



wwPDB X-ray Structure Validation Summary Report

Jun 19, 2024 – 10:19 AM EDT

PDB ID : 4BSS
Title : Structure of the ectodomain of LGR5 in complex with R-spondin-1 (Fu1Fu2) in P21 crystal form
Authors : Peng, W.C.; de Lau, W.; Forneris, F.; Granneman, J.C.M.; Huch, M.; Clevers, H.; Gros, P.
Deposited on : 2013-06-11
Resolution : 3.20 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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

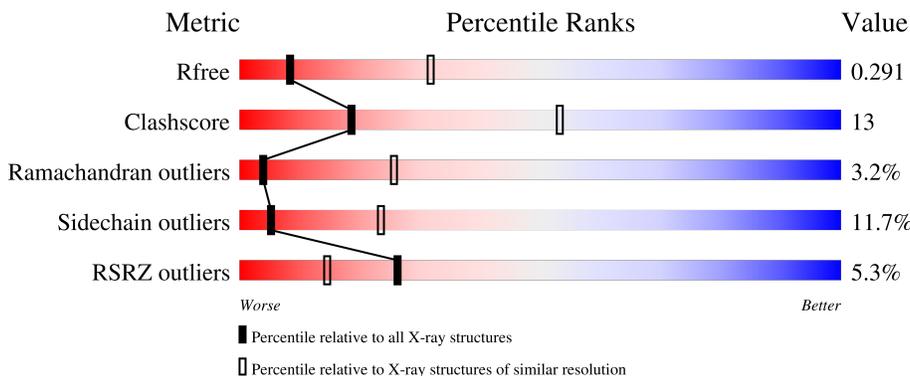
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	539	
1	B	539	
1	E	539	
1	F	539	
2	C	126	

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Mol	Chain	Length	Quality of chain
2	D	126	
2	G	126	
2	H	126	
3	I	2	
3	J	2	
3	K	2	
3	L	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
3	NAG	I	1	-	-	-	X
3	NAG	I	2	-	-	-	X
3	NAG	J	1	X	-	-	X
3	NAG	J	2	-	-	-	X
3	NAG	K	1	-	-	-	X
3	NAG	K	2	-	-	-	X
3	NAG	L	1	-	-	-	X
3	NAG	L	2	-	-	-	X
4	NAG	B	1208	-	-	-	X
4	NAG	F	1077	X	-	-	X

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 17925 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 LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	466	3653	2328	627	682	16	68	0	0
1	B	469	3671	2342	633	679	17	42	0	0
1	E	468	3672	2339	630	686	17	53	0	0
1	F	464	3637	2320	626	674	17	46	0	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	HIS	-	expression tag	UNP O75473
A	9	HIS	-	expression tag	UNP O75473
A	10	HIS	-	expression tag	UNP O75473
A	11	HIS	-	expression tag	UNP O75473
A	12	HIS	-	expression tag	UNP O75473
A	13	HIS	-	expression tag	UNP O75473
A	14	GLU	-	expression tag	UNP O75473
A	15	ASN	-	expression tag	UNP O75473
A	16	LEU	-	expression tag	UNP O75473
A	17	TYR	-	expression tag	UNP O75473
A	18	PHE	-	expression tag	UNP O75473
A	19	GLN	-	expression tag	UNP O75473
A	20	GLY	-	expression tag	UNP O75473
A	21	SER	-	expression tag	UNP O75473
A	544	ALA	-	expression tag	UNP O75473
A	545	ALA	-	expression tag	UNP O75473
A	546	ALA	-	expression tag	UNP O75473
B	8	HIS	-	expression tag	UNP O75473
B	9	HIS	-	expression tag	UNP O75473
B	10	HIS	-	expression tag	UNP O75473

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Chain	Residue	Modelled	Actual	Comment	Reference
B	11	HIS	-	expression tag	UNP O75473
B	12	HIS	-	expression tag	UNP O75473
B	13	HIS	-	expression tag	UNP O75473
B	14	GLU	-	expression tag	UNP O75473
B	15	ASN	-	expression tag	UNP O75473
B	16	LEU	-	expression tag	UNP O75473
B	17	TYR	-	expression tag	UNP O75473
B	18	PHE	-	expression tag	UNP O75473
B	19	GLN	-	expression tag	UNP O75473
B	20	GLY	-	expression tag	UNP O75473
B	21	SER	-	expression tag	UNP O75473
B	544	ALA	-	expression tag	UNP O75473
B	545	ALA	-	expression tag	UNP O75473
B	546	ALA	-	expression tag	UNP O75473
E	8	HIS	-	expression tag	UNP O75473
E	9	HIS	-	expression tag	UNP O75473
E	10	HIS	-	expression tag	UNP O75473
E	11	HIS	-	expression tag	UNP O75473
E	12	HIS	-	expression tag	UNP O75473
E	13	HIS	-	expression tag	UNP O75473
E	14	GLU	-	expression tag	UNP O75473
E	15	ASN	-	expression tag	UNP O75473
E	16	LEU	-	expression tag	UNP O75473
E	17	TYR	-	expression tag	UNP O75473
E	18	PHE	-	expression tag	UNP O75473
E	19	GLN	-	expression tag	UNP O75473
E	20	GLY	-	expression tag	UNP O75473
E	21	SER	-	expression tag	UNP O75473
E	544	ALA	-	expression tag	UNP O75473
E	545	ALA	-	expression tag	UNP O75473
E	546	ALA	-	expression tag	UNP O75473
F	8	HIS	-	expression tag	UNP O75473
F	9	HIS	-	expression tag	UNP O75473
F	10	HIS	-	expression tag	UNP O75473
F	11	HIS	-	expression tag	UNP O75473
F	12	HIS	-	expression tag	UNP O75473
F	13	HIS	-	expression tag	UNP O75473
F	14	GLU	-	expression tag	UNP O75473
F	15	ASN	-	expression tag	UNP O75473
F	16	LEU	-	expression tag	UNP O75473
F	17	TYR	-	expression tag	UNP O75473
F	18	PHE	-	expression tag	UNP O75473

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Chain	Residue	Modelled	Actual	Comment	Reference
F	19	GLN	-	expression tag	UNP O75473
F	20	GLY	-	expression tag	UNP O75473
F	21	SER	-	expression tag	UNP O75473
F	544	ALA	-	expression tag	UNP O75473
F	545	ALA	-	expression tag	UNP O75473
F	546	ALA	-	expression tag	UNP O75473

- Molecule 2 is a protein called R-SPONDIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	103	Total	C	N	O	S	0	0	0
			778	480	137	143	18			
2	D	104	Total	C	N	O	S	0	0	0
			784	483	138	145	18			
2	G	103	Total	C	N	O	S	0	0	0
			778	480	137	143	18			
2	H	104	Total	C	N	O	S	0	0	0
			784	483	138	145	18			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	29	GLY	-	expression tag	UNP Q2MKA7
C	30	SER	-	expression tag	UNP Q2MKA7
C	147	ALA	-	expression tag	UNP Q2MKA7
C	148	ALA	-	expression tag	UNP Q2MKA7
C	149	HIS	-	expression tag	UNP Q2MKA7
C	150	HIS	-	expression tag	UNP Q2MKA7
C	151	HIS	-	expression tag	UNP Q2MKA7
C	152	HIS	-	expression tag	UNP Q2MKA7
C	153	HIS	-	expression tag	UNP Q2MKA7
C	154	HIS	-	expression tag	UNP Q2MKA7
D	29	GLY	-	expression tag	UNP Q2MKA7
D	30	SER	-	expression tag	UNP Q2MKA7
D	147	ALA	-	expression tag	UNP Q2MKA7
D	148	ALA	-	expression tag	UNP Q2MKA7
D	149	HIS	-	expression tag	UNP Q2MKA7
D	150	HIS	-	expression tag	UNP Q2MKA7
D	151	HIS	-	expression tag	UNP Q2MKA7
D	152	HIS	-	expression tag	UNP Q2MKA7
D	153	HIS	-	expression tag	UNP Q2MKA7
D	154	HIS	-	expression tag	UNP Q2MKA7

