WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 02:40 AM EDT

PDB ID	:	4BLD
Title	:	Crystal structure of a human Suppressor of fused (SUFU)-GLI3p complex
Authors	:	Cherry, A.L.; Finta, C.; Karlstrom, M.; De Sanctis, D.; Toftgard, R.; Jovine, L.
Deposited on	:	2013-05-02
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

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 2.80 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.
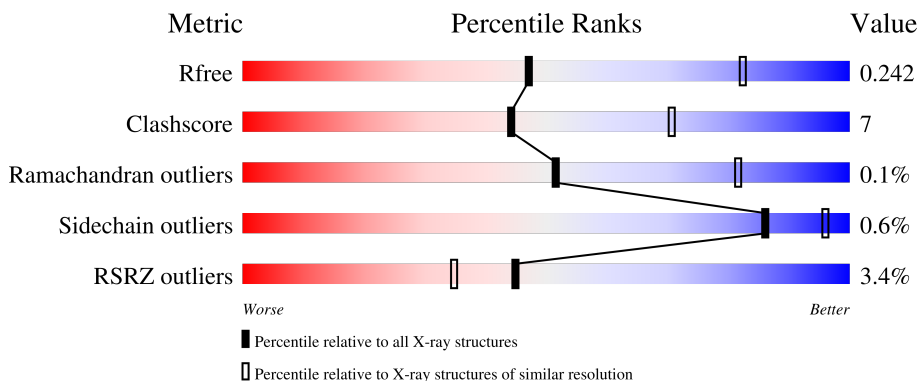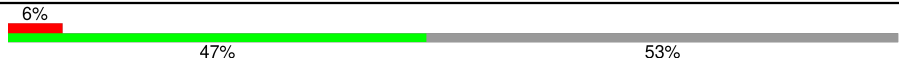

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	753	% 85% 12% ·
1	B	753	4% 81% 14% 5%
1	C	753	6% 82% 14% ·
1	D	753	2% 86% 11% ·
2	E	17	47% 53%

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Mol	Chain	Length	Quality of chain
2	F	17	6% 47% 53%
2	G	17	35% 12% 53%
2	H	17	47% 53%
3	I	2	100%
3	J	2	100%
3	K	2	100%
3	L	2	50% 50%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 23116 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 MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	734	Total 5757	C 3681	N 967	O 1090	S 19	0	0	0
1	B	717	Total 5621	C 3597	N 942	O 1064	S 18	0	0	0
1	C	725	Total 5687	C 3640	N 957	O 1072	S 18	0	0	0
1	D	730	Total 5727	C 3666	N 962	O 1081	S 18	0	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P0AEX9
A	3	THR	ILE	engineered mutation	UNP P0AEX9
A	360	ALA	GLU	engineered mutation	UNP P0AEX9
A	363	ALA	LYS	engineered mutation	UNP P0AEX9
A	364	ALA	ASP	engineered mutation	UNP P0AEX9
A	368	ASN	ARG	engineered mutation	UNP P0AEX9
A	369	ALA	-	linker	UNP P0AEX9
A	370	ALA	-	linker	UNP P0AEX9
A	371	ALA	-	linker	UNP P0AEX9
A	401	ASP	TRP	engineered mutation	UNP Q9UMX1
A	402	SER	LEU	engineered mutation	UNP Q9UMX1
A	403	PHE	GLY	engineered mutation	UNP Q9UMX1
A	619	PRO	-	linker	UNP Q9UMX1
A	620	SER	-	linker	UNP Q9UMX1
A	621	ARG	-	linker	UNP Q9UMX1
A	622	GLY	-	linker	UNP Q9UMX1
A	625	PRO	-	linker	UNP Q9UMX1
A	718	ALA	PRO	engineered mutation	UNP Q9UMX1
A	?	-	GLU	deletion	UNP Q9UMX1
A	?	-	GLU	deletion	UNP Q9UMX1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PHE	deletion	UNP Q9UMX1
A	719	ALA	LYS	engineered mutation	UNP Q9UMX1
A	746	VAL	-	expression tag	UNP Q9UMX1
A	747	GLU	-	expression tag	UNP Q9UMX1
A	748	HIS	-	expression tag	UNP Q9UMX1
A	749	HIS	-	expression tag	UNP Q9UMX1
A	750	HIS	-	expression tag	UNP Q9UMX1
A	751	HIS	-	expression tag	UNP Q9UMX1
A	752	HIS	-	expression tag	UNP Q9UMX1
A	753	HIS	-	expression tag	UNP Q9UMX1
B	1	MET	-	expression tag	UNP P0AEX9
B	3	THR	ILE	engineered mutation	UNP P0AEX9
B	360	ALA	GLU	engineered mutation	UNP P0AEX9
B	363	ALA	LYS	engineered mutation	UNP P0AEX9
B	364	ALA	ASP	engineered mutation	UNP P0AEX9
B	368	ASN	ARG	engineered mutation	UNP P0AEX9
B	369	ALA	-	linker	UNP P0AEX9
B	370	ALA	-	linker	UNP P0AEX9
B	371	ALA	-	linker	UNP P0AEX9
B	401	ASP	TRP	engineered mutation	UNP Q9UMX1
B	402	SER	LEU	engineered mutation	UNP Q9UMX1
B	403	PHE	GLY	engineered mutation	UNP Q9UMX1
B	619	PRO	-	linker	UNP Q9UMX1
B	620	SER	-	linker	UNP Q9UMX1
B	621	ARG	-	linker	UNP Q9UMX1
B	622	GLY	-	linker	UNP Q9UMX1
B	625	PRO	-	linker	UNP Q9UMX1
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B	?	-	PHE	deletion	UNP Q9UMX1
B	719	ALA	LYS	engineered mutation	UNP Q9UMX1
B	746	VAL	-	expression tag	UNP Q9UMX1
B	747	GLU	-	expression tag	UNP Q9UMX1
B	748	HIS	-	expression tag	UNP Q9UMX1
B	749	HIS	-	expression tag	UNP Q9UMX1
B	750	HIS	-	expression tag	UNP Q9UMX1
B	751	HIS	-	expression tag	UNP Q9UMX1
B	752	HIS	-	expression tag	UNP Q9UMX1
B	753	HIS	-	expression tag	UNP Q9UMX1
C	1	MET	-	expression tag	UNP P0AEX9
C	3	THR	ILE	engineered mutation	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	360	ALA	GLU	engineered mutation	UNP P0AEX9
C	363	ALA	LYS	engineered mutation	UNP P0AEX9
C	364	ALA	ASP	engineered mutation	UNP P0AEX9
C	368	ASN	ARG	engineered mutation	UNP P0AEX9
C	369	ALA	-	linker	UNP P0AEX9
C	370	ALA	-	linker	UNP P0AEX9
C	371	ALA	-	linker	UNP P0AEX9
C	401	ASP	TRP	engineered mutation	UNP Q9UMX1
C	402	SER	LEU	engineered mutation	UNP Q9UMX1
C	403	PHE	GLY	engineered mutation	UNP Q9UMX1
C	619	PRO	-	linker	UNP Q9UMX1
C	620	SER	-	linker	UNP Q9UMX1
C	621	ARG	-	linker	UNP Q9UMX1
C	622	GLY	-	linker	UNP Q9UMX1
C	625	PRO	-	linker	UNP Q9UMX1
C	718	ALA	PRO	engineered mutation	UNP Q9UMX1
C	?	-	GLU	deletion	UNP Q9UMX1
C	?	-	GLU	deletion	UNP Q9UMX1
C	?	-	PHE	deletion	UNP Q9UMX1
C	719	ALA	LYS	engineered mutation	UNP Q9UMX1
C	746	VAL	-	expression tag	UNP Q9UMX1
C	747	GLU	-	expression tag	UNP Q9UMX1
C	748	HIS	-	expression tag	UNP Q9UMX1
C	749	HIS	-	expression tag	UNP Q9UMX1
C	750	HIS	-	expression tag	UNP Q9UMX1
C	751	HIS	-	expression tag	UNP Q9UMX1
C	752	HIS	-	expression tag	UNP Q9UMX1
C	753	HIS	-	expression tag	UNP Q9UMX1
D	1	MET	-	expression tag	UNP P0AEX9
D	3	THR	ILE	engineered mutation	UNP P0AEX9
D	360	ALA	GLU	engineered mutation	UNP P0AEX9
D	363	ALA	LYS	engineered mutation	UNP P0AEX9
D	364	ALA	ASP	engineered mutation	UNP P0AEX9
D	368	ASN	ARG	engineered mutation	UNP P0AEX9
D	369	ALA	-	linker	UNP P0AEX9
D	370	ALA	-	linker	UNP P0AEX9
D	371	ALA	-	linker	UNP P0AEX9
D	401	ASP	TRP	engineered mutation	UNP Q9UMX1
D	402	SER	LEU	engineered mutation	UNP Q9UMX1
D	403	PHE	GLY	engineered mutation	UNP Q9UMX1
D	619	PRO	-	linker	UNP Q9UMX1
D	620	SER	-	linker	UNP Q9UMX1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	621	ARG	-	linker	UNP Q9UMX1
D	622	GLY	-	linker	UNP Q9UMX1
D	625	PRO	-	linker	UNP Q9UMX1
D	718	ALA	PRO	engineered mutation	UNP Q9UMX1
D	?	-	GLU	deletion	UNP Q9UMX1
D	?	-	GLU	deletion	UNP Q9UMX1
D	?	-	PHE	deletion	UNP Q9UMX1
D	719	ALA	LYS	engineered mutation	UNP Q9UMX1
D	746	VAL	-	expression tag	UNP Q9UMX1
D	747	GLU	-	expression tag	UNP Q9UMX1
D	748	HIS	-	expression tag	UNP Q9UMX1
D	749	HIS	-	expression tag	UNP Q9UMX1
D	750	HIS	-	expression tag	UNP Q9UMX1
D	751	HIS	-	expression tag	UNP Q9UMX1
D	752	HIS	-	expression tag	UNP Q9UMX1
D	753	HIS	-	expression tag	UNP Q9UMX1

