14,14,15	1.51	2 (14%)	17,19,21	1.42	3 (17%)
3	NAG	G	2	3	14,14,15	1.52	2 (14%)	17,19,21	1.22	3 (17%)

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	NAG	O5-C1	4.12	1.50	1.43
3	E	1	NAG	O5-C1	3.79	1.49	1.43
3	G	2	NAG	O5-C1	3.78	1.49	1.43
3	G	1	NAG	O5-C1	3.70	1.49	1.43
3	F	1	NAG	O5-C1	3.65	1.49	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	C8-C7-N2	2.77	120.78	116.10
3	F	1	NAG	C4-C3-C2	2.72	115.00	111.02
3	F	2	NAG	C1-O5-C5	2.67	115.81	112.19
3	E	1	NAG	C4-C3-C2	2.60	114.83	111.02
3	G	1	NAG	C1-O5-C5	2.55	115.65	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

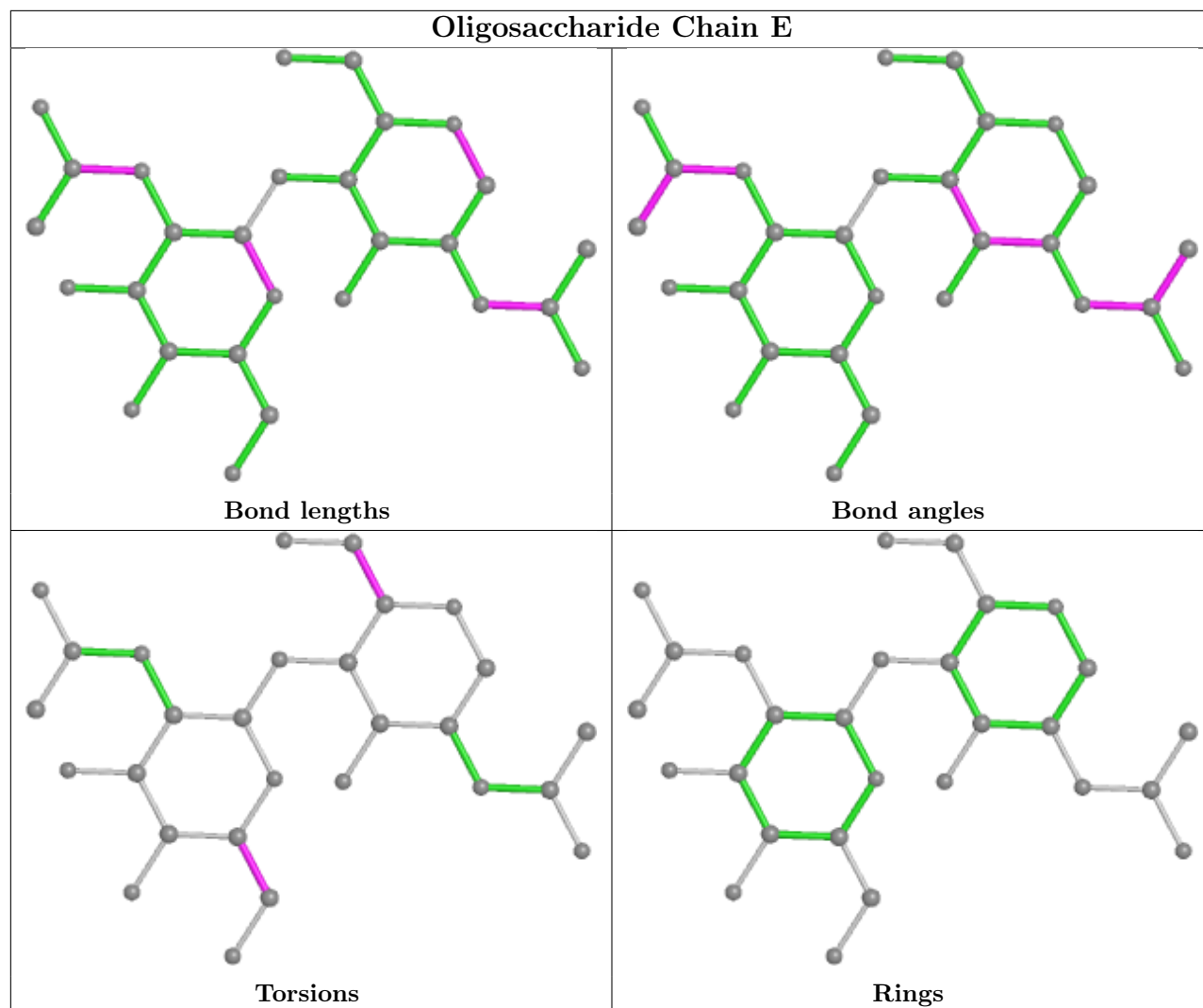
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6

There are no ring outliers.