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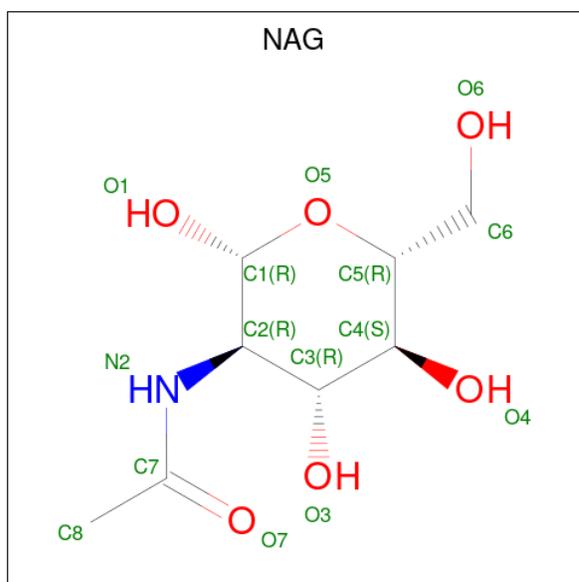
Chain	Residue	Modelled	Actual	Comment	Reference
G	29	GLY	-	expression tag	UNP Q2MKA7
G	30	SER	-	expression tag	UNP Q2MKA7
G	147	ALA	-	expression tag	UNP Q2MKA7
G	148	ALA	-	expression tag	UNP Q2MKA7
G	149	HIS	-	expression tag	UNP Q2MKA7
G	150	HIS	-	expression tag	UNP Q2MKA7
G	151	HIS	-	expression tag	UNP Q2MKA7
G	152	HIS	-	expression tag	UNP Q2MKA7
G	153	HIS	-	expression tag	UNP Q2MKA7
G	154	HIS	-	expression tag	UNP Q2MKA7
H	29	GLY	-	expression tag	UNP Q2MKA7
H	30	SER	-	expression tag	UNP Q2MKA7
H	147	ALA	-	expression tag	UNP Q2MKA7
H	148	ALA	-	expression tag	UNP Q2MKA7
H	149	HIS	-	expression tag	UNP Q2MKA7
H	150	HIS	-	expression tag	UNP Q2MKA7
H	151	HIS	-	expression tag	UNP Q2MKA7
H	152	HIS	-	expression tag	UNP Q2MKA7
H	153	HIS	-	expression tag	UNP Q2MKA7
H	154	HIS	-	expression tag	UNP Q2MKA7

- 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	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	L	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).

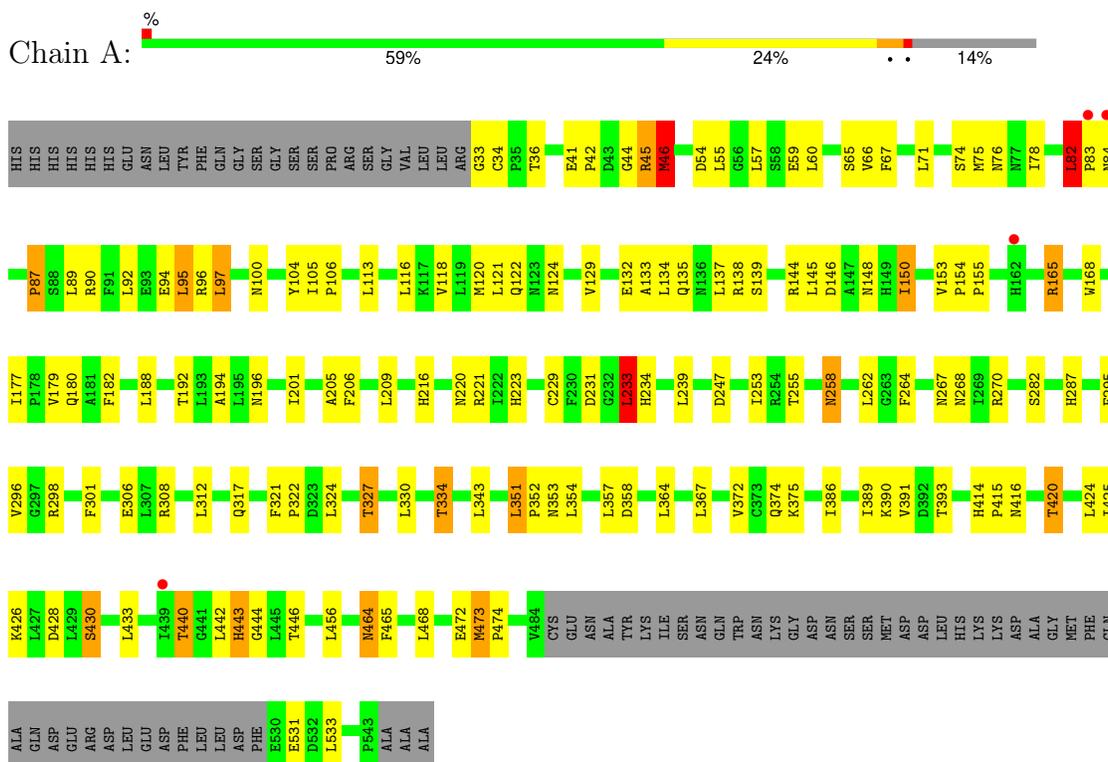


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	Total 14	C 8	N 1	O 5	0	0
4	B	1	Total 14	C 8	N 1	O 5	0	0
4	E	1	Total 14	C 8	N 1	O 5	0	0
4	F	1	Total 14	C 8	N 1	O 5	0	0