- Molecule 2 is a protein called TRANSCRIPTIONAL ACTIVATOR GLI3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	8	Total 57	C 35	N 10	O 12	0	0	0
2	F	8	Total 57	C 35	N 10	O 12	0	0	0
2	G	8	Total 57	C 35	N 10	O 12	0	0	0
2	H	8	Total 57	C 35	N 10	O 12	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	I	2	Total 23	C 12	O 11	0	0	0
3	J	2	Total 23	C 12	O 11	0	0	0
3	K	2	Total 23	C 12	O 11	0	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	L	2	Total 23	C 12	O 11	0	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

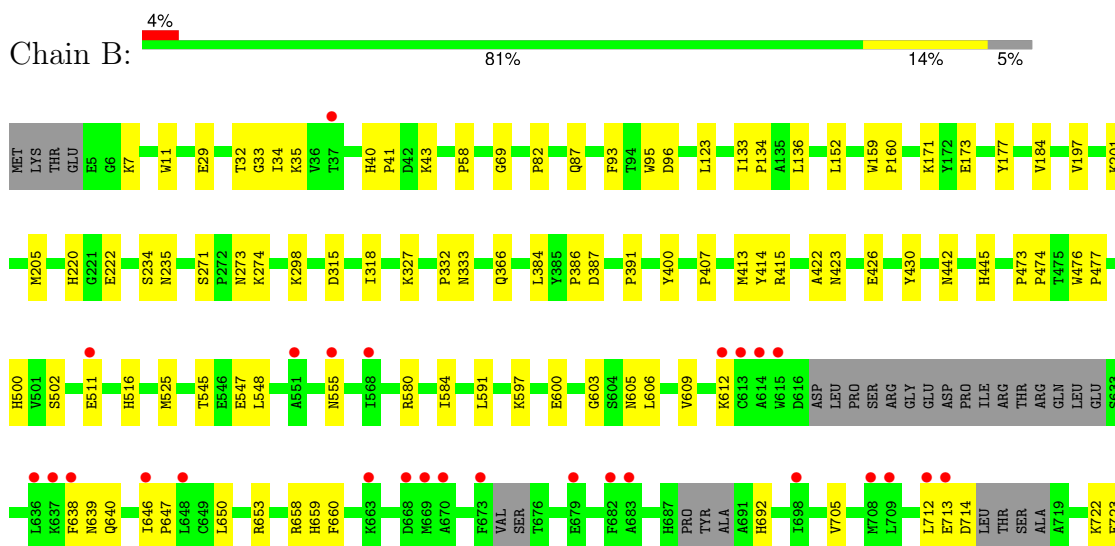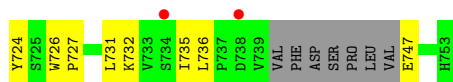| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Zn 1	0	0
4	B	1	Total 1	Zn 1	0	0
4	C	1	Total 1	Zn 1	0	0
4	D	1	Total 1	Zn 1	0	0

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.
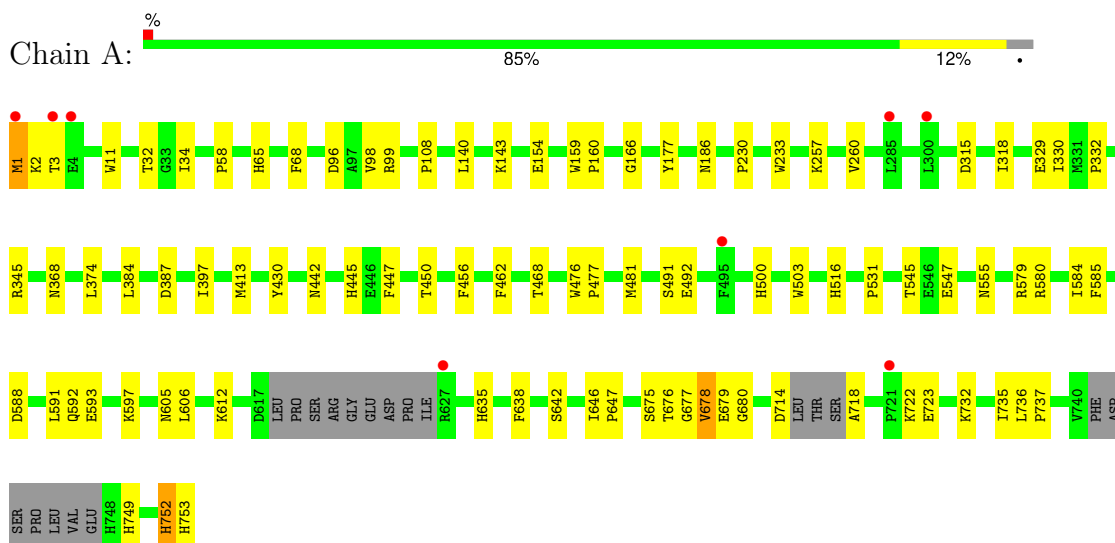
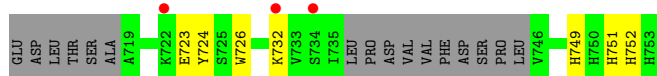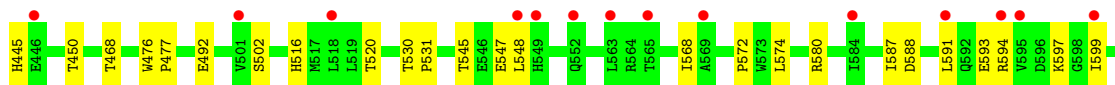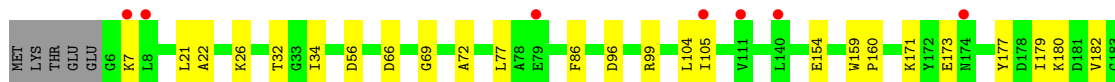• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG

• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG

Y724 S725 W726 P727 L731 K732 V733 S734 I735 L736 P737 D738 V739 VAL PHE ASP SER PRO LEU VAL E747 H753

• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG

Chain C:

6%
82%
14%

MET LYS THR GLU GLU G6 K7 L8 L21 A22 K26 T32 G33 I34 D56 D66 G69 A72 L77 A78 E79 F86 D96 R99 L104 I105 V111 L140 E154 W159 P160 K171 Y172 E173 N174 Y177 D178 I179 K180 D181 V182 G183

V184 N202 K203 H204 P230 W233 D237 K240 V245 P255 F259 S271 P272 N273 K274 L285 L286 L300 L312 K327 M331 P332 N333 R345 N350 Q366 A376 E380 R383 D387 N390 Y400 P407 I424

H445 E446 T450 T468 W476 P477 E492 V501 S502 H516 M517 L518 L519 T520 T530 P531 T545 E546 E547 L548 H549 Q552 L563 R564 T565 I568 A569 P572 W573 L574 R580 I584 I587 D588 L591 Q592 E593 R594 V595 D596 K597 G598 I599

G603 S604 N605 L606 A611 D616 D617 L618 PRO SER ARG GLU ASP P625 I626 R627 E632 S633 V634 H635 S642 I646 L650 R653 L654 R658 H659 T672 F682 A690 W695 L696 Q697 L700 T701 E702 E703 F704 V705 E706 K707 M708 L709 E710 D711 LEU

GLU ASP LEU THR SER ALA A719 K722 E723 Y724 S725 W726 K732 V733 S734 I735 LEU PRO ASP VAL VAL PHE ASP SER PRO LEU V746 H749 H750 H751 H752 H753

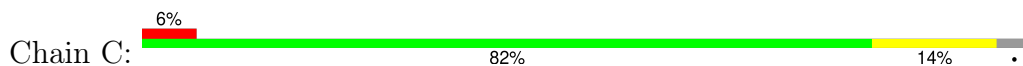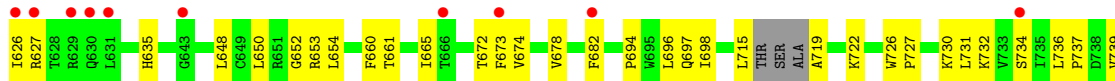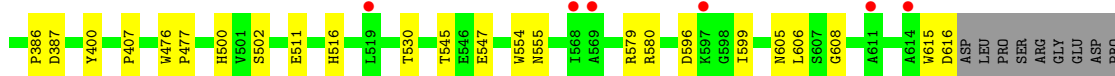• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG

Chain D:

2%
86%
11%

MET LYS THR GLU GLU G6 K7 K26 T32 G33 I34 K35 K43 V51 D56 D66 G69 K84 D88 G166 K171 Y172 E173 Y177 V182 G183 V184 D185 N186 P230 W233 E292 K296 M331 P332 N333 R355 Q366 A376

P386 D387 Y400 P407 W476 P477 H500 V501 S502 E511 H516 L519 T530 T545 E546 E547 W554 N555 I568 A569 R579 R580 D596 K597 G598 I599 N605 L606 S607 G608 A611 A614 W615 D616 ASP LEU PRO SER ARG GLU ASP PRO

I626 R627 T628 R629 Q630 L631 H635 G643 L648 C649 L650 R651 G652 R653 L654 F660 T661 I665 T666 T672 F673 V674 V678 F682 P694 W695 L696 Q697 I698 L715 THR SER ALA A719 K722 W726 P727 K730 L731 K732 V733 S734 I735 L736 P737 D738 V739

V740 PHE ASP SER PRO LEU VAL E747 H748 H753

• Molecule 2: TRANSCRIPTIONAL ACTIVATOR GLI3

Chain E:

47%
53%

SER SER ALA SER GLY **S333** **S340** ALA ILE SER PRO

• Molecule 2: TRANSCRIPTIONAL ACTIVATOR GLI3

Chain F:

6%

47%   53%

SER SER ALA SER GLY **S333** **Y334** **S340** ALA ILE SER PRO

• Molecule 2: TRANSCRIPTIONAL ACTIVATOR GLI3

Chain G:

35%   12%   53%

SER SER ALA SER GLY **S333** **L337** **S340** ALA ILE SER PRO

• Molecule 2: TRANSCRIPTIONAL ACTIVATOR GLI3

Chain H:

47%   53%

SER SER ALA SER GLY **S333** **S340** ALA ILE SER PRO

• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain I:

100%

GLC1 GLC2

• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain J:

100%

GLC1 GLC2

• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain K:

100%

GLC1 GLC2

• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain L:

50%   50%

GLC1 GLC2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	116.61Å 136.55Å 116.74Å 90.00° 105.25° 90.00°	Depositor
Resolution (Å)	19.94 – 2.80 46.36 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.94-2.80) 98.7 (46.36-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.201 , 0.234 0.209 , 0.242	Depositor DCC
R_{free} test set	1978 reflections (2.31%)	wwPDB-VP
Wilson B-factor (Å^2)	75.5	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 45.4	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.044 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	23116	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.05% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, ZN

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	0.32	0/5913	0.57	0/8040
1	B	0.32	1/5773 (0.0%)	0.56	0/7847
1	C	0.33	0/5843	0.58	0/7945
1	D	0.31	0/5883	0.55	0/8001
2	E	0.21	0/58	0.48	0/77
2	F	0.19	0/58	0.30	0/77
2	G	0.22	0/58	0.42	0/77
2	H	0.23	0/58	0.43	0/77
All	All	0.32	1/23644 (0.0%)	0.56	0/32141

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	41	PRO	N-CD	5.36	1.55	1.47

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	5757	0	5587	75	0
1	B	5621	0	5442	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5687	0	5522	88	0
1	D	5727	0	5562	57	0
2	E	57	0	49	0	0
2	F	57	0	49	0	0
2	G	57	0	49	1	0
2	H	57	0	49	0	0
3	I	23	0	21	0	0
3	J	23	0	21	0	0
3	K	23	0	21	0	0
3	L	23	0	21	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	23116	0	22393	301	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 7.