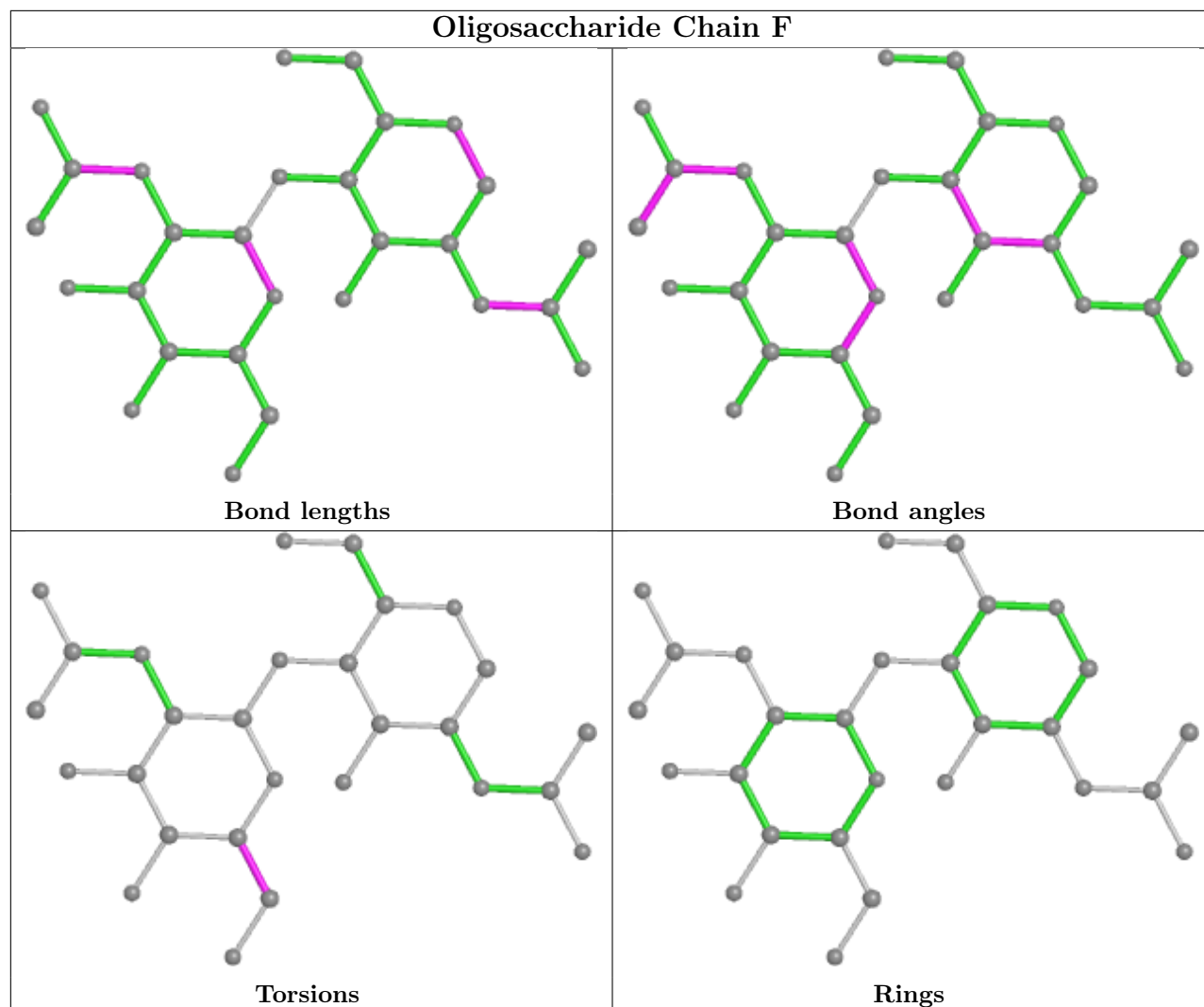
2 monomers are involved in 2 short contacts:

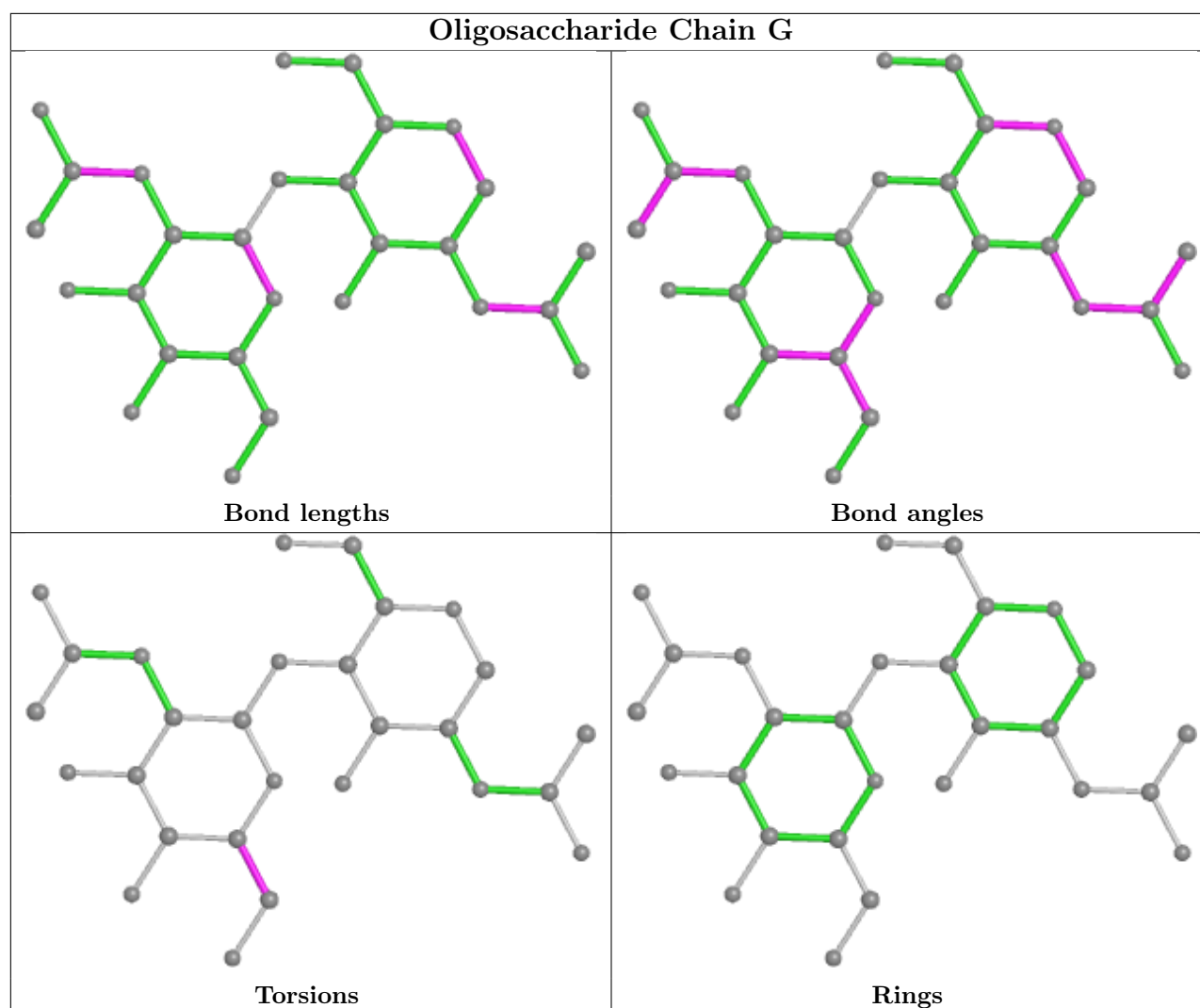
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	NAG	2	0
3	G	1	NAG	2	0

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



Oligosaccharide Chain F





5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
4	NAG	C	601	1	14,14,15	1.56	2 (14%)	17,19,21	1.07	1 (5%)
4	NAG	A	601	1	14,14,15	1.58	2 (14%)	17,19,21	1.08	1 (5%)
4	NAG	B	603	2	14,14,15	1.66	4 (28%)	17,19,21	1.86	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MES	A	604	-	12,12,12	2.26	1 (8%)	14,16,16	1.95	6 (42%)
4	NAG	C	602	1	14,14,15	1.57	2 (14%)	17,19,21	1.21	1 (5%)
5	MES	C	603	-	12,12,12	2.27	1 (8%)	14,16,16	1.92	3 (21%)