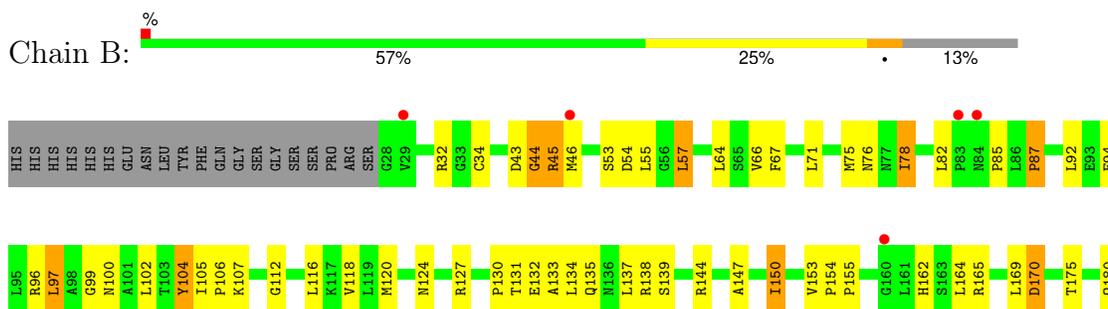
3 Residue-property plots

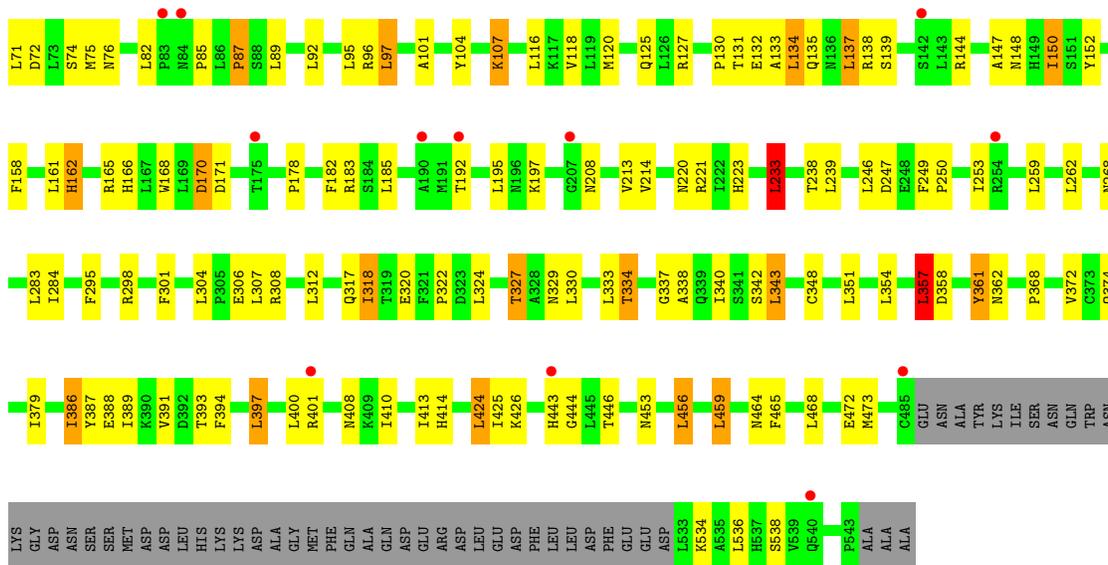
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR
5

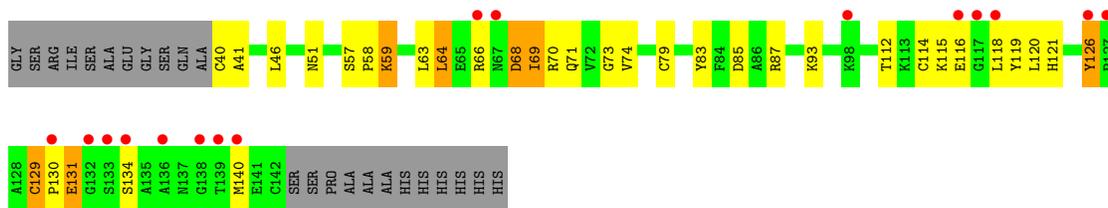


- Molecule 1: LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR
5

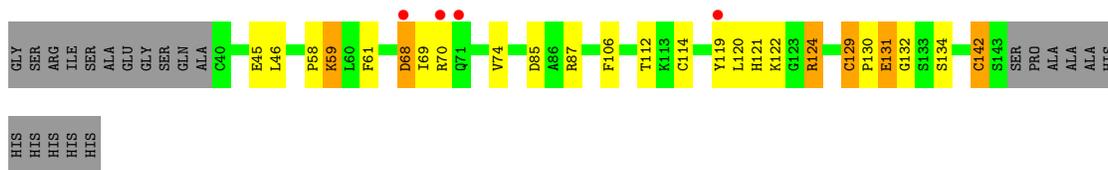




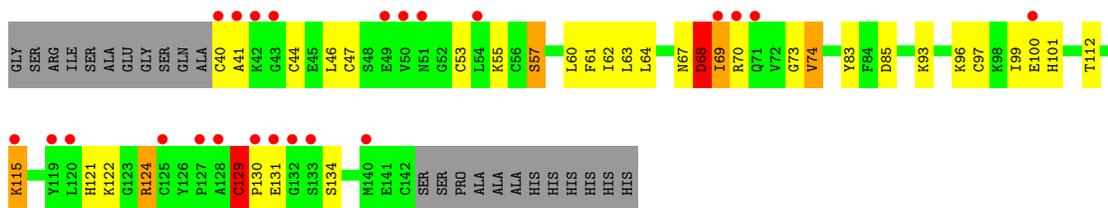
• Molecule 2: R-SPONDIN-1



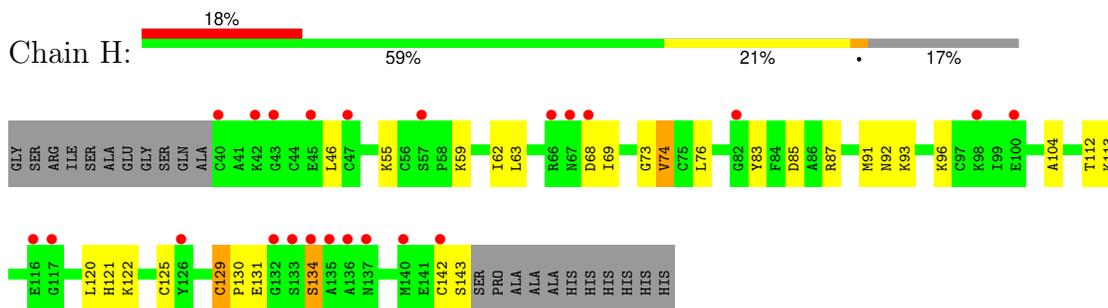
• Molecule 2: R-SPONDIN-1



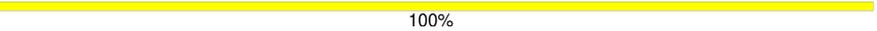
• Molecule 2: R-SPONDIN-1



• Molecule 2: R-SPONDIN-1



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

Chain I: 

MAG1
MAG2

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

Chain J: 

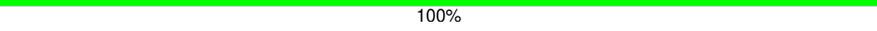
MAG1
MAG2

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

Chain K: 

MAG1
MAG2

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

Chain L: 

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.36Å 111.30Å 130.61Å 90.00° 109.19° 90.00°	Depositor
Resolution (Å)	28.90 – 3.20 28.90 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.1 (28.90-3.20) 97.1 (28.90-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.18Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.246 , 0.290 0.251 , 0.291	Depositor DCC
R_{free} test set	2664 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	87.3	Xtrriage
Anisotropy	0.455	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 80.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17925	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.84% 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	0.27	0/3734	0.58	3/5085 (0.1%)
1	B	0.27	0/3752	0.55	2/5109 (0.0%)
1	E	0.27	0/3753	0.61	1/5109 (0.0%)
1	F	0.27	0/3718	0.57	1/5062 (0.0%)
2	C	0.29	0/794	0.59	0/1066
2	D	0.27	0/800	0.54	0/1074
2	G	0.27	0/794	0.55	0/1066
2	H	0.29	0/800	0.56	0/1074
All	All	0.27	0/18145	0.57	7/24645 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	533	LEU	CA-CB-CG	6.58	130.44	115.30
1	A	82	LEU	CA-CB-CG	6.57	130.40	115.30
1	B	442	LEU	CA-CB-CG	5.89	128.85	115.30
1	A	433	LEU	CA-CB-CG	5.76	128.56	115.30
1	E	354	LEU	CA-CB-CG	5.58	128.14	115.30

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	3653	0	3652	74	9
1	B	3671	0	3685	94	0
1	E	3672	0	3674	142	1
1	F	3637	0	3652	96	8
2	C	778	0	744	22	0
2	D	784	0	749	16	0
2	G	778	0	744	21	0
2	H	784	0	749	20	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
4	B	28	0	26	2	0
4	E	14	0	13	1	0
4	F	14	0	13	0	0
All	All	17925	0	17801	467	9

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 13.