All (301) 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:C:72:ALA:CB	1:C:105:ILE:HD13	1.45	1.44
1:A:585:PHE:CD1	1:A:591:LEU:HD11	1.72	1.25
1:C:72:ALA:HB1	1:C:105:ILE:HD13	1.19	1.19
1:D:51:VAL:HB	1:D:56:ASP:OD1	1.41	1.18
1:B:413:MET:HE3	1:B:430:TYR:CE2	1.77	1.18
1:C:72:ALA:CB	1:C:105:ILE:CD1	2.24	1.15
1:A:714:ASP:HB3	1:A:722:LYS:HZ1	1.13	1.13
1:B:712:LEU:HD12	1:B:713:GLU:N	1.65	1.12
1:C:72:ALA:HB2	1:C:105:ILE:HD13	1.21	1.09
1:C:77:LEU:HD13	1:C:105:ILE:HG22	1.30	1.09
1:C:72:ALA:HB1	1:C:105:ILE:CD1	1.84	1.06
1:B:413:MET:HE3	1:B:430:TYR:HE2	1.06	1.06
1:B:413:MET:CE	1:B:473:PRO:HB2	1.86	1.04
1:B:413:MET:CE	1:B:430:TYR:CE2	2.42	1.01
1:C:350:ASN:HD21	1:C:390:ASN:ND2	1.60	0.97
1:A:584:ILE:O	1:A:591:LEU:HD21	1.67	0.95
1:C:77:LEU:CD1	1:C:105:ILE:CG2	2.45	0.94
1:C:77:LEU:HD12	1:C:105:ILE:HG21	1.48	0.93
1:A:714:ASP:HB3	1:A:722:LYS:NZ	1.85	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:ASN:ND2	1:C:390:ASN:HD21	1.67	0.91
1:A:588:ASP:HB3	1:A:591:LEU:HD23	1.55	0.89
1:C:77:LEU:CD1	1:C:105:ILE:HG22	2.03	0.88
1:B:413:MET:HE2	1:B:473:PRO:HB2	1.54	0.88
1:B:413:MET:HE1	1:B:473:PRO:HB2	1.54	0.88
1:C:77:LEU:HD13	1:C:105:ILE:CG2	2.02	0.87
1:A:585:PHE:CD1	1:A:591:LEU:CD1	2.56	0.87
1:B:712:LEU:HD12	1:B:713:GLU:H	1.41	0.85
1:C:350:ASN:HD21	1:C:390:ASN:HD21	0.89	0.85
1:B:413:MET:CE	1:B:430:TYR:HE2	1.85	0.81
1:C:72:ALA:HB2	1:C:105:ILE:CD1	2.00	0.81
1:D:51:VAL:CB	1:D:56:ASP:OD1	2.27	0.80
1:A:585:PHE:HD1	1:A:591:LEU:HD11	1.43	0.79
1:A:585:PHE:CE1	1:A:591:LEU:HD11	2.17	0.79
1:C:77:LEU:CD1	1:C:105:ILE:HG21	2.12	0.79
1:B:413:MET:CE	1:B:474:PRO:O	2.33	0.77
1:A:584:ILE:O	1:A:591:LEU:CD2	2.32	0.77
1:B:413:MET:HE3	1:B:474:PRO:O	1.89	0.73
1:D:739:VAL:HG23	1:D:740:VAL:HG23	1.69	0.73
1:B:235:ASN:OD1	1:B:298:LYS:NZ	2.22	0.72
1:A:714:ASP:CB	1:A:722:LYS:HZ1	1.99	0.72
1:B:7:LYS:O	1:B:273:ASN:ND2	2.22	0.72
1:B:422:ALA:O	1:B:423:ASN:ND2	2.24	0.70
1:B:43:LYS:NZ	1:B:386:PRO:O	2.25	0.70
1:D:596:ASP:O	1:D:599:ILE:HG13	1.92	0.69
1:C:7:LYS:O	1:C:273:ASN:ND2	2.25	0.69
1:D:84:LYS:NZ	1:D:88:ASP:OD1	2.25	0.69
1:D:292:GLU:OE2	1:D:296:LYS:NZ	2.25	0.69
1:A:585:PHE:CE1	1:A:591:LEU:CD1	2.76	0.68
1:A:678:VAL:O	1:A:680:GLY:N	2.27	0.68
1:A:547:GLU:OE2	1:A:580:ARG:NH2	2.28	0.66
1:B:547:GLU:OE2	1:B:580:ARG:NH2	2.30	0.65
1:A:1:MET:HA	1:A:1:MET:HE2	1.80	0.64
1:B:712:LEU:CD1	1:B:713:GLU:N	2.54	0.64
1:C:182:VAL:O	1:C:366:GLN:NE2	2.29	0.64
1:B:639:ASN:OD1	1:B:640:GLN:N	2.29	0.63
1:D:555:ASN:HB3	1:D:605:ASN:HB2	1.79	0.63
1:A:723:GLU:OE1	1:A:732:LYS:NZ	2.32	0.62
1:D:736:LEU:O	1:D:739:VAL:HG22	1.99	0.62
1:D:648:LEU:O	1:D:652:GLY:N	2.32	0.62
1:B:234:SER:HB3	1:B:298:LYS:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ILE:HG22	1:C:105:ILE:O	2.01	0.61
1:C:492:GLU:OE2	1:C:749:HIS:NE2	2.34	0.60
1:A:584:ILE:C	1:A:591:LEU:HD21	2.20	0.60
1:A:96:ASP:OD1	1:A:99:ARG:NH1	2.34	0.60
1:A:591:LEU:C	1:A:591:LEU:HD12	2.22	0.60
1:C:380:GLU:OE2	1:C:383:ARG:NH2	2.21	0.60
1:A:555:ASN:HB3	1:A:605:ASN:HB2	1.83	0.60
1:B:413:MET:HG2	1:B:430:TYR:CD2	2.36	0.60
1:C:154:GLU:OE1	1:C:345:ARG:NH1	2.34	0.60
1:B:413:MET:HE3	1:B:430:TYR:CZ	2.34	0.59
1:B:653:ARG:NE	1:B:659:HIS:O	2.33	0.59
1:D:7:LYS:HD3	1:D:35:LYS:HB3	1.83	0.59
1:C:547:GLU:OE2	1:C:580:ARG:NH2	2.35	0.59
1:D:674:VAL:CG1	1:D:678:VAL:HG21	2.32	0.59
1:C:350:ASN:ND2	1:C:390:ASN:ND2	2.37	0.59
1:B:413:MET:HE2	1:B:430:TYR:CE2	2.37	0.58
1:C:72:ALA:HB2	1:C:105:ILE:HG21	1.84	0.58
1:B:413:MET:HE1	1:B:474:PRO:O	2.02	0.58
1:B:712:LEU:CD1	1:B:713:GLU:H	2.16	0.58
1:A:492:GLU:OE2	1:A:749:HIS:CD2	2.57	0.58
1:B:82:PRO:HB2	1:B:87:GLN:HG3	1.85	0.58
1:A:468:THR:OG1	1:D:511:GLU:OE2	2.21	0.57
1:B:511:GLU:OE1	1:C:468:THR:OG1	2.22	0.57
1:A:154:GLU:OE1	1:A:345:ARG:NH1	2.37	0.57
1:B:502:SER:HA	1:B:516:HIS:HD2	1.68	0.57
1:C:271:SER:O	1:C:274:LYS:NZ	2.36	0.57
1:C:568:ILE:HD11	1:C:587:ILE:HD13	1.87	0.56
1:C:700:LEU:HD13	1:C:708:MET:HE1	1.87	0.56
1:B:234:SER:CB	1:B:298:LYS:HD3	2.35	0.55
1:B:413:MET:CE	1:B:430:TYR:CZ	2.89	0.55
1:C:682:PHE:CZ	1:C:697:GLN:HB2	2.41	0.55
1:C:77:LEU:CB	1:C:105:ILE:CG2	2.85	0.55
1:D:672:THR:HB	1:D:697:GLN:HG2	1.89	0.55
1:D:43:LYS:NZ	1:D:386:PRO:O	2.40	0.55
1:A:638:PHE:HB3	1:A:642:SER:OG	2.07	0.55
1:A:1:MET:HE1	1:A:2:LYS:H	1.71	0.55
1:A:585:PHE:CD1	1:A:592:GLN:OE1	2.59	0.54
1:A:585:PHE:HD1	1:A:591:LEU:CD1	2.11	0.54
1:D:608:GLY:HA3	1:D:661:THR:CG2	2.37	0.54
1:A:677:GLY:O	1:A:678:VAL:HG22	2.08	0.53
1:D:166:GLY:O	1:D:186:ASN:ND2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:730:LYS:O	1:D:731:LEU:HD12	2.09	0.53
1:D:696:LEU:HD21	1:D:698:ILE:HG23	1.90	0.53
1:D:608:GLY:HA3	1:D:661:THR:HG22	1.91	0.53
1:B:603:GLY:HA3	1:B:658:ARG:HH22	1.74	0.53
1:D:547:GLU:OE2	1:D:580:ARG:NH2	2.42	0.52
1:D:696:LEU:CD2	1:D:698:ILE:HG23	2.40	0.52
1:D:182:VAL:O	1:D:366:GLN:NE2	2.34	0.52
1:B:32:THR:HG22	1:B:34:ILE:HD13	1.92	0.51
1:C:635:HIS:CE1	1:C:732:LYS:HG3	2.45	0.51
1:B:555:ASN:HB3	1:B:605:ASN:HB2	1.92	0.51
1:B:271:SER:O	1:B:274:LYS:NZ	2.28	0.51
1:C:502:SER:HA	1:C:516:HIS:HD2	1.76	0.51
1:C:626:ILE:HG22	1:C:627:ARG:HG3	1.93	0.51
1:C:682:PHE:CE1	1:C:690:ALA:HB3	2.46	0.51
1:C:611:ALA:HB1	1:C:642:SER:HB3	1.93	0.51
1:D:719:ALA:O	1:D:722:LYS:HE3	2.11	0.51
1:A:65:HIS:HA	1:A:68:PHE:CD2	2.46	0.50
1:B:234:SER:HB3	1:B:298:LYS:CD	2.41	0.50
1:C:255:PRO:CB	1:C:327:LYS:HD3	2.41	0.50
1:C:599:ILE:O	1:C:603:GLY:N	2.44	0.50
1:C:516:HIS:CD2	1:C:548:LEU:HD22	2.47	0.50
1:D:616:ASP:O	1:D:635:HIS:N	2.43	0.50
1:B:184:VAL:HG23	1:B:366:GLN:HB2	1.94	0.49
1:B:650:LEU:HB3	1:B:705:VAL:HG13	1.93	0.49
1:C:77:LEU:CB	1:C:105:ILE:HG23	2.42	0.49
1:B:724:TYR:HB3	1:B:726:TRP:CH2	2.48	0.49
1:C:672:THR:HB	1:C:697:GLN:HG2	1.93	0.49
1:D:500:HIS:CE1	1:D:606:LEU:HD21	2.47	0.49
1:D:653:ARG:HD3	1:D:660:PHE:HB2	1.94	0.49
1:A:723:GLU:OE1	1:A:732:LYS:HG2	2.12	0.49
1:C:516:HIS:CE1	1:C:545:THR:HG22	2.49	0.48
1:D:69:GLY:HA3	1:D:333:ASN:O	2.13	0.48
1:D:673:PHE:CE2	1:D:698:ILE:HD11	2.48	0.48
1:B:653:ARG:HD3	1:B:660:PHE:HB2	1.95	0.48
1:D:606:LEU:O	1:D:653:ARG:HD2	2.14	0.48
1:C:255:PRO:HB2	1:C:327:LYS:HD3	1.94	0.48
1:C:724:TYR:HB3	1:C:726:TRP:CH2	2.49	0.48
1:B:612:LYS:NZ	1:B:736:LEU:HD22	2.27	0.48
1:A:503:TRP:H	1:A:516:HIS:HD2	1.61	0.48
1:A:456:PHE:CE1	1:A:752:HIS:HE1	2.32	0.48
1:C:387:ASP:OD1	1:C:387:ASP:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:HIS:NE2	1:A:732:LYS:HE2	2.30	0.47
1:A:736:LEU:N	1:A:737:PRO:HD3	2.29	0.47
1:A:753:HIS:HB3	1:B:220:HIS:CD2	2.50	0.47
1:B:11:TRP:CE2	1:B:58:PRO:HG3	2.49	0.47
1:B:606:LEU:HD21	1:B:609:VAL:HG22	1.95	0.47
1:C:72:ALA:HB1	1:C:105:ILE:HD11	1.87	0.47
1:B:29:GLU:O	1:B:33:GLY:N	2.41	0.47
1:B:11:TRP:CD2	1:B:58:PRO:HG3	2.49	0.47
1:C:66:ASP:HB3	1:C:331:MET:HE2	1.97	0.47
1:A:65:HIS:HA	1:A:68:PHE:HD2	1.80	0.47
1:A:387:ASP:N	1:A:387:ASP:OD1	2.48	0.47
1:B:724:TYR:CB	1:B:726:TRP:CH2	2.98	0.47
1:C:593:GLU:O	1:C:597:LYS:HG3	2.15	0.47
1:D:66:ASP:CB	1:D:331:MET:HE2	2.45	0.47
1:D:726:TRP:HB3	1:D:727:PRO:HD2	1.97	0.47
1:B:735:ILE:O	1:B:735:ILE:HG23	2.16	0.46
1:A:591:LEU:HD12	1:A:592:GLN:N	2.30	0.46
1:C:77:LEU:HB2	1:C:105:ILE:HG23	1.97	0.46
1:C:520:THR:HG21	1:C:574:LEU:HD13	1.97	0.46
1:C:604:SER:O	1:C:658:ARG:NH1	2.48	0.46
1:A:166:GLY:O	1:A:186:ASN:ND2	2.47	0.46
1:B:7:LYS:HD3	1:B:35:LYS:HD3	1.98	0.46
1:C:171:LYS:HG2	1:C:173:GLU:HG2	1.97	0.46
1:B:400:TYR:HB2	1:B:407:PRO:HA	1.98	0.46
1:D:387:ASP:OD1	1:D:387:ASP:N	2.45	0.46
1:A:257:LYS:CE	1:A:329:GLU:OE1	2.63	0.46
1:A:646:ILE:HB	1:A:647:PRO:HD3	1.97	0.46
1:C:96:ASP:OD1	1:C:99:ARG:NH2	2.48	0.46
1:D:26:LYS:HA	1:D:26:LYS:HD3	1.73	0.46
1:A:635:HIS:NE2	1:A:732:LYS:HG3	2.31	0.46
1:A:722:LYS:HG2	1:A:723:GLU:N	2.31	0.46
1:A:735:ILE:HG22	1:A:735:ILE:O	2.15	0.46
1:B:133:ILE:N	1:B:134:PRO:CD	2.79	0.46
1:B:315:ASP:HB3	1:B:318:ILE:HG12	1.98	0.46
1:C:708:MET:HG2	1:C:726:TRP:CZ2	2.50	0.46
1:A:450:THR:HG22	1:A:531:PRO:HA	1.97	0.46
1:B:606:LEU:HD21	1:B:609:VAL:CG2	2.46	0.46
1:D:171:LYS:HE2	1:D:173:GLU:CD	2.36	0.46
1:C:450:THR:HG22	1:C:531:PRO:HA	1.97	0.45
1:A:442:ASN:OD1	1:A:447:PHE:N	2.48	0.45
1:C:184:VAL:HG23	1:C:366:GLN:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:THR:HG22	1:A:34:ILE:HD13	1.98	0.45
1:D:500:HIS:HE1	1:D:606:LEU:HD21	1.79	0.45
1:A:11:TRP:CE2	1:A:58:PRO:HG3	2.51	0.45
1:C:21:LEU:CD1	1:C:285:LEU:HD13	2.46	0.45
1:C:159:TRP:N	1:C:160:PRO:CD	2.80	0.45
1:C:618:LEU:HD12	1:C:633:SER:HB2	1.98	0.45
1:B:584:ILE:O	1:B:591:LEU:CD1	2.65	0.45
1:C:86:PHE:HZ	1:C:286:LEU:HD13	1.81	0.45
1:C:653:ARG:HG2	1:C:658:ARG:HB2	1.98	0.45
1:D:736:LEU:HB2	1:D:737:PRO:HD3	1.97	0.45
1:A:612:LYS:HD2	1:A:736:LEU:HD22	1.98	0.45
1:C:22:ALA:O	1:C:26:LYS:HG3	2.17	0.45
1:C:69:GLY:HA3	1:C:333:ASN:O	2.17	0.45
1:B:692:HIS:O	1:B:692:HIS:CG	2.68	0.45
1:D:661:THR:HG23	1:D:661:THR:O	2.16	0.44
1:C:230:PRO:HA	1:C:233:TRP:CE2	2.52	0.44
1:D:555:ASN:CB	1:D:605:ASN:HB2	2.45	0.44
1:B:442:ASN:HA	1:B:445:HIS:O	2.18	0.44
1:D:650:LEU:HD23	1:D:654:LEU:HD12	2.00	0.44
1:D:502:SER:HA	1:D:516:HIS:HD2	1.83	0.44
1:B:152:LEU:HD11	1:B:205:MET:HE3	2.00	0.44
1:B:387:ASP:OD1	1:B:387:ASP:N	2.50	0.44
1:D:579:ARG:HA	1:D:579:ARG:NE	2.32	0.44
1:A:585:PHE:HA	1:A:591:LEU:HD21	2.00	0.44
1:C:626:ILE:HG22	1:C:627:ARG:N	2.33	0.44
1:D:177:TYR:CZ	1:D:332:PRO:HG3	2.53	0.44
1:B:413:MET:HE1	1:B:473:PRO:C	2.39	0.43
1:C:259:PHE:HB3	1:C:331:MET:CG	2.47	0.43
1:C:179:ILE:HG13	1:C:180:LYS:N	2.33	0.43
1:C:445:HIS:HA	1:C:752:HIS:HB3	2.00	0.43
1:C:616:ASP:OD1	1:C:617:ASP:N	2.45	0.43
1:C:700:LEU:HD22	1:C:704:PHE:CE2	2.53	0.43
1:A:635:HIS:CE1	1:A:732:LYS:HE2	2.53	0.43
1:D:516:HIS:CE1	1:D:545:THR:HG22	2.53	0.43
1:B:184:VAL:CG2	1:B:366:GLN:HB2	2.48	0.43
1:D:32:THR:HG22	1:D:34:ILE:HD13	2.00	0.43
1:A:230:PRO:HA	1:A:233:TRP:CE2	2.54	0.43
1:C:77:LEU:HB2	1:C:105:ILE:CG2	2.48	0.43
1:B:69:GLY:HA3	1:B:333:ASN:O	2.19	0.43
1:B:712:LEU:CD1	1:B:714:ASP:H	2.31	0.43
1:B:722:LYS:HD3	1:B:724:TYR:OH	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:682:PHE:CE1	1:C:697:GLN:HB2	2.54	0.43
1:A:516:HIS:CE1	1:A:545:THR:HG22	2.53	0.43
1:A:462:PHE:HB2	1:A:481:MET:HE3	2.01	0.43
1:B:712:LEU:HD12	1:B:713:GLU:CA	2.45	0.43
1:C:376:ALA:CB	1:C:530:THR:HG22	2.48	0.43
1:C:723:GLU:OE1	1:C:732:LYS:HG2	2.18	0.43
1:A:675:SER:OG	1:A:676:THR:N	2.51	0.43
1:A:413:MET:HG2	1:A:430:TYR:CD2	2.53	0.42
1:D:476:TRP:N	1:D:477:PRO:CD	2.82	0.42
1:D:554:TRP:HB2	1:D:599:ILE:HG22	2.01	0.42
1:A:736:LEU:N	1:A:737:PRO:CD	2.82	0.42
1:D:476:TRP:CG	1:D:477:PRO:HD3	2.54	0.42
1:A:177:TYR:CZ	1:A:332:PRO:HG3	2.54	0.42
1:D:635:HIS:CE1	1:D:732:LYS:HG3	2.54	0.42
1:A:718:ALA:HB1	1:A:722:LYS:HE2	2.01	0.42
1:B:177:TYR:CZ	1:B:332:PRO:HG3	2.55	0.42
1:B:726:TRP:HB3	1:B:727:PRO:HD2	1.99	0.42
1:B:597:LYS:HA	1:B:600:GLU:HG2	2.01	0.42
1:C:237:ASP:O	1:C:240:LYS:HD3	2.20	0.42
1:D:682:PHE:CE2	1:D:697:GLN:NE2	2.87	0.42
1:B:384:LEU:HD12	1:B:525:MET:SD	2.60	0.42
1:B:712:LEU:HD12	1:B:714:ASP:H	1.85	0.42
1:C:653:ARG:HG2	1:C:658:ARG:CB	2.50	0.42
1:D:184:VAL:HG23	1:D:366:GLN:HB2	2.01	0.42
1:A:635:HIS:CE1	1:A:732:LYS:CE	3.03	0.42
1:B:415:ARG:NH1	1:B:426:GLU:OE2	2.51	0.42
1:B:500:HIS:HD2	1:B:548:LEU:HD11	1.85	0.42
1:C:476:TRP:N	1:C:477:PRO:CD	2.83	0.42
1:A:159:TRP:N	1:A:160:PRO:CD	2.82	0.41
1:C:32:THR:HG22	1:C:34:ILE:HD13	2.02	0.41
1:A:476:TRP:N	1:A:477:PRO:CD	2.83	0.41
1:A:491:SER:O	1:A:492:GLU:HB2	2.20	0.41
1:C:177:TYR:CE1	1:C:332:PRO:HG3	2.55	0.41
1:C:594:ARG:HA	1:C:597:LYS:HD2	2.02	0.41
1:C:606:LEU:O	1:C:653:ARG:HD2	2.21	0.41
1:D:230:PRO:HA	1:D:233:TRP:CE2	2.55	0.41
1:D:696:LEU:HD21	1:D:698:ILE:CG2	2.50	0.41
1:C:202:ASN:HB2	1:C:204:HIS:CD2	2.55	0.41
1:A:11:TRP:CD2	1:A:58:PRO:HG3	2.56	0.41
1:A:368:ASN:OD1	1:A:374:LEU:CD2	2.69	0.41
1:C:424:ILE:HD11	1:C:572:PRO:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:400:TYR:HB2	1:D:407:PRO:HA	2.03	0.41
1:C:99:ARG:HG3	1:C:104:LEU:CD2	2.50	0.41
1:C:611:ALA:HB2	2:G:337:LEU:HD12	2.02	0.41
1:B:123:LEU:HD13	1:B:136:LEU:HD11	2.02	0.41
1:B:516:HIS:HE1	1:B:545:THR:HG22	1.85	0.41
1:B:159:TRP:N	1:B:160:PRO:CD	2.84	0.41
1:B:646:ILE:HB	1:B:647:PRO:HD3	2.03	0.41
1:C:400:TYR:CE2	1:C:751:HIS:HD2	2.39	0.41
1:D:626:ILE:HG22	1:D:627:ARG:N	2.36	0.41
1:A:315:ASP:HB3	1:A:318:ILE:HG12	2.03	0.41
1:A:397:ILE:H	1:A:397:ILE:HD12	1.86	0.41
1:A:500:HIS:HE1	1:A:606:LEU:HD21	1.86	0.41
1:B:40:HIS:CG	1:B:40:HIS:O	2.74	0.41
1:B:171:LYS:HE2	1:B:173:GLU:HG3	2.03	0.41
1:D:376:ALA:CB	1:D:530:THR:HG22	2.51	0.41
1:D:615:TRP:HZ2	1:D:694:PRO:HA	1.86	0.41
1:A:442:ASN:HA	1:A:445:HIS:O	2.21	0.41
1:B:476:TRP:N	1:B:477:PRO:CD	2.84	0.41
1:B:723:GLU:OE1	1:B:732:LYS:CG	2.69	0.41
1:C:400:TYR:HB2	1:C:407:PRO:HA	2.04	0.41
1:C:588:ASP:HB3	1:C:591:LEU:HD12	2.02	0.41
1:D:648:LEU:O	1:D:652:GLY:CA	2.68	0.41
1:A:476:TRP:CG	1:A:477:PRO:HD3	2.56	0.40
1:A:612:LYS:HD2	1:A:736:LEU:CD2	2.51	0.40
1:B:197:VAL:HG12	1:B:201:LYS:NZ	2.37	0.40
1:A:98:VAL:HG21	1:A:108:PRO:HD3	2.04	0.40
1:A:593:GLU:HG2	1:A:597:LYS:HE3	2.03	0.40
1:B:82:PRO:HG2	1:B:95:TRP:CH2	2.57	0.40
1:B:220:HIS:HB2	1:B:222:GLU:OE2	2.21	0.40
1:B:638:PHE:CD2	1:B:731:LEU:HD11	2.56	0.40
1:A:260:VAL:HB	1:A:330:ILE:HA	2.02	0.40
1:B:93:PHE:O	1:B:96:ASP:HB2	2.21	0.40
1:B:391:PRO:HG3	1:B:414:TYR:CE2	2.55	0.40
1:C:56:ASP:OD1	1:C:56:ASP:N	2.54	0.40
1:A:140:LEU:HD23	1:A:143:LYS:HE3	2.04	0.40
1:A:612:LYS:CD	1:A:736:LEU:HD22	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	726/753 (96%)	702 (97%)	22 (3%)	2 (0%)	41	72
1	B	705/753 (94%)	691 (98%)	14 (2%)	0	100	100
1	C	717/753 (95%)	703 (98%)	14 (2%)	0	100	100
1	D	722/753 (96%)	707 (98%)	15 (2%)	0	100	100
2	E	6/17 (35%)	6 (100%)	0	0	100	100
2	F	6/17 (35%)	6 (100%)	0	0	100	100
2	G	6/17 (35%)	6 (100%)	0	0	100	100
2	H	6/17 (35%)	6 (100%)	0	0	100	100
All	All	2894/3080 (94%)	2827 (98%)	65 (2%)	2 (0%)	51	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	679	GLU
1	A	678	VAL