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	C	601	1	-	2/6/23/26	0/1/1/1
4	NAG	A	601	1	-	1/6/23/26	0/1/1/1
4	NAG	B	603	2	-	2/6/23/26	0/1/1/1
5	MES	A	604	-	-	1/6/14/14	0/1/1/1
4	NAG	C	602	1	-	0/6/23/26	0/1/1/1
5	MES	C	603	-	-	4/6/14/14	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	603	MES	C8-S	-7.59	1.66	1.77
5	A	604	MES	C8-S	-7.55	1.66	1.77
4	B	603	NAG	O5-C1	4.14	1.50	1.43
4	C	602	NAG	O5-C1	4.05	1.50	1.43
4	A	601	NAG	O5-C1	4.04	1.50	1.43

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	603	NAG	C1-O5-C5	5.90	120.18	112.19
5	C	603	MES	C5-N4-C3	4.68	119.36	108.83
5	A	604	MES	C5-N4-C3	4.32	118.56	108.83
5	A	604	MES	C6-C5-N4	-2.73	105.96	110.10
4	B	603	NAG	O5-C1-C2	2.71	115.56	111.29

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	603	MES	C7-C8-S-O2S

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Mol	Chain	Res	Type	Atoms
5	C	603	MES	C7-C8-S-O3S
4	B	603	NAG	O5-C5-C6-O6
4	B	603	NAG	C4-C5-C6-O6
4	C	601	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	604	MES	1	0
5	C	603	MES	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	293/313 (93%)	-0.16	6 (2%) 64 49	21, 53, 97, 115	0
1	C	294/313 (93%)	-0.11	5 (1%) 69 53	25, 54, 96, 128	0
2	B	343/365 (93%)	-0.12	19 (5%) 32 20	17, 43, 123, 170	0
2	D	340/365 (93%)	-0.10	12 (3%) 47 32	17, 44, 126, 139	0
All	All	1270/1356 (93%)	-0.12	42 (3%) 49 34	17, 49, 114, 170	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	311	VAL	6.4
2	B	244	PRO	4.6
2	B	315	GLN	3.7
2	D	341	LEU	3.7
2	D	386	CYS	3.6

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.