The worst 5 of 467 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:F:408:ASN:HD21	1:F:410:ILE:HG13	1.23	1.01
1:E:343:LEU:HD11	1:E:368:PRO:HG3	1.53	0.87
1:A:282:SER:HA	1:A:306:GLU:HG3	1.58	0.86
1:E:259:LEU:HD13	1:E:262:LEU:HD11	1.57	0.85
1:B:107:LYS:HD2	1:B:132:GLU:HB2	1.57	0.85

The worst 5 of 9 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:GLU:OE2	1:F:67:PHE:CE2[1_454]	0.65	1.55
1:A:531:GLU:OE2	1:F:67:PHE:CZ[1_454]	0.80	1.40
1:A:531:GLU:CD	1:F:67:PHE:CE2[1_454]	1.47	0.73
1:A:531:GLU:CD	1:F:67:PHE:CZ[1_454]	1.67	0.53
1:A:531:GLU:OE2	1:F:67:PHE:CD2[1_454]	1.91	0.29

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	462/539 (86%)	383 (83%)	69 (15%)	10 (2%)	6	35
1	B	465/539 (86%)	385 (83%)	67 (14%)	13 (3%)	5	29
1	E	464/539 (86%)	386 (83%)	61 (13%)	17 (4%)	3	22
1	F	460/539 (85%)	377 (82%)	69 (15%)	14 (3%)	4	28
2	C	101/126 (80%)	81 (80%)	16 (16%)	4 (4%)	3	21
2	D	102/126 (81%)	81 (79%)	16 (16%)	5 (5%)	2	17
2	G	101/126 (80%)	79 (78%)	18 (18%)	4 (4%)	3	21
2	H	102/126 (81%)	82 (80%)	15 (15%)	5 (5%)	2	17
All	All	2257/2660 (85%)	1854 (82%)	331 (15%)	72 (3%)	4	26

5 of 72 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	133	ALA
1	A	138	ARG
1	B	45	ARG
1	B	54	ASP

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	421/484 (87%)	378 (90%)	43 (10%)	7	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	423/484 (87%)	374 (88%)	49 (12%)	5	24
1	E	424/484 (88%)	362 (85%)	62 (15%)	3	15
1	F	420/484 (87%)	374 (89%)	46 (11%)	6	26
2	C	89/105 (85%)	77 (86%)	12 (14%)	4	18
2	D	90/105 (86%)	83 (92%)	7 (8%)	12	43
2	G	89/105 (85%)	77 (86%)	12 (14%)	4	18
2	H	90/105 (86%)	82 (91%)	8 (9%)	9	35
All	All	2046/2356 (87%)	1807 (88%)	239 (12%)	5	23

5 of 239 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	78	ILE
2	G	55	LYS
1	E	312	LEU
2	G	44	CYS
2	H	120	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	135	GLN
1	E	302	GLN
1	F	135	GLN
1	E	339	GLN
1	B	76	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
3	NAG	I	1	3,1	14,14,15	0.83	1 (7%)	17,19,21	0.64	0
3	NAG	I	2	3	14,14,15	0.60	0	17,19,21	0.73	1 (5%)
3	NAG	J	1	3,1	14,14,15	0.44	0	17,19,21	0.67	0
3	NAG	J	2	3	14,14,15	0.64	0	17,19,21	0.60	0
3	NAG	K	1	3,1	14,14,15	0.36	0	17,19,21	0.92	0
3	NAG	K	2	3	14,14,15	0.61	0	17,19,21	0.46	0
3	NAG	L	1	3,1	14,14,15	0.52	0	17,19,21	0.54	0
3	NAG	L	2	3	14,14,15	0.34	0	17,19,21	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	3,1	1/1/5/7	1/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1	NAG	C1-C2	2.90	1.56	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	I	2	NAG	C1-O5-C5	2.15	115.06	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	J	1	NAG	C1

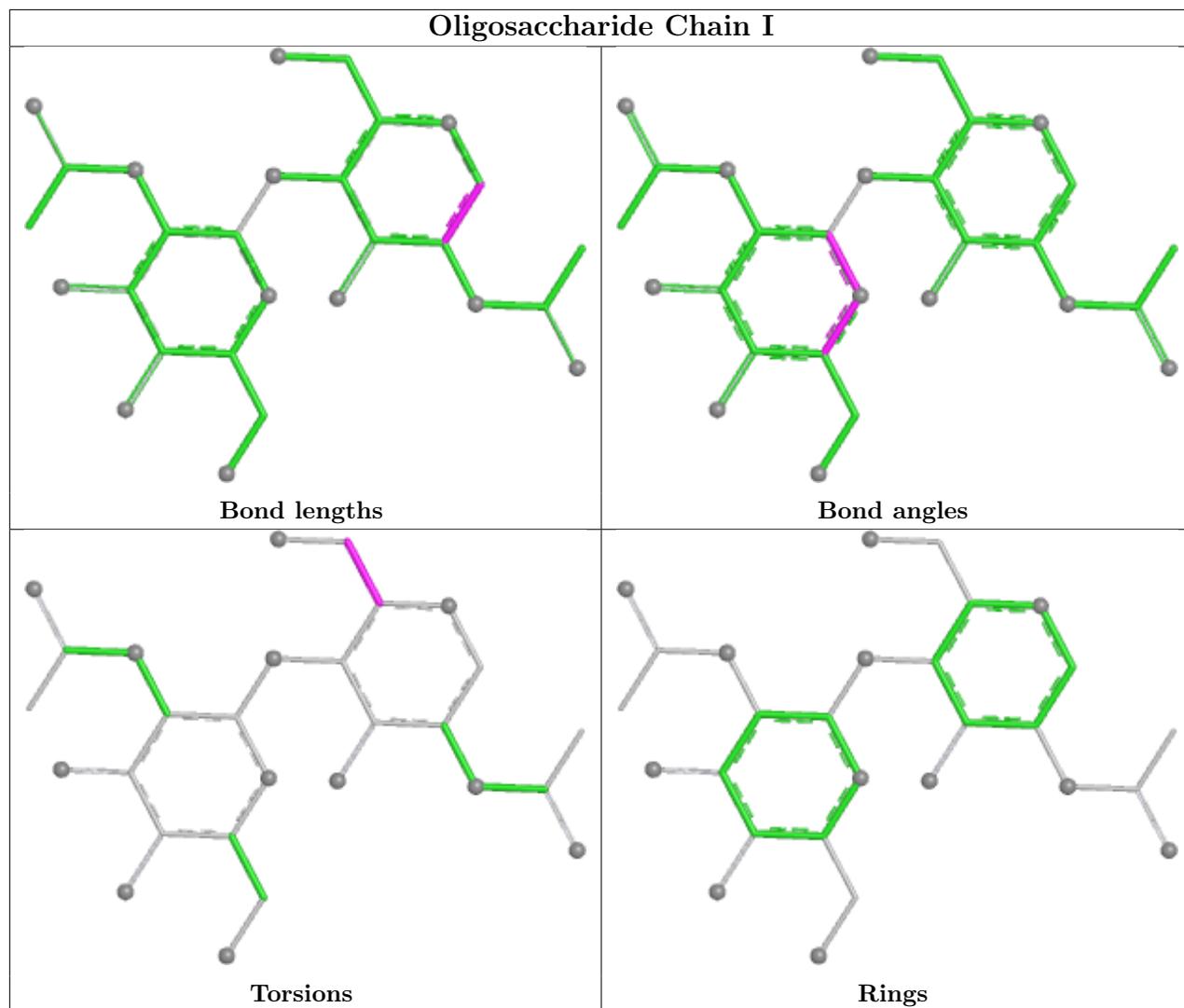
5 of 10 torsion outliers are listed below:

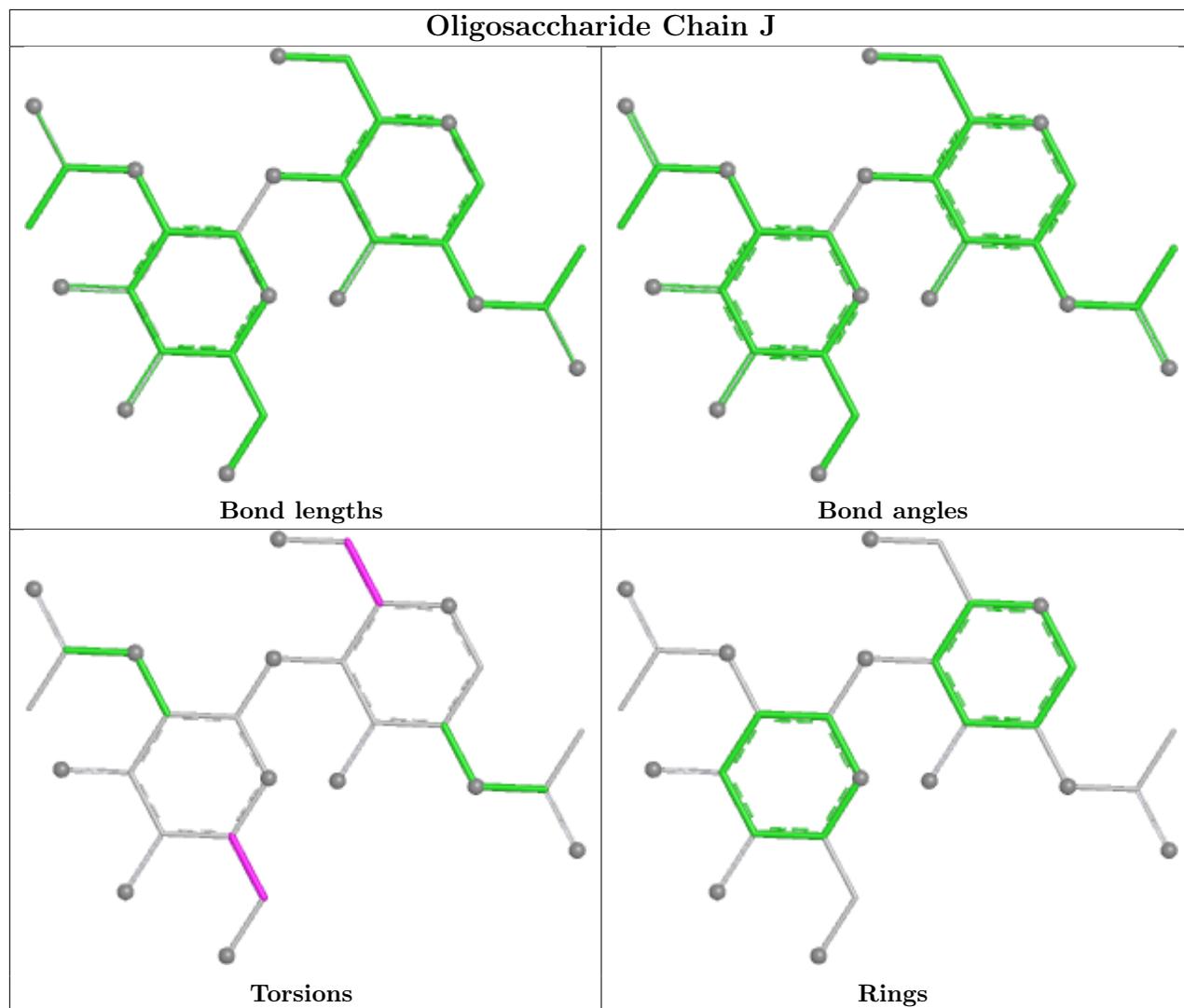
Mol	Chain	Res	Type	Atoms
3	L	1	NAG	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6

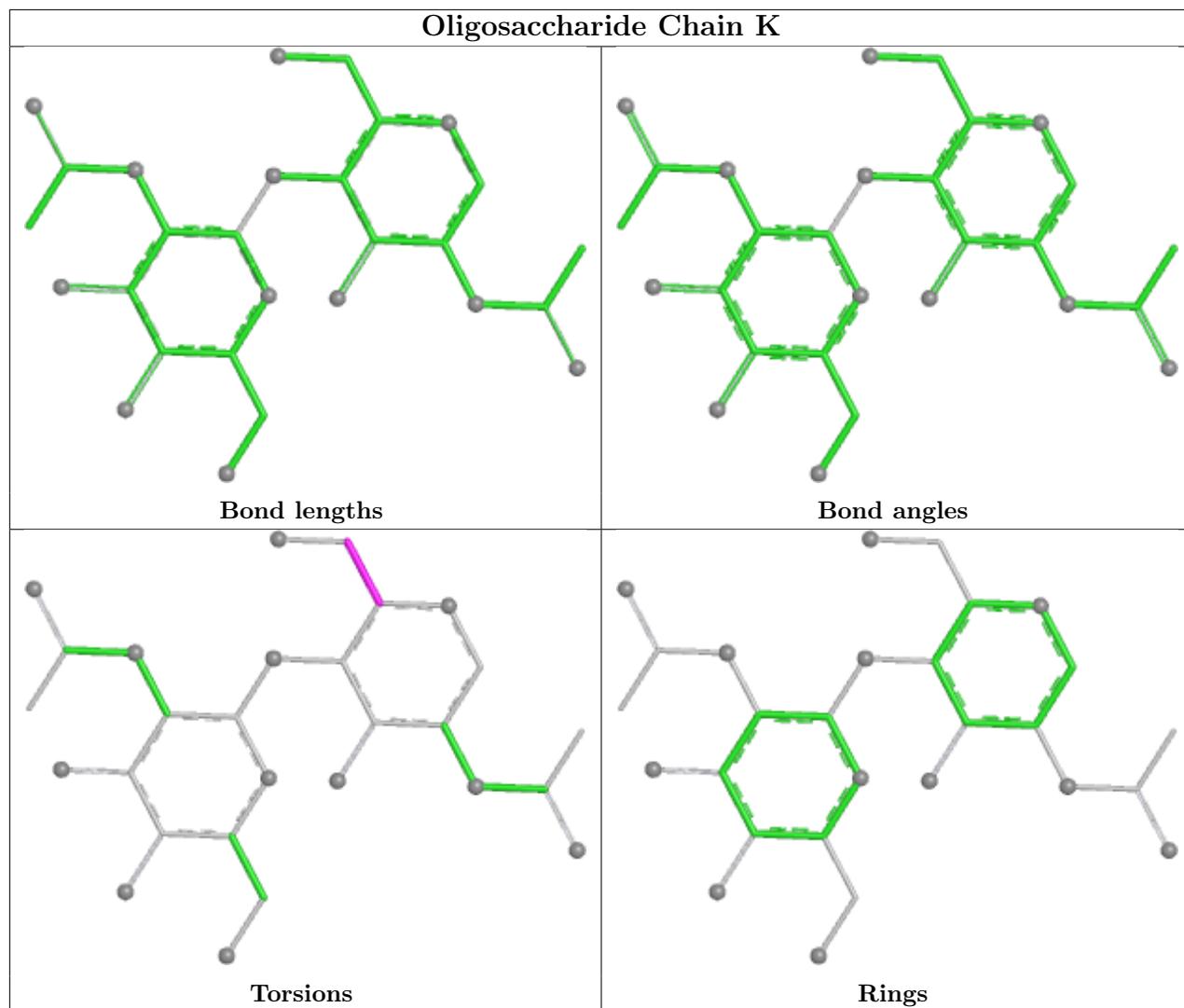
There are no ring outliers.