5.3.2 Protein sidechains ⓘ

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	608/626 (97%)	603 (99%)	5 (1%)	81	94
1	B	593/626 (95%)	591 (100%)	2 (0%)	92	98
1	C	600/626 (96%)	598 (100%)	2 (0%)	92	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	605/626 (97%)	601 (99%)	4 (1%)	84	95
2	E	6/12 (50%)	6 (100%)	0	100	100
2	F	6/12 (50%)	6 (100%)	0	100	100
2	G	6/12 (50%)	5 (83%)	1 (17%)	2	6
2	H	6/12 (50%)	6 (100%)	0	100	100
All	All	2430/2552 (95%)	2416 (99%)	14 (1%)	86	96

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	THR
1	A	384	LEU
1	A	579	ARG
1	A	752	HIS
1	B	327	LYS
1	B	747	GLU
1	C	653	ARG
1	C	695	TRP
1	D	355	ARG
1	D	665	ILE
1	D	715	LEU
1	D	734	SER
2	G	333	SER

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

Mol	Chain	Res	Type
1	A	500	HIS
1	A	516	HIS
1	A	748	HIS
1	A	749	HIS
1	A	752	HIS
1	B	273	ASN
1	B	423	ASN
1	B	516	HIS
1	C	204	HIS
1	C	350	ASN
1	C	516	HIS

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Mol	Chain	Res	Type
1	D	220	HIS
1	D	500	HIS
1	D	516	HIS
1	D	656	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	GLC	I	1	3	12,12,12	0.54	0	17,17,17	0.52	0
3	GLC	I	2	3	11,11,12	0.64	0	15,15,17	0.66	0
3	GLC	J	1	3	12,12,12	0.55	0	17,17,17	0.62	0
3	GLC	J	2	3	11,11,12	0.63	0	15,15,17	0.58	0
3	GLC	K	1	3	12,12,12	0.54	0	17,17,17	0.67	0
3	GLC	K	2	3	11,11,12	0.61	0	15,15,17	0.74	0
3	GLC	L	1	3	12,12,12	0.56	0	17,17,17	0.91	1 (5%)
3	GLC	L	2	3	11,11,12	0.60	0	15,15,17	0.80	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	GLC	I	1	3	-	0/2/22/22	0/1/1/1
3	GLC	I	2	3	-	1/2/19/22	0/1/1/1
3	GLC	J	1	3	-	2/2/22/22	0/1/1/1
3	GLC	J	2	3	-	0/2/19/22	0/1/1/1
3	GLC	K	1	3	-	2/2/22/22	0/1/1/1
3	GLC	K	2	3	-	0/2/19/22	0/1/1/1
3	GLC	L	1	3	-	2/2/22/22	0/1/1/1
3	GLC	L	2	3	-	0/2/19/22	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})
3	L	1	GLC	C1-C2-C3	2.20	114.84	110.36