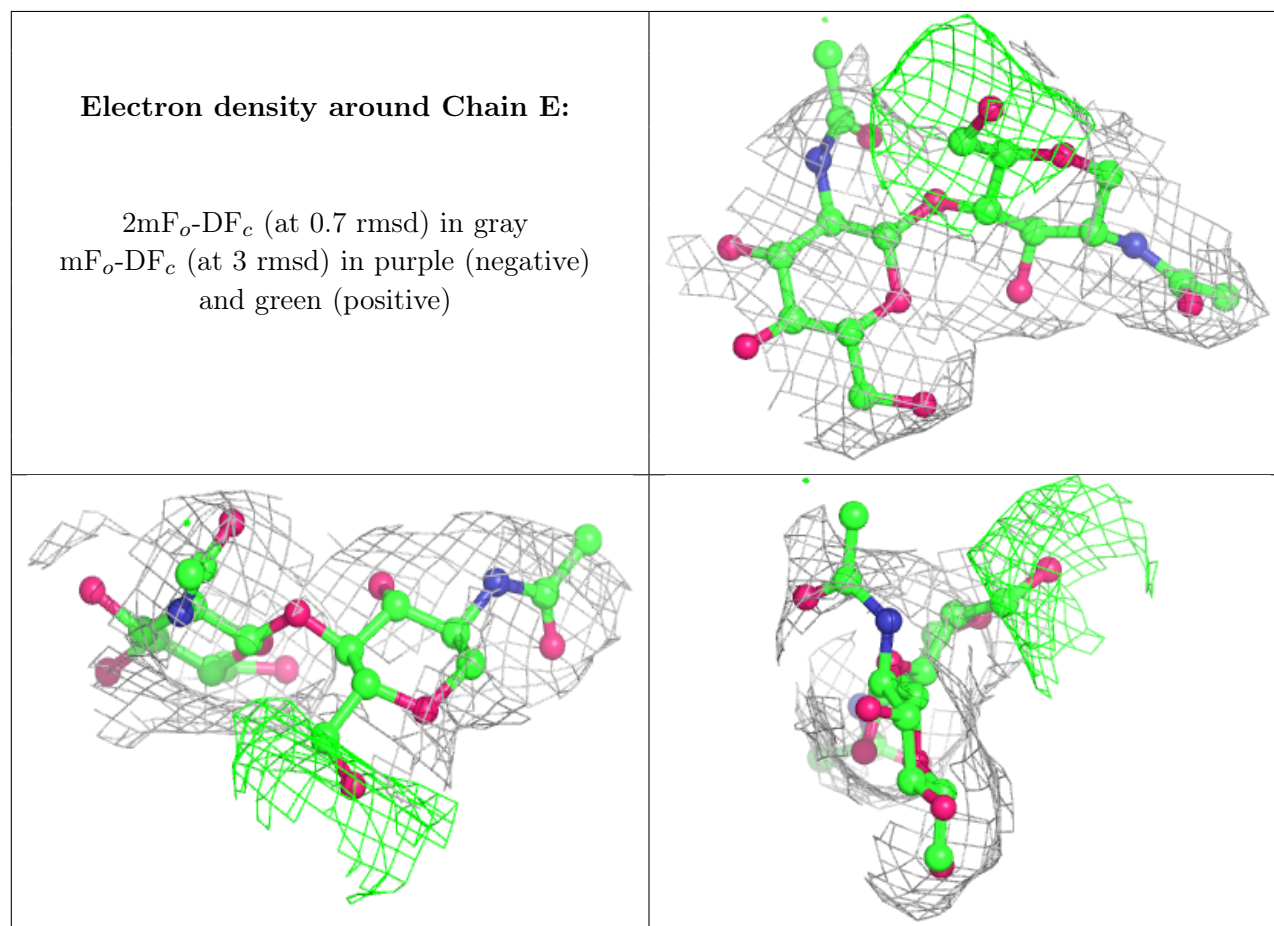
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	G	2	14/15	0.46	0.19	107,121,130,144	0
3	NAG	E	1	14/15	0.48	0.16	67,99,120,120	0

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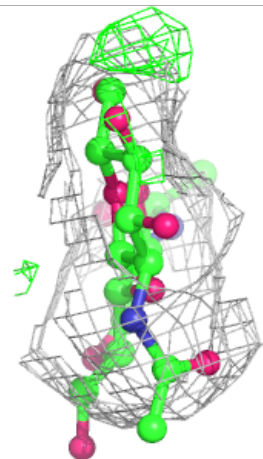
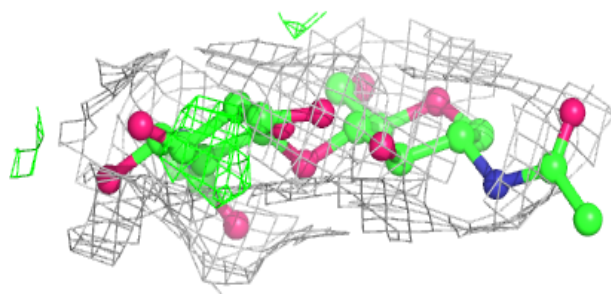
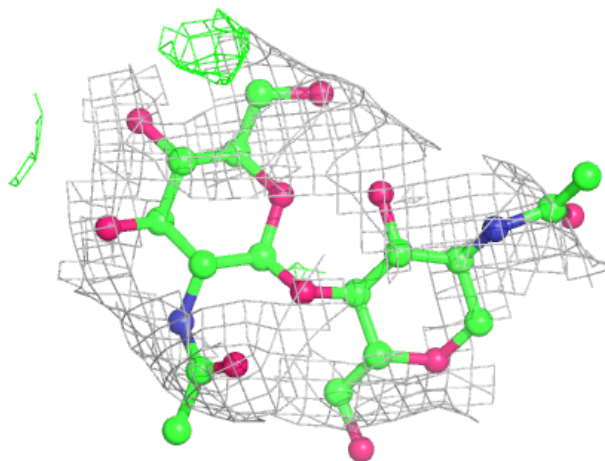
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	E	2	14/15	0.62	0.15	90,116,123,123	0
3	NAG	G	1	14/15	0.70	0.13	88,124,149,150	0
3	NAG	F	2	14/15	0.71	0.13	97,120,131,138	0
3	NAG	F	1	14/15	0.80	0.12	114,124,132,144	0