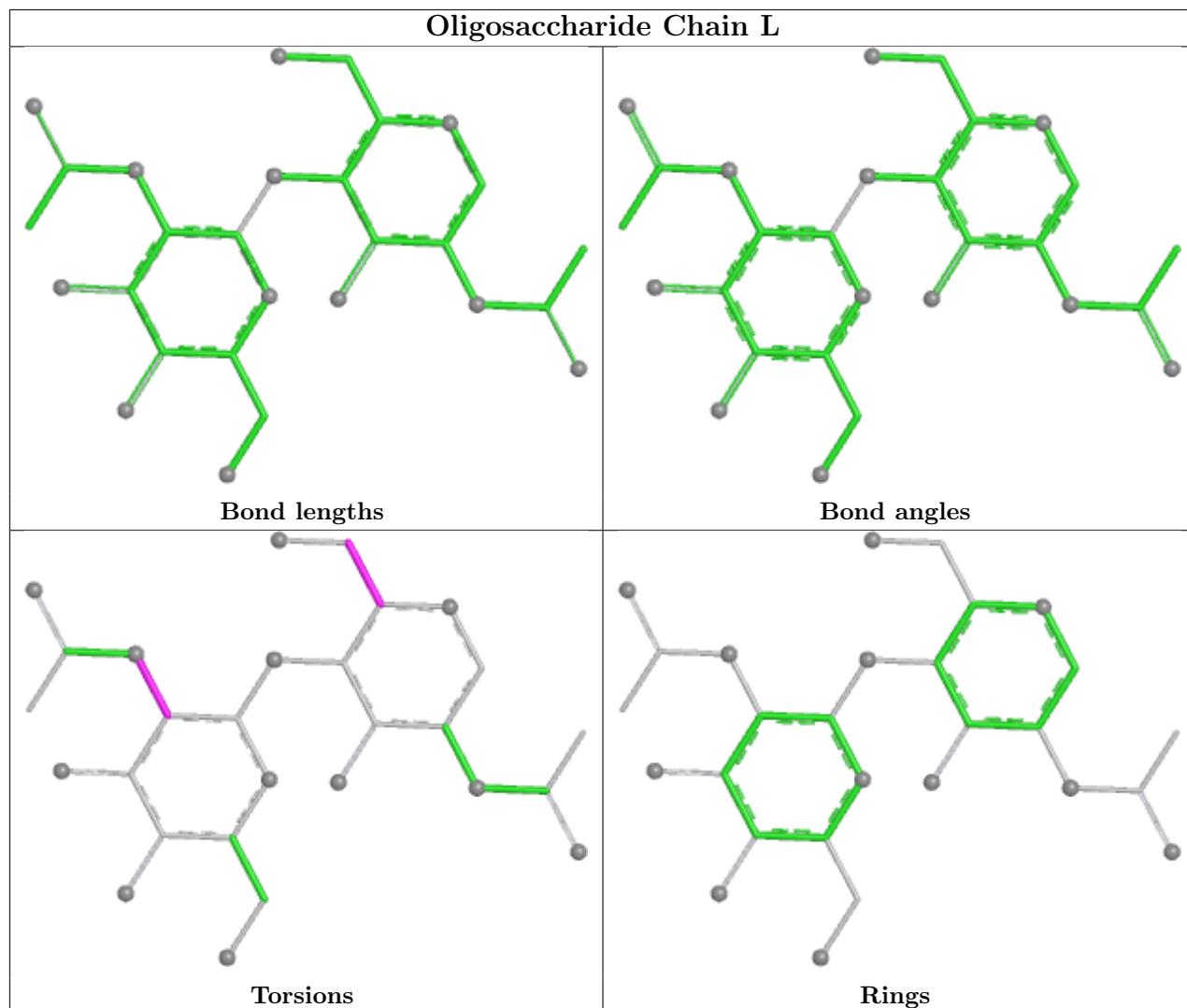
No monomer is involved in short contacts.

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	$\# Z > 2$
4	NAG	F	1077	1	14,14,15	0.74	1 (7%)	17,19,21	1.24	1 (5%)
4	NAG	B	1077	1	14,14,15	0.45	0	17,19,21	0.99	1 (5%)
4	NAG	E	1077	1	14,14,15	0.71	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1208	1	14,14,15	0.55	0	17,19,21	0.46	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	B	1208	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1077	1	-	1/6/23/26	0/1/1/1
4	NAG	E	1077	1	-	1/6/23/26	0/1/1/1
4	NAG	F	1077	1	1/1/5/7	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1077	NAG	O5-C1	-2.41	1.39	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1077	NAG	C3-C4-C5	3.51	116.59	110.23
4	B	1077	NAG	C2-N2-C7	-2.70	119.28	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	1077	NAG	C1

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1208	NAG	O5-C5-C6-O6
4	F	1077	NAG	C4-C5-C6-O6
4	B	1208	NAG	C4-C5-C6-O6
4	F	1077	NAG	O5-C5-C6-O6
4	B	1077	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1077	NAG	1	0
4	E	1077	NAG	1	0
4	B	1208	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	457/539 (84%)	-0.24	4 (0%) 84 75	36, 85, 149, 296	0
1	B	463/539 (85%)	-0.31	7 (1%) 73 61	42, 86, 161, 250	0
1	E	462/539 (85%)	0.23	26 (5%) 24 13	72, 152, 223, 276	1 (0%)
1	F	458/539 (84%)	0.05	17 (3%) 41 26	89, 143, 196, 310	0
2	C	103/126 (81%)	0.45	16 (15%) 2 1	64, 120, 210, 233	0
2	D	104/126 (82%)	0.09	4 (3%) 40 26	64, 113, 205, 350	0
2	G	103/126 (81%)	1.23	23 (22%) 0 0	112, 173, 257, 293	0
2	H	104/126 (82%)	1.05	23 (22%) 0 0	97, 160, 240, 267	0
All	All	2254/2660 (84%)	0.07	120 (5%) 26 14	36, 125, 210, 350	1 (0%)