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain J

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain K

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain L

Bond lengths   Bond angles

Torsions   Rings
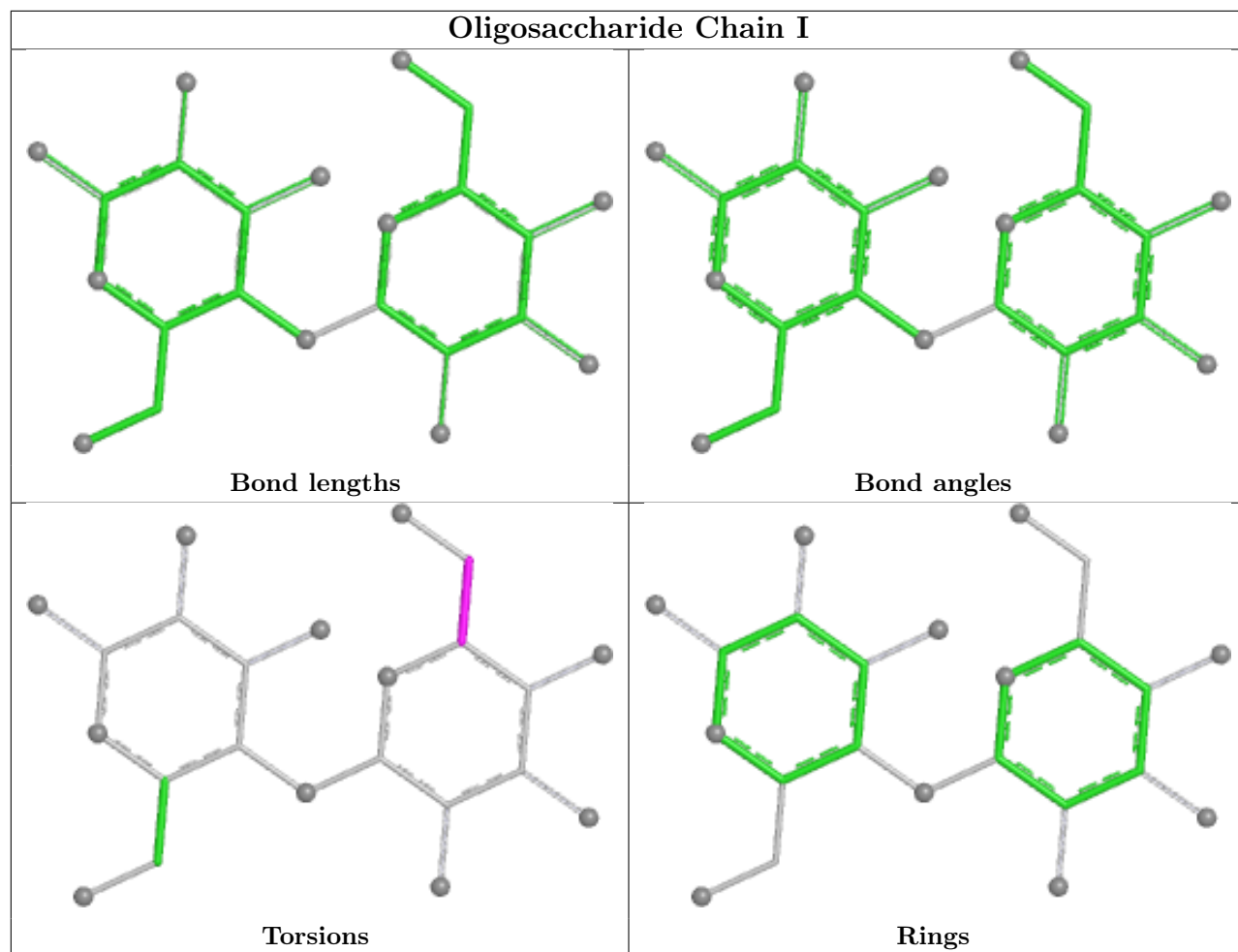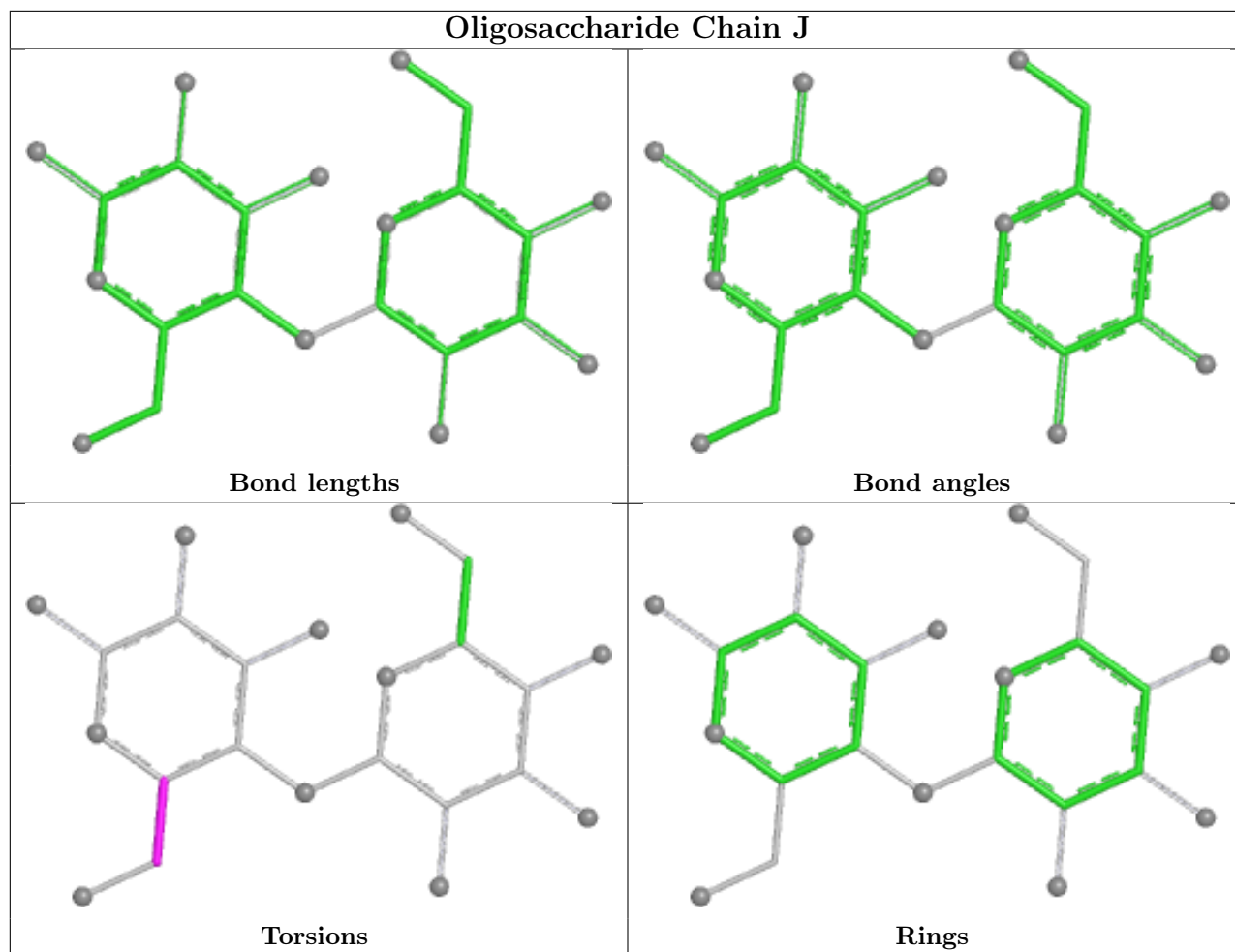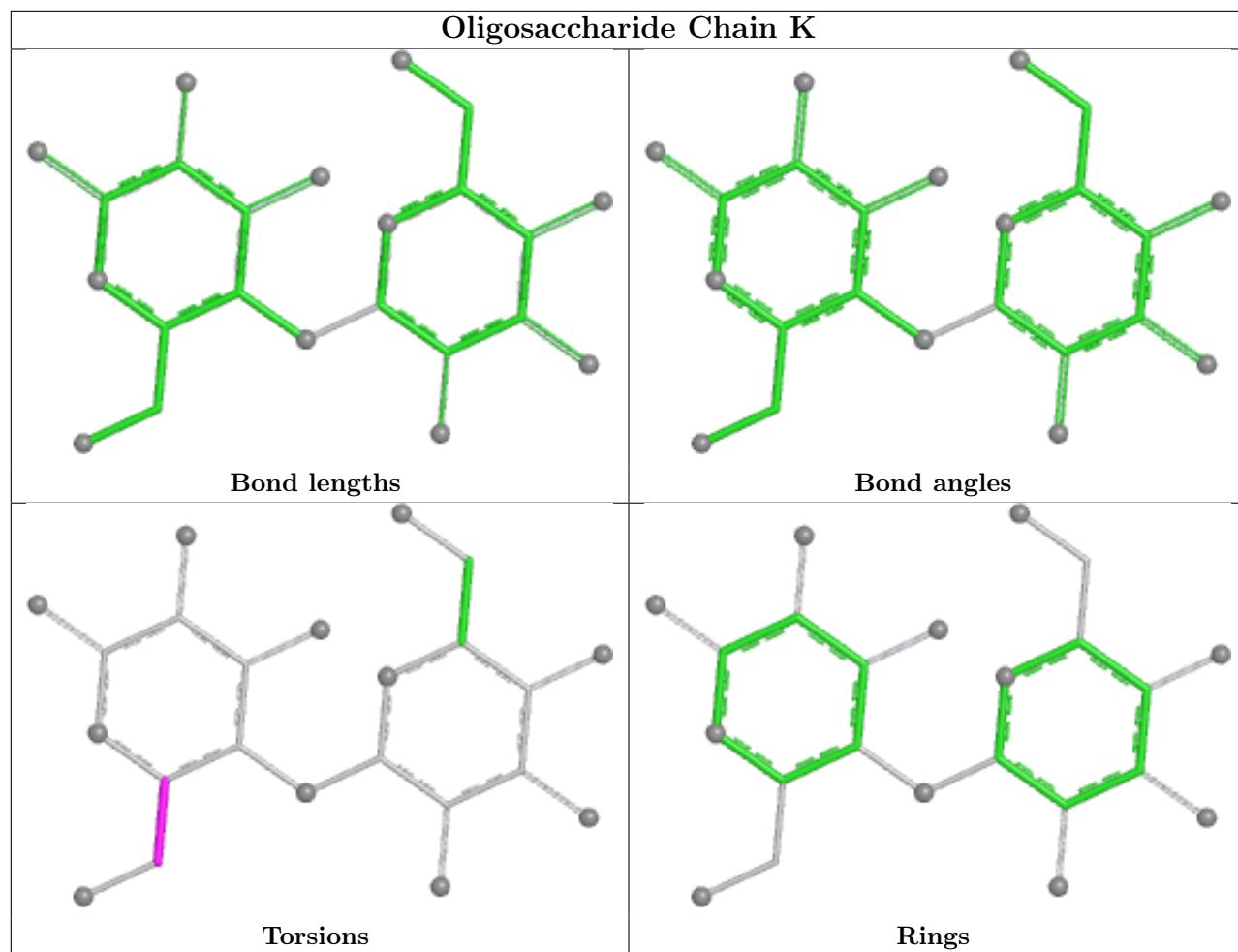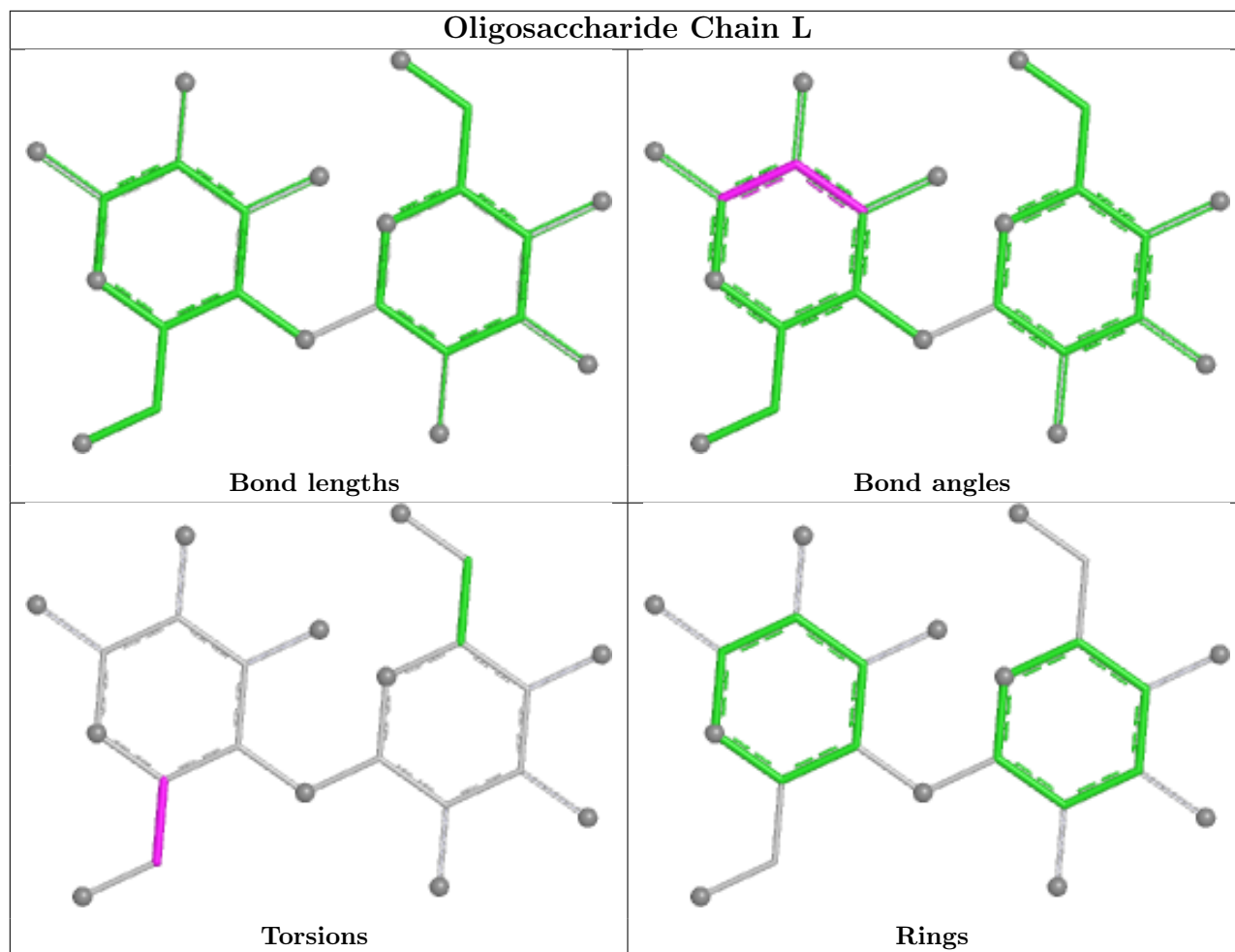
5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