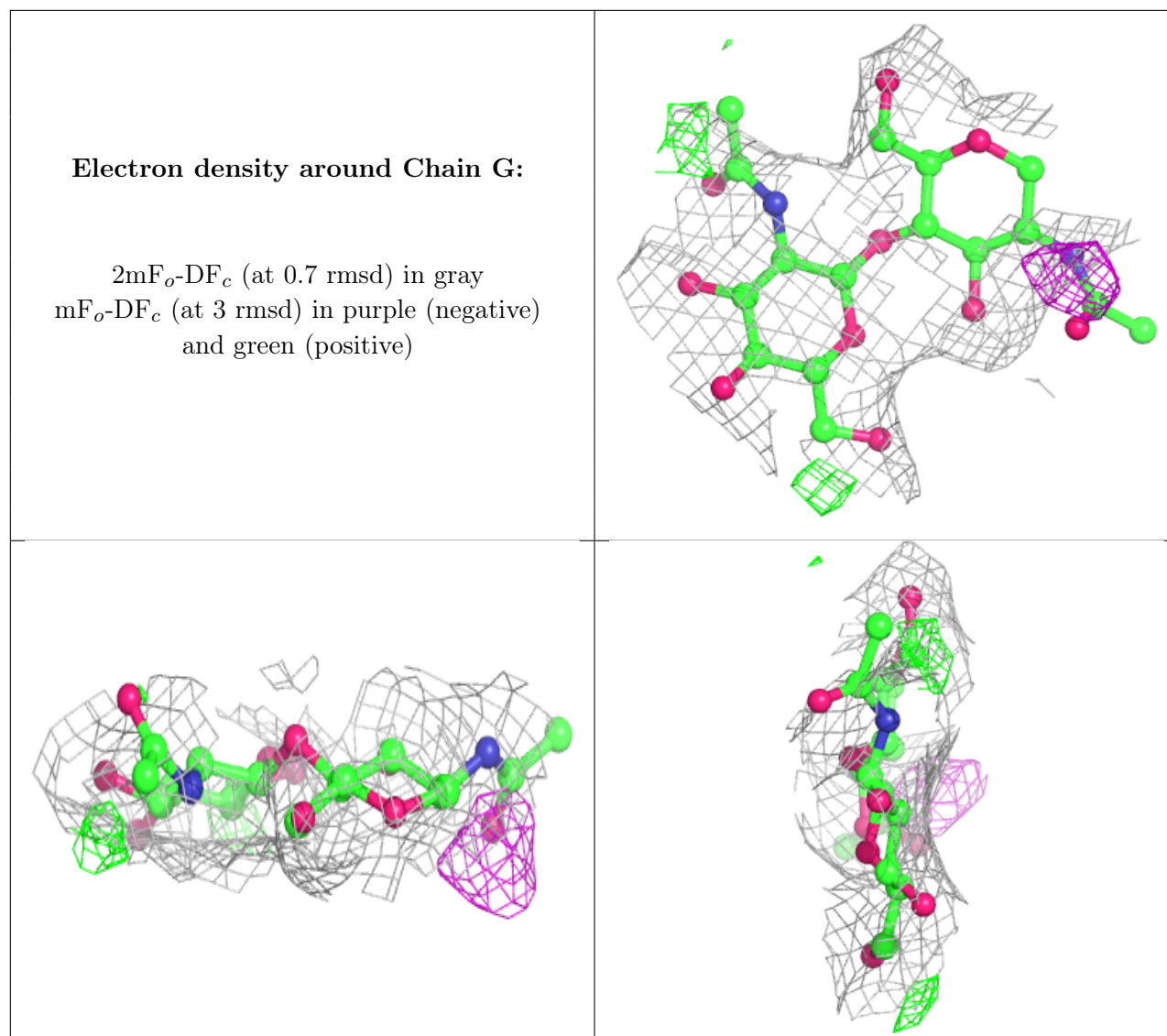
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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)





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(Å ²)	Q<0.9
4	NAG	A	601	14/15	0.33	0.18	64,117,126,126	0
4	NAG	B	603	14/15	0.60	0.14	101,107,129,130	0
4	NAG	C	601	14/15	0.76	0.11	87,101,118,128	0
4	NAG	C	602	14/15	0.77	0.12	56,81,90,97	0
5	MES	C	603	12/12	0.89	0.12	49,61,90,103	0
5	MES	A	604	12/12	0.92	0.10	52,71,93,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.