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	83	PRO	9.0
1	A	83	PRO	8.9
2	G	70	ARG	7.7
2	G	71	GLN	7.1
2	G	127	PRO	6.8

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

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

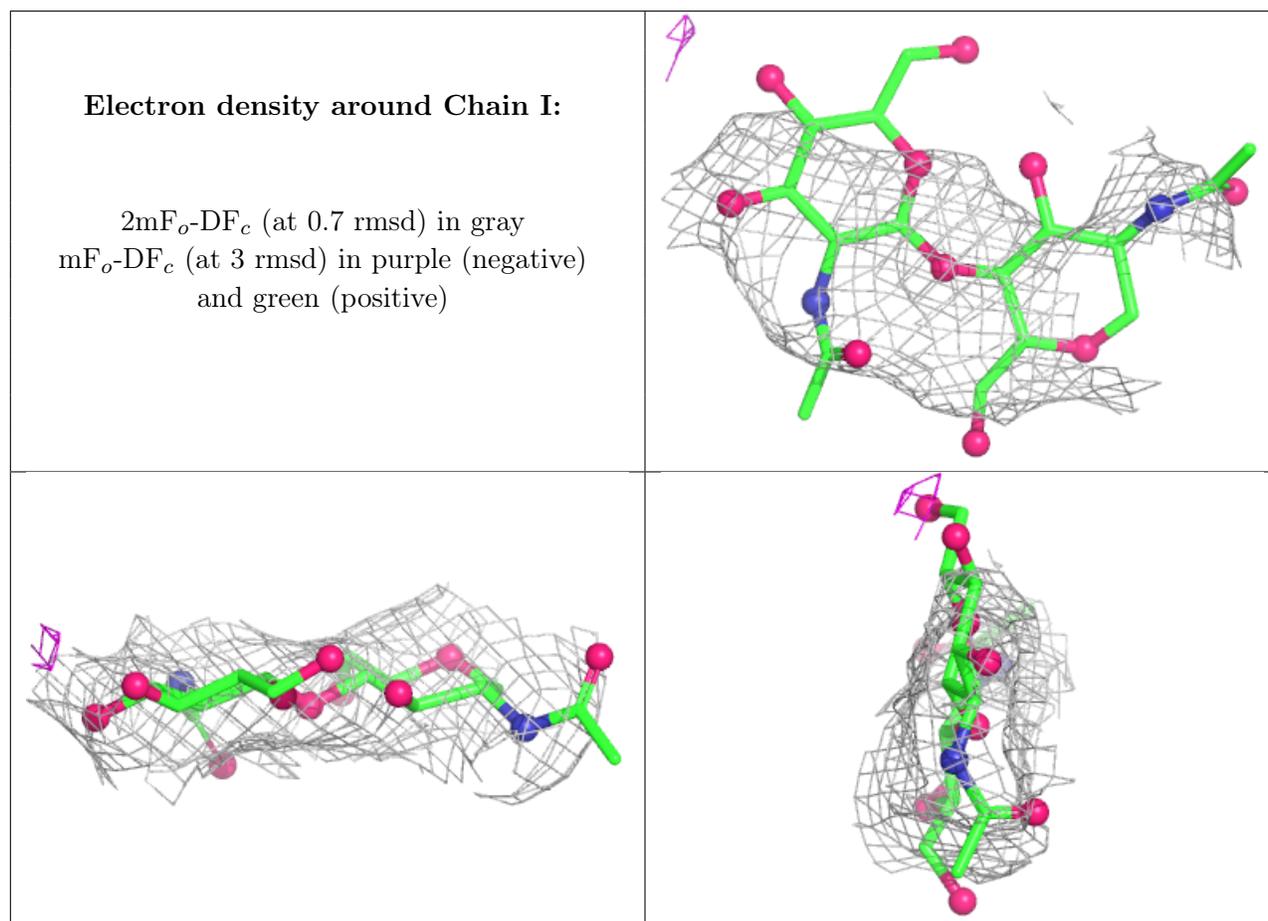
6.3 Carbohydrates [i](#)

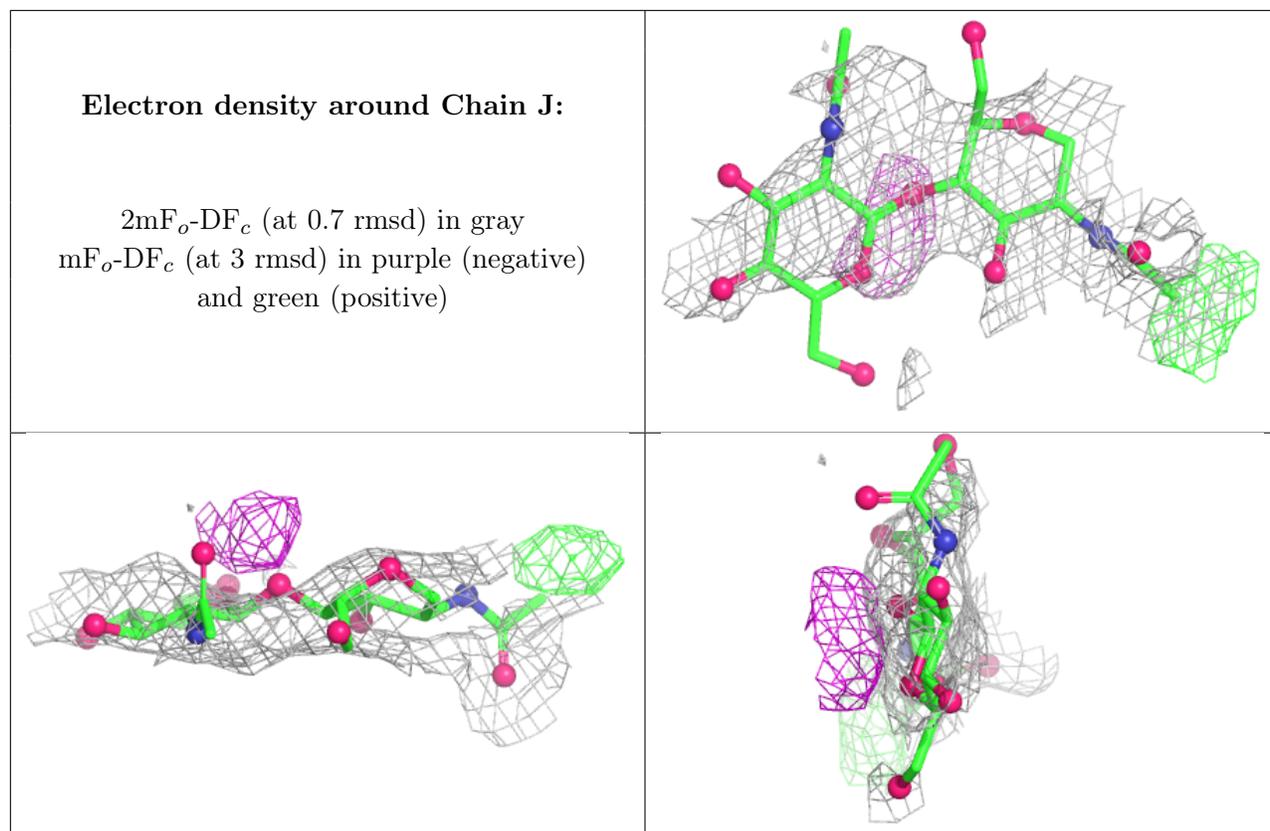
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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	J	1	14/15	0.44	0.53	167,181,192,200	0
3	NAG	J	2	14/15	0.58	0.68	173,191,200,201	0
3	NAG	K	1	14/15	0.60	0.58	174,189,216,220	0
3	NAG	K	2	14/15	0.62	0.74	219,230,233,235	0
3	NAG	L	2	14/15	0.66	0.98	202,216,225,228	0
3	NAG	L	1	14/15	0.71	0.49	191,204,213,213	0
3	NAG	I	2	14/15	0.71	0.65	188,200,224,227	0
3	NAG	I	1	14/15	0.80	0.49	141,178,197,205	0