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	734/753 (97%)	-0.26	8 (1%)	80	75	49, 79, 122, 165	0
1	B	717/753 (95%)	-0.09	29 (4%)	38	28	51, 92, 163, 199	0
1	C	725/753 (96%)	0.07	43 (5%)	22	14	54, 109, 174, 214	0
1	D	730/753 (96%)	-0.19	18 (2%)	57	47	46, 83, 142, 217	0
2	E	8/17 (47%)	-0.11	0	100	100	63, 73, 93, 94	0
2	F	8/17 (47%)	0.24	1 (12%)	3	2	89, 96, 118, 120	0
2	G	8/17 (47%)	-0.08	0	100	100	76, 88, 99, 108	0
2	H	8/17 (47%)	-0.30	0	100	100	77, 82, 96, 101	0
All	All	2938/3080 (95%)	-0.12	99 (3%)	45	35	46, 88, 158, 217	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	703	GLU	10.5
1	A	1	MET	6.9
1	B	614	ALA	6.0
1	C	710	GLU	5.8
1	C	709	LEU	5.7
1	B	712	LEU	5.1
1	C	594	ARG	5.0
1	C	711	ASP	5.0
1	B	615	TRP	4.9
1	C	300	LEU	4.8
1	C	704	PHE	4.7
1	B	734	SER	4.6
1	B	638	PHE	4.6
1	C	650	LEU	4.5
1	B	738	ASP	4.2
1	B	636	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	713	GLU	4.1
1	D	630	GLN	3.8
1	C	632	GLU	3.8
1	B	37	THR	3.8
1	B	670	ALA	3.8
1	C	646	ILE	3.7
1	C	569	ALA	3.7
1	C	595	VAL	3.7
1	D	682	PHE	3.6
1	C	708	MET	3.6
1	C	105	ILE	3.6
1	D	627	ARG	3.6
1	B	613	CYS	3.6
1	C	446	GLU	3.5
1	B	708	MET	3.5
1	C	701	THR	3.5
1	C	591	LEU	3.4
1	C	734	SER	3.4
1	C	634	VAL	3.4
1	D	629	ARG	3.3
1	A	3	THR	3.3
1	B	682	PHE	3.2
1	B	679	GLU	3.2
1	D	597	LYS	3.2
1	C	584	ILE	3.1
1	D	748	HIS	3.1
1	C	702	GLU	3.1
1	C	599	ILE	3.1
1	C	548	LEU	3.0
1	C	549	HIS	3.0
1	D	631	LEU	2.9
1	B	668	ASP	2.9
1	D	519	LEU	2.9
1	B	568	ILE	2.8
1	D	569	ALA	2.8
1	D	611	ALA	2.8
1	B	709	LEU	2.8
1	C	174	ASN	2.7
1	B	612	LYS	2.7
1	C	732	LYS	2.7
1	C	705	VAL	2.7
1	B	663	LYS	2.7

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type	RSRZ
1	C	659	HIS	2.7
1	C	552	GLN	2.6
1	C	79	GLU	2.6
1	A	627	ARG	2.6
1	B	698	ILE	2.5
1	D	643	GLY	2.5
1	C	8	LEU	2.5
1	B	683	ALA	2.5
1	C	7	LYS	2.5
1	C	565	THR	2.4
1	D	568	ILE	2.4
1	C	111	VAL	2.4
2	F	334	TYR	2.4
1	D	747	GLU	2.4
1	A	285	LEU	2.4
1	C	654	LEU	2.3
1	D	734	SER	2.3
1	C	563	LEU	2.3
1	C	501	VAL	2.3
1	D	626	ILE	2.3
1	A	721	PRO	2.2
1	B	637	LYS	2.2
1	C	707	LYS	2.2
1	C	518	LEU	2.2
1	D	666	THR	2.2
1	C	722	LYS	2.2
1	B	673	PHE	2.1
1	D	673	PHE	2.1
1	D	614	ALA	2.1
1	C	245	VAL	2.1
1	A	4	GLU	2.1
1	A	300	LEU	2.1
1	A	495	PHE	2.1
1	B	646	ILE	2.1
1	C	140	LEU	2.1
1	B	551	ALA	2.1
1	B	669	MET	2.1
1	C	312	LEU	2.0
1	B	511	GLU	2.0
1	B	555	ASN	2.0
1	B	648	LEU	2.0