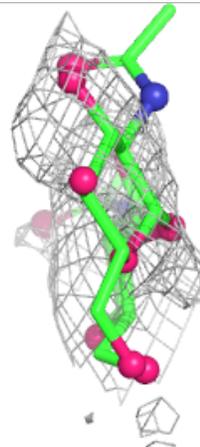
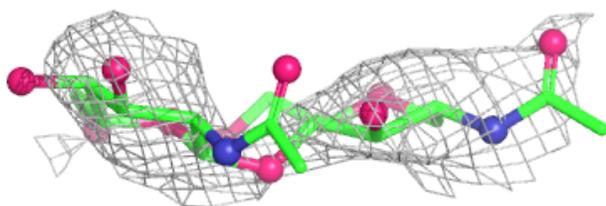
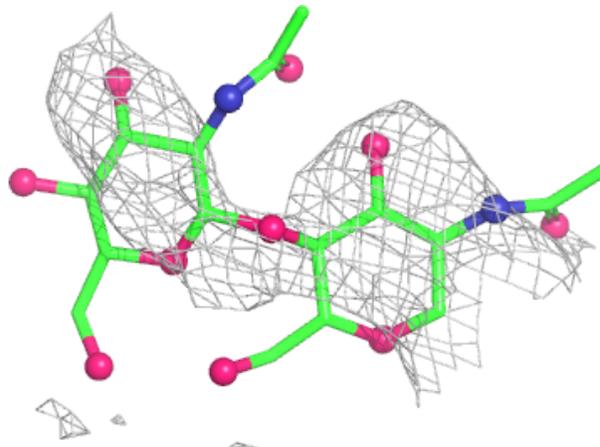
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

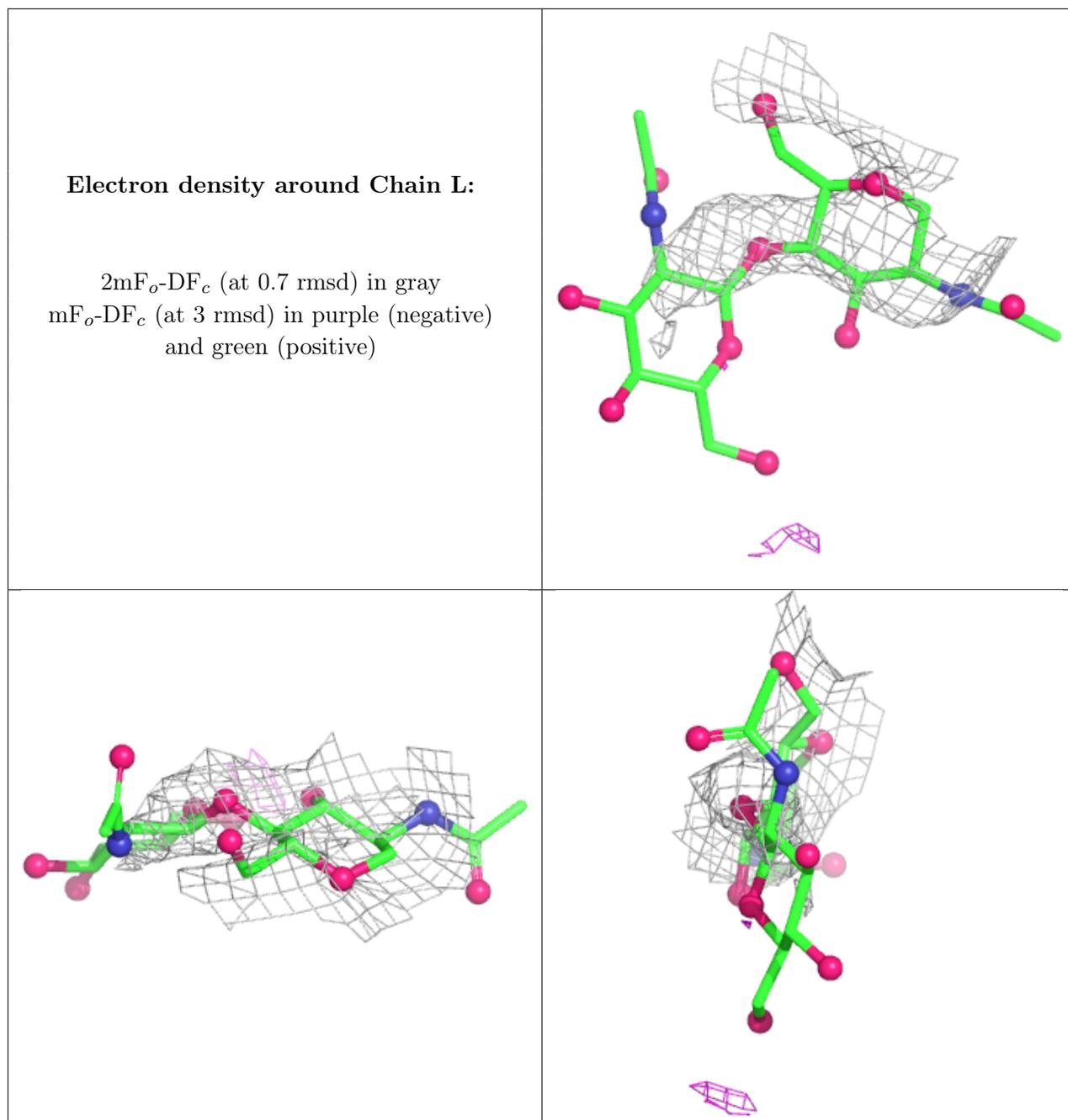




Electron density around Chain K:

$2mF_o-DF_c$ (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	F	1077	14/15	0.51	0.55	148,163,167,172	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	B	1208	14/15	0.54	0.54	144,191,199,206	0
4	NAG	E	1077	14/15	0.81	0.35	169,181,184,186	0
4	NAG	B	1077	14/15	0.81	0.35	109,149,161,170	0

6.5 Other polymers [i](#)

There are no such residues in this entry.