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

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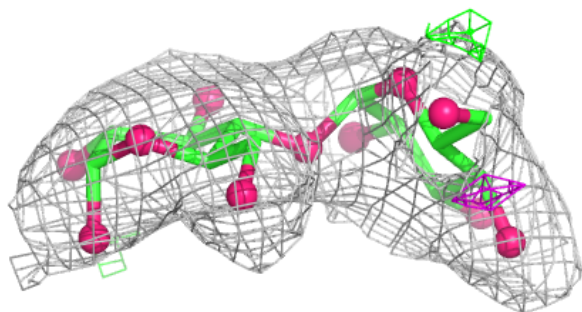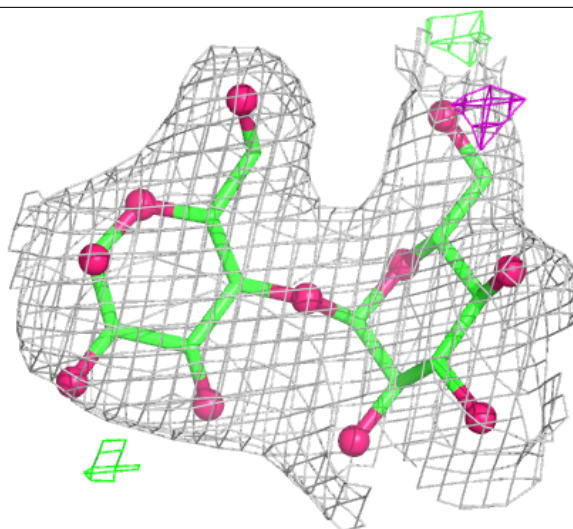
6.3 Carbohydrates ⓘ

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
3	GLC	K	1	12/12	0.95	0.19	67,77,85,86	0
3	GLC	K	2	11/12	0.95	0.13	61,73,84,94	0
3	GLC	I	2	11/12	0.96	0.11	48,56,65,69	0
3	GLC	J	1	12/12	0.96	0.21	51,63,80,93	0
3	GLC	L	1	12/12	0.96	0.17	52,59,69,69	0
3	GLC	L	2	11/12	0.96	0.14	47,56,71,73	0
3	GLC	J	2	11/12	0.97	0.14	50,57,67,70	0
3	GLC	I	1	12/12	0.98	0.17	48,60,73,84	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.
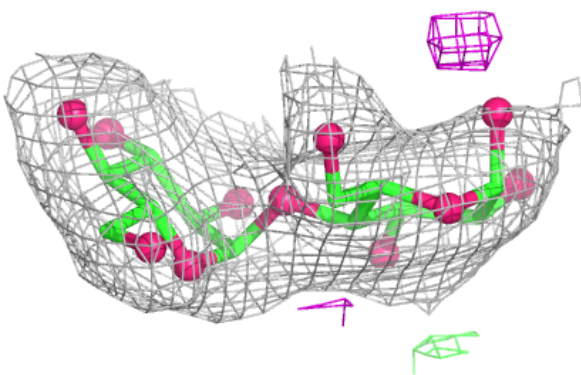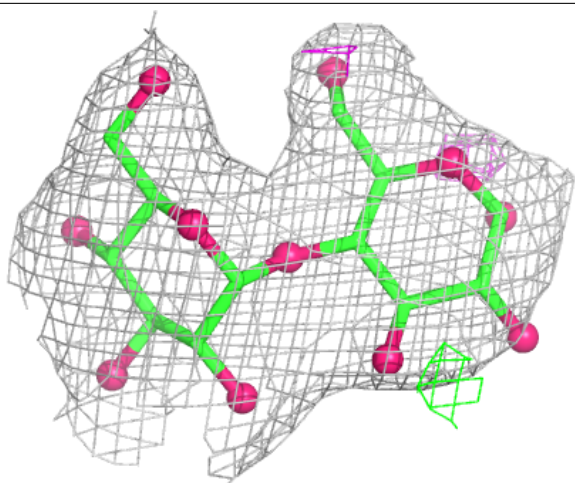
Electron density around Chain I:

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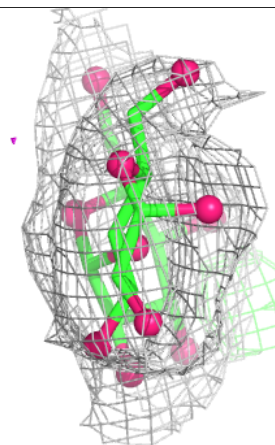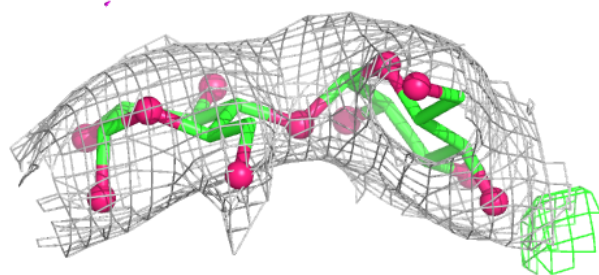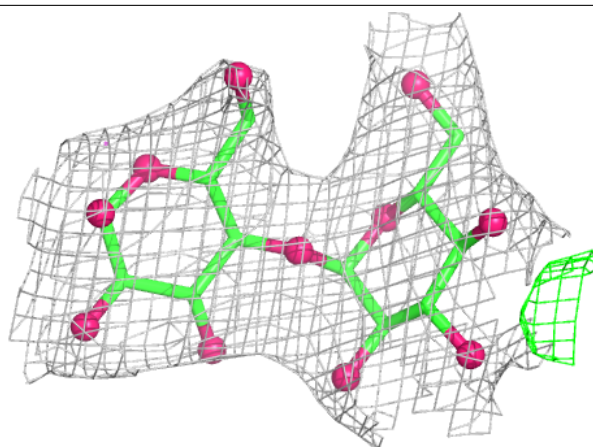mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
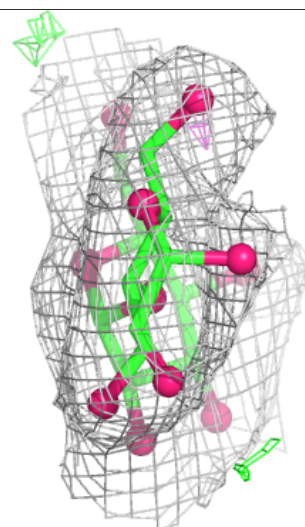
Electron density around Chain J:

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

Electron density around Chain K:
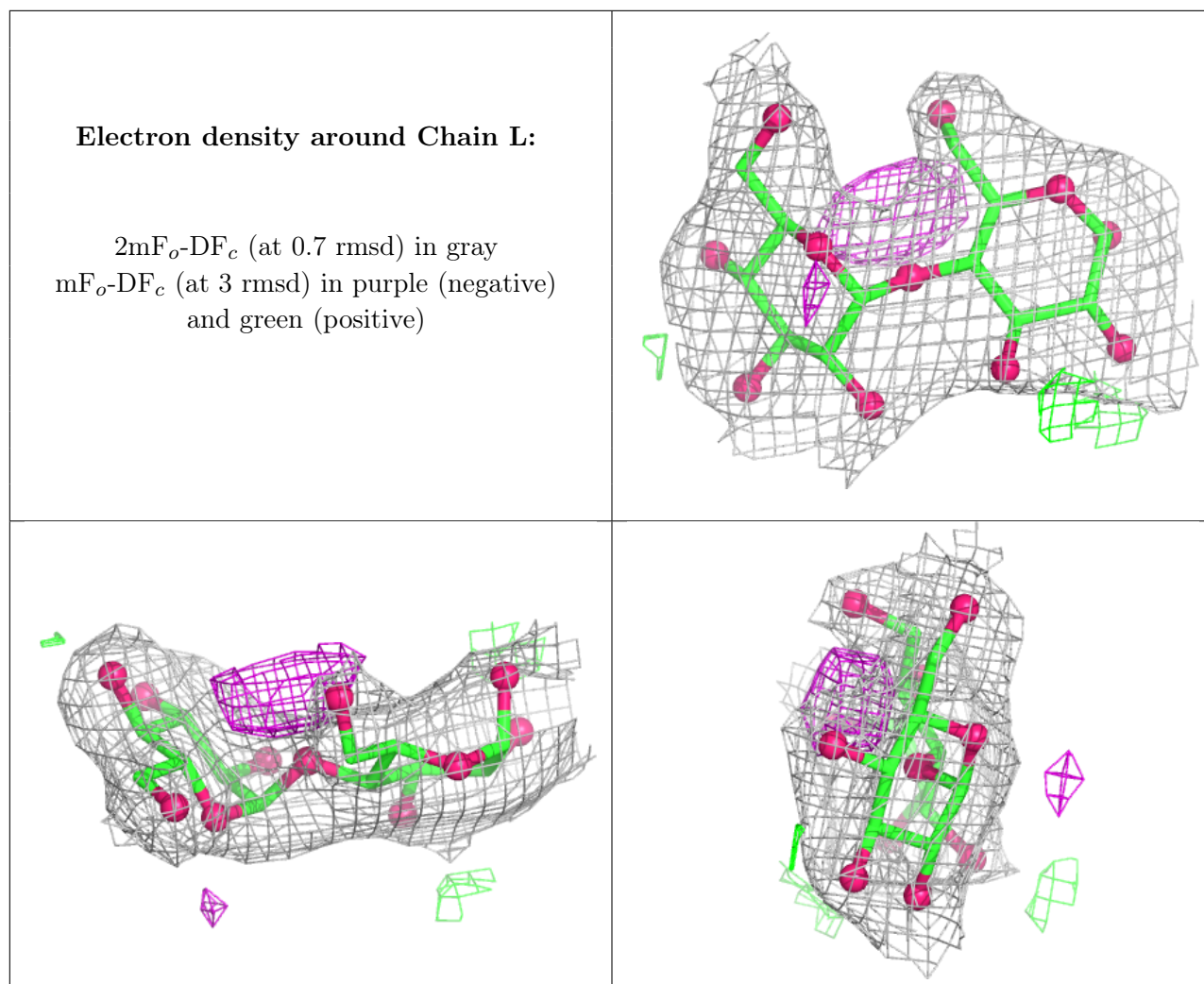
$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around Chain L:

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

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
4	ZN	A	910	1/1	0.79	0.13	65,65,65,65	0
4	ZN	B	910	1/1	0.99	0.17	75,75,75,75	0
4	ZN	C	910	1/1	0.99	0.17	57,57,57,57	0
4	ZN	D	910	1/1	1.00	0.14	74,74,74,74	0

6.5 Other polymers ⓘ

There are no such residues in this entry.